



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 09:25 AM UTC

PDB ID : 6CUF / pdb_00006cuf
EMDB ID : EMD-7622
Title : Cryo-EM structure at 4.2 Å resolution of vaccine-elicited antibody vFP1.01 in complex with HIV-1 Env BG505 DS-SOSIP, and antibodies VRC03 and PGT122
Authors : Acharya, P.; Carragher, B.; Potter, C.S.; Kwong, P.D.
Deposited on : 2018-03-26
Resolution : 4.00 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

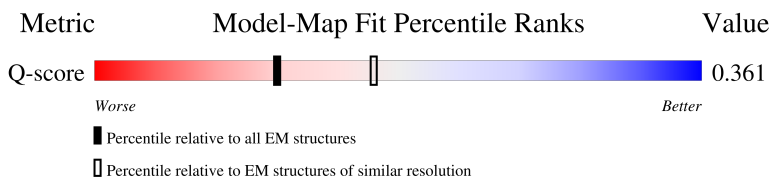
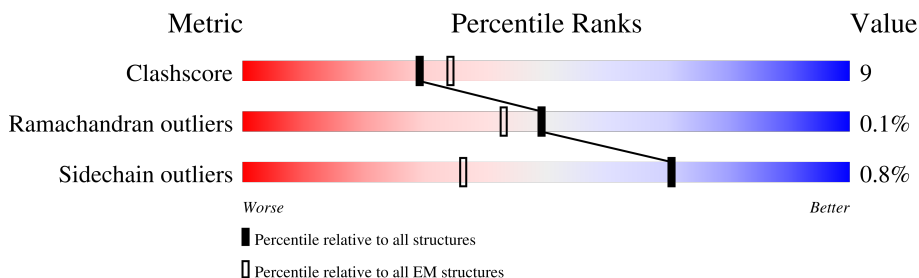
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.



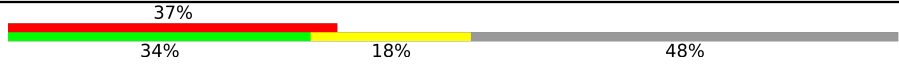
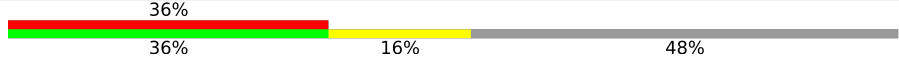
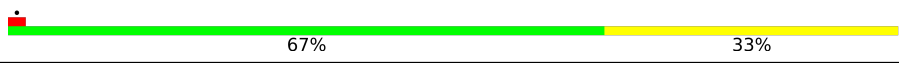

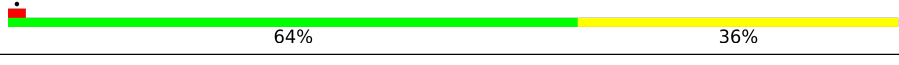
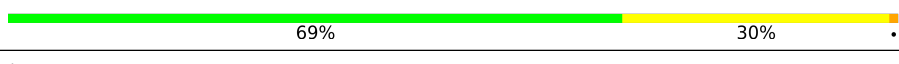
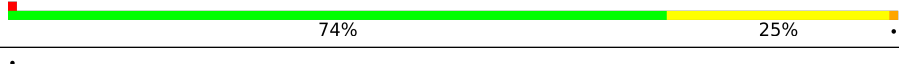

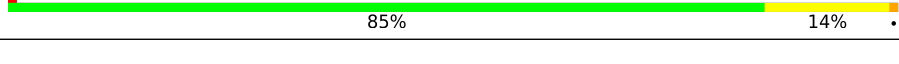


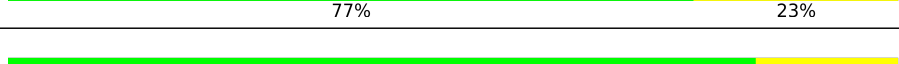
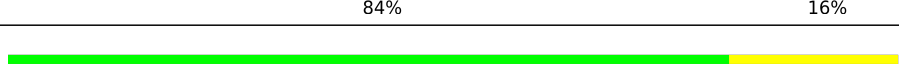
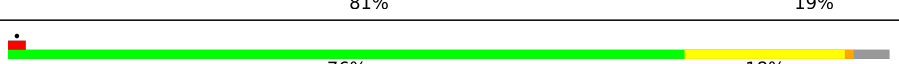

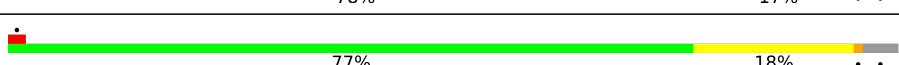
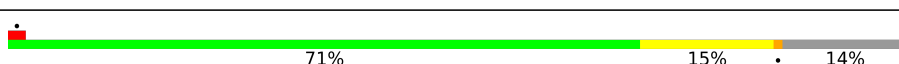
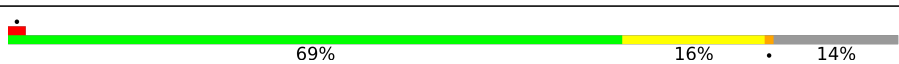
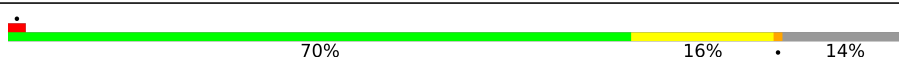


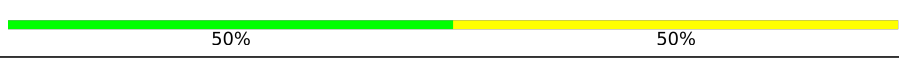
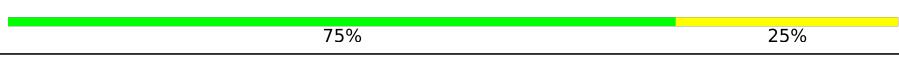


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	3	211	<p>14% (poor fit), 43% (0 outliers), 12% (1 outlier), 45% (2+ outliers)</p>
1	H	211	<p>13% (poor fit), 41% (0 outliers), 14% (1 outlier), 45% (2+ outliers)</p>
1	h	211	<p>14% (poor fit), 41% (0 outliers), 14% (1 outlier), 45% (2+ outliers)</p>
2	4	219	<p>36% (poor fit), 33% (0 outliers), 18% (1 outlier), 48% (2+ outliers)</p>

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Mol	Chain	Length	Quality of chain
2	L	219	
2	l	219	
3	5	132	
3	M	132	
3	m	132	
4	6	105	
4	N	105	
4	n	105	
5	7	102	
5	R	102	
5	r	102	
6	8	128	
6	Q	128	
6	q	128	
7	2	473	
7	C	473	
7	d	473	
8	A	153	
8	D	153	
8	c	153	
9	B	4	
9	DA	4	
9	E	4	
9	W	4	
9	X	4	

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Mol	Chain	Length	Quality of chain
9	Y	4	75% 25%
9	s	4	75% 25%
9	t	4	25% 75%
9	u	4	75% 25%
10	l	3	33% 67%
10	F	3	33% 100%
10	I	3	33% 67%
10	P	3	33% 67%
10	Z	3	33% 100%
10	b	3	33% 67%
10	i	3	33% 67%
10	v	3	33% 100%
10	x	3	33% 67%
11	0	2	100%
11	AA	2	50% 50%
11	CA	2	50% 50%
11	G	2	50% 100%
11	K	2	100%
11	O	2	100%
11	T	2	50% 50%
11	V	2	50% 50%
11	a	2	50% 100%
11	f	2	100%
11	g	2	100%
11	k	2	50% 50%

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Mol	Chain	Length	Quality of chain
11	p	2	50% 50%
11	w	2	50% 100%
11	z	2	100%
12	J	6	17% 33% 67%
12	e	6	17% 33% 67%
12	y	6	17% 33% 67%
13	9	5	100%
13	S	5	100%
13	j	5	100%
14	BA	9	11% 78% 11%
14	U	9	11% 78% 11%
14	o	9	11% 78% 11%

2 Entry composition i

There are 15 unique types of molecules in this entry. The entry contains 32325 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 vFP1.01 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3	116	930	597	154	176	3	0	0
1	H	116	930	597	154	176	3	0	0
1	h	116	930	597	154	176	3	0	0

- Molecule 2 is a protein called vFP1.01 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	113	882	560	149	170	3	0	0
2	L	113	882	560	149	170	3	0	0
2	l	113	882	560	149	170	3	0	0

- Molecule 3 is a protein called PGT122 Heavy chain.

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

- Molecule 4 is a protein called PGT122 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	105	805	504	139	160	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	105	Total	C	N	O	S	0	0
			805	504	139	160	2		
4	n	105	Total	C	N	O	S	0	0
			805	504	139	160	2		

- Molecule 5 is a protein called VRC03 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	102	Total	C	N	O	S	0	0
			802	510	137	152	3		
5	R	102	Total	C	N	O	S	0	0
			802	510	137	152	3		
5	r	102	Total	C	N	O	S	0	0
			802	510	137	152	3		

- Molecule 6 is a protein called VRC03 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		
6	Q	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		
6	q	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		

- Molecule 7 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	453	Total	C	N	O	S	0	0
			3565	2236	630	671	28		
7	2	453	Total	C	N	O	S	0	0
			3565	2236	630	671	28		
7	d	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
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
2	332	ASN	THR	conflict	UNP Q2N0S6
2	501	CYS	ALA	conflict	UNP Q2N0S6

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

- Molecule 8 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
8	A	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
8	c	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
D	605	CYS	THR	conflict	UNP Q2N0S7
A	605	CYS	THR	conflict	UNP Q2N0S7
c	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 9 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.



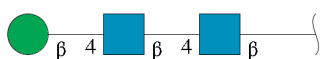
Mol	Chain	Residues	Atoms				AltConf	Trace
9	B	4	Total	C	N	O	0	0
			50	28	2	20		
9	E	4	Total	C	N	O	0	0
			50	28	2	20		
9	W	4	Total	C	N	O	0	0
			50	28	2	20		
9	X	4	Total	C	N	O	0	0
			50	28	2	20		
9	Y	4	Total	C	N	O	0	0
			50	28	2	20		
9	s	4	Total	C	N	O	0	0
			50	28	2	20		

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

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



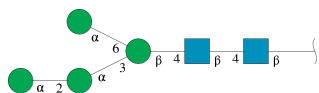
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	F	3	39	22	2	15	0	0
10	I	3	39	22	2	15	0	0
10	P	3	39	22	2	15	0	0
10	Z	3	39	22	2	15	0	0
10	b	3	39	22	2	15	0	0
10	i	3	39	22	2	15	0	0
10	v	3	39	22	2	15	0	0
10	x	3	39	22	2	15	0	0
10	1	3	39	22	2	15	0	0

- Molecule 11 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	2	28	16	2	10	0	0
11	K	2	28	16	2	10	0	0
11	O	2	28	16	2	10	0	0
11	T	2	28	16	2	10	0	0
11	V	2	28	16	2	10	0	0
11	a	2	28	16	2	10	0	0
11	f	2	28	16	2	10	0	0
11	g	2	28	16	2	10	0	0
11	k	2	28	16	2	10	0	0
11	p	2	28	16	2	10	0	0
11	w	2	28	16	2	10	0	0
11	z	2	28	16	2	10	0	0
11	0	2	28	16	2	10	0	0
11	AA	2	28	16	2	10	0	0
11	CA	2	28	16	2	10	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



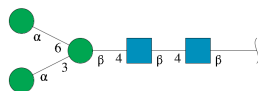
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	J	6	72	40	2	30	0	0
12	e	6	72	40	2	30	0	0

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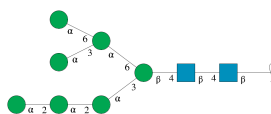
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	y	6	72	40	2	30	0	0

- Molecule 13 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.



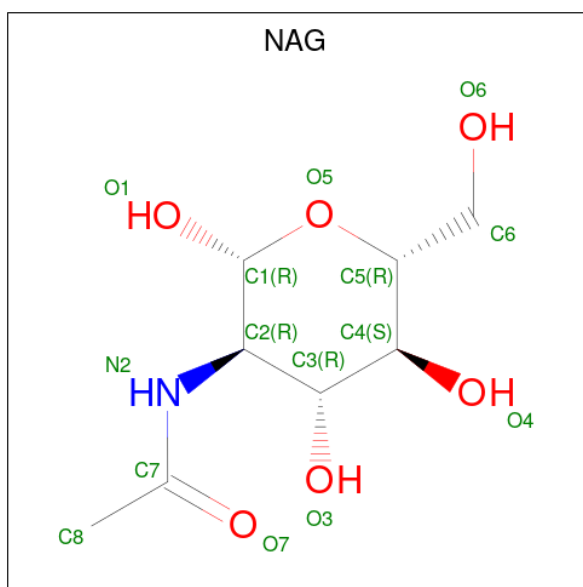
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	S	5	61	34	2	25	0	0
13	j	5	61	34	2	25	0	0
13	9	5	61	34	2	25	0	0

- Molecule 14 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
			Total	C	N	O		
14	U	9	105	58	2	45	0	0
14	o	9	105	58	2	45	0	0
14	BA	9	105	58	2	45	0	0

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

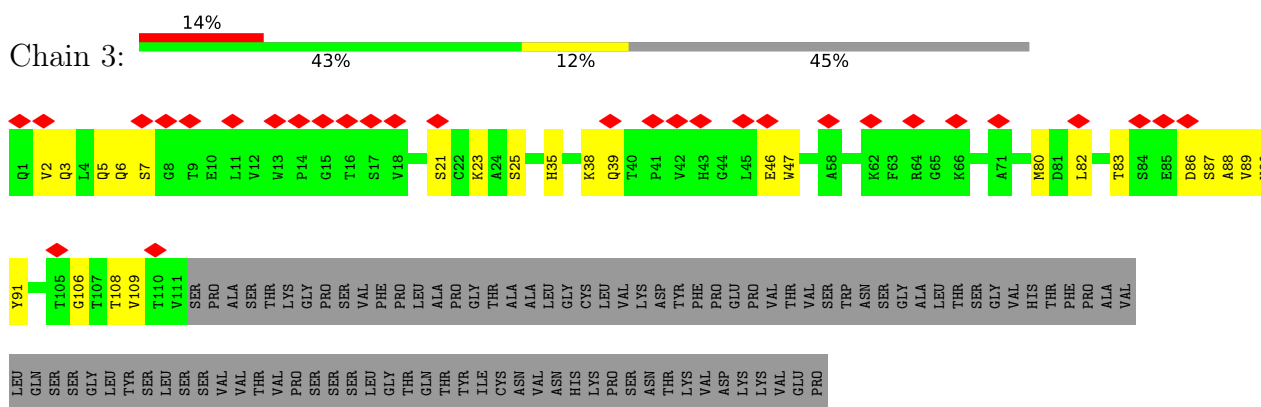


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
15	C	1	Total 14	C 8	N 1	O 5	0
15	C	1	Total 14	C 8	N 1	O 5	0
15	D	1	Total 14	C 8	N 1	O 5	0
15	2	1	Total 14	C 8	N 1	O 5	0
15	2	1	Total 14	C 8	N 1	O 5	0
15	A	1	Total 14	C 8	N 1	O 5	0
15	c	1	Total 14	C 8	N 1	O 5	0
15	d	1	Total 14	C 8	N 1	O 5	0
15	d	1	Total 14	C 8	N 1	O 5	0

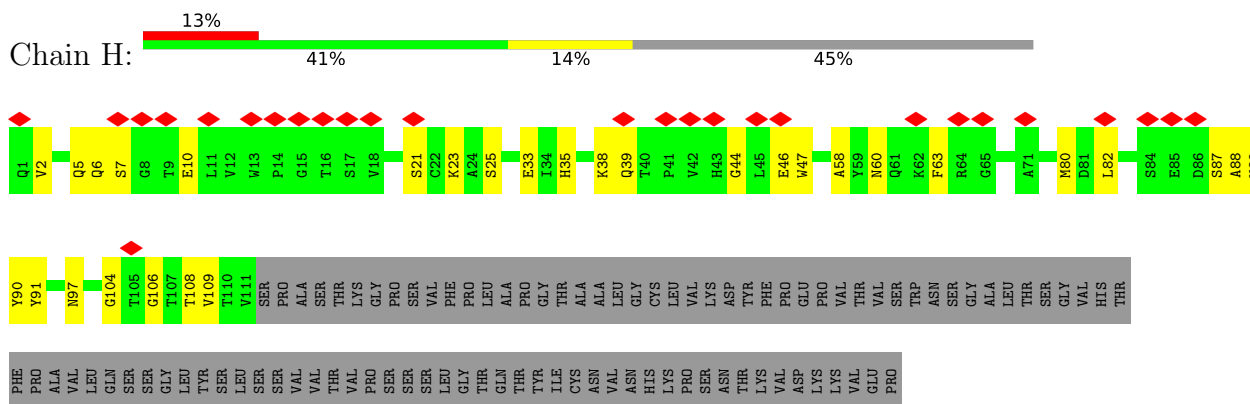
3 Residue-property plots i

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

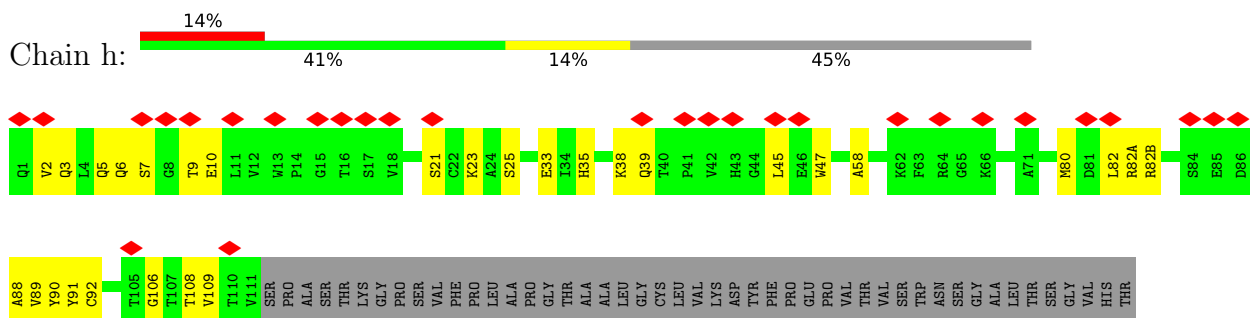
- Molecule 1: vFP1.01 heavy chain



- Molecule 1: vFP1.01 heavy chain

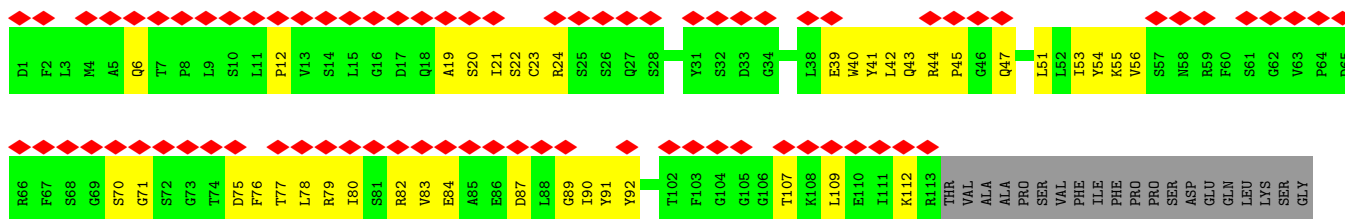
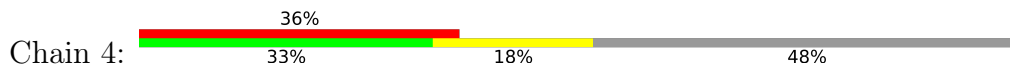


- Molecule 1: vFP1.01 heavy chain



THR PRO ALA VAL LEU GLN SER SER GLY TYR LEU SER SER SER VAL VAL THR VAL VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE ASN CYS ASN HIS PRO SER ASN THR LYS VAL ASP LYS LYS VAL VAL PRO

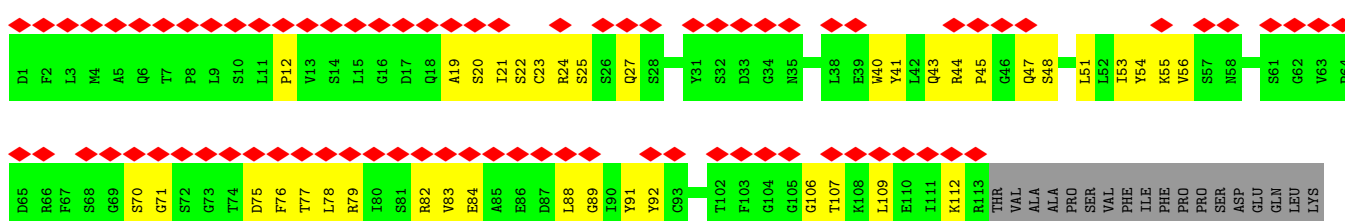
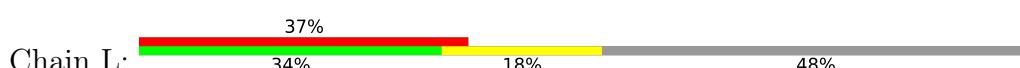
• Molecule 2: vFP1.01 Light chain



R66 F67 S68 G69 S70 G71 S72 G73 T74 D75 F76 T77 L78 R79 I80 S81 R82 V83 E84 A85 E86 D87 L88 G89 I90 Y91 Y92 T102 F103 G104 G105 G106 T107 K108 L109 E110 I111 K112 R113 THR VAL ALA PRO SER VAL PHE PHE PRO SER ASP ASP GLN LEU LEU LYS ASP THR

THR ALA VAL TYR ALA CYS VAL LEU THR ASN PHE LEU PRO ARG ALA PRO VAL THR VAL GLN TRP LYS VAL ASN ARG ALA LEU GLN SER GLY L88 C89 I90 Y91 Y92 T102 F103 G104 G105 G106 T107 K108 L109 E110 I111 K112 R113 THR VAL ALA PRO SER VAL PHE PHE PRO SER ASP ASP GLN LEU LEU LYS ASP THR

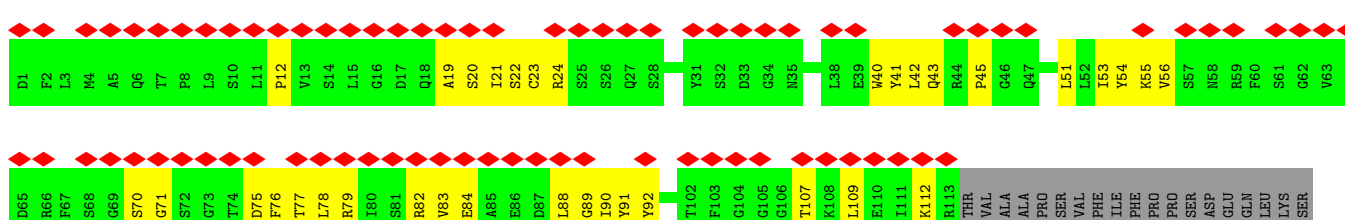
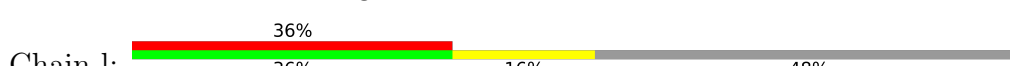
• Molecule 2: vFP1.01 Light chain



D65 R66 F67 S68 G69 S70 G71 S72 G73 T74 D75 F76 T77 L78 R79 I80 S81 R82 V83 E84 A85 E86 D87 L88 G89 I90 Y91 Y92 C93 T102 F103 G104 G105 G106 T107 K108 L109 E110 I111 K112 R113 THR VAL ALA PRO SER VAL PHE PHE PRO SER ASP ASP GLN LEU LEU LYS ASP THR

SER GLY THR ALA SER VAL VAL CYS LEU THR ASN PHE TYR PRO ARG ALA GLU VAL VAL THR LYS SER TRP LYS VAL ASN ARG ALA LEU GLN SER GLY CYS

• Molecule 2: vFP1.01 Light chain

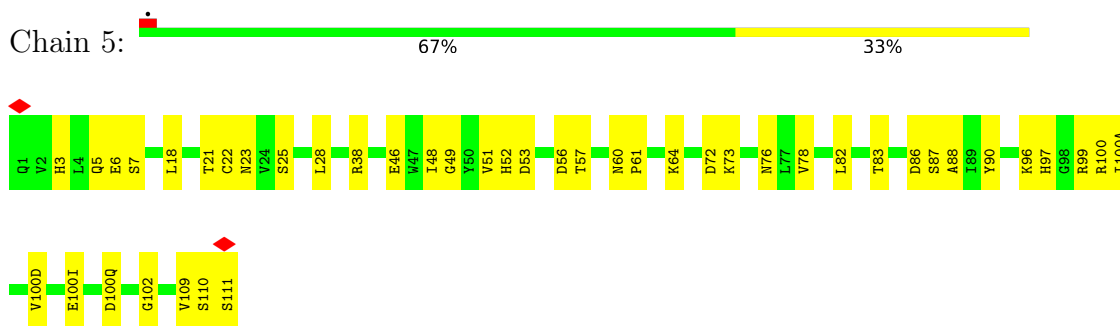


D65 R66 F67 S68 G69 S70 G71 S72 G73 T74 D75 F76 T77 L78 R79 I80 S81 R82 V83 E84 A85 E86 D87 L88 G89 I90 Y91 Y92 T102 F103 G104 G105 G106 T107 K108 L109 E110 I111 K112 R113 THR VAL ALA PRO SER VAL PHE PHE PRO SER ASP ASP GLN LEU LEU LYS ASP THR

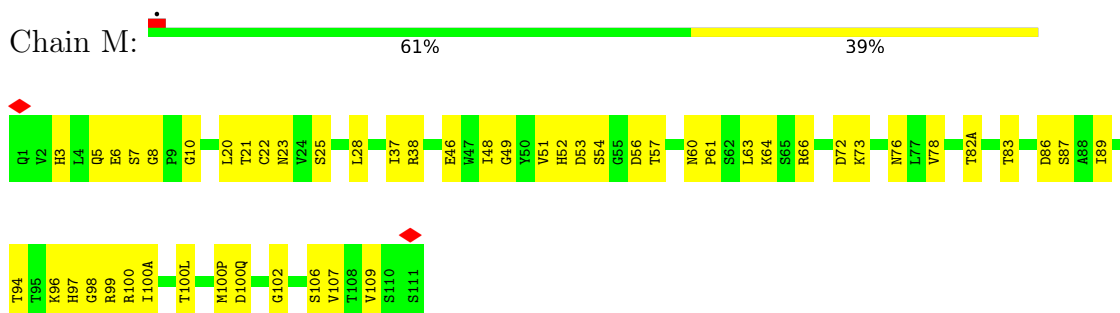
GLY THR ALA SER VAL VAL CYS LEU THR ASN PHE TYR PRO ARG ALA GLU VAL VAL THR LYS SER TRP LYS VAL ASN ARG ALA LEU GLN SER GLY CYS

LYS HIS VAL TYR ALA CYS VAL LEU THR HIS GLN PHE PRO VAL THR LYS SER PHE ASN ARG ALA LEU GLN CYS

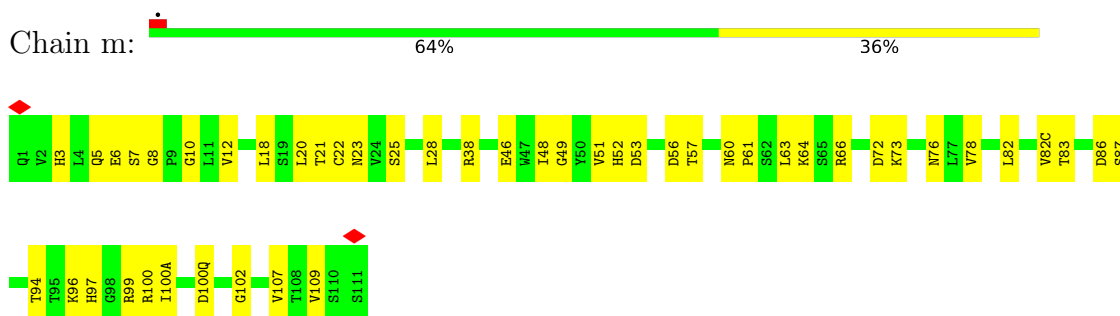
• Molecule 3: PGT122 Heavy chain



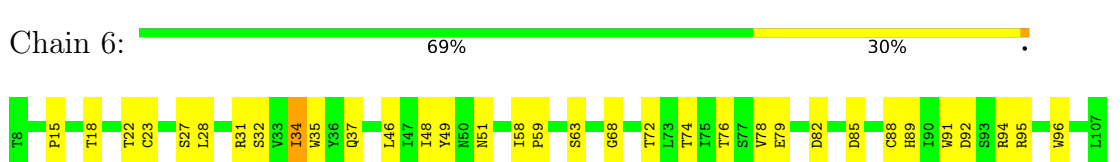
• Molecule 3: PGT122 Heavy chain



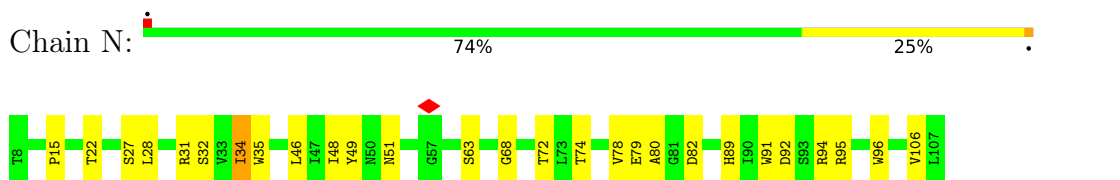
• Molecule 3: PGT122 Heavy chain



• Molecule 4: PGT122 light chain



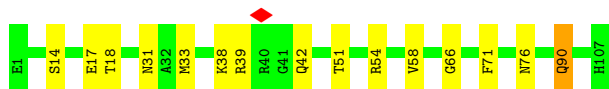
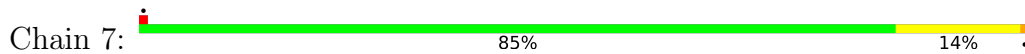
• Molecule 4: PGT122 light chain



• Molecule 4: PGT122 light chain



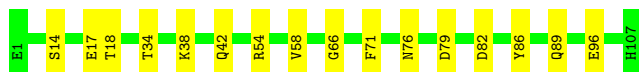
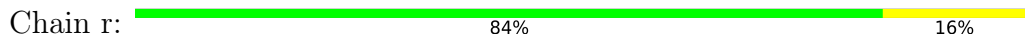
• Molecule 5: VRC03 light chain



• Molecule 5: VRC03 light chain



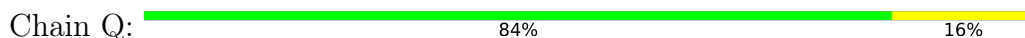
• Molecule 5: VRC03 light chain



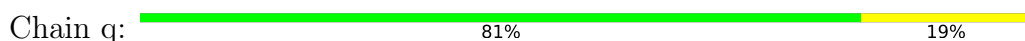
• Molecule 6: VRC03 heavy chain

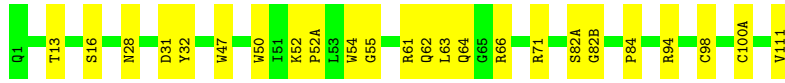


• Molecule 6: VRC03 heavy chain

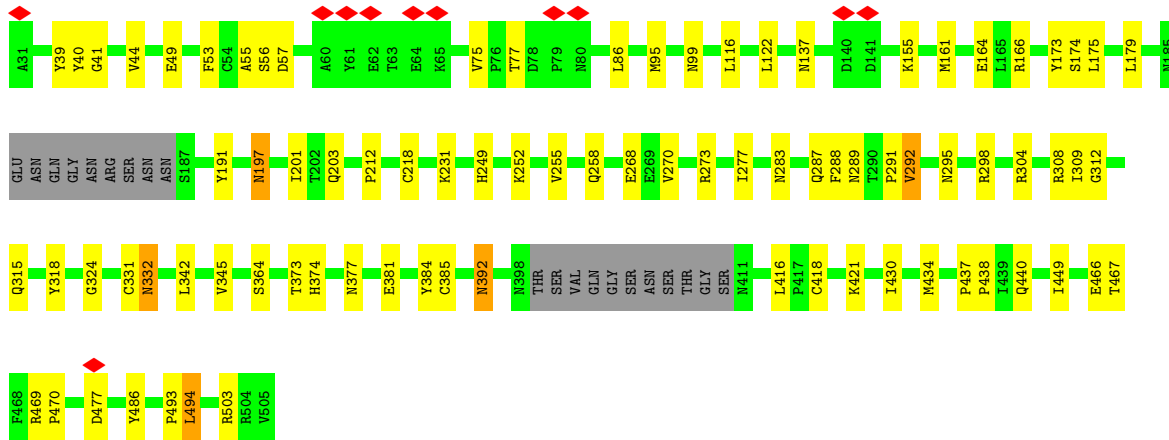
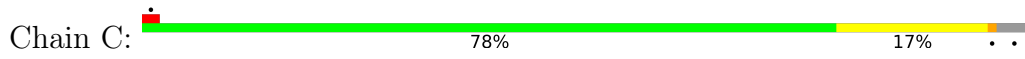


• Molecule 6: VRC03 heavy chain

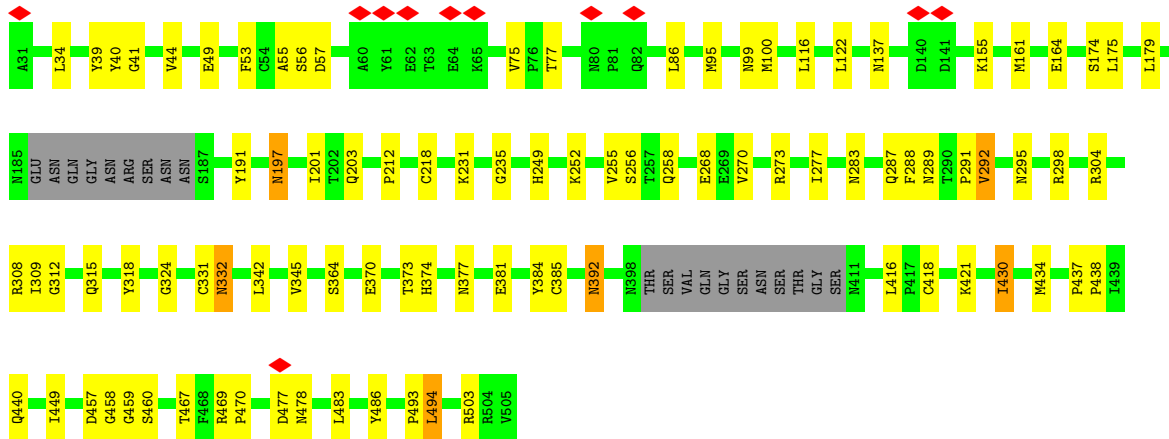
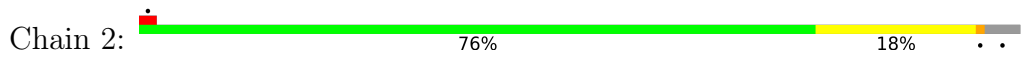




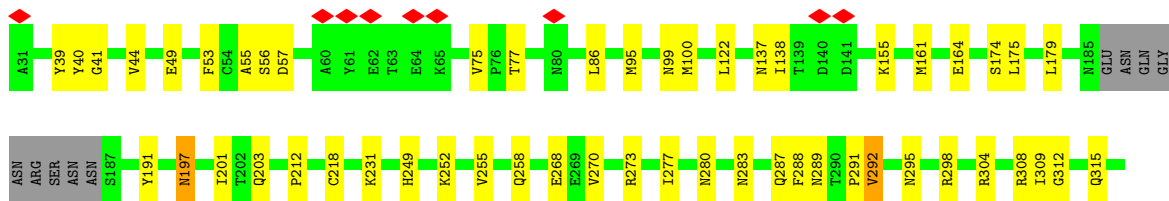
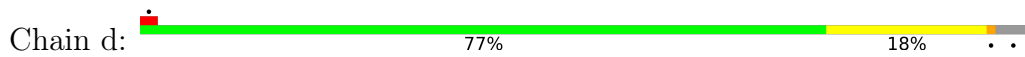
• Molecule 7: Envelope glycoprotein gp120

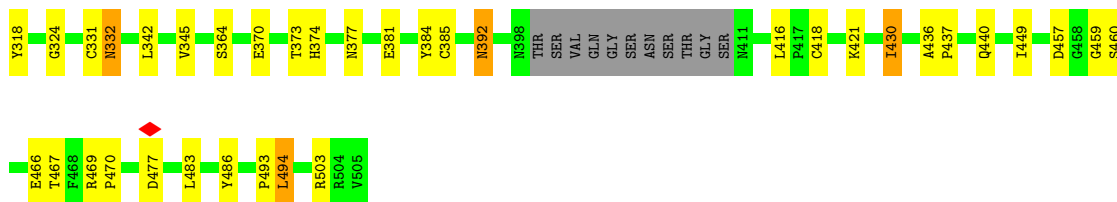


• Molecule 7: Envelope glycoprotein gp120

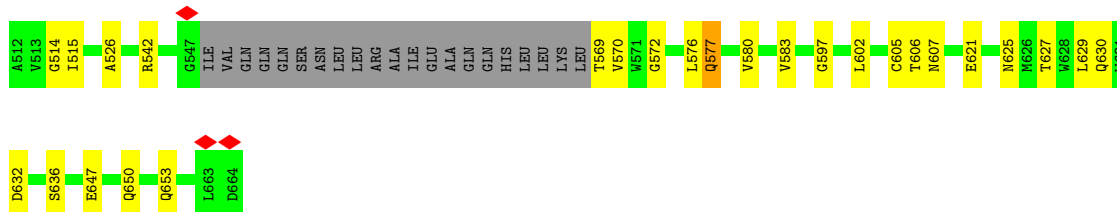


• Molecule 7: Envelope glycoprotein gp120

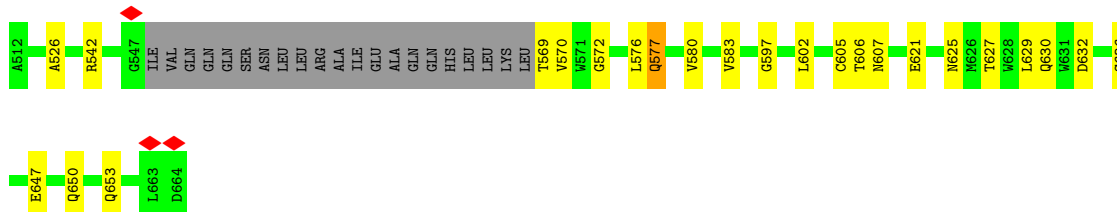




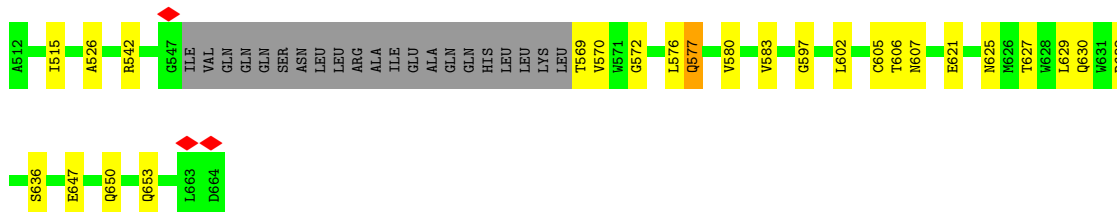
• Molecule 8: Envelope glycoprotein gp41



• Molecule 8: Envelope glycoprotein gp41



• Molecule 8: Envelope glycoprotein gp41



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




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

Chain E:  50% 50%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: 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 W:  75% 25%

MAG1
MAG2
BMA3
MAN4

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

Chain Y:  75% 25%

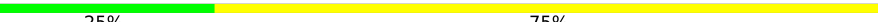
MAG1
MAG2
BMA3
MAN4

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

Chain s:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: 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:  25% 75%


MAG1
MAG2
BMA3
MAN4

- Molecule 9: 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 u:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: 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 DA:  75% 25%



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

Chain F:  33% 100%

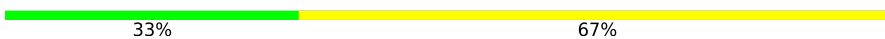


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%



- Molecule 10: 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%

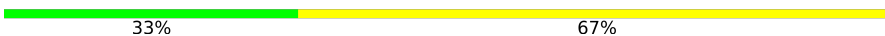


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  33% 100%

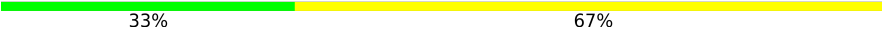


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  33% 67%



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

Chain i:  33% 67%


NAG1
NAG2
BMA3

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

Chain v:  33% 100%


NAG1
NAG2
BMA3

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

Chain x:  33% 67%


NAG1
NAG2
BMA3

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

Chain 1:  33% 67%


NAG1
NAG2
BMA3

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

Chain G:  50% 100%


NAG1
NAG2

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

Chain K:  100%


NAG1
NAG2

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

Chain O:  100%



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

Chain T:



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

Chain V:



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

Chain a:



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

Chain f:



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

Chain g:



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

Chain k:



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

Chain p:  50% 50%



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

Chain w:  50% 100%



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

Chain z:  100%



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

Chain 0:  100%



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

Chain AA:  50% 50% 50%



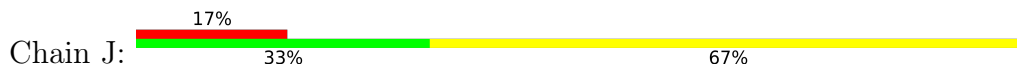
- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:  50% 50%



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-aceta

mido-2-deoxy-beta-D-glucopyranose



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



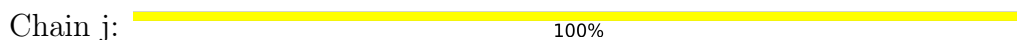
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

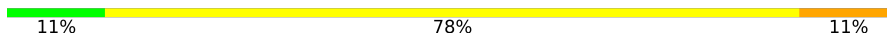


- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  11% 78% 11%

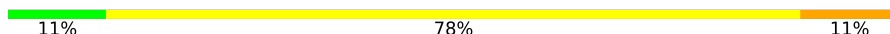
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 14: 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 o:  11% 78% 11%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 14: 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 BA:  11% 78% 11%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	44652	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 ($e^-/\text{\AA}^2$)	70.28	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.565	Depositor
Minimum map value	-1.291	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	1	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	3	0.21	0/956	0.49	0/1305
1	H	0.22	0/956	0.47	0/1305
1	h	0.22	0/956	0.47	0/1305
2	4	0.22	0/903	0.52	0/1221
2	L	0.22	0/903	0.51	0/1221
2	l	0.22	0/903	0.52	0/1221
3	5	0.27	0/1076	0.54	0/1465
3	M	0.27	0/1076	0.53	0/1465
3	m	0.26	0/1076	0.53	0/1465
4	6	0.29	0/826	0.48	0/1130
4	N	0.29	0/826	0.49	0/1130
4	n	0.29	0/826	0.48	0/1130
5	7	0.30	0/820	0.57	0/1107
5	R	0.30	0/820	0.58	0/1107
5	r	0.30	0/820	0.56	0/1107
6	8	0.37	0/1056	0.51	0/1439
6	Q	0.37	0/1056	0.49	0/1439
6	q	0.36	0/1056	0.48	0/1439
7	2	0.37	0/3639	0.59	1/4941 (0.0%)
7	C	0.37	0/3639	0.59	1/4941 (0.0%)
7	d	0.37	0/3639	0.59	1/4941 (0.0%)
8	A	0.37	0/1052	0.64	0/1427
8	D	0.37	0/1052	0.64	0/1427
8	c	0.37	0/1052	0.64	0/1427
All	All	0.33	0/30984	0.56	3/42105 (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
2	4	0	1
2	L	0	1
2	1	0	1
5	7	0	1
5	R	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	2	494	LEU	CA-CB-CG	5.22	134.56	116.30
7	d	494	LEU	CA-CB-CG	5.21	134.54	116.30
7	C	494	LEU	CA-CB-CG	5.21	134.53	116.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	55	LYS	Peptide
5	7	90	GLN	Peptide
2	L	55	LYS	Peptide
5	R	90	GLN	Peptide
2	1	55	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	930	0	900	15	0
1	H	930	0	900	20	0
1	h	930	0	900	21	0
2	4	882	0	860	28	0
2	L	882	0	860	28	0
2	1	882	0	860	26	0
3	5	1047	0	1026	24	0
3	M	1047	0	1026	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	m	1047	0	1026	27	0
4	6	805	0	761	21	0
4	N	805	0	761	17	0
4	n	805	0	761	23	0
5	7	802	0	780	8	0
5	R	802	0	780	6	0
5	r	802	0	780	9	0
6	8	1023	0	971	24	0
6	Q	1023	0	971	14	0
6	q	1023	0	971	19	0
7	2	3565	0	3494	83	0
7	C	3565	0	3494	74	0
7	d	3565	0	3494	80	0
8	A	1034	0	1014	18	0
8	D	1034	0	1014	19	0
8	c	1034	0	1014	19	0
9	B	50	0	43	0	0
9	DA	50	0	43	0	0
9	E	50	0	43	1	0
9	W	50	0	43	0	0
9	X	50	0	43	0	0
9	Y	50	0	43	0	0
9	s	50	0	43	0	0
9	t	50	0	43	0	0
9	u	50	0	43	0	0
10	l	39	0	34	0	0
10	F	39	0	34	0	0
10	I	39	0	34	1	0
10	P	39	0	34	0	0
10	Z	39	0	34	0	0
10	b	39	0	34	1	0
10	i	39	0	34	0	0
10	v	39	0	34	0	0
10	x	39	0	34	1	0
11	0	28	0	25	0	0
11	AA	28	0	25	1	0
11	CA	28	0	25	1	0
11	G	28	0	25	0	0
11	K	28	0	25	6	0
11	O	28	0	25	0	0
11	T	28	0	25	1	0
11	V	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	a	28	0	25	0	0
11	f	28	0	25	6	0
11	g	28	0	25	0	0
11	k	28	0	25	1	0
11	p	28	0	25	1	0
11	w	28	0	25	0	0
11	z	28	0	25	6	0
12	J	72	0	61	0	0
12	e	72	0	61	0	0
12	y	72	0	61	0	0
13	9	61	0	52	1	0
13	S	61	0	52	1	0
13	j	61	0	52	1	0
14	BA	105	0	88	1	0
14	U	105	0	88	2	0
14	o	105	0	88	1	0
15	2	28	0	25	0	0
15	A	14	0	13	0	0
15	C	28	0	25	0	0
15	D	14	0	13	0	0
15	c	14	0	13	0	0
15	d	28	0	25	0	0
All	All	32325	0	31203	590	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 590 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:295:ASN:HD21	11:f:1:NAG:C1	1.28	1.47
7:C:295:ASN:HD21	11:K:1:NAG:C1	1.28	1.47
7:d:295:ASN:HD21	11:z:1:NAG:C1	1.28	1.46
7:C:295:ASN:ND2	11:K:1:NAG:C1	1.85	1.39
7:d:295:ASN:ND2	11:z:1:NAG:C1	1.85	1.36

There are no symmetry-related clashes.

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	3	114/211 (54%)	106 (93%)	8 (7%)	0	100	100
1	H	114/211 (54%)	107 (94%)	7 (6%)	0	100	100
1	h	114/211 (54%)	105 (92%)	9 (8%)	0	100	100
2	4	111/219 (51%)	103 (93%)	7 (6%)	1 (1%)	14	48
2	L	111/219 (51%)	103 (93%)	7 (6%)	1 (1%)	14	48
2	l	111/219 (51%)	103 (93%)	7 (6%)	1 (1%)	14	48
3	5	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
3	M	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
3	m	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
4	6	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
4	N	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
4	n	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
5	7	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
5	R	100/102 (98%)	91 (91%)	9 (9%)	0	100	100
5	r	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
6	8	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
6	Q	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
6	q	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
7	2	447/473 (94%)	413 (92%)	34 (8%)	0	100	100
7	C	447/473 (94%)	413 (92%)	34 (8%)	0	100	100
7	d	447/473 (94%)	413 (92%)	34 (8%)	0	100	100
8	A	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
8	D	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
8	c	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
All	All	3777/4569 (83%)	3497 (93%)	277 (7%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	56	VAL
2	1	56	VAL
2	L	56	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	100/182 (55%)	100 (100%)	0	100	100
1	H	100/182 (55%)	100 (100%)	0	100	100
1	h	100/182 (55%)	100 (100%)	0	100	100
2	4	98/193 (51%)	98 (100%)	0	100	100
2	L	98/193 (51%)	98 (100%)	0	100	100
2	l	98/193 (51%)	98 (100%)	0	100	100
3	5	116/116 (100%)	116 (100%)	0	100	100
3	M	116/116 (100%)	116 (100%)	0	100	100
3	m	116/116 (100%)	116 (100%)	0	100	100
4	6	88/88 (100%)	87 (99%)	1 (1%)	65	74
4	N	88/88 (100%)	87 (99%)	1 (1%)	65	74
4	n	88/88 (100%)	87 (99%)	1 (1%)	65	74
5	7	86/86 (100%)	86 (100%)	0	100	100
5	R	86/86 (100%)	86 (100%)	0	100	100
5	r	86/86 (100%)	86 (100%)	0	100	100
6	8	108/108 (100%)	108 (100%)	0	100	100
6	Q	108/108 (100%)	108 (100%)	0	100	100
6	q	108/108 (100%)	108 (100%)	0	100	100
7	2	404/421 (96%)	397 (98%)	7 (2%)	53	68
7	C	404/421 (96%)	397 (98%)	7 (2%)	53	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	d	404/421 (96%)	397 (98%)	7 (2%)	53	68
8	A	110/129 (85%)	109 (99%)	1 (1%)	70	76
8	D	110/129 (85%)	109 (99%)	1 (1%)	70	76
8	c	110/129 (85%)	109 (99%)	1 (1%)	70	76
All	All	3330/3969 (84%)	3303 (99%)	27 (1%)	70	77

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	2	332	ASN
7	2	430	ILE
7	d	392	ASN
7	2	416	LEU
8	A	577	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
8	A	611	ASN
8	A	630	GLN
7	d	289	ASN
8	D	630	GLN
8	D	611	ASN

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](#)

153 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
11	NAG	0	1	7,11	14,14,15	0.21	0	17,19,21	0.58	0
11	NAG	0	2	11	14,14,15	0.22	0	17,19,21	0.49	0
10	NAG	1	1	7,10	14,14,15	0.51	0	17,19,21	0.49	0
10	NAG	1	2	10	14,14,15	0.17	0	17,19,21	0.68	1 (5%)
10	BMA	1	3	10	11,11,12	1.17	1 (9%)	15,15,17	1.22	2 (13%)
13	NAG	9	1	7,13	14,14,15	0.29	0	17,19,21	0.55	0
13	NAG	9	2	13	14,14,15	0.40	0	17,19,21	1.16	1 (5%)
13	BMA	9	3	13	11,11,12	0.75	0	15,15,17	1.03	2 (13%)
13	MAN	9	4	13	11,11,12	0.80	0	15,15,17	0.94	2 (13%)
13	MAN	9	5	13	11,11,12	0.79	0	15,15,17	0.96	2 (13%)
11	NAG	AA	1	7,11	14,14,15	0.44	0	17,19,21	0.69	0
11	NAG	AA	2	11	14,14,15	0.49	0	17,19,21	0.57	0
9	NAG	B	1	9,7	14,14,15	0.27	0	17,19,21	0.47	0
9	NAG	B	2	9	14,14,15	0.38	0	17,19,21	1.12	2 (11%)
9	BMA	B	3	9	11,11,12	0.75	0	15,15,17	1.54	1 (6%)
9	MAN	B	4	9	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
14	NAG	BA	1	7,14	14,14,15	0.32	0	17,19,21	0.56	0
14	NAG	BA	2	14	14,14,15	0.38	0	17,19,21	1.25	2 (11%)
14	BMA	BA	3	14	11,11,12	1.07	1 (9%)	15,15,17	1.24	2 (13%)
14	MAN	BA	4	14	11,11,12	0.55	0	15,15,17	1.40	2 (13%)
14	MAN	BA	5	14	11,11,12	0.73	0	15,15,17	1.31	2 (13%)
14	MAN	BA	6	14	11,11,12	0.84	0	15,15,17	1.14	2 (13%)
14	MAN	BA	7	14	11,11,12	0.69	0	15,15,17	1.17	2 (13%)
14	MAN	BA	8	14	11,11,12	0.71	0	15,15,17	1.00	2 (13%)
14	MAN	BA	9	14	11,11,12	0.87	0	15,15,17	0.99	2 (13%)
11	NAG	CA	1	7,11	14,14,15	0.32	0	17,19,21	1.05	1 (5%)
11	NAG	CA	2	11	14,14,15	0.26	0	17,19,21	0.56	0
9	NAG	DA	1	9,7	14,14,15	0.56	0	17,19,21	0.57	0
9	NAG	DA	2	9	14,14,15	0.32	0	17,19,21	0.81	0
9	BMA	DA	3	9	11,11,12	1.14	0	15,15,17	0.91	0
9	MAN	DA	4	9	11,11,12	0.79	1 (9%)	15,15,17	1.28	2 (13%)
9	NAG	E	1	9,7	14,14,15	0.41	0	17,19,21	0.46	0
9	NAG	E	2	9	14,14,15	0.33	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BMA	E	3	9	11,11,12	0.63	0	15,15,17	0.86	0
9	MAN	E	4	9	11,11,12	0.81	0	15,15,17	0.95	2 (13%)
10	NAG	F	1	7,10	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
10	NAG	F	2	10	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
10	BMA	F	3	10	11,11,12	0.77	0	15,15,17	0.83	1 (6%)
11	NAG	G	1	7,11	14,14,15	0.24	0	17,19,21	0.64	0
11	NAG	G	2	11	14,14,15	0.36	0	17,19,21	0.39	0
10	NAG	I	1	7,10	14,14,15	0.44	0	17,19,21	0.52	0
10	NAG	I	2	10	14,14,15	0.26	0	17,19,21	0.59	0
10	BMA	I	3	10	11,11,12	0.57	0	15,15,17	1.13	1 (6%)
12	NAG	J	1	12,7	14,14,15	0.31	0	17,19,21	0.58	0
12	NAG	J	2	12	14,14,15	0.21	0	17,19,21	0.49	0
12	BMA	J	3	12	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
12	MAN	J	4	12	11,11,12	0.80	1 (9%)	15,15,17	1.49	3 (20%)
12	MAN	J	5	12	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
12	MAN	J	6	12	11,11,12	0.70	0	15,15,17	1.28	2 (13%)
11	NAG	K	1	11	14,14,15	0.36	0	17,19,21	0.68	0
11	NAG	K	2	11	14,14,15	0.40	0	17,19,21	0.60	1 (5%)
11	NAG	O	1	7,11	14,14,15	0.21	0	17,19,21	0.57	0
11	NAG	O	2	11	14,14,15	0.22	0	17,19,21	0.50	0
10	NAG	P	1	7,10	14,14,15	0.50	0	17,19,21	0.50	0
10	NAG	P	2	10	14,14,15	0.18	0	17,19,21	0.67	1 (5%)
10	BMA	P	3	10	11,11,12	1.17	1 (9%)	15,15,17	1.21	2 (13%)
13	NAG	S	1	7,13	14,14,15	0.29	0	17,19,21	0.56	0
13	NAG	S	2	13	14,14,15	0.39	0	17,19,21	1.16	1 (5%)
13	BMA	S	3	13	11,11,12	0.73	0	15,15,17	1.03	2 (13%)
13	MAN	S	4	13	11,11,12	0.80	0	15,15,17	0.94	2 (13%)
13	MAN	S	5	13	11,11,12	0.78	0	15,15,17	0.95	2 (13%)
11	NAG	T	1	7,11	14,14,15	0.44	0	17,19,21	0.69	0
11	NAG	T	2	11	14,14,15	0.48	0	17,19,21	0.57	0
14	NAG	U	1	7,14	14,14,15	0.31	0	17,19,21	0.56	0
14	NAG	U	2	14	14,14,15	0.38	0	17,19,21	1.25	2 (11%)
14	BMA	U	3	14	11,11,12	1.08	1 (9%)	15,15,17	1.24	2 (13%)
14	MAN	U	4	14	11,11,12	0.56	0	15,15,17	1.40	2 (13%)
14	MAN	U	5	14	11,11,12	0.72	0	15,15,17	1.30	2 (13%)
14	MAN	U	6	14	11,11,12	0.84	0	15,15,17	1.14	2 (13%)
14	MAN	U	7	14	11,11,12	0.70	0	15,15,17	1.18	2 (13%)
14	MAN	U	8	14	11,11,12	0.71	0	15,15,17	0.99	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	MAN	U	9	14	11,11,12	0.88	0	15,15,17	0.99	2 (13%)
11	NAG	V	1	7,11	14,14,15	0.31	0	17,19,21	1.06	1 (5%)
11	NAG	V	2	11	14,14,15	0.25	0	17,19,21	0.56	0
9	NAG	W	1	9,7	14,14,15	0.56	0	17,19,21	0.56	0
9	NAG	W	2	9	14,14,15	0.32	0	17,19,21	0.81	0
9	BMA	W	3	9	11,11,12	1.14	0	15,15,17	0.91	0
9	MAN	W	4	9	11,11,12	0.79	1 (9%)	15,15,17	1.27	2 (13%)
9	NAG	X	1	9,7	14,14,15	0.27	0	17,19,21	0.46	0
9	NAG	X	2	9	14,14,15	0.38	0	17,19,21	1.12	2 (11%)
9	BMA	X	3	9	11,11,12	0.76	0	15,15,17	1.53	1 (6%)
9	MAN	X	4	9	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
9	NAG	Y	1	9,7	14,14,15	0.41	0	17,19,21	0.46	0
9	NAG	Y	2	9	14,14,15	0.33	0	17,19,21	0.63	0
9	BMA	Y	3	9	11,11,12	0.63	0	15,15,17	0.86	0
9	MAN	Y	4	9	11,11,12	0.81	0	15,15,17	0.95	2 (13%)
10	NAG	Z	1	7,10	14,14,15	0.51	0	17,19,21	1.02	1 (5%)
10	NAG	Z	2	10	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
10	BMA	Z	3	10	11,11,12	0.78	0	15,15,17	0.83	1 (6%)
11	NAG	a	1	7,11	14,14,15	0.24	0	17,19,21	0.63	0
11	NAG	a	2	11	14,14,15	0.37	0	17,19,21	0.39	0
10	NAG	b	1	7,10	14,14,15	0.42	0	17,19,21	0.52	0
10	NAG	b	2	10	14,14,15	0.26	0	17,19,21	0.59	0
10	BMA	b	3	10	11,11,12	0.58	0	15,15,17	1.12	1 (6%)
12	NAG	e	1	12,7	14,14,15	0.30	0	17,19,21	0.58	0
12	NAG	e	2	12	14,14,15	0.21	0	17,19,21	0.48	0
12	BMA	e	3	12	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
12	MAN	e	4	12	11,11,12	0.80	1 (9%)	15,15,17	1.49	3 (20%)
12	MAN	e	5	12	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
12	MAN	e	6	12	11,11,12	0.70	0	15,15,17	1.28	2 (13%)
11	NAG	f	1	11	14,14,15	0.36	0	17,19,21	0.68	0
11	NAG	f	2	11	14,14,15	0.40	0	17,19,21	0.60	1 (5%)
11	NAG	g	1	7,11	14,14,15	0.19	0	17,19,21	0.57	0
11	NAG	g	2	11	14,14,15	0.22	0	17,19,21	0.50	0
10	NAG	i	1	7,10	14,14,15	0.50	0	17,19,21	0.50	0
10	NAG	i	2	10	14,14,15	0.18	0	17,19,21	0.67	1 (5%)
10	BMA	i	3	10	11,11,12	1.16	1 (9%)	15,15,17	1.21	2 (13%)
13	NAG	j	1	7,13	14,14,15	0.29	0	17,19,21	0.55	0
13	NAG	j	2	13	14,14,15	0.39	0	17,19,21	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BMA	j	3	13	11,11,12	0.74	0	15,15,17	1.02	2 (13%)
13	MAN	j	4	13	11,11,12	0.80	0	15,15,17	0.94	2 (13%)
13	MAN	j	5	13	11,11,12	0.78	0	15,15,17	0.96	2 (13%)
11	NAG	k	1	7,11	14,14,15	0.43	0	17,19,21	0.68	0
11	NAG	k	2	11	14,14,15	0.49	0	17,19,21	0.57	0
14	NAG	o	1	7,14	14,14,15	0.32	0	17,19,21	0.56	0
14	NAG	o	2	14	14,14,15	0.37	0	17,19,21	1.26	2 (11%)
14	BMA	o	3	14	11,11,12	1.08	1 (9%)	15,15,17	1.25	2 (13%)
14	MAN	o	4	14	11,11,12	0.56	0	15,15,17	1.41	2 (13%)
14	MAN	o	5	14	11,11,12	0.73	0	15,15,17	1.30	2 (13%)
14	MAN	o	6	14	11,11,12	0.83	0	15,15,17	1.13	2 (13%)
14	MAN	o	7	14	11,11,12	0.69	0	15,15,17	1.19	2 (13%)
14	MAN	o	8	14	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
14	MAN	o	9	14	11,11,12	0.88	0	15,15,17	0.99	2 (13%)
11	NAG	p	1	7,11	14,14,15	0.31	0	17,19,21	1.05	1 (5%)
11	NAG	p	2	11	14,14,15	0.26	0	17,19,21	0.55	0
9	NAG	s	1	9,7	14,14,15	0.57	0	17,19,21	0.57	0
9	NAG	s	2	9	14,14,15	0.33	0	17,19,21	0.81	0
9	BMA	s	3	9	11,11,12	1.14	0	15,15,17	0.91	0
9	MAN	s	4	9	11,11,12	0.79	1 (9%)	15,15,17	1.28	2 (13%)
9	NAG	t	1	9,7	14,14,15	0.27	0	17,19,21	0.46	0
9	NAG	t	2	9	14,14,15	0.38	0	17,19,21	1.12	2 (11%)
9	BMA	t	3	9	11,11,12	0.75	0	15,15,17	1.53	1 (6%)
9	MAN	t	4	9	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
9	NAG	u	1	9,7	14,14,15	0.40	0	17,19,21	0.47	0
9	NAG	u	2	9	14,14,15	0.33	0	17,19,21	0.63	0
9	BMA	u	3	9	11,11,12	0.64	0	15,15,17	0.86	0
9	MAN	u	4	9	11,11,12	0.81	0	15,15,17	0.95	2 (13%)
10	NAG	v	1	7,10	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
10	NAG	v	2	10	14,14,15	0.26	0	17,19,21	0.74	1 (5%)
10	BMA	v	3	10	11,11,12	0.77	0	15,15,17	0.83	1 (6%)
11	NAG	w	1	7,11	14,14,15	0.26	0	17,19,21	0.64	0
11	NAG	w	2	11	14,14,15	0.38	0	17,19,21	0.39	0
10	NAG	x	1	7,10	14,14,15	0.45	0	17,19,21	0.52	0
10	NAG	x	2	10	14,14,15	0.25	0	17,19,21	0.59	0
10	BMA	x	3	10	11,11,12	0.57	0	15,15,17	1.13	1 (6%)
12	NAG	y	1	12,7	14,14,15	0.31	0	17,19,21	0.59	0
12	NAG	y	2	12	14,14,15	0.21	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	BMA	y	3	12	11,11,12	0.78	0	15,15,17	1.15	2 (13%)
12	MAN	y	4	12	11,11,12	0.80	1 (9%)	15,15,17	1.50	3 (20%)
12	MAN	y	5	12	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
12	MAN	y	6	12	11,11,12	0.71	0	15,15,17	1.28	2 (13%)
11	NAG	z	1	11	14,14,15	0.37	0	17,19,21	0.69	0
11	NAG	z	2	11	14,14,15	0.40	0	17,19,21	0.60	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
11	NAG	0	1	7,11	-	1/6/23/26	0/1/1/1
11	NAG	0	2	11	-	2/6/23/26	0/1/1/1
10	NAG	1	1	7,10	-	0/6/23/26	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
13	NAG	9	1	7,13	-	2/6/23/26	0/1/1/1
13	NAG	9	2	13	-	2/6/23/26	0/1/1/1
13	BMA	9	3	13	-	0/2/19/22	0/1/1/1
13	MAN	9	4	13	-	0/2/19/22	0/1/1/1
13	MAN	9	5	13	-	0/2/19/22	0/1/1/1
11	NAG	AA	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	AA	2	11	-	2/6/23/26	0/1/1/1
9	NAG	B	1	9,7	-	2/6/23/26	0/1/1/1
9	NAG	B	2	9	-	2/6/23/26	0/1/1/1
9	BMA	B	3	9	-	2/2/19/22	0/1/1/1
9	MAN	B	4	9	-	2/2/19/22	0/1/1/1
14	NAG	BA	1	7,14	-	2/6/23/26	0/1/1/1
14	NAG	BA	2	14	-	2/6/23/26	0/1/1/1
14	BMA	BA	3	14	-	0/2/19/22	0/1/1/1
14	MAN	BA	4	14	-	2/2/19/22	0/1/1/1
14	MAN	BA	5	14	-	2/2/19/22	0/1/1/1
14	MAN	BA	6	14	-	0/2/19/22	0/1/1/1
14	MAN	BA	7	14	-	2/2/19/22	0/1/1/1
14	MAN	BA	8	14	-	2/2/19/22	0/1/1/1
14	MAN	BA	9	14	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	CA	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	CA	2	11	-	2/6/23/26	0/1/1/1
9	NAG	DA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	DA	2	9	-	2/6/23/26	0/1/1/1
9	BMA	DA	3	9	-	2/2/19/22	0/1/1/1
9	MAN	DA	4	9	-	0/2/19/22	0/1/1/1
9	NAG	E	1	9,7	-	1/6/23/26	0/1/1/1
9	NAG	E	2	9	-	2/6/23/26	0/1/1/1
9	BMA	E	3	9	-	0/2/19/22	0/1/1/1
9	MAN	E	4	9	-	1/2/19/22	0/1/1/1
10	NAG	F	1	7,10	-	2/6/23/26	0/1/1/1
10	NAG	F	2	10	-	2/6/23/26	0/1/1/1
10	BMA	F	3	10	-	0/2/19/22	0/1/1/1
11	NAG	G	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	G	2	11	-	0/6/23/26	0/1/1/1
10	NAG	I	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	2/2/19/22	0/1/1/1
12	NAG	J	1	12,7	-	2/6/23/26	0/1/1/1
12	NAG	J	2	12	-	2/6/23/26	0/1/1/1
12	BMA	J	3	12	-	2/2/19/22	0/1/1/1
12	MAN	J	4	12	-	2/2/19/22	0/1/1/1
12	MAN	J	5	12	-	0/2/19/22	0/1/1/1
12	MAN	J	6	12	-	2/2/19/22	0/1/1/1
11	NAG	K	1	11	-	2/6/23/26	0/1/1/1
11	NAG	K	2	11	-	0/6/23/26	0/1/1/1
11	NAG	O	1	7,11	-	1/6/23/26	0/1/1/1
11	NAG	O	2	11	-	2/6/23/26	0/1/1/1
10	NAG	P	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	BMA	P	3	10	-	1/2/19/22	0/1/1/1
13	NAG	S	1	7,13	-	2/6/23/26	0/1/1/1
13	NAG	S	2	13	-	2/6/23/26	0/1/1/1
13	BMA	S	3	13	-	0/2/19/22	0/1/1/1
13	MAN	S	4	13	-	0/2/19/22	0/1/1/1
13	MAN	S	5	13	-	0/2/19/22	0/1/1/1
11	NAG	T	1	7,11	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	T	2	11	-	2/6/23/26	0/1/1/1
14	NAG	U	1	7,14	-	2/6/23/26	0/1/1/1
14	NAG	U	2	14	-	2/6/23/26	0/1/1/1
14	BMA	U	3	14	-	0/2/19/22	0/1/1/1
14	MAN	U	4	14	-	2/2/19/22	0/1/1/1
14	MAN	U	5	14	-	2/2/19/22	0/1/1/1
14	MAN	U	6	14	-	0/2/19/22	0/1/1/1
14	MAN	U	7	14	-	2/2/19/22	0/1/1/1
14	MAN	U	8	14	-	2/2/19/22	0/1/1/1
14	MAN	U	9	14	-	0/2/19/22	0/1/1/1
11	NAG	V	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	V	2	11	-	2/6/23/26	0/1/1/1
9	NAG	W	1	9,7	-	0/6/23/26	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
9	MAN	W	4	9	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,7	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
9	MAN	X	4	9	-	2/2/19/22	0/1/1/1
9	NAG	Y	1	9,7	-	1/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	4	9	-	1/2/19/22	0/1/1/1
10	NAG	Z	1	7,10	-	2/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	2/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
11	NAG	a	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	a	2	11	-	0/6/23/26	0/1/1/1
10	NAG	b	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	b	2	10	-	2/6/23/26	0/1/1/1
10	BMA	b	3	10	-	2/2/19/22	0/1/1/1
12	NAG	e	1	12,7	-	2/6/23/26	0/1/1/1
12	NAG	e	2	12	-	2/6/23/26	0/1/1/1
12	BMA	e	3	12	-	2/2/19/22	0/1/1/1
12	MAN	e	4	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	e	5	12	-	0/2/19/22	0/1/1/1
12	MAN	e	6	12	-	2/2/19/22	0/1/1/1
11	NAG	f	1	11	-	2/6/23/26	0/1/1/1
11	NAG	f	2	11	-	0/6/23/26	0/1/1/1
11	NAG	g	1	7,11	-	1/6/23/26	0/1/1/1
11	NAG	g	2	11	-	2/6/23/26	0/1/1/1
10	NAG	i	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	i	2	10	-	0/6/23/26	0/1/1/1
10	BMA	i	3	10	-	1/2/19/22	0/1/1/1
13	NAG	j	1	7,13	-	2/6/23/26	0/1/1/1
13	NAG	j	2	13	-	2/6/23/26	0/1/1/1
13	BMA	j	3	13	-	0/2/19/22	0/1/1/1
13	MAN	j	4	13	-	0/2/19/22	0/1/1/1
13	MAN	j	5	13	-	0/2/19/22	0/1/1/1
11	NAG	k	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	k	2	11	-	2/6/23/26	0/1/1/1
14	NAG	o	1	7,14	-	2/6/23/26	0/1/1/1
14	NAG	o	2	14	-	2/6/23/26	0/1/1/1
14	BMA	o	3	14	-	0/2/19/22	0/1/1/1
14	MAN	o	4	14	-	2/2/19/22	0/1/1/1
14	MAN	o	5	14	-	2/2/19/22	0/1/1/1
14	MAN	o	6	14	-	0/2/19/22	0/1/1/1
14	MAN	o	7	14	-	2/2/19/22	0/1/1/1
14	MAN	o	8	14	-	2/2/19/22	0/1/1/1
14	MAN	o	9	14	-	0/2/19/22	0/1/1/1
11	NAG	p	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	p	2	11	-	2/6/23/26	0/1/1/1
9	NAG	s	1	9,7	-	0/6/23/26	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
9	MAN	s	4	9	-	0/2/19/22	0/1/1/1
9	NAG	t	1	9,7	-	2/6/23/26	0/1/1/1
9	NAG	t	2	9	-	2/6/23/26	0/1/1/1
9	BMA	t	3	9	-	2/2/19/22	0/1/1/1
9	MAN	t	4	9	-	2/2/19/22	0/1/1/1
9	NAG	u	1	9,7	-	1/6/23/26	0/1/1/1
9	NAG	u	2	9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	u	3	9	-	0/2/19/22	0/1/1/1
9	MAN	u	4	9	-	1/2/19/22	0/1/1/1
10	NAG	v	1	7,10	-	2/6/23/26	0/1/1/1
10	NAG	v	2	10	-	2/6/23/26	0/1/1/1
10	BMA	v	3	10	-	0/2/19/22	0/1/1/1
11	NAG	w	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	w	2	11	-	0/6/23/26	0/1/1/1
10	NAG	x	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	x	2	10	-	2/6/23/26	0/1/1/1
10	BMA	x	3	10	-	2/2/19/22	0/1/1/1
12	NAG	y	1	12,7	-	2/6/23/26	0/1/1/1
12	NAG	y	2	12	-	2/6/23/26	0/1/1/1
12	BMA	y	3	12	-	2/2/19/22	0/1/1/1
12	MAN	y	4	12	-	2/2/19/22	0/1/1/1
12	MAN	y	5	12	-	0/2/19/22	0/1/1/1
12	MAN	y	6	12	-	2/2/19/22	0/1/1/1
11	NAG	z	1	11	-	2/6/23/26	0/1/1/1
11	NAG	z	2	11	-	0/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	3	BMA	C1-C2	2.63	1.58	1.52
10	P	3	BMA	C1-C2	2.62	1.58	1.52
10	i	3	BMA	C1-C2	2.61	1.58	1.52
12	J	4	MAN	O5-C5	2.13	1.47	1.43
12	y	4	MAN	O5-C5	2.13	1.47	1.43

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	3	BMA	C1-O5-C5	4.96	118.84	112.19
9	t	3	BMA	C1-O5-C5	4.96	118.84	112.19
9	X	3	BMA	C1-O5-C5	4.94	118.81	112.19
14	U	4	MAN	C1-O5-C5	4.52	118.25	112.19
14	o	4	MAN	C1-O5-C5	4.51	118.23	112.19

There are no chirality outliers.

5 of 201 torsion outliers are listed below:

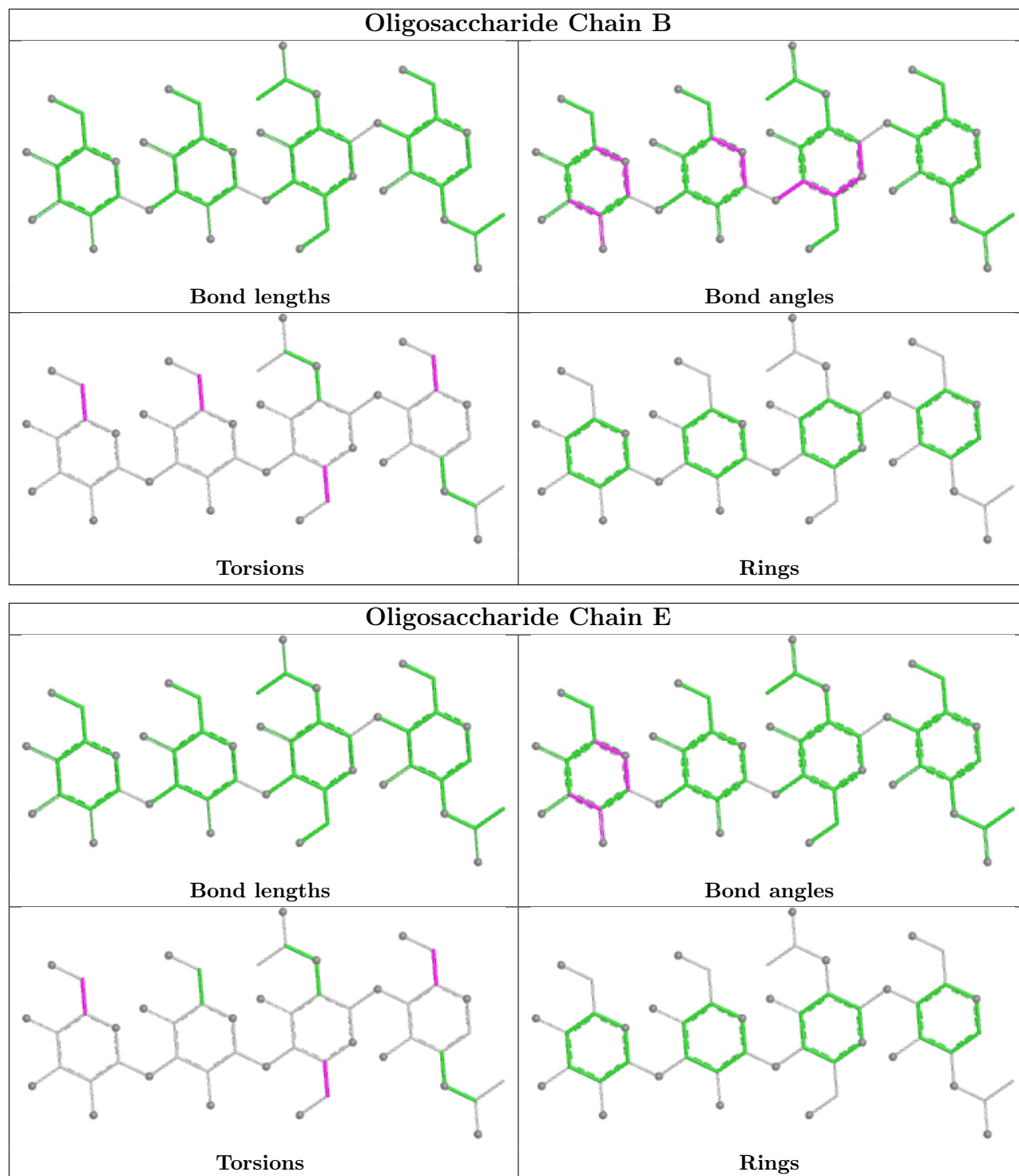
Mol	Chain	Res	Type	Atoms
13	S	2	NAG	O5-C5-C6-O6
13	j	2	NAG	O5-C5-C6-O6
13	9	2	NAG	O5-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
10	b	2	NAG	O5-C5-C6-O6

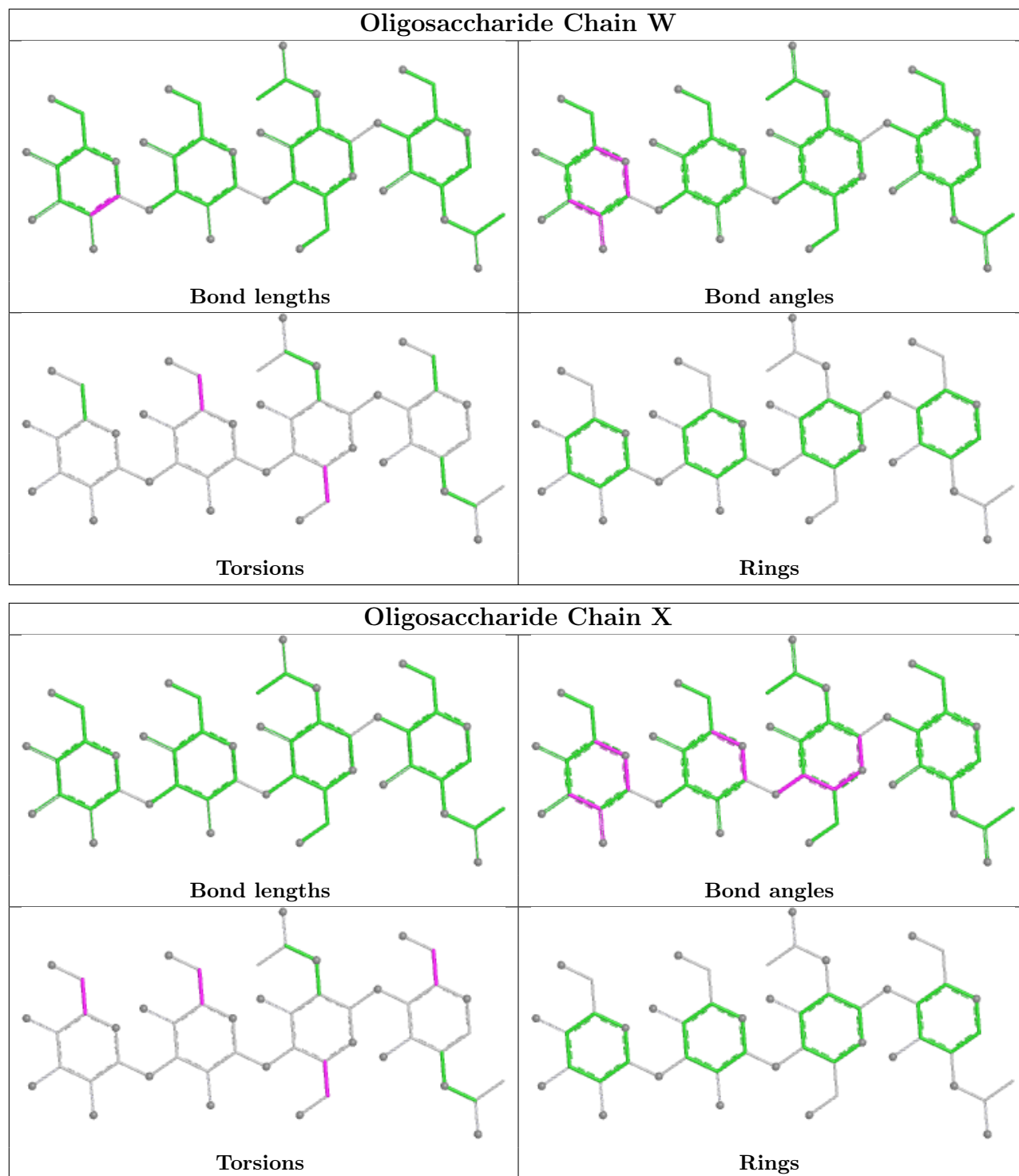
There are no ring outliers.

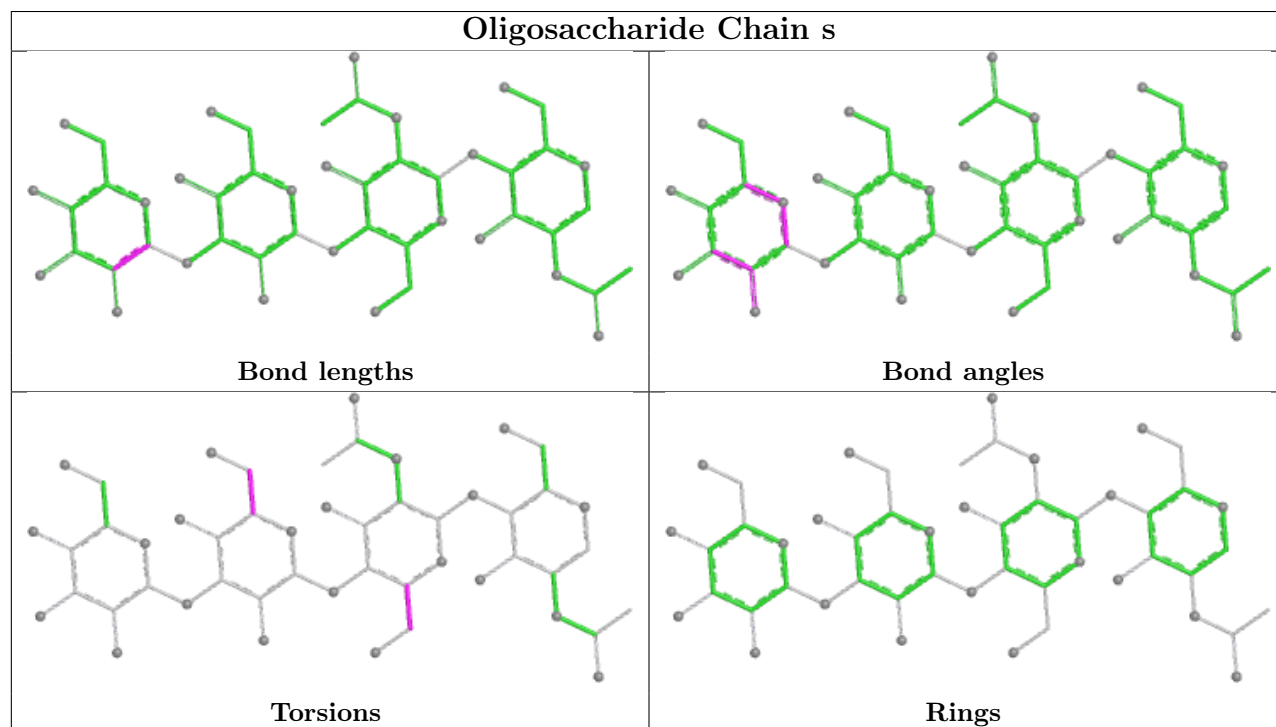
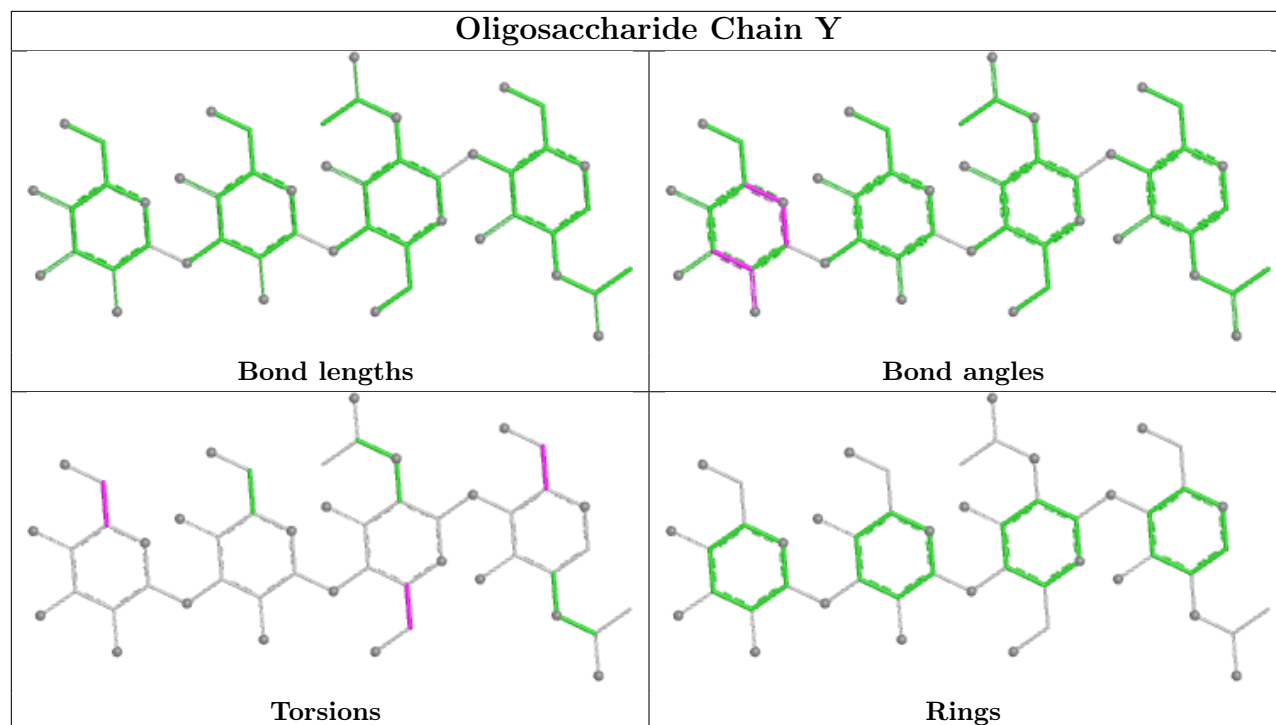
19 monomers are involved in 32 short contacts:

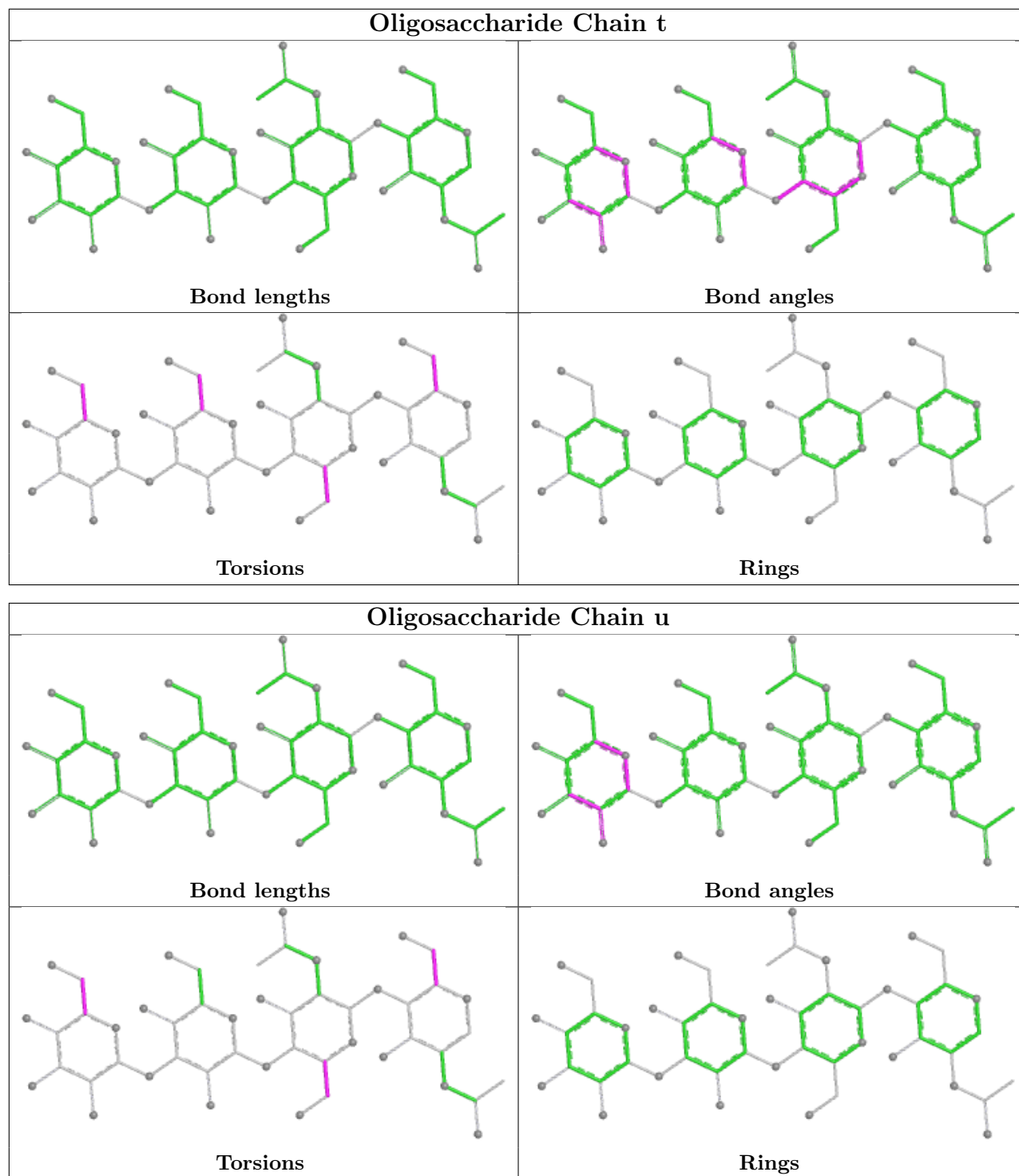
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	CA	1	NAG	1	0
10	I	1	NAG	1	0
11	K	1	NAG	6	0
11	V	1	NAG	1	0
11	AA	1	NAG	1	0
11	f	1	NAG	6	0
13	S	1	NAG	1	0
11	T	1	NAG	1	0
11	k	1	NAG	1	0
10	b	1	NAG	1	0
9	E	1	NAG	1	0
14	o	5	MAN	1	0
13	9	1	NAG	1	0
14	BA	5	MAN	1	0
13	j	1	NAG	1	0
11	p	1	NAG	1	0
10	x	1	NAG	1	0
14	U	5	MAN	2	0
11	z	1	NAG	6	0

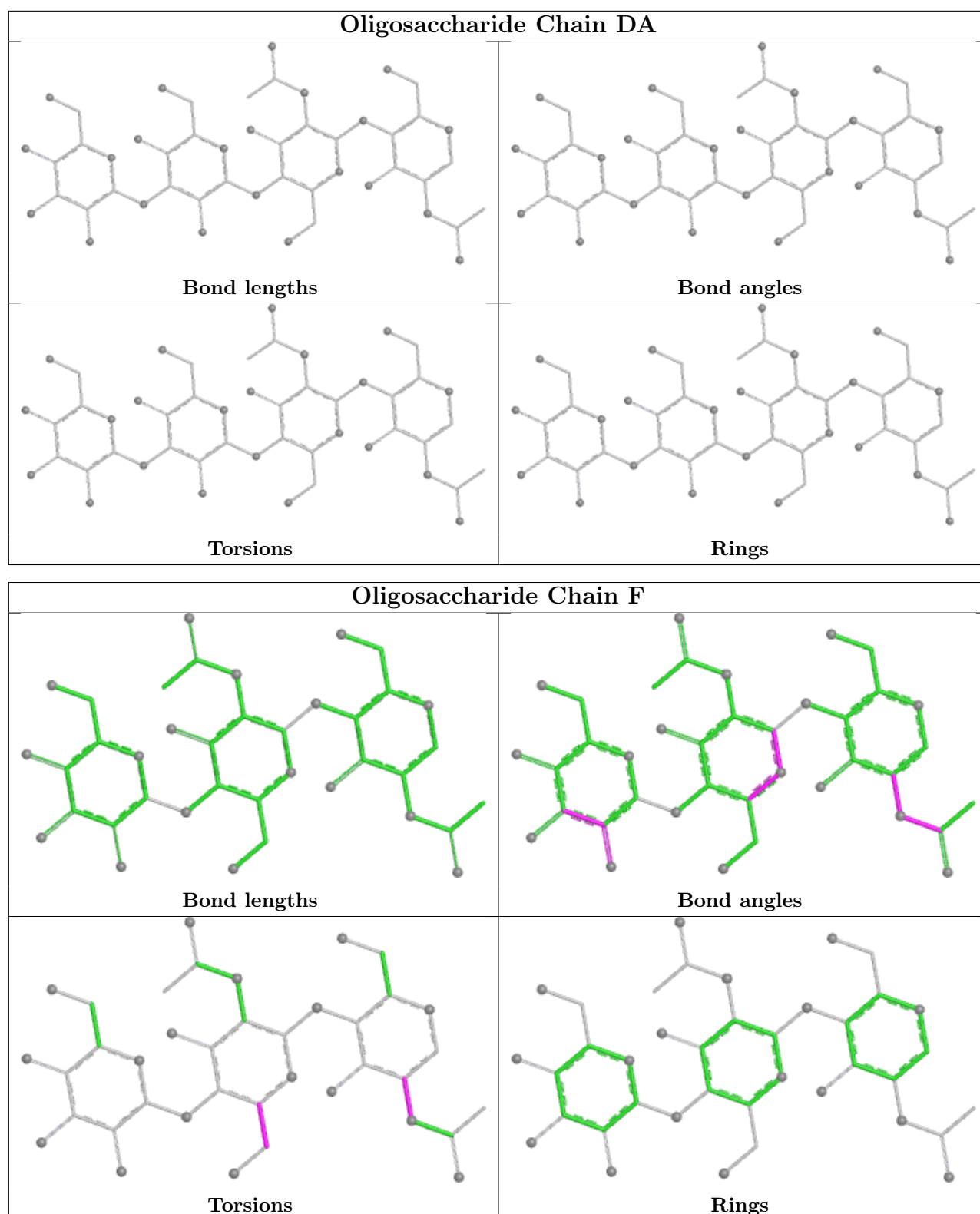
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

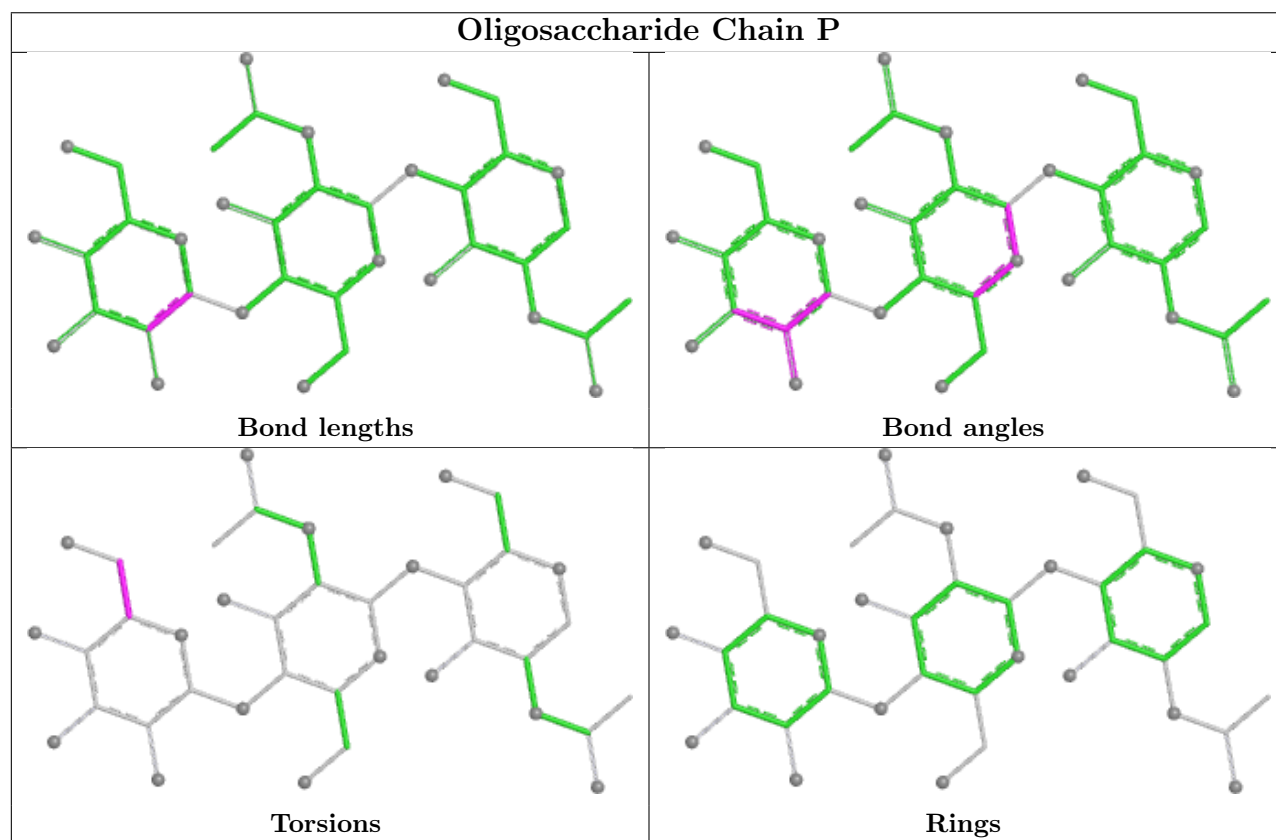
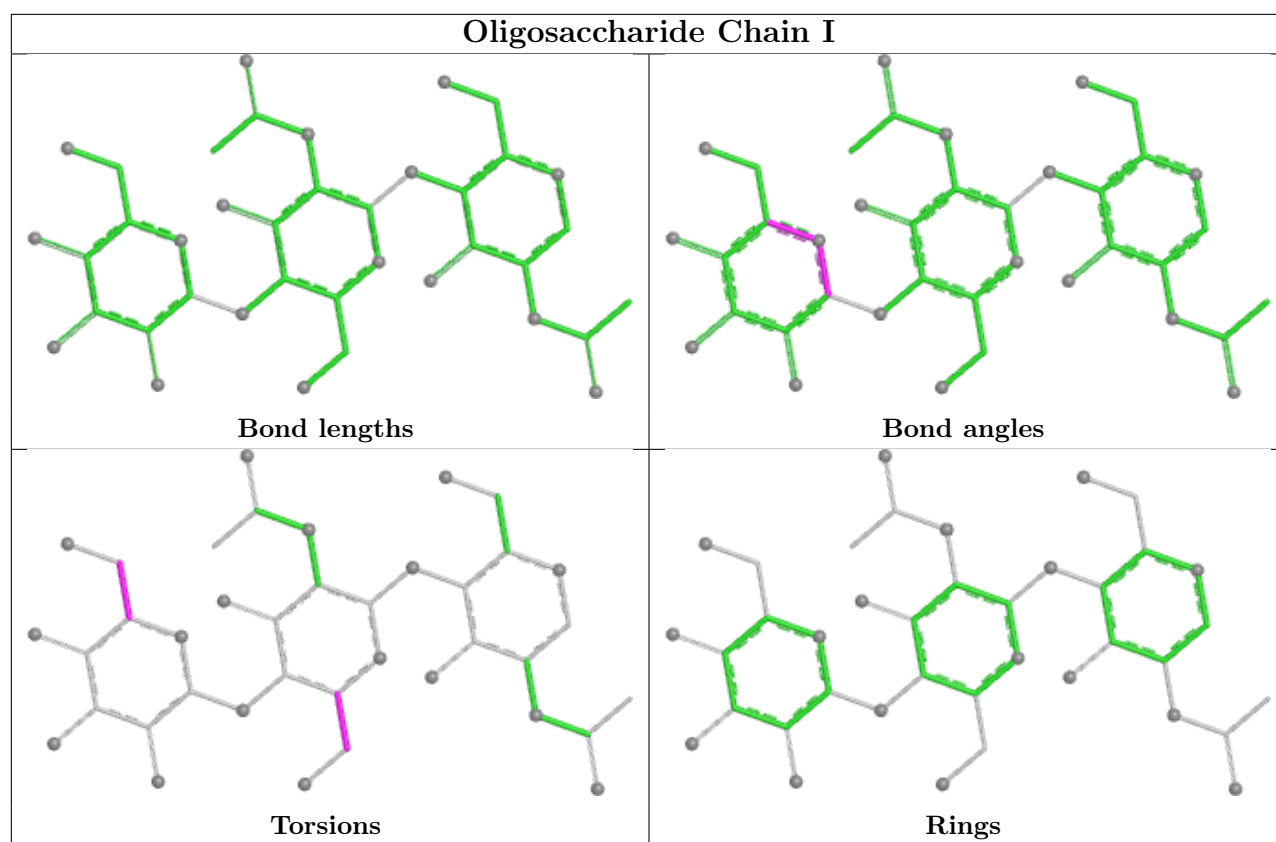


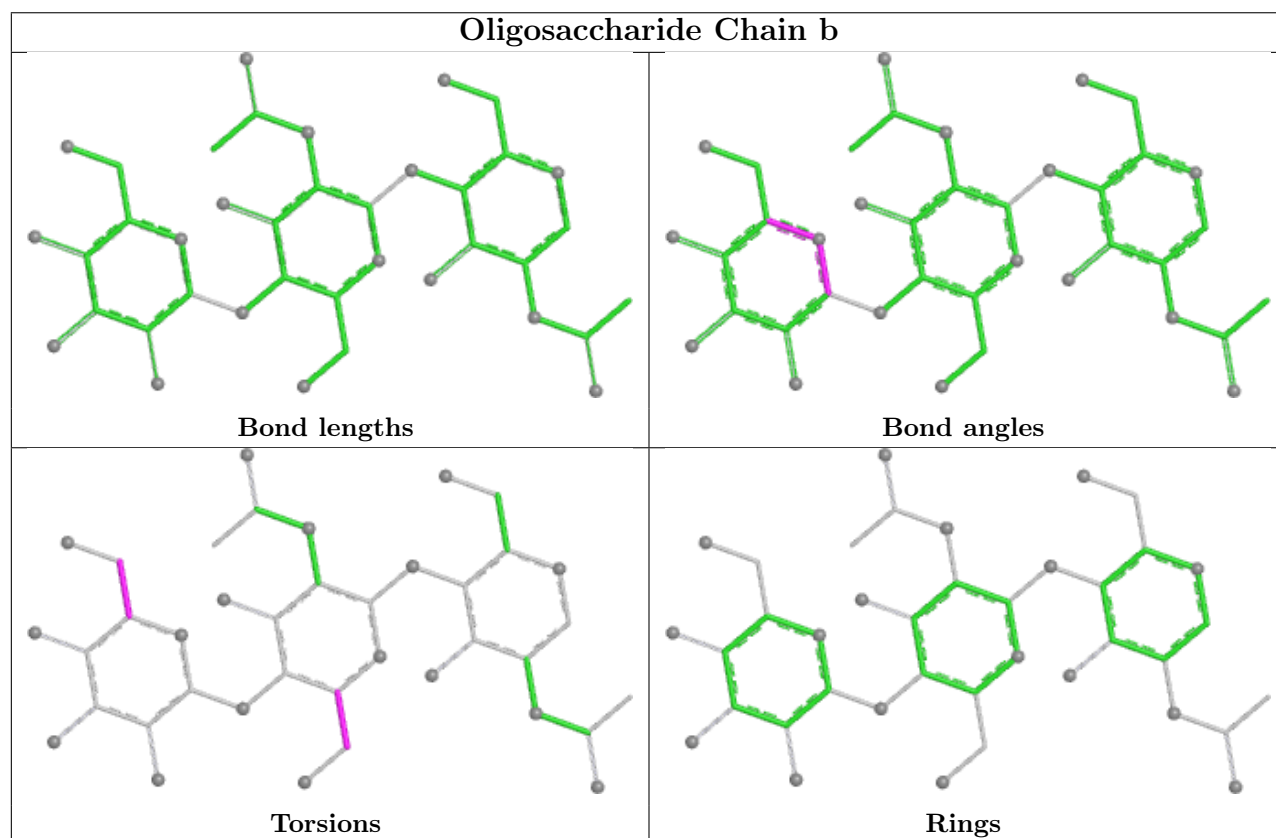
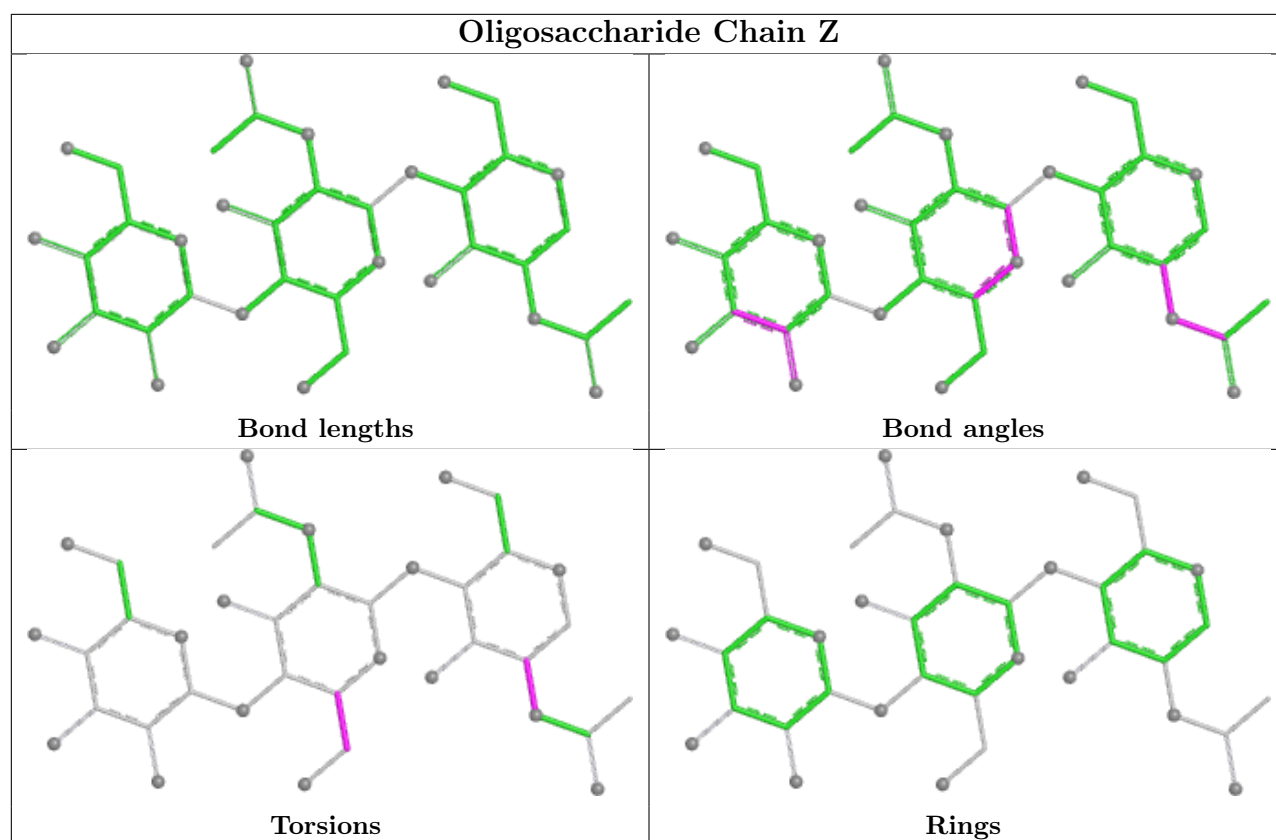


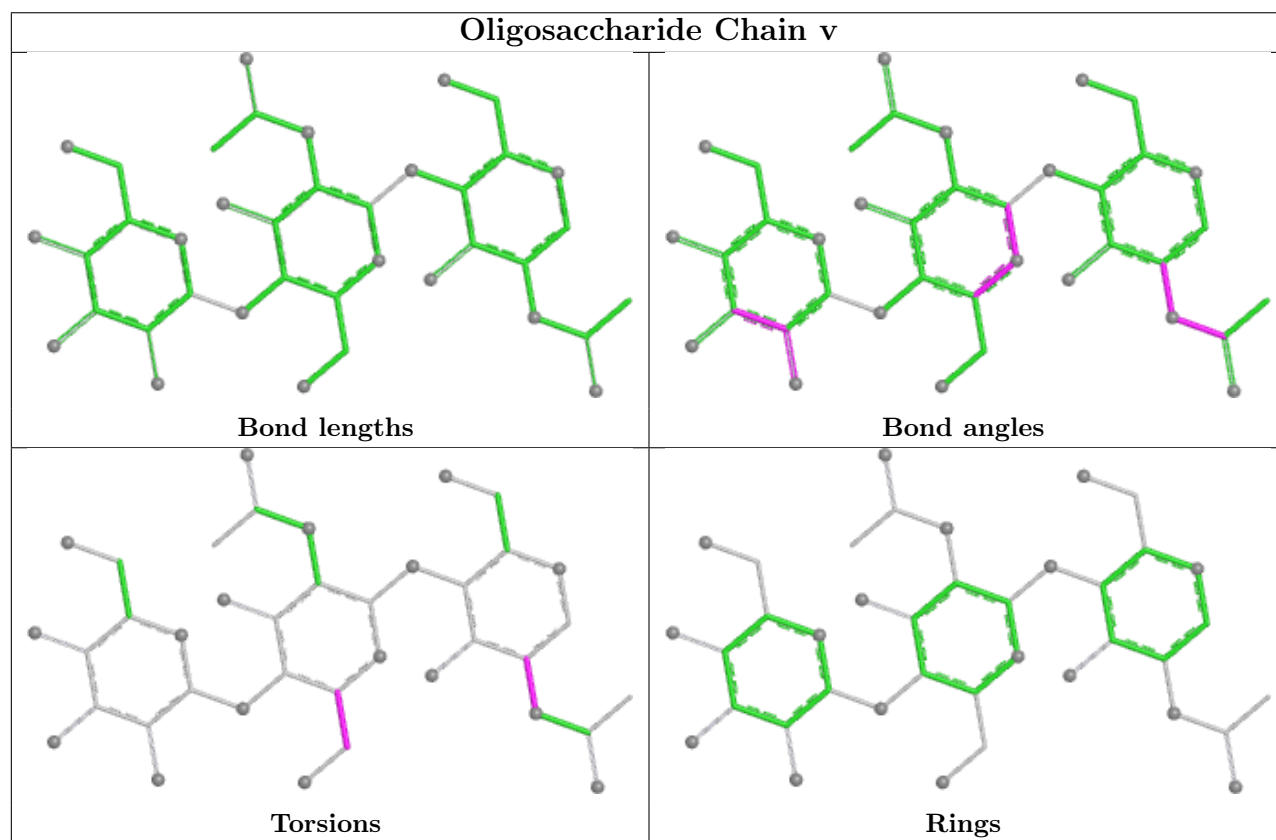
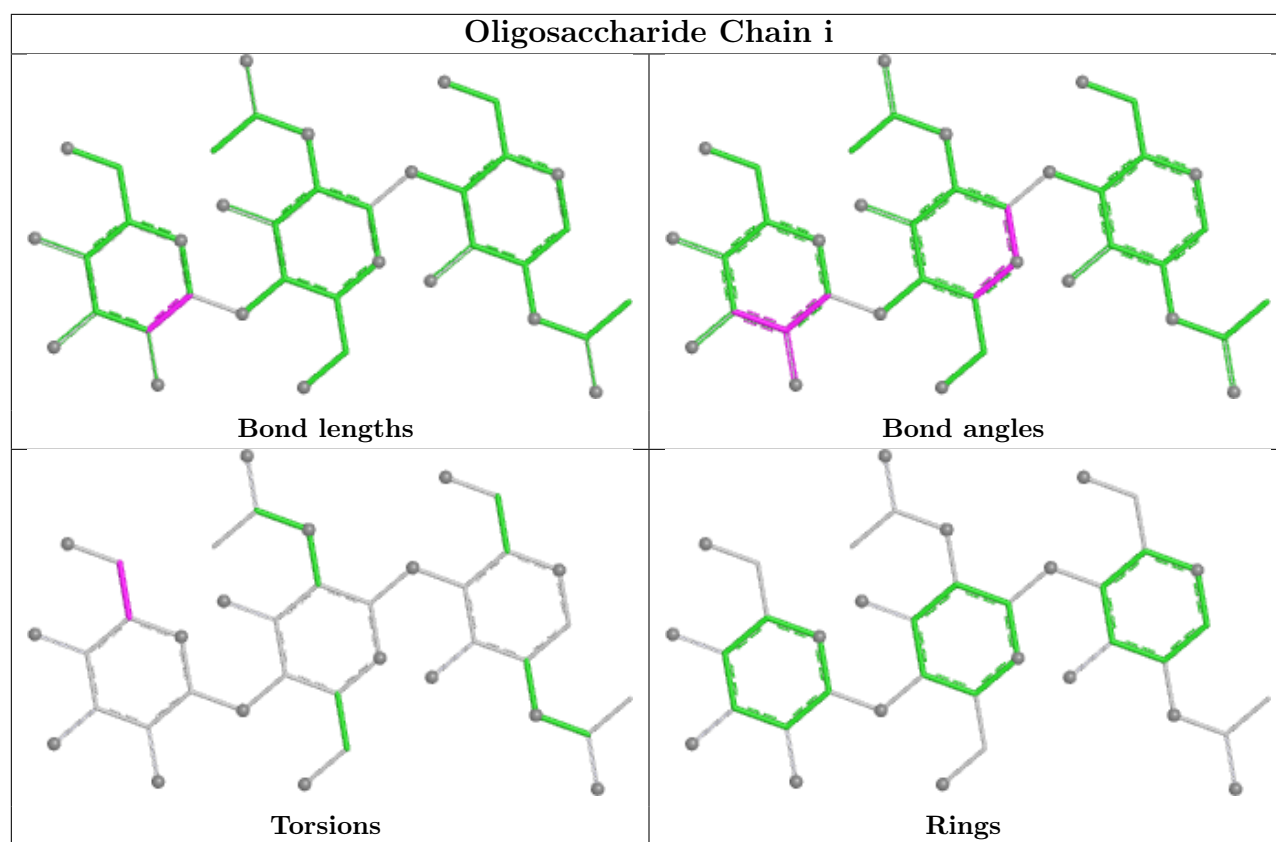


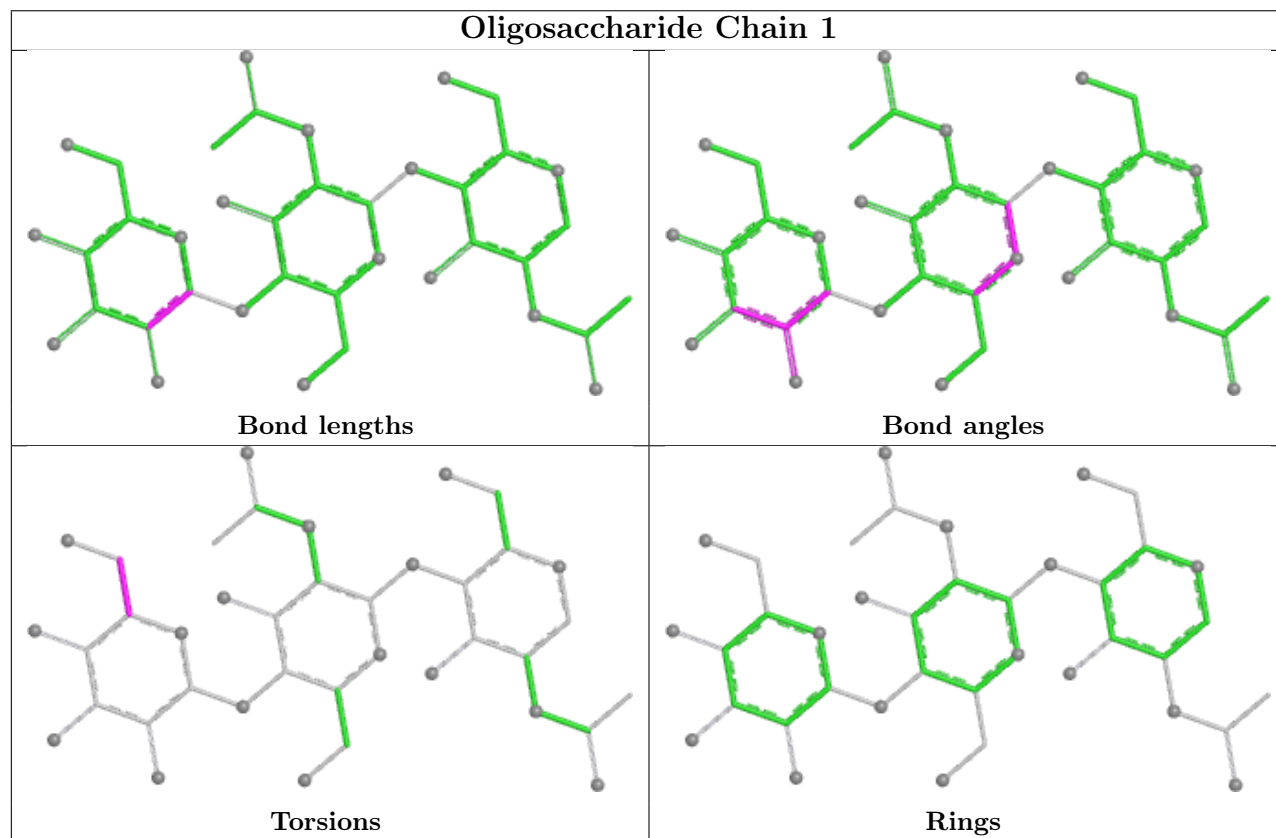
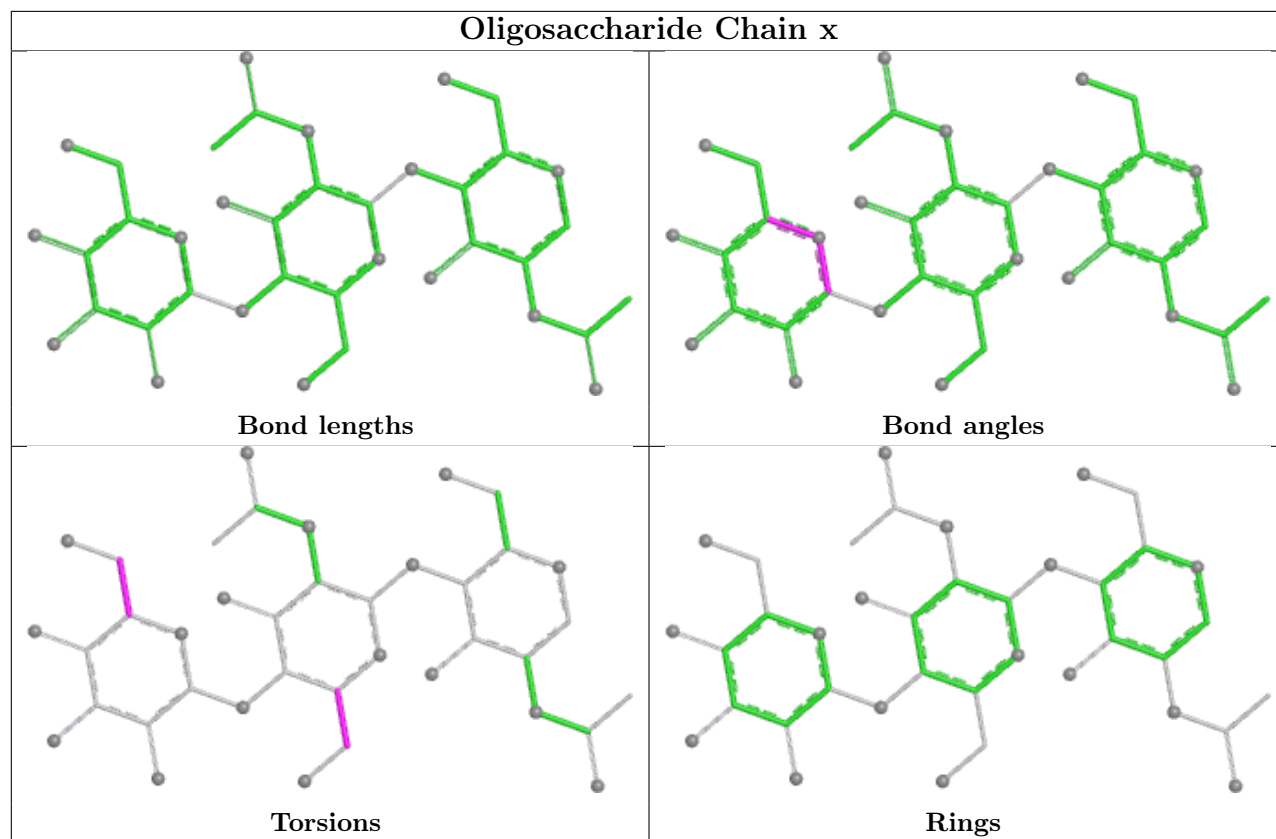


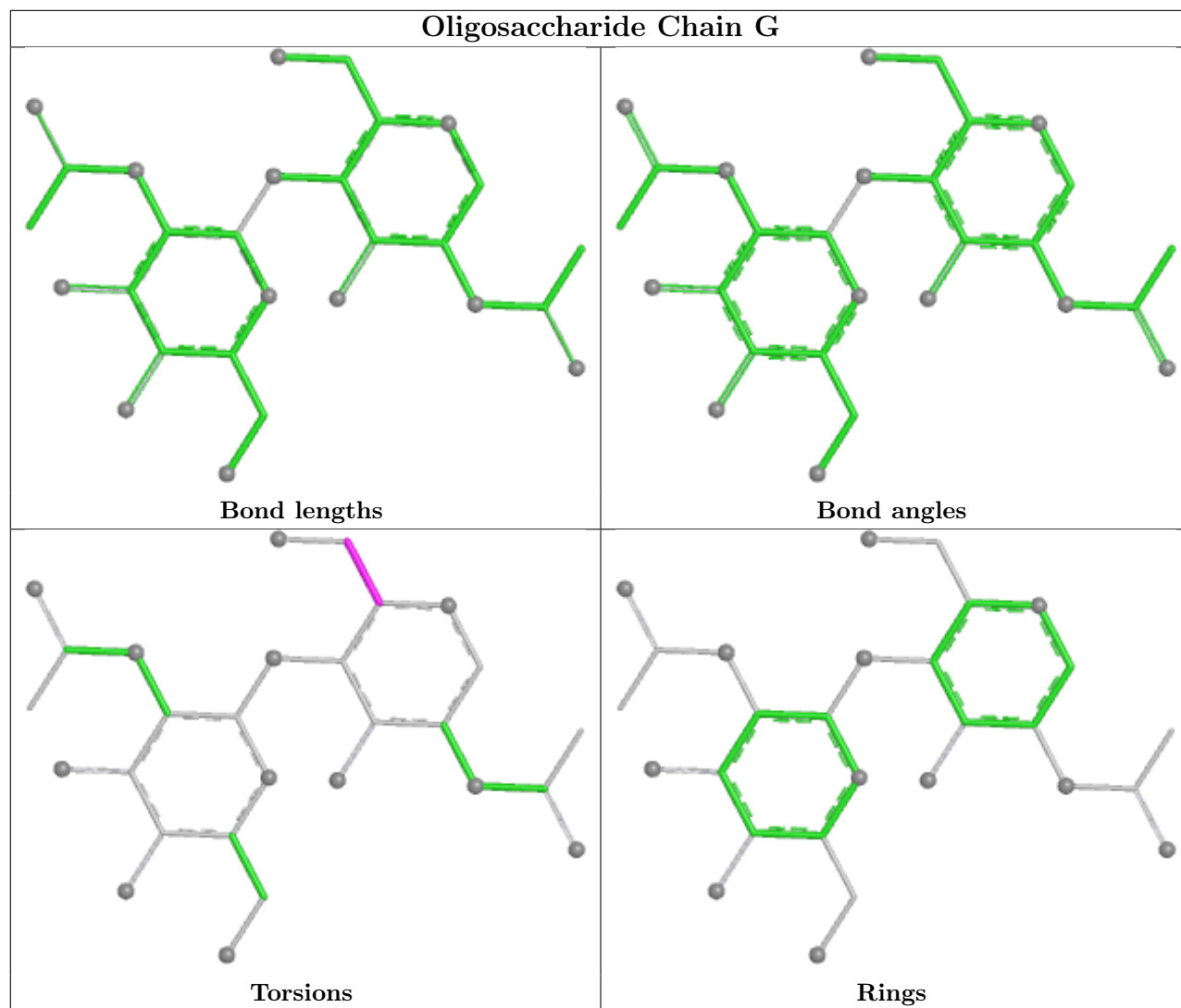


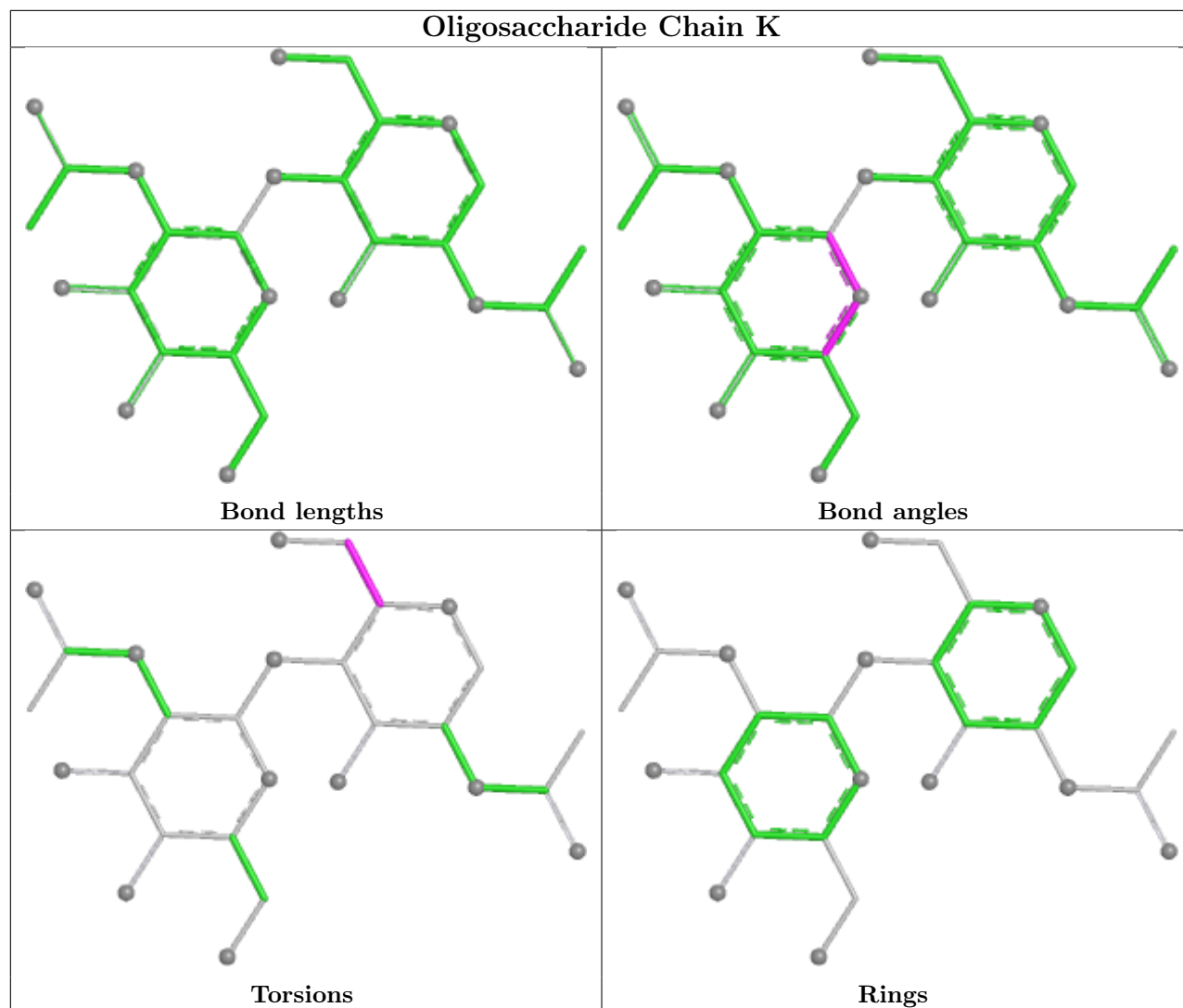


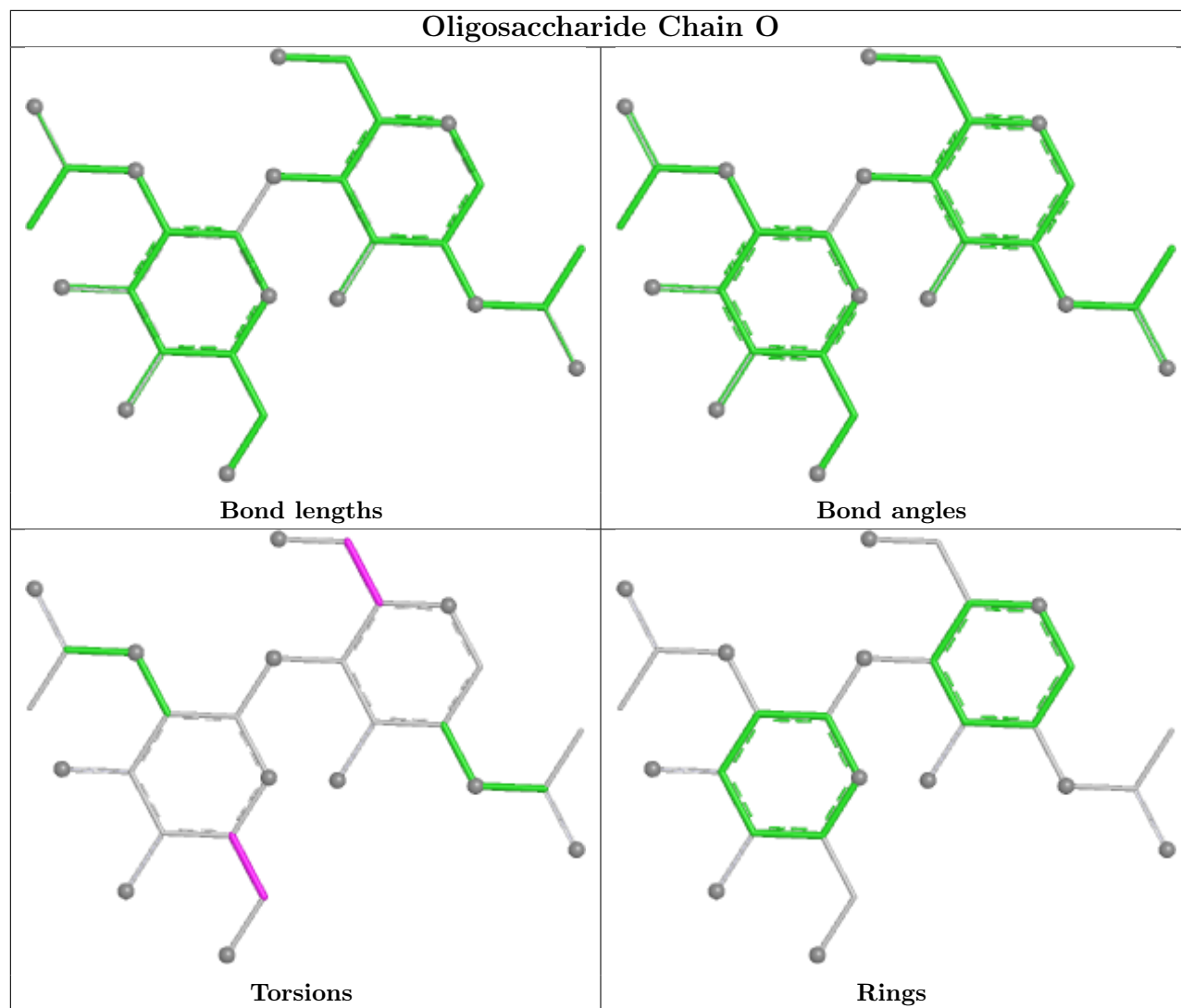


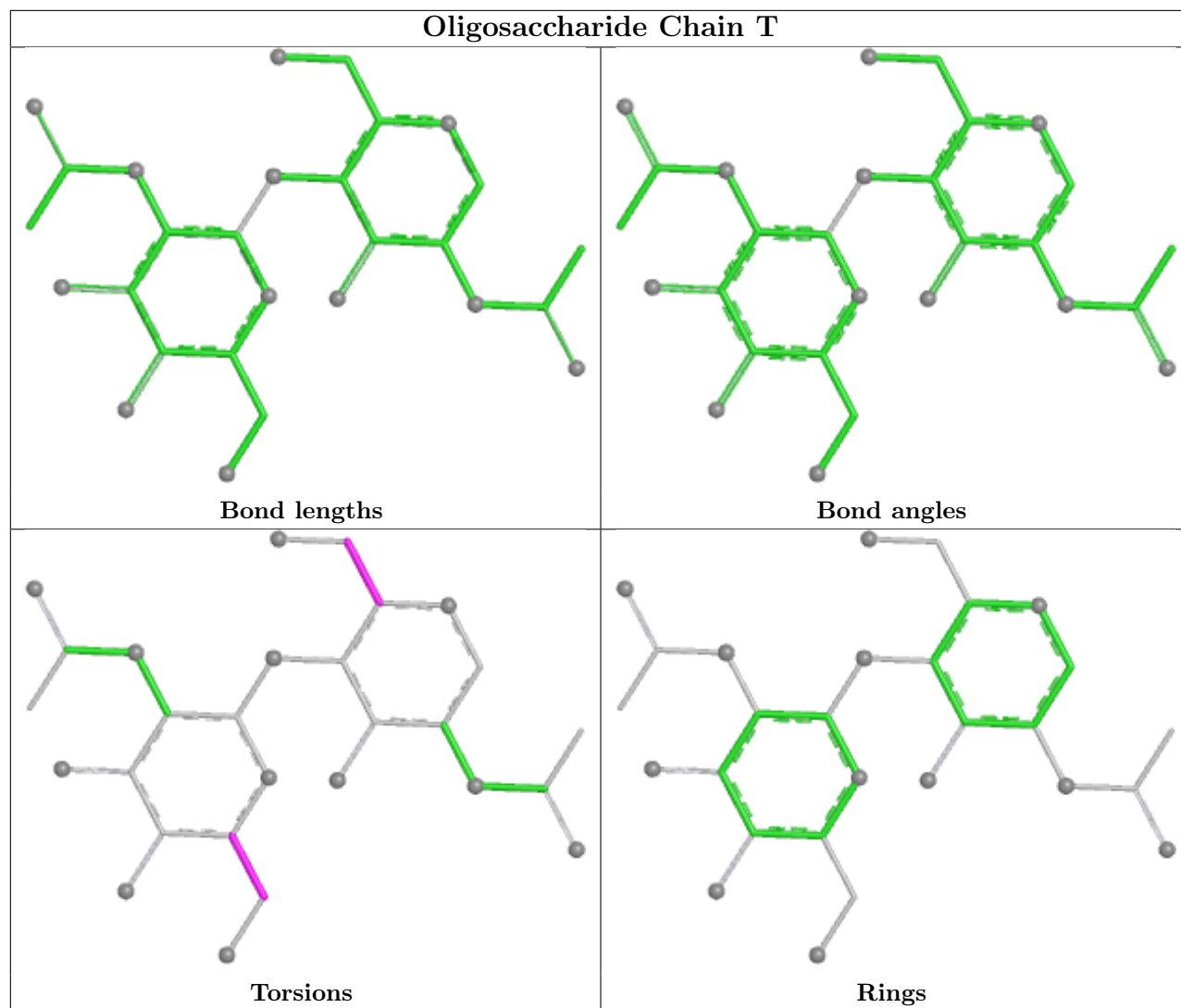


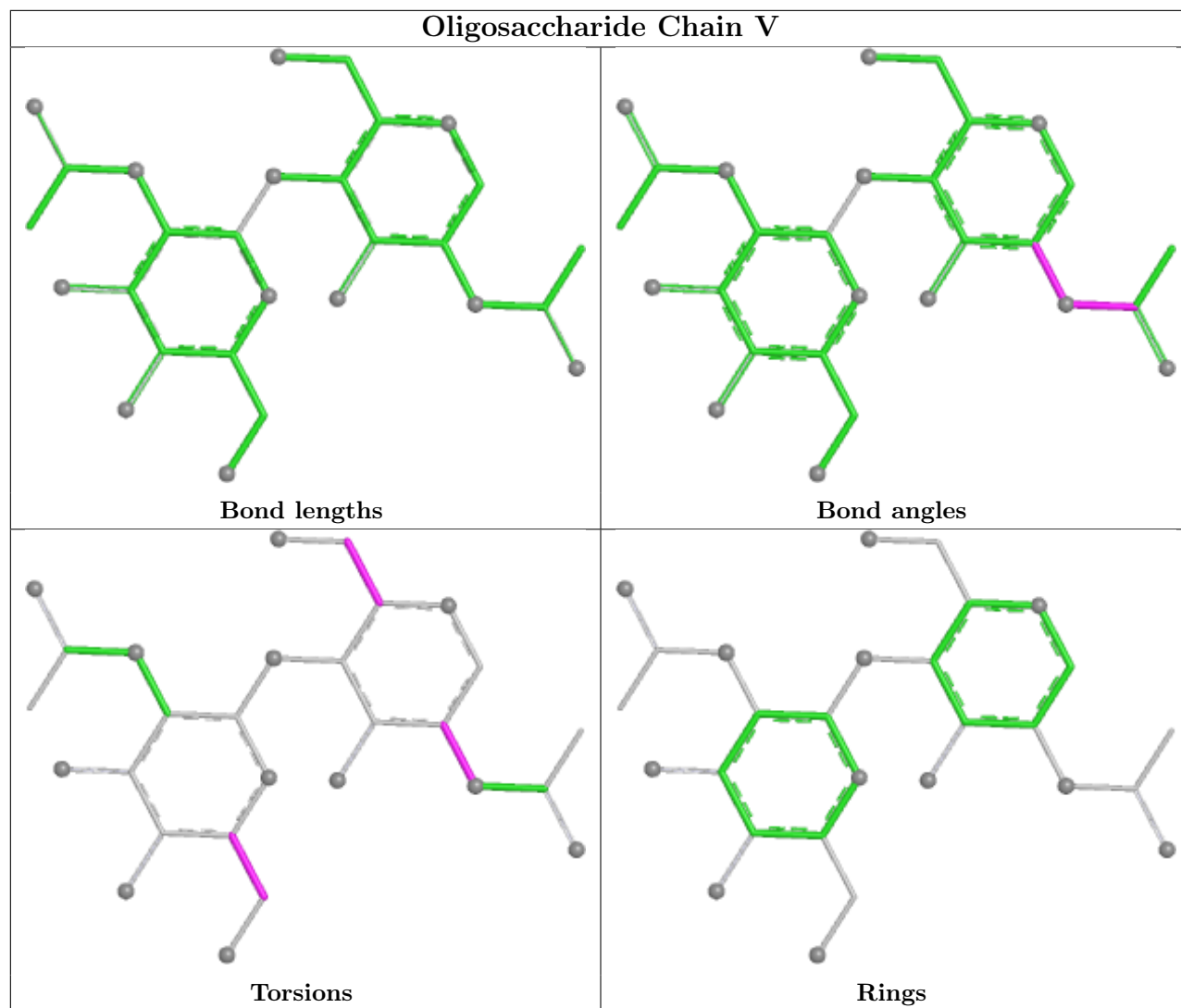


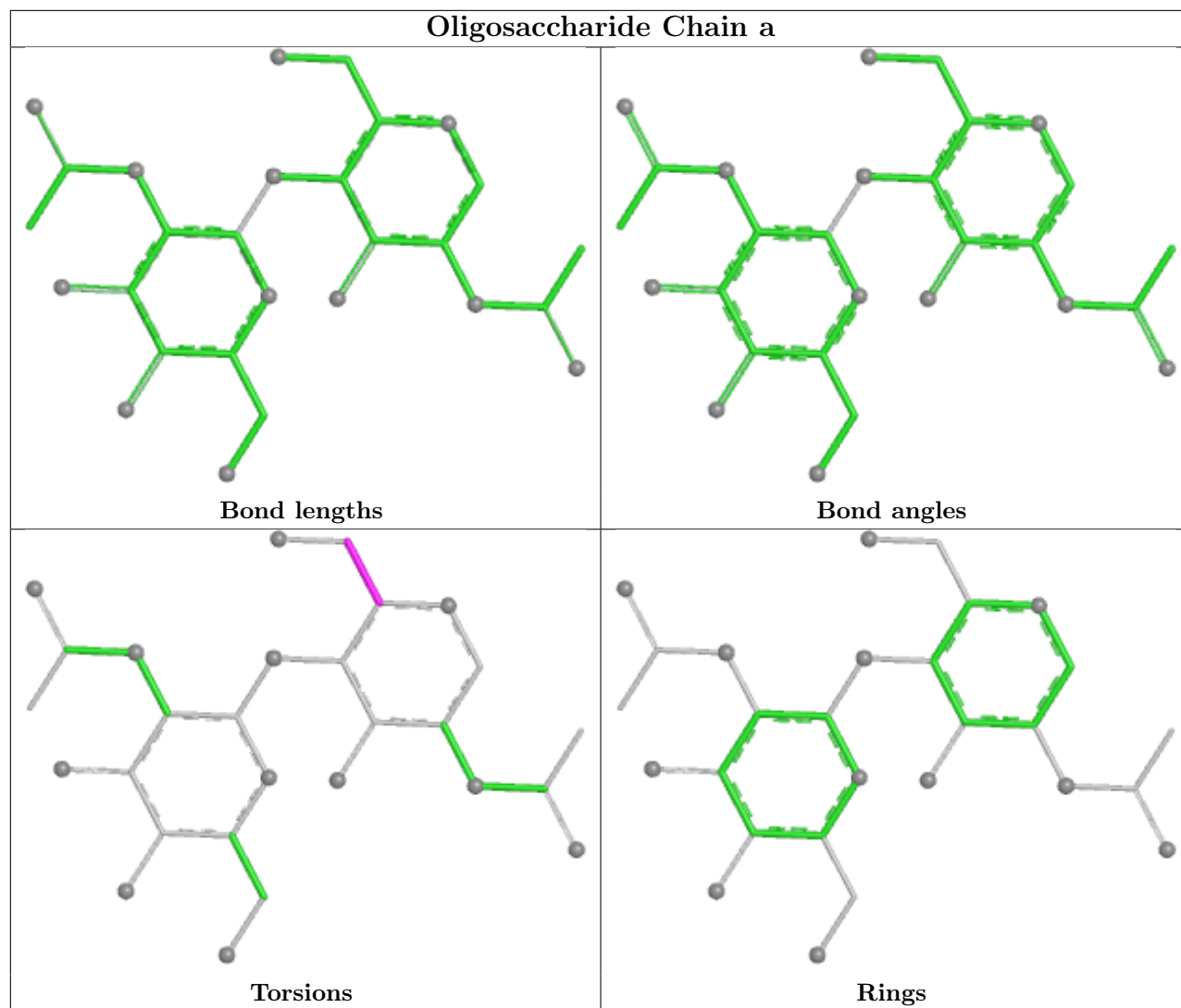


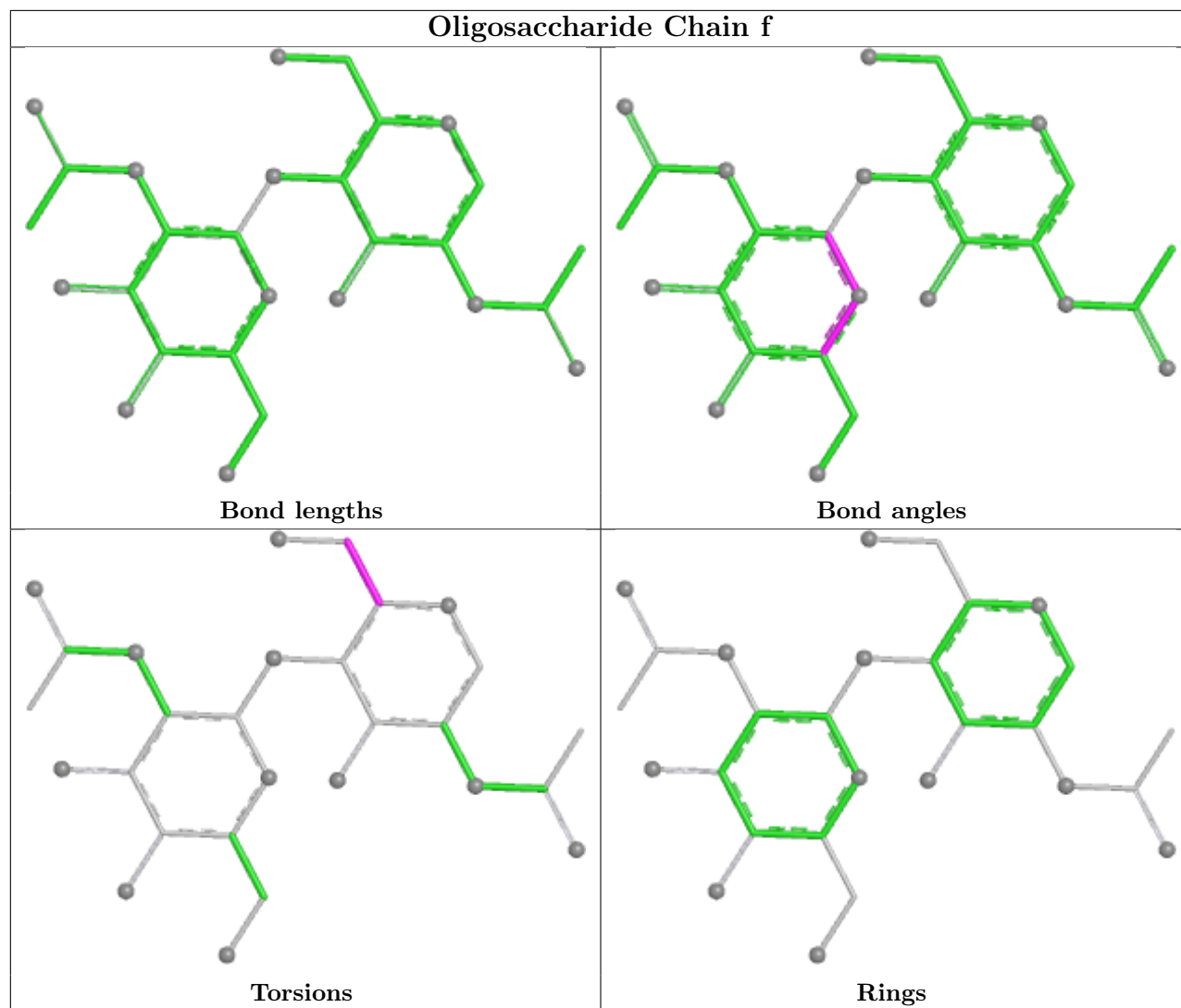


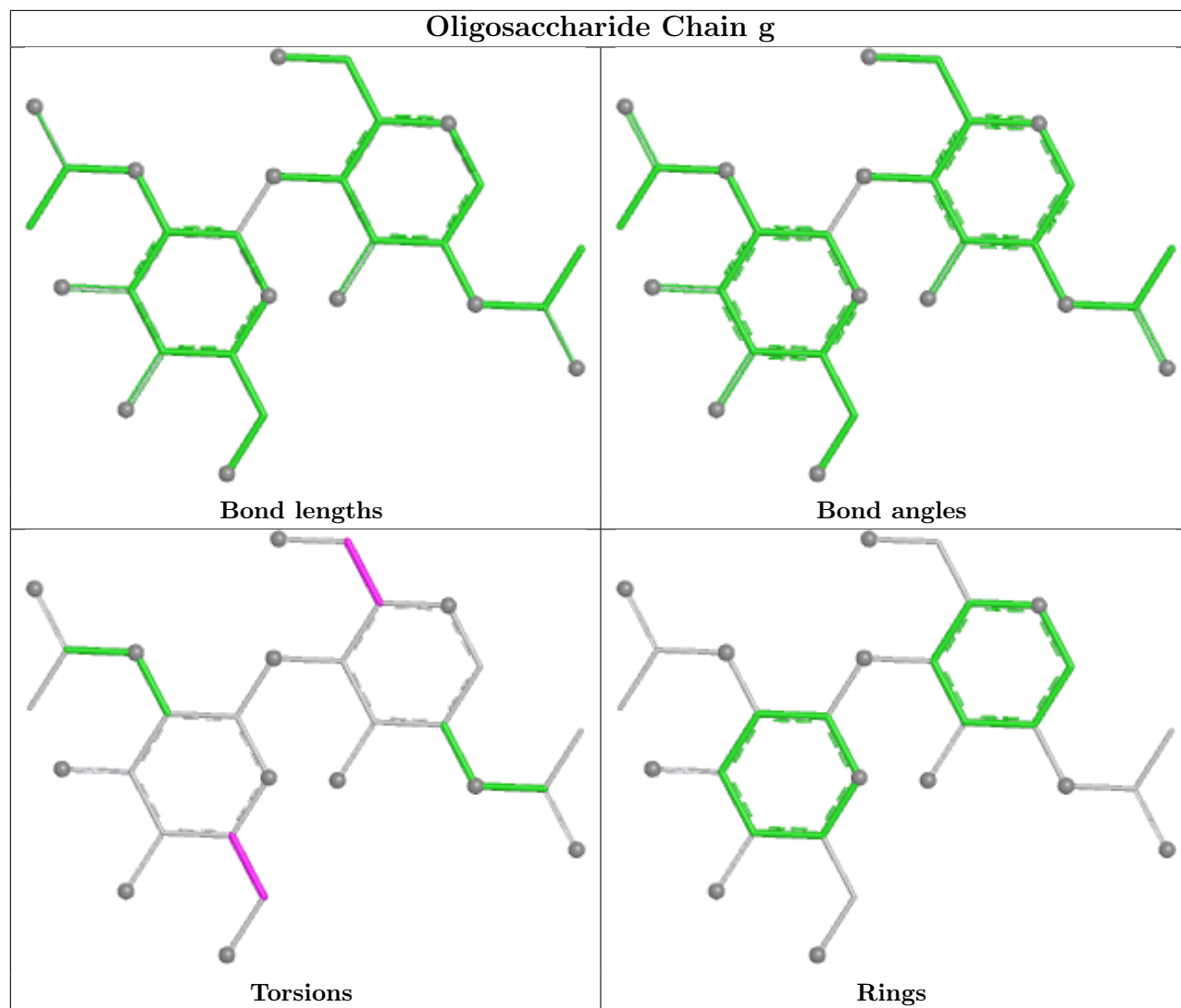


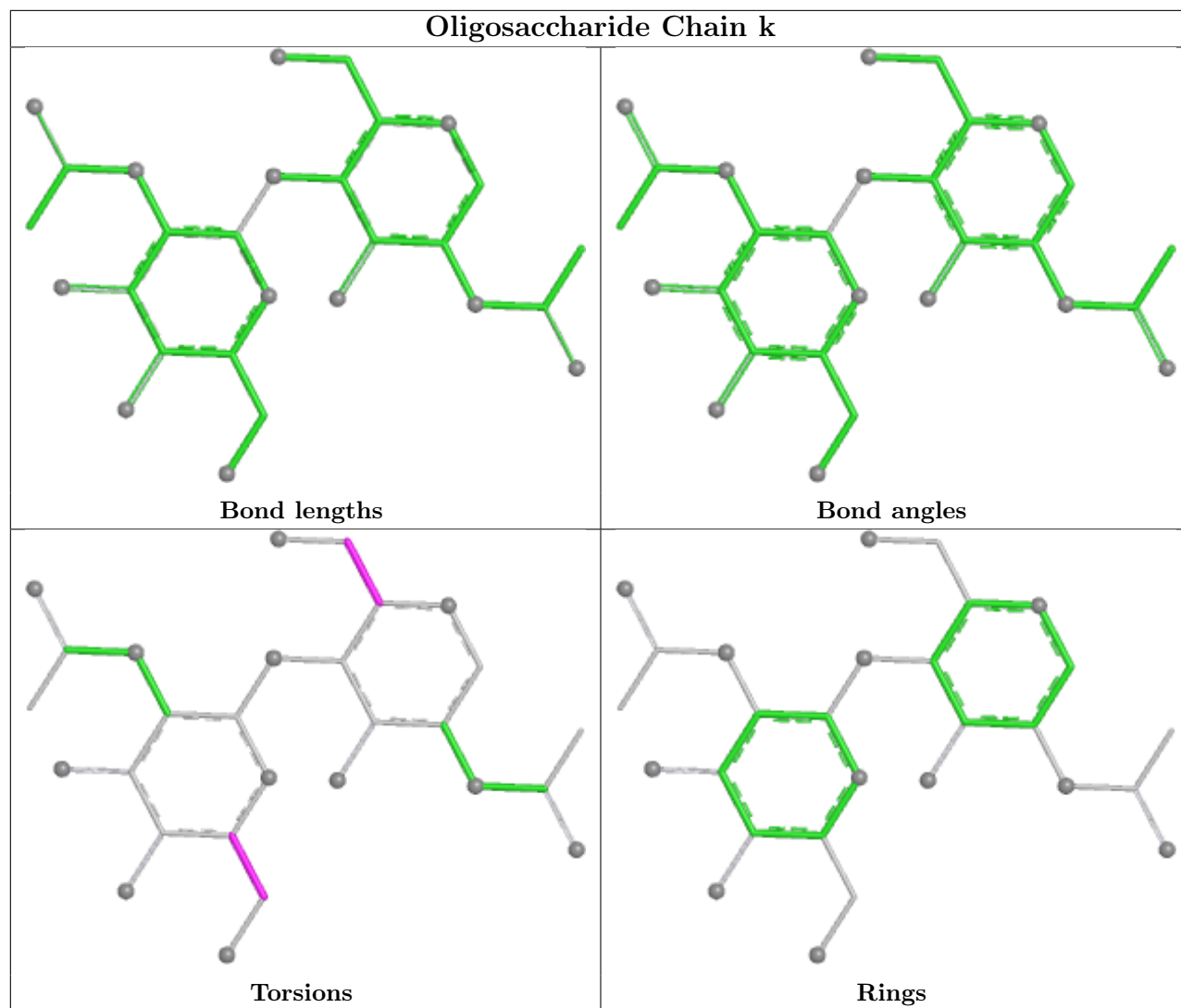


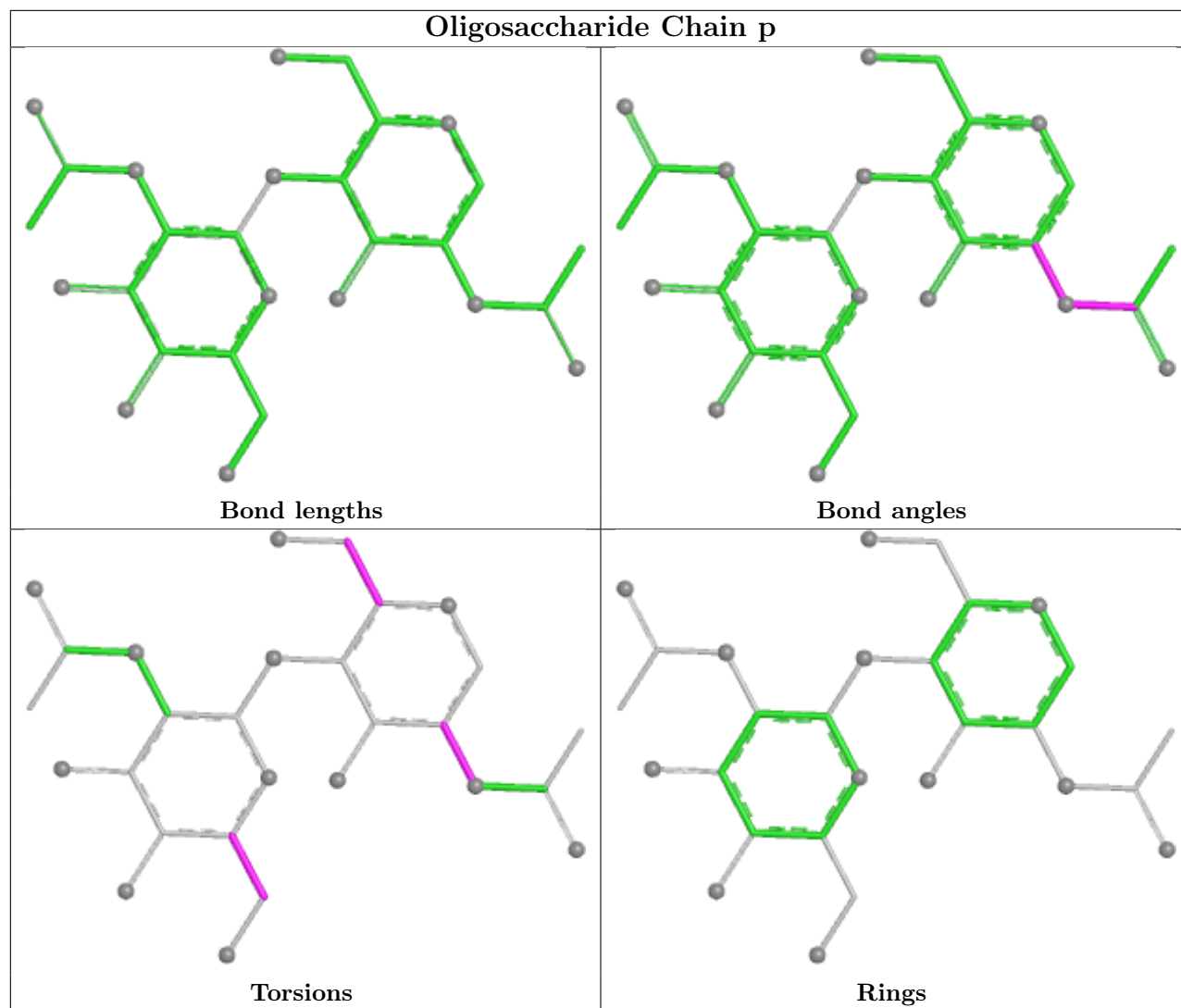


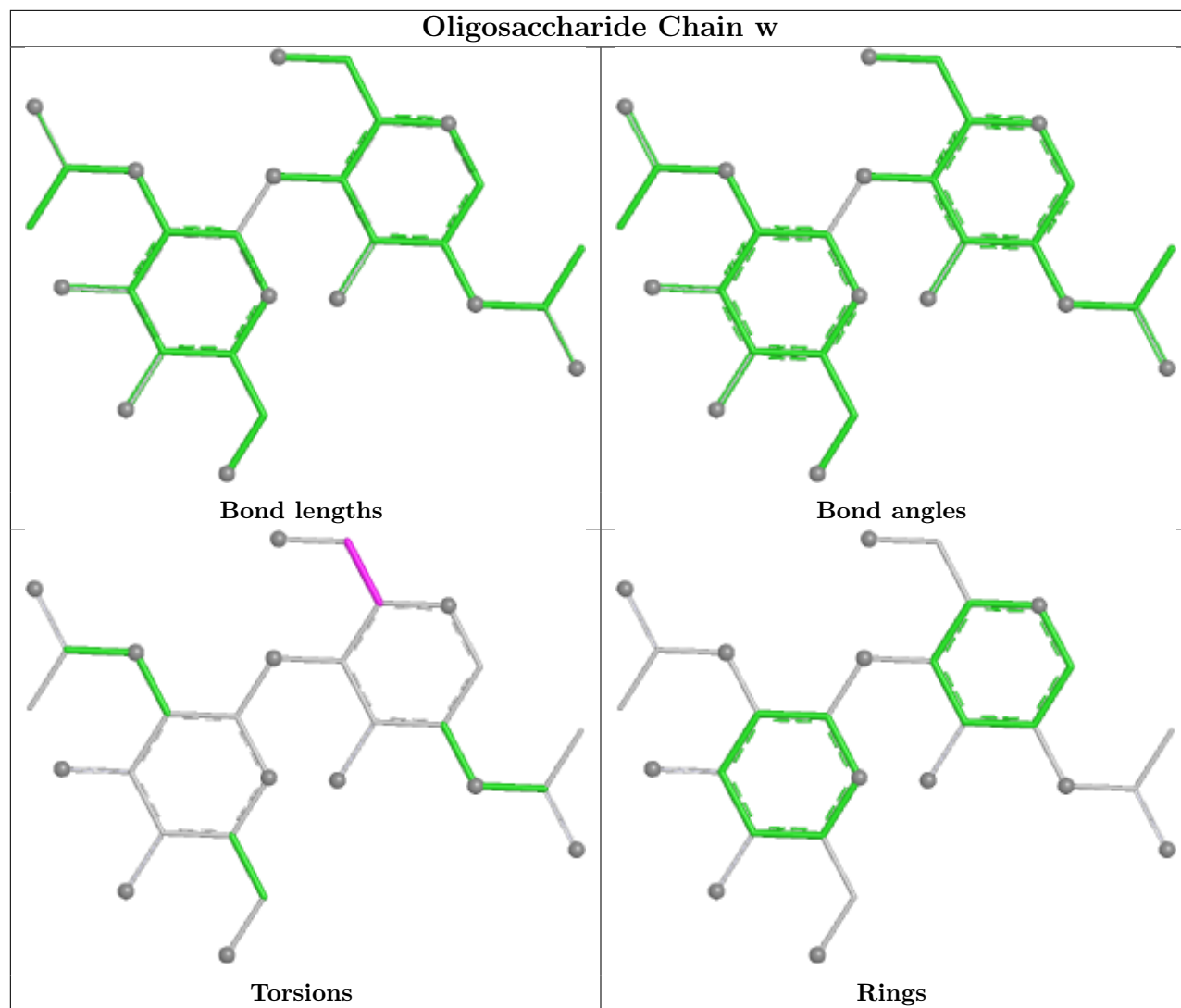


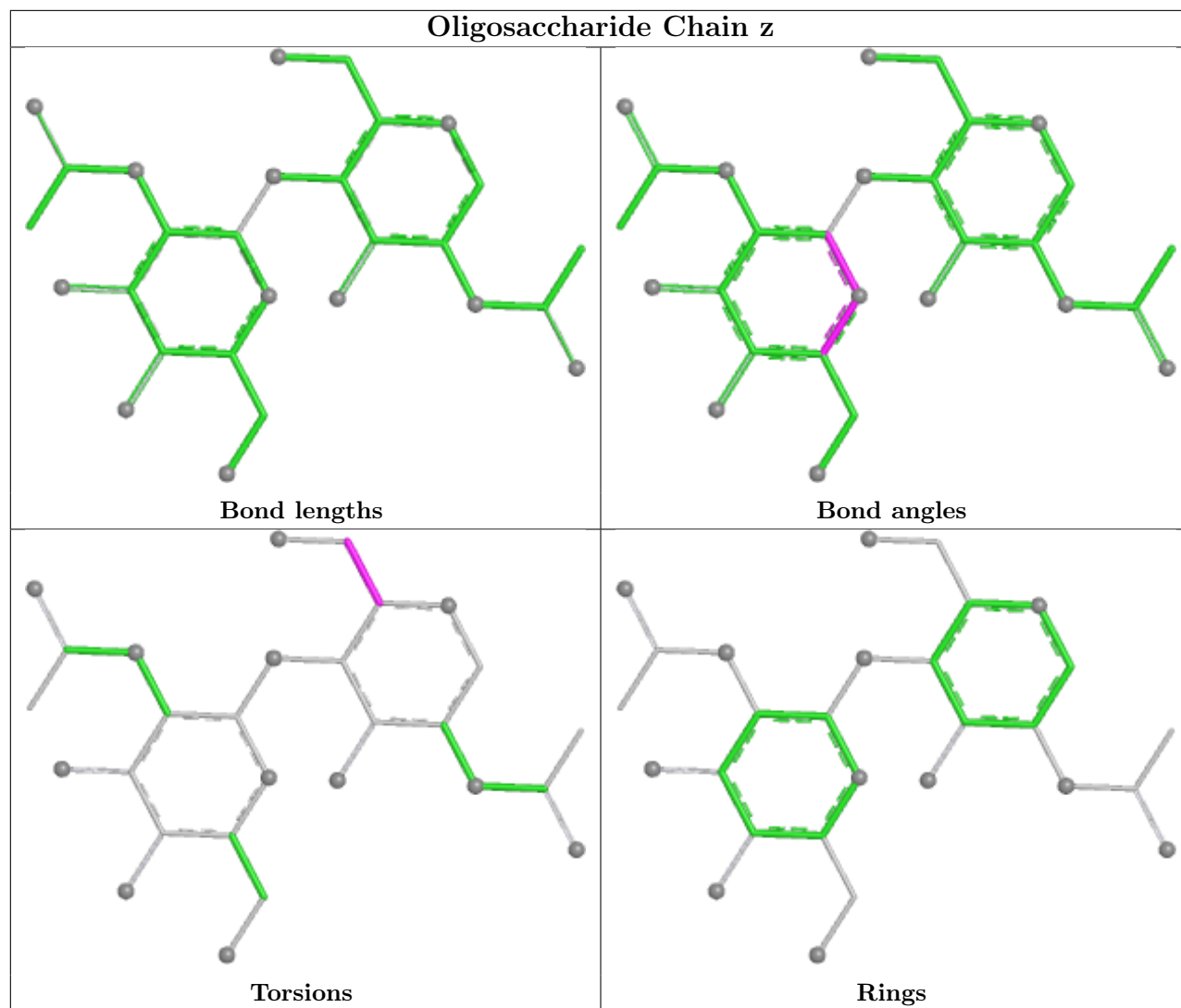


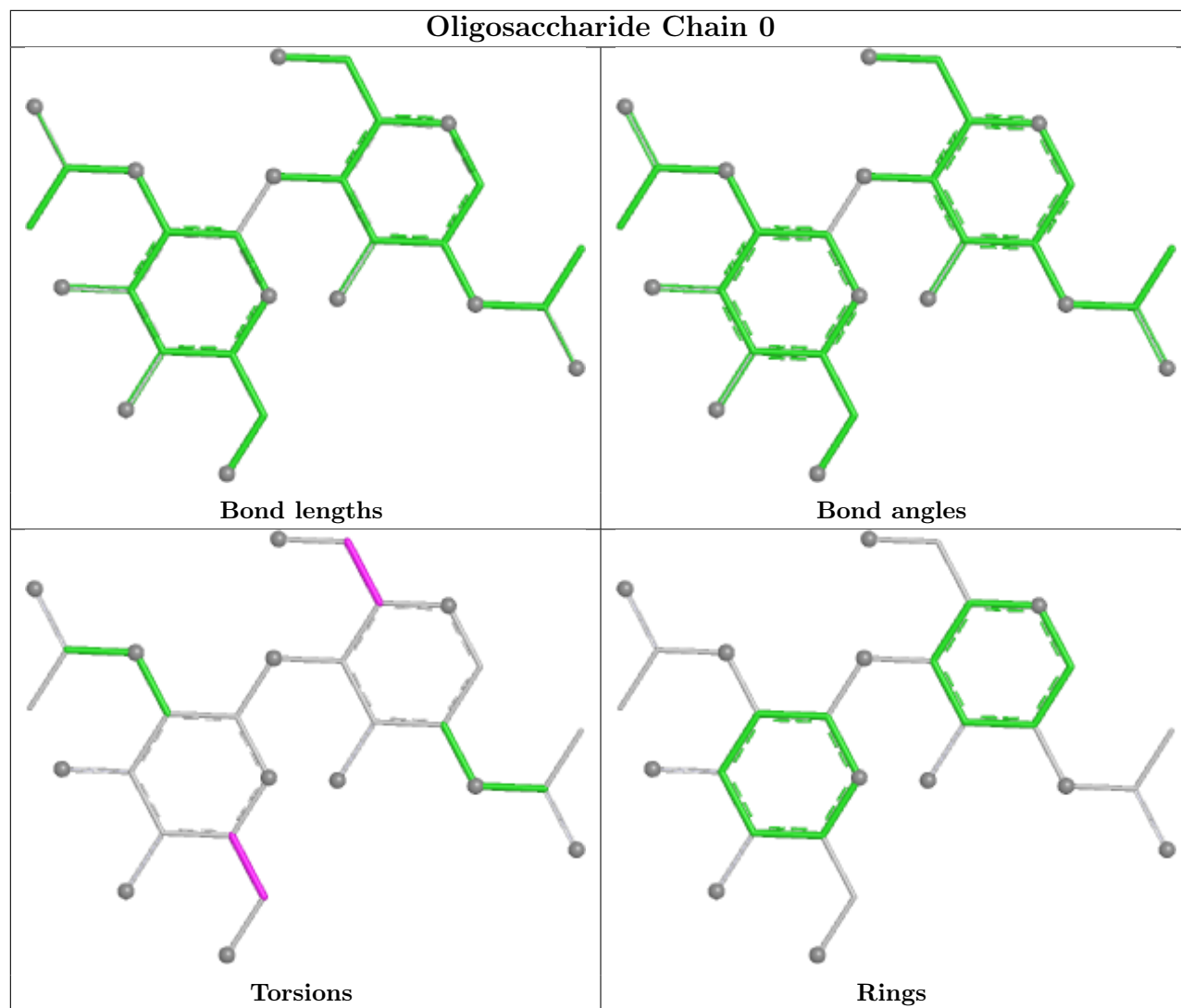


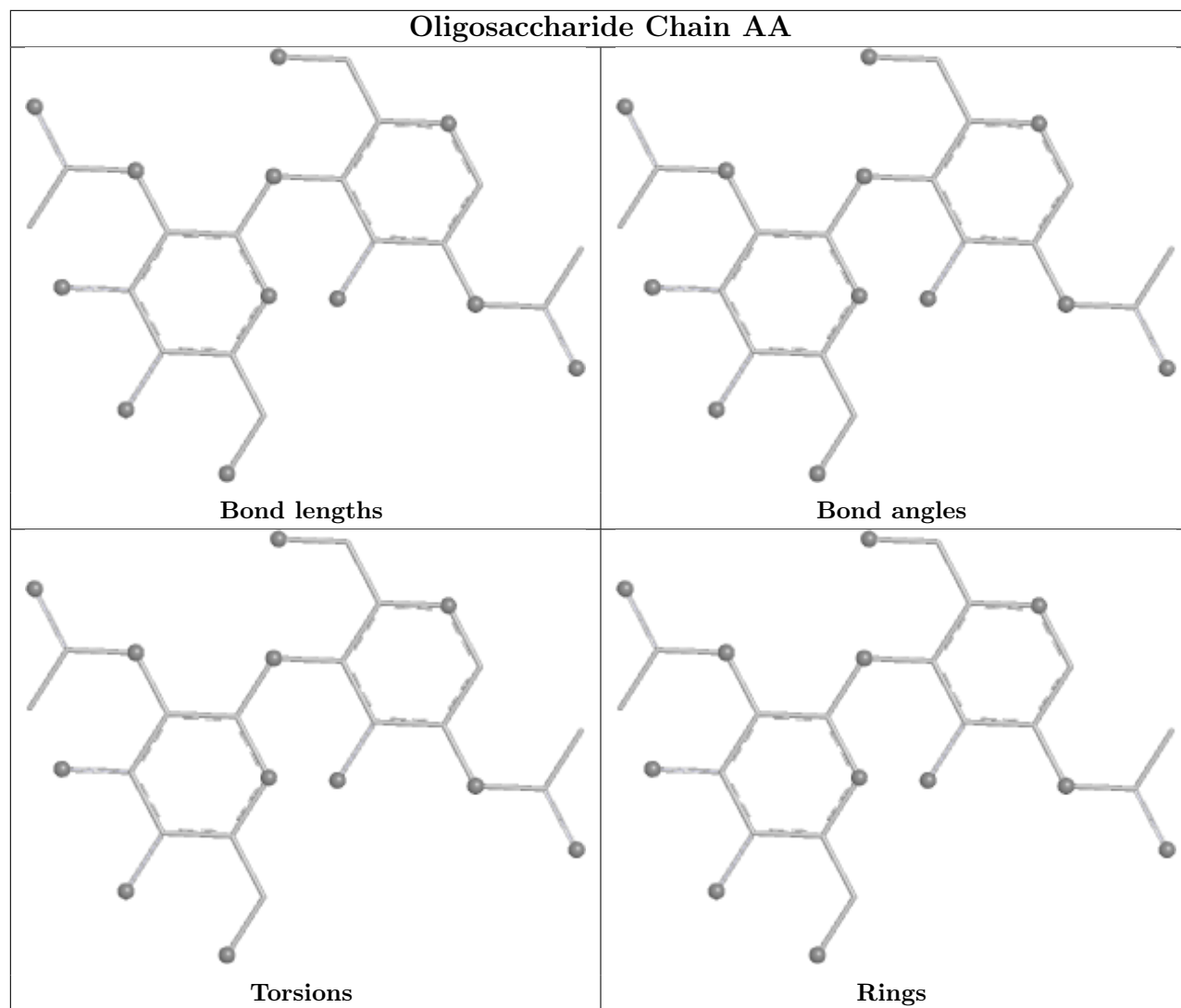


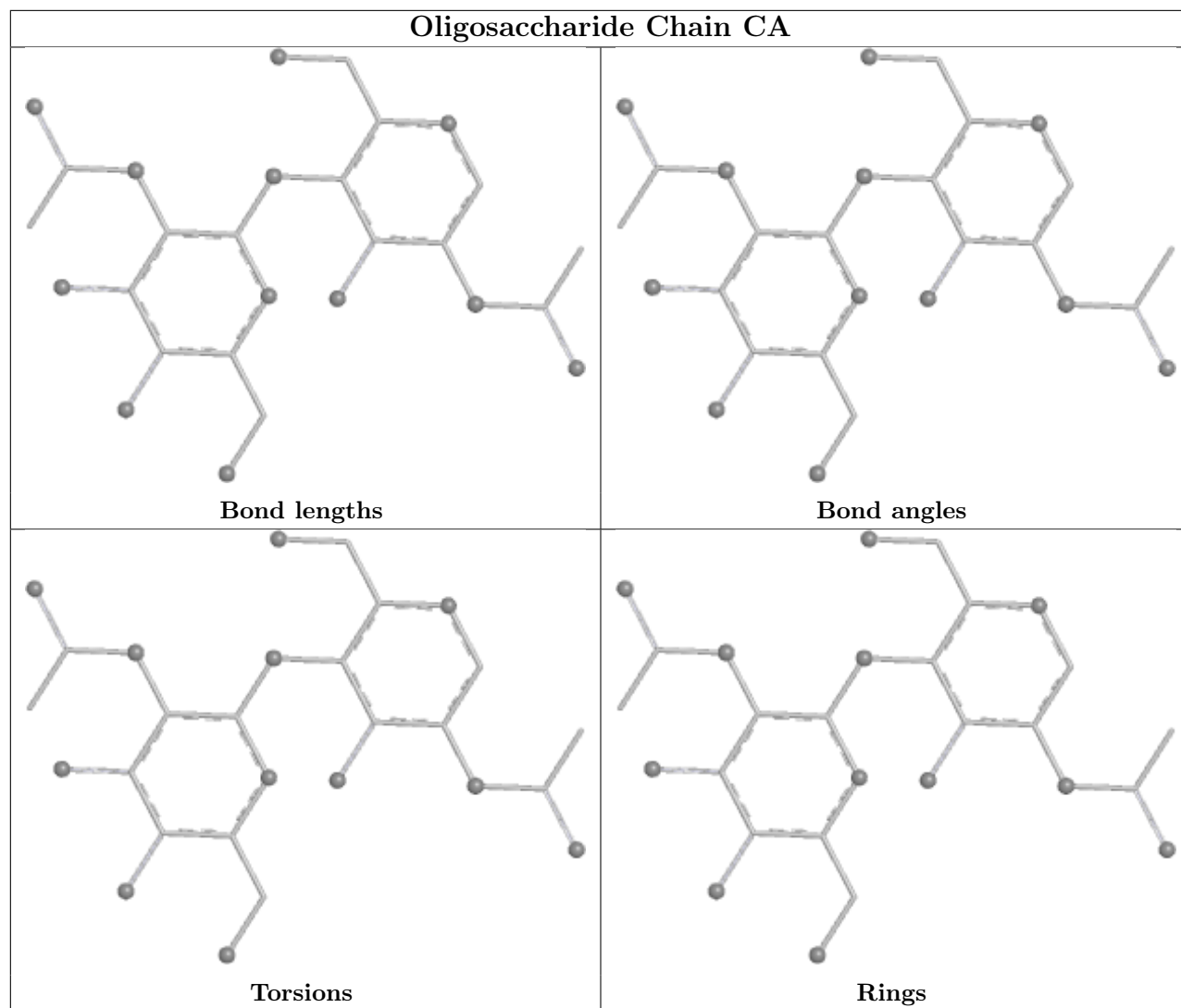


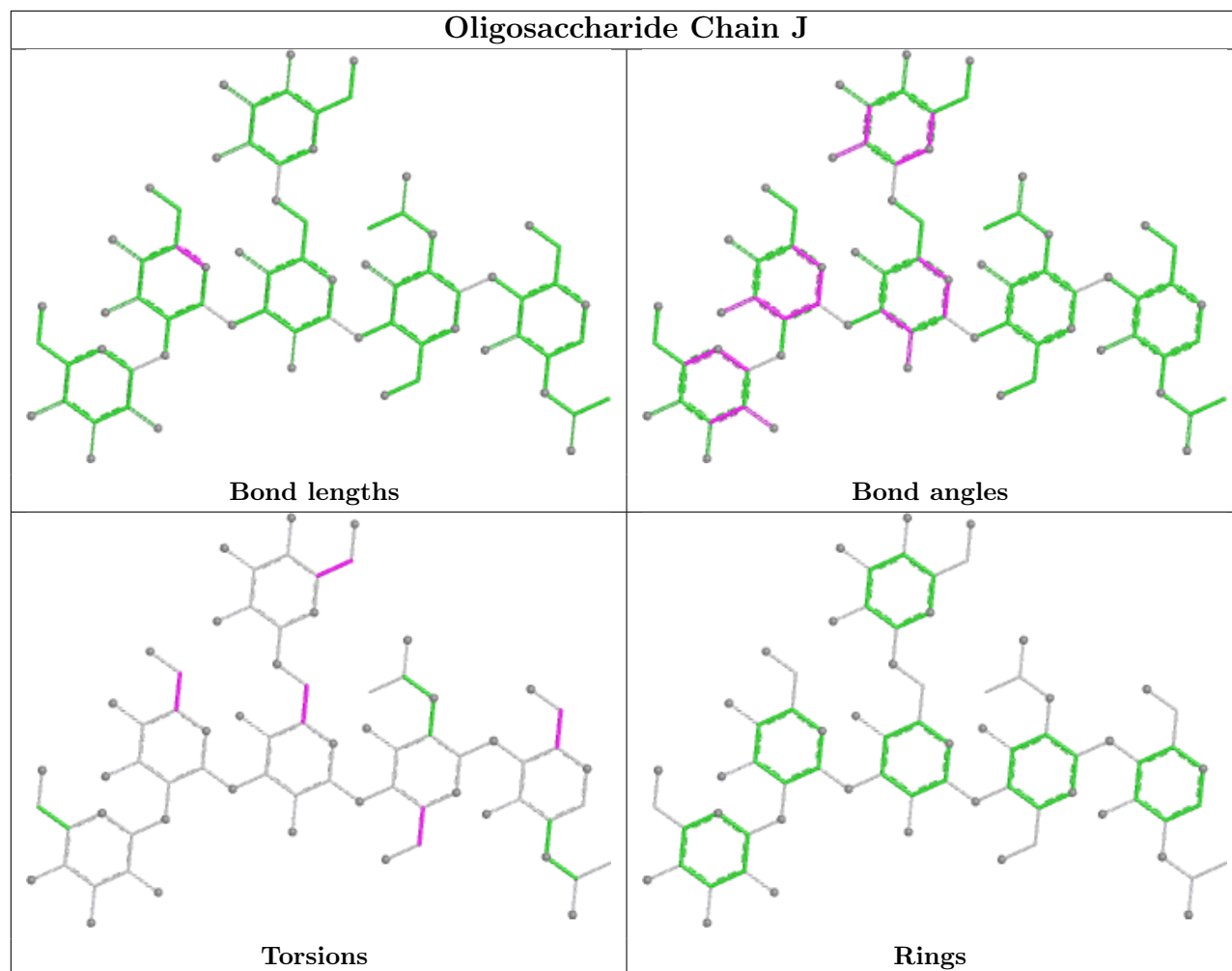


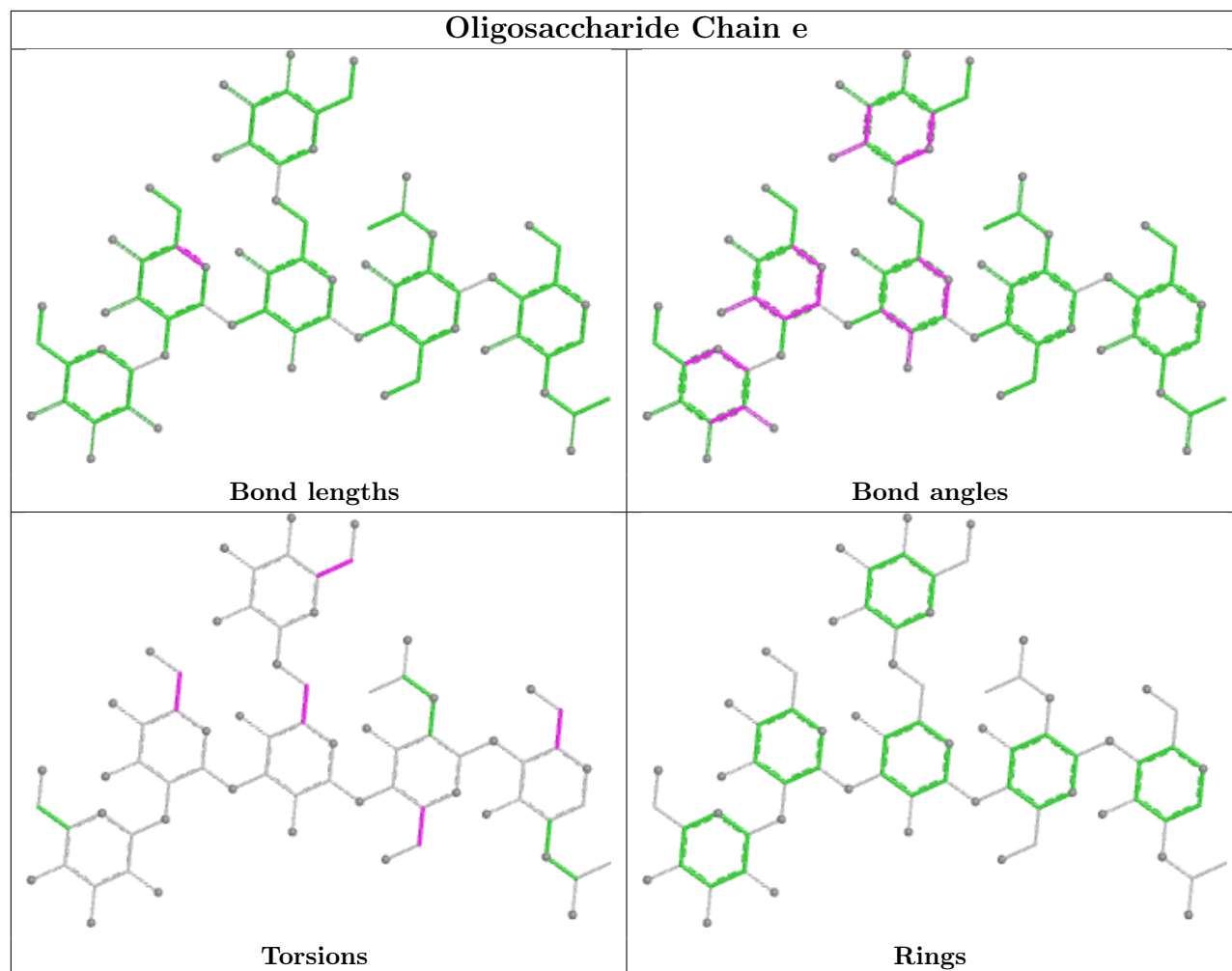


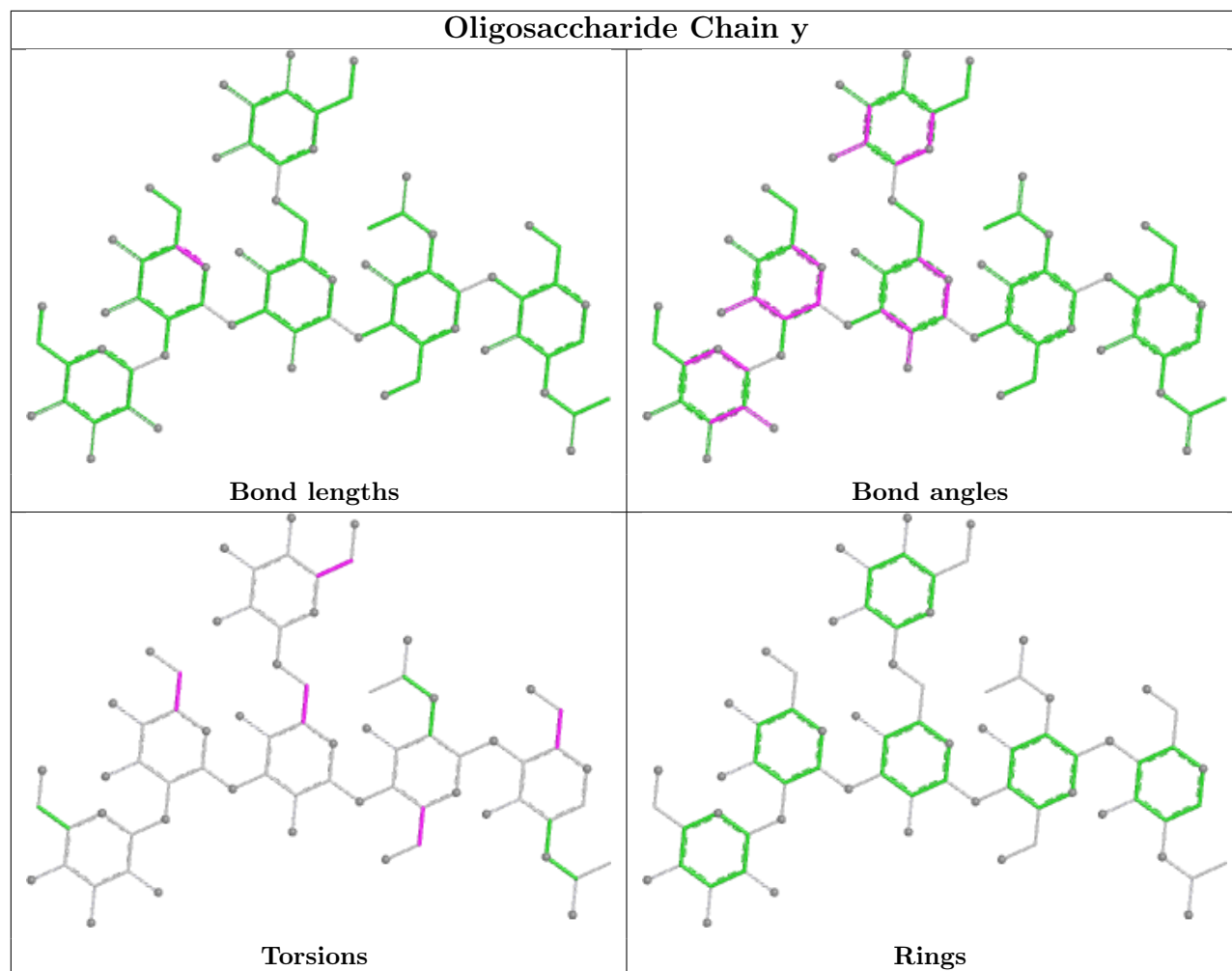


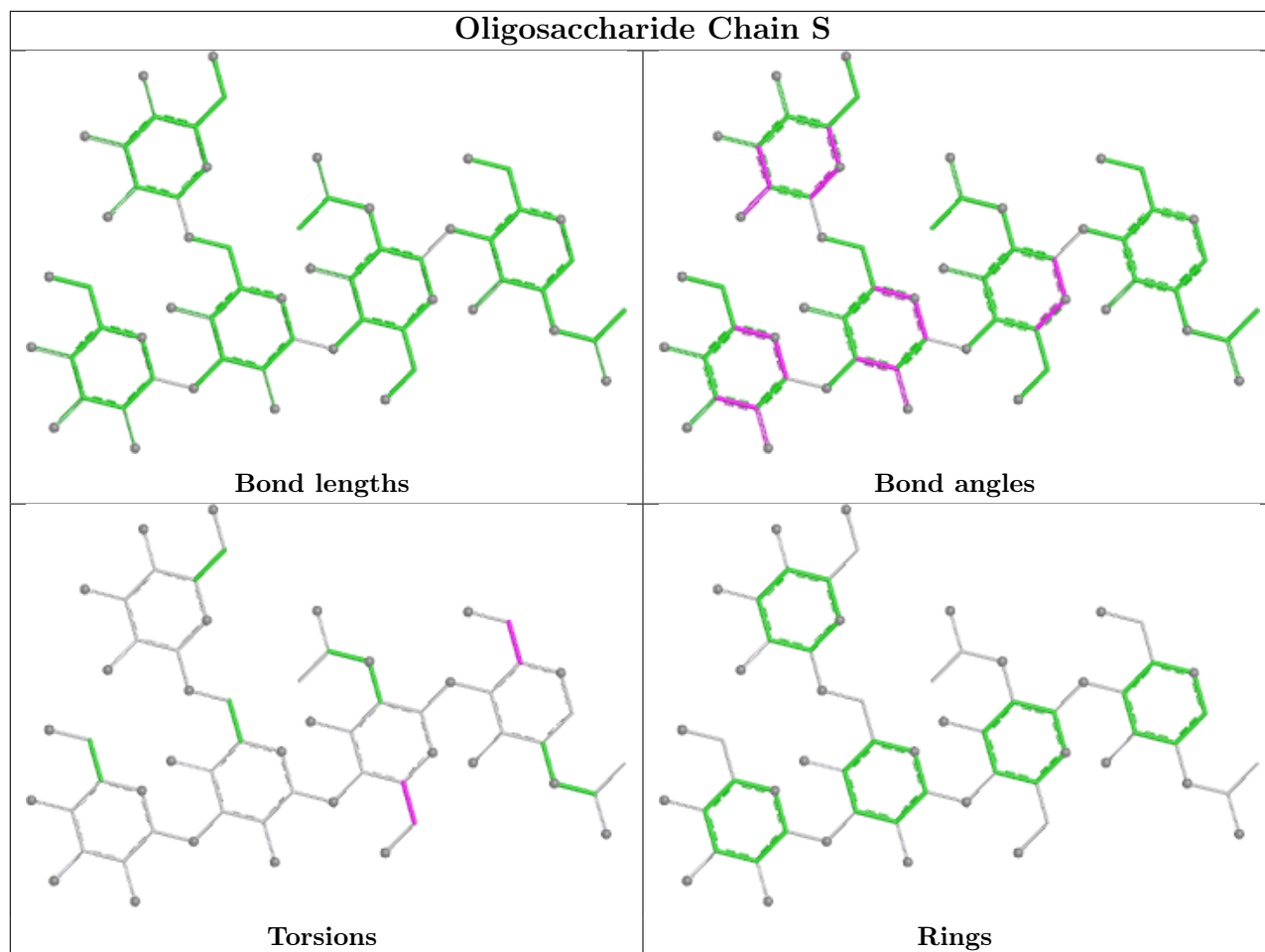


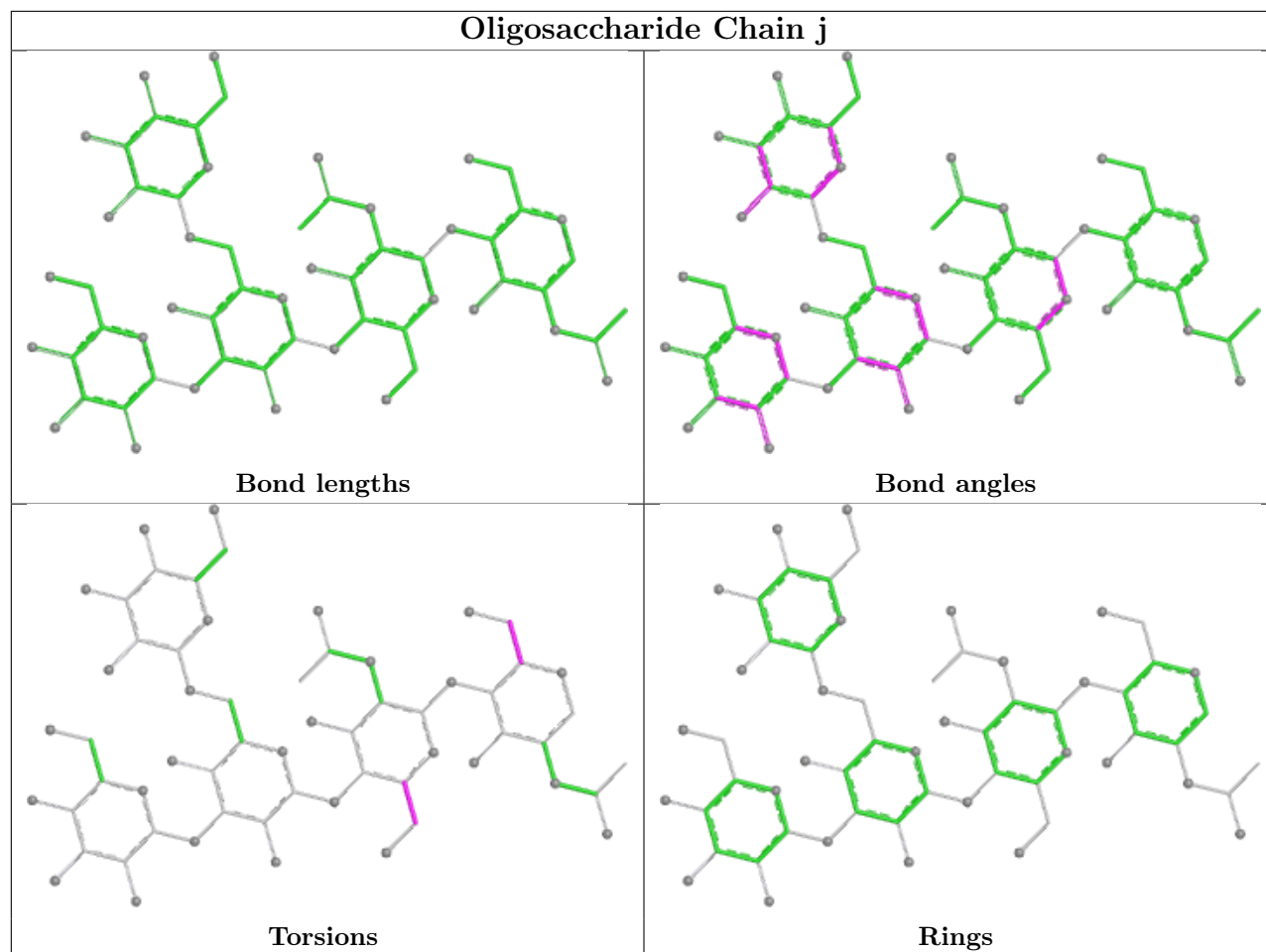


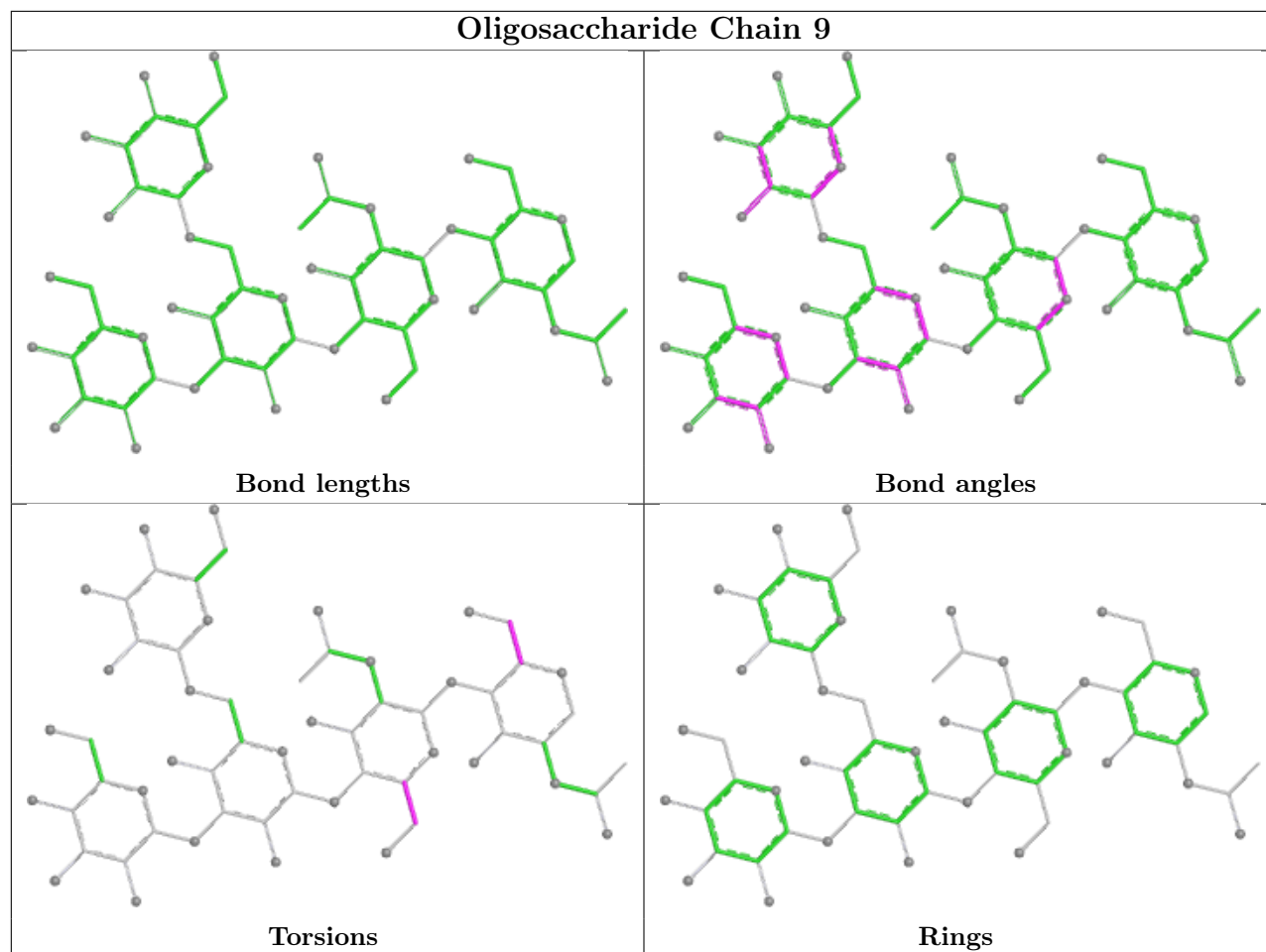


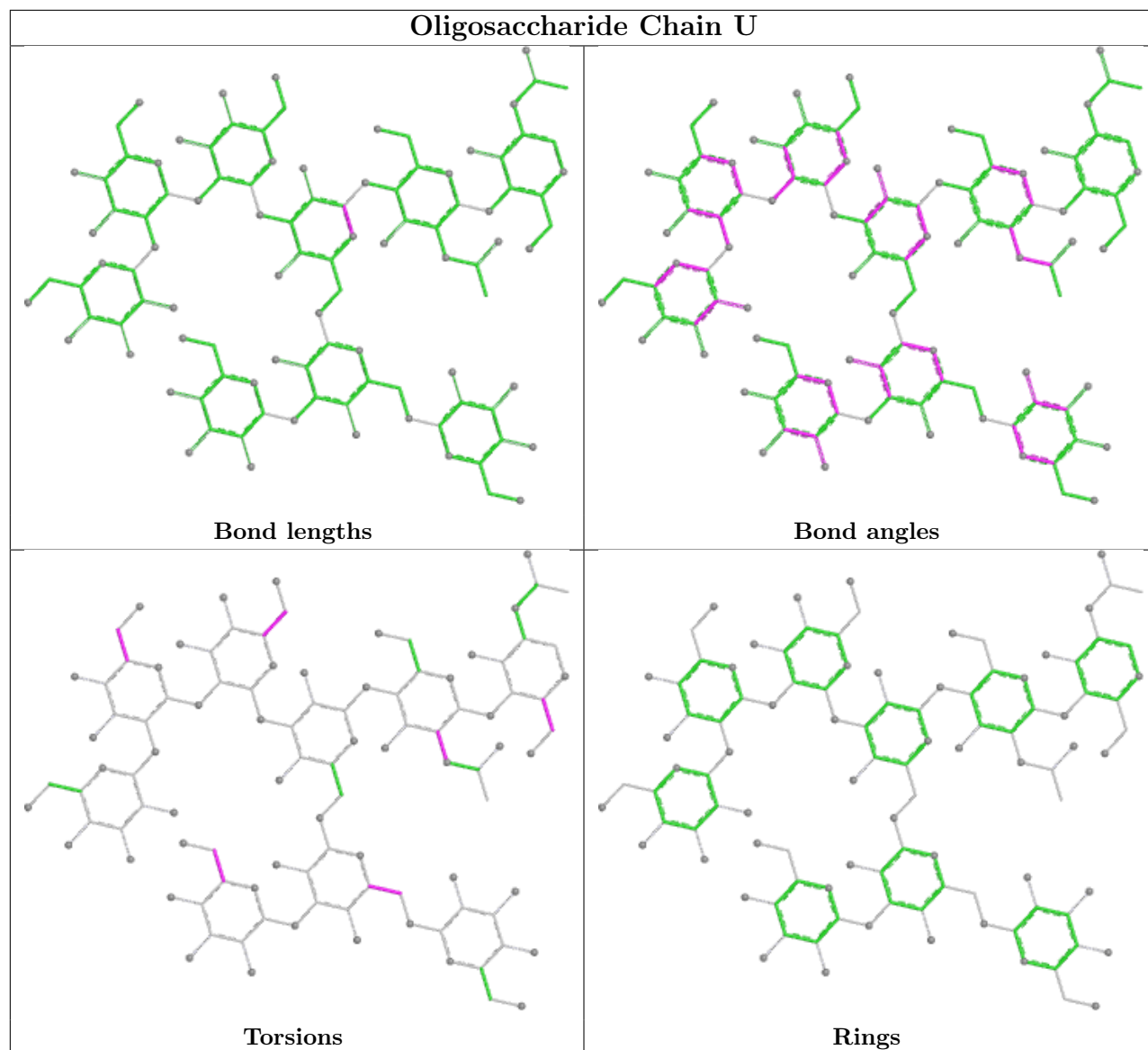


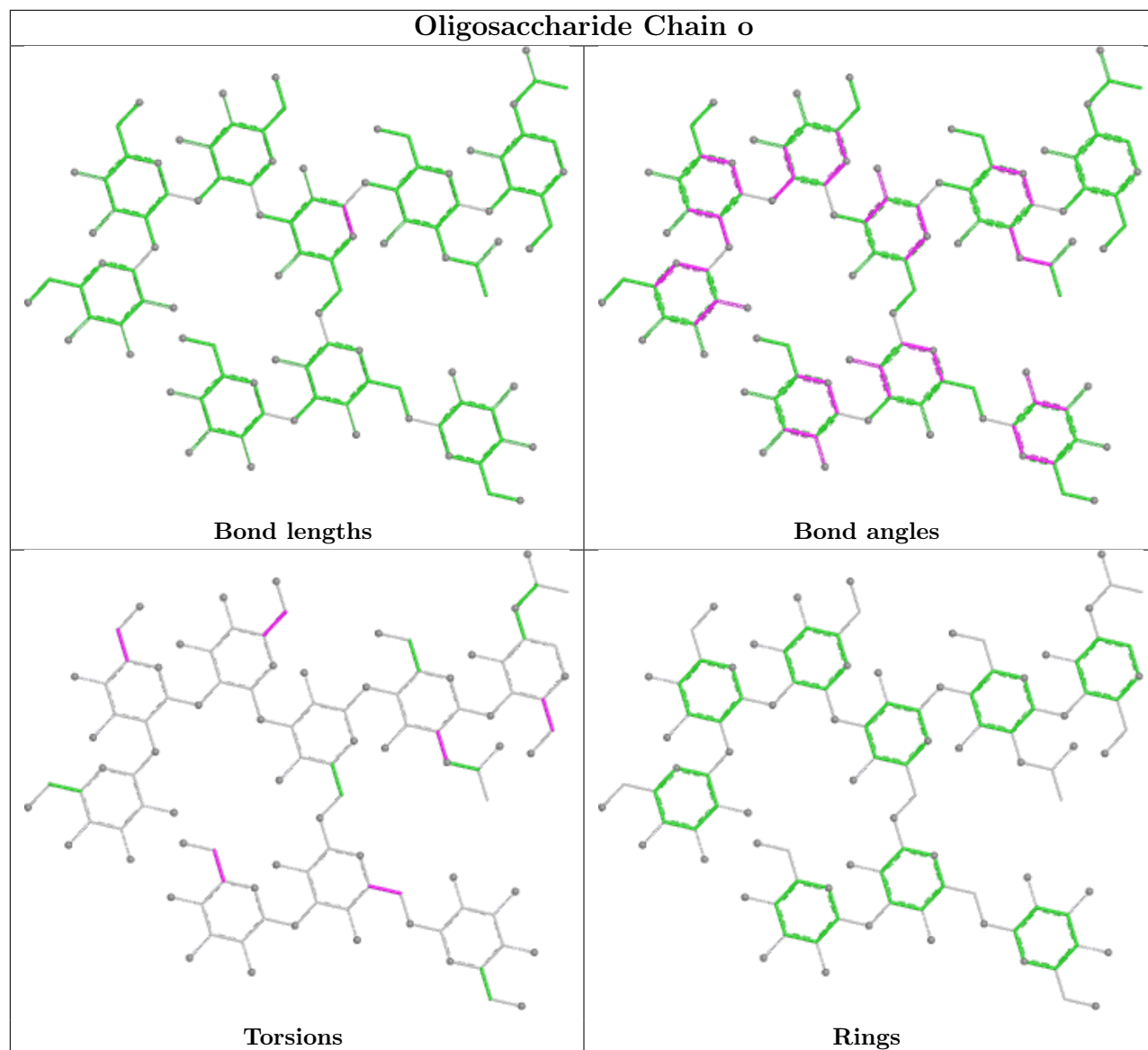


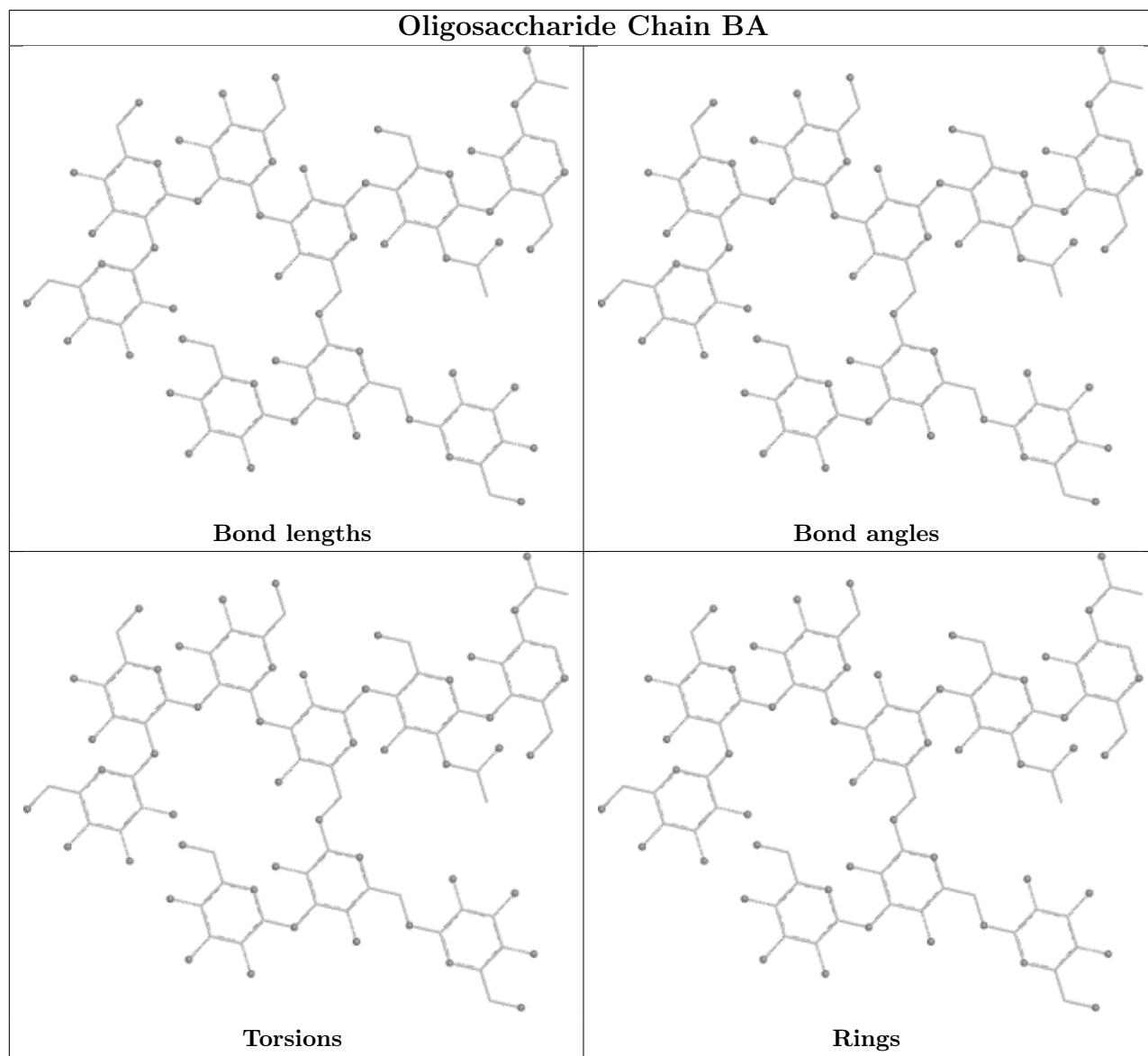












5.6 Ligand geometry [i](#)

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
15	NAG	A	701	8	14,14,15	0.19	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	d	601	7	14,14,15	0.32	0	17,19,21	1.09	1 (5%)
15	NAG	d	602	7	14,14,15	0.31	0	17,19,21	0.49	0
15	NAG	2	602	7	14,14,15	0.31	0	17,19,21	0.50	0
15	NAG	2	601	7	14,14,15	0.32	0	17,19,21	1.09	1 (5%)
15	NAG	D	701	8	14,14,15	0.19	0	17,19,21	0.47	0
15	NAG	C	601	7	14,14,15	0.32	0	17,19,21	1.09	1 (5%)
15	NAG	C	602	7	14,14,15	0.32	0	17,19,21	0.50	0
15	NAG	c	701	8	14,14,15	0.19	0	17,19,21	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	A	701	8	-	2/6/23/26	0/1/1/1
15	NAG	d	601	7	-	4/6/23/26	0/1/1/1
15	NAG	d	602	7	-	2/6/23/26	0/1/1/1
15	NAG	2	602	7	-	2/6/23/26	0/1/1/1
15	NAG	2	601	7	-	4/6/23/26	0/1/1/1
15	NAG	D	701	8	-	2/6/23/26	0/1/1/1
15	NAG	C	601	7	-	4/6/23/26	0/1/1/1
15	NAG	C	602	7	-	2/6/23/26	0/1/1/1
15	NAG	c	701	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	601	NAG	C2-N2-C7	3.29	127.30	122.90
15	2	601	NAG	C2-N2-C7	3.27	127.29	122.90
15	C	601	NAG	C2-N2-C7	3.26	127.27	122.90

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	D	701	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	A	701	NAG	O5-C5-C6-O6
15	c	701	NAG	O5-C5-C6-O6
15	D	701	NAG	C4-C5-C6-O6
15	A	701	NAG	C4-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.

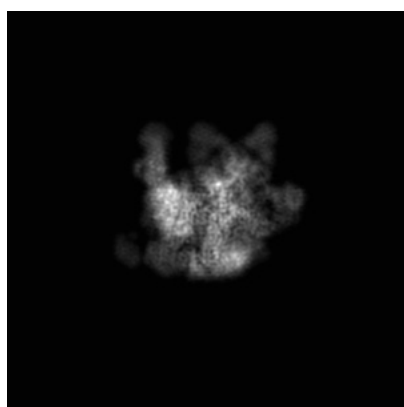
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7622. These allow visual inspection of the internal detail of the map and identification of artifacts.

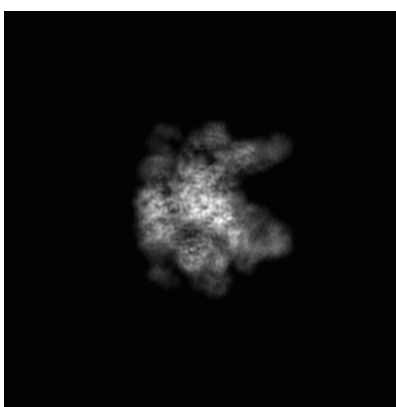
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

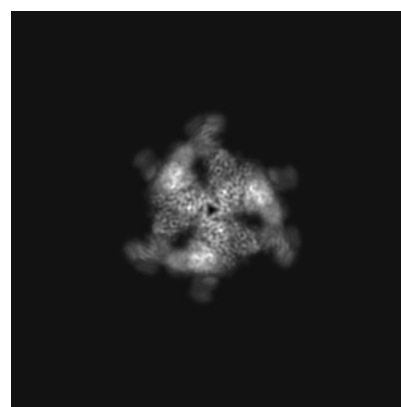
6.1.1 Primary map



X



Y

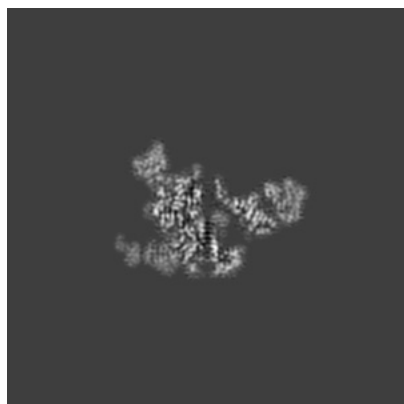


Z

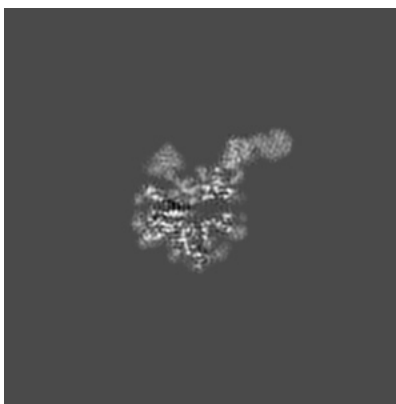
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

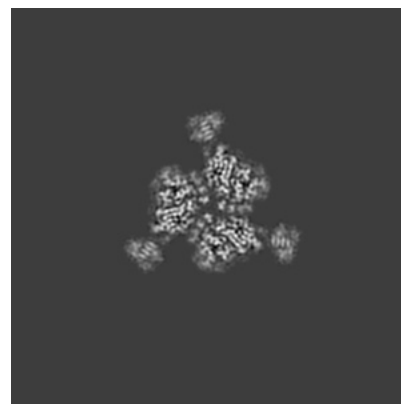
6.2.1 Primary map



X Index: 192



Y Index: 192

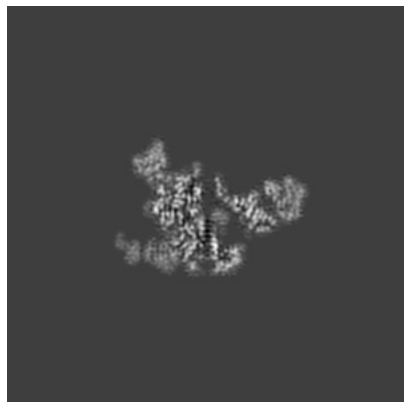


Z Index: 192

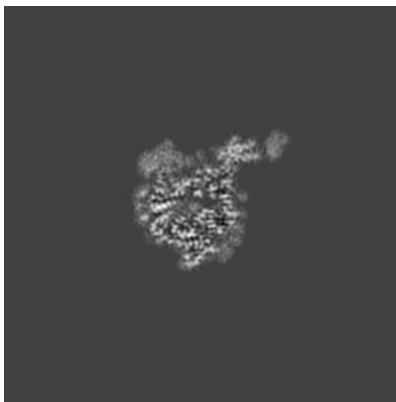
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

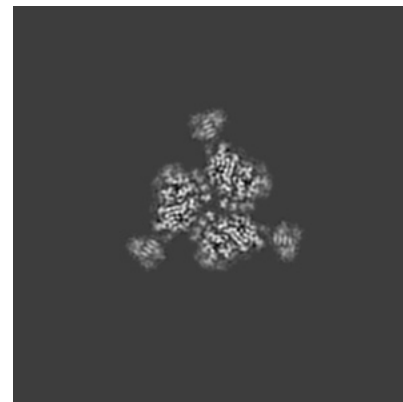
6.3.1 Primary map



X Index: 192



Y Index: 200

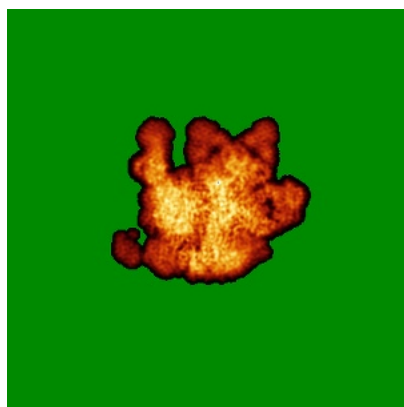


Z Index: 192

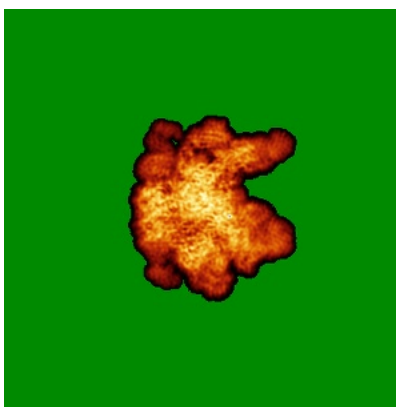
The images above show the largest variance slices of the map in three orthogonal directions.

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

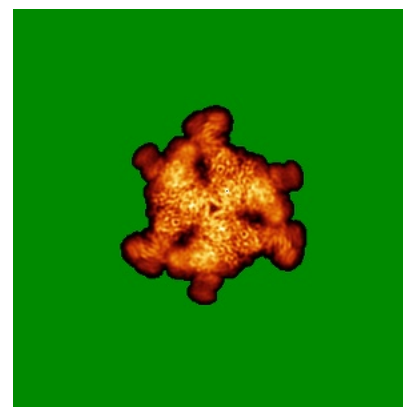
6.4.1 Primary map



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

This section was not generated.

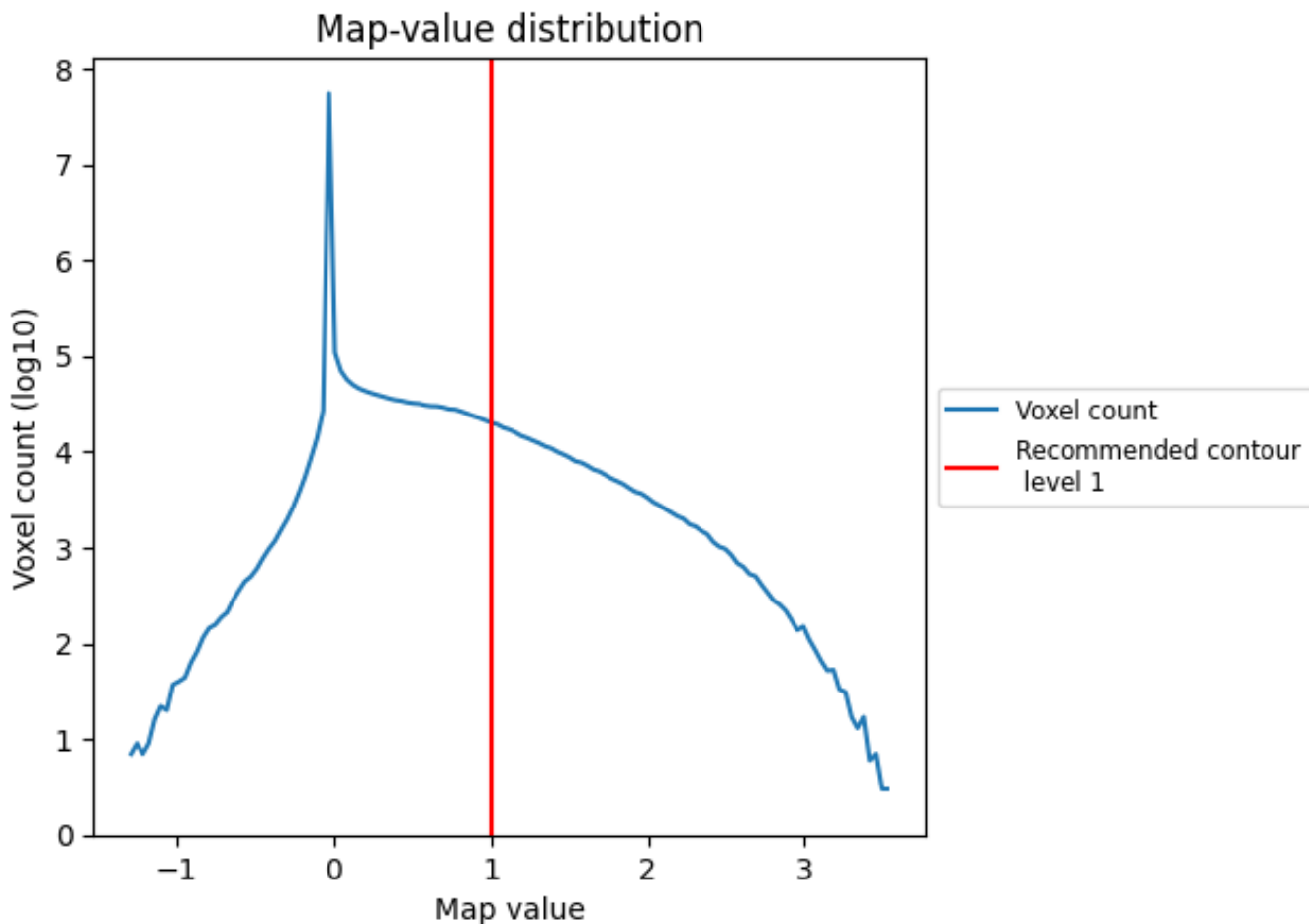
6.6 Mask visualisation

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

7 Map analysis [i](#)

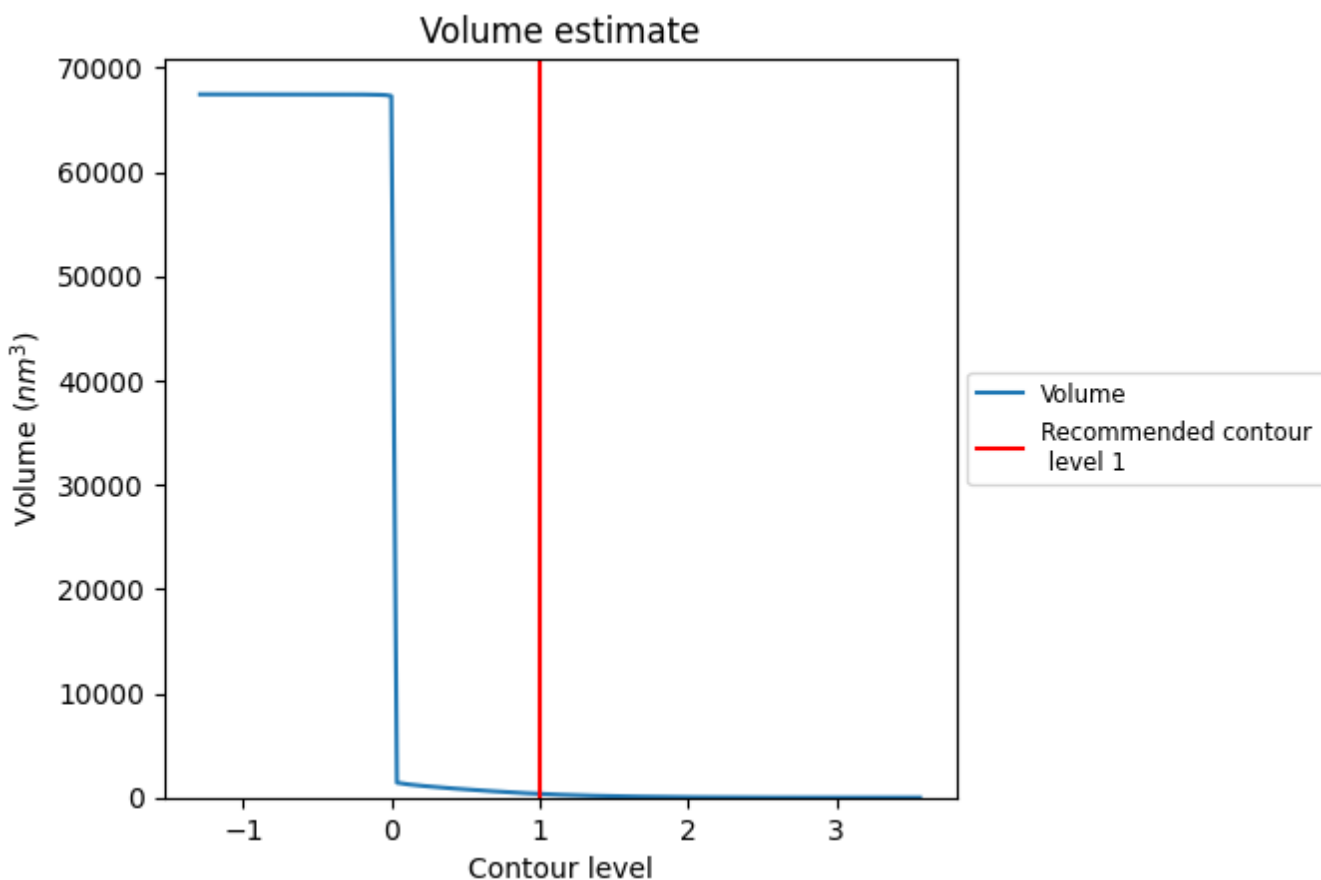
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

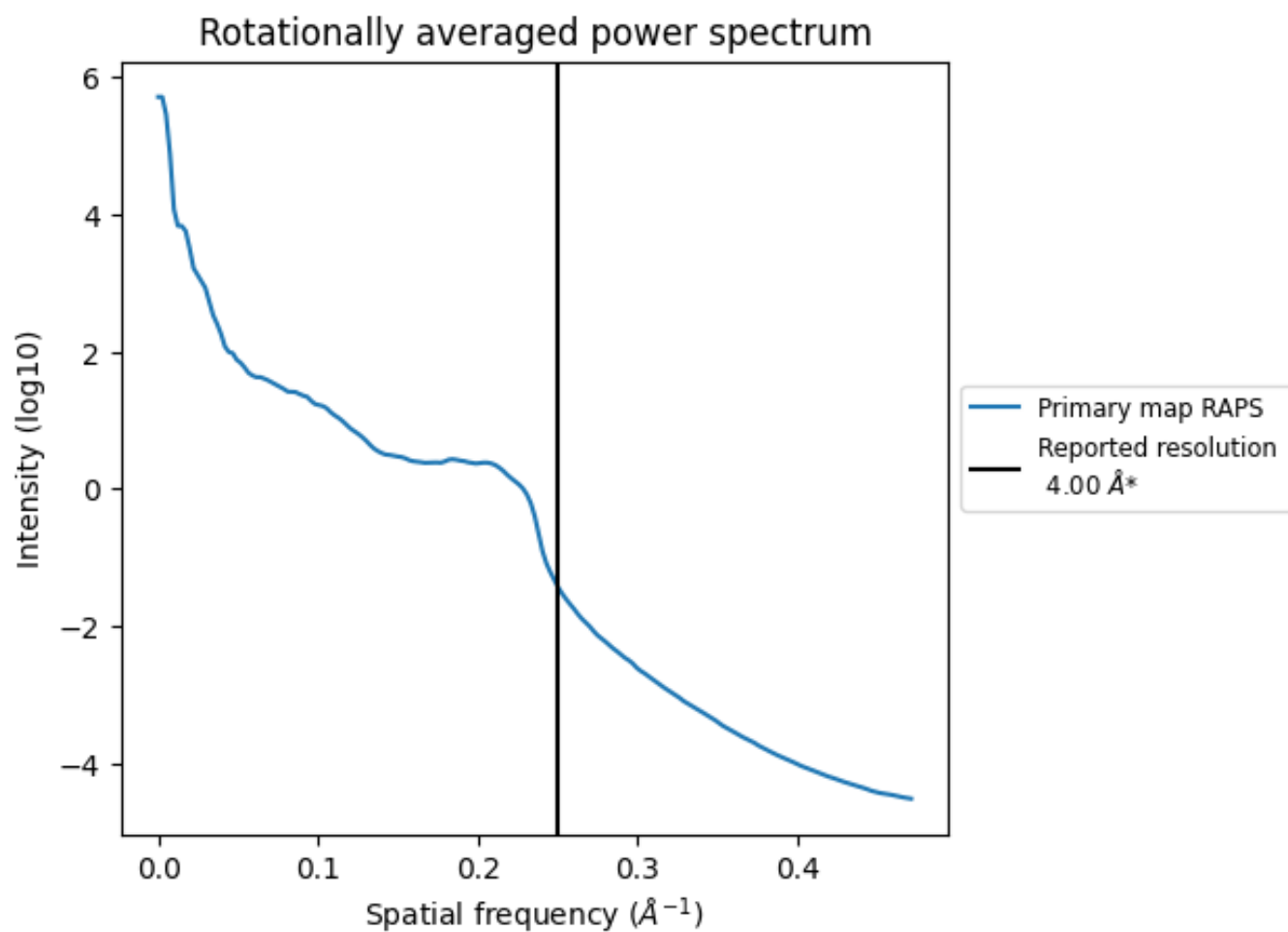
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 354 nm³; this corresponds to an approximate mass of 320 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

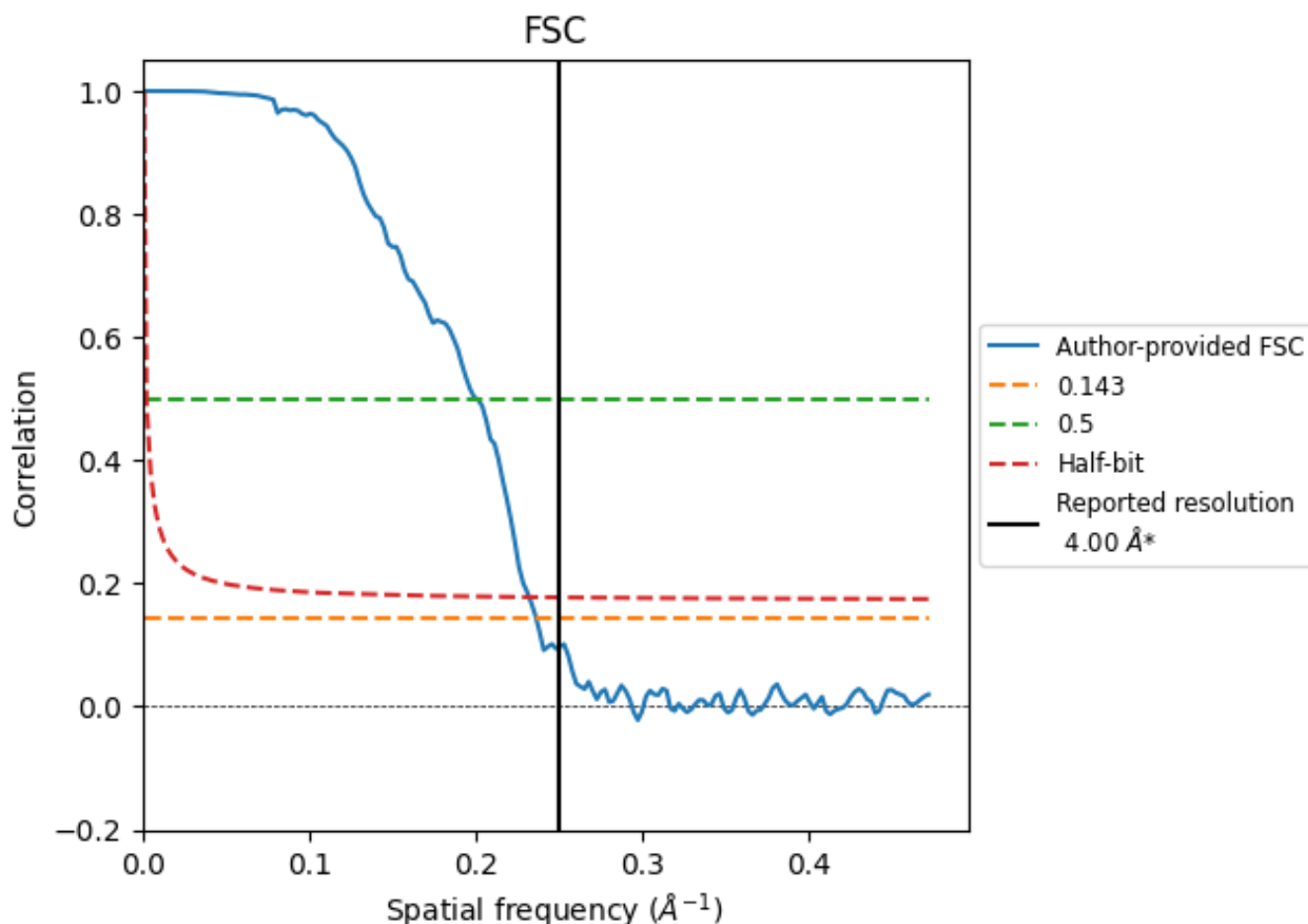


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.23	4.99	4.31
Unmasked-calculated*	-	-	-

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

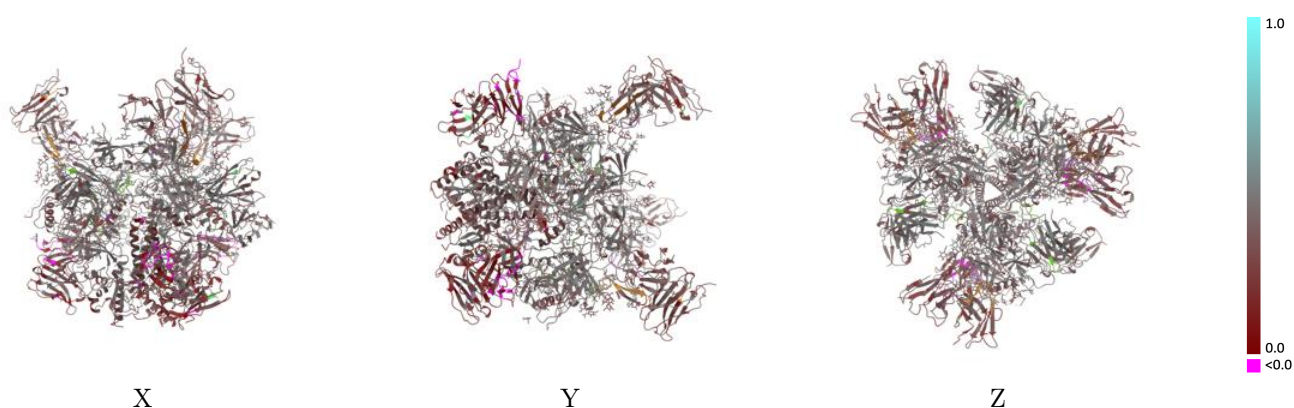
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7622 and PDB model 6CUF. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

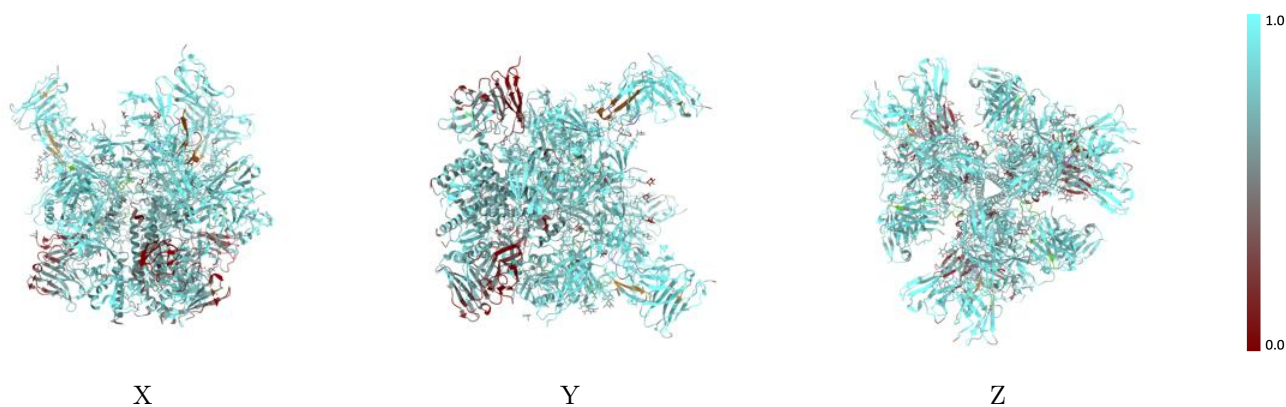
This section was not generated.

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



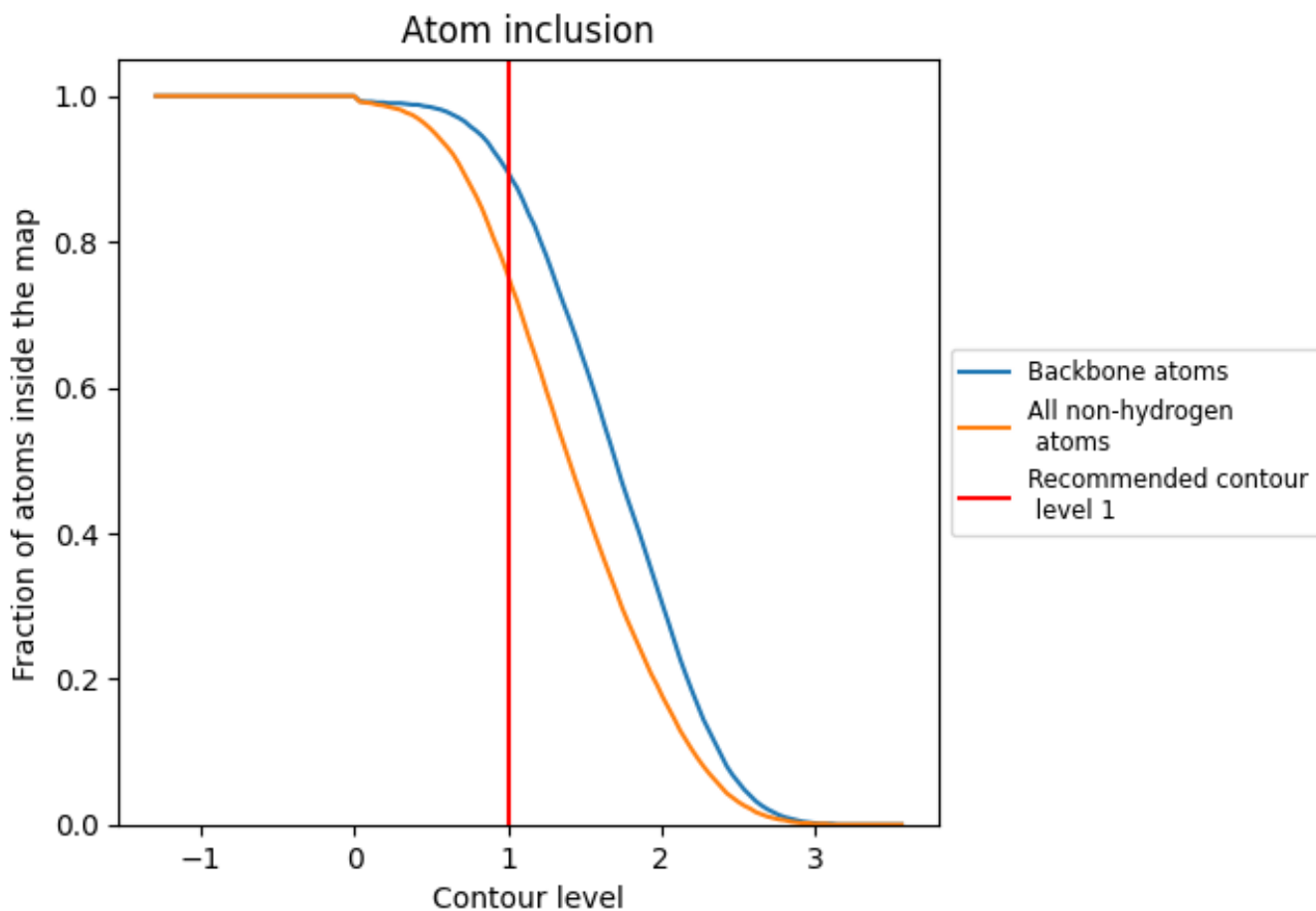
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 76% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.3610
0	 0.6790	 0.4260
1	 0.9490	 0.4560
2	 0.8070	 0.4080
3	 0.5750	 0.2560
4	 0.2880	 0.1720
5	 0.8470	 0.3370
6	 0.9060	 0.3640
7	 0.8280	 0.4010
8	 0.8530	 0.4230
9	 0.6720	 0.3740
A	 0.7970	 0.3550
AA	 0.5360	 0.3520
B	 0.8200	 0.4080
BA	 0.8760	 0.4310
C	 0.8100	 0.4090
CA	 0.6430	 0.3780
D	 0.7950	 0.3590
DA	 0.6600	 0.4040
E	 0.7600	 0.4350
F	 0.5380	 0.3540
G	 0.4290	 0.3670
H	 0.5760	 0.2580
I	 0.6920	 0.3770
J	 0.6940	 0.4310
K	 0.7500	 0.4430
L	 0.2810	 0.1700
M	 0.8480	 0.3370
N	 0.8920	 0.3620
O	 0.6430	 0.4190
P	 0.9490	 0.4660
Q	 0.8490	 0.4220
R	 0.8350	 0.4040
S	 0.6720	 0.3610
T	 0.5710	 0.3530



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Chain	Atom inclusion	Q-score
U	 0.8760	 0.4290
V	 0.6430	 0.3750
W	 0.6600	 0.4090
X	 0.8200	 0.4110
Y	 0.7400	 0.4330
Z	 0.5640	 0.3670
a	 0.3930	 0.3680
b	 0.6920	 0.3820
c	 0.7940	 0.3590
d	 0.8090	 0.4090
e	 0.6670	 0.4330
f	 0.7500	 0.4440
g	 0.6430	 0.4330
h	 0.5720	 0.2500
i	 0.9490	 0.4640
j	 0.6560	 0.3630
k	 0.5710	 0.3580
l	 0.2830	 0.1720
m	 0.8520	 0.3360
n	 0.8970	 0.3610
o	 0.8760	 0.4280
p	 0.6430	 0.3740
q	 0.8560	 0.4190
r	 0.8370	 0.4000
s	 0.6800	 0.4090
t	 0.8200	 0.4120
u	 0.7400	 0.4370
v	 0.5380	 0.3630
w	 0.4290	 0.3780
x	 0.6670	 0.3810
y	 0.6810	 0.4260
z	 0.7500	 0.4330