



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:23 AM UTC

PDB ID : 7Y6T / pdb_00007y6t
EMDB ID : EMD-33647
Title : Cryo-EM map of IPEC-J2 cell-derived PEDV PT52 S protein one D0-down and two D0-up
Authors : Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on : 2022-06-21
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

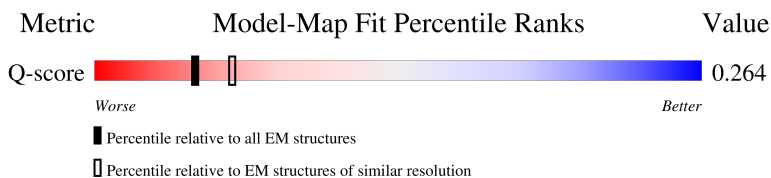
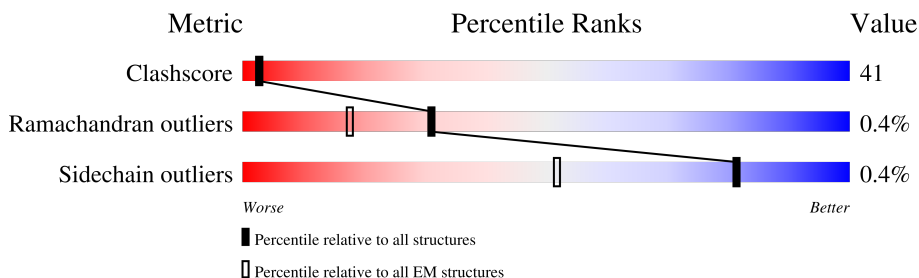
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



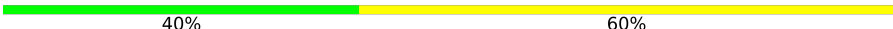
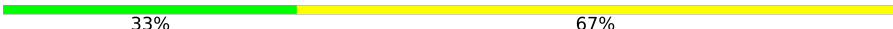
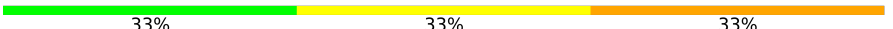
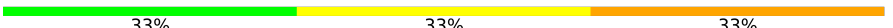
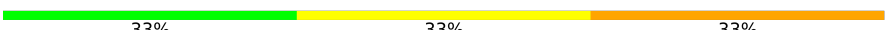
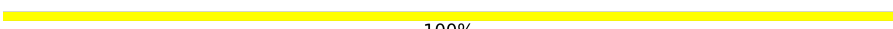
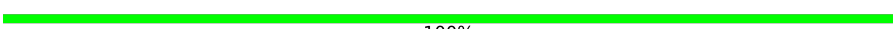
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	1402	
1	B	1402	
1	C	1402	
2	D	5	

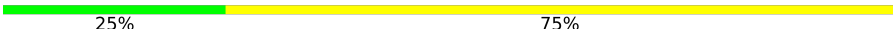
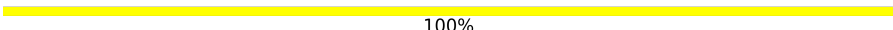
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Mol	Chain	Length	Quality of chain
2	O	5	 20% 80%
2	b	5	 40% 60%
3	E	3	 33% 67%
3	F	3	 33% 33% 33%
3	G	3	 33% 67%
3	K	3	 33% 67%
3	Q	3	 67% 33%
3	T	3	 33% 33% 33%
3	V	3	 33% 67%
3	X	3	 33% 67%
3	d	3	 67% 33%
3	g	3	 33% 67%
3	h	3	 33% 33% 33%
3	j	3	 33% 67%
4	H	2	 100%
4	I	2	 50% 50%
4	J	2	 50% 50%
4	L	2	 50% 50%
4	R	2	 50% 50%
4	U	2	 100%
4	W	2	 100%
4	Y	2	 100%
4	e	2	 50% 50%
4	i	2	 50% 50%
5	M	3	 33% 67%

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Mol	Chain	Length	Quality of chain
5	Z	3	 67%33%
6	N	4	 50%50%
6	a	4	 25%75%
6	k	4	 50%25%25%
7	P	2	 100%
7	S	2	 50%50%
7	c	2	 50%50%
7	f	2	 50%50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1124	Total	C	N	O	S	0	0
			8648	5493	1442	1676	37		
1	C	1098	Total	C	N	O	S	0	0
			8440	5359	1407	1637	37		
1	B	1224	Total	C	N	O	S	0	0
			9398	5972	1556	1829	41		

There are 231 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1076	PRO	ILE	engineered mutation	UNP A0A1Y0DD46
A	1077	PRO	LEU	engineered mutation	UNP A0A1Y0DD46
A	1328	GLU	-	expression tag	UNP A0A1Y0DD46
A	1329	PHE	-	expression tag	UNP A0A1Y0DD46
A	1330	GLY	-	expression tag	UNP A0A1Y0DD46
A	1331	SER	-	expression tag	UNP A0A1Y0DD46
A	1332	GLY	-	expression tag	UNP A0A1Y0DD46
A	1333	GLY	-	expression tag	UNP A0A1Y0DD46
A	1334	TYR	-	expression tag	UNP A0A1Y0DD46
A	1335	ILE	-	expression tag	UNP A0A1Y0DD46
A	1336	PRO	-	expression tag	UNP A0A1Y0DD46
A	1337	GLU	-	expression tag	UNP A0A1Y0DD46
A	1338	ALA	-	expression tag	UNP A0A1Y0DD46
A	1339	PRO	-	expression tag	UNP A0A1Y0DD46
A	1340	ARG	-	expression tag	UNP A0A1Y0DD46
A	1341	ASP	-	expression tag	UNP A0A1Y0DD46
A	1342	GLY	-	expression tag	UNP A0A1Y0DD46
A	1343	GLN	-	expression tag	UNP A0A1Y0DD46
A	1344	ALA	-	expression tag	UNP A0A1Y0DD46
A	1345	TYR	-	expression tag	UNP A0A1Y0DD46
A	1346	VAL	-	expression tag	UNP A0A1Y0DD46
A	1347	ARG	-	expression tag	UNP A0A1Y0DD46
A	1348	LYS	-	expression tag	UNP A0A1Y0DD46
A	1349	ASP	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1350	GLY	-	expression tag	UNP A0A1Y0DD46
A	1351	GLU	-	expression tag	UNP A0A1Y0DD46
A	1352	TRP	-	expression tag	UNP A0A1Y0DD46
A	1353	VAL	-	expression tag	UNP A0A1Y0DD46
A	1354	LEU	-	expression tag	UNP A0A1Y0DD46
A	1355	LEU	-	expression tag	UNP A0A1Y0DD46
A	1356	SER	-	expression tag	UNP A0A1Y0DD46
A	1357	THR	-	expression tag	UNP A0A1Y0DD46
A	1358	PHE	-	expression tag	UNP A0A1Y0DD46
A	1359	LEU	-	expression tag	UNP A0A1Y0DD46
A	1360	LYS	-	expression tag	UNP A0A1Y0DD46
A	1361	GLY	-	expression tag	UNP A0A1Y0DD46
A	1362	GLN	-	expression tag	UNP A0A1Y0DD46
A	1363	ASP	-	expression tag	UNP A0A1Y0DD46
A	1364	ASN	-	expression tag	UNP A0A1Y0DD46
A	1365	SER	-	expression tag	UNP A0A1Y0DD46
A	1366	ALA	-	expression tag	UNP A0A1Y0DD46
A	1367	ASP	-	expression tag	UNP A0A1Y0DD46
A	1368	ILE	-	expression tag	UNP A0A1Y0DD46
A	1369	GLN	-	expression tag	UNP A0A1Y0DD46
A	1370	HIS	-	expression tag	UNP A0A1Y0DD46
A	1371	SER	-	expression tag	UNP A0A1Y0DD46
A	1372	GLY	-	expression tag	UNP A0A1Y0DD46
A	1373	ARG	-	expression tag	UNP A0A1Y0DD46
A	1374	PRO	-	expression tag	UNP A0A1Y0DD46
A	1375	LEU	-	expression tag	UNP A0A1Y0DD46
A	1376	GLU	-	expression tag	UNP A0A1Y0DD46
A	1377	SER	-	expression tag	UNP A0A1Y0DD46
A	1378	ARG	-	expression tag	UNP A0A1Y0DD46
A	1379	GLY	-	expression tag	UNP A0A1Y0DD46
A	1380	PRO	-	expression tag	UNP A0A1Y0DD46
A	1381	PHE	-	expression tag	UNP A0A1Y0DD46
A	1382	GLU	-	expression tag	UNP A0A1Y0DD46
A	1383	GLN	-	expression tag	UNP A0A1Y0DD46
A	1384	LYS	-	expression tag	UNP A0A1Y0DD46
A	1385	LEU	-	expression tag	UNP A0A1Y0DD46
A	1386	ILE	-	expression tag	UNP A0A1Y0DD46
A	1387	SER	-	expression tag	UNP A0A1Y0DD46
A	1388	GLU	-	expression tag	UNP A0A1Y0DD46
A	1389	GLU	-	expression tag	UNP A0A1Y0DD46
A	1390	ASP	-	expression tag	UNP A0A1Y0DD46
A	1391	LEU	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1392	ASN	-	expression tag	UNP A0A1Y0DD46
A	1393	MET	-	expression tag	UNP A0A1Y0DD46
A	1394	HIS	-	expression tag	UNP A0A1Y0DD46
A	1395	THR	-	expression tag	UNP A0A1Y0DD46
A	1396	GLY	-	expression tag	UNP A0A1Y0DD46
A	1397	HIS	-	expression tag	UNP A0A1Y0DD46
A	1398	HIS	-	expression tag	UNP A0A1Y0DD46
A	1399	HIS	-	expression tag	UNP A0A1Y0DD46
A	1400	HIS	-	expression tag	UNP A0A1Y0DD46
A	1401	HIS	-	expression tag	UNP A0A1Y0DD46
A	1402	HIS	-	expression tag	UNP A0A1Y0DD46
C	1076	PRO	ILE	conflict	UNP A0A1Y0DD46
C	1077	PRO	LEU	conflict	UNP A0A1Y0DD46
C	1328	GLU	-	expression tag	UNP A0A1Y0DD46
C	1329	PHE	-	expression tag	UNP A0A1Y0DD46
C	1330	GLY	-	expression tag	UNP A0A1Y0DD46
C	1331	SER	-	expression tag	UNP A0A1Y0DD46
C	1332	GLY	-	expression tag	UNP A0A1Y0DD46
C	1333	GLY	-	expression tag	UNP A0A1Y0DD46
C	1334	TYR	-	expression tag	UNP A0A1Y0DD46
C	1335	ILE	-	expression tag	UNP A0A1Y0DD46
C	1336	PRO	-	expression tag	UNP A0A1Y0DD46
C	1337	GLU	-	expression tag	UNP A0A1Y0DD46
C	1338	ALA	-	expression tag	UNP A0A1Y0DD46
C	1339	PRO	-	expression tag	UNP A0A1Y0DD46
C	1340	ARG	-	expression tag	UNP A0A1Y0DD46
C	1341	ASP	-	expression tag	UNP A0A1Y0DD46
C	1342	GLY	-	expression tag	UNP A0A1Y0DD46
C	1343	GLN	-	expression tag	UNP A0A1Y0DD46
C	1344	ALA	-	expression tag	UNP A0A1Y0DD46
C	1345	TYR	-	expression tag	UNP A0A1Y0DD46
C	1346	VAL	-	expression tag	UNP A0A1Y0DD46
C	1347	ARG	-	expression tag	UNP A0A1Y0DD46
C	1348	LYS	-	expression tag	UNP A0A1Y0DD46
C	1349	ASP	-	expression tag	UNP A0A1Y0DD46
C	1350	GLY	-	expression tag	UNP A0A1Y0DD46
C	1351	GLU	-	expression tag	UNP A0A1Y0DD46
C	1352	TRP	-	expression tag	UNP A0A1Y0DD46
C	1353	VAL	-	expression tag	UNP A0A1Y0DD46
C	1354	LEU	-	expression tag	UNP A0A1Y0DD46
C	1355	LEU	-	expression tag	UNP A0A1Y0DD46
C	1356	SER	-	expression tag	UNP A0A1Y0DD46

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1357	THR	-	expression tag	UNP A0A1Y0DD46
C	1358	PHE	-	expression tag	UNP A0A1Y0DD46
C	1359	LEU	-	expression tag	UNP A0A1Y0DD46
C	1360	LYS	-	expression tag	UNP A0A1Y0DD46
C	1361	GLY	-	expression tag	UNP A0A1Y0DD46
C	1362	GLN	-	expression tag	UNP A0A1Y0DD46
C	1363	ASP	-	expression tag	UNP A0A1Y0DD46
C	1364	ASN	-	expression tag	UNP A0A1Y0DD46
C	1365	SER	-	expression tag	UNP A0A1Y0DD46
C	1366	ALA	-	expression tag	UNP A0A1Y0DD46
C	1367	ASP	-	expression tag	UNP A0A1Y0DD46
C	1368	ILE	-	expression tag	UNP A0A1Y0DD46
C	1369	GLN	-	expression tag	UNP A0A1Y0DD46
C	1370	HIS	-	expression tag	UNP A0A1Y0DD46
C	1371	SER	-	expression tag	UNP A0A1Y0DD46
C	1372	GLY	-	expression tag	UNP A0A1Y0DD46
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C	1375	LEU	-	expression tag	UNP A0A1Y0DD46
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C	1377	SER	-	expression tag	UNP A0A1Y0DD46
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C	1386	ILE	-	expression tag	UNP A0A1Y0DD46
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C	1389	GLU	-	expression tag	UNP A0A1Y0DD46
C	1390	ASP	-	expression tag	UNP A0A1Y0DD46
C	1391	LEU	-	expression tag	UNP A0A1Y0DD46
C	1392	ASN	-	expression tag	UNP A0A1Y0DD46
C	1393	MET	-	expression tag	UNP A0A1Y0DD46
C	1394	HIS	-	expression tag	UNP A0A1Y0DD46
C	1395	THR	-	expression tag	UNP A0A1Y0DD46
C	1396	GLY	-	expression tag	UNP A0A1Y0DD46
C	1397	HIS	-	expression tag	UNP A0A1Y0DD46
C	1398	HIS	-	expression tag	UNP A0A1Y0DD46

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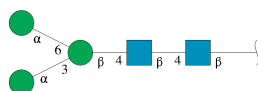
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C	1401	HIS	-	expression tag	UNP A0A1Y0DD46
C	1402	HIS	-	expression tag	UNP A0A1Y0DD46
B	1076	PRO	ILE	conflict	UNP A0A1Y0DD46
B	1077	PRO	LEU	conflict	UNP A0A1Y0DD46
B	1328	GLU	-	expression tag	UNP A0A1Y0DD46
B	1329	PHE	-	expression tag	UNP A0A1Y0DD46
B	1330	GLY	-	expression tag	UNP A0A1Y0DD46
B	1331	SER	-	expression tag	UNP A0A1Y0DD46
B	1332	GLY	-	expression tag	UNP A0A1Y0DD46
B	1333	GLY	-	expression tag	UNP A0A1Y0DD46
B	1334	TYR	-	expression tag	UNP A0A1Y0DD46
B	1335	ILE	-	expression tag	UNP A0A1Y0DD46
B	1336	PRO	-	expression tag	UNP A0A1Y0DD46
B	1337	GLU	-	expression tag	UNP A0A1Y0DD46
B	1338	ALA	-	expression tag	UNP A0A1Y0DD46
B	1339	PRO	-	expression tag	UNP A0A1Y0DD46
B	1340	ARG	-	expression tag	UNP A0A1Y0DD46
B	1341	ASP	-	expression tag	UNP A0A1Y0DD46
B	1342	GLY	-	expression tag	UNP A0A1Y0DD46
B	1343	GLN	-	expression tag	UNP A0A1Y0DD46
B	1344	ALA	-	expression tag	UNP A0A1Y0DD46
B	1345	TYR	-	expression tag	UNP A0A1Y0DD46
B	1346	VAL	-	expression tag	UNP A0A1Y0DD46
B	1347	ARG	-	expression tag	UNP A0A1Y0DD46
B	1348	LYS	-	expression tag	UNP A0A1Y0DD46
B	1349	ASP	-	expression tag	UNP A0A1Y0DD46
B	1350	GLY	-	expression tag	UNP A0A1Y0DD46
B	1351	GLU	-	expression tag	UNP A0A1Y0DD46
B	1352	TRP	-	expression tag	UNP A0A1Y0DD46
B	1353	VAL	-	expression tag	UNP A0A1Y0DD46
B	1354	LEU	-	expression tag	UNP A0A1Y0DD46
B	1355	LEU	-	expression tag	UNP A0A1Y0DD46
B	1356	SER	-	expression tag	UNP A0A1Y0DD46
B	1357	THR	-	expression tag	UNP A0A1Y0DD46
B	1358	PHE	-	expression tag	UNP A0A1Y0DD46
B	1359	LEU	-	expression tag	UNP A0A1Y0DD46
B	1360	LYS	-	expression tag	UNP A0A1Y0DD46
B	1361	GLY	-	expression tag	UNP A0A1Y0DD46
B	1362	GLN	-	expression tag	UNP A0A1Y0DD46
B	1363	ASP	-	expression tag	UNP A0A1Y0DD46

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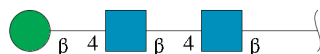
Chain	Residue	Modelled	Actual	Comment	Reference
B	1364	ASN	-	expression tag	UNP A0A1Y0DD46
B	1365	SER	-	expression tag	UNP A0A1Y0DD46
B	1366	ALA	-	expression tag	UNP A0A1Y0DD46
B	1367	ASP	-	expression tag	UNP A0A1Y0DD46
B	1368	ILE	-	expression tag	UNP A0A1Y0DD46
B	1369	GLN	-	expression tag	UNP A0A1Y0DD46
B	1370	HIS	-	expression tag	UNP A0A1Y0DD46
B	1371	SER	-	expression tag	UNP A0A1Y0DD46
B	1372	GLY	-	expression tag	UNP A0A1Y0DD46
B	1373	ARG	-	expression tag	UNP A0A1Y0DD46
B	1374	PRO	-	expression tag	UNP A0A1Y0DD46
B	1375	LEU	-	expression tag	UNP A0A1Y0DD46
B	1376	GLU	-	expression tag	UNP A0A1Y0DD46
B	1377	SER	-	expression tag	UNP A0A1Y0DD46
B	1378	ARG	-	expression tag	UNP A0A1Y0DD46
B	1379	GLY	-	expression tag	UNP A0A1Y0DD46
B	1380	PRO	-	expression tag	UNP A0A1Y0DD46
B	1381	PHE	-	expression tag	UNP A0A1Y0DD46
B	1382	GLU	-	expression tag	UNP A0A1Y0DD46
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B	1385	LEU	-	expression tag	UNP A0A1Y0DD46
B	1386	ILE	-	expression tag	UNP A0A1Y0DD46
B	1387	SER	-	expression tag	UNP A0A1Y0DD46
B	1388	GLU	-	expression tag	UNP A0A1Y0DD46
B	1389	GLU	-	expression tag	UNP A0A1Y0DD46
B	1390	ASP	-	expression tag	UNP A0A1Y0DD46
B	1391	LEU	-	expression tag	UNP A0A1Y0DD46
B	1392	ASN	-	expression tag	UNP A0A1Y0DD46
B	1393	MET	-	expression tag	UNP A0A1Y0DD46
B	1394	HIS	-	expression tag	UNP A0A1Y0DD46
B	1395	THR	-	expression tag	UNP A0A1Y0DD46
B	1396	GLY	-	expression tag	UNP A0A1Y0DD46
B	1397	HIS	-	expression tag	UNP A0A1Y0DD46
B	1398	HIS	-	expression tag	UNP A0A1Y0DD46
B	1399	HIS	-	expression tag	UNP A0A1Y0DD46
B	1400	HIS	-	expression tag	UNP A0A1Y0DD46
B	1401	HIS	-	expression tag	UNP A0A1Y0DD46
B	1402	HIS	-	expression tag	UNP A0A1Y0DD46

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	5	Total	C	N	O	0	0
			61	34	2	25		
2	O	5	Total	C	N	O	0	0
			61	34	2	25		
2	b	5	Total	C	N	O	0	0
			61	34	2	25		

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



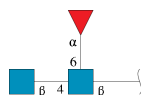
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		
3	T	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	d	3	Total	C	N	O	0	0
			39	22	2	15		
3	g	3	Total	C	N	O	0	0
			39	22	2	15		
3	h	3	Total	C	N	O	0	0
			39	22	2	15		
3	j	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		

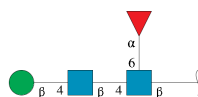
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	3	Total	C	N	O	0	0
			38	22	2	14		
5	Z	3	Total	C	N	O	0	0
			38	22	2	14		

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

ranose.



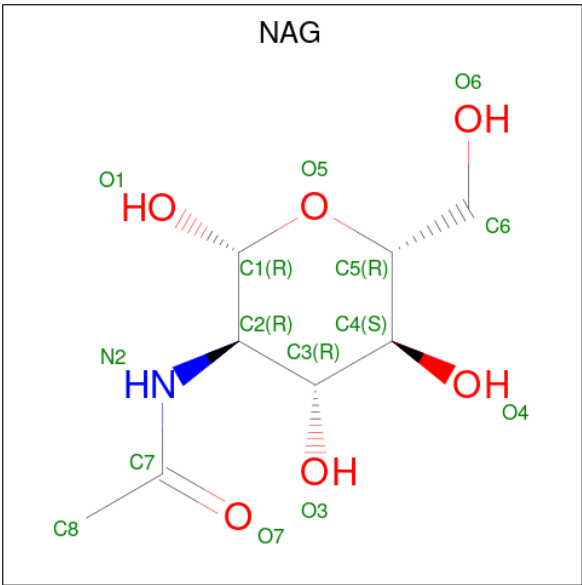
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	4	Total	C	N	O	0	0
			49	28	2	19		
6	a	4	Total	C	N	O	0	0
			49	28	2	19		
6	k	4	Total	C	N	O	0	0
			49	28	2	19		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	2	Total	C	N	O	0	0
			24	14	1	9		
7	S	2	Total	C	N	O	0	0
			24	14	1	9		
7	c	2	Total	C	N	O	0	0
			24	14	1	9		
7	f	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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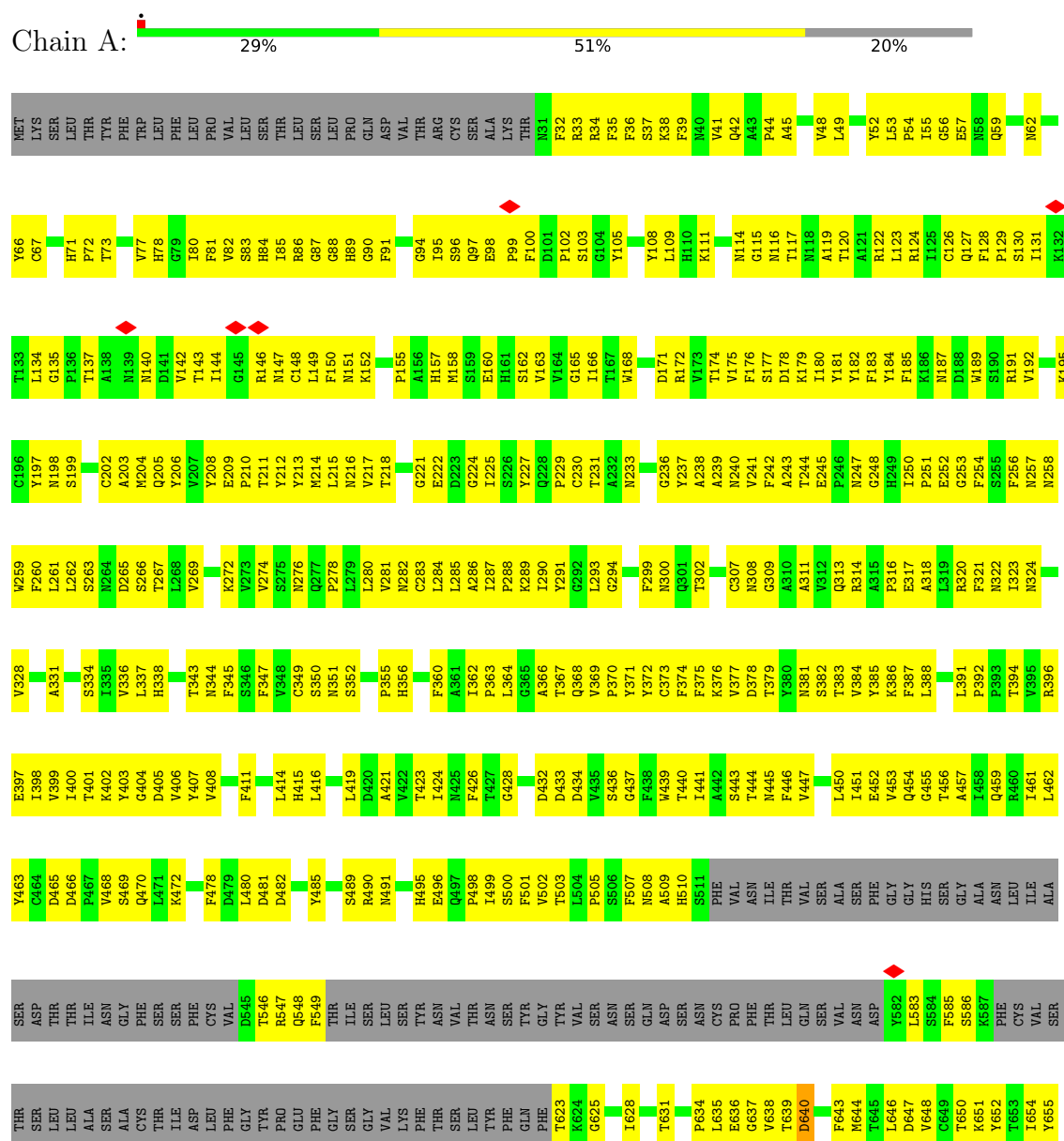
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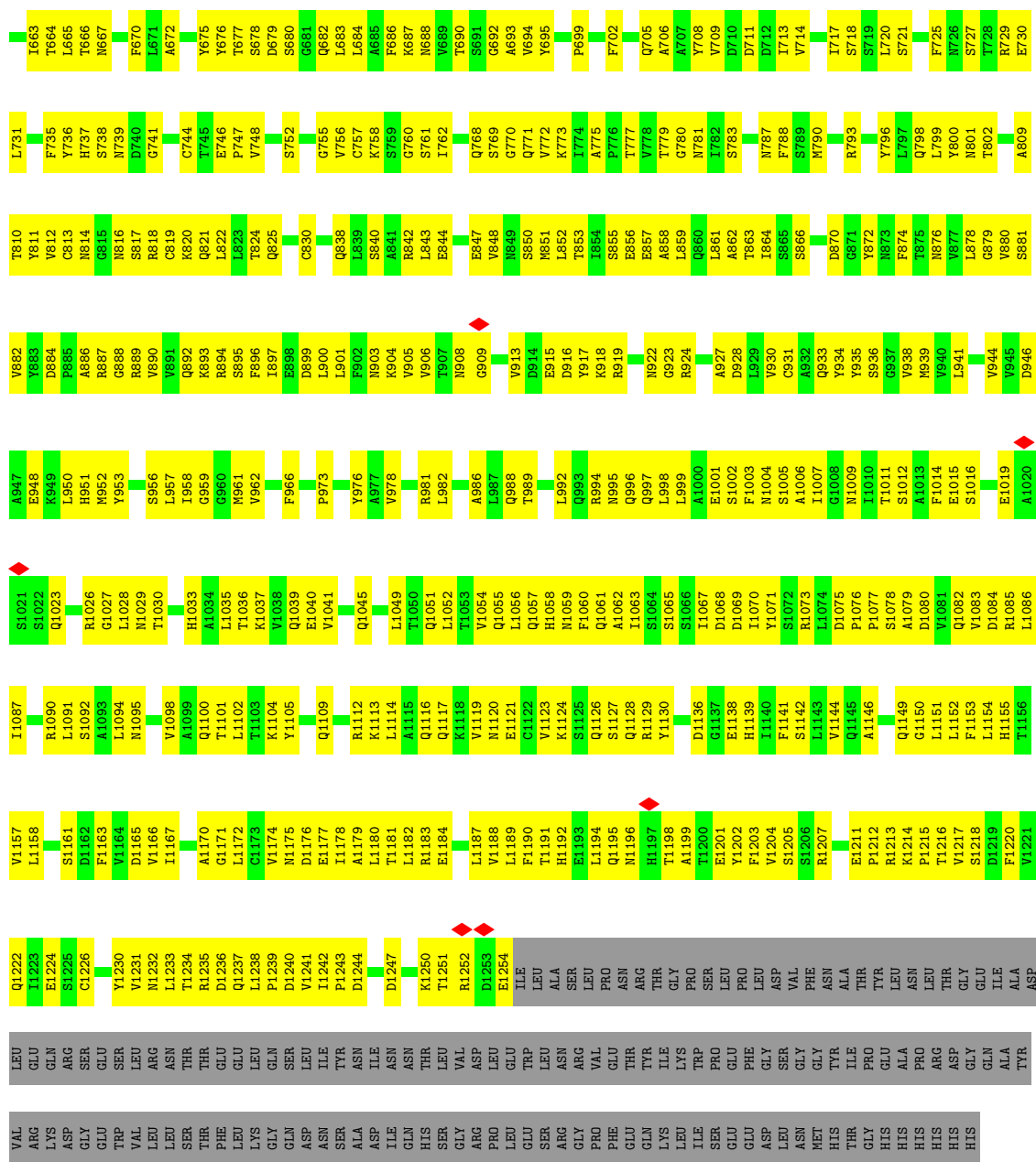
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	

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.

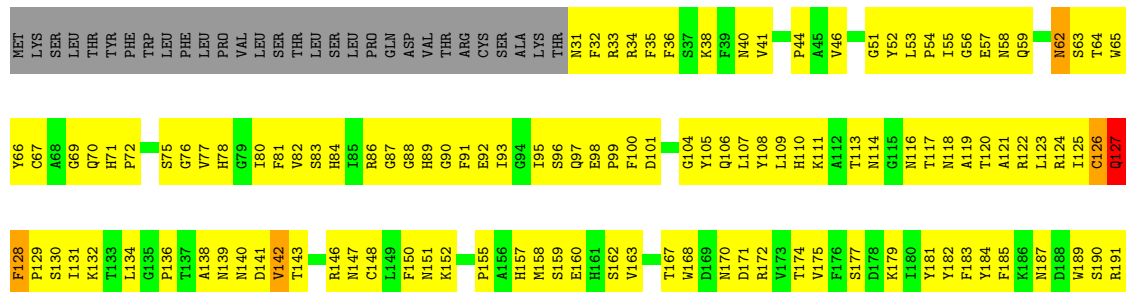
• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein

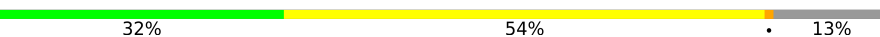
Chain C: 30% 48% 22%



C1173	V1105	A1032	L957	G888	C819	E746	S668	THR	SER	V476	F411	V336	L261	V192
V1174	T1106	H1033	I958	Q892	K820	P747	S669	ILE	SER	A477	H415	L337	L262	A193
N1175	Q1109	A1034	G959	Q893	Q821	L748	F670	LEU	PHE	D479	L416	H338	D265	K194
D1176	L1035	L1035	G960	K893	L822	V749	L671	ASP	CYS	L480	G417	T339	S266	K195
E1177	T1036	T1036	G961	R894	L823	Y750	A672	PHE	VAL	D481	L418	A340	C196	C196
I1178	K1037	K1037	N961	S895	T824	V751	G673	GLY	ASP	D482	L419	L341	Y197	Y197
A1179	V1038	V1038	F966	F896	Q825	S752	V674	THR	THR	G483	D420	G342	N198	N198
L1180	Q1039	Q1039	F966	I897	Q826	N753	Y675	PRO	ARG	G483	D420	G342	S199	S199
T1181	L972	E1040	L972	E998	T827	I754	Y676	GLU	THR	G483	D420	G342	C202	C202
L1182	Q1116	Q1116	P973	D899	T827	G755	T677	PHE	PHE	G483	D420	G342	A203	A203
R1183	Q1117	V1042	F973	L900	A828	G756	S678	GLY	THR	G483	D420	G342	M204	M204
E1184	Q1118	V1042	Y976	L901	K831	C757	D679	SER	ILE	S489	I424	N425	Q205	Q205
P1185	V1119	Q1051	Y976	F902	T832	K758	S680	GLY	SER	R490	N425	N274	M205	M205
G1186	N1120	L1052	R981	N903	I833	C758	S680	VAL	LEU	R490	N425	N274	Q206	Q206
L1187	E1121	T1053	R981	K904	I833	C758	S680	LYS	SER	R490	N425	N274	V207	V207
V1188	C1122	V1054	Y984	V905	E834	I762	L684	PHE	THR	L493	I424	N425	Y208	Y208
L1189	V1123	Q1055	L985	N906	S835	I762	A685	THR	ASN	L493	I424	N425	E209	E209
F1190	K1124	L1056	A986	T907	Q838	Q768	F686	SER	VAL	L493	I424	N425	P210	P210
T1191	S1126	Q1057	A986	N908	Q839	S769	K687	LEU	THR	L493	I424	N425	T211	T211
H1192	Q1126	H1058	Q988	C909	S840	G770	N688	THR	ASN	L493	I424	N425	Y212	Y212
E1193	Y1130	F1060	T989	L910	L843	T777	V689	PHE	SER	L493	I424	N425	Y213	Y213
L1194	G1131	Q1061	D990	V913	E844	T777	T690	GLN	GLY	L493	I424	N425	M214	M214
Q1195	Q1195	A1062	Y991	V913	E844	T777	T690	THR	TYR	L493	I424	N425	L215	L215
N1196	N1196	A1062	Y991	V913	E844	T777	T690	THR	TYR	L493	I424	N425	N216	N216
H1197	D1136	S1066	N985	D916	S845	G780	A693	LYS	VAL	L493	I424	N425	V217	V217
T1198	G1137	I1067	R986	Y917	E847	G780	A693	GLY	SER	L493	I424	N425	T218	T218
E1201	H1138	D1068	Q997	K918	E847	G780	A693	GLU	ASN	L493	I424	N425	G221	G221
Y1202	H1139	D1068	Q997	K918	E847	G780	A693	GLU	SER	L493	I424	N425	Y291	Y291
F1203	T1140	D1069	L999	R919	E847	G780	A693	GLU	SER	L493	I424	N425	G292	G292
V1204	F1141	I1070	L999	R919	E847	G780	A693	GLU	SER	L493	I424	N425	L293	L293
S1205	S1142	I1070	L999	R919	E847	G780	A693	GLU	SER	L493	I424	N425	G294	G294
L1206	L1143	R1073	F1003	A927	Q860	T790	A706	THR	THR	L493	I424	N425	Q295	Q295
R1207	V1144	D1075	M1004	A927	Q860	T790	A706	THR	THR	L493	I424	N425	Q296	Q296
L1208	Q1145	P1077	S1005	A927	Q860	T790	A706	THR	THR	L493	I424	N425	F297	F297
M1209	A1147	P1077	S1005	A927	Q860	T790	A706	THR	THR	L493	I424	N425	S298	S298
F1210	P1148	S1078	I1007	L928	L861	I792	Y708	LEU	THR	L493	I424	N425	N300	N300
E1211	Q1149	A1079	L1007	V930	A862	R793	Y709	GLN	VAL	L493	I424	N425	Q301	Q301
P1212	G1150	D1080	M1009	C931	A862	R793	Y709	GLN	VAL	L493	I424	N425	T302	T302
L1213	L1151	D1084	I1010	Q932	A862	R793	Y709	GLN	VAL	L493	I424	N425	N308	N308
K1214	F1152	D1084	I1011	Q932	A862	R793	Y709	GLN	VAL	L493	I424	N425	G309	G309
L1215	L1153	R1085	S1012	Y934	S865	L797	D711	VAL	ALA	L493	I424	N425	A310	A310
T1216	H1154	L1086	S1012	Y934	S865	L797	D711	VAL	ALA	L493	I424	N425	G310	G310
V1217	H1155	L1086	S1012	Y934	S865	L797	D711	VAL	ALA	L493	I424	N425	A238	A238
S1218	T1156	I1087	F1014	M939	D870	L799	S642	TYR	GLY	L493	I424	N425	A239	A239
D1219	V1157	T1088	E1015	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	N240	N240
L1220	L1158	G1089	S1016	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	V241	V241
F1220	V1159	R1090	V1017	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	F242	F242
Q1222	P1160	L1091	E1018	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	A243	A243
S1225	F1163	A1093	E1019	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	T244	T244
V1231	D1165	N1095	A1020	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	N247	N247
N1232	L1166	L1094	Q1023	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	G248	G248
L1233	T1167	N1095	T1024	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	H249	H249
L1234	L1168	A1098	S1025	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	E252	E252
R1235	T1169	Q1100	R1026	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	D325	D325
L1236	Q1170	L1028	G1027	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	T326	T326
Q1237	G1171	T1101	L1029	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	S327	S327
L1238	L1172	K1104	T1030	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	V328	V328
			Y1031	Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	N409	N409
				Y940	G871	Y800	S642	TYR	GLY	L493	I424	N425	G410	G410

P1239	D1240	V1241	I1242	P1243	D1244	Y1245	K1250	E1254	I1255	LEU	ALA	LEU	ARG	LEU	PRO	ASN	ARG	THR	GLY	PRO	LEU	PRO	LEU	LEU	ASP	ASP	VAL	PHE	ASN	GLY	GLY	TYR	ALA	THR	ILE	PRO	GLY	GLU	ALA	ASP	GLN	ARG	LEU	ASN	THR	THR	GLU	LEU	GLN	ASP
ILE	TYR	ASN	ASP	ILE	ASN	GLN	THR	LEU	VAL	ASP	PRO	LEU	TRP	LEU	ARG	GLY	GLY	THR	ILE	TRP	PRO	LEU	PRO	GLY	GLY	ASP	GLY	VAL	GLY	GLY	ASN	TYR	ALA	THR	ILE	PRO	GLY	GLU	ALA	ASP	GLN	ARG	LEU	ASN	THR	THR	GLU	LEU	GLN	ASP
ASN	SER	ALA	ASP	ILE	ASN	GLN	HIS	SER	GLY	ARG	PRO	LEU	TRP	LEU	ARG	GLY	GLY	THR	ILE	TRP	PRO	LEU	PRO	GLY	GLY	ASP	GLY	VAL	GLY	ASN	TYR	ALA	THR	ILE	PRO	GLY	GLU	ALA	ASP	GLN	ARG	LEU	ASN	THR	THR	GLU	LEU	GLN	ASP	

• Molecule 1: Spike glycoprotein

Chain B:  32% 54% 13%

MET	LYS	SER	LEU	THR	PHE	TRP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
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- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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

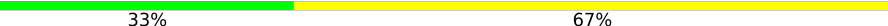


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  33% 67%

MAG1
MAG2
BMA3

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

Chain X:  33% 67%

MAG1
MAG2
BMA3

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

Chain d:  67% 33%

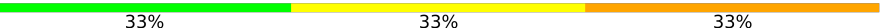
MAG1
MAG2
BMA3

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

Chain g:  33% 67%

MAG1
MAG2
BMA3

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

Chain h:  33% 33% 33%

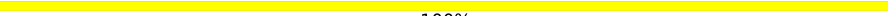
MAG1
MAG2
BMA3

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

Chain j:  33% 67%

MAG1
MAG2
BMA3

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

Chain H:  100%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

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

Chain L:  50% 50%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain W:  100%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain e:  50% 50%

MAG1
MAG2

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

Chain i:  50% 50%

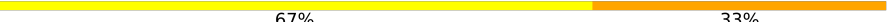
MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 67%

MAG1
MAG2
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  67% 33%

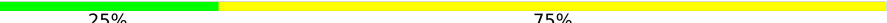
MAG1
MAG2
FUC3

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

Chain N:  50% 50%

MAG1
MAG2
BMA3
FUC4

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

Chain a:  25% 75%



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



- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.810	Depositor
Minimum map value	-0.175	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	385.83997, 385.83997, 385.83997	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/8838	0.52	0/12039
1	B	0.38	0/9610	0.51	0/13097
1	C	0.39	0/8626	0.53	1/11756 (0.0%)
All	All	0.38	0/27074	0.52	1/36892 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	GLN	N-CA-C	-5.42	99.26	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8648	0	8399	769	0
1	B	9398	0	9085	802	0
1	C	8440	0	8178	730	0
2	D	61	0	52	4	0
2	O	61	0	52	1	0
2	b	61	0	52	2	0
3	E	39	0	34	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	39	0	34	3	0
3	G	39	0	34	3	0
3	K	39	0	34	2	0
3	Q	39	0	34	1	0
3	T	39	0	34	3	0
3	V	39	0	34	6	0
3	X	39	0	34	1	0
3	d	39	0	34	2	0
3	g	39	0	34	3	0
3	h	39	0	34	3	0
3	j	39	0	34	2	0
4	H	28	0	25	0	0
4	I	28	0	25	2	0
4	J	28	0	25	4	0
4	L	28	0	25	2	0
4	R	28	0	25	1	0
4	U	28	0	25	4	0
4	W	28	0	25	0	0
4	Y	28	0	25	3	0
4	e	28	0	25	1	0
4	i	28	0	25	1	0
5	M	38	0	34	4	0
5	Z	38	0	34	2	0
6	N	49	0	43	3	0
6	a	49	0	43	6	0
6	k	49	0	43	5	0
7	P	24	0	22	3	0
7	S	24	0	22	6	0
7	c	24	0	22	1	0
7	f	24	0	22	1	0
8	A	84	0	78	5	0
8	B	98	0	91	4	0
8	C	70	0	65	2	0
All	All	27988	0	26995	2243	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 41.

The worst 5 of 2243 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:482:ASP:HA	1:A:708:TYR:O	1.52	1.06
1:C:218:THR:HG21	6:N:1:NAG:H62	1.40	1.00
1:A:510:HIS:HB2	1:A:634:PRO:HB3	1.45	0.97
1:B:482:ASP:HA	1:B:708:TYR:O	1.66	0.96
1:C:96:SER:O	1:C:191:ARG:HB3	1.63	0.96

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	1116/1402 (80%)	1005 (90%)	109 (10%)	2 (0%)	43	77
1	B	1222/1402 (87%)	1112 (91%)	103 (8%)	7 (1%)	21	58
1	C	1094/1402 (78%)	985 (90%)	103 (9%)	6 (0%)	24	62
All	All	3432/4206 (82%)	3102 (90%)	315 (9%)	15 (0%)	31	66

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	369	VAL
1	C	689	VAL
1	A	142	VAL
1	C	142	VAL
1	B	129	PRO

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	962/1209 (80%)	962 (100%)	0	100	100
1	B	1049/1209 (87%)	1040 (99%)	9 (1%)	70	75
1	C	938/1209 (78%)	935 (100%)	3 (0%)	86	84
All	All	2949/3627 (81%)	2937 (100%)	12 (0%)	81	82

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	133	THR
1	B	134	LEU
1	B	148	CYS
1	B	137	THR
1	B	128	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	258	ASN
1	B	979	GLN
1	B	445	ASN
1	B	566	ASN
1	B	993	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 ⓘ

97 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	0.44	0	17,19,21	1.38	2 (11%)
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.46	0
2	BMA	D	3	2	11,11,12	0.84	0	15,15,17	1.24	2 (13%)
2	MAN	D	4	2	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
2	MAN	D	5	2	11,11,12	0.57	0	15,15,17	0.99	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.39	0	17,19,21	0.73	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.59	0
3	BMA	E	3	3	11,11,12	0.57	0	15,15,17	0.80	0
3	NAG	F	1	3,1	14,14,15	0.53	0	17,19,21	1.43	2 (11%)
3	NAG	F	2	3	14,14,15	0.14	0	17,19,21	0.45	0
3	BMA	F	3	3	11,11,12	0.87	0	15,15,17	1.42	1 (6%)
3	NAG	G	1	3	14,14,15	0.82	1 (7%)	17,19,21	0.68	0
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	0.51	0
3	BMA	G	3	3	11,11,12	0.65	0	15,15,17	0.82	1 (6%)
4	NAG	H	1	1,4	14,14,15	1.43	2 (14%)	17,19,21	1.18	1 (5%)
4	NAG	H	2	4	14,14,15	0.61	0	17,19,21	0.90	1 (5%)
4	NAG	I	1	1,4	14,14,15	1.02	1 (7%)	17,19,21	1.65	3 (17%)
4	NAG	I	2	4	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	J	1	1,4	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	J	2	4	14,14,15	0.50	0	17,19,21	0.73	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.77	1 (7%)	17,19,21	0.60	0
3	NAG	K	2	3	14,14,15	0.40	0	17,19,21	1.43	2 (11%)
3	BMA	K	3	3	11,11,12	0.66	0	15,15,17	0.90	1 (6%)
4	NAG	L	1	1,4	14,14,15	0.27	0	17,19,21	0.55	0
4	NAG	L	2	4	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	M	1	5,1	14,14,15	1.36	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	M	2	5	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
5	FUC	M	3	5	10,10,11	0.94	0	14,14,16	1.23	2 (14%)
6	NAG	N	1	6,1	14,14,15	0.30	0	17,19,21	0.91	1 (5%)
6	NAG	N	2	6	14,14,15	0.23	0	17,19,21	0.47	0
6	BMA	N	3	6	11,11,12	0.51	0	15,15,17	0.75	0
6	FUC	N	4	6	10,10,11	0.45	0	14,14,16	0.82	1 (7%)
2	NAG	O	1	2,1	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	O	2	2	14,14,15	0.15	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	O	3	2	11,11,12	0.63	0	15,15,17	0.73	1 (6%)
2	MAN	O	4	2	11,11,12	0.71	1 (9%)	15,15,17	0.91	1 (6%)
2	MAN	O	5	2	11,11,12	0.62	0	15,15,17	0.96	1 (6%)
7	NAG	P	1	1,7	14,14,15	0.19	0	17,19,21	0.48	0
7	FUC	P	2	7	10,10,11	0.75	0	14,14,16	0.80	0
3	NAG	Q	1	3,1	14,14,15	0.50	0	17,19,21	0.40	0
3	NAG	Q	2	3	14,14,15	0.17	0	17,19,21	0.56	0
3	BMA	Q	3	3	11,11,12	0.61	0	15,15,17	0.80	0
4	NAG	R	1	1,4	14,14,15	0.36	0	17,19,21	0.52	0
4	NAG	R	2	4	14,14,15	0.26	0	17,19,21	0.42	0
7	NAG	S	1	1,7	14,14,15	0.65	1 (7%)	17,19,21	0.84	1 (5%)
7	FUC	S	2	7	10,10,11	0.56	0	14,14,16	0.76	0
3	NAG	T	1	3,1	14,14,15	1.44	1 (7%)	17,19,21	0.97	1 (5%)
3	NAG	T	2	3	14,14,15	0.28	0	17,19,21	0.50	0
3	BMA	T	3	3	11,11,12	0.50	0	15,15,17	0.85	0
4	NAG	U	1	1,4	14,14,15	0.28	0	17,19,21	1.40	1 (5%)
4	NAG	U	2	4	14,14,15	0.64	1 (7%)	17,19,21	0.97	1 (5%)
3	NAG	V	1	3,1	14,14,15	1.37	1 (7%)	17,19,21	1.50	2 (11%)
3	NAG	V	2	3	14,14,15	0.28	0	17,19,21	0.79	1 (5%)
3	BMA	V	3	3	11,11,12	0.69	0	15,15,17	0.68	0
4	NAG	W	1	1,4	14,14,15	0.58	0	17,19,21	0.75	0
4	NAG	W	2	4	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	X	1	3,1	14,14,15	0.39	0	17,19,21	0.81	0
3	NAG	X	2	3	14,14,15	0.33	0	17,19,21	0.40	0
3	BMA	X	3	3	11,11,12	0.83	0	15,15,17	0.93	1 (6%)
4	NAG	Y	1	1,4	14,14,15	0.72	1 (7%)	17,19,21	1.36	2 (11%)
4	NAG	Y	2	4	14,14,15	0.48	0	17,19,21	1.26	1 (5%)
5	NAG	Z	1	5,1	14,14,15	0.32	0	17,19,21	0.85	1 (5%)
5	NAG	Z	2	5	14,14,15	0.30	0	17,19,21	0.38	0
5	FUC	Z	3	5	10,10,11	0.49	0	14,14,16	0.87	0
6	NAG	a	1	6,1	14,14,15	0.63	0	17,19,21	0.67	0
6	NAG	a	2	6	14,14,15	0.23	0	17,19,21	0.49	0
6	BMA	a	3	6	11,11,12	0.50	0	15,15,17	0.68	0
6	FUC	a	4	6	10,10,11	0.51	0	14,14,16	0.70	0
2	NAG	b	1	2,1	14,14,15	0.18	0	17,19,21	0.38	0
2	NAG	b	2	2	14,14,15	0.21	0	17,19,21	0.48	0
2	BMA	b	3	2	11,11,12	0.64	0	15,15,17	0.92	0
2	MAN	b	4	2	11,11,12	0.82	1 (9%)	15,15,17	0.95	1 (6%)
2	MAN	b	5	2	11,11,12	0.58	0	15,15,17	1.02	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	c	1	1,7	14,14,15	0.30	0	17,19,21	0.34	0
7	FUC	c	2	7	10,10,11	0.64	0	14,14,16	0.90	0
3	NAG	d	1	3,1	14,14,15	0.42	0	17,19,21	0.41	0
3	NAG	d	2	3	14,14,15	0.18	0	17,19,21	0.50	0
3	BMA	d	3	3	11,11,12	0.56	0	15,15,17	0.91	0
4	NAG	e	1	1,4	14,14,15	0.40	0	17,19,21	0.58	0
4	NAG	e	2	4	14,14,15	0.20	0	17,19,21	0.45	0
7	NAG	f	1	1,7	14,14,15	0.16	0	17,19,21	0.52	0
7	FUC	f	2	7	10,10,11	0.76	0	14,14,16	0.69	0
3	NAG	g	1	3,1	14,14,15	0.30	0	17,19,21	0.54	0
3	NAG	g	2	3	14,14,15	0.19	0	17,19,21	0.38	0
3	BMA	g	3	3	11,11,12	0.50	0	15,15,17	0.80	0
3	NAG	h	1	3,1	14,14,15	0.77	1 (7%)	17,19,21	0.62	0
3	NAG	h	2	3	14,14,15	0.27	0	17,19,21	0.52	0
3	BMA	h	3	3	11,11,12	0.54	0	15,15,17	0.75	0
4	NAG	i	1	1,4	14,14,15	0.66	0	17,19,21	1.26	1 (5%)
4	NAG	i	2	4	14,14,15	0.22	0	17,19,21	0.38	0
3	NAG	j	1	3,1	14,14,15	0.56	0	17,19,21	1.29	1 (5%)
3	NAG	j	2	3	14,14,15	0.33	0	17,19,21	1.32	2 (11%)
3	BMA	j	3	3	11,11,12	1.31	2 (18%)	15,15,17	0.92	1 (6%)
6	NAG	k	1	6,1	14,14,15	0.68	1 (7%)	17,19,21	1.12	1 (5%)
6	NAG	k	2	6	14,14,15	0.30	0	17,19,21	0.50	0
6	BMA	k	3	6	11,11,12	0.58	0	15,15,17	0.64	0
6	FUC	k	4	6	10,10,11	0.59	0	14,14,16	0.84	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	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	6/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	6/6/23/26	0/1/1/1
5	FUC	M	3	5	-	-	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	FUC	N	4	6	-	-	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	BMA	O	3	2	-	2/2/19/22	0/1/1/1
2	MAN	O	4	2	-	0/2/19/22	0/1/1/1
2	MAN	O	5	2	-	2/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	P	2	7	-	-	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
7	NAG	S	1	1,7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUC	S	2	7	-	-	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	BMA	T	3	3	-	2/2/19/22	0/1/1/1
4	NAG	U	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	U	2	4	-	4/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
4	NAG	W	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	BMA	X	3	3	-	2/2/19/22	0/1/1/1
4	NAG	Y	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	5/6/23/26	0/1/1/1
5	NAG	Z	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	4/6/23/26	0/1/1/1
5	FUC	Z	3	5	-	-	0/1/1/1
6	NAG	a	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	BMA	a	3	6	-	0/2/19/22	0/1/1/1
6	FUC	a	4	6	-	-	0/1/1/1
2	NAG	b	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	BMA	b	3	2	-	0/2/19/22	0/1/1/1
2	MAN	b	4	2	-	0/2/19/22	0/1/1/1
2	MAN	b	5	2	-	0/2/19/22	0/1/1/1
7	NAG	c	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	c	2	7	-	-	0/1/1/1
3	NAG	d	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	BMA	d	3	3	-	0/2/19/22	0/1/1/1
4	NAG	e	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
7	NAG	f	1	1,7	-	2/6/23/26	0/1/1/1
7	FUC	f	2	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	g	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	BMA	g	3	3	-	0/2/19/22	0/1/1/1
3	NAG	h	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	h	2	3	-	4/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
4	NAG	i	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1
3	NAG	j	1	3,1	-	6/6/23/26	0/1/1/1
3	NAG	j	2	3	-	5/6/23/26	0/1/1/1
3	BMA	j	3	3	-	0/2/19/22	0/1/1/1
6	NAG	k	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	k	2	6	-	0/6/23/26	0/1/1/1
6	BMA	k	3	6	-	0/2/19/22	0/1/1/1
6	FUC	k	4	6	-	-	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	NAG	O5-C1	-5.06	1.35	1.43
3	V	1	NAG	O5-C1	-5.01	1.35	1.43
5	M	1	NAG	O5-C1	-4.90	1.35	1.43
4	H	1	NAG	O5-C1	-4.73	1.35	1.43
4	I	1	NAG	C1-C2	3.55	1.57	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C2-N2-C7	4.70	129.20	122.90
4	U	1	NAG	C2-N2-C7	4.67	129.16	122.90
4	i	1	NAG	C1-O5-C5	4.58	118.32	112.19
3	j	2	NAG	C2-N2-C7	4.52	128.96	122.90
3	V	1	NAG	C2-N2-C7	4.49	128.92	122.90

There are no chirality outliers.

5 of 204 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	c	1	NAG	C4-C5-C6-O6
2	O	5	MAN	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6

There are no ring outliers.

56 monomers are involved in 94 short contacts:

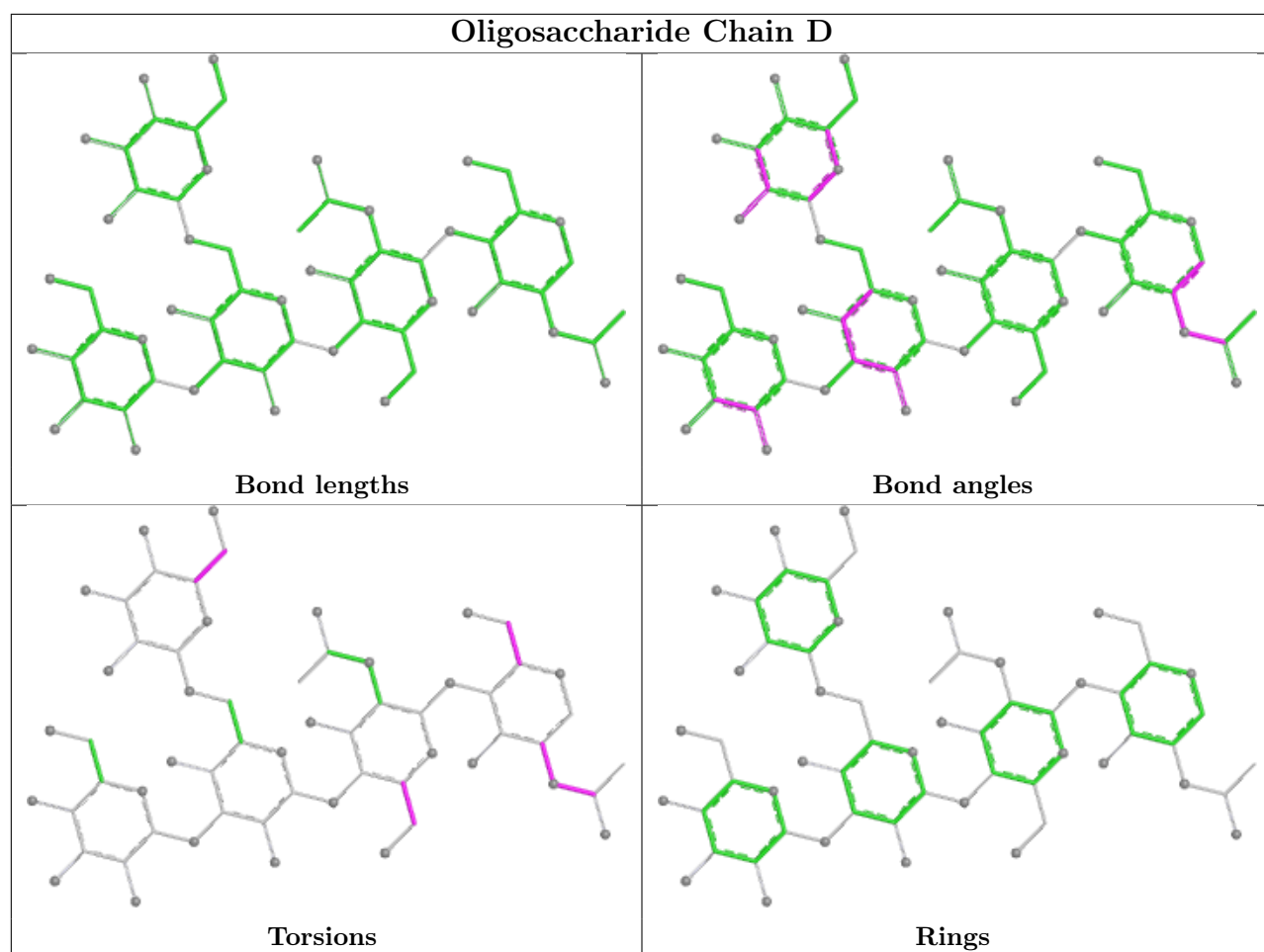
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0
6	N	1	NAG	2	0
3	j	2	NAG	1	0
3	E	2	NAG	3	0
7	P	1	NAG	1	0
3	T	1	NAG	2	0
5	Z	2	NAG	1	0
3	h	2	NAG	1	0
3	h	1	NAG	3	0
3	G	2	NAG	1	0
6	k	1	NAG	5	0
3	F	1	NAG	3	0
4	R	1	NAG	1	0
4	e	1	NAG	1	0
7	f	1	NAG	1	0
3	K	1	NAG	1	0
3	V	1	NAG	5	0
7	S	1	NAG	6	0
3	G	1	NAG	2	0
4	J	2	NAG	1	0
2	D	2	NAG	1	0
6	k	4	FUC	2	0
6	N	4	FUC	1	0
3	Q	3	BMA	1	0
7	P	2	FUC	3	0
4	Y	2	NAG	1	0
6	a	2	NAG	1	0
3	g	2	NAG	1	0
4	Y	1	NAG	2	0
5	Z	3	FUC	1	0
4	U	2	NAG	3	0
7	c	1	NAG	1	0
4	i	1	NAG	1	0
4	U	1	NAG	4	0

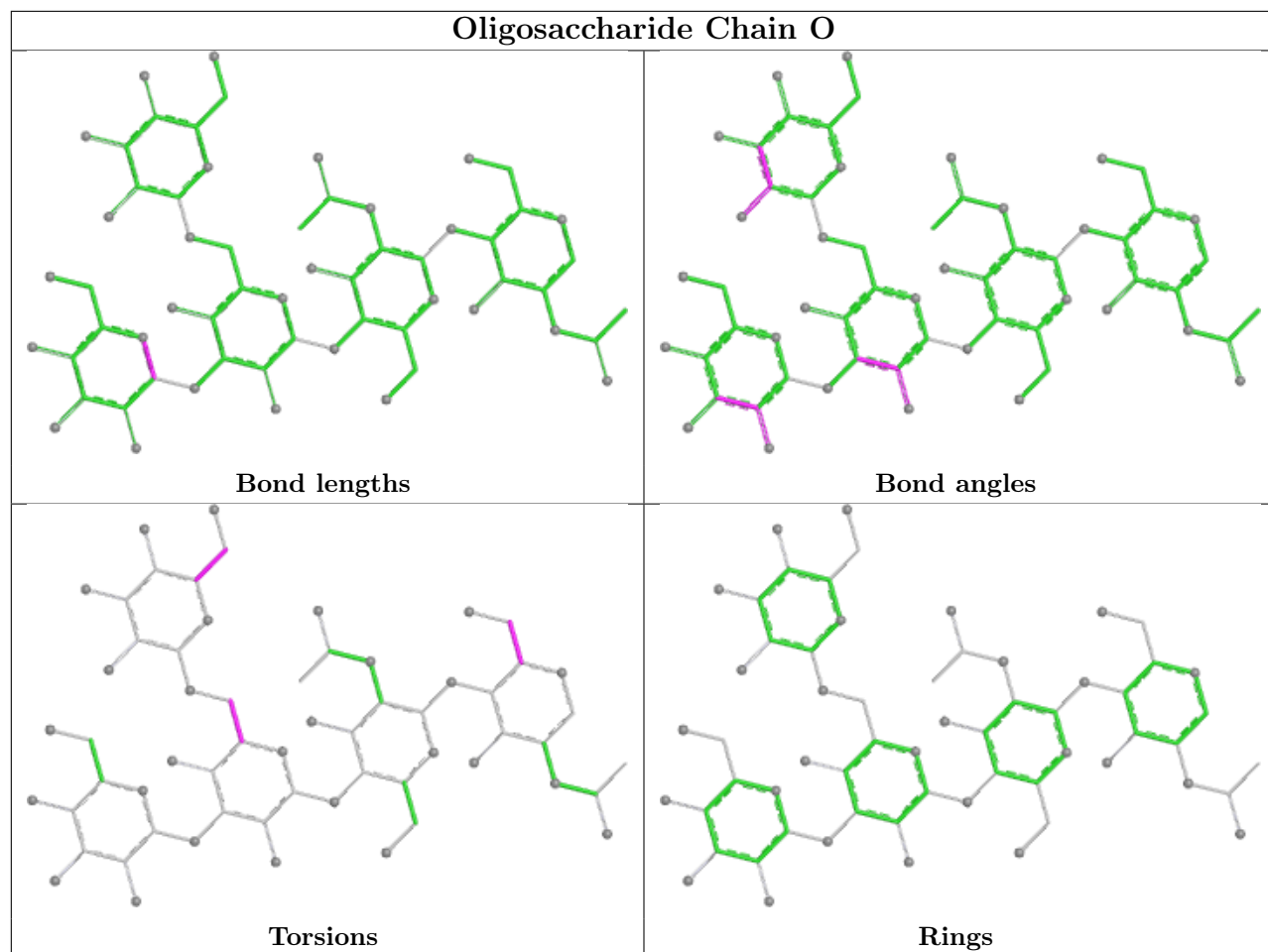
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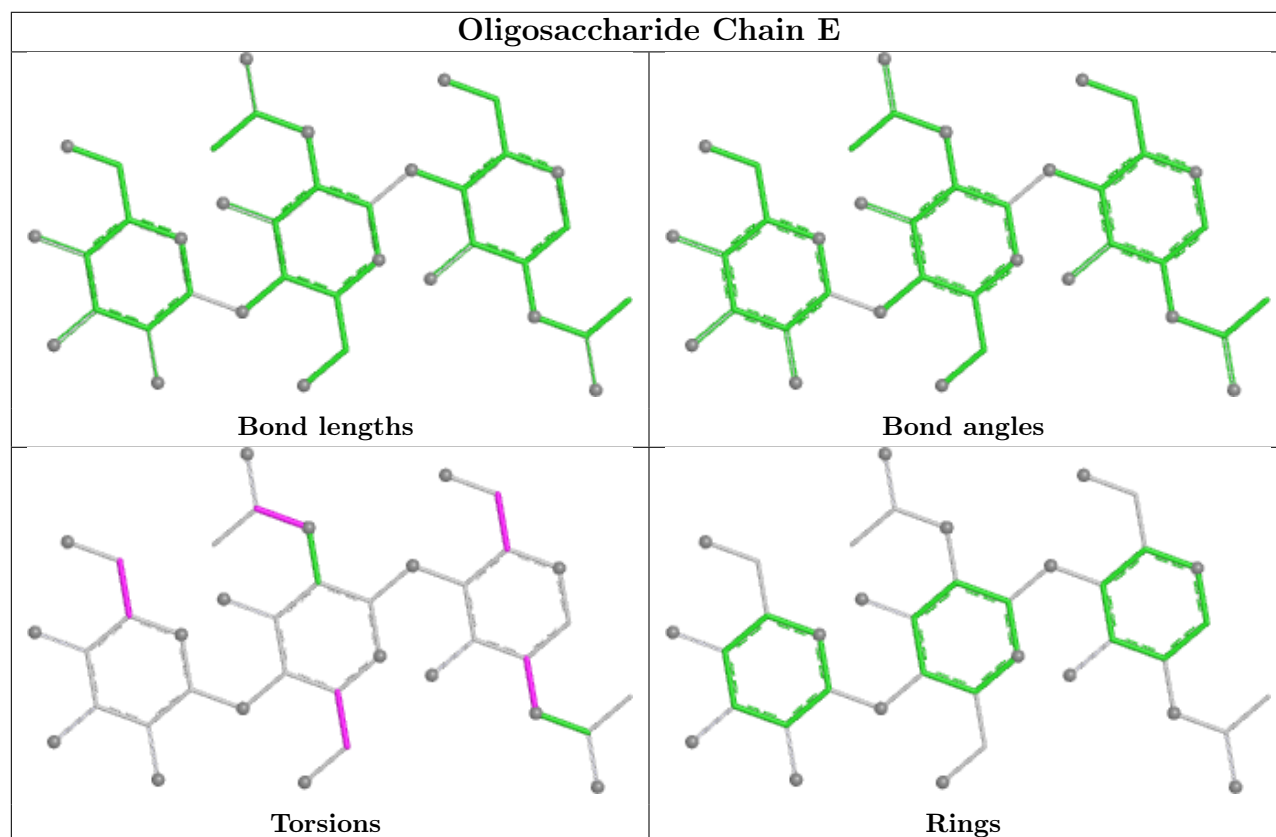
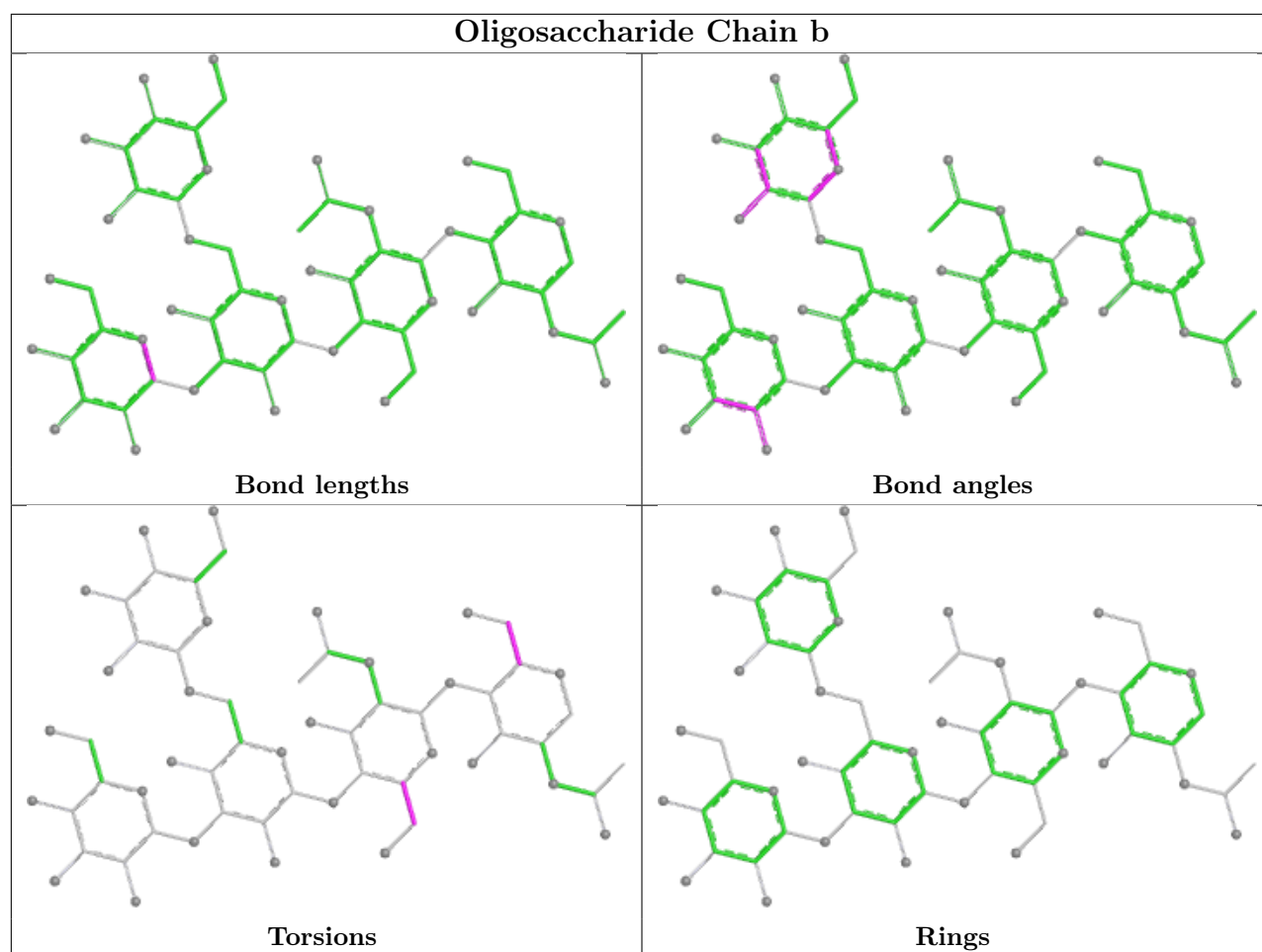
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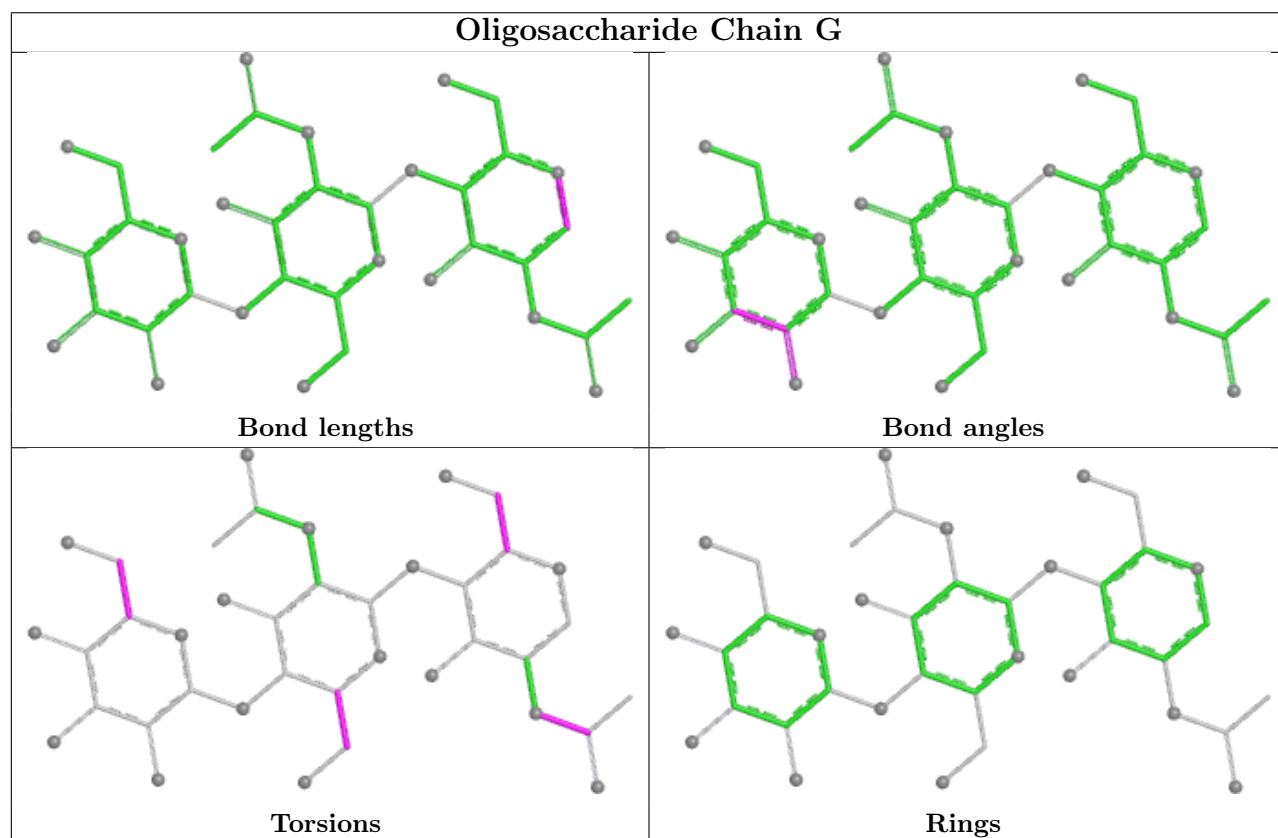
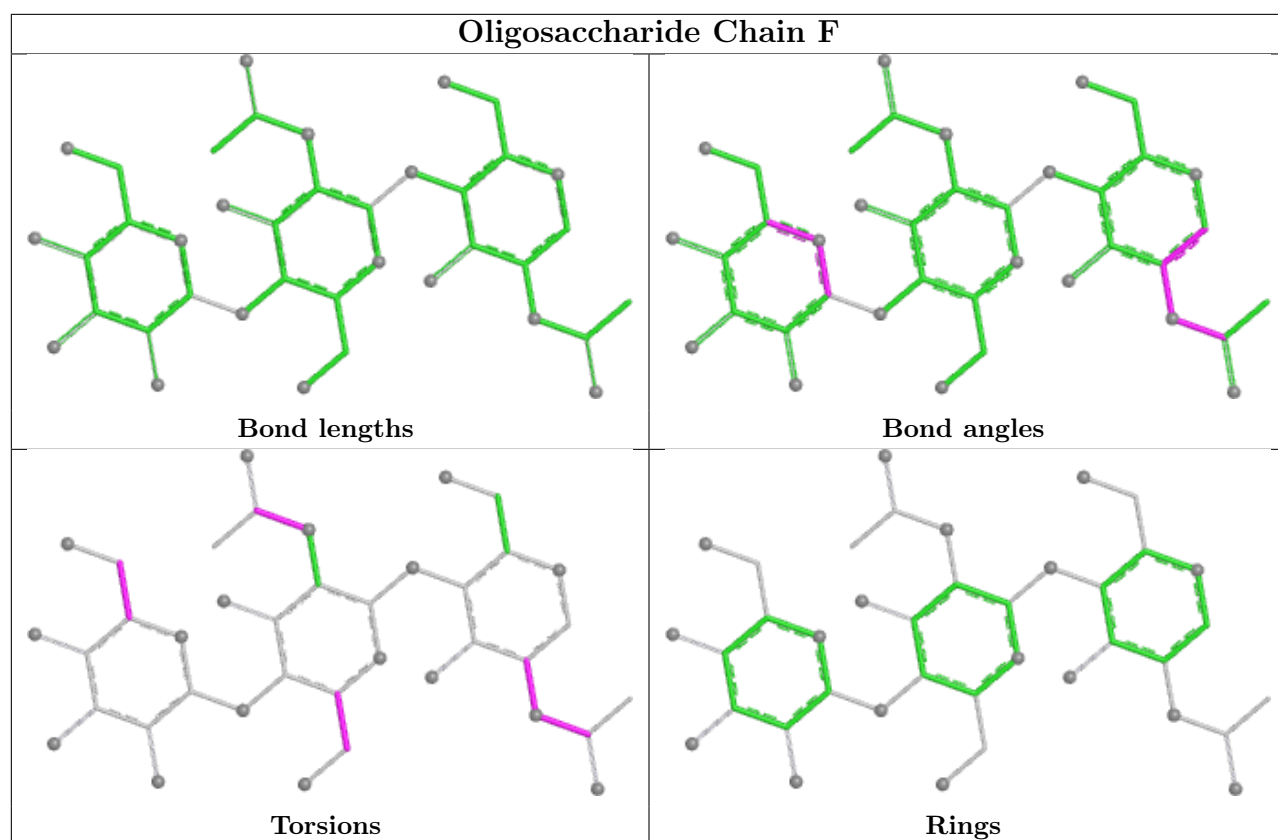
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	2	0
3	G	3	BMA	1	0
3	T	2	NAG	2	0
2	b	1	NAG	2	0
3	K	2	NAG	1	0
3	V	2	NAG	4	0
6	a	1	NAG	5	0
3	d	1	NAG	2	0
5	M	2	NAG	1	0
6	a	4	FUC	2	0
2	D	3	BMA	1	0
3	j	1	NAG	1	0
3	g	1	NAG	2	0
5	M	3	FUC	3	0
3	X	1	NAG	1	0
4	J	1	NAG	4	0
5	Z	1	NAG	2	0
2	D	5	MAN	1	0
2	O	1	NAG	1	0
4	L	1	NAG	2	0
3	E	1	NAG	6	0
3	V	3	BMA	1	0

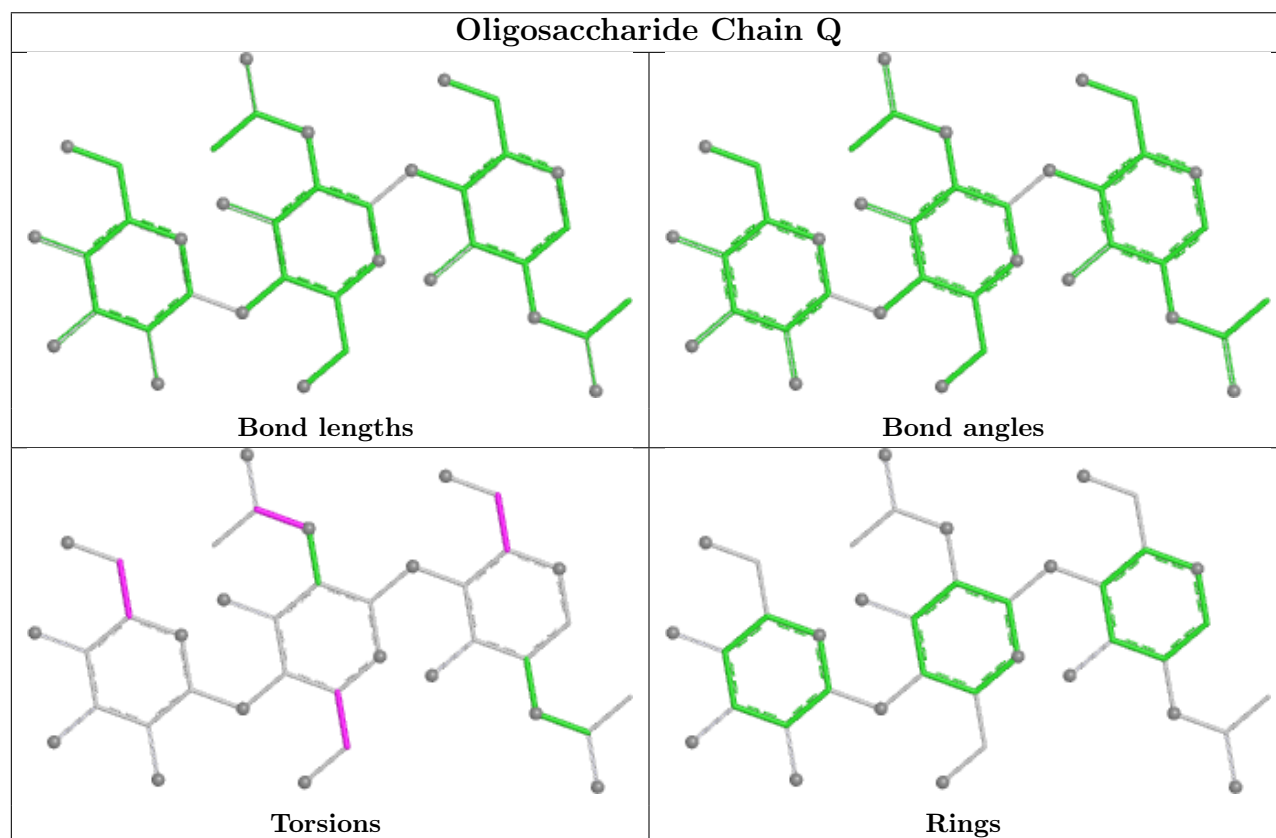
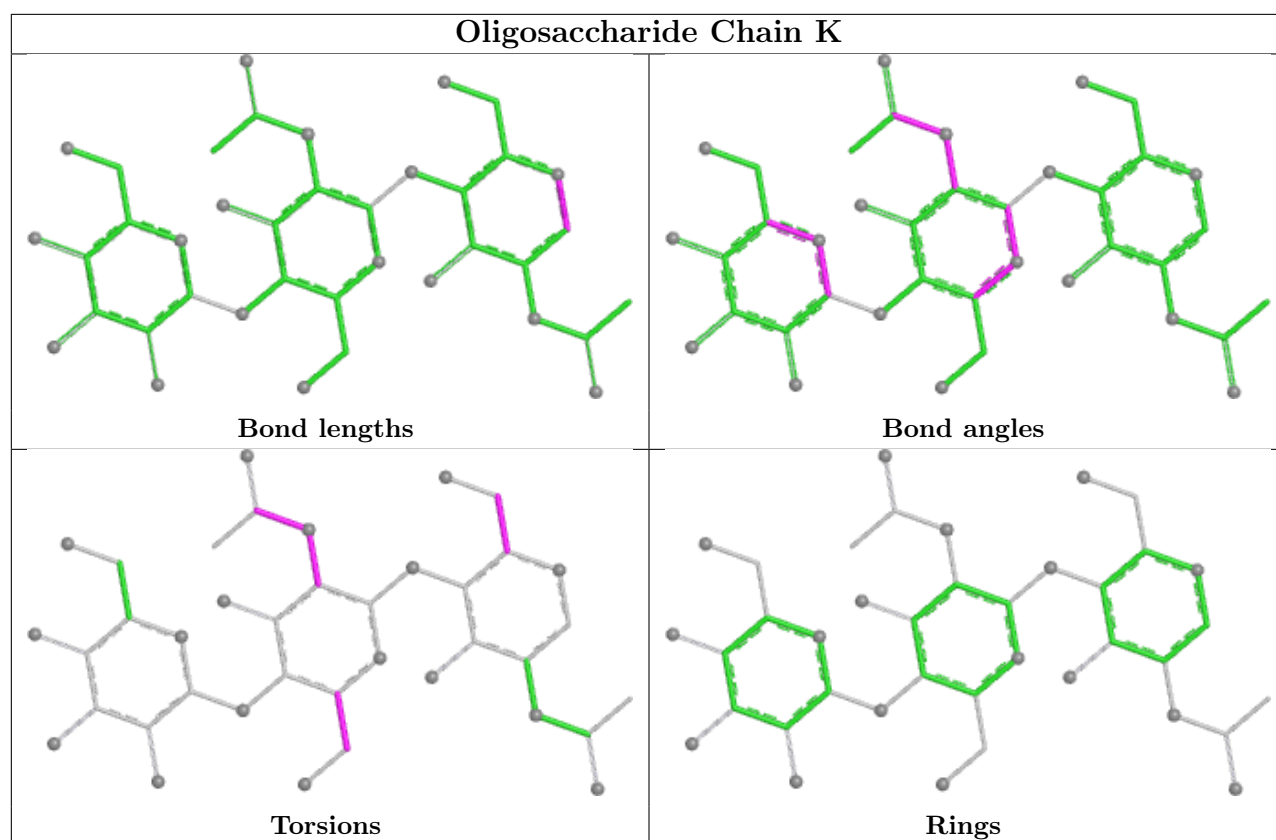
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

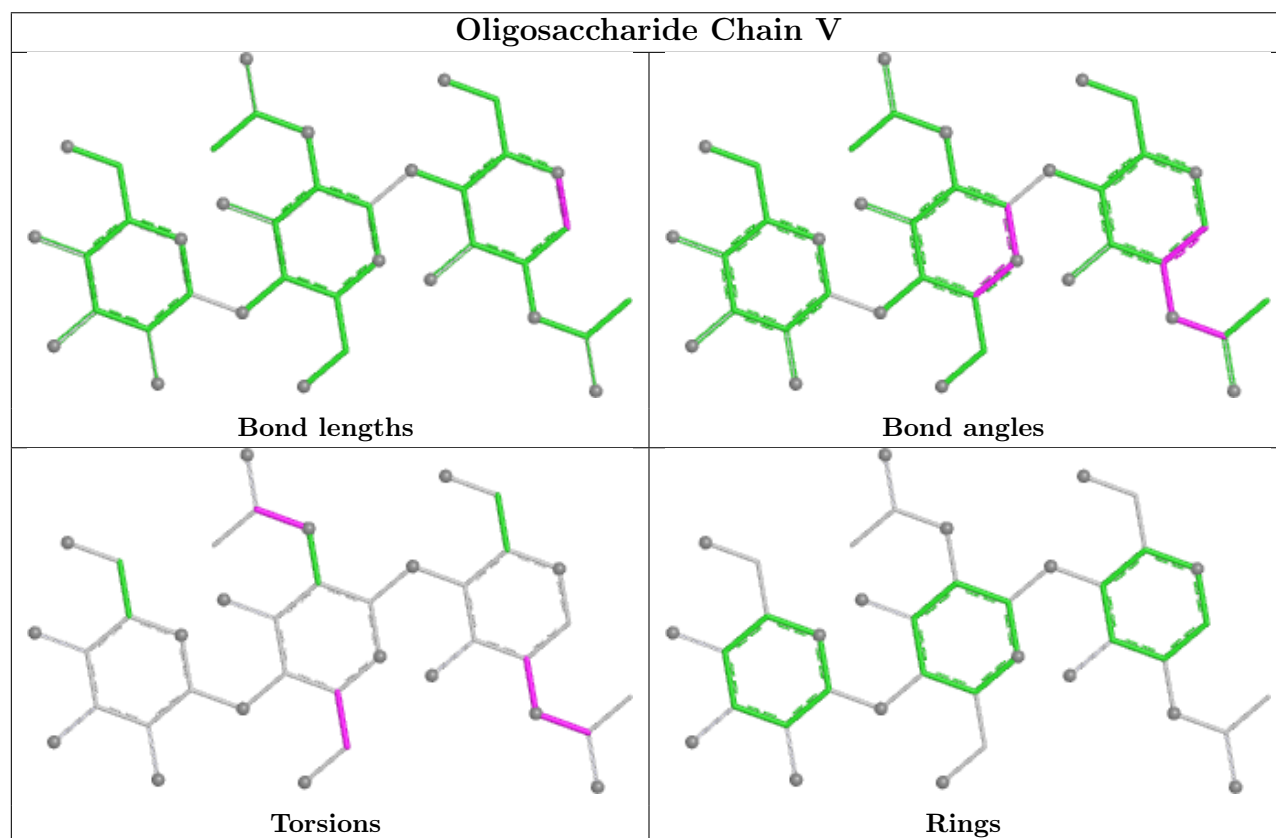
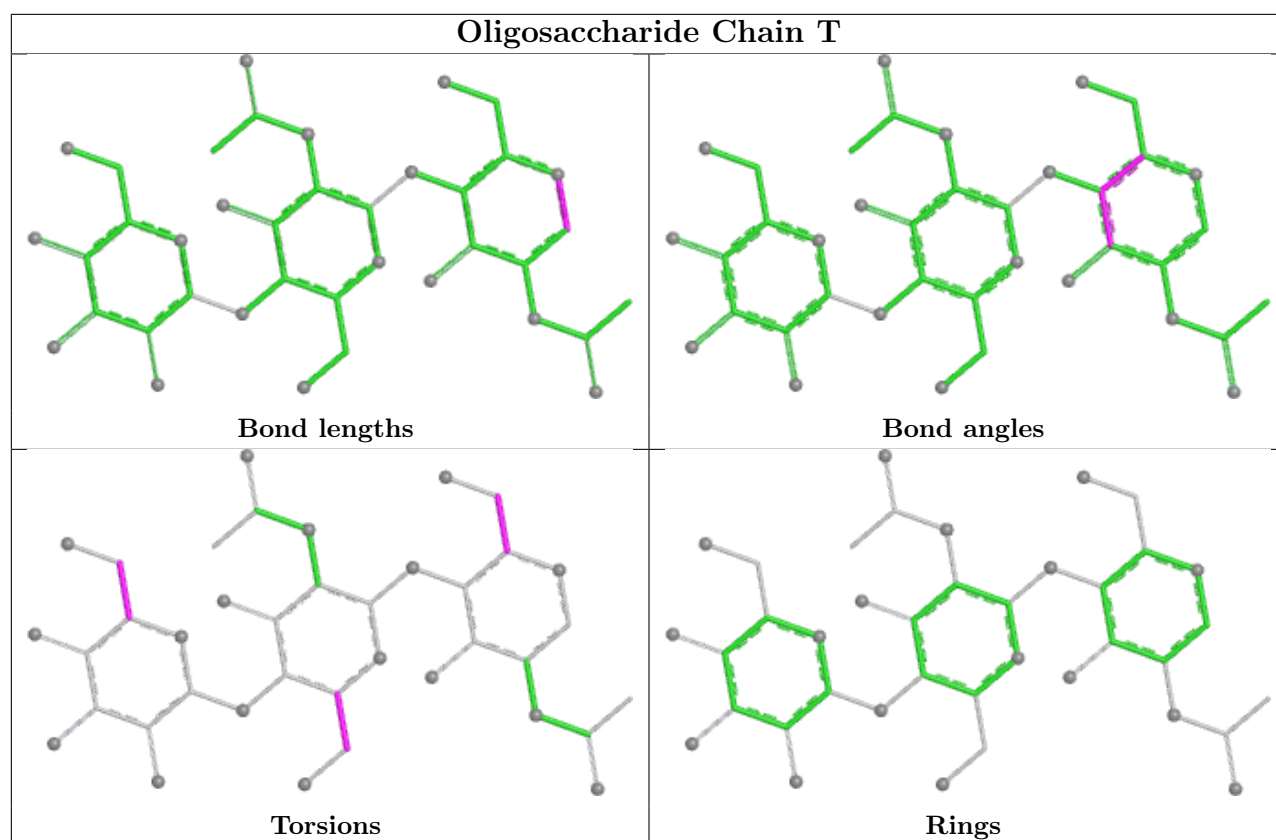


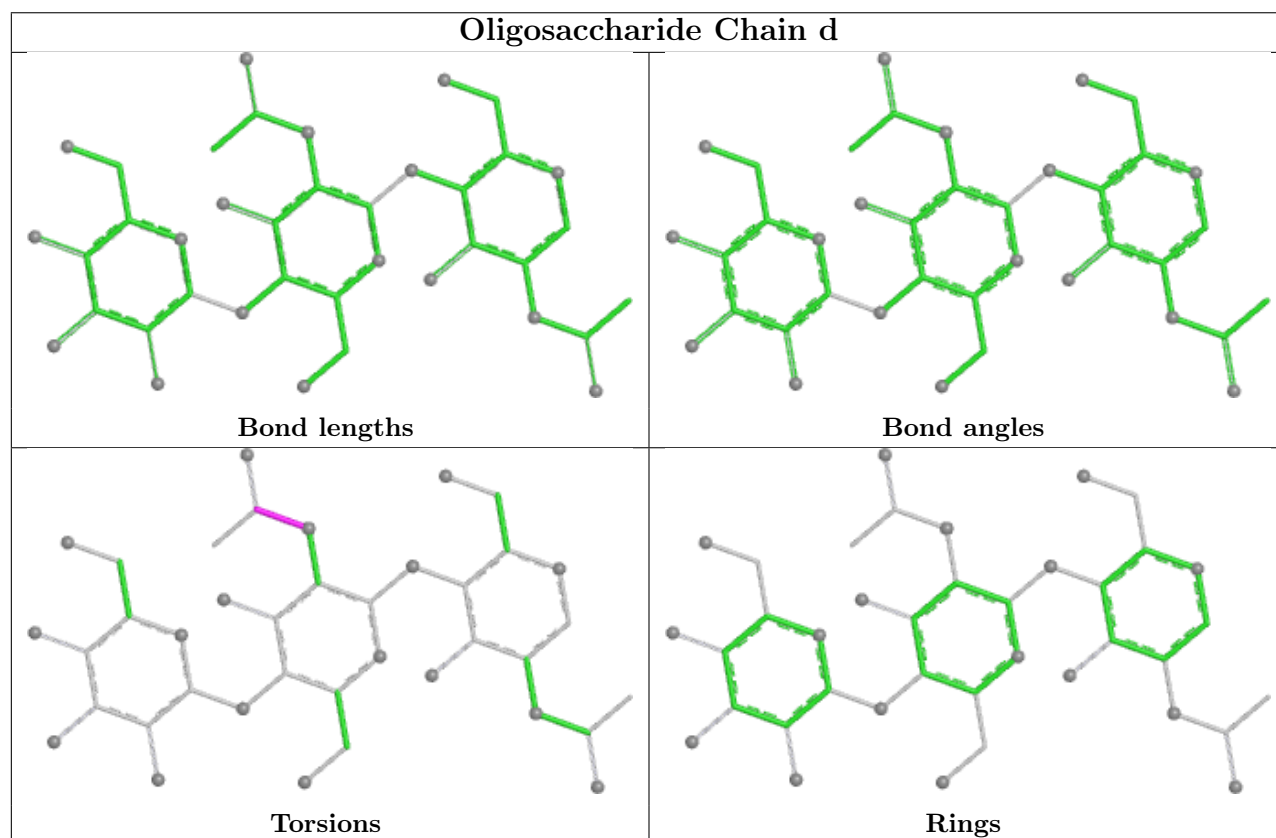
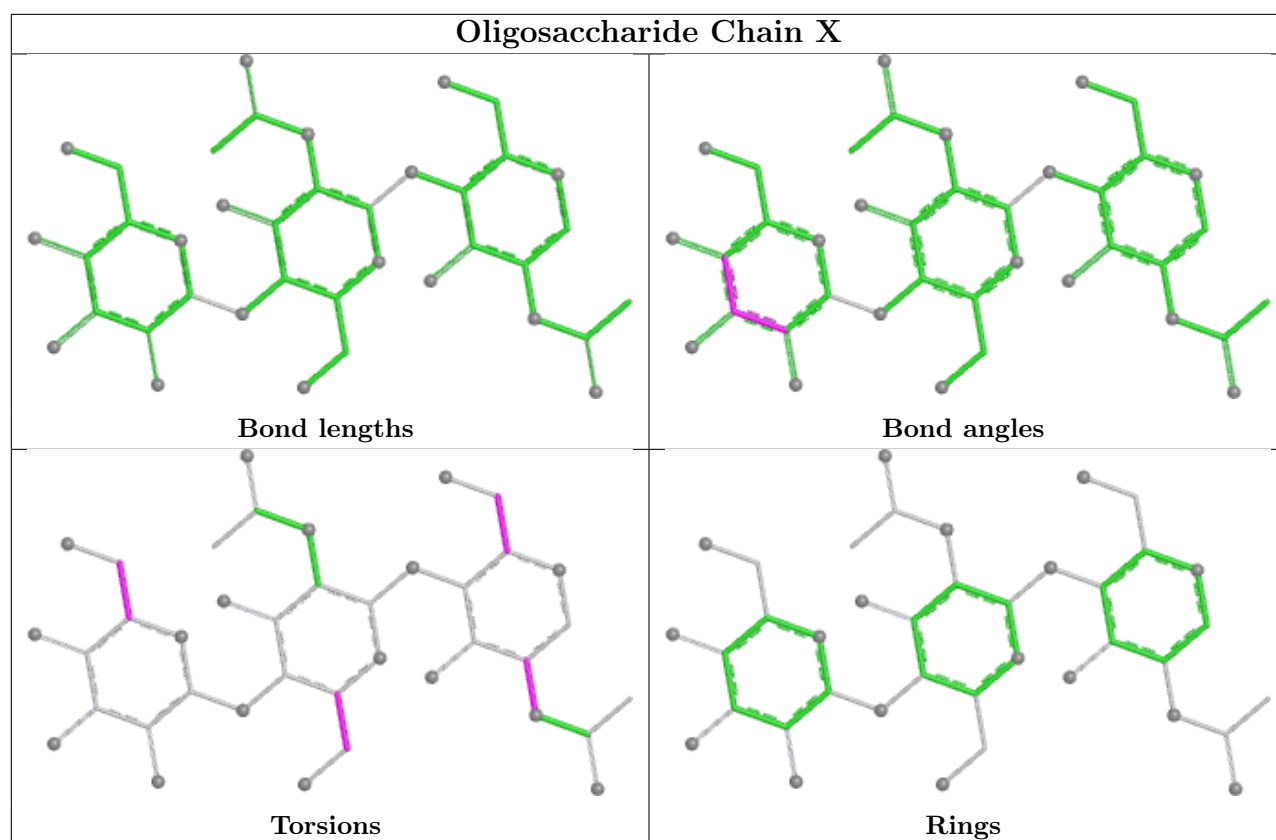


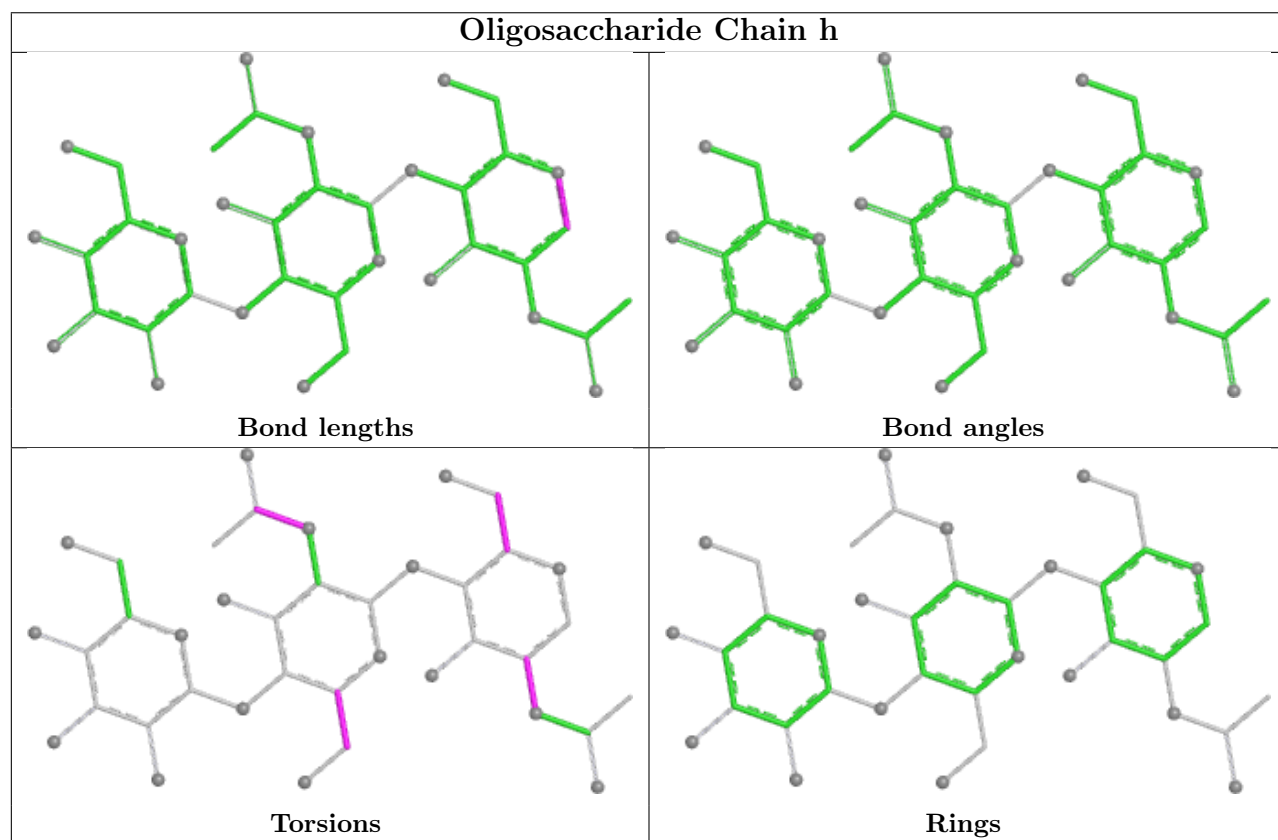
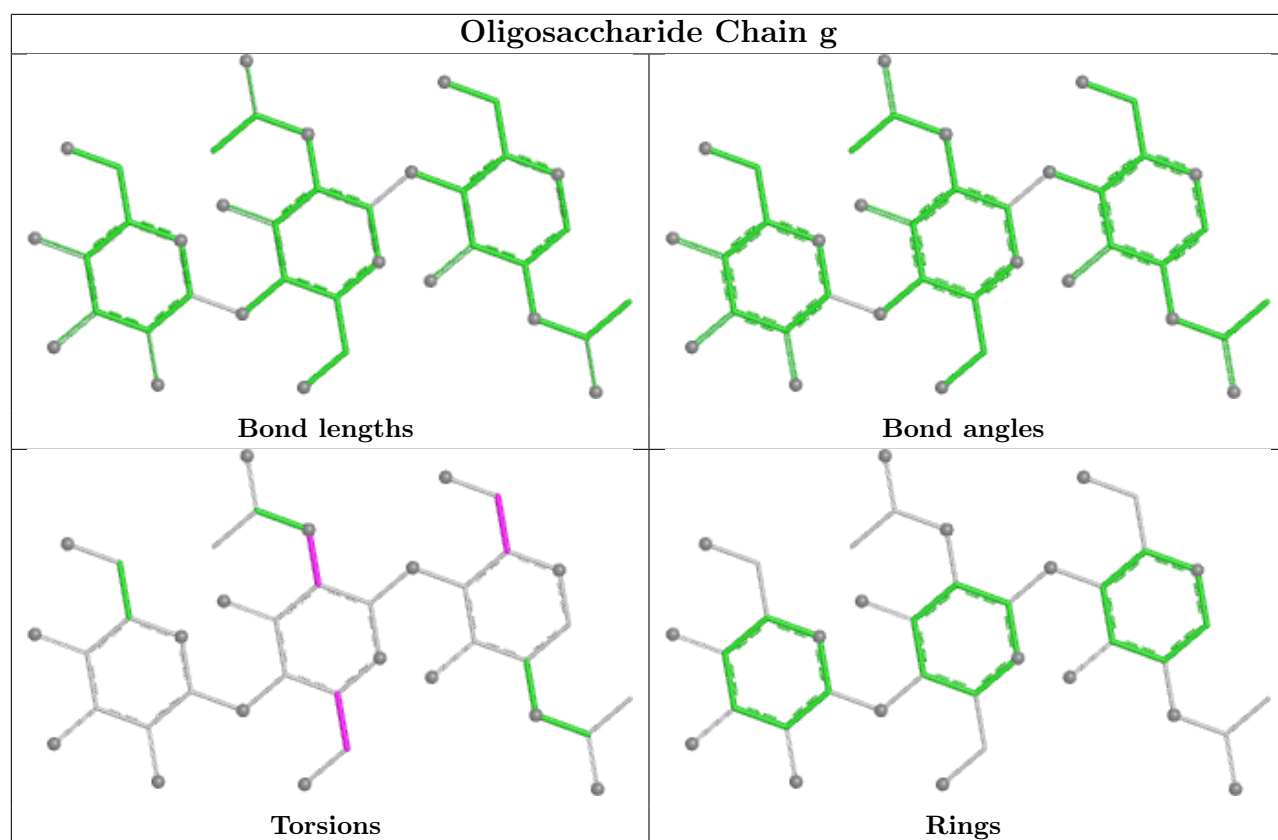


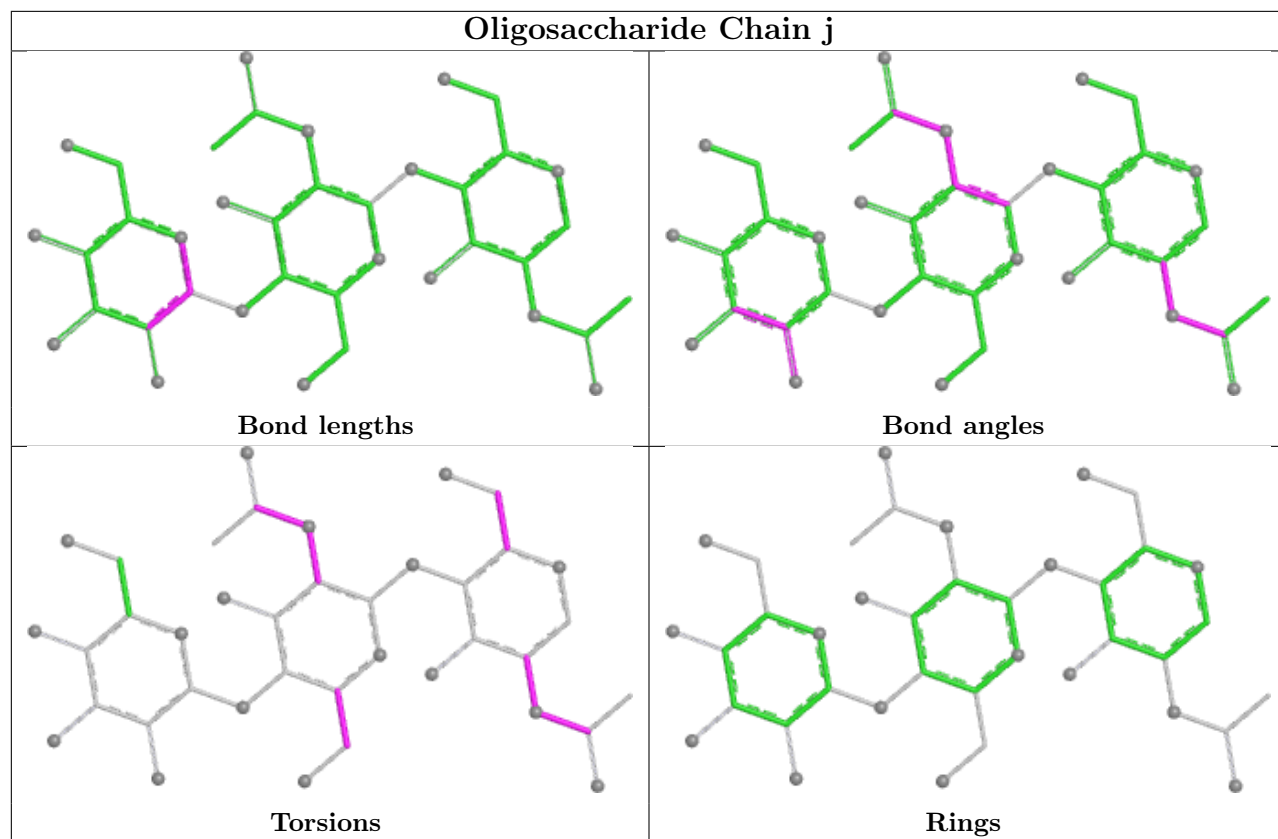


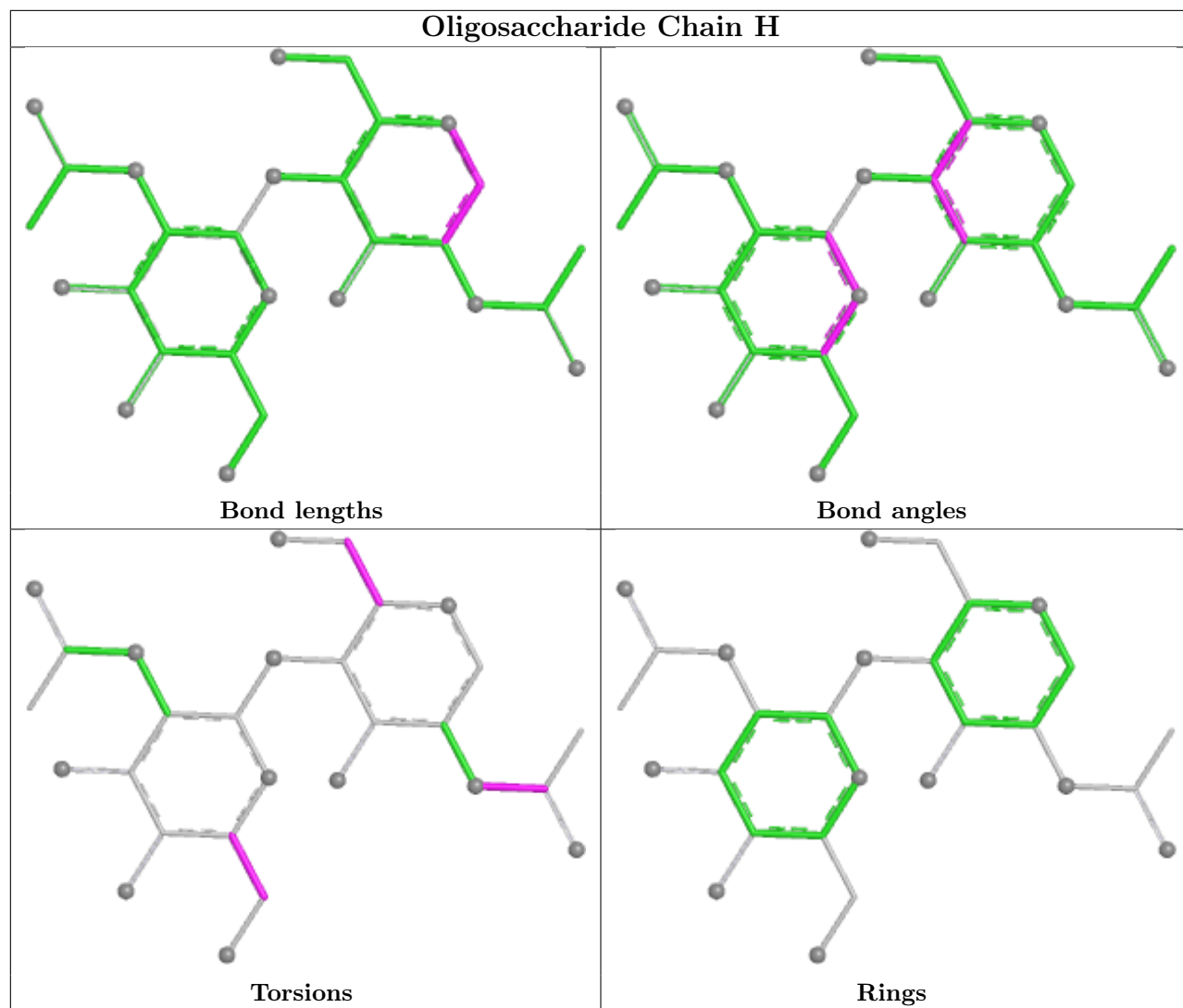


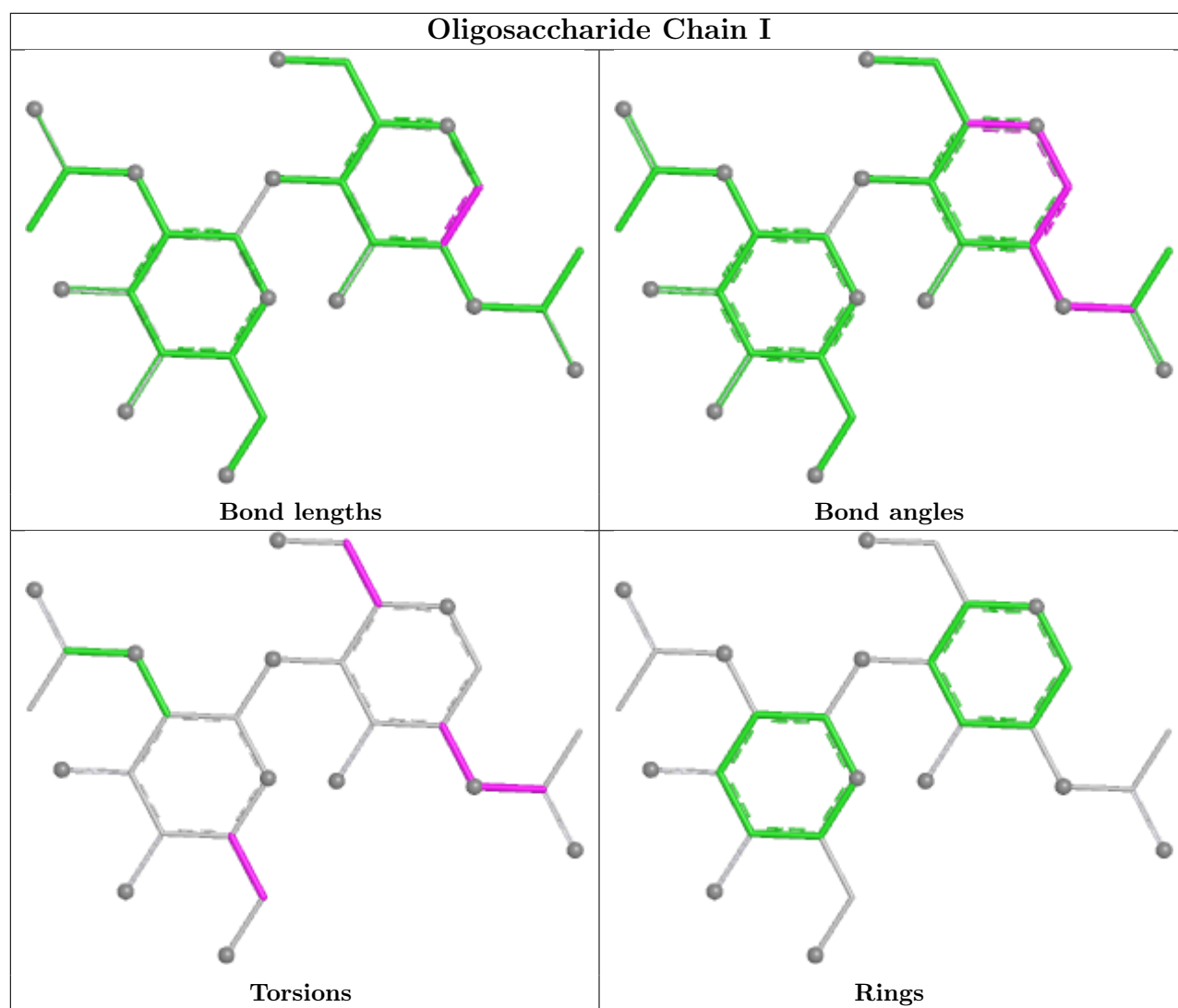


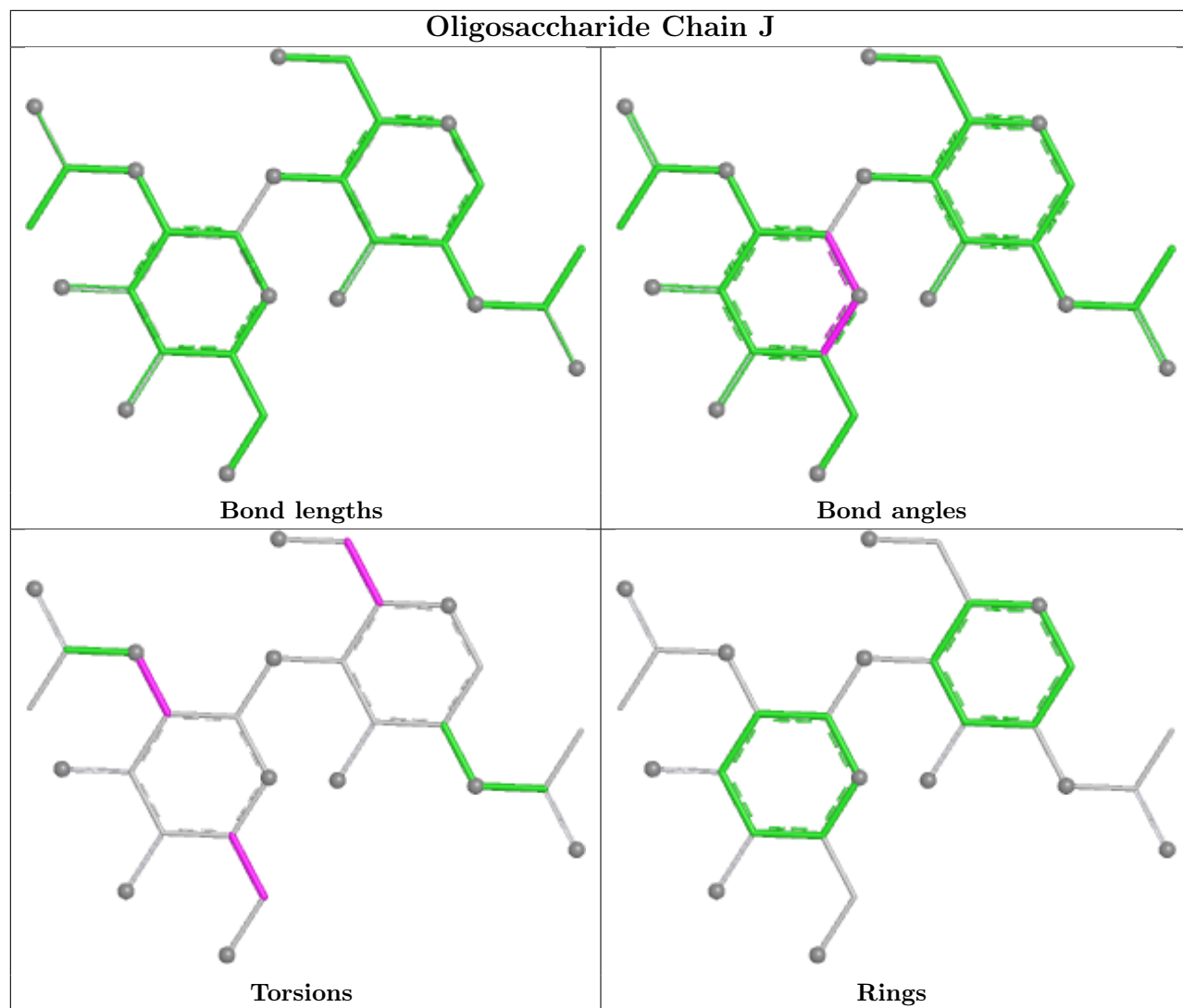


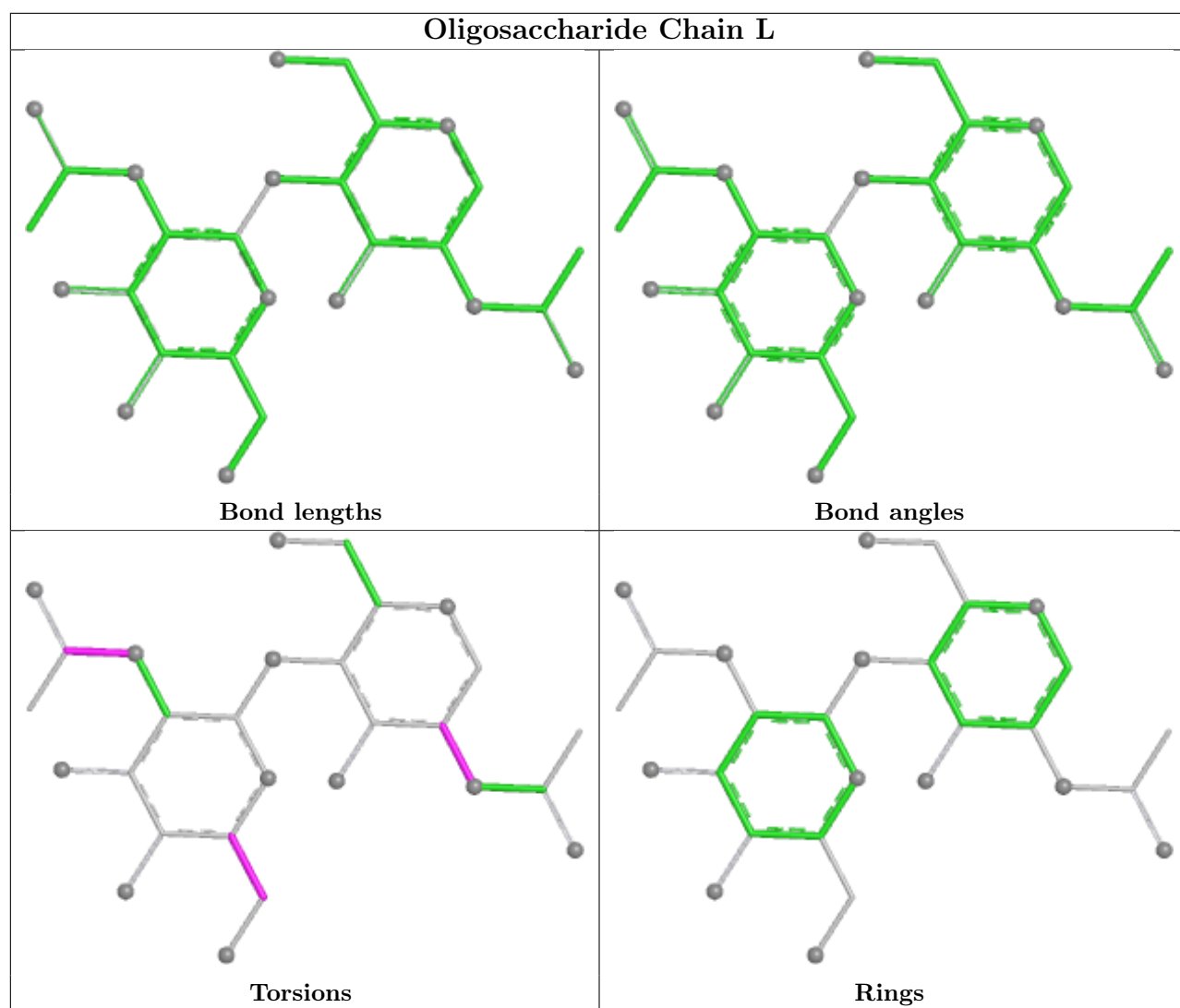


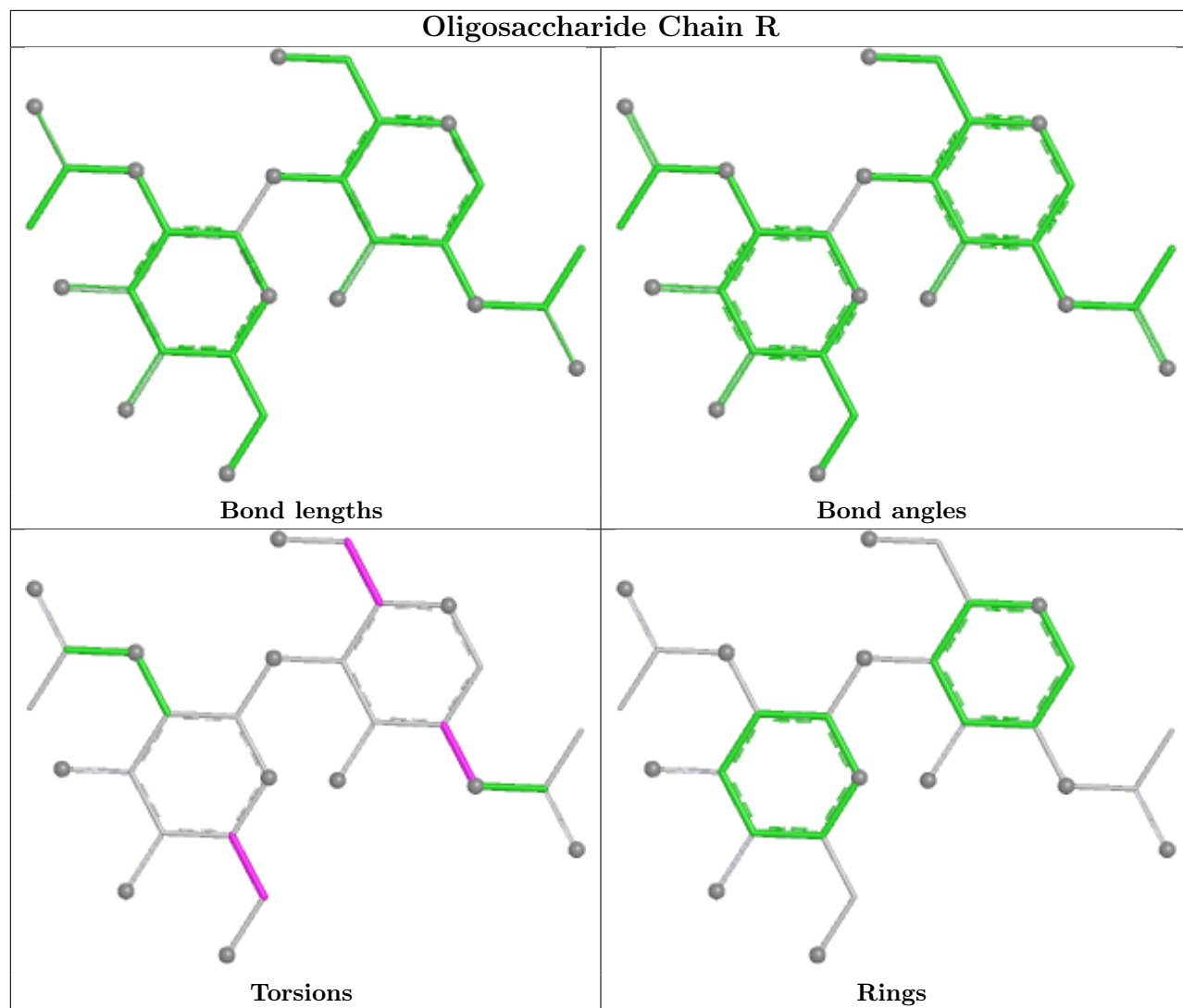


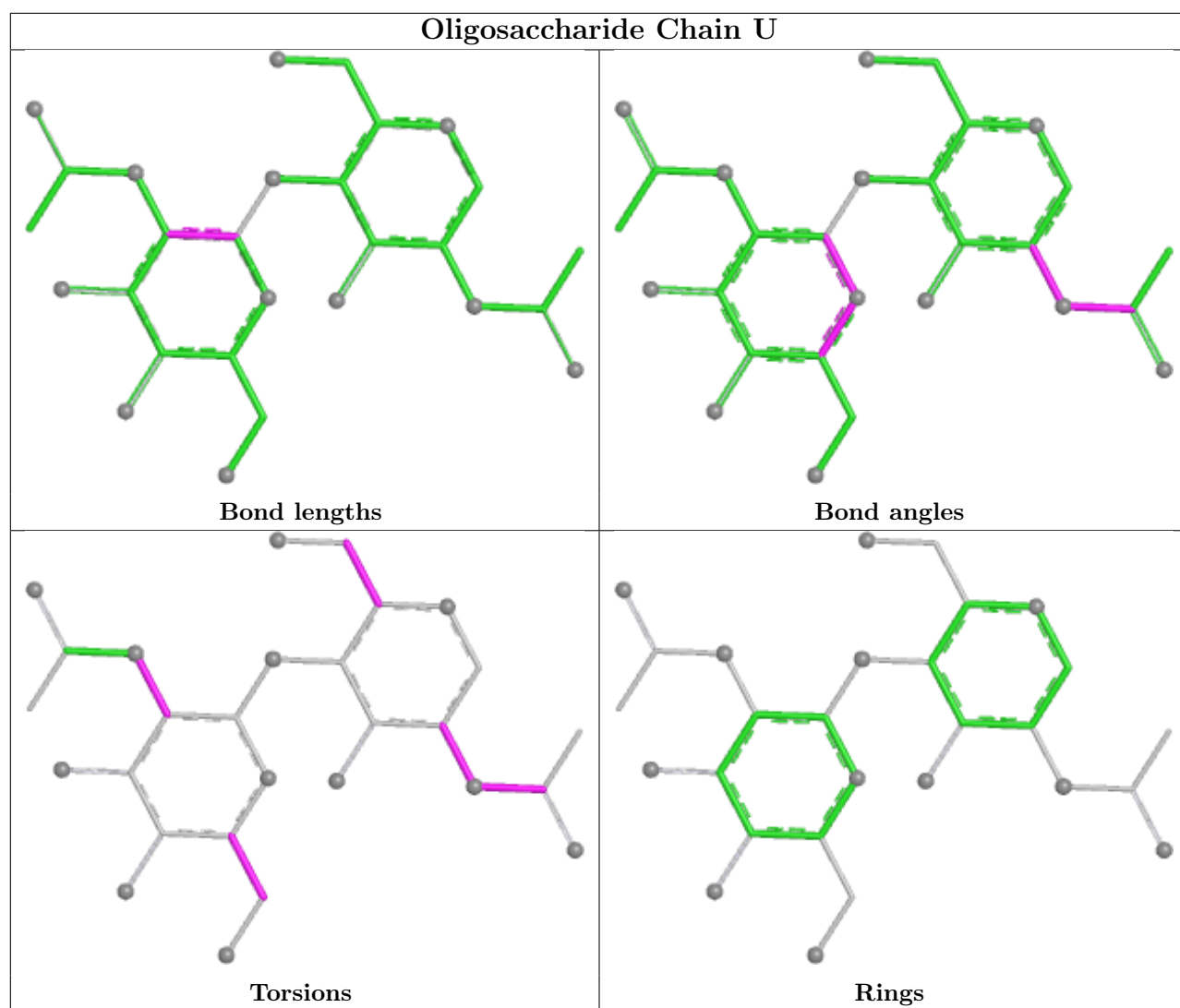


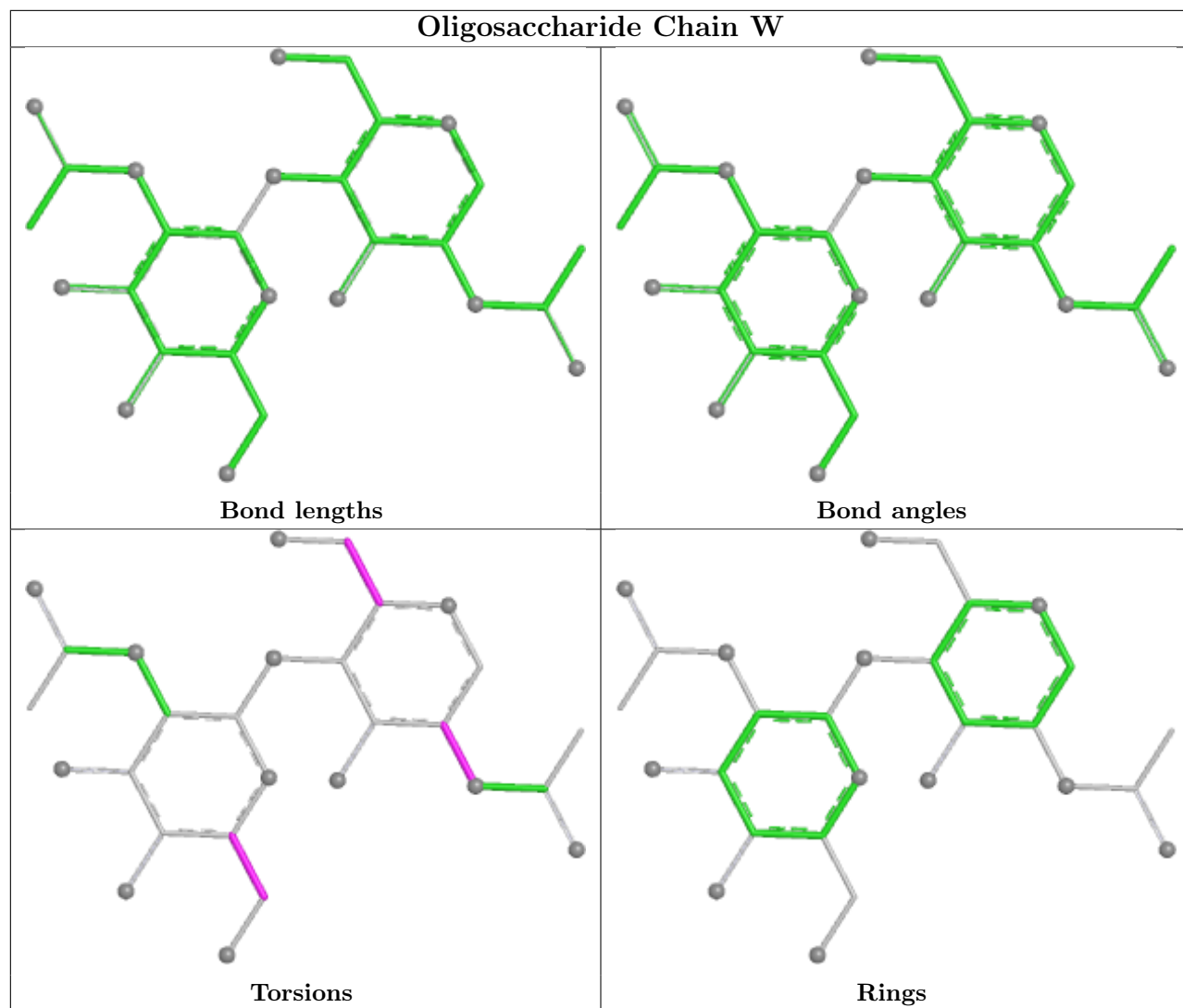


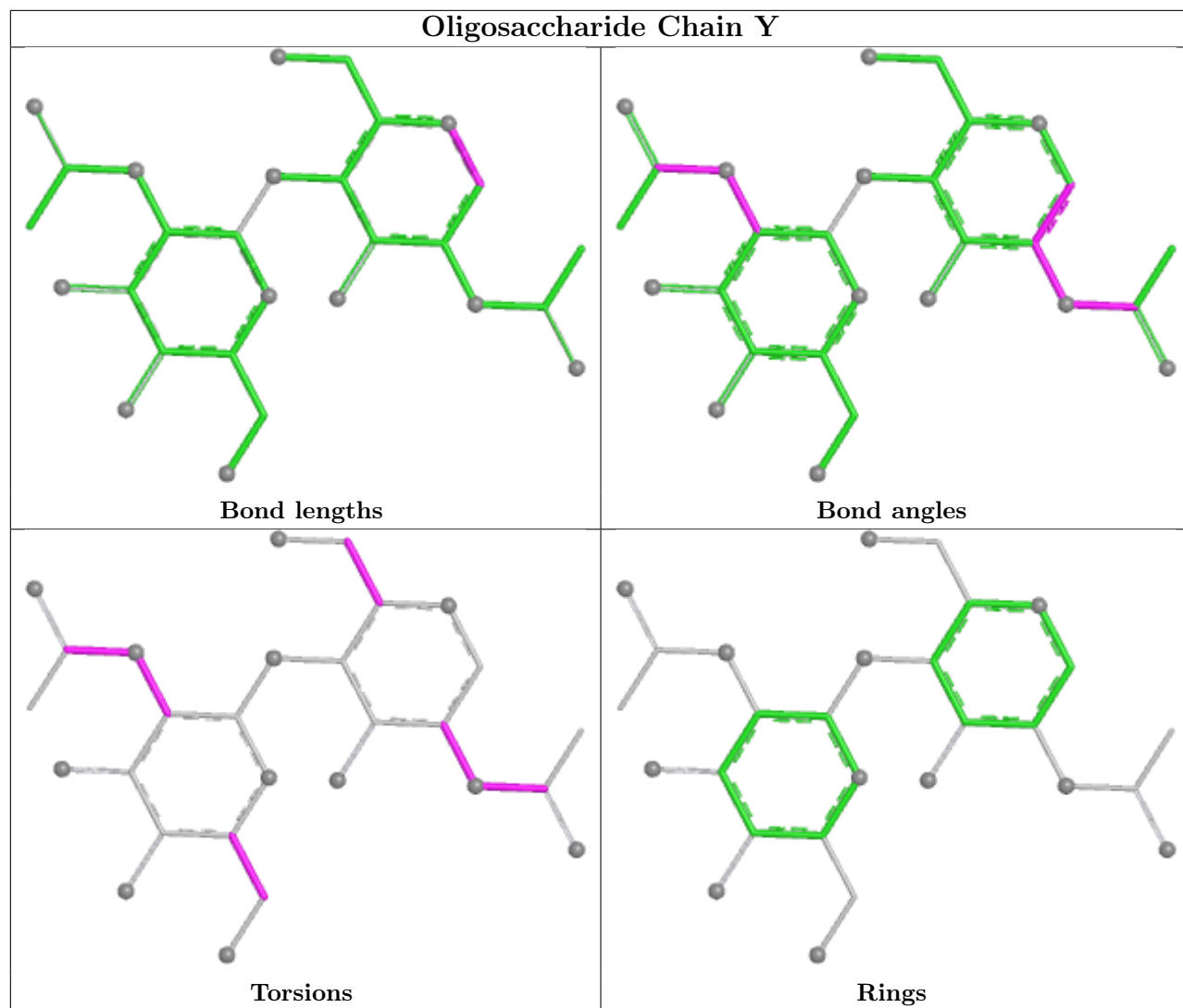


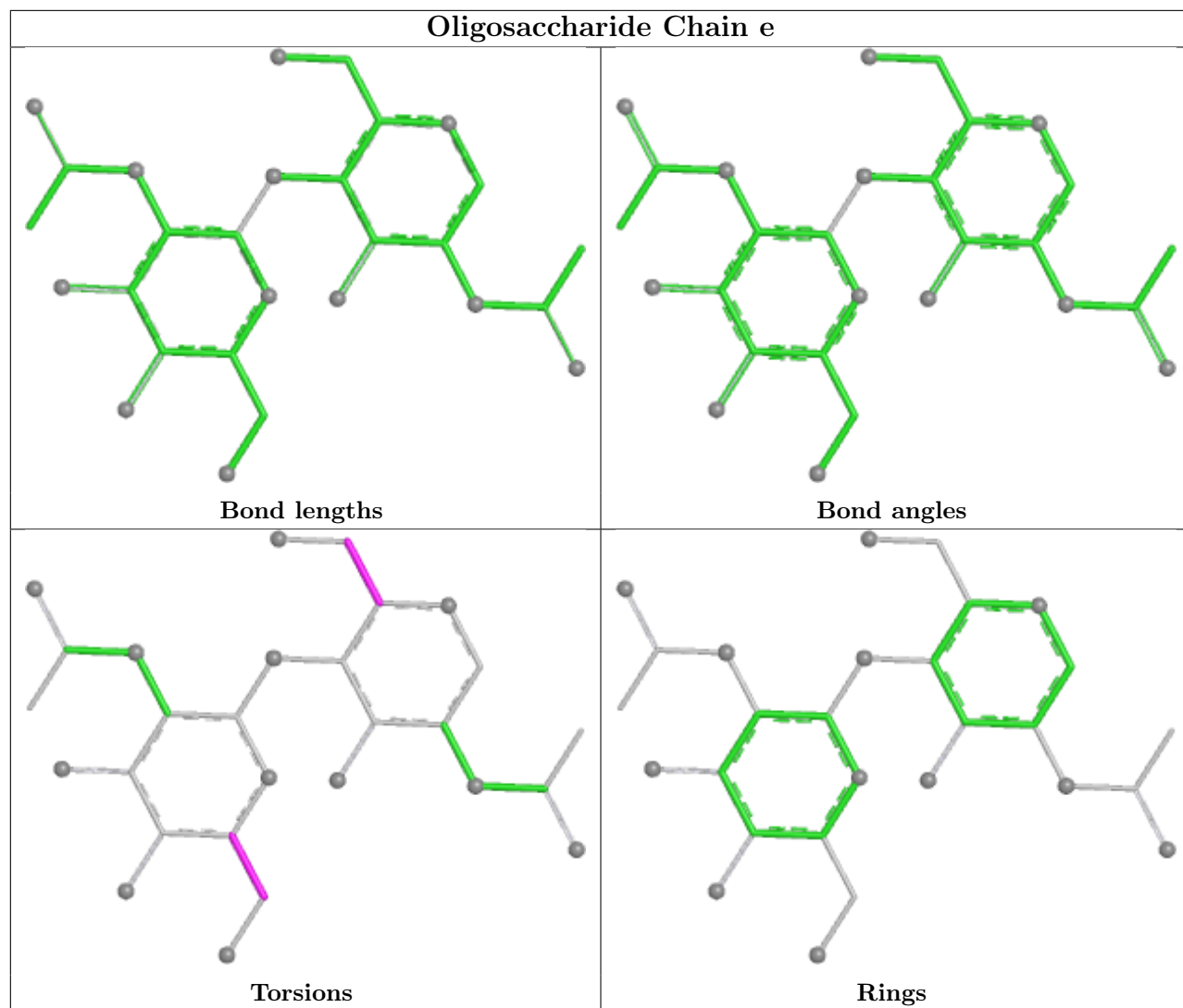


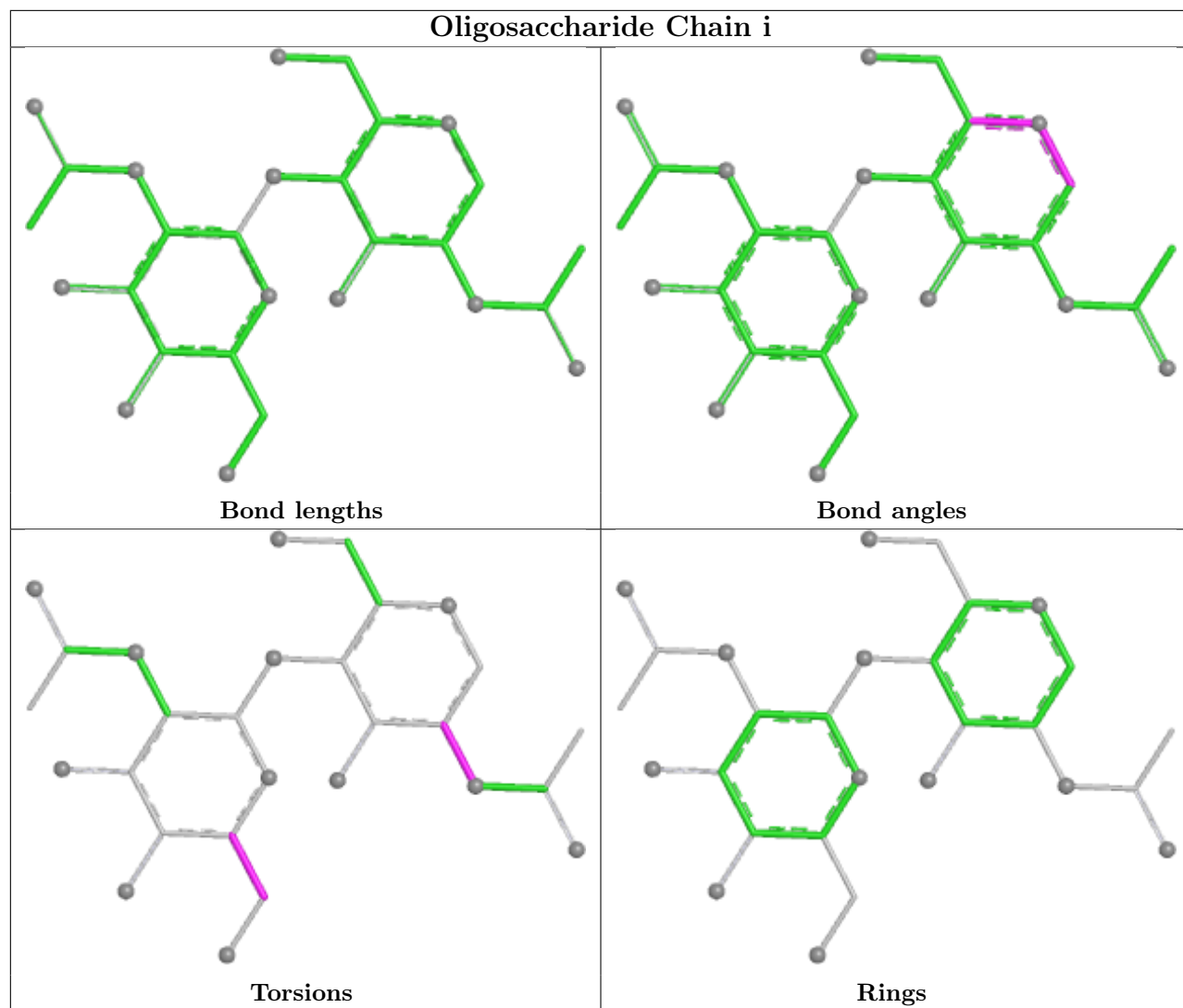


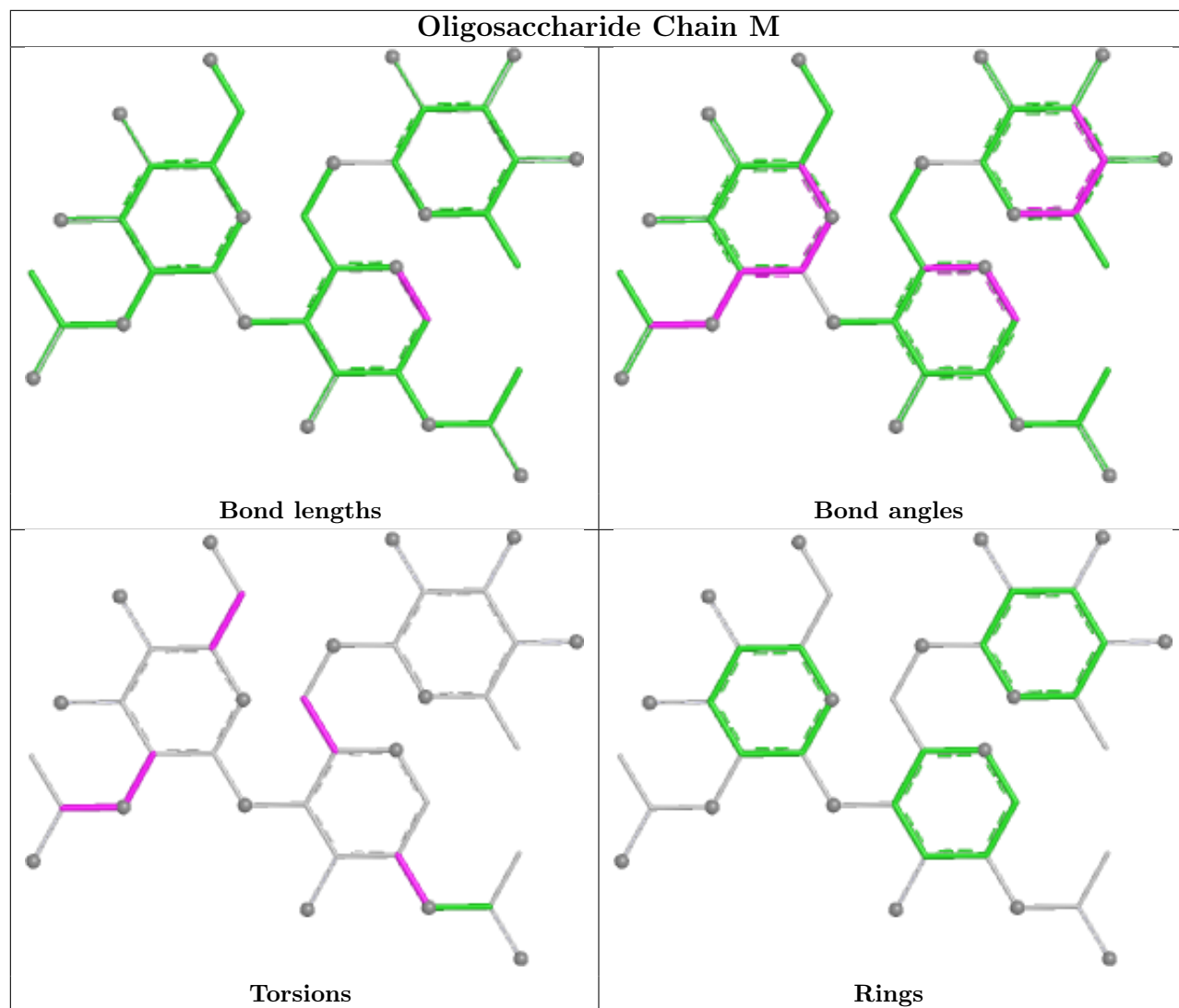


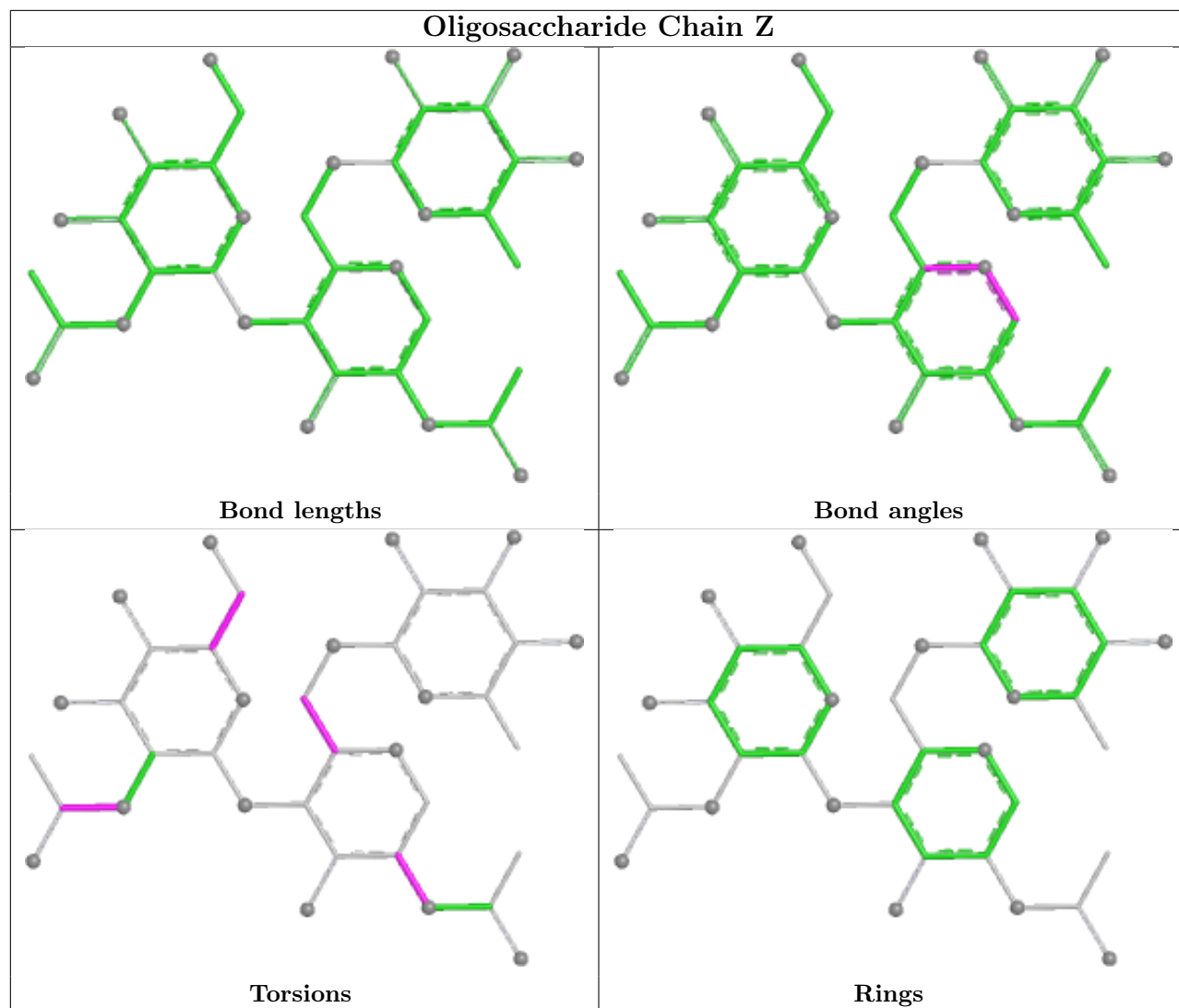


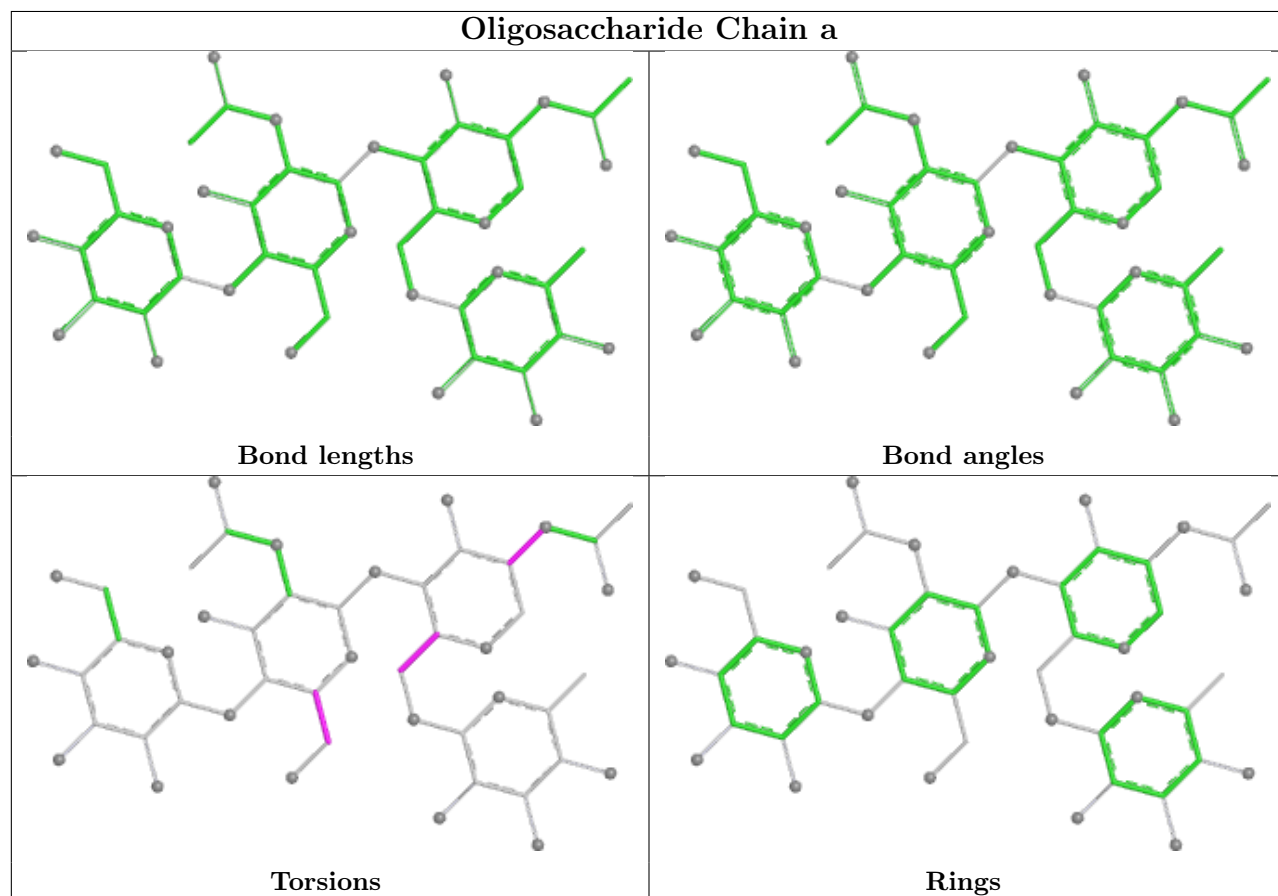
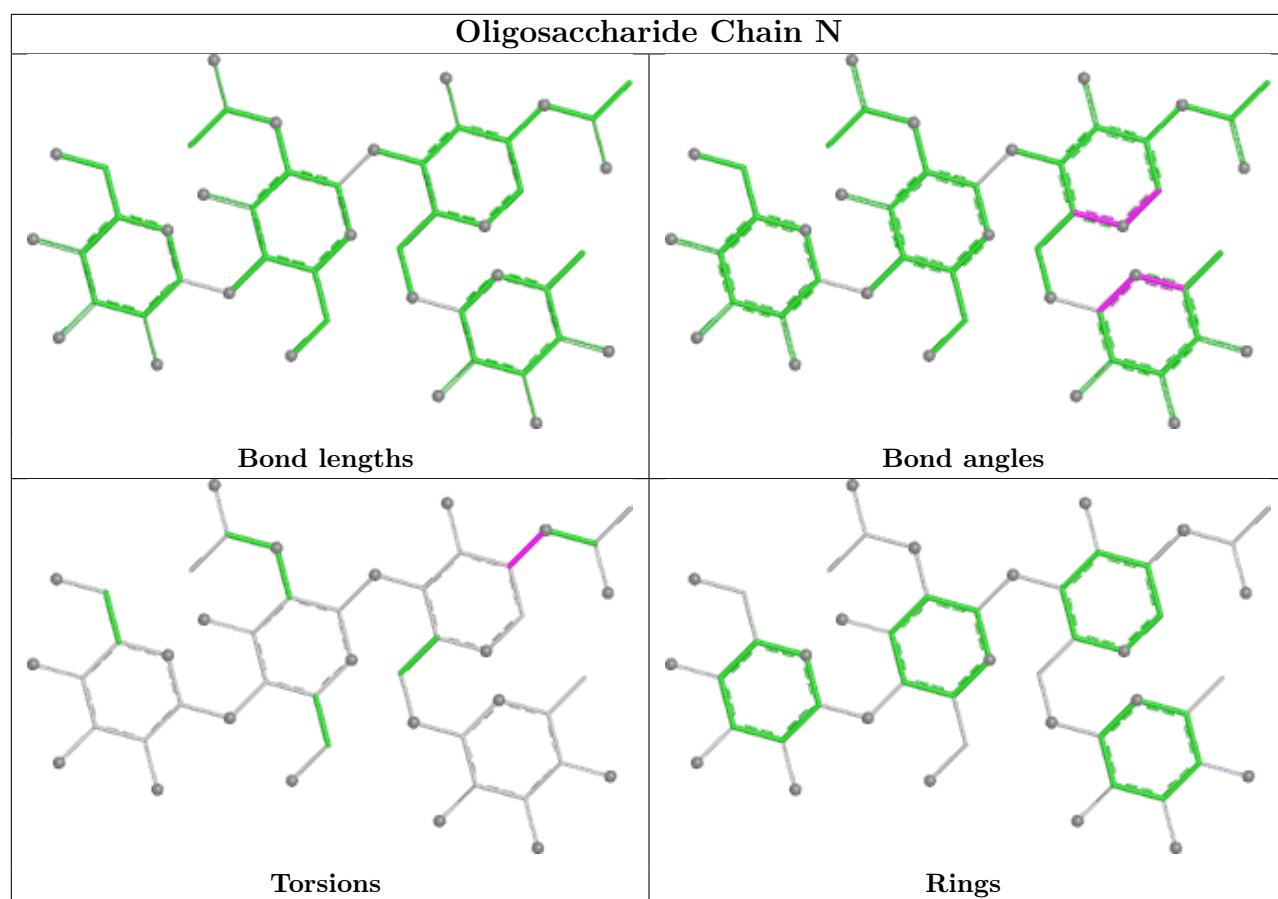


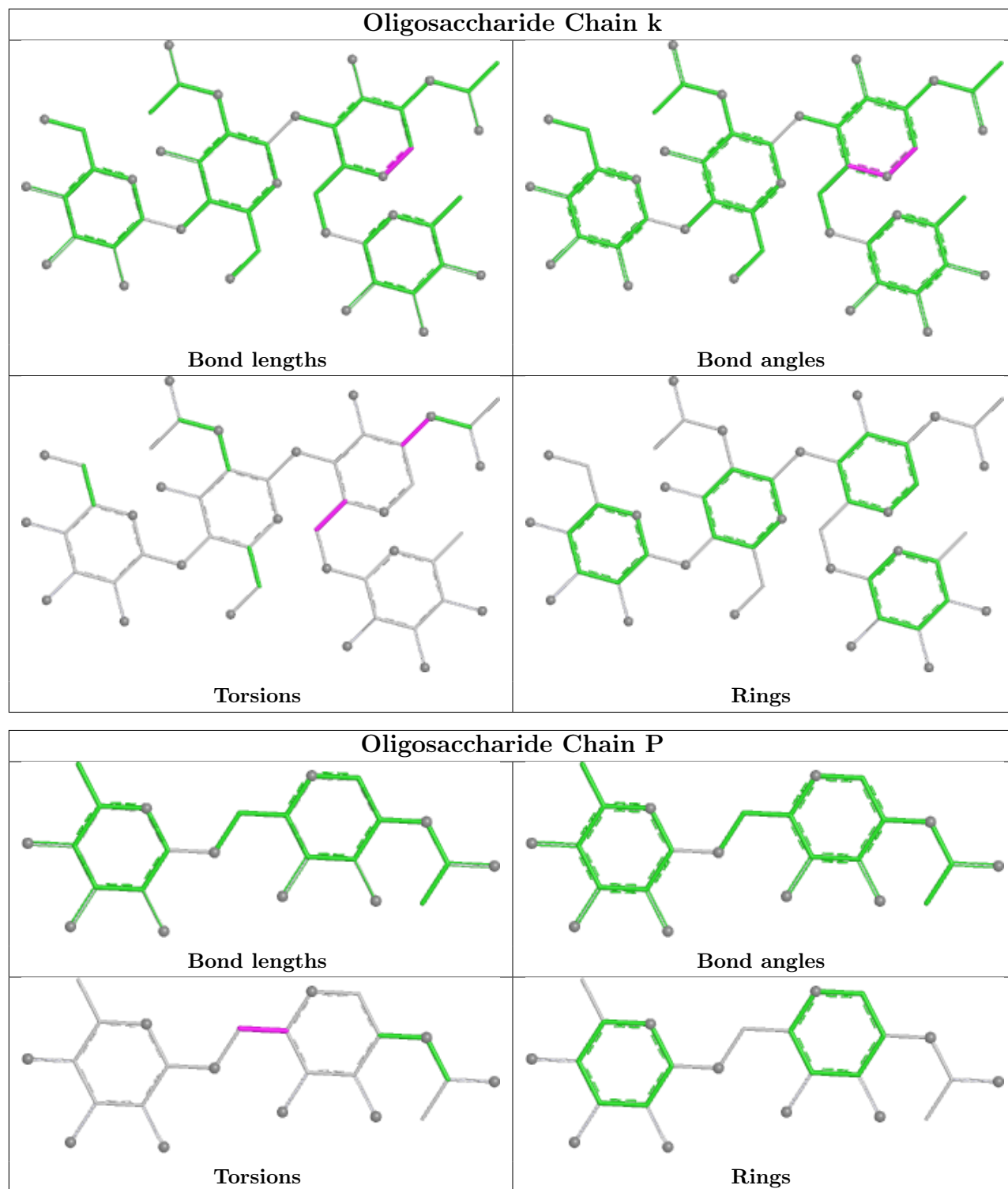


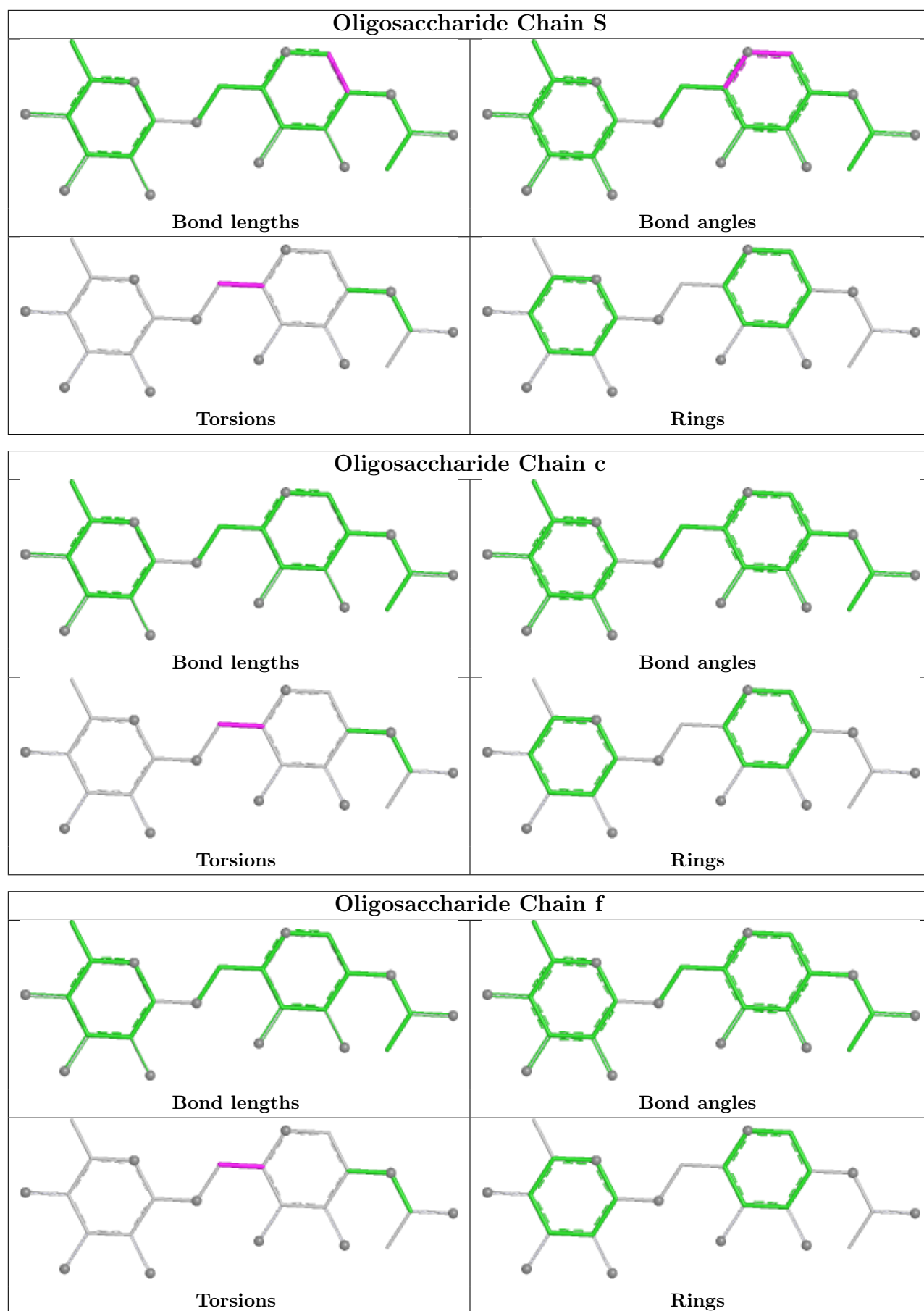












5.6 Ligand geometry

18 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
8	NAG	A	1502	1	14,14,15	0.51	0	17,19,21	0.59	0
8	NAG	A	1503	1	14,14,15	0.37	0	17,19,21	0.57	0
8	NAG	C	1504	1	14,14,15	0.24	0	17,19,21	0.51	0
8	NAG	A	1501	1	14,14,15	0.17	0	17,19,21	0.55	0
8	NAG	B	1505	1	14,14,15	0.31	0	17,19,21	0.52	0
8	NAG	B	1507	1	14,14,15	0.21	0	17,19,21	0.43	0
8	NAG	B	1503	1	14,14,15	0.24	0	17,19,21	0.40	0
8	NAG	A	1504	1	14,14,15	0.19	0	17,19,21	0.43	0
8	NAG	A	1506	1	14,14,15	0.48	0	17,19,21	0.61	0
8	NAG	C	1505	1	14,14,15	0.93	1 (7%)	17,19,21	0.60	0
8	NAG	B	1502	1	14,14,15	0.30	0	17,19,21	0.43	0
8	NAG	B	1506	1	14,14,15	0.26	0	17,19,21	0.41	0
8	NAG	B	1504	1	14,14,15	0.31	0	17,19,21	0.47	0
8	NAG	C	1502	1	14,14,15	0.22	0	17,19,21	0.45	0
8	NAG	A	1505	1	14,14,15	0.70	0	17,19,21	1.17	1 (5%)
8	NAG	B	1501	1	14,14,15	0.27	0	17,19,21	0.40	0
8	NAG	C	1501	1	14,14,15	0.28	0	17,19,21	0.40	0
8	NAG	C	1503	1	14,14,15	0.29	0	17,19,21	0.64	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1502	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1503	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1504	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1501	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1505	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	1507	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1503	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1504	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1506	1	-	4/6/23/26	0/1/1/1
8	NAG	C	1505	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1502	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1506	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1504	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1502	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1505	1	-	0/6/23/26	0/1/1/1
8	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1501	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1503	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1505	NAG	O5-C1	-3.13	1.38	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1505	NAG	C1-O5-C5	4.44	118.14	112.19
8	C	1503	NAG	C1-O5-C5	2.09	114.98	112.19

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1503	NAG	O5-C5-C6-O6
8	B	1503	NAG	O5-C5-C6-O6
8	B	1505	NAG	C4-C5-C6-O6
8	A	1506	NAG	C4-C5-C6-O6
8	C	1504	NAG	O5-C5-C6-O6

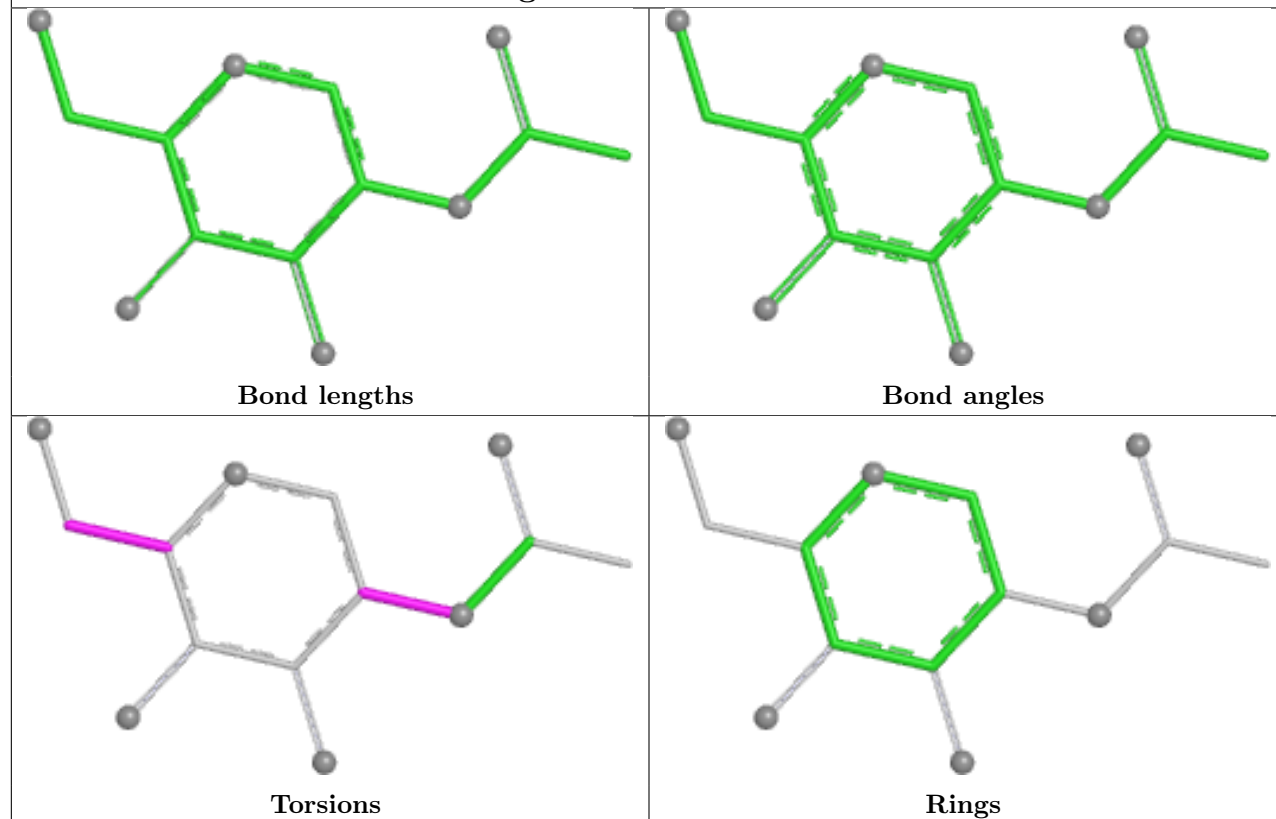
There are no ring outliers.

10 monomers are involved in 11 short contacts:

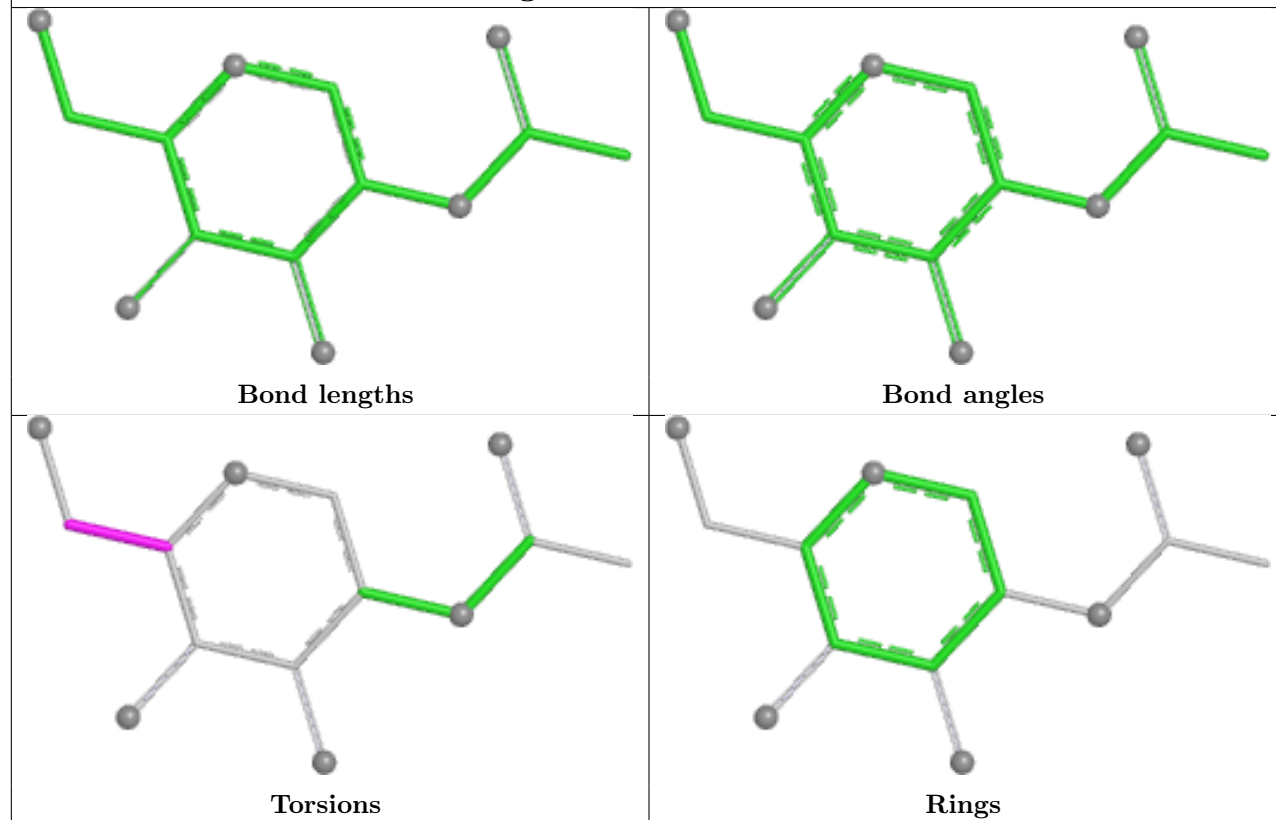
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1502	NAG	1	0
8	A	1501	NAG	1	0
8	B	1505	NAG	1	0
8	B	1503	NAG	1	0
8	A	1506	NAG	2	0
8	B	1502	NAG	1	0
8	A	1505	NAG	1	0
8	B	1501	NAG	1	0
8	C	1501	NAG	1	0
8	C	1503	NAG	1	0

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

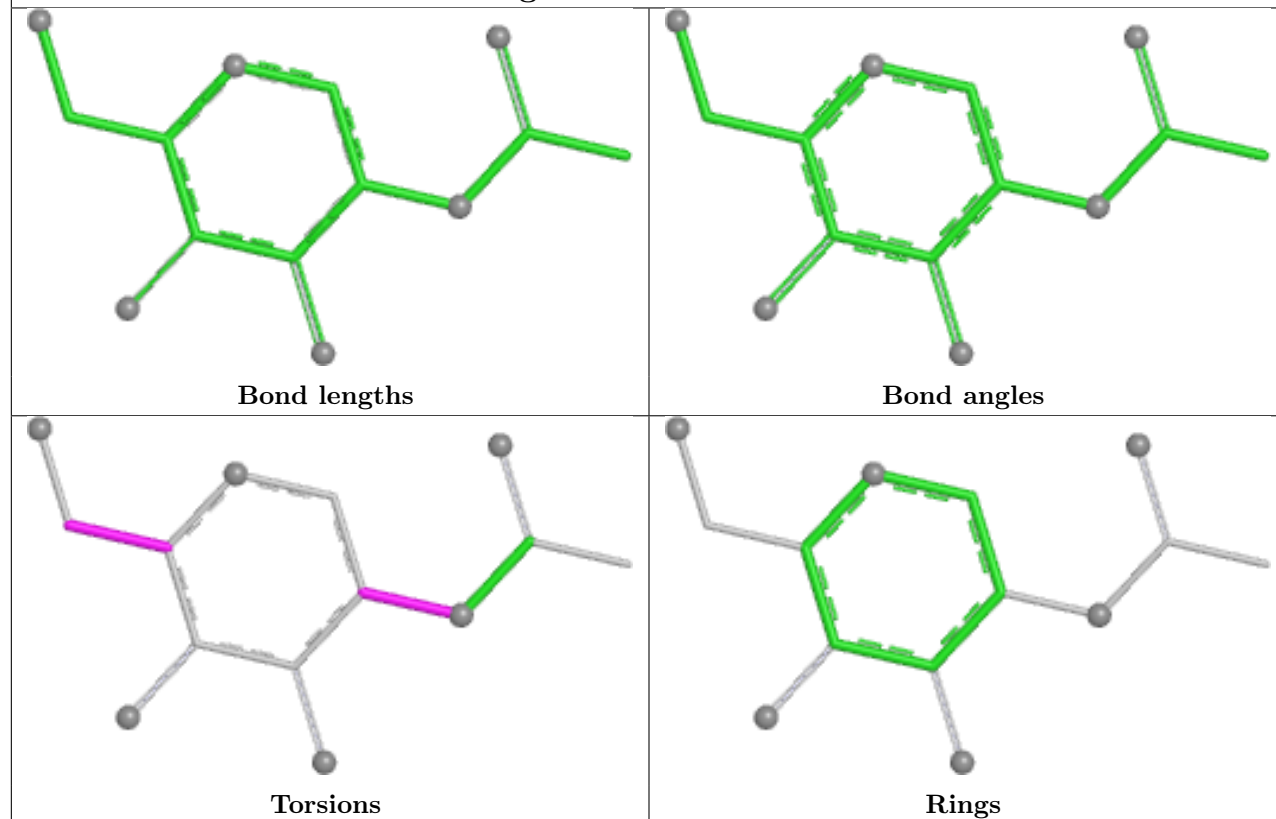
Ligand NAG A 1502



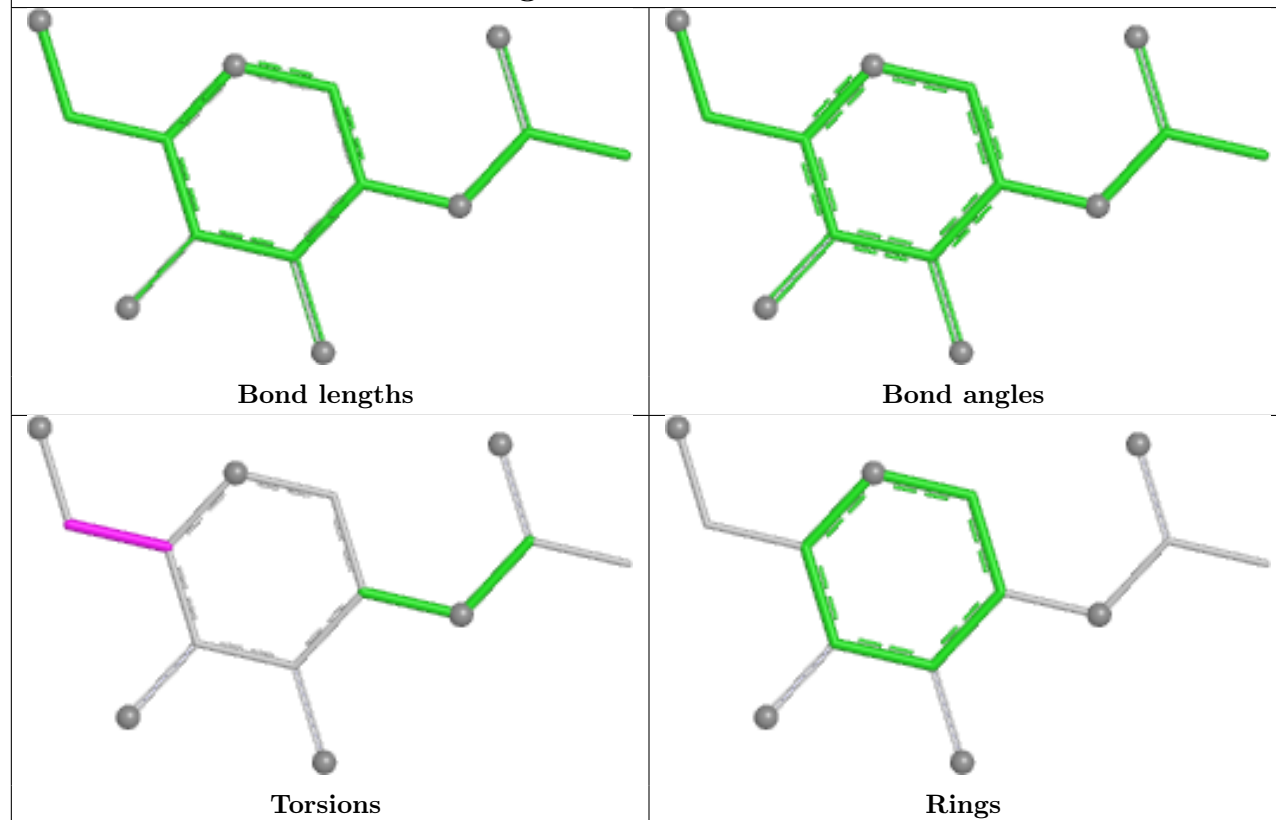
Ligand NAG A 1503

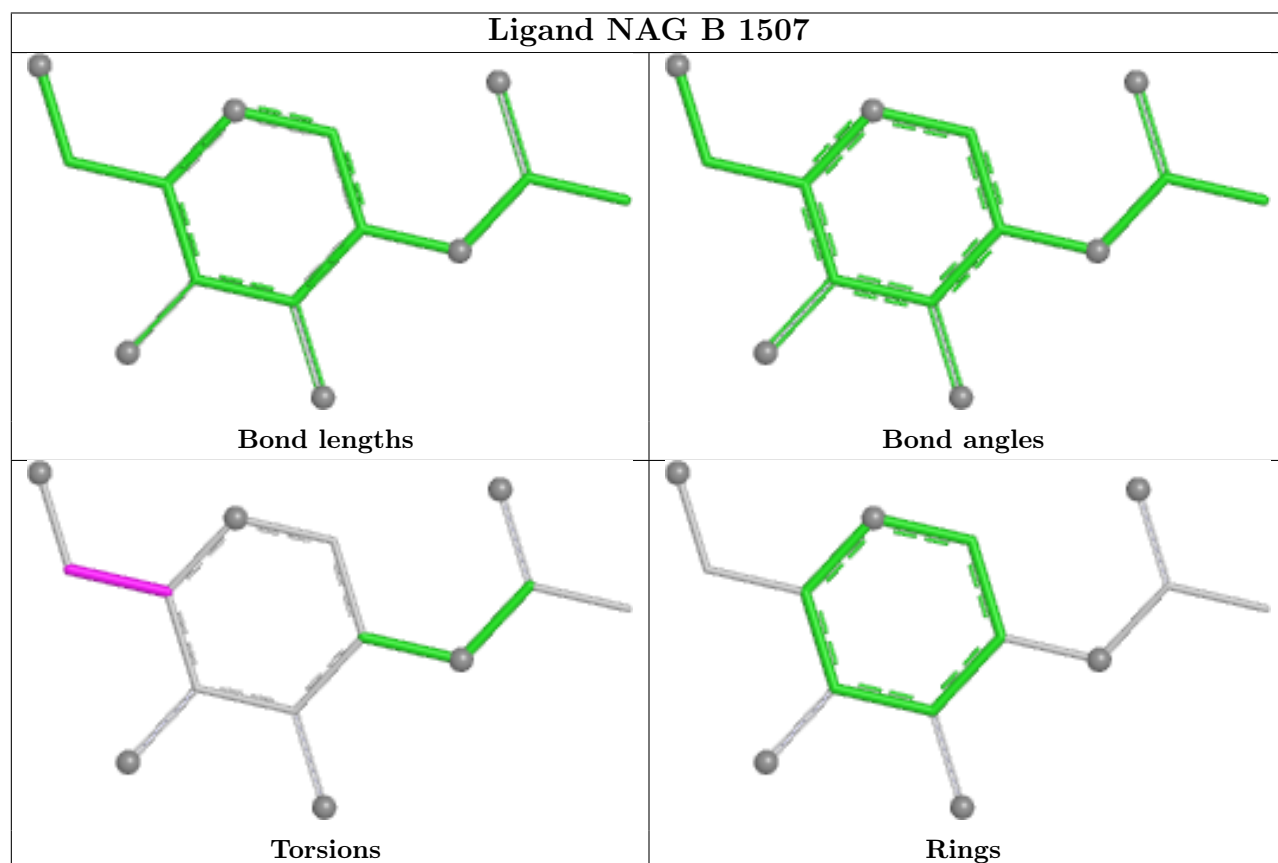
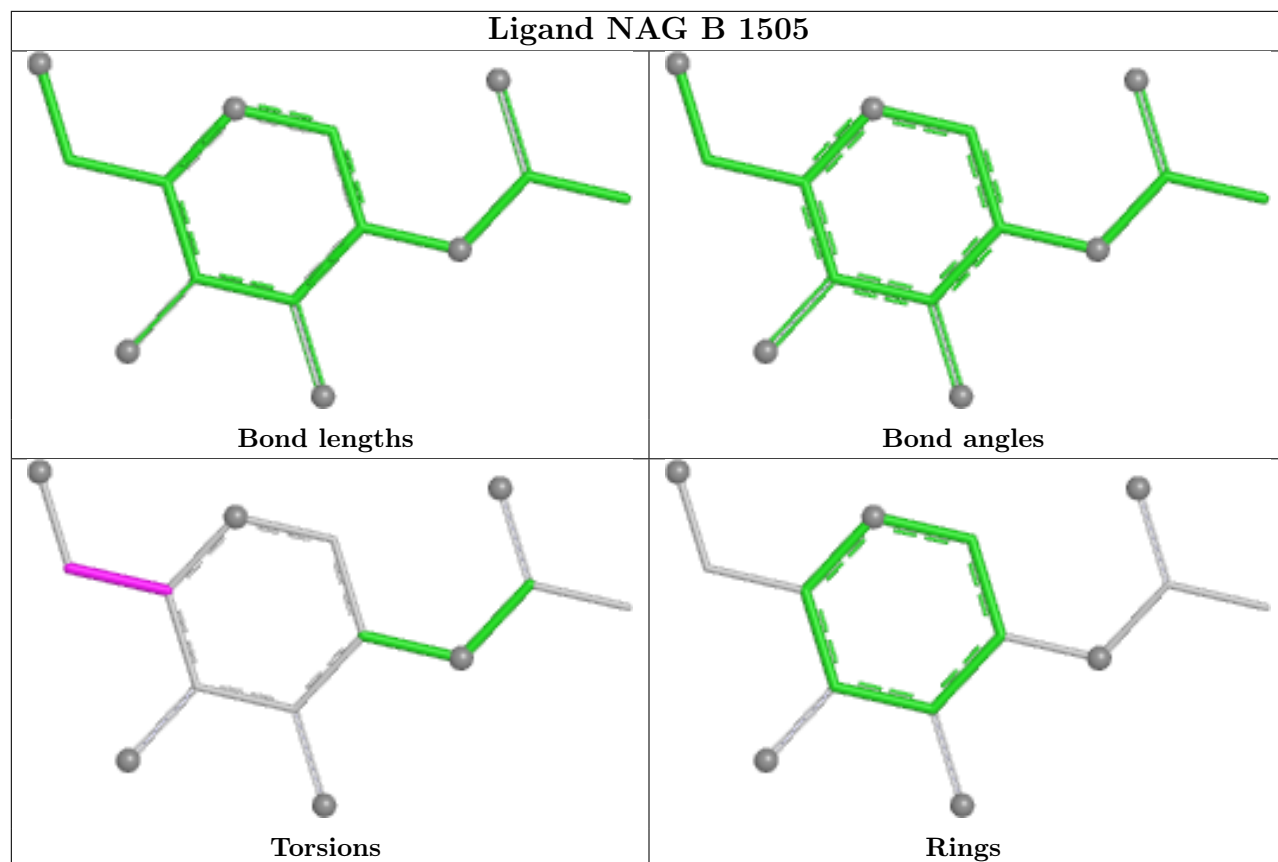


Ligand NAG C 1504

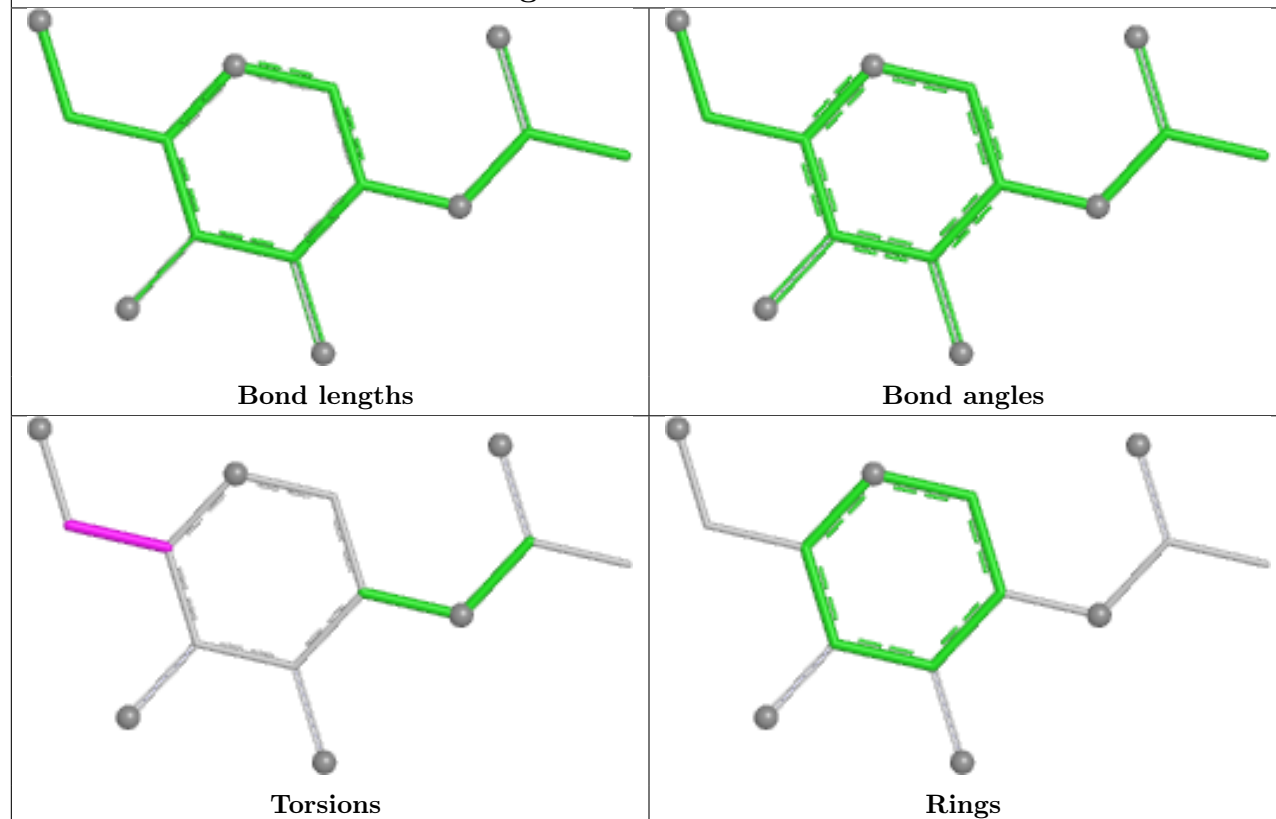


Ligand NAG A 1501

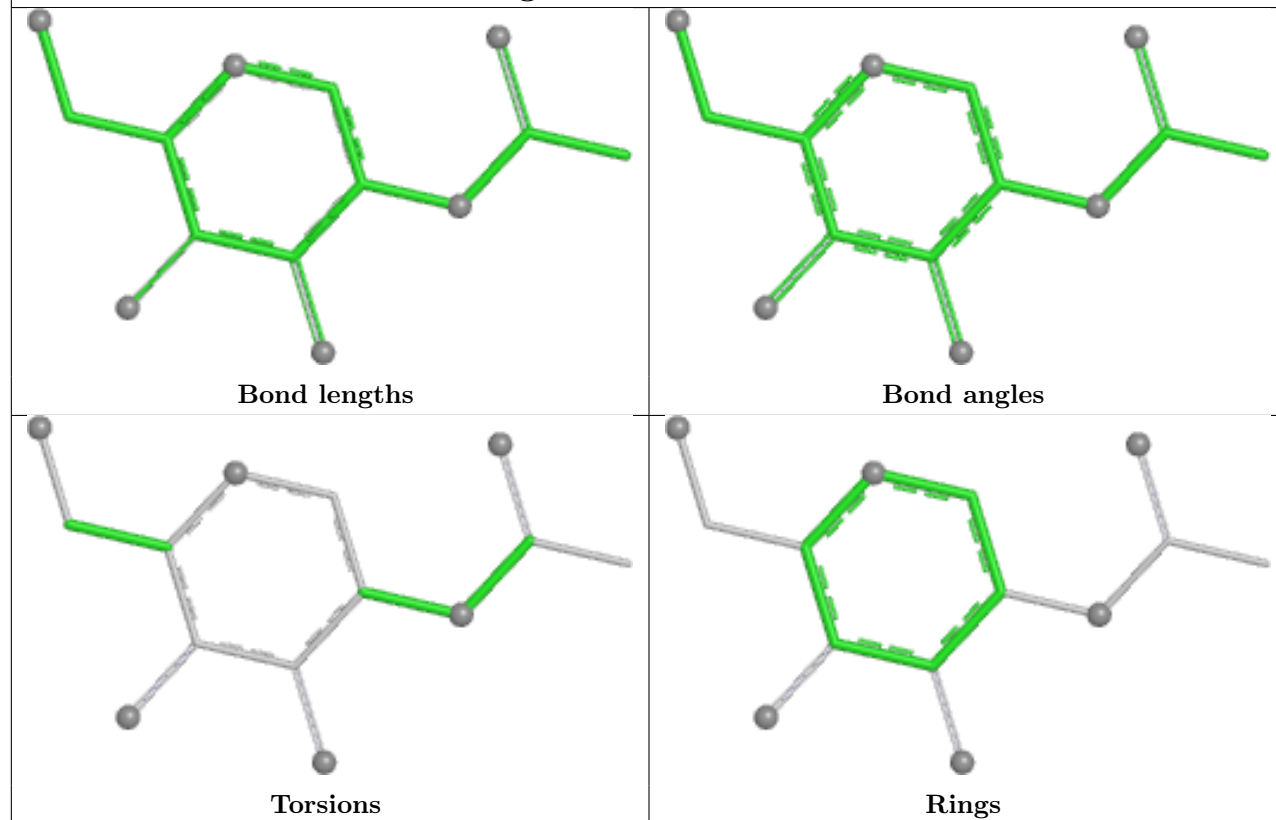




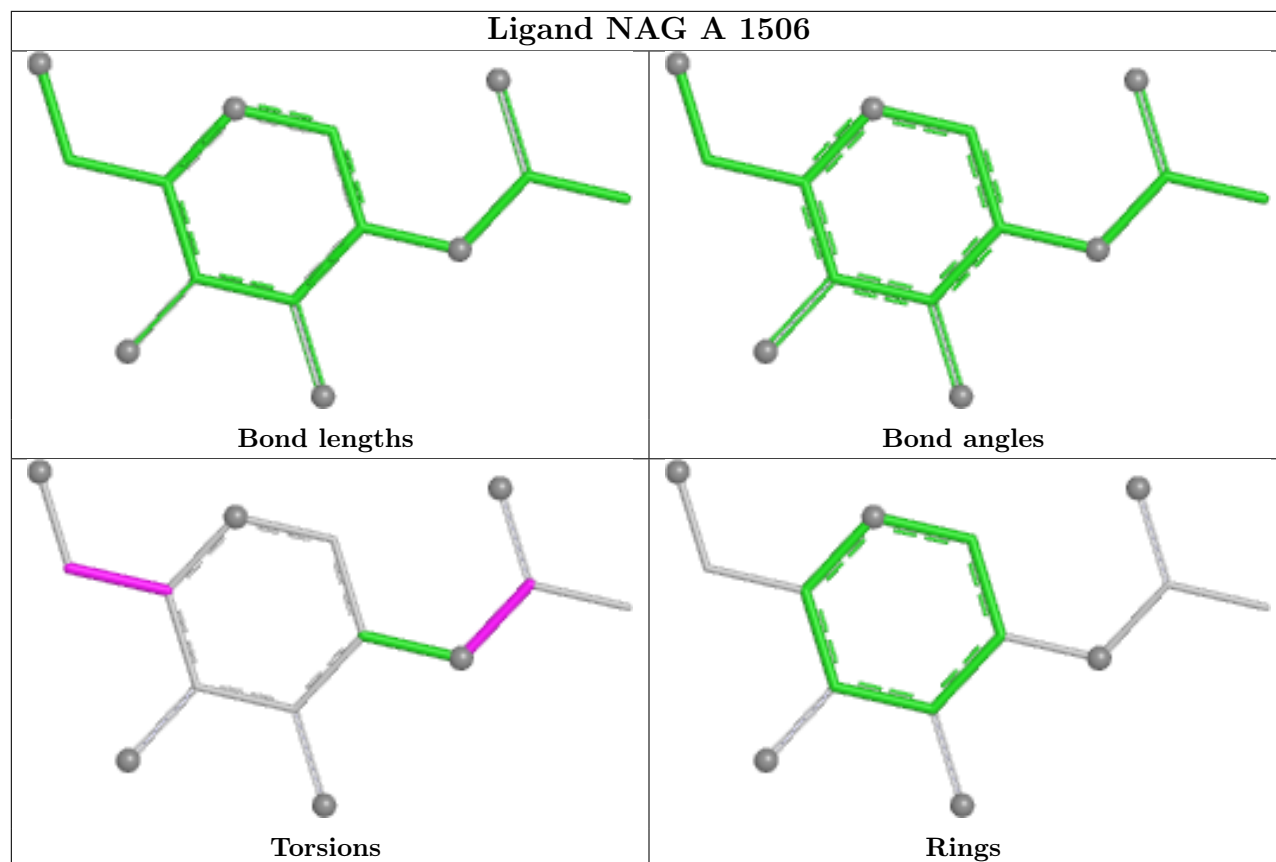
Ligand NAG B 1503



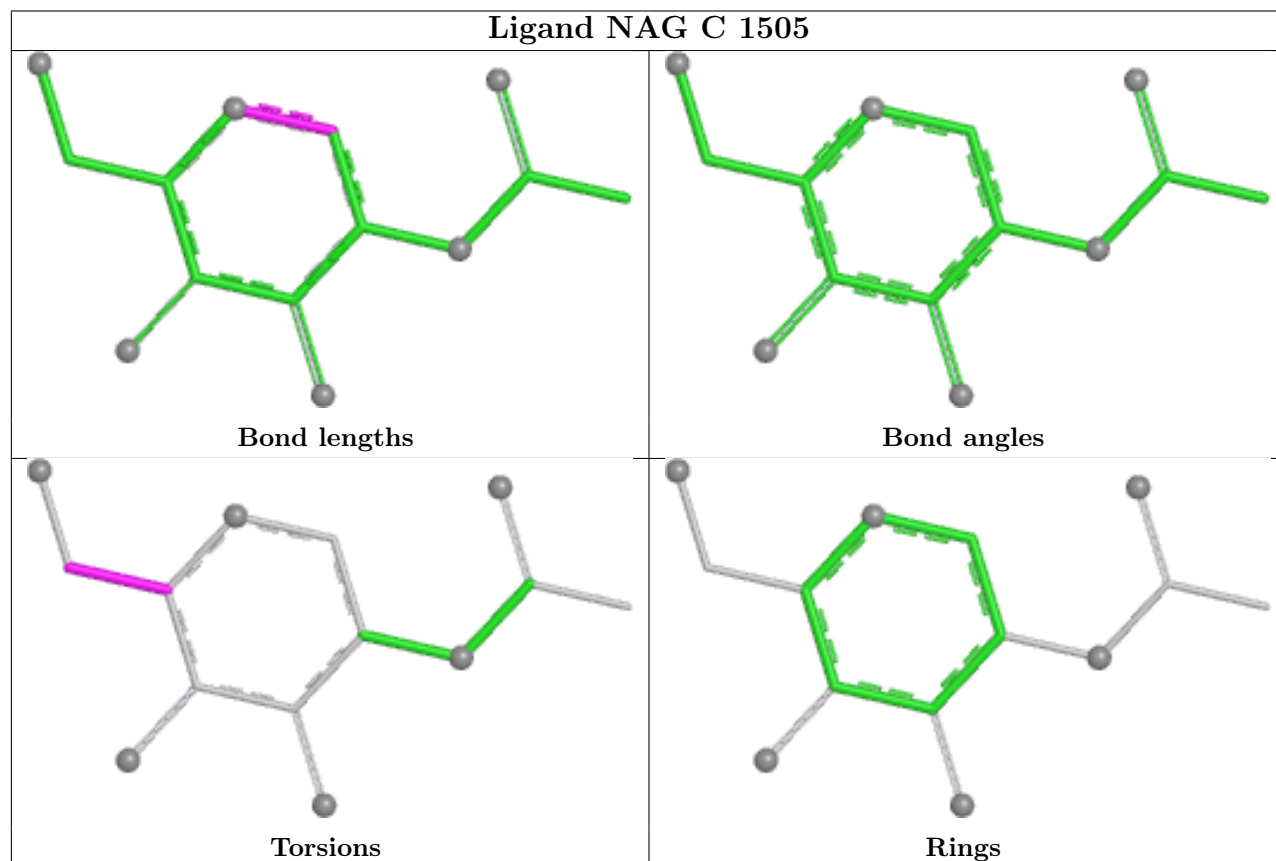
Ligand NAG A 1504

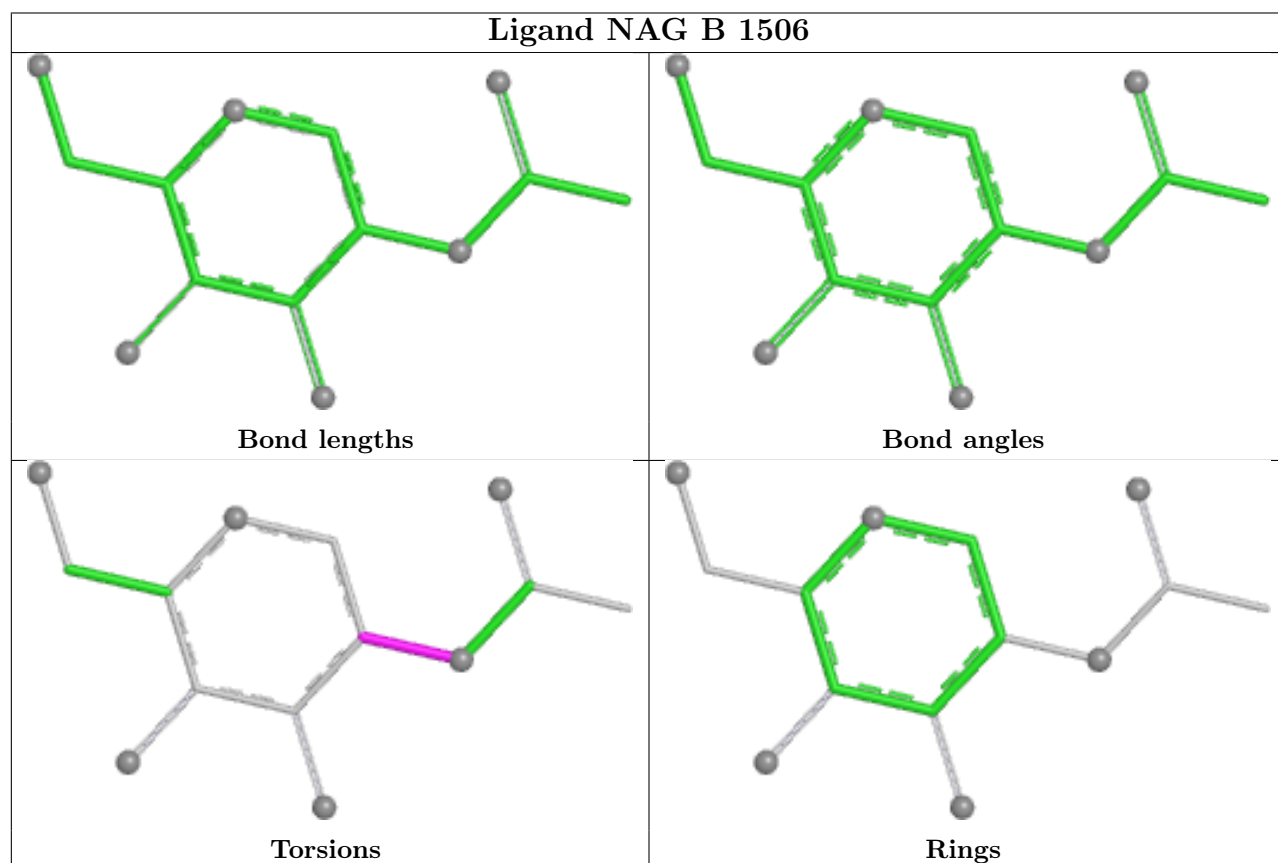
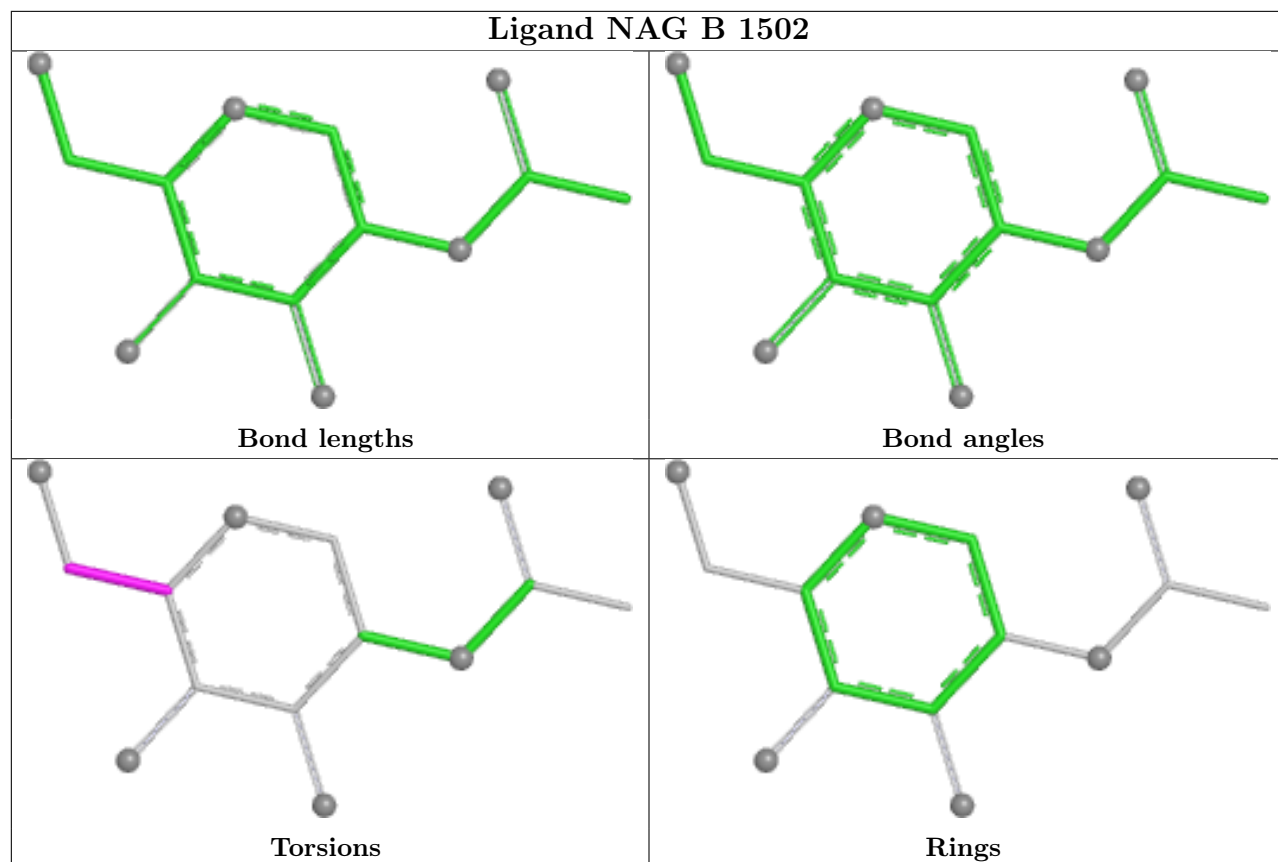


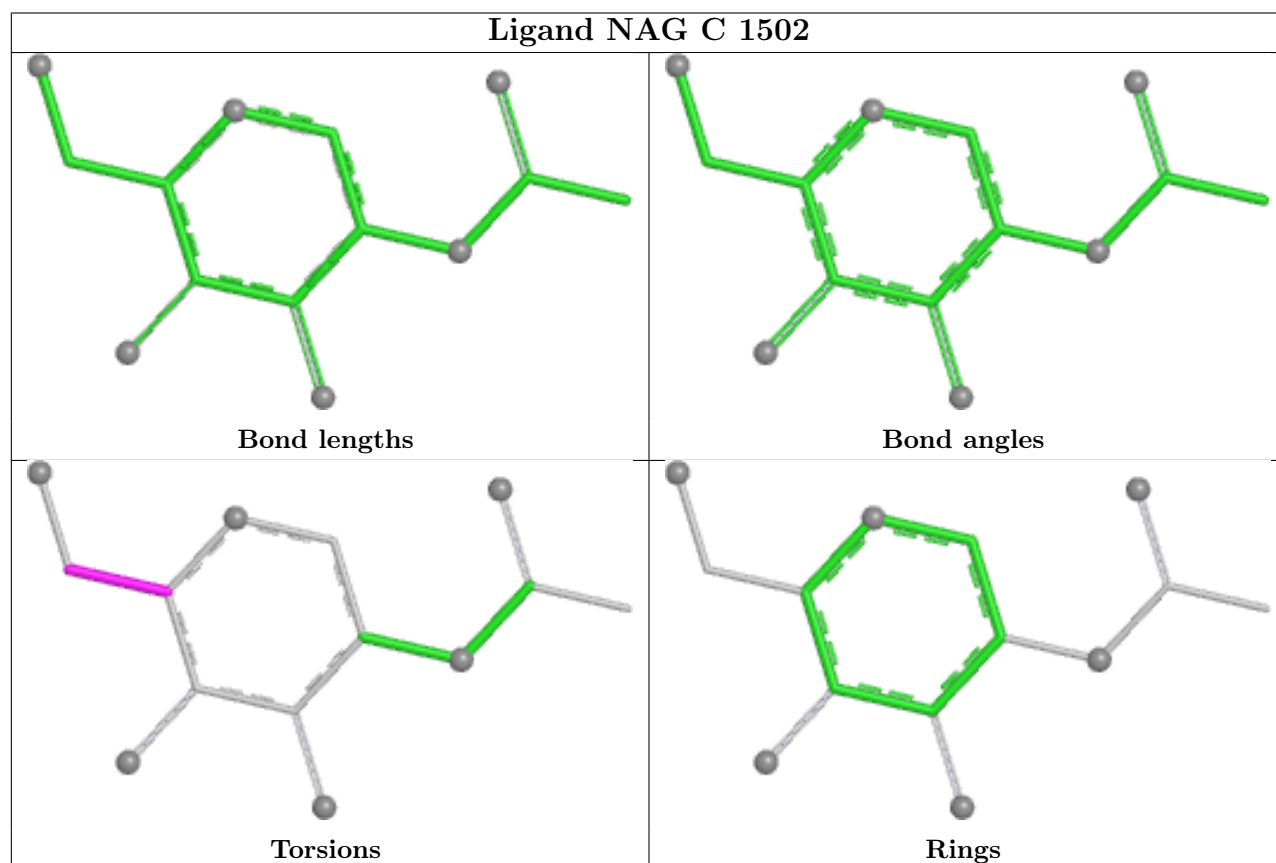
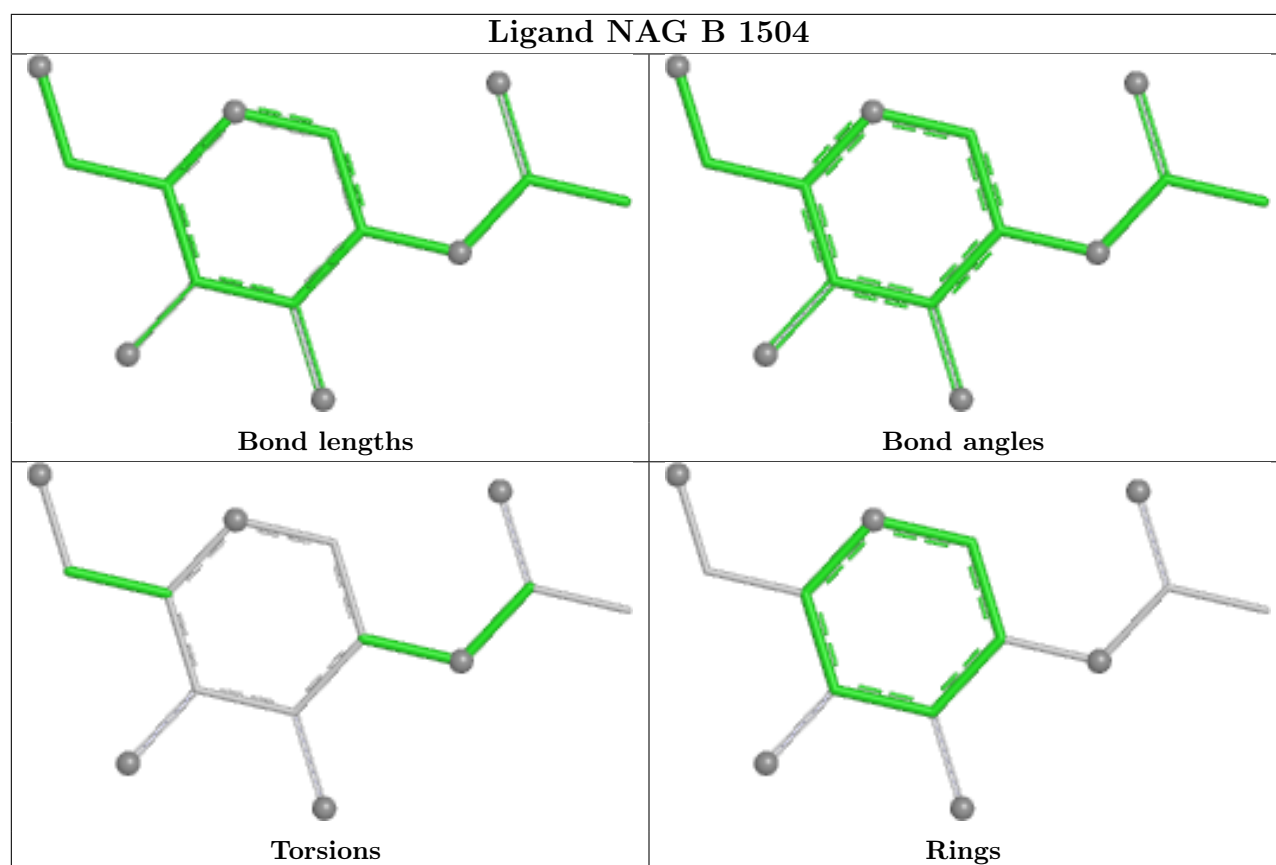
Ligand NAG A 1506



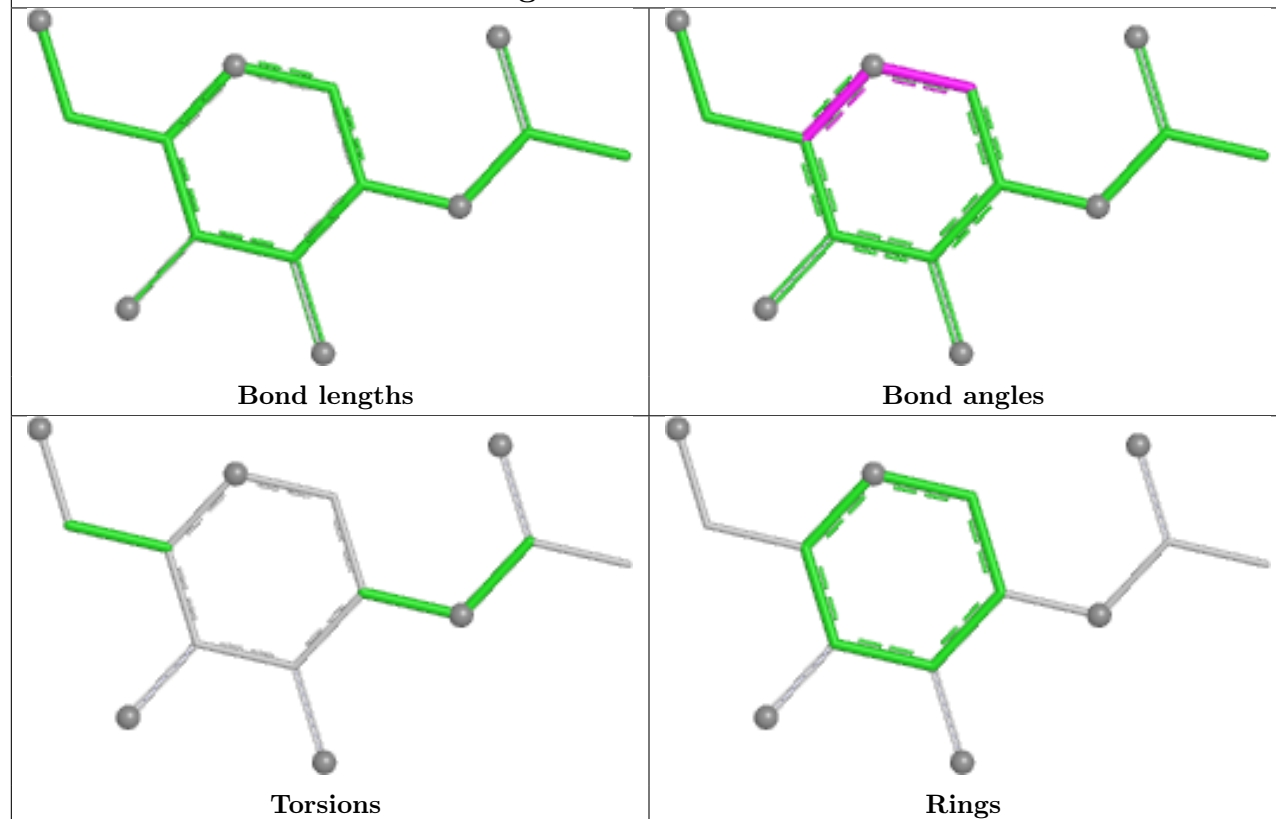
Ligand NAG C 1505



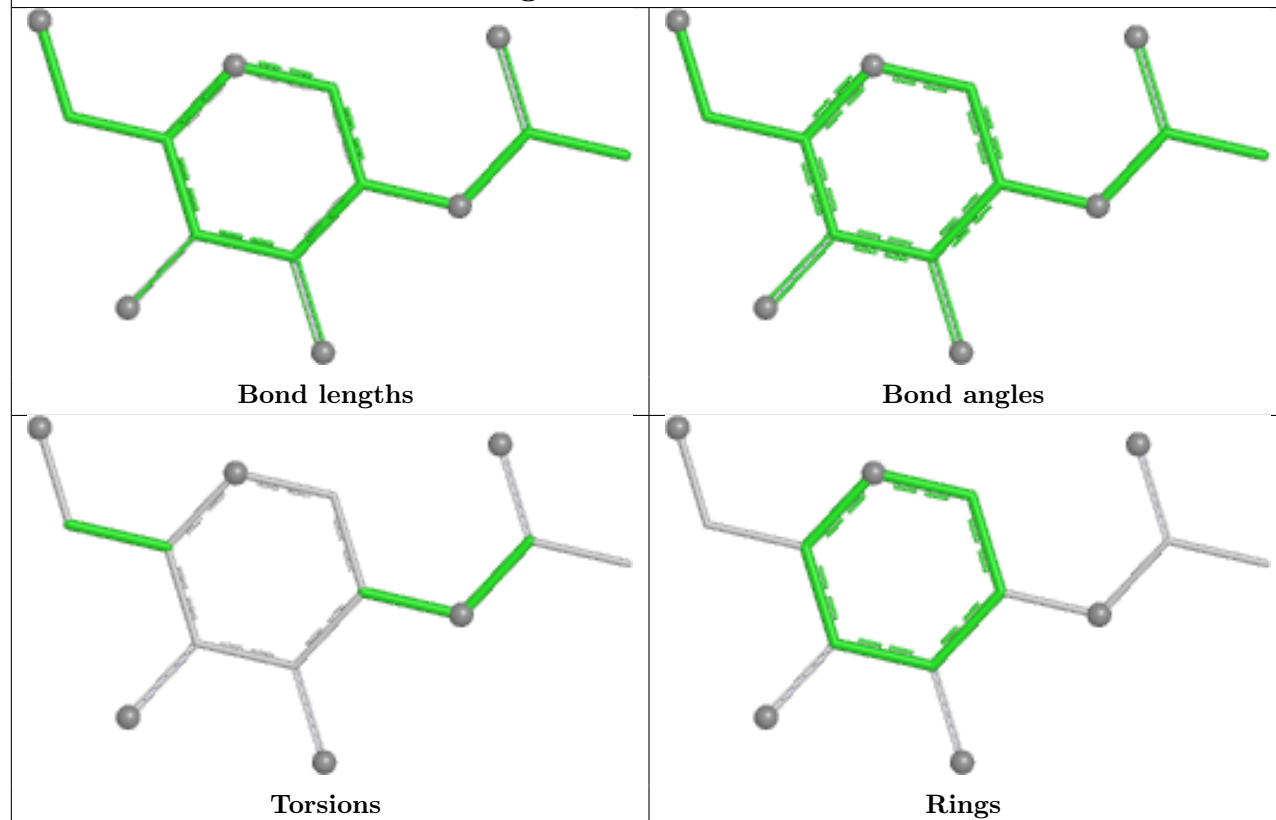




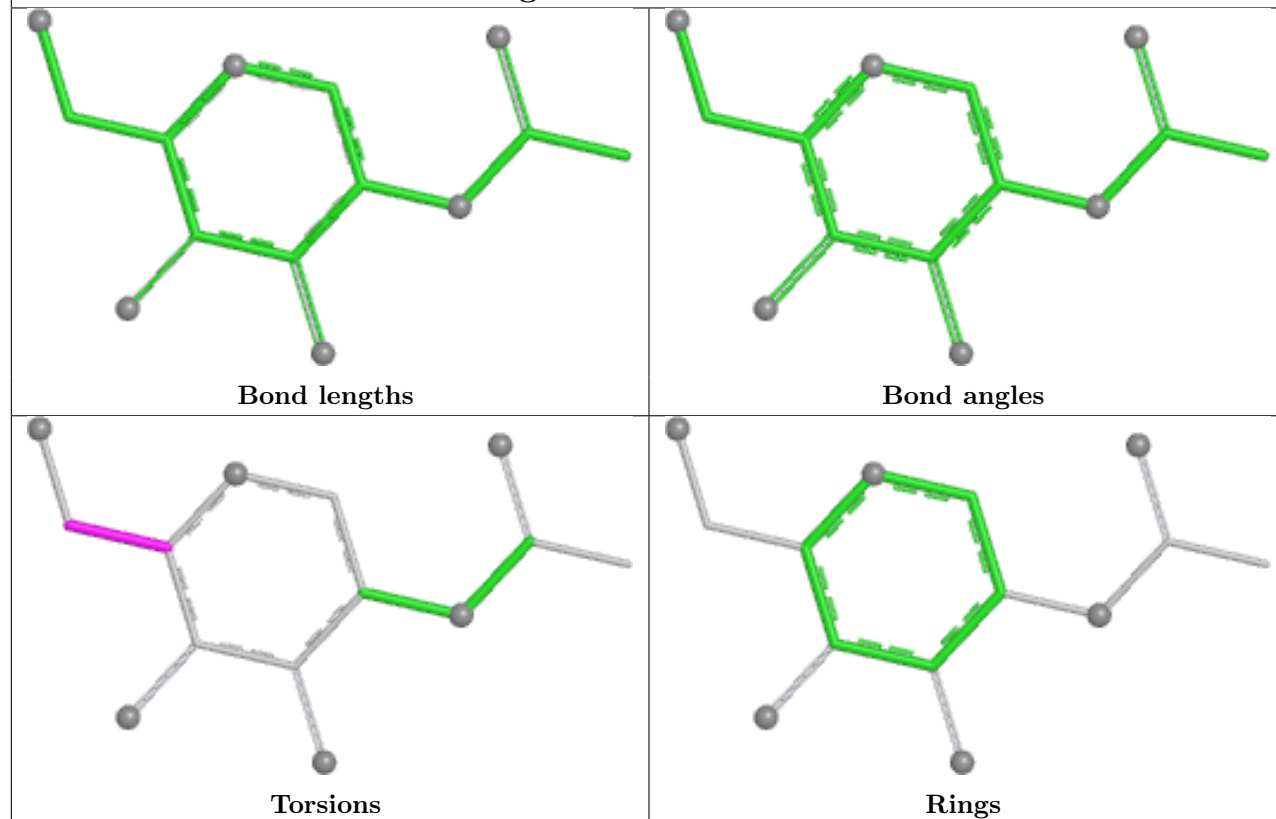
Ligand NAG A 1505



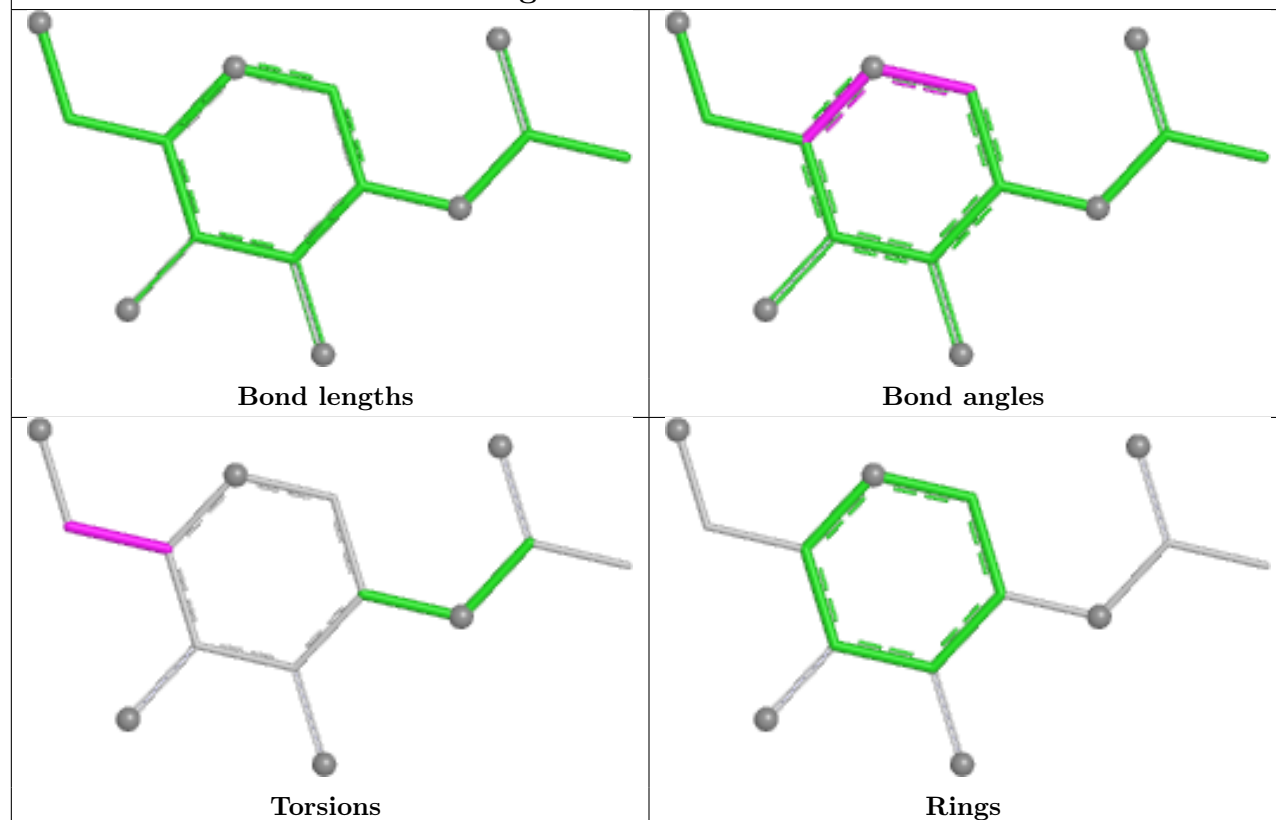
Ligand NAG B 1501



Ligand NAG C 1501



Ligand NAG C 1503



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.

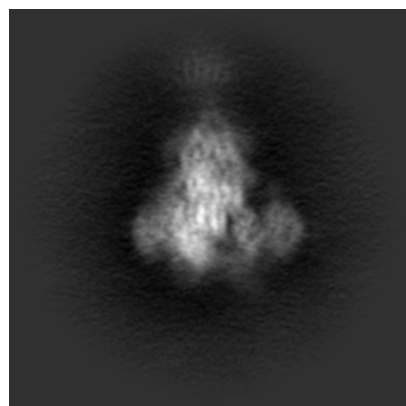
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33647. These allow visual inspection of the internal detail of the map and identification of artifacts.

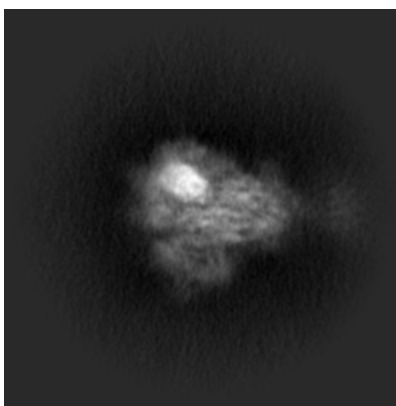
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

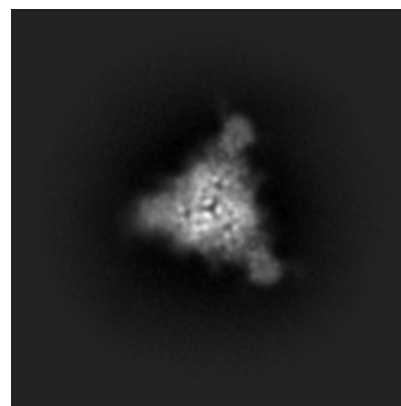
6.1.1 Primary map



X

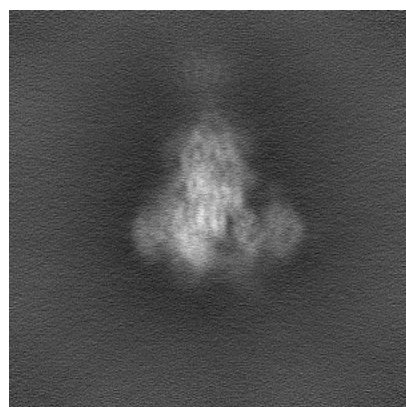


Y

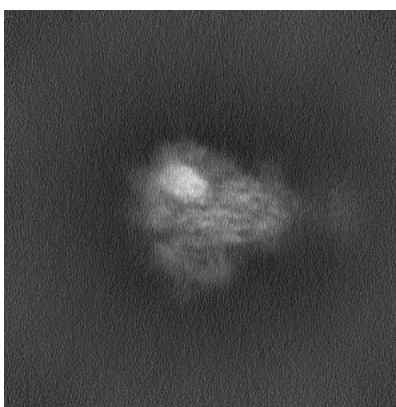


Z

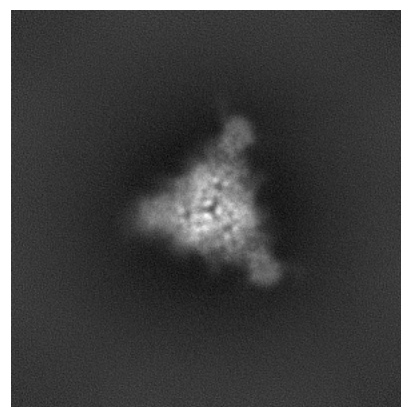
6.1.2 Raw map



X



Y

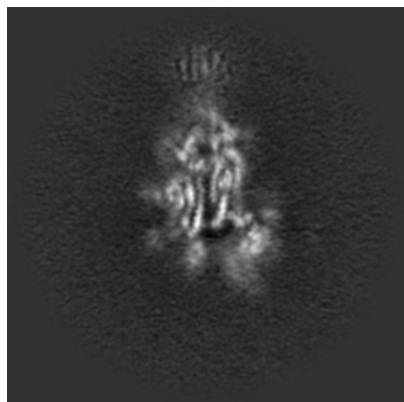


Z

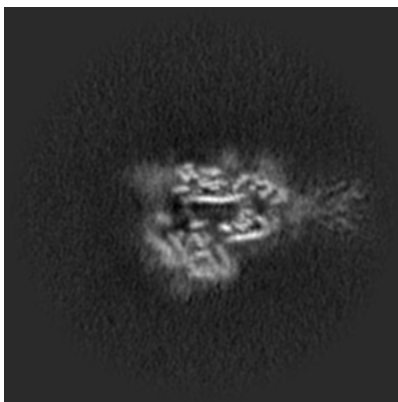
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

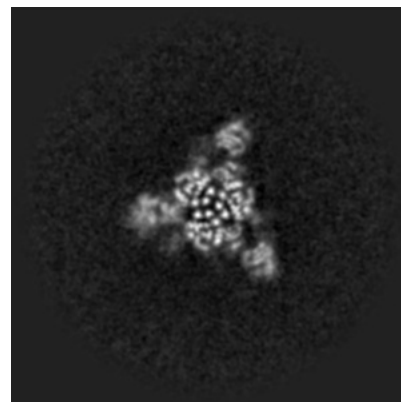
6.2.1 Primary map



X Index: 182

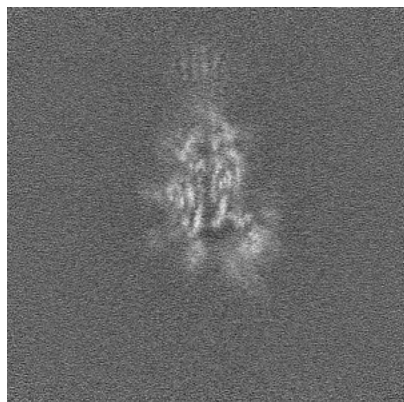


Y Index: 182



Z Index: 182

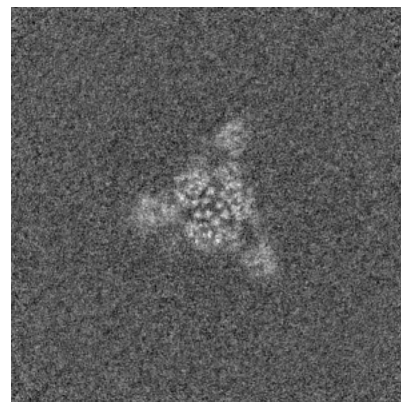
6.2.2 Raw map



X Index: 182



Y Index: 182

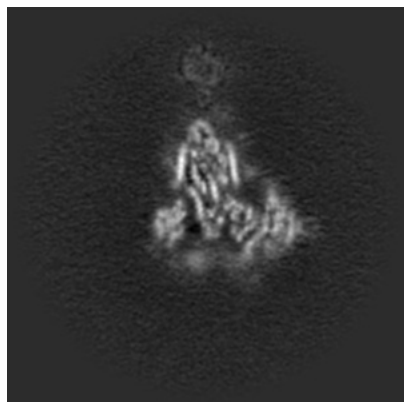


Z Index: 182

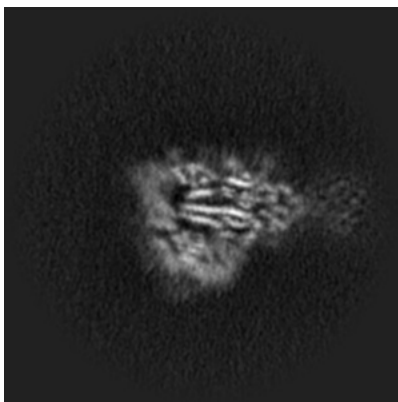
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

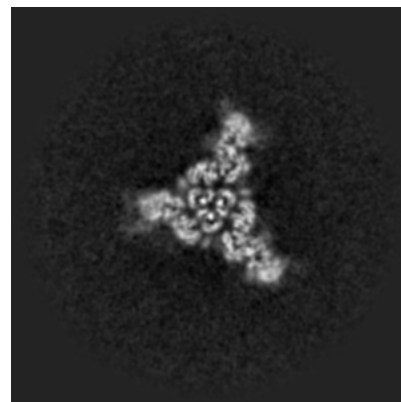
6.3.1 Primary map



X Index: 196

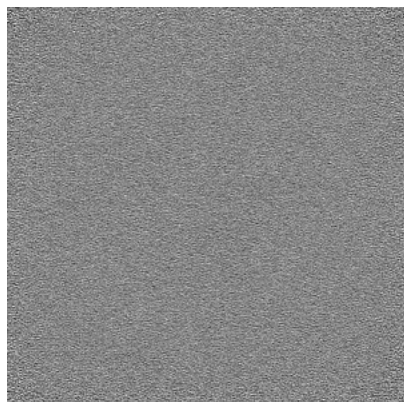


Y Index: 175

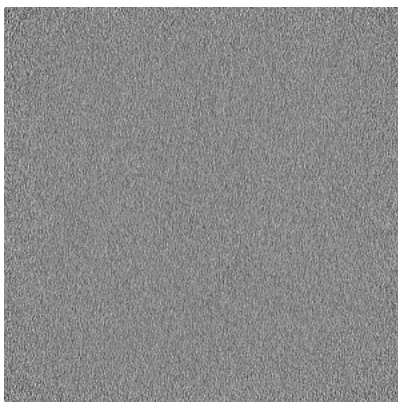


Z Index: 170

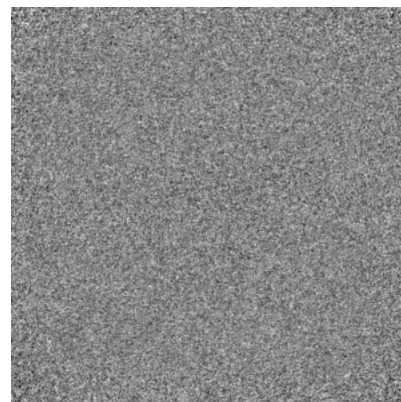
6.3.2 Raw map



X Index: 0



Y Index: 0

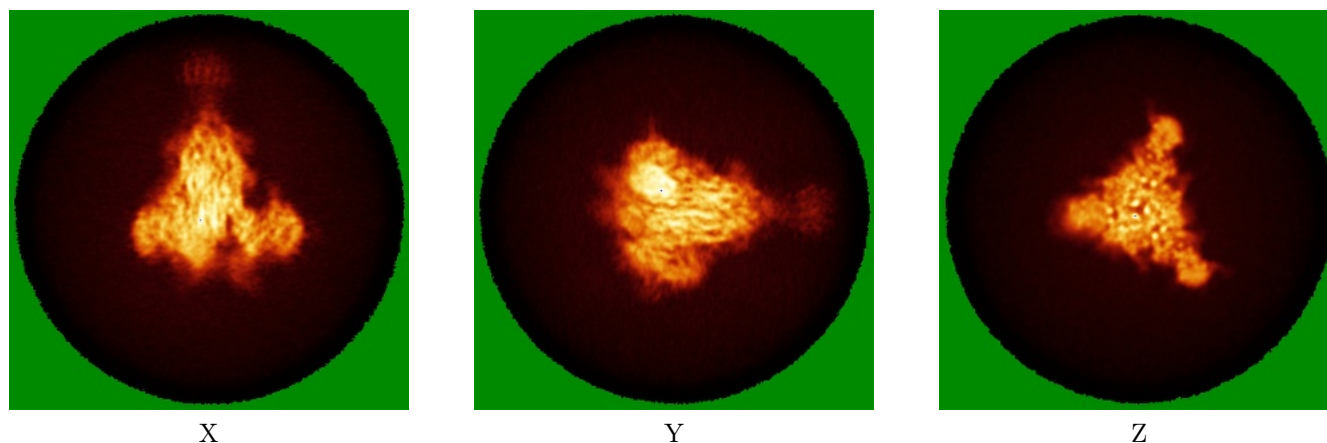


Z Index: 0

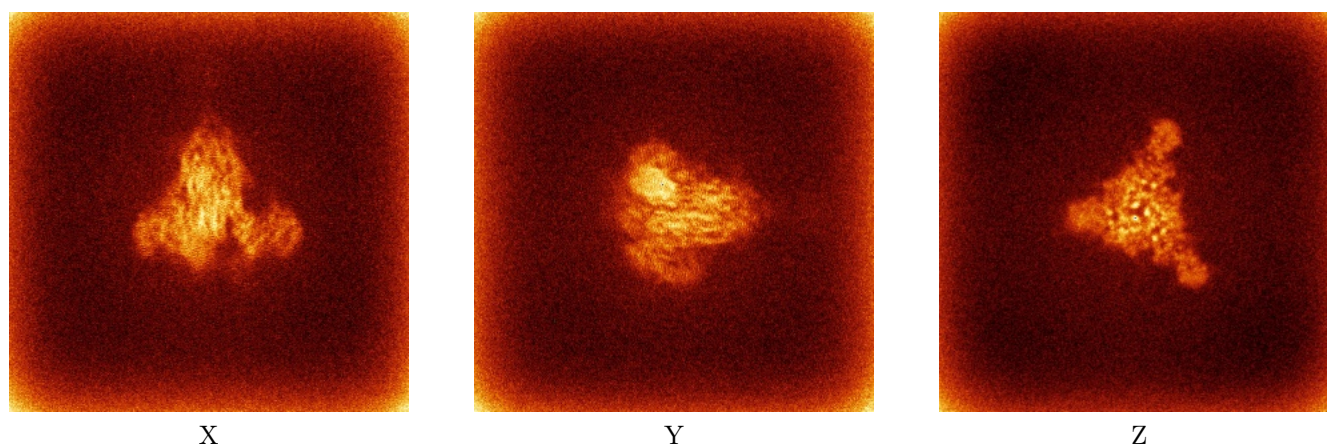
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

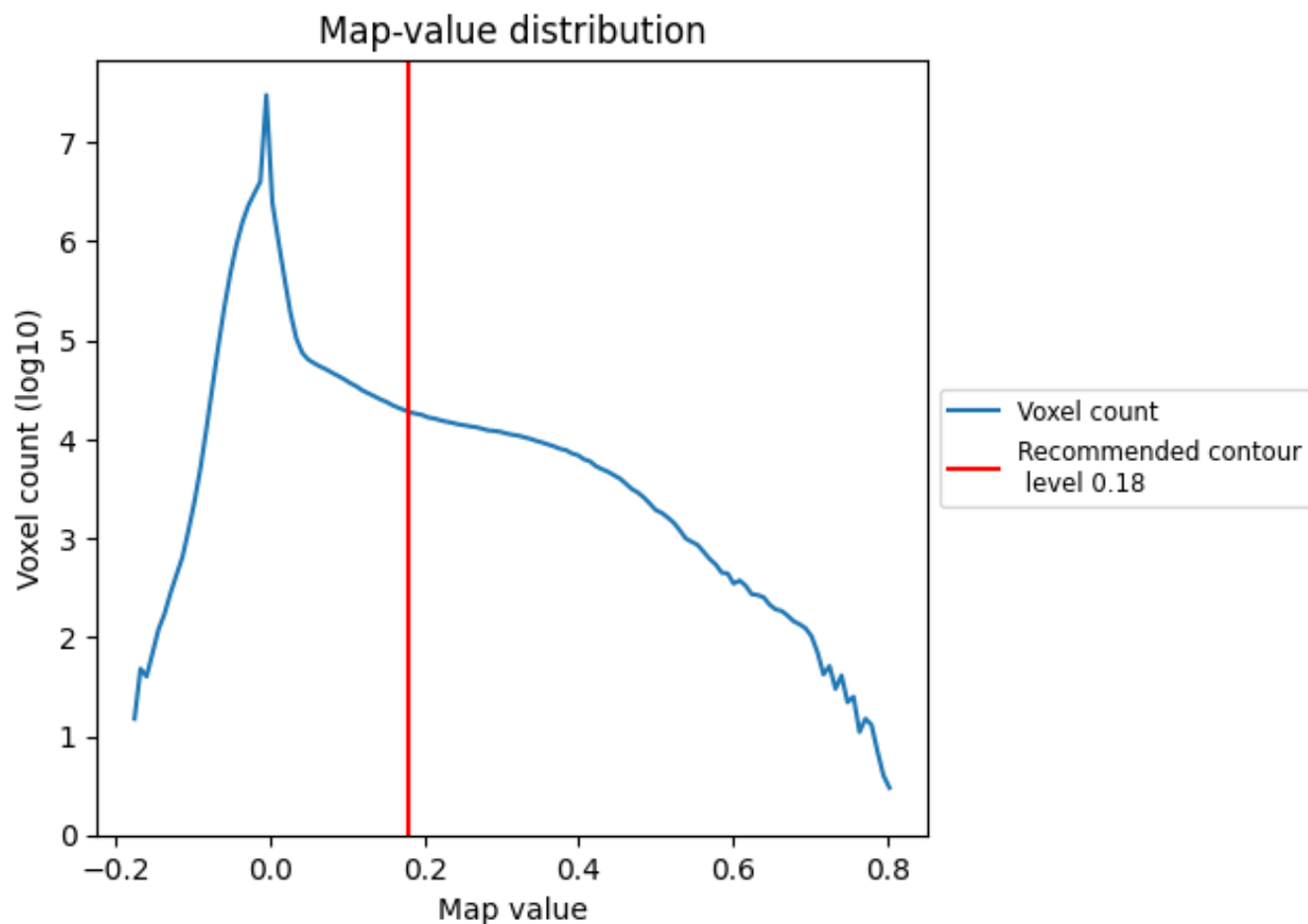
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

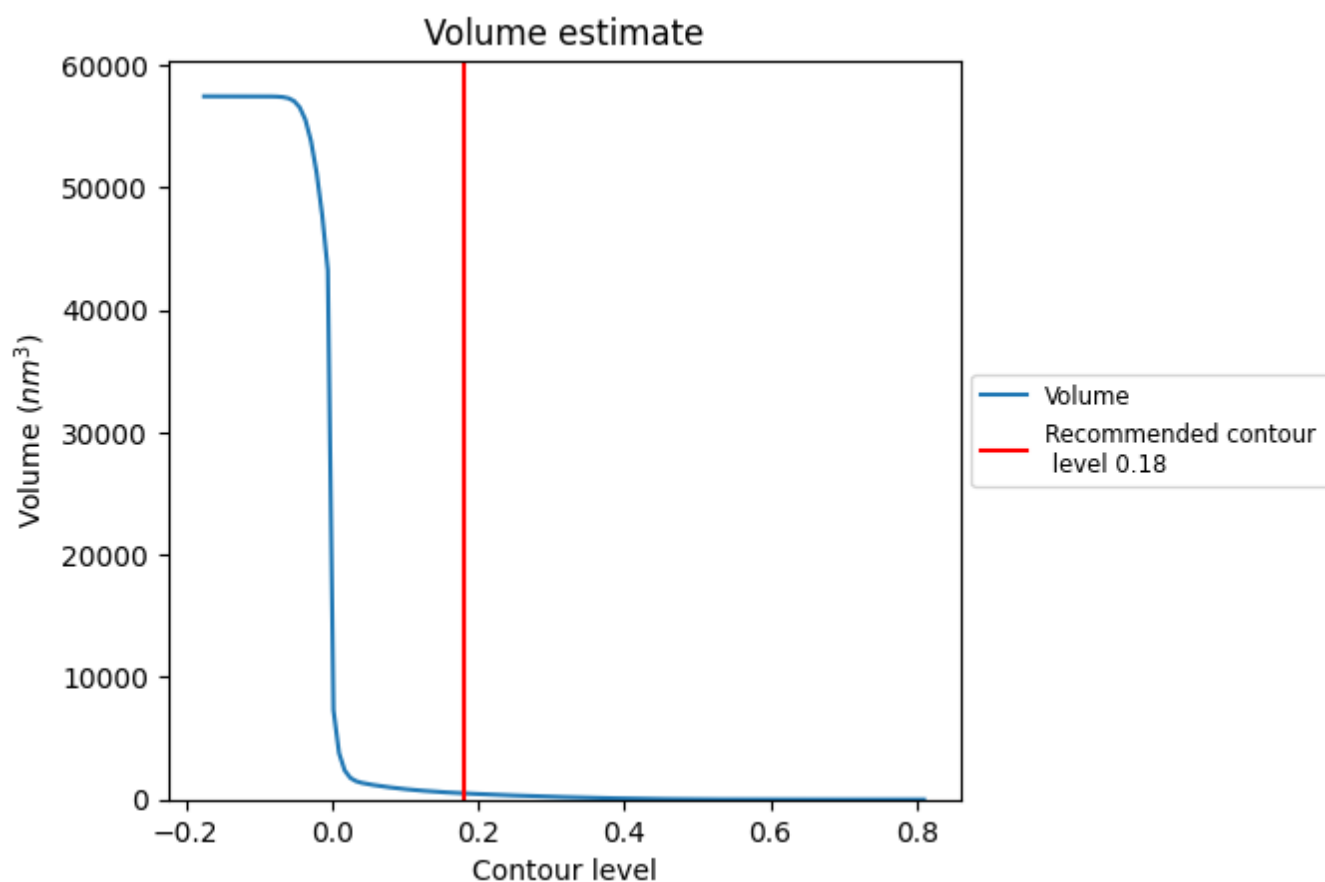
This section contains the results of statistical analysis of the map.

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.

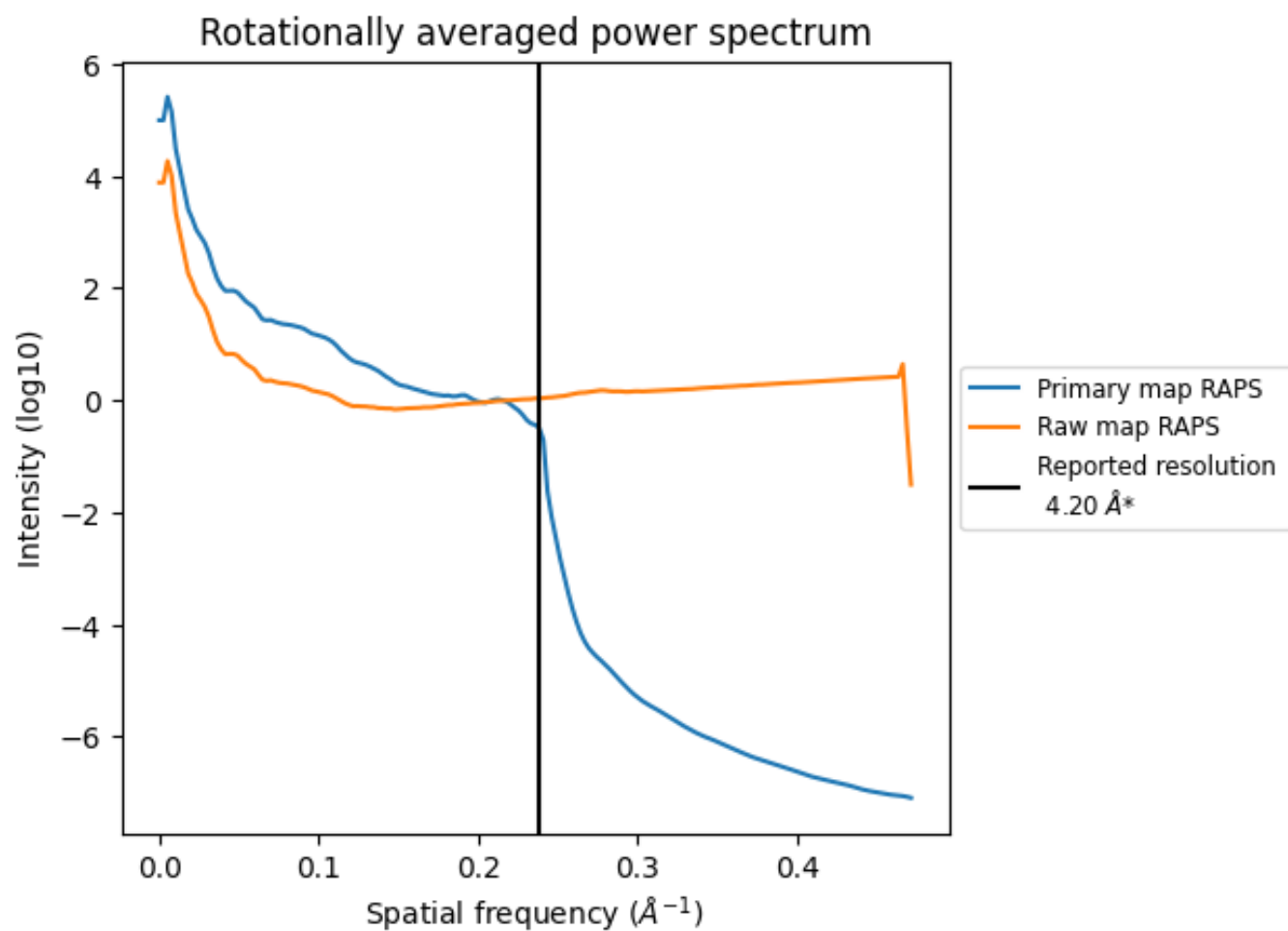
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 511 nm³; this corresponds to an approximate mass of 461 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 ⓘ

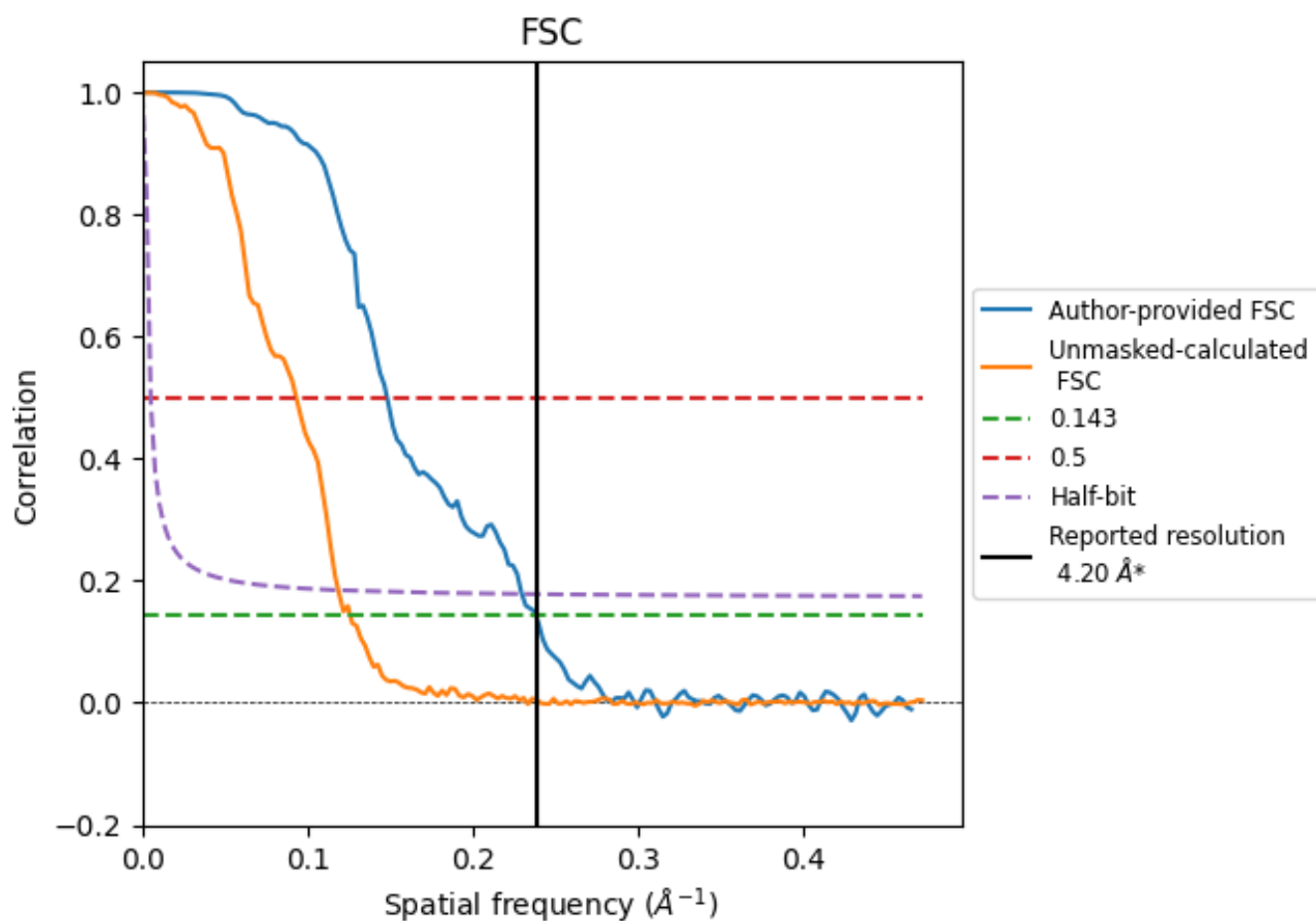


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

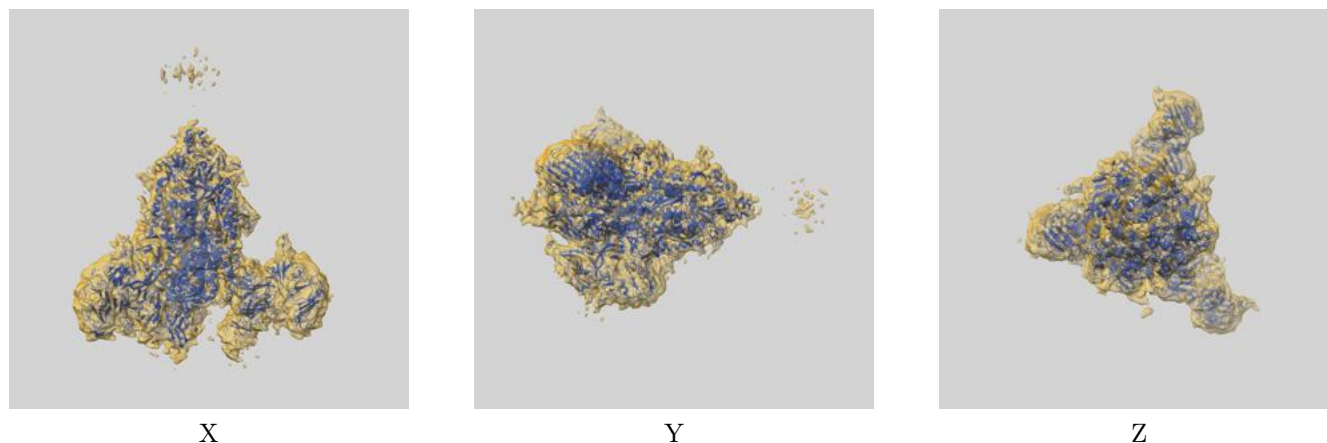
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	6.75	4.36
Unmasked-calculated*	7.95	10.74	8.43

*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 7.95 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

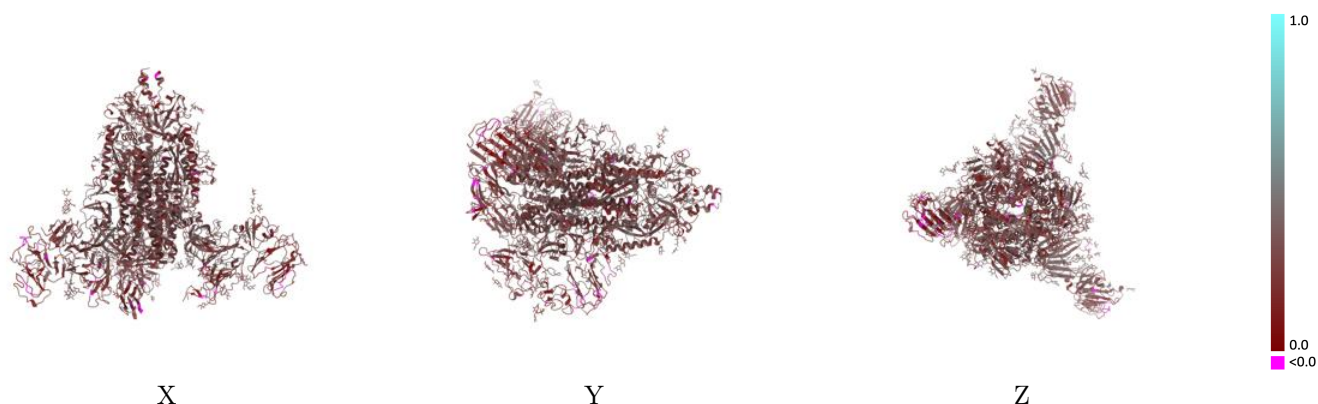
This section contains information regarding the fit between EMDB map EMD-33647 and PDB model 7Y6T. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.18 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](#)



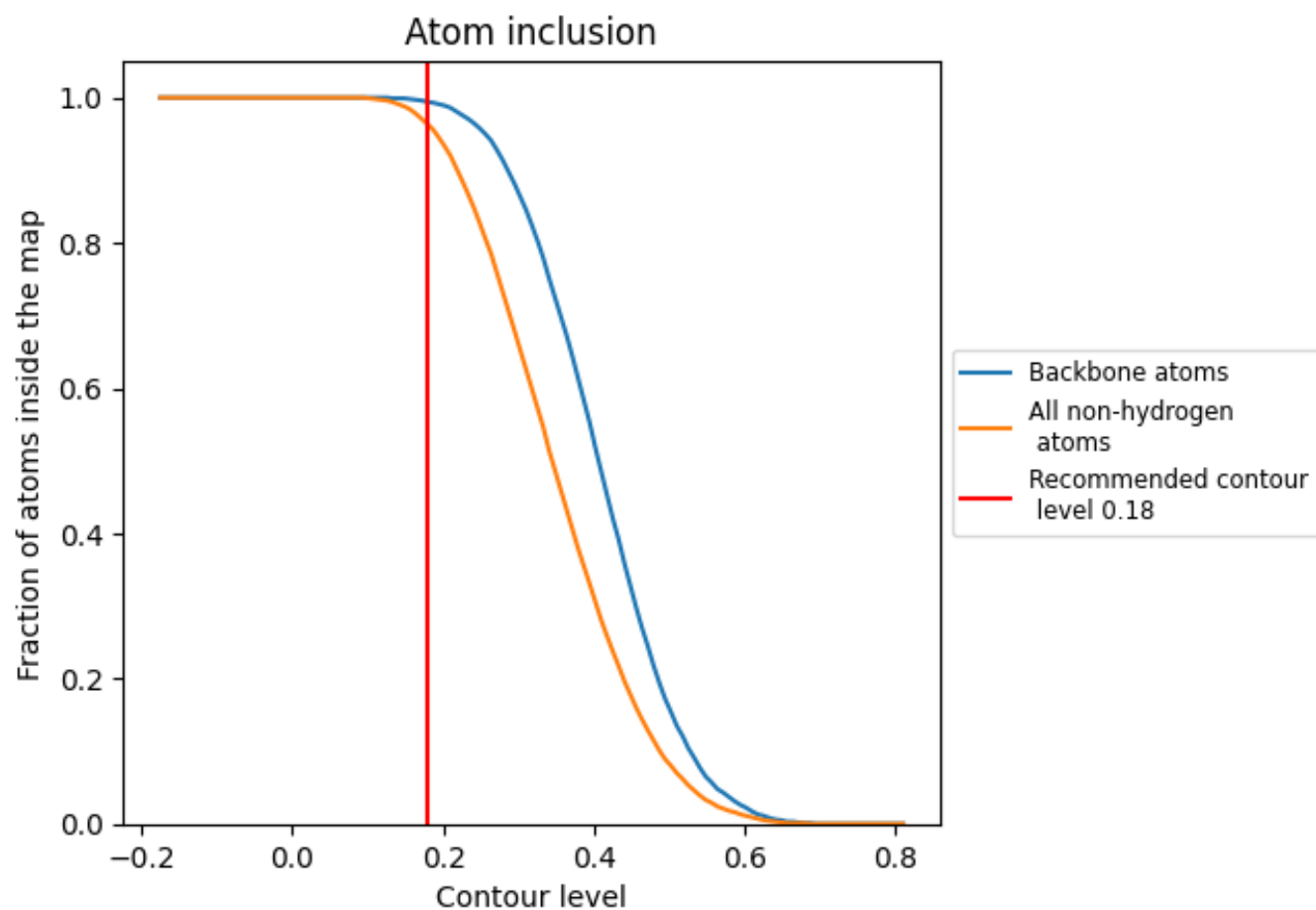
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.2640
A	 0.9590	 0.2440
B	 0.9670	 0.2670
C	 0.9650	 0.2740
D	 0.9840	 0.3490
E	 0.9490	 0.2130
F	 1.0000	 0.3190
G	 0.9740	 0.3540
H	 0.7860	 0.3230
I	 0.9640	 0.3110
J	 0.9290	 0.3290
K	 0.9740	 0.3700
L	 0.7860	 0.2950
M	 0.9740	 0.2390
N	 0.9390	 0.3040
O	 1.0000	 0.3950
P	 0.8750	 0.1870
Q	 0.9490	 0.3760
R	 0.9640	 0.3060
S	 0.9580	 0.2530
T	 0.9740	 0.3620
U	 1.0000	 0.3300
V	 0.9740	 0.3270
W	 0.8930	 0.3130
X	 0.9230	 0.2980
Y	 0.9640	 0.3150
Z	 0.8680	 0.3110
a	 0.9590	 0.3200
b	 1.0000	 0.4180
c	 0.7920	 0.2190
d	 0.9740	 0.3350
e	 0.9290	 0.2700
f	 0.8750	 0.2570
g	 0.9740	 0.3680
h	 1.0000	 0.3410



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Chain	Atom inclusion	Q-score
i	 1.0000	 0.3800
j	 0.9740	 0.3870
k	 0.8160	 0.2890