



Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 11:53 AM EDT

PDB ID : 6N1V
EMDB ID : EMD-9319
Title : Cryo-EM structure at 4.0 Å resolution of vaccine-elicited antibody A12V163-a.01 in complex with HIV-1 Env BG505 DS-SOSIP, and antibodies VRC03 and PGT122
Authors : Acharya, P.; Kwong, P.D.
Deposited on : 2018-11-12
Resolution : 4.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

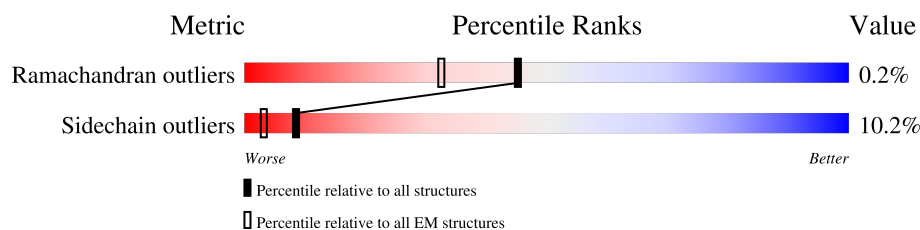
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 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.














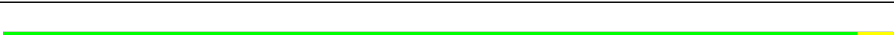

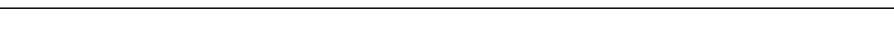
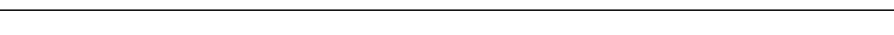
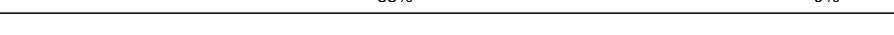

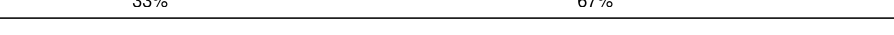
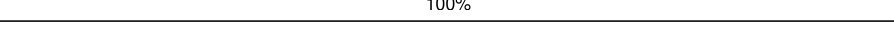
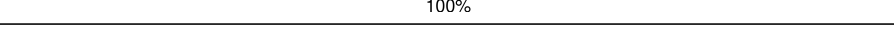





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	1	225	<div> <div>17%</div> <div>96%</div> <div>.</div> </div>
1	3	225	<div> <div>18%</div> <div>96%</div> <div>.</div> </div>
1	H	225	<div> <div>18%</div> <div>96%</div> <div>.</div> </div>
2	2	215	<div> <div>13%</div> <div>93%</div> <div>7%</div> </div>
2	4	215	<div> <div>13%</div> <div>93%</div> <div>7%</div> </div>
2	L	215	<div> <div>13%</div> <div>93%</div> <div>7%</div> </div>
3	A	473	<div> <div>83%</div> <div>12%</div> <div>.</div> </div>
3	B	473	<div> <div>83%</div> <div>12%</div> <div>.</div> </div>
3	C	473	<div> <div>83%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	153	
4	E	153	
4	F	153	
5	M	132	
5	X	132	
5	Y	132	
6	N	107	
6	Z	107	
6	a	107	
7	Q	129	
7	f	129	
7	g	129	
8	R	102	
8	h	102	
8	i	102	
9	5	3	
9	6	3	
9	8	3	
9	CA	3	
9	DA	3	
9	G	3	
9	J	3	
9	P	3	
9	S	3	
9	U	3	

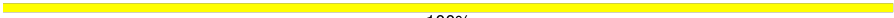



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Mol	Chain	Length	Quality of chain
9	c	3	100%
9	d	3	67% 33%
9	e	3	67% 33%
9	k	3	33% 67%
9	n	3	33% 67%
9	o	3	33% 67%
9	q	3	100%
9	u	3	100%
9	v	3	67% 33%
9	w	3	67% 33%
9	y	3	33% 67%
10	BA	4	100%
10	I	4	25% 25% 75%
10	b	4	100%
10	j	4	25% 75%
10	t	4	100%
10	x	4	25% 75%
11	AA	5	20% 80%
11	K	5	100%
11	W	5	20% 80%
11	l	5	100%
11	s	5	20% 80%
11	z	5	100%
12	0	2	100%
12	7	2	50% 50%

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Mol	Chain	Length	Quality of chain
12	9	2	 100%
12	O	2	 100%
12	T	2	 50%  50%
12	V	2	 100%
12	m	2	 100%
12	p	2	 50%  50%
12	r	2	 100%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 36498 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 A12V163-a.01 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	224	Total	C	N	O	S	0	0
			1669	1046	283	335	5		
1	1	224	Total	C	N	O	S	0	0
			1669	1046	283	335	5		
1	H	224	Total	C	N	O	S	0	0
			1669	1046	283	335	5		

- Molecule 2 is a protein called A12V163-a.01 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	215	Total	C	N	O	S	0	0
			1612	1008	266	332	6		
2	2	215	Total	C	N	O	S	0	0
			1612	1008	266	332	6		
2	L	215	Total	C	N	O	S	0	0
			1612	1008	266	332	6		

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	453	Total	C	N	O	S	0	0
			3565	2236	630	671	28		
3	A	453	Total	C	N	O	S	0	0
			3565	2236	630	671	28		
3	C	453	Total	C	N	O	S	0	0
			3565	2236	630	671	28		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	332	ASN	THR	conflict	UNP Q2N0S6
B	501	CYS	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	501	CYS	ALA	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 4 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
4	E	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
4	D	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	605	CYS	THR	conflict	UNP Q2N0S6
E	605	CYS	THR	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 5 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
5	X	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
5	M	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		

- Molecule 6 is a protein called PGT122 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	103	Total	C	N	O	S	0	0
			787	491	137	157	2		
6	Z	103	Total	C	N	O	S	0	0
			787	491	137	157	2		
6	N	103	Total	C	N	O	S	0	0
			787	491	137	157	2		

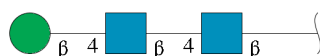
- Molecule 7 is a protein called VRC03 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	129	Total	C	N	O	S	0	0
			1029	660	176	187	6		
7	f	129	Total	C	N	O	S	0	0
			1029	660	176	187	6		
7	Q	129	Total	C	N	O	S	0	0
			1029	660	176	187	6		

- Molecule 8 is a protein called VRC03 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	102	Total	C	N	O	S	0	0
			802	510	137	152	3		
8	h	102	Total	C	N	O	S	0	0
			802	510	137	152	3		
8	R	102	Total	C	N	O	S	0	0
			802	510	137	152	3		

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	G	3	Total	C	N	O	0	0
			39	22	2	15		
9	J	3	Total	C	N	O	0	0
			39	22	2	15		
9	P	3	Total	C	N	O	0	0
			39	22	2	15		
9	S	3	Total	C	N	O	0	0
			39	22	2	15		
9	U	3	Total	C	N	O	0	0
			39	22	2	15		
9	c	3	Total	C	N	O	0	0
			39	22	2	15		
9	d	3	Total	C	N	O	0	0
			39	22	2	15		
9	e	3	Total	C	N	O	0	0
			39	22	2	15		
9	k	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	n	3	Total	C	N	O	0	0
			39	22	2	15		
9	o	3	Total	C	N	O	0	0
			39	22	2	15		
9	q	3	Total	C	N	O	0	0
			39	22	2	15		
9	u	3	Total	C	N	O	0	0
			39	22	2	15		
9	v	3	Total	C	N	O	0	0
			39	22	2	15		
9	w	3	Total	C	N	O	0	0
			39	22	2	15		
9	y	3	Total	C	N	O	0	0
			39	22	2	15		
9	5	3	Total	C	N	O	0	0
			39	22	2	15		
9	6	3	Total	C	N	O	0	0
			39	22	2	15		
9	8	3	Total	C	N	O	0	0
			39	22	2	15		
9	CA	3	Total	C	N	O	0	0
			39	22	2	15		
9	DA	3	Total	C	N	O	0	0
			39	22	2	15		

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



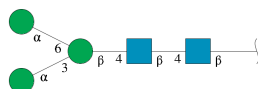
Mol	Chain	Residues	Atoms				AltConf	Trace
10	I	4	Total	C	N	O	0	0
			50	28	2	20		
10	b	4	Total	C	N	O	0	0
			50	28	2	20		
10	j	4	Total	C	N	O	0	0
			50	28	2	20		
10	t	4	Total	C	N	O	0	0
			50	28	2	20		

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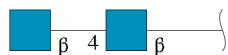
Mol	Chain	Residues	Atoms				AltConf	Trace
10	x	4	Total	C	N	O	0	0
			50	28	2	20		
10	BA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 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
11	K	5	Total	C	N	O	0	0
			61	34	2	25		
11	W	5	Total	C	N	O	0	0
			61	34	2	25		
11	l	5	Total	C	N	O	0	0
			61	34	2	25		
11	s	5	Total	C	N	O	0	0
			61	34	2	25		
11	z	5	Total	C	N	O	0	0
			61	34	2	25		
11	AA	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 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
12	O	2	Total	C	N	O	0	0
			28	16	2	10		
12	T	2	Total	C	N	O	0	0
			28	16	2	10		
12	V	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
12	m	2	Total	C	N	O	0	0
			28	16	2	10		
12	p	2	Total	C	N	O	0	0
			28	16	2	10		
12	r	2	Total	C	N	O	0	0
			28	16	2	10		
12	0	2	Total	C	N	O	0	0
			28	16	2	10		
12	7	2	Total	C	N	O	0	0
			28	16	2	10		
12	9	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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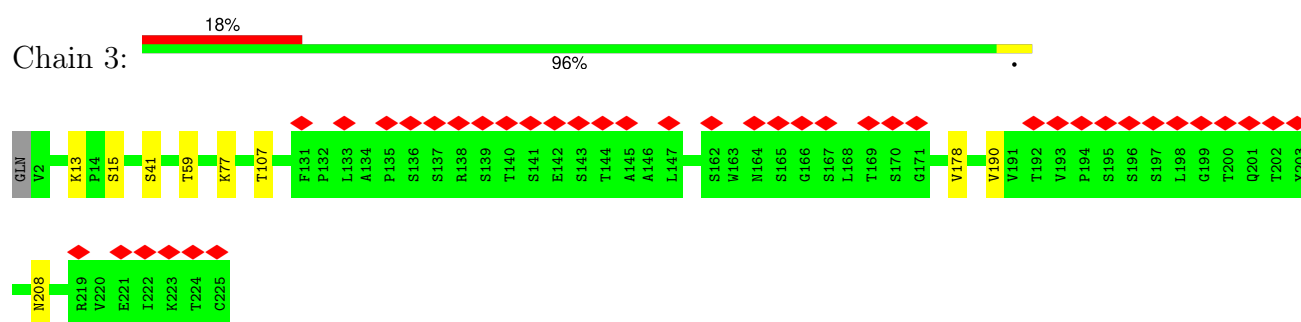
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Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	
13	C	1	Total	C	N	O	0
			14	8	1	5	

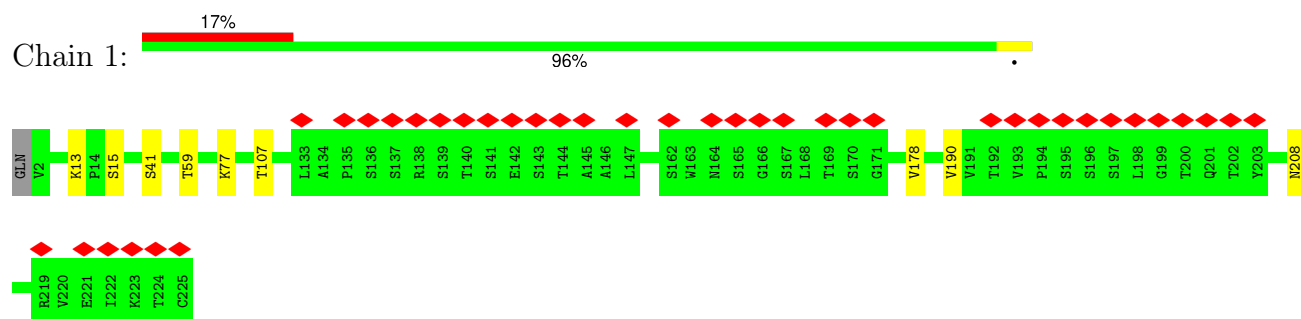
3 Residue-property plots [i](#)

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

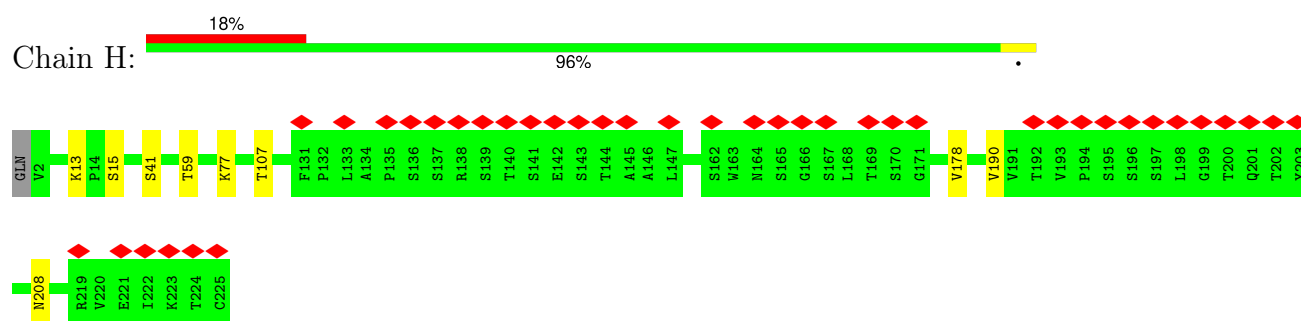
- Molecule 1: A12V163-a.01 Heavy chain



- Molecule 1: A12V163-a.01 Heavy chain

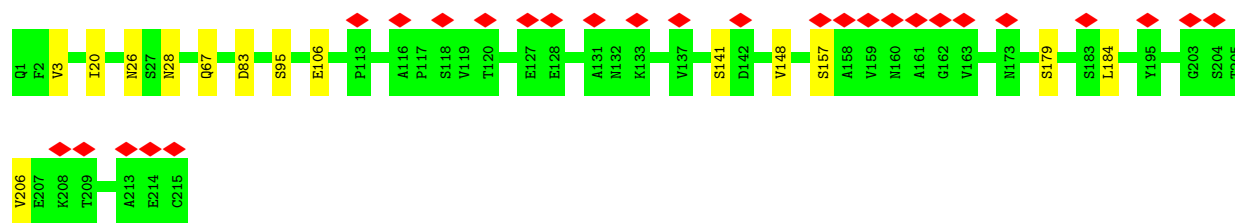


- Molecule 1: A12V163-a.01 Heavy chain

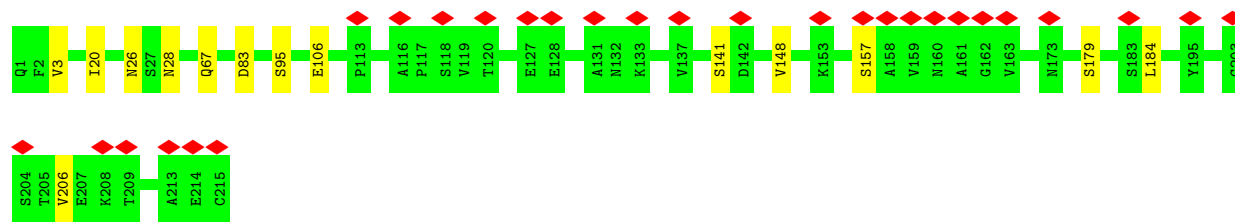


- Molecule 2: A12V163-a.01 Light chain

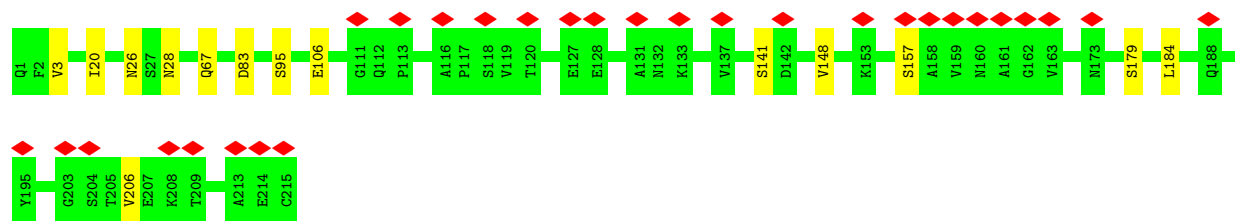
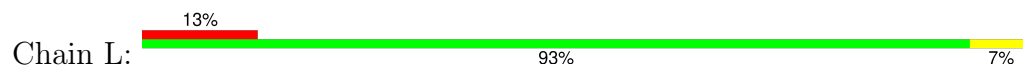




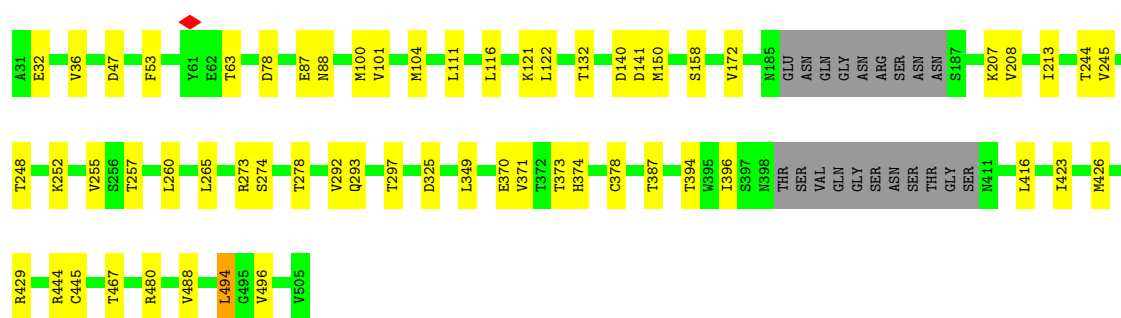
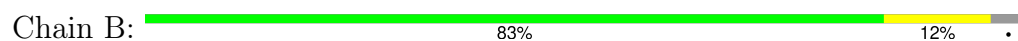
• Molecule 2: A12V163-a.01 Light chain



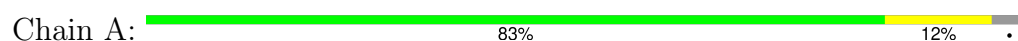
• Molecule 2: A12V163-a.01 Light chain

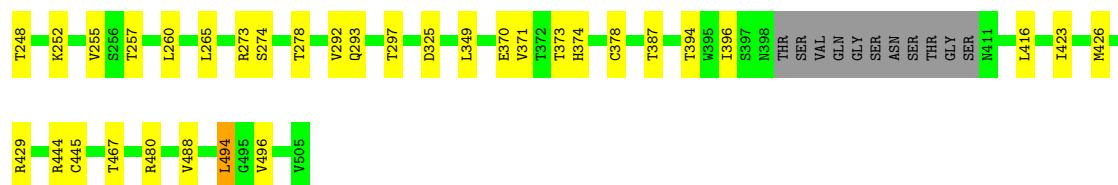


• Molecule 3: Envelope glycoprotein gp120



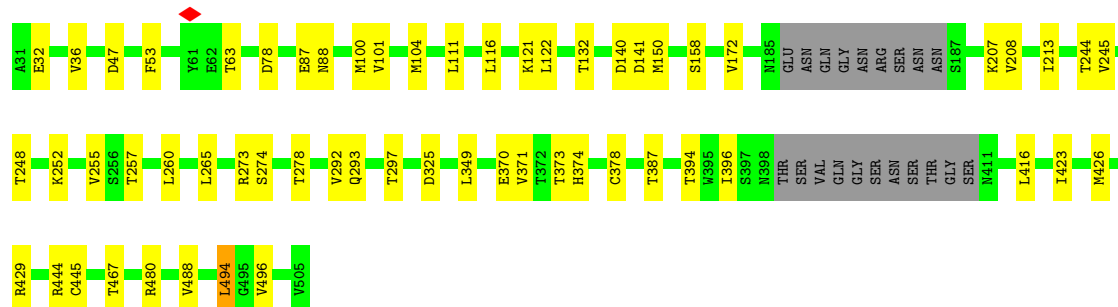
• Molecule 3: Envelope glycoprotein gp120





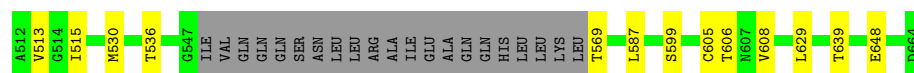
• Molecule 3: Envelope glycoprotein gp120

Chain C: 83% 12% •



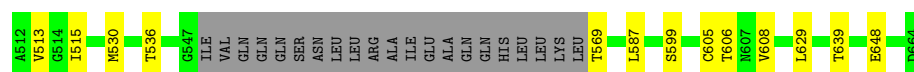
• Molecule 4: Envelope glycoprotein gp41

Chain F: 78% 8% 14%



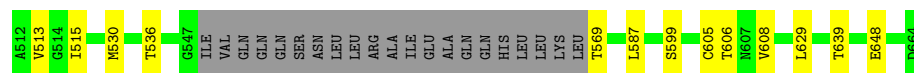
• Molecule 4: Envelope glycoprotein gp41

Chain E: 78% 8% 14%



• Molecule 4: Envelope glycoprotein gp41

Chain D: 78% 8% 14%



• Molecule 5: PGT122 Heavy chain

Chain Y: 91% 9%



• Molecule 5: PGT122 Heavy chain

Chain X:  91% 9%




- Molecule 5: PGT122 Heavy chain

Chain M:  91% 9%




- Molecule 6: PGT122 Light chain

Chain a:  86% 10% .




- Molecule 6: PGT122 Light chain

Chain Z:  86% 10% .



- Molecule 6: PGT122 Light chain

Chain N:  86% 10% .



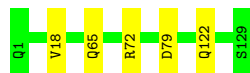
- Molecule 7: VRC03 Heavy chain

Chain g:  96% .



- Molecule 7: VRC03 Heavy chain

Chain f:  96% .




- Molecule 7: VRC03 Heavy chain

Chain Q:  95% 5%




- Molecule 8: VRC03 Light chain

Chain i:  88% 9% .




- Molecule 8: VRC03 Light chain

Chain h:  88% 9% .



- Molecule 8: VRC03 Light chain

Chain R:  88% 9% .



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

Chain G:  67% 33%



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

Chain J:  33% 67%



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

Chain P:  33% 67%



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

Chain S:  33% 67%

MAG1
MAG2
BMA3

- Molecule 9: 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

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

Chain c:  100%

MAG1
MAG2
BMA3

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

Chain d:  67% 33%

MAG1
MAG2
BMA3

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

Chain e:  67% 33%

MAG1
MAG2
BMA3

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

Chain k:  33% 67%

MAG1
MAG2
BMA3

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

Chain n:  33% 67%



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

Chain o:



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

Chain q:



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

Chain u:



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

Chain v:



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

Chain w:



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

Chain y:



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

Chain 5:  33% 67%



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

Chain 6:  33% 67%



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

Chain 8:  100%



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

Chain CA:  100%



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

Chain DA:  67% 33%




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

Chain I:  25% 25% 75%




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

Chain b:  100%

MAG1
MAG2
BMA3
MAN4

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

Chain j:  25% 75%

MAG1
MAG2
BMA3
MAN4

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

Chain t:  100%

MAG1
MAG2
BMA3
MAN4

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

Chain x:  25% 75%

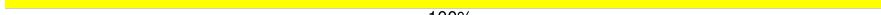
MAG1
MAG2
BMA3
MAN4

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

Chain BA:  100%


MAG1
MAG2
BMA3
MAN4

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

Chain K:  100%

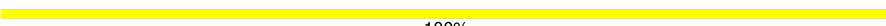
MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 11: 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:  20% 80%



- Molecule 11: 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 l:  100%

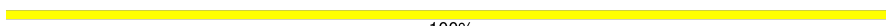


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  20% 80%



- Molecule 11: 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 z:  100%



- Molecule 11: 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 AA:  20% 80%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  50% 50%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  100%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:  50% 50%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:

100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	43895	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69.98	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.200	Depositor
Minimum map value	-1.386	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.73	Depositor
Map size (Å)	430.08002, 430.08002, 430.08002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	1	0.33	0/1708	0.58	0/2334
1	3	0.33	0/1708	0.58	0/2334
1	H	0.34	0/1708	0.58	0/2334
2	2	0.34	0/1650	0.54	0/2249
2	4	0.34	0/1650	0.54	0/2249
2	L	0.34	0/1650	0.54	0/2249
3	A	0.48	0/3639	0.58	1/4941 (0.0%)
3	B	0.48	0/3639	0.58	1/4941 (0.0%)
3	C	0.48	0/3639	0.58	1/4941 (0.0%)
4	D	0.44	0/1052	0.57	0/1427
4	E	0.44	0/1052	0.57	0/1427
4	F	0.44	0/1052	0.57	0/1427
5	M	0.37	0/1076	0.54	0/1465
5	X	0.37	0/1076	0.54	0/1465
5	Y	0.37	0/1076	0.54	0/1465
6	N	0.41	0/807	0.55	0/1104
6	Z	0.41	0/807	0.55	0/1104
6	a	0.41	0/807	0.55	0/1104
7	Q	0.52	0/1062	0.53	0/1447
7	f	0.52	0/1062	0.53	0/1447
7	g	0.52	0/1062	0.53	0/1447
8	R	0.44	0/820	0.60	1/1107 (0.1%)
8	h	0.45	0/820	0.60	1/1107 (0.1%)
8	i	0.44	0/820	0.60	1/1107 (0.1%)
All	All	0.43	0/35442	0.56	6/48222 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	R	0	3
8	h	0	3
8	i	0	3
All	All	0	9

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	494	LEU	CA-CB-CG	6.66	130.61	115.30
3	A	494	LEU	CA-CB-CG	6.65	130.60	115.30
3	C	494	LEU	CA-CB-CG	6.65	130.60	115.30
8	h	90	GLN	C-N-CA	5.13	134.53	121.70
8	i	90	GLN	C-N-CA	5.13	134.51	121.70
8	R	90	GLN	C-N-CA	5.12	134.50	121.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	R	7	SER	Peptide
8	R	89	GLN	Peptide
8	R	91	PHE	Mainchain
8	h	7	SER	Peptide
8	h	89	GLN	Peptide
8	h	91	PHE	Mainchain
8	i	7	SER	Peptide
8	i	89	GLN	Peptide
8	i	91	PHE	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	222/225 (99%)	214 (96%)	8 (4%)	0	100	100
1	3	222/225 (99%)	214 (96%)	8 (4%)	0	100	100
1	H	222/225 (99%)	214 (96%)	8 (4%)	0	100	100
2	2	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
2	4	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
2	L	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
3	A	447/473 (94%)	410 (92%)	36 (8%)	1 (0%)	44	76
3	B	447/473 (94%)	410 (92%)	36 (8%)	1 (0%)	44	76
3	C	447/473 (94%)	410 (92%)	36 (8%)	1 (0%)	44	76
4	D	128/153 (84%)	115 (90%)	13 (10%)	0	100	100
4	E	128/153 (84%)	115 (90%)	13 (10%)	0	100	100
4	F	128/153 (84%)	115 (90%)	13 (10%)	0	100	100
5	M	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
5	X	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
5	Y	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
6	N	101/107 (94%)	96 (95%)	5 (5%)	0	100	100
6	Z	101/107 (94%)	96 (95%)	5 (5%)	0	100	100
6	a	101/107 (94%)	96 (95%)	5 (5%)	0	100	100
7	Q	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
7	f	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
7	g	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
8	R	100/102 (98%)	89 (89%)	9 (9%)	2 (2%)	6	34
8	h	100/102 (98%)	89 (89%)	9 (9%)	2 (2%)	6	34
8	i	100/102 (98%)	89 (89%)	9 (9%)	2 (2%)	6	34
All	All	4404/4608 (96%)	4101 (93%)	294 (7%)	9 (0%)	45	76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	91	PHE
8	h	91	PHE
8	R	91	PHE

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Mol	Chain	Res	Type
3	B	88	ASN
3	A	88	ASN
3	C	88	ASN
8	i	8	PRO
8	h	8	PRO
8	R	8	PRO

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	1	194/195 (100%)	185 (95%)	9 (5%)	23	46
1	3	194/195 (100%)	185 (95%)	9 (5%)	23	46
1	H	194/195 (100%)	185 (95%)	9 (5%)	23	46
2	2	180/180 (100%)	166 (92%)	14 (8%)	10	33
2	4	180/180 (100%)	166 (92%)	14 (8%)	10	33
2	L	180/180 (100%)	166 (92%)	14 (8%)	10	33
3	A	404/421 (96%)	346 (86%)	58 (14%)	2	15
3	B	404/421 (96%)	346 (86%)	58 (14%)	2	15
3	C	404/421 (96%)	346 (86%)	58 (14%)	2	15
4	D	110/129 (85%)	97 (88%)	13 (12%)	4	19
4	E	110/129 (85%)	97 (88%)	13 (12%)	4	19
4	F	110/129 (85%)	97 (88%)	13 (12%)	4	19
5	M	116/116 (100%)	104 (90%)	12 (10%)	6	22
5	X	116/116 (100%)	104 (90%)	12 (10%)	6	22
5	Y	116/116 (100%)	104 (90%)	12 (10%)	6	22
6	N	86/89 (97%)	75 (87%)	11 (13%)	3	18
6	Z	86/89 (97%)	75 (87%)	11 (13%)	3	18
6	a	86/89 (97%)	75 (87%)	11 (13%)	3	18
7	Q	109/110 (99%)	103 (94%)	6 (6%)	18	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	f	109/110 (99%)	104 (95%)	5 (5%)	23	46
7	g	109/110 (99%)	104 (95%)	5 (5%)	23	46
8	R	86/86 (100%)	77 (90%)	9 (10%)	5	22
8	h	86/86 (100%)	77 (90%)	9 (10%)	5	22
8	i	86/86 (100%)	77 (90%)	9 (10%)	5	22
All	All	3855/3978 (97%)	3461 (90%)	394 (10%)	8	23

All (394) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	13	LYS
1	3	15	SER
1	3	41	SER
1	3	59	THR
1	3	77	LYS
1	3	107	THR
1	3	178	VAL
1	3	190	VAL
1	3	208	ASN
2	4	3	VAL
2	4	20	ILE
2	4	26	ASN
2	4	28	ASN
2	4	67	GLN
2	4	83	ASP
2	4	95	SER
2	4	106	GLU
2	4	141	SER
2	4	148	VAL
2	4	157	SER
2	4	179	SER
2	4	184	LEU
2	4	206	VAL
3	B	32	GLU
3	B	36	VAL
3	B	47	ASP
3	B	53	PHE
3	B	63	THR
3	B	78	ASP
3	B	87	GLU

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Mol	Chain	Res	Type
3	B	100	MET
3	B	101	VAL
3	B	104	MET
3	B	111	LEU
3	B	116	LEU
3	B	121	LYS
3	B	122	LEU
3	B	132	THR
3	B	140	ASP
3	B	141	ASP
3	B	150	MET
3	B	158	SER
3	B	172	VAL
3	B	207	LYS
3	B	208	VAL
3	B	213	ILE
3	B	244	THR
3	B	245	VAL
3	B	248	THR
3	B	252	LYS
3	B	255	VAL
3	B	257	THR
3	B	260	LEU
3	B	265	LEU
3	B	273	ARG
3	B	274	SER
3	B	278	THR
3	B	292	VAL
3	B	293	GLN
3	B	297	THR
3	B	325	ASP
3	B	349	LEU
3	B	370	GLU
3	B	371	VAL
3	B	373	THR
3	B	374	HIS
3	B	378	CYS
3	B	387	THR
3	B	394	THR
3	B	396	ILE
3	B	416	LEU
3	B	423	ILE

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Mol	Chain	Res	Type
3	B	426	MET
3	B	429	ARG
3	B	444	ARG
3	B	445	CYS
3	B	467	THR
3	B	480	ARG
3	B	488	VAL
3	B	494	LEU
3	B	496	VAL
4	F	513	VAL
4	F	515	ILE
4	F	530	MET
4	F	536	THR
4	F	569	THR
4	F	587	LEU
4	F	599	SER
4	F	605	CYS
4	F	606	THR
4	F	608	VAL
4	F	629	LEU
4	F	639	THR
4	F	648	GLU
5	Y	4	LEU
5	Y	32	ASN
5	Y	40	PRO
5	Y	41	LEU
5	Y	44	GLN
5	Y	57	THR
5	Y	67	VAL
5	Y	77	LEU
5	Y	82	LEU
5	Y	95	THR
5	Y	96	LYS
5	Y	109	VAL
6	a	26	GLU
6	a	47	ILE
6	a	58	ILE
6	a	63	SER
6	a	67(B)	THR
6	a	76	THR
6	a	85	ASP
6	a	93	SER

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Mol	Chain	Res	Type
6	a	97	VAL
6	a	105	ILE
6	a	106	VAL
7	g	18	VAL
7	g	65	GLN
7	g	72	ARG
7	g	79	ASP
7	g	122	GLN
8	i	6	GLN
8	i	7	SER
8	i	27	GLN
8	i	36	TYR
8	i	45	ARG
8	i	72	PHE
8	i	82	ASP
8	i	90	GLN
8	i	96	GLU
1	1	13	LYS
1	1	15	SER
1	1	41	SER
1	1	59	THR
1	1	77	LYS
1	1	107	THR
1	1	178	VAL
1	1	190	VAL
1	1	208	ASN
2	2	3	VAL
2	2	20	ILE
2	2	26	ASN
2	2	28	ASN
2	2	67	GLN
2	2	83	ASP
2	2	95	SER
2	2	106	GLU
2	2	141	SER
2	2	148	VAL
2	2	157	SER
2	2	179	SER
2	2	184	LEU
2	2	206	VAL
3	A	32	GLU
3	A	36	VAL

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Mol	Chain	Res	Type
3	A	47	ASP
3	A	53	PHE
3	A	63	THR
3	A	78	ASP
3	A	87	GLU
3	A	100	MET
3	A	101	VAL
3	A	104	MET
3	A	111	LEU
3	A	116	LEU
3	A	121	LYS
3	A	122	LEU
3	A	132	THR
3	A	140	ASP
3	A	141	ASP
3	A	150	MET
3	A	158	SER
3	A	172	VAL
3	A	207	LYS
3	A	208	VAL
3	A	213	ILE
3	A	244	THR
3	A	245	VAL
3	A	248	THR
3	A	252	LYS
3	A	255	VAL
3	A	257	THR
3	A	260	LEU
3	A	265	LEU
3	A	273	ARG
3	A	274	SER
3	A	278	THR
3	A	292	VAL
3	A	293	GLN
3	A	297	THR
3	A	325	ASP
3	A	349	LEU
3	A	370	GLU
3	A	371	VAL
3	A	373	THR
3	A	374	HIS
3	A	378	CYS

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Mol	Chain	Res	Type
3	A	387	THR
3	A	394	THR
3	A	396	ILE
3	A	416	LEU
3	A	423	ILE
3	A	426	MET
3	A	429	ARG
3	A	444	ARG
3	A	445	CYS
3	A	467	THR
3	A	480	ARG
3	A	488	VAL
3	A	494	LEU
3	A	496	VAL
4	E	513	VAL
4	E	515	ILE
4	E	530	MET
4	E	536	THR
4	E	569	THR
4	E	587	LEU
4	E	599	SER
4	E	605	CYS
4	E	606	THR
4	E	608	VAL
4	E	629	LEU
4	E	639	THR
4	E	648	GLU
5	X	4	LEU
5	X	32	ASN
5	X	40	PRO
5	X	41	LEU
5	X	44	GLN
5	X	57	THR
5	X	67	VAL
5	X	77	LEU
5	X	82	LEU
5	X	95	THR
5	X	96	LYS
5	X	109	VAL
6	Z	26	GLU
6	Z	47	ILE
6	Z	58	ILE

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Mol	Chain	Res	Type
6	Z	63	SER
6	Z	67(B)	THR
6	Z	76	THR
6	Z	85	ASP
6	Z	93	SER
6	Z	97	VAL
6	Z	105	ILE
6	Z	106	VAL
7	f	18	VAL
7	f	65	GLN
7	f	72	ARG
7	f	79	ASP
7	f	122	GLN
8	h	6	GLN
8	h	7	SER
8	h	27	GLN
8	h	36	TYR
8	h	45	ARG
8	h	72	PHE
8	h	82	ASP
8	h	90	GLN
8	h	96	GLU
3	C	32	GLU
3	C	36	VAL
3	C	47	ASP
3	C	53	PHE
3	C	63	THR
3	C	78	ASP
3	C	87	GLU
3	C	100	MET
3	C	101	VAL
3	C	104	MET
3	C	111	LEU
3	C	116	LEU
3	C	121	LYS
3	C	122	LEU
3	C	132	THR
3	C	140	ASP
3	C	141	ASP
3	C	150	MET
3	C	158	SER
3	C	172	VAL

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Mol	Chain	Res	Type
3	C	207	LYS
3	C	208	VAL
3	C	213	ILE
3	C	244	THR
3	C	245	VAL
3	C	248	THR
3	C	252	LYS
3	C	255	VAL
3	C	257	THR
3	C	260	LEU
3	C	265	LEU
3	C	273	ARG
3	C	274	SER
3	C	278	THR
3	C	292	VAL
3	C	293	GLN
3	C	297	THR
3	C	325	ASP
3	C	349	LEU
3	C	370	GLU
3	C	371	VAL
3	C	373	THR
3	C	374	HIS
3	C	378	CYS
3	C	387	THR
3	C	394	THR
3	C	396	ILE
3	C	416	LEU
3	C	423	ILE
3	C	426	MET
3	C	429	ARG
3	C	444	ARG
3	C	445	CYS
3	C	467	THR
3	C	480	ARG
3	C	488	VAL
3	C	494	LEU
3	C	496	VAL
4	D	513	VAL
4	D	515	ILE
4	D	530	MET
4	D	536	THR

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Mol	Chain	Res	Type
4	D	569	THR
4	D	587	LEU
4	D	599	SER
4	D	605	CYS
4	D	606	THR
4	D	608	VAL
4	D	629	LEU
4	D	639	THR
4	D	648	GLU
1	H	13	LYS
1	H	15	SER
1	H	41	SER
1	H	59	THR
1	H	77	LYS
1	H	107	THR
1	H	178	VAL
1	H	190	VAL
1	H	208	ASN
2	L	3	VAL
2	L	20	ILE
2	L	26	ASN
2	L	28	ASN
2	L	67	GLN
2	L	83	ASP
2	L	95	SER
2	L	106	GLU
2	L	141	SER
2	L	148	VAL
2	L	157	SER
2	L	179	SER
2	L	184	LEU
2	L	206	VAL
5	M	4	LEU
5	M	32	ASN
5	M	40	PRO
5	M	41	LEU
5	M	44	GLN
5	M	57	THR
5	M	67	VAL
5	M	77	LEU
5	M	82	LEU
5	M	95	THR

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Mol	Chain	Res	Type
5	M	96	LYS
5	M	109	VAL
6	N	26	GLU
6	N	47	ILE
6	N	58	ILE
6	N	63	SER
6	N	67(B)	THR
6	N	76	THR
6	N	85	ASP
6	N	93	SER
6	N	97	VAL
6	N	105	ILE
6	N	106	VAL
7	Q	18	VAL
7	Q	33	SER
7	Q	65	GLN
7	Q	72	ARG
7	Q	79	ASP
7	Q	122	GLN
8	R	6	GLN
8	R	7	SER
8	R	27	GLN
8	R	36	TYR
8	R	45	ARG
8	R	72	PHE
8	R	82	ASP
8	R	90	GLN
8	R	96	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	180	GLN
1	3	208	ASN
2	4	99	HIS
3	B	246	GLN
3	B	287	GLN
3	B	302	ASN
3	B	377	ASN
3	B	432	GLN
4	F	607	ASN
5	Y	1	GLN

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Mol	Chain	Res	Type
6	a	38	GLN
7	g	6	GLN
7	g	65	GLN
1	1	180	GLN
1	1	208	ASN
2	2	99	HIS
3	A	246	GLN
3	A	287	GLN
3	A	302	ASN
3	A	377	ASN
3	A	432	GLN
4	E	607	ASN
5	X	1	GLN
6	Z	38	GLN
7	f	6	GLN
7	f	65	GLN
3	C	246	GLN
3	C	287	GLN
3	C	302	ASN
3	C	377	ASN
3	C	432	GLN
4	D	607	ASN
1	H	180	GLN
1	H	208	ASN
2	L	99	HIS
5	M	1	GLN
6	N	38	GLN
7	Q	6	GLN
7	Q	65	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

135 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	$\# Z > 2$
12	NAG	0	1	12,3	14,14,15	0.22	0	17,19,21	0.70	0
12	NAG	0	2	12	14,14,15	0.30	0	17,19,21	0.65	0
9	NAG	5	1	9,3	14,14,15	0.28	0	17,19,21	1.05	1 (5%)
9	NAG	5	2	9	14,14,15	0.30	0	17,19,21	0.50	0
9	BMA	5	3	9	11,11,12	0.56	0	15,15,17	1.34	2 (13%)
9	NAG	6	1	9,3	14,14,15	1.15	2 (14%)	17,19,21	2.73	8 (47%)
9	NAG	6	2	9	14,14,15	0.51	0	17,19,21	0.58	0
9	BMA	6	3	9	11,11,12	0.44	0	15,15,17	1.27	2 (13%)
12	NAG	7	1	12,3	14,14,15	0.28	0	17,19,21	0.73	1 (5%)
12	NAG	7	2	12	14,14,15	0.39	0	17,19,21	0.58	0
9	NAG	8	1	9,3	14,14,15	0.31	0	17,19,21	1.08	1 (5%)
9	NAG	8	2	9	14,14,15	0.39	0	17,19,21	1.21	3 (17%)
9	BMA	8	3	9	11,11,12	0.91	0	15,15,17	1.00	1 (6%)
12	NAG	9	1	12,3	14,14,15	0.32	0	17,19,21	1.07	1 (5%)
12	NAG	9	2	12	14,14,15	0.43	0	17,19,21	1.01	1 (5%)
11	NAG	AA	1	3,11	14,14,15	0.41	0	17,19,21	0.71	0
11	NAG	AA	2	11	14,14,15	0.21	0	17,19,21	1.05	1 (5%)
11	BMA	AA	3	11	11,11,12	0.73	0	15,15,17	1.04	2 (13%)
11	MAN	AA	4	11	11,11,12	0.75	0	15,15,17	1.25	1 (6%)
11	MAN	AA	5	11	11,11,12	0.86	1 (9%)	15,15,17	1.20	2 (13%)
10	NAG	BA	1	3,10	14,14,15	0.74	1 (7%)	17,19,21	1.08	1 (5%)
10	NAG	BA	2	10	14,14,15	0.49	0	17,19,21	1.34	2 (11%)
10	BMA	BA	3	10	11,11,12	0.72	0	15,15,17	1.14	2 (13%)
10	MAN	BA	4	10	11,11,12	0.83	0	15,15,17	1.13	2 (13%)
9	NAG	CA	1	9,3	14,14,15	0.65	0	17,19,21	1.26	1 (5%)
9	NAG	CA	2	9	14,14,15	0.58	0	17,19,21	1.03	2 (11%)
9	BMA	CA	3	9	11,11,12	0.79	0	15,15,17	1.13	1 (6%)
9	NAG	DA	1	9,3	14,14,15	0.44	0	17,19,21	1.08	2 (11%)
9	NAG	DA	2	9	14,14,15	0.25	0	17,19,21	0.60	0
9	BMA	DA	3	9	11,11,12	0.91	0	15,15,17	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	G	1	9,3	14,14,15	0.58	1 (7%)	17,19,21	1.05	1 (5%)
9	NAG	G	2	9	14,14,15	0.23	0	17,19,21	0.65	0
9	BMA	G	3	9	11,11,12	0.74	0	15,15,17	0.80	0
10	NAG	I	1	3,10	14,14,15	0.74	1 (7%)	17,19,21	0.68	0
10	NAG	I	2	10	14,14,15	0.22	0	17,19,21	0.48	0
10	BMA	I	3	10	11,11,12	1.66	2 (18%)	15,15,17	1.49	3 (20%)
10	MAN	I	4	10	11,11,12	0.79	0	15,15,17	0.88	1 (6%)
9	NAG	J	1	9,3	14,14,15	0.42	0	17,19,21	0.77	1 (5%)
9	NAG	J	2	9	14,14,15	0.39	0	17,19,21	0.50	0
9	BMA	J	3	9	11,11,12	0.67	0	15,15,17	0.95	2 (13%)
11	NAG	K	1	3,11	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
11	NAG	K	2	11	14,14,15	0.55	0	17,19,21	1.26	1 (5%)
11	BMA	K	3	11	11,11,12	0.78	0	15,15,17	1.55	2 (13%)
11	MAN	K	4	11	11,11,12	0.74	0	15,15,17	1.09	2 (13%)
11	MAN	K	5	11	11,11,12	0.95	1 (9%)	15,15,17	1.09	1 (6%)
12	NAG	O	1	12,3	14,14,15	0.21	0	17,19,21	0.70	0
12	NAG	O	2	12	14,14,15	0.31	0	17,19,21	0.64	0
9	NAG	P	1	9,3	14,14,15	0.27	0	17,19,21	1.05	1 (5%)
9	NAG	P	2	9	14,14,15	0.30	0	17,19,21	0.50	0
9	BMA	P	3	9	11,11,12	0.54	0	15,15,17	1.34	2 (13%)
9	NAG	S	1	9,3	14,14,15	1.15	2 (14%)	17,19,21	2.72	8 (47%)
9	NAG	S	2	9	14,14,15	0.50	0	17,19,21	0.58	0
9	BMA	S	3	9	11,11,12	0.44	0	15,15,17	1.27	2 (13%)
12	NAG	T	1	12,3	14,14,15	0.28	0	17,19,21	0.72	1 (5%)
12	NAG	T	2	12	14,14,15	0.39	0	17,19,21	0.58	0
9	NAG	U	1	9,3	14,14,15	0.31	0	17,19,21	1.08	1 (5%)
9	NAG	U	2	9	14,14,15	0.38	0	17,19,21	1.21	3 (17%)
9	BMA	U	3	9	11,11,12	0.91	0	15,15,17	0.99	1 (6%)
12	NAG	V	1	12,3	14,14,15	0.32	0	17,19,21	1.07	1 (5%)
12	NAG	V	2	12	14,14,15	0.42	0	17,19,21	1.01	1 (5%)
11	NAG	W	1	3,11	14,14,15	0.41	0	17,19,21	0.71	0
11	NAG	W	2	11	14,14,15	0.21	0	17,19,21	1.05	1 (5%)
11	BMA	W	3	11	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
11	MAN	W	4	11	11,11,12	0.76	0	15,15,17	1.26	1 (6%)
11	MAN	W	5	11	11,11,12	0.87	1 (9%)	15,15,17	1.20	2 (13%)
10	NAG	b	1	3,10	14,14,15	0.73	1 (7%)	17,19,21	1.08	1 (5%)
10	NAG	b	2	10	14,14,15	0.49	0	17,19,21	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	b	3	10	11,11,12	0.72	0	15,15,17	1.14	2 (13%)
10	MAN	b	4	10	11,11,12	0.83	0	15,15,17	1.13	2 (13%)
9	NAG	c	1	9,3	14,14,15	0.65	0	17,19,21	1.26	1 (5%)
9	NAG	c	2	9	14,14,15	0.57	0	17,19,21	1.03	2 (11%)
9	BMA	c	3	9	11,11,12	0.79	0	15,15,17	1.13	1 (6%)
9	NAG	d	1	9,3	14,14,15	0.45	0	17,19,21	1.08	1 (5%)
9	NAG	d	2	9	14,14,15	0.25	0	17,19,21	0.60	0
9	BMA	d	3	9	11,11,12	0.92	0	15,15,17	0.66	0
9	NAG	e	1	9,3	14,14,15	0.59	1 (7%)	17,19,21	1.05	1 (5%)
9	NAG	e	2	9	14,14,15	0.23	0	17,19,21	0.65	0
9	BMA	e	3	9	11,11,12	0.73	0	15,15,17	0.80	0
10	NAG	j	1	3,10	14,14,15	0.75	1 (7%)	17,19,21	0.68	0
10	NAG	j	2	10	14,14,15	0.23	0	17,19,21	0.48	0
10	BMA	j	3	10	11,11,12	1.66	2 (18%)	15,15,17	1.49	3 (20%)
10	MAN	j	4	10	11,11,12	0.78	0	15,15,17	0.88	1 (6%)
9	NAG	k	1	9,3	14,14,15	0.43	0	17,19,21	0.77	1 (5%)
9	NAG	k	2	9	14,14,15	0.38	0	17,19,21	0.50	0
9	BMA	k	3	9	11,11,12	0.67	0	15,15,17	0.94	2 (13%)
11	NAG	l	1	3,11	14,14,15	0.31	0	17,19,21	0.66	1 (5%)
11	NAG	l	2	11	14,14,15	0.55	0	17,19,21	1.26	1 (5%)
11	BMA	l	3	11	11,11,12	0.79	0	15,15,17	1.55	2 (13%)
11	MAN	l	4	11	11,11,12	0.74	0	15,15,17	1.09	2 (13%)
11	MAN	l	5	11	11,11,12	0.95	1 (9%)	15,15,17	1.09	1 (6%)
12	NAG	m	1	12,3	14,14,15	0.21	0	17,19,21	0.70	0
12	NAG	m	2	12	14,14,15	0.30	0	17,19,21	0.64	0
9	NAG	n	1	9,3	14,14,15	0.27	0	17,19,21	1.05	1 (5%)
9	NAG	n	2	9	14,14,15	0.31	0	17,19,21	0.51	0
9	BMA	n	3	9	11,11,12	0.54	0	15,15,17	1.34	2 (13%)
9	NAG	o	1	9,3	14,14,15	1.15	2 (14%)	17,19,21	2.72	8 (47%)
9	NAG	o	2	9	14,14,15	0.51	0	17,19,21	0.58	0
9	BMA	o	3	9	11,11,12	0.44	0	15,15,17	1.27	2 (13%)
12	NAG	p	1	12,3	14,14,15	0.28	0	17,19,21	0.73	1 (5%)
12	NAG	p	2	12	14,14,15	0.38	0	17,19,21	0.59	0
9	NAG	q	1	9,3	14,14,15	0.32	0	17,19,21	1.08	1 (5%)
9	NAG	q	2	9	14,14,15	0.38	0	17,19,21	1.22	3 (17%)
9	BMA	q	3	9	11,11,12	0.91	0	15,15,17	1.00	1 (6%)
12	NAG	r	1	12,3	14,14,15	0.31	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	r	2	12	14,14,15	0.43	0	17,19,21	1.02	1 (5%)
11	NAG	s	1	3,11	14,14,15	0.41	0	17,19,21	0.71	0
11	NAG	s	2	11	14,14,15	0.21	0	17,19,21	1.05	1 (5%)
11	BMA	s	3	11	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
11	MAN	s	4	11	11,11,12	0.76	0	15,15,17	1.26	1 (6%)
11	MAN	s	5	11	11,11,12	0.86	1 (9%)	15,15,17	1.20	2 (13%)
10	NAG	t	1	3,10	14,14,15	0.72	1 (7%)	17,19,21	1.08	1 (5%)
10	NAG	t	2	10	14,14,15	0.50	0	17,19,21	1.35	2 (11%)
10	BMA	t	3	10	11,11,12	0.72	0	15,15,17	1.14	2 (13%)
10	MAN	t	4	10	11,11,12	0.83	0	15,15,17	1.13	2 (13%)
9	NAG	u	1	9,3	14,14,15	0.65	0	17,19,21	1.25	1 (5%)
9	NAG	u	2	9	14,14,15	0.58	0	17,19,21	1.04	2 (11%)
9	BMA	u	3	9	11,11,12	0.80	0	15,15,17	1.14	1 (6%)
9	NAG	v	1	9,3	14,14,15	0.45	0	17,19,21	1.07	1 (5%)
9	NAG	v	2	9	14,14,15	0.25	0	17,19,21	0.60	0
9	BMA	v	3	9	11,11,12	0.92	0	15,15,17	0.66	0
9	NAG	w	1	9,3	14,14,15	0.58	1 (7%)	17,19,21	1.05	1 (5%)
9	NAG	w	2	9	14,14,15	0.23	0	17,19,21	0.65	0
9	BMA	w	3	9	11,11,12	0.73	0	15,15,17	0.80	0
10	NAG	x	1	3,10	14,14,15	0.75	1 (7%)	17,19,21	0.68	0
10	NAG	x	2	10	14,14,15	0.22	0	17,19,21	0.48	0
10	BMA	x	3	10	11,11,12	1.67	2 (18%)	15,15,17	1.49	3 (20%)
10	MAN	x	4	10	11,11,12	0.78	0	15,15,17	0.88	1 (6%)
9	NAG	y	1	9,3	14,14,15	0.42	0	17,19,21	0.77	1 (5%)
9	NAG	y	2	9	14,14,15	0.38	0	17,19,21	0.50	0
9	BMA	y	3	9	11,11,12	0.66	0	15,15,17	0.94	2 (13%)
11	NAG	z	1	3,11	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
11	NAG	z	2	11	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
11	BMA	z	3	11	11,11,12	0.79	0	15,15,17	1.55	2 (13%)
11	MAN	z	4	11	11,11,12	0.74	0	15,15,17	1.08	2 (13%)
11	MAN	z	5	11	11,11,12	0.94	1 (9%)	15,15,17	1.09	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	0	1	12,3	-	0/6/23/26	0/1/1/1
12	NAG	0	2	12	-	2/6/23/26	0/1/1/1
9	NAG	5	1	9,3	-	4/6/23/26	0/1/1/1
9	NAG	5	2	9	-	1/6/23/26	0/1/1/1
9	BMA	5	3	9	-	2/2/19/22	0/1/1/1
9	NAG	6	1	9,3	-	6/6/23/26	0/1/1/1
9	NAG	6	2	9	-	2/6/23/26	0/1/1/1
9	BMA	6	3	9	-	2/2/19/22	0/1/1/1
12	NAG	7	1	12,3	-	2/6/23/26	0/1/1/1
12	NAG	7	2	12	-	0/6/23/26	0/1/1/1
9	NAG	8	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	8	2	9	-	2/6/23/26	0/1/1/1
9	BMA	8	3	9	-	2/2/19/22	0/1/1/1
12	NAG	9	1	12,3	-	4/6/23/26	0/1/1/1
12	NAG	9	2	12	-	2/6/23/26	0/1/1/1
11	NAG	AA	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	AA	2	11	-	4/6/23/26	0/1/1/1
11	BMA	AA	3	11	-	0/2/19/22	0/1/1/1
11	MAN	AA	4	11	-	2/2/19/22	0/1/1/1
11	MAN	AA	5	11	-	0/2/19/22	0/1/1/1
10	NAG	BA	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	BA	2	10	-	3/6/23/26	0/1/1/1
10	BMA	BA	3	10	-	2/2/19/22	0/1/1/1
10	MAN	BA	4	10	-	2/2/19/22	0/1/1/1
9	NAG	CA	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	CA	2	9	-	3/6/23/26	0/1/1/1
9	BMA	CA	3	9	-	1/2/19/22	0/1/1/1
9	NAG	DA	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	DA	2	9	-	3/6/23/26	0/1/1/1
9	BMA	DA	3	9	-	1/2/19/22	0/1/1/1
9	NAG	G	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	G	2	9	-	2/6/23/26	0/1/1/1
9	BMA	G	3	9	-	2/2/19/22	0/1/1/1
10	NAG	I	1	3,10	-	1/6/23/26	0/1/1/1
10	NAG	I	2	10	-	3/6/23/26	0/1/1/1
10	BMA	I	3	10	-	2/2/19/22	0/1/1/1
10	MAN	I	4	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	J	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
9	BMA	J	3	9	-	2/2/19/22	0/1/1/1
11	NAG	K	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	K	2	11	-	2/6/23/26	0/1/1/1
11	BMA	K	3	11	-	2/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
11	MAN	K	5	11	-	0/2/19/22	0/1/1/1
12	NAG	O	1	12,3	-	0/6/23/26	0/1/1/1
12	NAG	O	2	12	-	2/6/23/26	0/1/1/1
9	NAG	P	1	9,3	-	4/6/23/26	0/1/1/1
9	NAG	P	2	9	-	1/6/23/26	0/1/1/1
9	BMA	P	3	9	-	2/2/19/22	0/1/1/1
9	NAG	S	1	9,3	-	6/6/23/26	0/1/1/1
9	NAG	S	2	9	-	2/6/23/26	0/1/1/1
9	BMA	S	3	9	-	2/2/19/22	0/1/1/1
12	NAG	T	1	12,3	-	2/6/23/26	0/1/1/1
12	NAG	T	2	12	-	0/6/23/26	0/1/1/1
9	NAG	U	1	9,3	-	3/6/23/26	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
12	NAG	V	1	12,3	-	4/6/23/26	0/1/1/1
12	NAG	V	2	12	-	2/6/23/26	0/1/1/1
11	NAG	W	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	W	2	11	-	4/6/23/26	0/1/1/1
11	BMA	W	3	11	-	0/2/19/22	0/1/1/1
11	MAN	W	4	11	-	2/2/19/22	0/1/1/1
11	MAN	W	5	11	-	0/2/19/22	0/1/1/1
10	NAG	b	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	b	2	10	-	3/6/23/26	0/1/1/1
10	BMA	b	3	10	-	2/2/19/22	0/1/1/1
10	MAN	b	4	10	-	2/2/19/22	0/1/1/1
9	NAG	c	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	3/6/23/26	0/1/1/1
9	BMA	c	3	9	-	1/2/19/22	0/1/1/1
9	NAG	d	1	9,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	d	2	9	-	3/6/23/26	0/1/1/1
9	BMA	d	3	9	-	1/2/19/22	0/1/1/1
9	NAG	e	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	e	2	9	-	2/6/23/26	0/1/1/1
9	BMA	e	3	9	-	2/2/19/22	0/1/1/1
10	NAG	j	1	3,10	-	1/6/23/26	0/1/1/1
10	NAG	j	2	10	-	3/6/23/26	0/1/1/1
10	BMA	j	3	10	-	2/2/19/22	0/1/1/1
10	MAN	j	4	10	-	0/2/19/22	0/1/1/1
9	NAG	k	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	k	2	9	-	2/6/23/26	0/1/1/1
9	BMA	k	3	9	-	2/2/19/22	0/1/1/1
11	NAG	l	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	l	2	11	-	2/6/23/26	0/1/1/1
11	BMA	l	3	11	-	2/2/19/22	0/1/1/1
11	MAN	l	4	11	-	0/2/19/22	0/1/1/1
11	MAN	l	5	11	-	0/2/19/22	0/1/1/1
12	NAG	m	1	12,3	-	0/6/23/26	0/1/1/1
12	NAG	m	2	12	-	2/6/23/26	0/1/1/1
9	NAG	n	1	9,3	-	4/6/23/26	0/1/1/1
9	NAG	n	2	9	-	1/6/23/26	0/1/1/1
9	BMA	n	3	9	-	2/2/19/22	0/1/1/1
9	NAG	o	1	9,3	-	6/6/23/26	0/1/1/1
9	NAG	o	2	9	-	2/6/23/26	0/1/1/1
9	BMA	o	3	9	-	2/2/19/22	0/1/1/1
12	NAG	p	1	12,3	-	2/6/23/26	0/1/1/1
12	NAG	p	2	12	-	0/6/23/26	0/1/1/1
9	NAG	q	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	q	2	9	-	2/6/23/26	0/1/1/1
9	BMA	q	3	9	-	2/2/19/22	0/1/1/1
12	NAG	r	1	12,3	-	4/6/23/26	0/1/1/1
12	NAG	r	2	12	-	2/6/23/26	0/1/1/1
11	NAG	s	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	s	2	11	-	4/6/23/26	0/1/1/1
11	BMA	s	3	11	-	0/2/19/22	0/1/1/1
11	MAN	s	4	11	-	2/2/19/22	0/1/1/1
11	MAN	s	5	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	t	1	3,10	-	2/6/23/26	0/1/1/1
10	NAG	t	2	10	-	3/6/23/26	0/1/1/1
10	BMA	t	3	10	-	2/2/19/22	0/1/1/1
10	MAN	t	4	10	-	2/2/19/22	0/1/1/1
9	NAG	u	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	u	2	9	-	3/6/23/26	0/1/1/1
9	BMA	u	3	9	-	1/2/19/22	0/1/1/1
9	NAG	v	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	v	2	9	-	3/6/23/26	0/1/1/1
9	BMA	v	3	9	-	1/2/19/22	0/1/1/1
9	NAG	w	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	w	2	9	-	2/6/23/26	0/1/1/1
9	BMA	w	3	9	-	2/2/19/22	0/1/1/1
10	NAG	x	1	3,10	-	1/6/23/26	0/1/1/1
10	NAG	x	2	10	-	3/6/23/26	0/1/1/1
10	BMA	x	3	10	-	2/2/19/22	0/1/1/1
10	MAN	x	4	10	-	0/2/19/22	0/1/1/1
9	NAG	y	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	y	2	9	-	2/6/23/26	0/1/1/1
9	BMA	y	3	9	-	2/2/19/22	0/1/1/1
11	NAG	z	1	3,11	-	0/6/23/26	0/1/1/1
11	NAG	z	2	11	-	2/6/23/26	0/1/1/1
11	BMA	z	3	11	-	2/2/19/22	0/1/1/1
11	MAN	z	4	11	-	0/2/19/22	0/1/1/1
11	MAN	z	5	11	-	0/2/19/22	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	x	3	BMA	C4-C3	3.43	1.61	1.52
10	j	3	BMA	C4-C3	3.42	1.61	1.52
10	I	3	BMA	C4-C3	3.41	1.61	1.52
10	x	3	BMA	C2-C3	3.12	1.57	1.52
10	I	3	BMA	C2-C3	3.12	1.57	1.52
10	j	3	BMA	C2-C3	3.07	1.57	1.52
9	6	1	NAG	O5-C1	-2.77	1.39	1.43
9	S	1	NAG	O5-C1	-2.76	1.39	1.43
9	o	1	NAG	O5-C1	-2.74	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	BA	1	NAG	C1-C2	2.57	1.55	1.52
9	o	1	NAG	C1-C2	2.53	1.55	1.52
10	b	1	NAG	C1-C2	2.52	1.55	1.52
9	S	1	NAG	C1-C2	2.51	1.55	1.52
9	6	1	NAG	C1-C2	2.50	1.55	1.52
10	t	1	NAG	C1-C2	2.50	1.55	1.52
10	j	1	NAG	O5-C1	-2.44	1.39	1.43
10	x	1	NAG	O5-C1	-2.44	1.39	1.43
10	I	1	NAG	O5-C1	-2.43	1.39	1.43
11	W	5	MAN	C1-C2	2.15	1.57	1.52
11	AA	5	MAN	C1-C2	2.15	1.57	1.52
11	s	5	MAN	C1-C2	2.15	1.57	1.52
11	l	5	MAN	C1-C2	2.06	1.57	1.52
9	e	1	NAG	O5-C1	-2.05	1.40	1.43
11	K	5	MAN	C1-C2	2.04	1.57	1.52
9	G	1	NAG	O5-C1	-2.03	1.40	1.43
11	z	5	MAN	C1-C2	2.03	1.57	1.52
9	w	1	NAG	O5-C1	-2.03	1.40	1.43

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	6	1	NAG	C2-N2-C7	8.53	134.33	122.90
9	S	1	NAG	C2-N2-C7	8.51	134.30	122.90
9	o	1	NAG	C2-N2-C7	8.49	134.28	122.90
11	z	3	BMA	C1-O5-C5	4.48	118.18	112.19
11	l	3	BMA	C1-O5-C5	4.47	118.17	112.19
11	K	3	BMA	C1-O5-C5	4.46	118.17	112.19
11	s	4	MAN	C1-O5-C5	4.08	117.65	112.19
11	W	4	MAN	C1-O5-C5	4.07	117.65	112.19
11	AA	4	MAN	C1-O5-C5	4.06	117.62	112.19
9	o	3	BMA	C1-O5-C5	3.99	117.53	112.19
9	6	3	BMA	C1-O5-C5	3.98	117.53	112.19
9	S	3	BMA	C1-O5-C5	3.97	117.51	112.19
9	n	3	BMA	C1-O5-C5	3.87	117.38	112.19
9	P	3	BMA	C1-O5-C5	3.86	117.36	112.19
9	5	3	BMA	C1-O5-C5	3.85	117.35	112.19
10	j	3	BMA	C2-C3-C4	3.81	117.56	110.86
10	I	3	BMA	C2-C3-C4	3.79	117.52	110.86
10	x	3	BMA	C2-C3-C4	3.77	117.49	110.86
11	z	2	NAG	C1-O5-C5	3.68	117.12	112.19
9	6	1	NAG	C1-C2-N2	3.67	116.21	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	l	2	NAG	C1-O5-C5	3.66	117.09	112.19
11	K	2	NAG	C1-O5-C5	3.65	117.08	112.19
9	S	1	NAG	C1-C2-N2	3.65	116.19	110.43
9	o	1	NAG	C1-C2-N2	3.62	116.14	110.43
10	BA	2	NAG	C2-N2-C7	3.55	127.66	122.90
10	b	2	NAG	C2-N2-C7	3.55	127.65	122.90
10	t	2	NAG	C2-N2-C7	3.53	127.63	122.90
9	CA	1	NAG	C2-N2-C7	3.48	127.57	122.90
9	c	1	NAG	C2-N2-C7	3.46	127.54	122.90
9	G	1	NAG	C2-N2-C7	3.46	127.53	122.90
9	w	1	NAG	C2-N2-C7	3.46	127.53	122.90
9	e	1	NAG	C2-N2-C7	3.44	127.52	122.90
9	u	1	NAG	C2-N2-C7	3.42	127.49	122.90
9	n	1	NAG	C2-N2-C7	3.19	127.17	122.90
9	P	1	NAG	C2-N2-C7	3.19	127.17	122.90
9	u	3	BMA	C1-O5-C5	3.17	116.43	112.19
9	q	2	NAG	C2-N2-C7	3.16	127.14	122.90
9	q	1	NAG	C2-N2-C7	3.16	127.13	122.90
9	5	1	NAG	C2-N2-C7	3.16	127.13	122.90
9	U	2	NAG	C2-N2-C7	3.14	127.11	122.90
10	t	2	NAG	C1-O5-C5	3.14	116.39	112.19
9	U	1	NAG	C2-N2-C7	3.13	127.10	122.90
9	c	3	BMA	C1-O5-C5	3.13	116.38	112.19
9	8	2	NAG	C2-N2-C7	3.13	127.10	122.90
9	CA	3	BMA	C1-O5-C5	3.12	116.37	112.19
9	8	1	NAG	C2-N2-C7	3.11	127.07	122.90
10	b	2	NAG	C1-O5-C5	3.11	116.36	112.19
10	BA	2	NAG	C1-O5-C5	3.10	116.34	112.19
9	c	2	NAG	C2-N2-C7	3.06	127.00	122.90
9	u	2	NAG	C2-N2-C7	3.05	126.99	122.90
9	CA	2	NAG	C2-N2-C7	3.05	126.99	122.90
9	o	1	NAG	O4-C4-C3	-3.02	103.25	110.38
9	S	1	NAG	O4-C4-C3	-3.02	103.27	110.38
9	6	1	NAG	O4-C4-C3	-3.02	103.27	110.38
12	V	1	NAG	C2-N2-C7	3.00	126.92	122.90
10	b	1	NAG	C2-N2-C7	2.99	126.91	122.90
10	t	1	NAG	C2-N2-C7	2.99	126.91	122.90
12	r	1	NAG	C2-N2-C7	2.99	126.91	122.90
10	BA	1	NAG	C2-N2-C7	2.98	126.89	122.90
12	9	1	NAG	C2-N2-C7	2.98	126.89	122.90
11	W	2	NAG	C2-N2-C7	2.97	126.88	122.90
9	DA	1	NAG	C2-N2-C7	2.96	126.87	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BA	4	MAN	C1-O5-C5	2.96	116.15	112.19
11	AA	2	NAG	C2-N2-C7	2.94	126.85	122.90
10	t	4	MAN	C1-O5-C5	2.94	116.13	112.19
10	b	4	MAN	C1-O5-C5	2.94	116.13	112.19
9	d	1	NAG	C2-N2-C7	2.94	126.84	122.90
12	V	2	NAG	C2-N2-C7	2.93	126.83	122.90
11	s	2	NAG	C2-N2-C7	2.93	126.83	122.90
12	r	2	NAG	C2-N2-C7	2.93	126.82	122.90
12	9	2	NAG	C2-N2-C7	2.92	126.82	122.90
9	v	1	NAG	C2-N2-C7	2.91	126.80	122.90
11	z	4	MAN	C1-O5-C5	2.80	115.94	112.19
11	K	4	MAN	C1-O5-C5	2.80	115.94	112.19
11	l	4	MAN	C1-O5-C5	2.79	115.92	112.19
9	6	1	NAG	C1-O5-C5	-2.69	108.58	112.19
9	S	1	NAG	C1-O5-C5	-2.68	108.59	112.19
9	o	1	NAG	C1-O5-C5	-2.67	108.60	112.19
10	I	3	BMA	C1-C2-C3	2.60	113.44	109.64
10	x	3	BMA	C1-C2-C3	2.60	113.43	109.64
11	W	3	BMA	O2-C2-C3	-2.60	104.77	110.15
11	AA	3	BMA	O2-C2-C3	-2.60	104.77	110.15
10	j	3	BMA	C1-C2-C3	2.60	113.42	109.64
11	s	3	BMA	O2-C2-C3	-2.59	104.78	110.15
11	z	5	MAN	O2-C2-C3	-2.50	104.98	110.15
11	l	5	MAN	O2-C2-C3	-2.49	105.00	110.15
11	K	5	MAN	O2-C2-C3	-2.48	105.00	110.15
9	o	1	NAG	C4-C3-C2	2.47	114.64	111.02
10	BA	3	BMA	C1-O5-C5	2.47	115.49	112.19
9	S	1	NAG	C4-C3-C2	2.47	114.63	111.02
10	b	3	BMA	C1-O5-C5	2.46	115.48	112.19
10	t	3	BMA	C1-O5-C5	2.46	115.48	112.19
11	s	5	MAN	C1-O5-C5	2.46	115.48	112.19
9	6	1	NAG	C4-C3-C2	2.45	114.61	111.02
11	AA	5	MAN	C1-O5-C5	2.45	115.46	112.19
11	W	5	MAN	C1-O5-C5	2.44	115.46	112.19
11	l	4	MAN	O2-C2-C3	-2.41	105.16	110.15
11	K	4	MAN	O2-C2-C3	-2.40	105.18	110.15
9	y	3	BMA	O2-C2-C3	-2.39	105.20	110.15
10	BA	4	MAN	O2-C2-C3	-2.39	105.20	110.15
9	J	3	BMA	O2-C2-C3	-2.39	105.21	110.15
9	k	3	BMA	O2-C2-C3	-2.39	105.21	110.15
11	z	4	MAN	O2-C2-C3	-2.38	105.23	110.15
10	b	4	MAN	O2-C2-C3	-2.37	105.24	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	t	4	MAN	O2-C2-C3	-2.37	105.25	110.15
9	J	3	BMA	C1-O5-C5	2.36	115.35	112.19
9	k	3	BMA	C1-O5-C5	2.35	115.33	112.19
9	q	2	NAG	C1-O5-C5	2.34	115.32	112.19
9	y	3	BMA	C1-O5-C5	2.34	115.32	112.19
9	8	2	NAG	C1-O5-C5	2.32	115.29	112.19
9	U	2	NAG	C1-O5-C5	2.32	115.29	112.19
11	AA	3	BMA	C1-O5-C5	2.31	115.28	112.19
11	s	3	BMA	C1-O5-C5	2.30	115.28	112.19
11	W	3	BMA	C1-O5-C5	2.30	115.27	112.19
11	l	3	BMA	O2-C2-C3	-2.29	105.40	110.15
11	K	3	BMA	O2-C2-C3	-2.29	105.41	110.15
11	z	3	BMA	O2-C2-C3	-2.28	105.42	110.15
9	S	3	BMA	O2-C2-C3	-2.28	105.44	110.15
9	6	3	BMA	O2-C2-C3	-2.27	105.45	110.15
9	o	3	BMA	O2-C2-C3	-2.27	105.46	110.15
9	6	1	NAG	C3-C4-C5	2.25	114.32	110.23
9	S	1	NAG	C3-C4-C5	2.25	114.31	110.23
9	o	1	NAG	C3-C4-C5	2.24	114.30	110.23
11	AA	5	MAN	O2-C2-C3	-2.23	105.52	110.15
11	s	5	MAN	O2-C2-C3	-2.23	105.54	110.15
11	W	5	MAN	O2-C2-C3	-2.22	105.56	110.15
9	o	1	NAG	C8-C7-N2	2.20	119.77	116.12
12	7	1	NAG	C1-O5-C5	2.19	115.12	112.19
12	p	1	NAG	C1-O5-C5	2.19	115.11	112.19
9	S	1	NAG	C8-C7-N2	2.18	119.73	116.12
10	BA	3	BMA	O3-C3-C2	2.18	114.50	110.05
12	T	1	NAG	C1-O5-C5	2.18	115.10	112.19
10	b	3	BMA	O3-C3-C2	2.17	114.48	110.05
10	x	3	BMA	C3-C4-C5	2.17	114.16	110.23
10	t	3	BMA	O3-C3-C2	2.16	114.47	110.05
10	I	3	BMA	C3-C4-C5	2.16	114.14	110.23
10	x	4	MAN	O2-C2-C3	-2.15	105.69	110.15
9	6	1	NAG	C8-C7-N2	2.15	119.69	116.12
10	j	3	BMA	C3-C4-C5	2.15	114.12	110.23
9	n	3	BMA	O2-C2-C3	-2.14	105.72	110.15
9	P	3	BMA	O2-C2-C3	-2.14	105.72	110.15
9	u	2	NAG	C1-C2-N2	2.14	113.80	110.43
9	5	3	BMA	O2-C2-C3	-2.13	105.73	110.15
9	c	2	NAG	C1-C2-N2	2.13	113.79	110.43
9	y	1	NAG	C1-O5-C5	2.13	115.04	112.19
10	I	4	MAN	O2-C2-C3	-2.13	105.74	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	4	MAN	O2-C2-C3	-2.13	105.74	110.15
9	CA	2	NAG	C1-C2-N2	2.11	113.76	110.43
9	k	1	NAG	C1-O5-C5	2.11	115.01	112.19
9	J	1	NAG	C1-O5-C5	2.11	115.01	112.19
9	8	2	NAG	C1-C2-N2	2.09	113.72	110.43
9	U	2	NAG	C1-C2-N2	2.08	113.71	110.43
9	q	2	NAG	C1-C2-N2	2.07	113.69	110.43
9	q	3	BMA	C1-O5-C5	2.06	114.95	112.19
11	z	1	NAG	C1-O5-C5	2.05	114.93	112.19
11	K	1	NAG	C1-O5-C5	2.05	114.93	112.19
9	8	3	BMA	C1-O5-C5	2.04	114.92	112.19
11	l	1	NAG	C1-O5-C5	2.03	114.91	112.19
9	U	3	BMA	C1-O5-C5	2.03	114.91	112.19
9	S	1	NAG	O4-C4-C5	-2.02	104.34	109.32
9	DA	1	NAG	C1-C2-N2	2.01	113.61	110.43
9	o	1	NAG	O4-C4-C5	-2.01	104.37	109.32
9	6	1	NAG	O4-C4-C5	-2.01	104.37	109.32

There are no chirality outliers.

All (243) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	3	BMA	C4-C5-C6-O6
11	l	3	BMA	C4-C5-C6-O6
11	z	3	BMA	C4-C5-C6-O6
9	G	3	BMA	O5-C5-C6-O6
9	e	3	BMA	O5-C5-C6-O6
9	w	3	BMA	O5-C5-C6-O6
11	W	4	MAN	C4-C5-C6-O6
11	s	4	MAN	C4-C5-C6-O6
11	AA	4	MAN	C4-C5-C6-O6
11	W	2	NAG	O5-C5-C6-O6
11	s	2	NAG	O5-C5-C6-O6
11	AA	2	NAG	O5-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6
9	k	2	NAG	O5-C5-C6-O6
9	y	2	NAG	O5-C5-C6-O6
10	b	4	MAN	O5-C5-C6-O6
10	t	4	MAN	O5-C5-C6-O6
10	BA	4	MAN	O5-C5-C6-O6
11	K	3	BMA	O5-C5-C6-O6
11	l	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	z	3	BMA	O5-C5-C6-O6
9	G	3	BMA	C4-C5-C6-O6
9	e	3	BMA	C4-C5-C6-O6
9	w	3	BMA	C4-C5-C6-O6
9	P	3	BMA	O5-C5-C6-O6
9	S	3	BMA	O5-C5-C6-O6
9	n	3	BMA	O5-C5-C6-O6
9	o	3	BMA	O5-C5-C6-O6
9	5	3	BMA	O5-C5-C6-O6
9	6	3	BMA	O5-C5-C6-O6
11	K	2	NAG	O5-C5-C6-O6
11	l	2	NAG	O5-C5-C6-O6
11	z	2	NAG	O5-C5-C6-O6
11	K	2	NAG	C4-C5-C6-O6
11	l	2	NAG	C4-C5-C6-O6
11	z	2	NAG	C4-C5-C6-O6
9	P	1	NAG	O5-C5-C6-O6
9	n	1	NAG	O5-C5-C6-O6
9	5	1	NAG	O5-C5-C6-O6
11	W	4	MAN	O5-C5-C6-O6
11	s	4	MAN	O5-C5-C6-O6
11	AA	4	MAN	O5-C5-C6-O6
9	J	3	BMA	O5-C5-C6-O6
9	k	3	BMA	O5-C5-C6-O6
9	y	3	BMA	O5-C5-C6-O6
10	b	3	BMA	O5-C5-C6-O6
10	t	3	BMA	O5-C5-C6-O6
10	BA	3	BMA	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
9	v	2	NAG	O5-C5-C6-O6
9	DA	2	NAG	O5-C5-C6-O6
9	J	2	NAG	C4-C5-C6-O6
9	S	3	BMA	C4-C5-C6-O6
9	k	2	NAG	C4-C5-C6-O6
9	o	3	BMA	C4-C5-C6-O6
9	y	2	NAG	C4-C5-C6-O6
9	6	3	BMA	C4-C5-C6-O6
10	b	2	NAG	C4-C5-C6-O6
10	t	2	NAG	C4-C5-C6-O6
10	BA	2	NAG	C4-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
9	v	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	DA	2	NAG	C4-C5-C6-O6
11	W	2	NAG	C4-C5-C6-O6
11	s	2	NAG	C4-C5-C6-O6
11	AA	2	NAG	C4-C5-C6-O6
9	G	2	NAG	O5-C5-C6-O6
9	e	2	NAG	O5-C5-C6-O6
9	w	2	NAG	O5-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
10	x	2	NAG	O5-C5-C6-O6
9	S	1	NAG	O5-C5-C6-O6
9	o	1	NAG	O5-C5-C6-O6
9	6	1	NAG	O5-C5-C6-O6
10	j	2	NAG	O5-C5-C6-O6
10	BA	2	NAG	O5-C5-C6-O6
12	O	2	NAG	O5-C5-C6-O6
12	m	2	NAG	O5-C5-C6-O6
12	0	2	NAG	O5-C5-C6-O6
10	b	2	NAG	O5-C5-C6-O6
10	t	2	NAG	O5-C5-C6-O6
9	P	1	NAG	C4-C5-C6-O6
9	n	1	NAG	C4-C5-C6-O6
9	5	1	NAG	C4-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
10	j	2	NAG	C4-C5-C6-O6
10	x	2	NAG	C4-C5-C6-O6
9	S	1	NAG	C8-C7-N2-C2
9	S	1	NAG	O7-C7-N2-C2
9	o	1	NAG	C8-C7-N2-C2
9	o	1	NAG	O7-C7-N2-C2
9	6	1	NAG	C8-C7-N2-C2
9	6	1	NAG	O7-C7-N2-C2
12	T	1	NAG	C8-C7-N2-C2
12	T	1	NAG	O7-C7-N2-C2
12	p	1	NAG	C8-C7-N2-C2
12	p	1	NAG	O7-C7-N2-C2
12	7	1	NAG	C8-C7-N2-C2
12	7	1	NAG	O7-C7-N2-C2
9	S	2	NAG	O5-C5-C6-O6
9	o	2	NAG	O5-C5-C6-O6
9	6	2	NAG	O5-C5-C6-O6
9	G	2	NAG	C4-C5-C6-O6
12	V	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	r	1	NAG	O5-C5-C6-O6
12	9	1	NAG	O5-C5-C6-O6
9	e	2	NAG	C4-C5-C6-O6
9	w	2	NAG	C4-C5-C6-O6
9	U	3	BMA	O5-C5-C6-O6
9	q	3	BMA	O5-C5-C6-O6
9	8	3	BMA	O5-C5-C6-O6
12	O	2	NAG	C4-C5-C6-O6
12	m	2	NAG	C4-C5-C6-O6
12	0	2	NAG	C4-C5-C6-O6
9	c	3	BMA	O5-C5-C6-O6
9	u	3	BMA	O5-C5-C6-O6
9	CA	3	BMA	O5-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
10	j	1	NAG	O5-C5-C6-O6
10	x	1	NAG	O5-C5-C6-O6
9	P	2	NAG	O5-C5-C6-O6
9	n	2	NAG	O5-C5-C6-O6
9	5	2	NAG	O5-C5-C6-O6
10	I	3	BMA	O5-C5-C6-O6
10	j	3	BMA	O5-C5-C6-O6
10	x	3	BMA	O5-C5-C6-O6
9	U	1	NAG	O5-C5-C6-O6
9	q	1	NAG	O5-C5-C6-O6
9	8	1	NAG	O5-C5-C6-O6
9	d	3	BMA	O5-C5-C6-O6
9	v	3	BMA	O5-C5-C6-O6
9	DA	3	BMA	O5-C5-C6-O6
9	S	1	NAG	C4-C5-C6-O6
9	o	1	NAG	C4-C5-C6-O6
9	6	1	NAG	C4-C5-C6-O6
12	V	1	NAG	C4-C5-C6-O6
12	r	1	NAG	C4-C5-C6-O6
12	9	1	NAG	C4-C5-C6-O6
10	BA	4	MAN	C4-C5-C6-O6
10	t	4	MAN	C4-C5-C6-O6
10	b	4	MAN	C4-C5-C6-O6
9	U	3	BMA	C4-C5-C6-O6
9	q	3	BMA	C4-C5-C6-O6
9	8	3	BMA	C4-C5-C6-O6
10	I	3	BMA	C4-C5-C6-O6
10	x	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	j	3	BMA	C4-C5-C6-O6
9	P	1	NAG	C1-C2-N2-C7
9	U	1	NAG	C1-C2-N2-C7
9	c	2	NAG	C1-C2-N2-C7
9	n	1	NAG	C1-C2-N2-C7
9	q	1	NAG	C1-C2-N2-C7
9	u	2	NAG	C1-C2-N2-C7
9	5	1	NAG	C1-C2-N2-C7
9	8	1	NAG	C1-C2-N2-C7
9	CA	2	NAG	C1-C2-N2-C7
11	W	2	NAG	C1-C2-N2-C7
11	s	2	NAG	C1-C2-N2-C7
11	AA	2	NAG	C1-C2-N2-C7
10	BA	3	BMA	C4-C5-C6-O6
10	b	3	BMA	C4-C5-C6-O6
10	t	3	BMA	C4-C5-C6-O6
9	6	2	NAG	C4-C5-C6-O6
9	o	2	NAG	C4-C5-C6-O6
9	S	2	NAG	C4-C5-C6-O6
9	J	3	BMA	C4-C5-C6-O6
9	k	3	BMA	C4-C5-C6-O6
9	y	3	BMA	C4-C5-C6-O6
9	G	1	NAG	C3-C2-N2-C7
9	S	1	NAG	C3-C2-N2-C7
9	c	1	NAG	C3-C2-N2-C7
9	e	1	NAG	C3-C2-N2-C7
9	o	1	NAG	C3-C2-N2-C7
9	u	1	NAG	C3-C2-N2-C7
9	w	1	NAG	C3-C2-N2-C7
9	6	1	NAG	C3-C2-N2-C7
9	CA	1	NAG	C3-C2-N2-C7
10	b	2	NAG	C3-C2-N2-C7
10	t	2	NAG	C3-C2-N2-C7
10	BA	2	NAG	C3-C2-N2-C7
11	W	2	NAG	C3-C2-N2-C7
11	s	2	NAG	C3-C2-N2-C7
11	AA	2	NAG	C3-C2-N2-C7
12	V	1	NAG	C3-C2-N2-C7
12	r	1	NAG	C3-C2-N2-C7
12	9	1	NAG	C3-C2-N2-C7
9	5	3	BMA	C4-C5-C6-O6
9	P	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	n	3	BMA	C4-C5-C6-O6
9	G	1	NAG	C1-C2-N2-C7
9	S	1	NAG	C1-C2-N2-C7
9	U	2	NAG	C1-C2-N2-C7
9	c	1	NAG	C1-C2-N2-C7
9	d	1	NAG	C1-C2-N2-C7
9	d	2	NAG	C1-C2-N2-C7
9	e	1	NAG	C1-C2-N2-C7
9	o	1	NAG	C1-C2-N2-C7
9	q	2	NAG	C1-C2-N2-C7
9	u	1	NAG	C1-C2-N2-C7
9	v	1	NAG	C1-C2-N2-C7
9	v	2	NAG	C1-C2-N2-C7
9	w	1	NAG	C1-C2-N2-C7
9	6	1	NAG	C1-C2-N2-C7
9	8	2	NAG	C1-C2-N2-C7
9	CA	1	NAG	C1-C2-N2-C7
9	DA	1	NAG	C1-C2-N2-C7
9	DA	2	NAG	C1-C2-N2-C7
10	I	2	NAG	C1-C2-N2-C7
10	b	1	NAG	C1-C2-N2-C7
10	j	2	NAG	C1-C2-N2-C7
10	t	1	NAG	C1-C2-N2-C7
10	x	2	NAG	C1-C2-N2-C7
10	BA	1	NAG	C1-C2-N2-C7
12	V	1	NAG	C1-C2-N2-C7
12	V	2	NAG	C1-C2-N2-C7
12	r	1	NAG	C1-C2-N2-C7
12	r	2	NAG	C1-C2-N2-C7
12	9	1	NAG	C1-C2-N2-C7
12	9	2	NAG	C1-C2-N2-C7
9	CA	2	NAG	C4-C5-C6-O6
9	c	2	NAG	C4-C5-C6-O6
9	u	2	NAG	C4-C5-C6-O6
9	P	1	NAG	C3-C2-N2-C7
9	U	1	NAG	C3-C2-N2-C7
9	U	2	NAG	C3-C2-N2-C7
9	c	2	NAG	C3-C2-N2-C7
9	d	1	NAG	C3-C2-N2-C7
9	n	1	NAG	C3-C2-N2-C7
9	q	1	NAG	C3-C2-N2-C7
9	q	2	NAG	C3-C2-N2-C7

Continued on next page...

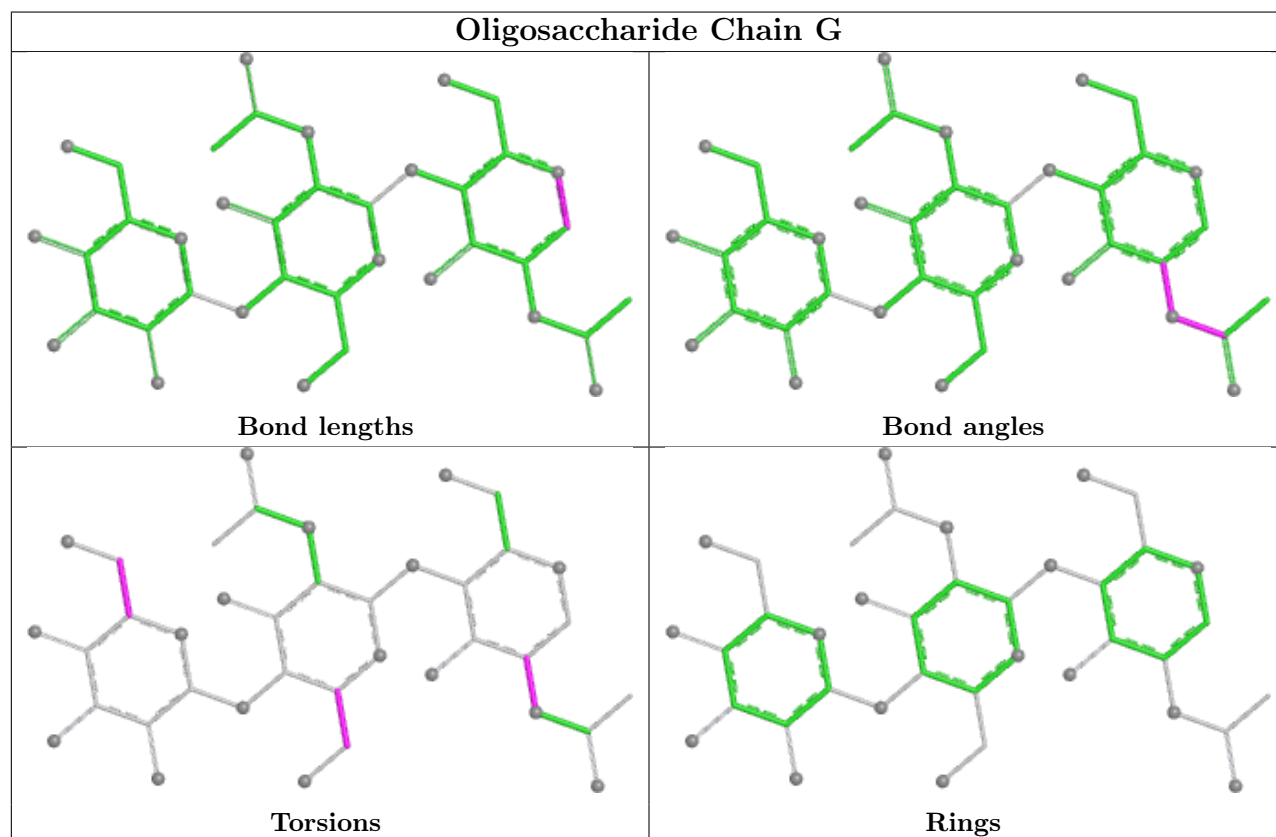
Continued from previous page...

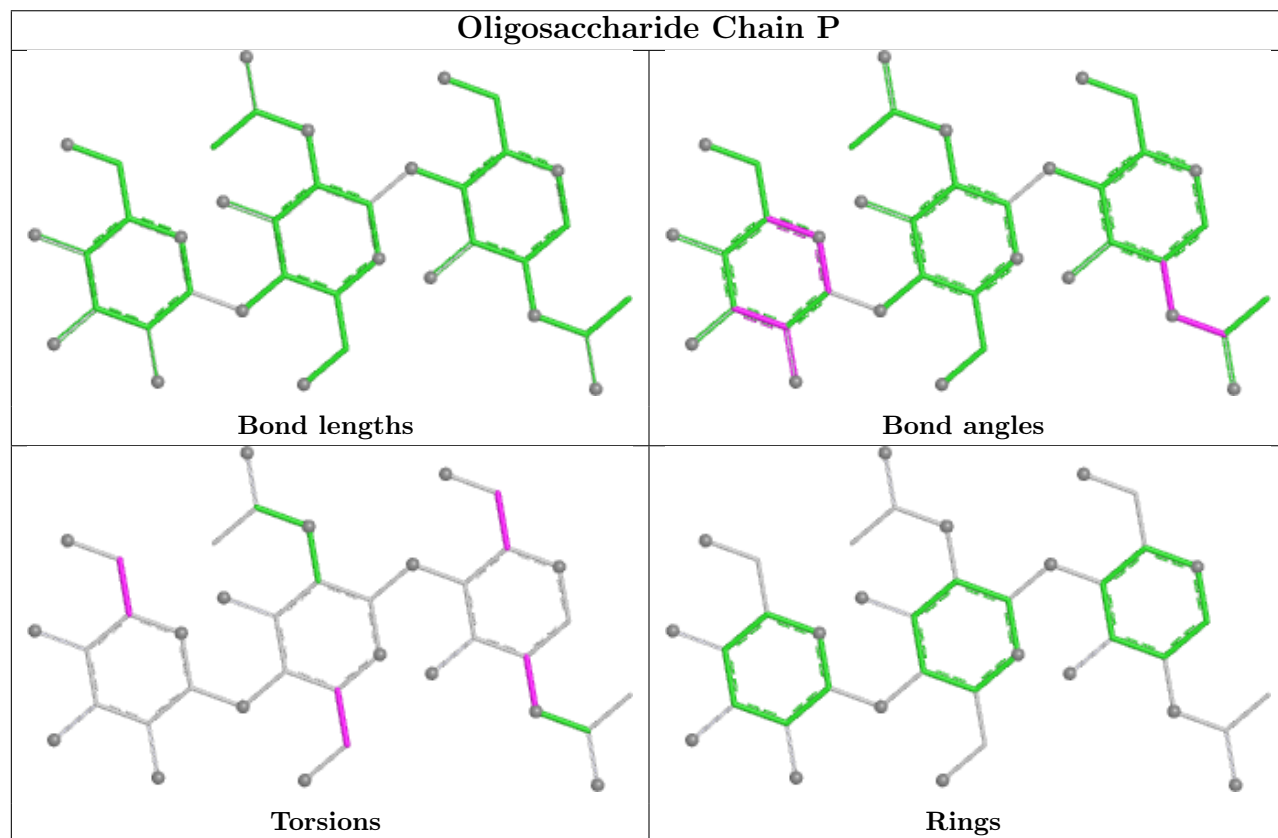
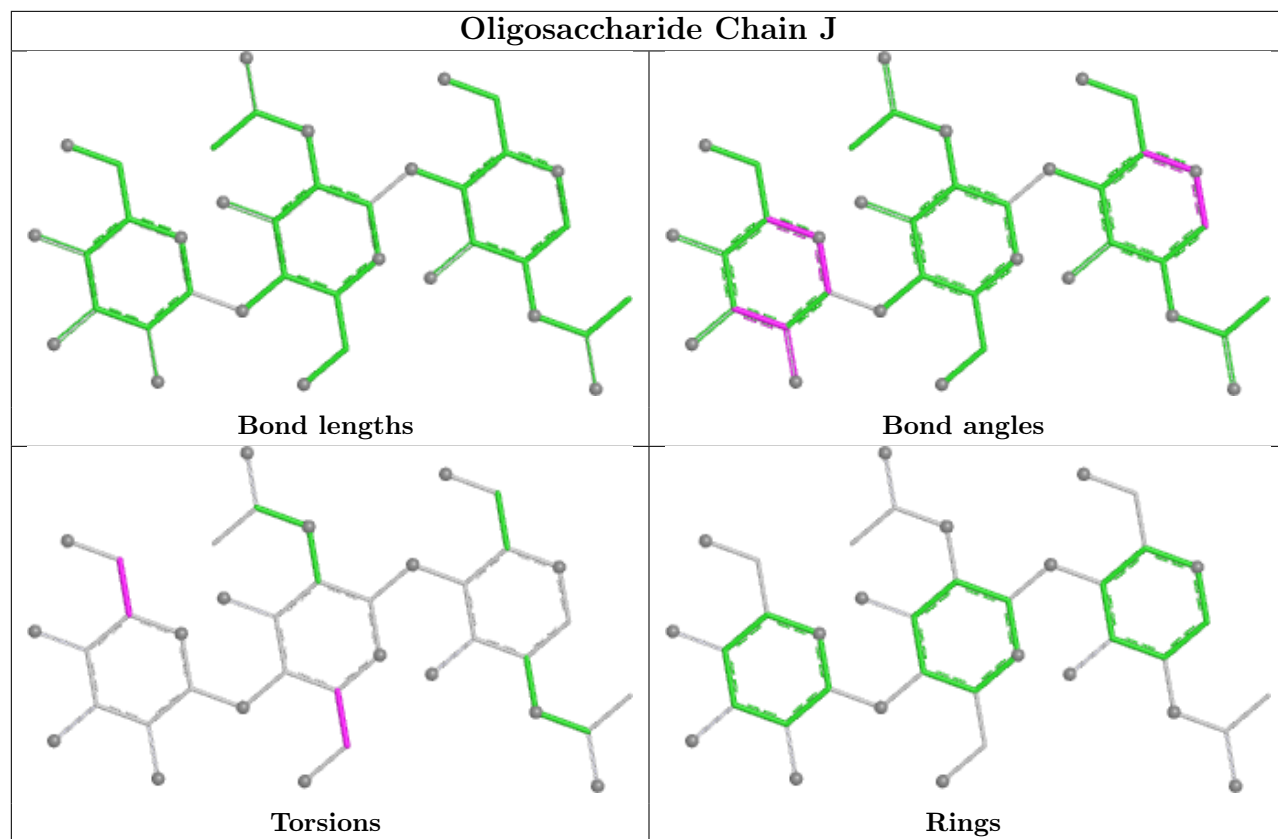
Mol	Chain	Res	Type	Atoms
9	u	2	NAG	C3-C2-N2-C7
9	v	1	NAG	C3-C2-N2-C7
9	5	1	NAG	C3-C2-N2-C7
9	8	1	NAG	C3-C2-N2-C7
9	8	2	NAG	C3-C2-N2-C7
9	CA	2	NAG	C3-C2-N2-C7
9	DA	1	NAG	C3-C2-N2-C7
10	b	1	NAG	C3-C2-N2-C7
10	t	1	NAG	C3-C2-N2-C7
10	BA	1	NAG	C3-C2-N2-C7
12	V	2	NAG	C3-C2-N2-C7
12	r	2	NAG	C3-C2-N2-C7
12	9	2	NAG	C3-C2-N2-C7

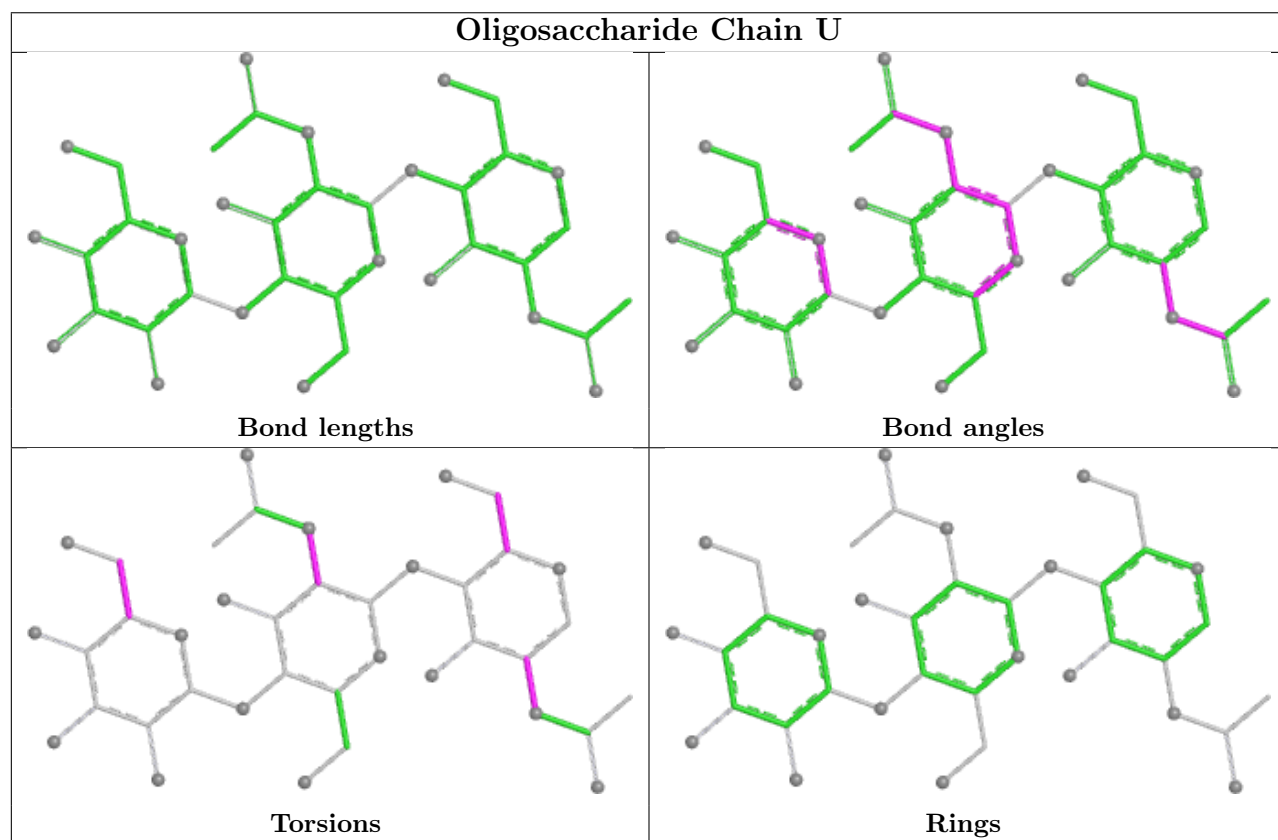
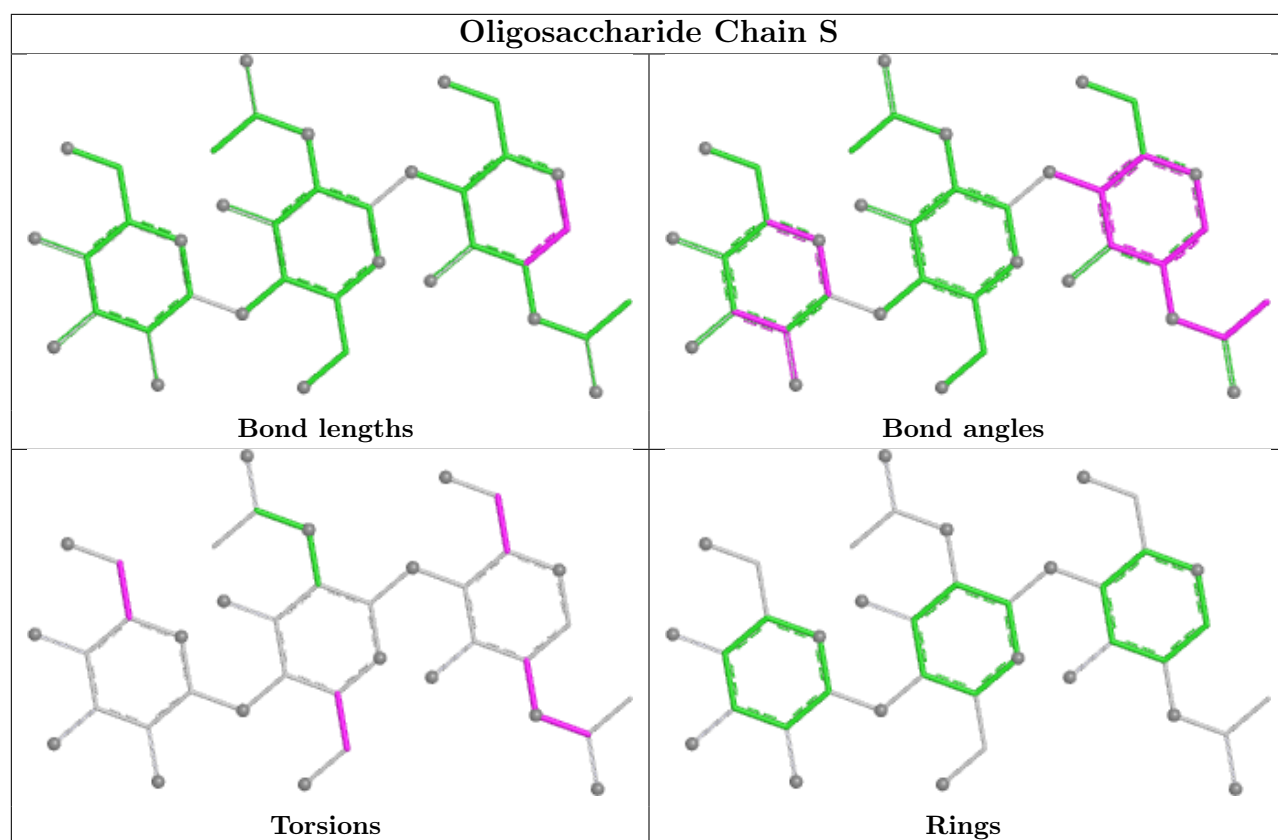
There are no ring outliers.

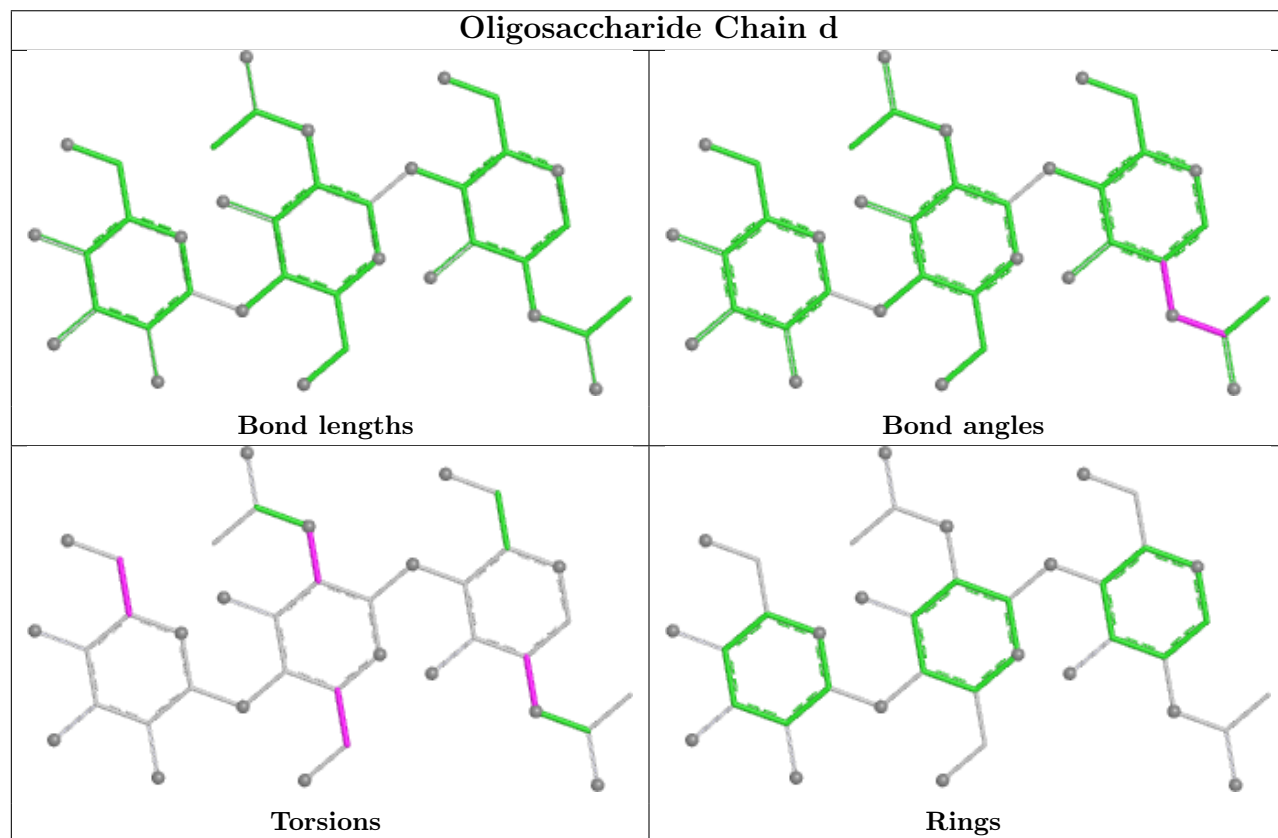
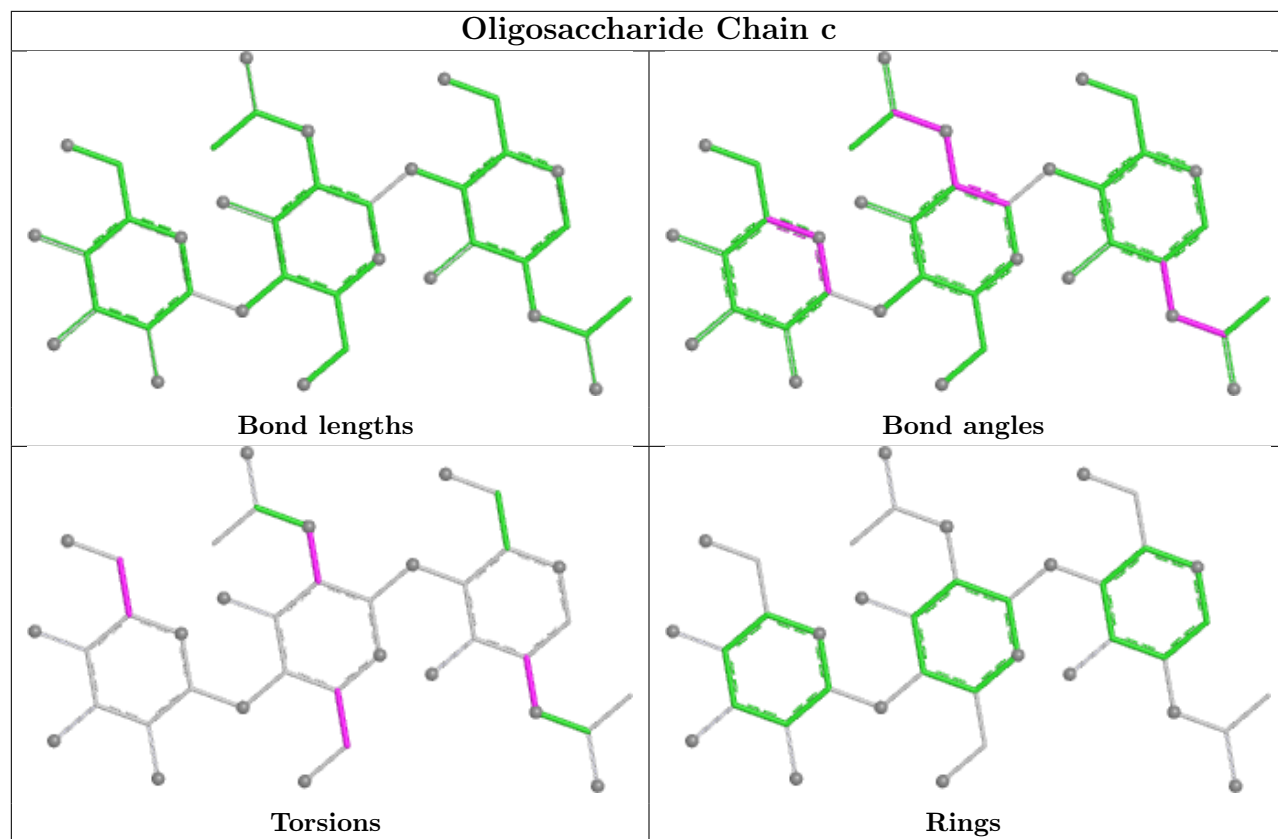
No monomer is involved in short contacts.

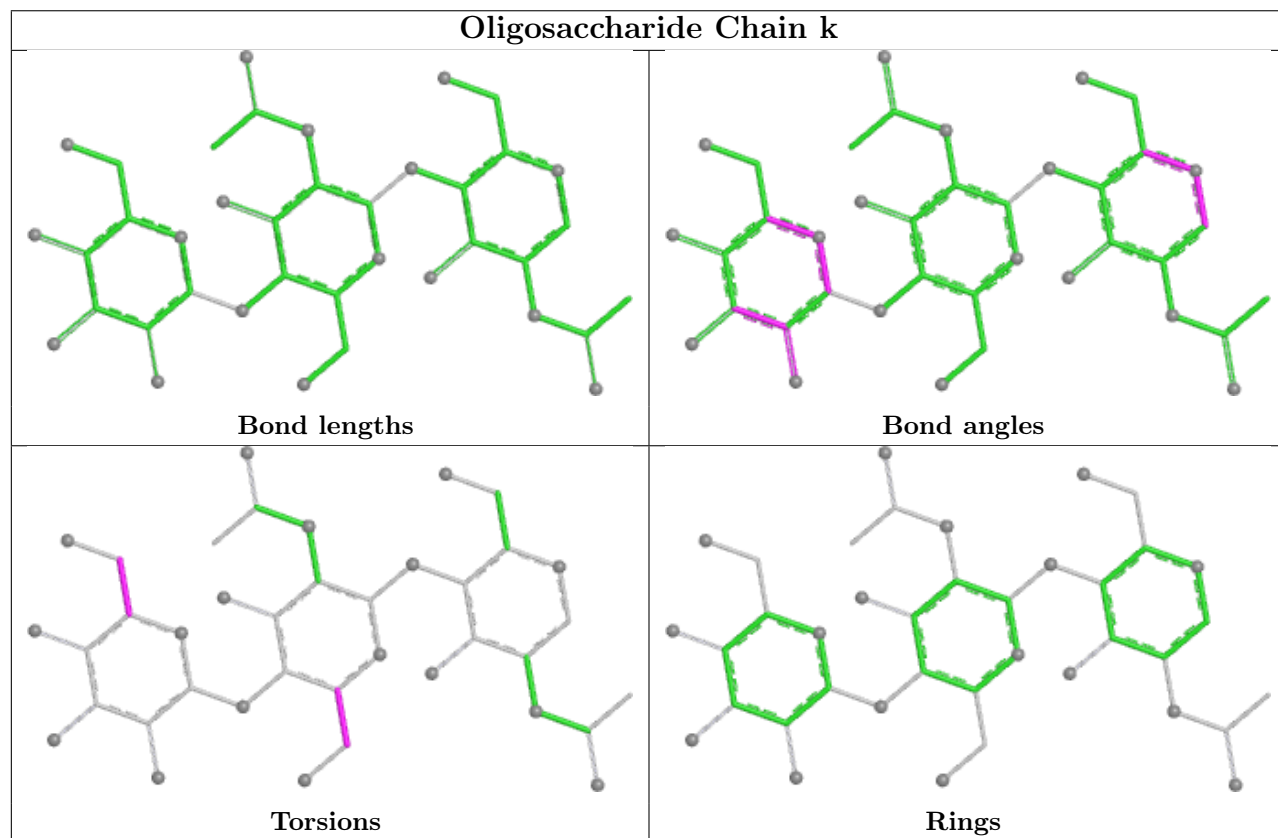
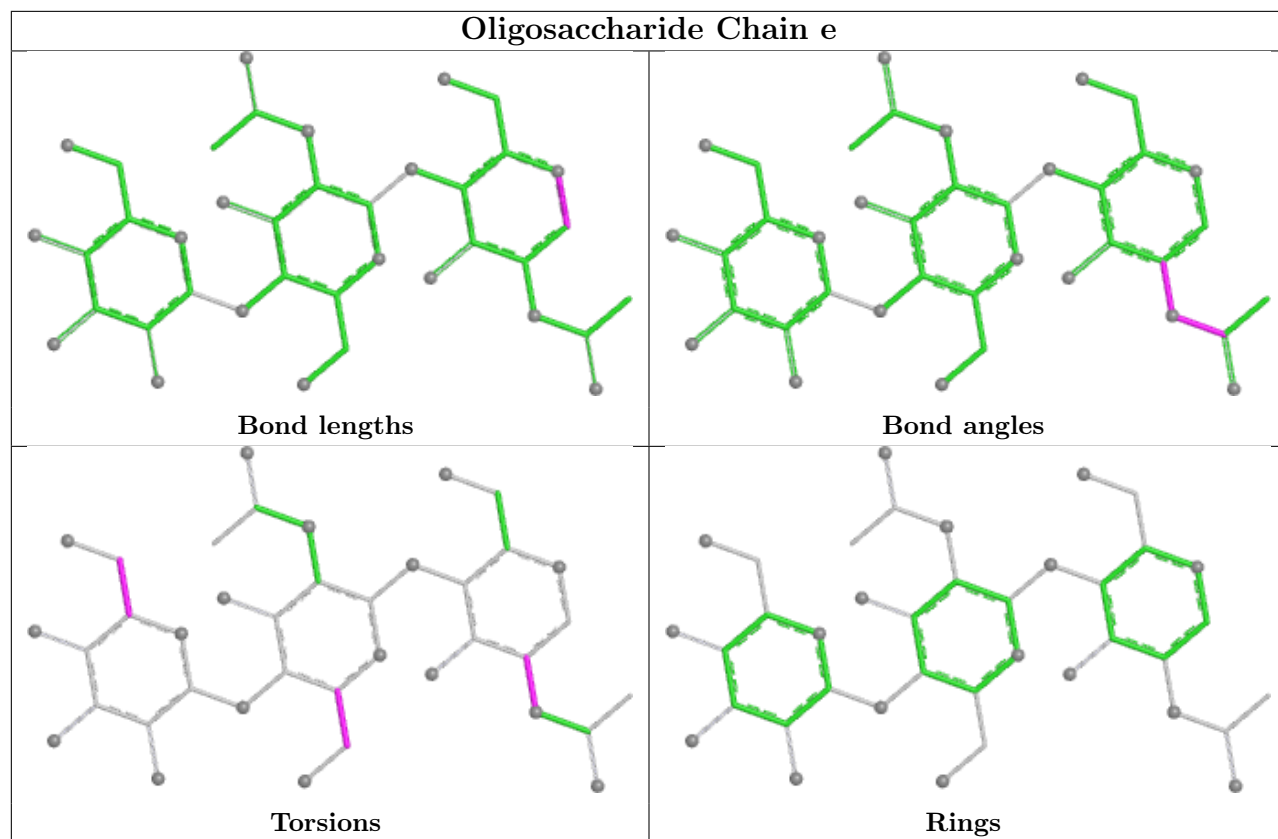
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

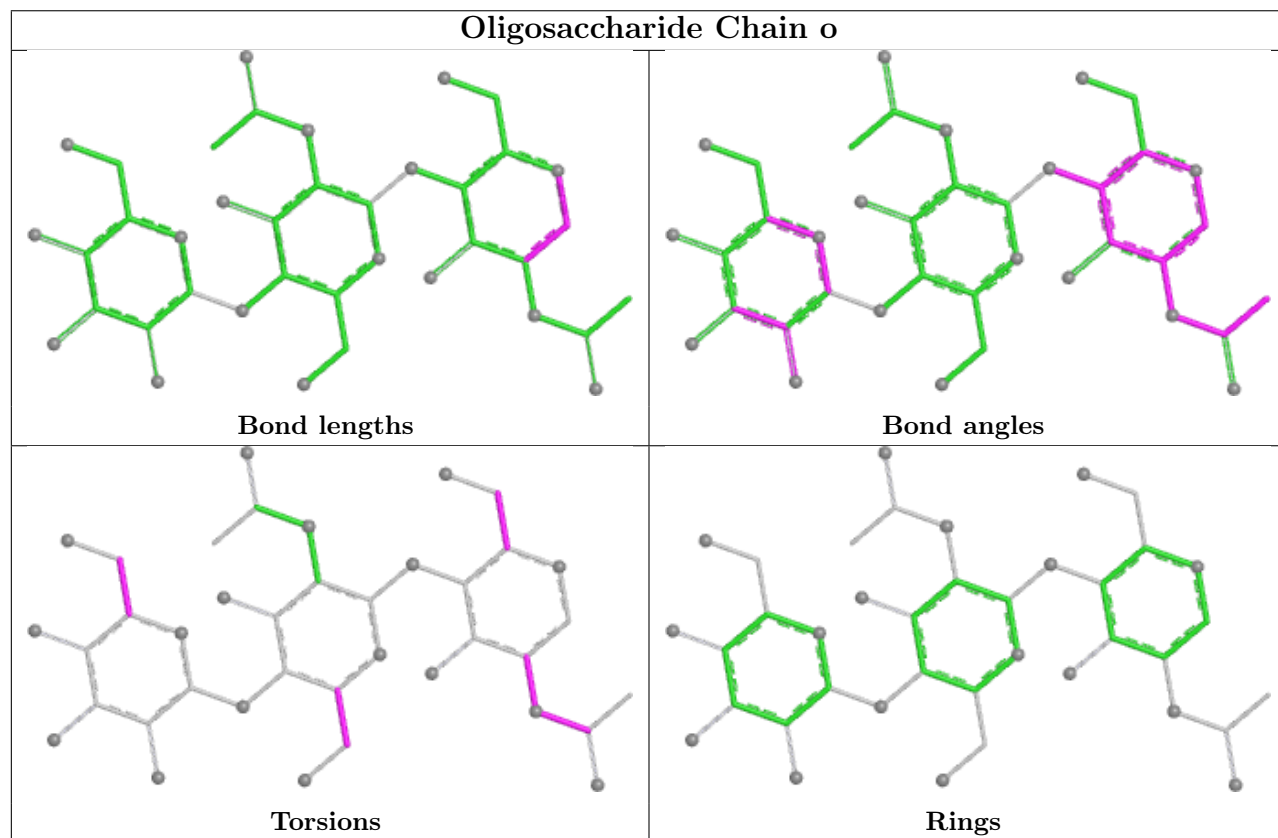
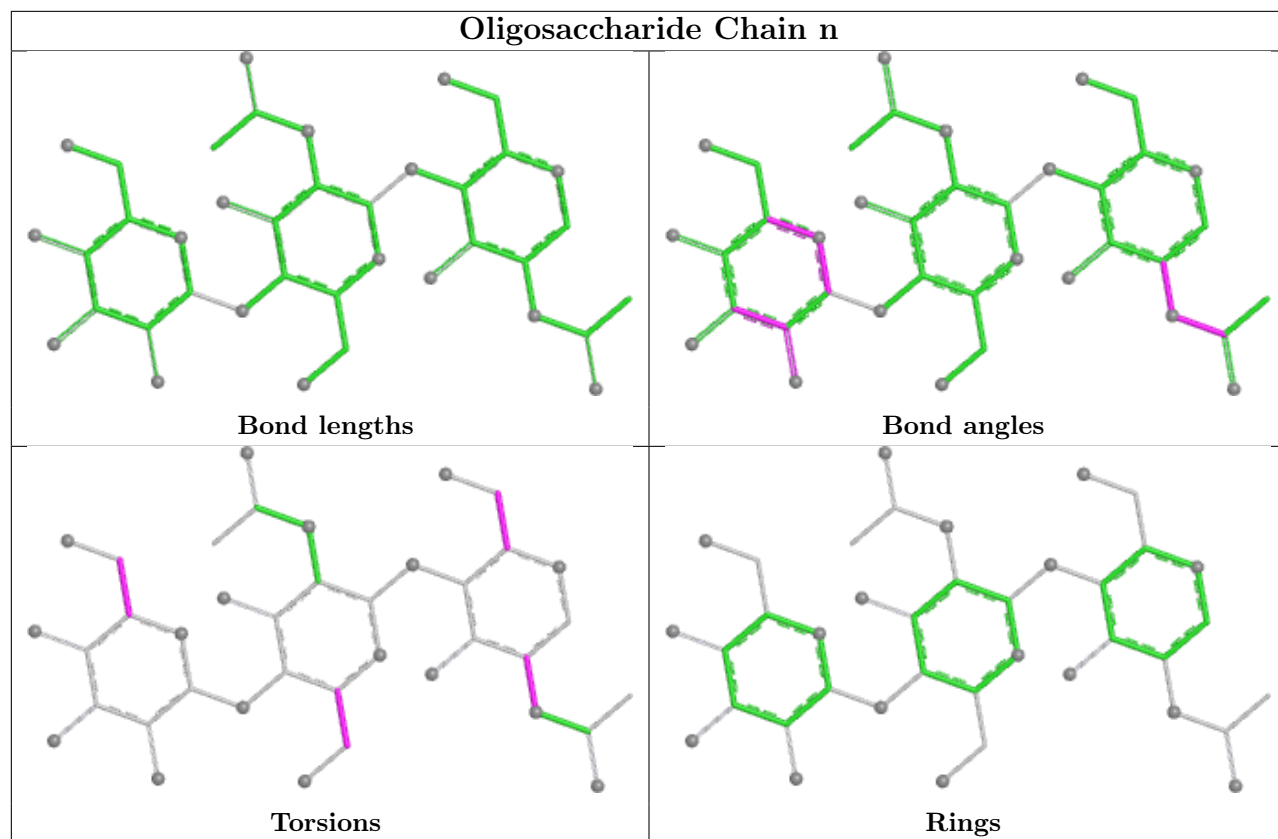


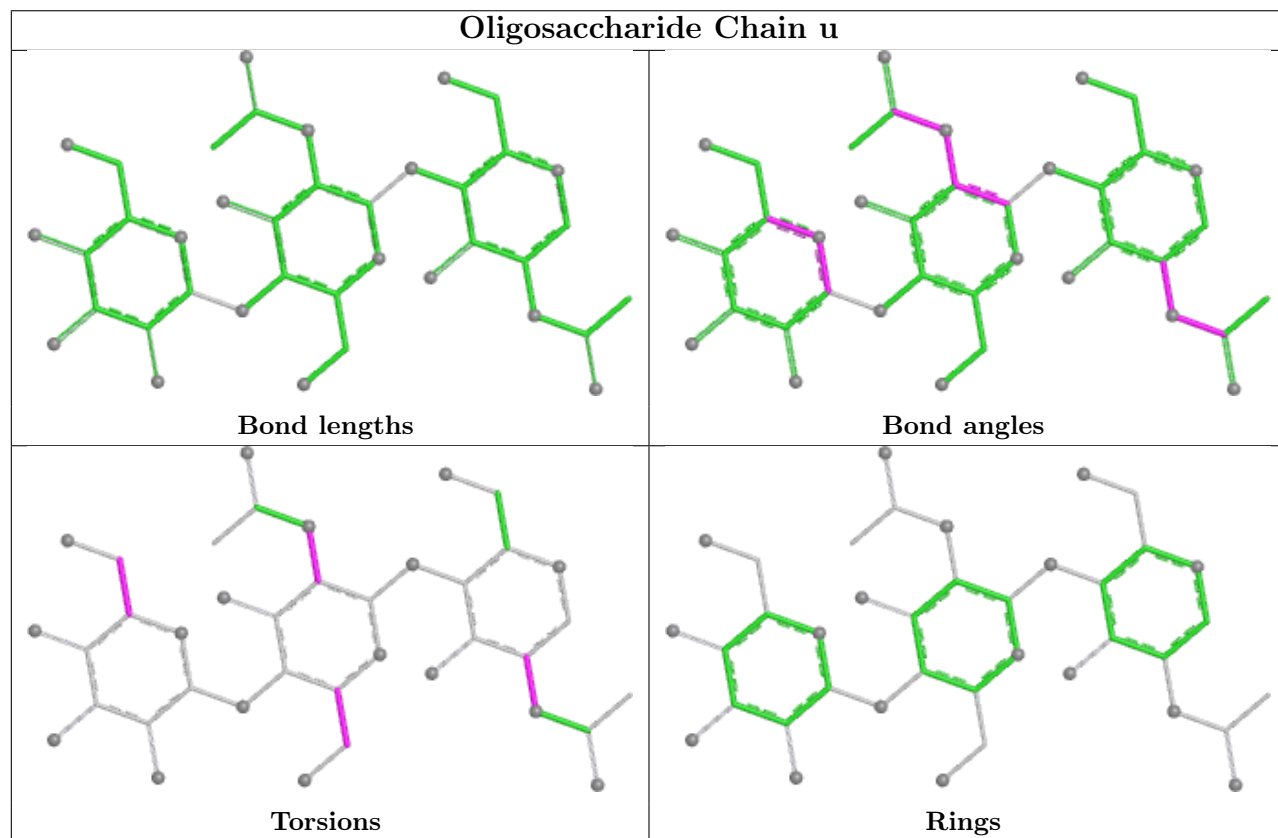
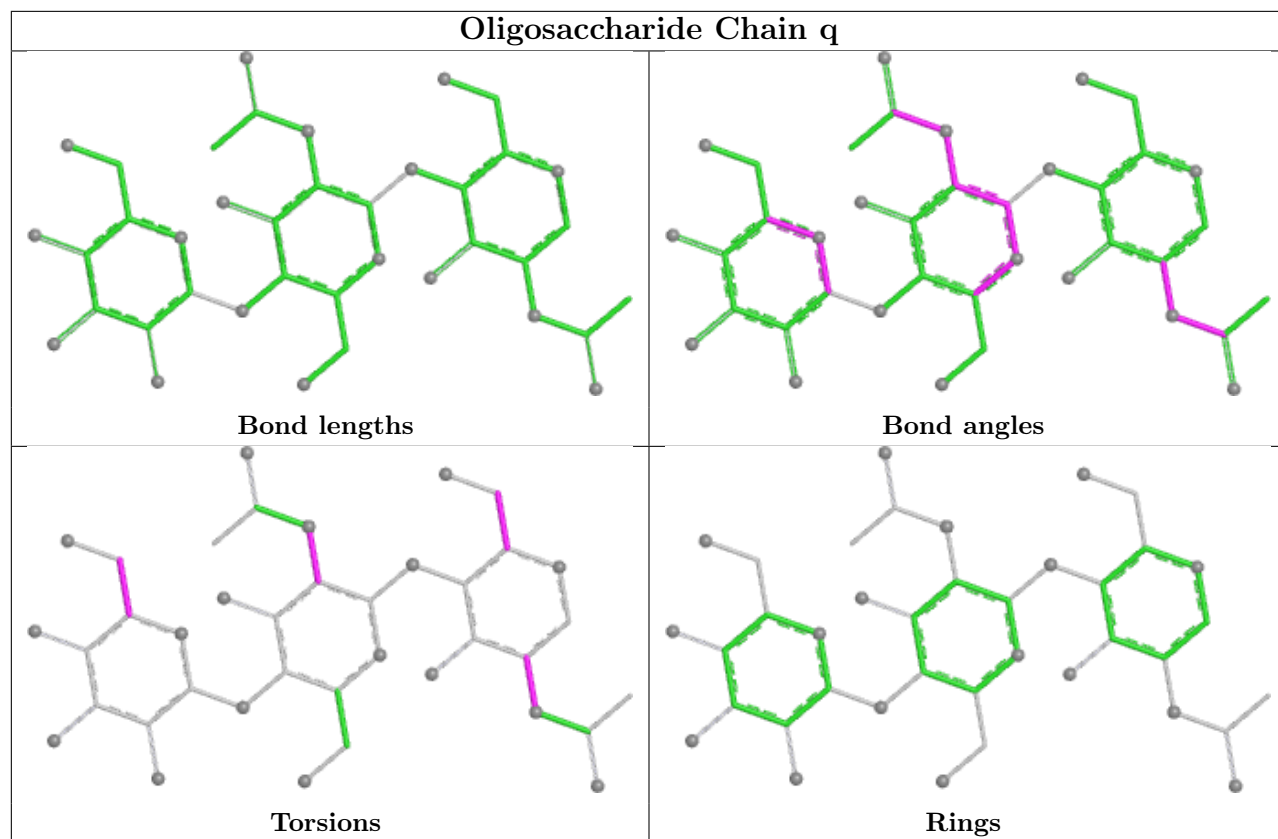


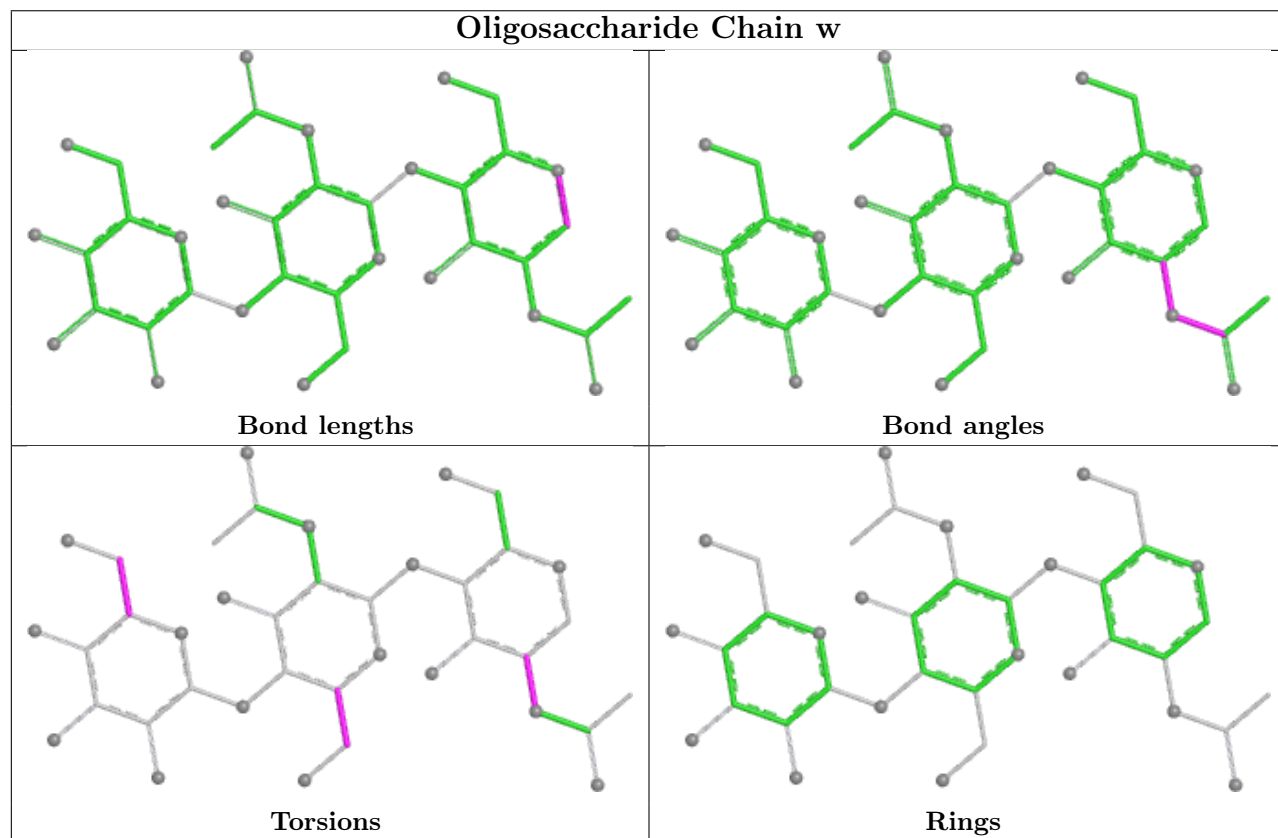
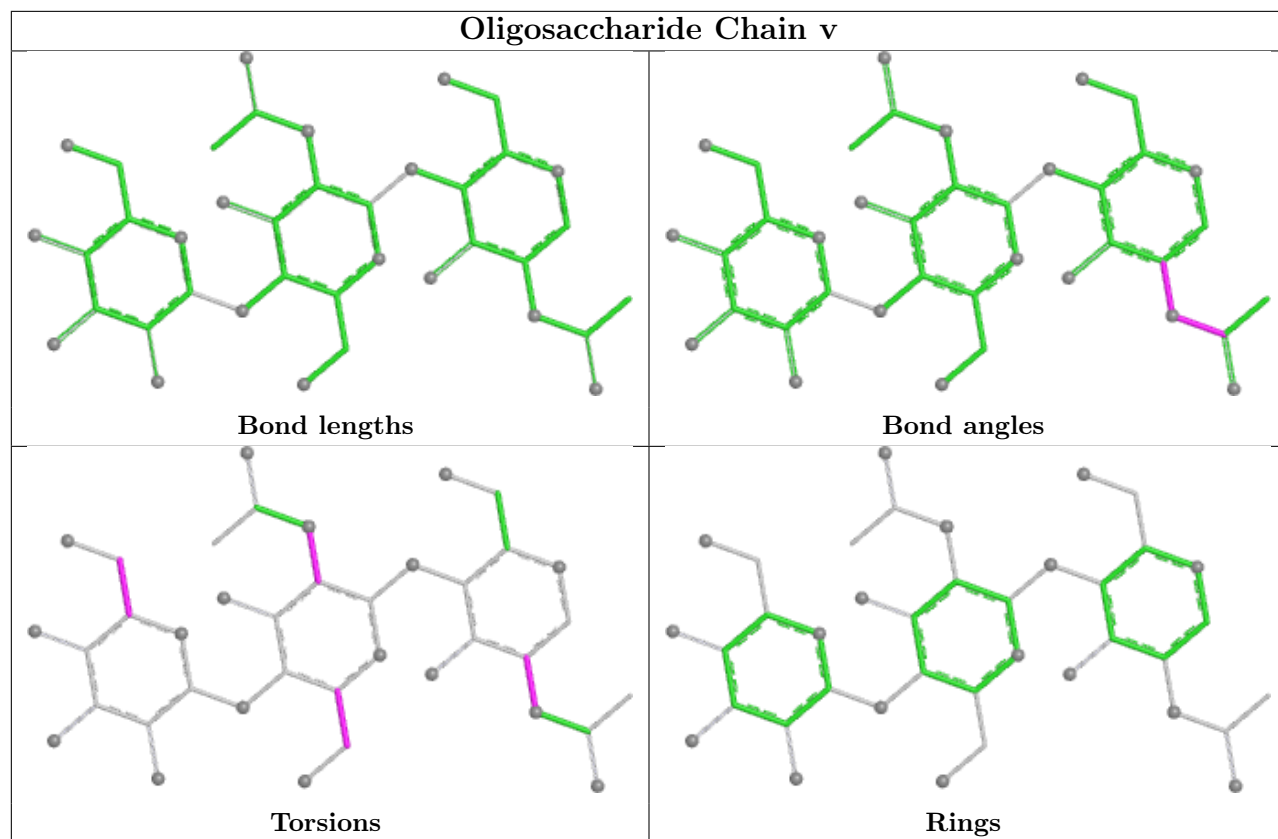


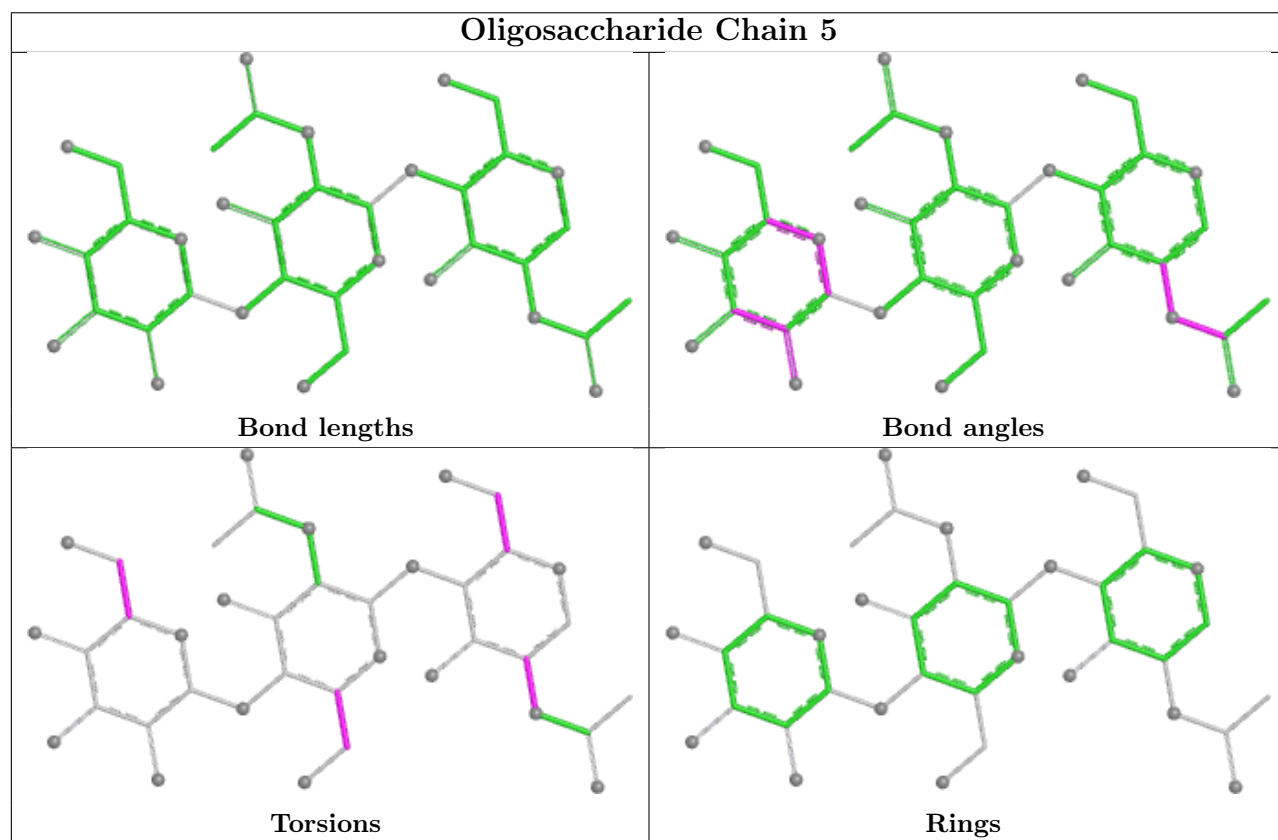
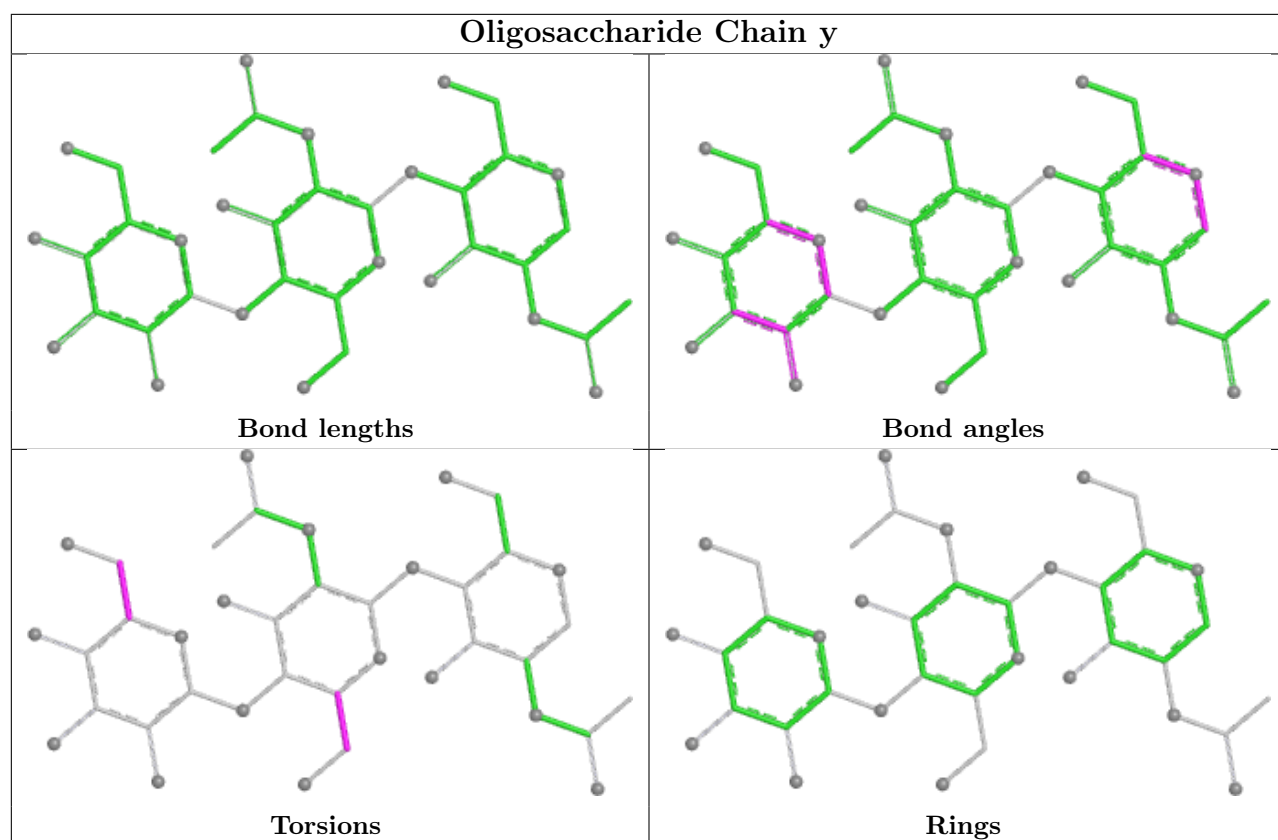


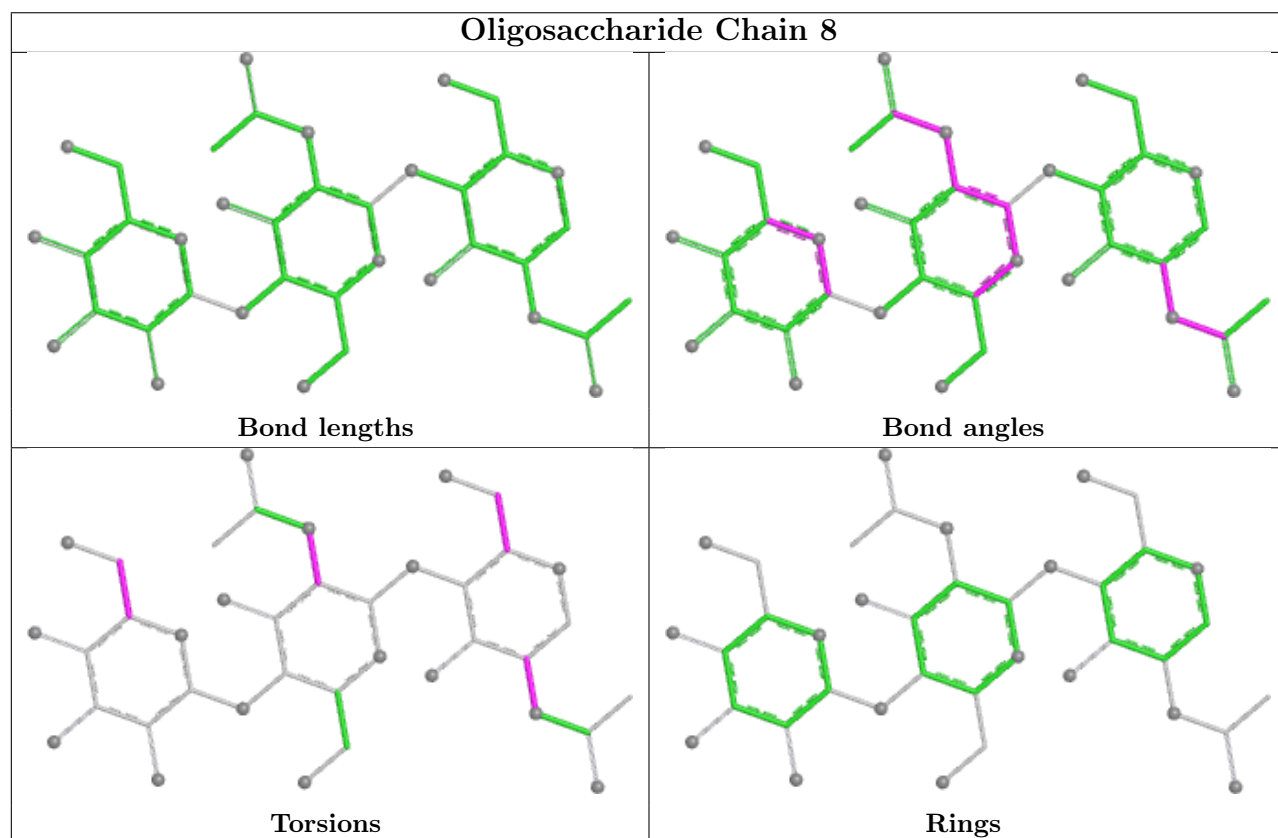
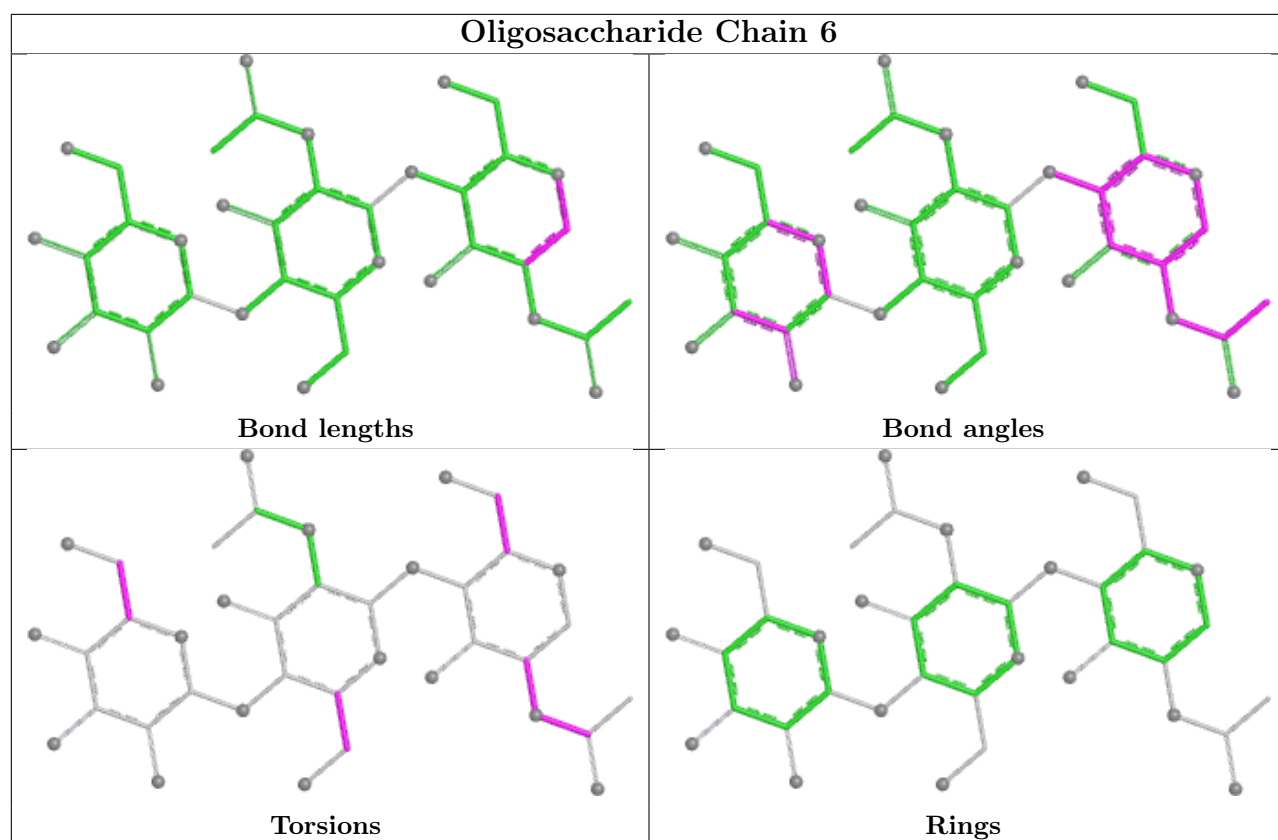


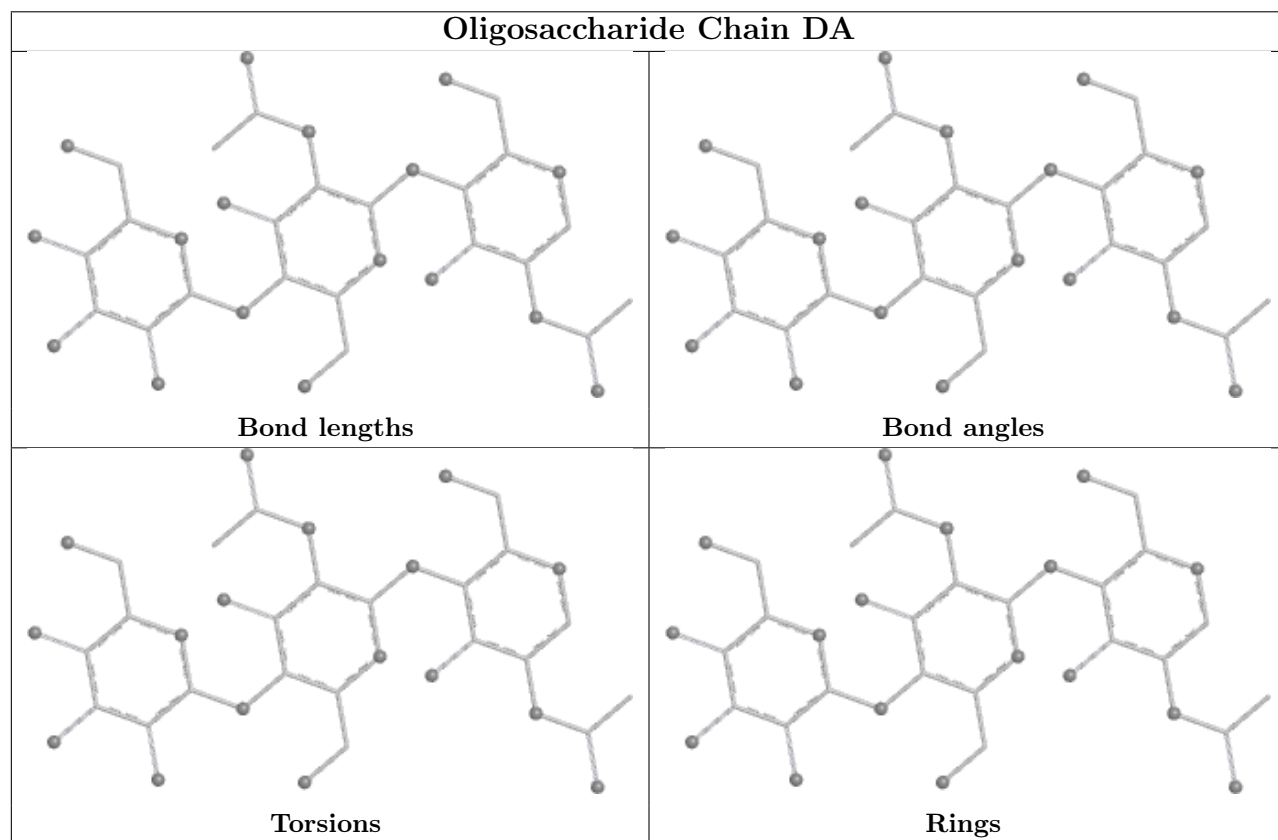
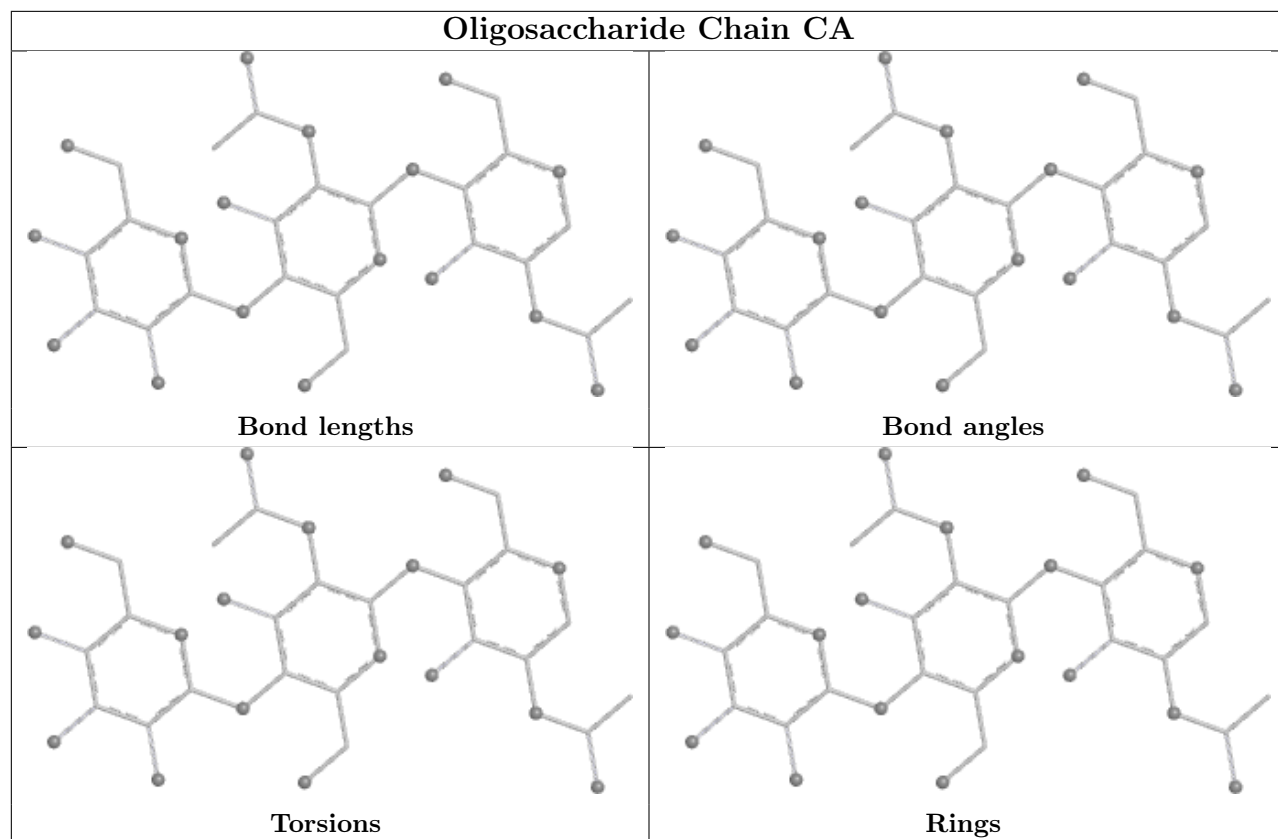


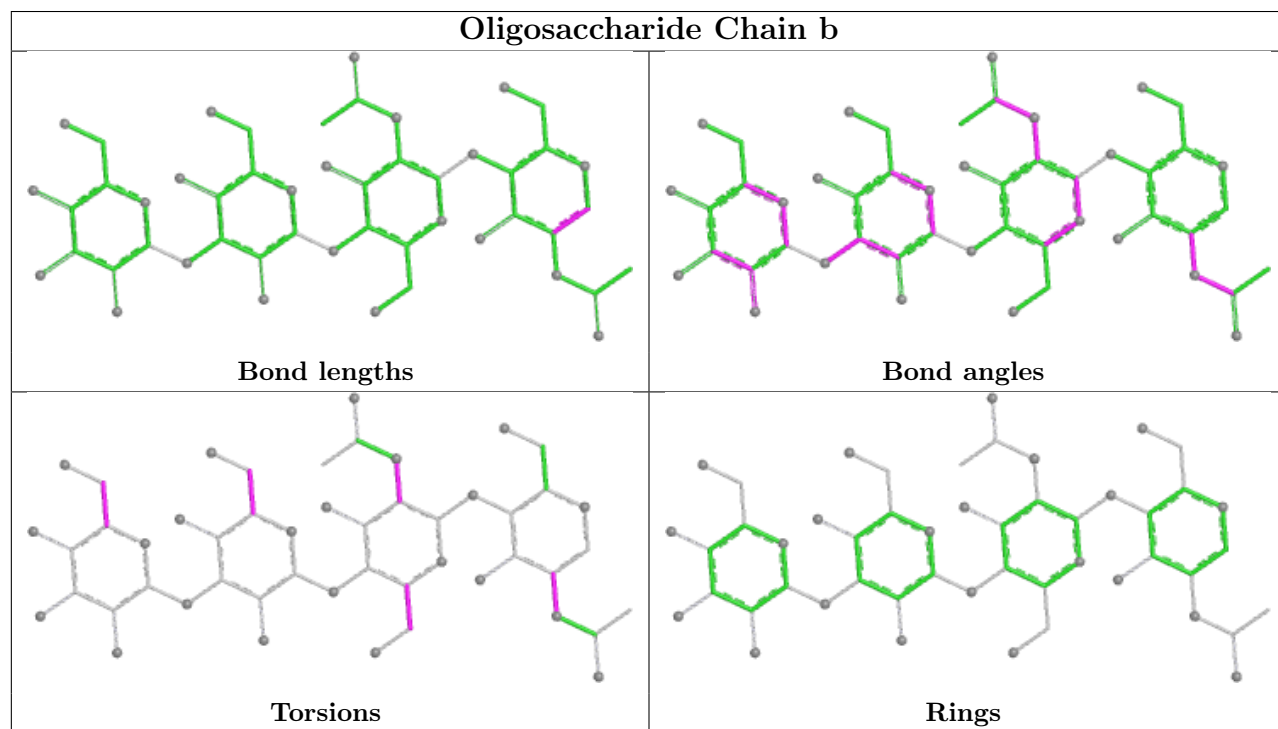
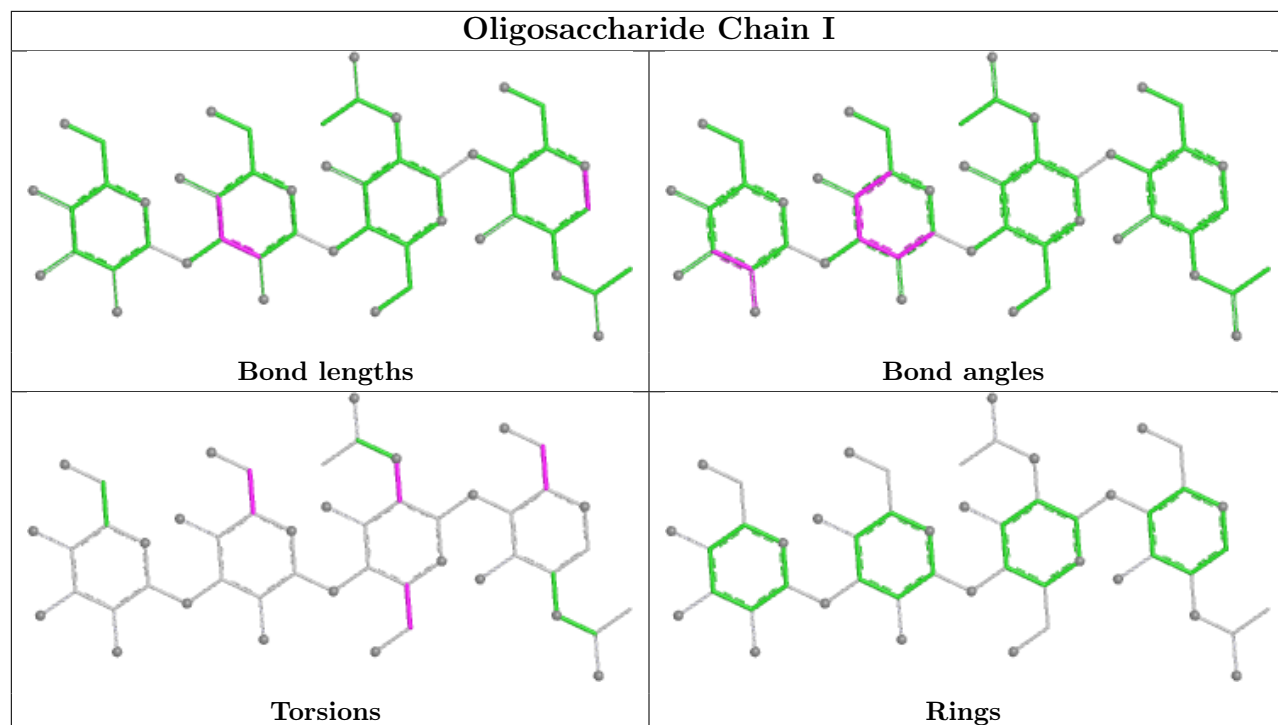


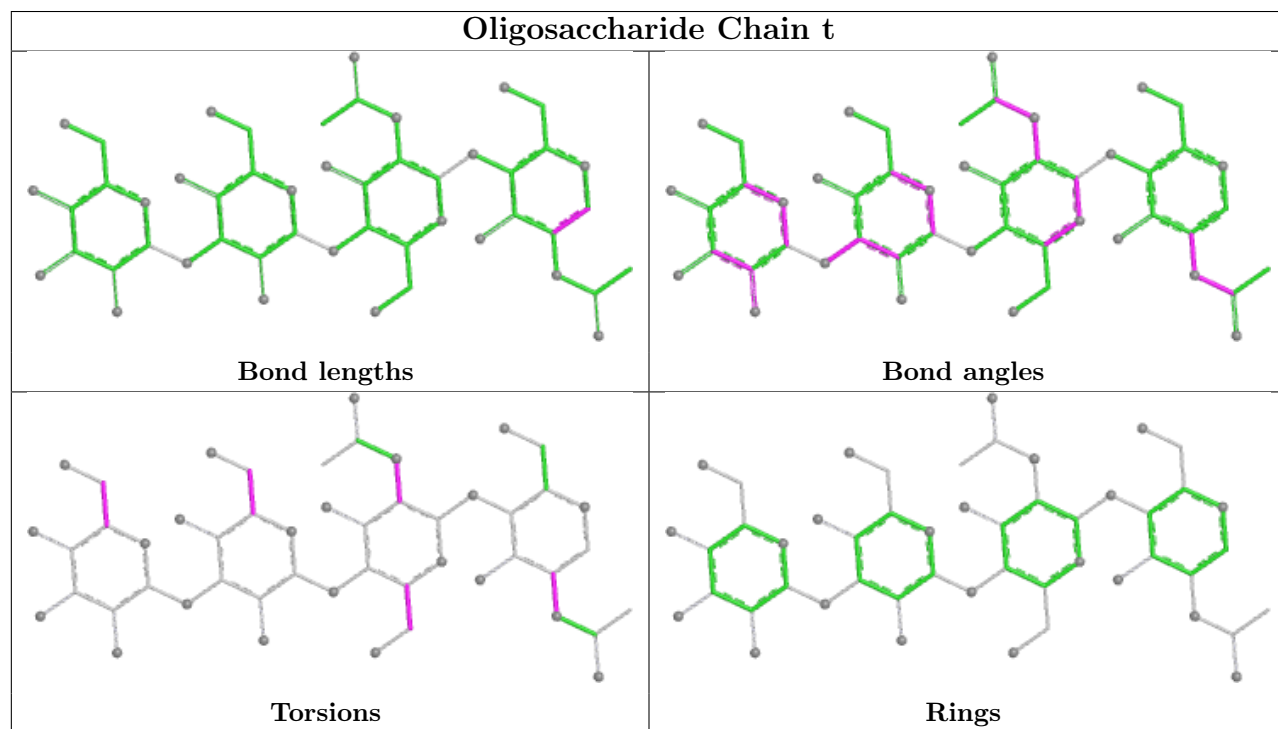
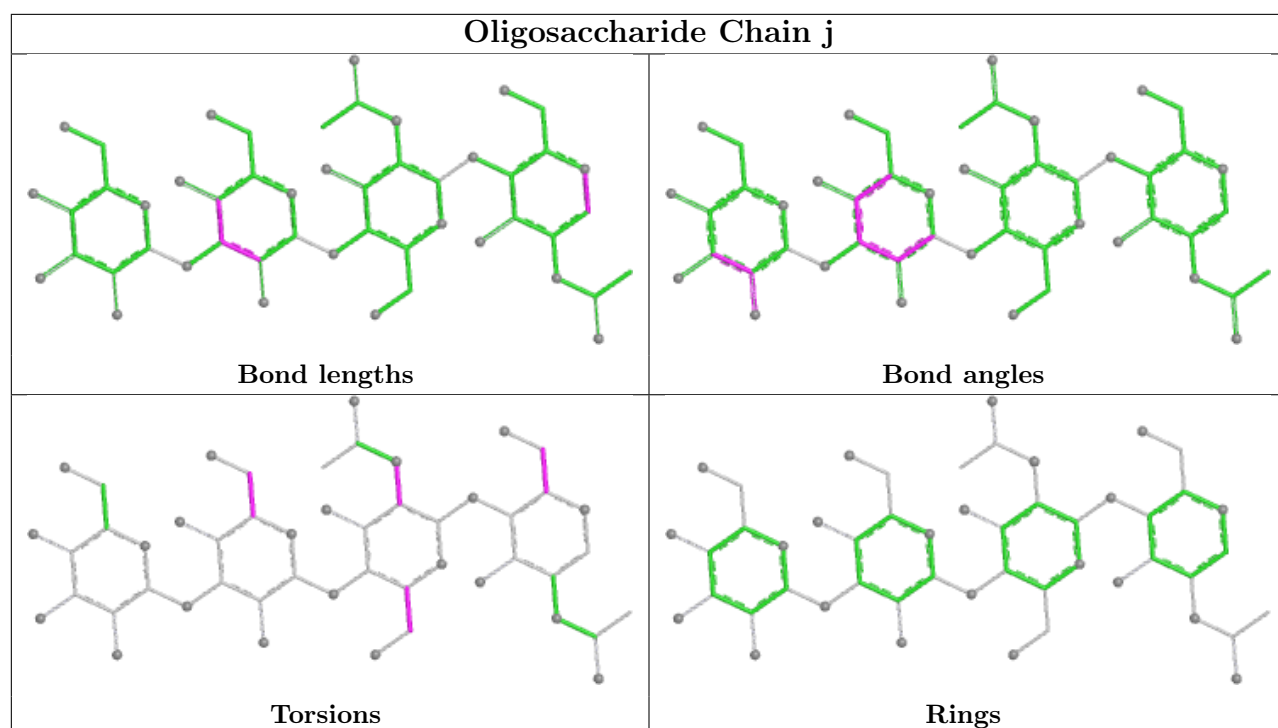


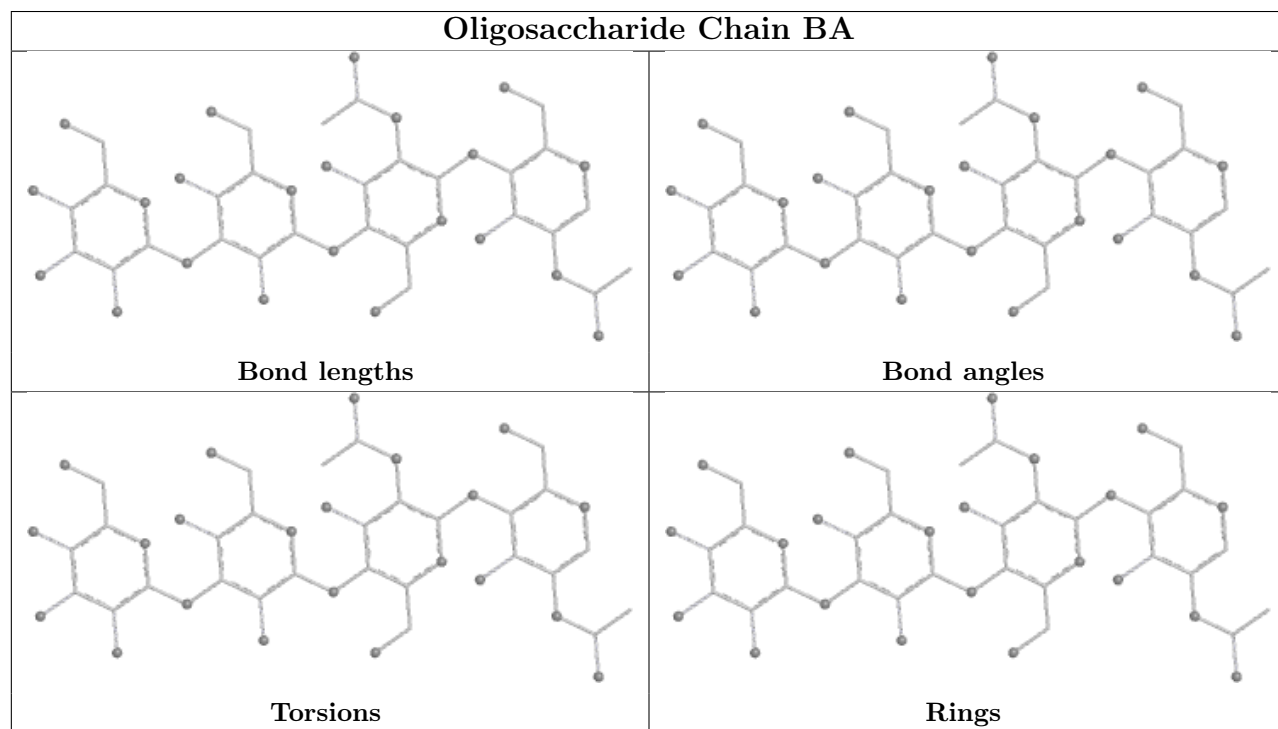
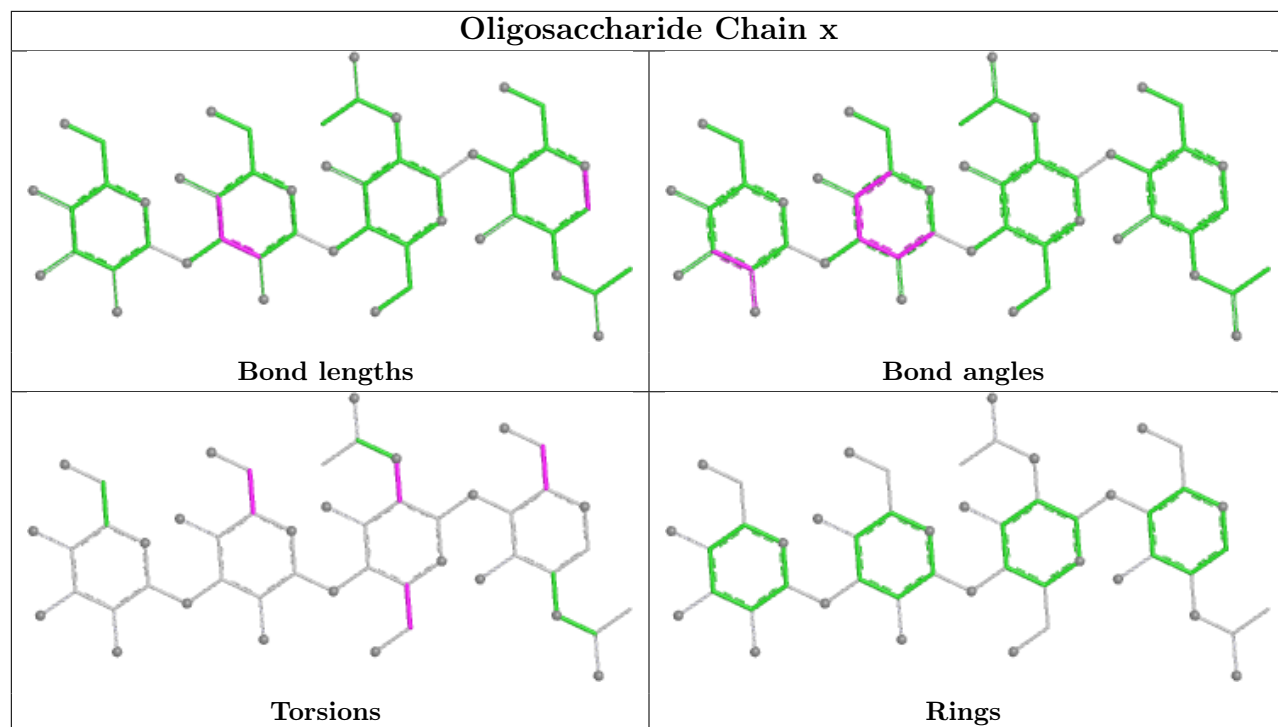


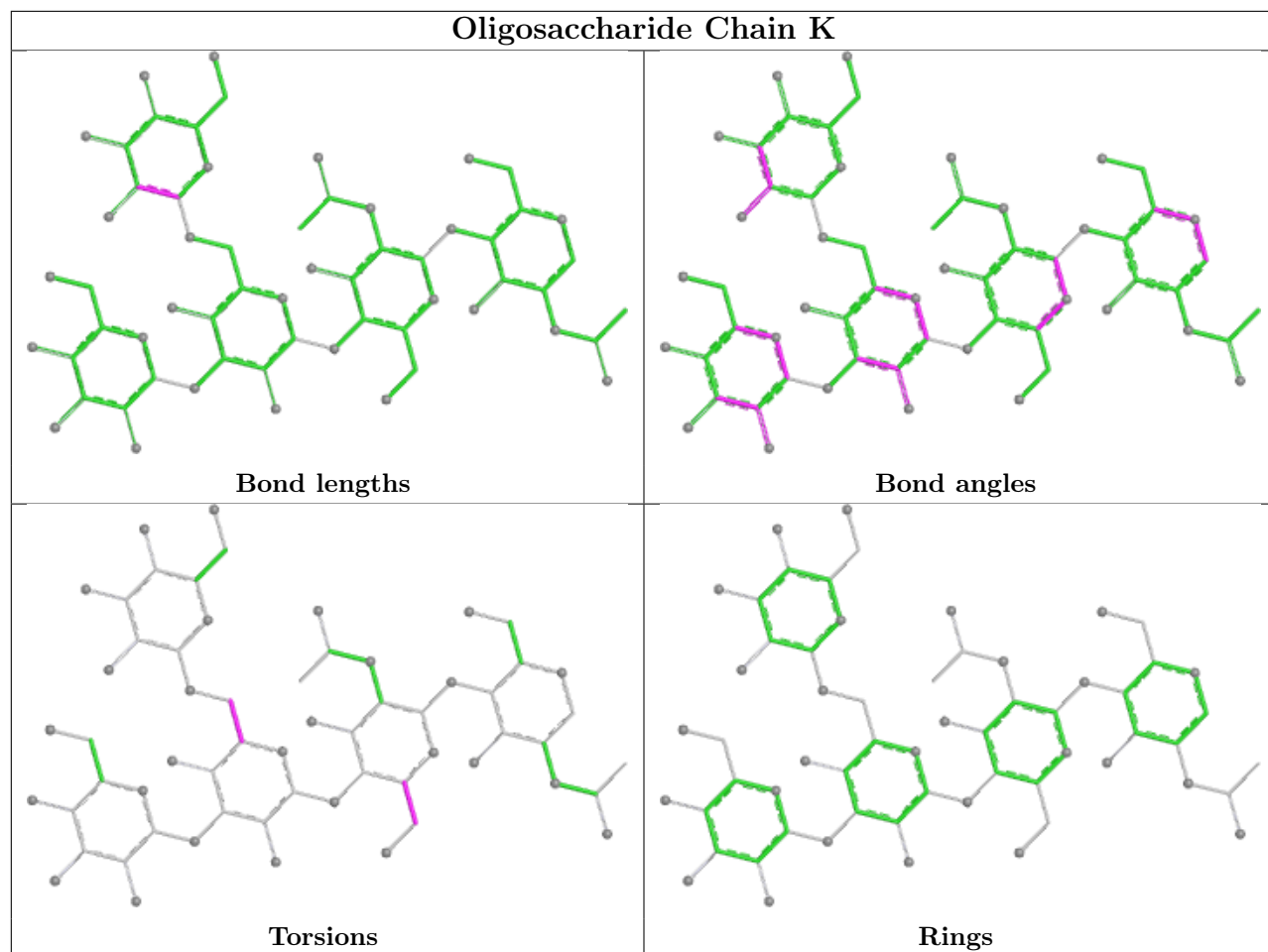


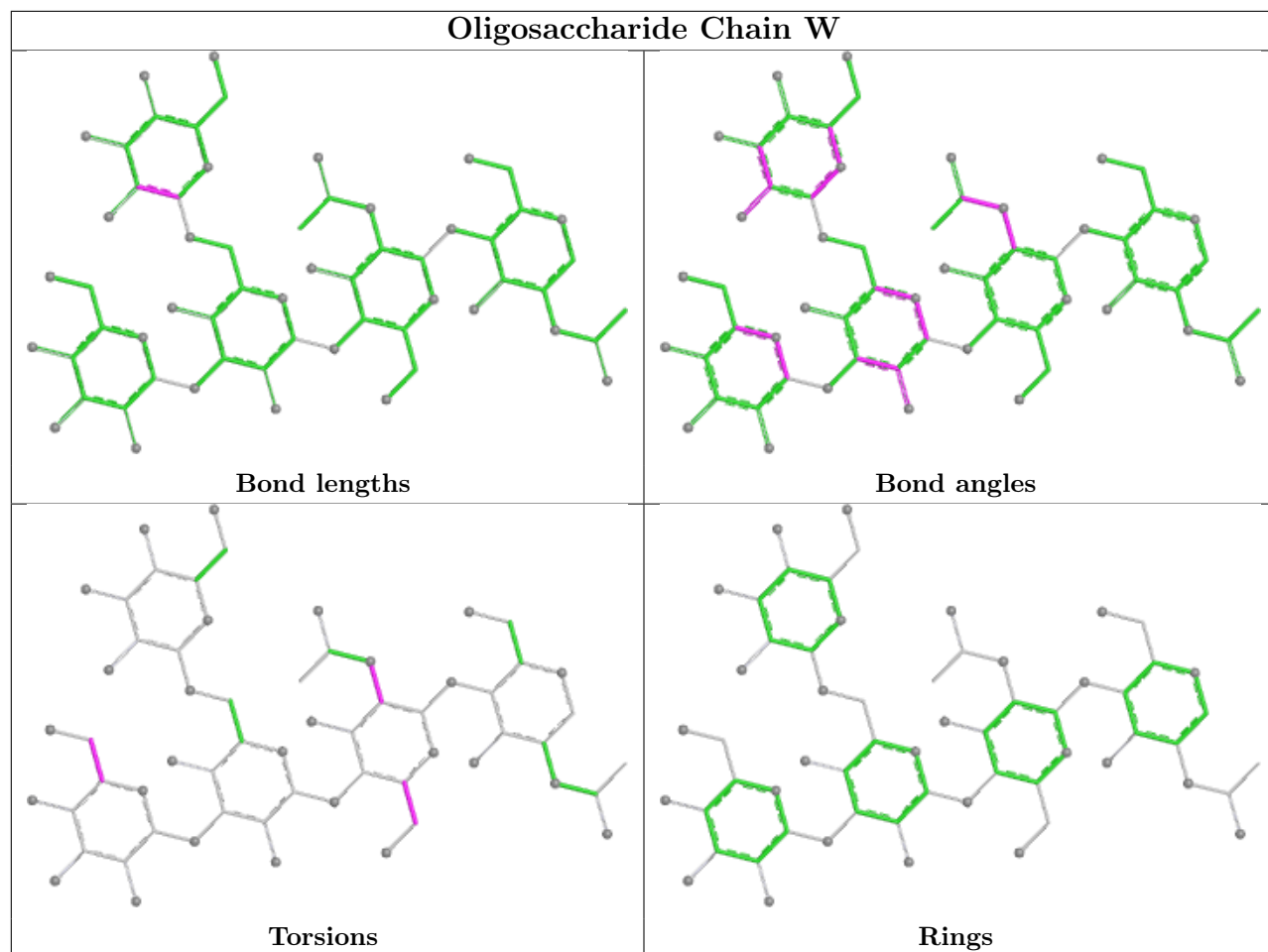


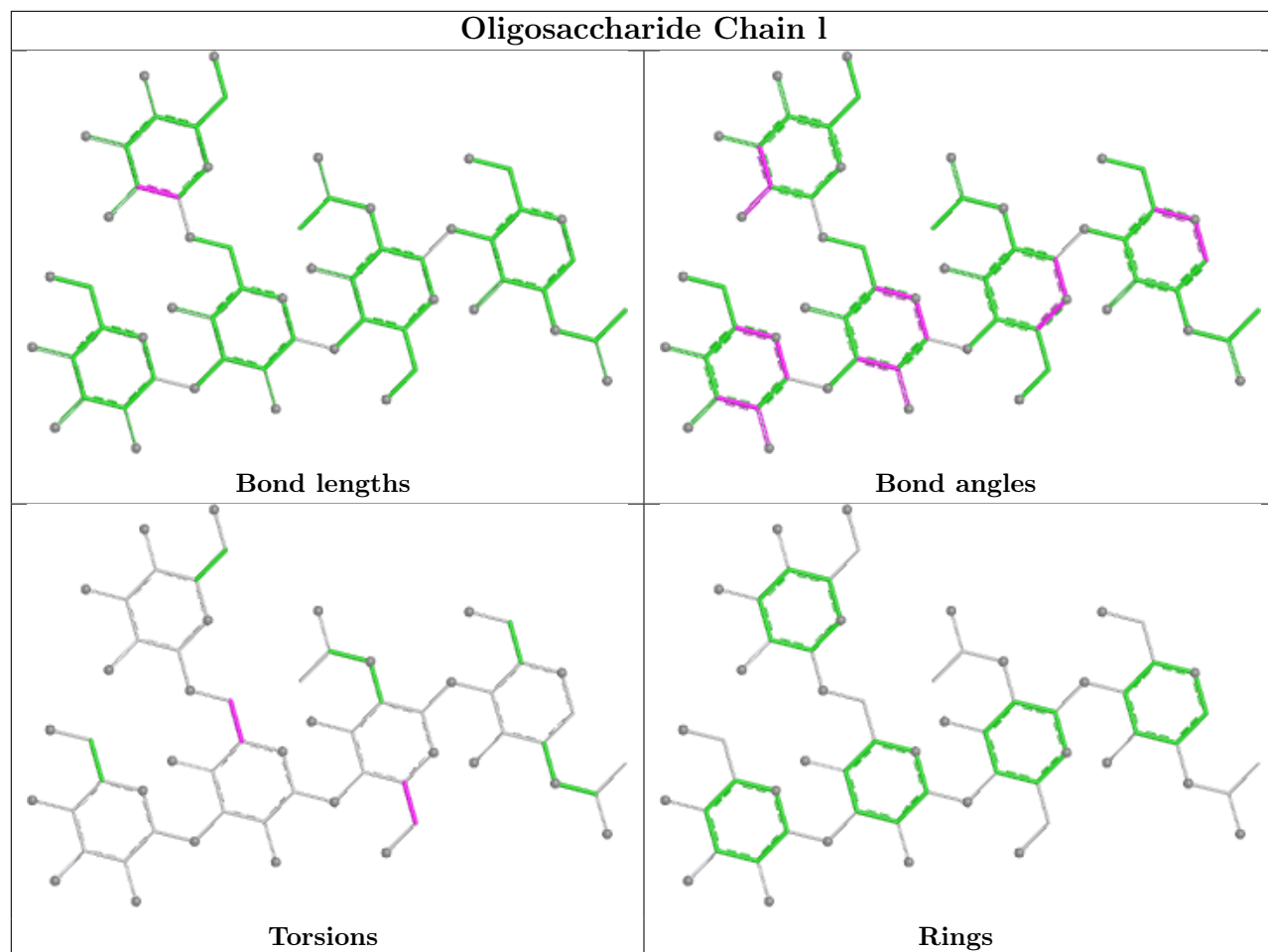


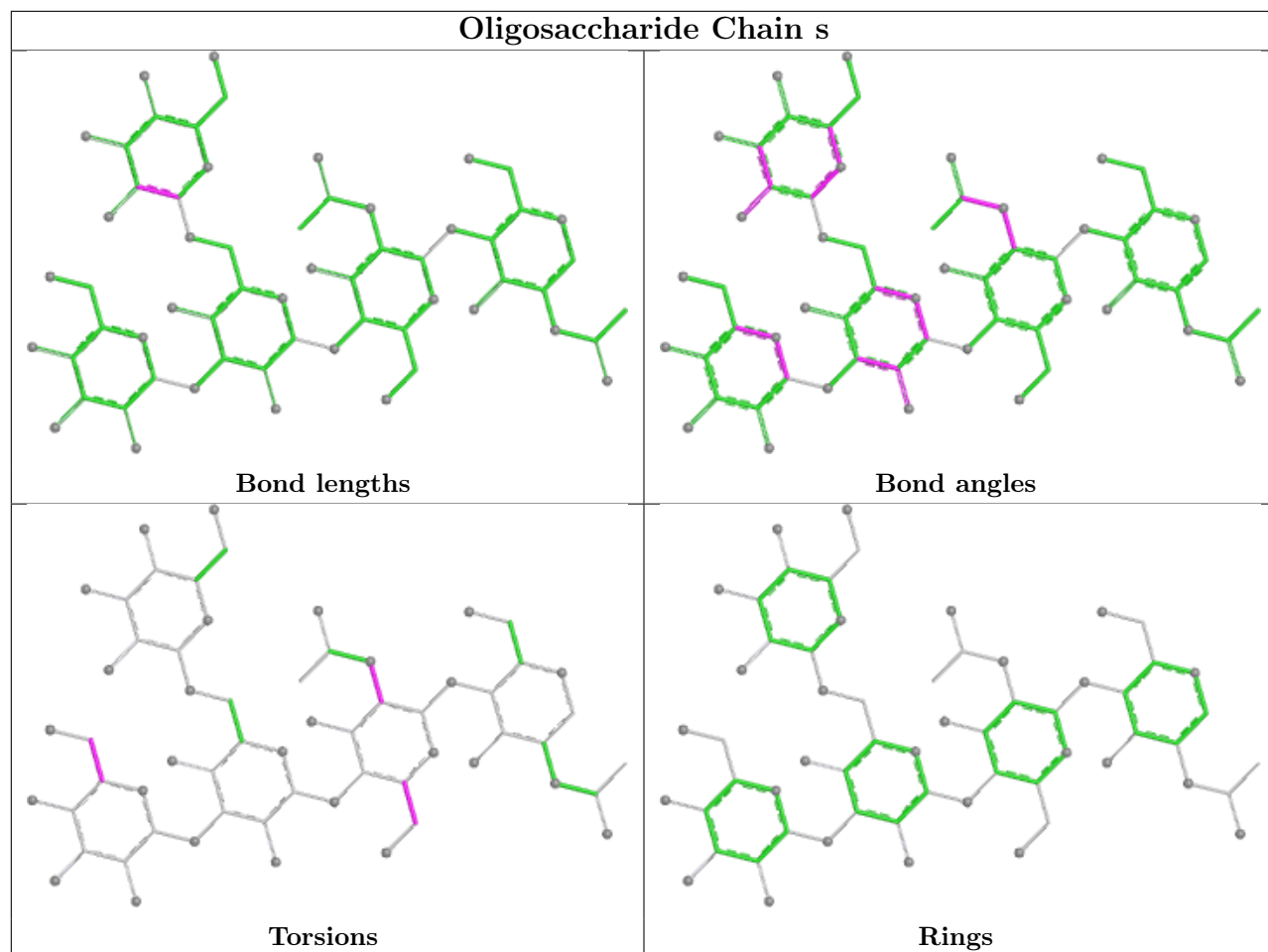


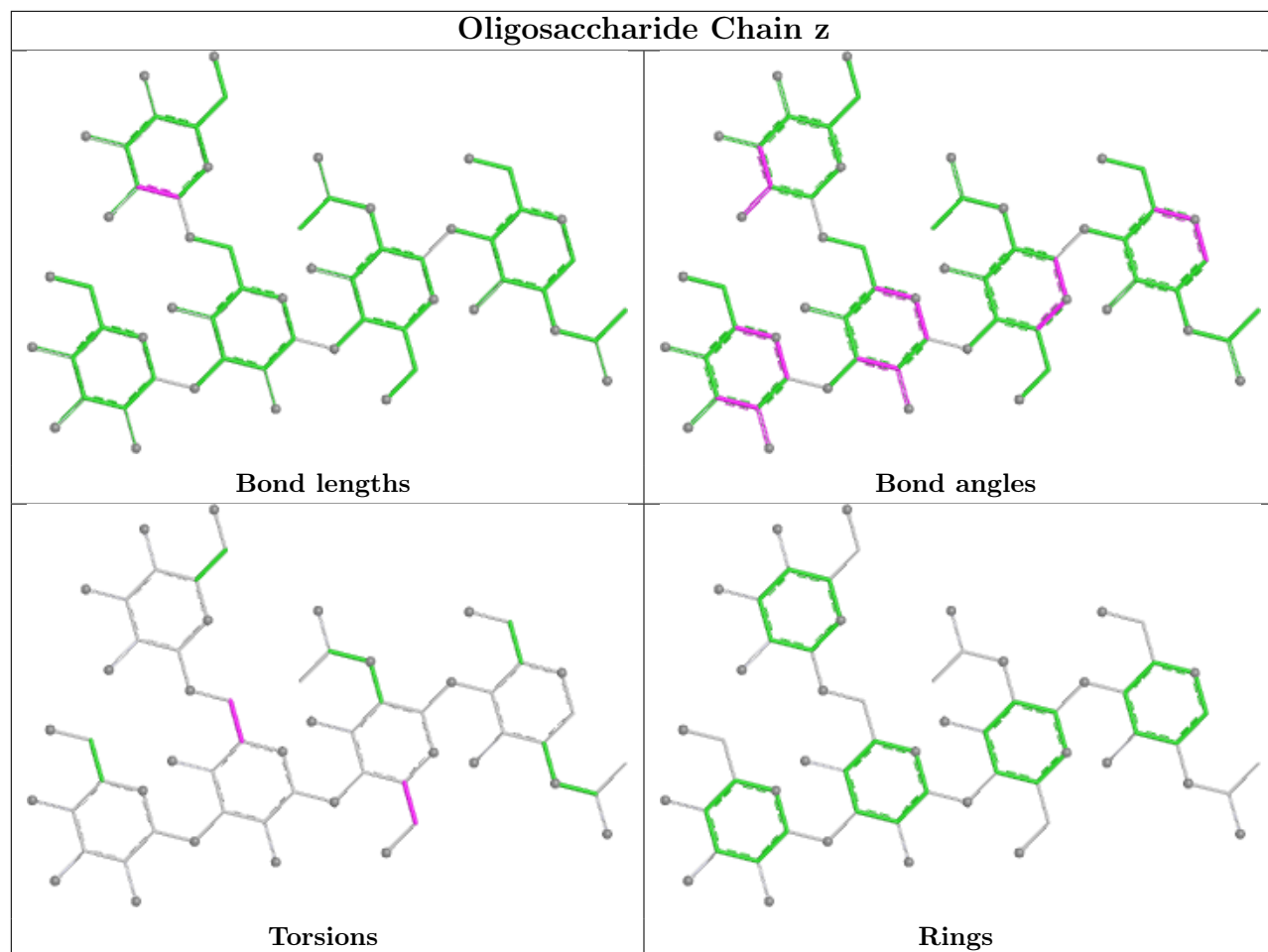


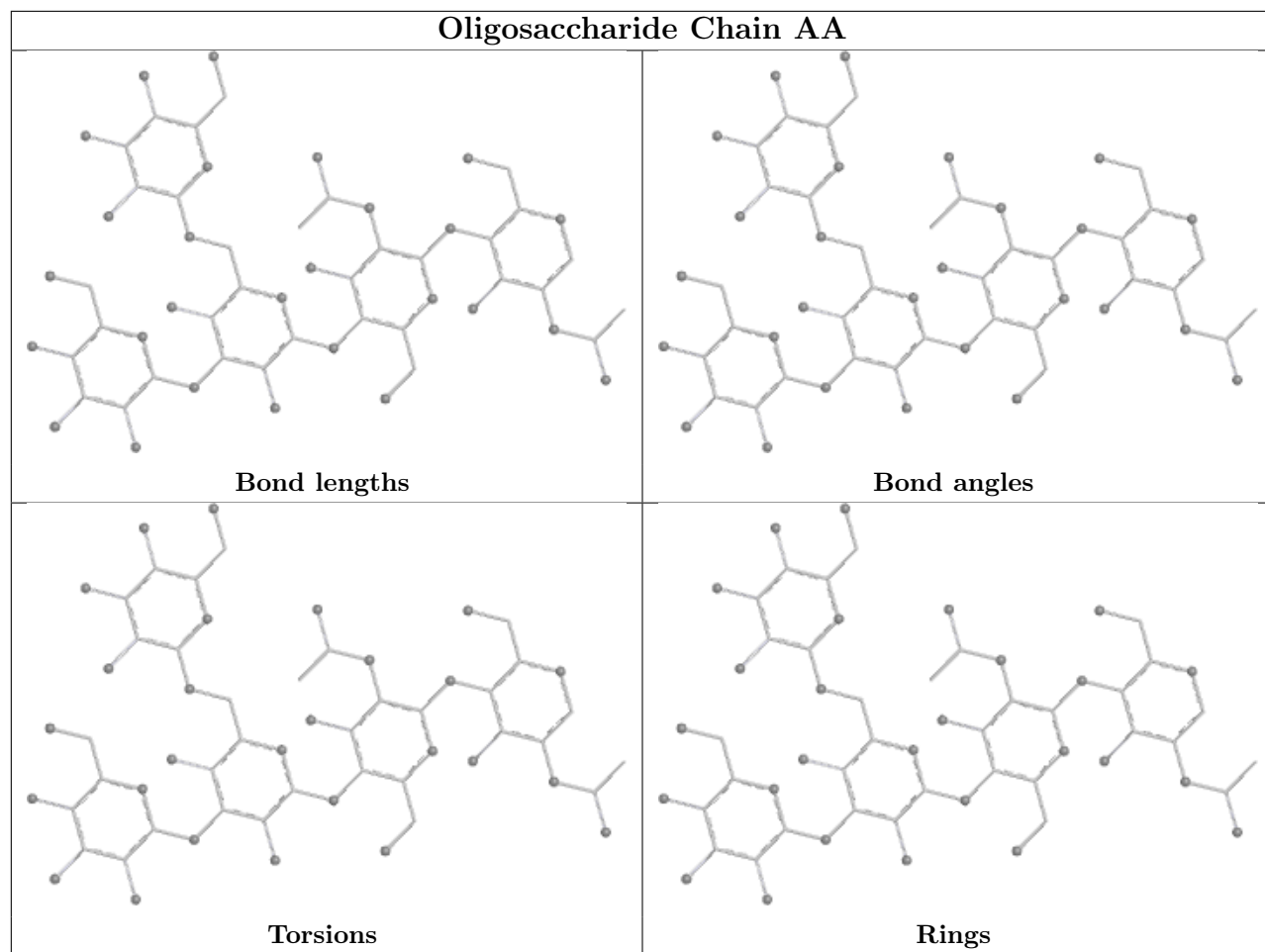


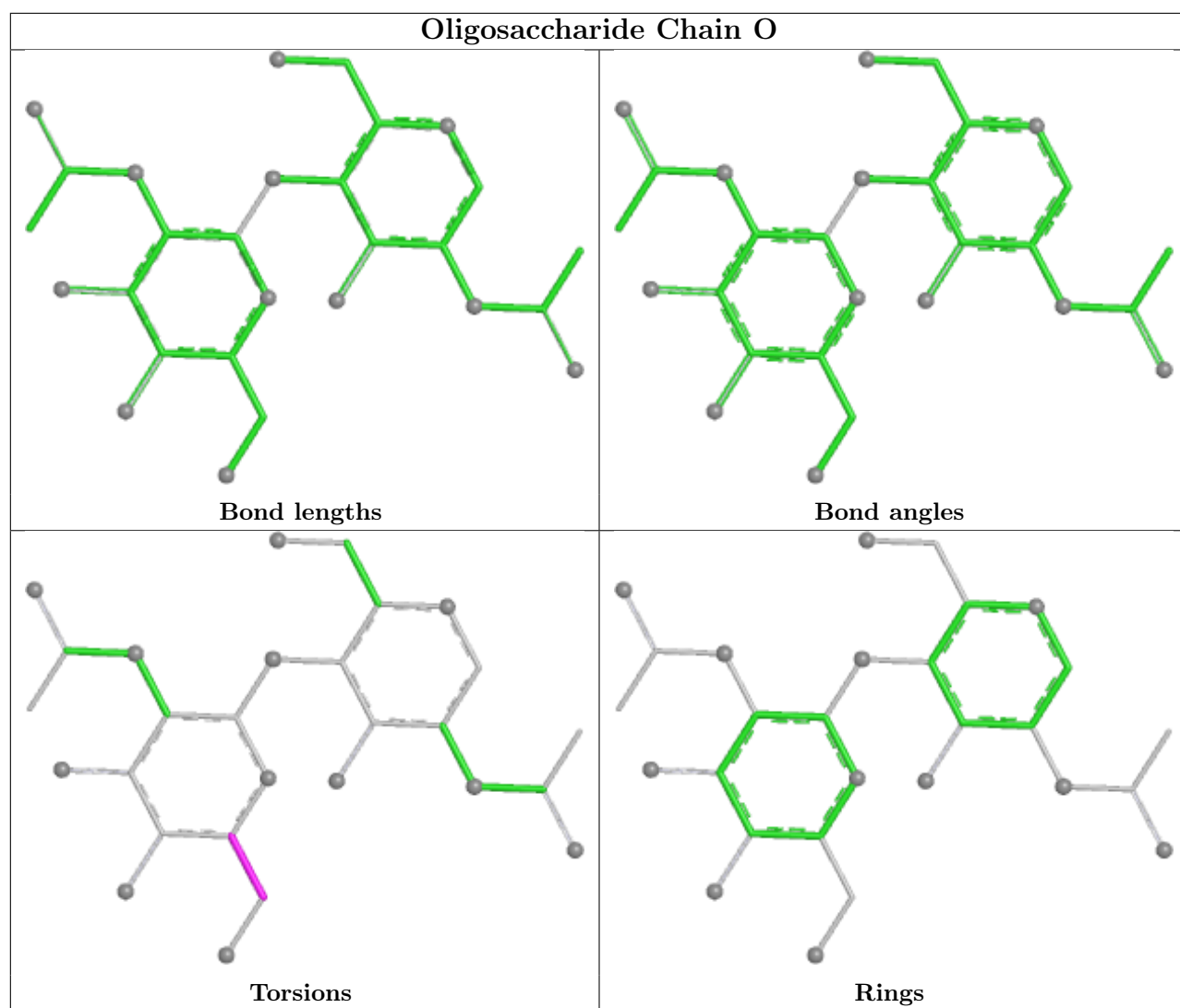


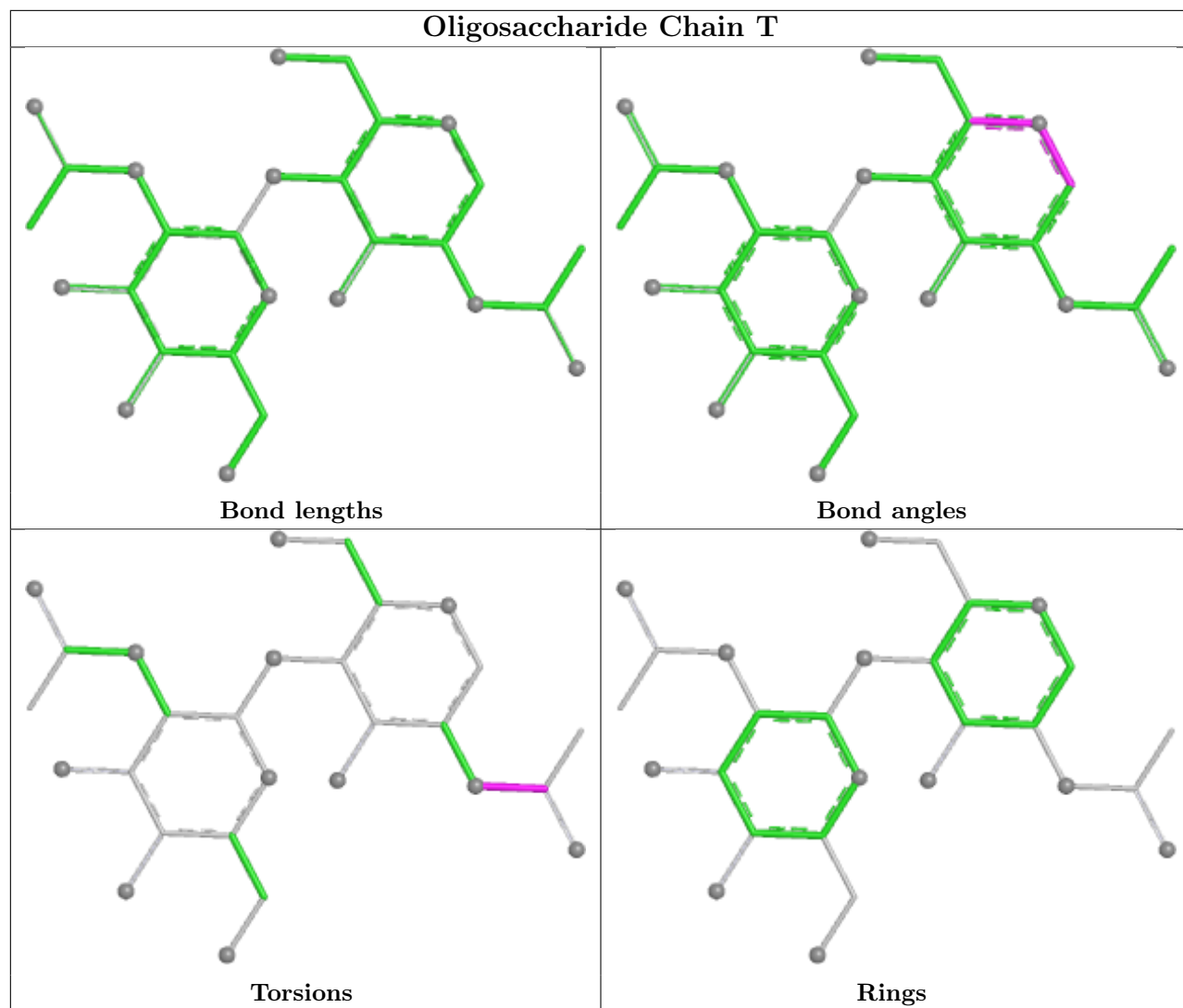


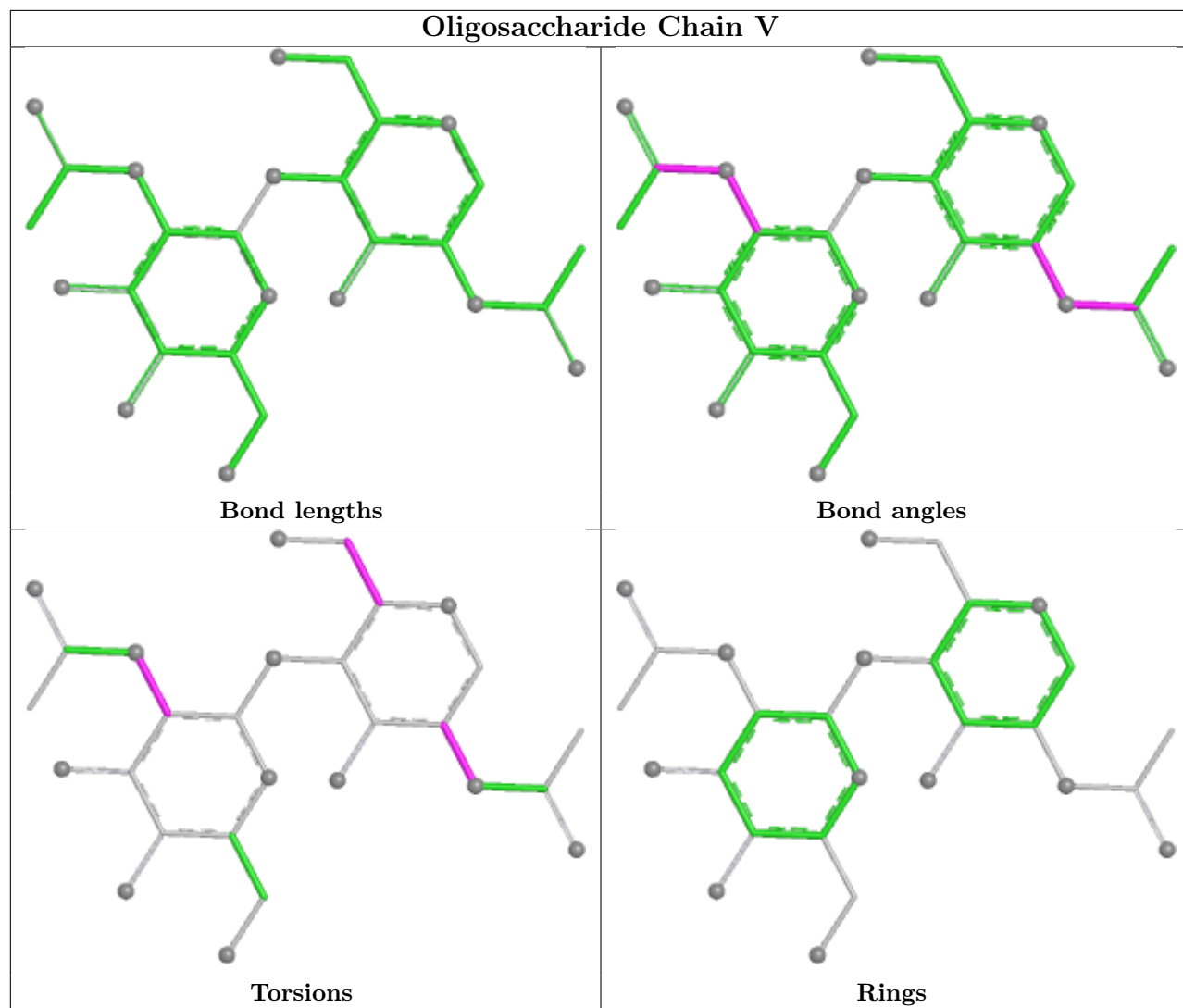


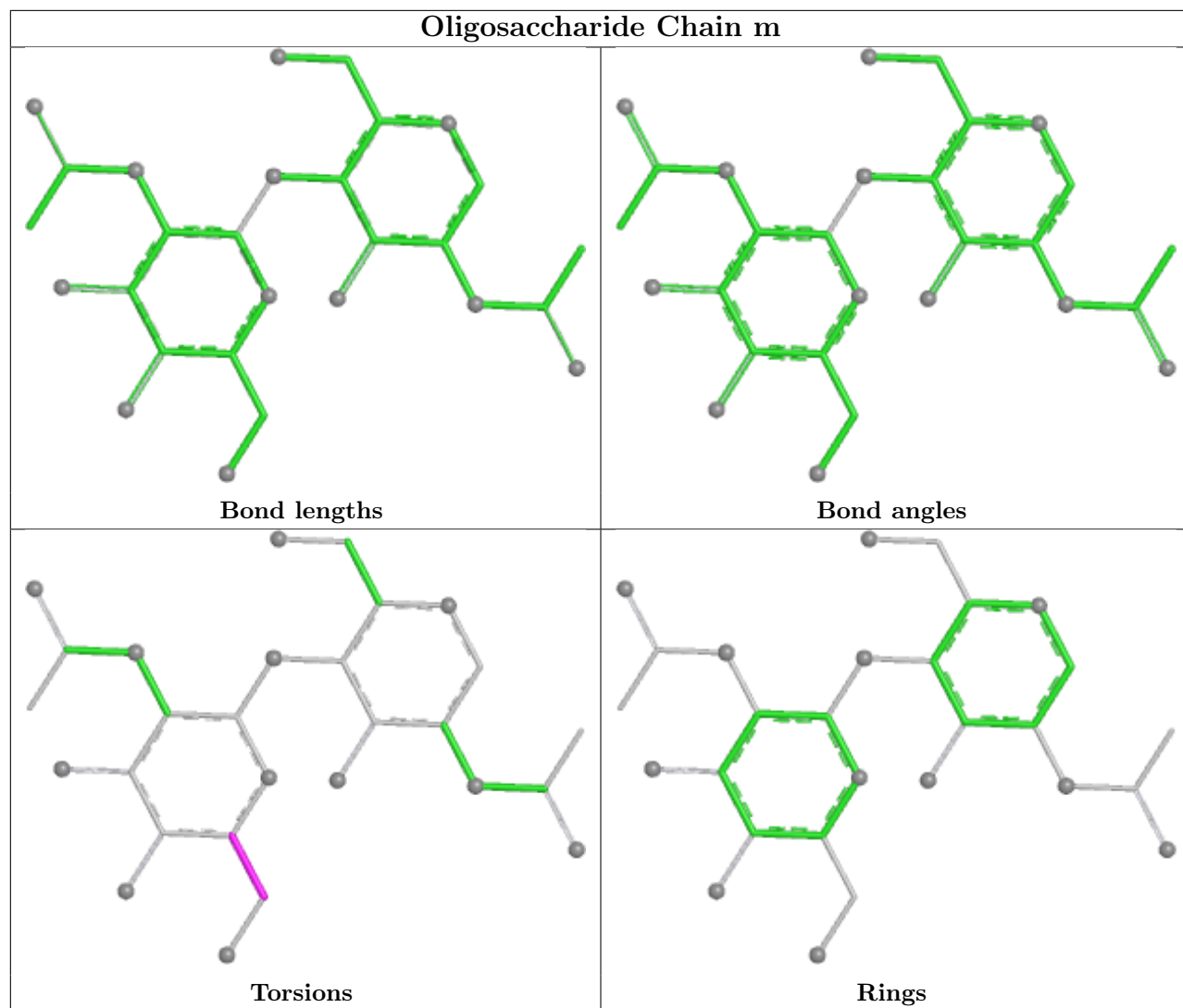


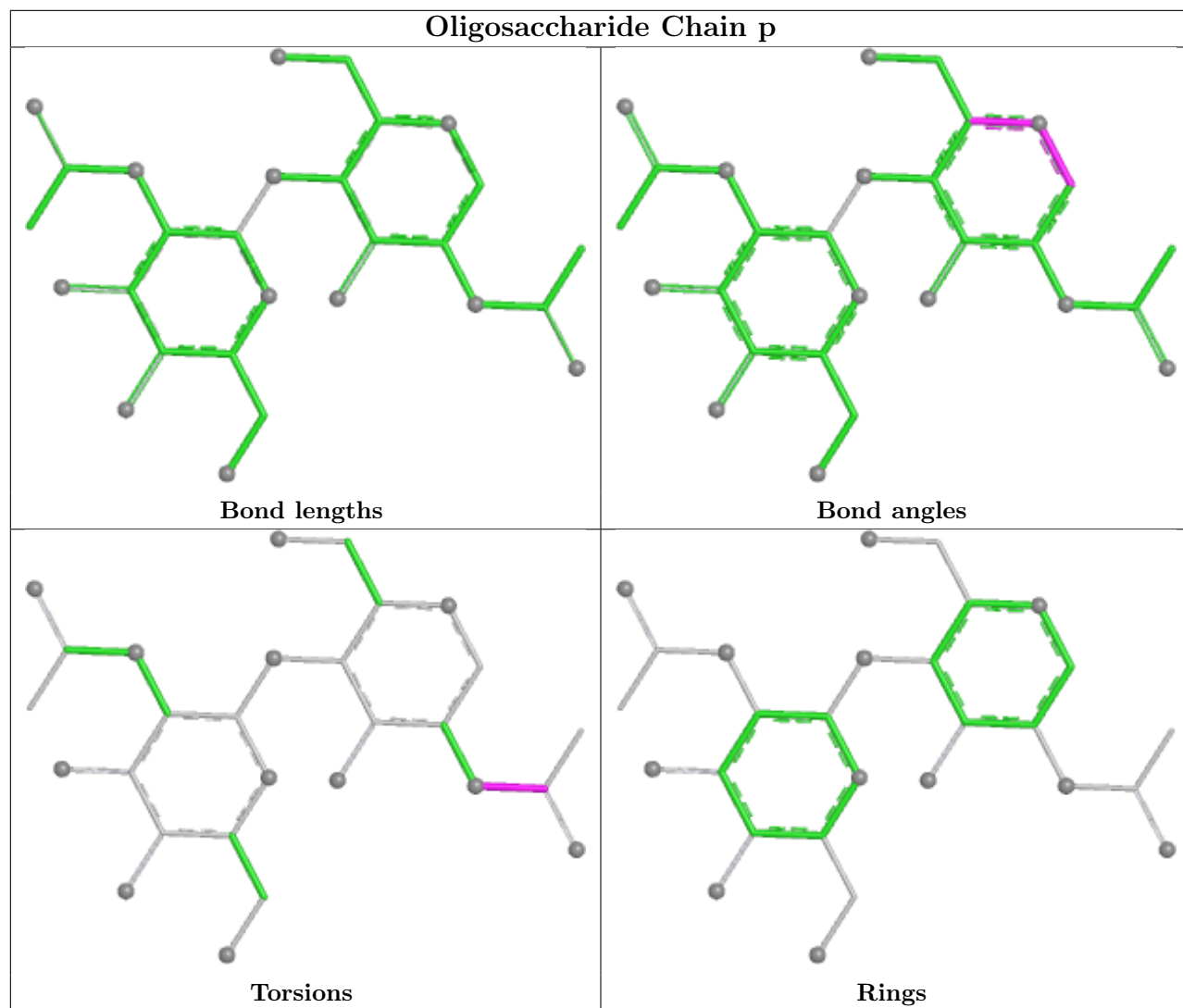


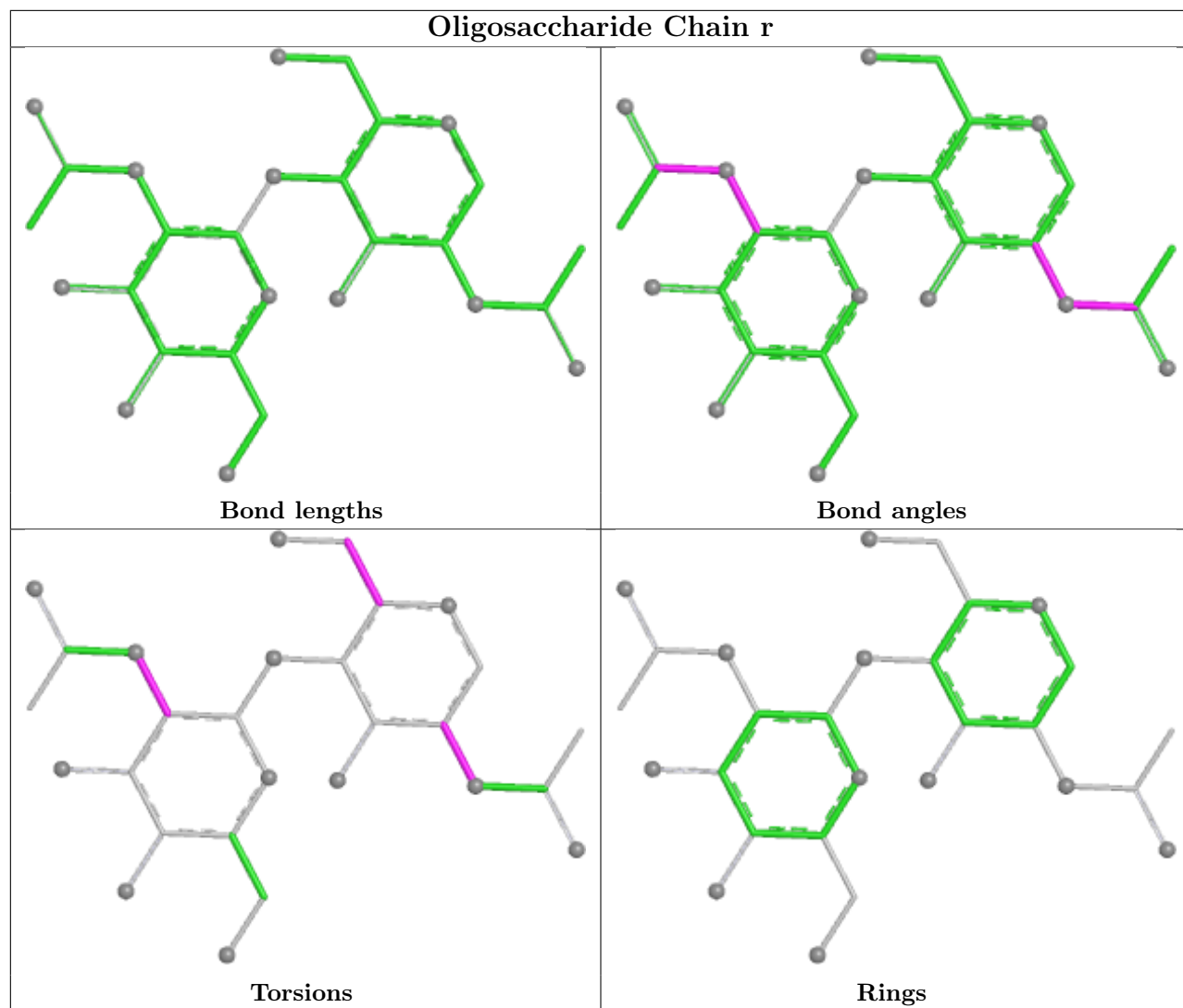


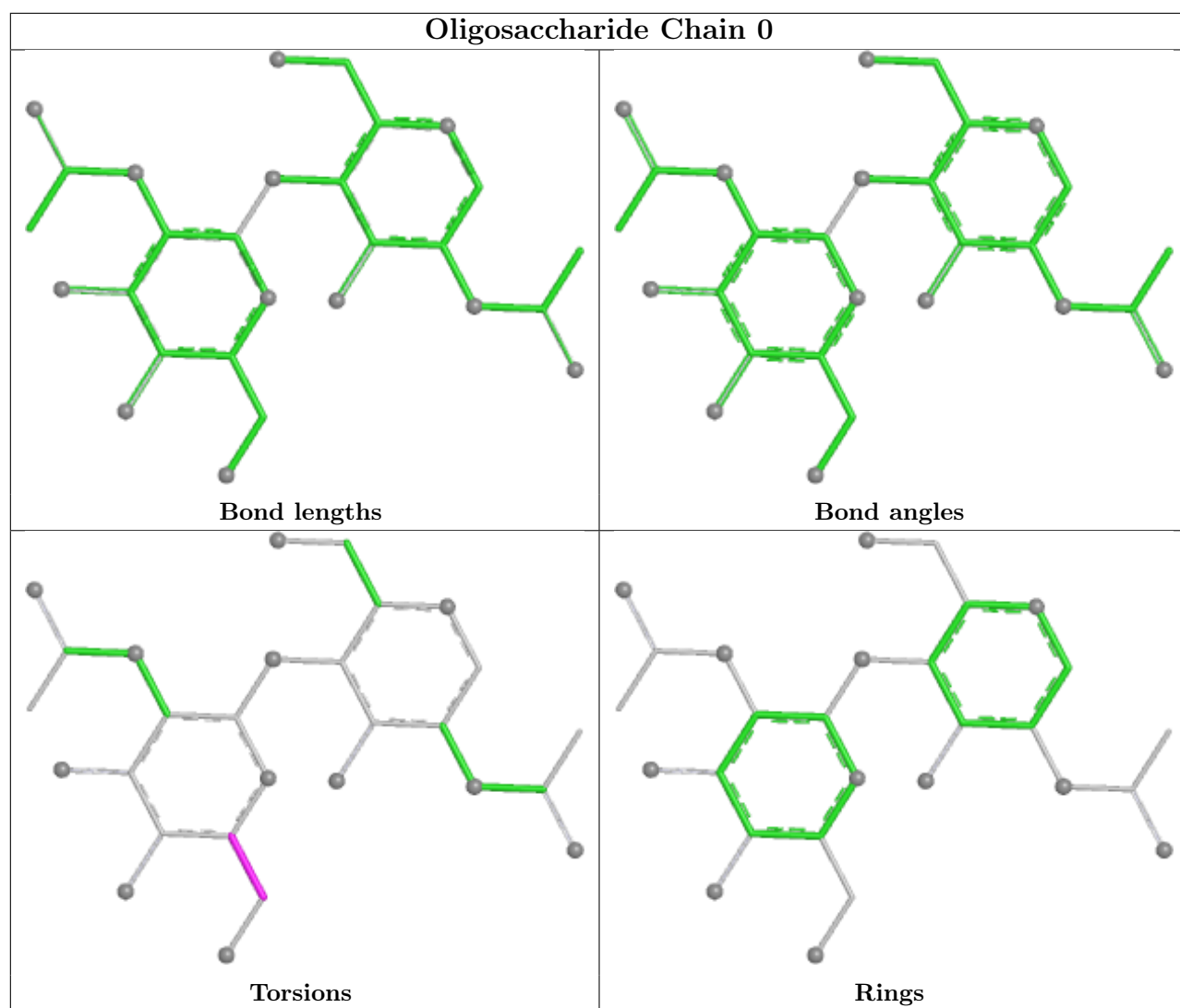


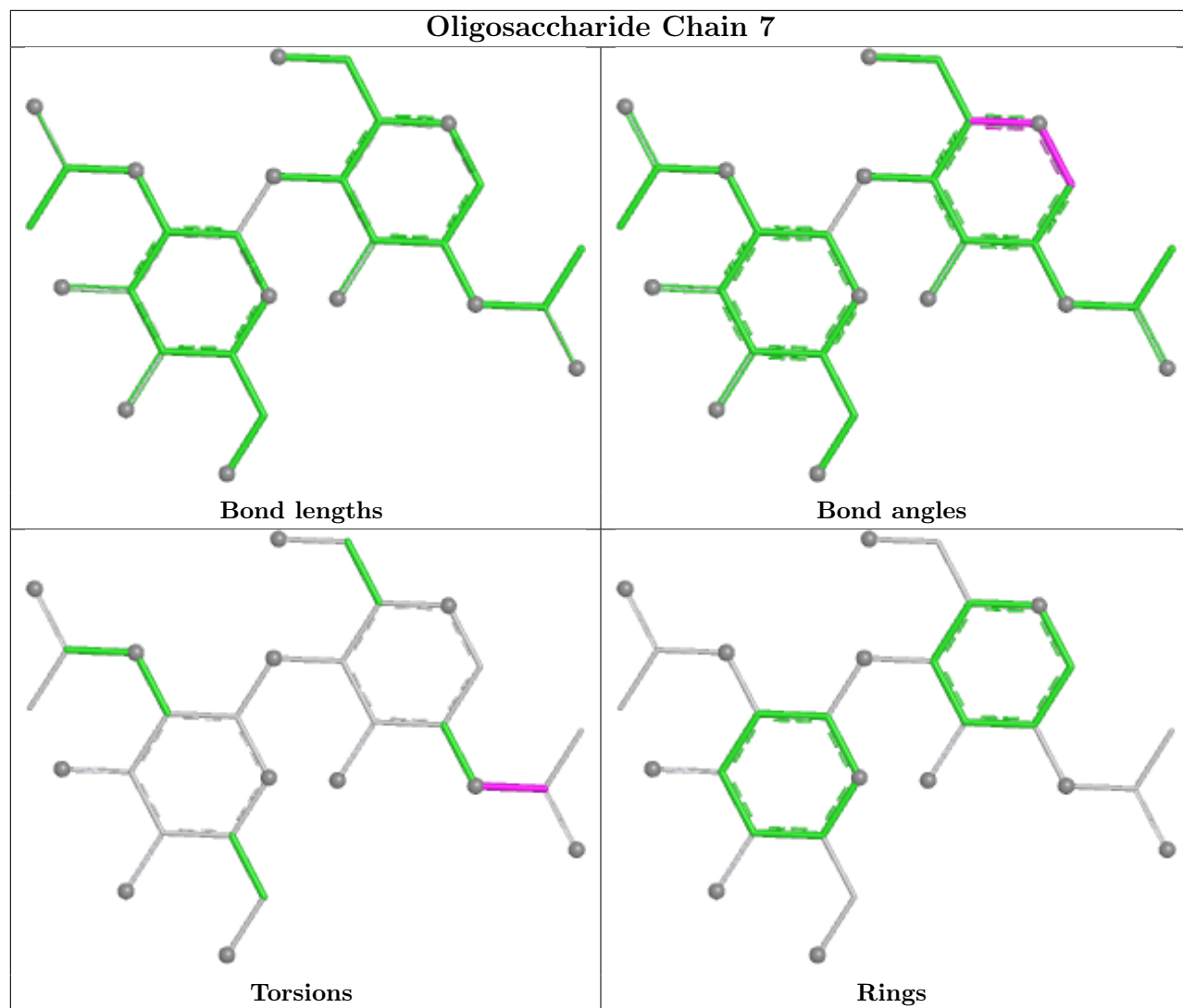


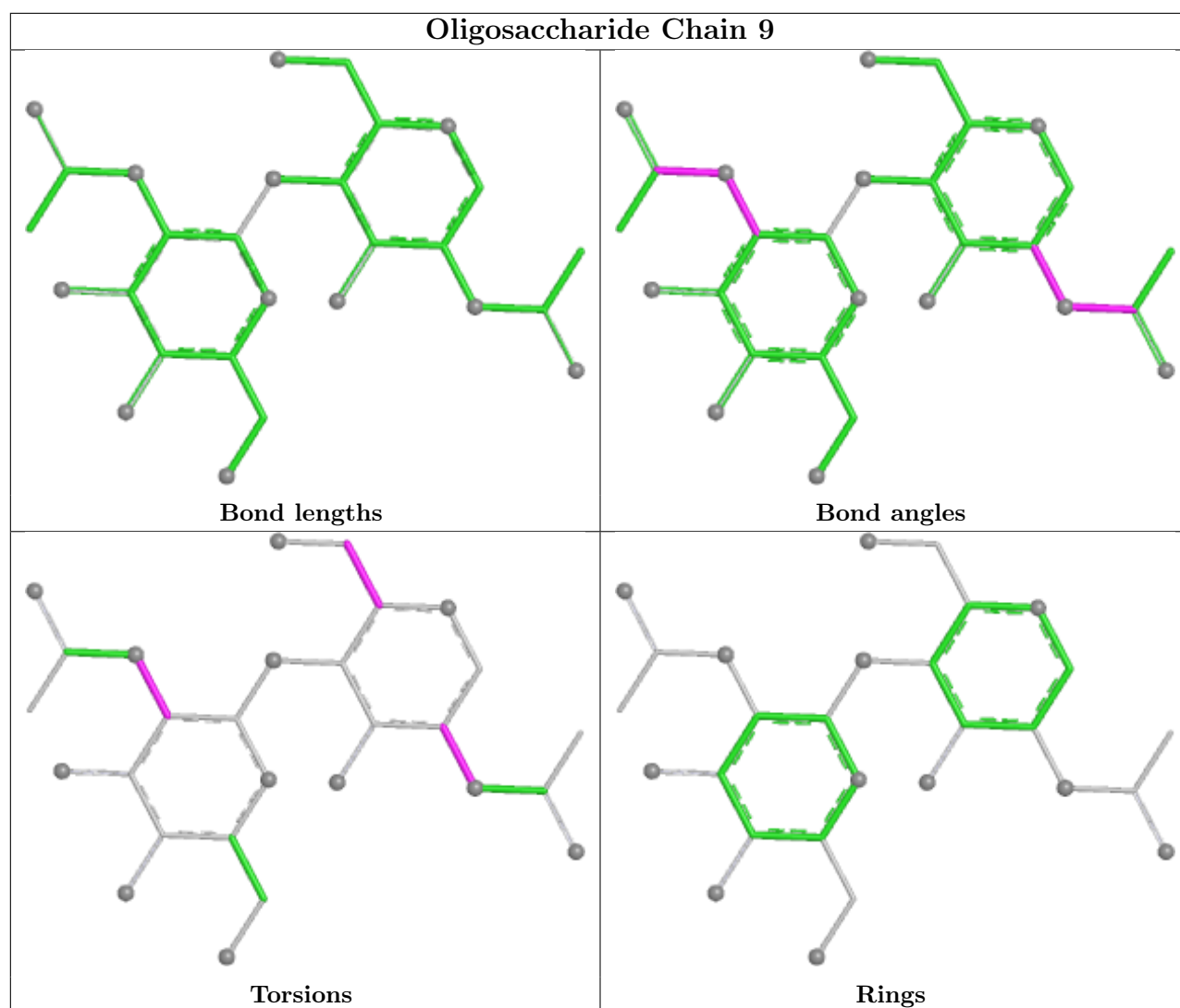












5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
13	NAG	A	608	3	14,14,15	0.37	0	17,19,21	0.57	0
13	NAG	B	623	3	14,14,15	0.26	0	17,19,21	0.60	0
13	NAG	A	623	3	14,14,15	0.26	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	C	623	3	14,14,15	0.26	0	17,19,21	0.60	0
13	NAG	B	617	3	14,14,15	0.48	0	17,19,21	1.54	2 (11%)
13	NAG	B	608	3	14,14,15	0.38	0	17,19,21	0.57	0
13	NAG	C	617	3	14,14,15	0.48	0	17,19,21	1.55	2 (11%)
13	NAG	C	608	3	14,14,15	0.39	0	17,19,21	0.57	0
13	NAG	A	617	3	14,14,15	0.49	0	17,19,21	1.54	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	608	3	-	2/6/23/26	0/1/1/1
13	NAG	B	623	3	-	2/6/23/26	0/1/1/1
13	NAG	A	623	3	-	2/6/23/26	0/1/1/1
13	NAG	C	623	3	-	2/6/23/26	0/1/1/1
13	NAG	B	617	3	-	2/6/23/26	0/1/1/1
13	NAG	B	608	3	-	2/6/23/26	0/1/1/1
13	NAG	C	617	3	-	2/6/23/26	0/1/1/1
13	NAG	C	608	3	-	2/6/23/26	0/1/1/1
13	NAG	A	617	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	617	NAG	C1-O5-C5	4.44	118.13	112.19
13	A	617	NAG	C1-O5-C5	4.41	118.10	112.19
13	B	617	NAG	C1-O5-C5	4.41	118.09	112.19
13	C	617	NAG	C3-C4-C5	3.50	116.58	110.23
13	A	617	NAG	C3-C4-C5	3.49	116.55	110.23
13	B	617	NAG	C3-C4-C5	3.48	116.54	110.23

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	623	NAG	O5-C5-C6-O6
13	A	623	NAG	O5-C5-C6-O6
13	C	623	NAG	O5-C5-C6-O6
13	C	623	NAG	C4-C5-C6-O6
13	B	623	NAG	C4-C5-C6-O6
13	A	623	NAG	C4-C5-C6-O6
13	B	617	NAG	C4-C5-C6-O6
13	A	617	NAG	C4-C5-C6-O6
13	C	617	NAG	C4-C5-C6-O6
13	B	608	NAG	O5-C5-C6-O6
13	A	608	NAG	O5-C5-C6-O6
13	C	608	NAG	O5-C5-C6-O6
13	B	608	NAG	C4-C5-C6-O6
13	A	608	NAG	C4-C5-C6-O6
13	C	608	NAG	C4-C5-C6-O6
13	C	617	NAG	O5-C5-C6-O6
13	B	617	NAG	O5-C5-C6-O6
13	A	617	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

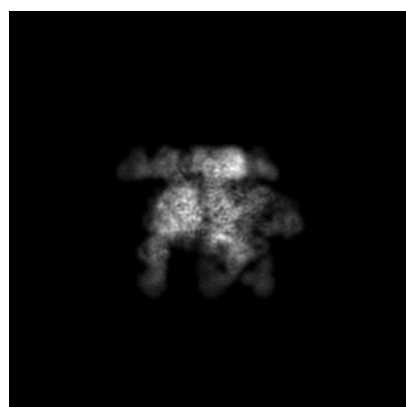
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9319. These allow visual inspection of the internal detail of the map and identification of artifacts.

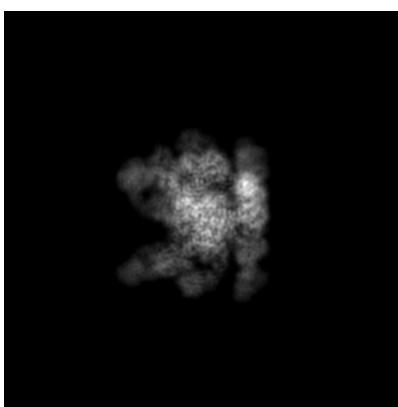
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

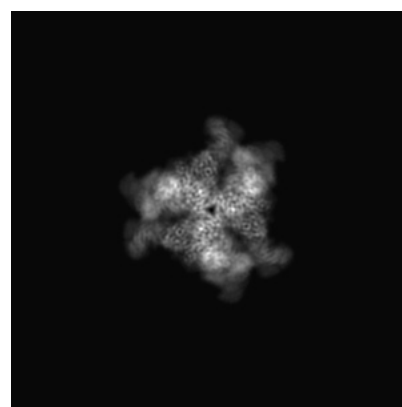
6.1.1 Primary map



X



Y

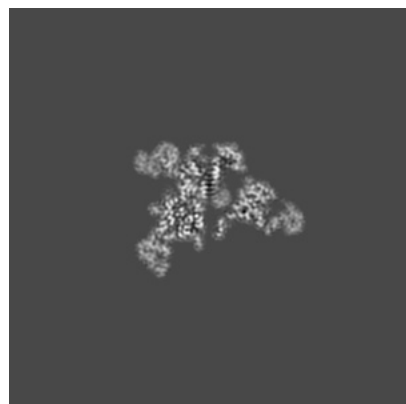


Z

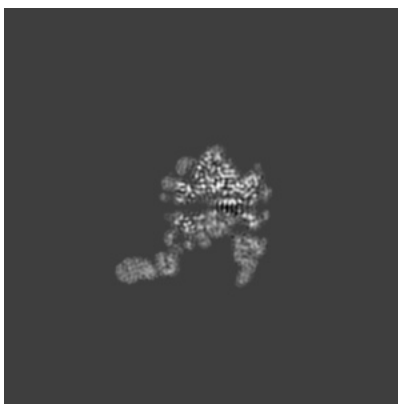
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

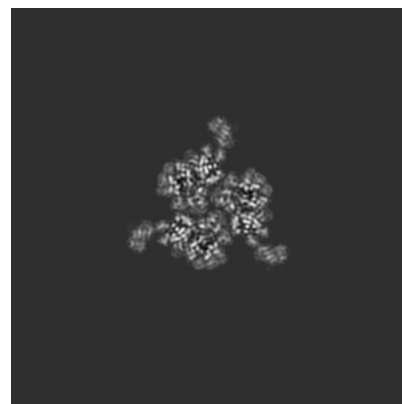
6.2.1 Primary map



X Index: 192



Y Index: 192

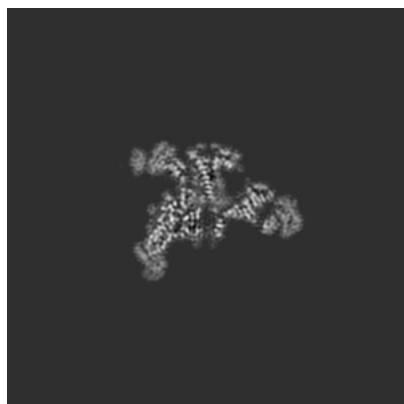


Z Index: 192

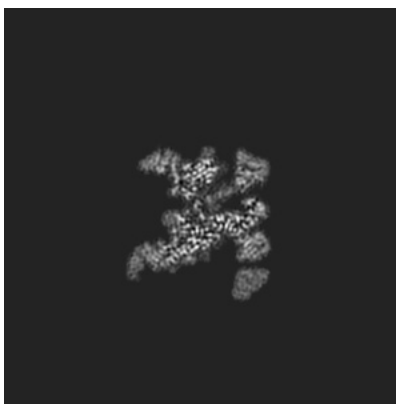
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

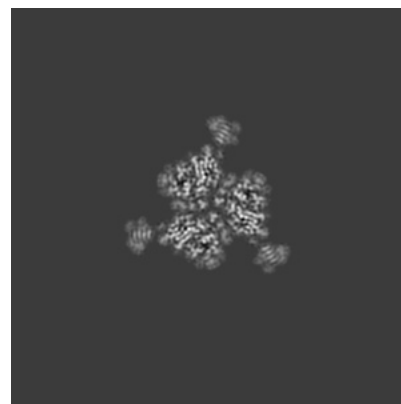
6.3.1 Primary map



X Index: 196



Y Index: 211

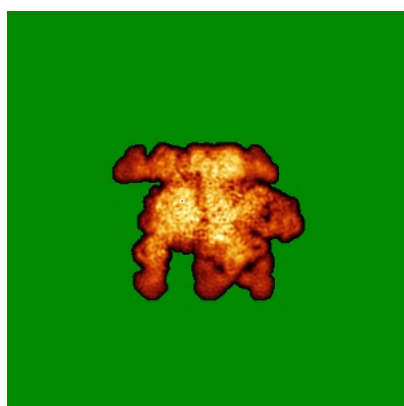


Z Index: 190

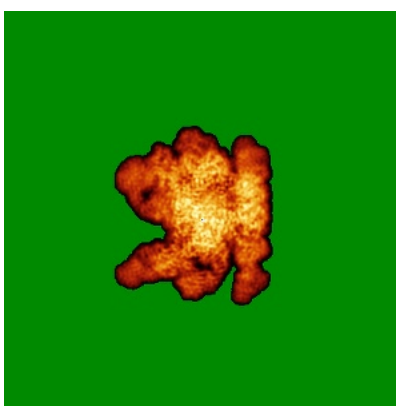
The images above show the largest variance slices of the map in three orthogonal directions.

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

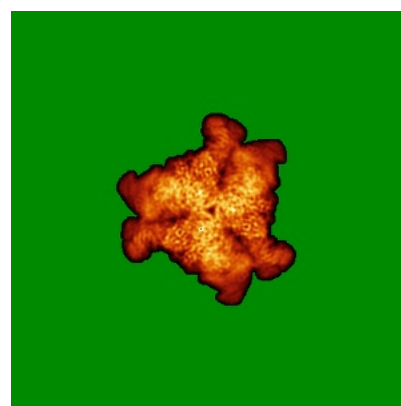
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.73. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

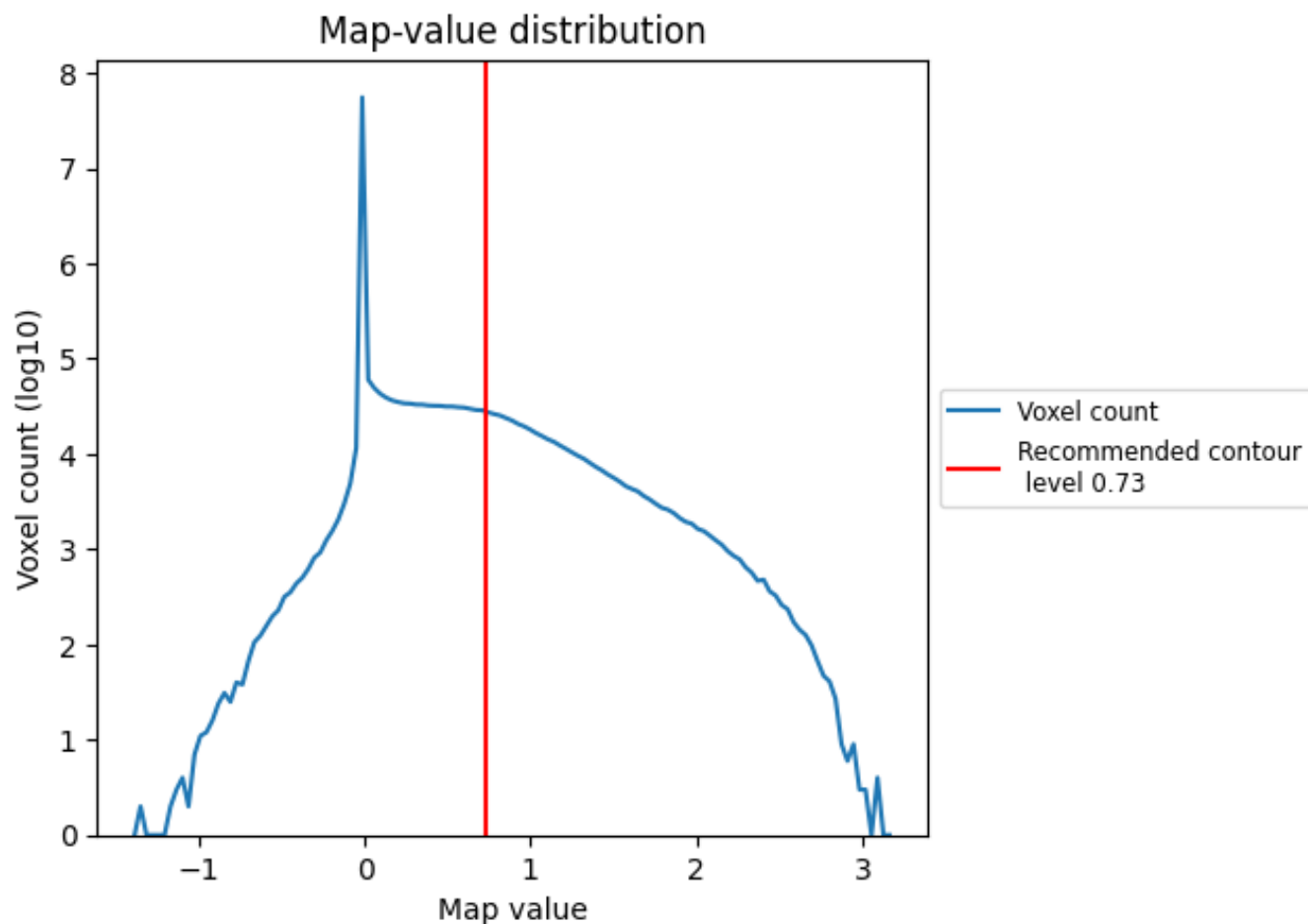
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

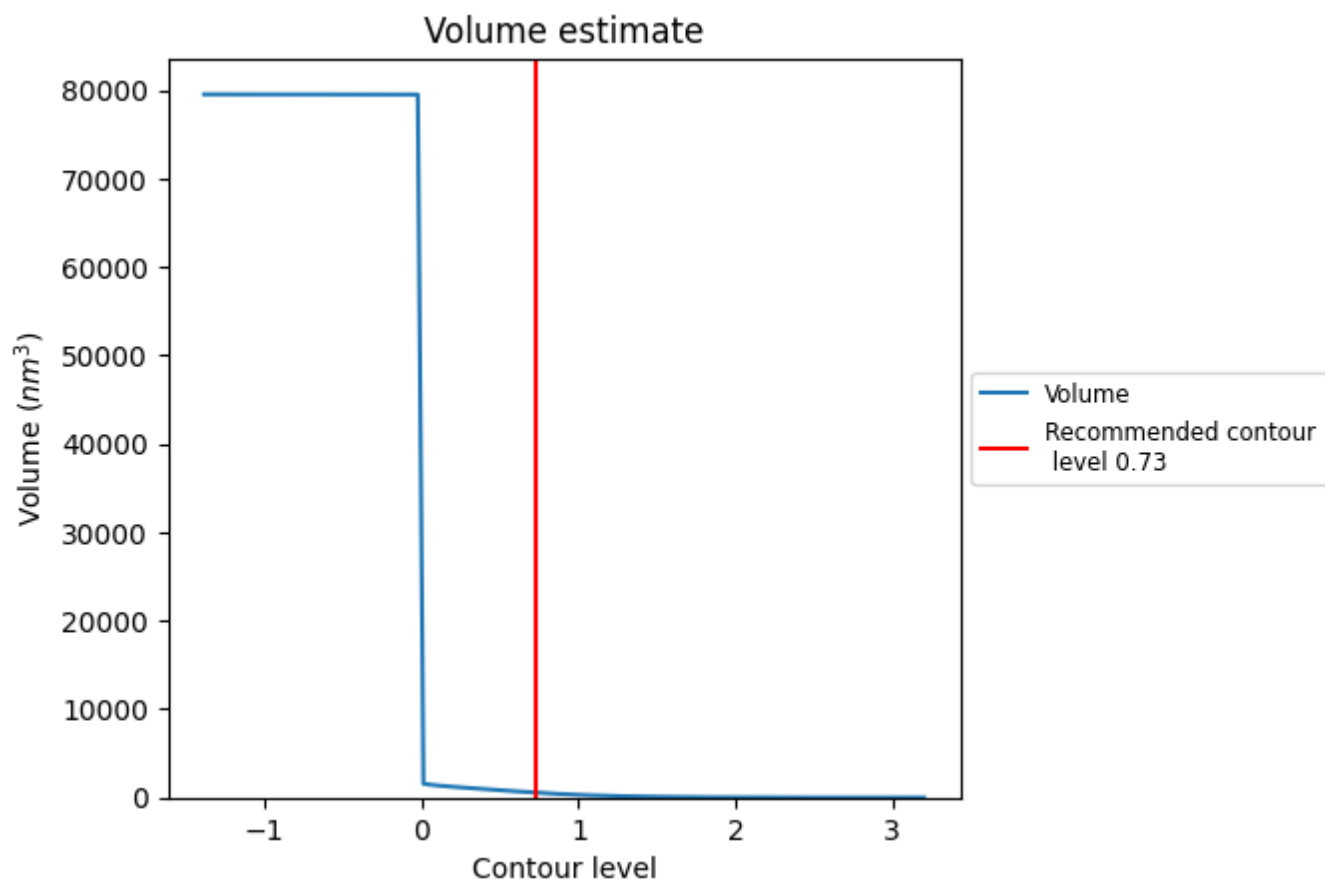
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

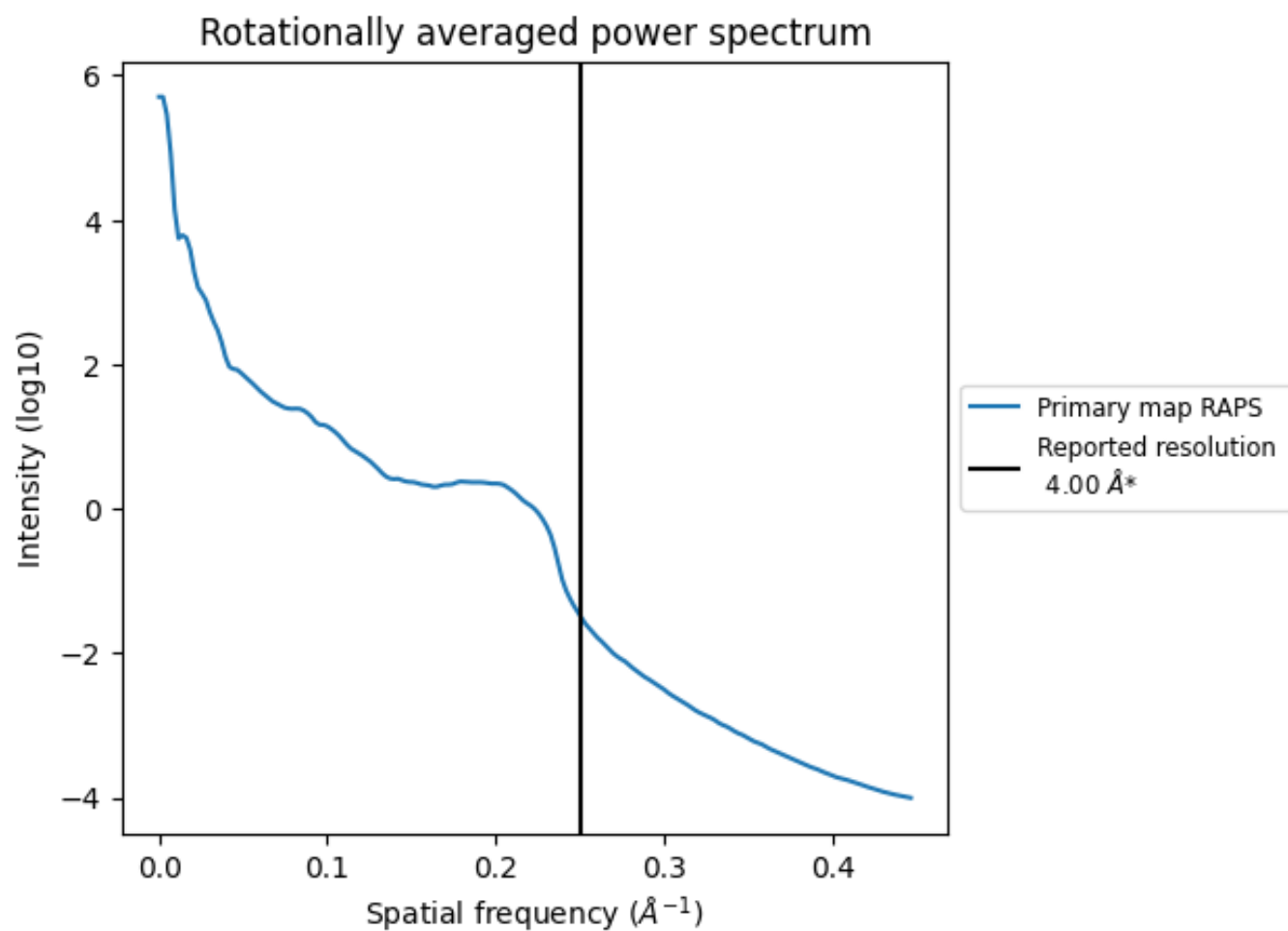
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 557 nm^3 ; this corresponds to an approximate mass of 503 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 0.250 Å⁻¹

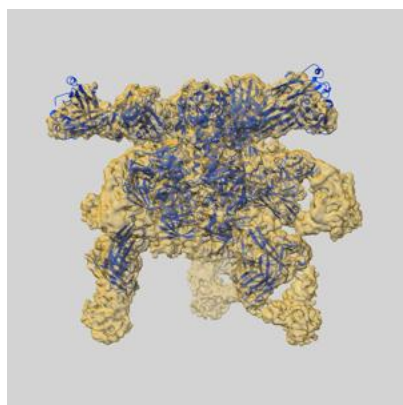
8 Fourier-Shell correlation

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

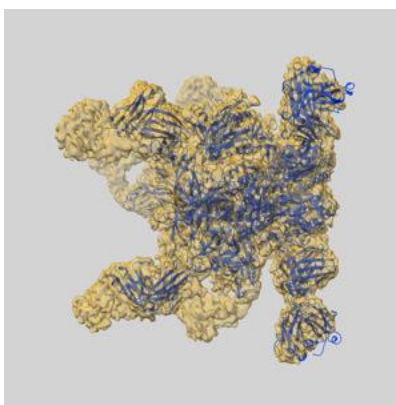
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9319 and PDB model 6N1V. Per-residue inclusion information can be found in section [3](#) on page [13](#).

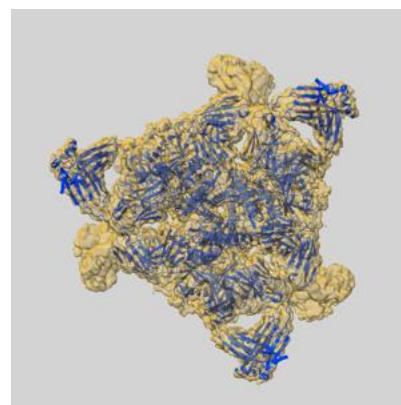
9.1 Map-model overlay [i](#)



X



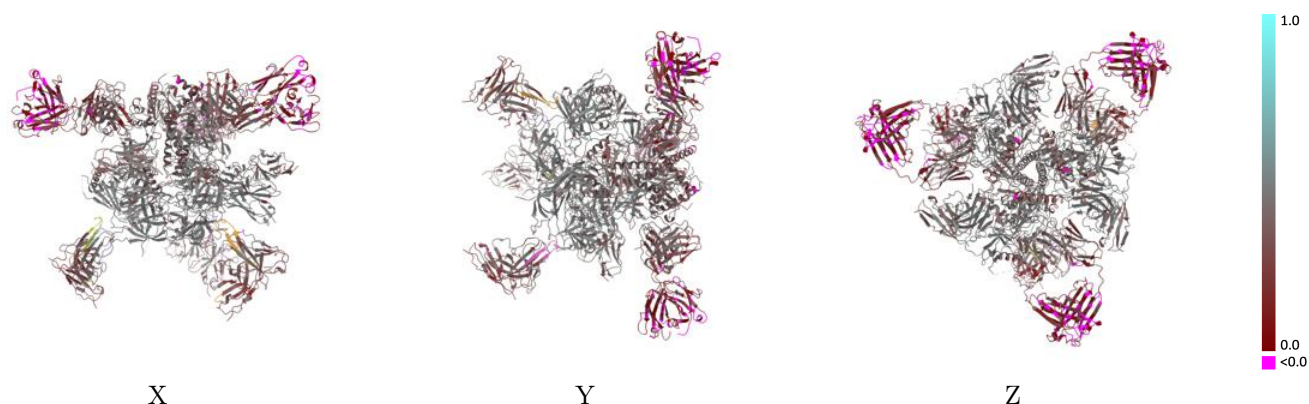
Y



Z

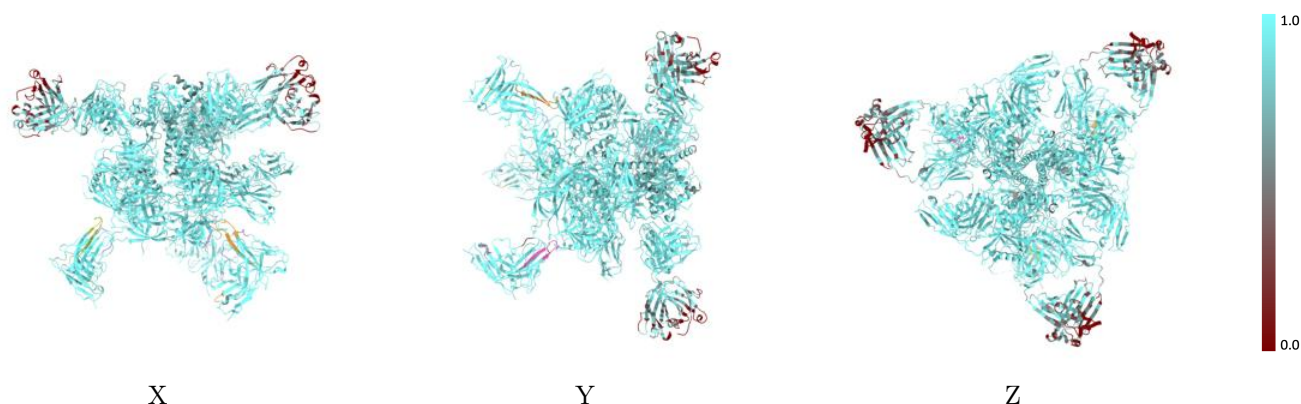
The images above show the 3D surface view of the map at the recommended contour level 0.73 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



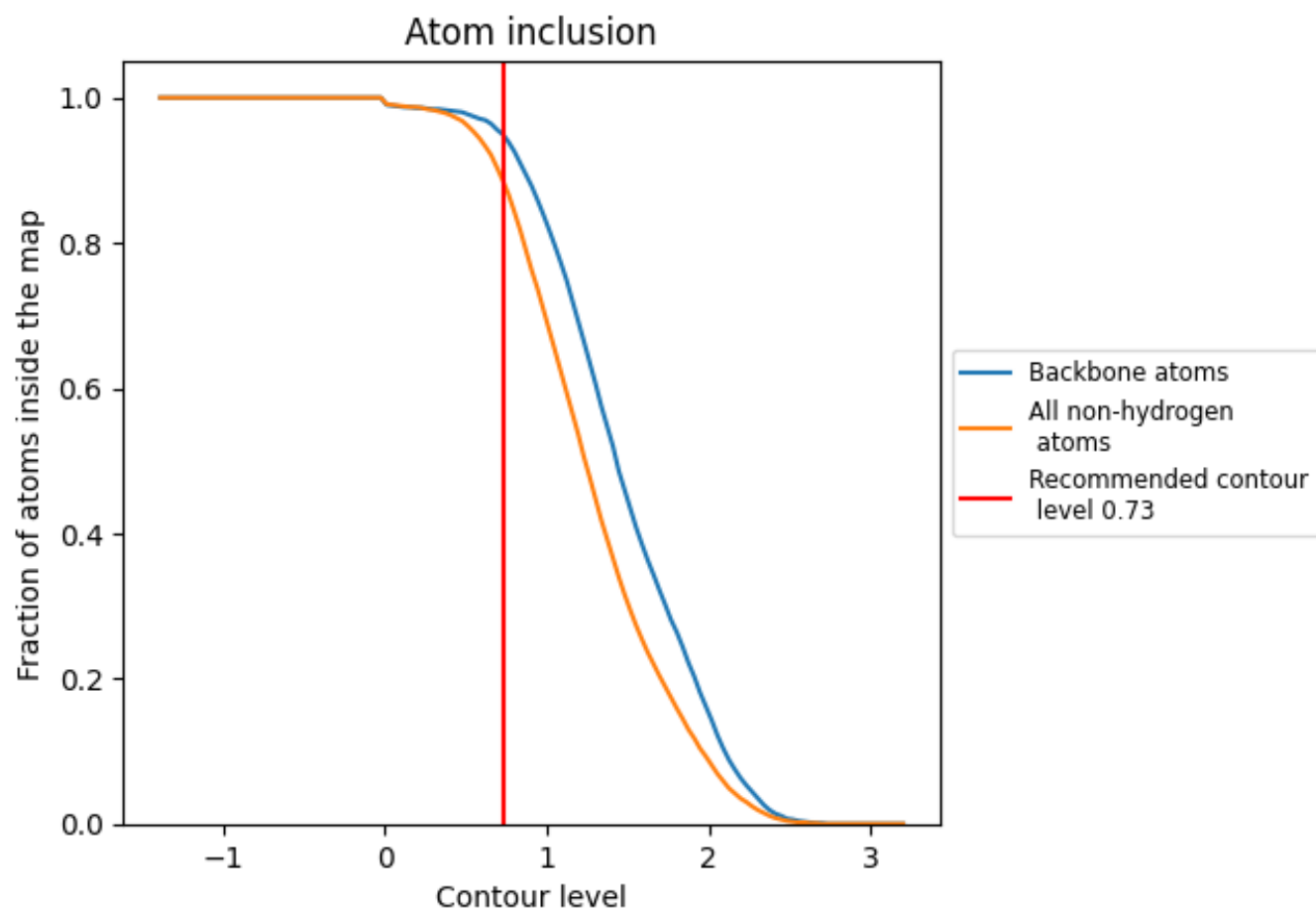
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.73).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.73) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.3730
0	 0.8570	 0.3640
1	 0.7410	 0.2360
2	 0.7740	 0.2400
3	 0.7420	 0.2390
4	 0.7710	 0.2430
5	 0.9230	 0.4660
6	 0.8720	 0.4570
7	 0.9290	 0.4830
8	 0.9740	 0.4630
9	 0.9640	 0.4740
A	 0.9340	 0.4480
AA	 0.9510	 0.4540
B	 0.9350	 0.4500
BA	 0.8600	 0.4220
C	 0.9350	 0.4490
CA	 0.9490	 0.4410
D	 0.9070	 0.3890
DA	 0.9490	 0.4080
E	 0.9080	 0.3930
F	 0.9080	 0.3940
G	 0.7440	 0.3900
H	 0.7400	 0.2380
I	 0.7200	 0.4080
J	 0.9490	 0.4590
K	 0.9180	 0.3530
L	 0.7690	 0.2420
M	 0.9320	 0.3480
N	 0.9610	 0.3920
O	 0.8570	 0.3830
P	 0.9230	 0.4530
Q	 0.9470	 0.4590
R	 0.9360	 0.4240
S	 0.8720	 0.4460
T	 0.9290	 0.4820



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Chain	Atom inclusion	Q-score
U	 0.9740	 0.4630
V	 0.9640	 0.4610
W	 0.9510	 0.4580
X	 0.9320	 0.3490
Y	 0.9330	 0.3470
Z	 0.9580	 0.3890
a	 0.9620	 0.3870
b	 0.8600	 0.4240
c	 0.9740	 0.4480
d	 0.9490	 0.4220
e	 0.7690	 0.3950
f	 0.9470	 0.4570
g	 0.9490	 0.4580
h	 0.9320	 0.4250
i	 0.9360	 0.4240
j	 0.7400	 0.4140
k	 0.9490	 0.4440
l	 0.9180	 0.3580
m	 0.8570	 0.3800
n	 0.9230	 0.4660
o	 0.8720	 0.4540
p	 0.9290	 0.4910
q	 0.9740	 0.4590
r	 1.0000	 0.4810
s	 0.9510	 0.4530
t	 0.8600	 0.4210
u	 0.9490	 0.4320
v	 0.9490	 0.4010
w	 0.7690	 0.3890
x	 0.7400	 0.4090
y	 0.9490	 0.4550
z	 0.9180	 0.3440