



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 02:58 AM EST

PDB ID : 6DID  
EMDB ID : EMD-7896  
Title : HIV Env BG505 SOSIP with polyclonal Fabs from immunized rabbit #3417  
post-boost#1  
Authors : Turner, H.L.; Cottrell, C.A.; Oyen, D.; Wilson, I.A.; Ward, A.B.  
Deposited on : 2018-05-23  
Resolution : 4.71 Å(reported)

This is a Full wwPDB EM Validation 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:

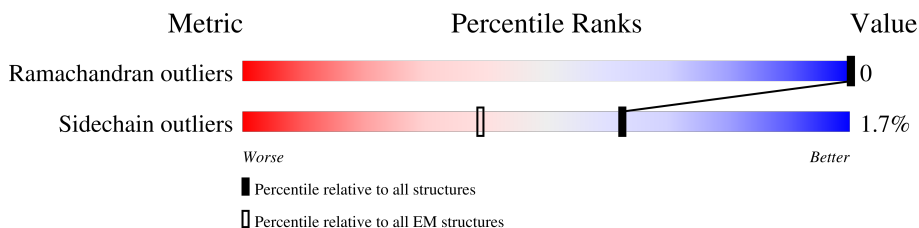
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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 4.71 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  $\geq 3$ , 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	481	92% 8%
1	F	481	92% 8%
1	G	481	92% 8%
2	B	153	84% 16%
2	I	153	84% 16%
2	J	153	84% 16%
3	C	217	41% 95% 5%
3	E	217	41% 95% 5%
3	H	217	41% 95% 5%

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Mol	Chain	Length	Quality of chain
4	D	214	41% 97%
4	K	214	41% 97%
4	L	214	41% 97%
5	M	3	67% 100%
5	Y	3	67% 100%
5	k	3	67% 100%
6	N	2	50% 50%
6	O	2	100%
6	P	2	100%
6	S	2	100%
6	T	2	50% 100%
6	U	2	50% 50%
6	X	2	100%
6	Z	2	50% 50%
6	a	2	100%
6	b	2	100%
6	e	2	100%
6	f	2	50% 100%
6	g	2	50% 50%
6	j	2	100%
6	l	2	50% 50%
6	m	2	100%
6	n	2	100%
6	q	2	100%
6	r	2	50% 100%

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Mol	Chain	Length	Quality of chain	
6	s	2	50%	50%
6	v	2	100%	
7	Q	7	14%	100%
7	c	7	14%	100%
7	o	7	14%	100%
8	R	8	12%	88%
8	d	8	12%	88%
8	p	8	12%	88%
9	V	6	17%	83%
9	h	6	17%	83%
9	t	6	17%	83%
10	W	4	25%	75%
10	i	4	25%	75%
10	u	4	25%	75%

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 34674 atoms, of which 9465 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 gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	444	3493	2192	617	656	28	0	0
1	F	444	3493	2192	617	656	28	0	0
1	G	444	3493	2192	617	656	28	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	511	ARG	-	expression tag	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	129	1024	646	177	195	6	0	0
2	I	129	1024	646	177	195	6	0	0
2	J	129	1024	646	177	195	6	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S7
B	605	CYS	THR	conflict	UNP Q2N0S7
I	559	PRO	ILE	conflict	UNP Q2N0S7
I	605	CYS	THR	conflict	UNP Q2N0S7
J	559	PRO	ILE	conflict	UNP Q2N0S7
J	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called Monoclonal antibody 10A light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	217	3258	1038	1596	272	343	9	7	0
3	E	217	3258	1038	1596	272	343	9	7	0
3	H	217	3258	1038	1596	272	343	9	7	0

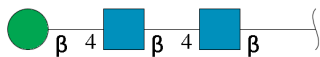
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	140	SER	THR	conflict	UNP P01840
E	140	SER	THR	conflict	UNP P01840
H	140	SER	THR	conflict	UNP P01840

- Molecule 4 is a protein called Monoclonal antibody 10A heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	213	3151	1001	1559	266	314	11	6	0
4	K	213	3151	1001	1559	266	314	11	6	0
4	L	213	3151	1001	1559	266	314	11	6	0

- Molecule 5 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		
5	M	3	39	22	2	15	0	0
5	Y	3	39	22	2	15	0	0
5	k	3	39	22	2	15	0	0

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



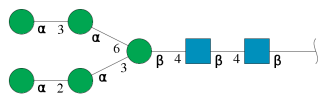
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	N	2	28	16	2	10	0	0
6	O	2	28	16	2	10	0	0
6	P	2	28	16	2	10	0	0
6	S	2	28	16	2	10	0	0
6	T	2	28	16	2	10	0	0
6	U	2	28	16	2	10	0	0
6	X	2	28	16	2	10	0	0
6	Z	2	28	16	2	10	0	0
6	a	2	28	16	2	10	0	0
6	b	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	e	2	Total 28	C 16	N 2	O 10	0	0
6	f	2	Total 28	C 16	N 2	O 10	0	0
6	g	2	Total 28	C 16	N 2	O 10	0	0
6	j	2	Total 28	C 16	N 2	O 10	0	0
6	l	2	Total 28	C 16	N 2	O 10	0	0
6	m	2	Total 28	C 16	N 2	O 10	0	0
6	n	2	Total 28	C 16	N 2	O 10	0	0
6	q	2	Total 28	C 16	N 2	O 10	0	0
6	r	2	Total 28	C 16	N 2	O 10	0	0
6	s	2	Total 28	C 16	N 2	O 10	0	0
6	v	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

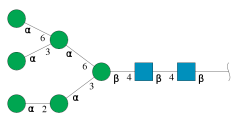


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	Q	7	Total 83	C 46	N 2	O 35	0	0
7	c	7	Total 83	C 46	N 2	O 35	0	0
7	o	7	Total 83	C 46	N 2	O 35	0	0

- Molecule 8 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-

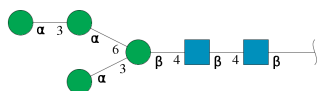


-acetamido-2-deoxy-beta-D-glucopyranose.



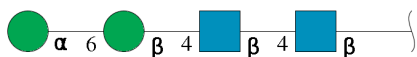
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	R	8	94	52	2	40	0	0
8	d	8	94	52	2	40	0	0
8	p	8	94	52	2	40	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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		
9	V	6	72	40	2	30	0	0
9	h	6	72	40	2	30	0	0
9	t	6	72	40	2	30	0	0

- Molecule 10 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.



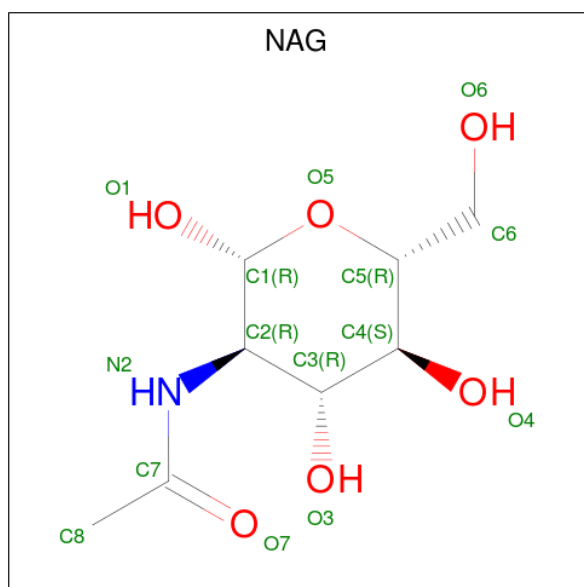
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	W	4	50	28	2	20	0	0
10	i	4	50	28	2	20	0	0

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

- Molecule 11 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
			Total	C	N	O	
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	A	1	Total	C	N	O	0
			70	40	5	25	
11	B	1	Total	C	N	O	0
			28	16	2	10	
11	B	1	Total	C	N	O	0
			28	16	2	10	
11	F	1	Total	C	N	O	0
			70	40	5	25	
11	F	1	Total	C	N	O	0
			70	40	5	25	
11	F	1	Total	C	N	O	0
			70	40	5	25	

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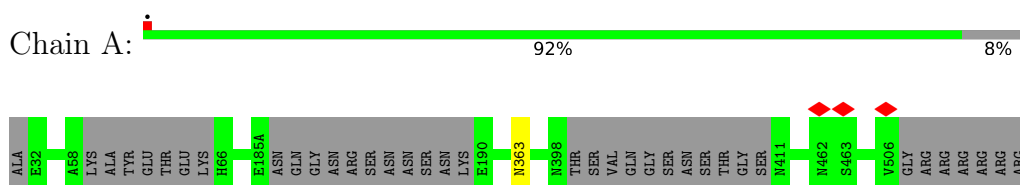
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>
11	F	1	Total 70	C 40	N 5	O 25	0
11	F	1	Total 70	C 40	N 5	O 25	0
11	I	1	Total 28	C 16	N 2	O 10	0
11	I	1	Total 28	C 16	N 2	O 10	0
11	G	1	Total 70	C 40	N 5	O 25	0
11	G	1	Total 70	C 40	N 5	O 25	0
11	G	1	Total 70	C 40	N 5	O 25	0
11	G	1	Total 70	C 40	N 5	O 25	0
11	G	1	Total 70	C 40	N 5	O 25	0
11	J	1	Total 28	C 16	N 2	O 10	0
11	J	1	Total 28	C 16	N 2	O 10	0

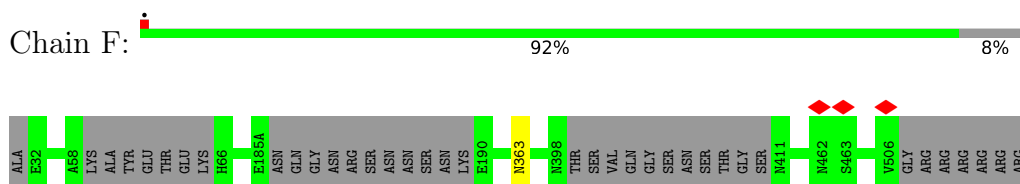
### 3 Residue-property plots [i](#)

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.

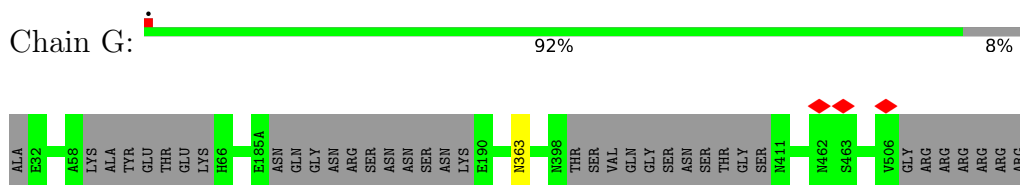
- Molecule 1: Envelope glycoprotein gp160



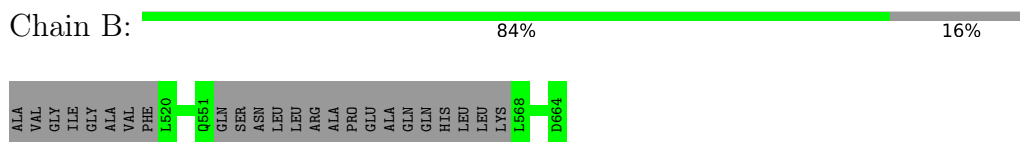
- Molecule 1: Envelope glycoprotein gp160



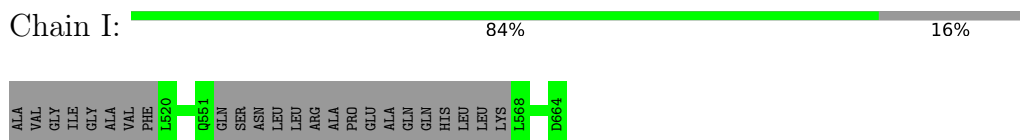
- Molecule 1: Envelope glycoprotein gp160




- Molecule 2: Envelope glycoprotein gp160

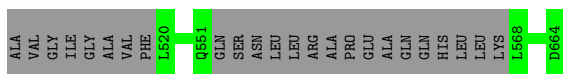


- Molecule 2: Envelope glycoprotein gp160

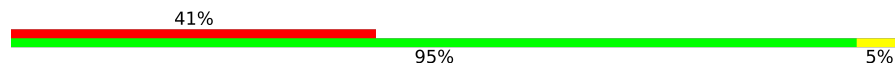


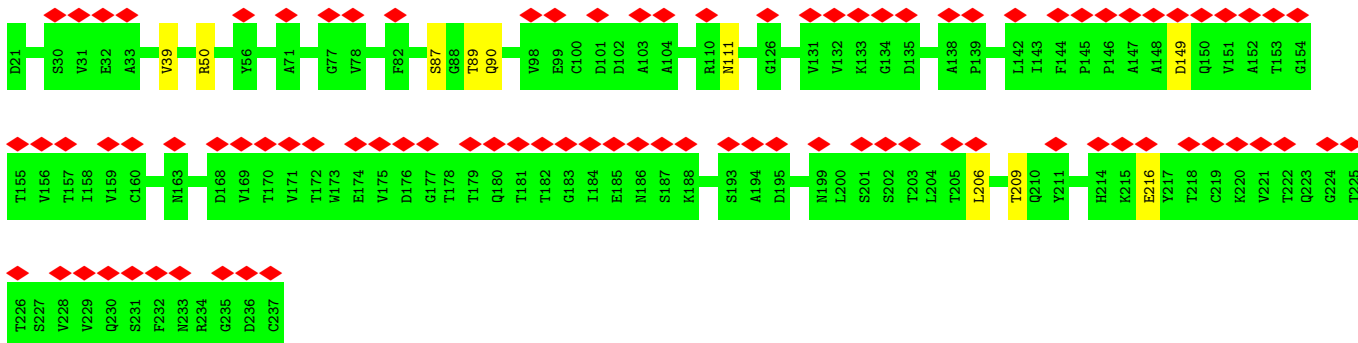
- Molecule 2: Envelope glycoprotein gp160

Chain J:  84% 16%

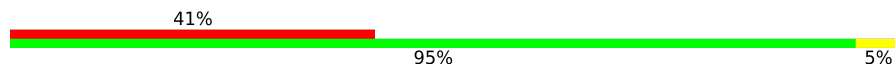


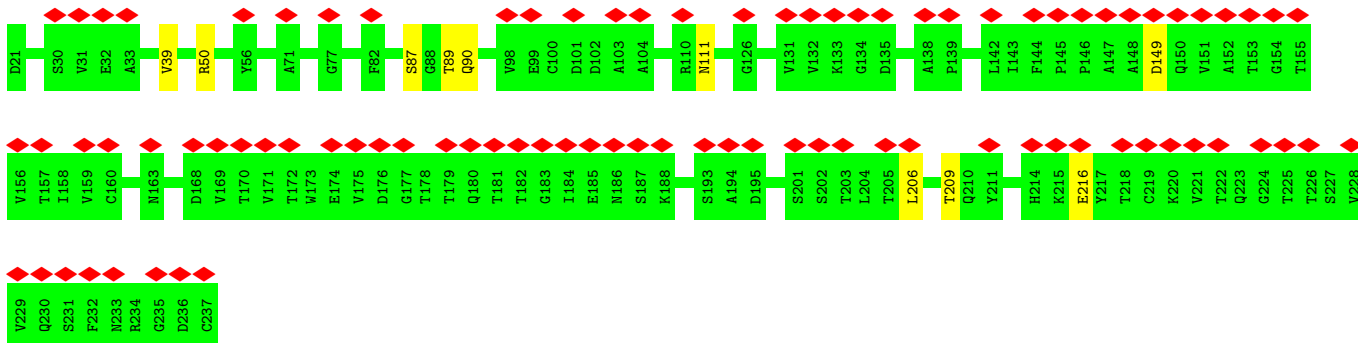
- Molecule 3: Monoclonal antibody 10A light chain

Chain C:  41% 95% 5%

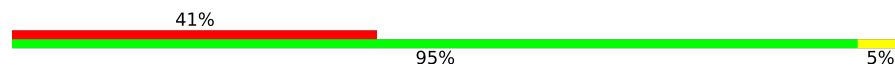


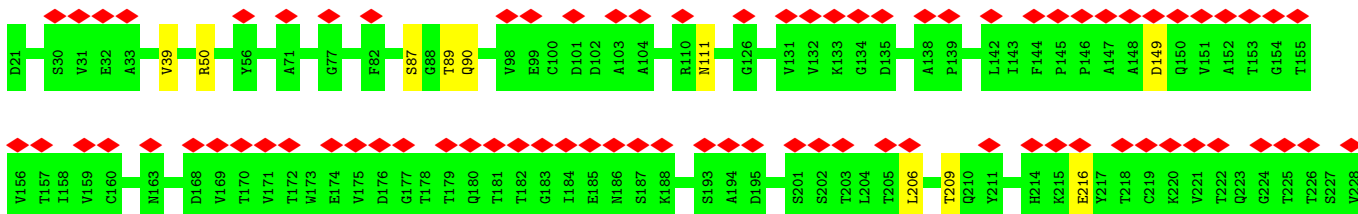
- Molecule 3: Monoclonal antibody 10A light chain

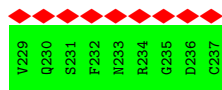
Chain E:  41% 95% 5%



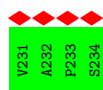
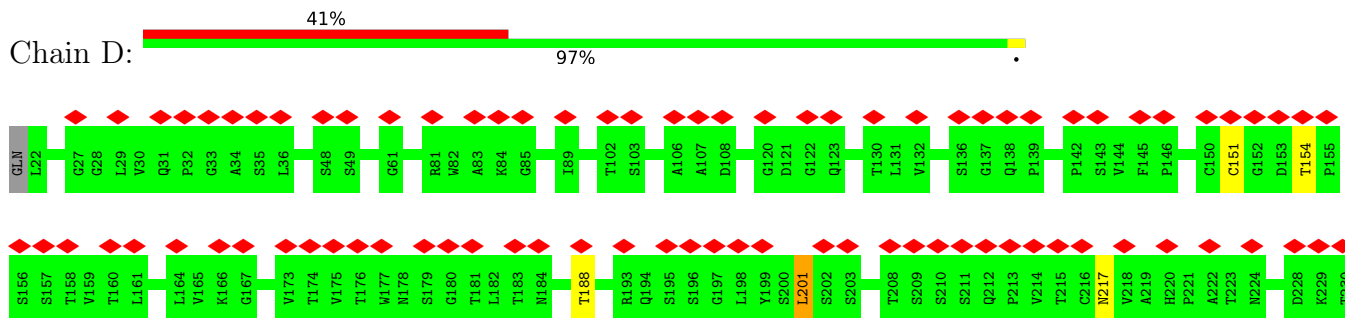
- Molecule 3: Monoclonal antibody 10A light chain

Chain H:  41% 95% 5%

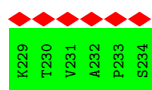
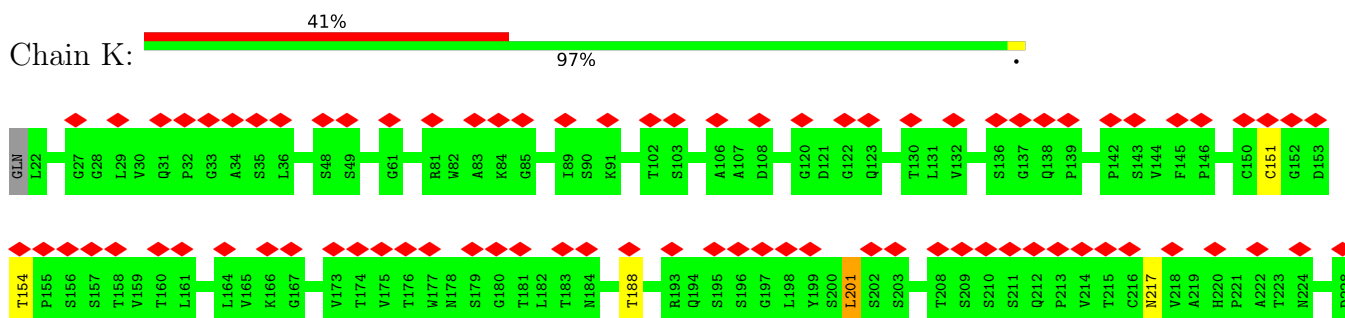




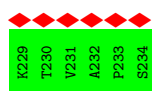
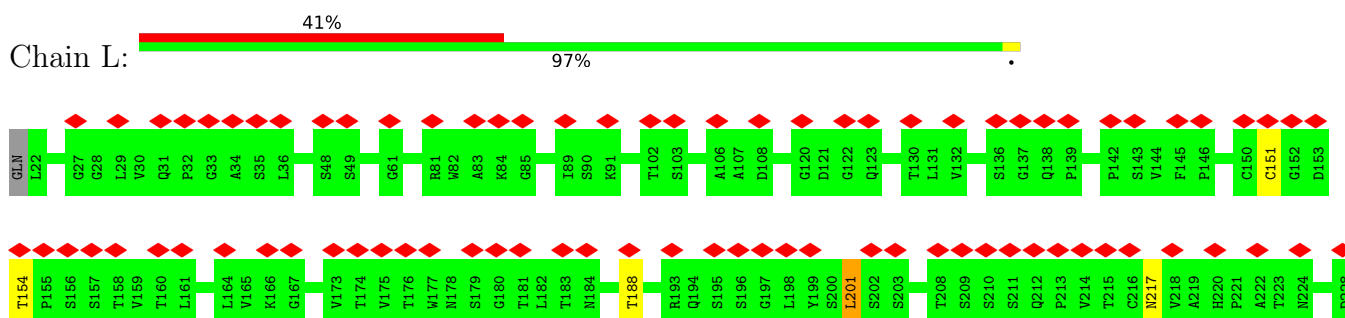
• Molecule 4: Monoclonal antibody 10A heavy chain



• Molecule 4: Monoclonal antibody 10A heavy chain



• Molecule 4: Monoclonal antibody 10A heavy chain



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



NAG1  
NAG2

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

Chain T: 

50%  
100%

NAG1  
NAG2

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

Chain U: 

50%  
50%

NAG1  
NAG2

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

Chain X: 

100%

NAG1  
NAG2

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

Chain Z: 

50%  
50%

NAG1  
NAG2

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

Chain a: 

100%

NAG1  
NAG2

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

Chain b: 

100%

NAG1  
NAG2



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

Chain e:  100%

  
NAG1  
NAG2

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

Chain f:  50% 100%

  
NAG1  
NAG2

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

Chain g:  50% 50%

  
NAG1  
NAG2

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

Chain j:  100%

  
NAG1  
NAG2

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

Chain l:  50% 50%

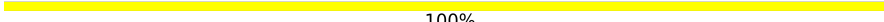
  
NAG1  
NAG2

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

Chain m:  100%

  
NAG1  
NAG2

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

Chain n:  100%

MAG1  
MAG2

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

Chain q:  100%

MAG1  
MAG2

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

Chain r:  50% 100%

MAG1  
MAG2

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

Chain s:  50% 50%

MAG1  
MAG2

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

Chain v:  100%

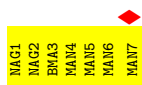
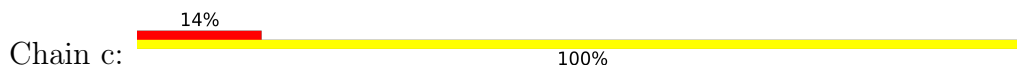
MAG1  
MAG2

- Molecule 7: 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

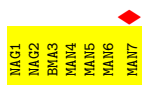
Chain Q:  14% 100%

MAG1  
MAG2  
EMAG3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 7: 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 7: 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 8: 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



- Molecule 8: 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

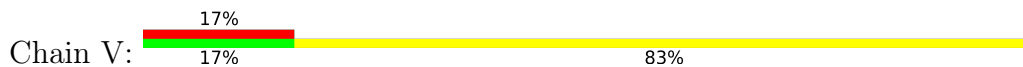


- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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

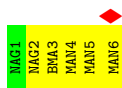
ido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 10: 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 10: 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 10: 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	161639	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.395	Depositor
Minimum map value	-0.402	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	345.0, 345.0, 345.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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	A	0.84	0/3565	0.82	0/4842
1	F	0.84	0/3565	0.82	0/4842
1	G	0.84	0/3565	0.82	0/4842
2	B	0.88	0/1041	0.80	0/1412
2	I	0.87	0/1041	0.80	0/1412
2	J	0.88	0/1041	0.80	0/1412
3	C	0.51	0/1697	0.66	0/2319
3	E	0.51	0/1697	0.66	0/2319
3	H	0.51	0/1697	0.66	0/2319
4	D	0.57	1/1641 (0.1%)	0.67	1/2249 (0.0%)
4	K	0.57	1/1641 (0.1%)	0.67	1/2249 (0.0%)
4	L	0.57	1/1641 (0.1%)	0.67	1/2249 (0.0%)
All	All	0.73	3/23832 (0.0%)	0.76	3/32466 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	188	THR	C-N	-5.53	1.21	1.34
4	D	188	THR	C-N	-5.52	1.21	1.34
4	K	188	THR	C-N	-5.51	1.21	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	K	201	LEU	CA-CB-CG	5.67	128.33	115.30
4	D	201	LEU	CA-CB-CG	5.66	128.32	115.30
4	L	201	LEU	CA-CB-CG	5.63	128.25	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
1	F	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
1	G	436/481 (91%)	427 (98%)	9 (2%)	0	100	100
2	B	125/153 (82%)	122 (98%)	3 (2%)	0	100	100
2	I	125/153 (82%)	123 (98%)	2 (2%)	0	100	100
2	J	125/153 (82%)	122 (98%)	3 (2%)	0	100	100
3	C	222/217 (102%)	214 (96%)	8 (4%)	0	100	100
3	E	222/217 (102%)	214 (96%)	8 (4%)	0	100	100
3	H	222/217 (102%)	214 (96%)	8 (4%)	0	100	100
4	D	217/214 (101%)	213 (98%)	4 (2%)	0	100	100
4	K	217/214 (101%)	213 (98%)	4 (2%)	0	100	100
4	L	217/214 (101%)	213 (98%)	4 (2%)	0	100	100
All	All	3000/3195 (94%)	2929 (98%)	71 (2%)	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	A	397/428 (93%)	396 (100%)	1 (0%)	92	95
1	F	397/428 (93%)	396 (100%)	1 (0%)	92	95
1	G	397/428 (93%)	396 (100%)	1 (0%)	92	95
2	B	111/129 (86%)	111 (100%)	0	100	100
2	I	111/129 (86%)	111 (100%)	0	100	100
2	J	111/129 (86%)	111 (100%)	0	100	100
3	C	186/181 (103%)	176 (95%)	10 (5%)	22	49
3	E	186/181 (103%)	176 (95%)	10 (5%)	22	49
3	H	186/181 (103%)	176 (95%)	10 (5%)	22	49
4	D	182/177 (103%)	178 (98%)	4 (2%)	52	71
4	K	182/177 (103%)	178 (98%)	4 (2%)	52	71
4	L	182/177 (103%)	178 (98%)	4 (2%)	52	71
All	All	2628/2745 (96%)	2583 (98%)	45 (2%)	62	78

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	ASN
1	F	363	ASN
1	G	363	ASN
3	C	39	VAL
3	C	50	ARG
3	C	87	SER
3	C	89	THR
3	C	90	GLN
3	C	111	ASN
3	C	149	ASP
3	C	206	LEU
3	C	209	THR
3	C	216	GLU
4	D	151	CYS
4	D	154	THR
4	D	201	LEU
4	D	217	ASN
3	E	39	VAL
3	E	50	ARG
3	E	87	SER
3	E	89	THR
3	E	90	GLN

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Mol	Chain	Res	Type
3	E	111	ASN
3	E	149	ASP
3	E	206	LEU
3	E	209	THR
3	E	216	GLU
4	K	151	CYS
4	K	154	THR
4	K	201	LEU
4	K	217	ASN
3	H	39	VAL
3	H	50	ARG
3	H	87	SER
3	H	89	THR
3	H	90	GLN
3	H	111	ASN
3	H	149	ASP
3	H	206	LEU
3	H	209	THR
3	H	216	GLU
4	L	151	CYS
4	L	154	THR
4	L	201	LEU
4	L	217	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	F	293	GLN
1	G	293	GLN
3	C	44	GLN
3	C	90	GLN
3	E	44	GLN
3	E	90	GLN
3	H	44	GLN
3	H	90	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](#)

126 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
5	NAG	M	1	1,5	14,14,15	0.80	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	M	2	5	14,14,15	0.45	0	17,19,21	1.48	3 (17%)
5	BMA	M	3	5	11,11,12	1.19	1 (9%)	15,15,17	1.51	2 (13%)
6	NAG	N	1	1,6	14,14,15	0.26	0	17,19,21	0.54	0
6	NAG	N	2	6	14,14,15	0.32	0	17,19,21	0.65	1 (5%)
6	NAG	O	1	1,6	14,14,15	0.41	0	17,19,21	0.44	0
6	NAG	O	2	6	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	P	1	1,6	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
6	NAG	P	2	6	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
7	NAG	Q	1	1,7	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
7	NAG	Q	2	7	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
7	BMA	Q	3	7	11,11,12	0.67	0	15,15,17	1.48	3 (20%)
7	MAN	Q	4	7	11,11,12	0.59	0	15,15,17	1.72	3 (20%)
7	MAN	Q	5	7	11,11,12	0.60	0	15,15,17	2.40	5 (33%)
7	MAN	Q	6	7	11,11,12	0.60	0	15,15,17	2.54	4 (26%)
7	MAN	Q	7	7	11,11,12	0.56	0	15,15,17	2.02	5 (33%)
8	NAG	R	1	1,8	14,14,15	0.79	1 (7%)	17,19,21	0.69	0
8	NAG	R	2	8	14,14,15	0.41	0	17,19,21	0.45	0
8	BMA	R	3	8	11,11,12	1.66	3 (27%)	15,15,17	1.84	2 (13%)
8	MAN	R	4	8	11,11,12	1.65	3 (27%)	15,15,17	1.32	2 (13%)
8	MAN	R	5	8	11,11,12	2.30	4 (36%)	15,15,17	1.84	5 (33%)
8	MAN	R	6	8	11,11,12	0.59	0	15,15,17	2.54	4 (26%)
8	MAN	R	7	8	11,11,12	0.59	0	15,15,17	2.03	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	R	8	8	11,11,12	0.63	0	15,15,17	2.42	7 (46%)
6	NAG	S	1	1,6	14,14,15	0.31	0	17,19,21	0.71	0
6	NAG	S	2	6	14,14,15	0.64	0	17,19,21	0.52	0
6	NAG	T	1	1,6	14,14,15	0.42	0	17,19,21	0.42	0
6	NAG	T	2	6	14,14,15	0.62	0	17,19,21	0.55	0
6	NAG	U	1	1,6	14,14,15	0.41	0	17,19,21	0.75	1 (5%)
6	NAG	U	2	6	14,14,15	0.55	0	17,19,21	0.53	0
9	NAG	V	1	1,9	14,14,15	0.33	0	17,19,21	0.58	0
9	NAG	V	2	9	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
9	BMA	V	3	9	11,11,12	0.66	0	15,15,17	1.48	3 (20%)
9	MAN	V	4	9	11,11,12	0.62	0	15,15,17	2.51	4 (26%)
9	MAN	V	5	9	11,11,12	0.56	0	15,15,17	2.03	6 (40%)
9	MAN	V	6	9	11,11,12	0.56	0	15,15,17	1.69	4 (26%)
10	NAG	W	1	1,10	14,14,15	1.00	1 (7%)	17,19,21	1.04	1 (5%)
10	NAG	W	2	10	14,14,15	0.48	0	17,19,21	0.55	0
10	BMA	W	3	10	11,11,12	0.65	0	15,15,17	1.46	3 (20%)
10	MAN	W	4	10	11,11,12	0.60	0	15,15,17	2.54	4 (26%)
6	NAG	X	1	1,6	14,14,15	0.53	0	17,19,21	0.56	0
6	NAG	X	2	6	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	Y	1	1,5	14,14,15	0.79	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	Y	2	5	14,14,15	0.43	0	17,19,21	1.48	3 (17%)
5	BMA	Y	3	5	11,11,12	1.20	1 (9%)	15,15,17	1.51	2 (13%)
6	NAG	Z	1	1,6	14,14,15	0.27	0	17,19,21	0.55	0
6	NAG	Z	2	6	14,14,15	0.31	0	17,19,21	0.66	1 (5%)
6	NAG	a	1	1,6	14,14,15	0.41	0	17,19,21	0.46	0
6	NAG	a	2	6	14,14,15	0.28	0	17,19,21	0.49	0
6	NAG	b	1	1,6	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
6	NAG	b	2	6	14,14,15	0.52	0	17,19,21	1.39	3 (17%)
7	NAG	c	1	1,7	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
7	NAG	c	2	7	14,14,15	0.50	0	17,19,21	1.39	3 (17%)
7	BMA	c	3	7	11,11,12	0.67	0	15,15,17	1.48	3 (20%)
7	MAN	c	4	7	11,11,12	0.59	0	15,15,17	1.72	4 (26%)
7	MAN	c	5	7	11,11,12	0.60	0	15,15,17	2.40	5 (33%)
7	MAN	c	6	7	11,11,12	0.60	0	15,15,17	2.54	4 (26%)
7	MAN	c	7	7	11,11,12	0.58	0	15,15,17	2.04	5 (33%)
8	NAG	d	1	1,8	14,14,15	0.79	1 (7%)	17,19,21	0.68	0
8	NAG	d	2	8	14,14,15	0.41	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BMA	d	3	8	11,11,12	1.67	4 (36%)	15,15,17	1.83	2 (13%)
8	MAN	d	4	8	11,11,12	1.65	3 (27%)	15,15,17	1.33	2 (13%)
8	MAN	d	5	8	11,11,12	2.31	4 (36%)	15,15,17	1.86	5 (33%)
8	MAN	d	6	8	11,11,12	0.61	0	15,15,17	2.54	4 (26%)
8	MAN	d	7	8	11,11,12	0.60	0	15,15,17	2.03	6 (40%)
8	MAN	d	8	8	11,11,12	0.63	0	15,15,17	2.42	7 (46%)
6	NAG	e	1	1,6	14,14,15	0.30	0	17,19,21	0.71	0
6	NAG	e	2	6	14,14,15	0.65	0	17,19,21	0.53	0
6	NAG	f	1	1,6	14,14,15	0.43	0	17,19,21	0.41	0
6	NAG	f	2	6	14,14,15	0.61	0	17,19,21	0.55	0
6	NAG	g	1	1,6	14,14,15	0.42	0	17,19,21	0.75	1 (5%)
6	NAG	g	2	6	14,14,15	0.57	0	17,19,21	0.53	0
9	NAG	h	1	1,9	14,14,15	0.32	0	17,19,21	0.58	0
9	NAG	h	2	9	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
9	BMA	h	3	9	11,11,12	0.66	0	15,15,17	1.49	3 (20%)
9	MAN	h	4	9	11,11,12	0.63	0	15,15,17	2.51	4 (26%)
9	MAN	h	5	9	11,11,12	0.55	0	15,15,17	2.03	7 (46%)
9	MAN	h	6	9	11,11,12	0.56	0	15,15,17	1.69	4 (26%)
10	NAG	i	1	1,10	14,14,15	1.01	1 (7%)	17,19,21	1.04	1 (5%)
10	NAG	i	2	10	14,14,15	0.48	0	17,19,21	0.55	0
10	BMA	i	3	10	11,11,12	0.64	0	15,15,17	1.47	3 (20%)
10	MAN	i	4	10	11,11,12	0.61	0	15,15,17	2.52	4 (26%)
6	NAG	j	1	1,6	14,14,15	0.50	0	17,19,21	0.56	0
6	NAG	j	2	6	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	k	1	1,5	14,14,15	0.81	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	k	2	5	14,14,15	0.45	0	17,19,21	1.47	3 (17%)
5	BMA	k	3	5	11,11,12	1.19	1 (9%)	15,15,17	1.51	2 (13%)
6	NAG	l	1	1,6	14,14,15	0.26	0	17,19,21	0.55	0
6	NAG	l	2	6	14,14,15	0.32	0	17,19,21	0.65	1 (5%)
6	NAG	m	1	1,6	14,14,15	0.42	0	17,19,21	0.45	0
6	NAG	m	2	6	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	n	1	1,6	14,14,15	0.50	0	17,19,21	2.23	3 (17%)
6	NAG	n	2	6	14,14,15	0.53	0	17,19,21	1.37	3 (17%)
7	NAG	o	1	1,7	14,14,15	0.51	0	17,19,21	2.23	3 (17%)
7	NAG	o	2	7	14,14,15	0.48	0	17,19,21	1.39	3 (17%)
7	BMA	o	3	7	11,11,12	0.66	0	15,15,17	1.47	3 (20%)
7	MAN	o	4	7	11,11,12	0.58	0	15,15,17	1.73	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	o	5	7	11,11,12	0.60	0	15,15,17	2.40	5 (33%)
7	MAN	o	6	7	11,11,12	0.60	0	15,15,17	2.53	4 (26%)
7	MAN	o	7	7	11,11,12	0.56	0	15,15,17	2.02	5 (33%)
8	NAG	p	1	1,8	14,14,15	0.80	1 (7%)	17,19,21	0.69	0
8	NAG	p	2	8	14,14,15	0.41	0	17,19,21	0.46	0
8	BMA	p	3	8	11,11,12	1.67	4 (36%)	15,15,17	1.82	2 (13%)
8	MAN	p	4	8	11,11,12	1.66	3 (27%)	15,15,17	1.31	2 (13%)
8	MAN	p	5	8	11,11,12	2.30	4 (36%)	15,15,17	1.85	5 (33%)
8	MAN	p	6	8	11,11,12	0.62	0	15,15,17	2.54	4 (26%)
8	MAN	p	7	8	11,11,12	0.59	0	15,15,17	2.03	6 (40%)
8	MAN	p	8	8	11,11,12	0.62	0	15,15,17	2.42	7 (46%)
6	NAG	q	1	1,6	14,14,15	0.32	0	17,19,21	0.70	0
6	NAG	q	2	6	14,14,15	0.64	0	17,19,21	0.52	0
6	NAG	r	1	1,6	14,14,15	0.44	0	17,19,21	0.41	0
6	NAG	r	2	6	14,14,15	0.62	0	17,19,21	0.55	0
6	NAG	s	1	1,6	14,14,15	0.41	0	17,19,21	0.76	1 (5%)
6	NAG	s	2	6	14,14,15	0.55	0	17,19,21	0.53	0
9	NAG	t	1	1,9	14,14,15	0.34	0	17,19,21	0.58	0
9	NAG	t	2	9	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
9	BMA	t	3	9	11,11,12	0.66	0	15,15,17	1.49	3 (20%)
9	MAN	t	4	9	11,11,12	0.62	0	15,15,17	2.52	4 (26%)
9	MAN	t	5	9	11,11,12	0.57	0	15,15,17	2.04	7 (46%)
9	MAN	t	6	9	11,11,12	0.56	0	15,15,17	1.68	3 (20%)
10	NAG	u	1	1,10	14,14,15	0.99	1 (7%)	17,19,21	1.04	1 (5%)
10	NAG	u	2	10	14,14,15	0.49	0	17,19,21	0.55	0
10	BMA	u	3	10	11,11,12	0.66	0	15,15,17	1.46	3 (20%)
10	MAN	u	4	10	11,11,12	0.63	0	15,15,17	2.53	4 (26%)
6	NAG	v	1	1,6	14,14,15	0.52	0	17,19,21	0.56	0
6	NAG	v	2	6	14,14,15	0.38	0	17,19,21	0.43	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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	6	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	7	7	-	0/2/19/22	0/1/1/1
8	NAG	R	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
8	BMA	R	3	8	-	0/2/19/22	0/1/1/1
8	MAN	R	4	8	-	2/2/19/22	0/1/1/1
8	MAN	R	5	8	-	0/2/19/22	0/1/1/1
8	MAN	R	6	8	-	0/2/19/22	0/1/1/1
8	MAN	R	7	8	-	0/2/19/22	0/1/1/1
8	MAN	R	8	8	-	0/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
9	NAG	V	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1
9	MAN	V	4	9	-	0/2/19/22	0/1/1/1
9	MAN	V	5	9	-	0/2/19/22	0/1/1/1
9	MAN	V	6	9	-	0/2/19/22	0/1/1/1
10	NAG	W	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	W	2	10	-	2/6/23/26	0/1/1/1
10	BMA	W	3	10	-	2/2/19/22	0/1/1/1
10	MAN	W	4	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	X	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
5	NAG	Y	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	5/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	NAG	b	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1
7	NAG	c	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	BMA	c	3	7	-	0/2/19/22	0/1/1/1
7	MAN	c	4	7	-	0/2/19/22	0/1/1/1
7	MAN	c	5	7	-	0/2/19/22	0/1/1/1
7	MAN	c	6	7	-	0/2/19/22	0/1/1/1
7	MAN	c	7	7	-	0/2/19/22	0/1/1/1
8	NAG	d	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
8	BMA	d	3	8	-	0/2/19/22	0/1/1/1
8	MAN	d	4	8	-	2/2/19/22	0/1/1/1
8	MAN	d	5	8	-	0/2/19/22	0/1/1/1
8	MAN	d	6	8	-	0/2/19/22	0/1/1/1
8	MAN	d	7	8	-	0/2/19/22	0/1/1/1
8	MAN	d	8	8	-	0/2/19/22	0/1/1/1
6	NAG	e	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	NAG	f	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	g	2	6	-	2/6/23/26	0/1/1/1
9	NAG	h	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	h	2	9	-	2/6/23/26	0/1/1/1
9	BMA	h	3	9	-	2/2/19/22	0/1/1/1
9	MAN	h	4	9	-	0/2/19/22	0/1/1/1
9	MAN	h	5	9	-	0/2/19/22	0/1/1/1
9	MAN	h	6	9	-	0/2/19/22	0/1/1/1

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

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

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	5	MAN	C4-C5	4.43	1.62	1.53
8	d	5	MAN	C4-C5	4.40	1.62	1.53
8	p	5	MAN	C4-C5	4.36	1.62	1.53
8	d	5	MAN	C4-C3	3.77	1.61	1.52
8	p	5	MAN	C4-C3	3.76	1.61	1.52
8	R	5	MAN	C4-C3	3.75	1.61	1.52
10	i	1	NAG	O5-C1	3.58	1.49	1.43
10	W	1	NAG	O5-C1	3.57	1.49	1.43
10	u	1	NAG	O5-C1	3.50	1.49	1.43
8	p	4	MAN	O5-C5	3.04	1.49	1.43
8	R	4	MAN	O5-C5	3.03	1.49	1.43
8	d	5	MAN	C2-C3	3.02	1.57	1.52
8	d	4	MAN	O5-C5	3.00	1.49	1.43
8	R	5	MAN	C2-C3	2.97	1.56	1.52
8	p	5	MAN	C2-C3	2.96	1.56	1.52
8	d	4	MAN	C4-C3	2.51	1.58	1.52
8	d	3	BMA	C2-C3	2.50	1.56	1.52
8	p	1	NAG	O5-C1	-2.49	1.39	1.43
8	R	4	MAN	C4-C5	2.48	1.58	1.53
8	p	4	MAN	C4-C5	2.48	1.58	1.53
8	d	4	MAN	C4-C5	2.48	1.58	1.53
8	p	4	MAN	C4-C3	2.48	1.58	1.52
5	k	3	BMA	C1-C2	2.46	1.57	1.52
8	R	4	MAN	C4-C3	2.46	1.58	1.52
8	d	1	NAG	O5-C1	-2.45	1.39	1.43
8	R	3	BMA	C2-C3	2.45	1.56	1.52
8	p	3	BMA	C2-C3	2.45	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	3	BMA	C1-C2	2.43	1.57	1.52
5	Y	3	BMA	C1-C2	2.43	1.57	1.52
8	R	1	NAG	O5-C1	-2.40	1.39	1.43
5	k	1	NAG	O5-C1	-2.34	1.40	1.43
8	d	3	BMA	O5-C5	2.33	1.48	1.43
8	p	3	BMA	O5-C5	2.33	1.48	1.43
8	R	3	BMA	O5-C5	2.32	1.48	1.43
5	M	1	NAG	O5-C1	-2.32	1.40	1.43
5	Y	1	NAG	O5-C1	-2.32	1.40	1.43
8	p	5	MAN	O5-C5	2.27	1.48	1.43
8	R	3	BMA	C4-C5	2.22	1.57	1.53
8	p	3	BMA	C4-C5	2.22	1.57	1.53
8	d	3	BMA	C4-C5	2.18	1.57	1.53
8	R	5	MAN	O5-C5	2.17	1.47	1.43
8	d	5	MAN	O5-C5	2.16	1.47	1.43
8	d	3	BMA	O2-C2	2.00	1.47	1.43
8	p	3	BMA	O2-C2	2.00	1.47	1.43

All (278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	c	1	NAG	O5-C1-C2	-7.36	99.66	111.29
7	o	1	NAG	O5-C1-C2	-7.36	99.66	111.29
7	Q	1	NAG	O5-C1-C2	-7.36	99.67	111.29
6	P	1	NAG	O5-C1-C2	-7.35	99.68	111.29
6	b	1	NAG	O5-C1-C2	-7.33	99.71	111.29
6	n	1	NAG	O5-C1-C2	-7.30	99.76	111.29
8	R	6	MAN	C1-C2-C3	7.00	118.27	109.67
8	p	6	MAN	C1-C2-C3	7.00	118.27	109.67
10	W	4	MAN	C1-C2-C3	6.99	118.26	109.67
7	Q	6	MAN	C1-C2-C3	6.97	118.24	109.67
8	d	6	MAN	C1-C2-C3	6.96	118.23	109.67
10	u	4	MAN	C1-C2-C3	6.96	118.22	109.67
10	i	4	MAN	C1-C2-C3	6.95	118.21	109.67
7	c	6	MAN	C1-C2-C3	6.93	118.18	109.67
7	o	6	MAN	C1-C2-C3	6.93	118.18	109.67
9	t	4	MAN	C1-C2-C3	6.92	118.18	109.67
9	V	4	MAN	C1-C2-C3	6.90	118.14	109.67
9	h	4	MAN	C1-C2-C3	6.87	118.12	109.67
8	R	3	BMA	C1-O5-C5	5.69	119.90	112.19
8	d	3	BMA	C1-O5-C5	5.66	119.86	112.19
8	p	3	BMA	C1-O5-C5	5.60	119.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	8	MAN	C6-C5-C4	-5.06	101.15	113.00
8	d	8	MAN	C6-C5-C4	-5.04	101.20	113.00
7	o	5	MAN	O2-C2-C1	5.03	119.45	109.15
8	p	8	MAN	C6-C5-C4	-5.03	101.22	113.00
7	c	5	MAN	O2-C2-C1	5.01	119.41	109.15
7	Q	5	MAN	O2-C2-C1	5.00	119.39	109.15
7	c	5	MAN	C1-O5-C5	4.79	118.68	112.19
7	Q	5	MAN	C1-O5-C5	4.78	118.67	112.19
7	o	5	MAN	C1-O5-C5	4.73	118.60	112.19
5	Y	2	NAG	C2-N2-C7	4.51	129.32	122.90
5	M	2	NAG	C2-N2-C7	4.50	129.31	122.90
5	k	2	NAG	C2-N2-C7	4.46	129.25	122.90
7	o	6	MAN	C2-C3-C4	-4.14	103.72	110.89
7	Q	6	MAN	C2-C3-C4	-4.14	103.73	110.89
7	c	6	MAN	C2-C3-C4	-4.14	103.73	110.89
10	W	4	MAN	C2-C3-C4	-4.12	103.77	110.89
8	d	6	MAN	C2-C3-C4	-4.11	103.78	110.89
8	R	6	MAN	C2-C3-C4	-4.11	103.79	110.89
8	p	6	MAN	C2-C3-C4	-4.10	103.80	110.89
10	u	4	MAN	C2-C3-C4	-4.10	103.80	110.89
10	i	4	MAN	C2-C3-C4	-4.09	103.82	110.89
9	h	4	MAN	C2-C3-C4	-4.08	103.83	110.89
7	o	5	MAN	O2-C2-C3	-4.08	101.97	110.14
7	Q	5	MAN	O2-C2-C3	-4.07	101.97	110.14
9	t	4	MAN	C2-C3-C4	-4.07	103.86	110.89
7	c	5	MAN	O2-C2-C3	-4.07	101.99	110.14
9	V	4	MAN	C2-C3-C4	-4.03	103.91	110.89
9	V	5	MAN	O4-C4-C3	-3.99	101.12	110.35
5	k	3	BMA	C1-O5-C5	3.98	117.59	112.19
5	M	3	BMA	C1-O5-C5	3.98	117.59	112.19
9	t	5	MAN	O4-C4-C3	-3.98	101.15	110.35
9	h	5	MAN	O4-C4-C3	-3.98	101.15	110.35
5	Y	3	BMA	C1-O5-C5	3.96	117.56	112.19
7	c	7	MAN	O4-C4-C3	-3.95	101.21	110.35
7	Q	7	MAN	O4-C4-C3	-3.95	101.22	110.35
8	d	7	MAN	O4-C4-C3	-3.93	101.27	110.35
7	o	7	MAN	O4-C4-C3	-3.92	101.28	110.35
8	d	5	MAN	C1-O5-C5	3.91	117.49	112.19
8	R	7	MAN	O4-C4-C3	-3.90	101.32	110.35
8	p	7	MAN	O4-C4-C3	-3.90	101.33	110.35
8	p	5	MAN	C1-O5-C5	3.90	117.47	112.19
8	R	5	MAN	C1-O5-C5	3.90	117.47	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	d	4	MAN	C1-O5-C5	3.78	117.32	112.19
8	R	4	MAN	C1-O5-C5	3.75	117.28	112.19
8	p	4	MAN	C1-O5-C5	3.69	117.20	112.19
7	o	2	NAG	O5-C5-C6	-3.60	101.55	107.20
8	p	8	MAN	O4-C4-C3	-3.60	102.04	110.35
8	R	8	MAN	O4-C4-C3	-3.59	102.05	110.35
7	c	2	NAG	O5-C5-C6	-3.59	101.58	107.20
8	d	8	MAN	O4-C4-C3	-3.58	102.08	110.35
7	Q	2	NAG	O5-C5-C6	-3.57	101.61	107.20
6	b	2	NAG	O5-C5-C6	-3.49	101.73	107.20
7	c	6	MAN	O5-C1-C2	-3.48	105.40	110.77
6	n	2	NAG	O5-C5-C6	-3.47	101.76	107.20
6	P	2	NAG	O5-C5-C6	-3.47	101.77	107.20
8	p	8	MAN	O5-C5-C6	3.45	112.62	107.20
7	Q	6	MAN	O5-C1-C2	-3.45	105.45	110.77
7	o	6	MAN	O5-C1-C2	-3.45	105.45	110.77
10	W	4	MAN	O5-C1-C2	-3.44	105.46	110.77
8	d	6	MAN	O5-C1-C2	-3.43	105.47	110.77
8	p	6	MAN	O5-C1-C2	-3.43	105.48	110.77
7	c	4	MAN	O5-C5-C6	3.42	112.57	107.20
8	R	6	MAN	O5-C1-C2	-3.41	105.50	110.77
7	o	4	MAN	O5-C5-C6	3.41	112.55	107.20
10	u	4	MAN	O5-C1-C2	-3.41	105.51	110.77
8	d	8	MAN	O5-C5-C6	3.39	112.52	107.20
8	R	8	MAN	O5-C5-C6	3.39	112.52	107.20
7	Q	4	MAN	O5-C5-C6	3.39	112.52	107.20
10	i	4	MAN	O5-C1-C2	-3.39	105.54	110.77
9	t	4	MAN	O5-C1-C2	-3.37	105.57	110.77
9	V	4	MAN	O5-C1-C2	-3.36	105.58	110.77
8	d	5	MAN	C1-C2-C3	-3.34	105.56	109.67
9	h	4	MAN	O5-C1-C2	-3.34	105.62	110.77
9	V	6	MAN	O5-C5-C6	3.30	112.38	107.20
9	h	6	MAN	O5-C5-C6	3.29	112.36	107.20
9	t	6	MAN	O5-C5-C6	3.28	112.35	107.20
8	R	5	MAN	C1-C2-C3	-3.26	105.65	109.67
8	p	5	MAN	C1-C2-C3	-3.26	105.66	109.67
7	c	7	MAN	O4-C4-C5	3.26	117.39	109.30
9	t	5	MAN	O4-C4-C5	3.23	117.33	109.30
7	o	7	MAN	O4-C4-C5	3.23	117.31	109.30
8	p	7	MAN	O4-C4-C5	3.22	117.29	109.30
7	Q	7	MAN	O4-C4-C5	3.21	117.27	109.30
9	h	5	MAN	O4-C4-C5	3.21	117.27	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	5	MAN	O4-C4-C5	3.21	117.26	109.30
8	R	7	MAN	O4-C4-C5	3.20	117.25	109.30
8	d	7	MAN	O4-C4-C5	3.19	117.22	109.30
8	R	8	MAN	C3-C4-C5	-3.17	104.59	110.24
8	d	8	MAN	C3-C4-C5	-3.14	104.64	110.24
10	W	1	NAG	C1-O5-C5	3.12	116.42	112.19
8	p	8	MAN	C3-C4-C5	-3.12	104.67	110.24
10	i	1	NAG	C1-O5-C5	3.11	116.41	112.19
10	u	1	NAG	C1-O5-C5	3.11	116.40	112.19
9	t	3	BMA	O2-C2-C3	3.09	116.33	110.14
7	c	3	BMA	O2-C2-C3	3.05	116.25	110.14
9	h	3	BMA	O2-C2-C3	3.04	116.23	110.14
7	o	3	BMA	O2-C2-C3	3.03	116.20	110.14
7	Q	3	BMA	O2-C2-C3	3.03	116.20	110.14
9	V	3	BMA	O2-C2-C3	3.02	116.19	110.14
8	d	8	MAN	O2-C2-C3	-2.96	104.20	110.14
8	p	8	MAN	O2-C2-C3	-2.96	104.22	110.14
10	W	3	BMA	O2-C2-C3	2.94	116.04	110.14
10	u	3	BMA	O2-C2-C3	2.94	116.03	110.14
10	i	3	BMA	O2-C2-C3	2.94	116.03	110.14
8	R	8	MAN	O2-C2-C3	-2.92	104.28	110.14
9	h	5	MAN	O5-C5-C6	-2.87	102.71	107.20
7	o	7	MAN	O5-C5-C6	-2.86	102.72	107.20
7	Q	7	MAN	O5-C5-C6	-2.85	102.74	107.20
8	d	7	MAN	O5-C5-C6	-2.84	102.75	107.20
8	p	7	MAN	O5-C5-C6	-2.84	102.75	107.20
8	R	7	MAN	O5-C5-C6	-2.84	102.75	107.20
9	V	5	MAN	O5-C5-C6	-2.83	102.78	107.20
7	c	7	MAN	O5-C5-C6	-2.82	102.78	107.20
9	t	5	MAN	O5-C5-C6	-2.82	102.79	107.20
7	Q	1	NAG	O7-C7-C8	-2.77	116.91	122.06
6	P	1	NAG	O7-C7-C8	-2.73	116.99	122.06
7	c	1	NAG	O7-C7-C8	-2.73	116.99	122.06
7	Q	5	MAN	O4-C4-C3	-2.72	104.06	110.35
7	c	5	MAN	O4-C4-C3	-2.72	104.06	110.35
6	b	1	NAG	O7-C7-C8	-2.72	117.01	122.06
7	o	1	NAG	O7-C7-C8	-2.71	117.03	122.06
6	P	1	NAG	C4-C3-C2	-2.71	107.05	111.02
6	n	1	NAG	O7-C7-C8	-2.71	117.03	122.06
6	n	1	NAG	C4-C3-C2	-2.70	107.06	111.02
7	o	5	MAN	O4-C4-C3	-2.70	104.11	110.35
7	Q	1	NAG	C4-C3-C2	-2.67	107.11	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	b	1	NAG	C4-C3-C2	-2.66	107.12	111.02
7	c	1	NAG	C4-C3-C2	-2.64	107.14	111.02
9	h	3	BMA	O4-C4-C5	-2.64	102.73	109.30
9	t	3	BMA	O4-C4-C5	-2.64	102.73	109.30
8	d	5	MAN	O5-C1-C2	2.64	114.84	110.77
9	V	3	BMA	O4-C4-C5	-2.64	102.75	109.30
8	p	5	MAN	O5-C1-C2	2.63	114.83	110.77
8	R	5	MAN	O5-C1-C2	2.63	114.83	110.77
10	i	3	BMA	O4-C4-C5	-2.62	102.78	109.30
7	c	3	BMA	O4-C4-C5	-2.61	102.80	109.30
7	Q	3	BMA	O4-C4-C5	-2.61	102.81	109.30
7	o	1	NAG	C4-C3-C2	-2.61	107.19	111.02
10	u	3	BMA	O4-C4-C5	-2.60	102.83	109.30
10	W	3	BMA	O4-C4-C5	-2.60	102.83	109.30
7	o	3	BMA	O4-C4-C5	-2.60	102.84	109.30
7	o	4	MAN	O5-C1-C2	2.54	114.69	110.77
7	c	4	MAN	O5-C1-C2	2.51	114.65	110.77
7	Q	4	MAN	O5-C1-C2	2.51	114.64	110.77
8	d	3	BMA	O2-C2-C1	2.50	114.27	109.15
8	R	3	BMA	O2-C2-C1	2.50	114.27	109.15
8	p	3	BMA	O2-C2-C1	2.49	114.25	109.15
7	Q	3	BMA	C6-C5-C4	-2.46	107.23	113.00
7	c	3	BMA	C6-C5-C4	-2.46	107.24	113.00
8	d	8	MAN	O2-C2-C1	2.45	114.17	109.15
10	u	3	BMA	C6-C5-C4	-2.45	107.26	113.00
7	o	3	BMA	C6-C5-C4	-2.45	107.26	113.00
8	p	8	MAN	O2-C2-C1	2.45	114.17	109.15
9	t	6	MAN	O5-C1-C2	2.45	114.55	110.77
9	V	6	MAN	O5-C1-C2	2.43	114.53	110.77
9	h	6	MAN	O5-C1-C2	2.43	114.52	110.77
8	R	8	MAN	O2-C2-C1	2.42	114.11	109.15
10	i	3	BMA	C6-C5-C4	-2.42	107.34	113.00
10	W	3	BMA	C6-C5-C4	-2.41	107.36	113.00
9	t	3	BMA	C6-C5-C4	-2.40	107.38	113.00
9	h	3	BMA	C6-C5-C4	-2.40	107.38	113.00
9	V	3	BMA	C6-C5-C4	-2.40	107.39	113.00
8	p	5	MAN	O3-C3-C4	2.40	115.89	110.35
5	M	2	NAG	C1-C2-N2	2.38	114.56	110.49
8	R	5	MAN	O3-C3-C4	2.37	115.84	110.35
8	d	5	MAN	O3-C3-C4	2.37	115.84	110.35
5	Y	3	BMA	O5-C1-C2	2.37	114.43	110.77
5	k	3	BMA	O5-C1-C2	2.37	114.43	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	k	2	NAG	C1-C2-N2	2.37	114.54	110.49
5	Y	2	NAG	C1-C2-N2	2.36	114.51	110.49
6	b	2	NAG	O5-C1-C2	-2.35	107.58	111.29
5	M	3	BMA	O5-C1-C2	2.35	114.40	110.77
5	k	1	NAG	C3-C4-C5	2.31	114.35	110.24
7	c	7	MAN	O3-C3-C2	-2.30	105.58	109.99
5	M	1	NAG	C3-C4-C5	2.30	114.34	110.24
5	Y	1	NAG	C3-C4-C5	2.30	114.34	110.24
7	o	2	NAG	O5-C1-C2	-2.29	107.67	111.29
9	V	5	MAN	C1-O5-C5	2.29	115.29	112.19
6	n	2	NAG	O5-C1-C2	-2.28	107.69	111.29
7	Q	5	MAN	O6-C6-C5	2.28	119.12	111.29
6	P	2	NAG	O5-C1-C2	-2.28	107.69	111.29
9	t	5	MAN	C1-O5-C5	2.27	115.27	112.19
8	d	7	MAN	C1-O5-C5	2.27	115.26	112.19
9	t	2	NAG	C1-O5-C5	2.27	115.26	112.19
7	o	5	MAN	O6-C6-C5	2.26	119.06	111.29
7	c	5	MAN	O6-C6-C5	2.26	119.04	111.29
7	o	7	MAN	O3-C3-C2	-2.26	105.67	109.99
7	Q	7	MAN	O3-C3-C2	-2.26	105.67	109.99
8	p	7	MAN	C1-O5-C5	2.25	115.25	112.19
7	Q	2	NAG	O5-C1-C2	-2.25	107.74	111.29
7	c	2	NAG	O5-C1-C2	-2.25	107.74	111.29
8	d	7	MAN	O3-C3-C2	-2.24	105.70	109.99
9	t	5	MAN	O3-C3-C2	-2.24	105.70	109.99
8	p	4	MAN	O2-C2-C3	-2.24	105.65	110.14
8	d	4	MAN	O2-C2-C3	-2.24	105.65	110.14
8	p	7	MAN	O3-C3-C2	-2.24	105.71	109.99
9	V	5	MAN	O3-C3-C2	-2.23	105.72	109.99
8	R	7	MAN	O3-C3-C2	-2.23	105.72	109.99
9	V	2	NAG	C1-O5-C5	2.23	115.22	112.19
8	R	4	MAN	O2-C2-C3	-2.23	105.67	110.14
9	h	5	MAN	O3-C3-C2	-2.23	105.72	109.99
8	d	5	MAN	O2-C2-C1	2.23	113.71	109.15
8	R	7	MAN	C1-O5-C5	2.23	115.21	112.19
8	p	5	MAN	O2-C2-C1	2.22	113.70	109.15
8	R	5	MAN	O2-C2-C1	2.21	113.68	109.15
9	h	2	NAG	C1-O5-C5	2.21	115.19	112.19
6	P	2	NAG	C4-C3-C2	-2.20	107.79	111.02
7	c	7	MAN	C1-O5-C5	2.20	115.18	112.19
6	b	2	NAG	C4-C3-C2	-2.20	107.79	111.02
9	h	5	MAN	C1-O5-C5	2.20	115.17	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	2	NAG	C4-C3-C2	-2.18	107.82	111.02
7	c	2	NAG	C4-C3-C2	-2.18	107.82	111.02
7	Q	7	MAN	C1-O5-C5	2.18	115.14	112.19
5	Y	2	NAG	O4-C4-C5	-2.17	103.90	109.30
7	o	4	MAN	O3-C3-C4	2.17	115.36	110.35
7	Q	4	MAN	O3-C3-C4	2.17	115.36	110.35
7	o	2	NAG	C4-C3-C2	-2.16	107.85	111.02
5	M	2	NAG	O4-C4-C5	-2.16	103.94	109.30
5	k	2	NAG	O4-C4-C5	-2.16	103.94	109.30
9	h	6	MAN	O3-C3-C4	2.15	115.33	110.35
9	V	6	MAN	O3-C3-C4	2.15	115.32	110.35
7	c	4	MAN	O3-C3-C4	2.15	115.32	110.35
6	g	1	NAG	O4-C4-C5	-2.15	103.97	109.30
7	o	7	MAN	C1-O5-C5	2.14	115.09	112.19
6	s	1	NAG	O4-C4-C5	-2.14	103.99	109.30
6	n	2	NAG	C4-C3-C2	-2.13	107.89	111.02
9	t	6	MAN	O3-C3-C4	2.13	115.28	110.35
6	U	1	NAG	O4-C4-C5	-2.13	104.01	109.30
7	c	6	MAN	O5-C5-C6	-2.10	103.91	107.20
8	R	6	MAN	O5-C5-C6	-2.07	103.96	107.20
7	Q	6	MAN	O5-C5-C6	-2.07	103.96	107.20
9	t	5	MAN	O3-C3-C4	2.05	115.09	110.35
10	W	4	MAN	O5-C5-C6	-2.05	103.99	107.20
7	o	6	MAN	O5-C5-C6	-2.05	103.99	107.20
8	d	6	MAN	O5-C5-C6	-2.04	104.00	107.20
9	h	5	MAN	O3-C3-C4	2.04	115.06	110.35
6	Z	2	NAG	C1-O5-C5	2.04	114.95	112.19
6	N	2	NAG	C1-O5-C5	2.03	114.95	112.19
9	V	5	MAN	O3-C3-C4	2.03	115.05	110.35
8	d	8	MAN	C2-C3-C4	2.03	114.41	110.89
9	h	4	MAN	O5-C5-C6	-2.03	104.02	107.20
10	i	4	MAN	O5-C5-C6	-2.03	104.03	107.20
8	R	8	MAN	C2-C3-C4	2.02	114.39	110.89
9	V	4	MAN	O5-C5-C6	-2.02	104.04	107.20
9	t	4	MAN	O5-C5-C6	-2.02	104.04	107.20
7	o	4	MAN	O4-C4-C3	-2.01	105.69	110.35
8	p	8	MAN	C2-C3-C4	2.01	114.38	110.89
7	c	4	MAN	O4-C4-C3	-2.01	105.70	110.35
9	h	6	MAN	O4-C4-C3	-2.01	105.70	110.35
8	p	7	MAN	O5-C1-C2	2.01	113.87	110.77
8	d	7	MAN	O3-C3-C4	2.01	115.00	110.35
9	h	5	MAN	O5-C1-C2	2.01	113.87	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	u	4	MAN	O5-C5-C6	-2.01	104.06	107.20
9	t	5	MAN	O5-C1-C2	2.01	113.87	110.77
8	p	6	MAN	O5-C5-C6	-2.00	104.06	107.20
9	V	6	MAN	O4-C4-C3	-2.00	105.72	110.35
6	l	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	3	BMA	C4-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
5	k	3	BMA	C4-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
6	q	1	NAG	O5-C5-C6-O6
6	r	1	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	m	2	NAG	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	k	3	BMA	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
5	k	1	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
6	s	2	NAG	O5-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
6	s	1	NAG	O5-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
6	m	2	NAG	C4-C5-C6-O6
8	R	1	NAG	C4-C5-C6-O6
8	d	1	NAG	C4-C5-C6-O6
8	p	1	NAG	C4-C5-C6-O6
8	d	2	NAG	O5-C5-C6-O6
8	p	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	S	1	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
6	f	1	NAG	C4-C5-C6-O6
6	q	1	NAG	C4-C5-C6-O6
6	r	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
9	V	1	NAG	O5-C5-C6-O6
9	h	1	NAG	O5-C5-C6-O6
9	t	1	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
6	l	1	NAG	O5-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
6	g	1	NAG	C4-C5-C6-O6
6	s	1	NAG	C4-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	r	2	NAG	O5-C5-C6-O6
9	V	1	NAG	C4-C5-C6-O6
9	h	1	NAG	C4-C5-C6-O6
9	t	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	g	2	NAG	C4-C5-C6-O6
6	s	2	NAG	C4-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
8	d	2	NAG	C4-C5-C6-O6
8	p	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	Y	2	NAG	C8-C7-N2-C2
5	Y	2	NAG	O7-C7-N2-C2
5	k	2	NAG	C8-C7-N2-C2
5	k	2	NAG	O7-C7-N2-C2
8	R	4	MAN	O5-C5-C6-O6
8	d	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	p	4	MAN	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6
5	k	1	NAG	C4-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
6	r	2	NAG	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	l	2	NAG	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	h	2	NAG	O5-C5-C6-O6
9	t	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
6	v	2	NAG	O5-C5-C6-O6
9	V	3	BMA	O5-C5-C6-O6
9	h	3	BMA	O5-C5-C6-O6
9	t	3	BMA	O5-C5-C6-O6
9	V	2	NAG	C4-C5-C6-O6
9	h	2	NAG	C4-C5-C6-O6
9	t	2	NAG	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	l	2	NAG	C4-C5-C6-O6
9	V	3	BMA	C4-C5-C6-O6
9	h	3	BMA	C4-C5-C6-O6
9	t	3	BMA	C4-C5-C6-O6
10	W	1	NAG	O5-C5-C6-O6
10	i	1	NAG	O5-C5-C6-O6
10	u	1	NAG	O5-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
6	j	2	NAG	C4-C5-C6-O6
6	v	2	NAG	C4-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
8	p	1	NAG	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	l	1	NAG	C4-C5-C6-O6
8	R	4	MAN	C4-C5-C6-O6
8	p	4	MAN	C4-C5-C6-O6

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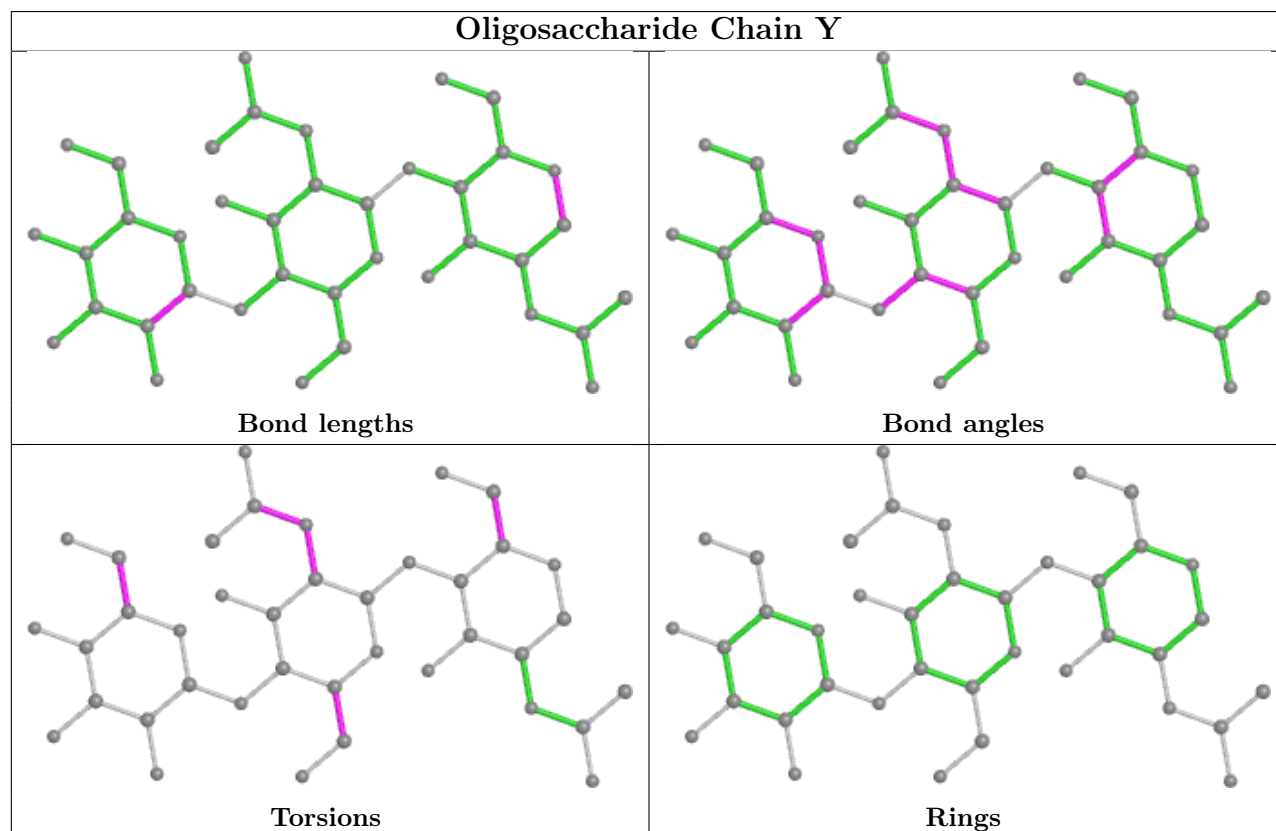
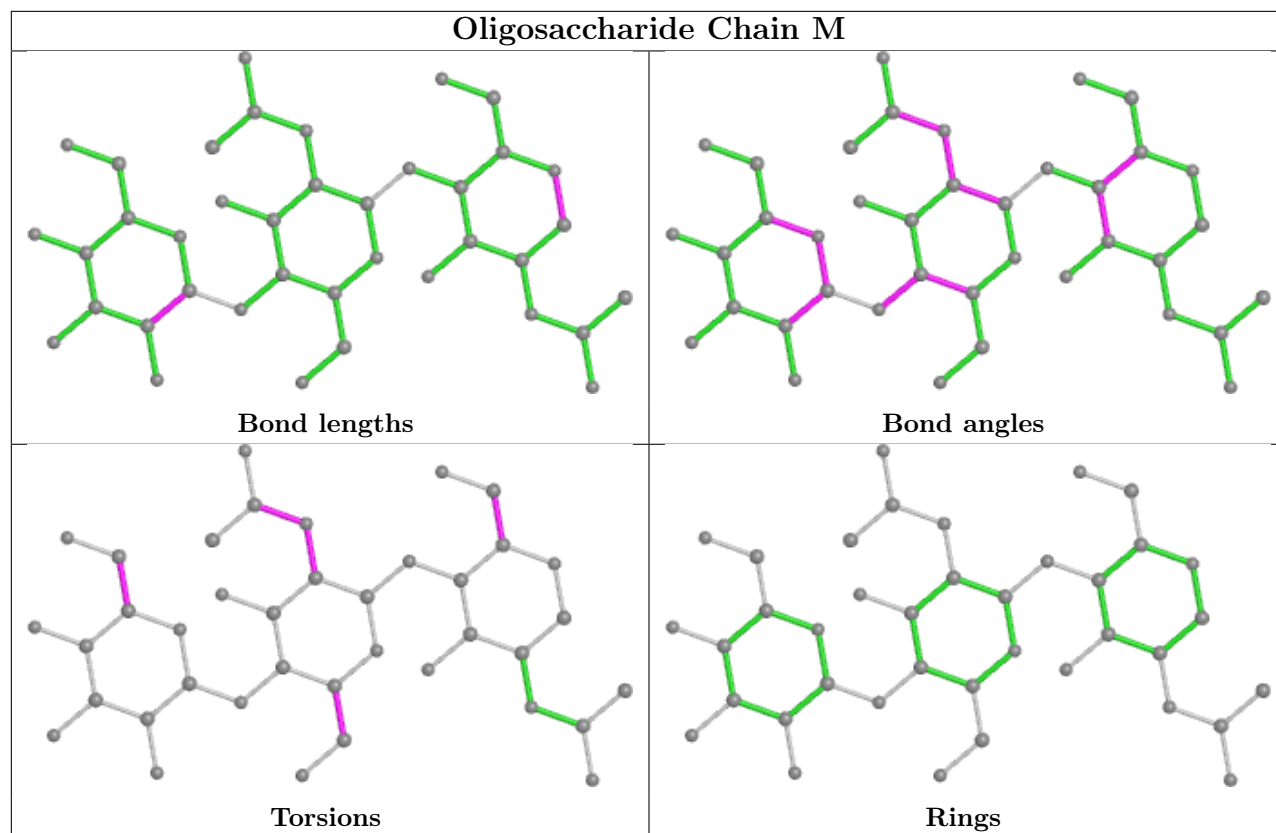
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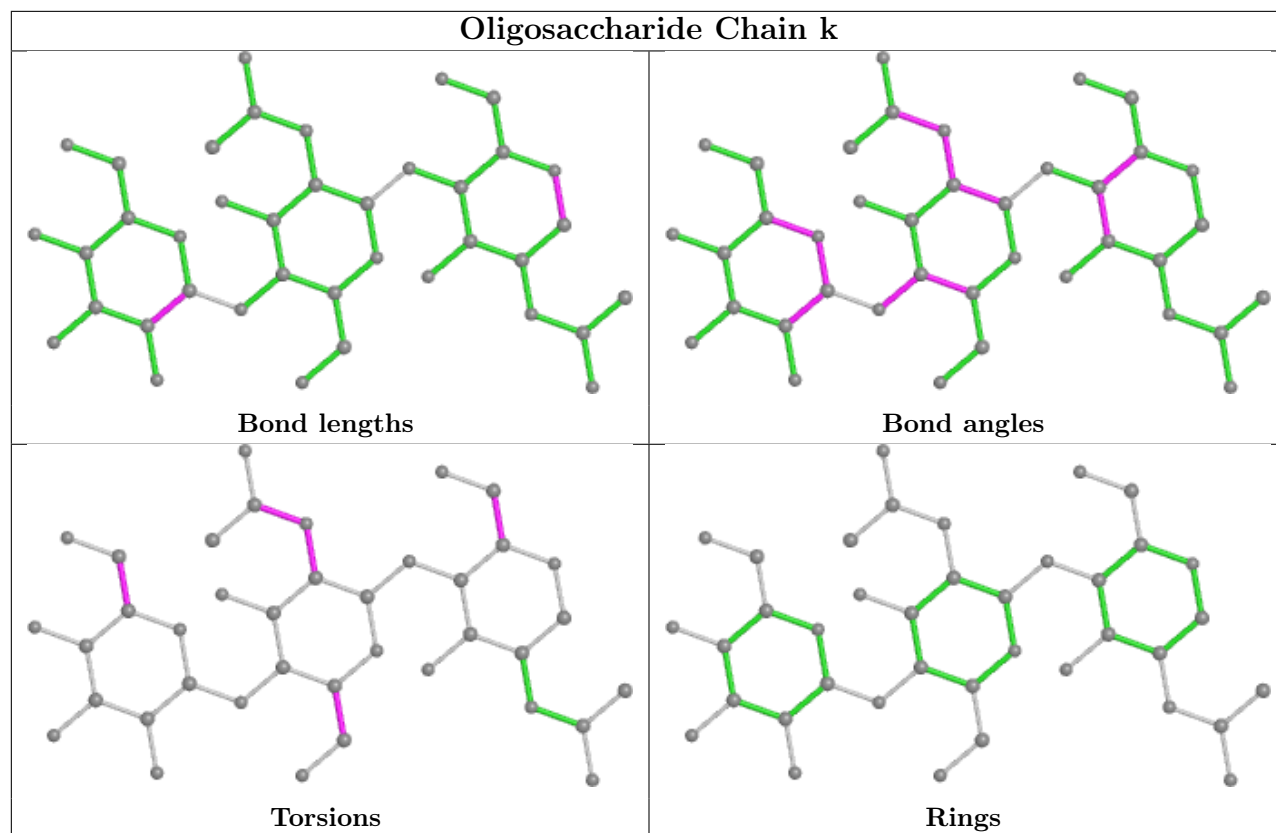
Mol	Chain	Res	Type	Atoms
8	d	4	MAN	C4-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
6	m	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
9	V	1	NAG	C1-C2-N2-C7
9	h	1	NAG	C1-C2-N2-C7
9	t	1	NAG	C1-C2-N2-C7
10	W	2	NAG	C4-C5-C6-O6
10	i	2	NAG	C4-C5-C6-O6
10	u	2	NAG	C4-C5-C6-O6
10	W	3	BMA	C4-C5-C6-O6
10	u	3	BMA	C4-C5-C6-O6
10	i	3	BMA	C4-C5-C6-O6
10	u	3	BMA	O5-C5-C6-O6
10	W	3	BMA	O5-C5-C6-O6
10	i	3	BMA	O5-C5-C6-O6
10	W	1	NAG	C4-C5-C6-O6
10	i	1	NAG	C4-C5-C6-O6
10	u	1	NAG	C4-C5-C6-O6
10	i	2	NAG	O5-C5-C6-O6
10	W	2	NAG	O5-C5-C6-O6
10	u	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7
5	k	2	NAG	C3-C2-N2-C7
9	V	1	NAG	C3-C2-N2-C7
9	h	1	NAG	C3-C2-N2-C7
9	t	1	NAG	C3-C2-N2-C7
6	P	1	NAG	O7-C7-N2-C2
6	b	1	NAG	O7-C7-N2-C2
7	Q	1	NAG	O7-C7-N2-C2
7	c	1	NAG	O7-C7-N2-C2

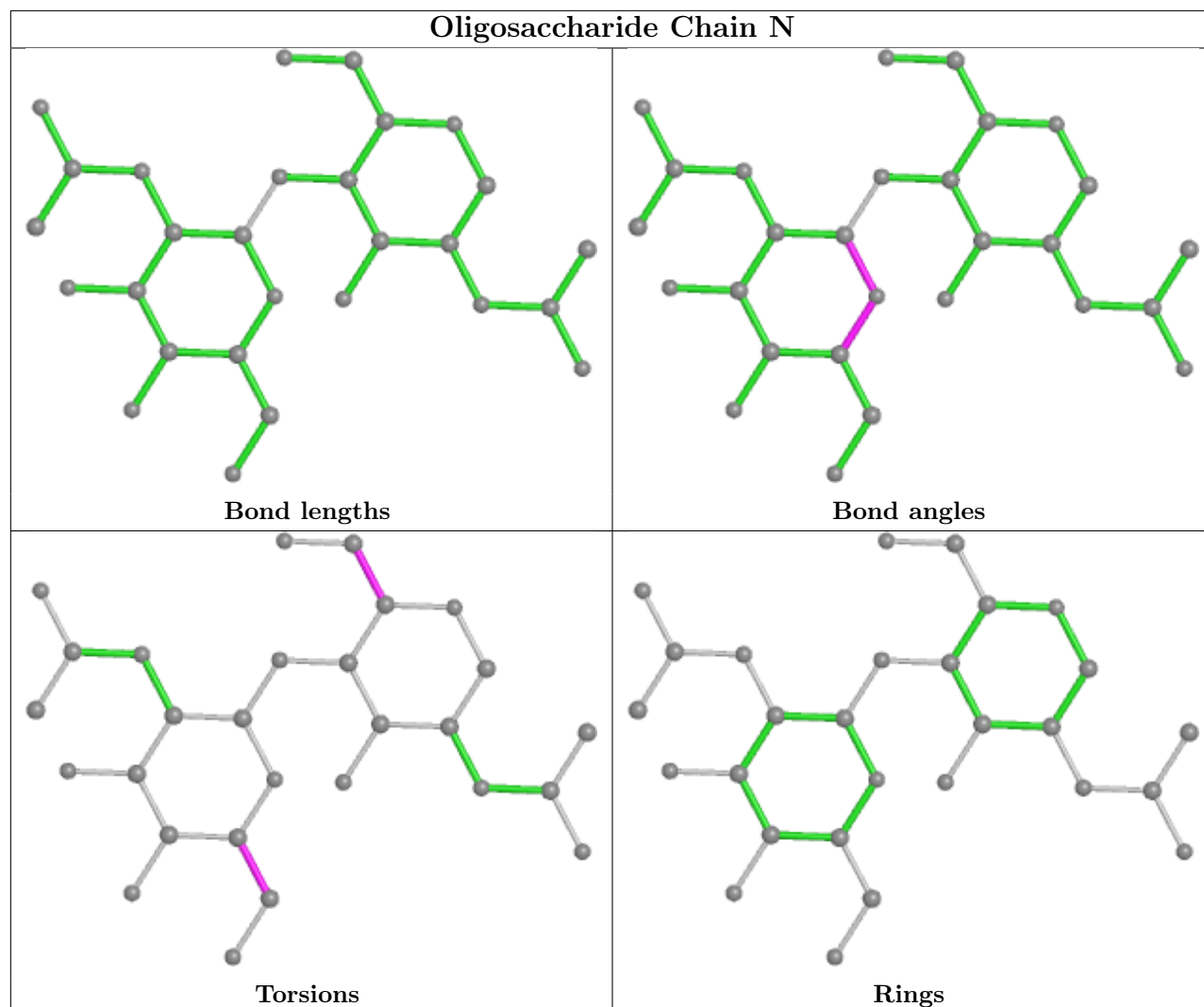
There are no ring outliers.

No monomer is involved in short contacts.

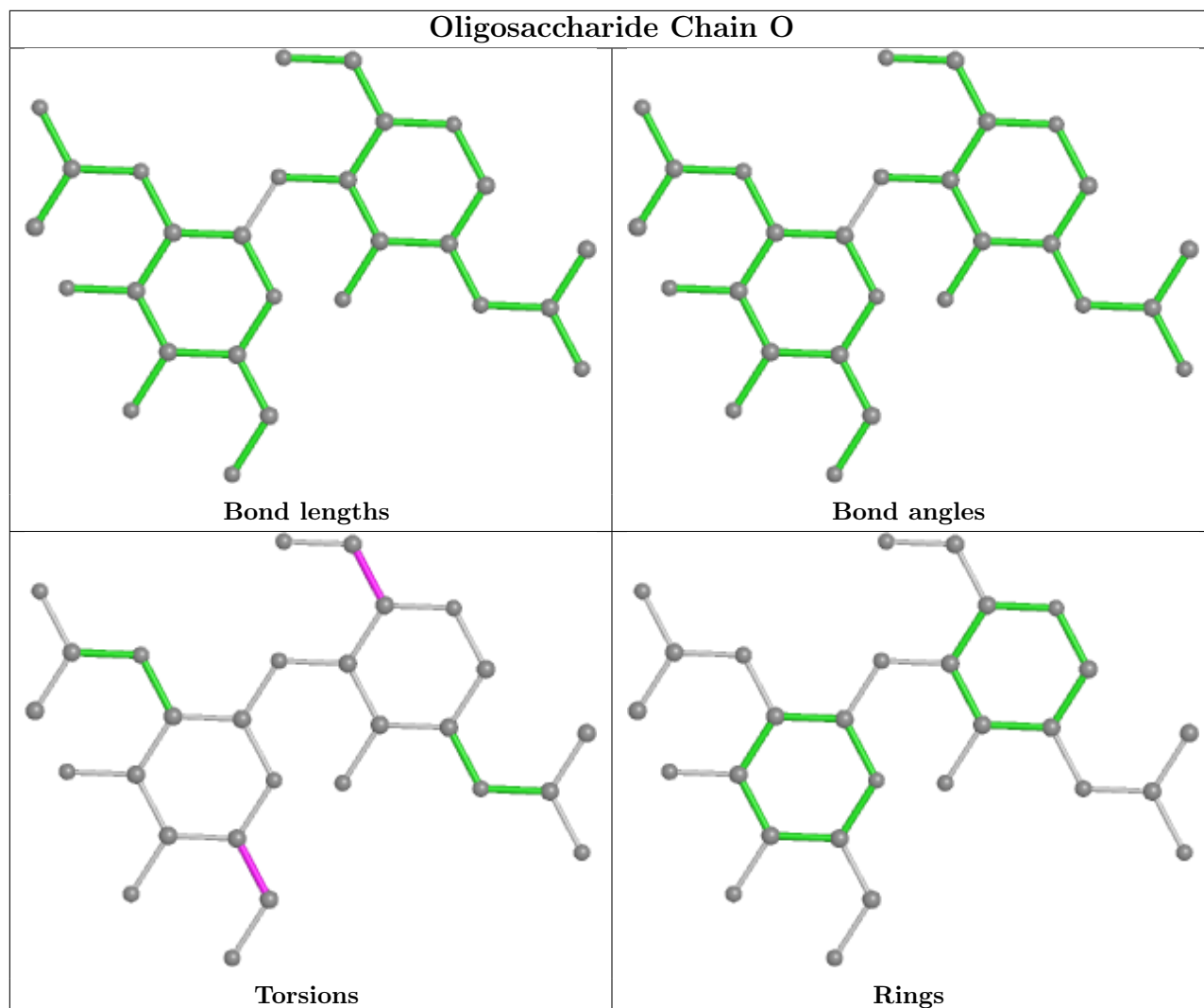
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

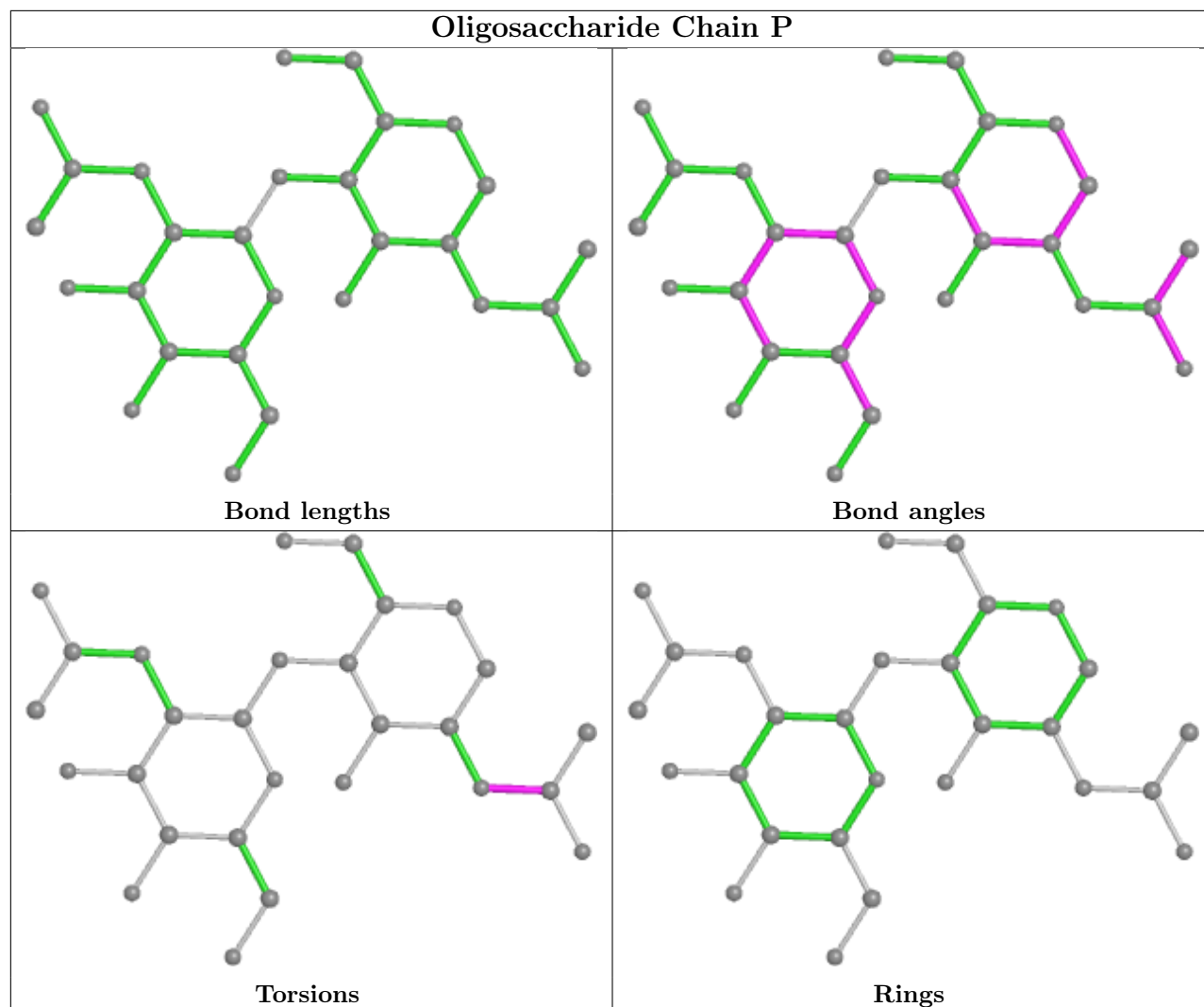


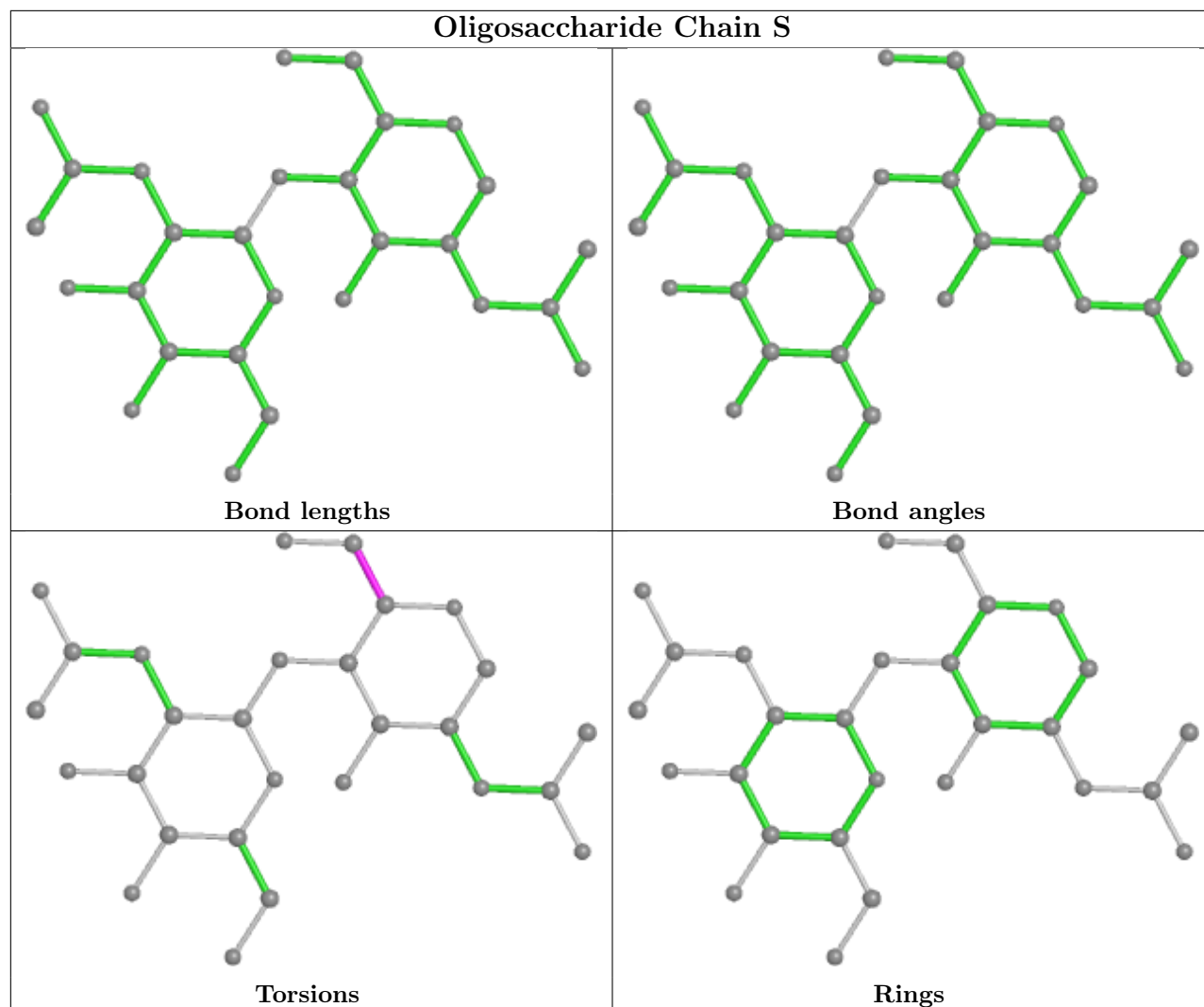


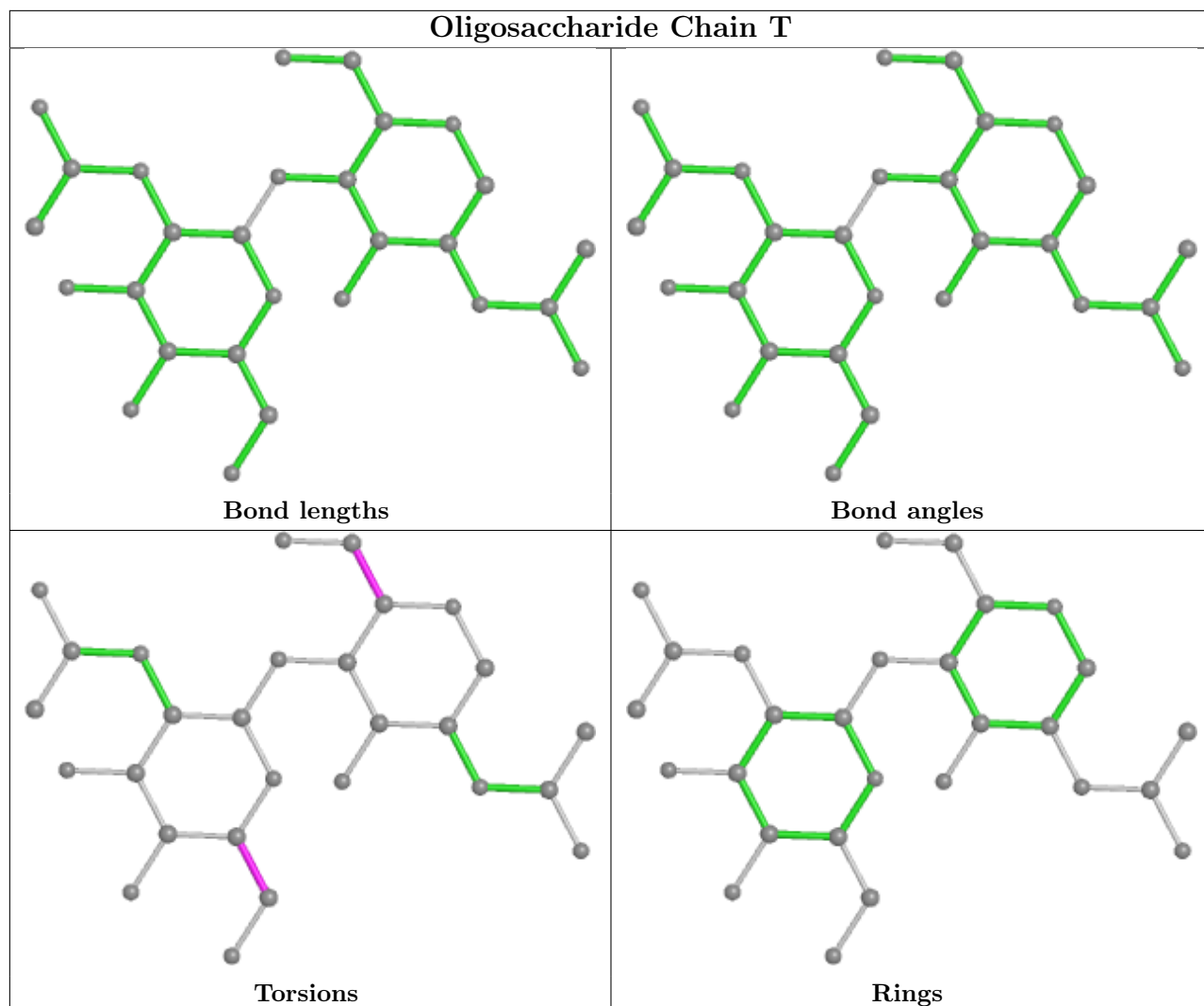


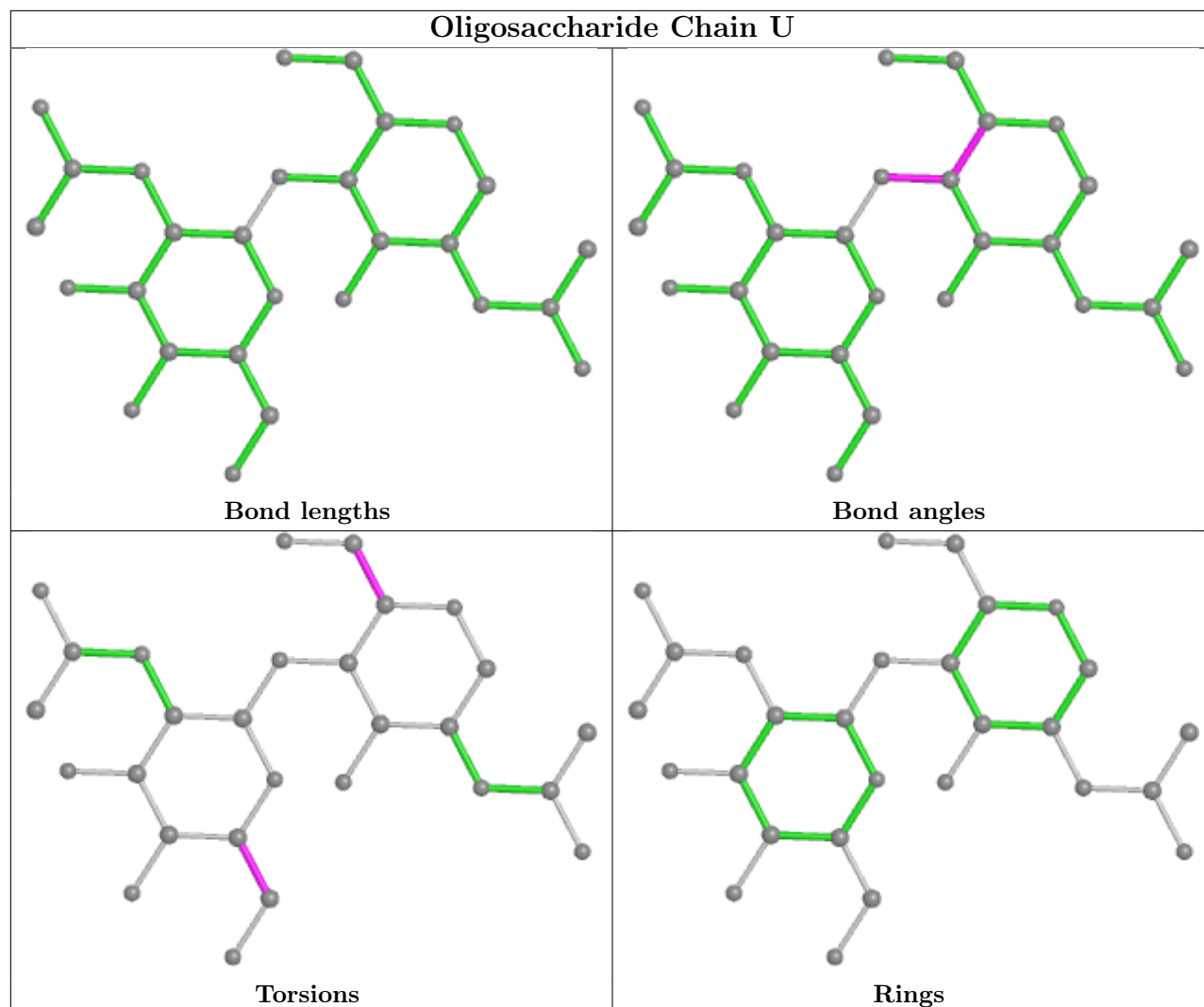


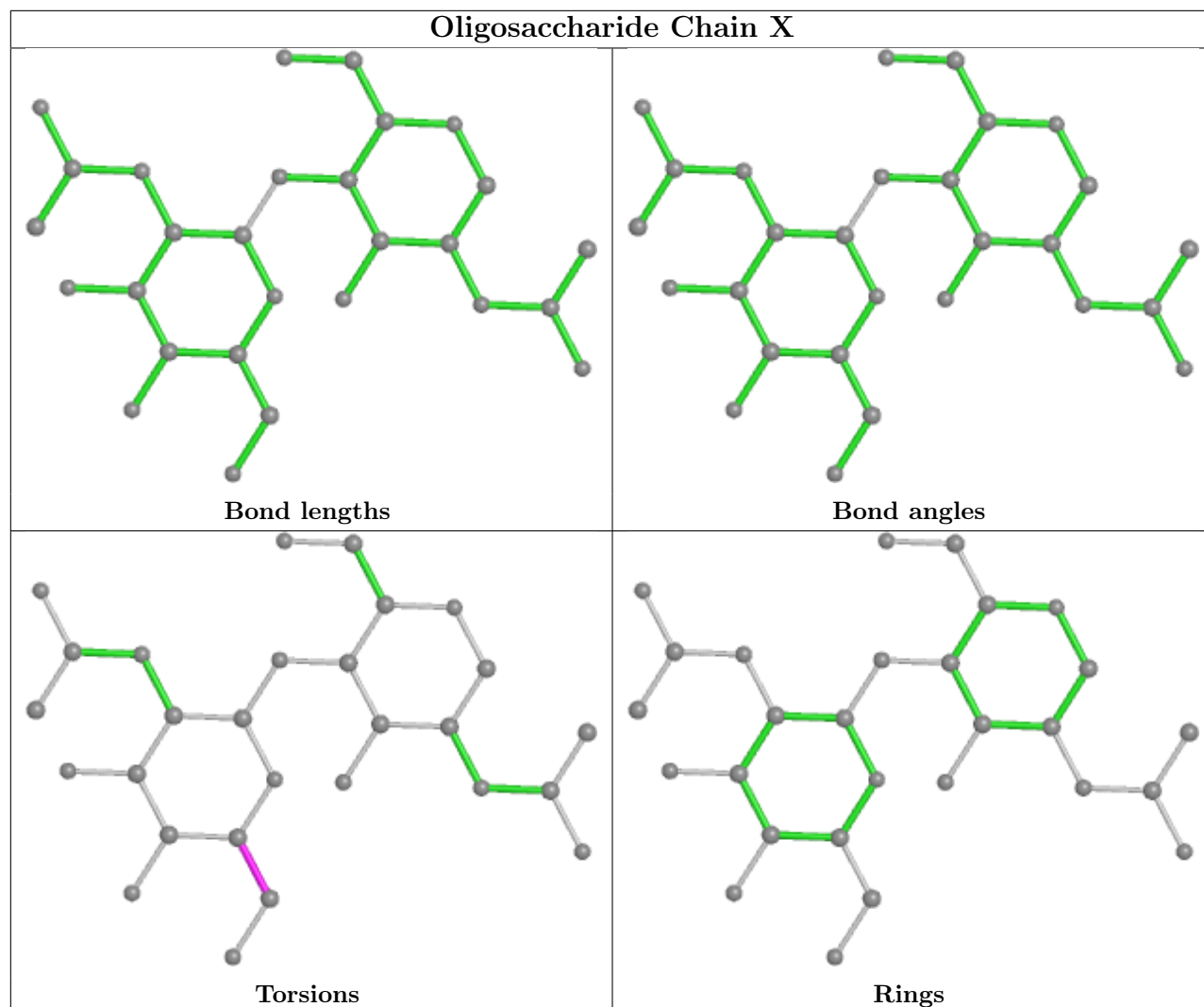


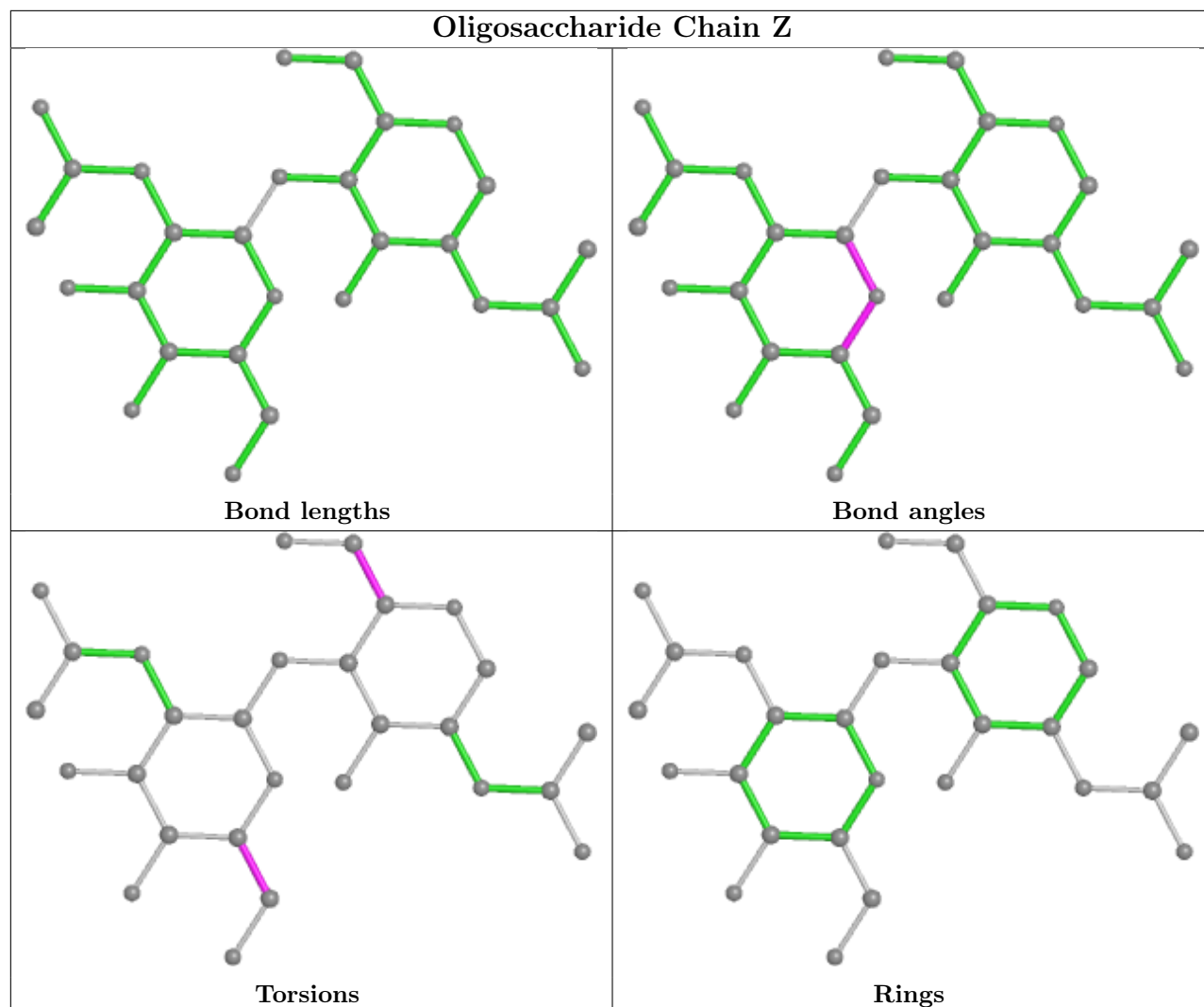


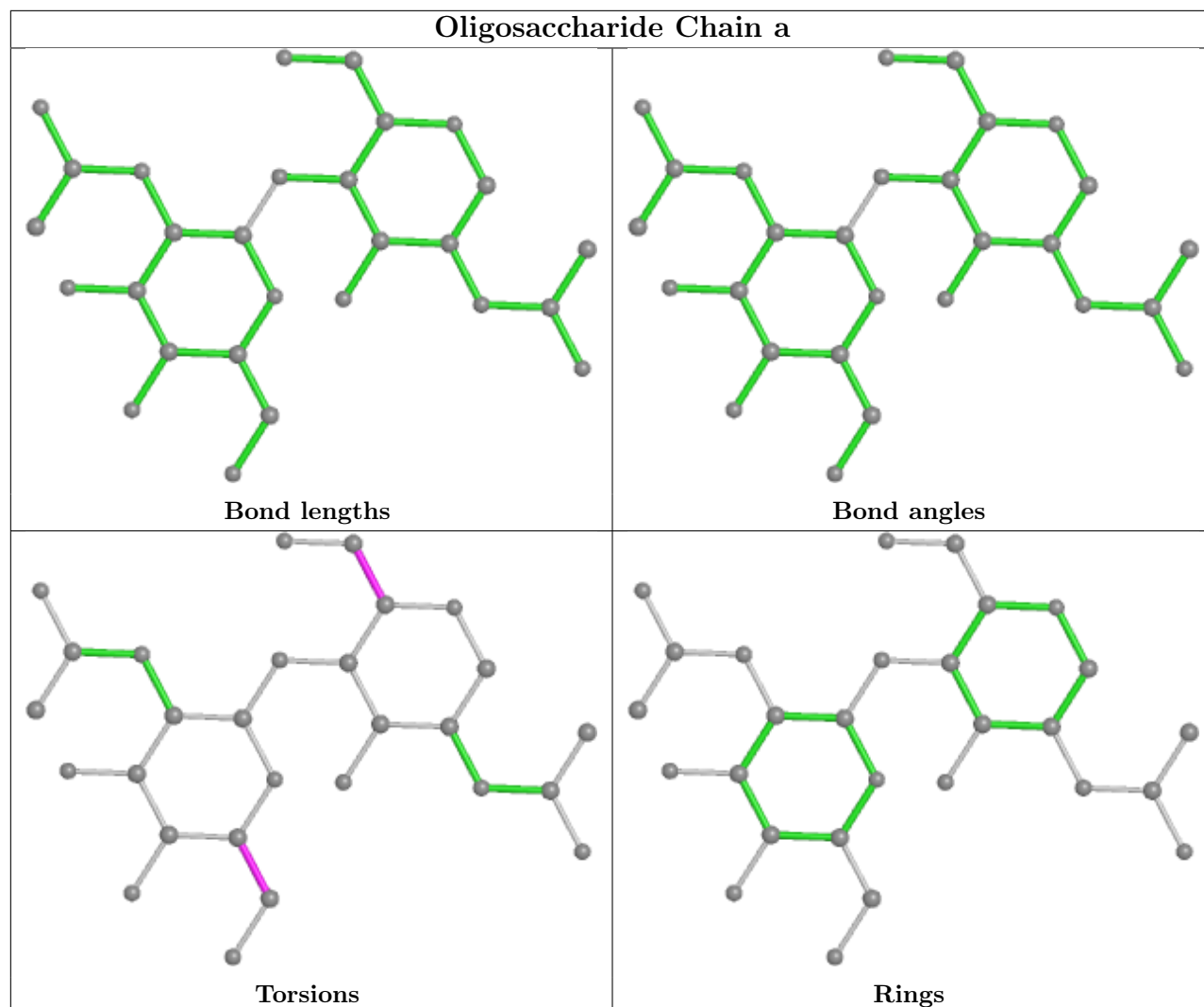




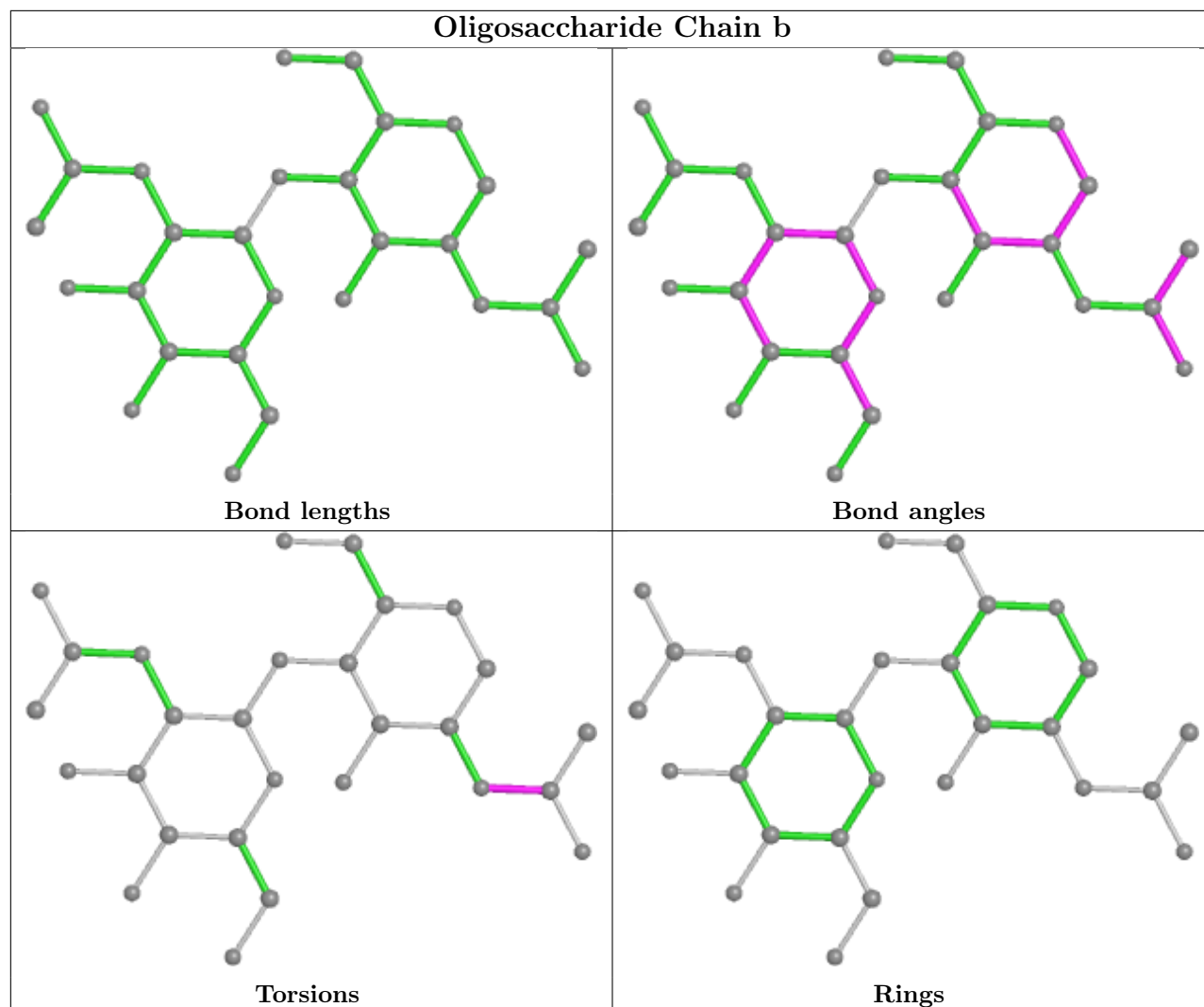


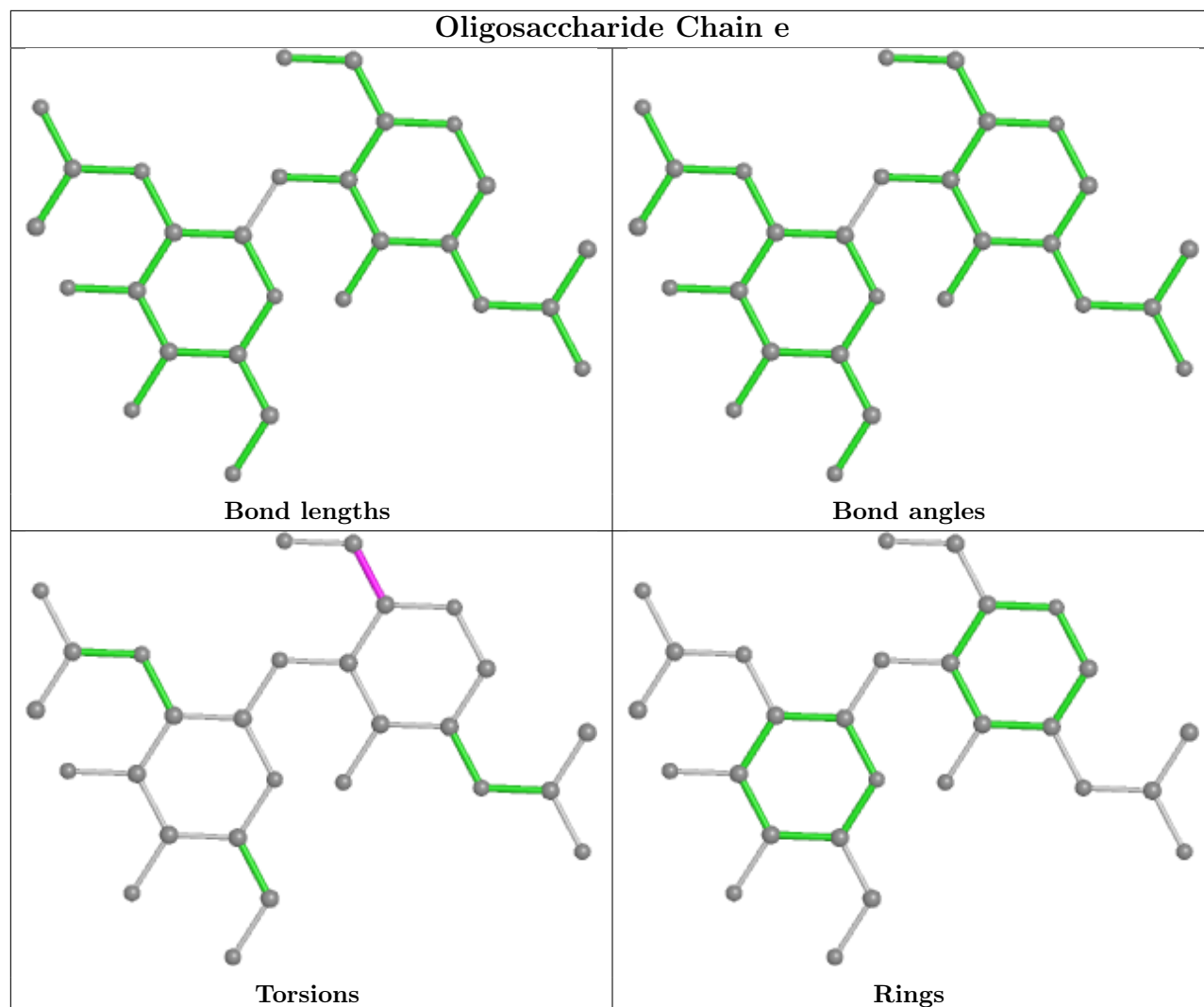


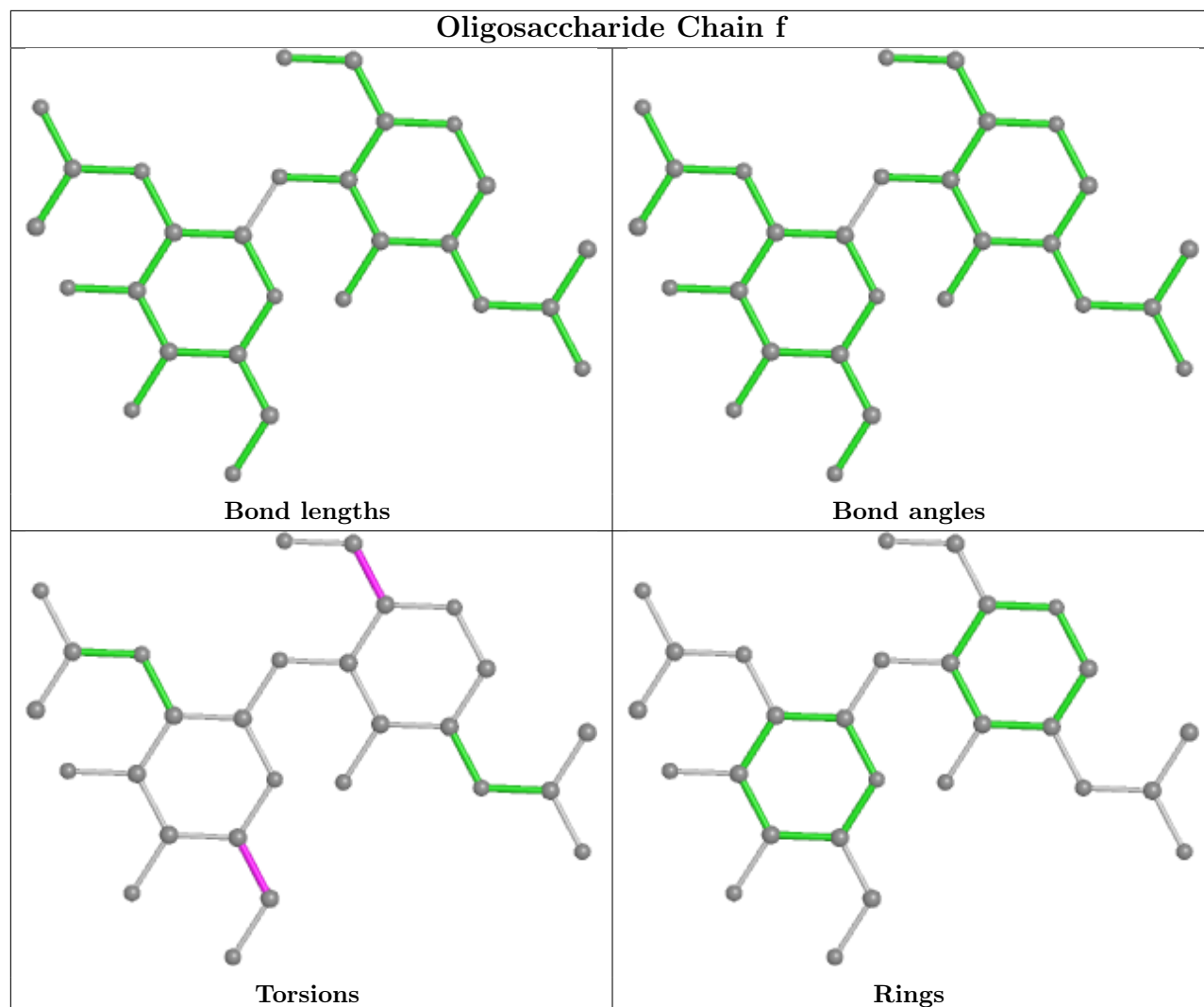


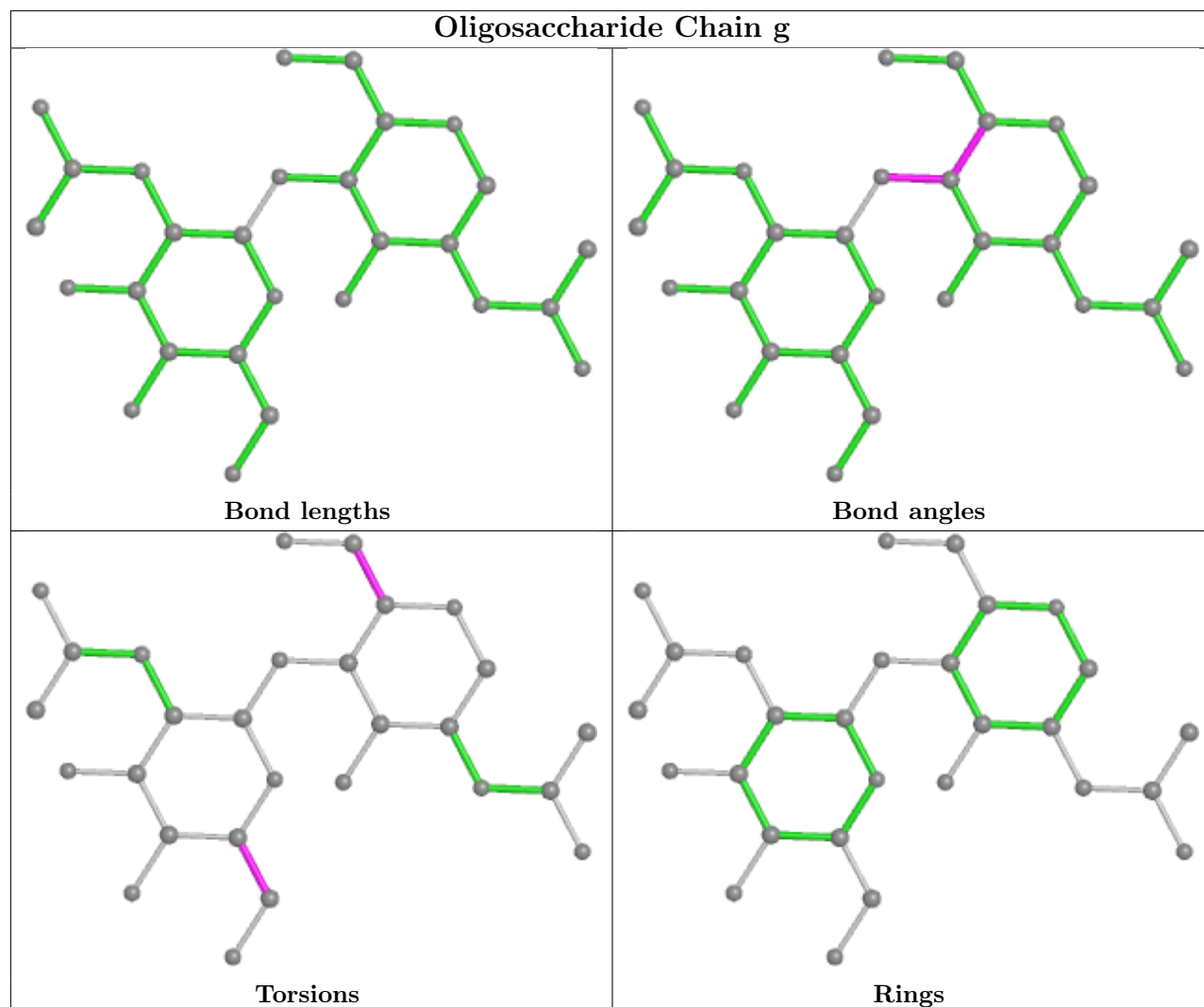


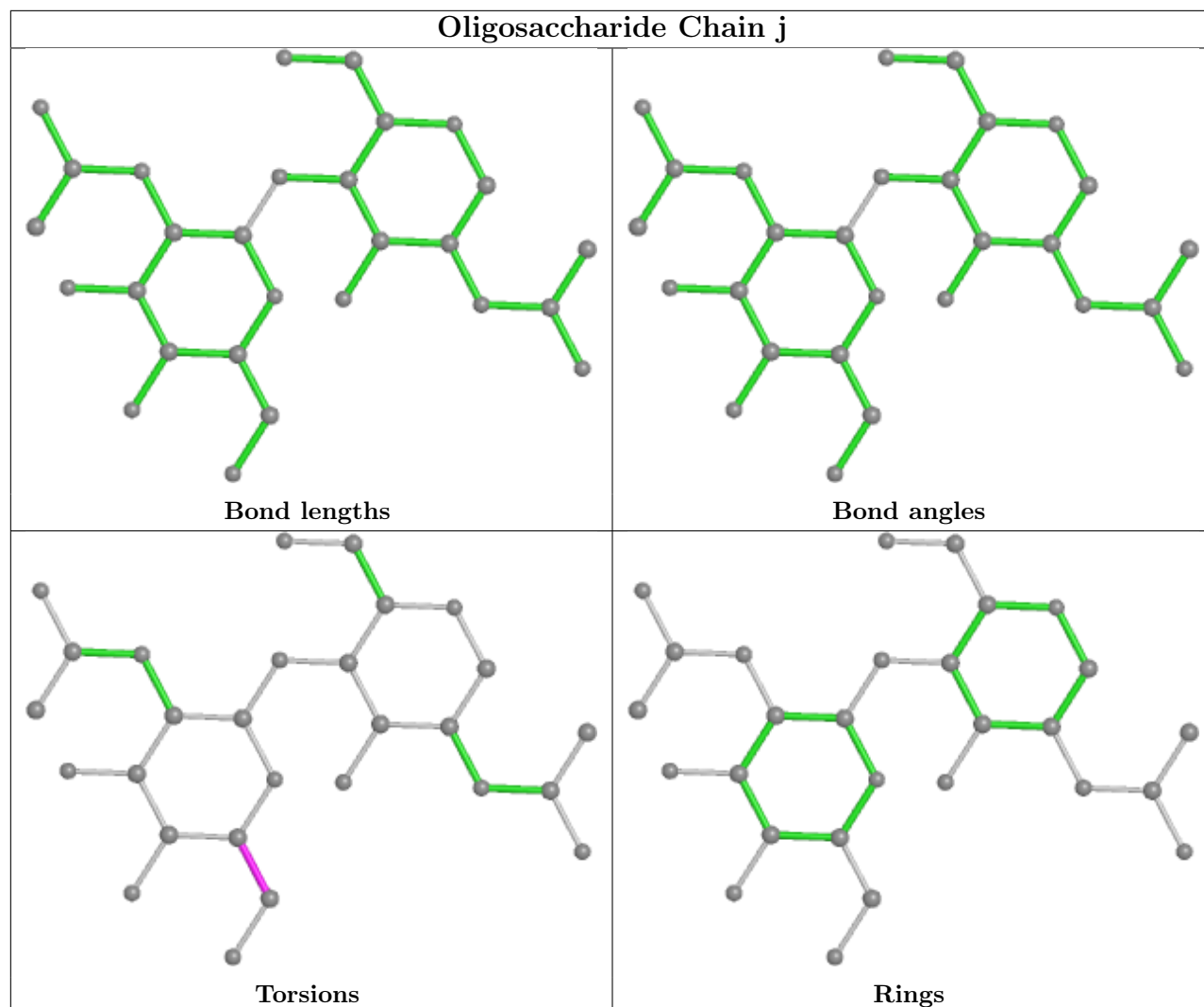


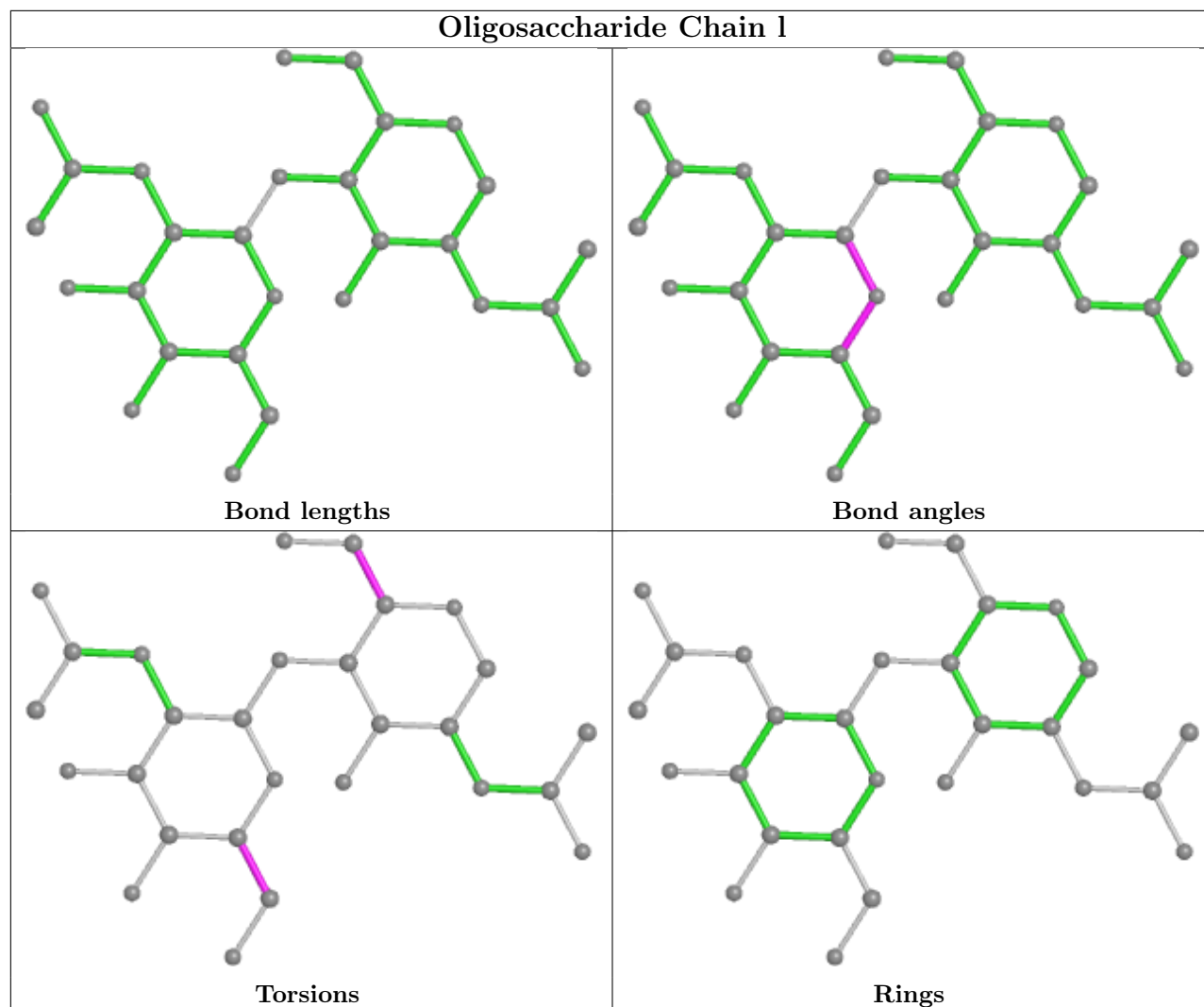


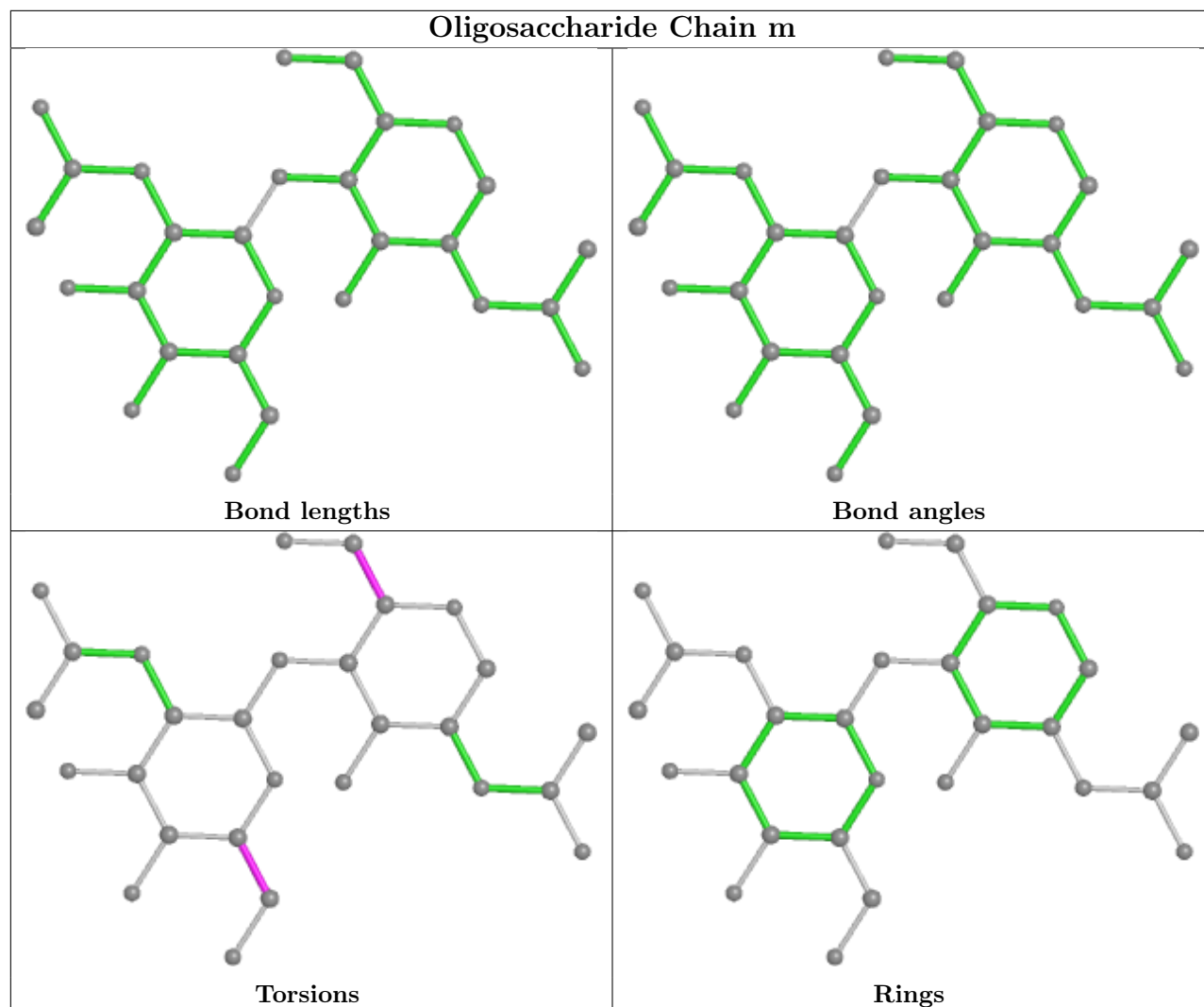


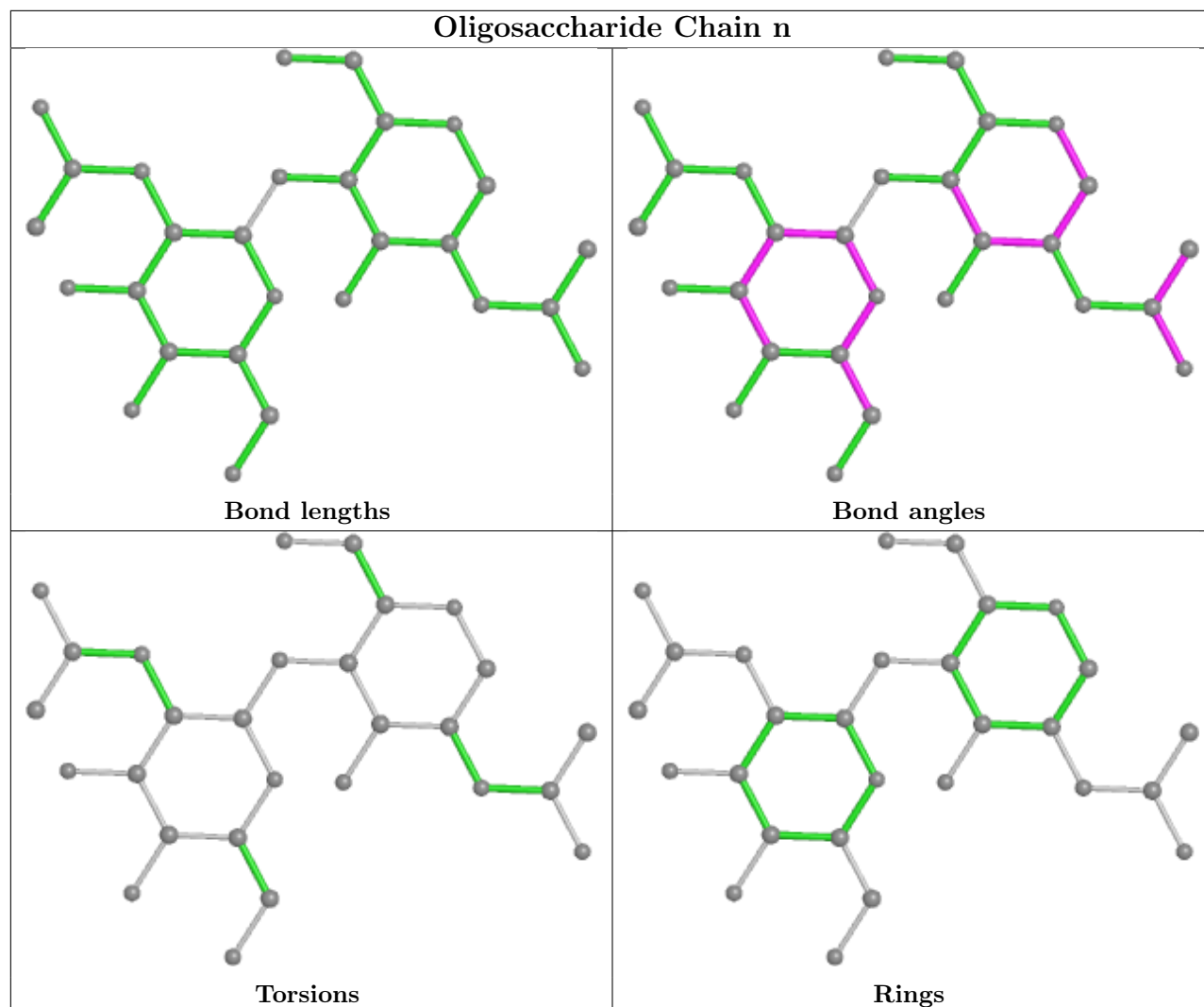




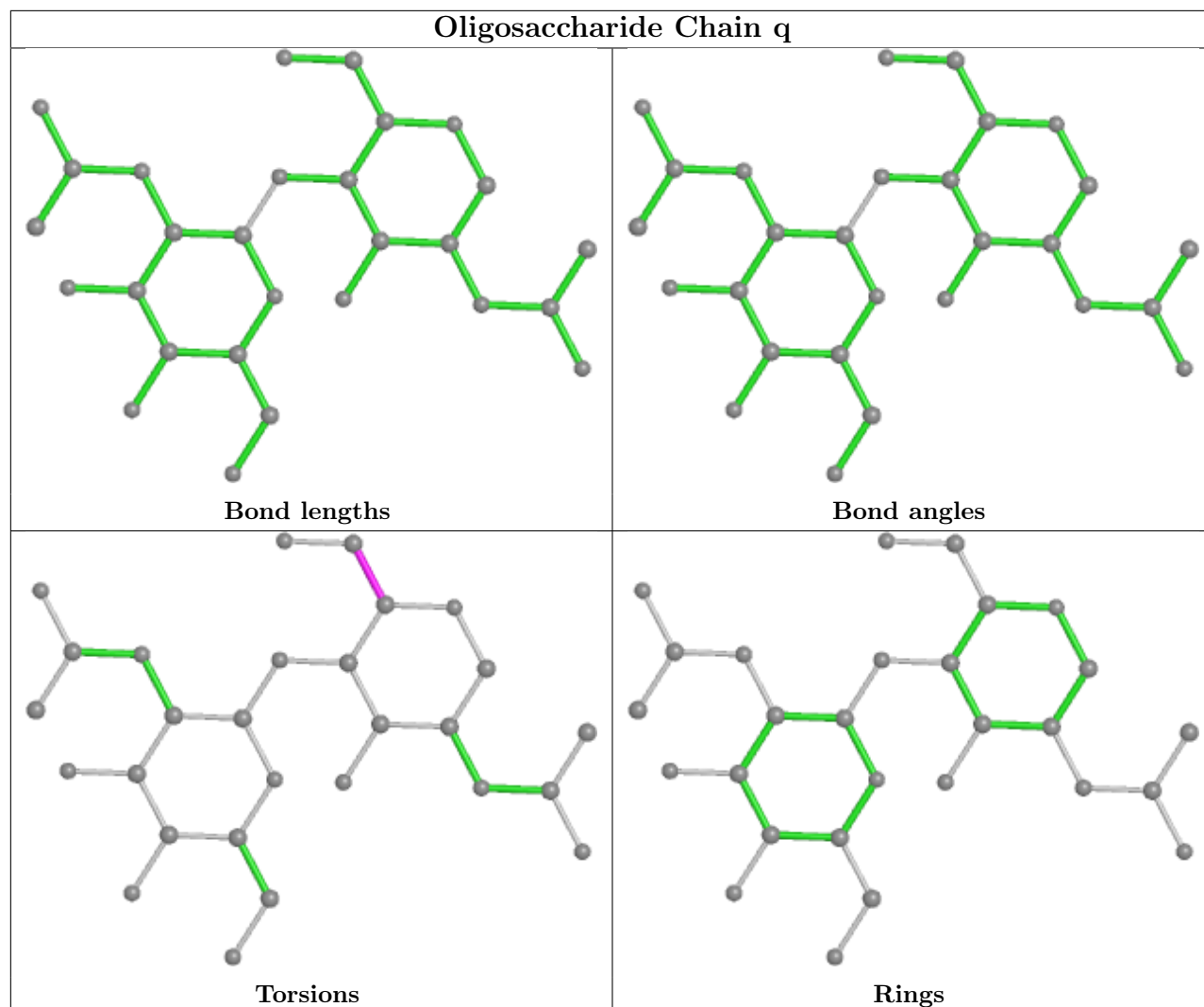


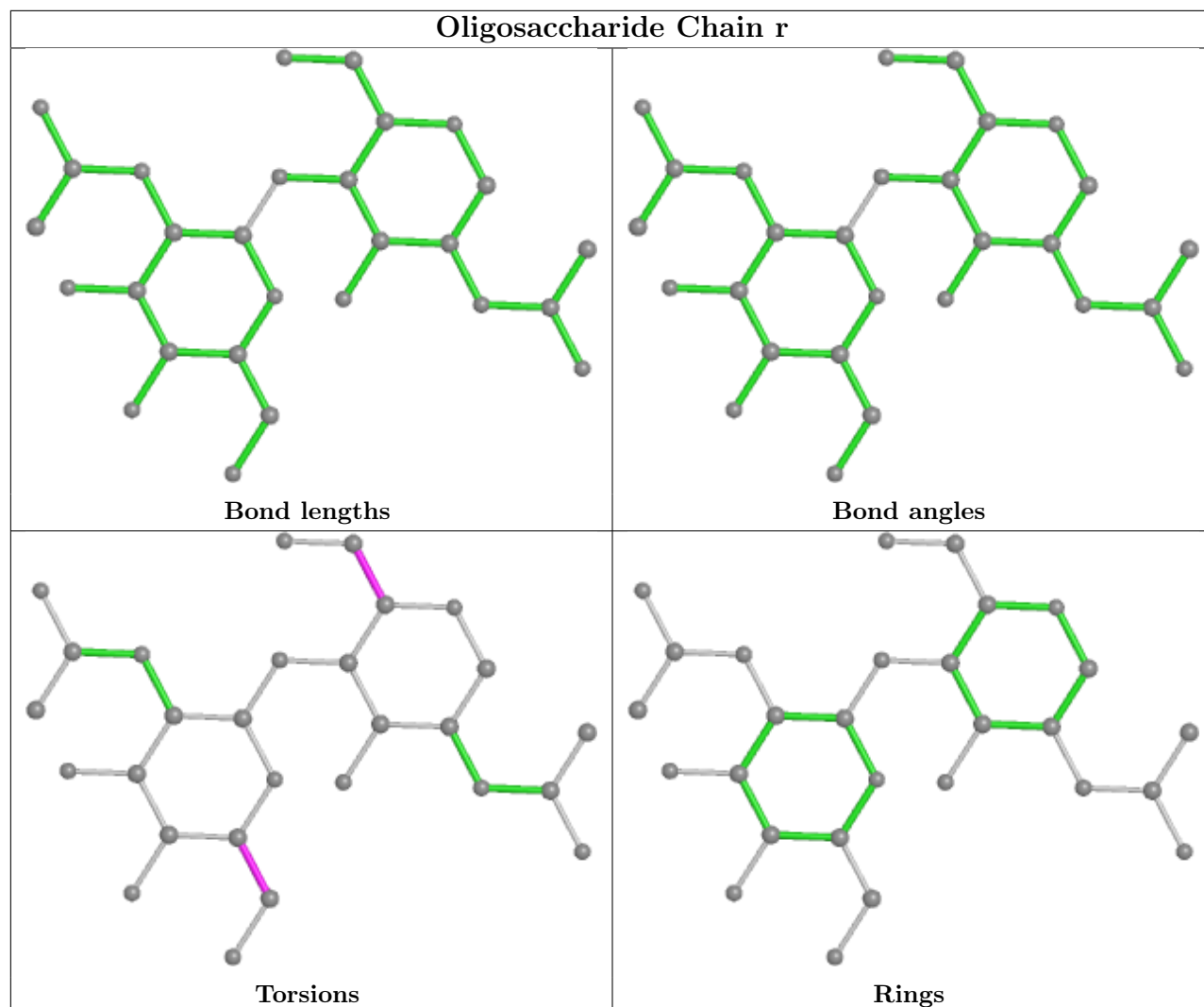


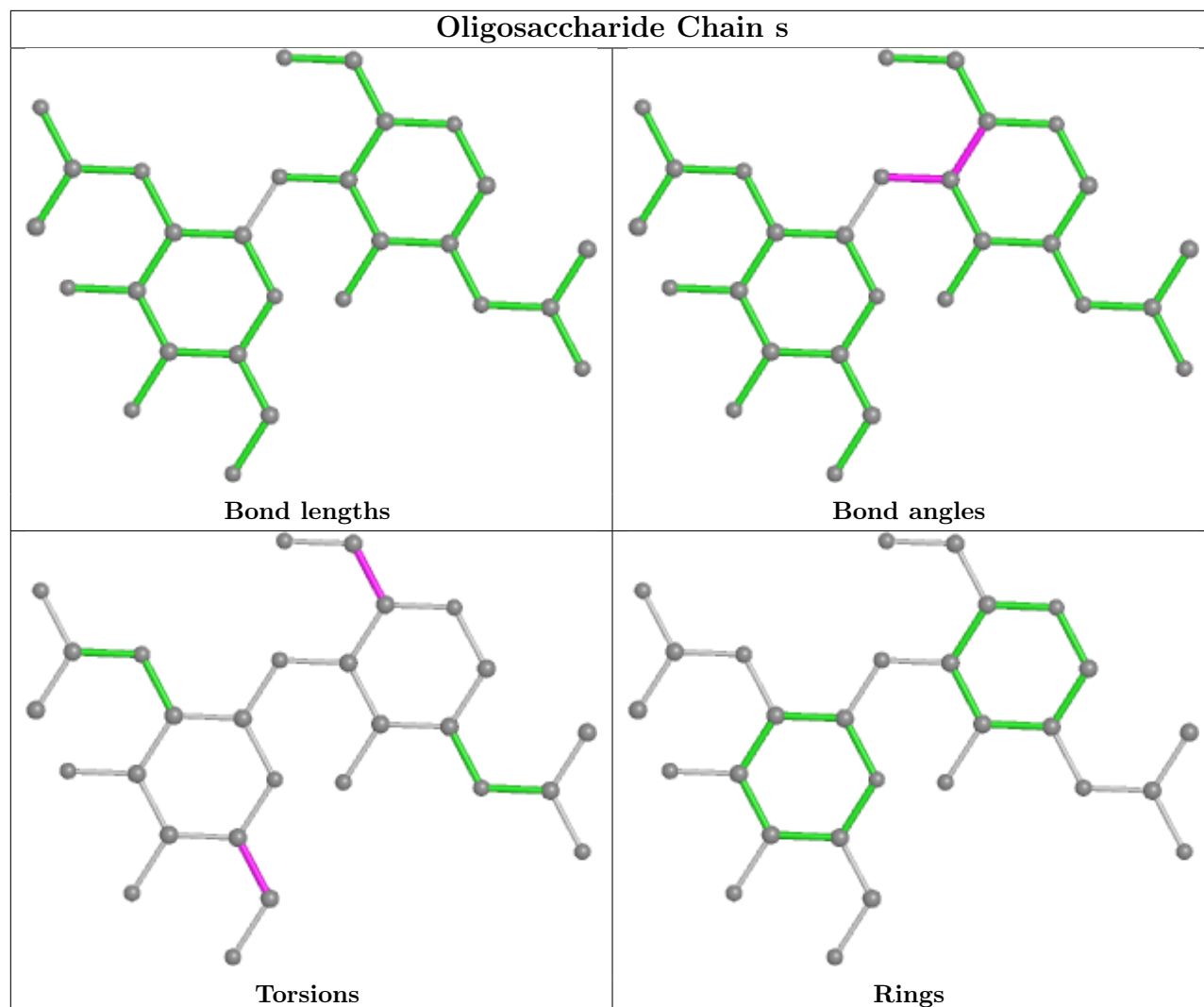


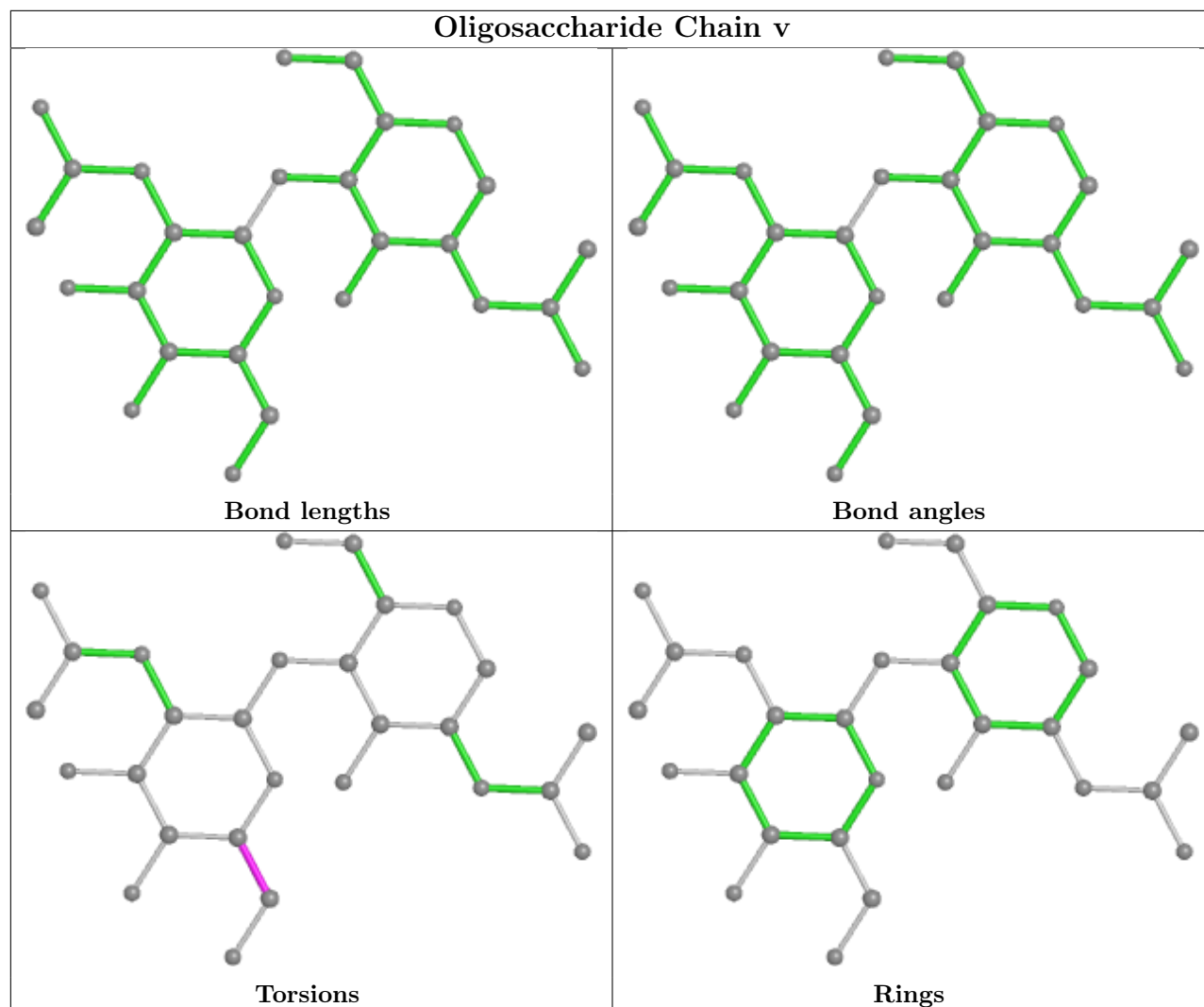


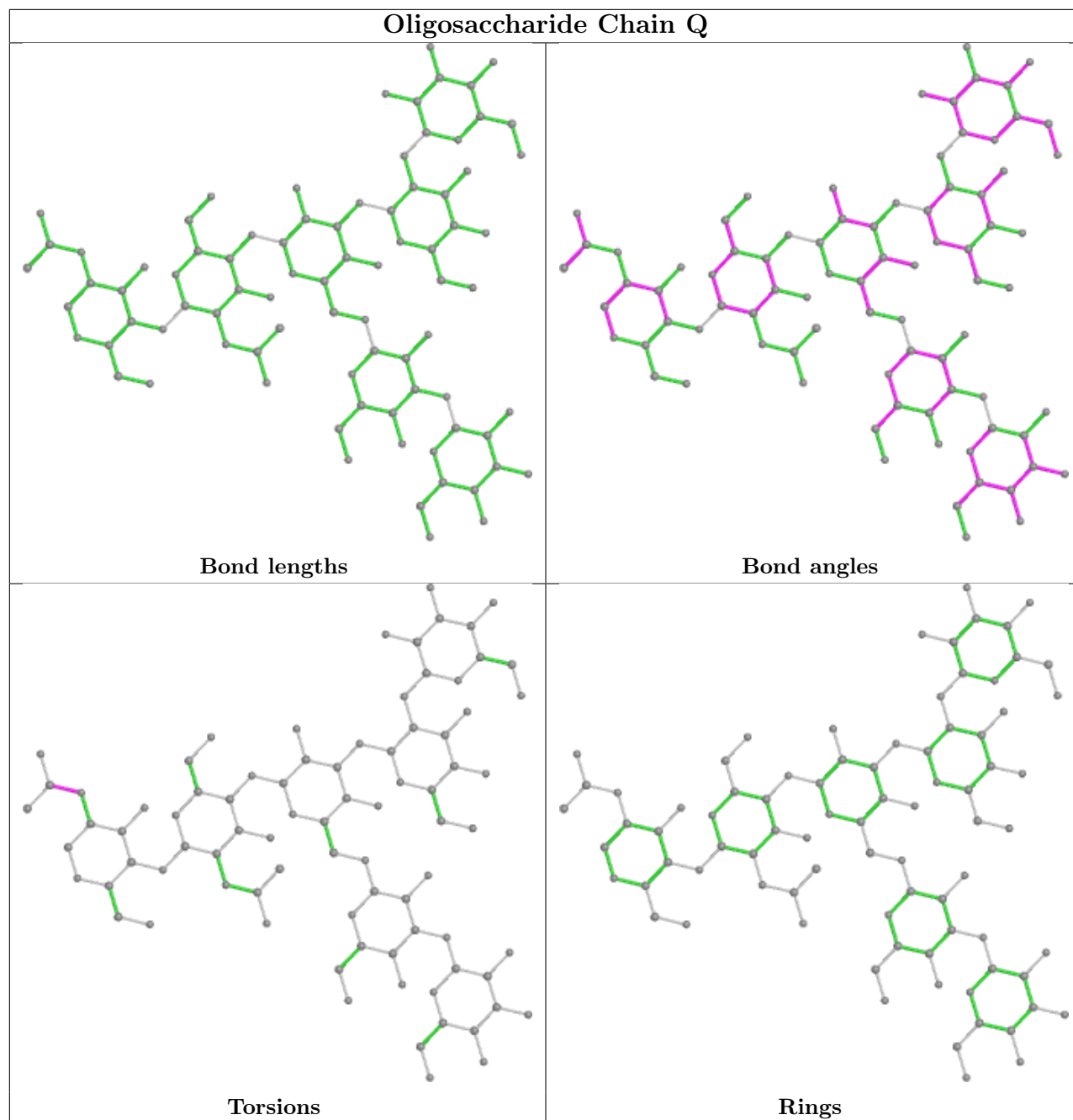


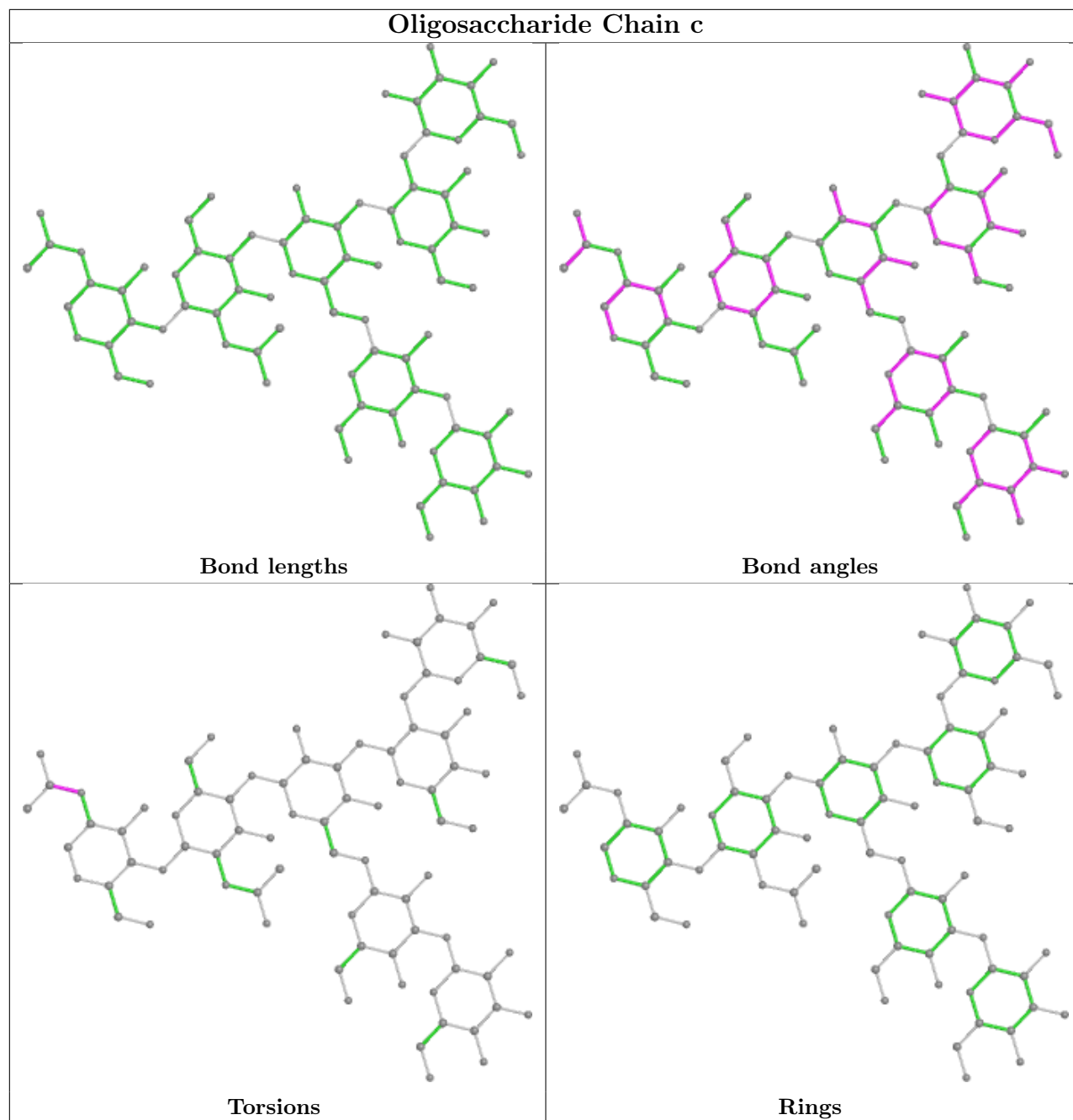


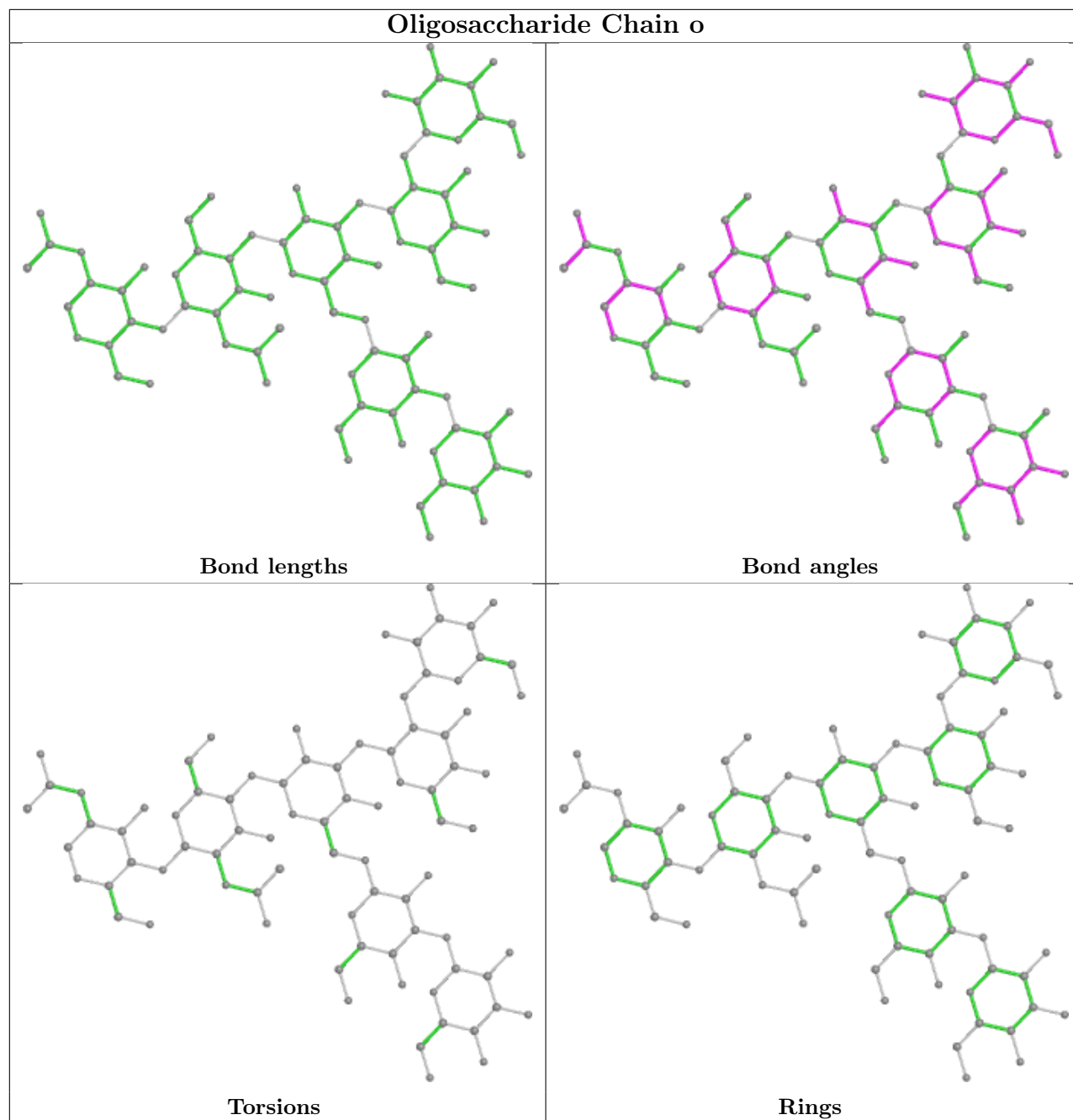


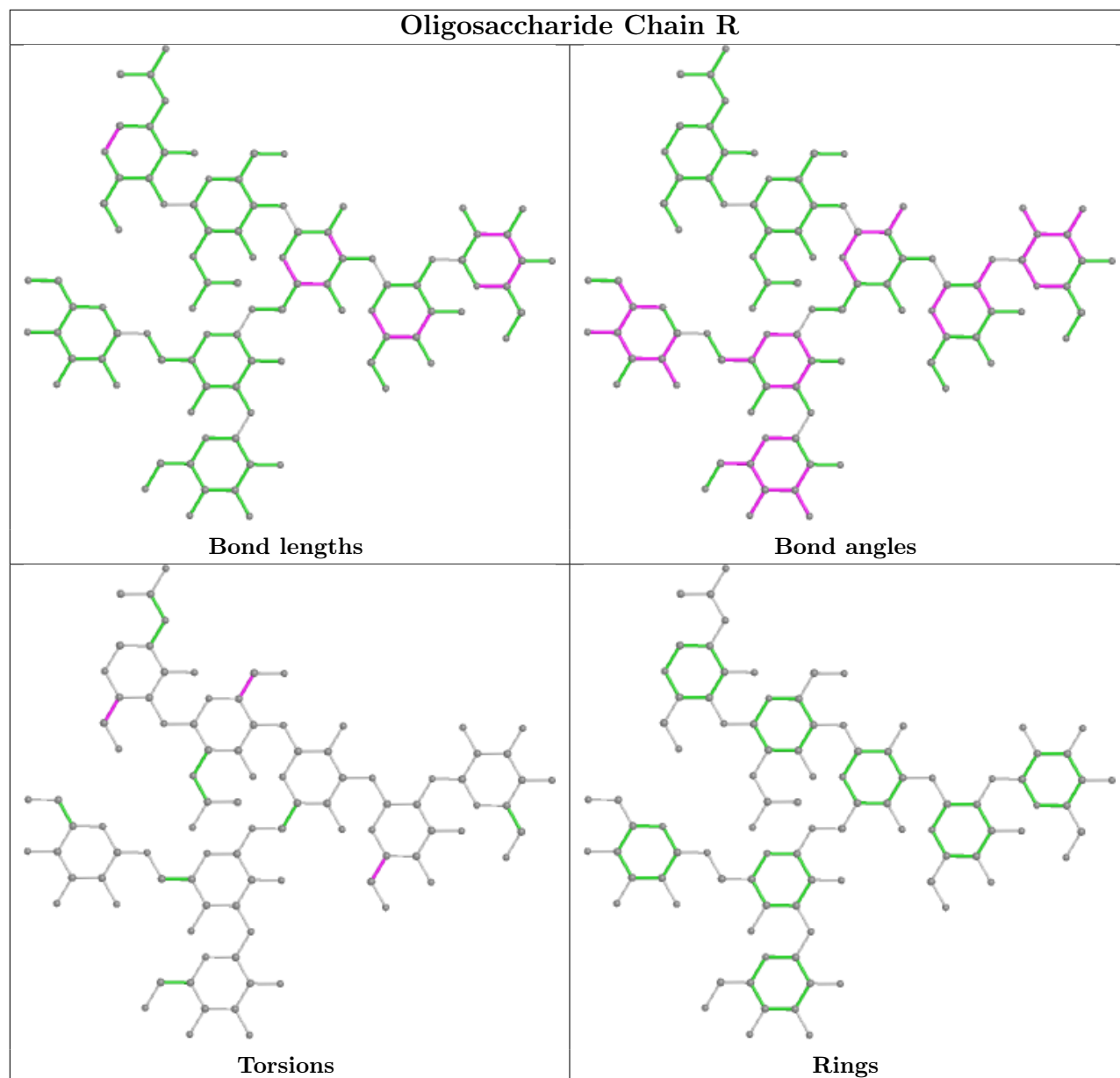




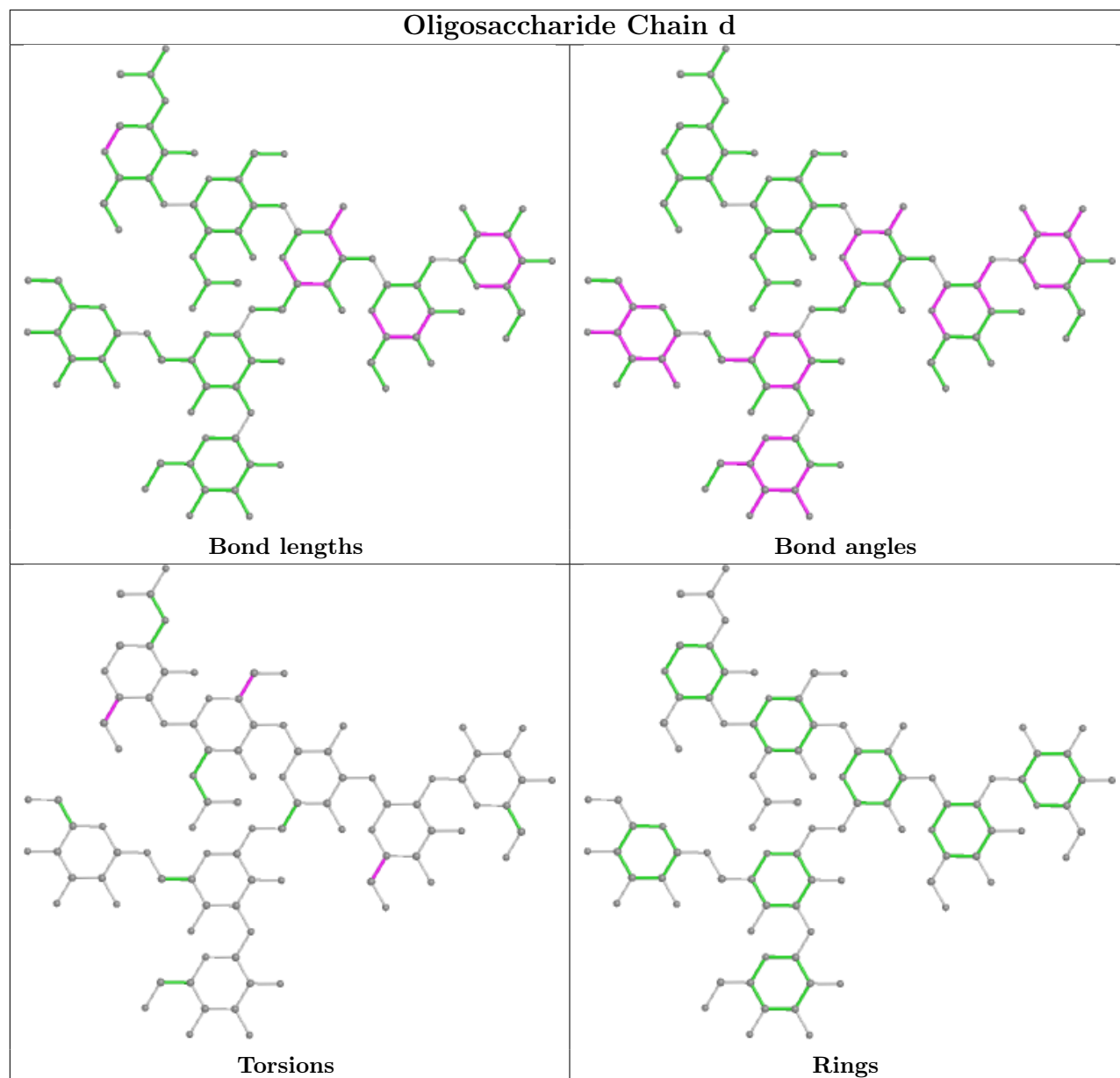


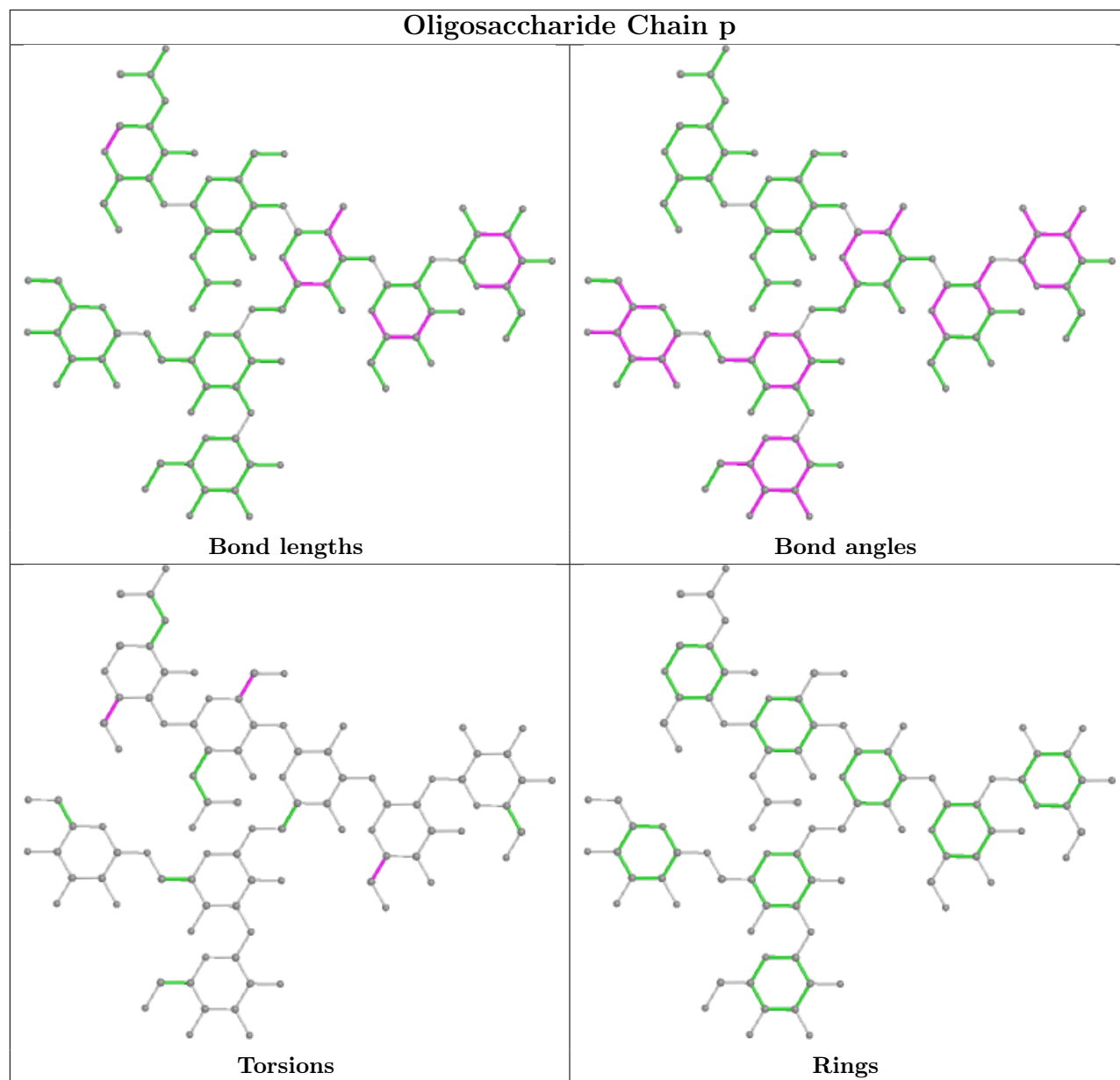


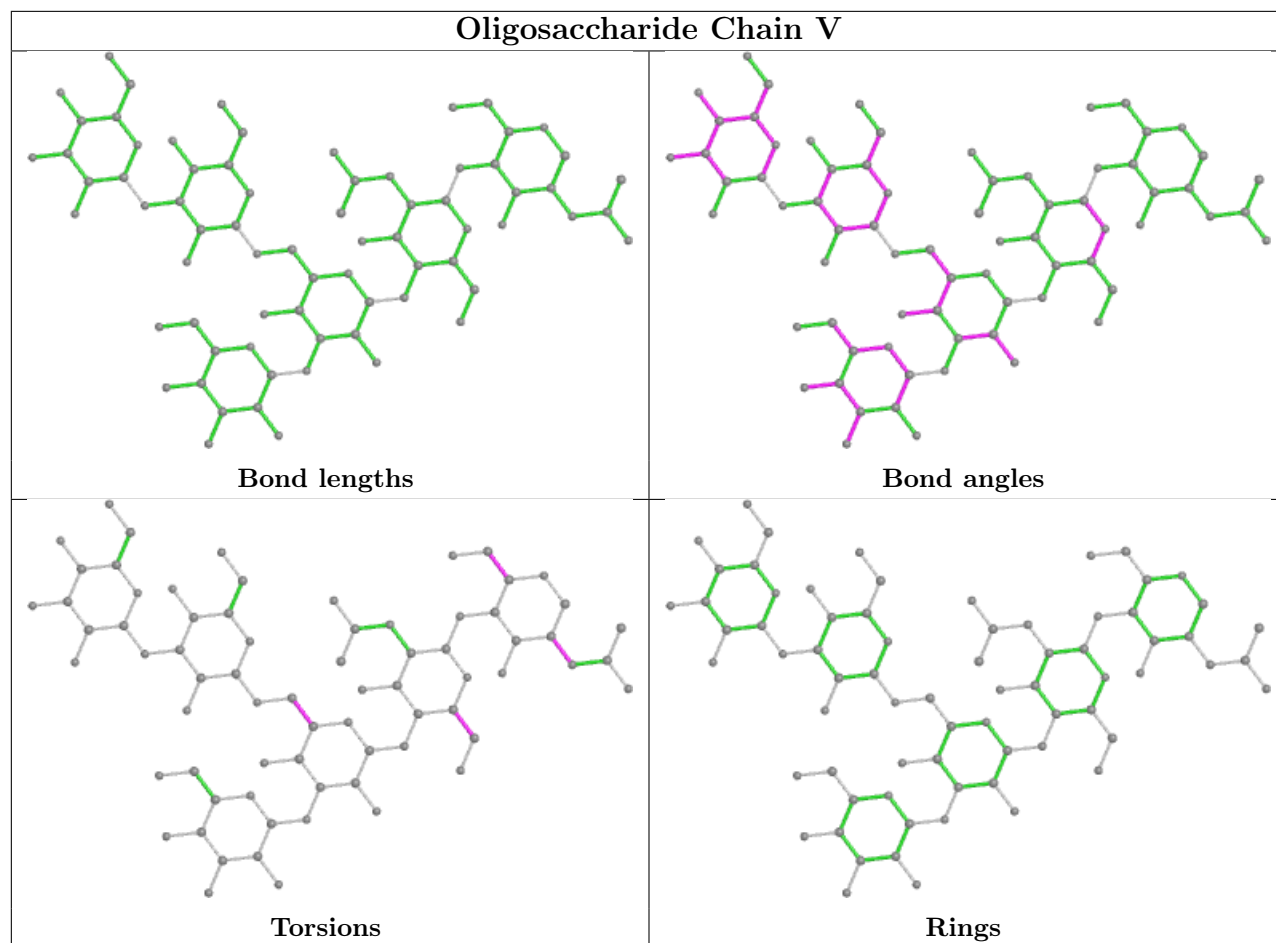


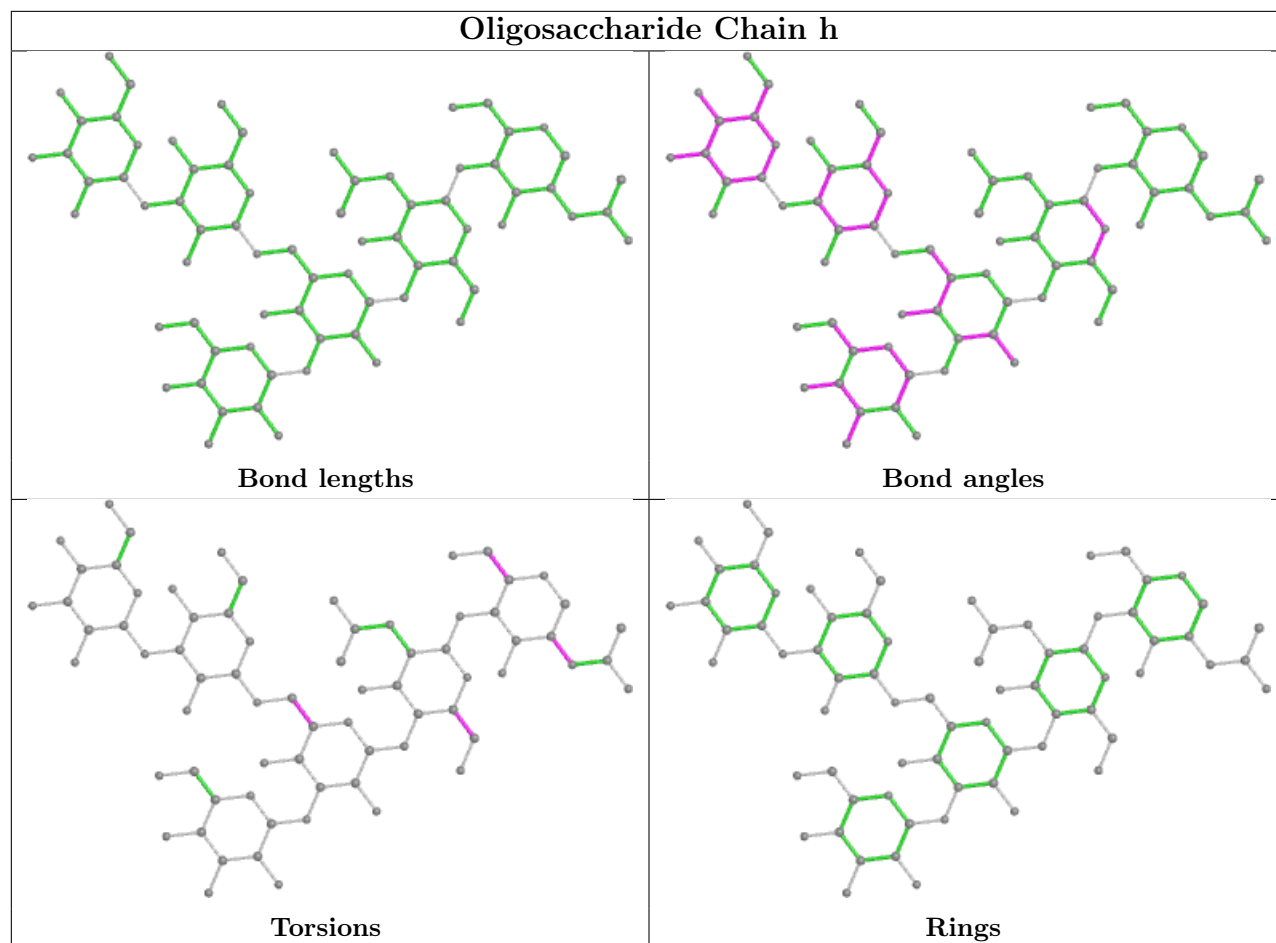


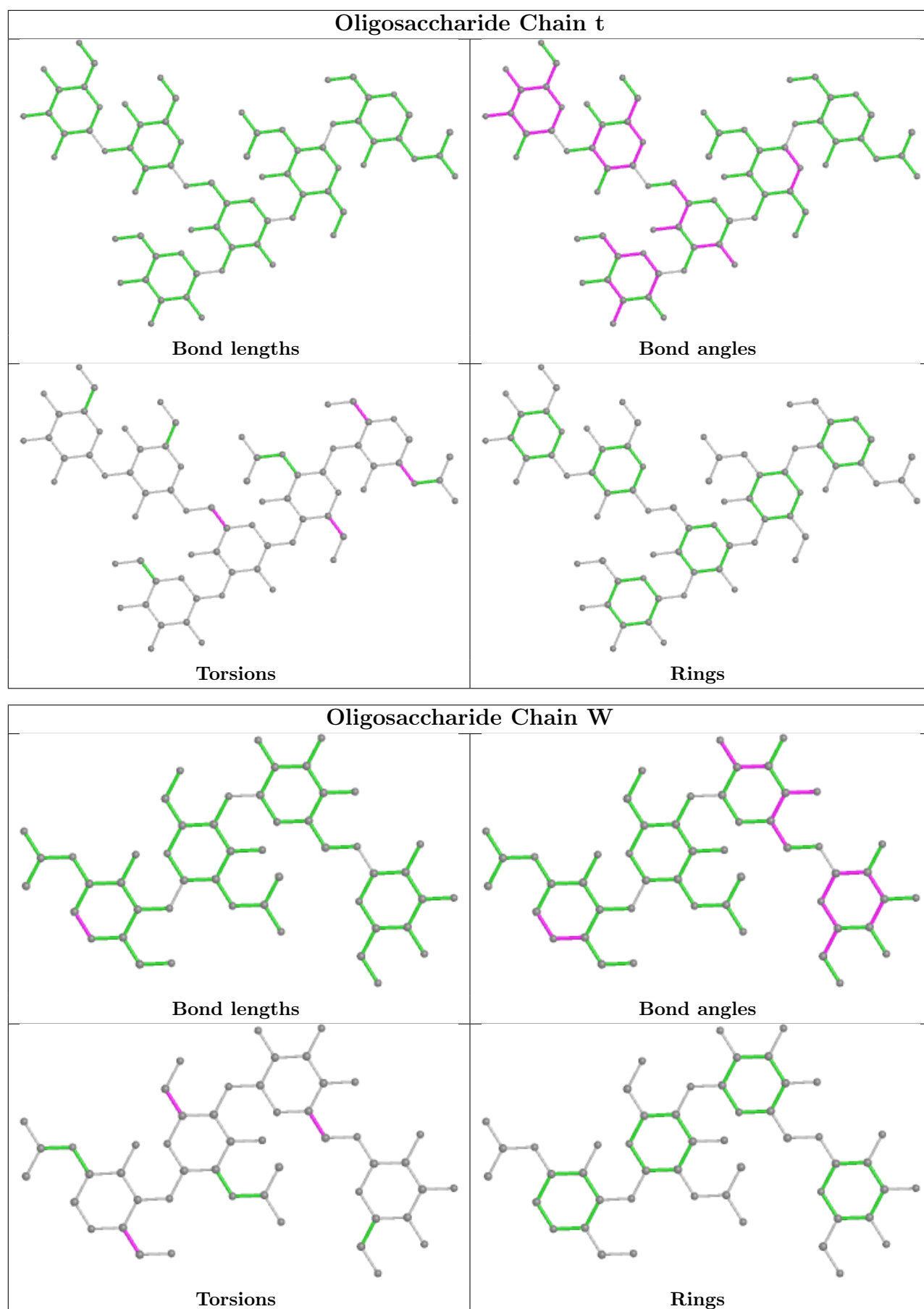


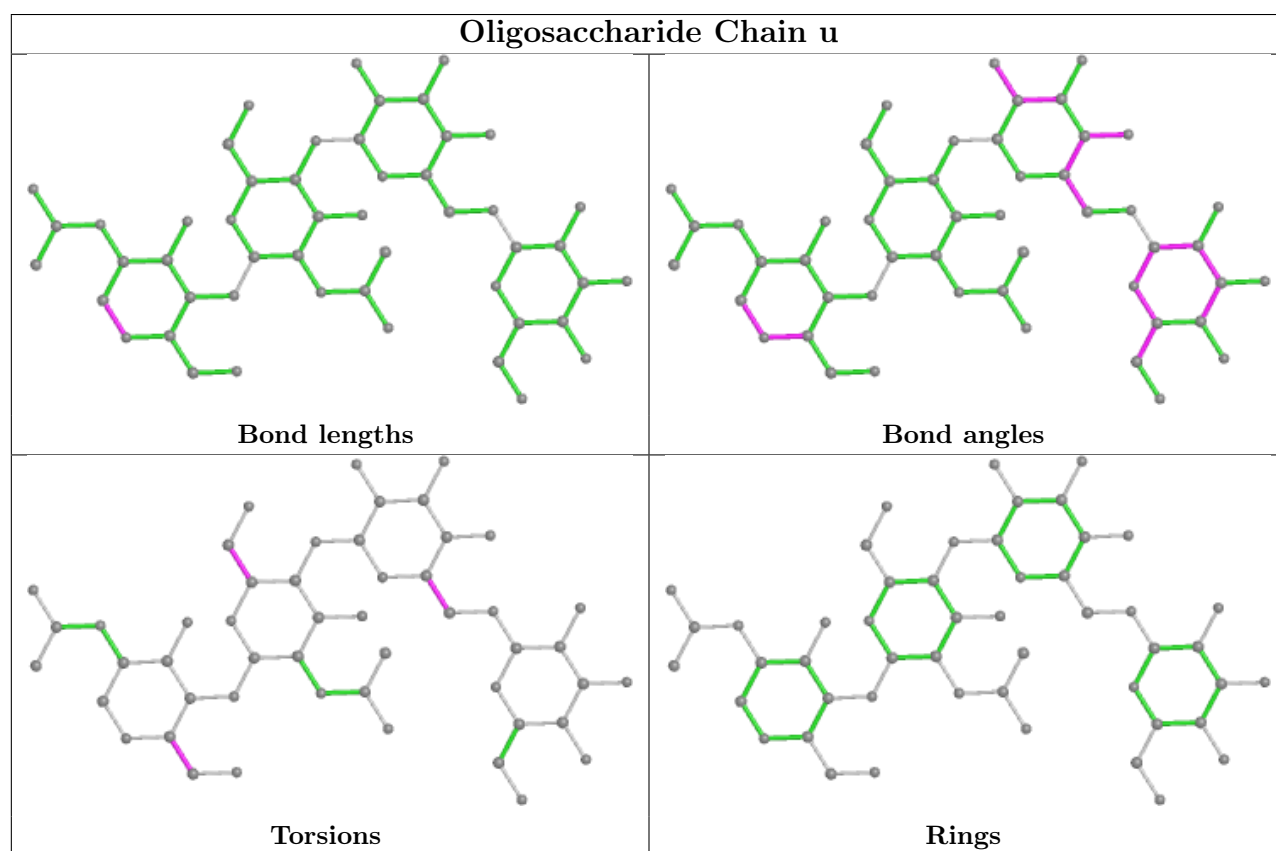
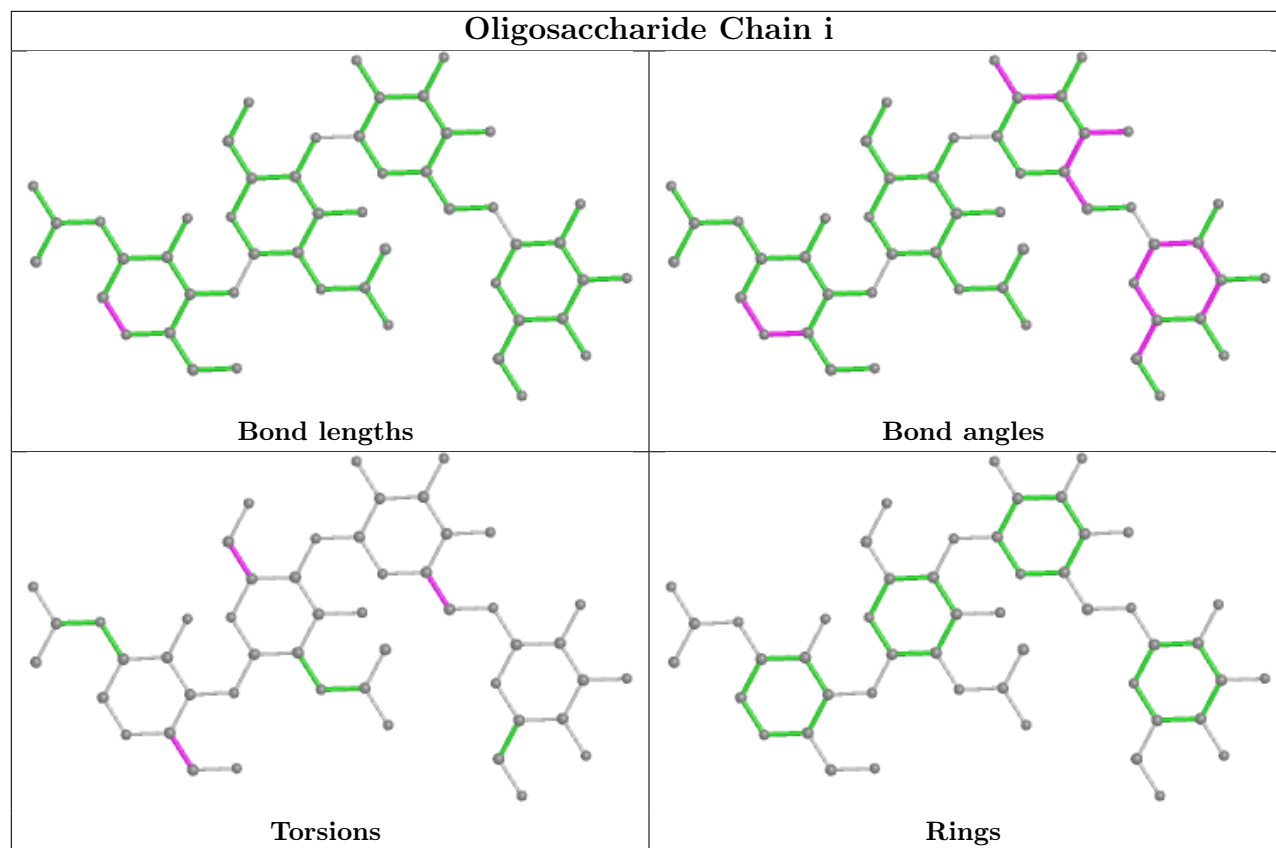












## 5.6 Ligand geometry

21 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
11	NAG	G	633	1	14,14,15	0.34	0	17,19,21	0.40	0
11	NAG	J	701	2	14,14,15	0.34	0	17,19,21	0.60	0
11	NAG	G	634	1	14,14,15	0.49	0	17,19,21	0.40	0
11	NAG	J	702	2	14,14,15	0.52	0	17,19,21	0.51	0
11	NAG	F	645	1	14,14,15	0.46	0	17,19,21	0.55	0
11	NAG	G	645	1	14,14,15	0.45	0	17,19,21	0.55	0
11	NAG	F	631	1	14,14,15	0.49	0	17,19,21	0.39	0
11	NAG	A	634	1	14,14,15	0.49	0	17,19,21	0.39	0
11	NAG	B	701	2	14,14,15	0.34	0	17,19,21	0.60	0
11	NAG	F	634	1	14,14,15	0.32	0	17,19,21	0.40	0
11	NAG	F	604	1	14,14,15	0.40	0	17,19,21	0.63	1 (5%)
11	NAG	G	611	1	14,14,15	0.52	0	17,19,21	0.50	0
11	NAG	G	604	1	14,14,15	0.42	0	17,19,21	0.63	1 (5%)
11	NAG	B	702	2	14,14,15	0.51	0	17,19,21	0.52	0
11	NAG	F	611	1	14,14,15	0.51	0	17,19,21	0.50	0
11	NAG	A	604	1	14,14,15	0.41	0	17,19,21	0.64	1 (5%)
11	NAG	A	611	1	14,14,15	0.51	0	17,19,21	0.50	0
11	NAG	I	701	2	14,14,15	0.34	0	17,19,21	0.60	0
11	NAG	A	645	1	14,14,15	0.47	0	17,19,21	0.54	0
11	NAG	A	633	1	14,14,15	0.32	0	17,19,21	0.39	0
11	NAG	I	702	2	14,14,15	0.51	0	17,19,21	0.52	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
11	NAG	G	633	1	-	2/6/23/26	0/1/1/1
11	NAG	J	701	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	G	634	1	-	2/6/23/26	0/1/1/1
11	NAG	J	702	2	-	2/6/23/26	0/1/1/1
11	NAG	F	645	1	-	0/6/23/26	0/1/1/1
11	NAG	G	645	1	-	0/6/23/26	0/1/1/1
11	NAG	F	631	1	-	2/6/23/26	0/1/1/1
11	NAG	A	634	1	-	2/6/23/26	0/1/1/1
11	NAG	B	701	2	-	3/6/23/26	0/1/1/1
11	NAG	F	634	1	-	2/6/23/26	0/1/1/1
11	NAG	F	604	1	-	2/6/23/26	0/1/1/1
11	NAG	G	611	1	-	2/6/23/26	0/1/1/1
11	NAG	G	604	1	-	2/6/23/26	0/1/1/1
11	NAG	B	702	2	-	2/6/23/26	0/1/1/1
11	NAG	F	611	1	-	2/6/23/26	0/1/1/1
11	NAG	A	604	1	-	2/6/23/26	0/1/1/1
11	NAG	A	611	1	-	2/6/23/26	0/1/1/1
11	NAG	I	701	2	-	3/6/23/26	0/1/1/1
11	NAG	A	645	1	-	0/6/23/26	0/1/1/1
11	NAG	A	633	1	-	2/6/23/26	0/1/1/1
11	NAG	I	702	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	604	NAG	C1-O5-C5	2.06	114.98	112.19
11	F	604	NAG	C1-O5-C5	2.04	114.95	112.19
11	G	604	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	634	NAG	O5-C5-C6-O6
11	F	631	NAG	O5-C5-C6-O6
11	G	634	NAG	O5-C5-C6-O6
11	A	633	NAG	O5-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	F	634	NAG	O5-C5-C6-O6
11	G	633	NAG	O5-C5-C6-O6
11	B	702	NAG	O5-C5-C6-O6
11	I	701	NAG	O5-C5-C6-O6
11	I	702	NAG	O5-C5-C6-O6
11	J	701	NAG	O5-C5-C6-O6
11	J	702	NAG	O5-C5-C6-O6
11	A	634	NAG	C4-C5-C6-O6
11	F	631	NAG	C4-C5-C6-O6
11	G	634	NAG	C4-C5-C6-O6
11	B	701	NAG	C4-C5-C6-O6
11	I	701	NAG	C4-C5-C6-O6
11	J	701	NAG	C4-C5-C6-O6
11	A	604	NAG	O5-C5-C6-O6
11	F	604	NAG	O5-C5-C6-O6
11	G	604	NAG	O5-C5-C6-O6
11	A	633	NAG	C4-C5-C6-O6
11	F	634	NAG	C4-C5-C6-O6
11	G	633	NAG	C4-C5-C6-O6
11	A	611	NAG	O5-C5-C6-O6
11	F	611	NAG	O5-C5-C6-O6
11	G	611	NAG	O5-C5-C6-O6
11	B	702	NAG	C4-C5-C6-O6
11	I	702	NAG	C4-C5-C6-O6
11	J	702	NAG	C4-C5-C6-O6
11	A	604	NAG	C4-C5-C6-O6
11	F	604	NAG	C4-C5-C6-O6
11	G	604	NAG	C4-C5-C6-O6
11	G	611	NAG	C4-C5-C6-O6
11	A	611	NAG	C4-C5-C6-O6
11	F	611	NAG	C4-C5-C6-O6
11	B	701	NAG	C3-C2-N2-C7
11	I	701	NAG	C3-C2-N2-C7
11	J	701	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

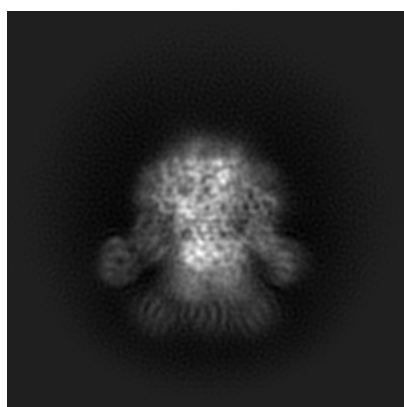
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7896. These allow visual inspection of the internal detail of the map and identification of artifacts.

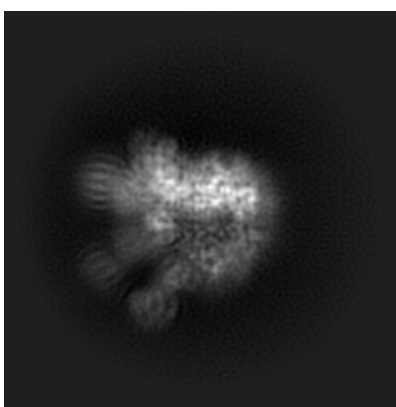
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

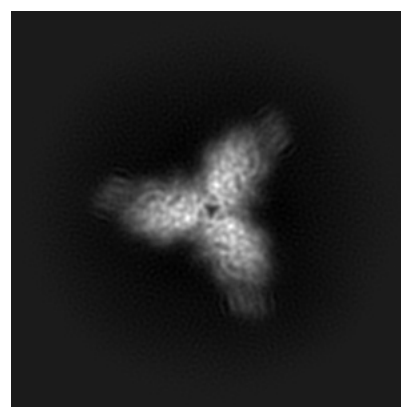
#### 6.1.1 Primary map



X



Y

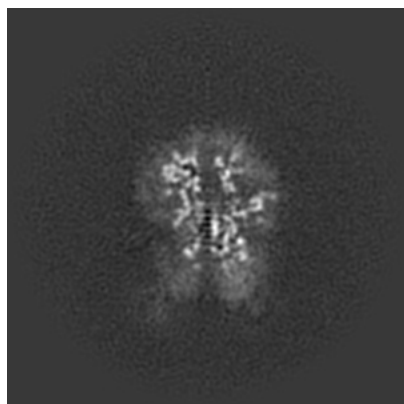


Z

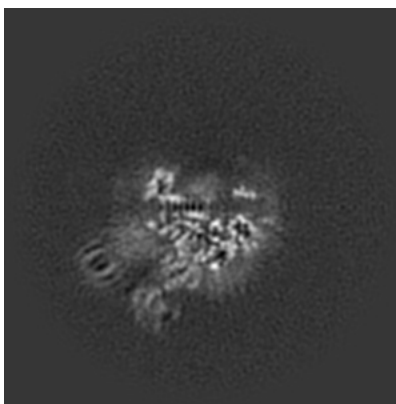
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

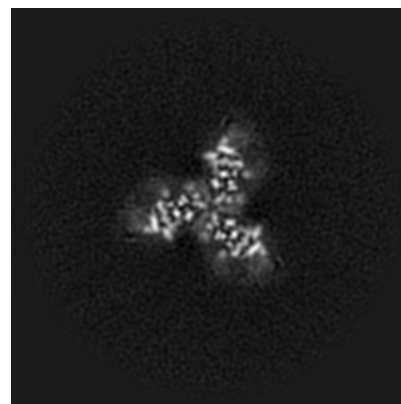
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

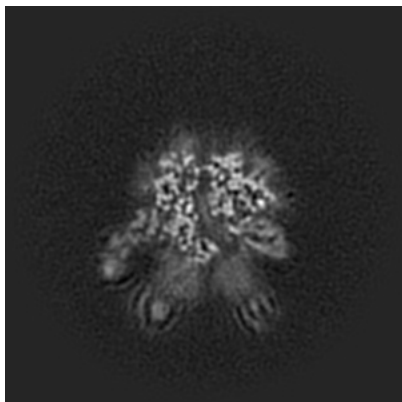


Z Index: 150

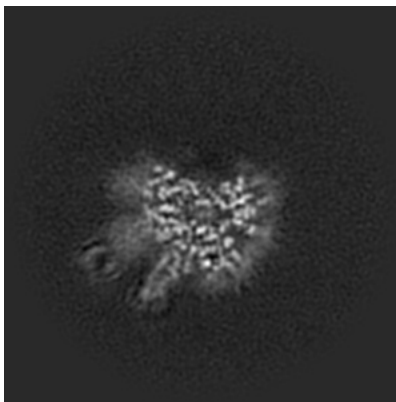
The images above show central slices of the map in three orthogonal directions.

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

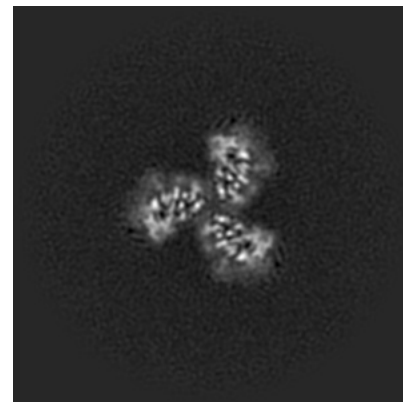
### 6.3.1 Primary map



X Index: 165



Y Index: 142

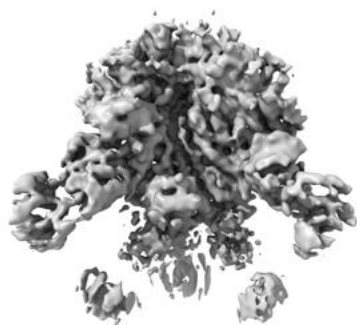


Z Index: 158

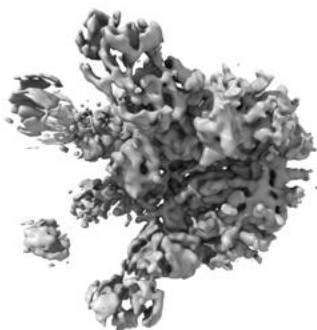
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

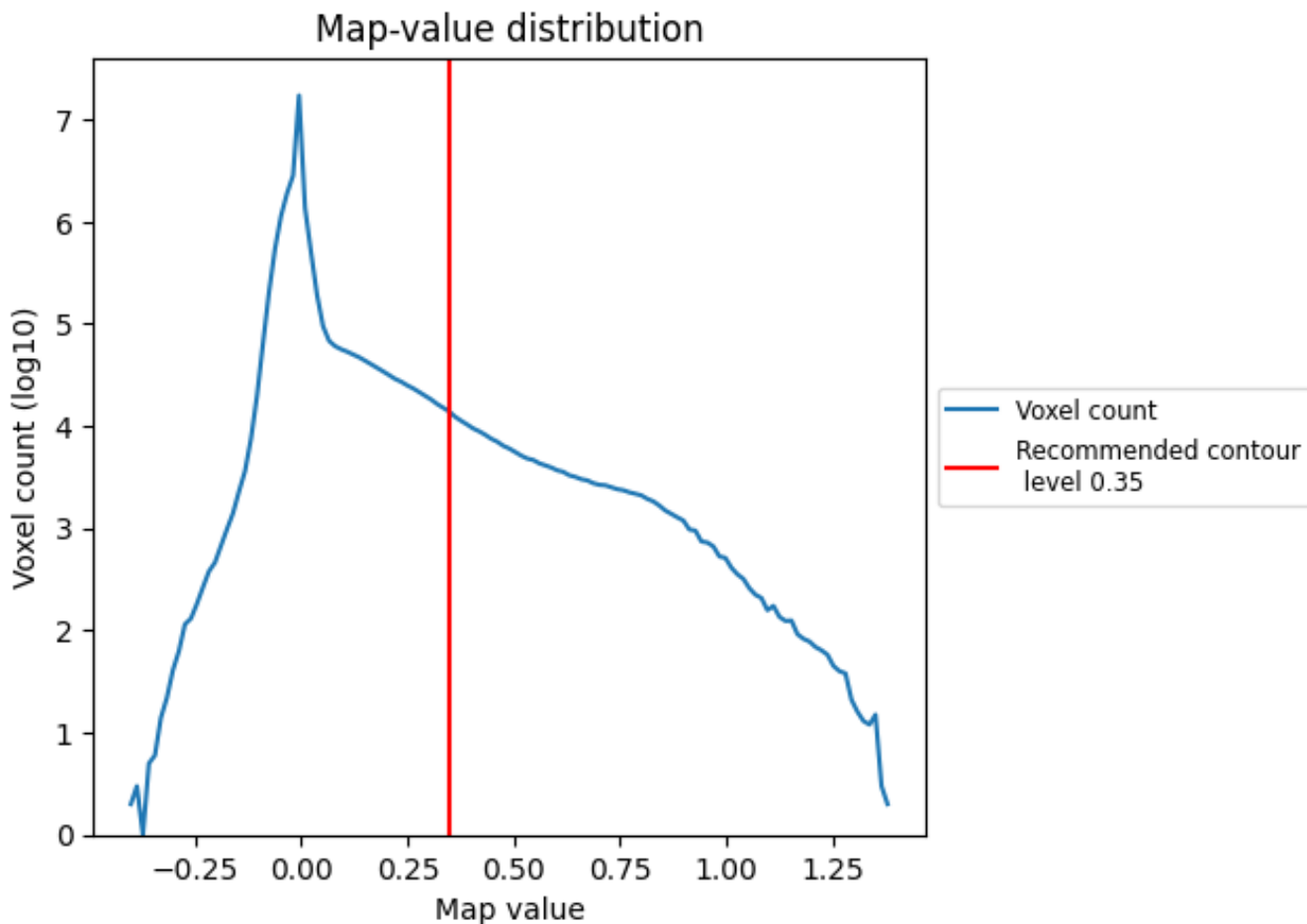
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

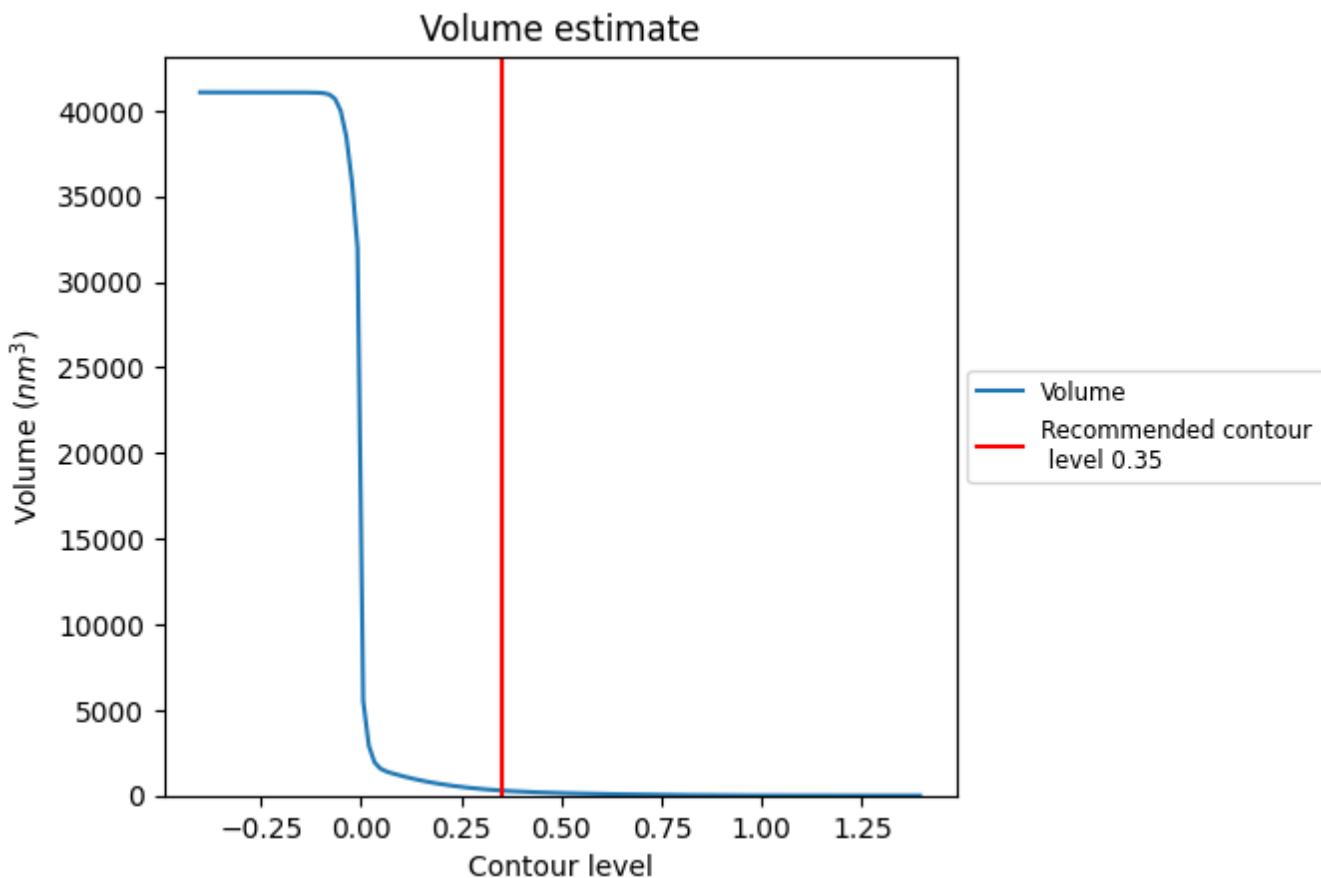
This section contains the results of statistical analysis of the map.

### 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.

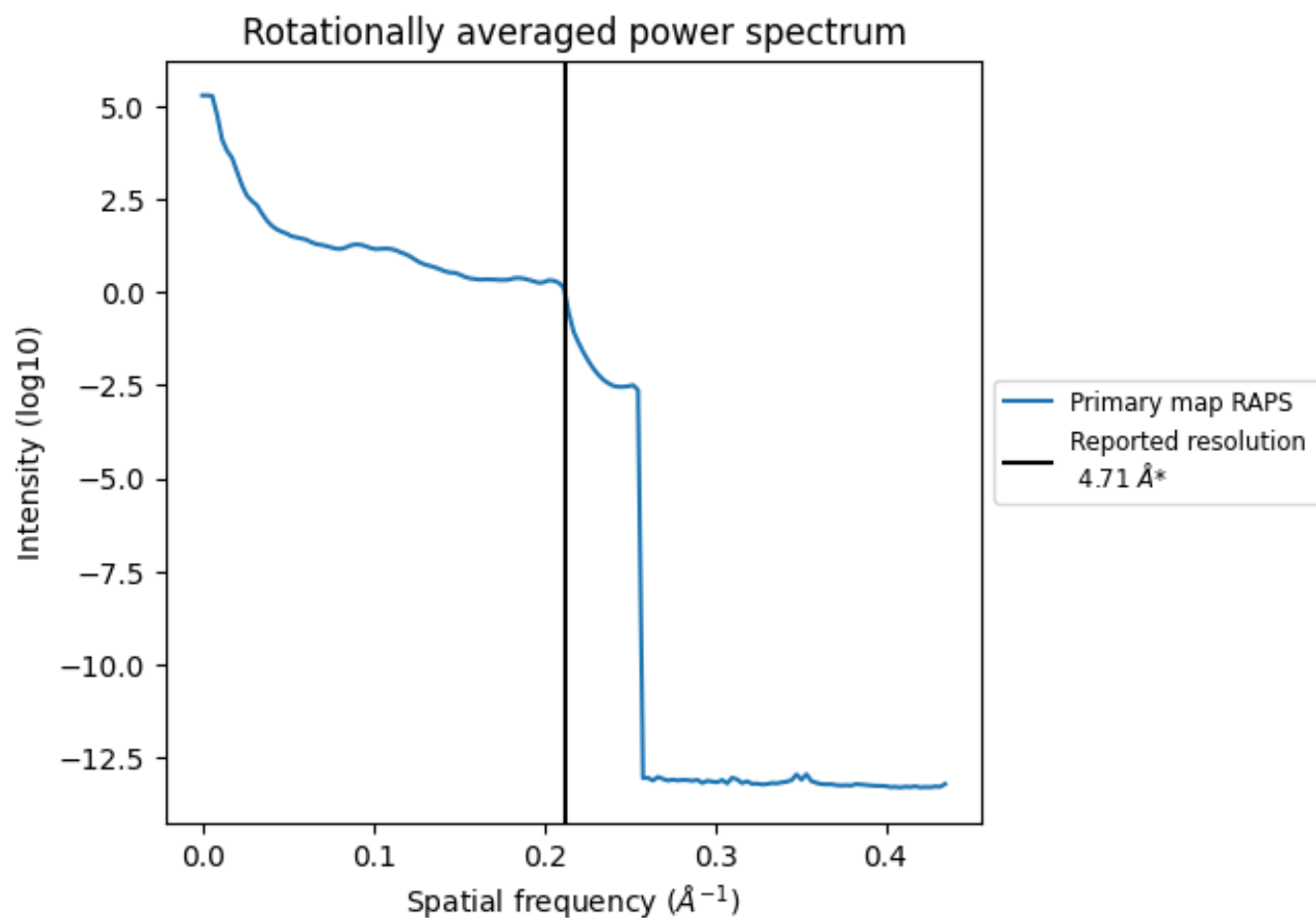
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 293 nm<sup>3</sup>; this corresponds to an approximate mass of 265 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  $0.212 \text{\AA}^{-1}$



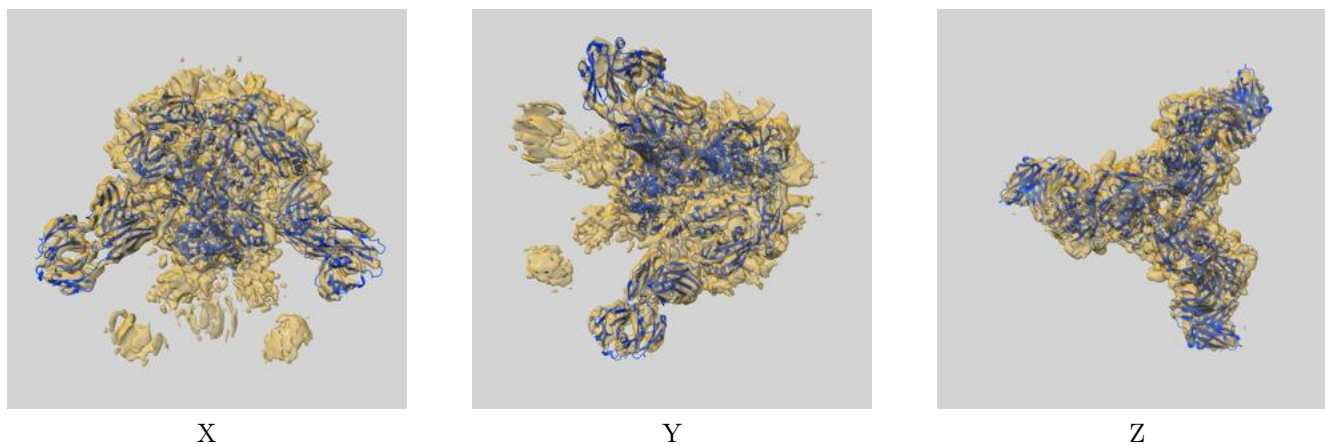
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

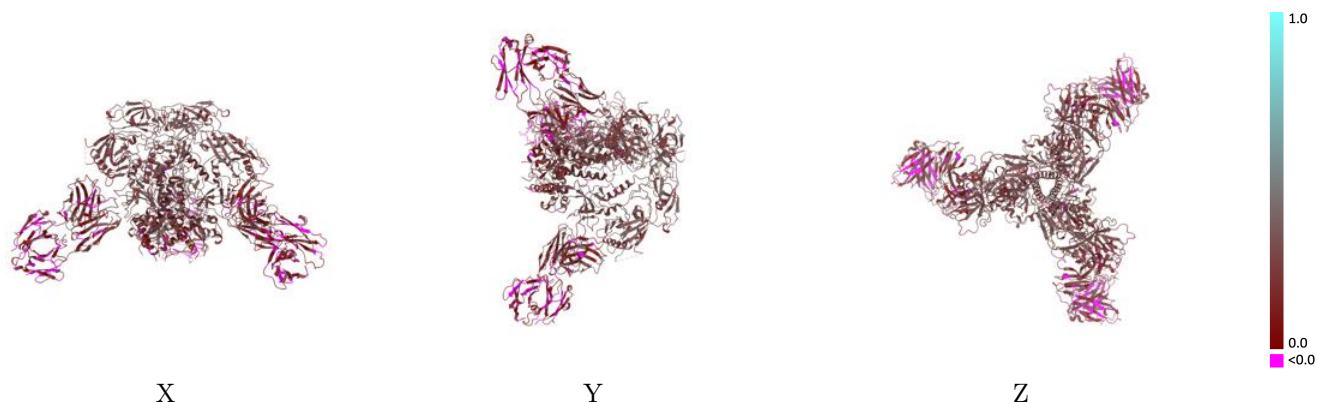
This section contains information regarding the fit between EMDB map EMD-7896 and PDB model 6DID. Per-residue inclusion information can be found in section 3 on page 12.

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



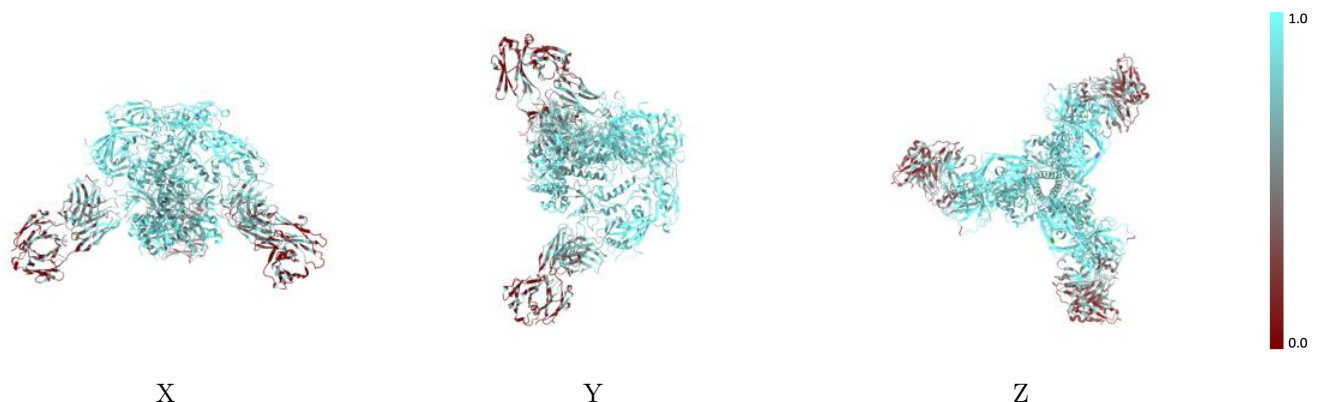
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



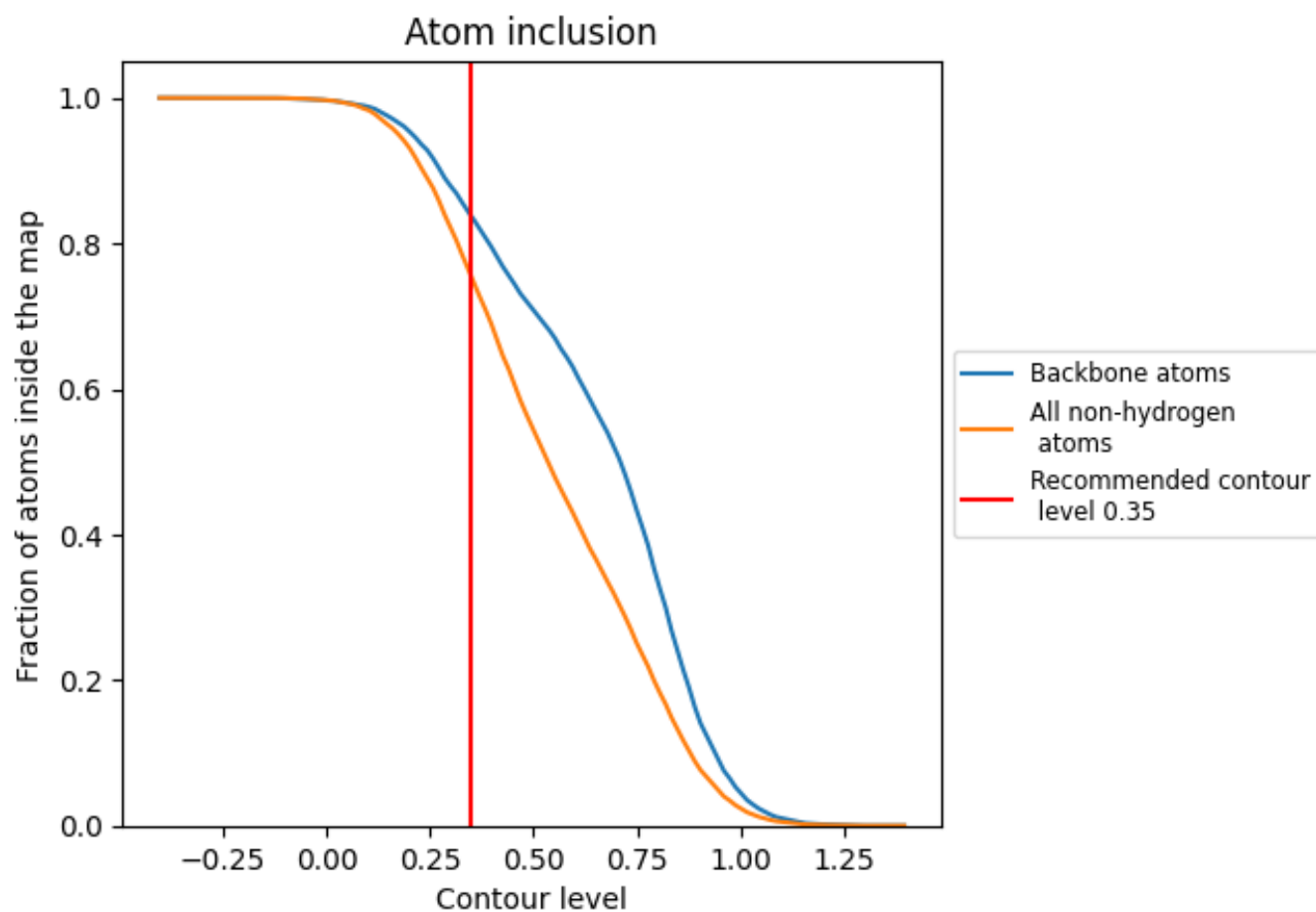
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7546	 0.2300
A	 0.8752	 0.3010
B	 0.8217	 0.2410
C	 0.4729	 0.1480
D	 0.4810	 0.1490
E	 0.4748	 0.1490
F	 0.8772	 0.3000
G	 0.8755	 0.3020
H	 0.4698	 0.1480
I	 0.8207	 0.2400
J	 0.8236	 0.2410
K	 0.4803	 0.1490
L	 0.4803	 0.1500
M	 0.3590	 0.1250
N	 0.8571	 0.3220
O	 0.7500	 0.3410
P	 0.8214	 0.3590
Q	 0.7590	 0.3320
R	 0.0000	 0.0070
S	 0.7857	 0.3000
T	 0.6071	 0.2720
U	 0.7857	 0.2600
V	 0.6806	 0.1890
W	 0.6600	 0.2010
X	 0.6786	 0.3210
Y	 0.3846	 0.1360
Z	 0.8571	 0.3200
a	 0.7857	 0.3220
b	 0.8214	 0.3660
c	 0.7590	 0.3340
d	 0.0000	 -0.0090
e	 0.7857	 0.2920
f	 0.6071	 0.2790
g	 0.7857	 0.2710
h	 0.6806	 0.1820



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Chain	Atom inclusion	Q-score
i	 0.6400	 0.1810
j	 0.7143	 0.2930
k	 0.3846	 0.1260
l	 0.8571	 0.3310
m	 0.7500	 0.3250
n	 0.8214	 0.3740
o	 0.7590	 0.3370
p	 0.0000	 -0.0000
q	 0.7857	 0.3090
r	 0.6071	 0.2750
s	 0.7857	 0.2840
t	 0.6806	 0.1810
u	 0.6400	 0.1880
v	 0.6786	 0.3220