



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 08:32 PM UTC

PDB ID : 8G3R / pdb_00008g3r
EMDB ID : EMD-29709
Title : N2 neuraminidase of A/Tanzania/205/2010 H3N2 with S245N S247T mutations in complex with one FNI17 Fab molecule
Authors : Dang, H.V.; Snell, G.
Deposited on : 2023-02-08
Resolution : 2.30 Å(reported)

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

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

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

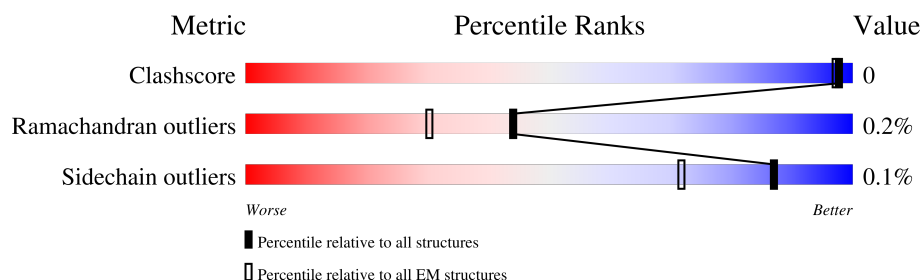
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	E	492	77% 21%
1	F	492	77% 21%
1	G	492	77% 21%
1	H	492	77% 21%
2	B	215	51% 49%
3	C	231	55% 44%
4	1	2	100%
4	2	2	50% 50%
4	4	2	100%

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Mol	Chain	Length	Quality of chain
4	5	2	100%
4	6	2	50%
4	7	2	50%
4	a	2	50%
4	b	2	100%
4	e	2	50%
4	f	2	100%
4	g	2	50%
4	i	2	100%
4	j	2	50%
4	l	2	100%
4	m	2	50%
4	n	2	100%
4	o	2	100%
4	q	2	100%
4	r	2	50%
4	t	2	100%
4	u	2	50%
4	v	2	100%
4	w	2	100%
5	3	8	25%
5	c	8	38%
5	k	8	38%
5	s	8	25%
6	d	3	33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14899 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 Neuraminidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	388	Total	C	N	O	S	0	0
			3004	1862	532	588	22		
1	G	388	Total	C	N	O	S	0	0
			3004	1862	532	588	22		
1	F	388	Total	C	N	O	S	0	0
			3004	1862	532	588	22		
1	H	388	Total	C	N	O	S	0	0
			3004	1862	532	588	22		

There are 424 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	MET	-	initiating methionine	UNP V9SNF2
E	-21	GLU	-	expression tag	UNP V9SNF2
E	-20	THR	-	expression tag	UNP V9SNF2
E	-19	ASP	-	expression tag	UNP V9SNF2
E	-18	THR	-	expression tag	UNP V9SNF2
E	-17	LEU	-	expression tag	UNP V9SNF2
E	-16	LEU	-	expression tag	UNP V9SNF2
E	-15	LEU	-	expression tag	UNP V9SNF2
E	-14	TRP	-	expression tag	UNP V9SNF2
E	-13	VAL	-	expression tag	UNP V9SNF2
E	-12	LEU	-	expression tag	UNP V9SNF2
E	-11	LEU	-	expression tag	UNP V9SNF2
E	-10	LEU	-	expression tag	UNP V9SNF2
E	-9	TRP	-	expression tag	UNP V9SNF2
E	-8	VAL	-	expression tag	UNP V9SNF2
E	-7	PRO	-	expression tag	UNP V9SNF2
E	-6	GLY	-	expression tag	UNP V9SNF2
E	-5	SER	-	expression tag	UNP V9SNF2
E	-4	THR	-	expression tag	UNP V9SNF2
E	-3	GLY	-	expression tag	UNP V9SNF2
E	-2	ASP	-	expression tag	UNP V9SNF2
E	-1	HIS	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP V9SNF2
E	1	HIS	-	expression tag	UNP V9SNF2
E	2	HIS	-	expression tag	UNP V9SNF2
E	3	HIS	-	expression tag	UNP V9SNF2
E	4	HIS	-	expression tag	UNP V9SNF2
E	5	GLY	-	expression tag	UNP V9SNF2
E	6	SER	-	expression tag	UNP V9SNF2
E	7	GLY	-	expression tag	UNP V9SNF2
E	8	LEU	-	expression tag	UNP V9SNF2
E	9	ASN	-	expression tag	UNP V9SNF2
E	10	ASP	-	expression tag	UNP V9SNF2
E	11	ILE	-	expression tag	UNP V9SNF2
E	12	PHE	-	expression tag	UNP V9SNF2
E	13	GLU	-	expression tag	UNP V9SNF2
E	14	ALA	-	expression tag	UNP V9SNF2
E	15	GLN	-	expression tag	UNP V9SNF2
E	16	LYS	-	expression tag	UNP V9SNF2
E	17	ILE	-	expression tag	UNP V9SNF2
E	18	GLU	-	expression tag	UNP V9SNF2
E	19	TRP	-	expression tag	UNP V9SNF2
E	20	HIS	-	expression tag	UNP V9SNF2
E	21	GLU	-	expression tag	UNP V9SNF2
E	22	GLY	-	expression tag	UNP V9SNF2
E	23	SER	-	expression tag	UNP V9SNF2
E	24	ILE	-	expression tag	UNP V9SNF2
E	25	ILE	-	expression tag	UNP V9SNF2
E	26	ASN	-	expression tag	UNP V9SNF2
E	27	GLU	-	expression tag	UNP V9SNF2
E	28	THR	-	expression tag	UNP V9SNF2
E	29	ALA	-	expression tag	UNP V9SNF2
E	30	ASP	-	expression tag	UNP V9SNF2
E	31	ASP	-	expression tag	UNP V9SNF2
E	32	ILE	-	expression tag	UNP V9SNF2
E	33	VAL	-	expression tag	UNP V9SNF2
E	34	TYR	-	expression tag	UNP V9SNF2
E	35	ARG	-	expression tag	UNP V9SNF2
E	36	LEU	-	expression tag	UNP V9SNF2
E	37	THR	-	expression tag	UNP V9SNF2
E	38	VAL	-	expression tag	UNP V9SNF2
E	39	ILE	-	expression tag	UNP V9SNF2
E	40	ILE	-	expression tag	UNP V9SNF2
E	41	ASP	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	42	ASP	-	expression tag	UNP V9SNF2
E	43	ARG	-	expression tag	UNP V9SNF2
E	44	TYR	-	expression tag	UNP V9SNF2
E	45	GLU	-	expression tag	UNP V9SNF2
E	46	SER	-	expression tag	UNP V9SNF2
E	47	LEU	-	expression tag	UNP V9SNF2
E	48	LYS	-	expression tag	UNP V9SNF2
E	49	ASN	-	expression tag	UNP V9SNF2
E	50	LEU	-	expression tag	UNP V9SNF2
E	51	ILE	-	expression tag	UNP V9SNF2
E	52	THR	-	expression tag	UNP V9SNF2
E	53	LEU	-	expression tag	UNP V9SNF2
E	54	ARG	-	expression tag	UNP V9SNF2
E	55	ALA	-	expression tag	UNP V9SNF2
E	56	ASP	-	expression tag	UNP V9SNF2
E	57	ARG	-	expression tag	UNP V9SNF2
E	58	LEU	-	expression tag	UNP V9SNF2
E	59	GLU	-	expression tag	UNP V9SNF2
E	60	MET	-	expression tag	UNP V9SNF2
E	61	ILE	-	expression tag	UNP V9SNF2
E	62	ILE	-	expression tag	UNP V9SNF2
E	63	ASN	-	expression tag	UNP V9SNF2
E	64	ASP	-	expression tag	UNP V9SNF2
E	65	ASN	-	expression tag	UNP V9SNF2
E	66	VAL	-	expression tag	UNP V9SNF2
E	67	SER	-	expression tag	UNP V9SNF2
E	68	THR	-	expression tag	UNP V9SNF2
E	69	ILE	-	expression tag	UNP V9SNF2
E	70	LEU	-	expression tag	UNP V9SNF2
E	71	ALA	-	expression tag	UNP V9SNF2
E	72	SER	-	expression tag	UNP V9SNF2
E	73	GLY	-	expression tag	UNP V9SNF2
E	74	LEU	-	expression tag	UNP V9SNF2
E	75	VAL	-	expression tag	UNP V9SNF2
E	76	PRO	-	expression tag	UNP V9SNF2
E	77	ARG	-	expression tag	UNP V9SNF2
E	78	GLY	-	expression tag	UNP V9SNF2
E	79	SER	-	expression tag	UNP V9SNF2
E	80	GLY	-	expression tag	UNP V9SNF2
E	81	SER	-	expression tag	UNP V9SNF2
E	245	ASN	SER	engineered mutation	UNP V9SNF2
E	247	THR	SER	engineered mutation	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-22	MET	-	initiating methionine	UNP V9SNF2
G	-21	GLU	-	expression tag	UNP V9SNF2
G	-20	THR	-	expression tag	UNP V9SNF2
G	-19	ASP	-	expression tag	UNP V9SNF2
G	-18	THR	-	expression tag	UNP V9SNF2
G	-17	LEU	-	expression tag	UNP V9SNF2
G	-16	LEU	-	expression tag	UNP V9SNF2
G	-15	LEU	-	expression tag	UNP V9SNF2
G	-14	TRP	-	expression tag	UNP V9SNF2
G	-13	VAL	-	expression tag	UNP V9SNF2
G	-12	LEU	-	expression tag	UNP V9SNF2
G	-11	LEU	-	expression tag	UNP V9SNF2
G	-10	LEU	-	expression tag	UNP V9SNF2
G	-9	TRP	-	expression tag	UNP V9SNF2
G	-8	VAL	-	expression tag	UNP V9SNF2
G	-7	PRO	-	expression tag	UNP V9SNF2
G	-6	GLY	-	expression tag	UNP V9SNF2
G	-5	SER	-	expression tag	UNP V9SNF2
G	-4	THR	-	expression tag	UNP V9SNF2
G	-3	GLY	-	expression tag	UNP V9SNF2
G	-2	ASP	-	expression tag	UNP V9SNF2
G	-1	HIS	-	expression tag	UNP V9SNF2
G	0	HIS	-	expression tag	UNP V9SNF2
G	1	HIS	-	expression tag	UNP V9SNF2
G	2	HIS	-	expression tag	UNP V9SNF2
G	3	HIS	-	expression tag	UNP V9SNF2
G	4	HIS	-	expression tag	UNP V9SNF2
G	5	GLY	-	expression tag	UNP V9SNF2
G	6	SER	-	expression tag	UNP V9SNF2
G	7	GLY	-	expression tag	UNP V9SNF2
G	8	LEU	-	expression tag	UNP V9SNF2
G	9	ASN	-	expression tag	UNP V9SNF2
G	10	ASP	-	expression tag	UNP V9SNF2
G	11	ILE	-	expression tag	UNP V9SNF2
G	12	PHE	-	expression tag	UNP V9SNF2
G	13	GLU	-	expression tag	UNP V9SNF2
G	14	ALA	-	expression tag	UNP V9SNF2
G	15	GLN	-	expression tag	UNP V9SNF2
G	16	LYS	-	expression tag	UNP V9SNF2
G	17	ILE	-	expression tag	UNP V9SNF2
G	18	GLU	-	expression tag	UNP V9SNF2
G	19	TRP	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	20	HIS	-	expression tag	UNP V9SNF2
G	21	GLU	-	expression tag	UNP V9SNF2
G	22	GLY	-	expression tag	UNP V9SNF2
G	23	SER	-	expression tag	UNP V9SNF2
G	24	ILE	-	expression tag	UNP V9SNF2
G	25	ILE	-	expression tag	UNP V9SNF2
G	26	ASN	-	expression tag	UNP V9SNF2
G	27	GLU	-	expression tag	UNP V9SNF2
G	28	THR	-	expression tag	UNP V9SNF2
G	29	ALA	-	expression tag	UNP V9SNF2
G	30	ASP	-	expression tag	UNP V9SNF2
G	31	ASP	-	expression tag	UNP V9SNF2
G	32	ILE	-	expression tag	UNP V9SNF2
G	33	VAL	-	expression tag	UNP V9SNF2
G	34	TYR	-	expression tag	UNP V9SNF2
G	35	ARG	-	expression tag	UNP V9SNF2
G	36	LEU	-	expression tag	UNP V9SNF2
G	37	THR	-	expression tag	UNP V9SNF2
G	38	VAL	-	expression tag	UNP V9SNF2
G	39	ILE	-	expression tag	UNP V9SNF2
G	40	ILE	-	expression tag	UNP V9SNF2
G	41	ASP	-	expression tag	UNP V9SNF2
G	42	ASP	-	expression tag	UNP V9SNF2
G	43	ARG	-	expression tag	UNP V9SNF2
G	44	TYR	-	expression tag	UNP V9SNF2
G	45	GLU	-	expression tag	UNP V9SNF2
G	46	SER	-	expression tag	UNP V9SNF2
G	47	LEU	-	expression tag	UNP V9SNF2
G	48	LYS	-	expression tag	UNP V9SNF2
G	49	ASN	-	expression tag	UNP V9SNF2
G	50	LEU	-	expression tag	UNP V9SNF2
G	51	ILE	-	expression tag	UNP V9SNF2
G	52	THR	-	expression tag	UNP V9SNF2
G	53	LEU	-	expression tag	UNP V9SNF2
G	54	ARG	-	expression tag	UNP V9SNF2
G	55	ALA	-	expression tag	UNP V9SNF2
G	56	ASP	-	expression tag	UNP V9SNF2
G	57	ARG	-	expression tag	UNP V9SNF2
G	58	LEU	-	expression tag	UNP V9SNF2
G	59	GLU	-	expression tag	UNP V9SNF2
G	60	MET	-	expression tag	UNP V9SNF2
G	61	ILE	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	62	ILE	-	expression tag	UNP V9SNF2
G	63	ASN	-	expression tag	UNP V9SNF2
G	64	ASP	-	expression tag	UNP V9SNF2
G	65	ASN	-	expression tag	UNP V9SNF2
G	66	VAL	-	expression tag	UNP V9SNF2
G	67	SER	-	expression tag	UNP V9SNF2
G	68	THR	-	expression tag	UNP V9SNF2
G	69	ILE	-	expression tag	UNP V9SNF2
G	70	LEU	-	expression tag	UNP V9SNF2
G	71	ALA	-	expression tag	UNP V9SNF2
G	72	SER	-	expression tag	UNP V9SNF2
G	73	GLY	-	expression tag	UNP V9SNF2
G	74	LEU	-	expression tag	UNP V9SNF2
G	75	VAL	-	expression tag	UNP V9SNF2
G	76	PRO	-	expression tag	UNP V9SNF2
G	77	ARG	-	expression tag	UNP V9SNF2
G	78	GLY	-	expression tag	UNP V9SNF2
G	79	SER	-	expression tag	UNP V9SNF2
G	80	GLY	-	expression tag	UNP V9SNF2
G	81	SER	-	expression tag	UNP V9SNF2
G	245	ASN	SER	engineered mutation	UNP V9SNF2
G	247	THR	SER	engineered mutation	UNP V9SNF2
F	-22	MET	-	initiating methionine	UNP V9SNF2
F	-21	GLU	-	expression tag	UNP V9SNF2
F	-20	THR	-	expression tag	UNP V9SNF2
F	-19	ASP	-	expression tag	UNP V9SNF2
F	-18	THR	-	expression tag	UNP V9SNF2
F	-17	LEU	-	expression tag	UNP V9SNF2
F	-16	LEU	-	expression tag	UNP V9SNF2
F	-15	LEU	-	expression tag	UNP V9SNF2
F	-14	TRP	-	expression tag	UNP V9SNF2
F	-13	VAL	-	expression tag	UNP V9SNF2
F	-12	LEU	-	expression tag	UNP V9SNF2
F	-11	LEU	-	expression tag	UNP V9SNF2
F	-10	LEU	-	expression tag	UNP V9SNF2
F	-9	TRP	-	expression tag	UNP V9SNF2
F	-8	VAL	-	expression tag	UNP V9SNF2
F	-7	PRO	-	expression tag	UNP V9SNF2
F	-6	GLY	-	expression tag	UNP V9SNF2
F	-5	SER	-	expression tag	UNP V9SNF2
F	-4	THR	-	expression tag	UNP V9SNF2
F	-3	GLY	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	ASP	-	expression tag	UNP V9SNF2
F	-1	HIS	-	expression tag	UNP V9SNF2
F	0	HIS	-	expression tag	UNP V9SNF2
F	1	HIS	-	expression tag	UNP V9SNF2
F	2	HIS	-	expression tag	UNP V9SNF2
F	3	HIS	-	expression tag	UNP V9SNF2
F	4	HIS	-	expression tag	UNP V9SNF2
F	5	GLY	-	expression tag	UNP V9SNF2
F	6	SER	-	expression tag	UNP V9SNF2
F	7	GLY	-	expression tag	UNP V9SNF2
F	8	LEU	-	expression tag	UNP V9SNF2
F	9	ASN	-	expression tag	UNP V9SNF2
F	10	ASP	-	expression tag	UNP V9SNF2
F	11	ILE	-	expression tag	UNP V9SNF2
F	12	PHE	-	expression tag	UNP V9SNF2
F	13	GLU	-	expression tag	UNP V9SNF2
F	14	ALA	-	expression tag	UNP V9SNF2
F	15	GLN	-	expression tag	UNP V9SNF2
F	16	LYS	-	expression tag	UNP V9SNF2
F	17	ILE	-	expression tag	UNP V9SNF2
F	18	GLU	-	expression tag	UNP V9SNF2
F	19	TRP	-	expression tag	UNP V9SNF2
F	20	HIS	-	expression tag	UNP V9SNF2
F	21	GLU	-	expression tag	UNP V9SNF2
F	22	GLY	-	expression tag	UNP V9SNF2
F	23	SER	-	expression tag	UNP V9SNF2
F	24	ILE	-	expression tag	UNP V9SNF2
F	25	ILE	-	expression tag	UNP V9SNF2
F	26	ASN	-	expression tag	UNP V9SNF2
F	27	GLU	-	expression tag	UNP V9SNF2
F	28	THR	-	expression tag	UNP V9SNF2
F	29	ALA	-	expression tag	UNP V9SNF2
F	30	ASP	-	expression tag	UNP V9SNF2
F	31	ASP	-	expression tag	UNP V9SNF2
F	32	ILE	-	expression tag	UNP V9SNF2
F	33	VAL	-	expression tag	UNP V9SNF2
F	34	TYR	-	expression tag	UNP V9SNF2
F	35	ARG	-	expression tag	UNP V9SNF2
F	36	LEU	-	expression tag	UNP V9SNF2
F	37	THR	-	expression tag	UNP V9SNF2
F	38	VAL	-	expression tag	UNP V9SNF2
F	39	ILE	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	40	ILE	-	expression tag	UNP V9SNF2
F	41	ASP	-	expression tag	UNP V9SNF2
F	42	ASP	-	expression tag	UNP V9SNF2
F	43	ARG	-	expression tag	UNP V9SNF2
F	44	TYR	-	expression tag	UNP V9SNF2
F	45	GLU	-	expression tag	UNP V9SNF2
F	46	SER	-	expression tag	UNP V9SNF2
F	47	LEU	-	expression tag	UNP V9SNF2
F	48	LYS	-	expression tag	UNP V9SNF2
F	49	ASN	-	expression tag	UNP V9SNF2
F	50	LEU	-	expression tag	UNP V9SNF2
F	51	ILE	-	expression tag	UNP V9SNF2
F	52	THR	-	expression tag	UNP V9SNF2
F	53	LEU	-	expression tag	UNP V9SNF2
F	54	ARG	-	expression tag	UNP V9SNF2
F	55	ALA	-	expression tag	UNP V9SNF2
F	56	ASP	-	expression tag	UNP V9SNF2
F	57	ARG	-	expression tag	UNP V9SNF2
F	58	LEU	-	expression tag	UNP V9SNF2
F	59	GLU	-	expression tag	UNP V9SNF2
F	60	MET	-	expression tag	UNP V9SNF2
F	61	ILE	-	expression tag	UNP V9SNF2
F	62	ILE	-	expression tag	UNP V9SNF2
F	63	ASN	-	expression tag	UNP V9SNF2
F	64	ASP	-	expression tag	UNP V9SNF2
F	65	ASN	-	expression tag	UNP V9SNF2
F	66	VAL	-	expression tag	UNP V9SNF2
F	67	SER	-	expression tag	UNP V9SNF2
F	68	THR	-	expression tag	UNP V9SNF2
F	69	ILE	-	expression tag	UNP V9SNF2
F	70	LEU	-	expression tag	UNP V9SNF2
F	71	ALA	-	expression tag	UNP V9SNF2
F	72	SER	-	expression tag	UNP V9SNF2
F	73	GLY	-	expression tag	UNP V9SNF2
F	74	LEU	-	expression tag	UNP V9SNF2
F	75	VAL	-	expression tag	UNP V9SNF2
F	76	PRO	-	expression tag	UNP V9SNF2
F	77	ARG	-	expression tag	UNP V9SNF2
F	78	GLY	-	expression tag	UNP V9SNF2
F	79	SER	-	expression tag	UNP V9SNF2
F	80	GLY	-	expression tag	UNP V9SNF2
F	81	SER	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	245	ASN	SER	engineered mutation	UNP V9SNF2
F	247	THR	SER	engineered mutation	UNP V9SNF2
H	-22	MET	-	initiating methionine	UNP V9SNF2
H	-21	GLU	-	expression tag	UNP V9SNF2
H	-20	THR	-	expression tag	UNP V9SNF2
H	-19	ASP	-	expression tag	UNP V9SNF2
H	-18	THR	-	expression tag	UNP V9SNF2
H	-17	LEU	-	expression tag	UNP V9SNF2
H	-16	LEU	-	expression tag	UNP V9SNF2
H	-15	LEU	-	expression tag	UNP V9SNF2
H	-14	TRP	-	expression tag	UNP V9SNF2
H	-13	VAL	-	expression tag	UNP V9SNF2
H	-12	LEU	-	expression tag	UNP V9SNF2
H	-11	LEU	-	expression tag	UNP V9SNF2
H	-10	LEU	-	expression tag	UNP V9SNF2
H	-9	TRP	-	expression tag	UNP V9SNF2
H	-8	VAL	-	expression tag	UNP V9SNF2
H	-7	PRO	-	expression tag	UNP V9SNF2
H	-6	GLY	-	expression tag	UNP V9SNF2
H	-5	SER	-	expression tag	UNP V9SNF2
H	-4	THR	-	expression tag	UNP V9SNF2
H	-3	GLY	-	expression tag	UNP V9SNF2
H	-2	ASP	-	expression tag	UNP V9SNF2
H	-1	HIS	-	expression tag	UNP V9SNF2
H	0	HIS	-	expression tag	UNP V9SNF2
H	1	HIS	-	expression tag	UNP V9SNF2
H	2	HIS	-	expression tag	UNP V9SNF2
H	3	HIS	-	expression tag	UNP V9SNF2
H	4	HIS	-	expression tag	UNP V9SNF2
H	5	GLY	-	expression tag	UNP V9SNF2
H	6	SER	-	expression tag	UNP V9SNF2
H	7	GLY	-	expression tag	UNP V9SNF2
H	8	LEU	-	expression tag	UNP V9SNF2
H	9	ASN	-	expression tag	UNP V9SNF2
H	10	ASP	-	expression tag	UNP V9SNF2
H	11	ILE	-	expression tag	UNP V9SNF2
H	12	PHE	-	expression tag	UNP V9SNF2
H	13	GLU	-	expression tag	UNP V9SNF2
H	14	ALA	-	expression tag	UNP V9SNF2
H	15	GLN	-	expression tag	UNP V9SNF2
H	16	LYS	-	expression tag	UNP V9SNF2
H	17	ILE	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	18	GLU	-	expression tag	UNP V9SNF2
H	19	TRP	-	expression tag	UNP V9SNF2
H	20	HIS	-	expression tag	UNP V9SNF2
H	21	GLU	-	expression tag	UNP V9SNF2
H	22	GLY	-	expression tag	UNP V9SNF2
H	23	SER	-	expression tag	UNP V9SNF2
H	24	ILE	-	expression tag	UNP V9SNF2
H	25	ILE	-	expression tag	UNP V9SNF2
H	26	ASN	-	expression tag	UNP V9SNF2
H	27	GLU	-	expression tag	UNP V9SNF2
H	28	THR	-	expression tag	UNP V9SNF2
H	29	ALA	-	expression tag	UNP V9SNF2
H	30	ASP	-	expression tag	UNP V9SNF2
H	31	ASP	-	expression tag	UNP V9SNF2
H	32	ILE	-	expression tag	UNP V9SNF2
H	33	VAL	-	expression tag	UNP V9SNF2
H	34	TYR	-	expression tag	UNP V9SNF2
H	35	ARG	-	expression tag	UNP V9SNF2
H	36	LEU	-	expression tag	UNP V9SNF2
H	37	THR	-	expression tag	UNP V9SNF2
H	38	VAL	-	expression tag	UNP V9SNF2
H	39	ILE	-	expression tag	UNP V9SNF2
H	40	ILE	-	expression tag	UNP V9SNF2
H	41	ASP	-	expression tag	UNP V9SNF2
H	42	ASP	-	expression tag	UNP V9SNF2
H	43	ARG	-	expression tag	UNP V9SNF2
H	44	TYR	-	expression tag	UNP V9SNF2
H	45	GLU	-	expression tag	UNP V9SNF2
H	46	SER	-	expression tag	UNP V9SNF2
H	47	LEU	-	expression tag	UNP V9SNF2
H	48	LYS	-	expression tag	UNP V9SNF2
H	49	ASN	-	expression tag	UNP V9SNF2
H	50	LEU	-	expression tag	UNP V9SNF2
H	51	ILE	-	expression tag	UNP V9SNF2
H	52	THR	-	expression tag	UNP V9SNF2
H	53	LEU	-	expression tag	UNP V9SNF2
H	54	ARG	-	expression tag	UNP V9SNF2
H	55	ALA	-	expression tag	UNP V9SNF2
H	56	ASP	-	expression tag	UNP V9SNF2
H	57	ARG	-	expression tag	UNP V9SNF2
H	58	LEU	-	expression tag	UNP V9SNF2
H	59	GLU	-	expression tag	UNP V9SNF2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	60	MET	-	expression tag	UNP V9SNF2
H	61	ILE	-	expression tag	UNP V9SNF2
H	62	ILE	-	expression tag	UNP V9SNF2
H	63	ASN	-	expression tag	UNP V9SNF2
H	64	ASP	-	expression tag	UNP V9SNF2
H	65	ASN	-	expression tag	UNP V9SNF2
H	66	VAL	-	expression tag	UNP V9SNF2
H	67	SER	-	expression tag	UNP V9SNF2
H	68	THR	-	expression tag	UNP V9SNF2
H	69	ILE	-	expression tag	UNP V9SNF2
H	70	LEU	-	expression tag	UNP V9SNF2
H	71	ALA	-	expression tag	UNP V9SNF2
H	72	SER	-	expression tag	UNP V9SNF2
H	73	GLY	-	expression tag	UNP V9SNF2
H	74	LEU	-	expression tag	UNP V9SNF2
H	75	VAL	-	expression tag	UNP V9SNF2
H	76	PRO	-	expression tag	UNP V9SNF2
H	77	ARG	-	expression tag	UNP V9SNF2
H	78	GLY	-	expression tag	UNP V9SNF2
H	79	SER	-	expression tag	UNP V9SNF2
H	80	GLY	-	expression tag	UNP V9SNF2
H	81	SER	-	expression tag	UNP V9SNF2
H	245	ASN	SER	engineered mutation	UNP V9SNF2
H	247	THR	SER	engineered mutation	UNP V9SNF2

- Molecule 2 is a protein called FNI17 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	109	Total	C	N	O	S	0	0
			834	526	145	160	3		

- Molecule 3 is a protein called FNI17 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	129	Total	C	N	O	S	0	0
			986	620	171	191	4		

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



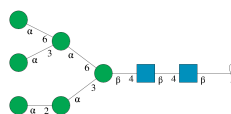
Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		
4	l	2	Total	C	N	O	0	0
			28	16	2	10		
4	n	2	Total	C	N	O	0	0
			28	16	2	10		
4	o	2	Total	C	N	O	0	0
			28	16	2	10		
4	q	2	Total	C	N	O	0	0
			28	16	2	10		
4	r	2	Total	C	N	O	0	0
			28	16	2	10		
4	t	2	Total	C	N	O	0	0
			28	16	2	10		
4	v	2	Total	C	N	O	0	0
			28	16	2	10		
4	w	2	Total	C	N	O	0	0
			28	16	2	10		
4	1	2	Total	C	N	O	0	0
			28	16	2	10		
4	2	2	Total	C	N	O	0	0
			28	16	2	10		
4	4	2	Total	C	N	O	0	0
			28	16	2	10		
4	6	2	Total	C	N	O	0	0
			28	16	2	10		
4	7	2	Total	C	N	O	0	0
			28	16	2	10		

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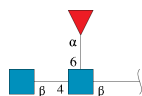
Mol	Chain	Residues	Atoms				AltConf	Trace
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		
4	u	2	Total	C	N	O	0	0
			28	16	2	10		
4	5	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 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
5	c	8	Total	C	N	O	0	0
			94	52	2	40		
5	k	8	Total	C	N	O	0	0
			94	52	2	40		
5	s	8	Total	C	N	O	0	0
			94	52	2	40		
5	3	8	Total	C	N	O	0	0
			94	52	2	40		

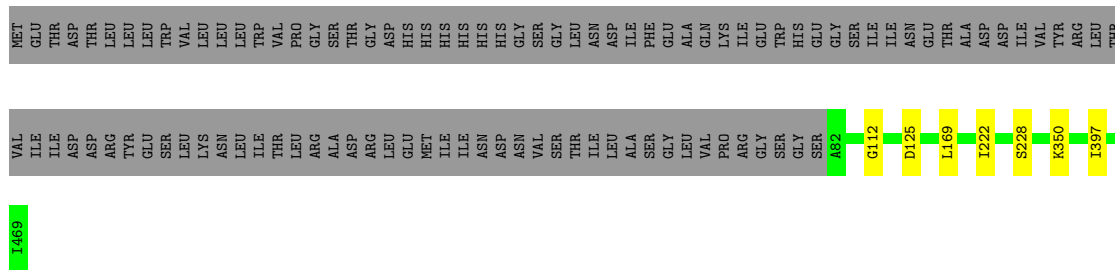
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



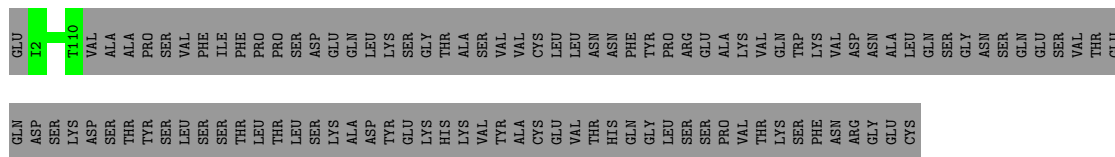
Mol	Chain	Residues	Atoms				AltConf	Trace
6	d	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

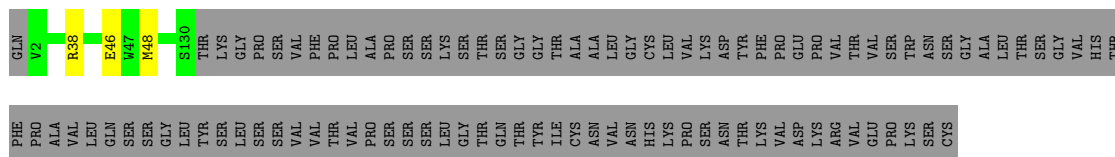
Mol	Chain	Residues	Atoms		AltConf
7	E	2	Total 2	Ca 2	0
7	G	1	Total 1	Ca 1	0
7	F	1	Total 1	Ca 1	0
7	H	1	Total 1	Ca 1	0



- Molecule 2: FNI17 Fab light chain



- Molecule 3: FNI17 Fab heavy chain



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



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



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



MAG1
MAG2

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

Chain g:  50% 50%MAG1
MAG2

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

Chain i:  100%MAG1
MAG2

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

Chain j:  50% 50%MAG1
MAG2

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

Chain l:  100%MAG1
MAG2

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

Chain n:  100%MAG1
MAG2

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

Chain o:  100%MAG1
MAG2

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

Chain q:  100%

MAG1
MAG2

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

Chain r:  50% 50%

MAG1
MAG2

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

Chain t:  100%

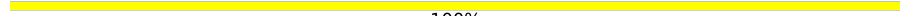
MAG1
MAG2

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

Chain v:  100%

MAG1
MAG2

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

Chain w:  100%

MAG1
MAG2

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

Chain 1:  100%

MAG1
MAG2

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

Chain 2:  50% 50%



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

Chain 4:  100%



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

Chain 6:  50% 50%



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

Chain 7:  50% 50%



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

Chain e:  50% 50%



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

Chain m:  50% 50%



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

Chain u:  50% 50%



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

Chain 5:  100%

MAG1
MAG2

- Molecule 5: 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 c:  38% 62%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 5: 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:  38% 62%

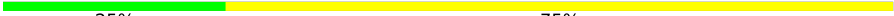
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 5: 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 s:  25% 75%

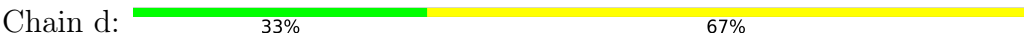
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 5: 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 3:  25% 75%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	528681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.81	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	E	0.96	0/3071	1.13	2/4167 (0.0%)
1	F	0.95	0/3071	1.14	2/4167 (0.0%)
1	G	0.98	0/3071	1.16	2/4167 (0.0%)
1	H	0.95	0/3071	1.14	2/4167 (0.0%)
2	B	0.98	0/856	1.08	0/1166
3	C	1.03	0/1008	1.16	0/1366
All	All	0.97	0/14148	1.14	8/19200 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	125	ASP	CA-CB-CG	6.65	119.25	112.60
1	H	397	ILE	N-CA-C	-5.86	106.10	111.67
1	E	397	ILE	N-CA-C	-5.77	106.19	111.67
1	G	397	ILE	N-CA-C	-5.61	106.34	111.67
1	F	397	ILE	N-CA-C	-5.58	106.36	111.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3004	0	2856	4	0
1	F	3004	0	2856	4	0
1	G	3004	0	2856	5	0
1	H	3004	0	2856	3	0
2	B	834	0	810	0	0
3	C	986	0	950	1	0
4	1	28	0	25	0	0
4	2	28	0	25	0	0
4	4	28	0	25	0	0
4	5	28	0	25	0	0
4	6	28	0	25	0	0
4	7	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	e	28	0	25	1	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
4	i	28	0	25	0	0
4	j	28	0	25	0	0
4	l	28	0	25	0	0
4	m	28	0	25	0	0
4	n	28	0	25	0	0
4	o	28	0	25	0	0
4	q	28	0	25	0	0
4	r	28	0	25	0	0
4	t	28	0	25	0	0
4	u	28	0	25	1	0
4	v	28	0	25	0	0
4	w	28	0	25	0	0
5	3	94	0	79	0	0
5	c	94	0	79	0	0
5	k	94	0	79	0	0
5	s	94	0	79	0	0
6	d	38	0	34	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
All	All	14899	0	14109	13	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 0.

The worst 5 of 13 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:G:112:GLY:HA3	1:H:169:LEU:HD11	1.83	0.59
1:E:244:GLY:HA3	4:e:1:NAG:H82	1.84	0.59
1:F:169:LEU:HD11	1:H:112:GLY:HA3	1.89	0.54
1:E:112:GLY:HA3	1:G:169:LEU:HD11	1.94	0.50
1:G:295:TRP:CE3	4:u:1:NAG:H81	2.47	0.49

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	386/492 (78%)	371 (96%)	14 (4%)	1 (0%)	36	46
1	F	386/492 (78%)	372 (96%)	13 (3%)	1 (0%)	36	46
1	G	386/492 (78%)	369 (96%)	16 (4%)	1 (0%)	36	46
1	H	386/492 (78%)	372 (96%)	13 (3%)	1 (0%)	36	46
2	B	107/215 (50%)	103 (96%)	4 (4%)	0	100	100
3	C	127/231 (55%)	127 (100%)	0	0	100	100
All	All	1778/2414 (74%)	1714 (96%)	60 (3%)	4 (0%)	44	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	222	ILE
1	G	222	ILE
1	F	222	ILE
1	H	222	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	338/430 (79%)	338 (100%)	0	100	100
1	F	338/430 (79%)	338 (100%)	0	100	100
1	G	338/430 (79%)	338 (100%)	0	100	100
1	H	338/430 (79%)	338 (100%)	0	100	100
2	B	91/186 (49%)	91 (100%)	0	100	100
3	C	105/194 (54%)	104 (99%)	1 (1%)	68	82
All	All	1548/2100 (74%)	1547 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	46	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	65	GLN
1	F	104	ASN
1	H	342	ASN
1	F	342	ASN
1	G	393	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

81 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	$\# Z > 2$
4	NAG	1	1	4,1	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
4	NAG	1	2	4	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
4	NAG	2	1	4,1	14,14,15	0.55	0	17,19,21	0.83	0
4	NAG	2	2	4	14,14,15	0.60	0	17,19,21	0.96	1 (5%)
5	NAG	3	1	5,1	14,14,15	0.52	0	17,19,21	1.06	1 (5%)
5	NAG	3	2	5	14,14,15	0.63	0	17,19,21	1.44	2 (11%)
5	BMA	3	3	5	11,11,12	0.50	0	15,15,17	0.73	1 (6%)
5	MAN	3	4	5	11,11,12	0.67	0	15,15,17	1.18	1 (6%)
5	MAN	3	5	5	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
5	MAN	3	6	5	11,11,12	0.54	0	15,15,17	0.77	0
5	MAN	3	7	5	11,11,12	0.65	0	15,15,17	0.99	1 (6%)
5	MAN	3	8	5	11,11,12	0.59	0	15,15,17	0.72	0
4	NAG	4	1	4,1	14,14,15	0.56	0	17,19,21	0.97	1 (5%)
4	NAG	4	2	4	14,14,15	0.65	0	17,19,21	0.97	1 (5%)
4	NAG	5	1	4,1	14,14,15	0.69	0	17,19,21	1.93	3 (17%)
4	NAG	5	2	4	14,14,15	0.65	0	17,19,21	0.81	1 (5%)
4	NAG	6	1	4,1	14,14,15	0.53	0	17,19,21	0.81	1 (5%)
4	NAG	6	2	4	14,14,15	0.55	0	17,19,21	0.92	0
4	NAG	7	1	4,1	14,14,15	0.53	0	17,19,21	0.76	0
4	NAG	7	2	4	14,14,15	0.71	0	17,19,21	0.99	1 (5%)
4	NAG	a	1	4,1	14,14,15	0.40	0	17,19,21	0.74	0
4	NAG	a	2	4	14,14,15	0.59	0	17,19,21	0.85	1 (5%)
4	NAG	b	1	4,1	14,14,15	0.50	0	17,19,21	0.64	0
4	NAG	b	2	4	14,14,15	0.57	0	17,19,21	0.80	0
5	NAG	c	1	5,1	14,14,15	0.60	0	17,19,21	0.82	0
5	NAG	c	2	5	14,14,15	0.76	0	17,19,21	1.44	2 (11%)
5	BMA	c	3	5	11,11,12	0.43	0	15,15,17	0.65	0
5	MAN	c	4	5	11,11,12	0.48	0	15,15,17	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	c	5	5	11,11,12	0.54	0	15,15,17	1.28	1 (6%)
5	MAN	c	6	5	11,11,12	0.62	0	15,15,17	0.72	0
5	MAN	c	7	5	11,11,12	0.78	0	15,15,17	1.27	2 (13%)
5	MAN	c	8	5	11,11,12	0.66	0	15,15,17	0.86	1 (6%)
6	NAG	d	1	6,1	14,14,15	0.51	0	17,19,21	1.19	1 (5%)
6	NAG	d	2	6	14,14,15	0.61	0	17,19,21	0.76	1 (5%)
6	FUC	d	3	6	10,10,11	0.85	0	14,14,16	0.72	0
4	NAG	e	1	4,1	14,14,15	0.68	0	17,19,21	1.30	1 (5%)
4	NAG	e	2	4	14,14,15	0.81	0	17,19,21	1.07	1 (5%)
4	NAG	f	1	4,1	14,14,15	0.57	0	17,19,21	1.21	1 (5%)
4	NAG	f	2	4	14,14,15	0.49	0	17,19,21	0.94	2 (11%)
4	NAG	g	1	4,1	14,14,15	0.51	0	17,19,21	0.72	0
4	NAG	g	2	4	14,14,15	0.65	0	17,19,21	0.84	1 (5%)
4	NAG	i	1	4,1	14,14,15	0.48	0	17,19,21	0.95	2 (11%)
4	NAG	i	2	4	14,14,15	0.75	0	17,19,21	0.98	2 (11%)
4	NAG	j	1	4,1	14,14,15	0.60	0	17,19,21	0.75	0
4	NAG	j	2	4	14,14,15	0.62	0	17,19,21	0.86	1 (5%)
5	NAG	k	1	5,1	14,14,15	0.53	0	17,19,21	1.03	0
5	NAG	k	2	5	14,14,15	0.72	0	17,19,21	1.35	1 (5%)
5	BMA	k	3	5	11,11,12	0.59	0	15,15,17	0.88	0
5	MAN	k	4	5	11,11,12	0.81	0	15,15,17	0.98	1 (6%)
5	MAN	k	5	5	11,11,12	0.50	0	15,15,17	1.01	1 (6%)
5	MAN	k	6	5	11,11,12	0.48	0	15,15,17	0.54	0
5	MAN	k	7	5	11,11,12	0.73	0	15,15,17	1.38	1 (6%)
5	MAN	k	8	5	11,11,12	0.65	0	15,15,17	0.97	1 (6%)
4	NAG	l	1	4,1	14,14,15	0.43	0	17,19,21	1.50	1 (5%)
4	NAG	l	2	4	14,14,15	0.55	0	17,19,21	0.72	1 (5%)
4	NAG	m	1	4,1	14,14,15	0.46	0	17,19,21	0.59	0
4	NAG	m	2	4	14,14,15	0.67	0	17,19,21	0.71	1 (5%)
4	NAG	n	1	4,1	14,14,15	0.51	0	17,19,21	0.87	1 (5%)
4	NAG	n	2	4	14,14,15	0.61	0	17,19,21	0.96	1 (5%)
4	NAG	o	1	4,1	14,14,15	0.46	0	17,19,21	0.73	1 (5%)
4	NAG	o	2	4	14,14,15	0.72	0	17,19,21	1.00	1 (5%)
4	NAG	q	1	4,1	14,14,15	0.49	0	17,19,21	1.05	1 (5%)
4	NAG	q	2	4	14,14,15	0.82	0	17,19,21	0.94	1 (5%)
4	NAG	r	1	4,1	14,14,15	0.57	0	17,19,21	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	r	2	4	14,14,15	0.55	0	17,19,21	0.90	1 (5%)
5	NAG	s	1	5,1	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
5	NAG	s	2	5	14,14,15	0.74	0	17,19,21	1.53	2 (11%)
5	BMA	s	3	5	11,11,12	0.48	0	15,15,17	0.78	0
5	MAN	s	4	5	11,11,12	0.55	0	15,15,17	1.18	2 (13%)
5	MAN	s	5	5	11,11,12	0.50	0	15,15,17	1.26	1 (6%)
5	MAN	s	6	5	11,11,12	0.62	0	15,15,17	0.79	0
5	MAN	s	7	5	11,11,12	0.67	0	15,15,17	1.04	1 (6%)
5	MAN	s	8	5	11,11,12	0.58	0	15,15,17	0.87	1 (6%)
4	NAG	t	1	4,1	14,14,15	0.53	0	17,19,21	1.54	1 (5%)
4	NAG	t	2	4	14,14,15	0.64	0	17,19,21	0.86	1 (5%)
4	NAG	u	1	4,1	14,14,15	0.43	0	17,19,21	0.76	1 (5%)
4	NAG	u	2	4	14,14,15	0.55	0	17,19,21	1.20	1 (5%)
4	NAG	v	1	4,1	14,14,15	0.62	0	17,19,21	1.15	1 (5%)
4	NAG	v	2	4	14,14,15	0.68	0	17,19,21	0.93	1 (5%)
4	NAG	w	1	4,1	14,14,15	0.61	0	17,19,21	0.91	1 (5%)
4	NAG	w	2	4	14,14,15	0.73	0	17,19,21	1.17	1 (5%)

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

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

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

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

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	t	1	NAG	C1-O5-C5	5.99	120.21	112.19
4	l	1	NAG	C1-O5-C5	5.42	119.44	112.19
4	5	1	NAG	C1-C2-N2	5.04	118.38	110.43
5	k	7	MAN	C1-O5-C5	4.86	118.70	112.19
4	5	1	NAG	C2-N2-C7	4.73	129.24	122.90

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5	1	NAG	C1-C2-N2-C7

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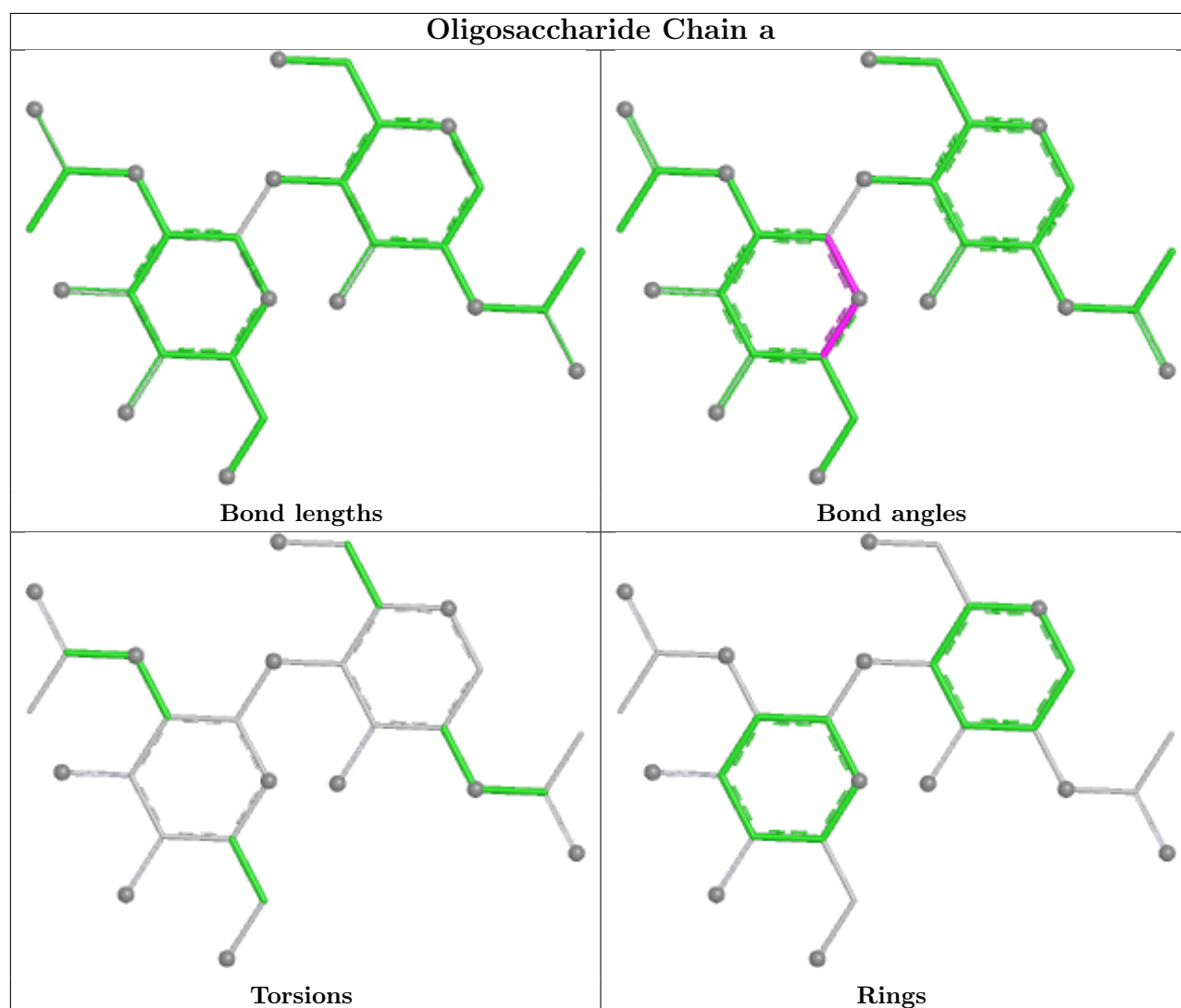
Mol	Chain	Res	Type	Atoms
5	k	2	NAG	O5-C5-C6-O6
5	s	2	NAG	O5-C5-C6-O6
5	3	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6

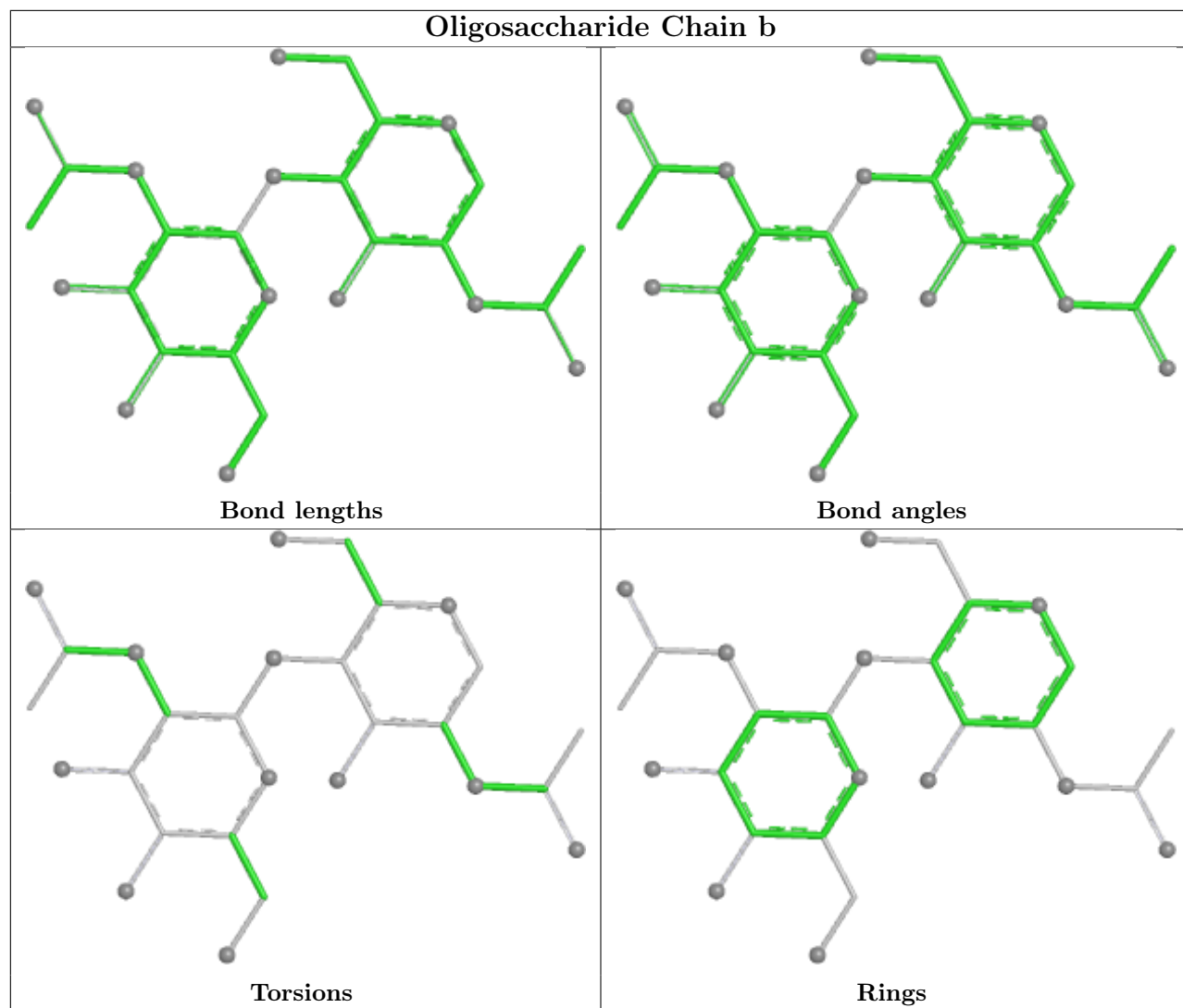
There are no ring outliers.

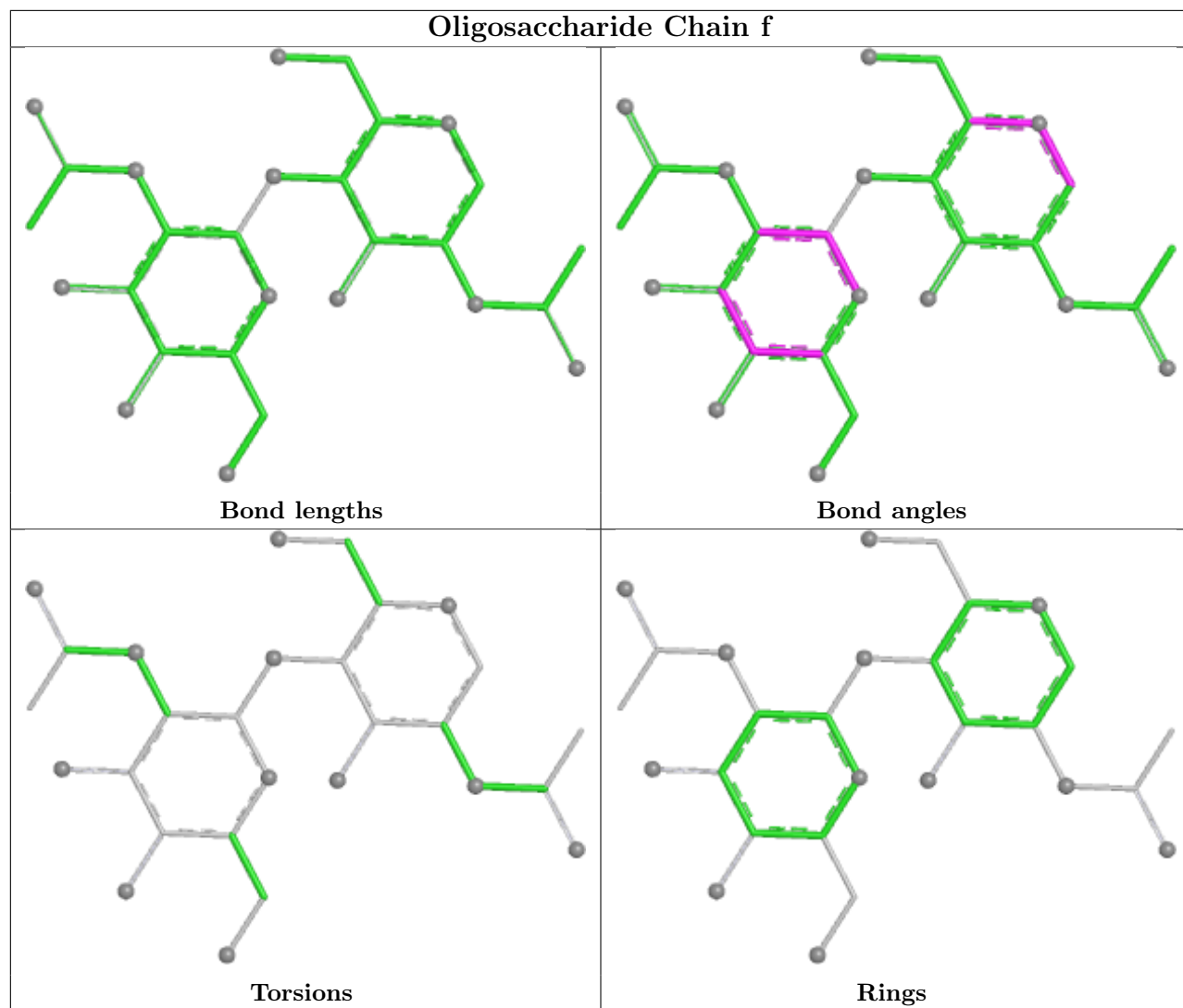
2 monomers are involved in 2 short contacts:

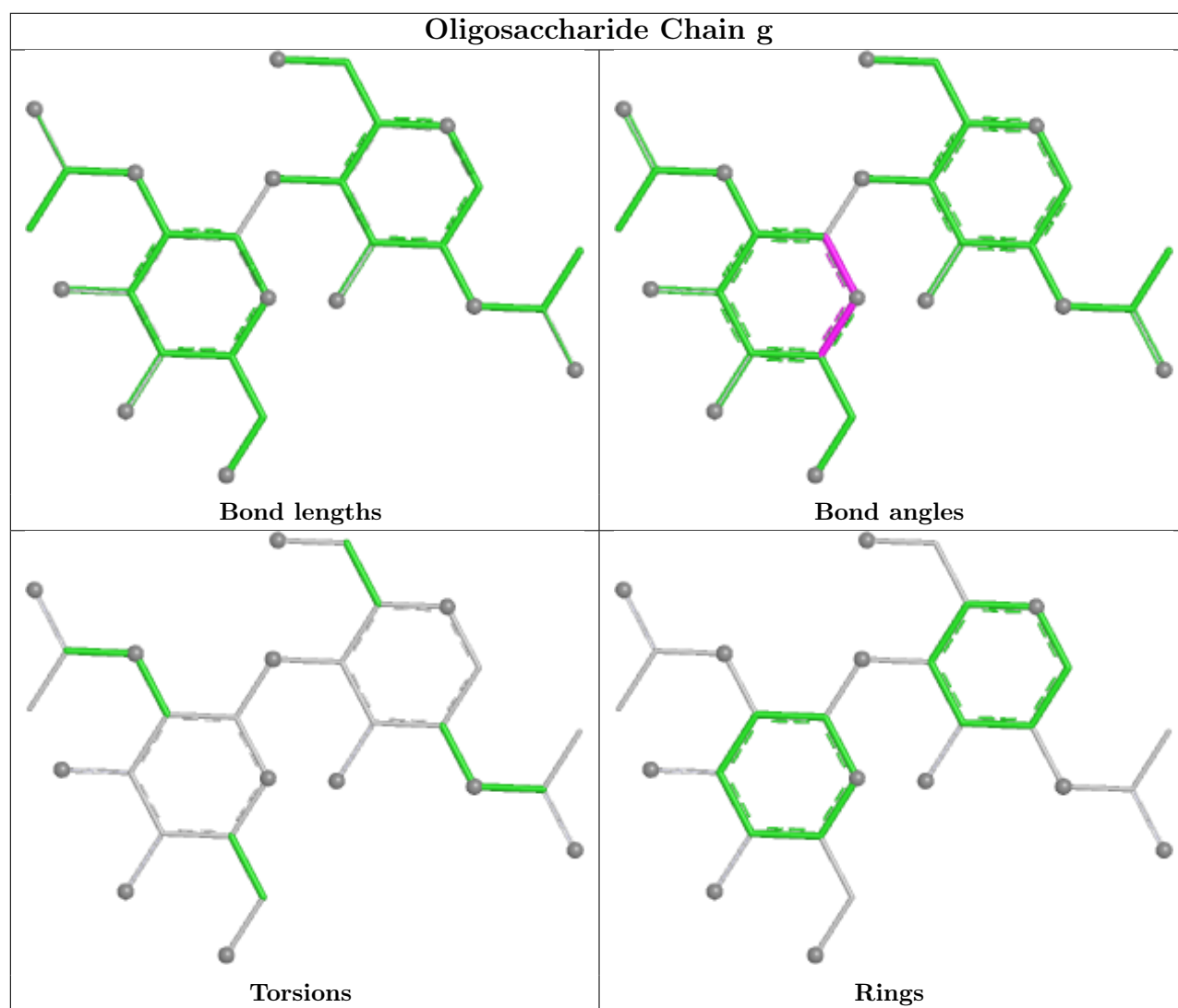
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	e	1	NAG	1	0
4	u	1	NAG	1	0

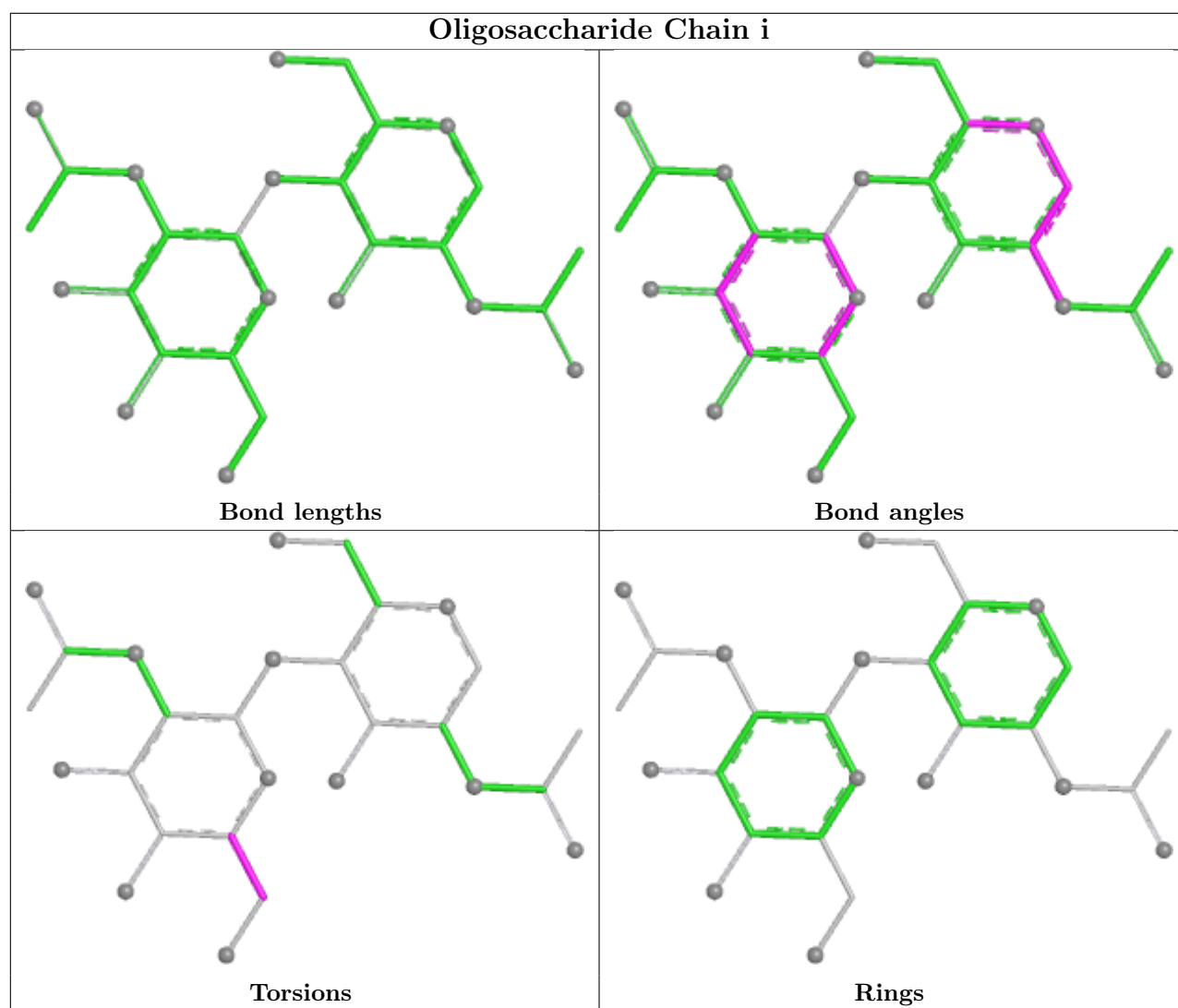
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

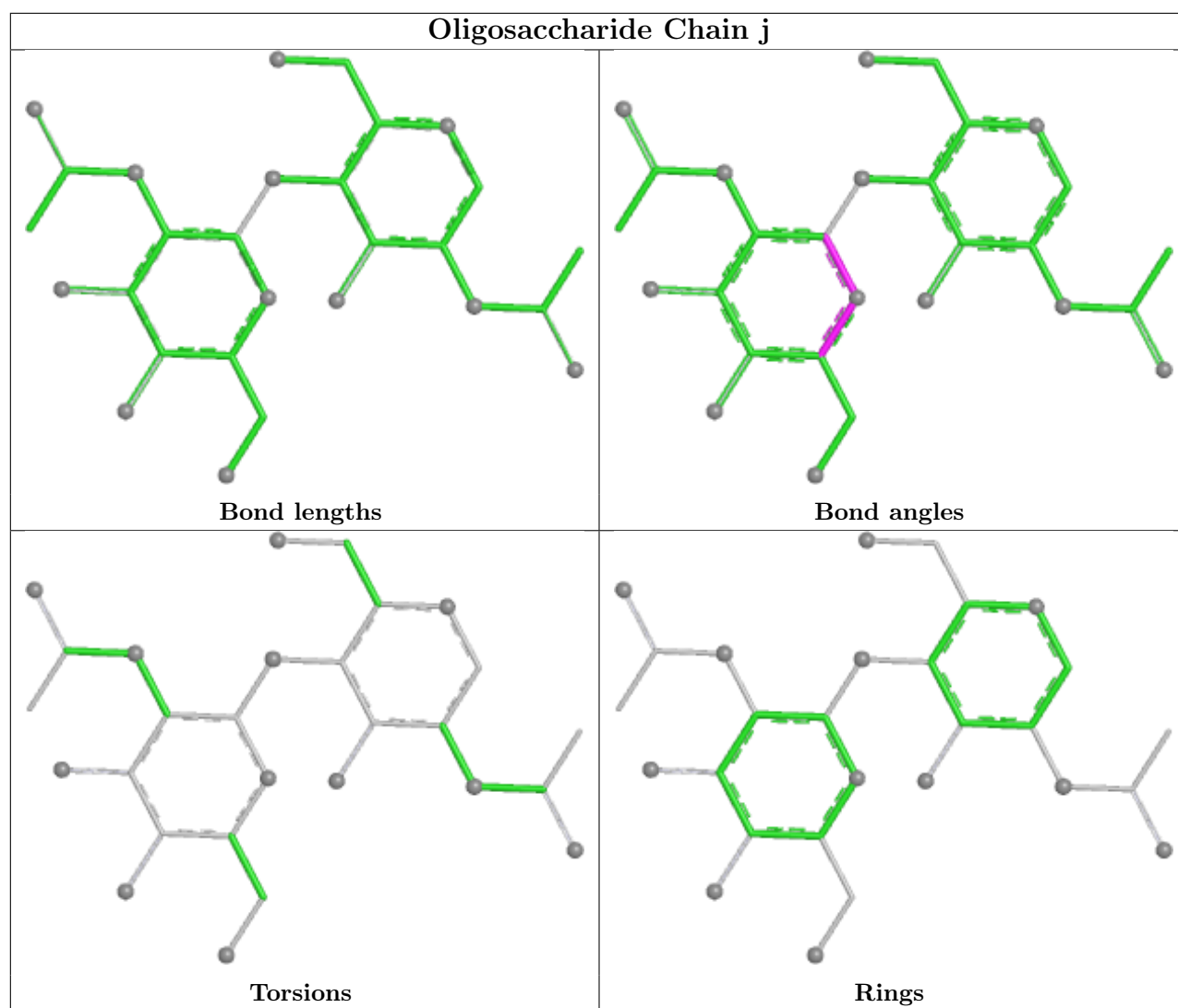


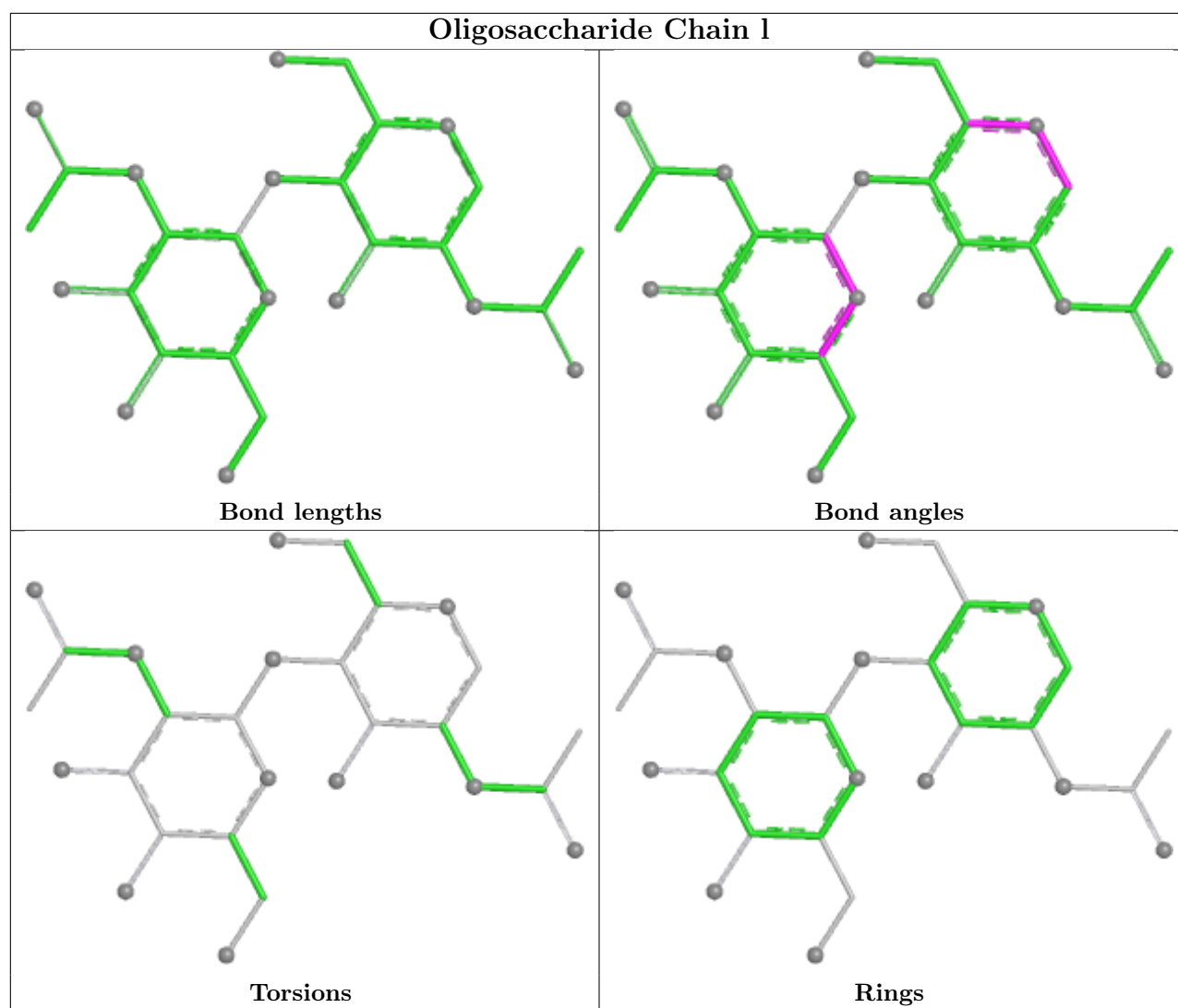


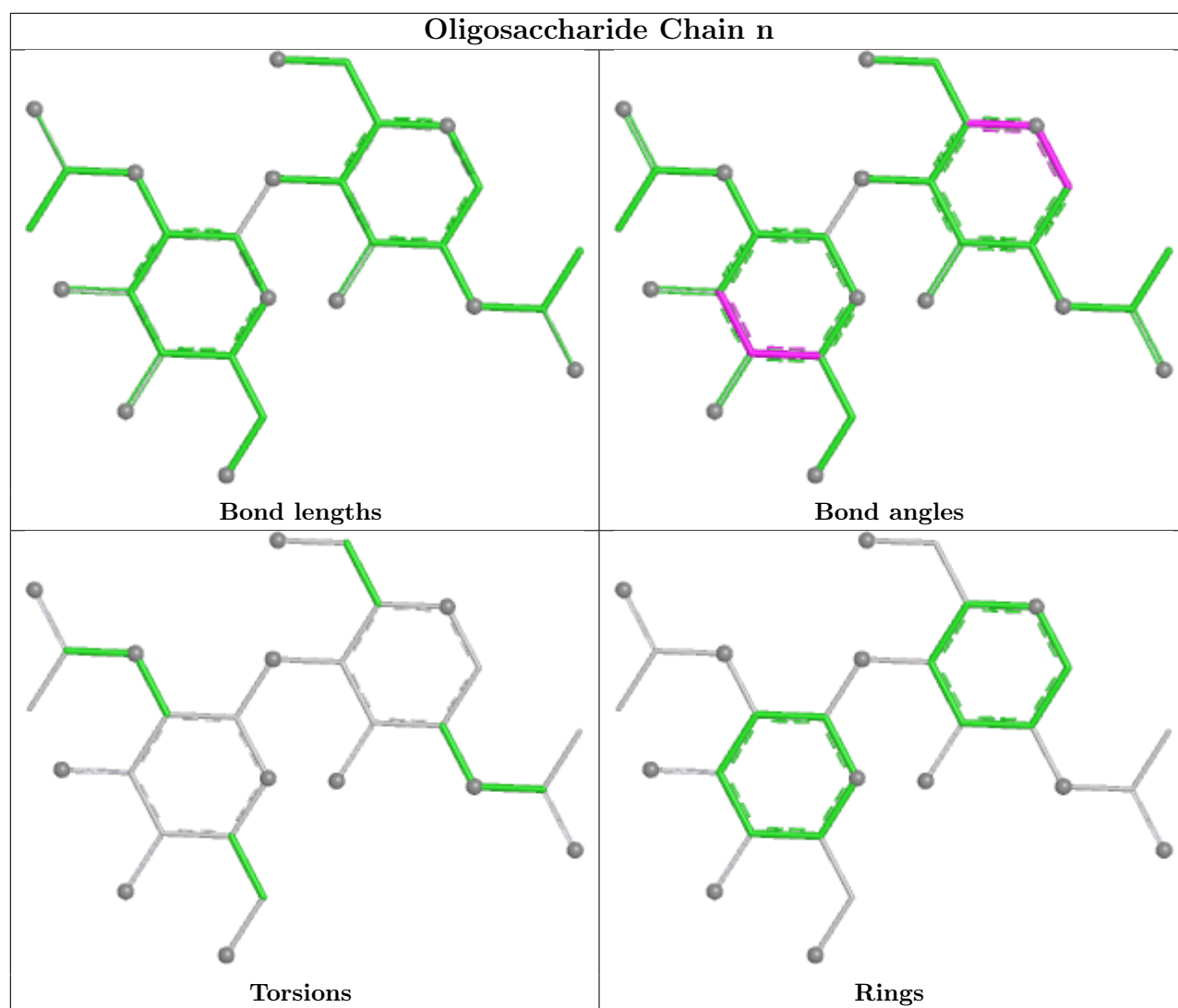


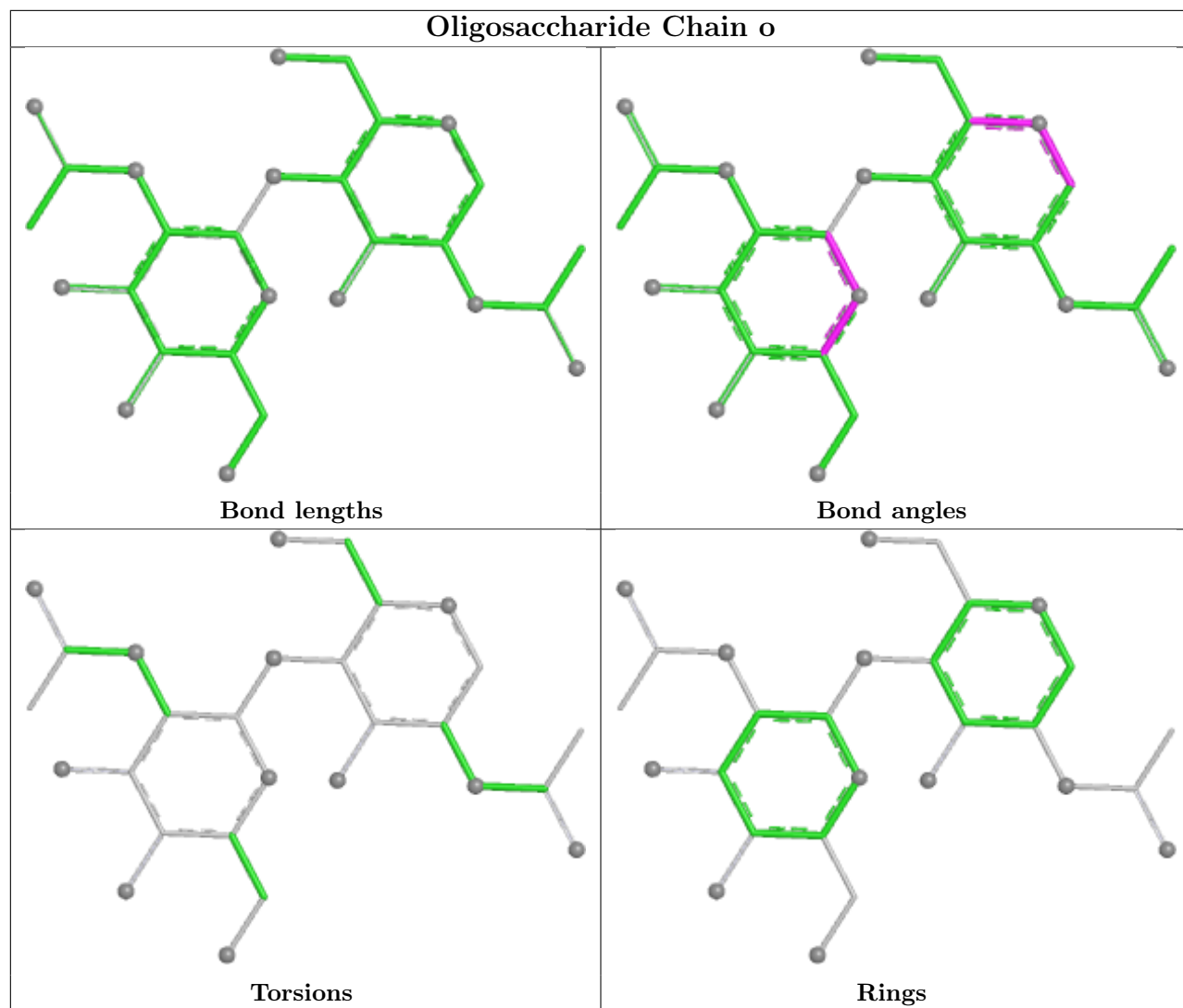


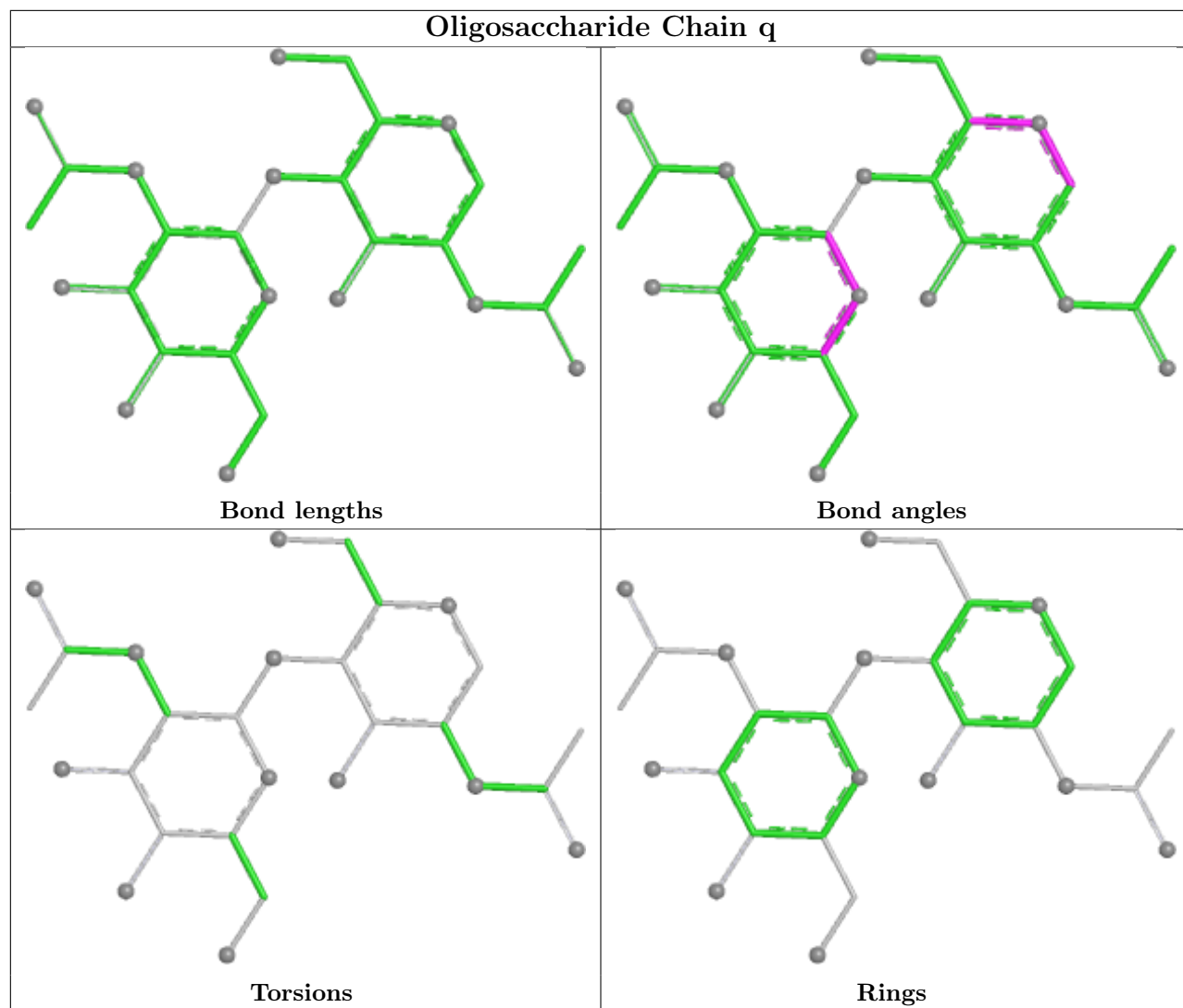


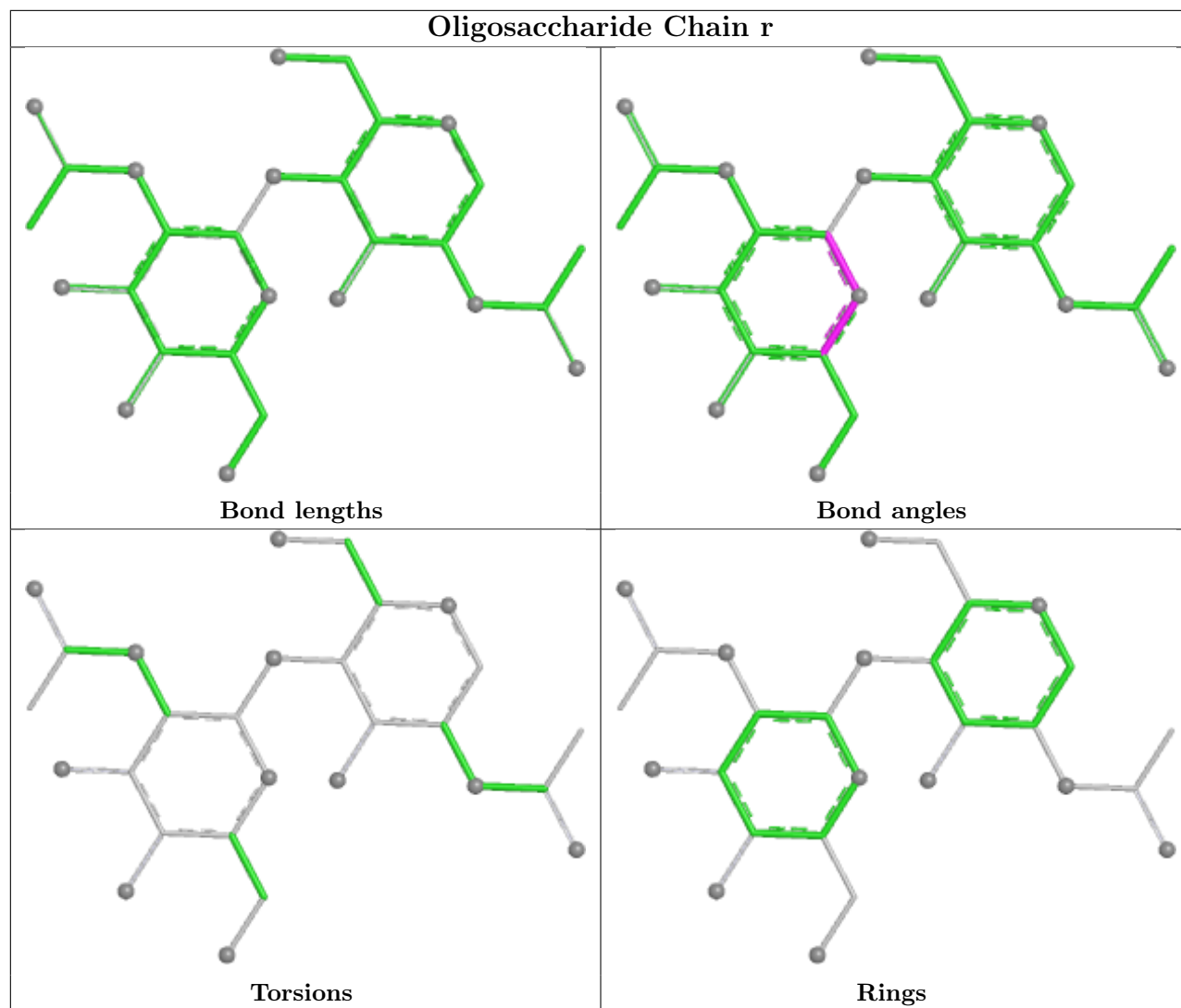


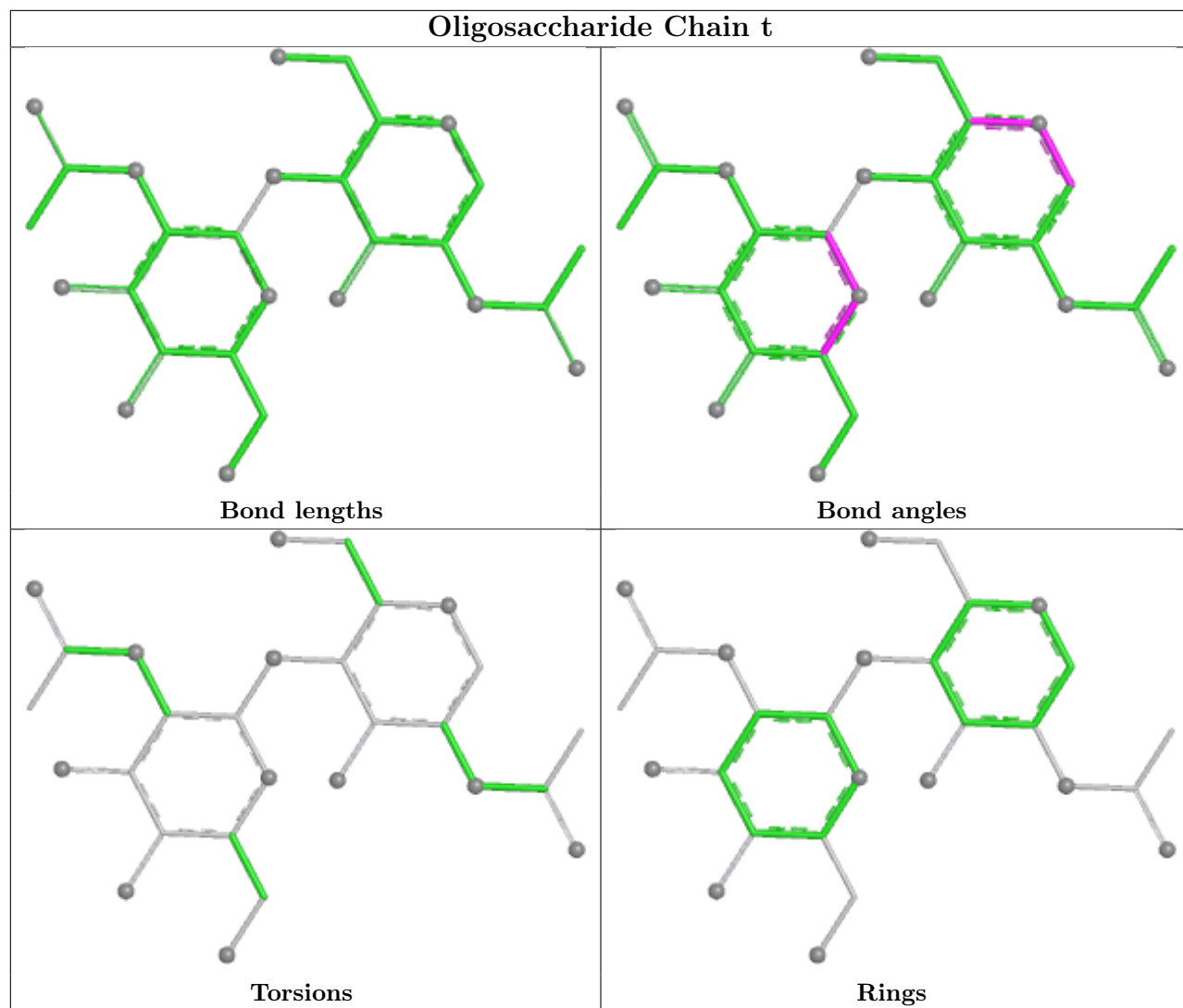


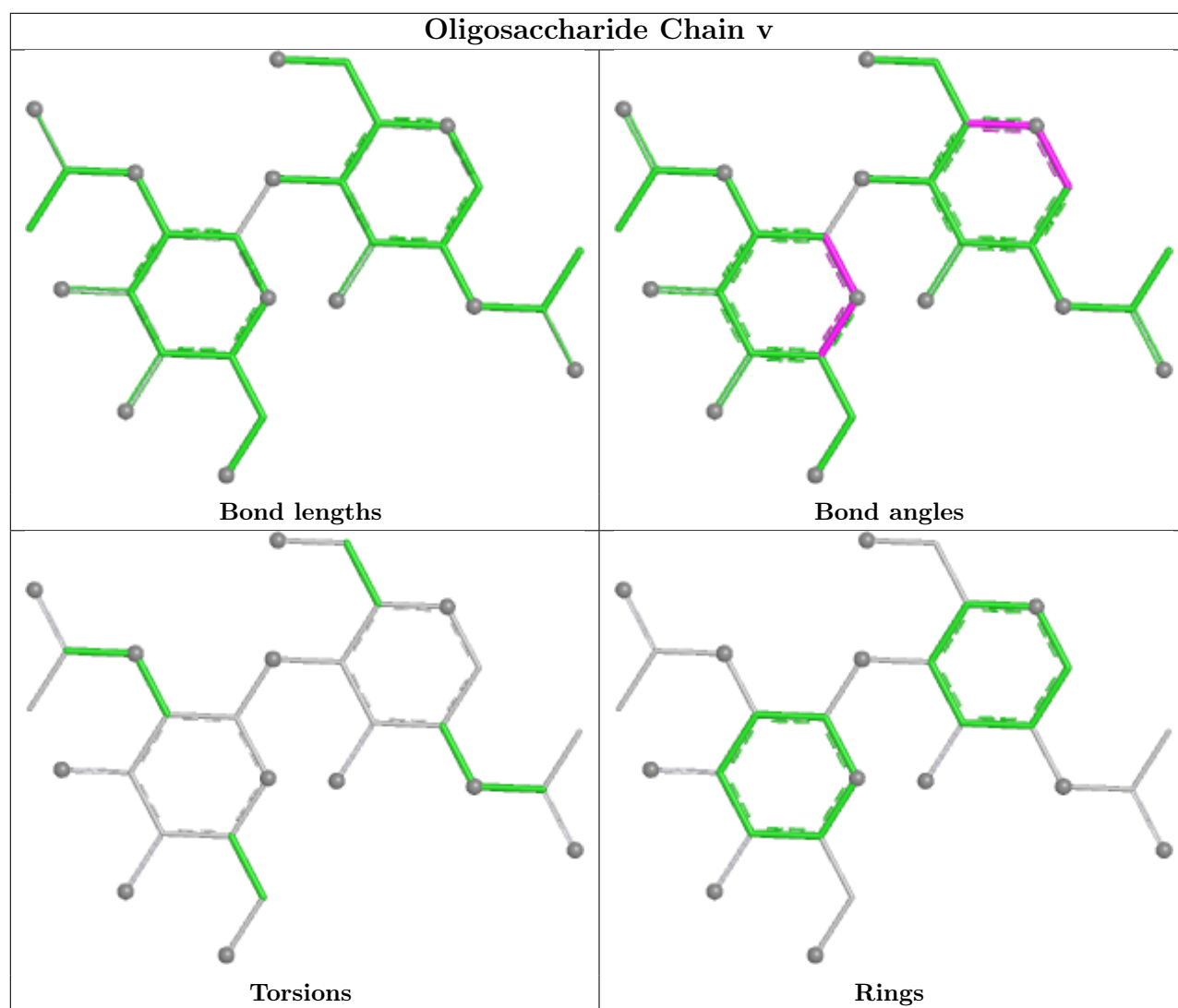


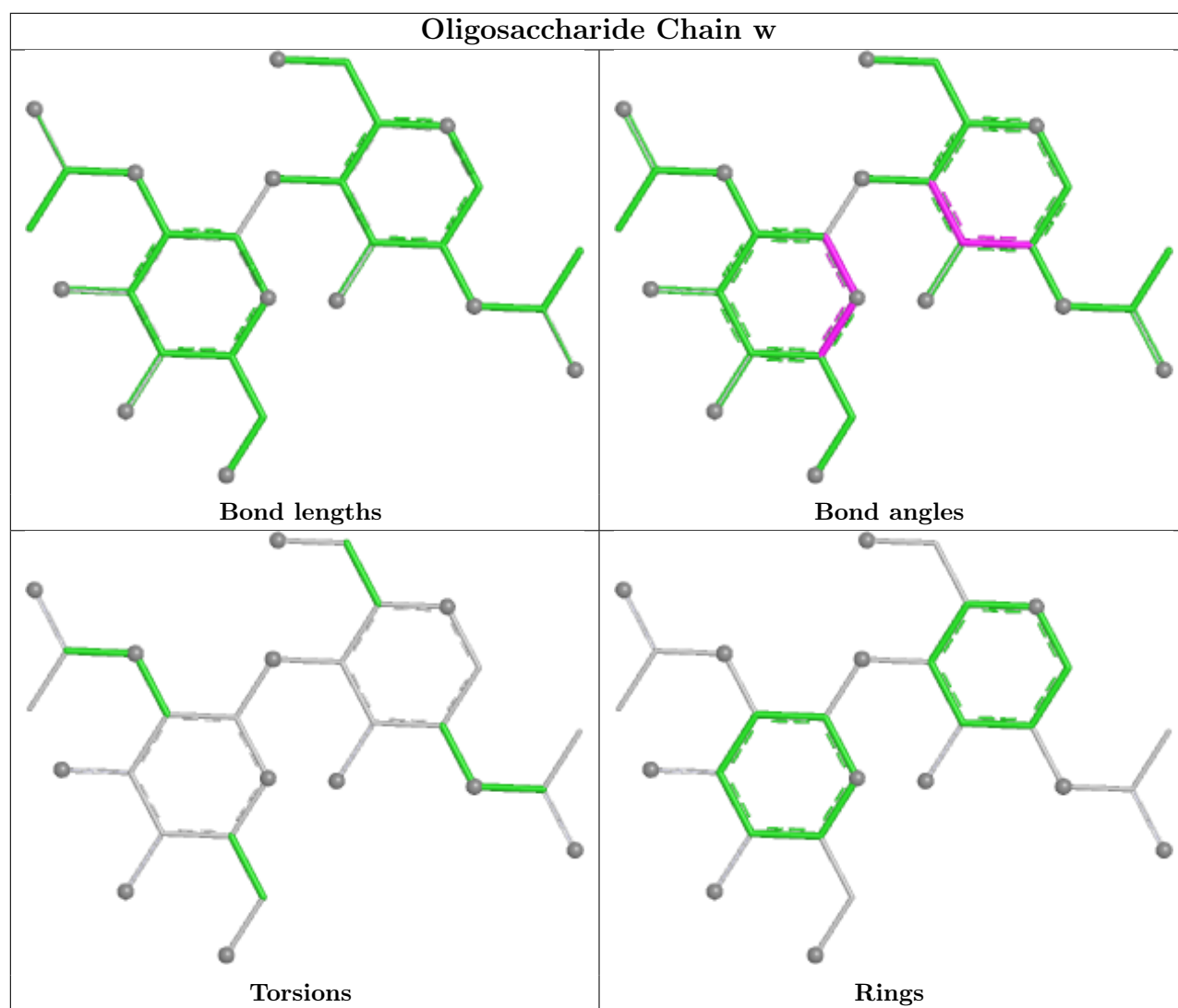


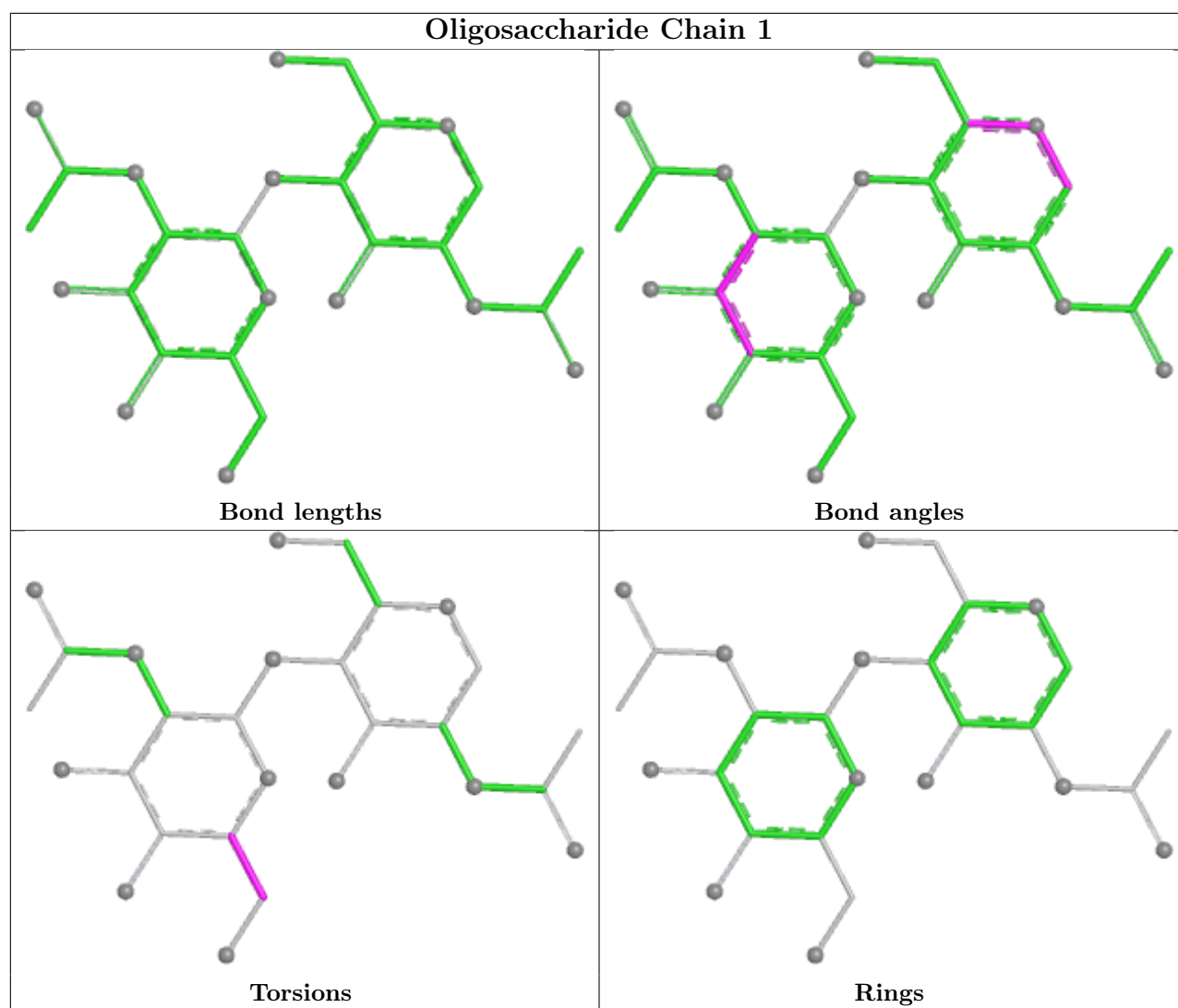


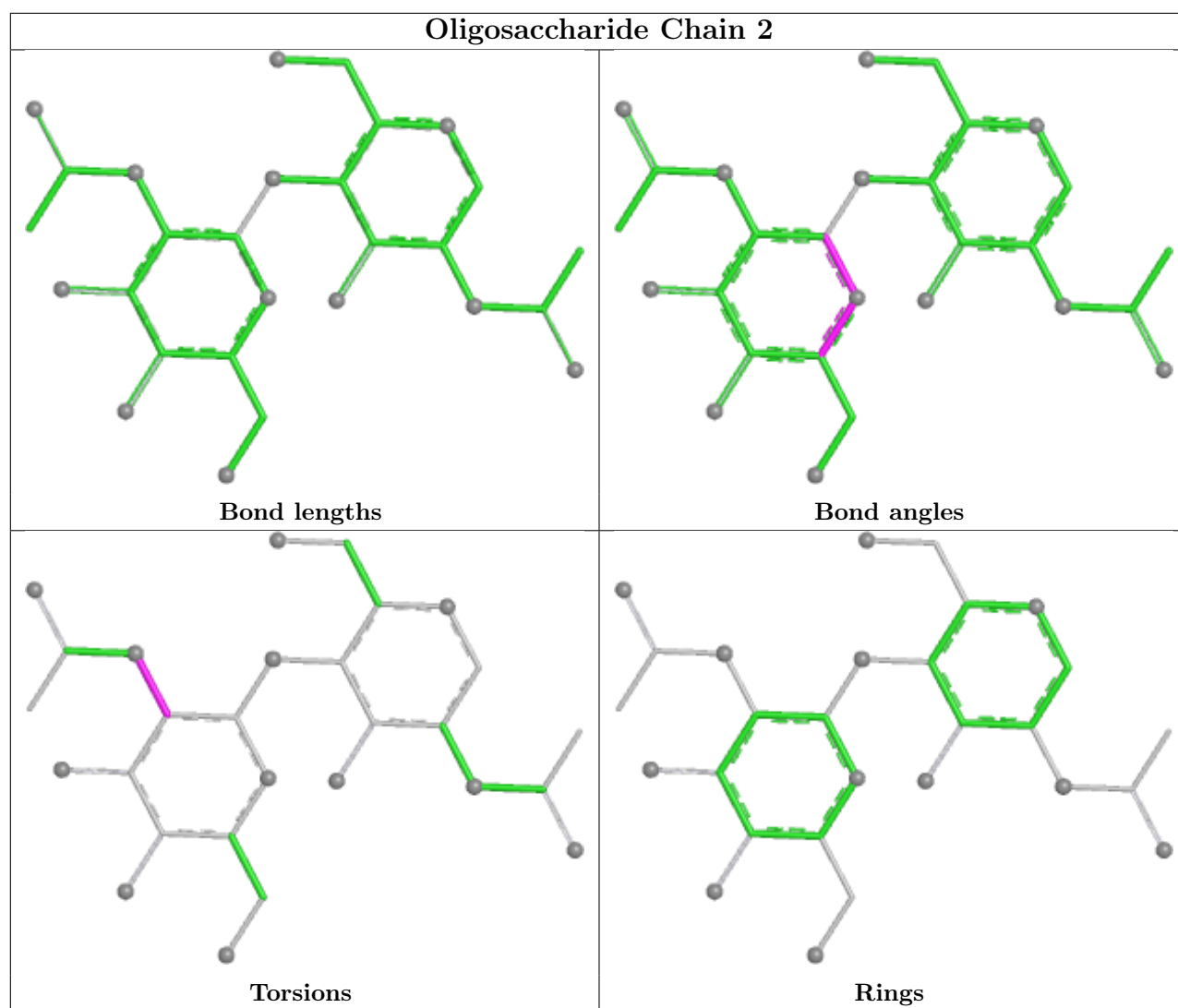


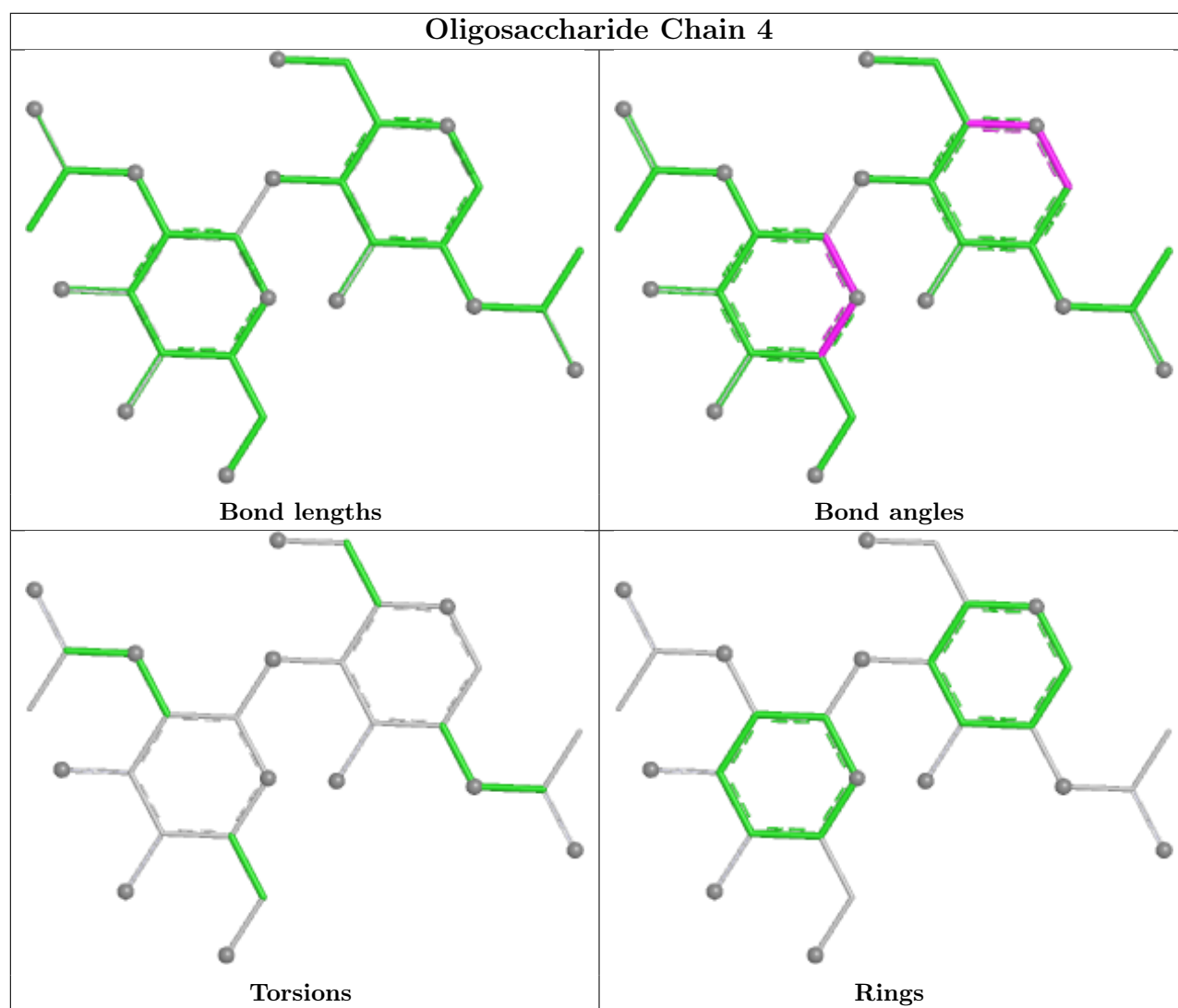


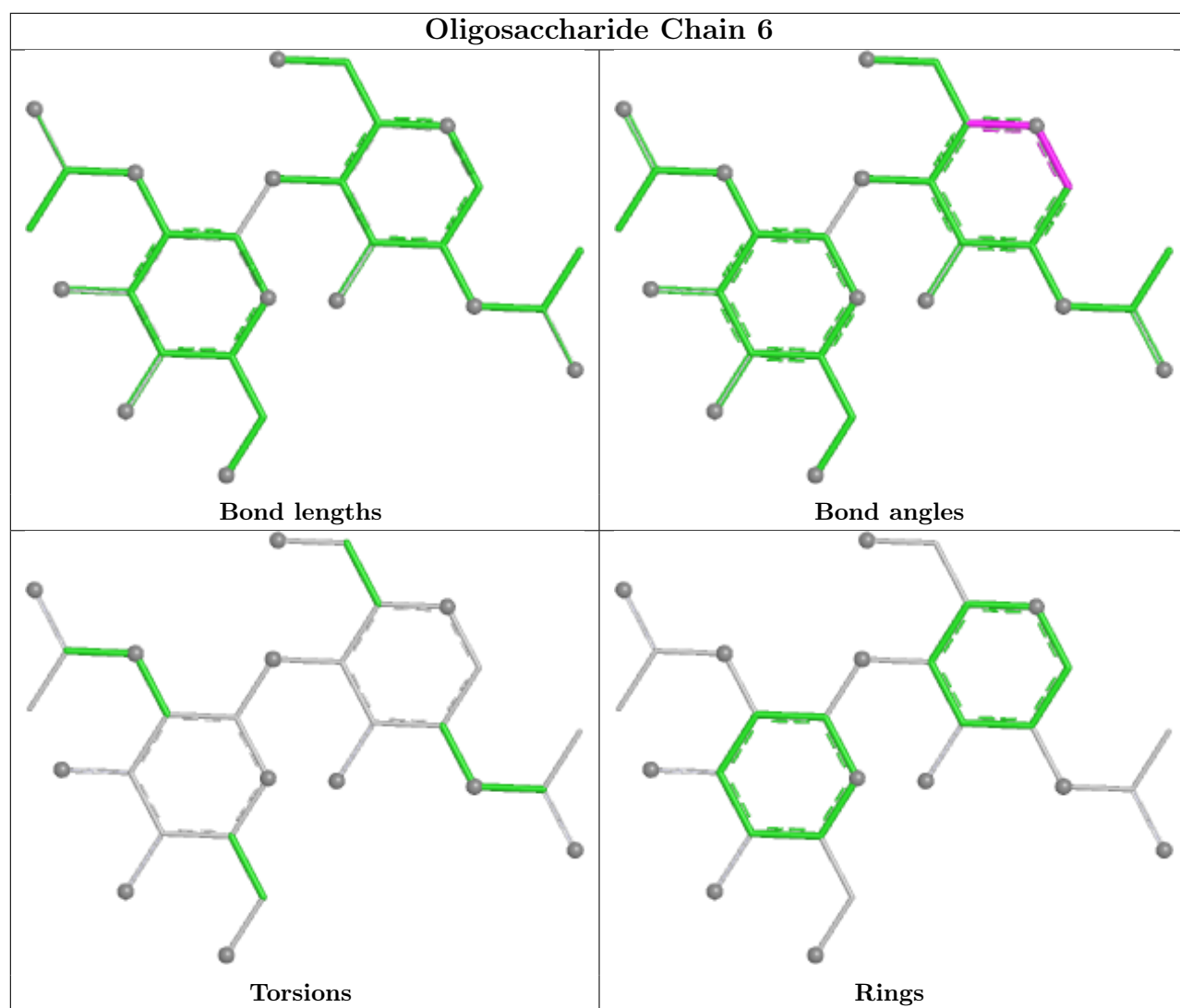


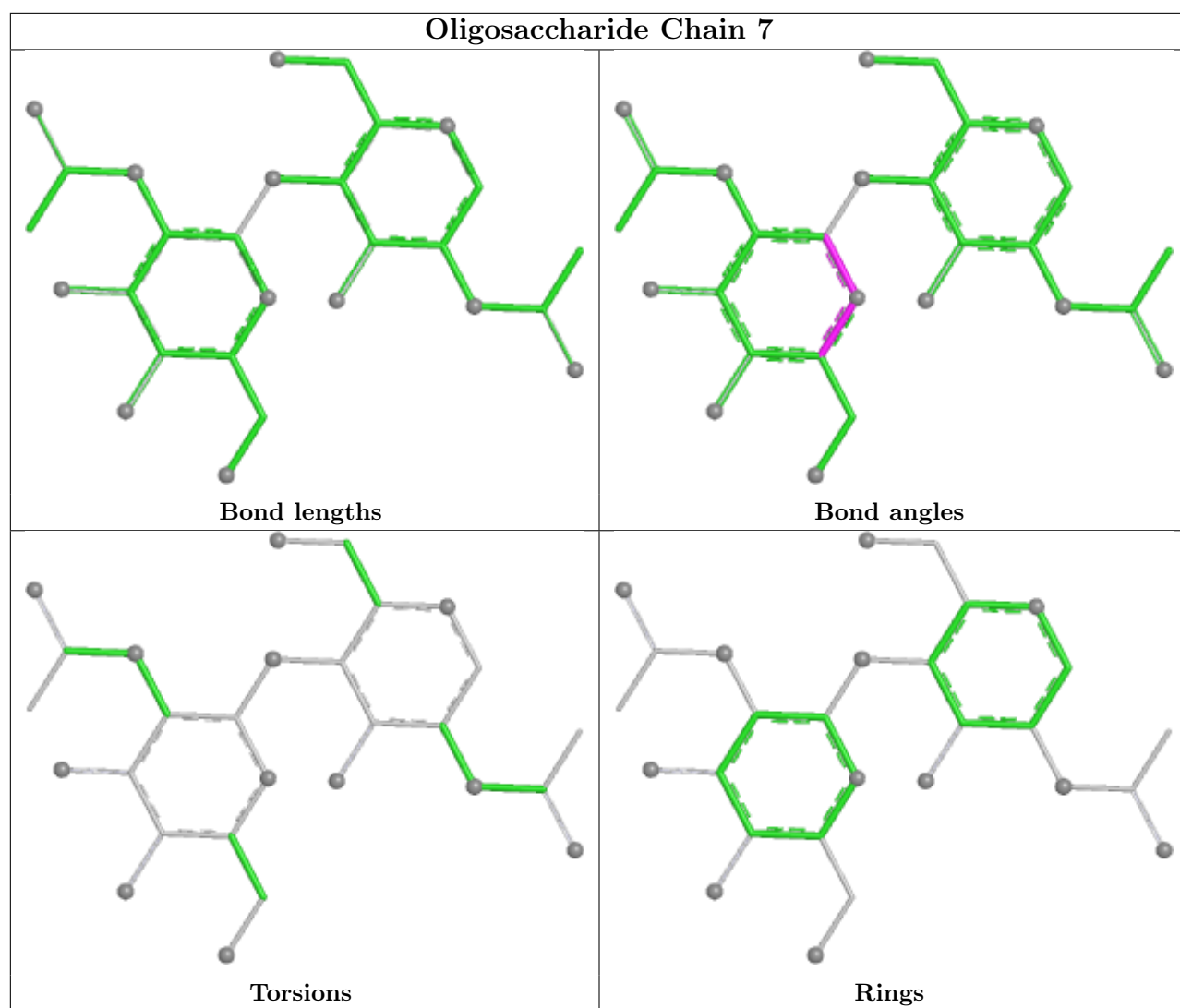


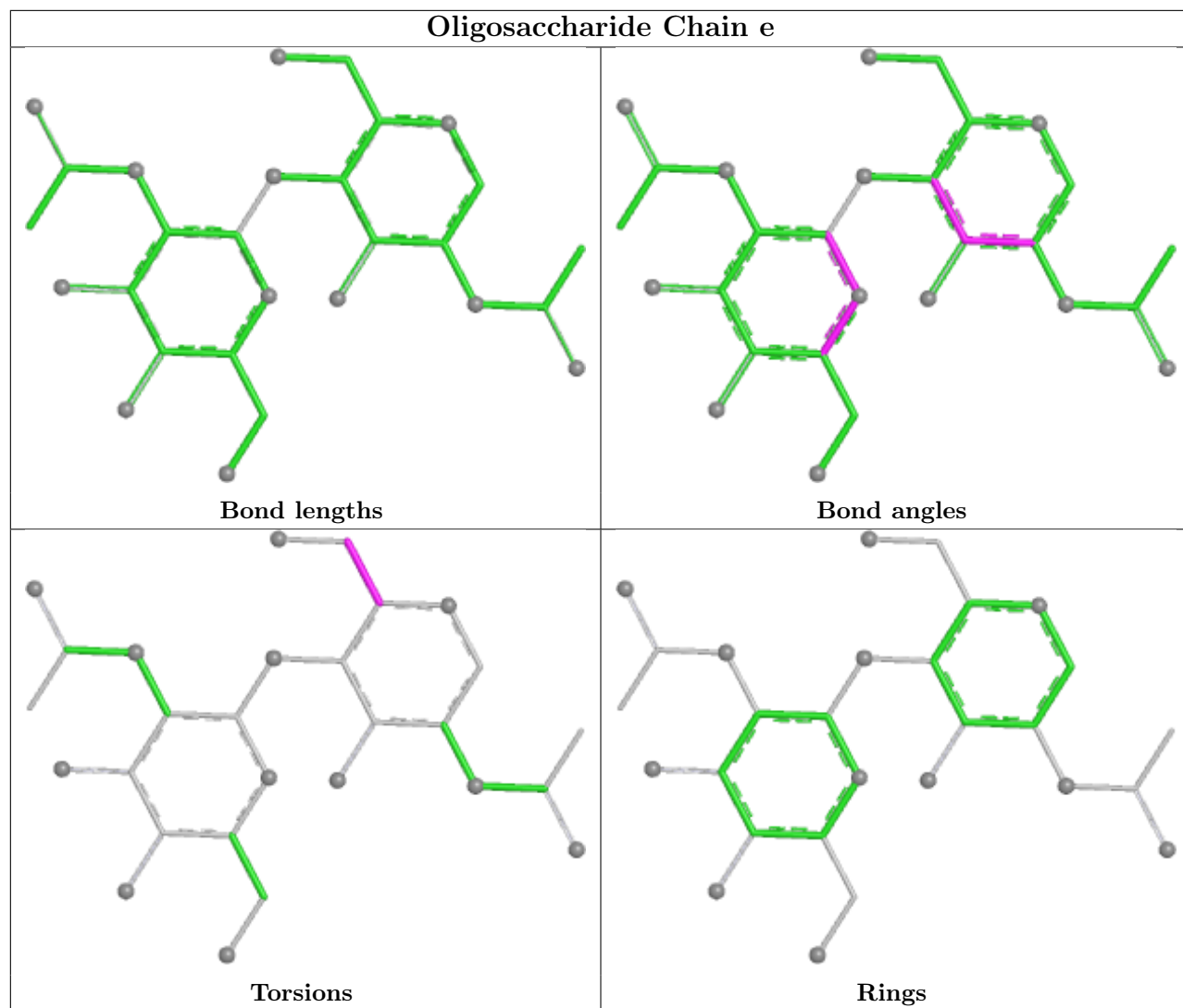


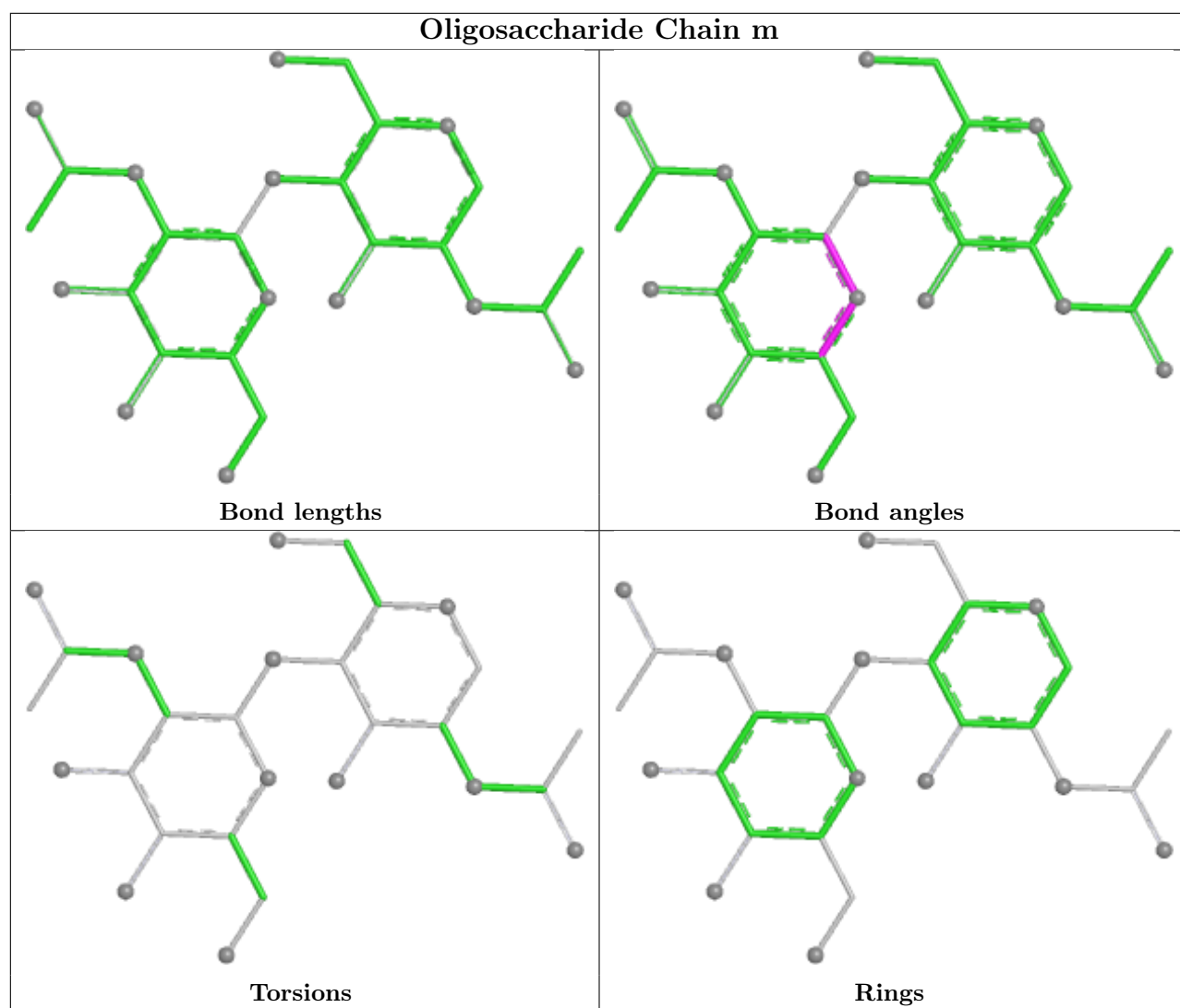


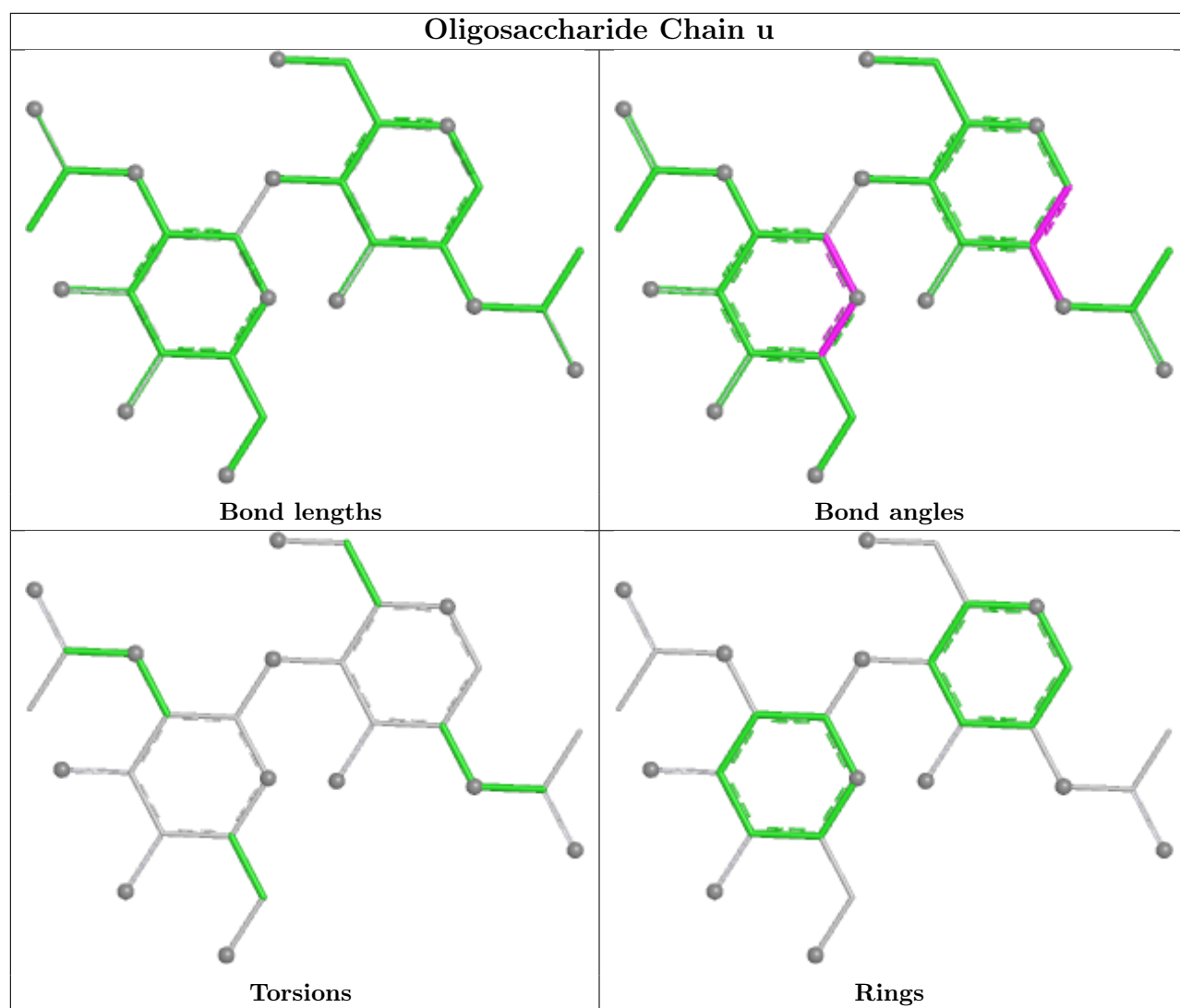


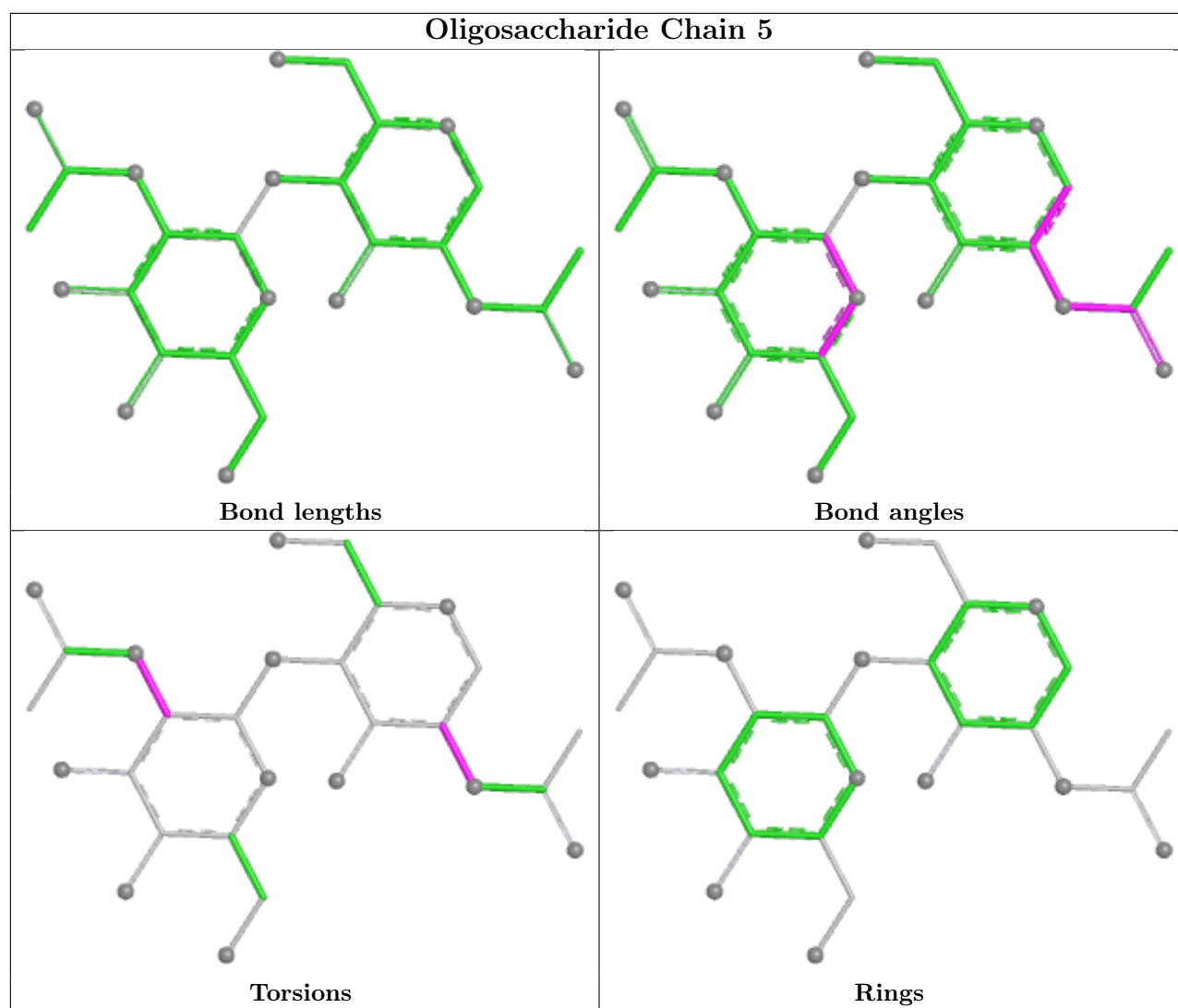


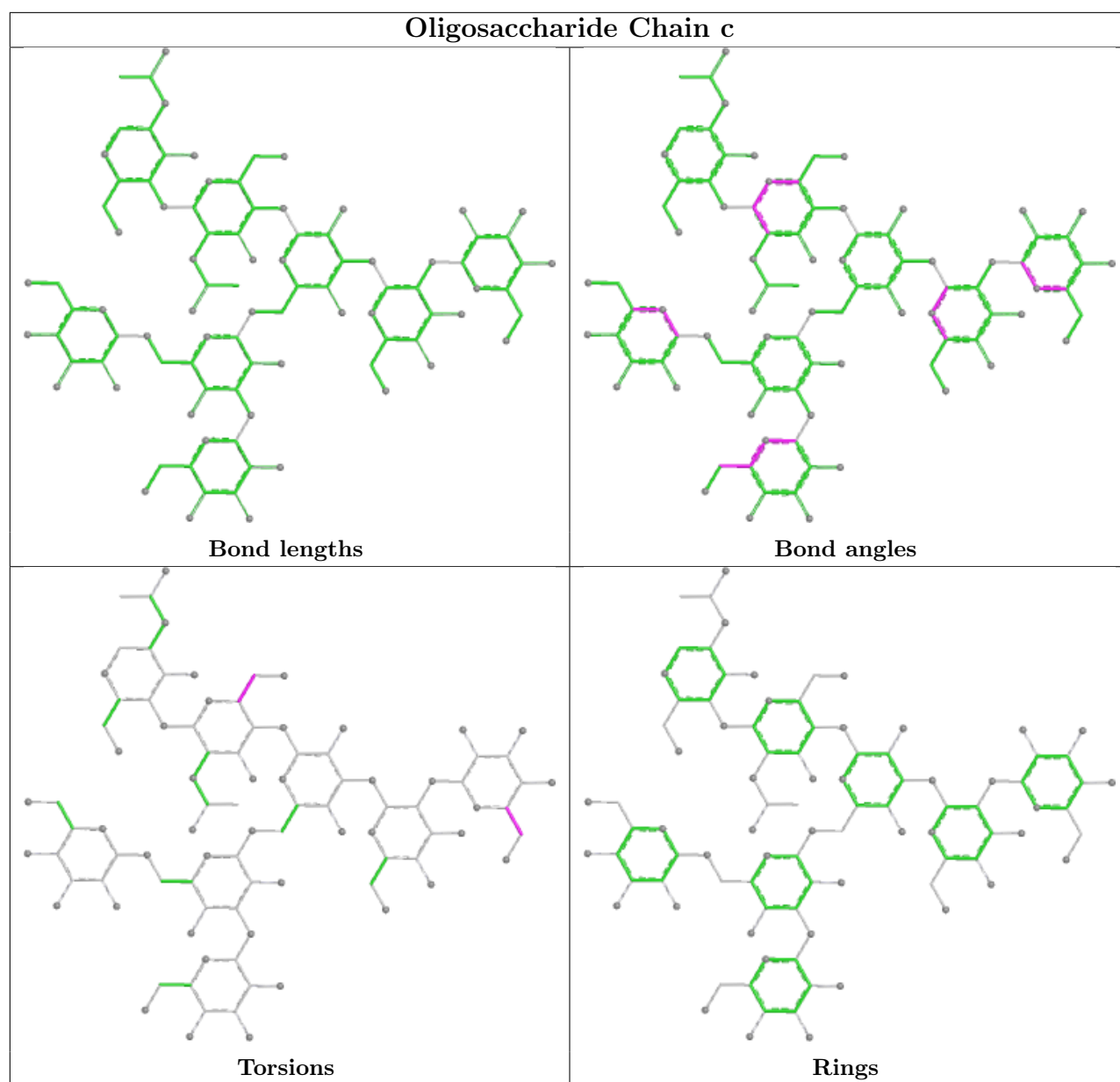


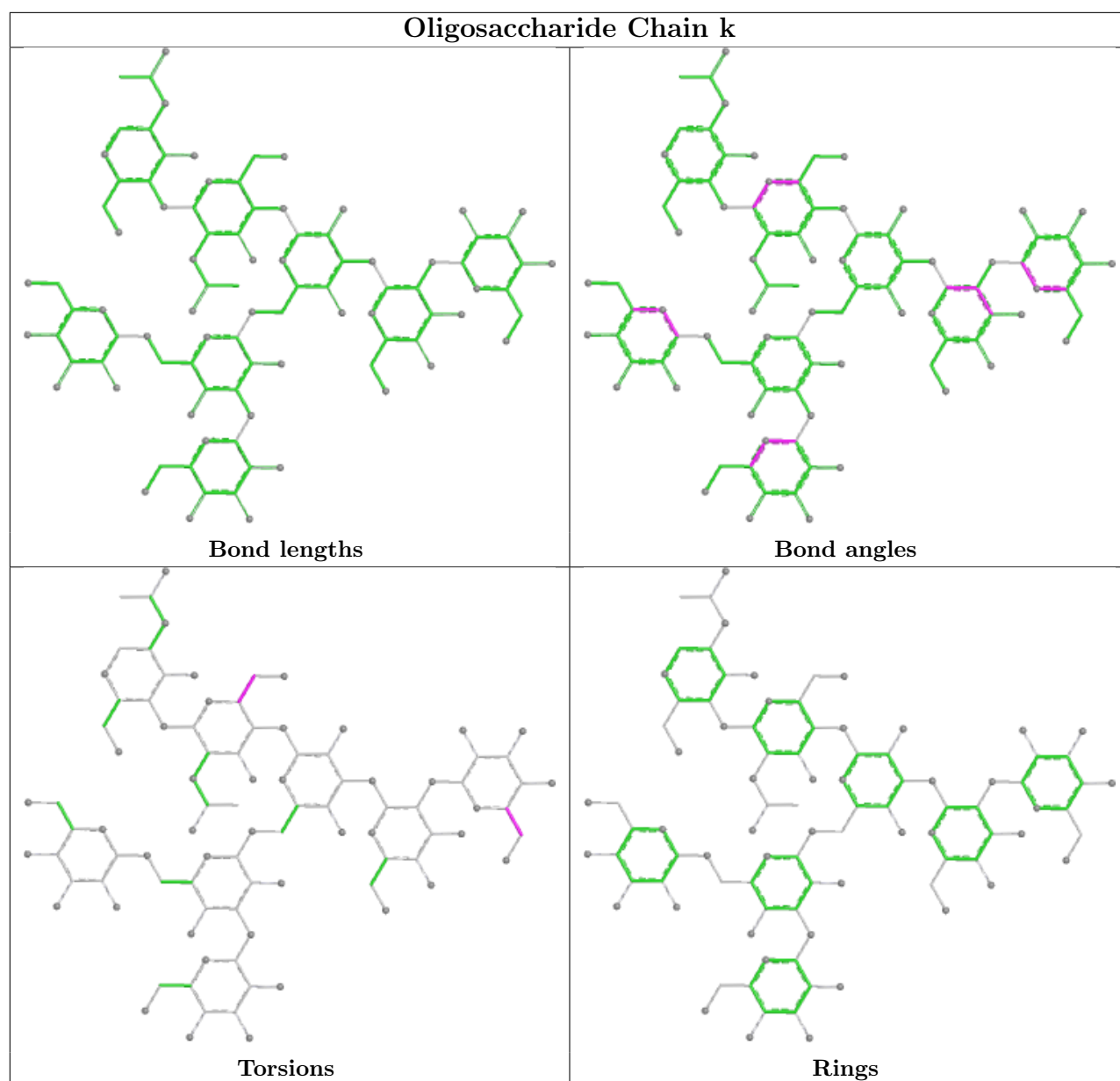


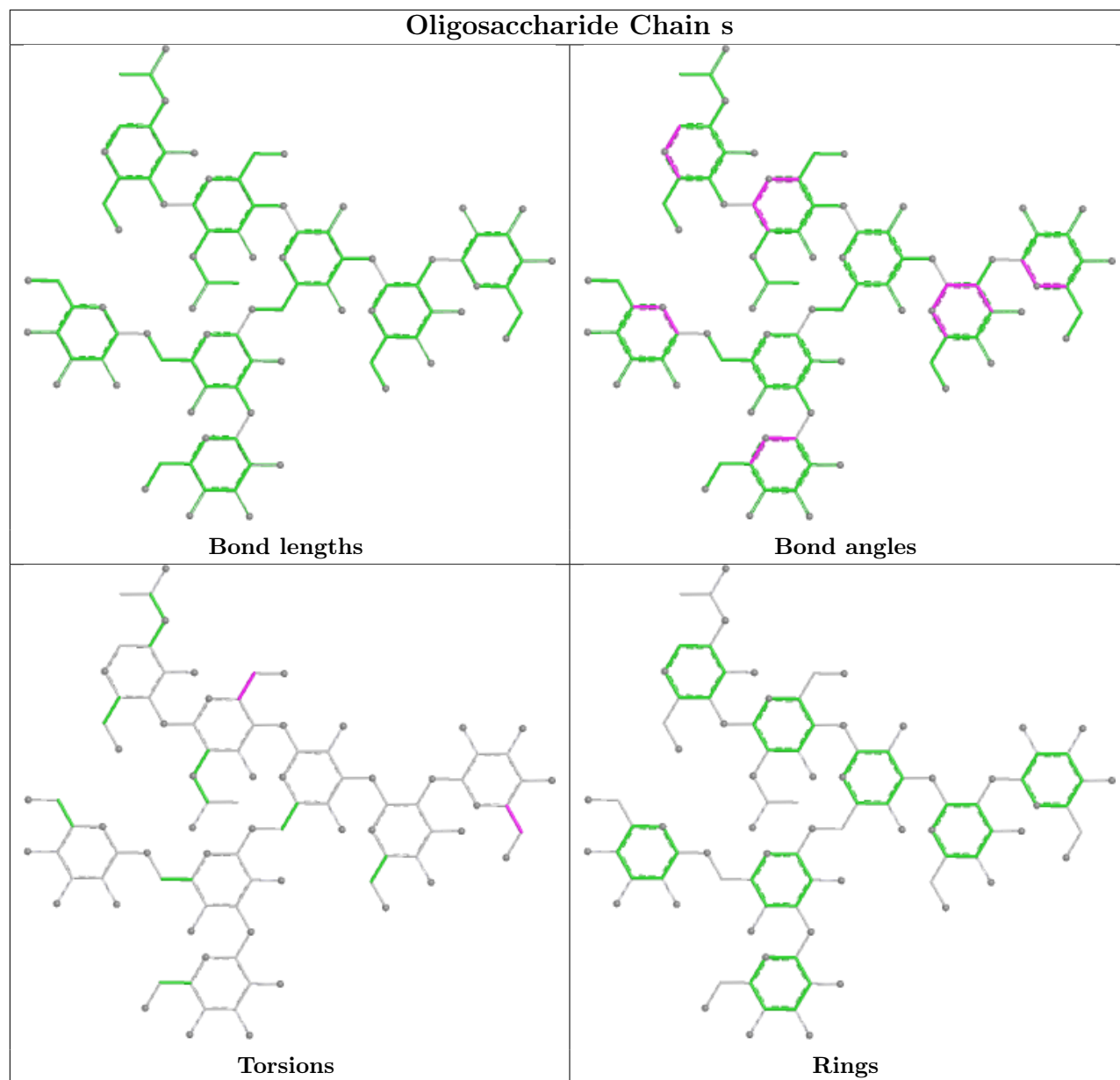


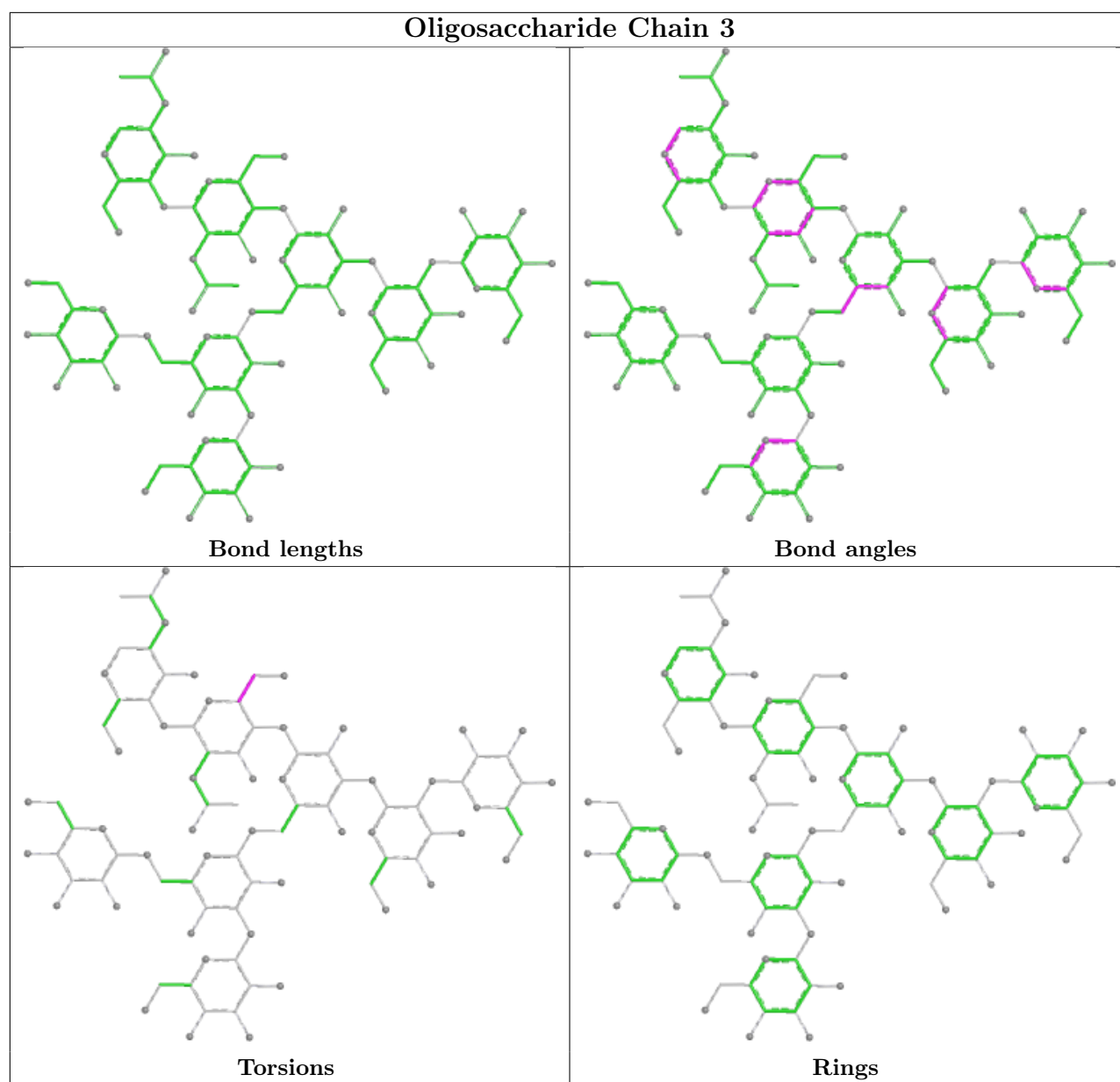


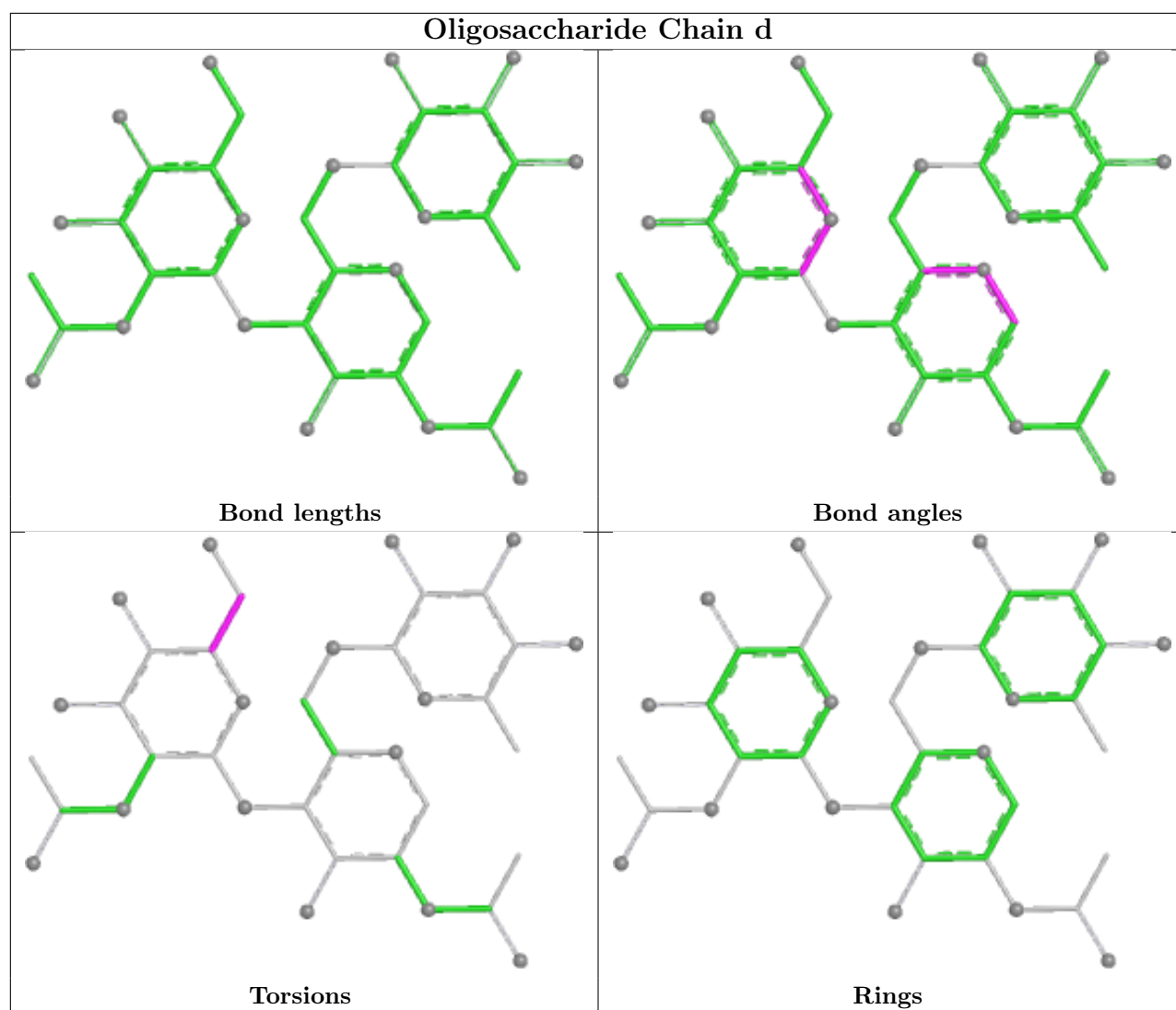












5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29709. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.