



wwPDB EM Validation Summary Report ⓘ

Oct 26, 2024 – 06:24 PM EDT

PDB ID : 6OZC
EMDB ID : EMD-20224
Title : BG505 SOSIP.664 with 2G12 Fab2
Authors : Cottrell, C.A.; Ward, A.B.
Deposited on : 2019-05-15
Resolution : 3.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

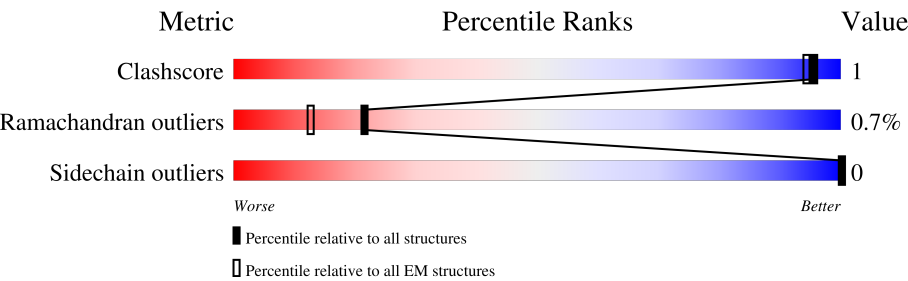
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.79 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 ≥ 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	<div><div>87%</div><div>8%</div></div>
1	E	475	<div><div>87%</div><div>5%</div><div>8%</div></div>
1	F	475	<div><div>86%</div><div>5%</div><div>8%</div></div>
2	B	153	<div><div>70%</div><div>8%</div><div>22%</div></div>
2	G	153	<div><div>70%</div><div>8%</div><div>22%</div></div>
2	I	153	<div><div>70%</div><div>8%</div><div>22%</div></div>
3	D	213	<div><div>8%</div><div>46%</div><div>51%</div></div>
3	L	213	<div><div>5%</div><div>47%</div><div>51%</div></div>

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Mol	Chain	Length	Quality of chain
3	M	213	
3	N	213	
3	Q	213	
3	R	213	
4	C	224	
4	H	224	
4	J	224	
4	K	224	
4	O	224	
4	P	224	
5	S	6	
5	c	6	
5	m	6	
6	T	5	
6	V	5	
6	d	5	
6	f	5	
6	n	5	
6	p	5	
7	U	9	
7	e	9	
7	o	9	
8	W	8	
8	g	8	
8	q	8	

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Mol	Chain	Length	Quality of chain
9	X	7	 100%
9	h	7	 100%
9	r	7	 100%
10	Y	9	 100%
10	i	9	 100%
10	s	9	 100%
11	Z	2	 100%
11	a	2	 100%
11	b	2	 100%
11	j	2	 100%
11	k	2	 100%
11	l	2	 100%
11	t	2	 100%
11	u	2	 100%
11	v	2	 100%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 25821 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 gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	435	Total	C	N	O	S	0	0
			3416	2148	600	640	28		
1	E	435	Total	C	N	O	S	0	0
			3416	2148	600	640	28		
1	F	435	Total	C	N	O	S	0	0
			3416	2148	600	640	28		

There are 6 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
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			956	601	167	182	6		
2	G	120	Total	C	N	O	S	0	0
			956	601	167	182	6		
2	I	120	Total	C	N	O	S	0	0
			956	601	167	182	6		

There are 6 discrepancies between the modelled and reference sequences:

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

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

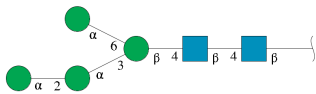
- Molecule 3 is a protein called 2G12 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	105	Total	C	N	O	S	0	0
			798	507	132	156	3		
3	D	105	Total	C	N	O	S	0	0
			798	507	132	156	3		
3	Q	105	Total	C	N	O	S	0	0
			798	507	132	156	3		
3	M	105	Total	C	N	O	S	0	0
			798	507	132	156	3		
3	R	105	Total	C	N	O	S	0	0
			798	507	132	156	3		
3	N	105	Total	C	N	O	S	0	0
			798	507	132	156	3		

- Molecule 4 is a protein called 2G12 Fab Heavy chain.

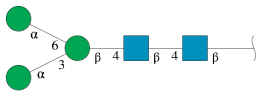
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	122	Total	C	N	O	S	0	0
			938	586	165	182	5		
4	C	122	Total	C	N	O	S	0	0
			938	586	165	182	5		
4	O	122	Total	C	N	O	S	0	0
			938	586	165	182	5		
4	J	122	Total	C	N	O	S	0	0
			938	586	165	182	5		
4	P	122	Total	C	N	O	S	0	0
			938	586	165	182	5		
4	K	122	Total	C	N	O	S	0	0
			938	586	165	182	5		

- Molecule 5 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.



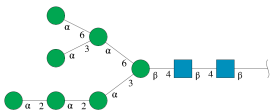
Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	6	Total	C	N	O	0	0
			72	40	2	30		
5	c	6	Total	C	N	O	0	0
			72	40	2	30		
5	m	6	Total	C	N	O	0	0
			72	40	2	30		

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



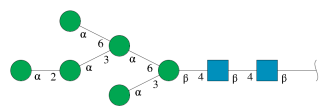
Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	5	Total	C	N	O	0	0
			61	34	2	25		
6	V	5	Total	C	N	O	0	0
			61	34	2	25		
6	d	5	Total	C	N	O	0	0
			61	34	2	25		
6	f	5	Total	C	N	O	0	0
			61	34	2	25		
6	n	5	Total	C	N	O	0	0
			61	34	2	25		
6	p	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



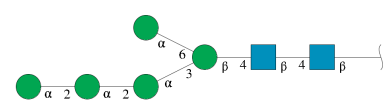
Mol	Chain	Residues	Atoms				AltConf	Trace
7	U	9	Total	C	N	O	0	0
			105	58	2	45		
7	e	9	Total	C	N	O	0	0
			105	58	2	45		
7	o	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
8	W	8	Total	C	N	O	0	0
			94	52	2	40		
8	g	8	Total	C	N	O	0	0
			94	52	2	40		
8	q	8	Total	C	N	O	0	0
			94	52	2	40		

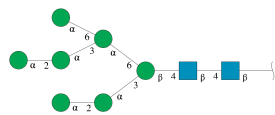
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	7	Total	C	N	O	0	0
			83	46	2	35		
9	h	7	Total	C	N	O	0	0
			83	46	2	35		
9	r	7	Total	C	N	O	0	0
			83	46	2	35		

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

ranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



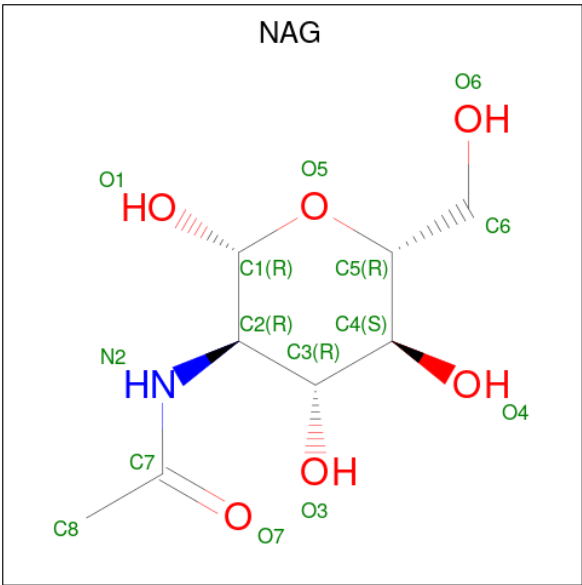
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Y	9	Total	C	N	O	0	0
			105	58	2	45		
10	i	9	Total	C	N	O	0	0
			105	58	2	45		
10	s	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 11 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
11	Z	2	Total	C	N	O	0	0
			28	16	2	10		
11	a	2	Total	C	N	O	0	0
			28	16	2	10		
11	b	2	Total	C	N	O	0	0
			28	16	2	10		
11	j	2	Total	C	N	O	0	0
			28	16	2	10		
11	k	2	Total	C	N	O	0	0
			28	16	2	10		
11	l	2	Total	C	N	O	0	0
			28	16	2	10		
11	t	2	Total	C	N	O	0	0
			28	16	2	10		
11	u	2	Total	C	N	O	0	0
			28	16	2	10		
11	v	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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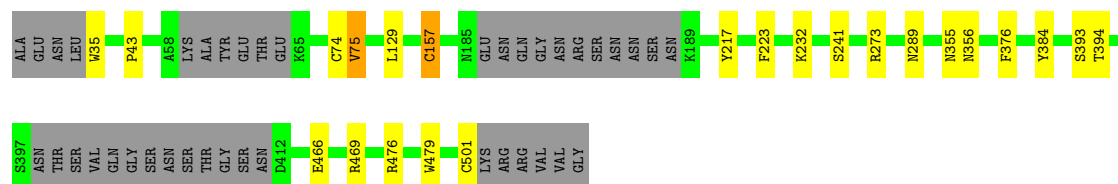
Mol	Chain	Residues	Atoms				AltConf
12	F	1	Total 14	C 8	N 1	O 5	0
12	F	1	Total 14	C 8	N 1	O 5	0
12	F	1	Total 14	C 8	N 1	O 5	0
12	F	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0

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.

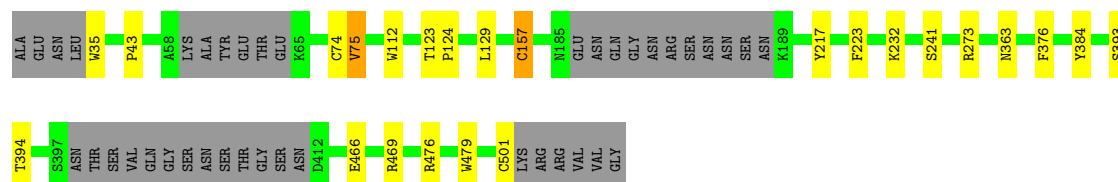
• Molecule 1: Envelope glycoprotein gp160

Chain A:  87% 8%



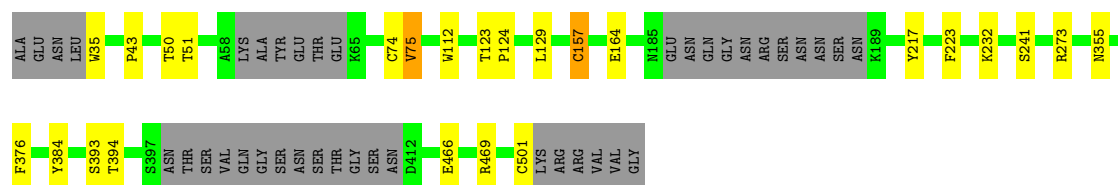
• Molecule 1: Envelope glycoprotein gp160

Chain E:  87% 5% 8%



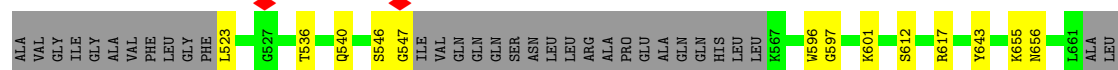
• Molecule 1: Envelope glycoprotein gp160

Chain F:  86% 5% 8%



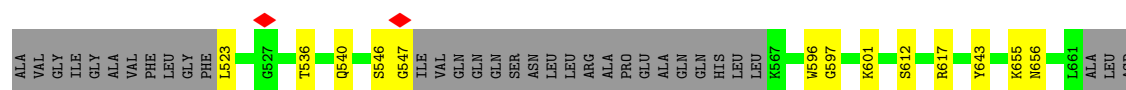
• Molecule 2: Envelope glycoprotein gp41

Chain B:  70% 8% 22%



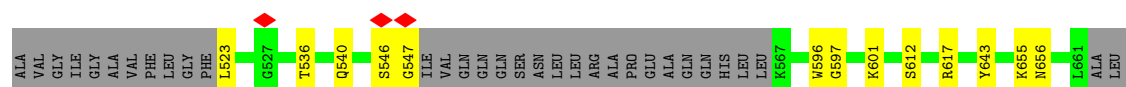
- Molecule 2: Envelope glycoprotein gp41

Chain G: 



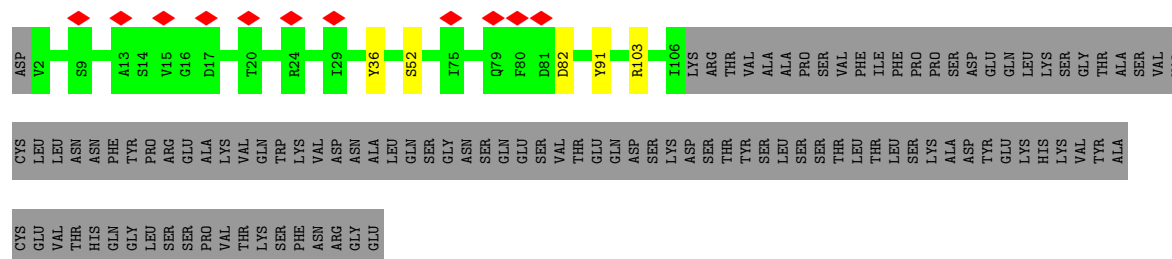
- Molecule 2: Envelope glycoprotein gp41

Chain I: 



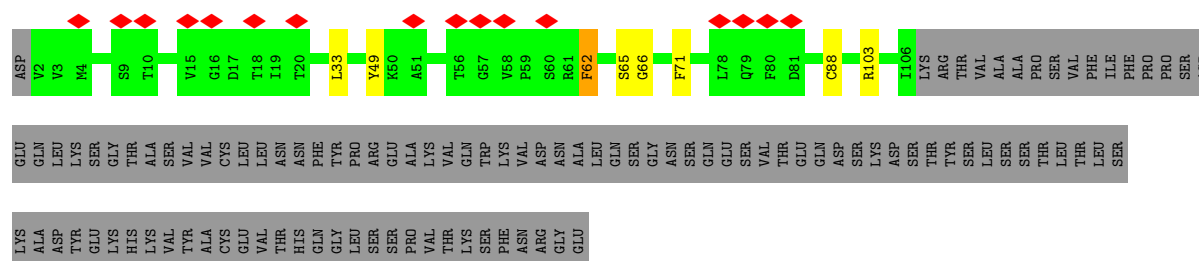
- Molecule 3: 2G12 Fab light chain

Chain L: 



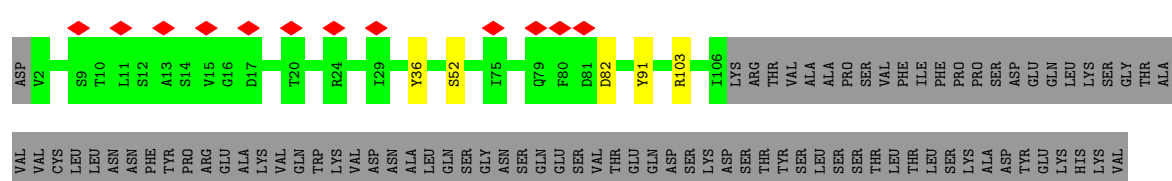
- Molecule 3: 2G12 Fab light chain

Chain D: 



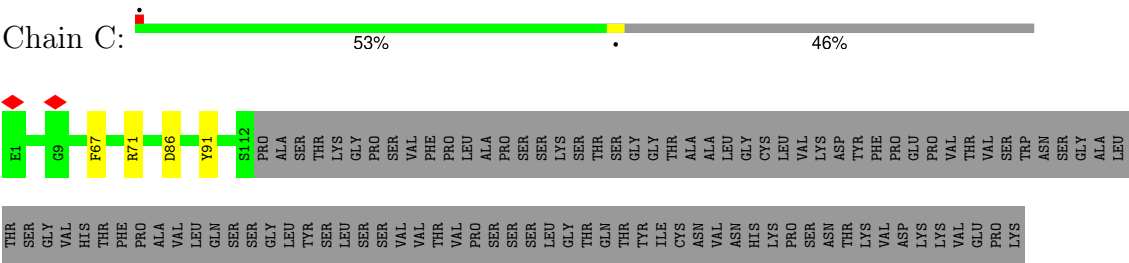
- Molecule 3: 2G12 Fab light chain

Chain Q: 

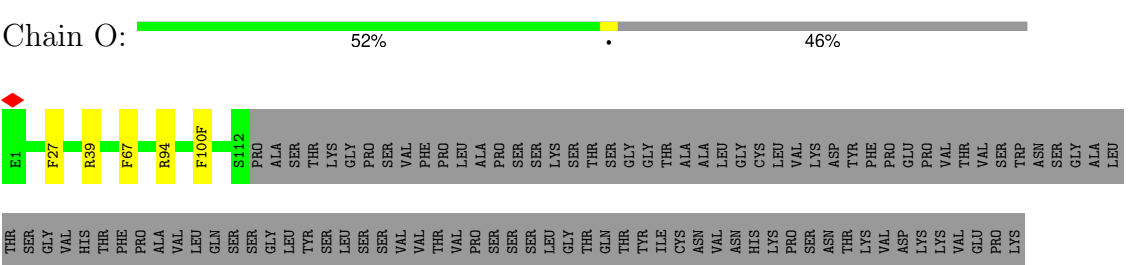


THR	THR	GLY	GLY	VAL	VAL	HIS	THR	PHE	PRO	PRO	ALA	ALA	VAL	VAL	LEU	GLN	SER	SER	SER	GLY	GLY	LEU	LEU	TYR	SER	SER	SER	LEU	LEU	SER	SER	VAL	VAL	VAL	VAL	THR	THR	VAL	VAL	GLY	GLY	THR	THR	GLN	THR	THR	TYR	ILE	CYS	ASN	ASN	VAL	VAL	ASN	ASN	HIS	HIS	LYS	PRO	PRO	SER	PRO	ASN	ASN	THR	THR	LYS	VAL	VAL	ASP	LYS	LYS	LYS	VAL	GLU	GLU	VAL	PRO	PRO	LYS
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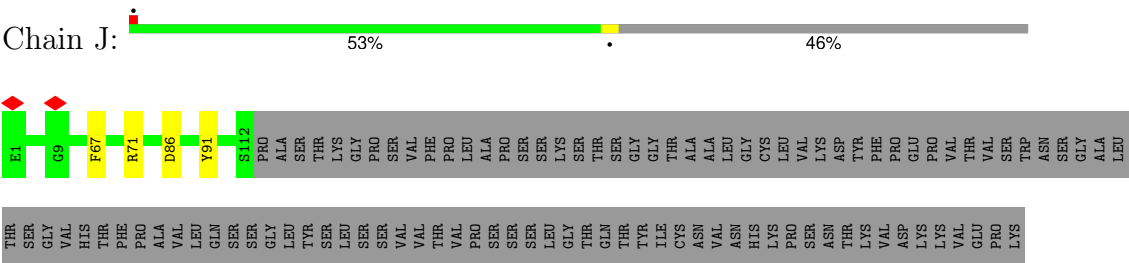
● Molecule 4: 2G12 Fab Heavy chain



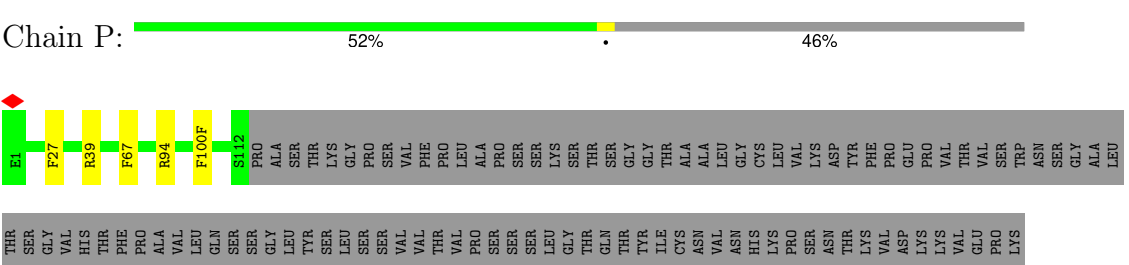
● Molecule 4: 2G12 Fab Heavy chain



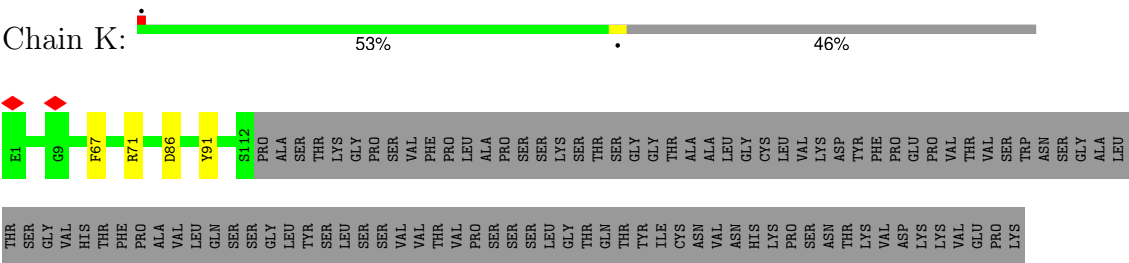
● Molecule 4: 2G12 Fab Heavy chain



● Molecule 4: 2G12 Fab Heavy chain



● Molecule 4: 2G12 Fab Heavy chain



● Molecule 5: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain S:

100%



● Molecule 5: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain c:

100%



● Molecule 5: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain m:

100%



● Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain T:

100%



● Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain V:

20%

100%




● Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain d:

100%


MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 6: 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 f:  20% 100%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 6: 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 n:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 6: 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 p:  20% 100%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 U:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 e:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 7: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain o:

100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

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

Chain W:

100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

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

Chain g:

100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

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

Chain q:

100%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

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

Chain X:

100%

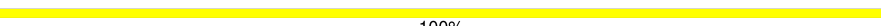
NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

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

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

Chain h:  100%

- Molecule 9: alpha-D-mannopyranose-(1-2)-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 r:  100%

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

Chain Y:  11%  100%

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

Chain i:  11%  100%

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

Chain s:  11%  100%

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

Chain Z:  100%

MAG1
MAG2

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

Chain a:  50% 100%

MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain j:  100%

MAG1
MAG2

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

Chain k:  50% 100%

MAG1
MAG2

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

Chain l:  100%

MAG1
MAG2

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

Chain t:  100%

NAG1
NAG2

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



NAG1
NAG2

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



NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	68155	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 ($e^-/\text{\AA}^2$)	76	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	3.0	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.713	Depositor
Minimum map value	-0.861	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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, BMA, NAG

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	1.04	5/3488 (0.1%)	0.88	5/4737 (0.1%)
1	E	1.04	6/3488 (0.2%)	0.88	5/4737 (0.1%)
1	F	1.04	7/3488 (0.2%)	0.88	5/4737 (0.1%)
2	B	1.09	1/972 (0.1%)	0.89	2/1317 (0.2%)
2	G	1.09	1/972 (0.1%)	0.89	2/1317 (0.2%)
2	I	1.09	1/972 (0.1%)	0.89	2/1317 (0.2%)
3	D	1.05	3/817 (0.4%)	1.00	2/1110 (0.2%)
3	L	1.02	2/817 (0.2%)	1.00	3/1110 (0.3%)
3	M	1.05	3/817 (0.4%)	1.00	2/1110 (0.2%)
3	N	1.05	3/817 (0.4%)	1.00	2/1110 (0.2%)
3	Q	1.02	2/817 (0.2%)	1.00	3/1110 (0.3%)
3	R	1.01	2/817 (0.2%)	1.00	3/1110 (0.3%)
4	C	1.12	0/957	1.09	5/1296 (0.4%)
4	H	1.13	3/957 (0.3%)	1.04	3/1296 (0.2%)
4	J	1.12	0/957	1.09	5/1296 (0.4%)
4	K	1.12	0/957	1.09	5/1296 (0.4%)
4	O	1.14	3/957 (0.3%)	1.04	3/1296 (0.2%)
4	P	1.13	3/957 (0.3%)	1.04	3/1296 (0.2%)
All	All	1.07	45/24024 (0.2%)	0.95	60/32598 (0.2%)

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	157	CYS	CB-SG	-13.07	1.60	1.82
1	E	157	CYS	CB-SG	-13.06	1.60	1.82
1	A	157	CYS	CB-SG	-13.06	1.60	1.82
3	L	91	TYR	CB-CG	-10.26	1.36	1.51
3	R	91	TYR	CB-CG	-10.24	1.36	1.51

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	71	ARG	NE-CZ-NH2	-11.89	114.36	120.30
4	K	71	ARG	NE-CZ-NH2	-11.84	114.38	120.30
4	C	71	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	E	469	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	F	469	ARG	NE-CZ-NH2	-8.83	115.88	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	3416	0	3354	9	0
1	E	3416	0	3354	8	0
1	F	3416	0	3354	8	0
2	B	956	0	939	5	0
2	G	956	0	939	5	0
2	I	956	0	939	5	0
3	D	798	0	779	3	0
3	L	798	0	779	0	0
3	M	798	0	779	2	0
3	N	798	0	779	2	0
3	Q	798	0	779	0	0
3	R	798	0	779	0	0
4	C	938	0	907	0	0
4	H	938	0	907	0	0
4	J	938	0	907	0	0
4	K	938	0	907	0	0
4	O	938	0	907	0	0
4	P	938	0	907	0	0
5	S	72	0	58	0	0
5	c	72	0	58	0	0
5	m	72	0	58	0	0
6	T	61	0	49	0	0
6	V	61	0	49	0	0
6	d	61	0	49	0	0
6	f	61	0	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	n	61	0	49	0	0
6	p	61	0	49	0	0
7	U	105	0	83	0	0
7	e	105	0	83	0	0
7	o	105	0	83	0	0
8	W	94	0	74	0	0
8	g	94	0	74	0	0
8	q	94	0	74	0	0
9	X	83	0	67	0	0
9	h	83	0	67	0	0
9	r	83	0	67	0	0
10	Y	105	0	83	0	0
10	i	105	0	83	0	0
10	s	105	0	83	0	0
11	Z	28	0	25	0	0
11	a	28	0	25	0	0
11	b	28	0	25	0	0
11	j	28	0	25	0	0
11	k	28	0	25	0	0
11	l	28	0	25	0	0
11	t	28	0	25	0	0
11	u	28	0	25	0	0
11	v	28	0	25	0	0
12	A	56	0	52	1	0
12	B	42	0	39	1	0
12	E	56	0	52	0	0
12	F	56	0	52	0	0
12	G	42	0	39	1	0
12	I	42	0	39	1	0
All	All	25821	0	24882	45	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 45 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)
3:N:33:LEU:HD13	3:N:71:PHE:CD1	2.46	0.51
3:M:33:LEU:HD13	3:M:71:PHE:CD1	2.46	0.50
3:D:33:LEU:HD13	3:D:71:PHE:CD1	2.46	0.50
1:A:393:SER:OG	1:A:394:THR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:393:SER:OG	1:E:394:THR:N	2.47	0.47

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	427/475 (90%)	409 (96%)	15 (4%)	3 (1%)	19	52
1	E	427/475 (90%)	409 (96%)	15 (4%)	3 (1%)	19	52
1	F	427/475 (90%)	409 (96%)	15 (4%)	3 (1%)	19	52
2	B	116/153 (76%)	103 (89%)	10 (9%)	3 (3%)	4	28
2	G	116/153 (76%)	103 (89%)	10 (9%)	3 (3%)	4	28
2	I	116/153 (76%)	103 (89%)	10 (9%)	3 (3%)	4	28
3	D	103/213 (48%)	100 (97%)	3 (3%)	0	100	100
3	L	103/213 (48%)	99 (96%)	3 (3%)	1 (1%)	13	44
3	M	103/213 (48%)	100 (97%)	3 (3%)	0	100	100
3	N	103/213 (48%)	100 (97%)	3 (3%)	0	100	100
3	Q	103/213 (48%)	99 (96%)	3 (3%)	1 (1%)	13	44
3	R	103/213 (48%)	99 (96%)	3 (3%)	1 (1%)	13	44
4	C	120/224 (54%)	120 (100%)	0	0	100	100
4	H	120/224 (54%)	120 (100%)	0	0	100	100
4	J	120/224 (54%)	120 (100%)	0	0	100	100
4	K	120/224 (54%)	120 (100%)	0	0	100	100
4	O	120/224 (54%)	120 (100%)	0	0	100	100
4	P	120/224 (54%)	120 (100%)	0	0	100	100
All	All	2967/4506 (66%)	2853 (96%)	93 (3%)	21 (1%)	21	52

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	597	GLY
2	G	597	GLY
2	I	597	GLY
2	B	536	THR
3	L	52	SER

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	388/422 (92%)	388 (100%)	0	100	100
1	E	388/422 (92%)	388 (100%)	0	100	100
1	F	388/422 (92%)	388 (100%)	0	100	100
2	B	104/129 (81%)	104 (100%)	0	100	100
2	G	104/129 (81%)	104 (100%)	0	100	100
2	I	104/129 (81%)	104 (100%)	0	100	100
3	D	87/184 (47%)	87 (100%)	0	100	100
3	L	87/184 (47%)	87 (100%)	0	100	100
3	M	87/184 (47%)	87 (100%)	0	100	100
3	N	87/184 (47%)	87 (100%)	0	100	100
3	Q	87/184 (47%)	87 (100%)	0	100	100
3	R	87/184 (47%)	87 (100%)	0	100	100
4	C	101/189 (53%)	101 (100%)	0	100	100
4	H	101/189 (53%)	101 (100%)	0	100	100
4	J	101/189 (53%)	101 (100%)	0	100	100
4	K	101/189 (53%)	101 (100%)	0	100	100
4	O	101/189 (53%)	101 (100%)	0	100	100
4	P	101/189 (53%)	101 (100%)	0	100	100
All	All	2604/3891 (67%)	2604 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
4	H	81	GLN
4	O	81	GLN
4	P	81	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 ⓘ

165 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	S	1	5,1	14,14,15	2.03	2 (14%)	17,19,21	0.82	1 (5%)
5	NAG	S	2	5	14,14,15	2.13	3 (21%)	17,19,21	0.84	1 (5%)
5	BMA	S	3	5	11,11,12	1.86	2 (18%)	15,15,17	1.10	1 (6%)
5	MAN	S	4	5	11,11,12	1.50	1 (9%)	15,15,17	0.99	1 (6%)
5	MAN	S	5	5	11,11,12	1.84	2 (18%)	15,15,17	1.06	2 (13%)
5	MAN	S	6	5	11,11,12	1.82	2 (18%)	15,15,17	0.99	1 (6%)
6	NAG	T	1	6,1	14,14,15	2.00	3 (21%)	17,19,21	1.01	1 (5%)
6	NAG	T	2	6	14,14,15	2.15	3 (21%)	17,19,21	1.06	2 (11%)
6	BMA	T	3	6	11,11,12	1.89	2 (18%)	15,15,17	1.16	2 (13%)
6	MAN	T	4	6	11,11,12	1.77	2 (18%)	15,15,17	1.05	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	T	5	6	11,11,12	1.81	2 (18%)	15,15,17	0.98	1 (6%)
7	NAG	U	1	7,1	14,14,15	2.01	3 (21%)	17,19,21	0.95	2 (11%)
7	NAG	U	2	7	14,14,15	2.08	3 (21%)	17,19,21	0.90	0
7	BMA	U	3	7	11,11,12	1.84	2 (18%)	15,15,17	0.96	1 (6%)
7	MAN	U	4	7	11,11,12	1.50	1 (9%)	15,15,17	0.80	0
7	MAN	U	5	7	11,11,12	1.69	2 (18%)	15,15,17	0.70	0
7	MAN	U	6	7	11,11,12	1.75	2 (18%)	15,15,17	1.07	0
7	MAN	U	7	7	11,11,12	1.87	3 (27%)	15,15,17	1.22	1 (6%)
7	MAN	U	8	7	11,11,12	1.83	2 (18%)	15,15,17	1.00	2 (13%)
7	MAN	U	9	7	11,11,12	1.80	2 (18%)	15,15,17	1.35	2 (13%)
6	NAG	V	1	6,1	14,14,15	2.04	3 (21%)	17,19,21	0.87	1 (5%)
6	NAG	V	2	6	14,14,15	2.07	5 (35%)	17,19,21	1.25	2 (11%)
6	BMA	V	3	6	11,11,12	1.88	2 (18%)	15,15,17	1.06	1 (6%)
6	MAN	V	4	6	11,11,12	1.90	3 (27%)	15,15,17	0.98	1 (6%)
6	MAN	V	5	6	11,11,12	1.77	1 (9%)	15,15,17	1.09	1 (6%)
8	NAG	W	1	8,1	14,14,15	2.00	2 (14%)	17,19,21	0.99	1 (5%)
8	NAG	W	2	8	14,14,15	2.13	3 (21%)	17,19,21	0.80	0
8	BMA	W	3	8	11,11,12	1.75	2 (18%)	15,15,17	0.93	1 (6%)
8	MAN	W	4	8	11,11,12	1.85	2 (18%)	15,15,17	1.14	1 (6%)
8	MAN	W	5	8	11,11,12	1.57	2 (18%)	15,15,17	1.00	0
8	MAN	W	6	8	11,11,12	1.81	2 (18%)	15,15,17	1.04	2 (13%)
8	MAN	W	7	8	11,11,12	1.76	2 (18%)	15,15,17	0.70	0
8	MAN	W	8	8	11,11,12	1.79	2 (18%)	15,15,17	0.92	1 (6%)
9	NAG	X	1	1,9	14,14,15	1.93	2 (14%)	17,19,21	1.00	1 (5%)
9	NAG	X	2	9	14,14,15	2.08	3 (21%)	17,19,21	0.90	1 (5%)
9	BMA	X	3	9	11,11,12	1.85	2 (18%)	15,15,17	0.80	0
9	MAN	X	4	9	11,11,12	1.62	1 (9%)	15,15,17	0.81	0
9	MAN	X	5	9	11,11,12	1.63	2 (18%)	15,15,17	0.83	0
9	MAN	X	6	9	11,11,12	1.71	2 (18%)	15,15,17	0.97	0
9	MAN	X	7	9	11,11,12	1.81	2 (18%)	15,15,17	1.08	1 (6%)
10	NAG	Y	1	1,10	14,14,15	1.97	4 (28%)	17,19,21	0.91	2 (11%)
10	NAG	Y	2	10	14,14,15	2.05	3 (21%)	17,19,21	1.06	1 (5%)
10	BMA	Y	3	10	11,11,12	1.85	2 (18%)	15,15,17	0.78	0
10	MAN	Y	4	10	11,11,12	1.88	2 (18%)	15,15,17	1.22	1 (6%)
10	MAN	Y	5	10	11,11,12	1.59	2 (18%)	15,15,17	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	Y	6	10	11,11,12	1.79	2 (18%)	15,15,17	1.04	2 (13%)
10	MAN	Y	7	10	11,11,12	1.74	1 (9%)	15,15,17	1.12	2 (13%)
10	MAN	Y	8	10	11,11,12	1.50	1 (9%)	15,15,17	0.81	0
10	MAN	Y	9	10	11,11,12	1.78	1 (9%)	15,15,17	1.03	1 (6%)
11	NAG	Z	1	1,11	14,14,15	2.02	2 (14%)	17,19,21	0.88	0
11	NAG	Z	2	11	14,14,15	2.14	3 (21%)	17,19,21	0.77	0
11	NAG	a	1	1,11	14,14,15	2.00	3 (21%)	17,19,21	0.82	1 (5%)
11	NAG	a	2	11	14,14,15	2.09	2 (14%)	17,19,21	0.84	1 (5%)
11	NAG	b	1	1,11	14,14,15	2.05	3 (21%)	17,19,21	1.12	2 (11%)
11	NAG	b	2	11	14,14,15	2.14	3 (21%)	17,19,21	0.77	0
5	NAG	c	1	5,1	14,14,15	2.03	2 (14%)	17,19,21	0.83	1 (5%)
5	NAG	c	2	5	14,14,15	2.14	3 (21%)	17,19,21	0.84	1 (5%)
5	BMA	c	3	5	11,11,12	1.85	2 (18%)	15,15,17	1.10	1 (6%)
5	MAN	c	4	5	11,11,12	1.50	1 (9%)	15,15,17	0.99	1 (6%)
5	MAN	c	5	5	11,11,12	1.84	2 (18%)	15,15,17	1.07	2 (13%)
5	MAN	c	6	5	11,11,12	1.82	2 (18%)	15,15,17	0.99	1 (6%)
6	NAG	d	1	6,1	14,14,15	2.00	3 (21%)	17,19,21	1.01	1 (5%)
6	NAG	d	2	6	14,14,15	2.15	3 (21%)	17,19,21	1.06	2 (11%)
6	BMA	d	3	6	11,11,12	1.89	2 (18%)	15,15,17	1.16	2 (13%)
6	MAN	d	4	6	11,11,12	1.77	2 (18%)	15,15,17	1.05	2 (13%)
6	MAN	d	5	6	11,11,12	1.81	2 (18%)	15,15,17	0.99	1 (6%)
7	NAG	e	1	7,1	14,14,15	2.00	3 (21%)	17,19,21	0.94	2 (11%)
7	NAG	e	2	7	14,14,15	2.09	3 (21%)	17,19,21	0.90	0
7	BMA	e	3	7	11,11,12	1.83	2 (18%)	15,15,17	0.97	1 (6%)
7	MAN	e	4	7	11,11,12	1.50	1 (9%)	15,15,17	0.80	0
7	MAN	e	5	7	11,11,12	1.69	2 (18%)	15,15,17	0.70	0
7	MAN	e	6	7	11,11,12	1.75	2 (18%)	15,15,17	1.07	0
7	MAN	e	7	7	11,11,12	1.87	3 (27%)	15,15,17	1.21	1 (6%)
7	MAN	e	8	7	11,11,12	1.83	2 (18%)	15,15,17	1.00	1 (6%)
7	MAN	e	9	7	11,11,12	1.79	2 (18%)	15,15,17	1.34	2 (13%)
6	NAG	f	1	6,1	14,14,15	2.03	3 (21%)	17,19,21	0.87	1 (5%)
6	NAG	f	2	6	14,14,15	2.07	5 (35%)	17,19,21	1.26	2 (11%)
6	BMA	f	3	6	11,11,12	1.87	2 (18%)	15,15,17	1.06	1 (6%)
6	MAN	f	4	6	11,11,12	1.89	3 (27%)	15,15,17	0.99	1 (6%)
6	MAN	f	5	6	11,11,12	1.77	1 (9%)	15,15,17	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	g	1	8,1	14,14,15	2.00	2 (14%)	17,19,21	0.99	1 (5%)
8	NAG	g	2	8	14,14,15	2.13	3 (21%)	17,19,21	0.80	0
8	BMA	g	3	8	11,11,12	1.75	2 (18%)	15,15,17	0.94	1 (6%)
8	MAN	g	4	8	11,11,12	1.84	2 (18%)	15,15,17	1.14	1 (6%)
8	MAN	g	5	8	11,11,12	1.57	2 (18%)	15,15,17	1.00	0
8	MAN	g	6	8	11,11,12	1.81	2 (18%)	15,15,17	1.04	2 (13%)
8	MAN	g	7	8	11,11,12	1.76	2 (18%)	15,15,17	0.70	0
8	MAN	g	8	8	11,11,12	1.79	2 (18%)	15,15,17	0.93	1 (6%)
9	NAG	h	1	1,9	14,14,15	1.93	2 (14%)	17,19,21	1.00	1 (5%)
9	NAG	h	2	9	14,14,15	2.08	3 (21%)	17,19,21	0.90	1 (5%)
9	BMA	h	3	9	11,11,12	1.86	2 (18%)	15,15,17	0.80	0
9	MAN	h	4	9	11,11,12	1.63	1 (9%)	15,15,17	0.81	0
9	MAN	h	5	9	11,11,12	1.62	2 (18%)	15,15,17	0.83	0
9	MAN	h	6	9	11,11,12	1.71	2 (18%)	15,15,17	0.97	0
9	MAN	h	7	9	11,11,12	1.81	2 (18%)	15,15,17	1.08	1 (6%)
10	NAG	i	1	1,10	14,14,15	1.97	4 (28%)	17,19,21	0.91	2 (11%)
10	NAG	i	2	10	14,14,15	2.04	3 (21%)	17,19,21	1.05	1 (5%)
10	BMA	i	3	10	11,11,12	1.86	2 (18%)	15,15,17	0.77	0
10	MAN	i	4	10	11,11,12	1.88	2 (18%)	15,15,17	1.22	1 (6%)
10	MAN	i	5	10	11,11,12	1.59	2 (18%)	15,15,17	1.13	0
10	MAN	i	6	10	11,11,12	1.78	2 (18%)	15,15,17	1.03	2 (13%)
10	MAN	i	7	10	11,11,12	1.75	1 (9%)	15,15,17	1.12	2 (13%)
10	MAN	i	8	10	11,11,12	1.51	1 (9%)	15,15,17	0.82	0
10	MAN	i	9	10	11,11,12	1.78	1 (9%)	15,15,17	1.03	1 (6%)
11	NAG	j	1	1,11	14,14,15	2.01	2 (14%)	17,19,21	0.88	0
11	NAG	j	2	11	14,14,15	2.14	2 (14%)	17,19,21	0.77	0
11	NAG	k	1	1,11	14,14,15	2.00	3 (21%)	17,19,21	0.82	1 (5%)
11	NAG	k	2	11	14,14,15	2.09	2 (14%)	17,19,21	0.84	1 (5%)
11	NAG	l	1	1,11	14,14,15	2.05	3 (21%)	17,19,21	1.12	2 (11%)
11	NAG	l	2	11	14,14,15	2.15	3 (21%)	17,19,21	0.77	0
5	NAG	m	1	5,1	14,14,15	2.03	2 (14%)	17,19,21	0.82	1 (5%)
5	NAG	m	2	5	14,14,15	2.13	3 (21%)	17,19,21	0.84	1 (5%)
5	BMA	m	3	5	11,11,12	1.86	2 (18%)	15,15,17	1.10	1 (6%)
5	MAN	m	4	5	11,11,12	1.50	1 (9%)	15,15,17	0.99	1 (6%)
5	MAN	m	5	5	11,11,12	1.85	2 (18%)	15,15,17	1.06	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	m	6	5	11,11,12	1.82	2 (18%)	15,15,17	0.99	1 (6%)
6	NAG	n	1	6,1	14,14,15	2.00	3 (21%)	17,19,21	1.00	1 (5%)
6	NAG	n	2	6	14,14,15	2.15	3 (21%)	17,19,21	1.07	2 (11%)
6	BMA	n	3	6	11,11,12	1.89	2 (18%)	15,15,17	1.16	2 (13%)
6	MAN	n	4	6	11,11,12	1.76	2 (18%)	15,15,17	1.05	2 (13%)
6	MAN	n	5	6	11,11,12	1.80	2 (18%)	15,15,17	0.98	1 (6%)
7	NAG	o	1	7,1	14,14,15	2.01	3 (21%)	17,19,21	0.94	2 (11%)
7	NAG	o	2	7	14,14,15	2.08	3 (21%)	17,19,21	0.90	0
7	BMA	o	3	7	11,11,12	1.84	2 (18%)	15,15,17	0.97	1 (6%)
7	MAN	o	4	7	11,11,12	1.49	1 (9%)	15,15,17	0.80	0
7	MAN	o	5	7	11,11,12	1.68	2 (18%)	15,15,17	0.70	0
7	MAN	o	6	7	11,11,12	1.76	2 (18%)	15,15,17	1.07	0
7	MAN	o	7	7	11,11,12	1.87	3 (27%)	15,15,17	1.21	1 (6%)
7	MAN	o	8	7	11,11,12	1.83	2 (18%)	15,15,17	1.00	1 (6%)
7	MAN	o	9	7	11,11,12	1.79	2 (18%)	15,15,17	1.35	2 (13%)
6	NAG	p	1	6,1	14,14,15	2.04	3 (21%)	17,19,21	0.87	1 (5%)
6	NAG	p	2	6	14,14,15	2.07	5 (35%)	17,19,21	1.26	2 (11%)
6	BMA	p	3	6	11,11,12	1.87	2 (18%)	15,15,17	1.07	1 (6%)
6	MAN	p	4	6	11,11,12	1.90	3 (27%)	15,15,17	0.98	1 (6%)
6	MAN	p	5	6	11,11,12	1.77	1 (9%)	15,15,17	1.09	1 (6%)
8	NAG	q	1	8,1	14,14,15	2.00	2 (14%)	17,19,21	0.99	1 (5%)
8	NAG	q	2	8	14,14,15	2.13	3 (21%)	17,19,21	0.80	0
8	BMA	q	3	8	11,11,12	1.75	2 (18%)	15,15,17	0.94	1 (6%)
8	MAN	q	4	8	11,11,12	1.84	2 (18%)	15,15,17	1.14	1 (6%)
8	MAN	q	5	8	11,11,12	1.57	2 (18%)	15,15,17	0.99	0
8	MAN	q	6	8	11,11,12	1.80	2 (18%)	15,15,17	1.04	2 (13%)
8	MAN	q	7	8	11,11,12	1.76	2 (18%)	15,15,17	0.70	0
8	MAN	q	8	8	11,11,12	1.79	2 (18%)	15,15,17	0.93	1 (6%)
9	NAG	r	1	1,9	14,14,15	1.93	2 (14%)	17,19,21	1.00	1 (5%)
9	NAG	r	2	9	14,14,15	2.07	3 (21%)	17,19,21	0.90	1 (5%)
9	BMA	r	3	9	11,11,12	1.85	2 (18%)	15,15,17	0.80	0
9	MAN	r	4	9	11,11,12	1.63	1 (9%)	15,15,17	0.81	0
9	MAN	r	5	9	11,11,12	1.62	2 (18%)	15,15,17	0.83	0
9	MAN	r	6	9	11,11,12	1.71	2 (18%)	15,15,17	0.97	0
9	MAN	r	7	9	11,11,12	1.81	2 (18%)	15,15,17	1.08	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	s	1	1,10	14,14,15	1.97	4 (28%)	17,19,21	0.91	2 (11%)
10	NAG	s	2	10	14,14,15	2.05	3 (21%)	17,19,21	1.06	1 (5%)
10	BMA	s	3	10	11,11,12	1.86	2 (18%)	15,15,17	0.77	0
10	MAN	s	4	10	11,11,12	1.88	2 (18%)	15,15,17	1.22	1 (6%)
10	MAN	s	5	10	11,11,12	1.59	2 (18%)	15,15,17	1.14	0
10	MAN	s	6	10	11,11,12	1.79	2 (18%)	15,15,17	1.04	2 (13%)
10	MAN	s	7	10	11,11,12	1.75	1 (9%)	15,15,17	1.12	2 (13%)
10	MAN	s	8	10	11,11,12	1.51	1 (9%)	15,15,17	0.81	0
10	MAN	s	9	10	11,11,12	1.78	1 (9%)	15,15,17	1.03	1 (6%)
11	NAG	t	1	1,11	14,14,15	2.01	2 (14%)	17,19,21	0.88	0
11	NAG	t	2	11	14,14,15	2.14	2 (14%)	17,19,21	0.77	0
11	NAG	u	1	1,11	14,14,15	2.00	3 (21%)	17,19,21	0.82	1 (5%)
11	NAG	u	2	11	14,14,15	2.09	2 (14%)	17,19,21	0.84	1 (5%)
11	NAG	v	1	1,11	14,14,15	2.05	3 (21%)	17,19,21	1.12	2 (11%)
11	NAG	v	2	11	14,14,15	2.14	3 (21%)	17,19,21	0.77	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
5	NAG	S	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	BMA	S	3	5	-	2/2/19/22	0/1/1/1
5	MAN	S	4	5	-	2/2/19/22	0/1/1/1
5	MAN	S	5	5	-	1/2/19/22	0/1/1/1
5	MAN	S	6	5	-	1/2/19/22	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	2/2/19/22	0/1/1/1
6	MAN	T	4	6	-	1/2/19/22	0/1/1/1
6	MAN	T	5	6	-	1/2/19/22	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	BMA	U	3	7	-	2/2/19/22	0/1/1/1
7	MAN	U	4	7	-	1/2/19/22	0/1/1/1
7	MAN	U	5	7	-	1/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	b	2	11	-	1/6/23/26	0/1/1/1
5	NAG	c	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	2/2/19/22	0/1/1/1
5	MAN	c	4	5	-	2/2/19/22	0/1/1/1
5	MAN	c	5	5	-	1/2/19/22	0/1/1/1
5	MAN	c	6	5	-	1/2/19/22	0/1/1/1
6	NAG	d	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	-	0/6/23/26	0/1/1/1
6	BMA	d	3	6	-	2/2/19/22	0/1/1/1
6	MAN	d	4	6	-	1/2/19/22	0/1/1/1
6	MAN	d	5	6	-	1/2/19/22	0/1/1/1
7	NAG	e	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
7	BMA	e	3	7	-	2/2/19/22	0/1/1/1
7	MAN	e	4	7	-	1/2/19/22	0/1/1/1
7	MAN	e	5	7	-	1/2/19/22	0/1/1/1
7	MAN	e	6	7	-	2/2/19/22	0/1/1/1
7	MAN	e	7	7	-	2/2/19/22	0/1/1/1
7	MAN	e	8	7	-	1/2/19/22	0/1/1/1
7	MAN	e	9	7	-	1/2/19/22	0/1/1/1
6	NAG	f	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	BMA	f	3	6	-	2/2/19/22	0/1/1/1
6	MAN	f	4	6	-	1/2/19/22	0/1/1/1
6	MAN	f	5	6	-	2/2/19/22	0/1/1/1
8	NAG	g	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1
8	BMA	g	3	8	-	2/2/19/22	0/1/1/1
8	MAN	g	4	8	-	2/2/19/22	0/1/1/1
8	MAN	g	5	8	-	2/2/19/22	0/1/1/1
8	MAN	g	6	8	-	1/2/19/22	0/1/1/1
8	MAN	g	7	8	-	2/2/19/22	0/1/1/1
8	MAN	g	8	8	-	1/2/19/22	0/1/1/1
9	NAG	h	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	h	2	9	-	0/6/23/26	0/1/1/1
9	BMA	h	3	9	-	2/2/19/22	0/1/1/1
9	MAN	h	4	9	-	1/2/19/22	0/1/1/1
9	MAN	h	5	9	-	1/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	p	3	6	-	2/2/19/22	0/1/1/1
6	MAN	p	4	6	-	1/2/19/22	0/1/1/1
6	MAN	p	5	6	-	2/2/19/22	0/1/1/1
8	NAG	q	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	q	2	8	-	0/6/23/26	0/1/1/1
8	BMA	q	3	8	-	2/2/19/22	0/1/1/1
8	MAN	q	4	8	-	2/2/19/22	0/1/1/1
8	MAN	q	5	8	-	2/2/19/22	0/1/1/1
8	MAN	q	6	8	-	1/2/19/22	0/1/1/1
8	MAN	q	7	8	-	2/2/19/22	0/1/1/1
8	MAN	q	8	8	-	1/2/19/22	0/1/1/1
9	NAG	r	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	r	2	9	-	0/6/23/26	0/1/1/1
9	BMA	r	3	9	-	2/2/19/22	0/1/1/1
9	MAN	r	4	9	-	1/2/19/22	0/1/1/1
9	MAN	r	5	9	-	1/2/19/22	0/1/1/1
9	MAN	r	6	9	-	0/2/19/22	0/1/1/1
9	MAN	r	7	9	-	2/2/19/22	0/1/1/1
10	NAG	s	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	s	2	10	-	0/6/23/26	0/1/1/1
10	BMA	s	3	10	-	2/2/19/22	0/1/1/1
10	MAN	s	4	10	-	2/2/19/22	0/1/1/1
10	MAN	s	5	10	-	1/2/19/22	0/1/1/1
10	MAN	s	6	10	-	1/2/19/22	0/1/1/1
10	MAN	s	7	10	-	1/2/19/22	0/1/1/1
10	MAN	s	8	10	-	1/2/19/22	0/1/1/1
10	MAN	s	9	10	-	1/2/19/22	0/1/1/1
11	NAG	t	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	t	2	11	-	2/6/23/26	0/1/1/1
11	NAG	u	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	u	2	11	-	2/6/23/26	0/1/1/1
11	NAG	v	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	v	2	11	-	1/6/23/26	0/1/1/1

The worst 5 of 367 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	t	2	NAG	O5-C1	6.74	1.55	1.43
6	n	2	NAG	O5-C1	6.74	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	d	2	NAG	O5-C1	6.73	1.55	1.43
11	Z	2	NAG	O5-C1	6.73	1.55	1.43
6	T	2	NAG	O5-C1	6.73	1.55	1.43

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	n	3	BMA	O3-C3-C4	2.81	116.99	110.38
6	T	3	BMA	O3-C3-C4	2.81	116.99	110.38
6	d	3	BMA	O3-C3-C4	2.81	116.99	110.38
8	W	4	MAN	C2-C3-C4	-2.78	105.97	110.86
7	U	9	MAN	C1-C2-C3	2.78	113.69	109.64

There are no chirality outliers.

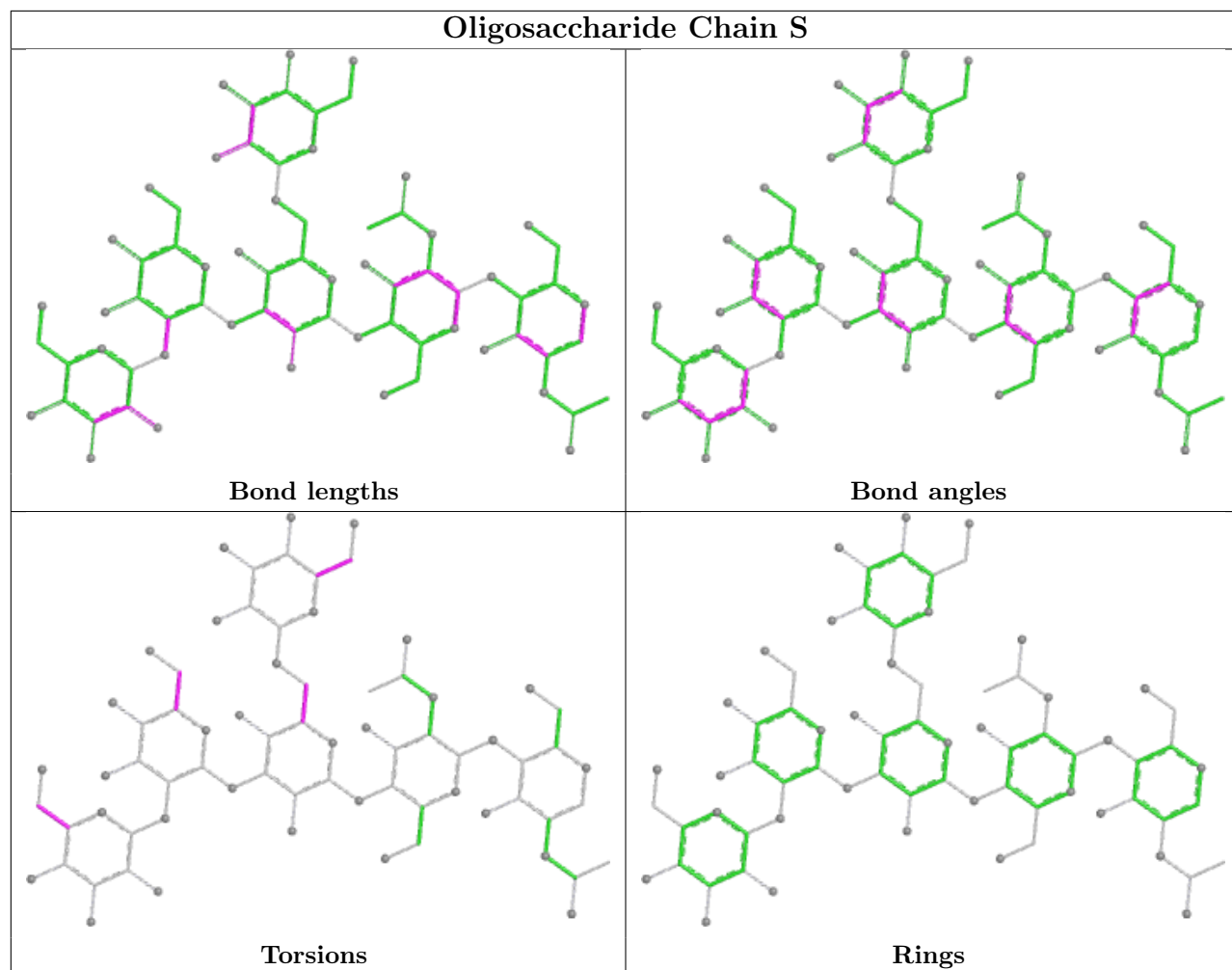
5 of 183 torsion outliers are listed below:

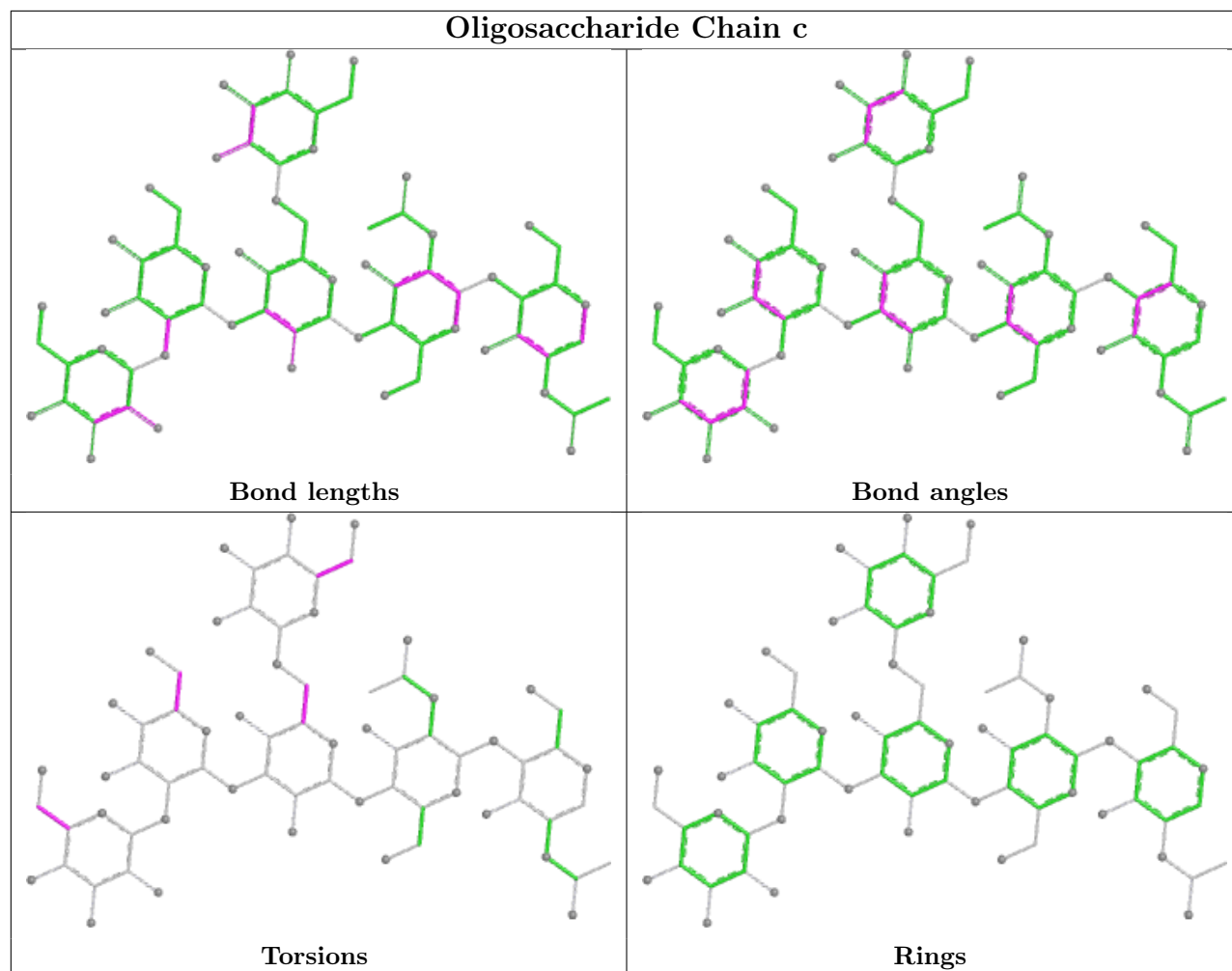
Mol	Chain	Res	Type	Atoms
7	U	3	BMA	C4-C5-C6-O6
7	e	3	BMA	C4-C5-C6-O6
7	o	3	BMA	C4-C5-C6-O6
7	U	3	BMA	O5-C5-C6-O6
7	U	7	MAN	O5-C5-C6-O6

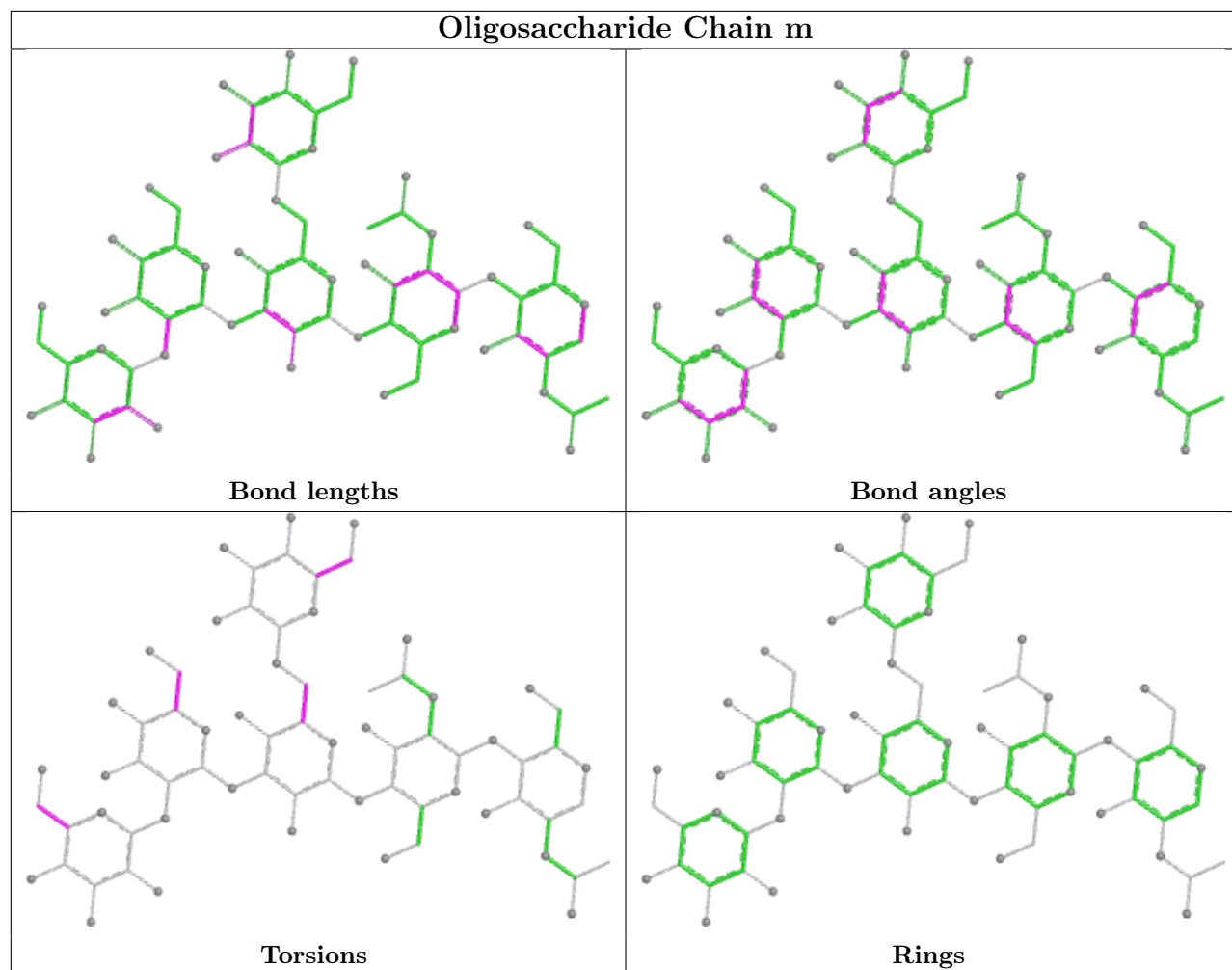
There are no ring outliers.

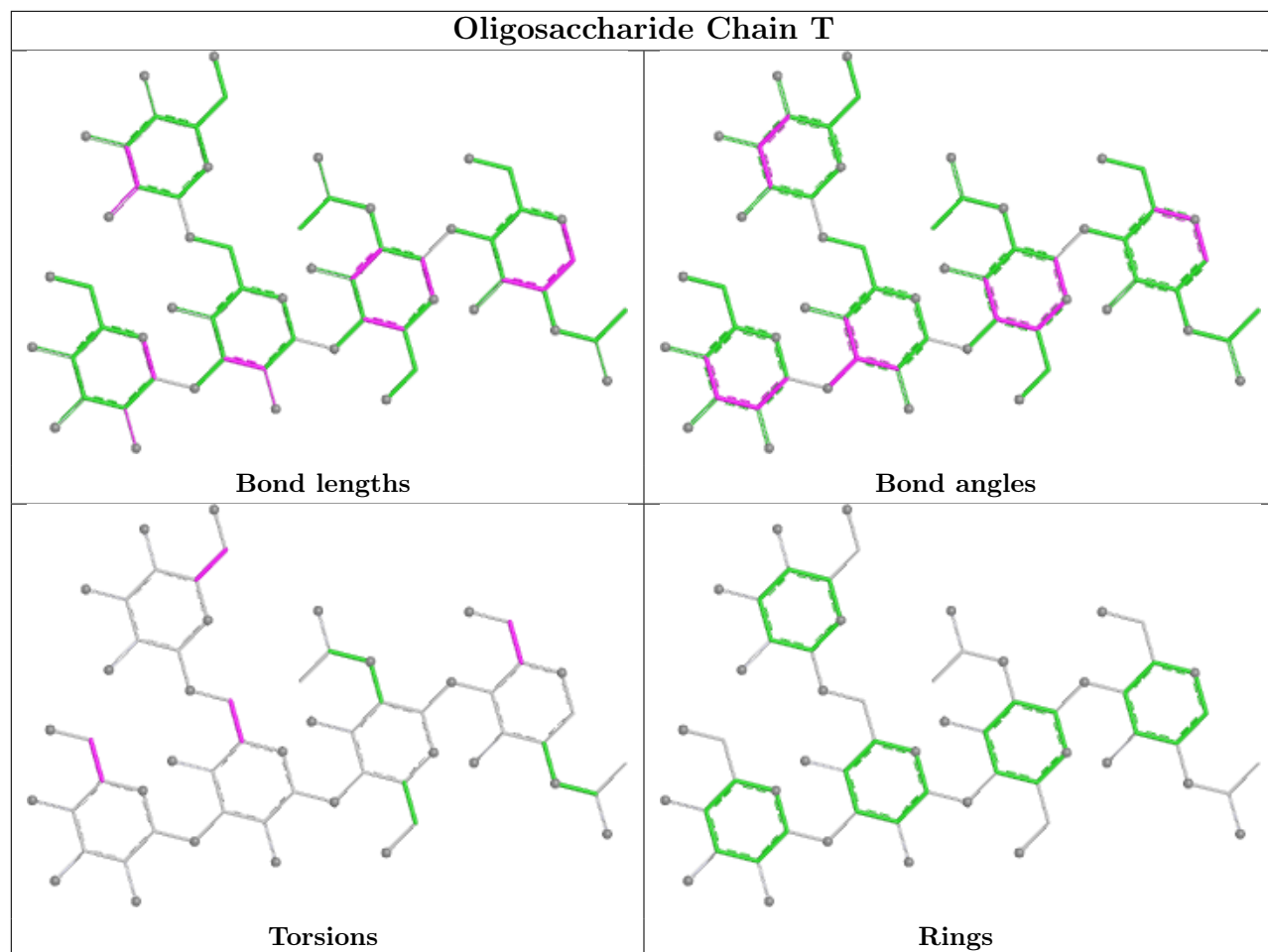
No monomer is involved in short contacts.

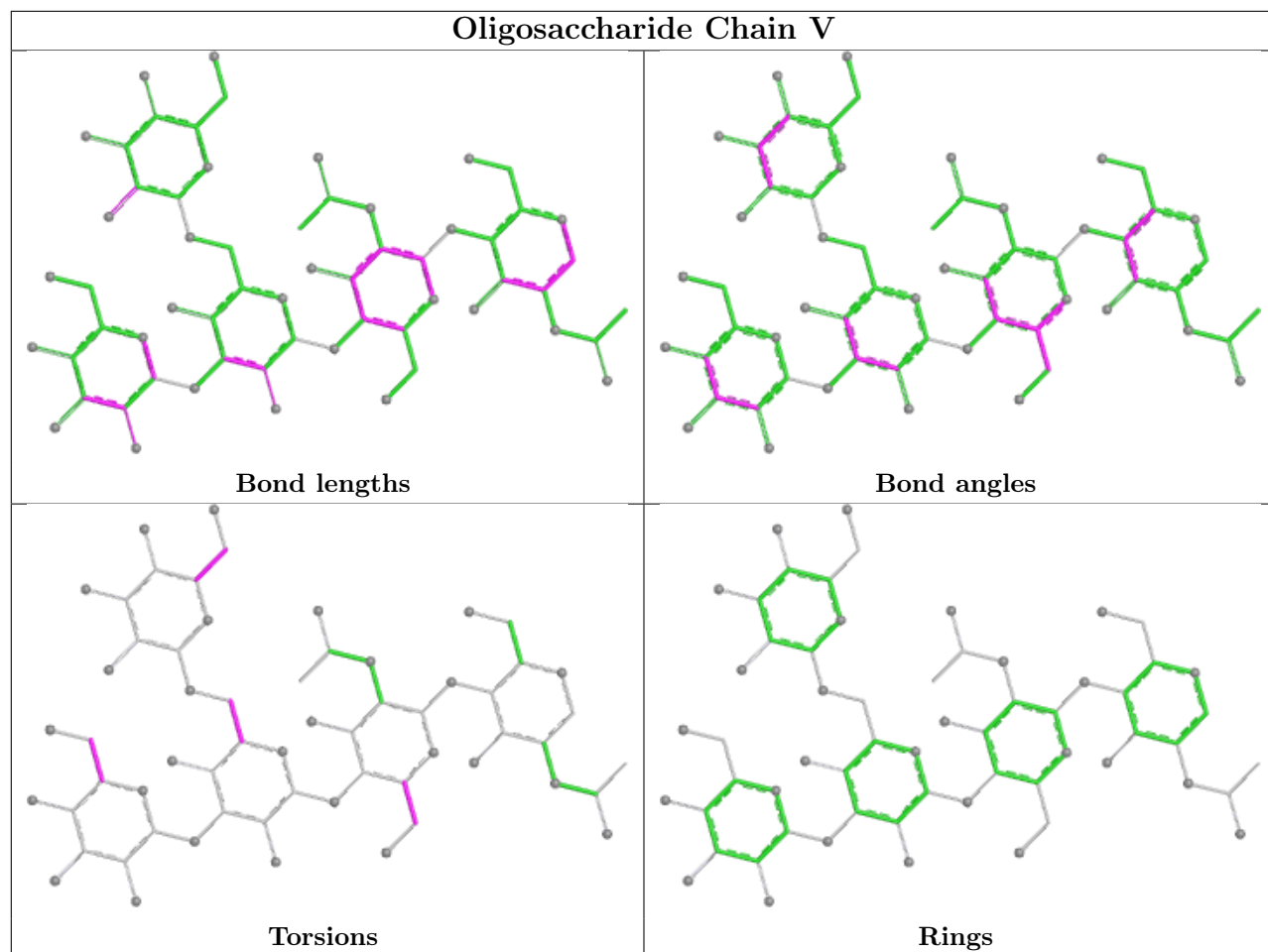
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

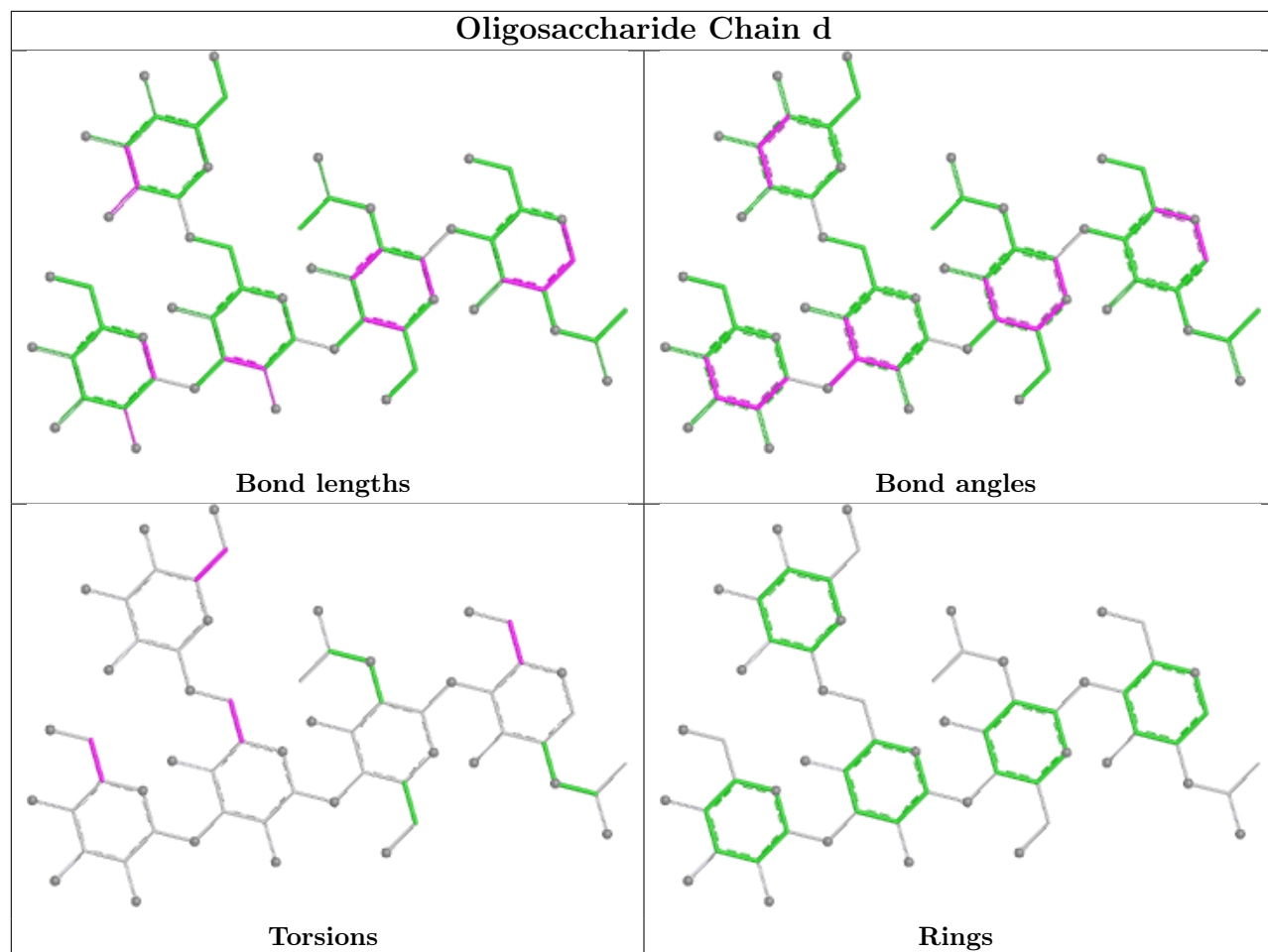


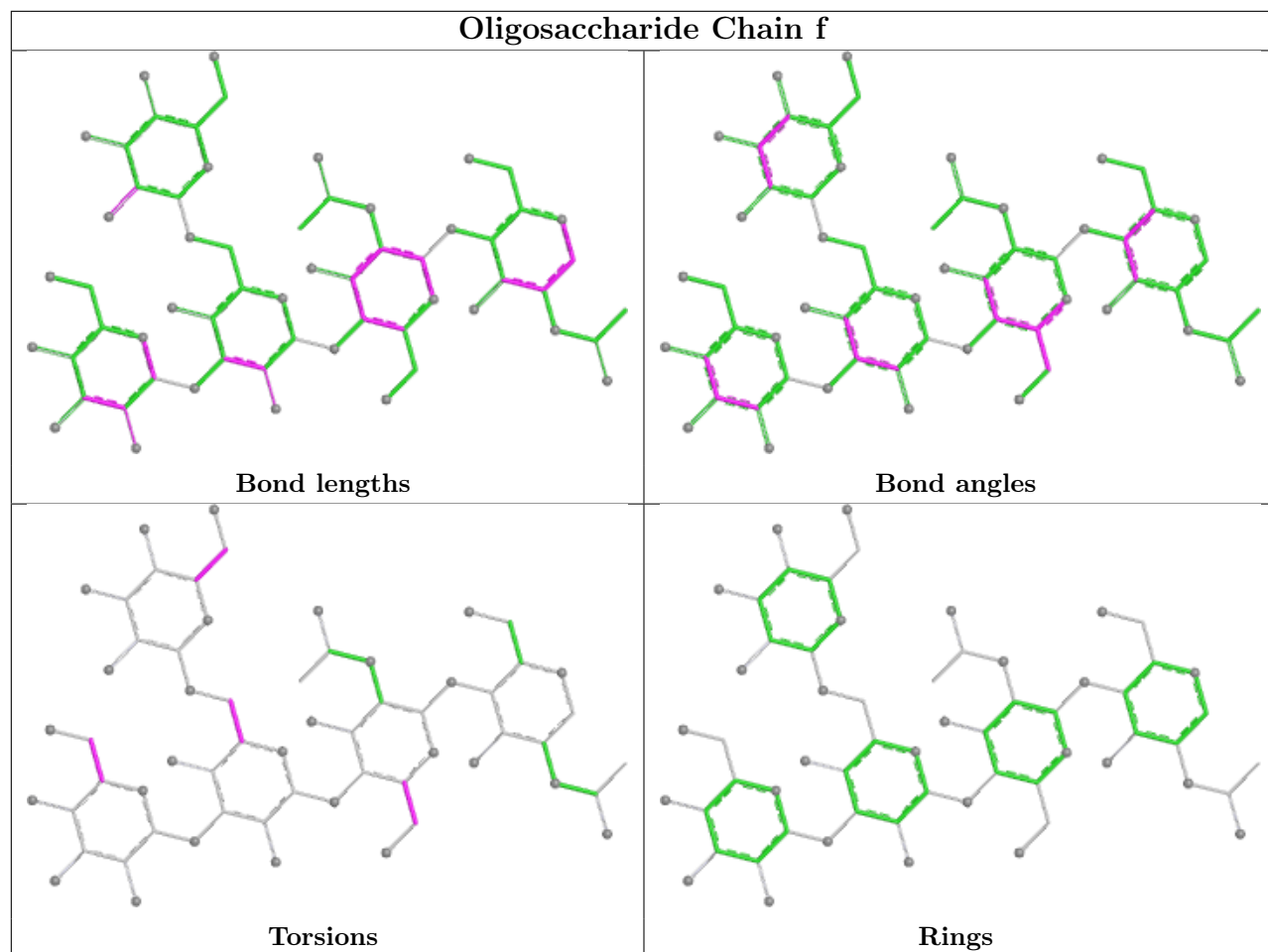


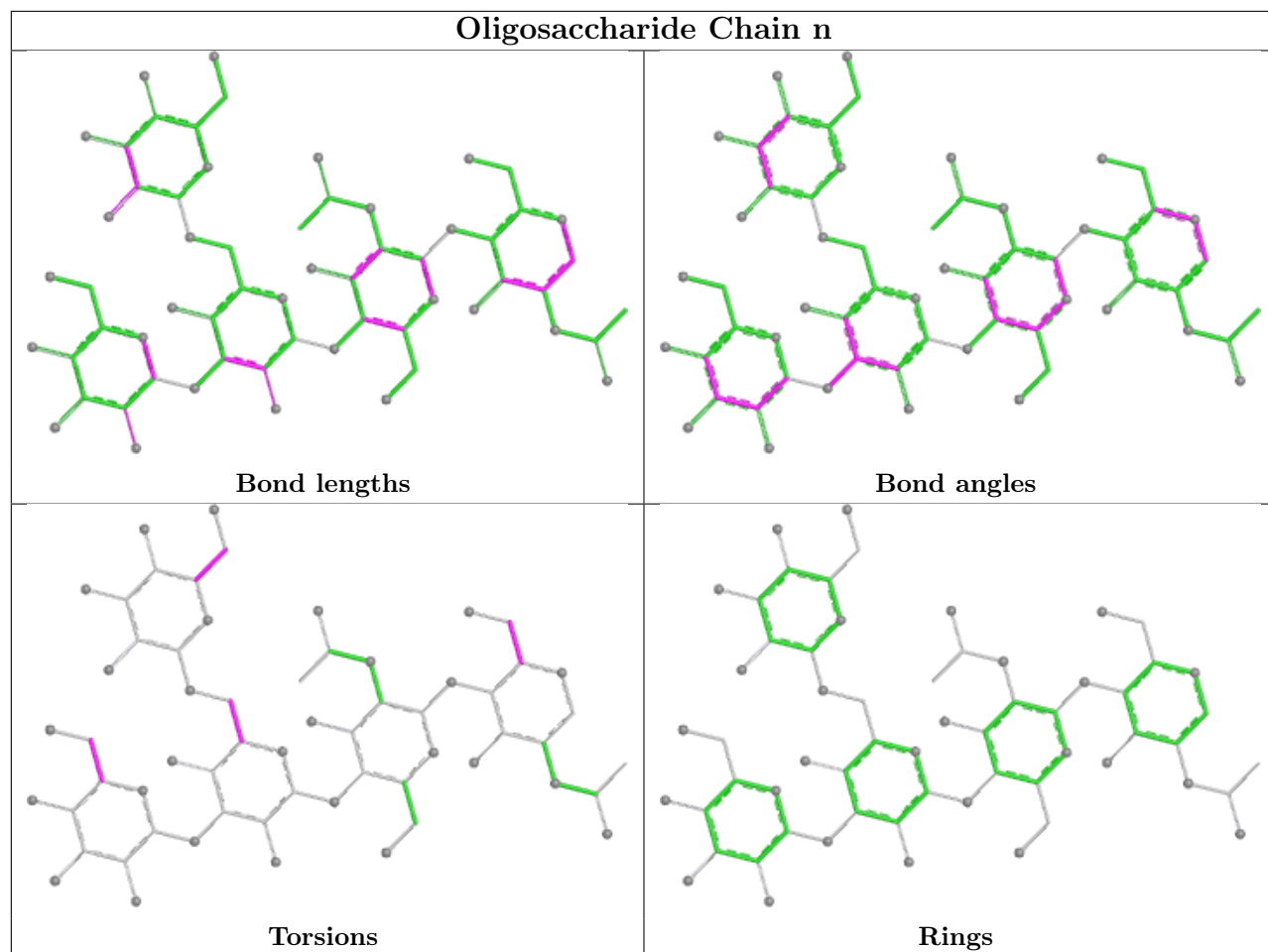


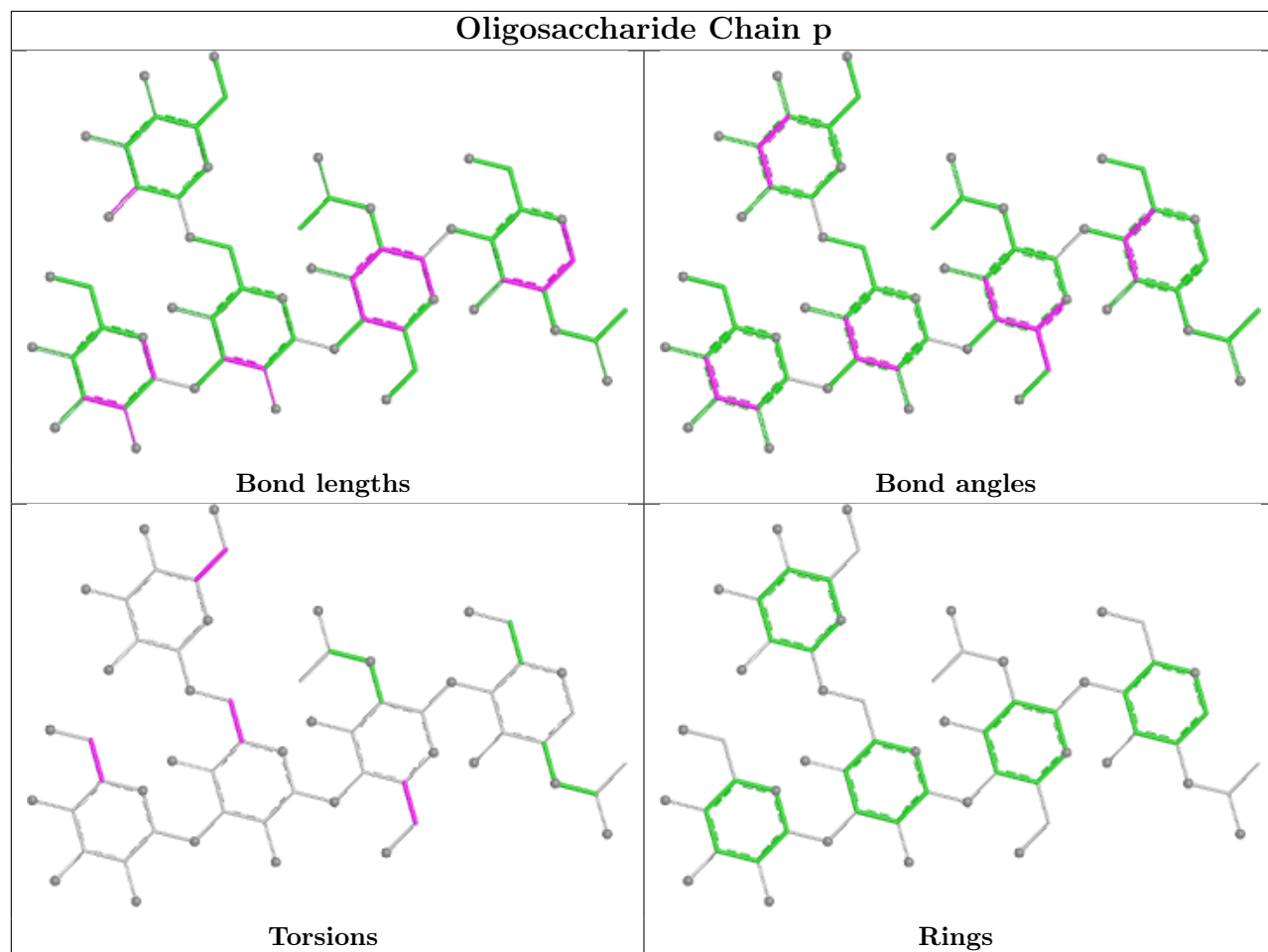


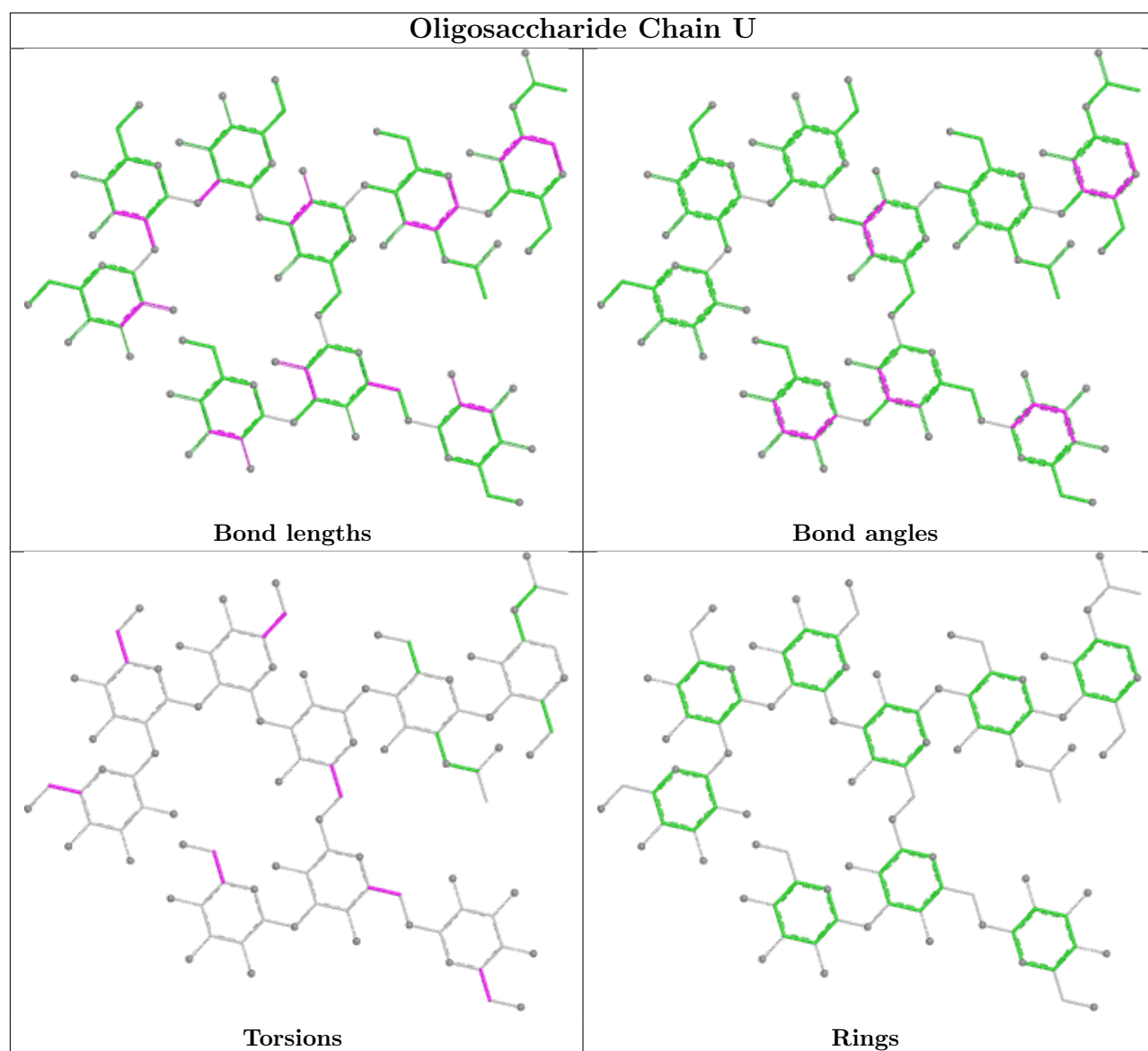


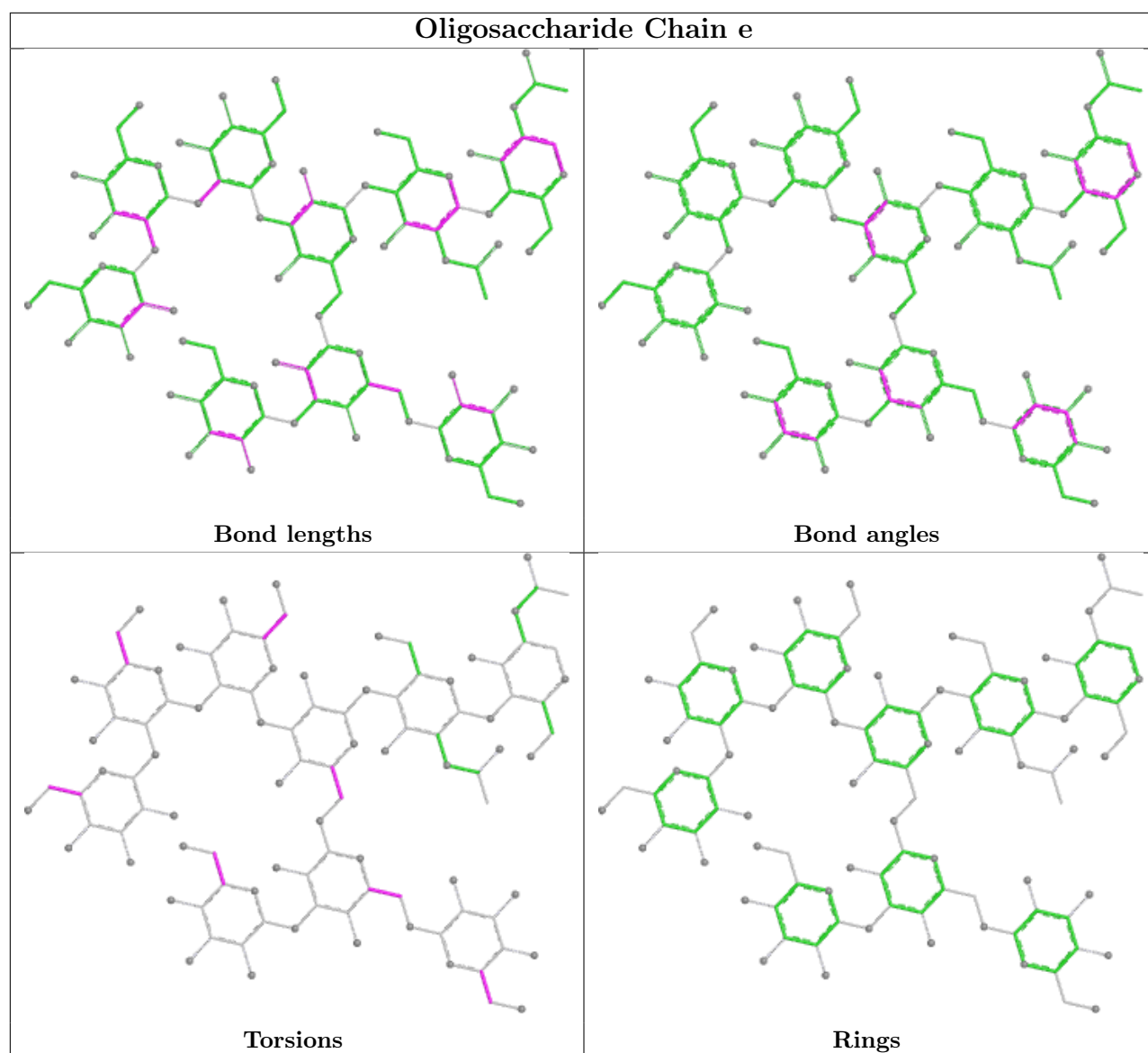


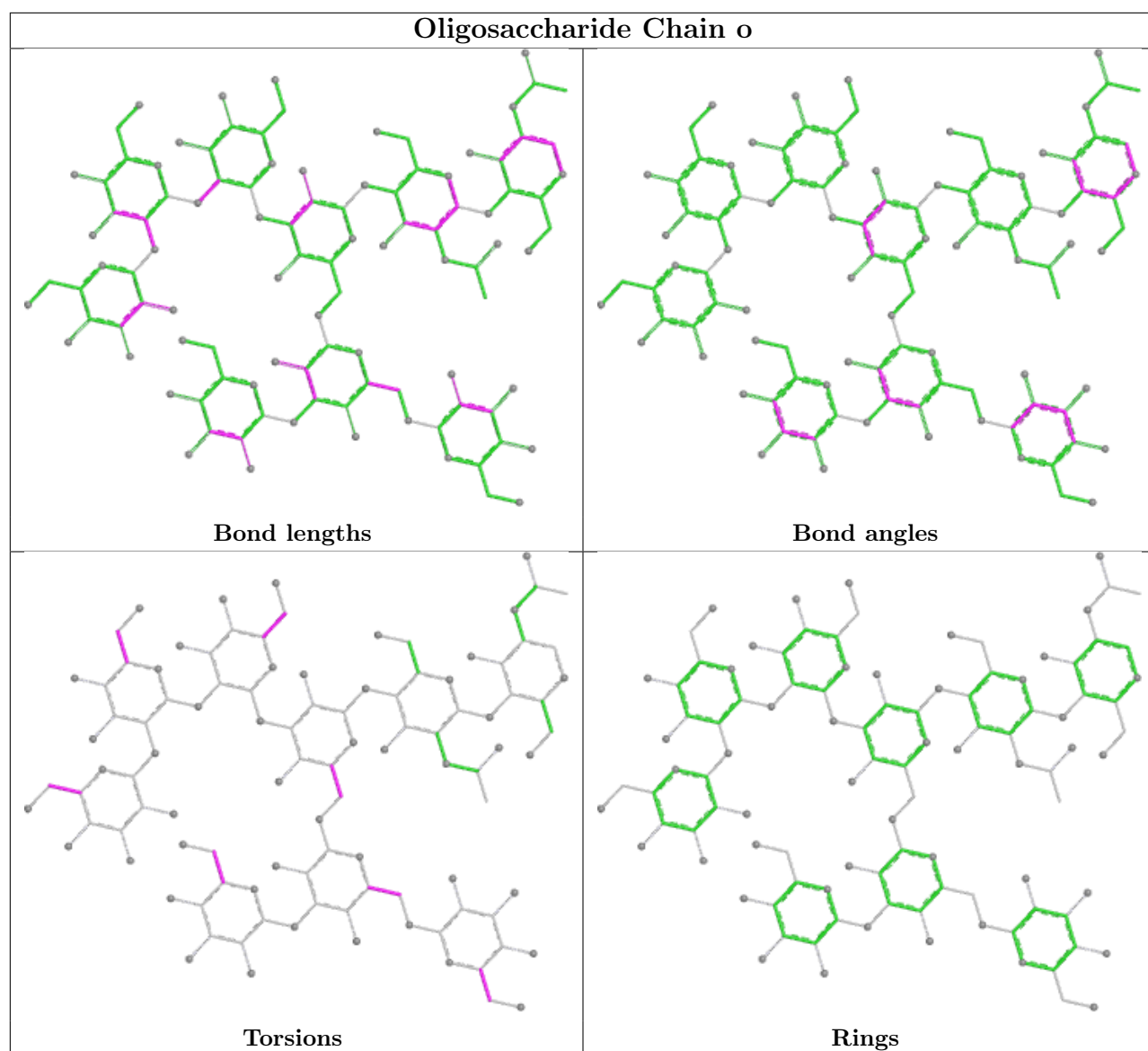


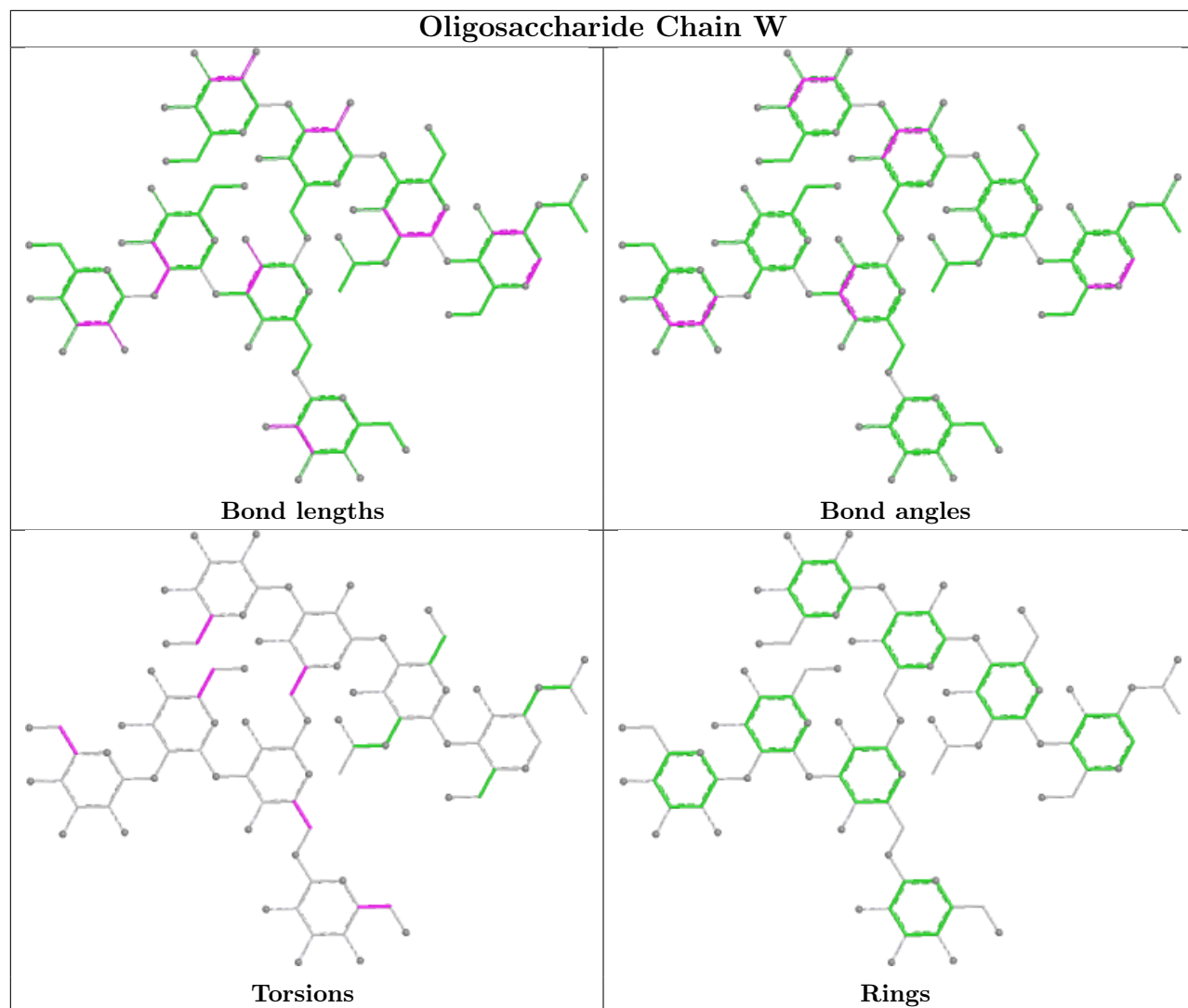


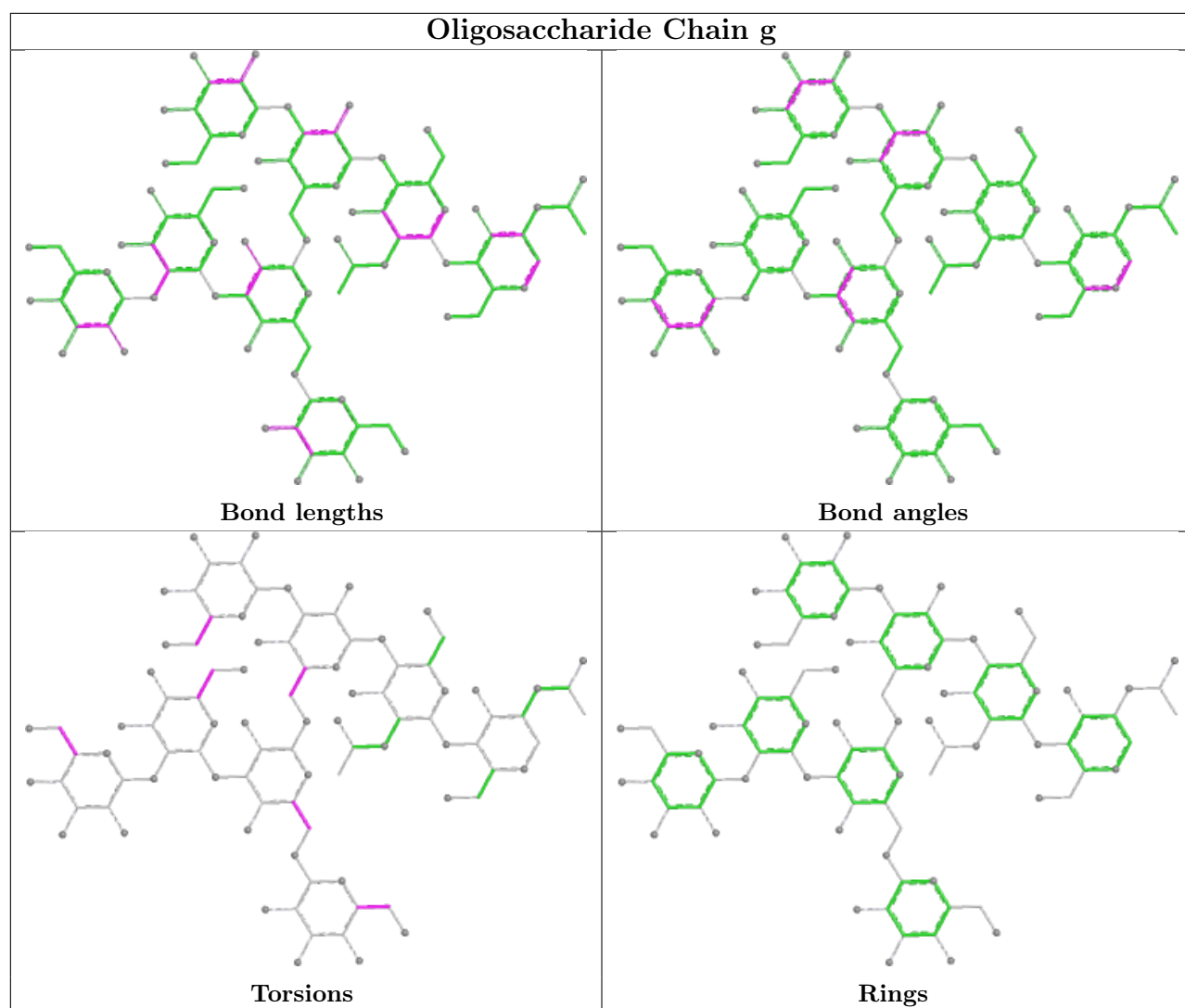


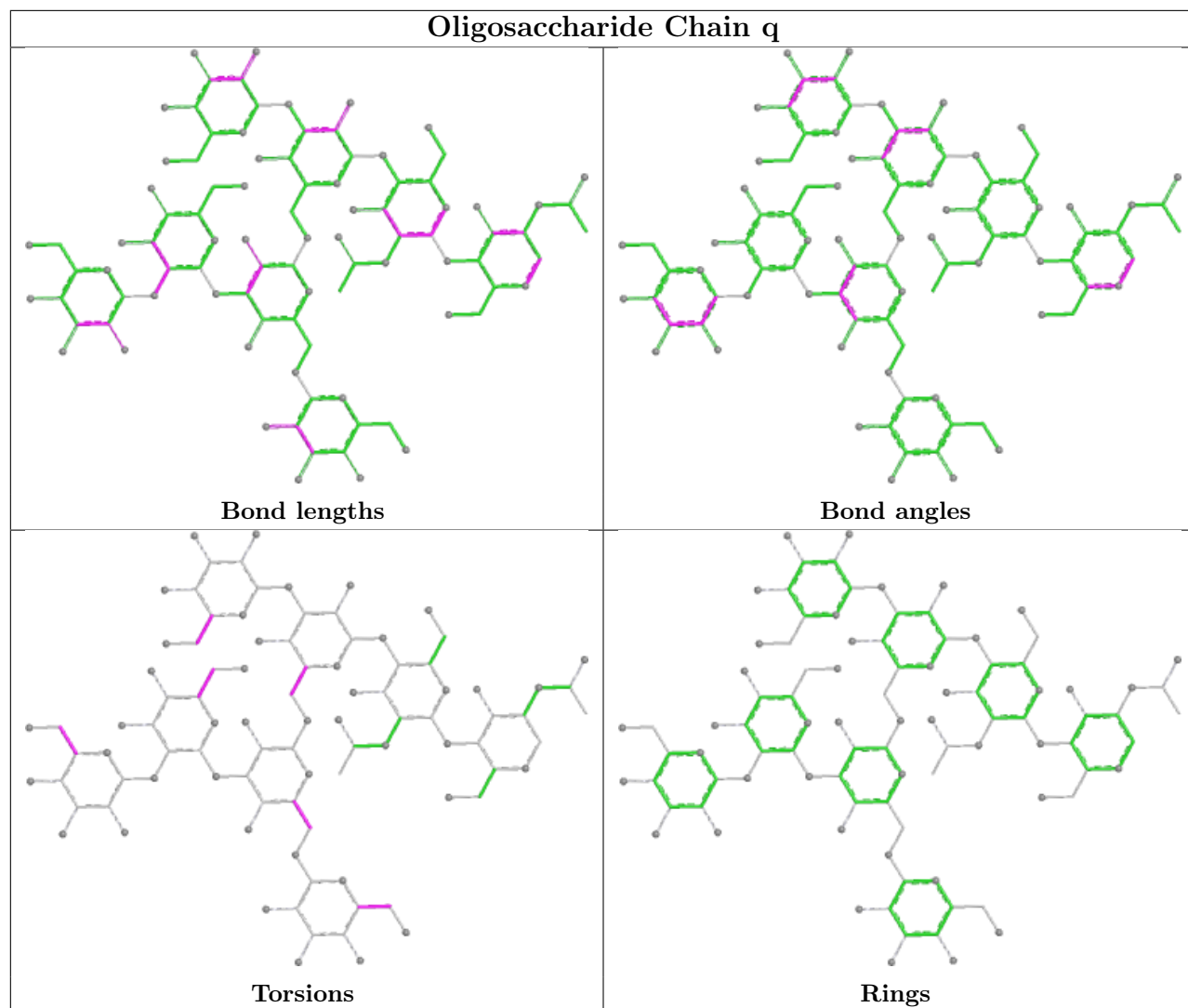


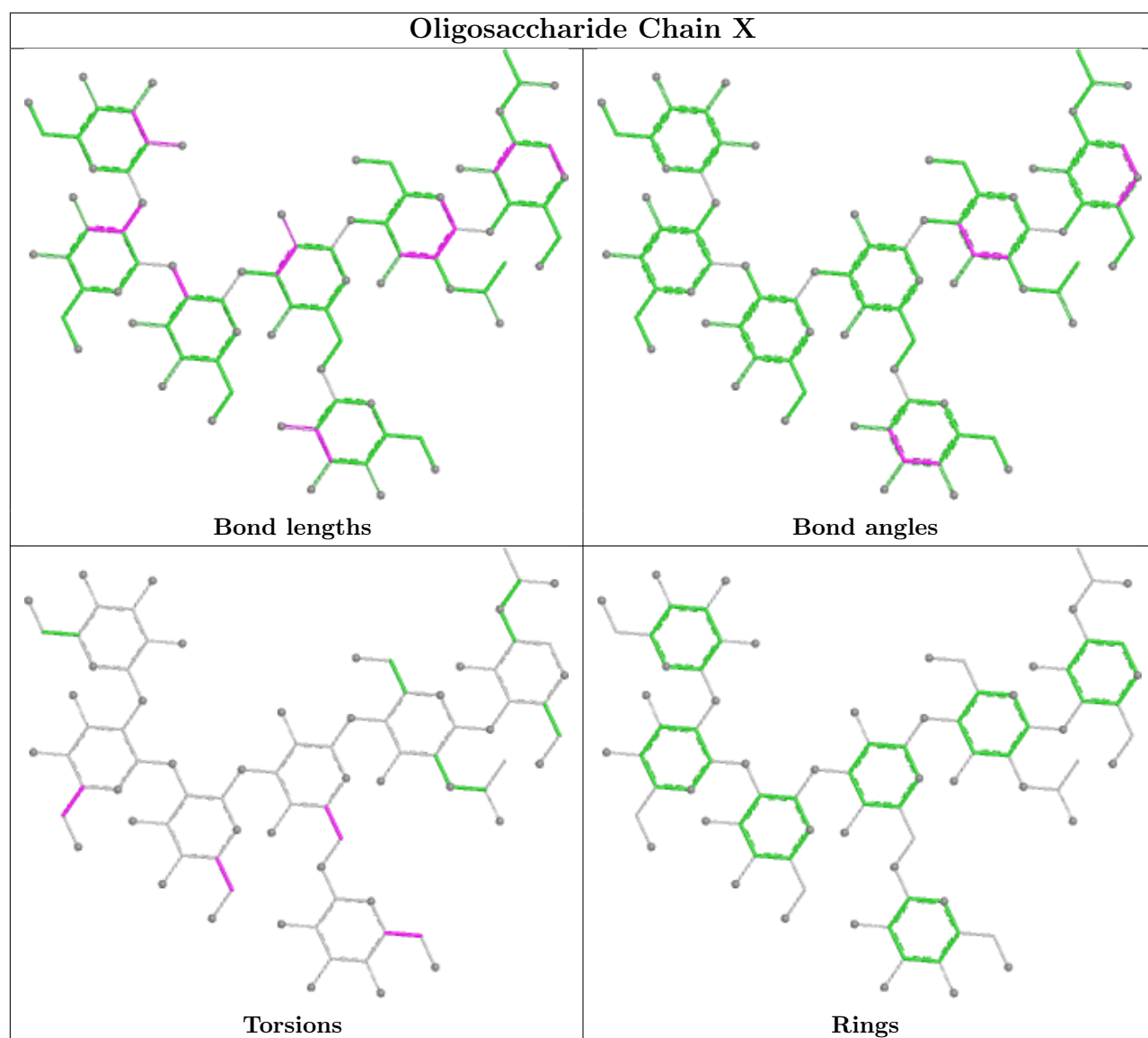


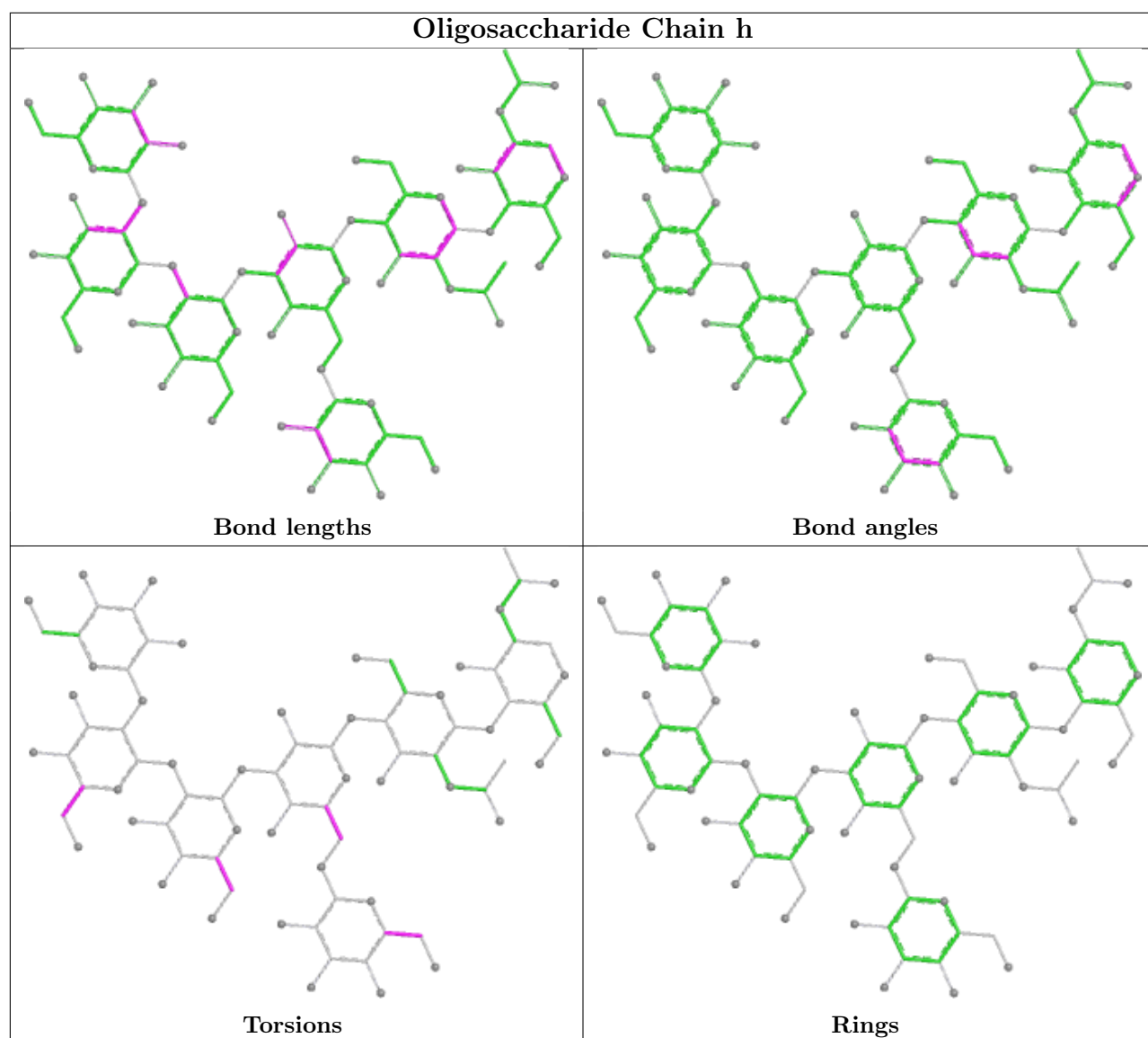


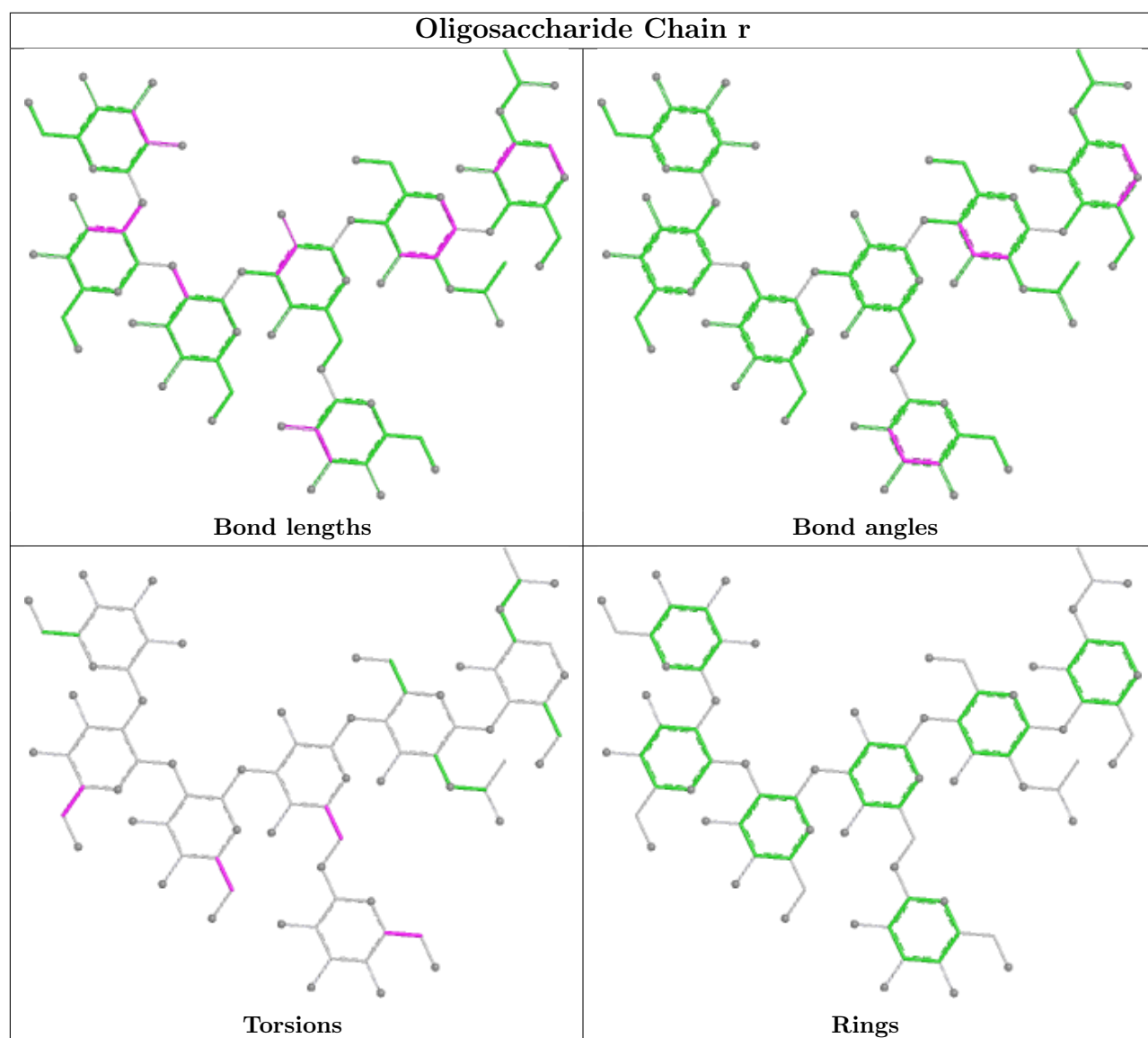


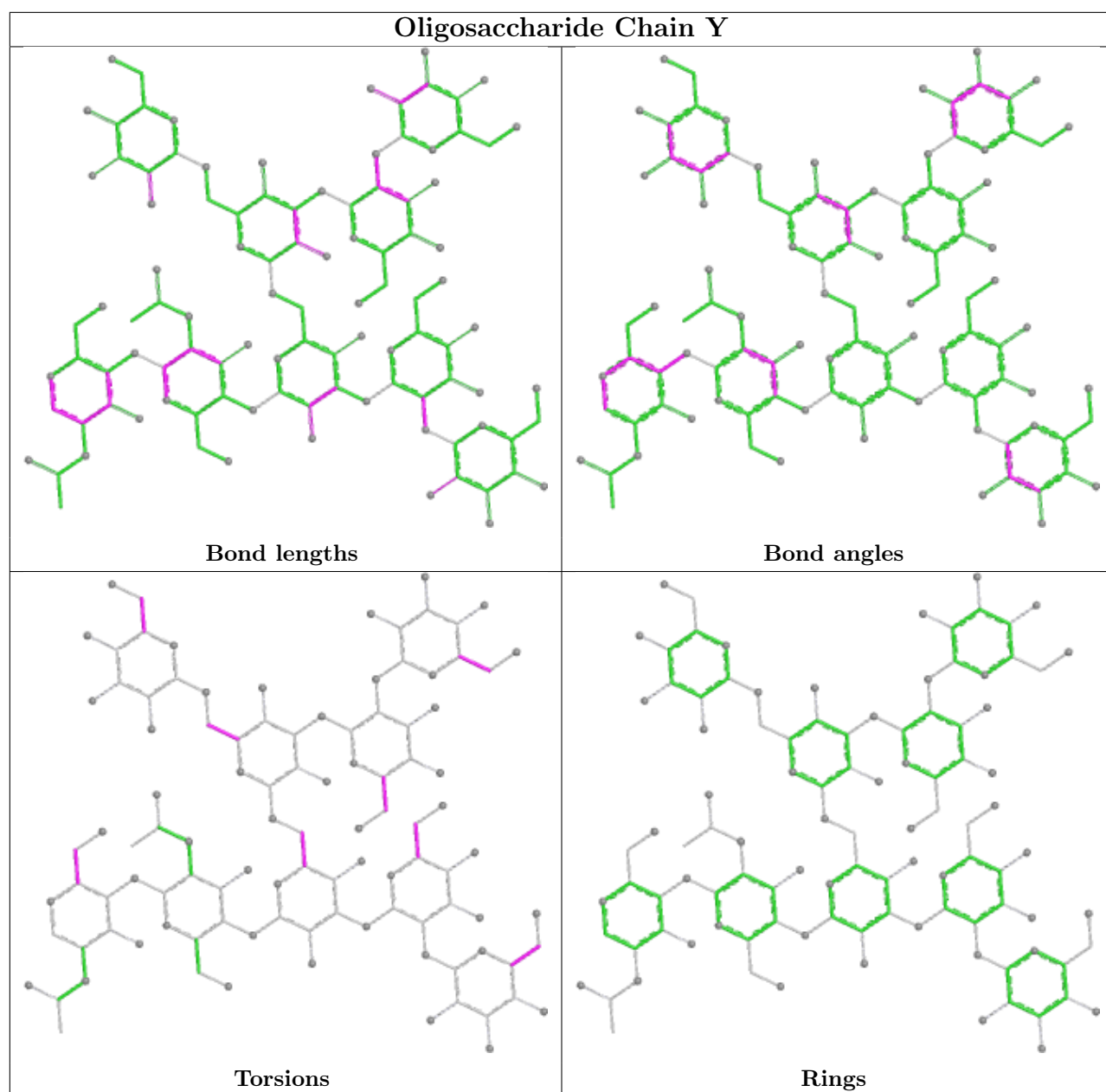


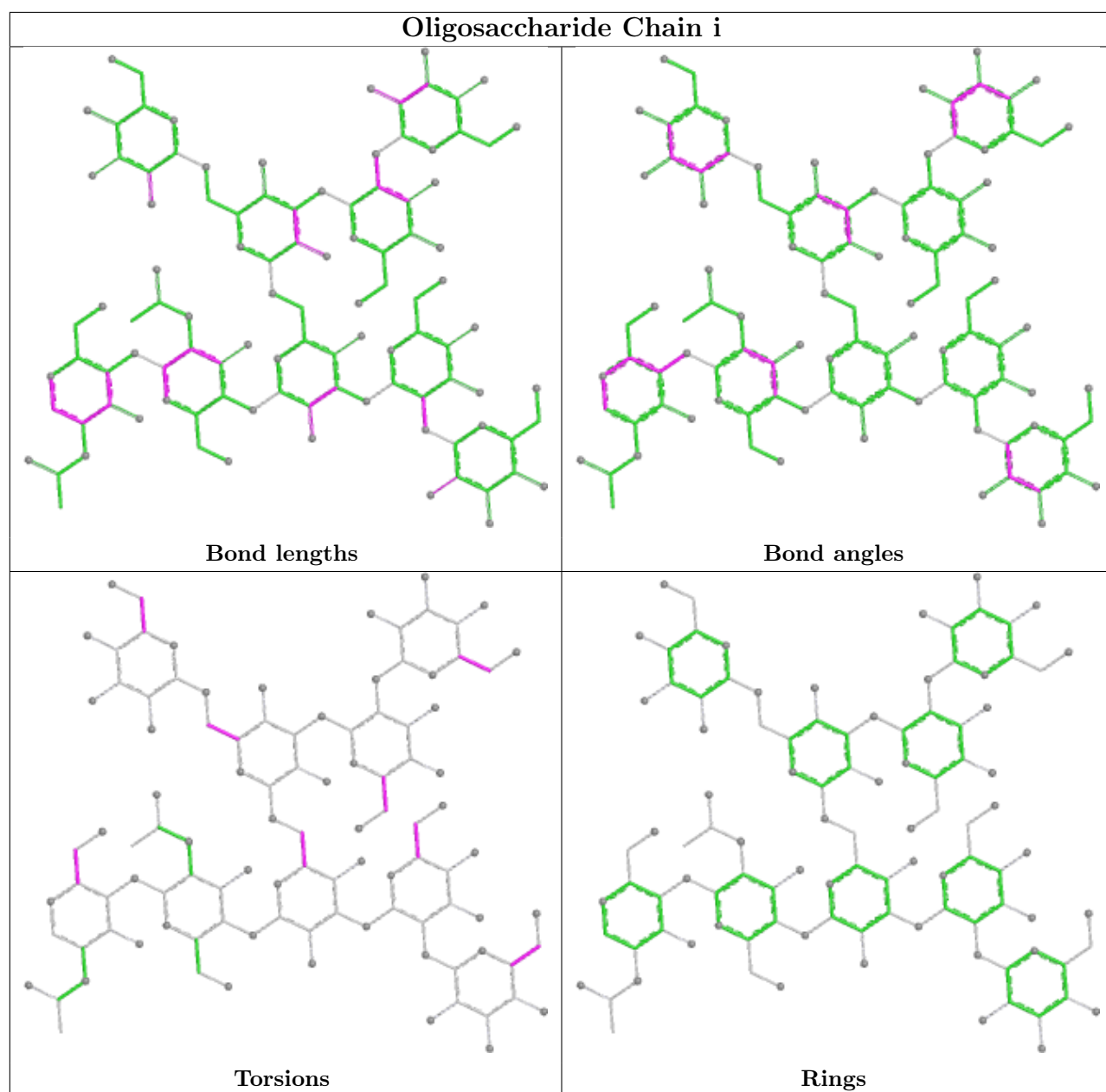


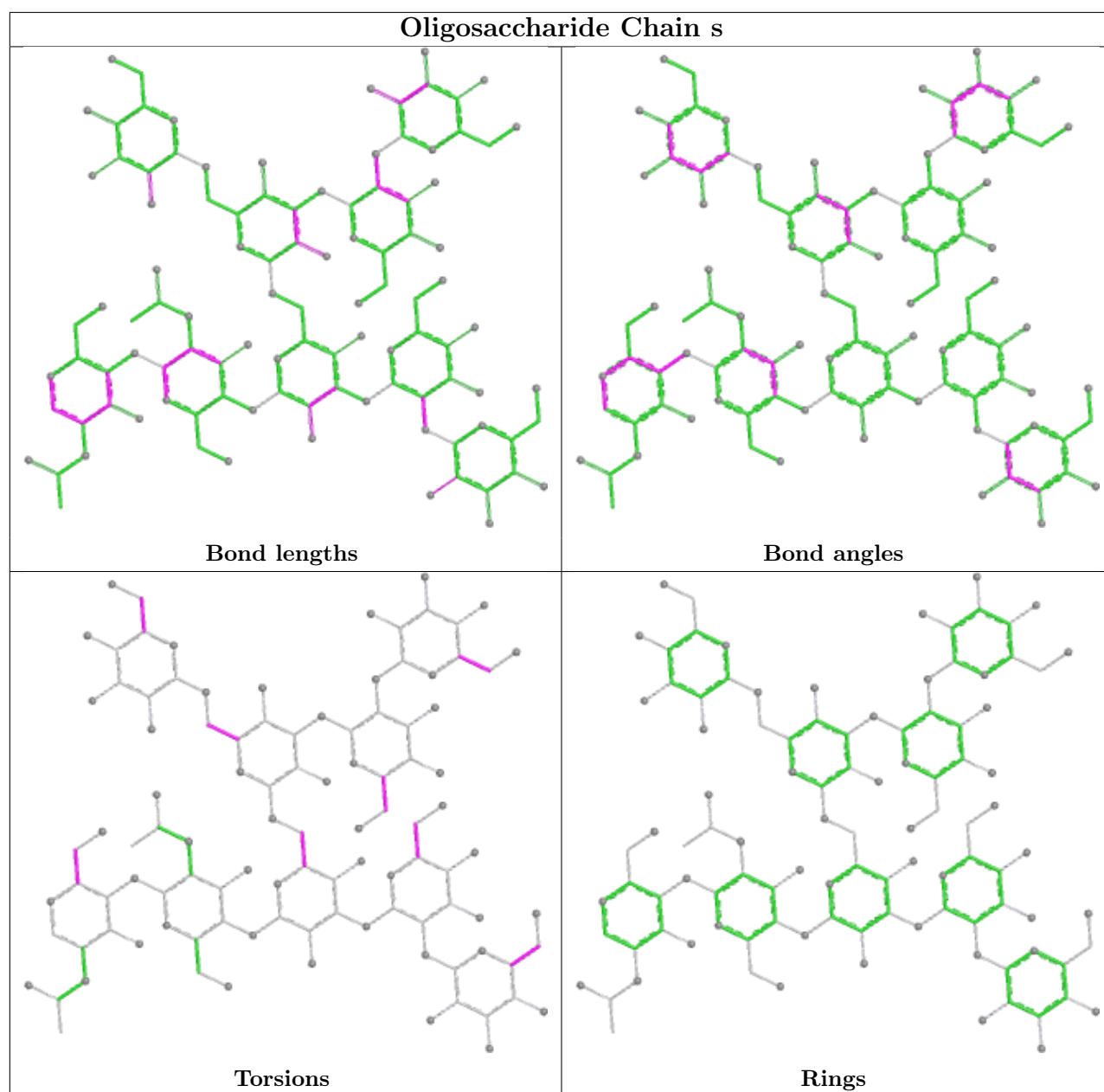


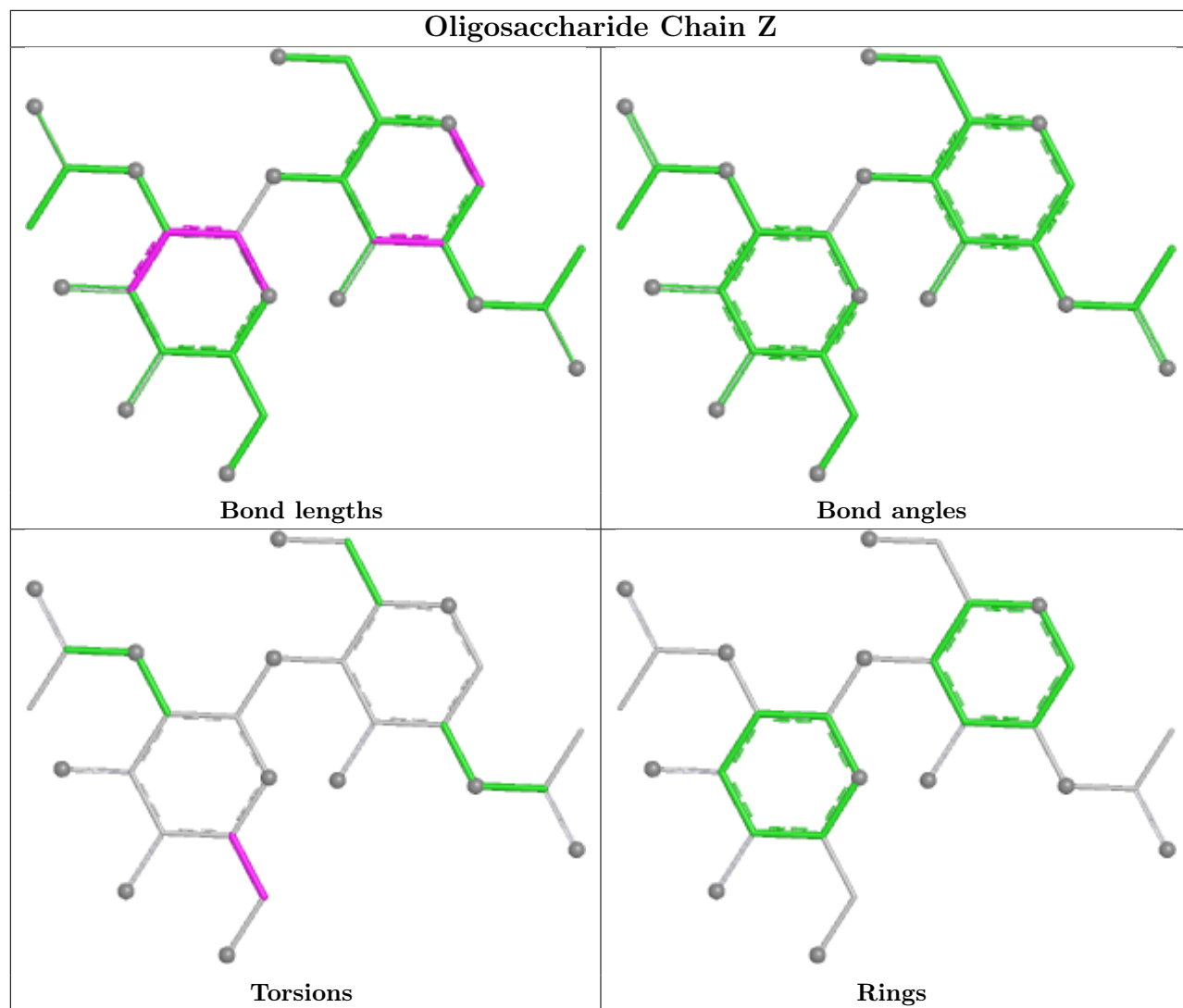


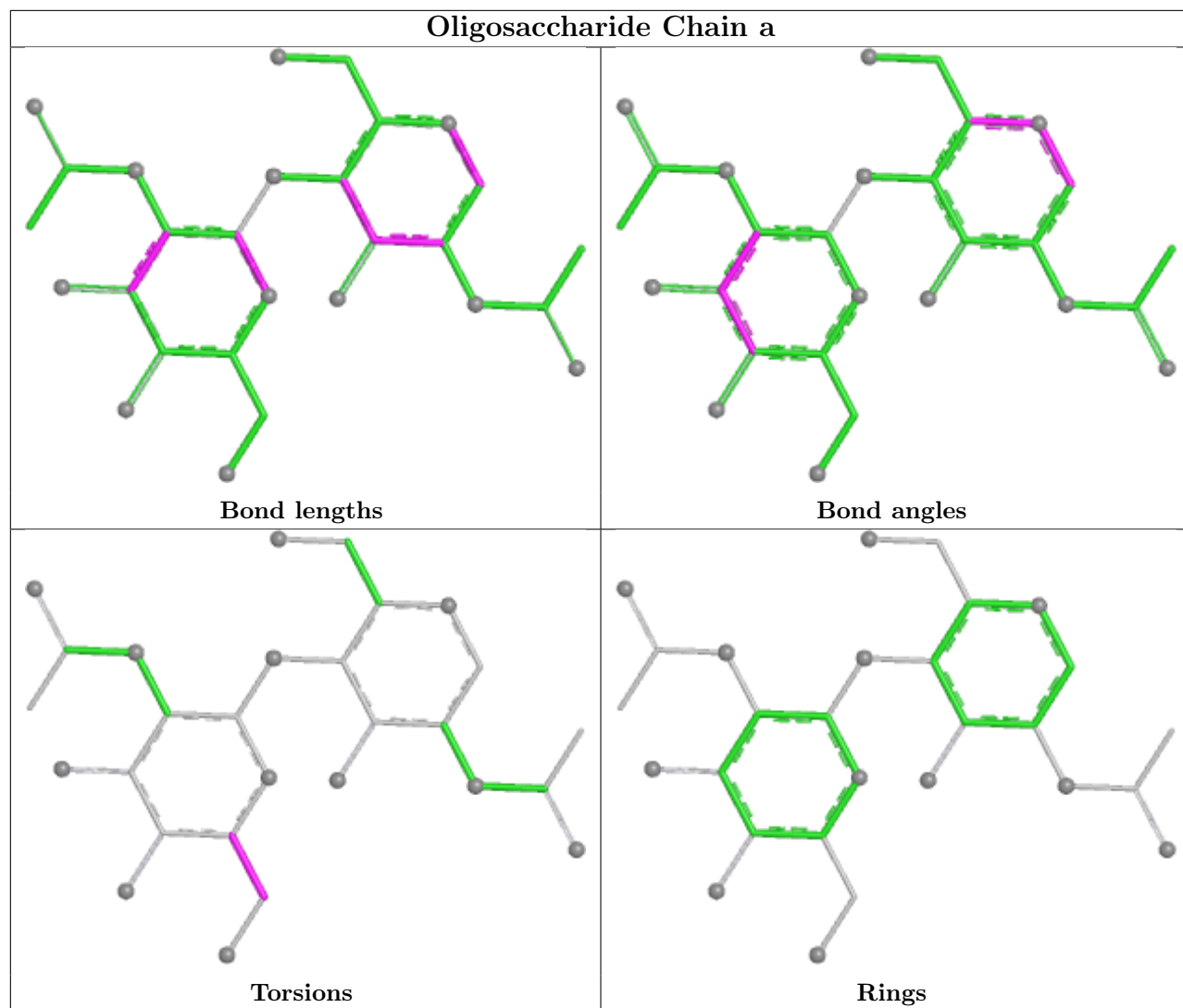


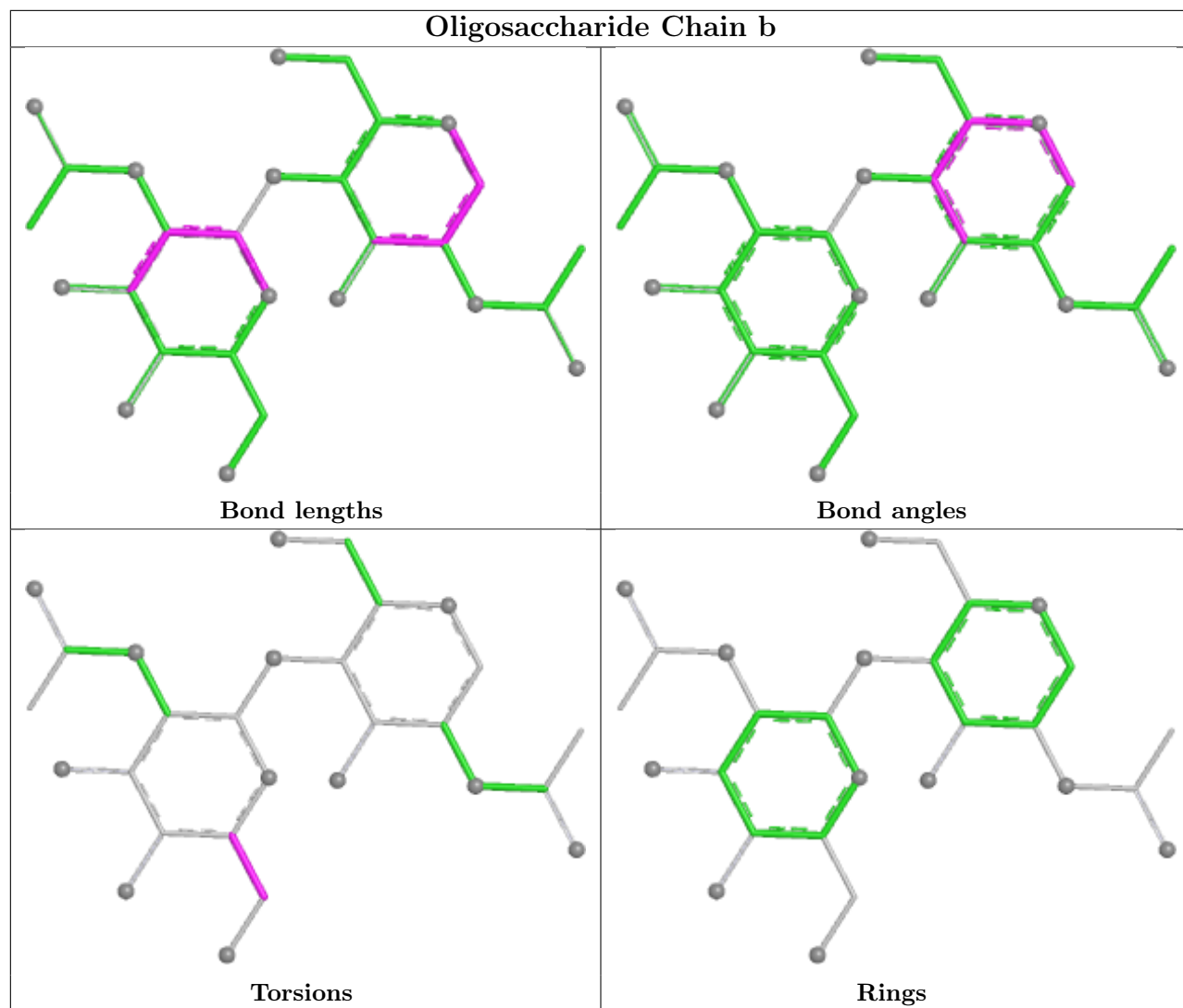


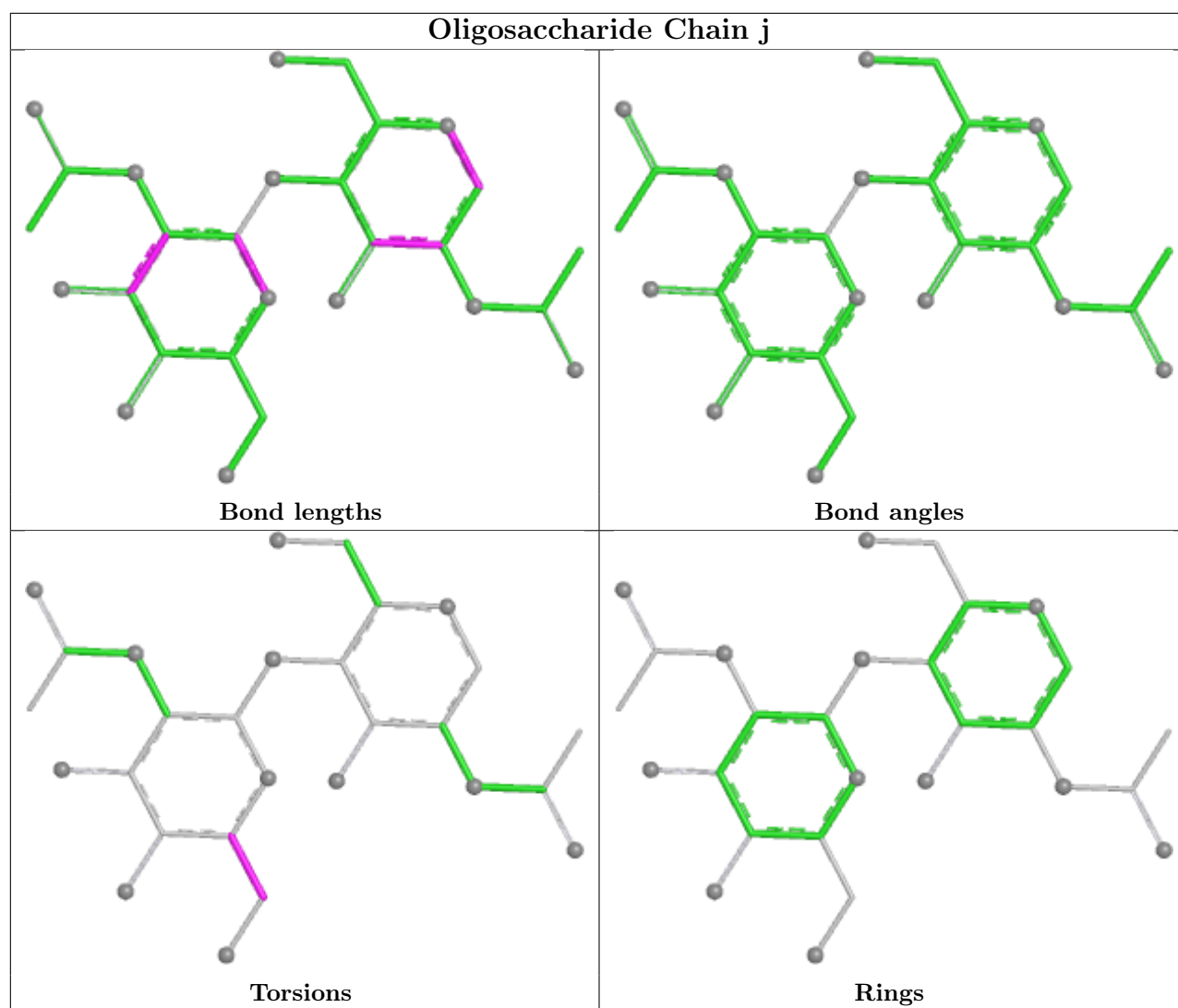


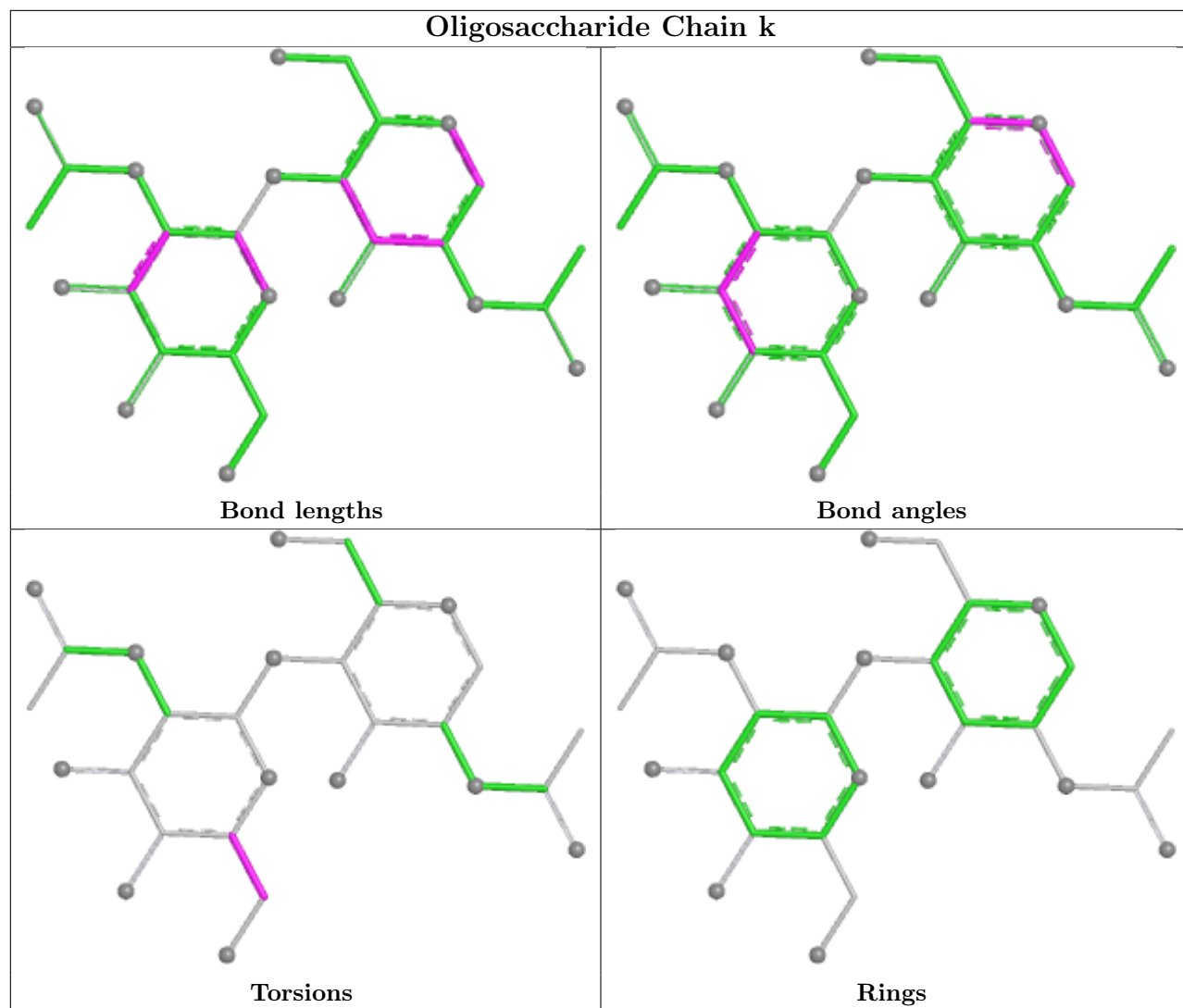


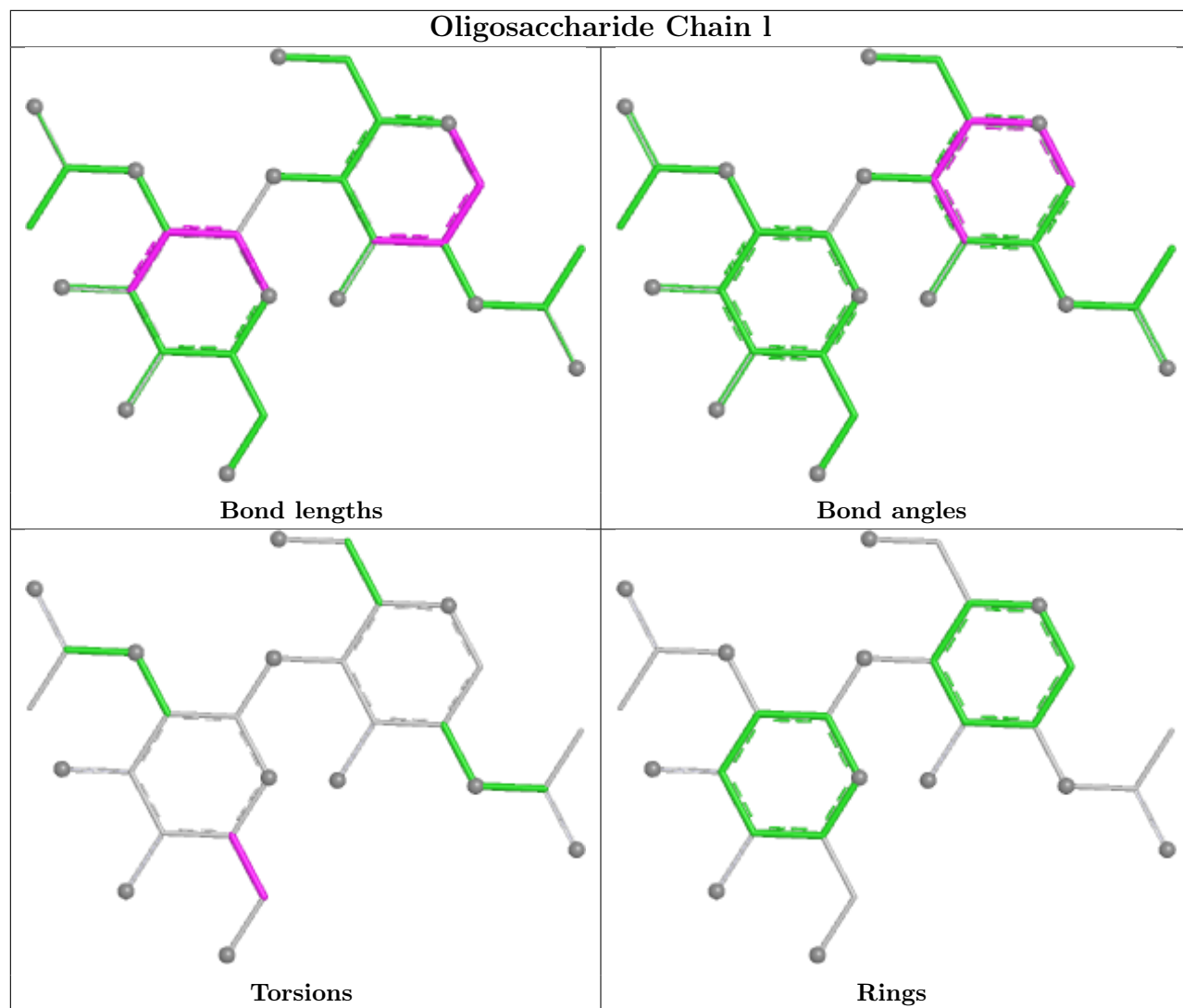


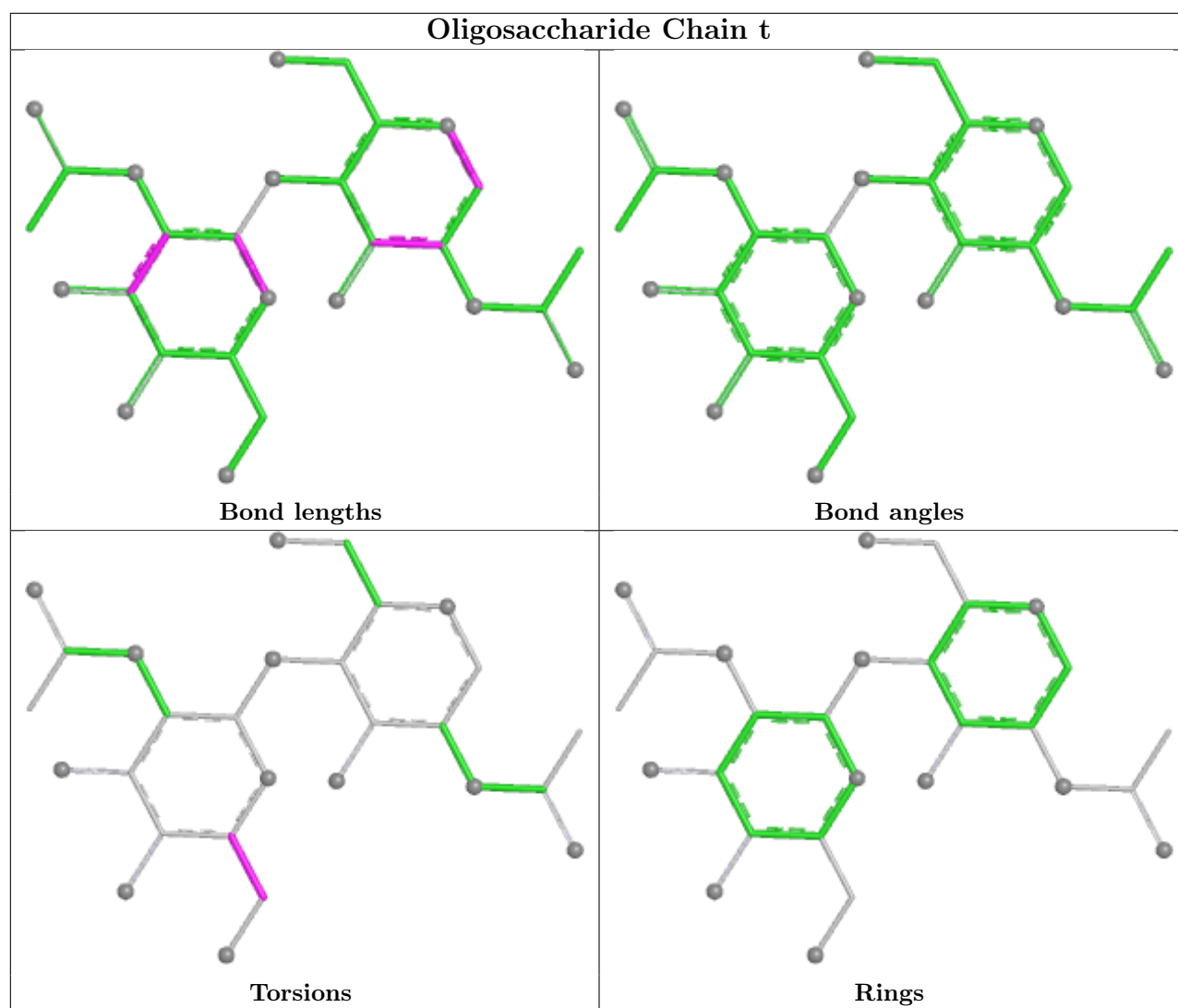


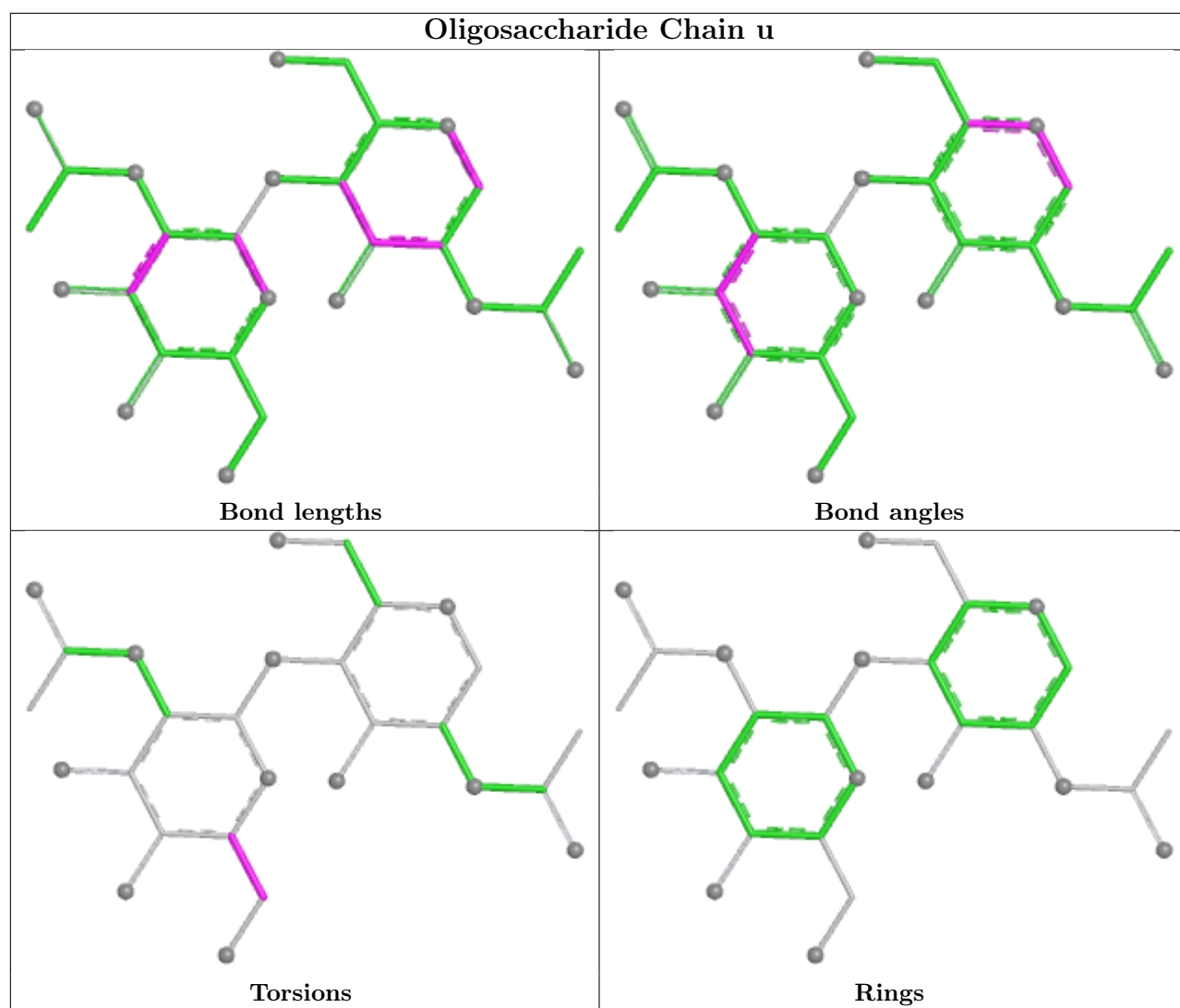


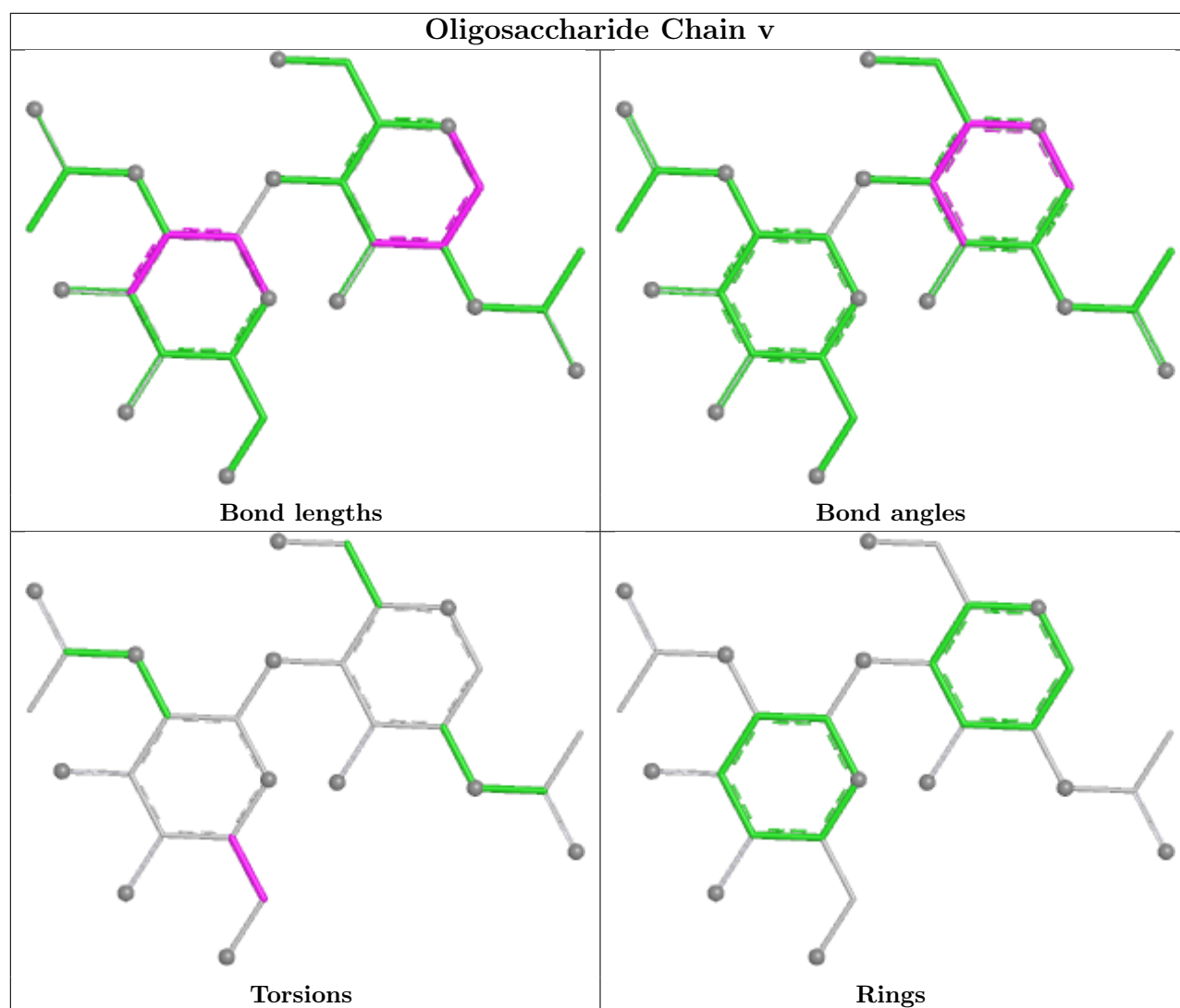












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
12	NAG	F	656	1	14,14,15	2.10	2 (14%)	17,19,21	0.63	0
12	NAG	B	702	2	14,14,15	2.06	2 (14%)	17,19,21	0.80	0
12	NAG	B	703	2	14,14,15	2.07	2 (14%)	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	A	653	1	14,14,15	1.99	2 (14%)	17,19,21	0.79	1 (5%)
12	NAG	F	653	1	14,14,15	1.99	2 (14%)	17,19,21	0.79	0
12	NAG	E	626	1	14,14,15	2.05	2 (14%)	17,19,21	0.82	0
12	NAG	E	659	1	14,14,15	2.11	2 (14%)	17,19,21	1.18	2 (11%)
12	NAG	I	701	2	14,14,15	2.07	2 (14%)	17,19,21	0.64	0
12	NAG	G	701	2	14,14,15	2.07	2 (14%)	17,19,21	0.64	0
12	NAG	E	656	1	14,14,15	2.10	2 (14%)	17,19,21	0.63	0
12	NAG	G	702	2	14,14,15	2.05	2 (14%)	17,19,21	0.80	1 (5%)
12	NAG	G	703	2	14,14,15	2.07	2 (14%)	17,19,21	0.71	0
12	NAG	I	703	2	14,14,15	2.07	2 (14%)	17,19,21	0.71	0
12	NAG	A	626	1	14,14,15	2.05	2 (14%)	17,19,21	0.82	0
12	NAG	A	659	1	14,14,15	2.11	2 (14%)	17,19,21	1.18	2 (11%)
12	NAG	F	626	1	14,14,15	2.06	2 (14%)	17,19,21	0.82	0
12	NAG	F	659	1	14,14,15	2.11	2 (14%)	17,19,21	1.18	2 (11%)
12	NAG	I	702	2	14,14,15	2.07	2 (14%)	17,19,21	0.80	0
12	NAG	A	656	1	14,14,15	2.10	2 (14%)	17,19,21	0.63	0
12	NAG	E	653	1	14,14,15	1.99	2 (14%)	17,19,21	0.79	0
12	NAG	B	701	2	14,14,15	2.07	2 (14%)	17,19,21	0.64	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
12	NAG	F	656	1	-	1/6/23/26	0/1/1/1
12	NAG	B	702	2	-	2/6/23/26	0/1/1/1
12	NAG	B	703	2	-	1/6/23/26	0/1/1/1
12	NAG	A	653	1	-	1/6/23/26	0/1/1/1
12	NAG	F	653	1	-	1/6/23/26	0/1/1/1
12	NAG	E	626	1	-	1/6/23/26	0/1/1/1
12	NAG	E	659	1	-	2/6/23/26	0/1/1/1
12	NAG	I	701	2	-	1/6/23/26	0/1/1/1
12	NAG	G	701	2	-	1/6/23/26	0/1/1/1
12	NAG	E	656	1	-	1/6/23/26	0/1/1/1
12	NAG	G	702	2	-	2/6/23/26	0/1/1/1
12	NAG	G	703	2	-	1/6/23/26	0/1/1/1
12	NAG	I	703	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	626	1	-	1/6/23/26	0/1/1/1
12	NAG	A	659	1	-	2/6/23/26	0/1/1/1
12	NAG	F	626	1	-	1/6/23/26	0/1/1/1
12	NAG	F	659	1	-	2/6/23/26	0/1/1/1
12	NAG	I	702	2	-	2/6/23/26	0/1/1/1
12	NAG	A	656	1	-	1/6/23/26	0/1/1/1
12	NAG	E	653	1	-	1/6/23/26	0/1/1/1
12	NAG	B	701	2	-	1/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	659	NAG	O5-C1	6.83	1.55	1.43
12	A	659	NAG	O5-C1	6.82	1.55	1.43
12	E	659	NAG	O5-C1	6.80	1.55	1.43
12	I	703	NAG	O5-C1	6.74	1.55	1.43
12	G	701	NAG	O5-C1	6.72	1.55	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	659	NAG	C4-C3-C2	-3.22	106.30	111.02
12	E	659	NAG	C4-C3-C2	-3.21	106.31	111.02
12	F	659	NAG	C4-C3-C2	-3.21	106.31	111.02
12	A	659	NAG	O5-C1-C2	-2.29	107.74	111.29
12	E	659	NAG	O5-C1-C2	-2.27	107.77	111.29

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	659	NAG	O5-C5-C6-O6
12	E	659	NAG	O5-C5-C6-O6
12	F	659	NAG	O5-C5-C6-O6
12	B	702	NAG	O5-C5-C6-O6
12	G	702	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	701	NAG	1	0
12	G	701	NAG	1	0
12	A	659	NAG	1	0
12	B	701	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.

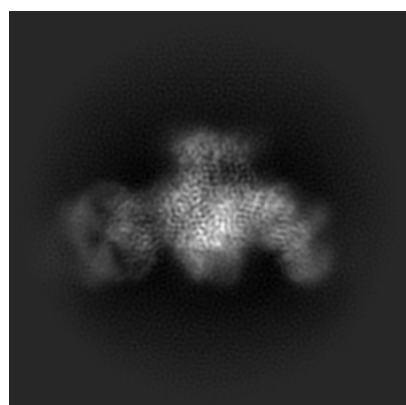
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20224. These allow visual inspection of the internal detail of the map and identification of artifacts.

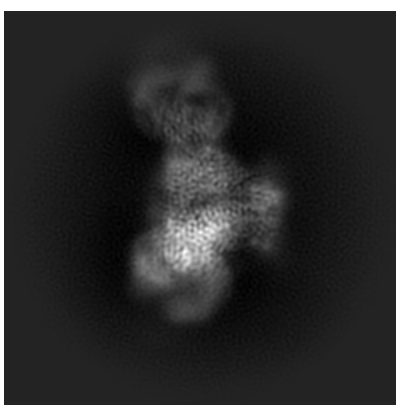
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

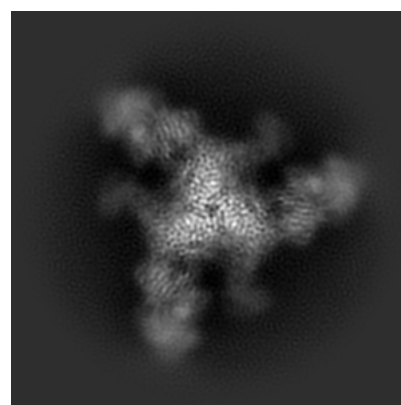
6.1.1 Primary map



X



Y

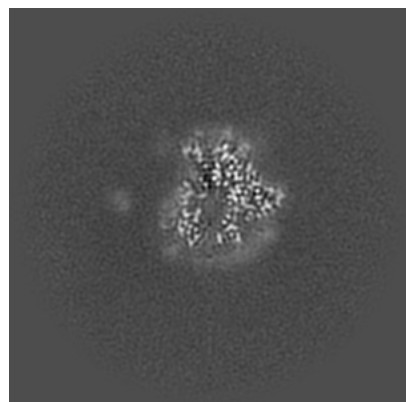


Z

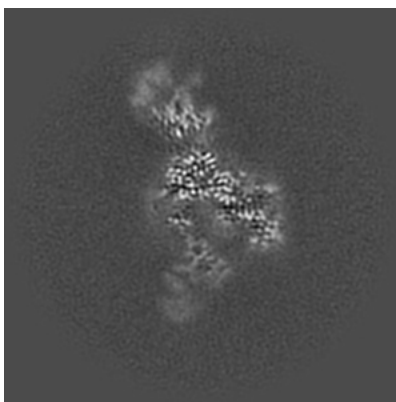
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

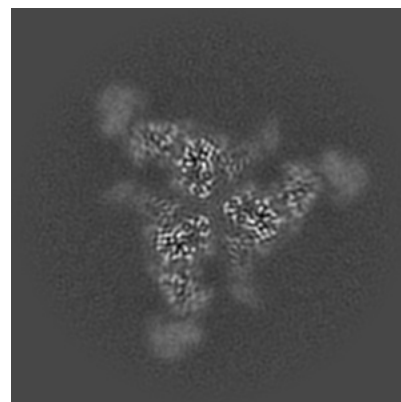
6.2.1 Primary map



X Index: 128



Y Index: 128

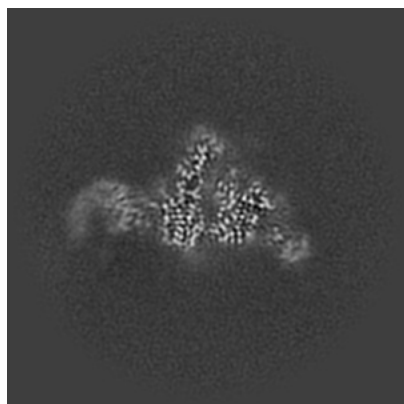


Z Index: 128

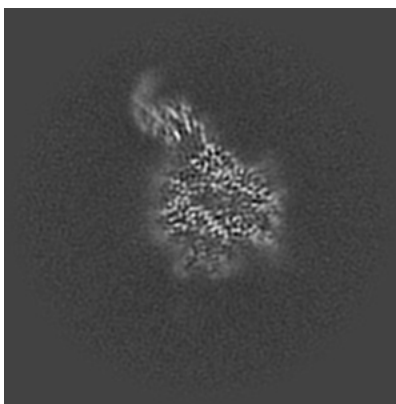
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

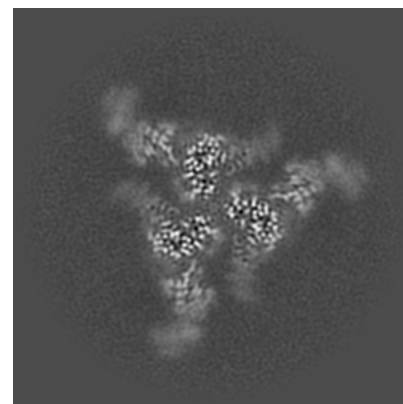
6.3.1 Primary map



X Index: 116



Y Index: 120

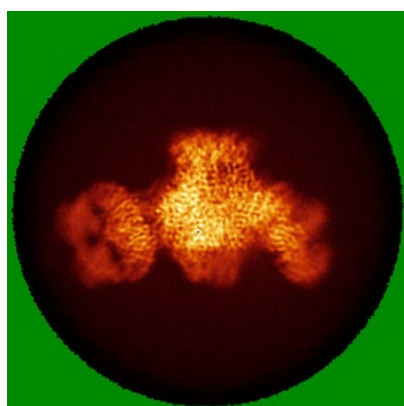


Z Index: 131

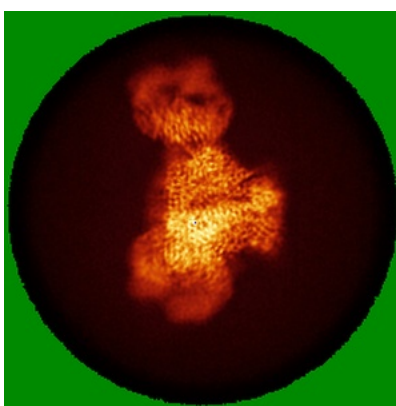
The images above show the largest variance slices of the map in three orthogonal directions.

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

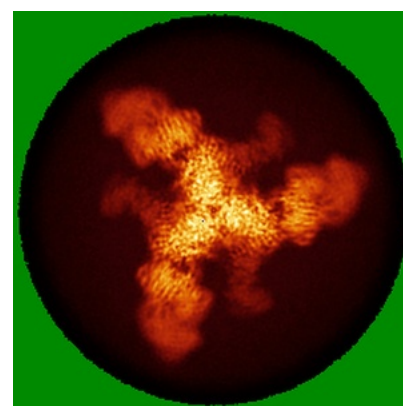
6.4.1 Primary map



X



Y

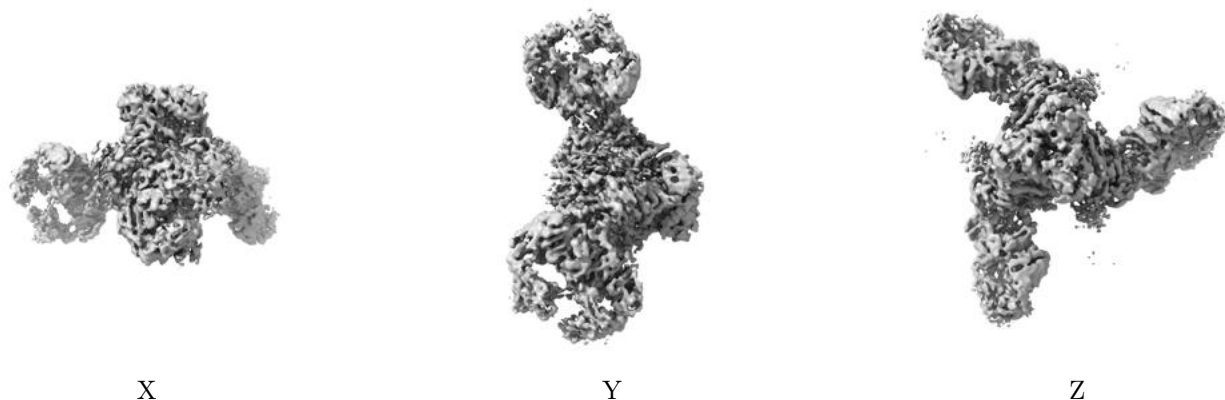


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

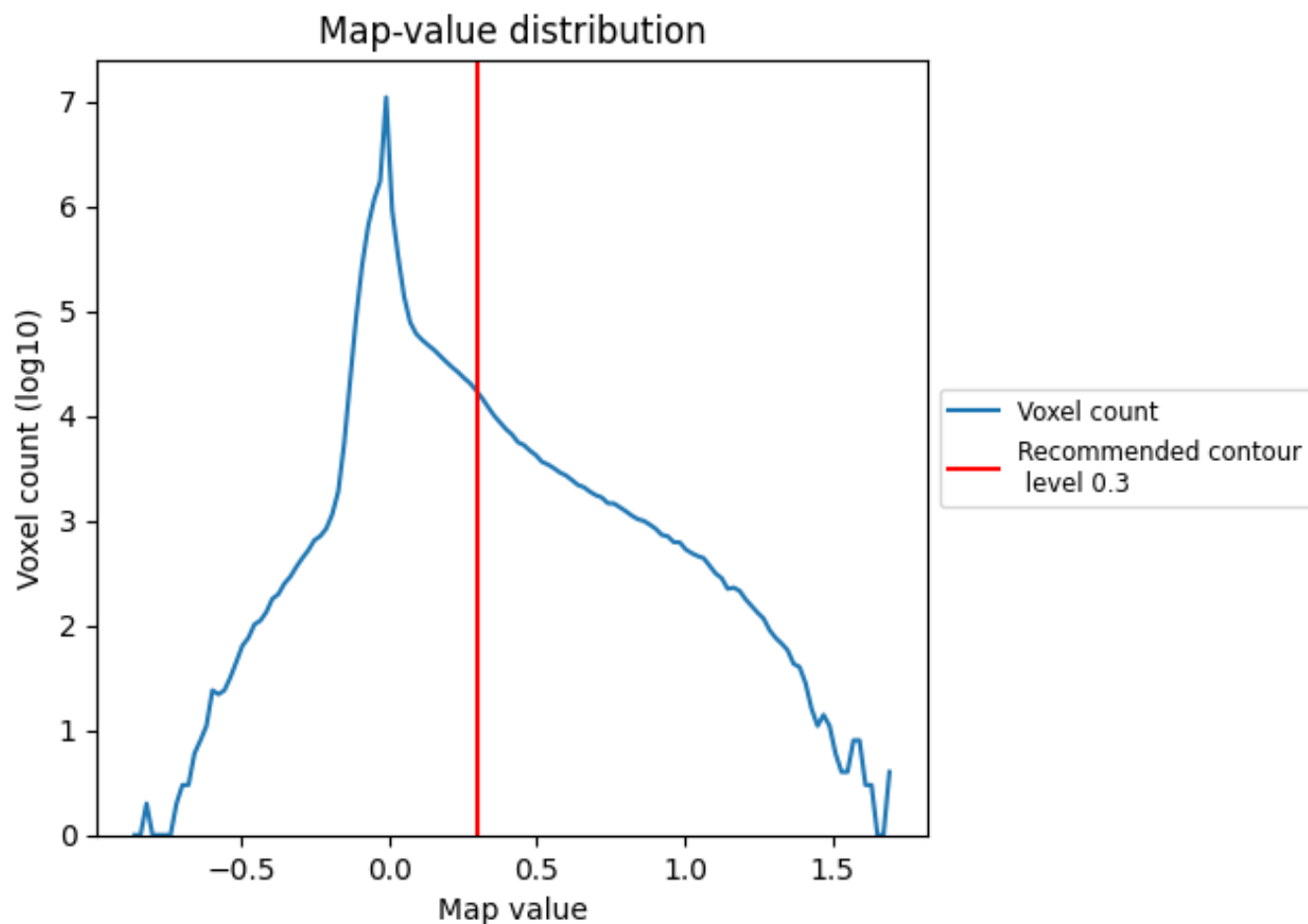
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

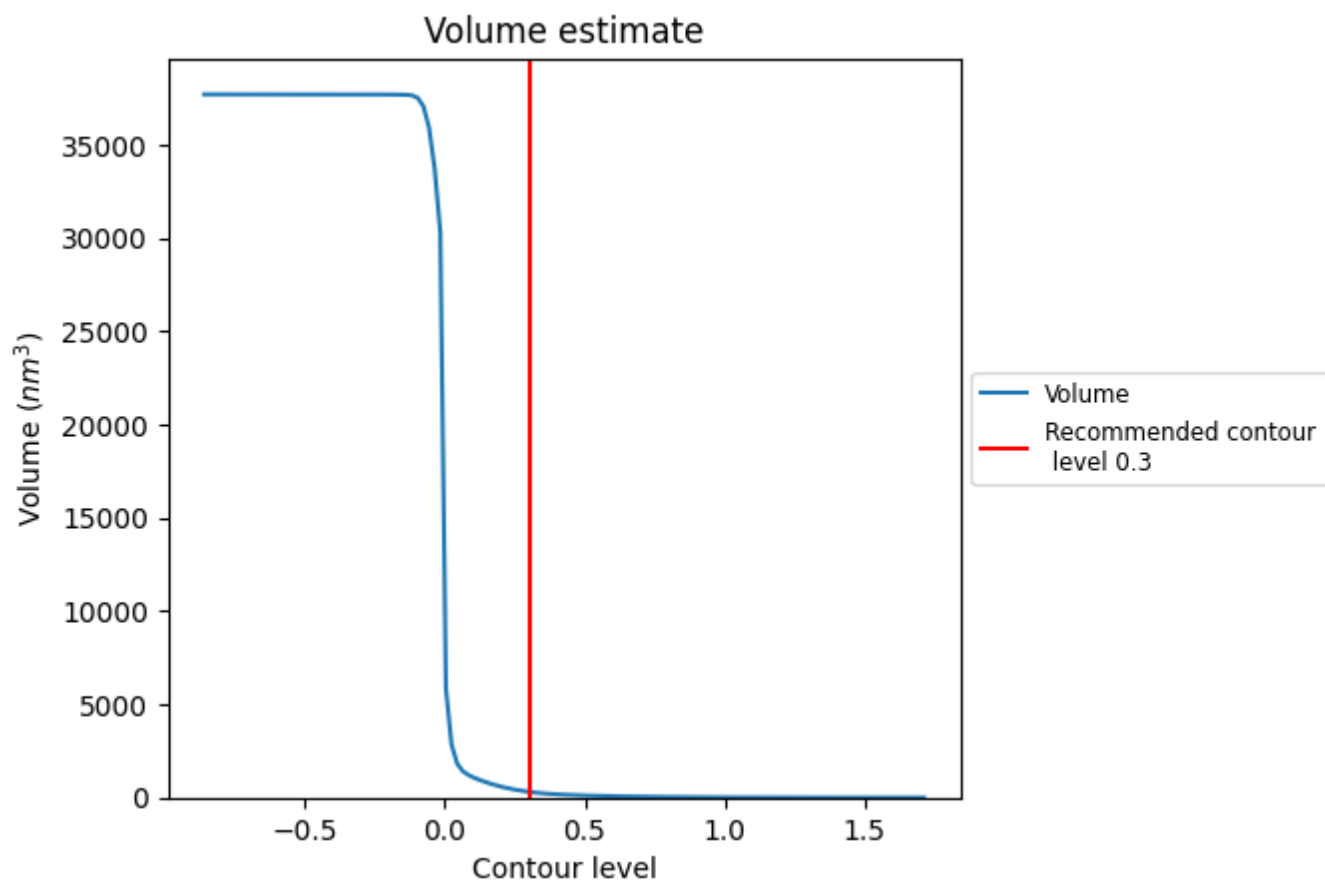
This section contains the results of statistical analysis of the map.

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.

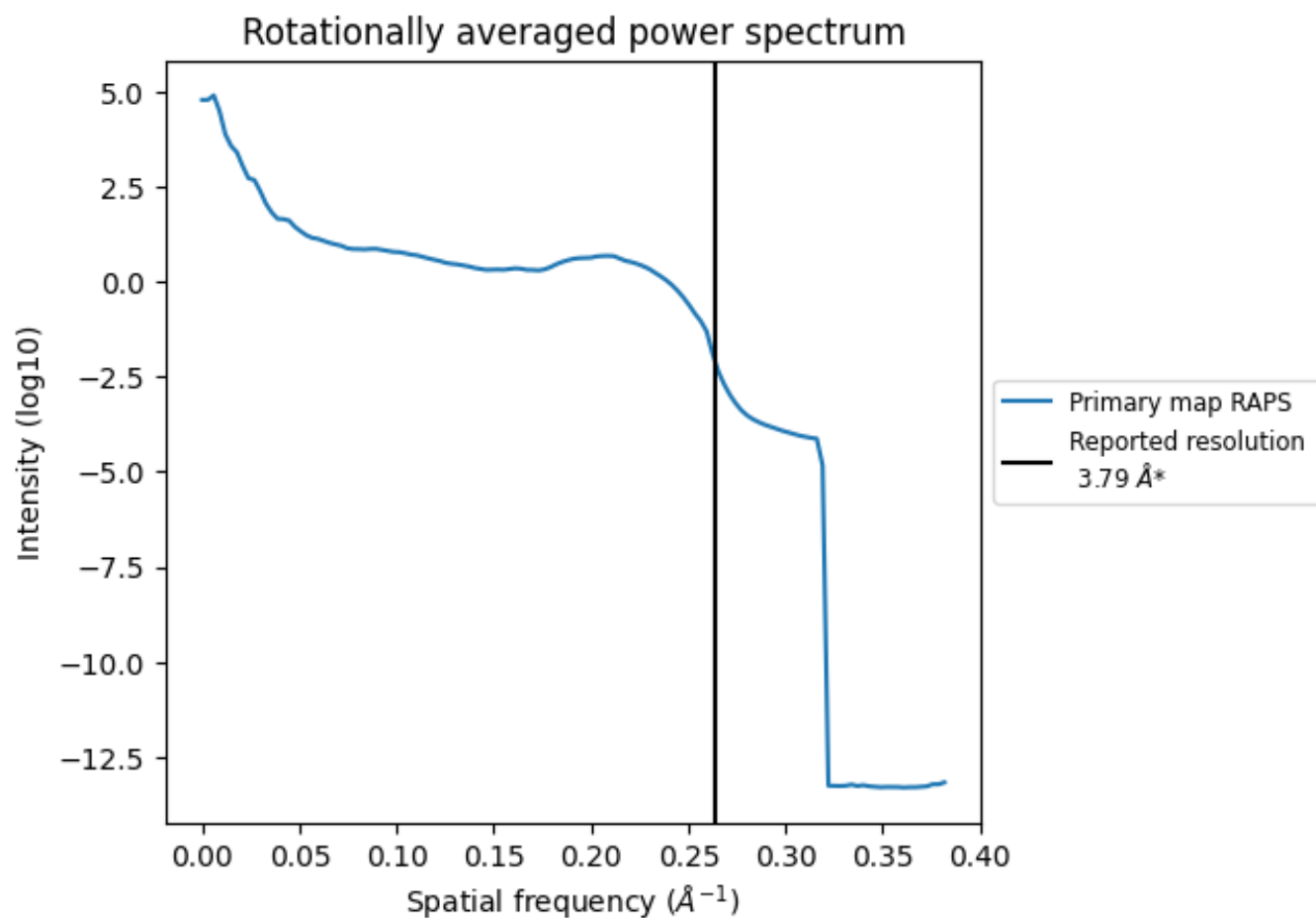
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm^3 ; this corresponds to an approximate mass of 278 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 0.264 Å⁻¹

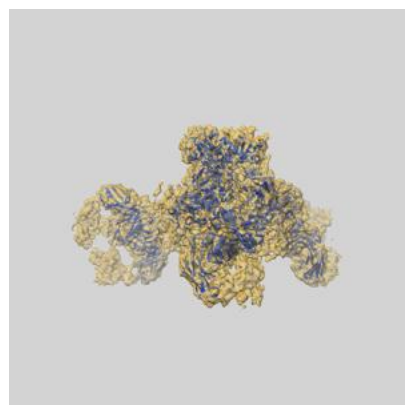
8 Fourier-Shell correlation

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

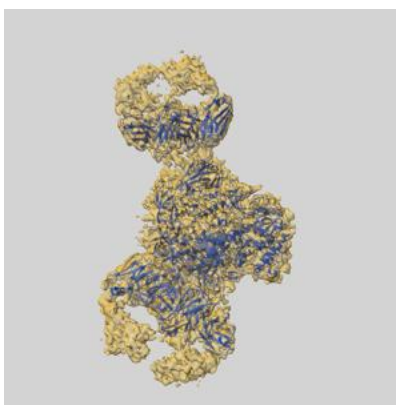
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20224 and PDB model 6OZC. Per-residue inclusion information can be found in section 3 on page 12.

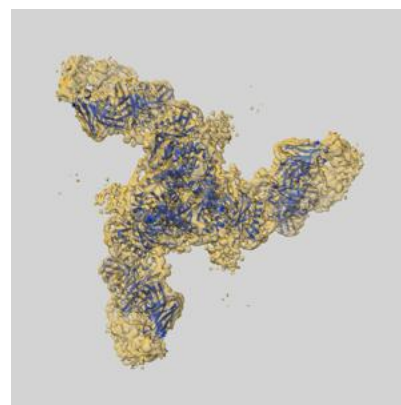
9.1 Map-model overlay [i](#)



X



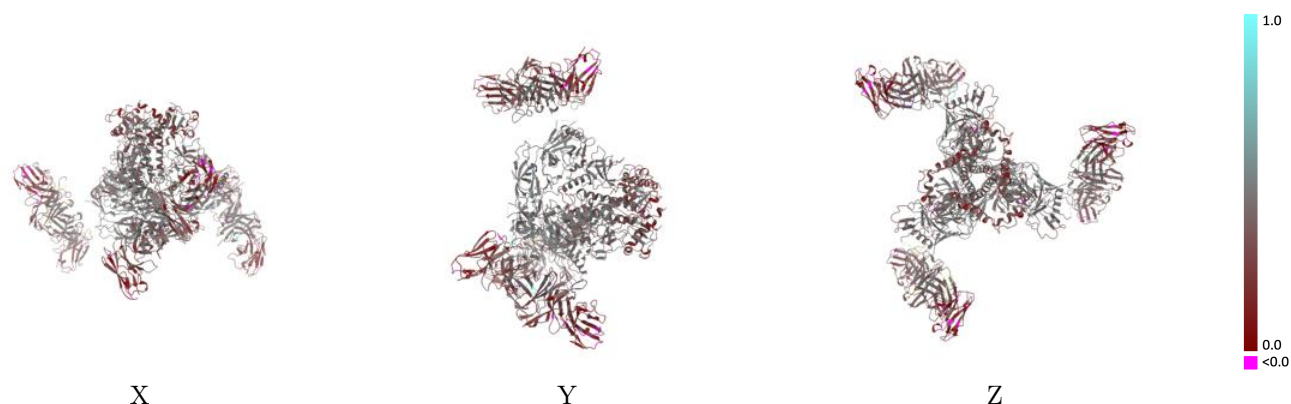
Y



Z

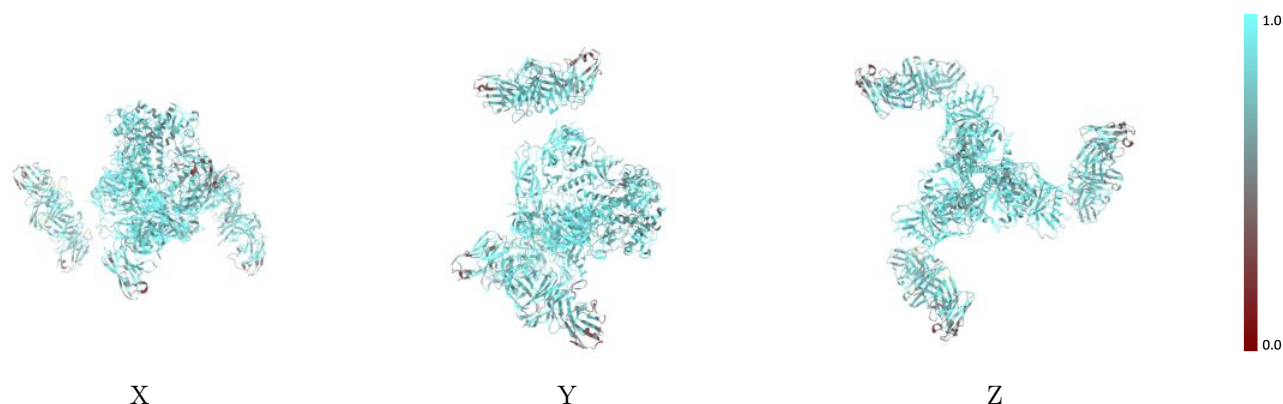
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



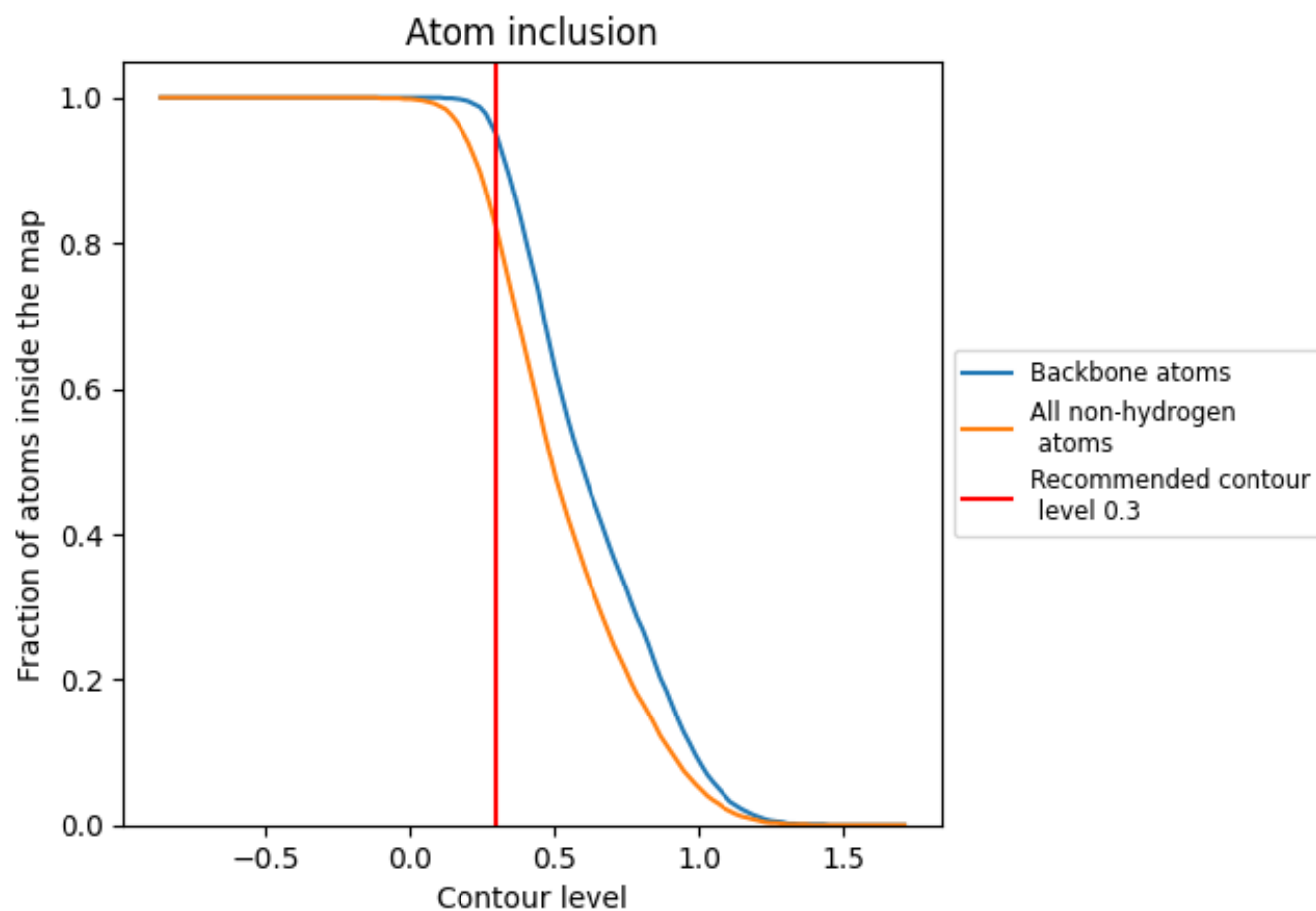
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).







































































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ





























The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8220	 0.3720
A	 0.8950	 0.4430
B	 0.7810	 0.3280
C	 0.8180	 0.3440
D	 0.6460	 0.2160
E	 0.8950	 0.4430
F	 0.8950	 0.4430
G	 0.7790	 0.3320
H	 0.8410	 0.3740
I	 0.7830	 0.3320
J	 0.8180	 0.3430
K	 0.8170	 0.3440
L	 0.7260	 0.2640
M	 0.6500	 0.2190
N	 0.6420	 0.2210
O	 0.8380	 0.3730
P	 0.8370	 0.3720
Q	 0.7220	 0.2630
R	 0.7210	 0.2630
S	 0.8330	 0.4280
T	 0.8200	 0.4390
U	 0.8480	 0.4260
V	 0.7700	 0.4240
W	 0.9040	 0.4550
X	 0.8430	 0.4030
Y	 0.7620	 0.3890
Z	 0.7500	 0.3870
a	 0.5360	 0.3960
b	 0.7500	 0.3800
c	 0.8470	 0.4380
d	 0.8360	 0.4370
e	 0.8380	 0.4210
f	 0.7540	 0.4230
g	 0.9150	 0.4540
h	 0.8550	 0.4130



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Chain	Atom inclusion	Q-score
i	 0.7620	 0.3930
j	 0.7500	 0.3830
k	 0.5710	 0.4040
l	 0.7860	 0.3770
m	 0.8470	 0.4350
n	 0.8200	 0.4370
o	 0.8290	 0.4260
p	 0.7700	 0.4260
q	 0.8940	 0.4540
r	 0.8430	 0.4060
s	 0.7520	 0.3910
t	 0.7500	 0.3960
u	 0.5360	 0.4050
v	 0.7500	 0.3990