



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 09:11 PM EDT

PDB ID : 6NB3
EMDB ID : EMD-0401
Title : MERS-CoV complex with human neutralizing LCA60 antibody Fab fragment (state 1)
Authors : Walls, A.C.; Xiong, X.; Park, Y.J.; Tortorici, M.A.; Snijder, S.; Quispe, J.; Cameroni, E.; Gopal, R.; Mian, D.; Lanzavecchia, A.; Zambon, M.; Rey, F.A.; Corti, D.; Veeler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-12-06
Resolution : 3.50 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:

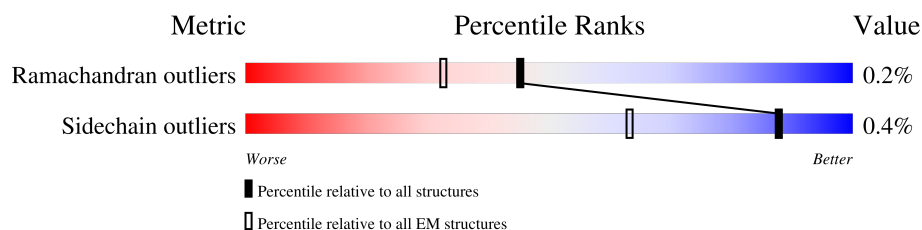
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.50 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1359	
1	B	1359	
1	C	1359	
2	E	109	
2	L	109	
3	D	127	
3	H	127	
4	F	2	
4	S	2	

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Mol	Chain	Length	Quality of chain
4	T	2	100% 50% 50%
4	U	2	50% 100%
4	X	2	50% 100%
4	f	2	100% 100%
4	h	2	50% 100%
4	i	2	50% 100%
4	l	2	50% 100%
4	r	2	100% 50% 50%
4	s	2	50% 100%
4	u	2	50% 100%
4	v	2	100% 100%
4	w	2	50% 100%
5	G	3	67% 100%
5	J	3	100% 100%
5	O	3	67% 100%
5	R	3	67% 67% 33%
5	V	3	67% 100%
5	Y	3	100% 67% 33%
5	a	3	100% 100%
5	e	3	67% 100%
5	g	3	100% 100%
5	j	3	67% 33% 67%
5	m	3	100% 33% 67%
5	o	3	100% 33% 67%
5	p	3	100% 100%

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Mol	Chain	Length	Quality of chain
5	t	3	
5	x	3	
6	I	6	
6	K	6	
6	M	6	
6	P	6	
6	Z	6	
6	b	6	
6	c	6	
6	n	6	
7	N	5	
7	W	5	
7	d	5	
7	k	5	
7	y	5	
8	Q	4	
9	q	5	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 30960 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	1169	Total	C	N	O	S	0	0
			9032	5739	1491	1752	50		
1	B	958	Total	C	N	O	S	0	0
			7402	4701	1232	1430	39		
1	C	1169	Total	C	N	O	S	0	0
			9032	5739	1491	1752	50		

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A0A140AYW5
A	-12	GLY	-	expression tag	UNP A0A140AYW5
A	-11	ILE	-	expression tag	UNP A0A140AYW5
A	-10	LEU	-	expression tag	UNP A0A140AYW5
A	-9	PRO	-	expression tag	UNP A0A140AYW5
A	-8	SER	-	expression tag	UNP A0A140AYW5
A	-7	PRO	-	expression tag	UNP A0A140AYW5
A	-6	GLY	-	expression tag	UNP A0A140AYW5
A	-5	MET	-	expression tag	UNP A0A140AYW5
A	-4	PRO	-	expression tag	UNP A0A140AYW5
A	-3	ALA	-	expression tag	UNP A0A140AYW5
A	-2	LEU	-	expression tag	UNP A0A140AYW5
A	-1	LEU	-	expression tag	UNP A0A140AYW5
A	0	SER	-	expression tag	UNP A0A140AYW5
A	1	LEU	-	expression tag	UNP A0A140AYW5
A	2	VAL	-	expression tag	UNP A0A140AYW5
A	3	SER	-	expression tag	UNP A0A140AYW5
A	4	LEU	-	expression tag	UNP A0A140AYW5
A	5	LEU	-	expression tag	UNP A0A140AYW5
A	6	SER	-	expression tag	UNP A0A140AYW5
A	7	VAL	-	expression tag	UNP A0A140AYW5
A	8	LEU	-	expression tag	UNP A0A140AYW5
A	9	LEU	-	expression tag	UNP A0A140AYW5
A	10	MET	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP A0A140AYW5
A	12	CYS	-	expression tag	UNP A0A140AYW5
A	13	VAL	-	expression tag	UNP A0A140AYW5
A	14	ALA	-	expression tag	UNP A0A140AYW5
A	15	GLU	-	expression tag	UNP A0A140AYW5
A	16	THR	-	expression tag	UNP A0A140AYW5
A	17	GLY	-	expression tag	UNP A0A140AYW5
A	18	THR	-	expression tag	UNP A0A140AYW5
A	529	ILE	THR	conflict	UNP A0A140AYW5
A	748	ALA	ARG	conflict	UNP A0A140AYW5
A	751	GLY	ARG	conflict	UNP A0A140AYW5
A	1020	GLN	ARG	conflict	UNP A0A140AYW5
A	1060	PRO	VAL	conflict	UNP A0A140AYW5
A	1061	PRO	LEU	conflict	UNP A0A140AYW5
A	1295	GLY	-	expression tag	UNP A0A140AYW5
A	1296	SER	-	expression tag	UNP A0A140AYW5
A	1297	GLY	-	expression tag	UNP A0A140AYW5
A	1298	ARG	-	expression tag	UNP A0A140AYW5
A	1299	GLU	-	expression tag	UNP A0A140AYW5
A	1300	ASN	-	expression tag	UNP A0A140AYW5
A	1301	LEU	-	expression tag	UNP A0A140AYW5
A	1302	TYR	-	expression tag	UNP A0A140AYW5
A	1303	PHE	-	expression tag	UNP A0A140AYW5
A	1304	GLN	-	expression tag	UNP A0A140AYW5
A	1305	GLY	-	expression tag	UNP A0A140AYW5
A	1306	GLY	-	expression tag	UNP A0A140AYW5
A	1307	GLY	-	expression tag	UNP A0A140AYW5
A	1308	GLY	-	expression tag	UNP A0A140AYW5
A	1309	SER	-	expression tag	UNP A0A140AYW5
A	1310	GLY	-	expression tag	UNP A0A140AYW5
A	1311	TYR	-	expression tag	UNP A0A140AYW5
A	1312	ILE	-	expression tag	UNP A0A140AYW5
A	1313	PRO	-	expression tag	UNP A0A140AYW5
A	1314	GLU	-	expression tag	UNP A0A140AYW5
A	1315	ALA	-	expression tag	UNP A0A140AYW5
A	1316	PRO	-	expression tag	UNP A0A140AYW5
A	1317	ARG	-	expression tag	UNP A0A140AYW5
A	1318	ASP	-	expression tag	UNP A0A140AYW5
A	1319	GLY	-	expression tag	UNP A0A140AYW5
A	1320	GLN	-	expression tag	UNP A0A140AYW5
A	1321	ALA	-	expression tag	UNP A0A140AYW5
A	1322	TYR	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1323	VAL	-	expression tag	UNP A0A140AYW5
A	1324	ARG	-	expression tag	UNP A0A140AYW5
A	1325	LYS	-	expression tag	UNP A0A140AYW5
A	1326	ASP	-	expression tag	UNP A0A140AYW5
A	1327	GLY	-	expression tag	UNP A0A140AYW5
A	1328	GLU	-	expression tag	UNP A0A140AYW5
A	1329	TRP	-	expression tag	UNP A0A140AYW5
A	1330	VAL	-	expression tag	UNP A0A140AYW5
A	1331	LEU	-	expression tag	UNP A0A140AYW5
A	1332	LEU	-	expression tag	UNP A0A140AYW5
A	1333	SER	-	expression tag	UNP A0A140AYW5
A	1334	THR	-	expression tag	UNP A0A140AYW5
A	1335	PHE	-	expression tag	UNP A0A140AYW5
A	1336	LEU	-	expression tag	UNP A0A140AYW5
A	1337	GLY	-	expression tag	UNP A0A140AYW5
A	1338	HIS	-	expression tag	UNP A0A140AYW5
A	1339	HIS	-	expression tag	UNP A0A140AYW5
A	1340	HIS	-	expression tag	UNP A0A140AYW5
A	1341	HIS	-	expression tag	UNP A0A140AYW5
A	1342	HIS	-	expression tag	UNP A0A140AYW5
A	1343	HIS	-	expression tag	UNP A0A140AYW5
A	1344	HIS	-	expression tag	UNP A0A140AYW5
A	1345	HIS	-	expression tag	UNP A0A140AYW5
B	-13	MET	-	initiating methionine	UNP A0A140AYW5
B	-12	GLY	-	expression tag	UNP A0A140AYW5
B	-11	ILE	-	expression tag	UNP A0A140AYW5
B	-10	LEU	-	expression tag	UNP A0A140AYW5
B	-9	PRO	-	expression tag	UNP A0A140AYW5
B	-8	SER	-	expression tag	UNP A0A140AYW5
B	-7	PRO	-	expression tag	UNP A0A140AYW5
B	-6	GLY	-	expression tag	UNP A0A140AYW5
B	-5	MET	-	expression tag	UNP A0A140AYW5
B	-4	PRO	-	expression tag	UNP A0A140AYW5
B	-3	ALA	-	expression tag	UNP A0A140AYW5
B	-2	LEU	-	expression tag	UNP A0A140AYW5
B	-1	LEU	-	expression tag	UNP A0A140AYW5
B	0	SER	-	expression tag	UNP A0A140AYW5
B	1	LEU	-	expression tag	UNP A0A140AYW5
B	2	VAL	-	expression tag	UNP A0A140AYW5
B	3	SER	-	expression tag	UNP A0A140AYW5
B	4	LEU	-	expression tag	UNP A0A140AYW5
B	5	LEU	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A0A140AYW5
B	7	VAL	-	expression tag	UNP A0A140AYW5
B	8	LEU	-	expression tag	UNP A0A140AYW5
B	9	LEU	-	expression tag	UNP A0A140AYW5
B	10	MET	-	expression tag	UNP A0A140AYW5
B	11	GLY	-	expression tag	UNP A0A140AYW5
B	12	CYS	-	expression tag	UNP A0A140AYW5
B	13	VAL	-	expression tag	UNP A0A140AYW5
B	14	ALA	-	expression tag	UNP A0A140AYW5
B	15	GLU	-	expression tag	UNP A0A140AYW5
B	16	THR	-	expression tag	UNP A0A140AYW5
B	17	GLY	-	expression tag	UNP A0A140AYW5
B	18	THR	-	expression tag	UNP A0A140AYW5
B	529	ILE	THR	conflict	UNP A0A140AYW5
B	748	ALA	ARG	conflict	UNP A0A140AYW5
B	751	GLY	ARG	conflict	UNP A0A140AYW5
B	1020	GLN	ARG	conflict	UNP A0A140AYW5
B	1060	PRO	VAL	conflict	UNP A0A140AYW5
B	1061	PRO	LEU	conflict	UNP A0A140AYW5
B	1295	GLY	-	expression tag	UNP A0A140AYW5
B	1296	SER	-	expression tag	UNP A0A140AYW5
B	1297	GLY	-	expression tag	UNP A0A140AYW5
B	1298	ARG	-	expression tag	UNP A0A140AYW5
B	1299	GLU	-	expression tag	UNP A0A140AYW5
B	1300	ASN	-	expression tag	UNP A0A140AYW5
B	1301	LEU	-	expression tag	UNP A0A140AYW5
B	1302	TYR	-	expression tag	UNP A0A140AYW5
B	1303	PHE	-	expression tag	UNP A0A140AYW5
B	1304	GLN	-	expression tag	UNP A0A140AYW5
B	1305	GLY	-	expression tag	UNP A0A140AYW5
B	1306	GLY	-	expression tag	UNP A0A140AYW5
B	1307	GLY	-	expression tag	UNP A0A140AYW5
B	1308	GLY	-	expression tag	UNP A0A140AYW5
B	1309	SER	-	expression tag	UNP A0A140AYW5
B	1310	GLY	-	expression tag	UNP A0A140AYW5
B	1311	TYR	-	expression tag	UNP A0A140AYW5
B	1312	ILE	-	expression tag	UNP A0A140AYW5
B	1313	PRO	-	expression tag	UNP A0A140AYW5
B	1314	GLU	-	expression tag	UNP A0A140AYW5
B	1315	ALA	-	expression tag	UNP A0A140AYW5
B	1316	PRO	-	expression tag	UNP A0A140AYW5
B	1317	ARG	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1318	ASP	-	expression tag	UNP A0A140AYW5
B	1319	GLY	-	expression tag	UNP A0A140AYW5
B	1320	GLN	-	expression tag	UNP A0A140AYW5
B	1321	ALA	-	expression tag	UNP A0A140AYW5
B	1322	TYR	-	expression tag	UNP A0A140AYW5
B	1323	VAL	-	expression tag	UNP A0A140AYW5
B	1324	ARG	-	expression tag	UNP A0A140AYW5
B	1325	LYS	-	expression tag	UNP A0A140AYW5
B	1326	ASP	-	expression tag	UNP A0A140AYW5
B	1327	GLY	-	expression tag	UNP A0A140AYW5
B	1328	GLU	-	expression tag	UNP A0A140AYW5
B	1329	TRP	-	expression tag	UNP A0A140AYW5
B	1330	VAL	-	expression tag	UNP A0A140AYW5
B	1331	LEU	-	expression tag	UNP A0A140AYW5
B	1332	LEU	-	expression tag	UNP A0A140AYW5
B	1333	SER	-	expression tag	UNP A0A140AYW5
B	1334	THR	-	expression tag	UNP A0A140AYW5
B	1335	PHE	-	expression tag	UNP A0A140AYW5
B	1336	LEU	-	expression tag	UNP A0A140AYW5
B	1337	GLY	-	expression tag	UNP A0A140AYW5
B	1338	HIS	-	expression tag	UNP A0A140AYW5
B	1339	HIS	-	expression tag	UNP A0A140AYW5
B	1340	HIS	-	expression tag	UNP A0A140AYW5
B	1341	HIS	-	expression tag	UNP A0A140AYW5
B	1342	HIS	-	expression tag	UNP A0A140AYW5
B	1343	HIS	-	expression tag	UNP A0A140AYW5
B	1344	HIS	-	expression tag	UNP A0A140AYW5
B	1345	HIS	-	expression tag	UNP A0A140AYW5
C	-13	MET	-	initiating methionine	UNP A0A140AYW5
C	-12	GLY	-	expression tag	UNP A0A140AYW5
C	-11	ILE	-	expression tag	UNP A0A140AYW5
C	-10	LEU	-	expression tag	UNP A0A140AYW5
C	-9	PRO	-	expression tag	UNP A0A140AYW5
C	-8	SER	-	expression tag	UNP A0A140AYW5
C	-7	PRO	-	expression tag	UNP A0A140AYW5
C	-6	GLY	-	expression tag	UNP A0A140AYW5
C	-5	MET	-	expression tag	UNP A0A140AYW5
C	-4	PRO	-	expression tag	UNP A0A140AYW5
C	-3	ALA	-	expression tag	UNP A0A140AYW5
C	-2	LEU	-	expression tag	UNP A0A140AYW5
C	-1	LEU	-	expression tag	UNP A0A140AYW5
C	0	SER	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	LEU	-	expression tag	UNP A0A140AYW5
C	2	VAL	-	expression tag	UNP A0A140AYW5
C	3	SER	-	expression tag	UNP A0A140AYW5
C	4	LEU	-	expression tag	UNP A0A140AYW5
C	5	LEU	-	expression tag	UNP A0A140AYW5
C	6	SER	-	expression tag	UNP A0A140AYW5
C	7	VAL	-	expression tag	UNP A0A140AYW5
C	8	LEU	-	expression tag	UNP A0A140AYW5
C	9	LEU	-	expression tag	UNP A0A140AYW5
C	10	MET	-	expression tag	UNP A0A140AYW5
C	11	GLY	-	expression tag	UNP A0A140AYW5
C	12	CYS	-	expression tag	UNP A0A140AYW5
C	13	VAL	-	expression tag	UNP A0A140AYW5
C	14	ALA	-	expression tag	UNP A0A140AYW5
C	15	GLU	-	expression tag	UNP A0A140AYW5
C	16	THR	-	expression tag	UNP A0A140AYW5
C	17	GLY	-	expression tag	UNP A0A140AYW5
C	18	THR	-	expression tag	UNP A0A140AYW5
C	529	ILE	THR	conflict	UNP A0A140AYW5
C	748	ALA	ARG	conflict	UNP A0A140AYW5
C	751	GLY	ARG	conflict	UNP A0A140AYW5
C	1020	GLN	ARG	conflict	UNP A0A140AYW5
C	1060	PRO	VAL	conflict	UNP A0A140AYW5
C	1061	PRO	LEU	conflict	UNP A0A140AYW5
C	1295	GLY	-	expression tag	UNP A0A140AYW5
C	1296	SER	-	expression tag	UNP A0A140AYW5
C	1297	GLY	-	expression tag	UNP A0A140AYW5
C	1298	ARG	-	expression tag	UNP A0A140AYW5
C	1299	GLU	-	expression tag	UNP A0A140AYW5
C	1300	ASN	-	expression tag	UNP A0A140AYW5
C	1301	LEU	-	expression tag	UNP A0A140AYW5
C	1302	TYR	-	expression tag	UNP A0A140AYW5
C	1303	PHE	-	expression tag	UNP A0A140AYW5
C	1304	GLN	-	expression tag	UNP A0A140AYW5
C	1305	GLY	-	expression tag	UNP A0A140AYW5
C	1306	GLY	-	expression tag	UNP A0A140AYW5
C	1307	GLY	-	expression tag	UNP A0A140AYW5
C	1308	GLY	-	expression tag	UNP A0A140AYW5
C	1309	SER	-	expression tag	UNP A0A140AYW5
C	1310	GLY	-	expression tag	UNP A0A140AYW5
C	1311	TYR	-	expression tag	UNP A0A140AYW5
C	1312	ILE	-	expression tag	UNP A0A140AYW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1313	PRO	-	expression tag	UNP A0A140AYW5
C	1314	GLU	-	expression tag	UNP A0A140AYW5
C	1315	ALA	-	expression tag	UNP A0A140AYW5
C	1316	PRO	-	expression tag	UNP A0A140AYW5
C	1317	ARG	-	expression tag	UNP A0A140AYW5
C	1318	ASP	-	expression tag	UNP A0A140AYW5
C	1319	GLY	-	expression tag	UNP A0A140AYW5
C	1320	GLN	-	expression tag	UNP A0A140AYW5
C	1321	ALA	-	expression tag	UNP A0A140AYW5
C	1322	TYR	-	expression tag	UNP A0A140AYW5
C	1323	VAL	-	expression tag	UNP A0A140AYW5
C	1324	ARG	-	expression tag	UNP A0A140AYW5
C	1325	LYS	-	expression tag	UNP A0A140AYW5
C	1326	ASP	-	expression tag	UNP A0A140AYW5
C	1327	GLY	-	expression tag	UNP A0A140AYW5
C	1328	GLU	-	expression tag	UNP A0A140AYW5
C	1329	TRP	-	expression tag	UNP A0A140AYW5
C	1330	VAL	-	expression tag	UNP A0A140AYW5
C	1331	LEU	-	expression tag	UNP A0A140AYW5
C	1332	LEU	-	expression tag	UNP A0A140AYW5
C	1333	SER	-	expression tag	UNP A0A140AYW5
C	1334	THR	-	expression tag	UNP A0A140AYW5
C	1335	PHE	-	expression tag	UNP A0A140AYW5
C	1336	LEU	-	expression tag	UNP A0A140AYW5
C	1337	GLY	-	expression tag	UNP A0A140AYW5
C	1338	HIS	-	expression tag	UNP A0A140AYW5
C	1339	HIS	-	expression tag	UNP A0A140AYW5
C	1340	HIS	-	expression tag	UNP A0A140AYW5
C	1341	HIS	-	expression tag	UNP A0A140AYW5
C	1342	HIS	-	expression tag	UNP A0A140AYW5
C	1343	HIS	-	expression tag	UNP A0A140AYW5
C	1344	HIS	-	expression tag	UNP A0A140AYW5
C	1345	HIS	-	expression tag	UNP A0A140AYW5

- Molecule 2 is a protein called LCA60 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	107	Total 773	C 479	N 129	O 161	S 4	0	0
2	E	107	Total 773	C 479	N 129	O 161	S 4	0	0

- Molecule 3 is a protein called LCA60 heavy chain.

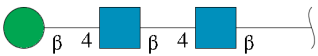
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	124	Total	C	N	O	S	0	0
			958	607	164	183	4		
3	D	123	Total	C	N	O	S	0	0
			951	602	163	182	4		

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



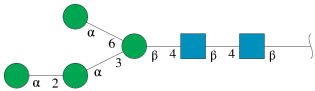
Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	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	s	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	v	2	Total	C	N	O	0	0
			28	16	2	10		
4	w	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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.



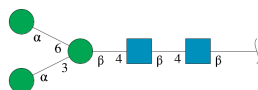
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	J	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	R	3	Total	C	N	O	0	0
			39	22	2	15		
5	V	3	Total	C	N	O	0	0
			39	22	2	15		
5	Y	3	Total	C	N	O	0	0
			39	22	2	15		
5	a	3	Total	C	N	O	0	0
			39	22	2	15		
5	e	3	Total	C	N	O	0	0
			39	22	2	15		
5	g	3	Total	C	N	O	0	0
			39	22	2	15		
5	j	3	Total	C	N	O	0	0
			39	22	2	15		
5	m	3	Total	C	N	O	0	0
			39	22	2	15		
5	o	3	Total	C	N	O	0	0
			39	22	2	15		
5	p	3	Total	C	N	O	0	0
			39	22	2	15		
5	t	3	Total	C	N	O	0	0
			39	22	2	15		
5	x	3	Total	C	N	O	0	0
			39	22	2	15		

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



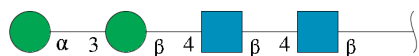
Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	6	Total	C	N	O	0	0
			72	40	2	30		
6	K	6	Total	C	N	O	0	0
			72	40	2	30		
6	M	6	Total	C	N	O	0	0
			72	40	2	30		
6	P	6	Total	C	N	O	0	0
			72	40	2	30		
6	Z	6	Total	C	N	O	0	0
			72	40	2	30		
6	b	6	Total	C	N	O	0	0
			72	40	2	30		
6	c	6	Total	C	N	O	0	0
			72	40	2	30		
6	n	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 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.



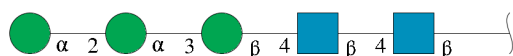
Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	5	Total	C	N	O	0	0
			61	34	2	25		
7	W	5	Total	C	N	O	0	0
			61	34	2	25		
7	d	5	Total	C	N	O	0	0
			61	34	2	25		
7	k	5	Total	C	N	O	0	0
			61	34	2	25		
7	y	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



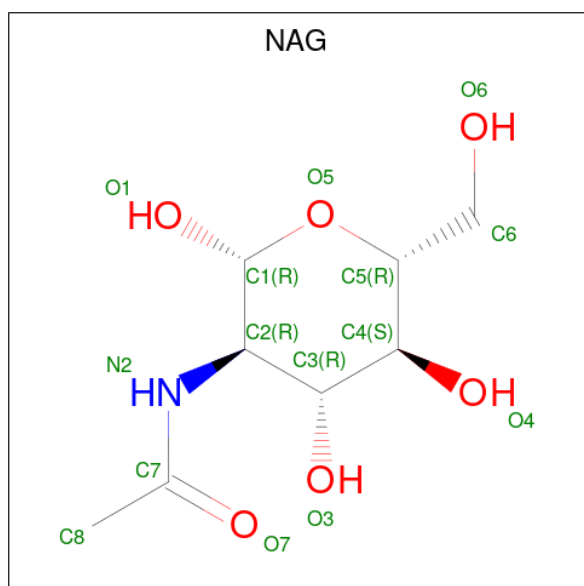
Mol	Chain	Residues	Atoms				AltConf	Trace
8	Q	4	Total	C	N	O	0	0
			50	28	2	20		

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



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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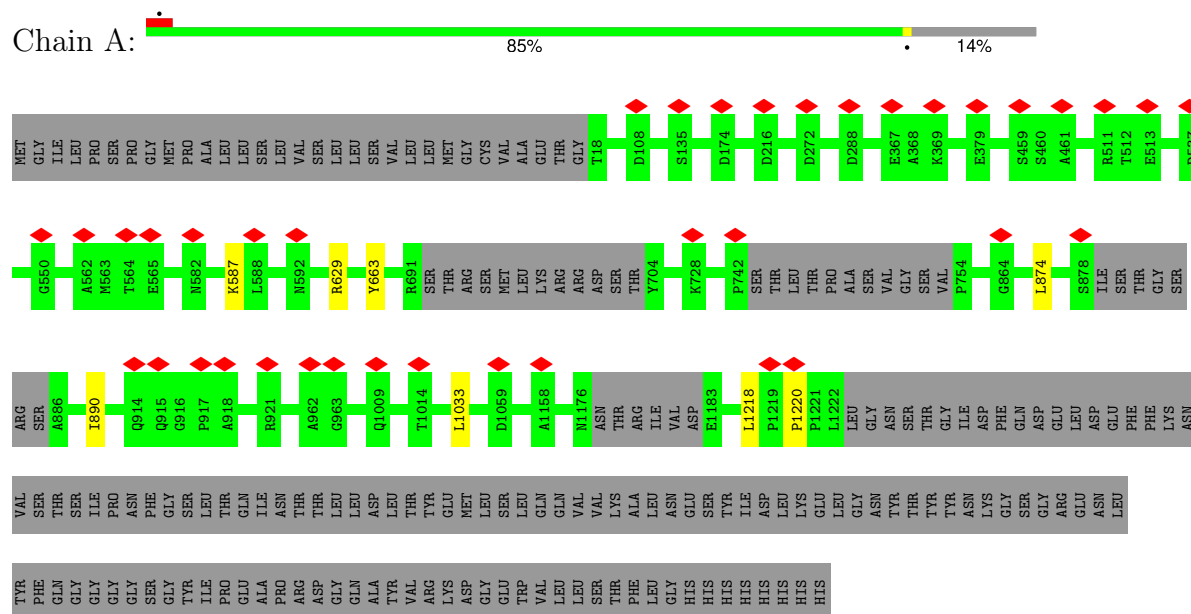
Continued from previous page...

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

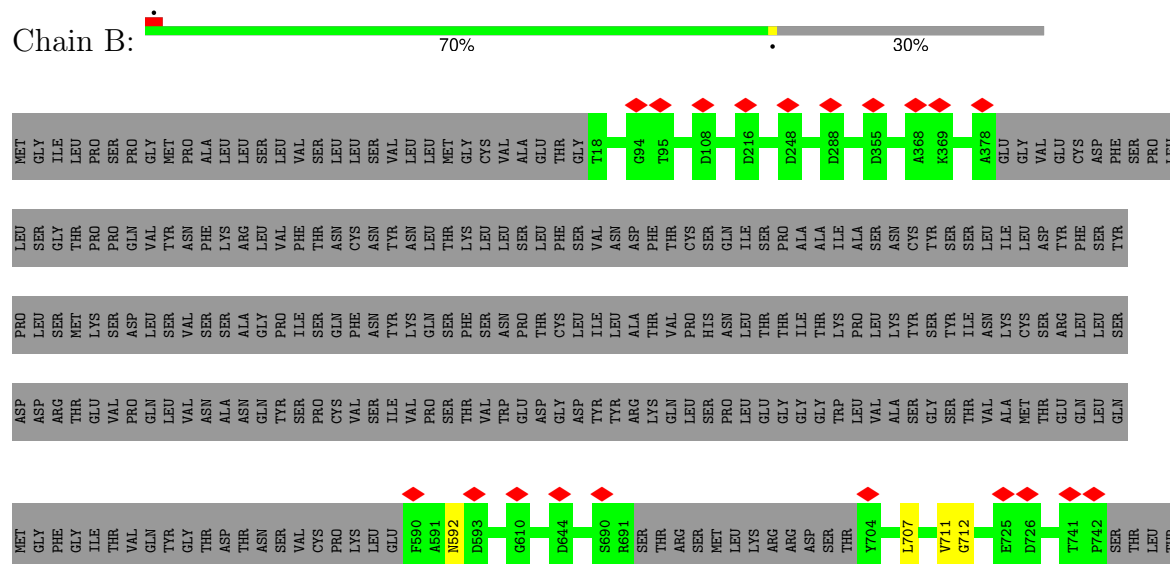
3 Residue-property plots [i](#)

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

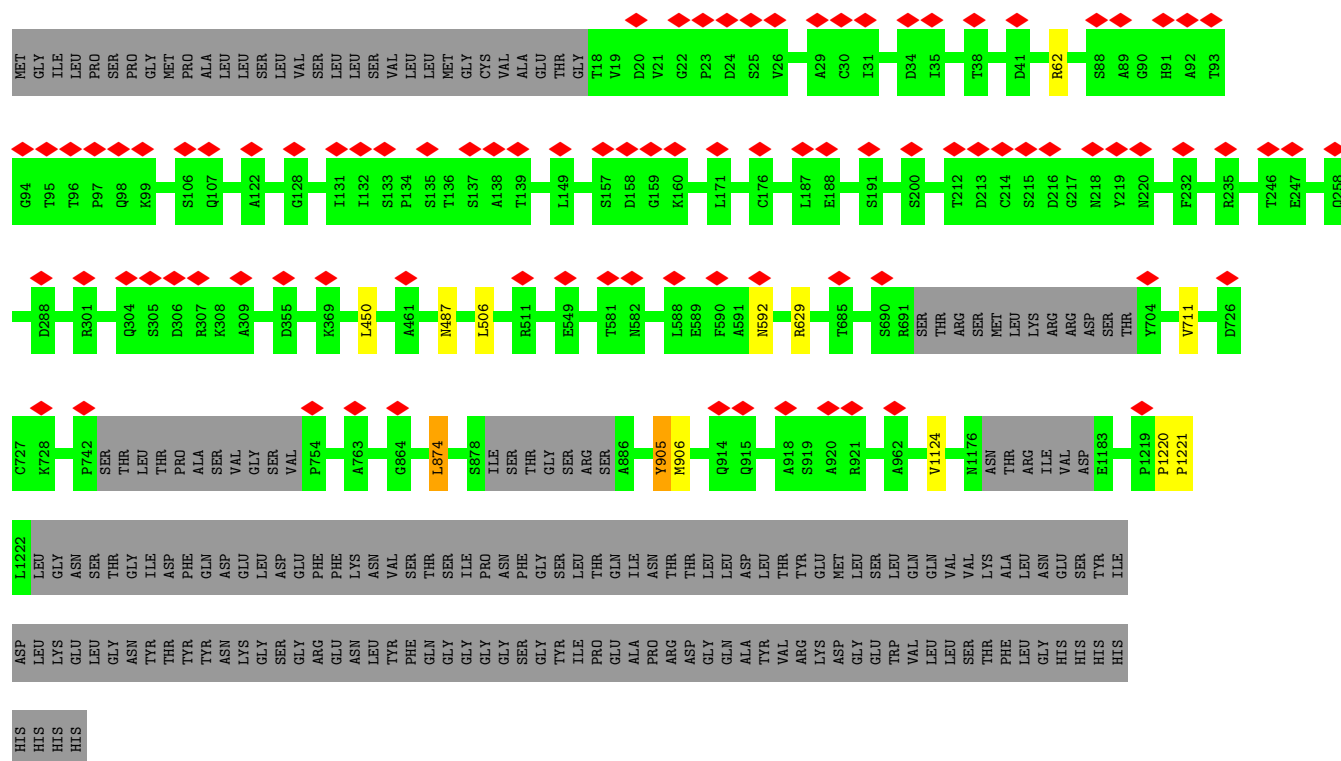
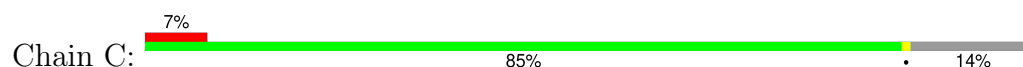
• Molecule 1: Spike glycoprotein



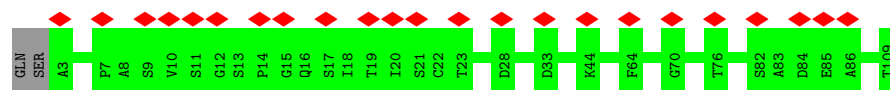
• Molecule 1: Spike glycoprotein



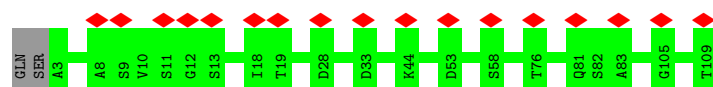
- Molecule 1: Spike glycoprotein



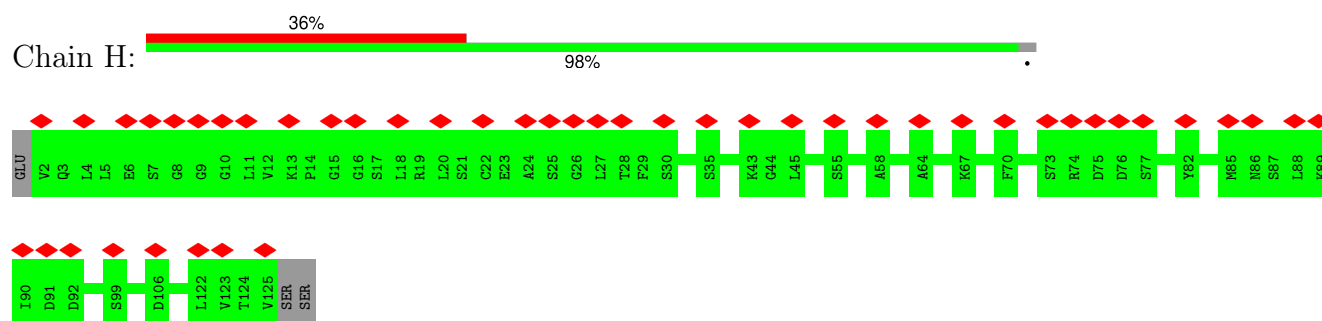
- Molecule 2: LCA60 light chain



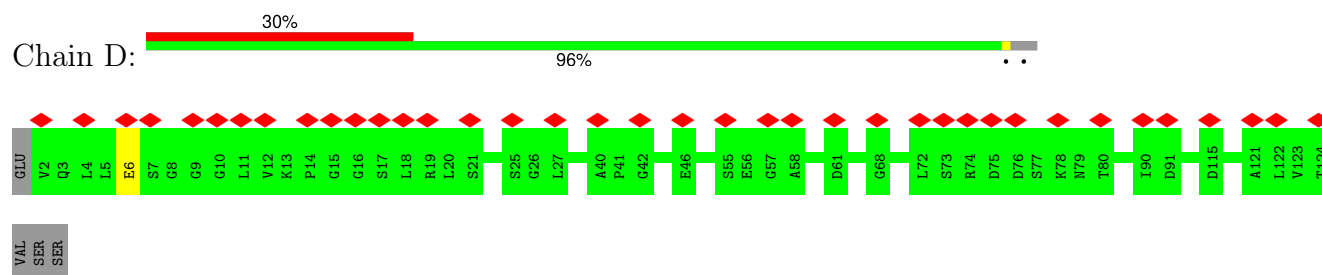
- Molecule 2: LCA60 light chain



- Molecule 3: LCA60 heavy chain



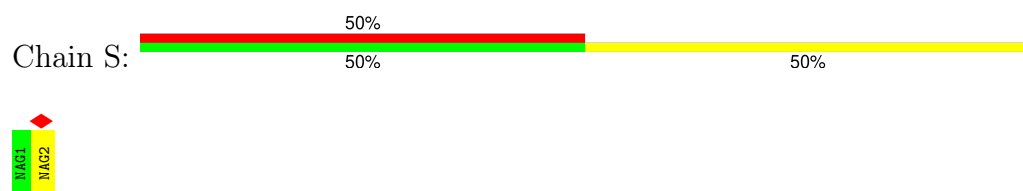
- Molecule 3: LCA60 heavy chain



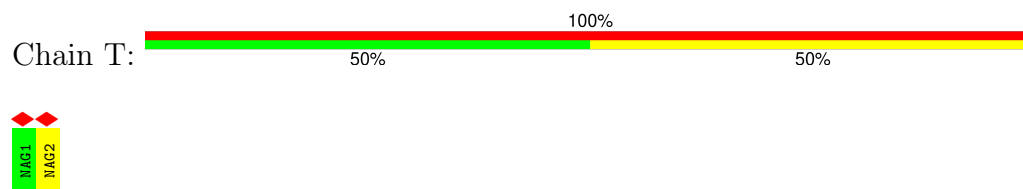
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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



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



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



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



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



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



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



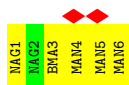
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



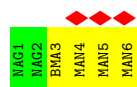
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





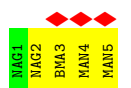
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



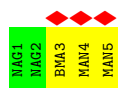
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

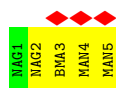


- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

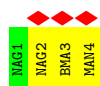
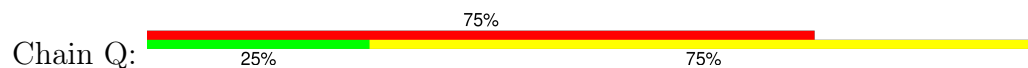


- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

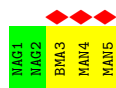
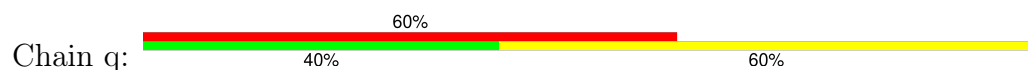




- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	54071	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.112	Depositor
Minimum map value	-2.972	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	526.08, 526.08, 526.08	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.69	0/9245	0.59	2/12582 (0.0%)
1	B	0.68	0/7574	0.60	3/10298 (0.0%)
1	C	0.69	1/9245 (0.0%)	0.62	6/12582 (0.0%)
2	E	0.62	0/789	0.61	0/1071
2	L	0.63	0/789	0.60	0/1071
3	D	0.77	1/973 (0.1%)	0.61	0/1317
3	H	0.75	0/980	0.61	0/1327
All	All	0.69	2/29595 (0.0%)	0.60	11/40248 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1221	PRO	N-CD	-5.16	1.40	1.47
3	D	6	GLU	CG-CD	-5.08	1.44	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	905	TYR	CB-CA-C	13.91	138.22	110.40
1	B	711	VAL	CB-CA-C	12.34	134.84	111.40
1	C	905	TYR	N-CA-C	-8.16	88.98	111.00
1	C	906	MET	N-CA-CB	-7.14	97.74	110.60
1	C	506	LEU	CD1-CG-CD2	7.02	131.55	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1159/1359 (85%)	1123 (97%)	35 (3%)	1 (0%)	48	79
1	B	946/1359 (70%)	920 (97%)	24 (2%)	2 (0%)	44	75
1	C	1159/1359 (85%)	1126 (97%)	29 (2%)	4 (0%)	37	68
2	E	105/109 (96%)	100 (95%)	5 (5%)	0	100	100
2	L	105/109 (96%)	102 (97%)	3 (3%)	0	100	100
3	D	121/127 (95%)	119 (98%)	2 (2%)	0	100	100
3	H	122/127 (96%)	120 (98%)	2 (2%)	0	100	100
All	All	3717/4549 (82%)	3610 (97%)	100 (3%)	7 (0%)	45	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1220	PRO
1	C	1220	PRO
1	B	1219	PRO
1	C	905	TYR
1	C	711	VAL

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	1003/1167 (86%)	998 (100%)	5 (0%)	86	93
1	B	811/1167 (70%)	808 (100%)	3 (0%)	89	95
1	C	1003/1167 (86%)	997 (99%)	6 (1%)	84	91
2	E	87/89 (98%)	87 (100%)	0	100	100
2	L	87/89 (98%)	87 (100%)	0	100	100
3	D	101/105 (96%)	101 (100%)	0	100	100
3	H	102/105 (97%)	102 (100%)	0	100	100
All	All	3194/3889 (82%)	3180 (100%)	14 (0%)	88	95

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1218	LEU
1	C	62	ARG
1	C	874	LEU
1	C	592	ASN
1	C	629	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	466	GLN
1	A	522	GLN
3	H	31	ASN
1	B	1129	ASN
1	C	708	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 ⓘ

155 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	F	1	4,1	14,14,15	0.74	0	17,19,21	0.88	0
4	NAG	F	2	4	14,14,15	0.78	0	17,19,21	1.05	1 (5%)
5	NAG	G	1	5,1	14,14,15	0.77	0	17,19,21	0.92	1 (5%)
5	NAG	G	2	5	14,14,15	0.80	0	17,19,21	1.13	2 (11%)
5	BMA	G	3	5	11,11,12	1.79	2 (18%)	15,15,17	0.94	1 (6%)
6	NAG	I	1	6,1	14,14,15	0.76	0	17,19,21	1.03	1 (5%)
6	NAG	I	2	6	14,14,15	0.84	0	17,19,21	1.02	0
6	BMA	I	3	6	11,11,12	1.83	1 (9%)	15,15,17	0.96	1 (6%)
6	MAN	I	4	6	11,11,12	1.56	1 (9%)	15,15,17	0.96	1 (6%)
6	MAN	I	5	6	11,11,12	1.79	2 (18%)	15,15,17	1.12	2 (13%)
6	MAN	I	6	6	11,11,12	1.83	2 (18%)	15,15,17	1.08	2 (13%)
5	NAG	J	1	5,1	14,14,15	0.74	0	17,19,21	0.95	1 (5%)
5	NAG	J	2	5	14,14,15	0.81	0	17,19,21	1.09	2 (11%)
5	BMA	J	3	5	11,11,12	1.79	2 (18%)	15,15,17	0.94	1 (6%)
6	NAG	K	1	6,1	14,14,15	0.74	0	17,19,21	1.50	3 (17%)
6	NAG	K	2	6	14,14,15	0.86	0	17,19,21	1.19	2 (11%)
6	BMA	K	3	6	11,11,12	1.83	2 (18%)	15,15,17	1.05	1 (6%)
6	MAN	K	4	6	11,11,12	1.63	2 (18%)	15,15,17	0.99	1 (6%)
6	MAN	K	5	6	11,11,12	1.79	2 (18%)	15,15,17	1.06	1 (6%)
6	MAN	K	6	6	11,11,12	1.83	2 (18%)	15,15,17	1.07	1 (6%)
6	NAG	M	1	6,1	14,14,15	0.78	0	17,19,21	1.03	0
6	NAG	M	2	6	14,14,15	0.88	1 (7%)	17,19,21	0.90	0
6	BMA	M	3	6	11,11,12	1.79	2 (18%)	15,15,17	1.04	1 (6%)
6	MAN	M	4	6	11,11,12	1.61	2 (18%)	15,15,17	0.80	0
6	MAN	M	5	6	11,11,12	1.82	2 (18%)	15,15,17	1.11	2 (13%)
6	MAN	M	6	6	11,11,12	1.81	2 (18%)	15,15,17	1.09	2 (13%)
7	NAG	N	1	1,7	14,14,15	0.73	0	17,19,21	1.04	1 (5%)
7	NAG	N	2	7	14,14,15	0.80	0	17,19,21	1.36	3 (17%)
7	BMA	N	3	7	11,11,12	1.77	2 (18%)	15,15,17	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	N	4	7	11,11,12	1.82	2 (18%)	15,15,17	1.10	2 (13%)
7	MAN	N	5	7	11,11,12	1.83	2 (18%)	15,15,17	1.20	2 (13%)
5	NAG	O	1	5,1	14,14,15	0.75	0	17,19,21	1.03	1 (5%)
5	NAG	O	2	5	14,14,15	0.79	0	17,19,21	1.00	1 (5%)
5	BMA	O	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.92	1 (6%)
6	NAG	P	1	6,1	14,14,15	0.67	0	17,19,21	1.15	1 (5%)
6	NAG	P	2	6	14,14,15	0.87	0	17,19,21	1.19	2 (11%)
6	BMA	P	3	6	11,11,12	1.78	1 (9%)	15,15,17	1.07	1 (6%)
6	MAN	P	4	6	11,11,12	1.57	2 (18%)	15,15,17	0.99	0
6	MAN	P	5	6	11,11,12	1.82	2 (18%)	15,15,17	1.27	2 (13%)
6	MAN	P	6	6	11,11,12	1.87	2 (18%)	15,15,17	1.17	2 (13%)
8	NAG	Q	1	8,1	14,14,15	0.75	0	17,19,21	0.79	0
8	NAG	Q	2	8	14,14,15	0.82	0	17,19,21	1.30	2 (11%)
8	BMA	Q	3	8	11,11,12	1.79	1 (9%)	15,15,17	1.01	1 (6%)
8	MAN	Q	4	8	11,11,12	1.79	2 (18%)	15,15,17	1.09	2 (13%)
5	NAG	R	1	5,1	14,14,15	0.81	0	17,19,21	0.92	0
5	NAG	R	2	5	14,14,15	0.80	0	17,19,21	0.92	0
5	BMA	R	3	5	11,11,12	1.80	2 (18%)	15,15,17	0.88	1 (6%)
4	NAG	S	1	4,1	14,14,15	0.77	0	17,19,21	0.96	0
4	NAG	S	2	4	14,14,15	0.79	0	17,19,21	1.05	1 (5%)
4	NAG	T	1	4,1	14,14,15	0.80	0	17,19,21	0.90	0
4	NAG	T	2	4	14,14,15	0.76	0	17,19,21	1.16	1 (5%)
4	NAG	U	1	4,1	14,14,15	0.81	0	17,19,21	1.18	2 (11%)
4	NAG	U	2	4	14,14,15	0.78	0	17,19,21	0.99	1 (5%)
5	NAG	V	1	5,1	14,14,15	0.77	0	17,19,21	1.05	2 (11%)
5	NAG	V	2	5	14,14,15	0.80	0	17,19,21	1.01	1 (5%)
5	BMA	V	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.92	1 (6%)
7	NAG	W	1	1,7	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
7	NAG	W	2	7	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
7	BMA	W	3	7	11,11,12	1.90	2 (18%)	15,15,17	0.94	1 (6%)
7	MAN	W	4	7	11,11,12	1.80	2 (18%)	15,15,17	0.92	0
7	MAN	W	5	7	11,11,12	1.82	2 (18%)	15,15,17	1.17	2 (13%)
4	NAG	X	1	4,1	14,14,15	0.77	0	17,19,21	1.13	1 (5%)
4	NAG	X	2	4	14,14,15	0.77	0	17,19,21	1.08	1 (5%)
5	NAG	Y	1	5,1	14,14,15	0.73	0	17,19,21	0.93	0
5	NAG	Y	2	5	14,14,15	0.80	0	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	Y	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.90	1 (6%)
6	NAG	Z	1	6,1	14,14,15	0.72	0	17,19,21	1.20	3 (17%)
6	NAG	Z	2	6	14,14,15	0.90	1 (7%)	17,19,21	1.10	2 (11%)
6	BMA	Z	3	6	11,11,12	1.86	2 (18%)	15,15,17	1.02	1 (6%)
6	MAN	Z	4	6	11,11,12	1.57	1 (9%)	15,15,17	0.97	1 (6%)
6	MAN	Z	5	6	11,11,12	1.80	2 (18%)	15,15,17	1.10	2 (13%)
6	MAN	Z	6	6	11,11,12	1.81	2 (18%)	15,15,17	1.15	2 (13%)
5	NAG	a	1	5,1	14,14,15	0.74	0	17,19,21	0.93	1 (5%)
5	NAG	a	2	5	14,14,15	0.80	0	17,19,21	1.07	2 (11%)
5	BMA	a	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.98	1 (6%)
6	NAG	b	1	6,1	14,14,15	0.80	0	17,19,21	1.67	3 (17%)
6	NAG	b	2	6	14,14,15	0.83	0	17,19,21	1.06	1 (5%)
6	BMA	b	3	6	11,11,12	1.79	1 (9%)	15,15,17	0.97	1 (6%)
6	MAN	b	4	6	11,11,12	1.61	2 (18%)	15,15,17	0.90	0
6	MAN	b	5	6	11,11,12	1.78	2 (18%)	15,15,17	1.10	2 (13%)
6	MAN	b	6	6	11,11,12	1.84	2 (18%)	15,15,17	1.08	2 (13%)
6	NAG	c	1	6,1	14,14,15	0.73	0	17,19,21	0.95	0
6	NAG	c	2	6	14,14,15	0.83	0	17,19,21	0.95	0
6	BMA	c	3	6	11,11,12	1.76	1 (9%)	15,15,17	1.01	1 (6%)
6	MAN	c	4	6	11,11,12	1.55	1 (9%)	15,15,17	0.78	0
6	MAN	c	5	6	11,11,12	1.83	2 (18%)	15,15,17	1.12	2 (13%)
6	MAN	c	6	6	11,11,12	1.83	2 (18%)	15,15,17	1.07	1 (6%)
7	NAG	d	1	1,7	14,14,15	0.79	0	17,19,21	0.99	0
7	NAG	d	2	7	14,14,15	0.87	0	17,19,21	1.43	3 (17%)
7	BMA	d	3	7	11,11,12	1.85	2 (18%)	15,15,17	1.00	1 (6%)
7	MAN	d	4	7	11,11,12	1.83	2 (18%)	15,15,17	1.10	2 (13%)
7	MAN	d	5	7	11,11,12	1.83	2 (18%)	15,15,17	1.05	1 (6%)
5	NAG	e	1	5,1	14,14,15	0.78	0	17,19,21	1.15	2 (11%)
5	NAG	e	2	5	14,14,15	0.85	0	17,19,21	1.06	1 (5%)
5	BMA	e	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.89	1 (6%)
4	NAG	f	1	4,1	14,14,15	0.85	0	17,19,21	0.90	1 (5%)
4	NAG	f	2	4	14,14,15	0.73	0	17,19,21	1.13	1 (5%)
5	NAG	g	1	5,1	14,14,15	0.78	0	17,19,21	1.06	1 (5%)
5	NAG	g	2	5	14,14,15	0.85	0	17,19,21	1.06	2 (11%)
5	BMA	g	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	h	1	4,1	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
4	NAG	h	2	4	14,14,15	0.79	0	17,19,21	1.06	1 (5%)
4	NAG	i	1	4,1	14,14,15	0.78	0	17,19,21	1.14	1 (5%)
4	NAG	i	2	4	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
5	NAG	j	1	5,1	14,14,15	0.79	0	17,19,21	1.05	2 (11%)
5	NAG	j	2	5	14,14,15	0.78	0	17,19,21	1.03	0
5	BMA	j	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.96	1 (6%)
7	NAG	k	1	1,7	14,14,15	0.78	0	17,19,21	0.90	0
7	NAG	k	2	7	14,14,15	0.78	0	17,19,21	0.99	0
7	BMA	k	3	7	11,11,12	1.83	1 (9%)	15,15,17	0.93	1 (6%)
7	MAN	k	4	7	11,11,12	1.83	2 (18%)	15,15,17	1.04	0
7	MAN	k	5	7	11,11,12	1.80	1 (9%)	15,15,17	1.09	1 (6%)
4	NAG	l	1	4,1	14,14,15	0.77	0	17,19,21	1.11	2 (11%)
4	NAG	l	2	4	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
5	NAG	m	1	5,1	14,14,15	0.72	0	17,19,21	0.94	0
5	NAG	m	2	5	14,14,15	0.75	0	17,19,21	0.92	1 (5%)
5	BMA	m	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.98	1 (6%)
6	NAG	n	1	6,1	14,14,15	0.76	0	17,19,21	1.13	1 (5%)
6	NAG	n	2	6	14,14,15	0.84	0	17,19,21	1.01	1 (5%)
6	BMA	n	3	6	11,11,12	1.75	1 (9%)	15,15,17	0.99	1 (6%)
6	MAN	n	4	6	11,11,12	1.57	1 (9%)	15,15,17	0.97	1 (6%)
6	MAN	n	5	6	11,11,12	1.81	2 (18%)	15,15,17	1.08	2 (13%)
6	MAN	n	6	6	11,11,12	1.82	2 (18%)	15,15,17	1.24	2 (13%)
5	NAG	o	1	5,1	14,14,15	0.78	0	17,19,21	1.06	2 (11%)
5	NAG	o	2	5	14,14,15	0.80	0	17,19,21	0.90	0
5	BMA	o	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.97	1 (6%)
5	NAG	p	1	5,1	14,14,15	0.80	0	17,19,21	1.24	2 (11%)
5	NAG	p	2	5	14,14,15	0.77	0	17,19,21	0.97	1 (5%)
5	BMA	p	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.92	1 (6%)
9	NAG	q	1	1,9	14,14,15	0.72	0	17,19,21	0.97	0
9	NAG	q	2	9	14,14,15	0.84	0	17,19,21	0.91	0
9	BMA	q	3	9	11,11,12	1.80	1 (9%)	15,15,17	1.17	1 (6%)
9	MAN	q	4	9	11,11,12	1.59	1 (9%)	15,15,17	0.86	0
9	MAN	q	5	9	11,11,12	1.79	2 (18%)	15,15,17	1.08	2 (13%)
4	NAG	r	1	4,1	14,14,15	0.83	0	17,19,21	0.80	0
4	NAG	r	2	4	14,14,15	0.76	0	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	s	1	4,1	14,14,15	0.78	0	17,19,21	1.11	1 (5%)
4	NAG	s	2	4	14,14,15	0.77	0	17,19,21	0.99	1 (5%)
5	NAG	t	1	5,1	14,14,15	0.83	0	17,19,21	0.85	0
5	NAG	t	2	5	14,14,15	0.82	0	17,19,21	0.96	0
5	BMA	t	3	5	11,11,12	1.80	2 (18%)	15,15,17	0.91	1 (6%)
4	NAG	u	1	4,1	14,14,15	0.80	0	17,19,21	0.97	1 (5%)
4	NAG	u	2	4	14,14,15	0.79	0	17,19,21	1.10	1 (5%)
4	NAG	v	1	4,1	14,14,15	0.77	0	17,19,21	1.01	1 (5%)
4	NAG	v	2	4	14,14,15	0.76	0	17,19,21	1.15	1 (5%)
4	NAG	w	1	4,1	14,14,15	0.81	0	17,19,21	1.27	2 (11%)
4	NAG	w	2	4	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
5	NAG	x	1	5,1	14,14,15	0.76	0	17,19,21	0.97	1 (5%)
5	NAG	x	2	5	14,14,15	0.80	0	17,19,21	0.94	0
5	BMA	x	3	5	11,11,12	1.80	2 (18%)	15,15,17	0.89	1 (6%)
7	NAG	y	1	1,7	14,14,15	0.84	0	17,19,21	0.98	0
7	NAG	y	2	7	14,14,15	0.81	1 (7%)	17,19,21	1.09	1 (5%)
7	BMA	y	3	7	11,11,12	1.84	2 (18%)	15,15,17	0.98	1 (6%)
7	MAN	y	4	7	11,11,12	1.78	2 (18%)	15,15,17	1.00	1 (6%)
7	MAN	y	5	7	11,11,12	1.82	1 (9%)	15,15,17	1.15	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
6	NAG	K	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	1/2/19/22	0/1/1/1
6	MAN	K	5	6	-	1/2/19/22	0/1/1/1
6	MAN	K	6	6	-	1/2/19/22	0/1/1/1
6	NAG	M	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	1/2/19/22	0/1/1/1
6	MAN	M	4	6	-	2/2/19/22	0/1/1/1
6	MAN	M	5	6	-	2/2/19/22	0/1/1/1
6	MAN	M	6	6	-	1/2/19/22	0/1/1/1
7	NAG	N	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	2/2/19/22	0/1/1/1
7	MAN	N	4	7	-	1/2/19/22	0/1/1/1
7	MAN	N	5	7	-	2/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	1/2/19/22	0/1/1/1
6	MAN	P	4	6	-	2/2/19/22	0/1/1/1
6	MAN	P	5	6	-	1/2/19/22	0/1/1/1
6	MAN	P	6	6	-	1/2/19/22	0/1/1/1
8	NAG	Q	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	1/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
5	BMA	R	3	5	-	1/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1

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

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

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

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	3	BMA	O2-C2	-4.60	1.33	1.43
6	Z	3	BMA	O2-C2	-4.35	1.34	1.43
6	I	3	BMA	O2-C2	-4.32	1.34	1.43
6	M	3	BMA	O2-C2	-4.29	1.34	1.43
7	d	3	BMA	O2-C2	-4.26	1.34	1.43

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	b	1	NAG	C3-C4-C5	-3.95	103.07	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	2	NAG	C4-C3-C2	-3.58	105.78	111.02
9	q	3	BMA	C2-C3-C4	-3.43	104.82	110.86
4	v	2	NAG	C4-C3-C2	-3.38	106.07	111.02
6	K	1	NAG	C3-C4-C5	-3.34	104.18	110.23

There are no chirality outliers.

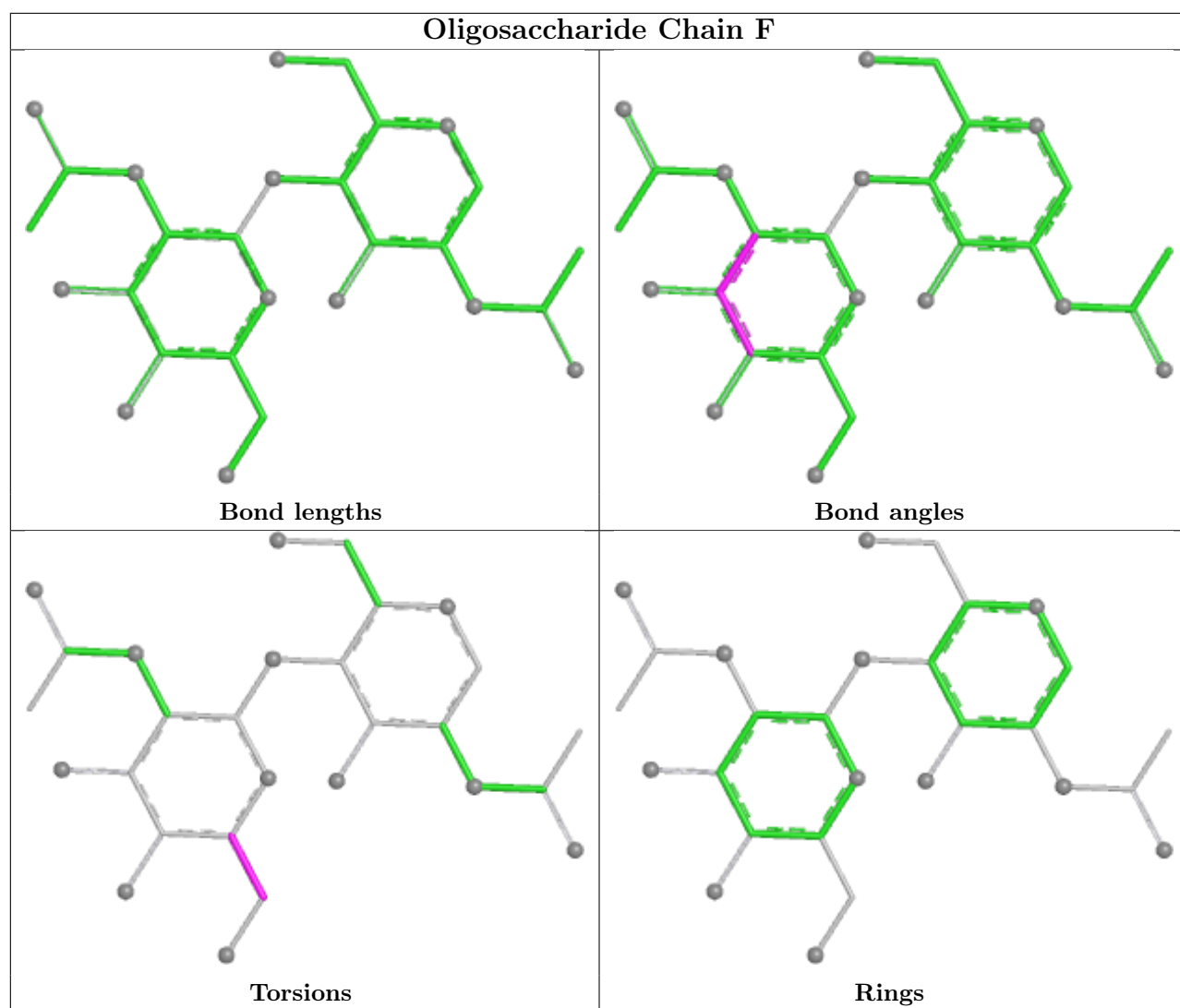
5 of 170 torsion outliers are listed below:

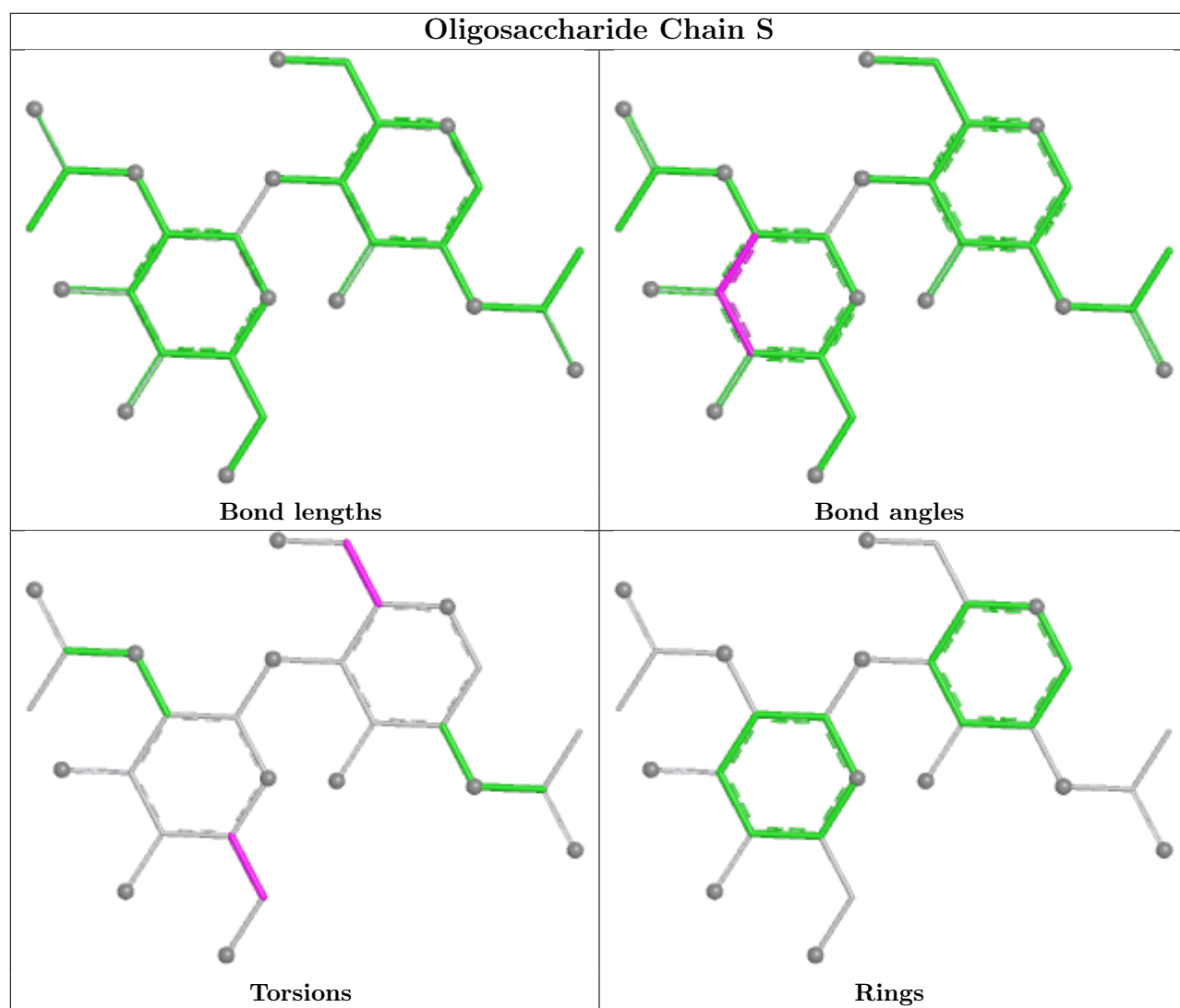
Mol	Chain	Res	Type	Atoms
7	N	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
4	l	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6

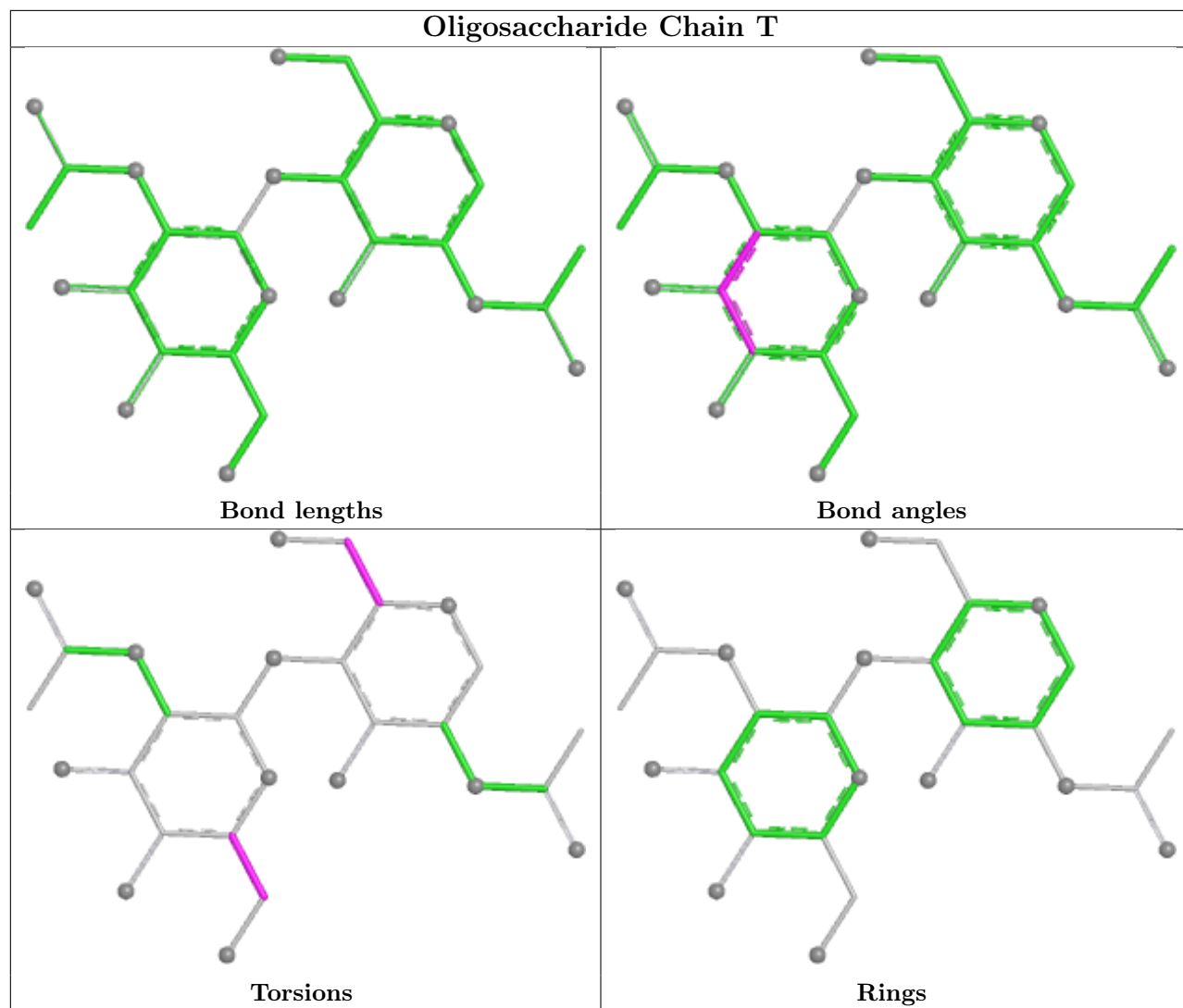
There are no ring outliers.

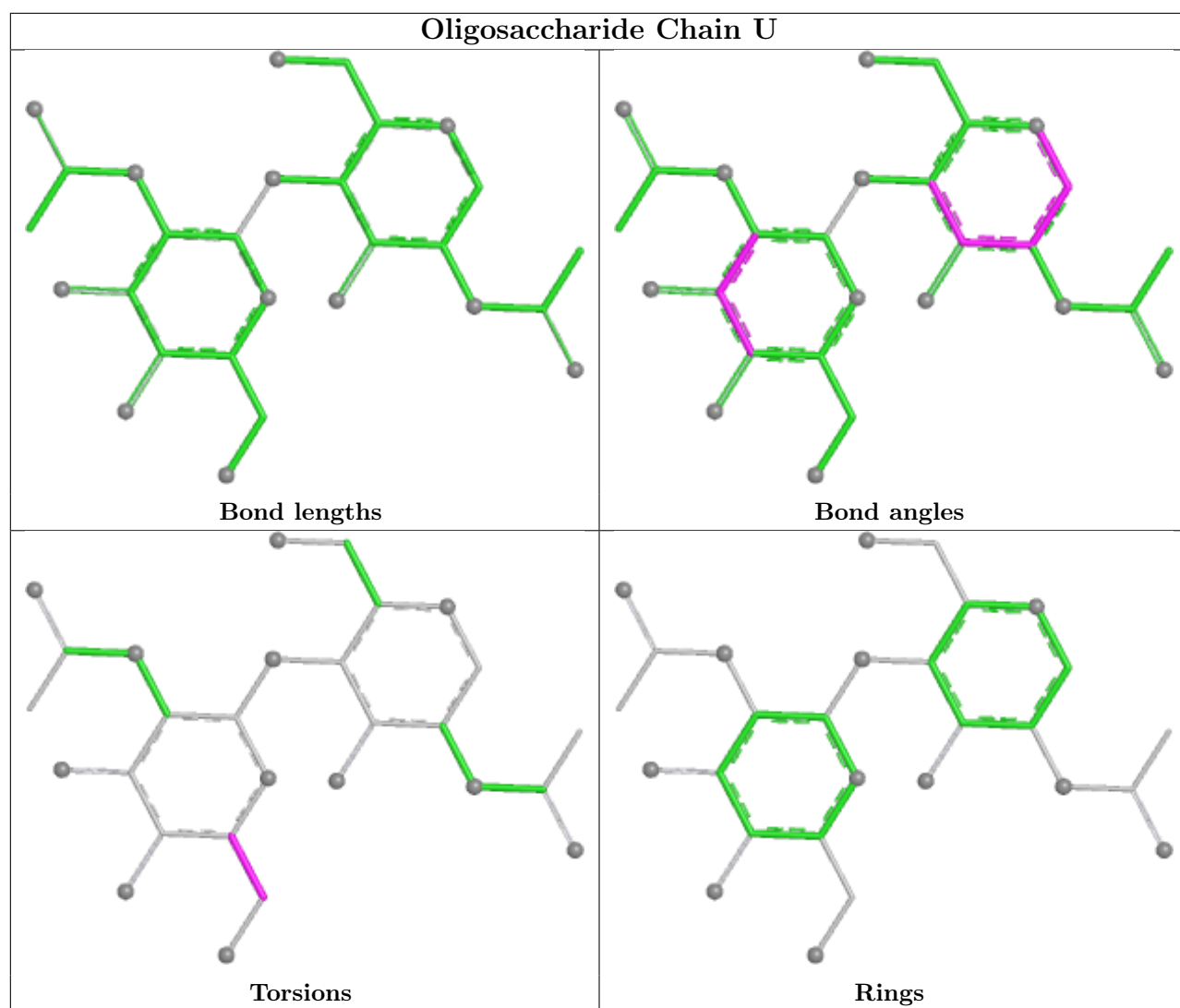
No monomer is involved in short contacts.

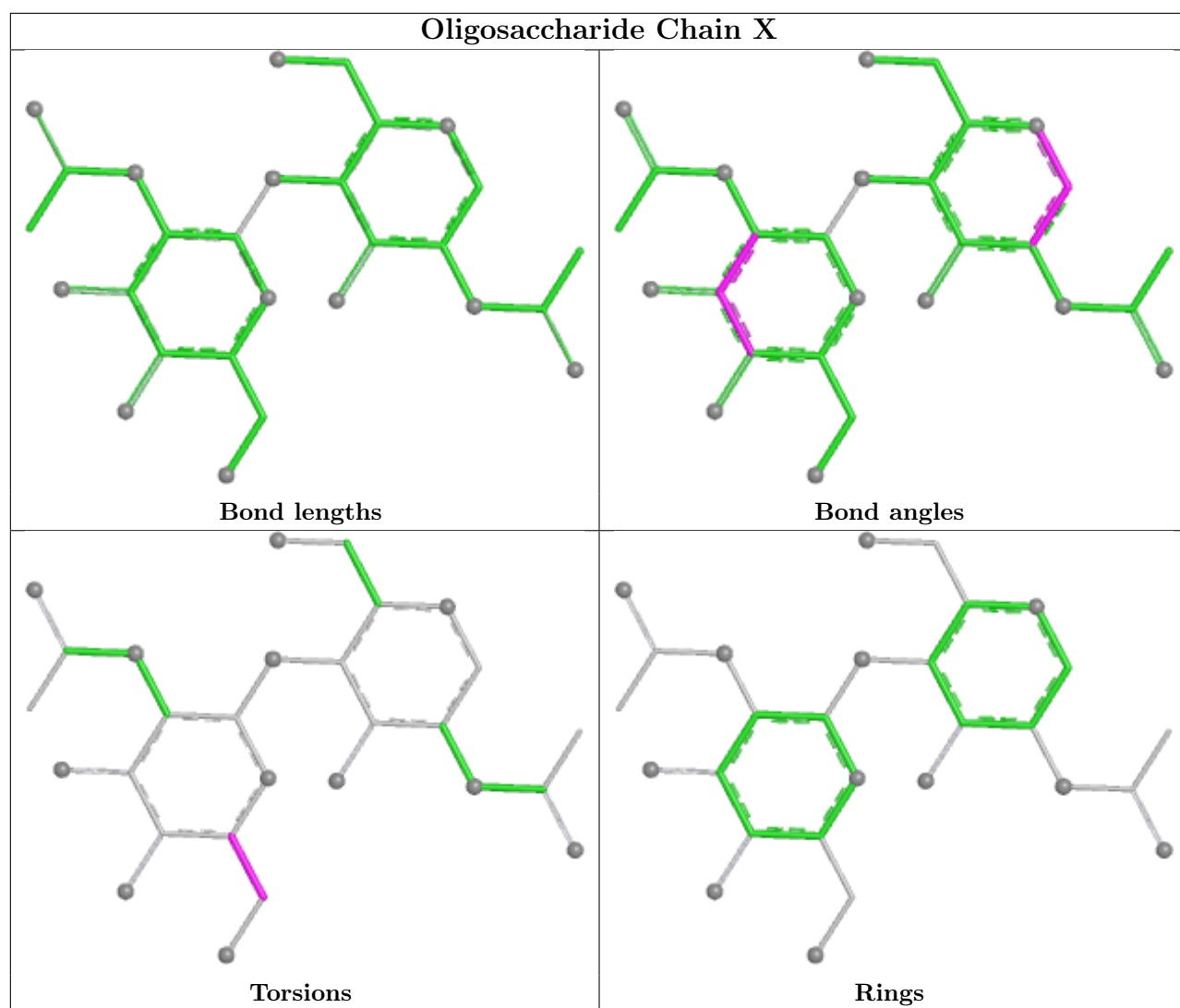
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

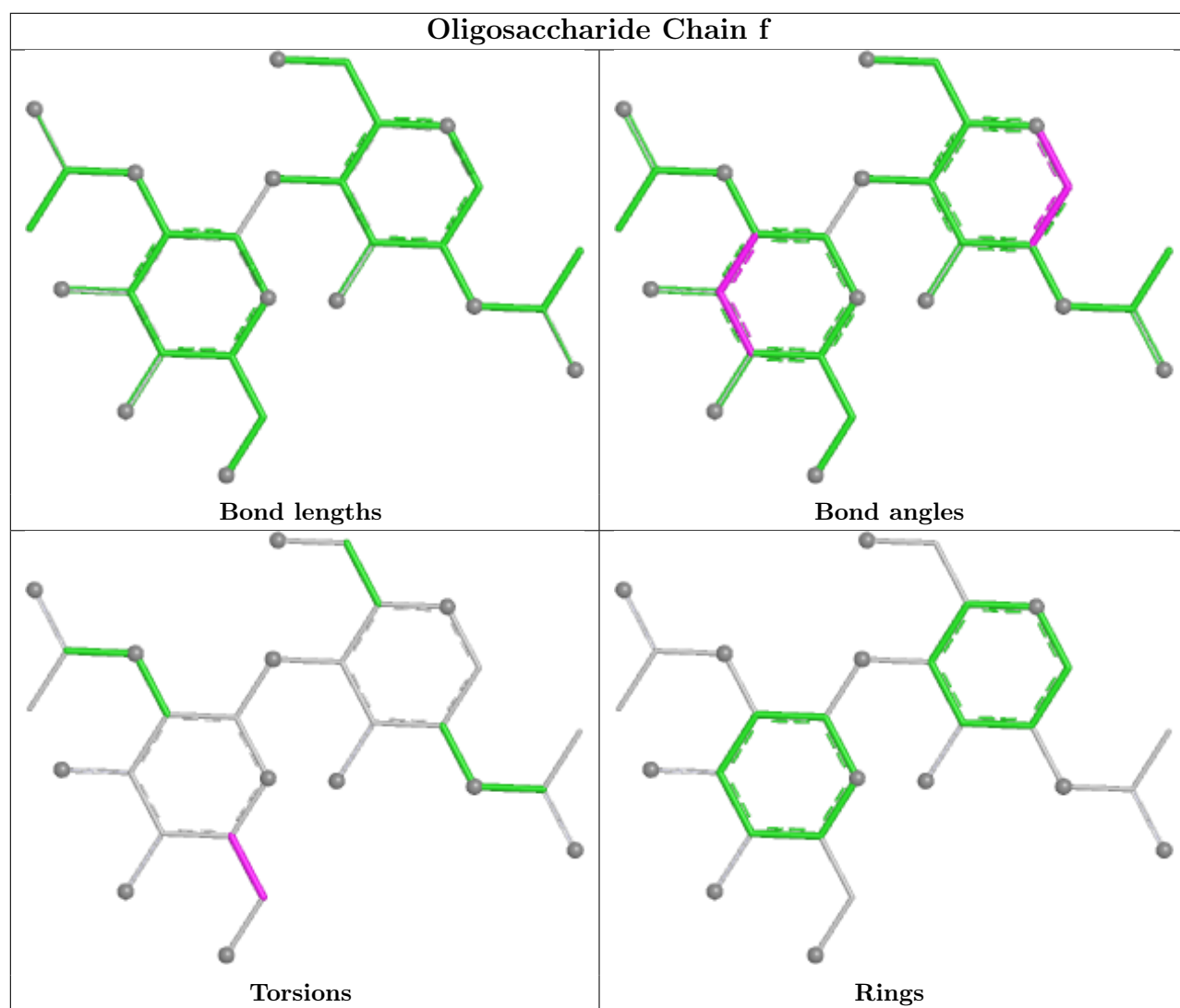


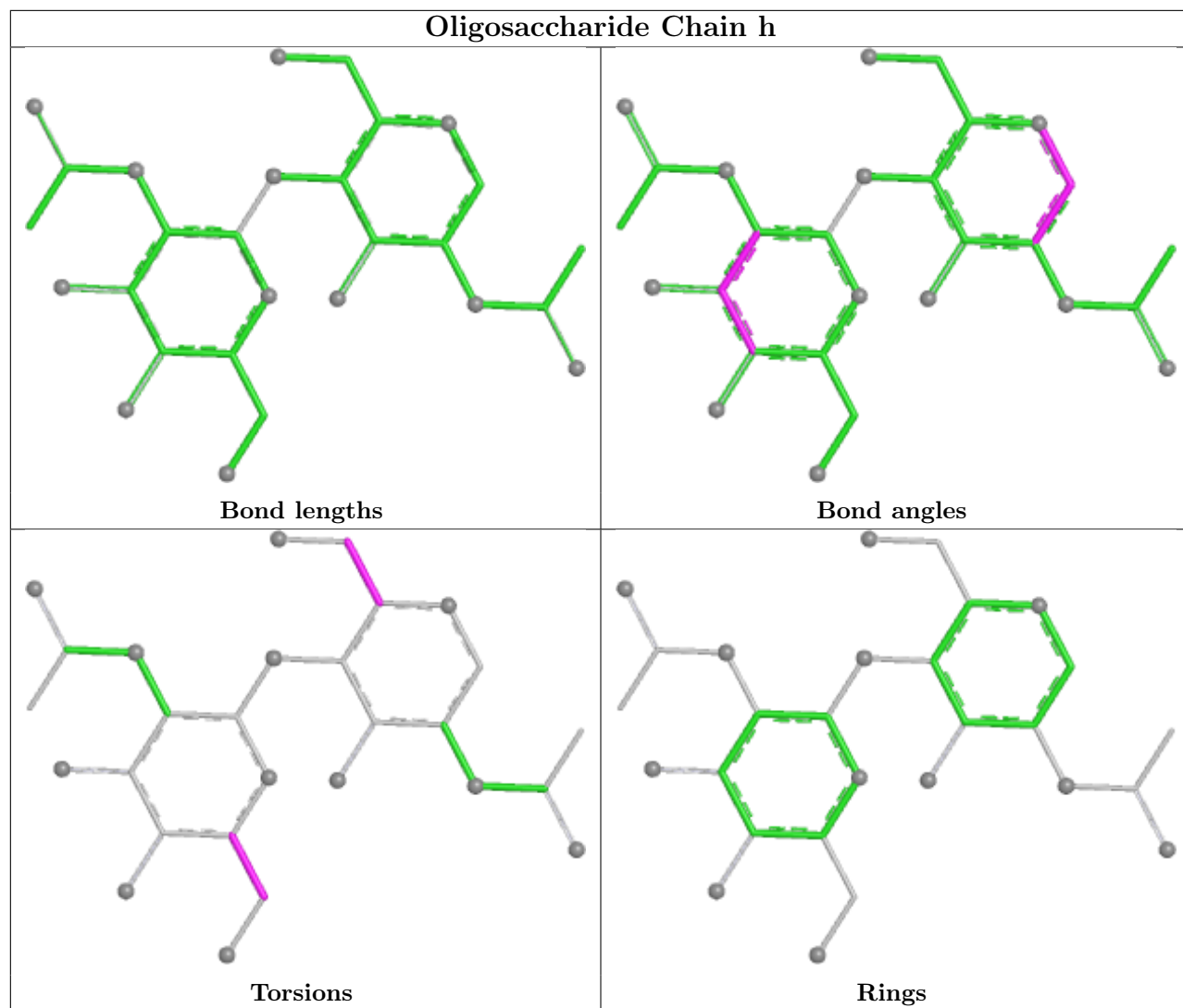


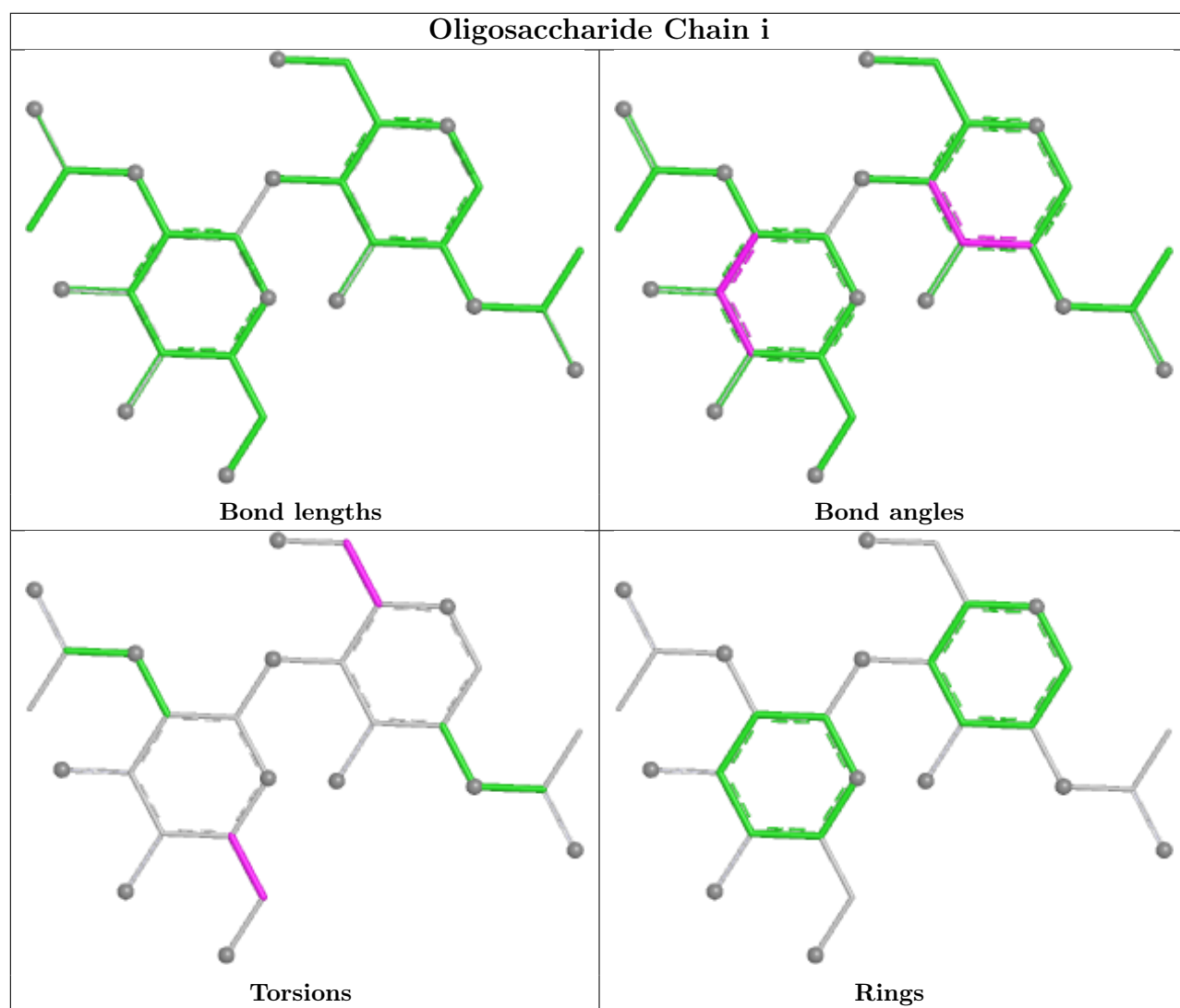


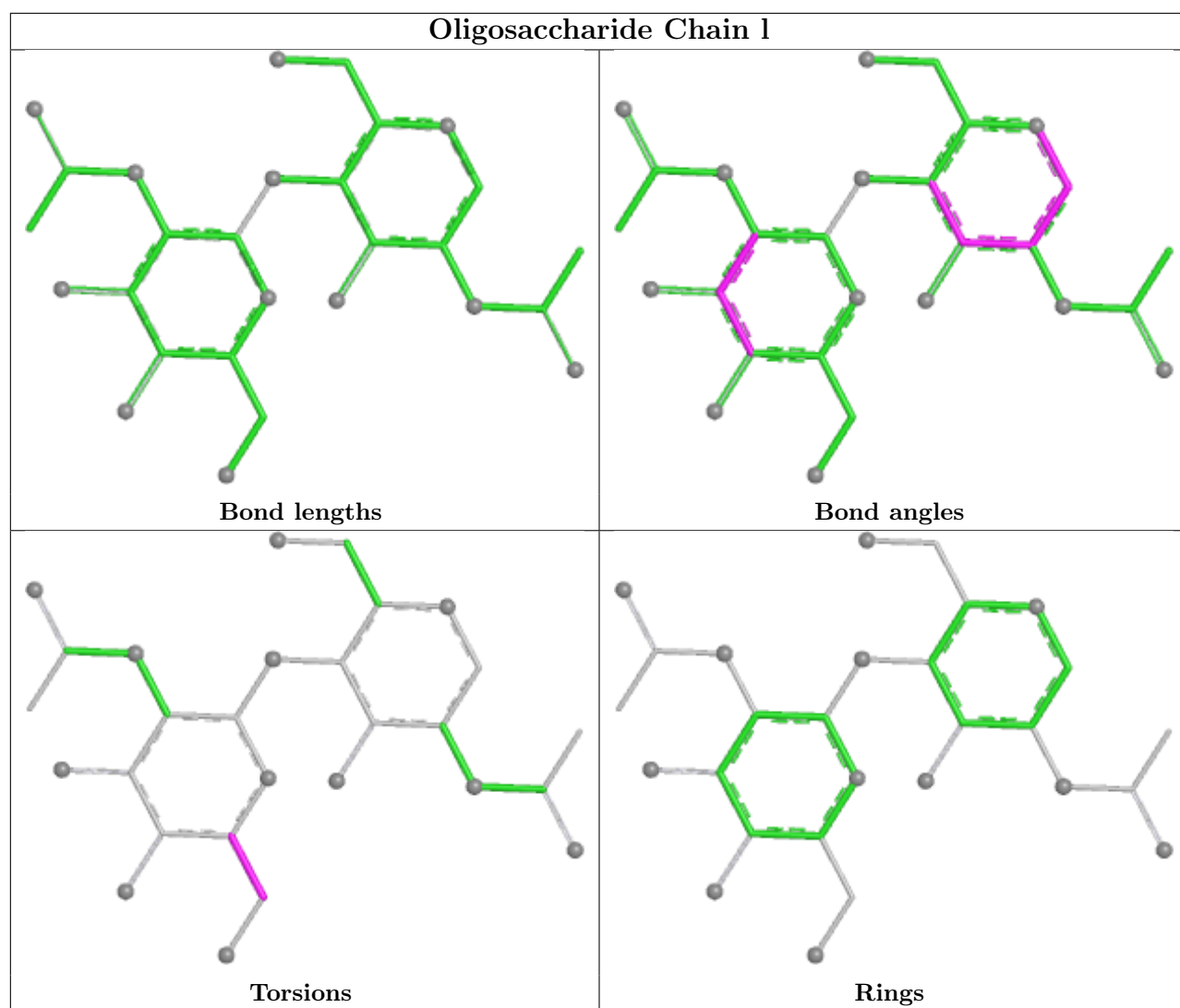


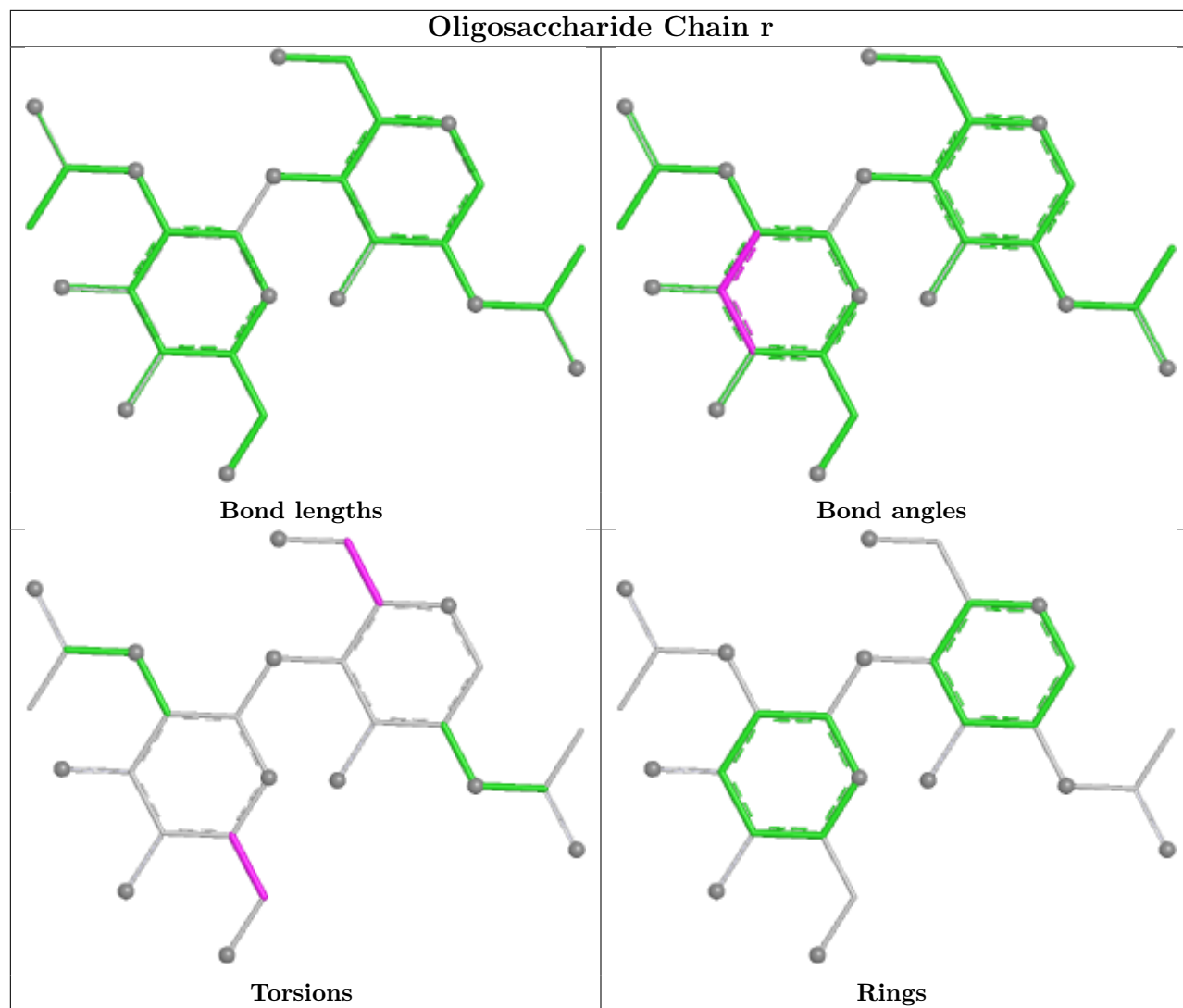


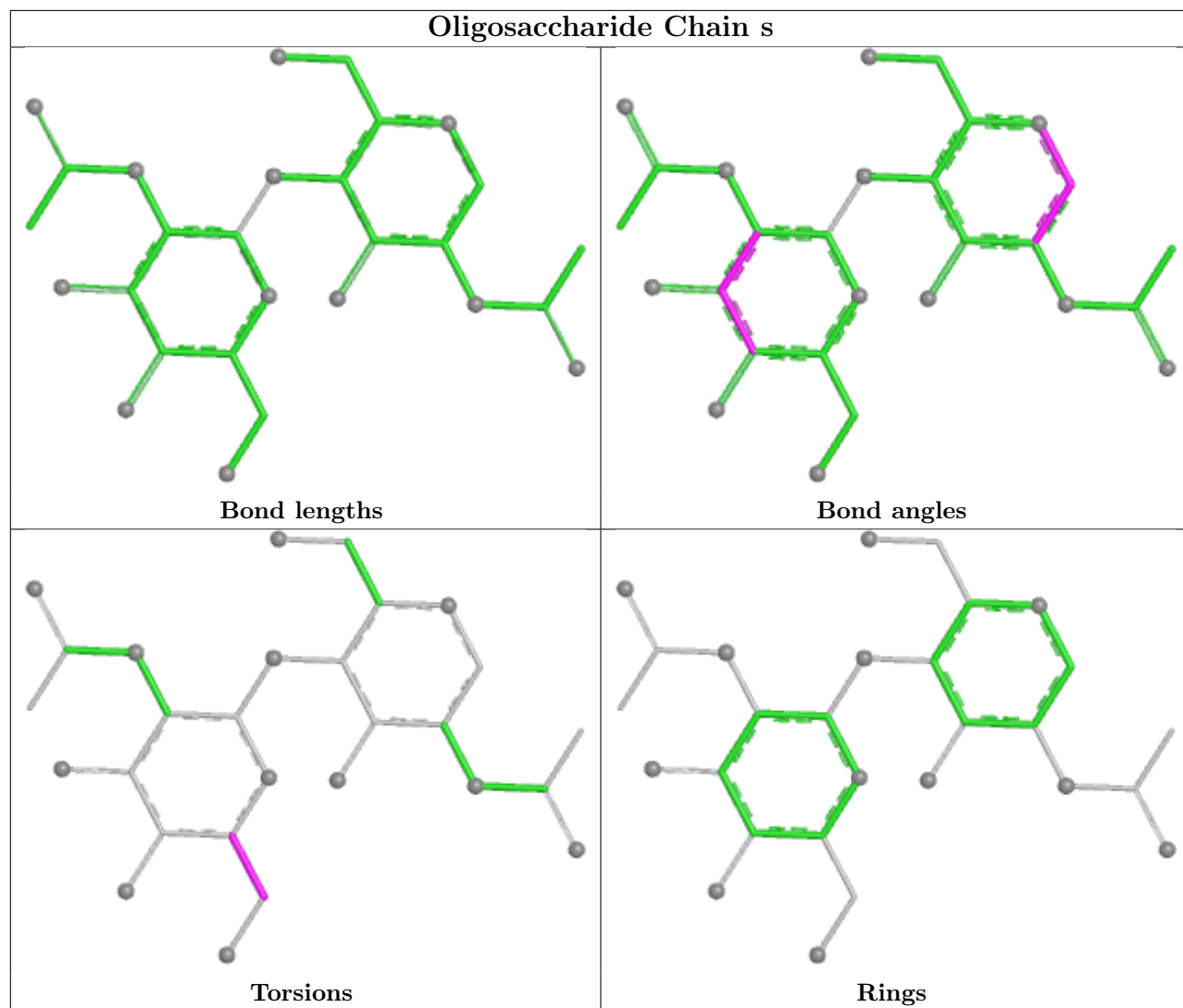


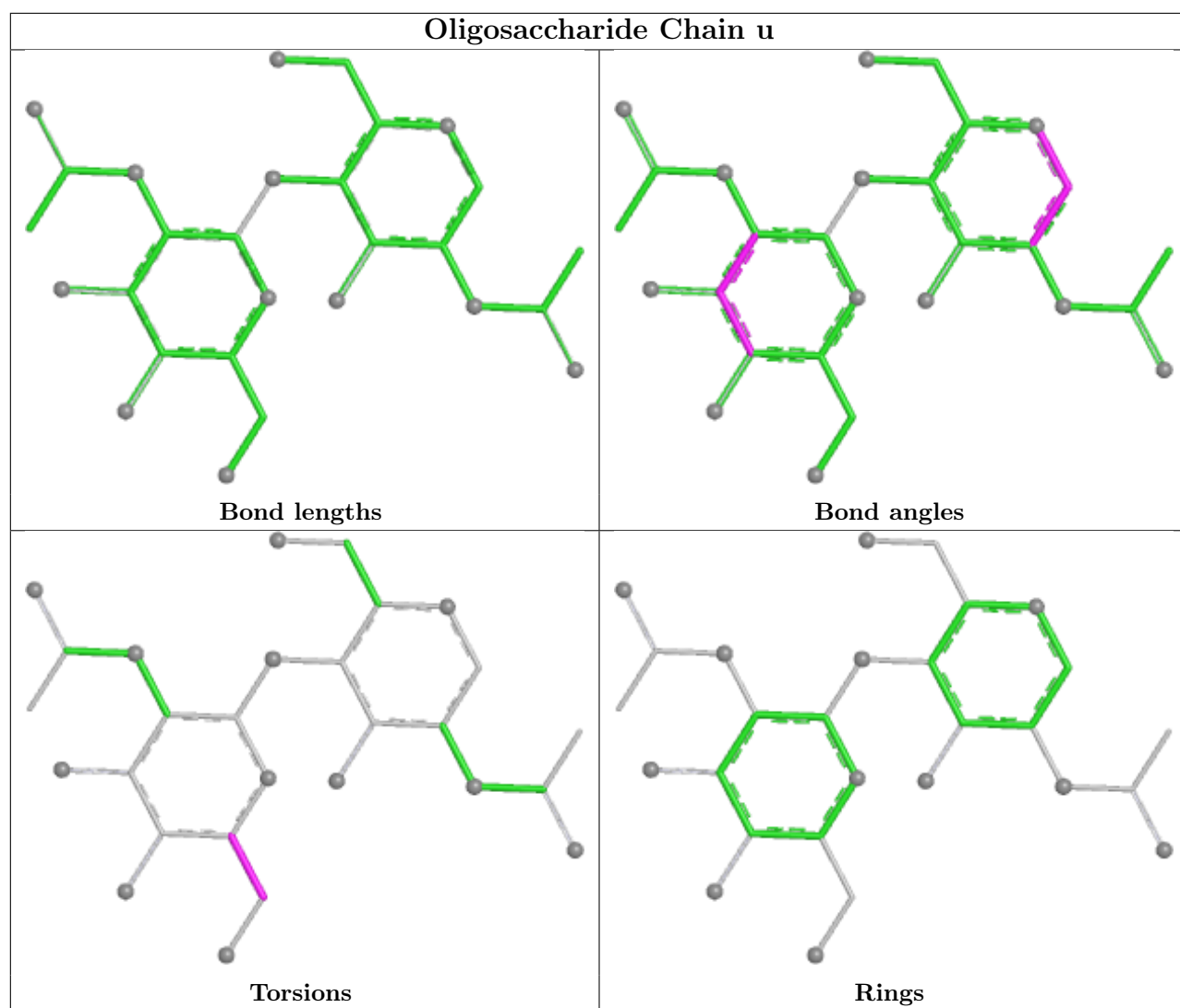


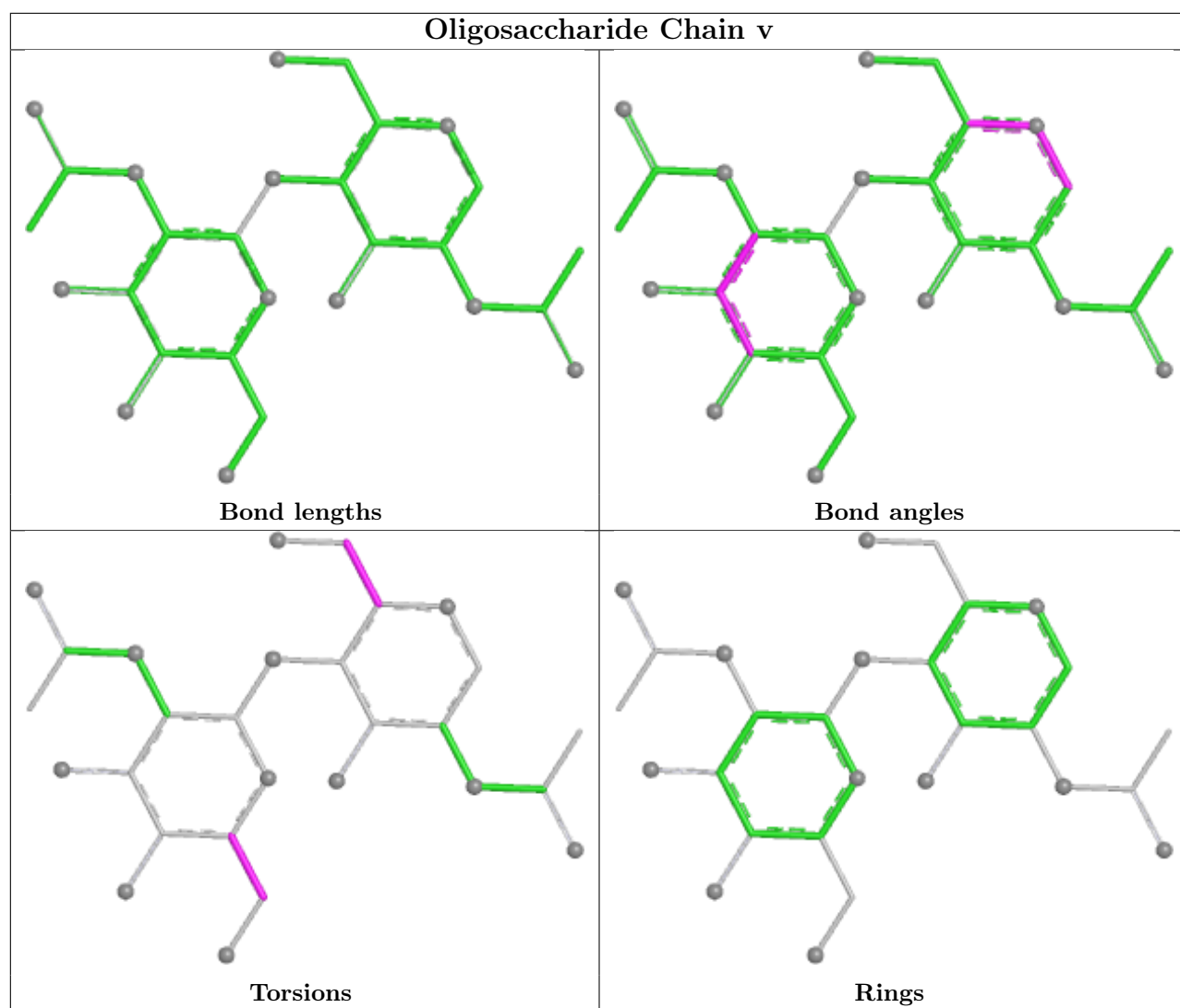


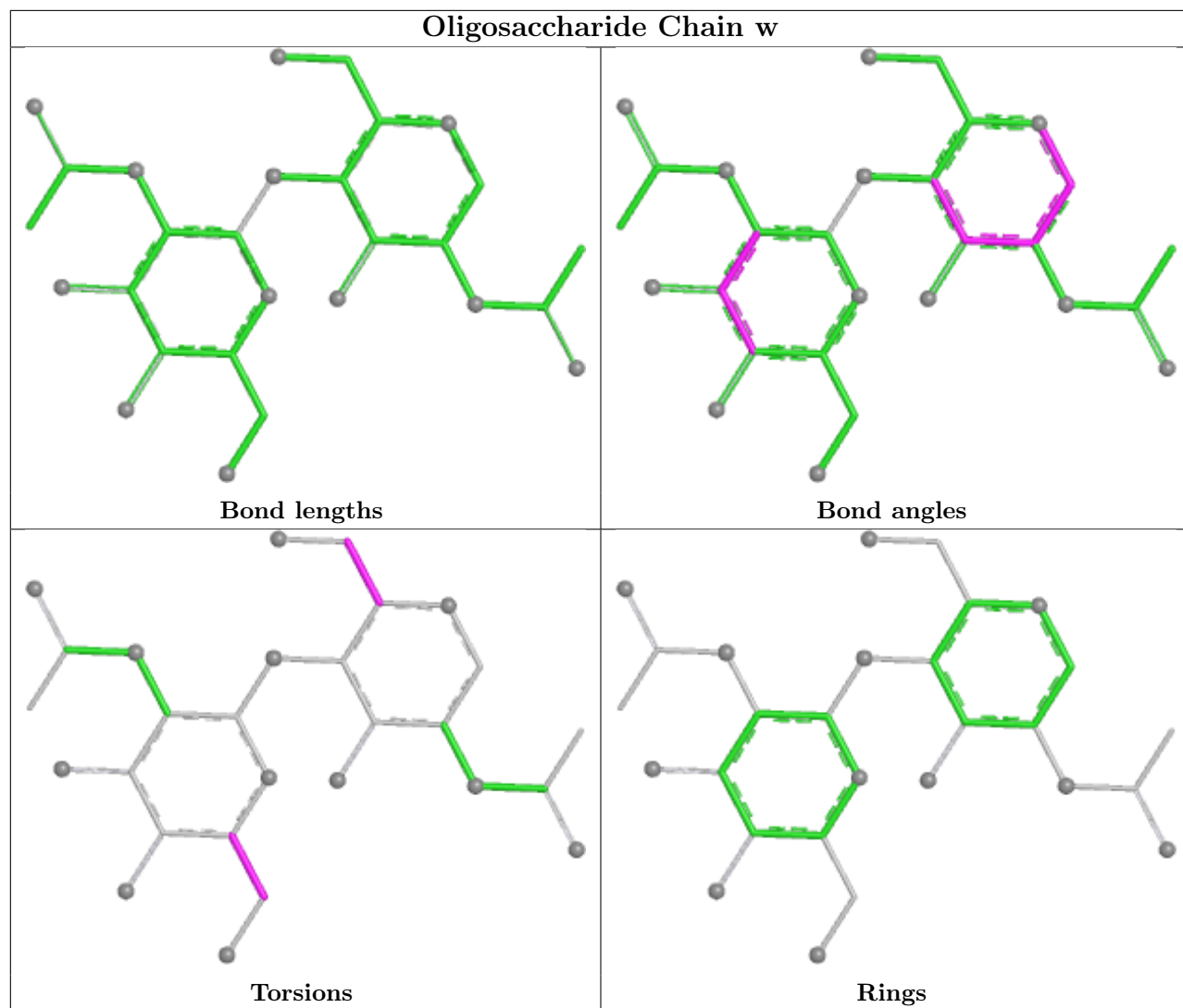


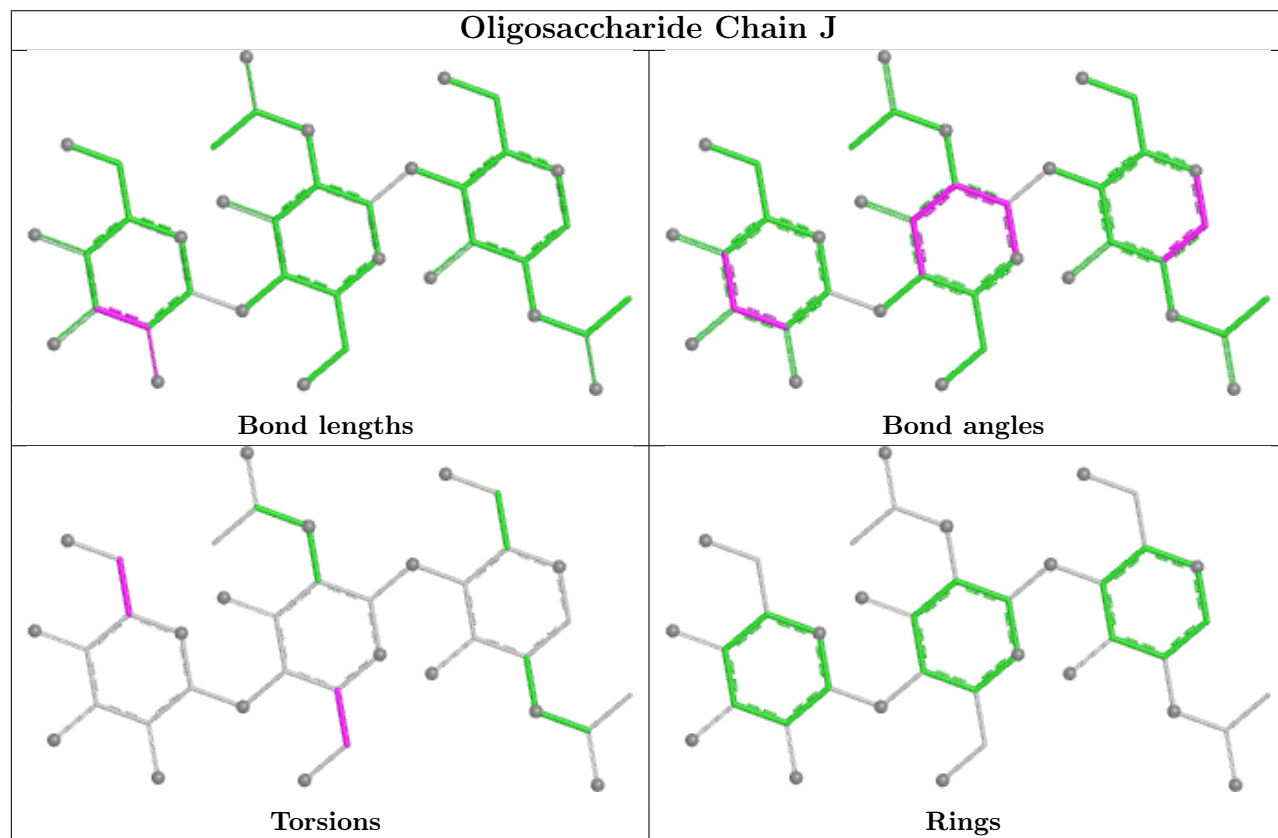
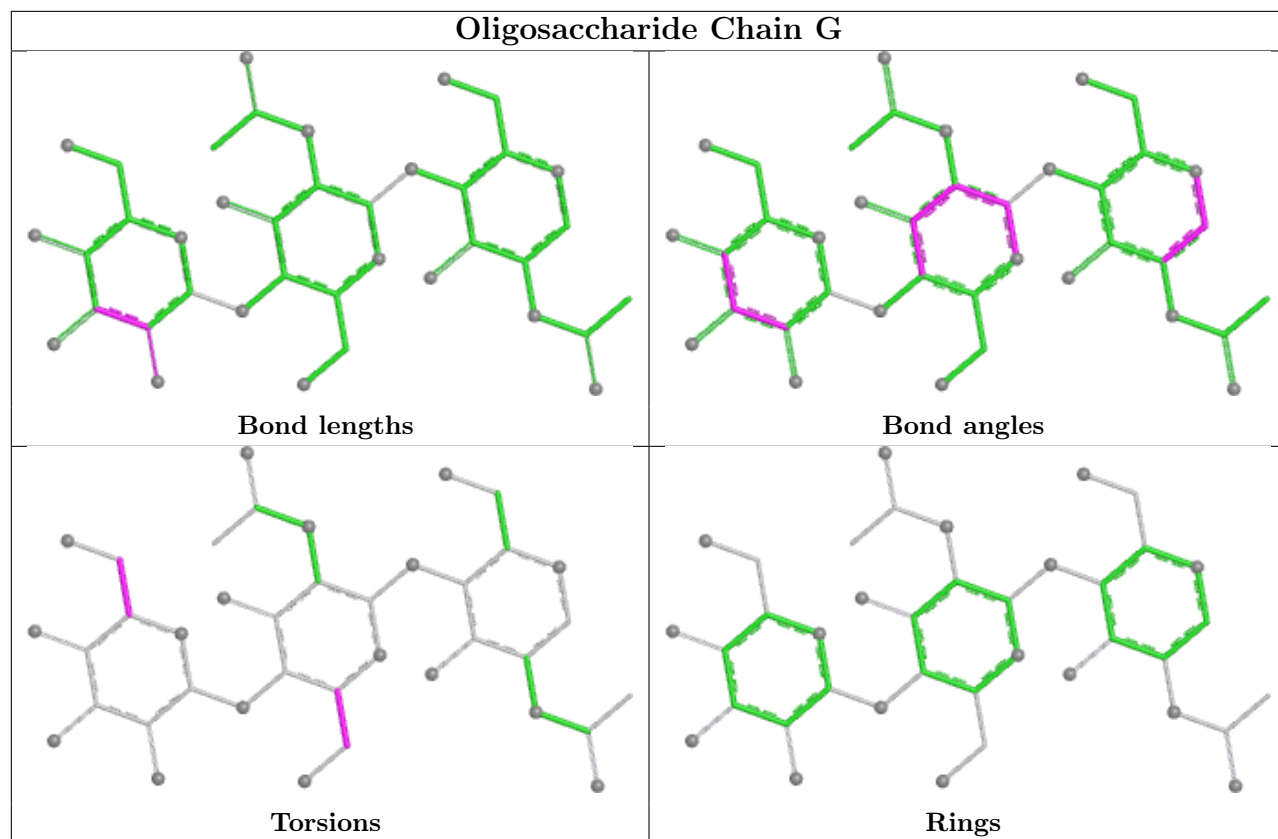


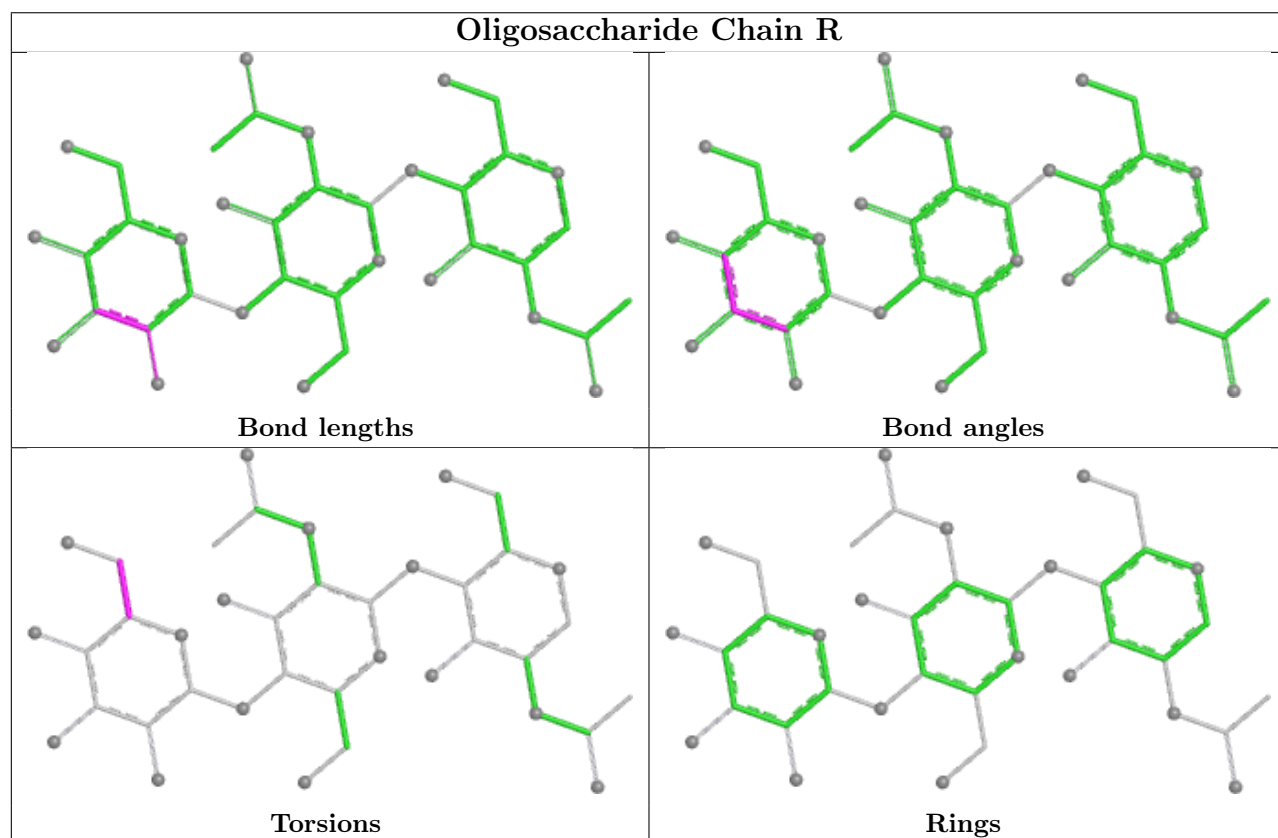
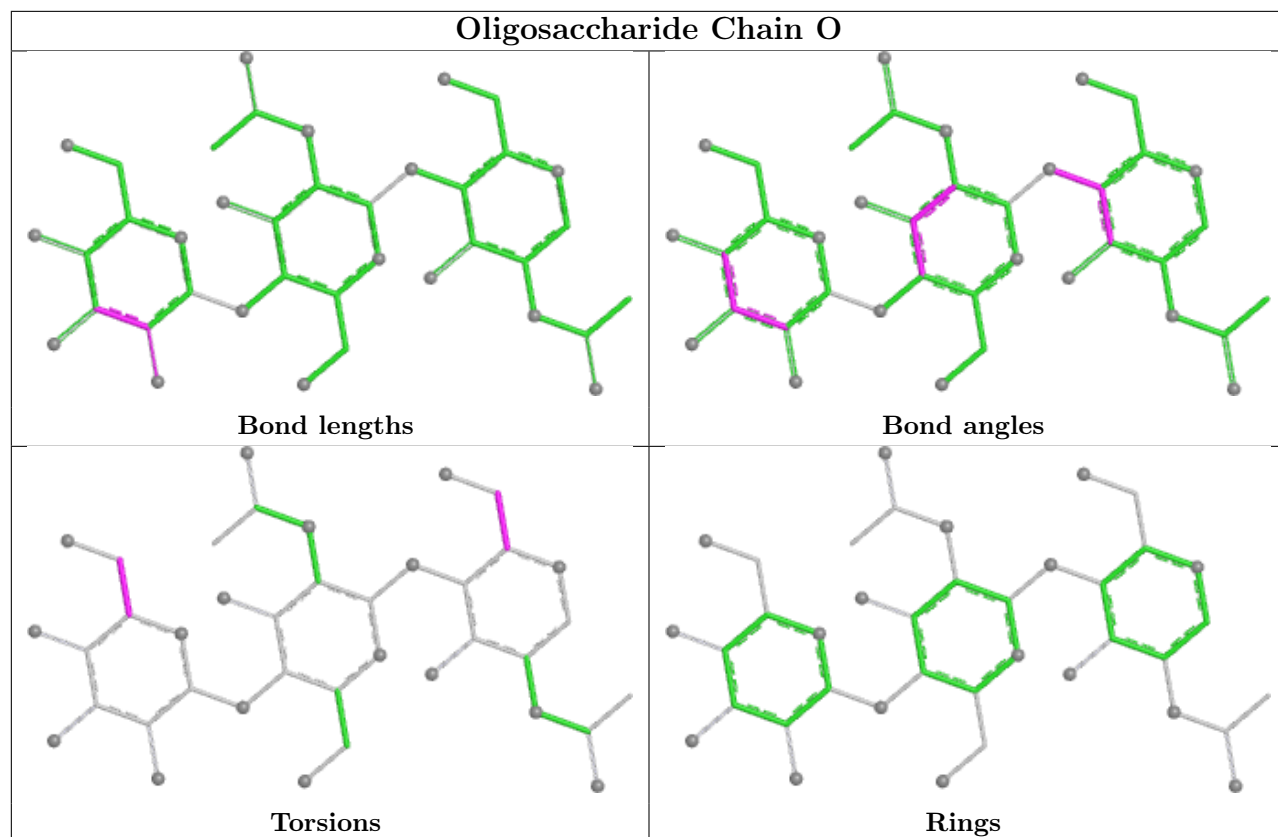


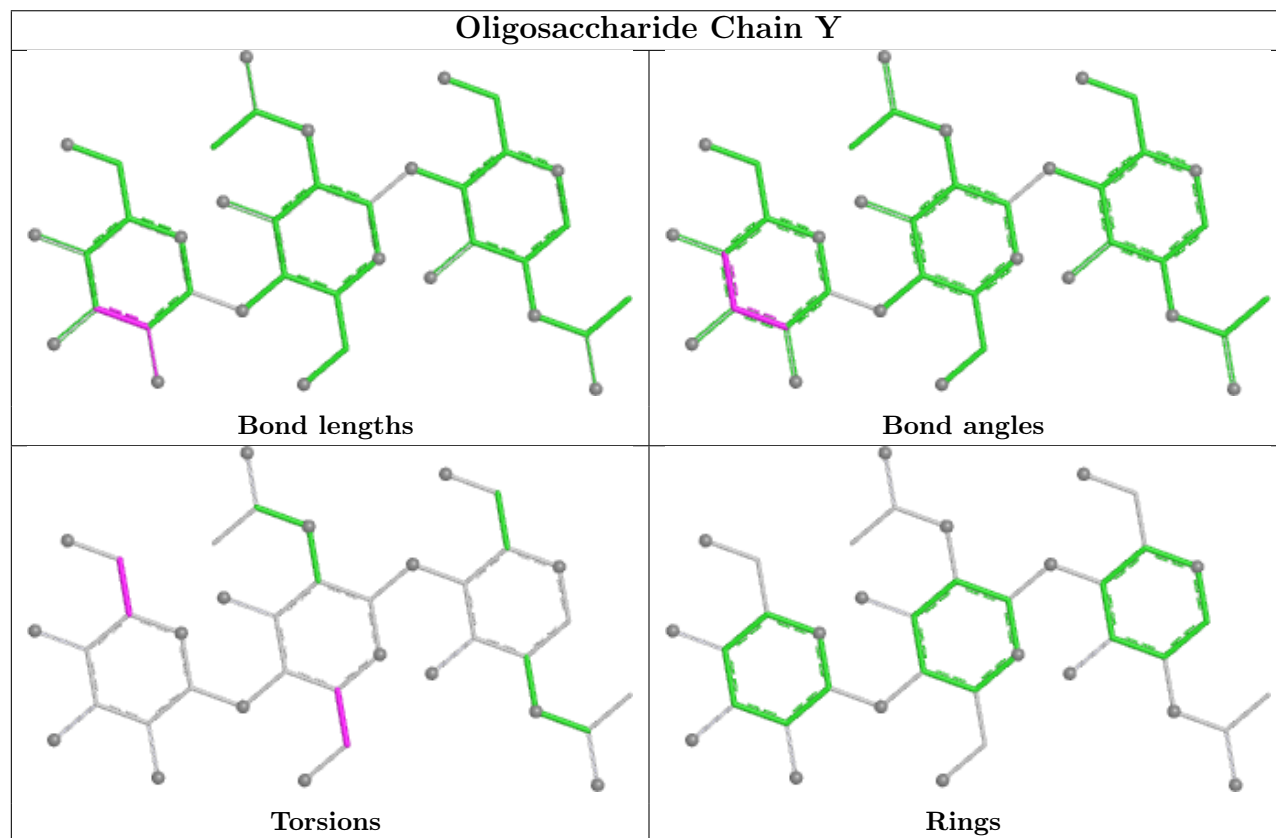
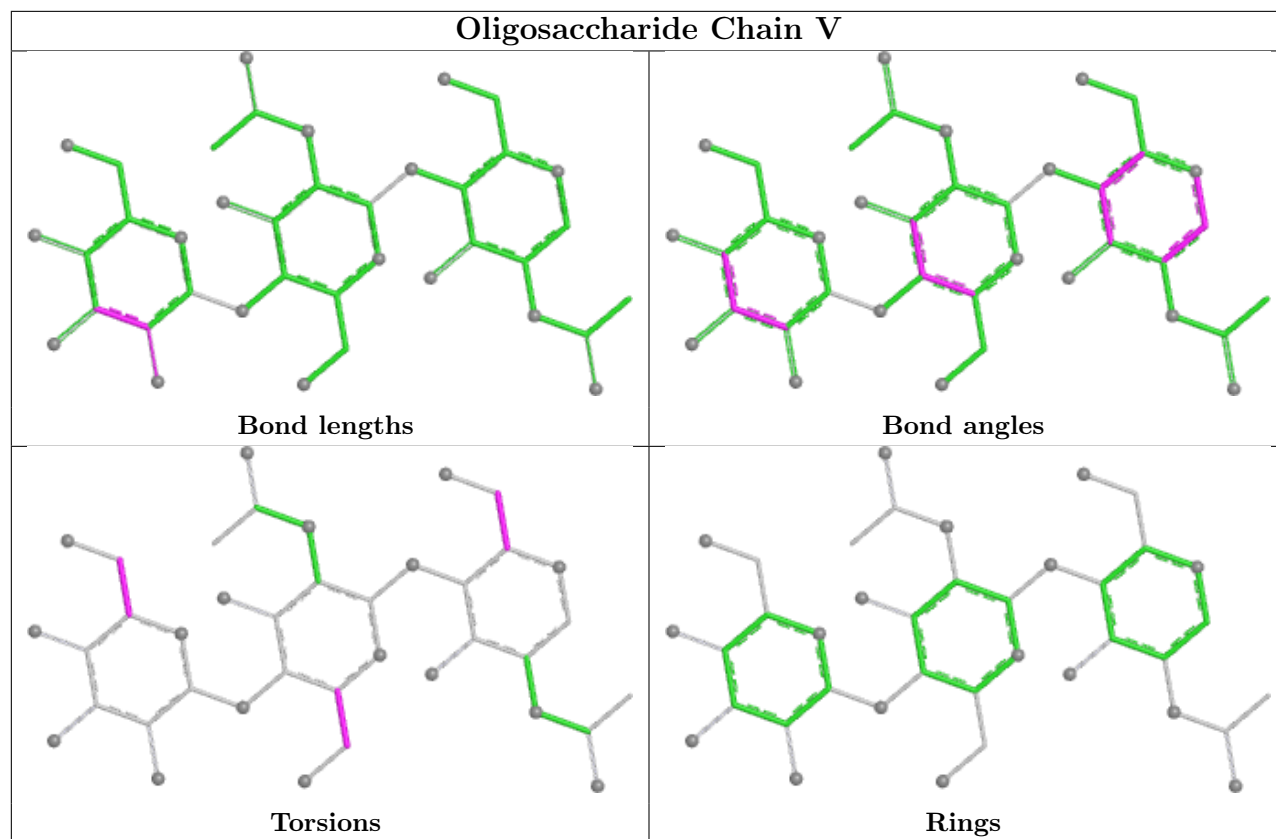


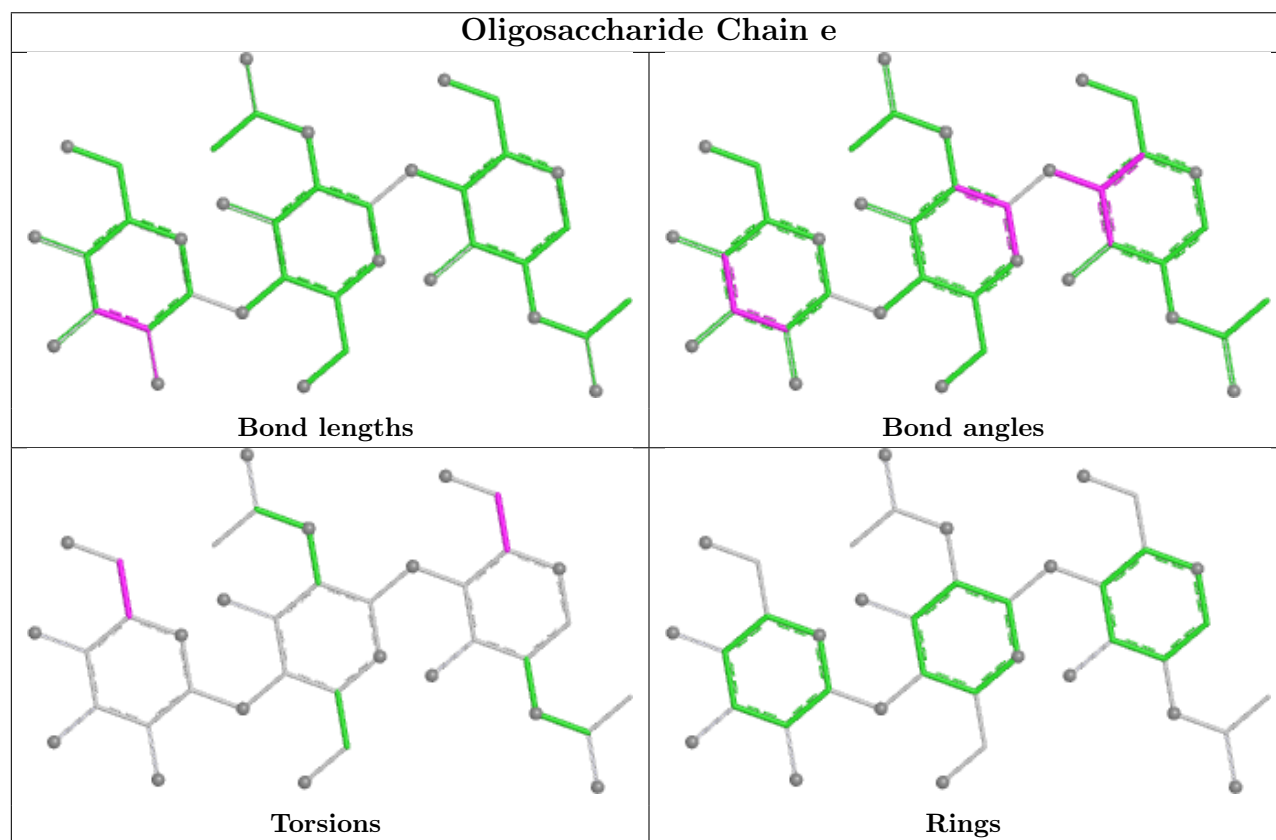
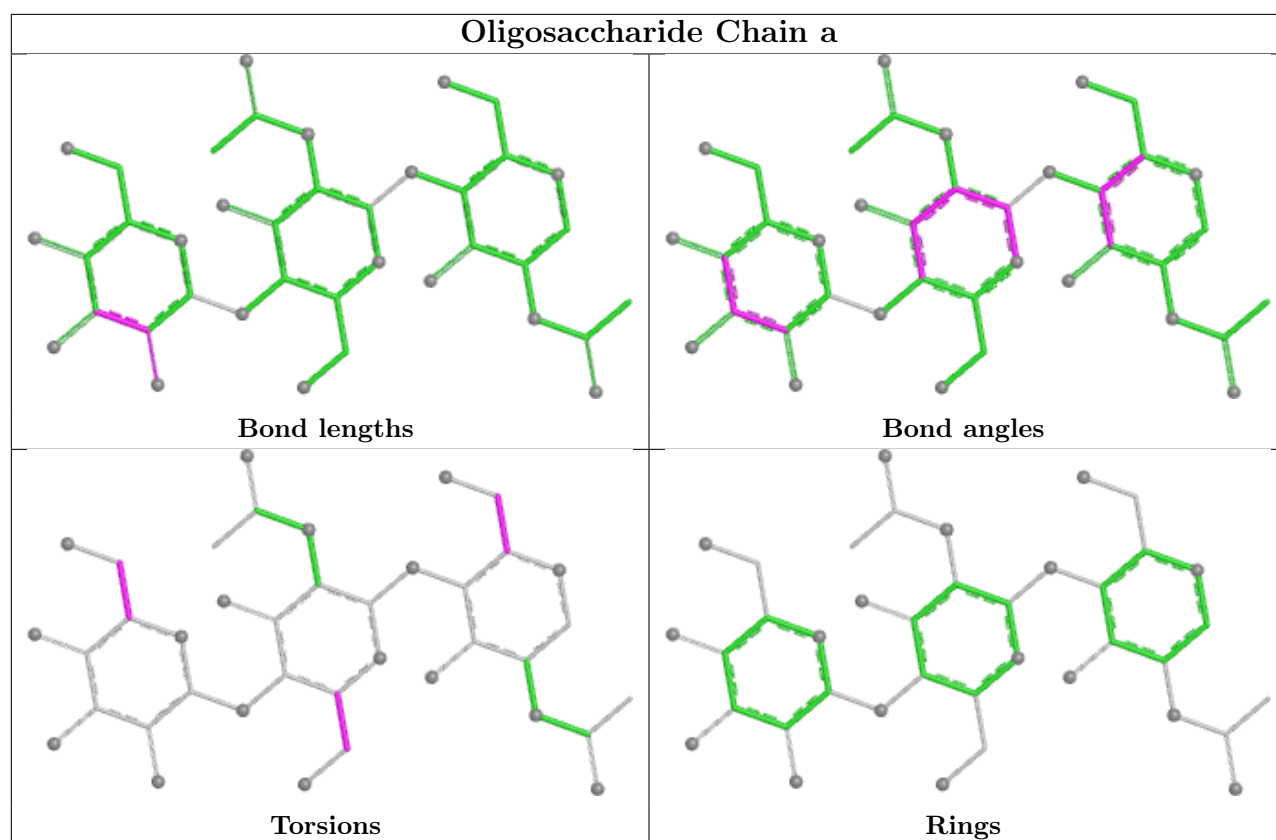


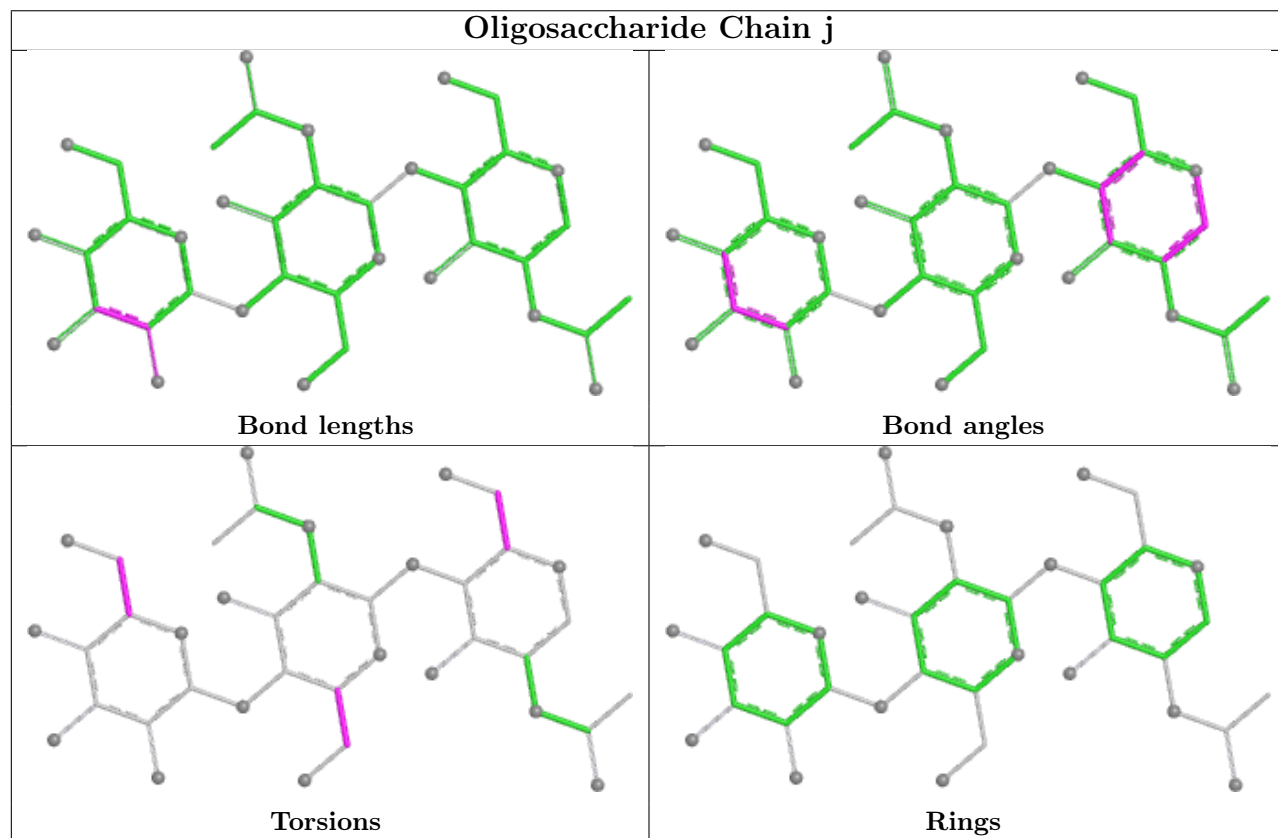
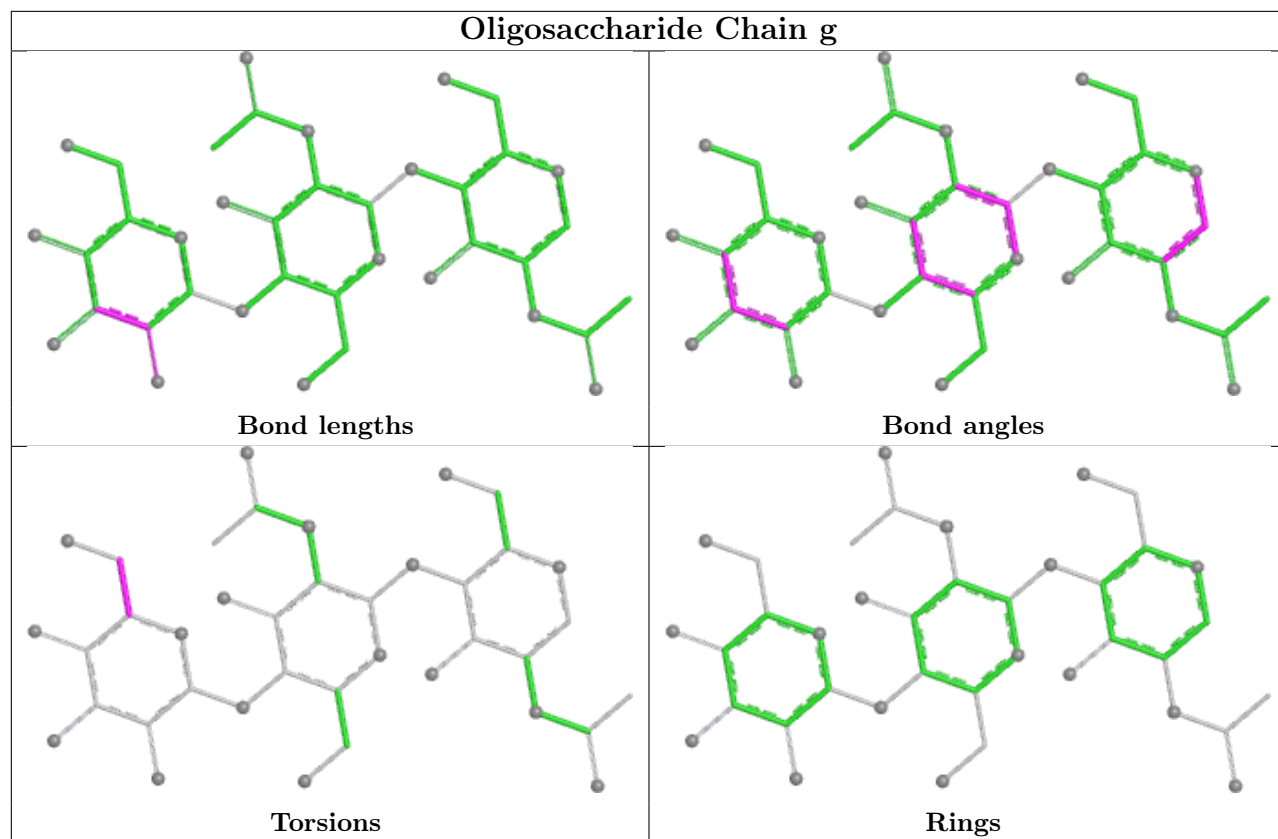


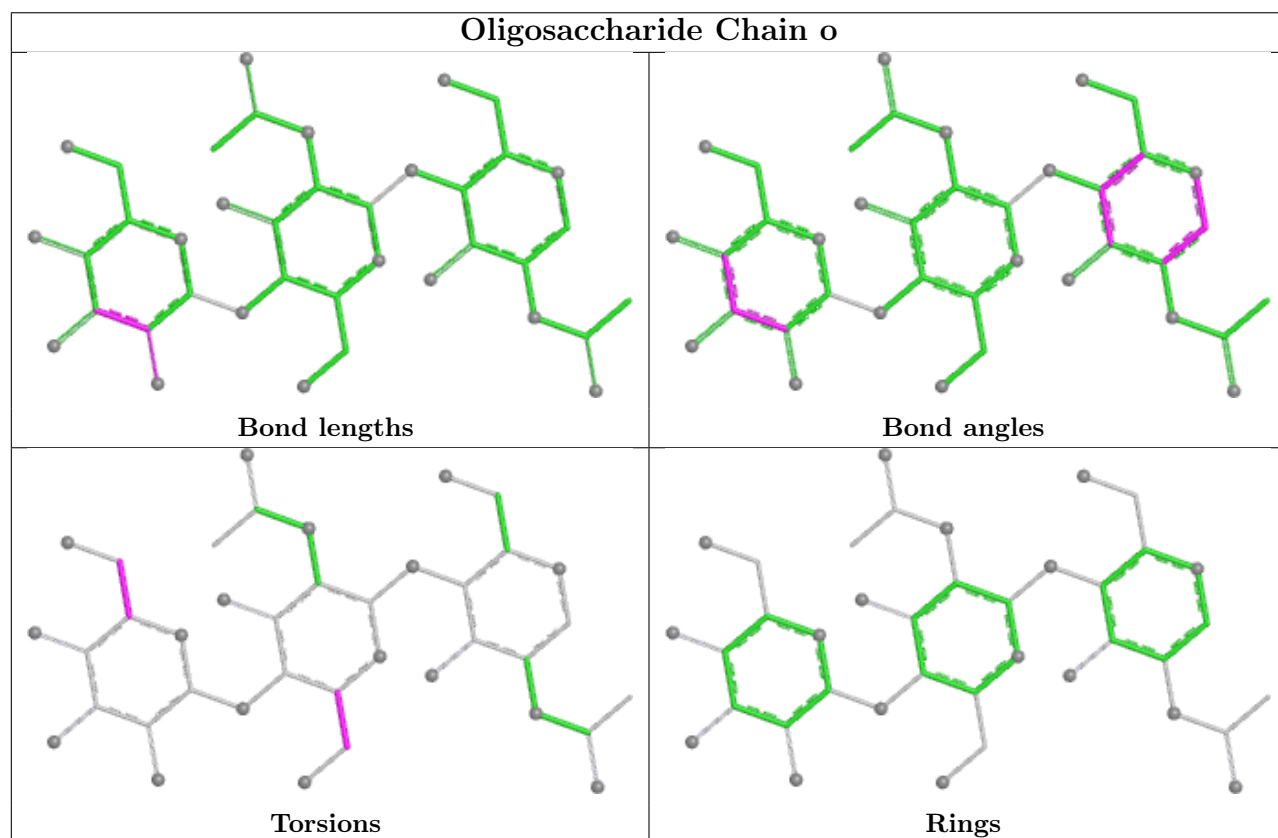
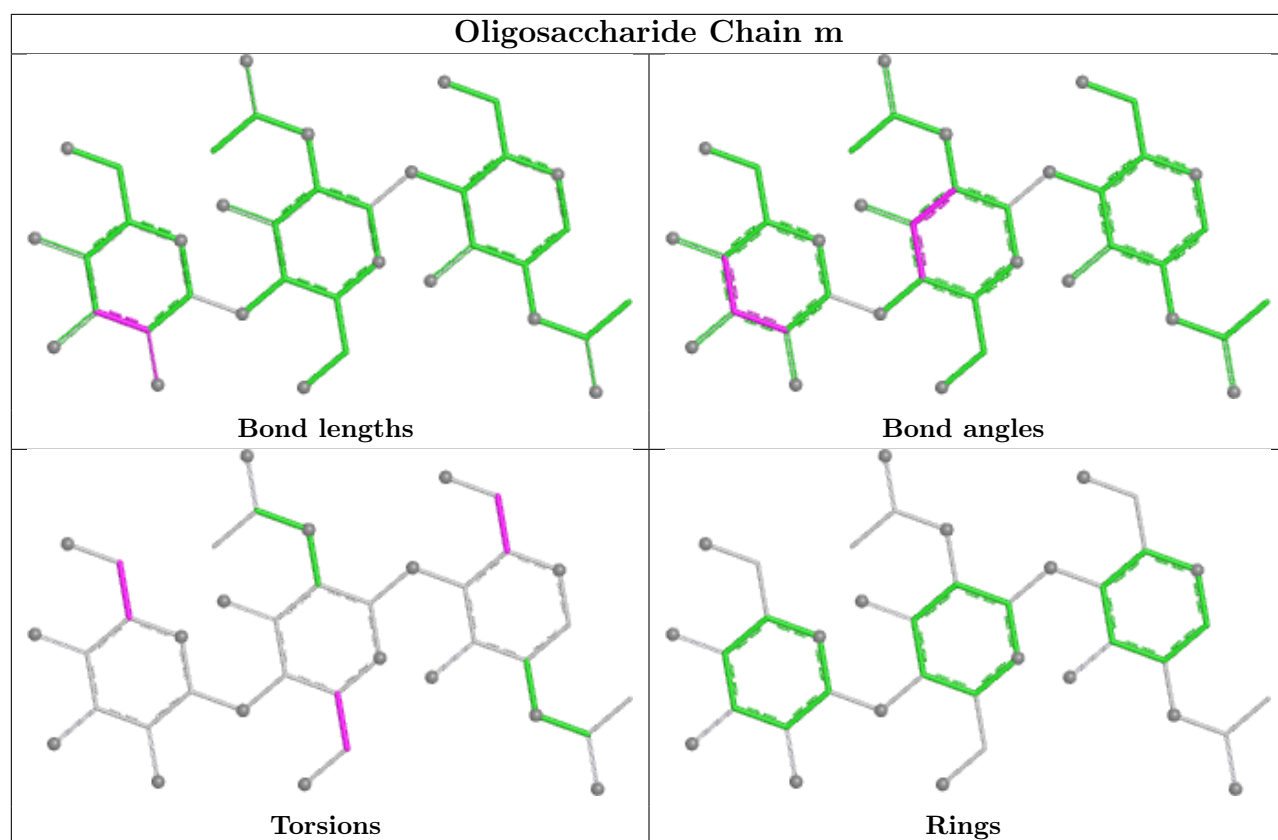


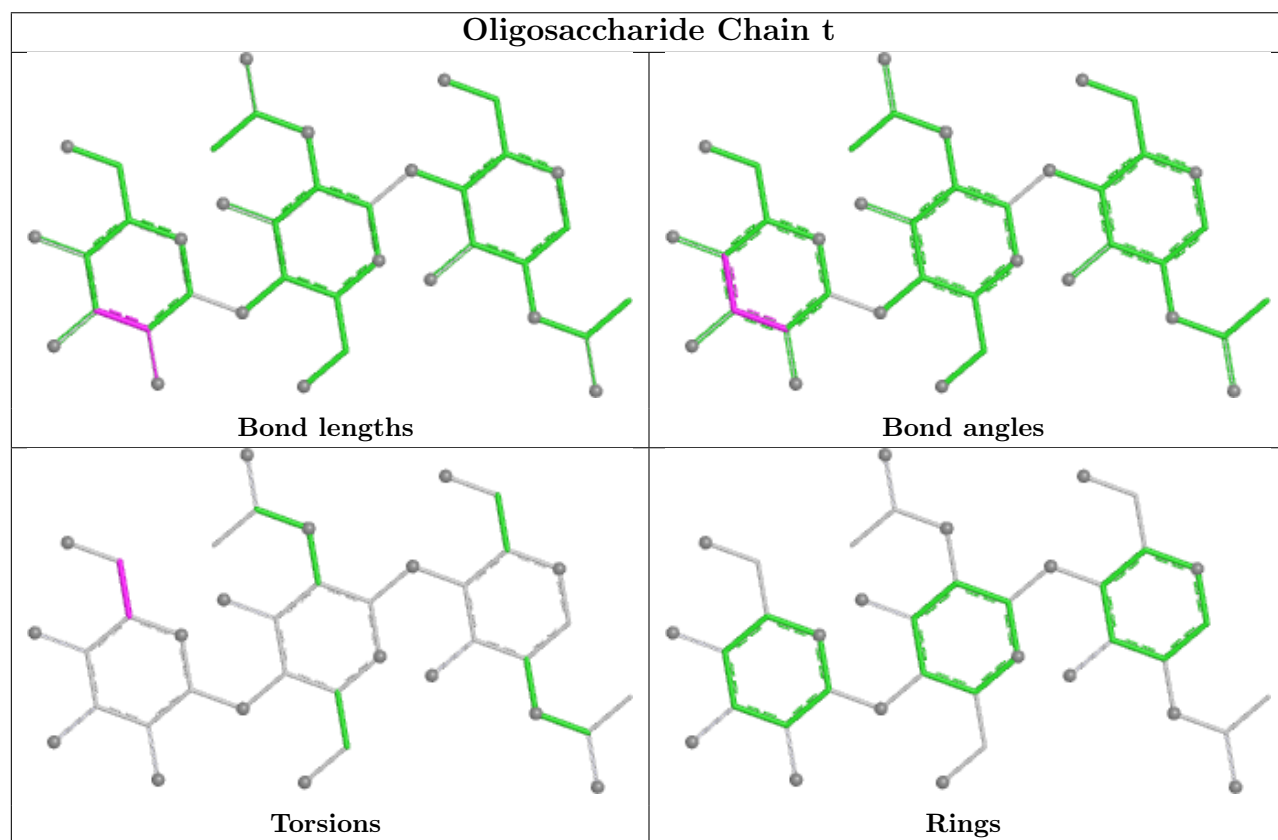
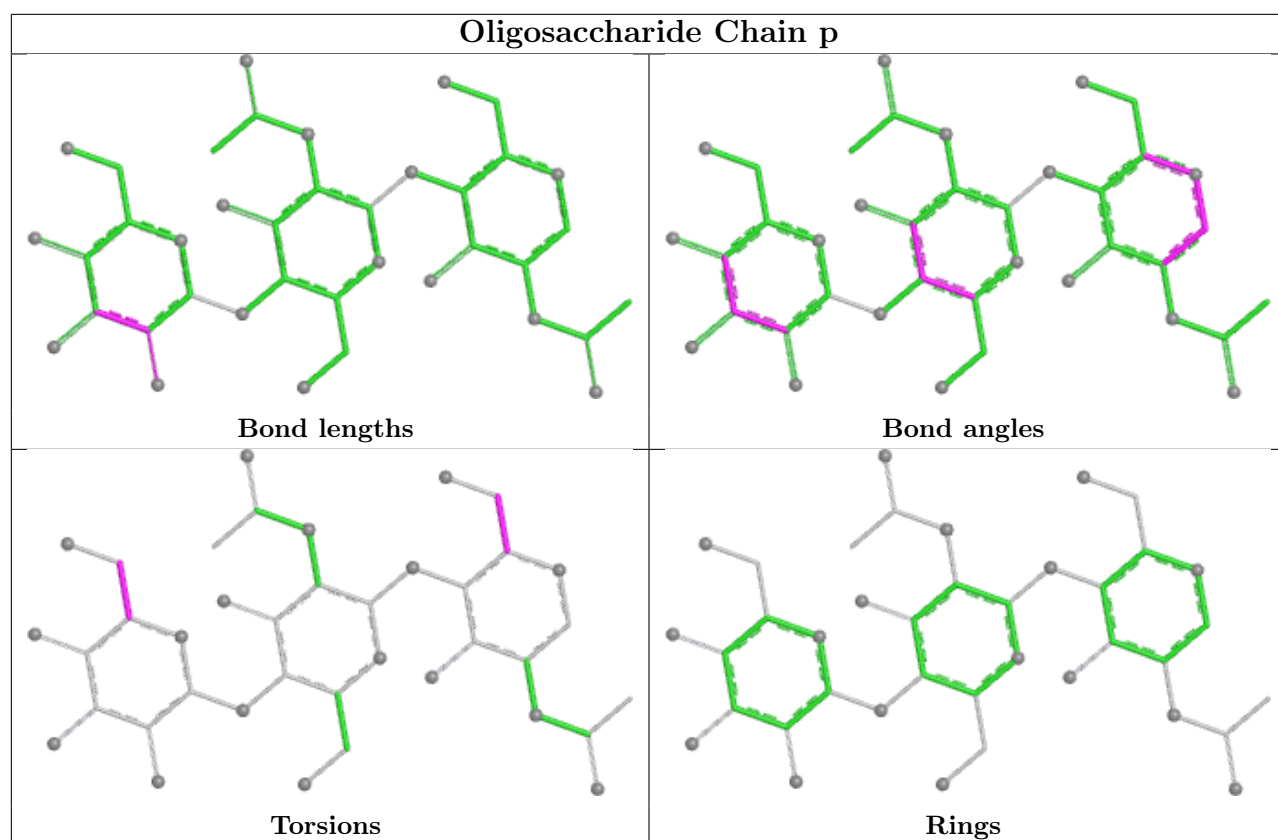


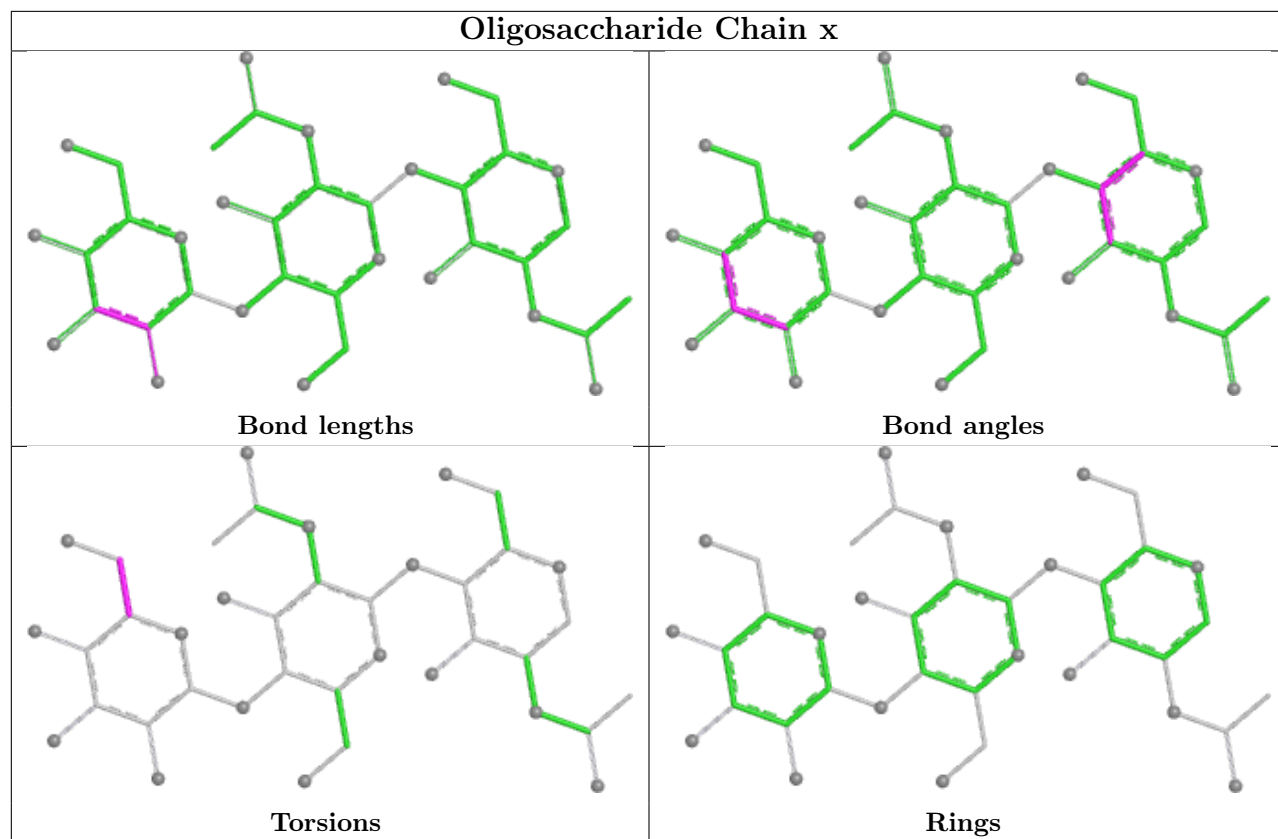


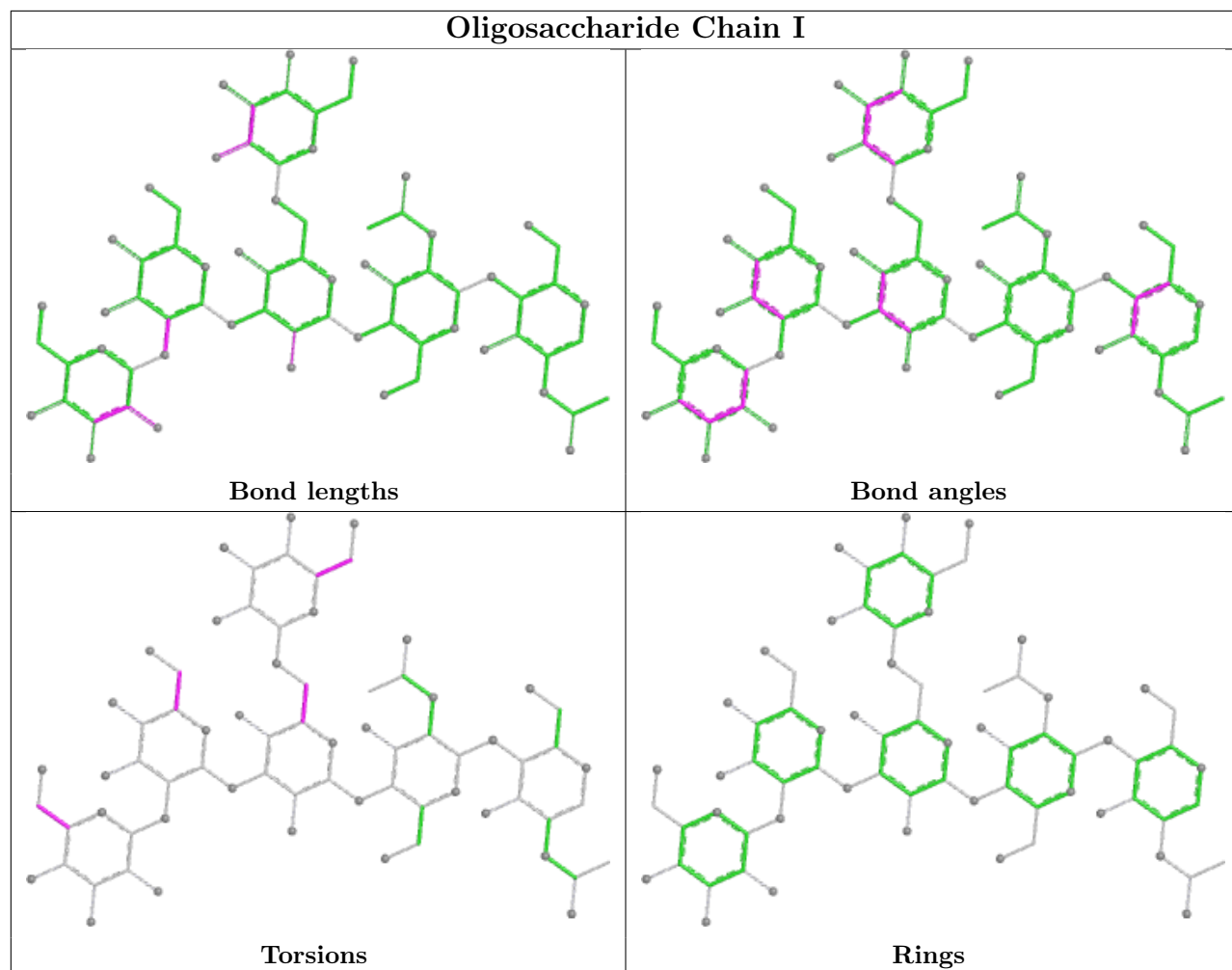




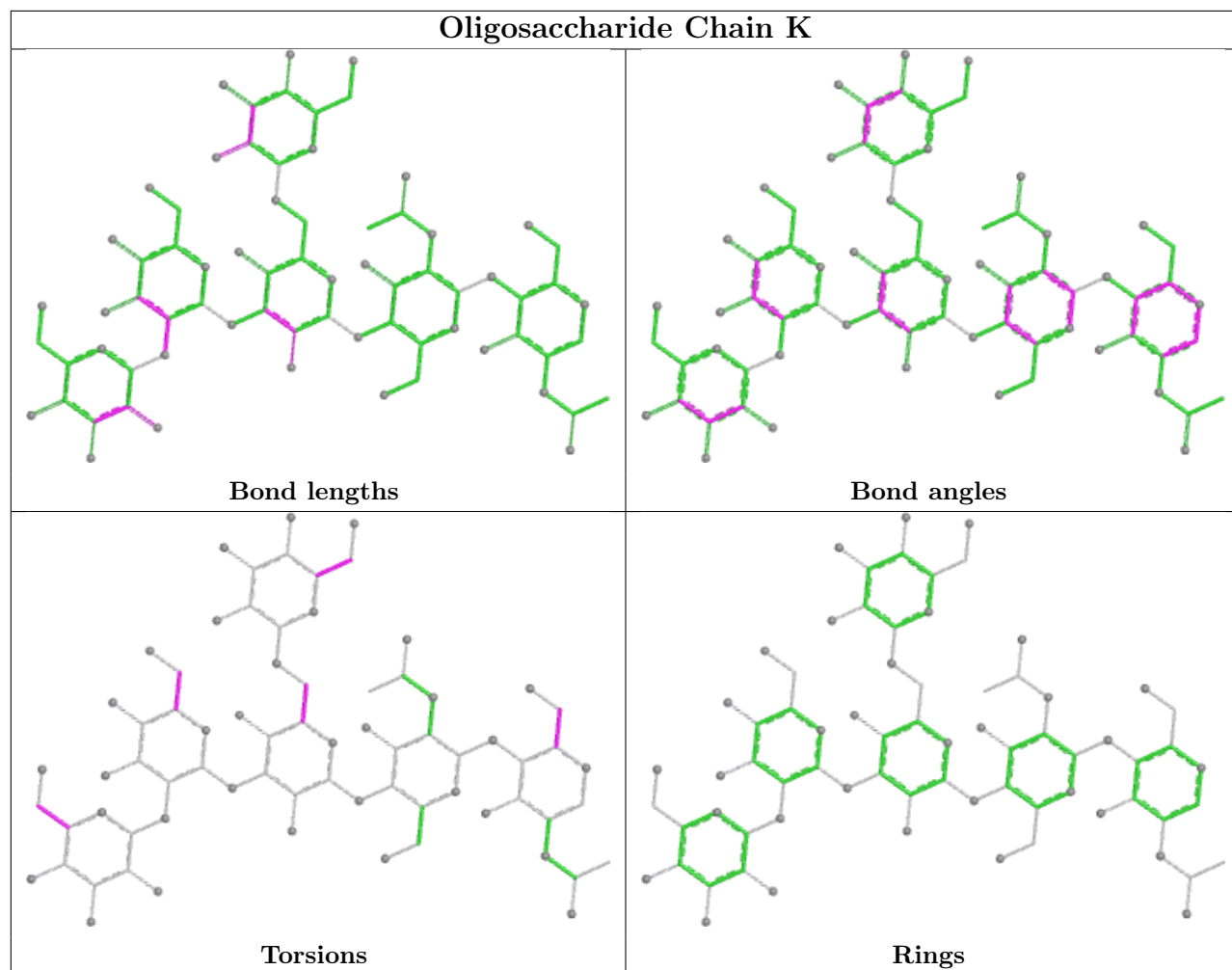


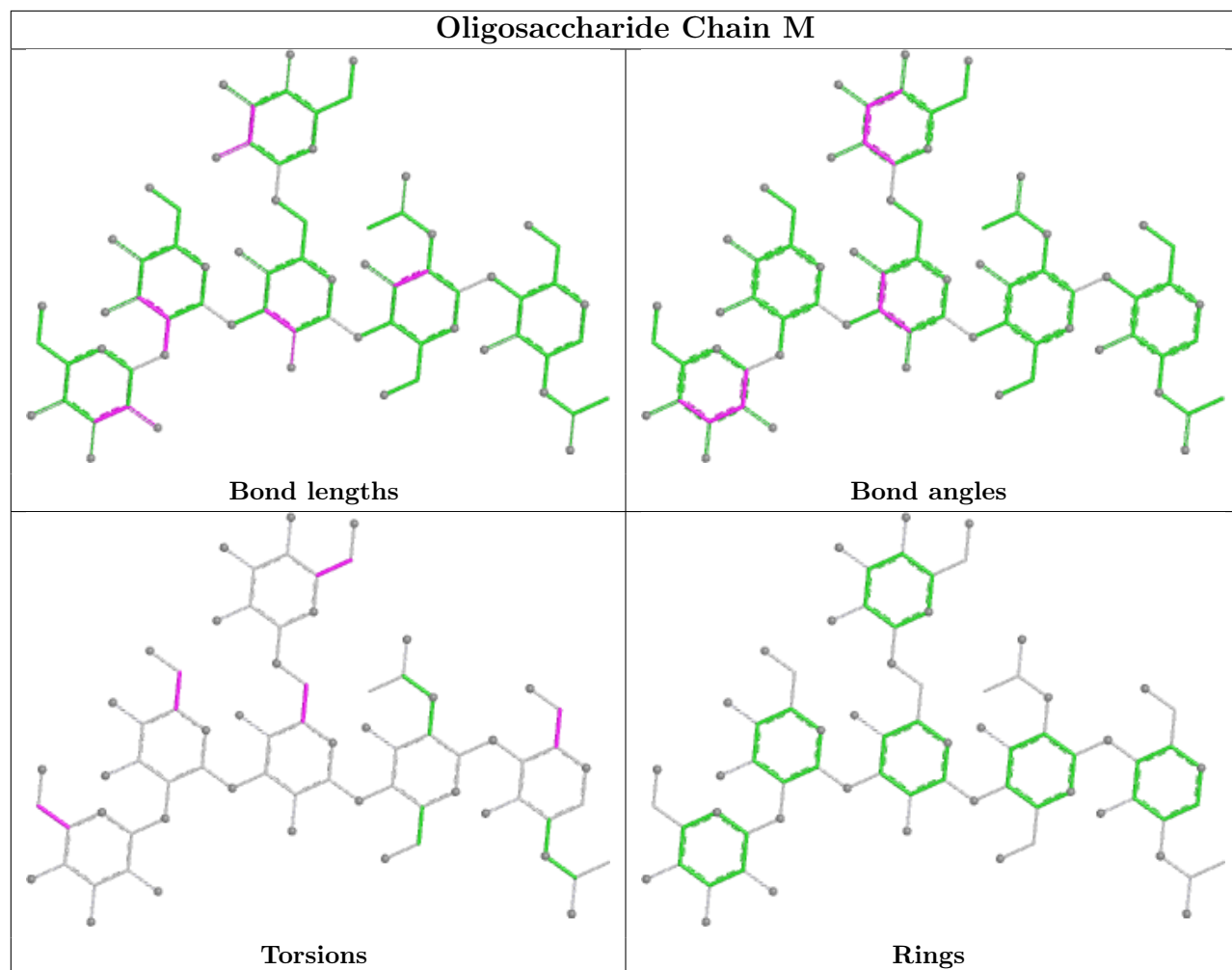


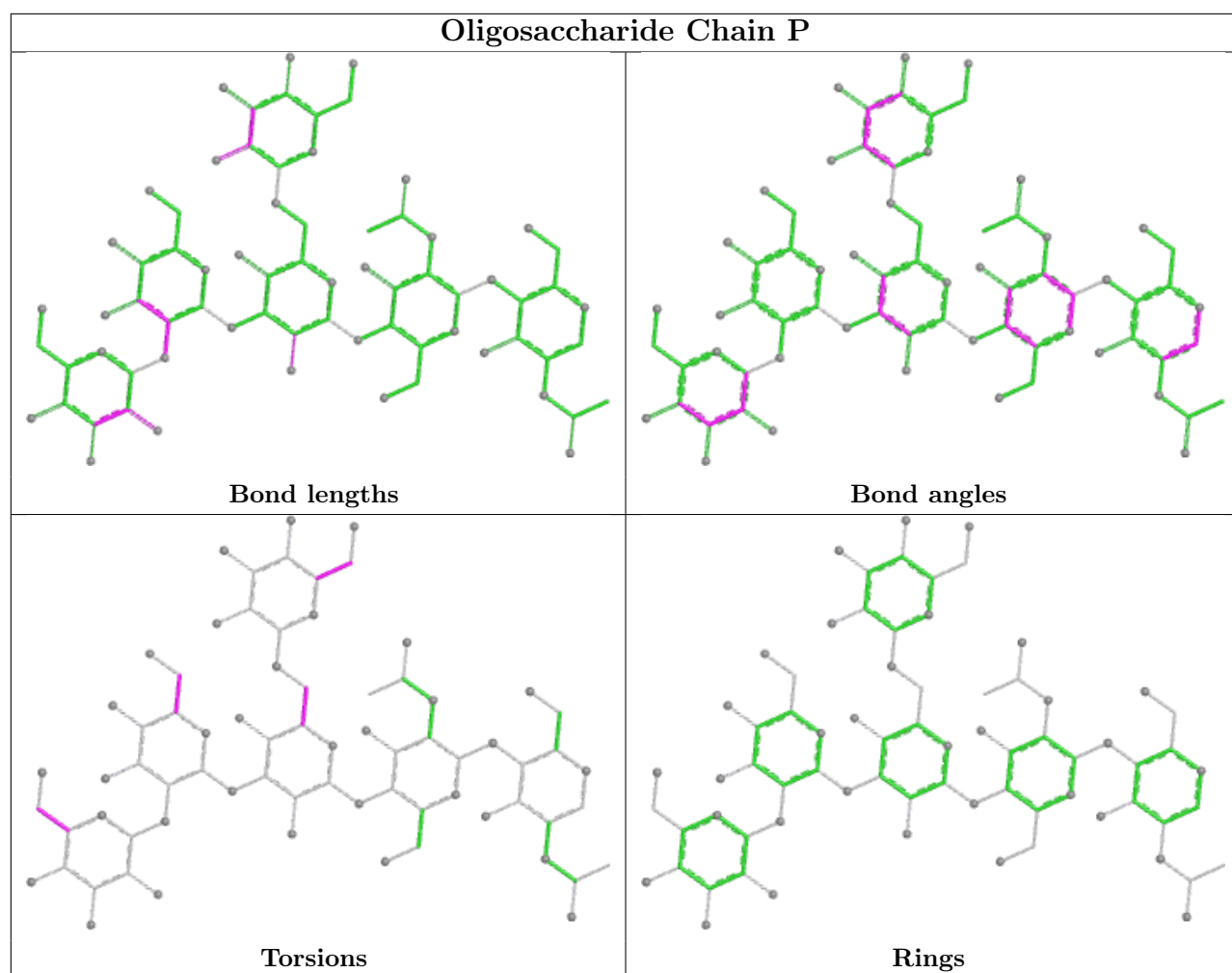


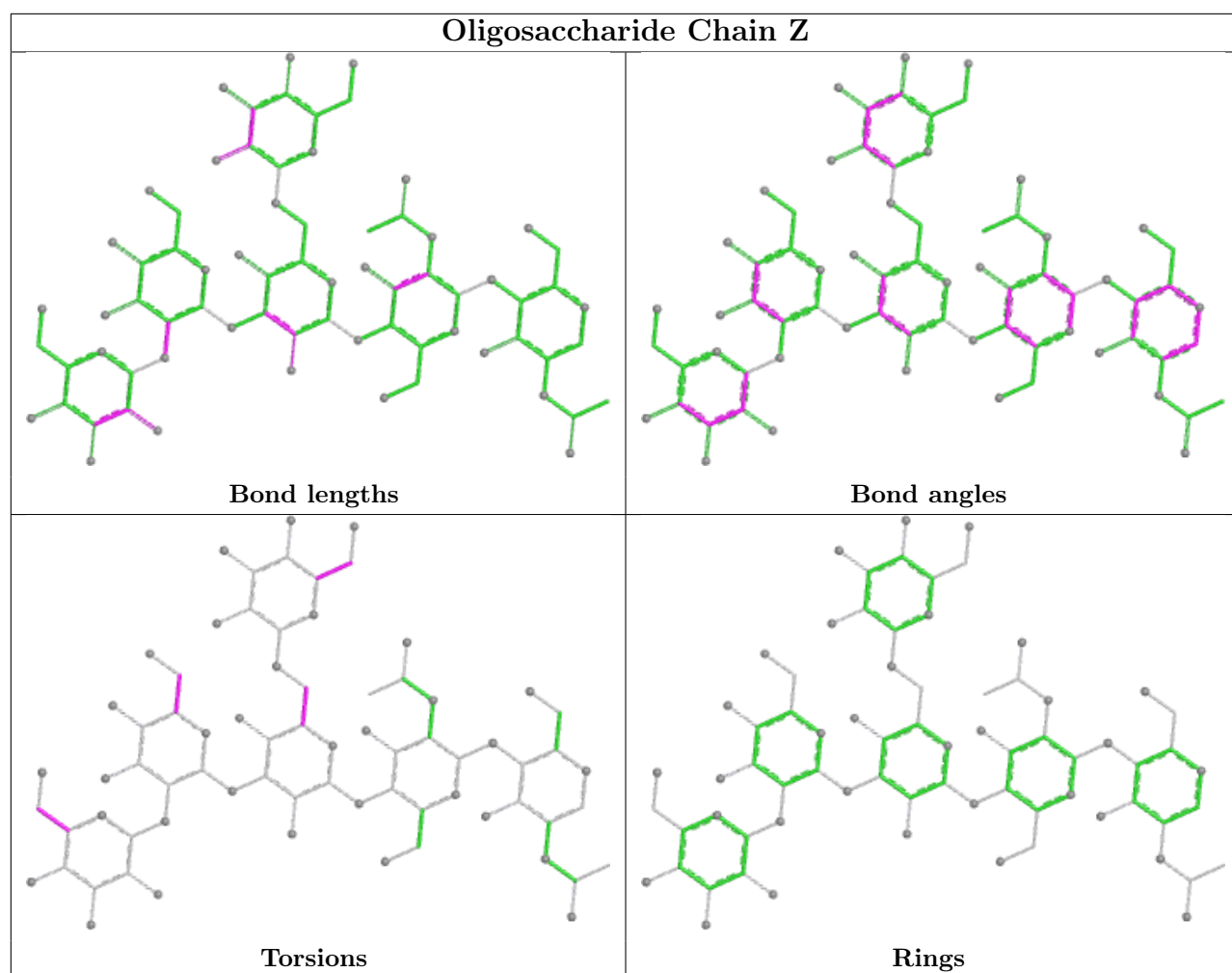


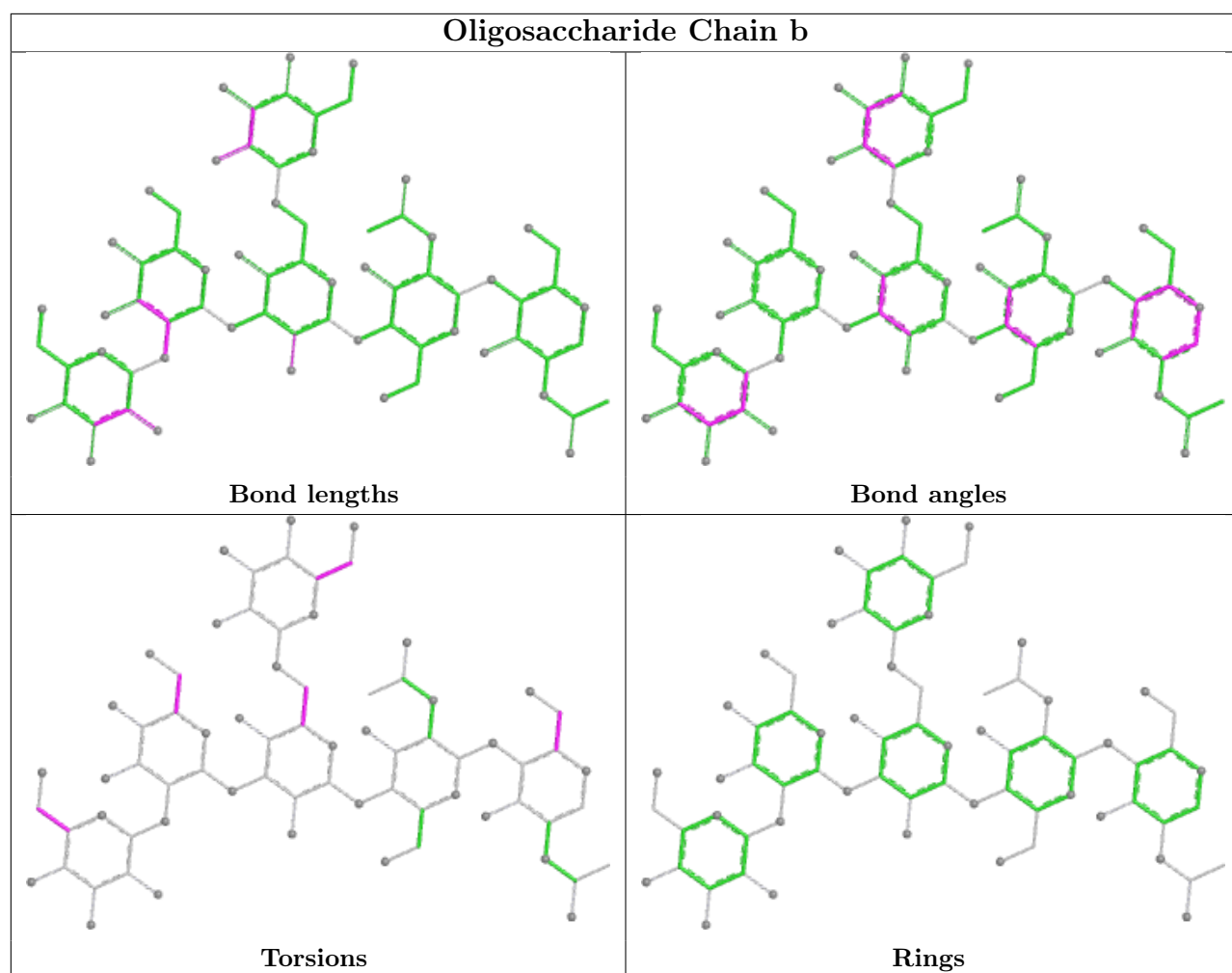
Oligosaccharide Chain K

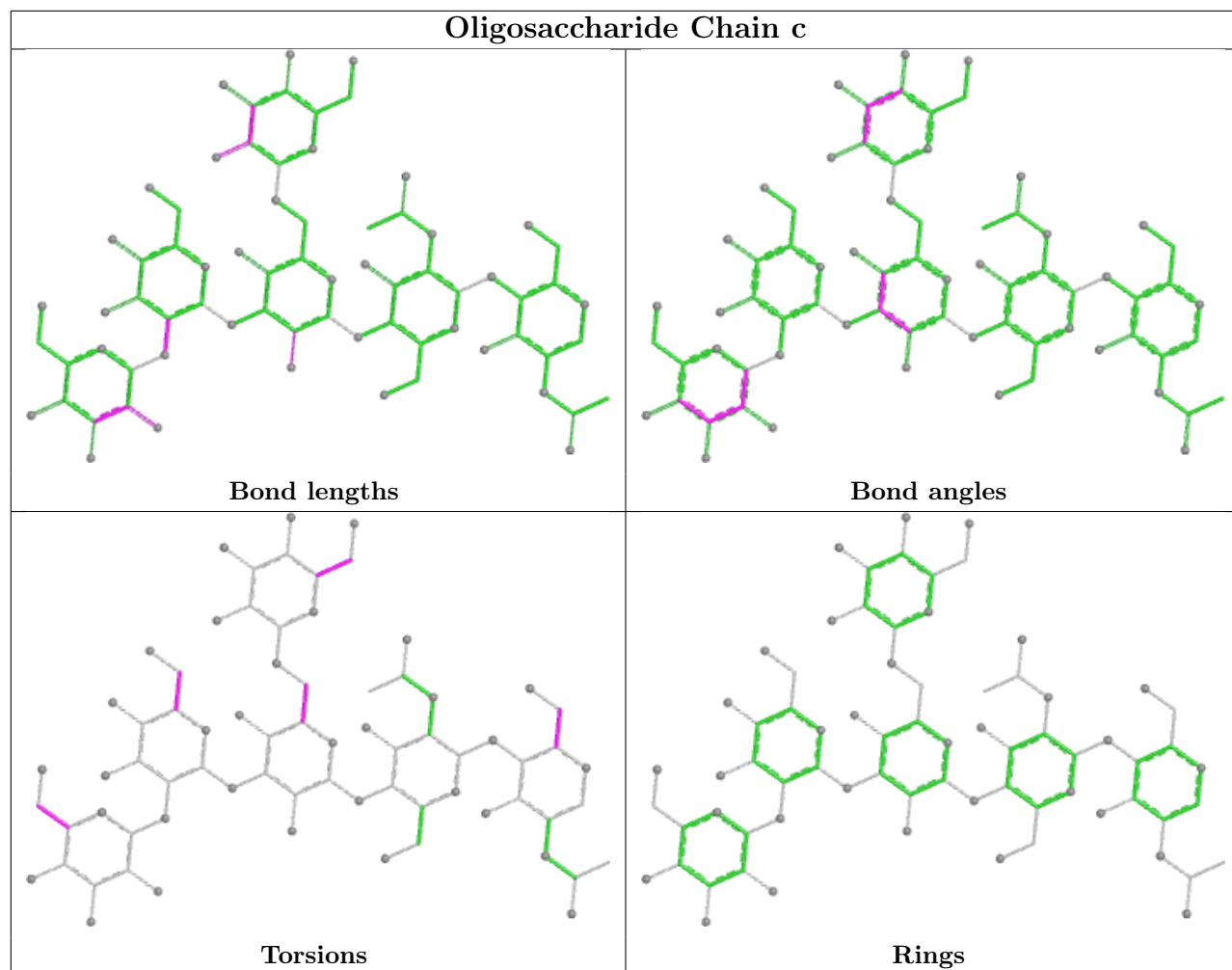


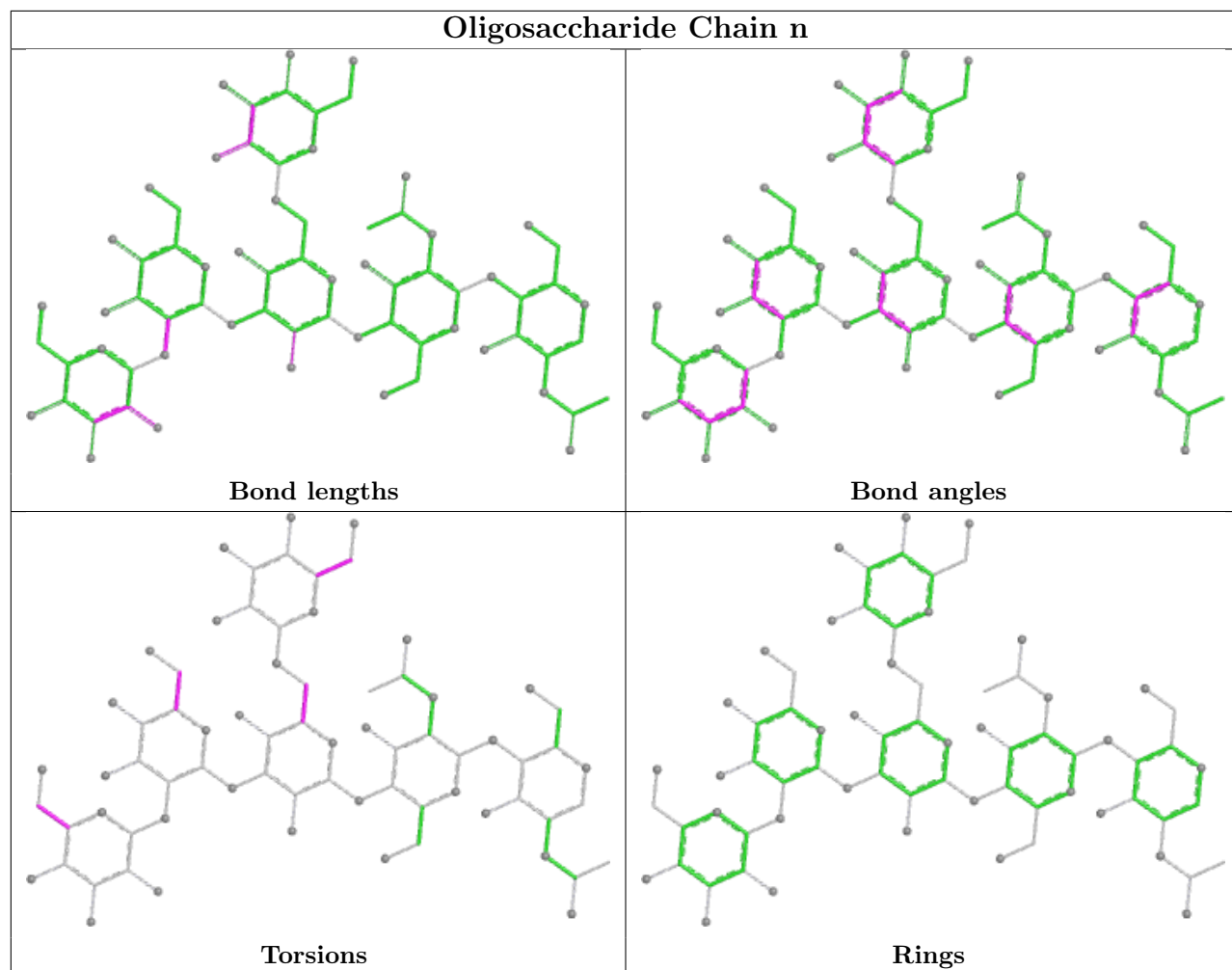


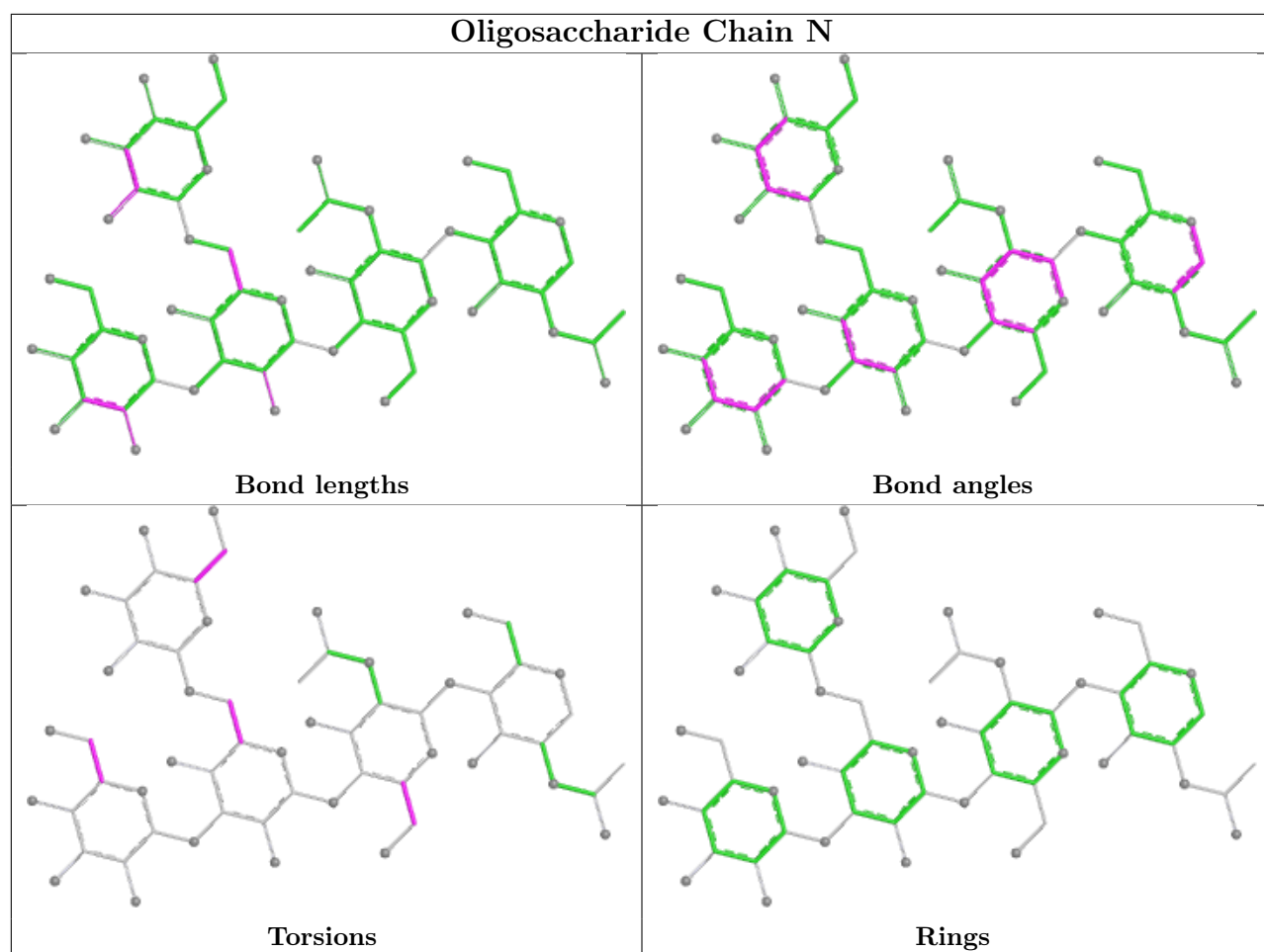


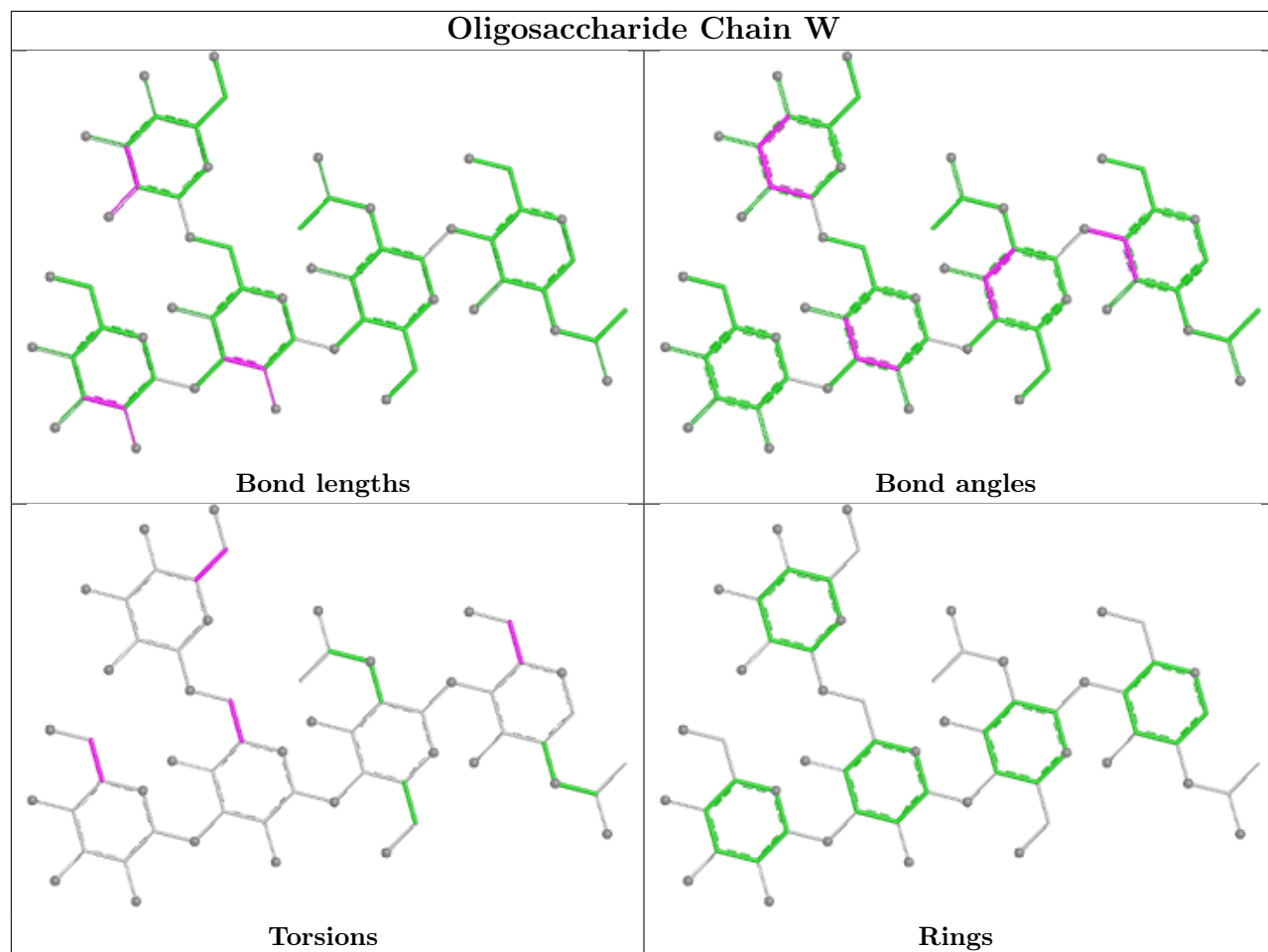


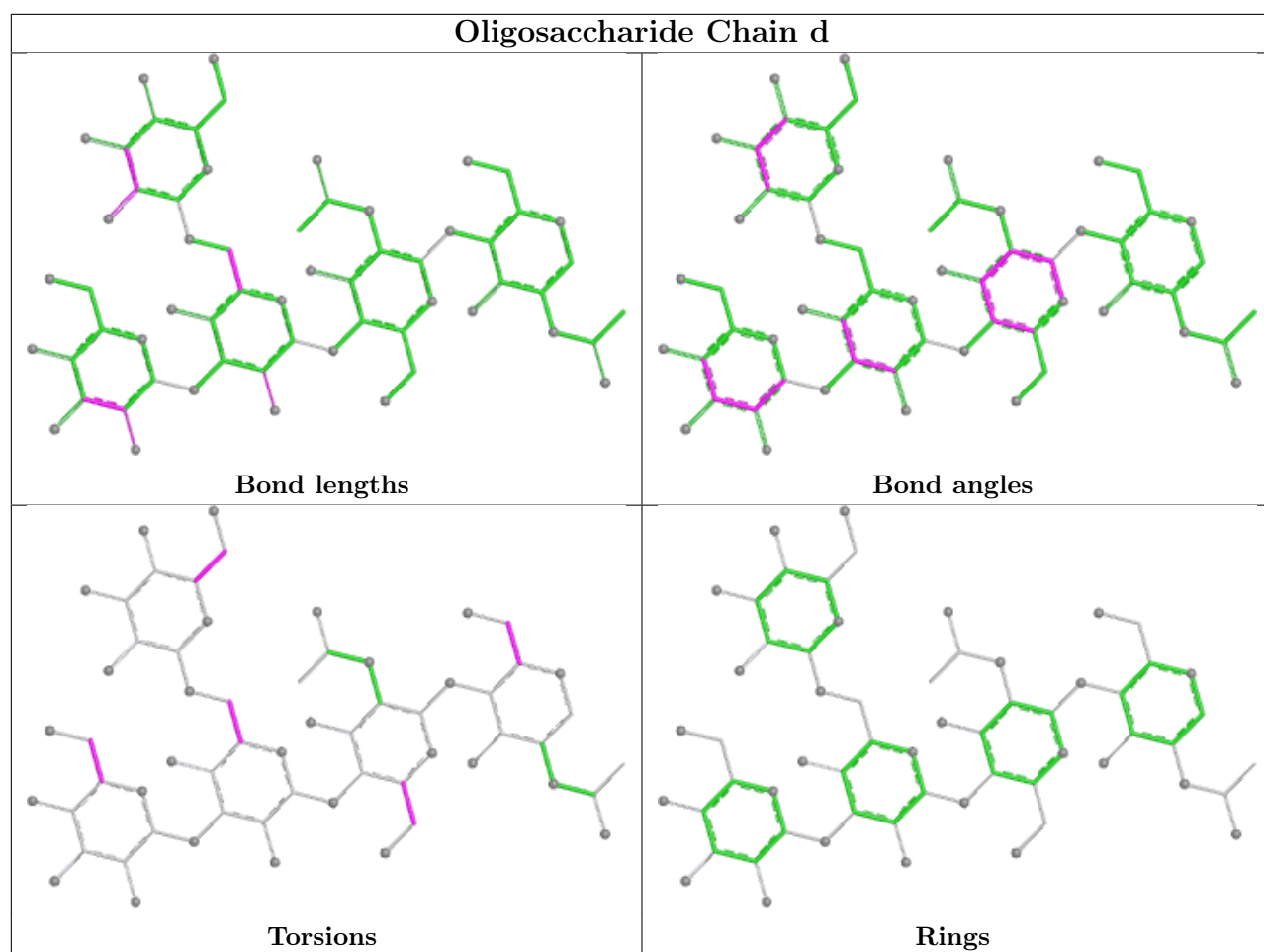


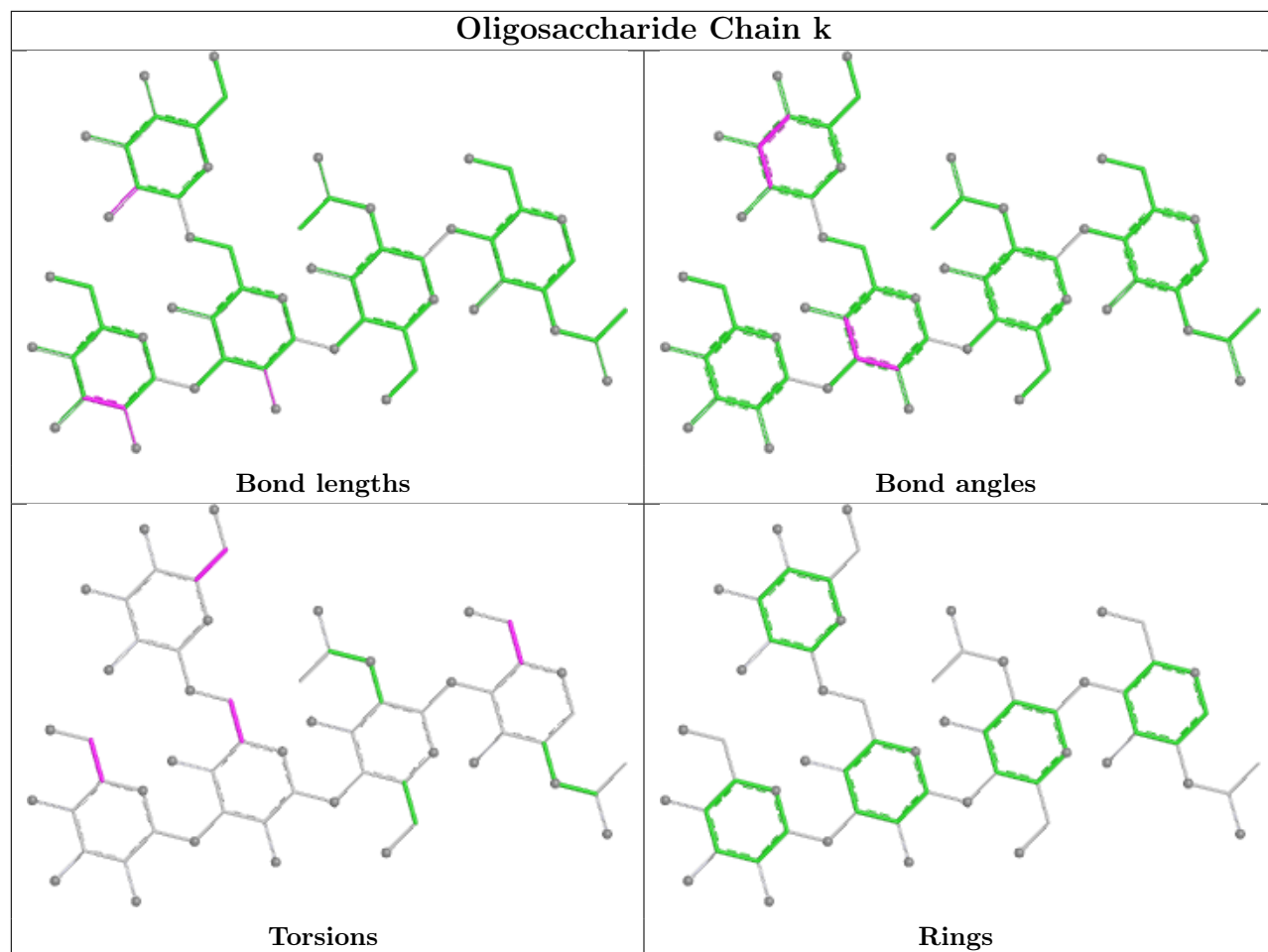


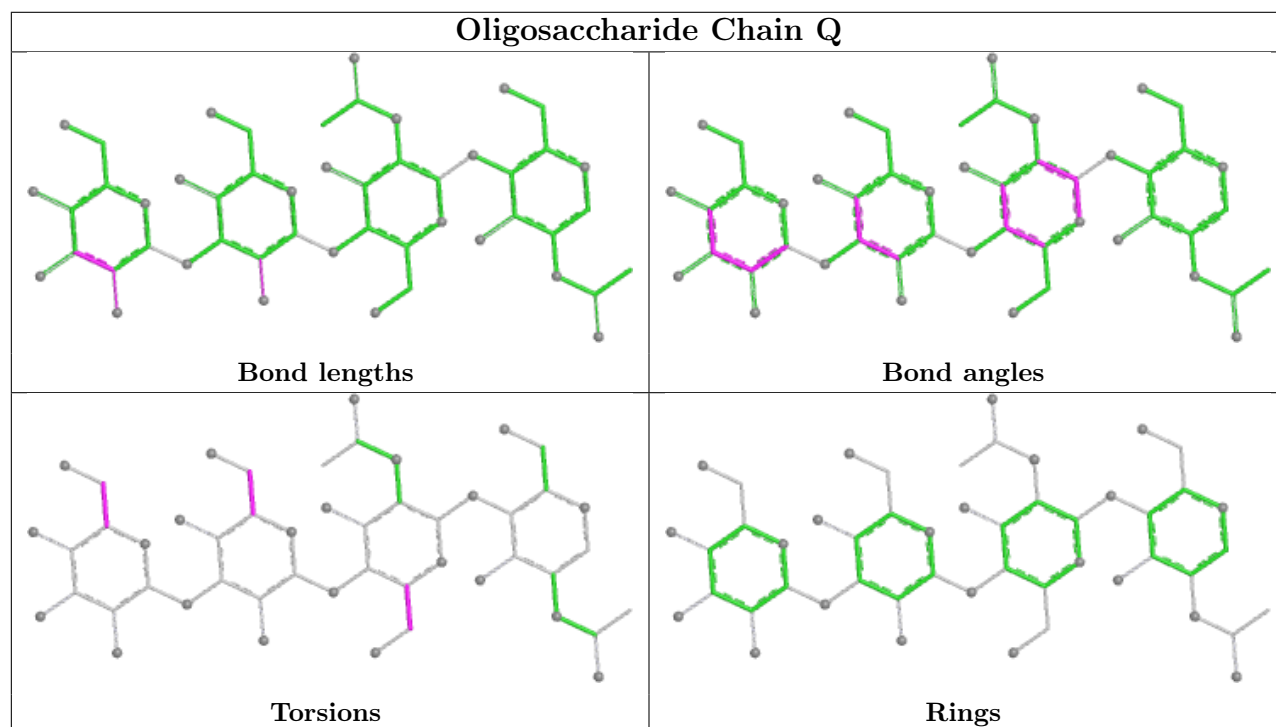
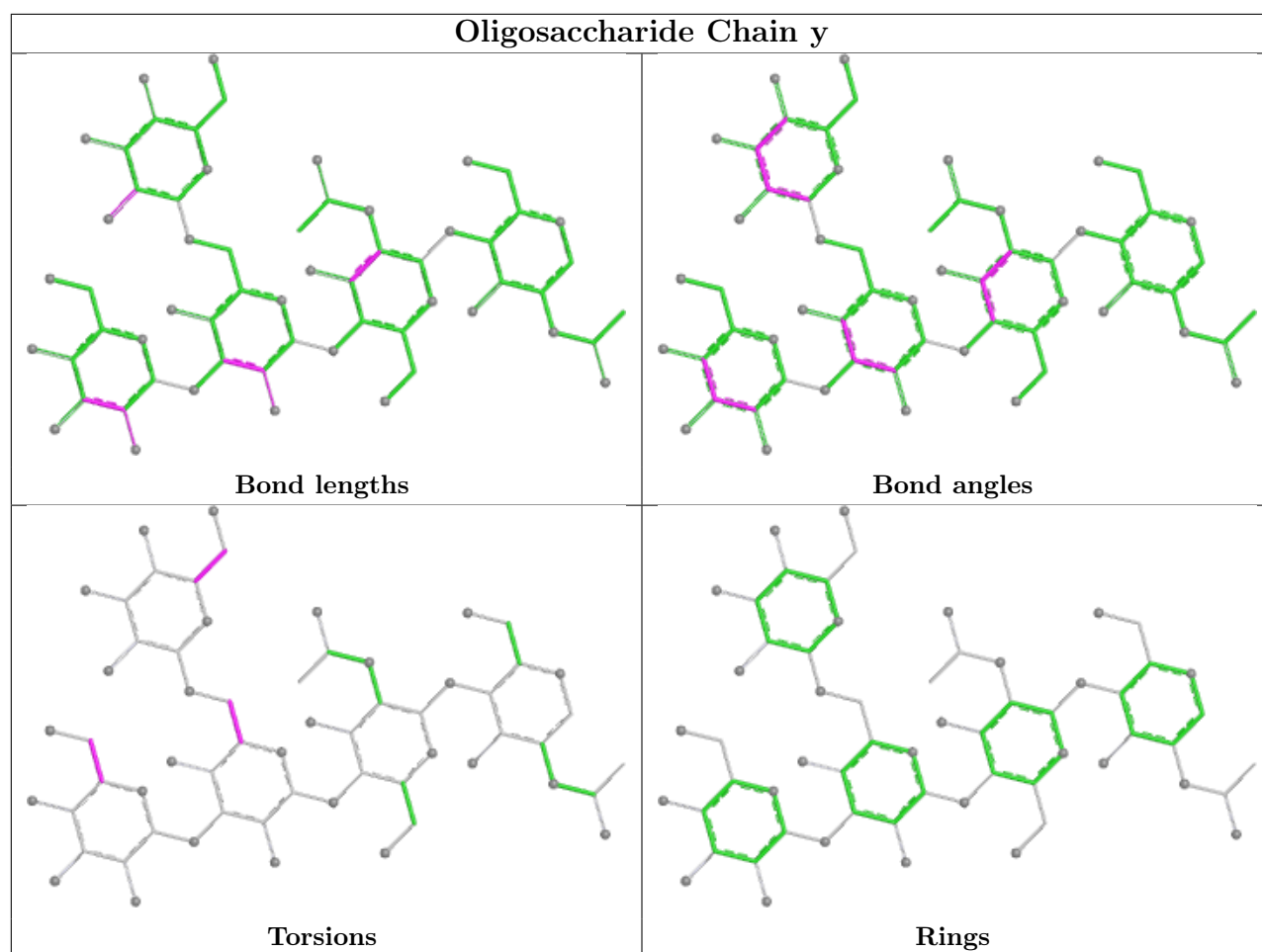


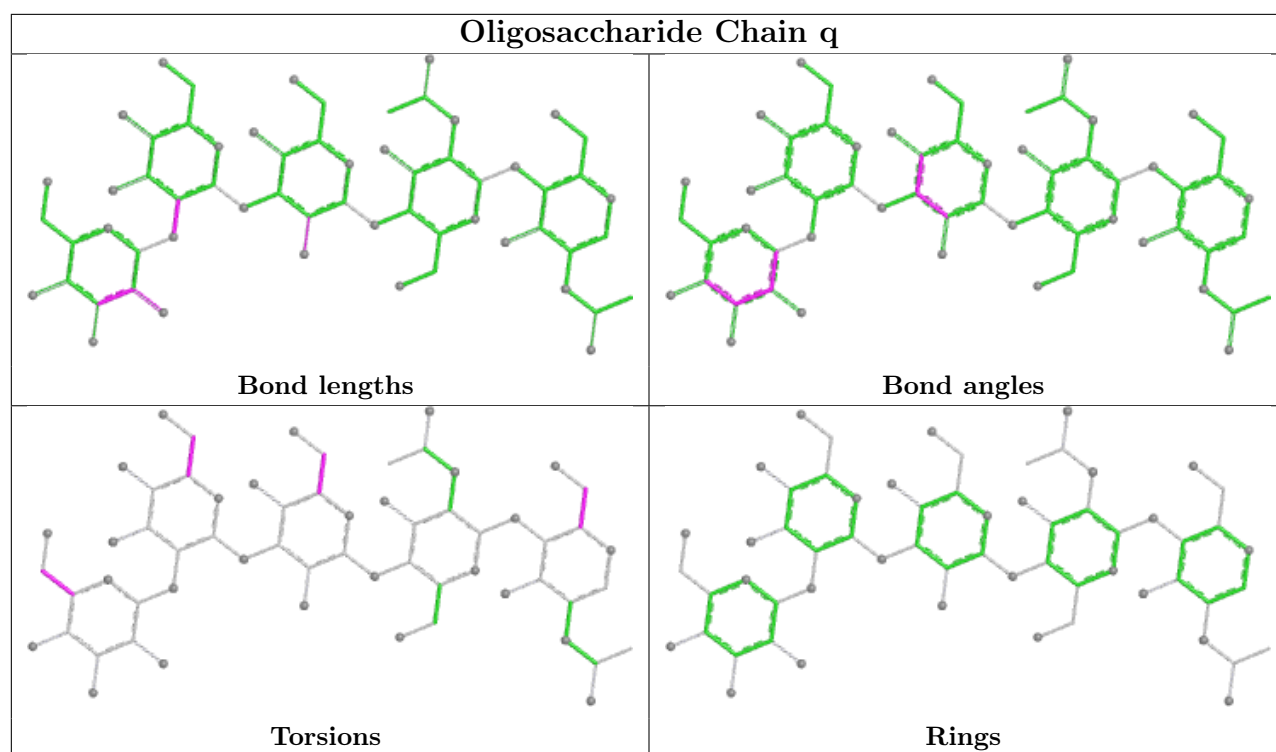












5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
10	NAG	C	1429	1	14,14,15	0.84	0	17,19,21	1.03	1 (5%)
10	NAG	B	1442	1	14,14,15	0.78	0	17,19,21	1.10	1 (5%)
10	NAG	C	1428	1	14,14,15	0.78	0	17,19,21	1.16	1 (5%)
10	NAG	A	1445	1	14,14,15	0.77	0	17,19,21	1.15	1 (5%)
10	NAG	C	1423	1	14,14,15	0.80	0	17,19,21	1.17	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	C	1429	1	-	1/6/23/26	0/1/1/1
10	NAG	B	1442	1	-	2/6/23/26	0/1/1/1
10	NAG	C	1428	1	-	1/6/23/26	0/1/1/1
10	NAG	A	1445	1	-	1/6/23/26	0/1/1/1
10	NAG	C	1423	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1428	NAG	C4-C3-C2	-3.70	105.60	111.02
10	C	1423	NAG	C4-C3-C2	-3.68	105.62	111.02
10	B	1442	NAG	C4-C3-C2	-3.39	106.06	111.02
10	A	1445	NAG	C4-C3-C2	-3.13	106.42	111.02
10	C	1429	NAG	C4-C3-C2	-2.92	106.73	111.02

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1423	NAG	O5-C5-C6-O6
10	B	1442	NAG	O5-C5-C6-O6
10	A	1445	NAG	O5-C5-C6-O6
10	C	1428	NAG	O5-C5-C6-O6
10	C	1429	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

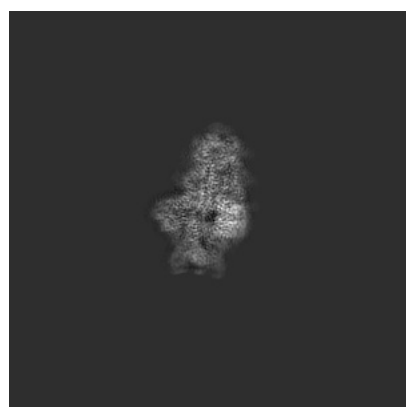
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0401. These allow visual inspection of the internal detail of the map and identification of artifacts.

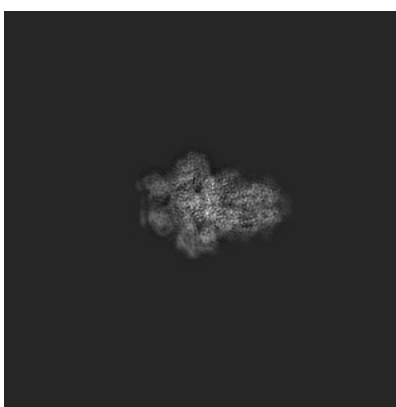
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

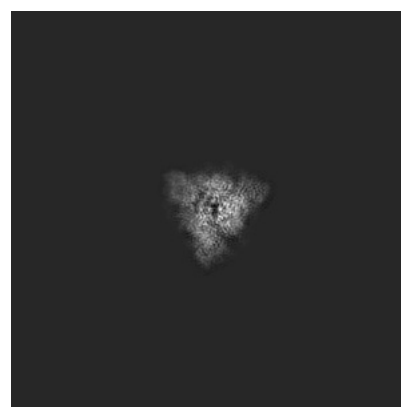
6.1.1 Primary map



X



Y

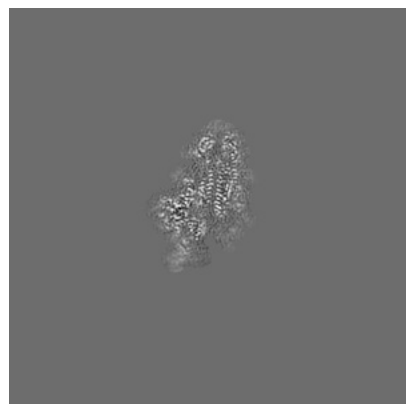


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192

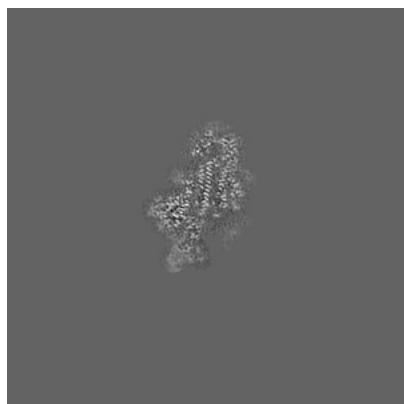


Z Index: 192

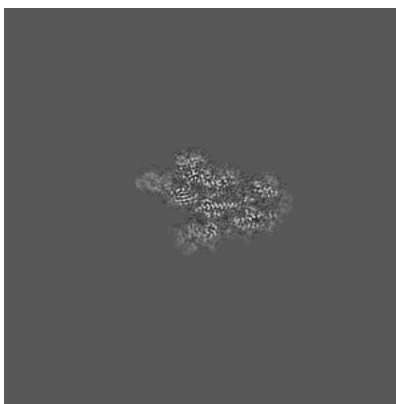
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 201

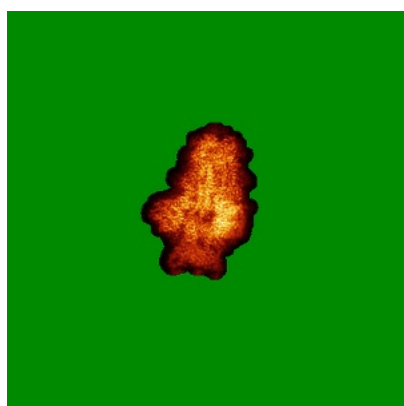


Z Index: 194

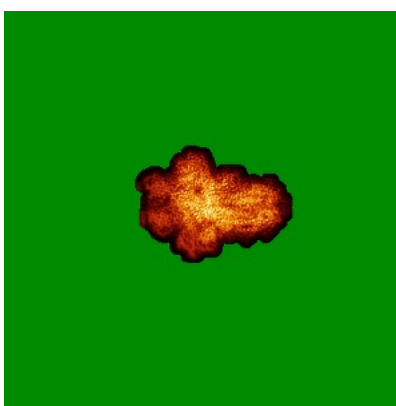
The images above show the largest variance slices of the map in three orthogonal directions.

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

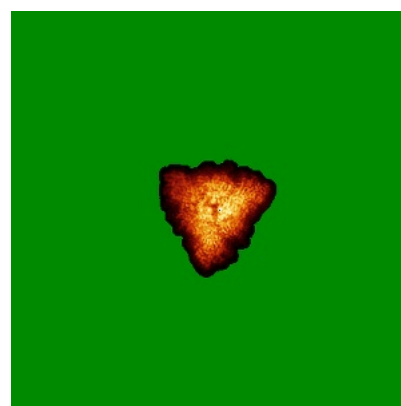
6.4.1 Primary map



X



Y

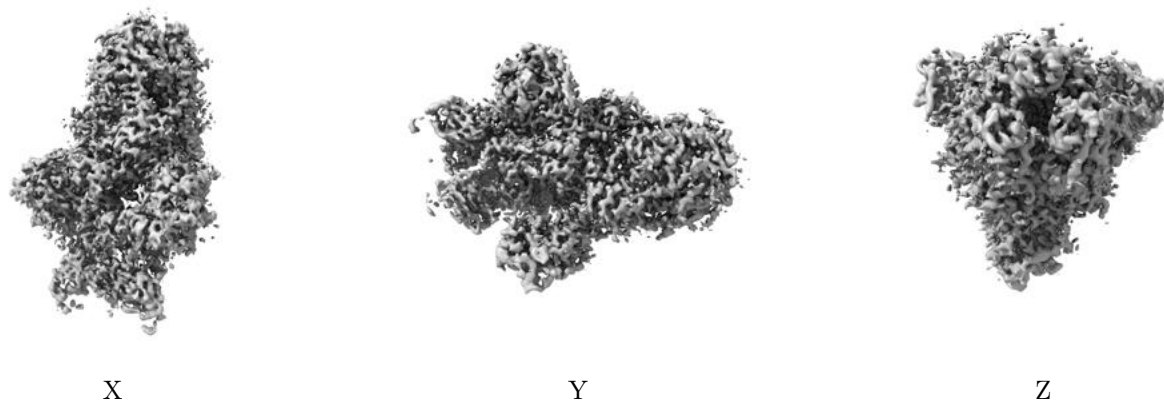


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

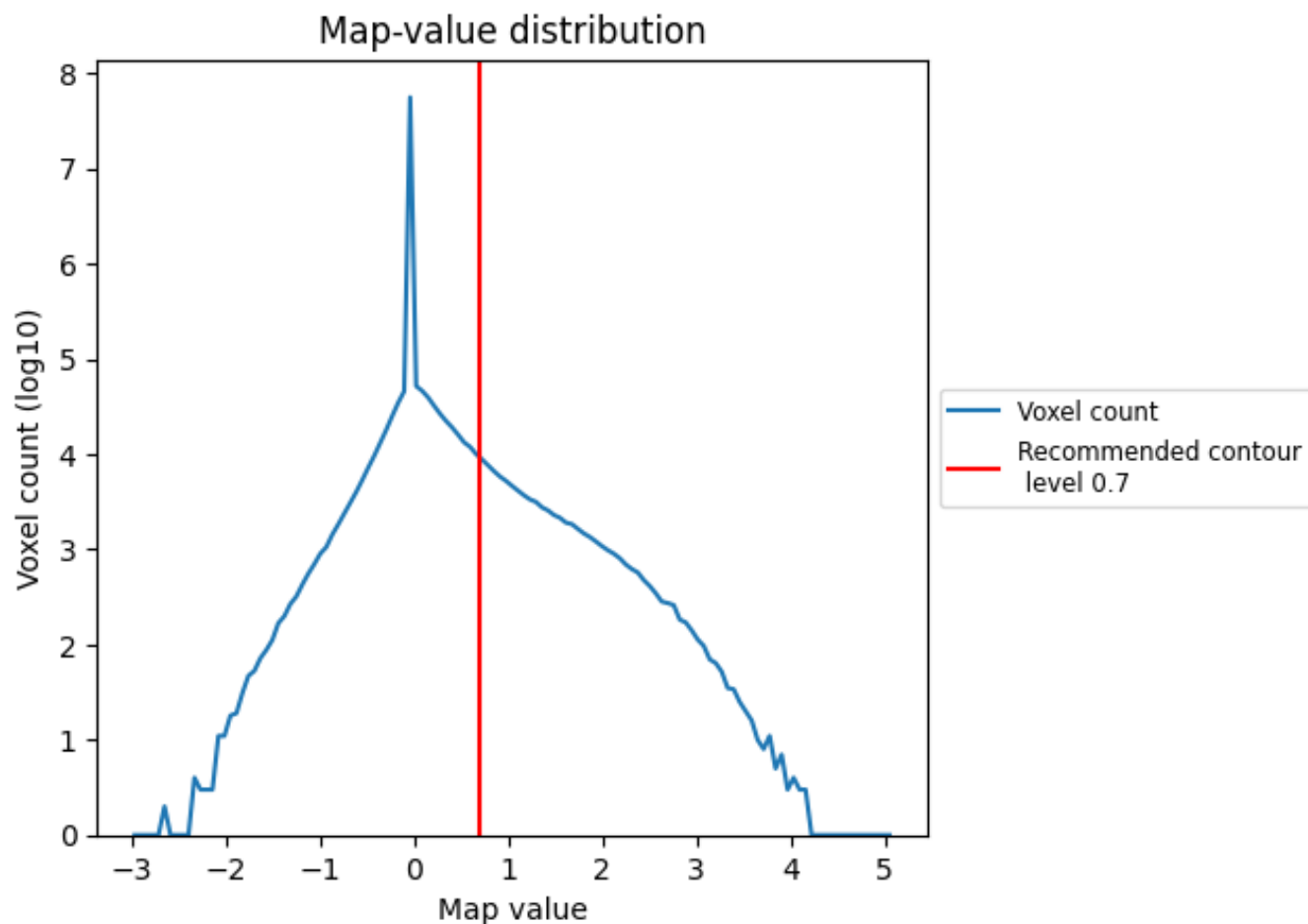
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

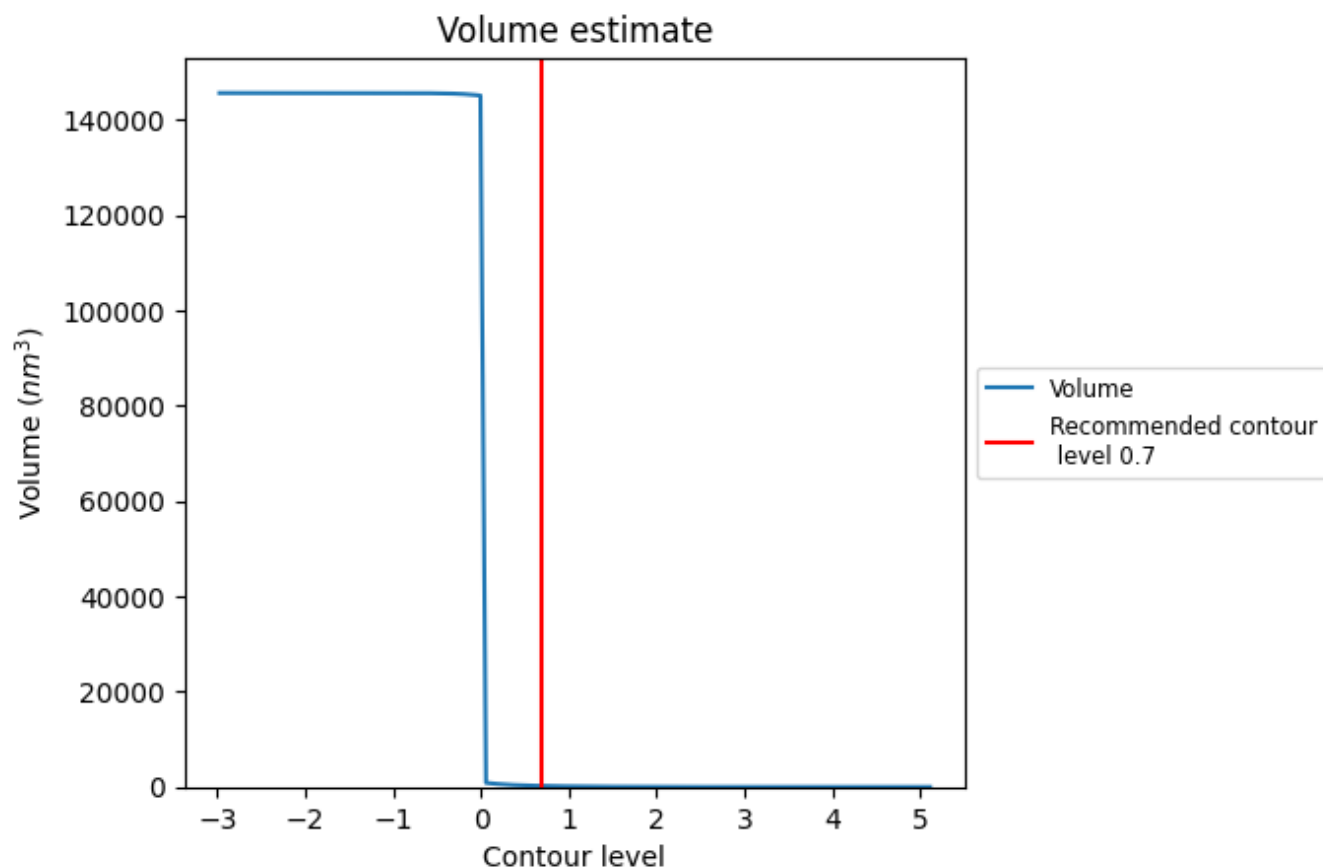
This section contains the results of statistical analysis of the map.

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.

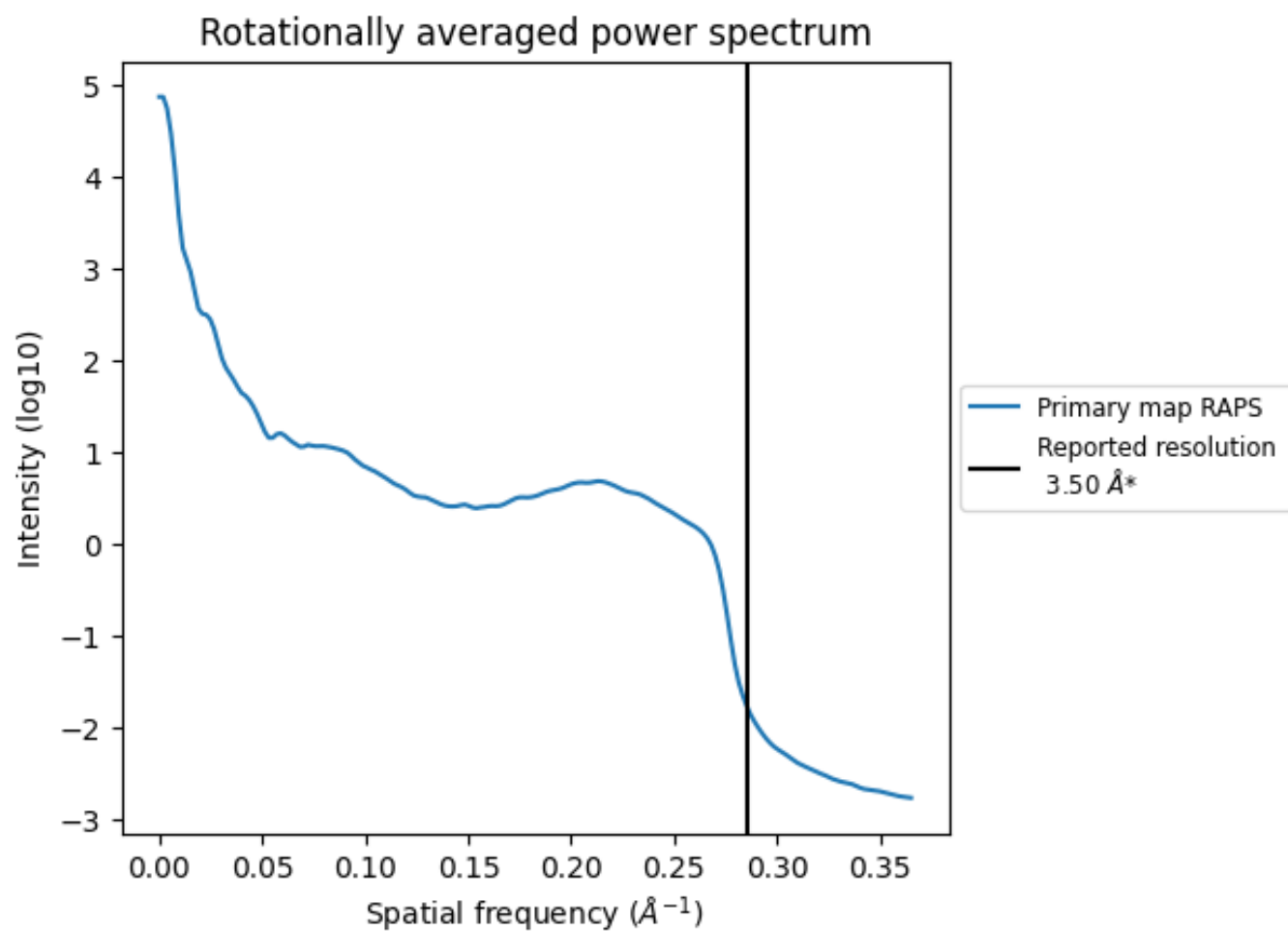
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 216 nm³; this corresponds to an approximate mass of 195 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 0.286 Å⁻¹

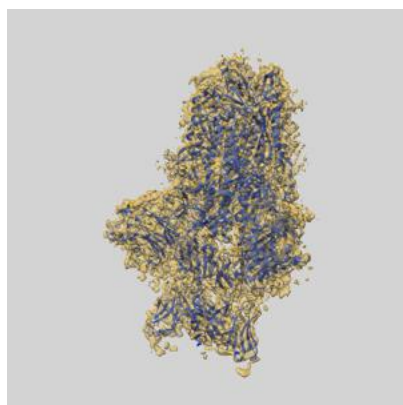
8 Fourier-Shell correlation

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

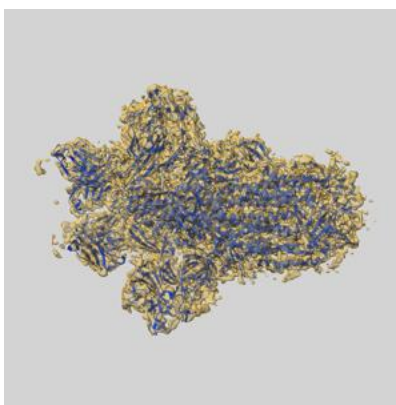
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0401 and PDB model 6NB3. Per-residue inclusion information can be found in section [3](#) on page [17](#).

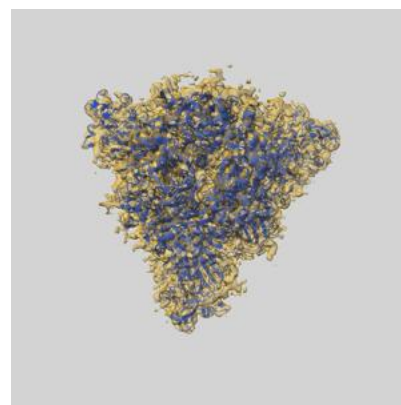
9.1 Map-model overlay [i](#)



X



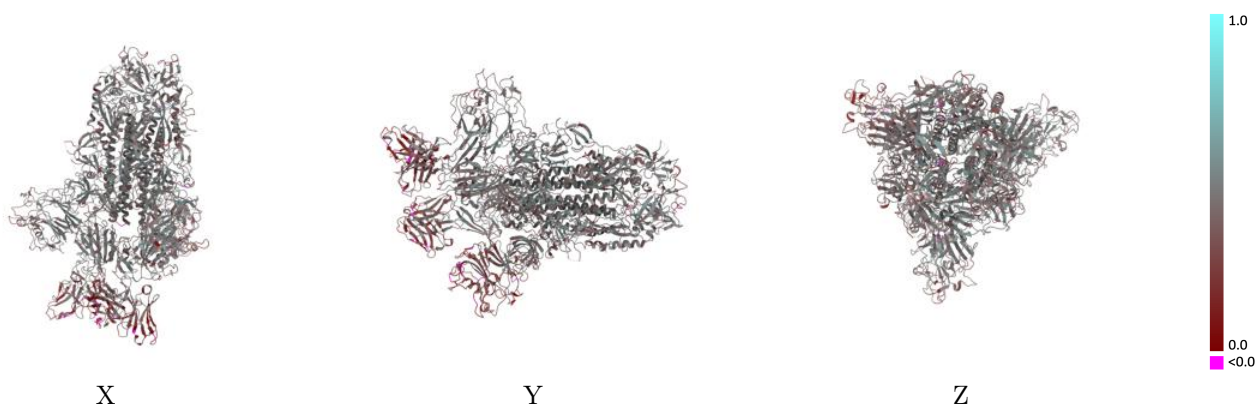
Y



Z

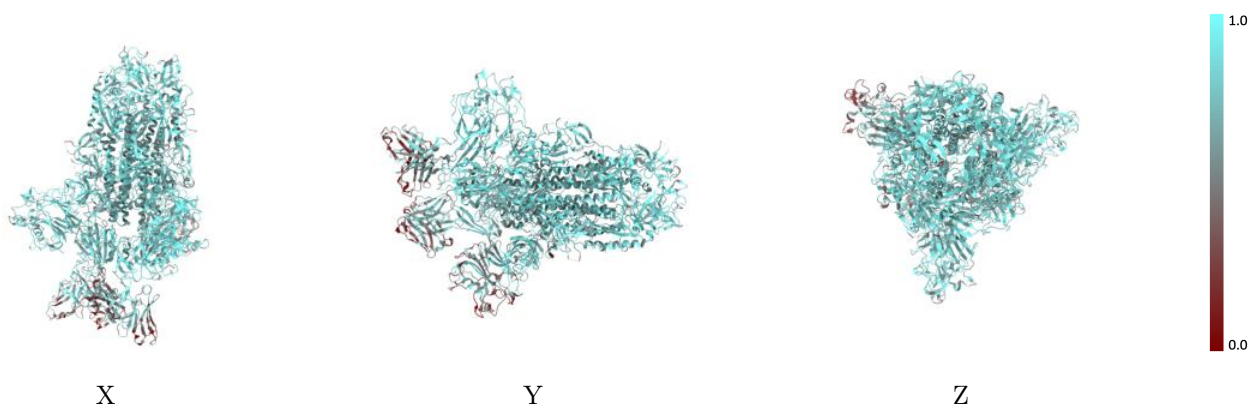
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



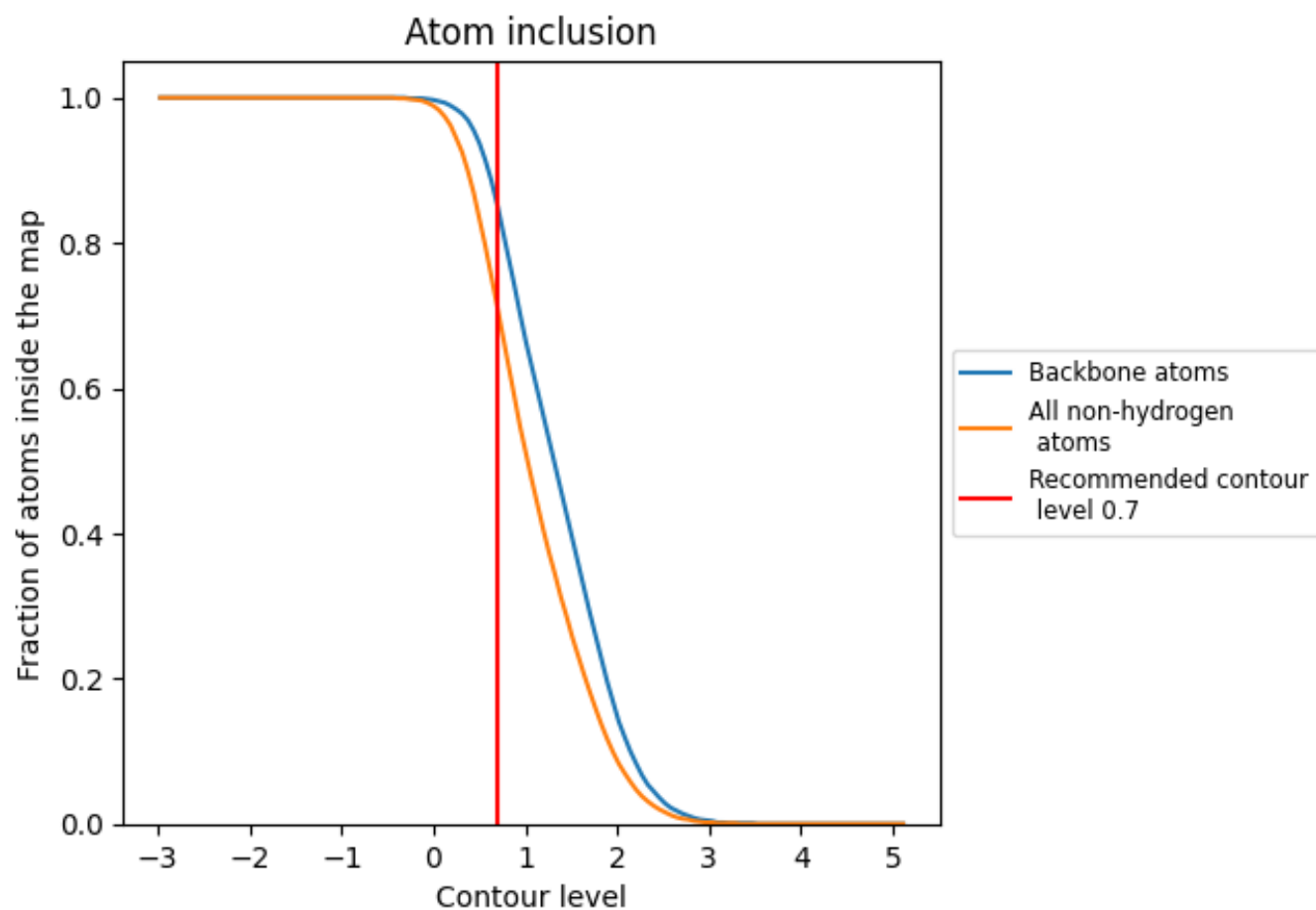
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



































The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7090	 0.4020
A	 0.7770	 0.4420
B	 0.7840	 0.4370
C	 0.7220	 0.4030
D	 0.5580	 0.3130
E	 0.6300	 0.2950
F	 0.5000	 0.2980
G	 0.2820	 0.3650
H	 0.5090	 0.2890
I	 0.6110	 0.3730
J	 0.0770	 0.0660
K	 0.4440	 0.3560
L	 0.5830	 0.2980
M	 0.4580	 0.3230
N	 0.2790	 0.2010
O	 0.3080	 0.1850
P	 0.5280	 0.2500
Q	 0.2400	 0.2870
R	 0.2560	 0.2200
S	 0.4640	 0.2910
T	 0.0000	 0.1630
U	 0.2860	 0.2780
V	 0.2560	 0.3390
W	 0.4430	 0.2840
X	 0.4290	 0.4030
Y	 0.1540	 0.2300
Z	 0.5140	 0.3330
a	 0.0260	 0.0680
b	 0.4310	 0.3130
c	 0.4310	 0.3080
d	 0.2620	 0.2590
e	 0.2820	 0.2080
f	 0.1070	 0.2740
g	 0.1030	 0.2030
h	 0.2860	 0.2650



Continued on next page...

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Chain	Atom inclusion	Q-score
i	 0.2140	 0.1640
j	 0.2820	 0.2910
k	 0.3770	 0.2330
l	 0.4290	 0.3060
m	 0.0260	 0.2420
n	 0.4310	 0.3040
o	 0.0510	 0.1540
p	 0.1030	 0.2870
q	 0.2300	 0.2180
r	 0.1430	 0.1110
s	 0.4640	 0.3510
t	 0.2560	 0.2700
u	 0.2500	 0.2810
v	 0.1070	 0.1740
w	 0.2500	 0.2250
x	 0.3080	 0.3560
y	 0.3610	 0.2530