



# wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 10:05 AM EST

PDB ID : 6NB6  
EMDB ID : EMD-0403  
Title : SARS-CoV complex with human neutralizing S230 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.; Veer, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2018-12-06  
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](mailto: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:

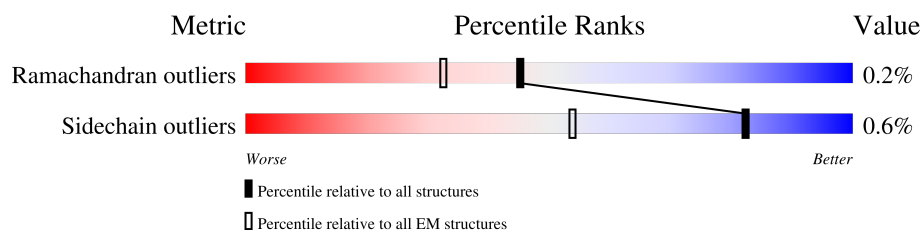
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson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



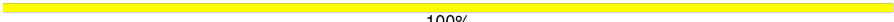


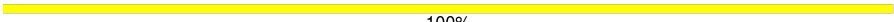





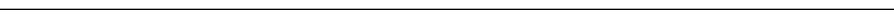
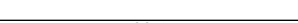



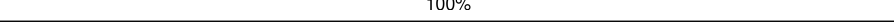
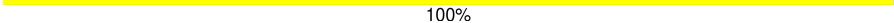
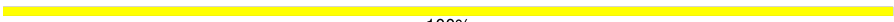



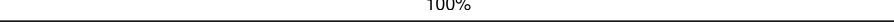
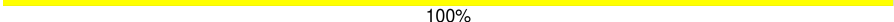

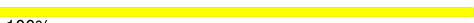




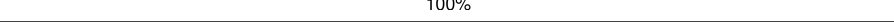
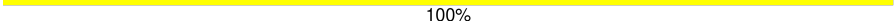
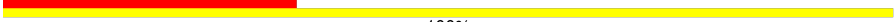
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1263	
1	B	1263	
1	C	1263	
2	H	127	
2	I	127	
3	L	112	
3	M	112	
4	D	3	
4	E	3	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	F	3	 100%
4	G	3	 33%  100%
4	J	3	 100%
4	N	3	 100%
4	S	3	 33%  100%
4	T	3	 100%
4	V	3	 100%
4	W	3	 100%
4	X	3	 33%  100%
4	Y	3	 33%  100%
4	Z	3	 100%
4	a	3	 100%
4	c	3	 100%
4	f	3	 100%
4	g	3	 100%
4	h	3	 100%
4	i	3	 100%
4	j	3	 100%
4	k	3	 33%  100%
4	l	3	 100%
4	m	3	 100%
4	n	3	 33%  100%
4	o	3	 100%
4	q	3	 100%
4	s	3	 100%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	K	5	<div><div>40%</div><div>100%</div></div>
5	O	5	<div><div>100%</div></div>
5	P	5	<div><div>40%</div><div>100%</div></div>
5	Q	5	<div><div>20%</div><div>100%</div></div>
5	R	5	<div><div>100%</div></div>
5	b	5	<div><div>100%</div></div>
5	e	5	<div><div>20%</div><div>100%</div></div>
5	p	5	<div><div>100%</div></div>
5	r	5	<div><div>100%</div></div>
6	U	2	<div><div>50%</div><div>100%</div></div>
7	d	4	<div><div>100%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25783 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	1052	Total	C	N	O	S	0	0
			7515	4786	1288	1399	42		
1	B	1026	Total	C	N	O	S	0	0
			6925	4354	1218	1313	40		
1	C	1055	Total	C	N	O	S	0	0
			7085	4479	1242	1322	42		

There are 261 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P59594
A	-17	GLY	-	expression tag	UNP P59594
A	-16	ILE	-	expression tag	UNP P59594
A	-15	LEU	-	expression tag	UNP P59594
A	-14	PRO	-	expression tag	UNP P59594
A	-13	SER	-	expression tag	UNP P59594
A	-12	PRO	-	expression tag	UNP P59594
A	-11	GLY	-	expression tag	UNP P59594
A	-10	MET	-	expression tag	UNP P59594
A	-9	PRO	-	expression tag	UNP P59594
A	-8	ALA	-	expression tag	UNP P59594
A	-7	LEU	-	expression tag	UNP P59594
A	-6	LEU	-	expression tag	UNP P59594
A	-5	SER	-	expression tag	UNP P59594
A	-4	LEU	-	expression tag	UNP P59594
A	-3	VAL	-	expression tag	UNP P59594
A	-2	SER	-	expression tag	UNP P59594
A	-1	LEU	-	expression tag	UNP P59594
A	0	LEU	-	expression tag	UNP P59594
A	1	SER	-	expression tag	UNP P59594
A	2	VAL	-	expression tag	UNP P59594
A	3	LEU	-	expression tag	UNP P59594
A	4	LEU	-	expression tag	UNP P59594
A	5	MET	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP P59594
A	7	CYS	-	expression tag	UNP P59594
A	8	VAL	-	expression tag	UNP P59594
A	9	ALA	-	expression tag	UNP P59594
A	10	GLU	-	expression tag	UNP P59594
A	11	THR	-	expression tag	UNP P59594
A	12	GLY	-	expression tag	UNP P59594
A	13	THR	-	expression tag	UNP P59594
A	77	ASP	GLY	conflict	UNP P59594
A	244	THR	ILE	conflict	UNP P59594
A	968	PRO	LYS	conflict	UNP P59594
A	969	PRO	VAL	conflict	UNP P59594
A	1194	GLY	-	expression tag	UNP P59594
A	1195	SER	-	expression tag	UNP P59594
A	1196	GLY	-	expression tag	UNP P59594
A	1197	ARG	-	expression tag	UNP P59594
A	1198	GLU	-	expression tag	UNP P59594
A	1199	ASN	-	expression tag	UNP P59594
A	1200	LEU	-	expression tag	UNP P59594
A	1201	TYR	-	expression tag	UNP P59594
A	1202	PHE	-	expression tag	UNP P59594
A	1203	GLN	-	expression tag	UNP P59594
A	1204	GLY	-	expression tag	UNP P59594
A	1205	GLY	-	expression tag	UNP P59594
A	1206	GLY	-	expression tag	UNP P59594
A	1207	GLY	-	expression tag	UNP P59594
A	1208	SER	-	expression tag	UNP P59594
A	1209	GLY	-	expression tag	UNP P59594
A	1210	TYR	-	expression tag	UNP P59594
A	1211	ILE	-	expression tag	UNP P59594
A	1212	PRO	-	expression tag	UNP P59594
A	1213	GLU	-	expression tag	UNP P59594
A	1214	ALA	-	expression tag	UNP P59594
A	1215	PRO	-	expression tag	UNP P59594
A	1216	ARG	-	expression tag	UNP P59594
A	1217	ASP	-	expression tag	UNP P59594
A	1218	GLY	-	expression tag	UNP P59594
A	1219	GLN	-	expression tag	UNP P59594
A	1220	ALA	-	expression tag	UNP P59594
A	1221	TYR	-	expression tag	UNP P59594
A	1222	VAL	-	expression tag	UNP P59594
A	1223	ARG	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	LYS	-	expression tag	UNP P59594
A	1225	ASP	-	expression tag	UNP P59594
A	1226	GLY	-	expression tag	UNP P59594
A	1227	GLU	-	expression tag	UNP P59594
A	1228	TRP	-	expression tag	UNP P59594
A	1229	VAL	-	expression tag	UNP P59594
A	1230	LEU	-	expression tag	UNP P59594
A	1231	LEU	-	expression tag	UNP P59594
A	1232	SER	-	expression tag	UNP P59594
A	1233	THR	-	expression tag	UNP P59594
A	1234	PHE	-	expression tag	UNP P59594
A	1235	LEU	-	expression tag	UNP P59594
A	1236	GLY	-	expression tag	UNP P59594
A	1237	HIS	-	expression tag	UNP P59594
A	1238	HIS	-	expression tag	UNP P59594
A	1239	HIS	-	expression tag	UNP P59594
A	1240	HIS	-	expression tag	UNP P59594
A	1241	HIS	-	expression tag	UNP P59594
A	1242	HIS	-	expression tag	UNP P59594
A	1243	HIS	-	expression tag	UNP P59594
A	1244	HIS	-	expression tag	UNP P59594
B	-18	MET	-	initiating methionine	UNP P59594
B	-17	GLY	-	expression tag	UNP P59594
B	-16	ILE	-	expression tag	UNP P59594
B	-15	LEU	-	expression tag	UNP P59594
B	-14	PRO	-	expression tag	UNP P59594
B	-13	SER	-	expression tag	UNP P59594
B	-12	PRO	-	expression tag	UNP P59594
B	-11	GLY	-	expression tag	UNP P59594
B	-10	MET	-	expression tag	UNP P59594
B	-9	PRO	-	expression tag	UNP P59594
B	-8	ALA	-	expression tag	UNP P59594
B	-7	LEU	-	expression tag	UNP P59594
B	-6	LEU	-	expression tag	UNP P59594
B	-5	SER	-	expression tag	UNP P59594
B	-4	LEU	-	expression tag	UNP P59594
B	-3	VAL	-	expression tag	UNP P59594
B	-2	SER	-	expression tag	UNP P59594
B	-1	LEU	-	expression tag	UNP P59594
B	0	LEU	-	expression tag	UNP P59594
B	1	SER	-	expression tag	UNP P59594
B	2	VAL	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LEU	-	expression tag	UNP P59594
B	4	LEU	-	expression tag	UNP P59594
B	5	MET	-	expression tag	UNP P59594
B	6	GLY	-	expression tag	UNP P59594
B	7	CYS	-	expression tag	UNP P59594
B	8	VAL	-	expression tag	UNP P59594
B	9	ALA	-	expression tag	UNP P59594
B	10	GLU	-	expression tag	UNP P59594
B	11	THR	-	expression tag	UNP P59594
B	12	GLY	-	expression tag	UNP P59594
B	13	THR	-	expression tag	UNP P59594
B	77	ASP	GLY	conflict	UNP P59594
B	244	THR	ILE	conflict	UNP P59594
B	968	PRO	LYS	conflict	UNP P59594
B	969	PRO	VAL	conflict	UNP P59594
B	1194	GLY	-	expression tag	UNP P59594
B	1195	SER	-	expression tag	UNP P59594
B	1196	GLY	-	expression tag	UNP P59594
B	1197	ARG	-	expression tag	UNP P59594
B	1198	GLU	-	expression tag	UNP P59594
B	1199	ASN	-	expression tag	UNP P59594
B	1200	LEU	-	expression tag	UNP P59594
B	1201	TYR	-	expression tag	UNP P59594
B	1202	PHE	-	expression tag	UNP P59594
B	1203	GLN	-	expression tag	UNP P59594
B	1204	GLY	-	expression tag	UNP P59594
B	1205	GLY	-	expression tag	UNP P59594
B	1206	GLY	-	expression tag	UNP P59594
B	1207	GLY	-	expression tag	UNP P59594
B	1208	SER	-	expression tag	UNP P59594
B	1209	GLY	-	expression tag	UNP P59594
B	1210	TYR	-	expression tag	UNP P59594
B	1211	ILE	-	expression tag	UNP P59594
B	1212	PRO	-	expression tag	UNP P59594
B	1213	GLU	-	expression tag	UNP P59594
B	1214	ALA	-	expression tag	UNP P59594
B	1215	PRO	-	expression tag	UNP P59594
B	1216	ARG	-	expression tag	UNP P59594
B	1217	ASP	-	expression tag	UNP P59594
B	1218	GLY	-	expression tag	UNP P59594
B	1219	GLN	-	expression tag	UNP P59594
B	1220	ALA	-	expression tag	UNP P59594

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	1221	TYR	-	expression tag	UNP P59594
B	1222	VAL	-	expression tag	UNP P59594
B	1223	ARG	-	expression tag	UNP P59594
B	1224	LYS	-	expression tag	UNP P59594
B	1225	ASP	-	expression tag	UNP P59594
B	1226	GLY	-	expression tag	UNP P59594
B	1227	GLU	-	expression tag	UNP P59594
B	1228	TRP	-	expression tag	UNP P59594
B	1229	VAL	-	expression tag	UNP P59594
B	1230	LEU	-	expression tag	UNP P59594
B	1231	LEU	-	expression tag	UNP P59594
B	1232	SER	-	expression tag	UNP P59594
B	1233	THR	-	expression tag	UNP P59594
B	1234	PHE	-	expression tag	UNP P59594
B	1235	LEU	-	expression tag	UNP P59594
B	1236	GLY	-	expression tag	UNP P59594
B	1237	HIS	-	expression tag	UNP P59594
B	1238	HIS	-	expression tag	UNP P59594
B	1239	HIS	-	expression tag	UNP P59594
B	1240	HIS	-	expression tag	UNP P59594
B	1241	HIS	-	expression tag	UNP P59594
B	1242	HIS	-	expression tag	UNP P59594
B	1243	HIS	-	expression tag	UNP P59594
B	1244	HIS	-	expression tag	UNP P59594
C	-18	MET	-	initiating methionine	UNP P59594
C	-17	GLY	-	expression tag	UNP P59594
C	-16	ILE	-	expression tag	UNP P59594
C	-15	LEU	-	expression tag	UNP P59594
C	-14	PRO	-	expression tag	UNP P59594
C	-13	SER	-	expression tag	UNP P59594
C	-12	PRO	-	expression tag	UNP P59594
C	-11	GLY	-	expression tag	UNP P59594
C	-10	MET	-	expression tag	UNP P59594
C	-9	PRO	-	expression tag	UNP P59594
C	-8	ALA	-	expression tag	UNP P59594
C	-7	LEU	-	expression tag	UNP P59594
C	-6	LEU	-	expression tag	UNP P59594
C	-5	SER	-	expression tag	UNP P59594
C	-4	LEU	-	expression tag	UNP P59594
C	-3	VAL	-	expression tag	UNP P59594
C	-2	SER	-	expression tag	UNP P59594
C	-1	LEU	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	LEU	-	expression tag	UNP P59594
C	1	SER	-	expression tag	UNP P59594
C	2	VAL	-	expression tag	UNP P59594
C	3	LEU	-	expression tag	UNP P59594
C	4	LEU	-	expression tag	UNP P59594
C	5	MET	-	expression tag	UNP P59594
C	6	GLY	-	expression tag	UNP P59594
C	7	CYS	-	expression tag	UNP P59594
C	8	VAL	-	expression tag	UNP P59594
C	9	ALA	-	expression tag	UNP P59594
C	10	GLU	-	expression tag	UNP P59594
C	11	THR	-	expression tag	UNP P59594
C	12	GLY	-	expression tag	UNP P59594
C	13	THR	-	expression tag	UNP P59594
C	77	ASP	GLY	conflict	UNP P59594
C	244	THR	ILE	conflict	UNP P59594
C	968	PRO	LYS	conflict	UNP P59594
C	969	PRO	VAL	conflict	UNP P59594
C	1194	GLY	-	expression tag	UNP P59594
C	1195	SER	-	expression tag	UNP P59594
C	1196	GLY	-	expression tag	UNP P59594
C	1197	ARG	-	expression tag	UNP P59594
C	1198	GLU	-	expression tag	UNP P59594
C	1199	ASN	-	expression tag	UNP P59594
C	1200	LEU	-	expression tag	UNP P59594
C	1201	TYR	-	expression tag	UNP P59594
C	1202	PHE	-	expression tag	UNP P59594
C	1203	GLN	-	expression tag	UNP P59594
C	1204	GLY	-	expression tag	UNP P59594
C	1205	GLY	-	expression tag	UNP P59594
C	1206	GLY	-	expression tag	UNP P59594
C	1207	GLY	-	expression tag	UNP P59594
C	1208	SER	-	expression tag	UNP P59594
C	1209	GLY	-	expression tag	UNP P59594
C	1210	TYR	-	expression tag	UNP P59594
C	1211	ILE	-	expression tag	UNP P59594
C	1212	PRO	-	expression tag	UNP P59594
C	1213	GLU	-	expression tag	UNP P59594
C	1214	ALA	-	expression tag	UNP P59594
C	1215	PRO	-	expression tag	UNP P59594
C	1216	ARG	-	expression tag	UNP P59594
C	1217	ASP	-	expression tag	UNP P59594

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	1218	GLY	-	expression tag	UNP P59594
C	1219	GLN	-	expression tag	UNP P59594
C	1220	ALA	-	expression tag	UNP P59594
C	1221	TYR	-	expression tag	UNP P59594
C	1222	VAL	-	expression tag	UNP P59594
C	1223	ARG	-	expression tag	UNP P59594
C	1224	LYS	-	expression tag	UNP P59594
C	1225	ASP	-	expression tag	UNP P59594
C	1226	GLY	-	expression tag	UNP P59594
C	1227	GLU	-	expression tag	UNP P59594
C	1228	TRP	-	expression tag	UNP P59594
C	1229	VAL	-	expression tag	UNP P59594
C	1230	LEU	-	expression tag	UNP P59594
C	1231	LEU	-	expression tag	UNP P59594
C	1232	SER	-	expression tag	UNP P59594
C	1233	THR	-	expression tag	UNP P59594
C	1234	PHE	-	expression tag	UNP P59594
C	1235	LEU	-	expression tag	UNP P59594
C	1236	GLY	-	expression tag	UNP P59594
C	1237	HIS	-	expression tag	UNP P59594
C	1238	HIS	-	expression tag	UNP P59594
C	1239	HIS	-	expression tag	UNP P59594
C	1240	HIS	-	expression tag	UNP P59594
C	1241	HIS	-	expression tag	UNP P59594
C	1242	HIS	-	expression tag	UNP P59594
C	1243	HIS	-	expression tag	UNP P59594
C	1244	HIS	-	expression tag	UNP P59594

- Molecule 2 is a protein called S230 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	123	Total	C	N	O	S	0	0
			613	365	123	123	2		
2	I	124	Total	C	N	O	S	0	0
			618	368	124	124	2		

- Molecule 3 is a protein called S230 light chain.

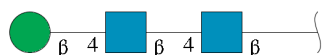
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	110	Total	C	N	O	S	0	0
			557	335	110	110	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	109	Total	C	N	O	S	0	0
			552	332	109	109	2		

- Molecule 4 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.



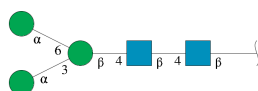
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	3	Total	C	N	O		0	0
			39	22	2	15			
4	E	3	Total	C	N	O		0	0
			39	22	2	15			
4	F	3	Total	C	N	O		0	0
			39	22	2	15			
4	G	3	Total	C	N	O		0	0
			39	22	2	15			
4	J	3	Total	C	N	O		0	0
			39	22	2	15			
4	N	3	Total	C	N	O		0	0
			39	22	2	15			
4	S	3	Total	C	N	O		0	0
			39	22	2	15			
4	T	3	Total	C	N	O		0	0
			39	22	2	15			
4	V	3	Total	C	N	O		0	0
			39	22	2	15			
4	W	3	Total	C	N	O		0	0
			39	22	2	15			
4	X	3	Total	C	N	O		0	0
			39	22	2	15			
4	Y	3	Total	C	N	O		0	0
			39	22	2	15			
4	Z	3	Total	C	N	O		0	0
			39	22	2	15			
4	a	3	Total	C	N	O		0	0
			39	22	2	15			
4	c	3	Total	C	N	O		0	0
			39	22	2	15			
4	f	3	Total	C	N	O		0	0
			39	22	2	15			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
4	g	3	Total	C	N	O	0	0
			39	22	2	15		
4	h	3	Total	C	N	O	0	0
			39	22	2	15		
4	i	3	Total	C	N	O	0	0
			39	22	2	15		
4	j	3	Total	C	N	O	0	0
			39	22	2	15		
4	k	3	Total	C	N	O	0	0
			39	22	2	15		
4	l	3	Total	C	N	O	0	0
			39	22	2	15		
4	m	3	Total	C	N	O	0	0
			39	22	2	15		
4	n	3	Total	C	N	O	0	0
			39	22	2	15		
4	o	3	Total	C	N	O	0	0
			39	22	2	15		
4	q	3	Total	C	N	O	0	0
			39	22	2	15		
4	s	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 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
5	K	5	Total	C	N	O	0	0
			61	34	2	25		
5	O	5	Total	C	N	O	0	0
			61	34	2	25		
5	P	5	Total	C	N	O	0	0
			61	34	2	25		
5	Q	5	Total	C	N	O	0	0
			61	34	2	25		
5	R	5	Total	C	N	O	0	0
			61	34	2	25		

*Continued on next page...*

*Continued from previous page...*

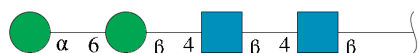
Mol	Chain	Residues	Atoms				AltConf	Trace
5	b	5	Total	C	N	O	0	0
			61	34	2	25		
5	e	5	Total	C	N	O	0	0
			61	34	2	25		
5	p	5	Total	C	N	O	0	0
			61	34	2	25		
5	r	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 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
6	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called 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	d	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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	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	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

*Continued from previous page...*

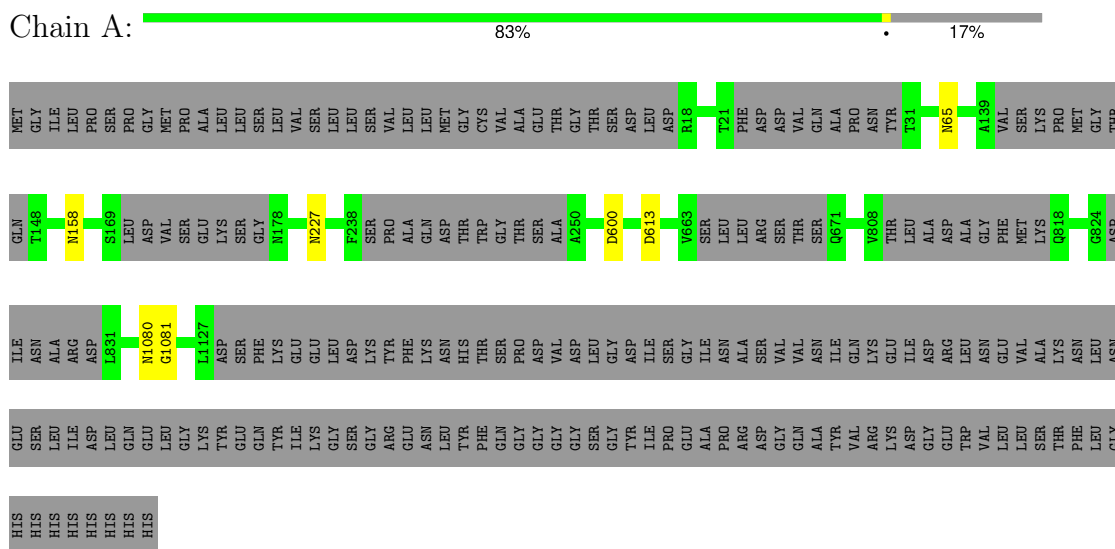
Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	



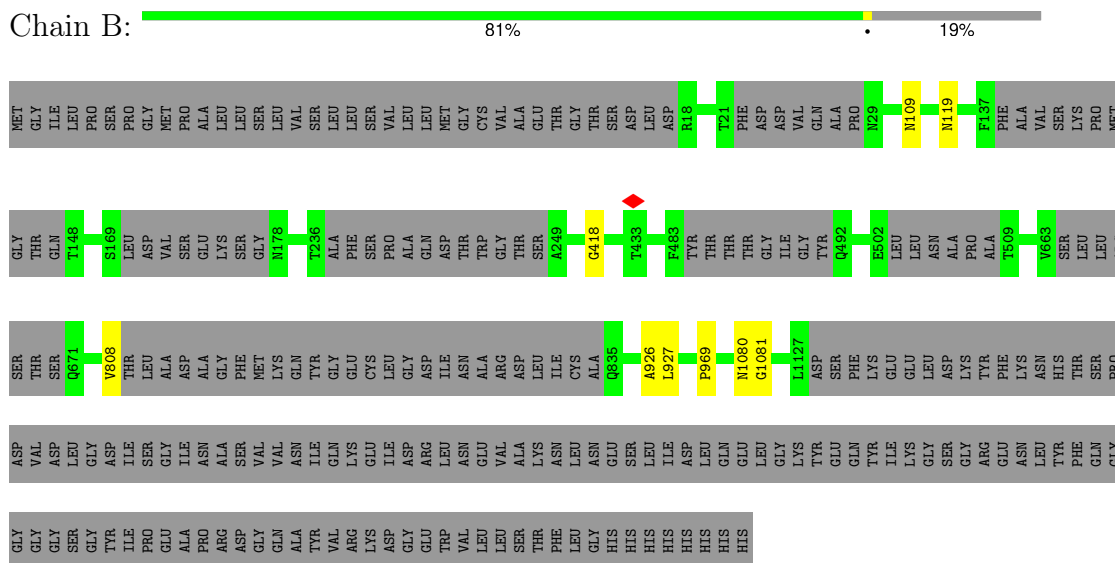
### 3 Residue-property plots

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


#### • Molecule 1: Spike glycoprotein

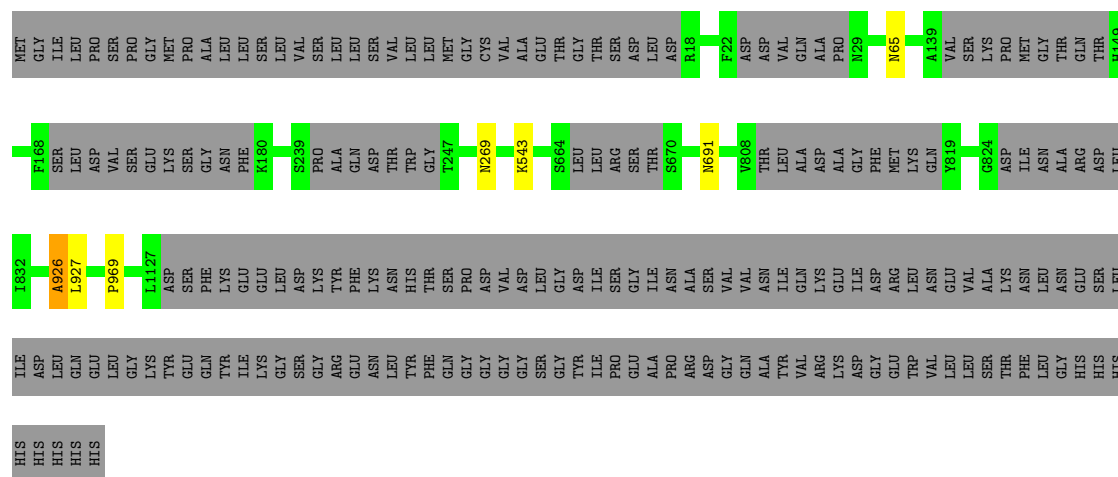


#### • Molecule 1: Spike glycoprotein



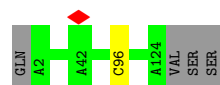
- Molecule 1: Spike glycoprotein

Chain C:  83% 16%



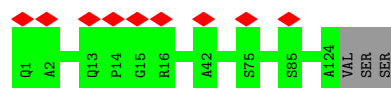
- Molecule 2: S230 heavy chain

Chain H:  96%



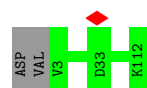
- Molecule 2: S230 heavy chain

Chain I:  7% 98%



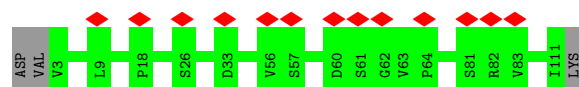
- Molecule 3: S230 light chain

Chain L:  98%



- Molecule 3: S230 light chain

Chain M:  12% 97%



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

Chain D:  67% 100%



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

Chain E:  100%



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

Chain F:  100%



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

Chain G:  33% 100%



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

Chain J:  100%



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

Chain N:  100%



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



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



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



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



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



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



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



NAG1  
NAG2  
BMA3

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

Chain a:  100%

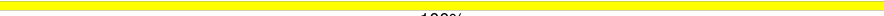
NAG1  
NAG2  
BMA3

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

Chain c:  100%

NAG1  
NAG2  
BMA3

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

Chain f:  100%


NAG1  
NAG2  
BMA3

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

Chain g:  100%


NAG1  
NAG2  
BMA3

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

Chain h:  100%

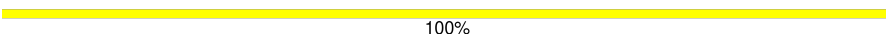
NAG1  
NAG2  
BMA3

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

Chain i:  100%

NAG1  
NAG2  
BMA3

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

Chain j:  100%

MAG1  
MAG2  
BMA3

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

Chain k:  33% 100%

MAG1  
MAG2  
BMA3

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

Chain l:  100%

MAG1  
MAG2  
BMA3

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

Chain m:  100%

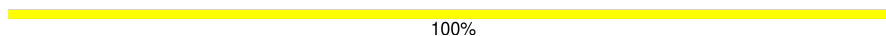
MAG1  
MAG2  
BMA3

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

Chain n:  33% 100%

MAG1  
MAG2  
BMA3

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

Chain o:  100%

MAG1  
MAG2  
BMA3

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

Chain q:  100%

NAG1  
NAG2  
BMA3

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

Chain s:  100%

NAG1  
NAG2  
BMA3

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  40%  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  40%  100%

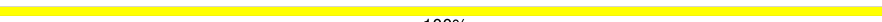
NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  20%  100%

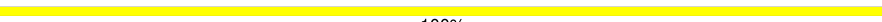
NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  20% 100%

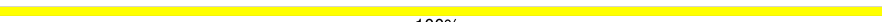
  
NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 100%





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

Chain d:

100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23071	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	2.618	Depositor
Minimum map value	-1.272	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.36	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: NAG, BMA, MAN

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	0.63	0/7687	0.60	0/10519
1	B	0.60	0/7056	0.61	3/9672 (0.0%)
1	C	0.60	0/7228	0.59	2/9917 (0.0%)
2	H	0.44	1/615 (0.2%)	0.51	0/855
2	I	0.42	0/620	0.51	0/862
3	L	0.41	0/564	0.52	0/787
3	M	0.40	0/559	0.52	0/780
All	All	0.60	1/24329 (0.0%)	0.59	5/33392 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	96	CYS	CB-SG	-5.07	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	808	VAL	CG1-CB-CG2	13.05	131.78	110.90
1	C	926	ALA	N-CA-C	10.14	138.37	111.00
1	B	926	ALA	N-CA-C	10.07	138.18	111.00
1	B	927	LEU	N-CA-CB	-9.69	91.02	110.40
1	C	927	LEU	N-CA-CB	-8.93	92.53	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1036/1263 (82%)	998 (96%)	35 (3%)	3 (0%)	37	71
1	B	1008/1263 (80%)	968 (96%)	37 (4%)	3 (0%)	37	71
1	C	1039/1263 (82%)	1000 (96%)	37 (4%)	2 (0%)	44	77
2	H	121/127 (95%)	120 (99%)	1 (1%)	0	100	100
2	I	122/127 (96%)	119 (98%)	3 (2%)	0	100	100
3	L	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
3	M	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
All	All	3541/4267 (83%)	3415 (96%)	118 (3%)	8 (0%)	45	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1081	GLY
1	A	600	ASP
1	B	1081	GLY
1	C	969	PRO
1	A	613	ASP

### 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	702/1092 (64%)	698 (99%)	4 (1%)	84	88
1	B	585/1092 (54%)	582 (100%)	3 (0%)	86	90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	581/1092 (53%)	577 (99%)	4 (1%)	81	86
2	H	5/106 (5%)	5 (100%)	0	100	100
2	I	5/106 (5%)	5 (100%)	0	100	100
3	L	10/99 (10%)	10 (100%)	0	100	100
3	M	10/99 (10%)	10 (100%)	0	100	100
All	All	1898/3686 (52%)	1887 (99%)	11 (1%)	82	88

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	65	ASN
1	C	269	ASN
1	C	691	ASN
1	C	543	LYS
1	B	109	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	917	GLN
1	C	786	GLN
1	A	786	GLN
1	A	1095	GLN
1	B	614	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 ⓘ

132 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	D	1	1,4	14,14,15	2.02	3 (21%)	17,19,21	1.01	1 (5%)
4	NAG	D	2	4	14,14,15	2.18	5 (35%)	17,19,21	1.22	2 (11%)
4	BMA	D	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.98	1 (6%)
4	NAG	E	1	1,4	14,14,15	2.06	4 (28%)	17,19,21	1.12	3 (17%)
4	NAG	E	2	4	14,14,15	2.20	5 (35%)	17,19,21	1.20	1 (5%)
4	BMA	E	3	4	11,11,12	1.79	2 (18%)	15,15,17	0.91	1 (6%)
4	NAG	F	1	1,4	14,14,15	2.10	3 (21%)	17,19,21	1.09	1 (5%)
4	NAG	F	2	4	14,14,15	2.22	3 (21%)	17,19,21	1.24	3 (17%)
4	BMA	F	3	4	11,11,12	1.80	2 (18%)	15,15,17	0.97	1 (6%)
4	NAG	G	1	1,4	14,14,15	2.19	3 (21%)	17,19,21	1.33	3 (17%)
4	NAG	G	2	4	14,14,15	2.22	5 (35%)	17,19,21	1.47	1 (5%)
4	BMA	G	3	4	11,11,12	1.79	2 (18%)	15,15,17	0.93	1 (6%)
4	NAG	J	1	1,4	14,14,15	1.80	2 (14%)	17,19,21	0.86	1 (5%)
4	NAG	J	2	4	14,14,15	2.11	3 (21%)	17,19,21	1.35	2 (11%)
4	BMA	J	3	4	11,11,12	1.79	2 (18%)	15,15,17	0.82	0
5	NAG	K	1	5,1	14,14,15	2.06	4 (28%)	17,19,21	1.07	1 (5%)
5	NAG	K	2	5	14,14,15	2.04	3 (21%)	17,19,21	1.35	2 (11%)
5	BMA	K	3	5	11,11,12	1.97	3 (27%)	15,15,17	1.04	1 (6%)
5	MAN	K	4	5	11,11,12	1.72	2 (18%)	15,15,17	1.12	2 (13%)
5	MAN	K	5	5	11,11,12	1.78	2 (18%)	15,15,17	1.03	1 (6%)
4	NAG	N	1	1,4	14,14,15	2.07	2 (14%)	17,19,21	1.02	1 (5%)
4	NAG	N	2	4	14,14,15	2.20	5 (35%)	17,19,21	1.74	3 (17%)
4	BMA	N	3	4	11,11,12	1.77	2 (18%)	15,15,17	0.96	1 (6%)
5	NAG	O	1	5,1	14,14,15	1.98	4 (28%)	17,19,21	1.26	3 (17%)
5	NAG	O	2	5	14,14,15	2.10	3 (21%)	17,19,21	1.32	2 (11%)
5	BMA	O	3	5	11,11,12	1.83	2 (18%)	15,15,17	1.09	1 (6%)
5	MAN	O	4	5	11,11,12	1.71	1 (9%)	15,15,17	1.32	2 (13%)
5	MAN	O	5	5	11,11,12	1.81	1 (9%)	15,15,17	1.13	2 (13%)
5	NAG	P	1	5,1	14,14,15	1.98	3 (21%)	17,19,21	1.44	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	P	2	5	14,14,15	2.07	4 (28%)	17,19,21	1.40	2 (11%)
5	BMA	P	3	5	11,11,12	1.89	2 (18%)	15,15,17	1.05	1 (6%)
5	MAN	P	4	5	11,11,12	1.78	2 (18%)	15,15,17	1.11	1 (6%)
5	MAN	P	5	5	11,11,12	1.86	3 (27%)	15,15,17	1.12	1 (6%)
5	NAG	Q	1	5,1	14,14,15	1.98	2 (14%)	17,19,21	0.79	0
5	NAG	Q	2	5	14,14,15	2.06	3 (21%)	17,19,21	1.24	3 (17%)
5	BMA	Q	3	5	11,11,12	1.81	2 (18%)	15,15,17	1.00	1 (6%)
5	MAN	Q	4	5	11,11,12	1.87	3 (27%)	15,15,17	1.25	2 (13%)
5	MAN	Q	5	5	11,11,12	1.69	1 (9%)	15,15,17	1.24	2 (13%)
5	NAG	R	1	5,1	14,14,15	2.03	3 (21%)	17,19,21	0.84	2 (11%)
5	NAG	R	2	5	14,14,15	2.16	3 (21%)	17,19,21	1.17	2 (11%)
5	BMA	R	3	5	11,11,12	2.08	3 (27%)	15,15,17	1.02	1 (6%)
5	MAN	R	4	5	11,11,12	1.79	1 (9%)	15,15,17	1.22	2 (13%)
5	MAN	R	5	5	11,11,12	1.73	1 (9%)	15,15,17	1.22	2 (13%)
4	NAG	S	1	1,4	14,14,15	2.07	3 (21%)	17,19,21	0.98	2 (11%)
4	NAG	S	2	4	14,14,15	2.19	5 (35%)	17,19,21	1.27	1 (5%)
4	BMA	S	3	4	11,11,12	1.80	2 (18%)	15,15,17	0.94	1 (6%)
4	NAG	T	1	1,4	14,14,15	2.13	3 (21%)	17,19,21	1.04	0
4	NAG	T	2	4	14,14,15	2.18	4 (28%)	17,19,21	1.11	1 (5%)
4	BMA	T	3	4	11,11,12	1.78	2 (18%)	15,15,17	0.90	1 (6%)
6	NAG	U	1	6,1	14,14,15	2.03	2 (14%)	17,19,21	0.84	0
6	NAG	U	2	6	14,14,15	2.14	3 (21%)	17,19,21	0.93	1 (5%)
4	NAG	V	1	1,4	14,14,15	2.09	3 (21%)	17,19,21	1.53	2 (11%)
4	NAG	V	2	4	14,14,15	2.32	5 (35%)	17,19,21	1.59	3 (17%)
4	BMA	V	3	4	11,11,12	1.78	2 (18%)	15,15,17	1.03	1 (6%)
4	NAG	W	1	1,4	14,14,15	2.00	2 (14%)	17,19,21	0.82	1 (5%)
4	NAG	W	2	4	14,14,15	2.16	5 (35%)	17,19,21	1.25	2 (11%)
4	BMA	W	3	4	11,11,12	1.78	2 (18%)	15,15,17	0.91	1 (6%)
4	NAG	X	1	1,4	14,14,15	2.09	2 (14%)	17,19,21	0.89	1 (5%)
4	NAG	X	2	4	14,14,15	2.16	5 (35%)	17,19,21	1.19	2 (11%)
4	BMA	X	3	4	11,11,12	1.77	2 (18%)	15,15,17	0.90	1 (6%)
4	NAG	Y	1	1,4	14,14,15	2.00	3 (21%)	17,19,21	1.24	2 (11%)
4	NAG	Y	2	4	14,14,15	2.13	4 (28%)	17,19,21	1.56	4 (23%)
4	BMA	Y	3	4	11,11,12	1.79	2 (18%)	15,15,17	0.97	1 (6%)
4	NAG	Z	1	1,4	14,14,15	2.06	3 (21%)	17,19,21	1.39	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	Z	2	4	14,14,15	2.16	5 (35%)	17,19,21	1.73	4 (23%)
4	BMA	Z	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.97	1 (6%)
4	NAG	a	1	1,4	14,14,15	1.98	1 (7%)	17,19,21	0.88	1 (5%)
4	NAG	a	2	4	14,14,15	2.27	3 (21%)	17,19,21	0.87	0
4	BMA	a	3	4	11,11,12	1.82	2 (18%)	15,15,17	1.02	1 (6%)
5	NAG	b	1	5,1	14,14,15	1.98	3 (21%)	17,19,21	1.04	1 (5%)
5	NAG	b	2	5	14,14,15	2.14	5 (35%)	17,19,21	1.42	2 (11%)
5	BMA	b	3	5	11,11,12	1.78	3 (27%)	15,15,17	0.80	0
5	MAN	b	4	5	11,11,12	1.88	3 (27%)	15,15,17	1.15	1 (6%)
5	MAN	b	5	5	11,11,12	1.73	1 (9%)	15,15,17	1.10	1 (6%)
4	NAG	c	1	1,4	14,14,15	2.09	3 (21%)	17,19,21	0.73	1 (5%)
4	NAG	c	2	4	14,14,15	2.16	4 (28%)	17,19,21	1.21	2 (11%)
4	BMA	c	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.88	0
7	NAG	d	1	7,1	14,14,15	2.03	3 (21%)	17,19,21	0.94	1 (5%)
7	NAG	d	2	7	14,14,15	2.11	4 (28%)	17,19,21	1.05	1 (5%)
7	BMA	d	3	7	11,11,12	1.92	3 (27%)	15,15,17	1.20	1 (6%)
7	MAN	d	4	7	11,11,12	1.79	2 (18%)	15,15,17	1.19	2 (13%)
5	NAG	e	1	5,1	14,14,15	1.95	3 (21%)	17,19,21	0.87	0
5	NAG	e	2	5	14,14,15	2.09	4 (28%)	17,19,21	1.48	3 (17%)
5	BMA	e	3	5	11,11,12	1.89	3 (27%)	15,15,17	0.86	0
5	MAN	e	4	5	11,11,12	1.79	2 (18%)	15,15,17	1.18	2 (13%)
5	MAN	e	5	5	11,11,12	1.78	1 (9%)	15,15,17	1.19	1 (6%)
4	NAG	f	1	1,4	14,14,15	1.99	3 (21%)	17,19,21	1.00	1 (5%)
4	NAG	f	2	4	14,14,15	2.17	4 (28%)	17,19,21	1.34	2 (11%)
4	BMA	f	3	4	11,11,12	1.79	2 (18%)	15,15,17	0.96	1 (6%)
4	NAG	g	1	1,4	14,14,15	2.15	3 (21%)	17,19,21	1.06	1 (5%)
4	NAG	g	2	4	14,14,15	2.13	4 (28%)	17,19,21	1.31	2 (11%)
4	BMA	g	3	4	11,11,12	1.80	2 (18%)	15,15,17	1.06	1 (6%)
4	NAG	h	1	1,4	14,14,15	2.01	2 (14%)	17,19,21	1.55	3 (17%)
4	NAG	h	2	4	14,14,15	2.16	5 (35%)	17,19,21	1.68	4 (23%)
4	BMA	h	3	4	11,11,12	1.81	2 (18%)	15,15,17	1.01	1 (6%)
4	NAG	i	1	1,4	14,14,15	2.07	3 (21%)	17,19,21	1.20	2 (11%)
4	NAG	i	2	4	14,14,15	2.13	4 (28%)	17,19,21	1.88	4 (23%)
4	BMA	i	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.98	1 (6%)
4	NAG	j	1	1,4	14,14,15	2.12	3 (21%)	17,19,21	1.03	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	j	2	4	14,14,15	2.22	3 (21%)	17,19,21	1.53	4 (23%)
4	BMA	j	3	4	11,11,12	1.80	2 (18%)	15,15,17	1.03	1 (6%)
4	NAG	k	1	1,4	14,14,15	1.92	2 (14%)	17,19,21	1.57	2 (11%)
4	NAG	k	2	4	14,14,15	2.37	5 (35%)	17,19,21	1.64	4 (23%)
4	BMA	k	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.97	1 (6%)
4	NAG	l	1	1,4	14,14,15	2.03	2 (14%)	17,19,21	0.96	1 (5%)
4	NAG	l	2	4	14,14,15	2.18	4 (28%)	17,19,21	1.16	2 (11%)
4	BMA	l	3	4	11,11,12	1.80	2 (18%)	15,15,17	0.94	1 (6%)
4	NAG	m	1	1,4	14,14,15	2.08	3 (21%)	17,19,21	0.81	1 (5%)
4	NAG	m	2	4	14,14,15	2.15	3 (21%)	17,19,21	1.25	3 (17%)
4	BMA	m	3	4	11,11,12	1.78	2 (18%)	15,15,17	1.01	1 (6%)
4	NAG	n	1	1,4	14,14,15	2.08	3 (21%)	17,19,21	0.94	1 (5%)
4	NAG	n	2	4	14,14,15	2.13	5 (35%)	17,19,21	1.23	2 (11%)
4	BMA	n	3	4	11,11,12	1.81	2 (18%)	15,15,17	0.99	1 (6%)
4	NAG	o	1	1,4	14,14,15	2.08	2 (14%)	17,19,21	1.06	2 (11%)
4	NAG	o	2	4	14,14,15	2.20	5 (35%)	17,19,21	1.51	3 (17%)
4	BMA	o	3	4	11,11,12	1.81	2 (18%)	15,15,17	1.12	1 (6%)
5	NAG	p	1	5,1	14,14,15	2.18	3 (21%)	17,19,21	1.14	2 (11%)
5	NAG	p	2	5	14,14,15	2.11	4 (28%)	17,19,21	1.46	3 (17%)
5	BMA	p	3	5	11,11,12	1.81	2 (18%)	15,15,17	1.08	1 (6%)
5	MAN	p	4	5	11,11,12	1.76	2 (18%)	15,15,17	1.27	2 (13%)
5	MAN	p	5	5	11,11,12	1.82	2 (18%)	15,15,17	1.20	2 (13%)
4	NAG	q	1	1,4	14,14,15	2.09	3 (21%)	17,19,21	0.83	1 (5%)
4	NAG	q	2	4	14,14,15	2.14	4 (28%)	17,19,21	1.42	2 (11%)
4	BMA	q	3	4	11,11,12	1.80	2 (18%)	15,15,17	1.03	1 (6%)
5	NAG	r	1	5,1	14,14,15	2.13	3 (21%)	17,19,21	0.83	0
5	NAG	r	2	5	14,14,15	2.10	5 (35%)	17,19,21	1.30	2 (11%)
5	BMA	r	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.92	0
5	MAN	r	4	5	11,11,12	1.73	2 (18%)	15,15,17	1.13	1 (6%)
5	MAN	r	5	5	11,11,12	1.85	2 (18%)	15,15,17	1.16	2 (13%)
4	NAG	s	1	1,4	14,14,15	2.09	3 (21%)	17,19,21	1.01	2 (11%)
4	NAG	s	2	4	14,14,15	2.11	3 (21%)	17,19,21	1.33	3 (17%)
4	BMA	s	3	4	11,11,12	1.79	2 (18%)	15,15,17	1.02	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
5	NAG	K	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	MAN	K	4	5	-	1/2/19/22	0/1/1/1
5	MAN	K	5	5	-	1/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	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	-	2/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	MAN	O	4	5	-	1/2/19/22	0/1/1/1
5	MAN	O	5	5	-	1/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	BMA	P	3	5	-	1/2/19/22	0/1/1/1
5	MAN	P	4	5	-	1/2/19/22	0/1/1/1
5	MAN	P	5	5	-	1/2/19/22	0/1/1/1
5	NAG	Q	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	1/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

The worst 5 of 374 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	2	NAG	O5-C1	7.52	1.56	1.43
4	k	2	NAG	O5-C1	7.49	1.56	1.43
4	F	2	NAG	O5-C1	7.17	1.55	1.43
4	V	2	NAG	O5-C1	7.08	1.55	1.43
4	j	2	NAG	O5-C1	7.08	1.55	1.43

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	2	NAG	C4-C3-C2	-5.25	103.32	111.02
4	G	2	NAG	C4-C3-C2	-4.62	104.25	111.02
4	V	2	NAG	C4-C3-C2	-4.51	104.41	111.02
4	o	2	NAG	C4-C3-C2	-4.38	104.59	111.02
4	V	1	NAG	C1-O5-C5	-4.36	106.34	112.19

There are no chirality outliers.

5 of 137 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	g	2	NAG	O5-C5-C6-O6

*Continued on next page...*

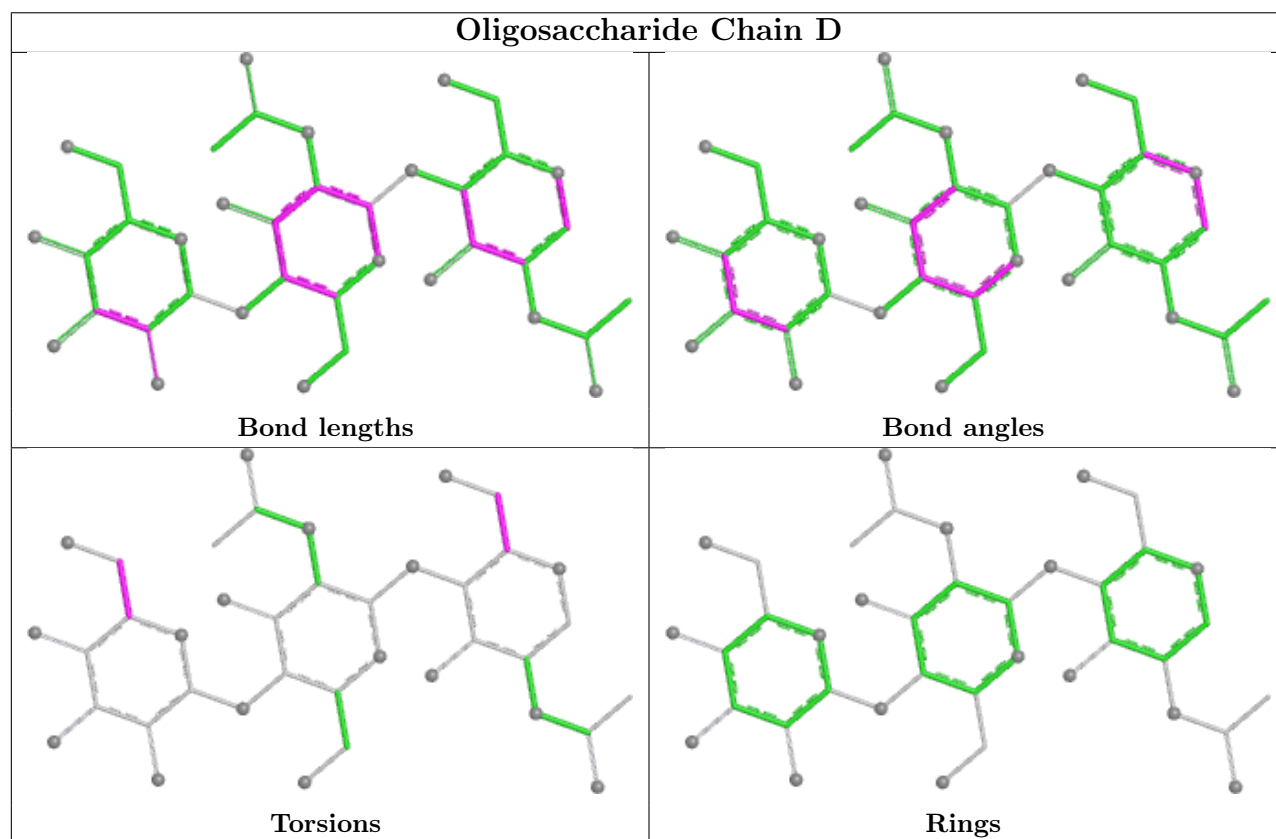
*Continued from previous page...*

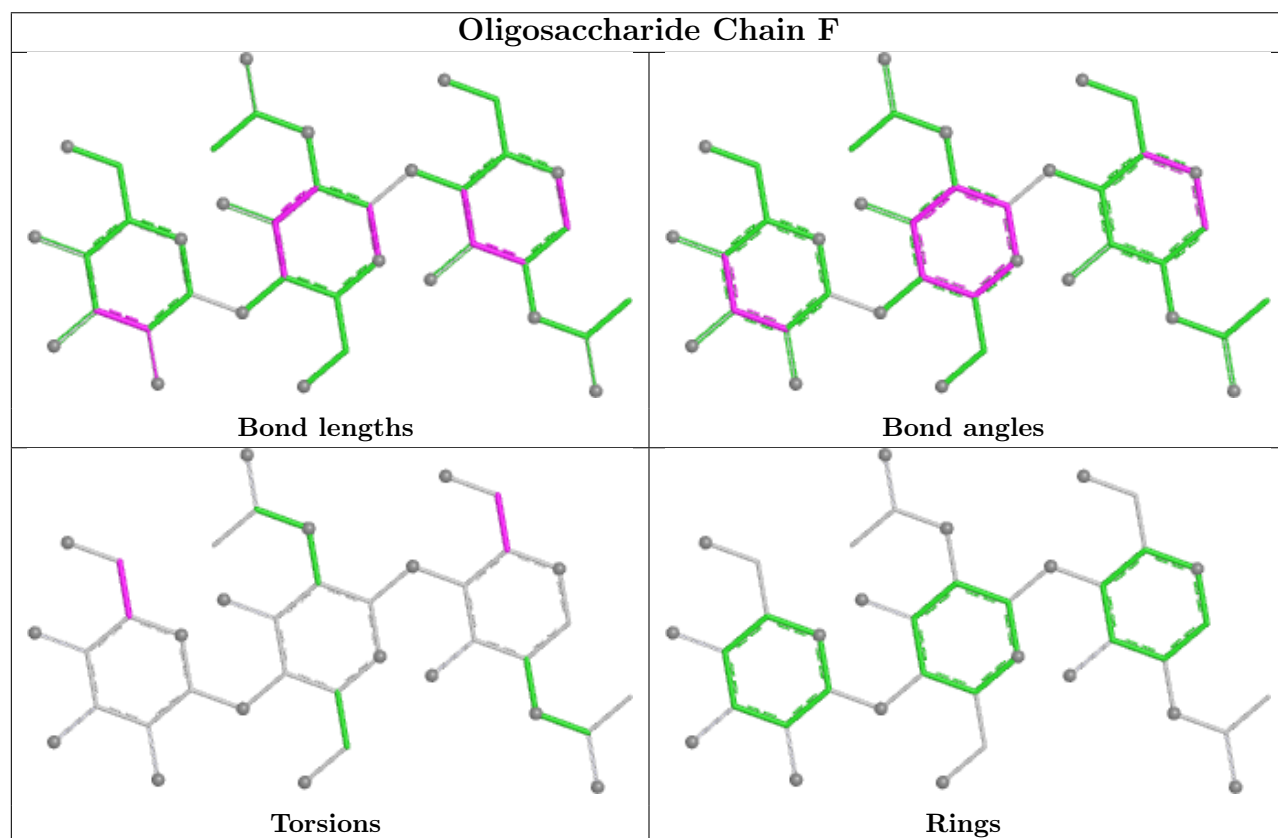
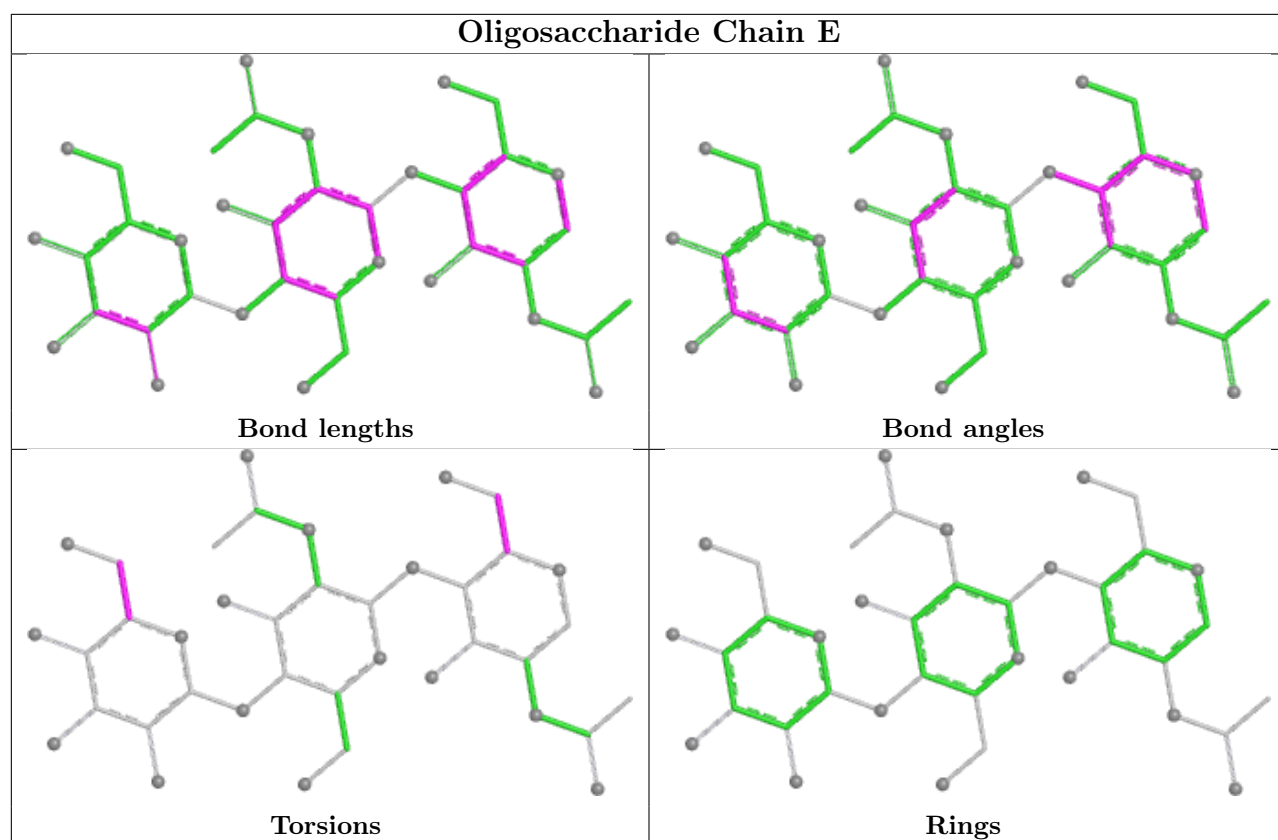
Mol	Chain	Res	Type	Atoms
4	a	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

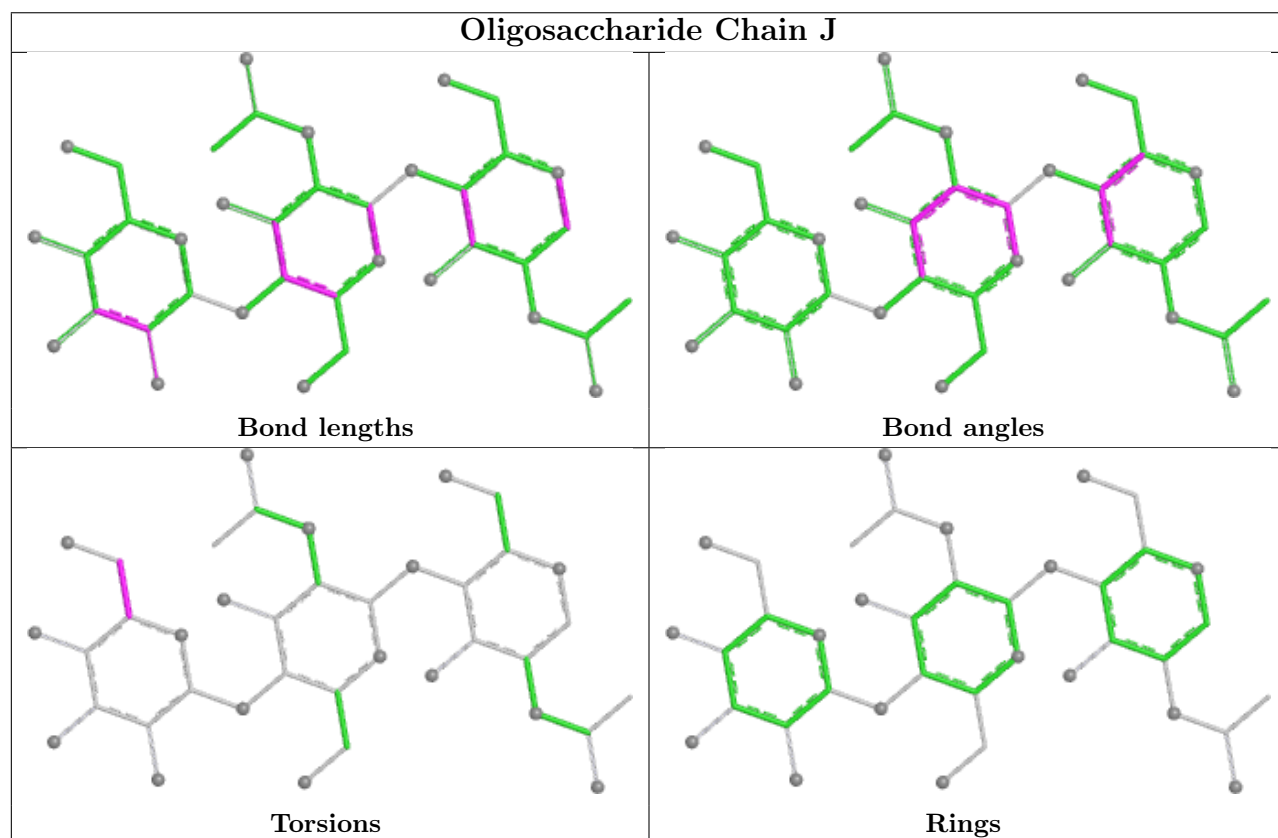
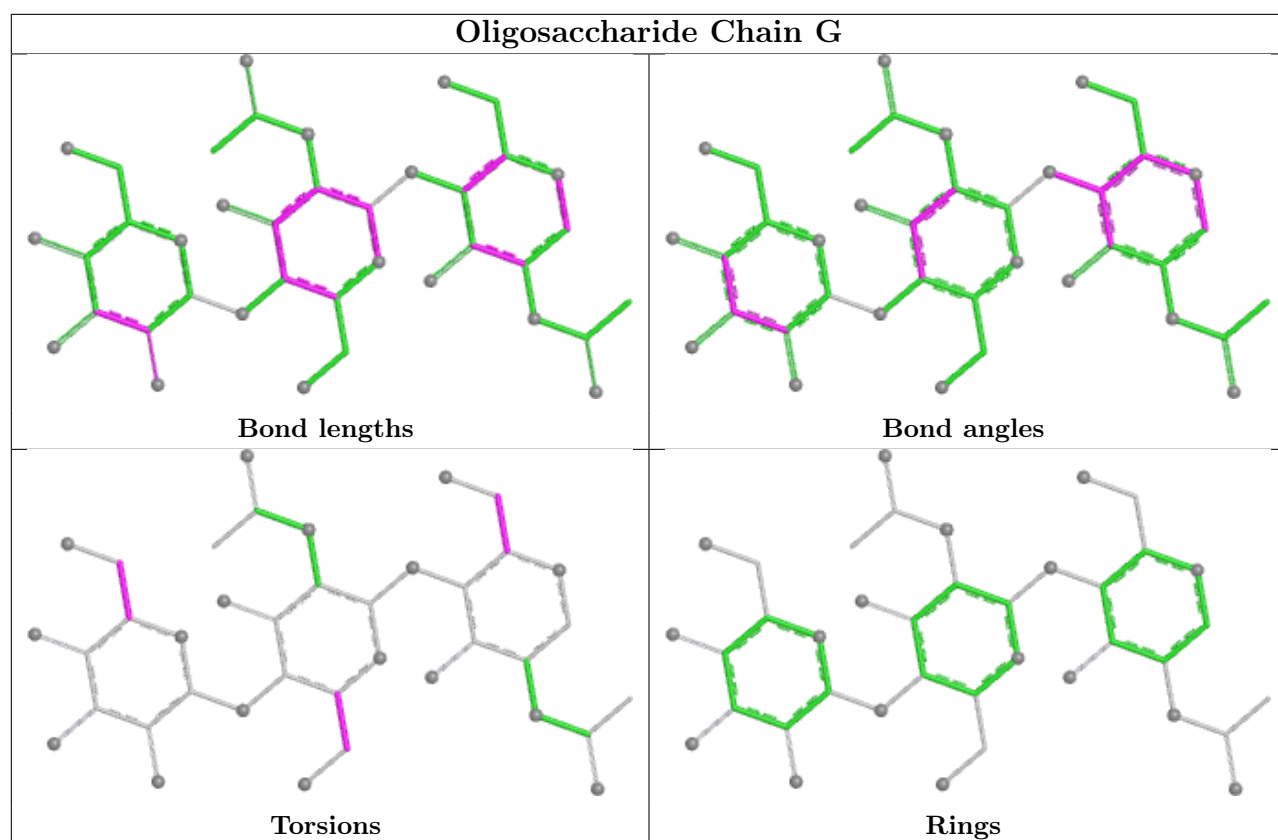
There are no ring outliers.

No monomer is involved in short contacts.

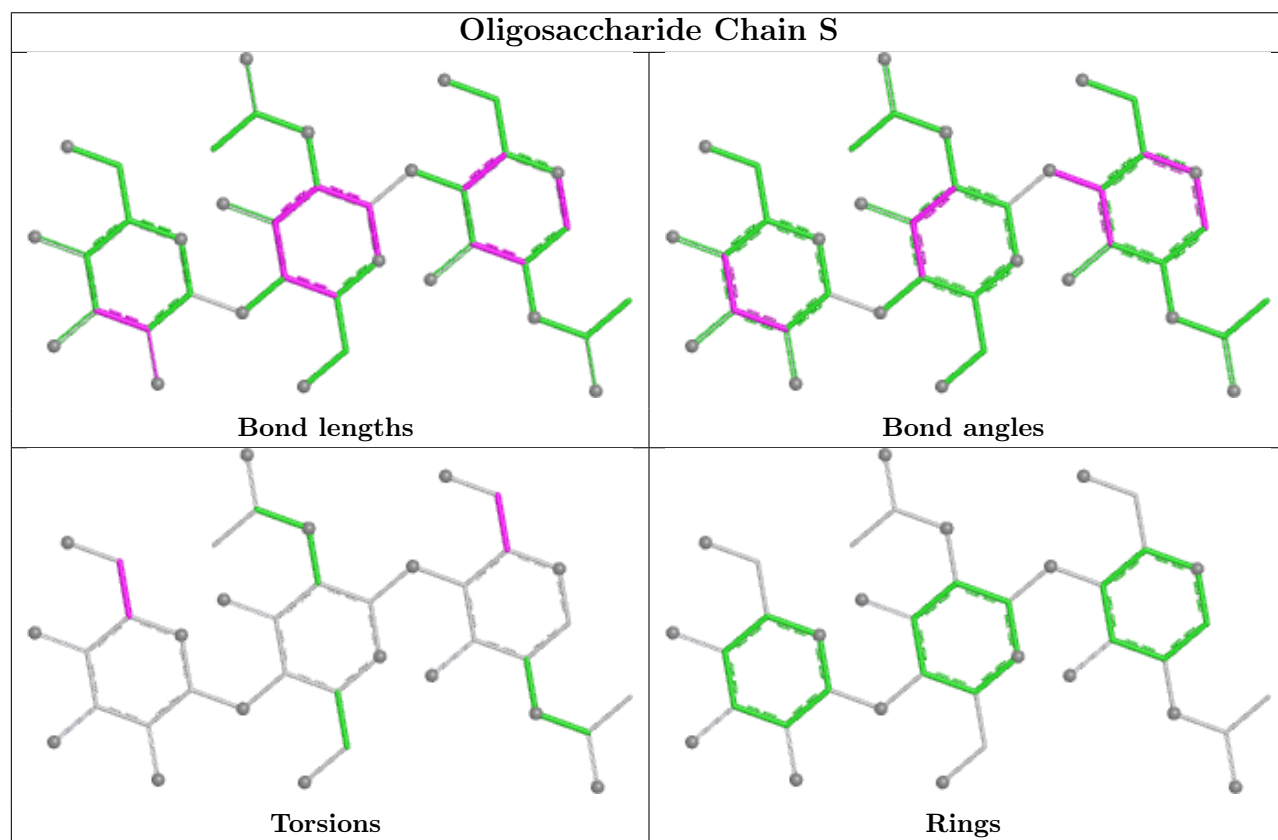
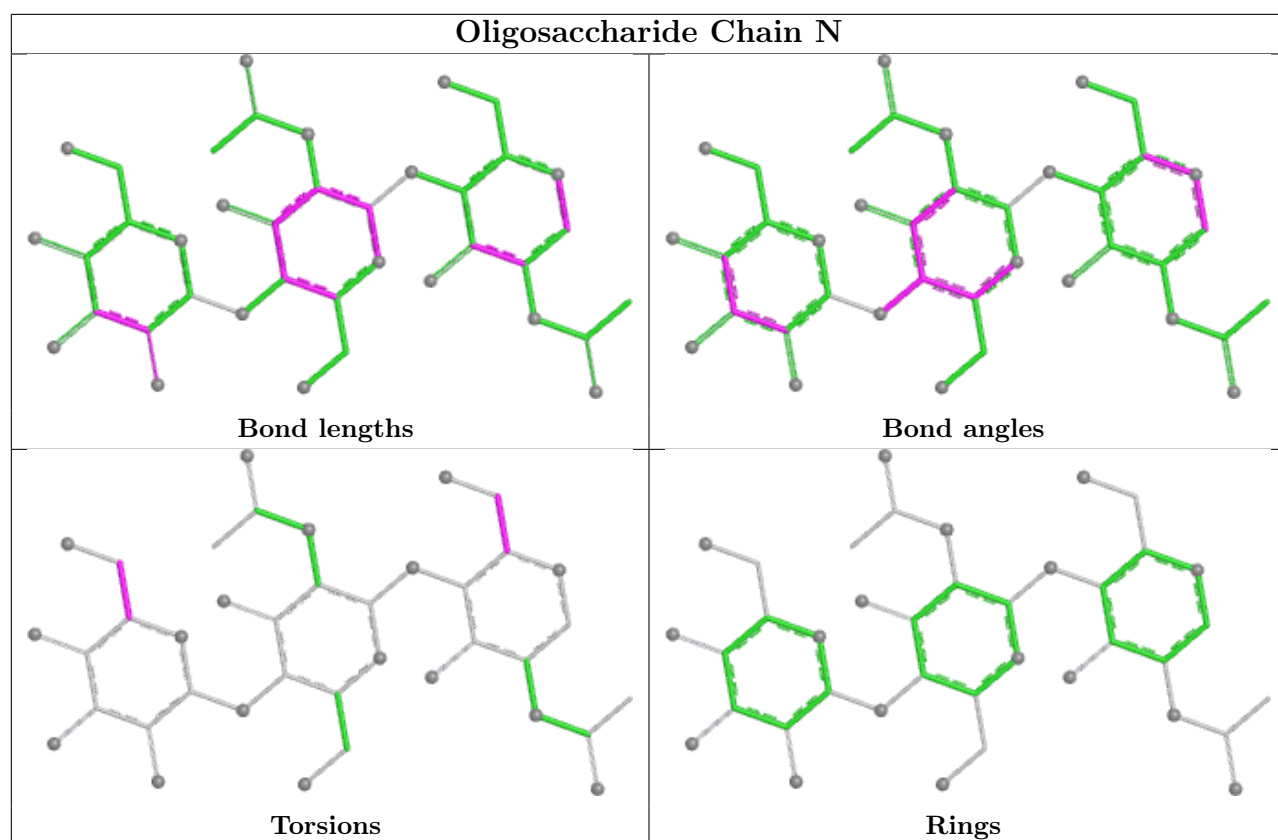
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

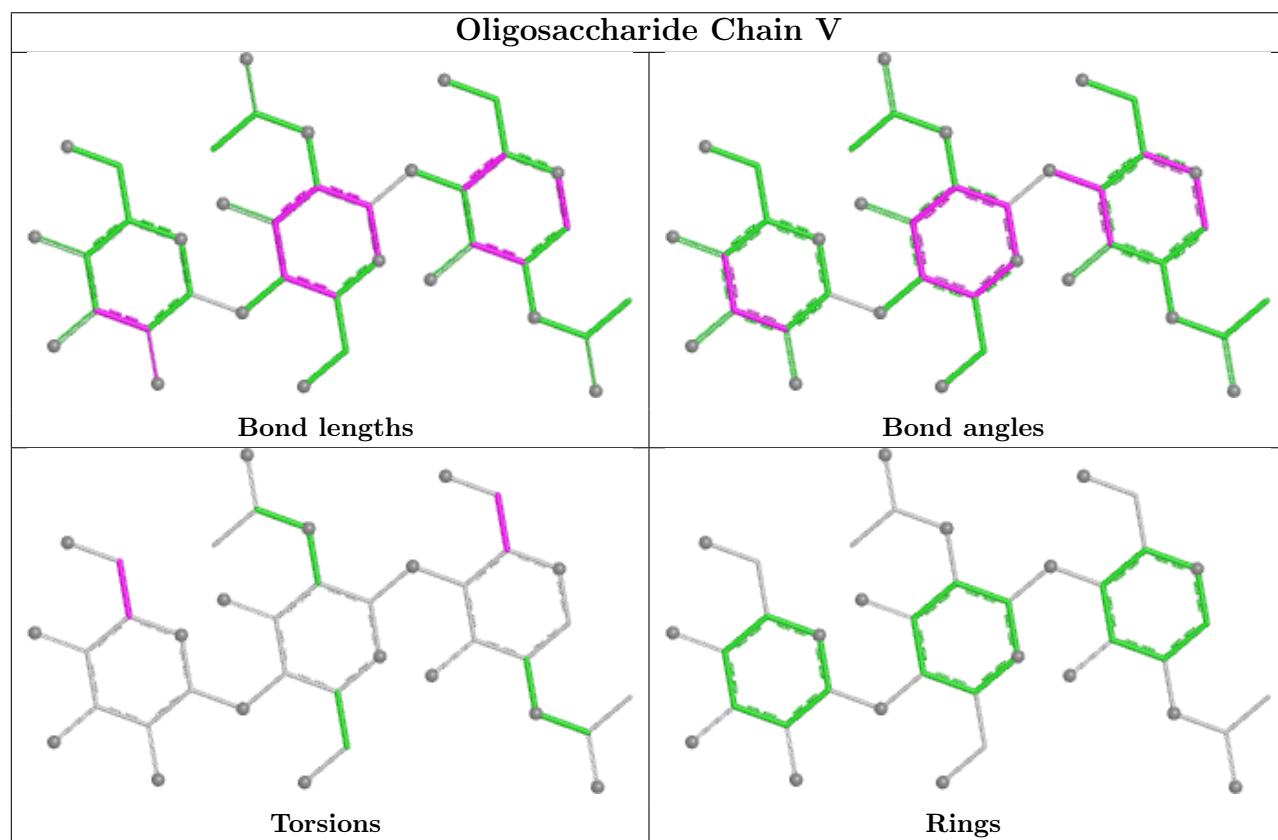
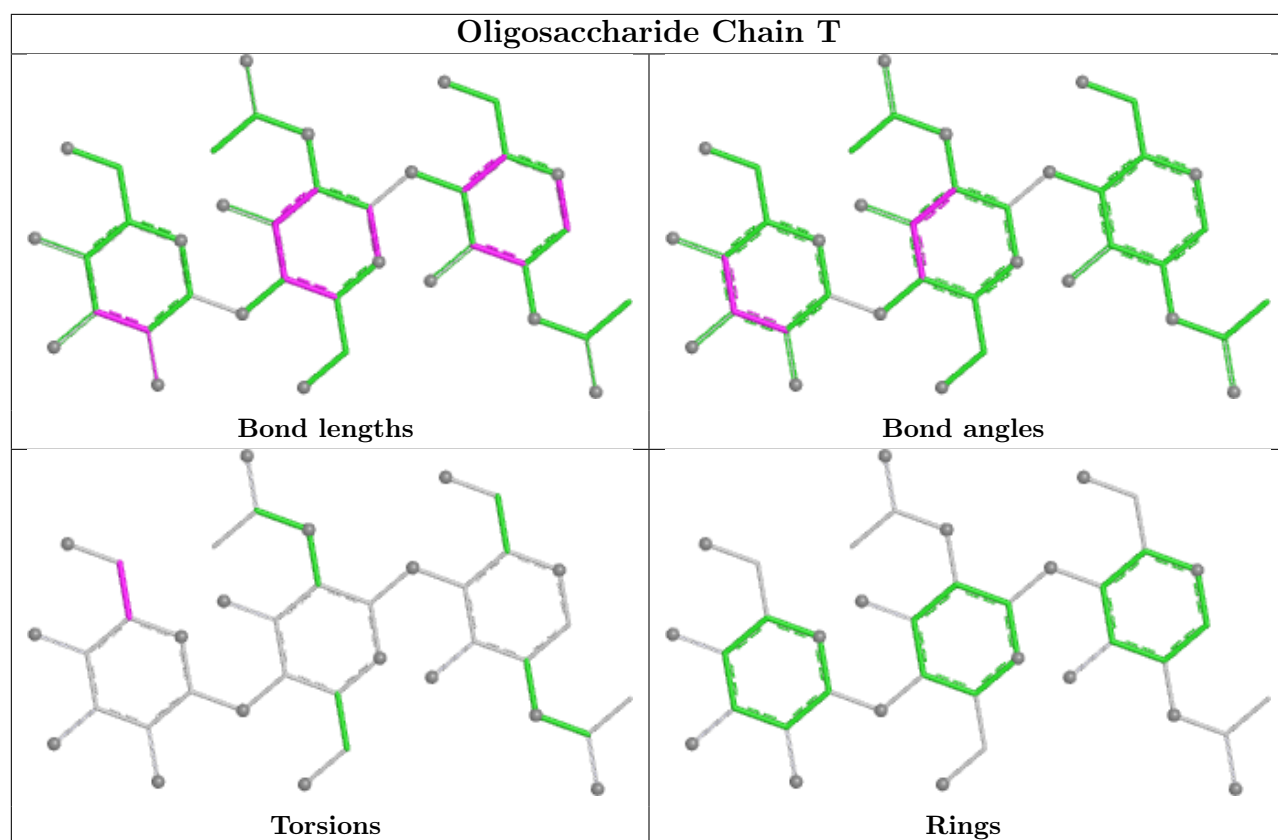


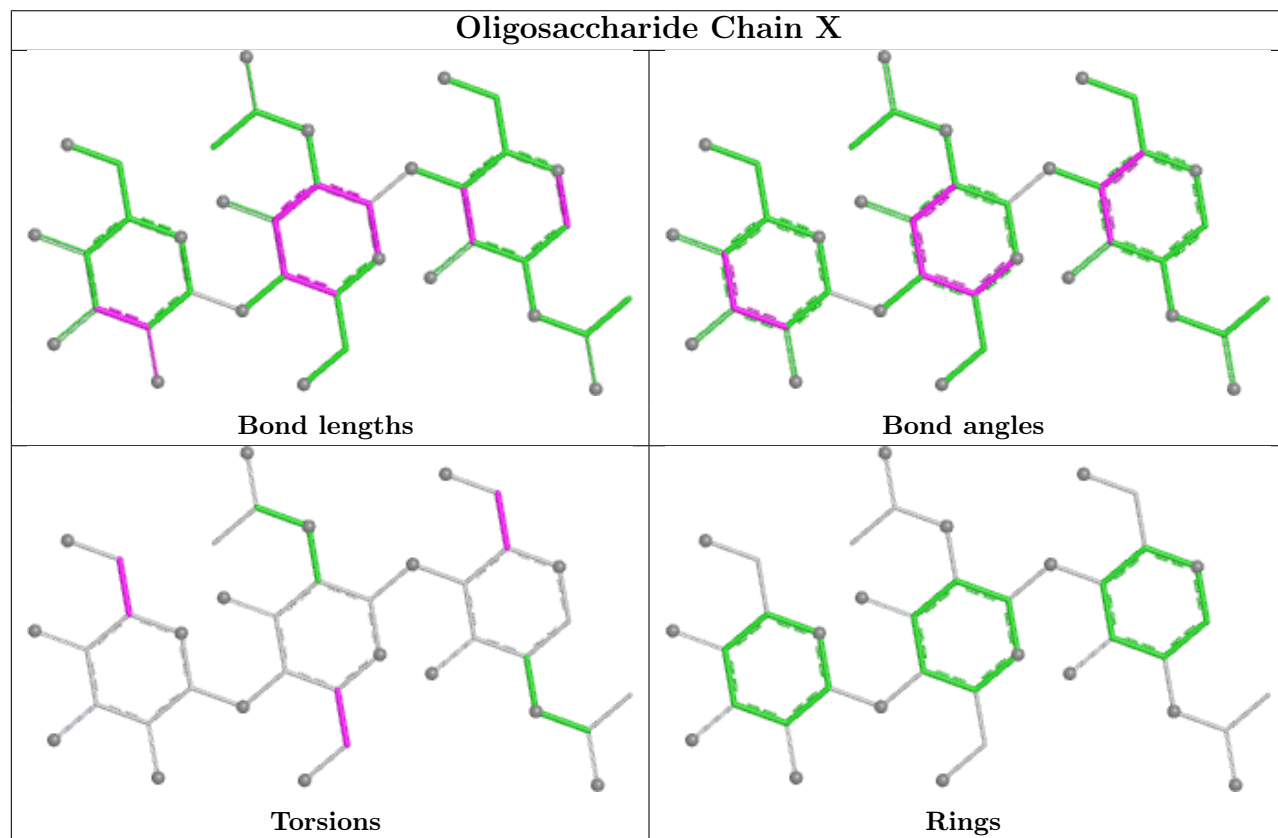
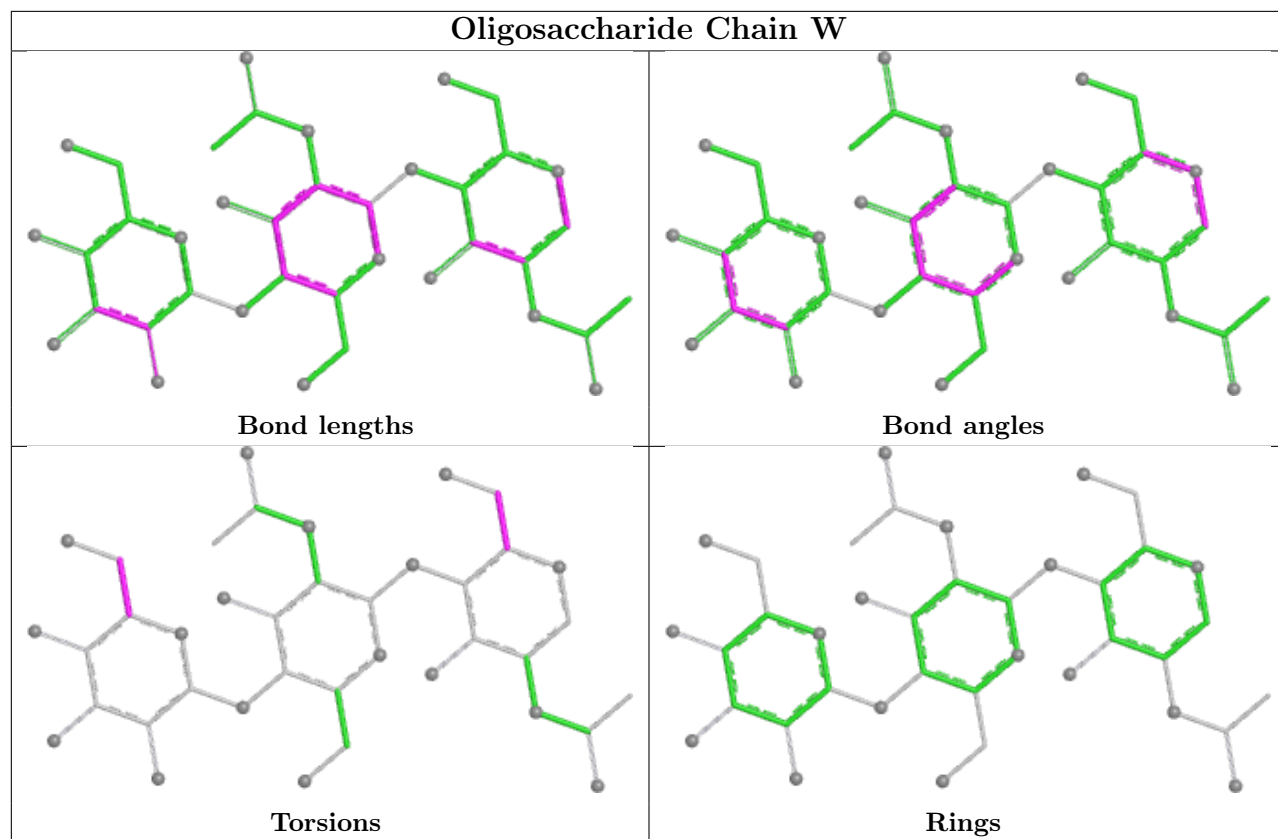


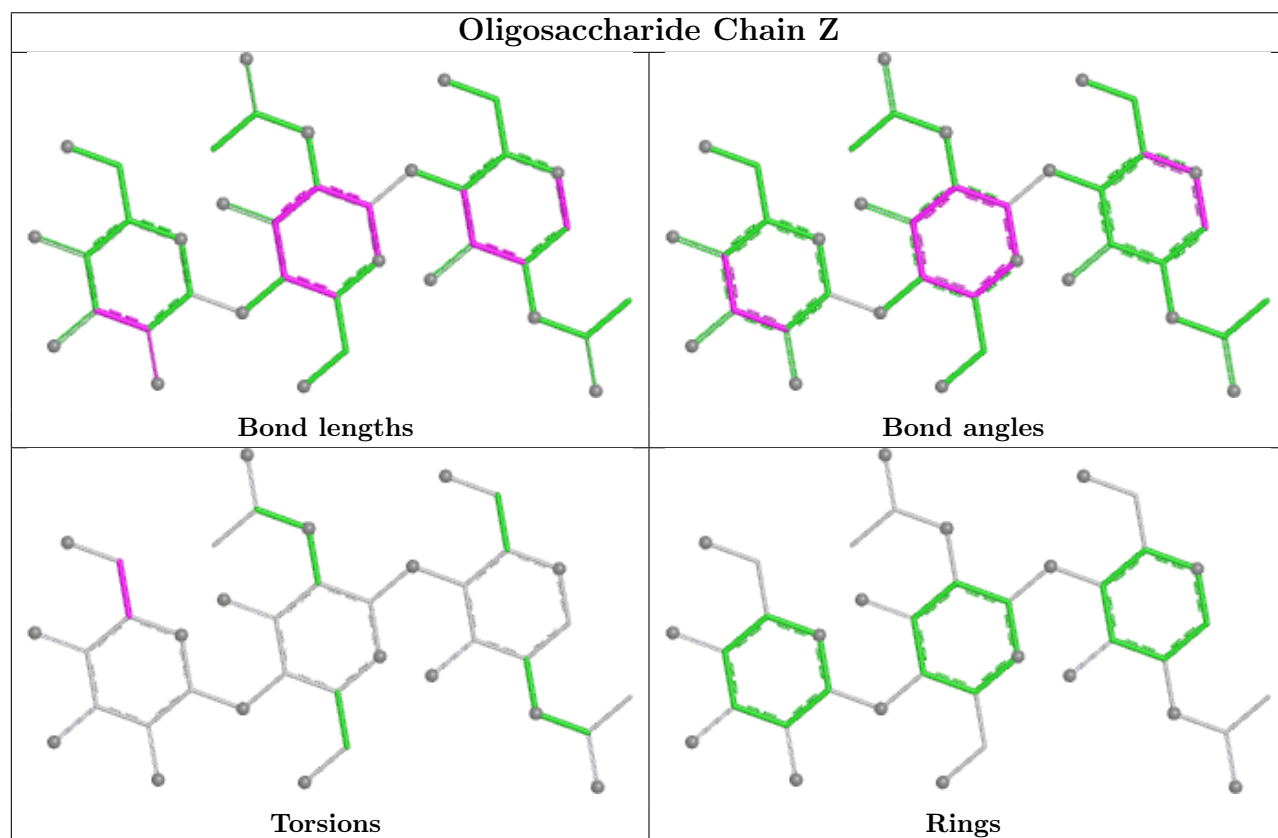
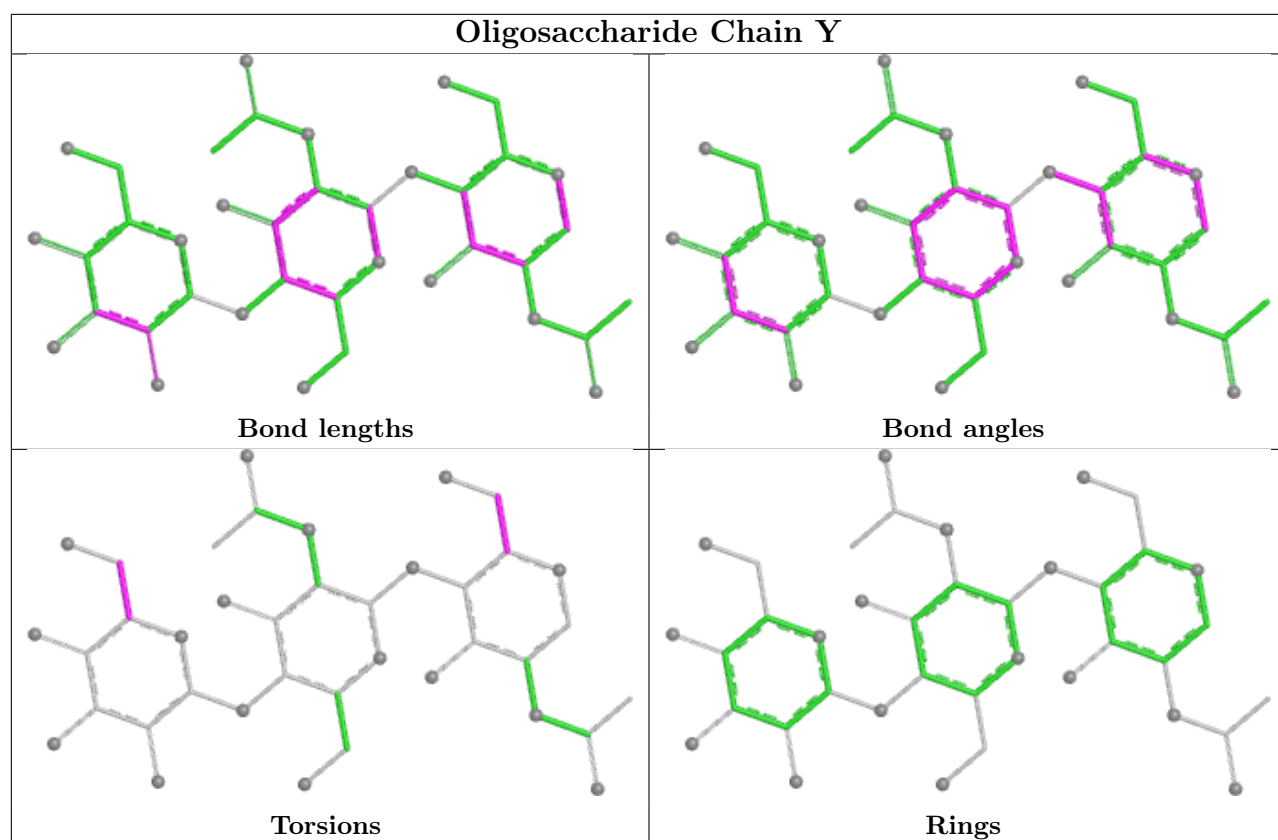


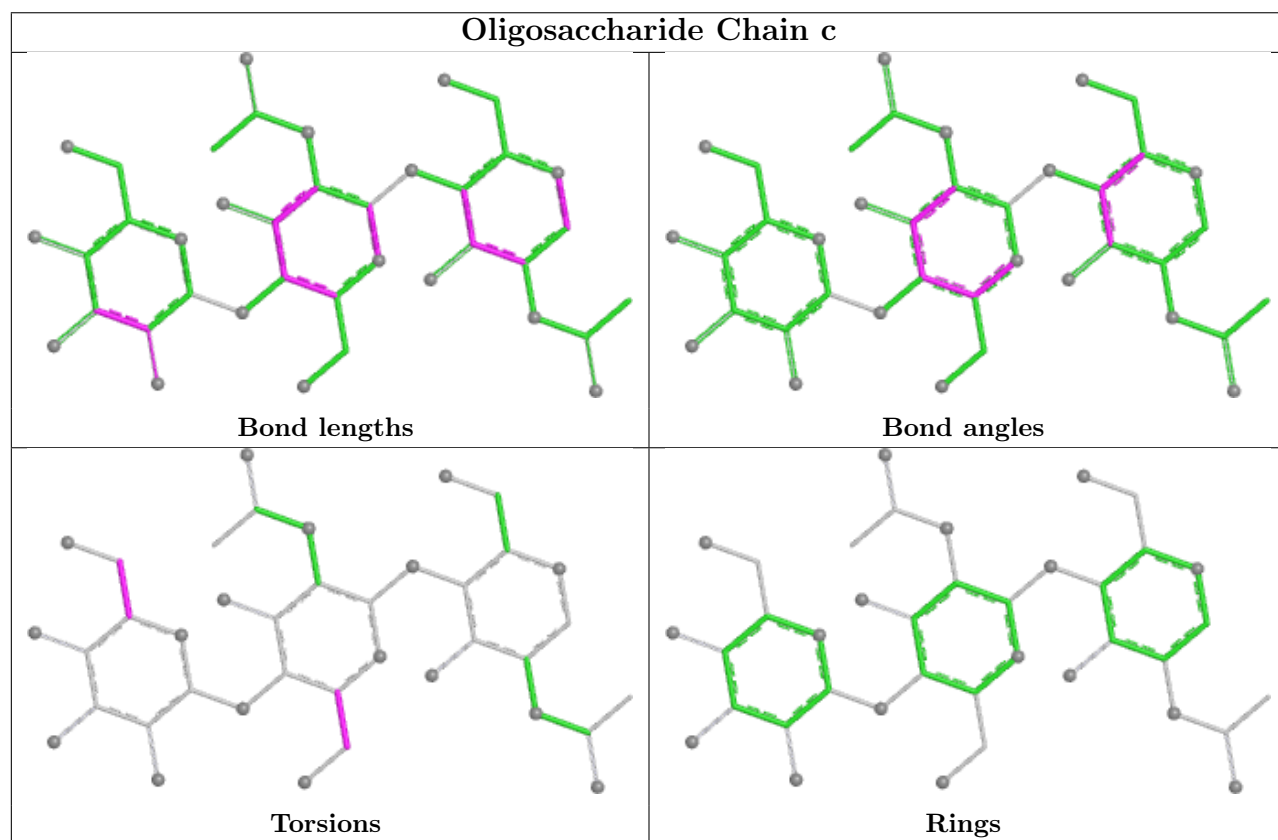
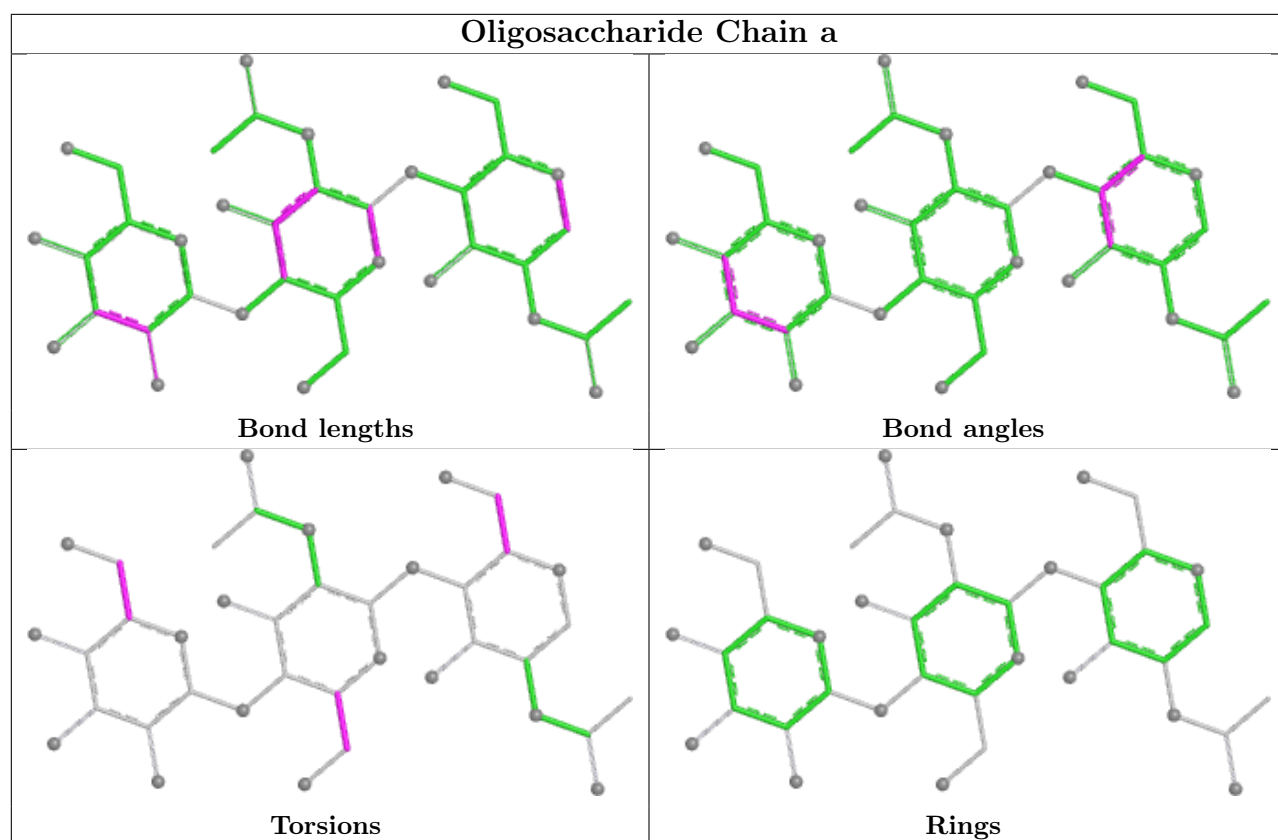


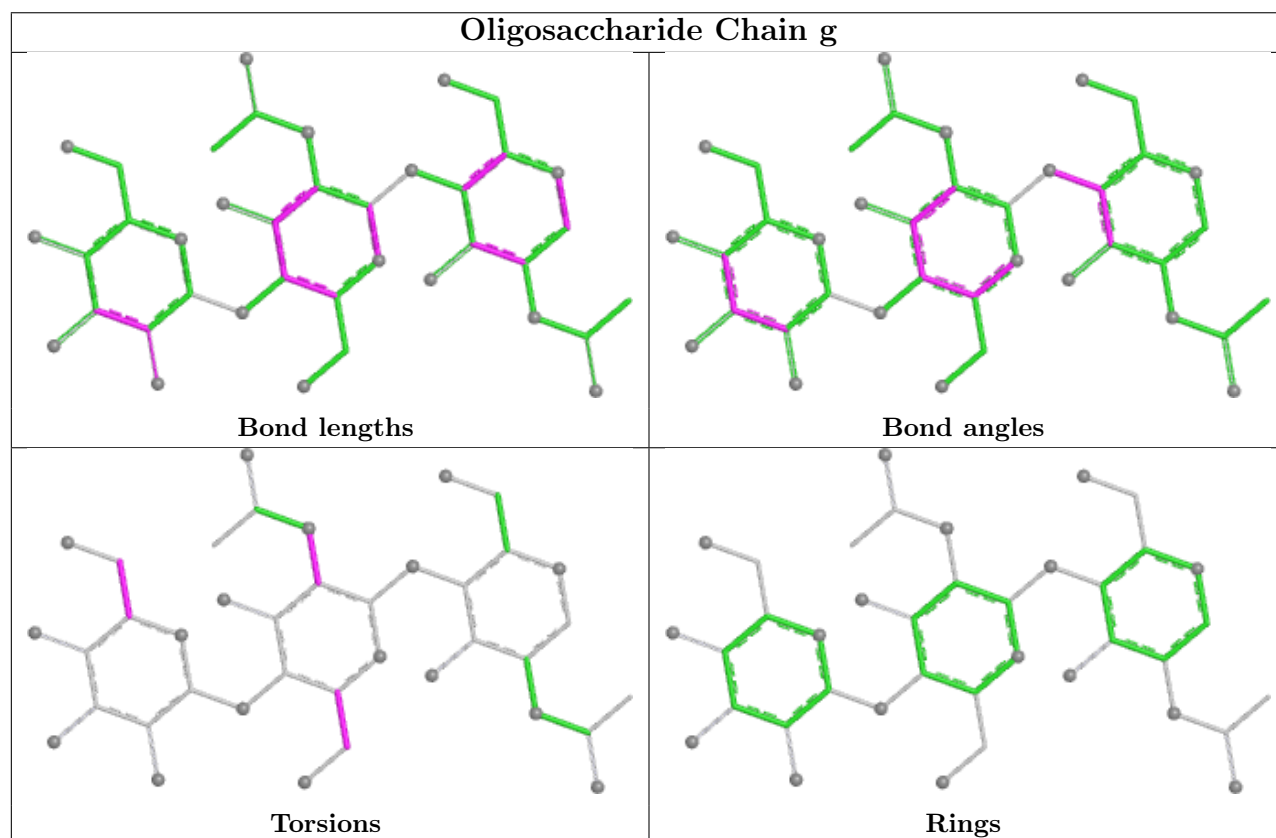
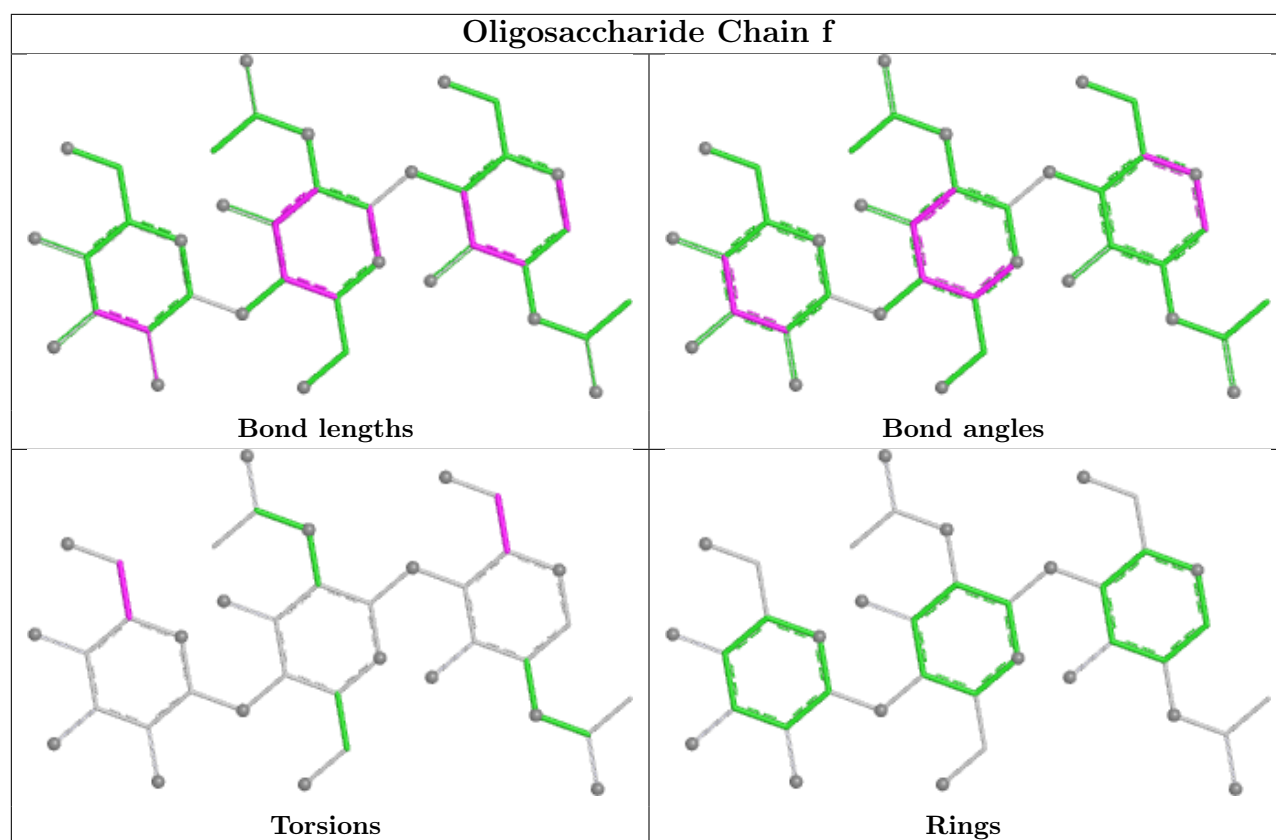


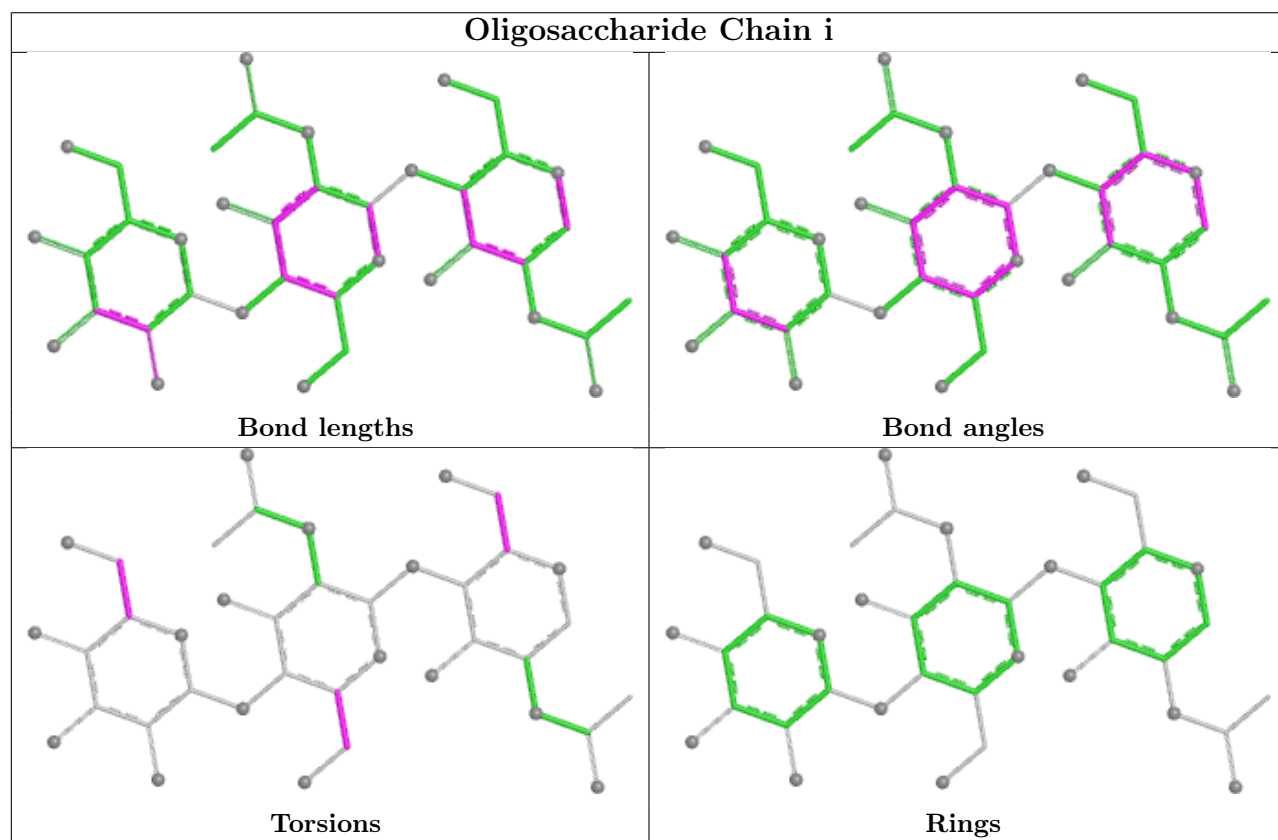
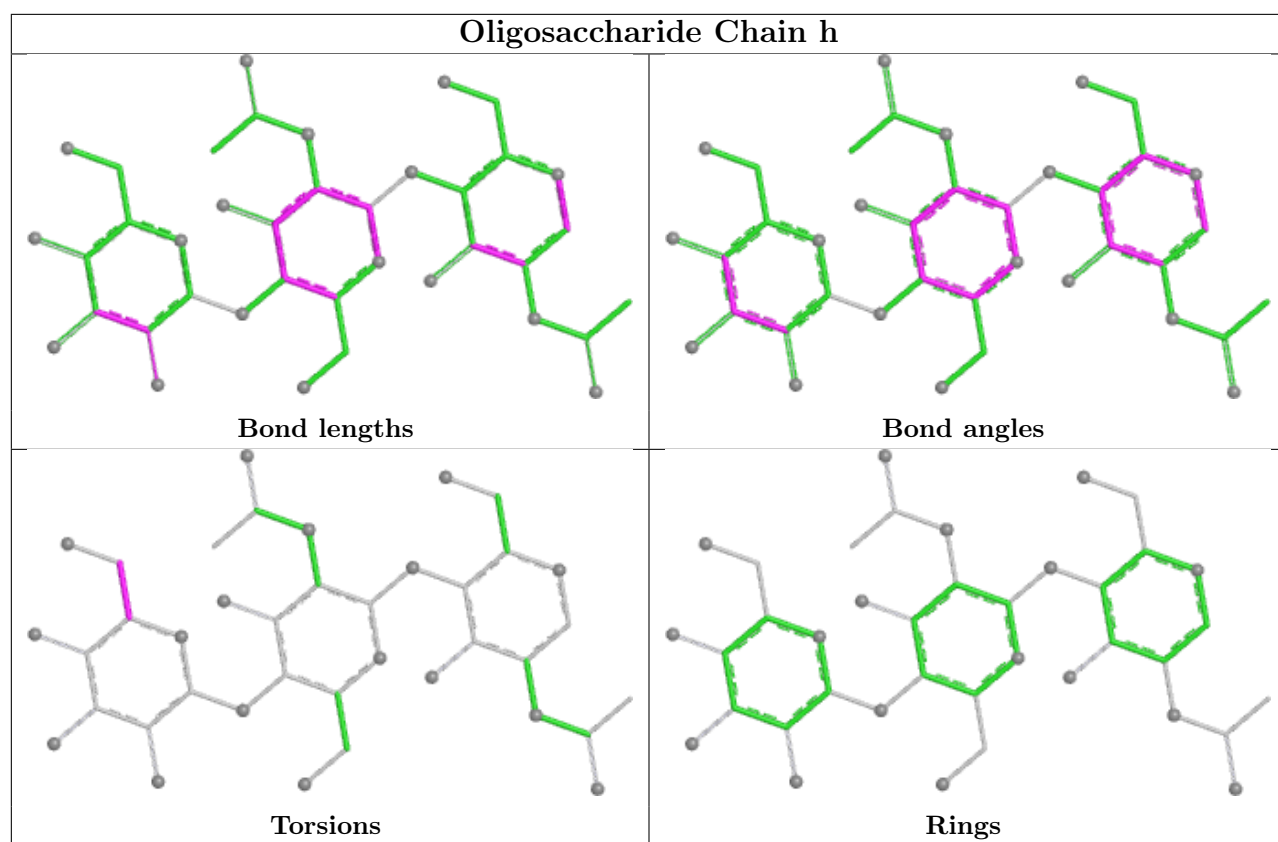


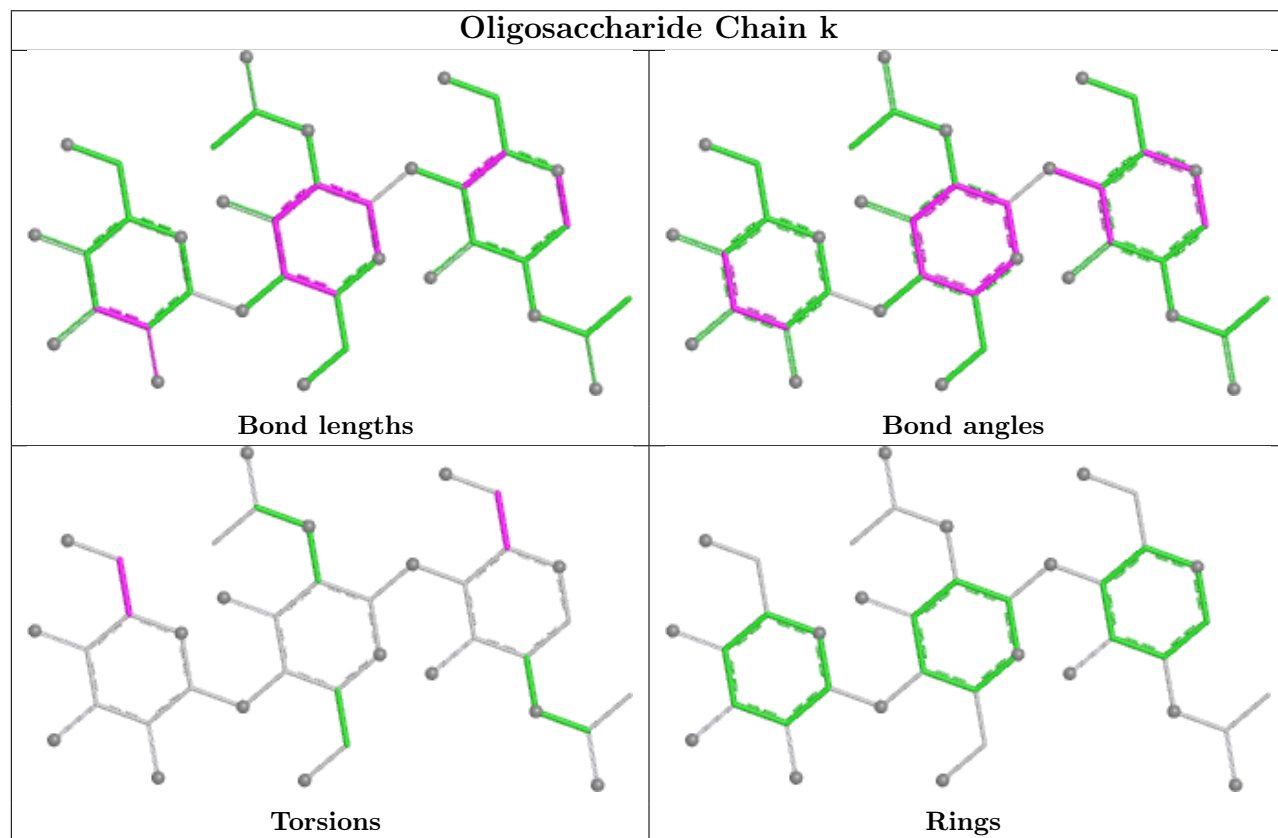
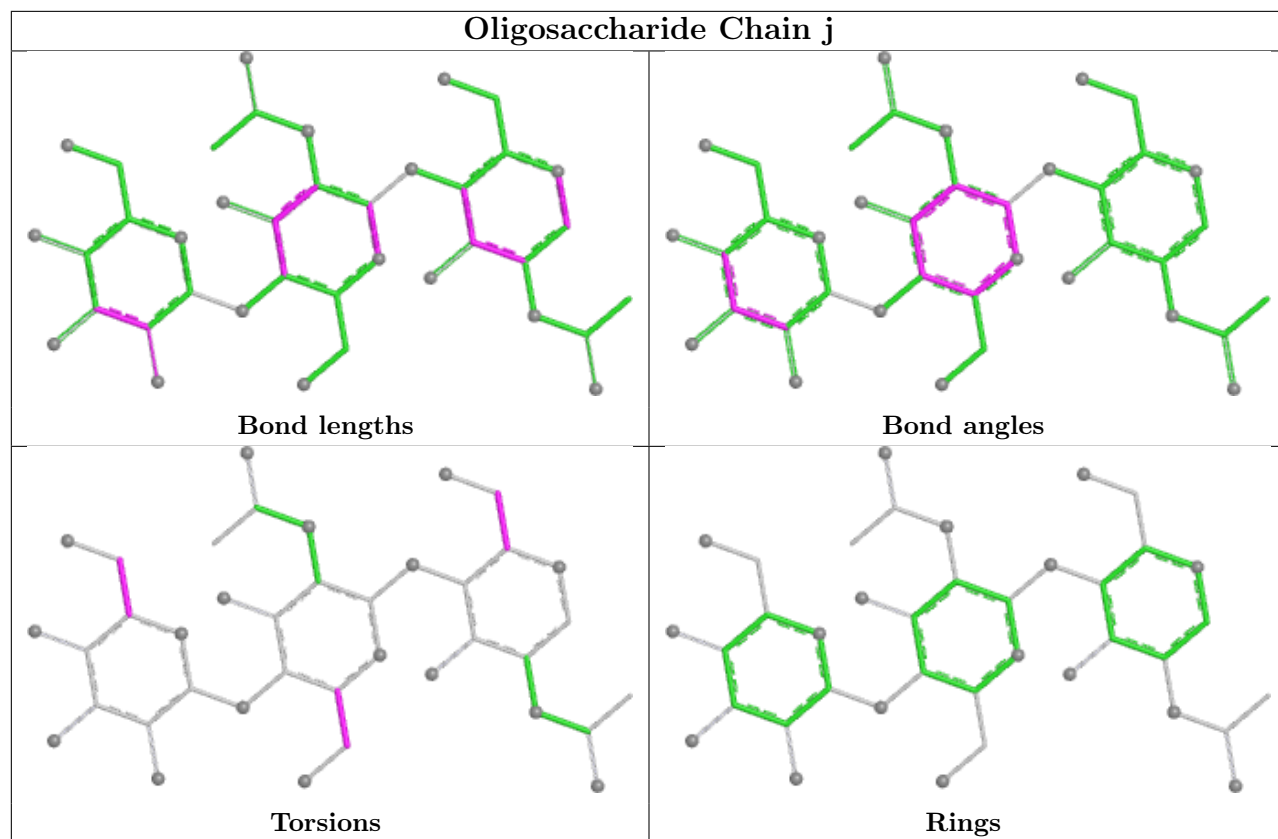




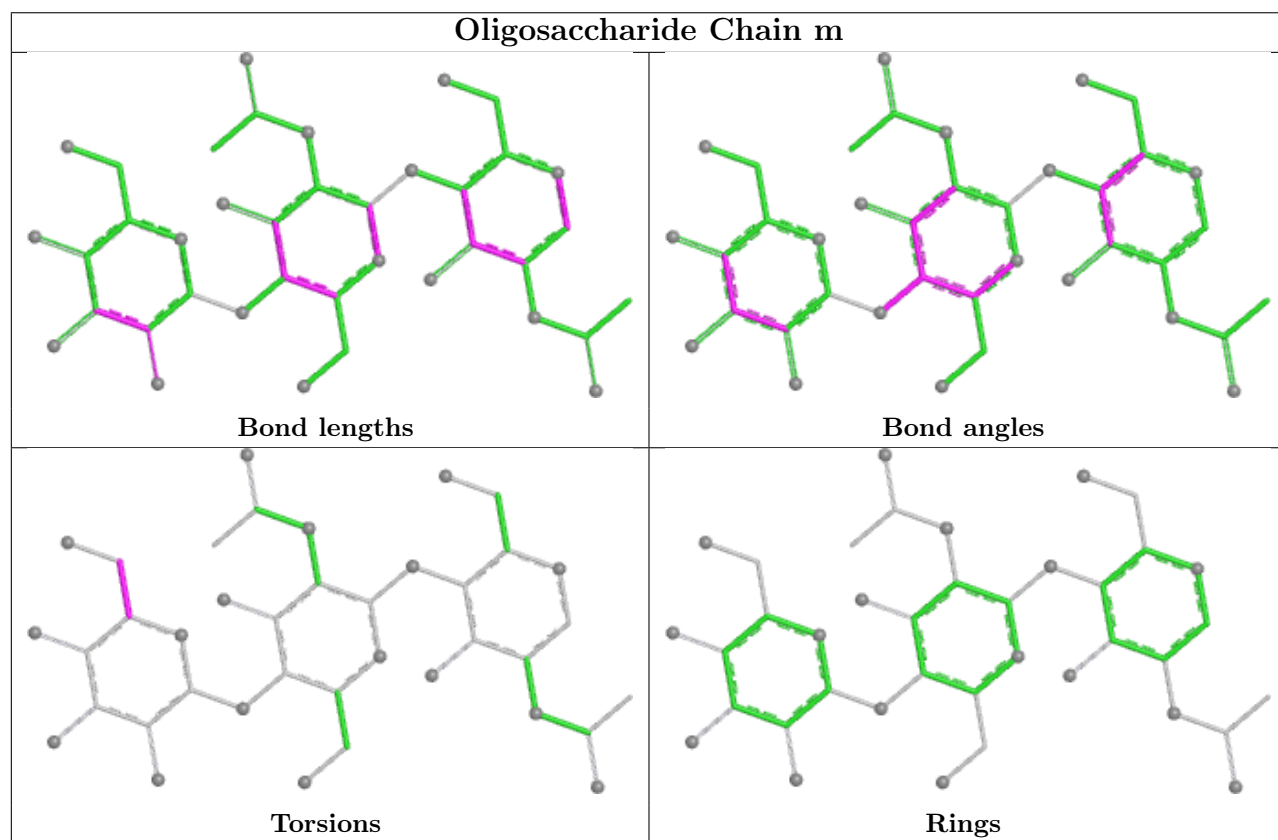
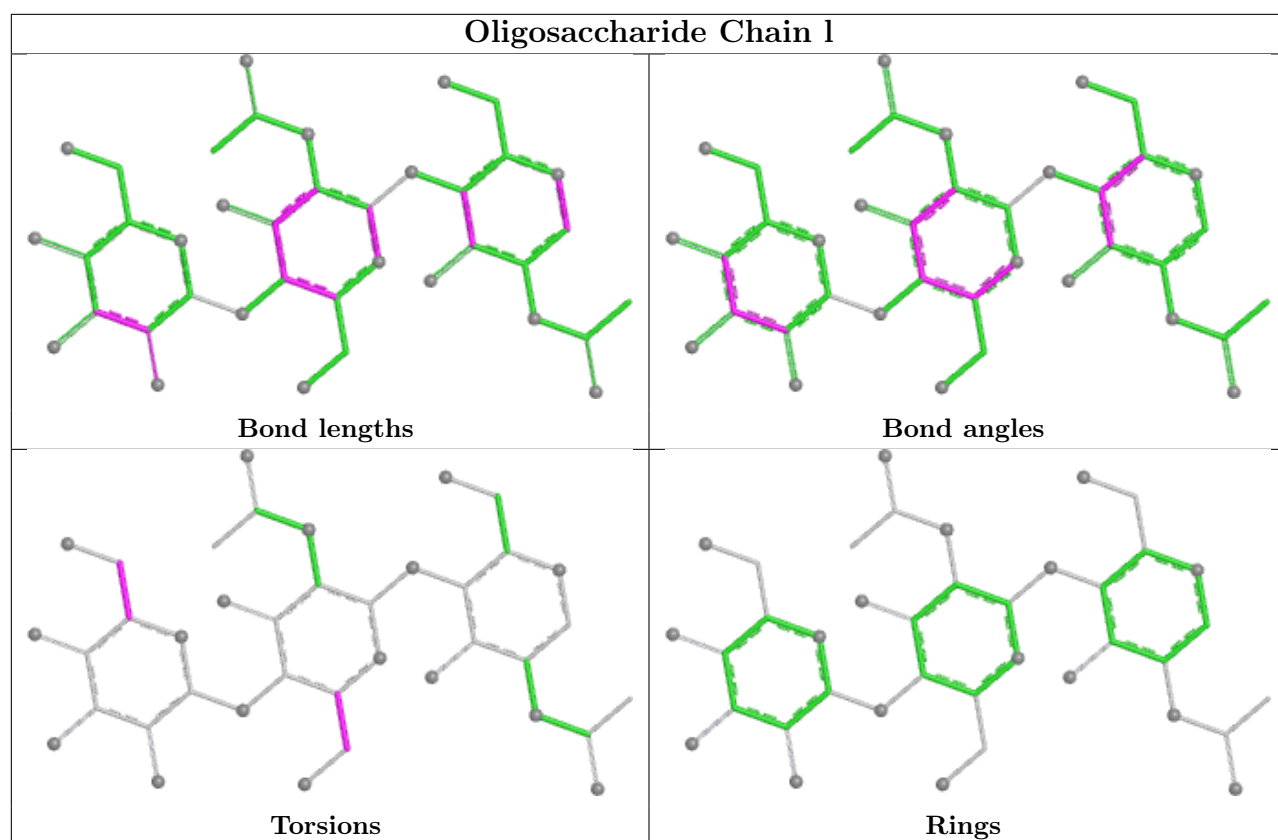


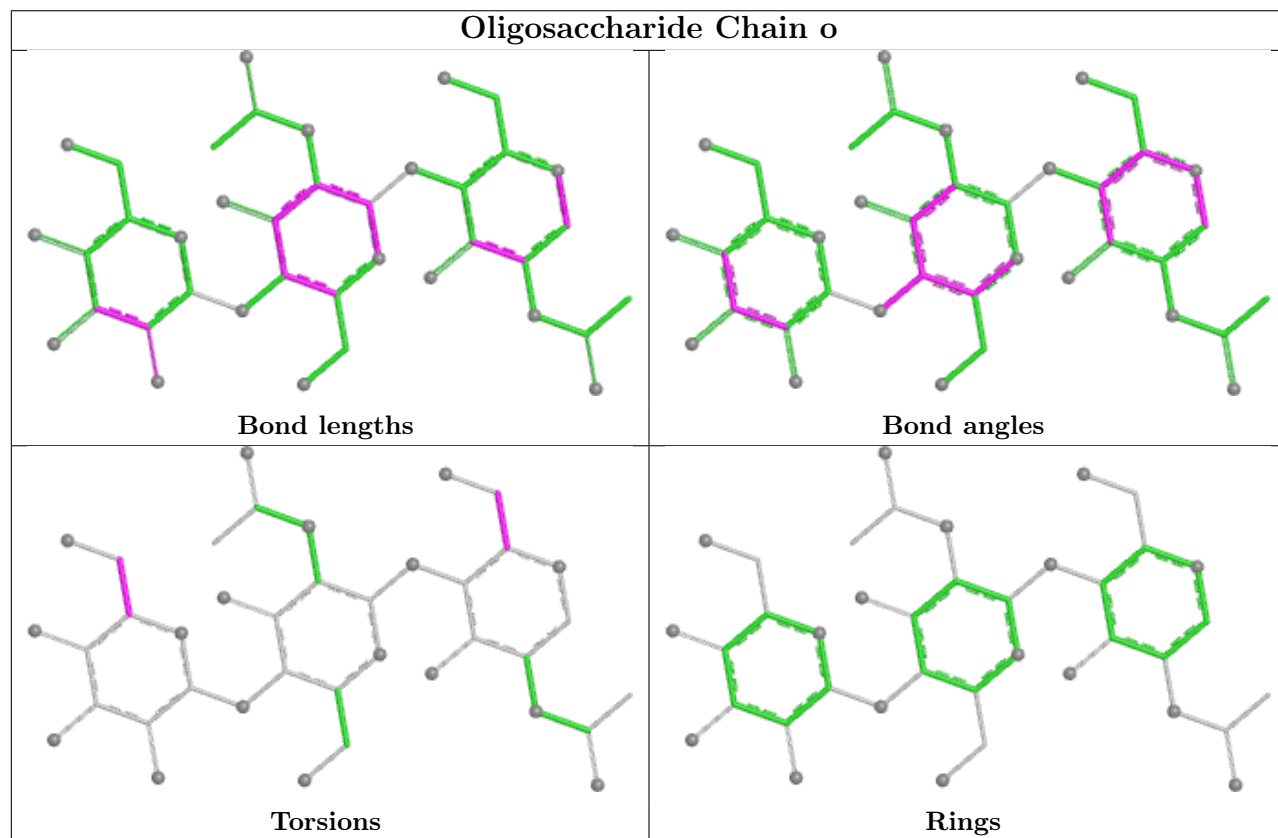
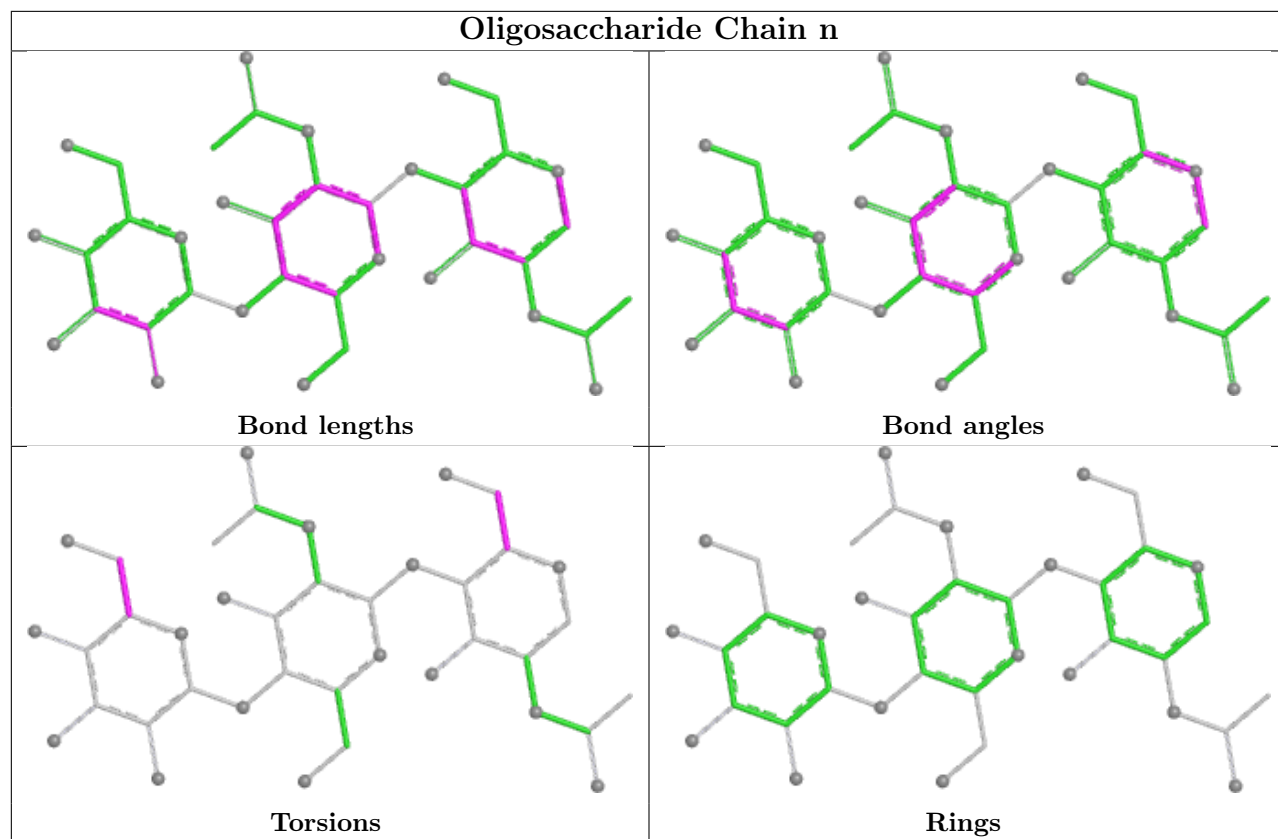


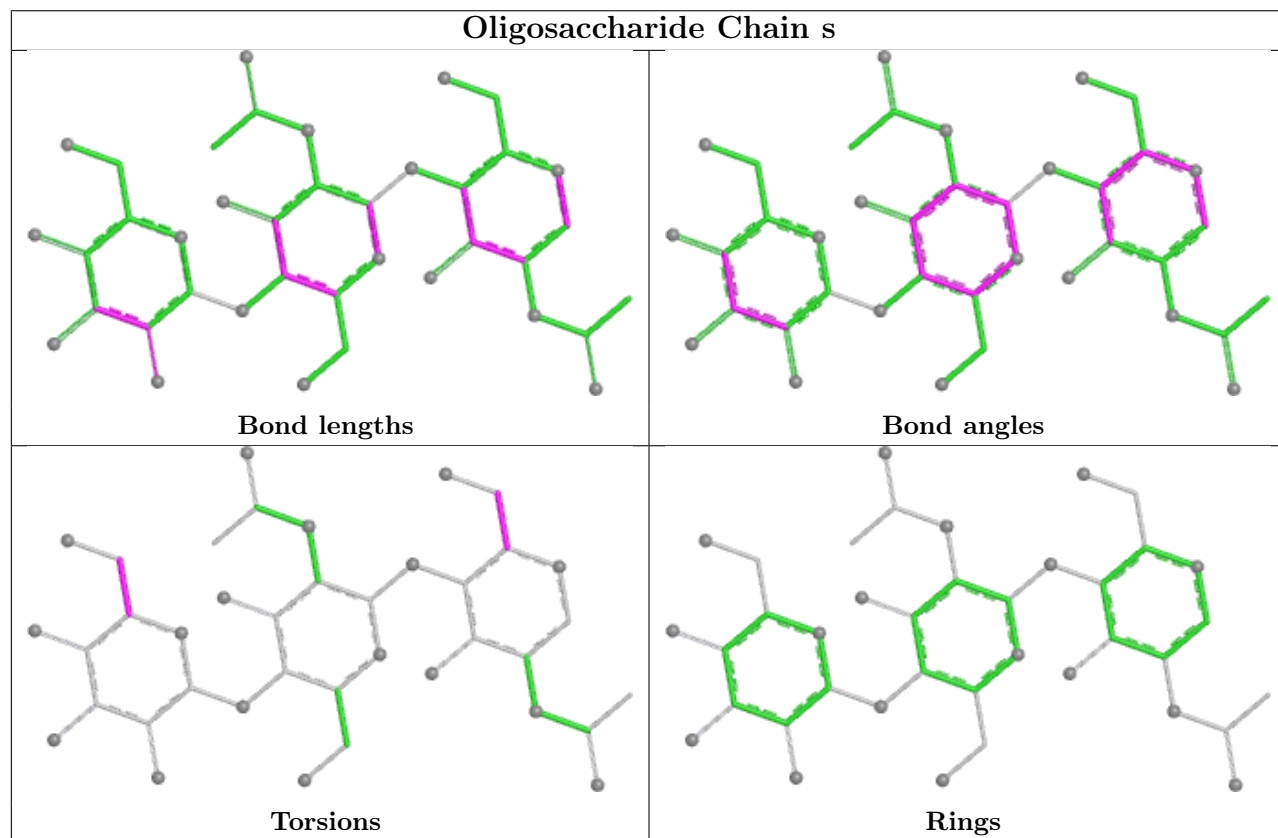
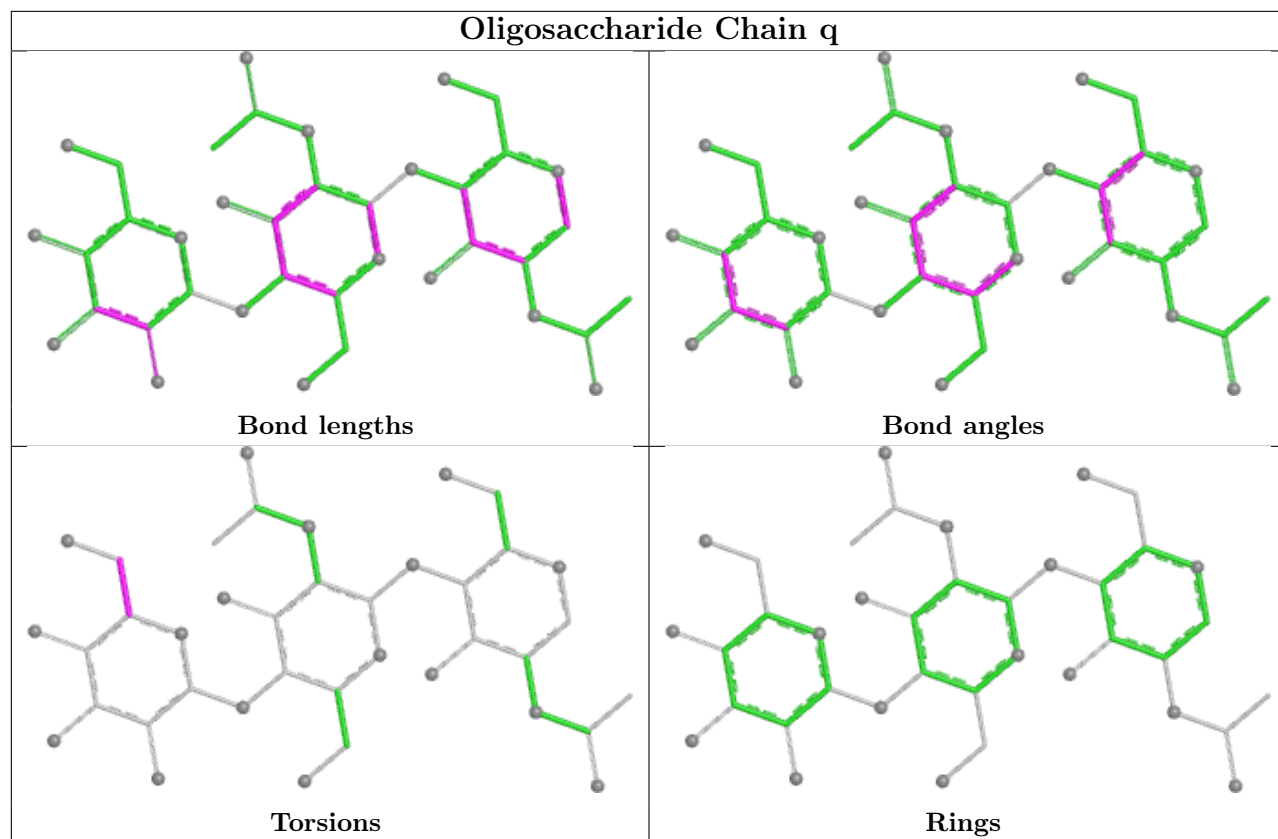


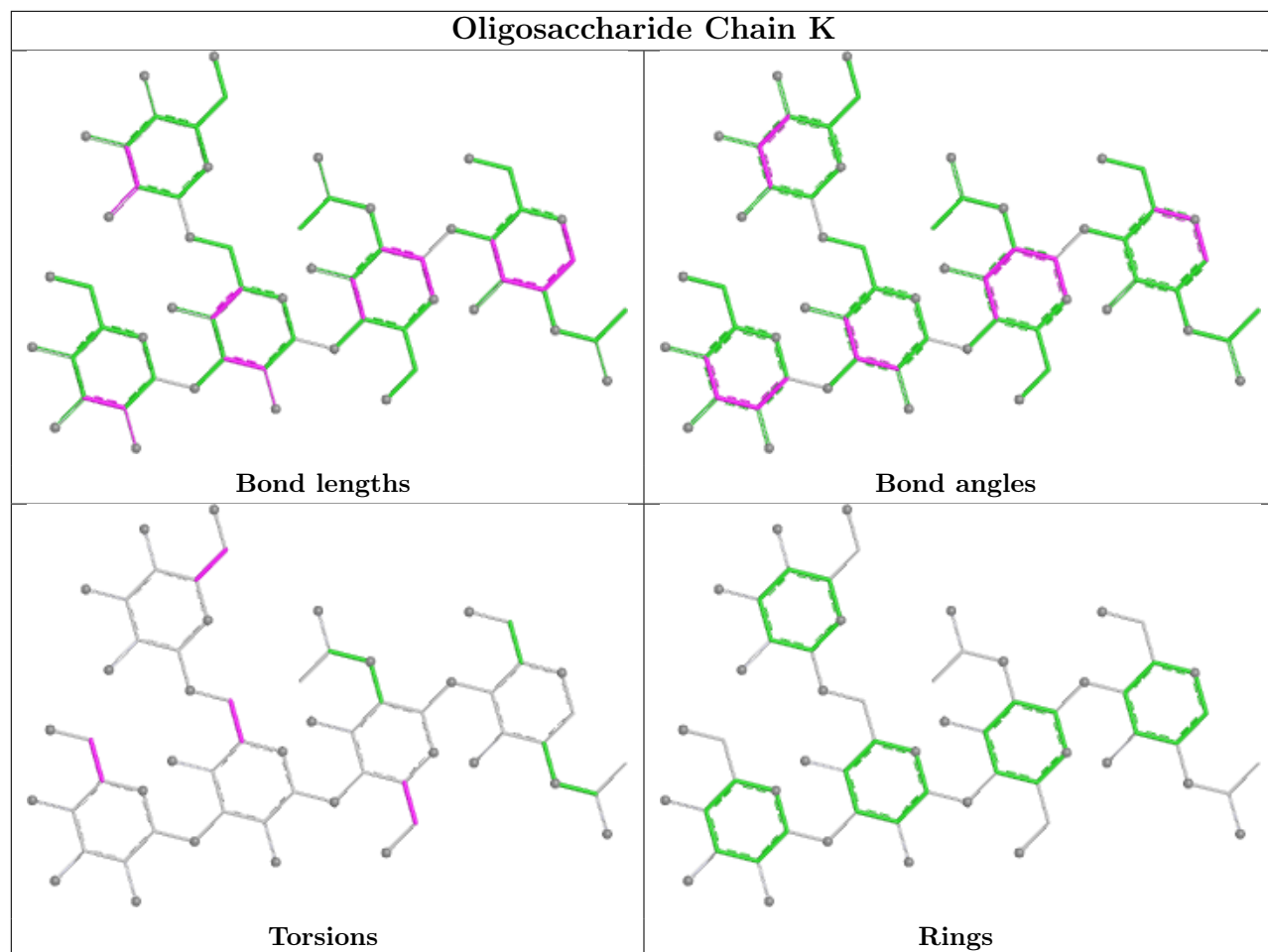


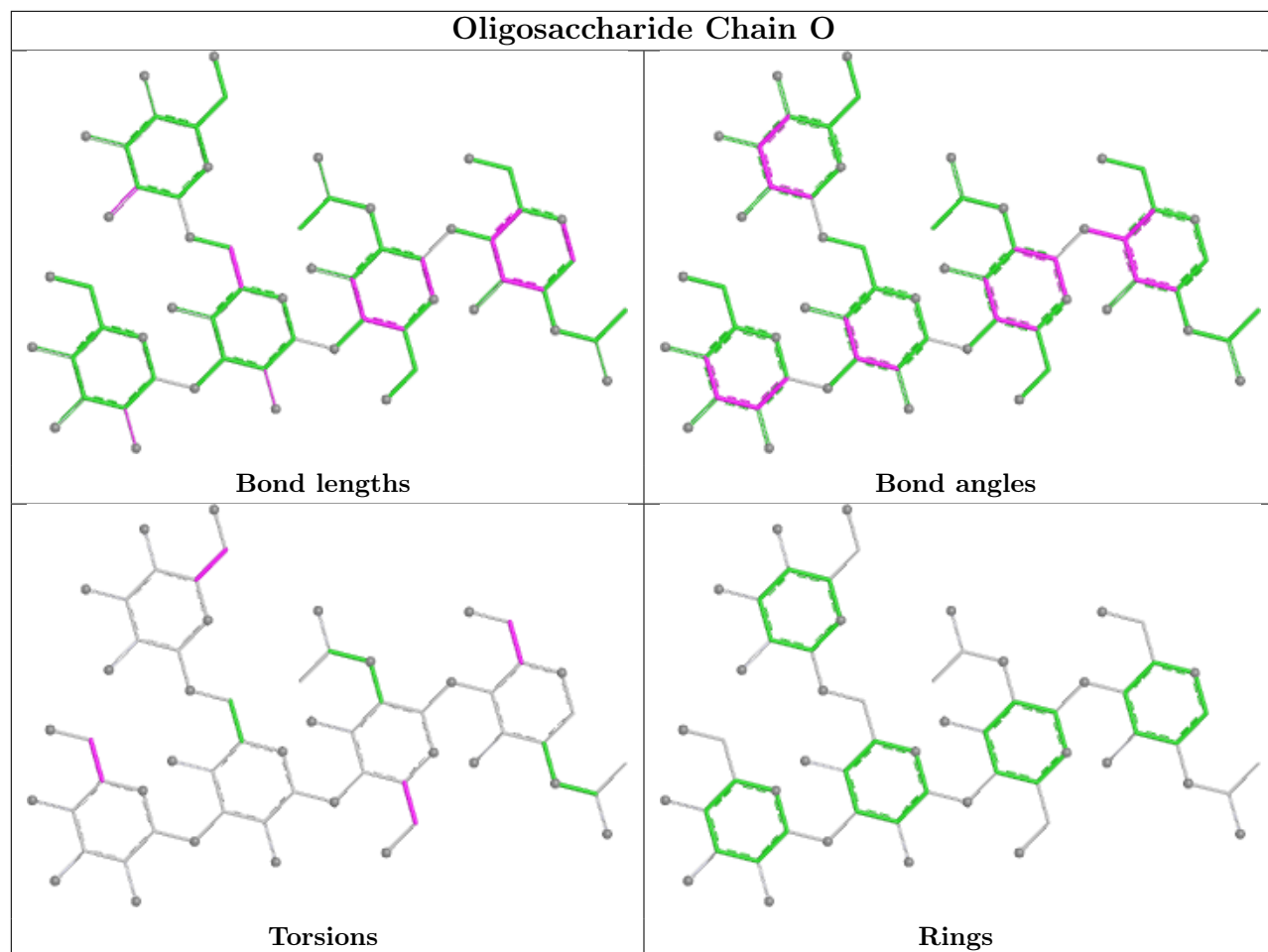


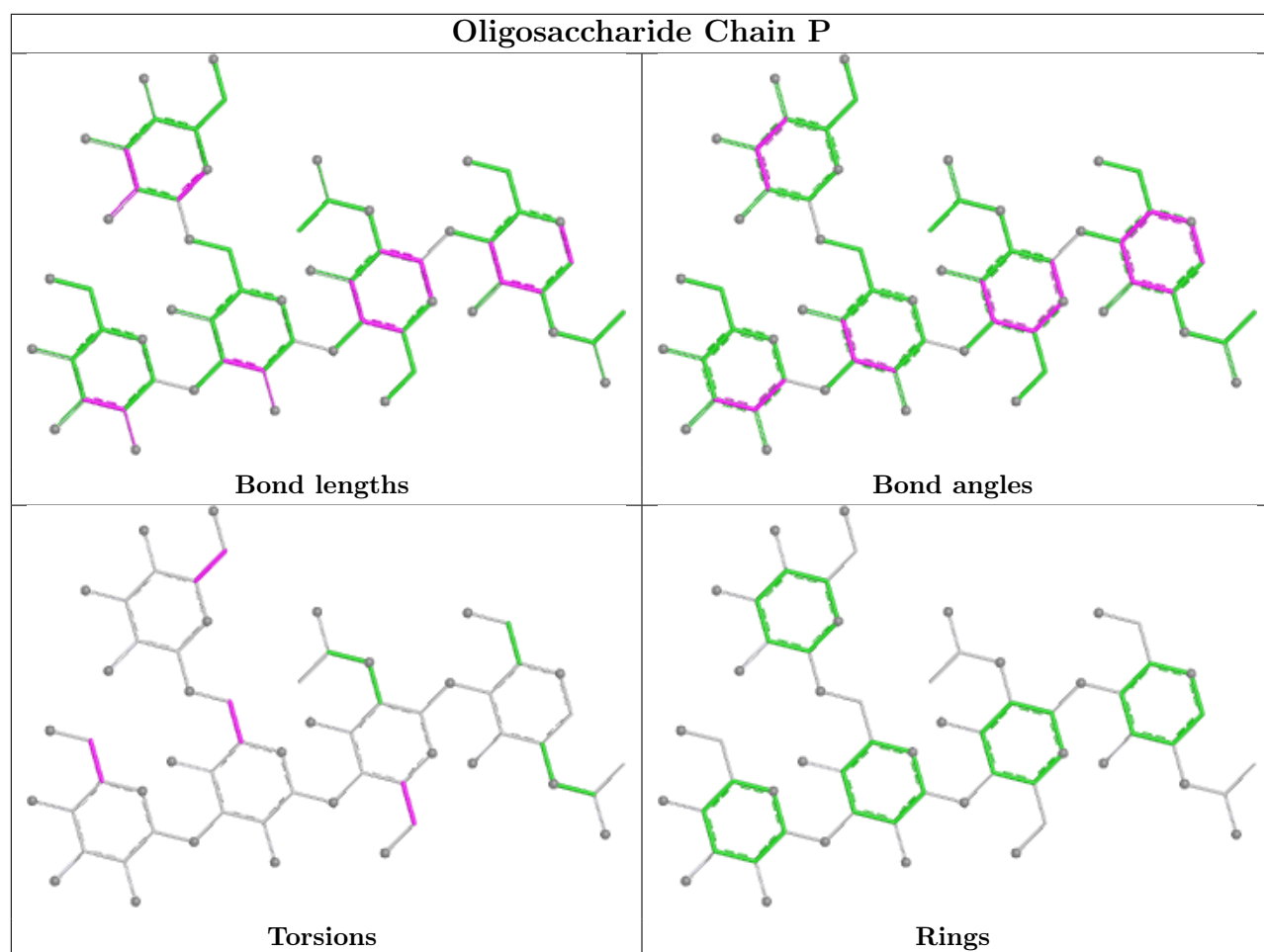


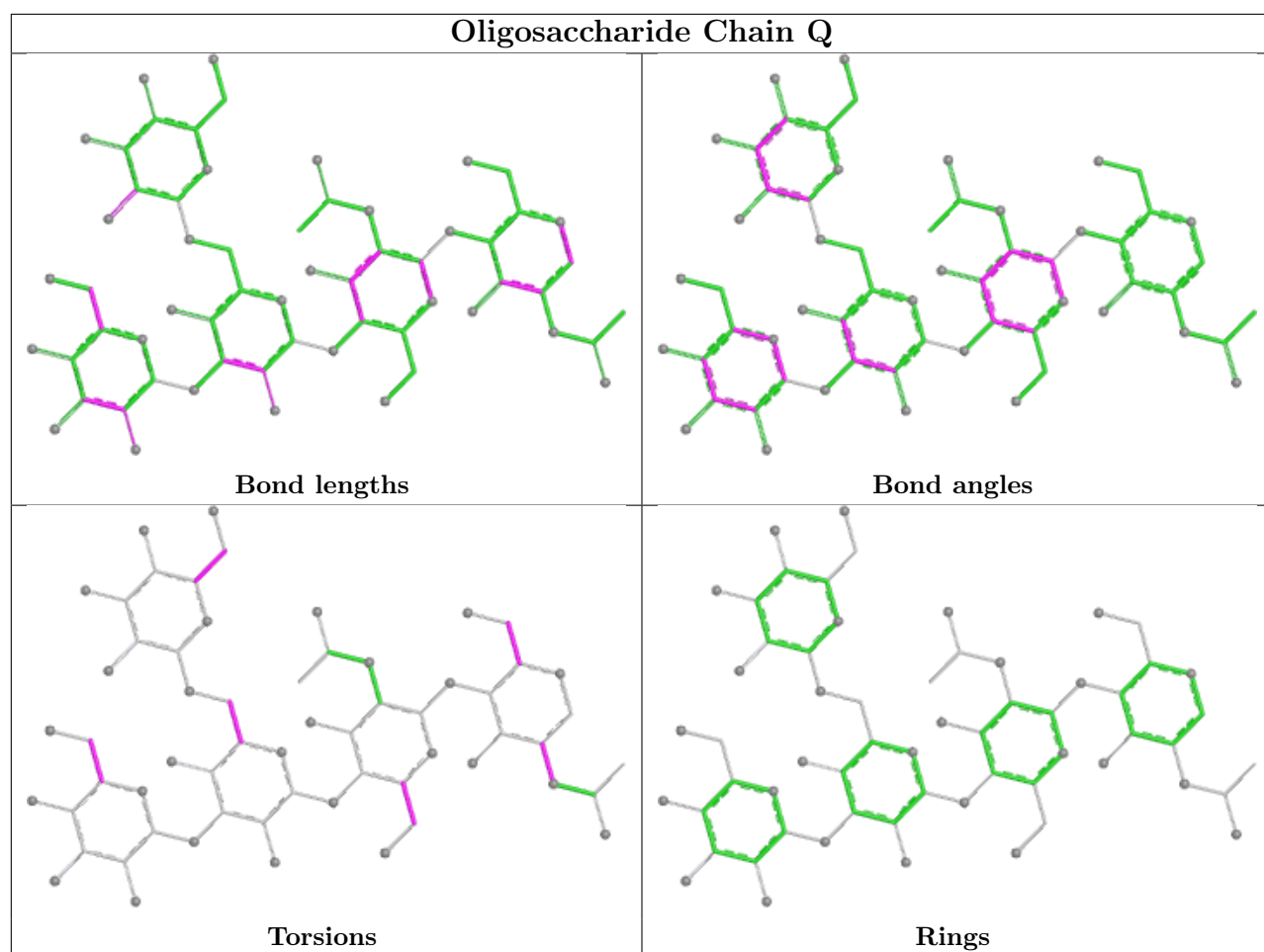


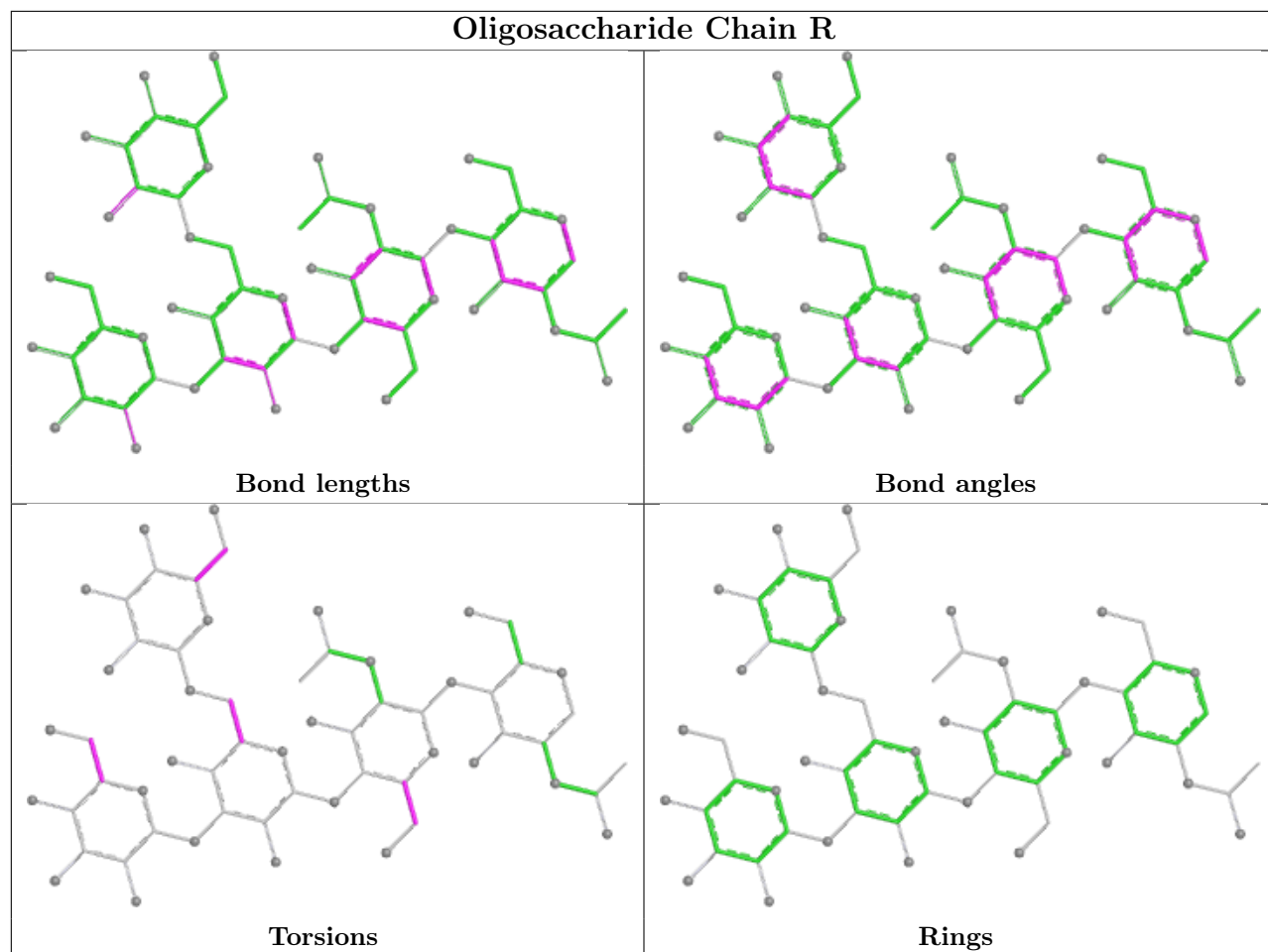




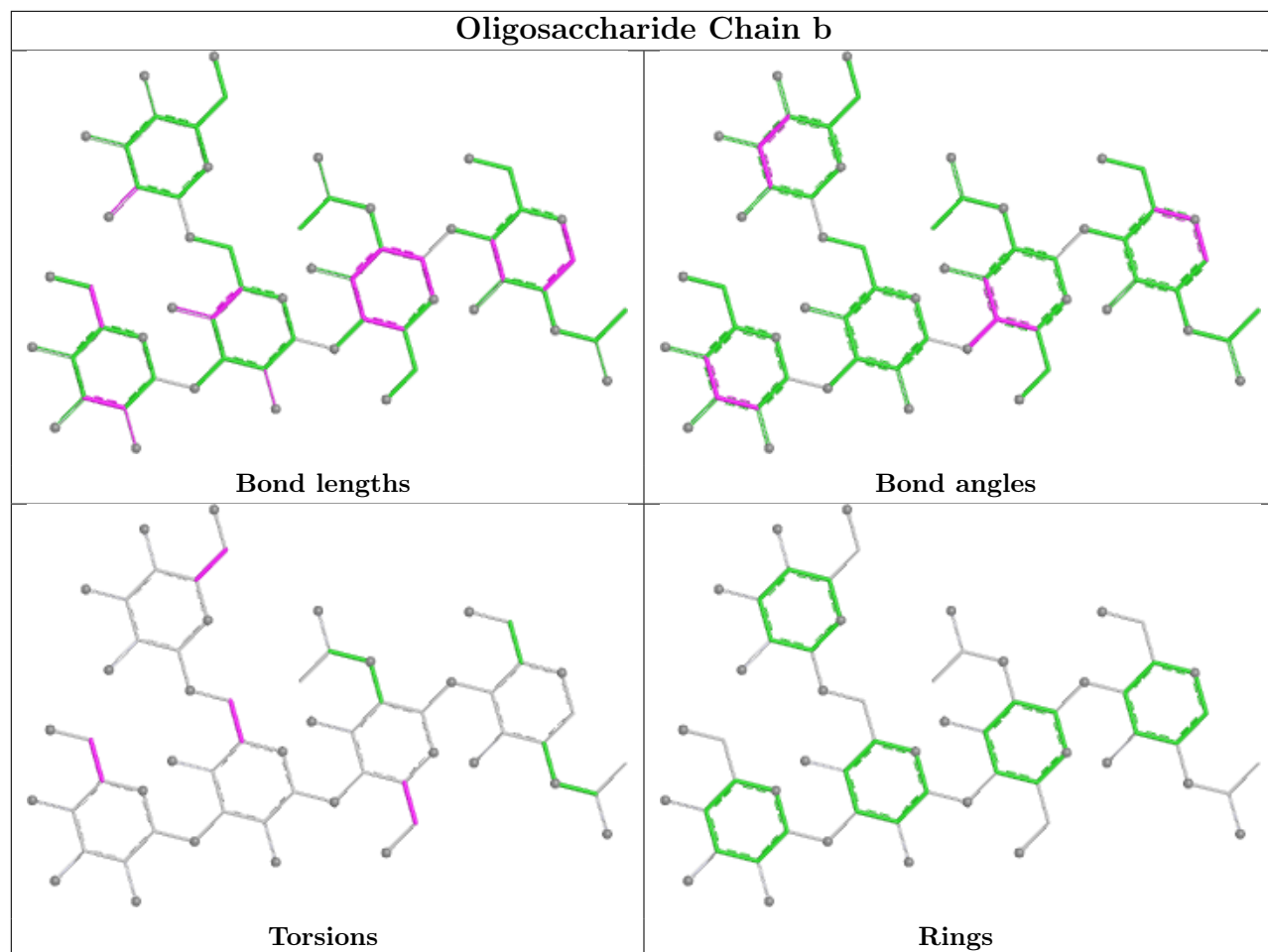


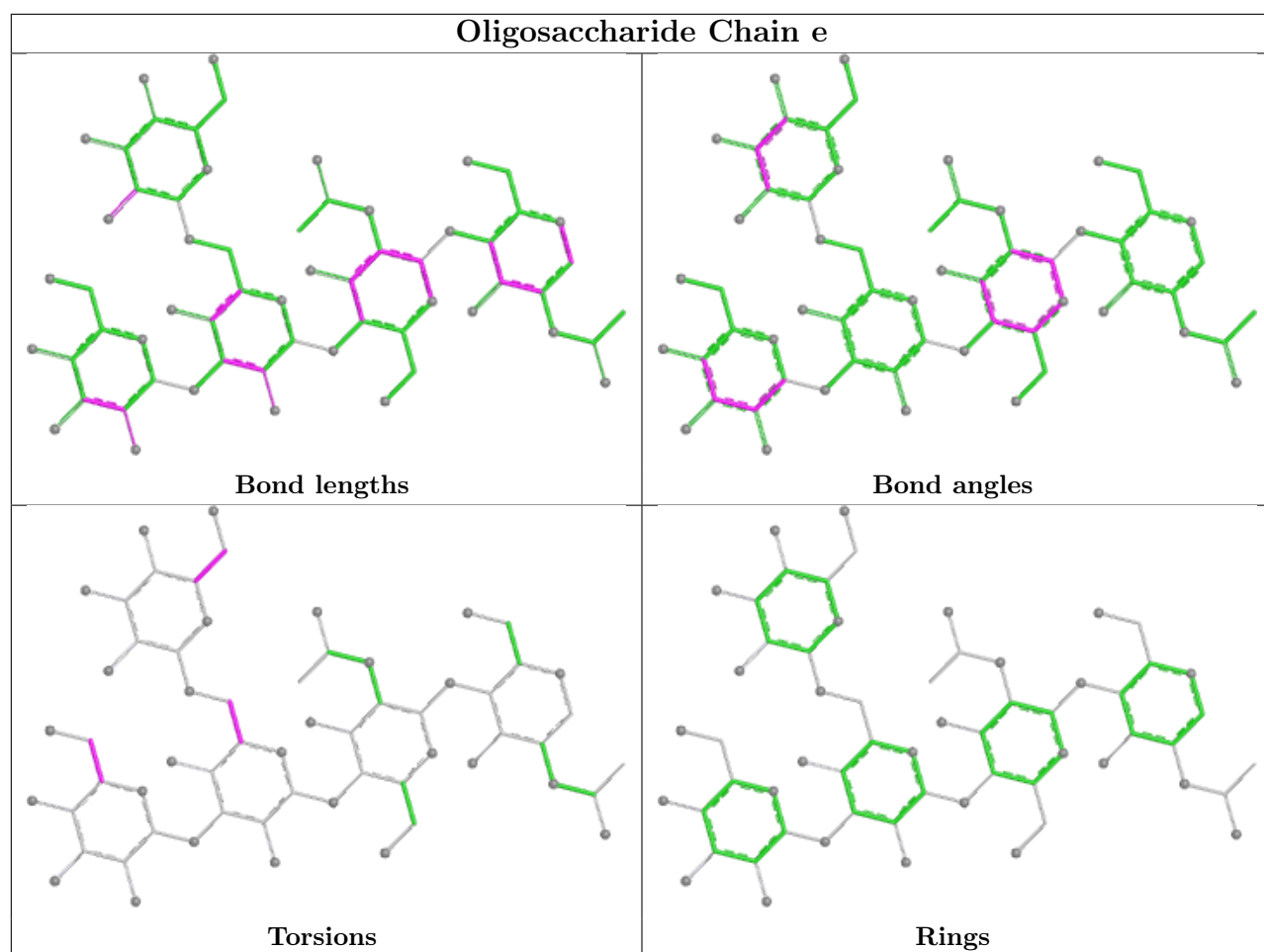


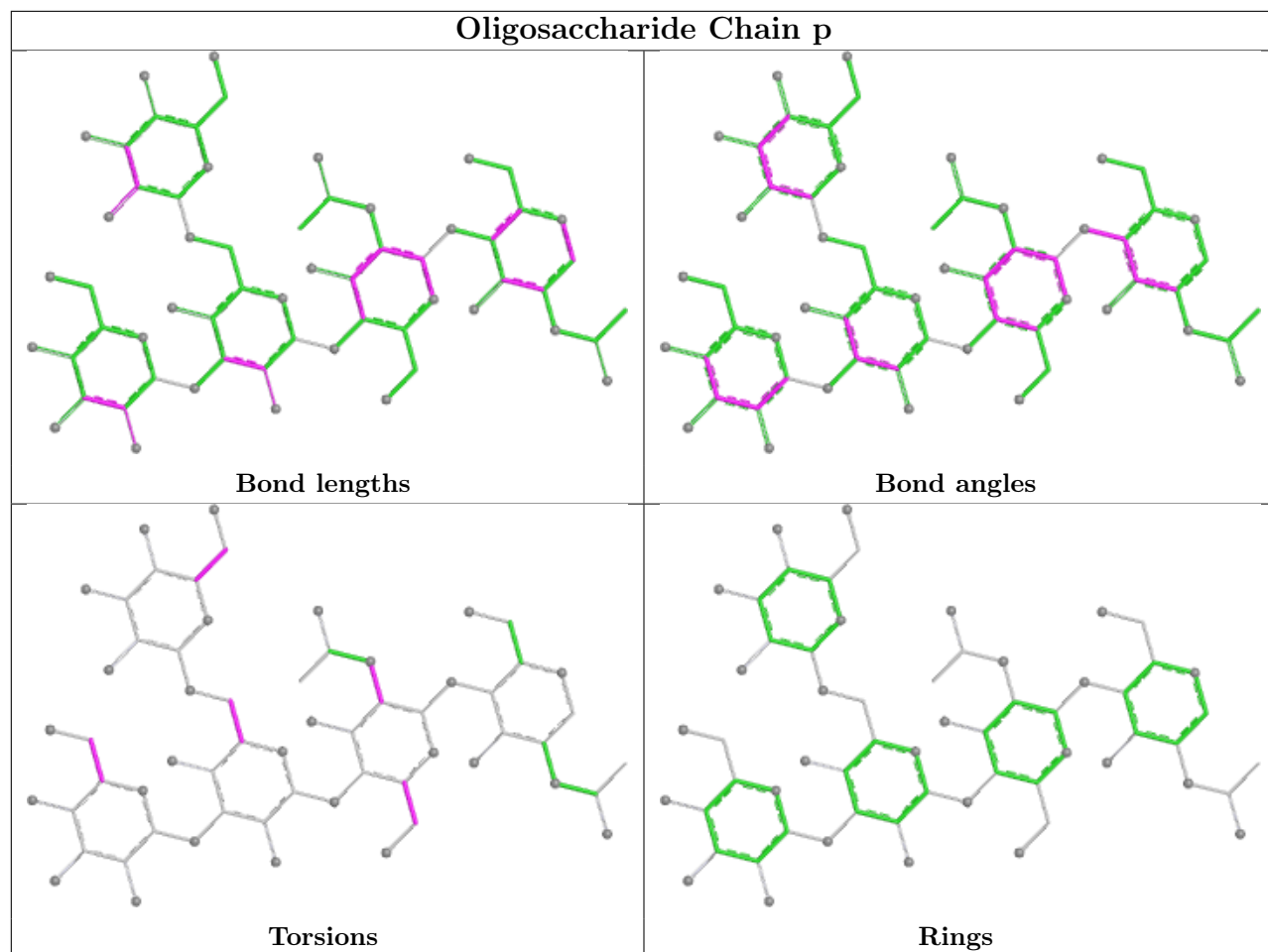


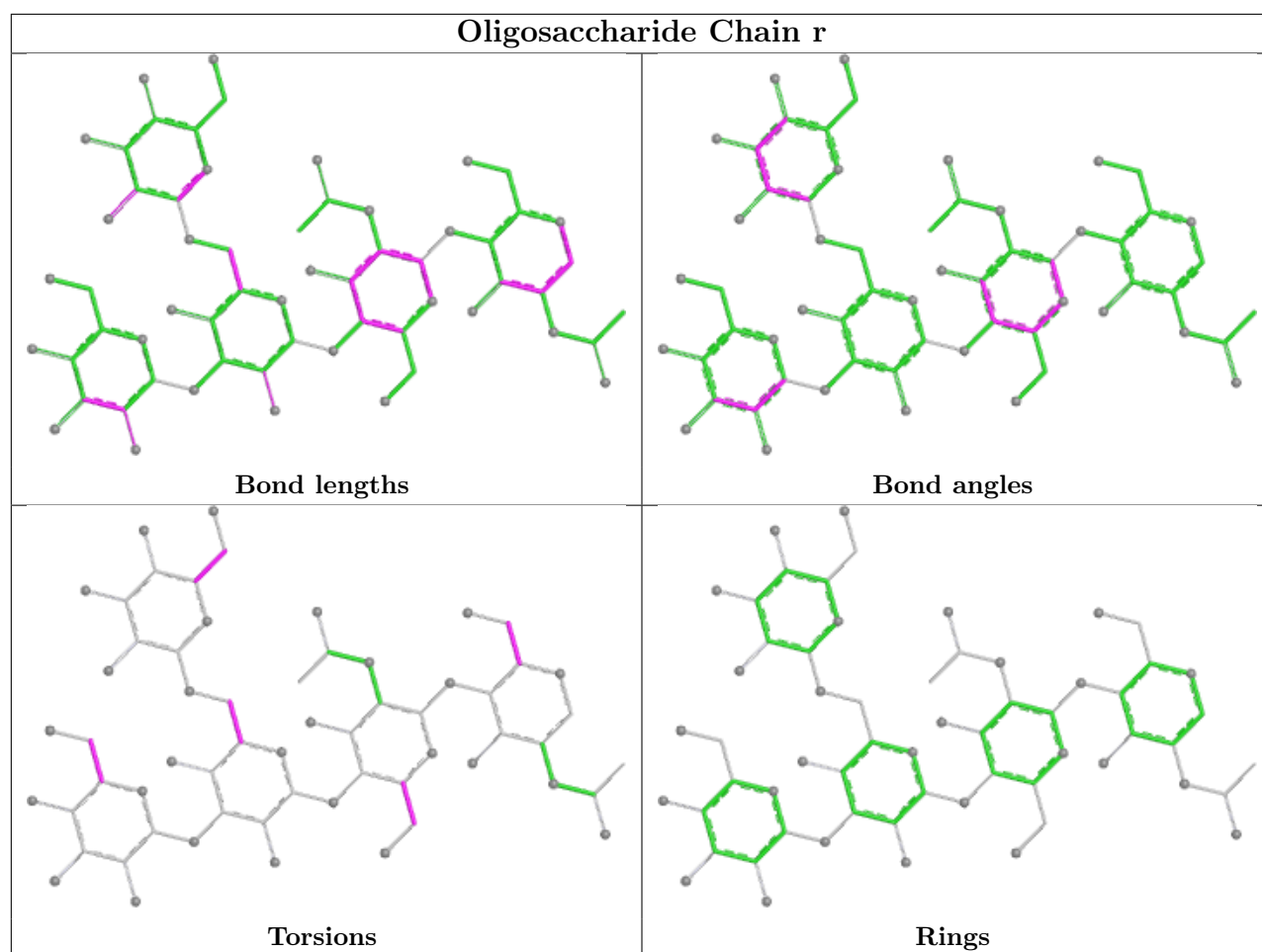


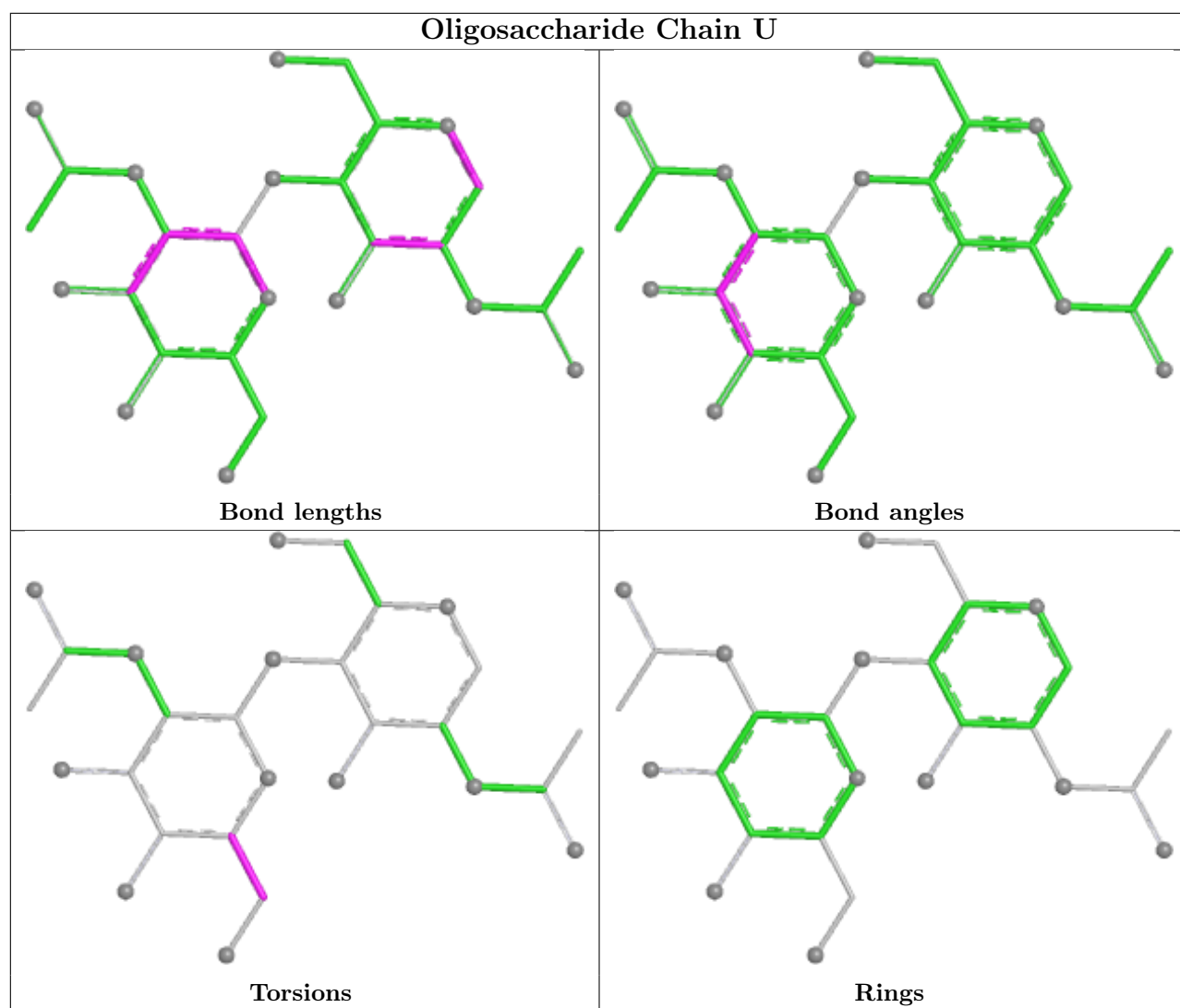


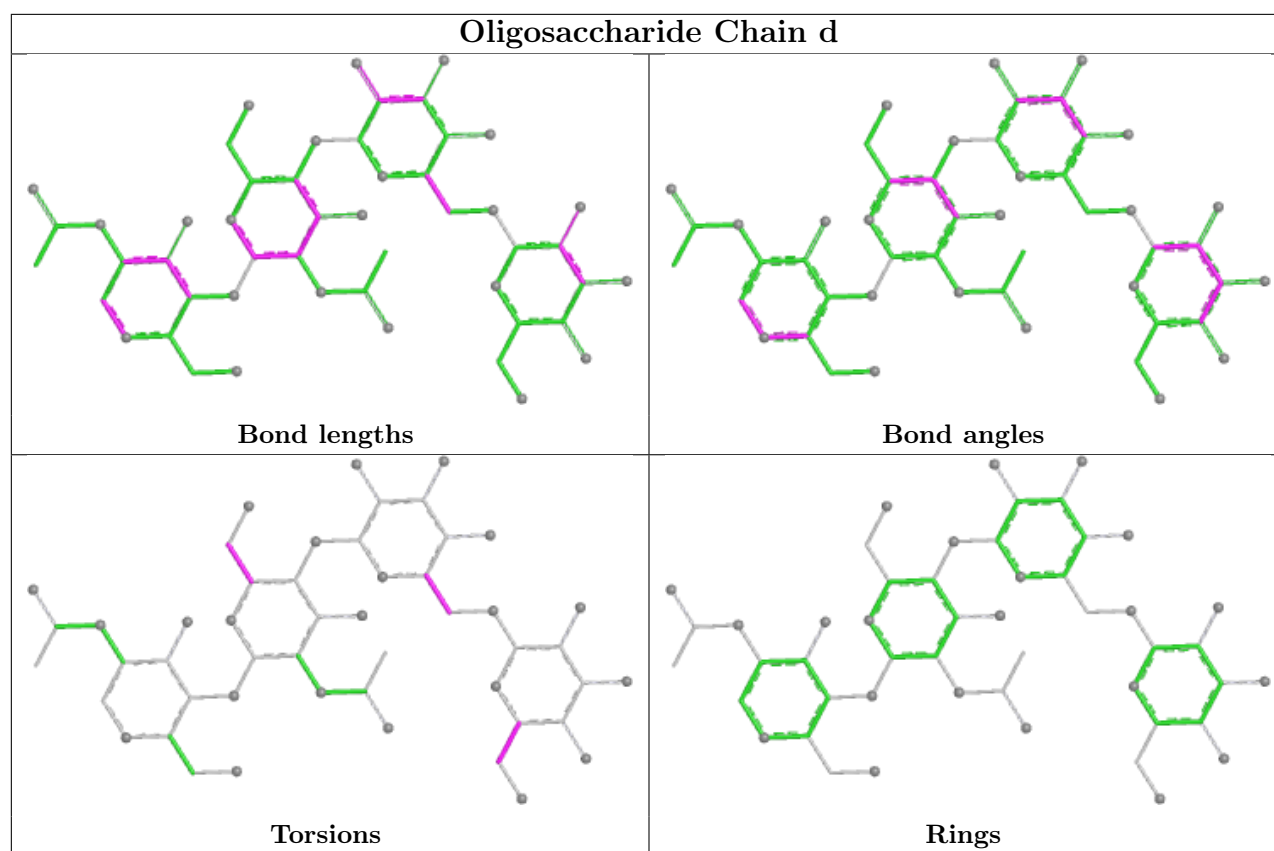












## 5.6 Ligand geometry [i](#)

17 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	1302	1	14,14,15	2.23	5 (35%)	17,19,21	1.32	2 (11%)
8	NAG	B	1303	1	14,14,15	2.05	2 (14%)	17,19,21	0.83	1 (5%)
8	NAG	A	1319	1	14,14,15	2.05	1 (7%)	17,19,21	0.87	1 (5%)
8	NAG	B	1312	1	14,14,15	2.06	2 (14%)	17,19,21	0.79	1 (5%)
8	NAG	A	1311	1	14,14,15	2.07	2 (14%)	17,19,21	1.03	1 (5%)
8	NAG	B	1301	1	14,14,15	2.07	2 (14%)	17,19,21	0.89	1 (5%)
8	NAG	B	1302	1	14,14,15	1.98	1 (7%)	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	C	1303	1	14,14,15	1.97	1 (7%)	17,19,21	0.86	1 (5%)
8	NAG	C	1304	1	14,14,15	2.05	2 (14%)	17,19,21	0.99	1 (5%)
8	NAG	A	1315	1	14,14,15	2.06	2 (14%)	17,19,21	0.87	1 (5%)
8	NAG	C	1302	1	14,14,15	2.08	2 (14%)	17,19,21	0.98	1 (5%)
8	NAG	C	1326	1	14,14,15	2.05	2 (14%)	17,19,21	0.96	1 (5%)
8	NAG	A	1301	1	14,14,15	2.02	2 (14%)	17,19,21	0.83	1 (5%)
8	NAG	A	1303	1	14,14,15	2.06	2 (14%)	17,19,21	0.95	1 (5%)
8	NAG	B	1322	1	14,14,15	2.02	1 (7%)	17,19,21	0.73	0
8	NAG	A	1310	1	14,14,15	2.05	2 (14%)	17,19,21	0.79	0
8	NAG	C	1301	1	14,14,15	1.97	1 (7%)	17,19,21	0.81	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	1302	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1319	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1315	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1326	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1322	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1301	1	-	1/6/23/26	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1303	NAG	O5-C1	6.67	1.54	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1310	NAG	O5-C1	6.67	1.54	1.43
8	B	1312	NAG	O5-C1	6.61	1.54	1.43
8	B	1301	NAG	O5-C1	6.61	1.54	1.43
8	C	1304	NAG	O5-C1	6.56	1.54	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1302	NAG	C1-O5-C5	3.61	117.02	112.19
8	A	1311	NAG	C4-C3-C2	-3.01	106.61	111.02
8	C	1302	NAG	C4-C3-C2	-3.01	106.61	111.02
8	C	1326	NAG	C4-C3-C2	-2.77	106.96	111.02
8	A	1302	NAG	O5-C1-C2	-2.75	107.03	111.29

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1302	NAG	O5-C5-C6-O6
8	A	1319	NAG	O5-C5-C6-O6
8	B	1312	NAG	O5-C5-C6-O6
8	C	1326	NAG	O5-C5-C6-O6
8	B	1302	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.



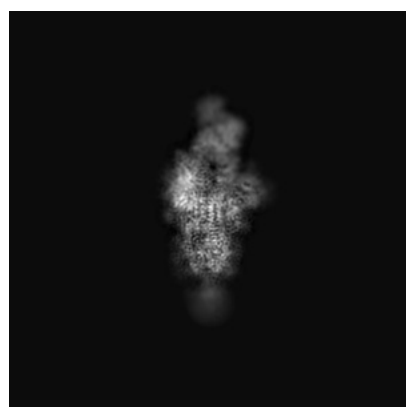
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0403. These allow visual inspection of the internal detail of the map and identification of artifacts.

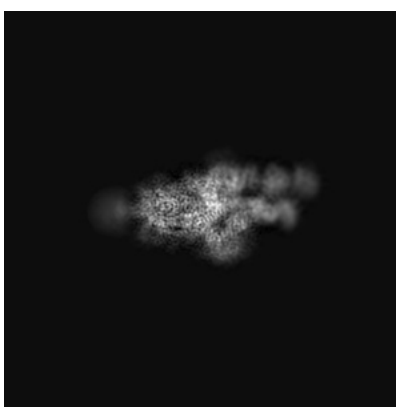
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

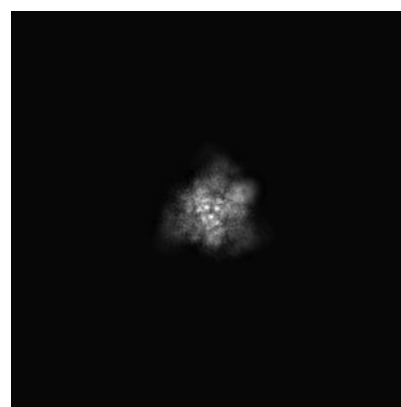
#### 6.1.1 Primary map



X



Y

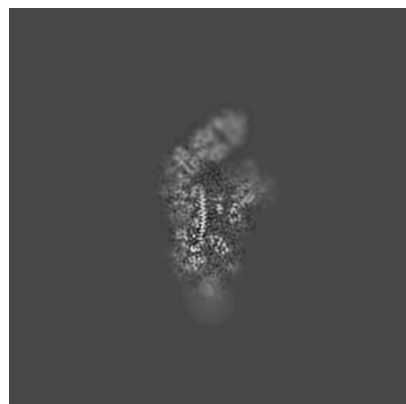


Z

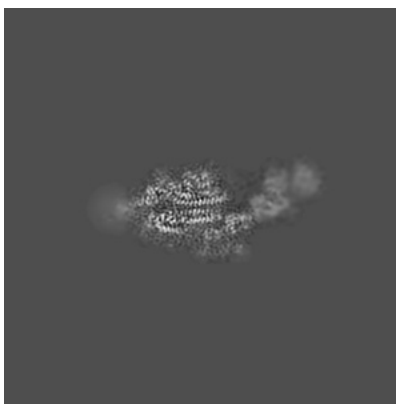
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

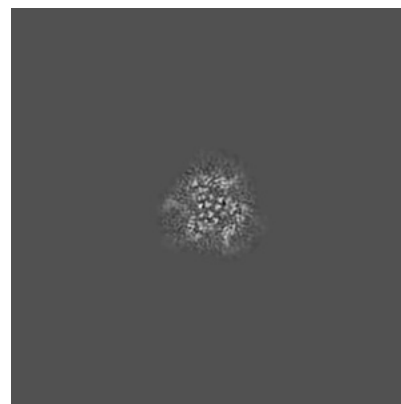
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

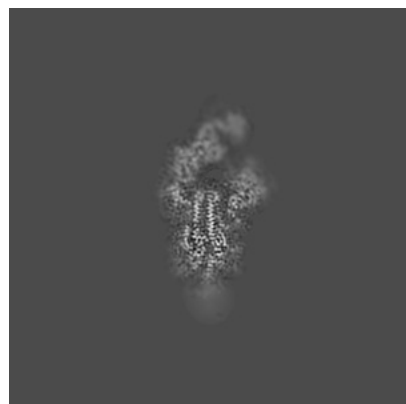


Z Index: 192

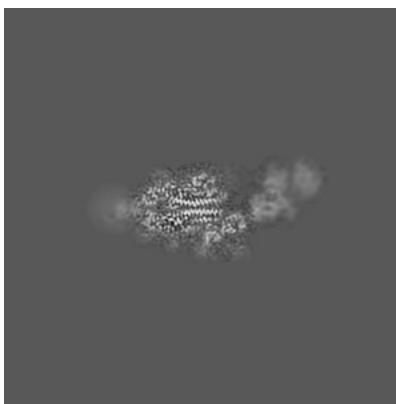
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

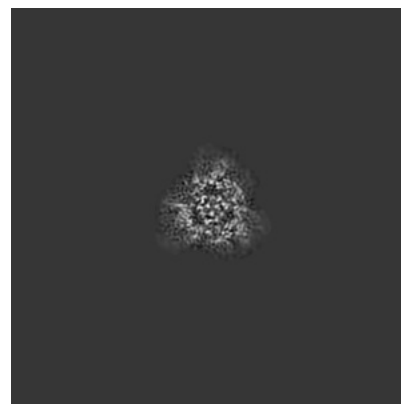
### 6.3.1 Primary map



X Index: 197



Y Index: 194

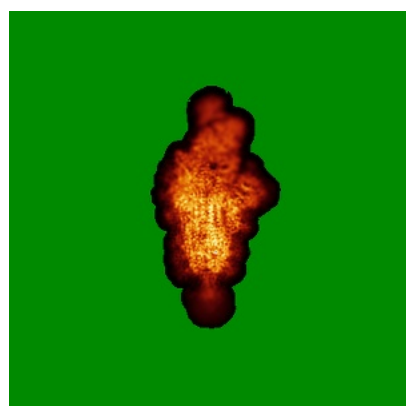


Z Index: 195

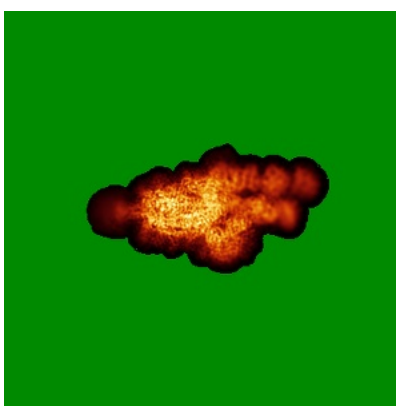
The images above show the largest variance slices of the map in three orthogonal directions.

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

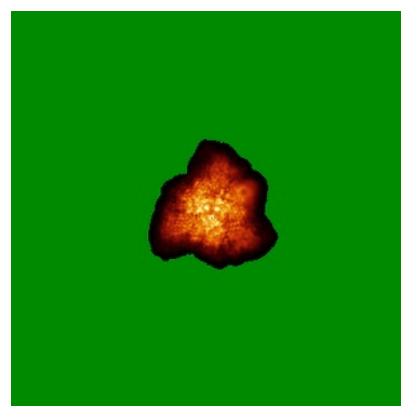
### 6.4.1 Primary map



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](#)

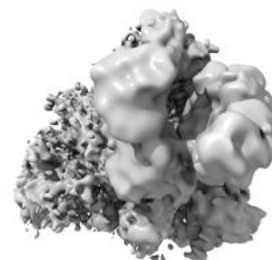
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

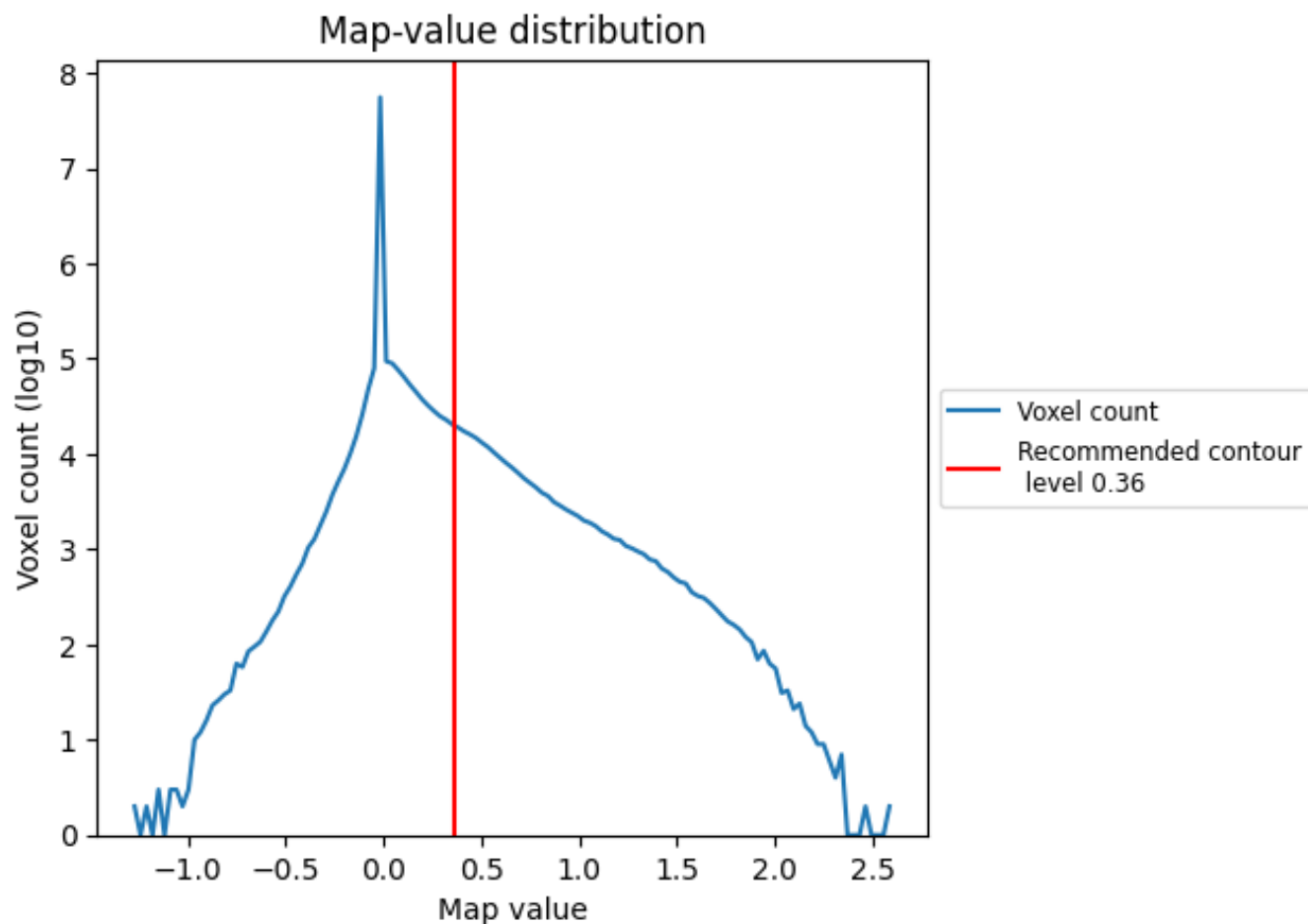
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

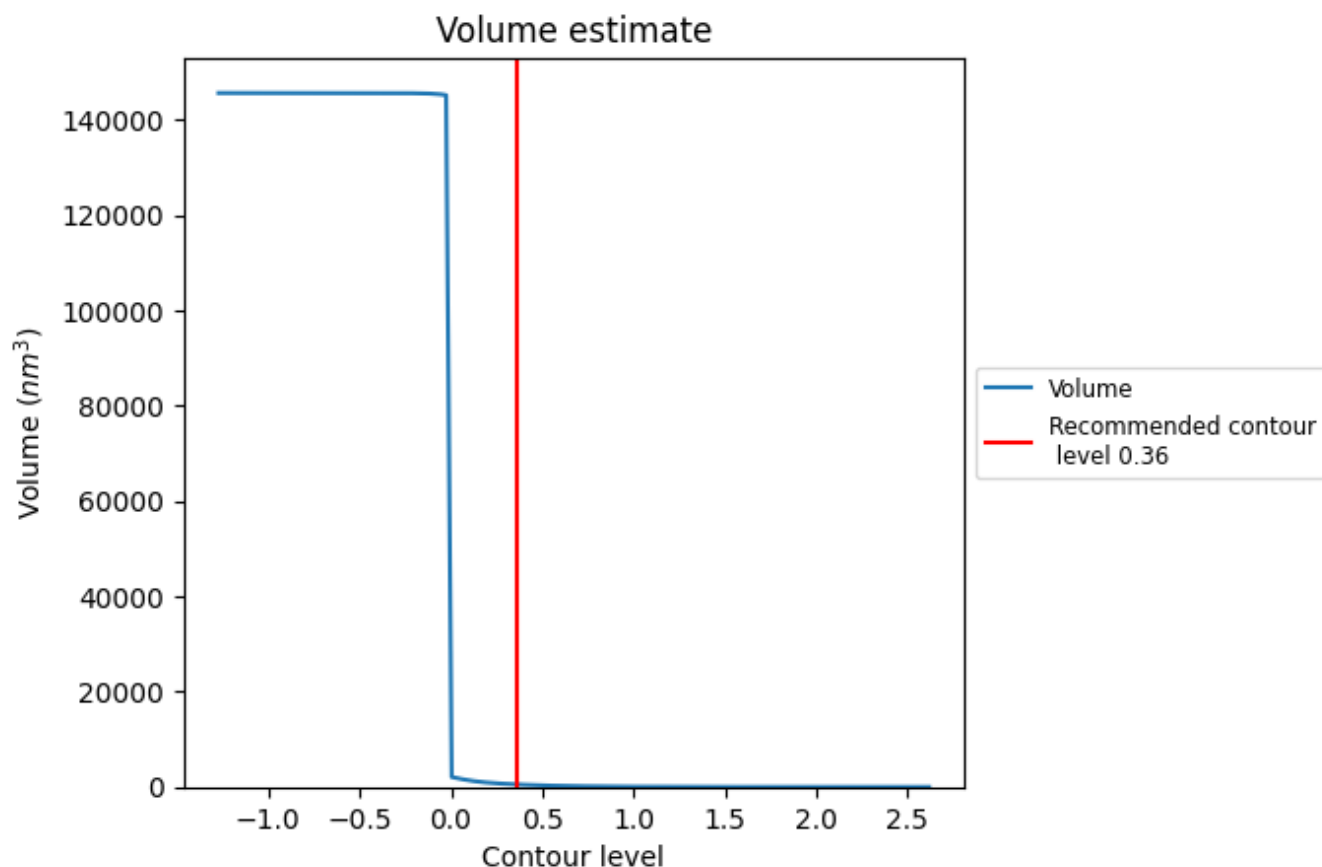
This section contains the results of statistical analysis of the map.

### 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.

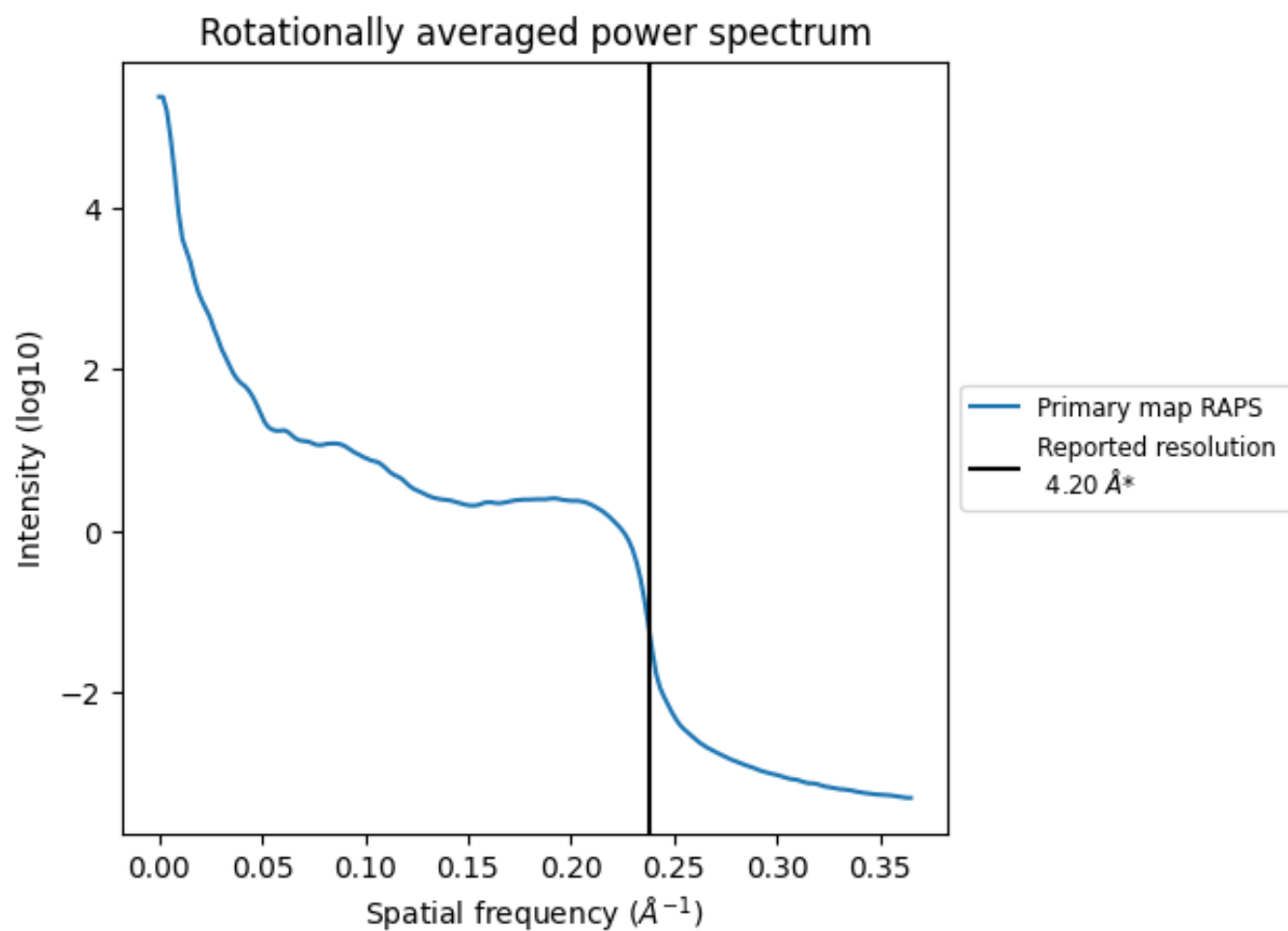
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 529 nm<sup>3</sup>; this corresponds to an approximate mass of 478 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<sup>-1</sup>

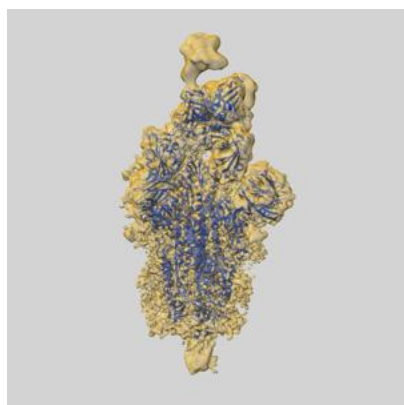
## 8 Fourier-Shell correlation

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

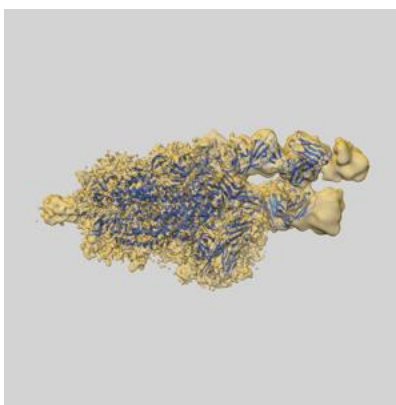
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0403 and PDB model 6NB6. Per-residue inclusion information can be found in section [3](#) on page [17](#).

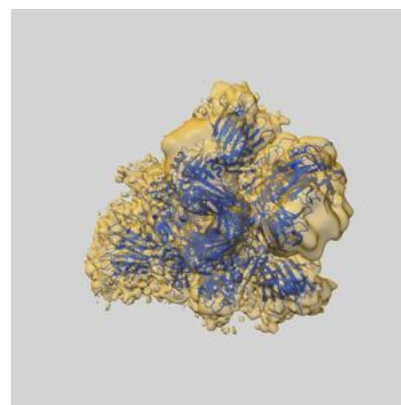
### 9.1 Map-model overlay [i](#)



X



Y

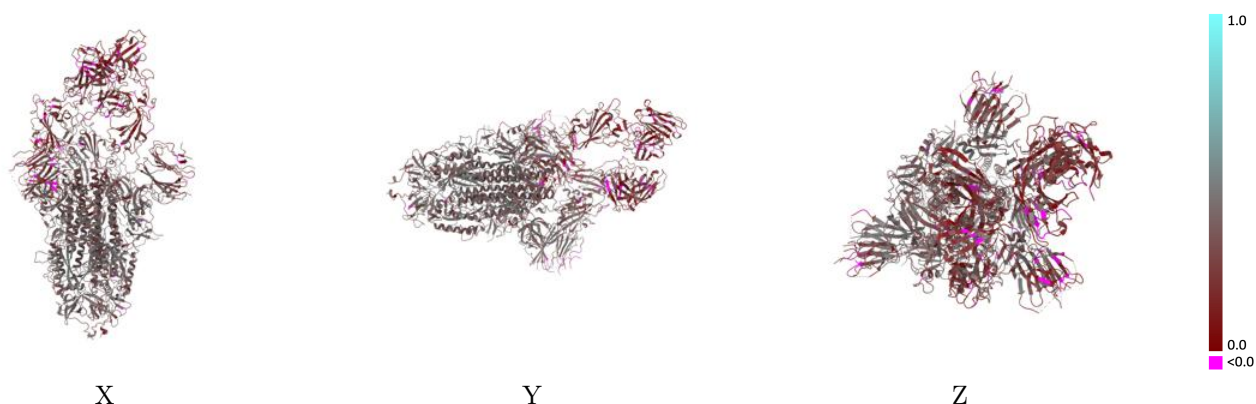


Z

The images above show the 3D surface view of the map at the recommended contour level 0.36 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.

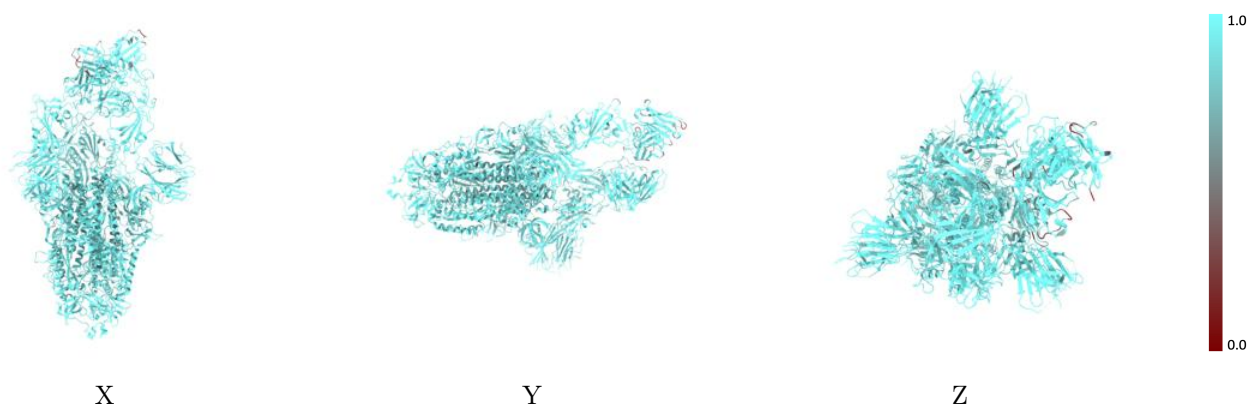


## 9.2 Q-score mapped to coordinate model [i](#)



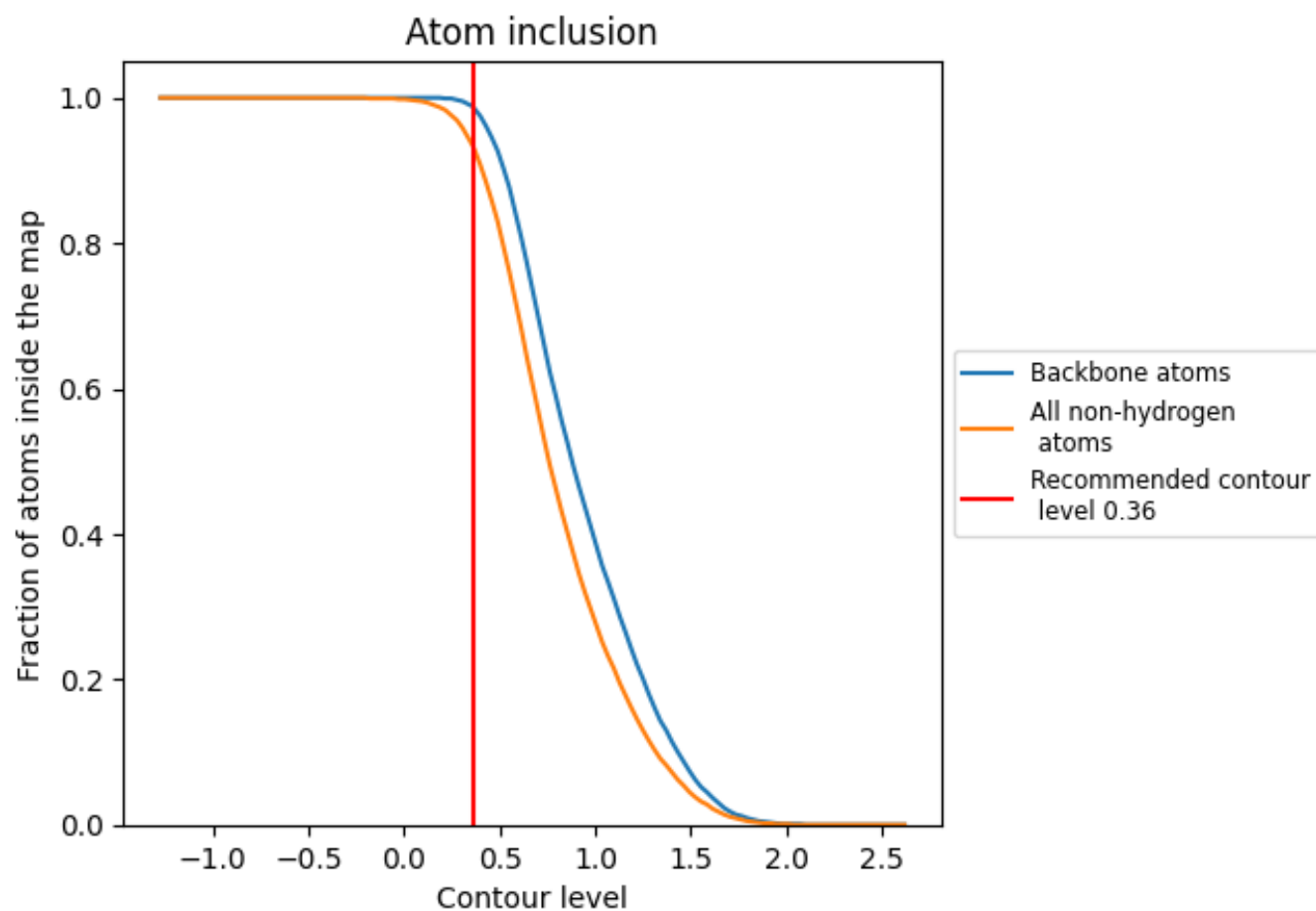
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.3380
A	 0.9420	 0.3630
B	 0.9520	 0.3470
C	 0.9500	 0.3610
D	 0.4620	 0.2070
E	 0.8460	 0.2300
F	 0.8970	 0.3100
G	 0.7950	 0.2500
H	 0.9760	 0.2340
I	 0.9210	 0.2020
J	 0.8970	 0.3190
K	 0.6720	 0.2870
L	 0.9710	 0.2040
M	 0.8410	 0.1500
N	 0.8720	 0.3630
O	 0.7380	 0.2290
P	 0.5570	 0.3190
Q	 0.7210	 0.2990
R	 0.8200	 0.2890
S	 0.5380	 0.2420
T	 0.7690	 0.1950
U	 0.5360	 0.2450
V	 0.8720	 0.3660
W	 0.9490	 0.3680
X	 0.6920	 0.1980
Y	 0.6410	 0.1890
Z	 0.7950	 0.1700
a	 0.9490	 0.4050
b	 0.8690	 0.3310
c	 0.7690	 0.3390
d	 0.8000	 0.3360
e	 0.7050	 0.3130
f	 0.7950	 0.2530
g	 0.8210	 0.2620
h	 0.9490	 0.2760



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.8460	 0.3100
j	 0.9230	 0.2960
k	 0.6410	 0.2330
l	 0.8210	 0.3310
m	 0.6920	 0.1860
n	 0.6920	 0.1700
o	 0.8210	 0.2620
p	 0.8030	 0.2860
q	 0.7440	 0.3120
r	 0.7380	 0.3130
s	 0.8460	 0.2670