



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 08:06 AM UTC

PDB ID : 9BIO / pdb_00009bio
EMDB ID : EMD-44595
Title : Structure of VRC44.01 Fab in complex with 3BNC117-purified C1080.c3 RnS
SOSIP.664 HIV-1 Env trimer
Authors : Gorman, J.; Kwong, P.D.
Deposited on : 2024-04-23
Resolution : 2.83 Å(reported)
Based on initial model : 6VTT

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.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

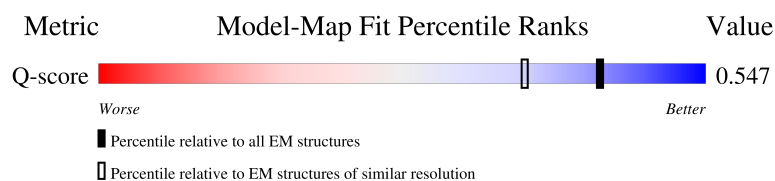
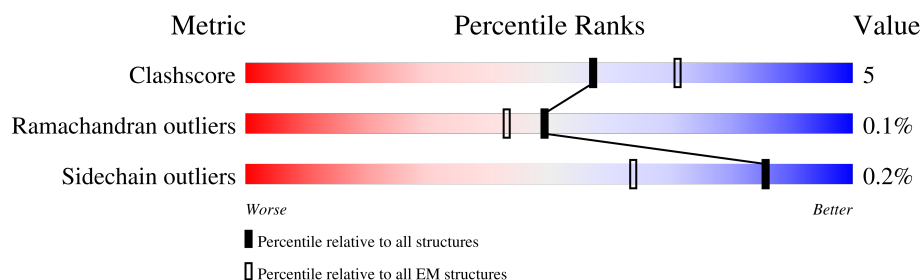
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

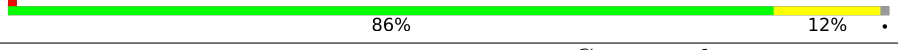
The reported resolution of this entry is 2.83 Å.

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.



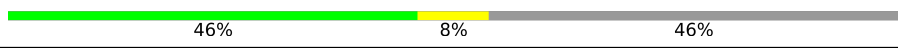
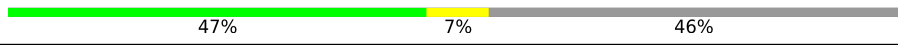
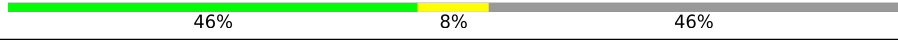
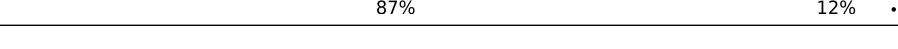
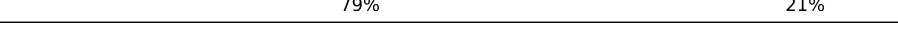
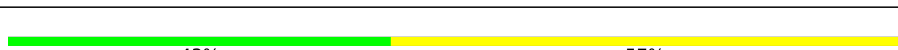
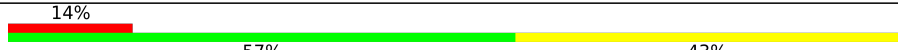
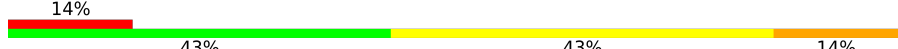
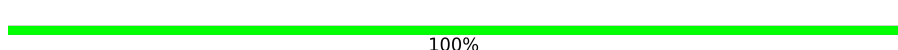
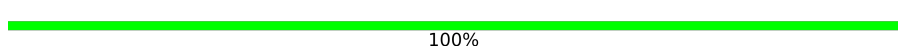
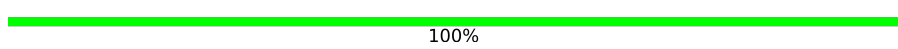
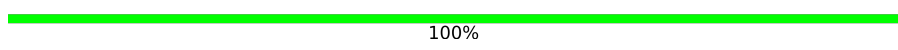
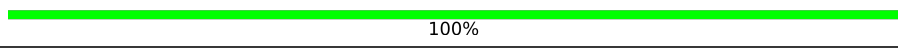
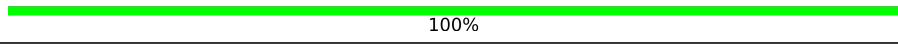
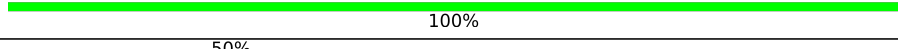
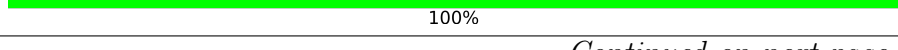
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	170	
1	B	170	
1	J	170	
2	C	478	

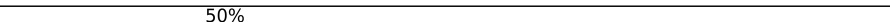
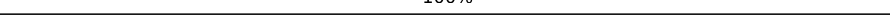
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	478	
2	K	478	
3	D	226	
3	M	226	
3	S	226	
4	E	206	
4	N	206	
4	U	206	
5	F	107	
5	L	107	
5	O	107	
6	H	124	
6	I	124	
6	P	124	
7	Q	7	
7	g	7	
7	u	7	
8	0	2	
8	2	2	
8	4	2	
8	5	2	
8	6	2	
8	R	2	
8	T	2	
8	Y	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	a	2	 100%
8	c	2	 100%
8	d	2	 100%
8	e	2	 100%
8	f	2	 50% 100%
8	h	2	 100%
8	i	2	 100%
8	m	2	 100%
8	o	2	 100%
8	q	2	 100%
8	r	2	 100%
8	s	2	 100%
8	t	2	 50% 100%
8	v	2	 100%
8	w	2	 100%
9	V	5	 60% 40%
9	j	5	 60% 40%
9	x	5	 60% 40%
10	W	9	 33% 67%
10	k	9	 33% 67%
10	y	9	 33% 67%
11	3	7	 14% 86%
11	X	7	 43% 43% 14%
11	b	7	 14% 86%
11	l	7	 43% 57%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	p	7	14% 14% 86%
11	z	7	43% 43% 14%
12	1	3	33% 100%
12	Z	3	33% 100%
12	n	3	100%



2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 27498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	136	Total	C	N	O	S	0	0
			1088	696	183	203	6		
1	A	136	Total	C	N	O	S	0	0
			1088	696	183	203	6		
1	J	136	Total	C	N	O	S	0	0
			1088	696	183	203	6		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	535	ASN	ILE	conflict	UNP I6NF57
B	556	PRO	LEU	conflict	UNP I6NF57
B	559	PRO	ILE	conflict	UNP I6NF57
B	588	GLU	LYS	conflict	UNP I6NF57
B	589	VAL	ASP	conflict	UNP I6NF57
B	605	CYS	THR	conflict	UNP I6NF57
B	651	PHE	ASN	conflict	UNP I6NF57
B	655	ILE	ARG	conflict	UNP I6NF57
B	658	VAL	LYS	conflict	UNP I6NF57
B	665	GLY	-	expression tag	UNP I6NF57
B	666	SER	-	expression tag	UNP I6NF57
B	667	ALA	-	expression tag	UNP I6NF57
B	668	PRO	-	expression tag	UNP I6NF57
B	669	THR	-	expression tag	UNP I6NF57
B	670	LYS	-	expression tag	UNP I6NF57
B	671	ALA	-	expression tag	UNP I6NF57
B	672	LYS	-	expression tag	UNP I6NF57
B	673	ARG	-	expression tag	UNP I6NF57
B	674	ARG	-	expression tag	UNP I6NF57
B	675	VAL	-	expression tag	UNP I6NF57
B	676	VAL	-	expression tag	UNP I6NF57
B	677	GLN	-	expression tag	UNP I6NF57
B	678	ARG	-	expression tag	UNP I6NF57
B	679	GLU	-	expression tag	UNP I6NF57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	680	LYS	-	expression tag	UNP I6NF57
B	681	ARG	-	expression tag	UNP I6NF57
A	535	ASN	ILE	conflict	UNP I6NF57
A	556	PRO	LEU	conflict	UNP I6NF57
A	559	PRO	ILE	conflict	UNP I6NF57
A	588	GLU	LYS	conflict	UNP I6NF57
A	589	VAL	ASP	conflict	UNP I6NF57
A	605	CYS	THR	conflict	UNP I6NF57
A	651	PHE	ASN	conflict	UNP I6NF57
A	655	ILE	ARG	conflict	UNP I6NF57
A	658	VAL	LYS	conflict	UNP I6NF57
A	665	GLY	-	expression tag	UNP I6NF57
A	666	SER	-	expression tag	UNP I6NF57
A	667	ALA	-	expression tag	UNP I6NF57
A	668	PRO	-	expression tag	UNP I6NF57
A	669	THR	-	expression tag	UNP I6NF57
A	670	LYS	-	expression tag	UNP I6NF57
A	671	ALA	-	expression tag	UNP I6NF57
A	672	LYS	-	expression tag	UNP I6NF57
A	673	ARG	-	expression tag	UNP I6NF57
A	674	ARG	-	expression tag	UNP I6NF57
A	675	VAL	-	expression tag	UNP I6NF57
A	676	VAL	-	expression tag	UNP I6NF57
A	677	GLN	-	expression tag	UNP I6NF57
A	678	ARG	-	expression tag	UNP I6NF57
A	679	GLU	-	expression tag	UNP I6NF57
A	680	LYS	-	expression tag	UNP I6NF57
A	681	ARG	-	expression tag	UNP I6NF57
J	535	ASN	ILE	conflict	UNP I6NF57
J	556	PRO	LEU	conflict	UNP I6NF57
J	559	PRO	ILE	conflict	UNP I6NF57
J	588	GLU	LYS	conflict	UNP I6NF57
J	589	VAL	ASP	conflict	UNP I6NF57
J	605	CYS	THR	conflict	UNP I6NF57
J	651	PHE	ASN	conflict	UNP I6NF57
J	655	ILE	ARG	conflict	UNP I6NF57
J	658	VAL	LYS	conflict	UNP I6NF57
J	665	GLY	-	expression tag	UNP I6NF57
J	666	SER	-	expression tag	UNP I6NF57
J	667	ALA	-	expression tag	UNP I6NF57
J	668	PRO	-	expression tag	UNP I6NF57
J	669	THR	-	expression tag	UNP I6NF57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	670	LYS	-	expression tag	UNP I6NF57
J	671	ALA	-	expression tag	UNP I6NF57
J	672	LYS	-	expression tag	UNP I6NF57
J	673	ARG	-	expression tag	UNP I6NF57
J	674	ARG	-	expression tag	UNP I6NF57
J	675	VAL	-	expression tag	UNP I6NF57
J	676	VAL	-	expression tag	UNP I6NF57
J	677	GLN	-	expression tag	UNP I6NF57
J	678	ARG	-	expression tag	UNP I6NF57
J	679	GLU	-	expression tag	UNP I6NF57
J	680	LYS	-	expression tag	UNP I6NF57
J	681	ARG	-	expression tag	UNP I6NF57

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	471	Total	C	N	O	S	0	0
			3722	2347	641	705	29		
2	C	471	Total	C	N	O	S	0	0
			3722	2347	641	705	29		
2	K	471	Total	C	N	O	S	0	0
			3722	2347	641	705	29		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	31	ALA	-	expression tag	UNP I6NF57
G	32	GLU	-	expression tag	UNP I6NF57
G	124	PRO	HIS	conflict	UNP I6NF57
G	179	LEU	THR	conflict	UNP I6NF57
G	201	CYS	ILE	conflict	UNP I6NF57
G	358	THR	LYS	conflict	UNP I6NF57
G	400	THR	GLY	conflict	UNP I6NF57
G	433	CYS	ALA	conflict	UNP I6NF57
G	501	CYS	ALA	conflict	UNP I6NF57
G	508	ARG	-	expression tag	UNP I6NF57
G	509	ARG	-	expression tag	UNP I6NF57
G	510	ARG	-	expression tag	UNP I6NF57
G	511	ARG	-	expression tag	UNP I6NF57
G	512	ARG	-	expression tag	UNP I6NF57
G	513	ARG	-	expression tag	UNP I6NF57
C	31	ALA	-	expression tag	UNP I6NF57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	GLU	-	expression tag	UNP I6NF57
C	124	PRO	HIS	conflict	UNP I6NF57
C	179	LEU	THR	conflict	UNP I6NF57
C	201	CYS	ILE	conflict	UNP I6NF57
C	358	THR	LYS	conflict	UNP I6NF57
C	400	THR	GLY	conflict	UNP I6NF57
C	433	CYS	ALA	conflict	UNP I6NF57
C	501	CYS	ALA	conflict	UNP I6NF57
C	508	ARG	-	expression tag	UNP I6NF57
C	509	ARG	-	expression tag	UNP I6NF57
C	510	ARG	-	expression tag	UNP I6NF57
C	511	ARG	-	expression tag	UNP I6NF57
C	512	ARG	-	expression tag	UNP I6NF57
C	513	ARG	-	expression tag	UNP I6NF57
K	31	ALA	-	expression tag	UNP I6NF57
K	32	GLU	-	expression tag	UNP I6NF57
K	124	PRO	HIS	conflict	UNP I6NF57
K	179	LEU	THR	conflict	UNP I6NF57
K	201	CYS	ILE	conflict	UNP I6NF57
K	358	THR	LYS	conflict	UNP I6NF57
K	400	THR	GLY	conflict	UNP I6NF57
K	433	CYS	ALA	conflict	UNP I6NF57
K	501	CYS	ALA	conflict	UNP I6NF57
K	508	ARG	-	expression tag	UNP I6NF57
K	509	ARG	-	expression tag	UNP I6NF57
K	510	ARG	-	expression tag	UNP I6NF57
K	511	ARG	-	expression tag	UNP I6NF57
K	512	ARG	-	expression tag	UNP I6NF57
K	513	ARG	-	expression tag	UNP I6NF57

- Molecule 3 is a protein called 3BNC117 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	D	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	M	121	Total	C	N	O	S	0	0
			985	626	177	179	3		

- Molecule 4 is a protein called 3BNC117 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
4	E	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
4	N	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

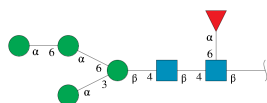
- Molecule 5 is a protein called VRC44.01 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	106	Total	C	N	O	S	0	0
			809	516	136	155	2		
5	F	106	Total	C	N	O	S	0	0
			809	516	136	155	2		
5	O	106	Total	C	N	O	S	0	0
			809	516	136	155	2		

- Molecule 6 is a protein called VRC44.01 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	119	Total	C	N	O	S	0	0
			951	604	165	178	4		
6	I	119	Total	C	N	O	S	0	0
			951	604	165	178	4		
6	P	119	Total	C	N	O	S	0	0
			951	604	165	178	4		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	7	Total	C	N	O	0	0
			82	46	2	34		
7	g	7	Total	C	N	O	0	0
			82	46	2	34		
7	u	7	Total	C	N	O	0	0
			82	46	2	34		

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



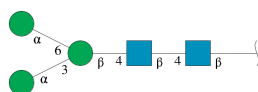
Mol	Chain	Residues	Atoms				AltConf	Trace
8	R	2	Total	C	N	O	0	0
			28	16	2	10		
8	T	2	Total	C	N	O	0	0
			28	16	2	10		
8	Y	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		
8	c	2	Total	C	N	O	0	0
			28	16	2	10		
8	d	2	Total	C	N	O	0	0
			28	16	2	10		
8	e	2	Total	C	N	O	0	0
			28	16	2	10		
8	f	2	Total	C	N	O	0	0
			28	16	2	10		
8	h	2	Total	C	N	O	0	0
			28	16	2	10		
8	i	2	Total	C	N	O	0	0
			28	16	2	10		
8	m	2	Total	C	N	O	0	0
			28	16	2	10		
8	o	2	Total	C	N	O	0	0
			28	16	2	10		
8	q	2	Total	C	N	O	0	0
			28	16	2	10		
8	r	2	Total	C	N	O	0	0
			28	16	2	10		
8	s	2	Total	C	N	O	0	0
			28	16	2	10		
8	t	2	Total	C	N	O	0	0
			28	16	2	10		
8	v	2	Total	C	N	O	0	0
			28	16	2	10		
8	w	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

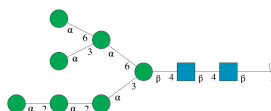
Mol	Chain	Residues	Atoms				AltConf	Trace
8	0	2	Total	C	N	O	0	0
			28	16	2	10		
8	2	2	Total	C	N	O	0	0
			28	16	2	10		
8	4	2	Total	C	N	O	0	0
			28	16	2	10		
8	5	2	Total	C	N	O	0	0
			28	16	2	10		
8	6	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

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



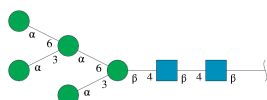
Mol	Chain	Residues	Atoms				AltConf	Trace
10	W	9	Total	C	N	O	0	0
			105	58	2	45		
10	k	9	Total	C	N	O	0	0
			105	58	2	45		

Continued on next page...

Continued from previous page...

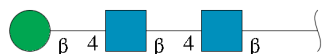
Mol	Chain	Residues	Atoms				AltConf	Trace
10	y	9	Total	C	N	O	0	0
			105	58	2	45		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	7	Total	C	N	O	0	0
			83	46	2	35		
11	b	7	Total	C	N	O	0	0
			83	46	2	35		
11	l	7	Total	C	N	O	0	0
			83	46	2	35		
11	p	7	Total	C	N	O	0	0
			83	46	2	35		
11	z	7	Total	C	N	O	0	0
			83	46	2	35		
11	3	7	Total	C	N	O	0	0
			83	46	2	35		

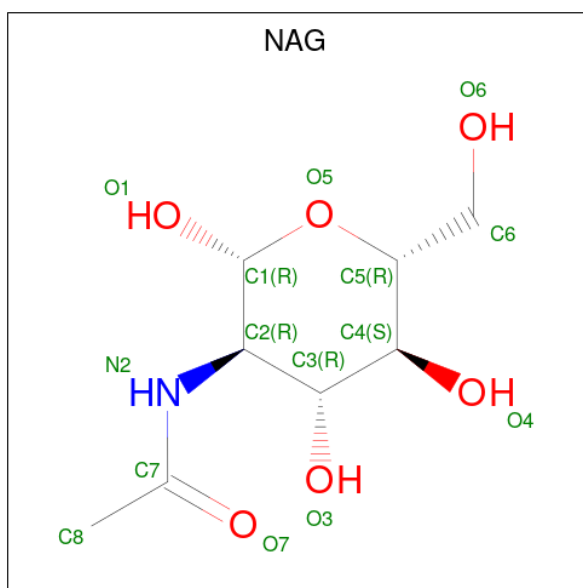
- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	Z	3	Total	C	N	O	0	0
			39	22	2	15		
12	n	3	Total	C	N	O	0	0
			39	22	2	15		
12	1	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



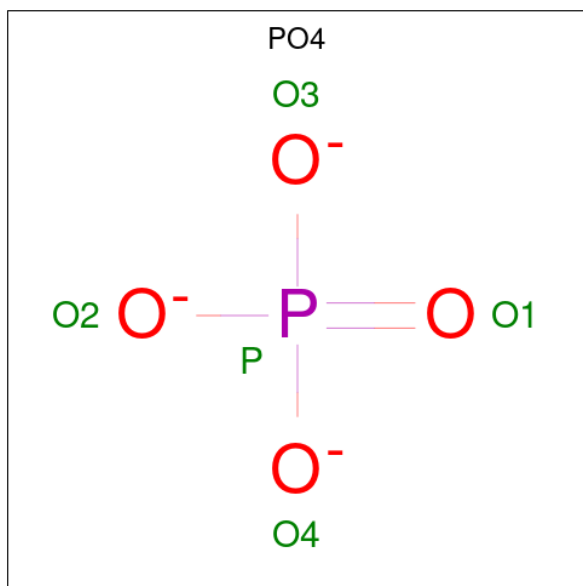
Mol	Chain	Residues	Atoms				AltConf
13	B	1	Total	C	N	O	0
			14	8	1	5	
13	B	1	Total	C	N	O	0
			14	8	1	5	
13	B	1	Total	C	N	O	0
			14	8	1	5	
13	G	1	Total	C	N	O	0
			14	8	1	5	
13	G	1	Total	C	N	O	0
			14	8	1	5	
13	G	1	Total	C	N	O	0
			14	8	1	5	
13	G	1	Total	C	N	O	0
			14	8	1	5	
13	G	1	Total	C	N	O	0
			14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

Continued on next page...

Continued from previous page...

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

- Molecule 14 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

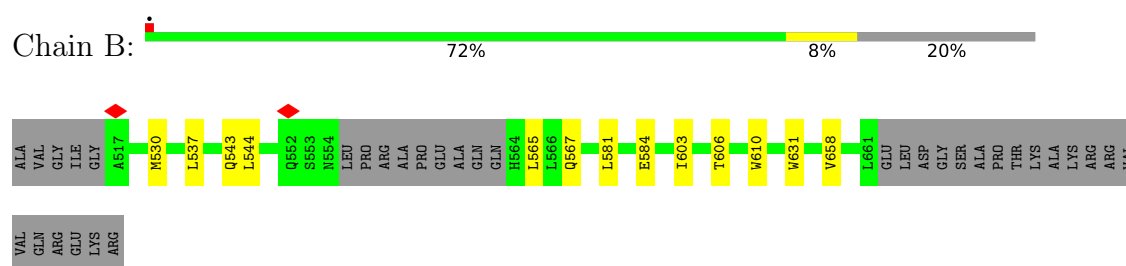


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
14	C	1	5	4	1	0

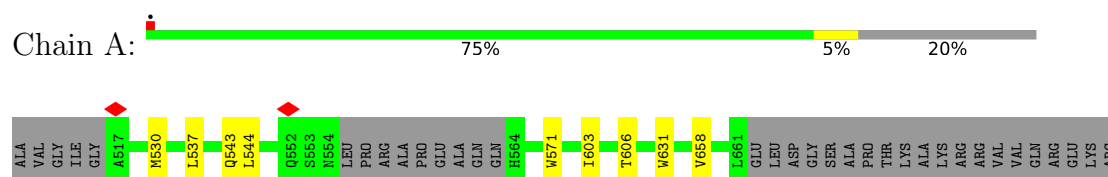
3 Residue-property plots [i](#)

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

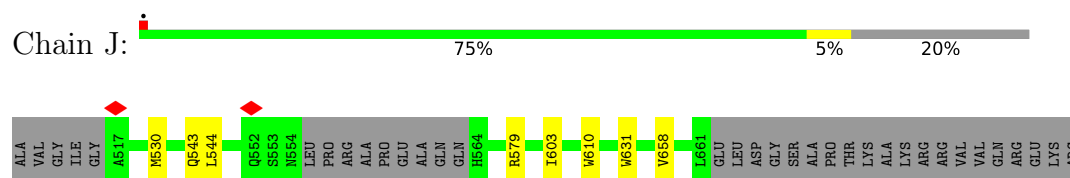
- Molecule 1: Envelope glycoprotein gp41



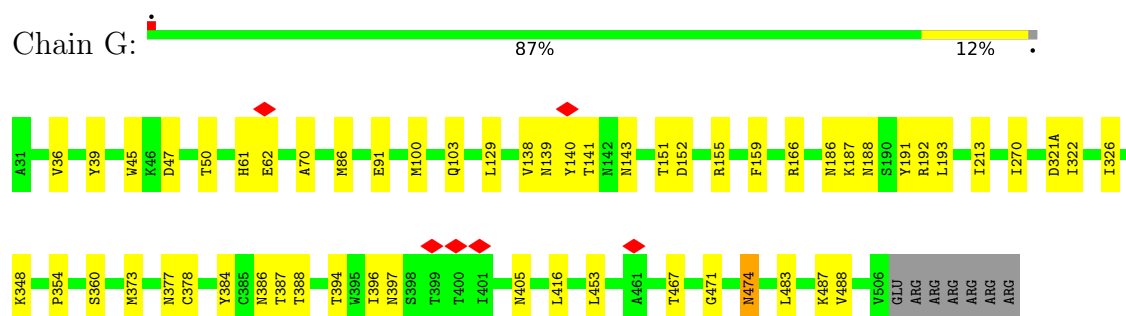
- Molecule 1: Envelope glycoprotein gp41



- Molecule 1: Envelope glycoprotein gp41

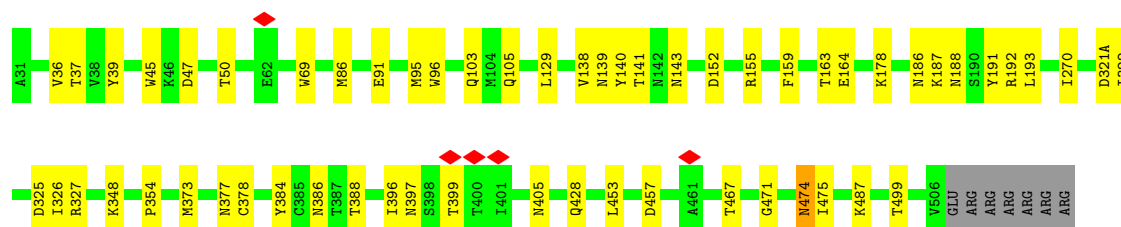


- Molecule 2: Envelope glycoprotein gp160



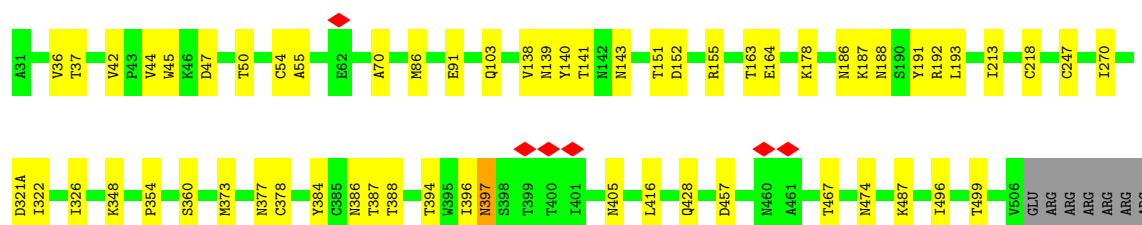
- Molecule 2: Envelope glycoprotein gp160

Chain C:  86% 12%

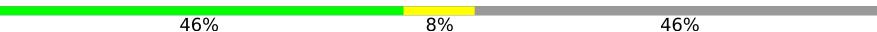


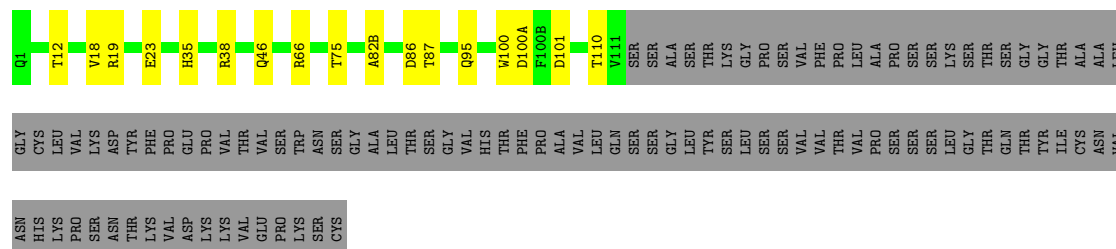
- Molecule 2: Envelope glycoprotein gp160

Chain K:  86% 12%

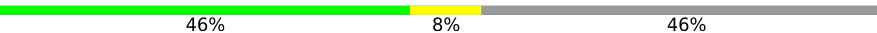


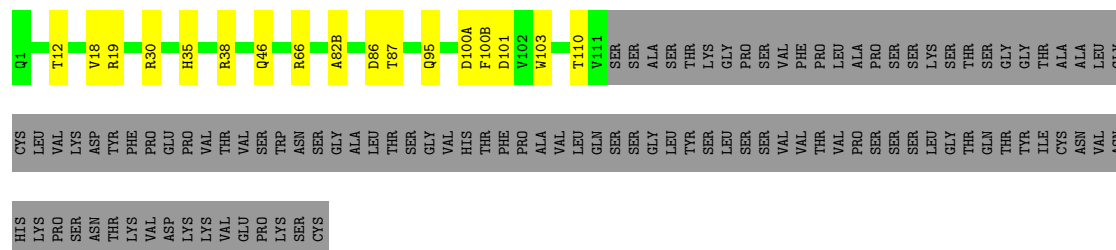
- Molecule 3: 3BNC117 heavy chain

Chain S:  46% 8% 46%

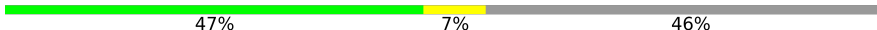


- Molecule 3: 3BNC117 heavy chain

Chain D:  46% 8% 46%



- Molecule 3: 3BNC117 heavy chain

Chain M:  47% 7% 46%

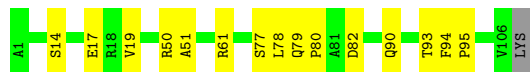
- Molecule 5: VRC44.01 light chain

Chain F:  87% 12%



- Molecule 5: VRC44.01 light chain

Chain O:  85% 14%



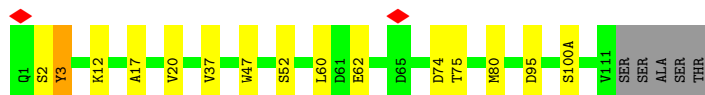
- Molecule 6: VRC44.01 heavy chain

Chain H:  86% 10%



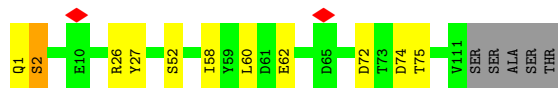
- Molecule 6: VRC44.01 heavy chain

Chain I:  84% 11%



- Molecule 6: VRC44.01 heavy chain

Chain P:  87% 8%



- Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

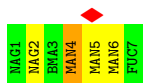
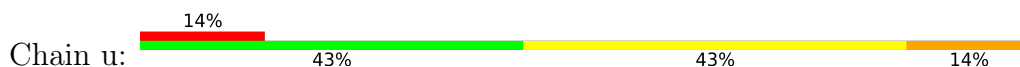
Chain Q:  43% 57%



- Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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

Chain c:  100%



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

Chain d:  100%



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

Chain e:  100%



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

Chain f:  50%
100%



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

Chain h:  100%



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

Chain i:  100%



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

Chain m:  100%



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

Chain o:  100%



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

Chain q:  100%



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

Chain r:  100%



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

Chain s:  100%



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

Chain t:  50% 100%



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

Chain v:  100%



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

Chain w:  100%



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

Chain 0:  100%



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

Chain 2:  100%



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

Chain 4:  100%



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

Chain 5:  100%



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

Chain 6:  100%



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

Chain V:  60% 40%



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

Chain j:  60% 40%

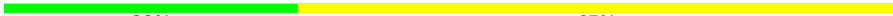


- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:  60% 40%



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

Chain W:  33% 67%



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

Chain k:  33% 67%



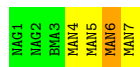
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  33% 67%



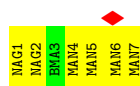
- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 43% 43% 14%



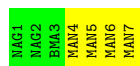
- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 14% 14% 86%



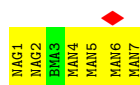
- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 43% 57%



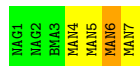
- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p: 14% 14% 86%

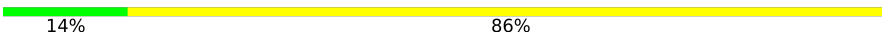


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z: 43% 43% 14%

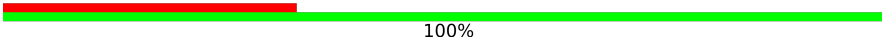


- Molecule 11: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain 3:  14% 86%

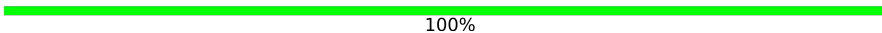
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

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

Chain Z:  33% 100%

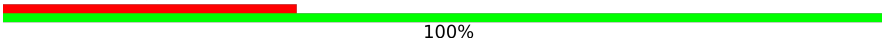
MAG1
MAG2
BMA3

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

Chain n:  100%

MAG1
MAG2
BMA3

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

Chain 1:  33% 100%

MAG1
MAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	90268	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 ($e^-/\text{\AA}^2$)	64.09	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.404	Depositor
Minimum map value	-2.888	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.7	Depositor
Map size ($\text{\AA}$)	438.44, 438.44, 438.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BMA, MAN, FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/1110	0.25	0/1507
1	B	0.19	0/1110	0.26	0/1507
1	J	0.19	0/1110	0.24	0/1507
2	C	0.17	0/3804	0.29	0/5176
2	G	0.18	0/3804	0.30	0/5176
2	K	0.17	0/3804	0.30	0/5176
3	D	0.16	0/1017	0.26	0/1386
3	M	0.16	0/1017	0.25	0/1386
3	S	0.16	0/1017	0.26	0/1386
4	E	0.12	0/800	0.28	0/1086
4	N	0.12	0/800	0.28	0/1086
4	U	0.12	0/800	0.27	0/1086
5	F	0.15	0/831	0.33	0/1132
5	L	0.15	0/831	0.37	0/1132
5	O	0.15	0/831	0.35	0/1132
6	H	0.14	0/978	0.26	0/1331
6	I	0.14	0/978	0.28	0/1331
6	P	0.14	0/978	0.27	0/1331
All	All	0.17	0/25620	0.29	0/34854

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	166	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1088	0	1061	7	0
1	B	1088	0	1061	11	0
1	J	1088	0	1061	7	0
2	C	3722	0	3644	40	0
2	G	3722	0	3644	39	0
2	K	3722	0	3644	43	0
3	D	985	0	919	12	0
3	M	985	0	919	10	0
3	S	985	0	919	12	0
4	E	783	0	763	13	0
4	N	783	0	763	13	0
4	U	783	0	763	16	0
5	F	809	0	787	7	0
5	L	809	0	787	14	0
5	O	809	0	787	10	0
6	H	951	0	913	8	0
6	I	951	0	913	9	0
6	P	951	0	913	8	0
7	Q	82	0	70	1	0
7	g	82	0	70	0	0
7	u	82	0	70	2	0
8	0	28	0	25	0	0
8	2	28	0	25	0	0
8	4	28	0	25	0	0
8	5	28	0	25	0	0
8	6	28	0	25	0	0
8	R	28	0	25	0	0
8	T	28	0	25	0	0
8	Y	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	a	28	0	25	0	0
8	c	28	0	25	0	0
8	d	28	0	25	0	0
8	e	28	0	25	0	0
8	f	28	0	25	0	0
8	h	28	0	25	0	0
8	i	28	0	25	0	0
8	m	28	0	25	0	0
8	o	28	0	25	0	0
8	q	28	0	25	0	0
8	r	28	0	25	0	0
8	s	28	0	25	0	0
8	t	28	0	25	0	0
8	v	28	0	25	0	0
8	w	28	0	25	0	0
9	V	61	0	52	0	0
9	j	61	0	52	0	0
9	x	61	0	52	0	0
10	W	105	0	88	0	0
10	k	105	0	88	0	0
10	y	105	0	88	0	0
11	3	83	0	70	1	0
11	X	83	0	70	1	0
11	b	83	0	70	1	0
11	l	83	0	70	0	0
11	p	83	0	70	1	0
11	z	83	0	70	1	0
12	1	39	0	34	0	0
12	Z	39	0	34	0	0
12	n	39	0	34	0	0
13	A	28	0	26	0	0
13	B	42	0	39	0	0
13	C	112	0	104	1	0
13	E	14	0	13	1	0
13	G	112	0	104	1	0
13	J	28	0	26	0	0
13	K	112	0	104	2	0
13	N	14	0	13	0	0
13	U	14	0	13	1	0
14	C	5	0	0	0	0
All	All	27498	0	26430	260	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 5.

All (260) 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)
1:B:606:THR:OG1	2:G:36:VAL:O	1.92	0.86
1:A:606:THR:OG1	2:C:36:VAL:O	1.97	0.82
5:F:90:GLN:NE2	5:F:95:PRO:O	2.14	0.80
5:O:90:GLN:NE2	5:O:95:PRO:O	2.19	0.75
4:U:22:THR:OG1	4:U:70:GLU:OE2	2.05	0.75
3:S:23:GLU:OE2	3:S:75:THR:OG1	2.08	0.71
2:C:47:ASP:OD1	2:C:487:LYS:NZ	2.19	0.71
4:E:90:VAL:HG12	4:E:91:TYR:H	1.56	0.70
4:N:90:VAL:HG12	4:N:91:TYR:H	1.55	0.70
4:U:90:VAL:HG12	4:U:91:TYR:H	1.56	0.70
4:U:65:ARG:NH1	13:U:301:NAG:O7	2.26	0.69
2:C:138:VAL:HG13	2:C:139:ASN:H	1.57	0.68
3:S:38:ARG:NH1	3:S:46:GLN:OE1	2.27	0.68
4:E:33:LEU:HD11	4:E:88:CYS:HB2	1.76	0.67
1:B:584:GLU:OE1	1:J:579:ARG:NH2	2.29	0.66
5:O:61:ARG:NH1	5:O:82:ASP:OD2	2.28	0.66
6:P:1:GLN:O	6:P:2:SER:OG	2.13	0.66
2:G:47:ASP:OD1	2:G:487:LYS:NZ	2.27	0.66
2:K:138:VAL:HG13	2:K:139:ASN:H	1.60	0.66
2:K:47:ASP:OD1	2:K:487:LYS:NZ	2.24	0.65
3:M:12:THR:HG21	3:M:18:VAL:HG22	1.79	0.64
2:G:138:VAL:HG13	2:G:139:ASN:H	1.61	0.64
2:G:100:MET:HE3	2:G:483:LEU:HD22	1.79	0.64
2:G:140:TYR:O	2:G:141:THR:OG1	2.16	0.63
2:C:140:TYR:O	2:C:141:THR:OG1	2.16	0.63
5:L:61:ARG:NH1	5:L:82:ASP:OD2	2.29	0.63
3:D:66:ARG:NH2	3:D:86:ASP:OD2	2.33	0.61
4:U:25:ALA:CB	4:U:33:LEU:HD13	2.30	0.61
3:M:87:THR:HG23	3:M:110:THR:HA	1.82	0.61
3:D:87:THR:HG23	3:D:110:THR:HA	1.81	0.61
2:K:321(A):ASP:OD1	2:K:322:ILE:N	2.33	0.61
2:K:163:THR:HG22	2:K:164:GLU:H	1.67	0.60
3:S:35:HIS:NE2	3:S:95:GLN:OE1	2.35	0.60
4:N:33:LEU:HD11	4:N:88:CYS:HB2	1.84	0.60
3:M:35:HIS:NE2	3:M:95:GLN:OE1	2.35	0.60
6:P:72:ASP:OD1	6:P:75:THR:HG22	2.02	0.60
2:G:321(A):ASP:OD1	2:G:322:ILE:N	2.34	0.59
3:D:100(A):ASP:OD1	4:E:34:ASN:ND2	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:543:GLN:O	1:J:544:LEU:HD22	2.01	0.59
3:S:87:THR:HG23	3:S:110:THR:HA	1.84	0.59
6:I:2:SER:O	6:I:3:TYR:HB2	2.01	0.59
2:K:386:ASN:OD1	2:K:388:THR:OG1	2.16	0.59
1:B:565:LEU:HD23	1:B:567:GLN:H	1.68	0.59
5:L:90:GLN:NE2	5:L:95:PRO:O	2.36	0.58
3:S:12:THR:HG21	3:S:18:VAL:HG22	1.85	0.58
1:A:543:GLN:O	1:A:544:LEU:HD22	2.03	0.58
6:P:74:ASP:OD1	6:P:75:THR:N	2.37	0.58
6:I:2:SER:OG	6:I:3:TYR:N	2.37	0.58
2:C:321(A):ASP:OD1	2:C:322:ILE:N	2.36	0.58
3:D:12:THR:HG21	3:D:18:VAL:HG22	1.84	0.58
3:M:66:ARG:NH2	3:M:86:ASP:OD2	2.36	0.58
4:E:20:THR:HG22	4:E:74:THR:HG22	1.86	0.58
5:L:39:GLN:OE1	5:L:42:ARG:NH1	2.37	0.57
2:K:91:GLU:OE2	2:K:487:LYS:NZ	2.37	0.57
2:G:91:GLU:OE2	2:G:487:LYS:NZ	2.37	0.57
6:H:72:ASP:OD1	6:H:75:THR:HG22	2.04	0.57
1:B:543:GLN:O	1:B:544:LEU:HD22	2.04	0.57
6:H:1:GLN:O	6:H:2:SER:OG	2.13	0.57
2:K:140:TYR:O	2:K:141:THR:OG1	2.15	0.57
2:C:163:THR:HG22	2:C:164:GLU:N	2.19	0.57
6:I:74:ASP:OD1	6:I:75:THR:N	2.38	0.56
2:C:396:ILE:HG23	2:C:397:ASN:N	2.20	0.56
2:G:396:ILE:HG23	2:G:397:ASN:N	2.20	0.56
2:C:270:ILE:O	2:C:348:LYS:NZ	2.38	0.56
3:M:100(A):ASP:OD1	4:N:34:ASN:ND2	2.37	0.56
2:K:377:ASN:OD1	2:K:378:CYS:N	2.38	0.56
2:G:474:ASN:N	2:G:474:ASN:OD1	2.38	0.56
6:I:12:LYS:NZ	6:I:17:ALA:O	2.39	0.56
2:K:396:ILE:HG23	2:K:397:ASN:H	1.70	0.56
3:S:66:ARG:NH2	3:S:86:ASP:OD2	2.39	0.56
4:N:20:THR:HG22	4:N:74:THR:HG22	1.86	0.56
4:U:37:GLN:HB2	4:U:47:LEU:HD11	1.87	0.55
2:C:325:ASP:OD2	2:C:327:ARG:NH2	2.37	0.55
2:K:396:ILE:HG23	2:K:397:ASN:N	2.21	0.55
2:C:377:ASN:OD1	2:C:378:CYS:N	2.40	0.55
5:O:19:VAL:HG11	5:O:78:LEU:HD12	1.89	0.55
2:K:50:THR:O	2:K:103:GLN:NE2	2.38	0.55
1:B:603:ILE:HG21	1:A:658:VAL:HG21	1.88	0.54
6:P:26:ARG:NH2	7:u:4:MAN:O3	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:397:ASN:OD1	2:C:397:ASN:O	2.26	0.54
4:U:67:TRP:NE1	11:X:6:MAN:O6	2.41	0.54
2:G:377:ASN:OD1	2:G:378:CYS:N	2.40	0.54
2:K:218:CYS:HA	2:K:247:CYS:CB	2.38	0.54
2:C:91:GLU:OE2	2:C:487:LYS:NZ	2.40	0.54
4:N:67:TRP:NE1	11:z:6:MAN:O6	2.41	0.54
1:B:658:VAL:HG21	1:J:603:ILE:HG21	1.90	0.53
2:C:396:ILE:HG23	2:C:397:ASN:H	1.71	0.53
2:K:37:THR:OG1	2:K:499:THR:OG1	2.19	0.53
2:G:192:ARG:NH1	2:G:193:LEU:O	2.42	0.53
2:C:50:THR:O	2:C:103:GLN:NE2	2.39	0.53
4:U:2:ILE:HG21	4:U:90:VAL:HG11	1.90	0.53
6:H:74:ASP:OD1	6:H:75:THR:N	2.41	0.53
2:G:138:VAL:HG13	2:G:139:ASN:N	2.24	0.53
3:S:100(A):ASP:OD1	4:U:34:ASN:ND2	2.40	0.53
2:G:50:THR:O	2:G:103:GLN:NE2	2.37	0.53
2:G:396:ILE:HG23	2:G:397:ASN:H	1.74	0.53
4:N:2:ILE:HG21	4:N:90:VAL:HG11	1.91	0.53
2:C:474:ASN:OD1	2:C:474:ASN:N	2.41	0.53
2:K:474:ASN:OD1	2:K:474:ASN:N	2.41	0.53
4:E:4:MET:HE1	4:E:88:CYS:O	2.09	0.52
4:E:4:MET:HE2	4:E:99:VAL:HG13	1.92	0.52
5:L:17:GLU:O	5:L:78:LEU:HD23	2.10	0.52
2:K:373:MET:HE2	2:K:384:TYR:O	2.09	0.52
2:K:138:VAL:HG13	2:K:139:ASN:N	2.24	0.52
2:C:163:THR:HG22	2:C:164:GLU:H	1.75	0.52
2:G:386:ASN:OD1	2:G:388:THR:OG1	2.20	0.52
2:K:428:GLN:O	3:M:30:ARG:NH2	2.42	0.52
2:K:163:THR:HG22	2:K:164:GLU:N	2.23	0.52
2:G:373:MET:HE2	2:G:384:TYR:O	2.10	0.52
2:K:270:ILE:O	2:K:348:LYS:NZ	2.42	0.52
3:M:66:ARG:NH2	3:M:82(B):ALA:O	2.43	0.51
2:K:187:LYS:O	2:K:188:ASN:HB2	2.11	0.51
2:C:354:PRO:HB2	13:C:607:NAG:H82	1.93	0.51
2:G:270:ILE:O	2:G:348:LYS:NZ	2.44	0.51
2:C:155:ARG:NH2	2:C:191:TYR:OH	2.42	0.51
4:E:2:ILE:HG21	4:E:90:VAL:HG11	1.92	0.51
4:U:25:ALA:HB2	4:U:33:LEU:HD13	1.92	0.50
4:E:40:ARG:NH2	4:E:85:THR:OG1	2.43	0.50
2:K:192:ARG:NH1	2:K:193:LEU:O	2.44	0.50
2:C:428:GLN:O	3:D:30:ARG:NH2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ILE:HG21	1:J:658:VAL:HG21	1.94	0.50
2:G:129:LEU:HD23	2:G:159:PHE:HB3	1.94	0.50
2:G:187:LYS:O	2:G:188:ASN:HB2	2.12	0.50
4:E:89:GLN:NE2	4:E:90:VAL:O	2.44	0.50
4:N:89:GLN:NE2	4:N:90:VAL:O	2.43	0.50
2:K:218:CYS:HA	2:K:247:CYS:HB2	1.93	0.50
2:G:354:PRO:HB2	13:G:606:NAG:H82	1.93	0.50
2:C:386:ASN:OD1	2:C:388:THR:OG1	2.17	0.50
2:C:187:LYS:O	2:C:188:ASN:HB2	2.11	0.49
3:S:101:ASP:OD1	3:S:101:ASP:N	2.46	0.49
2:G:141:THR:O	2:G:143:ASN:N	2.46	0.49
2:K:152:ASP:C	2:K:152:ASP:OD1	2.55	0.49
2:G:155:ARG:NH2	2:G:191:TYR:OH	2.41	0.49
4:U:20:THR:HG22	4:U:74:THR:HG22	1.95	0.49
2:K:54:CYS:SG	2:K:55:ALA:N	2.86	0.48
1:A:530:MET:HE1	1:A:631:TRP:CG	2.48	0.48
4:E:90:VAL:HG12	4:E:91:TYR:N	2.27	0.48
2:C:373:MET:HE2	2:C:384:TYR:O	2.14	0.48
5:O:79:GLN:HB3	5:O:80:PRO:HD2	1.96	0.48
2:K:354:PRO:HB2	13:K:606:NAG:H82	1.95	0.48
5:L:75:ILE:HB	5:L:78:LEU:HD21	1.96	0.48
2:C:152:ASP:OD1	2:C:152:ASP:C	2.57	0.48
2:K:141:THR:O	2:K:143:ASN:N	2.46	0.48
2:K:155:ARG:NH2	2:K:191:TYR:OH	2.41	0.47
6:I:52:SER:OG	11:p:2:NAG:O7	2.32	0.47
3:M:38:ARG:O	3:M:46:GLN:N	2.46	0.47
2:C:138:VAL:HG13	2:C:139:ASN:N	2.26	0.47
4:N:90:VAL:HG12	4:N:91:TYR:N	2.27	0.47
1:B:530:MET:HE1	1:B:631:TRP:CG	2.49	0.47
2:G:326:ILE:O	2:G:326:ILE:HG13	2.15	0.47
5:L:79:GLN:HB3	5:L:80:PRO:HD2	1.97	0.47
4:U:89:GLN:NE2	4:U:90:VAL:O	2.48	0.46
4:N:61:ARG:NE	4:N:82:ASP:OD2	2.47	0.46
2:G:387:THR:HG22	2:G:416:LEU:HD13	1.96	0.46
2:C:129:LEU:HD23	2:C:159:PHE:HB3	1.97	0.46
13:K:608:NAG:O7	13:K:608:NAG:O3	2.27	0.46
6:P:52:SER:OG	11:3:2:NAG:O7	2.33	0.46
5:O:77:SER:O	5:O:78:LEU:C	2.59	0.46
5:F:50:ARG:O	5:F:51:ALA:HB3	2.16	0.46
6:P:60:LEU:HD23	6:P:62:GLU:H	1.80	0.46
4:U:90:VAL:HG12	4:U:91:TYR:N	2.27	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:90:VAL:O	4:N:91:TYR:C	2.59	0.46
2:C:141:THR:O	2:C:143:ASN:N	2.49	0.45
2:G:70:ALA:HB3	2:G:213:ILE:HD11	1.98	0.45
2:K:155:ARG:HD3	2:K:178:LYS:HZ2	1.81	0.45
5:F:14:SER:N	5:F:17:GLU:OE2	2.35	0.45
2:K:139:ASN:O	2:K:141:THR:N	2.45	0.45
2:G:152:ASP:OD1	2:G:152:ASP:C	2.59	0.45
4:U:4:MET:HE1	4:U:88:CYS:O	2.16	0.45
4:U:90:VAL:O	4:U:91:TYR:C	2.59	0.45
5:F:2:ILE:HD12	5:F:93:THR:OG1	2.17	0.45
1:B:537:LEU:HD11	2:G:39:TYR:HD2	1.81	0.45
6:I:95:ASP:OD2	6:I:100(A):SER:HB3	2.17	0.45
2:G:45:TRP:CH2	2:G:86:MET:HE1	2.52	0.45
5:O:94:PHE:CE1	6:P:58:ILE:HG23	2.52	0.45
6:H:60:LEU:HD23	6:H:62:GLU:H	1.81	0.45
3:D:38:ARG:O	3:D:46:GLN:N	2.50	0.45
6:H:12:LYS:NZ	6:H:17:ALA:O	2.49	0.45
1:J:530:MET:HE1	1:J:631:TRP:CG	2.52	0.45
2:K:326:ILE:HG13	2:K:326:ILE:O	2.16	0.44
5:L:77:SER:O	5:L:79:GLN:N	2.50	0.44
3:D:100(B):PHE:O	3:D:103:TRP:NE1	2.50	0.44
3:M:101:ASP:OD1	3:M:101:ASP:N	2.47	0.44
4:U:61:ARG:NE	4:U:82:ASP:OD2	2.44	0.44
4:E:90:VAL:O	4:E:91:TYR:C	2.60	0.44
6:H:52:SER:OG	11:b:2:NAG:O7	2.34	0.44
2:C:45:TRP:CH2	2:C:86:MET:HE1	2.52	0.44
2:G:453:LEU:O	2:G:471:GLY:N	2.47	0.44
2:C:37:THR:OG1	2:C:499:THR:OG1	2.30	0.44
5:L:50:ARG:O	5:L:51:ALA:HB3	2.17	0.44
5:O:14:SER:N	5:O:17:GLU:OE2	2.35	0.44
2:G:50:THR:HG22	2:G:488:VAL:HG11	2.00	0.44
5:O:50:ARG:O	5:O:51:ALA:HB3	2.18	0.44
5:F:79:GLN:HB3	5:F:80:PRO:HD2	2.00	0.43
6:I:37:VAL:HG12	6:I:47:TRP:HA	1.99	0.43
2:G:186:ASN:O	2:G:187:LYS:C	2.61	0.43
5:L:29:ILE:HA	5:L:92:LYS:HD3	1.99	0.43
3:D:18:VAL:HG12	3:D:19:ARG:N	2.33	0.43
2:K:218:CYS:HA	2:K:247:CYS:HB3	2.00	0.43
2:K:457:ASP:OD2	2:K:467:THR:OG1	2.35	0.43
2:K:387:THR:HG22	2:K:416:LEU:HD13	1.99	0.43
5:O:78:LEU:HD23	5:O:79:GLN:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:18:VAL:HG12	3:S:19:ARG:N	2.34	0.43
2:C:139:ASN:O	2:C:141:THR:N	2.47	0.43
2:C:326:ILE:HG13	2:C:326:ILE:O	2.18	0.43
5:L:94:PHE:CE1	6:H:58:ILE:HG23	2.53	0.43
2:K:45:TRP:CH2	2:K:86:MET:HE1	2.54	0.43
6:H:27:TYR:HB2	7:Q:2:NAG:H81	2.01	0.43
2:C:186:ASN:O	2:C:187:LYS:C	2.62	0.43
4:N:4:MET:HE1	4:N:88:CYS:O	2.18	0.43
2:G:61:HIS:CG	2:G:62:GLU:H	2.37	0.42
3:D:66:ARG:NH2	3:D:82(B):ALA:O	2.50	0.42
2:G:138:VAL:CG1	2:G:139:ASN:H	2.30	0.42
4:E:65:ARG:NH1	13:E:301:NAG:O7	2.52	0.42
4:N:40:ARG:NH2	4:N:85:THR:OG1	2.50	0.42
2:K:360:SER:HB3	2:K:394:THR:HG23	2.01	0.42
1:B:610:TRP:HE3	2:G:36:VAL:HG22	1.84	0.42
2:K:186:ASN:O	2:K:187:LYS:C	2.62	0.42
2:K:386:ASN:O	2:K:387:THR:OG1	2.30	0.42
3:S:38:ARG:O	3:S:46:GLN:N	2.52	0.42
1:A:537:LEU:HD11	2:C:39:TYR:HD2	1.83	0.42
2:K:70:ALA:HB3	2:K:213:ILE:HD11	2.01	0.42
2:G:360:SER:HB3	2:G:394:THR:HG23	2.01	0.42
2:C:155:ARG:HD3	2:C:178:LYS:HZ2	1.84	0.42
2:G:360:SER:OG	2:G:467:THR:HG22	2.19	0.42
2:K:42:VAL:HG12	2:K:44:VAL:HG23	2.01	0.42
5:F:93:THR:HG22	5:F:94:PHE:N	2.35	0.42
4:E:61:ARG:NE	4:E:82:ASP:OD2	2.50	0.41
3:M:18:VAL:HG12	3:M:19:ARG:N	2.36	0.41
2:G:61:HIS:O	2:G:62:GLU:HG3	2.19	0.41
2:G:151:THR:O	2:G:152:ASP:CG	2.64	0.41
3:S:100:TRP:CE3	4:U:91:TYR:O	2.74	0.41
5:L:85:THR:HG1	5:L:102:THR:C	2.28	0.41
2:K:151:THR:O	2:K:152:ASP:CG	2.63	0.41
1:B:581:LEU:HD23	1:J:579:ARG:HH22	1.86	0.41
2:C:192:ARG:NH1	2:C:193:LEU:O	2.53	0.41
2:C:453:LEU:O	2:C:471:GLY:N	2.52	0.41
3:D:38:ARG:NH1	3:D:46:GLN:OE1	2.54	0.41
3:D:101:ASP:OD1	3:D:101:ASP:N	2.49	0.41
1:B:530:MET:CE	1:B:631:TRP:HB2	2.50	0.41
5:L:94:PHE:HB3	5:L:95:PRO:HD3	2.03	0.41
6:I:60:LEU:HD23	6:I:62:GLU:H	1.86	0.41
2:K:360:SER:OG	2:K:467:THR:HG22	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:93:THR:HG22	5:O:94:PHE:N	2.35	0.41
3:S:66:ARG:NH2	3:S:82(B):ALA:O	2.50	0.41
2:K:36:VAL:HG13	2:K:496:ILE:HG23	2.02	0.41
4:N:54:LEU:HD11	4:N:58:VAL:HG13	2.03	0.41
2:C:105:GLN:OE1	2:C:475:ILE:HG23	2.21	0.41
1:J:610:TRP:HE3	2:K:36:VAL:HG22	1.86	0.41
5:L:93:THR:HG22	5:L:95:PRO:HD2	2.03	0.40
2:C:397:ASN:HB3	2:C:399:THR:HG23	2.03	0.40
2:G:61:HIS:C	2:G:62:GLU:HG3	2.47	0.40
1:A:571:TRP:CZ3	2:C:69:TRP:O	2.74	0.40
5:F:82:ASP:OD1	5:F:86:TYR:OH	2.34	0.40
2:C:95:MET:HE3	2:C:96:TRP:CZ2	2.56	0.40
3:D:35:HIS:NE2	3:D:95:GLN:OE1	2.53	0.40
2:C:457:ASP:OD2	2:C:467:THR:OG1	2.39	0.40
6:I:20:VAL:CG1	6:I:80:MET:HE3	2.51	0.40
6:P:27:TYR:HB2	7:u:2:NAG:H81	2.03	0.40
5:L:7:SER:OG	5:L:8:PRO:HA	2.22	0.40

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	A	132/170 (78%)	126 (96%)	6 (4%)	0	100	100
1	B	132/170 (78%)	125 (95%)	7 (5%)	0	100	100
1	J	132/170 (78%)	127 (96%)	5 (4%)	0	100	100
2	C	469/478 (98%)	438 (93%)	31 (7%)	0	100	100
2	G	469/478 (98%)	440 (94%)	29 (6%)	0	100	100
2	K	469/478 (98%)	440 (94%)	29 (6%)	0	100	100
3	D	119/226 (53%)	115 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	119/226 (53%)	114 (96%)	5 (4%)	0	100	100
3	S	119/226 (53%)	114 (96%)	5 (4%)	0	100	100
4	E	96/206 (47%)	87 (91%)	9 (9%)	0	100	100
4	N	96/206 (47%)	89 (93%)	7 (7%)	0	100	100
4	U	96/206 (47%)	88 (92%)	8 (8%)	0	100	100
5	F	104/107 (97%)	96 (92%)	8 (8%)	0	100	100
5	L	104/107 (97%)	96 (92%)	8 (8%)	0	100	100
5	O	104/107 (97%)	95 (91%)	9 (9%)	0	100	100
6	H	117/124 (94%)	111 (95%)	6 (5%)	0	100	100
6	I	117/124 (94%)	112 (96%)	4 (3%)	1 (1%)	14	27
6	P	117/124 (94%)	112 (96%)	4 (3%)	1 (1%)	14	27
All	All	3111/3933 (79%)	2925 (94%)	184 (6%)	2 (0%)	49	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	I	3	TYR
6	P	2	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/144 (82%)	118 (100%)	0	100	100
1	B	118/144 (82%)	118 (100%)	0	100	100
1	J	118/144 (82%)	118 (100%)	0	100	100
2	C	425/432 (98%)	423 (100%)	2 (0%)	81	90
2	G	425/432 (98%)	423 (100%)	2 (0%)	81	90
2	K	425/432 (98%)	423 (100%)	2 (0%)	81	90
3	D	102/193 (53%)	102 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	102/193 (53%)	102 (100%)	0	100	100
3	S	102/193 (53%)	102 (100%)	0	100	100
4	E	86/183 (47%)	86 (100%)	0	100	100
4	N	86/183 (47%)	86 (100%)	0	100	100
4	U	86/183 (47%)	86 (100%)	0	100	100
5	F	89/90 (99%)	89 (100%)	0	100	100
5	L	89/90 (99%)	89 (100%)	0	100	100
5	O	89/90 (99%)	89 (100%)	0	100	100
6	H	101/105 (96%)	101 (100%)	0	100	100
6	I	101/105 (96%)	101 (100%)	0	100	100
6	P	101/105 (96%)	101 (100%)	0	100	100
All	All	2763/3441 (80%)	2757 (100%)	6 (0%)	85	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	405	ASN
2	G	474	ASN
2	C	405	ASN
2	C	474	ASN
2	K	397	ASN
2	K	405	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	67	ASN
2	G	72	HIS
2	G	139	ASN
2	G	183	GLN
2	G	258	GLN
2	G	460	ASN
3	S	59	ASN
3	S	64	GLN
4	U	37	GLN
4	U	69	GLN
4	U	79	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	6	GLN
6	H	56	HIS
2	C	67	ASN
2	C	72	HIS
2	C	139	ASN
2	C	258	GLN
2	C	460	ASN
3	D	64	GLN
5	F	6	GLN
1	J	564	HIS
1	J	577	GLN
2	K	61	HIS
2	K	99	ASN
2	K	139	ASN
2	K	258	GLN
3	M	3	GLN
3	M	59	ASN
4	N	3	GLN
5	O	6	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

160 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
8	NAG	0	1	8,2	14,14,15	0.22	0	17,19,21	0.48	0
8	NAG	0	2	8	14,14,15	0.21	0	17,19,21	0.47	0
12	NAG	1	1	12,2	14,14,15	0.27	0	17,19,21	0.44	0
12	NAG	1	2	12	14,14,15	0.22	0	17,19,21	0.51	0
12	BMA	1	3	12	11,11,12	0.47	0	15,15,17	0.73	0
8	NAG	2	1	8,2	14,14,15	0.22	0	17,19,21	0.48	0
8	NAG	2	2	8	14,14,15	0.19	0	17,19,21	0.45	0
11	NAG	3	1	11,2	14,14,15	0.26	0	17,19,21	0.68	1 (5%)
11	NAG	3	2	11	14,14,15	0.24	0	17,19,21	0.50	0
11	BMA	3	3	11	11,11,12	0.51	0	15,15,17	0.79	0
11	MAN	3	4	11	11,11,12	0.58	0	15,15,17	1.00	2 (13%)
11	MAN	3	5	11	11,11,12	0.64	0	15,15,17	0.96	2 (13%)
11	MAN	3	6	11	11,11,12	0.62	0	15,15,17	0.89	1 (6%)
11	MAN	3	7	11	11,11,12	0.61	0	15,15,17	0.91	2 (13%)
8	NAG	4	1	8,2	14,14,15	0.25	0	17,19,21	0.48	0
8	NAG	4	2	8	14,14,15	0.19	0	17,19,21	0.48	0
8	NAG	5	1	8,2	14,14,15	0.23	0	17,19,21	0.50	0
8	NAG	5	2	8	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	6	1	8,2	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	6	2	8	14,14,15	0.22	0	17,19,21	0.43	0
7	NAG	Q	1	1,7	14,14,15	0.24	0	17,19,21	0.51	0
7	NAG	Q	2	7	14,14,15	0.19	0	17,19,21	0.49	0
7	BMA	Q	3	7	11,11,12	0.45	0	15,15,17	0.64	0
7	MAN	Q	4	7	11,11,12	0.78	0	15,15,17	0.87	1 (6%)
7	MAN	Q	5	7	11,11,12	0.62	0	15,15,17	0.90	2 (13%)
7	MAN	Q	6	7	11,11,12	0.56	0	15,15,17	1.09	2 (13%)
7	FUC	Q	7	7	10,10,11	0.62	0	14,14,16	0.75	0
8	NAG	R	1	8,2	14,14,15	0.24	0	17,19,21	0.42	0
8	NAG	R	2	8	14,14,15	0.24	0	17,19,21	0.42	0
8	NAG	T	1	8,2	14,14,15	0.27	0	17,19,21	0.40	0
8	NAG	T	2	8	14,14,15	0.20	0	17,19,21	0.46	0
9	NAG	V	1	9,2	14,14,15	0.26	0	17,19,21	0.55	0
9	NAG	V	2	9	14,14,15	0.22	0	17,19,21	0.40	0
9	BMA	V	3	9	11,11,12	0.62	0	15,15,17	0.88	0
9	MAN	V	4	9	11,11,12	0.56	0	15,15,17	1.01	2 (13%)
9	MAN	V	5	9	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
10	NAG	W	1	2,10	14,14,15	0.26	0	17,19,21	0.48	0
10	NAG	W	2	10	14,14,15	0.20	0	17,19,21	0.42	0
10	BMA	W	3	10	11,11,12	0.52	0	15,15,17	0.69	0
10	MAN	W	4	10	11,11,12	0.60	0	15,15,17	0.96	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	W	5	10	11,11,12	0.66	0	15,15,17	0.90	1 (6%)
10	MAN	W	6	10	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
10	MAN	W	7	10	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
10	MAN	W	8	10	11,11,12	0.71	0	15,15,17	1.12	2 (13%)
10	MAN	W	9	10	11,11,12	0.60	0	15,15,17	1.03	2 (13%)
11	NAG	X	1	11,2	14,14,15	0.26	0	17,19,21	0.38	0
11	NAG	X	2	11	14,14,15	0.21	0	17,19,21	0.46	0
11	BMA	X	3	11	11,11,12	0.52	0	15,15,17	0.71	0
11	MAN	X	4	11	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
11	MAN	X	5	11	11,11,12	0.57	0	15,15,17	1.03	2 (13%)
11	MAN	X	6	11	11,11,12	0.57	0	15,15,17	0.97	2 (13%)
11	MAN	X	7	11	11,11,12	0.59	0	15,15,17	0.90	1 (6%)
8	NAG	Y	1	8,2	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	Y	2	8	14,14,15	0.20	0	17,19,21	0.47	0
12	NAG	Z	1	12,2	14,14,15	0.26	0	17,19,21	0.44	0
12	NAG	Z	2	12	14,14,15	0.21	0	17,19,21	0.52	0
12	BMA	Z	3	12	11,11,12	0.49	0	15,15,17	0.74	0
8	NAG	a	1	8,2	14,14,15	0.22	0	17,19,21	0.49	0
8	NAG	a	2	8	14,14,15	0.18	0	17,19,21	0.44	0
11	NAG	b	1	11,2	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
11	NAG	b	2	11	14,14,15	0.26	0	17,19,21	0.50	0
11	BMA	b	3	11	11,11,12	0.52	0	15,15,17	0.79	0
11	MAN	b	4	11	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
11	MAN	b	5	11	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
11	MAN	b	6	11	11,11,12	0.63	0	15,15,17	0.90	1 (6%)
11	MAN	b	7	11	11,11,12	0.60	0	15,15,17	0.91	2 (13%)
8	NAG	c	1	8,2	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	c	2	8	14,14,15	0.18	0	17,19,21	0.47	0
8	NAG	d	1	8,2	14,14,15	0.22	0	17,19,21	0.48	0
8	NAG	d	2	8	14,14,15	0.22	0	17,19,21	0.44	0
8	NAG	e	1	8,2	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	e	2	8	14,14,15	0.22	0	17,19,21	0.44	0
8	NAG	f	1	8,1	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	f	2	8	14,14,15	0.21	0	17,19,21	0.45	0
7	NAG	g	1	1,7	14,14,15	0.26	0	17,19,21	0.51	0
7	NAG	g	2	7	14,14,15	0.21	0	17,19,21	0.53	0
7	BMA	g	3	7	11,11,12	0.49	0	15,15,17	0.68	0
7	MAN	g	4	7	11,11,12	0.60	0	15,15,17	0.85	1 (6%)
7	MAN	g	5	7	11,11,12	0.61	0	15,15,17	0.89	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	g	6	7	11,11,12	0.70	0	15,15,17	0.81	1 (6%)
7	FUC	g	7	7	10,10,11	0.57	0	14,14,16	0.75	0
8	NAG	h	1	8,2	14,14,15	0.24	0	17,19,21	0.41	0
8	NAG	h	2	8	14,14,15	0.21	0	17,19,21	0.40	0
8	NAG	i	1	8,2	14,14,15	0.26	0	17,19,21	0.39	0
8	NAG	i	2	8	14,14,15	0.21	0	17,19,21	0.46	0
9	NAG	j	1	9,2	14,14,15	0.26	0	17,19,21	0.55	0
9	NAG	j	2	9	14,14,15	0.23	0	17,19,21	0.41	0
9	BMA	j	3	9	11,11,12	0.62	0	15,15,17	0.88	0
9	MAN	j	4	9	11,11,12	0.54	0	15,15,17	1.01	2 (13%)
9	MAN	j	5	9	11,11,12	0.63	0	15,15,17	0.94	1 (6%)
10	NAG	k	1	2,10	14,14,15	0.22	0	17,19,21	0.47	0
10	NAG	k	2	10	14,14,15	0.21	0	17,19,21	0.41	0
10	BMA	k	3	10	11,11,12	0.50	0	15,15,17	0.71	0
10	MAN	k	4	10	11,11,12	0.58	0	15,15,17	0.99	2 (13%)
10	MAN	k	5	10	11,11,12	0.63	0	15,15,17	0.91	1 (6%)
10	MAN	k	6	10	11,11,12	0.58	0	15,15,17	0.88	1 (6%)
10	MAN	k	7	10	11,11,12	0.64	0	15,15,17	0.95	2 (13%)
10	MAN	k	8	10	11,11,12	0.73	0	15,15,17	1.11	2 (13%)
10	MAN	k	9	10	11,11,12	0.62	0	15,15,17	1.02	2 (13%)
11	NAG	l	1	11,2	14,14,15	0.26	0	17,19,21	0.39	0
11	NAG	l	2	11	14,14,15	0.19	0	17,19,21	0.45	0
11	BMA	l	3	11	11,11,12	0.50	0	15,15,17	0.71	0
11	MAN	l	4	11	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
11	MAN	l	5	11	11,11,12	0.56	0	15,15,17	1.03	2 (13%)
11	MAN	l	6	11	11,11,12	0.58	0	15,15,17	0.98	2 (13%)
11	MAN	l	7	11	11,11,12	0.59	0	15,15,17	0.89	1 (6%)
8	NAG	m	1	8,2	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	m	2	8	14,14,15	0.20	0	17,19,21	0.46	0
12	NAG	n	1	12,2	14,14,15	0.27	0	17,19,21	0.45	0
12	NAG	n	2	12	14,14,15	0.22	0	17,19,21	0.51	0
12	BMA	n	3	12	11,11,12	0.49	0	15,15,17	0.73	0
8	NAG	o	1	8,2	14,14,15	0.21	0	17,19,21	0.49	0
8	NAG	o	2	8	14,14,15	0.19	0	17,19,21	0.45	0
11	NAG	p	1	11,2	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
11	NAG	p	2	11	14,14,15	0.25	0	17,19,21	0.47	0
11	BMA	p	3	11	11,11,12	0.50	0	15,15,17	0.77	0
11	MAN	p	4	11	11,11,12	0.58	0	15,15,17	1.01	2 (13%)
11	MAN	p	5	11	11,11,12	0.64	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
11	MAN	p	6	11	11,11,12	0.63	0	15,15,17	0.86	1 (6%)
11	MAN	p	7	11	11,11,12	0.59	0	15,15,17	0.93	2 (13%)
8	NAG	q	1	8,2	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	q	2	8	14,14,15	0.20	0	17,19,21	0.46	0
8	NAG	r	1	8,2	14,14,15	0.23	0	17,19,21	0.47	0
8	NAG	r	2	8	14,14,15	0.21	0	17,19,21	0.46	0
8	NAG	s	1	8,2	14,14,15	0.22	0	17,19,21	0.45	0
8	NAG	s	2	8	14,14,15	0.23	0	17,19,21	0.44	0
8	NAG	t	1	8,1	14,14,15	0.21	0	17,19,21	0.42	0
8	NAG	t	2	8	14,14,15	0.22	0	17,19,21	0.45	0
7	NAG	u	1	1,7	14,14,15	0.24	0	17,19,21	0.51	0
7	NAG	u	2	7	14,14,15	0.20	0	17,19,21	0.48	0
7	BMA	u	3	7	11,11,12	0.56	0	15,15,17	0.77	0
7	MAN	u	4	7	11,11,12	0.50	0	15,15,17	0.88	1 (6%)
7	MAN	u	5	7	11,11,12	0.67	0	15,15,17	1.01	2 (13%)
7	MAN	u	6	7	11,11,12	0.57	0	15,15,17	1.11	2 (13%)
7	FUC	u	7	7	10,10,11	0.61	0	14,14,16	0.75	0
8	NAG	v	1	8,2	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	v	2	8	14,14,15	0.22	0	17,19,21	0.41	0
8	NAG	w	1	8,2	14,14,15	0.25	0	17,19,21	0.39	0
8	NAG	w	2	8	14,14,15	0.20	0	17,19,21	0.46	0
9	NAG	x	1	9,2	14,14,15	0.24	0	17,19,21	0.57	0
9	NAG	x	2	9	14,14,15	0.23	0	17,19,21	0.41	0
9	BMA	x	3	9	11,11,12	0.60	0	15,15,17	0.86	0
9	MAN	x	4	9	11,11,12	0.56	0	15,15,17	1.00	2 (13%)
9	MAN	x	5	9	11,11,12	0.62	0	15,15,17	0.94	1 (6%)
10	NAG	y	1	2,10	14,14,15	0.24	0	17,19,21	0.44	0
10	NAG	y	2	10	14,14,15	0.21	0	17,19,21	0.40	0
10	BMA	y	3	10	11,11,12	0.50	0	15,15,17	0.71	0
10	MAN	y	4	10	11,11,12	0.60	0	15,15,17	0.98	2 (13%)
10	MAN	y	5	10	11,11,12	0.66	0	15,15,17	0.91	1 (6%)
10	MAN	y	6	10	11,11,12	0.61	0	15,15,17	0.88	1 (6%)
10	MAN	y	7	10	11,11,12	0.64	0	15,15,17	0.96	2 (13%)
10	MAN	y	8	10	11,11,12	0.71	0	15,15,17	1.11	2 (13%)
10	MAN	y	9	10	11,11,12	0.61	0	15,15,17	1.01	2 (13%)
11	NAG	z	1	11,2	14,14,15	0.24	0	17,19,21	0.38	0
11	NAG	z	2	11	14,14,15	0.21	0	17,19,21	0.45	0
11	BMA	z	3	11	11,11,12	0.50	0	15,15,17	0.70	0
11	MAN	z	4	11	11,11,12	0.64	0	15,15,17	0.98	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	z	5	11	11,11,12	0.57	0	15,15,17	1.04	2 (13%)
11	MAN	z	6	11	11,11,12	0.58	0	15,15,17	0.97	2 (13%)
11	MAN	z	7	11	11,11,12	0.60	0	15,15,17	0.89	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
8	NAG	0	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	0	2	8	-	2/6/23/26	0/1/1/1
12	NAG	1	1	12,2	-	1/6/23/26	0/1/1/1
12	NAG	1	2	12	-	2/6/23/26	0/1/1/1
12	BMA	1	3	12	-	1/2/19/22	0/1/1/1
8	NAG	2	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	2	2	8	-	0/6/23/26	0/1/1/1
11	NAG	3	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	3	2	11	-	2/6/23/26	0/1/1/1
11	BMA	3	3	11	-	0/2/19/22	0/1/1/1
11	MAN	3	4	11	-	0/2/19/22	0/1/1/1
11	MAN	3	5	11	-	2/2/19/22	0/1/1/1
11	MAN	3	6	11	-	0/2/19/22	0/1/1/1
11	MAN	3	7	11	-	1/2/19/22	0/1/1/1
8	NAG	4	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	4	2	8	-	4/6/23/26	0/1/1/1
8	NAG	5	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	5	2	8	-	4/6/23/26	0/1/1/1
8	NAG	6	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	6	2	8	-	0/6/23/26	0/1/1/1
7	NAG	Q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	1/2/19/22	0/1/1/1
7	MAN	Q	6	7	-	0/2/19/22	1/1/1/1
7	FUC	Q	7	7	-	-	0/1/1/1
8	NAG	R	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	R	2	8	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	m	2	8	-	2/6/23/26	0/1/1/1
12	NAG	n	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	n	2	12	-	2/6/23/26	0/1/1/1
12	BMA	n	3	12	-	2/2/19/22	0/1/1/1
8	NAG	o	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	0/6/23/26	0/1/1/1
11	NAG	p	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	p	2	11	-	2/6/23/26	0/1/1/1
11	BMA	p	3	11	-	0/2/19/22	0/1/1/1
11	MAN	p	4	11	-	0/2/19/22	0/1/1/1
11	MAN	p	5	11	-	2/2/19/22	0/1/1/1
11	MAN	p	6	11	-	0/2/19/22	0/1/1/1
11	MAN	p	7	11	-	1/2/19/22	0/1/1/1
8	NAG	q	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	q	2	8	-	4/6/23/26	0/1/1/1
8	NAG	r	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	r	2	8	-	4/6/23/26	0/1/1/1
8	NAG	s	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	s	2	8	-	0/6/23/26	0/1/1/1
8	NAG	t	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	t	2	8	-	2/6/23/26	0/1/1/1
7	NAG	u	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	u	2	7	-	0/6/23/26	0/1/1/1
7	BMA	u	3	7	-	2/2/19/22	0/1/1/1
7	MAN	u	4	7	-	1/2/19/22	0/1/1/1
7	MAN	u	5	7	-	2/2/19/22	0/1/1/1
7	MAN	u	6	7	-	0/2/19/22	1/1/1/1
7	FUC	u	7	7	-	-	0/1/1/1
8	NAG	v	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	v	2	8	-	4/6/23/26	0/1/1/1
8	NAG	w	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	w	2	8	-	0/6/23/26	0/1/1/1
9	NAG	x	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	x	2	9	-	0/6/23/26	0/1/1/1
9	BMA	x	3	9	-	0/2/19/22	0/1/1/1
9	MAN	x	4	9	-	0/2/19/22	0/1/1/1
9	MAN	x	5	9	-	1/2/19/22	0/1/1/1
10	NAG	y	1	2,10	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	y	2	10	-	2/6/23/26	0/1/1/1
10	BMA	y	3	10	-	0/2/19/22	0/1/1/1
10	MAN	y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	y	5	10	-	0/2/19/22	0/1/1/1
10	MAN	y	6	10	-	0/2/19/22	0/1/1/1
10	MAN	y	7	10	-	0/2/19/22	0/1/1/1
10	MAN	y	8	10	-	0/2/19/22	1/1/1/1
10	MAN	y	9	10	-	0/2/19/22	0/1/1/1
11	NAG	z	1	11,2	-	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	-	0/2/19/22	0/1/1/1
11	MAN	z	4	11	-	0/2/19/22	0/1/1/1
11	MAN	z	5	11	-	2/2/19/22	0/1/1/1
11	MAN	z	6	11	-	0/2/19/22	0/1/1/1
11	MAN	z	7	11	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	W	8	MAN	C1-O5-C5	3.31	116.62	112.19
10	k	8	MAN	C1-O5-C5	3.26	116.56	112.19
10	y	8	MAN	C1-O5-C5	3.25	116.54	112.19
7	u	6	MAN	C1-O5-C5	3.19	116.46	112.19
7	Q	6	MAN	C1-O5-C5	3.10	116.34	112.19
9	j	4	MAN	C1-O5-C5	2.65	115.74	112.19
9	V	4	MAN	C1-O5-C5	2.63	115.72	112.19
11	z	5	MAN	C1-O5-C5	2.61	115.69	112.19
9	x	4	MAN	C1-O5-C5	2.60	115.67	112.19
10	k	4	MAN	O2-C2-C3	-2.58	104.81	110.15
10	y	4	MAN	O2-C2-C3	-2.58	104.81	110.15
10	W	4	MAN	O2-C2-C3	-2.57	104.82	110.15
11	l	5	MAN	C1-O5-C5	2.57	115.62	112.19
11	X	5	MAN	C1-O5-C5	2.54	115.59	112.19
11	l	4	MAN	O2-C2-C3	-2.44	105.11	110.15
11	z	4	MAN	O2-C2-C3	-2.43	105.11	110.15
11	X	4	MAN	O2-C2-C3	-2.42	105.14	110.15
10	W	9	MAN	C1-O5-C5	2.39	115.39	112.19
7	u	5	MAN	C1-O5-C5	2.38	115.38	112.19
11	3	1	NAG	C1-O5-C5	2.38	115.38	112.19
10	k	9	MAN	C1-O5-C5	2.38	115.37	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1	NAG	C1-O5-C5	2.36	115.35	112.19
11	X	6	MAN	C1-O5-C5	2.36	115.34	112.19
10	y	9	MAN	C1-O5-C5	2.35	115.34	112.19
10	y	7	MAN	O2-C2-C3	-2.33	105.33	110.15
11	l	6	MAN	C1-O5-C5	2.32	115.29	112.19
11	l	5	MAN	O2-C2-C3	-2.31	105.36	110.15
11	z	5	MAN	O2-C2-C3	-2.31	105.38	110.15
11	p	4	MAN	C1-O5-C5	2.30	115.27	112.19
9	j	5	MAN	O2-C2-C3	-2.30	105.39	110.15
11	z	6	MAN	C1-O5-C5	2.29	115.25	112.19
10	W	7	MAN	O2-C2-C3	-2.29	105.42	110.15
10	k	5	MAN	O2-C2-C3	-2.29	105.42	110.15
11	X	5	MAN	O2-C2-C3	-2.29	105.42	110.15
11	3	4	MAN	C1-O5-C5	2.28	115.25	112.19
10	k	4	MAN	C1-O5-C5	2.28	115.25	112.19
9	V	5	MAN	O2-C2-C3	-2.28	105.43	110.15
9	x	5	MAN	O2-C2-C3	-2.28	105.44	110.15
10	k	7	MAN	O2-C2-C3	-2.27	105.44	110.15
10	y	4	MAN	C1-O5-C5	2.27	115.23	112.19
10	y	5	MAN	O2-C2-C3	-2.27	105.45	110.15
10	W	5	MAN	O2-C2-C3	-2.25	105.48	110.15
11	b	4	MAN	C1-O5-C5	2.25	115.20	112.19
11	b	5	MAN	C1-O5-C5	2.23	115.17	112.19
11	p	7	MAN	O2-C2-C3	-2.22	105.54	110.15
7	u	5	MAN	O2-C2-C3	-2.22	105.56	110.15
11	p	5	MAN	O2-C2-C3	-2.22	105.56	110.15
11	X	7	MAN	O2-C2-C3	-2.20	105.59	110.15
11	3	7	MAN	O2-C2-C3	-2.20	105.60	110.15
11	l	6	MAN	O2-C2-C3	-2.19	105.61	110.15
11	b	4	MAN	O2-C2-C3	-2.19	105.61	110.15
10	k	9	MAN	O2-C2-C3	-2.19	105.62	110.15
11	z	7	MAN	O2-C2-C3	-2.19	105.62	110.15
11	3	5	MAN	O2-C2-C3	-2.18	105.63	110.15
11	b	7	MAN	O2-C2-C3	-2.18	105.63	110.15
11	l	7	MAN	O2-C2-C3	-2.18	105.63	110.15
10	W	9	MAN	O2-C2-C3	-2.18	105.64	110.15
11	z	6	MAN	O2-C2-C3	-2.18	105.64	110.15
11	p	1	NAG	C1-O5-C5	2.17	115.10	112.19
10	W	4	MAN	C1-O5-C5	2.17	115.10	112.19
11	b	6	MAN	O2-C2-C3	-2.17	105.66	110.15
11	b	5	MAN	O2-C2-C3	-2.16	105.67	110.15
11	X	6	MAN	O2-C2-C3	-2.16	105.67	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	p	7	MAN	C1-O5-C5	2.16	115.08	112.19
10	y	9	MAN	O2-C2-C3	-2.16	105.68	110.15
9	x	4	MAN	O2-C2-C3	-2.16	105.69	110.15
11	3	4	MAN	O2-C2-C3	-2.16	105.69	110.15
11	3	6	MAN	O2-C2-C3	-2.15	105.70	110.15
9	V	4	MAN	O2-C2-C3	-2.15	105.70	110.15
7	Q	4	MAN	O2-C2-C3	-2.14	105.72	110.15
9	j	4	MAN	O2-C2-C3	-2.14	105.72	110.15
11	p	4	MAN	O2-C2-C3	-2.13	105.73	110.15
7	u	4	MAN	O2-C2-C3	-2.13	105.73	110.15
7	Q	5	MAN	O2-C2-C3	-2.13	105.74	110.15
10	W	8	MAN	O2-C2-C3	-2.12	105.75	110.15
10	k	7	MAN	C1-O5-C5	2.12	115.02	112.19
7	Q	6	MAN	O2-C2-C3	-2.11	105.77	110.15
10	y	7	MAN	C1-O5-C5	2.11	115.02	112.19
7	g	5	MAN	O2-C2-C3	-2.11	105.78	110.15
11	z	4	MAN	C1-O5-C5	2.11	115.01	112.19
11	p	6	MAN	O2-C2-C3	-2.11	105.79	110.15
10	k	8	MAN	O2-C2-C3	-2.10	105.79	110.15
11	b	7	MAN	C1-O5-C5	2.10	115.00	112.19
10	y	8	MAN	O2-C2-C3	-2.10	105.81	110.15
10	y	6	MAN	O2-C2-C3	-2.09	105.82	110.15
11	p	5	MAN	C1-O5-C5	2.09	114.98	112.19
10	W	6	MAN	O2-C2-C3	-2.08	105.84	110.15
7	u	6	MAN	O2-C2-C3	-2.08	105.84	110.15
11	l	4	MAN	C1-O5-C5	2.08	114.97	112.19
7	g	6	MAN	O2-C2-C3	-2.06	105.89	110.15
7	g	5	MAN	C1-O5-C5	2.06	114.94	112.19
7	g	4	MAN	O2-C2-C3	-2.05	105.90	110.15
11	X	4	MAN	C1-O5-C5	2.05	114.94	112.19
7	Q	5	MAN	C1-O5-C5	2.04	114.92	112.19
9	V	5	MAN	C1-O5-C5	2.03	114.91	112.19
11	3	5	MAN	C1-O5-C5	2.03	114.91	112.19
10	k	6	MAN	O2-C2-C3	-2.03	105.95	110.15
11	3	7	MAN	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	f	1	NAG	C1-C2-N2-C7
8	t	1	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	f	2	NAG	C4-C5-C6-O6
8	t	2	NAG	C4-C5-C6-O6
8	m	1	NAG	O5-C5-C6-O6
8	0	1	NAG	O5-C5-C6-O6
11	b	2	NAG	O5-C5-C6-O6
11	3	2	NAG	O5-C5-C6-O6
11	p	2	NAG	O5-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6
11	3	5	MAN	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
8	0	1	NAG	C4-C5-C6-O6
7	Q	4	MAN	O5-C5-C6-O6
8	r	2	NAG	O5-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
8	d	2	NAG	O5-C5-C6-O6
8	5	2	NAG	O5-C5-C6-O6
8	0	2	NAG	C4-C5-C6-O6
11	p	2	NAG	C4-C5-C6-O6
8	t	2	NAG	O5-C5-C6-O6
8	4	2	NAG	O5-C5-C6-O6
8	Y	2	NAG	C4-C5-C6-O6
8	c	2	NAG	O5-C5-C6-O6
8	m	1	NAG	C4-C5-C6-O6
11	b	2	NAG	C4-C5-C6-O6
8	0	2	NAG	O5-C5-C6-O6
11	3	2	NAG	C4-C5-C6-O6
8	q	2	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
12	Z	3	BMA	O5-C5-C6-O6
11	3	5	MAN	C4-C5-C6-O6
11	b	5	MAN	O5-C5-C6-O6
11	z	2	NAG	O5-C5-C6-O6
8	q	2	NAG	C4-C5-C6-O6
8	4	2	NAG	C4-C5-C6-O6
12	n	1	NAG	C4-C5-C6-O6
7	u	5	MAN	O5-C5-C6-O6
11	z	2	NAG	C4-C5-C6-O6
10	W	2	NAG	O5-C5-C6-O6
10	k	2	NAG	O5-C5-C6-O6
8	c	2	NAG	C4-C5-C6-O6
11	X	2	NAG	O5-C5-C6-O6
12	n	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	Q	1	NAG	C8-C7-N2-C2
7	Q	1	NAG	O7-C7-N2-C2
7	g	1	NAG	C8-C7-N2-C2
7	g	1	NAG	O7-C7-N2-C2
7	u	1	NAG	C8-C7-N2-C2
7	u	1	NAG	O7-C7-N2-C2
11	p	5	MAN	O5-C5-C6-O6
8	i	1	NAG	C4-C5-C6-O6
8	m	2	NAG	C4-C5-C6-O6
10	W	2	NAG	C4-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6
11	b	5	MAN	C4-C5-C6-O6
11	z	5	MAN	O5-C5-C6-O6
12	Z	1	NAG	C4-C5-C6-O6
8	w	1	NAG	C4-C5-C6-O6
11	X	5	MAN	O5-C5-C6-O6
11	l	2	NAG	O5-C5-C6-O6
12	l	3	BMA	O5-C5-C6-O6
7	u	5	MAN	C4-C5-C6-O6
10	k	2	NAG	C4-C5-C6-O6
11	X	2	NAG	C4-C5-C6-O6
12	n	1	NAG	O5-C5-C6-O6
7	Q	4	MAN	C4-C5-C6-O6
11	l	2	NAG	C4-C5-C6-O6
11	p	5	MAN	C4-C5-C6-O6
11	z	5	MAN	C4-C5-C6-O6
8	r	2	NAG	C4-C5-C6-O6
11	X	5	MAN	C4-C5-C6-O6
8	m	2	NAG	O5-C5-C6-O6
11	l	5	MAN	O5-C5-C6-O6
8	i	1	NAG	O5-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
12	Z	1	NAG	O5-C5-C6-O6
8	w	1	NAG	O5-C5-C6-O6
11	l	5	MAN	C4-C5-C6-O6
8	R	1	NAG	C4-C5-C6-O6
8	d	2	NAG	C4-C5-C6-O6
8	5	2	NAG	C4-C5-C6-O6
8	v	1	NAG	C4-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
11	3	1	NAG	O5-C5-C6-O6
11	p	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	3	1	NAG	C4-C5-C6-O6
11	p	1	NAG	C4-C5-C6-O6
11	p	7	MAN	O5-C5-C6-O6
7	g	4	MAN	O5-C5-C6-O6
9	j	5	MAN	O5-C5-C6-O6
9	x	5	MAN	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
9	V	5	MAN	O5-C5-C6-O6
11	3	7	MAN	O5-C5-C6-O6
7	u	4	MAN	O5-C5-C6-O6
11	b	7	MAN	O5-C5-C6-O6
8	h	1	NAG	C4-C5-C6-O6
11	b	1	NAG	C4-C5-C6-O6
8	v	1	NAG	O5-C5-C6-O6
11	b	1	NAG	O5-C5-C6-O6
10	W	1	NAG	C4-C5-C6-O6
10	W	1	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
8	R	2	NAG	C1-C2-N2-C7
8	d	1	NAG	C1-C2-N2-C7
8	d	2	NAG	C1-C2-N2-C7
8	h	2	NAG	C1-C2-N2-C7
8	r	1	NAG	C1-C2-N2-C7
8	r	2	NAG	C1-C2-N2-C7
8	v	2	NAG	C1-C2-N2-C7
8	5	1	NAG	C1-C2-N2-C7
8	5	2	NAG	C1-C2-N2-C7
8	v	2	NAG	C4-C5-C6-O6
10	y	2	NAG	C4-C5-C6-O6
8	h	2	NAG	C4-C5-C6-O6
7	u	3	BMA	C4-C5-C6-O6
10	y	2	NAG	O5-C5-C6-O6
8	R	2	NAG	C3-C2-N2-C7
8	c	2	NAG	C3-C2-N2-C7
8	d	1	NAG	C3-C2-N2-C7
8	h	2	NAG	C3-C2-N2-C7
8	q	2	NAG	C3-C2-N2-C7
8	r	1	NAG	C3-C2-N2-C7
8	t	1	NAG	C3-C2-N2-C7
8	v	2	NAG	C3-C2-N2-C7
8	4	2	NAG	C3-C2-N2-C7
12	Z	2	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	n	2	NAG	C3-C2-N2-C7
12	l	2	NAG	C3-C2-N2-C7
7	u	3	BMA	O5-C5-C6-O6
8	h	1	NAG	O5-C5-C6-O6
7	Q	5	MAN	O5-C5-C6-O6
12	Z	3	BMA	C4-C5-C6-O6
7	g	3	BMA	C4-C5-C6-O6
7	g	3	BMA	O5-C5-C6-O6
8	v	2	NAG	O5-C5-C6-O6
8	c	2	NAG	C1-C2-N2-C7
8	q	2	NAG	C1-C2-N2-C7
8	4	2	NAG	C1-C2-N2-C7
12	Z	2	NAG	C1-C2-N2-C7
12	n	2	NAG	C1-C2-N2-C7
12	l	2	NAG	C1-C2-N2-C7
8	h	2	NAG	O5-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
8	d	2	NAG	C3-C2-N2-C7
8	f	1	NAG	C3-C2-N2-C7
8	r	2	NAG	C3-C2-N2-C7
8	5	1	NAG	C3-C2-N2-C7
8	5	2	NAG	C3-C2-N2-C7
7	g	2	NAG	O5-C5-C6-O6
12	l	1	NAG	C4-C5-C6-O6
12	n	3	BMA	C4-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	W	8	MAN	C1-C2-C3-C4-C5-O5
10	k	8	MAN	C1-C2-C3-C4-C5-O5
10	y	8	MAN	C1-C2-C3-C4-C5-O5
7	Q	6	MAN	C1-C2-C3-C4-C5-O5
7	u	6	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 8 short contacts:

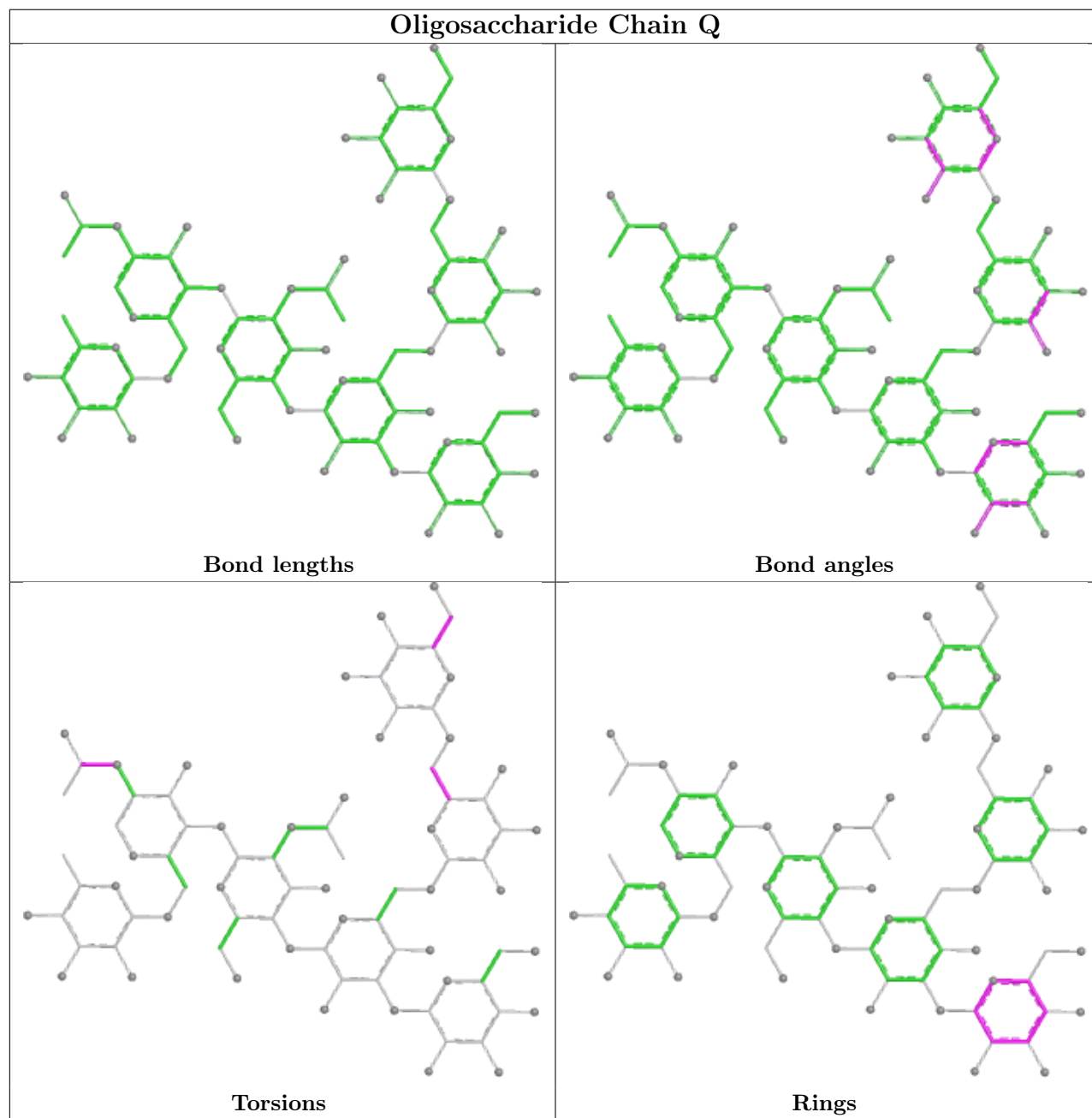
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	3	2	NAG	1	0
11	X	6	MAN	1	0
7	u	2	NAG	1	0
11	p	2	NAG	1	0

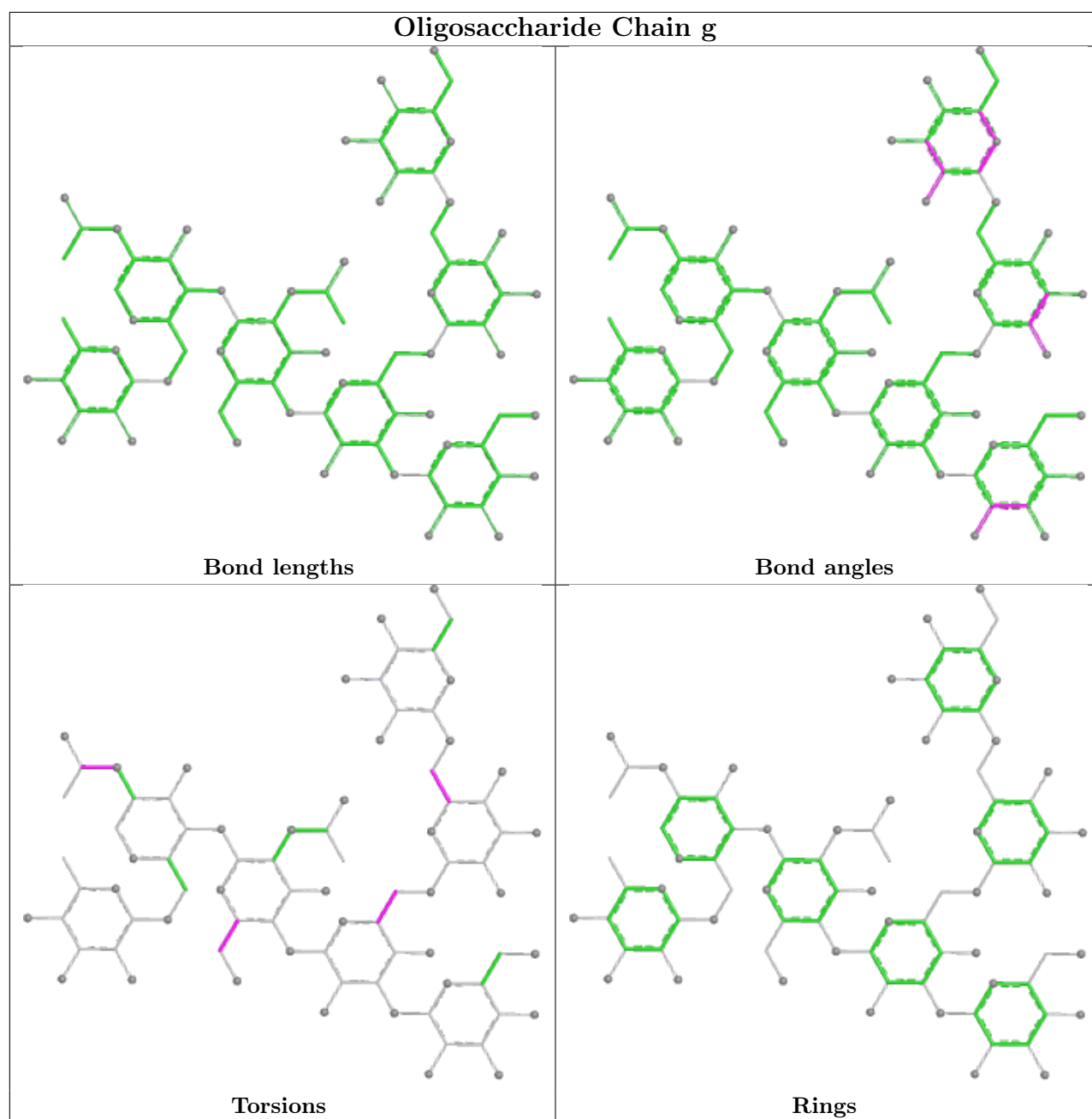
Continued on next page...

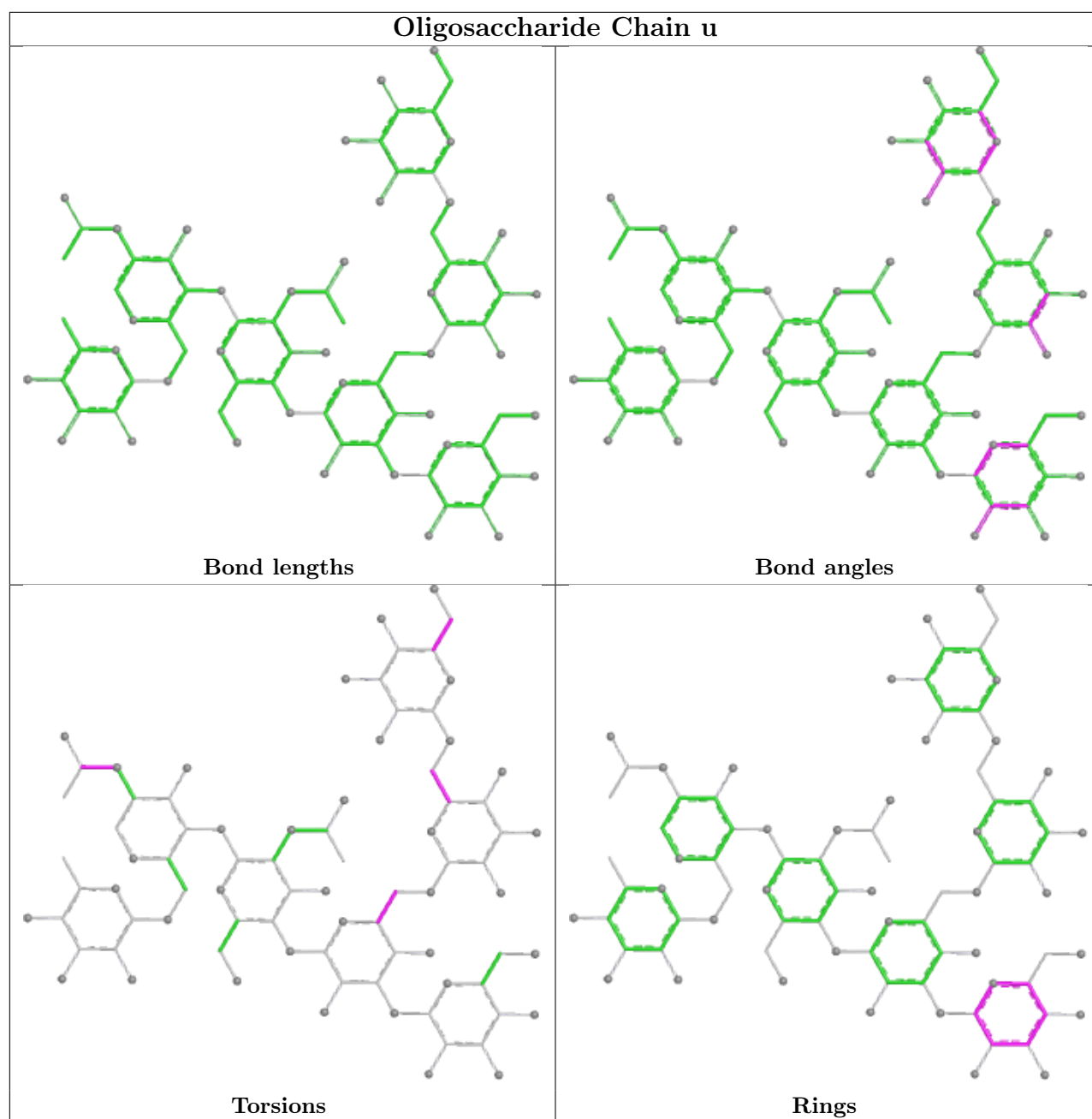
Continued from previous page...

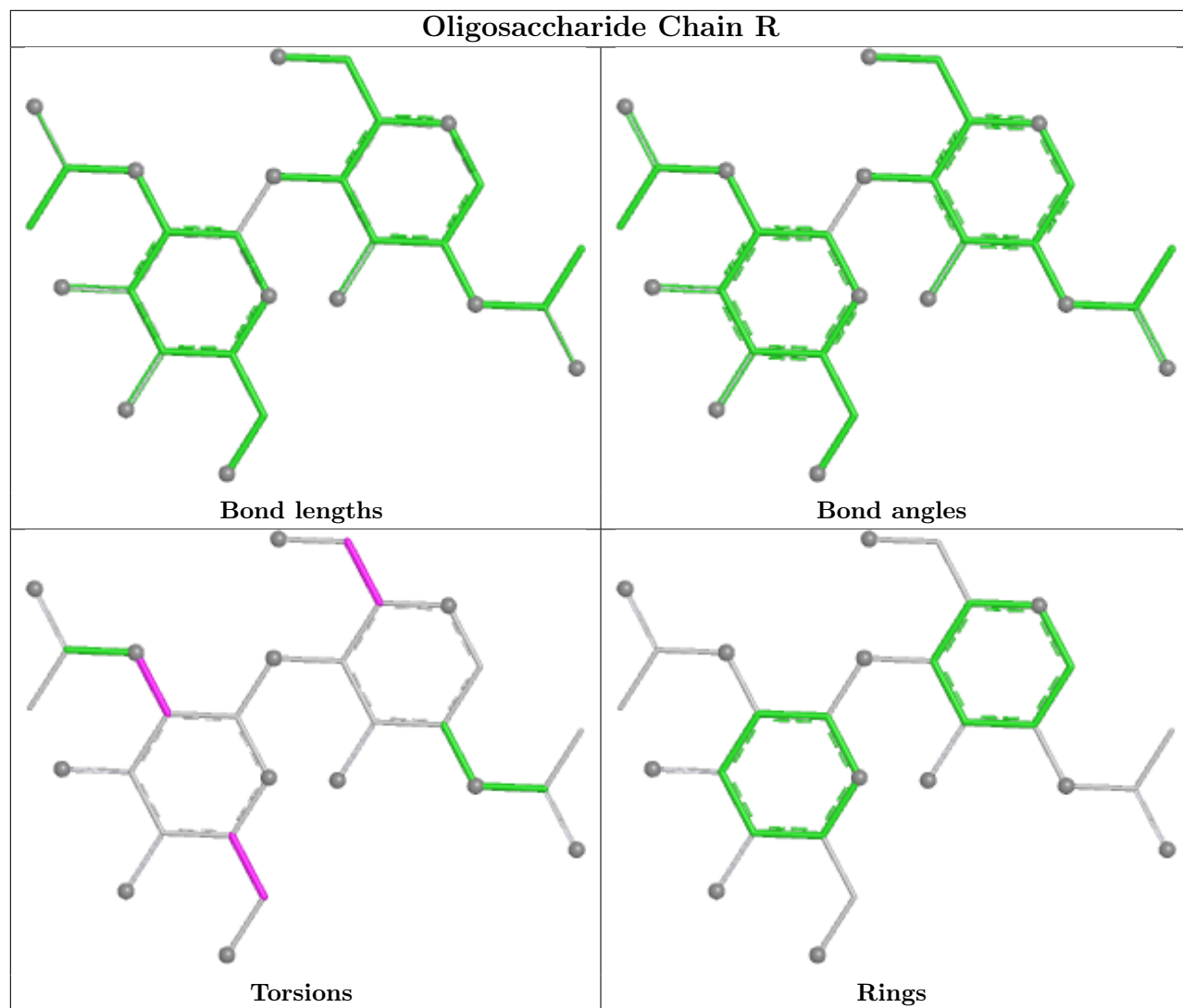
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	u	4	MAN	1	0
11	z	6	MAN	1	0
11	b	2	NAG	1	0
7	Q	2	NAG	1	0

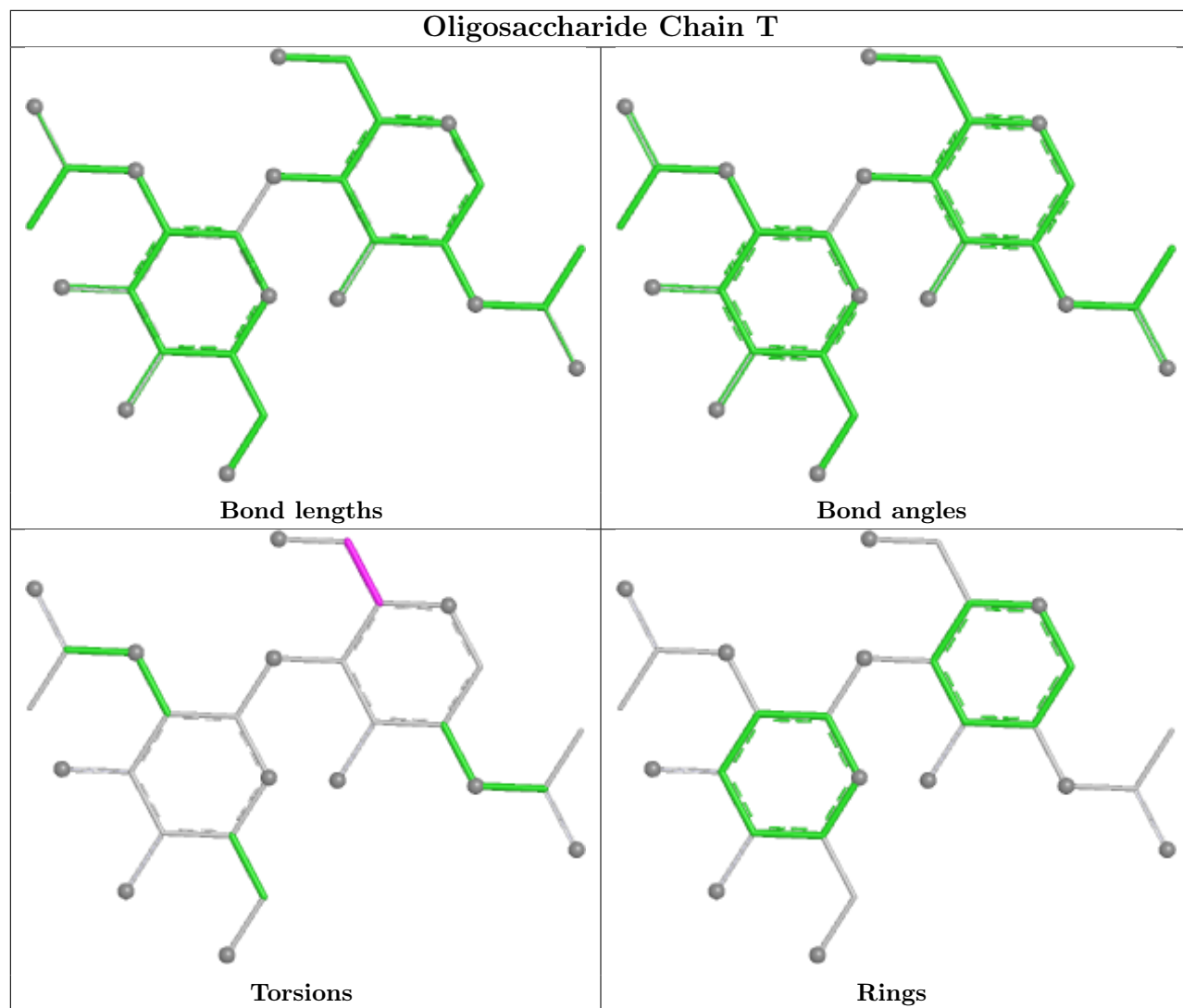
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

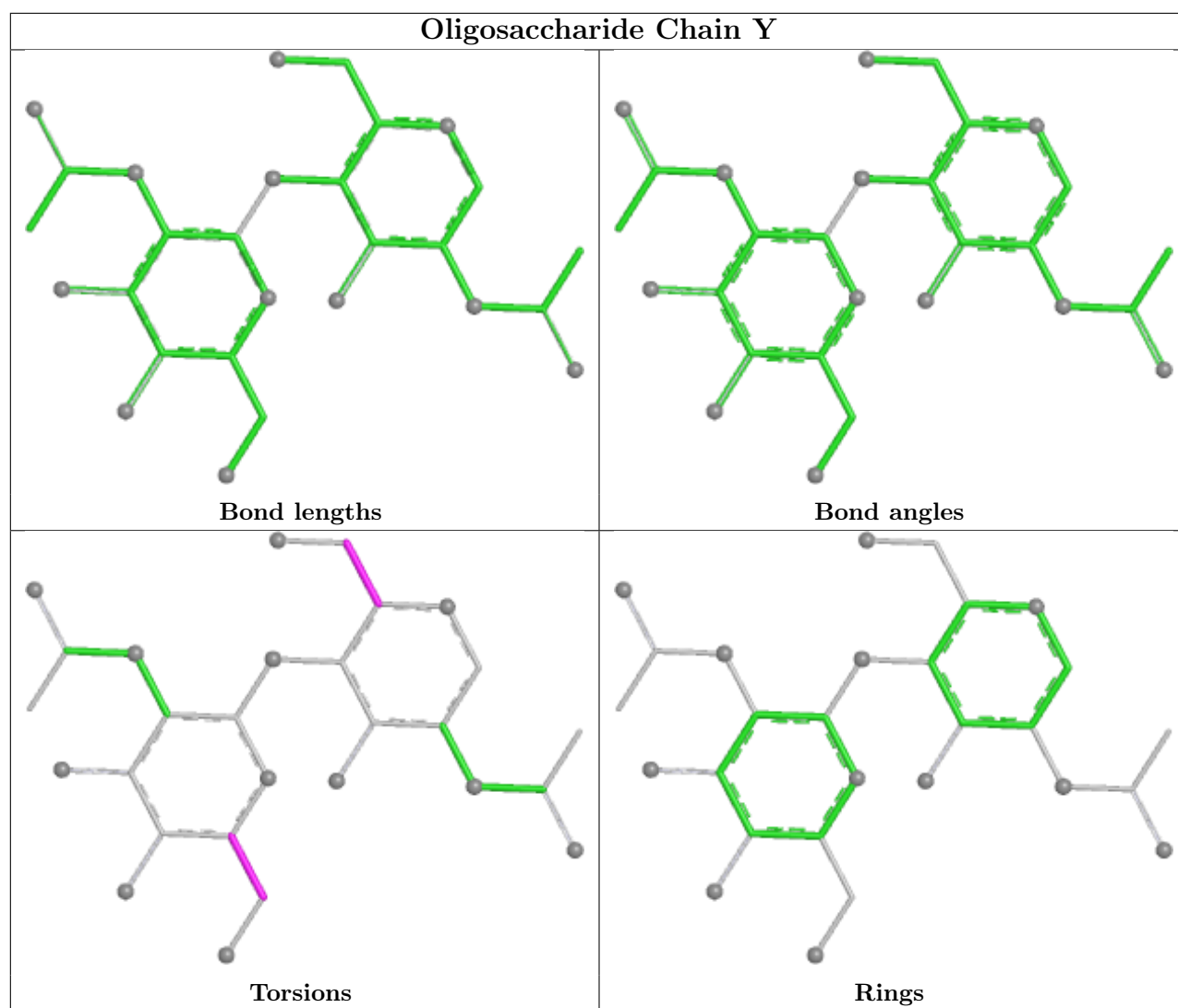


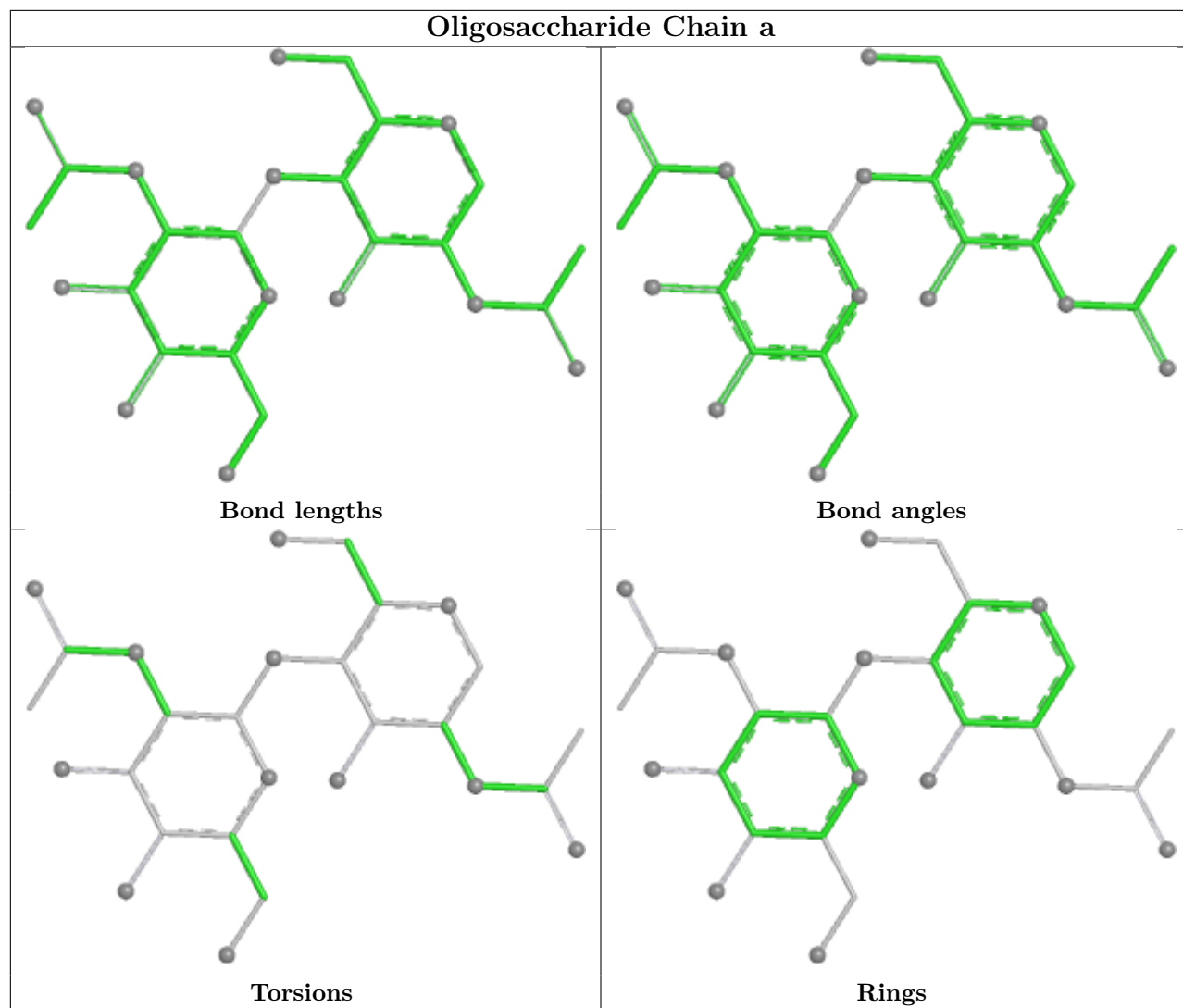


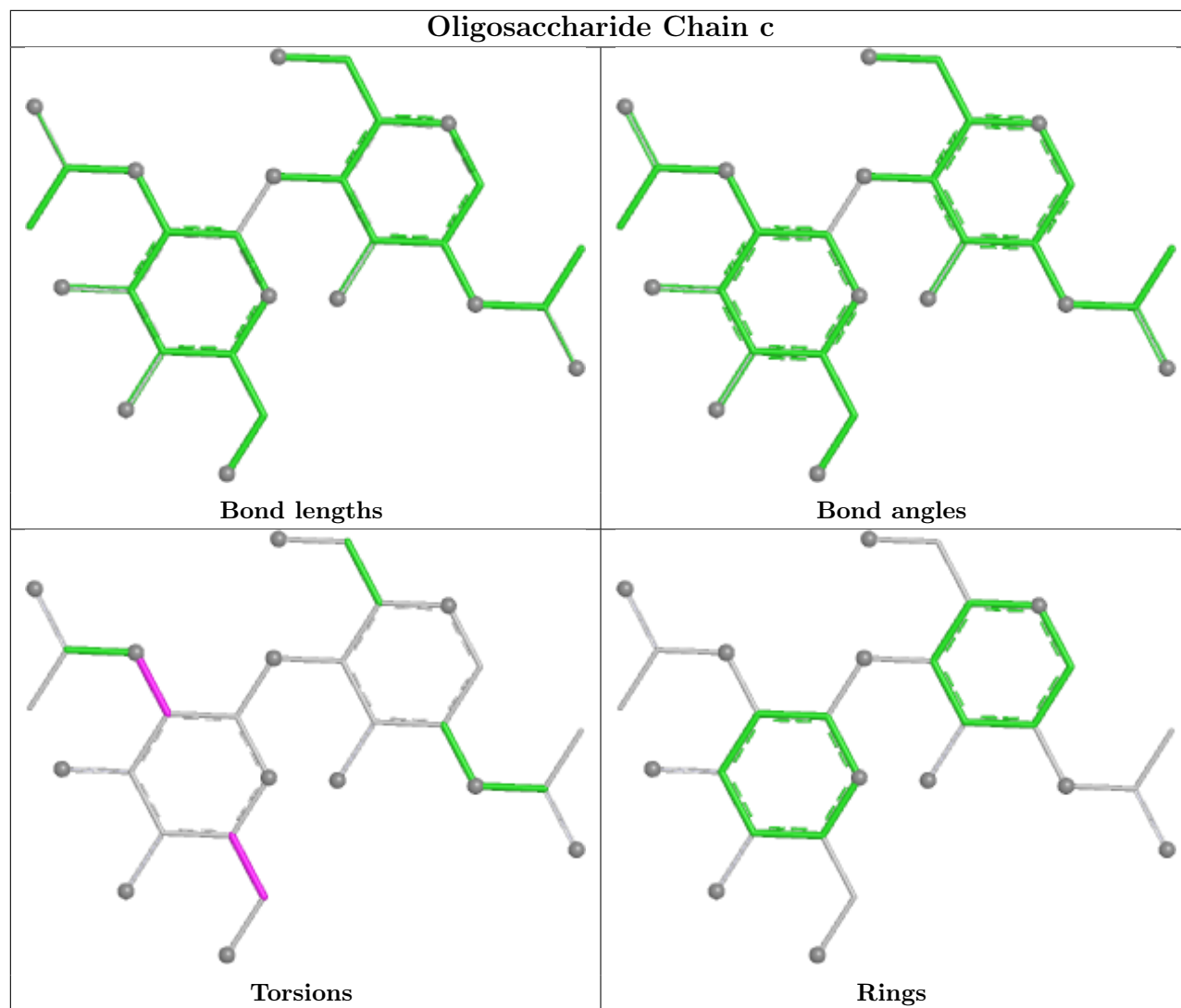


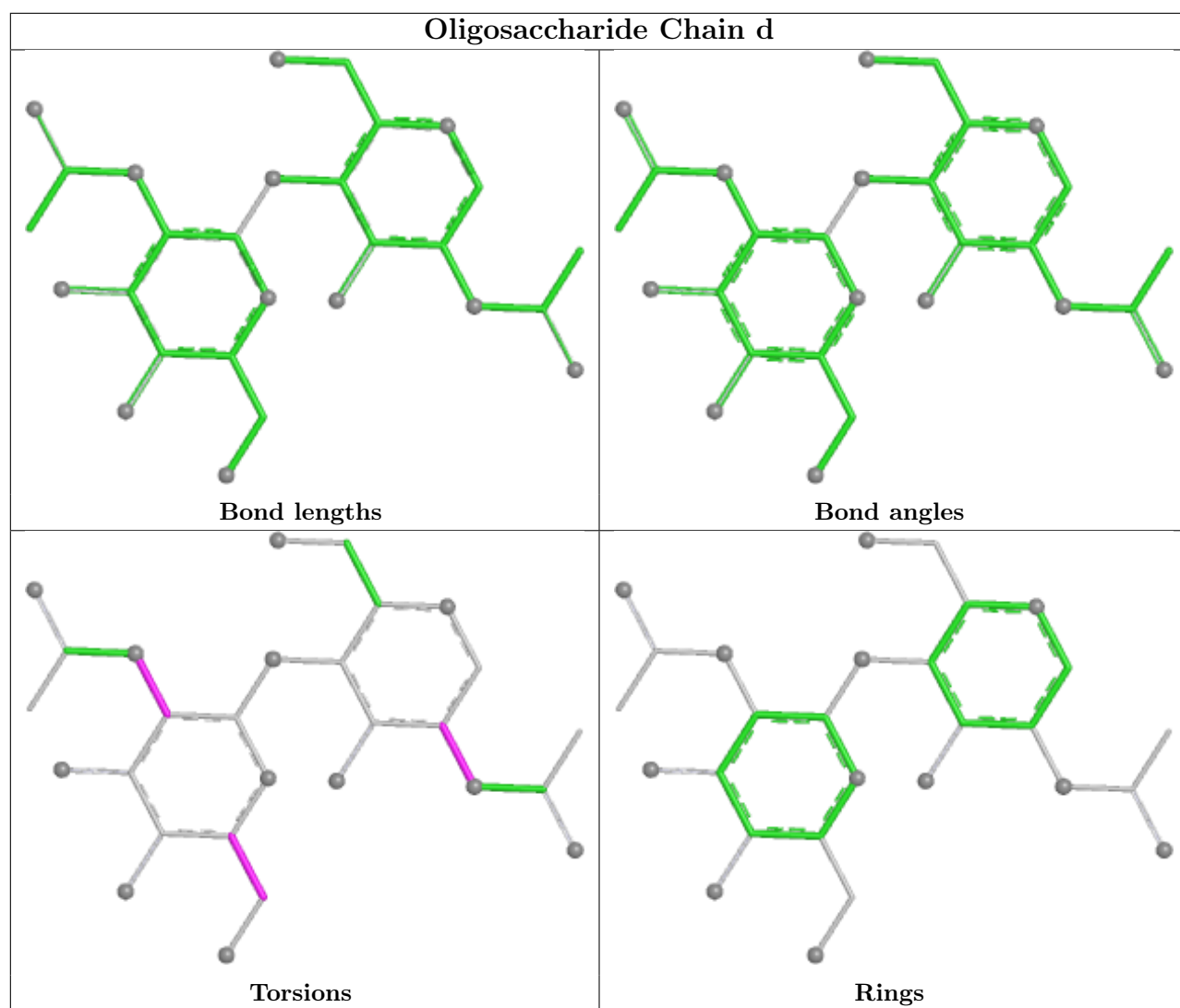


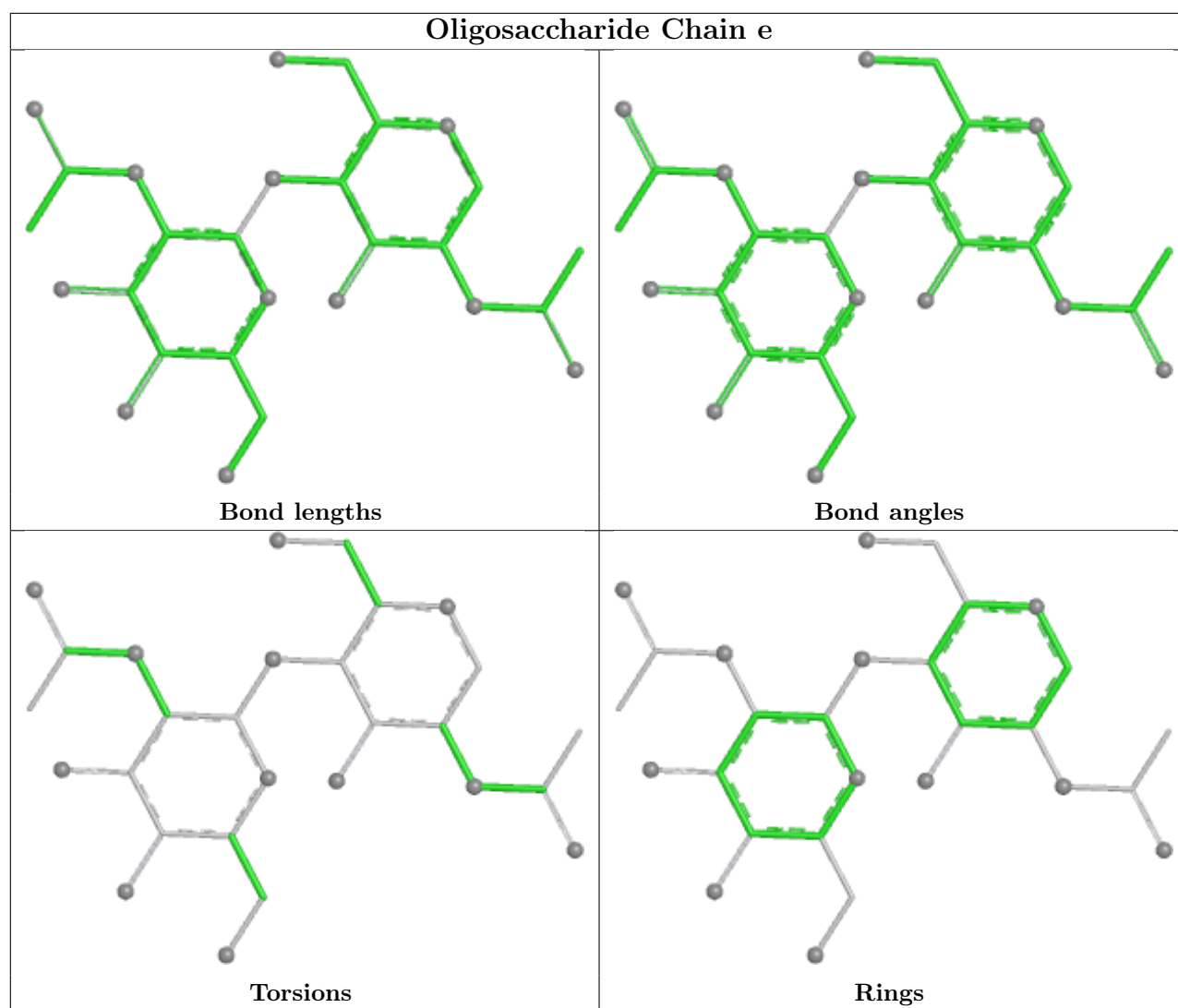


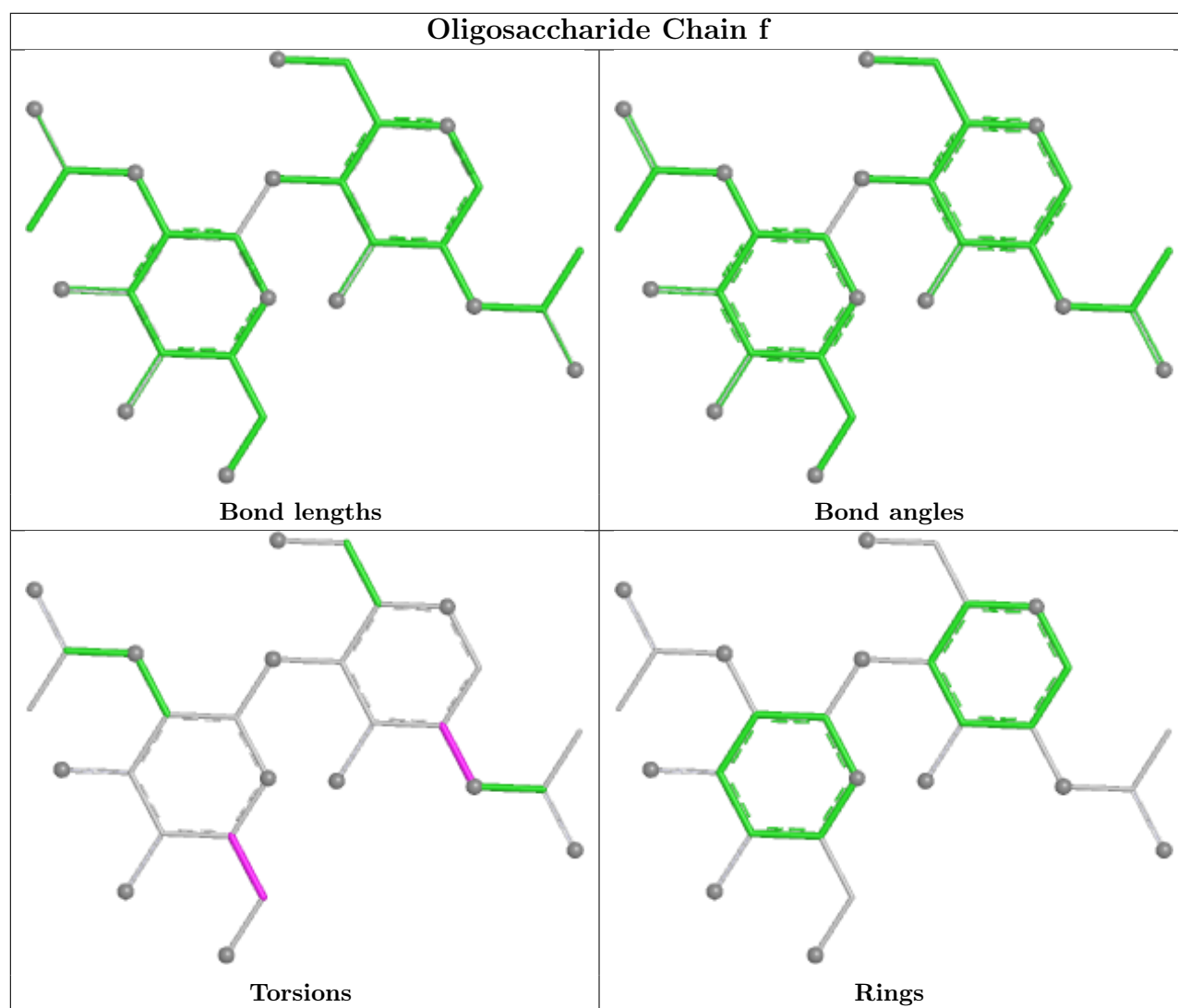


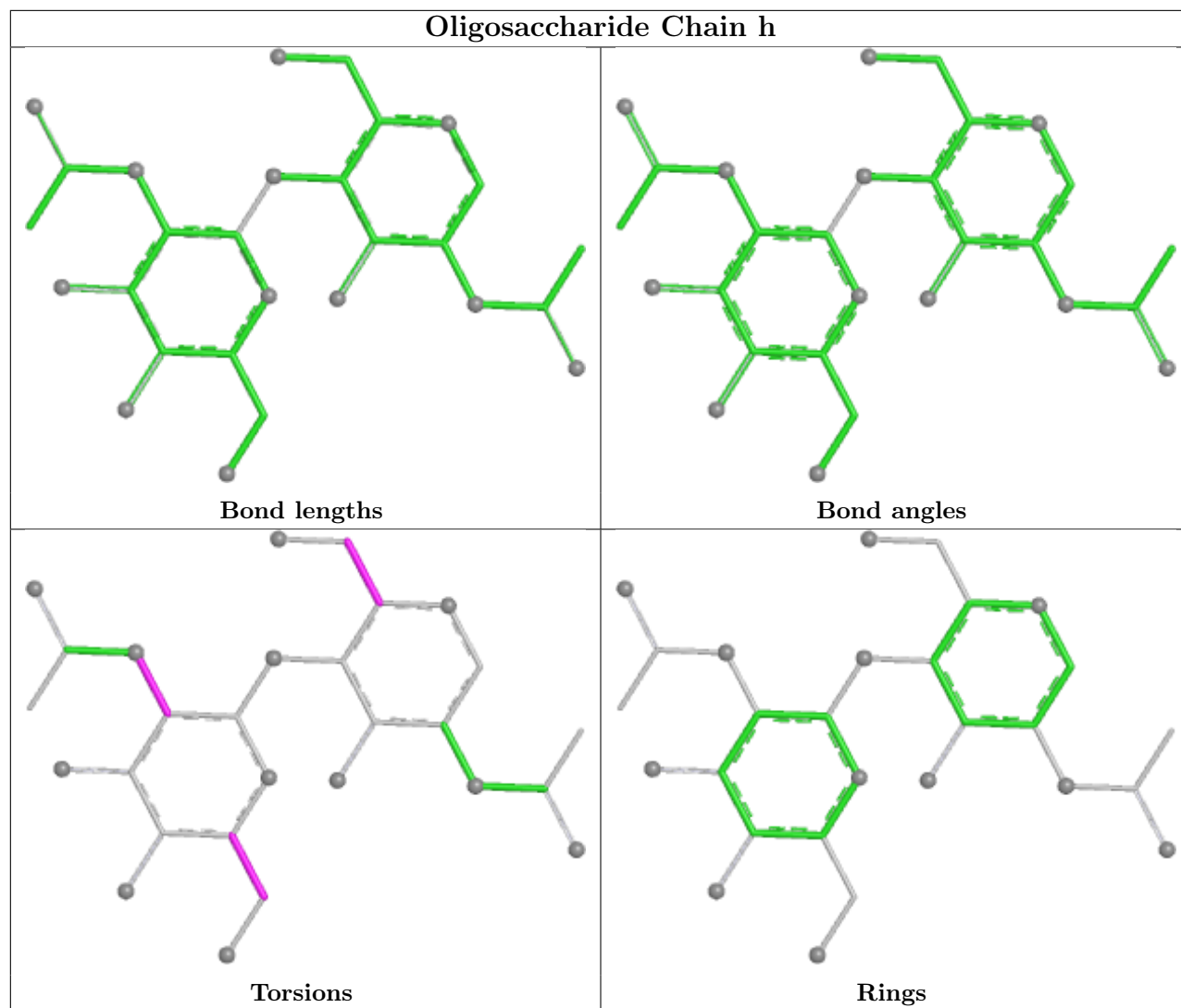


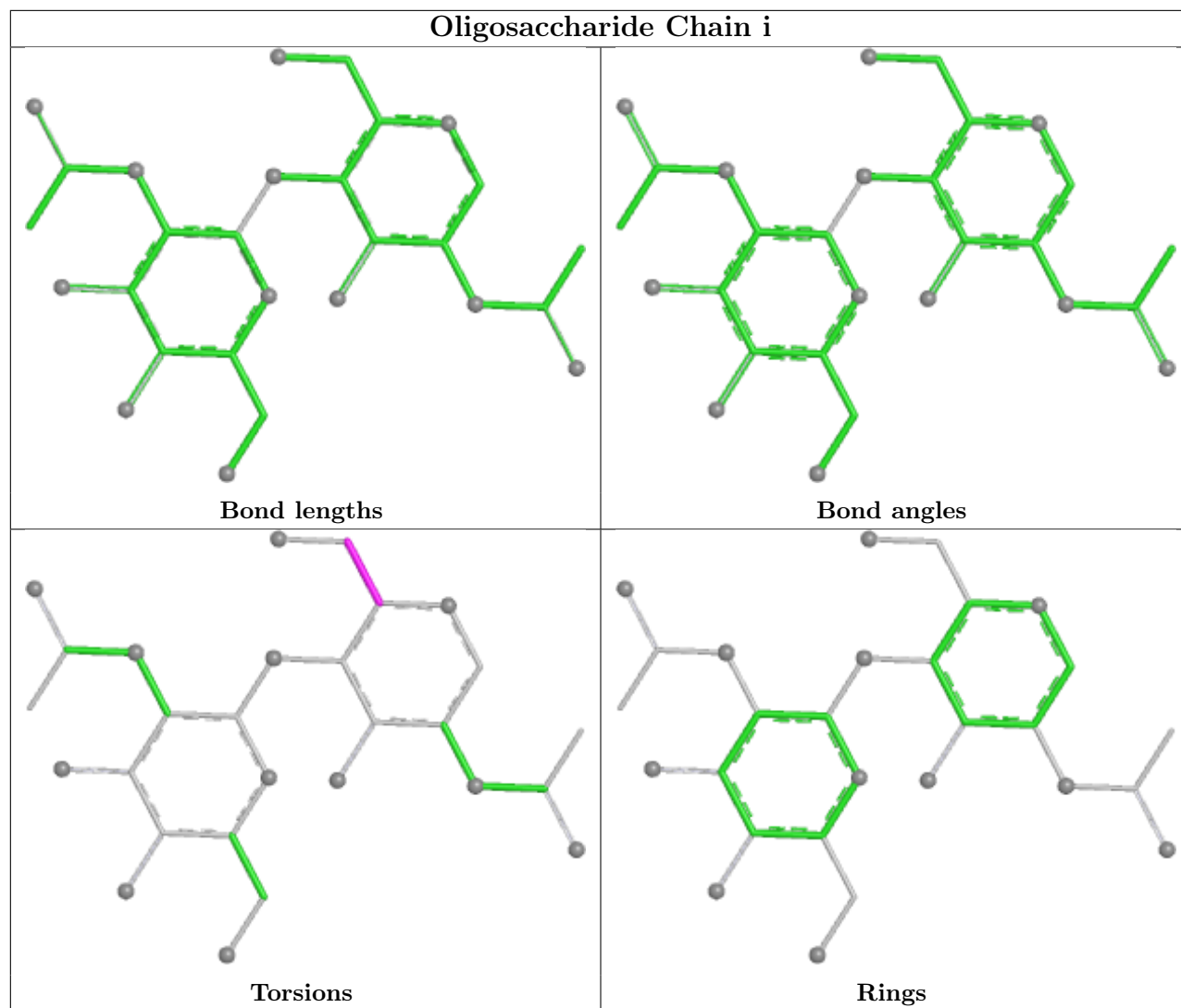


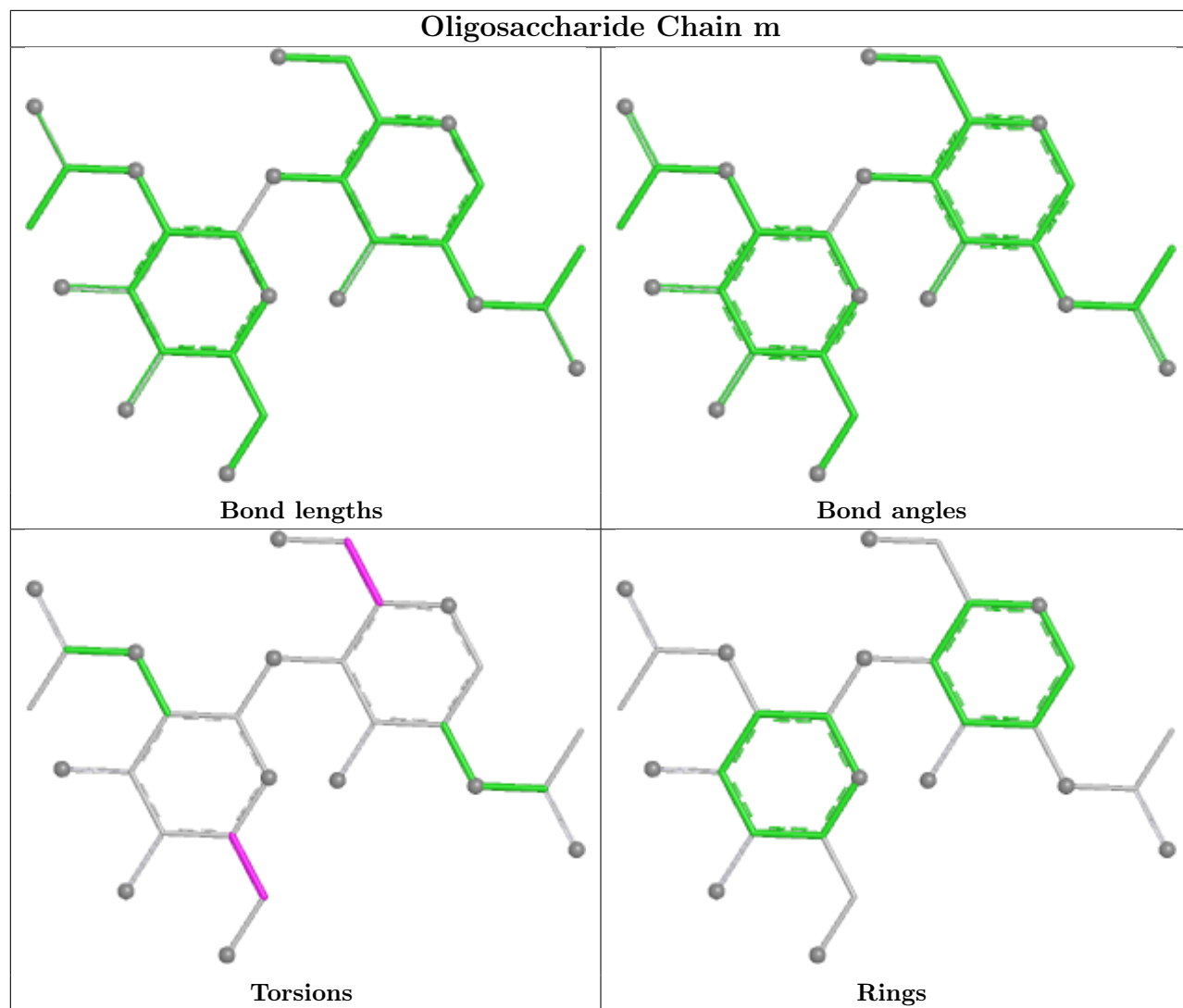


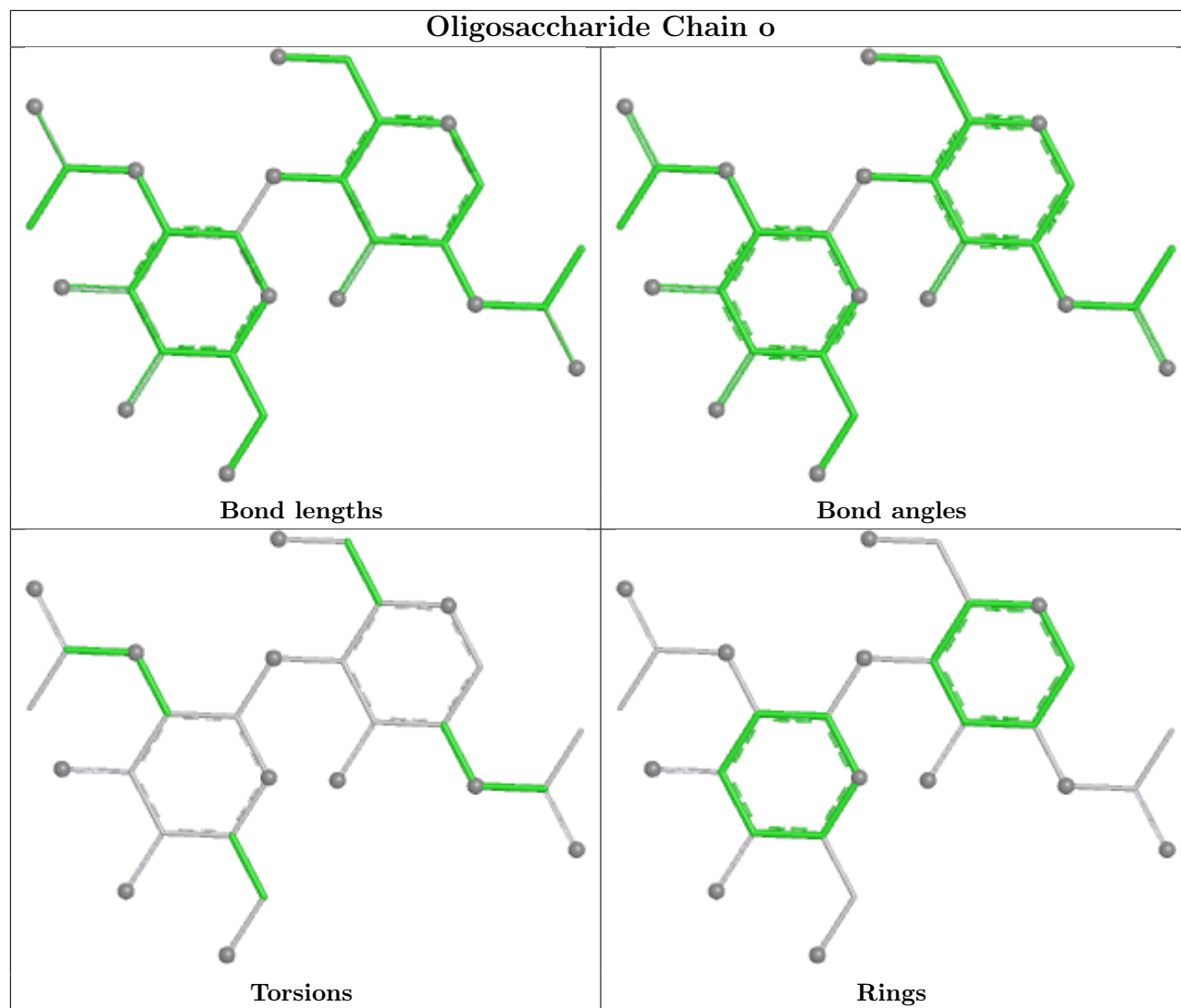


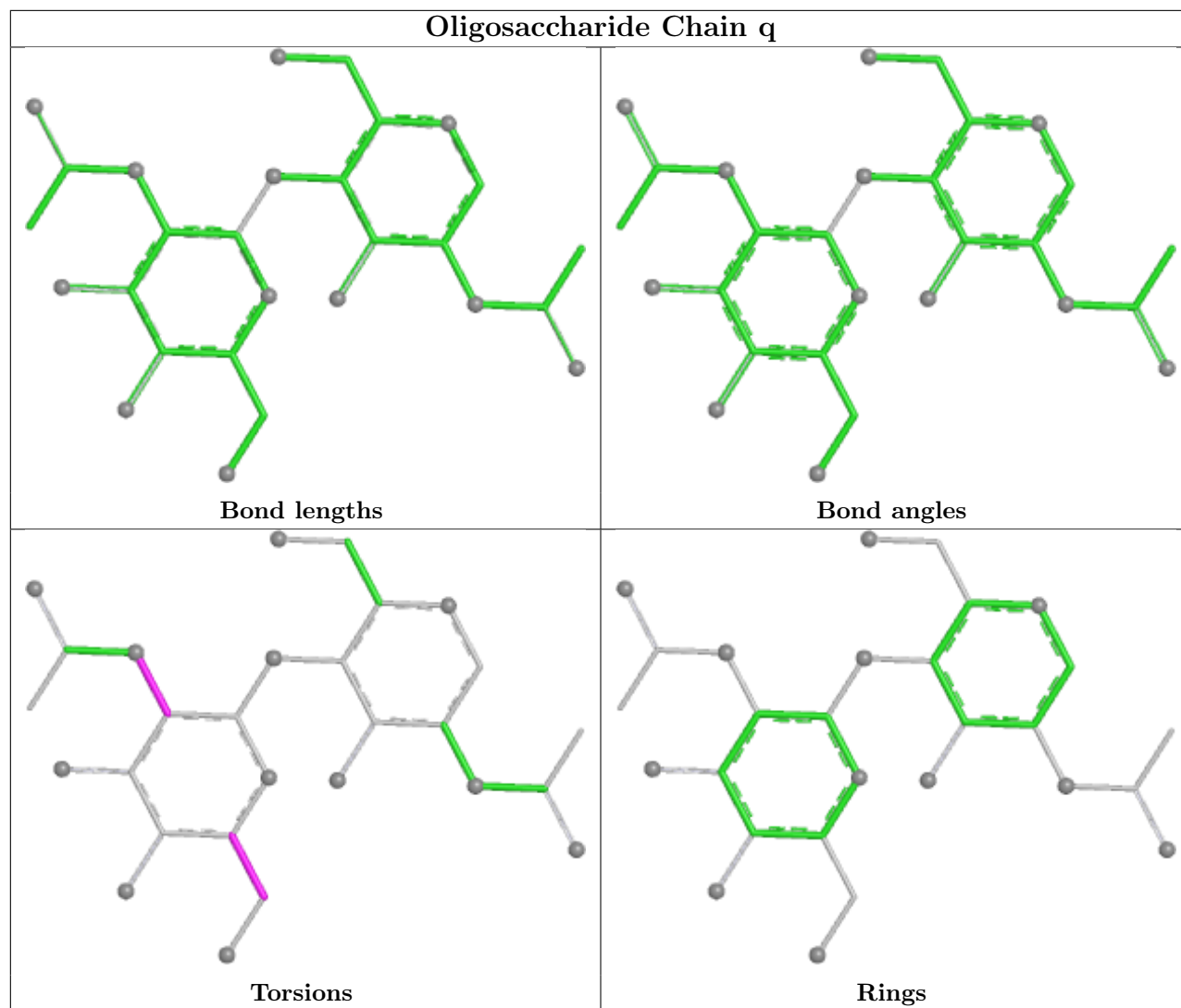


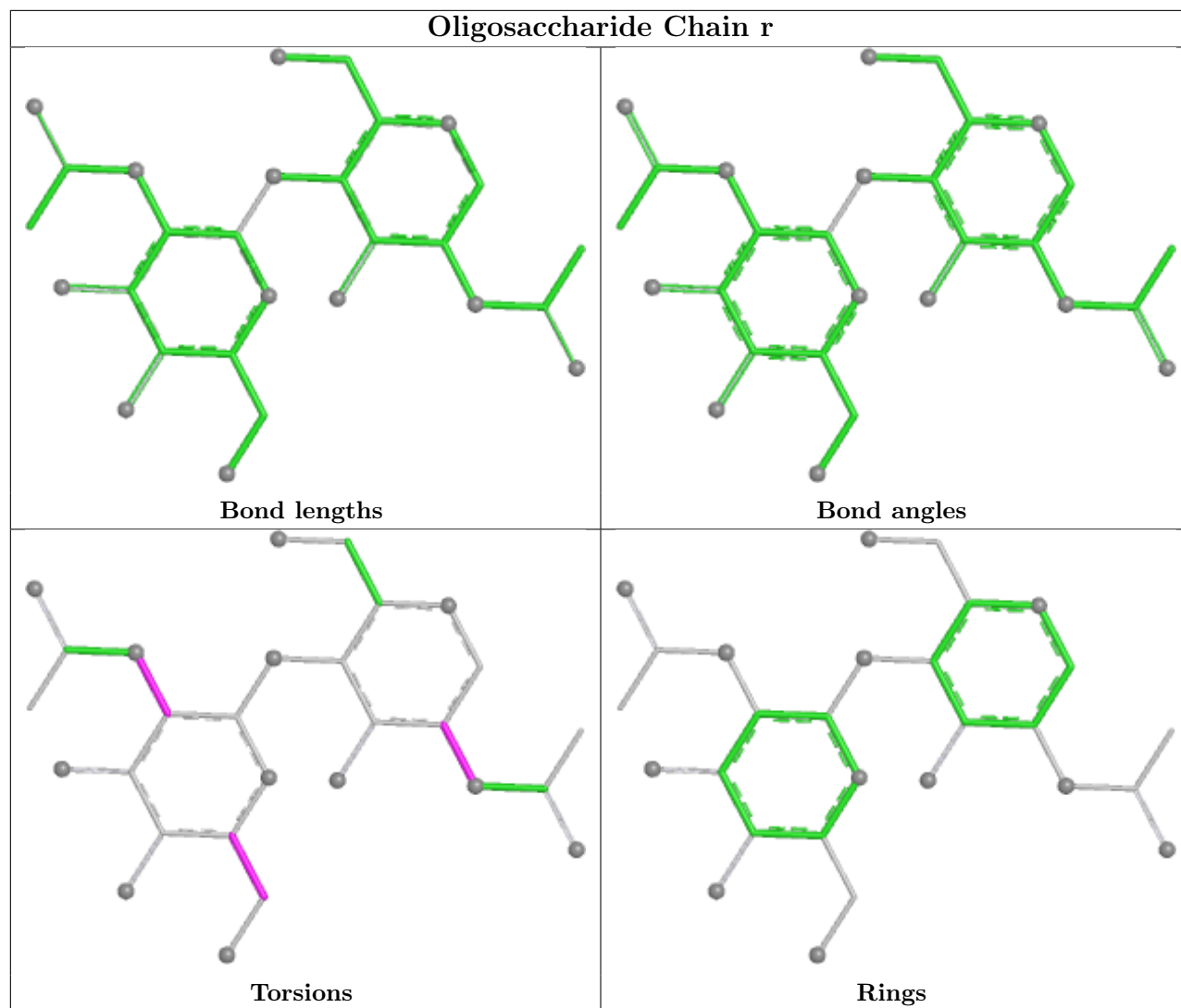


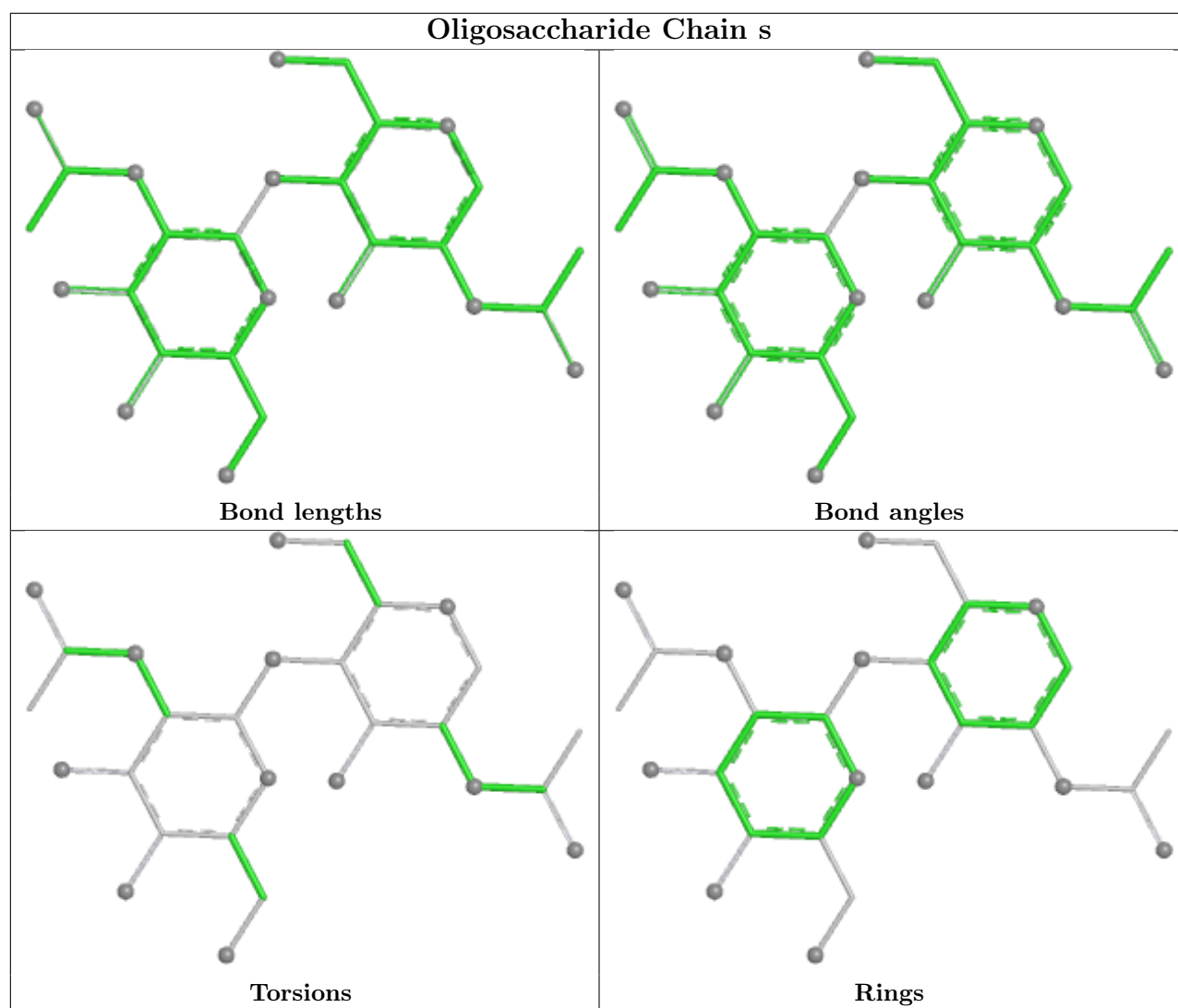


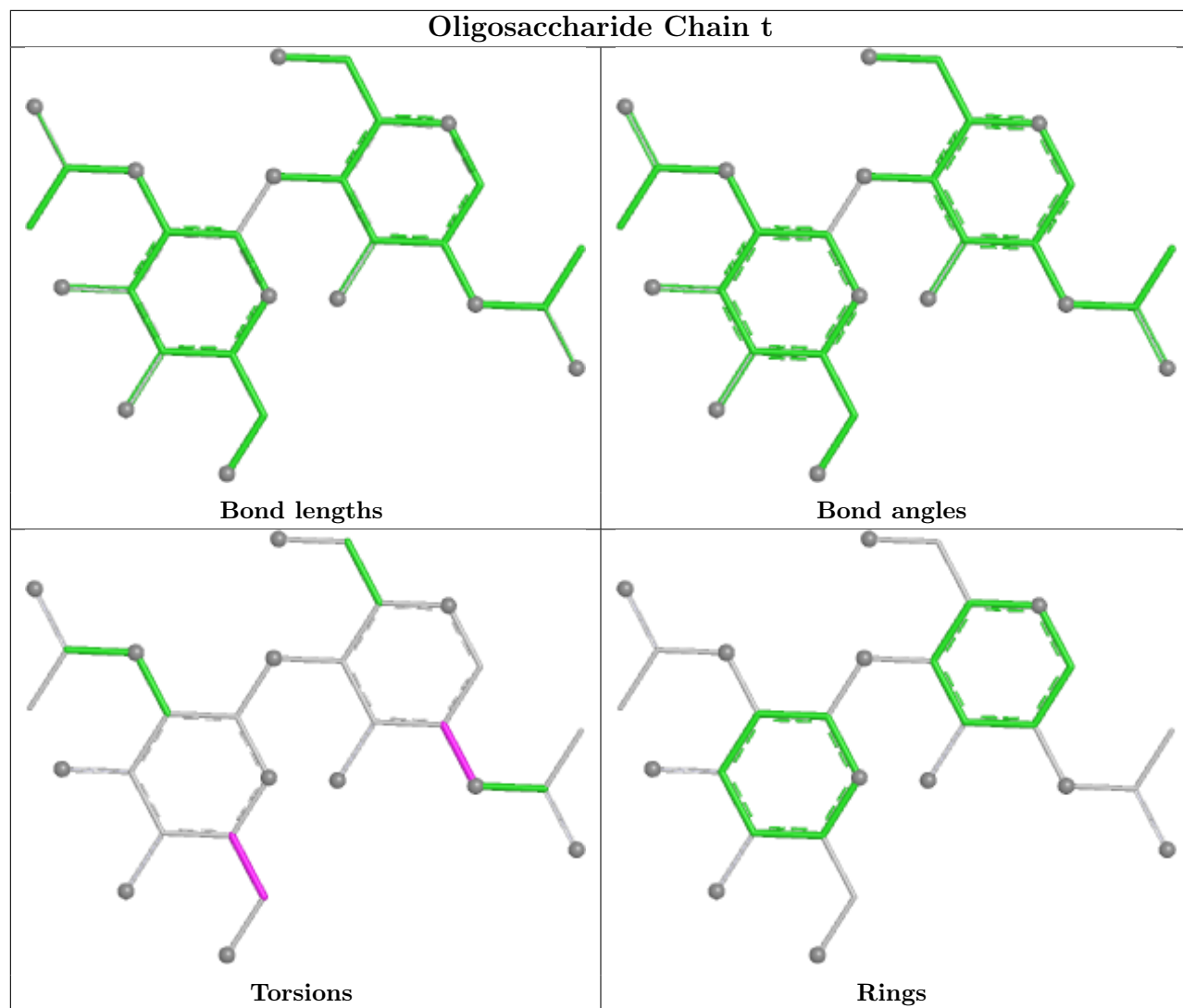


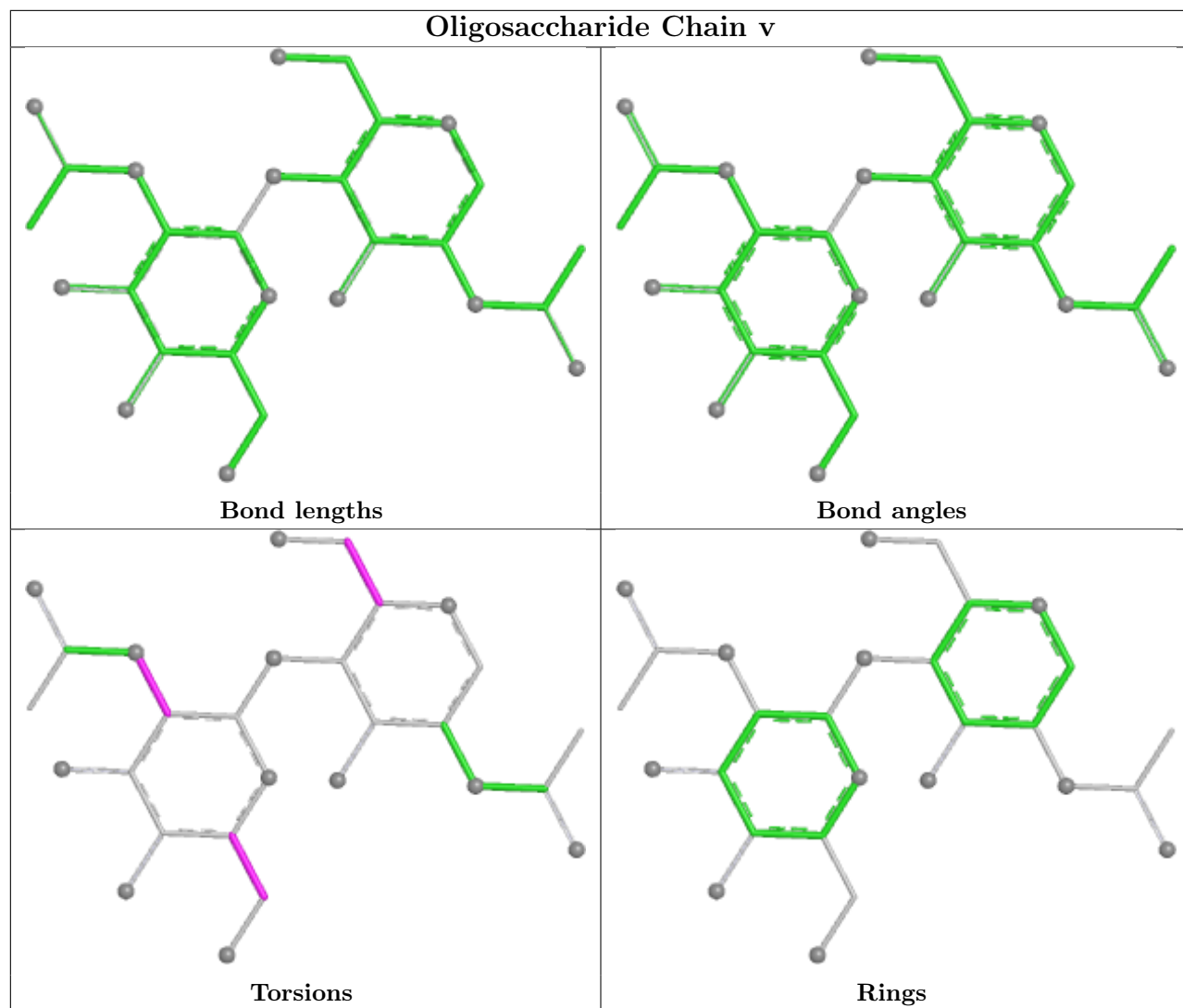


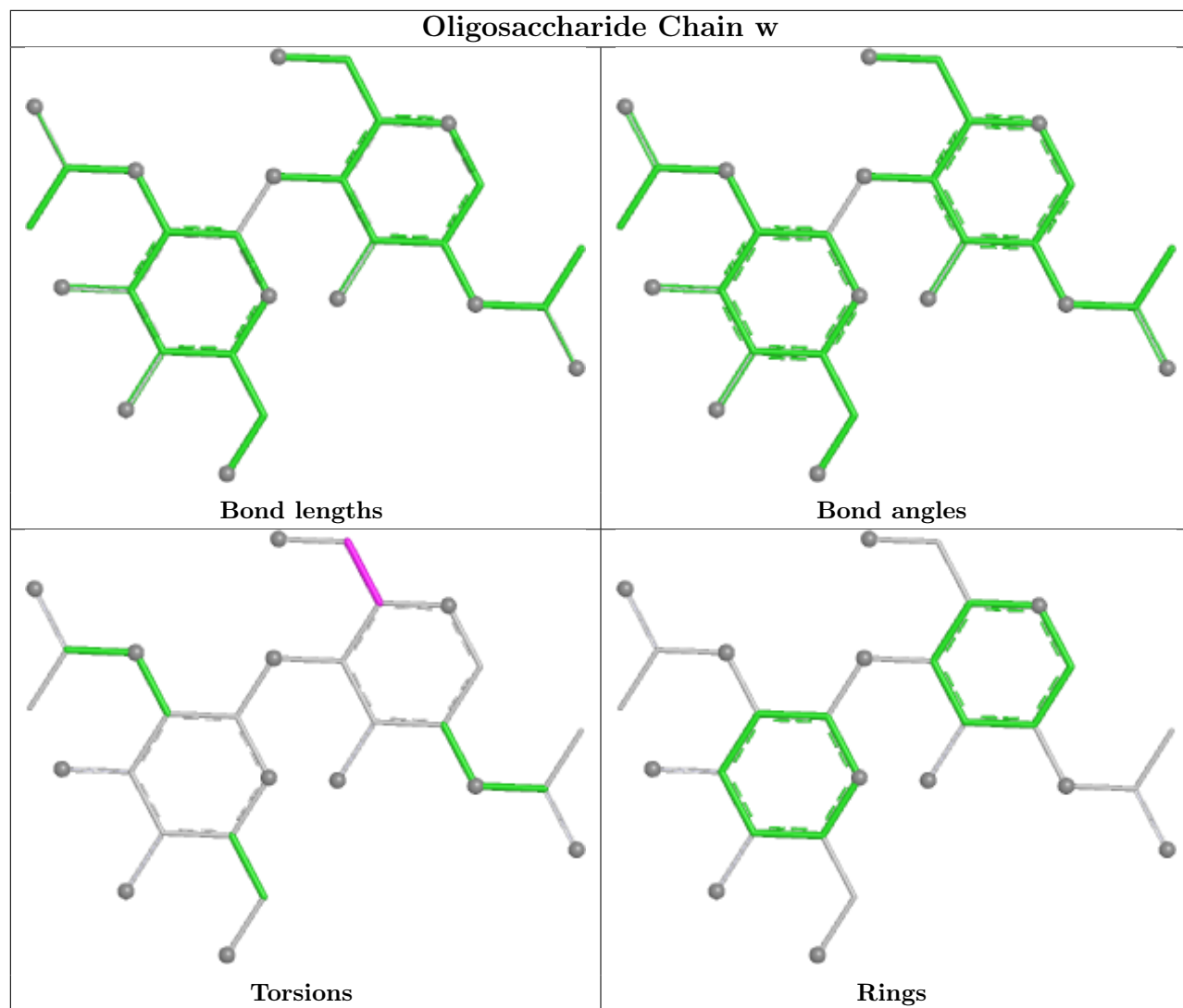


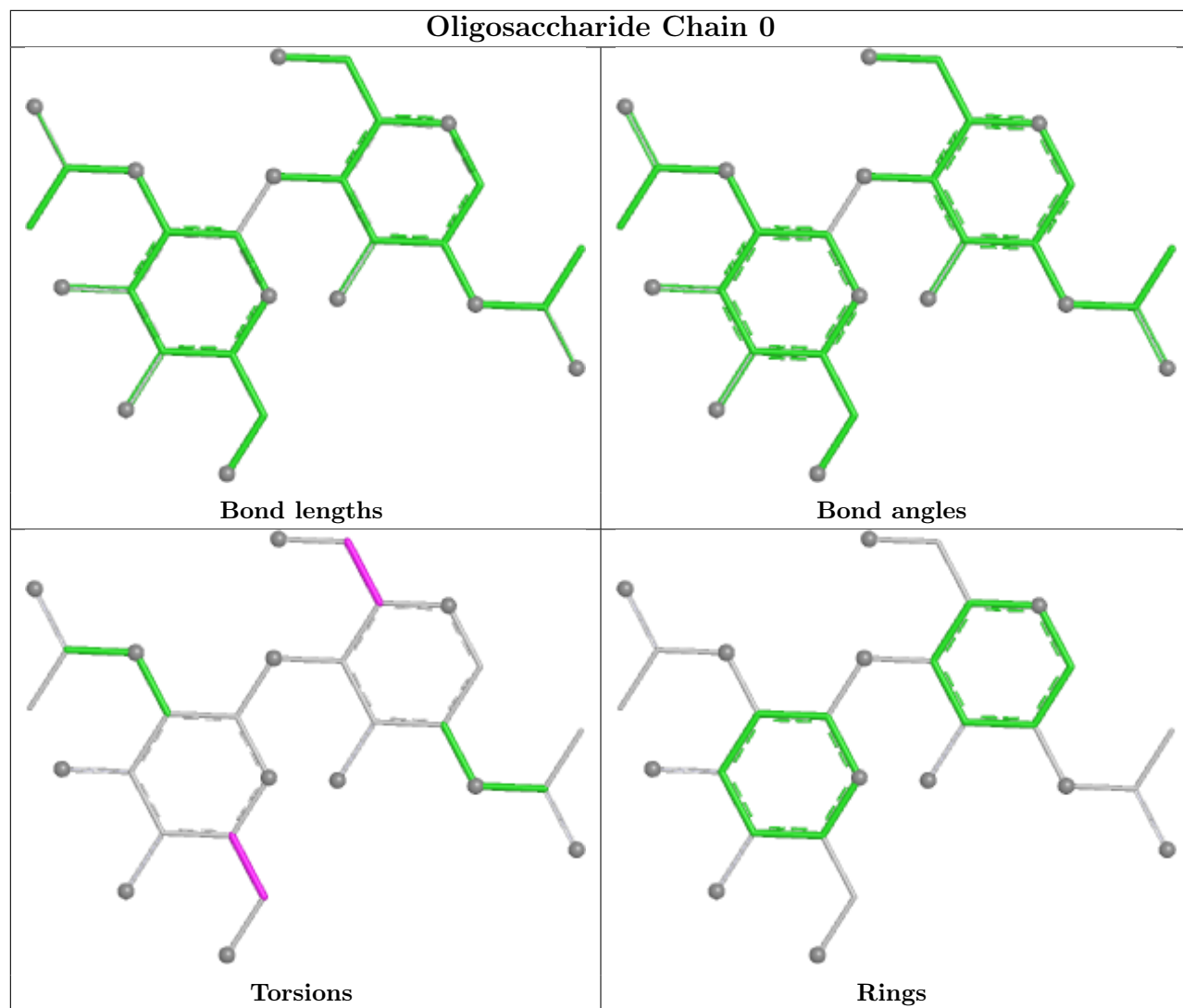


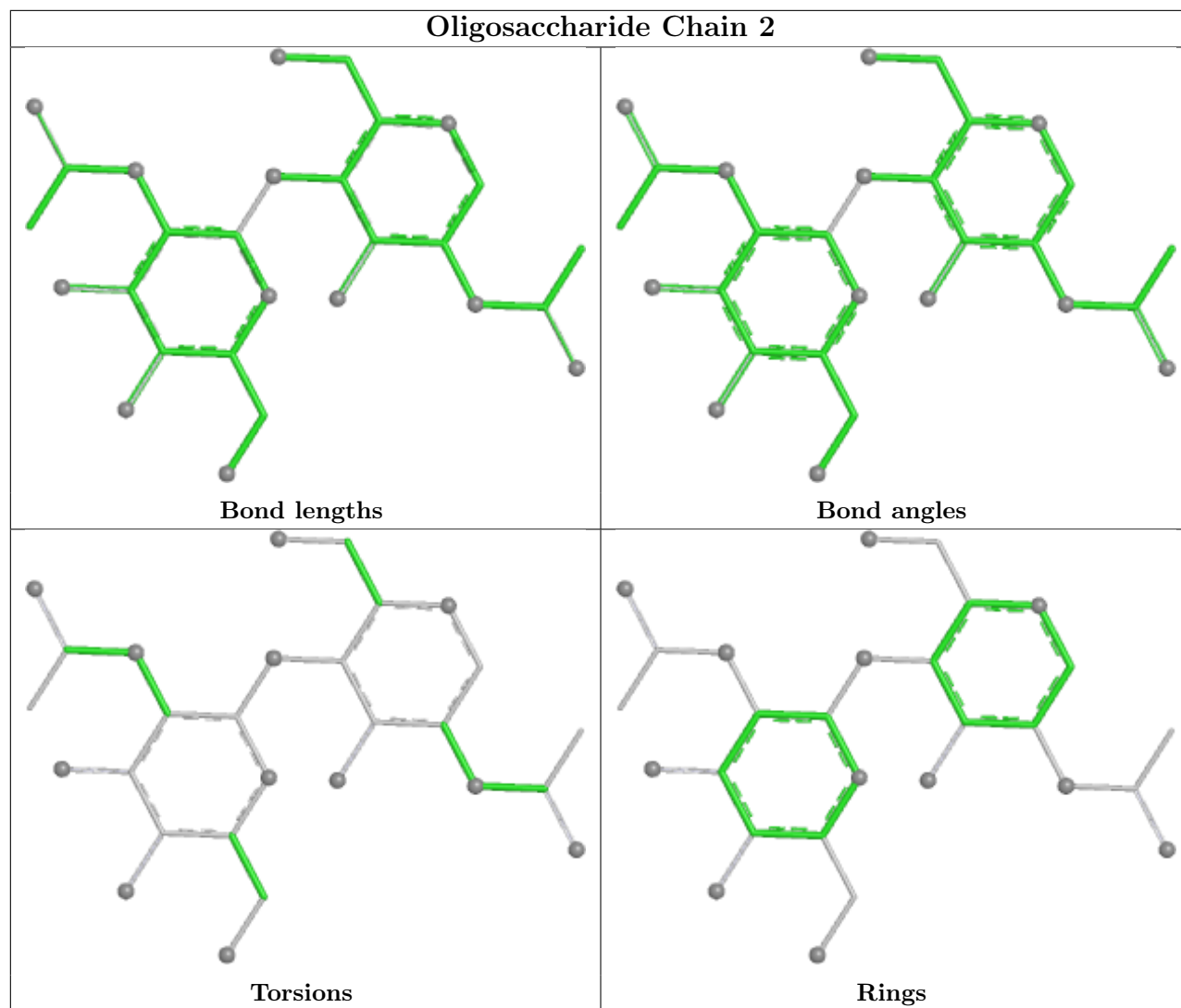


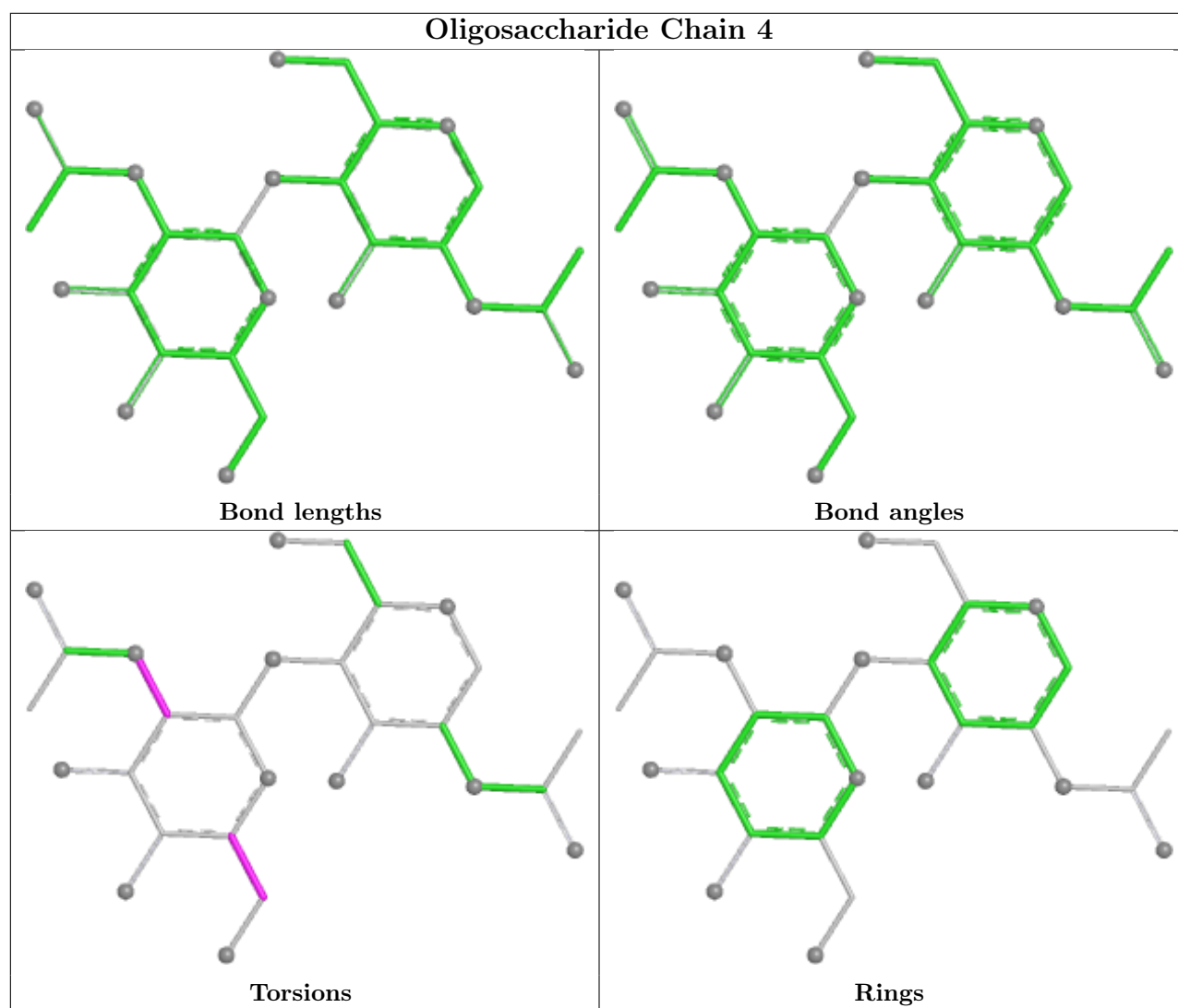


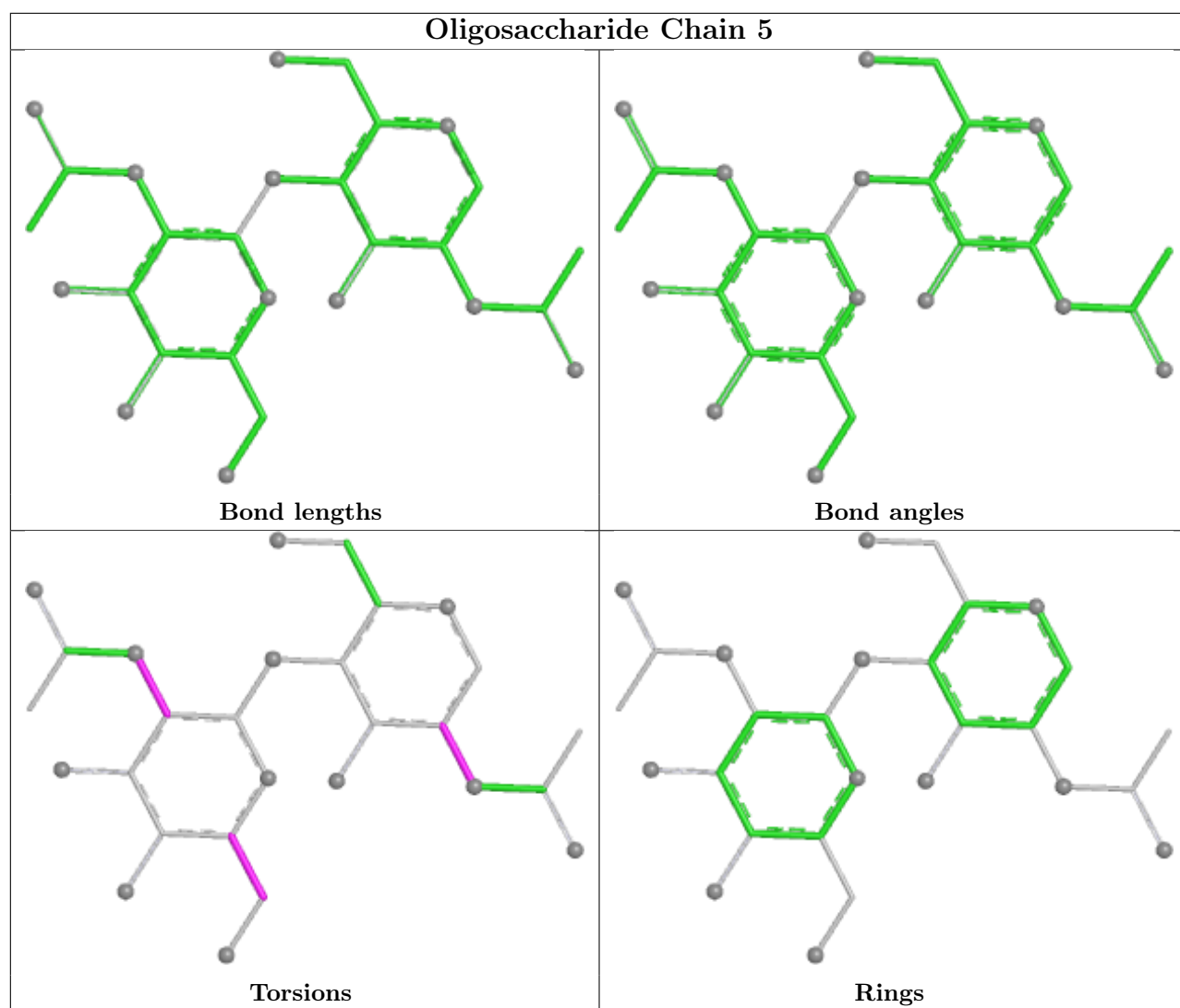


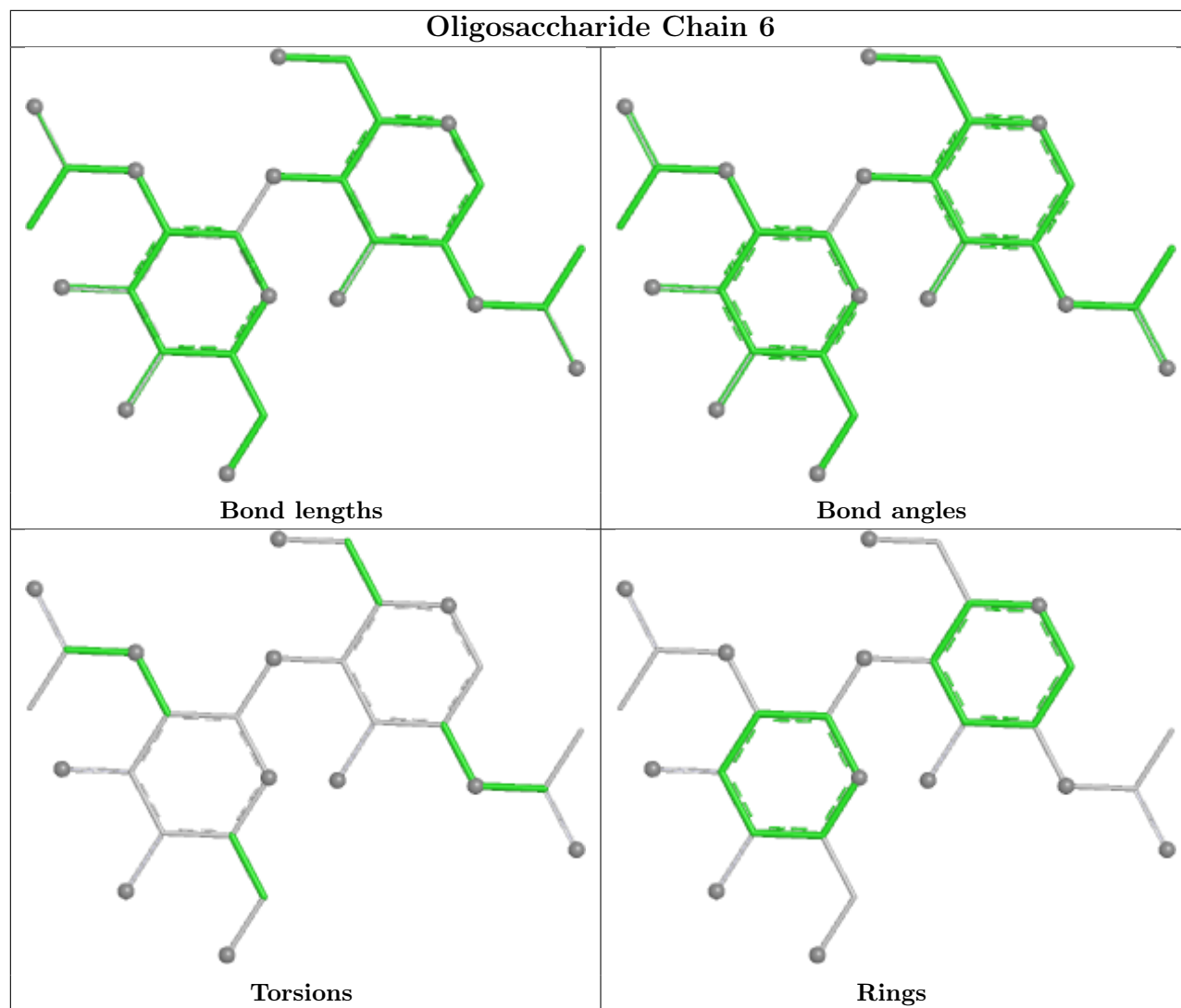


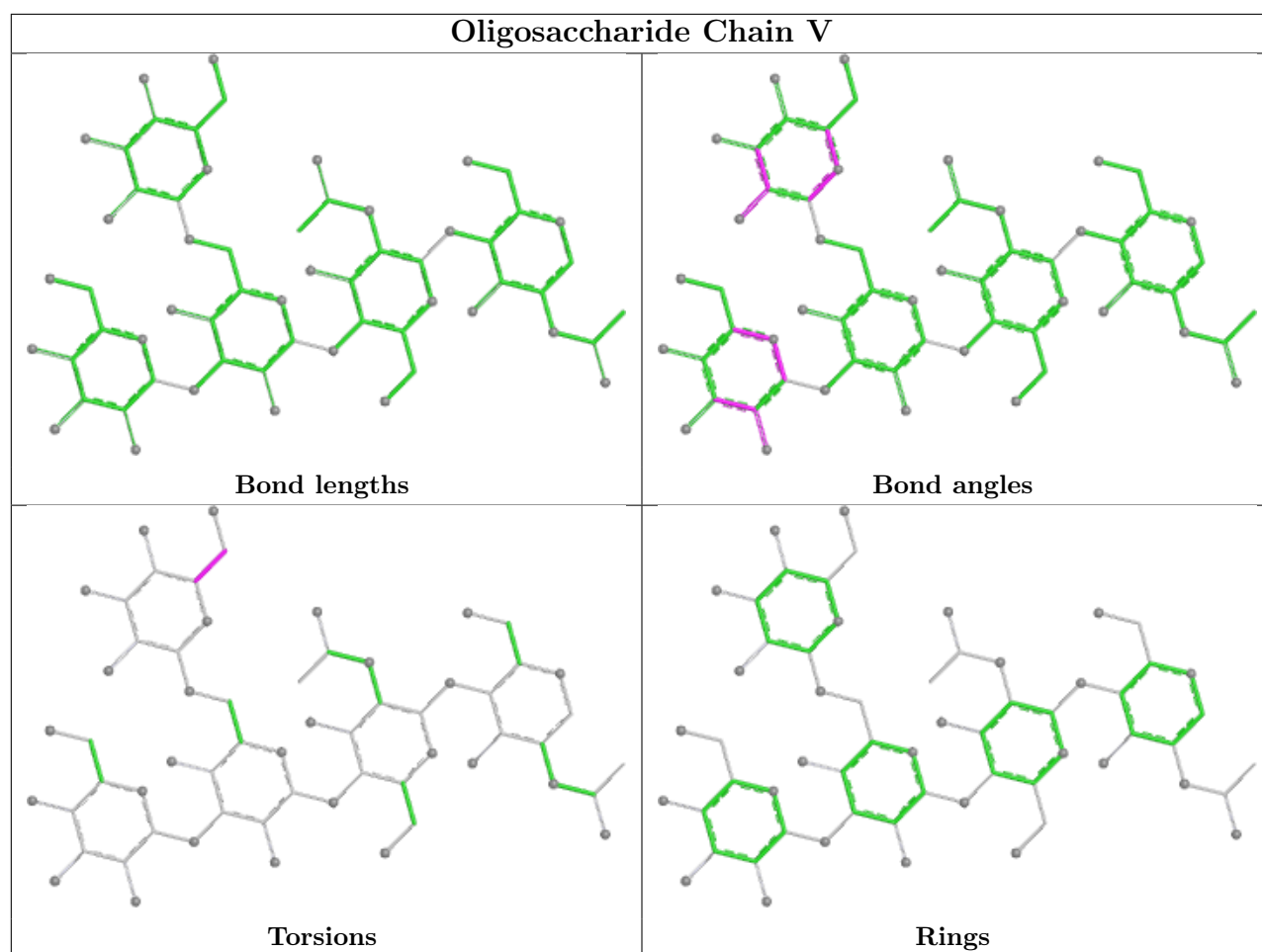


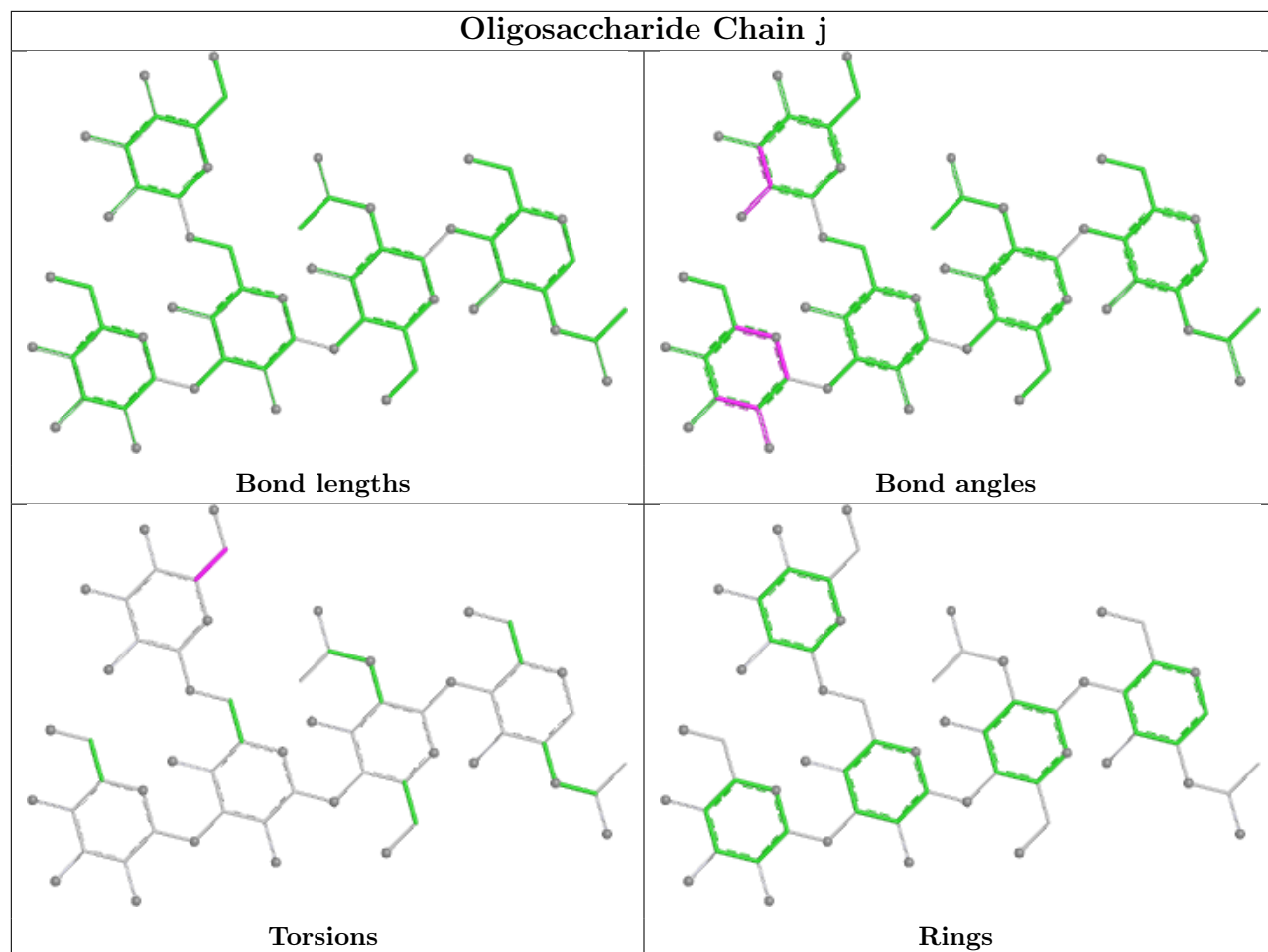


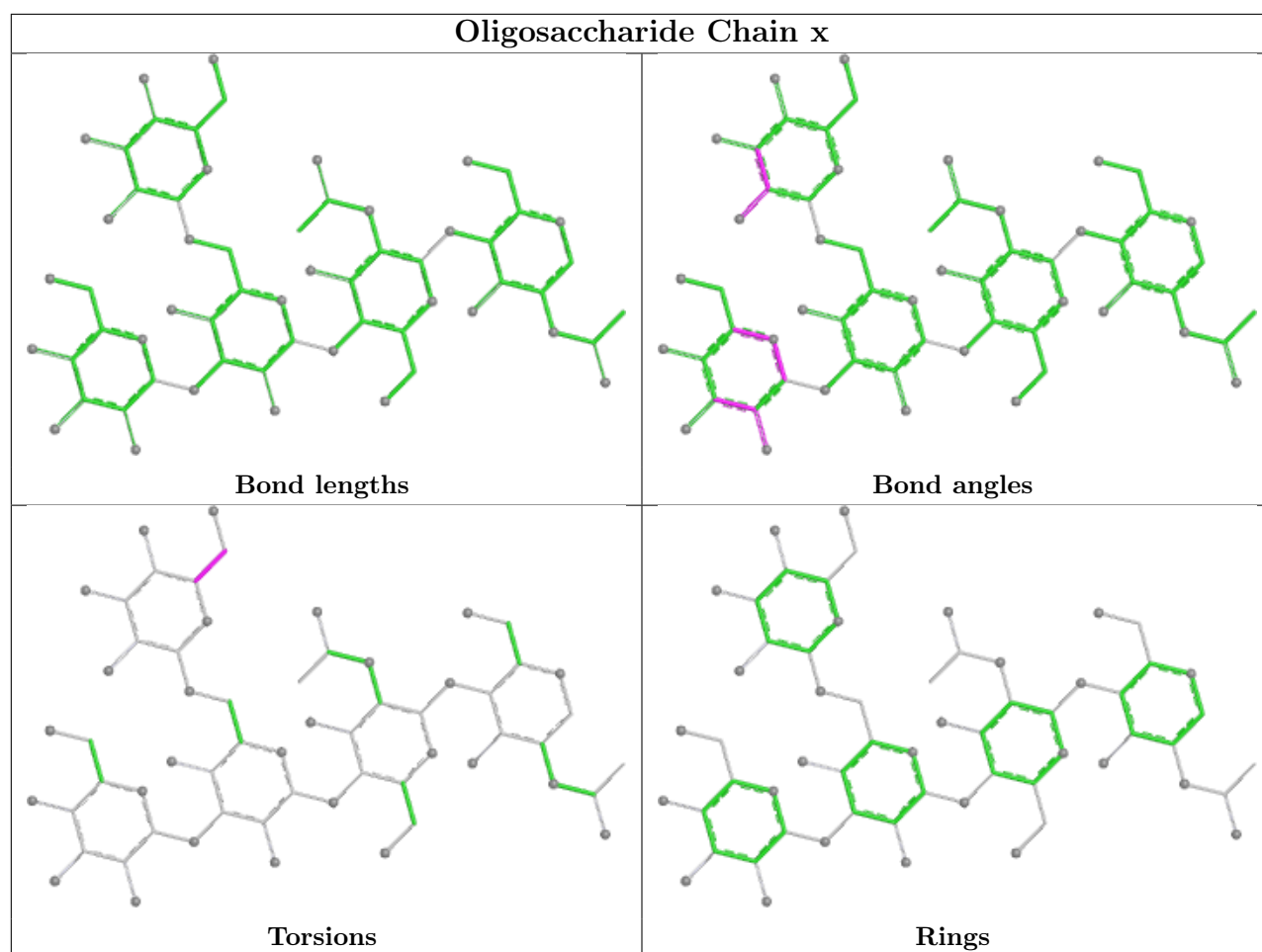


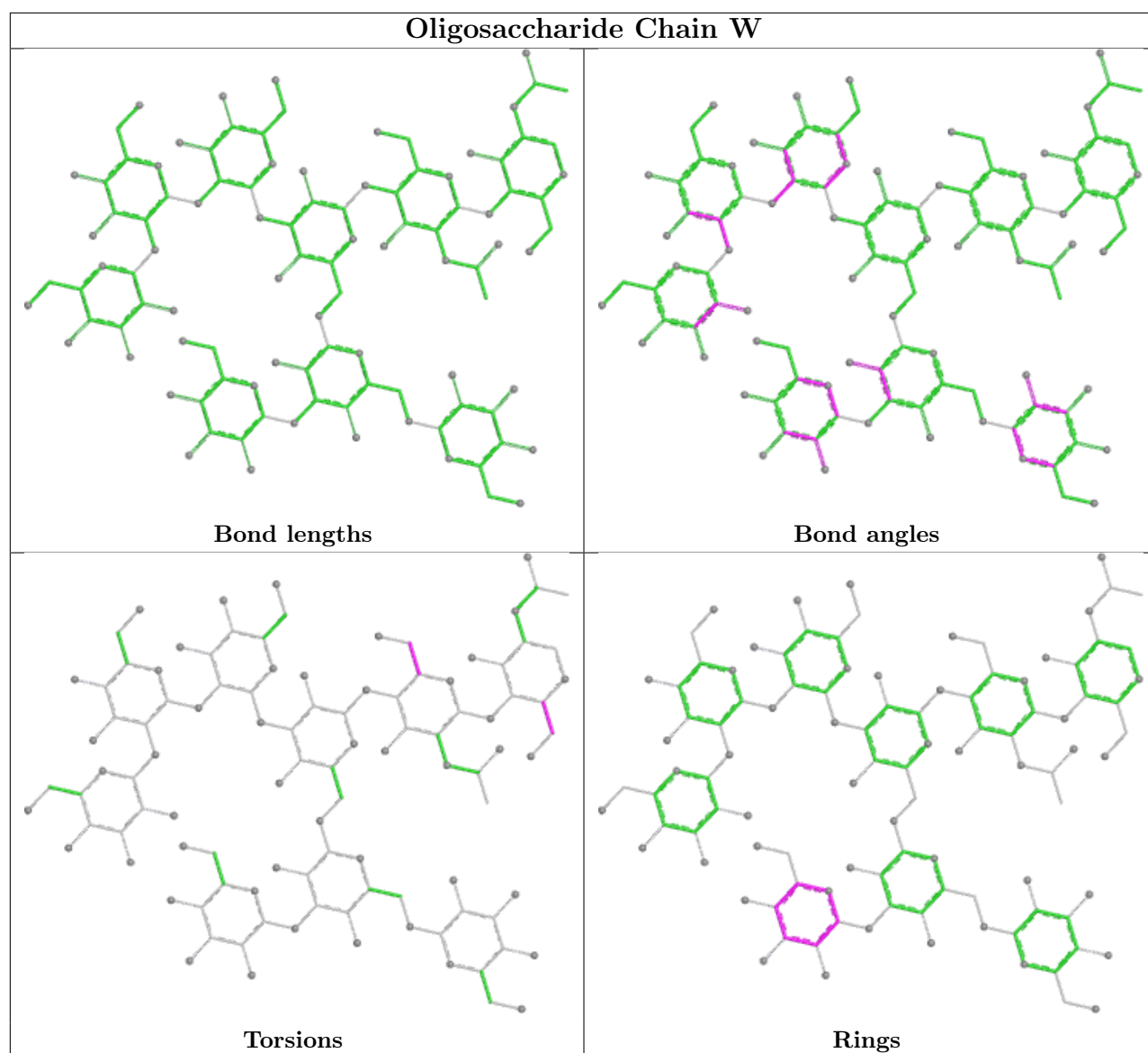


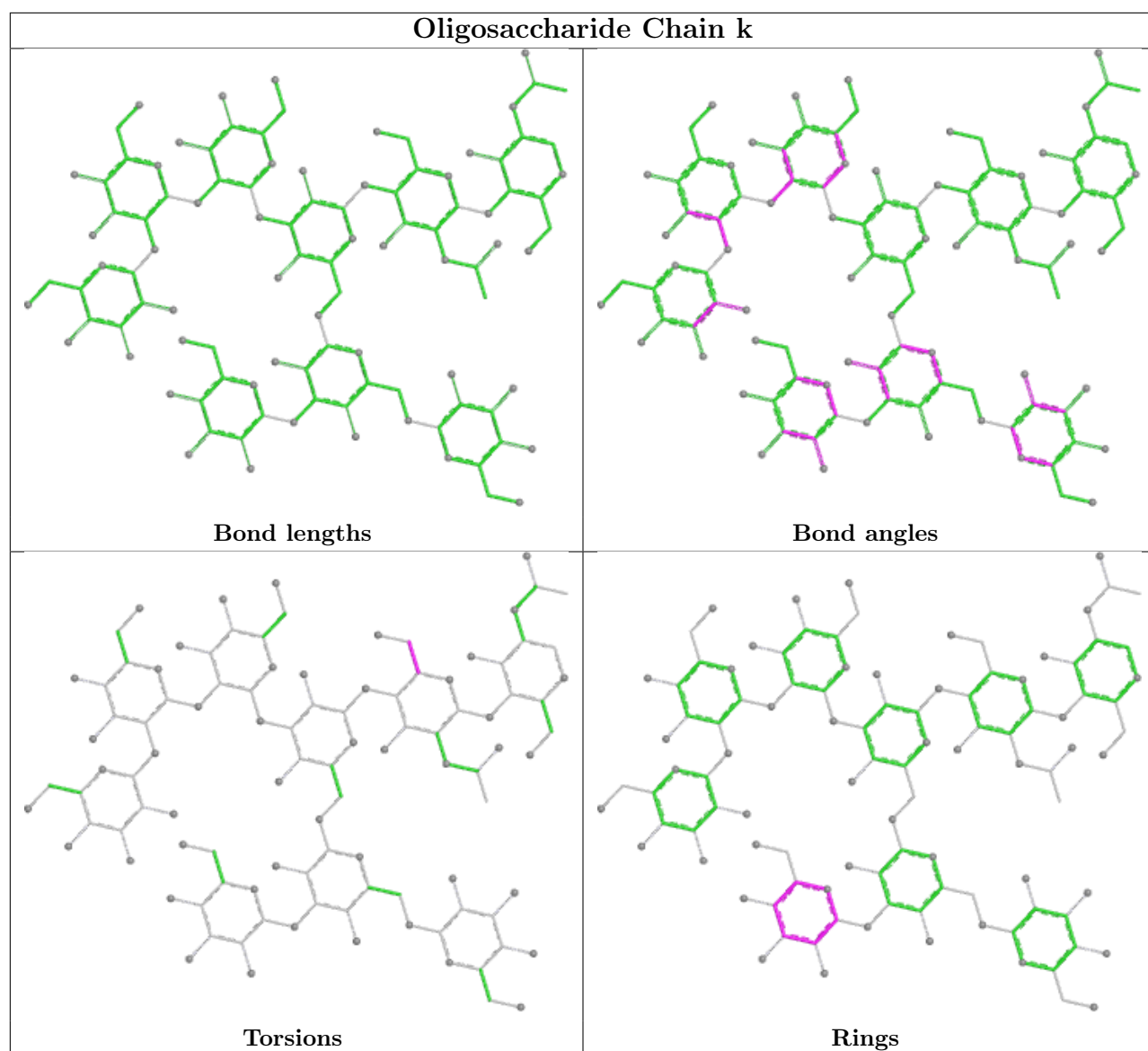


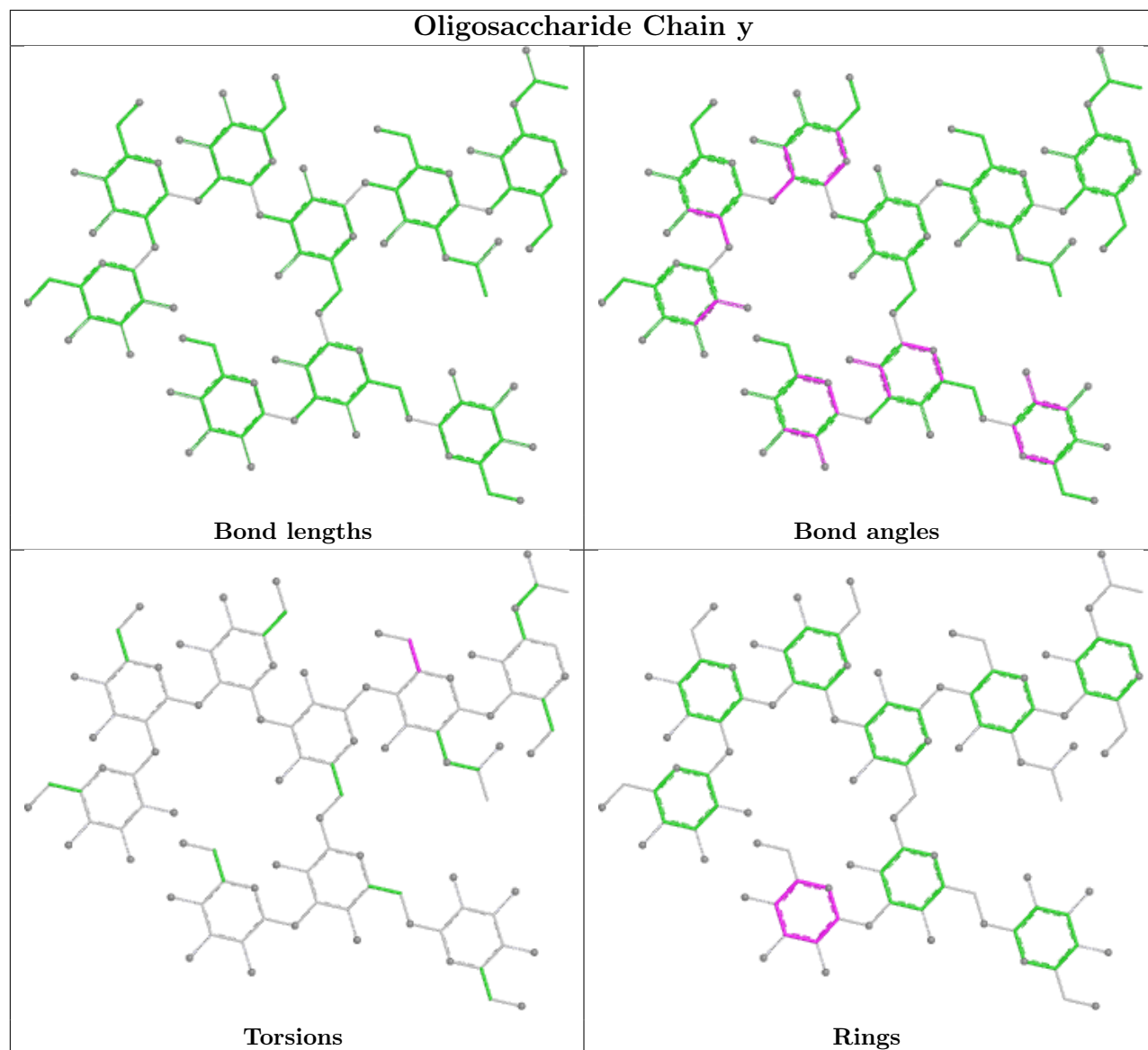


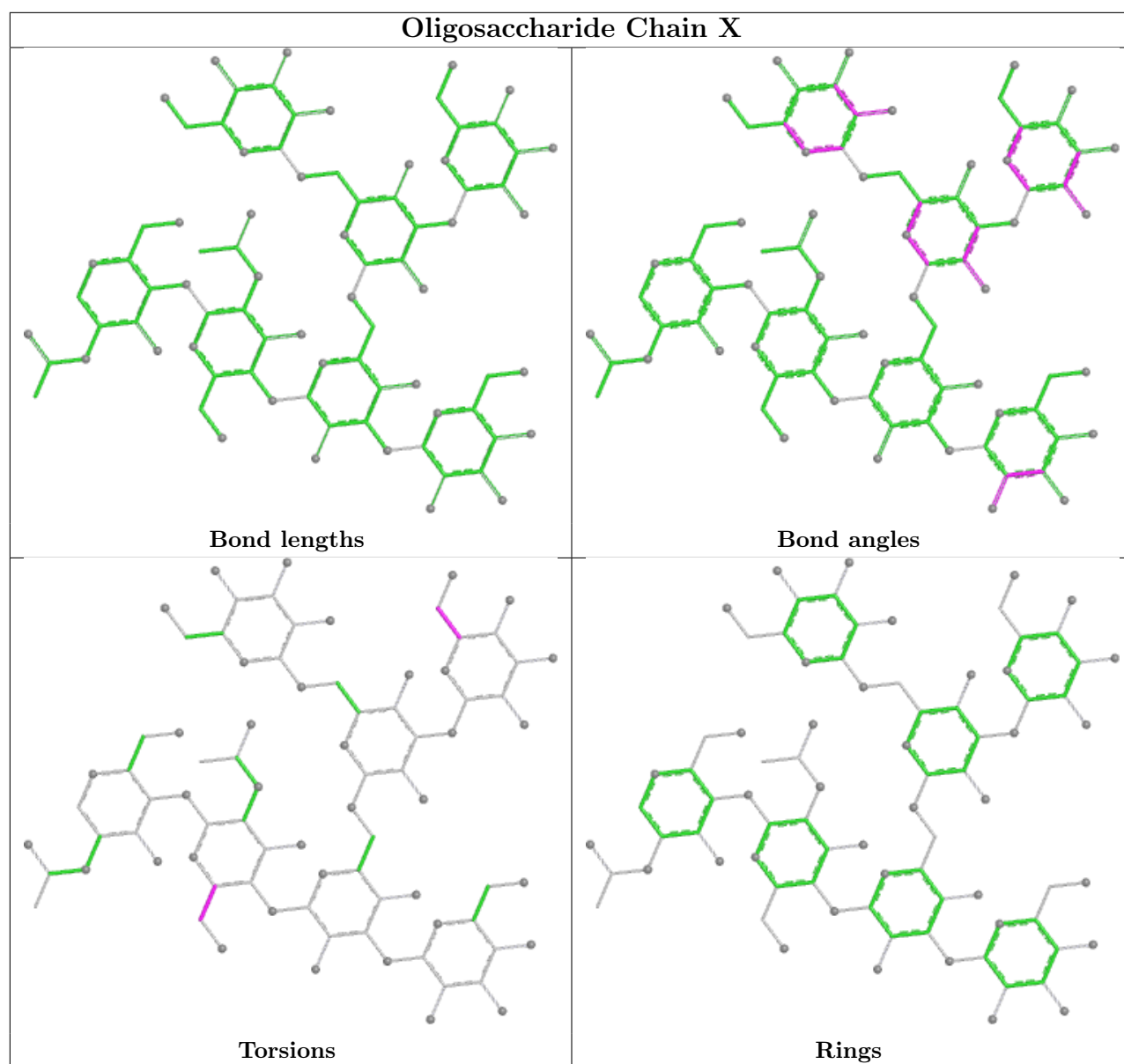


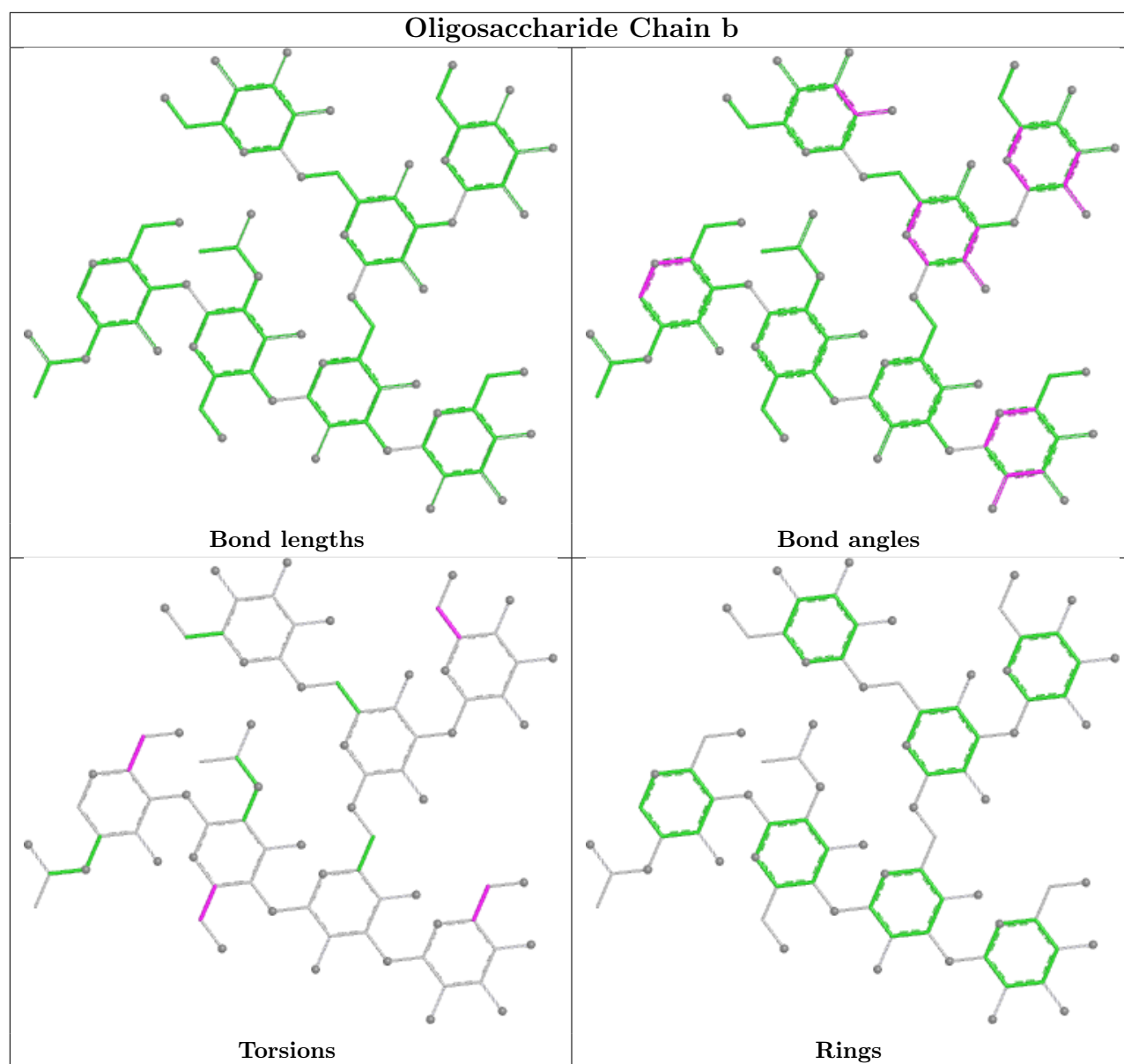


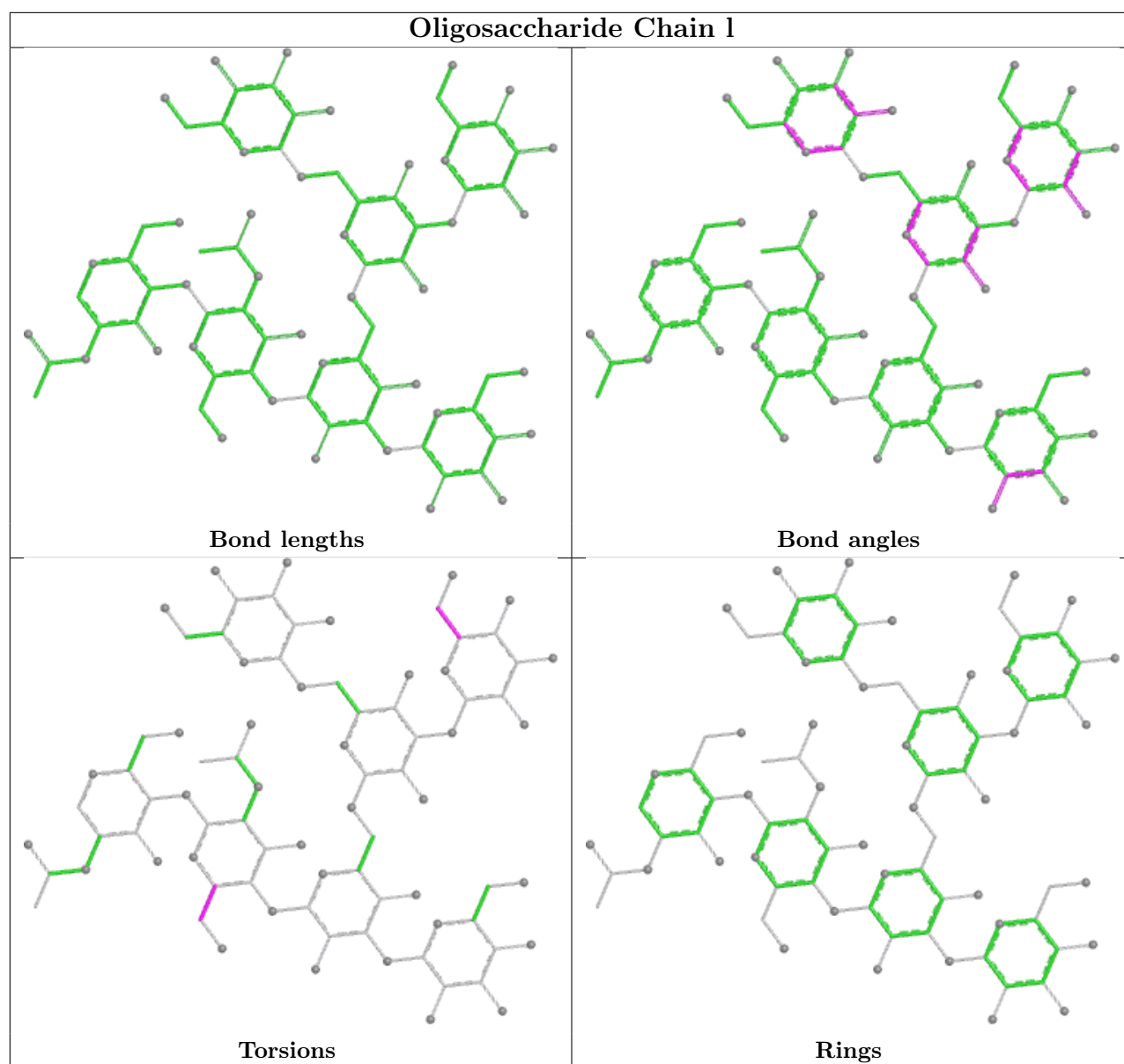


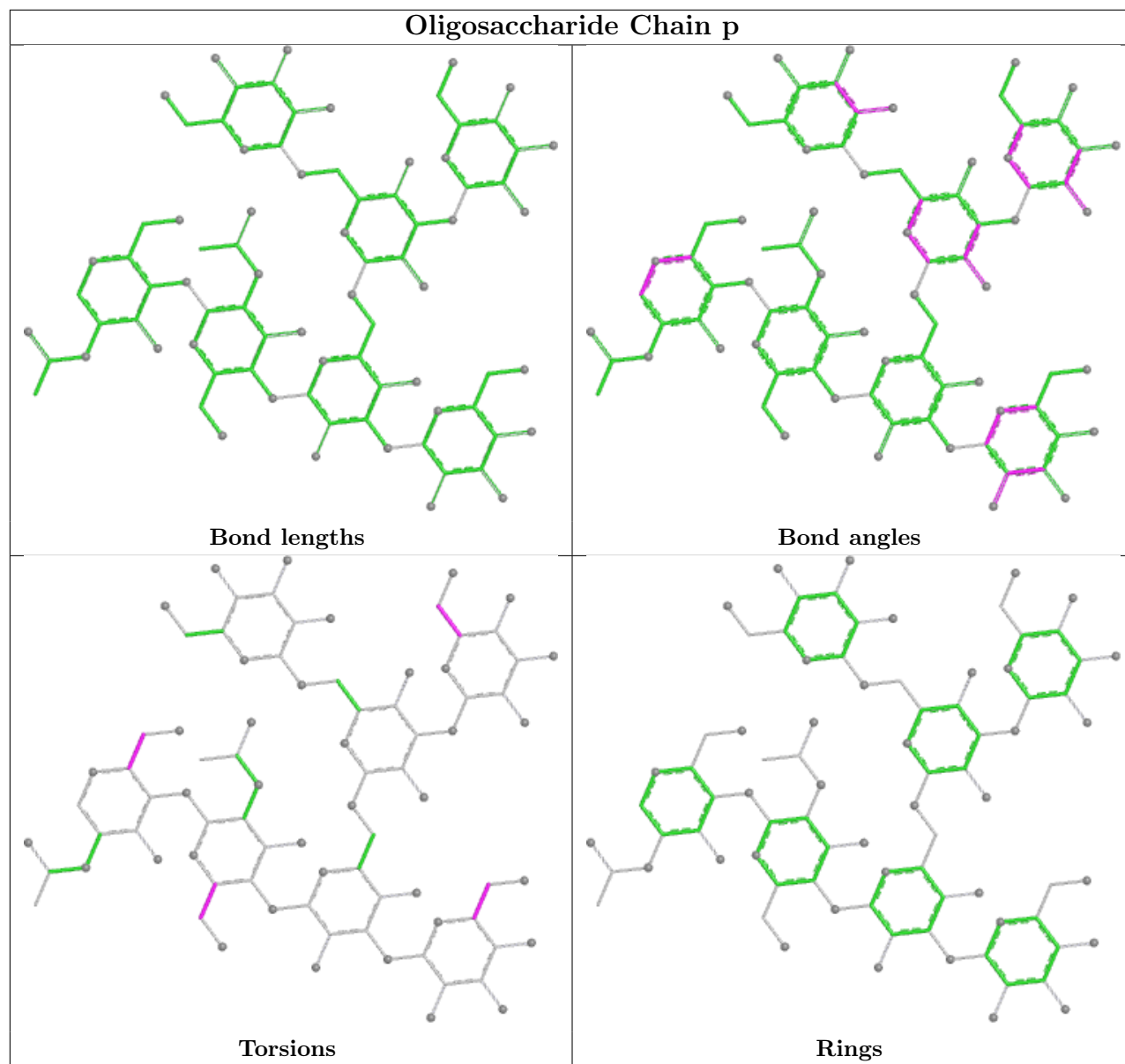


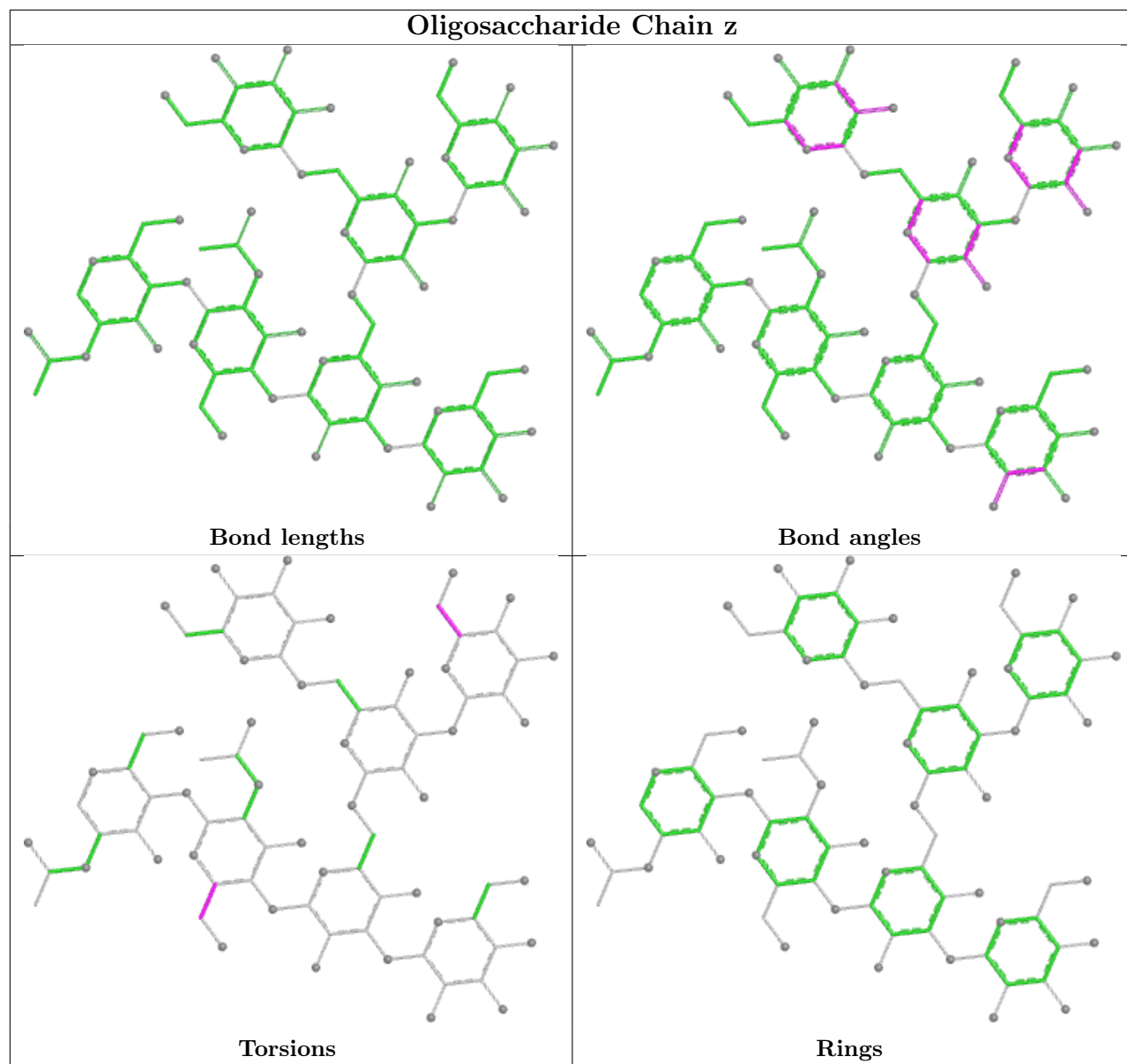


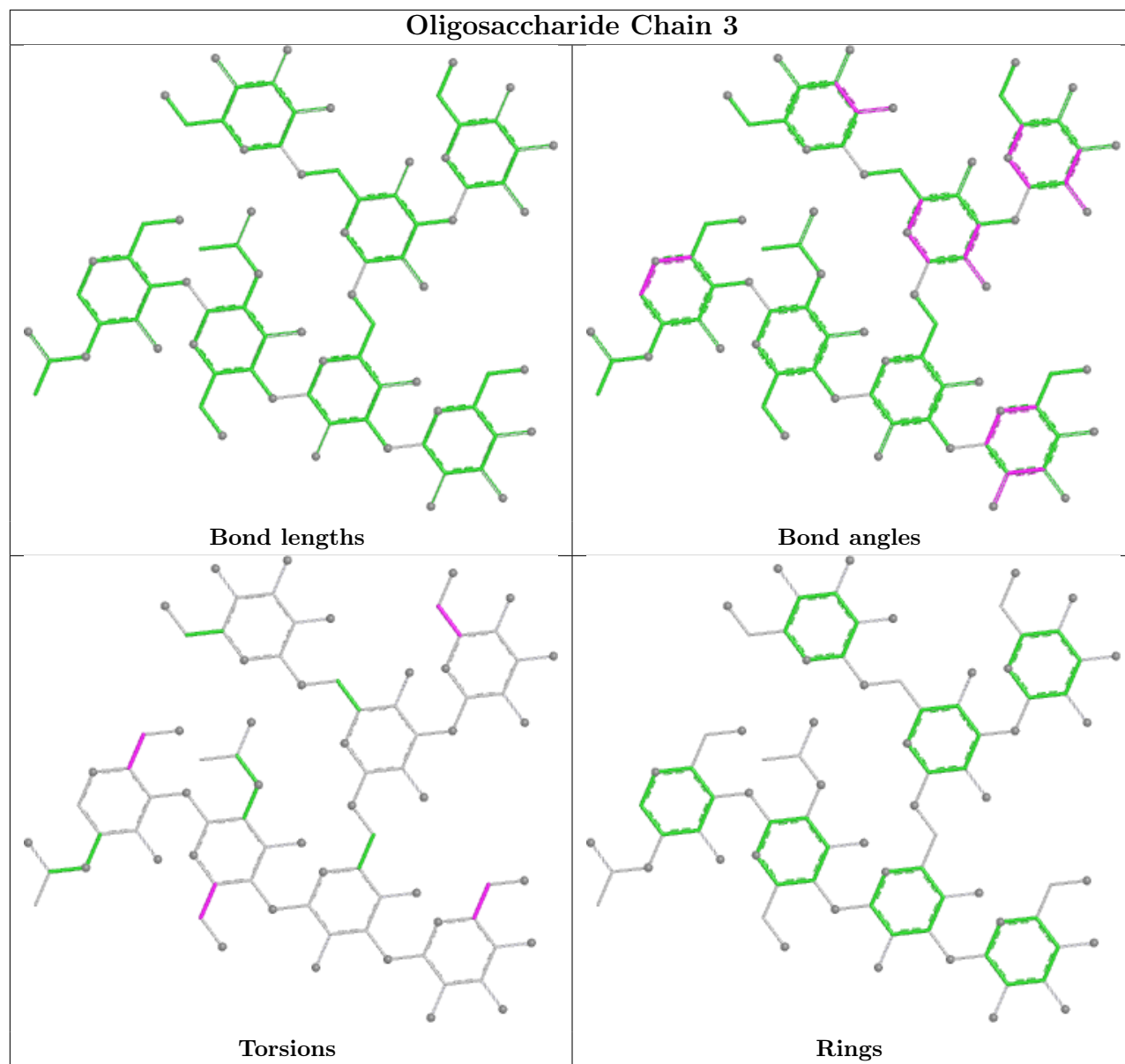


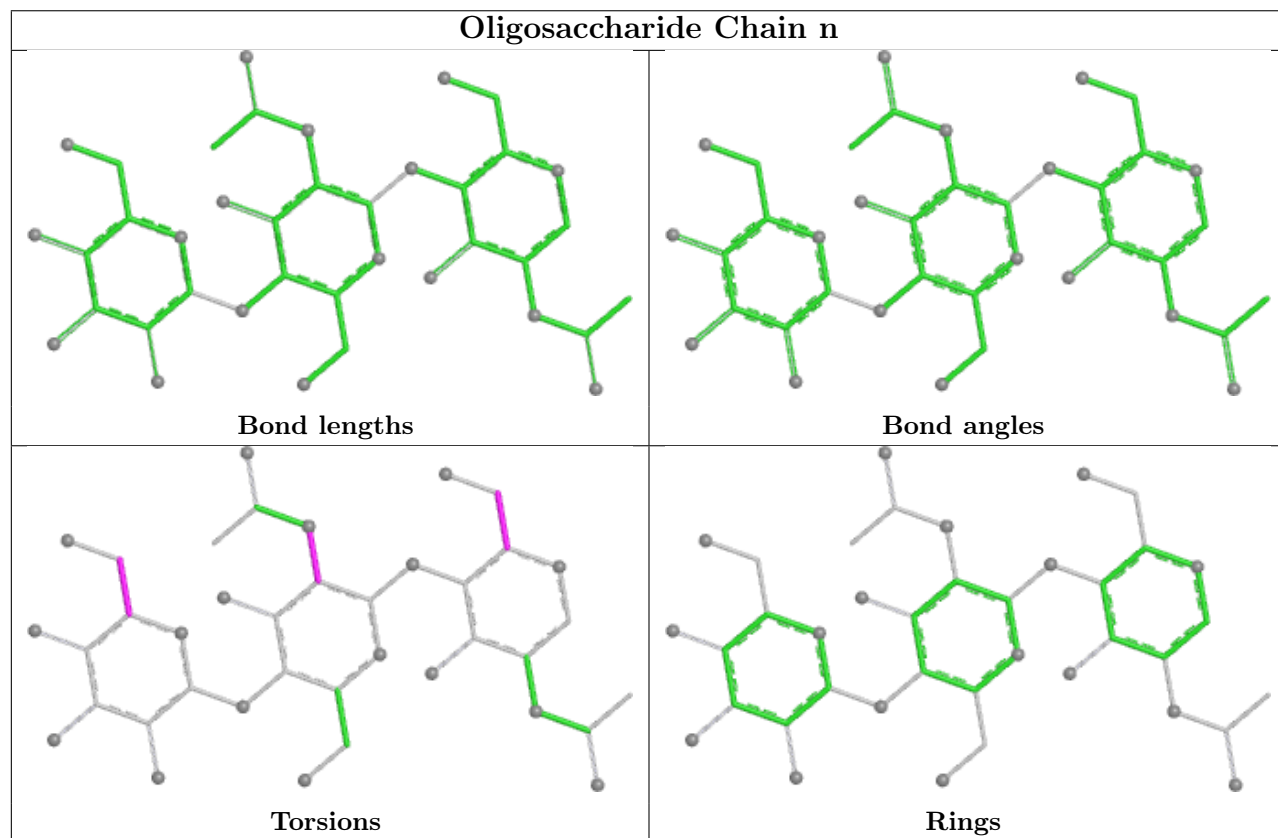
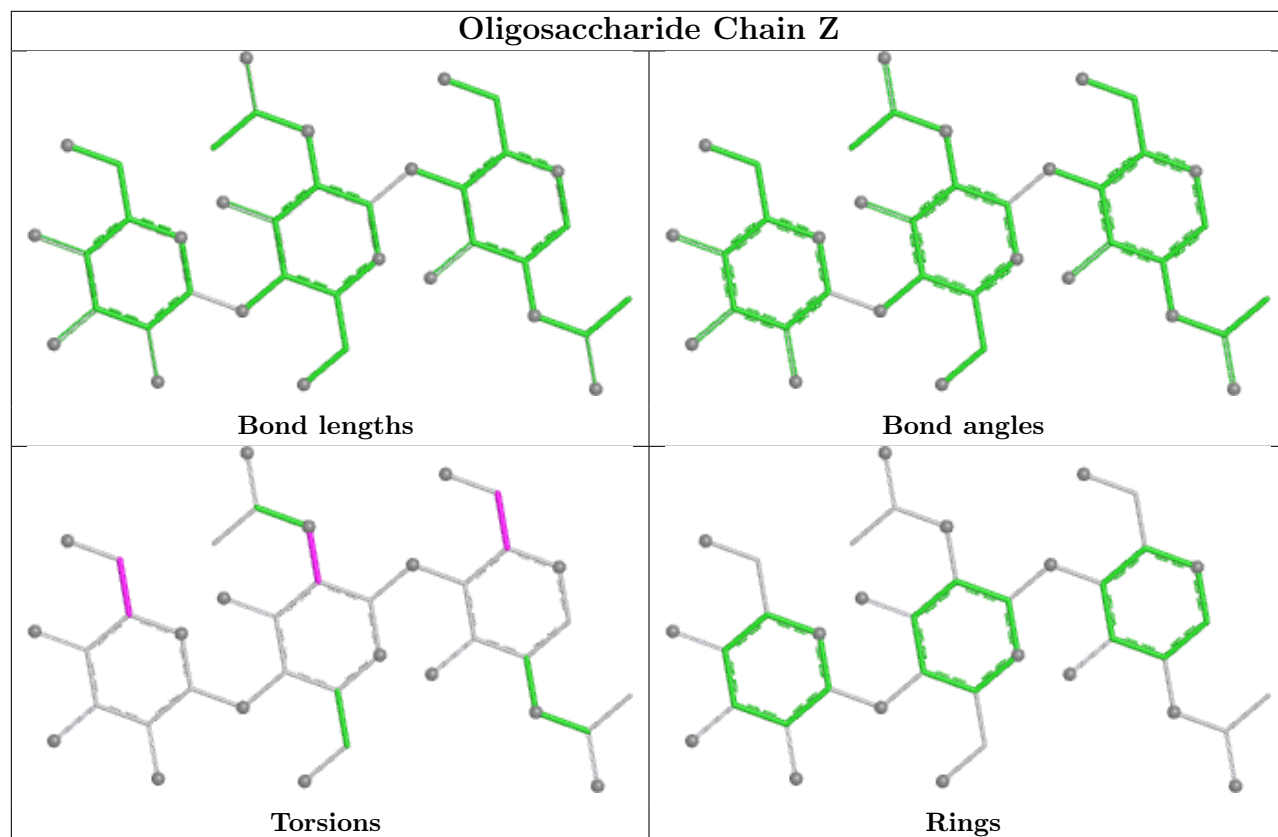


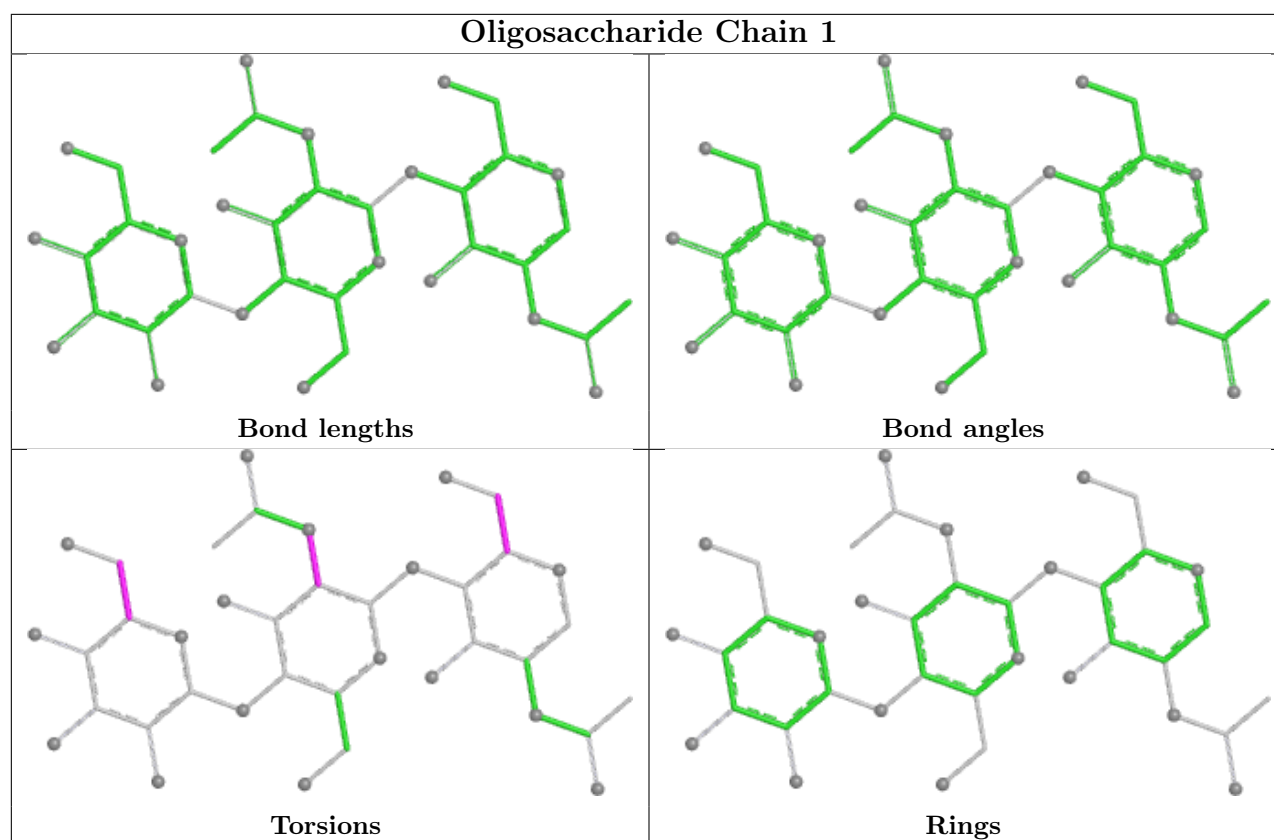












5.6 Ligand geometry [i](#)

35 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	701	1	14,14,15	0.22	0	17,19,21	0.45	0
13	NAG	C	603	2	14,14,15	0.19	0	17,19,21	0.45	0
13	NAG	B	701	1	14,14,15	0.23	0	17,19,21	0.47	0
13	NAG	B	702	1	14,14,15	0.21	0	17,19,21	0.43	0
13	NAG	J	701	1	14,14,15	0.21	0	17,19,21	0.44	0
13	NAG	C	605	2	14,14,15	0.28	0	17,19,21	0.46	0
13	NAG	G	603	2	14,14,15	0.21	0	17,19,21	0.42	0
13	NAG	G	604	2	14,14,15	0.28	0	17,19,21	0.46	0
13	NAG	K	604	2	14,14,15	0.28	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	G	605	2	14,14,15	0.19	0	17,19,21	0.42	0
13	NAG	K	601	2	14,14,15	0.19	0	17,19,21	0.44	0
13	NAG	K	602	2	14,14,15	0.21	0	17,19,21	0.45	0
13	NAG	C	606	2	14,14,15	0.16	0	17,19,21	0.43	0
14	PO4	C	601	-	4,4,4	0.76	0	6,6,6	0.46	0
13	NAG	G	608	2	14,14,15	0.22	0	17,19,21	0.42	0
13	NAG	G	607	2	14,14,15	0.25	0	17,19,21	0.50	0
13	NAG	B	703	1	14,14,15	0.22	0	17,19,21	0.53	0
13	NAG	C	608	2	14,14,15	0.22	0	17,19,21	0.46	0
13	NAG	C	602	2	14,14,15	0.20	0	17,19,21	0.42	0
13	NAG	G	606	2	14,14,15	0.22	0	17,19,21	0.43	0
13	NAG	A	702	1	14,14,15	0.22	0	17,19,21	0.49	0
13	NAG	K	608	2	14,14,15	0.27	0	17,19,21	0.39	0
13	NAG	J	702	1	14,14,15	0.22	0	17,19,21	0.54	0
13	NAG	K	607	2	14,14,15	0.22	0	17,19,21	0.47	0
13	NAG	K	603	2	14,14,15	0.18	0	17,19,21	0.41	0
13	NAG	K	606	2	14,14,15	0.21	0	17,19,21	0.43	0
13	NAG	E	301	4	14,14,15	0.15	0	17,19,21	0.51	0
13	NAG	U	301	4	14,14,15	0.20	0	17,19,21	0.41	0
13	NAG	G	602	2	14,14,15	0.20	0	17,19,21	0.44	0
13	NAG	K	605	2	14,14,15	0.19	0	17,19,21	0.42	0
13	NAG	C	607	2	14,14,15	0.21	0	17,19,21	0.41	0
13	NAG	C	609	2	14,14,15	0.28	0	17,19,21	0.38	0
13	NAG	C	604	2	14,14,15	0.22	0	17,19,21	0.41	0
13	NAG	G	601	2	14,14,15	0.19	0	17,19,21	0.42	0
13	NAG	N	301	4	14,14,15	0.22	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	A	701	1	-	2/6/23/26	0/1/1/1
13	NAG	C	603	2	-	0/6/23/26	0/1/1/1
13	NAG	B	701	1	-	2/6/23/26	0/1/1/1
13	NAG	B	702	1	-	2/6/23/26	0/1/1/1
13	NAG	J	701	1	-	2/6/23/26	0/1/1/1
13	NAG	C	605	2	-	3/6/23/26	0/1/1/1
13	NAG	G	603	2	-	2/6/23/26	0/1/1/1
13	NAG	G	604	2	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	K	604	2	-	3/6/23/26	0/1/1/1
13	NAG	G	605	2	-	2/6/23/26	0/1/1/1
13	NAG	K	601	2	-	1/6/23/26	0/1/1/1
13	NAG	K	602	2	-	0/6/23/26	0/1/1/1
13	NAG	C	606	2	-	2/6/23/26	0/1/1/1
13	NAG	G	608	2	-	0/6/23/26	0/1/1/1
13	NAG	G	607	2	-	2/6/23/26	0/1/1/1
13	NAG	B	703	1	-	2/6/23/26	0/1/1/1
13	NAG	C	608	2	-	2/6/23/26	0/1/1/1
13	NAG	C	602	2	-	0/6/23/26	0/1/1/1
13	NAG	G	606	2	-	0/6/23/26	0/1/1/1
13	NAG	A	702	1	-	0/6/23/26	0/1/1/1
13	NAG	K	608	2	-	2/6/23/26	0/1/1/1
13	NAG	J	702	1	-	1/6/23/26	0/1/1/1
13	NAG	K	607	2	-	2/6/23/26	0/1/1/1
13	NAG	K	603	2	-	2/6/23/26	0/1/1/1
13	NAG	K	606	2	-	0/6/23/26	0/1/1/1
13	NAG	E	301	4	-	3/6/23/26	0/1/1/1
13	NAG	U	301	4	-	2/6/23/26	0/1/1/1
13	NAG	G	602	2	-	0/6/23/26	0/1/1/1
13	NAG	K	605	2	-	2/6/23/26	0/1/1/1
13	NAG	C	607	2	-	0/6/23/26	0/1/1/1
13	NAG	C	609	2	-	1/6/23/26	0/1/1/1
13	NAG	C	604	2	-	2/6/23/26	0/1/1/1
13	NAG	G	601	2	-	0/6/23/26	0/1/1/1
13	NAG	N	301	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	604	NAG	C1-C2-N2-C7
13	C	605	NAG	C1-C2-N2-C7
13	K	604	NAG	C1-C2-N2-C7
13	A	701	NAG	O5-C5-C6-O6
13	J	701	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	K	607	NAG	O5-C5-C6-O6
13	B	702	NAG	C4-C5-C6-O6
13	U	301	NAG	C4-C5-C6-O6
13	C	608	NAG	C4-C5-C6-O6
13	K	607	NAG	C4-C5-C6-O6
13	N	301	NAG	C4-C5-C6-O6
13	U	301	NAG	O5-C5-C6-O6
13	C	608	NAG	O5-C5-C6-O6
13	B	702	NAG	O5-C5-C6-O6
13	N	301	NAG	O5-C5-C6-O6
13	A	701	NAG	C4-C5-C6-O6
13	J	701	NAG	C4-C5-C6-O6
13	E	301	NAG	C8-C7-N2-C2
13	E	301	NAG	O7-C7-N2-C2
13	B	703	NAG	O5-C5-C6-O6
13	E	301	NAG	O5-C5-C6-O6
13	K	604	NAG	O5-C5-C6-O6
13	G	607	NAG	C4-C5-C6-O6
13	G	604	NAG	O5-C5-C6-O6
13	C	605	NAG	O5-C5-C6-O6
13	J	702	NAG	O5-C5-C6-O6
13	B	701	NAG	C1-C2-N2-C7
13	G	603	NAG	C1-C2-N2-C7
13	G	605	NAG	C1-C2-N2-C7
13	C	604	NAG	C1-C2-N2-C7
13	C	606	NAG	C1-C2-N2-C7
13	K	603	NAG	C1-C2-N2-C7
13	K	605	NAG	C1-C2-N2-C7
13	B	703	NAG	C4-C5-C6-O6
13	G	607	NAG	O5-C5-C6-O6
13	B	701	NAG	C3-C2-N2-C7
13	C	609	NAG	C3-C2-N2-C7
13	K	603	NAG	C3-C2-N2-C7
13	K	608	NAG	O5-C5-C6-O6
13	K	601	NAG	C1-C2-N2-C7
13	G	603	NAG	C3-C2-N2-C7
13	G	604	NAG	C3-C2-N2-C7
13	G	605	NAG	C3-C2-N2-C7
13	C	604	NAG	C3-C2-N2-C7
13	C	605	NAG	C3-C2-N2-C7
13	C	606	NAG	C3-C2-N2-C7
13	K	604	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	K	605	NAG	C3-C2-N2-C7
13	K	608	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	606	NAG	1	0
13	K	608	NAG	1	0
13	K	606	NAG	1	0
13	E	301	NAG	1	0
13	U	301	NAG	1	0
13	C	607	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

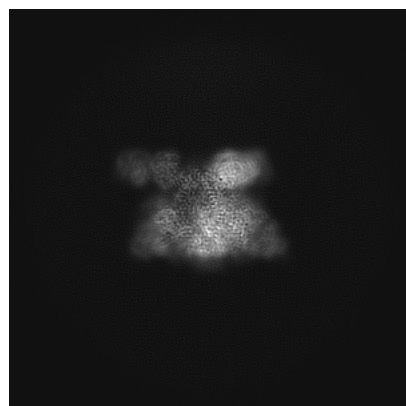
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44595. These allow visual inspection of the internal detail of the map and identification of artifacts.

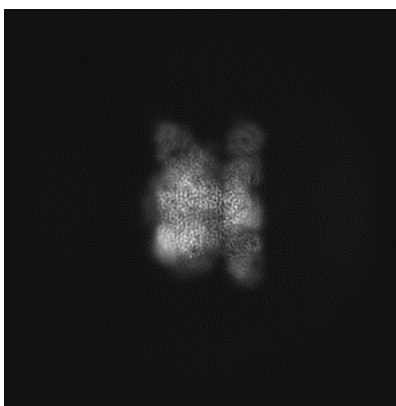
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

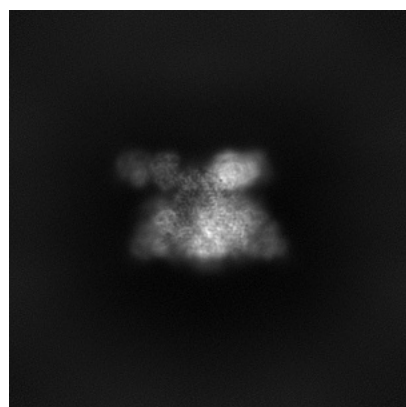


Y

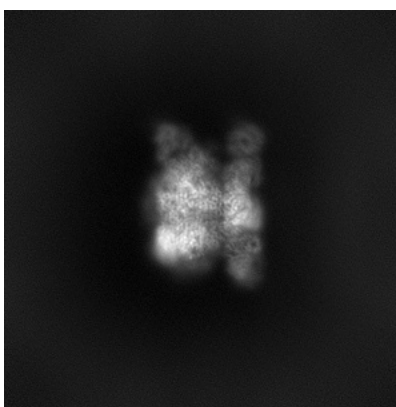


Z

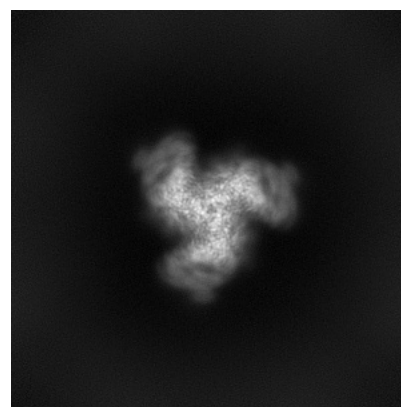
6.1.2 Raw map



X



Y

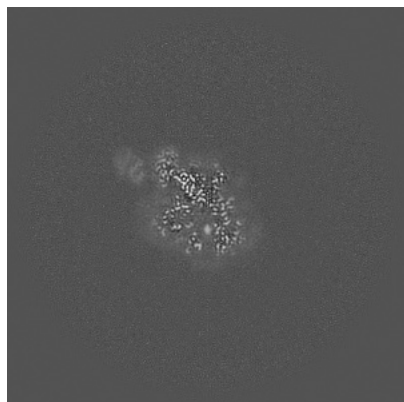


Z

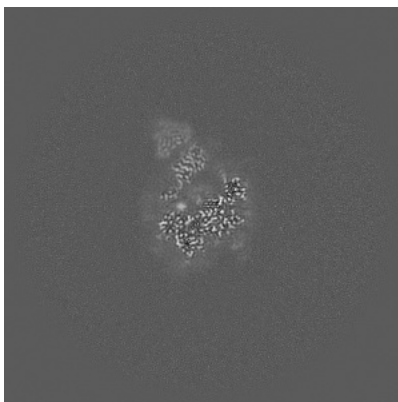
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

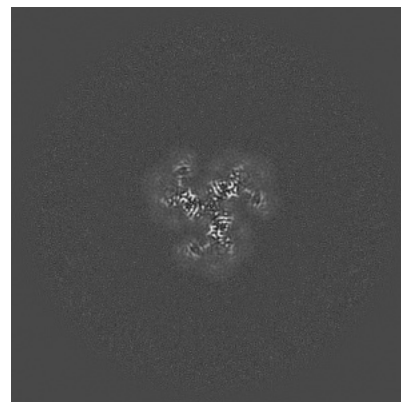
6.2.1 Primary map



X Index: 200

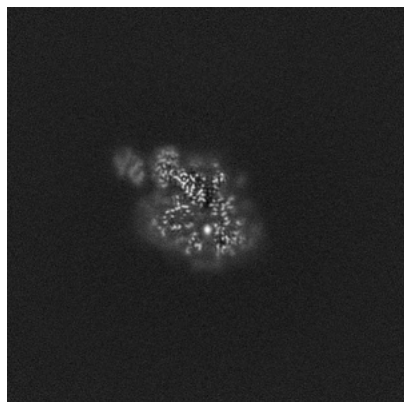


Y Index: 200

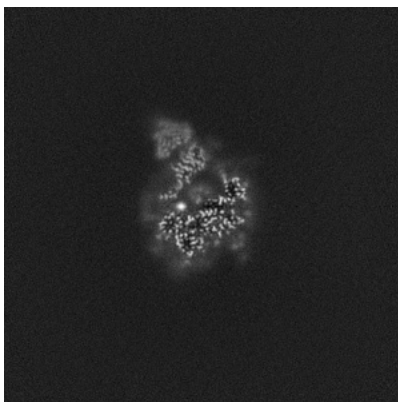


Z Index: 200

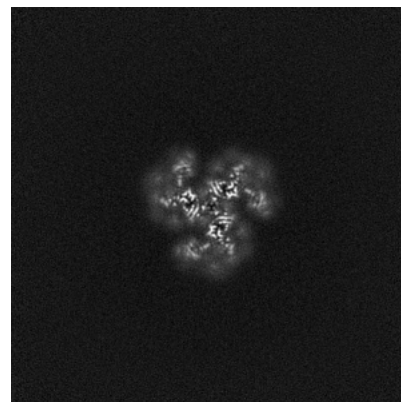
6.2.2 Raw map



X Index: 200



Y Index: 200

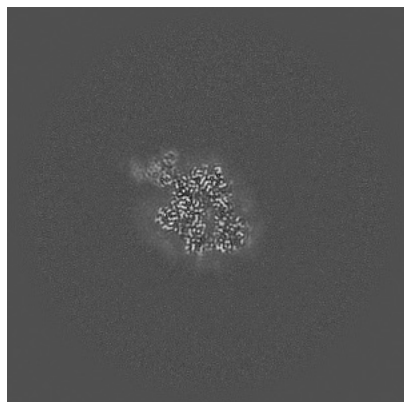


Z Index: 200

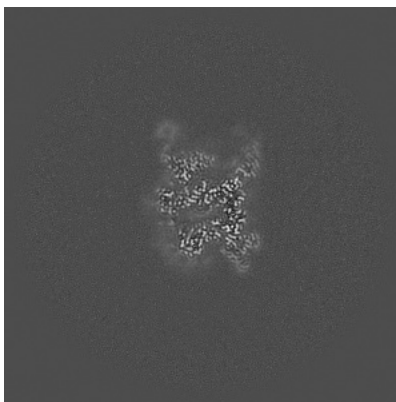
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

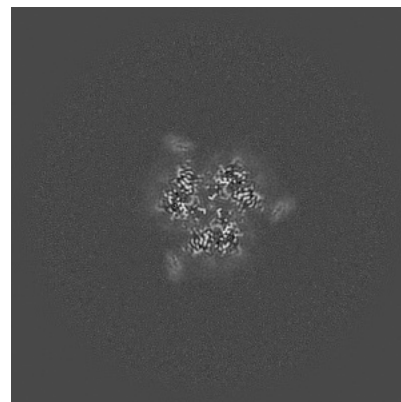
6.3.1 Primary map



X Index: 208

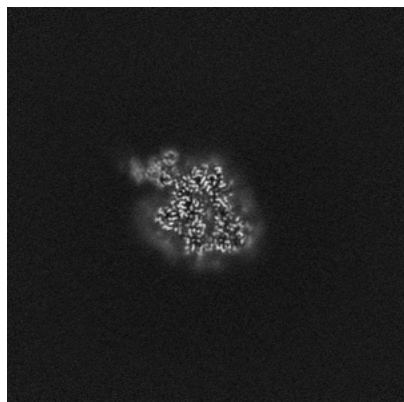


Y Index: 212

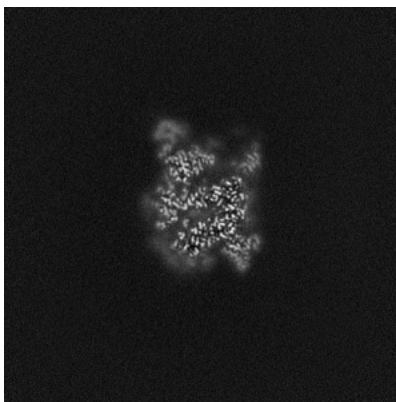


Z Index: 181

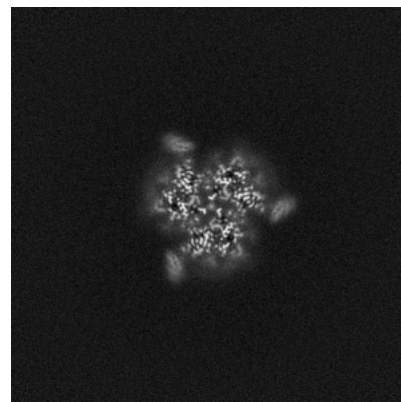
6.3.2 Raw map



X Index: 208



Y Index: 209

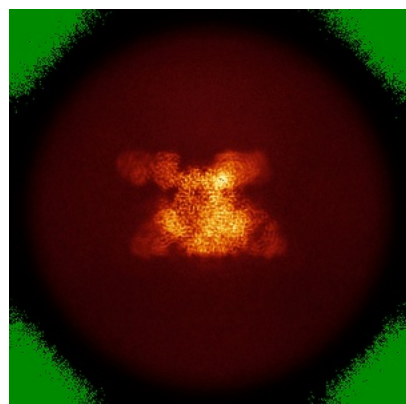


Z Index: 181

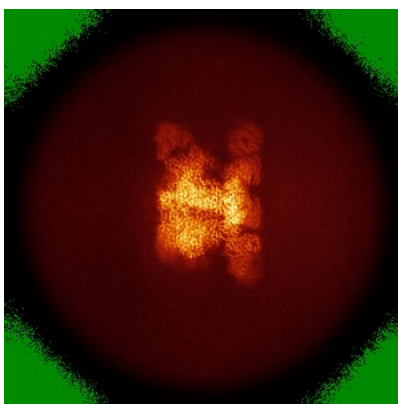
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

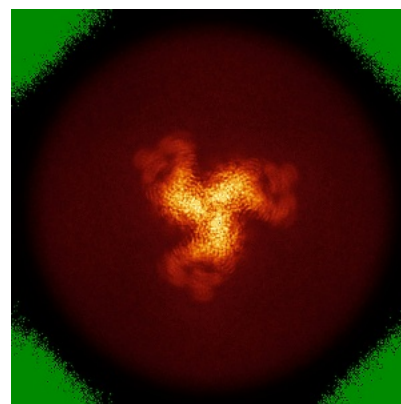
6.4.1 Primary map



X

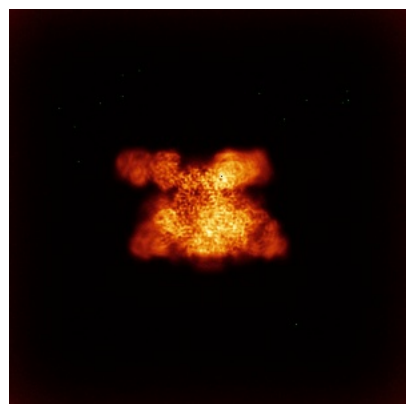


Y

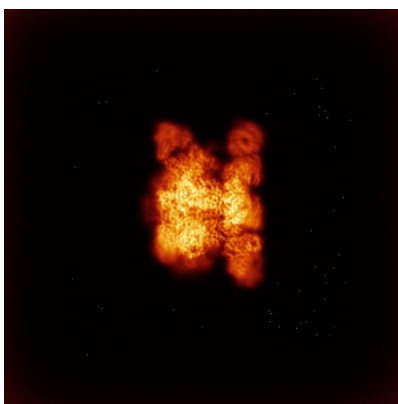


Z

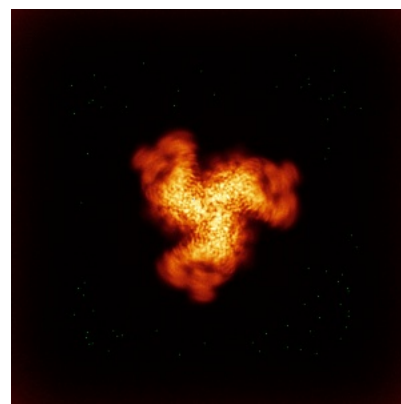
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



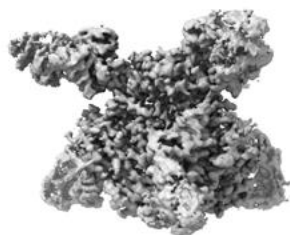
Y



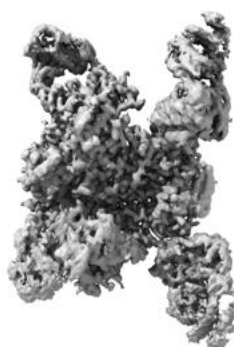
Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

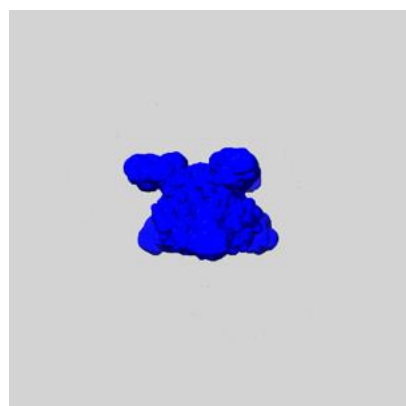
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

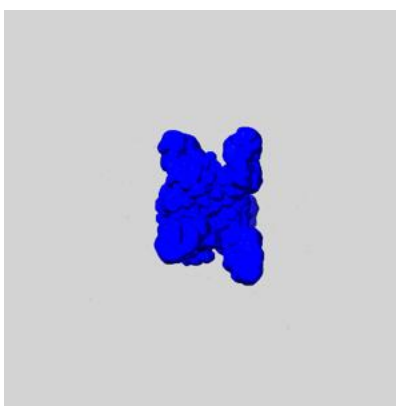
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

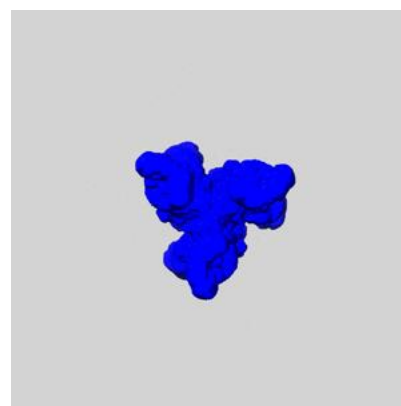
6.6.1 emd_44595_msk_1.map [i](#)



X



Y

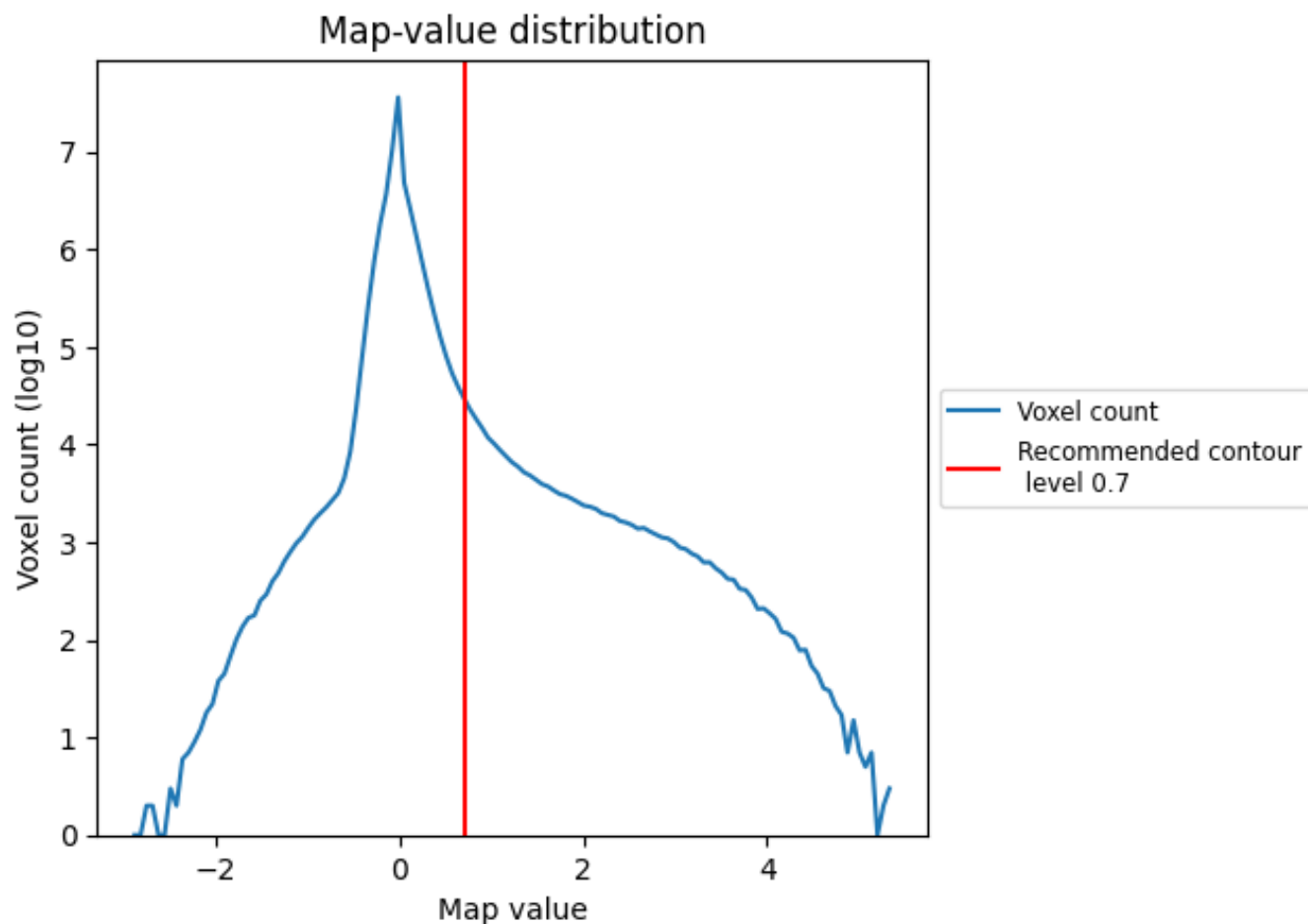


Z

7 Map analysis [i](#)

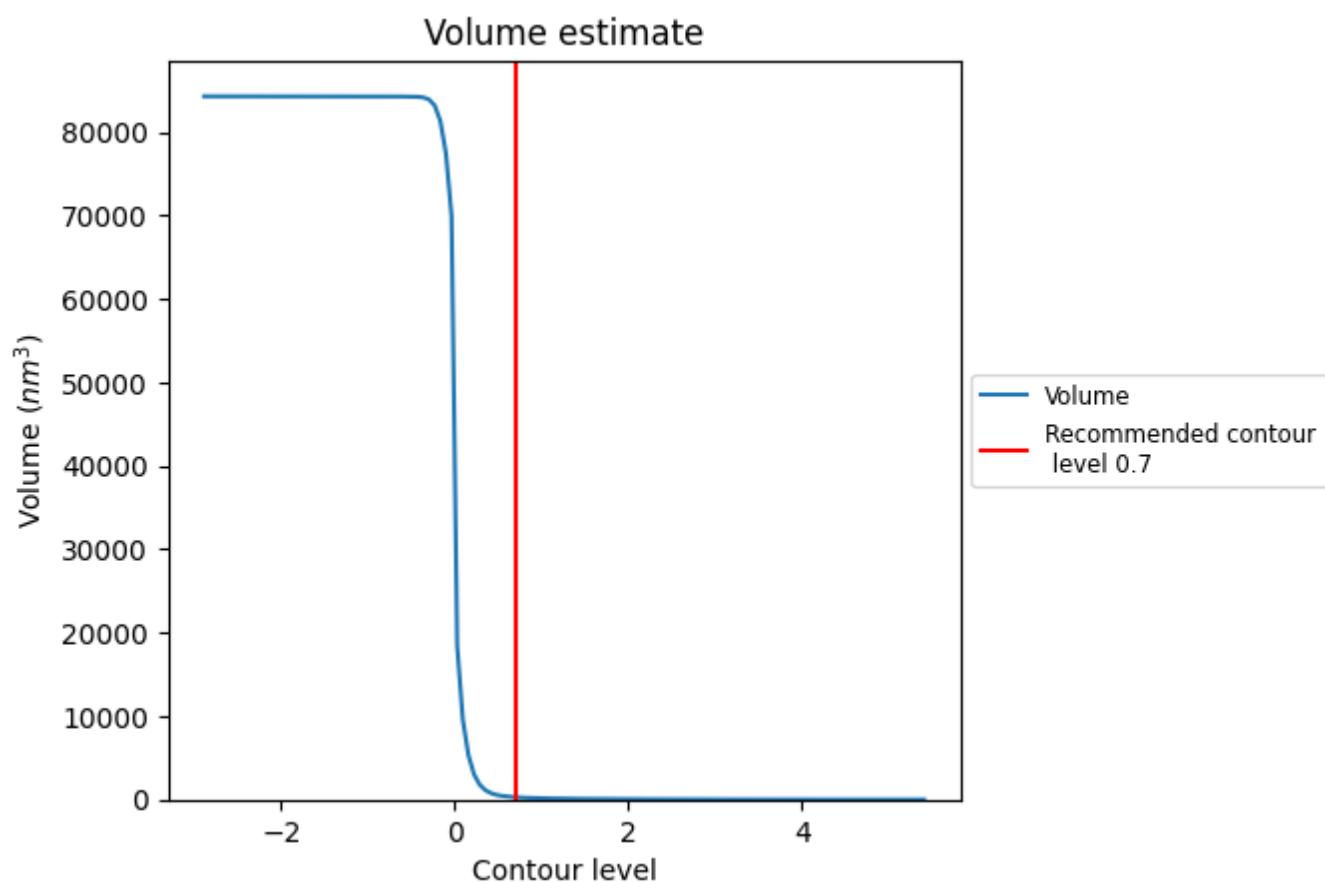
This section contains the results of statistical analysis of the map.

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.

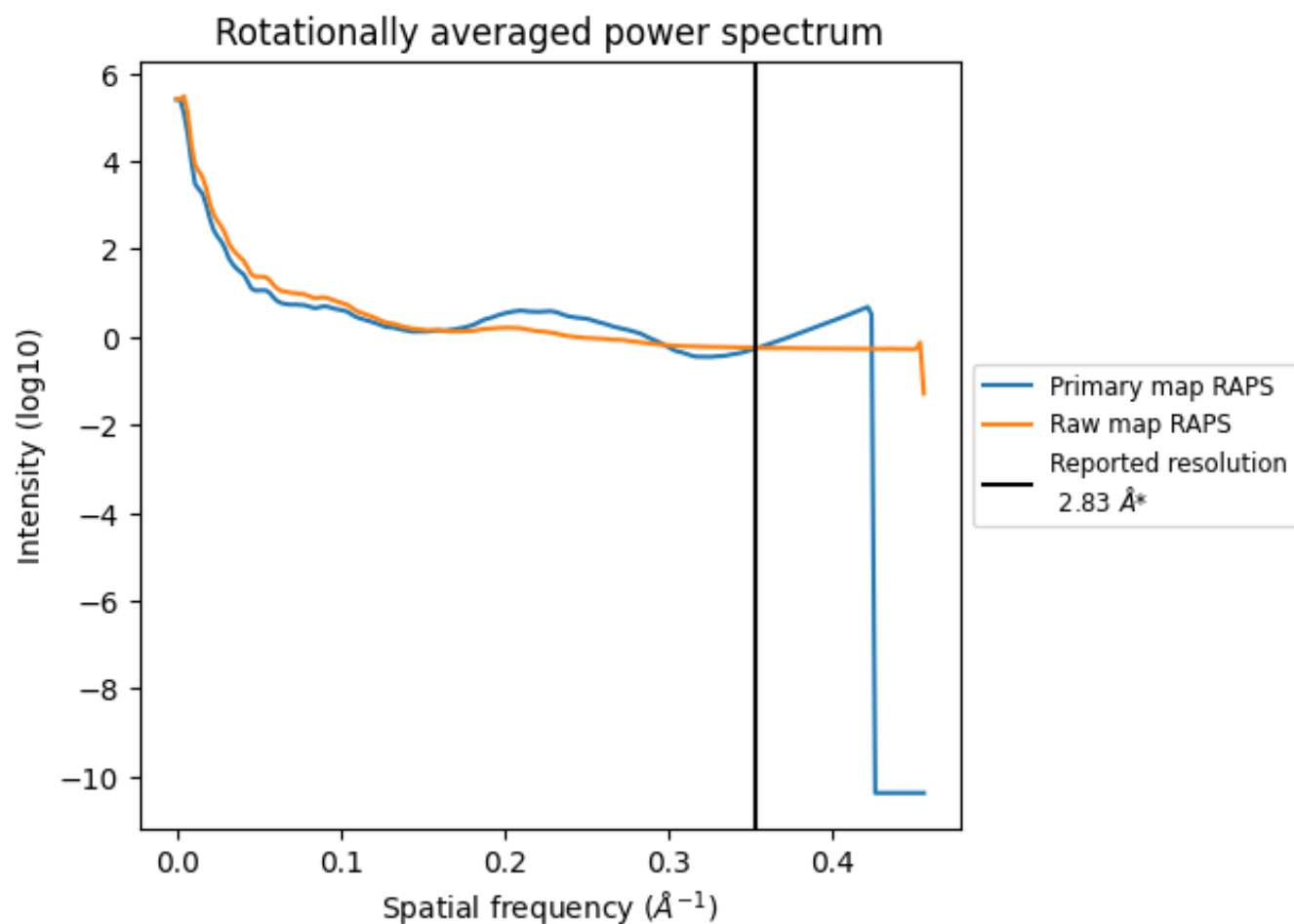
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm³; this corresponds to an approximate mass of 251 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 ⓘ

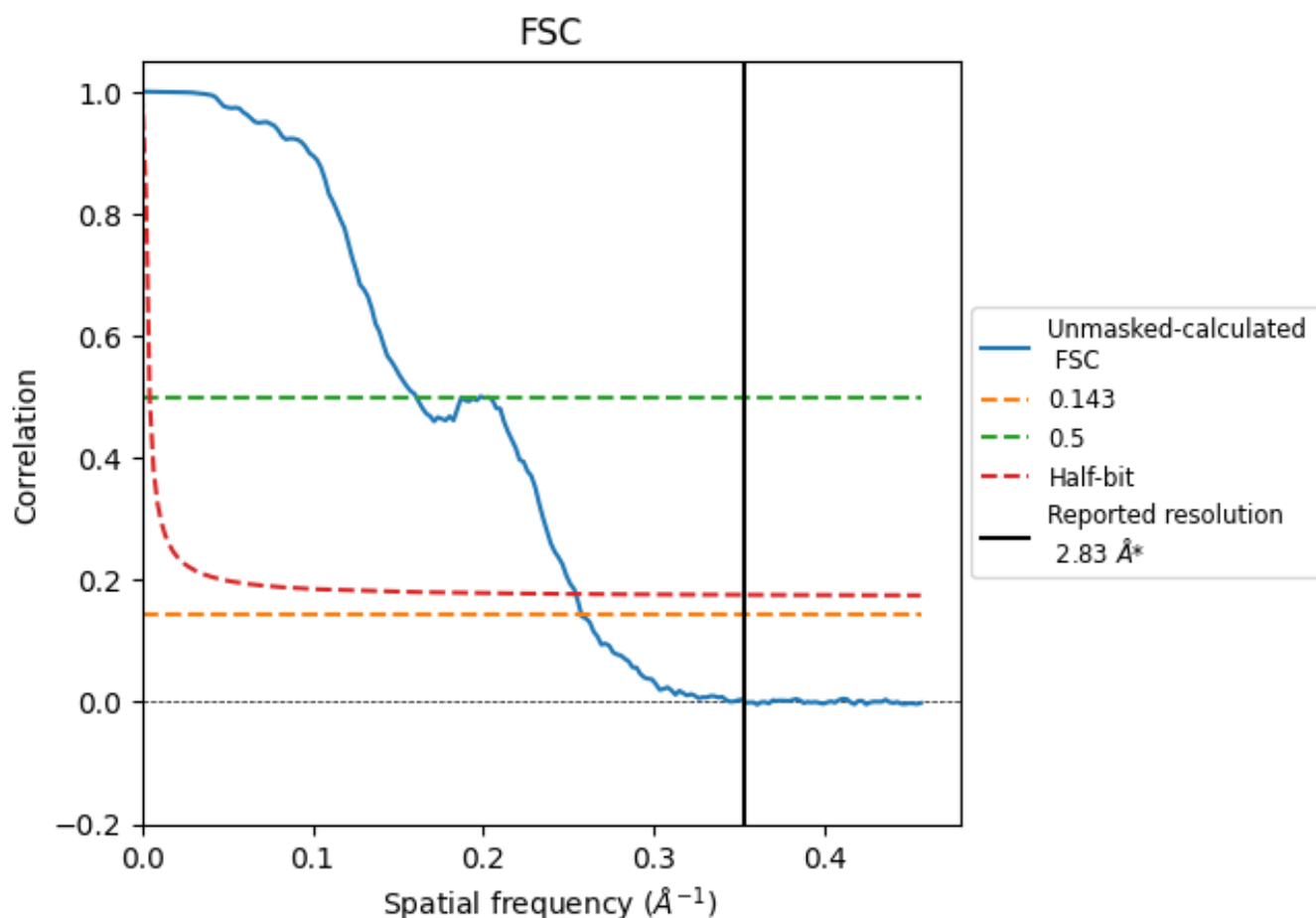


*Reported resolution corresponds to spatial frequency of $0.353 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.353 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

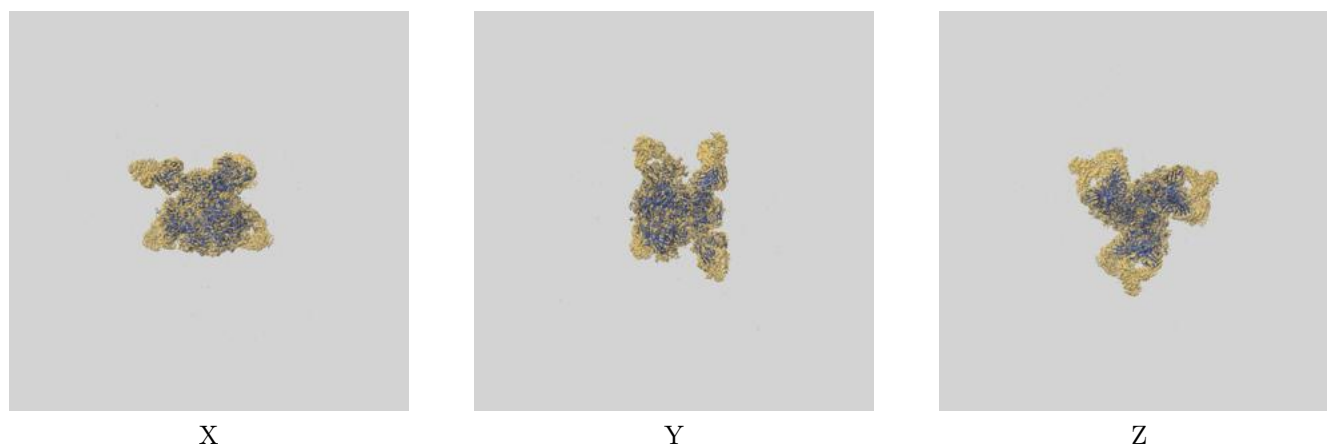
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	6.23	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

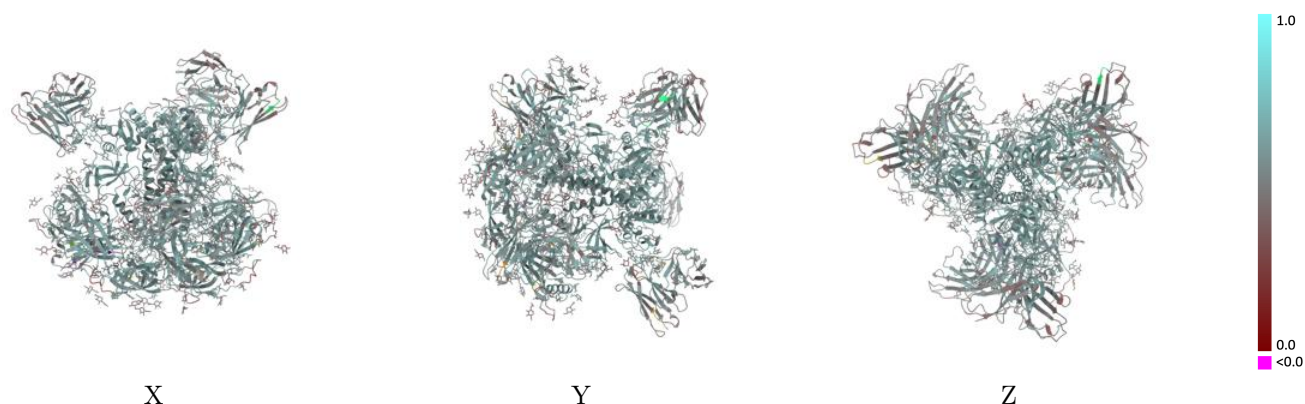
This section contains information regarding the fit between EMDB map EMD-44595 and PDB model 9BIO. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



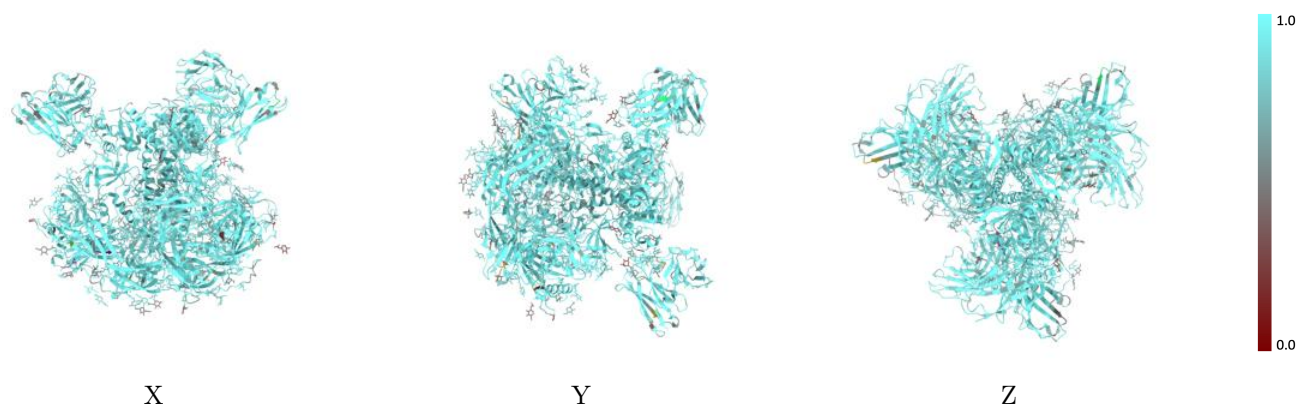
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



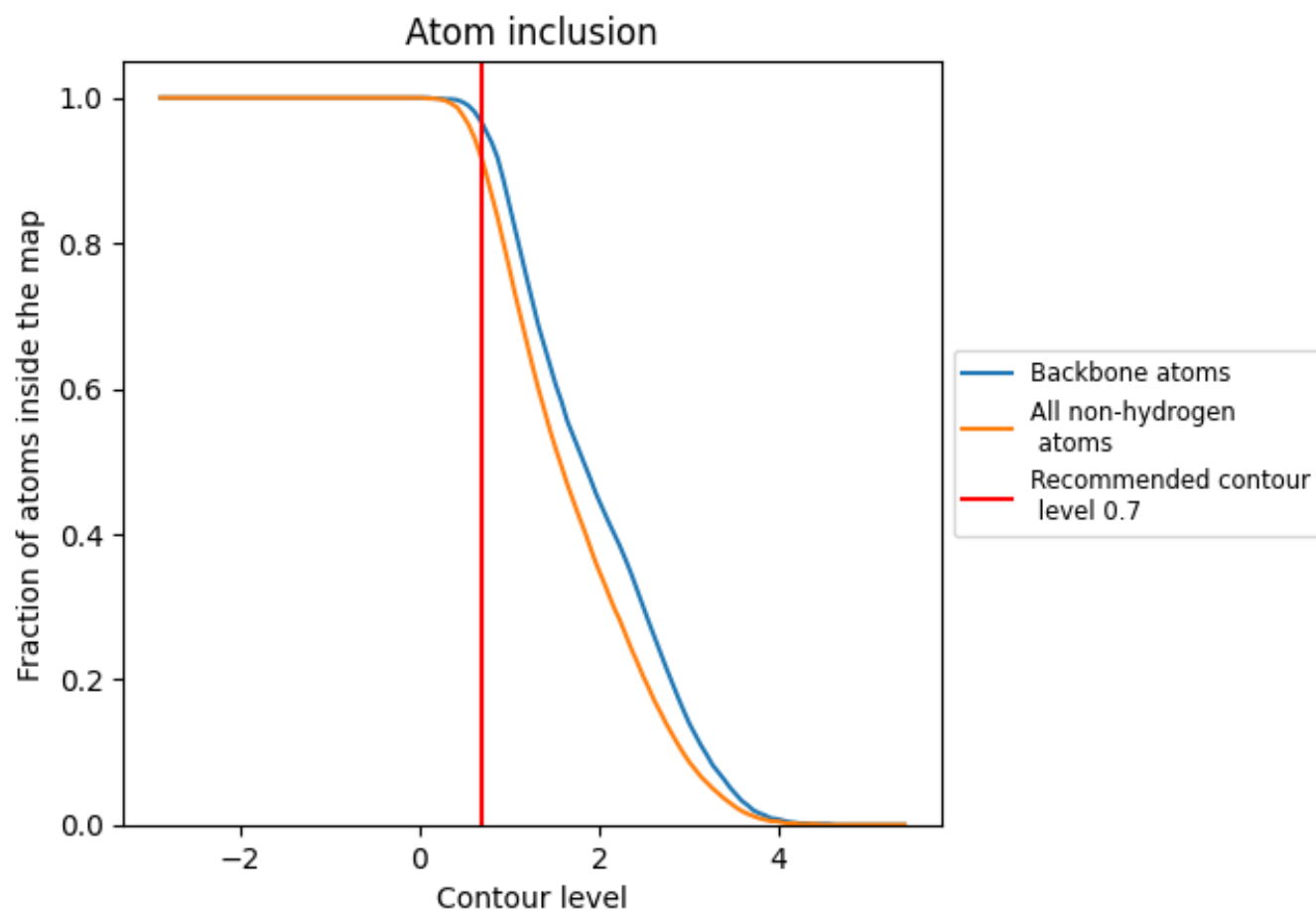
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.5470
0	 0.6790	 0.3910
1	 0.7180	 0.4900
2	 0.7500	 0.4370
3	 0.8920	 0.5500
4	 0.7500	 0.4680
5	 0.7860	 0.4740
6	 0.9640	 0.5690
A	 0.9440	 0.5870
B	 0.9380	 0.5820
C	 0.9340	 0.5650
D	 0.9430	 0.5690
E	 0.9120	 0.5120
F	 0.8690	 0.4960
G	 0.9340	 0.5680
H	 0.9000	 0.5160
I	 0.8950	 0.5160
J	 0.9400	 0.5850
K	 0.9360	 0.5660
L	 0.8670	 0.4960
M	 0.9410	 0.5670
N	 0.9010	 0.5130
O	 0.8600	 0.4940
P	 0.8940	 0.5170
Q	 0.8050	 0.4910
R	 0.8210	 0.4640
S	 0.9460	 0.5680
T	 0.6430	 0.4430
U	 0.9060	 0.5140
V	 0.6720	 0.4000
W	 0.8380	 0.5230
X	 0.8920	 0.5010
Y	 0.6430	 0.3830
Z	 0.7180	 0.4820
a	 0.6790	 0.4180



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.8790	 0.5460
c	 0.7500	 0.4740
d	 0.7860	 0.4910
e	 0.9640	 0.5600
f	 0.5000	 0.4000
g	 0.7800	 0.4740
h	 0.7500	 0.4590
i	 0.6430	 0.4380
j	 0.6720	 0.4120
k	 0.8190	 0.5220
l	 0.8790	 0.5030
m	 0.6790	 0.3760
n	 0.7690	 0.4750
o	 0.7140	 0.4380
p	 0.8790	 0.5480
q	 0.7860	 0.4570
r	 0.7500	 0.4880
s	 0.9640	 0.5610
t	 0.5360	 0.3940
u	 0.7320	 0.4710
v	 0.7860	 0.4720
w	 0.6430	 0.4420
x	 0.6230	 0.4030
y	 0.8290	 0.5220
z	 0.8790	 0.5050