



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 07:59 AM EDT

PDB ID : 7UGQ  
EMDB ID : EMD-26496  
Title : Cryo-EM structure of BG24 Fabs with an inferred germline CDRL1 and 10-1074 Fabs in complex with HIV-1 Env 6405-SOSIP.664  
Authors : Dam, K.A.; Bjorkman, P.J.  
Deposited on : 2022-03-25  
Resolution : 3.40 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:

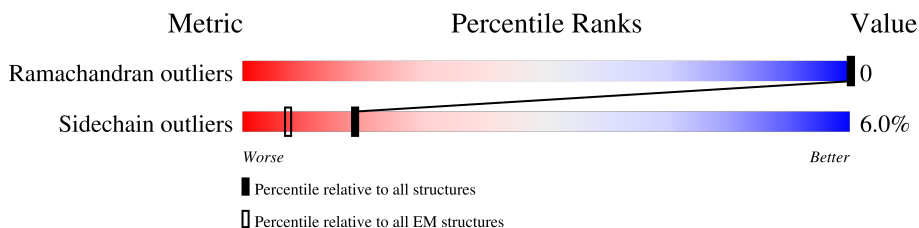
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



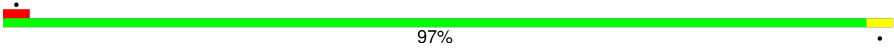
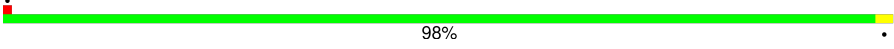
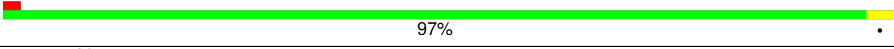
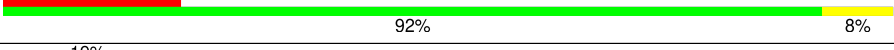
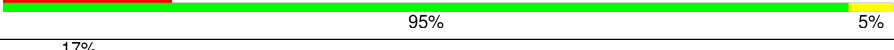
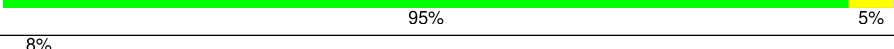
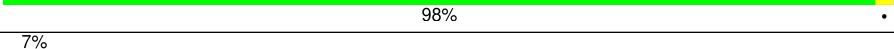
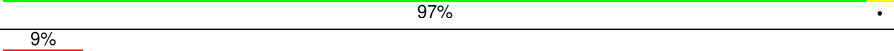
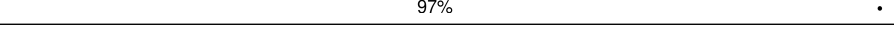
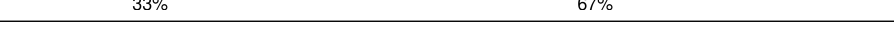
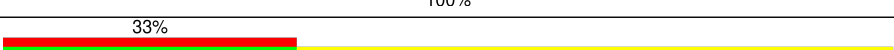
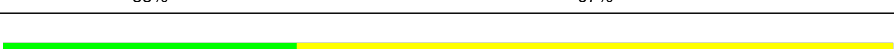
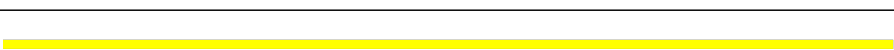
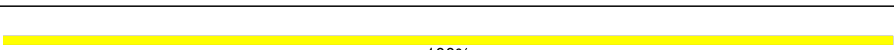
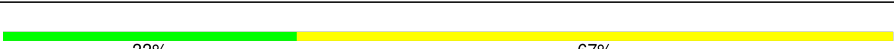
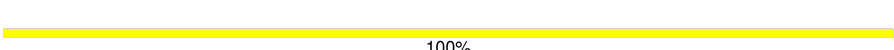
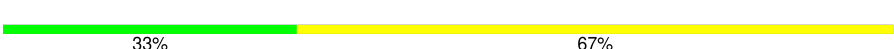
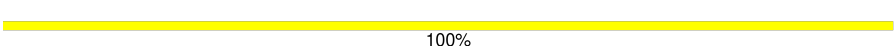
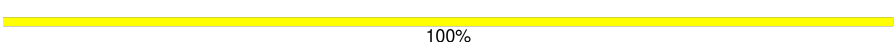
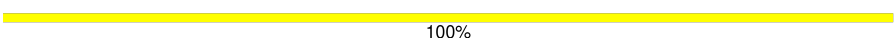
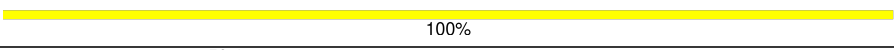


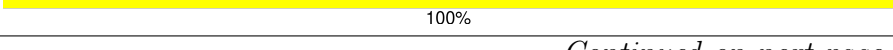

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	447	94% 6%
1	B	447	94% 6%
1	C	447	93% 7%
2	D	129	95% 5%
2	E	129	95% 5%
2	F	129	95% 5%
3	G	125	96% .
3	H	125	94% 6%
3	I	125	95% 5%

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Mol	Chain	Length	Quality of chain
4	J	105	 97%
4	K	105	 98%
4	L	105	 97%
5	M	133	 20% 92% 8%
5	N	133	 19% 95% 5%
5	O	133	 17% 95% 5%
6	P	107	 8% 98%
6	Q	107	 7% 97%
6	R	107	 9% 97%
7	0	3	 33% 67%
7	S	3	 100%
7	V	3	 33% 33% 67%
7	c	3	 33% 67%
7	e	3	 100%
7	h	3	 100%
7	o	3	 33% 67%
7	q	3	 100%
7	t	3	 33% 67%
8	T	2	 100%
8	U	2	 100%
8	X	2	 100%
8	Y	2	 100%
8	Z	2	 50% 50% 50%
8	a	2	 50% 50%
8	b	2	 100%

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Mol	Chain	Length	Quality of chain
8	f	2	100%
8	g	2	100%
8	j	2	100%
8	k	2	50%
8	l	2	50%
8	m	2	50%
8	n	2	100%
8	r	2	100%
8	s	2	100%
8	v	2	100%
8	w	2	50%
8	x	2	50%
8	y	2	50%
8	z	2	100%
9	W	5	100%
9	i	5	100%
9	u	5	100%
10	1	9	11% 89%
10	d	9	11% 89%
11	p	8	12% 88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	0	1	X	-	-	-
7	NAG	c	1	X	-	-	-
7	NAG	o	1	X	-	-	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 26113 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	447	Total	C	N	O	S	0	0
			3498	2191	616	662	29		
1	B	447	Total	C	N	O	S	0	0
			3498	2191	616	662	29		
1	C	447	Total	C	N	O	S	0	0
			3498	2191	616	662	29		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ASN	ASP	conflict	UNP D7S1H2
A	?	-	GLU	deletion	UNP D7S1H2
A	?	-	THR	deletion	UNP D7S1H2
A	?	-	GLU	deletion	UNP D7S1H2
A	?	-	ARG	deletion	UNP D7S1H2
A	?	-	GLY	deletion	UNP D7S1H2
A	?	-	ALA	deletion	UNP D7S1H2
A	?	-	SER	deletion	UNP D7S1H2
A	?	-	ASN	deletion	UNP D7S1H2
A	?	-	SER	deletion	UNP D7S1H2
A	?	-	THR	deletion	UNP D7S1H2
A	?	-	GLY	deletion	UNP D7S1H2
A	?	-	THR	deletion	UNP D7S1H2
A	?	-	ASN	deletion	UNP D7S1H2
A	?	-	ASN	deletion	UNP D7S1H2
A	?	-	GLY	deletion	UNP D7S1H2
A	?	-	THR	deletion	UNP D7S1H2
A	?	-	ILE	deletion	UNP D7S1H2
A	?	-	SER	deletion	UNP D7S1H2
A	?	-	SER	deletion	UNP D7S1H2
A	?	-	THR	deletion	UNP D7S1H2
A	?	-	GLY	deletion	UNP D7S1H2
A	?	-	PRO	deletion	UNP D7S1H2
A	?	-	GLY	deletion	UNP D7S1H2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP D7S1H2
A	?	-	ALA	deletion	UNP D7S1H2
A	?	-	ILE	deletion	UNP D7S1H2
A	?	-	TRP	deletion	UNP D7S1H2
A	496	VAL	ILE	conflict	UNP D7S1H2
A	500	ARG	LYS	conflict	UNP D7S1H2
A	501	CYS	ALA	conflict	UNP D7S1H2
A	502	LYS	ARG	conflict	UNP D7S1H2
B	33	ASN	ASP	conflict	UNP D7S1H2
B	?	-	GLU	deletion	UNP D7S1H2
B	?	-	THR	deletion	UNP D7S1H2
B	?	-	GLU	deletion	UNP D7S1H2
B	?	-	ARG	deletion	UNP D7S1H2
B	?	-	GLY	deletion	UNP D7S1H2
B	?	-	ALA	deletion	UNP D7S1H2
B	?	-	SER	deletion	UNP D7S1H2
B	?	-	ASN	deletion	UNP D7S1H2
B	?	-	SER	deletion	UNP D7S1H2
B	?	-	THR	deletion	UNP D7S1H2
B	?	-	GLY	deletion	UNP D7S1H2
B	?	-	THR	deletion	UNP D7S1H2
B	?	-	ASN	deletion	UNP D7S1H2
B	?	-	ASN	deletion	UNP D7S1H2
B	?	-	GLY	deletion	UNP D7S1H2
B	?	-	THR	deletion	UNP D7S1H2
B	?	-	ILE	deletion	UNP D7S1H2
B	?	-	SER	deletion	UNP D7S1H2
B	?	-	SER	deletion	UNP D7S1H2
B	?	-	THR	deletion	UNP D7S1H2
B	?	-	GLY	deletion	UNP D7S1H2
B	?	-	PRO	deletion	UNP D7S1H2
B	?	-	GLY	deletion	UNP D7S1H2
B	?	-	GLN	deletion	UNP D7S1H2
B	?	-	ALA	deletion	UNP D7S1H2
B	?	-	ILE	deletion	UNP D7S1H2
B	?	-	TRP	deletion	UNP D7S1H2
B	496	VAL	ILE	conflict	UNP D7S1H2
B	500	ARG	LYS	conflict	UNP D7S1H2
B	501	CYS	ALA	conflict	UNP D7S1H2
B	502	LYS	ARG	conflict	UNP D7S1H2
C	33	ASN	ASP	conflict	UNP D7S1H2
C	?	-	GLU	deletion	UNP D7S1H2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	THR	deletion	UNP D7S1H2
C	?	-	GLU	deletion	UNP D7S1H2
C	?	-	ARG	deletion	UNP D7S1H2
C	?	-	GLY	deletion	UNP D7S1H2
C	?	-	ALA	deletion	UNP D7S1H2
C	?	-	SER	deletion	UNP D7S1H2
C	?	-	ASN	deletion	UNP D7S1H2
C	?	-	SER	deletion	UNP D7S1H2
C	?	-	THR	deletion	UNP D7S1H2
C	?	-	GLY	deletion	UNP D7S1H2
C	?	-	THR	deletion	UNP D7S1H2
C	?	-	ASN	deletion	UNP D7S1H2
C	?	-	ASN	deletion	UNP D7S1H2
C	?	-	GLY	deletion	UNP D7S1H2
C	?	-	THR	deletion	UNP D7S1H2
C	?	-	ILE	deletion	UNP D7S1H2
C	?	-	SER	deletion	UNP D7S1H2
C	?	-	SER	deletion	UNP D7S1H2
C	?	-	THR	deletion	UNP D7S1H2
C	?	-	GLY	deletion	UNP D7S1H2
C	?	-	PRO	deletion	UNP D7S1H2
C	?	-	GLY	deletion	UNP D7S1H2
C	?	-	GLN	deletion	UNP D7S1H2
C	?	-	ALA	deletion	UNP D7S1H2
C	?	-	ILE	deletion	UNP D7S1H2
C	?	-	TRP	deletion	UNP D7S1H2
C	496	VAL	ILE	conflict	UNP D7S1H2
C	500	ARG	LYS	conflict	UNP D7S1H2
C	501	CYS	ALA	conflict	UNP D7S1H2
C	502	LYS	ARG	conflict	UNP D7S1H2

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	129	Total	C	N	O	S	0	0
			1030	655	176	193	6		
2	E	129	Total	C	N	O	S	0	0
			1030	655	176	193	6		
2	F	129	Total	C	N	O	S	0	0
			1030	655	176	193	6		

- Molecule 3 is a protein called BG24 with an inferred germline CDRL1 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	125	Total	C	N	O	S	0	0
			966	605	172	183	6		
3	H	125	Total	C	N	O	S	0	0
			966	605	172	183	6		
3	I	125	Total	C	N	O	S	0	0
			966	605	172	183	6		

- Molecule 4 is a protein called BG24 with an inferred germline CDRL1 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	105	Total	C	N	O	S	0	0
			758	468	135	153	2		
4	K	105	Total	C	N	O	S	0	0
			758	468	135	153	2		
4	L	105	Total	C	N	O	S	0	0
			758	468	135	153	2		

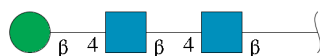
- Molecule 5 is a protein called 10-1074 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
5	N	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
5	O	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		

- Molecule 6 is a protein called 10-1074 Fab light chain.

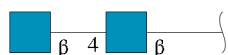
Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
6	Q	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
6	R	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

- Molecule 7 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
7	S	3	Total	C	N	O	0	0
			39	22	2	15		
7	V	3	Total	C	N	O	0	0
			39	22	2	15		
7	c	3	Total	C	N	O	0	0
			39	22	2	15		
7	e	3	Total	C	N	O	0	0
			39	22	2	15		
7	h	3	Total	C	N	O	0	0
			39	22	2	15		
7	o	3	Total	C	N	O	0	0
			39	22	2	15		
7	q	3	Total	C	N	O	0	0
			39	22	2	15		
7	t	3	Total	C	N	O	0	0
			39	22	2	15		
7	0	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



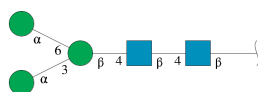
Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	2	Total	C	N	O	0	0
			28	16	2	10		
8	U	2	Total	C	N	O	0	0
			28	16	2	10		
8	X	2	Total	C	N	O	0	0
			28	16	2	10		
8	Y	2	Total	C	N	O	0	0
			28	16	2	10		
8	Z	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		
8	b	2	Total	C	N	O	0	0
			28	16	2	10		
8	f	2	Total	C	N	O	0	0
			28	16	2	10		

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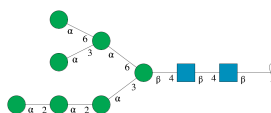
Mol	Chain	Residues	Atoms				AltConf	Trace
8	g	2	Total	C	N	O	0	0
			28	16	2	10		
8	j	2	Total	C	N	O	0	0
			28	16	2	10		
8	k	2	Total	C	N	O	0	0
			28	16	2	10		
8	l	2	Total	C	N	O	0	0
			28	16	2	10		
8	m	2	Total	C	N	O	0	0
			28	16	2	10		
8	n	2	Total	C	N	O	0	0
			28	16	2	10		
8	r	2	Total	C	N	O	0	0
			28	16	2	10		
8	s	2	Total	C	N	O	0	0
			28	16	2	10		
8	v	2	Total	C	N	O	0	0
			28	16	2	10		
8	w	2	Total	C	N	O	0	0
			28	16	2	10		
8	x	2	Total	C	N	O	0	0
			28	16	2	10		
8	y	2	Total	C	N	O	0	0
			28	16	2	10		
8	z	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 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.



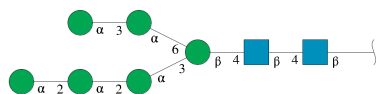
Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	5	Total	C	N	O	0	0
			61	34	2	25		
9	i	5	Total	C	N	O	0	0
			61	34	2	25		
9	u	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 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.



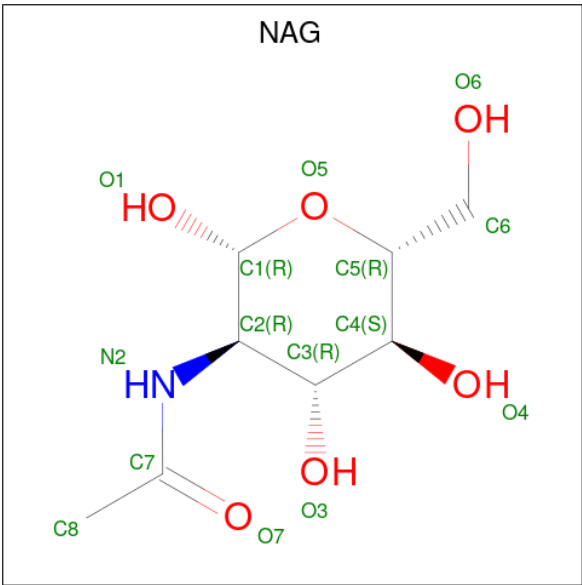
Mol	Chain	Residues	Atoms				AltConf	Trace
10	d	9	Total	C	N	O	0	0
			105	58	2	45		
10	1	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



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

Continued on next page...

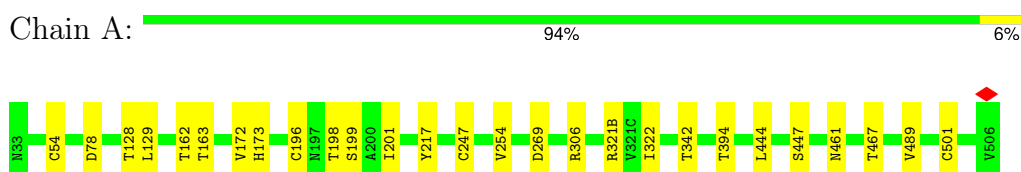
*Continued from previous page...*

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

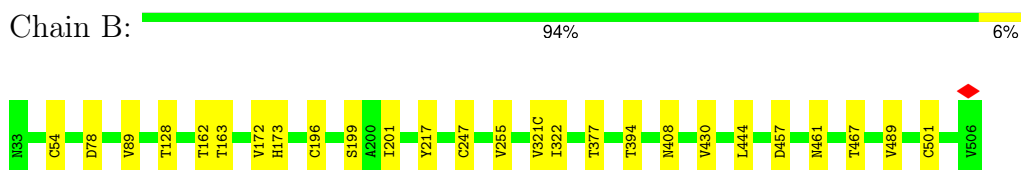
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

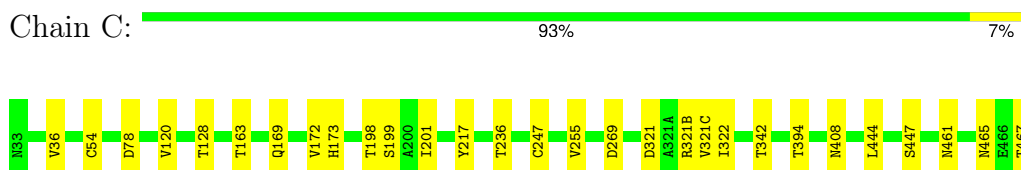
- Molecule 1: Envelope glycoprotein gp120



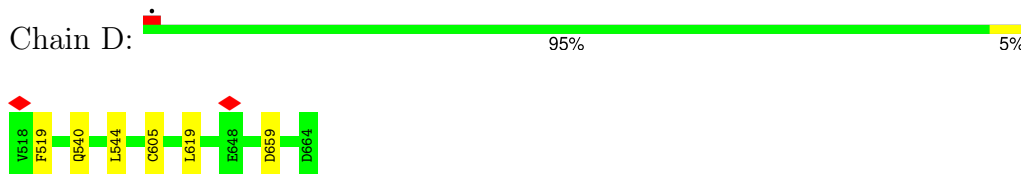
- Molecule 1: Envelope glycoprotein gp120



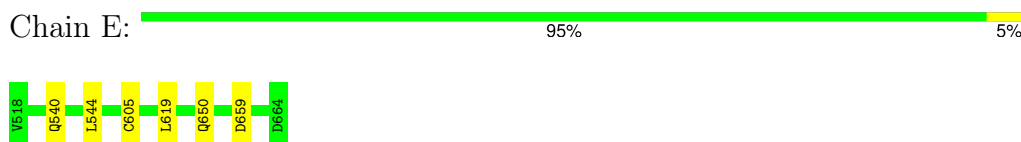
- Molecule 1: Envelope glycoprotein gp120



- Molecule 2: Envelope glycoprotein gp41



- Molecule 2: Envelope glycoprotein gp41



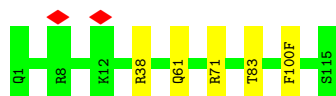
- Molecule 2: Envelope glycoprotein gp41

Chain F:  95% 5%



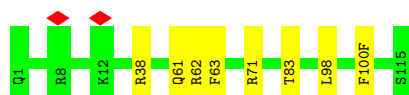
- Molecule 3: BG24 with an inferred germline CDRL1 Fab heavy chain

Chain G:  96% 4%



- Molecule 3: BG24 with an inferred germline CDRL1 Fab heavy chain

Chain H:  94% 6%



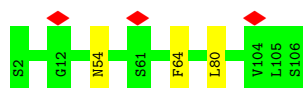
- Molecule 3: BG24 with an inferred germline CDRL1 Fab heavy chain

Chain I:  95% 5%



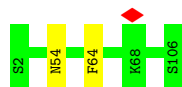
- Molecule 4: BG24 with an inferred germline CDRL1 Fab light chain

Chain J:  97% 3%



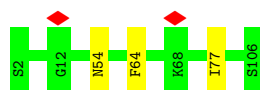
- Molecule 4: BG24 with an inferred germline CDRL1 Fab light chain

Chain K:  98% 2%

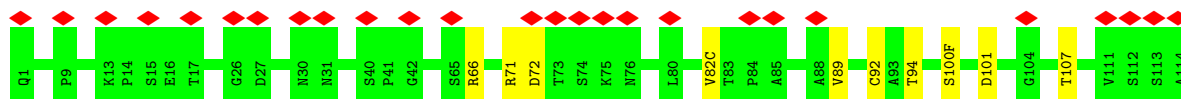
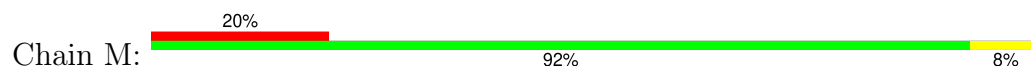


- Molecule 4: BG24 with an inferred germline CDRL1 Fab light chain

Chain L:  97% 3%



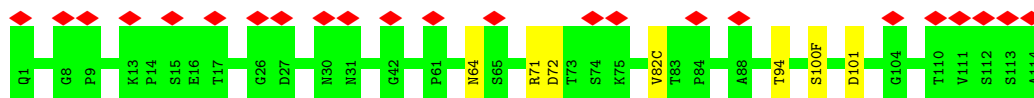
- Molecule 5: 10-1074 Fab heavy chain



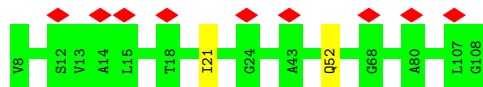
- Molecule 5: 10-1074 Fab heavy chain



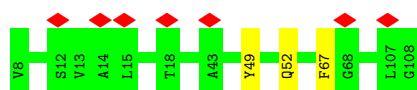
- Molecule 5: 10-1074 Fab heavy chain



- Molecule 6: 10-1074 Fab light chain



- Molecule 6: 10-1074 Fab light chain



- Molecule 6: 10-1074 Fab light chain



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

Chain S:  100%

NAG1  
NAG2  
BMA3

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

Chain V:  33% 33% 67%

NAG1  
NAG2  
BMA3

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

Chain c:  33% 67%

NAG1  
NAG2  
BMA3

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

Chain e:  100%

NAG1  
NAG2  
BMA3

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

Chain h:  100%

NAG1  
NAG2  
BMA3

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

Chain o:  33% 67%

NAG1  
NAG2  
BMA3

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

Chain q:  100%

NAG1  
NAG2  
BMA3

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

Chain t:  33% 67%

NAG1  
NAG2  
BMA3

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

Chain 0:  33% 67%

NAG1  
NAG2  
BMA3

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

Chain T:  100%

NAG1  
NAG2

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

Chain U:  100%

NAG1  
NAG2

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

Chain X:  100%

NAG1  
NAG2

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

Chain Y:  100%

NAG1  
NAG2

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

Chain Z: 



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

Chain a: 



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

Chain b: 

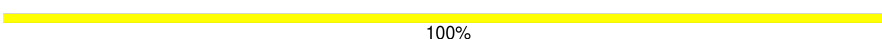


- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 



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

Chain g: 



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

Chain j: 



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

Chain k:  50% 50%



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

Chain l:  50% 50% 50%



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

Chain m:  50% 50%



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

Chain n:  100%

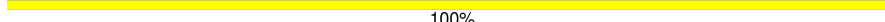


- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%



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

Chain s:  100%



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

Chain v:  100%

NAG1  
NAG2

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

Chain w:  50% 50%

NAG1  
NAG2

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

Chain x:  50% 50% 50%

NAG1  
NAG2

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

Chain y:  50% 50%

NAG1  
NAG2

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

Chain z:  100%

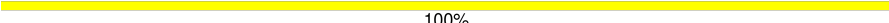
NAG1  
NAG2

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

Chain W:  100%


NAG1  
NAG2  
MAN3  
MAN4  
MAN5

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

Chain i:  100%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 9:  $\alpha$ -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 u:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 10:  $\alpha$ -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 d:  11%  89%



MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

- Molecule 10:  $\alpha$ -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 1:  11%  89%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

- Molecule 11:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain p:  12%  88%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170897	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0115	Depositor
Map size ( $\text{\AA}$ )	312.84, 312.84, 312.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.869, 0.869, 0.869	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: BMA, NAG, MAN

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	0.31	0/3572	0.55	0/4859
1	B	0.31	0/3572	0.55	0/4859
1	C	0.31	0/3572	0.55	0/4859
2	D	0.27	0/1048	0.54	0/1421
2	E	0.33	0/1048	0.54	0/1421
2	F	0.27	0/1048	0.54	0/1421
3	G	0.30	0/990	0.53	0/1346
3	H	0.30	0/990	0.54	0/1346
3	I	0.29	0/990	0.52	0/1346
4	J	0.28	0/773	0.54	0/1047
4	K	0.28	0/773	0.55	0/1047
4	L	0.29	0/773	0.56	0/1047
5	M	0.28	0/1066	0.54	0/1451
5	N	0.27	0/1066	0.55	0/1451
5	O	0.27	0/1066	0.55	0/1451
6	P	0.27	0/845	0.50	0/1148
6	Q	0.28	0/845	0.55	0/1148
6	R	0.28	0/845	0.53	0/1148
All	All	0.29	0/24882	0.54	0/33816

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

### 5.3.1 Protein backbone ⓘ

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	439/447 (98%)	405 (92%)	34 (8%)	0	100	100
1	B	439/447 (98%)	404 (92%)	35 (8%)	0	100	100
1	C	439/447 (98%)	407 (93%)	32 (7%)	0	100	100
2	D	125/129 (97%)	116 (93%)	9 (7%)	0	100	100
2	E	125/129 (97%)	118 (94%)	7 (6%)	0	100	100
2	F	125/129 (97%)	115 (92%)	10 (8%)	0	100	100
3	G	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
3	H	123/125 (98%)	112 (91%)	11 (9%)	0	100	100
3	I	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
4	J	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
4	K	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
4	L	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
5	M	131/133 (98%)	129 (98%)	2 (2%)	0	100	100
5	N	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
5	O	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
6	P	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
6	Q	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
6	R	105/107 (98%)	94 (90%)	11 (10%)	0	100	100
All	All	3078/3138 (98%)	2852 (93%)	226 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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	397/397 (100%)	370 (93%)	27 (7%)	13	38
1	B	397/397 (100%)	371 (94%)	26 (6%)	14	39
1	C	397/397 (100%)	367 (92%)	30 (8%)	11	34
2	D	112/112 (100%)	106 (95%)	6 (5%)	18	44
2	E	112/112 (100%)	106 (95%)	6 (5%)	18	44
2	F	112/112 (100%)	106 (95%)	6 (5%)	18	44
3	G	102/102 (100%)	97 (95%)	5 (5%)	21	48
3	H	102/102 (100%)	94 (92%)	8 (8%)	10	33
3	I	102/102 (100%)	96 (94%)	6 (6%)	16	41
4	J	79/87 (91%)	76 (96%)	3 (4%)	28	54
4	K	79/87 (91%)	77 (98%)	2 (2%)	42	65
4	L	79/87 (91%)	76 (96%)	3 (4%)	28	54
5	M	116/116 (100%)	106 (91%)	10 (9%)	8	29
5	N	116/116 (100%)	109 (94%)	7 (6%)	16	41
5	O	116/116 (100%)	109 (94%)	7 (6%)	16	41
6	P	85/85 (100%)	83 (98%)	2 (2%)	44	66
6	Q	85/85 (100%)	82 (96%)	3 (4%)	31	56
6	R	85/85 (100%)	82 (96%)	3 (4%)	31	56
All	All	2673/2697 (99%)	2513 (94%)	160 (6%)	18	41

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS
1	A	78	ASP
1	A	128	THR
1	A	129	LEU
1	A	162	THR
1	A	163	THR
1	A	172	VAL
1	A	173	HIS
1	A	196	CYS
1	A	198	THR
1	A	199	SER

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Mol	Chain	Res	Type
1	A	201	ILE
1	A	217	TYR
1	A	247	CYS
1	A	254	VAL
1	A	269	ASP
1	A	306	ARG
1	A	321(B)	ARG
1	A	322	ILE
1	A	342	THR
1	A	394	THR
1	A	444	LEU
1	A	447	SER
1	A	461	ASN
1	A	467	THR
1	A	489	VAL
1	A	501	CYS
1	B	54	CYS
1	B	78	ASP
1	B	89	VAL
1	B	128	THR
1	B	162	THR
1	B	163	THR
1	B	172	VAL
1	B	173	HIS
1	B	196	CYS
1	B	199	SER
1	B	201	ILE
1	B	217	TYR
1	B	247	CYS
1	B	255	VAL
1	B	321(C)	VAL
1	B	322	ILE
1	B	377	THR
1	B	394	THR
1	B	408	ASN
1	B	430	VAL
1	B	444	LEU
1	B	457	ASP
1	B	461	ASN
1	B	467	THR
1	B	489	VAL
1	B	501	CYS

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Mol	Chain	Res	Type
1	C	36	VAL
1	C	54	CYS
1	C	78	ASP
1	C	120	VAL
1	C	128	THR
1	C	163	THR
1	C	169	GLN
1	C	172	VAL
1	C	173	HIS
1	C	198	THR
1	C	199	SER
1	C	201	ILE
1	C	217	TYR
1	C	236	THR
1	C	247	CYS
1	C	255	VAL
1	C	269	ASP
1	C	321	ASP
1	C	321(B)	ARG
1	C	321(C)	VAL
1	C	322	ILE
1	C	342	THR
1	C	394	THR
1	C	408	ASN
1	C	444	LEU
1	C	447	SER
1	C	461	ASN
1	C	465	ASN
1	C	467	THR
1	C	501	CYS
2	D	519	PHE
2	D	540	GLN
2	D	544	LEU
2	D	605	CYS
2	D	619	LEU
2	D	659	ASP
2	E	540	GLN
2	E	544	LEU
2	E	605	CYS
2	E	619	LEU
2	E	650	GLN
2	E	659	ASP

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Mol	Chain	Res	Type
2	F	519	PHE
2	F	544	LEU
2	F	570	VAL
2	F	605	CYS
2	F	619	LEU
2	F	627	THR
3	G	38	ARG
3	G	61	GLN
3	G	71	ARG
3	G	83	THR
3	G	100(F)	PHE
3	H	38	ARG
3	H	61	GLN
3	H	62	ARG
3	H	63	PHE
3	H	71	ARG
3	H	83	THR
3	H	98	LEU
3	H	100(F)	PHE
3	I	1	GLN
3	I	38	ARG
3	I	71	ARG
3	I	73	THR
3	I	83	THR
3	I	100(F)	PHE
4	J	54	ASN
4	J	64	PHE
4	J	80	LEU
4	K	54	ASN
4	K	64	PHE
4	L	54	ASN
4	L	64	PHE
4	L	77	ILE
5	M	66	ARG
5	M	71	ARG
5	M	72	ASP
5	M	82(C)	VAL
5	M	89	VAL
5	M	92	CYS
5	M	94	THR
5	M	100(F)	SER
5	M	101	ASP

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Mol	Chain	Res	Type
5	M	107	THR
5	N	71	ARG
5	N	72	ASP
5	N	92	CYS
5	N	94	THR
5	N	100(F)	SER
5	N	101	ASP
5	N	107	THR
5	O	64	ASN
5	O	71	ARG
5	O	72	ASP
5	O	82(C)	VAL
5	O	94	THR
5	O	100(F)	SER
5	O	101	ASP
6	P	21	ILE
6	P	52	GLN
6	Q	49	TYR
6	Q	52	GLN
6	Q	67	PHE
6	R	49	TYR
6	R	51	ASN
6	R	52	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	130	GLN
1	A	258	GLN
1	A	408	ASN
1	B	105	HIS
1	B	130	GLN
1	B	258	GLN
1	B	408	ASN
1	C	105	HIS
1	C	130	GLN
1	C	258	GLN
1	C	408	ASN
2	D	651	ASN
2	E	540	GLN
2	E	650	GLN

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Mol	Chain	Res	Type
2	E	652	GLN
2	F	651	ASN
3	G	43	GLN
3	G	46	GLN
3	H	43	GLN
3	I	43	GLN
3	I	64	GLN
4	J	16	GLN
4	J	39	GLN
4	K	16	GLN
4	L	16	GLN
5	M	39	GLN
5	M	76	ASN
5	N	30	ASN
5	O	5	GLN
6	Q	51	ASN
6	Q	66(C)	ASN
6	R	50	ASN
6	R	51	ASN
6	R	52	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](#)

110 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	0	1	7,1	14,14,15	2.24	1 (7%)	17,19,21	1.93	2 (11%)
7	NAG	0	2	7	14,14,15	0.43	0	17,19,21	1.40	4 (23%)
7	BMA	0	3	7	11,11,12	0.23	0	15,15,17	0.82	0
10	NAG	1	1	10,1	14,14,15	0.27	0	17,19,21	0.76	0
10	NAG	1	2	10	14,14,15	0.28	0	17,19,21	0.83	1 (5%)
10	BMA	1	3	10	11,11,12	1.34	3 (27%)	15,15,17	1.78	3 (20%)
10	MAN	1	4	10	11,11,12	0.85	0	15,15,17	1.37	1 (6%)
10	MAN	1	5	10	11,11,12	0.84	0	15,15,17	1.28	1 (6%)
10	MAN	1	6	10	11,11,12	0.96	0	15,15,17	1.16	2 (13%)
10	MAN	1	7	10	11,11,12	1.59	3 (27%)	15,15,17	2.21	2 (13%)
10	MAN	1	8	10	11,11,12	1.03	1 (9%)	15,15,17	1.28	2 (13%)
10	MAN	1	9	10	11,11,12	1.08	0	15,15,17	1.15	2 (13%)
7	NAG	S	1	7,1	14,14,15	0.57	0	17,19,21	0.83	1 (5%)
7	NAG	S	2	7	14,14,15	1.15	1 (7%)	17,19,21	2.77	3 (17%)
7	BMA	S	3	7	11,11,12	1.03	0	15,15,17	1.02	1 (6%)
8	NAG	T	1	8,1	14,14,15	1.01	1 (7%)	17,19,21	2.74	3 (17%)
8	NAG	T	2	8	14,14,15	0.62	0	17,19,21	0.64	1 (5%)
8	NAG	U	1	8,1	14,14,15	1.03	1 (7%)	17,19,21	2.78	4 (23%)
8	NAG	U	2	8	14,14,15	0.51	0	17,19,21	0.63	1 (5%)
7	NAG	V	1	7,1	14,14,15	0.41	0	17,19,21	0.77	0
7	NAG	V	2	7	14,14,15	0.78	1 (7%)	17,19,21	1.42	3 (17%)
7	BMA	V	3	7	11,11,12	1.02	1 (9%)	15,15,17	1.14	1 (6%)
9	NAG	W	1	9,1	14,14,15	0.78	0	17,19,21	2.89	4 (23%)
9	NAG	W	2	9	14,14,15	0.46	0	17,19,21	0.64	1 (5%)
9	BMA	W	3	9	11,11,12	0.89	0	15,15,17	1.06	1 (6%)
9	MAN	W	4	9	11,11,12	1.27	2 (18%)	15,15,17	1.74	1 (6%)
9	MAN	W	5	9	11,11,12	1.13	0	15,15,17	1.02	2 (13%)
8	NAG	X	1	8,1	14,14,15	0.39	0	17,19,21	0.68	1 (5%)
8	NAG	X	2	8	14,14,15	1.11	1 (7%)	17,19,21	2.76	3 (17%)
8	NAG	Y	1	8,1	14,14,15	0.89	1 (7%)	17,19,21	1.29	3 (17%)
8	NAG	Y	2	8	14,14,15	0.53	0	17,19,21	0.61	1 (5%)
8	NAG	Z	1	8,1	14,14,15	0.33	0	17,19,21	0.64	0
8	NAG	Z	2	8	14,14,15	0.55	0	17,19,21	0.87	2 (11%)
8	NAG	a	1	8,1	14,14,15	0.47	0	17,19,21	0.62	0
8	NAG	a	2	8	14,14,15	0.63	0	17,19,21	0.61	1 (5%)
8	NAG	b	1	8,1	14,14,15	0.39	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	b	2	8	14,14,15	0.55	0	17,19,21	0.91	2 (11%)
7	NAG	c	1	7,1	14,14,15	2.31	1 (7%)	17,19,21	2.33	5 (29%)
7	NAG	c	2	7	14,14,15	0.40	0	17,19,21	1.48	3 (17%)
7	BMA	c	3	7	11,11,12	0.23	0	15,15,17	0.84	0
10	NAG	d	1	10,1	14,14,15	0.28	0	17,19,21	0.78	0
10	NAG	d	2	10	14,14,15	0.27	0	17,19,21	0.84	1 (5%)
10	BMA	d	3	10	11,11,12	1.30	2 (18%)	15,15,17	1.83	4 (26%)
10	MAN	d	4	10	11,11,12	0.84	0	15,15,17	1.42	1 (6%)
10	MAN	d	5	10	11,11,12	0.86	0	15,15,17	1.26	1 (6%)
10	MAN	d	6	10	11,11,12	0.90	0	15,15,17	1.16	2 (13%)
10	MAN	d	7	10	11,11,12	1.50	3 (27%)	15,15,17	2.10	2 (13%)
10	MAN	d	8	10	11,11,12	1.04	1 (9%)	15,15,17	1.30	2 (13%)
10	MAN	d	9	10	11,11,12	1.05	0	15,15,17	1.17	2 (13%)
7	NAG	e	1	7,1	14,14,15	0.58	0	17,19,21	0.82	1 (5%)
7	NAG	e	2	7	14,14,15	1.13	1 (7%)	17,19,21	2.76	3 (17%)
7	BMA	e	3	7	11,11,12	1.02	0	15,15,17	1.04	1 (6%)
8	NAG	f	1	8,1	14,14,15	1.01	1 (7%)	17,19,21	2.75	3 (17%)
8	NAG	f	2	8	14,14,15	0.61	0	17,19,21	0.63	1 (5%)
8	NAG	g	1	8,1	14,14,15	1.03	1 (7%)	17,19,21	2.78	4 (23%)
8	NAG	g	2	8	14,14,15	0.49	0	17,19,21	0.83	2 (11%)
7	NAG	h	1	7,1	14,14,15	0.33	0	17,19,21	1.08	1 (5%)
7	NAG	h	2	7	14,14,15	0.68	0	17,19,21	0.75	1 (5%)
7	BMA	h	3	7	11,11,12	1.01	1 (9%)	15,15,17	1.14	1 (6%)
9	NAG	i	1	9,1	14,14,15	0.83	1 (7%)	17,19,21	2.87	4 (23%)
9	NAG	i	2	9	14,14,15	0.48	0	17,19,21	0.65	1 (5%)
9	BMA	i	3	9	11,11,12	0.85	0	15,15,17	1.09	1 (6%)
9	MAN	i	4	9	11,11,12	1.18	1 (9%)	15,15,17	1.77	1 (6%)
9	MAN	i	5	9	11,11,12	1.02	0	15,15,17	1.09	2 (13%)
8	NAG	j	1	8,1	14,14,15	0.39	0	17,19,21	0.68	1 (5%)
8	NAG	j	2	8	14,14,15	1.11	1 (7%)	17,19,21	2.75	3 (17%)
8	NAG	k	1	8,1	14,14,15	0.99	1 (7%)	17,19,21	1.39	4 (23%)
8	NAG	k	2	8	14,14,15	0.60	0	17,19,21	0.56	0
8	NAG	l	1	8,1	14,14,15	0.33	0	17,19,21	0.62	0
8	NAG	l	2	8	14,14,15	0.54	0	17,19,21	0.87	2 (11%)
8	NAG	m	1	8,1	14,14,15	0.31	0	17,19,21	0.82	0
8	NAG	m	2	8	14,14,15	0.72	1 (7%)	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	n	1	8,1	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
8	NAG	n	2	8	14,14,15	0.54	0	17,19,21	0.89	2 (11%)
7	NAG	o	1	7,1	14,14,15	2.30	1 (7%)	17,19,21	1.91	2 (11%)
7	NAG	o	2	7	14,14,15	0.45	0	17,19,21	1.75	4 (23%)
7	BMA	o	3	7	11,11,12	0.23	0	15,15,17	0.81	0
11	NAG	p	1	11,1	14,14,15	0.28	0	17,19,21	0.79	0
11	NAG	p	2	11	14,14,15	0.28	0	17,19,21	0.86	2 (11%)
11	BMA	p	3	11	11,11,12	1.40	3 (27%)	15,15,17	1.86	4 (26%)
11	MAN	p	4	11	11,11,12	0.89	0	15,15,17	1.32	1 (6%)
11	MAN	p	5	11	11,11,12	0.82	0	15,15,17	1.24	2 (13%)
11	MAN	p	6	11	11,11,12	0.97	0	15,15,17	1.16	2 (13%)
11	MAN	p	7	11	11,11,12	1.35	3 (27%)	15,15,17	1.92	2 (13%)
11	MAN	p	8	11	11,11,12	1.04	1 (9%)	15,15,17	1.31	2 (13%)
7	NAG	q	1	7,1	14,14,15	0.60	0	17,19,21	0.82	1 (5%)
7	NAG	q	2	7	14,14,15	1.15	1 (7%)	17,19,21	2.77	3 (17%)
7	BMA	q	3	7	11,11,12	1.03	0	15,15,17	1.02	1 (6%)
8	NAG	r	1	8,1	14,14,15	1.02	1 (7%)	17,19,21	2.75	3 (17%)
8	NAG	r	2	8	14,14,15	0.61	0	17,19,21	0.65	1 (5%)
8	NAG	s	1	8,1	14,14,15	1.04	1 (7%)	17,19,21	2.78	4 (23%)
8	NAG	s	2	8	14,14,15	0.52	0	17,19,21	0.64	1 (5%)
7	NAG	t	1	7,1	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
7	NAG	t	2	7	14,14,15	0.50	0	17,19,21	0.76	0
7	BMA	t	3	7	11,11,12	1.04	1 (9%)	15,15,17	1.11	1 (6%)
9	NAG	u	1	9,1	14,14,15	0.79	1 (7%)	17,19,21	2.89	4 (23%)
9	NAG	u	2	9	14,14,15	0.48	0	17,19,21	0.65	1 (5%)
9	BMA	u	3	9	11,11,12	0.98	0	15,15,17	0.93	1 (6%)
9	MAN	u	4	9	11,11,12	1.11	1 (9%)	15,15,17	1.59	2 (13%)
9	MAN	u	5	9	11,11,12	0.99	0	15,15,17	1.16	2 (13%)
8	NAG	v	1	8,1	14,14,15	0.40	0	17,19,21	0.66	1 (5%)
8	NAG	v	2	8	14,14,15	1.12	1 (7%)	17,19,21	2.76	3 (17%)
8	NAG	w	1	8,1	14,14,15	0.99	1 (7%)	17,19,21	1.38	4 (23%)
8	NAG	w	2	8	14,14,15	0.57	0	17,19,21	0.57	0
8	NAG	x	1	8,1	14,14,15	0.34	0	17,19,21	0.64	0
8	NAG	x	2	8	14,14,15	0.55	0	17,19,21	0.87	2 (11%)
8	NAG	y	1	8,1	14,14,15	0.47	0	17,19,21	0.61	0
8	NAG	y	2	8	14,14,15	0.63	0	17,19,21	0.60	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	z	1	8,1	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
8	NAG	z	2	8	14,14,15	0.53	0	17,19,21	0.90	1 (5%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	NAG	Z	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	4/6/23/26	0/1/1/1
8	NAG	a	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1
8	NAG	b	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
7	NAG	c	1	7,1	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	c	2	7	-	2/6/23/26	0/1/1/1
7	BMA	c	3	7	-	2/2/19/22	0/1/1/1
10	NAG	d	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	d	2	10	-	0/6/23/26	0/1/1/1
10	BMA	d	3	10	-	1/2/19/22	0/1/1/1
10	MAN	d	4	10	-	0/2/19/22	0/1/1/1
10	MAN	d	5	10	-	2/2/19/22	0/1/1/1
10	MAN	d	6	10	-	0/2/19/22	0/1/1/1
10	MAN	d	7	10	-	2/2/19/22	0/1/1/1
10	MAN	d	8	10	-	0/2/19/22	0/1/1/1
10	MAN	d	9	10	-	0/2/19/22	0/1/1/1
7	NAG	e	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	e	2	7	-	6/6/23/26	0/1/1/1
7	BMA	e	3	7	-	0/2/19/22	0/1/1/1
8	NAG	f	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	NAG	g	1	8,1	-	6/6/23/26	0/1/1/1
8	NAG	g	2	8	-	2/6/23/26	0/1/1/1
7	NAG	h	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	h	2	7	-	2/6/23/26	0/1/1/1
7	BMA	h	3	7	-	2/2/19/22	0/1/1/1
9	NAG	i	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	i	2	9	-	1/6/23/26	0/1/1/1
9	BMA	i	3	9	-	0/2/19/22	0/1/1/1
9	MAN	i	4	9	-	0/2/19/22	0/1/1/1
9	MAN	i	5	9	-	0/2/19/22	0/1/1/1
8	NAG	j	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	6/6/23/26	0/1/1/1
8	NAG	k	1	8,1	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	x	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	x	2	8	-	4/6/23/26	0/1/1/1
8	NAG	y	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	y	2	8	-	0/6/23/26	0/1/1/1
8	NAG	z	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	z	2	8	-	2/6/23/26	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	1	NAG	C1-C2	8.57	1.64	1.52
7	o	1	NAG	C1-C2	8.50	1.63	1.52
7	0	1	NAG	C1-C2	8.31	1.63	1.52
10	1	7	MAN	O5-C5	3.34	1.49	1.43
7	q	2	NAG	C1-C2	3.24	1.56	1.52
8	k	1	NAG	O5-C1	-3.23	1.38	1.43
7	S	2	NAG	C1-C2	3.20	1.56	1.52
10	d	7	MAN	O5-C5	3.20	1.49	1.43
10	1	7	MAN	O5-C1	3.20	1.49	1.43
8	w	1	NAG	O5-C1	-3.19	1.38	1.43
7	e	2	NAG	C1-C2	3.12	1.56	1.52
8	v	2	NAG	C1-C2	3.11	1.56	1.52
8	X	2	NAG	C1-C2	3.10	1.56	1.52
8	j	2	NAG	C1-C2	3.07	1.56	1.52
8	s	1	NAG	C1-C2	2.99	1.56	1.52
8	g	1	NAG	C1-C2	2.94	1.56	1.52
10	d	7	MAN	O5-C1	2.93	1.48	1.43
9	i	4	MAN	O5-C5	2.92	1.49	1.43
8	U	1	NAG	C1-C2	2.91	1.56	1.52
8	r	1	NAG	C1-C2	2.91	1.56	1.52
11	p	7	MAN	O5-C5	2.89	1.49	1.43
8	f	1	NAG	C1-C2	2.85	1.56	1.52
8	T	1	NAG	C1-C2	2.83	1.56	1.52
8	Y	1	NAG	O5-C1	-2.83	1.38	1.43
11	p	3	BMA	O5-C1	-2.73	1.39	1.43
9	u	4	MAN	O5-C5	2.68	1.48	1.43
9	W	4	MAN	O5-C5	2.67	1.48	1.43
11	p	7	MAN	O5-C1	2.54	1.48	1.43
11	p	3	BMA	C4-C3	2.53	1.58	1.52
10	d	3	BMA	C4-C3	2.53	1.58	1.52
10	1	3	BMA	C4-C3	2.52	1.58	1.52
10	1	7	MAN	C1-C2	2.44	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	2	NAG	C1-C2	2.43	1.55	1.52
10	d	3	BMA	O5-C1	-2.43	1.39	1.43
10	l	3	BMA	O5-C1	-2.41	1.39	1.43
10	d	7	MAN	C1-C2	2.35	1.57	1.52
7	V	3	BMA	C2-C3	2.29	1.56	1.52
10	l	3	BMA	C2-C3	2.27	1.56	1.52
11	p	3	BMA	C2-C3	2.27	1.56	1.52
11	p	8	MAN	C1-C2	2.25	1.57	1.52
9	i	1	NAG	C1-C2	2.22	1.55	1.52
10	d	8	MAN	C1-C2	2.22	1.57	1.52
7	t	3	BMA	C2-C3	2.20	1.55	1.52
7	h	3	BMA	C2-C3	2.15	1.55	1.52
10	l	8	MAN	C1-C2	2.15	1.57	1.52
11	p	7	MAN	C1-C2	2.15	1.57	1.52
9	W	4	MAN	C1-C2	2.14	1.57	1.52
8	m	2	NAG	O5-C1	2.10	1.47	1.43
9	u	1	NAG	C1-C2	2.02	1.55	1.52

All (184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	r	1	NAG	C2-N2-C7	9.67	135.86	122.90
8	f	1	NAG	C2-N2-C7	9.66	135.84	122.90
9	W	1	NAG	C2-N2-C7	9.66	135.84	122.90
9	u	1	NAG	C2-N2-C7	9.65	135.84	122.90
9	i	1	NAG	C2-N2-C7	9.65	135.83	122.90
8	U	1	NAG	C2-N2-C7	9.64	135.82	122.90
7	S	2	NAG	C2-N2-C7	9.64	135.82	122.90
8	g	1	NAG	C2-N2-C7	9.64	135.82	122.90
8	T	1	NAG	C2-N2-C7	9.64	135.81	122.90
8	s	1	NAG	C2-N2-C7	9.63	135.80	122.90
7	q	2	NAG	C2-N2-C7	9.61	135.78	122.90
8	v	2	NAG	C2-N2-C7	9.61	135.78	122.90
8	X	2	NAG	C2-N2-C7	9.58	135.74	122.90
7	e	2	NAG	C2-N2-C7	9.57	135.72	122.90
8	j	2	NAG	C2-N2-C7	9.57	135.72	122.90
10	l	7	MAN	C1-O5-C5	7.75	122.57	112.19
10	d	7	MAN	C1-O5-C5	7.32	122.00	112.19
11	p	7	MAN	C1-O5-C5	6.59	121.02	112.19
7	c	1	NAG	O5-C1-C2	-6.57	101.13	111.29
7	o	1	NAG	O5-C1-C2	-6.46	101.30	111.29
7	0	1	NAG	O5-C1-C2	-6.14	101.78	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	4	MAN	C1-O5-C5	6.09	120.35	112.19
9	W	4	MAN	C1-O5-C5	5.88	120.06	112.19
9	u	4	MAN	C1-O5-C5	5.50	119.56	112.19
9	W	1	NAG	C1-C2-N2	5.18	118.59	110.43
9	u	1	NAG	C1-C2-N2	5.14	118.53	110.43
9	i	1	NAG	C1-C2-N2	5.09	118.45	110.43
7	e	2	NAG	C1-C2-N2	4.93	118.21	110.43
7	q	2	NAG	C1-C2-N2	4.93	118.20	110.43
7	S	2	NAG	C1-C2-N2	4.88	118.12	110.43
8	X	2	NAG	C1-C2-N2	4.82	118.04	110.43
8	j	2	NAG	C1-C2-N2	4.81	118.01	110.43
10	d	4	MAN	C1-O5-C5	4.80	118.61	112.19
8	v	2	NAG	C1-C2-N2	4.77	117.95	110.43
10	d	3	BMA	C1-O5-C5	4.75	118.56	112.19
11	p	3	BMA	C1-O5-C5	4.73	118.52	112.19
8	T	1	NAG	C1-C2-N2	4.59	117.66	110.43
10	l	4	MAN	C1-O5-C5	4.58	118.33	112.19
8	f	1	NAG	C1-C2-N2	4.58	117.65	110.43
8	r	1	NAG	C1-C2-N2	4.57	117.64	110.43
8	g	1	NAG	C1-C2-N2	4.45	117.45	110.43
8	U	1	NAG	C1-C2-N2	4.45	117.44	110.43
10	l	3	BMA	C1-O5-C5	4.44	118.13	112.19
8	s	1	NAG	C1-C2-N2	4.42	117.39	110.43
7	o	2	NAG	C1-O5-C5	4.39	118.08	112.19
7	c	2	NAG	C1-O5-C5	4.32	117.97	112.19
11	p	4	MAN	C1-O5-C5	4.27	117.91	112.19
10	l	5	MAN	C1-O5-C5	4.15	117.75	112.19
7	V	2	NAG	C2-N2-C7	4.13	128.43	122.90
10	d	5	MAN	C1-O5-C5	4.01	117.56	112.19
11	p	8	MAN	C1-O5-C5	4.01	117.56	112.19
7	c	1	NAG	C2-N2-C7	3.96	128.21	122.90
10	d	8	MAN	C1-O5-C5	3.92	117.44	112.19
10	l	8	MAN	C1-O5-C5	3.83	117.32	112.19
11	p	5	MAN	C1-O5-C5	3.80	117.28	112.19
7	o	2	NAG	O5-C5-C6	-3.71	100.44	107.66
11	p	6	MAN	C1-O5-C5	3.51	116.89	112.19
10	d	9	MAN	C1-O5-C5	3.48	116.85	112.19
10	l	6	MAN	C1-O5-C5	3.40	116.75	112.19
9	u	5	MAN	C1-O5-C5	3.40	116.74	112.19
7	h	3	BMA	C1-O5-C5	3.37	116.70	112.19
7	0	1	NAG	C1-O5-C5	3.34	116.67	112.19
10	l	9	MAN	C1-O5-C5	3.33	116.65	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	3	BMA	C1-O5-C5	3.32	116.64	112.19
10	d	6	MAN	C1-O5-C5	3.30	116.61	112.19
7	c	1	NAG	C1-O5-C5	3.29	116.59	112.19
9	u	1	NAG	C1-O5-C5	3.27	116.57	112.19
9	W	1	NAG	C1-O5-C5	3.23	116.52	112.19
7	t	3	BMA	C1-O5-C5	3.23	116.51	112.19
9	i	1	NAG	C1-O5-C5	3.13	116.38	112.19
7	o	1	NAG	C1-O5-C5	3.04	116.27	112.19
7	0	2	NAG	C1-O5-C5	3.03	116.25	112.19
9	i	5	MAN	C1-O5-C5	3.02	116.24	112.19
11	p	3	BMA	C2-C3-C4	2.98	116.10	110.86
7	c	2	NAG	O5-C1-C2	-2.95	106.73	111.29
7	o	2	NAG	O5-C1-C2	-2.89	106.82	111.29
10	l	3	BMA	C2-C3-C4	2.81	115.81	110.86
7	e	3	BMA	C1-O5-C5	2.81	115.95	112.19
8	b	2	NAG	C1-O5-C5	2.79	115.92	112.19
7	c	1	NAG	C1-C2-N2	2.77	114.81	110.43
8	w	1	NAG	C3-C4-C5	2.75	115.22	110.23
8	k	1	NAG	O4-C4-C3	-2.74	103.91	110.38
8	k	1	NAG	C3-C4-C5	2.74	115.20	110.23
8	z	2	NAG	C1-O5-C5	2.73	115.85	112.19
7	S	3	BMA	C1-O5-C5	2.73	115.84	112.19
7	q	3	BMA	C1-O5-C5	2.72	115.83	112.19
8	n	2	NAG	C1-O5-C5	2.69	115.79	112.19
8	w	1	NAG	O4-C4-C3	-2.68	104.06	110.38
10	d	3	BMA	C2-C3-C4	2.66	115.54	110.86
8	k	1	NAG	C4-C3-C2	2.65	114.91	111.02
8	Y	1	NAG	C3-C4-C5	2.64	115.02	110.23
7	V	2	NAG	C1-C2-N2	2.60	114.53	110.43
8	w	1	NAG	C4-C3-C2	2.58	114.80	111.02
8	s	1	NAG	C8-C7-N2	2.57	120.38	116.12
8	l	2	NAG	C1-O5-C5	2.57	115.63	112.19
7	e	2	NAG	C8-C7-N2	2.57	120.37	116.12
8	U	1	NAG	C8-C7-N2	2.56	120.36	116.12
8	g	1	NAG	C8-C7-N2	2.56	120.36	116.12
7	q	2	NAG	C8-C7-N2	2.55	120.35	116.12
8	Z	2	NAG	C1-O5-C5	2.55	115.60	112.19
8	f	1	NAG	C8-C7-N2	2.55	120.34	116.12
7	S	2	NAG	C8-C7-N2	2.54	120.34	116.12
8	r	1	NAG	C8-C7-N2	2.54	120.33	116.12
8	x	2	NAG	C1-O5-C5	2.53	115.58	112.19
8	j	2	NAG	C8-C7-N2	2.53	120.32	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	0	2	NAG	O5-C1-C2	-2.53	107.38	111.29
8	T	1	NAG	C8-C7-N2	2.52	120.30	116.12
11	p	3	BMA	C1-C2-C3	2.51	113.30	109.64
8	X	2	NAG	C8-C7-N2	2.51	120.28	116.12
10	l	3	BMA	C1-C2-C3	2.51	113.30	109.64
8	v	2	NAG	C8-C7-N2	2.49	120.25	116.12
8	Y	1	NAG	O4-C4-C3	-2.45	104.60	110.38
9	u	1	NAG	C8-C7-N2	2.44	120.16	116.12
7	q	1	NAG	C1-O5-C5	2.43	115.44	112.19
10	d	3	BMA	C1-C2-C3	2.43	113.18	109.64
7	S	1	NAG	C1-O5-C5	2.43	115.44	112.19
9	i	3	BMA	C1-O5-C5	2.42	115.43	112.19
9	i	1	NAG	C8-C7-N2	2.42	120.13	116.12
7	e	1	NAG	C1-O5-C5	2.42	115.42	112.19
9	W	1	NAG	C8-C7-N2	2.41	120.12	116.12
8	Y	1	NAG	C4-C3-C2	2.39	114.53	111.02
7	h	2	NAG	C1-O5-C5	2.39	115.39	112.19
8	r	2	NAG	C1-O5-C5	2.31	115.29	112.19
8	s	2	NAG	C1-O5-C5	2.29	115.26	112.19
8	g	2	NAG	C1-O5-C5	2.29	115.26	112.19
8	T	2	NAG	C1-O5-C5	2.28	115.25	112.19
7	o	2	NAG	O4-C4-C3	-2.28	105.01	110.38
8	f	2	NAG	C1-O5-C5	2.27	115.22	112.19
7	h	1	NAG	O4-C4-C5	-2.26	103.75	109.32
9	W	5	MAN	C1-O5-C5	2.25	115.21	112.19
9	W	5	MAN	O2-C2-C3	-2.25	105.48	110.15
8	U	2	NAG	C1-O5-C5	2.25	115.20	112.19
9	u	2	NAG	C1-O5-C5	2.24	115.19	112.19
8	k	1	NAG	C1-O5-C5	2.24	115.19	112.19
7	V	2	NAG	C1-O5-C5	2.24	115.19	112.19
8	w	1	NAG	C1-O5-C5	2.23	115.18	112.19
7	c	1	NAG	C3-C4-C5	-2.23	106.19	110.23
9	i	2	NAG	C1-O5-C5	2.22	115.16	112.19
10	l	7	MAN	O2-C2-C3	-2.22	105.56	110.15
8	z	1	NAG	C1-O5-C5	2.21	115.15	112.19
8	n	1	NAG	C1-O5-C5	2.20	115.14	112.19
9	u	5	MAN	O2-C2-C3	-2.20	105.59	110.15
9	i	5	MAN	O2-C2-C3	-2.18	105.63	110.15
11	p	3	BMA	O5-C5-C6	-2.18	103.41	107.66
10	d	7	MAN	O2-C2-C3	-2.18	105.63	110.15
11	p	7	MAN	O2-C2-C3	-2.17	105.66	110.15
8	Y	2	NAG	C1-O5-C5	2.16	115.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	1	8	MAN	O2-C2-C3	-2.14	105.72	110.15
10	1	6	MAN	O2-C2-C3	-2.14	105.72	110.15
10	d	6	MAN	O2-C2-C3	-2.14	105.73	110.15
10	d	8	MAN	O2-C2-C3	-2.14	105.73	110.15
9	u	4	MAN	O2-C2-C3	-2.13	105.73	110.15
9	W	2	NAG	C1-O5-C5	2.13	115.04	112.19
8	X	1	NAG	C1-O5-C5	2.13	115.03	112.19
8	j	1	NAG	C1-O5-C5	2.12	115.03	112.19
7	0	2	NAG	C3-C4-C5	-2.11	106.41	110.23
7	c	2	NAG	O5-C5-C6	-2.10	103.57	107.66
10	d	3	BMA	O5-C5-C6	-2.10	103.57	107.66
7	0	2	NAG	O5-C5-C6	-2.10	103.58	107.66
9	u	3	BMA	C1-O5-C5	2.10	115.00	112.19
10	1	2	NAG	C1-O5-C5	2.10	115.00	112.19
7	t	1	NAG	C2-N2-C7	2.10	125.71	122.90
11	p	6	MAN	O2-C2-C3	-2.09	105.83	110.15
8	a	2	NAG	C1-O5-C5	2.08	114.98	112.19
11	p	8	MAN	O2-C2-C3	-2.08	105.85	110.15
9	W	3	BMA	C1-O5-C5	2.07	114.97	112.19
11	p	5	MAN	O2-C2-C3	-2.07	105.86	110.15
10	d	9	MAN	O2-C2-C3	-2.06	105.87	110.15
8	b	1	NAG	C1-O5-C5	2.06	114.95	112.19
8	s	1	NAG	C1-O5-C5	2.06	114.95	112.19
10	d	2	NAG	C1-O5-C5	2.06	114.94	112.19
8	g	2	NAG	C2-N2-C7	2.05	125.65	122.90
8	Z	2	NAG	C2-N2-C7	2.05	125.65	122.90
10	1	9	MAN	O2-C2-C3	-2.04	105.92	110.15
11	p	2	NAG	C1-O5-C5	2.04	114.92	112.19
8	b	2	NAG	C2-N2-C7	2.04	125.63	122.90
11	p	2	NAG	O4-C4-C5	-2.04	104.30	109.32
8	y	2	NAG	C1-O5-C5	2.04	114.92	112.19
8	l	2	NAG	C2-N2-C7	2.03	125.63	122.90
8	v	1	NAG	C1-O5-C5	2.03	114.91	112.19
8	x	2	NAG	C2-N2-C7	2.03	125.62	122.90
8	n	2	NAG	C2-N2-C7	2.02	125.61	122.90
8	U	1	NAG	C1-O5-C5	2.01	114.88	112.19
8	g	1	NAG	C1-O5-C5	2.00	114.87	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	c	1	NAG	C1

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Mol	Chain	Res	Type	Atom
7	o	1	NAG	C1
7	0	1	NAG	C1

All (208) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	c	1	NAG	C8-C7-N2-C2
7	c	1	NAG	O7-C7-N2-C2
7	c	2	NAG	C8-C7-N2-C2
7	c	2	NAG	O7-C7-N2-C2
7	o	1	NAG	C8-C7-N2-C2
7	o	1	NAG	O7-C7-N2-C2
7	0	1	NAG	C8-C7-N2-C2
8	Y	2	NAG	O5-C5-C6-O6
8	w	2	NAG	O5-C5-C6-O6
10	d	7	MAN	O5-C5-C6-O6
7	0	1	NAG	O7-C7-N2-C2
8	k	2	NAG	O5-C5-C6-O6
8	x	2	NAG	O5-C5-C6-O6
10	l	7	MAN	O5-C5-C6-O6
7	t	1	NAG	O5-C5-C6-O6
7	t	3	BMA	O5-C5-C6-O6
8	Z	2	NAG	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
7	q	2	NAG	O5-C5-C6-O6
8	k	1	NAG	O5-C5-C6-O6
8	l	2	NAG	O5-C5-C6-O6
8	m	1	NAG	O5-C5-C6-O6
8	w	1	NAG	O5-C5-C6-O6
10	d	5	MAN	O5-C5-C6-O6
10	l	5	MAN	O5-C5-C6-O6
11	p	5	MAN	O5-C5-C6-O6
7	t	3	BMA	C4-C5-C6-O6
8	l	2	NAG	C4-C5-C6-O6
8	x	2	NAG	C4-C5-C6-O6
8	Z	2	NAG	C4-C5-C6-O6
8	Y	2	NAG	C4-C5-C6-O6
8	k	2	NAG	C4-C5-C6-O6
8	w	2	NAG	C4-C5-C6-O6
10	d	7	MAN	C4-C5-C6-O6
11	p	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	Y	1	NAG	O5-C5-C6-O6
10	1	7	MAN	C4-C5-C6-O6
7	0	2	NAG	O5-C5-C6-O6
7	t	1	NAG	C4-C5-C6-O6
7	V	1	NAG	O5-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
8	w	1	NAG	C4-C5-C6-O6
7	q	2	NAG	C4-C5-C6-O6
8	k	1	NAG	C4-C5-C6-O6
7	V	1	NAG	C4-C5-C6-O6
7	h	1	NAG	C4-C5-C6-O6
7	0	2	NAG	C8-C7-N2-C2
7	h	2	NAG	O5-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
10	d	5	MAN	C4-C5-C6-O6
10	1	5	MAN	C4-C5-C6-O6
10	1	3	BMA	O5-C5-C6-O6
7	h	2	NAG	C4-C5-C6-O6
7	V	3	BMA	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	S	2	NAG	C8-C7-N2-C2
7	S	2	NAG	O7-C7-N2-C2
7	e	2	NAG	C8-C7-N2-C2
7	e	2	NAG	O7-C7-N2-C2
7	h	1	NAG	C8-C7-N2-C2
7	h	1	NAG	O7-C7-N2-C2
7	o	2	NAG	C8-C7-N2-C2
7	o	2	NAG	O7-C7-N2-C2
7	q	2	NAG	C8-C7-N2-C2
7	q	2	NAG	O7-C7-N2-C2
7	t	1	NAG	C8-C7-N2-C2
7	t	1	NAG	O7-C7-N2-C2
7	0	2	NAG	O7-C7-N2-C2
8	T	1	NAG	C8-C7-N2-C2
8	T	1	NAG	O7-C7-N2-C2
8	U	1	NAG	C8-C7-N2-C2
8	U	1	NAG	O7-C7-N2-C2
8	X	2	NAG	C8-C7-N2-C2
8	X	2	NAG	O7-C7-N2-C2
8	Z	2	NAG	C8-C7-N2-C2
8	Z	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	b	2	NAG	C8-C7-N2-C2
8	b	2	NAG	O7-C7-N2-C2
8	f	1	NAG	C8-C7-N2-C2
8	f	1	NAG	O7-C7-N2-C2
8	g	1	NAG	C8-C7-N2-C2
8	g	1	NAG	O7-C7-N2-C2
8	g	2	NAG	C8-C7-N2-C2
8	g	2	NAG	O7-C7-N2-C2
8	j	2	NAG	C8-C7-N2-C2
8	j	2	NAG	O7-C7-N2-C2
8	l	2	NAG	C8-C7-N2-C2
8	l	2	NAG	O7-C7-N2-C2
8	n	2	NAG	C8-C7-N2-C2
8	n	2	NAG	O7-C7-N2-C2
8	r	1	NAG	C8-C7-N2-C2
8	r	1	NAG	O7-C7-N2-C2
8	s	1	NAG	C8-C7-N2-C2
8	s	1	NAG	O7-C7-N2-C2
8	v	2	NAG	C8-C7-N2-C2
8	v	2	NAG	O7-C7-N2-C2
8	x	2	NAG	C8-C7-N2-C2
8	x	2	NAG	O7-C7-N2-C2
8	z	2	NAG	C8-C7-N2-C2
8	z	2	NAG	O7-C7-N2-C2
9	W	1	NAG	C8-C7-N2-C2
9	W	1	NAG	O7-C7-N2-C2
9	i	1	NAG	C8-C7-N2-C2
9	i	1	NAG	O7-C7-N2-C2
9	u	1	NAG	C8-C7-N2-C2
9	u	1	NAG	O7-C7-N2-C2
8	U	1	NAG	O5-C5-C6-O6
8	a	1	NAG	O5-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
8	g	1	NAG	C4-C5-C6-O6
7	V	3	BMA	C4-C5-C6-O6
9	u	3	BMA	O5-C5-C6-O6
8	m	1	NAG	C4-C5-C6-O6
7	V	2	NAG	C4-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
8	s	1	NAG	C4-C5-C6-O6
8	s	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	u	3	BMA	C4-C5-C6-O6
11	p	7	MAN	O5-C5-C6-O6
7	0	2	NAG	C4-C5-C6-O6
8	X	2	NAG	C4-C5-C6-O6
7	h	3	BMA	O5-C5-C6-O6
8	y	1	NAG	O5-C5-C6-O6
10	d	3	BMA	O5-C5-C6-O6
8	v	2	NAG	C4-C5-C6-O6
8	f	2	NAG	C4-C5-C6-O6
8	X	2	NAG	O5-C5-C6-O6
11	p	3	BMA	O5-C5-C6-O6
7	c	1	NAG	C3-C2-N2-C7
8	f	2	NAG	O5-C5-C6-O6
10	l	1	NAG	C4-C5-C6-O6
7	o	3	BMA	C4-C5-C6-O6
9	u	2	NAG	C4-C5-C6-O6
7	t	2	NAG	C4-C5-C6-O6
8	r	2	NAG	C4-C5-C6-O6
8	v	2	NAG	O5-C5-C6-O6
8	r	2	NAG	O5-C5-C6-O6
9	u	2	NAG	O5-C5-C6-O6
7	o	1	NAG	C1-C2-N2-C7
7	0	1	NAG	C1-C2-N2-C7
8	z	1	NAG	O5-C5-C6-O6
7	c	3	BMA	C4-C5-C6-O6
8	j	2	NAG	C4-C5-C6-O6
7	0	1	NAG	C4-C5-C6-O6
8	a	1	NAG	C4-C5-C6-O6
10	l	4	MAN	C4-C5-C6-O6
10	l	1	NAG	O5-C5-C6-O6
7	t	2	NAG	O5-C5-C6-O6
8	T	2	NAG	C4-C5-C6-O6
10	l	4	MAN	O5-C5-C6-O6
8	n	1	NAG	O5-C5-C6-O6
9	W	5	MAN	C4-C5-C6-O6
11	p	1	NAG	C4-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
7	h	3	BMA	C4-C5-C6-O6
7	o	3	BMA	O5-C5-C6-O6
8	j	2	NAG	O5-C5-C6-O6
8	j	1	NAG	C4-C5-C6-O6
7	0	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	S	2	NAG	C1-C2-N2-C7
7	V	2	NAG	C1-C2-N2-C7
7	e	2	NAG	C1-C2-N2-C7
7	q	2	NAG	C1-C2-N2-C7
7	0	2	NAG	C1-C2-N2-C7
8	T	1	NAG	C1-C2-N2-C7
8	U	1	NAG	C1-C2-N2-C7
8	X	2	NAG	C1-C2-N2-C7
8	f	1	NAG	C1-C2-N2-C7
8	g	1	NAG	C1-C2-N2-C7
8	j	2	NAG	C1-C2-N2-C7
8	r	1	NAG	C1-C2-N2-C7
8	s	1	NAG	C1-C2-N2-C7
8	v	2	NAG	C1-C2-N2-C7
9	W	1	NAG	C1-C2-N2-C7
9	i	1	NAG	C1-C2-N2-C7
9	u	1	NAG	C1-C2-N2-C7
7	S	2	NAG	C3-C2-N2-C7
7	V	2	NAG	C3-C2-N2-C7
7	e	2	NAG	C3-C2-N2-C7
7	o	1	NAG	C3-C2-N2-C7
7	q	2	NAG	C3-C2-N2-C7
7	0	1	NAG	C3-C2-N2-C7
8	T	1	NAG	C3-C2-N2-C7
8	U	1	NAG	C3-C2-N2-C7
8	X	2	NAG	C3-C2-N2-C7
8	f	1	NAG	C3-C2-N2-C7
8	g	1	NAG	C3-C2-N2-C7
8	j	2	NAG	C3-C2-N2-C7
8	r	1	NAG	C3-C2-N2-C7
8	s	1	NAG	C3-C2-N2-C7
8	v	2	NAG	C3-C2-N2-C7
9	W	1	NAG	C3-C2-N2-C7
9	i	1	NAG	C3-C2-N2-C7
9	u	1	NAG	C3-C2-N2-C7
8	m	2	NAG	C4-C5-C6-O6
7	0	3	BMA	C4-C5-C6-O6
11	p	7	MAN	C4-C5-C6-O6
9	i	2	NAG	C4-C5-C6-O6
8	j	1	NAG	O5-C5-C6-O6
7	c	3	BMA	O5-C5-C6-O6
10	d	1	NAG	C4-C5-C6-O6

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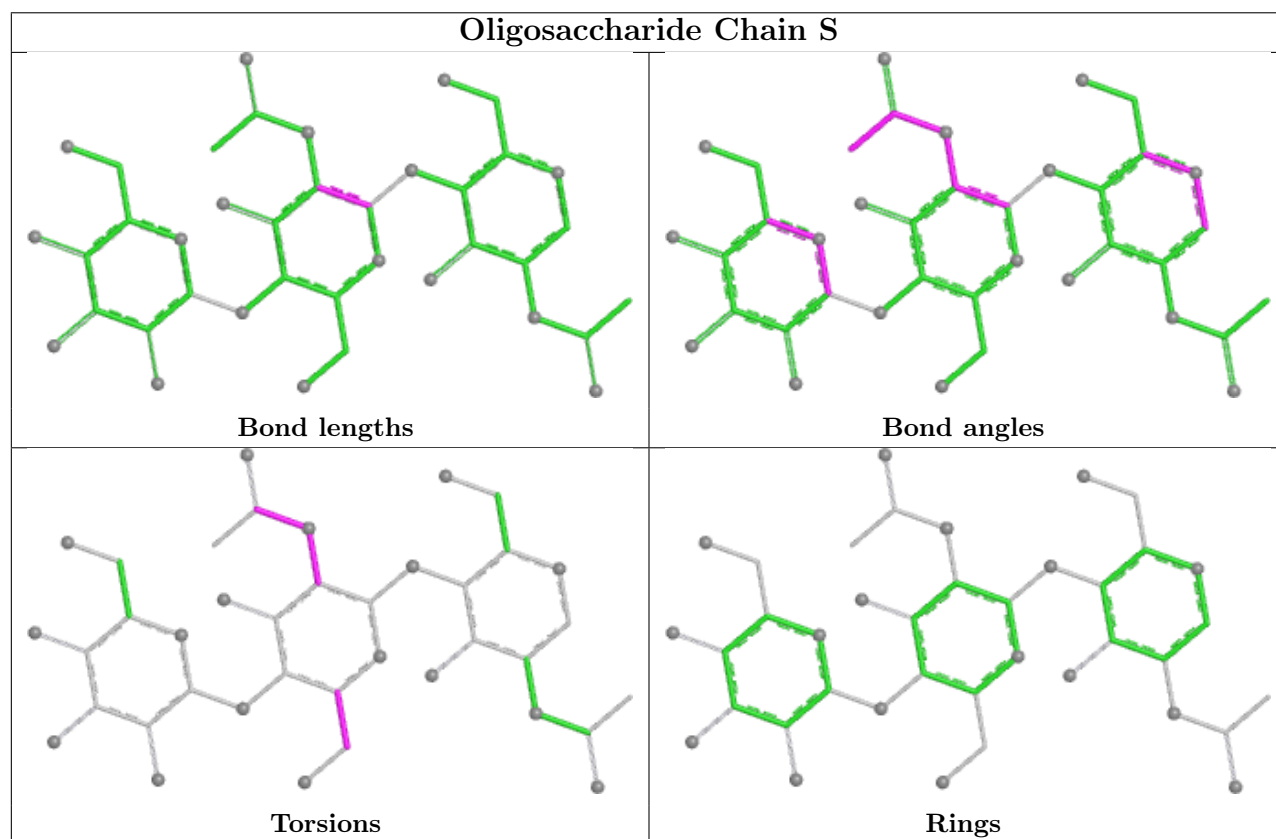
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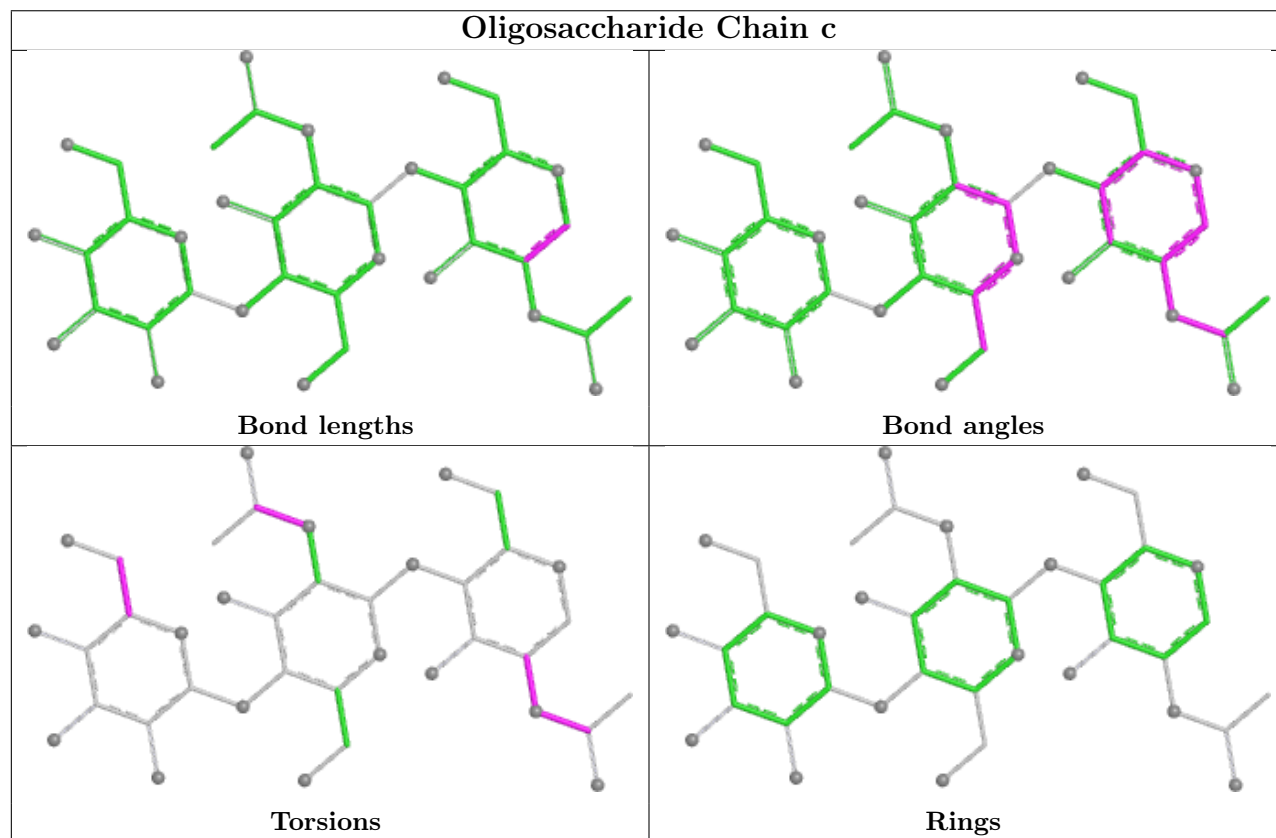
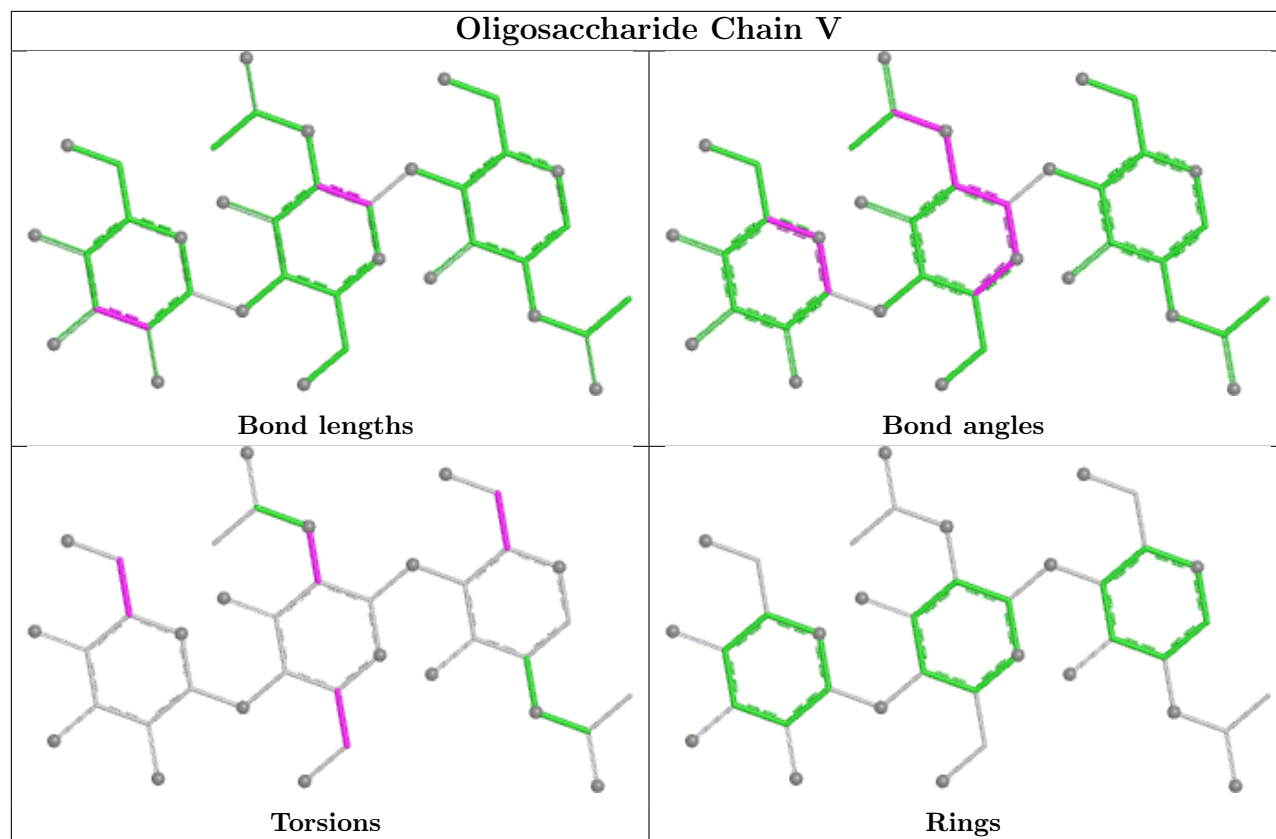
Mol	Chain	Res	Type	Atoms
8	X	1	NAG	C4-C5-C6-O6
8	v	1	NAG	C4-C5-C6-O6
11	p	1	NAG	O5-C5-C6-O6
11	p	8	MAN	O5-C5-C6-O6

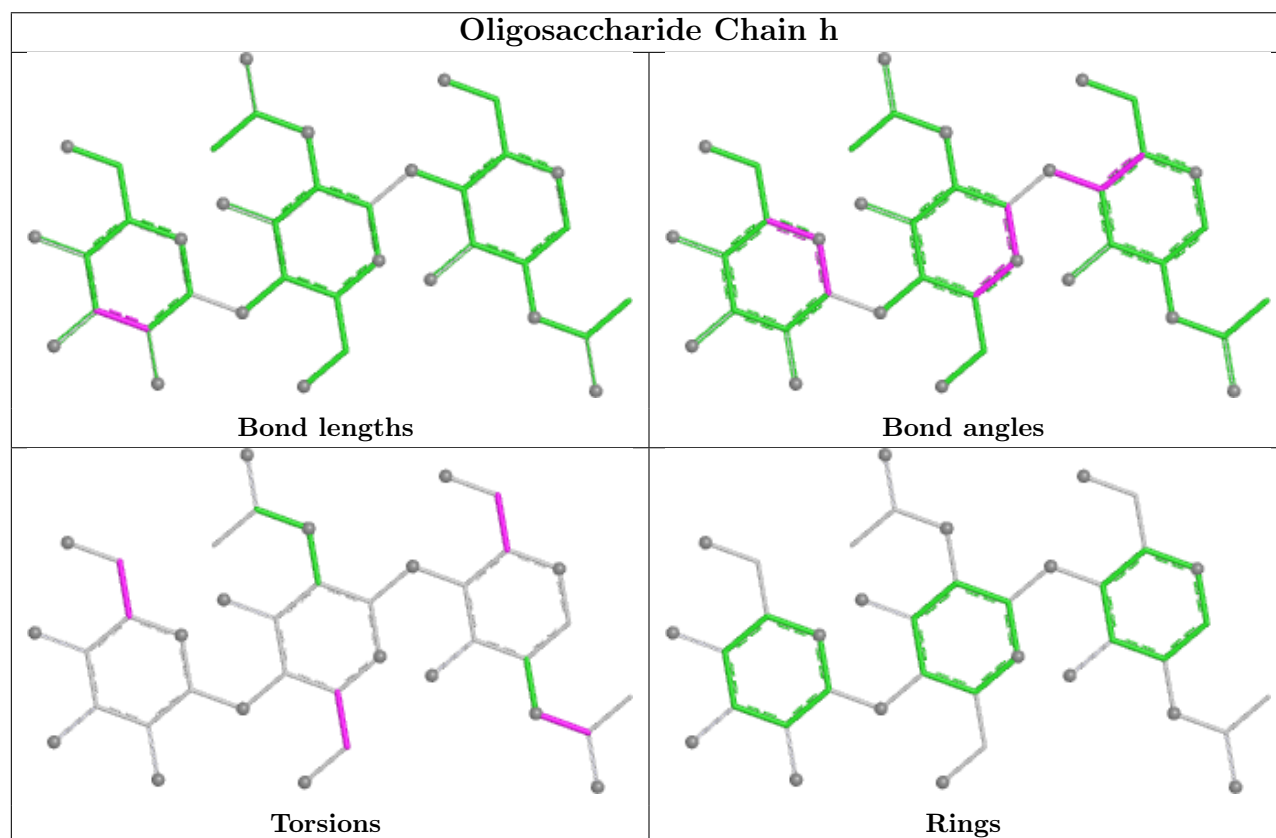
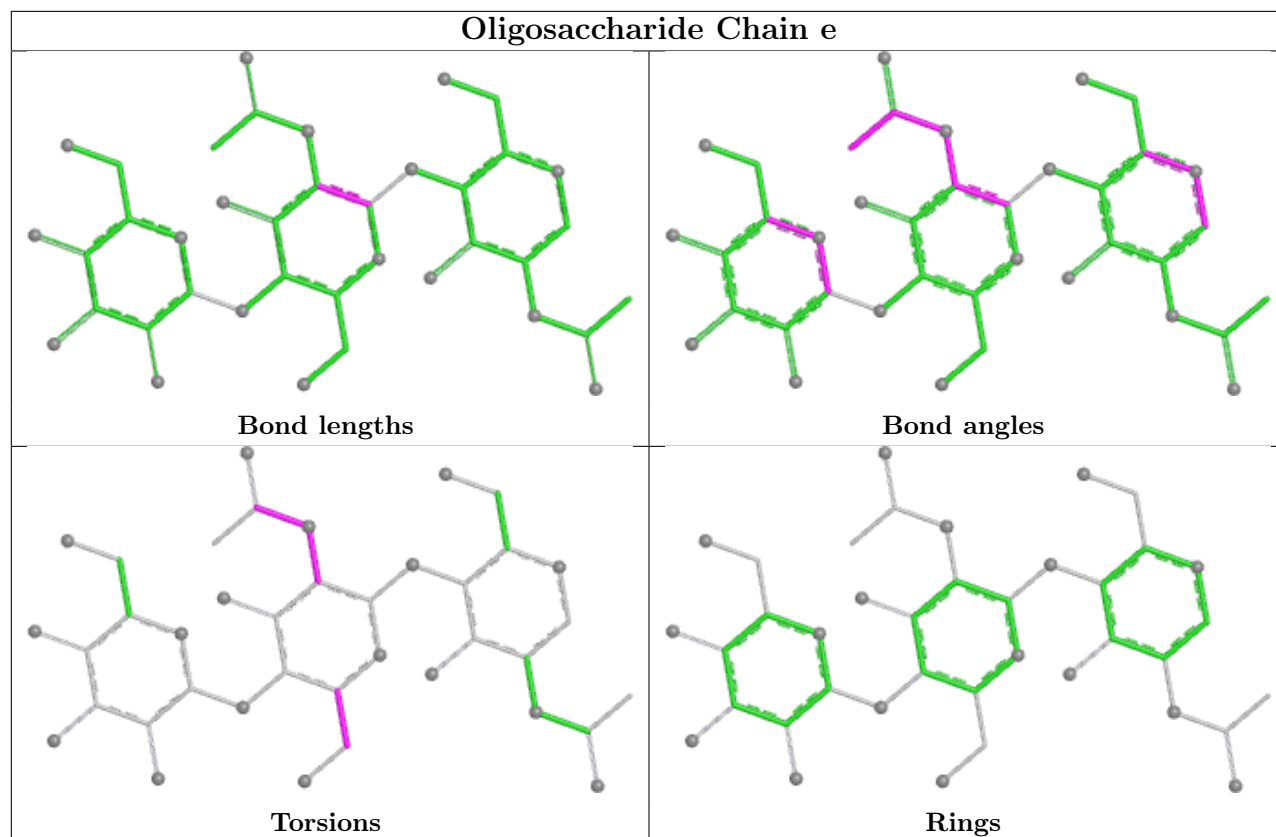
There are no ring outliers.

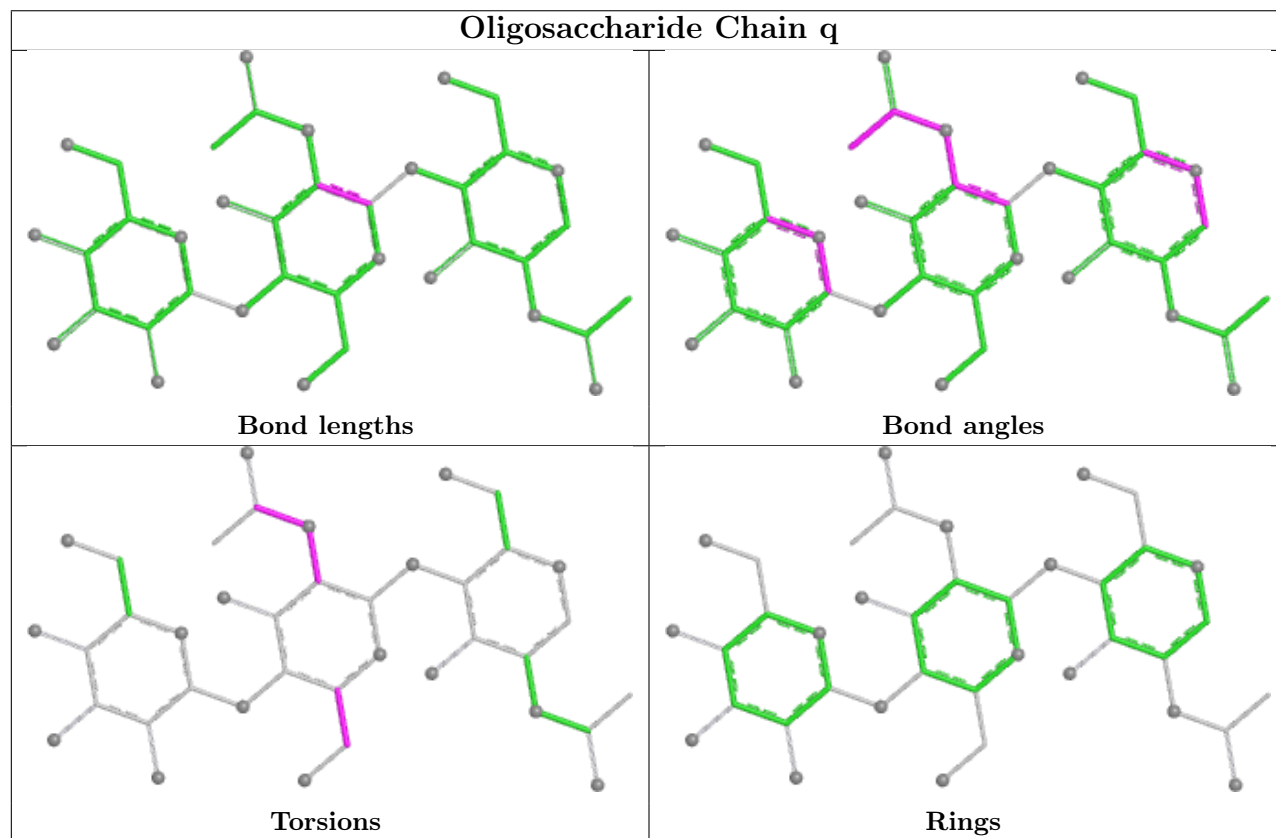
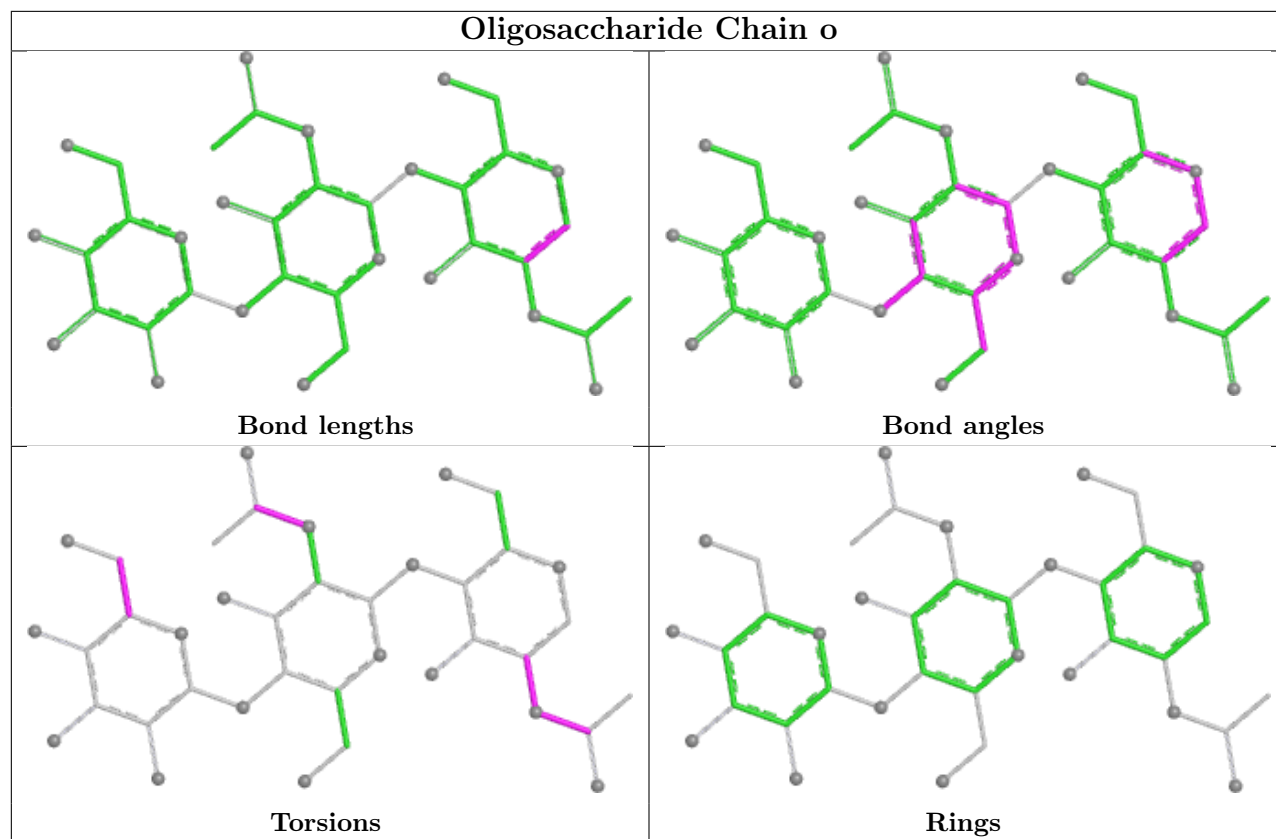
No monomer is involved in short contacts.

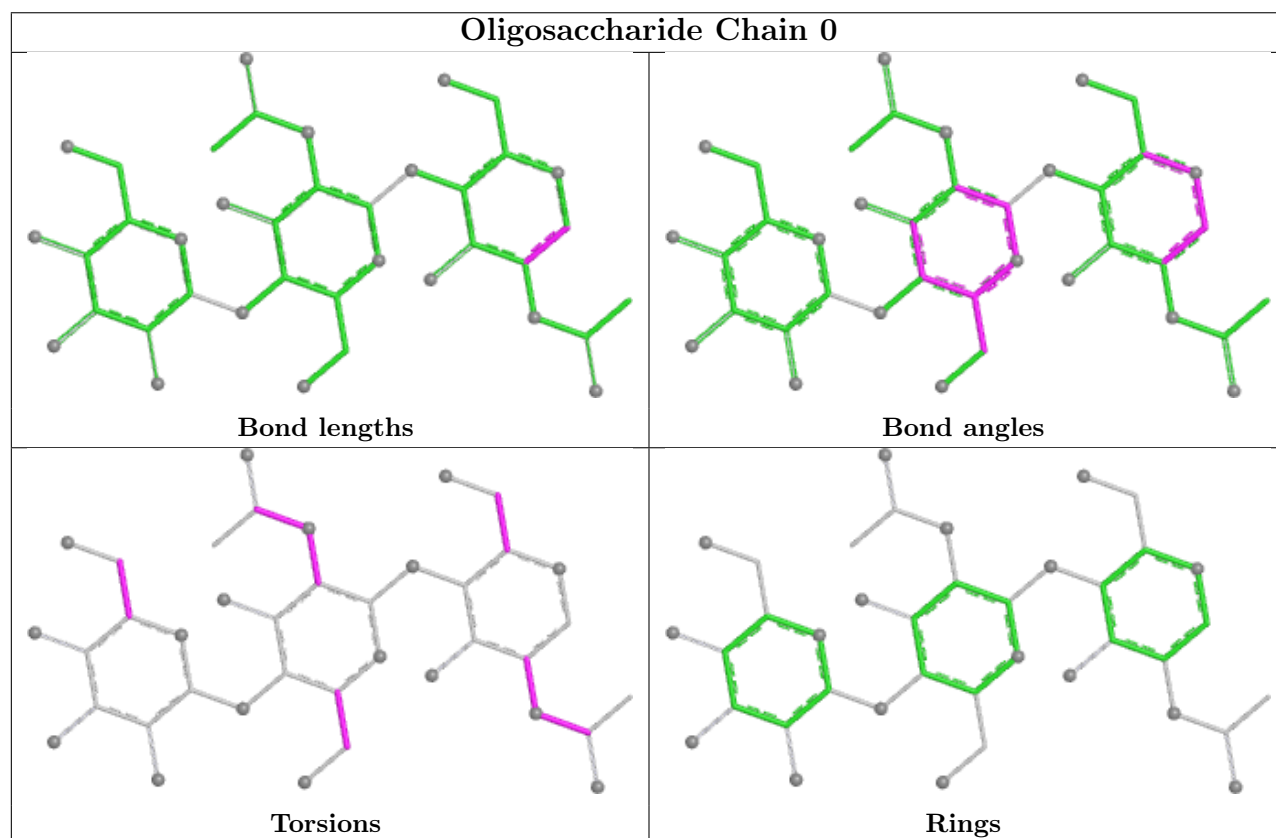
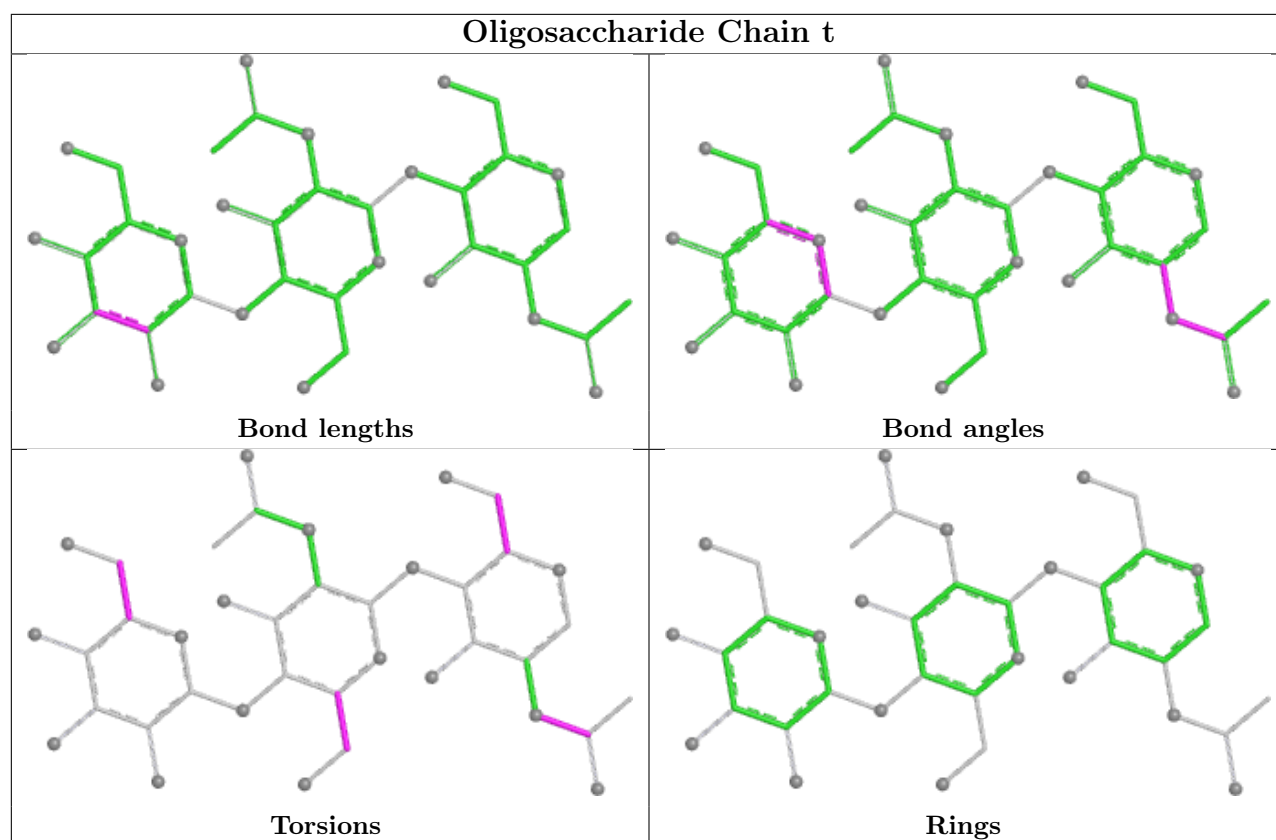
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

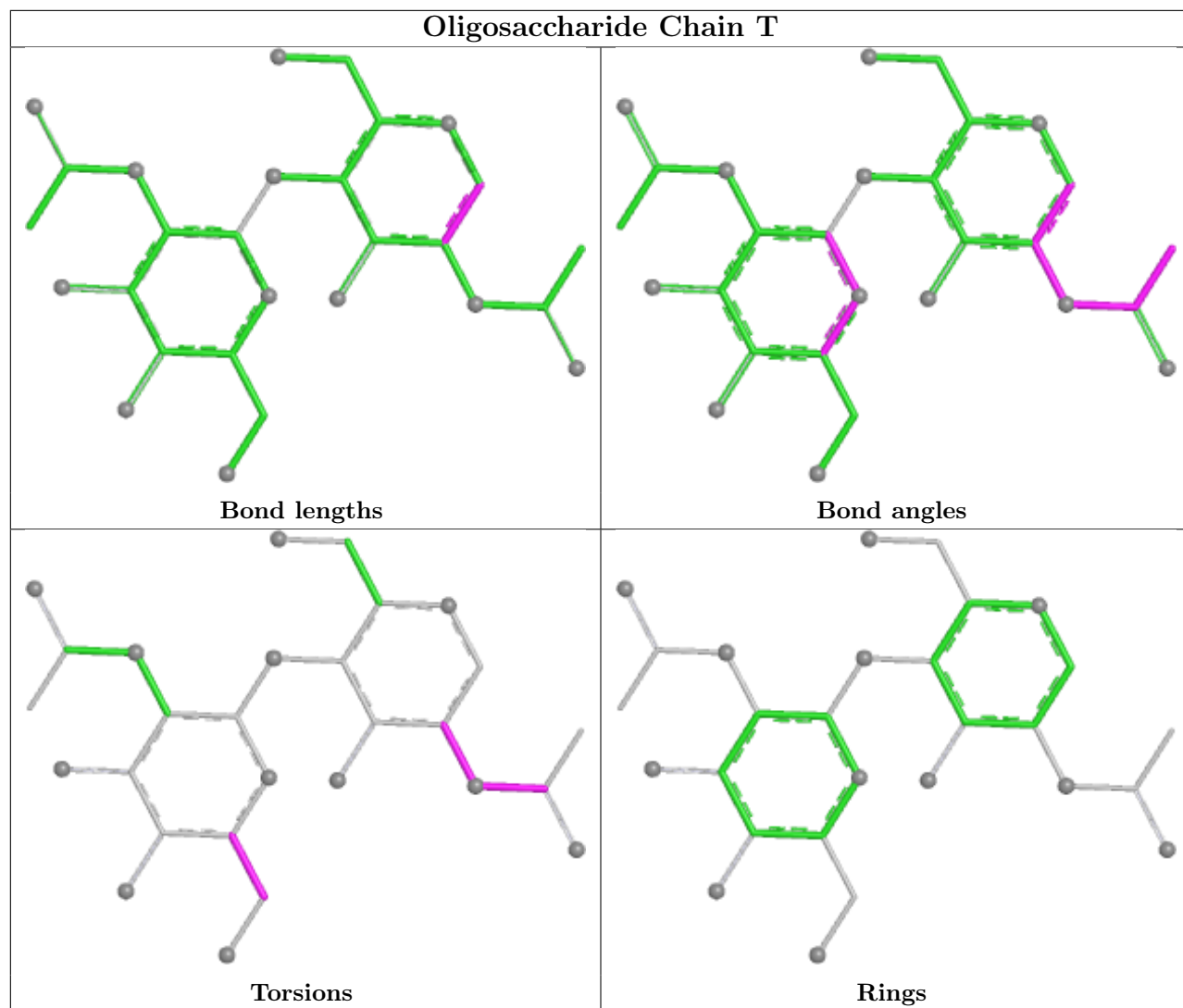


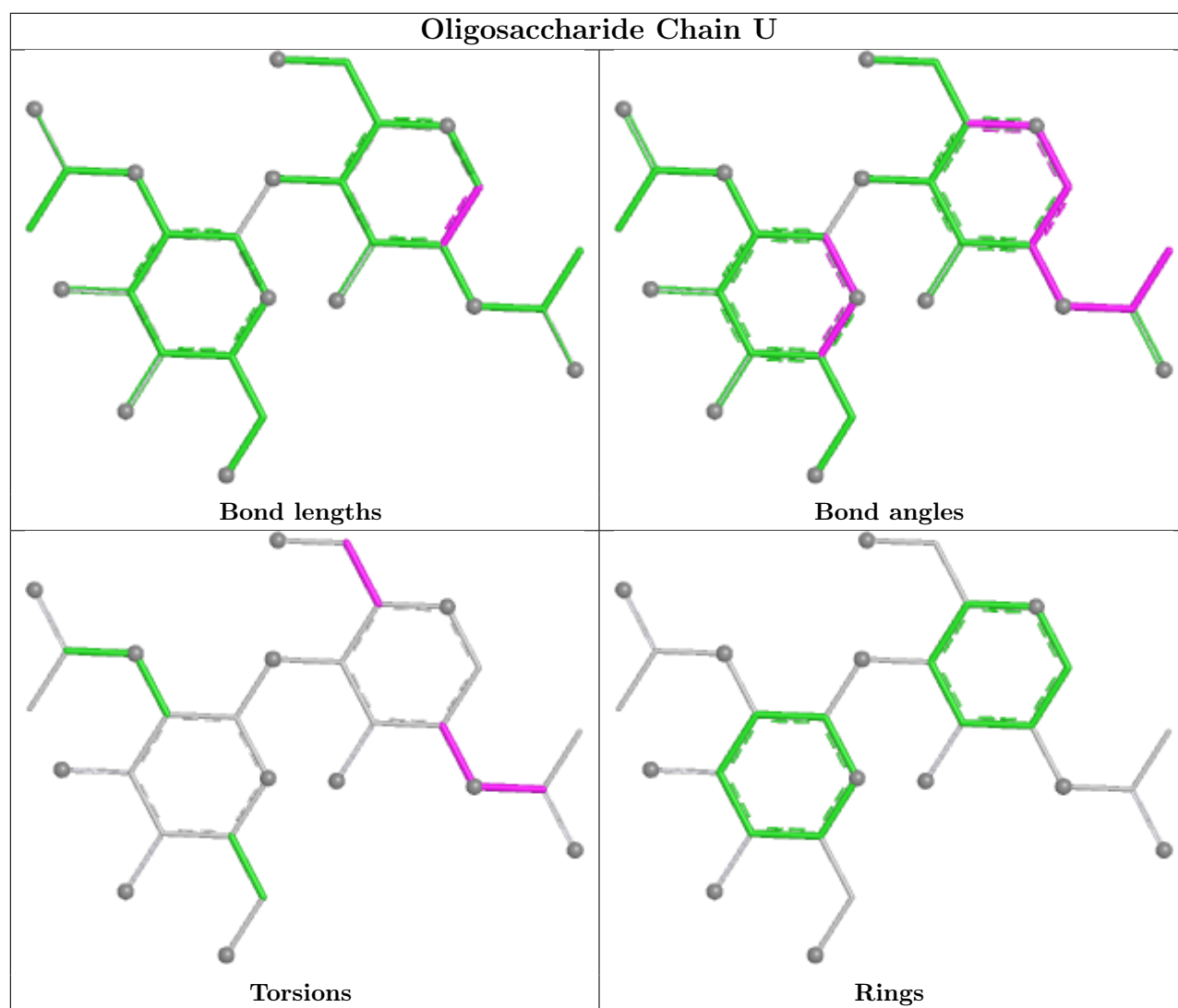


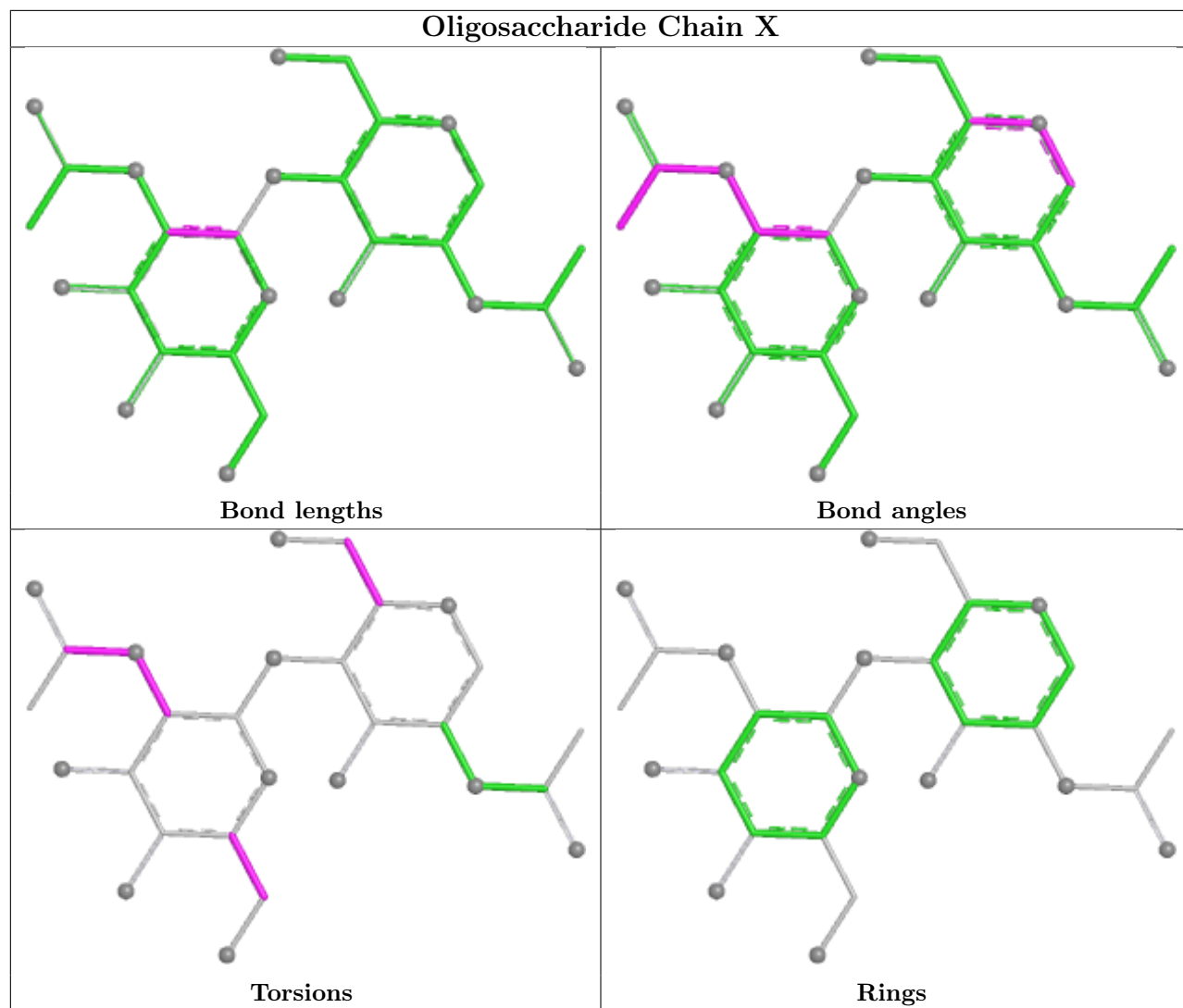


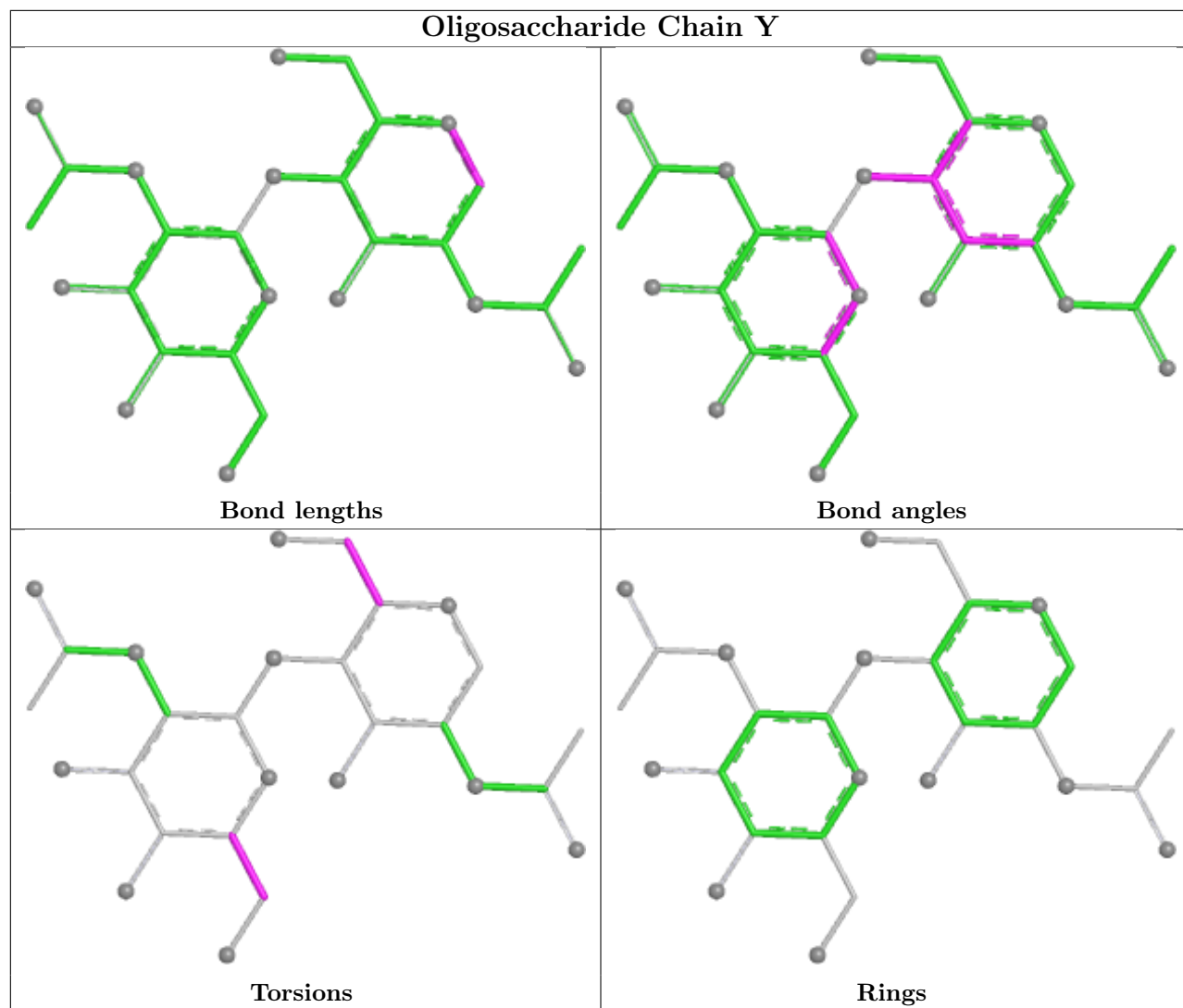


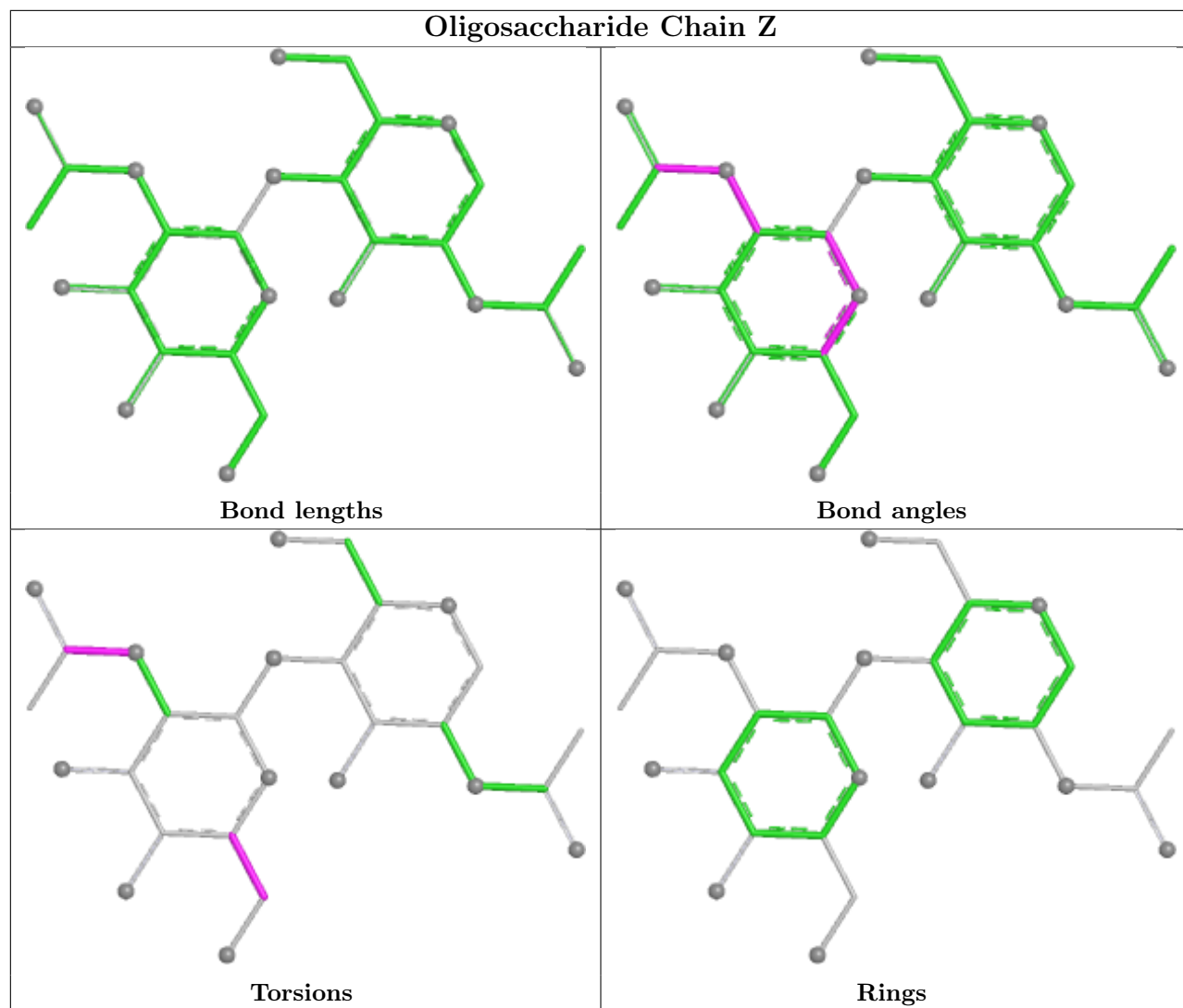


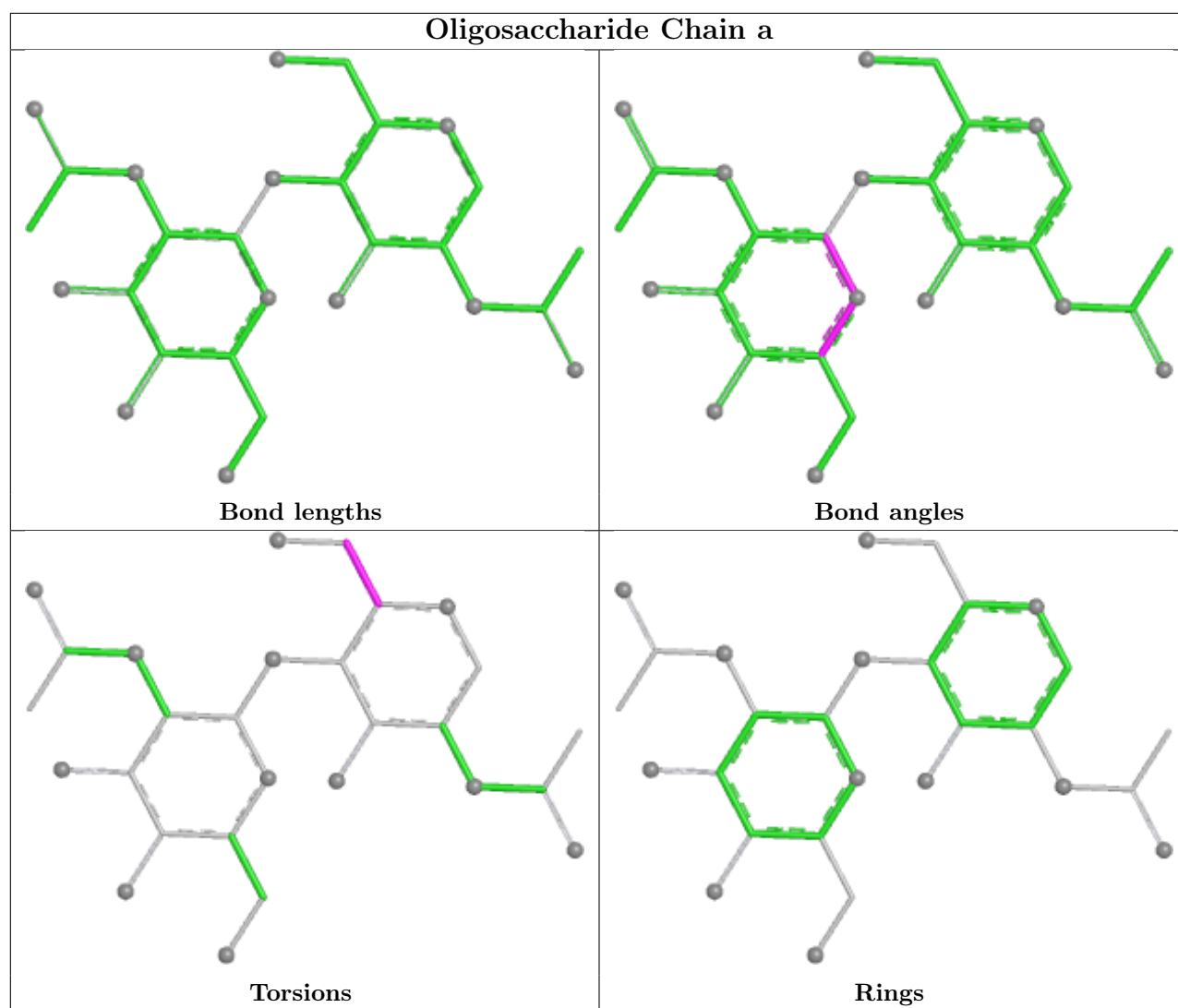


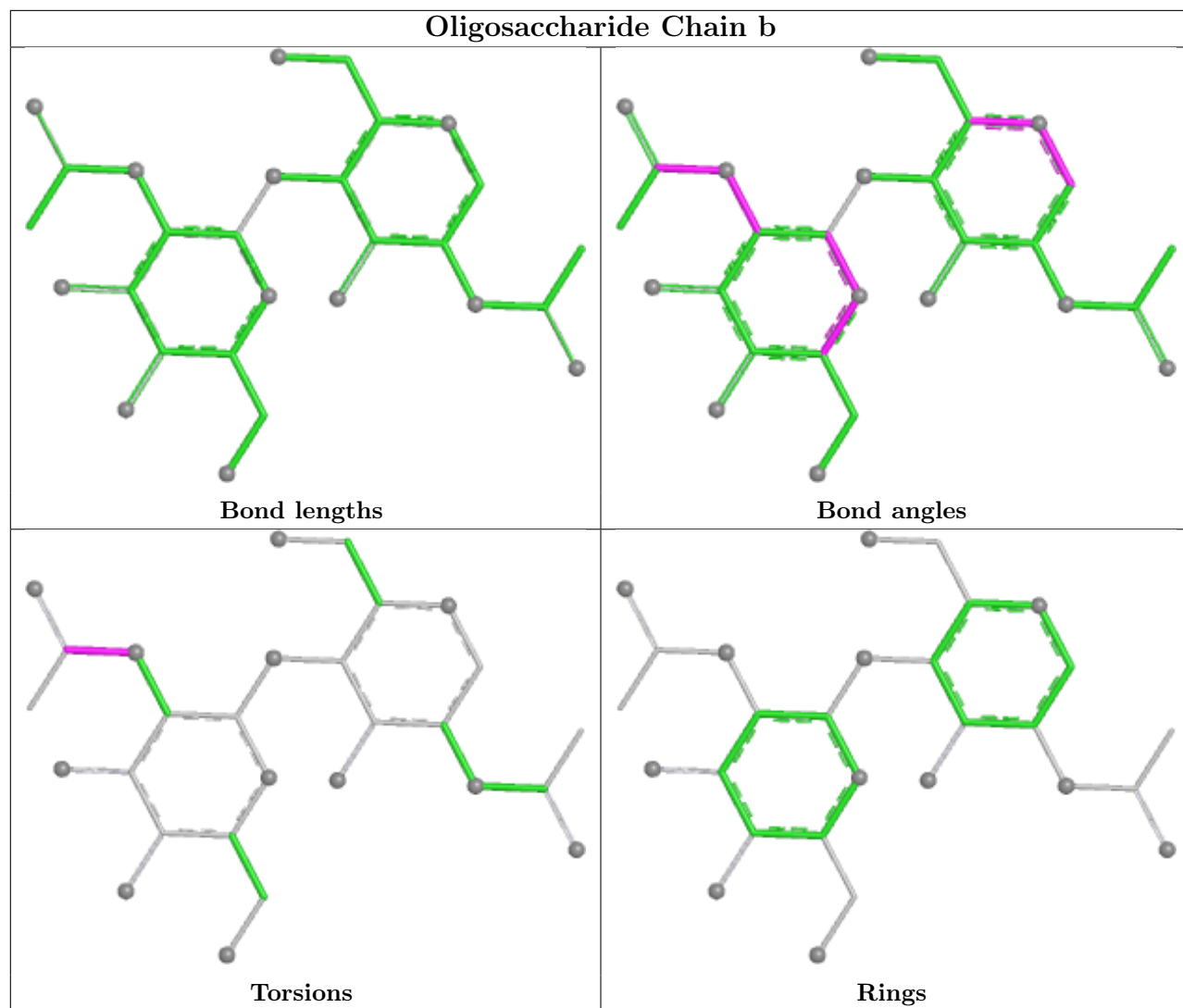


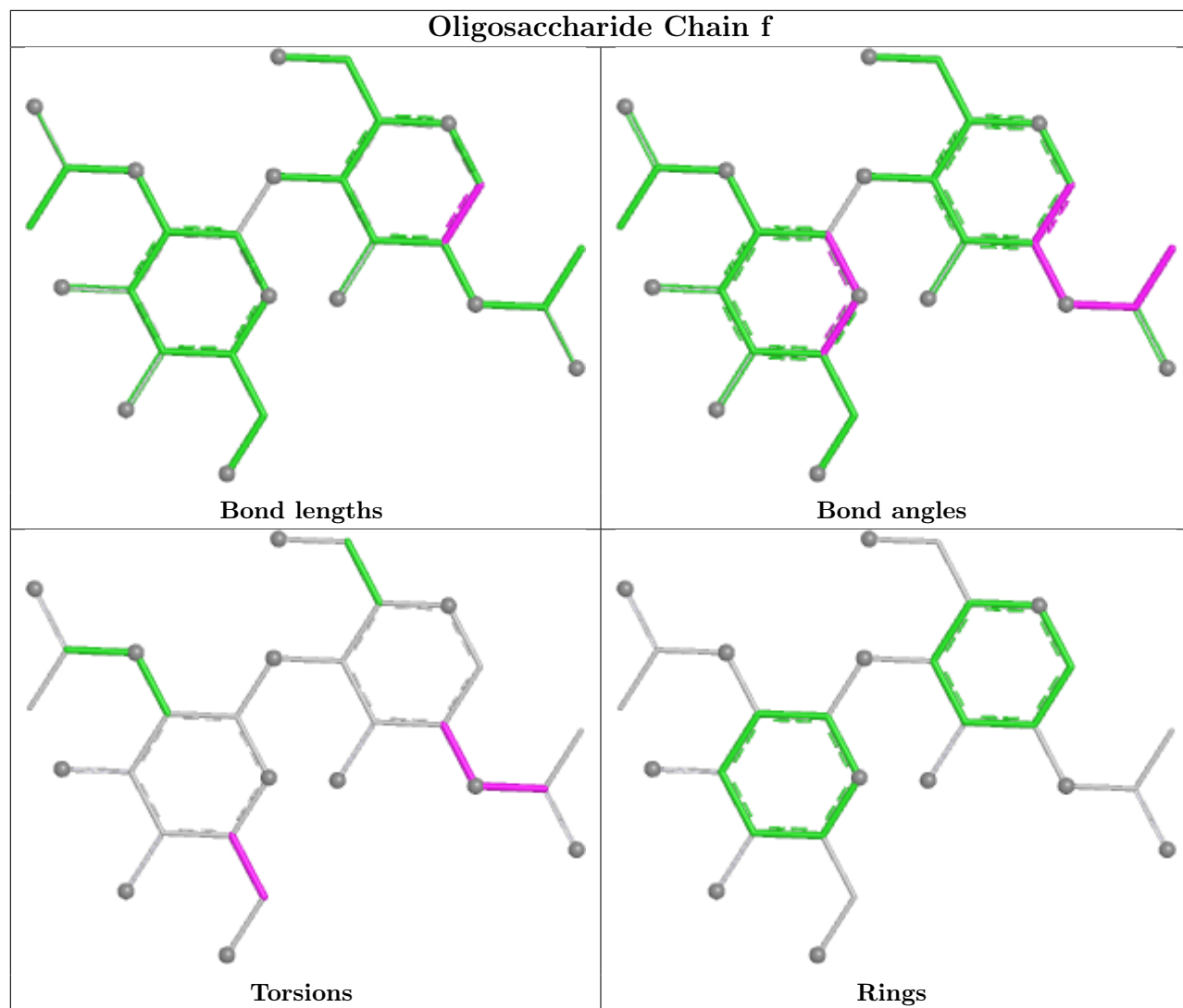


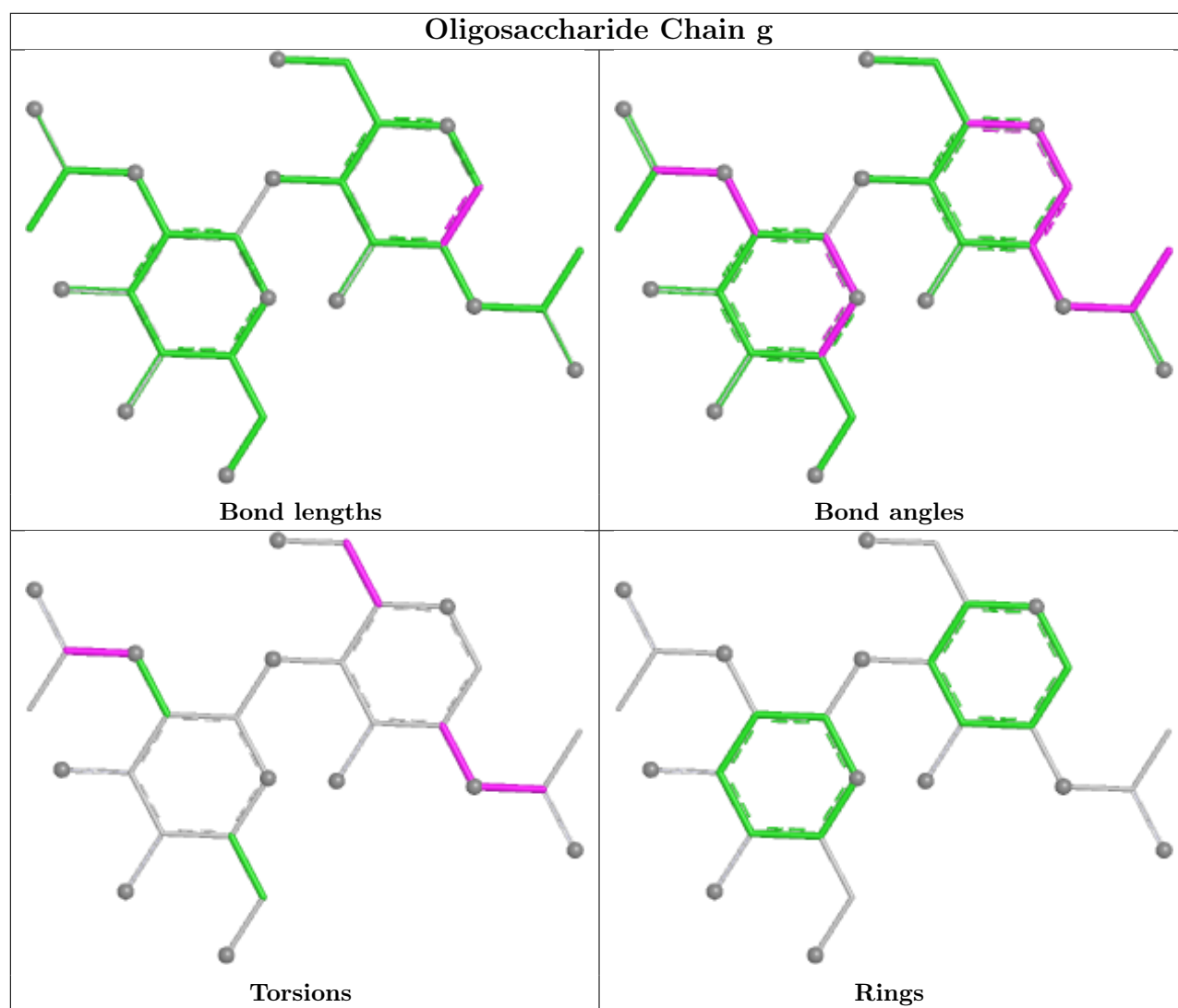


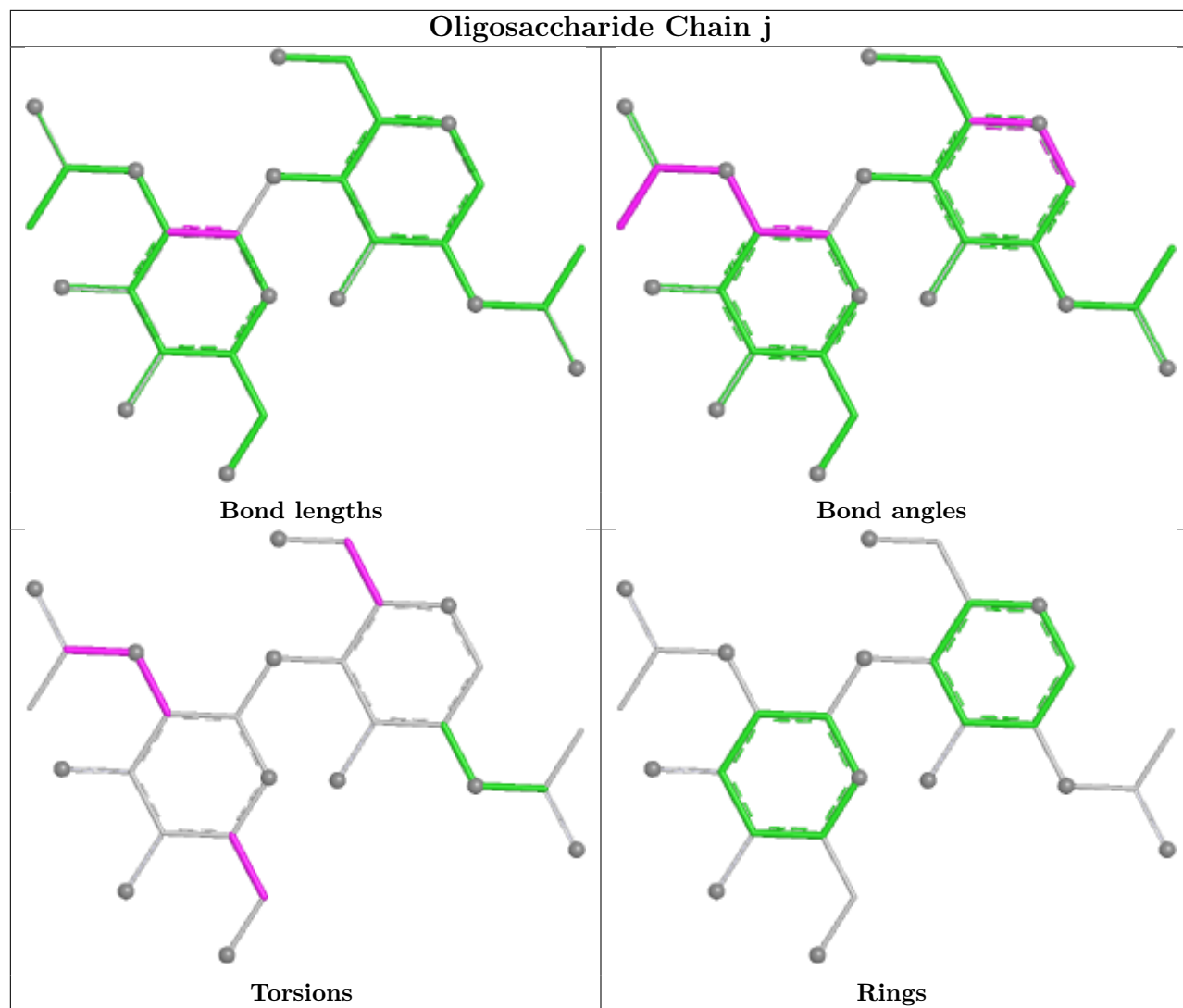


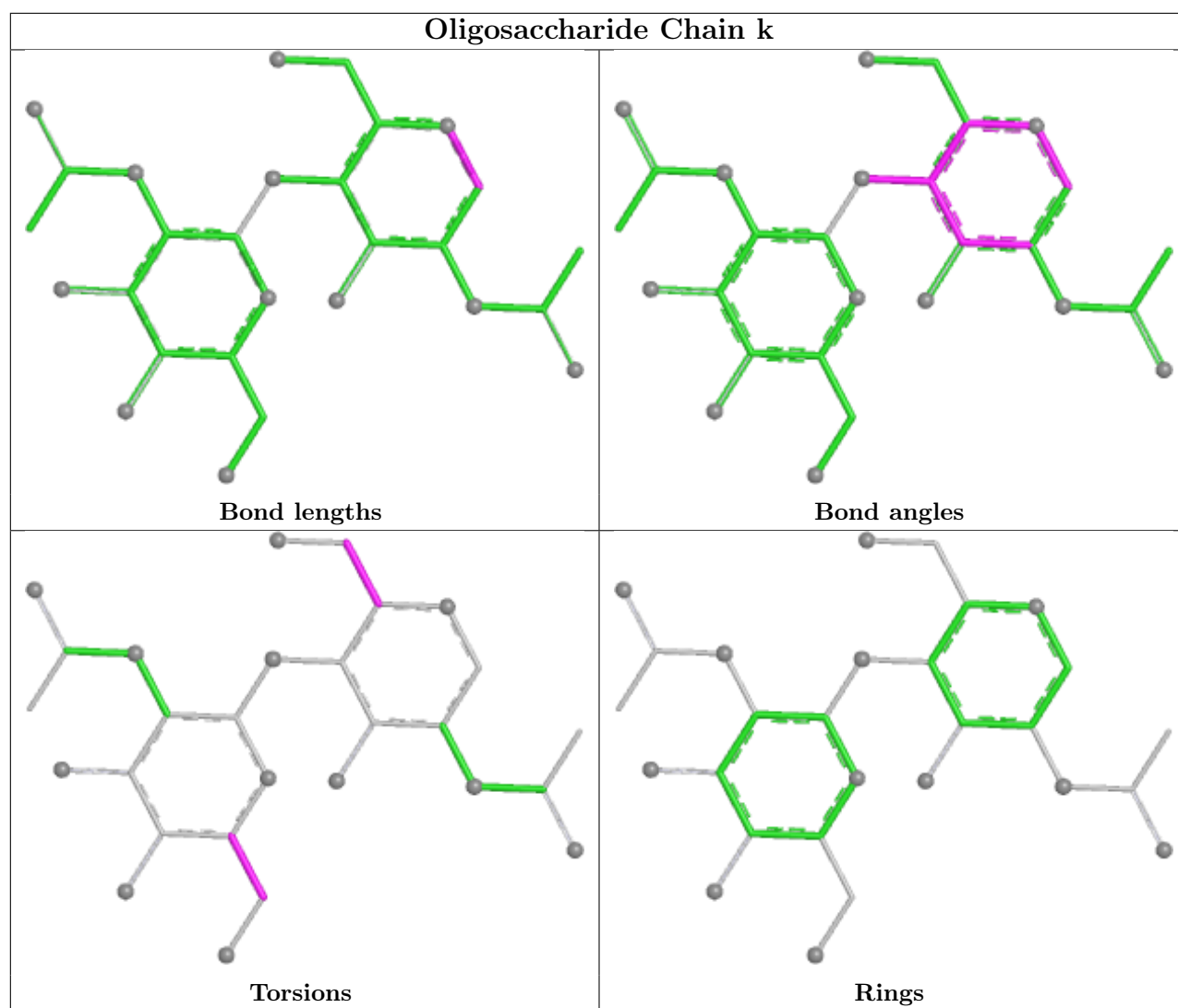


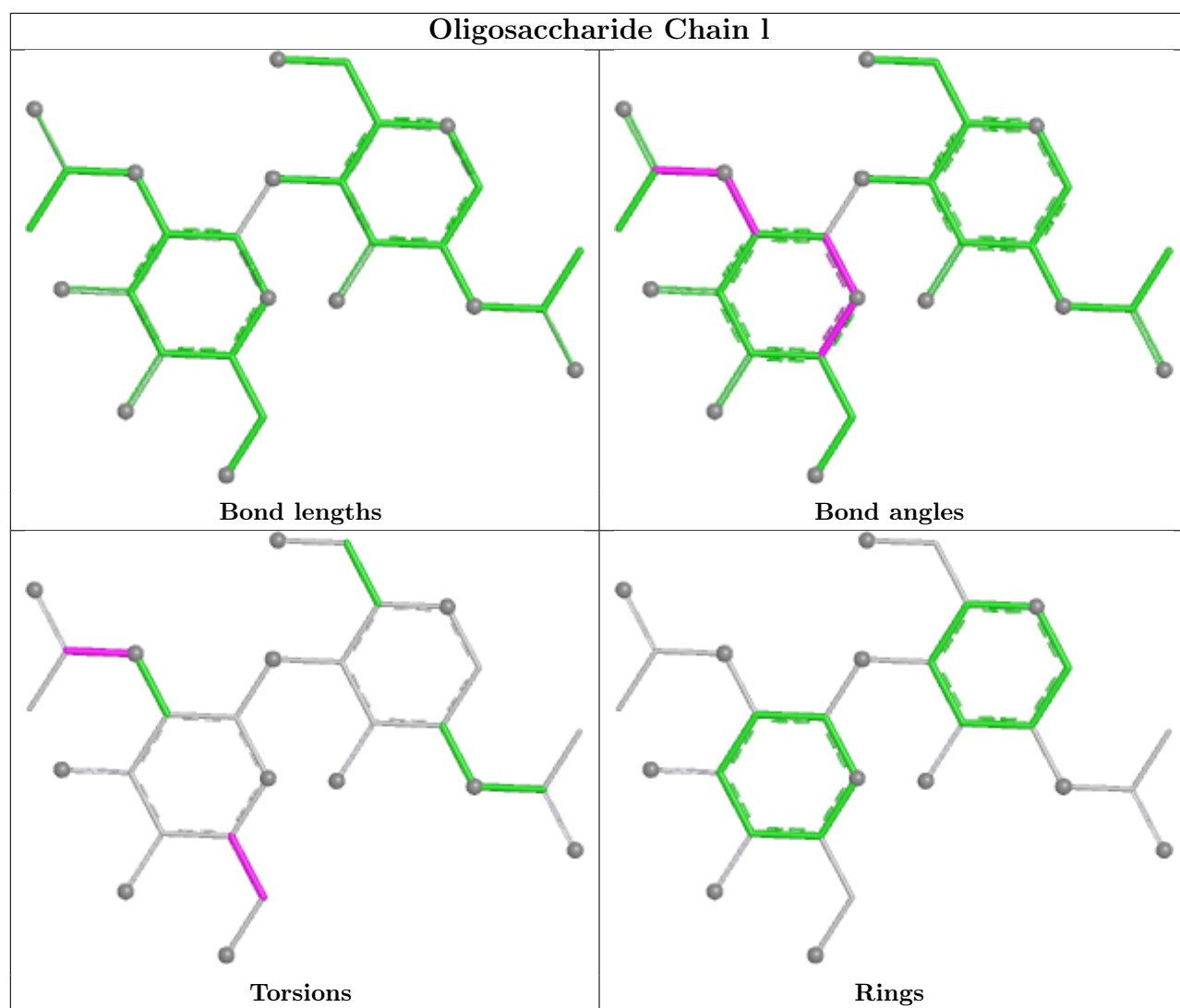


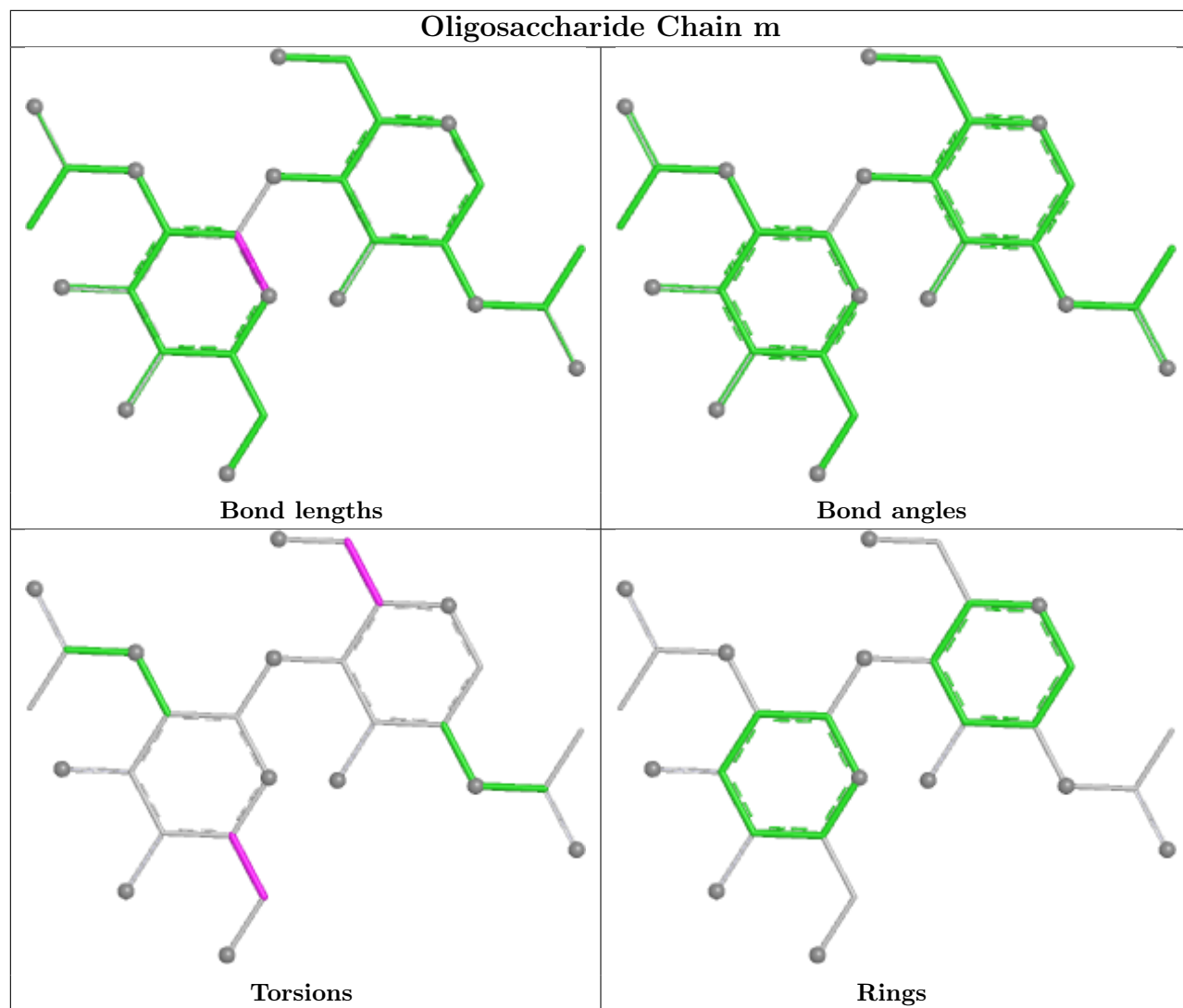


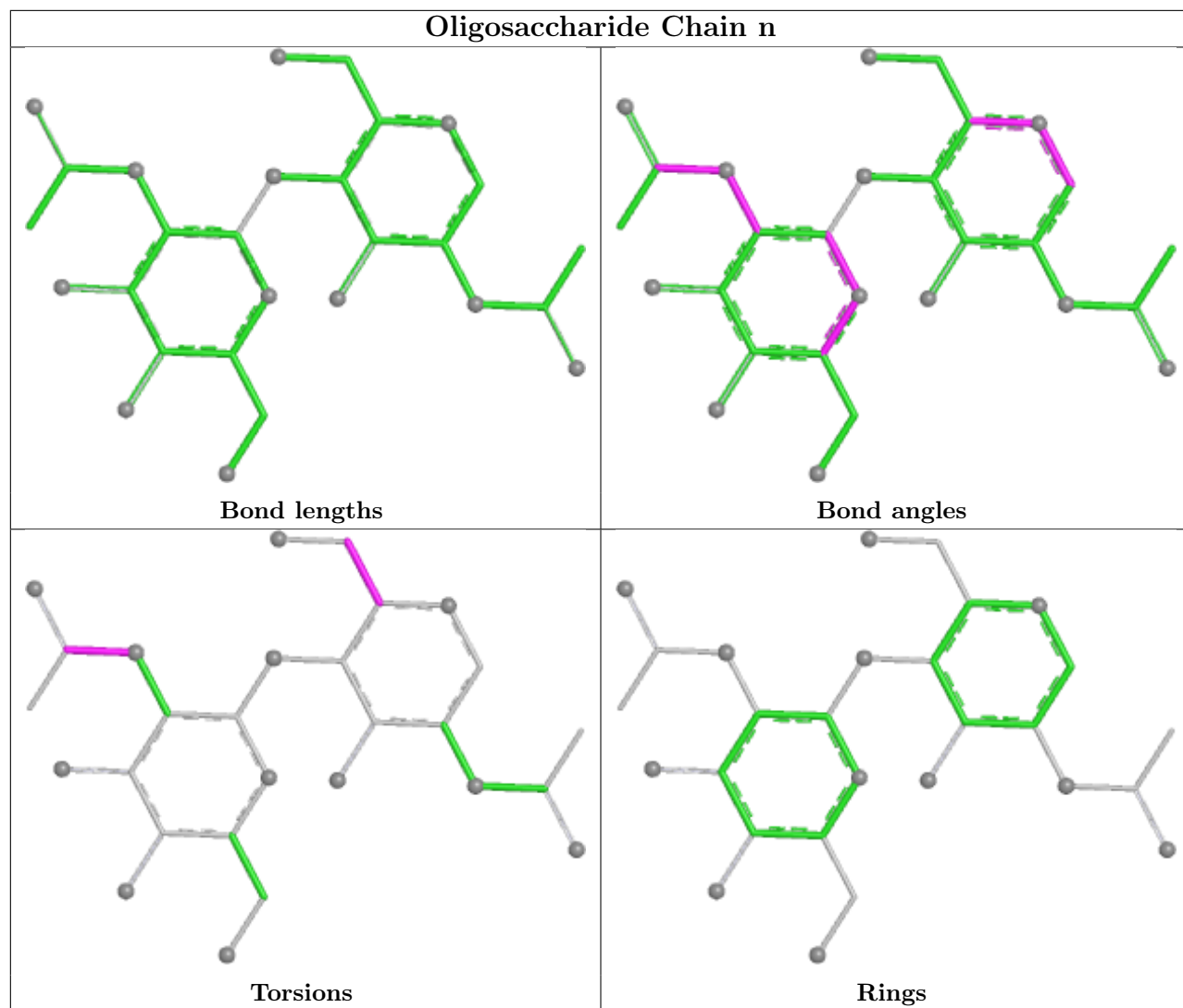


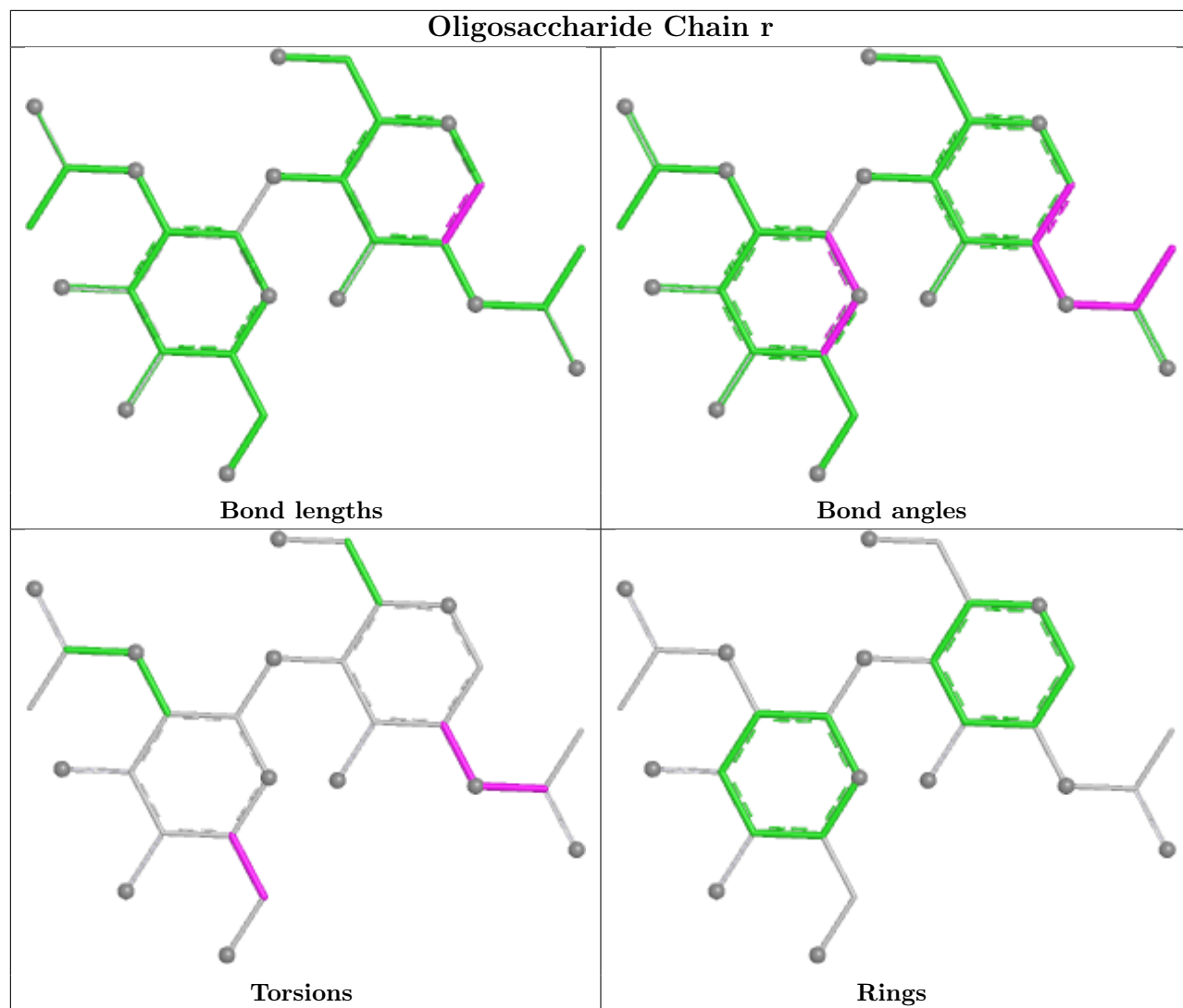


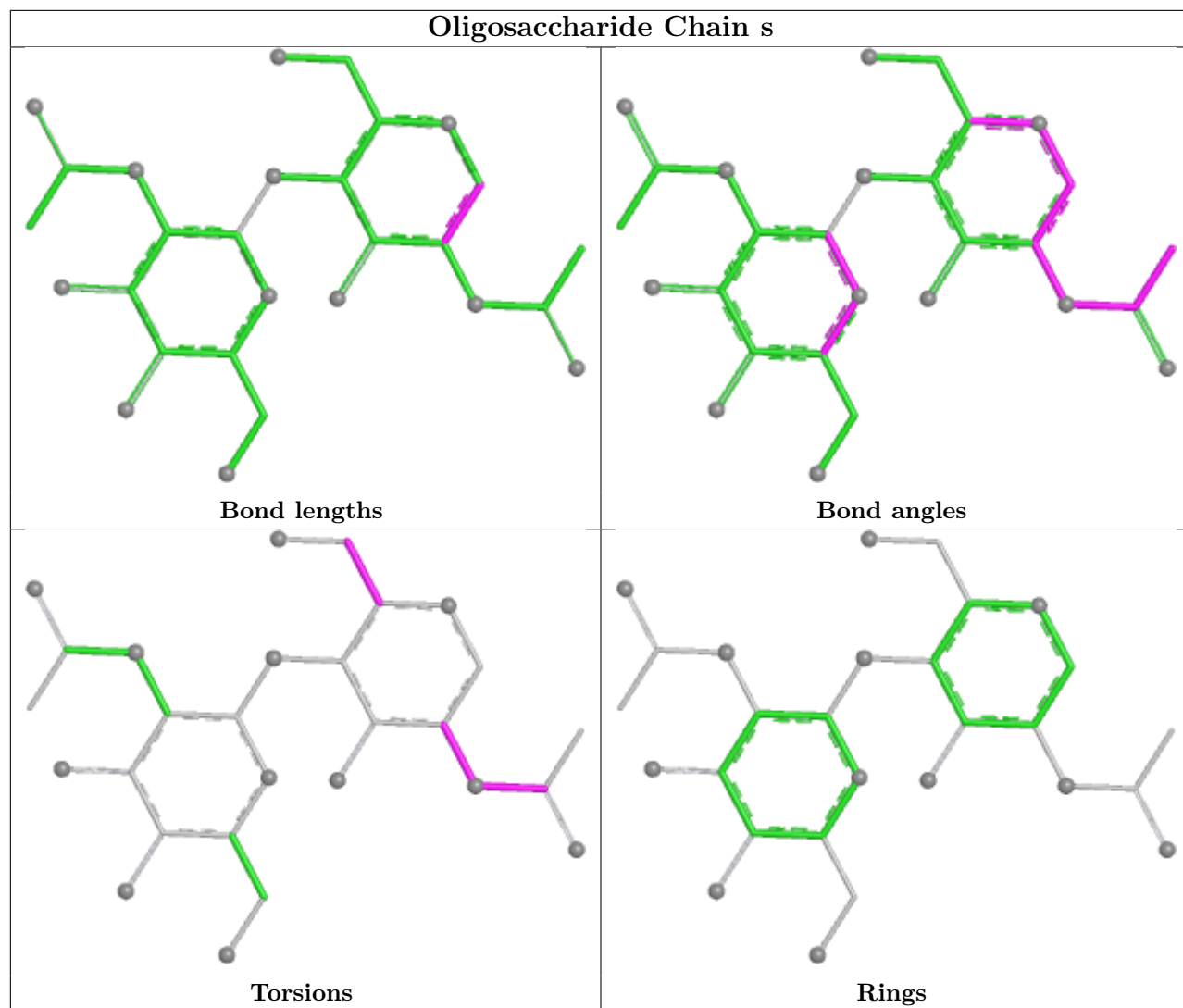


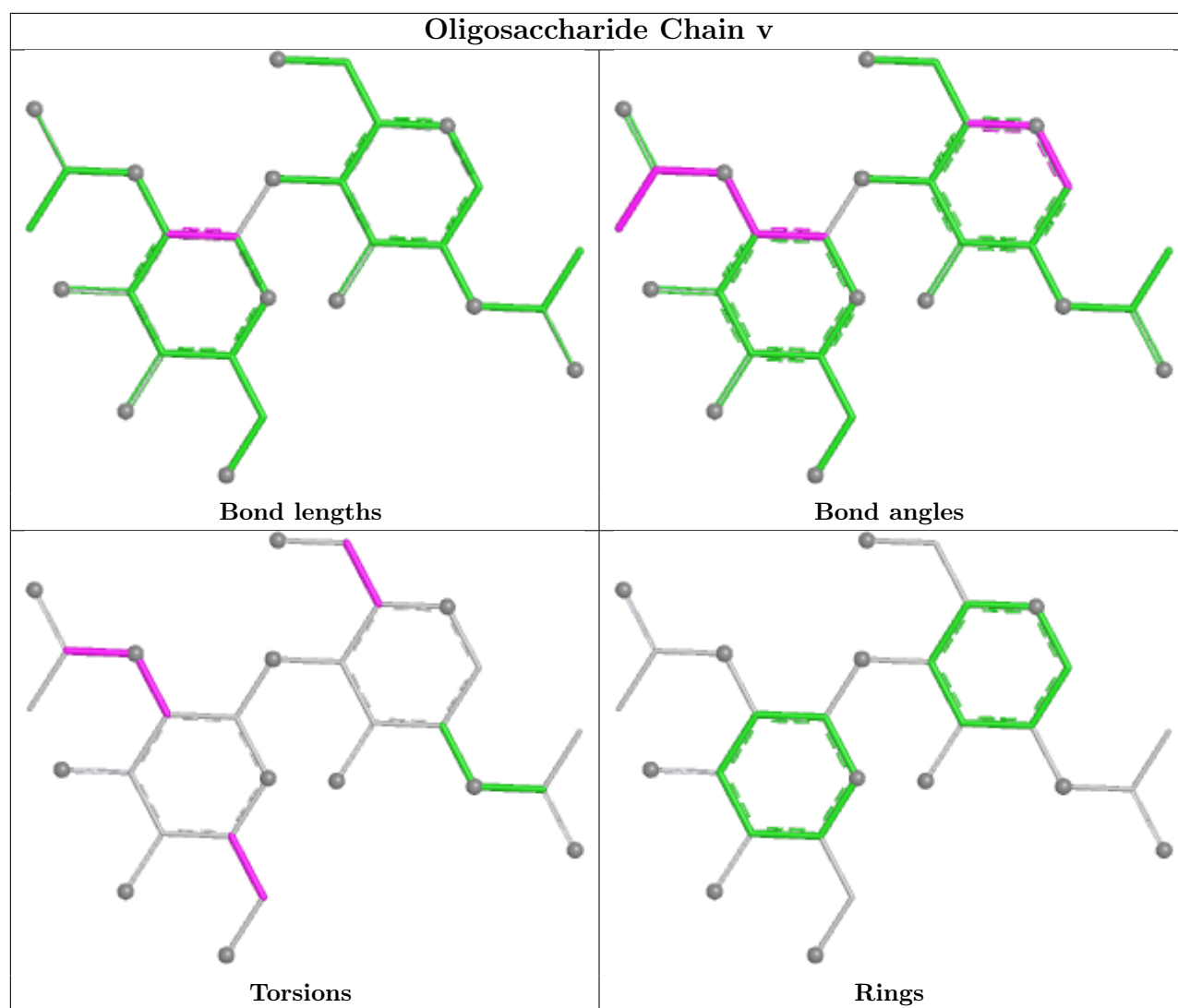


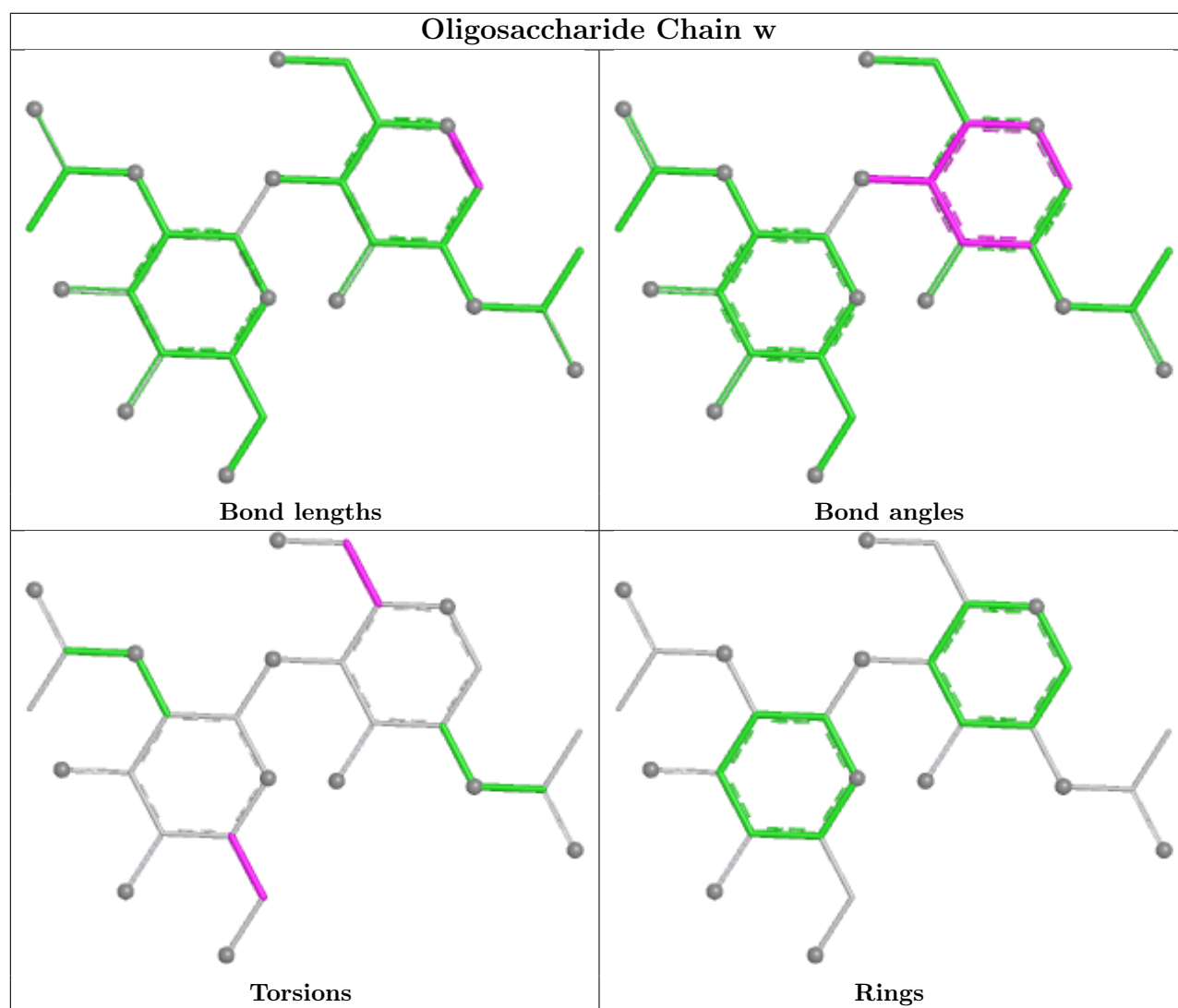


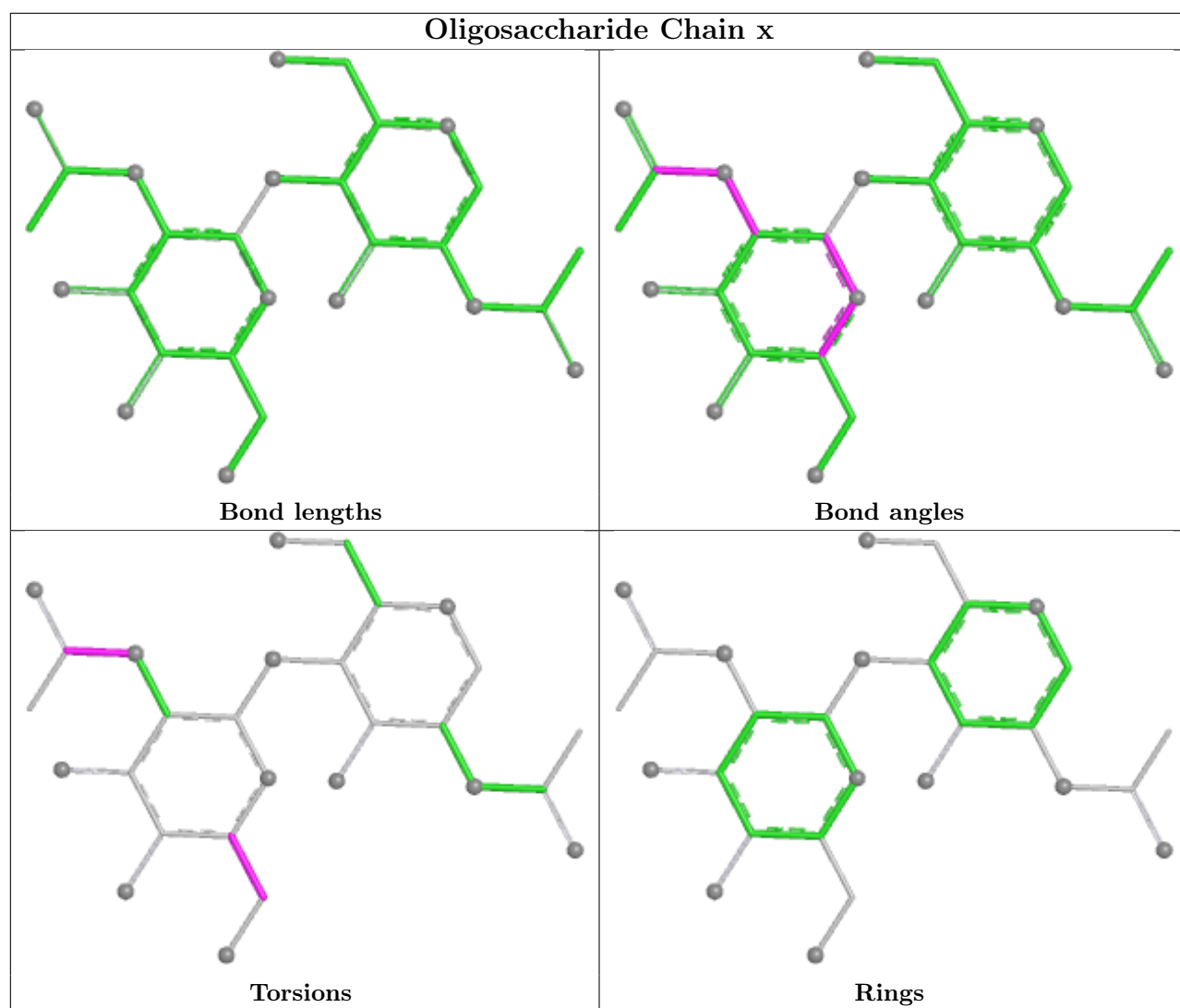


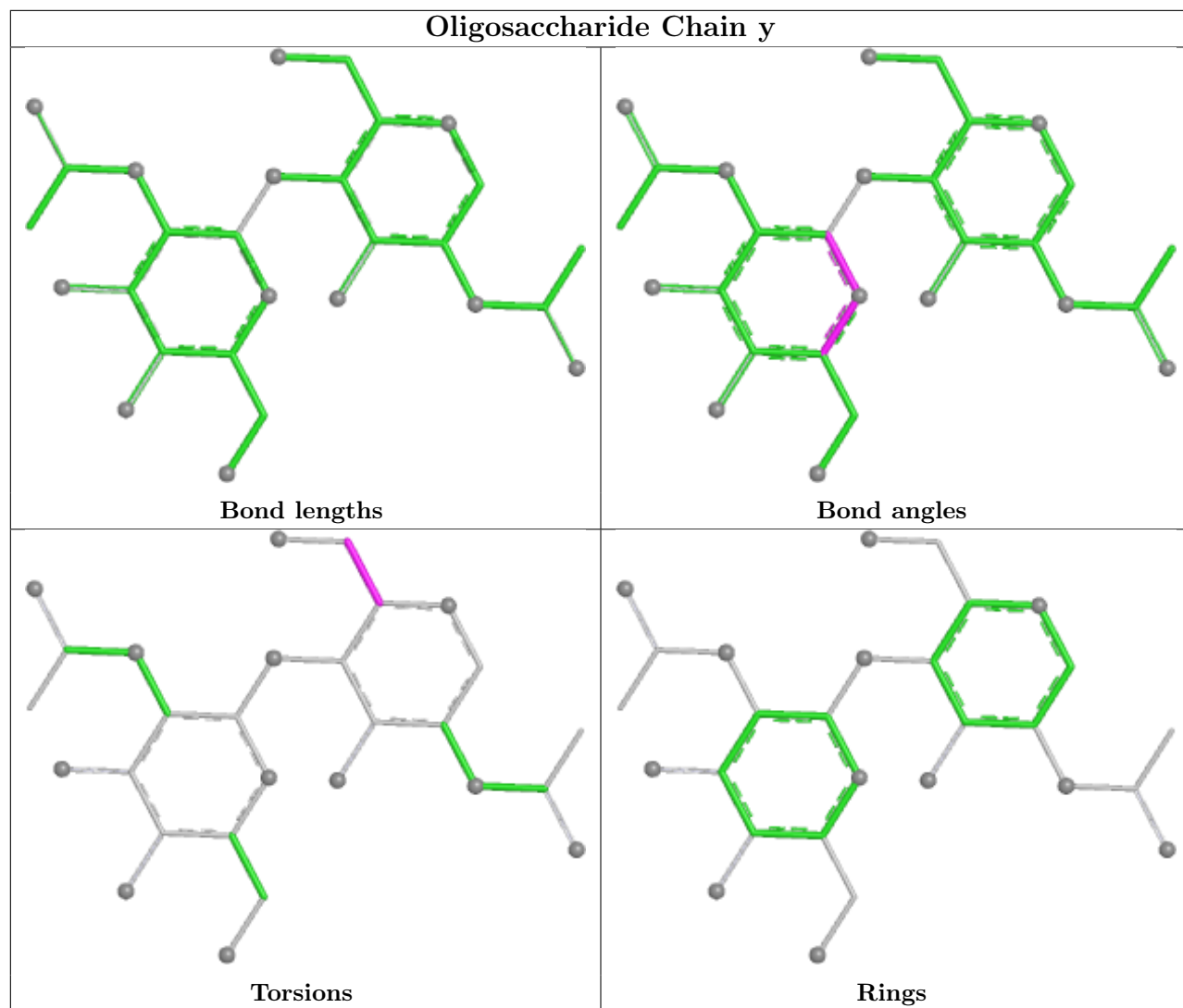


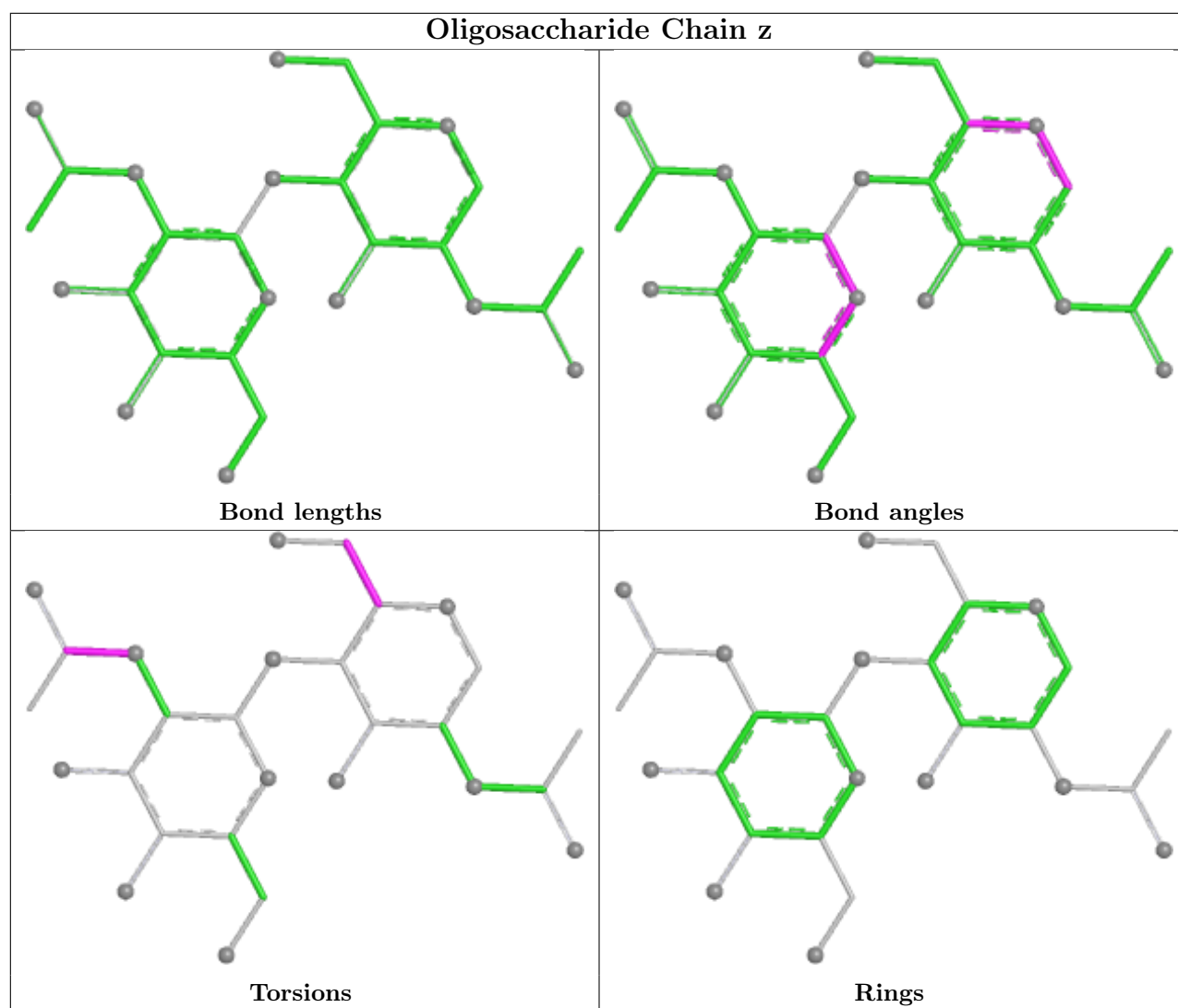


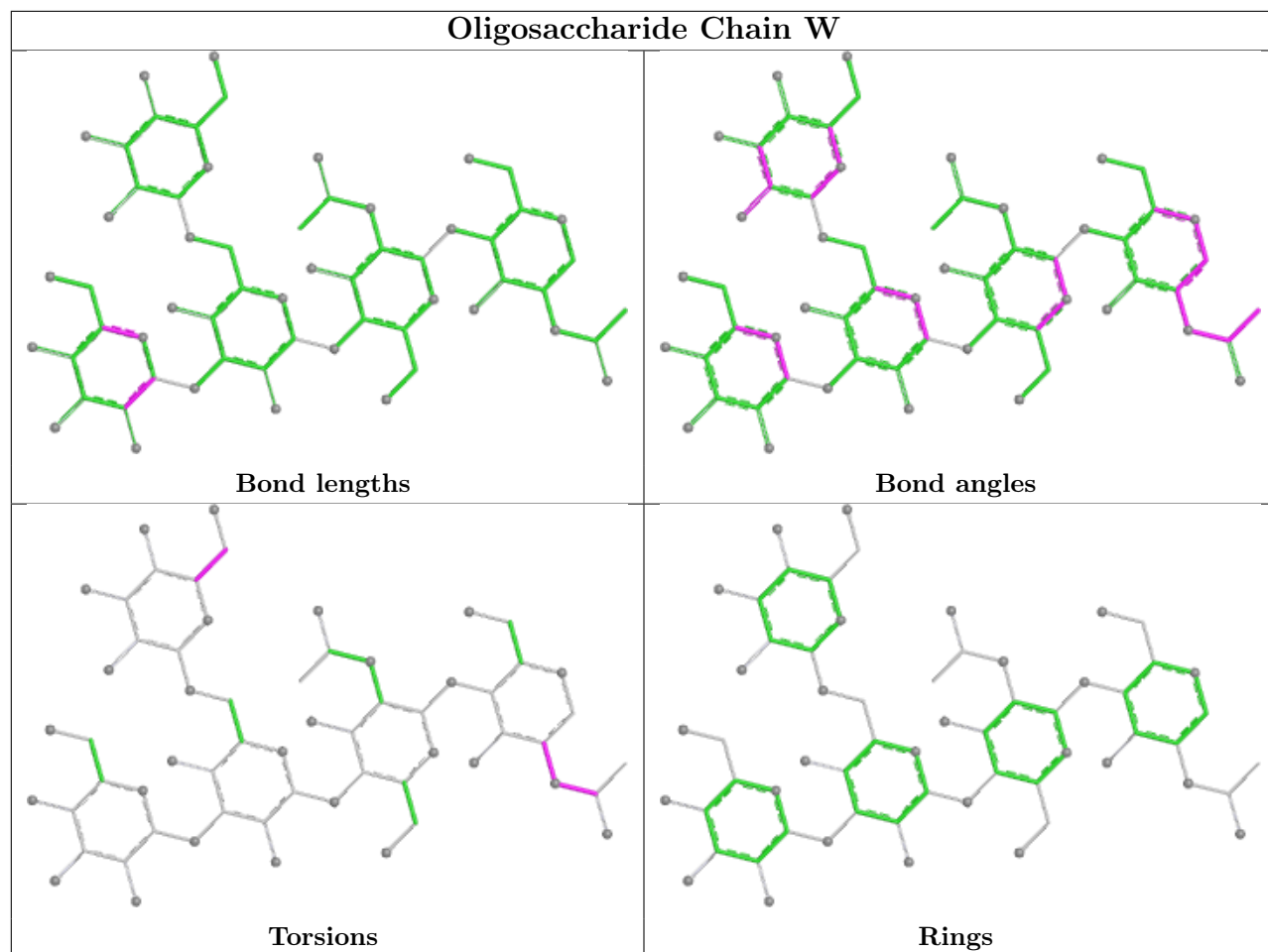


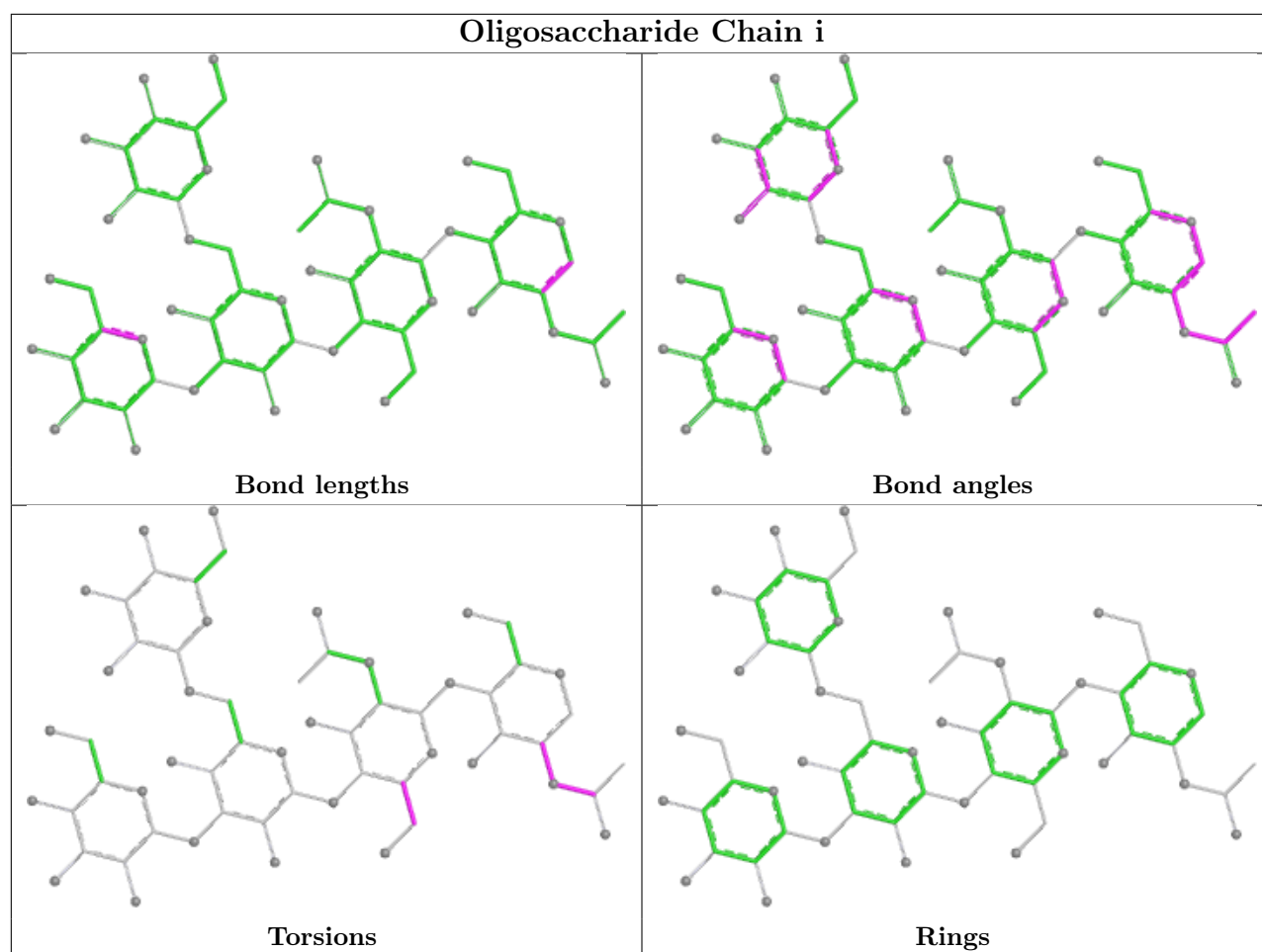


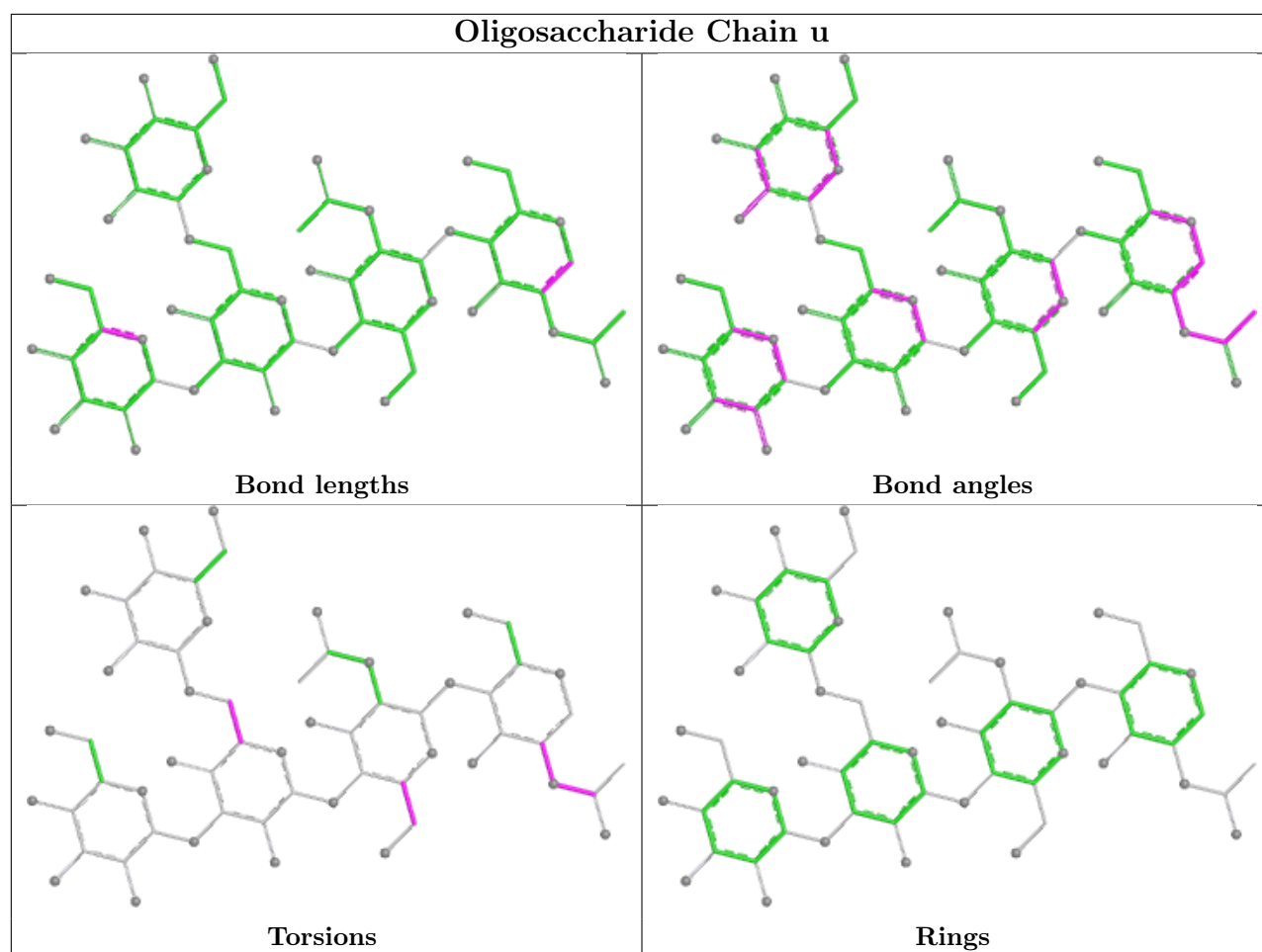


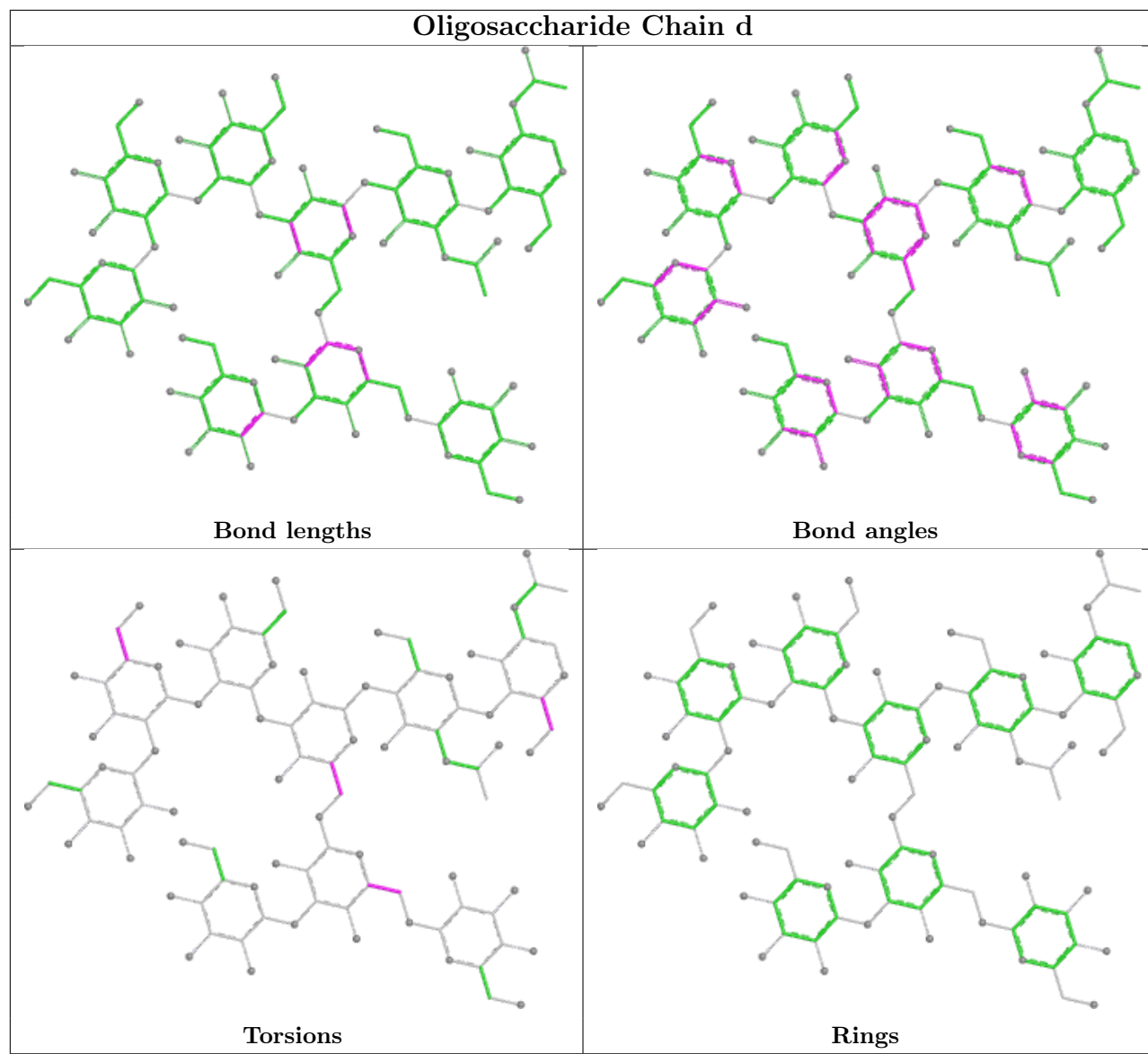


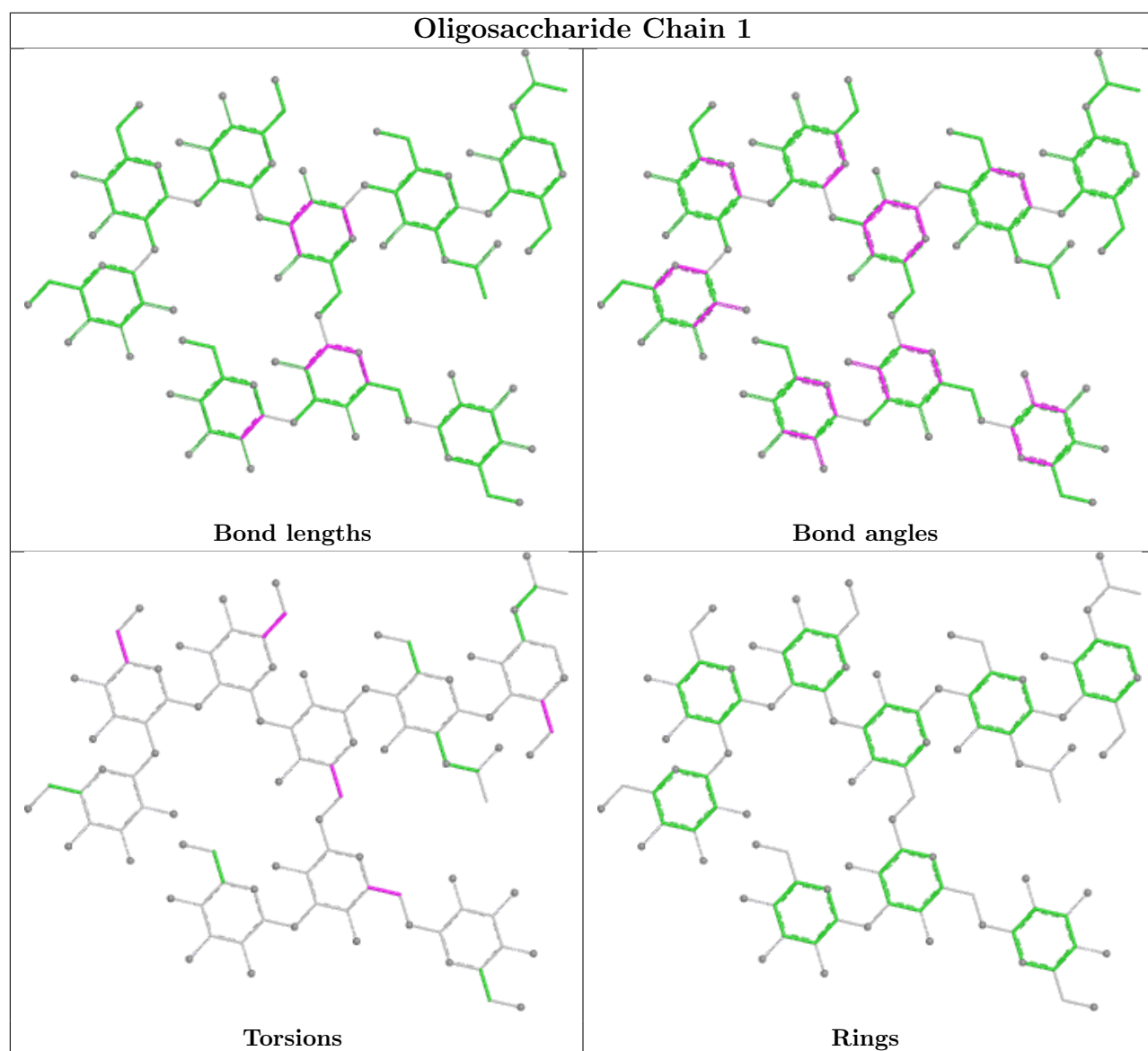


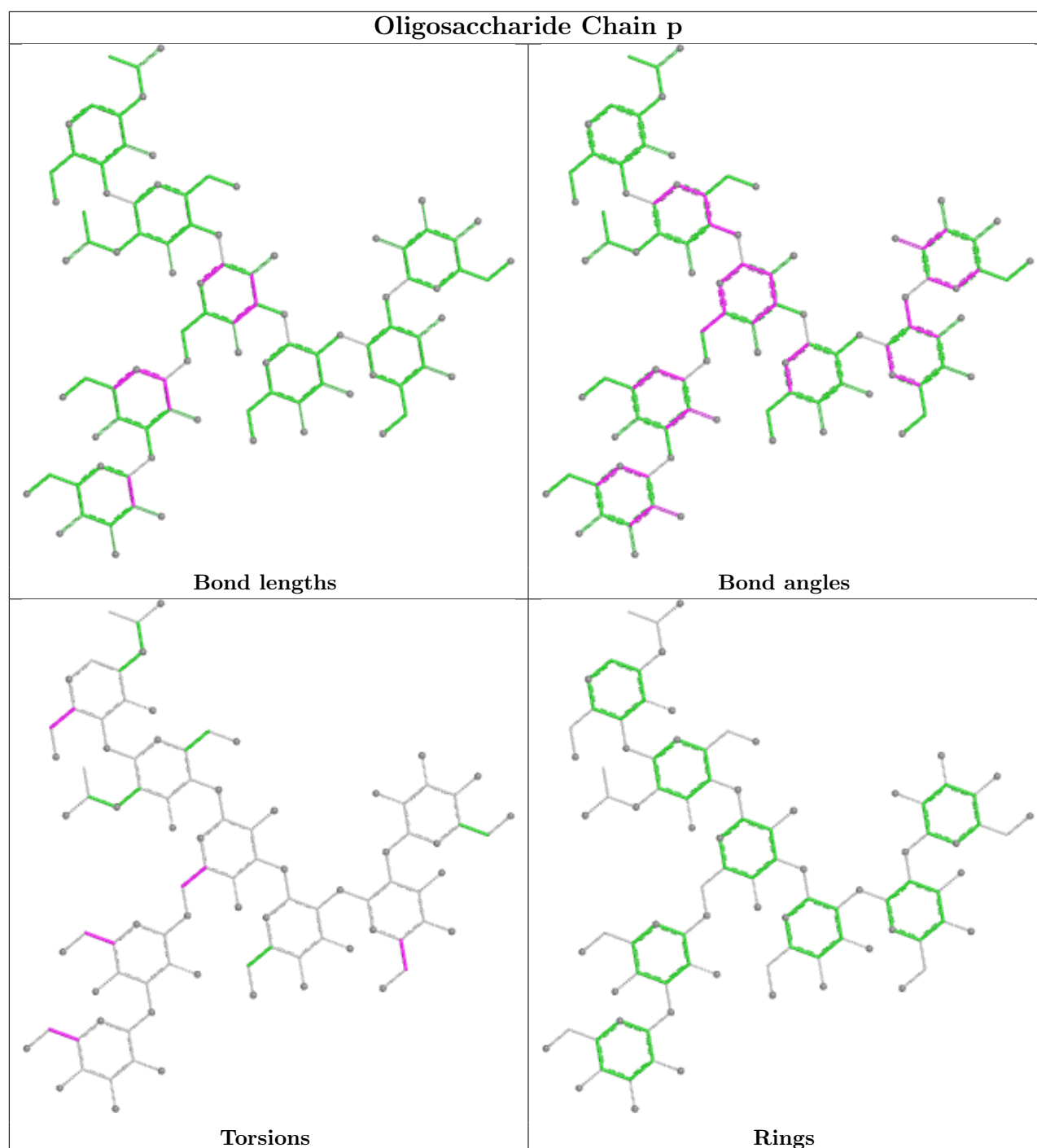












## 5.6 Ligand geometry [i](#)

24 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	C	602	1	14,14,15	0.61	0	17,19,21	0.60	1 (5%)
12	NAG	A	605	1	14,14,15	0.59	0	17,19,21	0.73	1 (5%)
12	NAG	A	601	1	14,14,15	0.77	1 (7%)	17,19,21	1.36	3 (17%)
12	NAG	B	607	1	14,14,15	0.62	0	17,19,21	0.71	1 (5%)
12	NAG	A	607	1	14,14,15	0.82	1 (7%)	17,19,21	0.68	1 (5%)
12	NAG	A	602	1	14,14,15	0.62	0	17,19,21	0.62	1 (5%)
12	NAG	B	604	1	14,14,15	0.72	0	17,19,21	1.36	3 (17%)
12	NAG	B	602	1	14,14,15	0.62	0	17,19,21	0.62	1 (5%)
12	NAG	C	605	1	14,14,15	0.57	0	17,19,21	0.73	1 (5%)
12	NAG	C	603	1	14,14,15	0.57	0	17,19,21	0.57	0
12	NAG	A	604	1	14,14,15	0.72	0	17,19,21	1.36	3 (17%)
12	NAG	E	701	2	14,14,15	0.90	1 (7%)	17,19,21	1.29	2 (11%)
12	NAG	B	605	1	14,14,15	0.58	0	17,19,21	0.72	1 (5%)
12	NAG	C	601	1	14,14,15	0.77	1 (7%)	17,19,21	1.40	3 (17%)
12	NAG	C	607	1	14,14,15	0.63	0	17,19,21	0.71	1 (5%)
12	NAG	D	701	2	14,14,15	0.86	1 (7%)	17,19,21	1.29	2 (11%)
12	NAG	C	606	1	14,14,15	1.21	1 (7%)	17,19,21	2.75	3 (17%)
12	NAG	A	603	1	14,14,15	0.60	0	17,19,21	0.66	1 (5%)
12	NAG	B	601	1	14,14,15	0.76	1 (7%)	17,19,21	1.39	3 (17%)
12	NAG	B	603	1	14,14,15	0.56	0	17,19,21	0.56	0
12	NAG	F	701	2	14,14,15	0.88	1 (7%)	17,19,21	1.30	2 (11%)
12	NAG	B	606	1	14,14,15	1.11	1 (7%)	17,19,21	2.77	4 (23%)
12	NAG	C	604	1	14,14,15	0.72	0	17,19,21	1.36	3 (17%)
12	NAG	A	606	1	14,14,15	0.63	0	17,19,21	0.70	1 (5%)

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	C	602	1	-	1/6/23/26	0/1/1/1
12	NAG	A	605	1	-	2/6/23/26	0/1/1/1
12	NAG	A	601	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	B	607	1	-	2/6/23/26	0/1/1/1
12	NAG	A	607	1	-	0/6/23/26	0/1/1/1
12	NAG	A	602	1	-	1/6/23/26	0/1/1/1
12	NAG	B	604	1	-	4/6/23/26	0/1/1/1
12	NAG	B	602	1	-	1/6/23/26	0/1/1/1
12	NAG	C	605	1	-	2/6/23/26	0/1/1/1
12	NAG	C	603	1	-	0/6/23/26	0/1/1/1
12	NAG	A	604	1	-	4/6/23/26	0/1/1/1
12	NAG	E	701	2	-	2/6/23/26	0/1/1/1
12	NAG	B	605	1	-	2/6/23/26	0/1/1/1
12	NAG	C	601	1	-	4/6/23/26	0/1/1/1
12	NAG	C	607	1	-	2/6/23/26	0/1/1/1
12	NAG	D	701	2	-	2/6/23/26	0/1/1/1
12	NAG	C	606	1	-	5/6/23/26	0/1/1/1
12	NAG	A	603	1	-	2/6/23/26	0/1/1/1
12	NAG	B	601	1	-	4/6/23/26	0/1/1/1
12	NAG	B	603	1	-	0/6/23/26	0/1/1/1
12	NAG	F	701	2	-	2/6/23/26	0/1/1/1
12	NAG	B	606	1	-	6/6/23/26	0/1/1/1
12	NAG	C	604	1	-	4/6/23/26	0/1/1/1
12	NAG	A	606	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	606	NAG	C1-C2	3.44	1.57	1.52
12	B	606	NAG	C1-C2	3.02	1.56	1.52
12	E	701	NAG	C1-C2	2.51	1.55	1.52
12	F	701	NAG	C1-C2	2.46	1.55	1.52
12	D	701	NAG	C1-C2	2.35	1.55	1.52
12	A	607	NAG	O5-C1	2.32	1.47	1.43
12	C	601	NAG	C1-C2	2.07	1.55	1.52
12	A	601	NAG	C1-C2	2.06	1.55	1.52
12	B	601	NAG	C1-C2	2.06	1.55	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	606	NAG	C2-N2-C7	9.60	135.77	122.90
12	C	606	NAG	C2-N2-C7	9.53	135.68	122.90
12	C	606	NAG	C1-C2-N2	4.91	118.18	110.43
12	B	606	NAG	C1-C2-N2	4.72	117.88	110.43
12	C	604	NAG	C2-N2-C7	4.25	128.60	122.90
12	A	604	NAG	C2-N2-C7	4.24	128.58	122.90
12	B	601	NAG	C2-N2-C7	4.23	128.57	122.90
12	C	601	NAG	C2-N2-C7	4.23	128.57	122.90
12	B	604	NAG	C2-N2-C7	4.22	128.56	122.90
12	A	601	NAG	C2-N2-C7	4.21	128.54	122.90
12	F	701	NAG	C2-N2-C7	4.18	128.50	122.90
12	D	701	NAG	C2-N2-C7	4.16	128.48	122.90
12	E	701	NAG	C2-N2-C7	4.16	128.47	122.90
12	A	605	NAG	C1-O5-C5	2.68	115.77	112.19
12	C	601	NAG	C1-O5-C5	2.66	115.75	112.19
12	C	605	NAG	C1-O5-C5	2.65	115.73	112.19
12	B	605	NAG	C1-O5-C5	2.64	115.72	112.19
12	B	601	NAG	C1-O5-C5	2.63	115.71	112.19
12	C	607	NAG	C1-O5-C5	2.57	115.64	112.19
12	B	607	NAG	C1-O5-C5	2.55	115.61	112.19
12	A	606	NAG	C1-O5-C5	2.53	115.58	112.19
12	C	606	NAG	C8-C7-N2	2.50	120.26	116.12
12	C	604	NAG	C1-O5-C5	2.45	115.47	112.19
12	A	601	NAG	C1-O5-C5	2.45	115.46	112.19
12	B	606	NAG	C8-C7-N2	2.43	120.15	116.12
12	B	604	NAG	C1-O5-C5	2.41	115.41	112.19
12	A	604	NAG	C1-O5-C5	2.40	115.41	112.19
12	A	603	NAG	C1-O5-C5	2.34	115.32	112.19
12	A	607	NAG	C1-O5-C5	2.33	115.31	112.19
12	F	701	NAG	C1-C2-N2	2.30	114.06	110.43
12	E	701	NAG	C1-C2-N2	2.29	114.05	110.43
12	C	601	NAG	C1-C2-N2	2.27	114.02	110.43
12	B	606	NAG	C1-O5-C5	2.27	115.23	112.19
12	B	601	NAG	C1-C2-N2	2.27	114.00	110.43
12	D	701	NAG	C1-C2-N2	2.26	114.00	110.43
12	A	601	NAG	C1-C2-N2	2.23	113.95	110.43
12	B	602	NAG	C1-O5-C5	2.18	115.11	112.19
12	A	602	NAG	C1-O5-C5	2.17	115.09	112.19
12	B	604	NAG	C1-C2-N2	2.13	113.79	110.43
12	C	604	NAG	C1-C2-N2	2.11	113.75	110.43
12	A	604	NAG	C1-C2-N2	2.10	113.74	110.43
12	C	602	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	601	NAG	O5-C5-C6-O6
12	B	606	NAG	O5-C5-C6-O6
12	B	601	NAG	O5-C5-C6-O6
12	C	601	NAG	O5-C5-C6-O6
12	A	603	NAG	O5-C5-C6-O6
12	B	607	NAG	O5-C5-C6-O6
12	C	607	NAG	O5-C5-C6-O6
12	B	606	NAG	C4-C5-C6-O6
12	A	606	NAG	O5-C5-C6-O6
12	A	601	NAG	C4-C5-C6-O6
12	A	603	NAG	C4-C5-C6-O6
12	B	601	NAG	C4-C5-C6-O6
12	C	601	NAG	C4-C5-C6-O6
12	A	606	NAG	C4-C5-C6-O6
12	B	607	NAG	C4-C5-C6-O6
12	C	607	NAG	C4-C5-C6-O6
12	B	604	NAG	O5-C5-C6-O6
12	C	604	NAG	O5-C5-C6-O6
12	A	605	NAG	O5-C5-C6-O6
12	C	605	NAG	O5-C5-C6-O6
12	A	604	NAG	O5-C5-C6-O6
12	B	605	NAG	O5-C5-C6-O6
12	B	606	NAG	C8-C7-N2-C2
12	B	606	NAG	O7-C7-N2-C2
12	C	606	NAG	C8-C7-N2-C2
12	C	606	NAG	O7-C7-N2-C2
12	B	604	NAG	C4-C5-C6-O6
12	B	605	NAG	C4-C5-C6-O6
12	C	604	NAG	C4-C5-C6-O6
12	A	604	NAG	C4-C5-C6-O6
12	A	605	NAG	C4-C5-C6-O6
12	C	605	NAG	C4-C5-C6-O6
12	B	602	NAG	O5-C5-C6-O6
12	A	602	NAG	O5-C5-C6-O6
12	C	602	NAG	O5-C5-C6-O6
12	C	606	NAG	O5-C5-C6-O6
12	A	601	NAG	C1-C2-N2-C7
12	A	604	NAG	C1-C2-N2-C7
12	B	601	NAG	C1-C2-N2-C7
12	B	604	NAG	C1-C2-N2-C7
12	B	606	NAG	C1-C2-N2-C7
12	C	601	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
12	C	604	NAG	C1-C2-N2-C7
12	C	606	NAG	C1-C2-N2-C7
12	D	701	NAG	C1-C2-N2-C7
12	E	701	NAG	C1-C2-N2-C7
12	F	701	NAG	C1-C2-N2-C7
12	A	601	NAG	C3-C2-N2-C7
12	A	604	NAG	C3-C2-N2-C7
12	B	601	NAG	C3-C2-N2-C7
12	B	604	NAG	C3-C2-N2-C7
12	B	606	NAG	C3-C2-N2-C7
12	C	601	NAG	C3-C2-N2-C7
12	C	604	NAG	C3-C2-N2-C7
12	C	606	NAG	C3-C2-N2-C7
12	D	701	NAG	C3-C2-N2-C7
12	E	701	NAG	C3-C2-N2-C7
12	F	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	B	3
1	A	3
2	E	1
2	F	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	546:SER	C	565:LEU	N	25.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	546:SER	C	565:LEU	N	25.01
1	D	546:SER	C	565:LEU	N	24.75
1	C	137:GLY	C	152:THR	N	13.35
1	B	137:GLY	C	152:THR	N	13.34
1	A	137:GLY	C	152:THR	N	13.30
1	B	309:ILE	C	319:THR	N	7.51
1	C	309:ILE	C	319:THR	N	7.46
1	A	309:ILE	C	319:THR	N	7.38
1	A	61:TYR	C	65:ALA	N	6.48
1	C	61:TYR	C	65:ALA	N	6.11
1	B	61:TYR	C	65:ALA	N	5.88

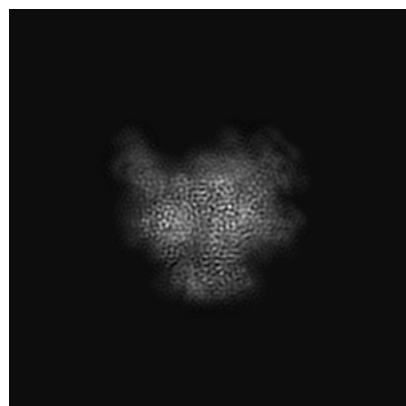
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26496. These allow visual inspection of the internal detail of the map and identification of artifacts.

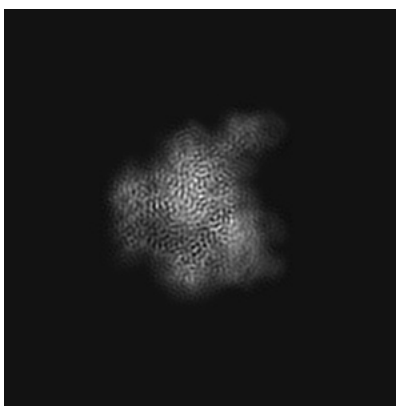
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

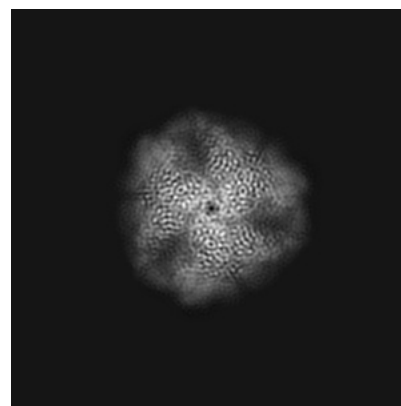
#### 6.1.1 Primary map



X

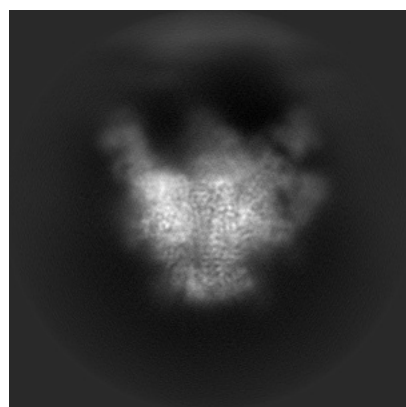


Y

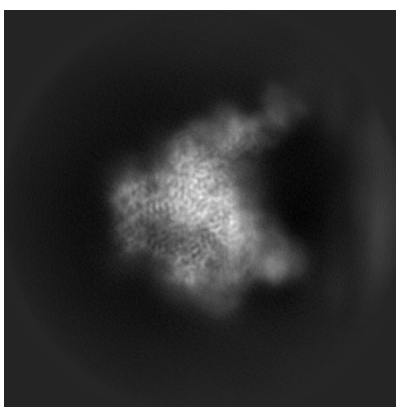


Z

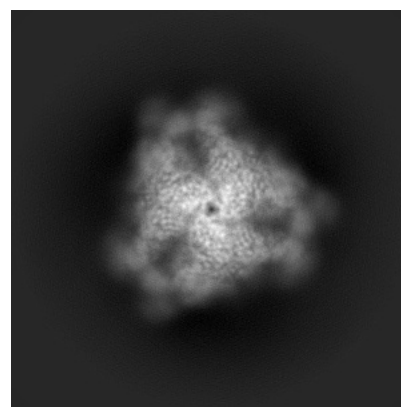
#### 6.1.2 Raw map



X



Y

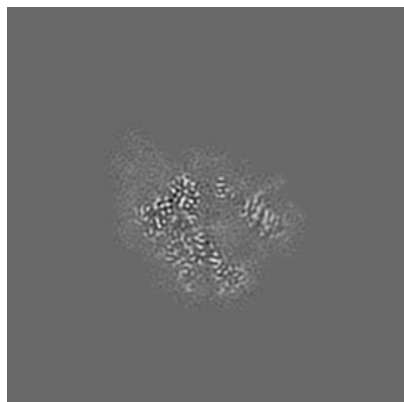


Z

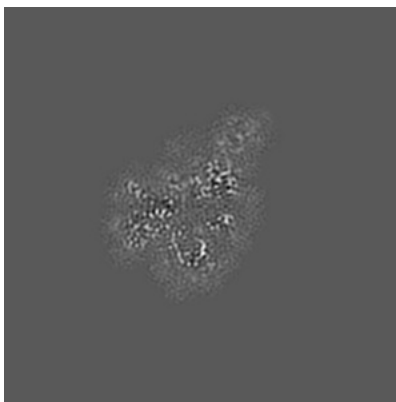
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

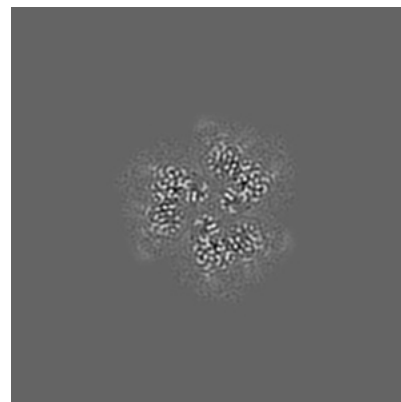
### 6.2.1 Primary map



X Index: 180

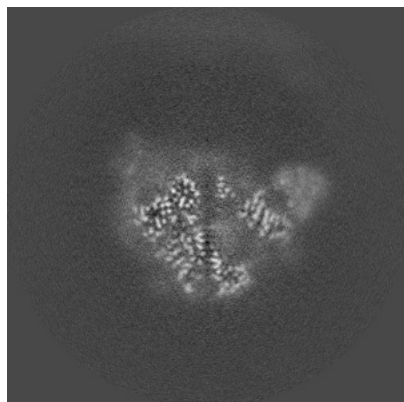


Y Index: 180

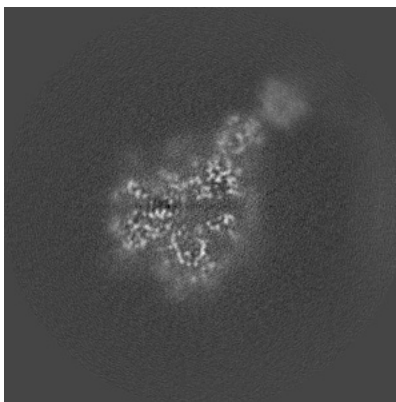


Z Index: 180

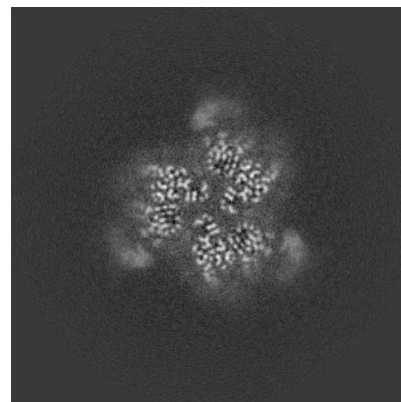
### 6.2.2 Raw map



X Index: 180



Y Index: 180

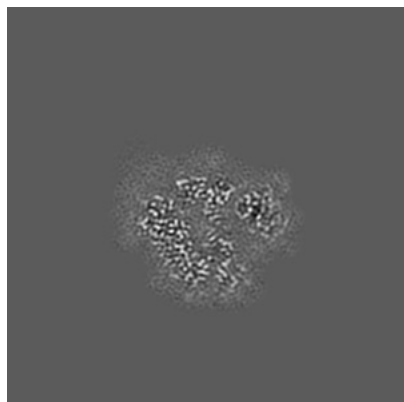


Z Index: 180

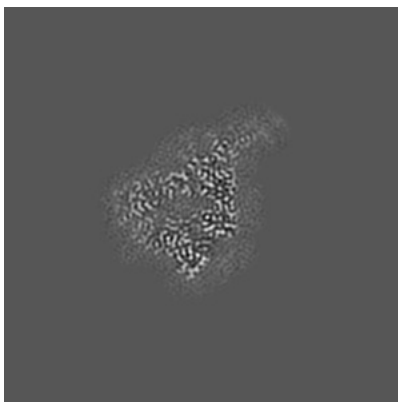
The images above show central slices of the map in three orthogonal directions.

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

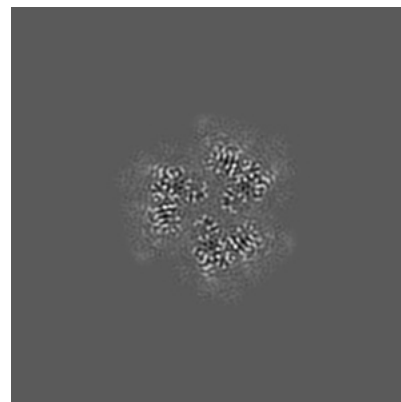
### 6.3.1 Primary map



X Index: 189

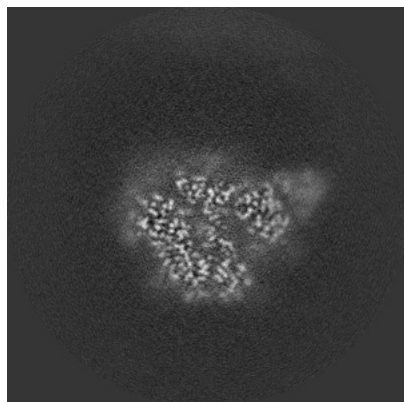


Y Index: 191

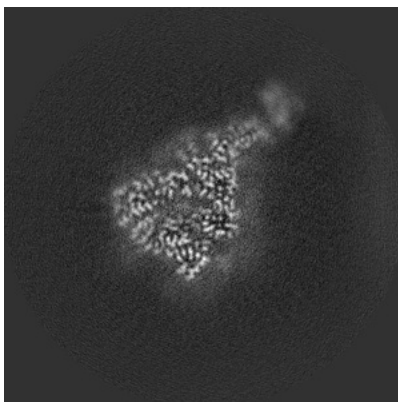


Z Index: 179

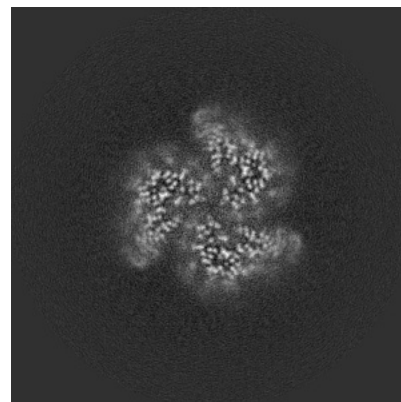
### 6.3.2 Raw map



X Index: 189



Y Index: 191

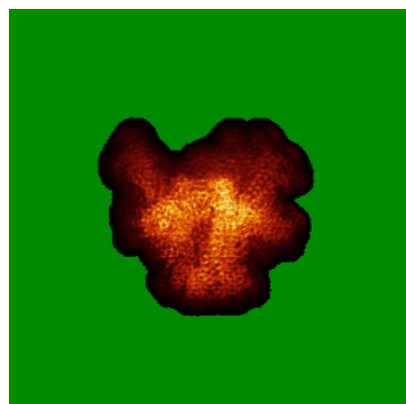


Z Index: 168

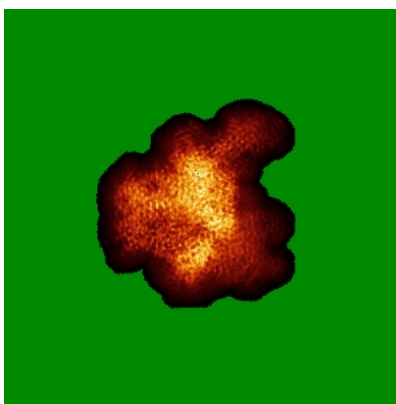
The images above show the largest variance slices of the map in three orthogonal directions.

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

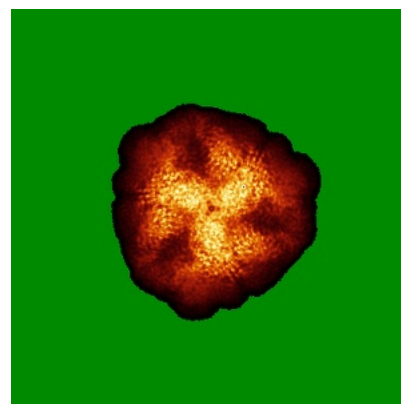
### 6.4.1 Primary map



X

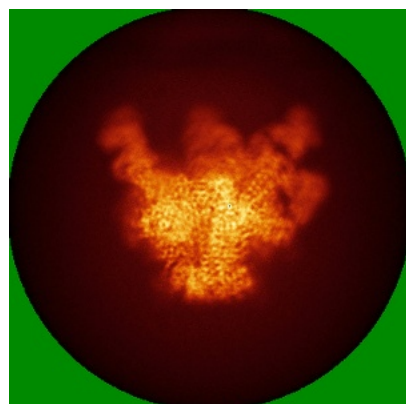


Y

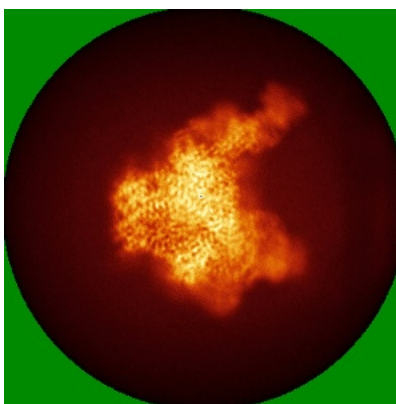


Z

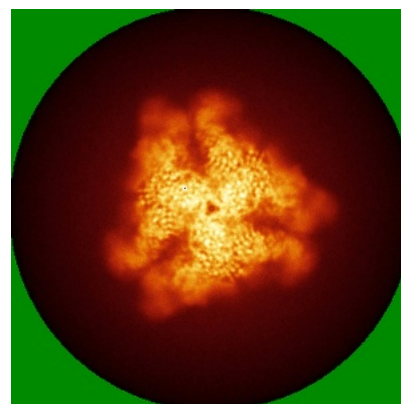
### 6.4.2 Raw map



X



Y



Z

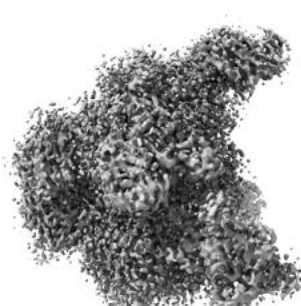
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

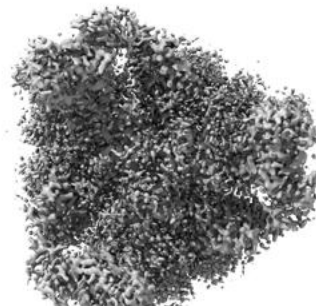
### 6.5.1 Primary map



X



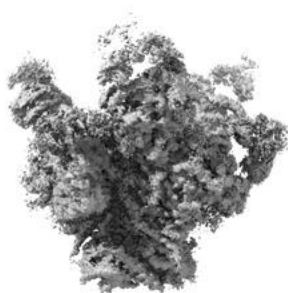
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

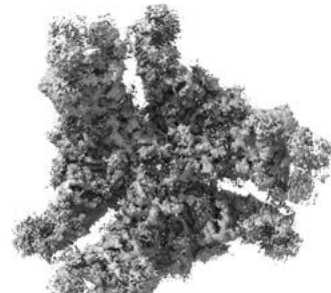
### 6.5.2 Raw map



X



Y



Z

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

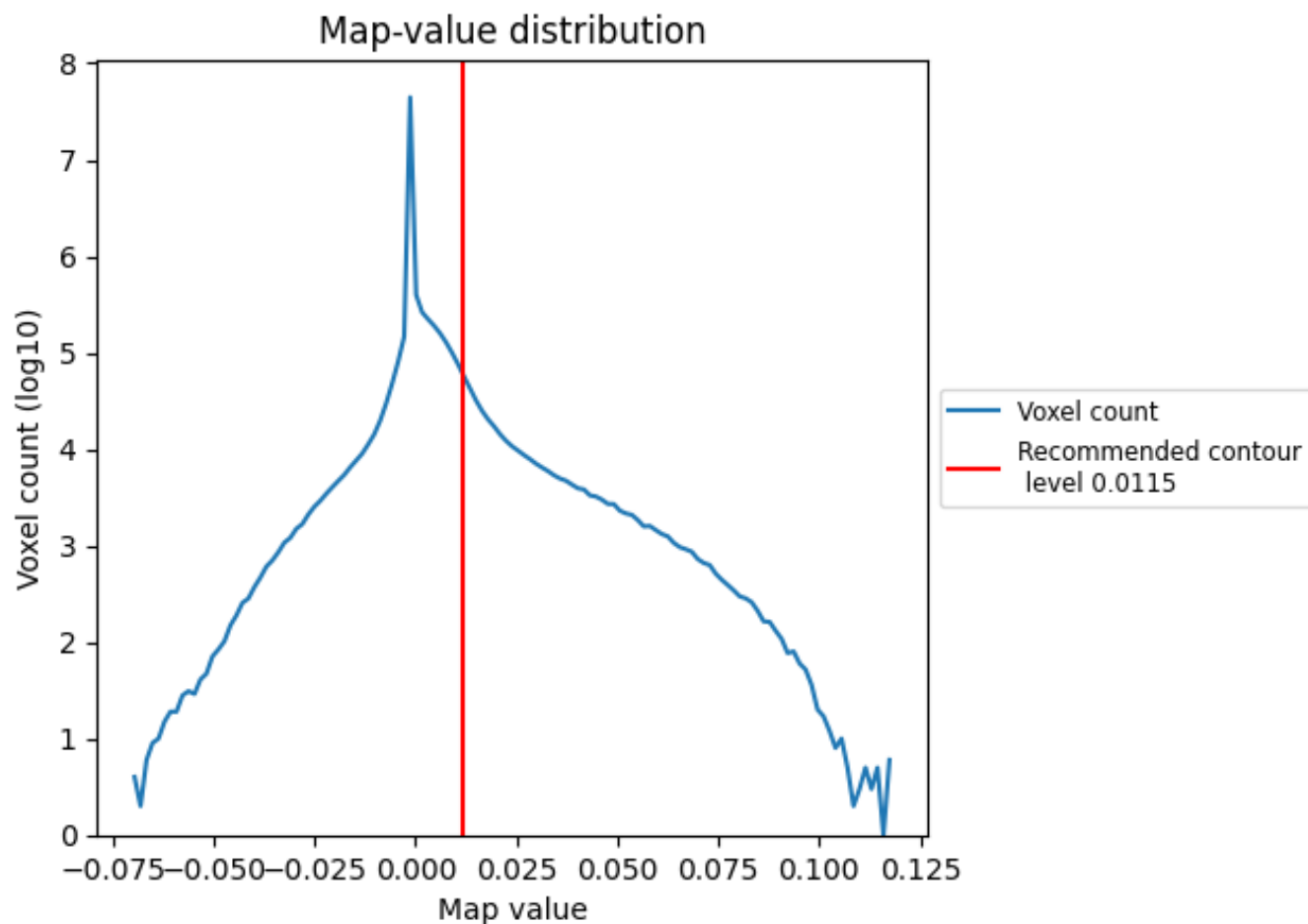
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

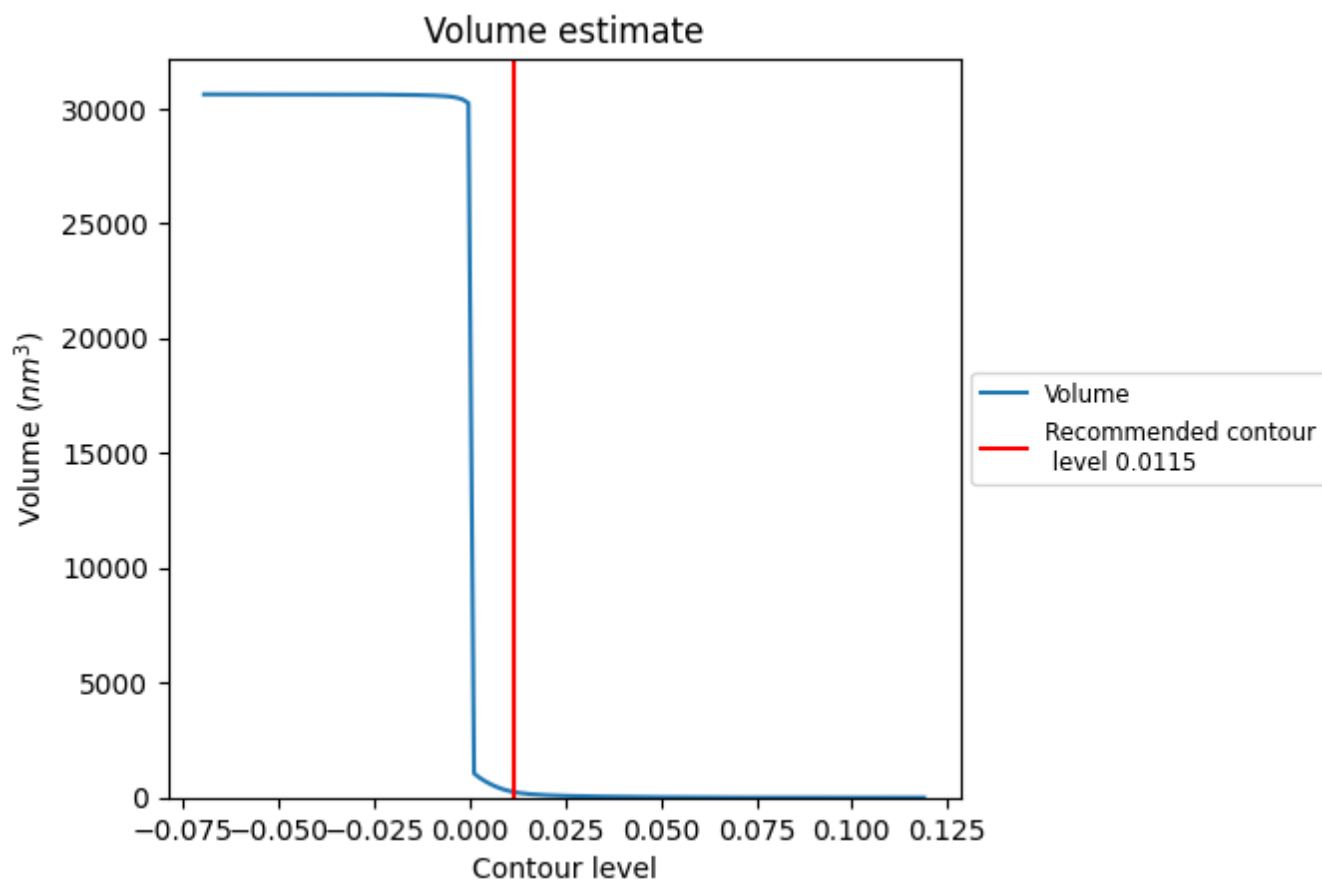
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

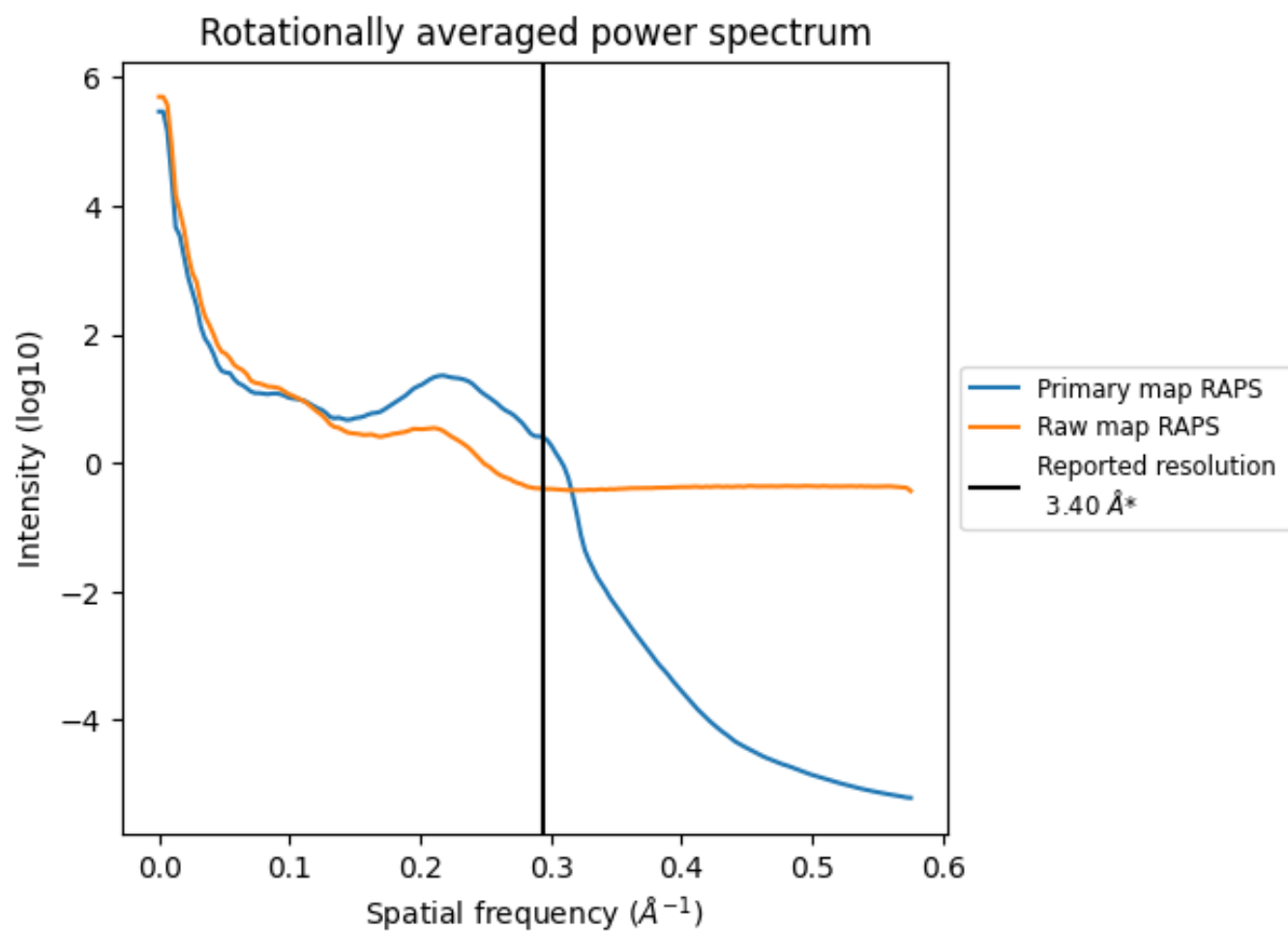
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243  $\text{nm}^3$ ; this corresponds to an approximate mass of 219 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 ⓘ

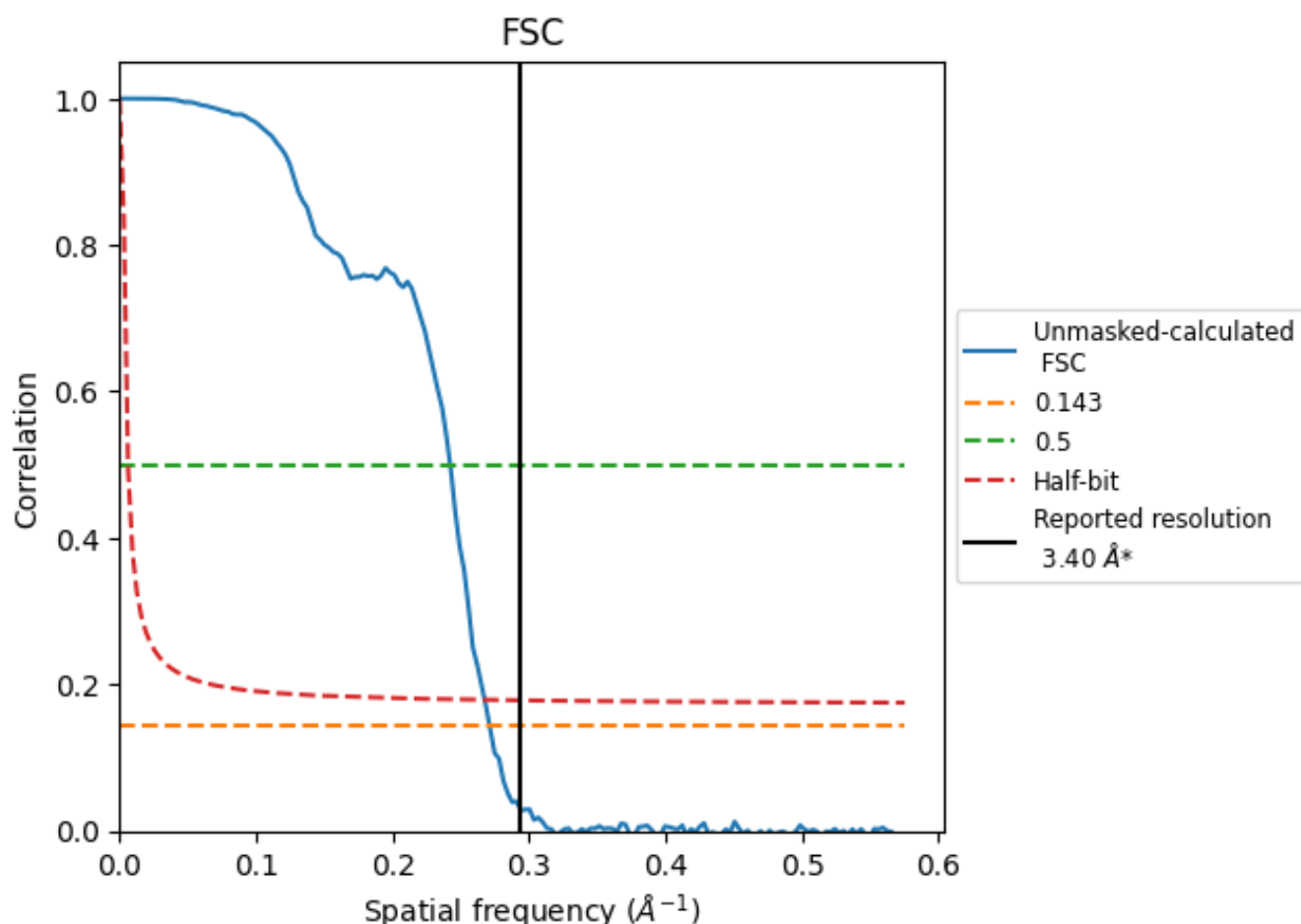


\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

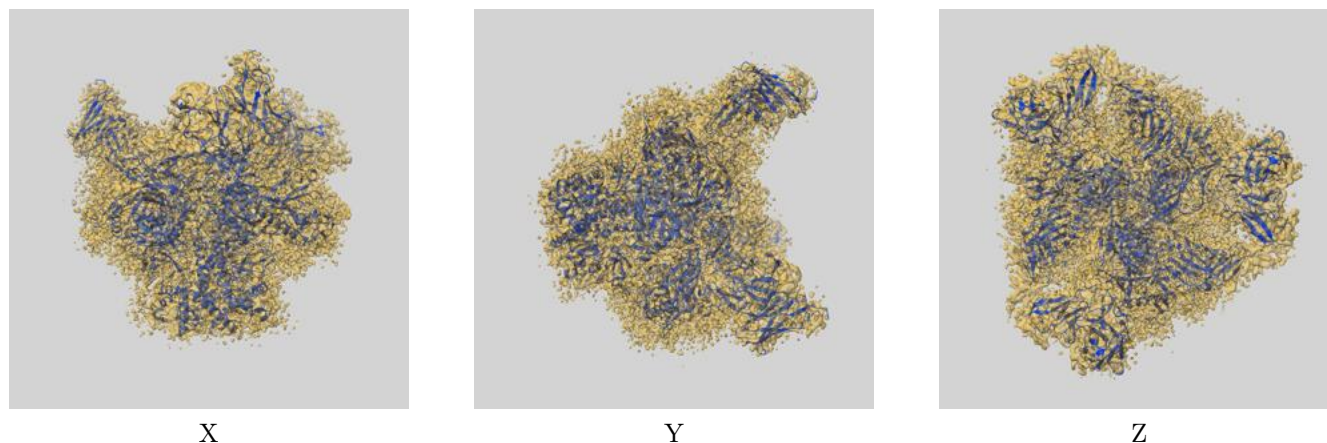
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	4.13	3.74

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

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

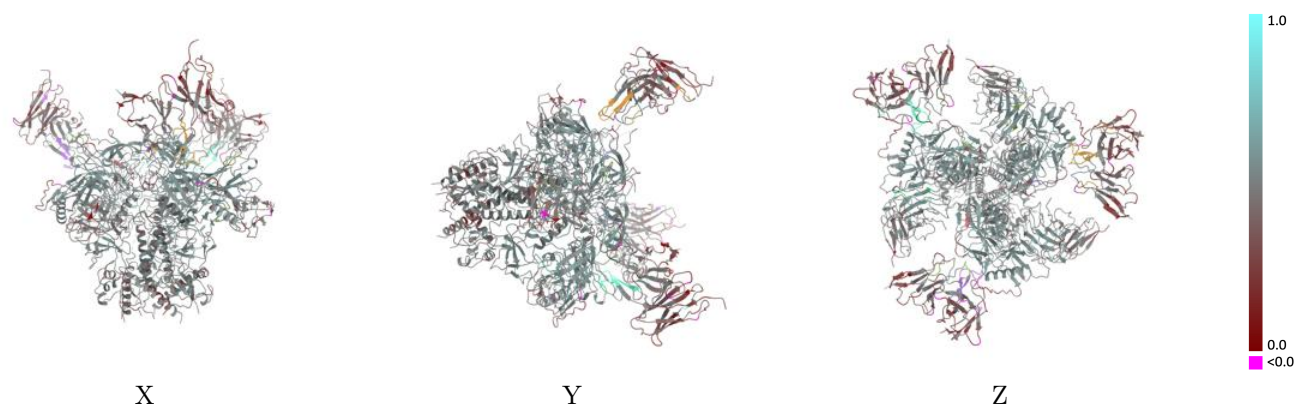
This section contains information regarding the fit between EMDB map EMD-26496 and PDB model 7UGQ. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



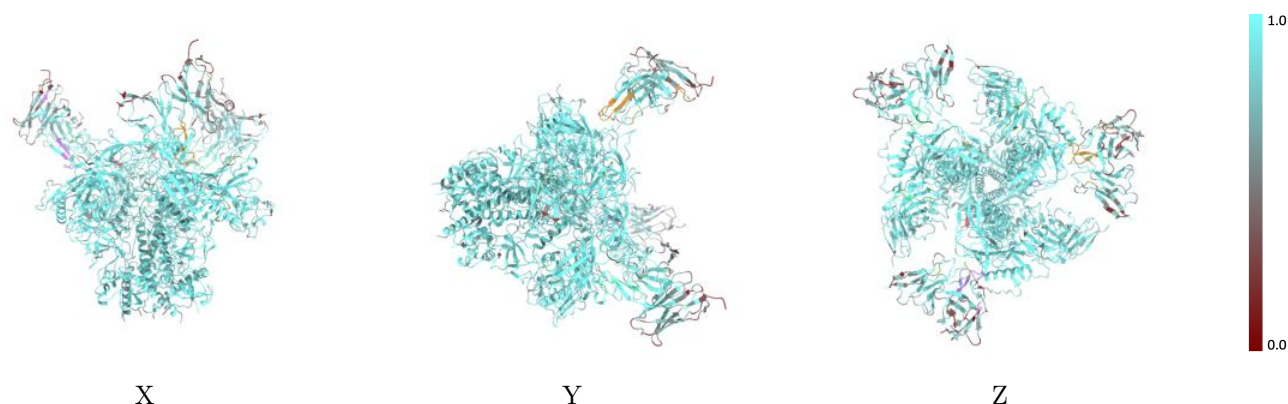
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



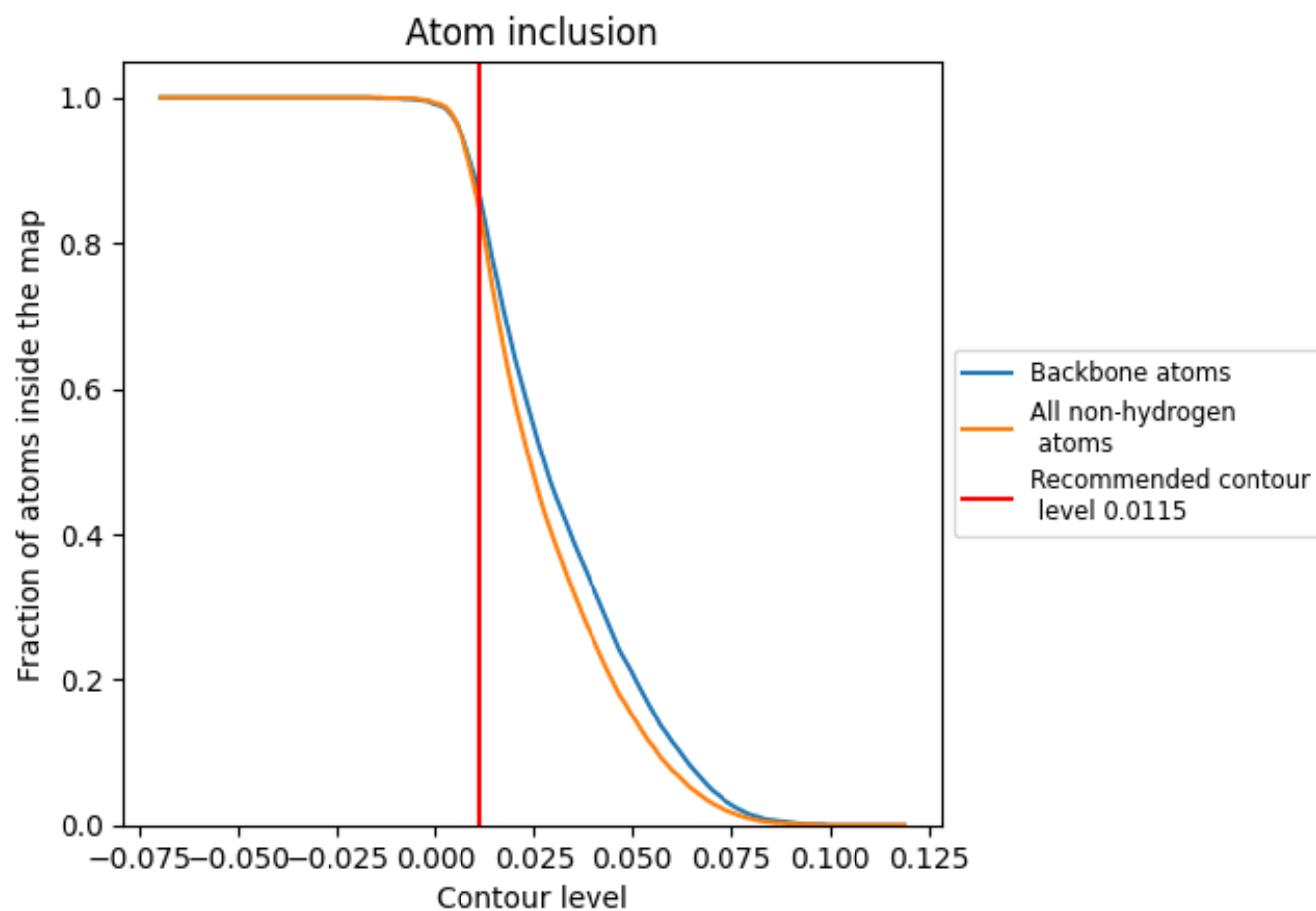
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0115).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.4700
0	 0.6150	 0.3230
1	 0.8000	 0.4520
A	 0.8890	 0.5090
B	 0.8920	 0.5090
C	 0.8910	 0.5100
D	 0.8520	 0.4660
E	 0.8560	 0.4690
F	 0.8530	 0.4680
G	 0.9000	 0.5280
H	 0.8990	 0.5230
I	 0.8960	 0.5230
J	 0.8350	 0.4460
K	 0.8390	 0.4470
L	 0.8440	 0.4460
M	 0.6580	 0.3690
N	 0.6510	 0.3690
O	 0.6530	 0.3640
P	 0.7900	 0.4220
Q	 0.7930	 0.4170
R	 0.7900	 0.4170
S	 0.8210	 0.4340
T	 0.8570	 0.4680
U	 0.7860	 0.4400
V	 0.6670	 0.3180
W	 0.8200	 0.4350
X	 0.8210	 0.4790
Y	 0.7860	 0.3310
Z	 0.5000	 0.3260
a	 0.7140	 0.3840
b	 0.8930	 0.4870
c	 0.7180	 0.3190
d	 0.8000	 0.4460
e	 0.8210	 0.4350
f	 0.8570	 0.4600



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Chain	Atom inclusion	Q-score
g	 0.7860	 0.4220
h	 0.7440	 0.3850
i	 0.8530	 0.4370
j	 0.7860	 0.4660
k	 0.7500	 0.3370
l	 0.5000	 0.3130
m	 0.8570	 0.4290
n	 0.8570	 0.4750
o	 0.6670	 0.3470
p	 0.8300	 0.4660
q	 0.8210	 0.4400
r	 0.8570	 0.4590
s	 0.7860	 0.4300
t	 0.6670	 0.3360
u	 0.8530	 0.4360
v	 0.7860	 0.4850
w	 0.7500	 0.3560
x	 0.5360	 0.3360
y	 0.7140	 0.3920
z	 0.8570	 0.4750