



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 06:08 AM UTC

PDB ID : 7W73 / pdb_00007w73
EMDB ID : EMD-32338
Title : Cryo-EM map of PEDV S protein with one protomer in the D0-up conformation while the other two in the D0-down conformation
Authors : Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on : 2021-12-03
Resolution : 6.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

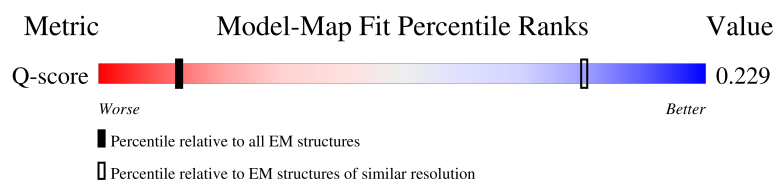
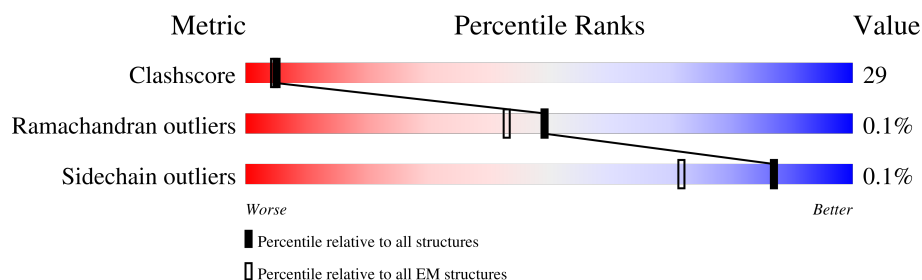
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.40 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.



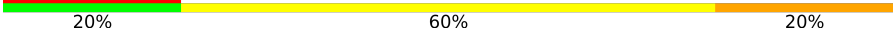
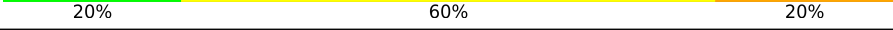
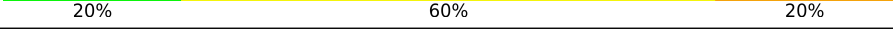
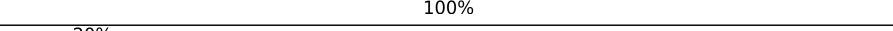
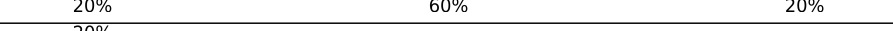
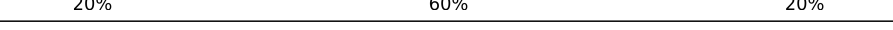
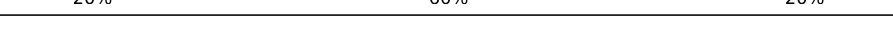
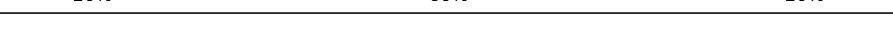
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	544 (5.90 - 6.90)

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	1386	
1	B	1386	
1	C	1386	
2	D	5	

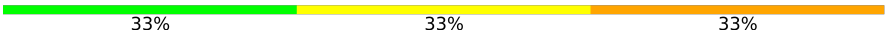
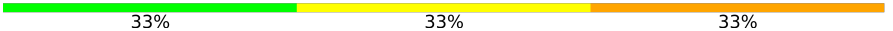
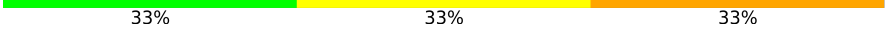
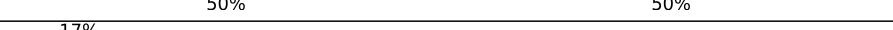
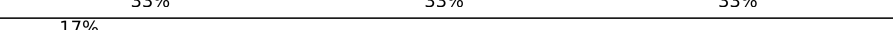
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Mol	Chain	Length	Quality of chain
2	F	5	
2	G	5	
2	H	5	
2	J	5	
2	N	5	
2	P	5	
2	R	5	
2	T	5	
2	U	5	
2	W	5	
2	X	5	
2	Y	5	
2	a	5	
2	b	5	
2	d	5	
2	g	5	
2	h	5	
2	j	5	
2	k	5	
2	m	5	
2	n	5	
2	o	5	
2	p	5	
2	u	5	
3	E	3	

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Mol	Chain	Length	Quality of chain
3	K	3	 67% 33%
3	Q	3	 33% 33% 33%
3	V	3	 33% 33% 33%
3	c	3	 33% 67%
3	f	3	 33% 33% 33%
3	l	3	 67% 33%
3	q	3	 67% 33%
3	r	3	 67% 33%
4	I	4	 25% 50% 50%
4	M	4	 50% 25% 25%
4	Z	4	 50% 50%
4	t	4	 25% 25% 75%
5	L	4	 25% 75%
6	O	6	 17% 50% 50%
6	S	6	 17% 50% 33% 17%
6	e	6	 17% 33% 33% 33%
6	i	6	 17% 67% 33%
7	s	2	 50% 50%

2 Entry composition [i](#)

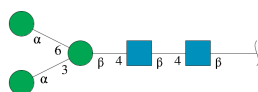
There are 8 unique types of molecules in this entry. The entry contains 30896 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1224	Total	C	N	O	S	0	0
			9400	5974	1556	1829	41		
1	B	1224	Total	C	N	O	S	0	0
			9400	5974	1556	1829	41		
1	C	1224	Total	C	N	O	S	0	0
			9400	5974	1556	1829	41		

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



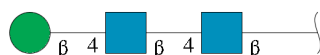
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	5	Total	C	N	O	0	0
			61	34	2	25		
2	F	5	Total	C	N	O	0	0
			61	34	2	25		
2	G	5	Total	C	N	O	0	0
			61	34	2	25		
2	H	5	Total	C	N	O	0	0
			61	34	2	25		
2	J	5	Total	C	N	O	0	0
			61	34	2	25		
2	N	5	Total	C	N	O	0	0
			61	34	2	25		
2	P	5	Total	C	N	O	0	0
			61	34	2	25		
2	R	5	Total	C	N	O	0	0
			61	34	2	25		
2	T	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	U	5	Total	C	N	O	0	0
			61	34	2	25		
2	W	5	Total	C	N	O	0	0
			61	34	2	25		
2	X	5	Total	C	N	O	0	0
			61	34	2	25		
2	Y	5	Total	C	N	O	0	0
			61	34	2	25		
2	a	5	Total	C	N	O	0	0
			61	34	2	25		
2	b	5	Total	C	N	O	0	0
			61	34	2	25		
2	d	5	Total	C	N	O	0	0
			61	34	2	25		
2	g	5	Total	C	N	O	0	0
			61	34	2	25		
2	h	5	Total	C	N	O	0	0
			61	34	2	25		
2	j	5	Total	C	N	O	0	0
			61	34	2	25		
2	k	5	Total	C	N	O	0	0
			61	34	2	25		
2	m	5	Total	C	N	O	0	0
			61	34	2	25		
2	n	5	Total	C	N	O	0	0
			61	34	2	25		
2	o	5	Total	C	N	O	0	0
			61	34	2	25		
2	p	5	Total	C	N	O	0	0
			61	34	2	25		
2	u	5	Total	C	N	O	0	0
			61	34	2	25		

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



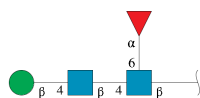
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	c	3	Total	C	N	O	0	0
			39	22	2	15		
3	f	3	Total	C	N	O	0	0
			39	22	2	15		
3	l	3	Total	C	N	O	0	0
			39	22	2	15		
3	q	3	Total	C	N	O	0	0
			39	22	2	15		
3	r	3	Total	C	N	O	0	0
			39	22	2	15		

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



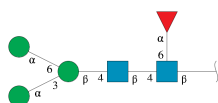
Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	4	Total	C	N	O	0	0
			49	28	2	19		
4	M	4	Total	C	N	O	0	0
			49	28	2	19		
4	Z	4	Total	C	N	O	0	0
			49	28	2	19		
4	t	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 5 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
5	L	4	Total	C	N	O	0	0
			50	28	2	20		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	6	Total	C	N	O	0	0
			71	40	2	29		
6	S	6	Total	C	N	O	0	0
			71	40	2	29		
6	e	6	Total	C	N	O	0	0
			71	40	2	29		
6	i	6	Total	C	N	O	0	0
			71	40	2	29		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
7	s	2	Total	C	N	O	0	0
			24	14	1	9		

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



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

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

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein

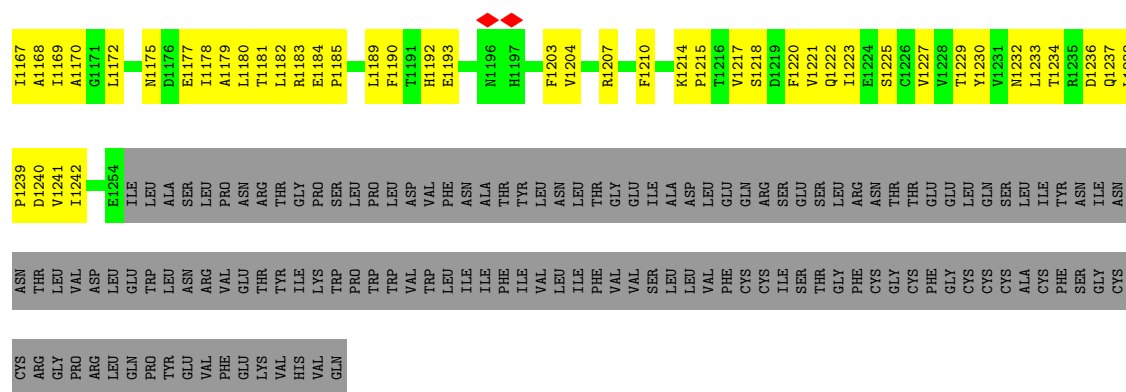


GLU	PHE	T1156	V1231	T1157	S1092	T1030	E948	Q860	P785	A693	Y606	G522	E452	K376
GLU	GLY	V1157	N1232	V1158	A1093	V1031	H951	L861	T785	V694	Y606	G522	V453	V377
GLN	CYS	L1158	L1233	V1159	L1094	H1032	N952	A862	F787	Y695	G612	HS24	G455	V384
SER	CYS	P1160	R1235	P1161	A1096	H1033	Y953	D870	M788	S696	V613	L529	A457	Y385
ALA	CYS	D1236	R1236	S1161	F1097	L1035	S954	G871	S789	E704	S817	I530	I458	K386
CYS	CYS	Q1237	Q1237		V1098	T1036		Y872	M790	Q705	L618	A531	F387	L388
THR	PHE	V1164		D1165	A1099	K1037	L957	T875	S791	A707	Y619	D533	I461	L391
ASN	SER	D1166		V1166	Q1100	V1038	L958	T876	R792	A707	Y619	D533	I461	L391
ASN	GLY	I1167		I1167	T1101	Q1039	L963	V877	E795	Q709	Y620	D533	I461	L391
CYS	CYS	D1244			L1102	E1040		L878	Q709	Q709	Y620	D533	I461	L391
ASN	CYS	L1172		L1172	T1103	V1041	F966	G879	Y796	D711	Q621	D533	I461	L391
THR	ARG	C1173		C1173	L1104	V1042	T967	L878	Q709	D711	Q621	D533	I461	L391
LEU	GLY	N1174		N1174	Y1105	V1042	S881	V880	L797	D712	Q621	D533	I461	L391
ASP	ARG	N1175		N1175	T1106	Q1045	A969	V882	Q798	D712	Q621	D533	I461	L391
LEU	LEU	E1254		E1254	E1107				Y800	L713	Q621	D533	I461	L391
GLU	GLN	L1180		L1180	V1108	A1048	P973	P885	C808	G715	L627	D545	K402	K402
TRP	PRO	T1181		T1181	Q109	L1049	F974		S817	T546	Q470	T546	Y403	Y403
LEU	ALA	L1182		L1182	A1110	T1050	S975	G888	R818	T546	Q470	T546	Y403	Y403
ASN	SER	R1183		R1183	S1111	Q1051		R889	S817	T546	Q470	T546	Y403	Y403
ARG	LEU	E1184		E1184	R1112	T1053	A977	V890	R818	T546	Q470	T546	Y403	Y403
GLU	PHE	L1187		L1187	K1113	V1054	Y978	Q892	C819	T546	Q470	T546	Y403	Y403
THR	GLY	Q1116		Q1116	A1115	Q1055		K893	K820	T546	Q470	T546	Y403	Y403
LYS	VAL	L1188		L1188	Q1117	Q1057	L982	R894	Q821	T546	Q470	T546	Y403	Y403
VAL	VAL	F1190		F1190	H1059	Q1057	N983	S895	L822	T546	Q470	T546	Y403	Y403
VAL	VAL	L1194		L1194	V1119	H1059	Y984	F896	L823	T546	Q470	T546	Y403	Y403
PRO	SER	L1197		L1197	F1120	Q1061	A986	I897	T824	T546	Q470	T546	Y403	Y403
TRP	LEU	T1198		T1198	V1123	Q1062	L987	D899	A829	T546	Q470	T546	Y403	Y403
ASP	LEU	A1199		A1199	Q1126	I1063	Q988		C830	T546	Q470	T546	Y403	Y403
VAL	VAL	Y1202		Y1202	S1127	S1064	L989	F902	K831	T546	Q470	T546	Y403	Y403
LEU	PHE	F1203		F1203	Q1128	S1066	L992	K904	T832	T546	Q470	T546	Y403	Y403
ALA	ASN	V1204		V1204	R1129	I1067	Q993	V906	E834	T546	Q470	T546	Y403	Y403
THR	THR	S1205		S1205	Y1130	D1068	R994	V906	S835	T546	Q470	T546	Y403	Y403
LEU	LEU	M1209		M1209	G1131	D1069	N995	T907	A836	T546	Q470	T546	Y403	Y403
ASN	THR	F1210		F1210	F1132	I1070	Q996	N908	L837	T546	Q470	T546	Y403	Y403
LEU	THR	E1211		E1211		Y1071	L998	G909	Q838	T546	Q470	T546	Y403	Y403
THR	THR	P1212		P1212	G1135	S1072	L998	D916	L839	T546	Q470	T546	Y403	Y403
GLY	GLY	K1213		K1213	D1136	R1073	L999	Y917	S840	T546	Q470	T546	Y403	Y403
VAL	VAL	P1215		P1215	E1137	L1074	A1000	K918	A841	T546	Q470	T546	Y403	Y403
SER	SER	T1216		T1216	H1139	I1076	S1002	N222	E842	T546	Q470	T546	Y403	Y403
LEU	LEU	V1217		V1217	I1140	S1078	F1003	G823	E844	T546	Q470	T546	Y403	Y403
VAL	VAL	S1216		S1216	F1141	A1079	G1008	R924	V846	T546	Q470	T546	Y403	Y403
GLN	GLN	F1220		F1220	L1143	D1080	N1009	L929	E847	T546	Q470	T546	Y403	Y403
ARG	ARG	V1221		V1221	V1144	V1081			V848	T546	Q470	T546	Y403	Y403
SER	SER	I1223		I1223	Q1145	Q1082	A1013	A832	N849	T546	Q470	T546	Y403	Y403
THR	THR	E1224		E1224	Q1149	D1084	F1014	Q933	L852	T546	Q470	T546	Y403	Y403
GLY	GLY	S1225		S1225	G1150	L1086	S1022	Y934	T853	T546	Q470	T546	Y403	Y403
PHE	PHE	C1226		C1226	L1151	I1087	D1023	Y935	R854	T546	Q470	T546	Y403	Y403
CYS	CYS	V1227		V1227	L1152	T1088	T1024	S936	E855	T546	Q470	T546	Y403	Y403
THR	THR				F1153	Q1089	S1025	V838	E857	T546	Q470	T546	Y403	Y403
CYS	CYS				L1154	R1090			E858	T546	Q470	T546	Y403	Y403
									L859	T546	Q470	T546	Y403	Y403
										T784	G692	G605	F521	I451

• Molecule 1: Spike glycoprotein







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

Chain D: 60% 40%



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

Chain F: 40% 60%



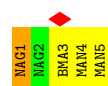
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 20% 80%

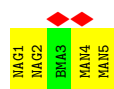


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 20% 20% 60%



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



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



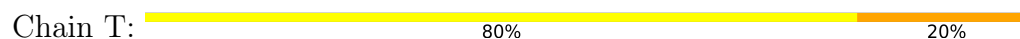
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



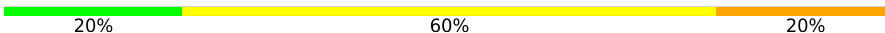
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

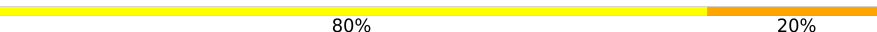


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 

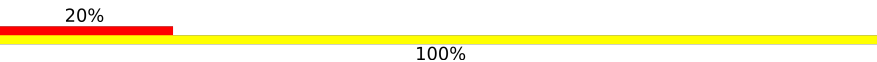


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

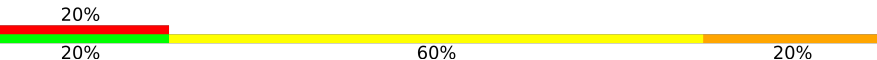


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

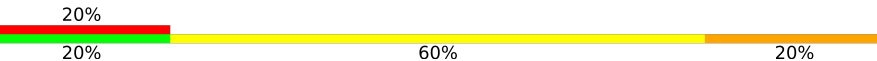


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

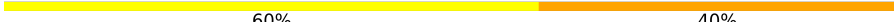


- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 



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

Chain d:  60% 40%

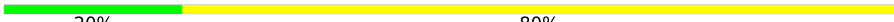


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  40% 60%

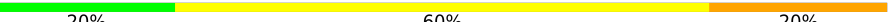


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  20% 80%

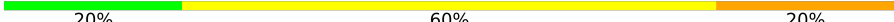


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  20% 60% 20%

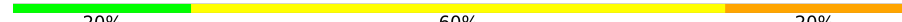


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  20% 60% 20%



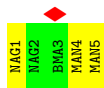
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  20% 60% 20%



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

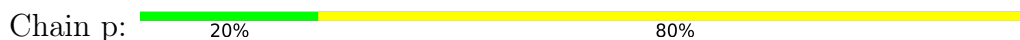
nose



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



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



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



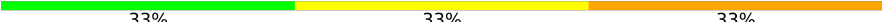
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

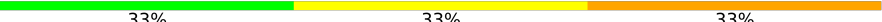


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  33% 33% 33%



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

Chain V:  33% 33% 33%

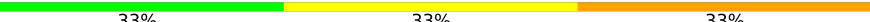


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  33% 67%



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

Chain f:  33% 33% 33%



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

Chain l:  67% 33%



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

Chain q:  67% 33%



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

Chain r:  67% 33%



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

Chain I:  25% 50% 50%



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

Chain M:  50% 25% 25%



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

Chain Z:  50% 50%

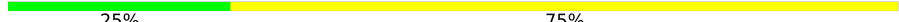


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  25% 25% 75%

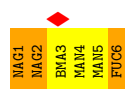


- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

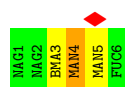
Chain L:  25% 75%



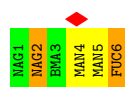
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



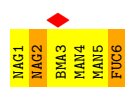
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9319	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.512	Depositor
Minimum map value	-0.687	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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, FUC, 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	0.26	0/9610	0.48	0/13095
1	B	0.25	0/9610	0.46	0/13095
1	C	0.26	0/9610	0.47	0/13095
All	All	0.25	0/28830	0.47	0/39285

There are no bond length outliers.

There are no bond angle outliers.

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	9400	0	9090	606	0
1	B	9400	0	9090	595	0
1	C	9400	0	9090	569	0
2	D	61	0	52	3	0
2	F	61	0	52	3	0
2	G	61	0	52	8	0
2	H	61	0	52	1	0
2	J	61	0	52	1	0
2	N	61	0	52	2	0
2	P	61	0	52	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	61	0	52	4	0
2	T	61	0	52	2	0
2	U	61	0	52	4	0
2	W	61	0	52	2	0
2	X	61	0	52	4	0
2	Y	61	0	52	1	0
2	a	61	0	52	1	0
2	b	61	0	52	1	0
2	d	61	0	52	4	0
2	g	61	0	52	1	0
2	h	61	0	52	2	0
2	j	61	0	52	2	0
2	k	61	0	52	3	0
2	m	61	0	52	1	0
2	n	61	0	52	0	0
2	o	61	0	52	5	0
2	p	61	0	52	0	0
2	u	61	0	52	7	0
3	E	39	0	34	2	0
3	K	39	0	34	0	0
3	Q	39	0	34	2	0
3	V	39	0	34	4	0
3	c	39	0	34	1	0
3	f	39	0	34	3	0
3	l	39	0	34	1	0
3	q	39	0	34	1	0
3	r	39	0	34	1	0
4	I	49	0	43	3	0
4	M	49	0	43	1	0
4	Z	49	0	43	0	0
4	t	49	0	43	4	0
5	L	50	0	43	6	0
6	O	71	0	61	5	0
6	S	71	0	61	1	0
6	e	71	0	61	2	0
6	i	71	0	61	2	0
7	s	24	0	22	5	0
8	A	84	0	78	6	0
8	B	98	0	91	10	0
8	C	84	0	78	1	0
All	All	30896	0	29604	1756	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 29.

The worst 5 of 1756 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:VAL:HG12	1:B:472:LYS:HZ2	1.35	0.90
1:C:795:GLU:HB3	1:C:1153:PHE:HB2	1.51	0.90
1:A:337:LEU:HB2	1:A:345:PHE:HB2	1.55	0.87
1:A:1140:ILE:HG13	1:A:1158:LEU:HD23	1.55	0.85
1:B:1069:ASP:O	1:B:1073:ARG:NH1	2.09	0.85

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	1222/1386 (88%)	1127 (92%)	93 (8%)	2 (0%)	43	77
1	B	1222/1386 (88%)	1119 (92%)	101 (8%)	2 (0%)	43	77
1	C	1222/1386 (88%)	1124 (92%)	97 (8%)	1 (0%)	48	83
All	All	3666/4158 (88%)	3370 (92%)	291 (8%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	ALA
1	A	710	ASP
1	B	353	SER
1	C	710	ASP
1	B	710	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1049/1199 (88%)	1049 (100%)	0	100	100
1	B	1049/1199 (88%)	1048 (100%)	1 (0%)	88	89
1	C	1049/1199 (88%)	1047 (100%)	2 (0%)	87	87
All	All	3147/3597 (88%)	3144 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	351	ASN
1	C	126	CYS
1	C	127	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	445	ASN
1	C	524	HIS
1	C	1128	GLN
1	C	508	ASN
1	C	768	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

198 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	D	1	2,1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.51	0
2	BMA	D	3	2	11,11,12	0.86	0	15,15,17	1.04	2 (13%)
2	MAN	D	4	2	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
2	MAN	D	5	2	11,11,12	0.59	0	15,15,17	1.00	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.94	2 (14%)	17,19,21	1.53	1 (5%)
3	NAG	E	2	3	14,14,15	0.30	0	17,19,21	0.89	1 (5%)
3	BMA	E	3	3	11,11,12	0.58	0	15,15,17	0.88	0
2	NAG	F	1	2,1	14,14,15	0.62	1 (7%)	17,19,21	1.43	1 (5%)
2	NAG	F	2	2	14,14,15	0.46	0	17,19,21	0.42	0
2	BMA	F	3	2	11,11,12	1.09	1 (9%)	15,15,17	1.05	1 (6%)
2	MAN	F	4	2	11,11,12	0.76	1 (9%)	15,15,17	1.15	2 (13%)
2	MAN	F	5	2	11,11,12	0.79	0	15,15,17	1.03	2 (13%)
2	NAG	G	1	2,1	14,14,15	0.60	1 (7%)	17,19,21	0.85	0
2	NAG	G	2	2	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
2	BMA	G	3	2	11,11,12	0.72	0	15,15,17	1.46	3 (20%)
2	MAN	G	4	2	11,11,12	0.60	0	15,15,17	1.07	2 (13%)
2	MAN	G	5	2	11,11,12	1.60	2 (18%)	15,15,17	1.85	3 (20%)
2	NAG	H	1	2,1	14,14,15	0.76	1 (7%)	17,19,21	0.79	0
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.59	0
2	BMA	H	3	2	11,11,12	0.79	0	15,15,17	0.89	1 (6%)
2	MAN	H	4	2	11,11,12	0.87	1 (9%)	15,15,17	1.33	2 (13%)
2	MAN	H	5	2	11,11,12	0.78	0	15,15,17	0.95	2 (13%)
4	NAG	I	1	4,1	14,14,15	0.57	0	17,19,21	0.69	1 (5%)
4	NAG	I	2	4	14,14,15	0.57	0	17,19,21	0.79	1 (5%)
4	BMA	I	3	4	11,11,12	0.84	0	15,15,17	0.83	0
4	FUC	I	4	4	10,10,11	0.74	0	14,14,16	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	J	1	2,1	14,14,15	0.24	0	17,19,21	0.54	0
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.55	0
2	BMA	J	3	2	11,11,12	0.71	0	15,15,17	0.91	0
2	MAN	J	4	2	11,11,12	0.71	0	15,15,17	0.87	1 (6%)
2	MAN	J	5	2	11,11,12	0.73	1 (9%)	15,15,17	1.09	2 (13%)
3	NAG	K	1	3,1	14,14,15	0.64	1 (7%)	17,19,21	0.58	0
3	NAG	K	2	3	14,14,15	0.19	0	17,19,21	0.47	0
3	BMA	K	3	3	11,11,12	0.50	0	15,15,17	0.73	0
5	NAG	L	1	5,1	14,14,15	0.51	0	17,19,21	0.77	0
5	NAG	L	2	5	14,14,15	0.46	0	17,19,21	0.50	0
5	BMA	L	3	5	11,11,12	0.48	0	15,15,17	0.67	0
5	MAN	L	4	5	11,11,12	0.58	0	15,15,17	1.01	2 (13%)
4	NAG	M	1	4,1	14,14,15	0.60	0	17,19,21	1.07	1 (5%)
4	NAG	M	2	4	14,14,15	0.46	0	17,19,21	0.41	0
4	BMA	M	3	4	11,11,12	0.47	0	15,15,17	0.79	0
4	FUC	M	4	4	10,10,11	0.69	0	14,14,16	0.93	1 (7%)
2	NAG	N	1	2,1	14,14,15	0.44	0	17,19,21	0.72	0
2	NAG	N	2	2	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
2	BMA	N	3	2	11,11,12	0.88	1 (9%)	15,15,17	1.03	2 (13%)
2	MAN	N	4	2	11,11,12	0.94	1 (9%)	15,15,17	1.03	1 (6%)
2	MAN	N	5	2	11,11,12	0.91	1 (9%)	15,15,17	1.25	1 (6%)
6	NAG	O	1	6,1	14,14,15	0.71	1 (7%)	17,19,21	0.94	1 (5%)
6	NAG	O	2	6	14,14,15	0.62	1 (7%)	17,19,21	0.94	1 (5%)
6	BMA	O	3	6	11,11,12	0.89	1 (9%)	15,15,17	1.48	3 (20%)
6	MAN	O	4	6	11,11,12	0.77	0	15,15,17	1.56	2 (13%)
6	MAN	O	5	6	11,11,12	0.86	1 (9%)	15,15,17	1.84	3 (20%)
6	FUC	O	6	6	10,10,11	0.71	0	14,14,16	0.92	1 (7%)
2	NAG	P	1	2,1	14,14,15	1.02	1 (7%)	17,19,21	2.13	4 (23%)
2	NAG	P	2	2	14,14,15	0.96	2 (14%)	17,19,21	1.47	2 (11%)
2	BMA	P	3	2	11,11,12	0.59	0	15,15,17	1.03	0
2	MAN	P	4	2	11,11,12	1.21	1 (9%)	15,15,17	2.17	5 (33%)
2	MAN	P	5	2	11,11,12	0.68	0	15,15,17	0.85	1 (6%)
3	NAG	Q	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.58	0
3	NAG	Q	2	3	14,14,15	0.27	0	17,19,21	0.53	0
3	BMA	Q	3	3	11,11,12	0.51	0	15,15,17	0.87	1 (6%)
2	NAG	R	1	2,1	14,14,15	0.97	1 (7%)	17,19,21	0.78	0
2	NAG	R	2	2	14,14,15	0.28	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	R	3	2	11,11,12	0.67	0	15,15,17	0.89	1 (6%)
2	MAN	R	4	2	11,11,12	0.70	0	15,15,17	1.36	2 (13%)
2	MAN	R	5	2	11,11,12	0.60	0	15,15,17	0.91	1 (6%)
6	NAG	S	1	6,1	14,14,15	0.29	0	17,19,21	0.40	0
6	NAG	S	2	6	14,14,15	0.22	0	17,19,21	0.48	0
6	BMA	S	3	6	11,11,12	0.69	0	15,15,17	0.89	0
6	MAN	S	4	6	11,11,12	0.70	0	15,15,17	1.00	1 (6%)
6	MAN	S	5	6	11,11,12	0.75	0	15,15,17	1.05	2 (13%)
6	FUC	S	6	6	10,10,11	0.67	0	14,14,16	0.75	0
2	NAG	T	1	2,1	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
2	NAG	T	2	2	14,14,15	0.31	0	17,19,21	0.51	0
2	BMA	T	3	2	11,11,12	0.94	0	15,15,17	1.31	2 (13%)
2	MAN	T	4	2	11,11,12	0.80	0	15,15,17	1.06	2 (13%)
2	MAN	T	5	2	11,11,12	0.64	0	15,15,17	1.09	2 (13%)
2	NAG	U	1	2,1	14,14,15	0.40	0	17,19,21	1.34	2 (11%)
2	NAG	U	2	2	14,14,15	0.22	0	17,19,21	0.58	0
2	BMA	U	3	2	11,11,12	0.70	0	15,15,17	0.66	0
2	MAN	U	4	2	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
2	MAN	U	5	2	11,11,12	0.63	0	15,15,17	0.89	1 (6%)
3	NAG	V	1	3,1	14,14,15	0.40	0	17,19,21	1.36	1 (5%)
3	NAG	V	2	3	14,14,15	0.24	0	17,19,21	0.47	0
3	BMA	V	3	3	11,11,12	0.58	0	15,15,17	0.69	0
2	NAG	W	1	2,1	14,14,15	0.33	0	17,19,21	0.70	0
2	NAG	W	2	2	14,14,15	1.11	1 (7%)	17,19,21	1.14	1 (5%)
2	BMA	W	3	2	11,11,12	0.83	0	15,15,17	0.92	0
2	MAN	W	4	2	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
2	MAN	W	5	2	11,11,12	0.55	0	15,15,17	0.99	2 (13%)
2	NAG	X	1	2,1	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	X	2	2	14,14,15	0.38	0	17,19,21	0.77	0
2	BMA	X	3	2	11,11,12	0.58	0	15,15,17	0.74	0
2	MAN	X	4	2	11,11,12	0.52	0	15,15,17	1.01	2 (13%)
2	MAN	X	5	2	11,11,12	0.64	0	15,15,17	1.13	2 (13%)
2	NAG	Y	1	2,1	14,14,15	0.18	0	17,19,21	0.58	0
2	NAG	Y	2	2	14,14,15	0.82	1 (7%)	17,19,21	1.43	1 (5%)
2	BMA	Y	3	2	11,11,12	0.97	0	15,15,17	0.86	1 (6%)
2	MAN	Y	4	2	11,11,12	0.53	0	15,15,17	1.03	2 (13%)
2	MAN	Y	5	2	11,11,12	0.68	0	15,15,17	1.02	2 (13%)
4	NAG	Z	1	4,1	14,14,15	0.48	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	Z	2	4	14,14,15	0.29	0	17,19,21	0.41	0
4	BMA	Z	3	4	11,11,12	0.57	0	15,15,17	0.76	0
4	FUC	Z	4	4	10,10,11	0.71	0	14,14,16	1.43	2 (14%)
2	NAG	a	1	2,1	14,14,15	0.49	0	17,19,21	0.50	0
2	NAG	a	2	2	14,14,15	0.49	0	17,19,21	1.41	2 (11%)
2	BMA	a	3	2	11,11,12	0.94	0	15,15,17	0.97	0
2	MAN	a	4	2	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
2	MAN	a	5	2	11,11,12	0.75	1 (9%)	15,15,17	1.11	2 (13%)
2	NAG	b	1	2,1	14,14,15	0.56	0	17,19,21	0.74	1 (5%)
2	NAG	b	2	2	14,14,15	0.35	0	17,19,21	1.49	1 (5%)
2	BMA	b	3	2	11,11,12	0.64	0	15,15,17	0.79	0
2	MAN	b	4	2	11,11,12	0.68	0	15,15,17	1.29	2 (13%)
2	MAN	b	5	2	11,11,12	0.87	0	15,15,17	1.14	2 (13%)
3	NAG	c	1	3,1	14,14,15	0.40	0	17,19,21	0.40	0
3	NAG	c	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	BMA	c	3	3	11,11,12	0.85	1 (9%)	15,15,17	0.90	0
2	NAG	d	1	2,1	14,14,15	1.07	1 (7%)	17,19,21	1.06	1 (5%)
2	NAG	d	2	2	14,14,15	0.71	1 (7%)	17,19,21	0.74	0
2	BMA	d	3	2	11,11,12	0.49	0	15,15,17	1.03	1 (6%)
2	MAN	d	4	2	11,11,12	0.61	0	15,15,17	0.90	1 (6%)
2	MAN	d	5	2	11,11,12	0.63	0	15,15,17	0.94	1 (6%)
6	NAG	e	1	6,1	14,14,15	0.33	0	17,19,21	0.52	0
6	NAG	e	2	6	14,14,15	0.61	1 (7%)	17,19,21	1.38	2 (11%)
6	BMA	e	3	6	11,11,12	0.71	0	15,15,17	0.72	0
6	MAN	e	4	6	11,11,12	0.57	0	15,15,17	0.98	2 (13%)
6	MAN	e	5	6	11,11,12	0.72	0	15,15,17	1.07	2 (13%)
6	FUC	e	6	6	10,10,11	1.61	2 (20%)	14,14,16	1.59	3 (21%)
3	NAG	f	1	3,1	14,14,15	0.77	1 (7%)	17,19,21	0.80	1 (5%)
3	NAG	f	2	3	14,14,15	0.22	0	17,19,21	0.38	0
3	BMA	f	3	3	11,11,12	0.65	0	15,15,17	0.72	0
2	NAG	g	1	2,1	14,14,15	0.18	0	17,19,21	0.56	0
2	NAG	g	2	2	14,14,15	0.19	0	17,19,21	0.52	0
2	BMA	g	3	2	11,11,12	0.70	0	15,15,17	0.75	0
2	MAN	g	4	2	11,11,12	0.50	0	15,15,17	1.10	2 (13%)
2	MAN	g	5	2	11,11,12	0.71	1 (9%)	15,15,17	1.25	2 (13%)
2	NAG	h	1	2,1	14,14,15	0.18	0	17,19,21	0.67	0
2	NAG	h	2	2	14,14,15	0.21	0	17,19,21	0.46	0
2	BMA	h	3	2	11,11,12	0.65	0	15,15,17	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	h	4	2	11,11,12	0.66	0	15,15,17	0.96	1 (6%)
2	MAN	h	5	2	11,11,12	0.81	1 (9%)	15,15,17	1.22	2 (13%)
6	NAG	i	1	6,1	14,14,15	0.57	0	17,19,21	0.71	0
6	NAG	i	2	6	14,14,15	0.30	0	17,19,21	1.26	1 (5%)
6	BMA	i	3	6	11,11,12	0.64	0	15,15,17	0.63	0
6	MAN	i	4	6	11,11,12	0.92	1 (9%)	15,15,17	1.45	2 (13%)
6	MAN	i	5	6	11,11,12	0.66	0	15,15,17	1.16	2 (13%)
6	FUC	i	6	6	10,10,11	0.63	0	14,14,16	1.02	2 (14%)
2	NAG	j	1	2,1	14,14,15	0.39	0	17,19,21	0.43	0
2	NAG	j	2	2	14,14,15	0.24	0	17,19,21	0.41	0
2	BMA	j	3	2	11,11,12	0.78	0	15,15,17	0.71	0
2	MAN	j	4	2	11,11,12	0.84	0	15,15,17	1.32	2 (13%)
2	MAN	j	5	2	11,11,12	0.82	1 (9%)	15,15,17	1.25	2 (13%)
2	NAG	k	1	2,1	14,14,15	0.27	0	17,19,21	0.47	0
2	NAG	k	2	2	14,14,15	0.35	0	17,19,21	0.54	0
2	BMA	k	3	2	11,11,12	0.58	0	15,15,17	0.73	0
2	MAN	k	4	2	11,11,12	0.59	0	15,15,17	0.98	2 (13%)
2	MAN	k	5	2	11,11,12	0.68	0	15,15,17	1.24	2 (13%)
3	NAG	l	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	1.89	1 (5%)
3	NAG	l	2	3	14,14,15	0.65	0	17,19,21	1.12	1 (5%)
3	BMA	l	3	3	11,11,12	0.91	1 (9%)	15,15,17	1.03	1 (6%)
2	NAG	m	1	2,1	14,14,15	0.52	0	17,19,21	1.35	1 (5%)
2	NAG	m	2	2	14,14,15	0.27	0	17,19,21	0.59	0
2	BMA	m	3	2	11,11,12	0.57	0	15,15,17	0.64	0
2	MAN	m	4	2	11,11,12	0.62	0	15,15,17	1.10	2 (13%)
2	MAN	m	5	2	11,11,12	0.73	0	15,15,17	0.92	1 (6%)
2	NAG	n	1	2,1	14,14,15	0.64	1 (7%)	17,19,21	0.69	0
2	NAG	n	2	2	14,14,15	0.16	0	17,19,21	0.49	0
2	BMA	n	3	2	11,11,12	1.10	0	15,15,17	0.79	0
2	MAN	n	4	2	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
2	MAN	n	5	2	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
2	NAG	o	1	2,1	14,14,15	0.70	1 (7%)	17,19,21	0.53	0
2	NAG	o	2	2	14,14,15	0.34	0	17,19,21	0.73	0
2	BMA	o	3	2	11,11,12	1.12	2 (18%)	15,15,17	1.05	2 (13%)
2	MAN	o	4	2	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
2	MAN	o	5	2	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
2	NAG	p	1	2,1	14,14,15	0.58	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	p	2	2	14,14,15	0.57	0	17,19,21	0.99	1 (5%)
2	BMA	p	3	2	11,11,12	0.73	0	15,15,17	1.10	0
2	MAN	p	4	2	11,11,12	0.64	0	15,15,17	1.15	2 (13%)
2	MAN	p	5	2	11,11,12	0.68	0	15,15,17	1.11	2 (13%)
3	NAG	q	1	3,1	14,14,15	0.29	0	17,19,21	0.44	0
3	NAG	q	2	3	14,14,15	0.20	0	17,19,21	0.45	0
3	BMA	q	3	3	11,11,12	0.72	0	15,15,17	0.67	0
3	NAG	r	1	3,1	14,14,15	0.25	0	17,19,21	0.54	0
3	NAG	r	2	3	14,14,15	0.28	0	17,19,21	0.55	0
3	BMA	r	3	3	11,11,12	0.61	0	15,15,17	0.65	0
7	NAG	s	1	7,1	14,14,15	0.48	0	17,19,21	0.57	0
7	FUC	s	2	7	10,10,11	0.90	0	14,14,16	0.95	1 (7%)
4	NAG	t	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.56	0
4	NAG	t	2	4	14,14,15	0.64	0	17,19,21	1.35	2 (11%)
4	BMA	t	3	4	11,11,12	0.61	0	15,15,17	0.97	2 (13%)
4	FUC	t	4	4	10,10,11	0.88	1 (10%)	14,14,16	1.04	1 (7%)
2	NAG	u	1	2,1	14,14,15	0.87	2 (14%)	17,19,21	0.60	0
2	NAG	u	2	2	14,14,15	0.46	0	17,19,21	1.44	3 (17%)
2	BMA	u	3	2	11,11,12	1.19	2 (18%)	15,15,17	0.99	0
2	MAN	u	4	2	11,11,12	0.71	0	15,15,17	0.85	1 (6%)
2	MAN	u	5	2	11,11,12	0.93	0	15,15,17	1.35	3 (20%)

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	O	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	1/2/19/22	0/1/1/1
6	MAN	O	4	6	-	2/2/19/22	1/1/1/1
6	MAN	O	5	6	-	1/2/19/22	0/1/1/1
6	FUC	O	6	6	-	-	0/1/1/1
2	NAG	P	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	P	2	2	-	6/6/23/26	0/1/1/1
2	BMA	P	3	2	-	2/2/19/22	0/1/1/1
2	MAN	P	4	2	-	0/2/19/22	0/1/1/1
2	MAN	P	5	2	-	0/2/19/22	1/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
2	NAG	R	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	BMA	R	3	2	-	2/2/19/22	0/1/1/1
2	MAN	R	4	2	-	0/2/19/22	0/1/1/1
2	MAN	R	5	2	-	0/2/19/22	0/1/1/1
6	NAG	S	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
6	MAN	S	4	6	-	0/2/19/22	0/1/1/1
6	MAN	S	5	6	-	0/2/19/22	1/1/1/1
6	FUC	S	6	6	-	-	0/1/1/1
2	NAG	T	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	BMA	T	3	2	-	0/2/19/22	0/1/1/1
2	MAN	T	4	2	-	2/2/19/22	1/1/1/1
2	MAN	T	5	2	-	0/2/19/22	0/1/1/1
2	NAG	U	1	2,1	-	6/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	BMA	U	3	2	-	2/2/19/22	0/1/1/1
2	MAN	U	4	2	-	0/2/19/22	0/1/1/1
2	MAN	U	5	2	-	0/2/19/22	0/1/1/1
3	NAG	V	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	m	3	2	-	2/2/19/22	0/1/1/1
2	MAN	m	4	2	-	0/2/19/22	0/1/1/1
2	MAN	m	5	2	-	0/2/19/22	0/1/1/1
2	NAG	n	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	n	2	2	-	4/6/23/26	0/1/1/1
2	BMA	n	3	2	-	2/2/19/22	0/1/1/1
2	MAN	n	4	2	-	2/2/19/22	0/1/1/1
2	MAN	n	5	2	-	0/2/19/22	0/1/1/1
2	NAG	o	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	o	2	2	-	2/6/23/26	0/1/1/1
2	BMA	o	3	2	-	1/2/19/22	0/1/1/1
2	MAN	o	4	2	-	0/2/19/22	0/1/1/1
2	MAN	o	5	2	-	0/2/19/22	0/1/1/1
2	NAG	p	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	p	2	2	-	0/6/23/26	0/1/1/1
2	BMA	p	3	2	-	2/2/19/22	0/1/1/1
2	MAN	p	4	2	-	0/2/19/22	0/1/1/1
2	MAN	p	5	2	-	2/2/19/22	1/1/1/1
3	NAG	q	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	q	3	3	-	0/2/19/22	0/1/1/1
3	NAG	r	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	0/6/23/26	0/1/1/1
3	BMA	r	3	3	-	0/2/19/22	0/1/1/1
7	NAG	s	1	7,1	-	2/6/23/26	0/1/1/1
7	FUC	s	2	7	-	-	0/1/1/1
4	NAG	t	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	t	2	4	-	6/6/23/26	0/1/1/1
4	BMA	t	3	4	-	2/2/19/22	0/1/1/1
4	FUC	t	4	4	-	-	0/1/1/1
2	NAG	u	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	u	2	2	-	6/6/23/26	0/1/1/1
2	BMA	u	3	2	-	2/2/19/22	0/1/1/1
2	MAN	u	4	2	-	0/2/19/22	0/1/1/1
2	MAN	u	5	2	-	1/2/19/22	0/1/1/1

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	5	MAN	C1-C2	4.41	1.62	1.52
2	d	1	NAG	O5-C1	-3.81	1.37	1.43
6	e	6	FUC	C1-C2	3.69	1.61	1.52
2	P	1	NAG	O5-C1	-3.60	1.37	1.43
2	R	1	NAG	O5-C1	-3.45	1.37	1.43

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	l	1	NAG	C1-O5-C5	7.47	122.20	112.19
2	P	4	MAN	C1-O5-C5	6.35	120.69	112.19
6	O	5	MAN	C1-O5-C5	5.87	120.05	112.19
3	E	1	NAG	C1-O5-C5	5.74	119.88	112.19
2	b	2	NAG	C1-O5-C5	5.69	119.81	112.19

There are no chirality outliers.

5 of 263 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	2	NAG	C4-C5-C6-O6
2	k	3	BMA	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	o	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6

5 of 18 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	j	5	MAN	C1-C2-C3-C4-C5-O5
6	i	4	MAN	C1-C2-C3-C4-C5-O5
2	P	5	MAN	C1-C2-C3-C4-C5-O5
6	O	4	MAN	C1-C2-C3-C4-C5-O5
2	H	5	MAN	C1-C2-C3-C4-C5-O5

88 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	2	NAG	2	0
4	M	4	FUC	1	0
2	u	4	MAN	2	0
6	i	1	NAG	1	0
4	I	2	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	k	2	NAG	1	0
2	P	2	NAG	2	0
2	a	2	NAG	1	0
2	F	2	NAG	1	0
2	J	2	NAG	1	0
2	d	1	NAG	4	0
2	k	5	MAN	1	0
2	G	3	BMA	3	0
3	f	1	NAG	3	0
2	H	1	NAG	1	0
2	J	1	NAG	1	0
2	U	1	NAG	3	0
5	L	1	NAG	3	0
3	f	2	NAG	2	0
2	N	1	NAG	1	0
6	S	3	BMA	1	0
2	u	5	MAN	1	0
2	N	5	MAN	1	0
2	W	2	NAG	1	0
2	u	2	NAG	1	0
3	V	1	NAG	3	0
2	N	2	NAG	1	0
2	j	2	NAG	1	0
2	X	1	NAG	2	0
2	g	1	NAG	1	0
2	m	2	NAG	1	0
2	T	1	NAG	2	0
2	o	1	NAG	4	0
2	X	5	MAN	1	0
2	m	4	MAN	1	0
2	R	2	NAG	1	0
2	D	1	NAG	2	0
3	l	1	NAG	1	0
2	h	1	NAG	1	0
7	s	1	NAG	3	0
4	t	3	BMA	1	0
6	i	3	BMA	1	0
2	j	1	NAG	1	0
6	O	1	NAG	3	0
4	t	2	NAG	1	0
2	D	4	MAN	1	0
2	U	2	NAG	1	0

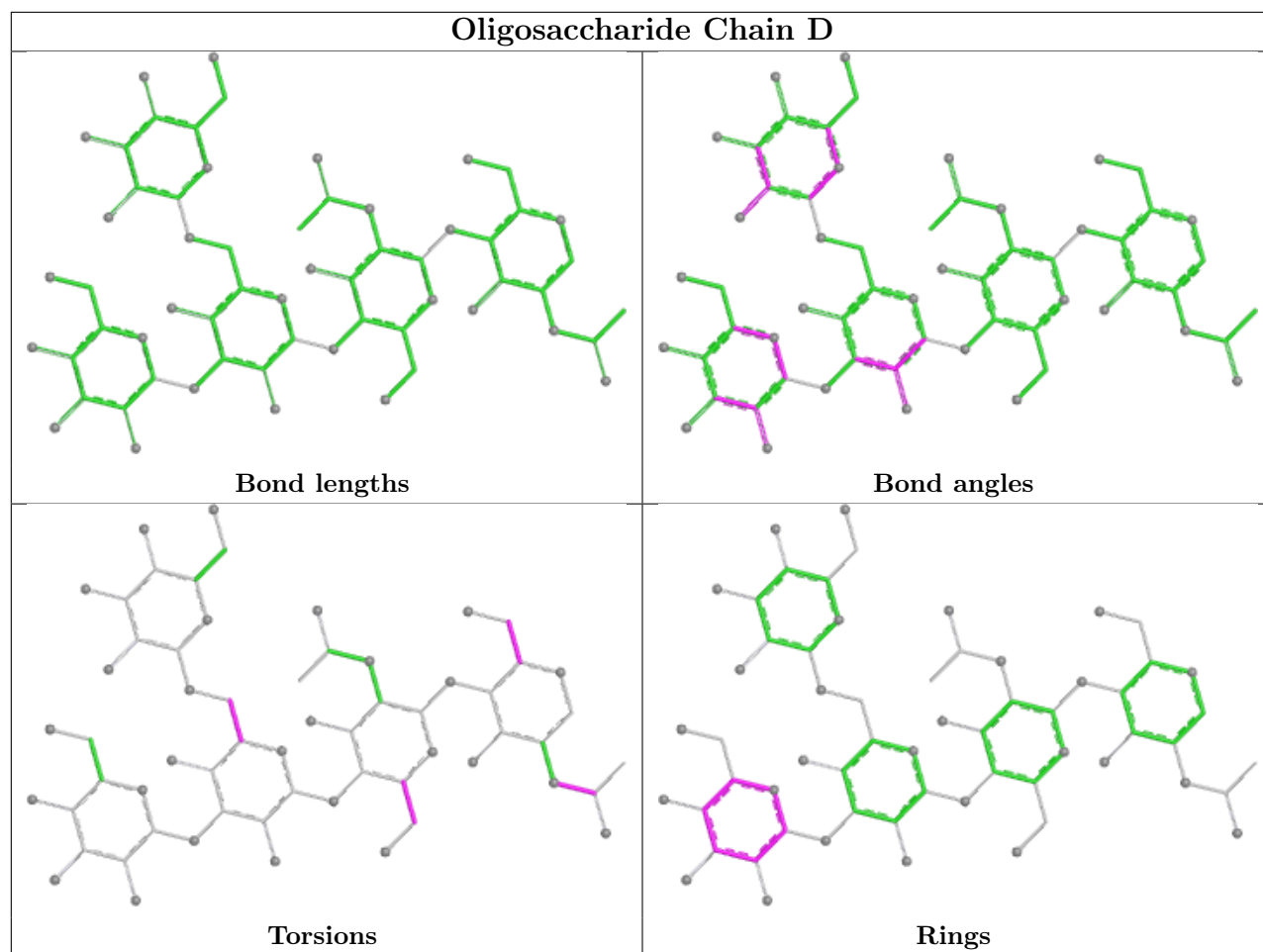
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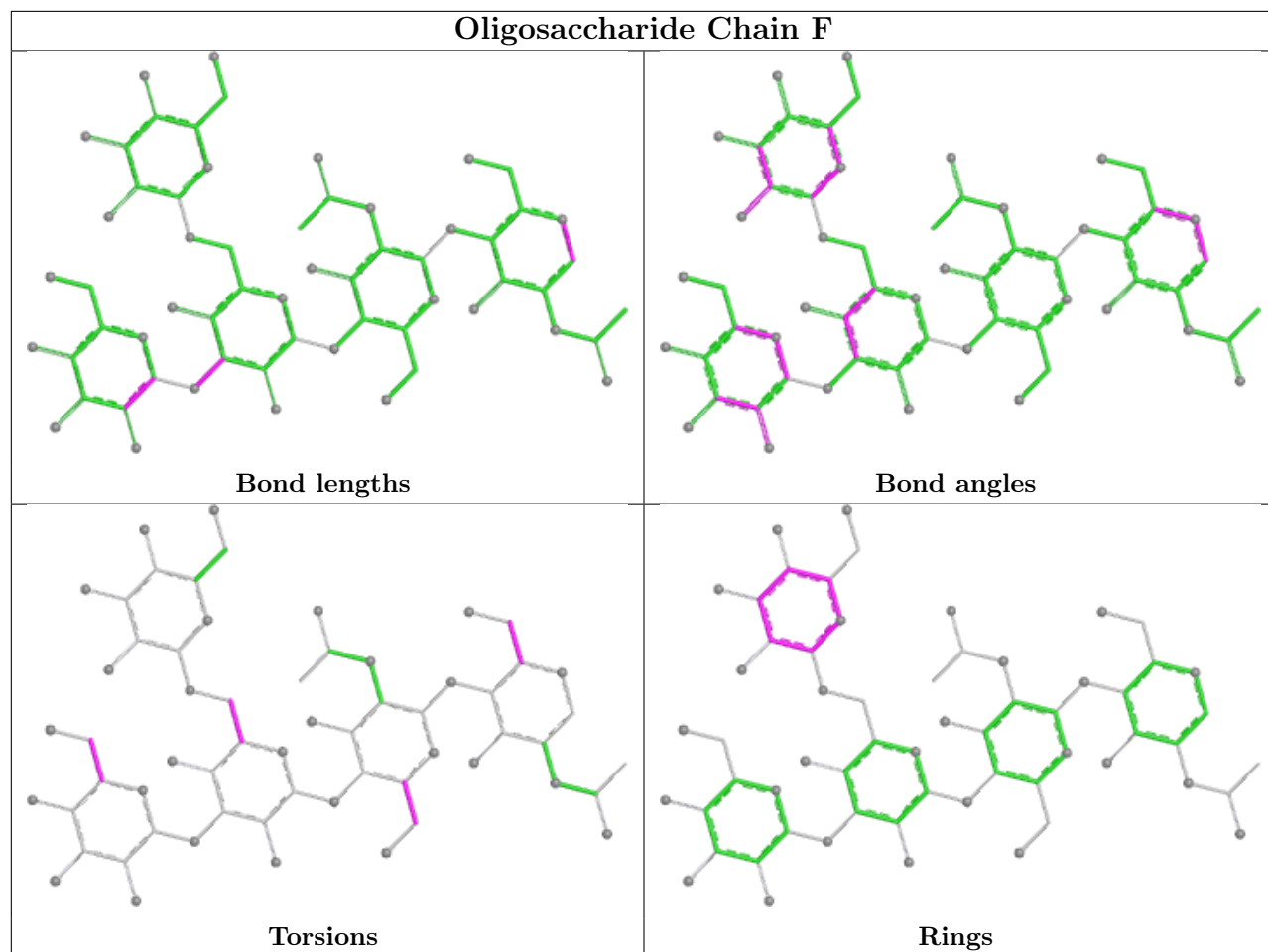
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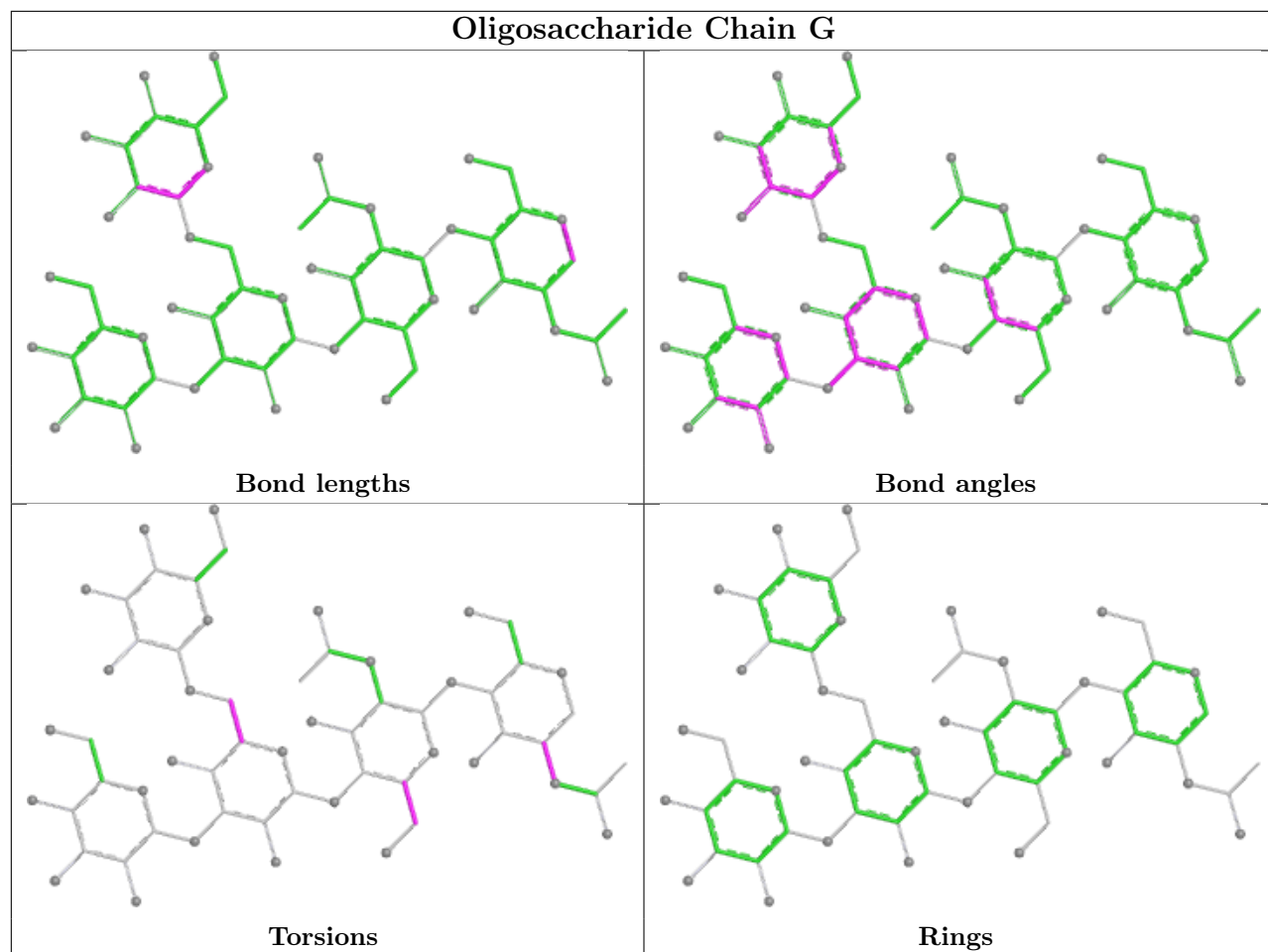
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	1	NAG	2	0
2	G	2	NAG	2	0
2	R	1	NAG	3	0
2	j	5	MAN	1	0
6	O	2	NAG	2	0
2	b	1	NAG	1	0
2	Y	1	NAG	1	0
6	S	4	MAN	1	0
4	I	1	NAG	3	0
2	h	3	BMA	1	0
2	o	3	BMA	1	0
2	X	2	NAG	1	0
5	L	2	NAG	5	0
2	F	5	MAN	1	0
2	u	1	NAG	4	0
2	F	4	MAN	1	0
2	T	2	NAG	1	0
4	t	1	NAG	2	0
2	G	1	NAG	4	0
2	P	1	NAG	2	0
2	F	1	NAG	2	0
3	c	2	NAG	1	0
7	s	2	FUC	2	0
6	i	6	FUC	1	0
2	a	3	BMA	1	0
3	E	1	NAG	2	0
6	i	2	NAG	1	0
6	O	6	FUC	2	0
3	r	1	NAG	1	0
2	W	1	NAG	2	0
2	o	2	NAG	1	0
2	k	1	NAG	2	0
3	q	1	NAG	1	0
2	D	5	MAN	1	0
2	P	3	BMA	1	0
6	e	6	FUC	1	0
2	X	3	BMA	2	0
2	D	2	NAG	1	0
2	G	5	MAN	2	0
6	e	2	NAG	2	0
2	d	2	NAG	1	0

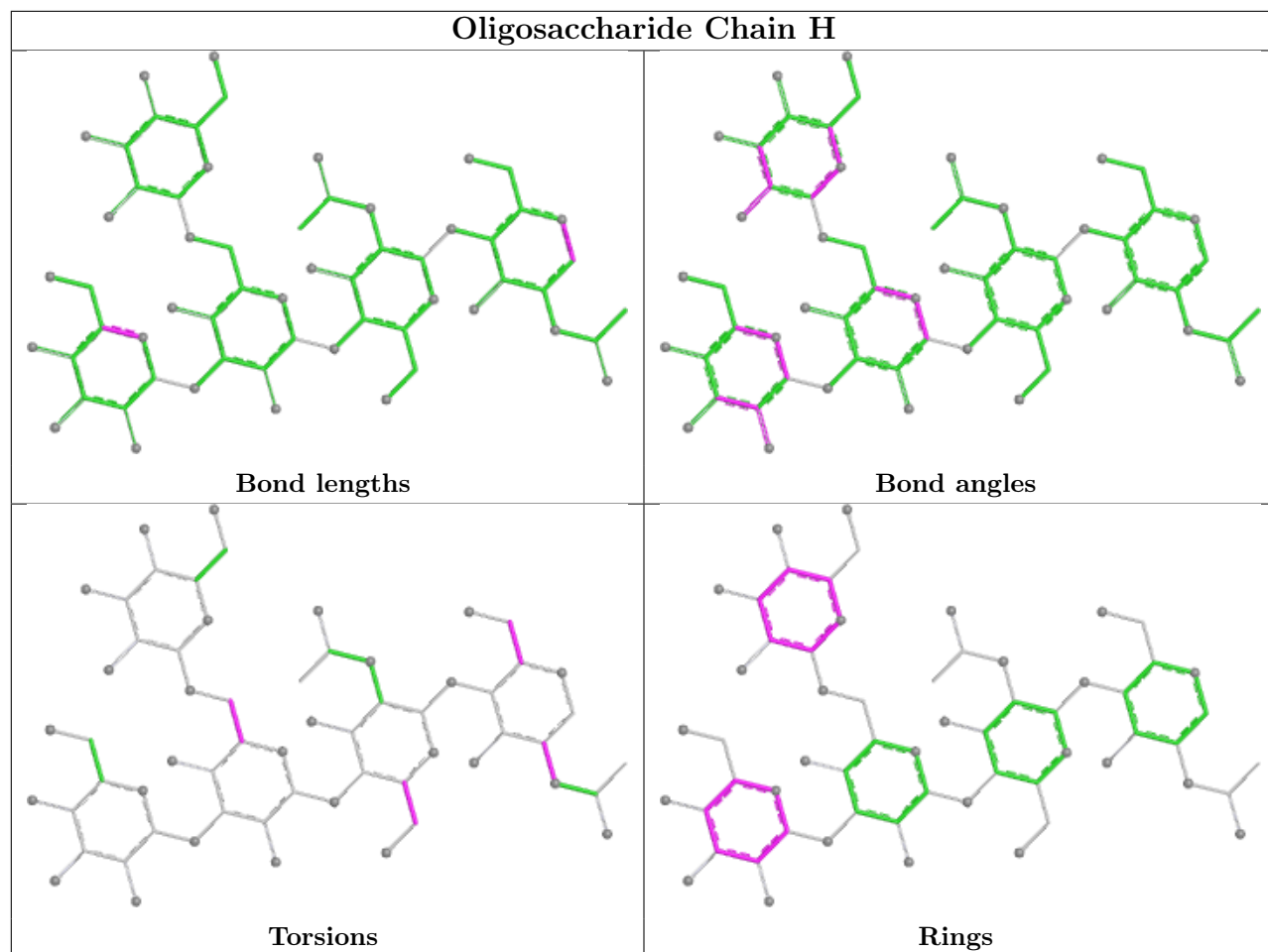
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

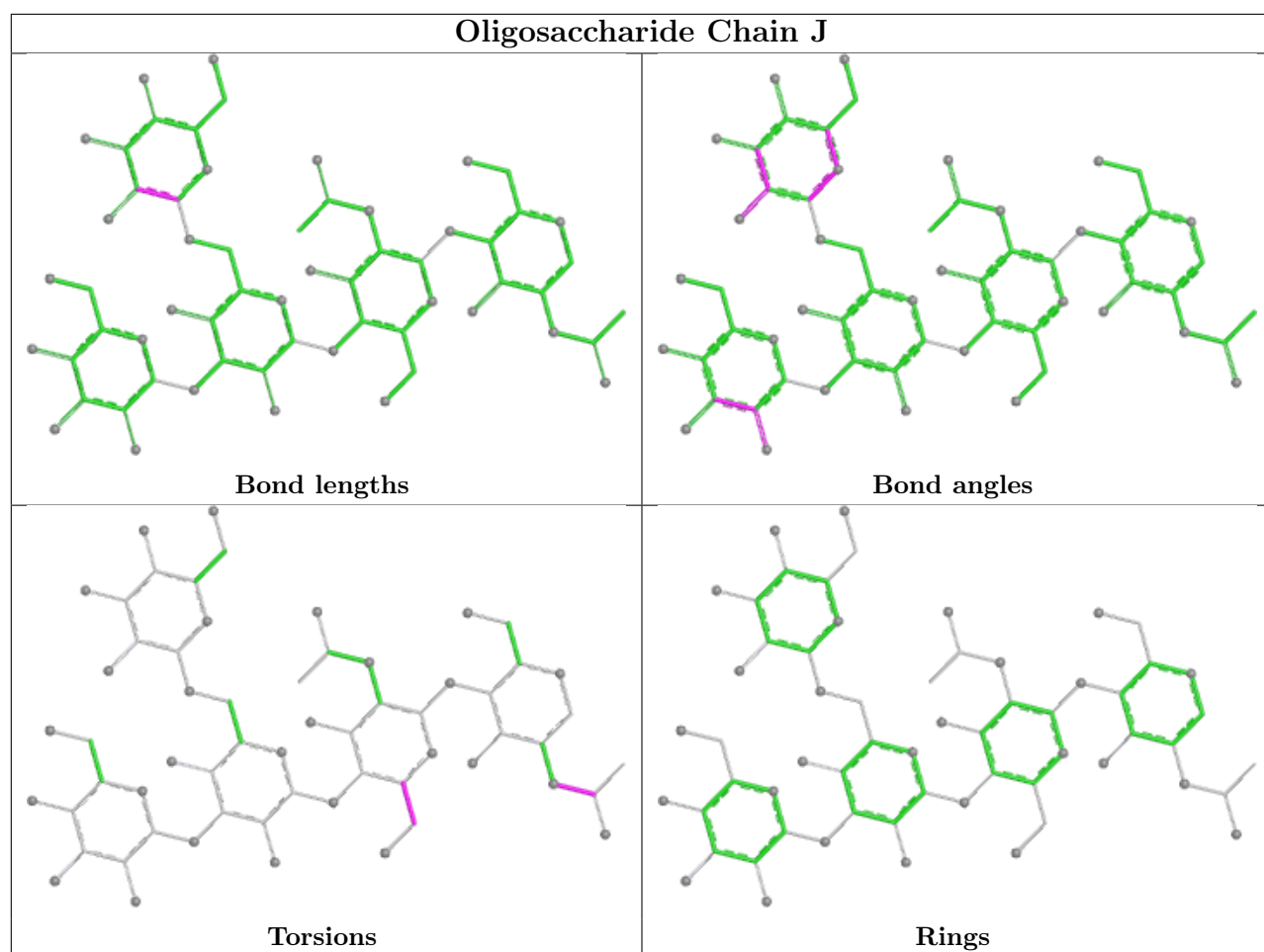
bond angles, torsion angles, and ring geometry for oligosaccharide.

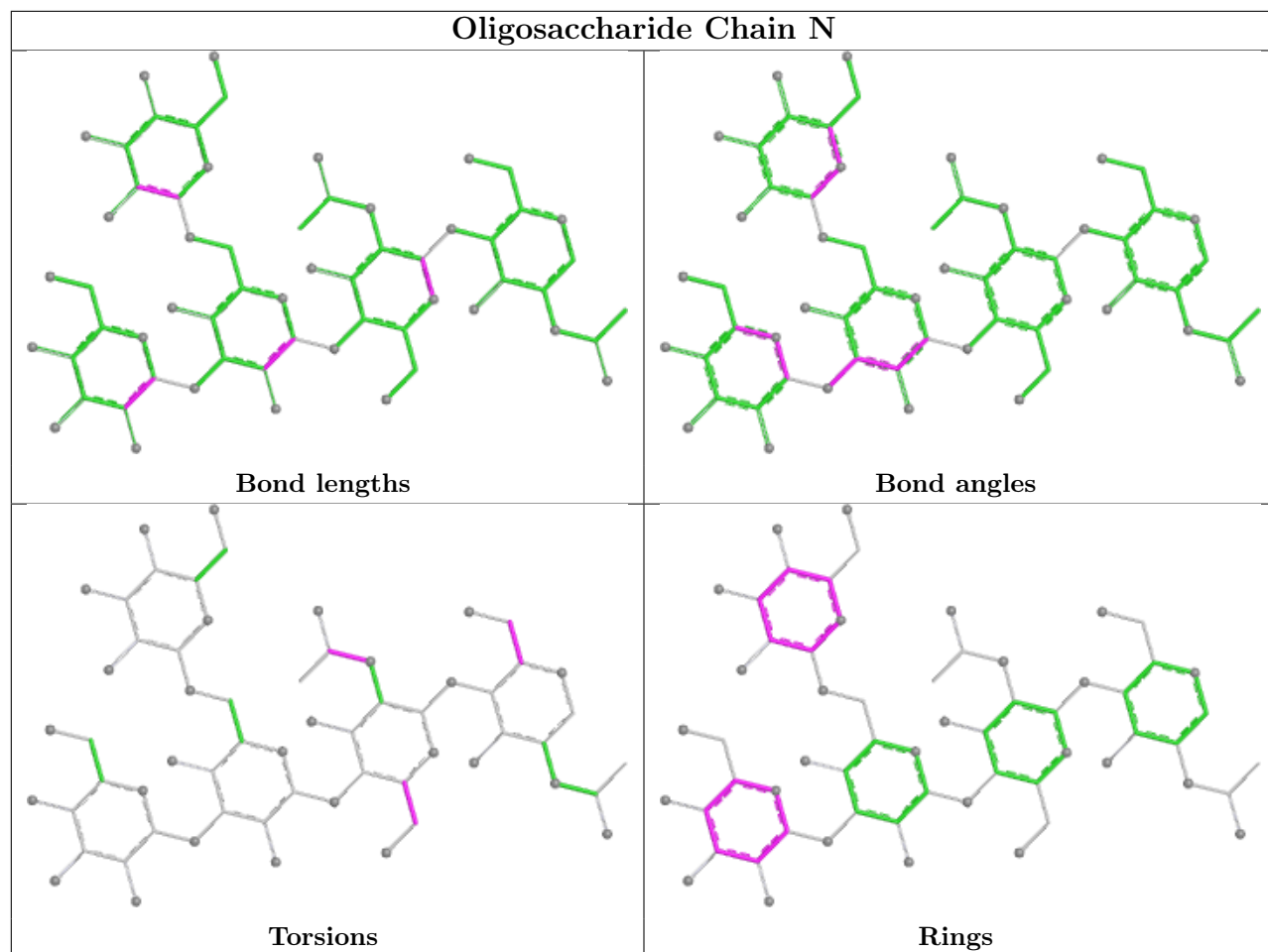


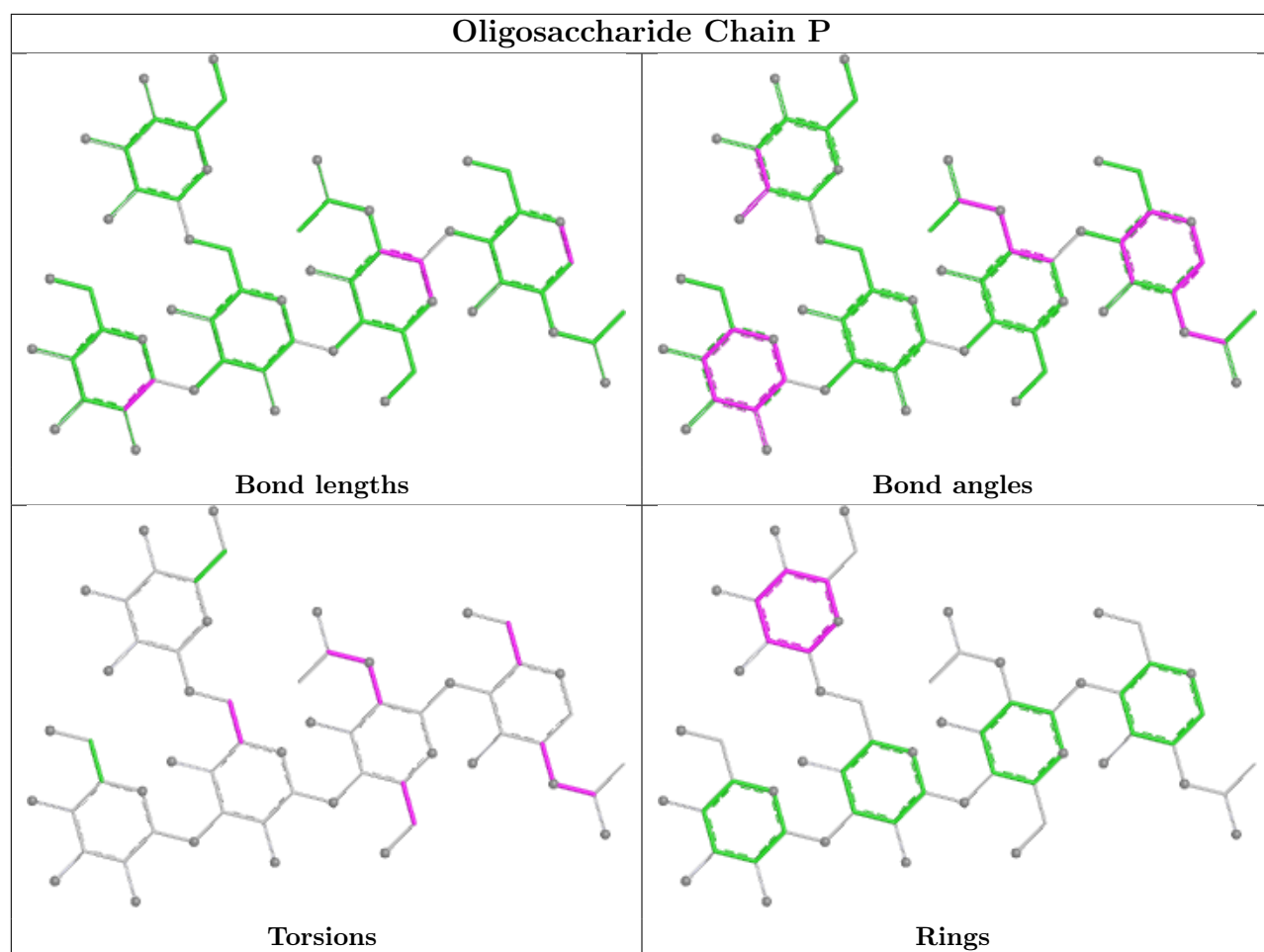


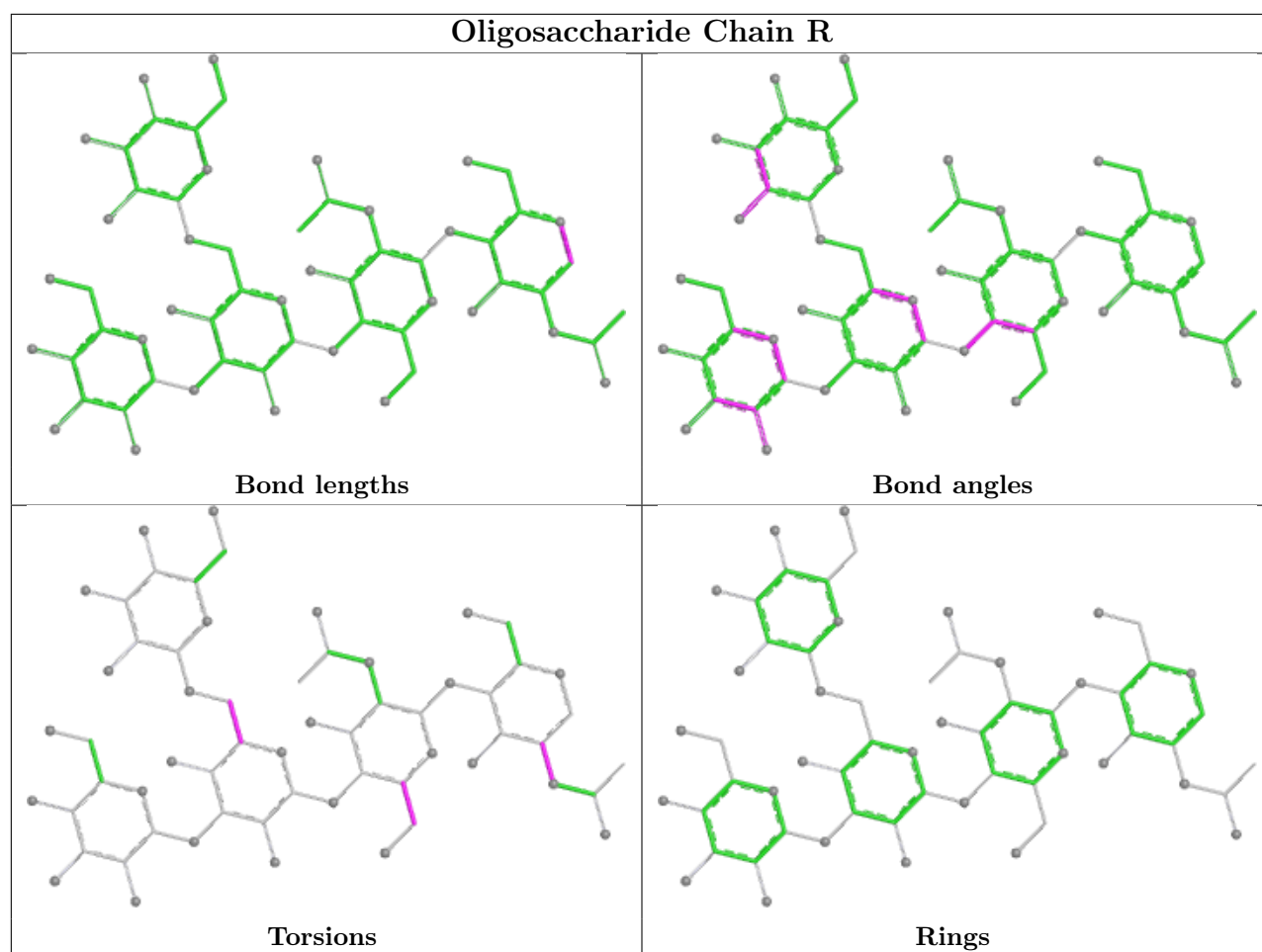


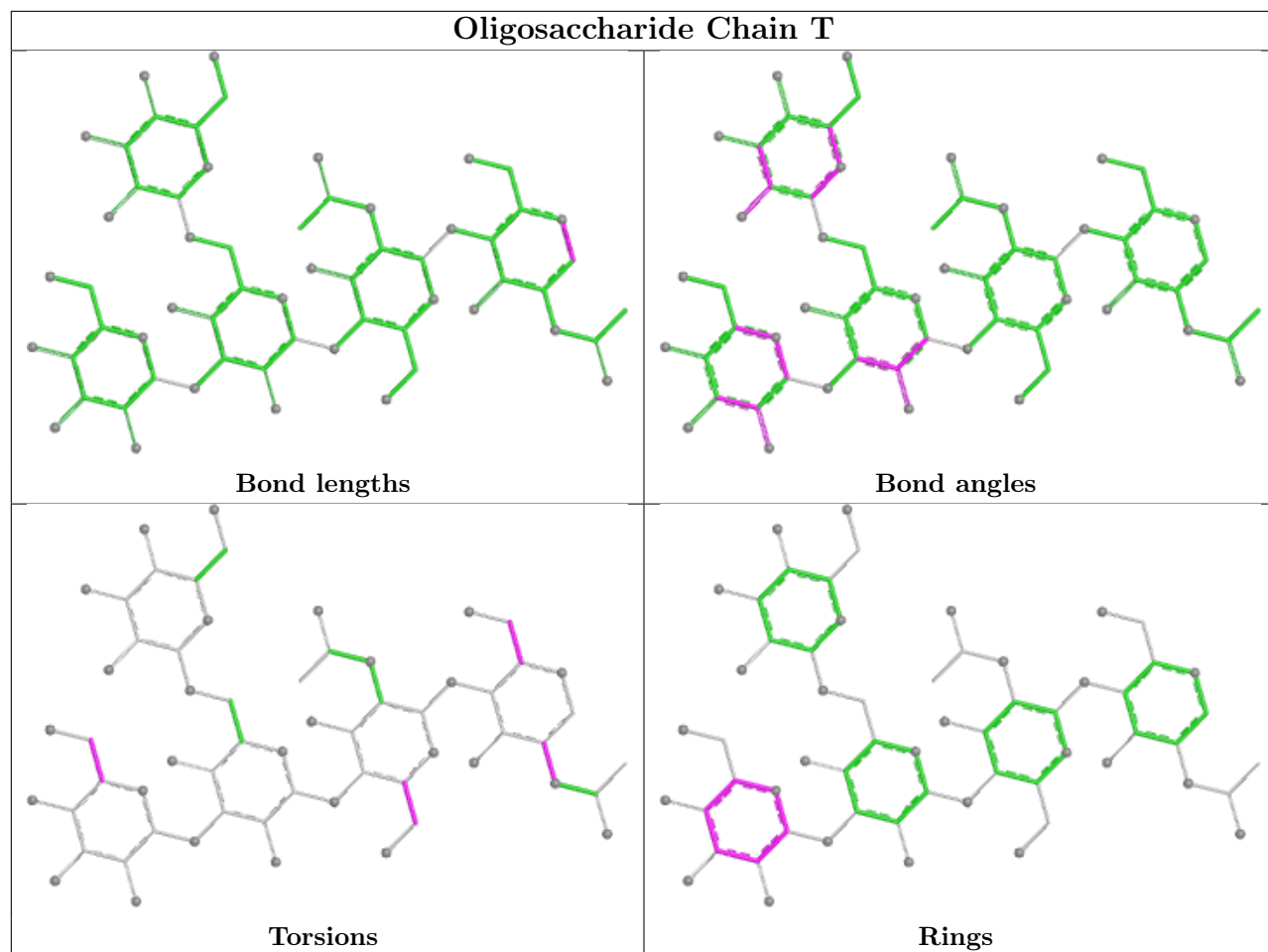


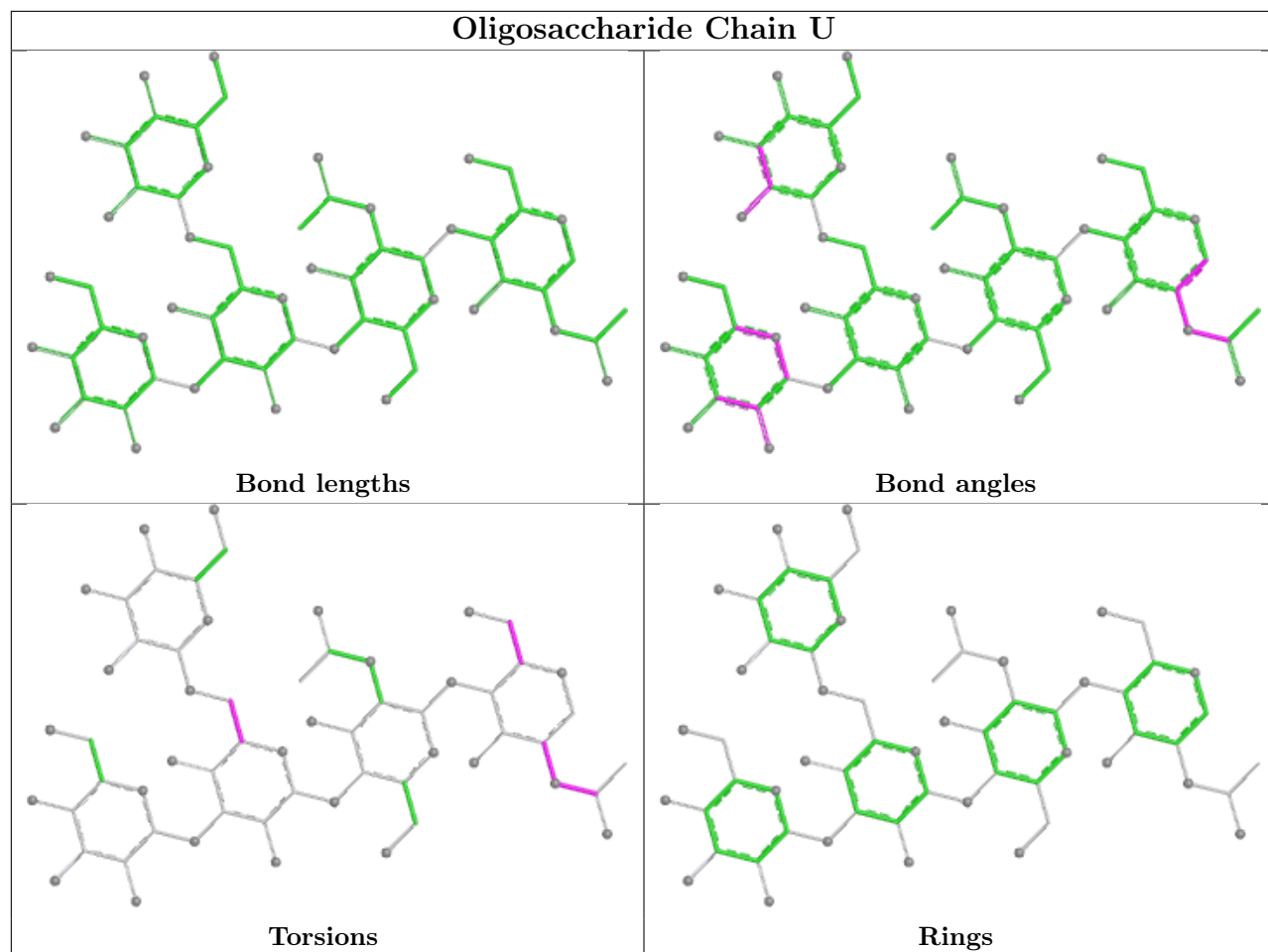


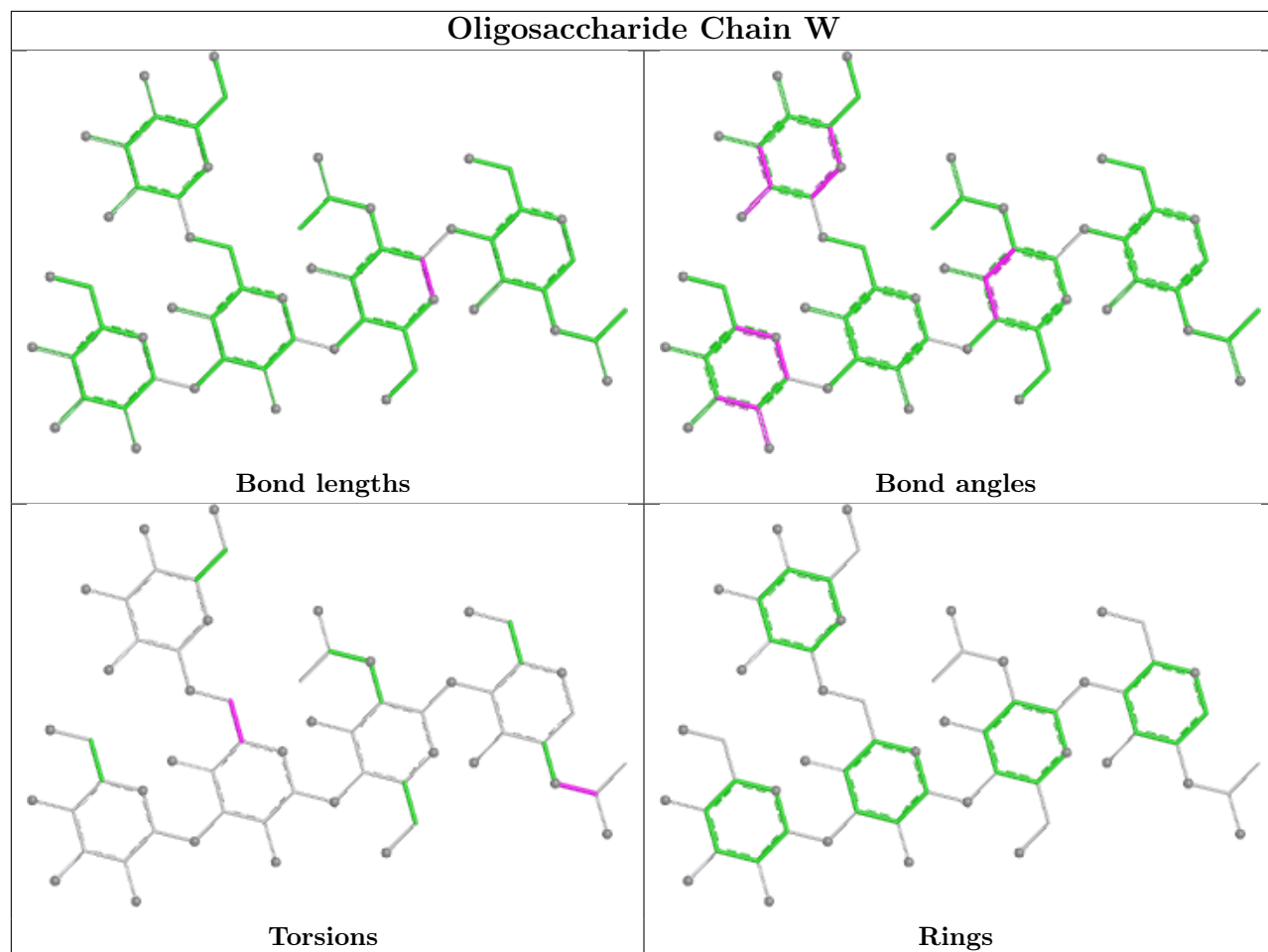


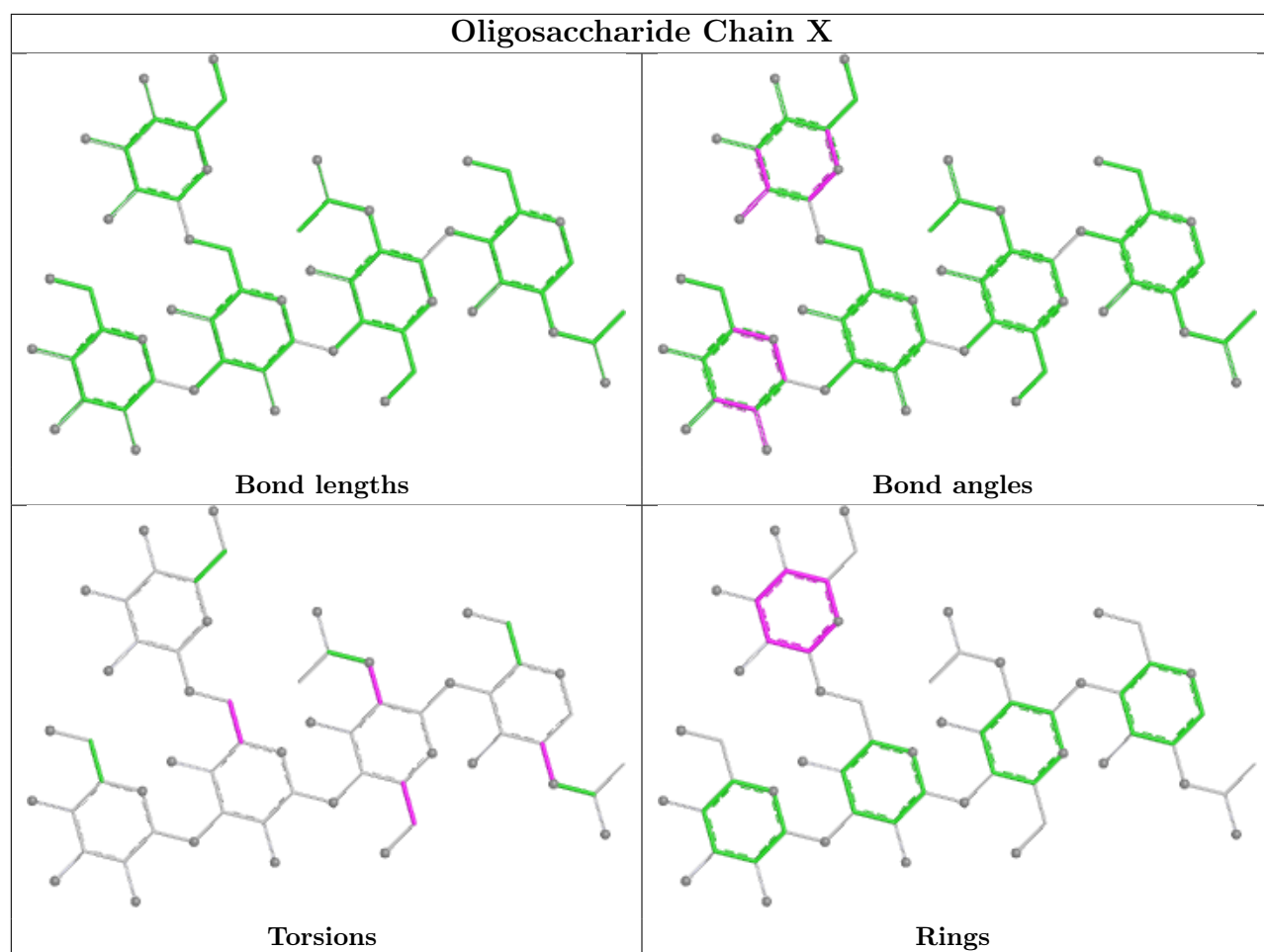


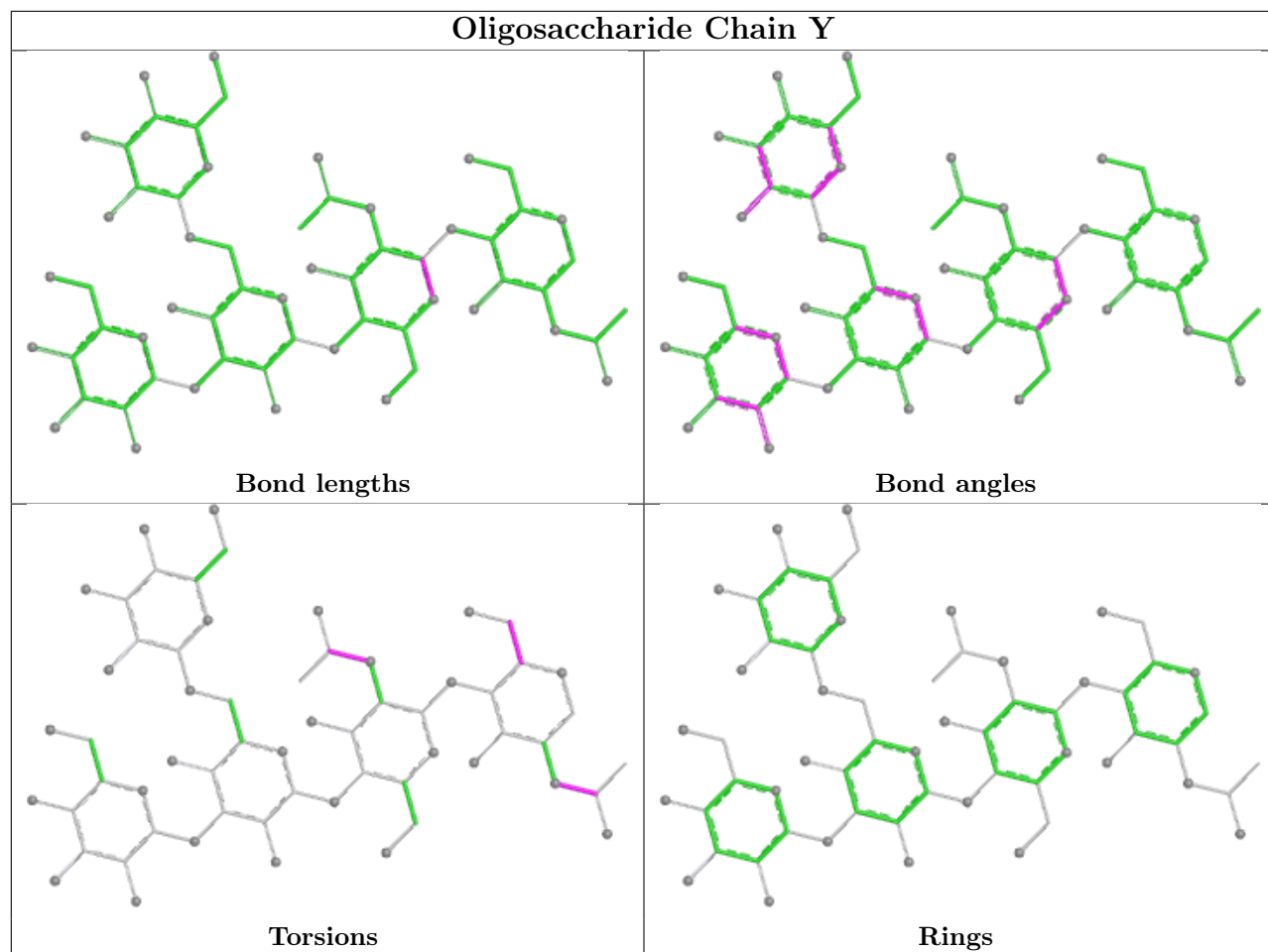


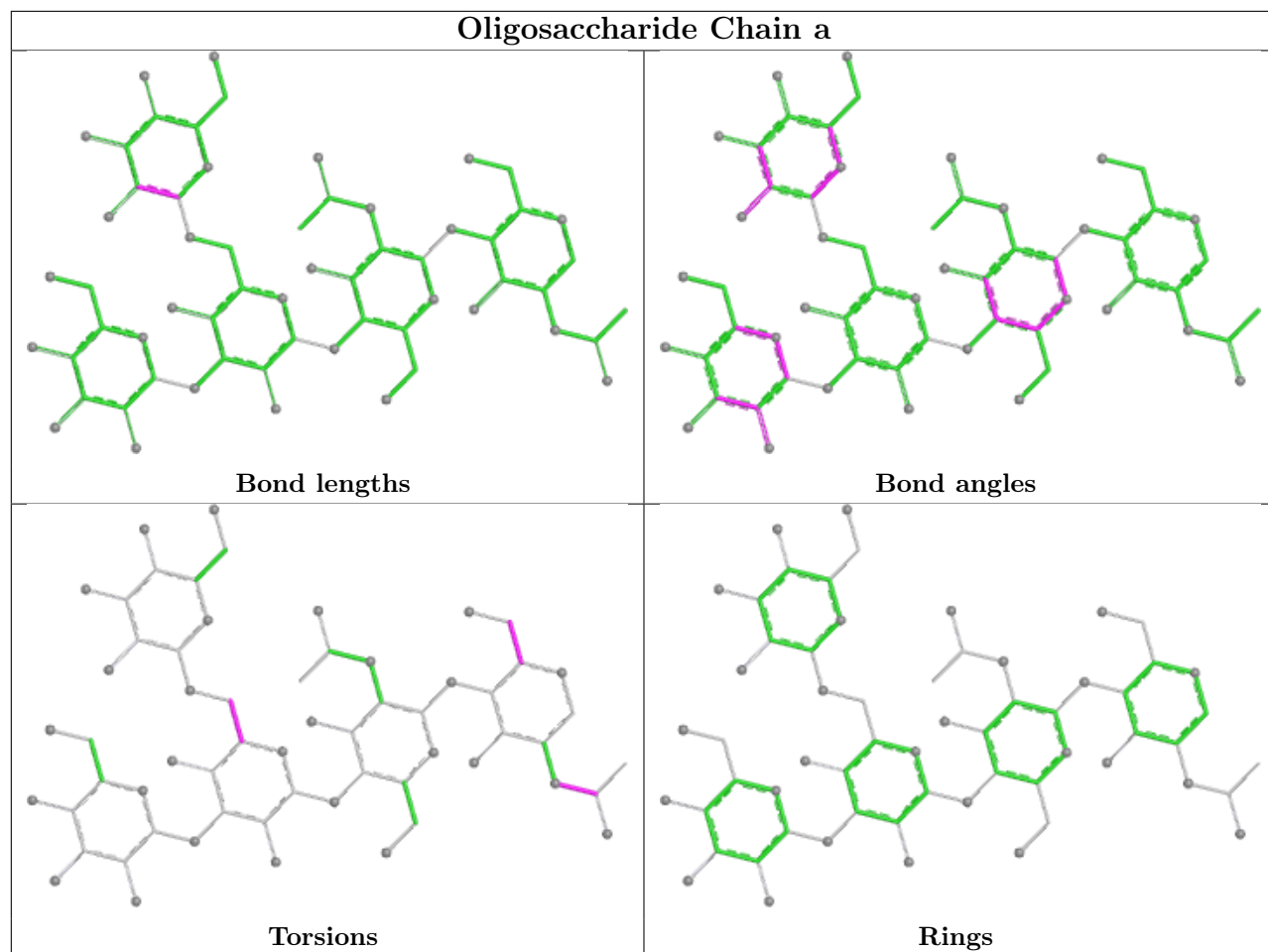


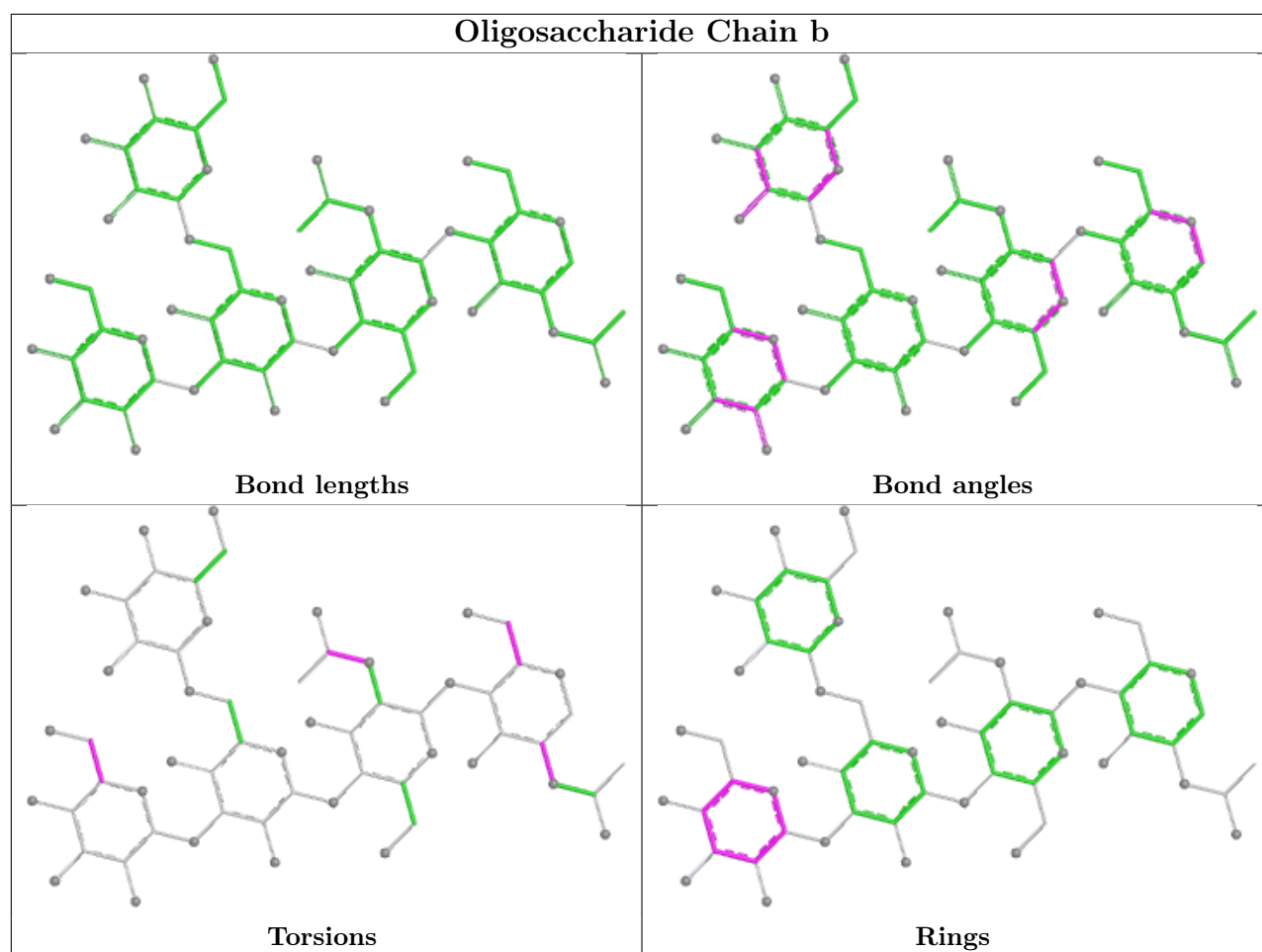


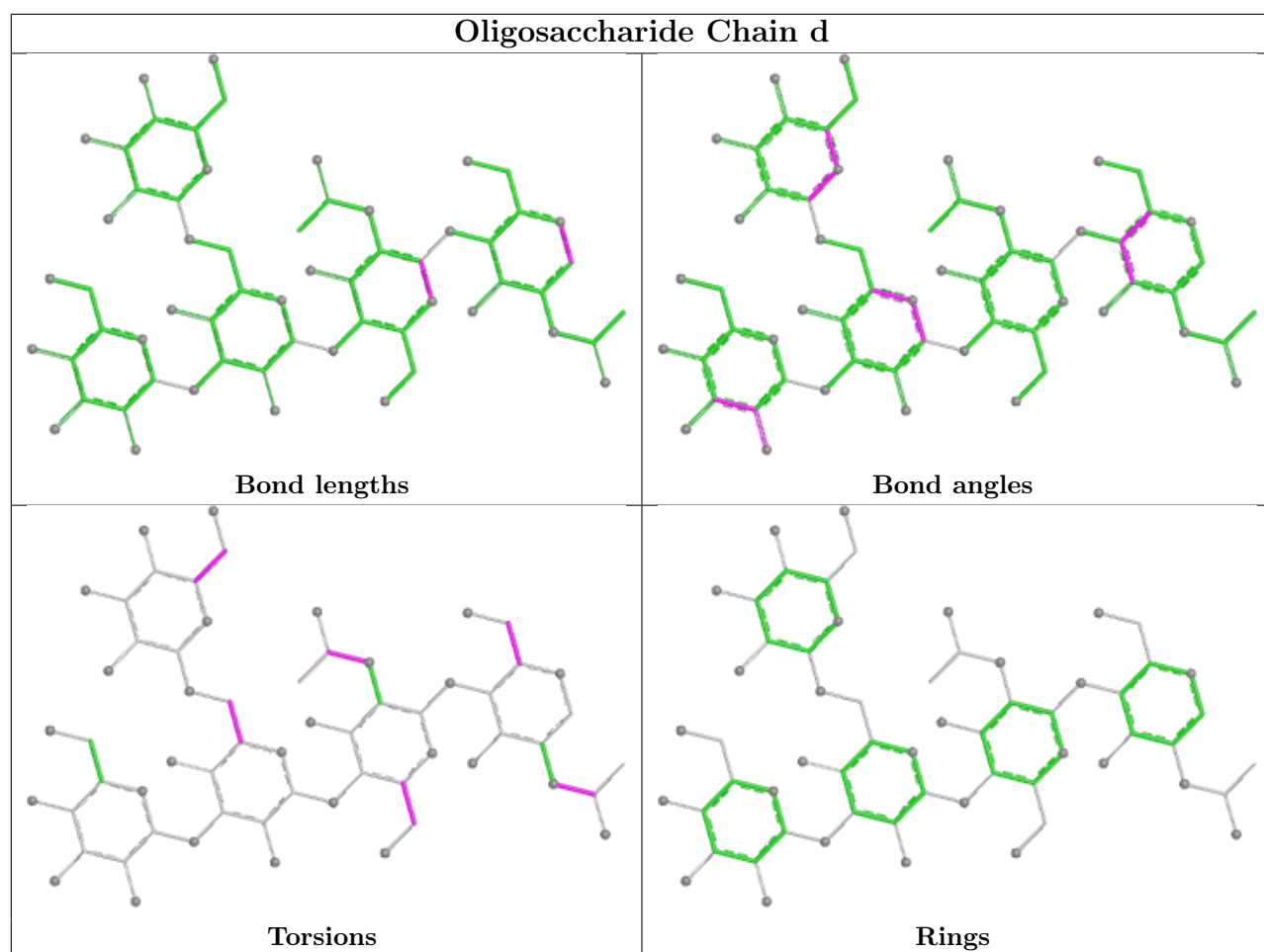


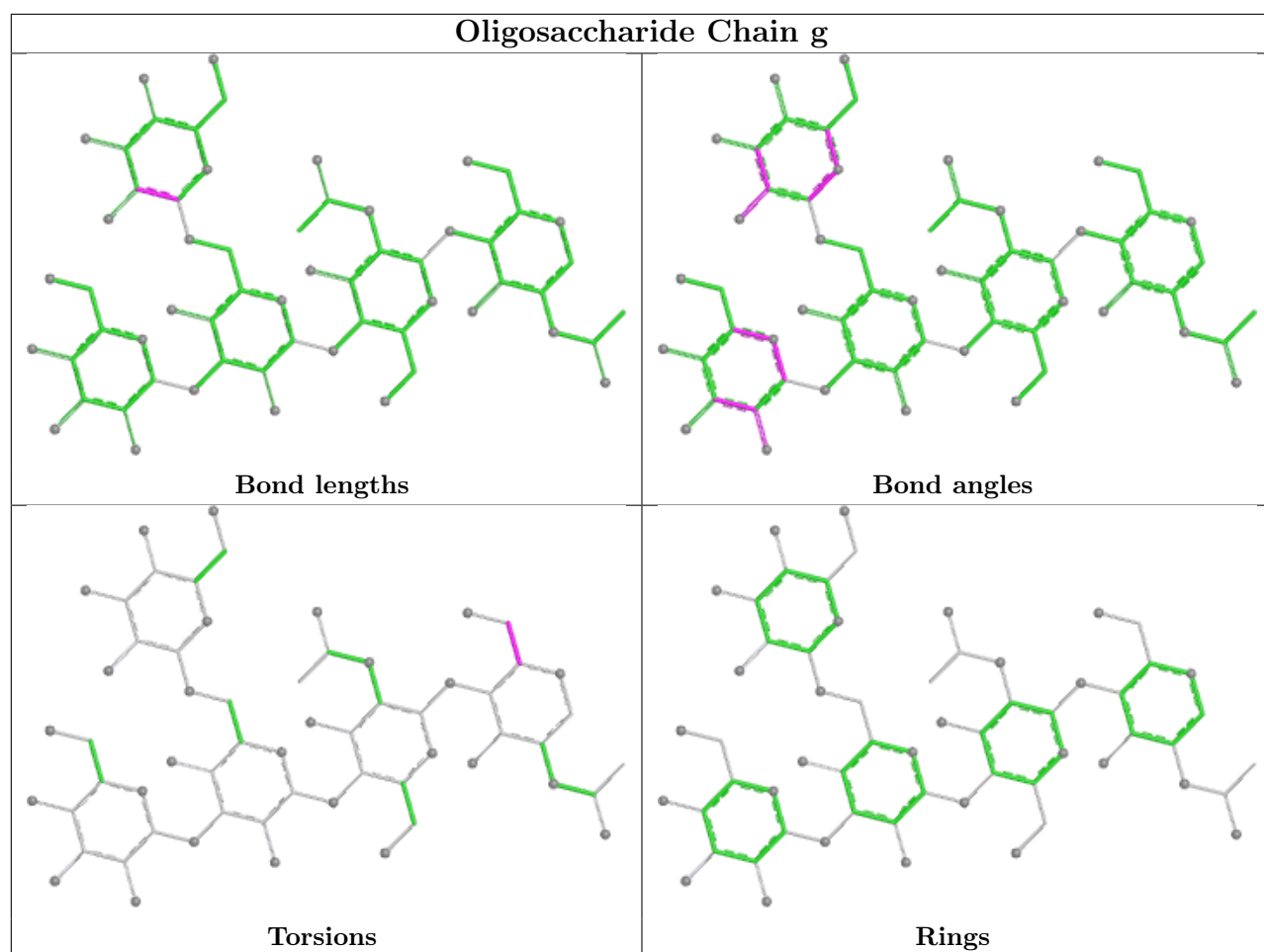


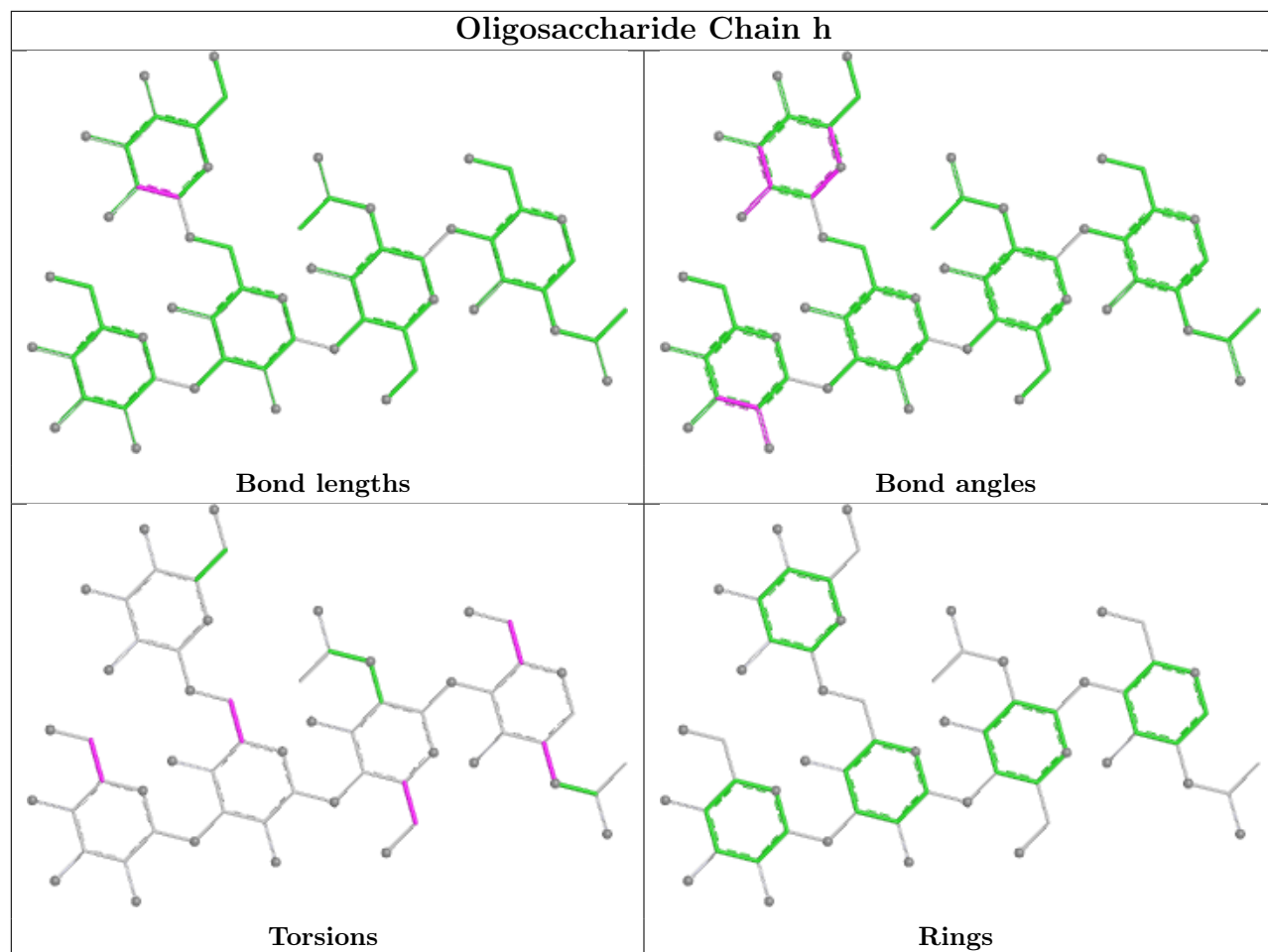


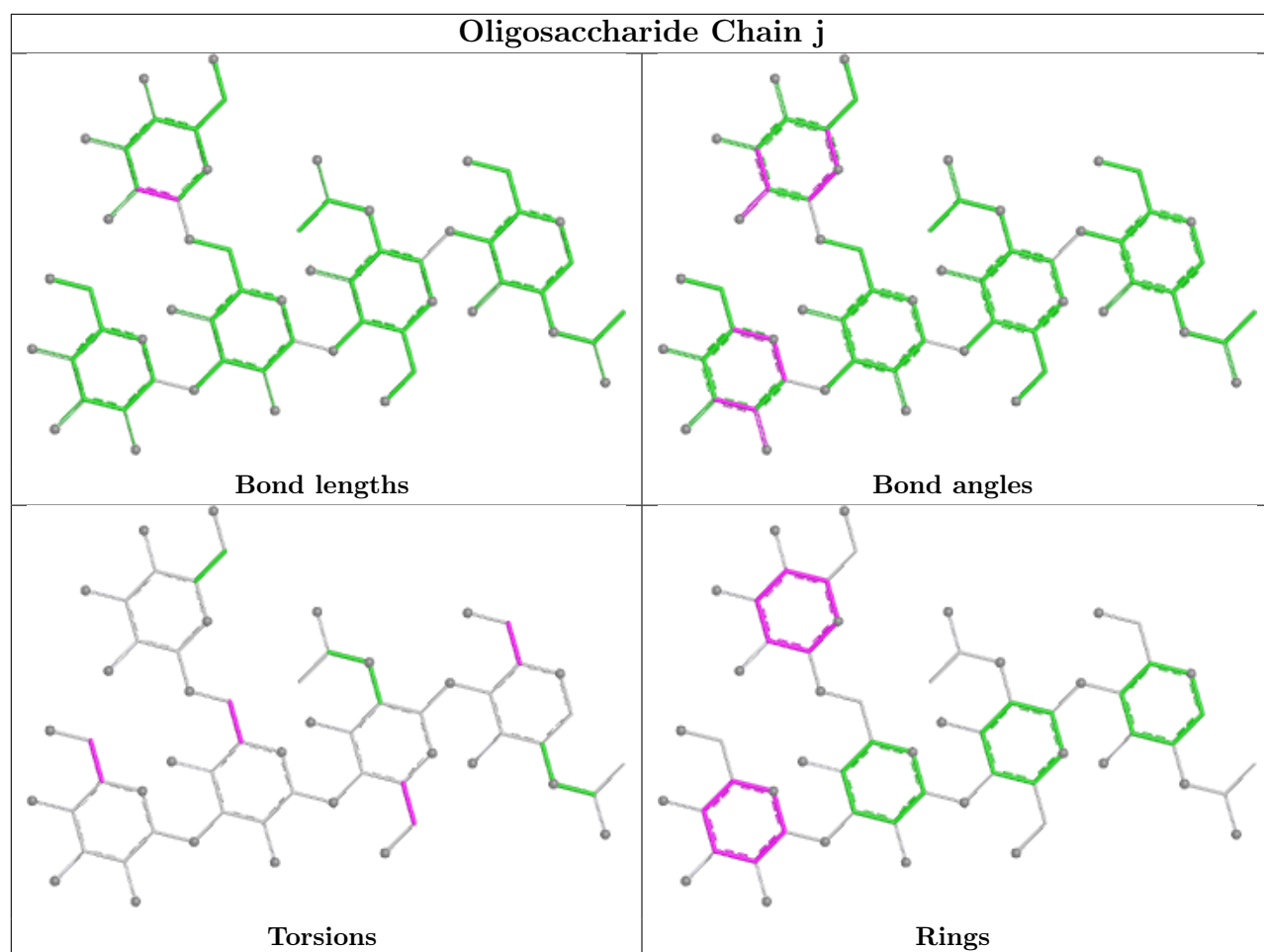


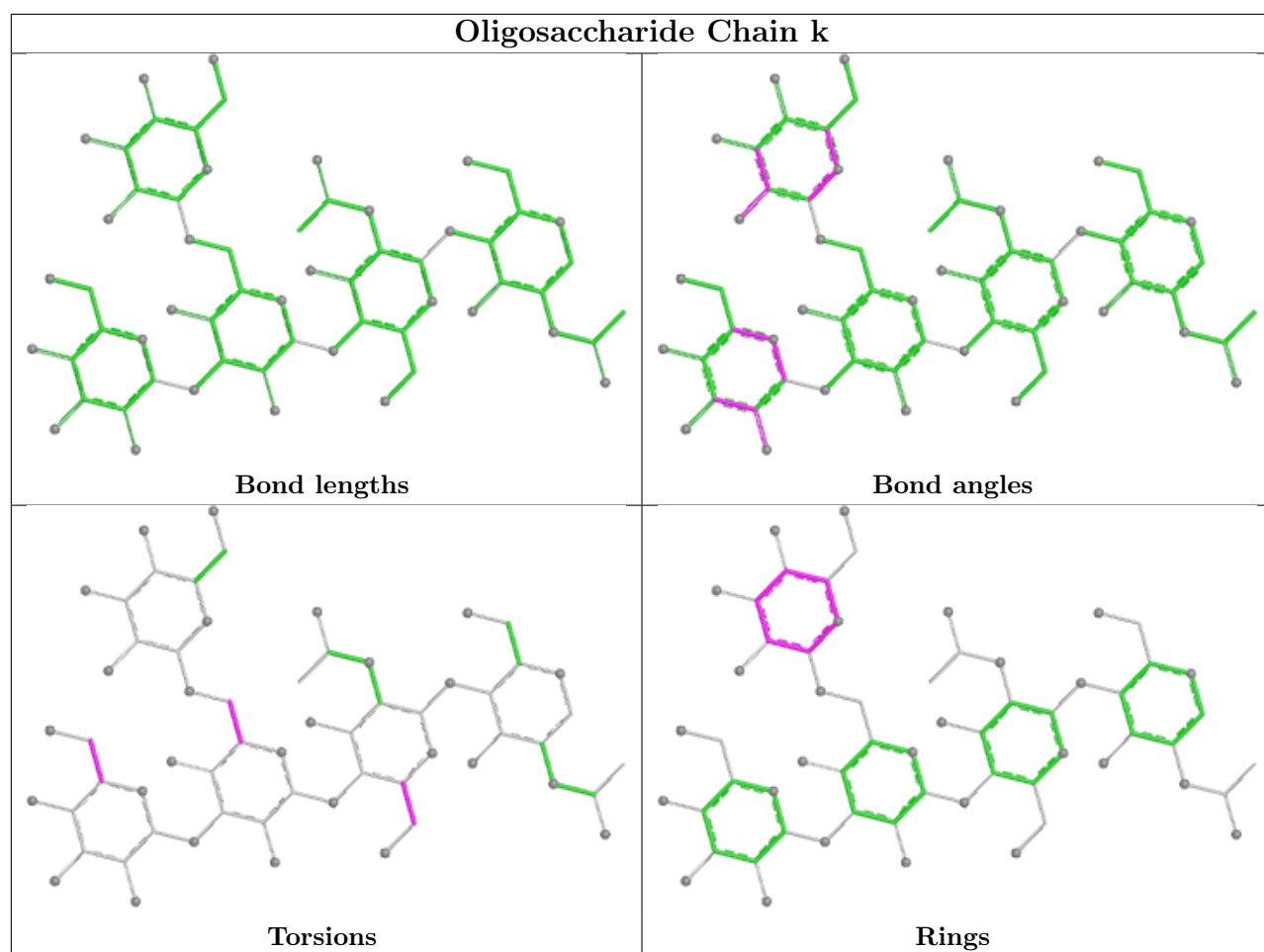


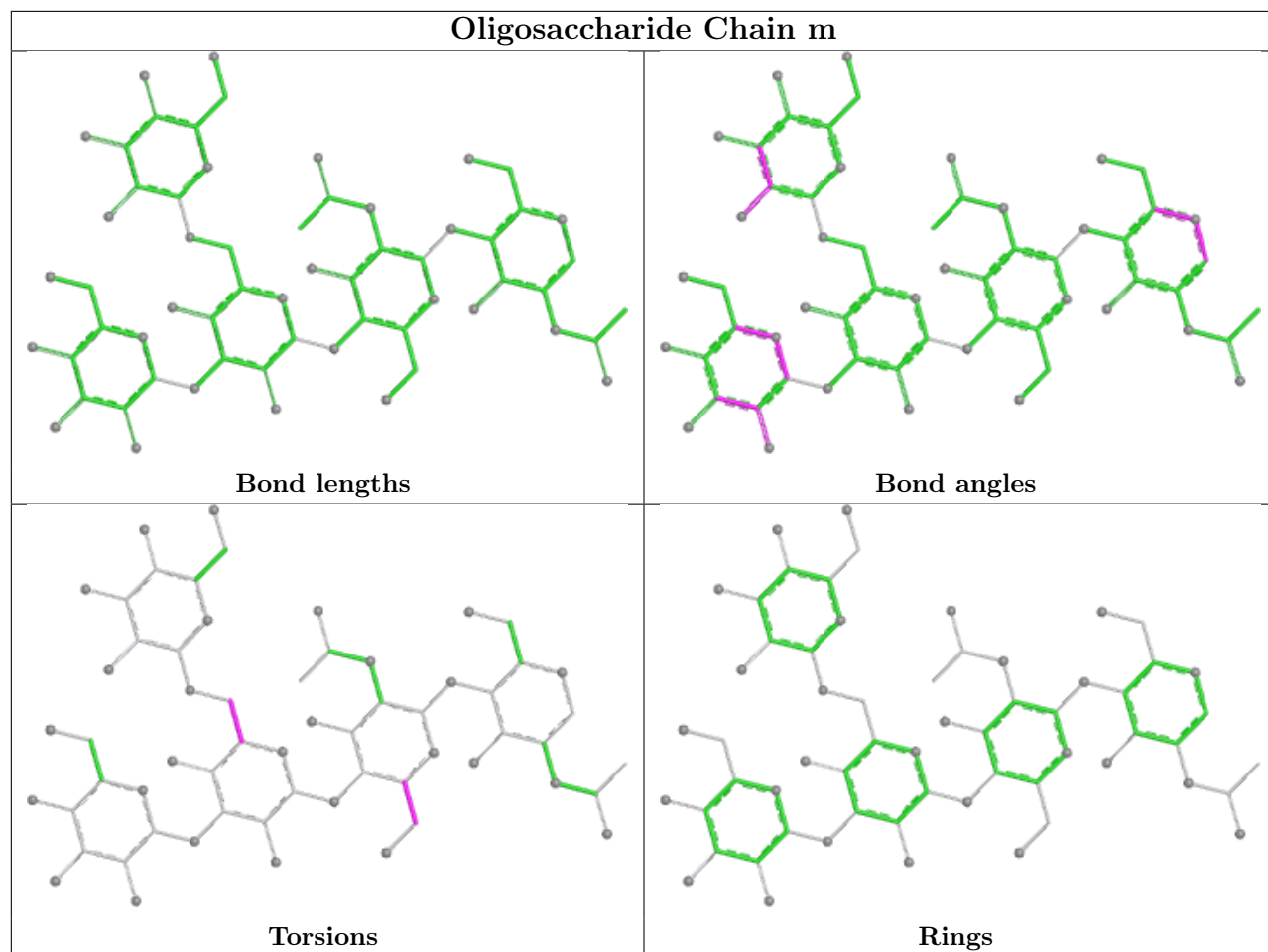


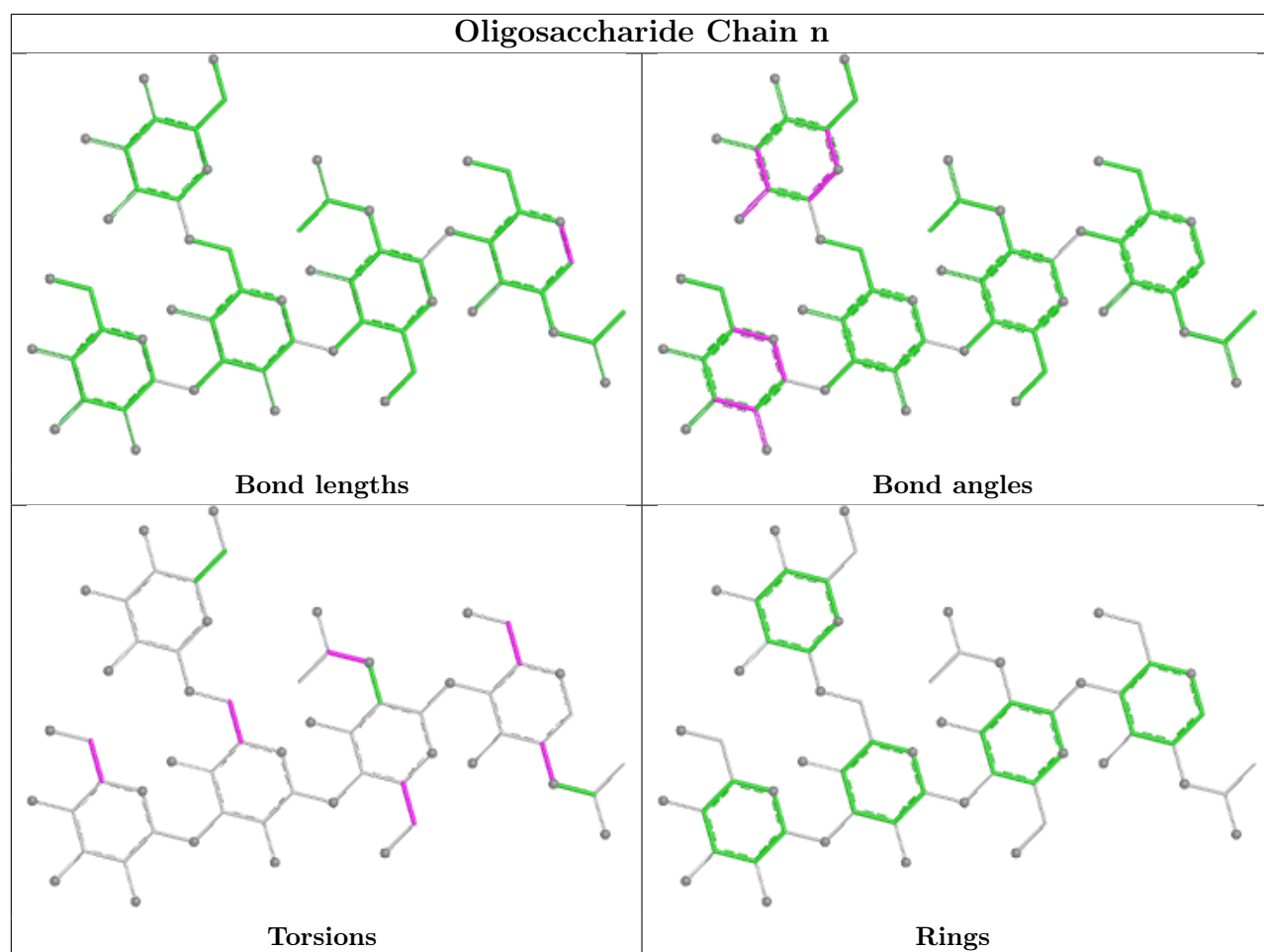


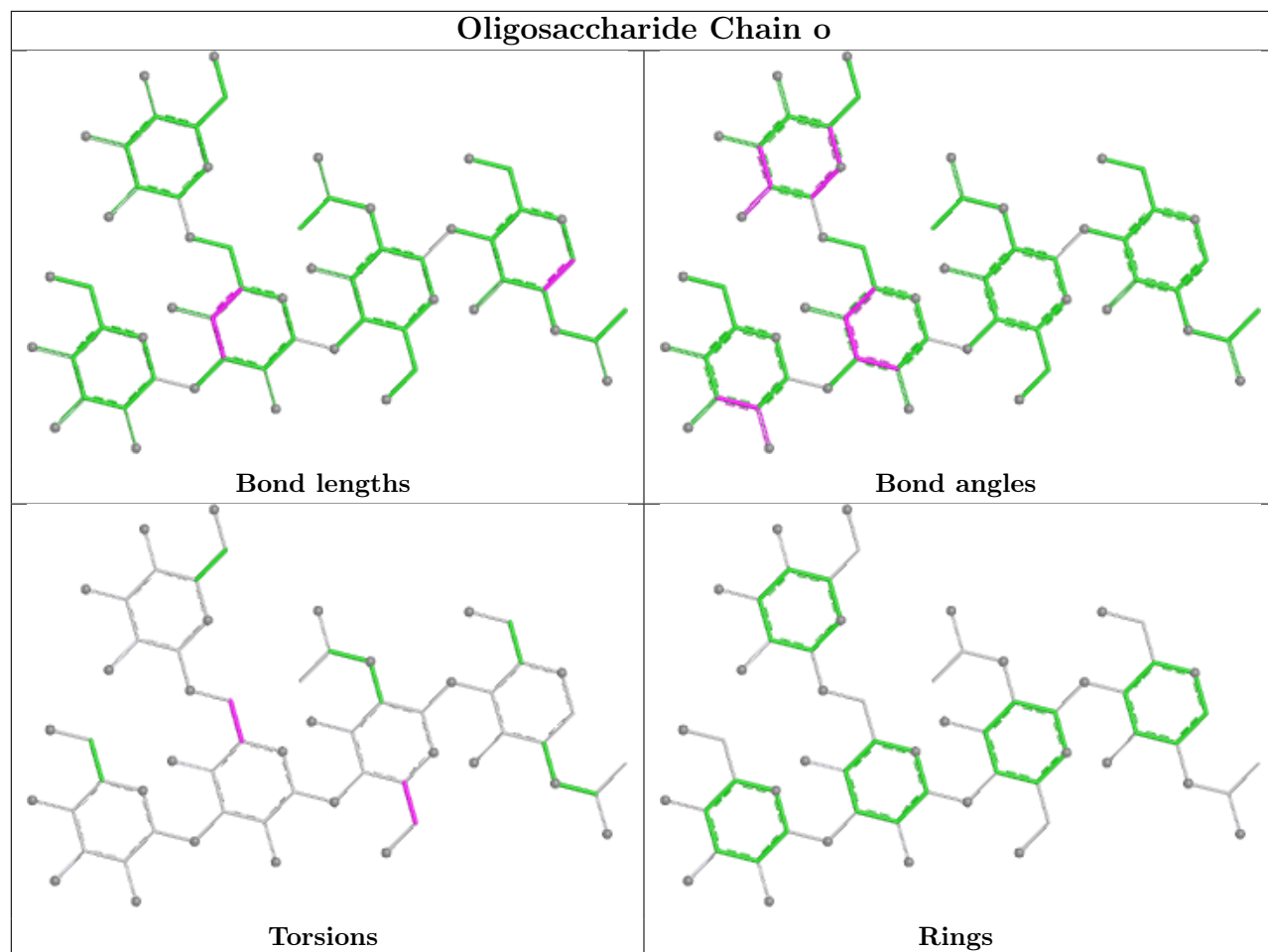


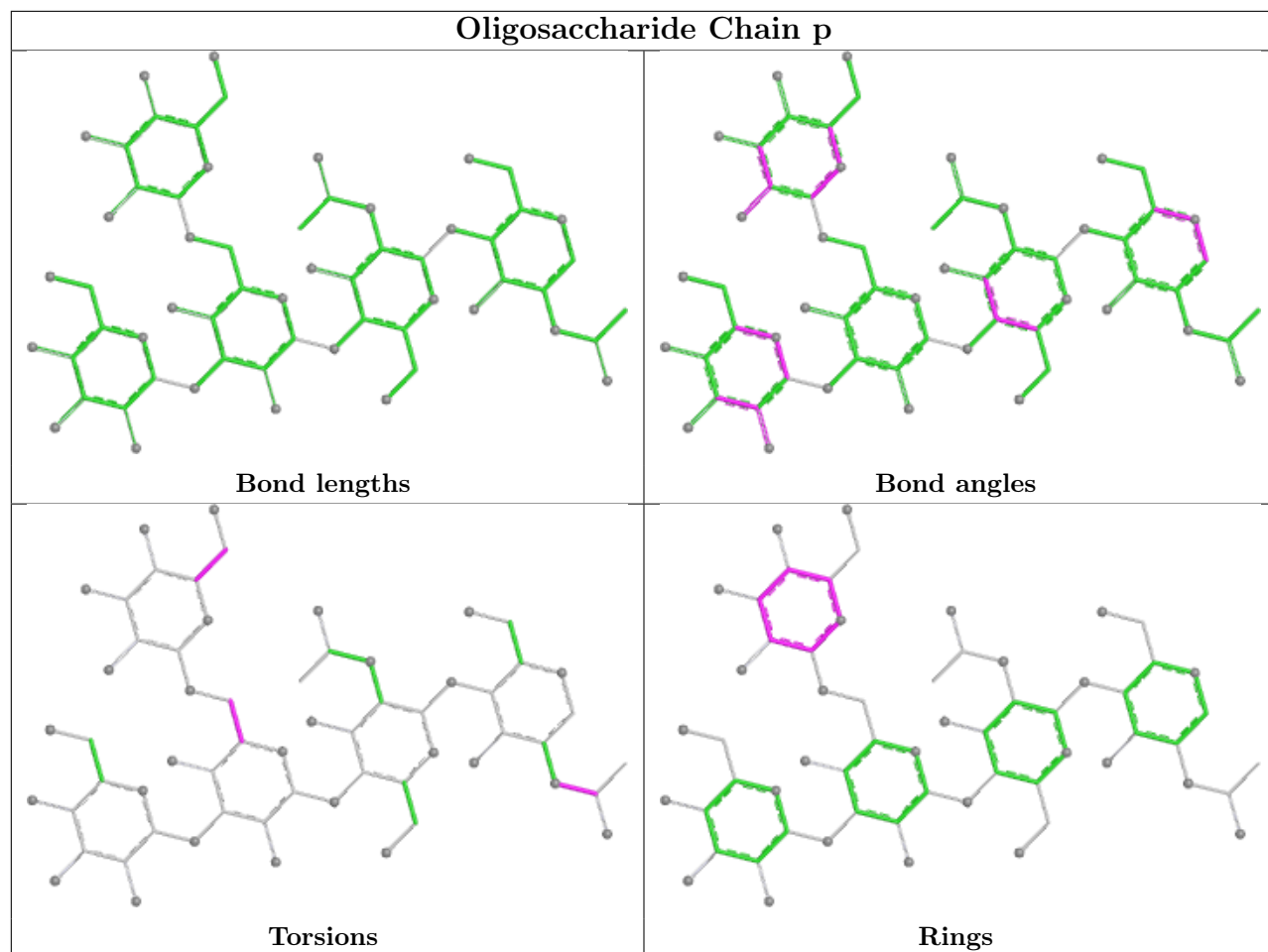


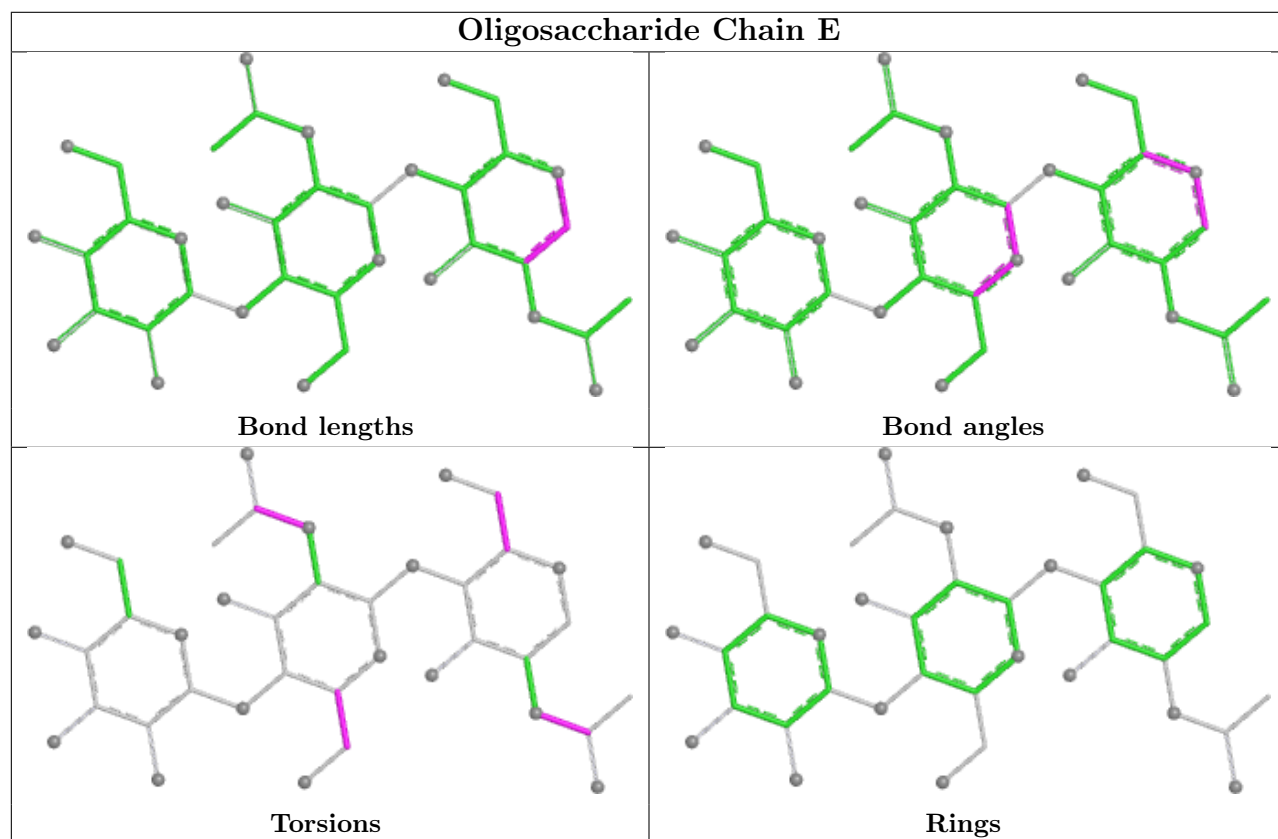
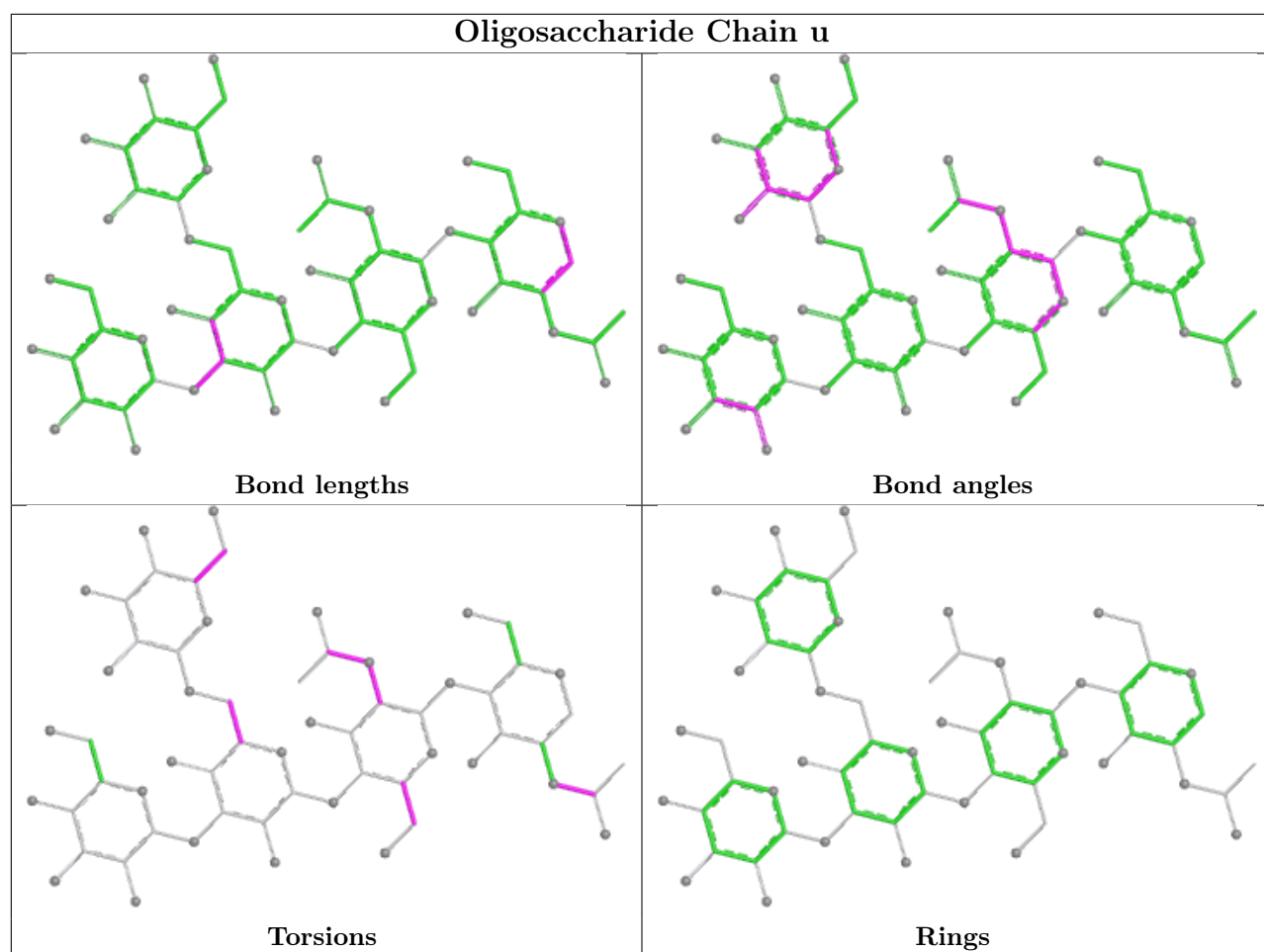


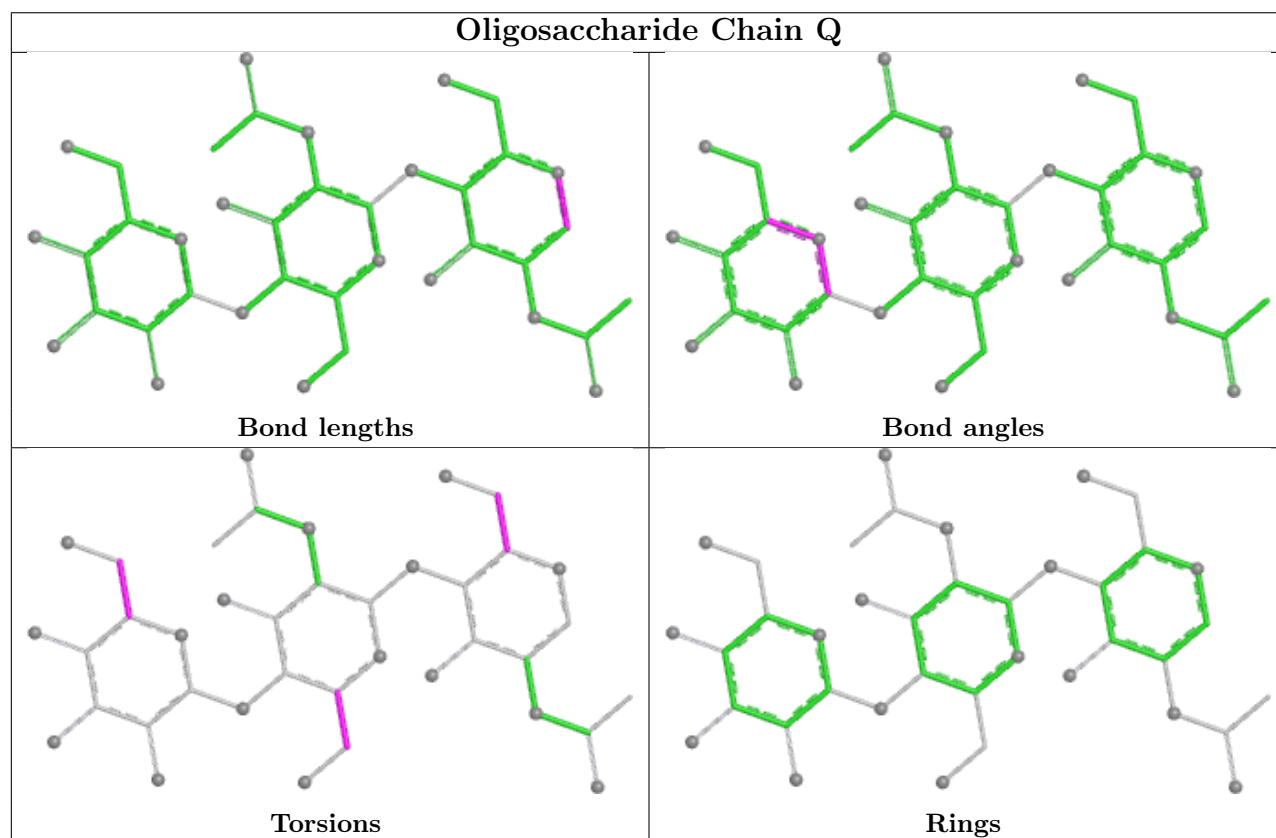
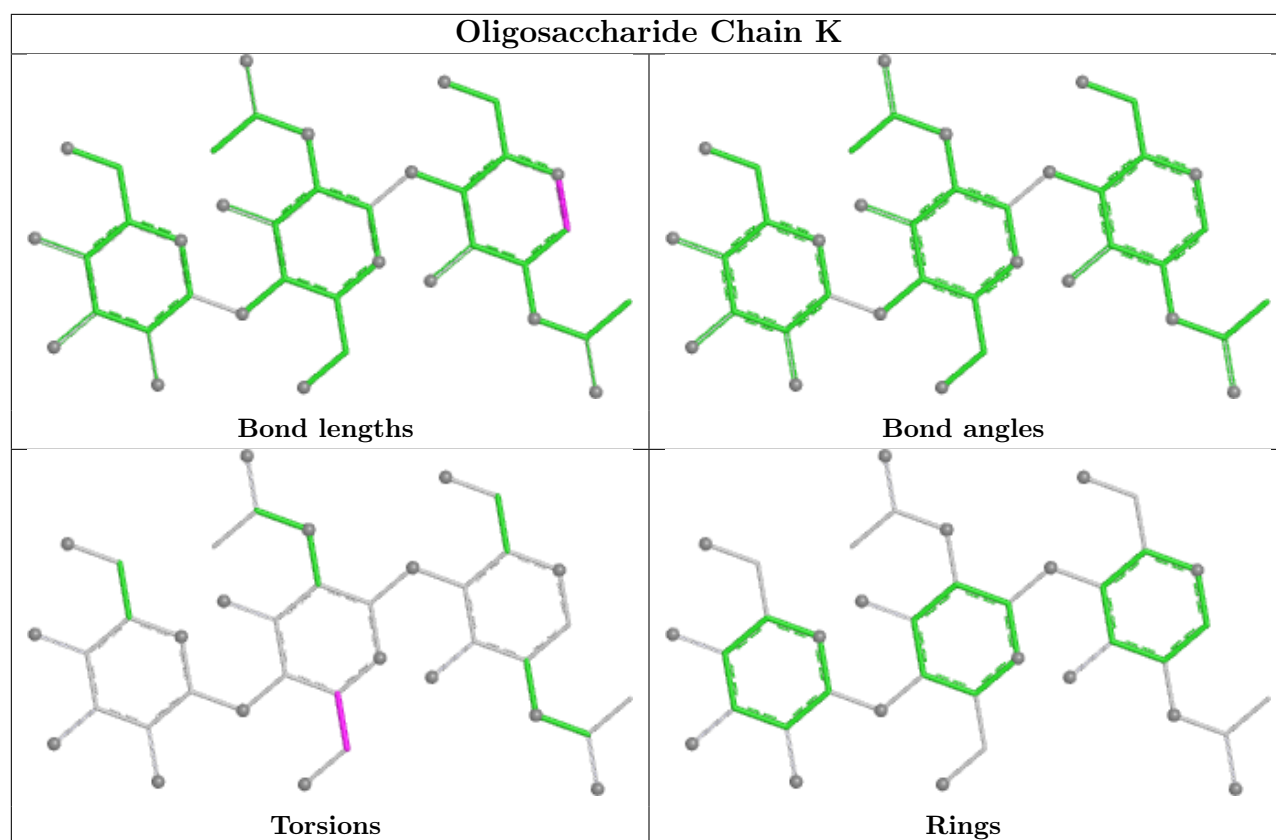


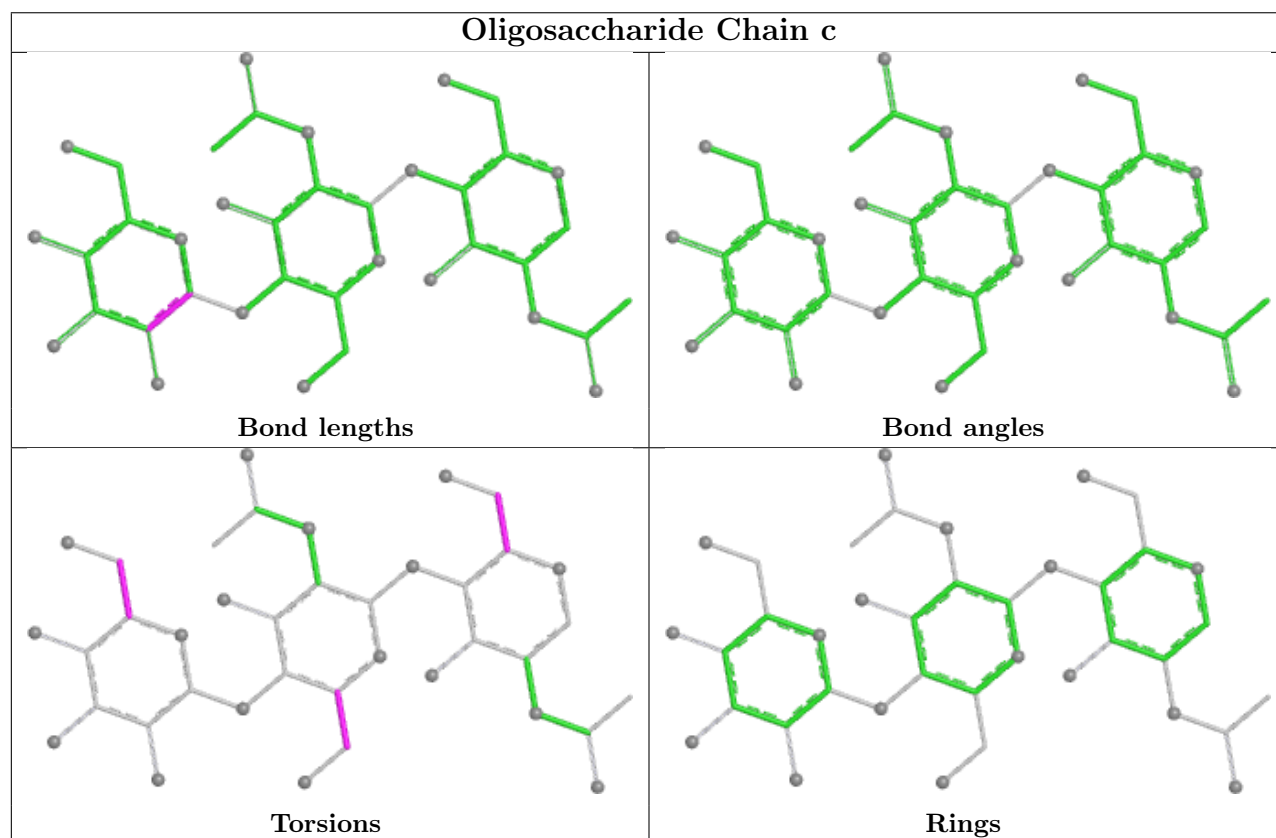
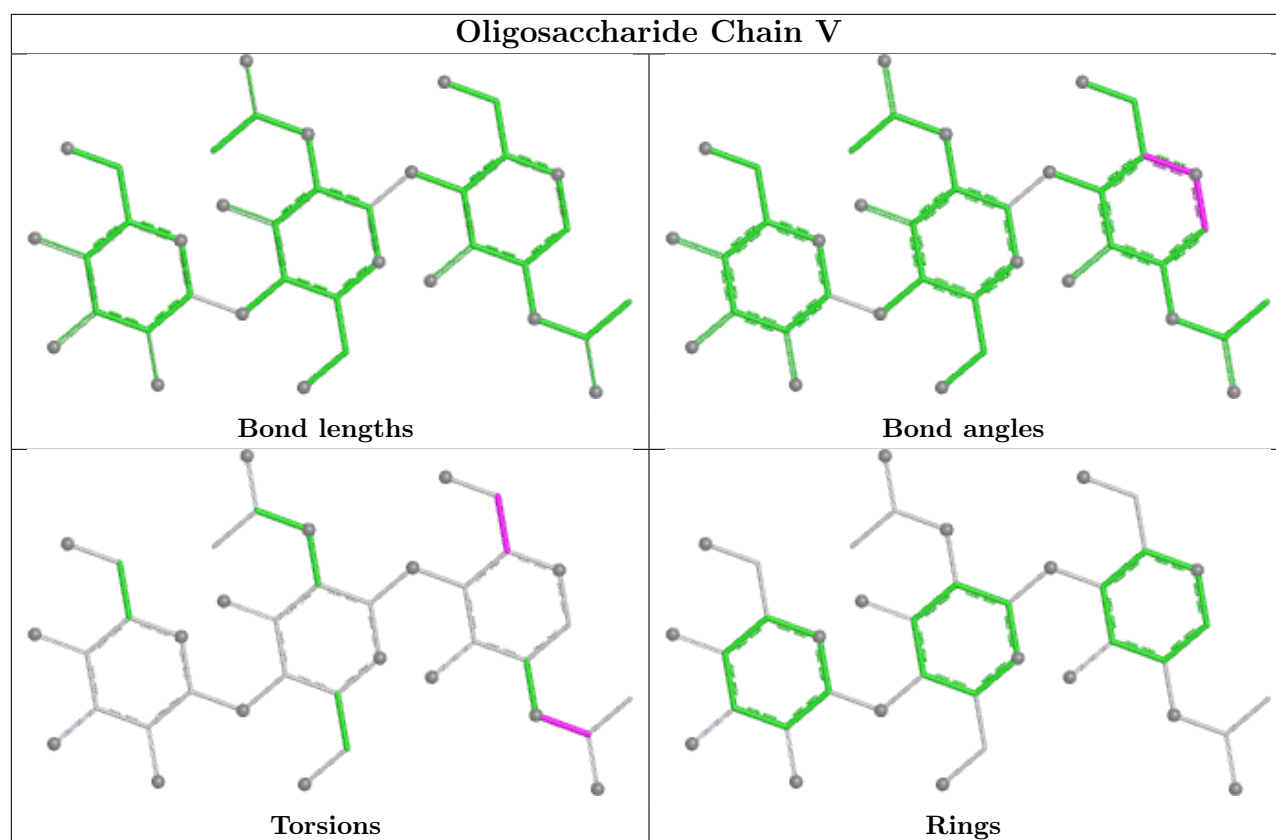


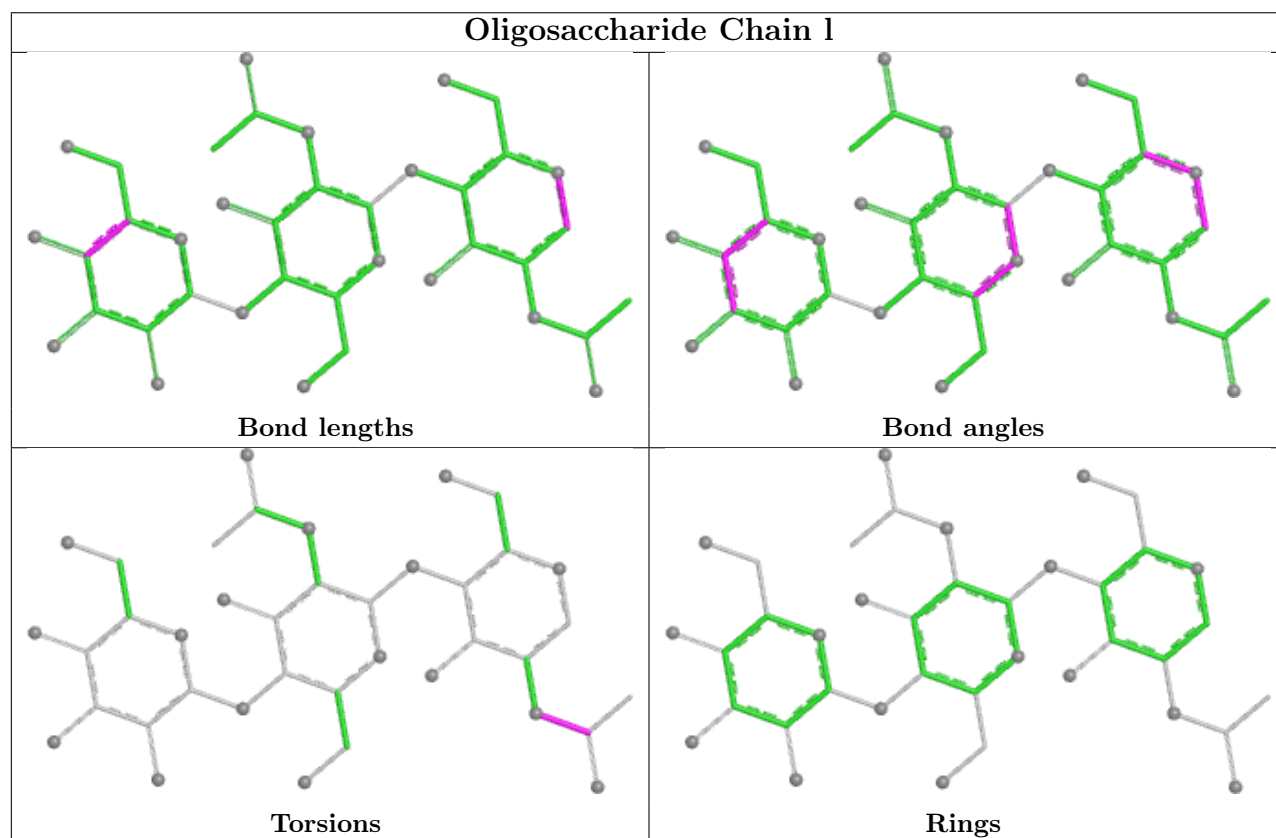
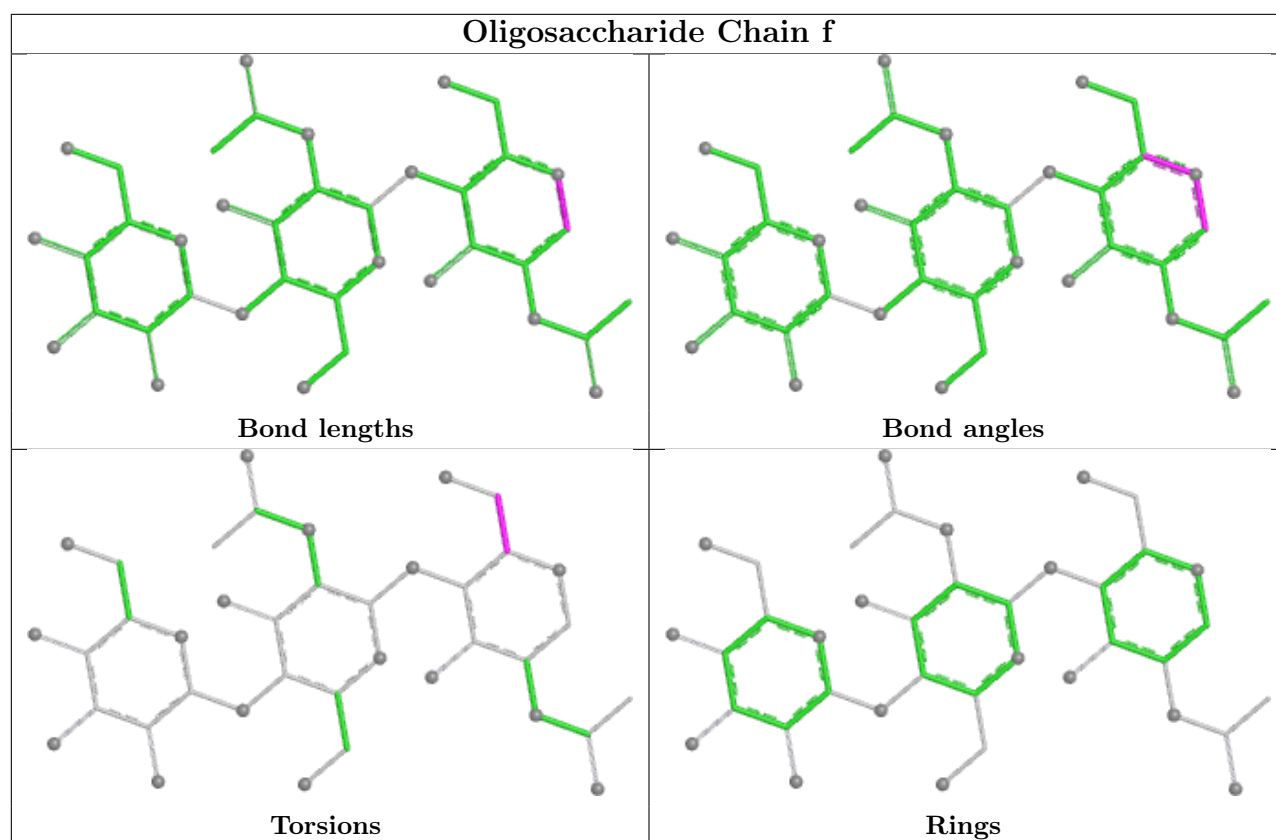


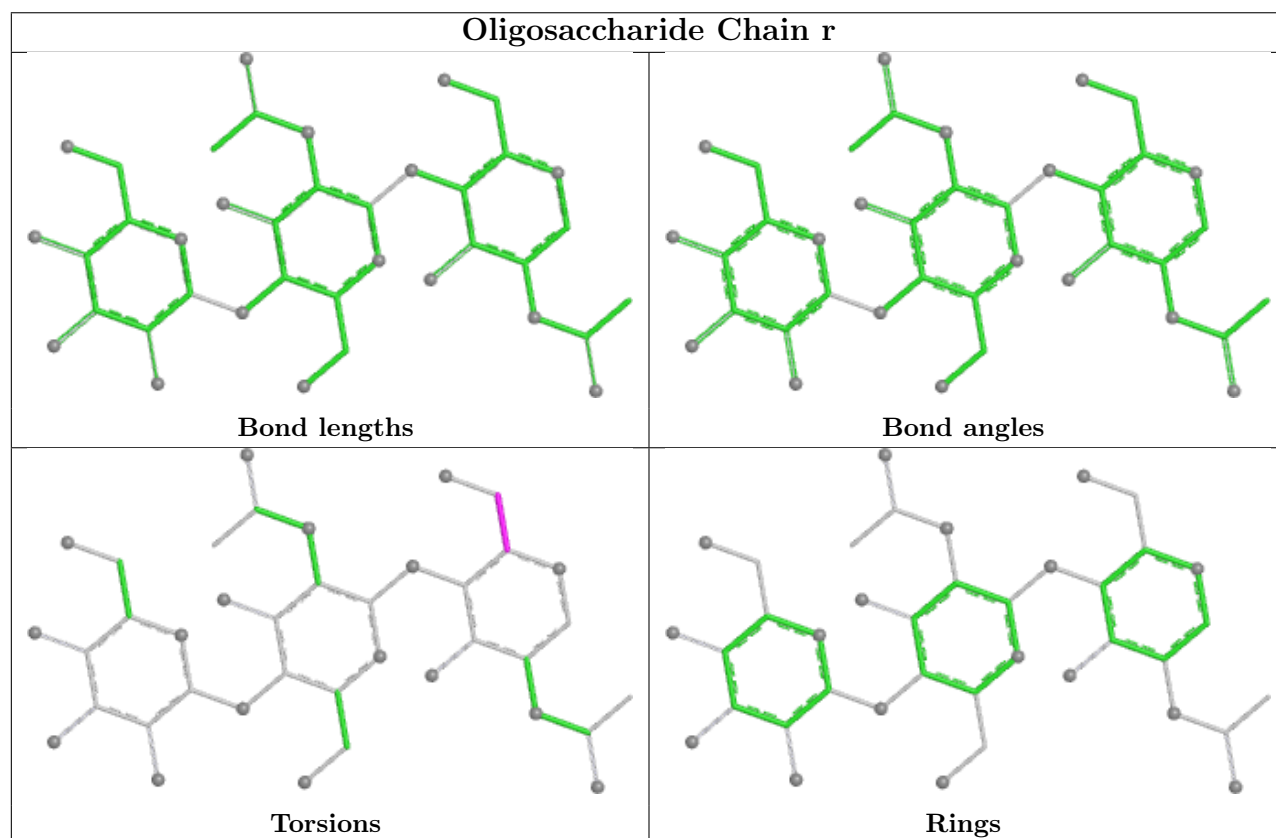
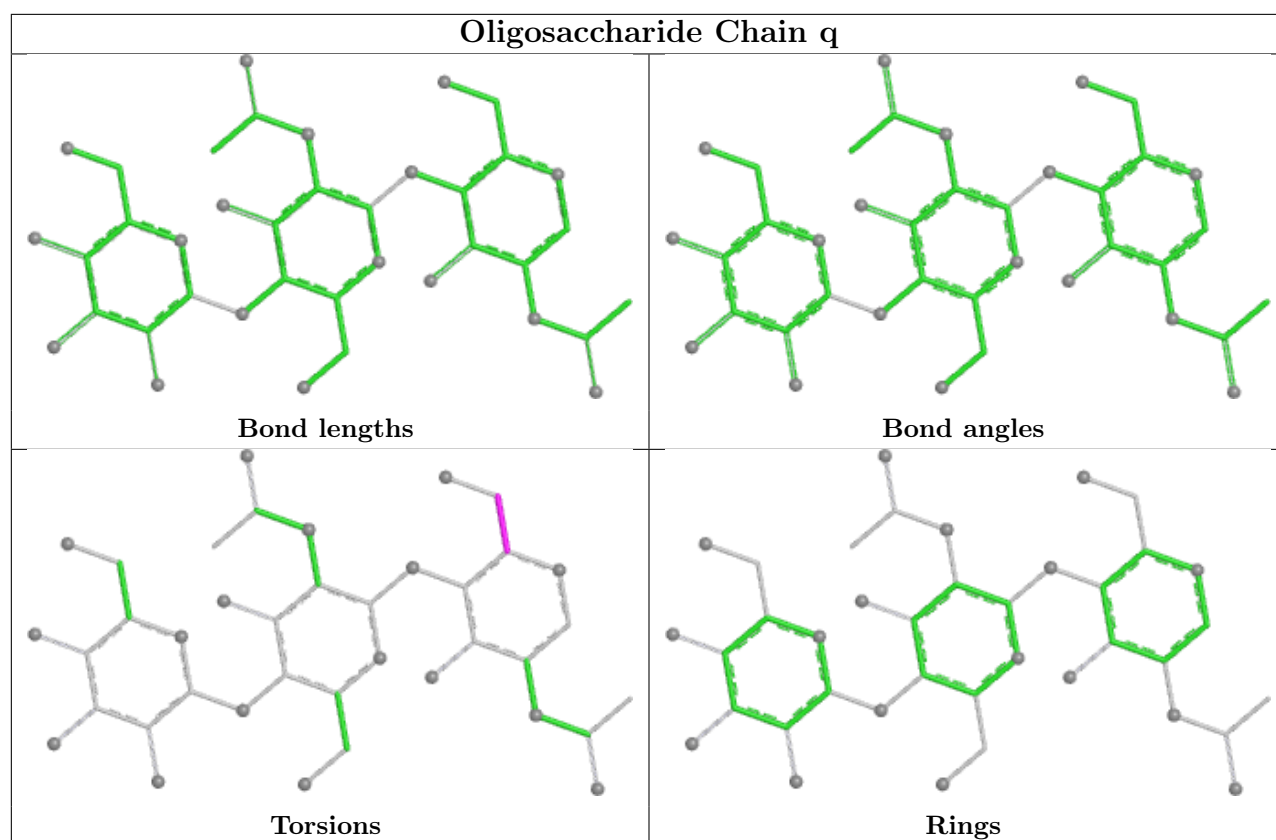


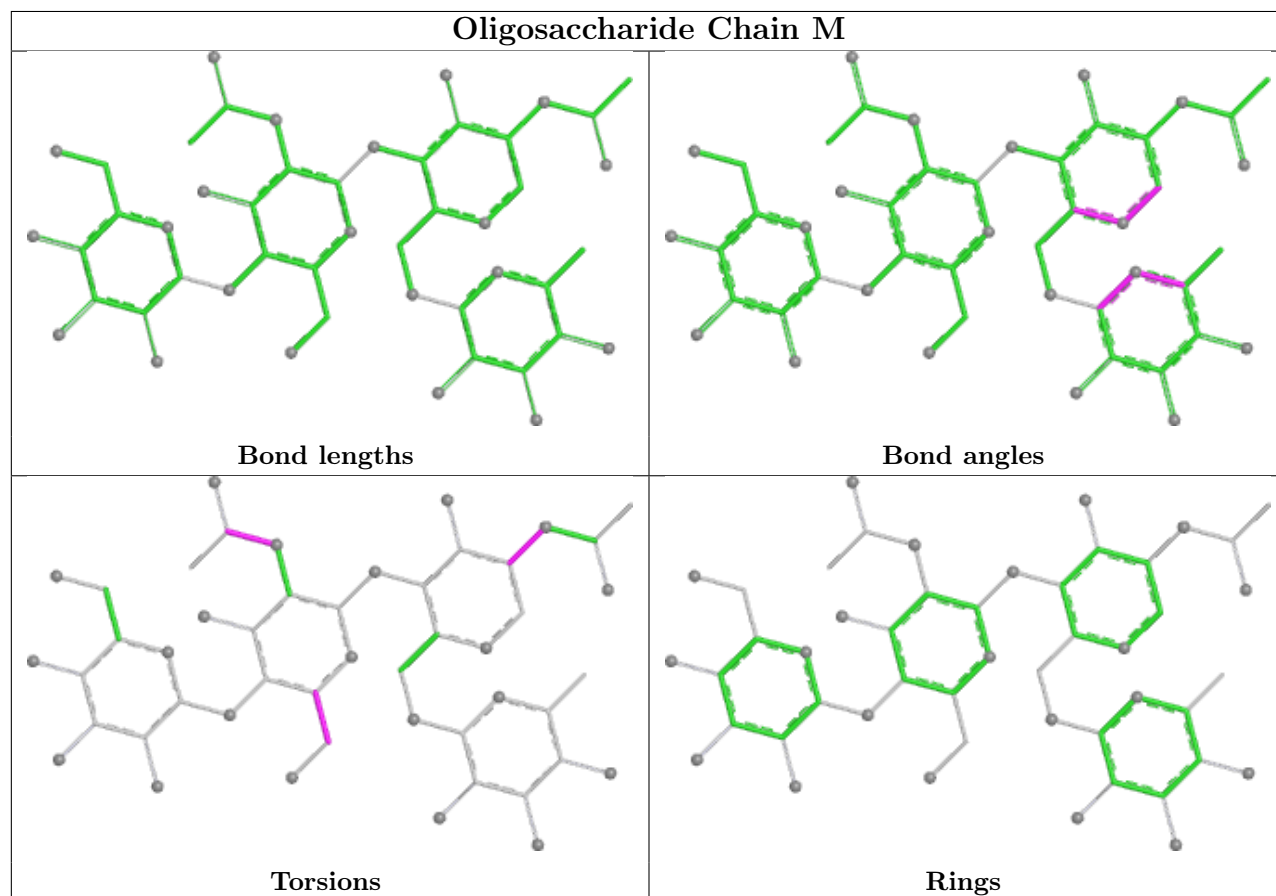
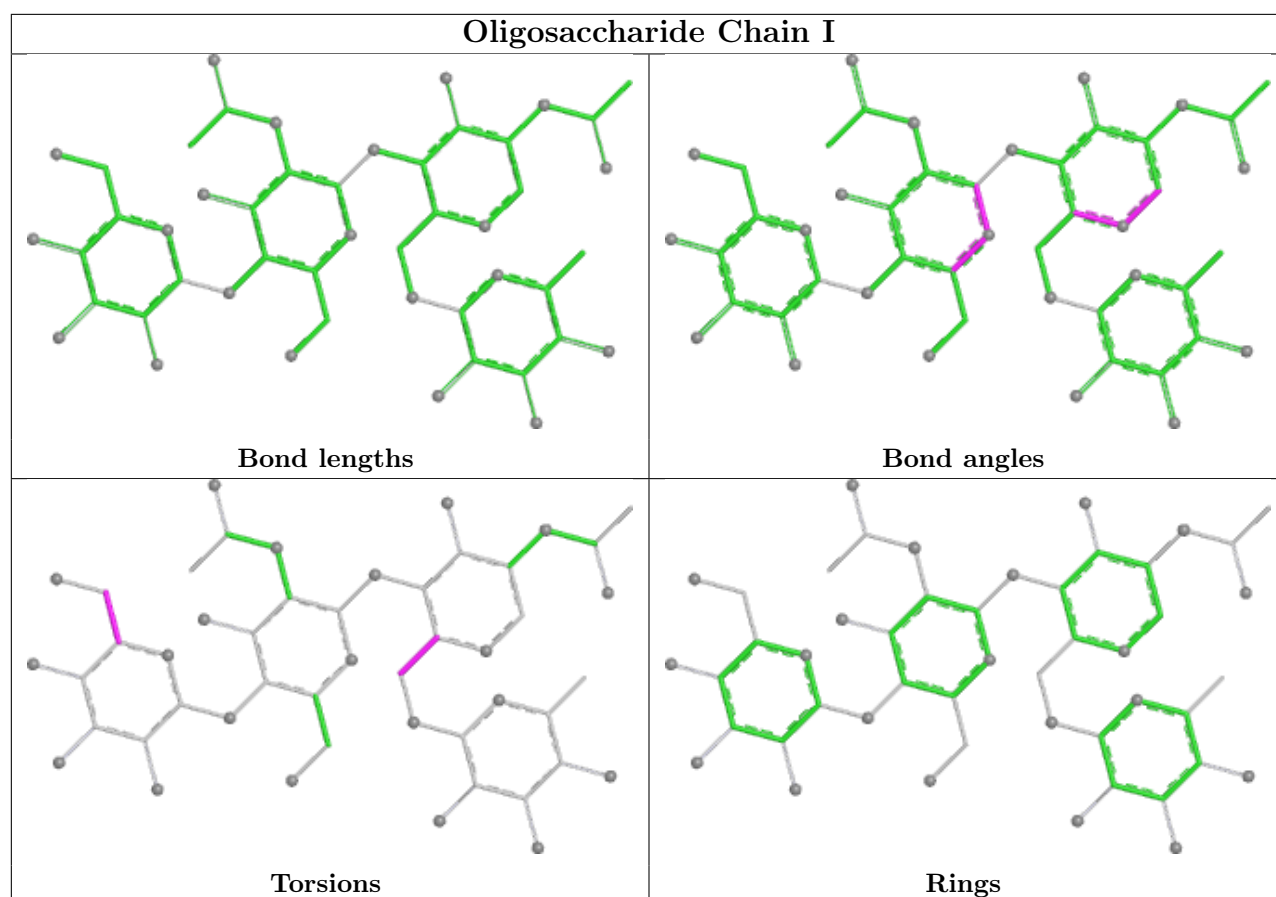


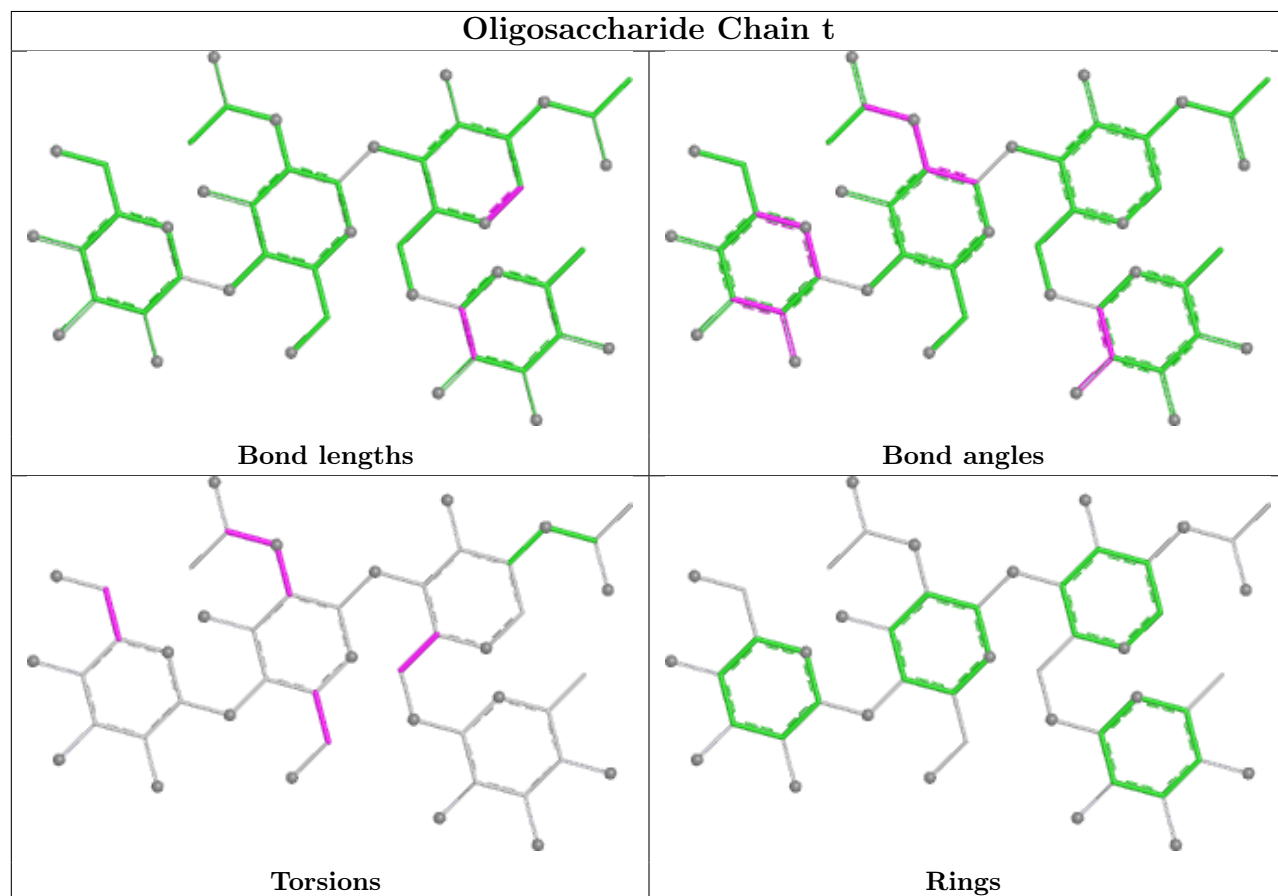
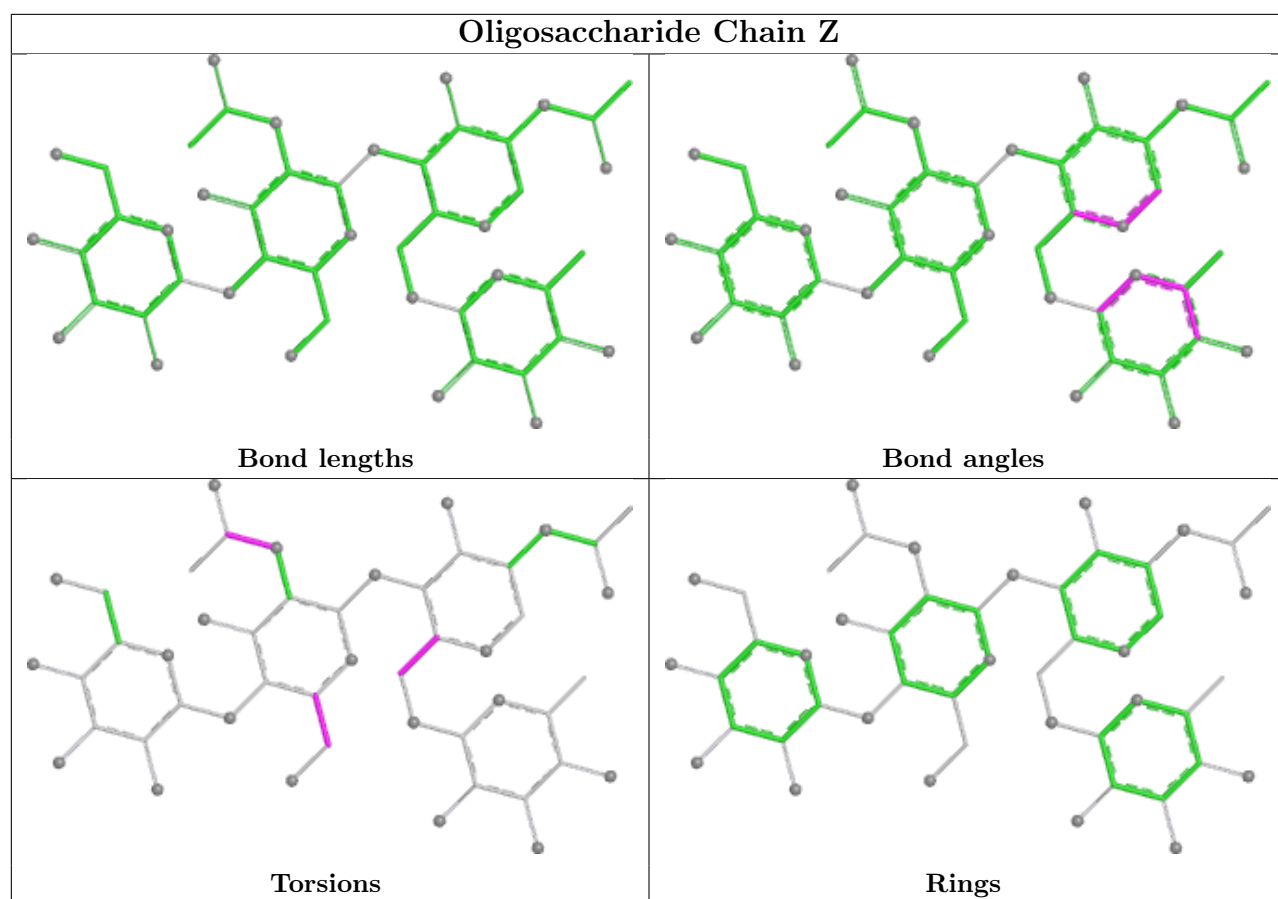


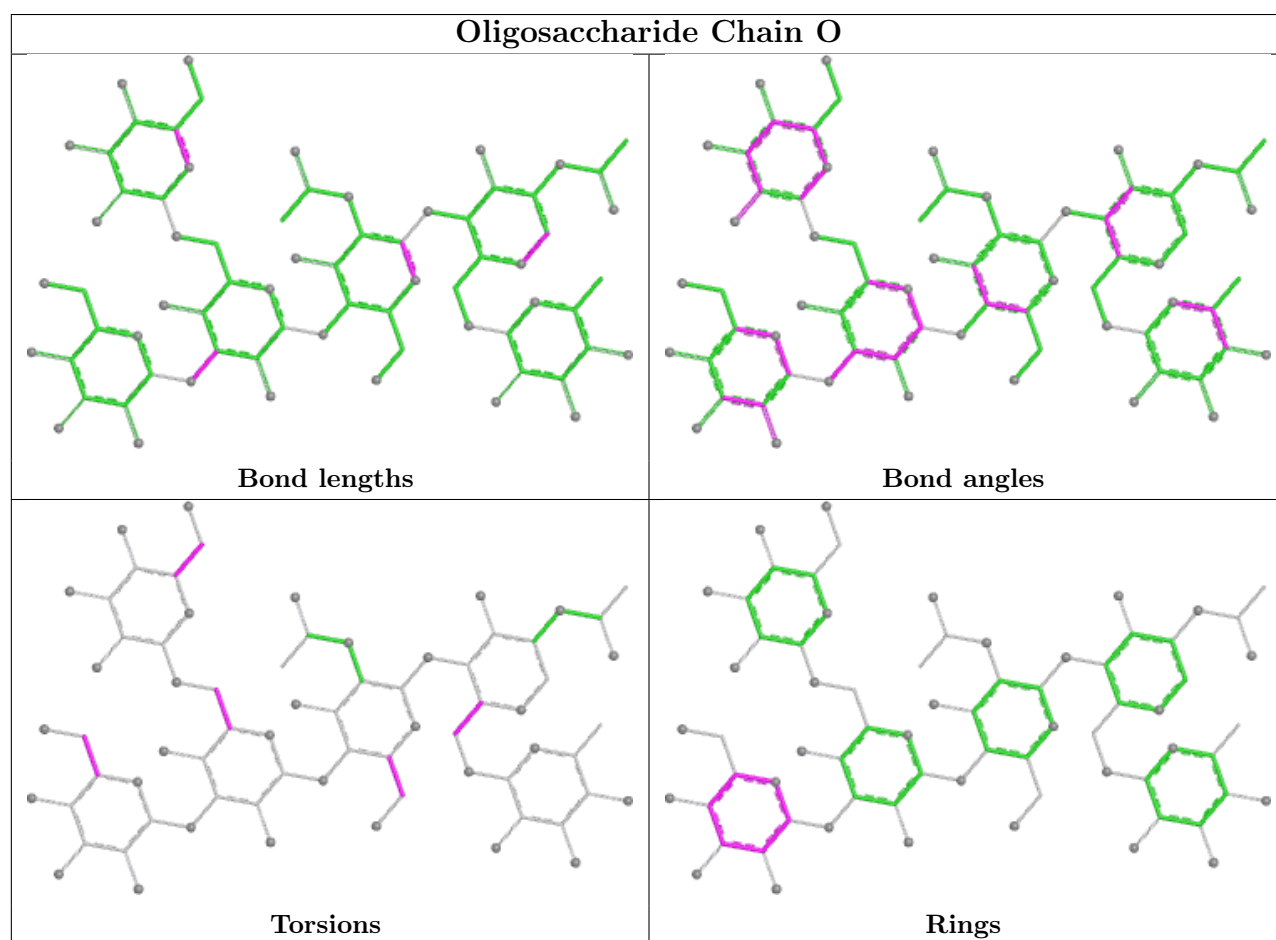
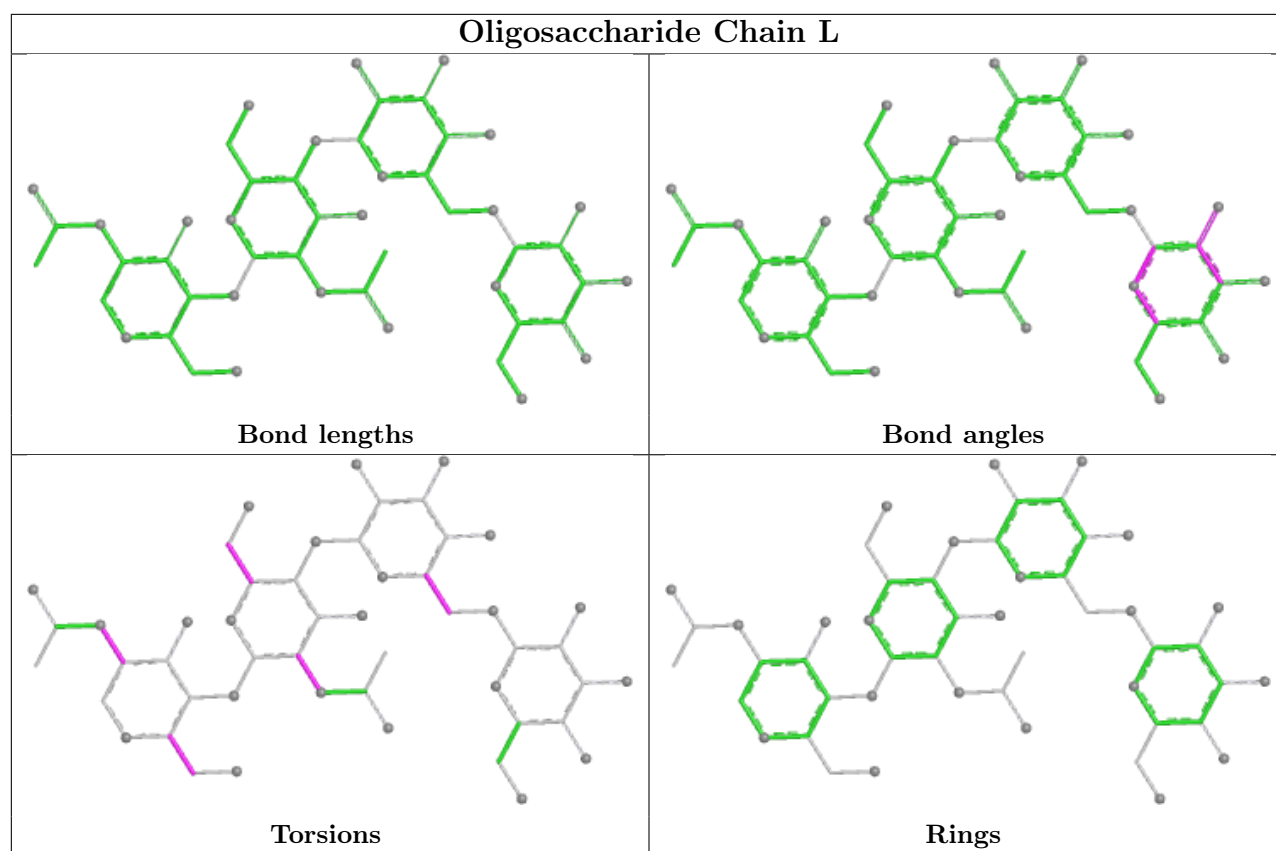


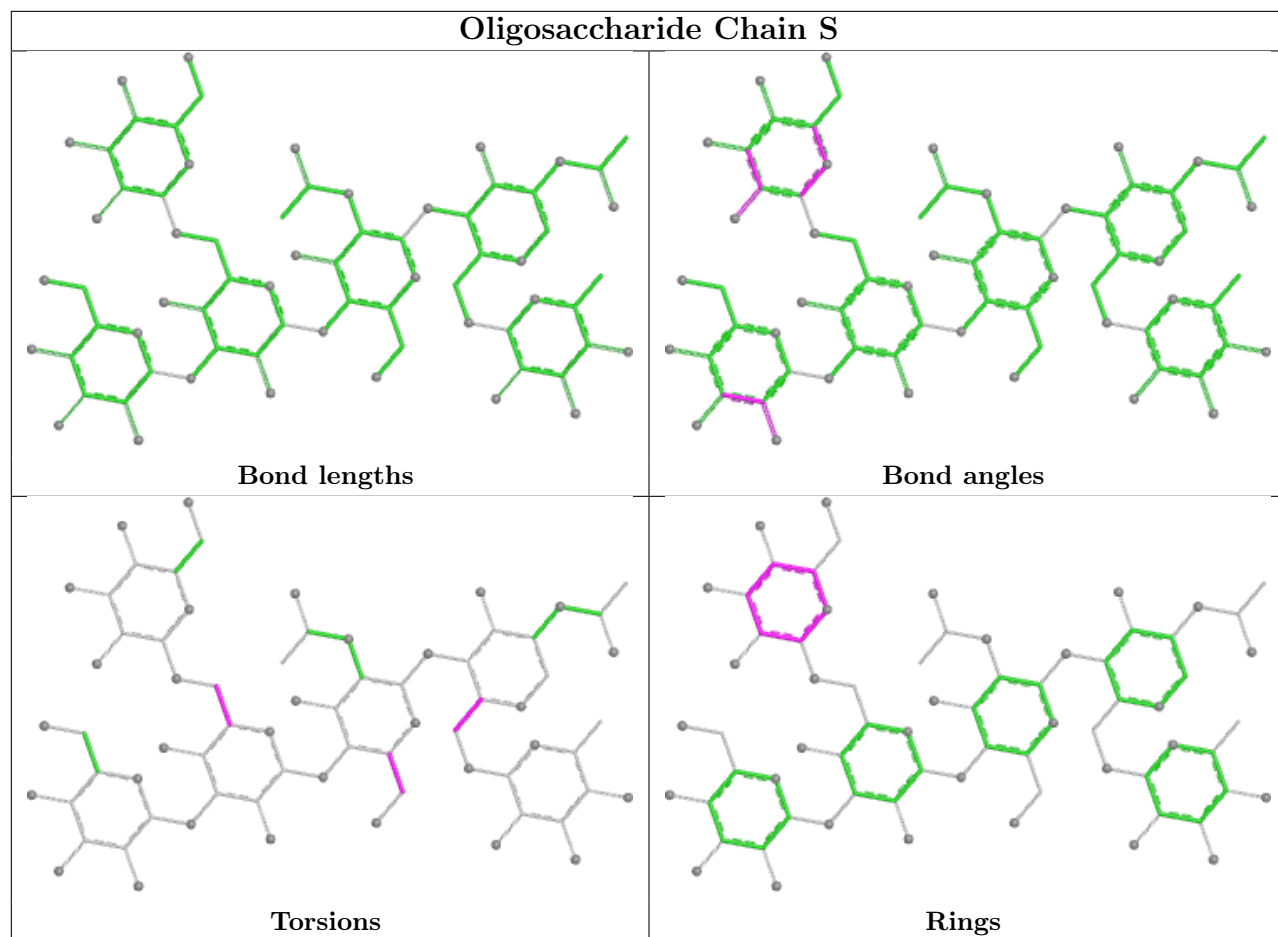


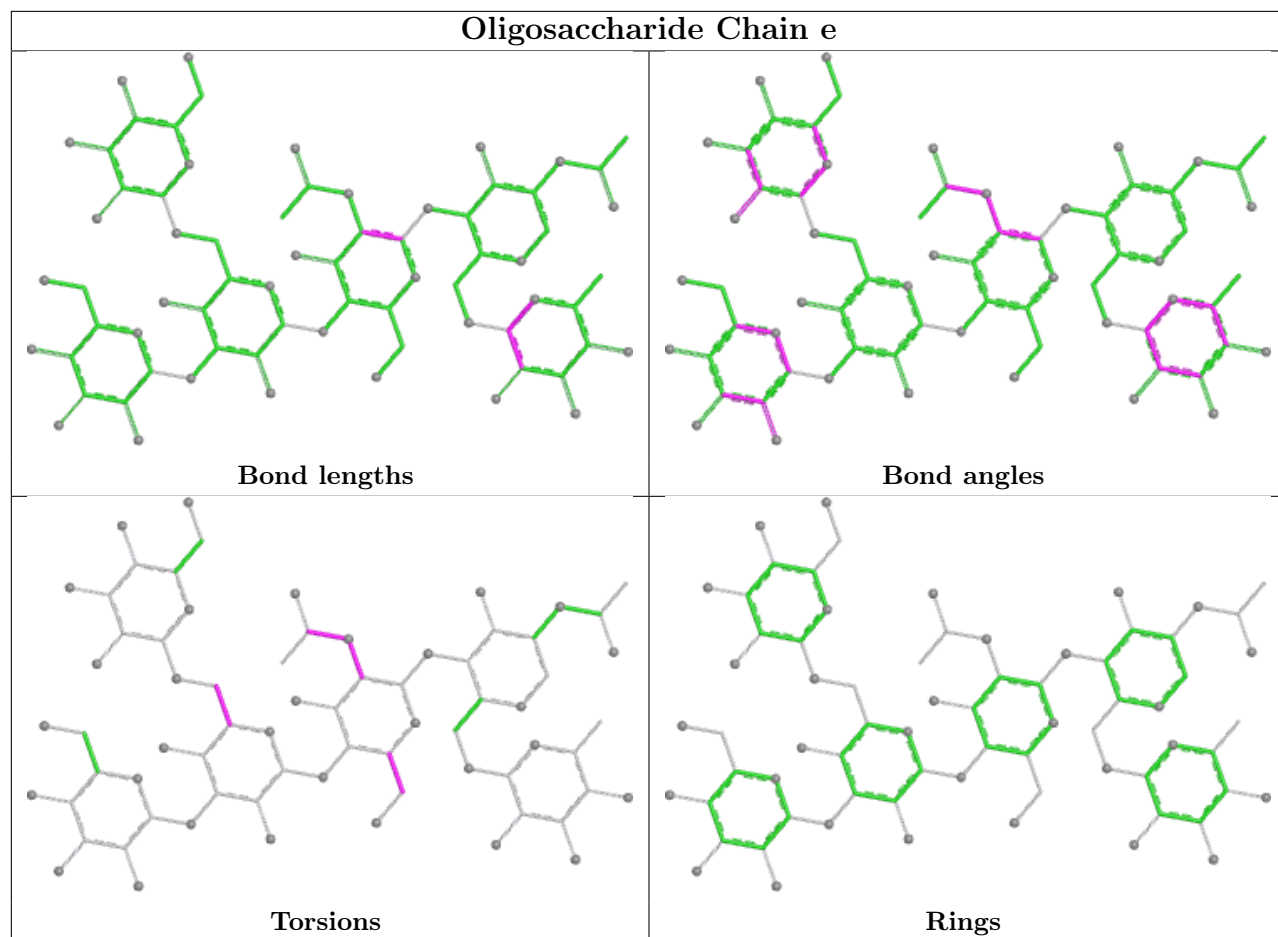


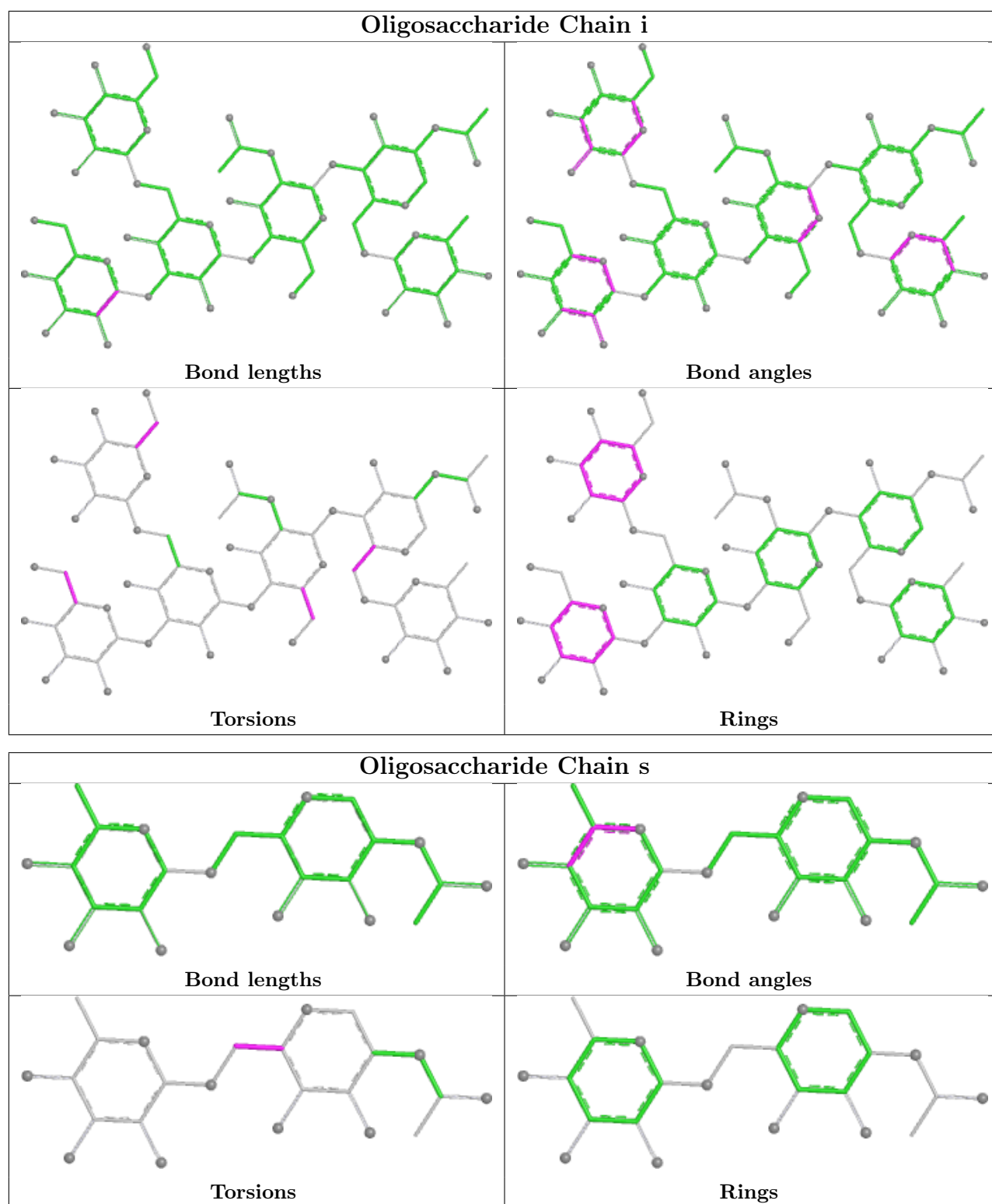












5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	B	1404	1	14,14,15	0.27	0	17,19,21	0.46	0
8	NAG	A	1402	1	14,14,15	0.50	0	17,19,21	0.47	0
8	NAG	B	1407	1	14,14,15	0.82	1 (7%)	17,19,21	0.62	0
8	NAG	A	1406	1	14,14,15	0.27	0	17,19,21	0.47	0
8	NAG	A	1404	1	14,14,15	0.21	0	17,19,21	0.41	0
8	NAG	B	1406	1	14,14,15	0.19	0	17,19,21	0.42	0
8	NAG	C	1406	1	14,14,15	1.16	1 (7%)	17,19,21	0.59	0
8	NAG	B	1401	1	14,14,15	0.26	0	17,19,21	0.48	0
8	NAG	C	1403	1	14,14,15	0.27	0	17,19,21	0.55	0
8	NAG	A	1403	1	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	C	1405	1	14,14,15	0.42	0	17,19,21	0.48	0
8	NAG	A	1405	1	14,14,15	0.24	0	17,19,21	0.36	0
8	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.40	0
8	NAG	C	1404	1	14,14,15	0.20	0	17,19,21	0.44	0
8	NAG	B	1403	1	14,14,15	0.26	0	17,19,21	0.46	0
8	NAG	C	1402	1	14,14,15	0.29	0	17,19,21	0.34	0
8	NAG	C	1401	1	14,14,15	0.26	0	17,19,21	0.55	0
8	NAG	B	1405	1	14,14,15	0.26	0	17,19,21	0.52	0
8	NAG	A	1401	1	14,14,15	0.28	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1402	1	-	4/6/23/26	0/1/1/1
8	NAG	B	1407	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1406	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1404	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
8	NAG	C	1406	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1401	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
8	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1402	1	-	3/6/23/26	0/1/1/1
8	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
8	NAG	B	1405	1	-	4/6/23/26	0/1/1/1
8	NAG	A	1401	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1406	NAG	C1-C2	3.91	1.57	1.52
8	B	1407	NAG	C1-C2	2.99	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1403	NAG	O5-C5-C6-O6
8	C	1401	NAG	O5-C5-C6-O6
8	A	1401	NAG	C4-C5-C6-O6
8	A	1401	NAG	O5-C5-C6-O6
8	B	1404	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 17 short contacts:

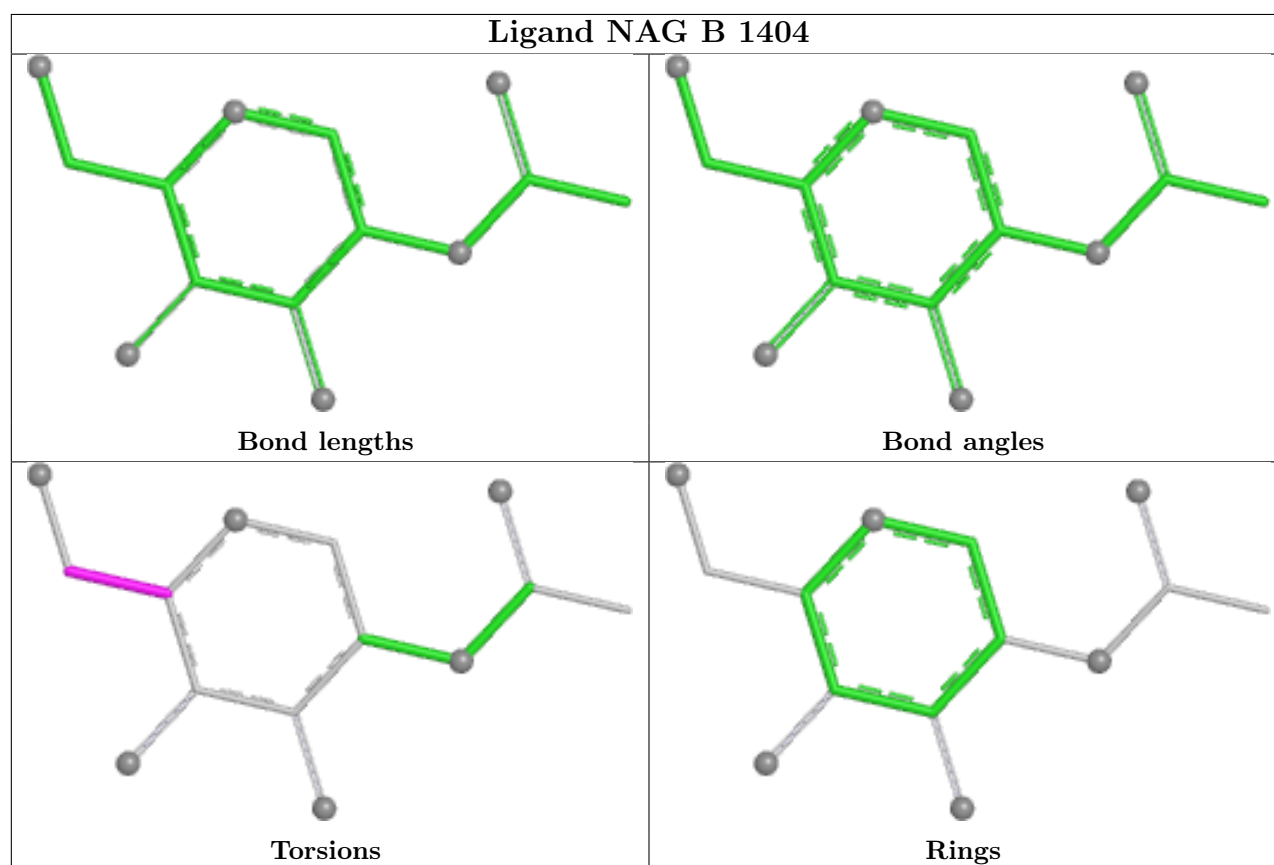
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1404	NAG	1	0
8	A	1402	NAG	4	0
8	B	1407	NAG	2	0
8	A	1406	NAG	1	0
8	B	1406	NAG	1	0
8	C	1406	NAG	1	0

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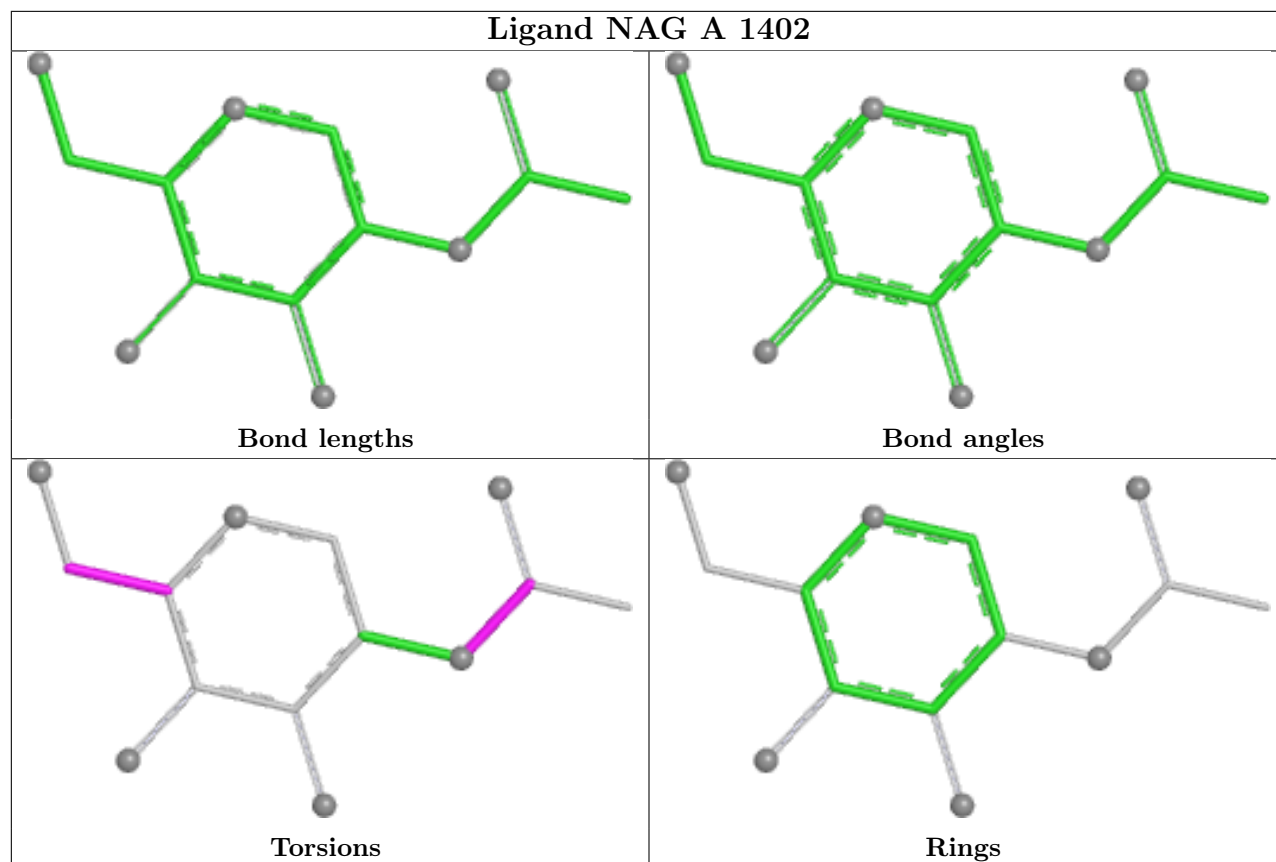
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1401	NAG	1	0
8	B	1402	NAG	4	0
8	B	1403	NAG	1	0
8	A	1401	NAG	1	0

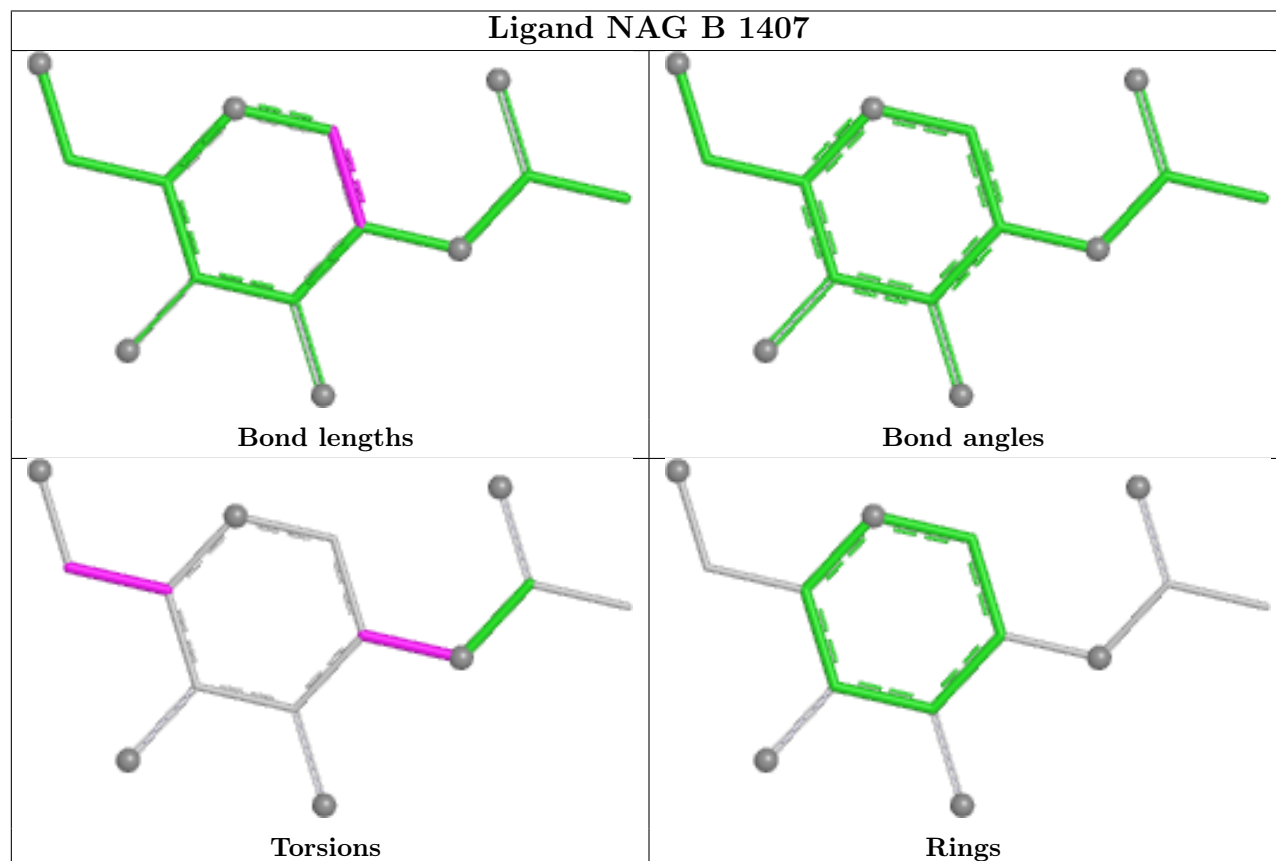
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



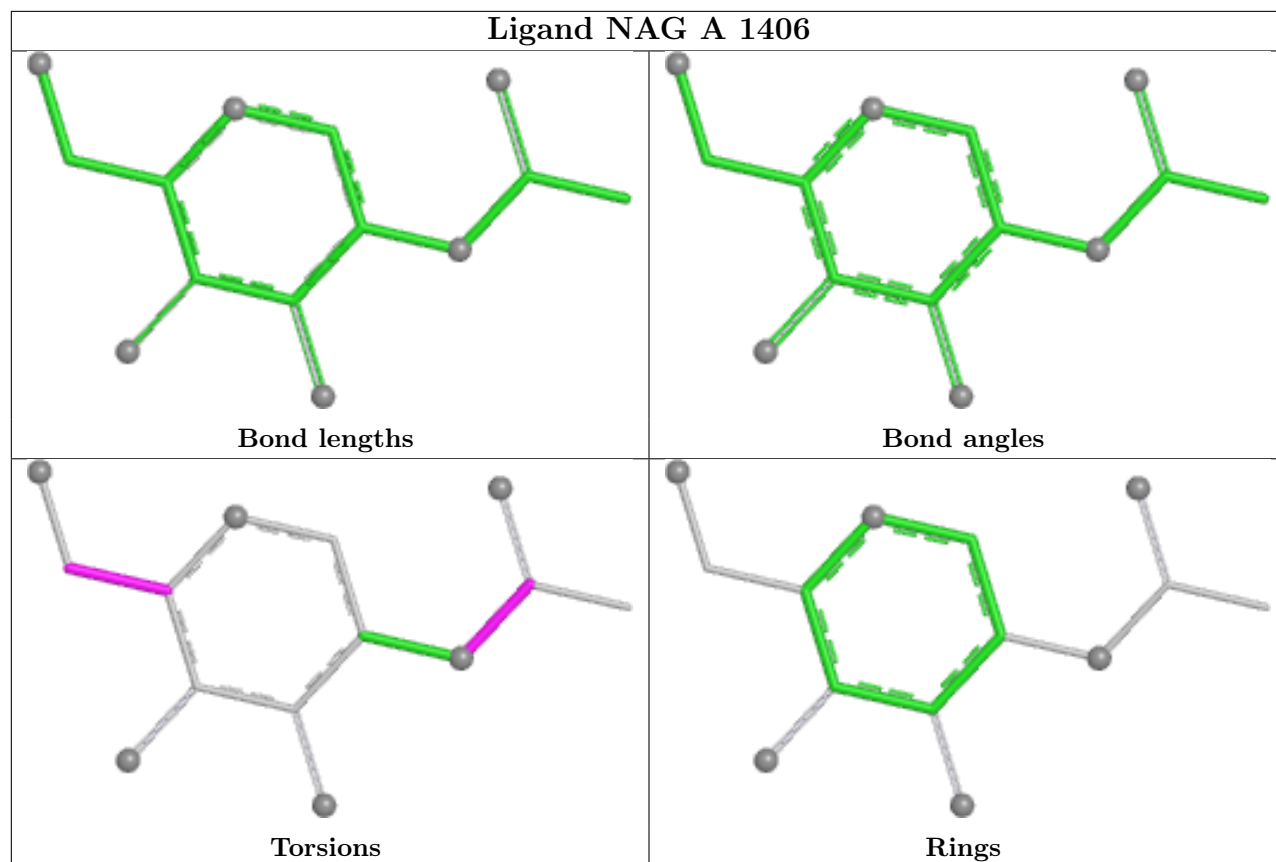
Ligand NAG A 1402



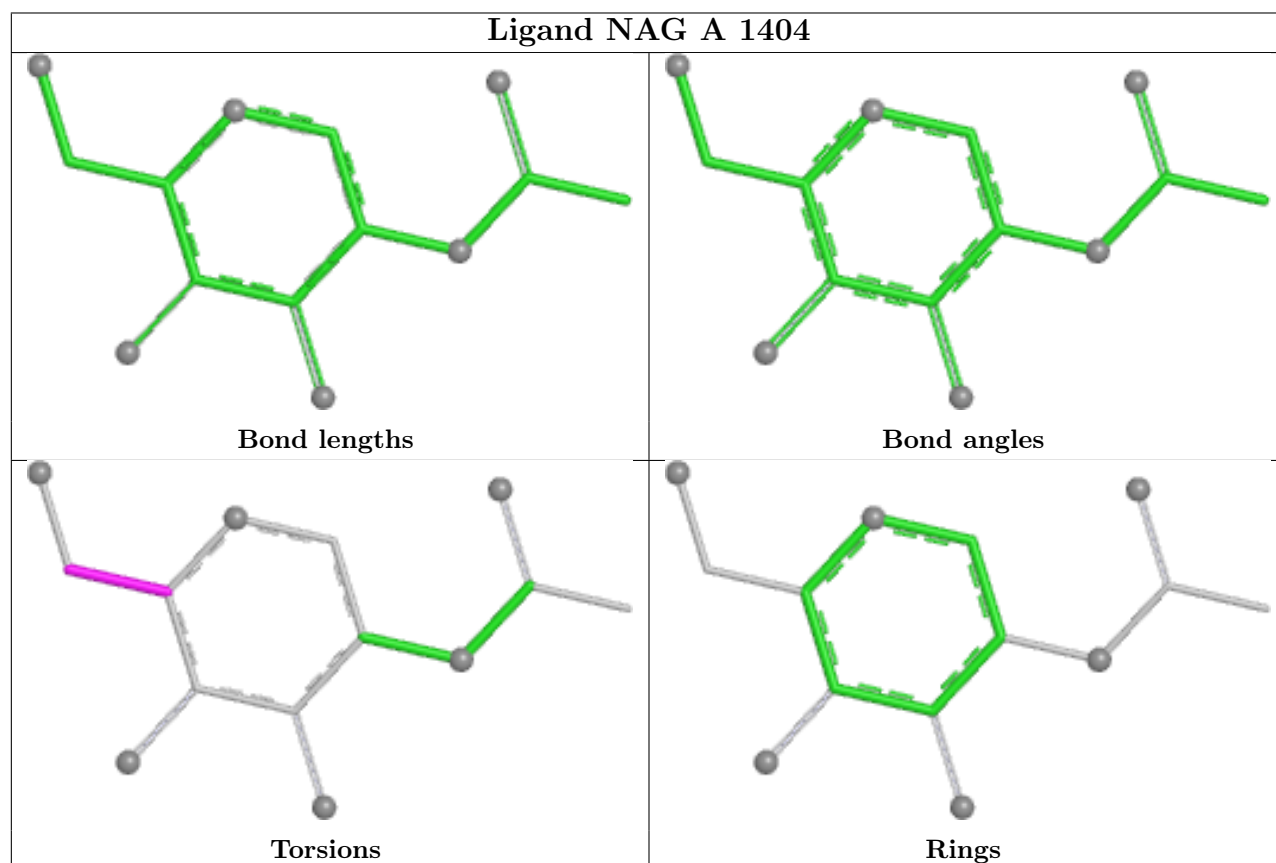
Ligand NAG B 1407



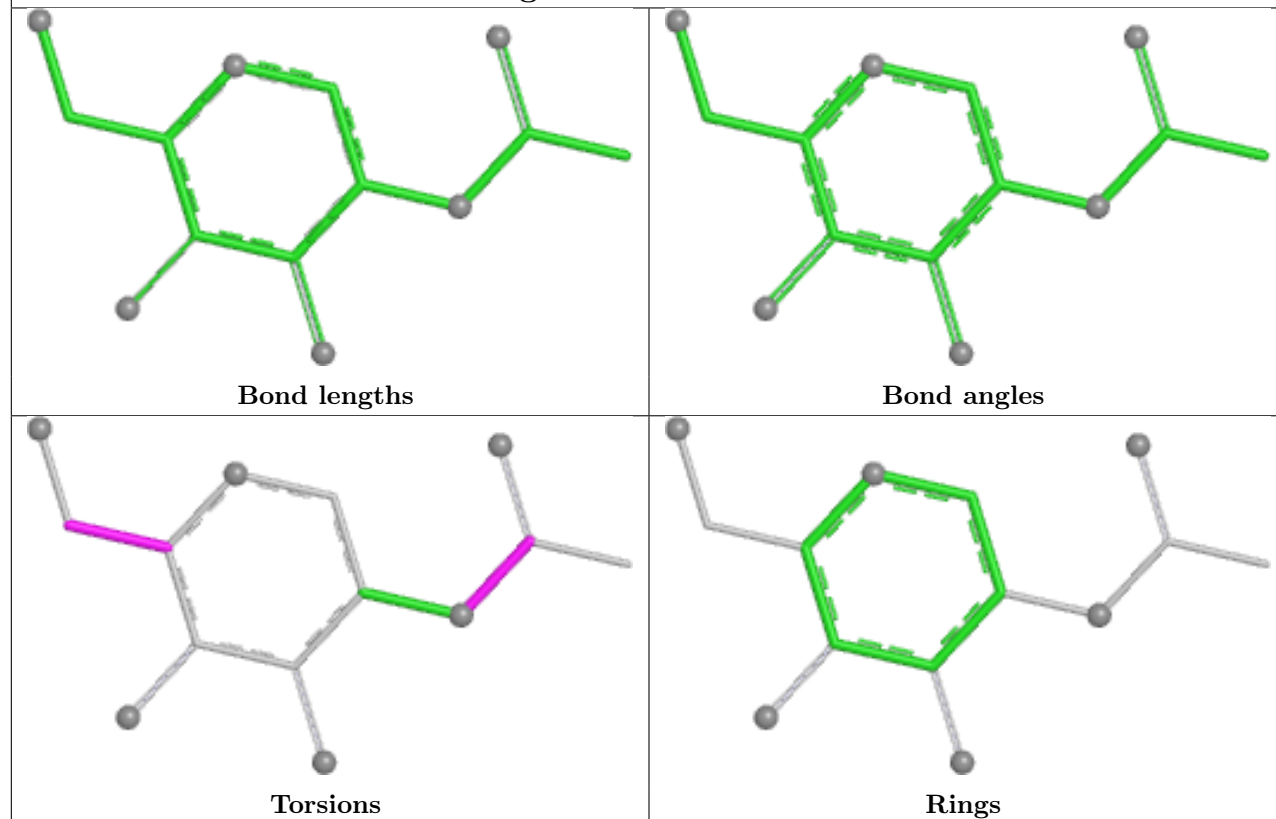
Ligand NAG A 1406



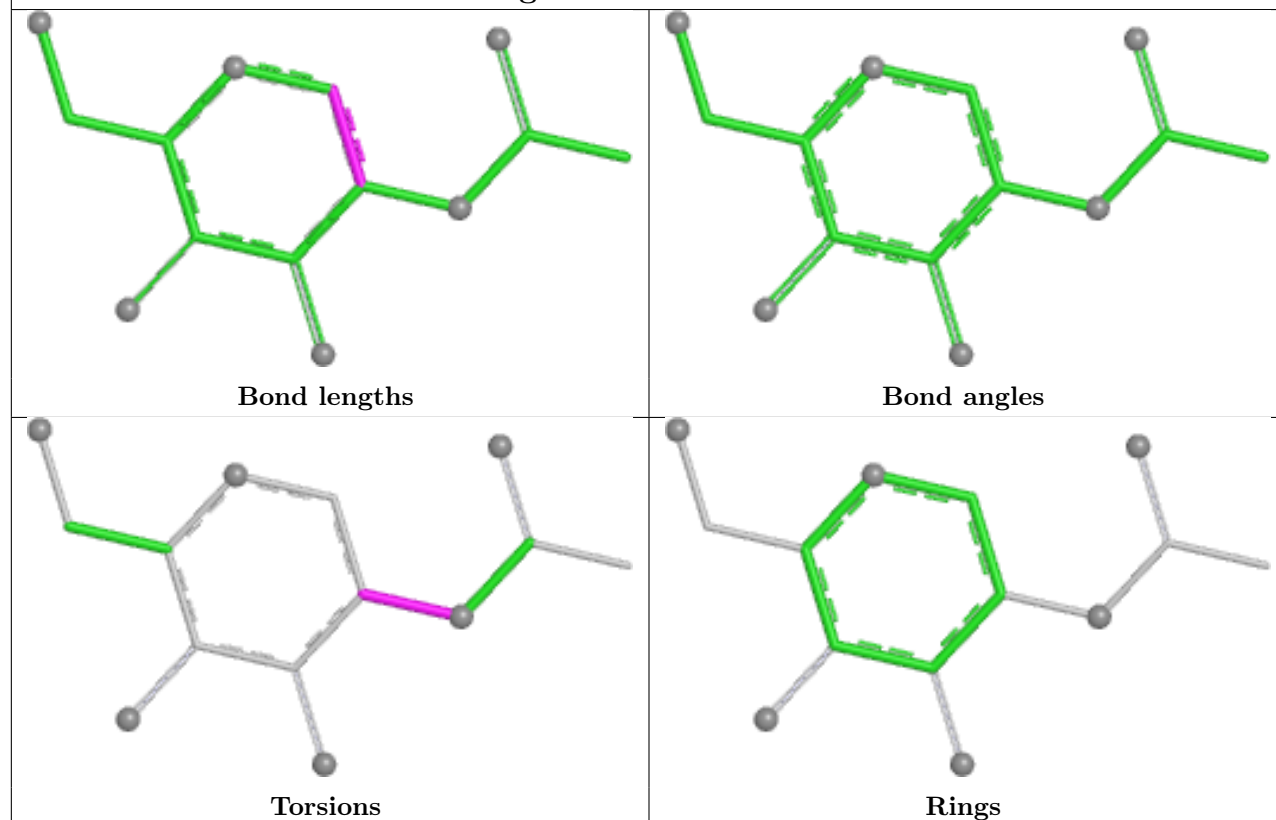
Ligand NAG A 1404



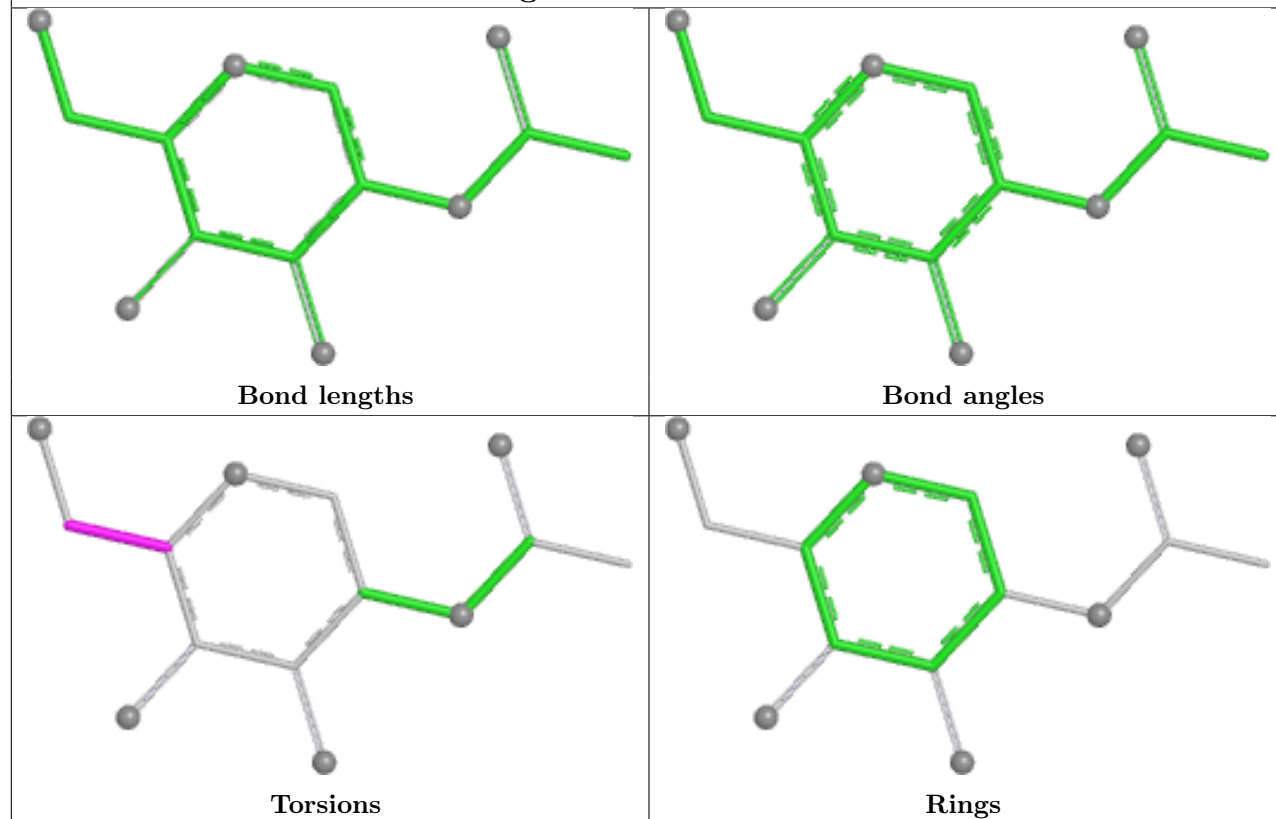
Ligand NAG B 1406



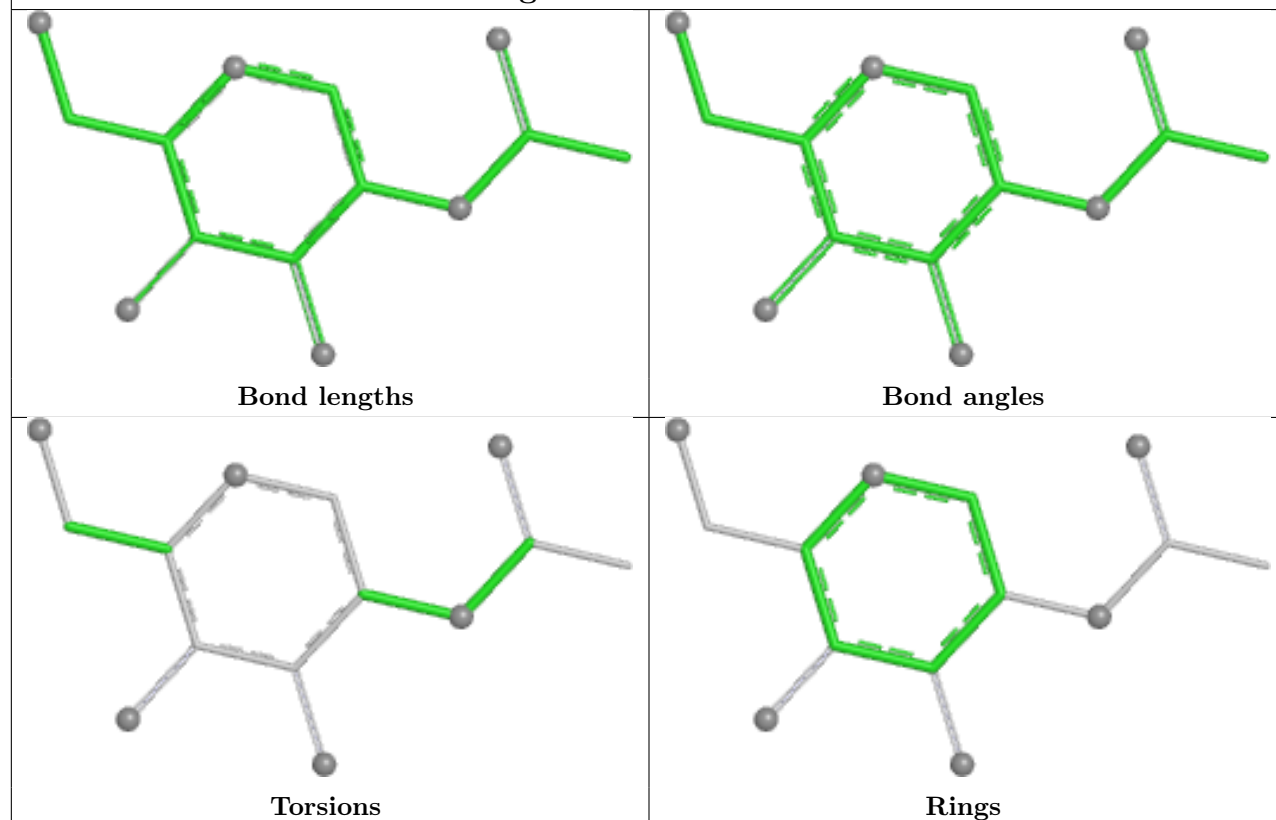
Ligand NAG C 1406



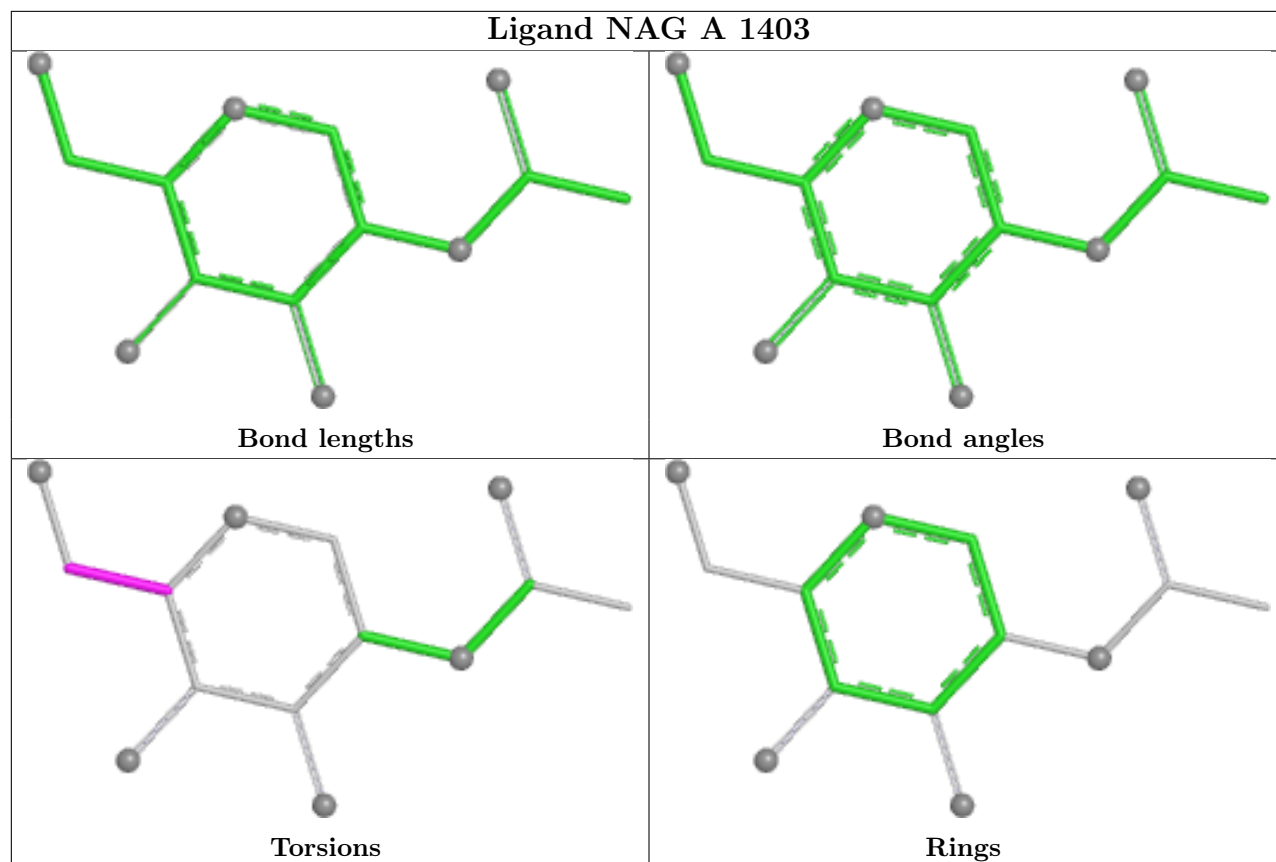
Ligand NAG B 1401



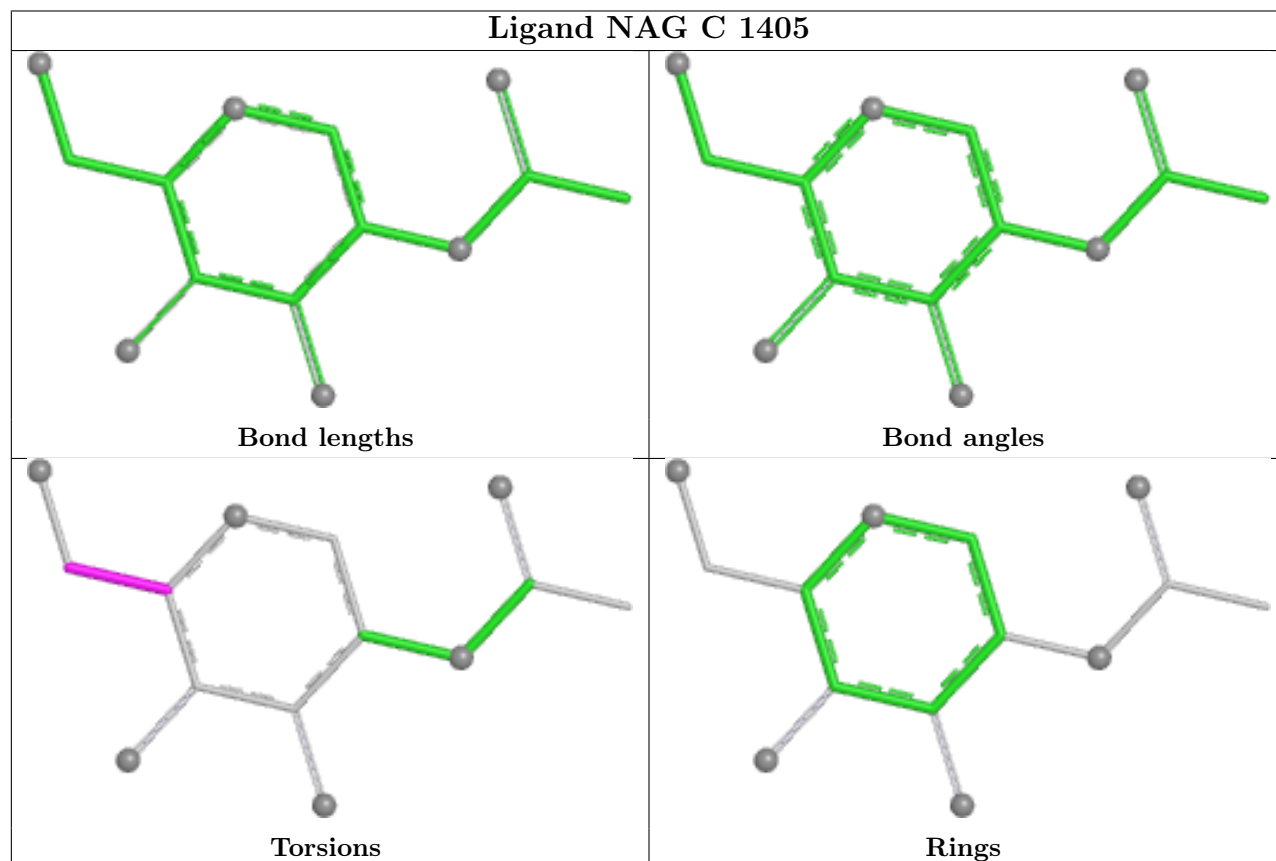
Ligand NAG C 1403



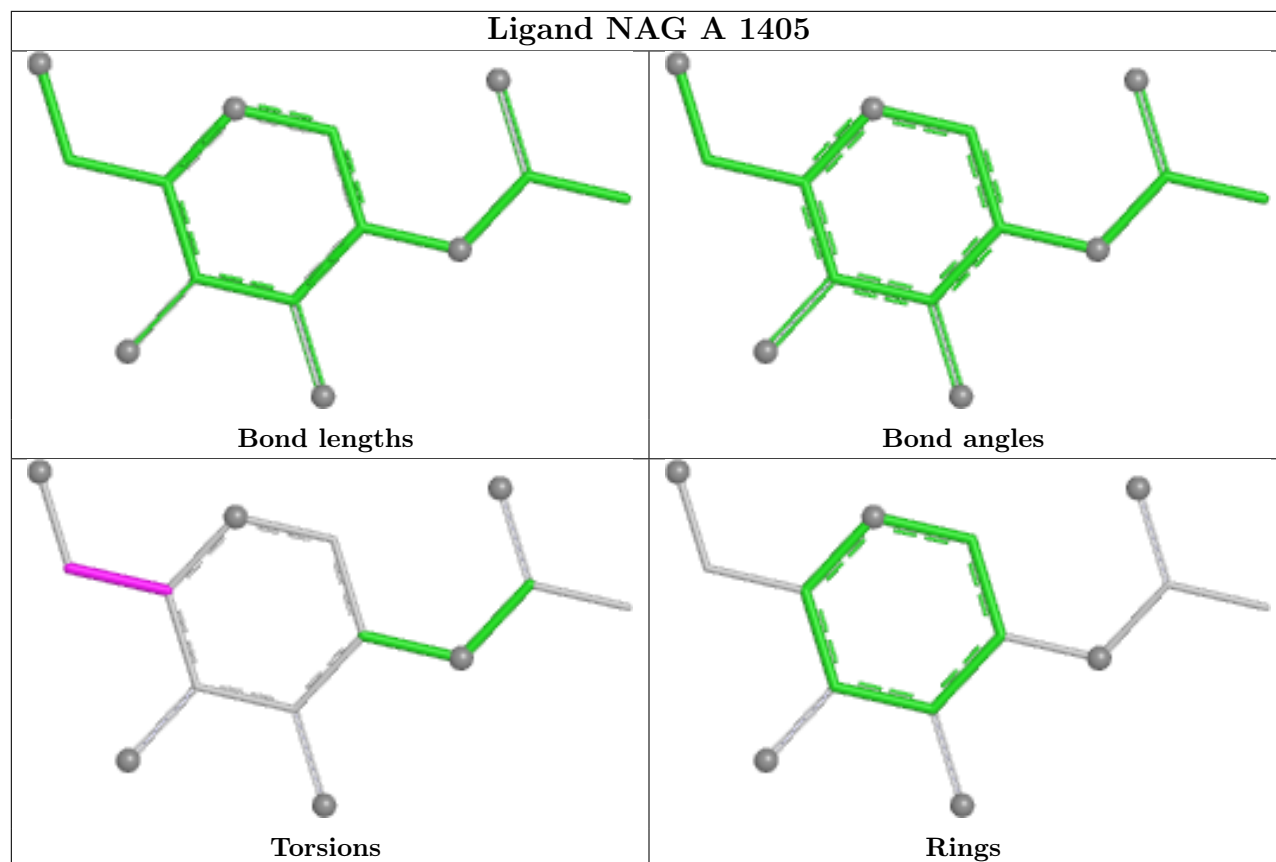
Ligand NAG A 1403



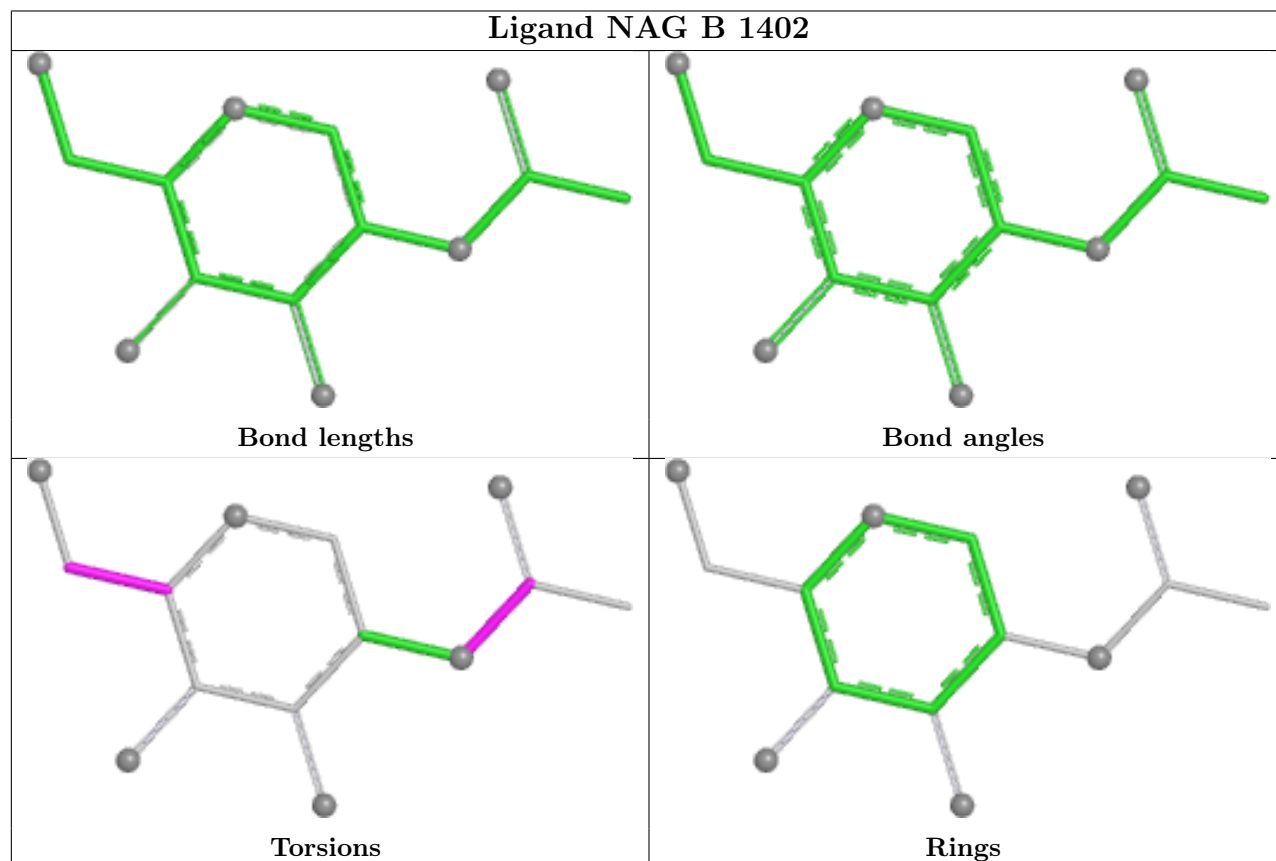
Ligand NAG C 1405



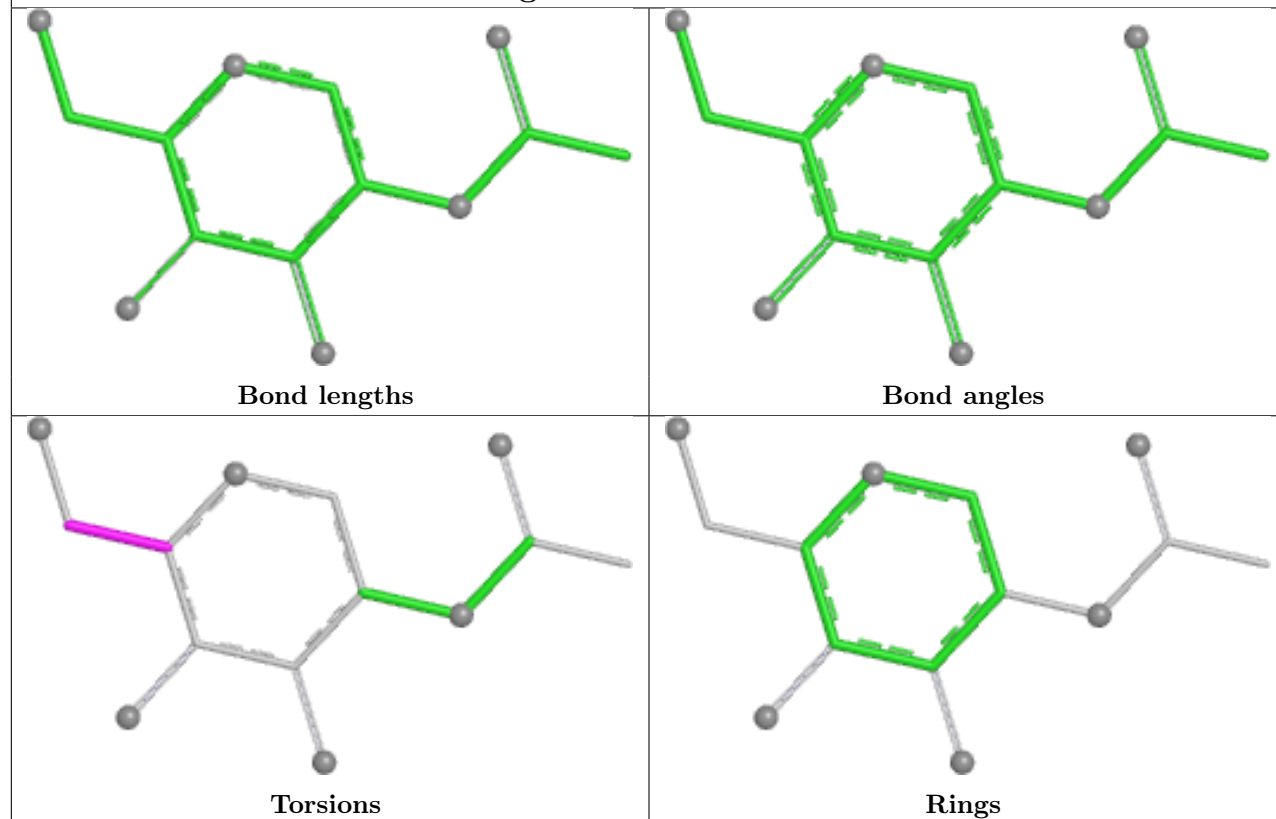
Ligand NAG A 1405



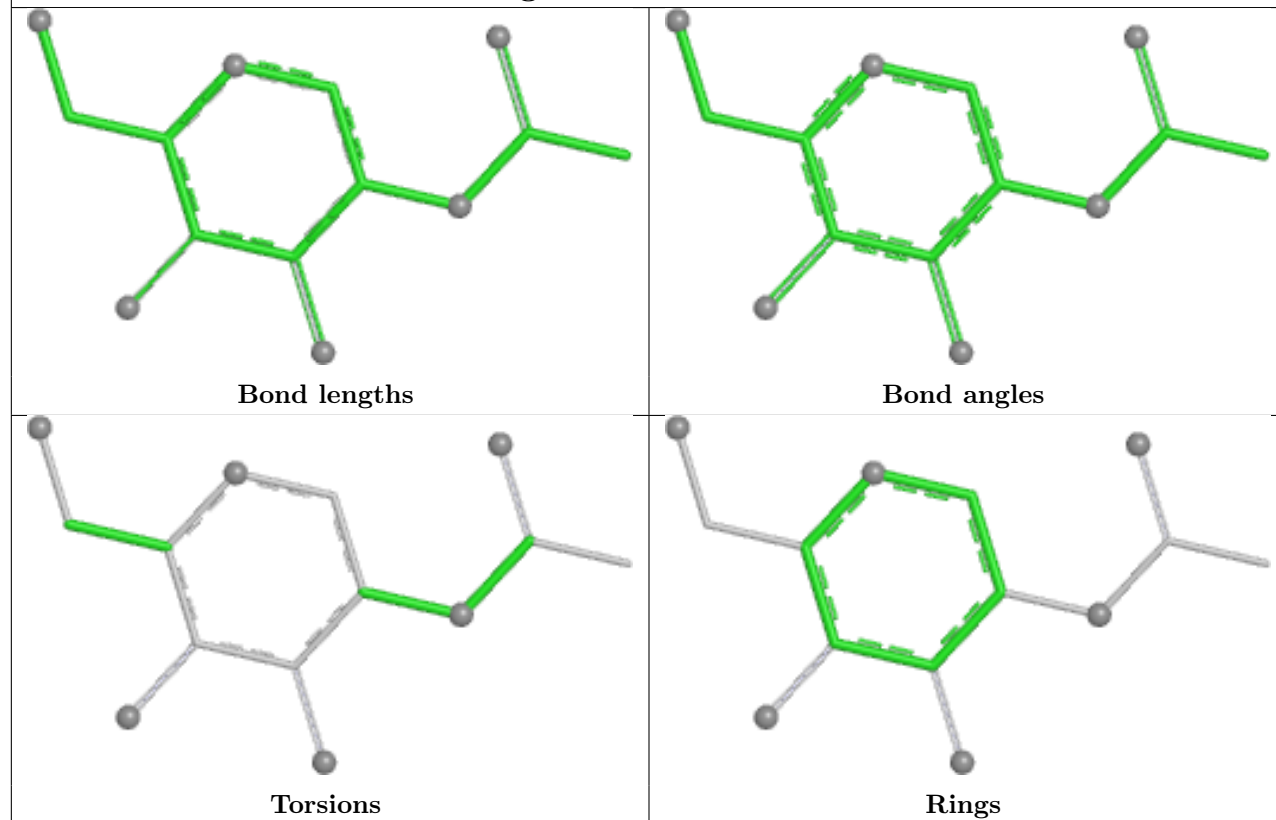
Ligand NAG B 1402



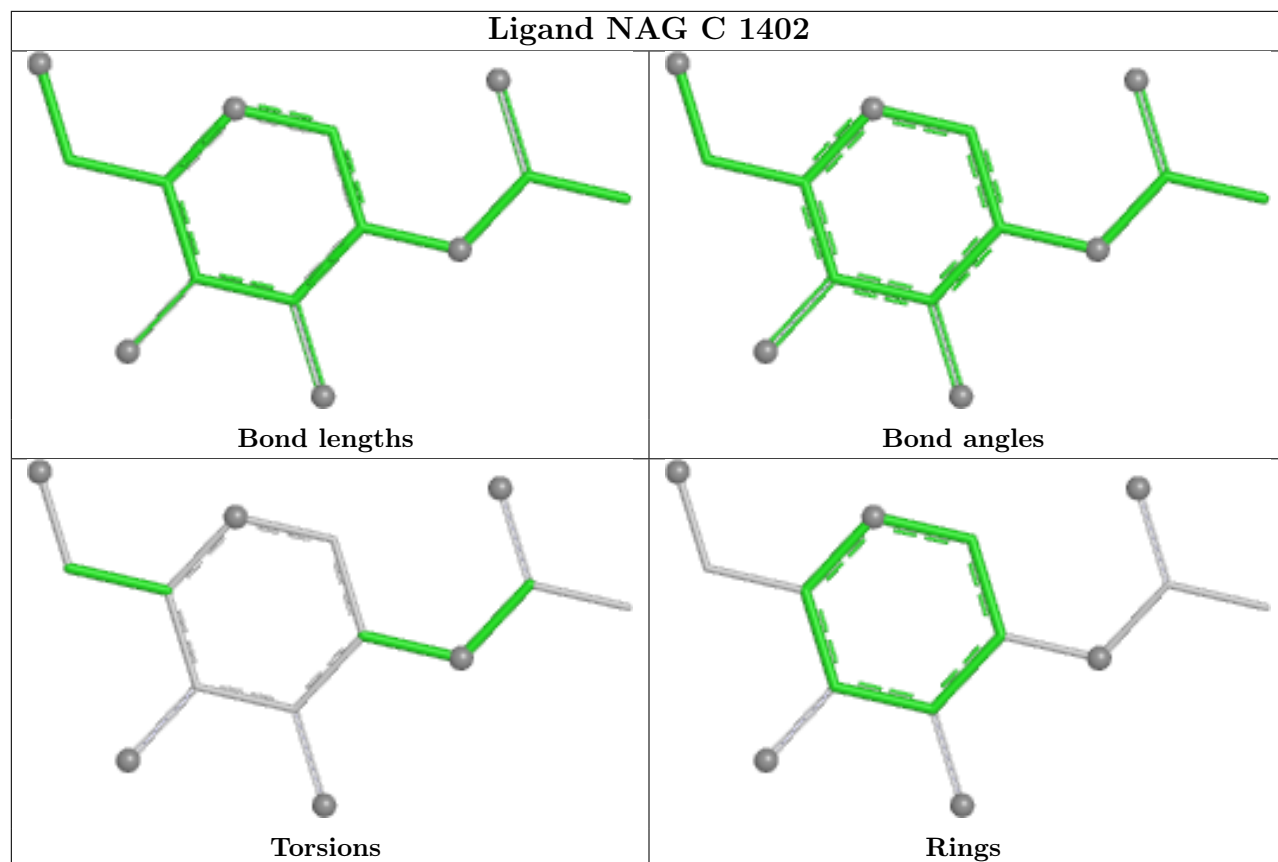
Ligand NAG C 1404



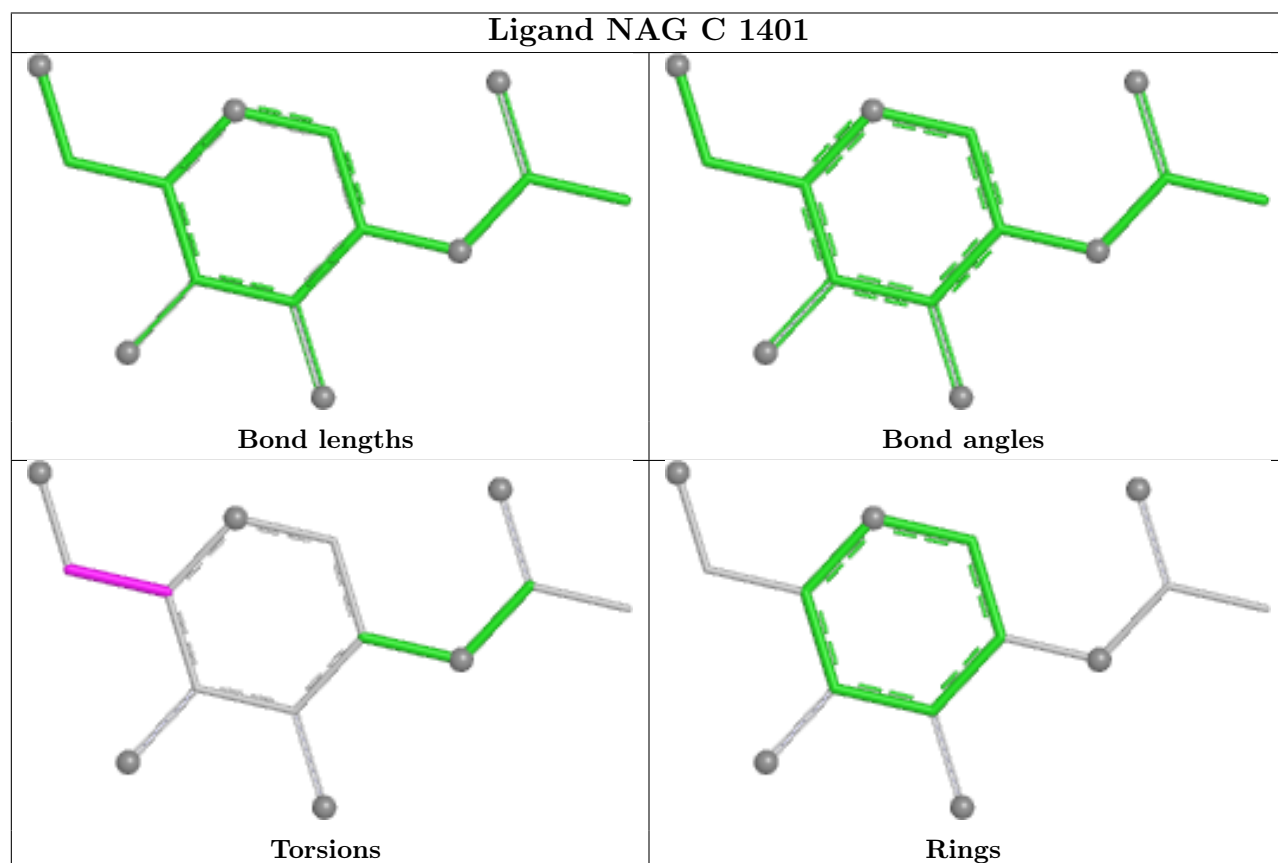
Ligand NAG B 1403



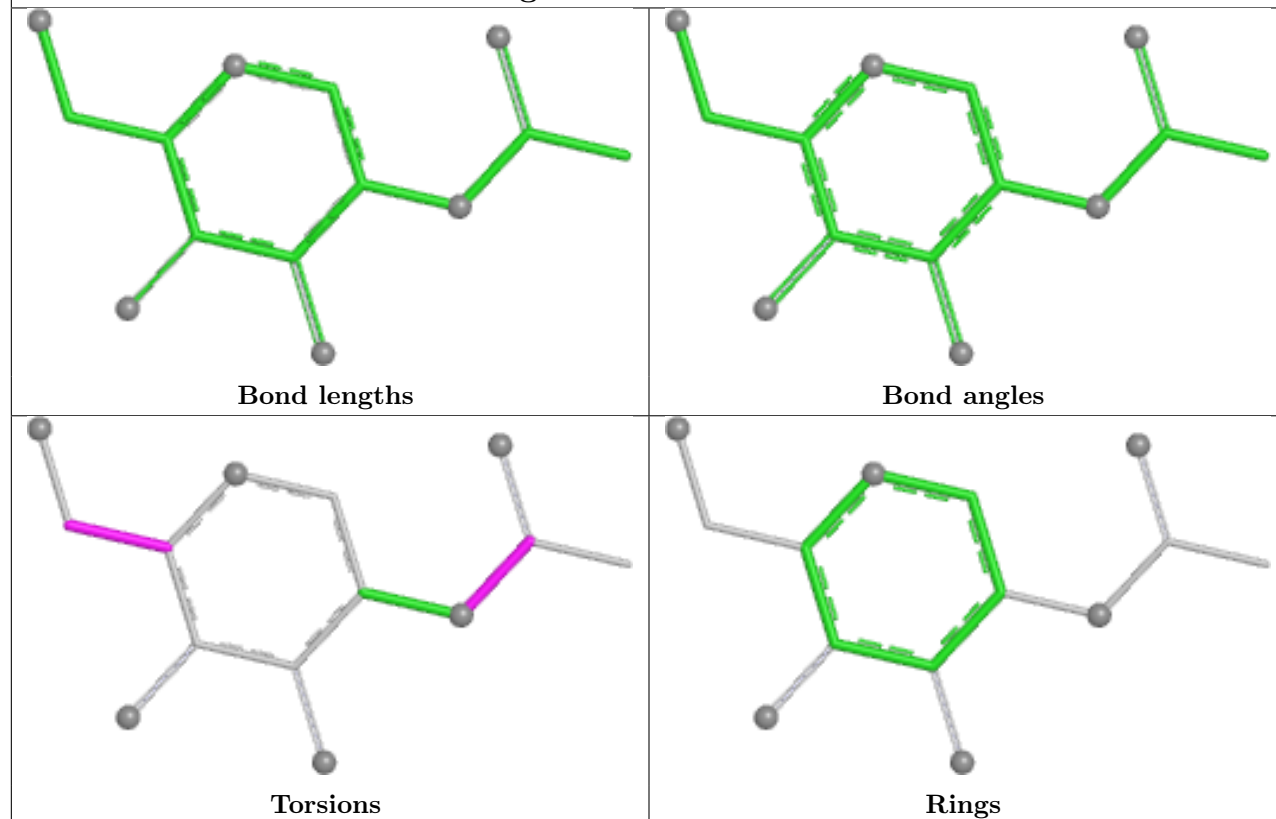
Ligand NAG C 1402



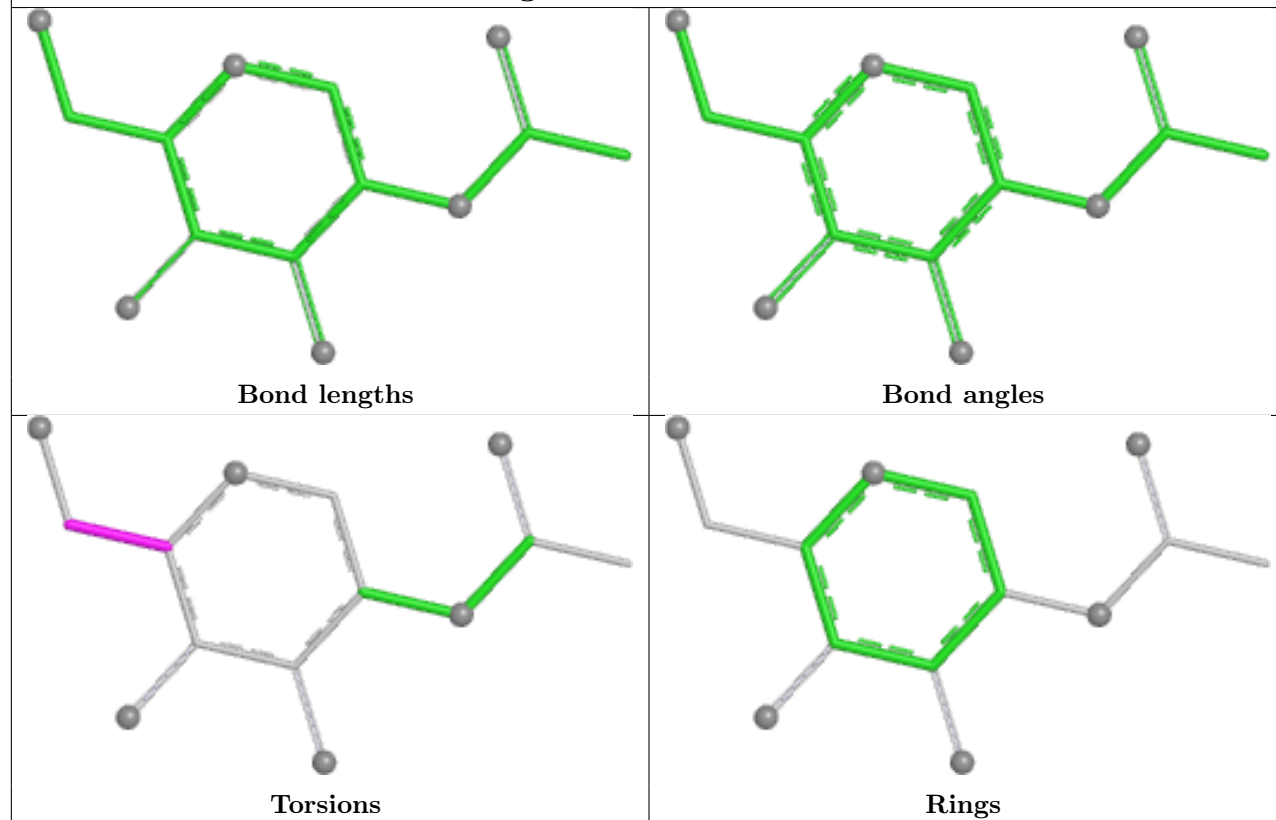
Ligand NAG C 1401



Ligand NAG B 1405



Ligand NAG A 1401



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.

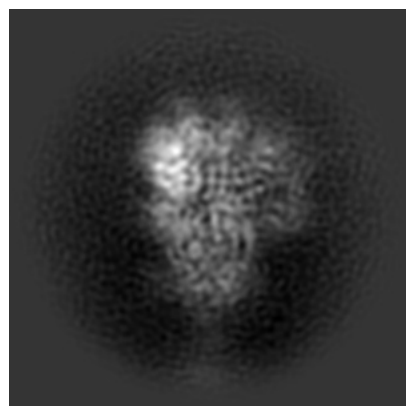
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32338. These allow visual inspection of the internal detail of the map and identification of artifacts.

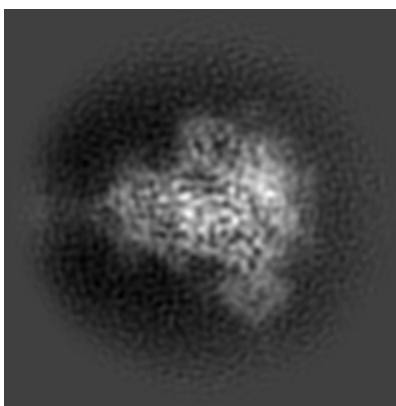
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

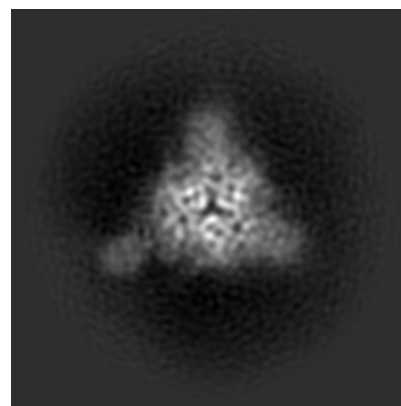
6.1.1 Primary map



X

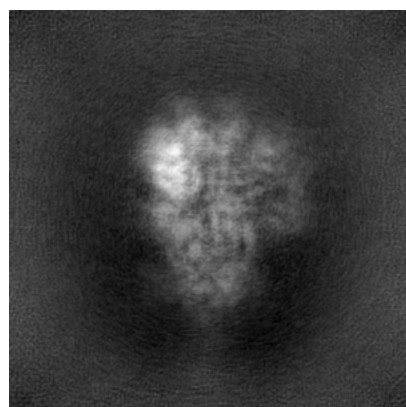


Y

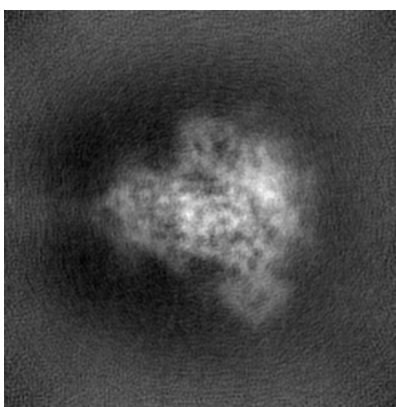


Z

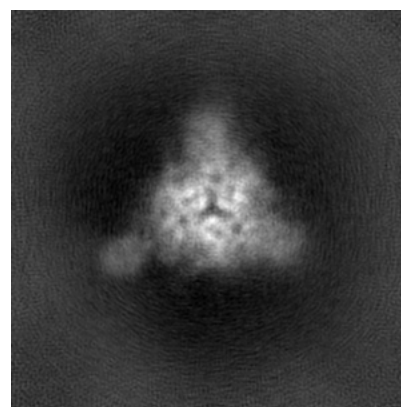
6.1.2 Raw map



X



Y

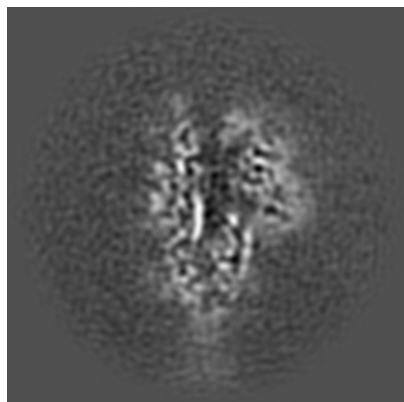


Z

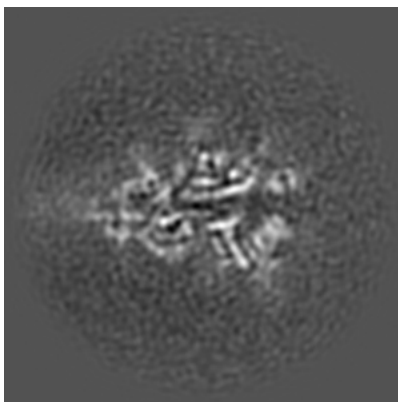
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

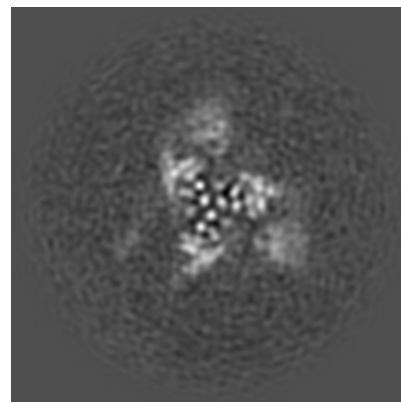
6.2.1 Primary map



X Index: 110

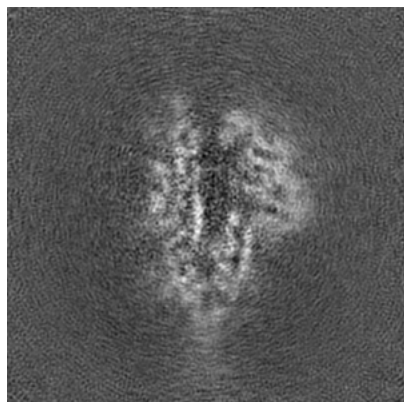


Y Index: 110

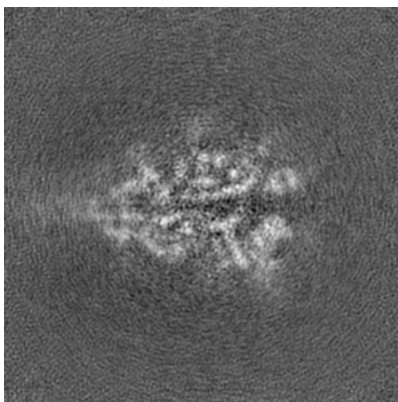


Z Index: 110

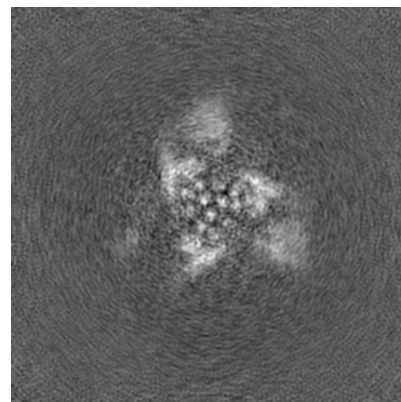
6.2.2 Raw map



X Index: 110



Y Index: 110

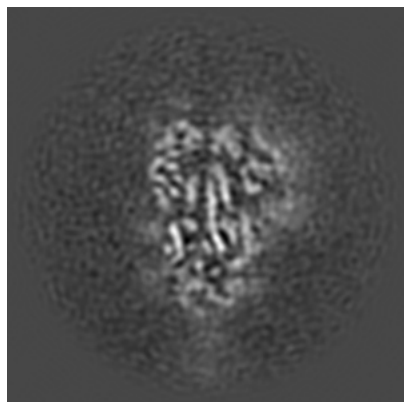


Z Index: 110

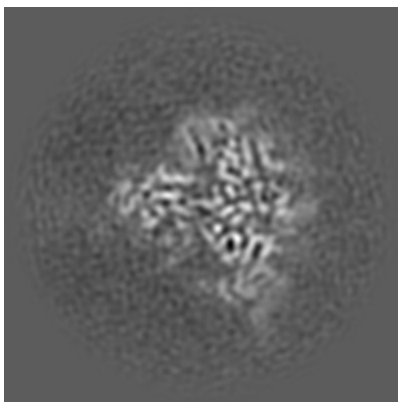
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

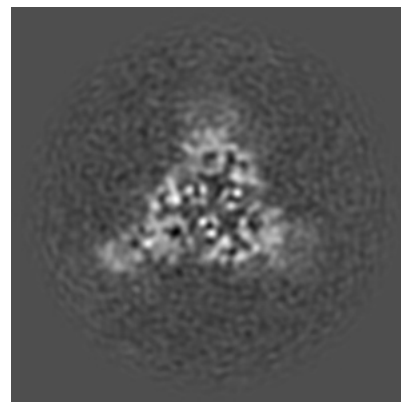
6.3.1 Primary map



X Index: 116

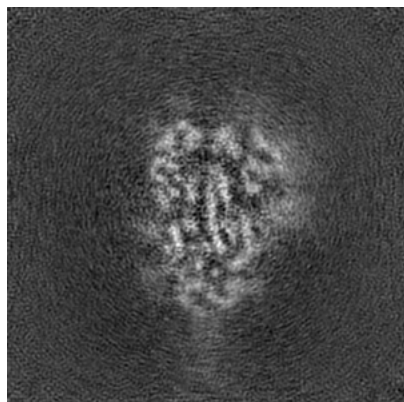


Y Index: 94

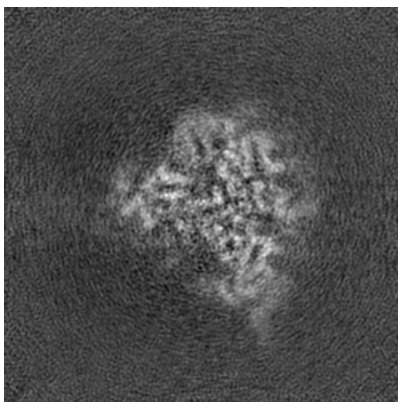


Z Index: 132

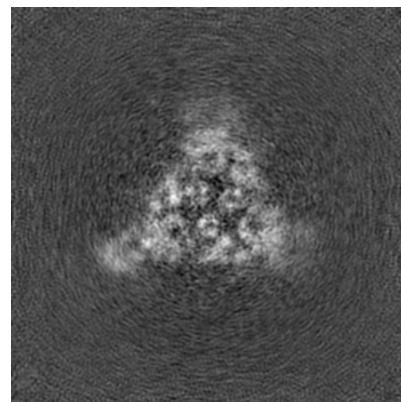
6.3.2 Raw map



X Index: 116



Y Index: 93

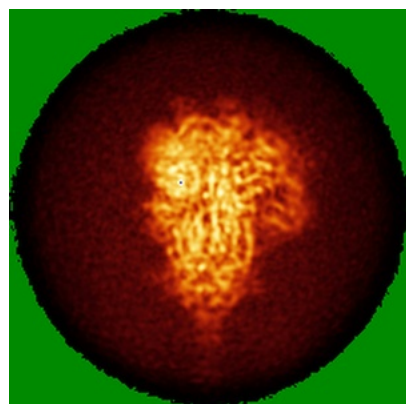


Z Index: 132

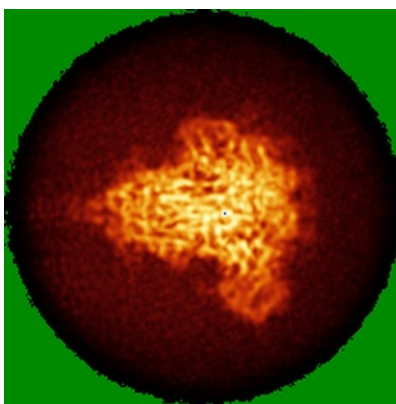
The images above show the largest variance slices of the map in three orthogonal directions.

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

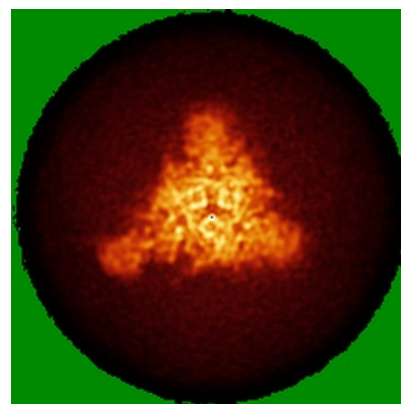
6.4.1 Primary map



X

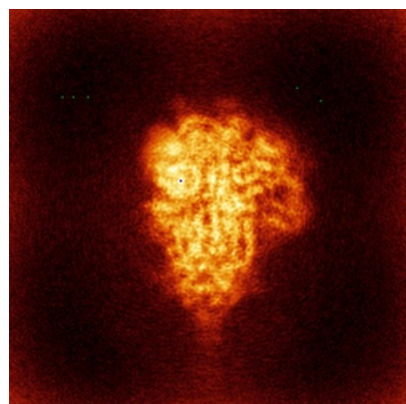


Y

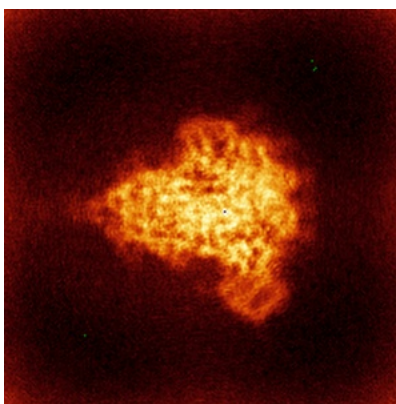


Z

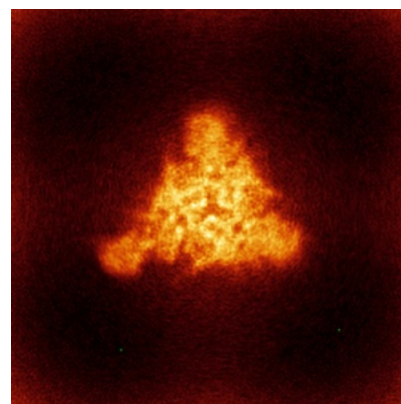
6.4.2 Raw map



X



Y



Z

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

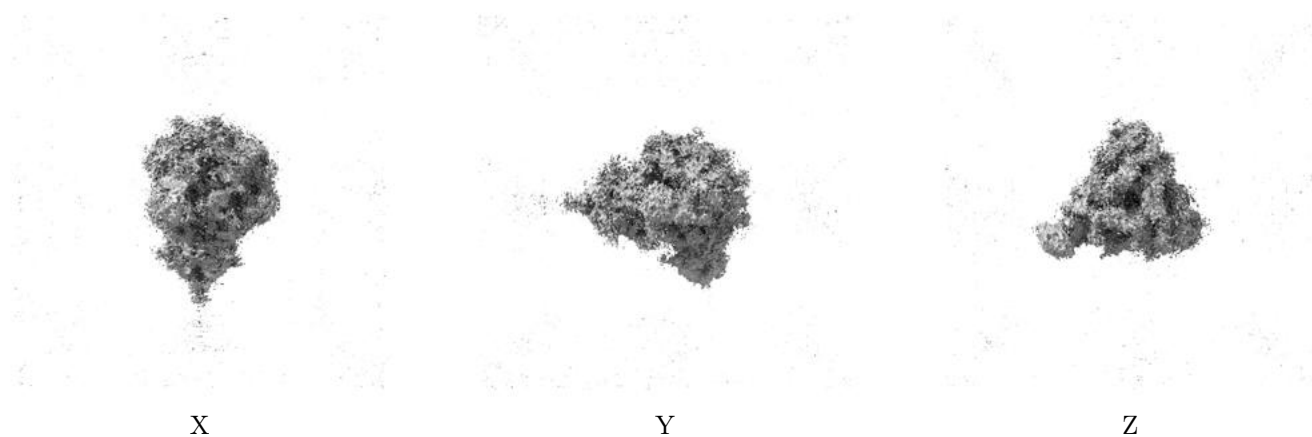
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

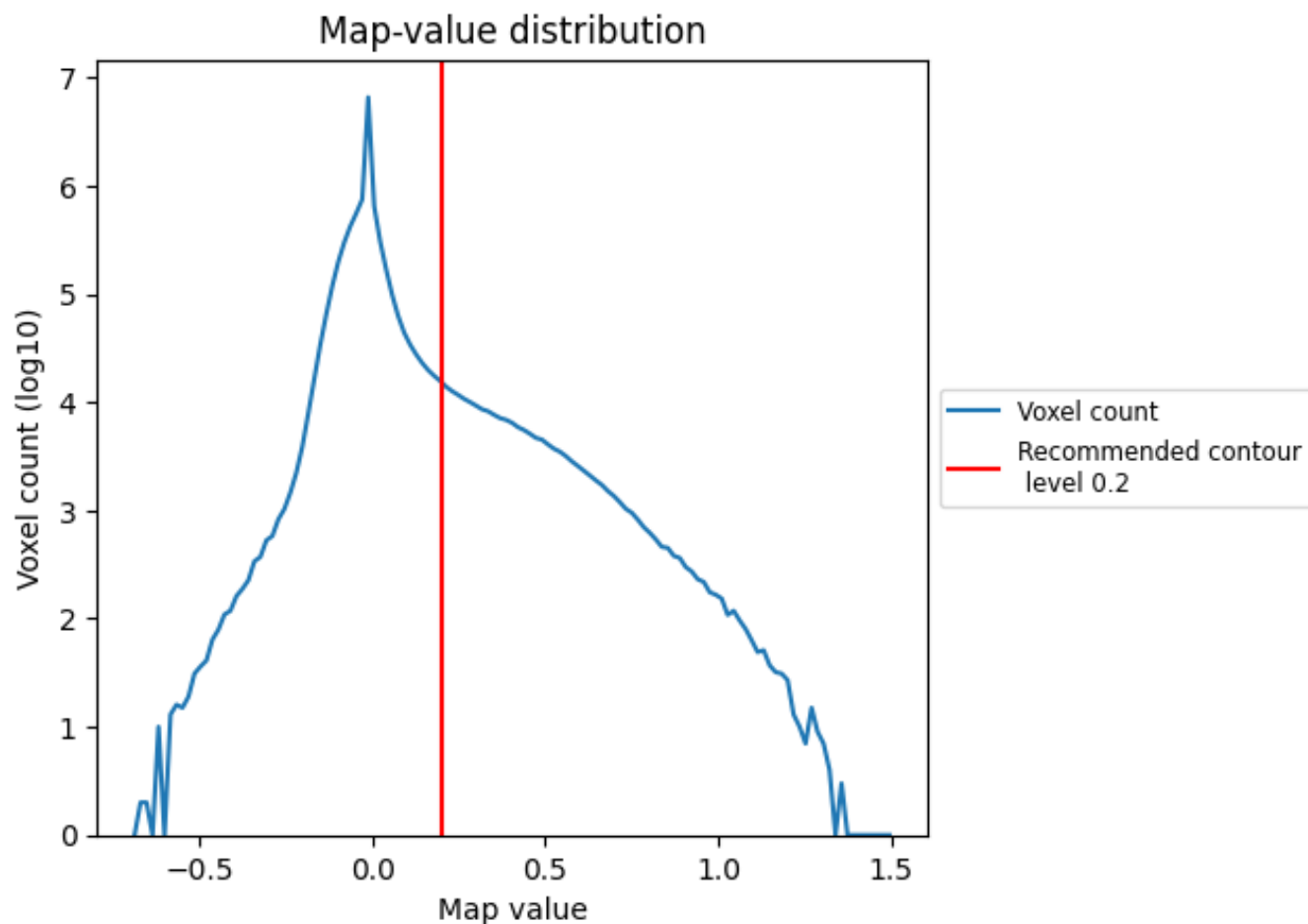
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

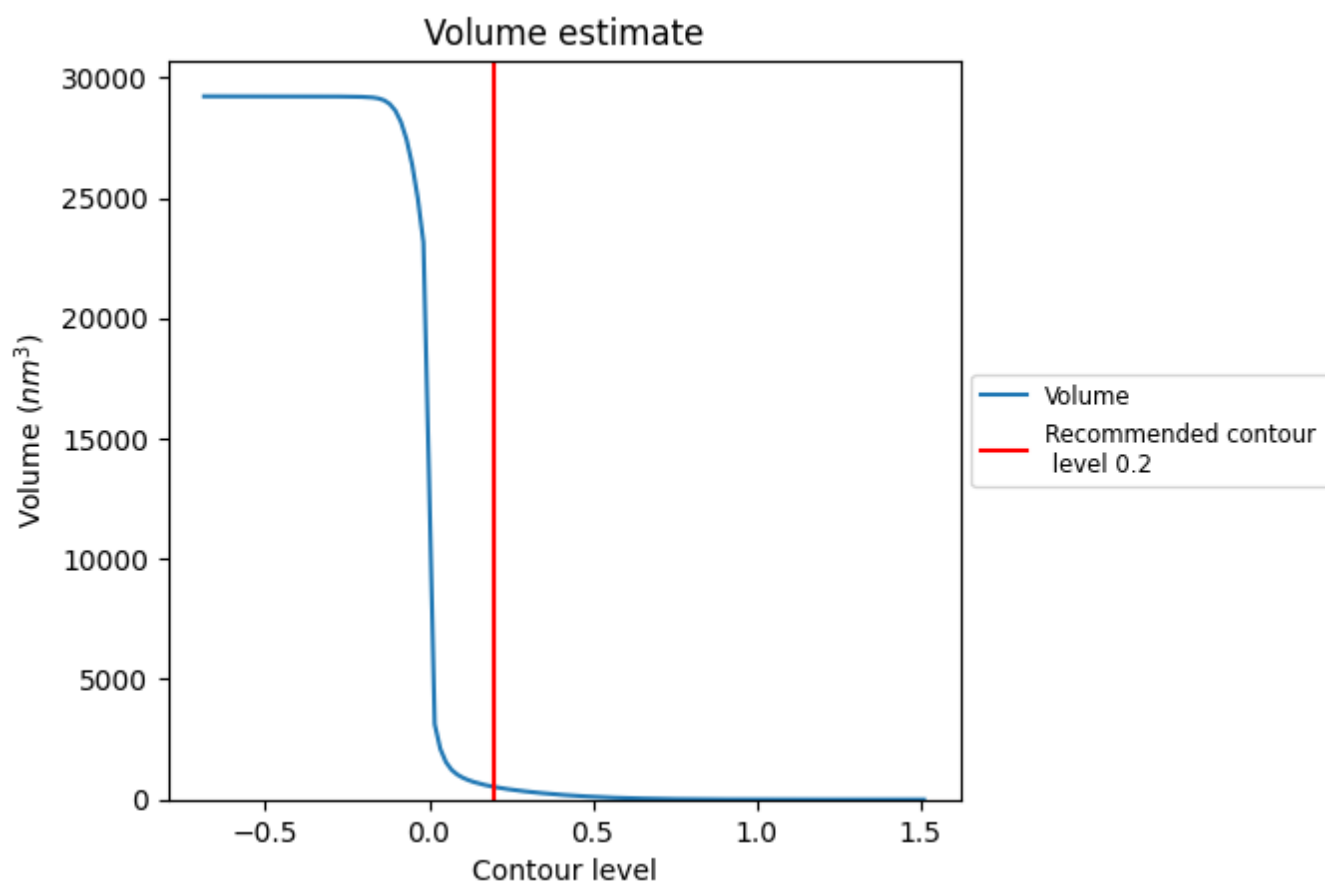
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

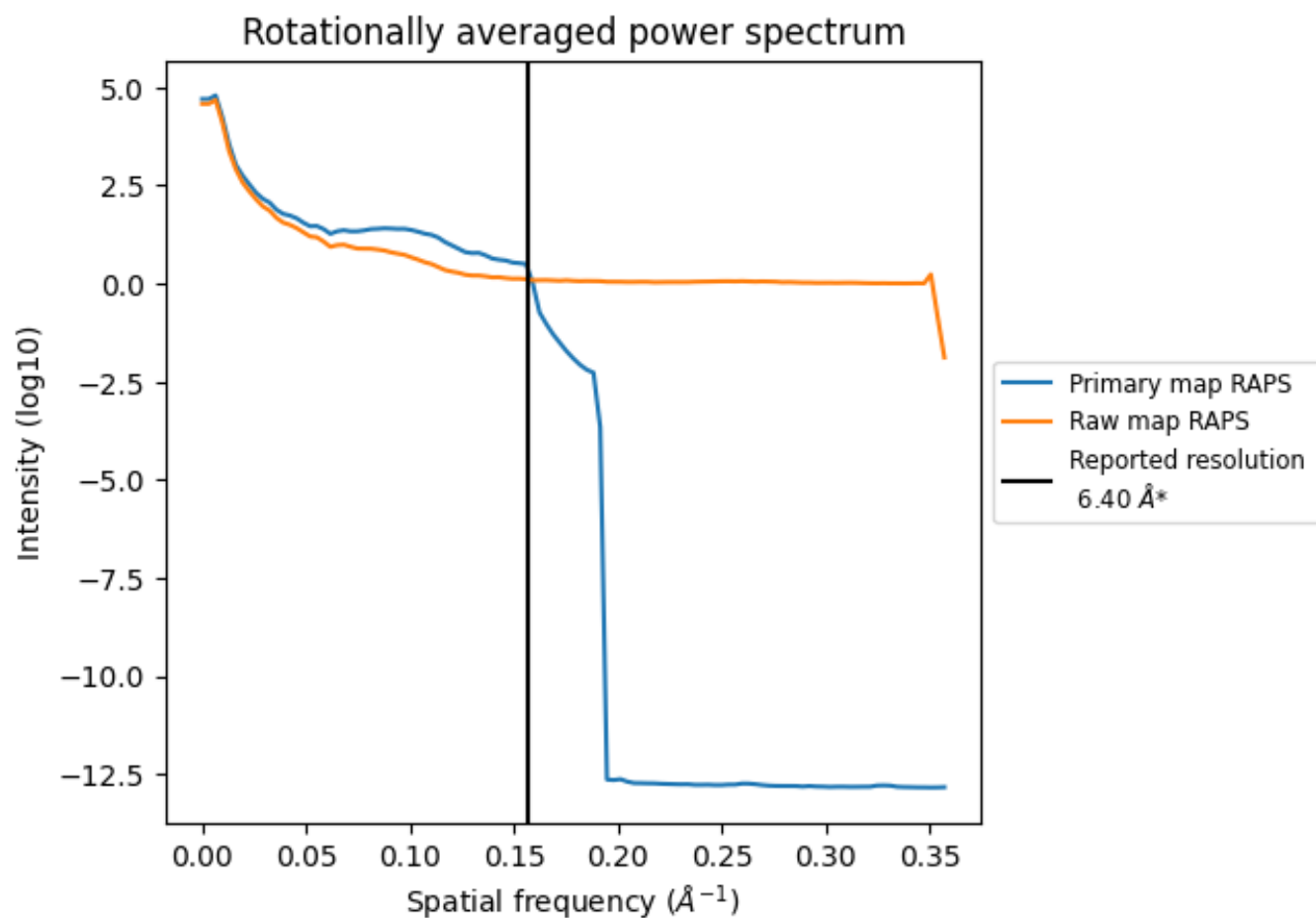
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 524 nm³; this corresponds to an approximate mass of 473 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 ⓘ

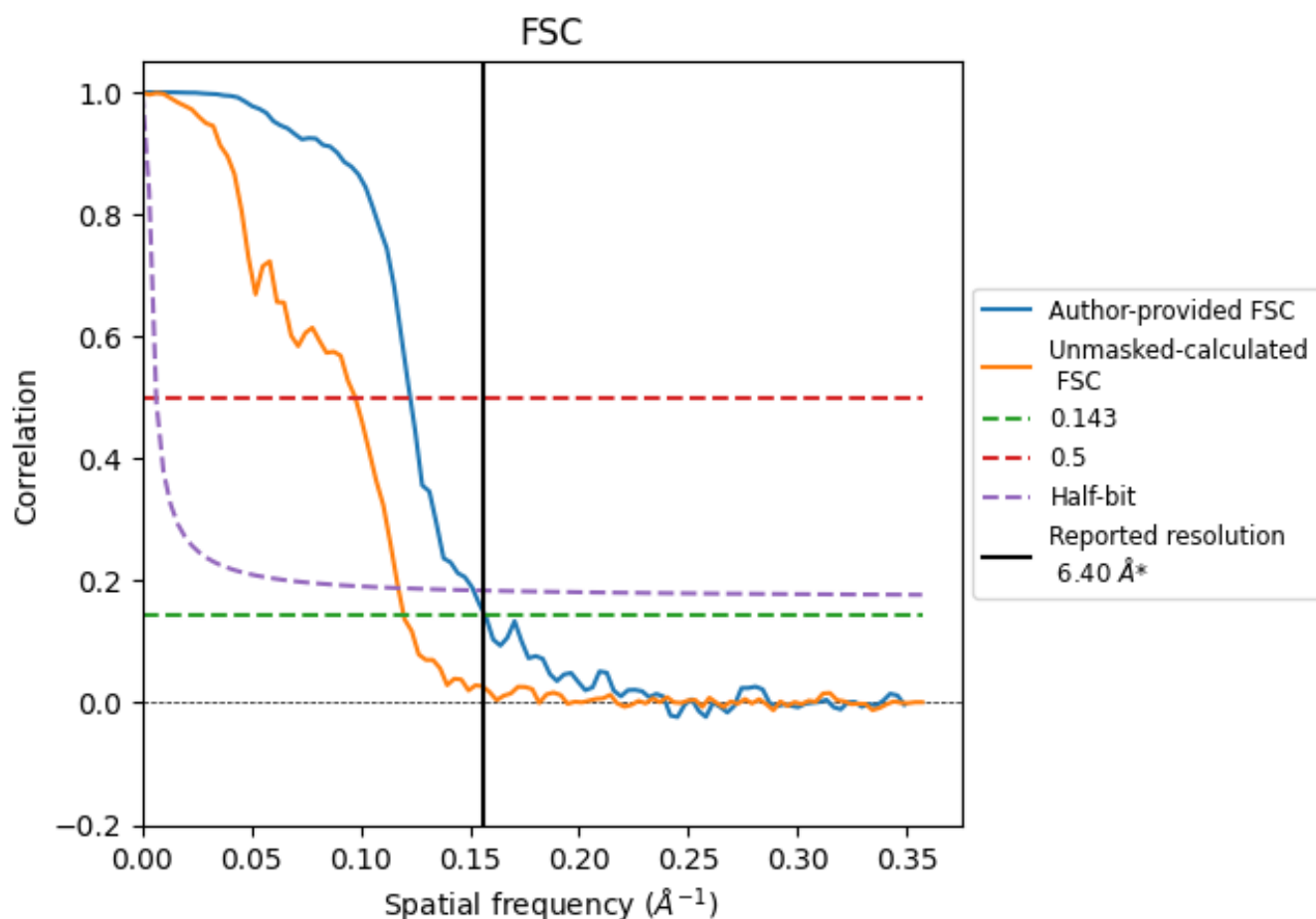


*Reported resolution corresponds to spatial frequency of 0.156 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.156 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

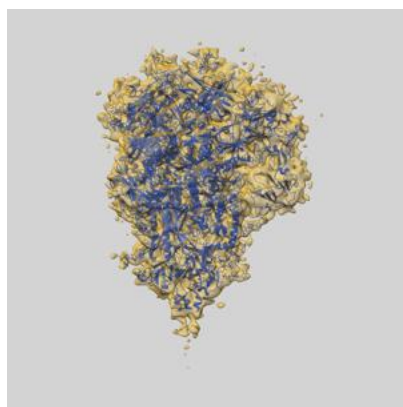
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	6.37	8.15	6.60
Unmasked-calculated*	8.35	10.26	8.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.35 differs from the reported value 6.4 by more than 10 %

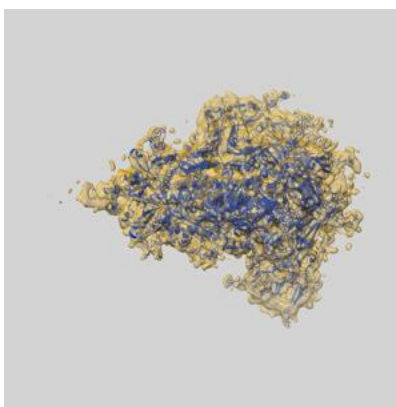
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32338 and PDB model 7W73. Per-residue inclusion information can be found in section [3](#) on page [11](#).

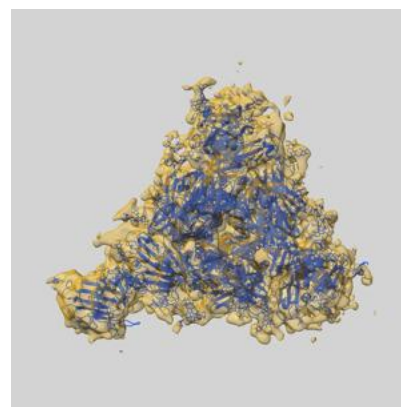
9.1 Map-model overlay [i](#)



X



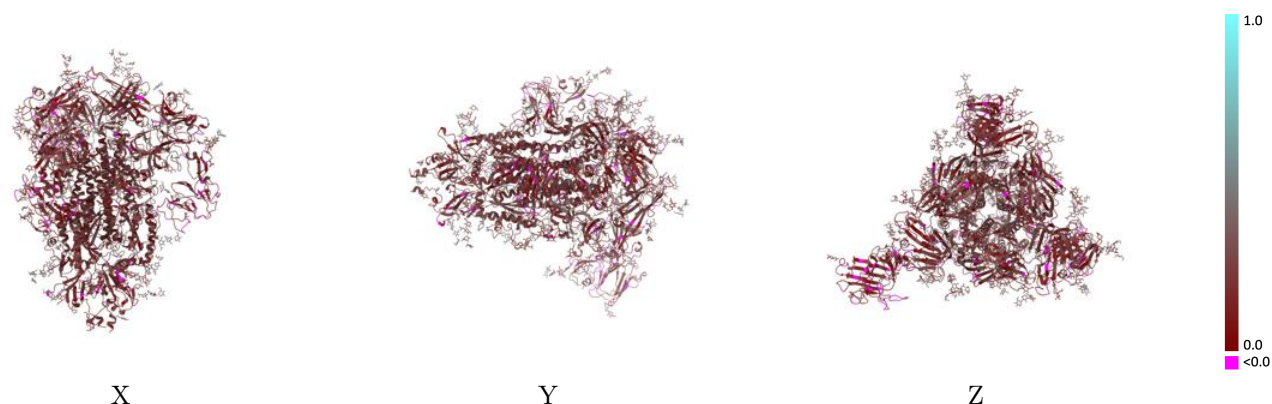
Y



Z

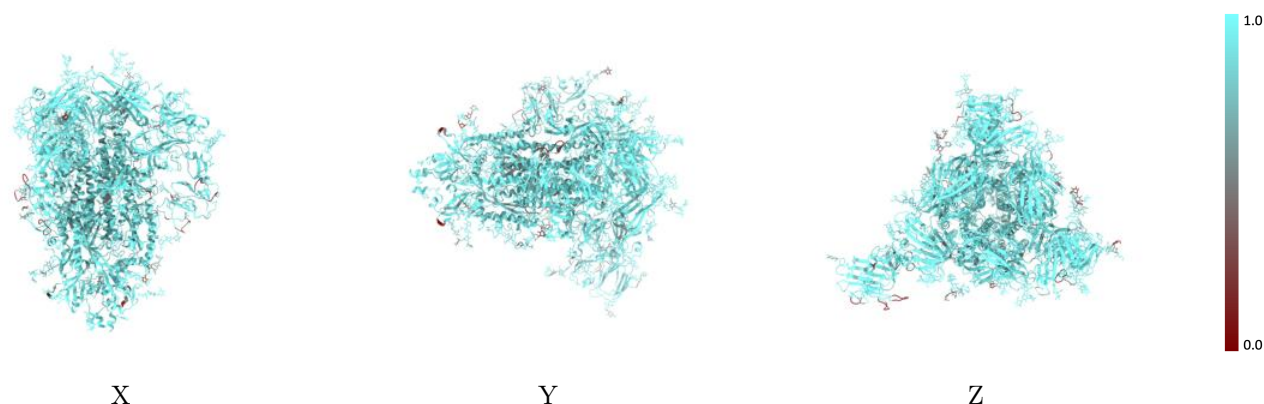
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



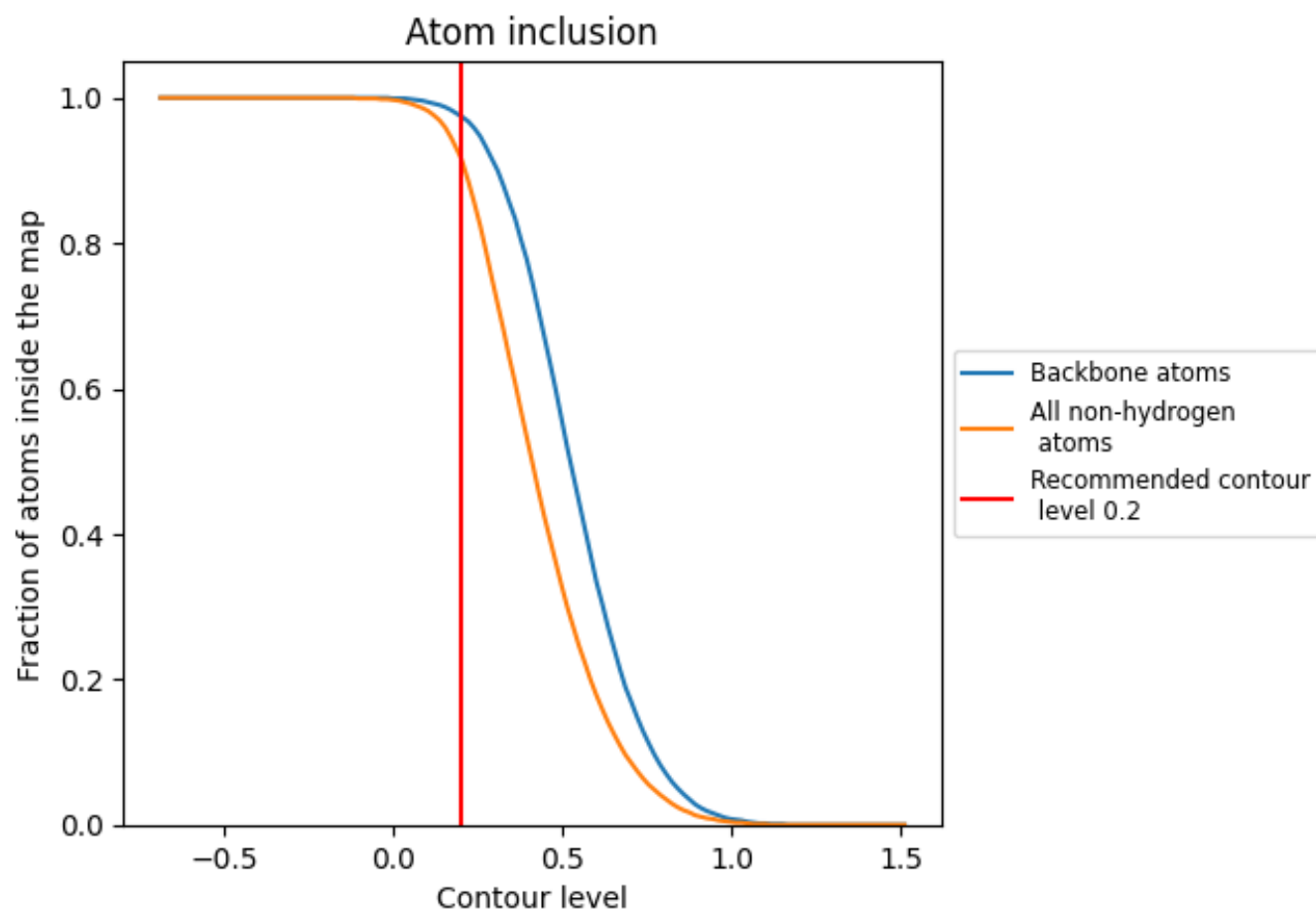
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.2290
A	 0.9250	 0.2190
B	 0.9180	 0.2210
C	 0.9240	 0.2230
D	 0.9840	 0.3790
E	 0.9490	 0.3570
F	 0.9840	 0.2650
G	 0.9670	 0.3020
H	 0.7050	 0.3130
I	 0.6330	 0.2430
J	 0.6390	 0.2700
K	 0.9490	 0.4320
L	 0.9400	 0.3350
M	 0.8570	 0.3100
N	 0.9840	 0.2810
O	 0.8450	 0.2370
P	 0.9020	 0.2930
Q	 1.0000	 0.2760
R	 0.9020	 0.3530
S	 0.7180	 0.3240
T	 0.9840	 0.4080
U	 0.9840	 0.3230
V	 0.9230	 0.2930
W	 1.0000	 0.3490
X	 0.9510	 0.3330
Y	 0.7050	 0.2440
Z	 0.8980	 0.3360
a	 0.8200	 0.3270
b	 0.7210	 0.2970
c	 1.0000	 0.3650
d	 0.9670	 0.2600
e	 0.7320	 0.3460
f	 0.9490	 0.3120
g	 0.8530	 0.3540
h	 0.9840	 0.4160



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Chain	Atom inclusion	Q-score
i	 0.7040	 0.3660
j	 0.9840	 0.2680
k	 0.9020	 0.3110
l	 0.9230	 0.3220
m	 0.9020	 0.3260
n	 0.6890	 0.2970
o	 0.8200	 0.3050
p	 0.7380	 0.3410
q	 0.9490	 0.3860
r	 0.8720	 0.3840
s	 0.9580	 0.2960
t	 0.7550	 0.2920
u	 0.8690	 0.2270