



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:49 AM UTC

PDB ID : 9OFQ / pdb_00009ofq
EMDB ID : EMD-70442
Title : HCoV-229E S2P bound by one DH1533 Fab
Authors : Wrapp, D.
Deposited on : 2025-04-30
Resolution : 2.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

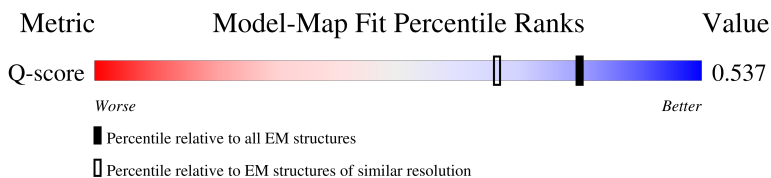
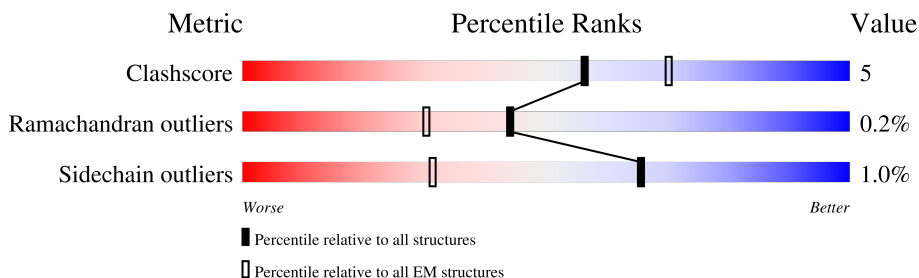
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 Å.

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



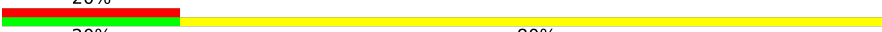
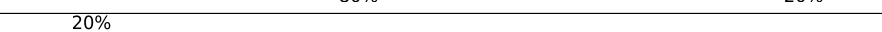
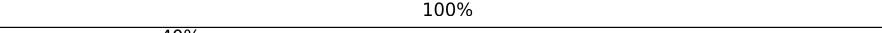
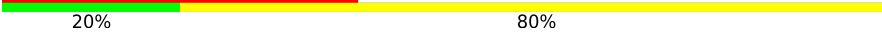
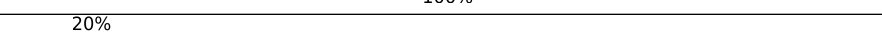
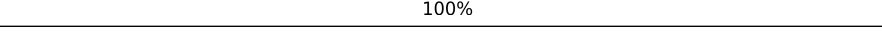
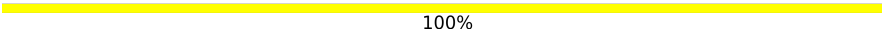
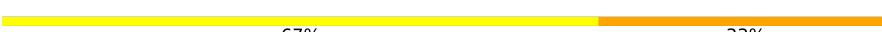
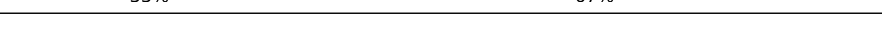
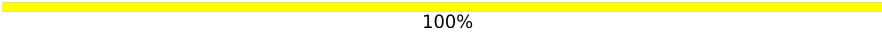
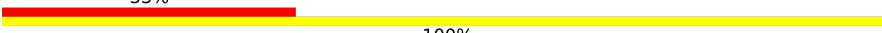
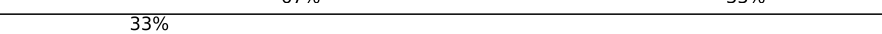
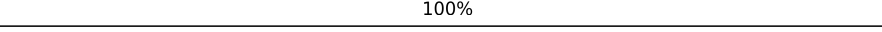
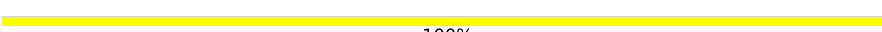
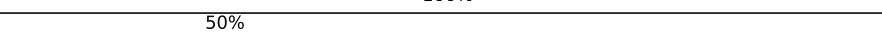
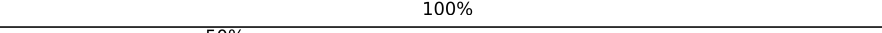
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12111 (2.38 - 3.38)

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	1134	
1	B	1134	
1	C	1134	
2	H	239	

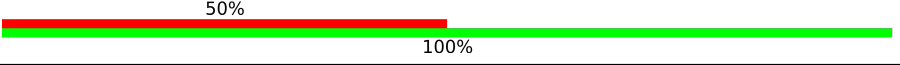
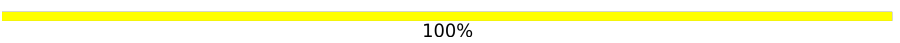
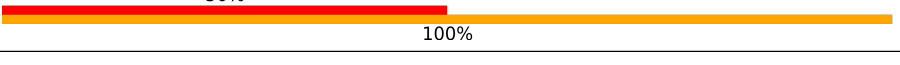
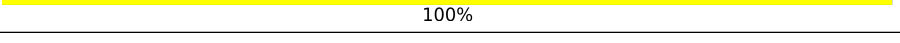
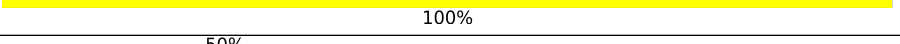
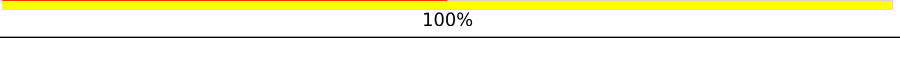
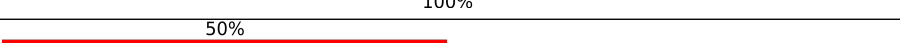
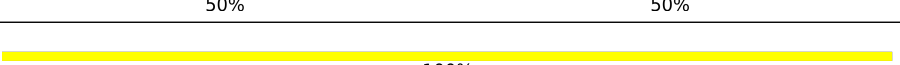
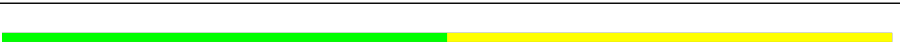
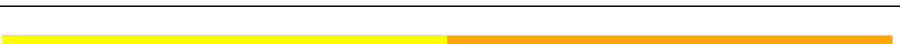
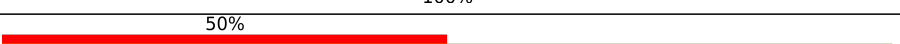
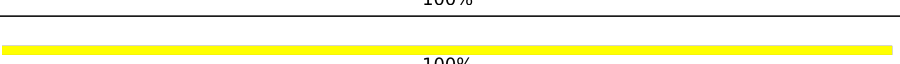
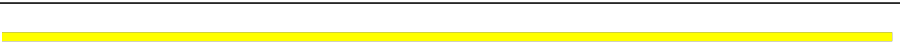
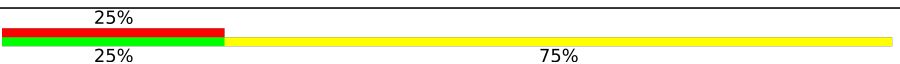
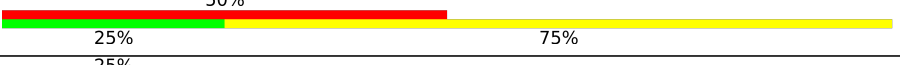
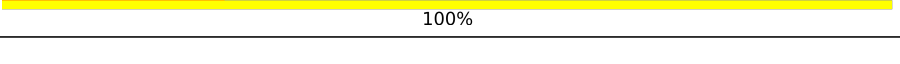
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Mol	Chain	Length	Quality of chain
3	L	214	
4	1	5	
4	3	5	
4	D	5	
4	T	5	
4	V	5	
4	k	5	
4	o	5	
5	E	3	
5	F	3	
5	W	3	
5	b	3	
5	c	3	
5	m	3	
5	r	3	
5	v	3	
6	4	2	
6	G	2	
6	I	2	
6	J	2	
6	K	2	
6	M	2	
6	N	2	
6	O	2	
6	P	2	

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Mol	Chain	Length	Quality of chain
6	Q	2	
6	R	2	
6	Z	2	
6	a	2	
6	d	2	
6	e	2	
6	f	2	
6	g	2	
6	h	2	
6	i	2	
6	n	2	
6	p	2	
6	q	2	
6	s	2	
6	u	2	
6	w	2	
6	x	2	
6	y	2	
6	z	2	
7	0	4	
7	2	4	
7	S	4	
7	U	4	
7	l	4	
8	X	6	

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Mol	Chain	Length	Quality of chain
9	Y	4	75% 25%
9	j	4	50% 25% 75%
9	t	4	25% 75% 25%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25152 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 Surface glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	873	Total	C	N	O	S	0	0
			6694	4242	1116	1304	32		
1	A	1012	Total	C	N	O	S	0	0
			7768	4930	1302	1496	40		
1	B	872	Total	C	N	O	S	0	0
			6688	4239	1115	1302	32		

There are 246 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	869	PRO	ILE	conflict	UNP A0A1B3TN99
C	870	PRO	ILE	conflict	UNP A0A1B3TN99
C	1055	GLY	-	expression tag	UNP A0A1B3TN99
C	1056	SER	-	expression tag	UNP A0A1B3TN99
C	1057	GLY	-	expression tag	UNP A0A1B3TN99
C	1058	TYR	-	expression tag	UNP A0A1B3TN99
C	1059	ILE	-	expression tag	UNP A0A1B3TN99
C	1060	PRO	-	expression tag	UNP A0A1B3TN99
C	1061	GLU	-	expression tag	UNP A0A1B3TN99
C	1062	ALA	-	expression tag	UNP A0A1B3TN99
C	1063	PRO	-	expression tag	UNP A0A1B3TN99
C	1064	ARG	-	expression tag	UNP A0A1B3TN99
C	1065	ASP	-	expression tag	UNP A0A1B3TN99
C	1066	GLY	-	expression tag	UNP A0A1B3TN99
C	1067	GLN	-	expression tag	UNP A0A1B3TN99
C	1068	ALA	-	expression tag	UNP A0A1B3TN99
C	1069	TYR	-	expression tag	UNP A0A1B3TN99
C	1070	VAL	-	expression tag	UNP A0A1B3TN99
C	1071	ARG	-	expression tag	UNP A0A1B3TN99
C	1072	LYS	-	expression tag	UNP A0A1B3TN99
C	1073	ASP	-	expression tag	UNP A0A1B3TN99
C	1074	GLY	-	expression tag	UNP A0A1B3TN99
C	1075	GLU	-	expression tag	UNP A0A1B3TN99
C	1076	TRP	-	expression tag	UNP A0A1B3TN99

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1077	VAL	-	expression tag	UNP A0A1B3TN99
C	1078	LEU	-	expression tag	UNP A0A1B3TN99
C	1079	LEU	-	expression tag	UNP A0A1B3TN99
C	1080	SER	-	expression tag	UNP A0A1B3TN99
C	1081	THR	-	expression tag	UNP A0A1B3TN99
C	1082	PHE	-	expression tag	UNP A0A1B3TN99
C	1083	LEU	-	expression tag	UNP A0A1B3TN99
C	1084	GLY	-	expression tag	UNP A0A1B3TN99
C	1085	ARG	-	expression tag	UNP A0A1B3TN99
C	1086	SER	-	expression tag	UNP A0A1B3TN99
C	1087	LEU	-	expression tag	UNP A0A1B3TN99
C	1088	GLU	-	expression tag	UNP A0A1B3TN99
C	1089	VAL	-	expression tag	UNP A0A1B3TN99
C	1090	LEU	-	expression tag	UNP A0A1B3TN99
C	1091	PHE	-	expression tag	UNP A0A1B3TN99
C	1092	GLN	-	expression tag	UNP A0A1B3TN99
C	1093	GLY	-	expression tag	UNP A0A1B3TN99
C	1094	PRO	-	expression tag	UNP A0A1B3TN99
C	1095	GLY	-	expression tag	UNP A0A1B3TN99
C	1096	HIS	-	expression tag	UNP A0A1B3TN99
C	1097	HIS	-	expression tag	UNP A0A1B3TN99
C	1098	HIS	-	expression tag	UNP A0A1B3TN99
C	1099	HIS	-	expression tag	UNP A0A1B3TN99
C	1100	HIS	-	expression tag	UNP A0A1B3TN99
C	1101	HIS	-	expression tag	UNP A0A1B3TN99
C	1102	HIS	-	expression tag	UNP A0A1B3TN99
C	1103	HIS	-	expression tag	UNP A0A1B3TN99
C	1104	SER	-	expression tag	UNP A0A1B3TN99
C	1105	ALA	-	expression tag	UNP A0A1B3TN99
C	1106	TRP	-	expression tag	UNP A0A1B3TN99
C	1107	SER	-	expression tag	UNP A0A1B3TN99
C	1108	HIS	-	expression tag	UNP A0A1B3TN99
C	1109	PRO	-	expression tag	UNP A0A1B3TN99
C	1110	GLN	-	expression tag	UNP A0A1B3TN99
C	1111	PHE	-	expression tag	UNP A0A1B3TN99
C	1112	GLU	-	expression tag	UNP A0A1B3TN99
C	1113	LYS	-	expression tag	UNP A0A1B3TN99
C	1114	GLY	-	expression tag	UNP A0A1B3TN99
C	1115	GLY	-	expression tag	UNP A0A1B3TN99
C	1116	GLY	-	expression tag	UNP A0A1B3TN99
C	1117	SER	-	expression tag	UNP A0A1B3TN99
C	1118	GLY	-	expression tag	UNP A0A1B3TN99

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1119	GLY	-	expression tag	UNP A0A1B3TN99
C	1120	GLY	-	expression tag	UNP A0A1B3TN99
C	1121	GLY	-	expression tag	UNP A0A1B3TN99
C	1122	SER	-	expression tag	UNP A0A1B3TN99
C	1123	GLY	-	expression tag	UNP A0A1B3TN99
C	1124	GLY	-	expression tag	UNP A0A1B3TN99
C	1125	SER	-	expression tag	UNP A0A1B3TN99
C	1126	ALA	-	expression tag	UNP A0A1B3TN99
C	1127	TRP	-	expression tag	UNP A0A1B3TN99
C	1128	SER	-	expression tag	UNP A0A1B3TN99
C	1129	HIS	-	expression tag	UNP A0A1B3TN99
C	1130	PRO	-	expression tag	UNP A0A1B3TN99
C	1131	GLN	-	expression tag	UNP A0A1B3TN99
C	1132	PHE	-	expression tag	UNP A0A1B3TN99
C	1133	GLU	-	expression tag	UNP A0A1B3TN99
C	1134	LYS	-	expression tag	UNP A0A1B3TN99
A	869	PRO	ILE	conflict	UNP A0A1B3TN99
A	870	PRO	ILE	conflict	UNP A0A1B3TN99
A	1055	GLY	-	expression tag	UNP A0A1B3TN99
A	1056	SER	-	expression tag	UNP A0A1B3TN99
A	1057	GLY	-	expression tag	UNP A0A1B3TN99
A	1058	TYR	-	expression tag	UNP A0A1B3TN99
A	1059	ILE	-	expression tag	UNP A0A1B3TN99
A	1060	PRO	-	expression tag	UNP A0A1B3TN99
A	1061	GLU	-	expression tag	UNP A0A1B3TN99
A	1062	ALA	-	expression tag	UNP A0A1B3TN99
A	1063	PRO	-	expression tag	UNP A0A1B3TN99
A	1064	ARG	-	expression tag	UNP A0A1B3TN99
A	1065	ASP	-	expression tag	UNP A0A1B3TN99
A	1066	GLY	-	expression tag	UNP A0A1B3TN99
A	1067	GLN	-	expression tag	UNP A0A1B3TN99
A	1068	ALA	-	expression tag	UNP A0A1B3TN99
A	1069	TYR	-	expression tag	UNP A0A1B3TN99
A	1070	VAL	-	expression tag	UNP A0A1B3TN99
A	1071	ARG	-	expression tag	UNP A0A1B3TN99
A	1072	LYS	-	expression tag	UNP A0A1B3TN99
A	1073	ASP	-	expression tag	UNP A0A1B3TN99
A	1074	GLY	-	expression tag	UNP A0A1B3TN99
A	1075	GLU	-	expression tag	UNP A0A1B3TN99
A	1076	TRP	-	expression tag	UNP A0A1B3TN99
A	1077	VAL	-	expression tag	UNP A0A1B3TN99
A	1078	LEU	-	expression tag	UNP A0A1B3TN99

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1079	LEU	-	expression tag	UNP A0A1B3TN99
A	1080	SER	-	expression tag	UNP A0A1B3TN99
A	1081	THR	-	expression tag	UNP A0A1B3TN99
A	1082	PHE	-	expression tag	UNP A0A1B3TN99
A	1083	LEU	-	expression tag	UNP A0A1B3TN99
A	1084	GLY	-	expression tag	UNP A0A1B3TN99
A	1085	ARG	-	expression tag	UNP A0A1B3TN99
A	1086	SER	-	expression tag	UNP A0A1B3TN99
A	1087	LEU	-	expression tag	UNP A0A1B3TN99
A	1088	GLU	-	expression tag	UNP A0A1B3TN99
A	1089	VAL	-	expression tag	UNP A0A1B3TN99
A	1090	LEU	-	expression tag	UNP A0A1B3TN99
A	1091	PHE	-	expression tag	UNP A0A1B3TN99
A	1092	GLN	-	expression tag	UNP A0A1B3TN99
A	1093	GLY	-	expression tag	UNP A0A1B3TN99
A	1094	PRO	-	expression tag	UNP A0A1B3TN99
A	1095	GLY	-	expression tag	UNP A0A1B3TN99
A	1096	HIS	-	expression tag	UNP A0A1B3TN99
A	1097	HIS	-	expression tag	UNP A0A1B3TN99
A	1098	HIS	-	expression tag	UNP A0A1B3TN99
A	1099	HIS	-	expression tag	UNP A0A1B3TN99
A	1100	HIS	-	expression tag	UNP A0A1B3TN99
A	1101	HIS	-	expression tag	UNP A0A1B3TN99
A	1102	HIS	-	expression tag	UNP A0A1B3TN99
A	1103	HIS	-	expression tag	UNP A0A1B3TN99
A	1104	SER	-	expression tag	UNP A0A1B3TN99
A	1105	ALA	-	expression tag	UNP A0A1B3TN99
A	1106	TRP	-	expression tag	UNP A0A1B3TN99
A	1107	SER	-	expression tag	UNP A0A1B3TN99
A	1108	HIS	-	expression tag	UNP A0A1B3TN99
A	1109	PRO	-	expression tag	UNP A0A1B3TN99
A	1110	GLN	-	expression tag	UNP A0A1B3TN99
A	1111	PHE	-	expression tag	UNP A0A1B3TN99
A	1112	GLU	-	expression tag	UNP A0A1B3TN99
A	1113	LYS	-	expression tag	UNP A0A1B3TN99
A	1114	GLY	-	expression tag	UNP A0A1B3TN99
A	1115	GLY	-	expression tag	UNP A0A1B3TN99
A	1116	GLY	-	expression tag	UNP A0A1B3TN99
A	1117	SER	-	expression tag	UNP A0A1B3TN99
A	1118	GLY	-	expression tag	UNP A0A1B3TN99
A	1119	GLY	-	expression tag	UNP A0A1B3TN99
A	1120	GLY	-	expression tag	UNP A0A1B3TN99

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1121	GLY	-	expression tag	UNP A0A1B3TN99
A	1122	SER	-	expression tag	UNP A0A1B3TN99
A	1123	GLY	-	expression tag	UNP A0A1B3TN99
A	1124	GLY	-	expression tag	UNP A0A1B3TN99
A	1125	SER	-	expression tag	UNP A0A1B3TN99
A	1126	ALA	-	expression tag	UNP A0A1B3TN99
A	1127	TRP	-	expression tag	UNP A0A1B3TN99
A	1128	SER	-	expression tag	UNP A0A1B3TN99
A	1129	HIS	-	expression tag	UNP A0A1B3TN99
A	1130	PRO	-	expression tag	UNP A0A1B3TN99
A	1131	GLN	-	expression tag	UNP A0A1B3TN99
A	1132	PHE	-	expression tag	UNP A0A1B3TN99
A	1133	GLU	-	expression tag	UNP A0A1B3TN99
A	1134	LYS	-	expression tag	UNP A0A1B3TN99
B	869	PRO	ILE	conflict	UNP A0A1B3TN99
B	870	PRO	ILE	conflict	UNP A0A1B3TN99
B	1055	GLY	-	expression tag	UNP A0A1B3TN99
B	1056	SER	-	expression tag	UNP A0A1B3TN99
B	1057	GLY	-	expression tag	UNP A0A1B3TN99
B	1058	TYR	-	expression tag	UNP A0A1B3TN99
B	1059	ILE	-	expression tag	UNP A0A1B3TN99
B	1060	PRO	-	expression tag	UNP A0A1B3TN99
B	1061	GLU	-	expression tag	UNP A0A1B3TN99
B	1062	ALA	-	expression tag	UNP A0A1B3TN99
B	1063	PRO	-	expression tag	UNP A0A1B3TN99
B	1064	ARG	-	expression tag	UNP A0A1B3TN99
B	1065	ASP	-	expression tag	UNP A0A1B3TN99
B	1066	GLY	-	expression tag	UNP A0A1B3TN99
B	1067	GLN	-	expression tag	UNP A0A1B3TN99
B	1068	ALA	-	expression tag	UNP A0A1B3TN99
B	1069	TYR	-	expression tag	UNP A0A1B3TN99
B	1070	VAL	-	expression tag	UNP A0A1B3TN99
B	1071	ARG	-	expression tag	UNP A0A1B3TN99
B	1072	LYS	-	expression tag	UNP A0A1B3TN99
B	1073	ASP	-	expression tag	UNP A0A1B3TN99
B	1074	GLY	-	expression tag	UNP A0A1B3TN99
B	1075	GLU	-	expression tag	UNP A0A1B3TN99
B	1076	TRP	-	expression tag	UNP A0A1B3TN99
B	1077	VAL	-	expression tag	UNP A0A1B3TN99
B	1078	LEU	-	expression tag	UNP A0A1B3TN99
B	1079	LEU	-	expression tag	UNP A0A1B3TN99
B	1080	SER	-	expression tag	UNP A0A1B3TN99

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1081	THR	-	expression tag	UNP A0A1B3TN99
B	1082	PHE	-	expression tag	UNP A0A1B3TN99
B	1083	LEU	-	expression tag	UNP A0A1B3TN99
B	1084	GLY	-	expression tag	UNP A0A1B3TN99
B	1085	ARG	-	expression tag	UNP A0A1B3TN99
B	1086	SER	-	expression tag	UNP A0A1B3TN99
B	1087	LEU	-	expression tag	UNP A0A1B3TN99
B	1088	GLU	-	expression tag	UNP A0A1B3TN99
B	1089	VAL	-	expression tag	UNP A0A1B3TN99
B	1090	LEU	-	expression tag	UNP A0A1B3TN99
B	1091	PHE	-	expression tag	UNP A0A1B3TN99
B	1092	GLN	-	expression tag	UNP A0A1B3TN99
B	1093	GLY	-	expression tag	UNP A0A1B3TN99
B	1094	PRO	-	expression tag	UNP A0A1B3TN99
B	1095	GLY	-	expression tag	UNP A0A1B3TN99
B	1096	HIS	-	expression tag	UNP A0A1B3TN99
B	1097	HIS	-	expression tag	UNP A0A1B3TN99
B	1098	HIS	-	expression tag	UNP A0A1B3TN99
B	1099	HIS	-	expression tag	UNP A0A1B3TN99
B	1100	HIS	-	expression tag	UNP A0A1B3TN99
B	1101	HIS	-	expression tag	UNP A0A1B3TN99
B	1102	HIS	-	expression tag	UNP A0A1B3TN99
B	1103	HIS	-	expression tag	UNP A0A1B3TN99
B	1104	SER	-	expression tag	UNP A0A1B3TN99
B	1105	ALA	-	expression tag	UNP A0A1B3TN99
B	1106	TRP	-	expression tag	UNP A0A1B3TN99
B	1107	SER	-	expression tag	UNP A0A1B3TN99
B	1108	HIS	-	expression tag	UNP A0A1B3TN99
B	1109	PRO	-	expression tag	UNP A0A1B3TN99
B	1110	GLN	-	expression tag	UNP A0A1B3TN99
B	1111	PHE	-	expression tag	UNP A0A1B3TN99
B	1112	GLU	-	expression tag	UNP A0A1B3TN99
B	1113	LYS	-	expression tag	UNP A0A1B3TN99
B	1114	GLY	-	expression tag	UNP A0A1B3TN99
B	1115	GLY	-	expression tag	UNP A0A1B3TN99
B	1116	GLY	-	expression tag	UNP A0A1B3TN99
B	1117	SER	-	expression tag	UNP A0A1B3TN99
B	1118	GLY	-	expression tag	UNP A0A1B3TN99
B	1119	GLY	-	expression tag	UNP A0A1B3TN99
B	1120	GLY	-	expression tag	UNP A0A1B3TN99
B	1121	GLY	-	expression tag	UNP A0A1B3TN99
B	1122	SER	-	expression tag	UNP A0A1B3TN99

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1123	GLY	-	expression tag	UNP A0A1B3TN99
B	1124	GLY	-	expression tag	UNP A0A1B3TN99
B	1125	SER	-	expression tag	UNP A0A1B3TN99
B	1126	ALA	-	expression tag	UNP A0A1B3TN99
B	1127	TRP	-	expression tag	UNP A0A1B3TN99
B	1128	SER	-	expression tag	UNP A0A1B3TN99
B	1129	HIS	-	expression tag	UNP A0A1B3TN99
B	1130	PRO	-	expression tag	UNP A0A1B3TN99
B	1131	GLN	-	expression tag	UNP A0A1B3TN99
B	1132	PHE	-	expression tag	UNP A0A1B3TN99
B	1133	GLU	-	expression tag	UNP A0A1B3TN99
B	1134	LYS	-	expression tag	UNP A0A1B3TN99

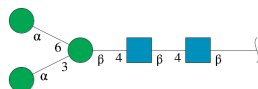
- Molecule 2 is a protein called DH1533 FAB heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	124	Total	C	N	O	S	0	0
			944	598	159	183	4		

- Molecule 3 is a protein called DH1533 FAB light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	106	Total	C	N	O	S	0	0
			811	511	130	167	3		

- Molecule 4 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.



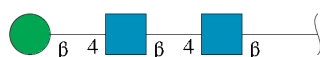
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	5	Total	C	N	O		0	0
			61	34	2	25			
4	T	5	Total	C	N	O		0	0
			61	34	2	25			
4	V	5	Total	C	N	O		0	0
			61	34	2	25			
4	k	5	Total	C	N	O		0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	o	5	Total	C	N	O	0	0
			61	34	2	25		
4	1	5	Total	C	N	O	0	0
			61	34	2	25		
4	3	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	F	3	Total	C	N	O	0	0
			39	22	2	15		
5	W	3	Total	C	N	O	0	0
			39	22	2	15		
5	b	3	Total	C	N	O	0	0
			39	22	2	15		
5	c	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	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		

- 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	G	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		
6	M	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		
6	d	2	Total	C	N	O	0	0
			28	16	2	10		
6	e	2	Total	C	N	O	0	0
			28	16	2	10		
6	f	2	Total	C	N	O	0	0
			28	16	2	10		
6	g	2	Total	C	N	O	0	0
			28	16	2	10		
6	h	2	Total	C	N	O	0	0
			28	16	2	10		
6	i	2	Total	C	N	O	0	0
			28	16	2	10		
6	n	2	Total	C	N	O	0	0
			28	16	2	10		
6	p	2	Total	C	N	O	0	0
			28	16	2	10		
6	q	2	Total	C	N	O	0	0
			28	16	2	10		
6	s	2	Total	C	N	O	0	0
			28	16	2	10		

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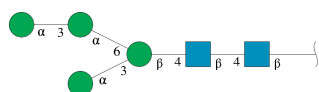
Mol	Chain	Residues	Atoms				AltConf	Trace
6	u	2	Total	C	N	O	0	0
			28	16	2	10		
6	w	2	Total	C	N	O	0	0
			28	16	2	10		
6	x	2	Total	C	N	O	0	0
			28	16	2	10		
6	y	2	Total	C	N	O	0	0
			28	16	2	10		
6	z	2	Total	C	N	O	0	0
			28	16	2	10		
6	4	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	S	4	Total	C	N	O	0	0
			50	28	2	20		
7	U	4	Total	C	N	O	0	0
			50	28	2	20		
7	1	4	Total	C	N	O	0	0
			50	28	2	20		
7	0	4	Total	C	N	O	0	0
			50	28	2	20		
7	2	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



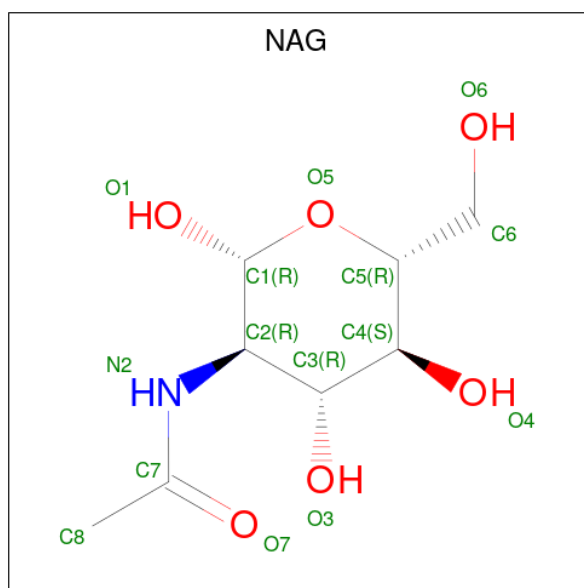
Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 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
9	Y	4	Total	C	N	O	0	0
			50	28	2	20		
9	j	4	Total	C	N	O	0	0
			50	28	2	20		
9	t	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

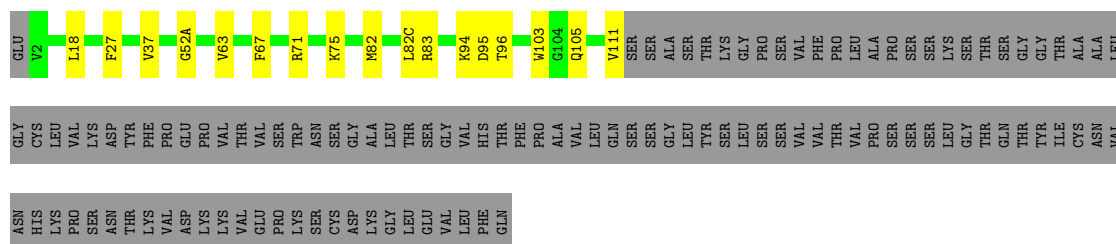


Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	

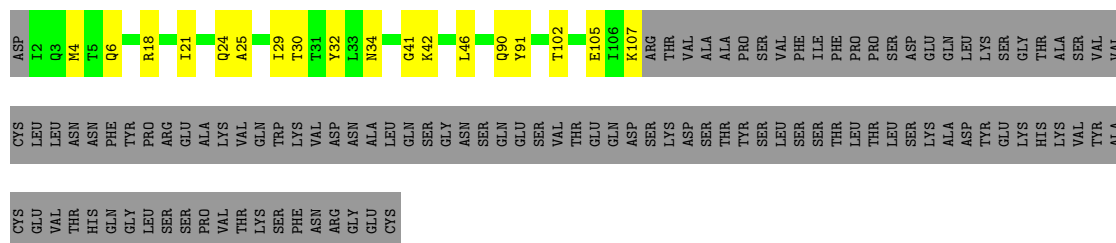
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Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total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



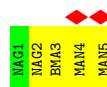
• Molecule 3: DH1533 FAB light chain



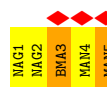
• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: 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 4: 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 4: 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



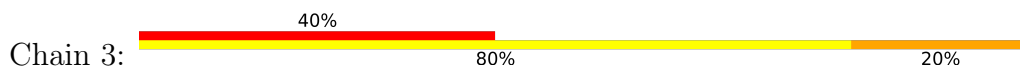
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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 4: 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 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

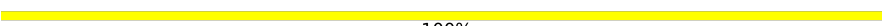


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain G:  100%



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

Chain I:  100%

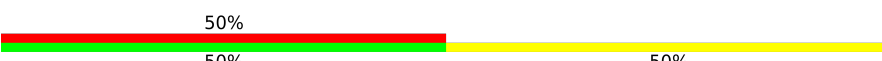


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 100%



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

Chain K:  50% 50% 50%



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

Chain M:  50% 50%



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

Chain N:  100%



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



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



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



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



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



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



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



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



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



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



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



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



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

Chain n:  100%

MAG1
MAG2

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

Chain p:  50% 50%

MAG1
MAG2

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

Chain q:  50% 50%

MAG1
MAG2

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

Chain s:  50% 50%

MAG1
MAG2

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

Chain u:  100%

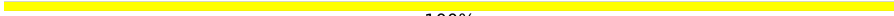
MAG1
MAG2

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

Chain w:  50% 100%

MAG1
MAG2

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

Chain x:  100%

NAG1
NAG2

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

Chain y:  50% 50%

NAG1
NAG2

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

Chain z:  50% 50%

NAG1
NAG2

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

Chain 4:  100%

NAG1
NAG2

- 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 S:  25% 25% 75%

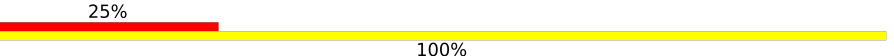
NAG1
NAG2
BMA3
MAN4

- 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 U:  25% 50% 75%

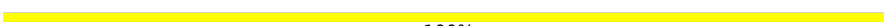
NAG1
NAG2
BMA3
MAN4

- 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 I:  25% 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 0:  100%

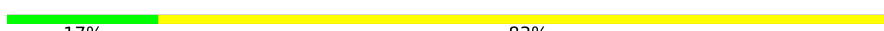


- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:  25% 50% 75%

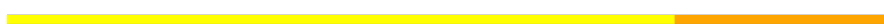


- Molecule 8: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  17% 83%



- Molecule 9: 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

Chain Y:  75% 25%



- Molecule 9: 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

Chain j:  25% 50% 75%



- Molecule 9: 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

Chain t:  25% 75% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	202873	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF Estimation	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	110.218	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.080	Depositor
Recommended contour level	10	Depositor
Map size (Å)	466.56003, 466.56003, 466.56003	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.21	0/7928	0.54	4/10805 (0.0%)
1	B	0.25	0/6816	0.57	3/9291 (0.0%)
1	C	0.21	0/6822	0.55	1/9299 (0.0%)
2	H	0.25	0/969	0.50	0/1317
3	L	0.26	0/827	0.62	0/1124
All	All	0.22	0/23362	0.55	8/31836 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	GLU	N-CA-C	-6.66	104.98	113.23
1	A	35	HIS	N-CA-C	-6.22	106.06	113.21
1	A	928	ASN	N-CA-CB	5.53	118.35	110.44
1	B	242	ASN	CB-CG-ND2	5.49	124.63	116.40
1	B	242	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	927	GLY	CA-C-N	-5.38	109.93	121.45
1	A	927	GLY	C-N-CA	-5.38	109.93	121.45
1	C	34	GLY	CA-C-O	-5.03	116.98	121.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7768	0	7600	81	0
1	B	6688	0	6548	69	0
1	C	6694	0	6551	74	0
2	H	944	0	898	11	0
3	L	811	0	787	15	0
4	1	61	0	52	0	0
4	3	61	0	52	1	0
4	D	61	0	52	0	0
4	T	61	0	52	0	0
4	V	61	0	52	1	0
4	k	61	0	52	0	0
4	o	61	0	52	0	0
5	E	39	0	34	0	0
5	F	39	0	34	1	0
5	W	39	0	34	0	0
5	b	39	0	34	0	0
5	c	39	0	34	1	0
5	m	39	0	34	0	0
5	r	39	0	34	1	0
5	v	39	0	34	0	0
6	4	28	0	25	1	0
6	G	28	0	25	0	0
6	I	28	0	25	0	0
6	J	28	0	25	0	0
6	K	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
6	O	28	0	25	0	0
6	P	28	0	25	0	0
6	Q	28	0	25	0	0
6	R	28	0	25	0	0
6	Z	28	0	25	1	0
6	a	28	0	25	0	0
6	d	28	0	25	1	0
6	e	28	0	25	0	0
6	f	28	0	25	0	0
6	g	28	0	25	0	0
6	h	28	0	25	0	0
6	i	28	0	25	1	0
6	n	28	0	25	0	0
6	p	28	0	25	0	0
6	q	28	0	25	1	0
6	s	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	u	28	0	25	0	0
6	w	28	0	25	0	0
6	x	28	0	25	0	0
6	y	28	0	25	1	0
6	z	28	0	25	0	0
7	0	50	0	43	0	0
7	2	50	0	43	0	0
7	S	50	0	43	0	0
7	U	50	0	43	0	0
7	l	50	0	43	0	0
8	X	72	0	61	0	0
9	Y	50	0	43	1	0
9	j	50	0	43	0	0
9	t	50	0	43	2	0
10	A	112	0	104	4	0
10	B	70	0	65	1	0
10	C	70	0	65	0	0
All	All	25152	0	24359	243	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1204:NAG:O7	1:B:717:LEU:HD21	1.24	1.29
10:A:1204:NAG:C7	1:B:717:LEU:HD21	1.63	1.27
10:A:1204:NAG:O7	1:B:717:LEU:CD2	1.85	1.24
3:L:25:ALA:CB	3:L:29:ILE:HD12	1.83	1.09
3:L:25:ALA:HB2	3:L:29:ILE:HD12	1.36	1.05
1:A:33:VAL:HG12	1:A:229:CYS:HA	1.39	1.00
3:L:25:ALA:CB	3:L:29:ILE:CD1	2.44	0.95
3:L:25:ALA:HB1	3:L:29:ILE:CD1	1.99	0.91
3:L:25:ALA:HB1	3:L:29:ILE:HD11	1.58	0.85
1:B:32:CYS:N	1:B:38:ASN:HB3	1.91	0.83
1:B:32:CYS:N	1:B:229:CYS:SG	2.52	0.82
1:A:153:GLY:HA2	6:Z:2:NAG:H83	1.64	0.79
1:B:579:ASN:CG	6:y:1:NAG:C1	2.48	0.79
1:A:715:LYS:HE3	1:A:715:LYS:HA	1.63	0.77
1:C:516:ASN:HB2	1:C:532:PHE:CE2	2.21	0.76
2:H:82:MET:HB3	2:H:82(C):LEU:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:VAL:N	1:C:229:CYS:SG	2.60	0.75
1:B:33:VAL:N	1:B:229:CYS:SG	2.62	0.73
10:A:1204:NAG:O7	1:B:717:LEU:HD23	1.90	0.70
1:A:33:VAL:CG1	1:A:229:CYS:HA	2.18	0.70
1:C:117:ILE:HG12	1:C:233:LEU:CD2	2.21	0.70
1:C:127:LEU:HG	1:C:128:ARG:H	1.56	0.70
1:B:36:SER:HA	1:B:39:VAL:HG12	1.72	0.70
1:B:114:SER:HB2	1:B:233:LEU:HD12	1.75	0.69
1:C:833:ASP:O	1:C:837:GLN:HG2	1.92	0.69
1:A:33:VAL:N	1:A:229:CYS:SG	2.66	0.68
1:A:1013:ASN:HB2	1:B:784:VAL:HG22	1.79	0.65
1:A:33:VAL:CG2	1:A:122:ASN:HD21	2.10	0.64
1:C:240:LEU:HB3	1:C:252:ILE:CG2	2.27	0.64
1:C:34:GLY:C	1:C:36:SER:H	2.07	0.63
1:A:824:VAL:O	1:A:828:LEU:HD13	1.98	0.63
1:C:117:ILE:HG12	1:C:233:LEU:HD23	1.80	0.63
1:A:38:ASN:ND2	1:A:229:CYS:HB3	2.15	0.61
1:A:33:VAL:HG13	1:A:229:CYS:SG	2.40	0.61
1:B:146:THR:HG21	1:B:151:VAL:HB	1.83	0.60
1:B:33:VAL:HG13	1:B:35:HIS:ND1	2.15	0.60
1:C:252:ILE:CD1	1:C:262:ARG:NH1	2.65	0.59
1:A:34:GLY:C	1:A:36:SER:H	2.09	0.59
1:C:528:MET:HE3	1:C:529:PRO:HD2	1.85	0.59
1:A:515:GLU:HG2	1:A:517:PHE:HD1	1.68	0.59
3:L:25:ALA:HB2	3:L:29:ILE:CD1	2.16	0.59
1:B:32:CYS:SG	1:B:86:SER:HB2	2.43	0.58
1:B:142:VAL:HG12	1:B:171:ASN:HB2	1.85	0.58
1:A:386:SER:HB3	1:A:390:ILE:HD11	1.86	0.58
1:C:126:ASN:HD21	1:C:128:ARG:HG3	1.69	0.58
1:A:1002:THR:HG23	1:A:1030:GLU:OE2	2.05	0.57
1:C:1034:VAL:HG13	1:A:1032:ILE:HD12	1.86	0.56
1:A:33:VAL:HB	1:A:86:SER:OG	2.06	0.56
1:A:422:VAL:HG13	1:A:423:ILE:HG13	1.88	0.56
1:C:1034:VAL:HG21	1:A:1034:VAL:HG22	1.88	0.56
1:B:469:ILE:HG13	1:B:470:THR:HG23	1.87	0.56
1:B:32:CYS:SG	1:B:33:VAL:N	2.79	0.56
1:A:854:GLN:HB2	1:A:878:ARG:HH21	1.71	0.55
1:B:597:ILE:HG12	1:B:942:GLY:HA2	1.89	0.55
1:C:709:ASP:OD1	1:C:711:LYS:HG2	2.06	0.55
3:L:21:ILE:HG12	3:L:102:THR:HG21	1.89	0.55
2:H:52(A):GLY:HA2	2:H:71:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ILE:HD11	1:C:262:ARG:NH1	2.22	0.55
1:A:1013:ASN:HB2	1:B:784:VAL:CG2	2.37	0.54
1:B:157:ILE:HG13	1:B:157:ILE:O	2.07	0.54
1:C:680:SER:HB2	1:C:683:ARG:NH2	2.22	0.54
1:C:1013:ASN:HD22	1:A:784:VAL:HG22	1.73	0.54
1:A:119:TYR:HB2	1:A:193:PHE:HB3	1.89	0.54
1:C:188:LYS:H	1:C:188:LYS:HD2	1.73	0.54
1:A:288:SER:HB3	1:A:439:VAL:HG12	1.89	0.54
1:C:197:ARG:HG3	1:C:197:ARG:HH11	1.73	0.53
1:A:145:CYS:HA	1:A:168:CYS:HA	1.90	0.53
1:B:32:CYS:O	1:B:35:HIS:N	2.42	0.53
1:C:222:THR:OG1	1:C:223:ASN:N	2.42	0.53
1:A:851:GLN:OE1	1:A:853:PHE:CZ	2.62	0.53
1:B:241:VAL:HG12	1:B:243:VAL:HG23	1.91	0.53
1:B:33:VAL:C	1:B:35:HIS:H	2.18	0.52
1:C:122:ASN:ND2	1:C:227:THR:HA	2.24	0.52
3:L:107:LYS:HE2	3:L:107:LYS:HA	1.91	0.51
1:A:165:ASN:OD1	1:A:167:TYR:HE1	1.94	0.51
3:L:32:TYR:HB3	3:L:91:TYR:CE1	2.44	0.51
1:B:224:ALA:HA	1:B:227:THR:HG22	1.91	0.51
1:A:540:ASN:OD1	1:A:540:ASN:O	2.28	0.51
1:B:83:TRP:HB3	1:B:105:CYS:HA	1.93	0.51
1:C:154:ASP:OD2	5:F:2:NAG:H83	2.10	0.51
3:L:41:GLY:C	3:L:42:LYS:HD2	2.36	0.51
1:B:127:LEU:HD12	1:B:190:VAL:HG11	1.92	0.51
1:A:195:ILE:HG21	1:A:217:VAL:HG21	1.91	0.50
6:4:1:NAG:H5	6:4:2:NAG:C7	2.41	0.50
2:H:67:PHE:CE2	2:H:82:MET:HG2	2.46	0.50
1:A:584:PHE:CZ	6:i:1:NAG:H83	2.46	0.50
1:B:33:VAL:HB	1:B:122:ASN:OD1	2.11	0.50
1:A:461:SER:HB2	1:B:717:LEU:O	2.12	0.50
2:H:63:VAL:CG2	2:H:67:PHE:CG	2.95	0.49
1:A:33:VAL:CG1	1:A:86:SER:HB2	2.42	0.49
1:A:687:ARG:HG2	1:A:687:ARG:HH11	1.78	0.49
1:C:52:PHE:CD1	1:C:53:ALA:N	2.80	0.49
2:H:37:VAL:HG11	2:H:103:TRP:CZ3	2.48	0.48
1:C:121:ILE:HG22	1:C:122:ASN:H	1.78	0.48
1:A:964:LEU:HB3	1:A:972:TYR:HB2	1.95	0.48
1:B:244:SER:HB2	9:t:1:NAG:H62	1.95	0.48
1:B:800:MET:HE1	1:B:946:LEU:HD13	1.95	0.48
1:C:473:SER:HB3	1:C:479:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:ASN:HB2	1:C:532:PHE:CD2	2.47	0.48
1:A:655:LYS:NZ	1:A:762:ALA:HB3	2.28	0.48
1:C:34:GLY:C	1:C:36:SER:N	2.71	0.48
1:C:252:ILE:HD11	1:C:259:ASN:OD1	2.14	0.48
1:C:270:VAL:H	1:C:506:GLN:HE22	1.62	0.48
1:C:127:LEU:C	1:C:129:ARG:H	2.22	0.48
1:A:147:ASN:C	1:A:147:ASN:OD1	2.57	0.48
2:H:27:PHE:CZ	2:H:94:LYS:HD2	2.48	0.48
1:C:470:THR:HG22	1:A:64:SER:HB3	1.95	0.48
1:B:125:GLU:HG2	1:B:227:THR:OG1	2.14	0.48
1:B:82:LEU:HD12	1:B:232:ALA:HB2	1.95	0.47
1:A:33:VAL:HG12	1:A:86:SER:HB2	1.97	0.47
1:A:586:TRP:CZ2	1:A:995:MET:HG2	2.50	0.47
1:A:715:LYS:HA	1:A:715:LYS:CE	2.41	0.47
1:B:151:VAL:HA	5:r:2:NAG:H82	1.97	0.47
1:B:62:ASN:HD22	1:B:207:ARG:HH11	1.62	0.47
1:C:80:ASN:O	1:C:109:TYR:HA	2.15	0.47
1:C:866:ARG:O	1:C:867:LEU:HD12	2.15	0.47
1:A:97:PHE:CE2	1:A:197:ARG:HA	2.50	0.47
1:B:242:ASN:OD1	1:B:249:ALA:HB3	2.15	0.47
1:A:98:ASN:HD22	9:Y:1:NAG:C7	2.28	0.46
1:A:144:TYR:HE1	1:A:171:ASN:OD1	1.98	0.46
1:C:252:ILE:HD12	1:C:262:ARG:NH1	2.30	0.46
1:A:134:PHE:CD1	1:A:217:VAL:HG22	2.50	0.46
1:B:94:PHE:CD1	1:B:218:ASN:HB2	2.51	0.46
1:B:268:PHE:HB2	9:t:1:NAG:H81	1.97	0.46
1:C:150:LEU:H	1:C:150:LEU:HD23	1.81	0.46
1:B:563:GLN:OE1	1:B:563:GLN:HA	2.15	0.46
4:V:3:BMA:H61	4:V:5:MAN:H2	1.52	0.46
1:C:197:ARG:HG3	1:C:197:ARG:NH1	2.30	0.46
1:A:33:VAL:HB	1:A:86:SER:CB	2.46	0.46
1:C:197:ARG:HD2	1:C:197:ARG:C	2.41	0.46
1:C:252:ILE:HD12	1:C:262:ARG:CZ	2.45	0.46
1:C:528:MET:HE3	1:C:529:PRO:CD	2.45	0.46
3:L:32:TYR:HB3	3:L:91:TYR:CD1	2.50	0.46
1:C:721:ASP:OD1	1:C:722:LEU:N	2.49	0.45
1:B:81:CYS:HB3	1:B:109:TYR:HA	1.97	0.45
1:A:33:VAL:HG21	1:A:122:ASN:HD21	1.81	0.45
1:A:77:LEU:HD13	1:A:251:ILE:HD13	1.98	0.45
1:A:379:LYS:HE3	1:A:424:THR:HB	1.99	0.45
1:C:628:CYS:O	1:C:632:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LYS:O	1:A:342:THR:HB	2.17	0.45
1:A:655:LYS:O	1:A:658:THR:HG22	2.17	0.45
1:A:655:LYS:HZ2	1:A:762:ALA:HB3	1.82	0.45
1:B:166:PHE:HE1	6:q:1:NAG:H61	1.80	0.45
1:C:145:CYS:HA	1:C:168:CYS:HA	1.99	0.45
1:C:224:ALA:HA	1:C:227:THR:OG1	2.16	0.45
1:B:110:SER:HA	10:B:1201:NAG:H82	1.99	0.45
1:B:32:CYS:O	1:B:33:VAL:C	2.60	0.45
1:B:224:ALA:C	1:B:226:THR:H	2.25	0.45
1:A:1041:LEU:HD13	1:A:1041:LEU:O	2.17	0.45
1:B:528:MET:HE3	1:B:529:PRO:HD2	1.98	0.45
1:C:194:VAL:HB	1:C:202:TYR:HB2	1.99	0.45
1:A:684:VAL:HG11	1:A:745:MET:SD	2.57	0.45
1:B:522:PHE:CG	1:B:535:SER:HA	2.52	0.44
1:A:194:VAL:HB	1:A:202:TYR:HB2	1.99	0.44
1:B:522:PHE:CD1	1:B:535:SER:HA	2.52	0.44
1:B:628:CYS:O	1:B:632:GLU:HG3	2.17	0.44
6:d:1:NAG:H61	6:d:2:NAG:N2	2.32	0.44
1:C:81:CYS:HB2	1:C:105:CYS:HB3	1.44	0.44
1:A:33:VAL:CG1	1:A:122:ASN:ND2	2.81	0.44
1:B:142:VAL:CG1	1:B:171:ASN:HB2	2.46	0.44
1:B:619:GLU:HA	1:B:619:GLU:OE1	2.17	0.44
1:B:1018:ASN:OD1	4:3:1:NAG:O5	2.34	0.44
1:C:127:LEU:CG	1:C:128:ARG:H	2.24	0.44
1:C:677:LEU:CD2	1:C:678:PRO:HD2	2.48	0.44
1:C:811:ASN:OD1	1:C:814:ILE:HD13	2.17	0.44
1:A:132:ILE:HD12	1:A:143:PHE:HD2	1.82	0.44
1:A:127:LEU:HB3	1:A:128:ARG:H	1.50	0.44
1:A:811:ASN:O	1:A:815:THR:HG23	2.16	0.44
1:B:765:ILE:H	1:B:765:ILE:HG13	1.61	0.44
1:C:52:PHE:HD1	1:C:53:ALA:H	1.66	0.43
1:A:370:SER:O	1:A:374:VAL:HG23	2.17	0.43
1:B:227:THR:HG23	1:B:228:VAL:HG23	1.99	0.43
1:B:615:VAL:O	1:B:618:VAL:HG22	2.18	0.43
1:A:126:ASN:OD1	1:A:128:ARG:HD3	2.18	0.43
1:C:39:VAL:HG22	1:C:39:VAL:O	2.18	0.43
1:C:683:ARG:HB2	1:C:741:GLU:OE1	2.19	0.43
1:A:375:ASN:HB3	1:A:427:PRO:HA	2.00	0.43
1:A:677:LEU:HD22	1:A:678:PRO:HD2	2.01	0.43
1:A:811:ASN:OD1	1:A:814:ILE:HB	2.17	0.43
1:C:818:SER:HB3	1:C:821:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:HA	1:C:177:GLU:O	2.18	0.43
1:C:240:LEU:HB3	1:C:252:ILE:HG22	1.99	0.43
1:C:437:MET:HE3	1:C:439:VAL:HG22	2.00	0.43
1:A:33:VAL:HG22	1:A:122:ASN:HD21	1.82	0.43
2:H:105:GLN:OE1	2:H:105:GLN:HA	2.18	0.43
1:B:134:PHE:CD2	1:B:217:VAL:HG12	2.54	0.43
1:C:34:GLY:O	1:C:35:HIS:CD2	2.72	0.43
2:H:18:LEU:HA	2:H:18:LEU:HD23	1.90	0.43
1:A:650:LEU:HD11	1:A:743:MET:HE1	2.00	0.42
1:A:108:PHE:CD1	1:A:108:PHE:C	2.97	0.42
1:C:678:PRO:HB3	1:C:683:ARG:HG2	2.01	0.42
3:L:18:ARG:O	3:L:18:ARG:HD3	2.19	0.42
1:C:560:ILE:C	1:C:560:ILE:HD12	2.44	0.42
1:A:518:THR:HB	1:A:522:PHE:O	2.20	0.42
1:A:597:ILE:HG12	1:A:942:GLY:HA2	2.02	0.42
1:B:743:MET:HE1	1:B:943:LEU:HD21	2.01	0.42
1:C:252:ILE:CD1	1:C:262:ARG:CZ	2.96	0.42
2:H:95:ASP:OD1	2:H:96:THR:N	2.51	0.42
3:L:34:ASN:OD1	3:L:46:LEU:HD11	2.19	0.42
1:B:128:ARG:HD3	1:B:128:ARG:HA	1.89	0.42
1:B:473:SER:HB3	1:B:479:LEU:HD11	2.02	0.42
1:C:811:ASN:HD21	1:C:814:ILE:HB	1.84	0.42
1:A:32:CYS:N	1:A:122:ASN:OD1	2.53	0.42
1:C:222:THR:HG23	1:C:223:ASN:OD1	2.19	0.42
1:C:548:TYR:CD1	1:C:548:TYR:C	2.97	0.42
1:A:327:THR:HG21	5:c:1:NAG:H5	2.02	0.42
1:B:667:ASP:OD2	1:B:667:ASP:N	2.52	0.42
1:C:554:CYS:SG	1:C:555:ALA:N	2.93	0.42
1:A:515:GLU:N	1:A:515:GLU:OE1	2.52	0.42
1:A:814:ILE:HG22	1:A:817:THR:HB	2.02	0.42
1:C:60:LEU:HD21	1:C:194:VAL:HG11	2.01	0.41
1:A:757:GLY:HA3	1:A:765:ILE:HD13	2.01	0.41
1:C:221:VAL:O	1:C:222:THR:O	2.38	0.41
1:A:35:HIS:O	1:A:37:GLU:HG3	2.20	0.41
2:H:63:VAL:HG22	2:H:63:VAL:O	2.20	0.41
1:B:769:LEU:HD12	1:B:769:LEU:HA	1.86	0.41
1:A:1034:VAL:HG11	1:B:1034:VAL:HG12	2.03	0.41
2:H:83:ARG:O	2:H:111:VAL:HG11	2.21	0.41
1:B:163:LEU:HD13	1:B:163:LEU:HA	1.91	0.41
1:A:109:TYR:CD1	1:A:109:TYR:C	2.98	0.41
1:C:116:VAL:HG13	1:C:194:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:4:MET:HE2	3:L:90:GLN:HB3	2.02	0.41
3:L:105:GLU:OE2	3:L:105:GLU:HA	2.21	0.41
1:C:614:ASN:O	1:C:618:VAL:HG23	2.20	0.41
1:C:1032:ILE:HD13	1:B:1034:VAL:HG23	2.03	0.41
1:A:32:CYS:HB2	1:A:38:ASN:CB	2.50	0.41
1:A:134:PHE:CE1	1:A:217:VAL:HG22	2.56	0.41
1:A:431:GLU:OE1	1:A:431:GLU:N	2.47	0.41
1:B:33:VAL:O	1:B:33:VAL:HG22	2.21	0.41
1:A:677:LEU:HD13	1:A:678:PRO:CD	2.51	0.41
1:B:443:LYS:HE3	1:B:443:LYS:HB3	1.84	0.41
1:B:842:LEU:HA	1:B:842:LEU:HD12	1.81	0.41
1:B:956:LYS:HD3	1:B:996:PHE:CE1	2.56	0.41
1:C:32:CYS:C	1:C:34:GLY:N	2.79	0.40
1:C:518:THR:HG22	1:C:525:VAL:HG23	2.02	0.40
1:C:711:LYS:HG2	1:C:711:LYS:H	1.67	0.40
1:A:33:VAL:C	1:A:35:HIS:N	2.78	0.40
1:A:588:THR:HG22	1:A:795:SER:HB3	2.03	0.40
1:C:182:PHE:HE1	1:B:294:VAL:HA	1.87	0.40
1:C:539:TYR:CD1	1:C:539:TYR:N	2.89	0.40
1:C:122:ASN:HB3	1:C:227:THR:O	2.20	0.40
1:B:128:ARG:HD2	1:B:166:PHE:CD2	2.57	0.40
1:B:606:CYS:O	1:B:610:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1010/1134 (89%)	969 (96%)	40 (4%)	1 (0%)	48	74
1	B	868/1134 (76%)	831 (96%)	37 (4%)	0	100	100
1	C	869/1134 (77%)	831 (96%)	34 (4%)	4 (0%)	24	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	122/239 (51%)	118 (97%)	4 (3%)	0	100	100
3	L	104/214 (49%)	95 (91%)	8 (8%)	1 (1%)	12	35
All	All	2973/3855 (77%)	2844 (96%)	123 (4%)	6 (0%)	44	70

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	127	LEU
1	C	158	PRO
1	C	222	THR
1	A	333	GLU
1	C	121	ILE
3	L	30	THR

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	873/969 (90%)	865 (99%)	8 (1%)	70	88
1	B	751/969 (78%)	742 (99%)	9 (1%)	63	84
1	C	752/969 (78%)	746 (99%)	6 (1%)	73	89
2	H	99/199 (50%)	98 (99%)	1 (1%)	68	87
3	L	92/189 (49%)	90 (98%)	2 (2%)	45	75
All	All	2567/3295 (78%)	2541 (99%)	26 (1%)	65	87

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	CYS
1	C	35	HIS
1	C	37	GLU
1	C	102	ARG
1	C	486	ASN

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Mol	Chain	Res	Type
1	C	814	ILE
1	A	35	HIS
1	A	111	ASN
1	A	147	ASN
1	A	266	LEU
1	A	541	CYS
1	A	622	LYS
1	A	743	MET
1	A	811	ASN
2	H	75	LYS
3	L	6	GLN
3	L	24	GLN
1	B	82	LEU
1	B	154	ASP
1	B	159	SER
1	B	443	LYS
1	B	541	CYS
1	B	642	GLU
1	B	677	LEU
1	B	697	LYS
1	B	765	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	126	ASN
1	C	200	HIS
1	C	281	GLN
1	C	442	ASN
1	C	496	ASN
1	C	506	GLN
1	C	837	GLN
1	C	852	ASN
1	C	913	ASN
1	A	120	ASN
1	A	296	HIS
1	A	348	GLN
1	A	591	GLN
1	A	786	GLN
1	A	838	GLN
1	A	861	GLN
1	A	888	ASN

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Mol	Chain	Res	Type
1	A	919	GLN
1	A	954	GLN
2	H	39	GLN
3	L	3	GLN
3	L	38	GLN
1	B	38	ASN
1	B	89	GLN
1	B	120	ASN
1	B	786	GLN
1	B	819	GLN
1	B	875	GLN
1	B	919	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

153 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	$\# Z > 2$
7	NAG	0	1	1,7	14,14,15	0.69	0	17,19,21	1.16	2 (11%)
7	NAG	0	2	7	14,14,15	0.70	0	17,19,21	0.88	1 (5%)
7	BMA	0	3	7	11,11,12	0.83	0	15,15,17	2.69	7 (46%)
7	MAN	0	4	7	11,11,12	0.73	0	15,15,17	1.05	1 (6%)
4	NAG	1	1	1,4	14,14,15	0.83	0	17,19,21	1.33	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	1	2	4	14,14,15	0.61	0	17,19,21	1.31	2 (11%)
4	BMA	1	3	4	11,11,12	0.87	0	15,15,17	2.45	6 (40%)
4	MAN	1	4	4	11,11,12	0.66	0	15,15,17	1.26	1 (6%)
4	MAN	1	5	4	11,11,12	0.78	0	15,15,17	0.96	0
7	NAG	2	1	1,7	14,14,15	0.78	0	17,19,21	0.99	1 (5%)
7	NAG	2	2	7	14,14,15	0.72	0	17,19,21	0.85	0
7	BMA	2	3	7	11,11,12	0.82	0	15,15,17	2.69	7 (46%)
7	MAN	2	4	7	11,11,12	0.71	0	15,15,17	1.02	1 (6%)
4	NAG	3	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	1.12	2 (11%)
4	NAG	3	2	4	14,14,15	0.73	0	17,19,21	1.44	2 (11%)
4	BMA	3	3	4	11,11,12	0.81	0	15,15,17	2.25	4 (26%)
4	MAN	3	4	4	11,11,12	0.66	0	15,15,17	1.50	1 (6%)
4	MAN	3	5	4	11,11,12	0.72	0	15,15,17	1.05	1 (6%)
6	NAG	4	1	6,1	14,14,15	0.82	0	17,19,21	2.89	3 (17%)
6	NAG	4	2	6	14,14,15	1.00	1 (7%)	17,19,21	1.36	1 (5%)
4	NAG	D	1	1,4	14,14,15	0.66	0	17,19,21	1.41	3 (17%)
4	NAG	D	2	4	14,14,15	0.75	0	17,19,21	1.38	2 (11%)
4	BMA	D	3	4	11,11,12	0.77	0	15,15,17	1.36	2 (13%)
4	MAN	D	4	4	11,11,12	0.69	0	15,15,17	1.38	2 (13%)
4	MAN	D	5	4	11,11,12	0.65	0	15,15,17	1.34	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.71	0	17,19,21	1.64	2 (11%)
5	NAG	E	2	5	14,14,15	0.65	0	17,19,21	1.67	2 (11%)
5	BMA	E	3	5	11,11,12	0.86	0	15,15,17	2.66	5 (33%)
5	NAG	F	1	1,5	14,14,15	0.71	0	17,19,21	1.19	2 (11%)
5	NAG	F	2	5	14,14,15	0.80	1 (7%)	17,19,21	1.06	1 (5%)
5	BMA	F	3	5	11,11,12	0.80	0	15,15,17	2.46	7 (46%)
6	NAG	G	1	6,1	14,14,15	0.85	1 (7%)	17,19,21	1.16	2 (11%)
6	NAG	G	2	6	14,14,15	0.71	0	17,19,21	0.93	1 (5%)
6	NAG	I	1	6,1	14,14,15	0.89	0	17,19,21	1.31	1 (5%)
6	NAG	I	2	6	14,14,15	0.68	0	17,19,21	1.28	2 (11%)
6	NAG	J	1	6,1	14,14,15	0.74	0	17,19,21	1.51	3 (17%)
6	NAG	J	2	6	14,14,15	0.67	0	17,19,21	0.96	1 (5%)
6	NAG	K	1	6,1	14,14,15	0.83	1 (7%)	17,19,21	1.39	2 (11%)
6	NAG	K	2	6	14,14,15	0.77	0	17,19,21	0.94	0
6	NAG	M	1	6,1	14,14,15	0.70	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	M	2	6	14,14,15	0.71	0	17,19,21	1.38	3 (17%)
6	NAG	N	1	6,1	14,14,15	0.79	0	17,19,21	1.72	3 (17%)
6	NAG	N	2	6	14,14,15	0.76	0	17,19,21	1.25	2 (11%)
6	NAG	O	1	6,1	14,14,15	0.72	0	17,19,21	0.73	0
6	NAG	O	2	6	14,14,15	0.68	0	17,19,21	1.08	2 (11%)
6	NAG	P	1	6,1	14,14,15	0.75	0	17,19,21	0.84	0
6	NAG	P	2	6	14,14,15	0.84	1 (7%)	17,19,21	1.38	2 (11%)
6	NAG	Q	1	6,1	14,14,15	0.86	0	17,19,21	1.28	3 (17%)
6	NAG	Q	2	6	14,14,15	0.77	0	17,19,21	1.04	0
6	NAG	R	1	6,1	14,14,15	0.73	0	17,19,21	0.79	0
6	NAG	R	2	6	14,14,15	0.72	0	17,19,21	0.86	0
7	NAG	S	1	1,7	14,14,15	0.74	0	17,19,21	0.92	0
7	NAG	S	2	7	14,14,15	0.68	0	17,19,21	1.01	2 (11%)
7	BMA	S	3	7	11,11,12	0.86	0	15,15,17	2.46	7 (46%)
7	MAN	S	4	7	11,11,12	0.65	0	15,15,17	1.16	1 (6%)
4	NAG	T	1	1,4	14,14,15	0.78	0	17,19,21	0.83	0
4	NAG	T	2	4	14,14,15	0.64	0	17,19,21	1.24	3 (17%)
4	BMA	T	3	4	11,11,12	0.86	0	15,15,17	2.47	5 (33%)
4	MAN	T	4	4	11,11,12	0.80	0	15,15,17	1.21	1 (6%)
4	MAN	T	5	4	11,11,12	0.70	0	15,15,17	1.23	1 (6%)
7	NAG	U	1	1,7	14,14,15	0.72	0	17,19,21	1.21	3 (17%)
7	NAG	U	2	7	14,14,15	0.67	0	17,19,21	1.04	1 (5%)
7	BMA	U	3	7	11,11,12	0.83	0	15,15,17	2.49	6 (40%)
7	MAN	U	4	7	11,11,12	0.80	0	15,15,17	0.89	0
4	NAG	V	1	1,4	14,14,15	0.65	0	17,19,21	1.17	2 (11%)
4	NAG	V	2	4	14,14,15	0.70	0	17,19,21	1.15	1 (5%)
4	BMA	V	3	4	11,11,12	0.84	0	15,15,17	2.92	6 (40%)
4	MAN	V	4	4	11,11,12	0.79	0	15,15,17	1.28	2 (13%)
4	MAN	V	5	4	11,11,12	0.59	0	15,15,17	1.64	1 (6%)
5	NAG	W	1	1,5	14,14,15	0.72	0	17,19,21	1.24	1 (5%)
5	NAG	W	2	5	14,14,15	0.80	0	17,19,21	0.83	0
5	BMA	W	3	5	11,11,12	0.86	0	15,15,17	2.80	6 (40%)
8	NAG	X	1	8,1	14,14,15	0.71	0	17,19,21	1.14	2 (11%)
8	NAG	X	2	8	14,14,15	0.70	0	17,19,21	0.75	0
8	BMA	X	3	8	11,11,12	0.84	0	15,15,17	1.57	3 (20%)
8	MAN	X	4	8	11,11,12	0.64	0	15,15,17	1.69	1 (6%)
8	MAN	X	5	8	11,11,12	0.69	0	15,15,17	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	X	6	8	11,11,12	0.70	0	15,15,17	1.50	1 (6%)
9	NAG	Y	1	1,9	14,14,15	0.80	1 (7%)	17,19,21	0.84	1 (5%)
9	NAG	Y	2	9	14,14,15	0.67	0	17,19,21	1.33	1 (5%)
9	BMA	Y	3	9	11,11,12	0.78	0	15,15,17	2.72	4 (26%)
9	MAN	Y	4	9	11,11,12	0.66	0	15,15,17	1.20	1 (6%)
6	NAG	Z	1	6,1	14,14,15	0.71	0	17,19,21	1.44	3 (17%)
6	NAG	Z	2	6	14,14,15	0.82	1 (7%)	17,19,21	1.41	3 (17%)
6	NAG	a	1	6,1	14,14,15	0.76	0	17,19,21	1.62	2 (11%)
6	NAG	a	2	6	14,14,15	0.80	0	17,19,21	1.22	1 (5%)
5	NAG	b	1	1,5	14,14,15	0.79	0	17,19,21	1.35	2 (11%)
5	NAG	b	2	5	14,14,15	0.72	0	17,19,21	0.85	0
5	BMA	b	3	5	11,11,12	0.80	0	15,15,17	2.54	6 (40%)
5	NAG	c	1	1,5	14,14,15	0.75	0	17,19,21	0.84	0
5	NAG	c	2	5	14,14,15	0.71	0	17,19,21	1.12	2 (11%)
5	BMA	c	3	5	11,11,12	0.84	0	15,15,17	2.38	6 (40%)
6	NAG	d	1	6,1	14,14,15	0.71	0	17,19,21	2.04	4 (23%)
6	NAG	d	2	6	14,14,15	0.62	0	17,19,21	0.95	1 (5%)
6	NAG	e	1	6,1	14,14,15	0.88	1 (7%)	17,19,21	1.46	3 (17%)
6	NAG	e	2	6	14,14,15	0.63	0	17,19,21	1.46	1 (5%)
6	NAG	f	1	6,1	14,14,15	0.80	0	17,19,21	0.98	1 (5%)
6	NAG	f	2	6	14,14,15	0.67	0	17,19,21	1.33	2 (11%)
6	NAG	g	1	6,1	14,14,15	0.69	0	17,19,21	1.31	2 (11%)
6	NAG	g	2	6	14,14,15	0.72	0	17,19,21	1.58	4 (23%)
6	NAG	h	1	6,1	14,14,15	0.81	0	17,19,21	0.81	1 (5%)
6	NAG	h	2	6	14,14,15	0.69	0	17,19,21	1.27	2 (11%)
6	NAG	i	1	6,1	14,14,15	0.59	0	17,19,21	1.95	3 (17%)
6	NAG	i	2	6	14,14,15	0.74	0	17,19,21	1.02	1 (5%)
9	NAG	j	1	1,9	14,14,15	0.71	0	17,19,21	1.39	2 (11%)
9	NAG	j	2	9	14,14,15	0.68	0	17,19,21	1.29	2 (11%)
9	BMA	j	3	9	11,11,12	0.83	0	15,15,17	2.05	6 (40%)
9	MAN	j	4	9	11,11,12	0.77	0	15,15,17	0.96	0
4	NAG	k	1	1,4	14,14,15	0.90	1 (7%)	17,19,21	1.68	4 (23%)
4	NAG	k	2	4	14,14,15	0.67	0	17,19,21	1.23	2 (11%)
4	BMA	k	3	4	11,11,12	0.88	0	15,15,17	2.38	5 (33%)
4	MAN	k	4	4	11,11,12	0.75	0	15,15,17	1.05	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	k	5	4	11,11,12	0.65	0	15,15,17	1.10	1 (6%)
7	NAG	l	1	1,7	14,14,15	0.85	0	17,19,21	1.50	5 (29%)
7	NAG	l	2	7	14,14,15	0.67	0	17,19,21	0.98	1 (5%)
7	BMA	l	3	7	11,11,12	0.79	0	15,15,17	2.99	7 (46%)
7	MAN	l	4	7	11,11,12	0.77	0	15,15,17	0.93	1 (6%)
5	NAG	m	1	1,5	14,14,15	0.71	0	17,19,21	1.18	2 (11%)
5	NAG	m	2	5	14,14,15	0.67	0	17,19,21	1.34	2 (11%)
5	BMA	m	3	5	11,11,12	0.77	0	15,15,17	3.00	7 (46%)
6	NAG	n	1	6,1	14,14,15	0.72	0	17,19,21	1.09	2 (11%)
6	NAG	n	2	6	14,14,15	0.76	0	17,19,21	1.46	1 (5%)
4	NAG	o	1	1,4	14,14,15	0.81	0	17,19,21	0.85	1 (5%)
4	NAG	o	2	4	14,14,15	0.75	0	17,19,21	1.28	2 (11%)
4	BMA	o	3	4	11,11,12	0.78	0	15,15,17	1.91	4 (26%)
4	MAN	o	4	4	11,11,12	0.65	0	15,15,17	1.28	1 (6%)
4	MAN	o	5	4	11,11,12	0.56	0	15,15,17	2.53	1 (6%)
6	NAG	p	1	6,1	14,14,15	0.76	0	17,19,21	1.48	2 (11%)
6	NAG	p	2	6	14,14,15	0.74	0	17,19,21	0.84	0
6	NAG	q	1	6,1	14,14,15	0.60	0	17,19,21	2.02	3 (17%)
6	NAG	q	2	6	14,14,15	0.70	0	17,19,21	1.08	1 (5%)
5	NAG	r	1	1,5	14,14,15	0.83	0	17,19,21	1.10	2 (11%)
5	NAG	r	2	5	14,14,15	1.04	1 (7%)	17,19,21	1.27	2 (11%)
5	BMA	r	3	5	11,11,12	0.85	0	15,15,17	2.35	5 (33%)
6	NAG	s	1	6,1	14,14,15	0.78	0	17,19,21	0.95	0
6	NAG	s	2	6	14,14,15	0.75	0	17,19,21	2.22	4 (23%)
9	NAG	t	1	1,9	14,14,15	0.85	1 (7%)	17,19,21	1.11	2 (11%)
9	NAG	t	2	9	14,14,15	0.74	0	17,19,21	0.91	1 (5%)
9	BMA	t	3	9	11,11,12	0.80	0	15,15,17	3.23	5 (33%)
9	MAN	t	4	9	11,11,12	0.76	0	15,15,17	1.22	1 (6%)
6	NAG	u	1	6,1	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
6	NAG	u	2	6	14,14,15	0.76	1 (7%)	17,19,21	1.19	1 (5%)
5	NAG	v	1	1,5	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
5	NAG	v	2	5	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
5	BMA	v	3	5	11,11,12	0.83	0	15,15,17	2.63	7 (46%)
6	NAG	w	1	6,1	14,14,15	0.82	0	17,19,21	1.33	1 (5%)
6	NAG	w	2	6	14,14,15	0.73	0	17,19,21	1.79	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	x	1	6,1	14,14,15	0.59	0	17,19,21	1.17	1 (5%)
6	NAG	x	2	6	14,14,15	0.78	1 (7%)	17,19,21	1.45	1 (5%)
6	NAG	y	1	6	14,14,15	0.80	1 (7%)	17,19,21	0.93	1 (5%)
6	NAG	y	2	6	14,14,15	0.75	0	17,19,21	0.98	1 (5%)
6	NAG	z	1	6,1	14,14,15	0.77	0	17,19,21	0.86	0
6	NAG	z	2	6	14,14,15	0.75	0	17,19,21	1.32	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
7	NAG	0	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	0	2	7	-	0/6/23/26	0/1/1/1
7	BMA	0	3	7	-	0/2/19/22	0/1/1/1
7	MAN	0	4	7	-	1/2/19/22	0/1/1/1
4	NAG	1	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	1	2	4	-	2/6/23/26	0/1/1/1
4	BMA	1	3	4	-	0/2/19/22	0/1/1/1
4	MAN	1	4	4	-	0/2/19/22	0/1/1/1
4	MAN	1	5	4	-	1/2/19/22	0/1/1/1
7	NAG	2	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	2	2	7	-	0/6/23/26	0/1/1/1
7	BMA	2	3	7	-	0/2/19/22	0/1/1/1
7	MAN	2	4	7	-	0/2/19/22	0/1/1/1
4	NAG	3	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	3	2	4	-	2/6/23/26	0/1/1/1
4	BMA	3	3	4	-	2/2/19/22	0/1/1/1
4	MAN	3	4	4	-	0/2/19/22	0/1/1/1
4	MAN	3	5	4	-	2/2/19/22	0/1/1/1
6	NAG	4	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	4	2	6	-	0/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	V	4	4	-	0/2/19/22	0/1/1/1
4	MAN	V	5	4	-	0/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
5	BMA	W	3	5	-	0/2/19/22	0/1/1/1
8	NAG	X	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	0/2/19/22	0/1/1/1
8	MAN	X	4	8	-	1/2/19/22	0/1/1/1
8	MAN	X	5	8	-	1/2/19/22	0/1/1/1
8	MAN	X	6	8	-	2/2/19/22	0/1/1/1
9	NAG	Y	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	1/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	4	9	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	0/6/23/26	0/1/1/1
5	NAG	b	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	BMA	b	3	5	-	1/2/19/22	0/1/1/1
5	NAG	c	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	2/2/19/22	0/1/1/1
6	NAG	d	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	d	2	6	-	0/6/23/26	0/1/1/1
6	NAG	e	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	NAG	f	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	g	2	6	-	4/6/23/26	0/1/1/1
6	NAG	h	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	h	2	6	-	1/6/23/26	0/1/1/1
6	NAG	i	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	i	2	6	-	3/6/23/26	0/1/1/1
9	NAG	j	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	j	2	9	-	1/6/23/26	0/1/1/1
9	BMA	j	3	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	j	4	9	-	1/2/19/22	0/1/1/1
4	NAG	k	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	k	2	4	-	0/6/23/26	0/1/1/1
4	BMA	k	3	4	-	0/2/19/22	0/1/1/1
4	MAN	k	4	4	-	0/2/19/22	0/1/1/1
4	MAN	k	5	4	-	0/2/19/22	0/1/1/1
7	NAG	l	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	l	2	7	-	2/6/23/26	0/1/1/1
7	BMA	l	3	7	-	1/2/19/22	0/1/1/1
7	MAN	l	4	7	-	0/2/19/22	0/1/1/1
5	NAG	m	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	m	2	5	-	3/6/23/26	0/1/1/1
5	BMA	m	3	5	-	1/2/19/22	0/1/1/1
6	NAG	n	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	n	2	6	-	0/6/23/26	0/1/1/1
4	NAG	o	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	o	2	4	-	2/6/23/26	0/1/1/1
4	BMA	o	3	4	-	1/2/19/22	0/1/1/1
4	MAN	o	4	4	-	2/2/19/22	0/1/1/1
4	MAN	o	5	4	-	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	NAG	q	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	q	2	6	-	0/6/23/26	0/1/1/1
5	NAG	r	1	1,5	-	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	-	0/2/19/22	0/1/1/1
6	NAG	s	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	s	2	6	-	2/6/23/26	0/1/1/1
9	NAG	t	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	t	2	9	-	0/6/23/26	0/1/1/1
9	BMA	t	3	9	-	1/2/19/22	0/1/1/1
9	MAN	t	4	9	-	0/2/19/22	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
5	NAG	v	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	v	2	5	-	3/6/23/26	0/1/1/1
5	BMA	v	3	5	-	1/2/19/22	0/1/1/1
6	NAG	w	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	w	2	6	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	x	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	x	2	6	-	0/6/23/26	0/1/1/1
6	NAG	y	1	6	-	0/6/23/26	0/1/1/1
6	NAG	y	2	6	-	0/6/23/26	0/1/1/1
6	NAG	z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	z	2	6	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	r	2	NAG	C1-C2	3.46	1.57	1.52
6	4	2	NAG	C1-C2	3.06	1.56	1.52
4	k	1	NAG	C1-C2	2.61	1.55	1.52
6	P	2	NAG	C1-C2	2.53	1.55	1.52
6	G	1	NAG	C1-C2	2.42	1.55	1.52
9	t	1	NAG	C1-C2	2.36	1.55	1.52
6	y	1	NAG	C1-C2	2.34	1.55	1.52
6	x	2	NAG	C1-C2	2.20	1.55	1.52
9	Y	1	NAG	O5-C1	-2.19	1.40	1.43
6	u	2	NAG	C1-C2	2.08	1.55	1.52
6	K	1	NAG	C1-C2	2.07	1.55	1.52
6	e	1	NAG	O5-C1	-2.05	1.40	1.43
6	Z	2	NAG	C1-C2	2.03	1.55	1.52
5	F	2	NAG	C1-C2	2.03	1.55	1.52
4	3	1	NAG	C1-C2	2.01	1.55	1.52

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	t	3	BMA	C1-O5-C5	10.39	126.11	112.19
6	4	1	NAG	C1-O5-C5	10.36	126.07	112.19
5	m	3	BMA	C1-O5-C5	9.57	125.01	112.19
4	V	3	BMA	C1-O5-C5	9.31	124.67	112.19
7	l	3	BMA	C1-O5-C5	9.18	124.49	112.19
4	o	5	MAN	C1-O5-C5	8.99	124.23	112.19
5	W	3	BMA	C1-O5-C5	8.90	124.11	112.19
9	Y	3	BMA	C1-O5-C5	8.88	124.09	112.19
5	E	3	BMA	C1-O5-C5	8.36	123.39	112.19
7	2	3	BMA	C1-O5-C5	8.10	123.04	112.19
7	0	3	BMA	C1-O5-C5	7.90	122.78	112.19
5	v	3	BMA	C1-O5-C5	7.75	122.57	112.19
5	b	3	BMA	C1-O5-C5	7.41	122.12	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	3	BMA	C1-O5-C5	7.41	122.12	112.19
4	1	3	BMA	C1-O5-C5	7.37	122.06	112.19
4	3	3	BMA	C1-O5-C5	7.35	122.03	112.19
5	F	3	BMA	C1-O5-C5	7.20	121.84	112.19
4	T	3	BMA	C1-O5-C5	7.05	121.63	112.19
5	r	3	BMA	C1-O5-C5	6.75	121.24	112.19
5	c	3	BMA	C1-O5-C5	6.60	121.03	112.19
4	k	3	BMA	C1-O5-C5	6.59	121.02	112.19
7	S	3	BMA	C1-O5-C5	6.48	120.88	112.19
6	i	1	NAG	C1-O5-C5	6.37	120.72	112.19
6	s	2	NAG	C2-N2-C7	6.12	131.10	122.90
8	X	4	MAN	C1-O5-C5	5.55	119.62	112.19
4	V	5	MAN	C1-O5-C5	5.45	119.49	112.19
6	q	1	NAG	O5-C1-C2	-5.25	103.17	111.29
6	d	1	NAG	C2-N2-C7	5.10	129.74	122.90
5	E	2	NAG	C2-N2-C7	4.95	129.53	122.90
5	E	1	NAG	O5-C1-C2	-4.92	103.67	111.29
6	x	2	NAG	C1-O5-C5	4.76	118.56	112.19
6	4	2	NAG	C1-O5-C5	4.74	118.55	112.19
6	s	2	NAG	C1-O5-C5	4.69	118.47	112.19
6	w	2	NAG	C2-N2-C7	4.62	129.09	122.90
6	N	1	NAG	O5-C1-C2	-4.53	104.29	111.29
8	X	6	MAN	C1-O5-C5	4.45	118.16	112.19
4	3	4	MAN	C1-O5-C5	4.44	118.13	112.19
6	w	1	NAG	O5-C1-C2	-4.43	104.44	111.29
6	e	2	NAG	C1-O5-C5	4.36	118.03	112.19
4	D	5	MAN	C1-O5-C5	4.21	117.82	112.19
9	j	3	BMA	C1-O5-C5	4.20	117.82	112.19
6	q	1	NAG	C1-O5-C5	4.19	117.81	112.19
6	K	1	NAG	C2-N2-C7	3.98	128.23	122.90
6	a	1	NAG	C2-N2-C7	3.97	128.22	122.90
4	o	4	MAN	C1-O5-C5	3.97	117.51	112.19
6	N	1	NAG	C1-O5-C5	3.96	117.49	112.19
6	d	1	NAG	C1-C2-N2	3.95	116.66	110.43
6	a	2	NAG	C1-O5-C5	3.94	117.46	112.19
6	p	1	NAG	C1-O5-C5	3.94	117.46	112.19
6	n	2	NAG	C2-N2-C7	3.93	128.16	122.90
6	h	2	NAG	C1-O5-C5	3.92	117.43	112.19
4	1	4	MAN	C1-O5-C5	3.92	117.43	112.19
4	k	1	NAG	O5-C1-C2	-3.87	105.30	111.29
6	a	1	NAG	C1-O5-C5	3.80	117.28	112.19
6	u	2	NAG	C1-O5-C5	3.80	117.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-O5-C5	3.75	117.21	112.19
5	W	1	NAG	O5-C1-C2	-3.71	105.55	111.29
9	j	1	NAG	C1-O5-C5	3.69	117.13	112.19
9	Y	2	NAG	O5-C1-C2	-3.66	105.62	111.29
4	T	5	MAN	C1-O5-C5	3.62	117.03	112.19
9	j	2	NAG	C4-C3-C2	-3.58	105.77	111.02
4	o	3	BMA	O5-C5-C6	-3.55	100.76	107.66
6	z	2	NAG	C2-N2-C7	3.54	127.64	122.90
9	Y	4	MAN	C1-O5-C5	3.52	116.90	112.19
6	P	2	NAG	C2-N2-C7	3.48	127.57	122.90
6	g	2	NAG	C4-C3-C2	-3.45	105.96	111.02
6	I	1	NAG	C1-O5-C5	3.43	116.78	112.19
9	t	3	BMA	C3-C4-C5	3.42	116.44	110.23
9	j	3	BMA	C3-C4-C5	3.41	116.42	110.23
5	r	2	NAG	C1-O5-C5	3.39	116.74	112.19
6	Z	1	NAG	C2-N2-C7	3.39	127.45	122.90
7	S	3	BMA	C3-C4-C5	3.39	116.37	110.23
6	M	2	NAG	C2-N2-C7	3.38	127.42	122.90
6	J	1	NAG	O4-C4-C3	-3.37	102.43	110.38
7	U	3	BMA	C3-C4-C5	3.37	116.34	110.23
4	k	2	NAG	O5-C1-C2	-3.35	106.11	111.29
4	V	3	BMA	C3-C4-C5	3.33	116.27	110.23
4	3	2	NAG	C2-N2-C7	3.32	127.35	122.90
5	r	3	BMA	C3-C4-C5	3.32	116.25	110.23
5	F	1	NAG	C4-C3-C2	-3.31	106.17	111.02
7	S	4	MAN	C1-O5-C5	3.31	116.62	112.19
7	0	3	BMA	C3-C4-C5	3.29	116.20	110.23
4	o	3	BMA	C3-C4-C5	3.26	116.14	110.23
4	V	2	NAG	O5-C1-C2	-3.25	106.26	111.29
4	D	4	MAN	C1-O5-C5	3.25	116.54	112.19
4	k	3	BMA	C3-C4-C5	3.24	116.11	110.23
4	T	3	BMA	C3-C4-C5	3.24	116.10	110.23
5	v	3	BMA	C3-C4-C5	3.22	116.07	110.23
7	S	3	BMA	C2-C3-C4	3.21	116.52	110.86
6	d	1	NAG	C4-C3-C2	-3.19	106.35	111.02
5	c	3	BMA	C3-C4-C5	3.19	116.01	110.23
4	o	3	BMA	O4-C4-C5	-3.18	101.48	109.32
8	X	5	MAN	C1-O5-C5	3.18	116.45	112.19
6	d	1	NAG	O5-C1-C2	-3.18	106.37	111.29
4	1	2	NAG	C2-N2-C7	3.15	127.12	122.90
5	b	3	BMA	C3-C4-C5	3.14	115.93	110.23
7	l	3	BMA	C3-C4-C5	3.12	115.89	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	q	1	NAG	C2-N2-C7	3.12	127.08	122.90
4	o	3	BMA	O4-C4-C3	-3.11	103.04	110.38
6	J	1	NAG	C2-N2-C7	3.11	127.07	122.90
5	E	1	NAG	C1-O5-C5	3.11	116.35	112.19
6	4	1	NAG	O5-C1-C2	3.11	116.10	111.29
6	P	2	NAG	C1-O5-C5	3.07	116.30	112.19
5	m	3	BMA	C3-C4-C5	3.04	115.73	110.23
5	c	2	NAG	C4-C3-C2	-3.03	106.58	111.02
6	N	2	NAG	C2-N2-C7	3.01	126.93	122.90
9	t	3	BMA	O5-C5-C4	3.01	118.14	110.83
4	k	3	BMA	C2-C3-C4	3.00	116.14	110.86
6	d	2	NAG	C1-O5-C5	2.99	116.19	112.19
6	I	2	NAG	C2-N2-C7	2.99	126.90	122.90
6	f	1	NAG	C2-N2-C7	2.99	126.90	122.90
4	k	5	MAN	C1-O5-C5	2.98	116.18	112.19
5	E	3	BMA	C3-C4-C5	2.97	115.62	110.23
4	D	3	BMA	O4-C4-C3	-2.97	103.38	110.38
9	t	3	BMA	C1-C2-C3	2.96	113.96	109.64
6	g	2	NAG	C2-N2-C7	2.96	126.86	122.90
6	Q	1	NAG	O5-C1-C2	-2.95	106.72	111.29
6	w	2	NAG	C4-C3-C2	-2.95	106.69	111.02
7	2	3	BMA	C3-C4-C5	2.94	115.57	110.23
4	1	3	BMA	O3-C3-C4	2.94	117.31	110.38
5	v	1	NAG	C2-N2-C7	2.93	126.83	122.90
6	f	2	NAG	C1-O5-C5	2.93	116.11	112.19
6	g	1	NAG	C3-C4-C5	-2.92	104.94	110.23
4	k	1	NAG	C2-N2-C7	2.92	126.81	122.90
5	m	2	NAG	C2-N2-C7	2.92	126.81	122.90
8	X	3	BMA	C3-C4-C5	2.92	115.52	110.23
6	f	2	NAG	C2-N2-C7	2.92	126.81	122.90
4	T	2	NAG	C1-O5-C5	2.91	116.09	112.19
8	X	3	BMA	O4-C4-C3	-2.90	103.54	110.38
6	u	1	NAG	C4-C3-C2	-2.90	106.77	111.02
6	p	1	NAG	C4-C3-C2	-2.89	106.78	111.02
6	s	2	NAG	C1-C2-N2	2.88	114.97	110.43
6	g	2	NAG	C1-O5-C5	2.87	116.04	112.19
6	4	1	NAG	O5-C5-C4	2.86	117.78	110.83
5	r	1	NAG	O5-C1-C2	-2.84	106.90	111.29
5	W	3	BMA	C2-C3-C4	2.84	115.85	110.86
6	e	1	NAG	O5-C1-C2	-2.84	106.90	111.29
7	2	3	BMA	C2-C3-C4	2.84	115.85	110.86
6	Z	2	NAG	O5-C1-C2	-2.83	106.91	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	2	NAG	C1-C2-N2	2.83	114.89	110.43
7	0	3	BMA	C2-C3-C4	2.83	115.84	110.86
5	c	3	BMA	C2-C3-C4	2.82	115.82	110.86
4	T	3	BMA	C2-C3-C4	2.80	115.79	110.86
4	D	1	NAG	O5-C1-C2	-2.80	106.95	111.29
4	1	1	NAG	C2-N2-C7	2.80	126.65	122.90
6	Z	2	NAG	C2-N2-C7	2.80	126.65	122.90
9	j	3	BMA	C2-C3-C4	2.79	115.77	110.86
5	v	3	BMA	C2-C3-C4	2.78	115.74	110.86
5	F	3	BMA	C3-C4-C5	2.77	115.25	110.23
5	m	2	NAG	O5-C1-C2	-2.76	107.02	111.29
4	D	1	NAG	C4-C3-C2	-2.75	106.99	111.02
7	l	1	NAG	C3-C4-C5	-2.75	105.25	110.23
7	0	4	MAN	C1-O5-C5	2.74	115.86	112.19
7	U	1	NAG	C1-O5-C5	2.74	115.86	112.19
5	E	3	BMA	C2-C3-C4	2.74	115.68	110.86
4	k	3	BMA	O4-C4-C3	-2.73	103.94	110.38
4	T	4	MAN	C1-C2-C3	2.73	113.62	109.64
5	W	3	BMA	C3-C4-C5	2.72	115.17	110.23
5	b	3	BMA	C2-C3-C4	2.71	115.62	110.86
5	v	2	NAG	C2-N2-C7	2.69	126.51	122.90
7	2	4	MAN	C1-O5-C5	2.69	115.79	112.19
6	w	2	NAG	C1-O5-C5	2.68	115.78	112.19
4	V	3	BMA	O5-C5-C4	2.67	117.33	110.83
7	l	3	BMA	O5-C5-C4	2.67	117.33	110.83
5	b	1	NAG	C2-N2-C7	2.67	126.48	122.90
5	b	3	BMA	O3-C3-C2	-2.65	104.64	110.05
4	1	1	NAG	C1-O5-C5	-2.65	108.63	112.19
9	j	1	NAG	O5-C1-C2	-2.64	107.21	111.29
4	3	5	MAN	C1-O5-C5	2.62	115.70	112.19
4	V	1	NAG	C1-O5-C5	2.61	115.69	112.19
4	3	2	NAG	O5-C1-C2	-2.60	107.27	111.29
9	Y	3	BMA	O4-C4-C3	-2.60	104.24	110.38
7	l	3	BMA	C2-C3-C4	2.59	115.41	110.86
5	m	3	BMA	C2-C3-C4	2.58	115.40	110.86
6	G	1	NAG	C1-O5-C5	2.57	115.64	112.19
7	l	3	BMA	O3-C3-C2	-2.57	104.82	110.05
7	l	1	NAG	O5-C5-C4	-2.56	104.59	110.83
4	1	1	NAG	O4-C4-C3	-2.56	104.35	110.38
6	e	1	NAG	C2-N2-C7	2.55	126.32	122.90
6	M	2	NAG	O5-C1-C2	-2.55	107.34	111.29
5	m	3	BMA	O5-C5-C4	2.55	117.02	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	m	3	BMA	O3-C3-C2	-2.55	104.86	110.05
7	S	3	BMA	O3-C3-C2	-2.54	104.87	110.05
4	V	4	MAN	C1-C2-C3	2.54	113.34	109.64
9	j	3	BMA	O4-C4-C3	-2.54	104.39	110.38
6	x	1	NAG	C4-C3-C2	-2.52	107.32	111.02
7	l	3	BMA	O4-C4-C3	-2.51	104.46	110.38
7	U	3	BMA	C2-C3-C4	2.51	115.27	110.86
5	c	3	BMA	O3-C3-C2	-2.49	104.96	110.05
5	r	3	BMA	C2-C3-C4	2.49	115.25	110.86
4	k	1	NAG	O4-C4-C3	-2.49	104.50	110.38
6	n	1	NAG	C4-C3-C2	-2.49	107.36	111.02
4	1	2	NAG	O5-C1-C2	-2.49	107.44	111.29
4	T	3	BMA	O5-C5-C4	2.49	116.87	110.83
7	0	3	BMA	O3-C3-C2	-2.48	105.00	110.05
7	U	3	BMA	O5-C5-C4	2.47	116.83	110.83
7	0	3	BMA	O5-C5-C4	2.46	116.82	110.83
9	Y	3	BMA	O5-C5-C4	2.46	116.82	110.83
4	T	2	NAG	O5-C1-C2	-2.46	107.49	111.29
5	v	3	BMA	O3-C3-C2	-2.45	105.05	110.05
4	3	1	NAG	C1-O5-C5	2.45	115.47	112.19
7	l	3	BMA	C1-C2-C3	2.45	113.21	109.64
4	V	1	NAG	O4-C4-C3	-2.45	104.61	110.38
4	1	3	BMA	O4-C4-C3	-2.45	104.61	110.38
4	k	2	NAG	C1-O5-C5	2.44	115.46	112.19
5	F	3	BMA	O4-C4-C3	-2.44	104.62	110.38
6	Z	1	NAG	C3-C4-C5	-2.44	105.81	110.23
7	0	1	NAG	C1-O5-C5	2.42	115.43	112.19
4	D	4	MAN	C1-C2-C3	2.42	113.17	109.64
4	o	1	NAG	C4-C3-C2	-2.42	107.48	111.02
5	r	3	BMA	O5-C5-C4	2.41	116.70	110.83
9	t	1	NAG	C2-N2-C7	2.41	126.13	122.90
7	S	3	BMA	C1-C2-C3	2.41	113.15	109.64
7	U	2	NAG	C1-O5-C5	2.41	115.41	112.19
4	o	2	NAG	C1-O5-C5	2.40	115.40	112.19
7	l	1	NAG	C2-N2-C7	2.39	126.11	122.90
5	F	3	BMA	C2-C3-C4	2.39	115.07	110.86
5	F	3	BMA	C1-C2-C3	2.39	113.12	109.64
9	j	3	BMA	O3-C3-C2	-2.39	105.18	110.05
4	T	3	BMA	O4-C4-C3	-2.38	104.75	110.38
9	t	3	BMA	C2-C3-C4	2.38	115.05	110.86
9	Y	1	NAG	O4-C4-C3	-2.38	104.77	110.38
5	m	3	BMA	C1-C2-C3	2.37	113.10	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	2	NAG	C1-O5-C5	2.37	115.36	112.19
4	V	3	BMA	O4-C4-C3	-2.36	104.81	110.38
6	q	2	NAG	O5-C1-C2	-2.36	107.64	111.29
4	3	3	BMA	O5-C5-C4	2.35	116.55	110.83
7	0	1	NAG	C2-N2-C7	2.35	126.05	122.90
6	g	1	NAG	C6-C5-C4	2.35	118.79	113.02
7	2	3	BMA	O3-C3-C2	-2.35	105.26	110.05
9	t	1	NAG	O5-C1-C2	-2.34	107.66	111.29
7	U	1	NAG	C3-C4-C5	-2.34	105.98	110.23
6	J	2	NAG	O5-C1-C2	-2.34	107.67	111.29
4	k	3	BMA	O5-C5-C4	2.34	116.51	110.83
5	m	1	NAG	O4-C4-C3	-2.33	104.87	110.38
4	k	4	MAN	C1-O5-C5	2.33	115.31	112.19
5	m	1	NAG	C2-N2-C7	2.32	126.00	122.90
6	G	1	NAG	C4-C3-C2	-2.31	107.63	111.02
5	b	1	NAG	C1-O5-C5	2.30	115.27	112.19
4	k	1	NAG	C3-C4-C5	-2.30	106.06	110.23
6	K	1	NAG	O5-C1-C2	-2.30	107.73	111.29
5	E	3	BMA	O4-C4-C3	-2.30	104.96	110.38
4	1	3	BMA	O2-C2-C3	2.30	114.91	110.15
8	X	1	NAG	C1-O5-C5	2.29	115.26	112.19
9	t	4	MAN	C1-C2-C3	2.29	112.98	109.64
5	r	3	BMA	O4-C4-C3	-2.28	105.00	110.38
5	v	3	BMA	O4-C4-C3	-2.28	105.00	110.38
6	N	1	NAG	C3-C4-C5	-2.28	106.10	110.23
7	U	1	NAG	O4-C4-C3	-2.28	105.01	110.38
8	X	1	NAG	C3-C4-C5	-2.27	106.11	110.23
5	v	3	BMA	O5-C5-C4	2.27	116.34	110.83
4	V	3	BMA	C2-C3-C4	2.27	114.85	110.86
7	2	3	BMA	O4-C4-C3	-2.27	105.03	110.38
5	W	3	BMA	O3-C3-C2	-2.27	105.43	110.05
4	o	2	NAG	C1-C2-N2	2.26	114.00	110.43
7	U	3	BMA	O4-C4-C3	-2.26	105.04	110.38
7	l	2	NAG	C1-O5-C5	2.25	115.20	112.19
5	W	3	BMA	C1-C2-C3	2.25	112.92	109.64
7	0	3	BMA	C1-C2-C3	2.25	112.92	109.64
5	E	3	BMA	O3-C3-C2	-2.25	105.47	110.05
5	r	2	NAG	C2-N2-C7	2.25	125.91	122.90
7	0	3	BMA	O4-C4-C3	-2.24	105.10	110.38
9	Y	3	BMA	C2-C3-C4	2.23	114.79	110.86
7	S	3	BMA	O4-C4-C3	-2.23	105.11	110.38
4	1	3	BMA	O5-C5-C4	2.23	116.25	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	g	2	NAG	C1-C2-N2	2.23	113.95	110.43
4	3	1	NAG	C2-N2-C7	2.23	125.89	122.90
6	J	1	NAG	O5-C1-C2	-2.22	107.85	111.29
7	2	3	BMA	O5-C5-C4	2.22	116.22	110.83
5	W	3	BMA	O4-C4-C3	-2.21	105.17	110.38
5	b	3	BMA	O4-C4-C3	-2.21	105.17	110.38
6	i	1	NAG	C2-N2-C7	2.20	125.85	122.90
5	r	1	NAG	O4-C4-C3	-2.20	105.19	110.38
6	w	2	NAG	O7-C7-N2	2.20	125.87	121.98
5	m	3	BMA	O4-C4-C3	-2.20	105.20	110.38
6	I	2	NAG	C1-O5-C5	2.19	115.12	112.19
6	y	2	NAG	C1-O5-C5	2.19	115.11	112.19
4	V	3	BMA	O3-C3-C4	2.18	115.53	110.38
4	T	2	NAG	C4-C3-C2	-2.18	107.82	111.02
5	c	3	BMA	O5-C5-C4	2.18	116.14	110.83
5	c	3	BMA	O4-C4-C3	-2.18	105.24	110.38
4	D	3	BMA	C3-C4-C5	2.17	114.17	110.23
6	M	2	NAG	C4-C3-C2	-2.17	107.84	111.02
4	D	1	NAG	C1-C2-N2	2.17	113.85	110.43
9	j	2	NAG	C1-O5-C5	2.16	115.08	112.19
7	2	3	BMA	C1-C2-C3	2.16	112.79	109.64
5	E	2	NAG	O7-C7-N2	2.16	125.80	121.98
4	V	4	MAN	C1-O5-C5	2.16	115.08	112.19
7	S	2	NAG	C1-O5-C5	2.15	115.07	112.19
4	3	3	BMA	C3-C4-C5	2.15	114.14	110.23
6	n	1	NAG	C2-N2-C7	2.14	125.77	122.90
5	F	2	NAG	O4-C4-C3	-2.14	105.33	110.38
7	l	1	NAG	O4-C4-C5	2.13	114.58	109.32
6	y	1	NAG	O5-C1-C2	-2.13	108.00	111.29
6	Q	1	NAG	C2-N2-C7	2.13	125.75	122.90
6	N	2	NAG	C4-C3-C2	-2.13	107.90	111.02
6	G	2	NAG	C1-O5-C5	2.12	115.03	112.19
7	S	3	BMA	O5-C5-C4	2.12	115.98	110.83
7	0	2	NAG	C1-O5-C5	2.12	115.02	112.19
5	F	3	BMA	O3-C3-C2	-2.11	105.75	110.05
5	F	1	NAG	C1-O5-C5	2.11	115.01	112.19
4	1	3	BMA	C3-C4-C5	2.10	114.04	110.23
4	3	3	BMA	O4-C4-C3	-2.10	105.44	110.38
5	b	3	BMA	O5-C5-C4	2.10	115.93	110.83
7	l	4	MAN	C1-O5-C5	2.09	114.99	112.19
6	s	2	NAG	C4-C3-C2	-2.09	107.96	111.02
9	t	2	NAG	O4-C4-C3	-2.09	105.46	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	2	NAG	O5-C1-C2	-2.08	108.07	111.29
7	U	3	BMA	O3-C3-C2	-2.07	105.83	110.05
4	D	2	NAG	C4-C3-C2	-2.07	107.99	111.02
6	e	1	NAG	C1-O5-C5	2.07	114.96	112.19
6	O	2	NAG	C1-O5-C5	2.06	114.95	112.19
5	F	3	BMA	O5-C5-C4	2.06	115.84	110.83
5	v	3	BMA	C1-C2-C3	2.06	112.64	109.64
6	Z	1	NAG	C4-C3-C2	2.05	114.02	111.02
6	Q	1	NAG	O5-C5-C4	-2.04	105.86	110.83
6	h	1	NAG	C2-N2-C7	2.04	125.63	122.90
7	2	1	NAG	O4-C4-C3	-2.04	105.57	110.38
8	X	3	BMA	C6-C5-C4	-2.04	108.02	113.02
6	i	1	NAG	O4-C4-C3	-2.03	105.58	110.38
6	i	2	NAG	C2-N2-C7	2.03	125.62	122.90
7	l	1	NAG	C6-C5-C4	2.03	118.00	113.02
6	h	2	NAG	C2-N2-C7	2.02	125.60	122.90
7	S	2	NAG	C4-C3-C2	-2.01	108.07	111.02
9	j	3	BMA	O5-C5-C4	2.01	115.71	110.83

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C1-C2-N2-C7
6	d	1	NAG	C1-C2-N2-C7
6	s	2	NAG	C1-C2-N2-C7
6	w	2	NAG	C3-C2-N2-C7
4	o	1	NAG	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
7	S	4	MAN	O5-C5-C6-O6
4	o	5	MAN	O5-C5-C6-O6
5	v	3	BMA	O5-C5-C6-O6
4	V	3	BMA	C4-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
8	X	6	MAN	O5-C5-C6-O6
9	Y	4	MAN	O5-C5-C6-O6
4	o	1	NAG	C4-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
4	o	4	MAN	O5-C5-C6-O6
5	m	3	BMA	O5-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	3	3	BMA	C4-C5-C6-O6
6	4	1	NAG	O5-C5-C6-O6
4	T	3	BMA	O5-C5-C6-O6
6	f	1	NAG	O5-C5-C6-O6
4	3	5	MAN	O5-C5-C6-O6
4	o	2	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	n	1	NAG	O5-C5-C6-O6
6	g	2	NAG	C4-C5-C6-O6
7	S	4	MAN	C4-C5-C6-O6
9	j	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
8	X	4	MAN	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
8	X	5	MAN	O5-C5-C6-O6
4	T	5	MAN	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	s	2	NAG	O5-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
4	o	3	BMA	O5-C5-C6-O6
7	0	4	MAN	O5-C5-C6-O6
9	t	3	BMA	O5-C5-C6-O6
5	v	1	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
6	u	2	NAG	O5-C5-C6-O6
6	i	2	NAG	O5-C5-C6-O6
6	q	1	NAG	O5-C5-C6-O6
6	i	1	NAG	C3-C2-N2-C7
6	O	2	NAG	O5-C5-C6-O6
6	g	1	NAG	C4-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
4	o	5	MAN	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	1	2	NAG	C1-C2-N2-C7
5	F	2	NAG	C1-C2-N2-C7
5	m	2	NAG	C1-C2-N2-C7
5	v	2	NAG	C1-C2-N2-C7
6	M	2	NAG	C1-C2-N2-C7
6	a	1	NAG	C1-C2-N2-C7
6	g	2	NAG	C1-C2-N2-C7
6	q	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	z	2	NAG	C1-C2-N2-C7
6	4	1	NAG	C1-C2-N2-C7
6	O	1	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
9	Y	4	MAN	C4-C5-C6-O6
4	o	4	MAN	C4-C5-C6-O6
5	c	3	BMA	C4-C5-C6-O6
4	V	3	BMA	O5-C5-C6-O6
4	1	2	NAG	C3-C2-N2-C7
4	3	2	NAG	C3-C2-N2-C7
5	m	2	NAG	C3-C2-N2-C7
5	v	2	NAG	C3-C2-N2-C7
6	I	2	NAG	C3-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7
6	Z	2	NAG	C3-C2-N2-C7
6	f	2	NAG	C3-C2-N2-C7
6	4	1	NAG	C3-C2-N2-C7
6	Z	1	NAG	C4-C5-C6-O6
4	3	2	NAG	O5-C5-C6-O6
7	l	3	BMA	O5-C5-C6-O6
9	Y	2	NAG	O5-C5-C6-O6
9	j	4	MAN	O5-C5-C6-O6
6	I	2	NAG	C1-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
6	N	2	NAG	C1-C2-N2-C7
6	P	2	NAG	C1-C2-N2-C7
6	Z	2	NAG	C1-C2-N2-C7
6	f	2	NAG	C1-C2-N2-C7
6	i	2	NAG	C1-C2-N2-C7
6	f	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C3-C2-N2-C7
6	M	2	NAG	C3-C2-N2-C7
6	N	2	NAG	C3-C2-N2-C7
6	P	2	NAG	C3-C2-N2-C7
6	a	1	NAG	C3-C2-N2-C7
6	g	2	NAG	C3-C2-N2-C7
6	i	2	NAG	C3-C2-N2-C7
6	q	1	NAG	C3-C2-N2-C7
6	z	2	NAG	C3-C2-N2-C7
4	3	3	BMA	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6

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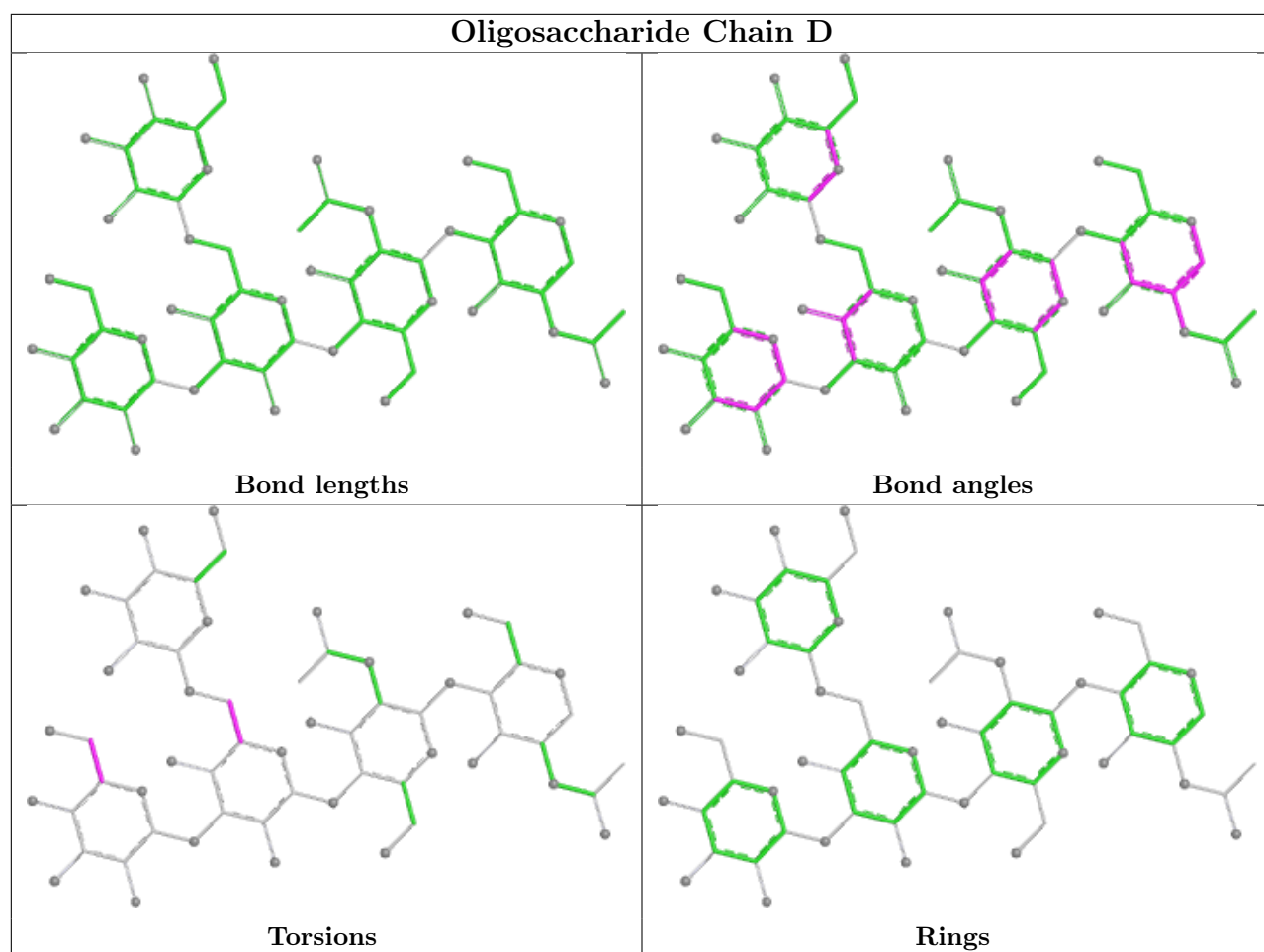
Mol	Chain	Res	Type	Atoms
6	K	1	NAG	C4-C5-C6-O6
4	o	2	NAG	C4-C5-C6-O6
7	l	2	NAG	C4-C5-C6-O6
5	v	2	NAG	O5-C5-C6-O6
8	X	6	MAN	C4-C5-C6-O6
4	3	5	MAN	C4-C5-C6-O6
7	S	3	BMA	O5-C5-C6-O6
4	1	5	MAN	O5-C5-C6-O6

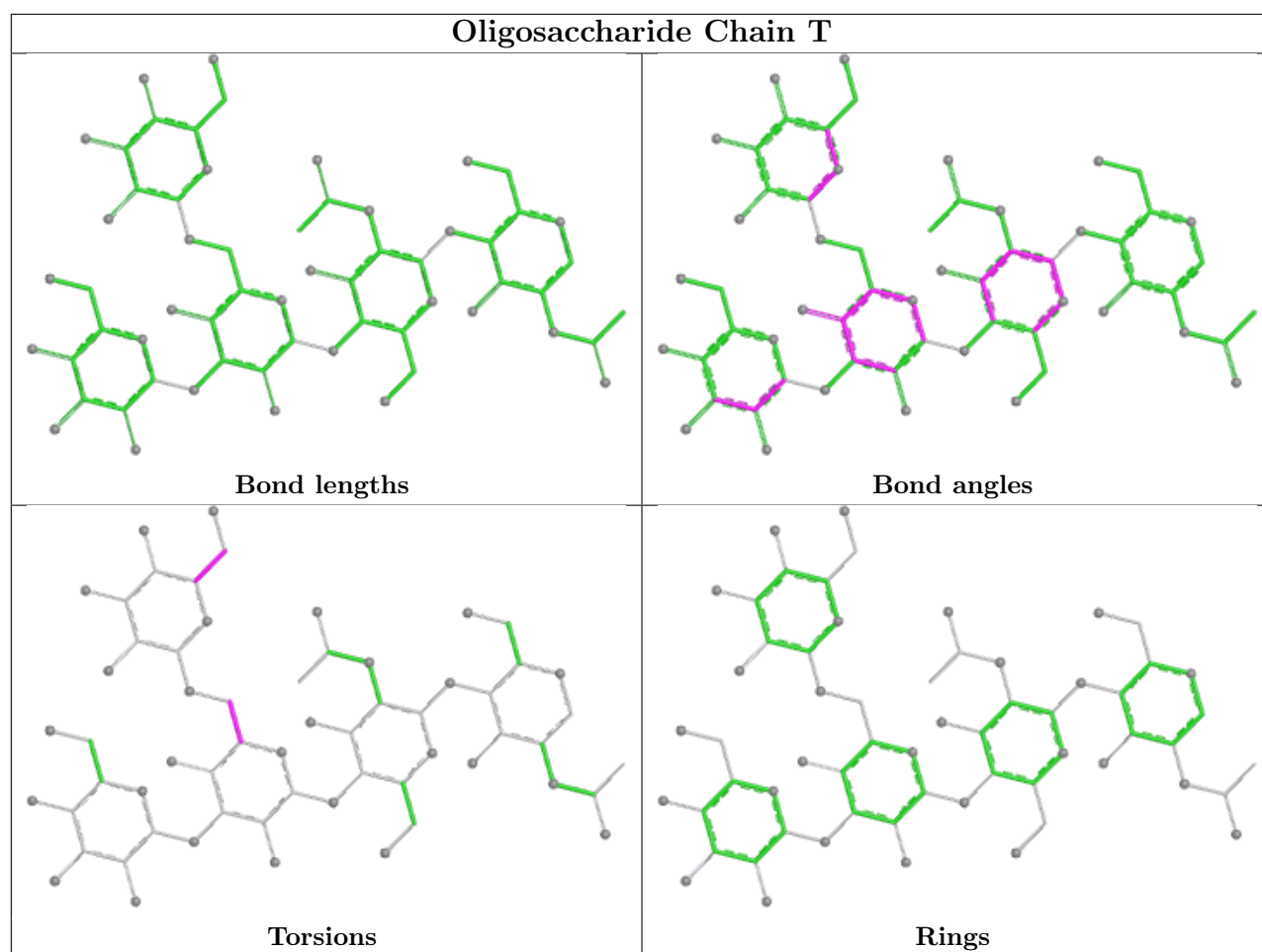
There are no ring outliers.

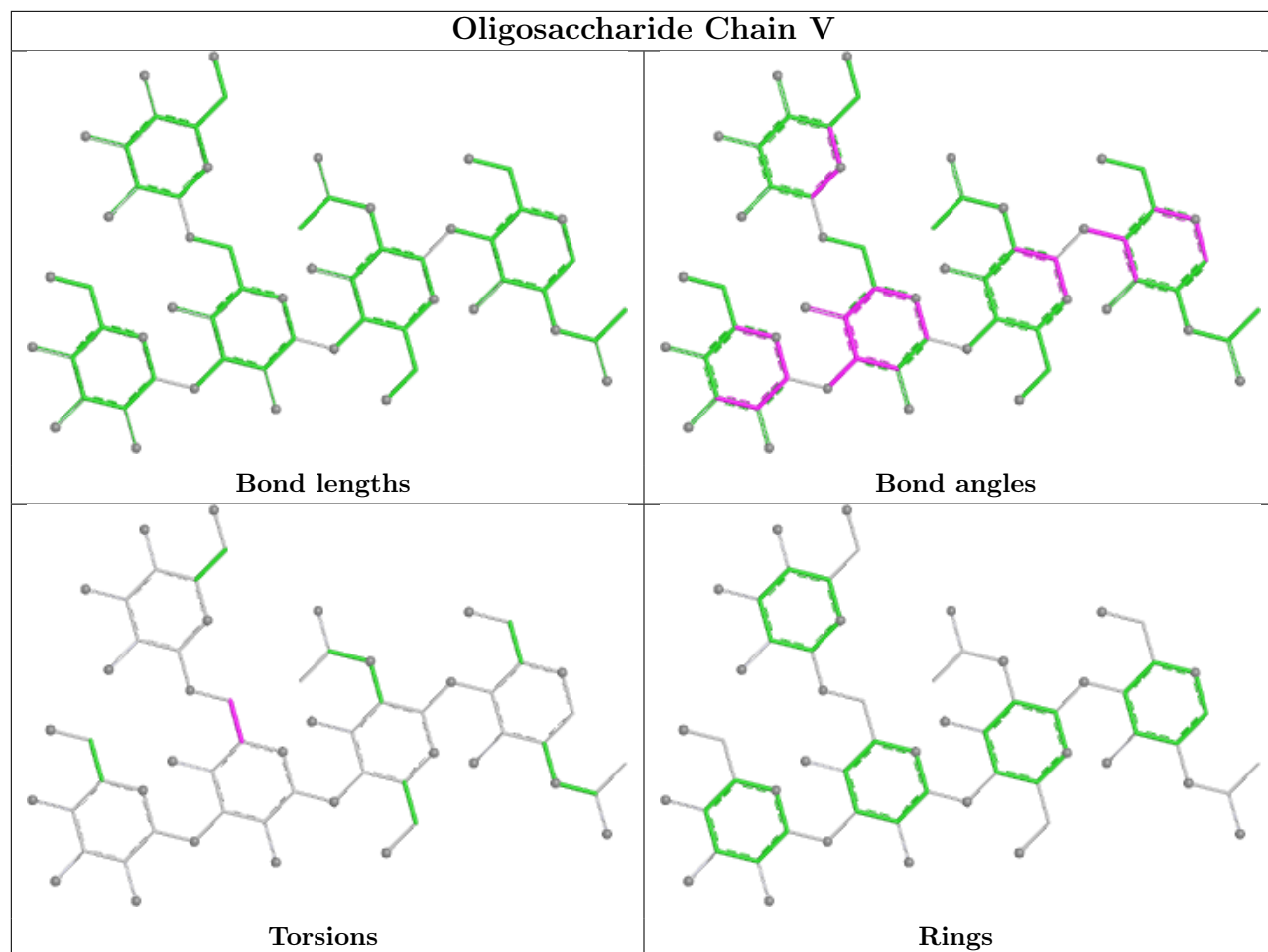
16 monomers are involved in 14 short contacts:

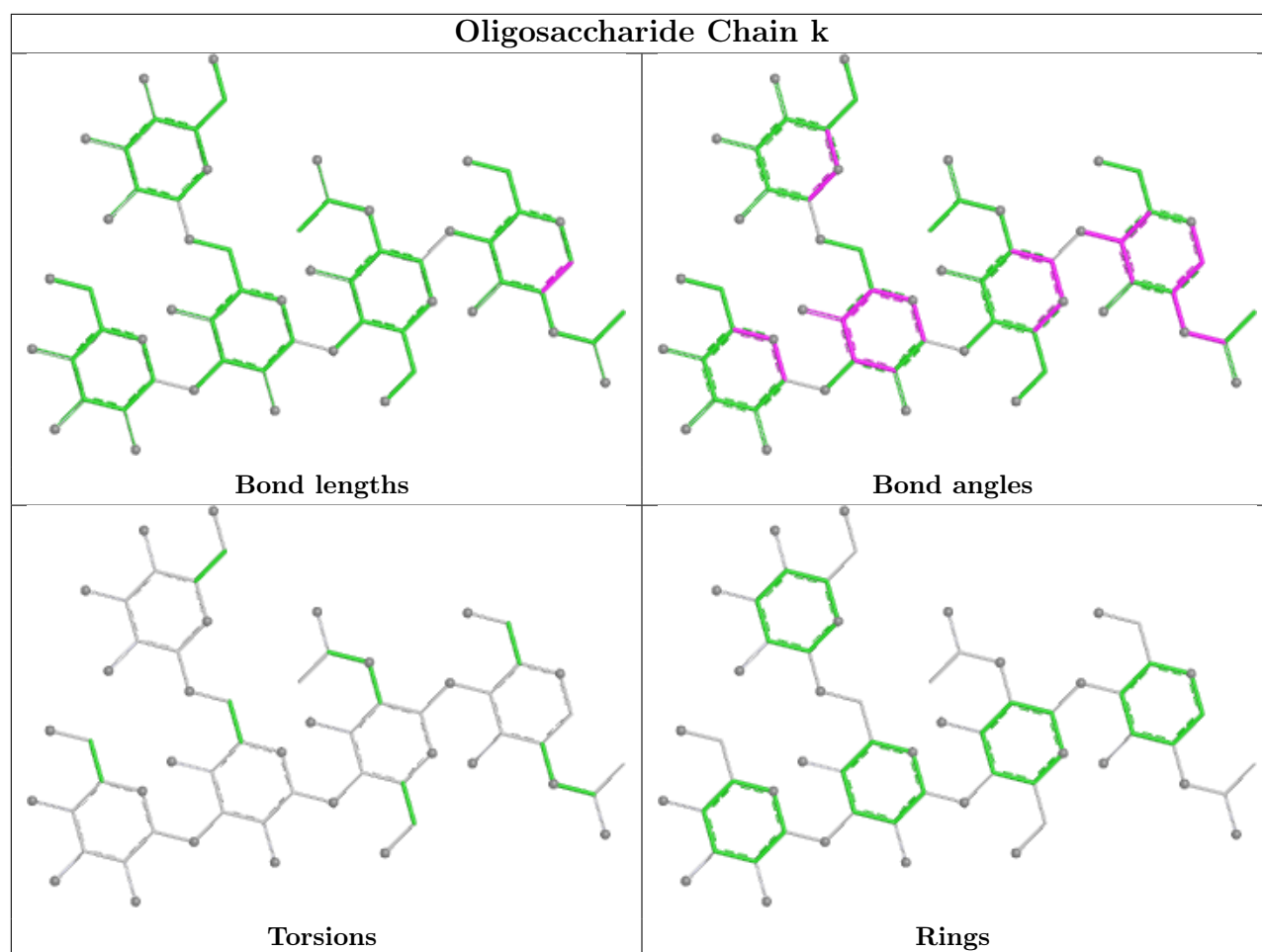
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	2	NAG	1	0
9	t	1	NAG	2	0
9	Y	1	NAG	1	0
6	d	1	NAG	1	0
6	4	1	NAG	1	0
5	F	2	NAG	1	0
6	q	1	NAG	1	0
4	V	3	BMA	1	0
6	y	1	NAG	1	0
6	i	1	NAG	1	0
5	r	2	NAG	1	0
6	4	2	NAG	1	0
4	3	1	NAG	1	0
6	d	2	NAG	1	0
4	V	5	MAN	1	0
5	c	1	NAG	1	0

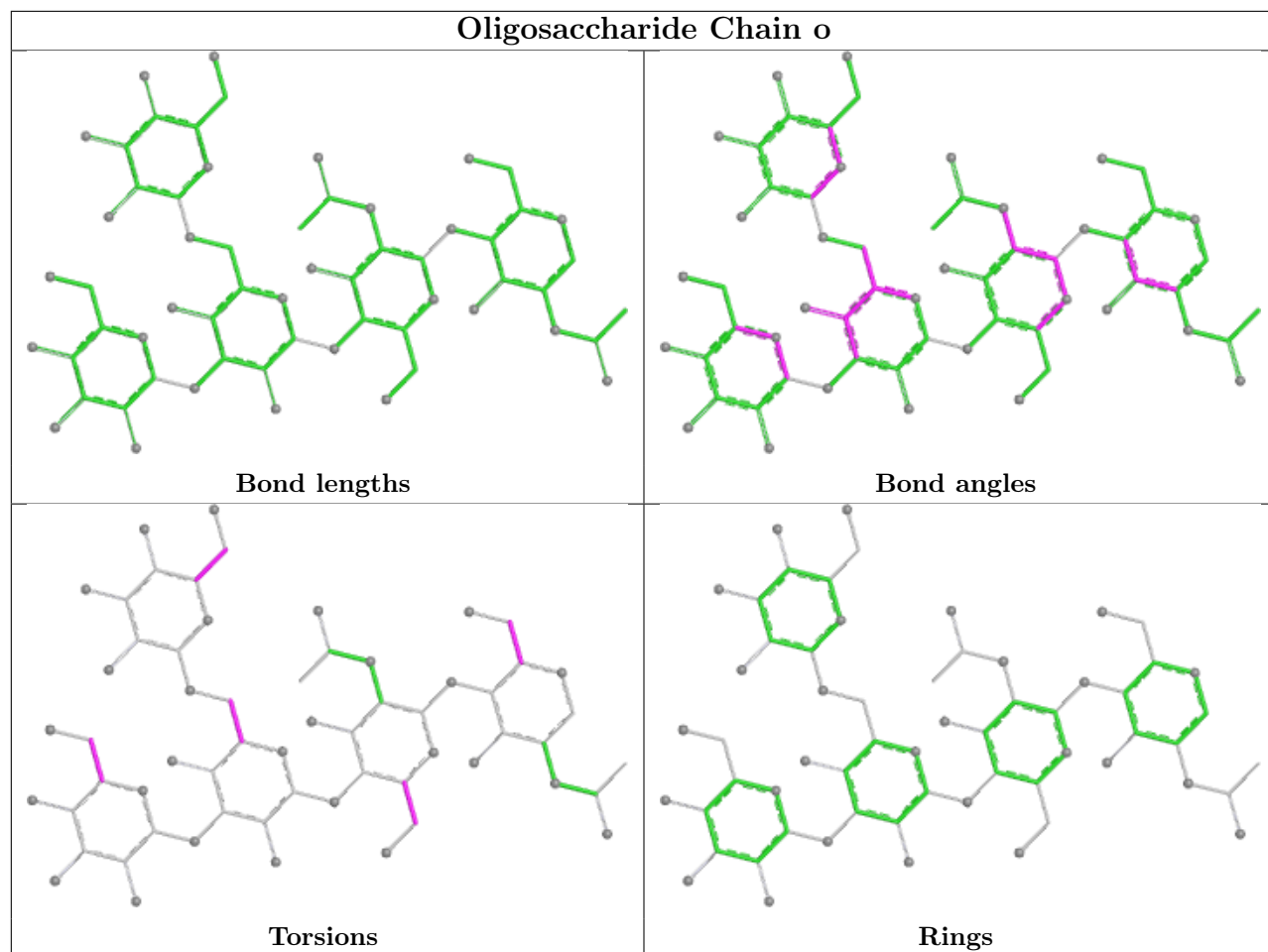
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

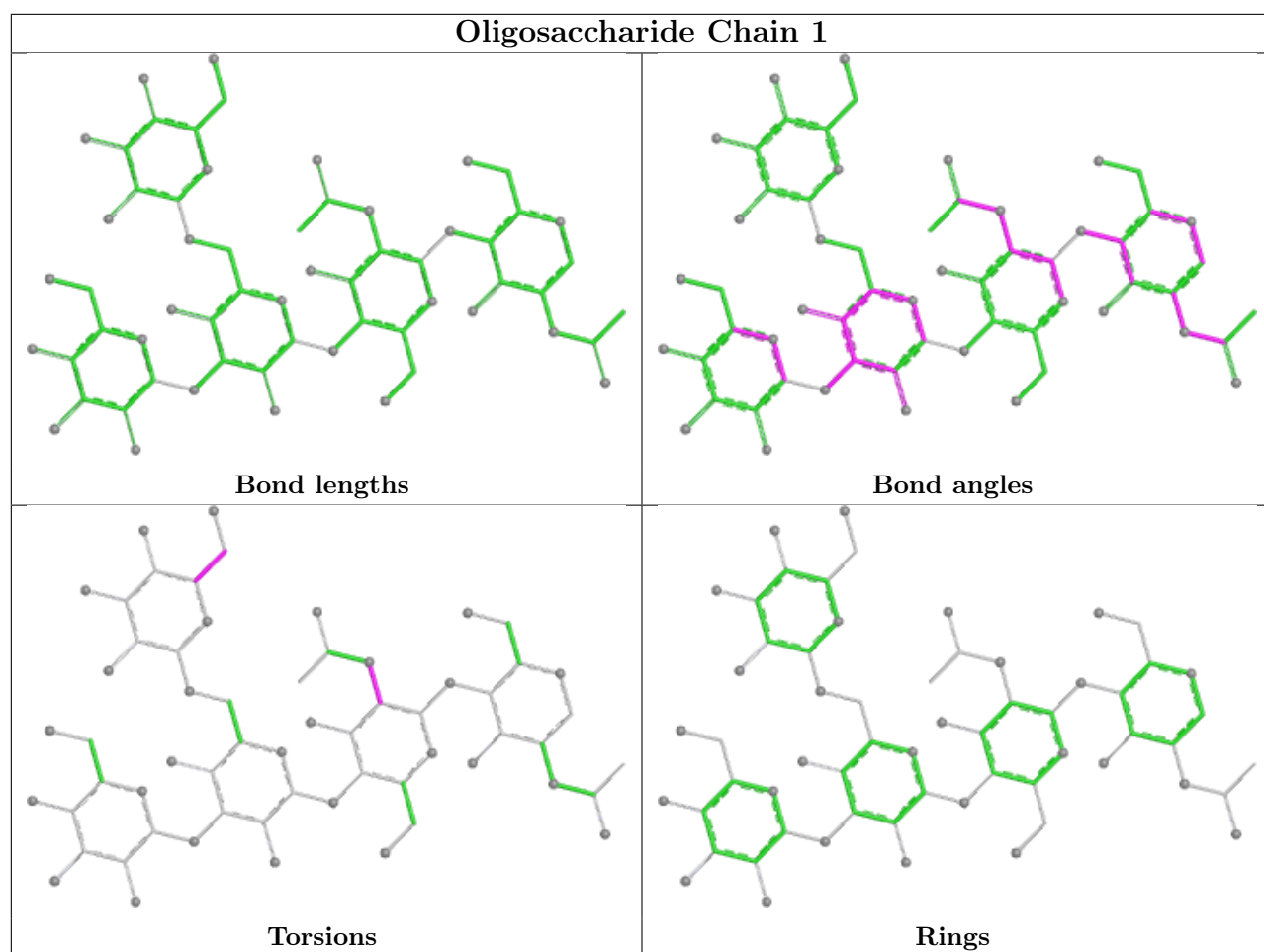




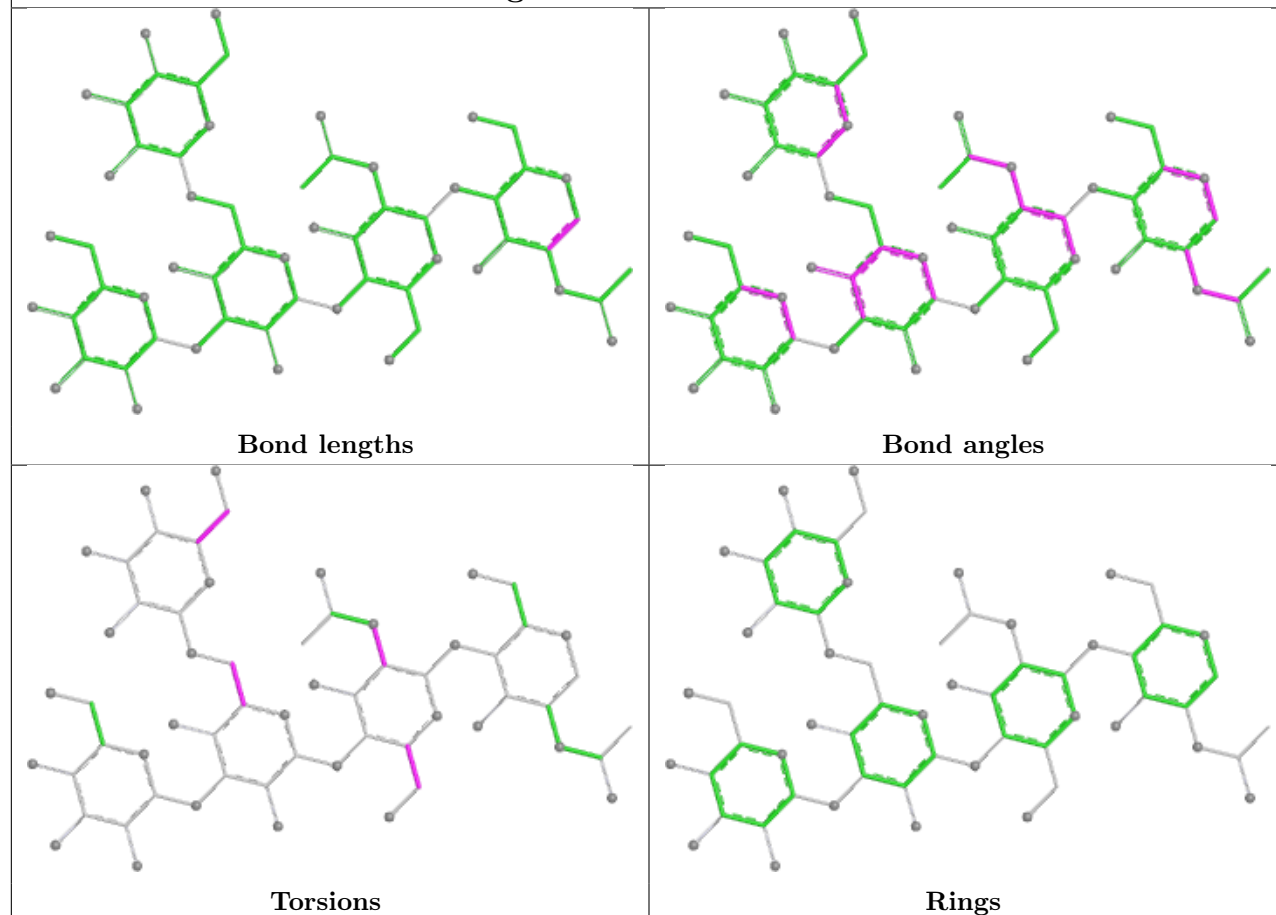




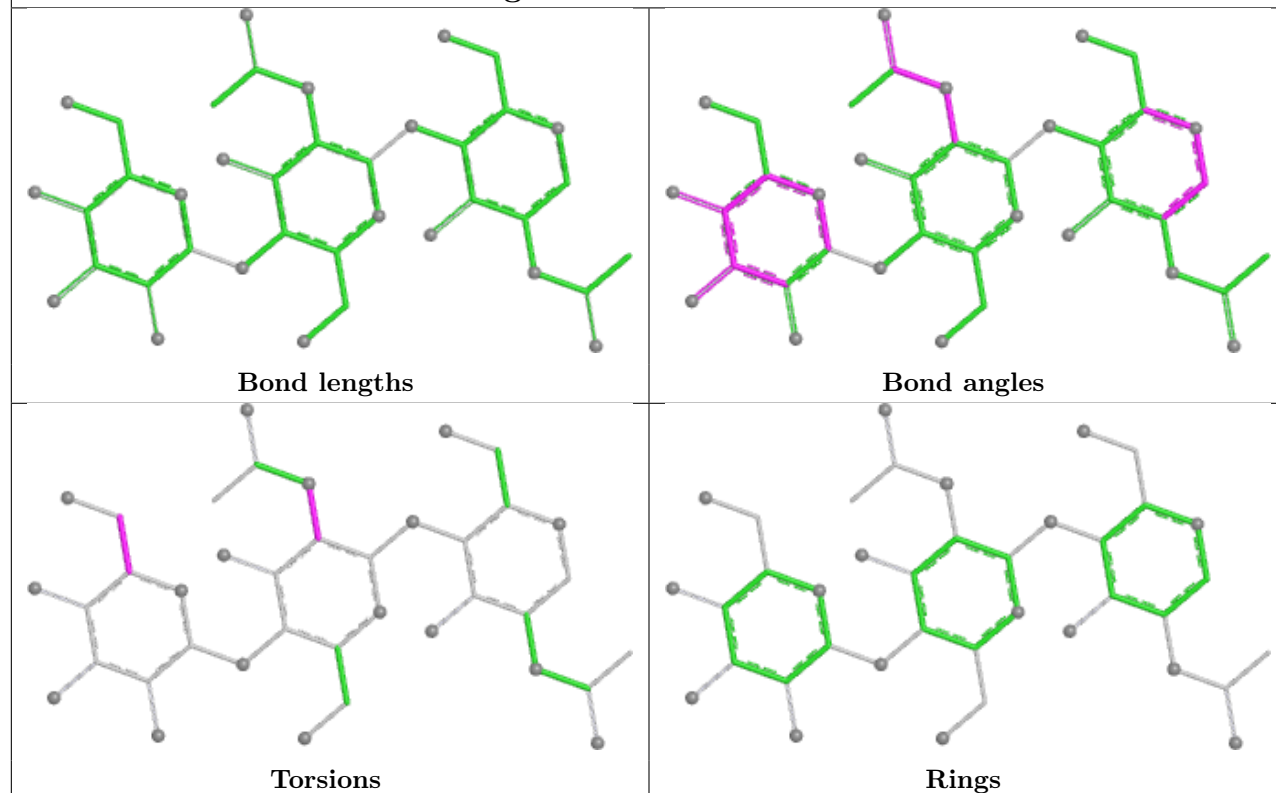


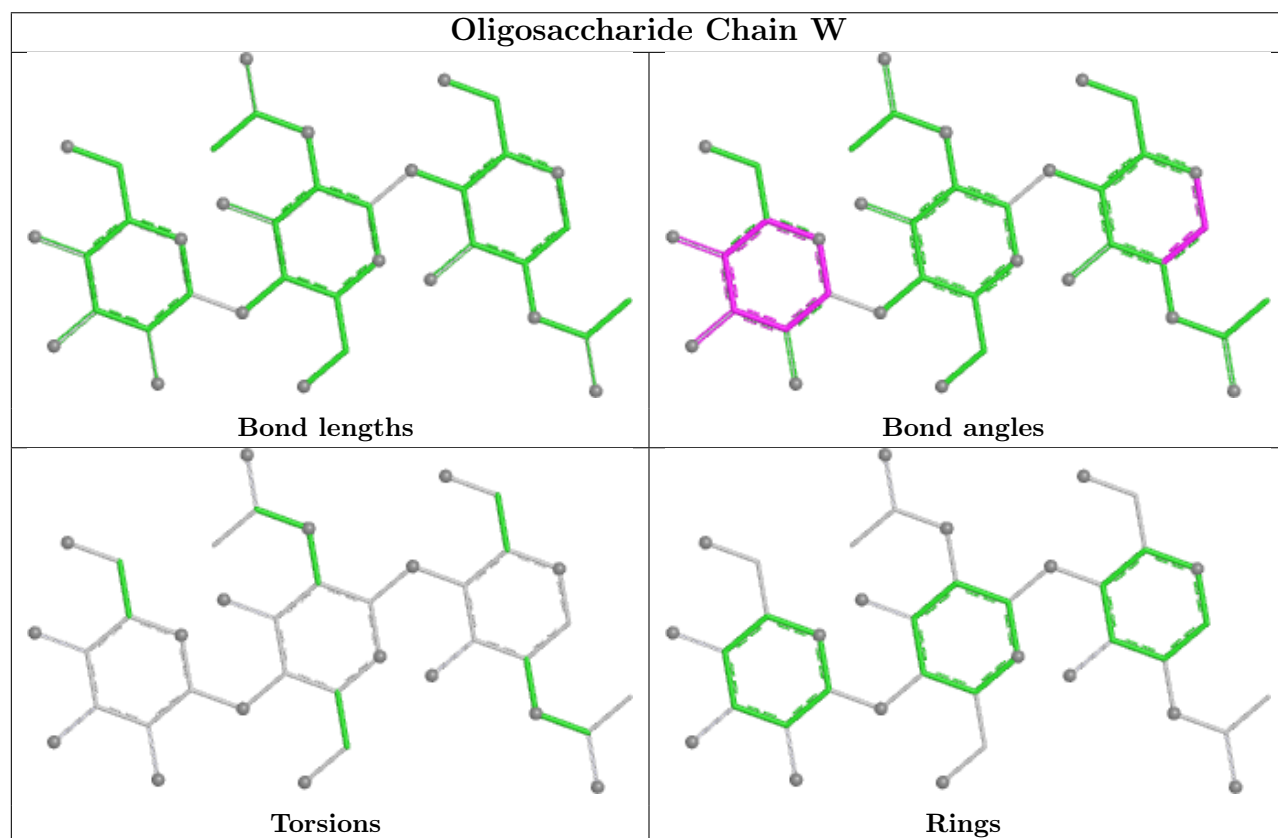
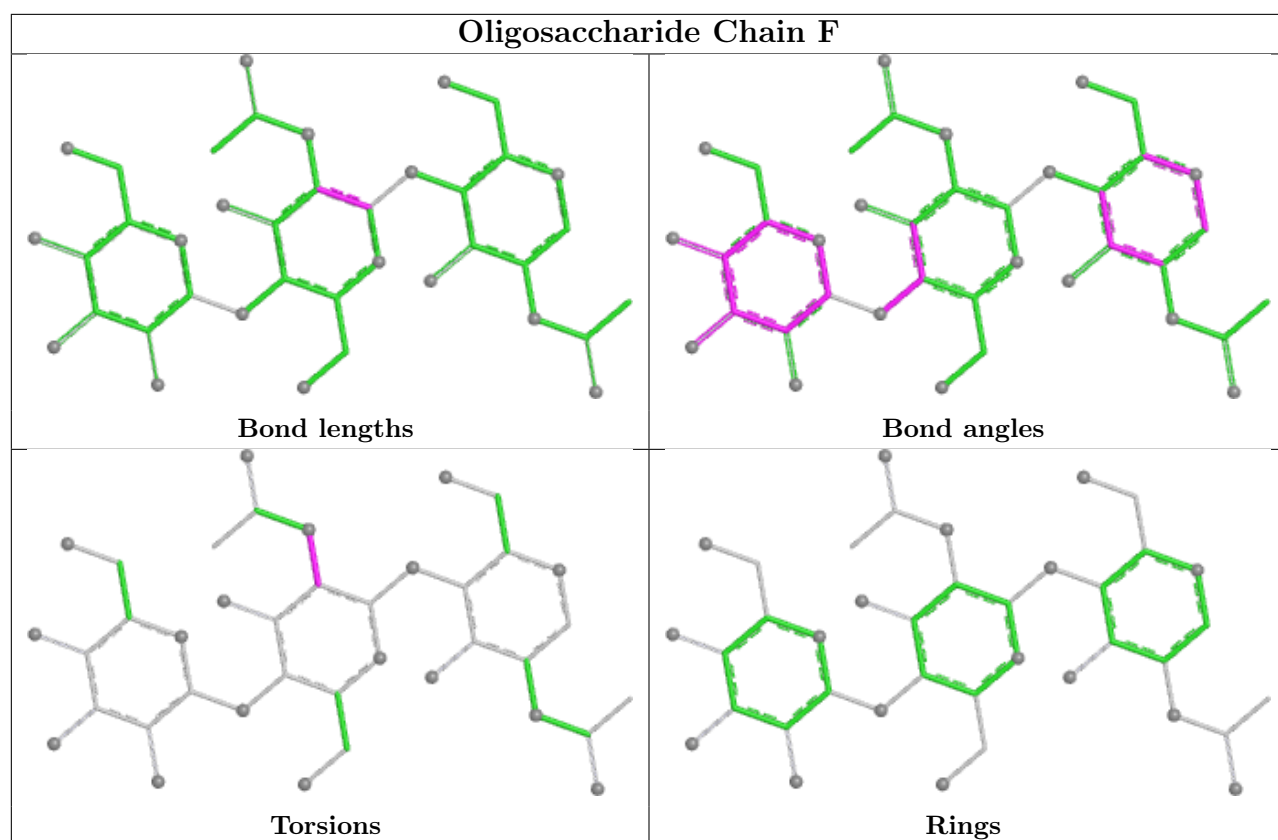


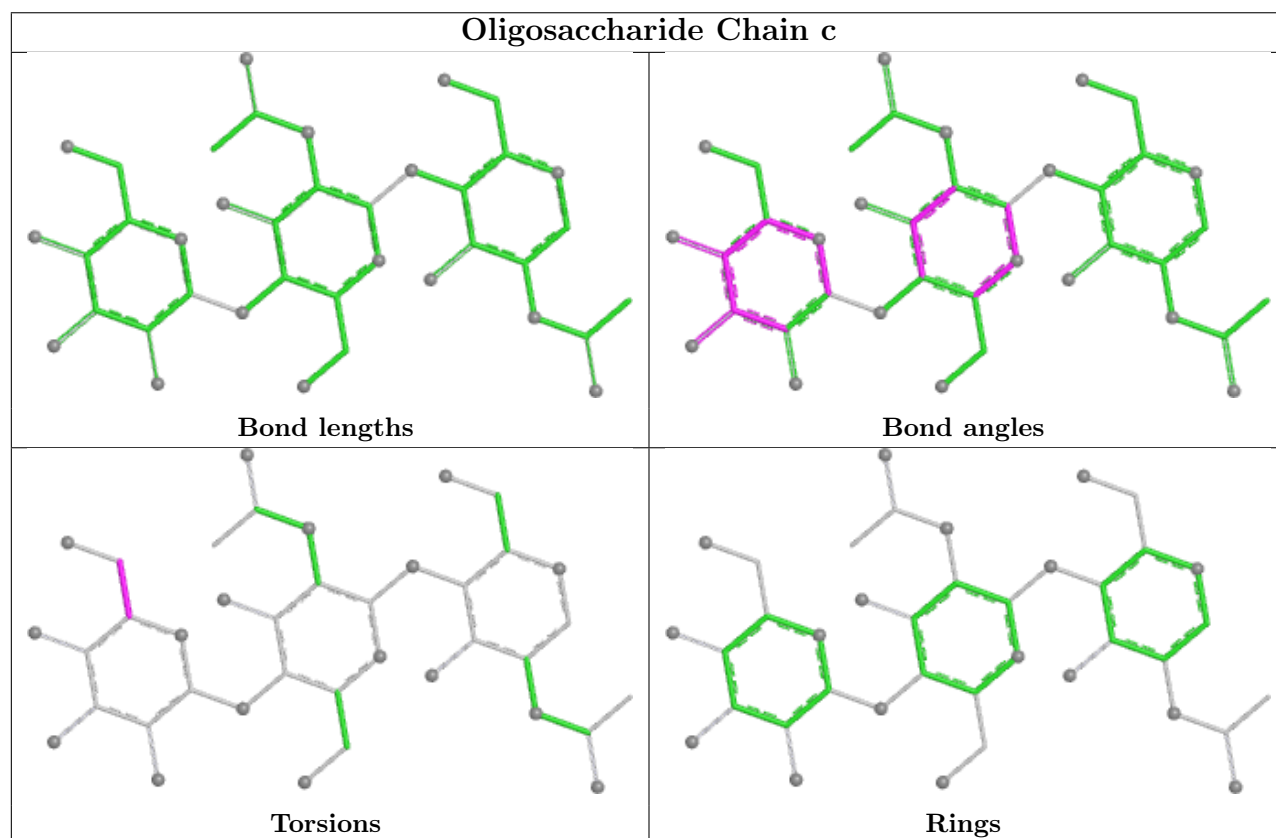
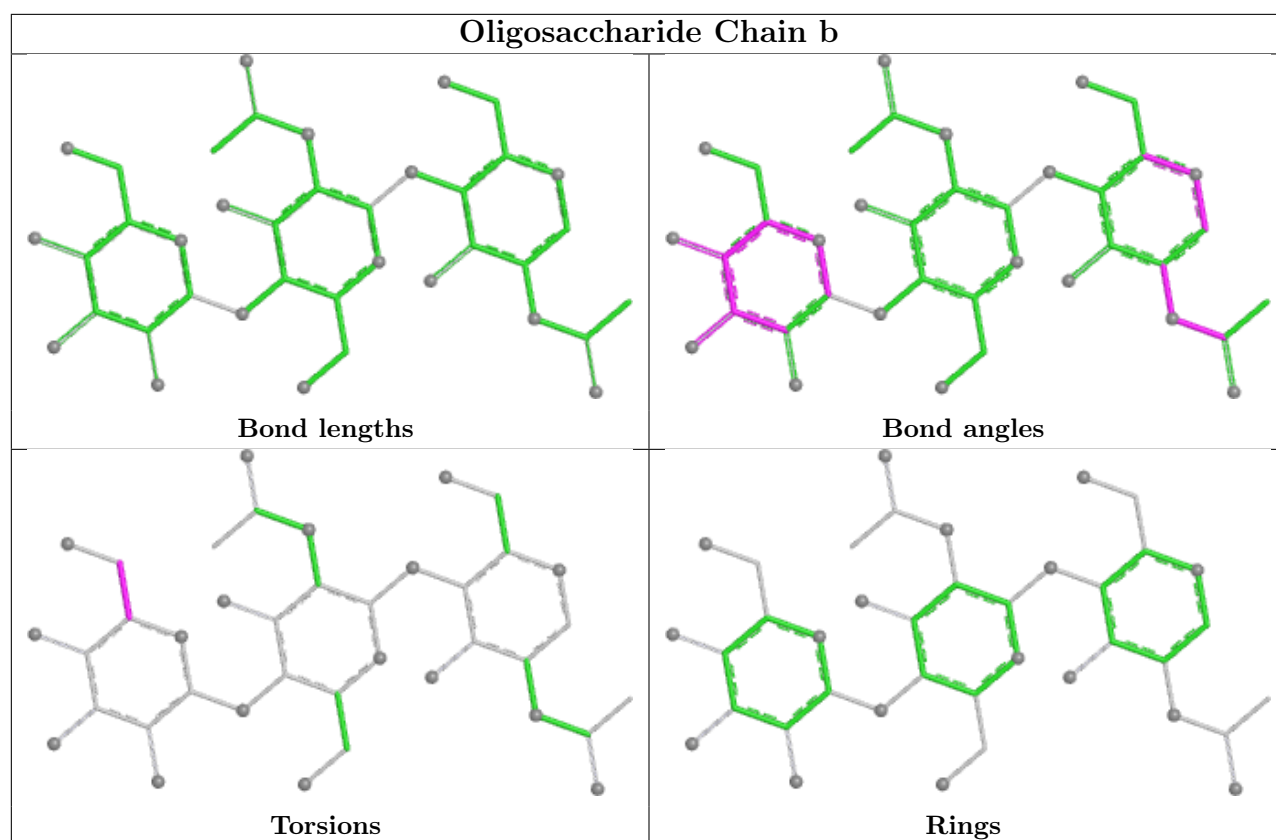
Oligosaccharide Chain 3

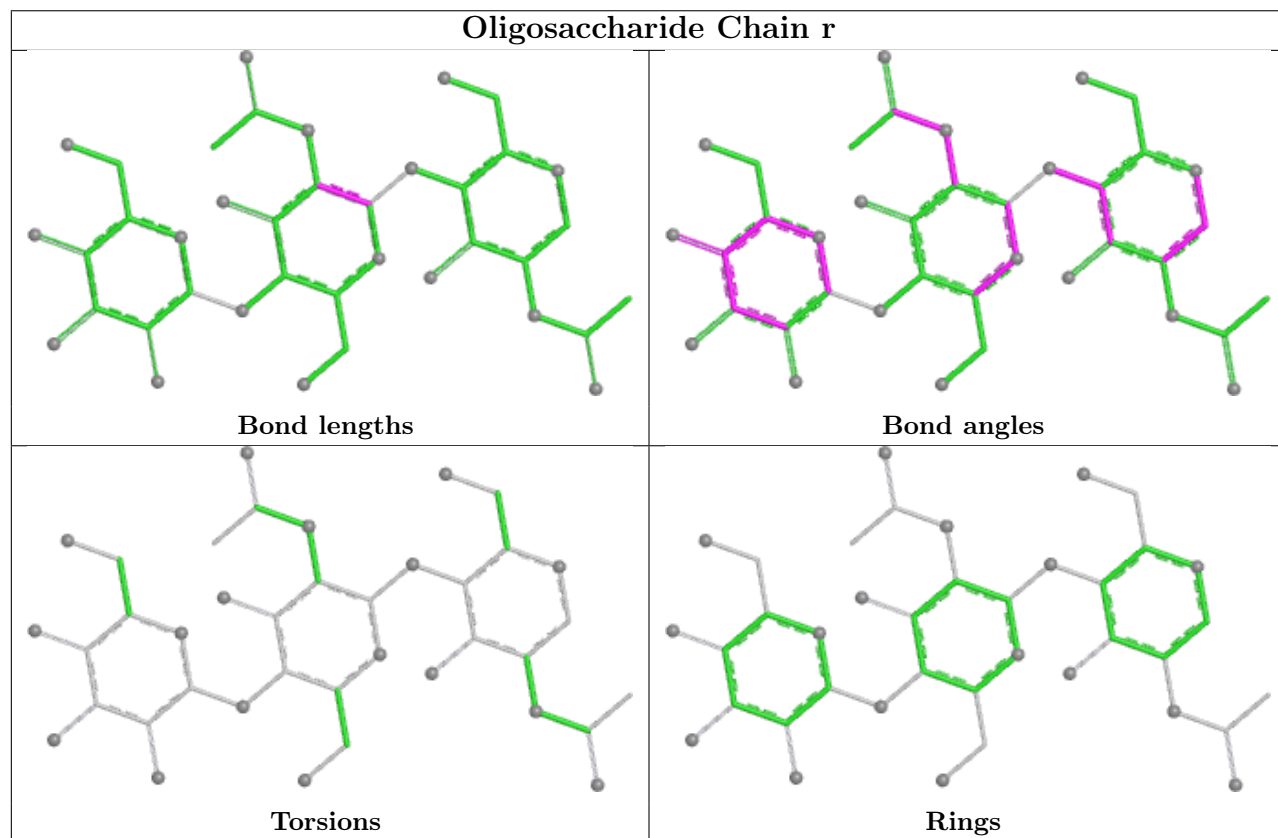
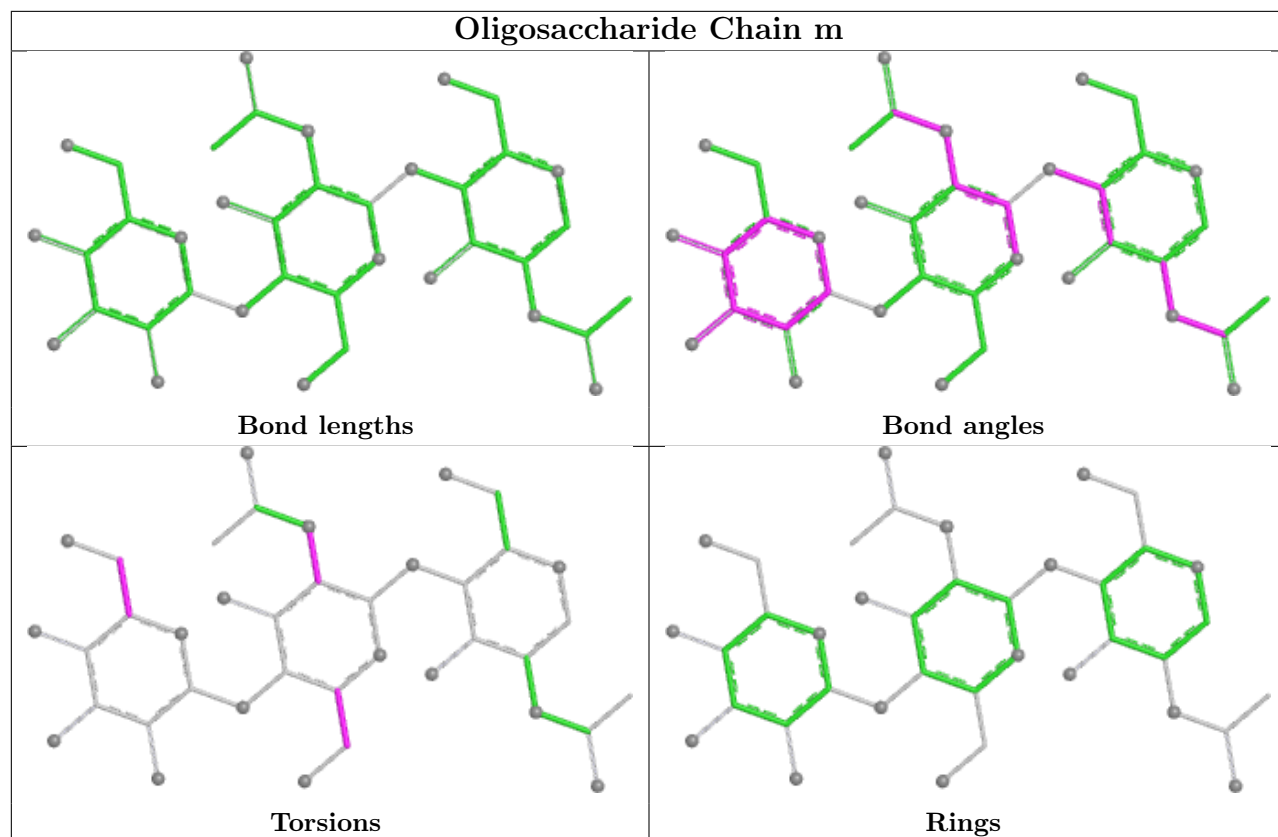


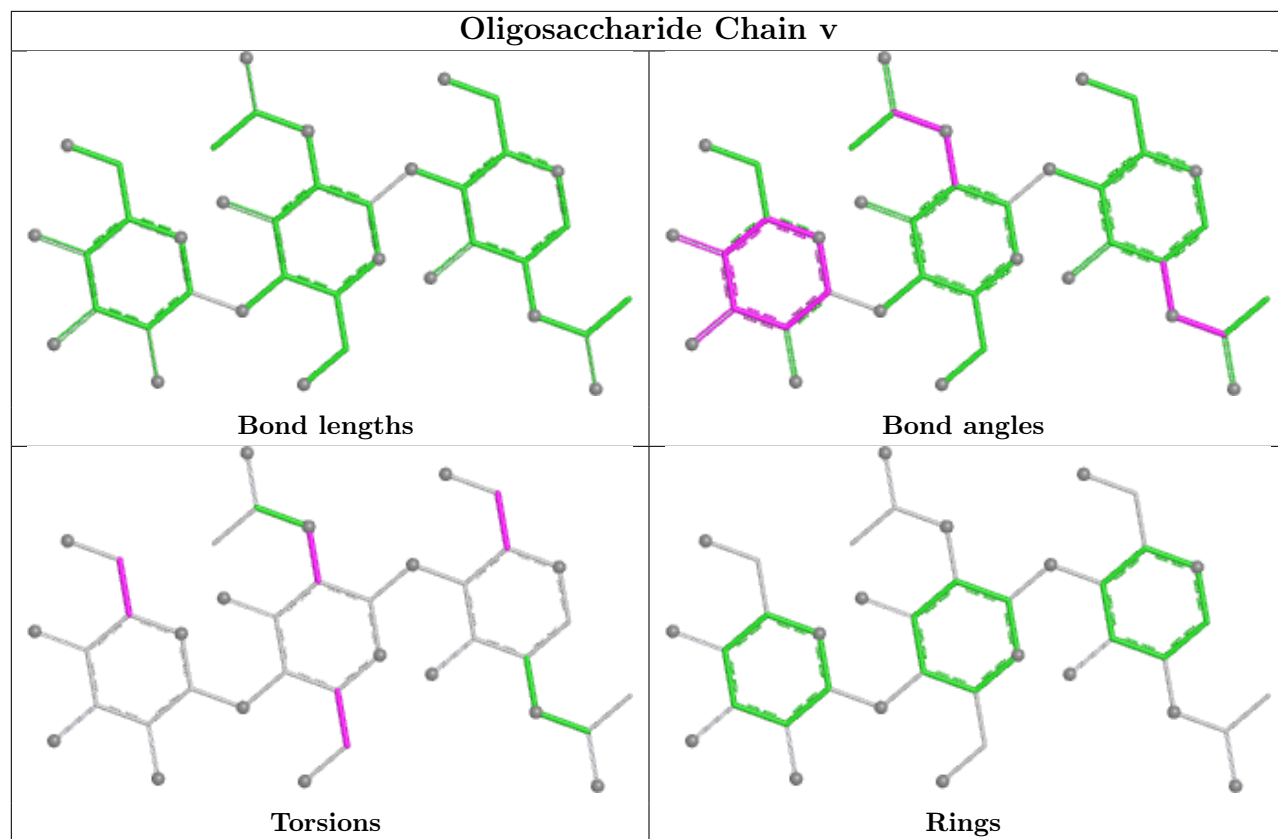
Oligosaccharide Chain E

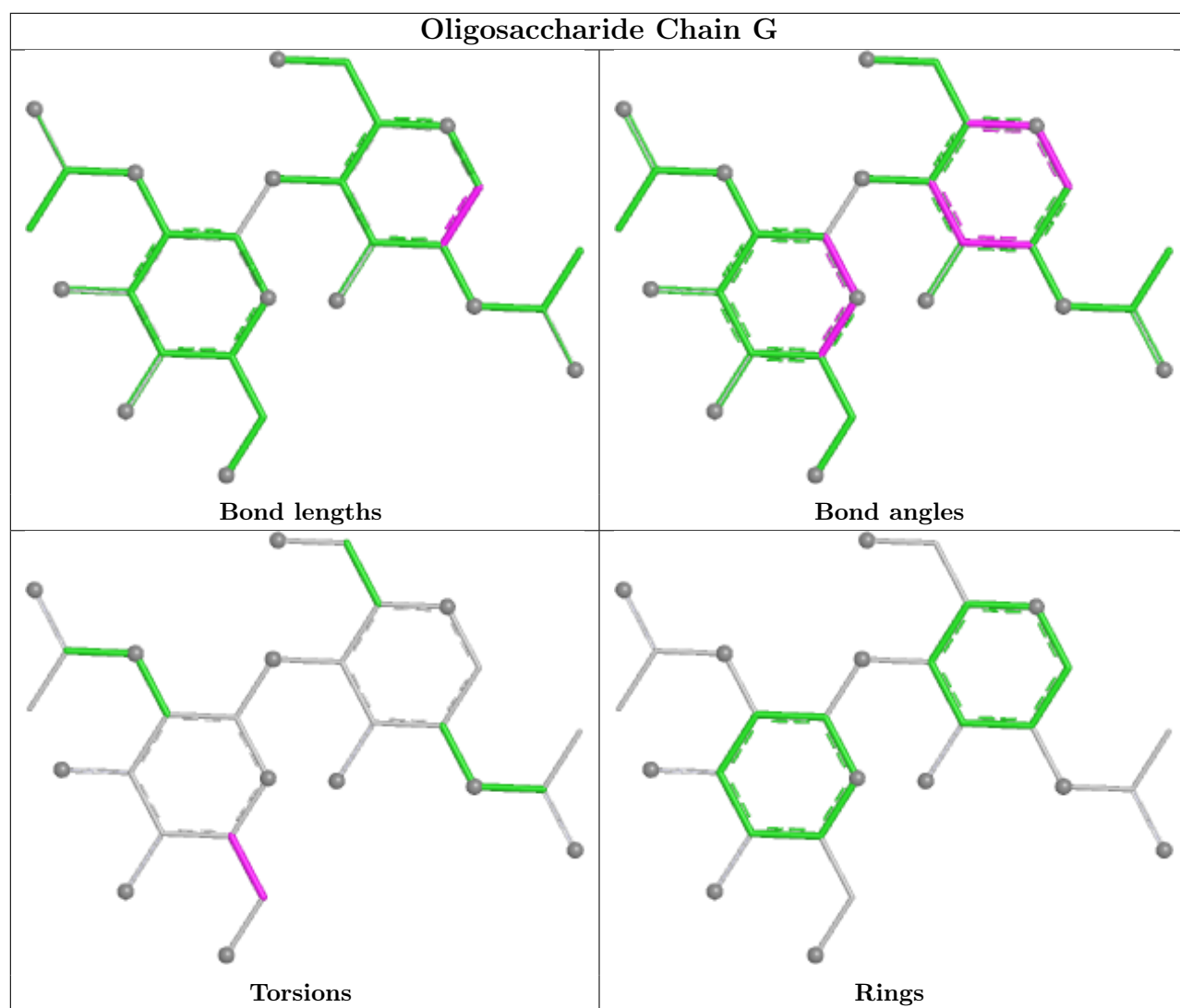


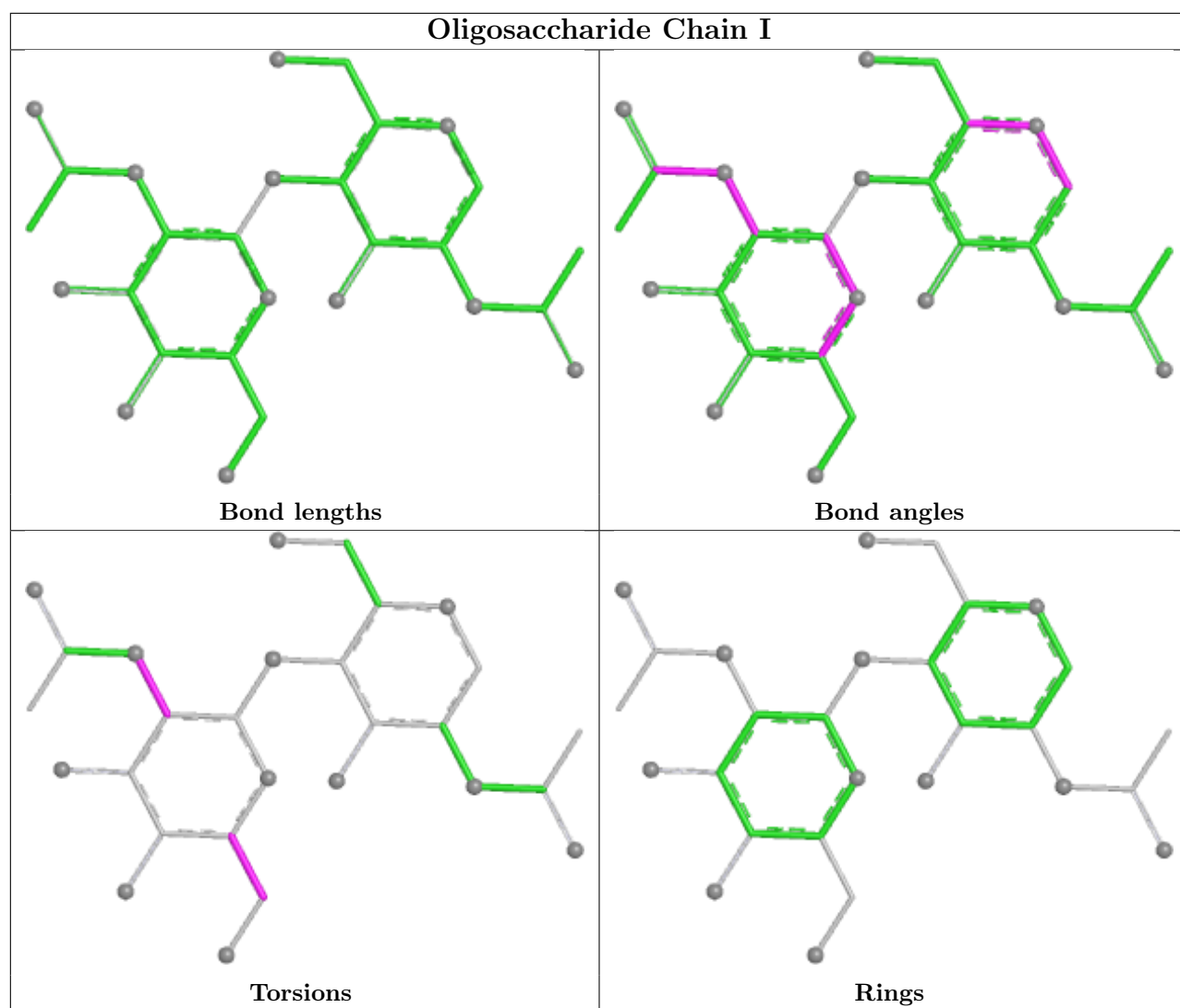


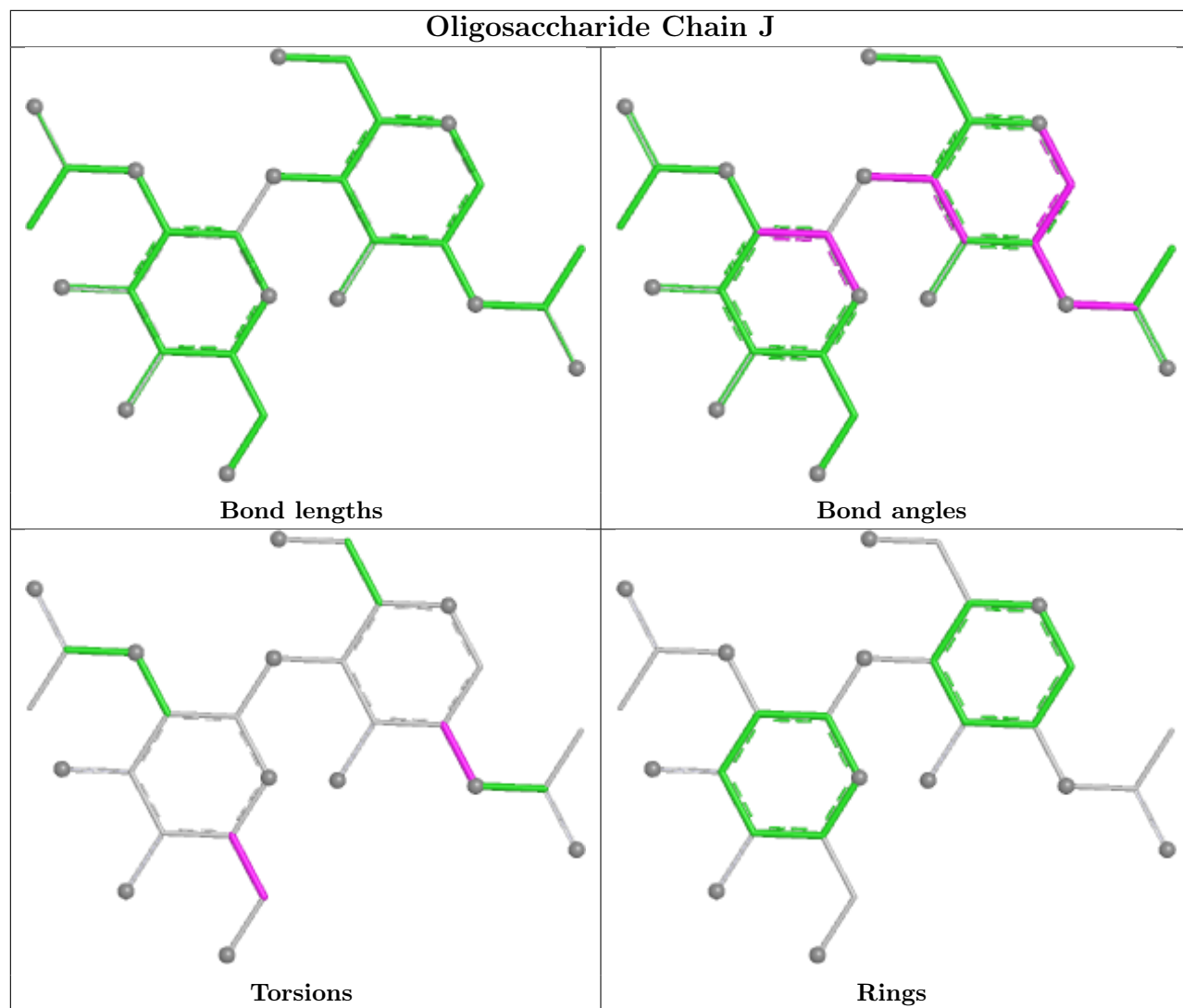


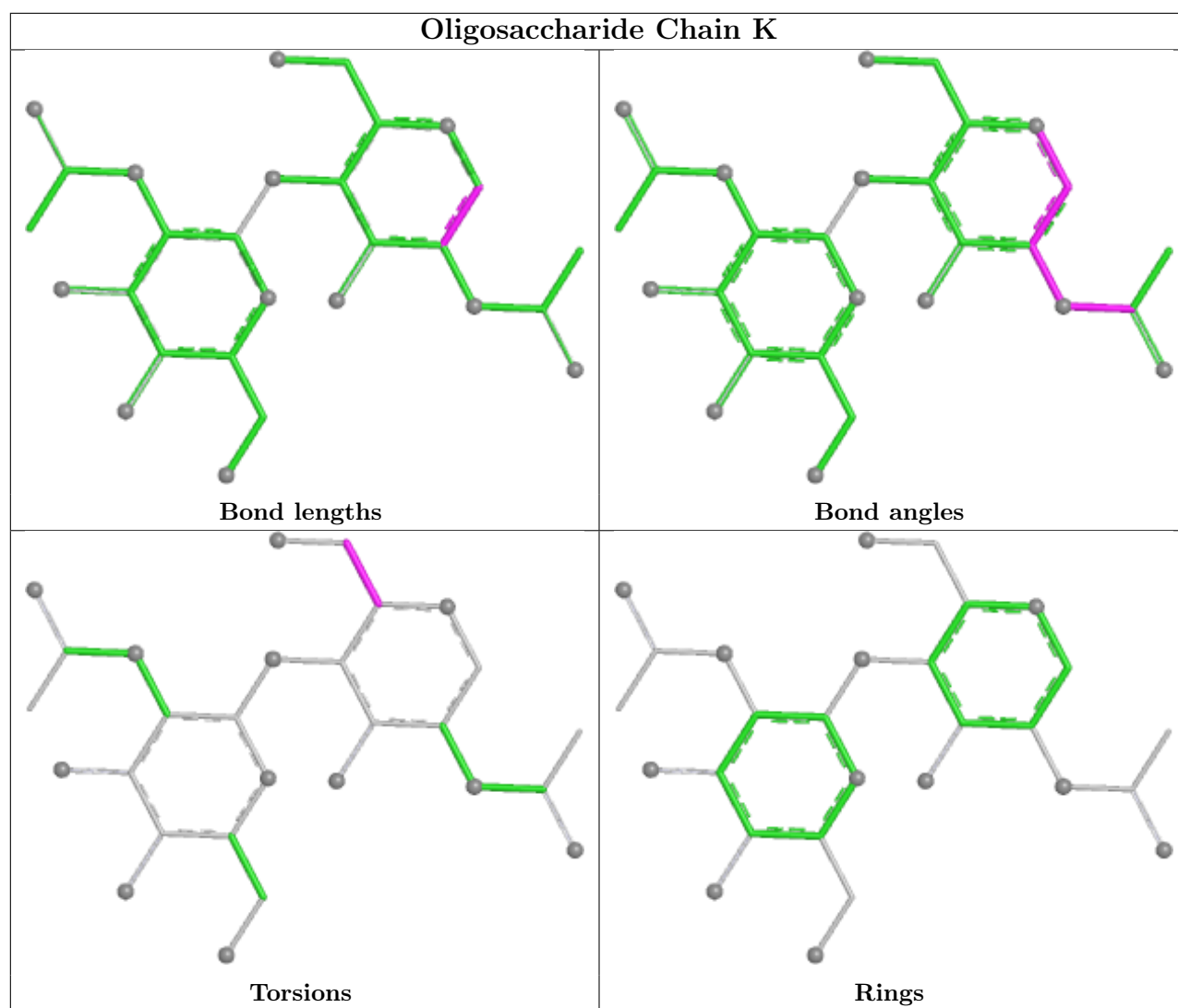


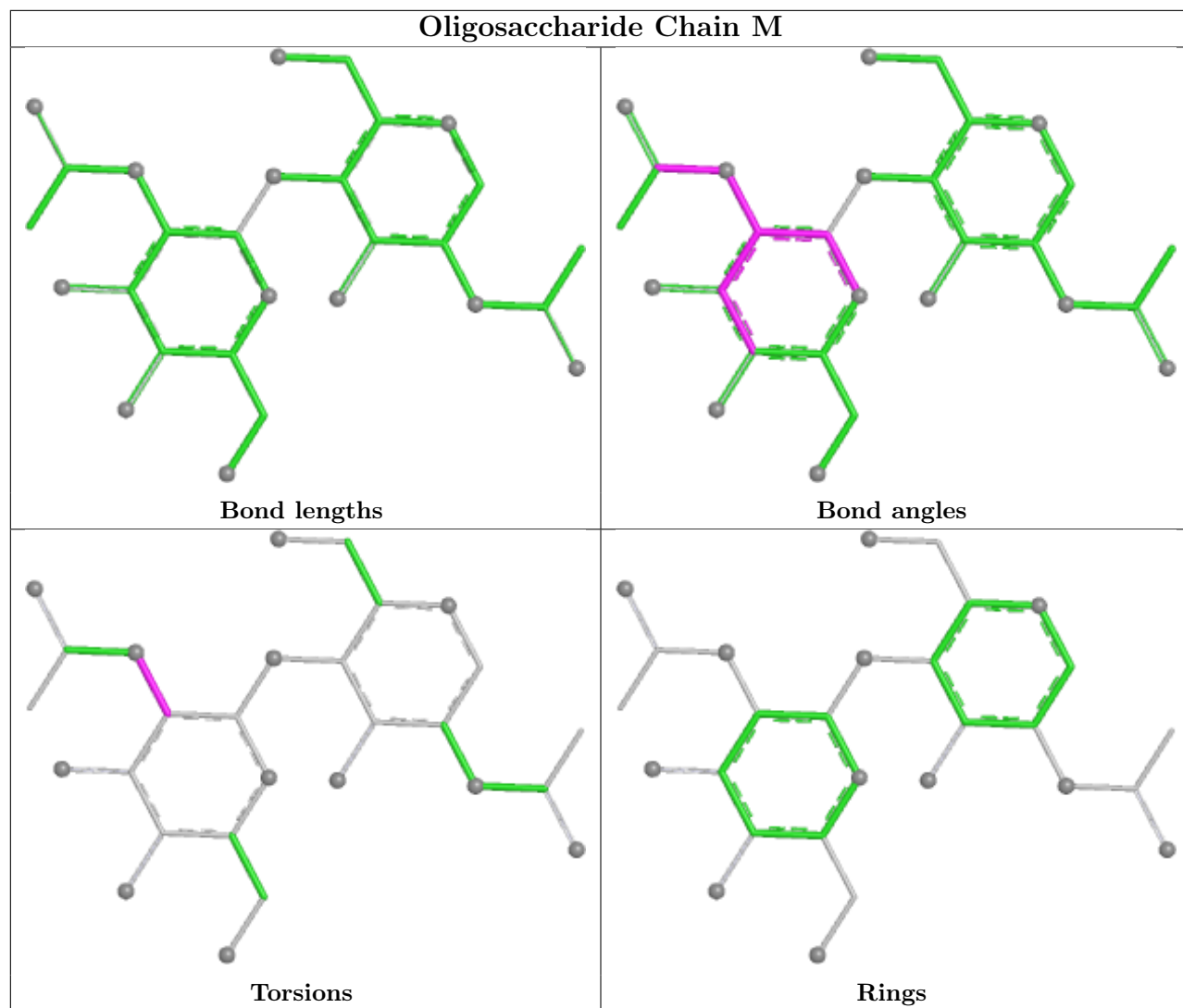


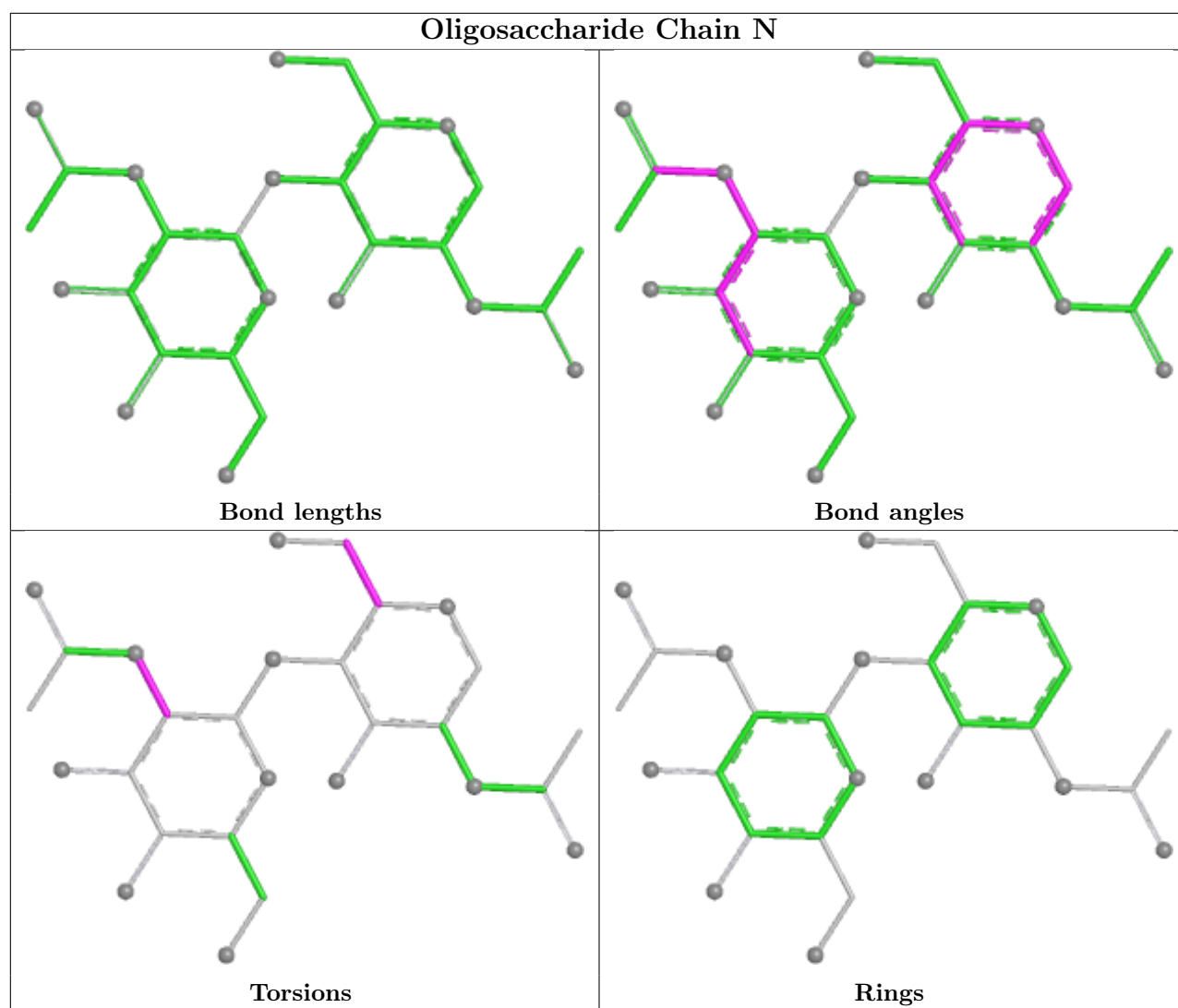


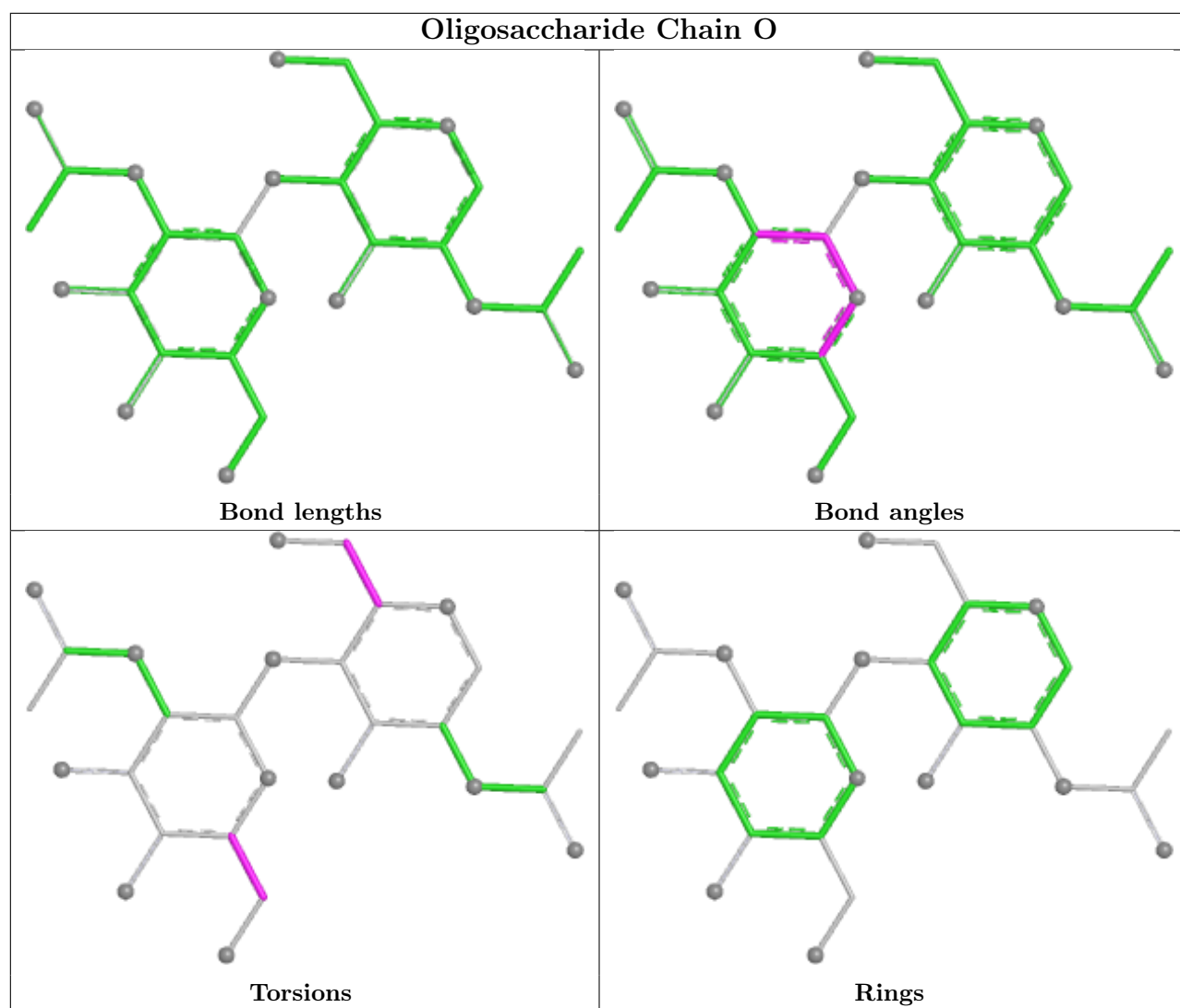


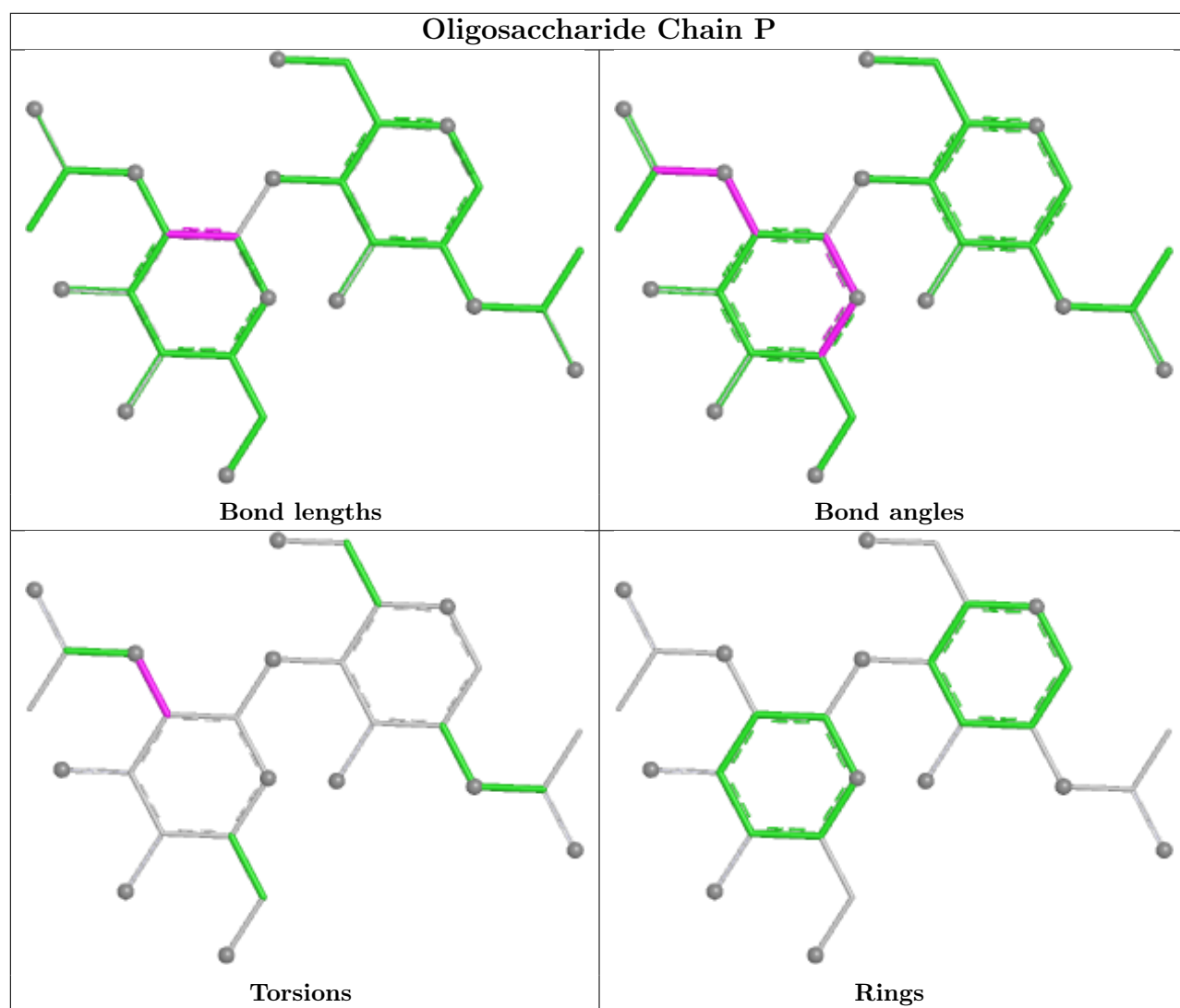


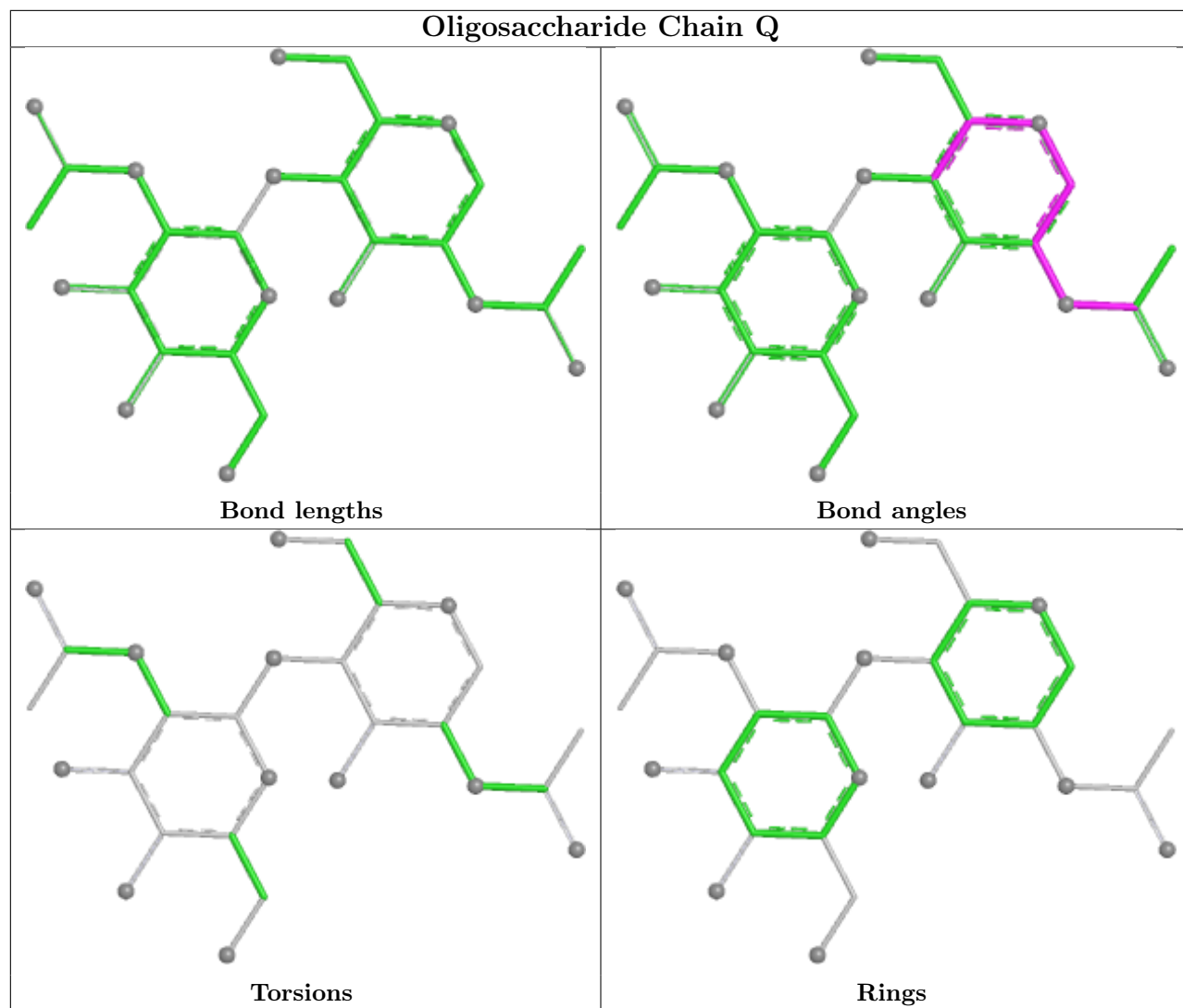


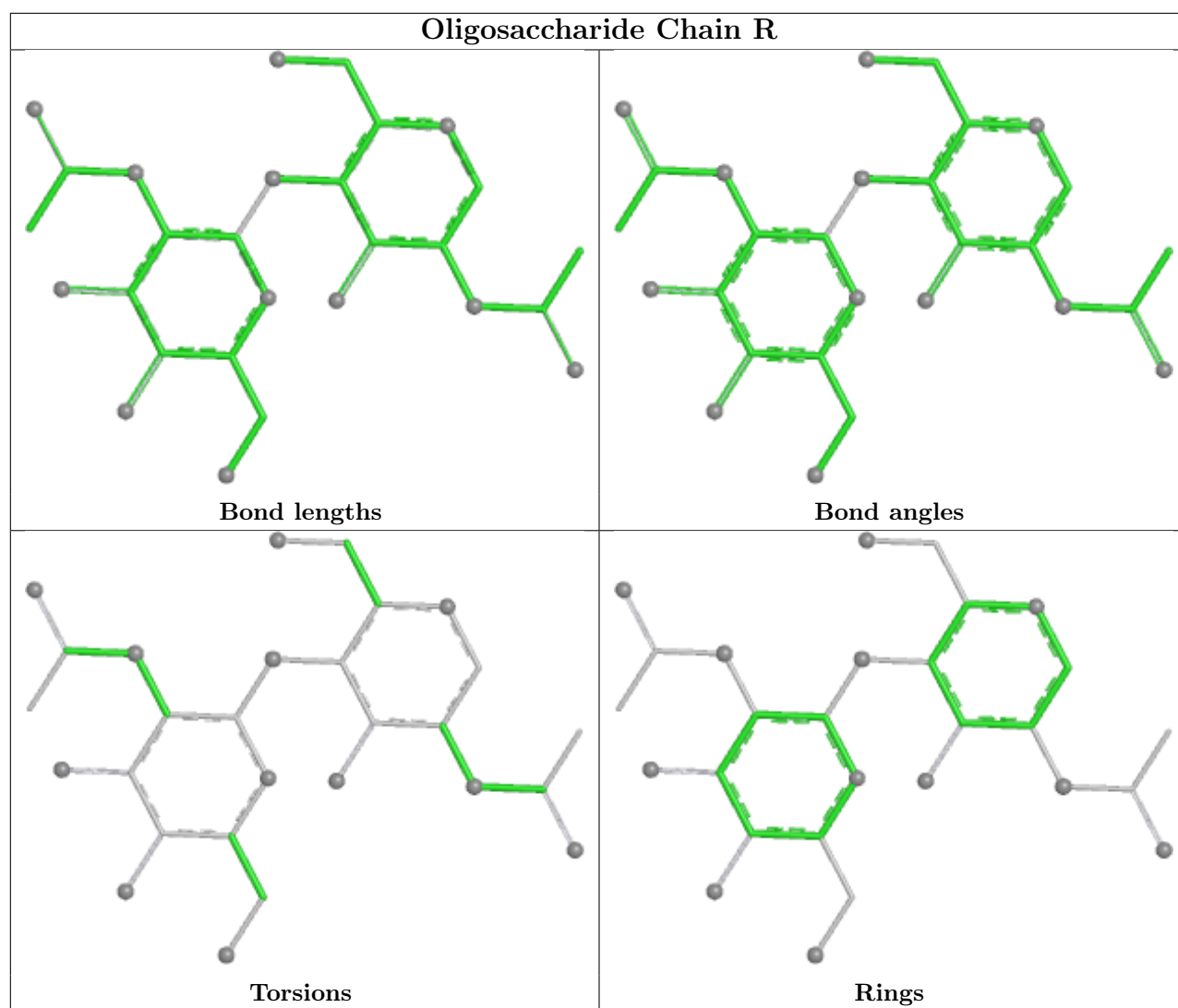


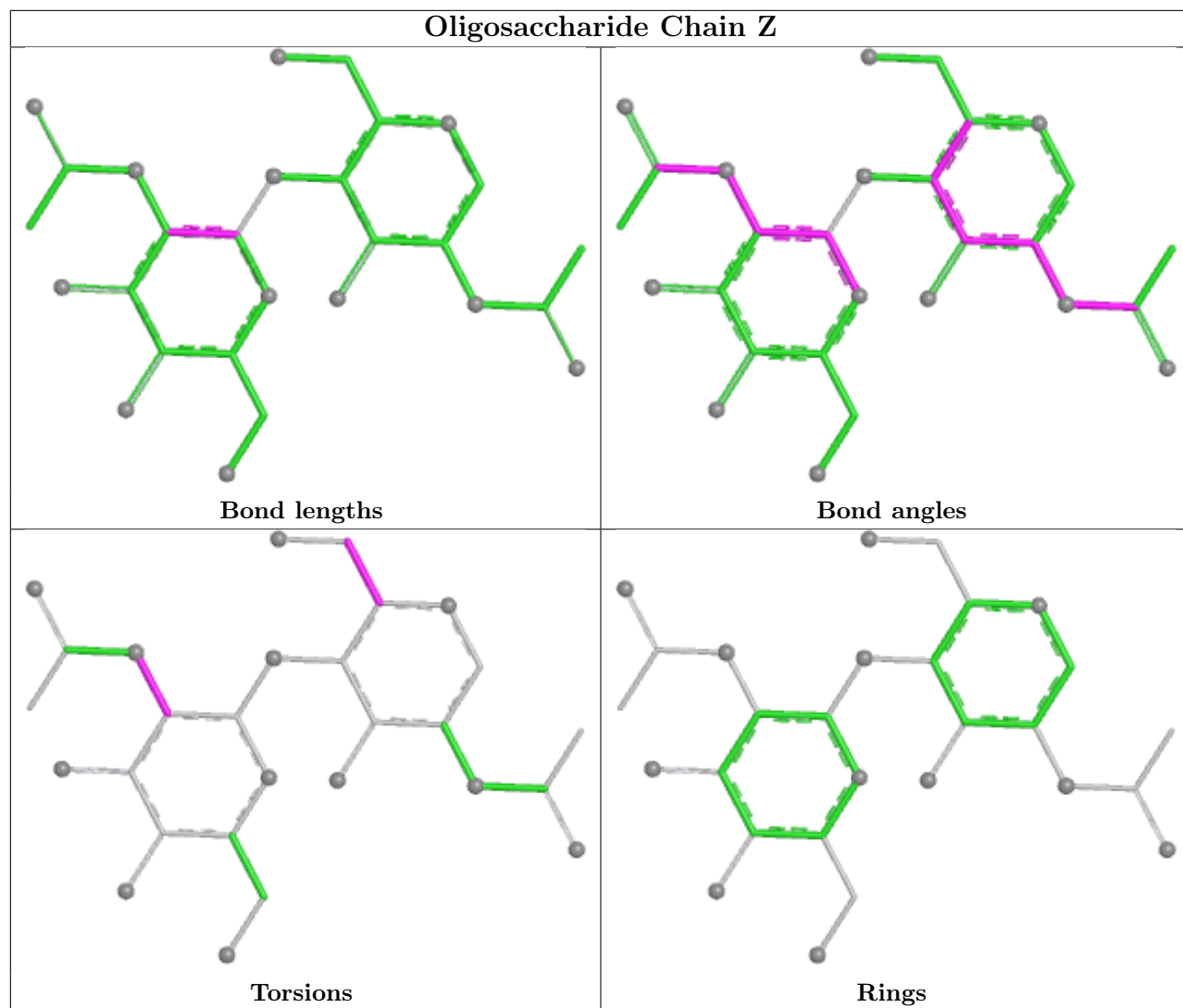


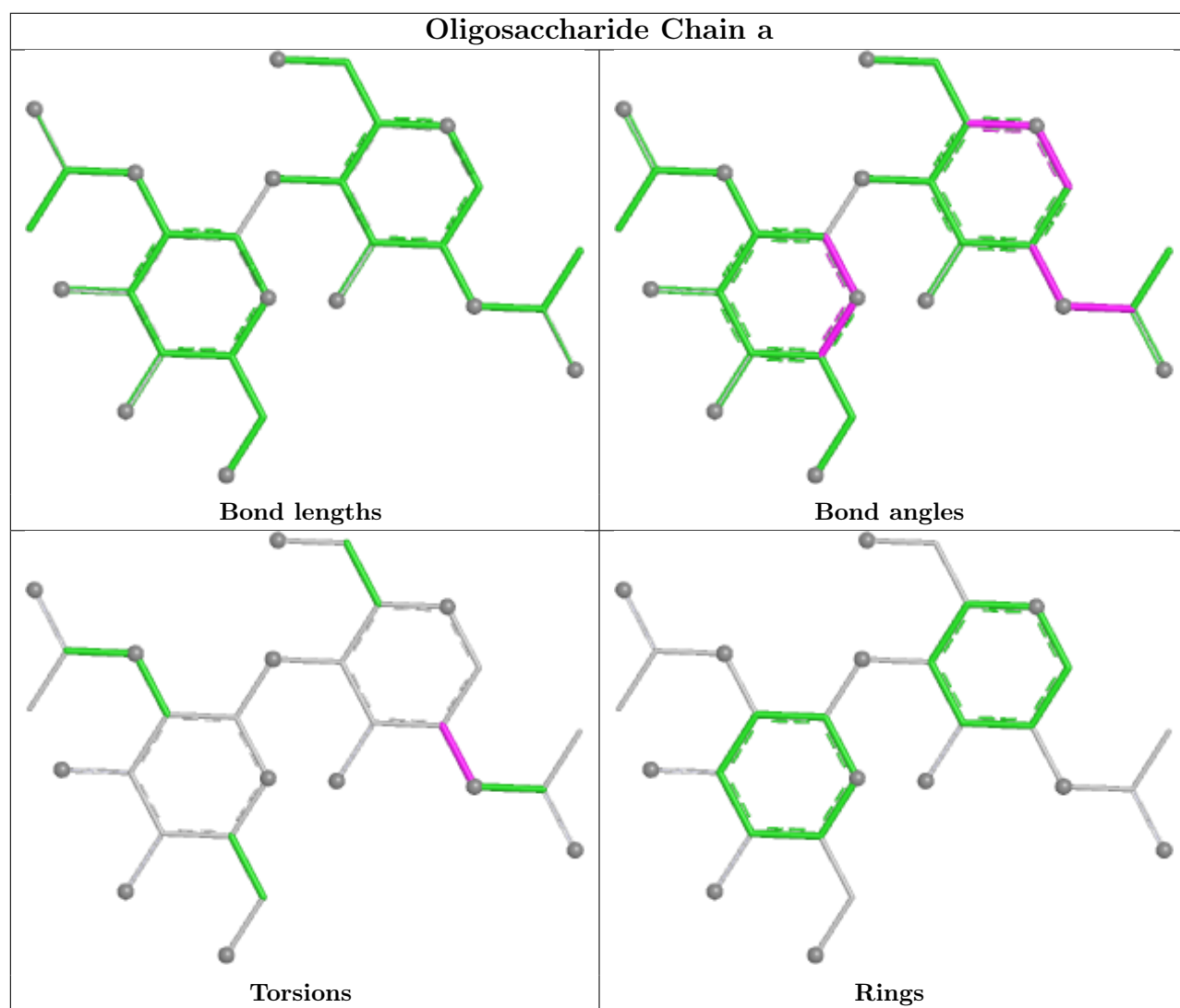


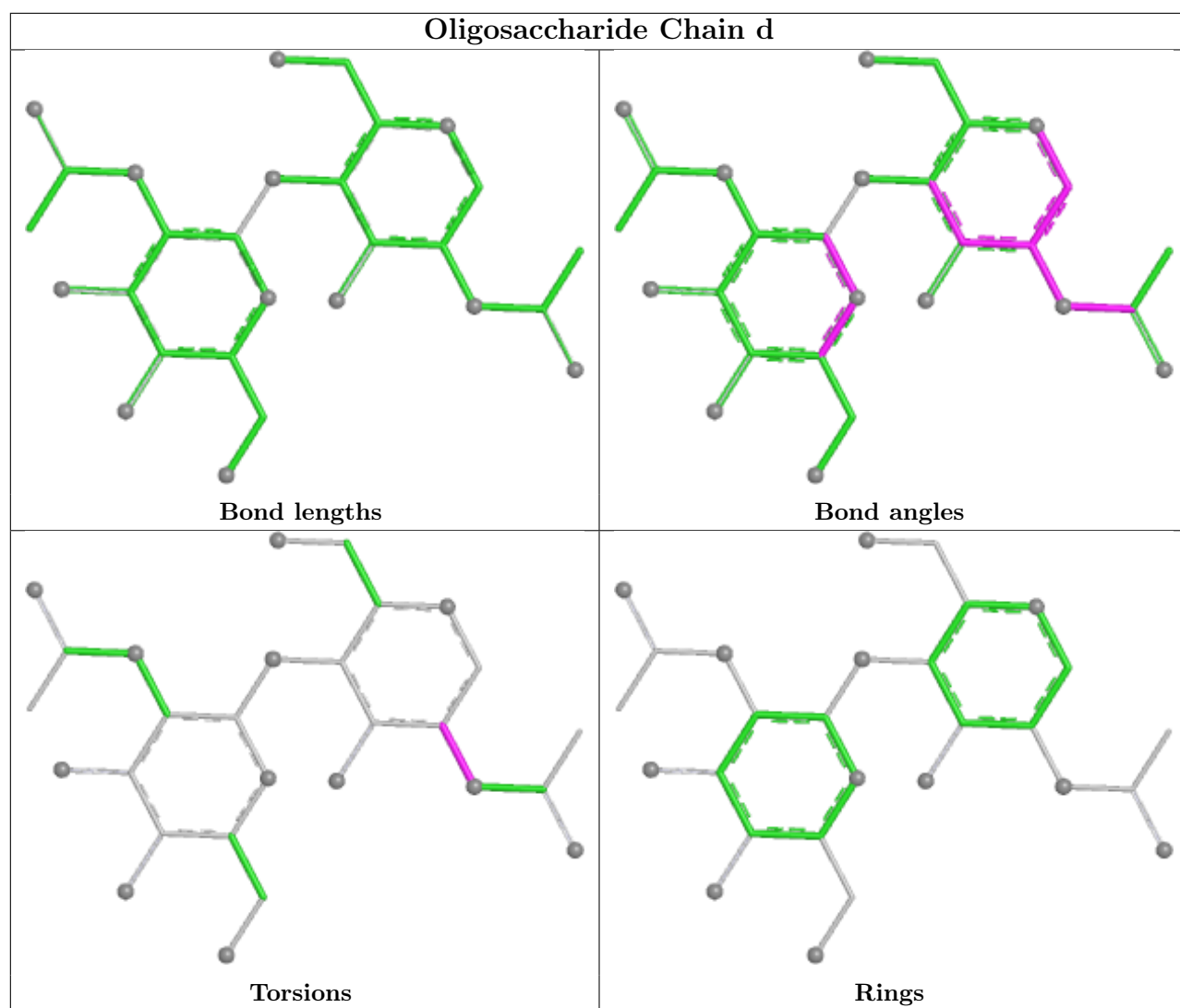


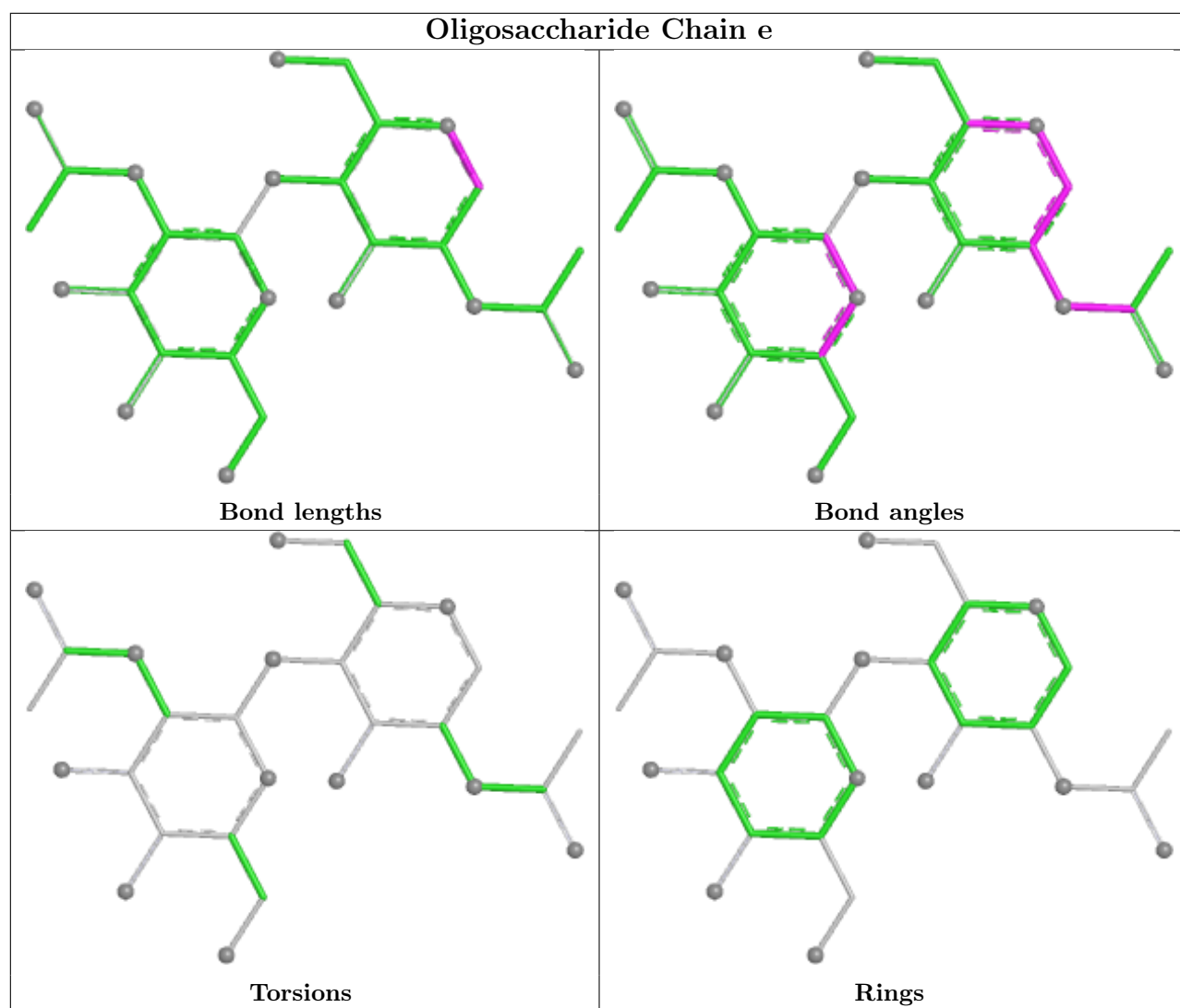


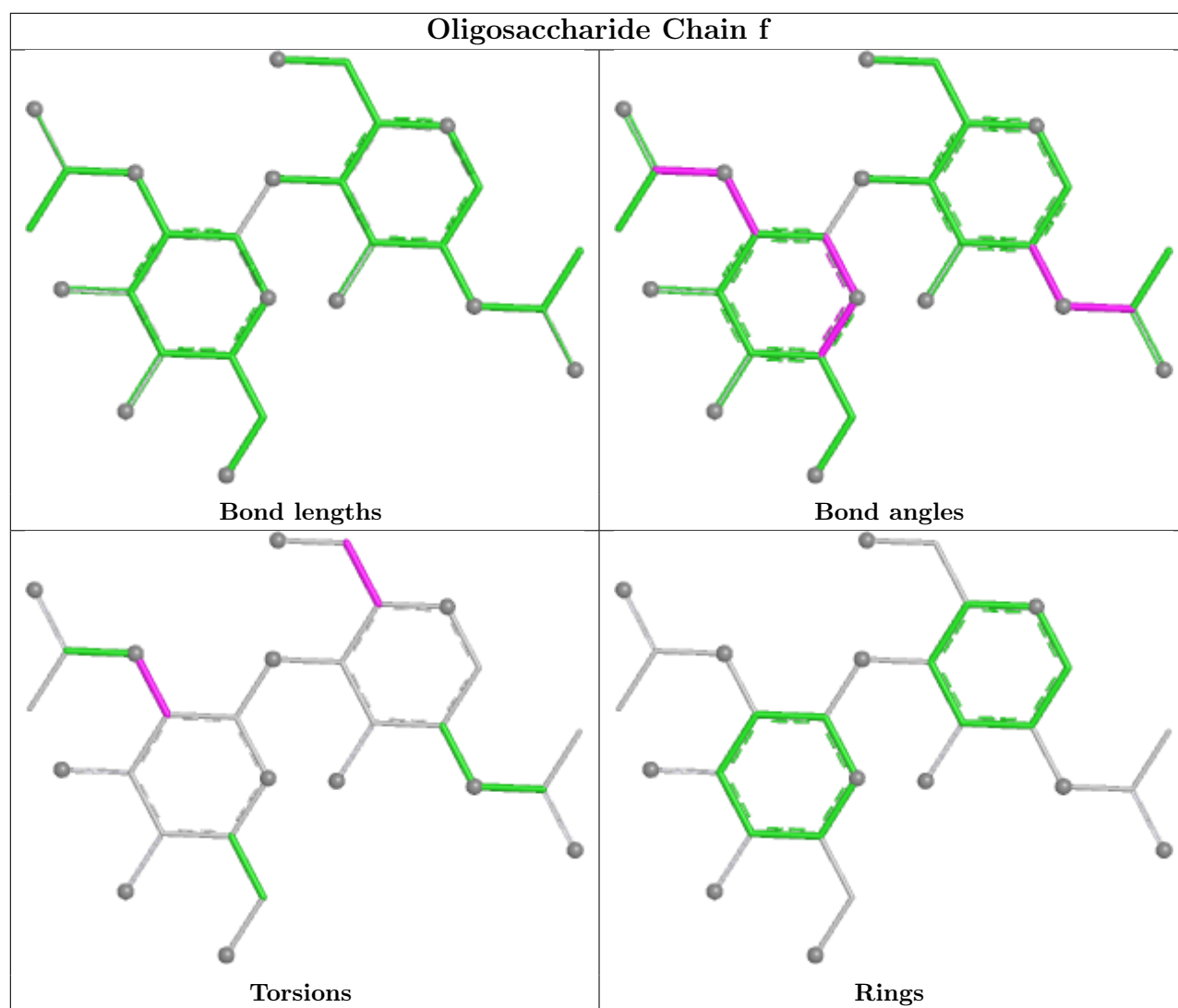


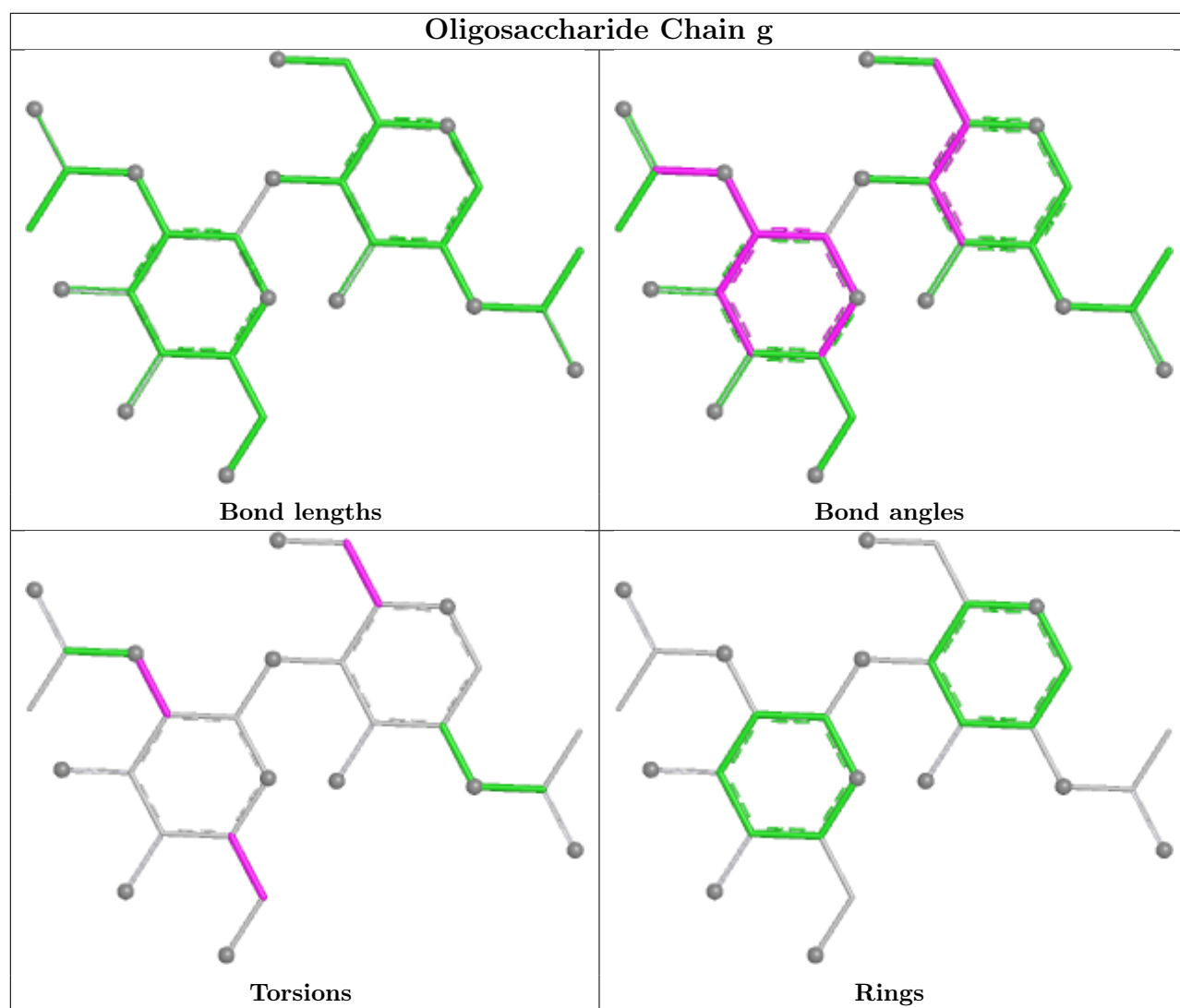


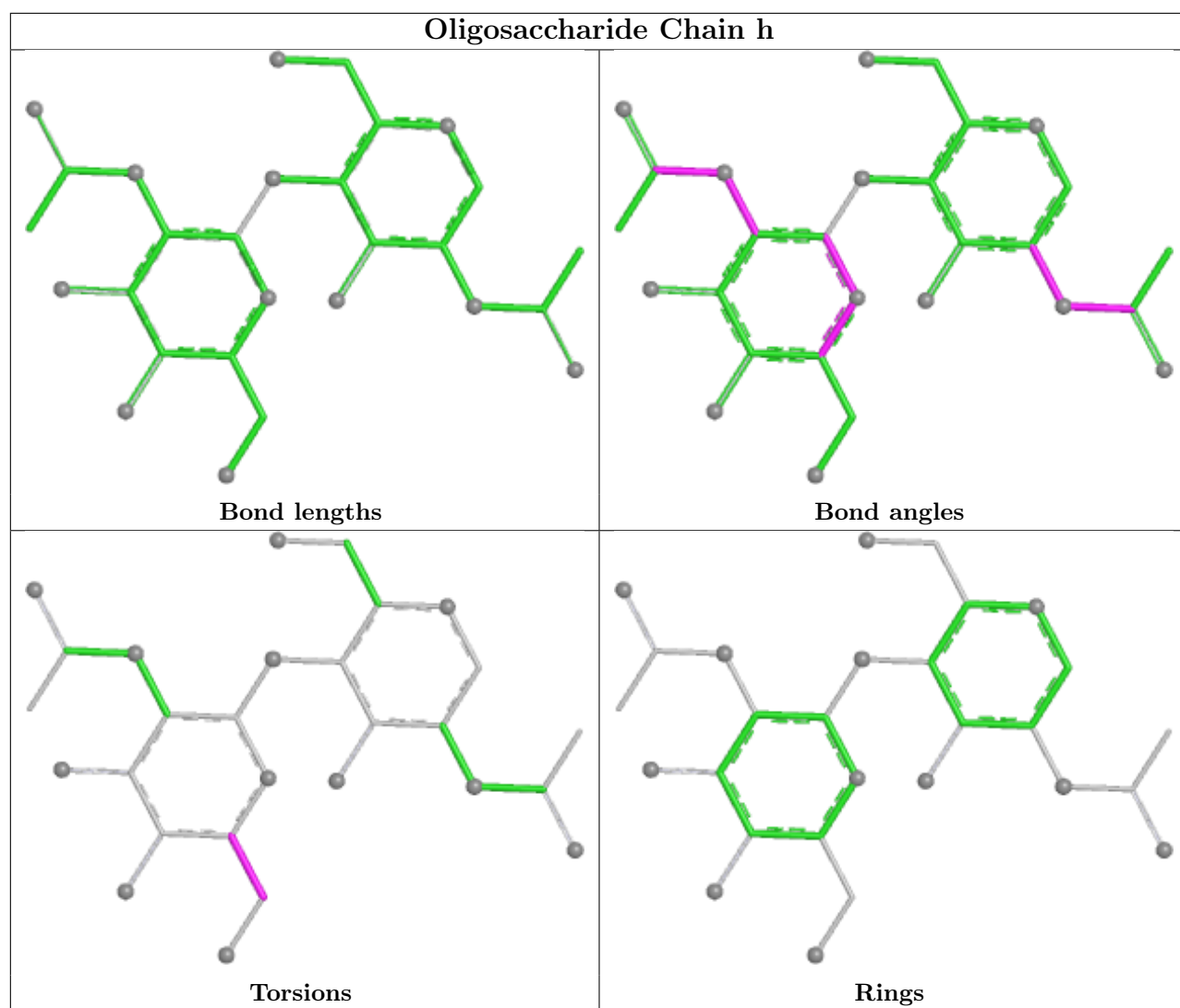


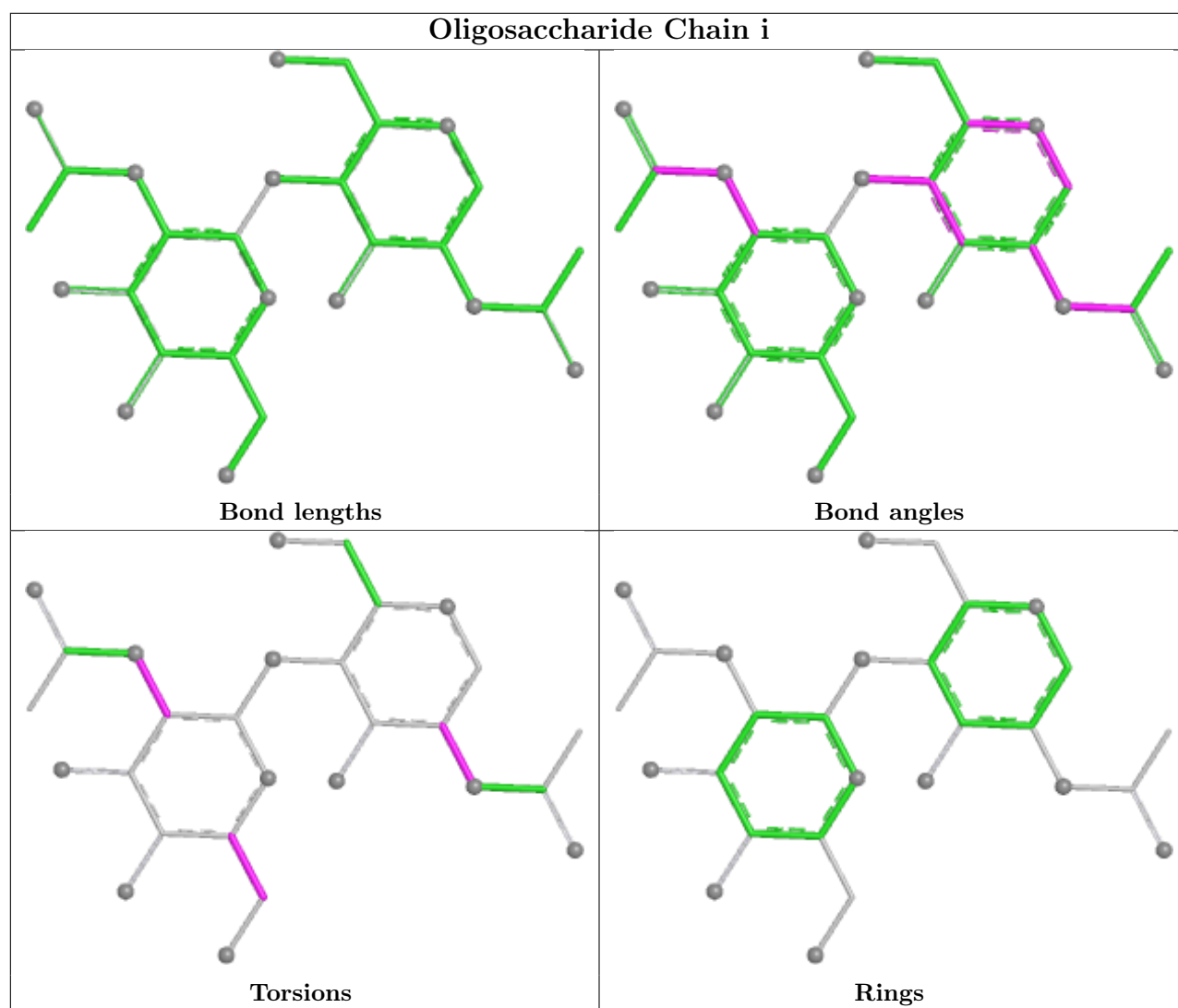


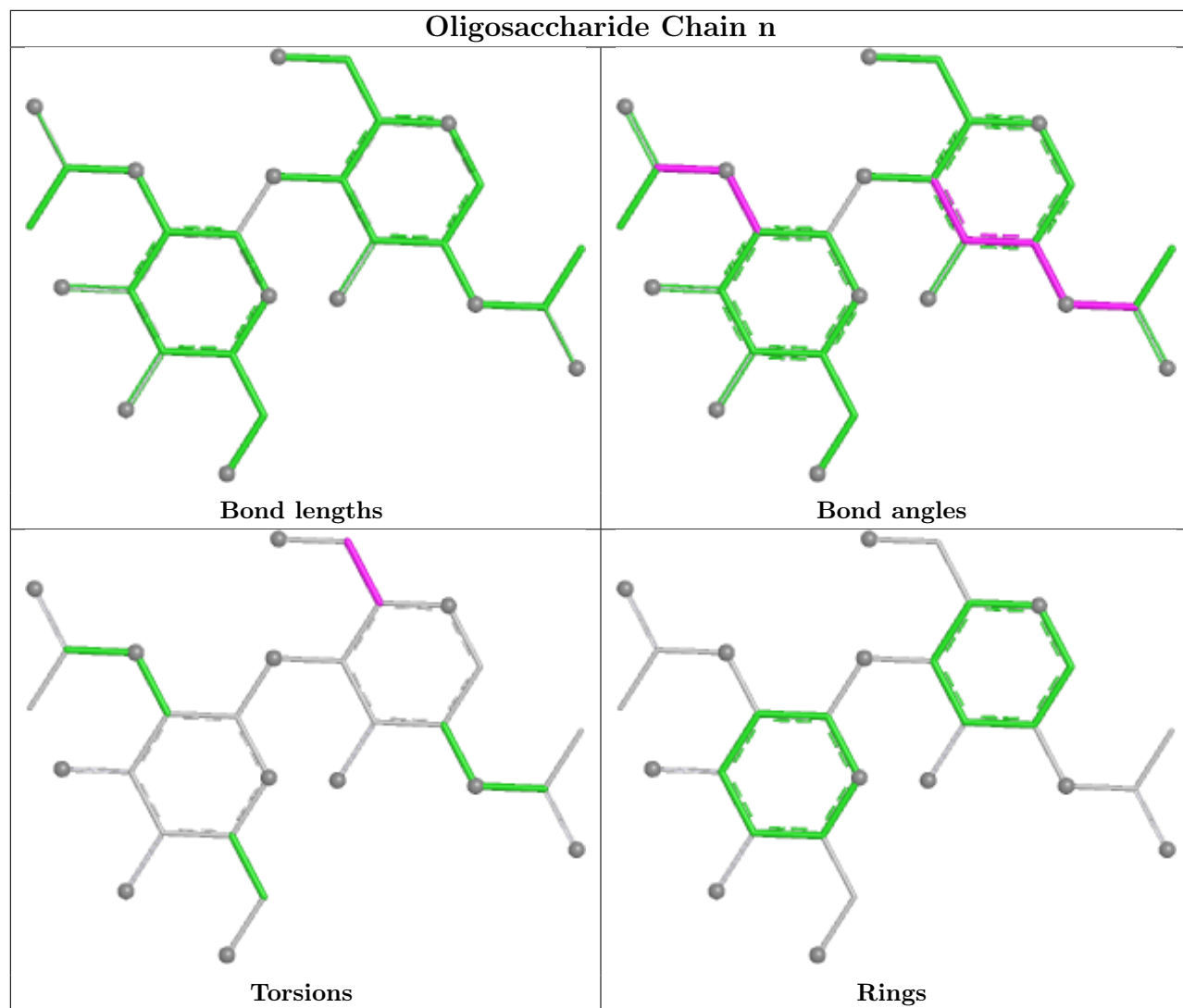


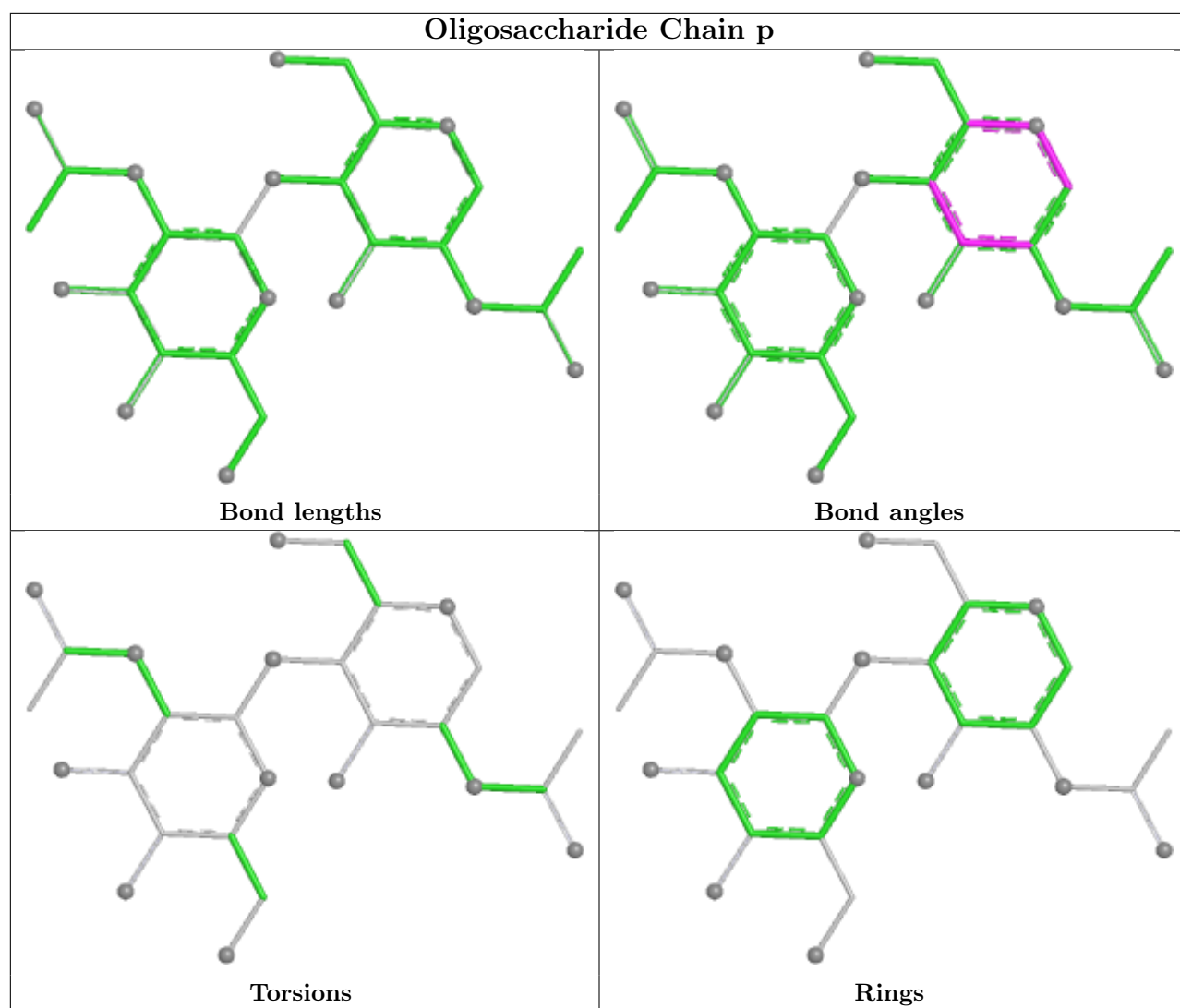


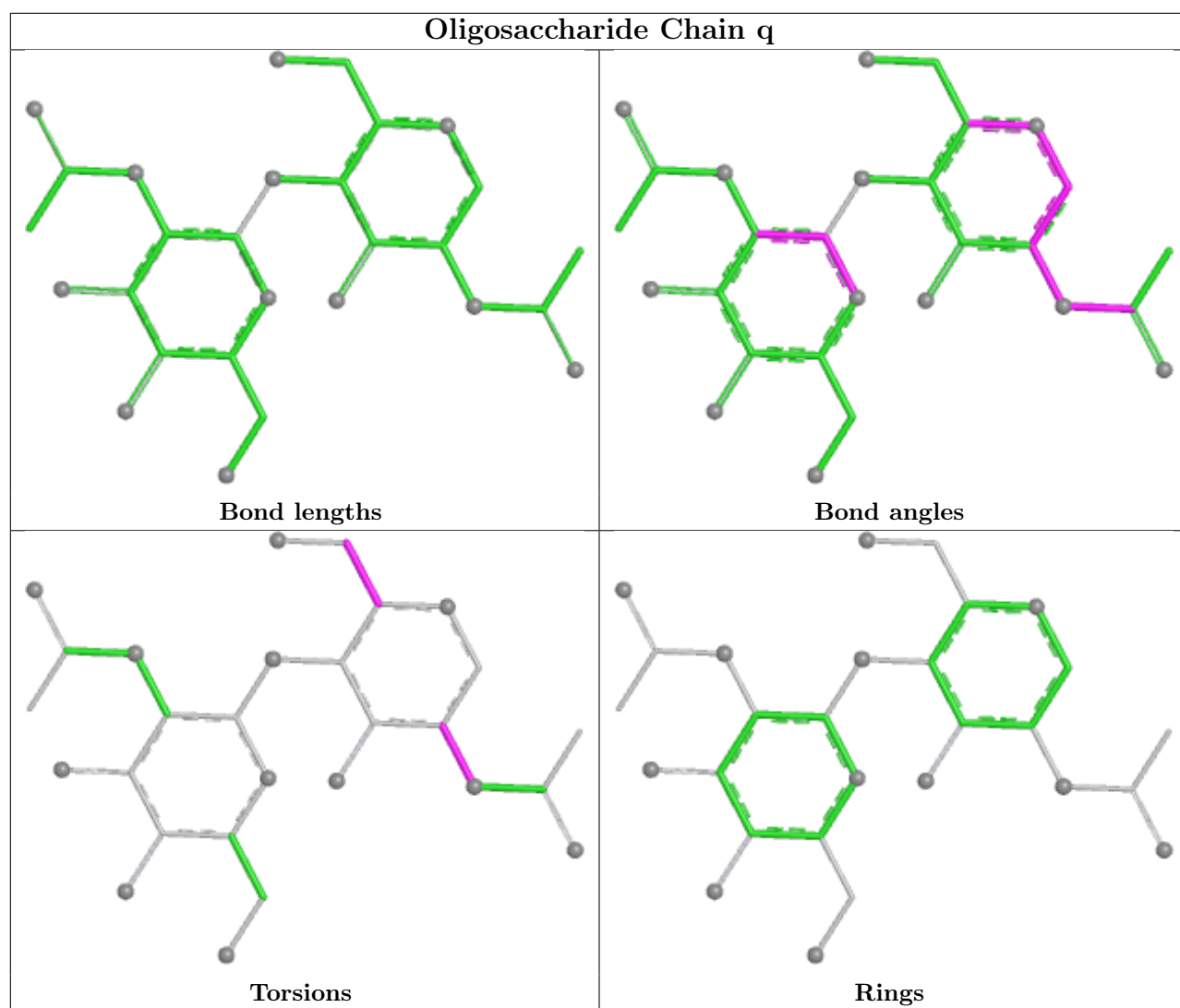


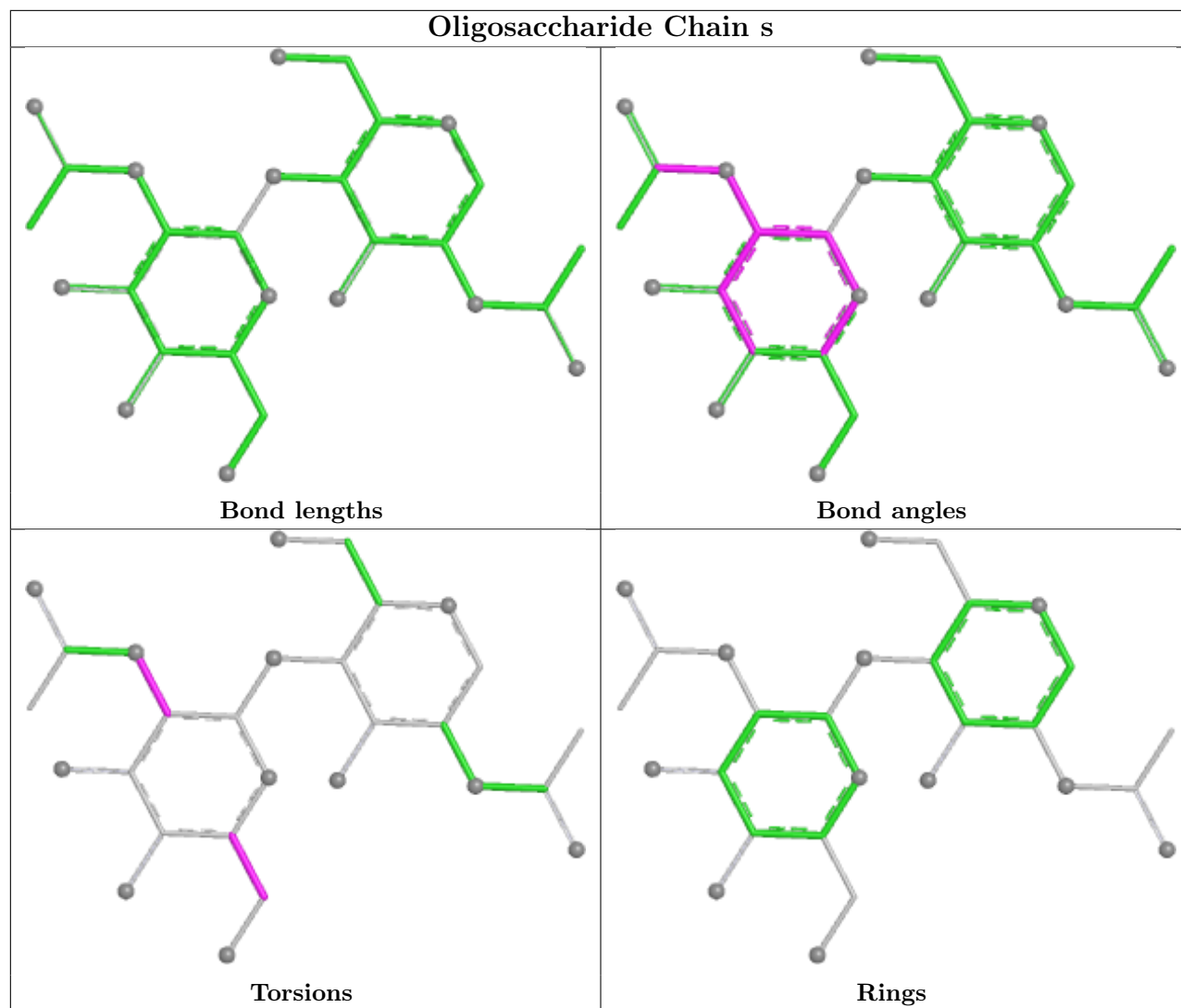


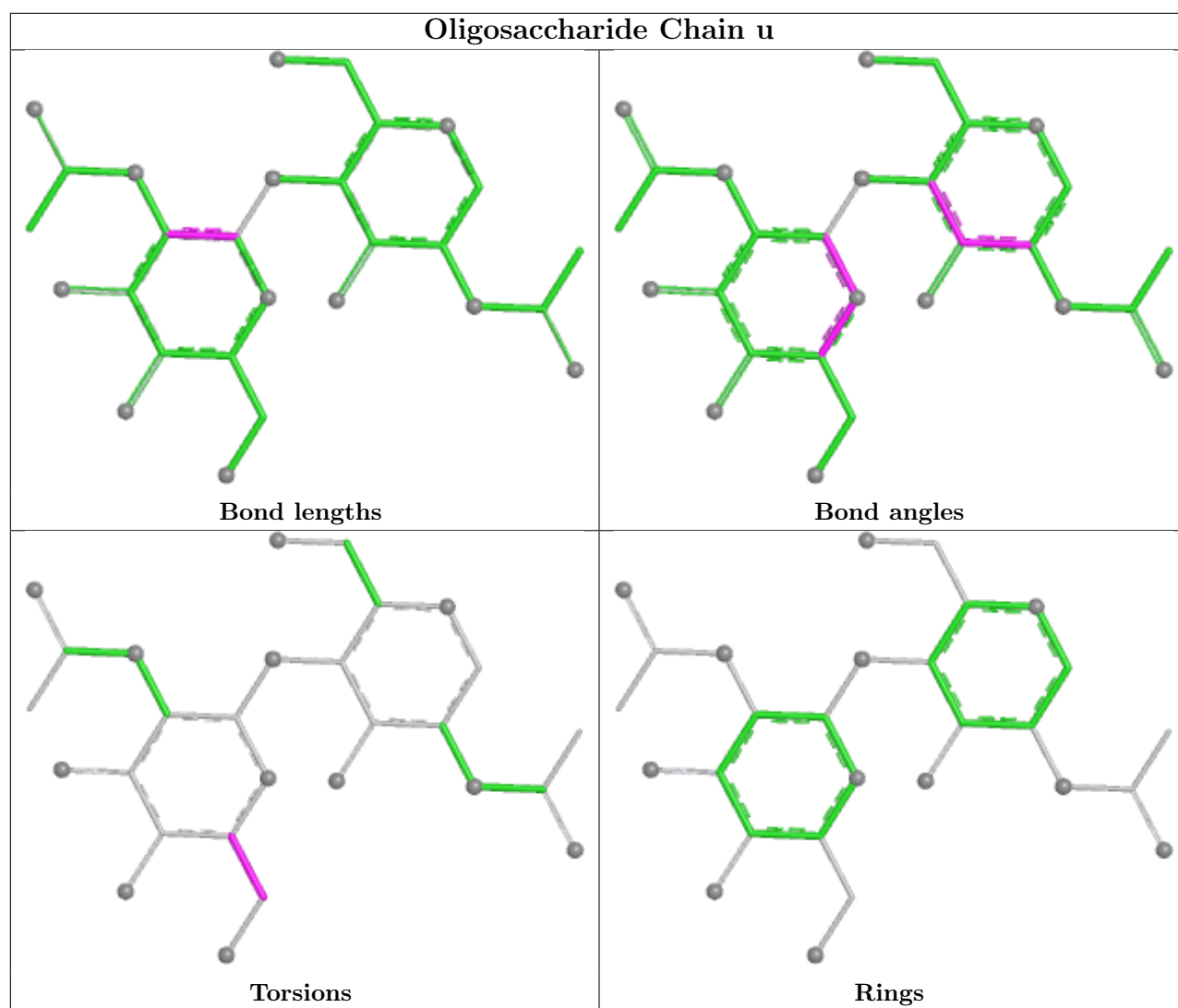


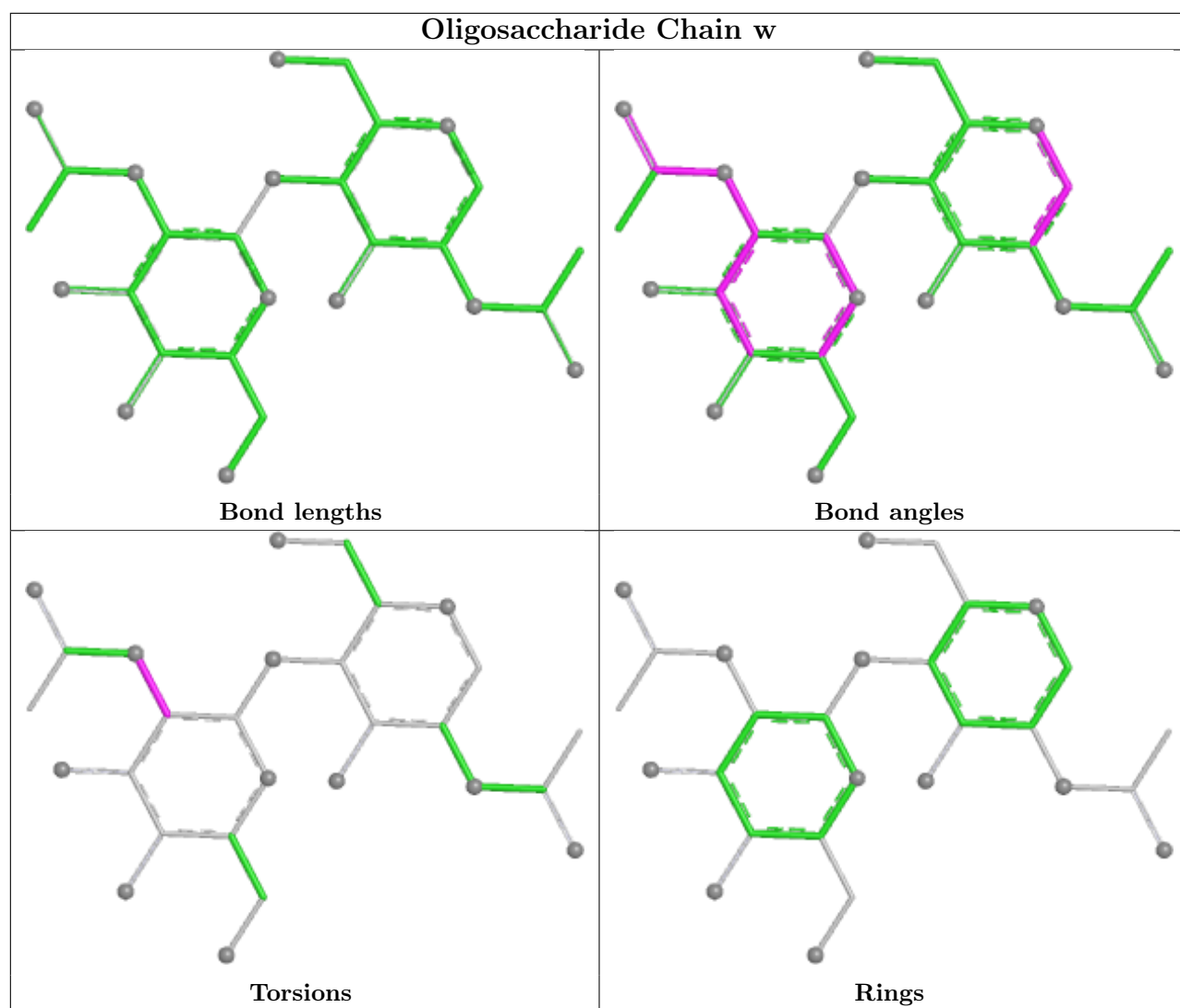


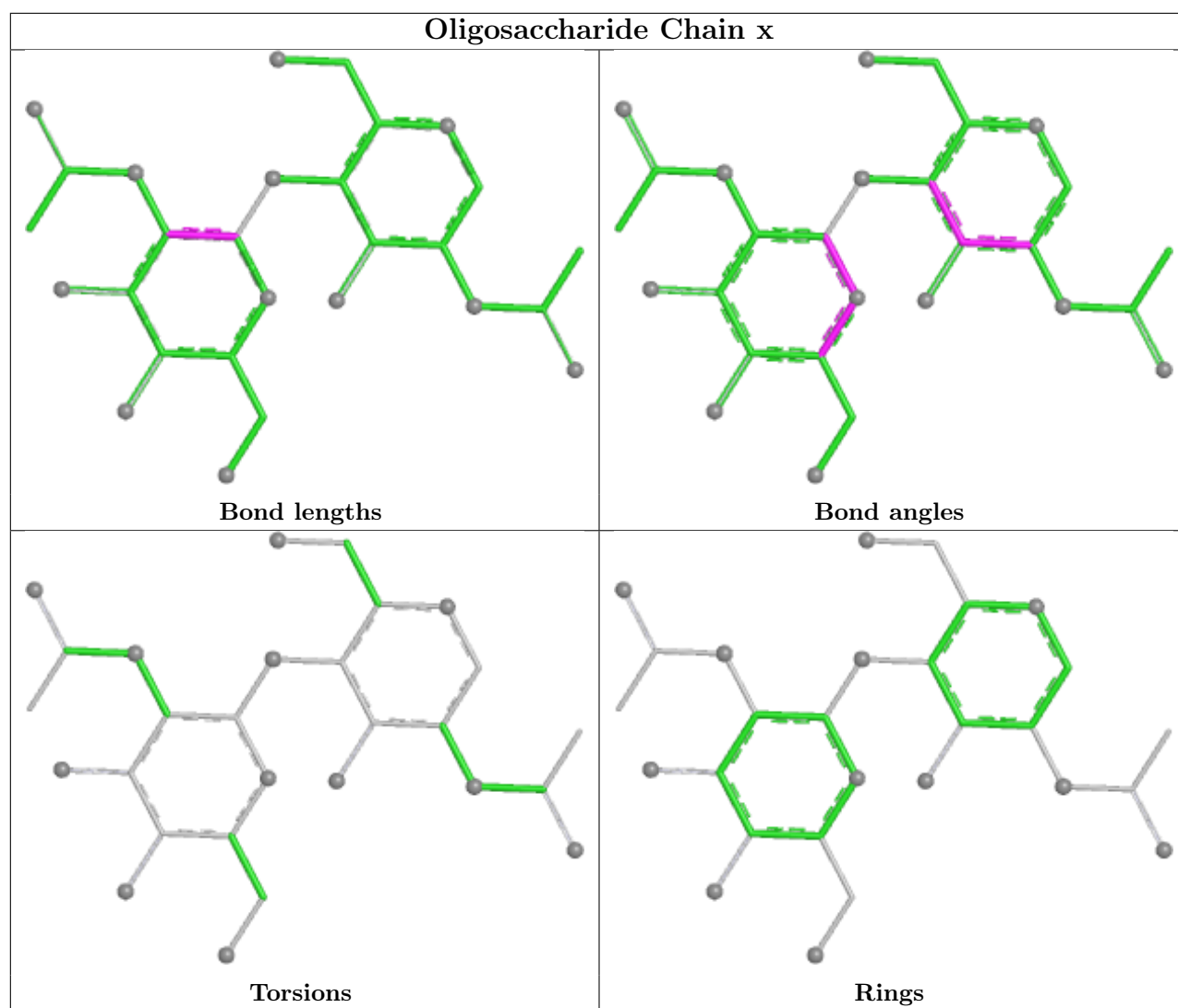


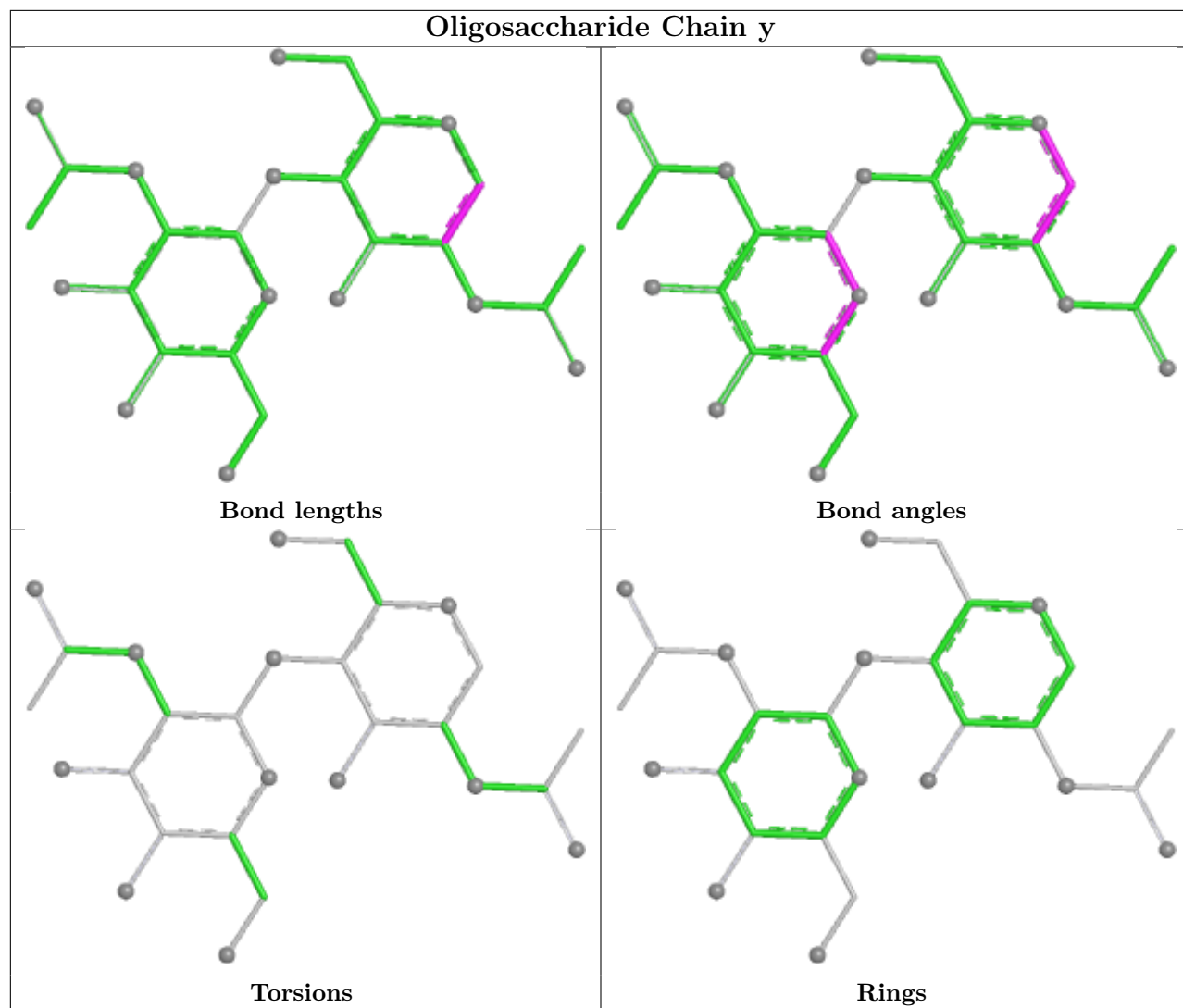


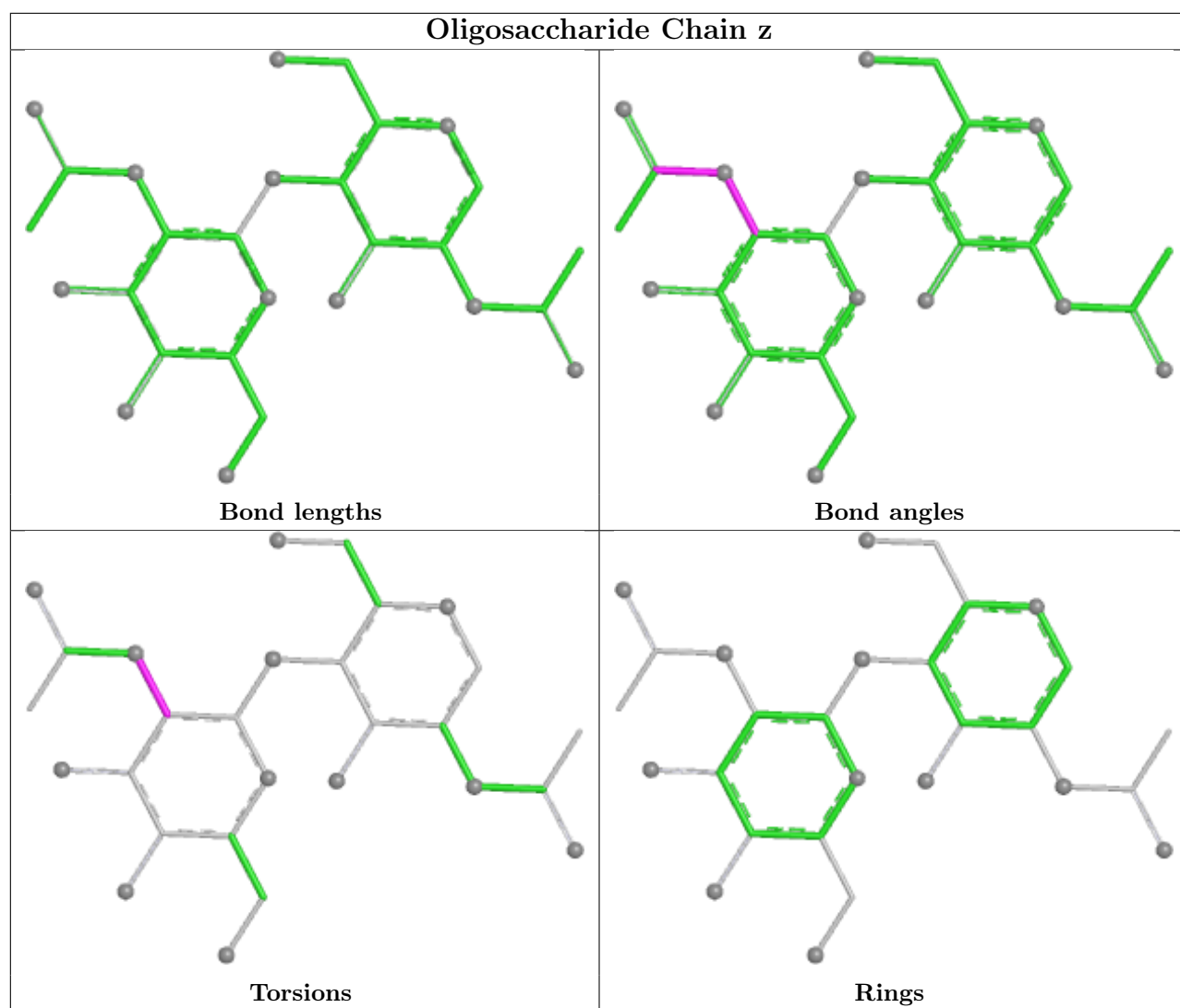


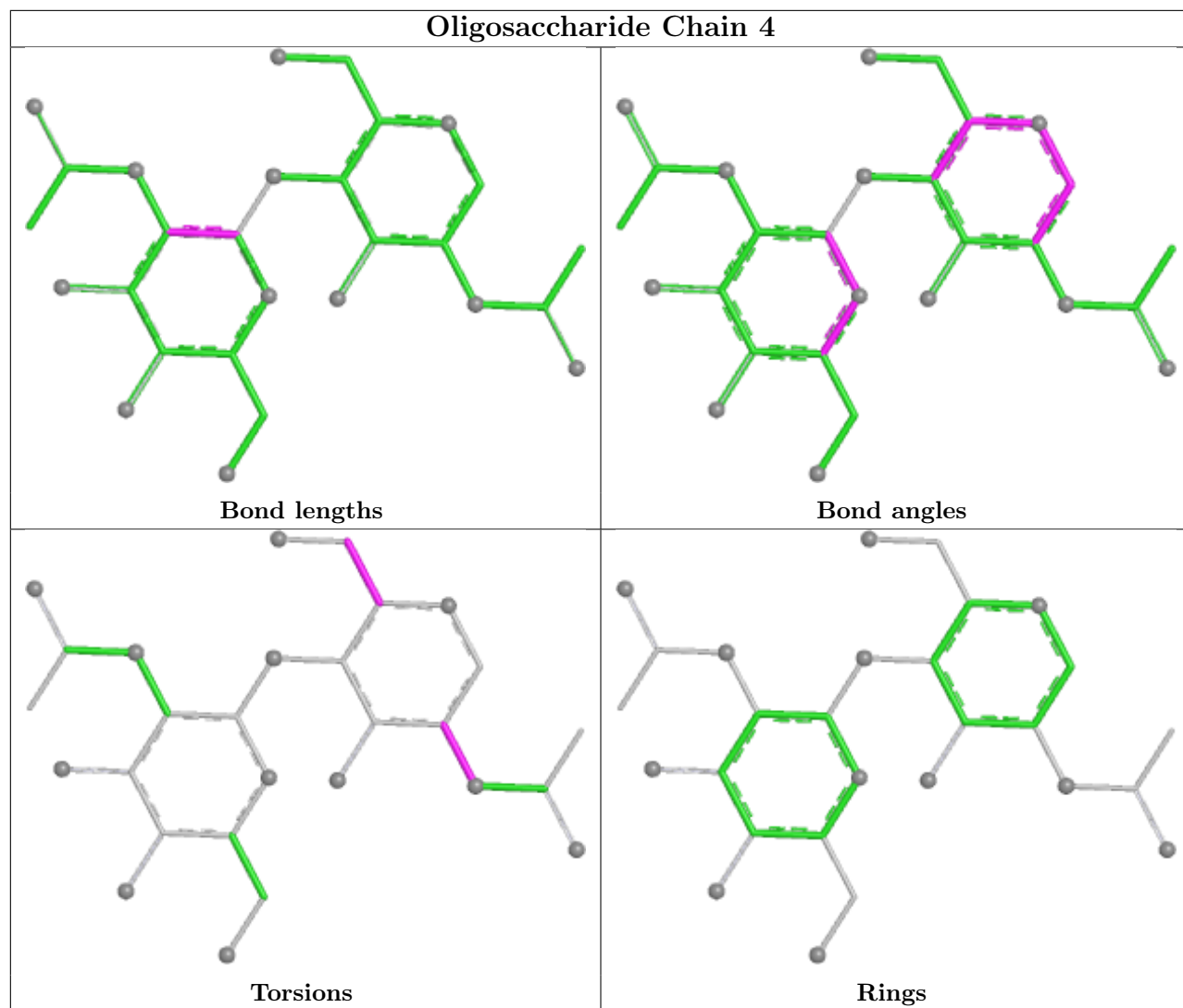


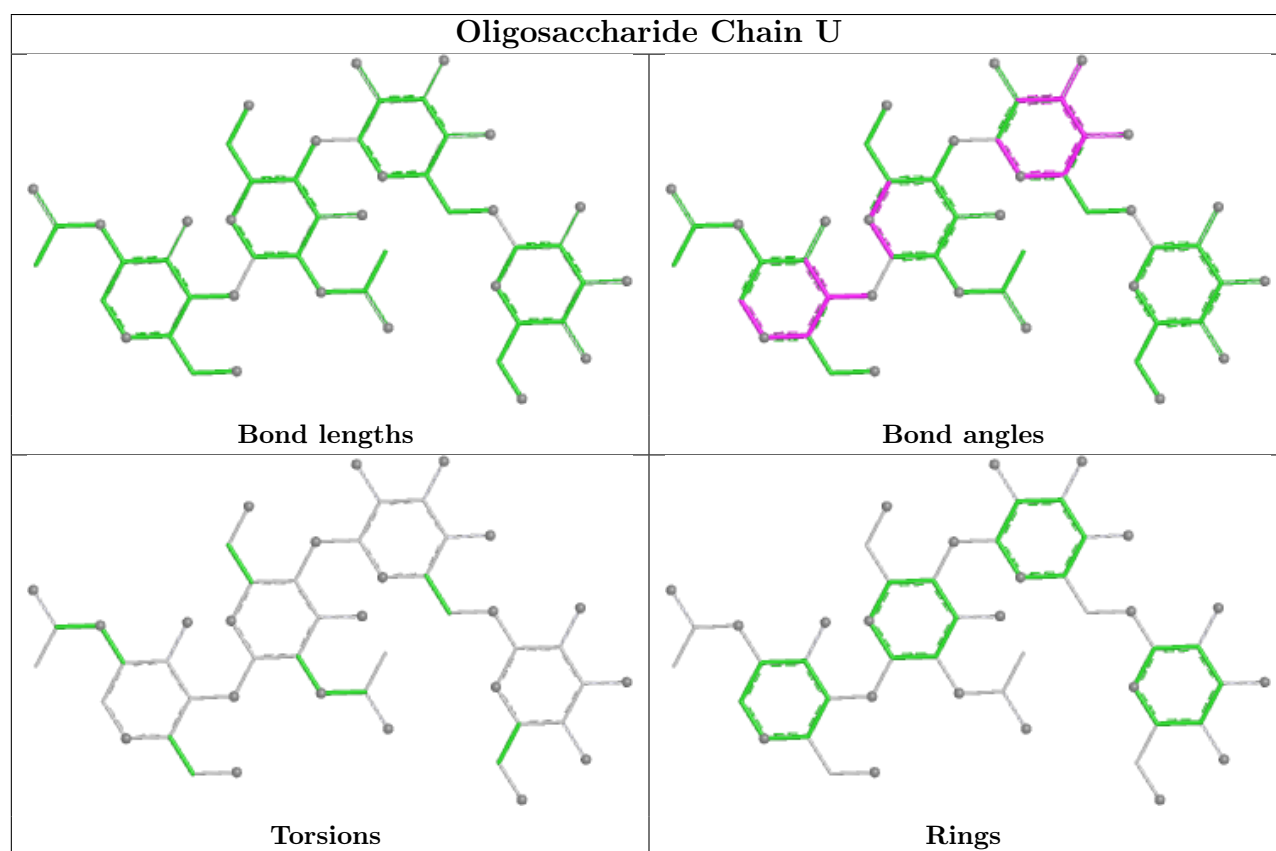
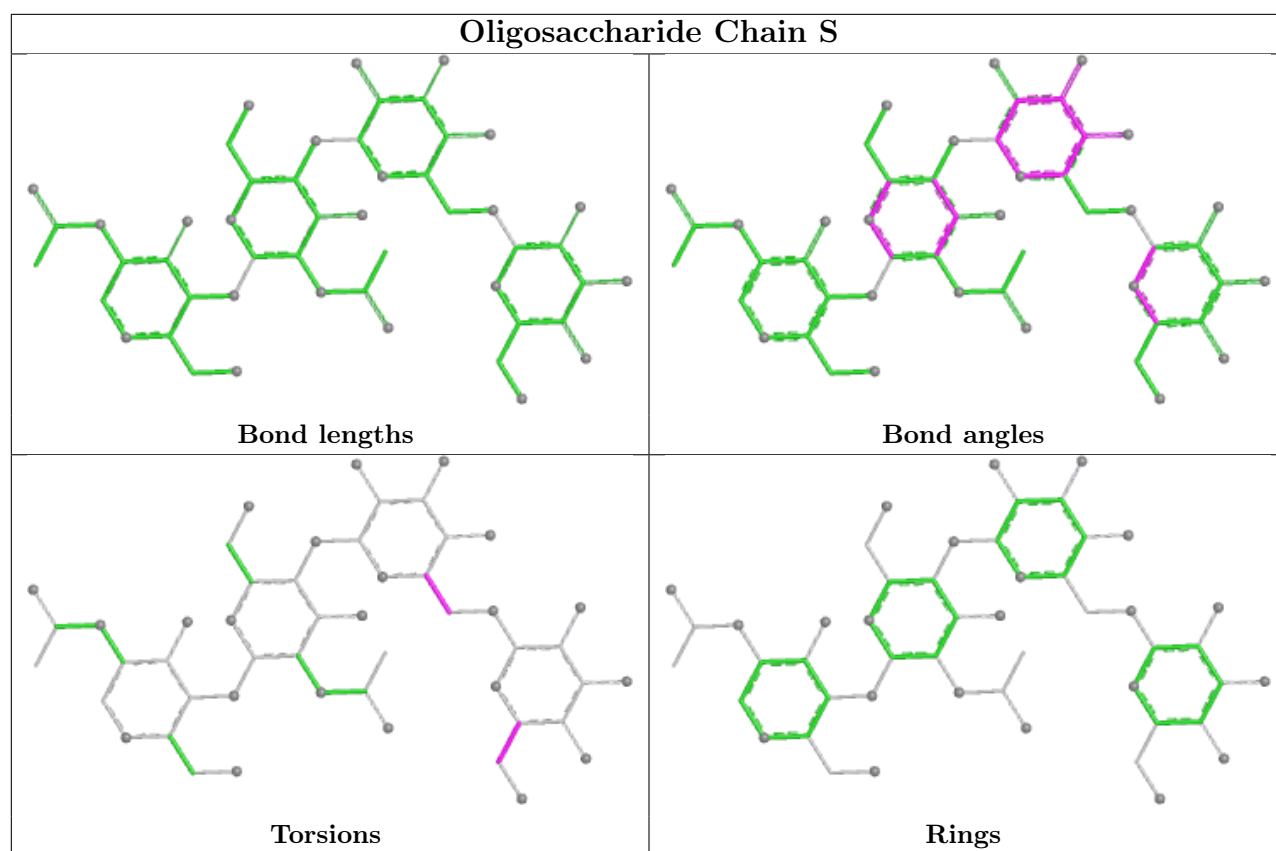


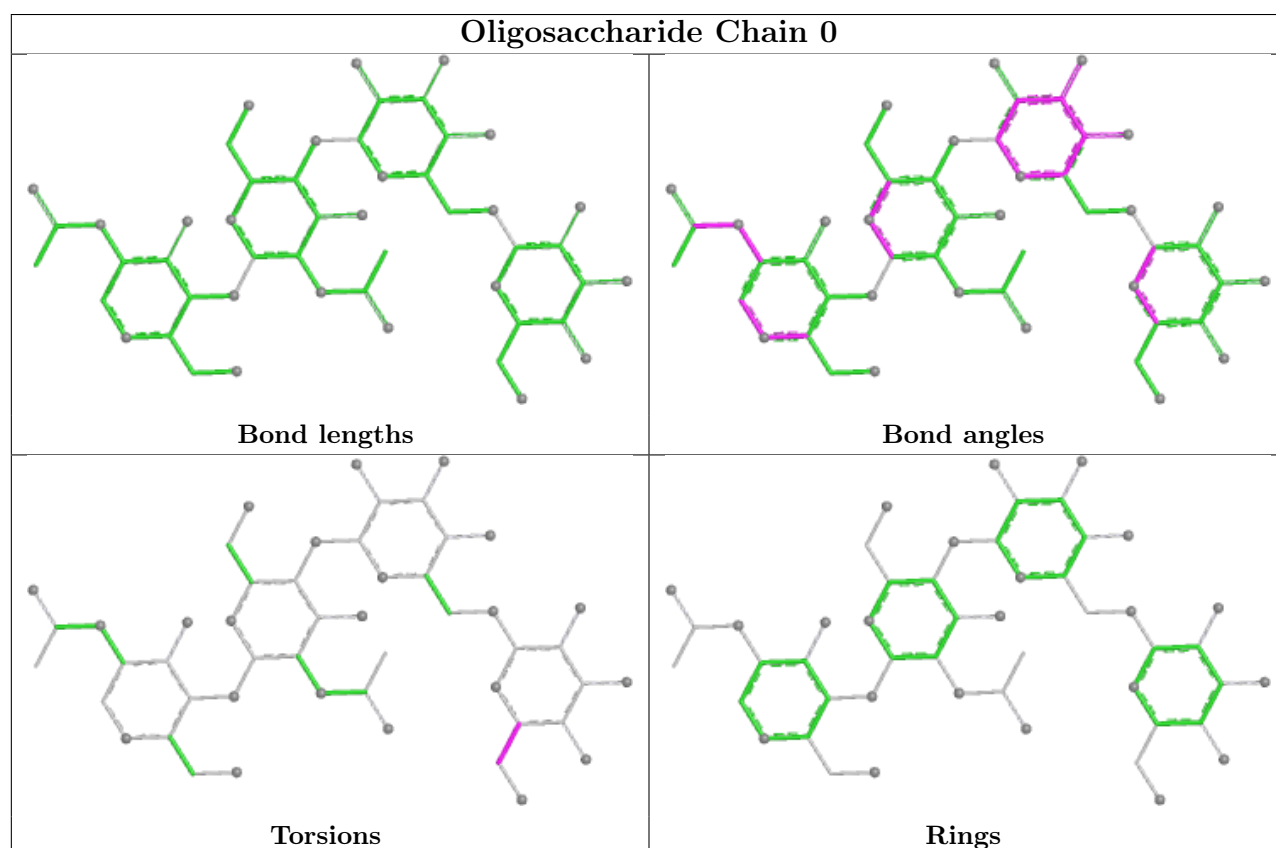
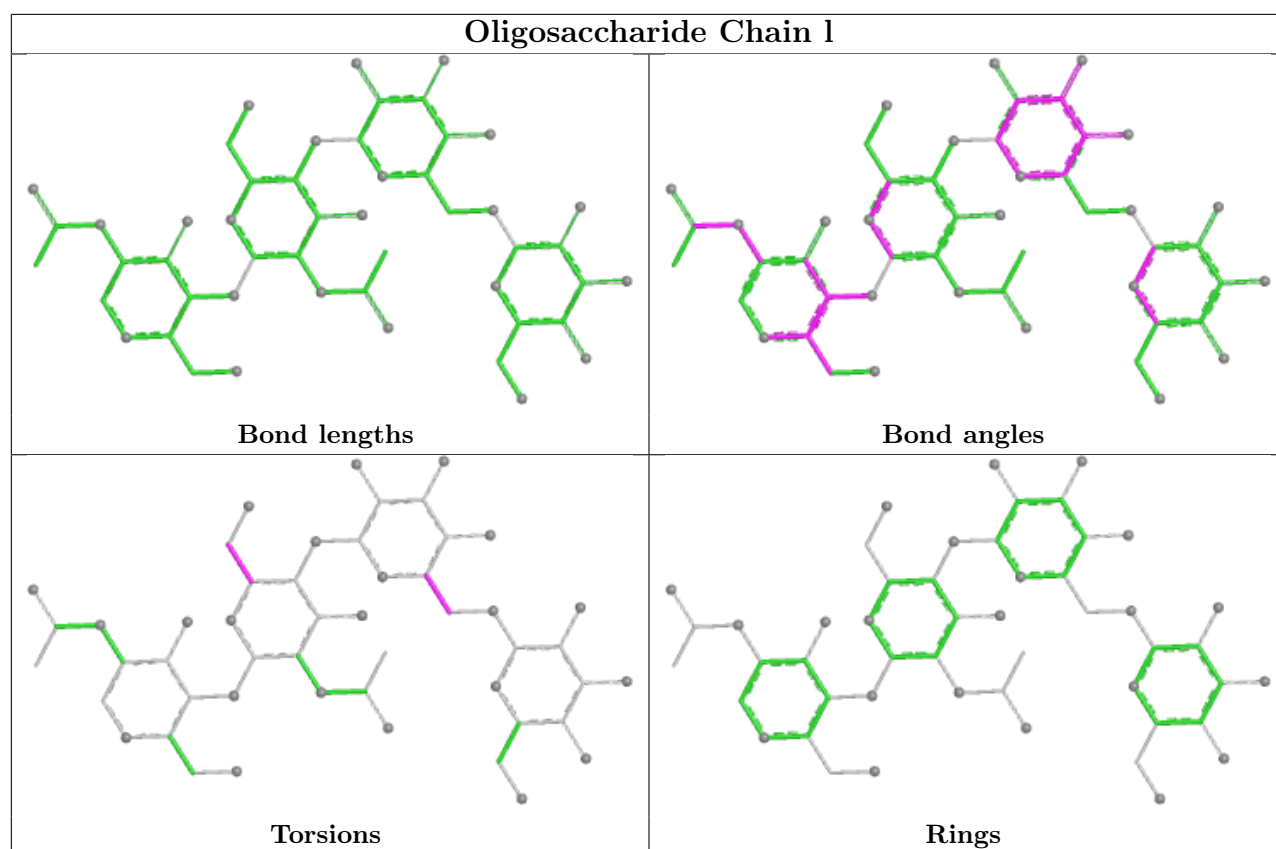


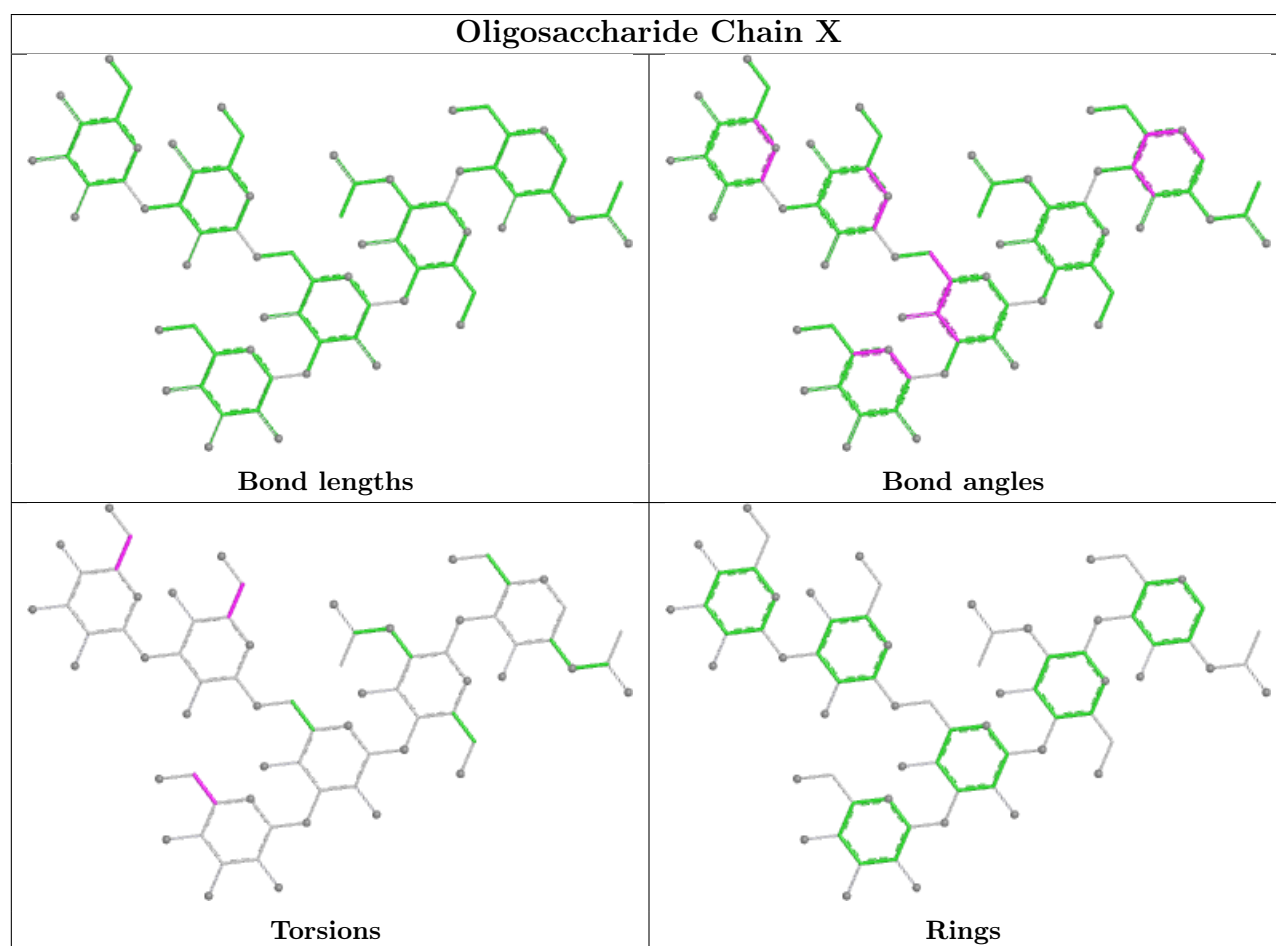
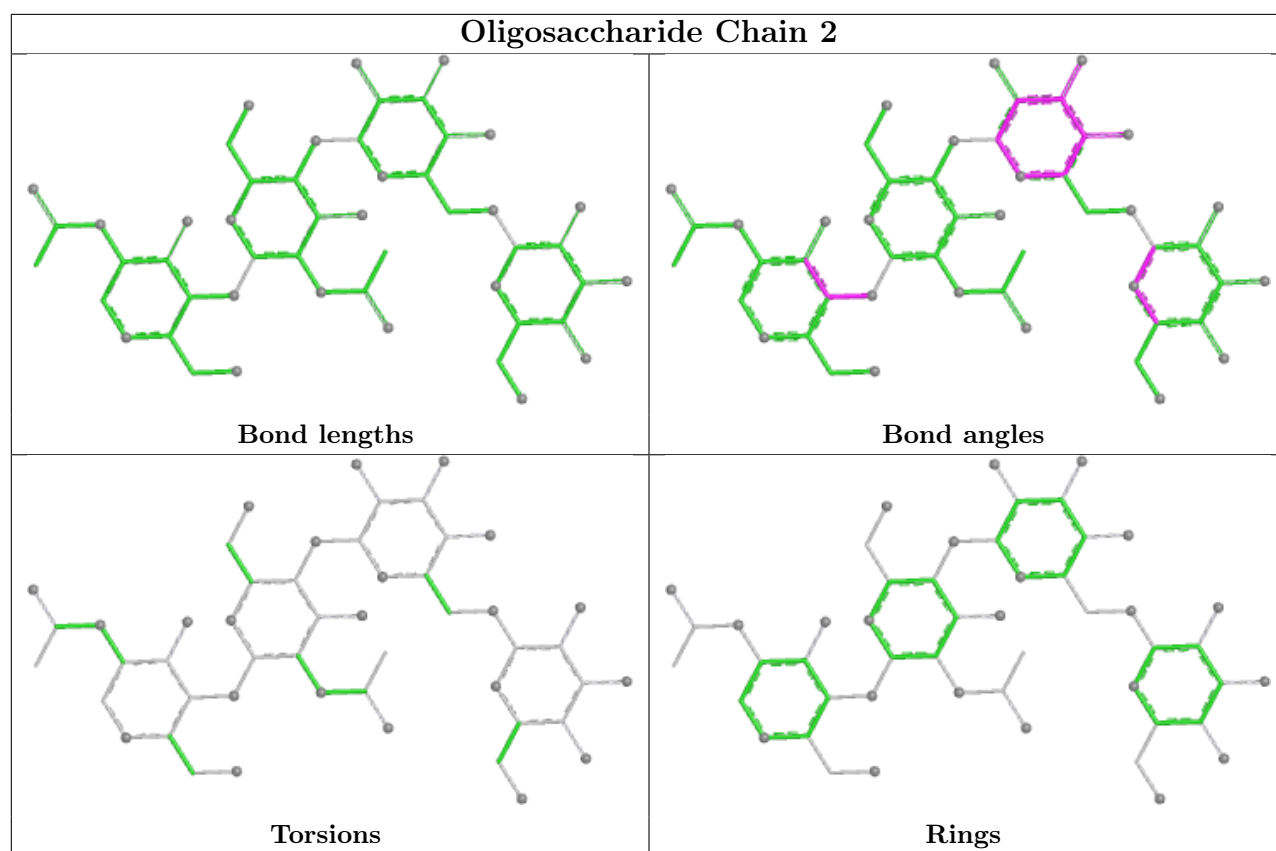


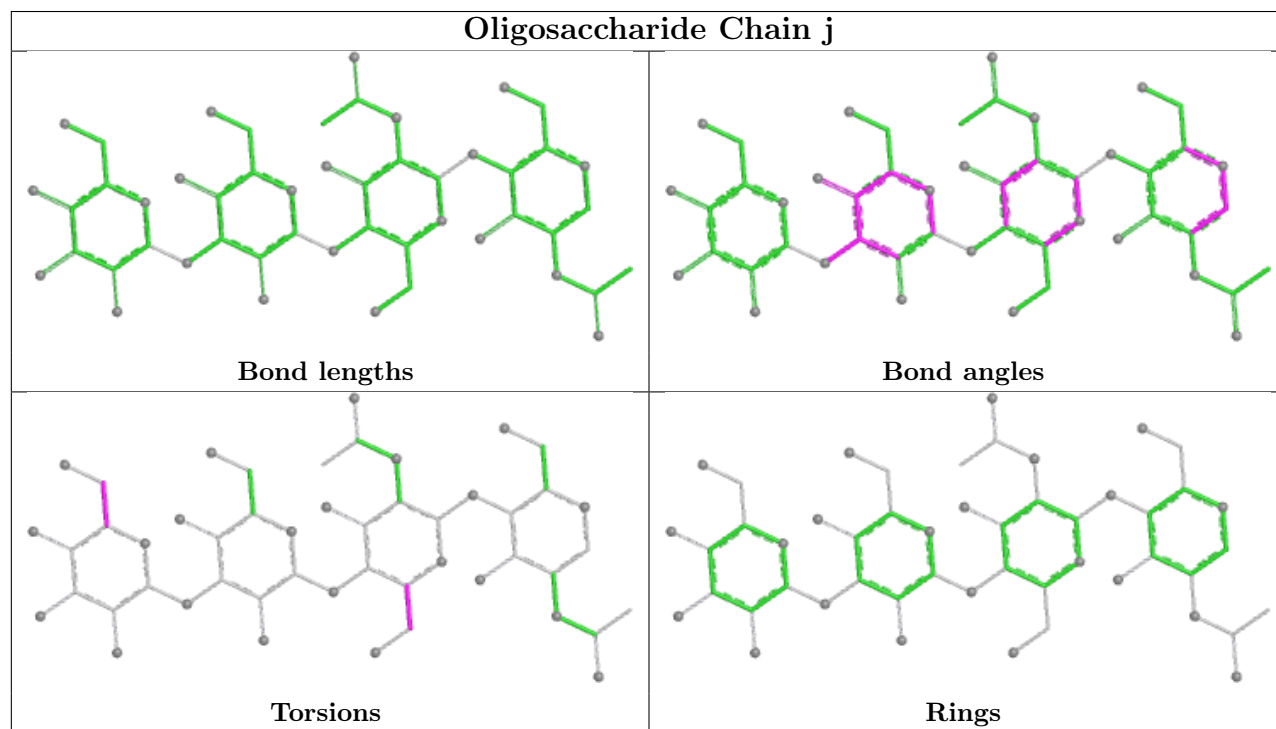
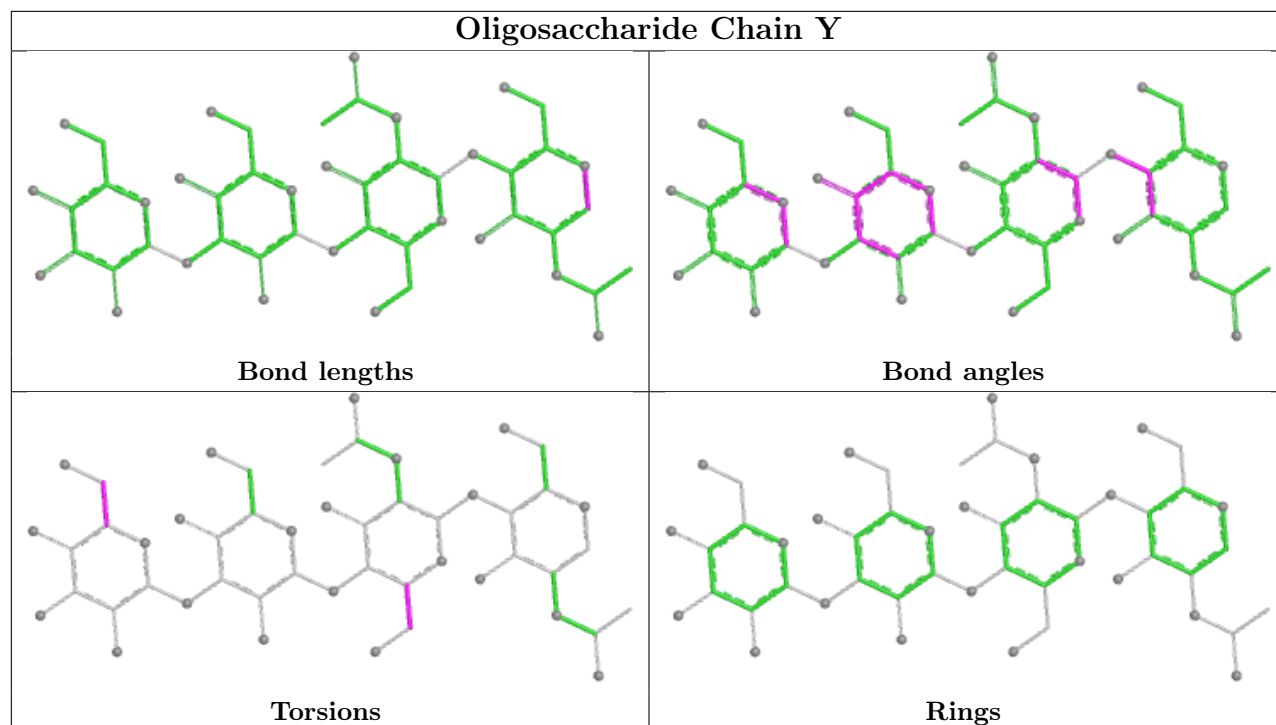


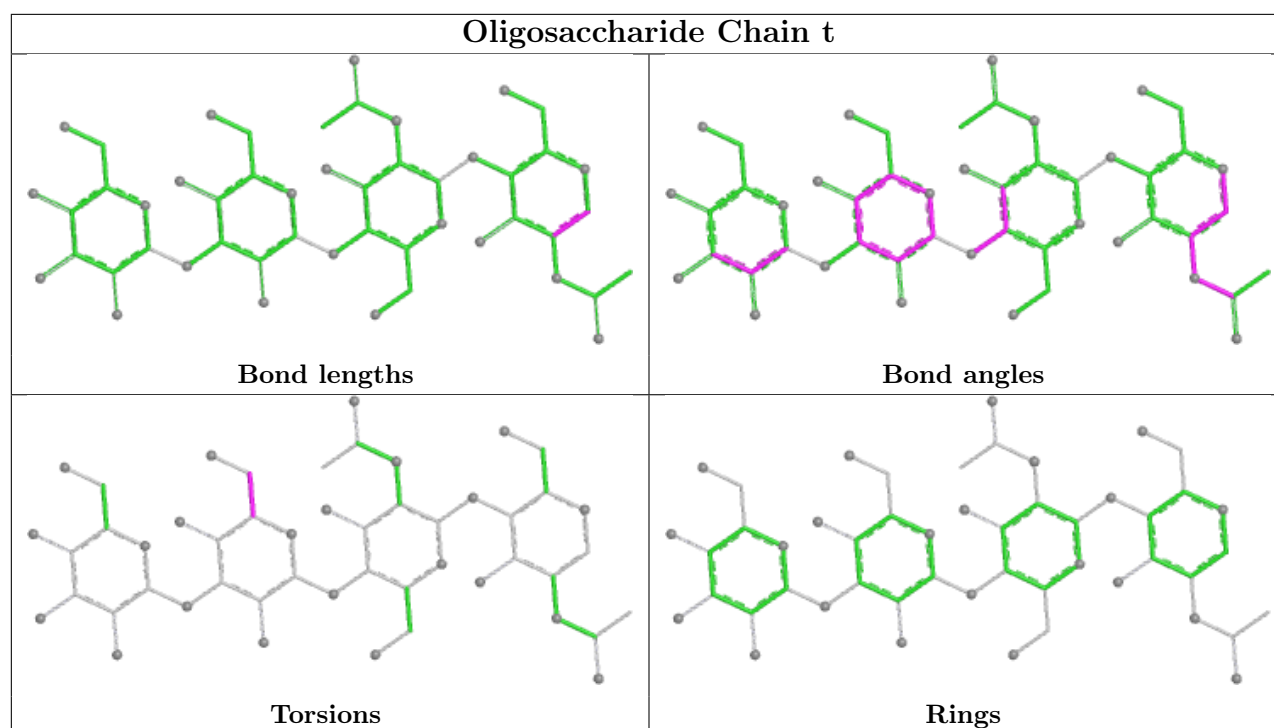












5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	NAG	B	1205	1	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
10	NAG	C	1202	1	14,14,15	0.71	0	17,19,21	1.41	2 (11%)
10	NAG	A	1208	1	14,14,15	0.74	0	17,19,21	1.71	3 (17%)
10	NAG	B	1202	1	14,14,15	0.73	0	17,19,21	1.25	2 (11%)
10	NAG	A	1203	1	14,14,15	0.75	0	17,19,21	1.22	2 (11%)
10	NAG	A	1206	1	14,14,15	0.79	0	17,19,21	0.94	0
10	NAG	A	1207	1	14,14,15	0.75	0	17,19,21	0.87	0
10	NAG	C	1204	1	14,14,15	0.71	0	17,19,21	1.48	1 (5%)
10	NAG	A	1204	1	14,14,15	0.72	0	17,19,21	2.94	5 (29%)
10	NAG	A	1202	1	14,14,15	0.72	0	17,19,21	1.54	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	A	1205	1	14,14,15	0.84	0	17,19,21	1.61	3 (17%)
10	NAG	B	1203	1	14,14,15	0.79	0	17,19,21	1.60	3 (17%)
10	NAG	A	1201	1	14,14,15	0.95	1 (7%)	17,19,21	1.51	3 (17%)
10	NAG	B	1204	1	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
10	NAG	C	1205	1	14,14,15	0.76	0	17,19,21	1.15	1 (5%)
10	NAG	B	1201	1	14,14,15	0.68	0	17,19,21	0.93	1 (5%)
10	NAG	C	1203	1	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
10	NAG	C	1201	1	14,14,15	0.68	0	17,19,21	1.49	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	1205	1	-	1/6/23/26	0/1/1/1
10	NAG	C	1202	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1208	1	-	3/6/23/26	0/1/1/1
10	NAG	B	1202	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1206	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1207	1	-	0/6/23/26	0/1/1/1
10	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1204	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1202	1	-	1/6/23/26	0/1/1/1
10	NAG	A	1205	1	-	2/6/23/26	0/1/1/1
10	NAG	B	1203	1	-	1/6/23/26	0/1/1/1
10	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
10	NAG	B	1204	1	-	0/6/23/26	0/1/1/1
10	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
10	NAG	B	1201	1	-	0/6/23/26	0/1/1/1
10	NAG	C	1203	1	-	0/6/23/26	0/1/1/1
10	NAG	C	1201	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1201	NAG	C1-C2	2.12	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1204	NAG	C2-N2-C7	7.48	132.92	122.90
10	A	1204	NAG	C1-O5-C5	6.67	121.12	112.19
10	A	1208	NAG	C2-N2-C7	5.25	129.93	122.90
10	A	1204	NAG	C1-C2-N2	-4.63	103.13	110.43
10	C	1204	NAG	C1-O5-C5	-4.61	106.01	112.19
10	B	1203	NAG	C2-N2-C7	4.60	129.07	122.90
10	A	1202	NAG	C2-N2-C7	4.29	128.65	122.90
10	C	1201	NAG	C1-O5-C5	3.91	117.43	112.19
10	A	1205	NAG	C2-N2-C7	3.86	128.08	122.90
10	A	1201	NAG	C1-O5-C5	3.59	117.00	112.19
10	A	1205	NAG	C1-O5-C5	3.53	116.92	112.19
10	A	1203	NAG	C2-N2-C7	3.22	127.22	122.90
10	C	1202	NAG	C2-N2-C7	3.22	127.22	122.90
10	A	1202	NAG	C1-O5-C5	3.14	116.40	112.19
10	C	1203	NAG	C2-N2-C7	3.02	126.95	122.90
10	A	1201	NAG	C1-C2-N2	3.00	115.16	110.43
10	C	1205	NAG	C2-N2-C7	2.97	126.88	122.90
10	A	1204	NAG	C8-C7-N2	-2.88	111.34	116.12
10	A	1201	NAG	C4-C3-C2	-2.84	106.86	111.02
10	B	1202	NAG	C2-N2-C7	2.67	126.47	122.90
10	C	1201	NAG	C2-N2-C7	2.60	126.39	122.90
10	C	1202	NAG	C1-O5-C5	2.51	115.55	112.19
10	B	1202	NAG	C1-O5-C5	2.46	115.49	112.19
10	A	1203	NAG	C1-O5-C5	2.44	115.46	112.19
10	A	1208	NAG	C1-C2-N2	2.38	114.19	110.43
10	B	1203	NAG	C1-O5-C5	2.31	115.28	112.19
10	A	1204	NAG	C3-C4-C5	-2.26	106.13	110.23
10	B	1204	NAG	C4-C3-C2	-2.25	107.71	111.02
10	A	1205	NAG	O5-C1-C2	2.21	114.71	111.29
10	B	1205	NAG	C1-O5-C5	2.16	115.09	112.19
10	B	1201	NAG	O5-C1-C2	-2.05	108.12	111.29
10	A	1208	NAG	O7-C7-N2	2.02	125.55	121.98
10	B	1203	NAG	C1-C2-N2	2.01	113.61	110.43

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1208	NAG	C1-C2-N2-C7
10	B	1205	NAG	O5-C5-C6-O6
10	C	1201	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	1202	NAG	O5-C5-C6-O6
10	A	1208	NAG	C4-C5-C6-O6
10	A	1208	NAG	O5-C5-C6-O6
10	C	1201	NAG	C1-C2-N2-C7
10	A	1205	NAG	C1-C2-N2-C7
10	B	1202	NAG	C1-C2-N2-C7
10	C	1202	NAG	C3-C2-N2-C7
10	B	1202	NAG	C3-C2-N2-C7
10	C	1202	NAG	C1-C2-N2-C7
10	C	1205	NAG	C1-C2-N2-C7
10	B	1203	NAG	C1-C2-N2-C7
10	C	1201	NAG	C3-C2-N2-C7
10	C	1205	NAG	C3-C2-N2-C7
10	A	1205	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1204	NAG	4	0
10	B	1201	NAG	1	0

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.

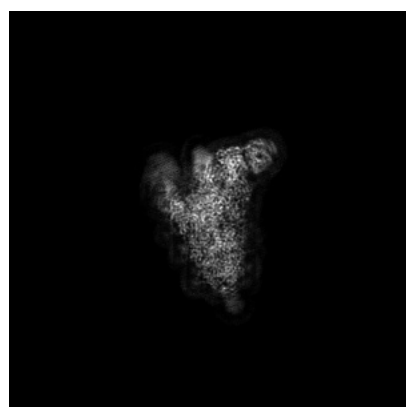
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70442. These allow visual inspection of the internal detail of the map and identification of artifacts.

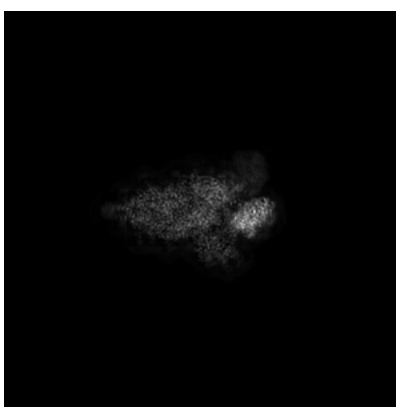
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

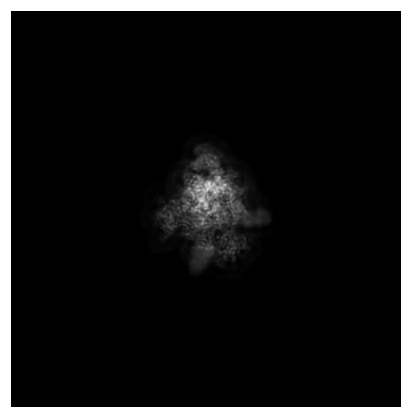
6.1.1 Primary map



X



Y

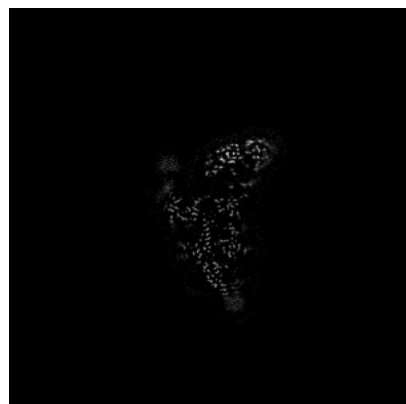


Z

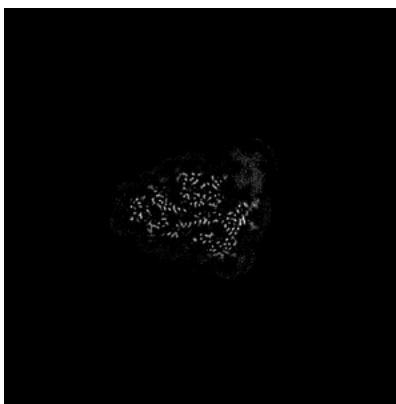
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

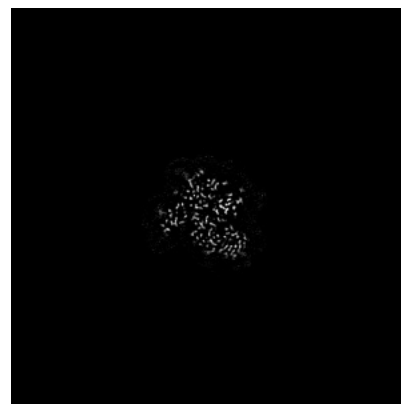
6.2.1 Primary map



X Index: 216



Y Index: 216



Z Index: 216

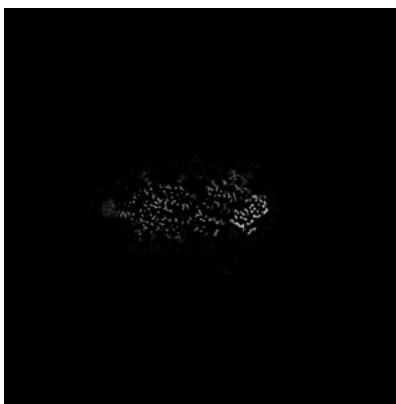
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 209



Y Index: 238

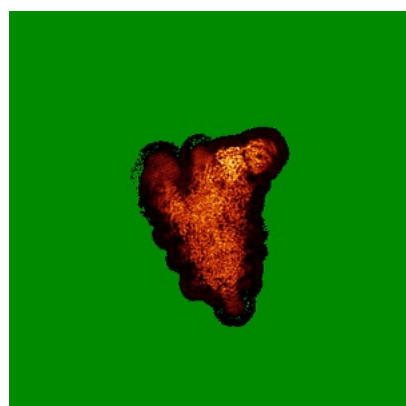


Z Index: 270

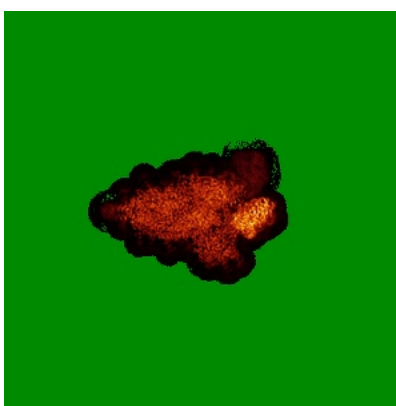
The images above show the largest variance slices of the map in three orthogonal directions.

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

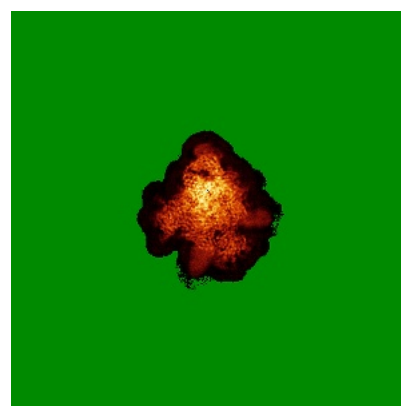
6.4.1 Primary map



X



Y

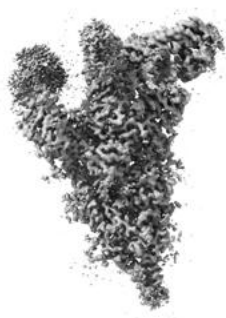


Z

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 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

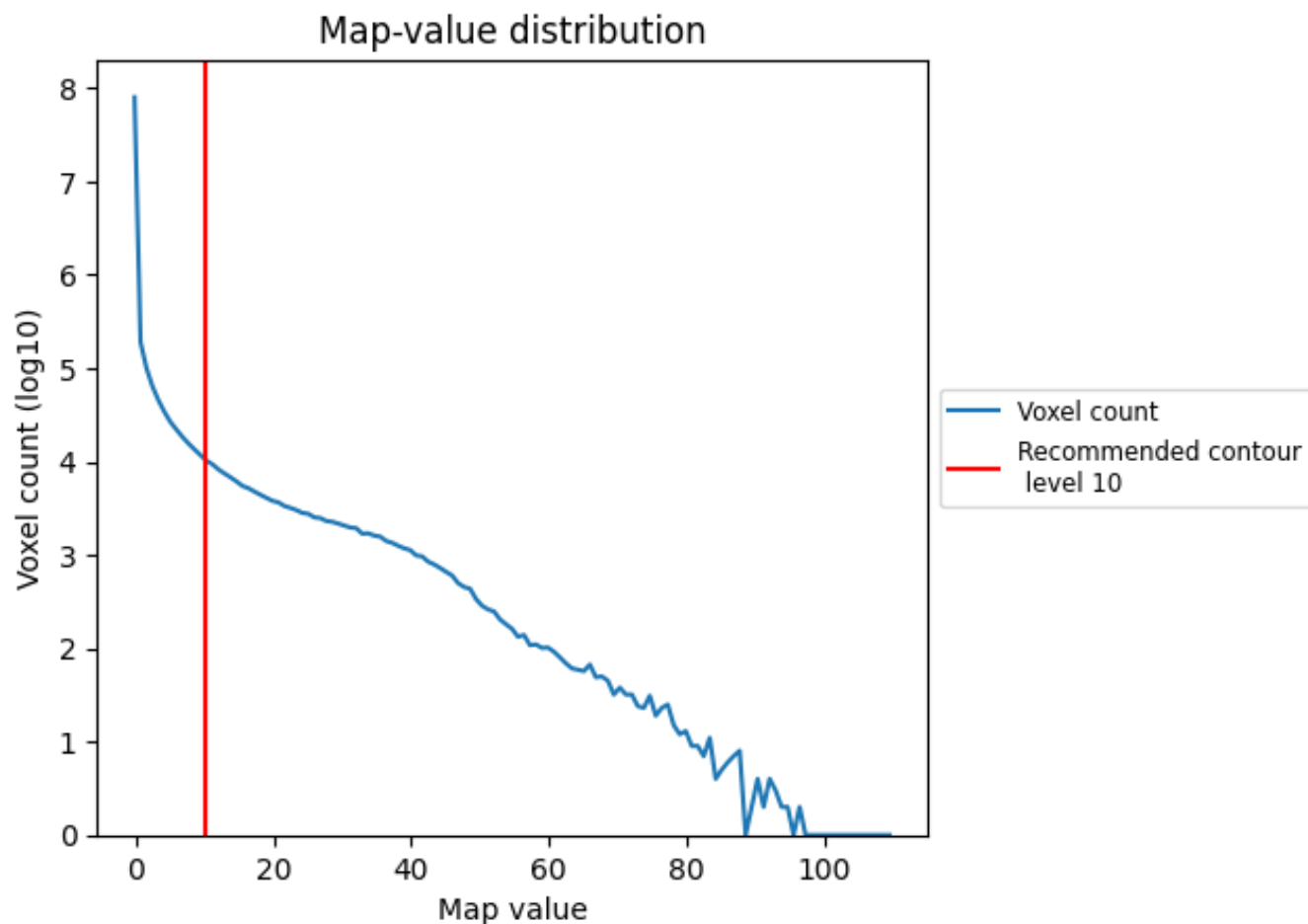
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

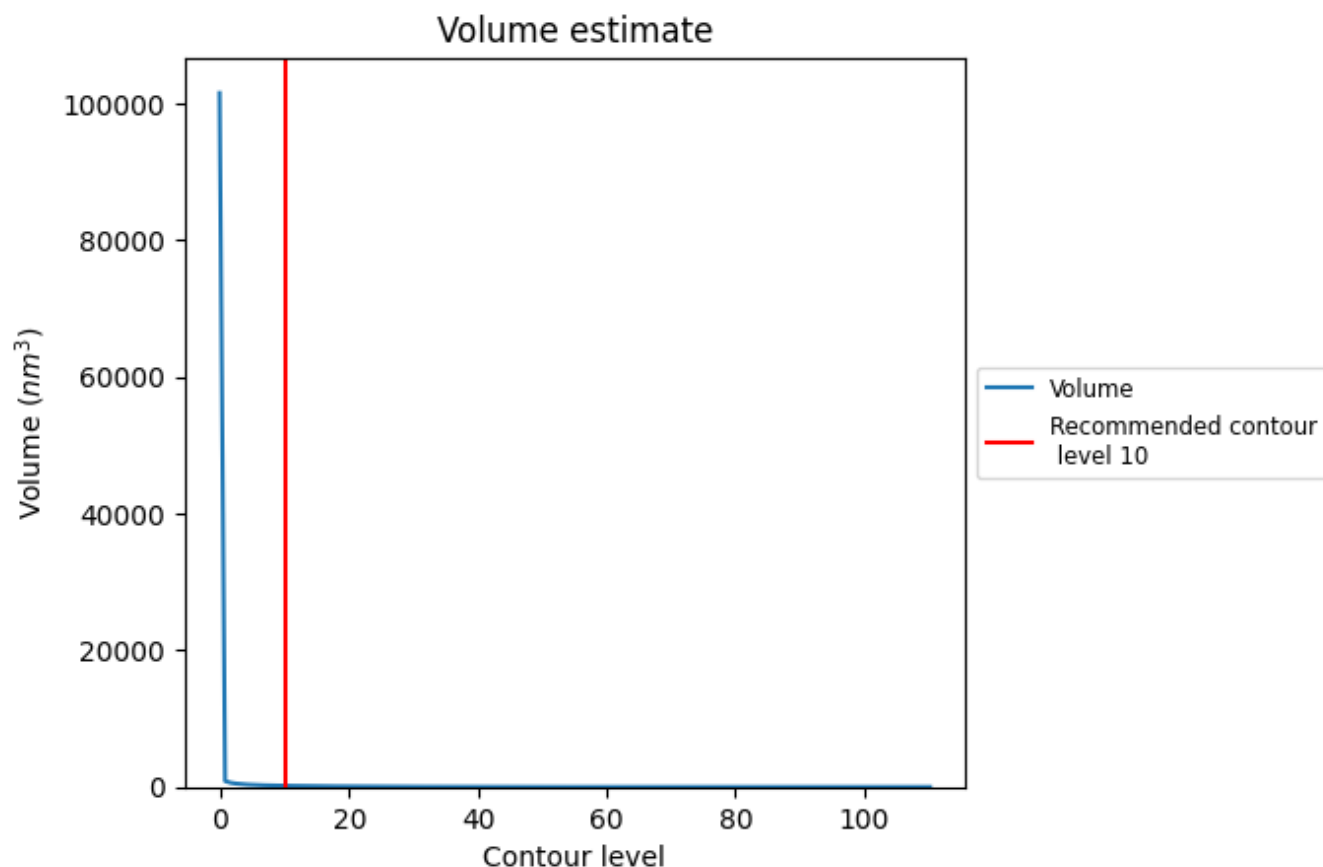
This section contains the results of statistical analysis of the map.

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.

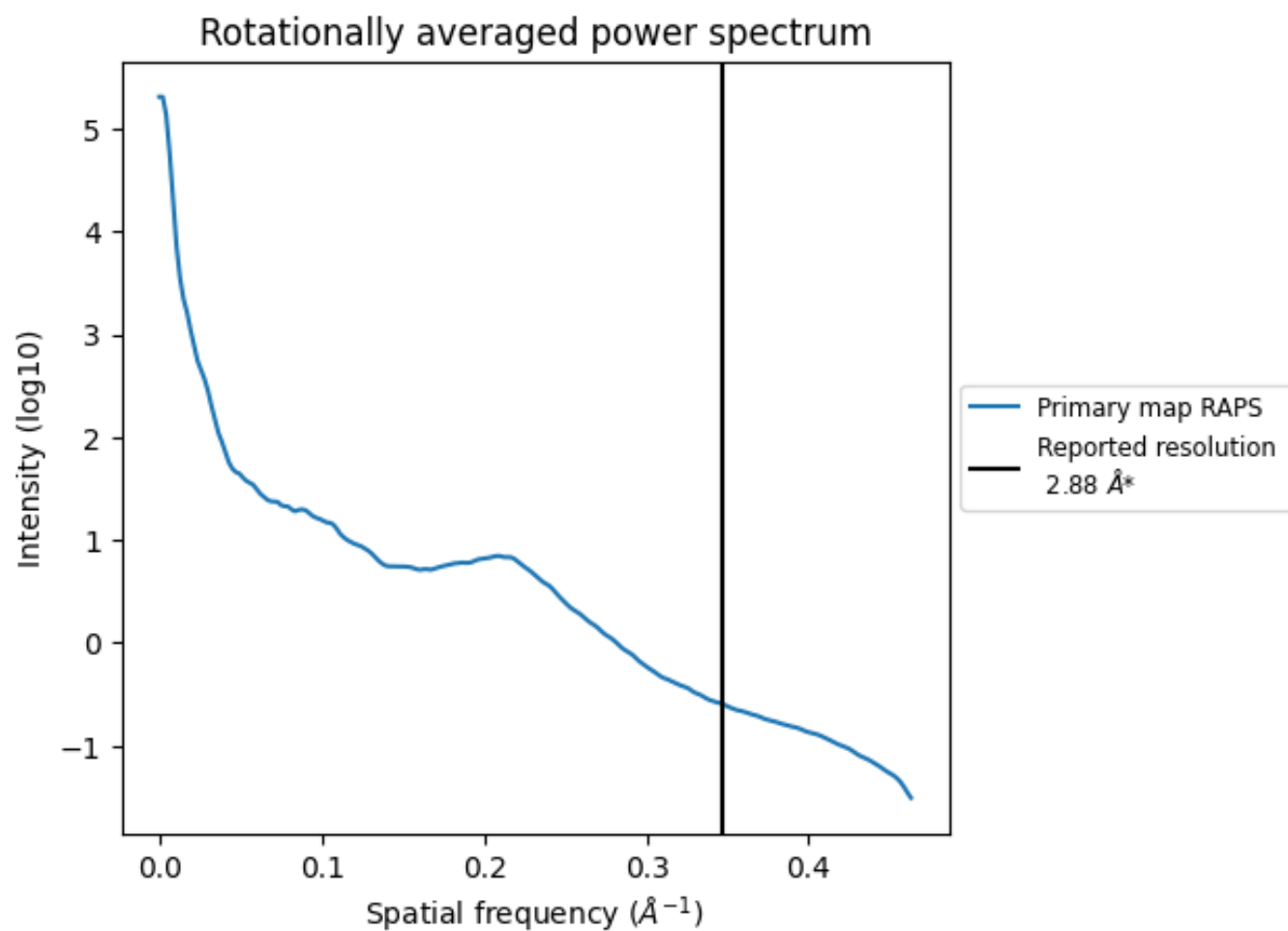
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm^3 ; this corresponds to an approximate mass of 159 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 0.347 Å⁻¹

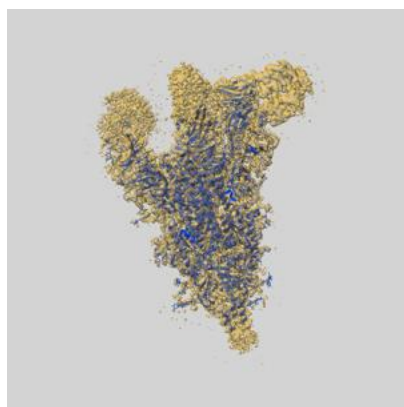
8 Fourier-Shell correlation

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

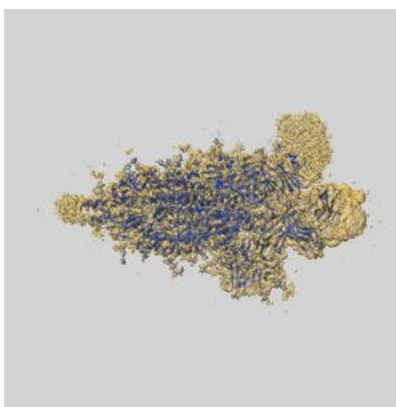
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70442 and PDB model 9OFQ. Per-residue inclusion information can be found in section 3 on page 18.

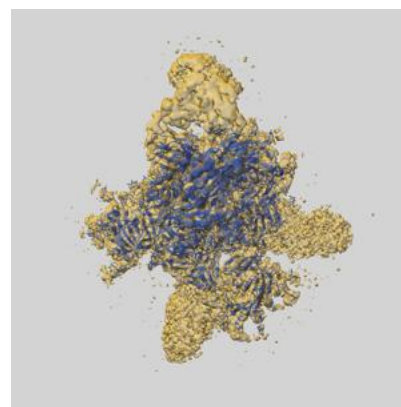
9.1 Map-model overlay [i](#)



X



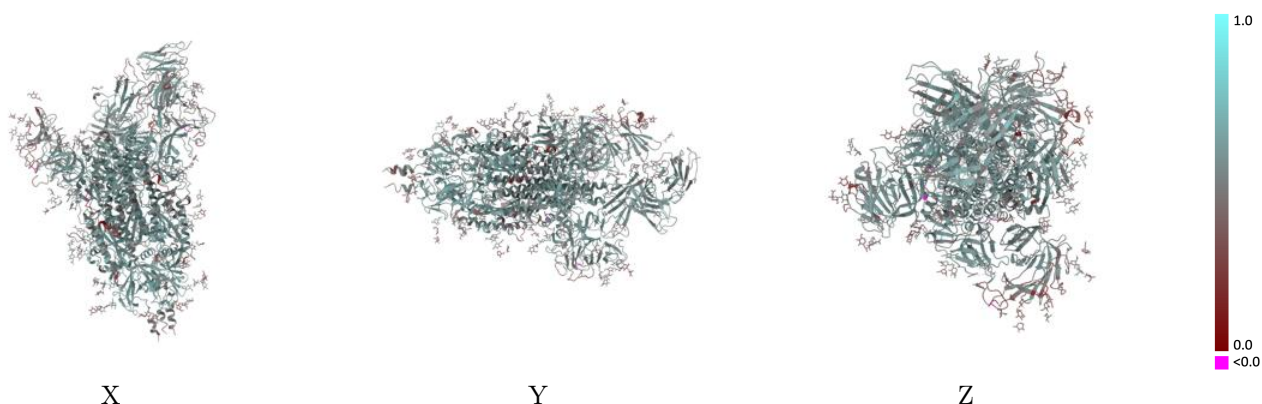
Y



Z

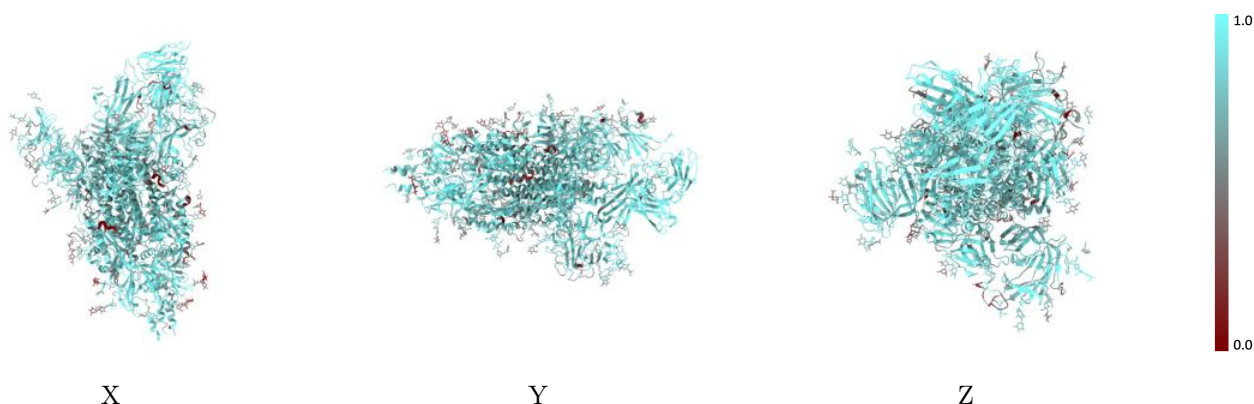
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



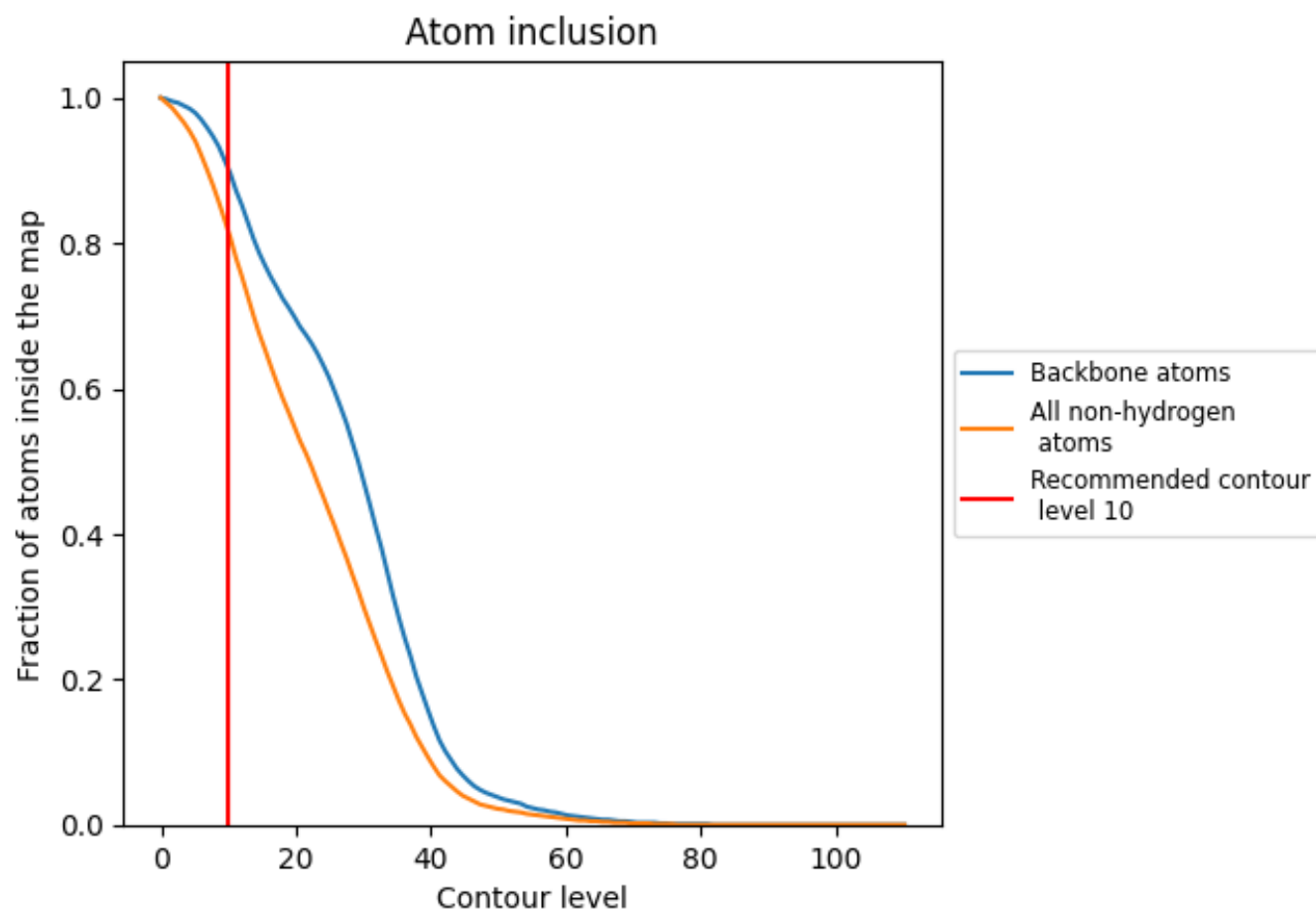
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.5370
0	 0.6600	 0.4420
1	 0.6070	 0.4830
2	 0.5000	 0.5050
3	 0.5570	 0.4220
4	 0.7500	 0.3410
A	 0.8280	 0.5450
B	 0.8320	 0.5560
C	 0.8040	 0.5350
D	 0.6390	 0.4330
E	 0.8720	 0.4440
F	 0.7180	 0.3910
G	 0.5710	 0.4200
H	 0.9610	 0.5620
I	 0.7500	 0.5080
J	 0.5710	 0.4320
K	 0.3930	 0.4330
L	 0.9410	 0.5300
M	 0.7140	 0.5170
N	 0.6790	 0.4250
O	 0.5000	 0.4480
P	 0.5000	 0.3720
Q	 0.6430	 0.5060
R	 0.5000	 0.4660
S	 0.6000	 0.4720
T	 0.5570	 0.4780
U	 0.4800	 0.4380
V	 0.4260	 0.4370
W	 0.2310	 0.3470
X	 0.8330	 0.5330
Y	 0.7800	 0.4260
Z	 0.6790	 0.3590
a	 0.6070	 0.4040
b	 0.7440	 0.5120
c	 0.9490	 0.4580



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Chain	Atom inclusion	Q-score
d	 0.5360	 0.4220
e	 0.6430	 0.4240
f	 0.5710	 0.4210
g	 0.3930	 0.3100
h	 0.6070	 0.4020
i	 0.5710	 0.4470
j	 0.5400	 0.4440
k	 0.5740	 0.4510
l	 0.5800	 0.4510
m	 0.5380	 0.4400
n	 0.6430	 0.3480
o	 0.6230	 0.4570
p	 0.7500	 0.4280
q	 0.7140	 0.4460
r	 0.7180	 0.3380
s	 0.6070	 0.4040
t	 0.7000	 0.4640
u	 0.5360	 0.5020
v	 0.6410	 0.3900
w	 0.4640	 0.4010
x	 0.4640	 0.4400
y	 0.7860	 0.4140
z	 0.6430	 0.4790