



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:21 AM UTC

PDB ID : 9LVS / pdb_00009lvs
EMDB ID : EMD-63424
Title : Cryo-EM structure of the SARS-CoV-2 spike protein in complex with S416
Authors : Fang, Y.; Binghao, Z.
Deposited on : 2025-02-12
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

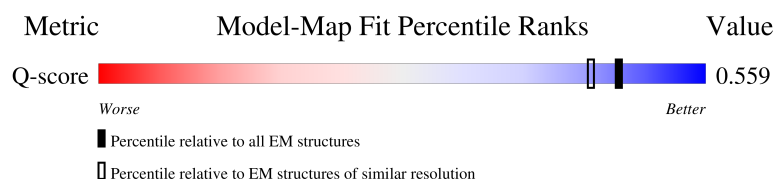
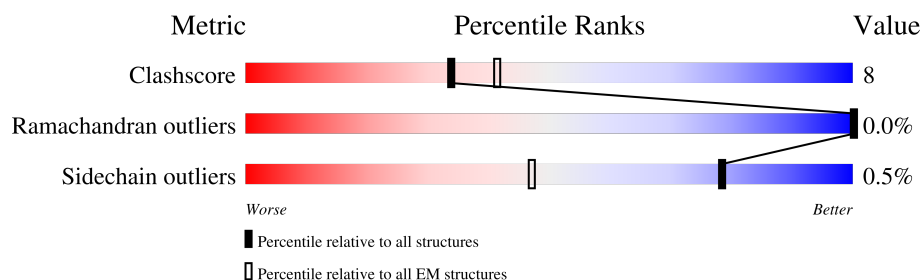
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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	13114 (2.45 - 3.45)

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	1275	 71% 16% 13%
1	B	1275	 69% 18% 13%
1	C	1275	 72% 15% • 13%
2	D	2	 100%




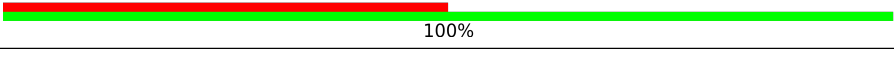

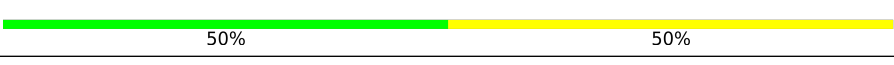


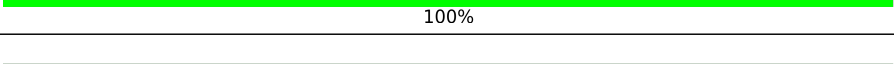
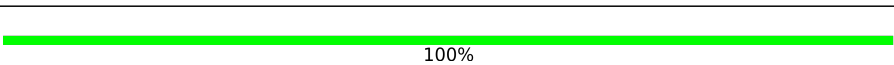
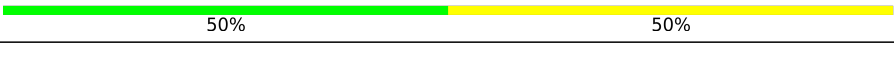

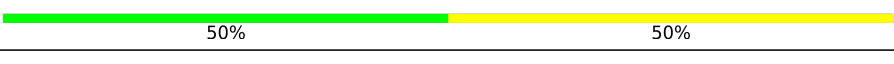
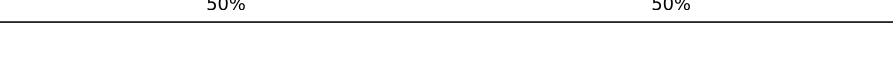
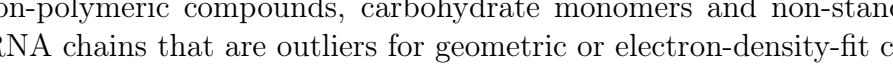
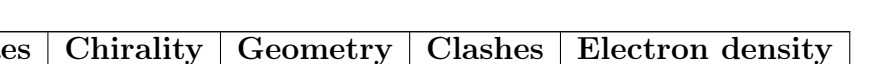
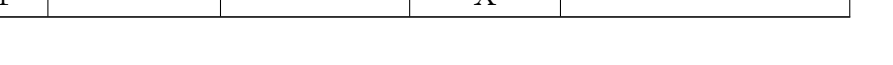


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Mol	Chain	Length	Quality of chain
2	E	2	100%
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	100%
2	I	2	100%
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	50% 50%
2	M	2	50% 50%
2	N	2	50% 50%
2	O	2	100%
2	P	2	50% 50%
2	Q	2	100%
2	R	2	100%
2	S	2	100%
2	T	2	50% 50%
2	U	2	50% 50%
2	V	2	100%
2	W	2	100%
2	X	2	100%
2	Y	2	100%
2	Z	2	100%
2	a	2	100%
2	b	2	100%
2	c	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	d	2	
2	e	2	
2	f	2	
2	g	2	
2	h	2	
2	i	2	
2	j	2	
2	k	2	
2	l	2	
2	m	2	
2	n	2	
2	o	2	
2	p	2	
2	q	2	
2	r	2	
2	s	2	
2	t	2	
2	u	2	
2	v	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	r	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27462 atoms, of which 39 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1109	Total	C	N	O	S	0	0
			8657	5516	1448	1653	40		
1	B	1109	Total	C	N	O	S	0	0
			8657	5516	1448	1653	40		
1	C	1109	Total	C	N	O	S	0	0
			8657	5516	1448	1653	40		

There are 246 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P0DTC2
A	-23	LEU	-	expression tag	UNP P0DTC2
A	-22	LEU	-	expression tag	UNP P0DTC2
A	-21	VAL	-	expression tag	UNP P0DTC2
A	-20	ASN	-	expression tag	UNP P0DTC2
A	-19	GLN	-	expression tag	UNP P0DTC2
A	-18	SER	-	expression tag	UNP P0DTC2
A	-17	HIS	-	expression tag	UNP P0DTC2
A	-16	GLN	-	expression tag	UNP P0DTC2
A	-15	GLY	-	expression tag	UNP P0DTC2
A	-14	PHE	-	expression tag	UNP P0DTC2
A	-13	ASN	-	expression tag	UNP P0DTC2
A	-12	LYS	-	expression tag	UNP P0DTC2
A	-11	GLU	-	expression tag	UNP P0DTC2
A	-10	HIS	-	expression tag	UNP P0DTC2
A	-9	THR	-	expression tag	UNP P0DTC2
A	-8	SER	-	expression tag	UNP P0DTC2
A	-7	LYS	-	expression tag	UNP P0DTC2
A	-6	MET	-	expression tag	UNP P0DTC2
A	-5	VAL	-	expression tag	UNP P0DTC2
A	-4	SER	-	expression tag	UNP P0DTC2
A	-3	ALA	-	expression tag	UNP P0DTC2
A	-2	ILE	-	expression tag	UNP P0DTC2
A	-1	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	TYR	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	ALA	-	expression tag	UNP P0DTC2
A	6	ALA	-	expression tag	UNP P0DTC2
A	7	ALA	-	expression tag	UNP P0DTC2
A	8	ALA	-	expression tag	UNP P0DTC2
A	9	HIS	-	expression tag	UNP P0DTC2
A	10	SER	-	expression tag	UNP P0DTC2
A	11	ALA	-	expression tag	UNP P0DTC2
A	12	PHE	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	TYR	-	expression tag	UNP P0DTC2
A	1217	ILE	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	GLU	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	ASP	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLN	-	expression tag	UNP P0DTC2
A	1226	ALA	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	LYS	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLU	-	expression tag	UNP P0DTC2
A	1234	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	THR	-	expression tag	UNP P0DTC2
A	1240	PHE	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
B	-24	MET	-	initiating methionine	UNP P0DTC2
B	-23	LEU	-	expression tag	UNP P0DTC2
B	-22	LEU	-	expression tag	UNP P0DTC2
B	-21	VAL	-	expression tag	UNP P0DTC2
B	-20	ASN	-	expression tag	UNP P0DTC2
B	-19	GLN	-	expression tag	UNP P0DTC2
B	-18	SER	-	expression tag	UNP P0DTC2
B	-17	HIS	-	expression tag	UNP P0DTC2
B	-16	GLN	-	expression tag	UNP P0DTC2
B	-15	GLY	-	expression tag	UNP P0DTC2
B	-14	PHE	-	expression tag	UNP P0DTC2
B	-13	ASN	-	expression tag	UNP P0DTC2
B	-12	LYS	-	expression tag	UNP P0DTC2
B	-11	GLU	-	expression tag	UNP P0DTC2
B	-10	HIS	-	expression tag	UNP P0DTC2
B	-9	THR	-	expression tag	UNP P0DTC2
B	-8	SER	-	expression tag	UNP P0DTC2
B	-7	LYS	-	expression tag	UNP P0DTC2
B	-6	MET	-	expression tag	UNP P0DTC2
B	-5	VAL	-	expression tag	UNP P0DTC2
B	-4	SER	-	expression tag	UNP P0DTC2
B	-3	ALA	-	expression tag	UNP P0DTC2
B	-2	ILE	-	expression tag	UNP P0DTC2
B	-1	VAL	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2
B	1	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	ALA	-	expression tag	UNP P0DTC2
B	6	ALA	-	expression tag	UNP P0DTC2
B	7	ALA	-	expression tag	UNP P0DTC2
B	8	ALA	-	expression tag	UNP P0DTC2
B	9	HIS	-	expression tag	UNP P0DTC2
B	10	SER	-	expression tag	UNP P0DTC2
B	11	ALA	-	expression tag	UNP P0DTC2
B	12	PHE	-	expression tag	UNP P0DTC2
B	13	ALA	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	TYR	-	expression tag	UNP P0DTC2
B	1217	ILE	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	GLU	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	PRO	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	ASP	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLN	-	expression tag	UNP P0DTC2
B	1226	ALA	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2
B	1230	LYS	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLU	-	expression tag	UNP P0DTC2
B	1234	TRP	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	THR	-	expression tag	UNP P0DTC2
B	1240	PHE	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLY	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
C	-24	MET	-	initiating methionine	UNP P0DTC2
C	-23	LEU	-	expression tag	UNP P0DTC2
C	-22	LEU	-	expression tag	UNP P0DTC2
C	-21	VAL	-	expression tag	UNP P0DTC2
C	-20	ASN	-	expression tag	UNP P0DTC2
C	-19	GLN	-	expression tag	UNP P0DTC2
C	-18	SER	-	expression tag	UNP P0DTC2
C	-17	HIS	-	expression tag	UNP P0DTC2
C	-16	GLN	-	expression tag	UNP P0DTC2
C	-15	GLY	-	expression tag	UNP P0DTC2
C	-14	PHE	-	expression tag	UNP P0DTC2
C	-13	ASN	-	expression tag	UNP P0DTC2
C	-12	LYS	-	expression tag	UNP P0DTC2
C	-11	GLU	-	expression tag	UNP P0DTC2
C	-10	HIS	-	expression tag	UNP P0DTC2
C	-9	THR	-	expression tag	UNP P0DTC2
C	-8	SER	-	expression tag	UNP P0DTC2
C	-7	LYS	-	expression tag	UNP P0DTC2
C	-6	MET	-	expression tag	UNP P0DTC2
C	-5	VAL	-	expression tag	UNP P0DTC2
C	-4	SER	-	expression tag	UNP P0DTC2
C	-3	ALA	-	expression tag	UNP P0DTC2
C	-2	ILE	-	expression tag	UNP P0DTC2
C	-1	VAL	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	TYR	-	expression tag	UNP P0DTC2
C	2	VAL	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	ALA	-	expression tag	UNP P0DTC2
C	6	ALA	-	expression tag	UNP P0DTC2
C	7	ALA	-	expression tag	UNP P0DTC2
C	8	ALA	-	expression tag	UNP P0DTC2
C	9	HIS	-	expression tag	UNP P0DTC2
C	10	SER	-	expression tag	UNP P0DTC2
C	11	ALA	-	expression tag	UNP P0DTC2
C	12	PHE	-	expression tag	UNP P0DTC2
C	13	ALA	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	TYR	-	expression tag	UNP P0DTC2
C	1217	ILE	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	GLU	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2
C	1221	PRO	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	ASP	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLN	-	expression tag	UNP P0DTC2
C	1226	ALA	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	LYS	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLU	-	expression tag	UNP P0DTC2
C	1234	TRP	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1239	THR	-	expression tag	UNP P0DTC2
C	1240	PHE	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	h	2	Total	C	N	O	0	0
			28	16	2	10		

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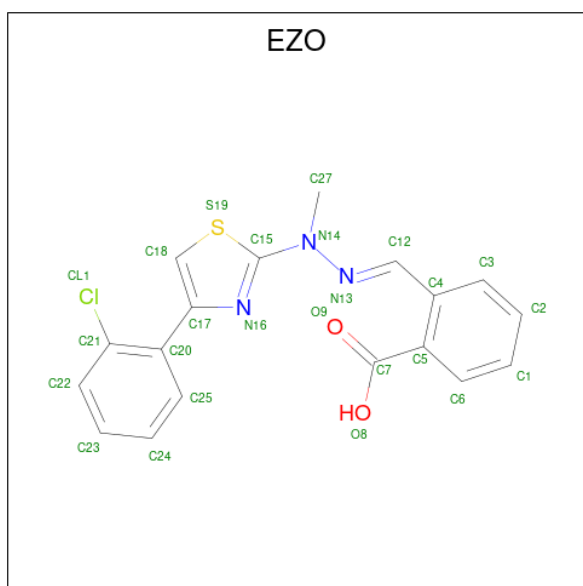
Mol	Chain	Residues	Atoms				AltConf	Trace
2	i	2	Total	C	N	O	0	0
			28	16	2	10		
2	j	2	Total	C	N	O	0	0
			28	16	2	10		
2	k	2	Total	C	N	O	0	0
			28	16	2	10		
2	l	2	Total	C	N	O	0	0
			28	16	2	10		
2	m	2	Total	C	N	O	0	0
			28	16	2	10		
2	n	2	Total	C	N	O	0	0
			28	16	2	10		
2	o	2	Total	C	N	O	0	0
			28	16	2	10		
2	p	2	Total	C	N	O	0	0
			28	16	2	10		
2	q	2	Total	C	N	O	0	0
			28	16	2	10		
2	r	2	Total	C	N	O	0	0
			28	16	2	10		
2	s	2	Total	C	N	O	0	0
			28	16	2	10		
2	t	2	Total	C	N	O	0	0
			28	16	2	10		
2	u	2	Total	C	N	O	0	0
			28	16	2	10		
2	v	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 2-[(E)-[[4-(2-chlorophenyl)-1,3-thiazol-2-yl]-methyl-hydrazinylidene]methyl]benzoic acid (CCD ID: EZO) (formula: $C_{18}H_{14}ClN_3O_2S$).

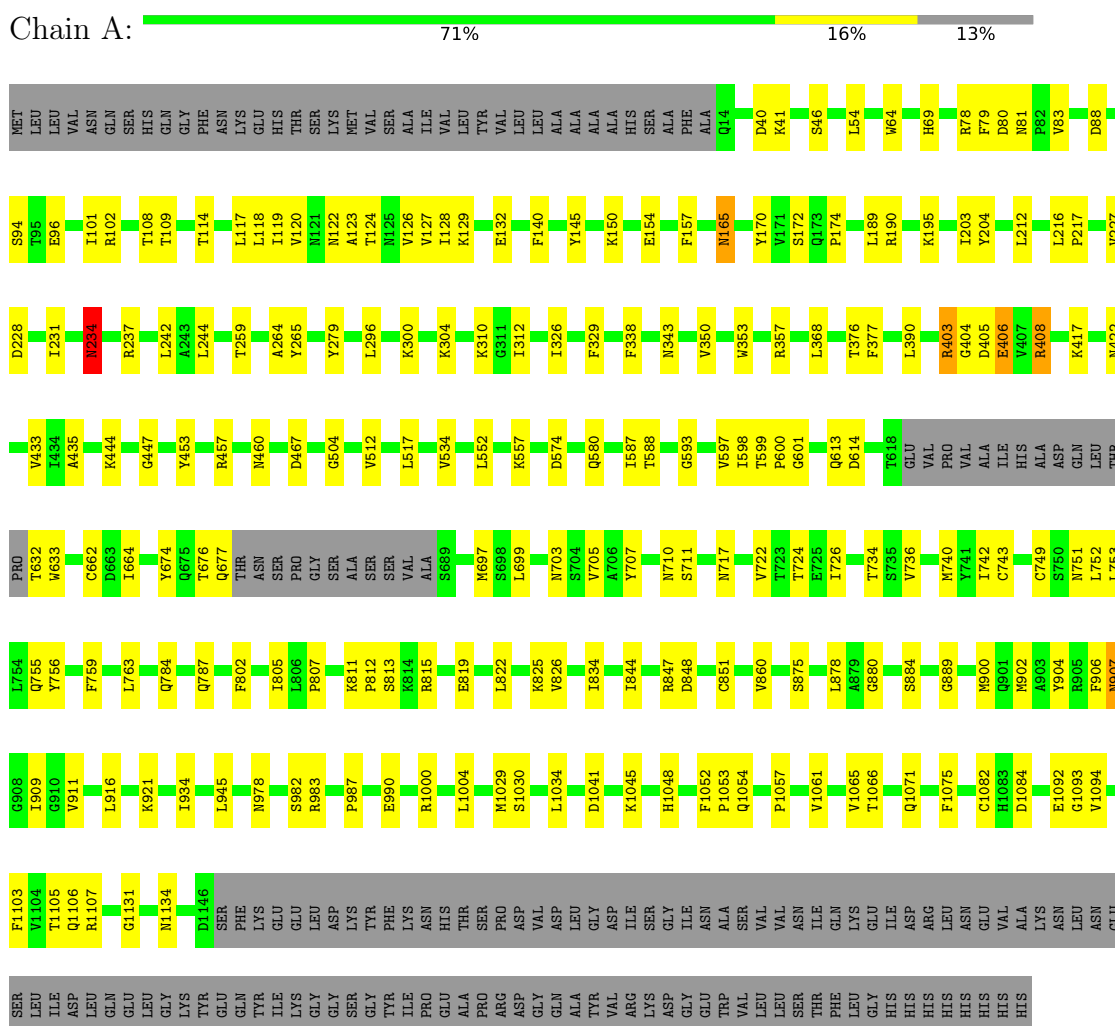


Mol	Chain	Residues	Atoms							AltConf
4	A	1	Total	C	Cl	H	N	O	S	0
			38	18	1	13	3	2	1	
4	A	1	Total	C	Cl	N	O	S		0
			25	18	1	3	2	1		
4	B	1	Total	C	Cl	H	N	O	S	0
			38	18	1	13	3	2	1	
4	B	1	Total	C	Cl	N	O	S		0
			25	18	1	3	2	1		
4	C	1	Total	C	Cl	H	N	O	S	0
			38	18	1	13	3	2	1	
4	C	1	Total	C	Cl	N	O	S		0
			25	18	1	3	2	1		

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



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

Chain I:  100%



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

Chain J:  50%



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

Chain K:  50%



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

Chain L:  50%



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

Chain M:  50%



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

Chain N:  50%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain Q:  100%



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

Chain R:  100%



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

Chain S:  100%



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

Chain T:  50% 50%



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

Chain U:  50% 50% 50%



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

Chain V:  100%



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

Chain W:  100%



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

Chain X:  100%



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

Chain Y:  100%



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

Chain Z:  100%



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

Chain a:  100%



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

Chain b:  100%



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



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



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



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



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



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





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

Chain i:  50% 50%



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

Chain j:  50% 50%



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

Chain k:  50% 50%



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

Chain l:  50% 50%



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

Chain m:  100%



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

Chain n:  50% 50%



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

Chain o:  100%



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

Chain p:  100%



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

Chain q:  100%



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

Chain r:  50% 50%



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

Chain s:  50% 50%



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

Chain t:  50% 50%



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

Chain u:  50% 50%

HA01
HA02

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

Chain v:  50% 50%

HA01
HA02

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5921528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.13	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.652	Depositor
Minimum map value	-0.366	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.0505	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EZO, 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	0.21	2/8859 (0.0%)	0.36	1/12059 (0.0%)
1	B	0.19	0/8859	0.38	3/12059 (0.0%)
1	C	0.22	1/8859 (0.0%)	0.38	5/12059 (0.0%)
All	All	0.21	3/26577 (0.0%)	0.37	9/36177 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	ASN	CA-C	-5.32	1.46	1.52
1	A	234	ASN	C-N	-5.23	1.26	1.33
1	C	234	ASN	N-CA	-5.08	1.39	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	ASN	N-CA-C	10.28	123.87	111.02
1	B	166	CYS	N-CA-C	7.40	120.95	108.23
1	C	233	ILE	CB-CA-C	-6.70	102.62	111.13
1	C	234	ASN	N-CA-CB	-6.12	101.43	110.85
1	B	165	ASN	CB-CA-C	-5.83	101.58	112.30
1	C	340	GLU	N-CA-C	-5.75	106.89	114.31
1	C	235	ILE	N-CA-C	5.52	115.94	107.77
1	C	164	ASN	O-C-N	5.15	129.40	123.17
1	A	406	GLU	N-CA-C	5.07	119.32	113.18

There are no chirality outliers.

There are no planarity outliers.

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	8657	0	8422	154	0
1	B	8657	0	8420	162	0
1	C	8657	0	8427	147	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	24	0	0
2	J	28	0	25	0	0
2	K	28	0	25	1	0
2	L	28	0	25	0	0
2	M	28	0	25	3	0
2	N	28	0	25	2	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	Q	28	0	24	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	1	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	1	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	2	0
2	d	28	0	25	1	0
2	e	28	0	25	4	0
2	f	28	0	22	1	0
2	g	28	0	25	2	0
2	h	28	0	25	0	0
2	i	28	0	25	1	0
2	j	28	0	25	1	0
2	k	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	l	28	0	25	3	0
2	m	28	0	25	0	0
2	n	28	0	25	0	0
2	o	28	0	25	0	0
2	p	28	0	25	0	0
2	q	28	0	25	0	0
2	r	28	0	25	7	0
2	s	28	0	25	1	0
2	t	28	0	25	0	0
2	u	28	0	23	0	0
2	v	28	0	25	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
4	A	50	13	0	8	0
4	B	50	13	0	4	0
4	C	50	13	0	5	0
All	All	27423	39	26426	439	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 8.

All (439) 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:A:377:PHE:CZ	4:A:1303:EZO:C27	2.24	1.21
1:A:711:SER:HA	1:A:1075:PHE:O	1.57	1.03
1:B:24:LEU:HB3	1:B:78:ARG:HH12	1.37	0.89
4:A:1303:EZO:O9	1:B:408:ARG:NH2	2.12	0.83
1:B:165:ASN:HD21	2:e:1:NAG:C1	1.93	0.81
1:C:130:VAL:HG12	1:C:168:PHE:HB3	1.63	0.79
1:C:234:ASN:C	1:C:234:ASN:ND2	2.41	0.79
1:C:377:PHE:CZ	4:C:1303:EZO:C27	2.65	0.78
1:A:377:PHE:HZ	4:A:1303:EZO:C27	1.93	0.78
1:B:377:PHE:CZ	4:B:1303:EZO:C27	2.67	0.78
1:A:377:PHE:CE2	4:A:1303:EZO:C27	2.67	0.76
1:A:123:ALA:HB3	2:M:1:NAG:H82	1.67	0.76
1:B:165:ASN:ND2	2:e:1:NAG:C1	2.48	0.76
1:C:403:ARG:HG2	1:C:406:GLU:HG3	1.67	0.76
1:A:1030:SER:HB3	1:B:1041:ASP:HB2	1.69	0.74
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:PRO:HD3	1:C:711:SER:O	1.89	0.73
1:C:234:ASN:ND2	2:r:1:NAG:C1	2.52	0.72
1:C:343:ASN:OD1	2:j:1:NAG:H4	1.90	0.72
1:A:1082:CYS:HB3	1:A:1134:ASN:HB3	1.72	0.71
1:C:234:ASN:C	1:C:234:ASN:HD22	1.99	0.70
1:C:234:ASN:CG	2:r:1:NAG:C1	2.65	0.70
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.74	0.69
1:B:406:GLU:OE2	1:B:417:LYS:NZ	2.27	0.68
1:A:1041:ASP:HB2	1:C:1030:SER:HB3	1.74	0.68
1:C:111:ASP:HB3	1:C:113:LYS:HG2	1.76	0.68
1:A:403:ARG:HD2	1:A:406:GLU:CD	2.19	0.68
1:A:752:LEU:HD21	1:A:990:GLU:HG2	1.75	0.67
1:C:717:ASN:HD22	2:l:1:NAG:C1	2.08	0.67
1:C:770:ILE:HD11	1:C:1012:LEU:HD12	1.76	0.67
1:C:766:ALA:HB1	1:C:1012:LEU:HD11	1.78	0.66
1:C:720:ILE:HG13	1:C:923:ILE:HG23	1.77	0.66
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.77	0.66
1:A:844:ILE:HG13	1:A:847:ARG:HH21	1.60	0.65
1:B:96:GLU:OE1	1:B:190:ARG:NH1	2.30	0.65
1:A:69:HIS:ND1	1:A:259:THR:OG1	2.25	0.65
1:A:1131:GLY:HA3	2:G:1:NAG:H83	1.78	0.65
1:C:129:LYS:HG2	1:C:169:GLU:HG3	1.80	0.64
1:C:632:THR:OG1	1:C:633:TRP:N	2.27	0.64
1:B:165:ASN:OD1	2:e:1:NAG:C1	2.46	0.64
1:B:167:THR:HG21	1:C:466:ARG:NH1	2.12	0.64
1:C:926:GLN:HE21	2:l:1:NAG:H61	1.61	0.64
1:A:123:ALA:HB2	1:A:154:GLU:HG3	1.80	0.64
1:A:599:THR:HG22	1:A:601:GLY:H	1.63	0.64
1:C:310:LYS:HE2	1:C:664:ILE:HD11	1.80	0.63
1:A:102:ARG:NH2	1:A:154:GLU:OE2	2.31	0.63
1:B:563:GLN:O	1:B:577:ARG:NH2	2.32	0.63
1:B:165:ASN:CG	2:e:1:NAG:C1	2.73	0.62
1:C:130:VAL:CG1	1:C:168:PHE:HB3	2.29	0.62
1:A:632:THR:OG1	1:A:633:TRP:N	2.33	0.62
1:C:108:THR:HB	2:r:1:NAG:H62	1.81	0.62
1:A:751:ASN:OD1	1:B:52:GLN:NE2	2.33	0.62
1:B:24:LEU:HD13	1:B:25:PRO:HD2	1.81	0.62
1:B:903:ALA:HB2	1:B:916:LEU:HD22	1.81	0.62
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.82	0.61
1:B:644:GLN:NE2	1:B:645:THR:O	2.32	0.61
1:A:132:GLU:OE1	1:A:165:ASN:ND2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD22	1:A:217:PRO:HG2	1.81	0.61
1:B:1030:SER:HB3	1:C:1041:ASP:HB2	1.82	0.60
1:B:902:MET:HE1	1:B:1050:MET:SD	2.41	0.60
1:B:338:PHE:HE1	4:B:1303:EZO:CL1	2.22	0.60
1:B:642:VAL:HG22	1:B:651:ILE:HG12	1.82	0.60
1:A:338:PHE:HB3	1:A:368:LEU:HD21	1.82	0.60
1:A:1093:GLY:HA3	1:A:1105:THR:O	2.02	0.59
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.35	0.59
1:B:17:ASN:HB2	2:f:1:NAG:N2	2.17	0.59
1:C:801:ASN:OD1	1:C:802:PHE:N	2.35	0.59
1:A:343:ASN:ND2	2:F:1:NAG:O4	2.32	0.59
1:C:338:PHE:HE1	4:C:1303:EZO:CL1	2.22	0.59
1:A:807:PRO:HG3	1:A:875:SER:HB2	1.85	0.59
1:B:1115:ILE:HG23	1:B:1120:THR:HG21	1.84	0.59
1:B:708:SER:HB3	1:B:711:SER:HB3	1.84	0.59
1:A:787:GLN:OE1	1:B:703:ASN:ND2	2.35	0.58
1:C:644:GLN:NE2	1:C:645:THR:O	2.36	0.58
1:B:1106:GLN:NE2	1:B:1111:GLU:OE1	2.36	0.58
4:A:1303:EZO:C18	4:A:1303:EZO:CL1	2.89	0.57
4:B:1303:EZO:CL1	4:B:1303:EZO:C18	2.89	0.57
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.86	0.57
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.87	0.57
1:C:563:GLN:O	1:C:577:ARG:NH2	2.38	0.57
4:C:1303:EZO:CL1	4:C:1303:EZO:C18	2.90	0.57
1:A:711:SER:CA	1:A:1075:PHE:O	2.45	0.57
1:B:914:ASN:O	1:B:918:GLU:HG2	2.05	0.57
1:C:67:ALA:O	1:C:262:ALA:HA	2.04	0.57
1:B:834:ILE:HD12	2:i:1:NAG:H82	1.86	0.57
1:C:815:ARG:HG2	1:C:819:GLU:HB3	1.88	0.56
1:C:919:ASN:O	1:C:923:ILE:HD12	2.05	0.56
1:A:557:LYS:NZ	1:A:574:ASP:OD1	2.39	0.56
1:B:811:LYS:NZ	1:B:820:ASP:OD1	2.37	0.56
1:A:96:GLU:OE2	1:A:190:ARG:NE	2.37	0.56
1:A:457:ARG:NH2	2:r:1:NAG:O7	2.38	0.56
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.87	0.56
1:A:848:ASP:HB3	1:A:851:CYS:HB2	1.88	0.56
1:A:753:LEU:HD12	1:A:756:TYR:HB2	1.88	0.56
1:B:598:ILE:HG12	1:B:666:ILE:HD11	1.88	0.56
1:B:120:VAL:HG11	1:B:157:PHE:HE1	1.71	0.56
1:A:880:GLY:O	1:A:884:SER:OG	2.23	0.55
1:B:894:LEU:HB3	1:C:713:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ILE:HG21	1:B:488:CYS:HB3	1.89	0.55
1:A:377:PHE:CE2	4:A:1303:EZO:N14	2.74	0.55
1:B:376:THR:HB	1:B:435:ALA:HB3	1.88	0.55
1:B:47:VAL:HG12	1:B:279:TYR:HB2	1.89	0.55
1:B:906:PHE:O	1:B:909:ILE:HG22	2.06	0.55
1:C:203:ILE:O	1:C:226:LEU:HB3	2.06	0.55
1:C:332:ILE:HD11	1:C:525:CYS:HB2	1.88	0.55
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.88	0.55
1:B:598:ILE:HG23	1:B:664:ILE:HG21	1.89	0.54
1:B:915:VAL:O	1:B:919:ASN:ND2	2.40	0.54
1:A:46:SER:HA	1:A:279:TYR:O	2.07	0.54
1:B:632:THR:OG1	1:B:633:TRP:N	2.26	0.54
1:A:444:LYS:HG3	1:A:447:GLY:H	1.73	0.54
1:B:807:PRO:HG3	1:B:875:SER:HB2	1.88	0.54
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.89	0.54
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.38	0.54
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	1.90	0.54
1:A:127:VAL:HG21	2:M:1:NAG:H62	1.90	0.54
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.73	0.54
1:B:981:LEU:O	1:C:386:LYS:NZ	2.40	0.54
1:C:28:TYR:HB3	1:C:61:ASN:ND2	2.23	0.53
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.89	0.53
1:A:118:LEU:HD11	1:A:120:VAL:HB	1.90	0.53
1:B:752:LEU:HD21	1:B:990:GLU:HG2	1.91	0.53
1:A:815:ARG:HG2	1:A:819:GLU:HB3	1.91	0.53
1:B:295:PRO:HA	1:B:298:GLU:HG3	1.91	0.53
1:A:978:ASN:O	1:A:982:SER:OG	2.21	0.52
1:C:470:THR:O	1:C:470:THR:OG1	2.27	0.52
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.36	0.52
1:A:403:ARG:HG3	1:A:504:GLY:O	2.10	0.52
1:B:375:SER:O	1:C:408:ARG:HD3	2.09	0.52
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.92	0.52
1:A:329:PHE:O	1:A:580:GLN:NE2	2.42	0.52
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.91	0.52
1:C:825:LYS:HB3	1:C:945:LEU:HD13	1.92	0.52
1:B:718:PHE:HZ	1:B:919:ASN:ND2	2.08	0.52
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.90	0.52
1:A:408:ARG:HD3	1:C:375:SER:O	2.10	0.52
1:B:599:THR:HG22	1:B:601:GLY:H	1.74	0.52
1:B:706:ALA:HB2	2:Y:2:NAG:H62	1.92	0.51
1:C:390:LEU:HD22	1:C:517:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:HB3	1:A:242:LEU:HD12	1.93	0.51
1:B:170:TYR:CZ	4:B:1302:EZO:N13	2.78	0.51
1:B:868:GLU:OE2	1:B:868:GLU:N	2.38	0.51
1:C:227:VAL:HG22	1:C:228:ASP:N	2.25	0.51
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.74	0.51
1:C:406:GLU:OE1	1:C:495:TYR:OH	2.24	0.51
1:A:1084:ASP:OD1	1:A:1084:ASP:N	2.44	0.51
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.93	0.51
1:A:234:ASN:ND2	2:N:1:NAG:C1	2.74	0.51
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.93	0.51
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.76	0.51
1:A:983:ARG:HD2	1:B:517:LEU:HD13	1.93	0.51
1:B:143:VAL:HG11	1:B:179:LEU:HB3	1.93	0.51
1:A:703:ASN:ND2	1:C:787:GLN:OE1	2.35	0.50
1:B:880:GLY:O	1:B:884:SER:OG	2.24	0.50
1:B:1100:THR:HG23	1:B:1101:HIS:ND1	2.27	0.50
1:C:462:LYS:HG3	2:c:1:NAG:H82	1.94	0.50
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.92	0.50
1:C:909:ILE:HD11	1:C:1047:TYR:HB3	1.93	0.50
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.93	0.50
1:B:406:GLU:OE1	1:B:495:TYR:OH	2.28	0.50
1:B:212:LEU:HG	1:B:217:PRO:HG3	1.93	0.50
1:C:206:LYS:HB3	1:C:223:LEU:HD22	1.94	0.50
1:A:234:ASN:ND2	1:A:234:ASN:C	2.70	0.50
1:C:350:VAL:HG22	1:C:422:ASN:HB3	1.92	0.50
1:A:117:LEU:HD22	1:A:231:ILE:HD13	1.92	0.50
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.94	0.50
1:C:79:PHE:CZ	1:C:242:LEU:HB2	2.47	0.50
1:A:165:ASN:CG	2:P:1:NAG:C1	2.85	0.49
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.93	0.49
1:B:724:THR:HG23	1:B:934:ILE:HD12	1.92	0.49
1:C:280:ASN:HD22	2:s:1:NAG:H82	1.77	0.49
1:A:755:GLN:OE1	1:A:755:GLN:N	2.46	0.49
1:C:903:ALA:HB2	1:C:916:LEU:HD22	1.93	0.49
1:A:552:LEU:HD23	1:A:587:ILE:HG12	1.94	0.49
1:A:710:ASN:OD1	1:A:710:ASN:N	2.45	0.49
1:C:825:LYS:HD3	1:C:942:ALA:HA	1.95	0.49
1:B:108:THR:O	1:B:237:ARG:NH1	2.39	0.49
1:B:822:LEU:HD22	1:B:1061:VAL:HG21	1.95	0.49
1:C:204:TYR:CD2	1:C:225:PRO:HA	2.48	0.49
1:C:376:THR:HB	1:C:435:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:LYS:HE3	1:C:575:ALA:HB2	1.95	0.49
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.94	0.49
1:B:146:HIS:ND1	2:g:1:NAG:O6	2.46	0.48
1:B:613:GLN:HA	1:B:648:GLY:HA3	1.95	0.48
1:B:1051:SER:OG	1:B:1064:HIS:ND1	2.33	0.48
1:B:738:CYS:HB3	1:B:742:ILE:HD12	1.95	0.48
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.77	0.48
1:C:34:ARG:NH1	1:C:217:PRO:O	2.47	0.48
1:A:404:GLY:O	1:A:405:ASP:C	2.56	0.48
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	1.94	0.48
1:B:18:LEU:HD12	1:B:21:ARG:HH21	1.78	0.48
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.32	0.48
1:A:588:THR:HG21	1:C:842:GLY:H	1.79	0.48
1:C:444:LYS:O	1:C:499:PRO:HD3	2.13	0.48
1:A:724:THR:HG23	1:A:934:ILE:HD12	1.95	0.48
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.47	0.48
1:A:40:ASP:OD1	1:A:41:LYS:N	2.41	0.48
1:A:127:VAL:CG2	2:M:1:NAG:H62	2.43	0.48
1:A:1103:PHE:HZ	2:K:1:NAG:H62	1.79	0.48
1:B:784:GLN:HG3	1:B:1029:MET:HG2	1.96	0.48
1:C:102:ARG:NH2	1:C:154:GLU:OE1	2.47	0.48
1:A:227:VAL:HG22	1:A:228:ASP:N	2.29	0.47
1:C:127:VAL:HG12	1:C:129:LYS:HG3	1.96	0.47
1:A:759:PHE:O	1:A:763:LEU:HG	2.14	0.47
1:A:126:VAL:HG12	1:A:172:SER:OG	2.15	0.47
1:B:884:SER:OG	1:B:888:PHE:HB3	2.14	0.47
1:A:119:ILE:HG23	1:A:128:ILE:HG12	1.97	0.47
1:A:734:THR:HG22	1:A:860:VAL:HG22	1.95	0.47
1:C:62:VAL:CG1	1:C:266:TYR:HB3	2.44	0.47
1:A:41:LYS:HG2	1:B:562:PHE:HD1	1.79	0.47
1:B:1134:ASN:OD1	1:B:1134:ASN:N	2.44	0.47
1:A:46:SER:CA	1:A:279:TYR:O	2.63	0.47
1:A:108:THR:HB	1:A:114:THR:HG21	1.95	0.47
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.77	0.47
1:C:123:ALA:HB2	1:C:179:LEU:HD21	1.97	0.47
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.64	0.47
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.47	0.47
1:B:234:ASN:H	1:B:234:ASN:ND2	2.12	0.47
1:B:370:ASN:HB2	1:C:455:LEU:HD21	1.97	0.47
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.96	0.47
1:A:889:GLY:HA3	1:A:1034:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:SER:HB3	1:C:62:VAL:CG2	2.45	0.47
1:C:156:GLU:OE1	1:C:246:ARG:NH2	2.41	0.47
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.97	0.47
1:A:987:PRO:HD3	1:C:427:ASP:HB3	1.97	0.47
1:B:920:GLN:O	1:B:921:LYS:C	2.57	0.47
1:B:963:VAL:O	1:B:966:LEU:HB2	2.15	0.47
1:B:1029:MET:HE2	1:B:1029:MET:HB2	1.77	0.46
1:C:28:TYR:HD2	1:C:61:ASN:HD21	1.61	0.46
1:A:784:GLN:HG3	1:A:1029:MET:HG2	1.97	0.46
1:A:834:ILE:HD12	2:T:1:NAG:H82	1.96	0.46
1:B:317:ASN:ND2	1:B:593:GLY:O	2.48	0.46
1:C:170:TYR:CE2	4:C:1302:EZO:N13	2.83	0.46
1:B:296:LEU:HB2	1:B:608:VAL:HG11	1.97	0.46
1:C:632:THR:HG1	1:C:633:TRP:H	1.56	0.46
1:C:985:ASP:OD1	1:C:988:GLU:HG3	2.15	0.46
1:A:78:ARG:NH2	1:A:80:ASP:OD1	2.48	0.46
1:A:707:TYR:HB2	1:C:883:THR:HG23	1.96	0.46
1:C:613:GLN:H	1:C:613:GLN:HG2	1.59	0.46
1:C:901:GLN:O	1:C:905:ARG:HG2	2.16	0.46
1:B:303:LEU:HD12	1:B:308:VAL:HG22	1.98	0.46
1:B:878:LEU:O	1:B:882:ILE:HG13	2.16	0.46
1:B:991:VAL:HG23	1:B:992:GLN:HE21	1.81	0.46
1:A:145:TYR:HE1	1:A:150:LYS:HA	1.81	0.46
1:A:907:ASN:HD22	1:A:907:ASN:HA	1.53	0.46
1:B:153:MET:HE1	2:g:1:NAG:H5	1.97	0.46
1:C:339:GLY:O	1:C:343:ASN:ND2	2.43	0.46
1:C:1097:SER:C	1:C:1099:GLY:H	2.24	0.46
1:A:906:PHE:HA	1:A:909:ILE:HG22	1.98	0.46
1:B:792:PRO:HG2	1:B:797:PHE:CZ	2.50	0.46
1:C:612:TYR:HB2	1:C:615:VAL:HG12	1.98	0.46
1:C:206:LYS:NZ	1:C:222:ALA:O	2.39	0.45
1:A:1045:LYS:HE3	1:C:890:ALA:HA	1.98	0.45
1:B:113:LYS:HB3	1:B:113:LYS:HE2	1.34	0.45
1:A:613:GLN:H	1:A:613:GLN:HG2	1.51	0.45
1:B:989:ALA:O	1:B:993:ILE:HG12	2.16	0.45
1:C:258:TRP:HZ3	1:C:260:ALA:HB2	1.82	0.45
1:B:718:PHE:CZ	1:B:919:ASN:ND2	2.84	0.45
1:B:742:ILE:HA	1:B:1000:ARG:HD3	1.98	0.45
1:A:310:LYS:HA	1:A:599:THR:O	2.17	0.45
1:A:900:MET:HE1	1:B:1077:THR:OG1	2.17	0.45
1:B:231:ILE:HD12	1:B:233:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HB	1:A:435:ALA:HB3	1.99	0.45
1:B:226:LEU:HG	1:B:227:VAL:HG13	1.99	0.45
1:B:1038:LYS:HE3	1:B:1038:LYS:HB3	1.58	0.45
1:A:94:SER:HB2	1:A:101:ILE:HG13	1.98	0.45
1:A:338:PHE:CG	1:A:368:LEU:HD11	2.50	0.45
1:A:705:VAL:HB	1:C:883:THR:HG21	1.99	0.45
1:A:1029:MET:HB2	1:A:1029:MET:HE2	1.78	0.45
1:A:1092:GLU:OE1	1:A:1107:ARG:NH1	2.45	0.45
1:B:30:ASN:HD21	1:B:59:PHE:HD1	1.64	0.45
1:A:304:LYS:HA	1:A:304:LYS:HD3	1.68	0.45
1:A:405:ASP:O	1:A:408:ARG:HG3	2.17	0.45
1:B:405:ASP:O	1:B:408:ARG:HG2	2.17	0.45
1:B:120:VAL:HG22	1:B:241:LEU:HD13	1.99	0.44
1:A:742:ILE:HG12	1:A:1000:ARG:HB3	1.99	0.44
1:B:568:ASP:OD1	1:B:572:THR:HG22	2.17	0.44
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.98	0.44
1:C:327:VAL:HG21	1:C:528:LYS:HD3	2.00	0.44
1:C:335:LEU:HD21	1:C:364:ASP:HB3	2.00	0.44
1:C:973:ILE:HD12	1:C:983:ARG:HH21	1.81	0.44
1:A:593:GLY:HA2	1:A:614:ASP:OD2	2.17	0.44
1:A:676:THR:HG22	1:A:677:GLN:HG2	1.98	0.44
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.76	0.44
1:B:108:THR:HG21	1:B:234:ASN:OD1	2.17	0.44
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.82	0.44
1:C:926:GLN:NE2	2:l:1:NAG:H61	2.28	0.44
1:A:878:LEU:HD11	1:A:1054:GLN:HE22	1.82	0.44
1:A:909:ILE:HG23	1:A:911:VAL:HG23	1.99	0.44
1:B:124:THR:HG22	1:B:125:ASN:OD1	2.17	0.44
1:B:792:PRO:HG2	1:B:797:PHE:HZ	1.82	0.44
1:C:438:SER:O	1:C:438:SER:OG	2.35	0.44
1:A:699:LEU:HD21	1:C:869:MET:HB3	1.99	0.44
1:A:736:VAL:HG11	1:A:1004:LEU:HD22	1.99	0.44
1:B:29:THR:OG1	1:B:30:ASN:N	2.51	0.44
1:B:354:ASN:O	1:B:398:ASP:HA	2.18	0.44
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.52	0.44
1:C:117:LEU:HA	1:C:130:VAL:HA	1.99	0.44
1:C:343:ASN:O	1:C:344:ALA:C	2.59	0.44
1:B:312:ILE:HA	1:B:597:VAL:O	2.18	0.44
1:B:612:TYR:HB2	1:B:615:VAL:HG22	2.00	0.44
1:A:813:SER:O	1:A:815:ARG:N	2.50	0.44
1:A:921:LYS:HE2	1:A:921:LYS:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASN:ND2	1:B:177:MET:SD	2.91	0.43
1:B:438:SER:O	1:B:438:SER:OG	2.34	0.43
1:B:81:ASN:HB3	1:B:242:LEU:HD12	1.99	0.43
1:C:529:LYS:HB3	1:C:529:LYS:HE2	1.57	0.43
1:A:1094:VAL:HG13	1:C:900:MET:HE1	2.01	0.43
1:B:982:SER:OG	1:C:545:GLY:O	2.35	0.43
1:A:170:TYR:CE2	4:A:1302:EZO:N13	2.86	0.43
1:B:117:LEU:HD22	1:B:231:ILE:HD13	2.00	0.43
1:B:472:ILE:CG2	1:B:488:CYS:HB3	2.48	0.43
1:B:825:LYS:HE2	1:B:938:LEU:O	2.19	0.43
1:C:338:PHE:HB3	1:C:368:LEU:HD11	2.00	0.43
1:A:126:VAL:HG11	4:A:1302:EZO:C2	2.48	0.43
1:A:811:LYS:HD2	1:A:812:PRO:HD2	2.00	0.43
1:A:69:HIS:CG	1:A:259:THR:HG1	2.33	0.43
1:A:195:LYS:HD3	1:A:204:TYR:HE1	1.83	0.43
1:A:1045:LYS:HE2	1:A:1045:LYS:HB3	1.79	0.43
1:C:30:ASN:HD21	1:C:59:PHE:HD1	1.66	0.43
1:C:381:GLY:HA3	1:C:430:THR:HG23	2.01	0.43
1:A:46:SER:N	1:A:279:TYR:O	2.51	0.43
1:B:703:ASN:OD1	1:B:704:SER:N	2.52	0.43
1:B:962:LEU:HD23	1:B:962:LEU:HA	1.81	0.43
1:B:731:MET:HE2	1:B:955:ASN:HD21	1.84	0.43
1:B:921:LYS:HE2	1:B:921:LYS:HB2	1.77	0.43
1:C:734:THR:HG22	1:C:860:VAL:HG22	2.00	0.43
1:A:711:SER:O	1:A:711:SER:OG	2.27	0.43
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.50	0.43
1:C:460:ASN:O	2:c:1:NAG:H81	2.19	0.43
1:A:740:MET:HE2	1:A:740:MET:HB3	1.92	0.43
1:A:1105:THR:OG1	1:A:1106:GLN:N	2.51	0.43
1:B:503:VAL:HG21	1:C:503:VAL:HG21	2.01	0.43
1:B:1027:THR:O	1:B:1031:GLU:HG3	2.19	0.43
1:A:80:ASP:O	1:A:265:TYR:OH	2.25	0.42
1:A:203:ILE:HB	1:A:227:VAL:HG12	2.00	0.42
1:A:353:TRP:CD1	1:A:353:TRP:H	2.36	0.42
1:C:74:ASN:OD1	1:C:74:ASN:N	2.52	0.42
1:C:108:THR:CB	2:r:1:NAG:H62	2.48	0.42
1:C:148:ASN:ND2	2:v:1:NAG:O6	2.51	0.42
1:C:327:VAL:HG11	1:C:528:LYS:HG2	2.00	0.42
1:A:433:VAL:HG22	1:A:512:VAL:HG13	2.01	0.42
1:B:759:PHE:O	1:B:763:LEU:HG	2.20	0.42
1:A:902:MET:HB3	1:A:916:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:LEU:HD22	1:B:993:ILE:HD12	2.02	0.42
1:B:1072:GLU:OE1	1:B:1072:GLU:N	2.50	0.42
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.54	0.42
1:A:165:ASN:OD1	1:A:165:ASN:N	2.52	0.42
1:B:353:TRP:H	1:B:353:TRP:CD1	2.37	0.42
1:C:336:CYS:HB2	1:C:338:PHE:CZ	2.54	0.42
1:A:296:LEU:O	1:A:300:LYS:HG3	2.20	0.42
1:A:417:LYS:HD2	1:A:453:TYR:CD2	2.54	0.42
1:B:187:LYS:HE2	1:B:187:LYS:HB3	1.78	0.42
1:B:569:ILE:HG23	1:B:570:ALA:N	2.33	0.42
1:B:676:THR:OG1	1:B:677:GLN:N	2.53	0.42
1:B:740:MET:HA	1:B:744:GLY:HA2	2.02	0.42
1:C:234:ASN:OD1	2:r:1:NAG:C1	2.67	0.42
1:C:108:THR:OG1	1:C:114:THR:HG21	2.20	0.42
1:B:407:VAL:HG12	1:B:407:VAL:O	2.19	0.42
1:C:79:PHE:HB2	1:C:258:TRP:CH2	2.54	0.42
1:C:724:THR:HG22	1:C:934:ILE:HD13	2.02	0.42
1:A:460:ASN:O	2:r:1:NAG:H81	2.19	0.42
1:B:120:VAL:O	1:B:126:VAL:HA	2.20	0.42
1:A:390:LEU:HD22	1:A:517:LEU:HD22	2.01	0.42
1:B:980:ILE:HG23	1:B:984:LEU:HD12	2.01	0.42
1:B:127:VAL:HG12	1:B:129:LYS:HG3	2.02	0.42
1:C:353:TRP:CD1	1:C:353:TRP:H	2.36	0.42
1:A:79:PHE:CZ	1:A:242:LEU:HB2	2.55	0.41
1:A:83:VAL:HG11	1:A:237:ARG:HH21	1.84	0.41
1:A:312:ILE:HA	1:A:597:VAL:O	2.20	0.41
1:A:811:LYS:HG3	1:A:813:SER:O	2.19	0.41
1:B:471:GLU:O	1:B:472:ILE:C	2.62	0.41
1:B:901:GLN:O	1:B:905:ARG:HG2	2.19	0.41
1:C:1138:TYR:OH	1:C:1143:PRO:HG2	2.20	0.41
1:A:904:TYR:CE2	1:B:1107:ARG:HG2	2.56	0.41
1:B:578:ASP:HB3	1:B:581:THR:O	2.20	0.41
1:A:212:LEU:HD21	1:A:217:PRO:HD3	2.03	0.41
1:A:822:LEU:HD23	1:A:945:LEU:HD11	2.01	0.41
1:A:878:LEU:HD21	1:A:1052:PHE:HB3	2.02	0.41
1:B:472:ILE:N	1:B:472:ILE:HD12	2.36	0.41
1:C:312:ILE:HA	1:C:597:VAL:O	2.20	0.41
1:C:866:THR:OG1	1:C:869:MET:HG3	2.20	0.41
1:C:1126:CYS:HB2	1:C:1132:ILE:HG12	2.01	0.41
1:A:811:LYS:HD2	1:A:812:PRO:CD	2.50	0.41
1:A:878:LEU:HD11	1:A:1054:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:HB2	1:B:563:GLN:HG3	2.01	0.41
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.88	0.41
1:C:643:PHE:CE2	1:C:645:THR:HG22	2.55	0.41
1:A:357:ARG:HD3	4:C:1302:EZO:C23	2.49	0.41
1:B:726:ILE:HD12	1:B:1061:VAL:HG22	2.03	0.41
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.20	0.41
1:A:108:THR:HG23	2:N:1:NAG:H62	2.02	0.41
1:A:350:VAL:HG22	1:A:422:ASN:HB3	2.02	0.41
1:B:214:ARG:HD2	1:B:214:ARG:HA	1.82	0.41
1:C:31:SER:HB3	1:C:62:VAL:HG21	2.02	0.41
1:C:216:LEU:HD12	1:C:216:LEU:HA	1.91	0.41
1:A:825:LYS:HA	1:A:825:LYS:HD3	1.86	0.41
1:B:281:GLU:HG2	2:d:1:NAG:HN2	1.85	0.41
1:C:343:ASN:O	1:C:343:ASN:CG	2.64	0.41
1:C:662:CYS:HB2	1:C:697:MET:HG3	2.02	0.41
1:A:122:ASN:HB3	1:A:157:PHE:HE2	1.86	0.41
1:A:231:ILE:O	1:A:231:ILE:HG13	2.20	0.41
1:A:326:ILE:HG21	1:A:534:VAL:HG22	2.02	0.41
1:A:662:CYS:HB2	1:A:697:MET:HE3	2.03	0.41
1:C:53:ASP:HB2	1:C:55:PHE:CE2	2.56	0.41
1:C:401:VAL:HG22	1:C:509:ARG:HG2	2.03	0.41
1:C:823:PHE:CD1	1:C:823:PHE:C	2.99	0.41
1:C:962:LEU:HD23	1:C:962:LEU:HA	1.83	0.41
1:C:1086:LYS:HE3	1:C:1086:LYS:HB2	1.82	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:CZ2	2.56	0.41
1:A:408:ARG:HH11	1:A:408:ARG:HB2	1.86	0.41
1:C:226:LEU:HG	1:C:227:VAL:N	2.36	0.41
1:B:244:LEU:HD21	1:B:258:TRP:CE3	2.55	0.40
1:B:338:PHE:HB3	1:B:368:LEU:HD21	2.03	0.40
1:B:421:TYR:HB3	1:B:454:ARG:HG2	2.03	0.40
1:C:444:LYS:HB3	1:C:444:LYS:HE3	1.88	0.40
1:C:731:MET:H	1:C:774:GLN:HG3	1.85	0.40
1:B:20:THR:O	1:B:20:THR:OG1	2.35	0.40
1:B:24:LEU:HB3	1:B:78:ARG:NH1	2.20	0.40
1:B:42:VAL:HG11	1:C:567:ARG:HG3	2.03	0.40
1:B:111:ASP:HB3	1:B:113:LYS:HD2	2.04	0.40
1:B:244:LEU:HA	1:B:244:LEU:HD23	1.76	0.40
1:B:920:GLN:O	1:B:923:ILE:N	2.55	0.40
1:C:214:ARG:HD3	1:C:214:ARG:HA	1.98	0.40
1:C:709:ASN:CG	2:k:1:NAG:C1	2.94	0.40
1:C:980:ILE:HG21	1:C:992:GLN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:CE1	1:A:244:LEU:HD22	2.57	0.40
1:A:600:PRO:HB3	1:A:674:TYR:HB2	2.04	0.40
1:A:717:ASN:HB2	1:A:1071:GLN:HB2	2.04	0.40
1:C:722:VAL:HA	1:C:1064:HIS:O	2.21	0.40
1:A:108:THR:HG22	1:A:109:THR:HG23	2.02	0.40
1:C:37:TYR:OH	1:C:54:LEU:O	2.37	0.40
1:C:327:VAL:HG22	1:C:542:ASN:HB3	2.02	0.40
1:A:54:LEU:HD22	1:A:88:ASP:HB3	2.02	0.40
1:A:124:THR:O	1:A:174:PRO:HA	2.20	0.40
1:B:146:HIS:HB3	1:B:148:ASN:ND2	2.37	0.40
1:B:475:ALA:O	1:B:487:ASN:HB3	2.21	0.40
1:C:201:PHE:HB2	1:C:231:ILE:HD11	2.02	0.40
1:C:825:LYS:HE3	1:C:938:LEU:O	2.21	0.40

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	A	1103/1275 (86%)	1053 (96%)	50 (4%)	0	100	100
1	B	1103/1275 (86%)	1058 (96%)	45 (4%)	0	100	100
1	C	1103/1275 (86%)	1050 (95%)	52 (5%)	1 (0%)	48	72
All	All	3309/3825 (86%)	3161 (96%)	147 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1132	ILE

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	964/1104 (87%)	958 (99%)	6 (1%)	78	89
1	B	964/1104 (87%)	961 (100%)	3 (0%)	86	92
1	C	964/1104 (87%)	958 (99%)	6 (1%)	78	89
All	All	2892/3312 (87%)	2877 (100%)	15 (0%)	78	90

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	165	ASN
1	A	234	ASN
1	A	403	ARG
1	A	408	ARG
1	A	907	ASN
1	B	113	LYS
1	B	234	ASN
1	B	919	ASN
1	C	61	ASN
1	C	113	LYS
1	C	234	ASN
1	C	343	ASN
1	C	408	ARG
1	C	709	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	234	ASN
1	A	487	ASN
1	A	657	ASN
1	A	658	ASN
1	A	764	ASN

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Mol	Chain	Res	Type
1	A	856	ASN
1	A	907	ASN
1	A	913	GLN
1	A	1058	HIS
1	A	1142	GLN
1	B	148	ASN
1	B	165	ASN
1	B	606	ASN
1	B	856	ASN
1	B	872	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	1005	GLN
1	B	1071	GLN
1	B	1125	ASN
1	B	1142	GLN
1	C	61	ASN
1	C	99	ASN
1	C	234	ASN
1	C	331	ASN
1	C	544	ASN
1	C	658	ASN
1	C	717	ASN
1	C	935	GLN
1	C	955	ASN
1	C	1005	GLN
1	C	1142	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

90 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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.42	0
2	NAG	E	1	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	E	2	2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	F	1	2	14,14,15	0.50	0	17,19,21	0.43	0
2	NAG	F	2	2	14,14,15	0.40	0	17,19,21	0.41	0
2	NAG	G	1	2,1	14,14,15	0.23	0	17,19,21	0.38	0
2	NAG	G	2	2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	H	1	2	14,14,15	0.36	0	17,19,21	0.41	0
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	I	1	2,1	14,14,15	0.27	0	17,19,21	0.38	0
2	NAG	I	2	2	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	J	1	2,1	14,14,15	0.54	0	17,19,21	0.87	1 (5%)
2	NAG	J	2	2	14,14,15	0.22	0	17,19,21	0.53	0
2	NAG	K	1	2,1	14,14,15	0.33	0	17,19,21	0.55	0
2	NAG	K	2	2	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	L	1	2,1	14,14,15	0.77	1 (7%)	17,19,21	0.86	1 (5%)
2	NAG	L	2	2	14,14,15	0.23	0	17,19,21	0.50	0
2	NAG	M	1	2,1	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	M	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	N	1	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	N	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	O	1	2,1	14,14,15	0.33	0	17,19,21	0.47	0
2	NAG	O	2	2	14,14,15	0.27	0	17,19,21	0.43	0
2	NAG	P	1	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	P	2	2	14,14,15	0.37	0	17,19,21	0.40	0
2	NAG	Q	1	2,1	14,14,15	0.30	0	17,19,21	0.41	0
2	NAG	Q	2	2	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	R	1	2	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	R	2	2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	S	1	2,1	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	S	2	2	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	T	1	2,1	14,14,15	0.32	0	17,19,21	0.46	0
2	NAG	T	2	2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	U	1	2,1	14,14,15	0.81	1 (7%)	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	U	2	2	14,14,15	0.25	0	17,19,21	0.60	0
2	NAG	V	1	2,1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	V	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	W	1	2,1	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	W	2	2	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	X	1	2,1	14,14,15	0.24	0	17,19,21	0.39	0
2	NAG	X	2	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	Y	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	0.96	1 (5%)
2	NAG	Y	2	2	14,14,15	0.19	0	17,19,21	0.54	0
2	NAG	Z	1	2,1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	Z	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	a	1	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	a	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	b	1	2,1	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	b	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	c	1	2	14,14,15	0.62	0	17,19,21	0.82	0
2	NAG	c	2	2	14,14,15	0.27	0	17,19,21	0.42	0
2	NAG	d	1	2,1	14,14,15	0.42	0	17,19,21	1.13	2 (11%)
2	NAG	d	2	2	14,14,15	0.24	0	17,19,21	0.43	0
2	NAG	e	1	2	14,14,15	0.71	1 (7%)	17,19,21	0.89	1 (5%)
2	NAG	e	2	2	14,14,15	0.20	0	17,19,21	0.49	0
2	NAG	f	1	2,1	14,14,15	0.53	0	17,19,21	0.50	0
2	NAG	f	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	g	1	2,1	14,14,15	0.39	0	17,19,21	0.36	0
2	NAG	g	2	2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	h	1	2	14,14,15	0.32	0	17,19,21	0.43	0
2	NAG	h	2	2	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	i	1	2,1	14,14,15	0.31	0	17,19,21	0.46	0
2	NAG	i	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	j	1	2	14,14,15	1.54	2 (14%)	17,19,21	1.40	1 (5%)
2	NAG	j	2	2	14,14,15	1.16	2 (14%)	17,19,21	0.91	1 (5%)
2	NAG	k	1	2	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	k	2	2	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	l	1	2	14,14,15	0.37	0	17,19,21	0.72	0
2	NAG	l	2	2	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	m	1	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	m	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	n	1	2,1	14,14,15	0.74	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	n	2	2	14,14,15	0.21	0	17,19,21	0.55	0
2	NAG	o	1	2	14,14,15	0.27	0	17,19,21	0.40	0
2	NAG	o	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	p	1	2,1	14,14,15	0.19	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	p	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	q	1	2,1	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	q	2	2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	r	1	2	14,14,15	0.36	0	17,19,21	0.64	0
2	NAG	r	2	2	14,14,15	0.28	0	17,19,21	0.42	0
2	NAG	s	1	2,1	14,14,15	0.19	0	17,19,21	0.45	0
2	NAG	s	2	2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	t	1	2	14,14,15	0.45	0	17,19,21	0.68	1 (5%)
2	NAG	t	2	2	14,14,15	0.43	0	17,19,21	0.39	0
2	NAG	u	1	2,1	14,14,15	0.55	0	17,19,21	0.73	1 (5%)
2	NAG	u	2	2	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	v	1	2,1	14,14,15	0.37	0	17,19,21	0.46	0
2	NAG	v	2	2	14,14,15	0.21	0	17,19,21	0.50	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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	1/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	4/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	4/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
2	NAG	W	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	1/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	NAG	a	1	2	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	NAG	b	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	NAG	c	1	2	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	2/6/23/26	0/1/1/1
2	NAG	d	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
2	NAG	e	1	2	-	4/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	g	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	NAG	h	1	2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	2/6/23/26	0/1/1/1
2	NAG	i	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	i	2	2	-	2/6/23/26	0/1/1/1
2	NAG	j	1	2	-	4/6/23/26	0/1/1/1
2	NAG	j	2	2	-	4/6/23/26	0/1/1/1
2	NAG	k	1	2	-	0/6/23/26	0/1/1/1
2	NAG	k	2	2	-	0/6/23/26	0/1/1/1
2	NAG	l	1	2	-	2/6/23/26	0/1/1/1
2	NAG	l	2	2	-	2/6/23/26	0/1/1/1
2	NAG	m	1	2	-	2/6/23/26	0/1/1/1
2	NAG	m	2	2	-	3/6/23/26	0/1/1/1
2	NAG	n	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	n	2	2	-	2/6/23/26	0/1/1/1
2	NAG	o	1	2	-	2/6/23/26	0/1/1/1
2	NAG	o	2	2	-	0/6/23/26	0/1/1/1
2	NAG	p	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	p	2	2	-	0/6/23/26	0/1/1/1
2	NAG	q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	r	1	2	-	2/6/23/26	0/1/1/1
2	NAG	r	2	2	-	0/6/23/26	0/1/1/1
2	NAG	s	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	s	2	2	-	0/6/23/26	0/1/1/1
2	NAG	t	1	2	-	2/6/23/26	0/1/1/1
2	NAG	t	2	2	-	0/6/23/26	0/1/1/1
2	NAG	u	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	u	2	2	-	0/6/23/26	0/1/1/1
2	NAG	v	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	v	2	2	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	1	NAG	O5-C1	5.09	1.52	1.43
2	j	2	NAG	O5-C1	3.48	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1	NAG	O5-C1	-2.68	1.39	1.43
2	j	1	NAG	C1-C2	2.58	1.55	1.52
2	j	2	NAG	C1-C2	2.44	1.55	1.52
2	U	1	NAG	O5-C1	2.43	1.47	1.43
2	Y	1	NAG	C1-C2	2.24	1.55	1.52
2	n	1	NAG	C1-C2	2.06	1.55	1.52
2	e	1	NAG	C1-C2	2.00	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	1	NAG	C1-O5-C5	5.32	119.32	112.19
2	d	1	NAG	C1-O5-C5	3.47	116.83	112.19
2	j	2	NAG	C1-O5-C5	3.43	116.79	112.19
2	U	1	NAG	C1-O5-C5	3.12	116.37	112.19
2	n	1	NAG	C1-O5-C5	3.00	116.21	112.19
2	Y	1	NAG	C1-O5-C5	2.92	116.10	112.19
2	e	1	NAG	C1-O5-C5	2.87	116.03	112.19
2	J	1	NAG	C1-O5-C5	2.85	116.01	112.19
2	d	1	NAG	C3-C4-C5	2.39	114.57	110.23
2	u	1	NAG	C1-O5-C5	2.27	115.23	112.19
2	L	1	NAG	C3-C4-C5	2.06	113.98	110.23
2	t	1	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	v	1	NAG	O5-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	m	1	NAG	O5-C5-C6-O6
2	o	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	U	1	NAG	C4-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	j	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	u	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	o	1	NAG	C4-C5-C6-O6
2	v	1	NAG	C4-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
2	f	1	NAG	C4-C5-C6-O6
2	s	1	NAG	O5-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6
2	m	1	NAG	C4-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
2	l	2	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	j	1	NAG	C4-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	P	2	NAG	C8-C7-N2-C2
2	P	2	NAG	O7-C7-N2-C2
2	S	2	NAG	C8-C7-N2-C2
2	S	2	NAG	O7-C7-N2-C2
2	e	1	NAG	C8-C7-N2-C2
2	e	1	NAG	O7-C7-N2-C2
2	h	2	NAG	C8-C7-N2-C2
2	h	2	NAG	O7-C7-N2-C2
2	j	1	NAG	C8-C7-N2-C2
2	j	1	NAG	O7-C7-N2-C2
2	j	2	NAG	C8-C7-N2-C2
2	j	2	NAG	O7-C7-N2-C2
2	t	1	NAG	C8-C7-N2-C2
2	t	1	NAG	O7-C7-N2-C2
2	V	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	u	1	NAG	C4-C5-C6-O6
2	r	1	NAG	C4-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	i	2	NAG	C4-C5-C6-O6
2	s	1	NAG	C4-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	q	2	NAG	C4-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
2	r	1	NAG	O5-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	n	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	q	2	NAG	O5-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	i	1	NAG	O5-C5-C6-O6
2	l	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	l	1	NAG	O5-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	n	2	NAG	C4-C5-C6-O6
2	U	2	NAG	C3-C2-N2-C7
2	n	2	NAG	O5-C5-C6-O6
2	n	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C1-C2-N2-C7
2	U	2	NAG	C1-C2-N2-C7
2	l	1	NAG	C1-C2-N2-C7
2	m	2	NAG	C1-C2-N2-C7
2	f	1	NAG	C3-C2-N2-C7
2	E	2	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	j	2	NAG	O5-C5-C6-O6
2	j	2	NAG	C4-C5-C6-O6
2	m	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

20 monomers are involved in 36 short contacts:

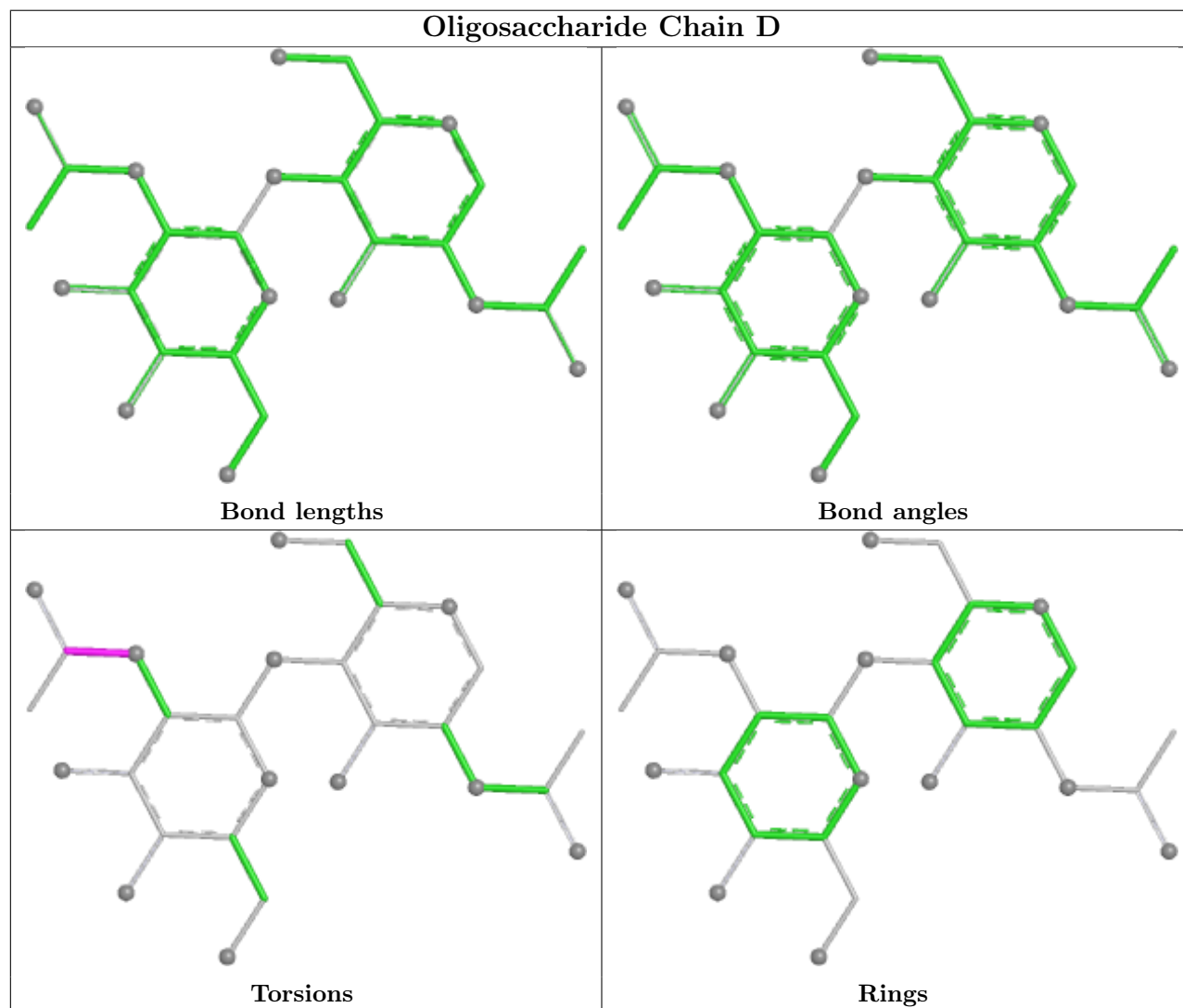
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	j	1	NAG	1	0
2	T	1	NAG	1	0
2	Y	2	NAG	1	0
2	f	1	NAG	1	0
2	s	1	NAG	1	0
2	v	1	NAG	1	0
2	l	1	NAG	3	0
2	c	1	NAG	2	0
2	G	1	NAG	1	0
2	k	1	NAG	1	0
2	M	1	NAG	3	0
2	K	1	NAG	1	0
2	P	1	NAG	1	0
2	d	1	NAG	1	0
2	F	1	NAG	1	0
2	i	1	NAG	1	0

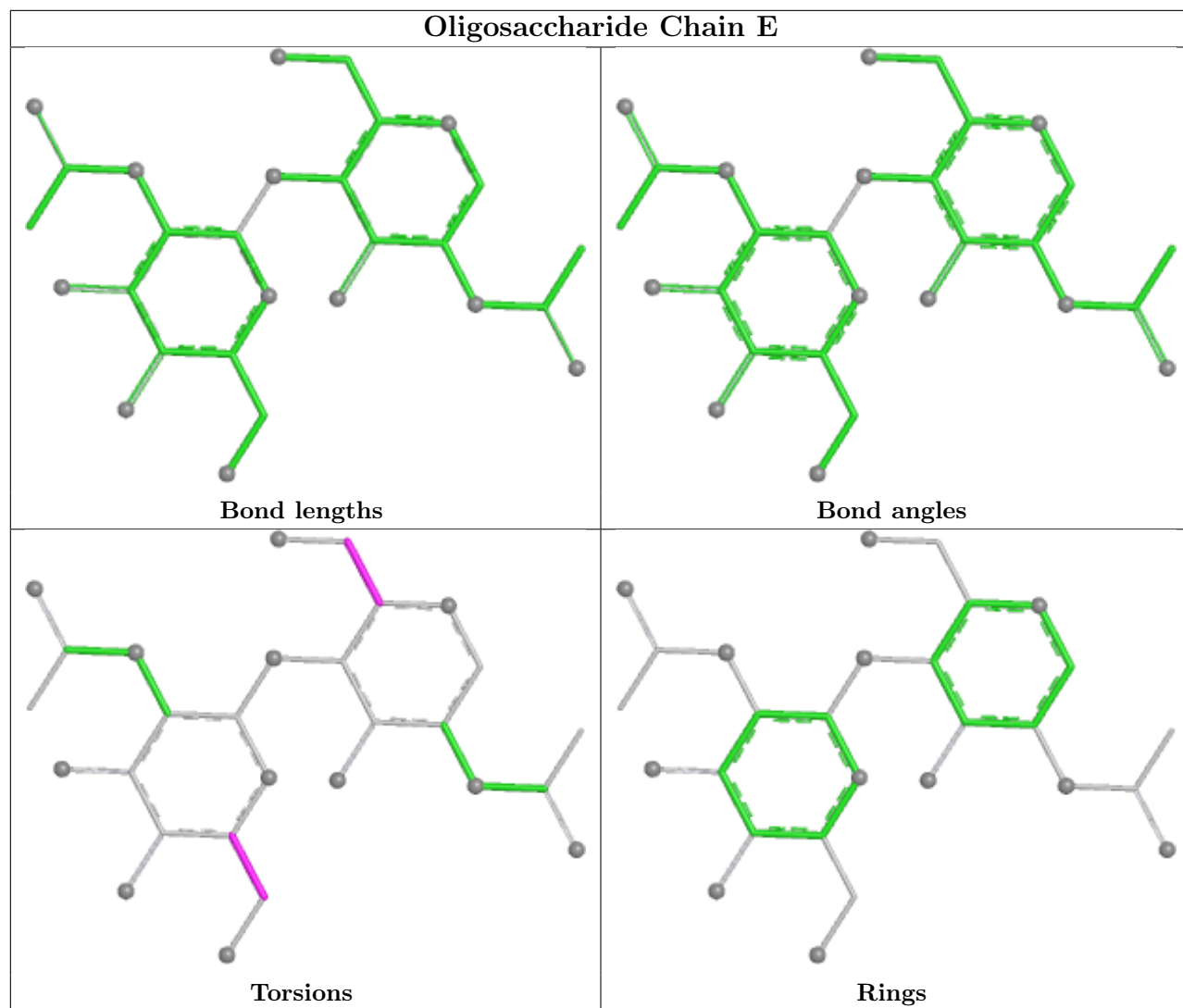
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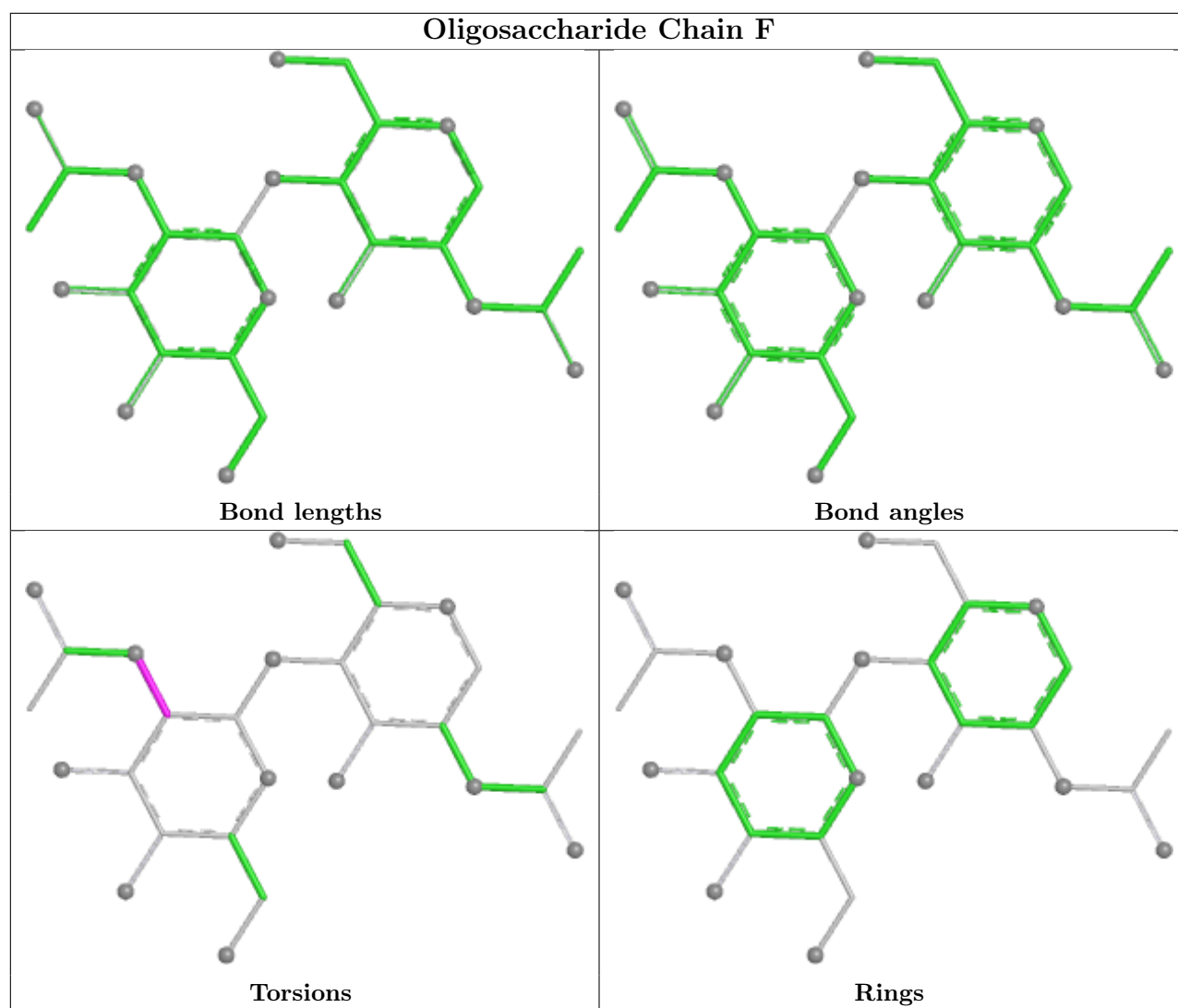
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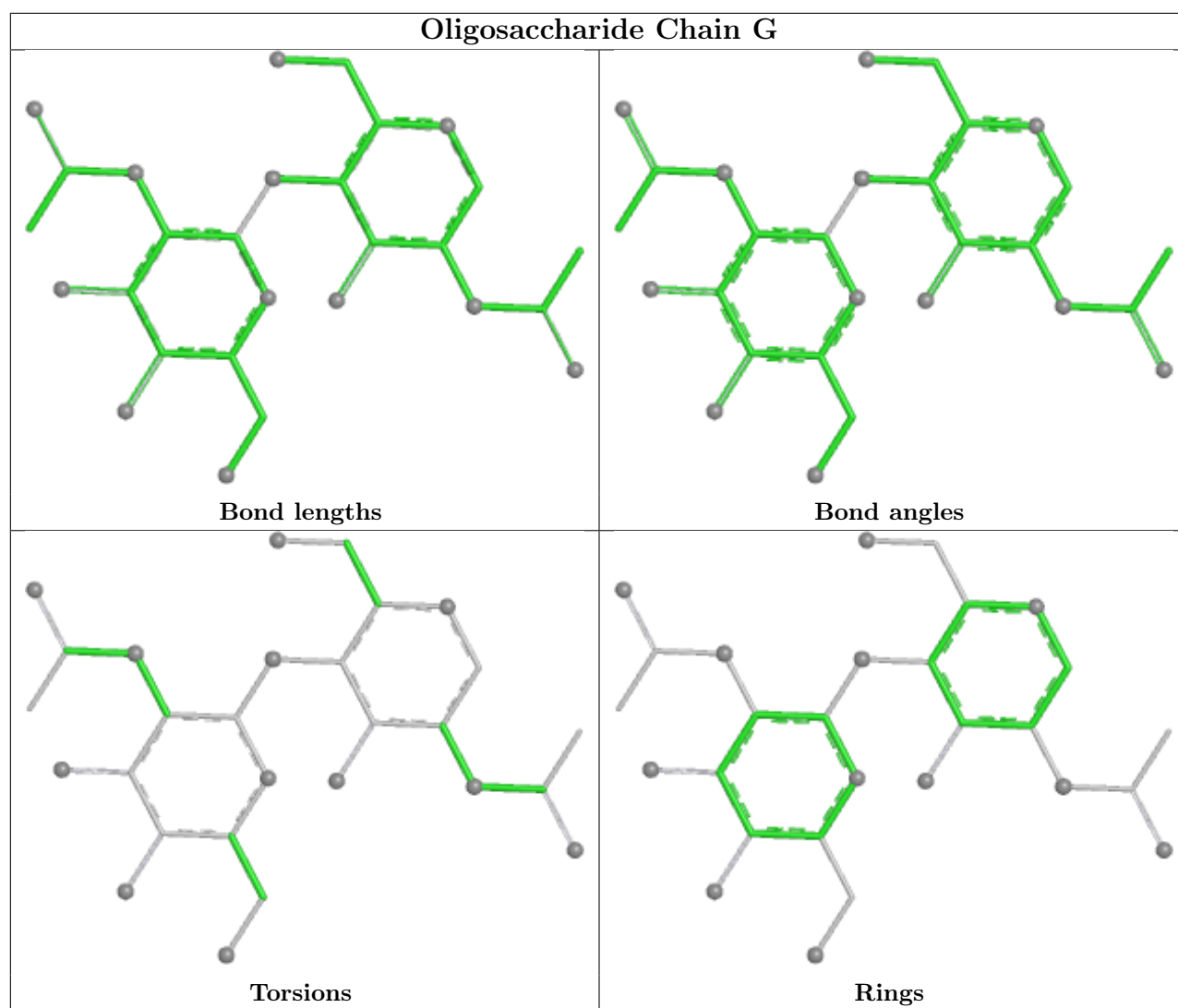
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	g	1	NAG	2	0
2	r	1	NAG	7	0
2	e	1	NAG	4	0
2	N	1	NAG	2	0

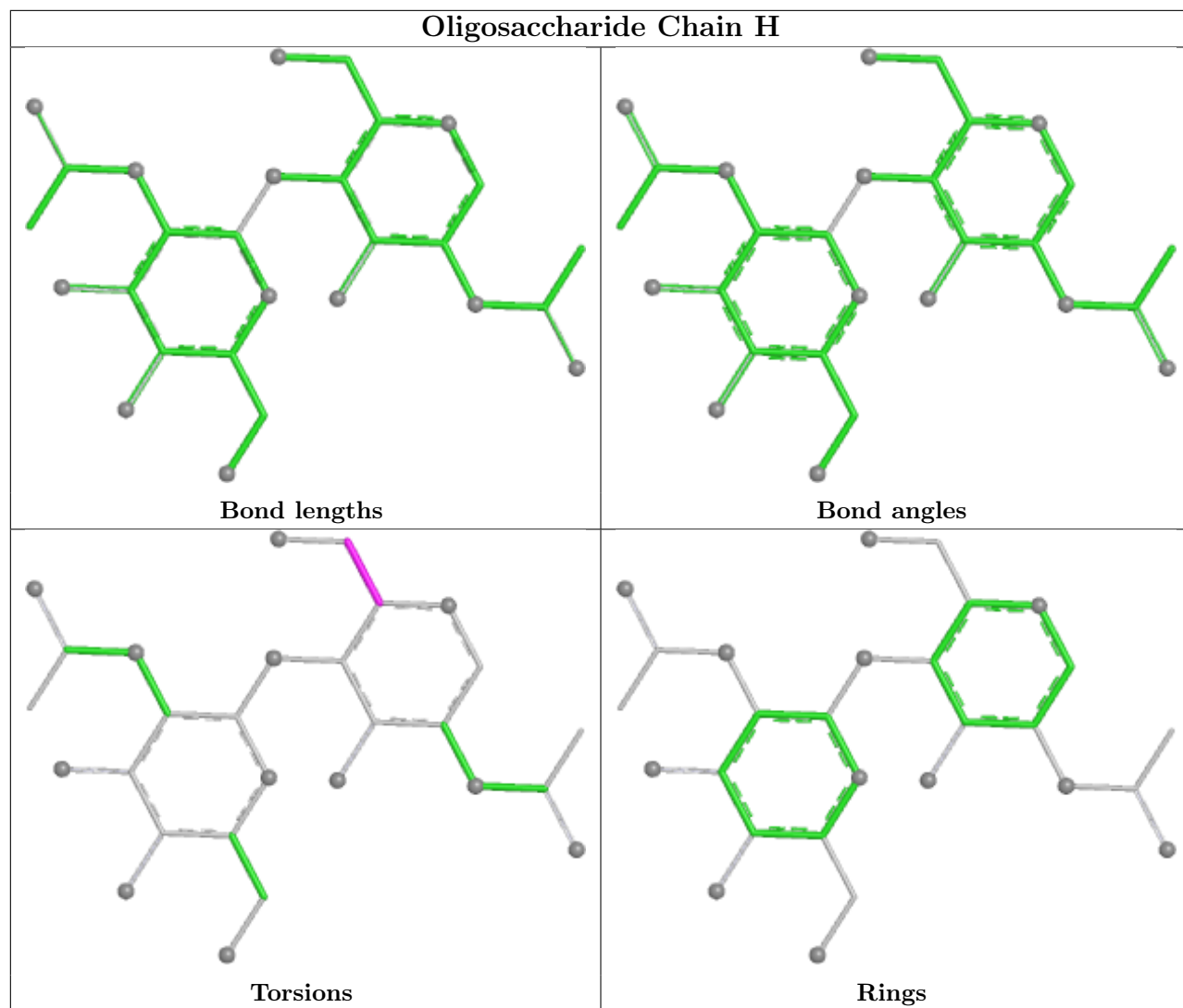
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

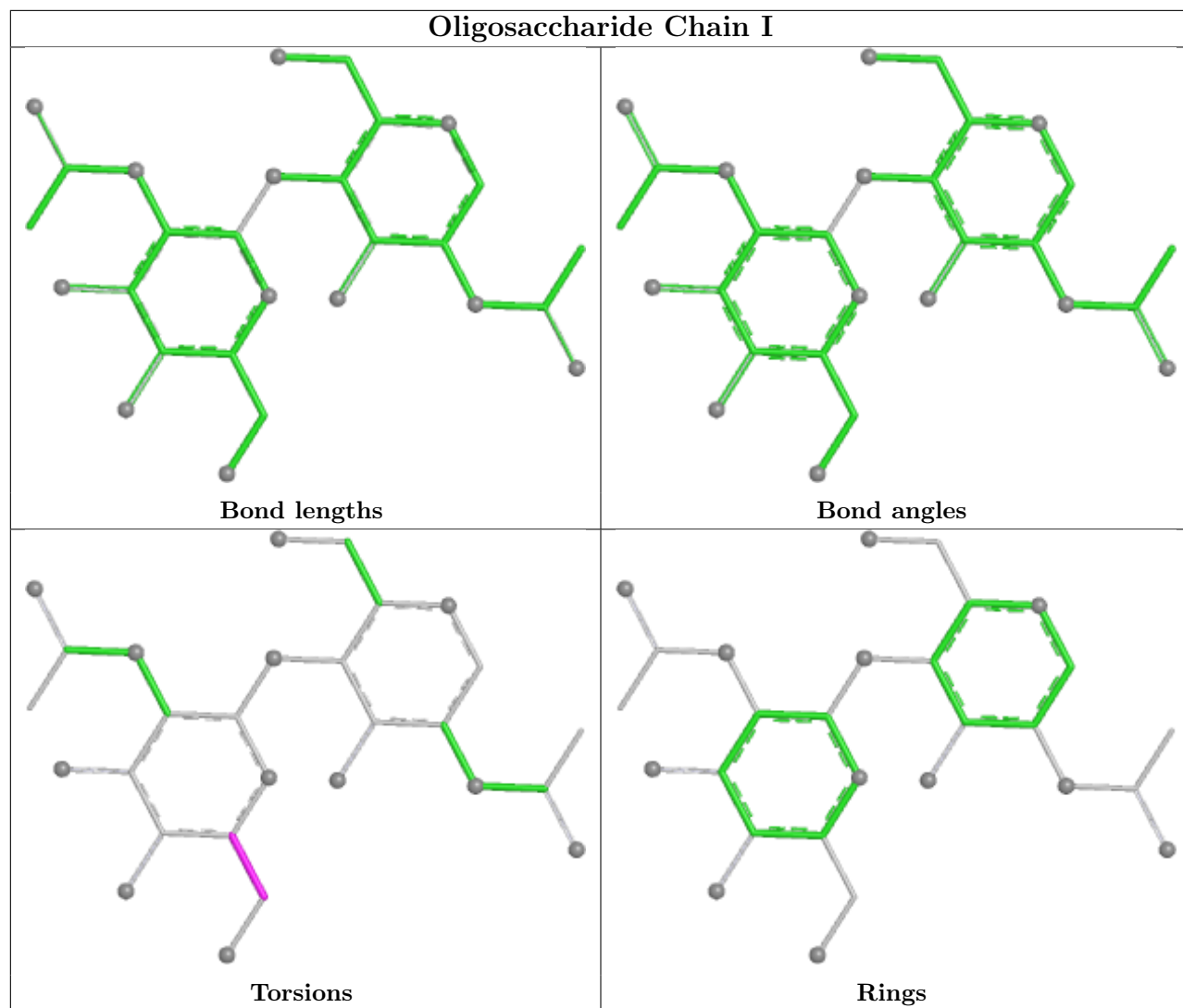


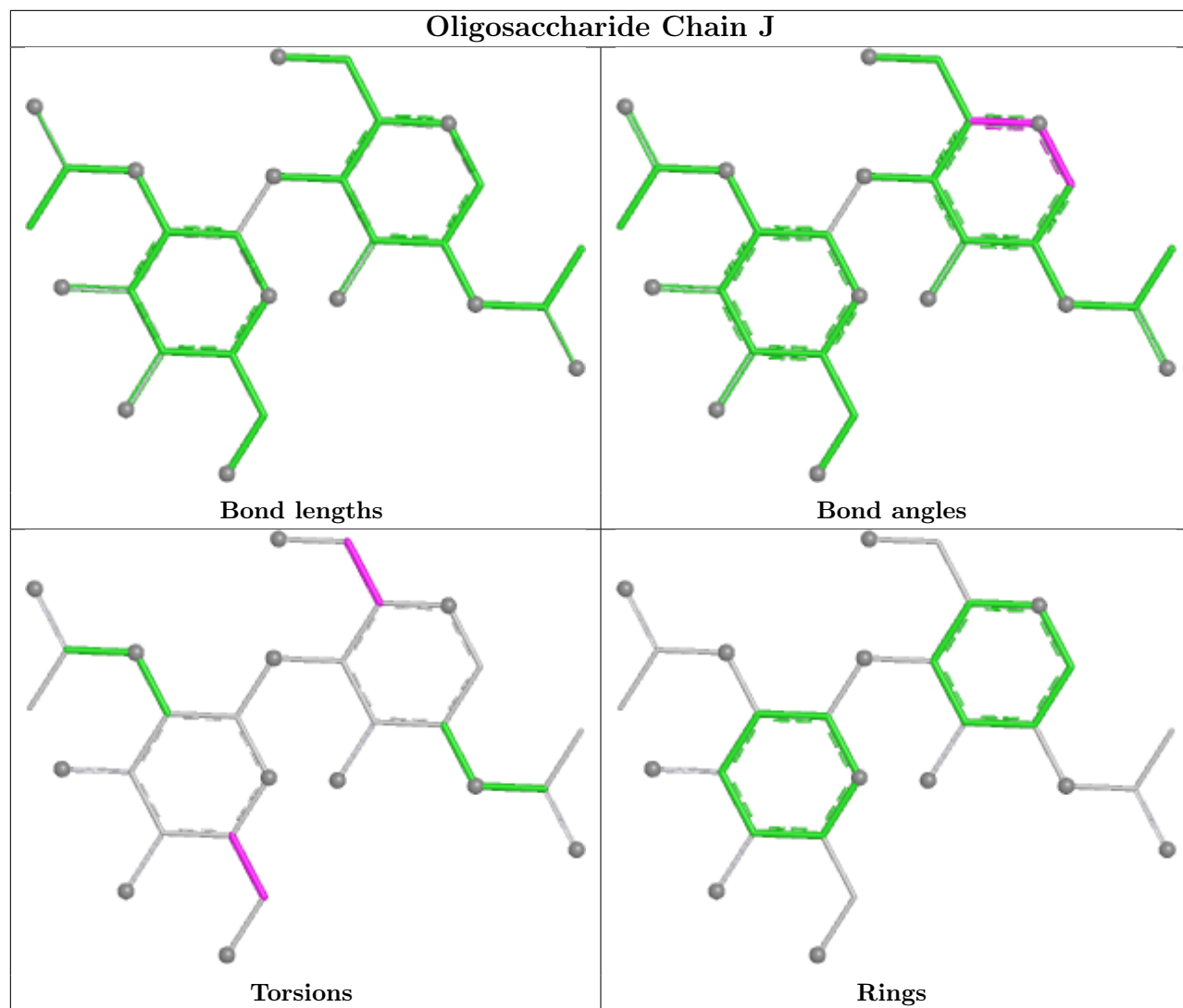


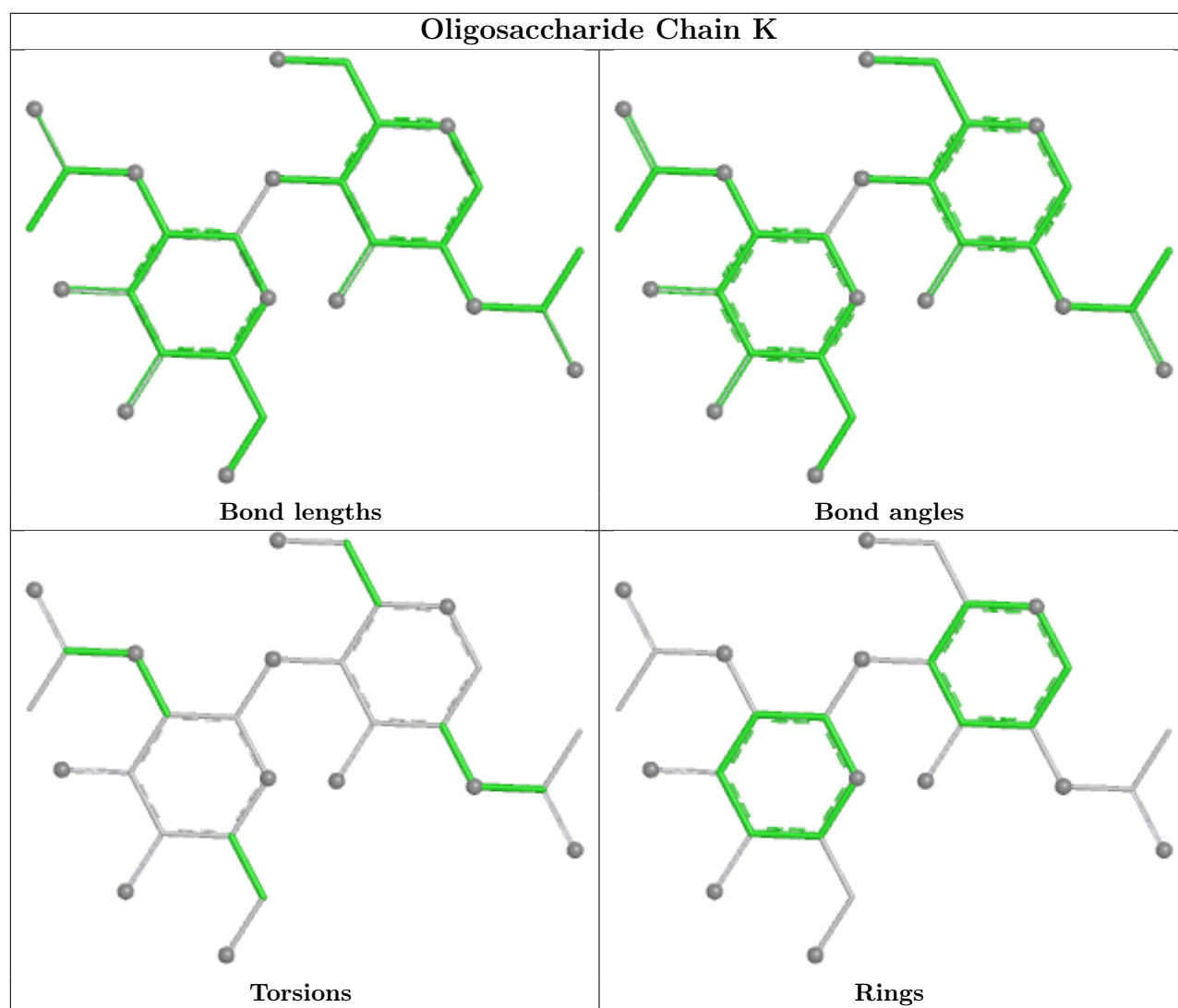


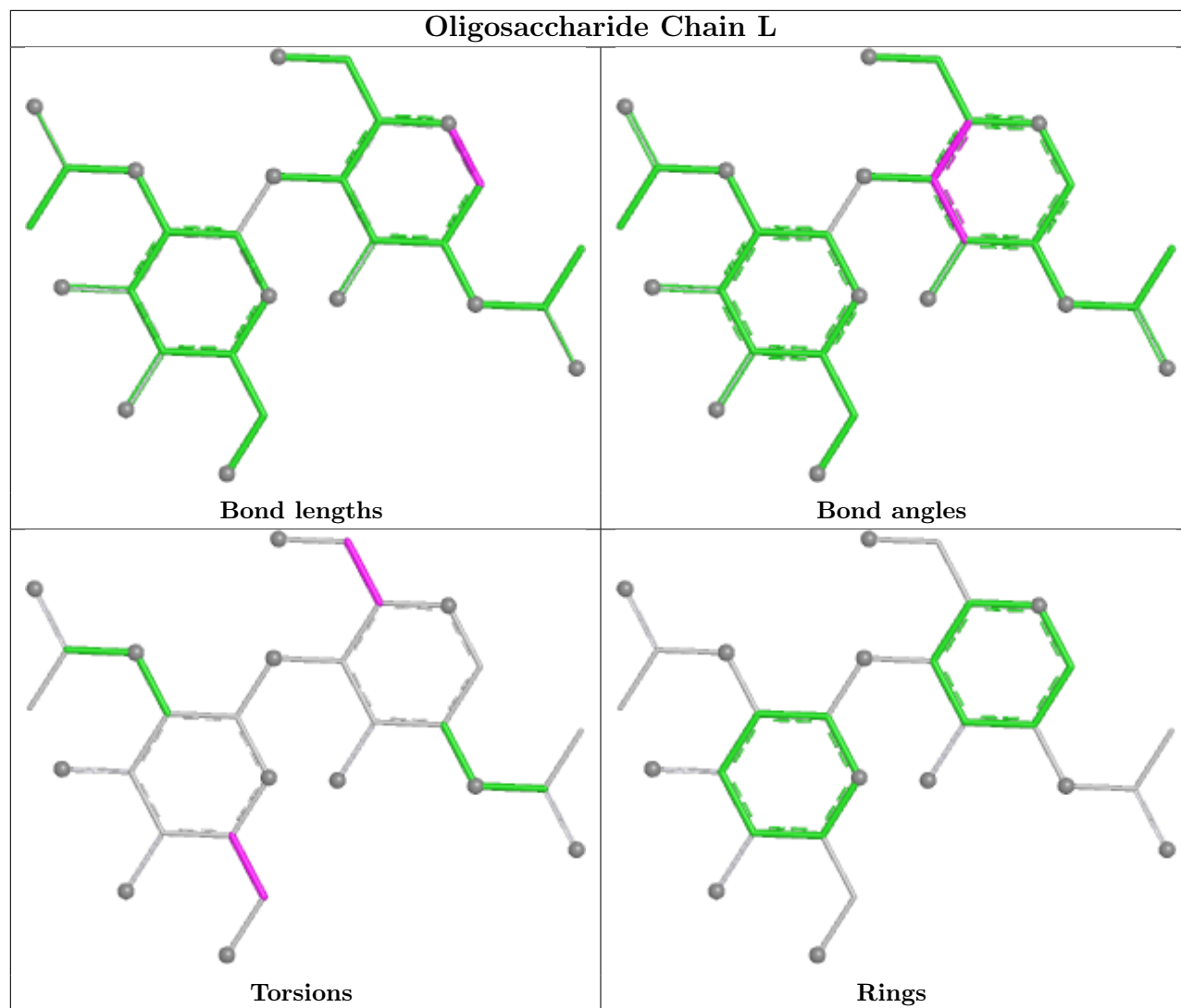


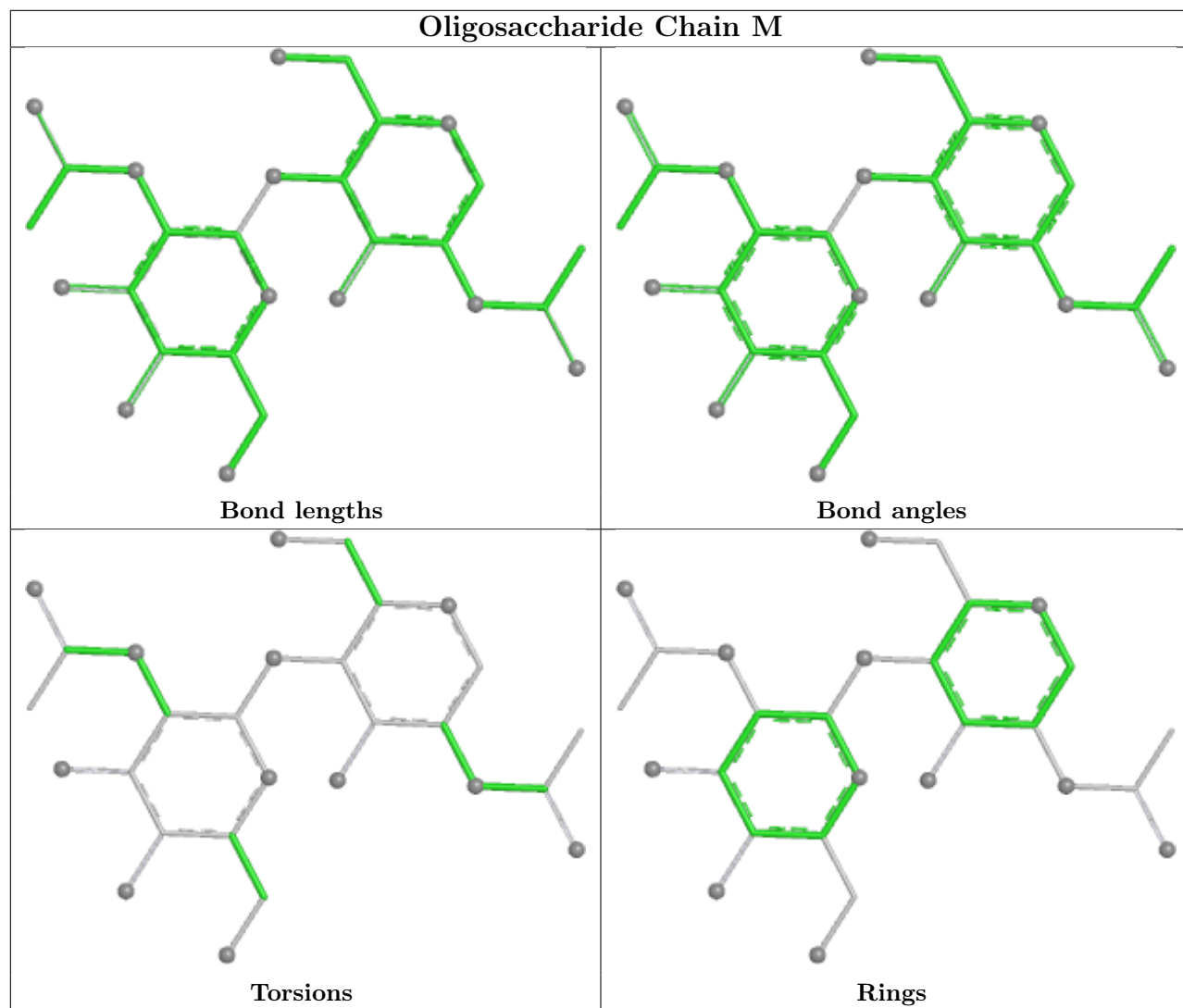


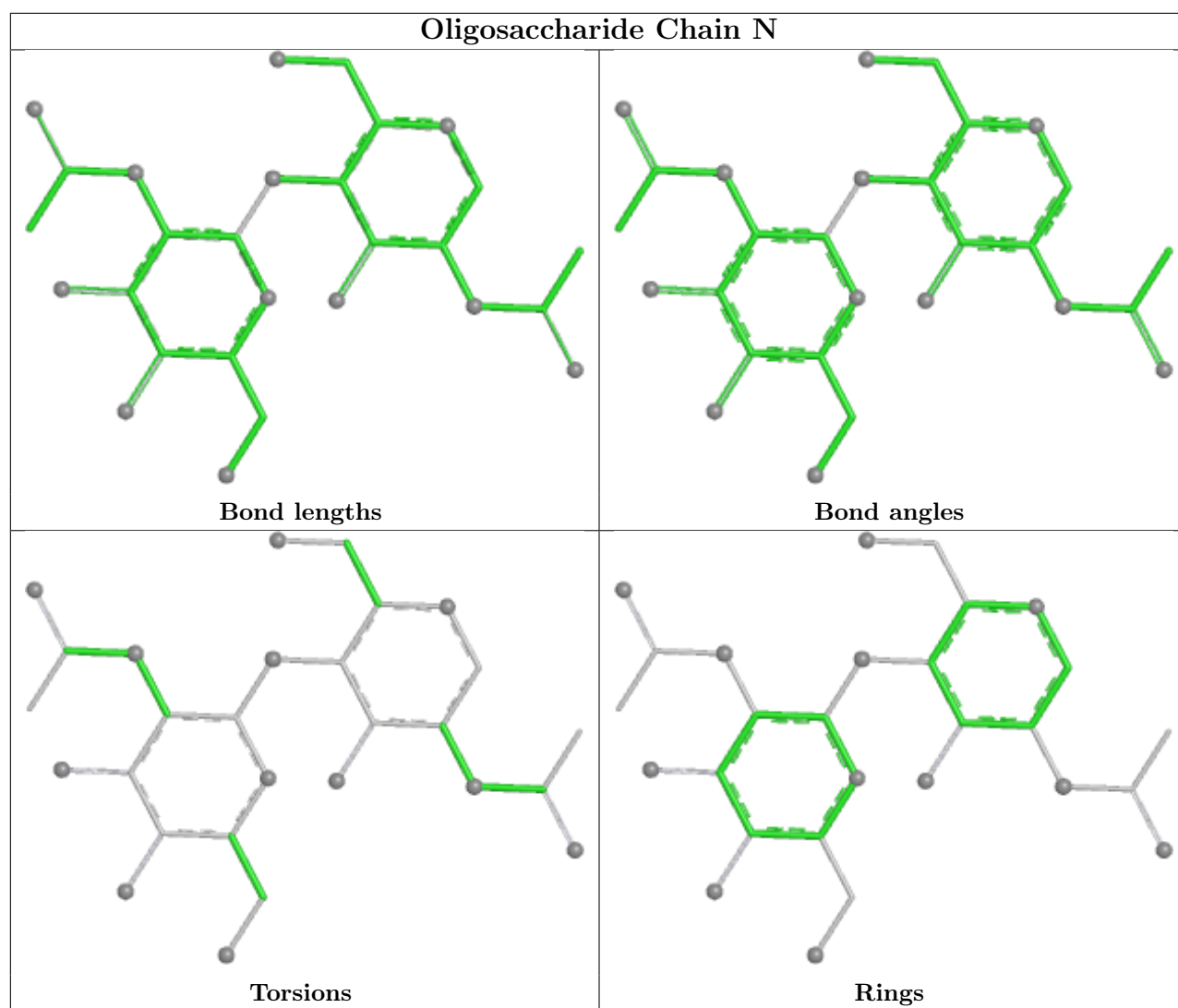


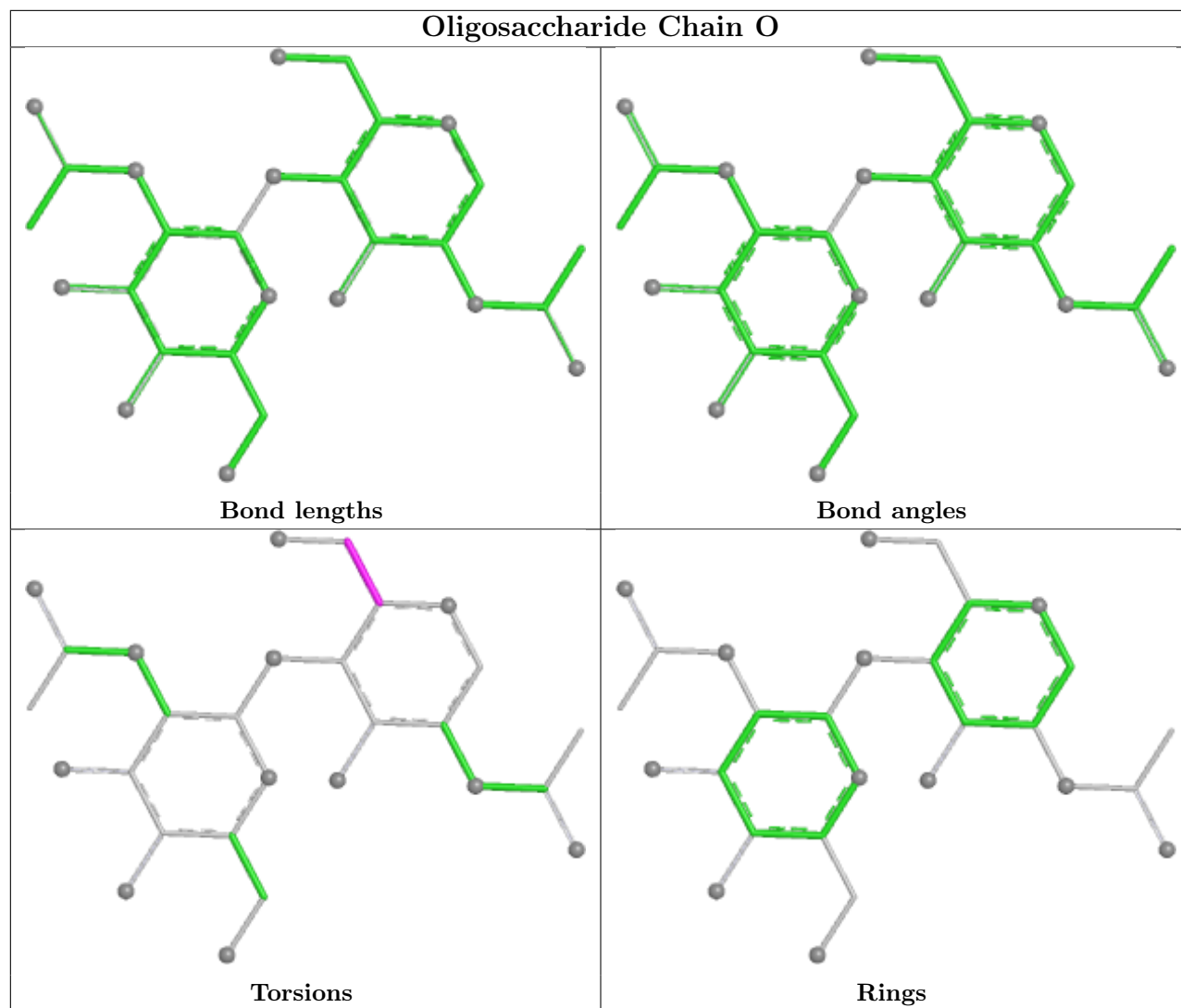


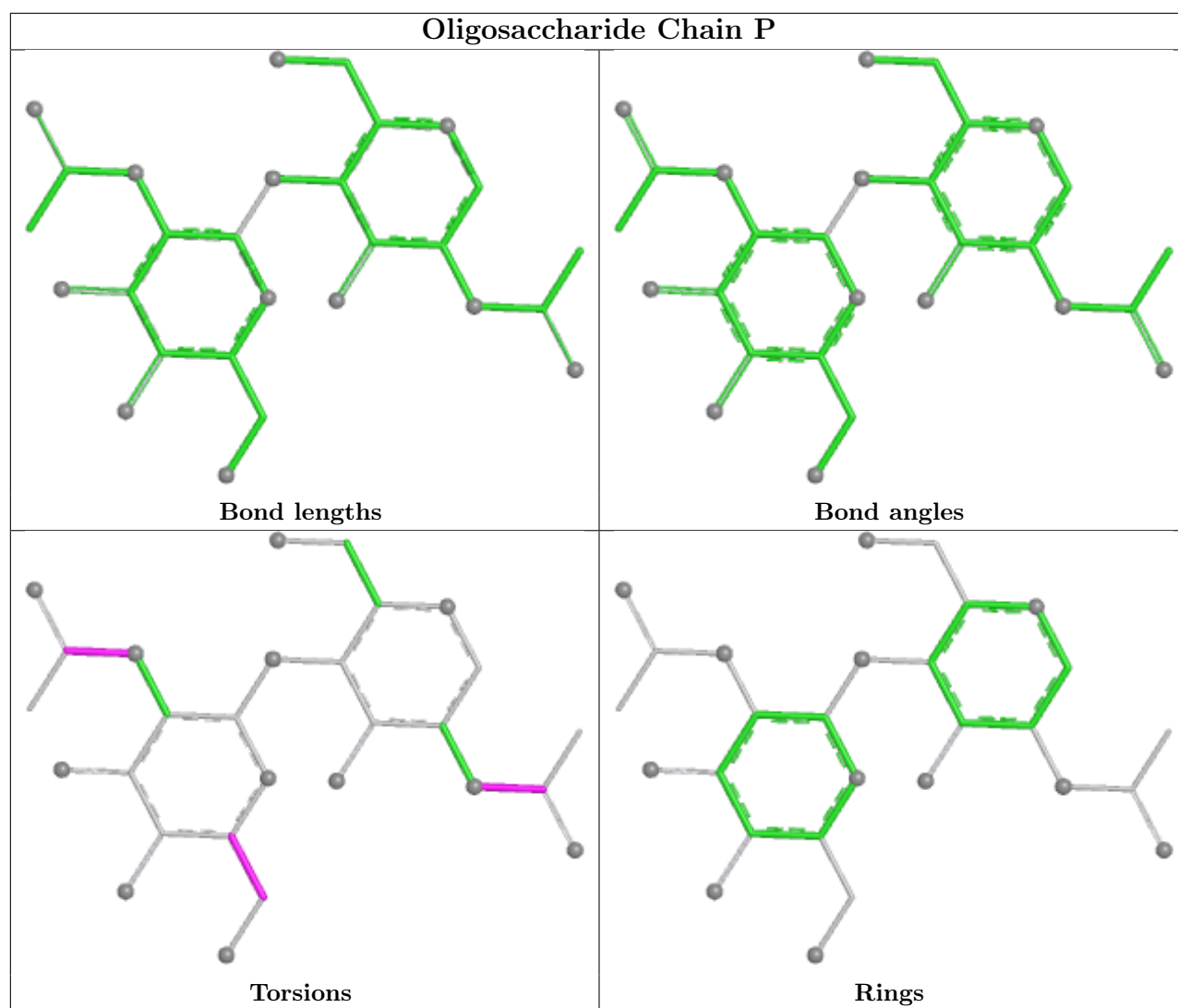


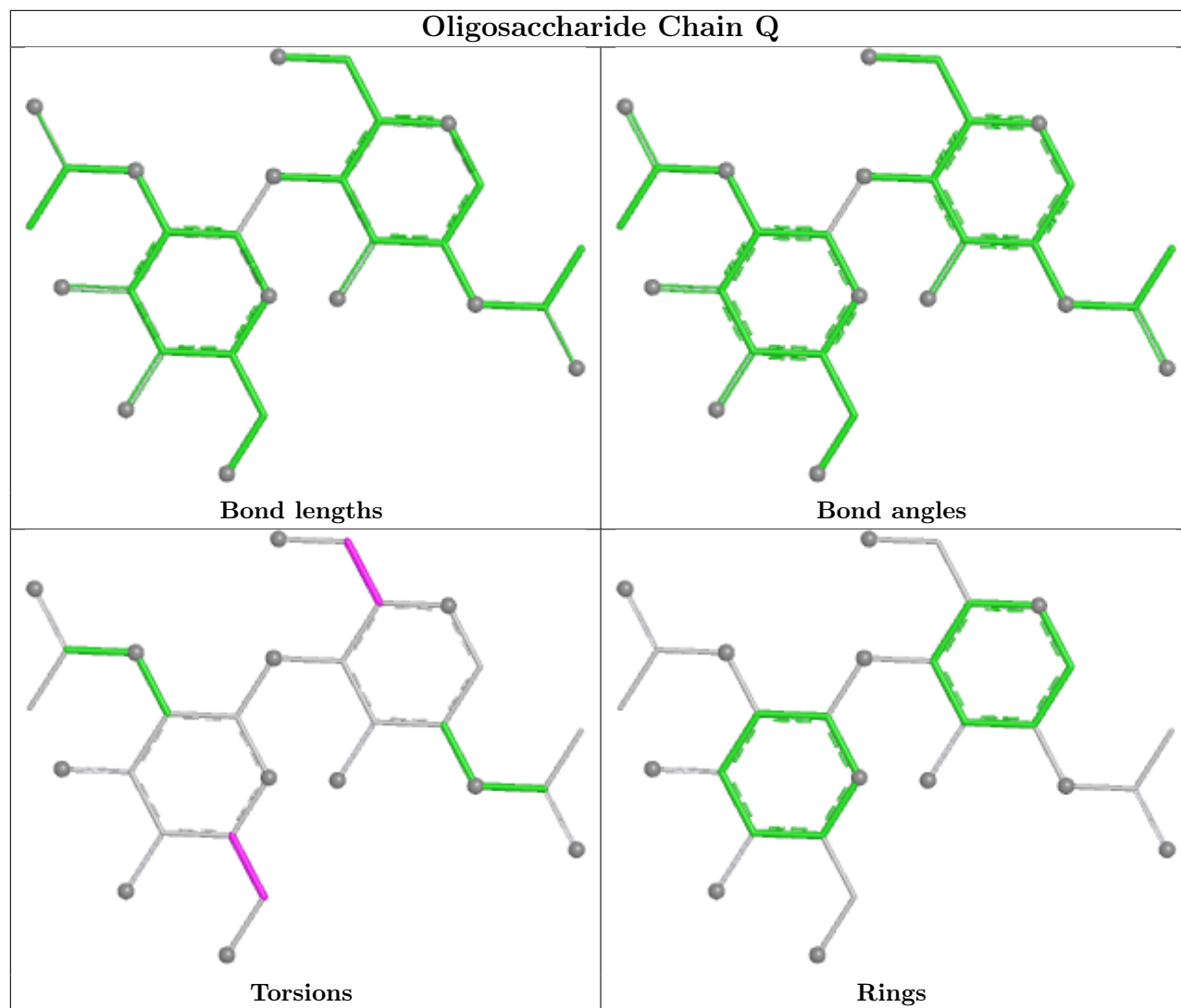


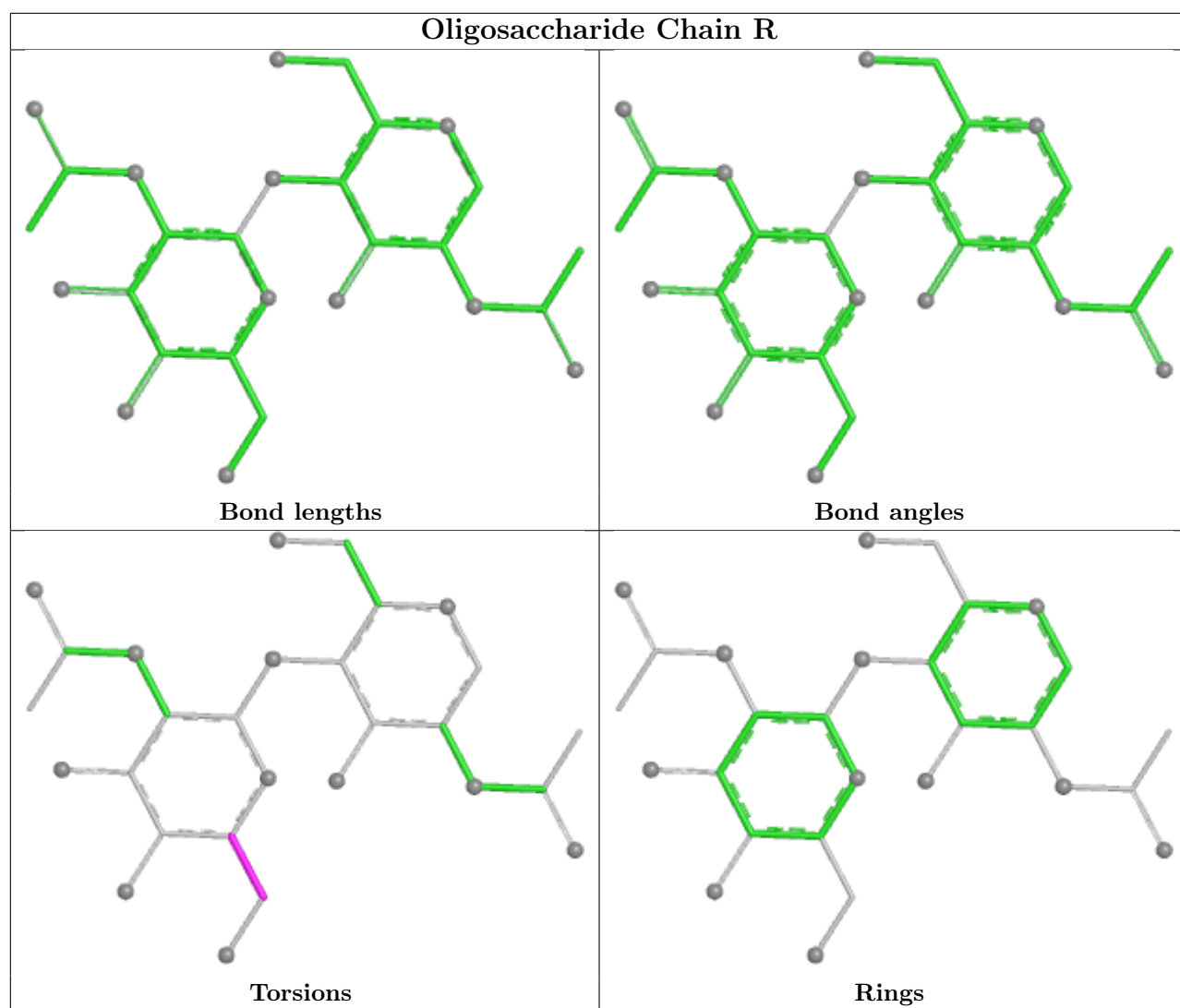


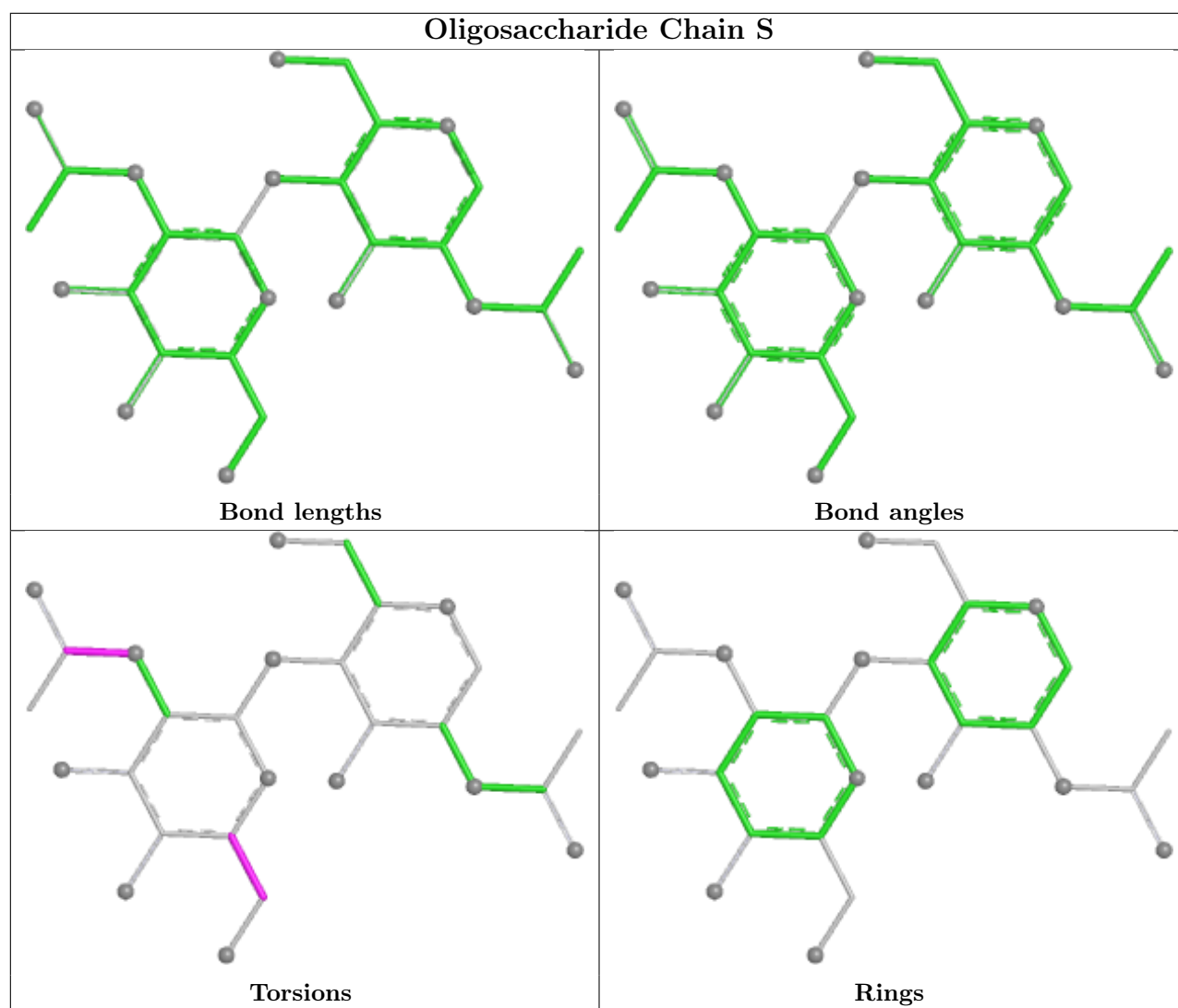


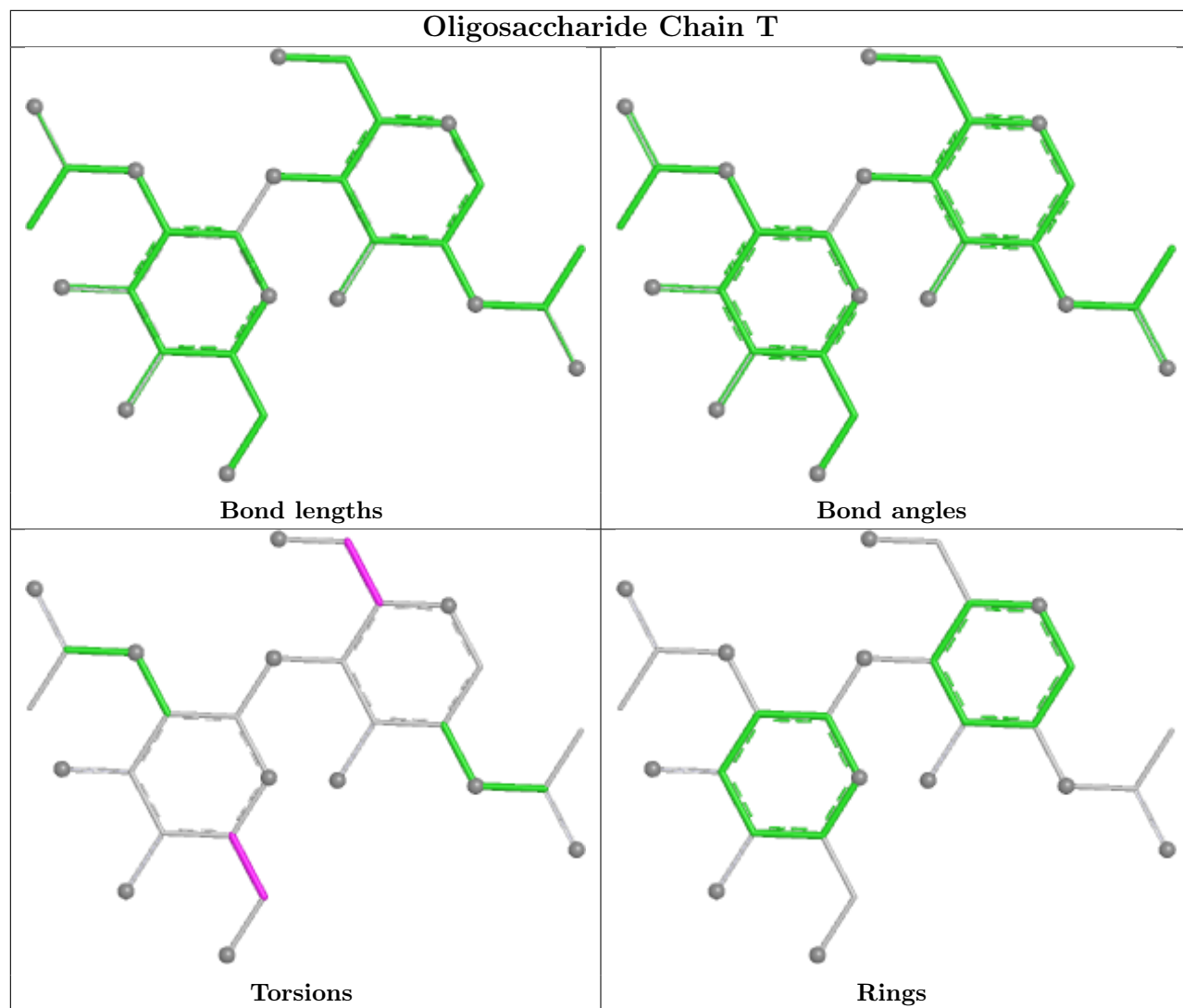


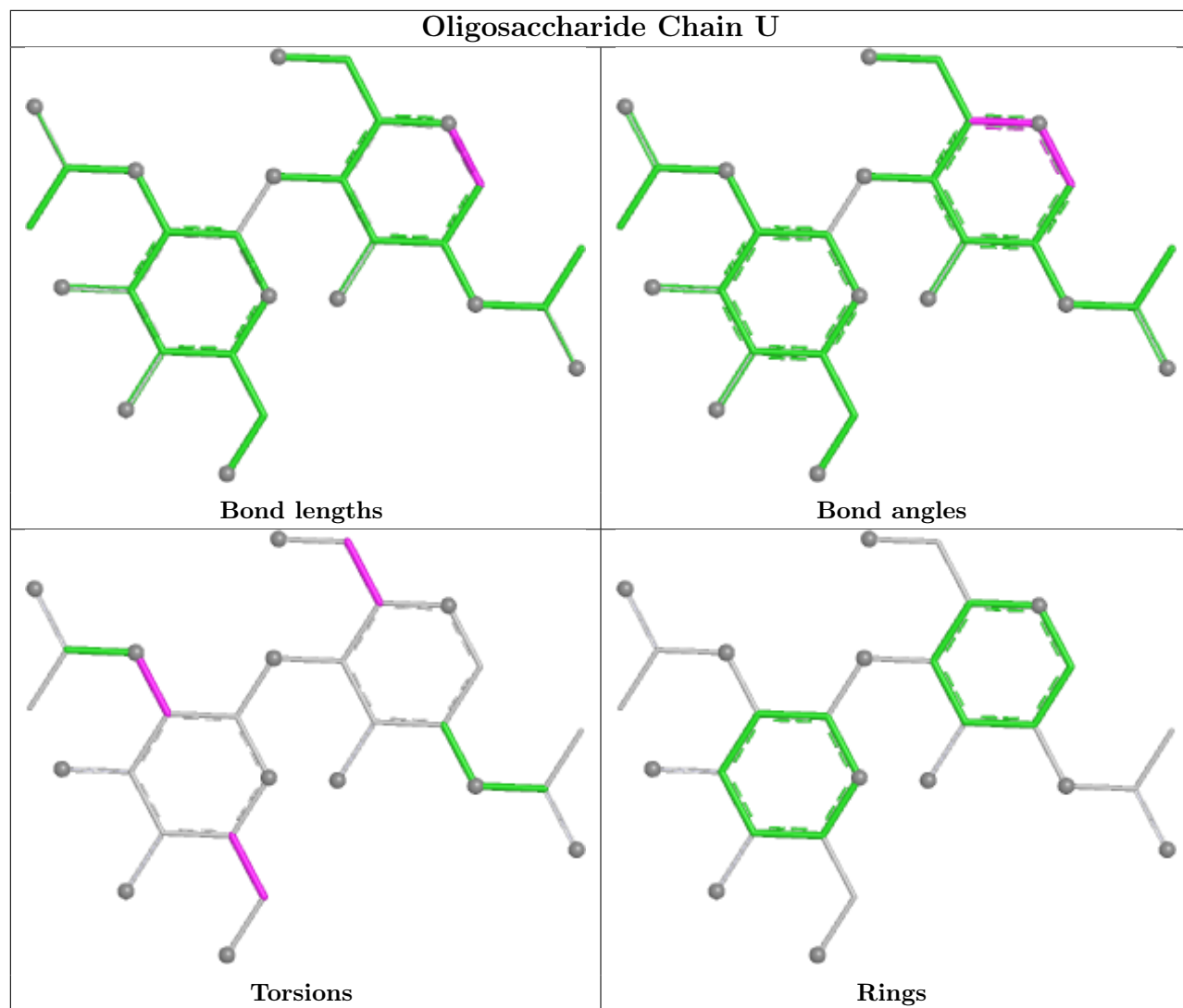


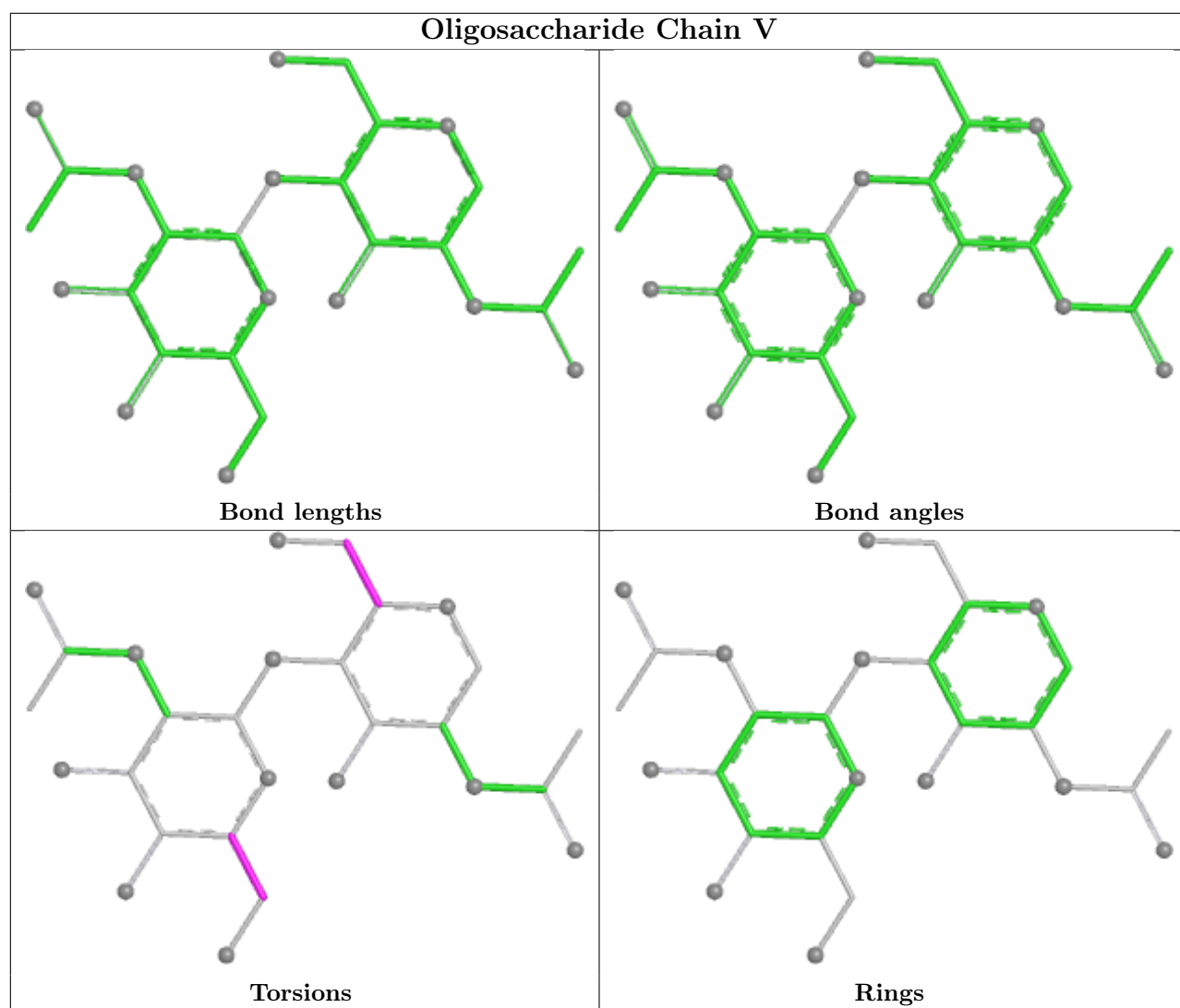


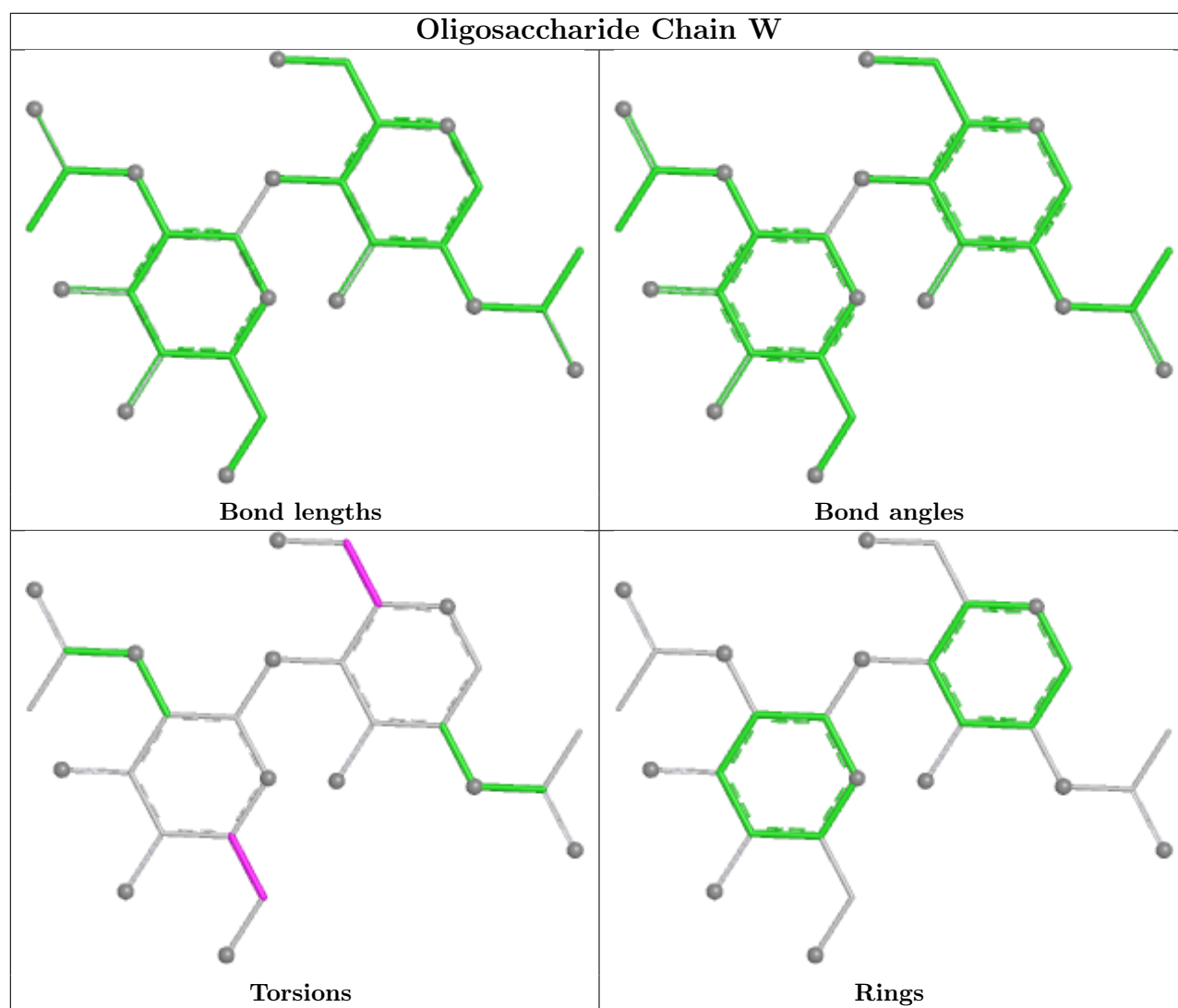


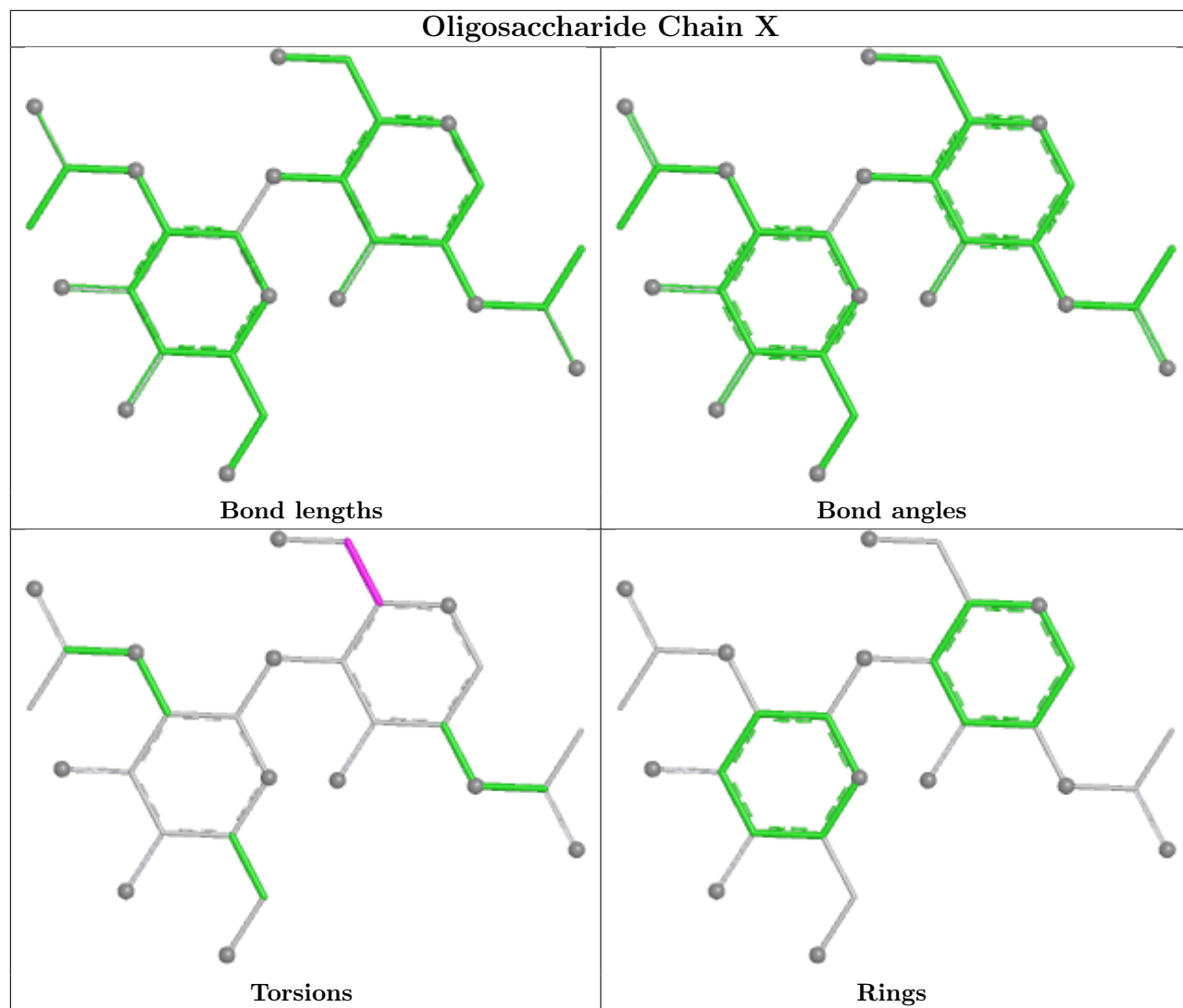


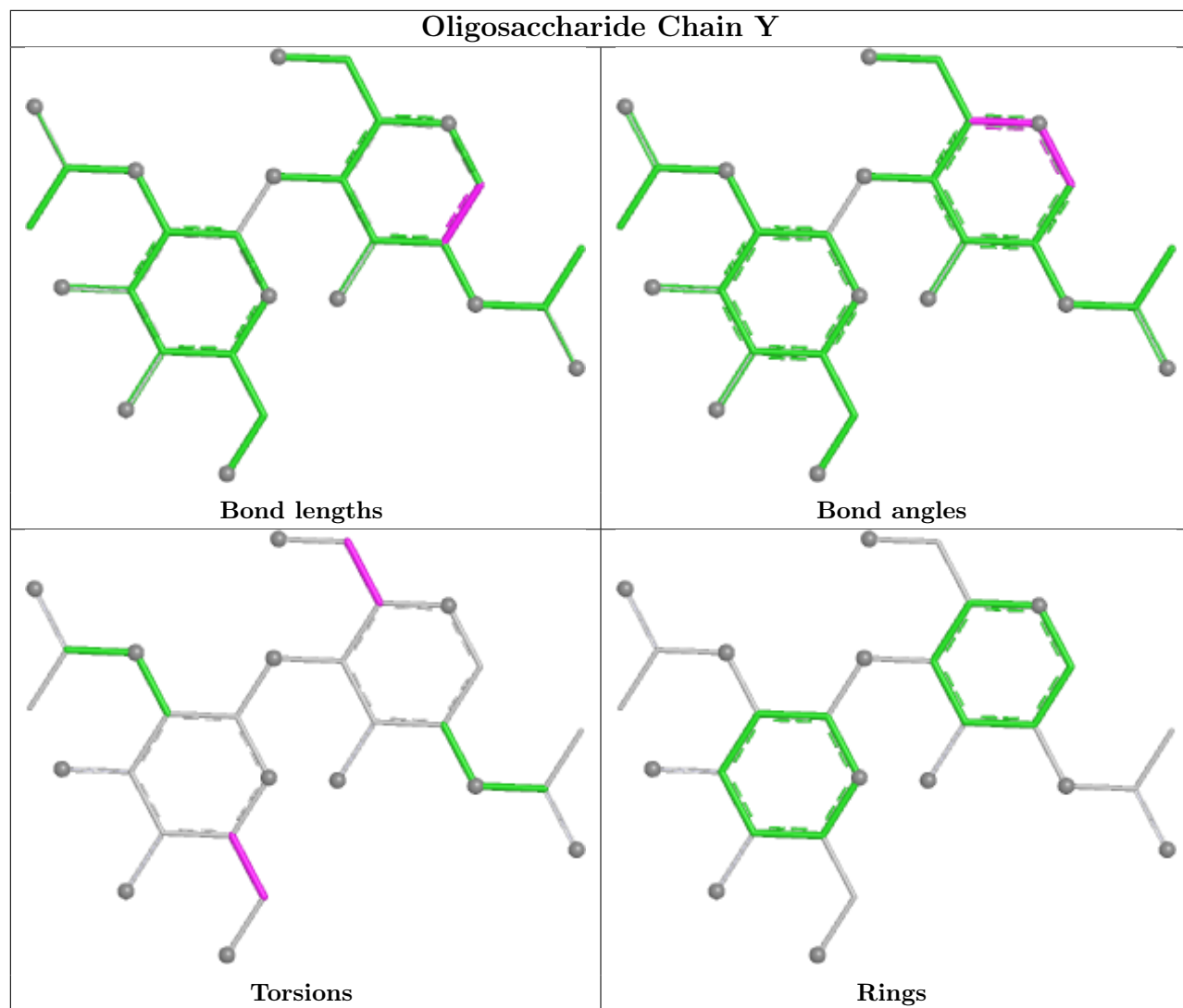


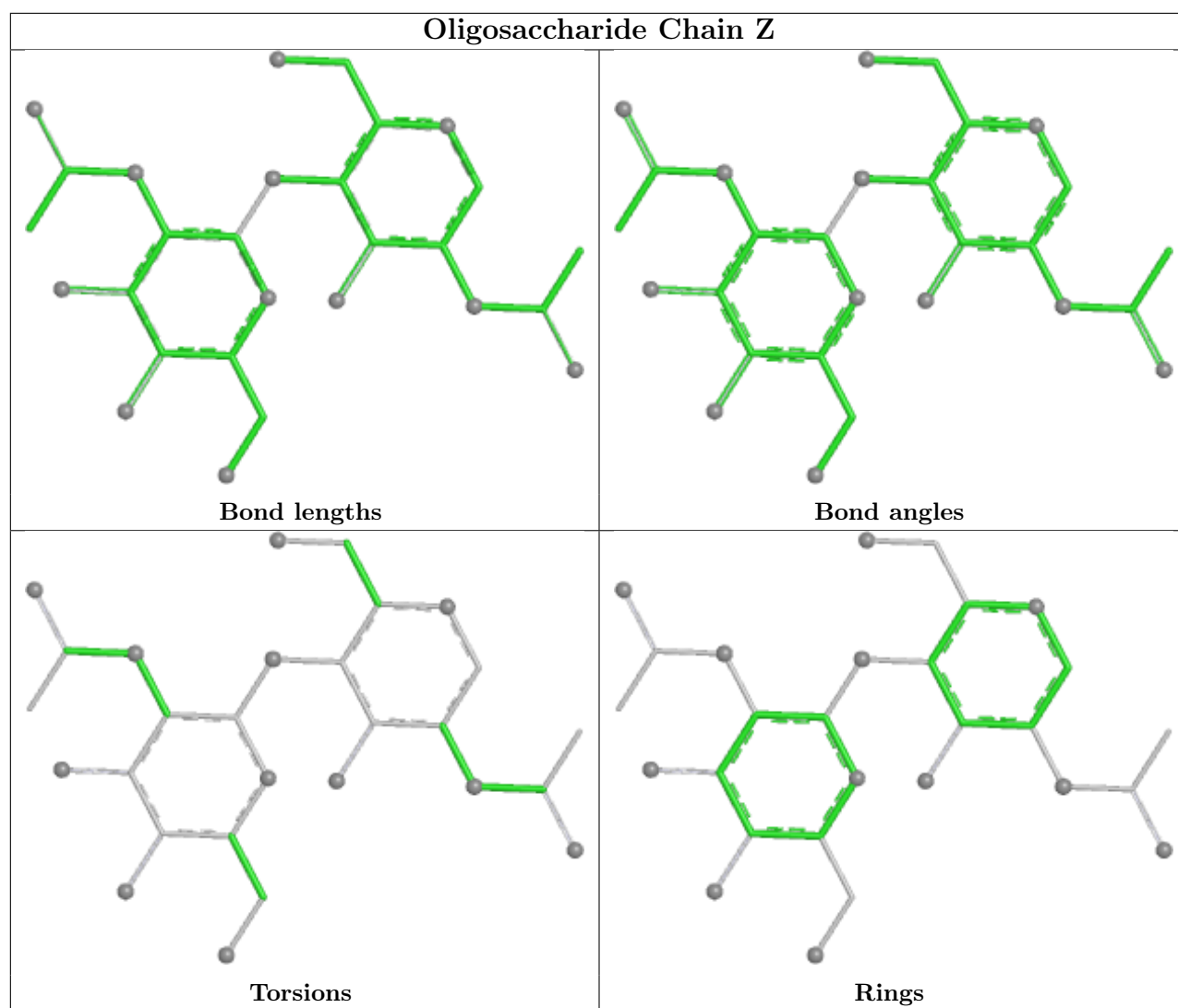


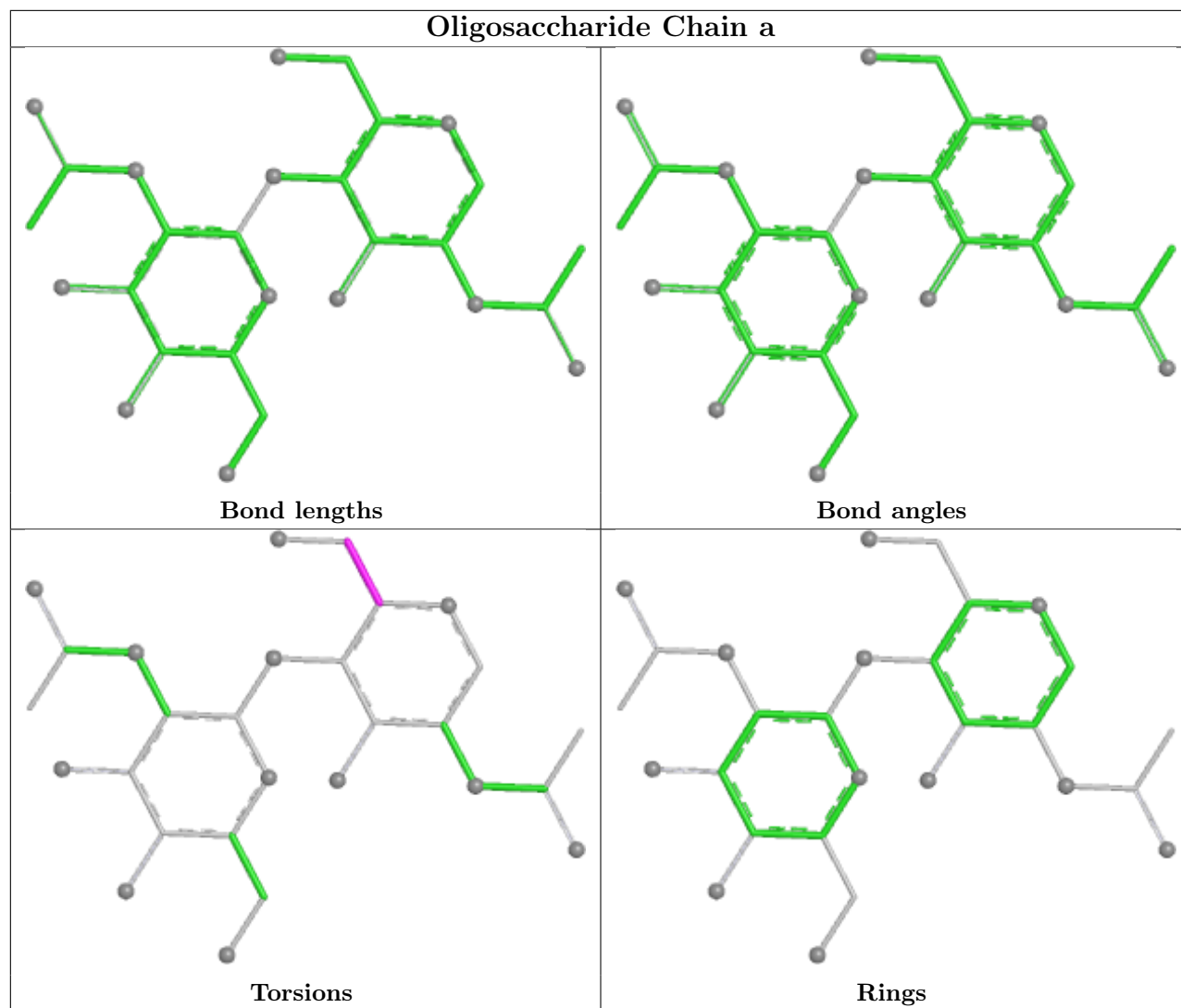


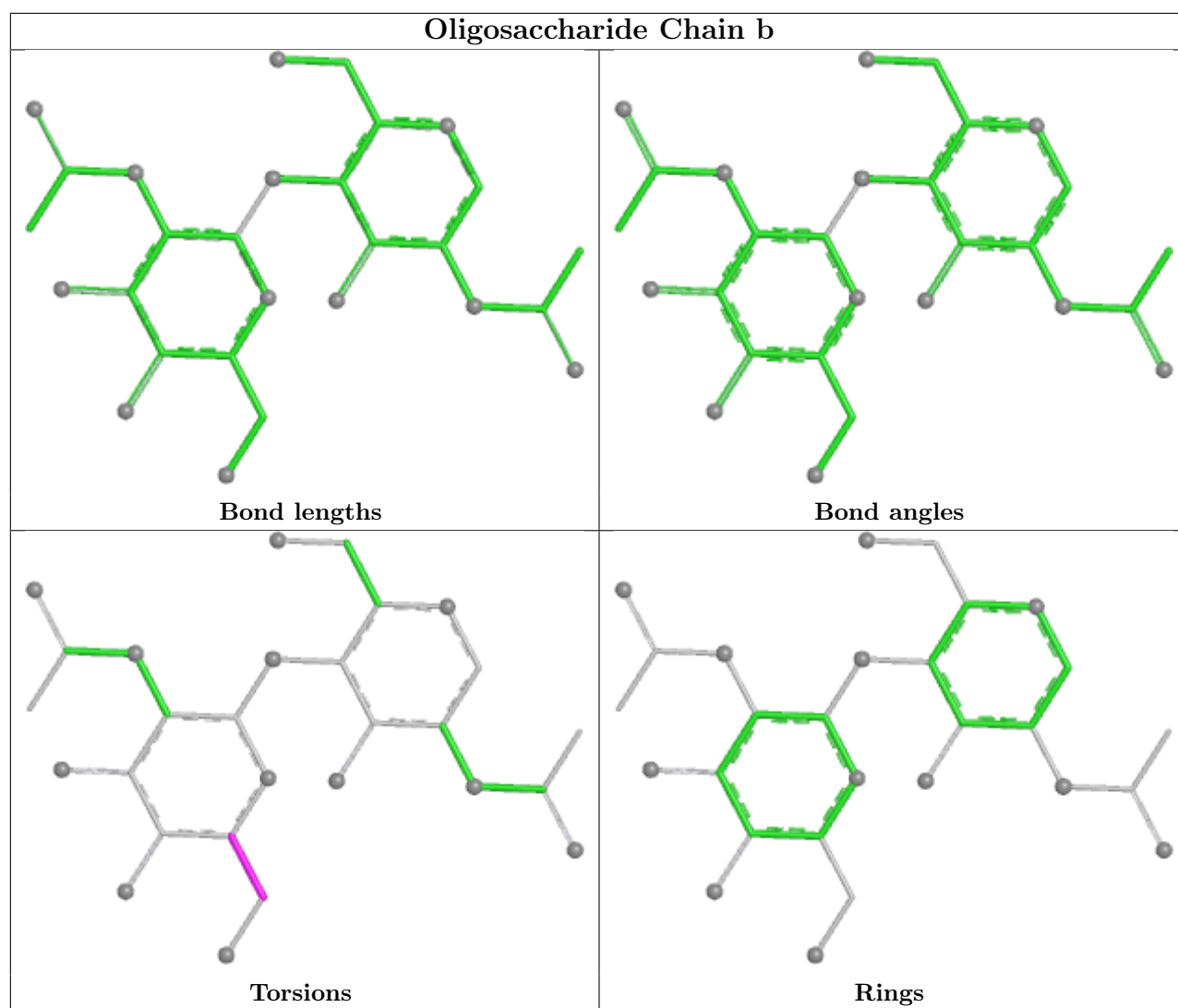


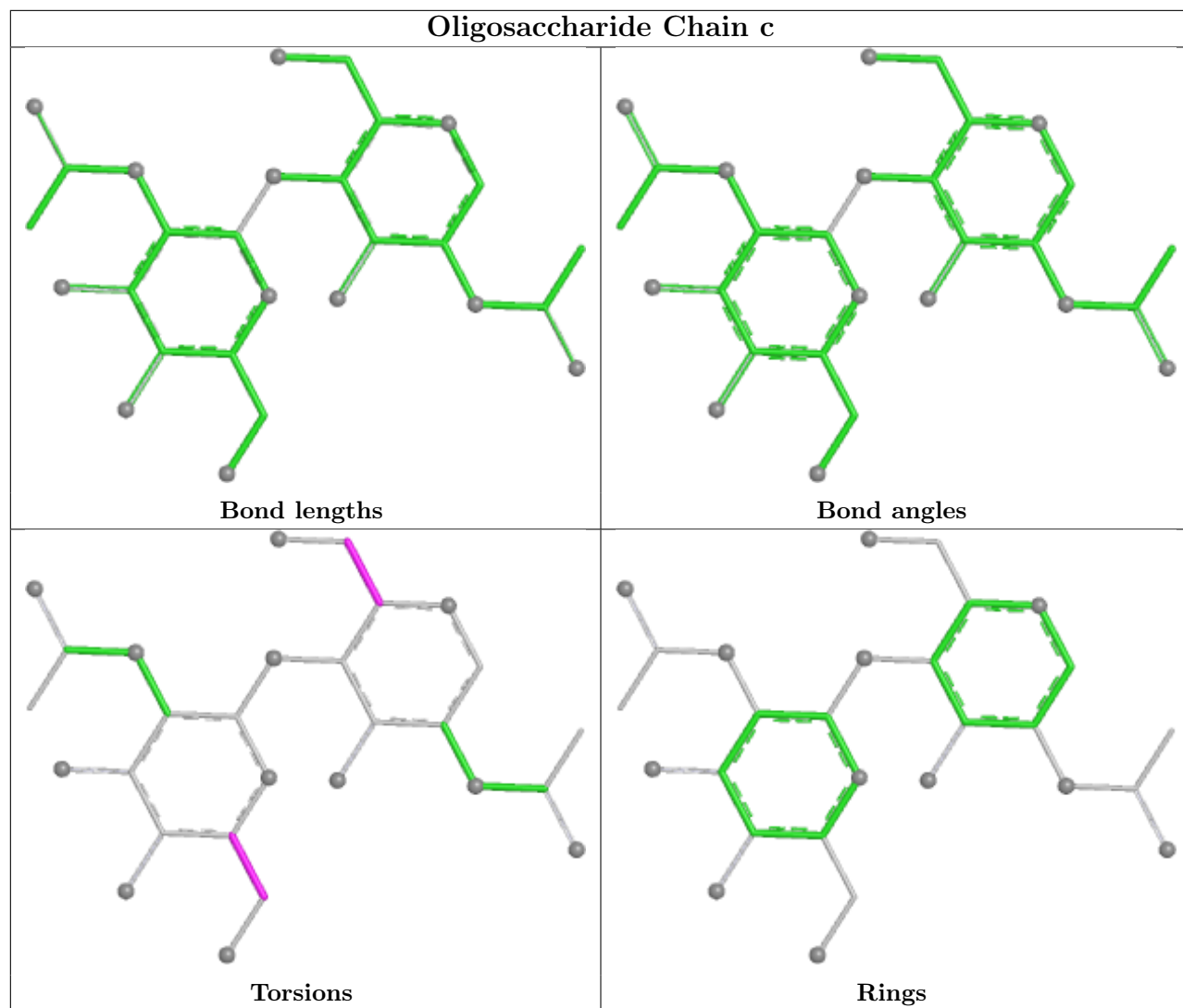


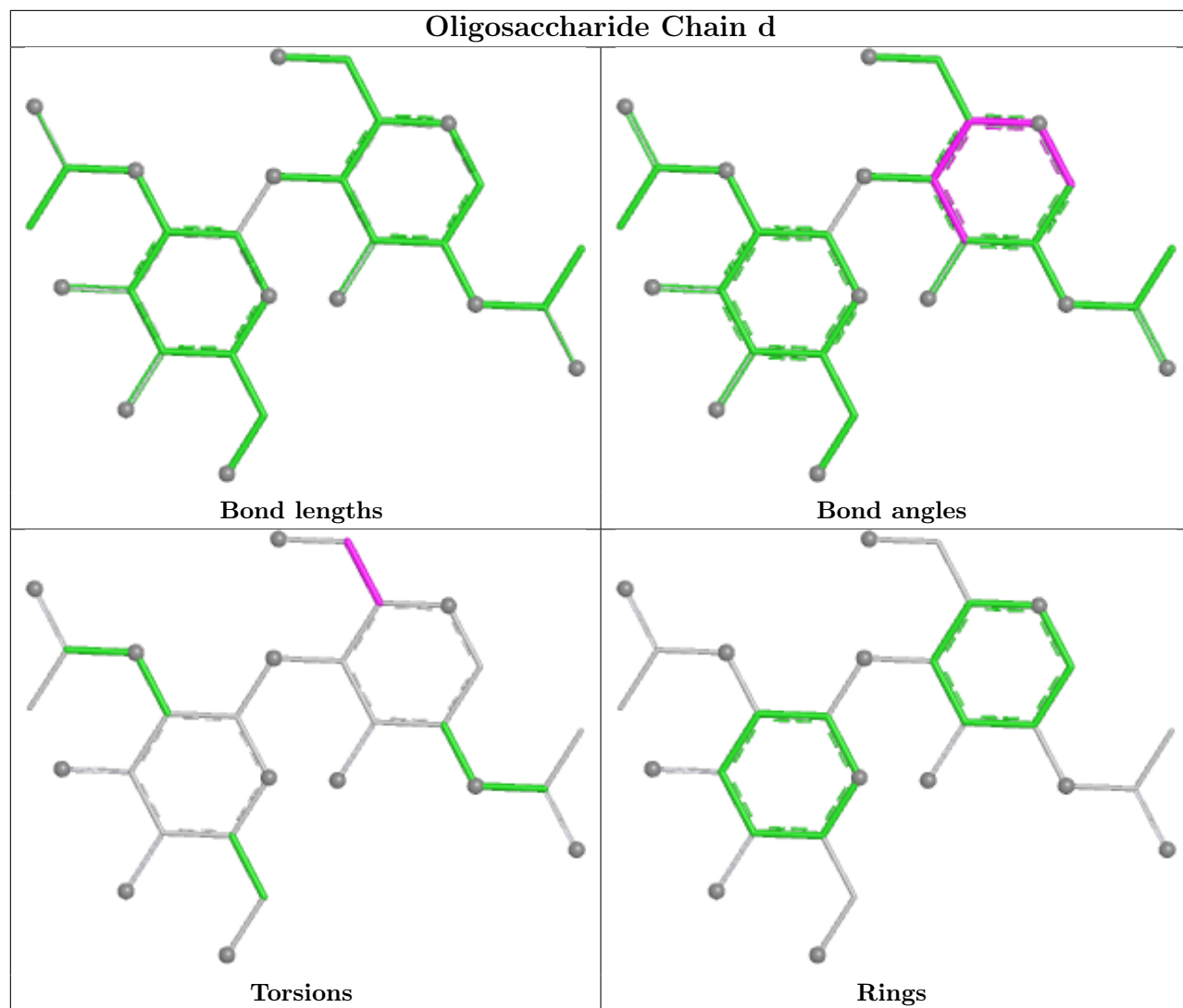


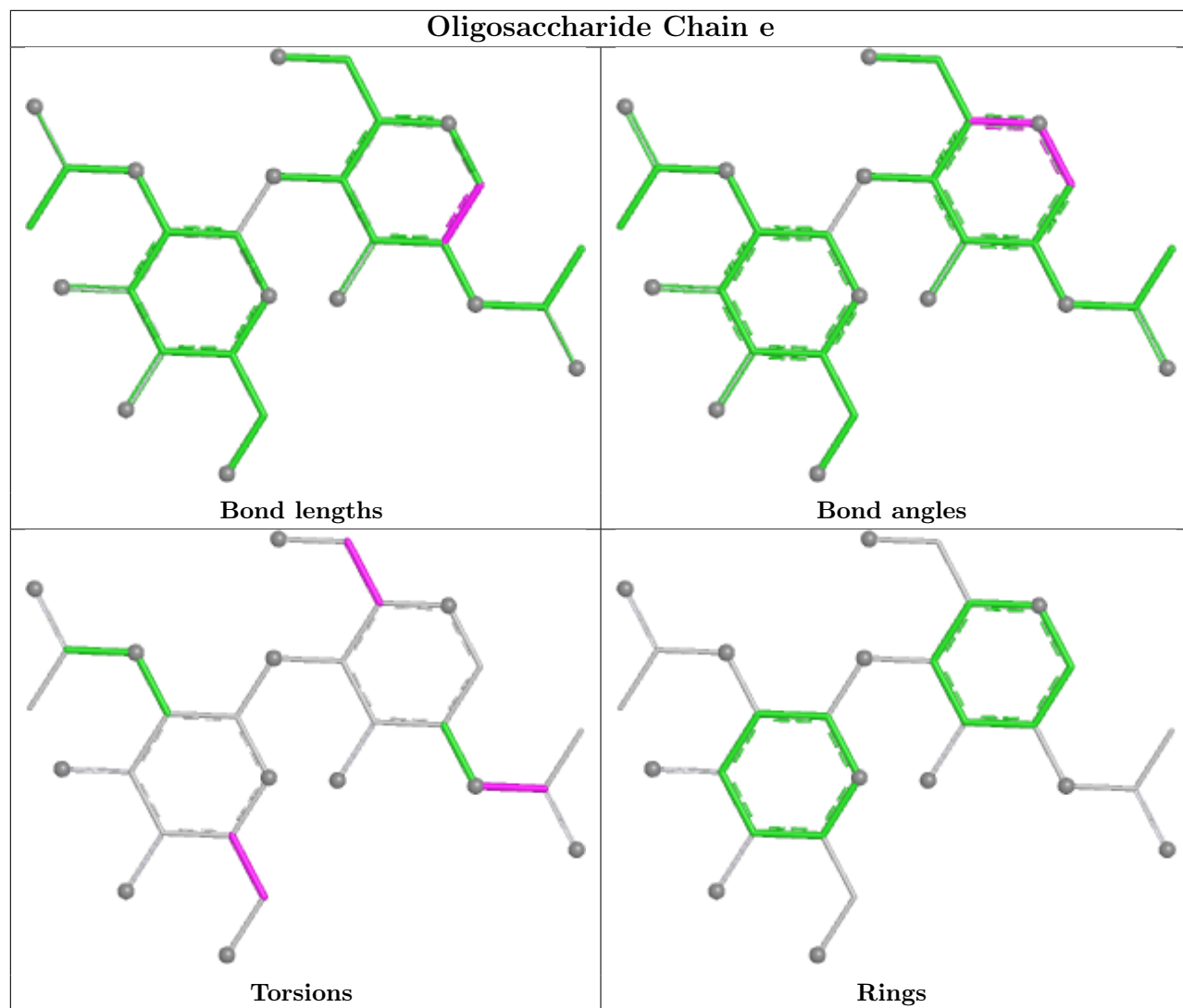


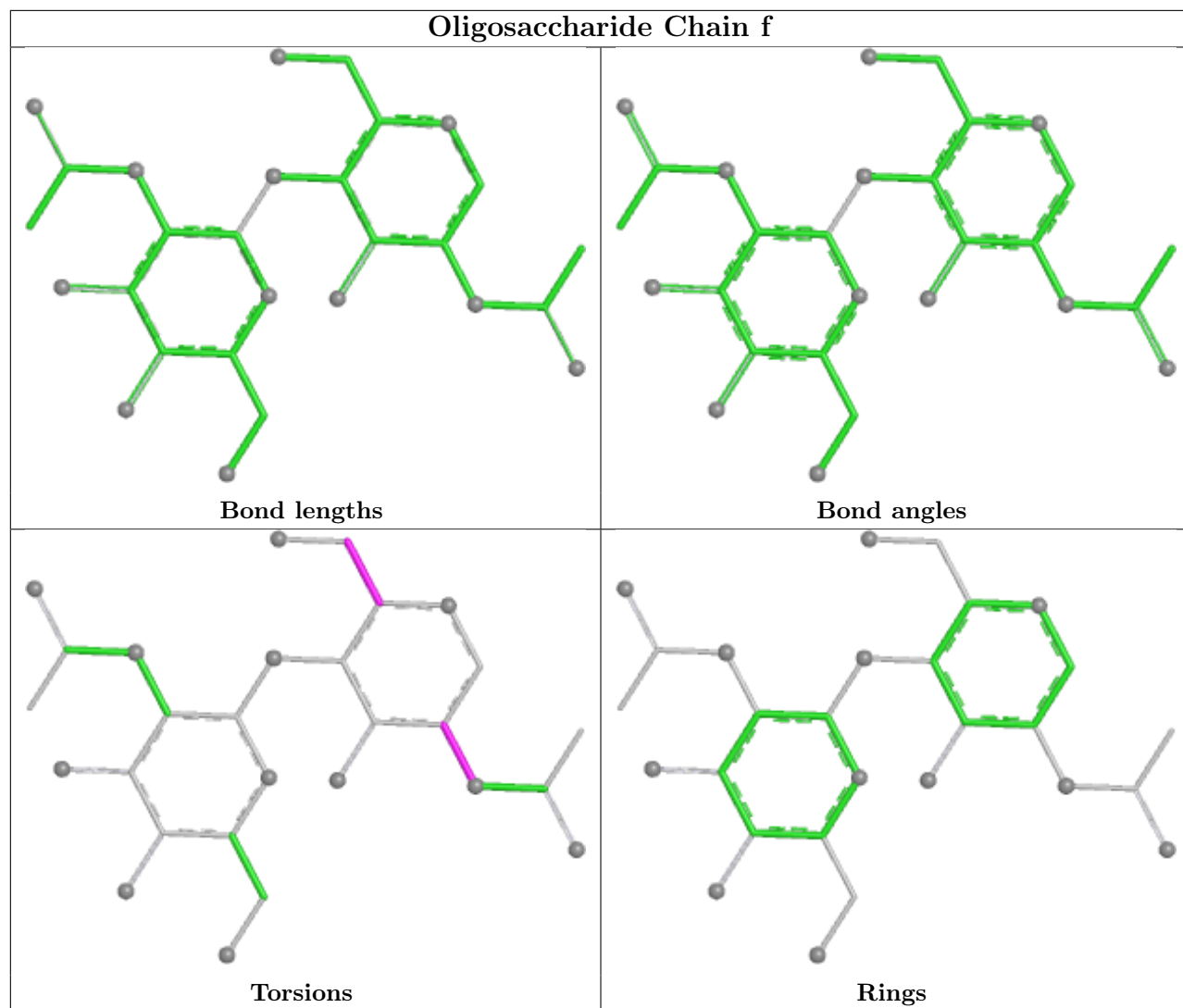


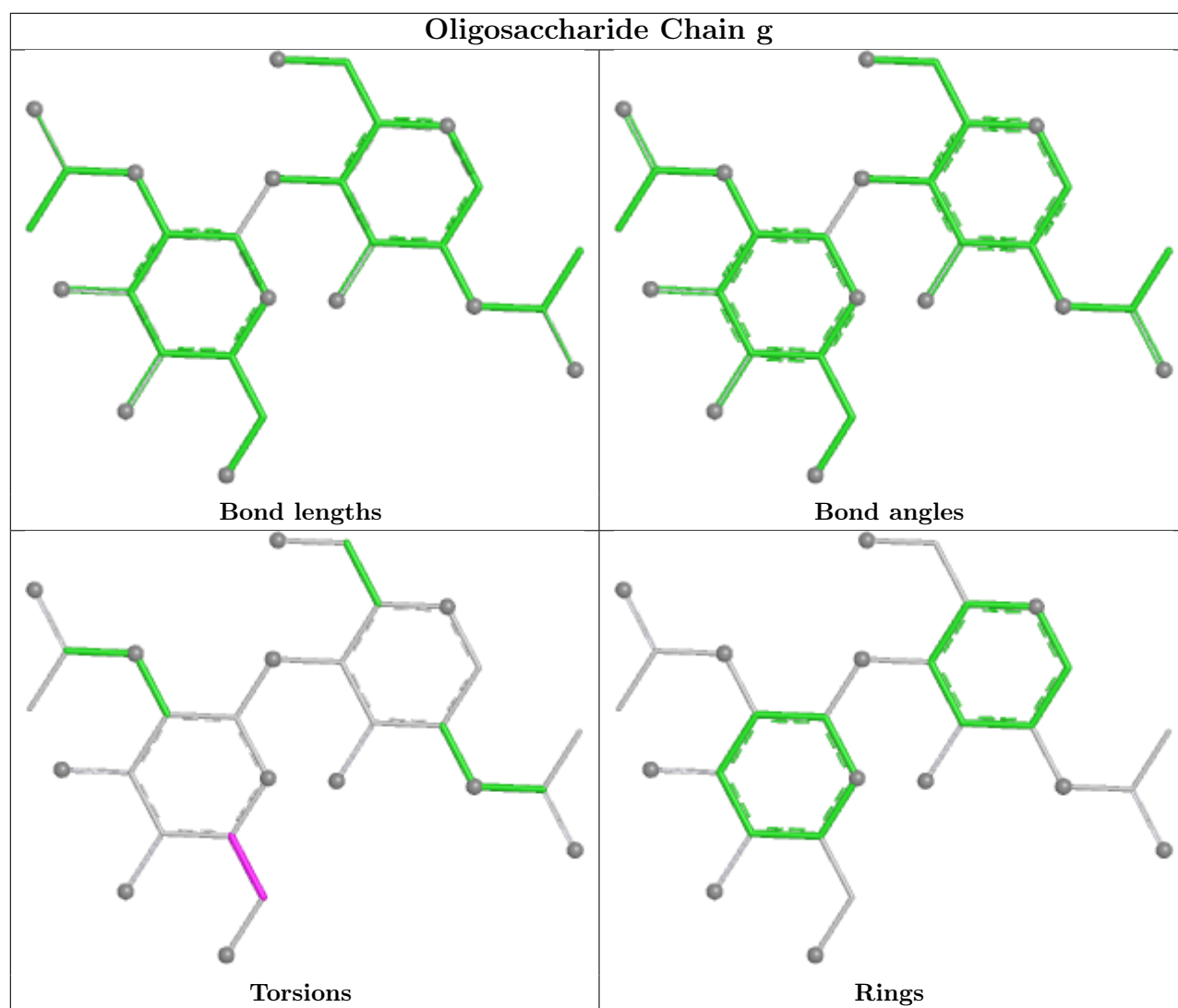


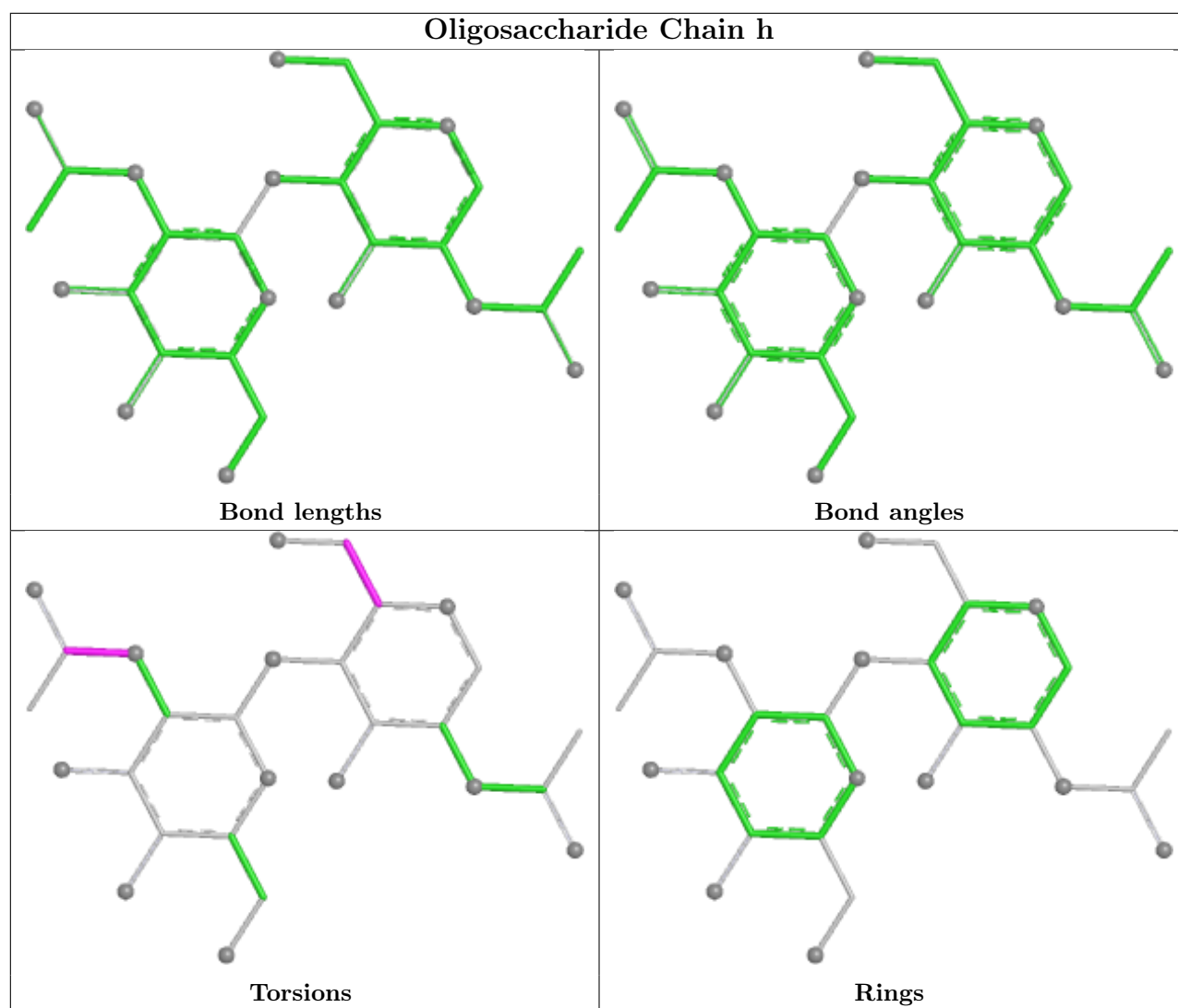


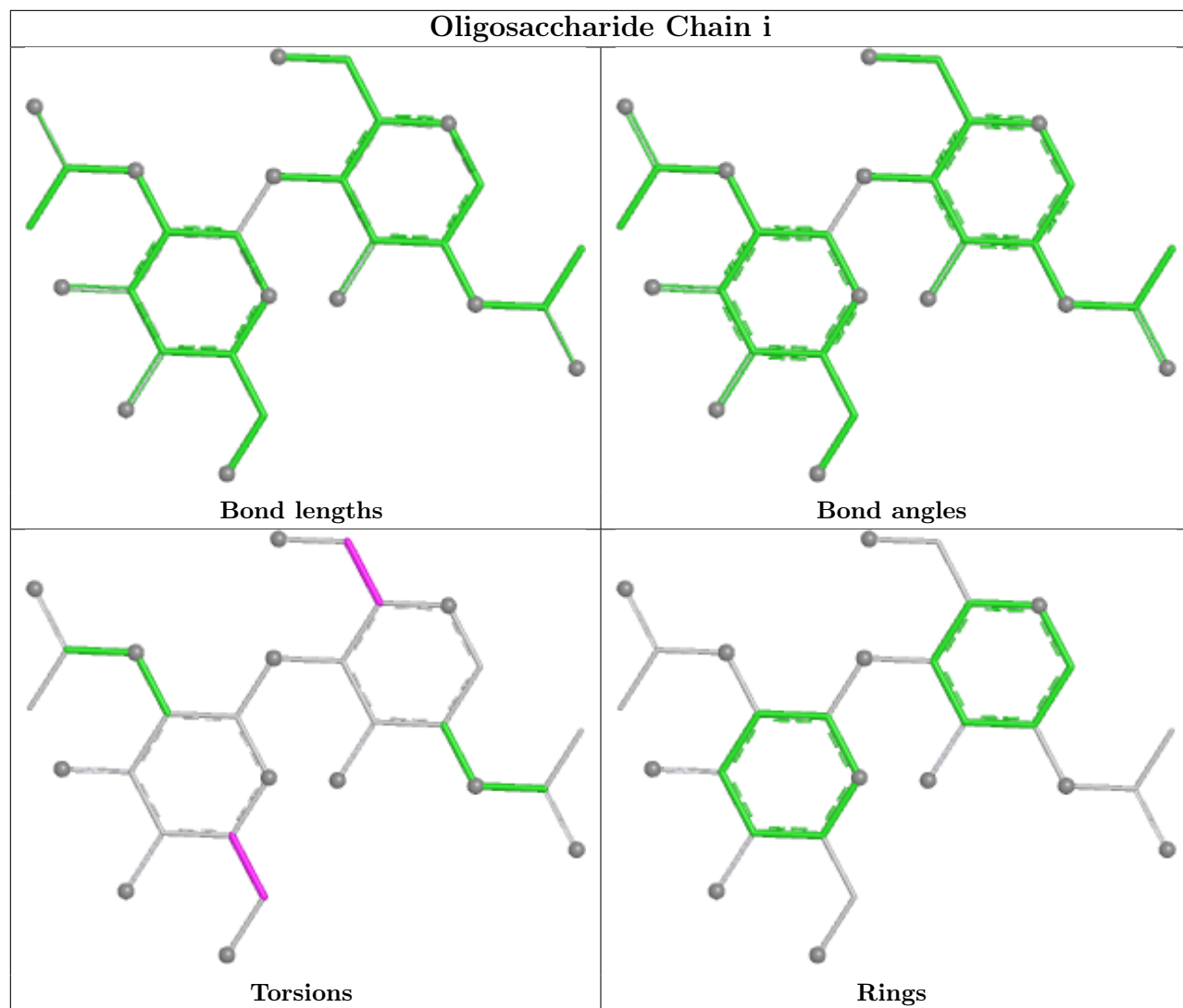


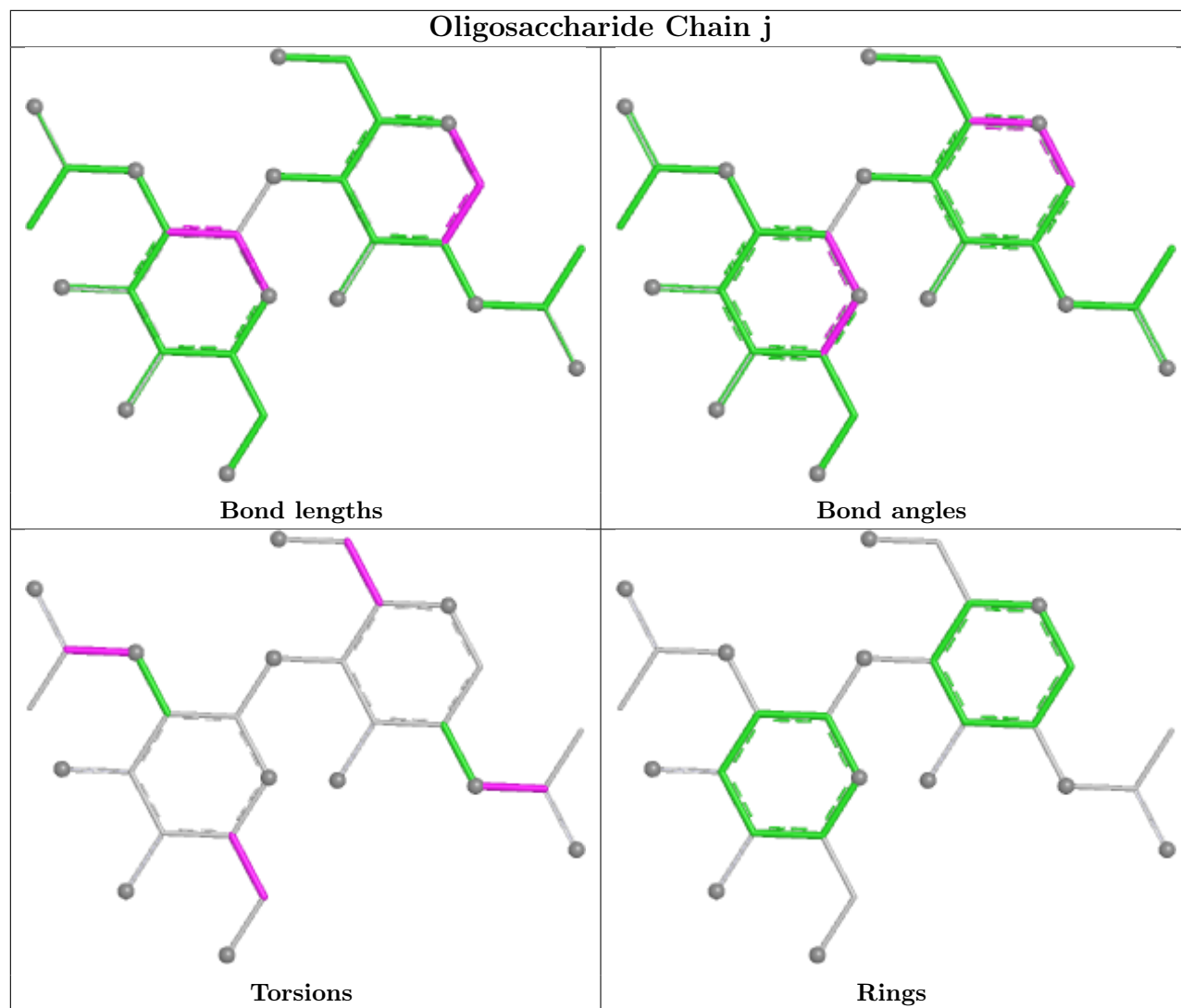


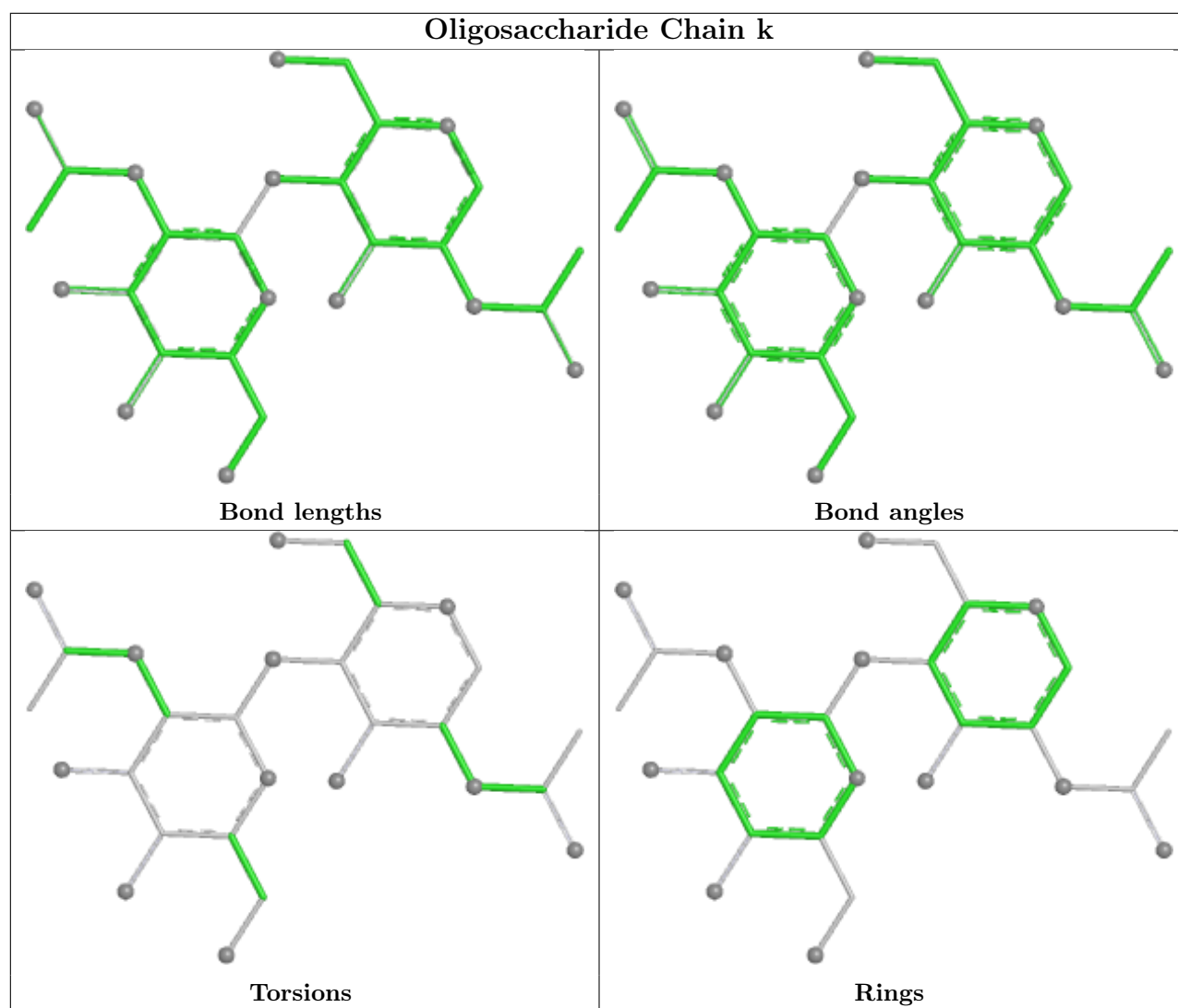


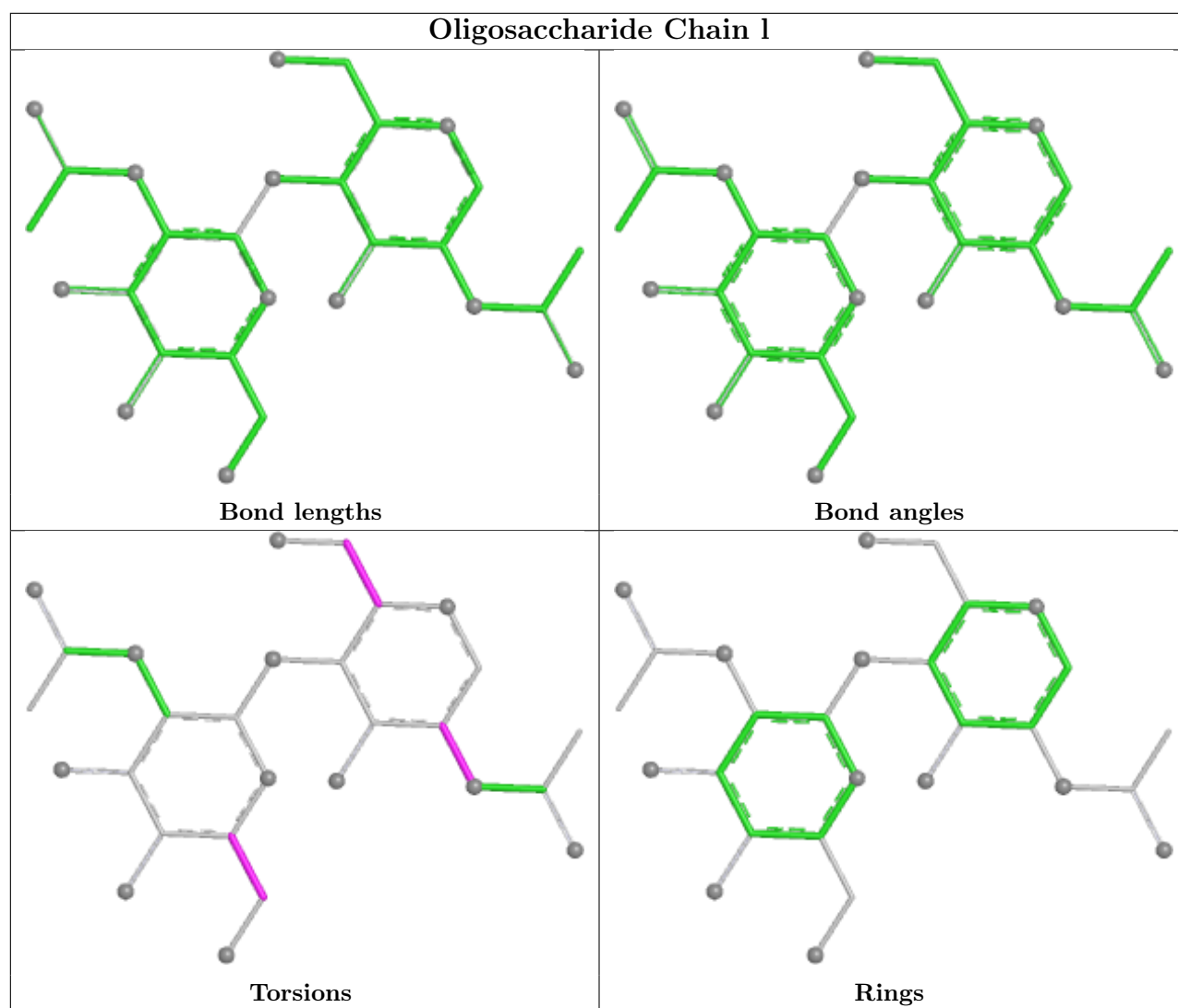


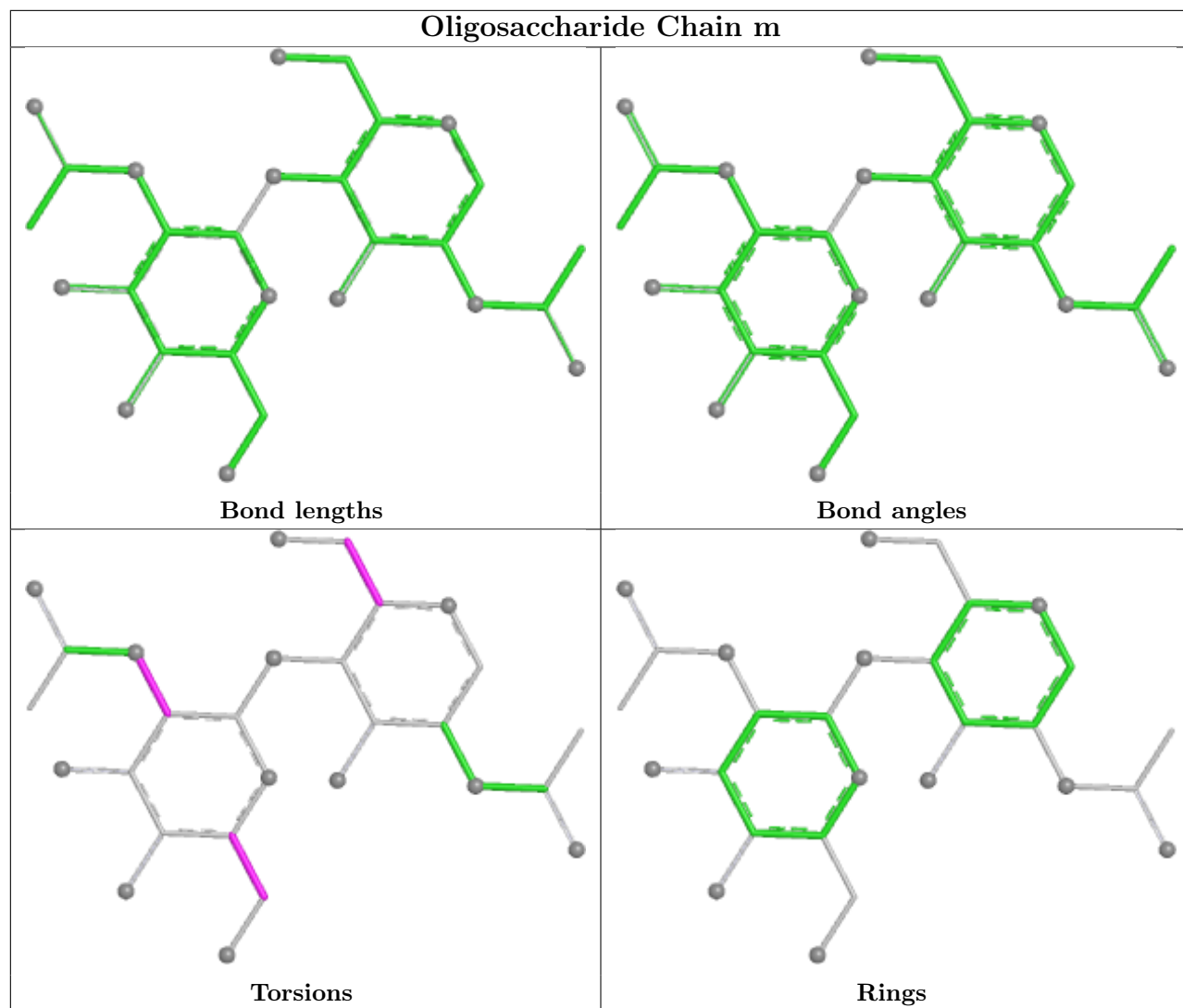


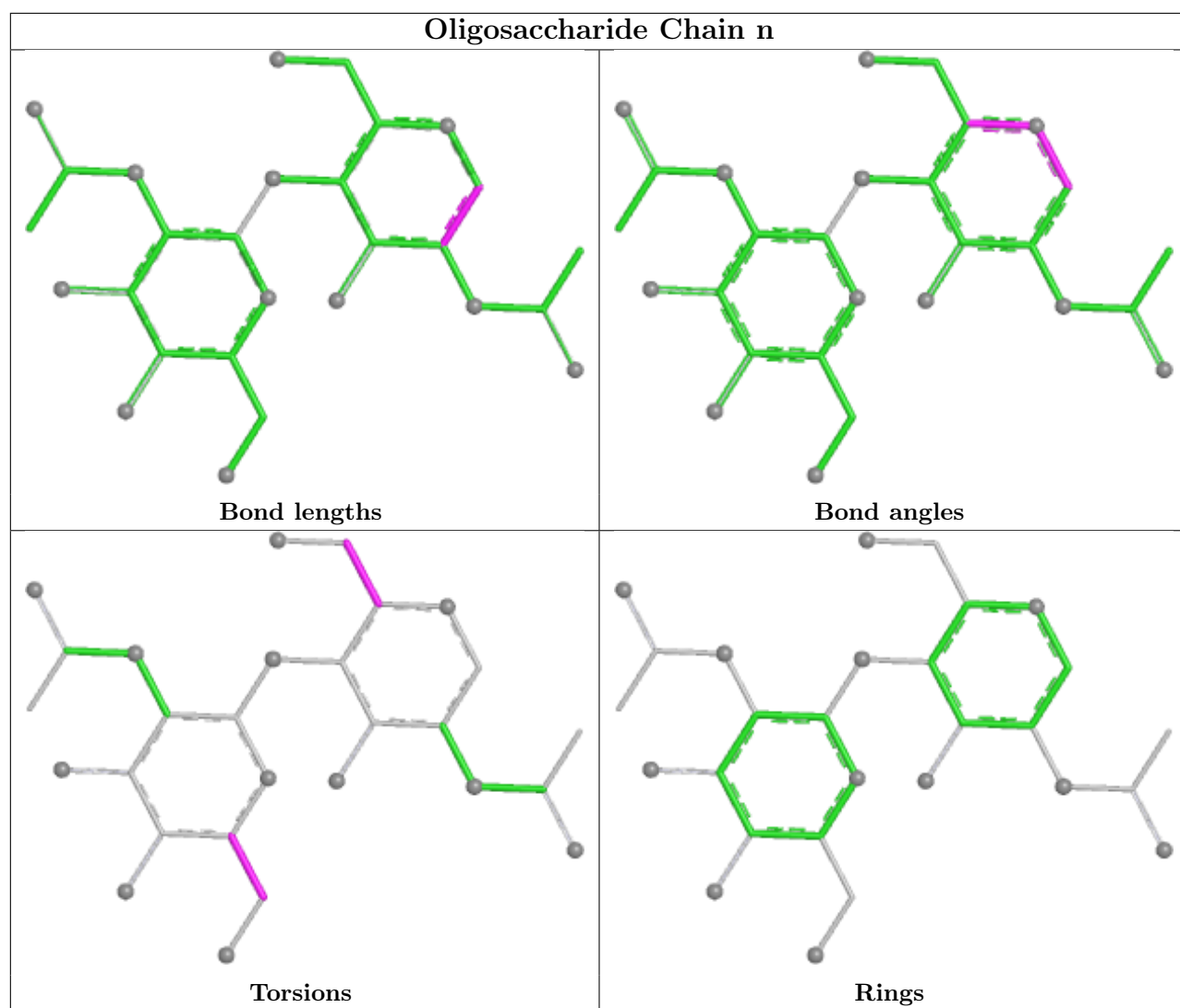


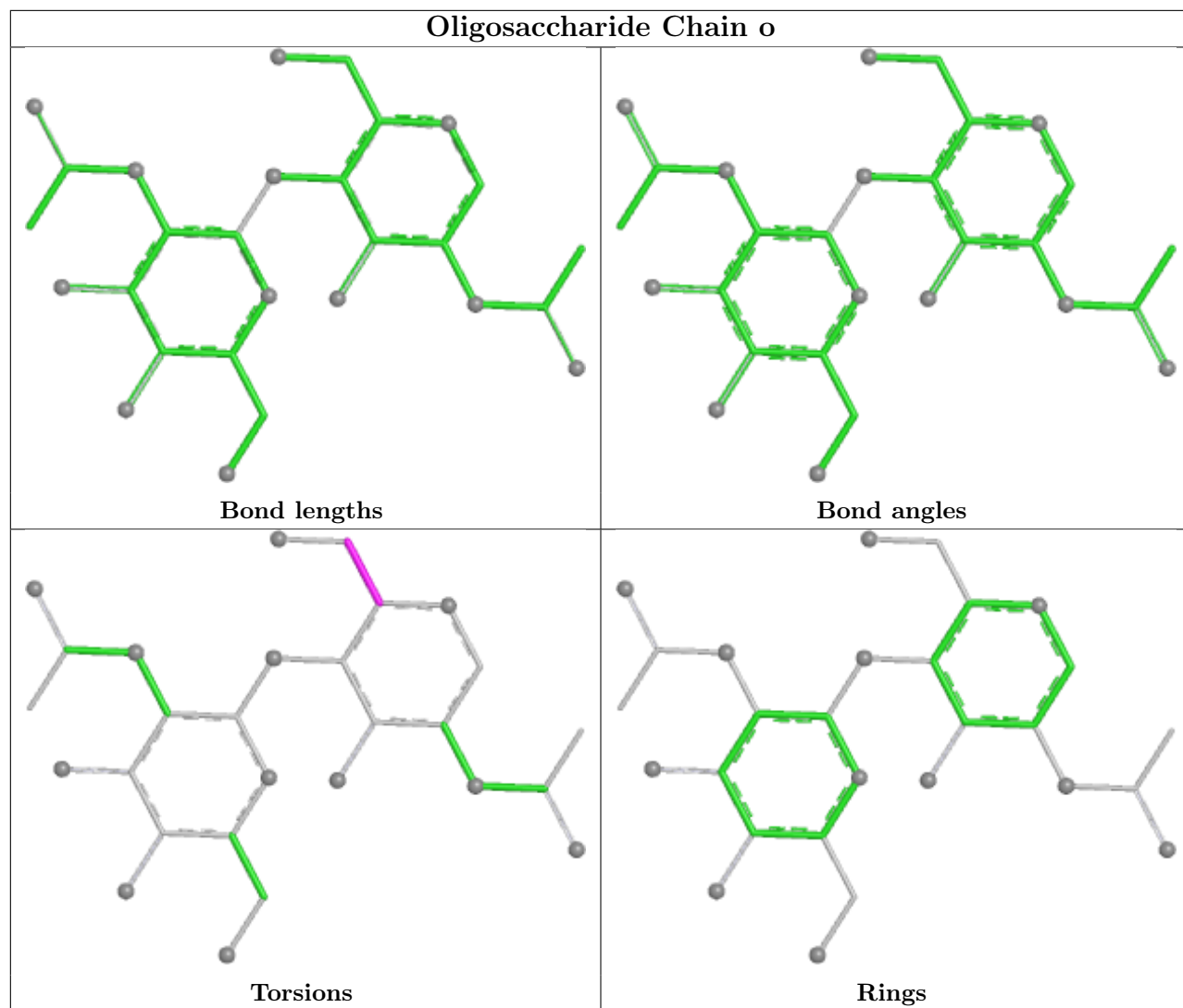


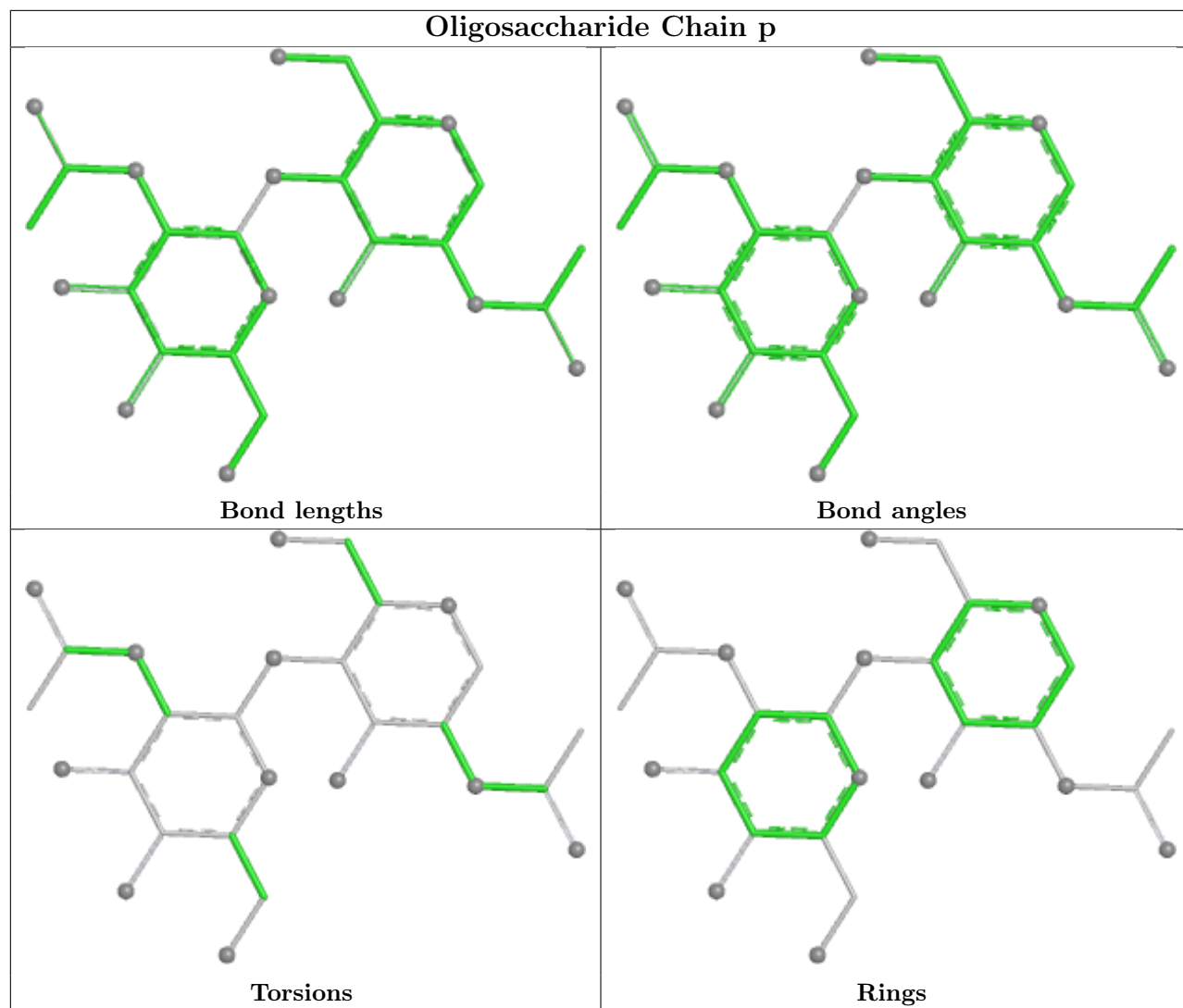


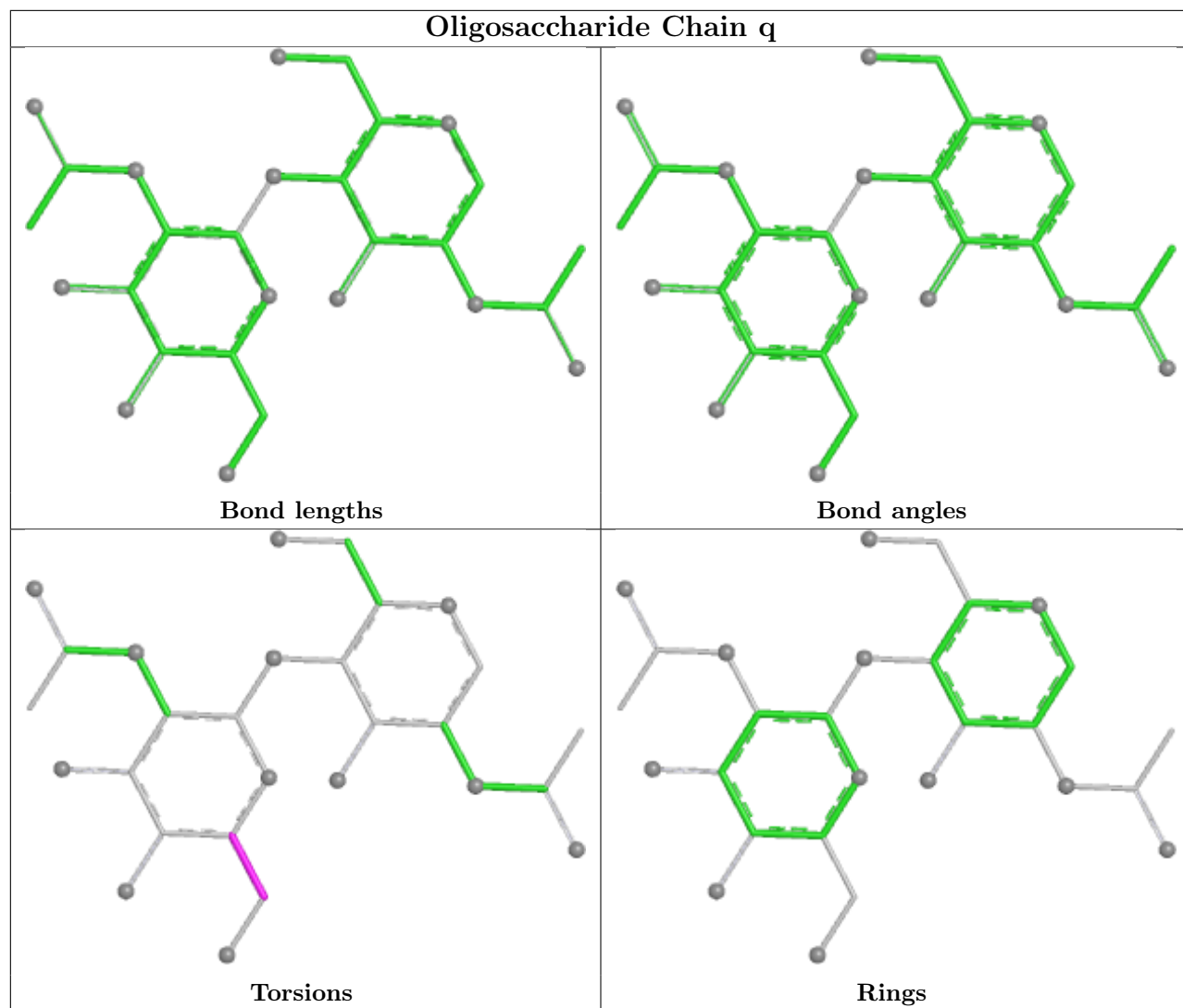


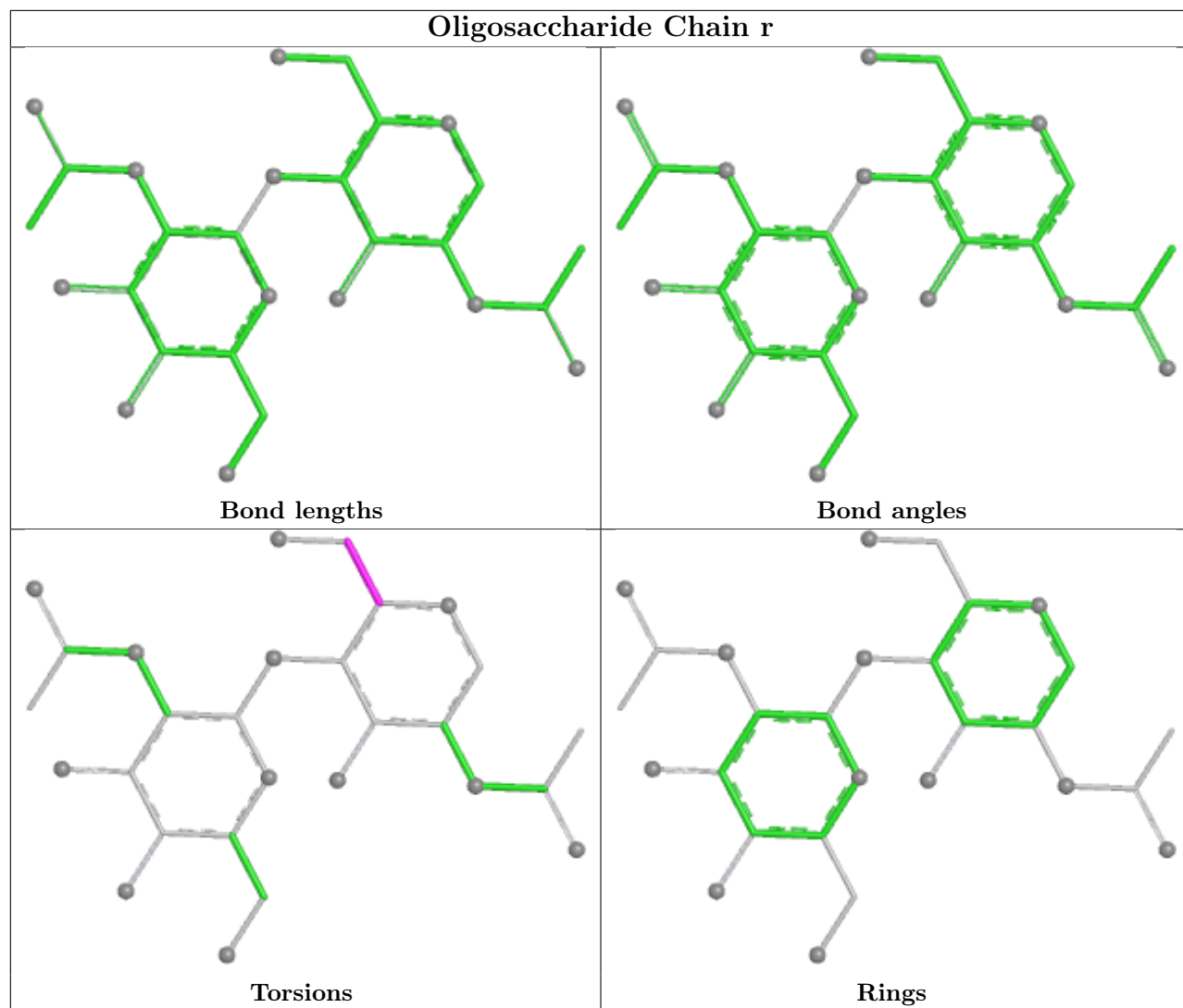


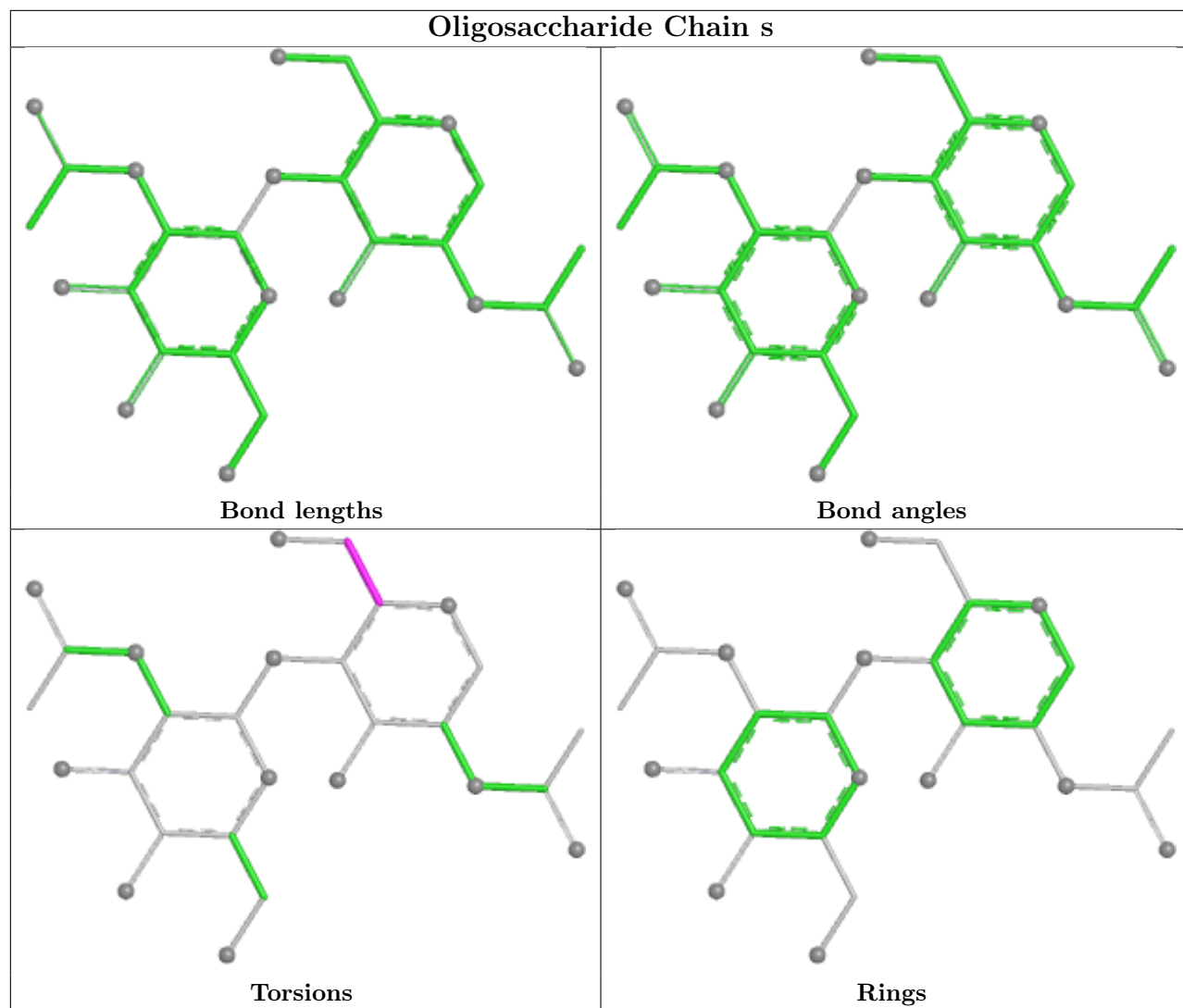


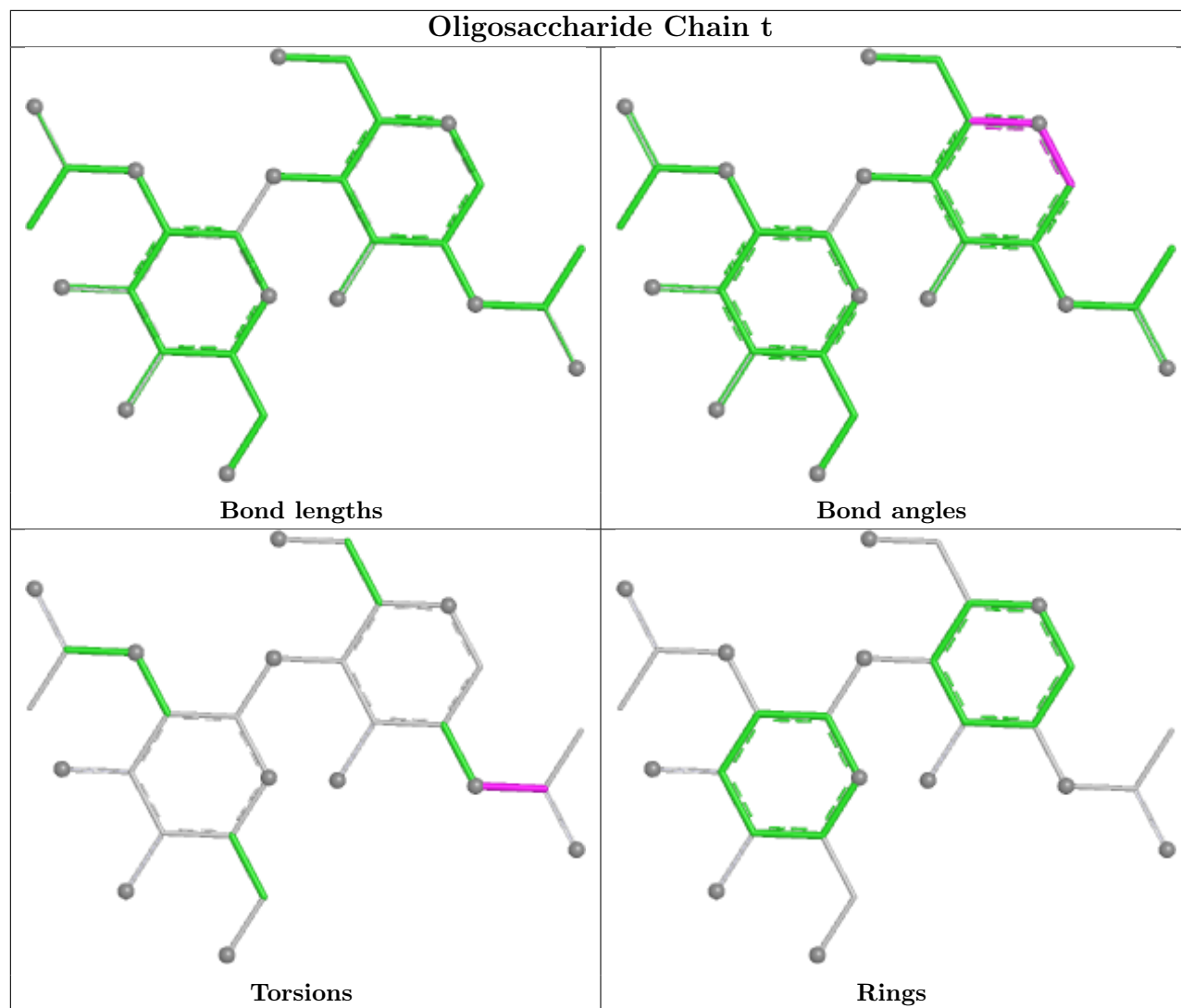


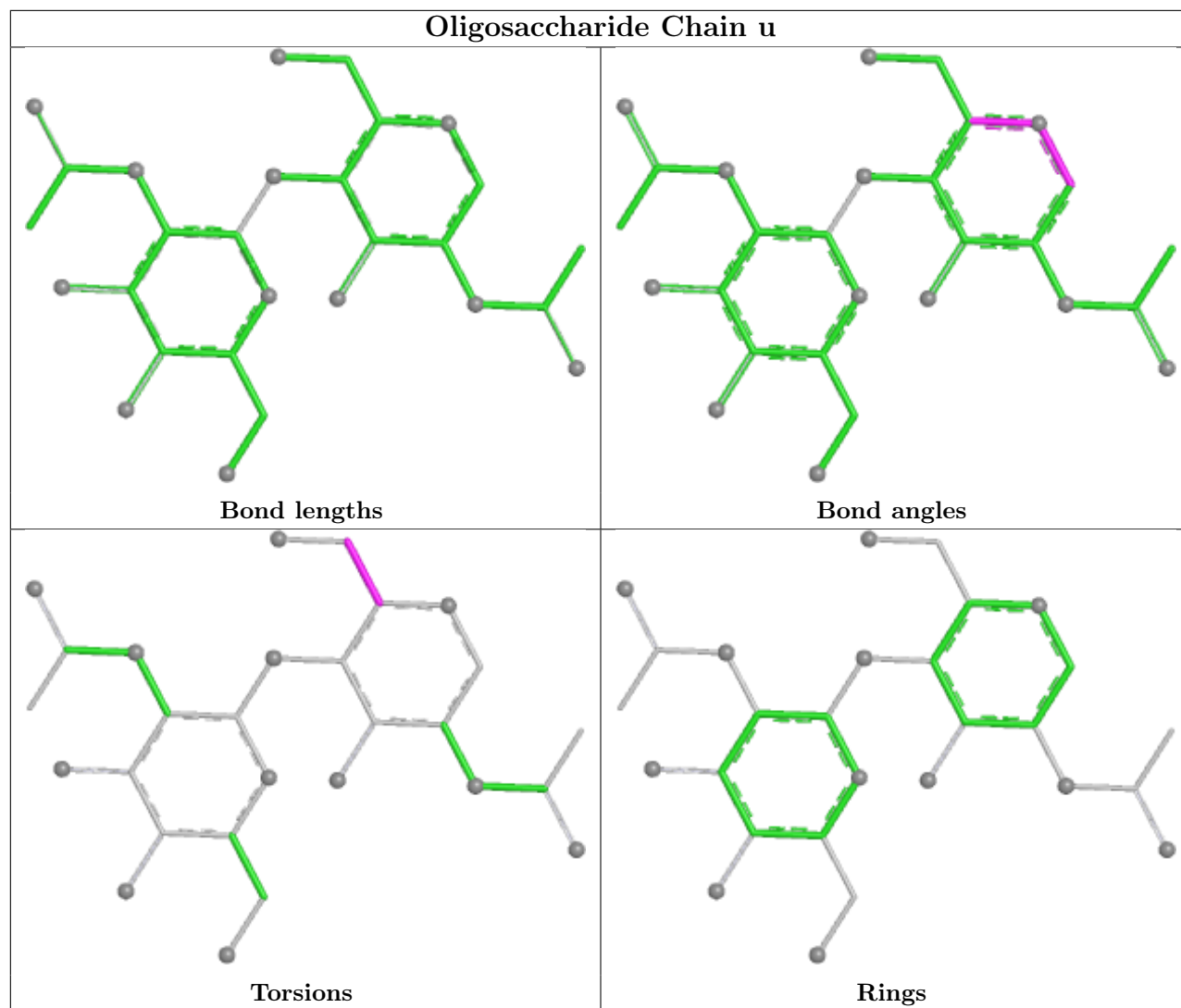


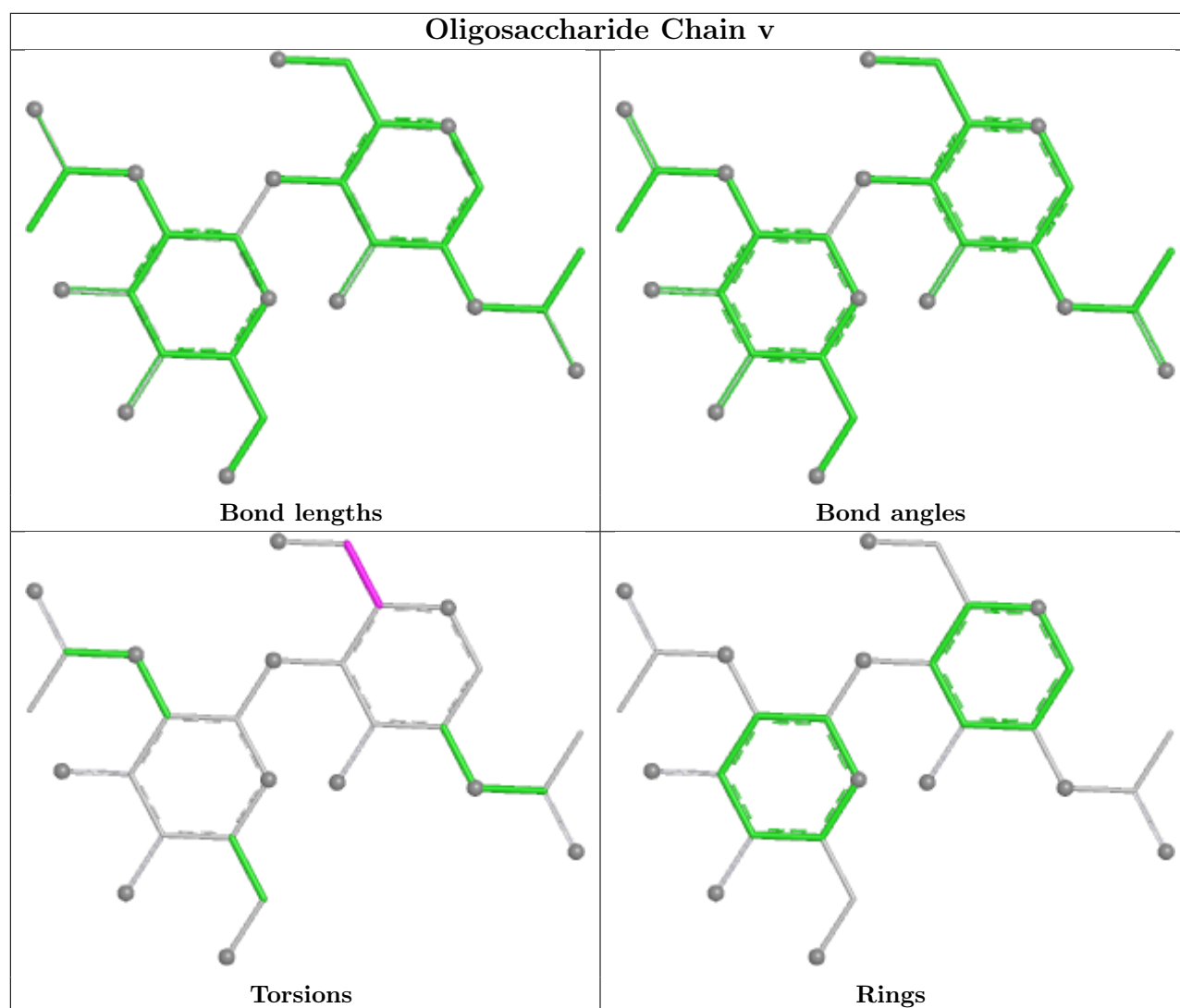












5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EZO	C	1303	-	27,27,27	1.56	6 (22%)	36,37,37	1.55	10 (27%)
4	EZO	A	1302	-	27,27,27	1.70	7 (25%)	36,37,37	1.57	10 (27%)
4	EZO	A	1303	-	27,27,27	1.60	7 (25%)	36,37,37	1.61	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1301	1	14,14,15	0.26	0	17,19,21	0.40	0
4	EZO	B	1302	-	27,27,27	1.66	6 (22%)	36,37,37	1.53	10 (27%)
4	EZO	C	1302	-	27,27,27	1.72	8 (29%)	36,37,37	1.59	8 (22%)
3	NAG	C	1301	-	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	A	1301	1	14,14,15	0.95	1 (7%)	17,19,21	1.94	1 (5%)
4	EZO	B	1303	-	27,27,27	1.40	5 (18%)	36,37,37	1.42	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EZO	C	1303	-	-	1/17/17/17	0/3/3/3
4	EZO	A	1302	-	-	13/17/17/17	0/3/3/3
4	EZO	A	1303	-	-	2/17/17/17	0/3/3/3
3	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	EZO	B	1302	-	-	14/17/17/17	0/3/3/3
4	EZO	C	1302	-	-	10/17/17/17	0/3/3/3
3	NAG	C	1301	-	-	4/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	EZO	B	1303	-	-	2/17/17/17	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1302	EZO	C15-N14	3.76	1.45	1.35
4	B	1302	EZO	C15-N14	3.65	1.44	1.35
4	C	1302	EZO	C15-N14	3.63	1.44	1.35
4	C	1302	EZO	C4-C12	3.47	1.52	1.45
4	A	1302	EZO	C4-C12	3.43	1.52	1.45
4	A	1303	EZO	O8-C7	-3.39	1.20	1.30
4	B	1303	EZO	C5-C4	-3.35	1.36	1.41
4	B	1302	EZO	C4-C12	3.32	1.52	1.45
4	A	1303	EZO	O9-C7	3.27	1.32	1.22
4	C	1303	EZO	O8-C7	-3.25	1.20	1.30
3	A	1301	NAG	O5-C1	3.25	1.49	1.43
4	C	1302	EZO	C17-N16	-3.12	1.33	1.39
4	C	1303	EZO	O9-C7	3.11	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1302	EZO	C17-N16	-3.06	1.33	1.39
4	A	1302	EZO	C17-N16	-2.98	1.34	1.39
4	A	1303	EZO	C5-C4	-2.97	1.37	1.41
4	C	1302	EZO	C20-C17	2.84	1.52	1.47
4	B	1302	EZO	C20-C17	2.80	1.52	1.47
4	A	1302	EZO	C20-C17	2.78	1.52	1.47
4	C	1303	EZO	C5-C4	-2.76	1.37	1.41
4	C	1303	EZO	C15-S19	-2.73	1.68	1.74
4	A	1303	EZO	C15-S19	-2.66	1.68	1.74
4	B	1303	EZO	C15-S19	-2.63	1.69	1.74
4	B	1302	EZO	C18-C17	2.58	1.39	1.36
4	C	1303	EZO	C18-C17	2.57	1.39	1.36
4	B	1303	EZO	C18-C17	2.50	1.39	1.36
4	C	1302	EZO	C18-C17	2.49	1.39	1.36
4	A	1303	EZO	C18-C17	2.41	1.39	1.36
4	A	1302	EZO	C18-C17	2.41	1.39	1.36
4	C	1302	EZO	C5-C4	-2.36	1.38	1.41
4	B	1303	EZO	O8-C7	-2.22	1.23	1.30
4	C	1302	EZO	N14-N13	2.21	1.41	1.37
4	A	1302	EZO	C5-C4	-2.13	1.38	1.41
4	B	1303	EZO	C3-C4	-2.11	1.37	1.41
4	B	1302	EZO	C5-C4	-2.09	1.38	1.41
4	A	1303	EZO	C21-CL1	2.08	1.78	1.73
4	A	1303	EZO	C3-C4	-2.06	1.37	1.41
4	C	1303	EZO	C3-C4	-2.05	1.37	1.41
4	C	1302	EZO	C21-CL1	2.04	1.78	1.73
4	A	1302	EZO	C21-CL1	2.02	1.78	1.73

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	NAG	C1-O5-C5	7.49	122.22	112.19
4	A	1303	EZO	C17-C18-S19	-3.95	106.38	111.16
4	C	1303	EZO	C17-C18-S19	-3.90	106.44	111.16
4	A	1302	EZO	S19-C15-N16	-3.88	111.48	116.28
4	B	1302	EZO	S19-C15-N16	-3.66	111.74	116.28
4	C	1302	EZO	C21-C20-C17	-3.61	120.27	125.02
4	C	1303	EZO	S19-C15-N16	-3.58	111.85	116.28
4	C	1302	EZO	S19-C15-N16	-3.57	111.86	116.28
4	A	1303	EZO	S19-C15-N16	-3.56	111.87	116.28
4	B	1303	EZO	S19-C15-N16	-3.40	112.07	116.28
4	B	1302	EZO	C21-C20-C17	-3.14	120.90	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1303	EZO	C17-C18-S19	-3.08	107.43	111.16
4	C	1302	EZO	C4-C5-C7	-3.07	119.09	122.51
4	B	1303	EZO	C4-C12-N13	-3.04	114.51	119.93
4	A	1302	EZO	C4-C5-C7	-2.93	119.26	122.51
4	A	1302	EZO	C15-N16-C17	2.89	115.04	106.26
4	B	1302	EZO	C15-N16-C17	2.86	114.95	106.26
4	A	1302	EZO	C21-C20-C17	-2.86	121.27	125.02
4	C	1302	EZO	C15-N16-C17	2.83	114.84	106.26
4	C	1302	EZO	C5-C4-C12	-2.78	119.23	122.49
4	A	1302	EZO	C20-C17-C18	-2.65	123.34	128.24
4	A	1303	EZO	C4-C12-N13	-2.65	115.21	119.93
4	A	1302	EZO	C20-C17-N16	2.61	124.16	118.86
4	C	1303	EZO	O8-C7-C5	2.56	122.56	115.28
4	C	1302	EZO	C20-C17-C18	-2.46	123.70	128.24
4	A	1303	EZO	O8-C7-C5	2.44	122.22	115.28
4	A	1303	EZO	C18-S19-C15	2.42	93.52	89.41
4	A	1303	EZO	O8-C7-O9	-2.42	118.16	123.35
4	A	1302	EZO	C5-C4-C12	-2.41	119.67	122.49
4	B	1302	EZO	C4-C5-C7	-2.40	119.84	122.51
4	C	1302	EZO	C20-C17-N16	2.38	123.70	118.86
4	C	1303	EZO	C18-S19-C15	2.35	93.41	89.41
4	A	1303	EZO	C25-C20-C21	2.32	120.50	117.79
4	C	1303	EZO	O8-C7-O9	-2.29	118.42	123.35
4	B	1302	EZO	C5-C4-C12	-2.28	119.81	122.49
4	B	1302	EZO	C20-C17-N16	2.25	123.43	118.86
4	B	1302	EZO	C20-C17-C18	-2.24	124.11	128.24
4	C	1303	EZO	C25-C20-C21	2.21	120.38	117.79
4	A	1303	EZO	C25-C20-C17	-2.18	115.54	119.25
4	A	1303	EZO	N14-C15-N16	2.17	124.96	122.82
4	C	1303	EZO	S19-C15-N14	2.16	123.84	120.22
4	A	1302	EZO	N14-C15-N16	2.14	124.93	122.82
4	B	1303	EZO	C15-N16-C17	2.14	112.75	106.26
4	C	1302	EZO	S19-C15-N14	2.11	123.75	120.22
4	C	1303	EZO	C25-C20-C17	-2.11	115.66	119.25
4	A	1302	EZO	C27-N14-N13	-2.10	119.55	122.19
4	C	1303	EZO	C15-N16-C17	2.08	112.56	106.26
4	B	1302	EZO	C25-C20-C21	2.06	120.20	117.79
4	C	1303	EZO	C20-C17-C18	-2.05	124.45	128.24
4	A	1302	EZO	S19-C15-N14	2.02	123.59	120.22
4	B	1302	EZO	S19-C15-N14	2.01	123.59	120.22
4	B	1302	EZO	O8-C7-C5	2.00	120.97	115.28

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	EZO	N13-C12-C4-C3
4	A	1302	EZO	N13-C12-C4-C5
4	A	1302	EZO	N16-C15-N14-N13
4	A	1302	EZO	S19-C15-N14-N13
4	A	1302	EZO	C12-N13-N14-C15
4	A	1302	EZO	C12-N13-N14-C27
4	A	1303	EZO	N13-C12-C4-C5
4	B	1302	EZO	N13-C12-C4-C5
4	B	1302	EZO	N16-C15-N14-N13
4	B	1302	EZO	S19-C15-N14-N13
4	B	1302	EZO	C12-N13-N14-C15
4	B	1302	EZO	C12-N13-N14-C27
4	C	1302	EZO	N13-C12-C4-C5
4	B	1302	EZO	N13-C12-C4-C3
3	A	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	C	1301	NAG	C8-C7-N2-C2
3	C	1301	NAG	O7-C7-N2-C2
4	C	1302	EZO	N13-C12-C4-C3
4	A	1303	EZO	N13-C12-C4-C3
4	B	1303	EZO	N13-C12-C4-C5
4	B	1302	EZO	C6-C5-C7-O9
4	B	1303	EZO	N13-C12-C4-C3
4	B	1302	EZO	C6-C5-C7-O8
4	A	1302	EZO	C6-C5-C7-O9
4	A	1302	EZO	S19-C15-N14-C27
4	B	1302	EZO	S19-C15-N14-C27
4	A	1302	EZO	C6-C5-C7-O8
4	C	1302	EZO	C6-C5-C7-O9
4	C	1302	EZO	C6-C5-C7-O8
4	C	1303	EZO	N13-C12-C4-C3
4	B	1302	EZO	C4-C5-C7-O9
4	B	1302	EZO	N16-C15-N14-C27
4	C	1302	EZO	C12-N13-N14-C27

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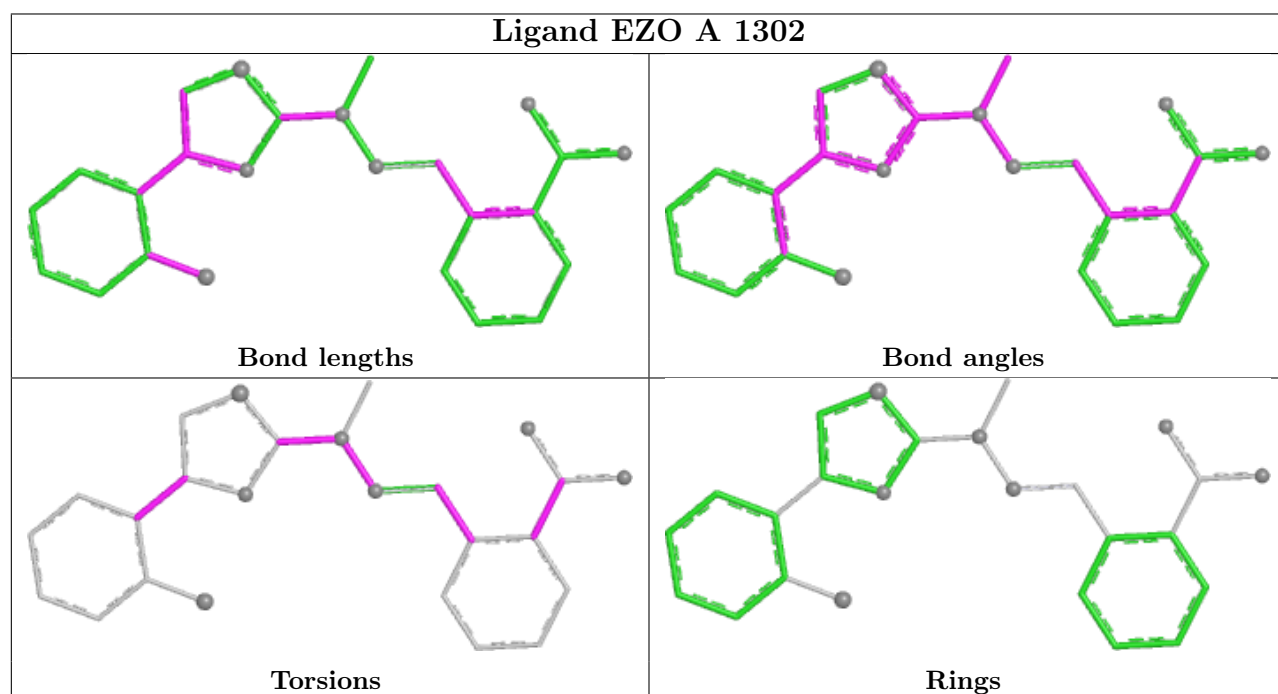
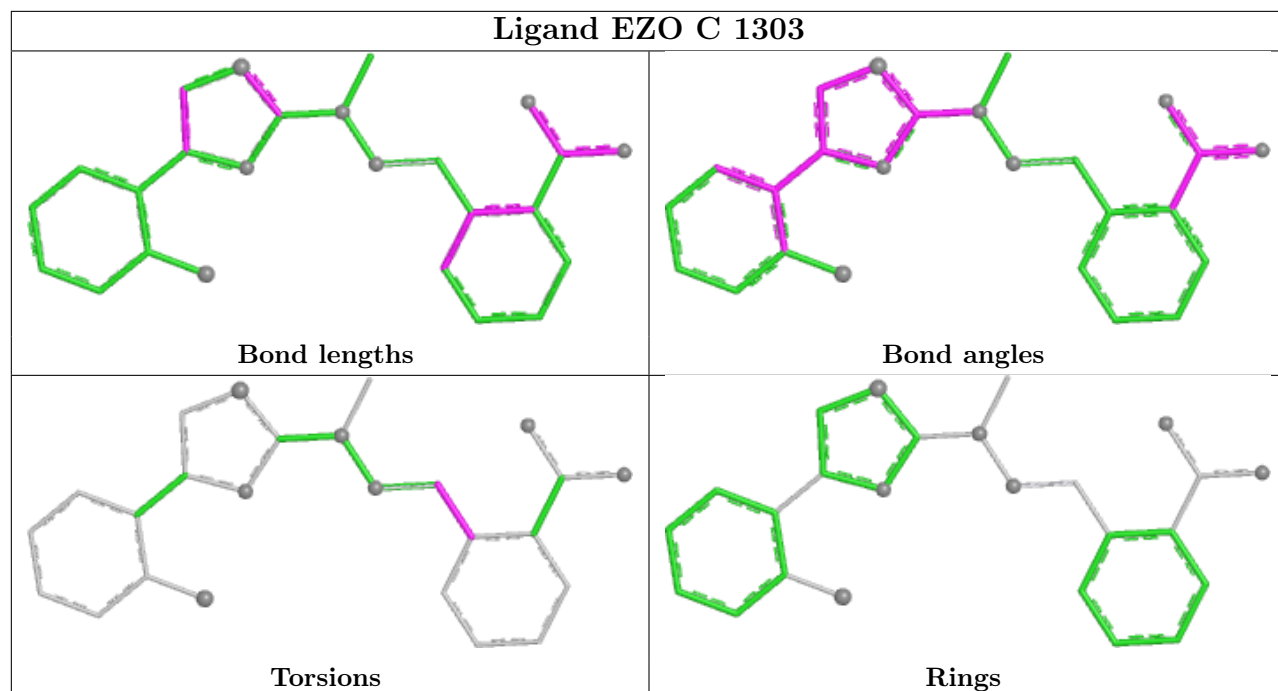
Mol	Chain	Res	Type	Atoms
4	A	1302	EZO	N16-C17-C20-C25
4	B	1302	EZO	N16-C17-C20-C25
4	C	1302	EZO	N16-C17-C20-C25
4	B	1302	EZO	C4-C5-C7-O8
4	A	1302	EZO	C4-C5-C7-O8
4	A	1302	EZO	C4-C5-C7-O9
4	A	1302	EZO	N16-C17-C20-C21
4	B	1302	EZO	N16-C17-C20-C21
4	C	1302	EZO	N16-C17-C20-C21
4	C	1302	EZO	C4-C5-C7-O9
4	C	1302	EZO	C18-C17-C20-C25
4	C	1302	EZO	C4-C5-C7-O8

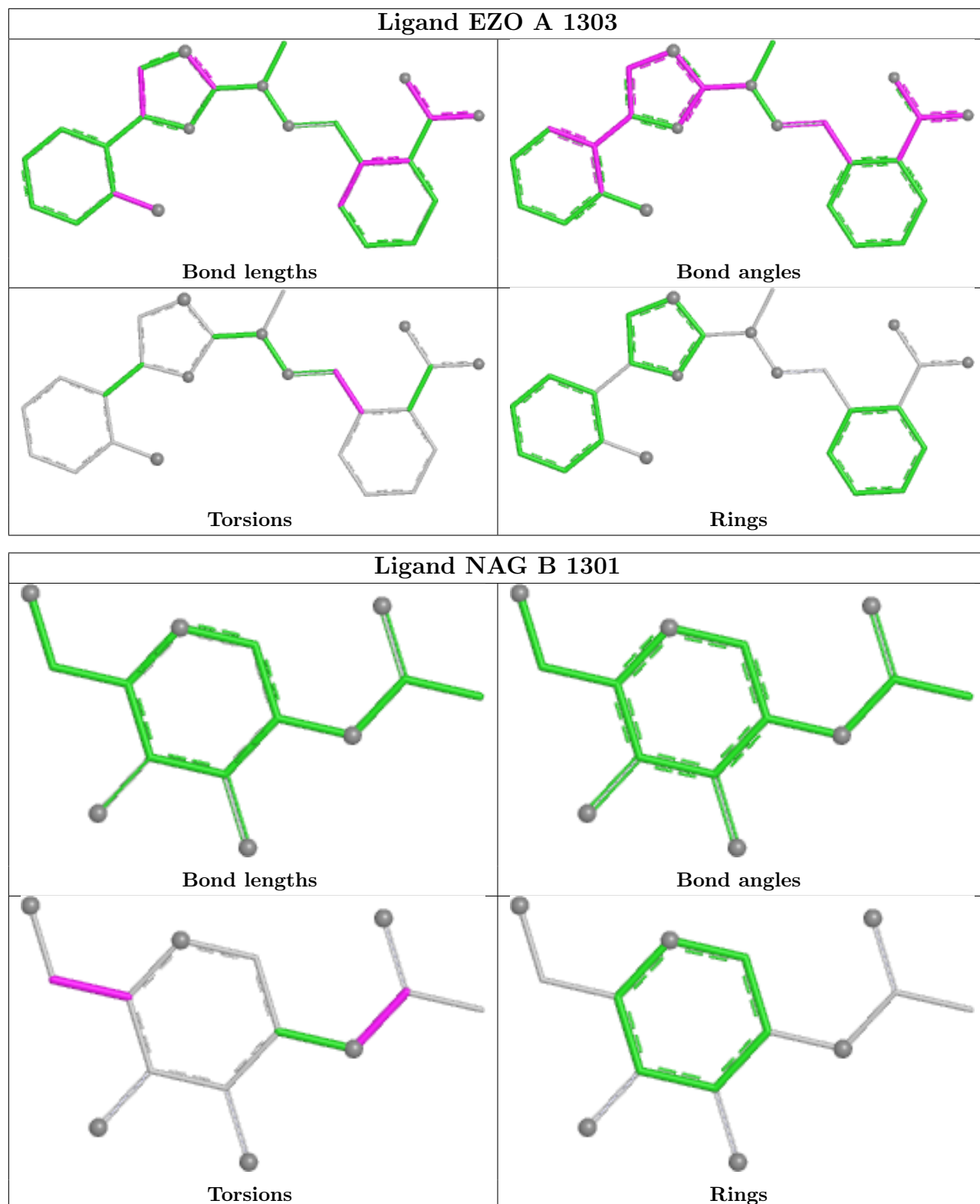
There are no ring outliers.

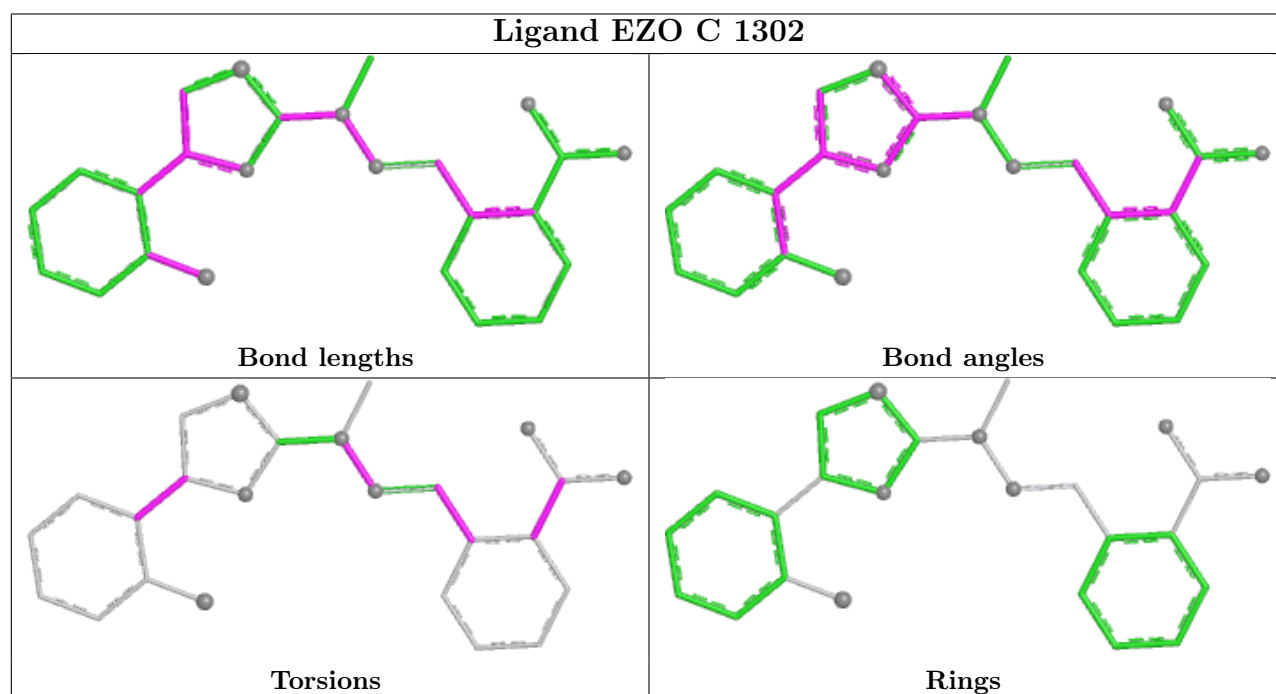
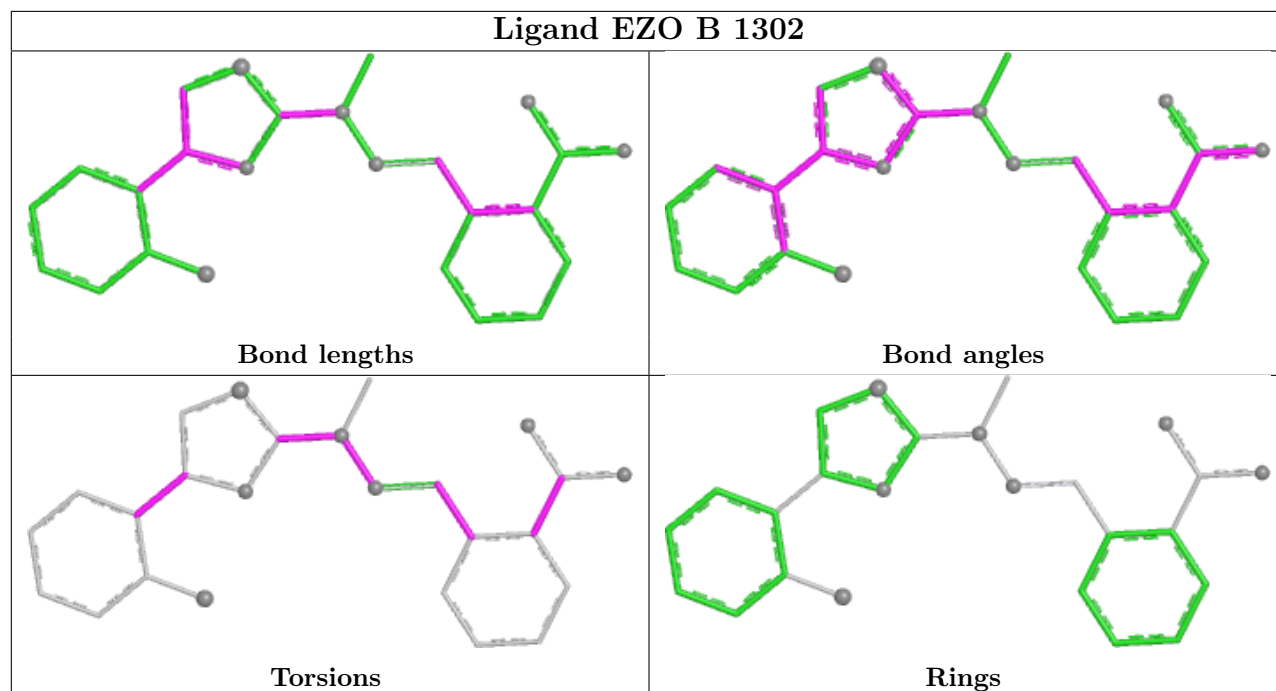
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1303	EZO	3	0
4	A	1302	EZO	2	0
4	A	1303	EZO	6	0
4	B	1302	EZO	1	0
4	C	1302	EZO	2	0
4	B	1303	EZO	3	0

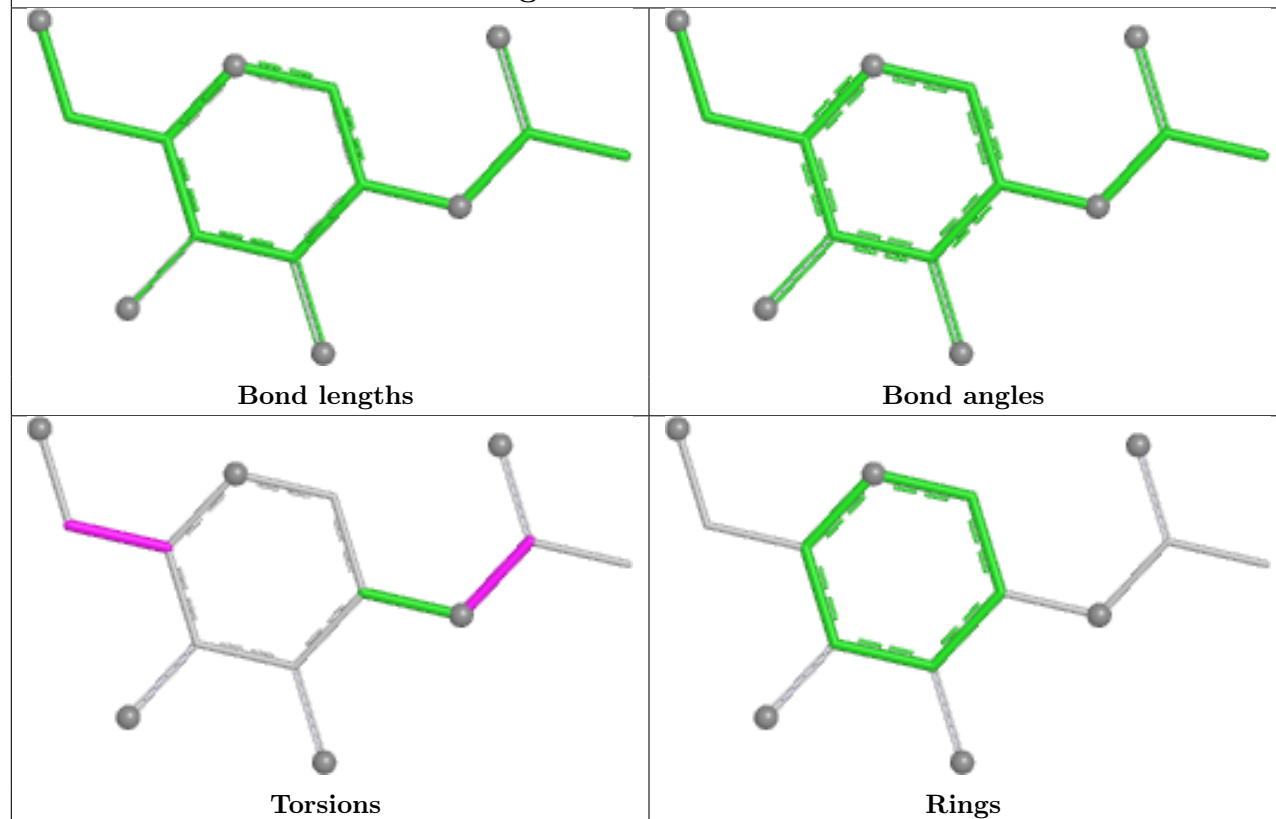
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



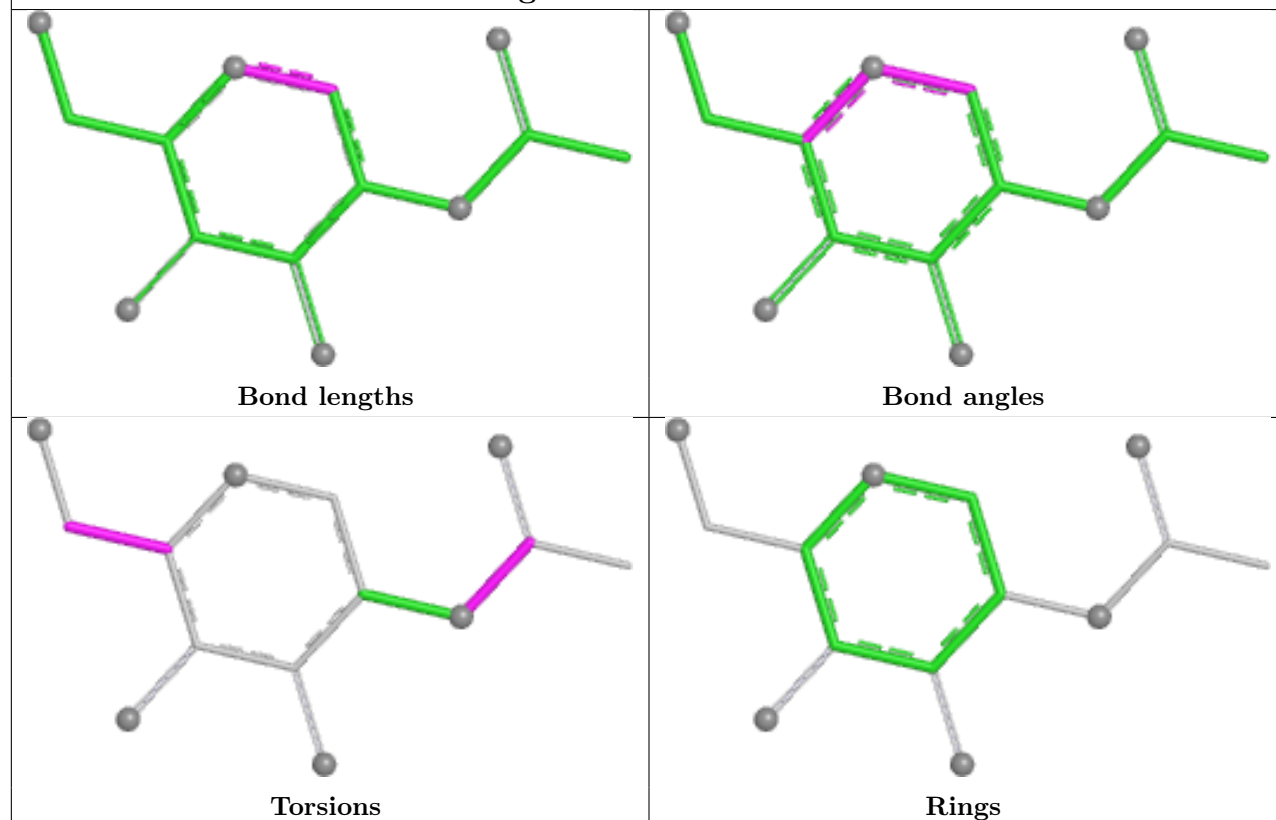


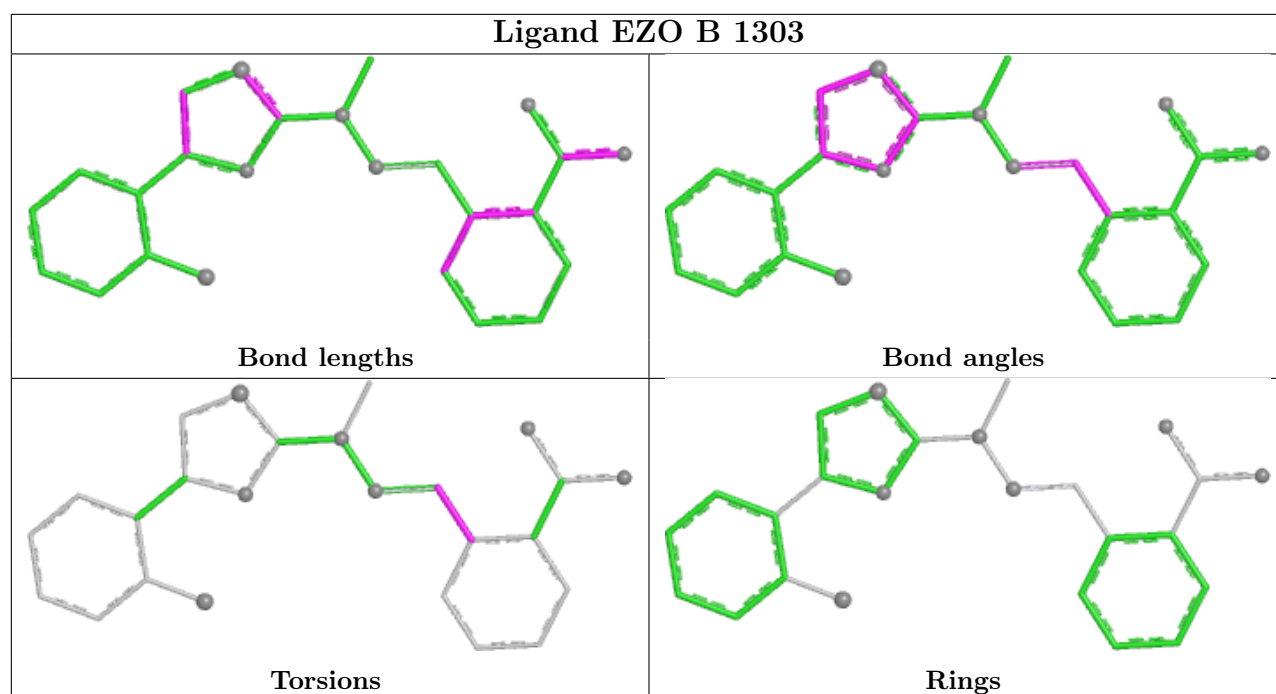


Ligand NAG C 1301



Ligand NAG A 1301





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.

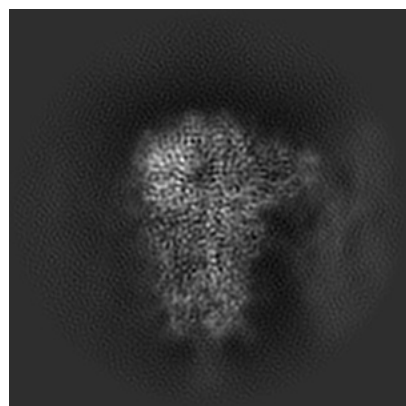
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63424. These allow visual inspection of the internal detail of the map and identification of artifacts.

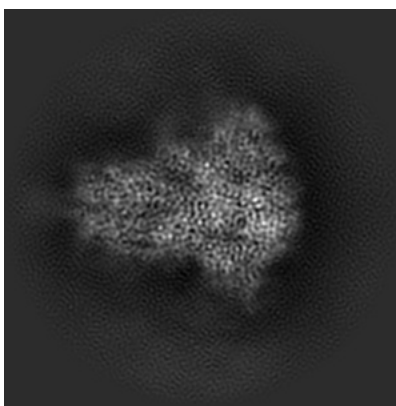
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

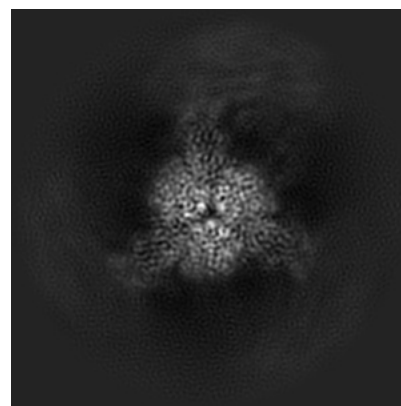
6.1.1 Primary map



X

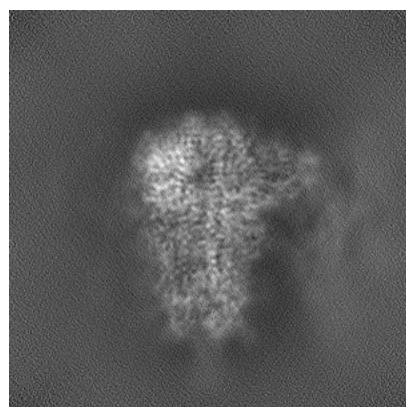


Y

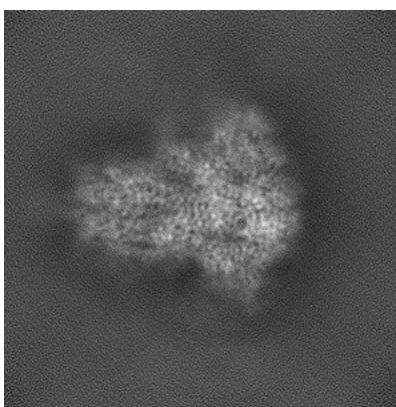


Z

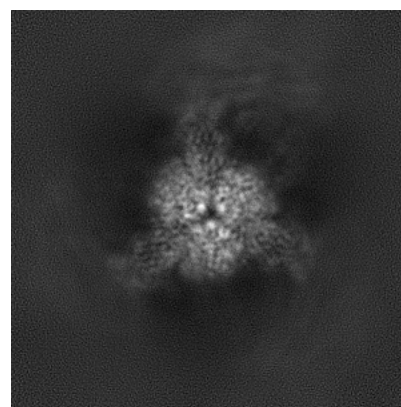
6.1.2 Raw map



X



Y

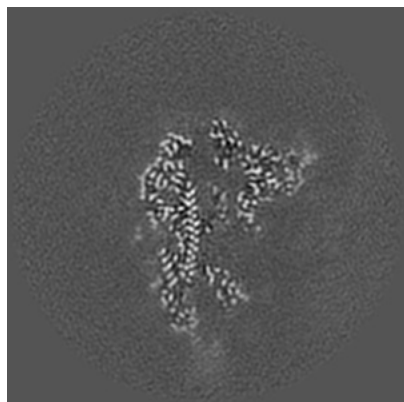


Z

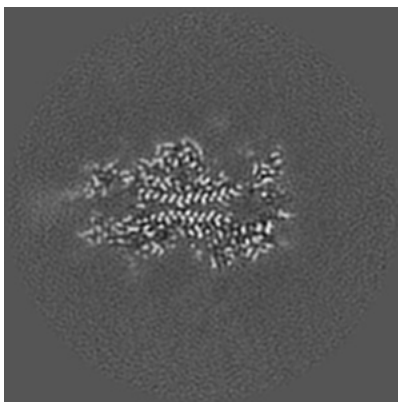
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

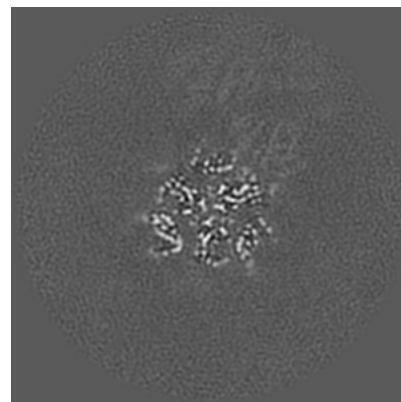
6.2.1 Primary map



X Index: 160

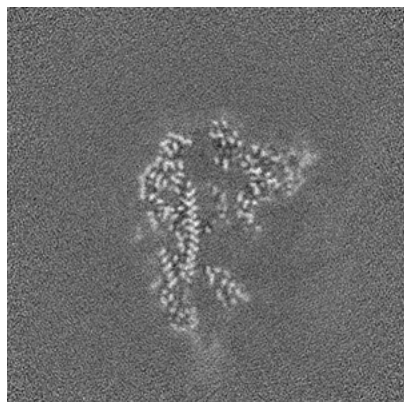


Y Index: 160

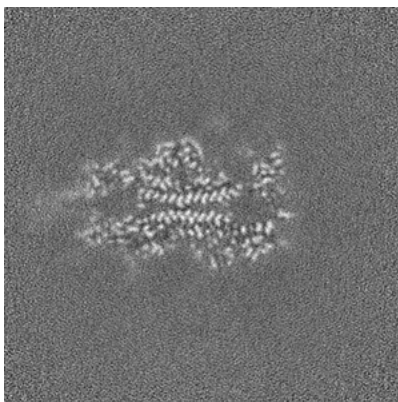


Z Index: 160

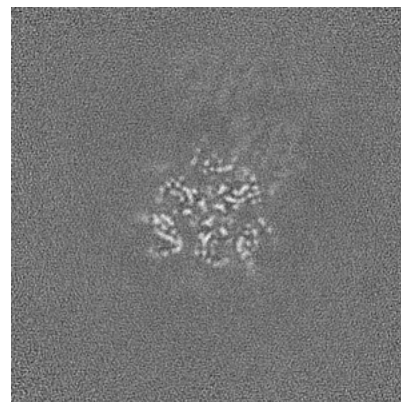
6.2.2 Raw map



X Index: 160



Y Index: 160

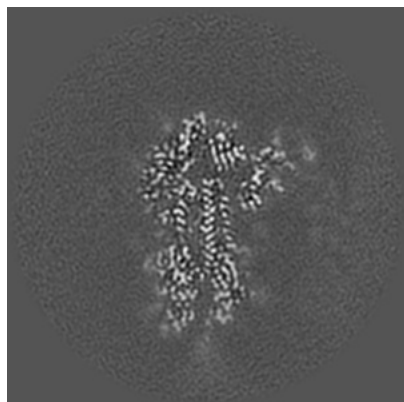


Z Index: 160

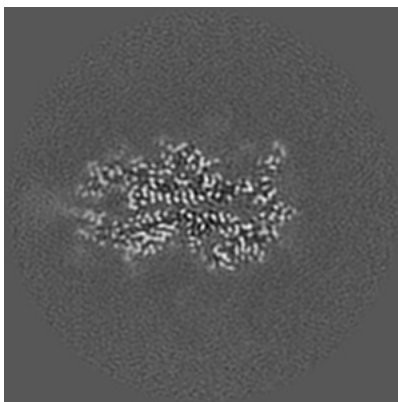
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

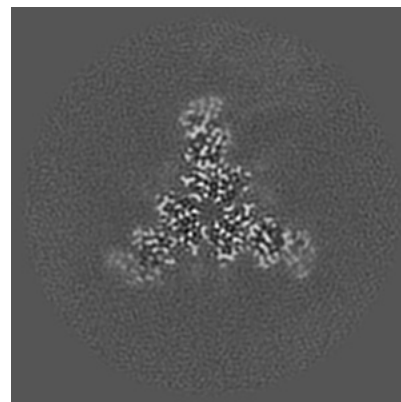
6.3.1 Primary map



X Index: 167

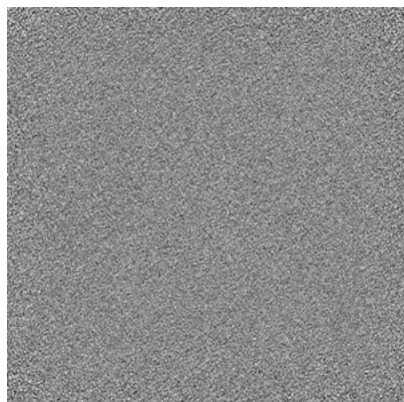


Y Index: 164

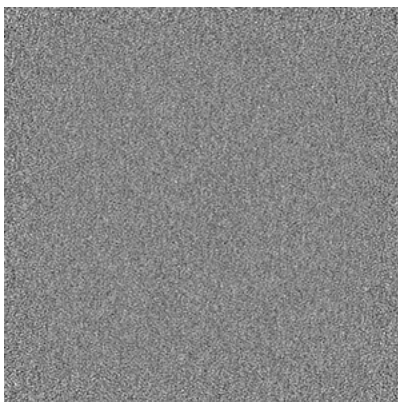


Z Index: 200

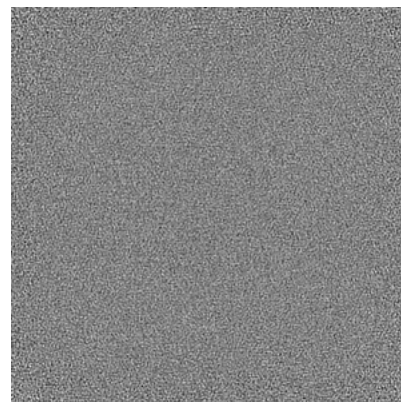
6.3.2 Raw map



X Index: 0



Y Index: 0

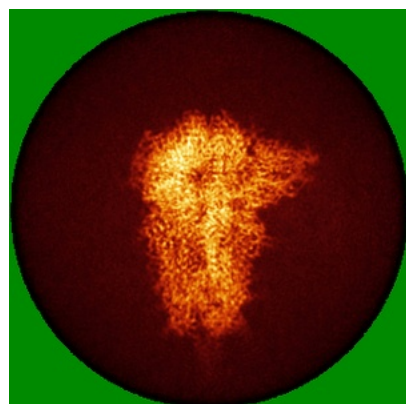


Z Index: 319

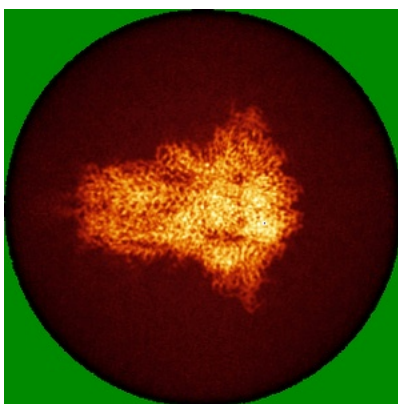
The images above show the largest variance slices of the map in three orthogonal directions.

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

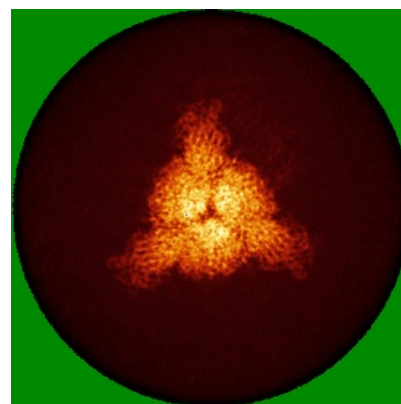
6.4.1 Primary map



X

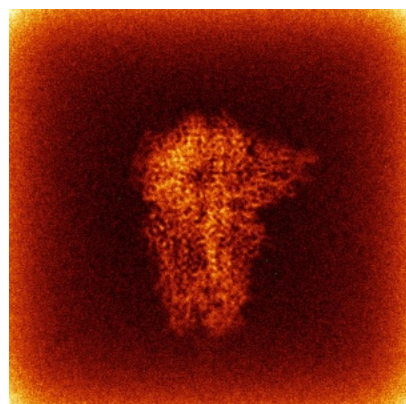


Y

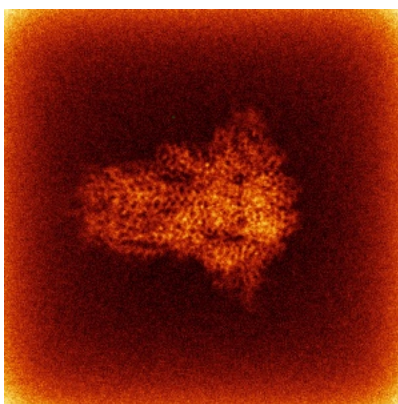


Z

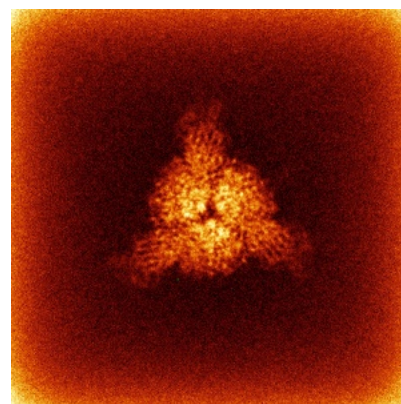
6.4.2 Raw map



X



Y

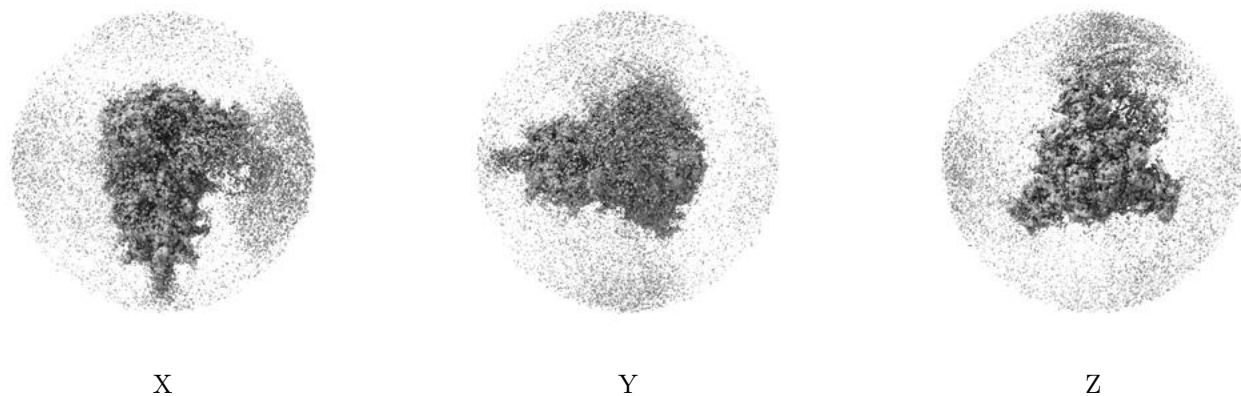


Z

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

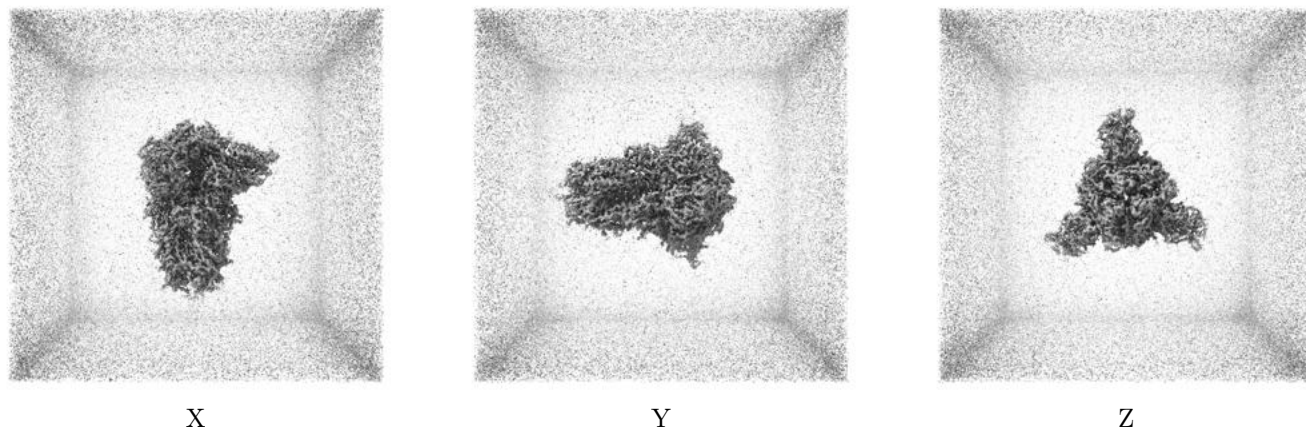
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0505. 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



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

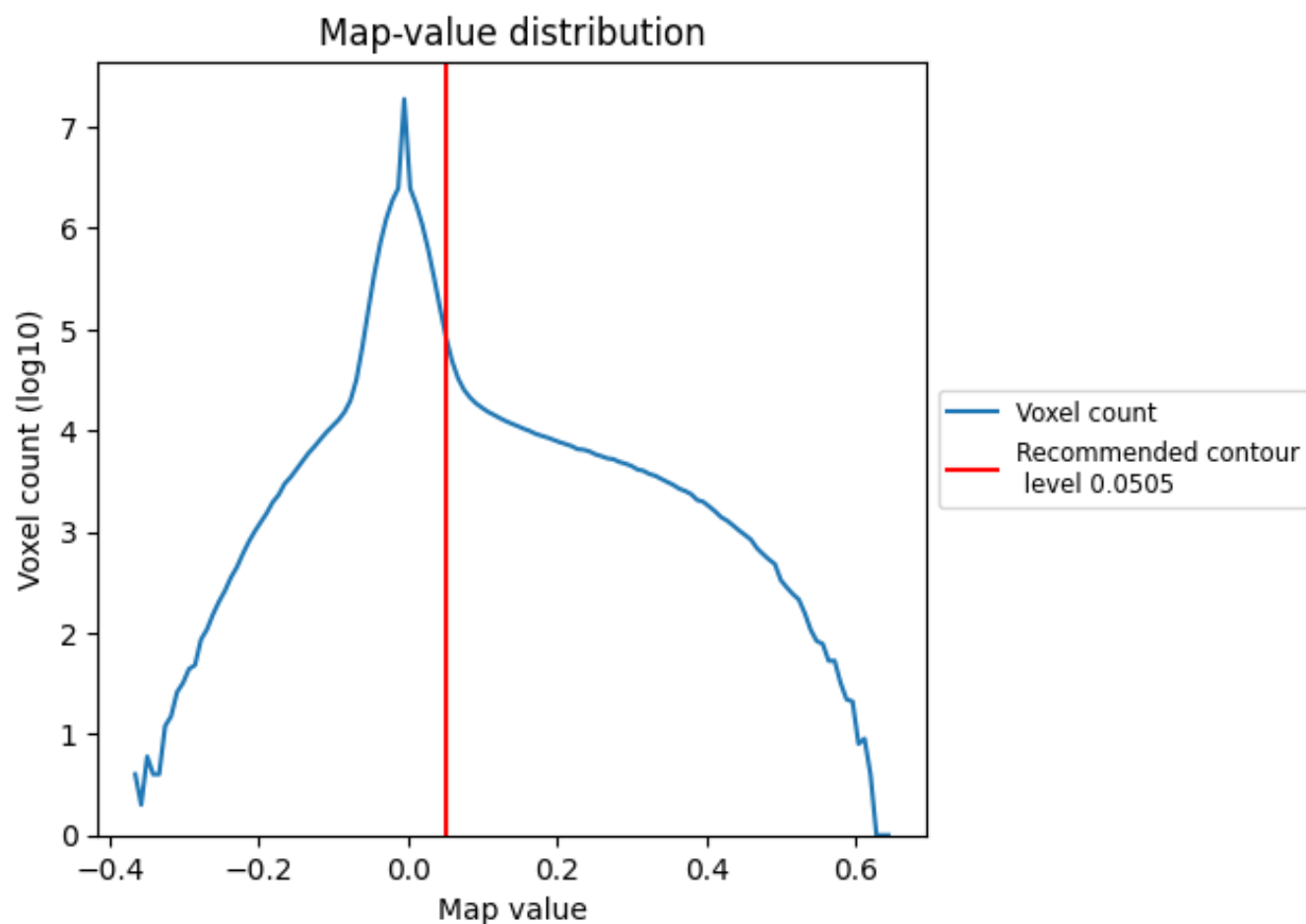
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

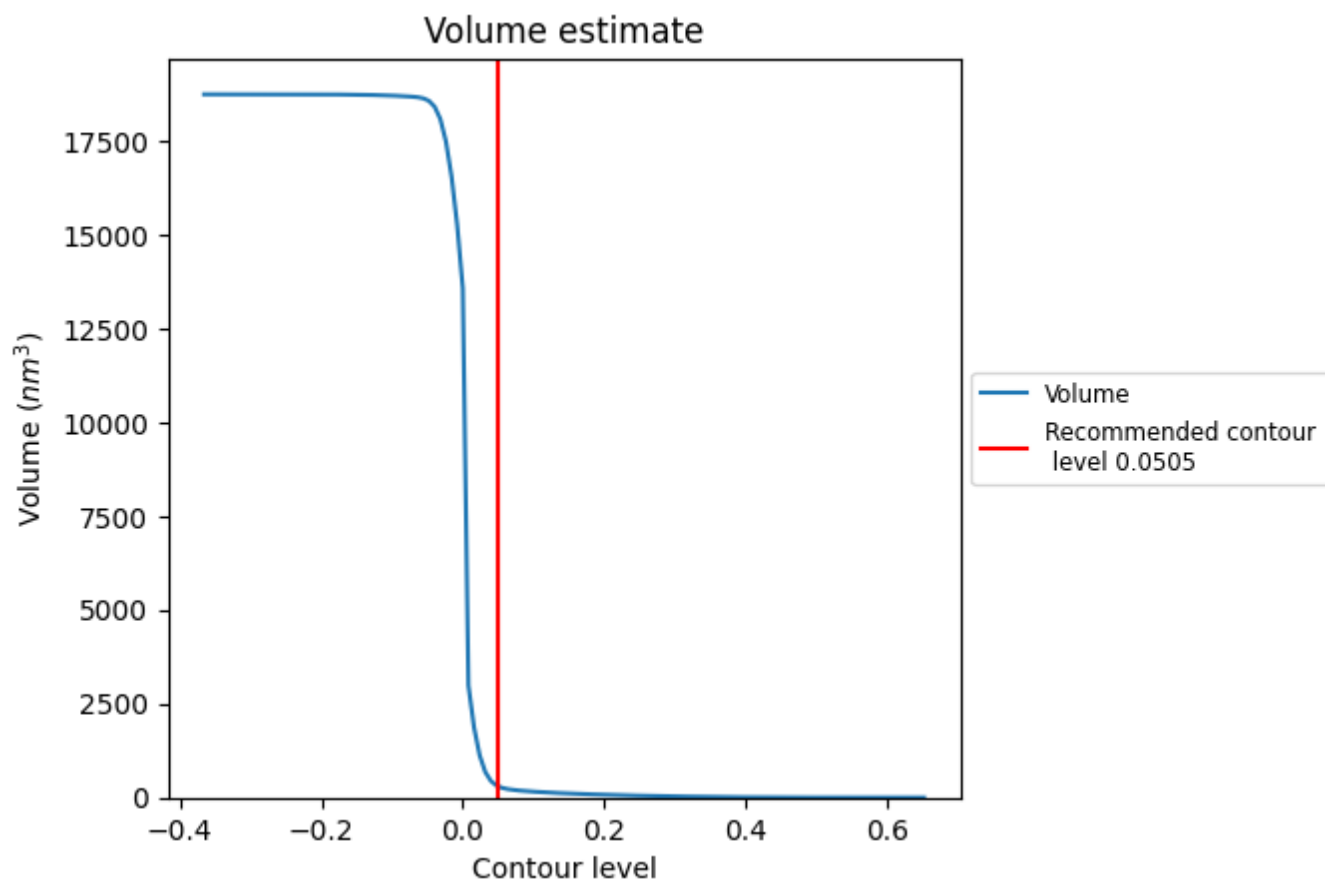
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

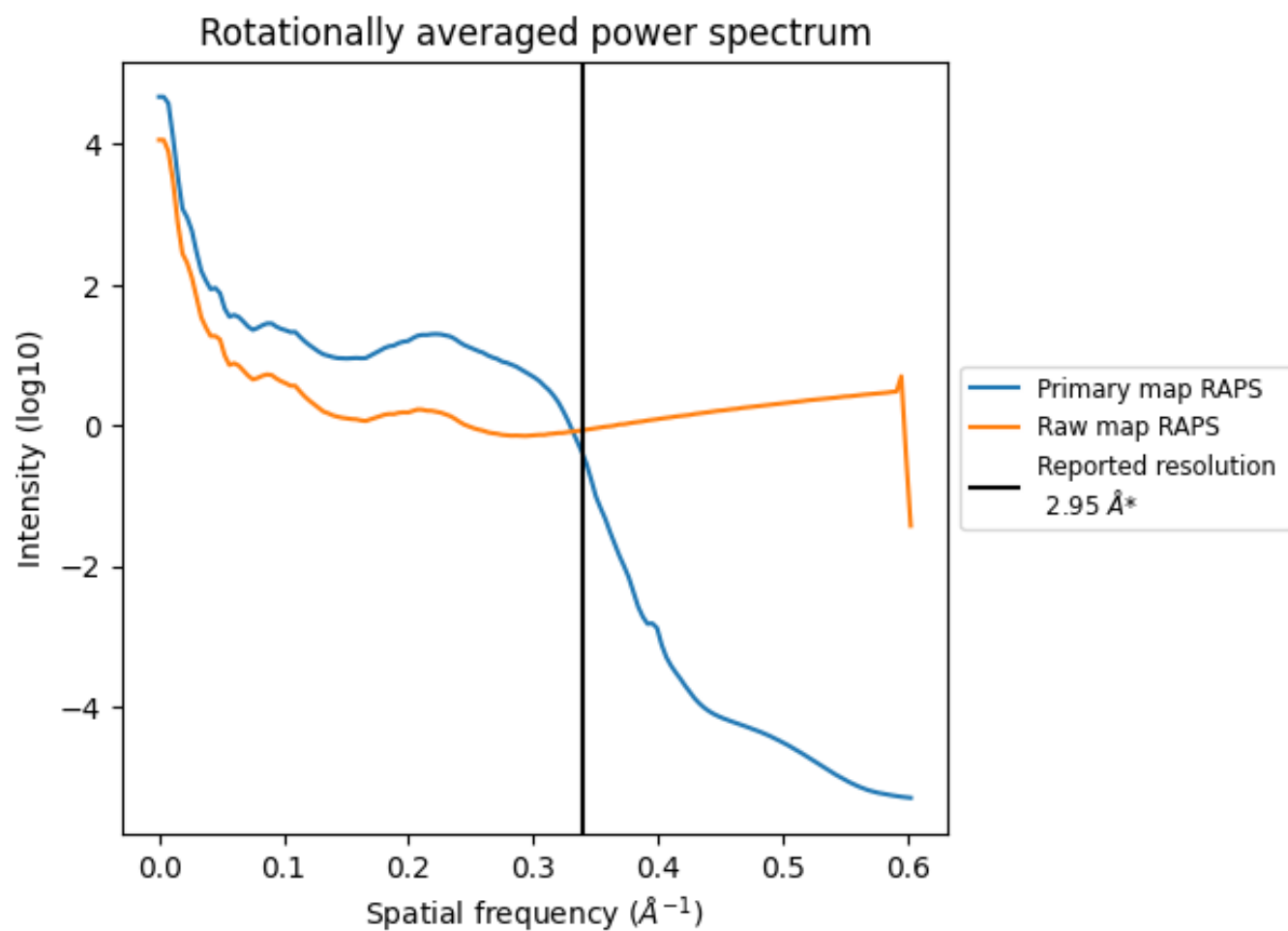
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 298 nm³; this corresponds to an approximate mass of 269 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 ⓘ

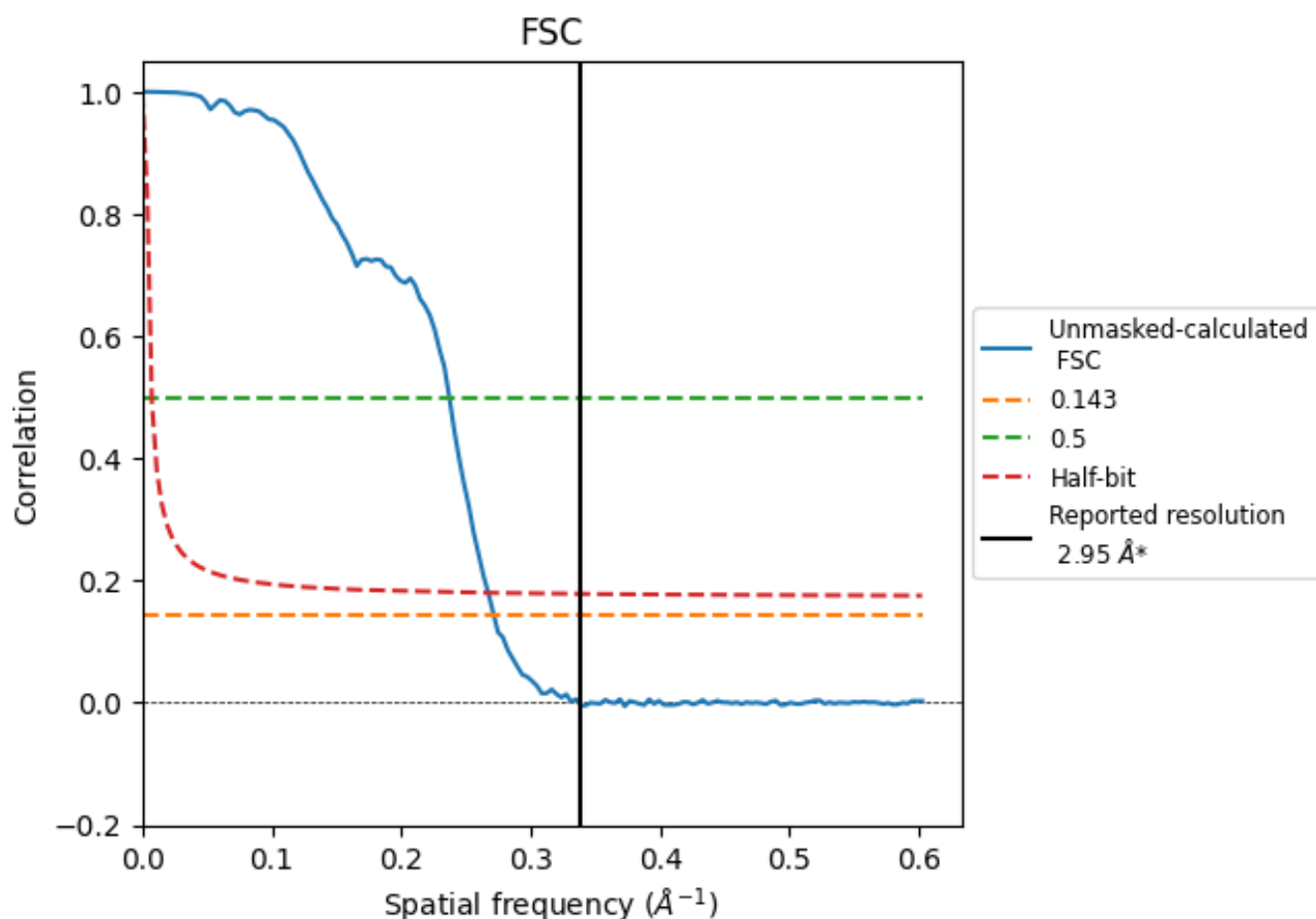


*Reported resolution corresponds to spatial frequency of 0.339 \AA^{-1}

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 0.339 Å⁻¹

8.2 Resolution estimates [i](#)

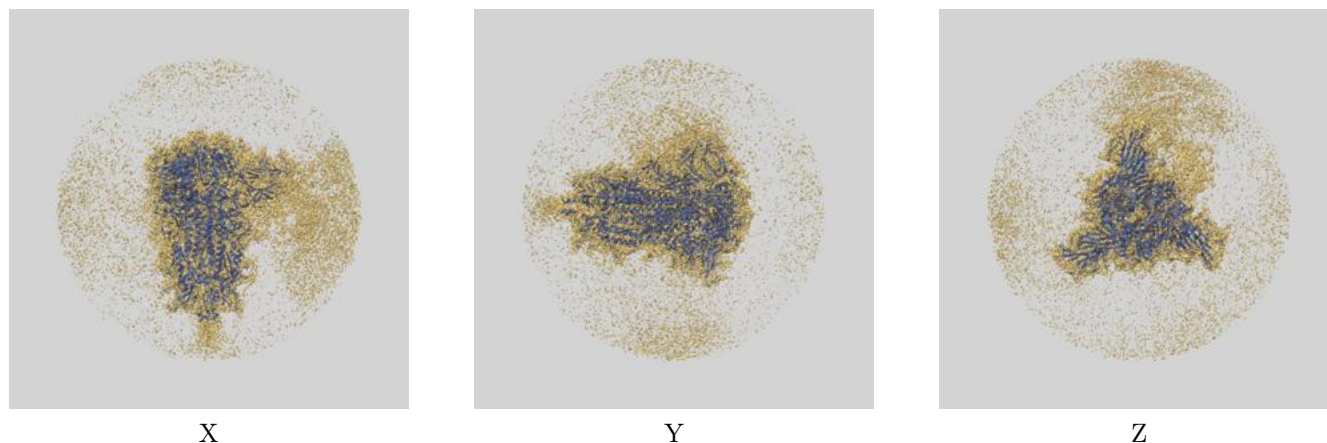
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	4.22	3.74

*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 3.68 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

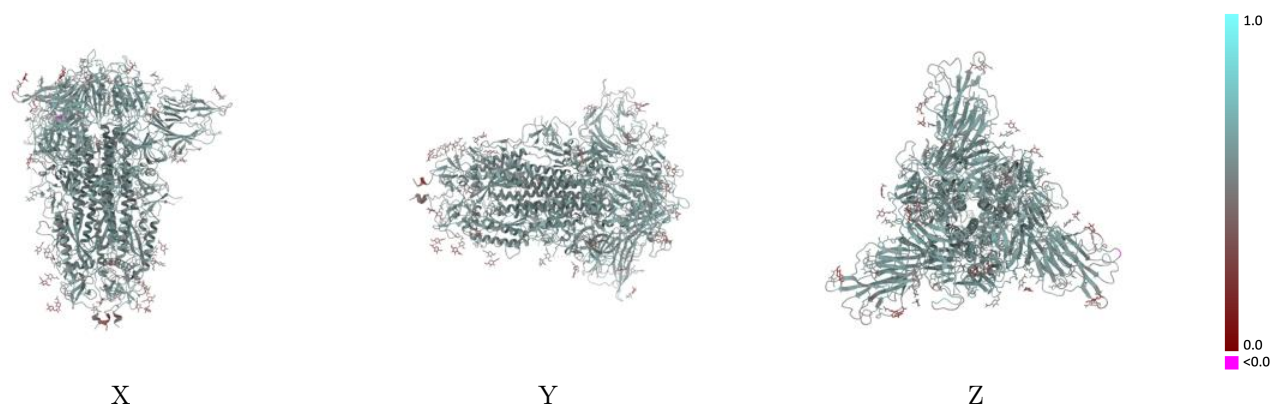
This section contains information regarding the fit between EMDB map EMD-63424 and PDB model 9LVS. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



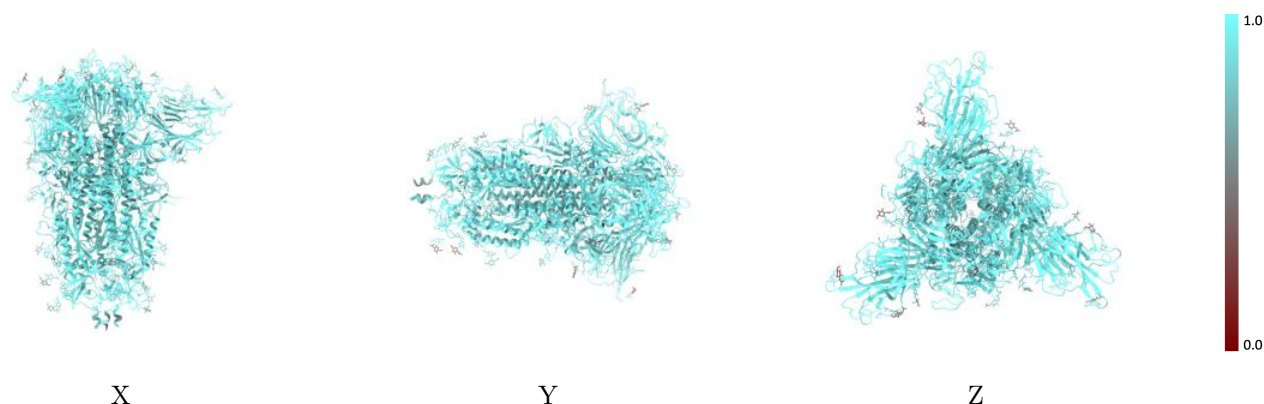
The images above show the 3D surface view of the map at the recommended contour level 0.0505 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



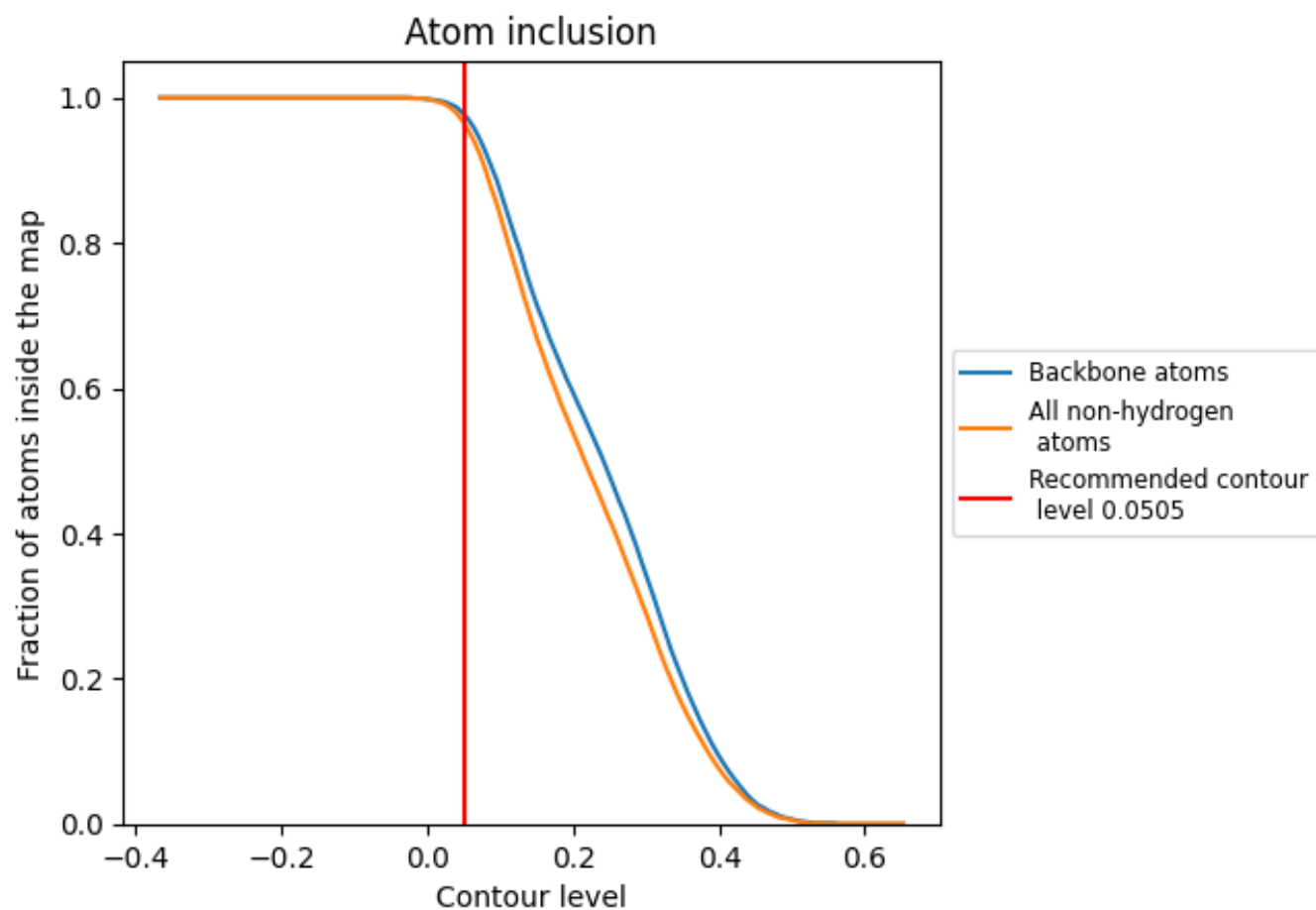
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0505).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.0505) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9650	 0.5590
A	 0.9740	 0.5660
B	 0.9730	 0.5690
C	 0.9760	 0.5680
D	 0.7500	 0.4010
E	 0.9640	 0.5070
F	 0.6790	 0.3170
G	 0.7140	 0.3810
H	 0.8930	 0.5120
I	 0.8570	 0.4250
J	 0.7140	 0.3730
K	 0.9290	 0.3900
L	 0.7860	 0.3490
M	 0.9640	 0.5210
N	 0.9290	 0.4750
O	 0.7860	 0.3450
P	 0.8930	 0.4870
Q	 0.6790	 0.3310
R	 0.6790	 0.2850
S	 0.7860	 0.4140
T	 0.9640	 0.5390
U	 0.5360	 0.2060
V	 0.6790	 0.3220
W	 0.8930	 0.5070
X	 0.8210	 0.3630
Y	 0.6790	 0.3970
Z	 0.7140	 0.4510
a	 0.7860	 0.2660
b	 0.9640	 0.5360
c	 0.8930	 0.4660
d	 0.6430	 0.3850
e	 1.0000	 0.4160
f	 0.5710	 0.2230
g	 0.5710	 0.3010
h	 0.6070	 0.3100



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Chain	Atom inclusion	Q-score
i	 0.8930	 0.4970
j	 0.5710	 0.1920
k	 0.6430	 0.2960
l	 0.8570	 0.4200
m	 0.8570	 0.4200
n	 0.7860	 0.3710
o	 0.8570	 0.3220
p	 0.6790	 0.2670
q	 0.9290	 0.5640
r	 0.8570	 0.4350
s	 0.7500	 0.4000
t	 0.8210	 0.4360
u	 0.7500	 0.3770
v	 0.8210	 0.3960