



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 08:31 PM EST

PDB ID : 8DZH
EMDB ID : EMD-27798
Title : Structure of SARS-CoV-2 Omicron BA.1.1.529 Spike trimer with two RBDs down in complex with the Fab fragment of human neutralizing antibody MB.02
Authors : Hu, Y.; Xiong, Y.
Deposited on : 2022-08-07
Resolution : 3.20 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:

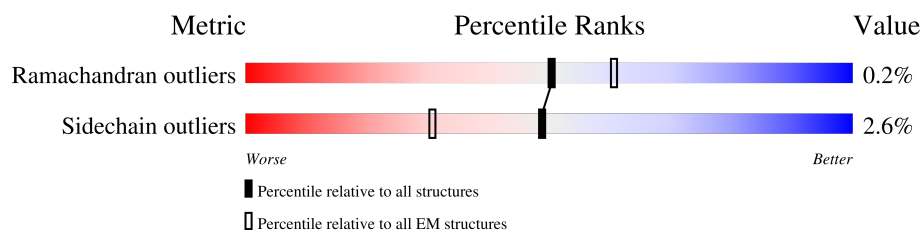
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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




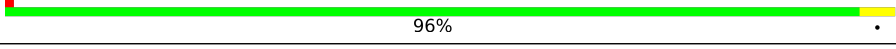
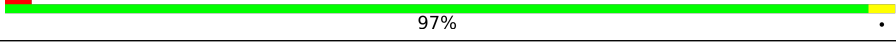
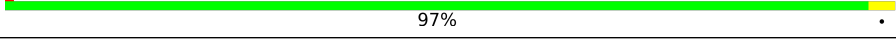
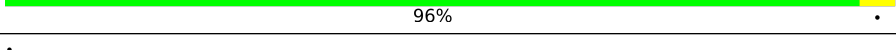
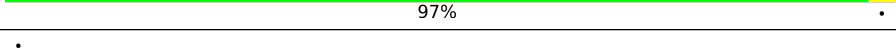
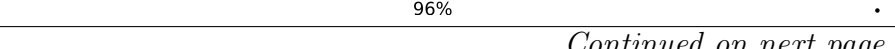
The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1285	 84% 14%
1	B	1285	 83% 15%
1	C	1285	 82% 15%
2	E	118	 96% .
2	H	118	 97% .
2	I	118	 97% .
3	D	109	 96% .
3	J	109	 97% .
3	L	109	 96% .

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Mol	Chain	Length	Quality of chain
4	F	2	100%
4	G	2	100%
4	K	2	50% 50%
4	M	2	50% 100%
4	N	2	50% 100%
4	O	2	50% 50%
4	P	2	50% 50%
4	Q	2	100% 50%
4	R	2	50% 50%
4	S	2	100%
4	T	2	100% 50%
4	U	2	50% 50%
4	V	2	50% 50%
4	W	2	50% 100%
4	X	2	100%
4	Y	2	50% 50%
4	Z	2	100%
4	a	2	50% 50%
4	b	2	50% 50%
4	c	2	50% 100%
4	d	2	50% 100%
4	e	2	100%
4	f	2	50% 100%
4	g	2	50% 50%
4	h	2	100% 100%

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Mol	Chain	Length	Quality of chain	
4	i	2	<div><div></div></div>	50%
4	j	2	<div><div></div></div>	50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31956 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	B	1092	Total	C	N	O	S	0	0
			8562	5476	1429	1618	39		
1	A	1100	Total	C	N	O	S	0	0
			8606	5501	1439	1627	39		
1	C	1093	Total	C	N	O	S	0	0
			8561	5475	1430	1618	38		

There are 387 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	93	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	140	ASP	TYR	conflict	UNP P0DTC2
B	206	ILE	-	insertion	UNP P0DTC2
B	207	VAL	-	insertion	UNP P0DTC2
B	208	ARG	ASN	conflict	UNP P0DTC2
B	209	GLU	LEU	conflict	UNP P0DTC2
B	210	PRO	VAL	conflict	UNP P0DTC2
B	211	GLU	ARG	conflict	UNP P0DTC2
B	336	ASP	GLY	conflict	UNP P0DTC2
B	368	LEU	SER	conflict	UNP P0DTC2
B	370	PRO	SER	conflict	UNP P0DTC2
B	372	PHE	SER	conflict	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	conflict	UNP P0DTC2
B	443	SER	GLY	conflict	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	490	ARG	GLN	conflict	UNP P0DTC2
B	493	SER	GLY	conflict	UNP P0DTC2
B	495	ARG	GLN	conflict	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	conflict	UNP P0DTC2
B	544	LYS	THR	conflict	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	conflict	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	761	LYS	ASN	conflict	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	conflict	UNP P0DTC2
B	853	LYS	ASN	conflict	UNP P0DTC2
B	889	PRO	ALA	conflict	UNP P0DTC2
B	896	PRO	ALA	conflict	UNP P0DTC2
B	939	PRO	ALA	conflict	UNP P0DTC2
B	951	HIS	GLN	conflict	UNP P0DTC2
B	966	LYS	ASN	conflict	UNP P0DTC2
B	978	PHE	LEU	conflict	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1206	GLY	-	expression tag	UNP P0DTC2
B	1207	SER	-	expression tag	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	TYR	-	expression tag	UNP P0DTC2
B	1210	ILE	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	GLU	-	expression tag	UNP P0DTC2
B	1213	ALA	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	ASP	-	expression tag	UNP P0DTC2
B	1217	GLY	-	expression tag	UNP P0DTC2
B	1218	GLN	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	TYR	-	expression tag	UNP P0DTC2
B	1221	VAL	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1223	LYS	-	expression tag	UNP P0DTC2
B	1224	ASP	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	GLU	-	expression tag	UNP P0DTC2
B	1227	TRP	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	LEU	-	expression tag	UNP P0DTC2
B	1230	LEU	-	expression tag	UNP P0DTC2
B	1231	SER	-	expression tag	UNP P0DTC2
B	1232	THR	-	expression tag	UNP P0DTC2
B	1233	PHE	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	ARG	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	GLU	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	PRO	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	SER	-	expression tag	UNP P0DTC2
B	1256	ALA	-	expression tag	UNP P0DTC2
B	1257	TRP	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	PRO	-	expression tag	UNP P0DTC2
B	1261	GLN	-	expression tag	UNP P0DTC2
B	1262	PHE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1265	GLY	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	GLY	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	SER	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	ALA	-	expression tag	UNP P0DTC2
B	1278	TRP	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
B	1281	PRO	-	expression tag	UNP P0DTC2
B	1282	GLN	-	expression tag	UNP P0DTC2
B	1283	PHE	-	expression tag	UNP P0DTC2
B	1284	GLU	-	expression tag	UNP P0DTC2
B	1285	LYS	-	expression tag	UNP P0DTC2
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	140	ASP	TYR	conflict	UNP P0DTC2
A	206	ILE	-	insertion	UNP P0DTC2
A	207	VAL	-	insertion	UNP P0DTC2
A	208	ARG	ASN	conflict	UNP P0DTC2
A	209	GLU	LEU	conflict	UNP P0DTC2
A	210	PRO	VAL	conflict	UNP P0DTC2
A	211	GLU	ARG	conflict	UNP P0DTC2
A	336	ASP	GLY	conflict	UNP P0DTC2
A	368	LEU	SER	conflict	UNP P0DTC2
A	370	PRO	SER	conflict	UNP P0DTC2
A	372	PHE	SER	conflict	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	conflict	UNP P0DTC2
A	443	SER	GLY	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	conflict	UNP P0DTC2
A	490	ARG	GLN	conflict	UNP P0DTC2
A	493	SER	GLY	conflict	UNP P0DTC2
A	495	ARG	GLN	conflict	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	conflict	UNP P0DTC2
A	544	LYS	THR	conflict	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	conflict	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	761	LYS	ASN	conflict	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	853	LYS	ASN	conflict	UNP P0DTC2
A	889	PRO	ALA	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	939	PRO	ALA	conflict	UNP P0DTC2
A	951	HIS	GLN	conflict	UNP P0DTC2
A	966	LYS	ASN	conflict	UNP P0DTC2
A	978	PHE	LEU	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1206	GLY	-	expression tag	UNP P0DTC2
A	1207	SER	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	TYR	-	expression tag	UNP P0DTC2
A	1210	ILE	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	GLU	-	expression tag	UNP P0DTC2
A	1213	ALA	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	ASP	-	expression tag	UNP P0DTC2
A	1217	GLY	-	expression tag	UNP P0DTC2
A	1218	GLN	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	TYR	-	expression tag	UNP P0DTC2
A	1221	VAL	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	LYS	-	expression tag	UNP P0DTC2
A	1224	ASP	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2
A	1227	TRP	-	expression tag	UNP P0DTC2
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	LEU	-	expression tag	UNP P0DTC2
A	1230	LEU	-	expression tag	UNP P0DTC2
A	1231	SER	-	expression tag	UNP P0DTC2
A	1232	THR	-	expression tag	UNP P0DTC2
A	1233	PHE	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	PRO	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	SER	-	expression tag	UNP P0DTC2
A	1256	ALA	-	expression tag	UNP P0DTC2
A	1257	TRP	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	PRO	-	expression tag	UNP P0DTC2
A	1261	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1262	PHE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	LYS	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	SER	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	ALA	-	expression tag	UNP P0DTC2
A	1278	TRP	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	PRO	-	expression tag	UNP P0DTC2
A	1282	GLN	-	expression tag	UNP P0DTC2
A	1283	PHE	-	expression tag	UNP P0DTC2
A	1284	GLU	-	expression tag	UNP P0DTC2
A	1285	LYS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	140	ASP	TYR	conflict	UNP P0DTC2
C	206	ILE	-	insertion	UNP P0DTC2
C	207	VAL	-	insertion	UNP P0DTC2
C	208	ARG	ASN	conflict	UNP P0DTC2
C	209	GLU	LEU	conflict	UNP P0DTC2
C	210	PRO	VAL	conflict	UNP P0DTC2
C	211	GLU	ARG	conflict	UNP P0DTC2
C	336	ASP	GLY	conflict	UNP P0DTC2
C	368	LEU	SER	conflict	UNP P0DTC2
C	370	PRO	SER	conflict	UNP P0DTC2
C	372	PHE	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	conflict	UNP P0DTC2
C	443	SER	GLY	conflict	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
C	481	ALA	GLU	conflict	UNP P0DTC2
C	490	ARG	GLN	conflict	UNP P0DTC2
C	493	SER	GLY	conflict	UNP P0DTC2
C	495	ARG	GLN	conflict	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	conflict	UNP P0DTC2
C	544	LYS	THR	conflict	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	conflict	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	761	LYS	ASN	conflict	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2
C	814	PRO	PHE	conflict	UNP P0DTC2
C	853	LYS	ASN	conflict	UNP P0DTC2
C	889	PRO	ALA	conflict	UNP P0DTC2
C	896	PRO	ALA	conflict	UNP P0DTC2
C	939	PRO	ALA	conflict	UNP P0DTC2
C	951	HIS	GLN	conflict	UNP P0DTC2
C	966	LYS	ASN	conflict	UNP P0DTC2
C	978	PHE	LEU	conflict	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1206	GLY	-	expression tag	UNP P0DTC2
C	1207	SER	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	TYR	-	expression tag	UNP P0DTC2
C	1210	ILE	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	ALA	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	GLN	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	TYR	-	expression tag	UNP P0DTC2
C	1221	VAL	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	LYS	-	expression tag	UNP P0DTC2
C	1224	ASP	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	TRP	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	LEU	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	SER	-	expression tag	UNP P0DTC2
C	1232	THR	-	expression tag	UNP P0DTC2
C	1233	PHE	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	PRO	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	SER	-	expression tag	UNP P0DTC2
C	1256	ALA	-	expression tag	UNP P0DTC2
C	1257	TRP	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	PRO	-	expression tag	UNP P0DTC2
C	1261	GLN	-	expression tag	UNP P0DTC2
C	1262	PHE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	LYS	-	expression tag	UNP P0DTC2
C	1265	GLY	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	SER	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	ALA	-	expression tag	UNP P0DTC2
C	1278	TRP	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	PRO	-	expression tag	UNP P0DTC2
C	1282	GLN	-	expression tag	UNP P0DTC2
C	1283	PHE	-	expression tag	UNP P0DTC2
C	1284	GLU	-	expression tag	UNP P0DTC2
C	1285	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called antibody MB.02 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	118	Total	C	N	O	S	0	0
			912	581	146	179	6		
2	H	118	Total	C	N	O	S	0	0
			912	581	146	179	6		
2	I	118	Total	C	N	O	S	0	0
			912	581	146	179	6		

- Molecule 3 is a protein called antibody MB.02 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	109	Total	C	N	O	S	0	0
			823	515	142	164	2		
3	L	109	Total	C	N	O	S	0	0
			823	515	142	164	2		
3	J	109	Total	C	N	O	S	0	0
			823	515	142	164	2		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			98	56	7	35	
5	B	1	Total	C	N	O	0
			98	56	7	35	
5	B	1	Total	C	N	O	0
			98	56	7	35	
5	B	1	Total	C	N	O	0
			98	56	7	35	
5	B	1	Total	C	N	O	0
			98	56	7	35	
5	B	1	Total	C	N	O	0
			98	56	7	35	
5	B	1	Total	C	N	O	0
			98	56	7	35	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	A	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	

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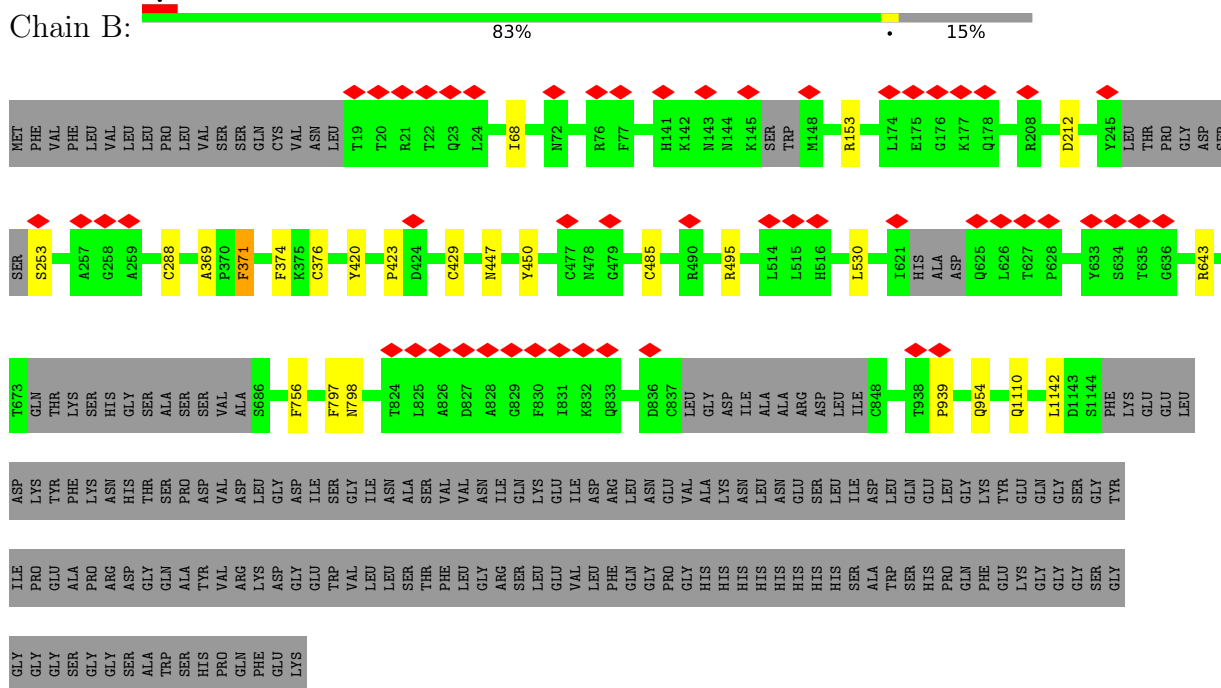
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	
5	C	1	Total	C	N	O	0
			84	48	6	30	

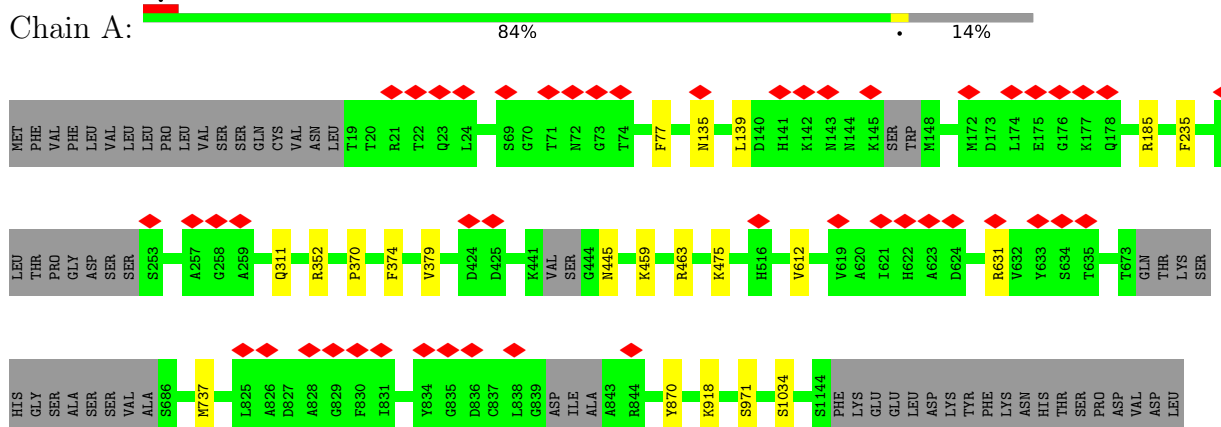
3 Residue-property plots

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

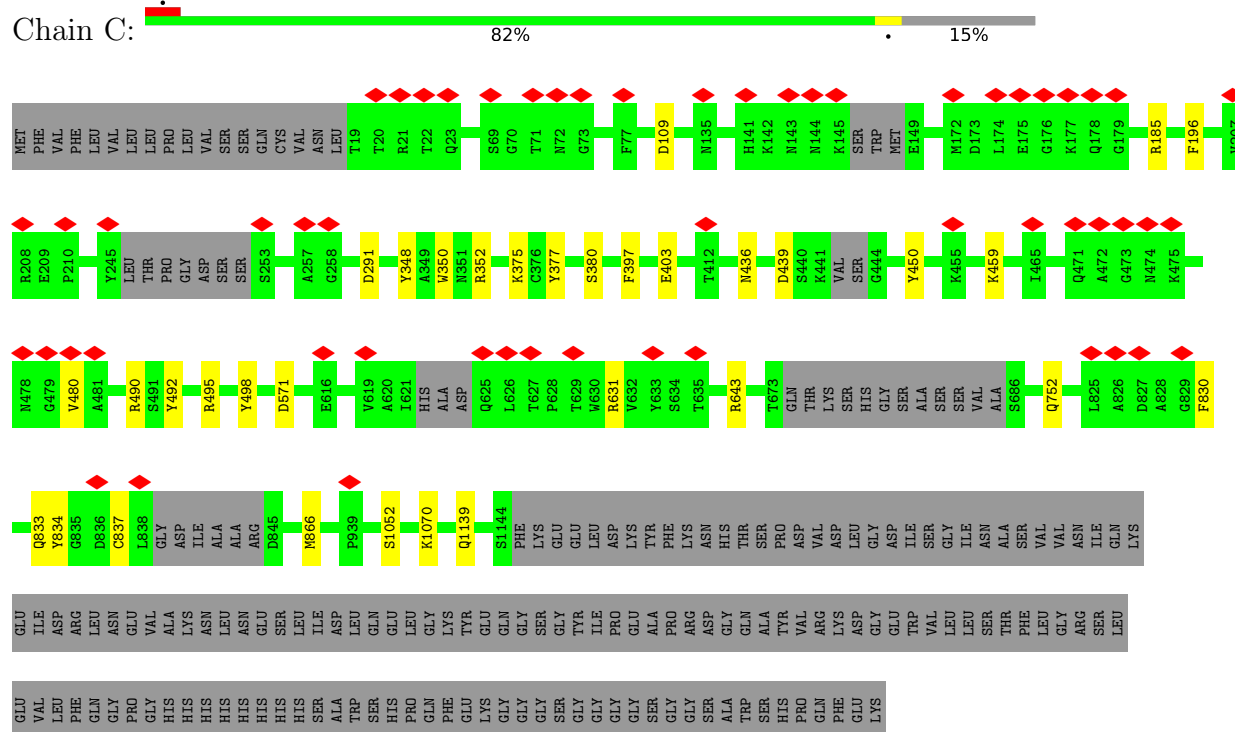
• Molecule 1: Spike glycoprotein



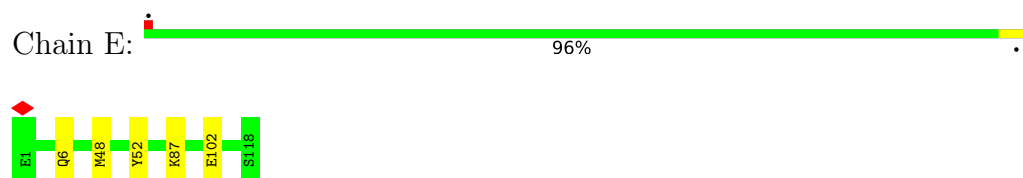
• Molecule 1: Spike glycoprotein



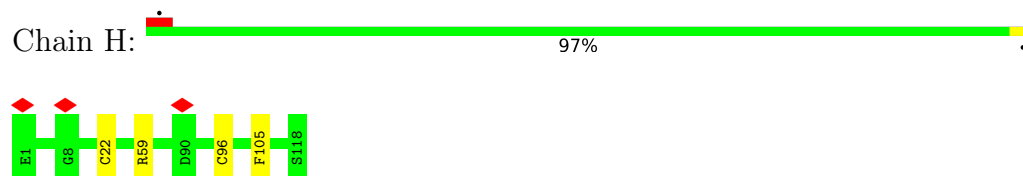
- Molecule 1: Spike glycoprotein



- Molecule 2: antibody MB.02 heavy chain

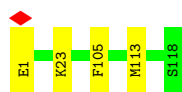


- Molecule 2: antibody MB.02 heavy chain



- Molecule 2: antibody MB.02 heavy chain

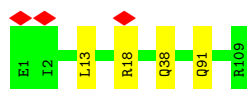




- Molecule 3: antibody MB.02 light chain



- Molecule 3: antibody MB.02 light chain



- Molecule 3: antibody MB.02 light chain



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



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



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



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



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



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



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



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



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



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

Chain S:  100%



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

Chain T:  100%
50% 50%



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

Chain U:  50%
50% 50%



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

Chain V:  50%
50% 50%



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

Chain W:  50%
100%



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

Chain X:  100%



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

Chain Y:  50% 50%



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

Chain Z:  100%



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

Chain a:  50% 50%



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

Chain b:  50% 50%



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

Chain c:  50% 100%



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

Chain d:  50% 100%



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

Chain e:  100%



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

Chain f:  50%
100%



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

Chain g:  50%
50% 50%



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

Chain h:  100%
100%



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

Chain i:  50% 50%



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

Chain j:  50%
50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	465702	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.30	0/8810	0.50	0/11984
1	B	0.81	6/8767 (0.1%)	0.88	8/11928 (0.1%)
1	C	0.74	6/8765 (0.1%)	0.73	8/11925 (0.1%)
2	E	0.30	0/936	0.53	0/1265
2	H	0.28	0/936	0.51	0/1265
2	I	0.29	0/936	0.54	0/1265
3	D	0.28	0/842	0.55	0/1141
3	J	0.27	0/842	0.55	0/1141
3	L	0.27	0/842	0.54	0/1141
All	All	0.61	12/31676 (0.0%)	0.69	16/43055 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
3	D	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	450	TYR	CD2-CE2	44.98	2.06	1.39
1	B	450	TYR	CD1-CE1	44.95	2.06	1.39
1	C	830	PHE	CD1-CE1	35.90	2.11	1.39
1	C	830	PHE	CD2-CE2	35.81	2.10	1.39
1	C	830	PHE	CE2-CZ	-21.98	0.95	1.37
1	C	830	PHE	CE1-CZ	-21.97	0.95	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	450	TYR	CG-CD2	-14.80	1.20	1.39
1	B	450	TYR	CG-CD1	-14.77	1.20	1.39
1	C	830	PHE	CG-CD1	-14.66	1.16	1.38
1	C	830	PHE	CG-CD2	-14.64	1.16	1.38
1	B	450	TYR	CE1-CZ	-14.28	1.20	1.38
1	B	450	TYR	CE2-CZ	-14.25	1.20	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	TYR	CE1-CZ-CE2	-46.04	46.13	119.80
1	B	450	TYR	CG-CD1-CE1	-30.25	97.10	121.30
1	B	450	TYR	CG-CD2-CE2	-30.16	97.17	121.30
1	C	830	PHE	CE1-CZ-CE2	-28.63	68.46	120.00
1	B	450	TYR	CD1-CG-CD2	-27.38	87.79	117.90
1	B	450	TYR	CB-CG-CD1	25.09	136.05	121.00
1	B	450	TYR	CB-CG-CD2	24.50	135.70	121.00
1	C	830	PHE	CD1-CG-CD2	-23.22	88.11	118.30
1	C	830	PHE	CG-CD1-CE1	-22.37	96.19	120.80
1	C	830	PHE	CG-CD2-CE2	-22.25	96.32	120.80
1	C	830	PHE	CB-CG-CD1	21.63	135.94	120.80
1	C	830	PHE	CB-CG-CD2	21.54	135.87	120.80
1	C	830	PHE	CZ-CE2-CD2	-11.69	106.07	120.10
1	C	830	PHE	CD1-CE1-CZ	-11.66	106.11	120.10
1	B	450	TYR	CE1-CZ-OH	-8.66	96.70	120.10
1	B	450	TYR	OH-CZ-CE2	8.42	142.83	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	612	VAL	Peptide
1	B	797	PHE	Peptide
1	B	798	ASN	Peptide
3	D	95	SER	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1085/1285 (84%)	1027 (95%)	56 (5%)	2 (0%)	47	79
1	B	1080/1285 (84%)	1014 (94%)	61 (6%)	5 (0%)	29	67
1	C	1079/1285 (84%)	1029 (95%)	49 (4%)	1 (0%)	51	83
2	E	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
2	H	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	I	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
3	D	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
3	J	107/109 (98%)	99 (92%)	8 (8%)	0	100	100
3	L	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
All	All	3913/4536 (86%)	3697 (94%)	208 (5%)	8 (0%)	50	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	423	PRO
1	A	370	PRO
1	A	379	VAL
1	C	480	VAL
1	B	68	ILE
1	B	447	ASN
1	B	369	ALA
1	B	371	PHE

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	956/1116 (86%)	938 (98%)	18 (2%)	57	81
1	B	956/1116 (86%)	938 (98%)	18 (2%)	57	81
1	C	953/1116 (85%)	922 (97%)	31 (3%)	38	71
2	E	98/98 (100%)	93 (95%)	5 (5%)	24	60
2	H	98/98 (100%)	94 (96%)	4 (4%)	30	66
2	I	98/98 (100%)	94 (96%)	4 (4%)	30	66
3	D	90/90 (100%)	87 (97%)	3 (3%)	38	71
3	J	90/90 (100%)	87 (97%)	3 (3%)	38	71
3	L	90/90 (100%)	86 (96%)	4 (4%)	28	64
All	All	3429/3912 (88%)	3339 (97%)	90 (3%)	49	76

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	153	ARG
1	B	212	ASP
1	B	253	SER
1	B	288	CYS
1	B	371	PHE
1	B	374	PHE
1	B	376	CYS
1	B	420	TYR
1	B	429	CYS
1	B	485	CYS
1	B	495	ARG
1	B	530	LEU
1	B	643	ARG
1	B	756	PHE
1	B	939	PRO
1	B	954	GLN
1	B	1110	GLN
1	B	1142	LEU
1	A	77	PHE
1	A	135	ASN
1	A	139	LEU
1	A	185	ARG
1	A	235	PHE
1	A	311	GLN

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Mol	Chain	Res	Type
1	A	352	ARG
1	A	374	PHE
1	A	445	ASN
1	A	459	LYS
1	A	463	ARG
1	A	475	LYS
1	A	631	ARG
1	A	737	MET
1	A	870	TYR
1	A	918	LYS
1	A	971	SER
1	A	1034	SER
1	C	109	ASP
1	C	185	ARG
1	C	196	PHE
1	C	291	ASP
1	C	348	TYR
1	C	350	TRP
1	C	352	ARG
1	C	375	LYS
1	C	377	TYR
1	C	380	SER
1	C	397	PHE
1	C	403	GLU
1	C	436	ASN
1	C	439	ASP
1	C	450	TYR
1	C	459	LYS
1	C	490	ARG
1	C	492	TYR
1	C	495	ARG
1	C	498	TYR
1	C	571	ASP
1	C	631	ARG
1	C	643	ARG
1	C	752	GLN
1	C	833	GLN
1	C	834	TYR
1	C	837	CYS
1	C	866	MET
1	C	1052	SER
1	C	1070	LYS

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Mol	Chain	Res	Type
1	C	1139	GLN
2	E	6	GLN
2	E	48	MET
2	E	52	TYR
2	E	87	LYS
2	E	102	GLU
3	D	13	LEU
3	D	46	ARG
3	D	90	GLN
2	H	22	CYS
2	H	59	ARG
2	H	96	CYS
2	H	105	PHE
3	L	13	LEU
3	L	18	ARG
3	L	38	GLN
3	L	91	GLN
2	I	1	GLU
2	I	23	LYS
2	I	105	PHE
2	I	113	MET
3	J	13	LEU
3	J	50	TYR
3	J	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	178	GLN
1	B	357	ASN
1	B	391	ASN
1	B	406	GLN
1	B	474	ASN
1	B	478	ASN
1	B	625	GLN
1	B	687	GLN
1	B	781	GLN
1	B	910	GLN
1	B	923	GLN
1	B	952	ASN
1	B	989	GLN
1	B	1103	GLN

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	123	ASN
1	A	242	HIS
1	A	318	GLN
1	A	367	ASN
1	A	406	GLN
1	A	411	GLN
1	A	471	GLN
1	A	625	GLN
1	A	687	GLN
1	A	869	GLN
1	A	952	ASN
1	A	954	GLN
1	A	1002	GLN
1	A	1008	GLN
1	C	484	ASN
1	C	625	GLN
1	C	638	ASN
1	C	687	GLN
1	C	707	ASN
1	C	850	GLN
3	L	38	GLN
3	J	38	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 ⓘ

54 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	F	1	4,1	14,14,15	0.36	0	17,19,21	0.38	0
4	NAG	F	2	4	14,14,15	0.43	0	17,19,21	0.34	0
4	NAG	G	1	4,1	14,14,15	1.37	1 (7%)	17,19,21	1.47	1 (5%)
4	NAG	G	2	4	14,14,15	1.01	1 (7%)	17,19,21	0.86	0
4	NAG	K	1	4,1	14,14,15	1.20	1 (7%)	17,19,21	1.01	2 (11%)
4	NAG	K	2	4	14,14,15	0.16	0	17,19,21	0.41	0
4	NAG	M	1	4,1	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	N	1	4,1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	N	2	4	14,14,15	0.19	0	17,19,21	0.42	0
4	NAG	O	1	4,1	14,14,15	1.19	1 (7%)	17,19,21	1.55	1 (5%)
4	NAG	O	2	4	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	P	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	0.77	0
4	NAG	P	2	4	14,14,15	0.19	0	17,19,21	0.46	0
4	NAG	Q	1	4,1	14,14,15	0.66	1 (7%)	17,19,21	0.71	1 (5%)
4	NAG	Q	2	4	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	R	1	4,1	14,14,15	0.42	0	17,19,21	0.58	0
4	NAG	R	2	4	14,14,15	0.82	1 (7%)	17,19,21	0.82	0
4	NAG	S	1	4,1	14,14,15	0.40	0	17,19,21	0.35	0
4	NAG	S	2	4	14,14,15	0.42	0	17,19,21	0.39	0
4	NAG	T	1	4,1	14,14,15	0.40	0	17,19,21	0.50	0
4	NAG	T	2	4	14,14,15	0.98	2 (14%)	17,19,21	0.82	1 (5%)
4	NAG	U	1	4,1	14,14,15	0.20	0	17,19,21	0.90	1 (5%)
4	NAG	U	2	4	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	V	1	4,1	14,14,15	0.35	0	17,19,21	0.59	0
4	NAG	V	2	4	14,14,15	1.09	1 (7%)	17,19,21	1.60	1 (5%)
4	NAG	W	1	4,1	14,14,15	0.40	0	17,19,21	0.50	0
4	NAG	W	2	4	14,14,15	0.55	0	17,19,21	0.38	0
4	NAG	X	1	4,1	14,14,15	0.32	0	17,19,21	0.56	0
4	NAG	X	2	4	14,14,15	0.17	0	17,19,21	0.38	0
4	NAG	Y	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	1.33	1 (5%)
4	NAG	Y	2	4	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	Z	1	4,1	14,14,15	0.35	0	17,19,21	0.56	0
4	NAG	Z	2	4	14,14,15	0.18	0	17,19,21	0.50	0
4	NAG	a	1	4,1	14,14,15	0.35	0	17,19,21	0.51	0
4	NAG	a	2	4	14,14,15	0.81	1 (7%)	17,19,21	0.99	1 (5%)
4	NAG	b	1	4,1	14,14,15	0.37	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	b	2	4	14,14,15	0.16	0	17,19,21	0.44	0
4	NAG	c	1	4,1	14,14,15	0.57	0	17,19,21	0.51	0
4	NAG	c	2	4	14,14,15	0.41	0	17,19,21	0.48	0
4	NAG	d	1	4,1	14,14,15	0.56	0	17,19,21	0.49	0
4	NAG	d	2	4	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	e	1	4,1	14,14,15	0.56	0	17,19,21	0.45	0
4	NAG	e	2	4	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	f	1	4,1	14,14,15	0.65	0	17,19,21	0.48	0
4	NAG	f	2	4	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	g	1	4,1	14,14,15	0.37	0	17,19,21	0.66	1 (5%)
4	NAG	g	2	4	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	h	1	4,1	14,14,15	0.59	1 (7%)	17,19,21	0.52	0
4	NAG	h	2	4	14,14,15	0.68	1 (7%)	17,19,21	0.82	0
4	NAG	i	1	4,1	14,14,15	0.93	2 (14%)	17,19,21	0.89	1 (5%)
4	NAG	i	2	4	14,14,15	0.31	0	17,19,21	0.37	0
4	NAG	j	1	4,1	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	j	2	4	14,14,15	0.82	1 (7%)	17,19,21	1.00	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
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	S	2	4	-	4/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	a	2	4	-	0/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	c	2	4	-	3/6/23/26	0/1/1/1
4	NAG	d	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	d	2	4	-	2/6/23/26	0/1/1/1
4	NAG	e	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
4	NAG	f	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	NAG	h	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	4/6/23/26	0/1/1/1
4	NAG	i	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1
4	NAG	j	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	j	2	4	-	2/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	O5-C1	-4.81	1.36	1.43
4	K	1	NAG	O5-C1	-4.27	1.36	1.43
4	O	1	NAG	O5-C1	4.21	1.50	1.43
4	V	2	NAG	O5-C1	3.90	1.49	1.43
4	G	2	NAG	O5-C1	-3.18	1.38	1.43
4	R	2	NAG	O5-C1	-2.89	1.39	1.43
4	Y	1	NAG	O5-C1	2.70	1.48	1.43
4	T	2	NAG	O5-C1	2.67	1.48	1.43
4	a	2	NAG	O5-C1	2.65	1.47	1.43
4	j	2	NAG	O5-C1	2.52	1.47	1.43
4	P	1	NAG	O5-C1	-2.39	1.39	1.43
4	i	1	NAG	C1-C2	2.34	1.55	1.52
4	T	2	NAG	C1-C2	2.34	1.55	1.52
4	i	1	NAG	O5-C1	-2.23	1.40	1.43
4	h	1	NAG	O5-C1	-2.15	1.40	1.43
4	h	2	NAG	O5-C1	-2.14	1.40	1.43
4	Q	1	NAG	C1-C2	2.06	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	2	NAG	C1-O5-C5	6.25	120.65	112.19
4	O	1	NAG	C1-O5-C5	6.00	120.31	112.19
4	Y	1	NAG	C1-O5-C5	5.26	119.32	112.19
4	G	1	NAG	C2-N2-C7	4.66	129.54	122.90
4	a	2	NAG	C1-O5-C5	3.84	117.39	112.19
4	j	2	NAG	C1-O5-C5	3.76	117.29	112.19
4	T	2	NAG	C1-O5-C5	3.10	116.39	112.19
4	b	1	NAG	C1-O5-C5	2.83	116.03	112.19
4	U	1	NAG	C1-O5-C5	2.64	115.77	112.19
4	K	1	NAG	C3-C4-C5	2.31	114.37	110.24
4	i	1	NAG	O3-C3-C2	-2.31	104.69	109.47
4	Q	1	NAG	C1-O5-C5	2.29	115.30	112.19
4	g	1	NAG	C1-O5-C5	2.17	115.13	112.19
4	K	1	NAG	O4-C4-C5	-2.01	104.31	109.30

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	f	2	NAG	C4-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	S	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	S	1	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	T	2	NAG	C8-C7-N2-C2
4	T	2	NAG	O7-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2
4	d	1	NAG	O7-C7-N2-C2
4	a	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	d	2	NAG	C4-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C1-C2-N2-C7
4	d	1	NAG	O5-C5-C6-O6
4	g	1	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	j	1	NAG	O5-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C1-C2-N2-C7
4	f	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	c	2	NAG	C1-C2-N2-C7

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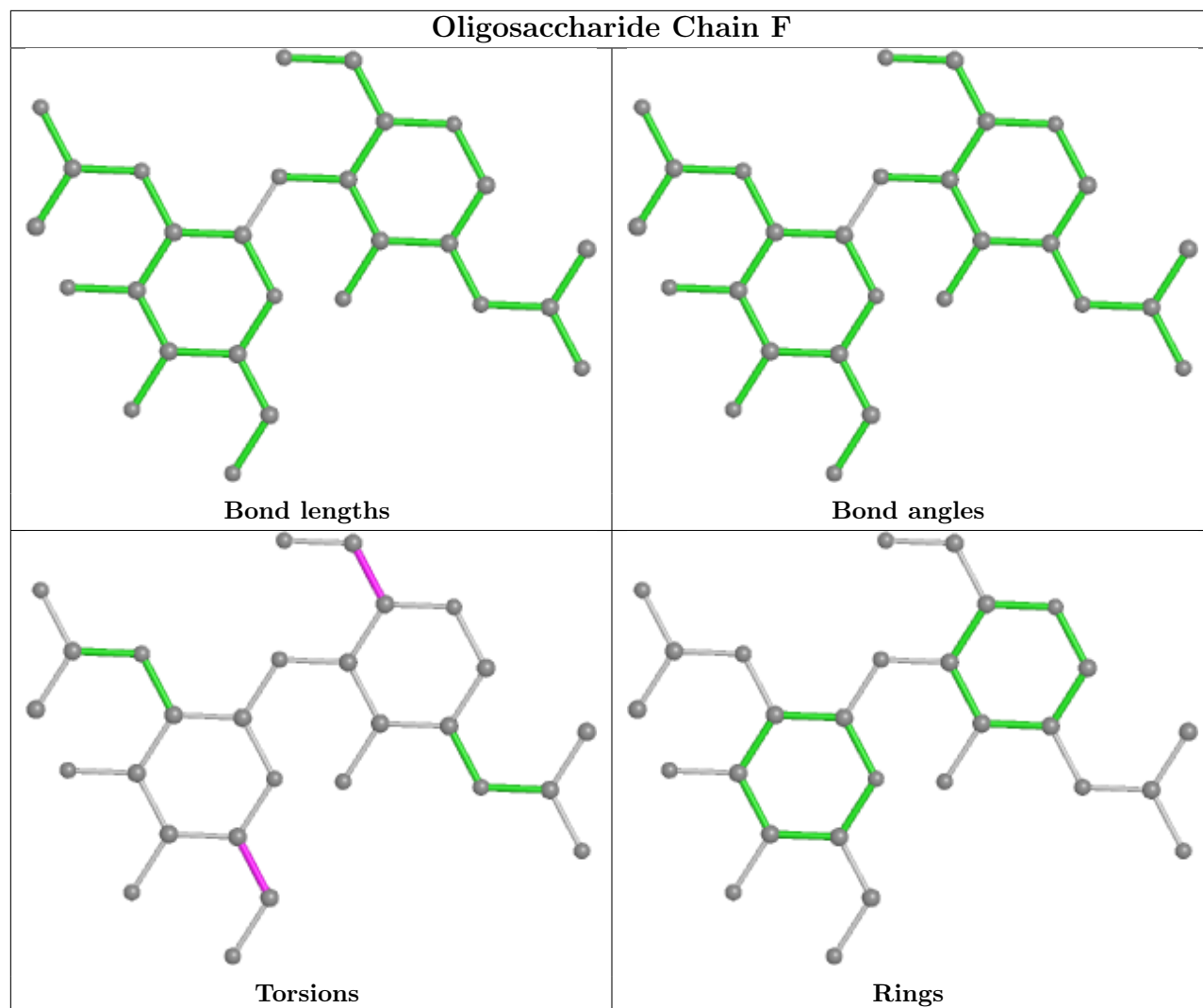
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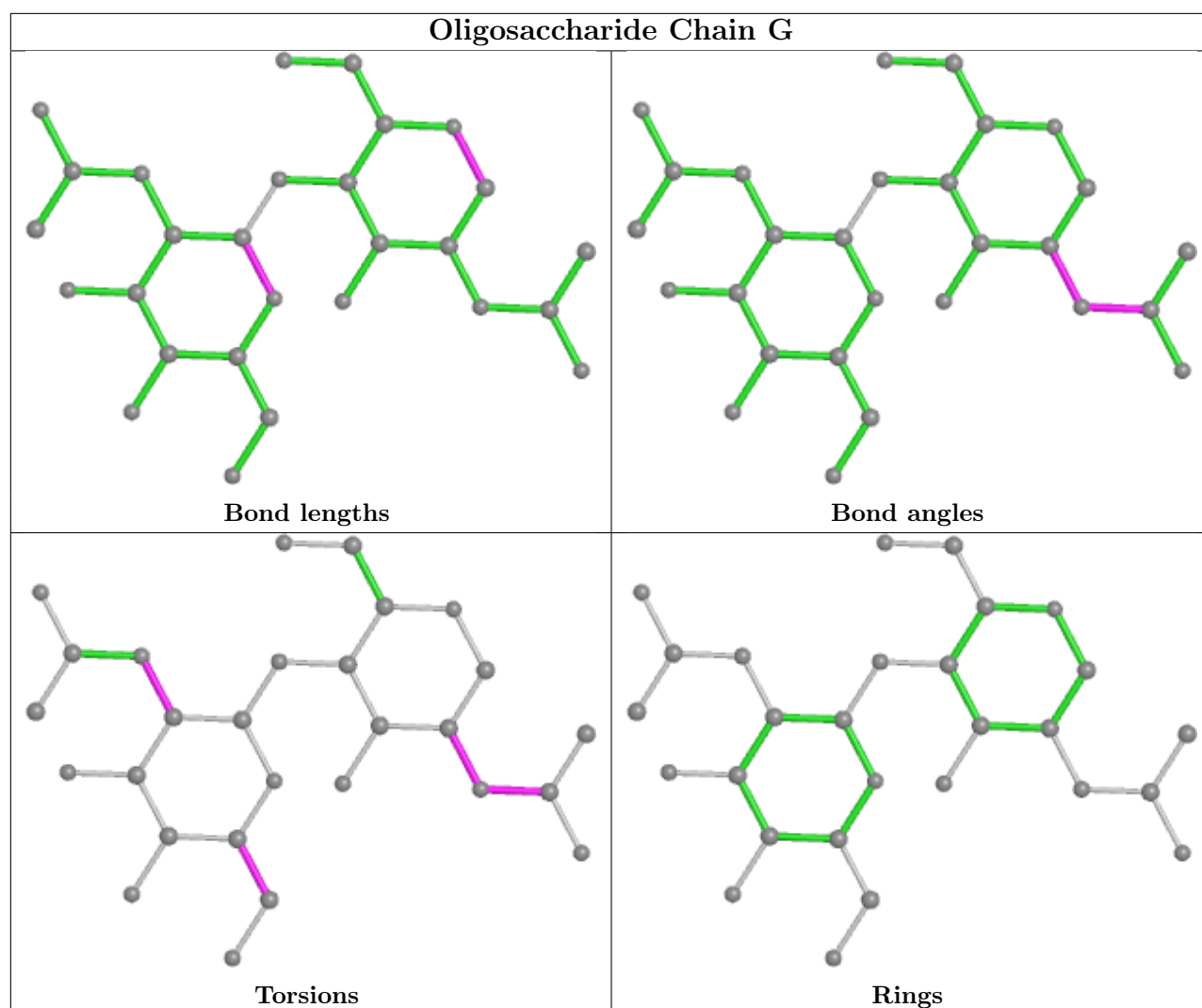
Mol	Chain	Res	Type	Atoms
4	g	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C1-C2-N2-C7
4	Y	1	NAG	O5-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	U	1	NAG	C3-C2-N2-C7
4	W	1	NAG	C3-C2-N2-C7
4	Z	1	NAG	C3-C2-N2-C7
4	j	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
4	h	2	NAG	C1-C2-N2-C7
4	e	2	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	R	2	NAG	C3-C2-N2-C7
4	V	1	NAG	C3-C2-N2-C7
4	h	2	NAG	C3-C2-N2-C7
4	V	1	NAG	C1-C2-N2-C7
4	a	1	NAG	C1-C2-N2-C7
4	j	2	NAG	C1-C2-N2-C7
4	f	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6

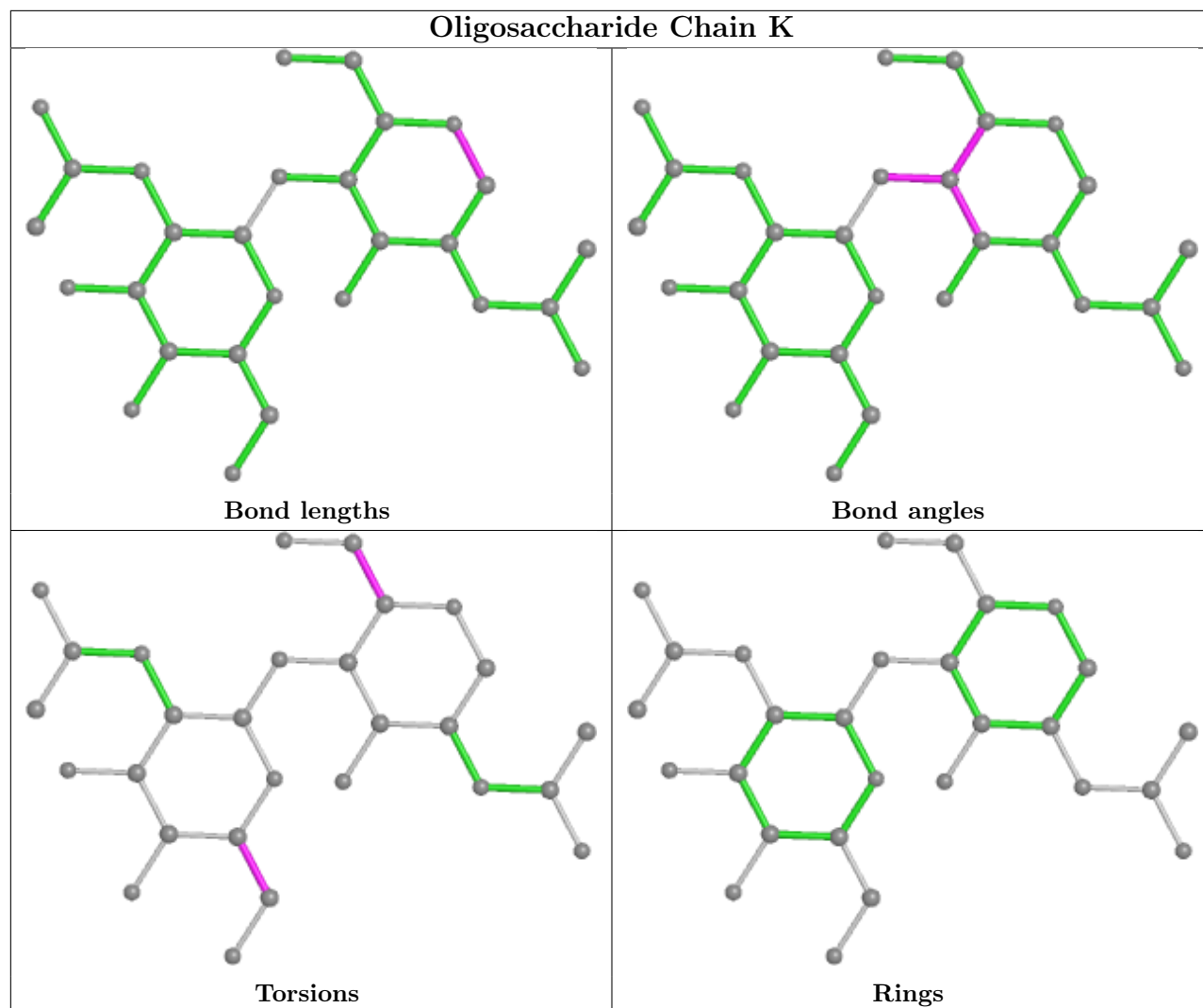
There are no ring outliers.

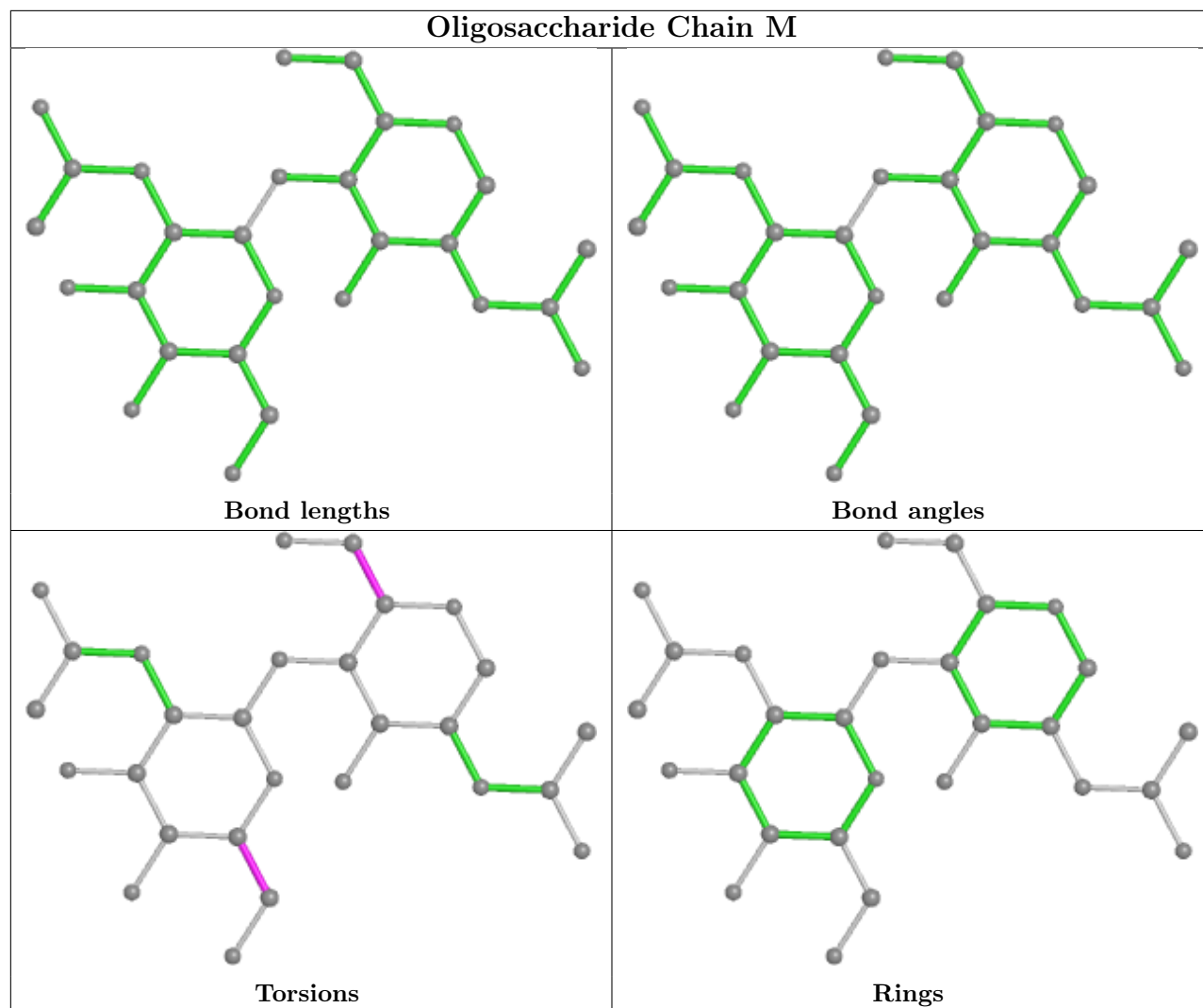
No monomer is involved in short contacts.

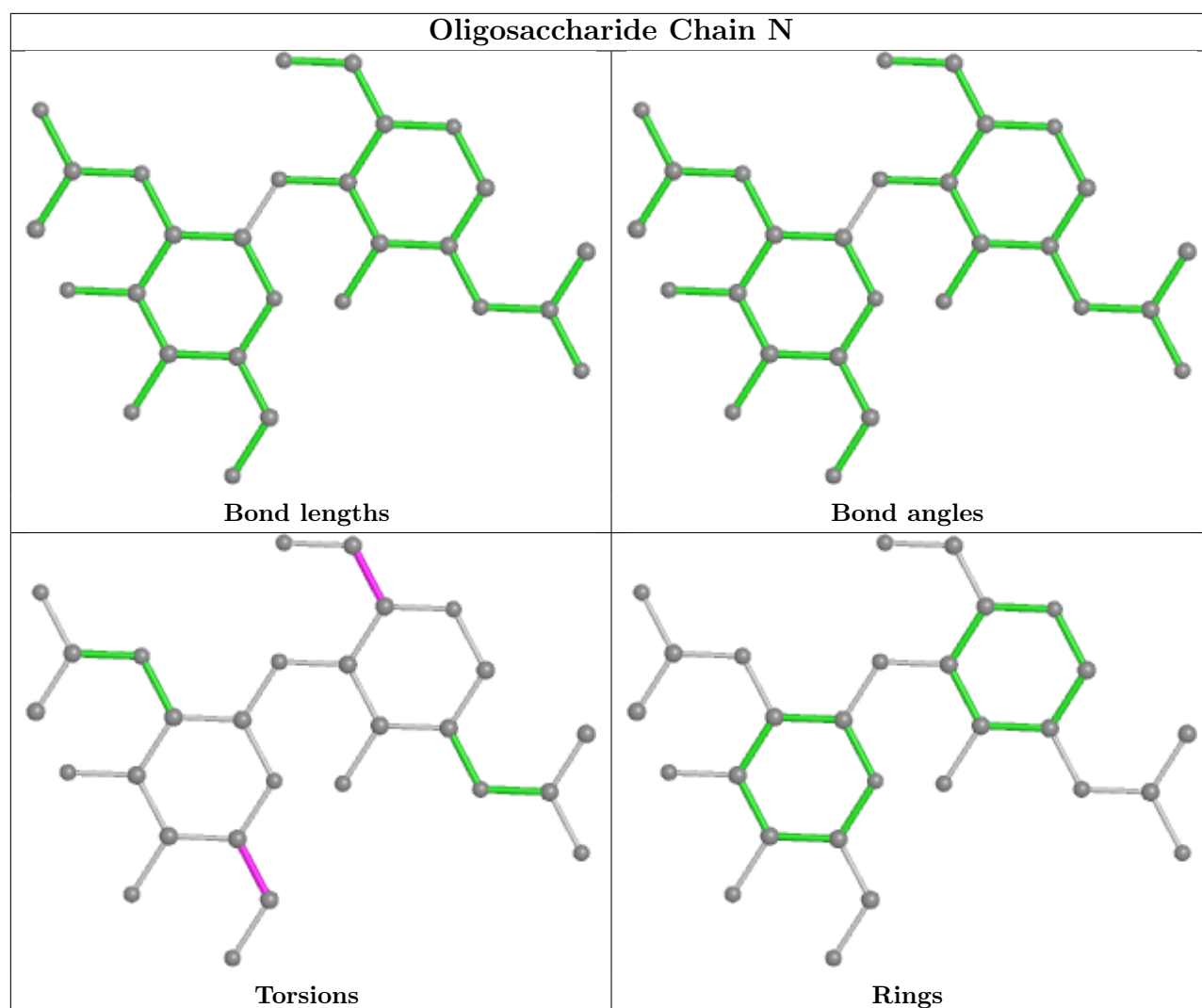
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

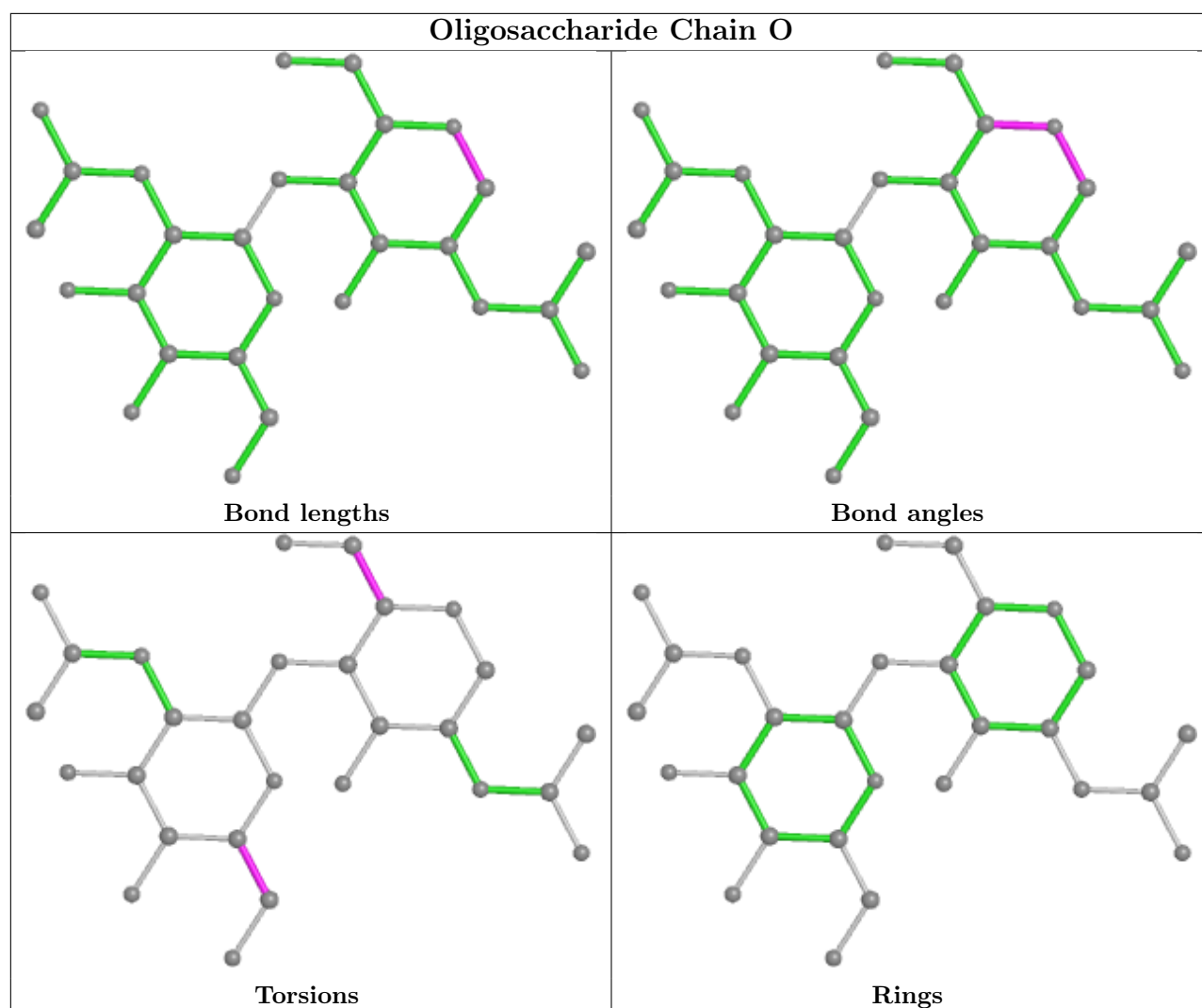


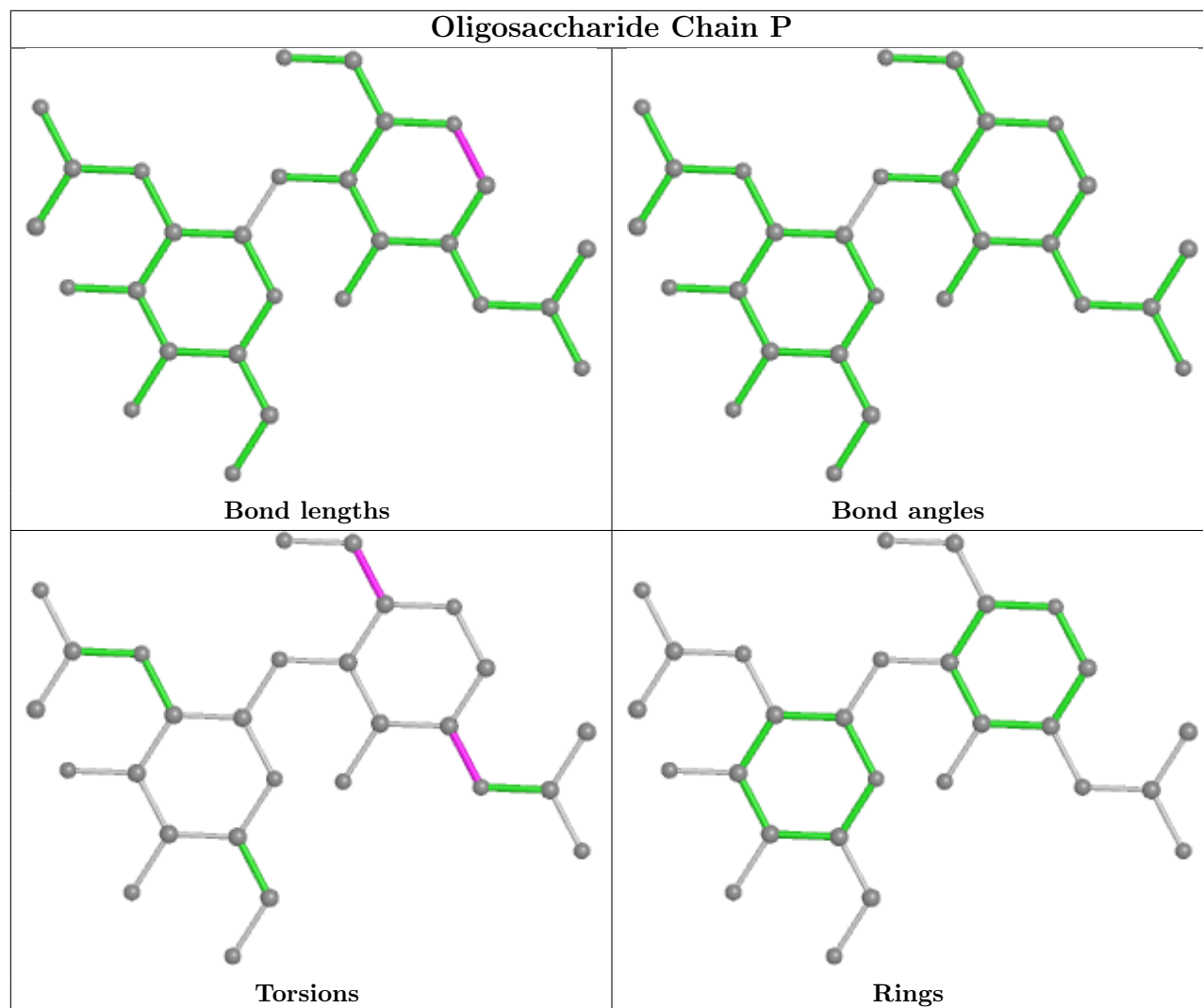


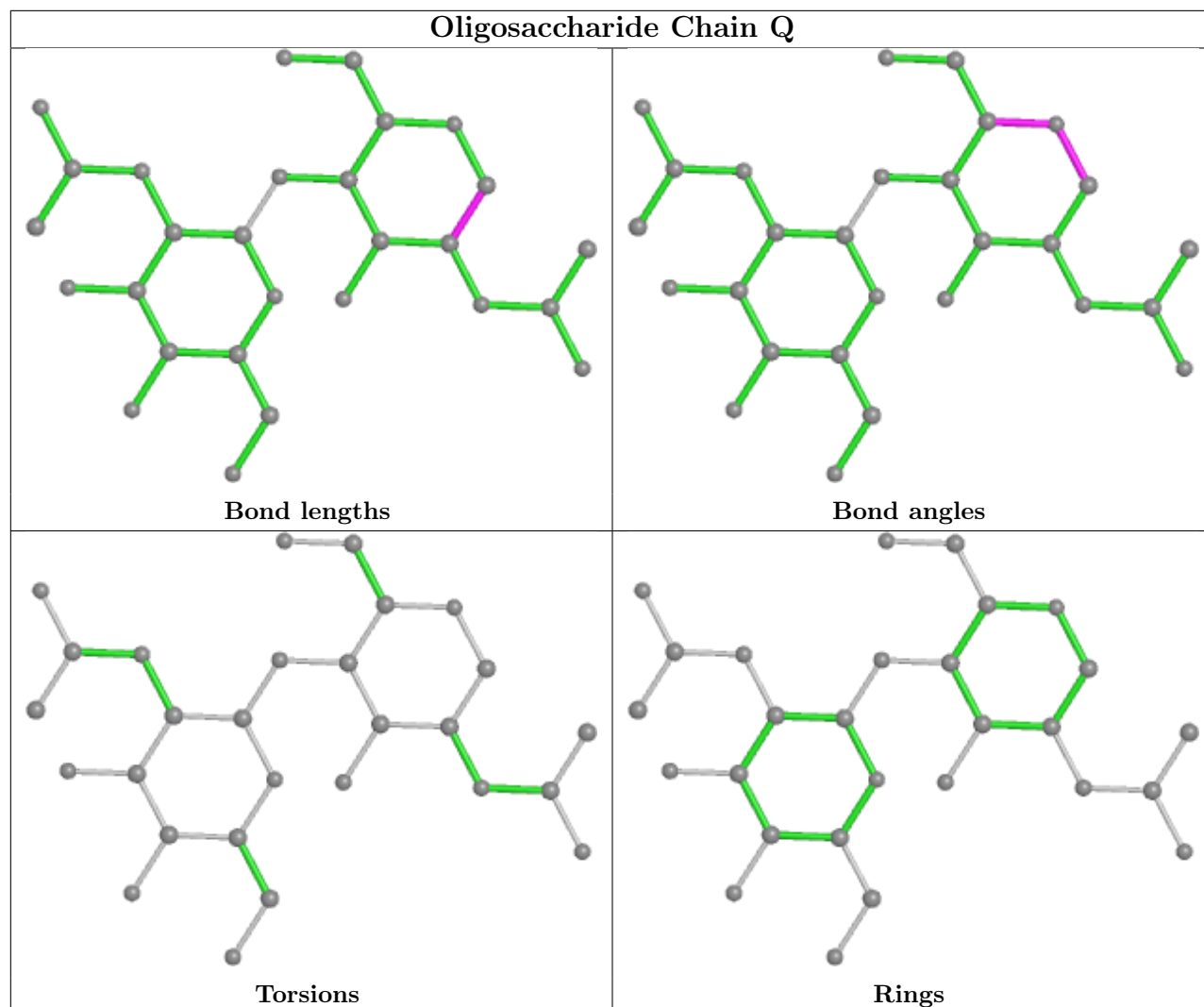


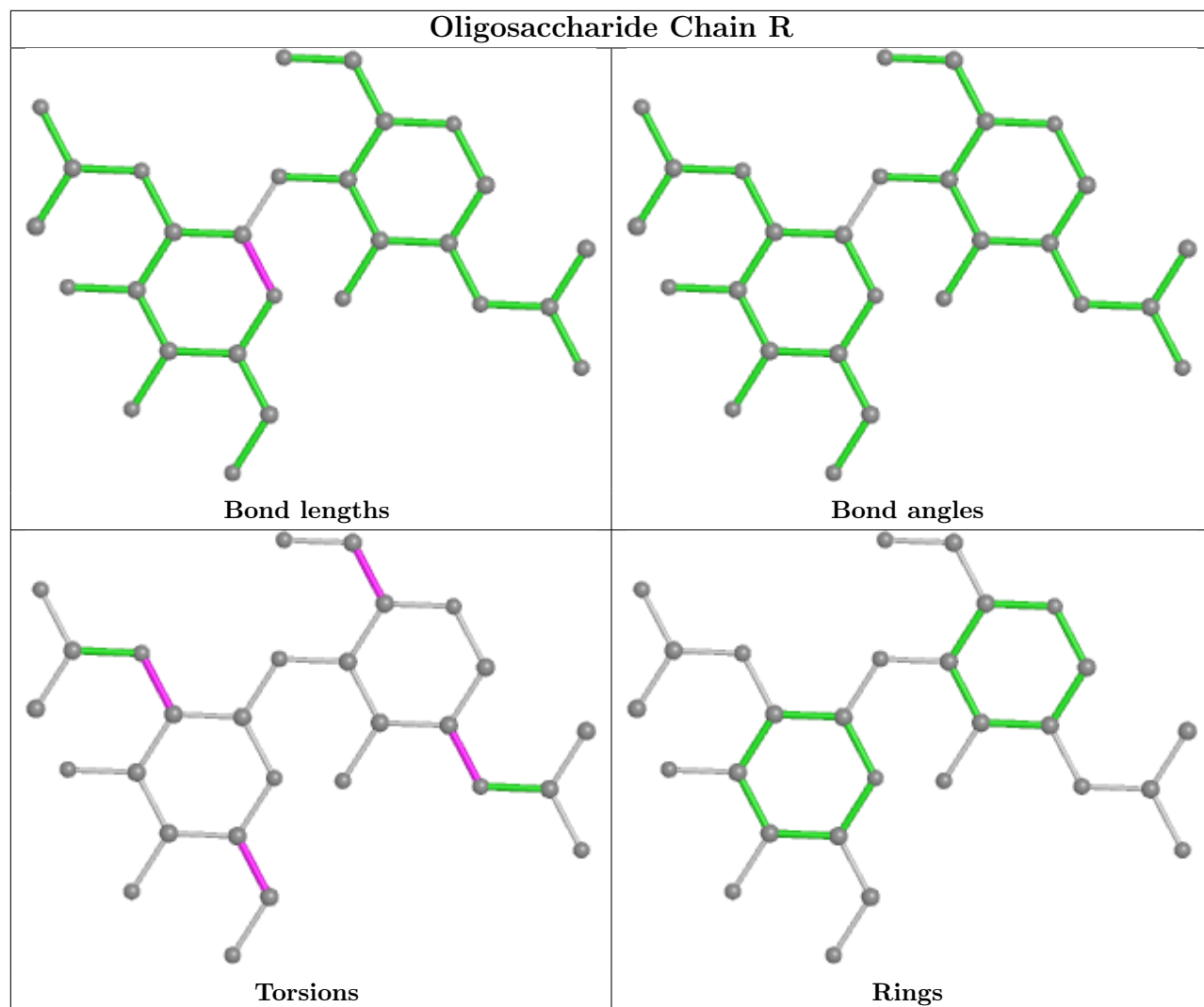


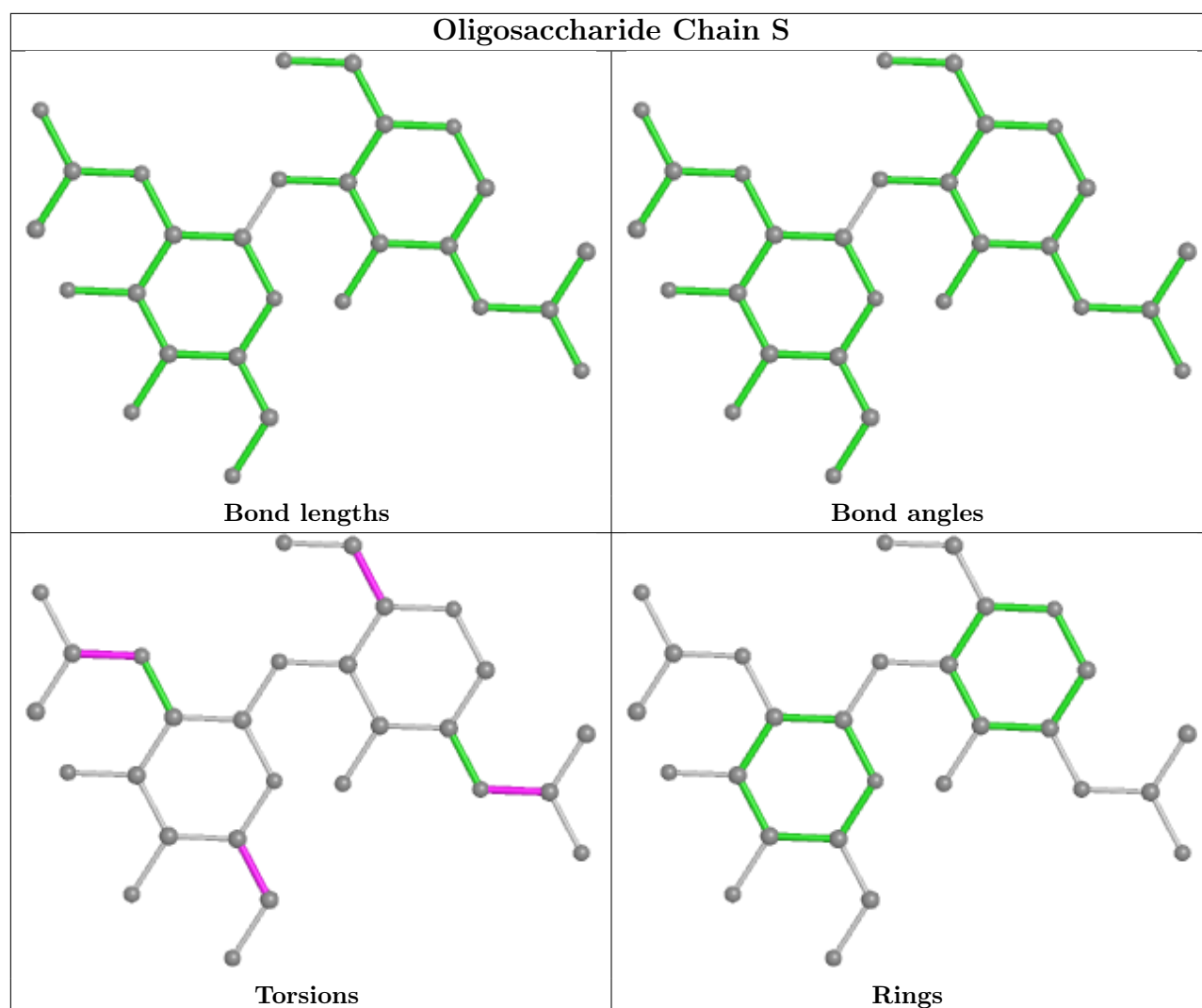


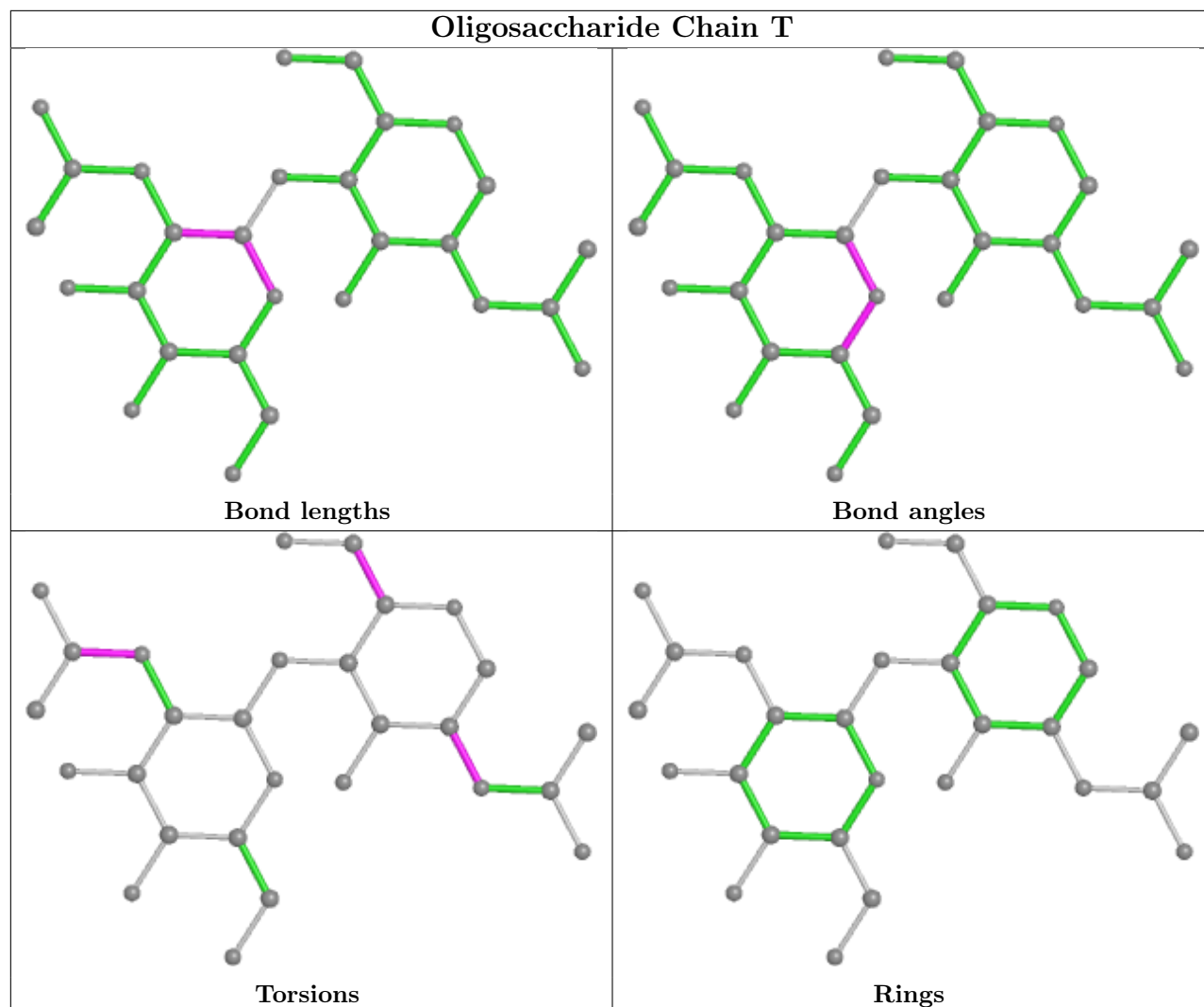


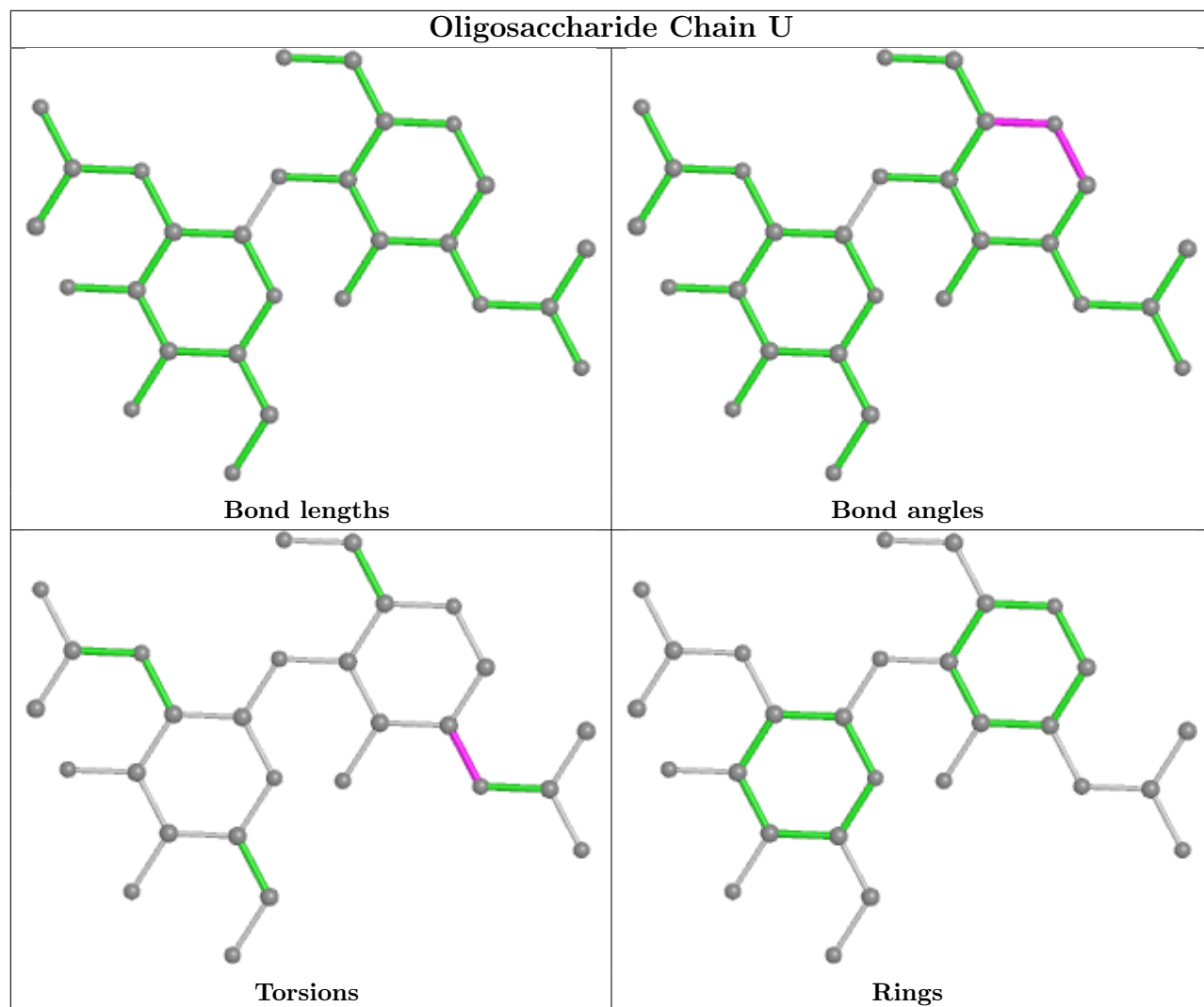


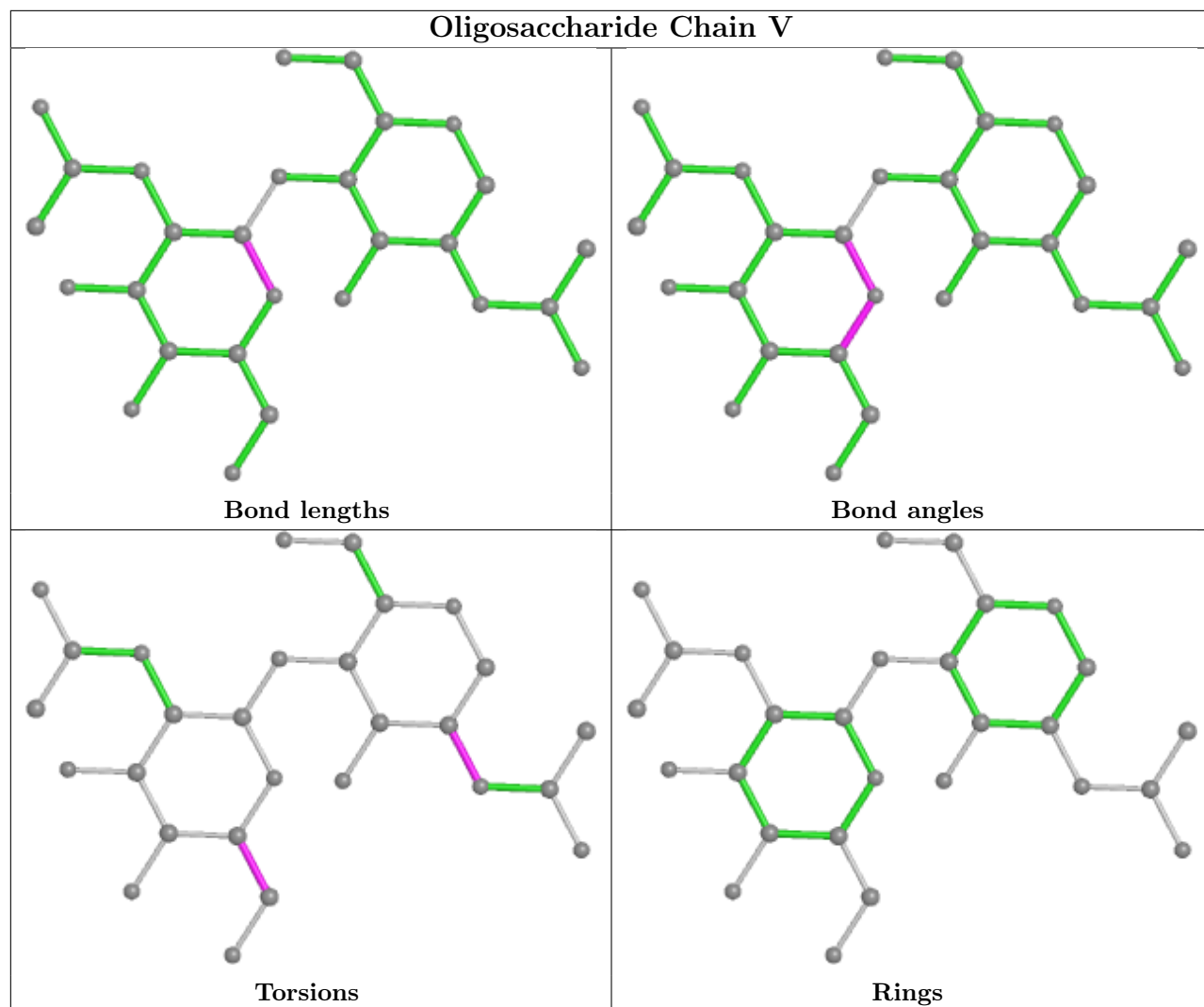


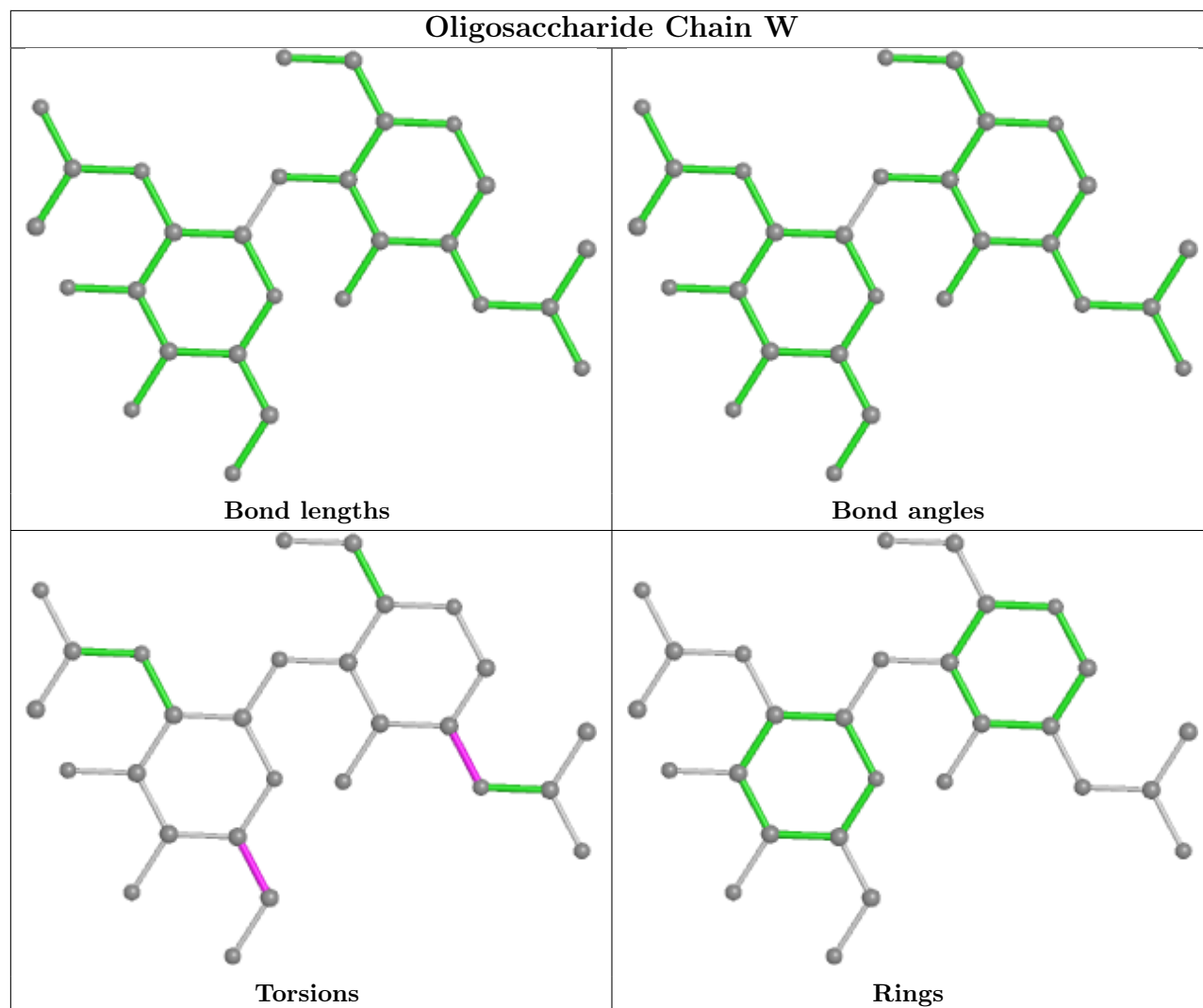


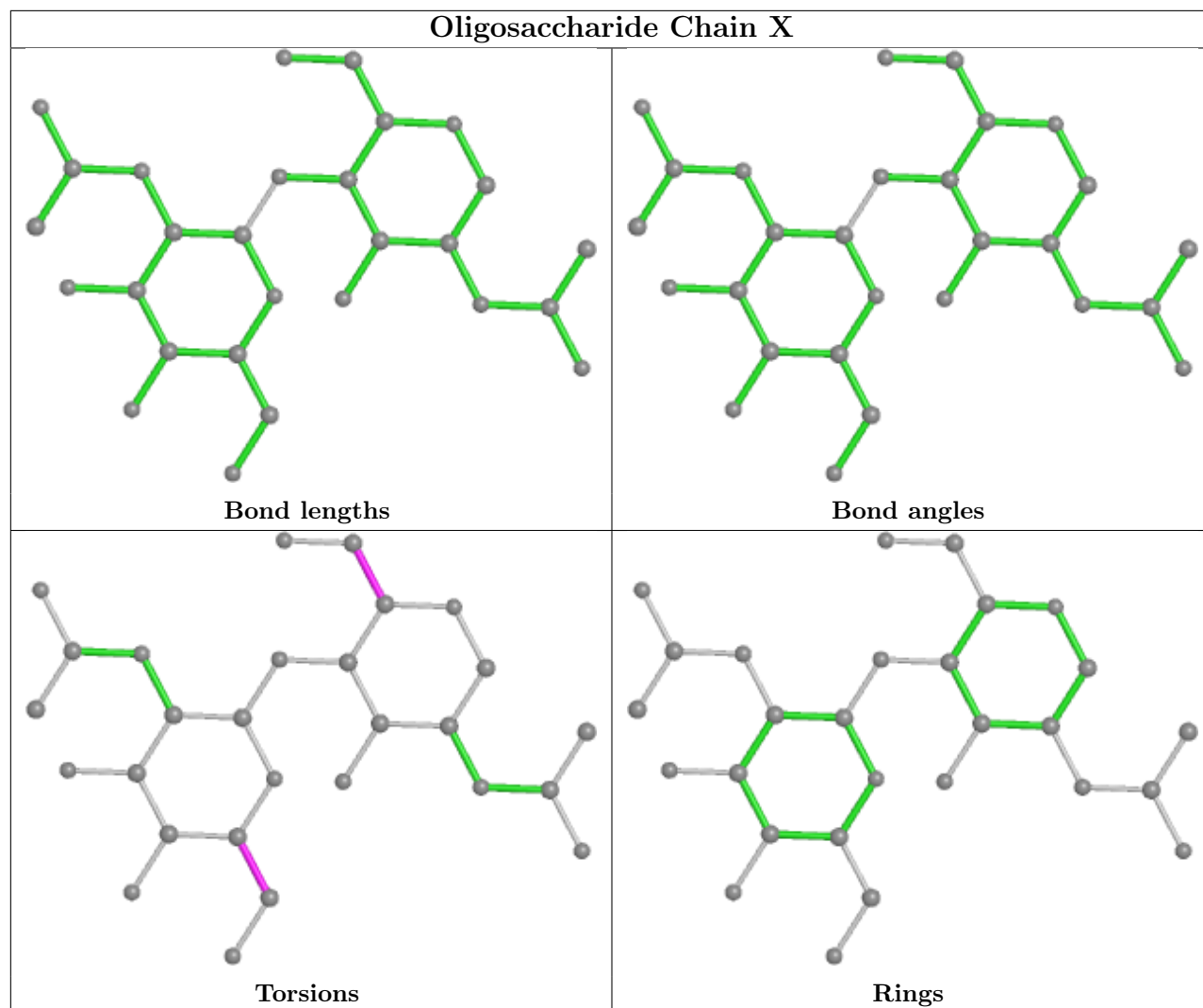


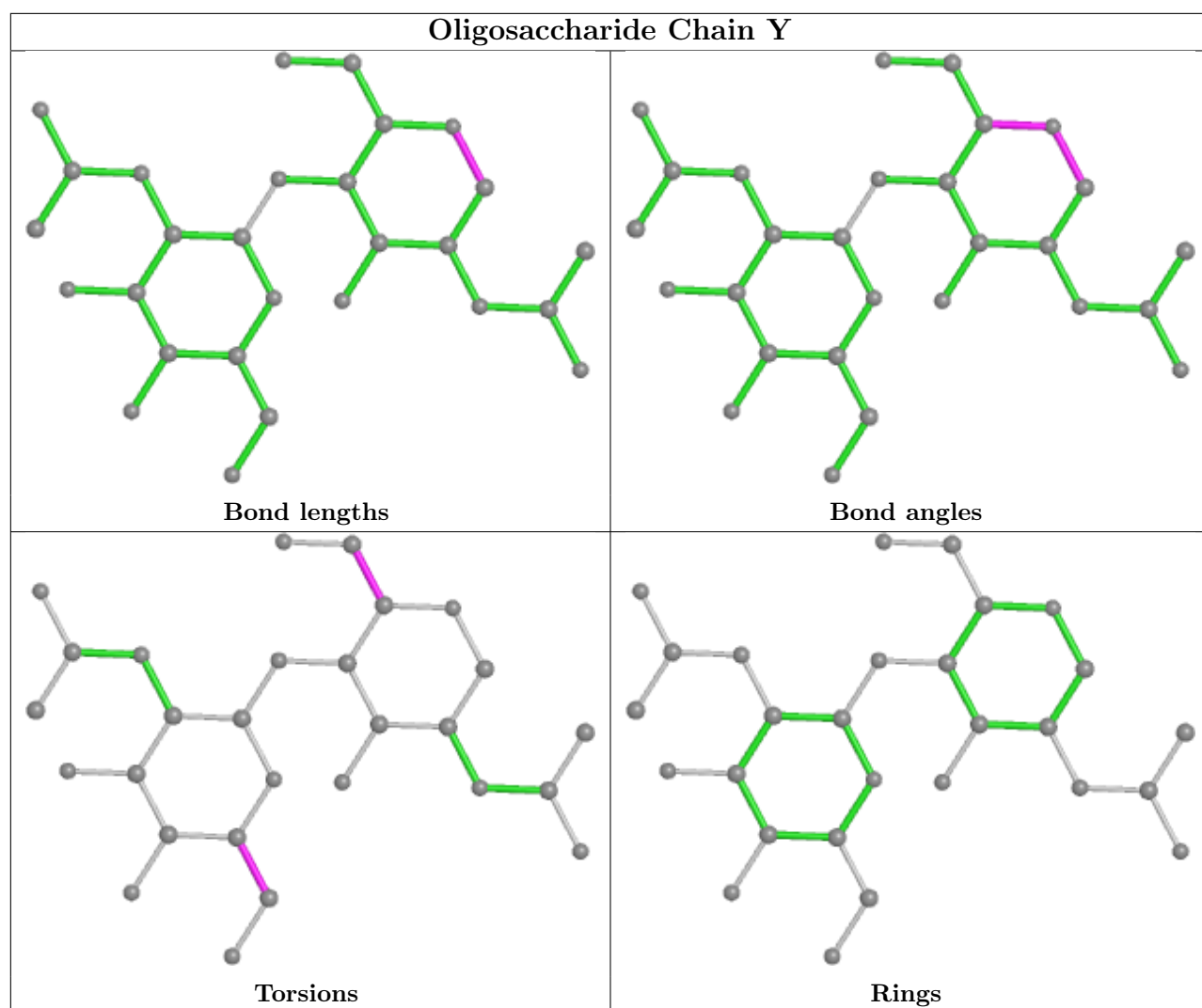


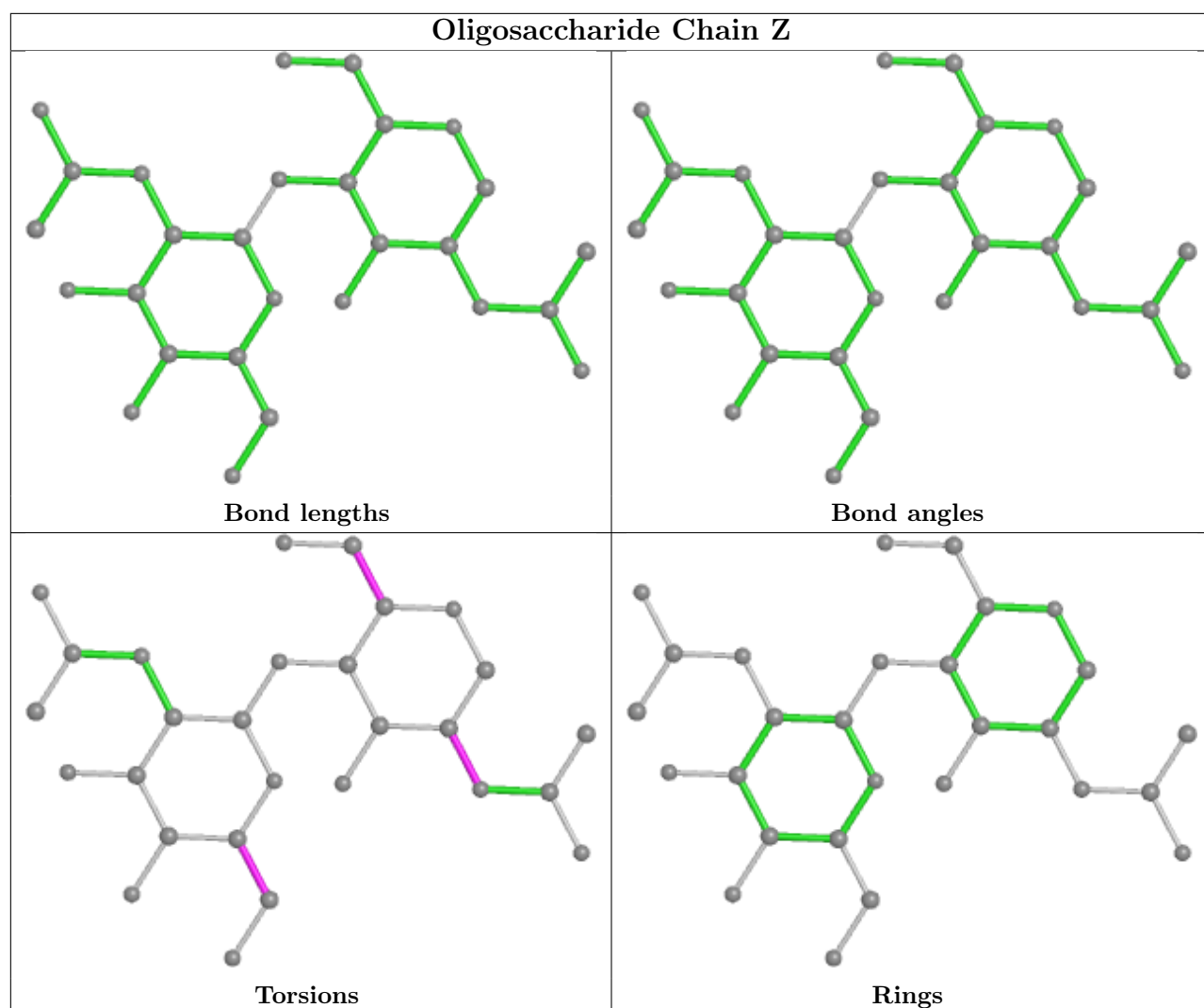


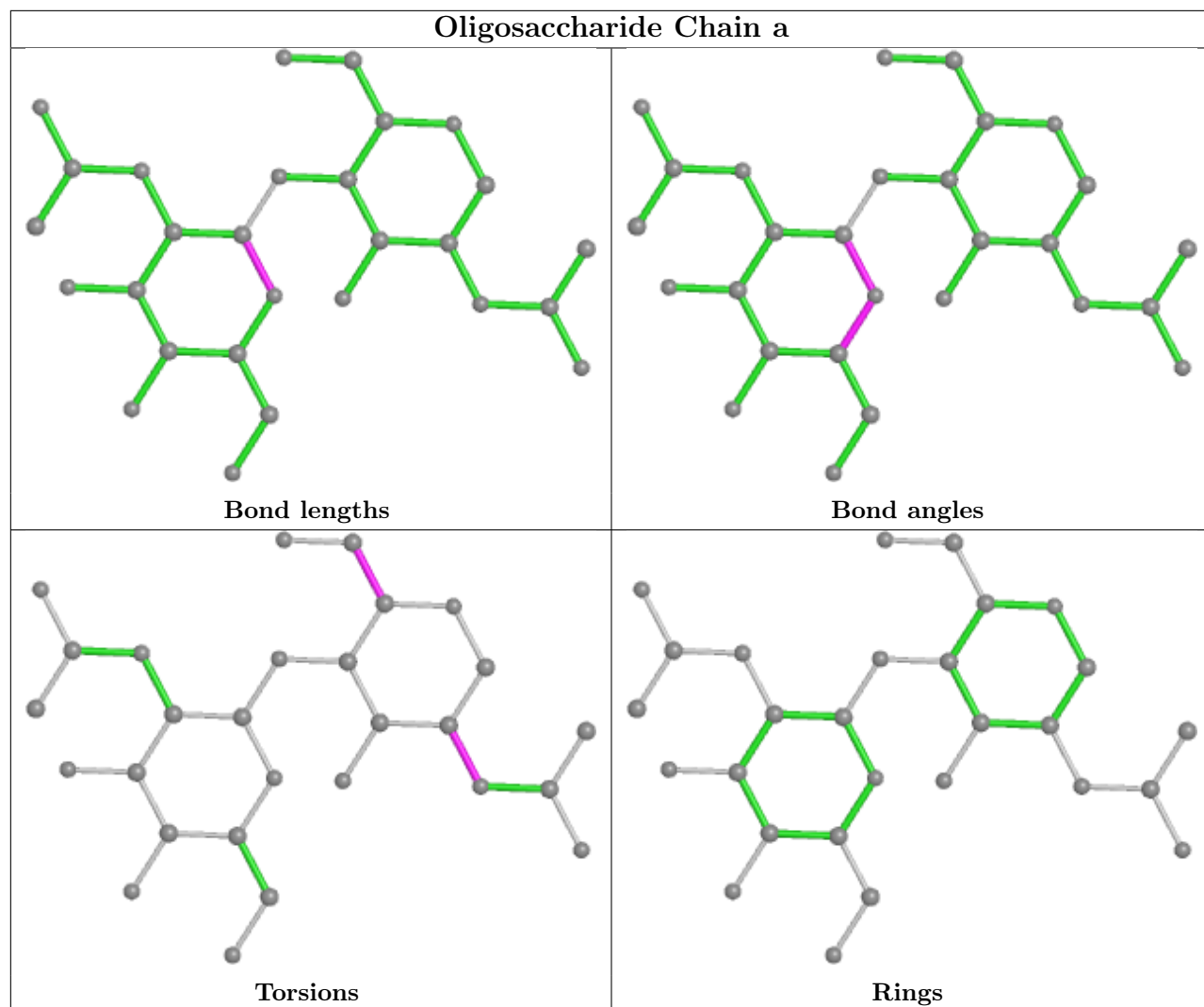


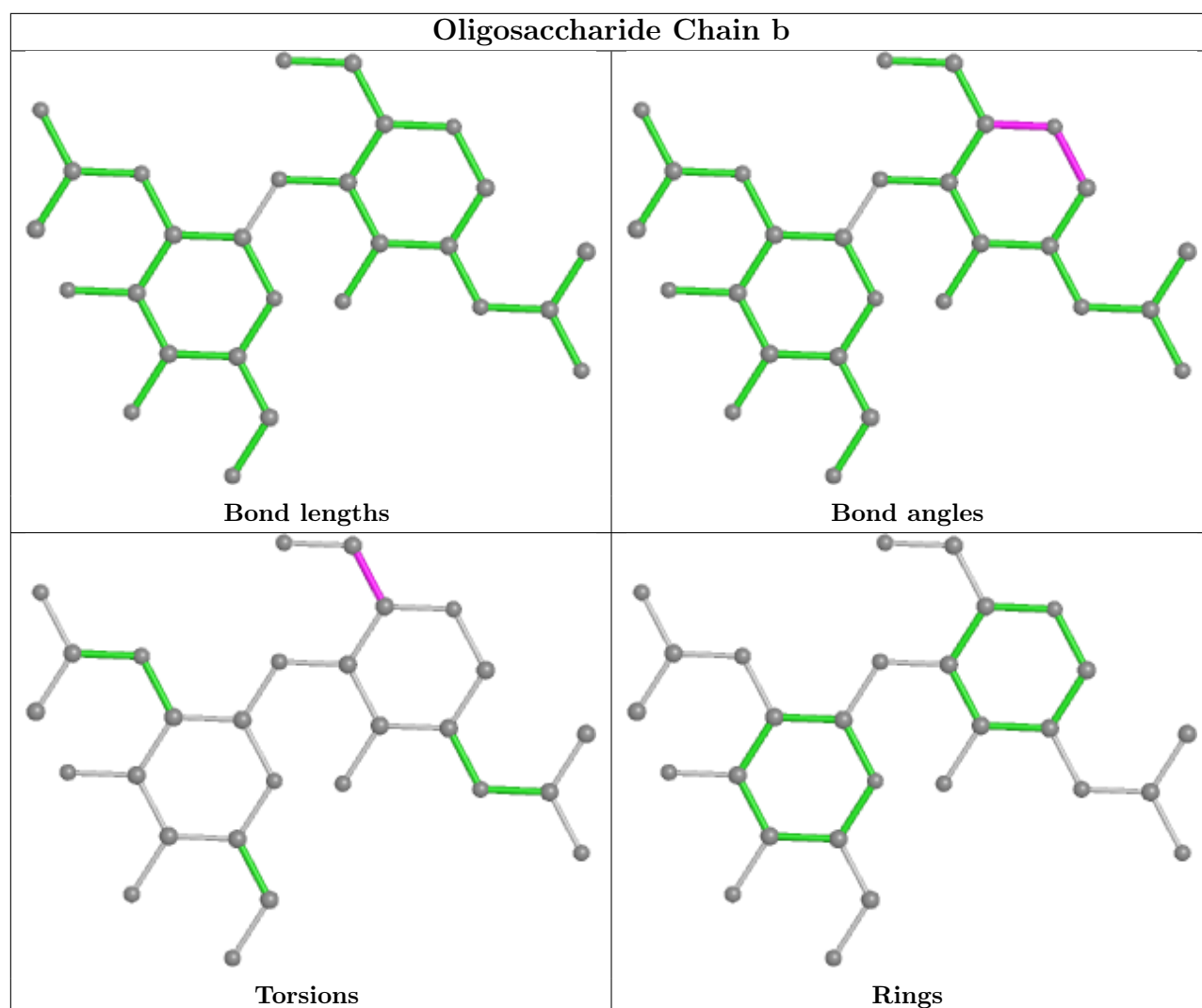


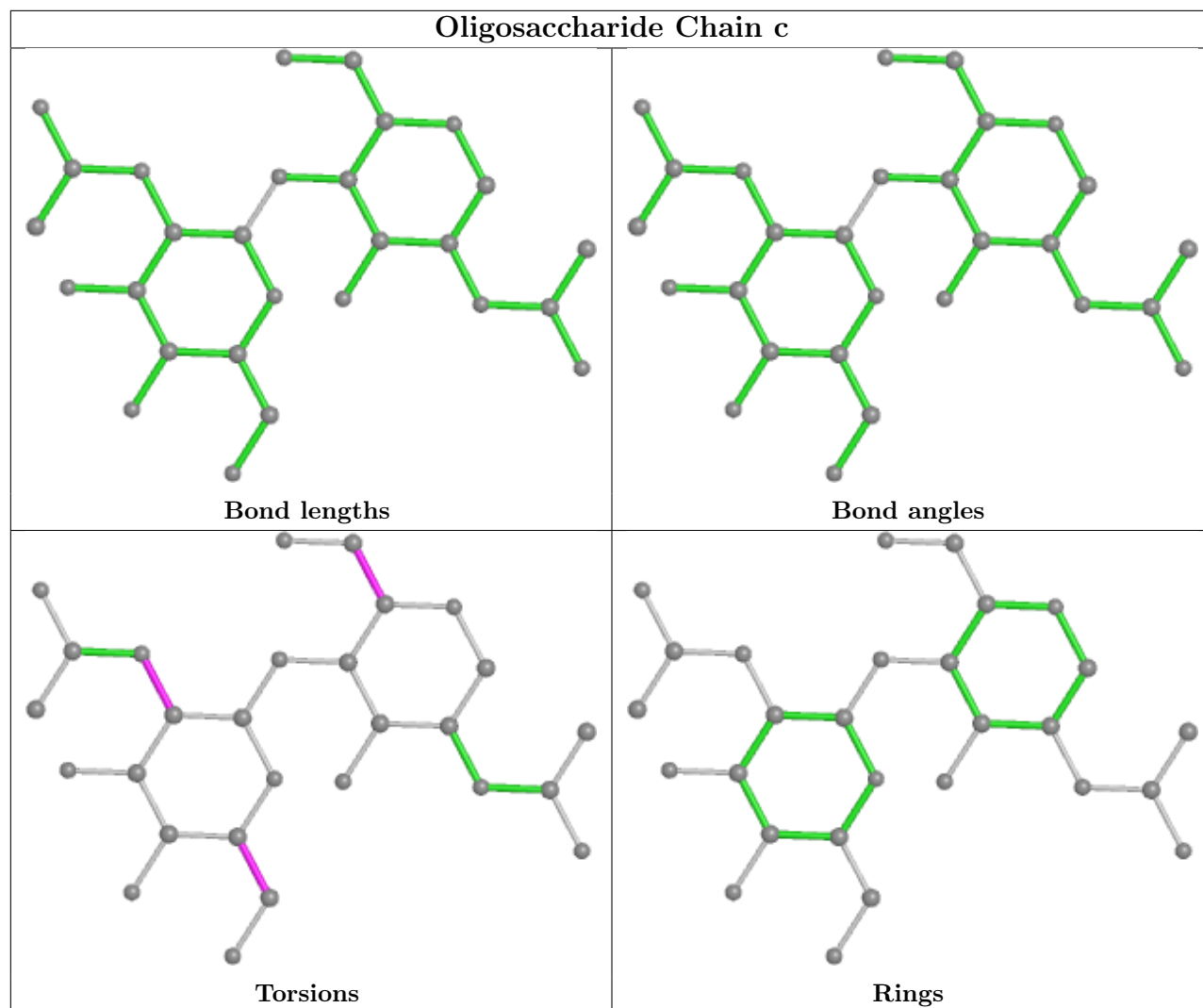


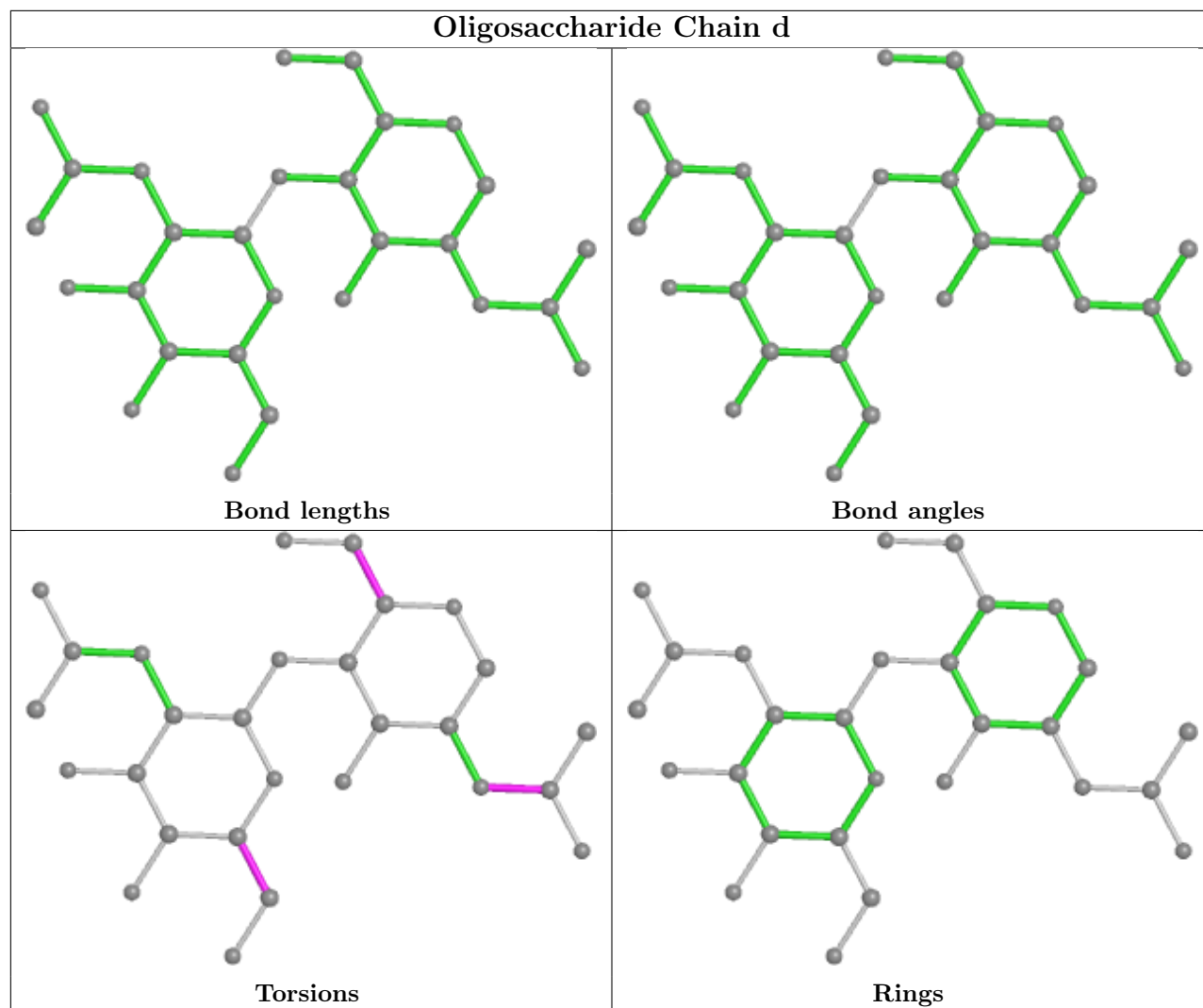


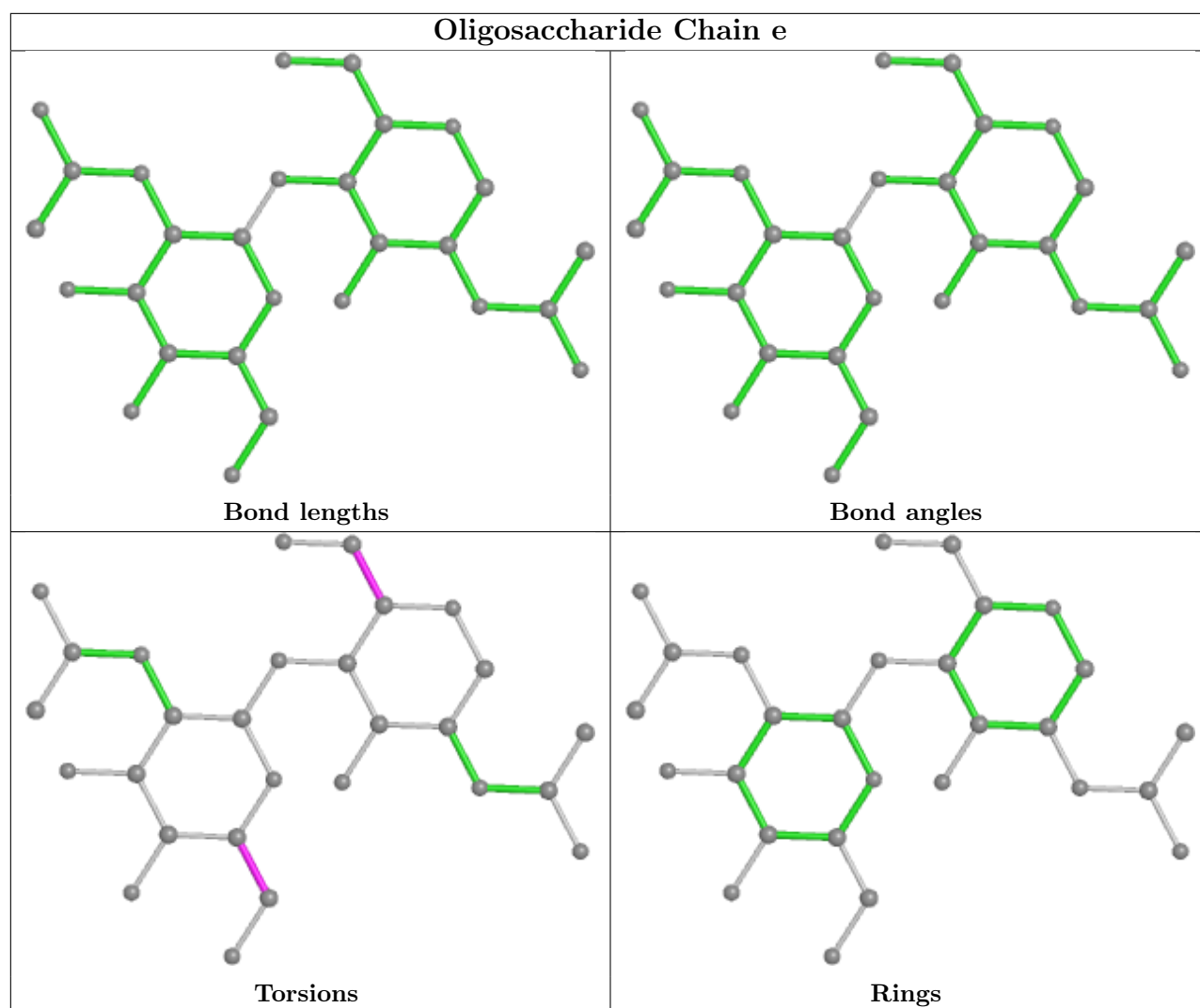


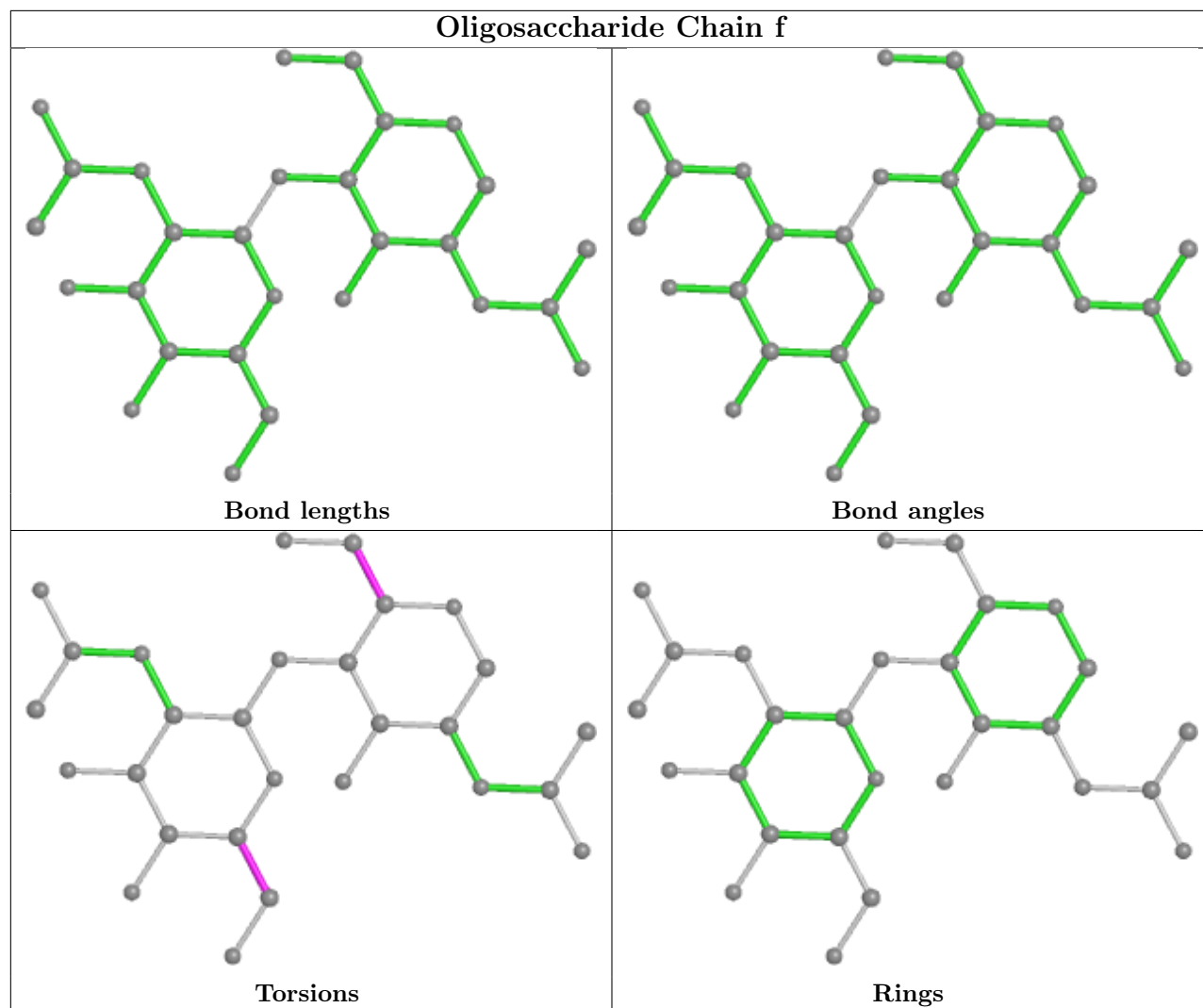


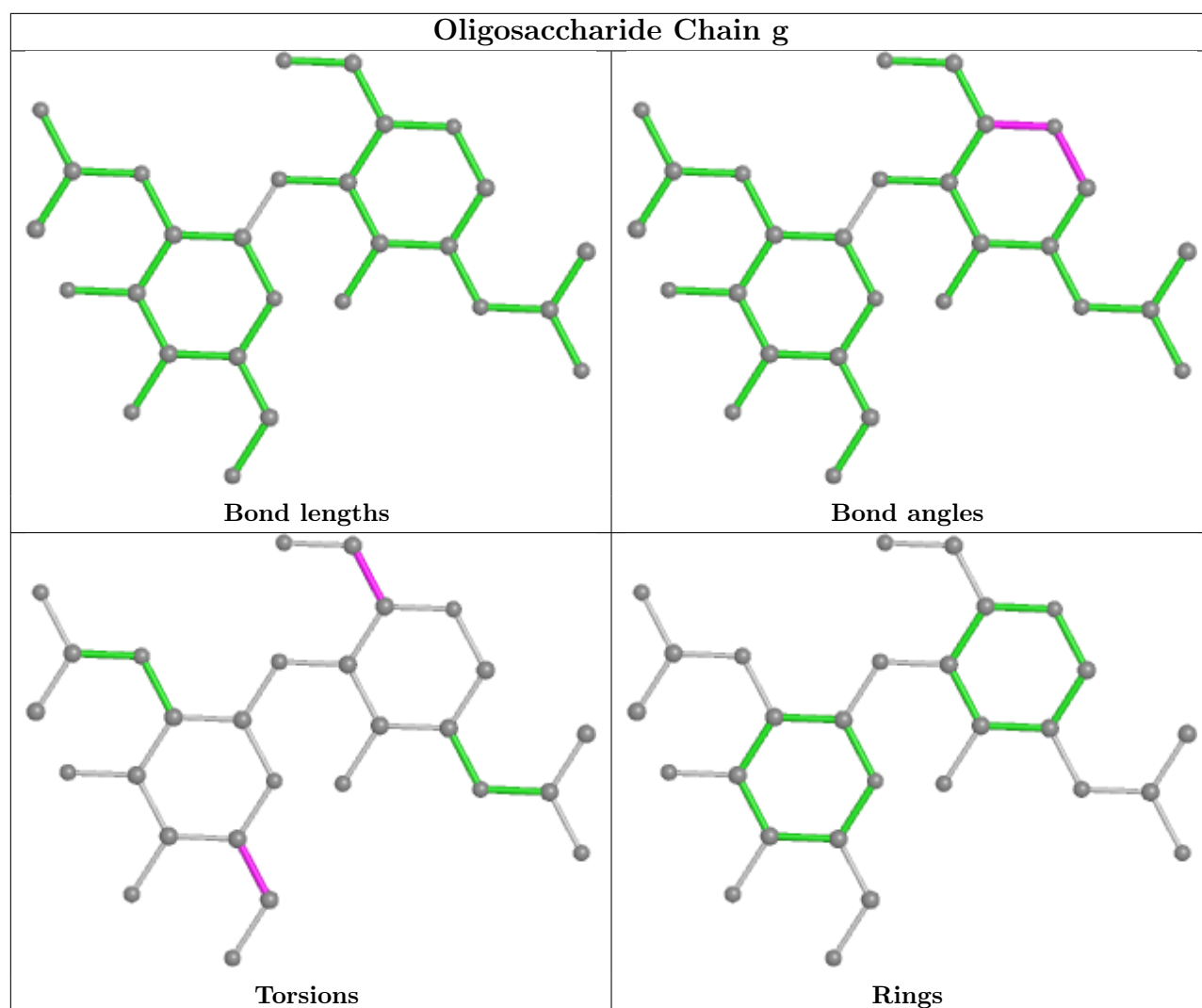


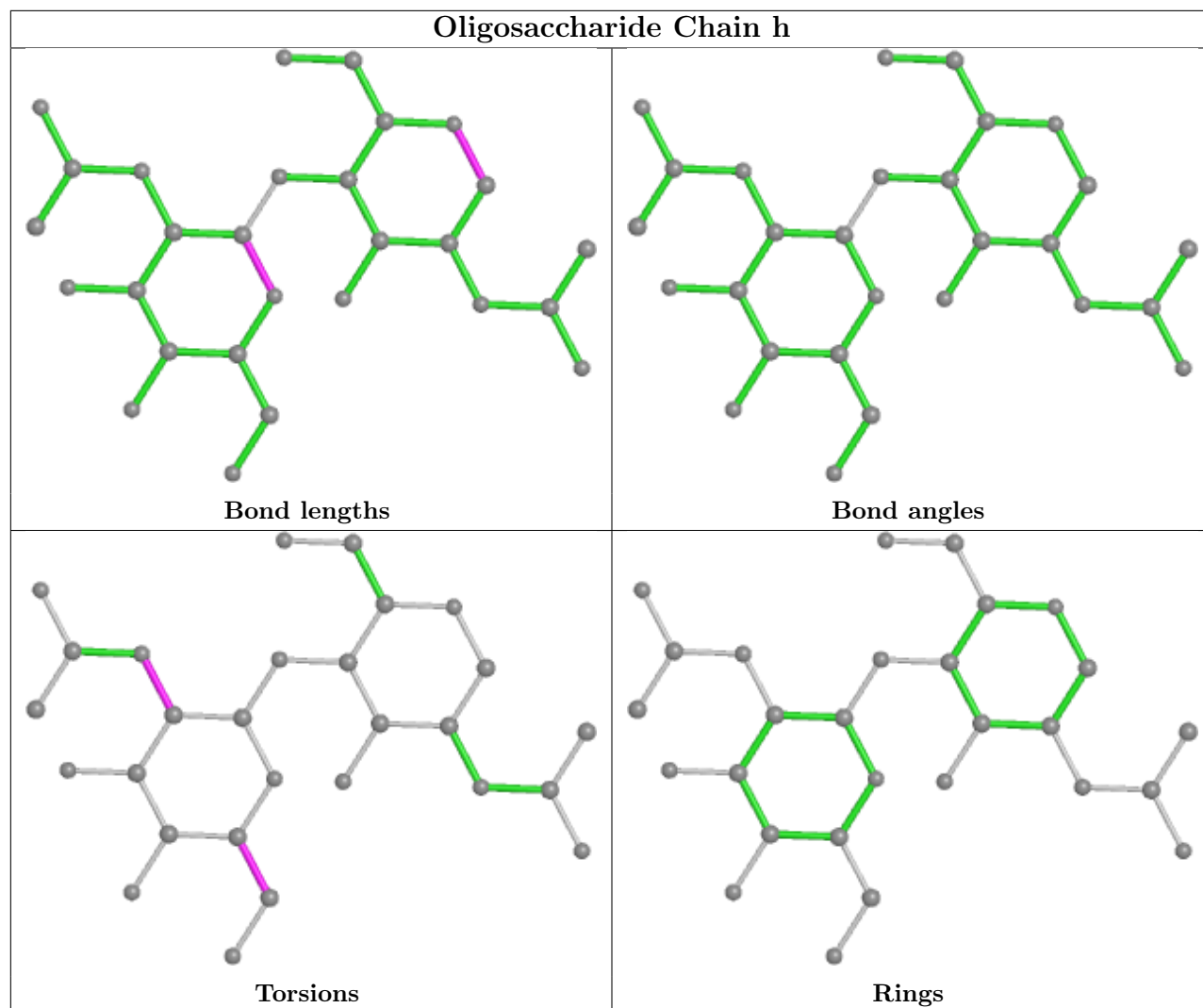


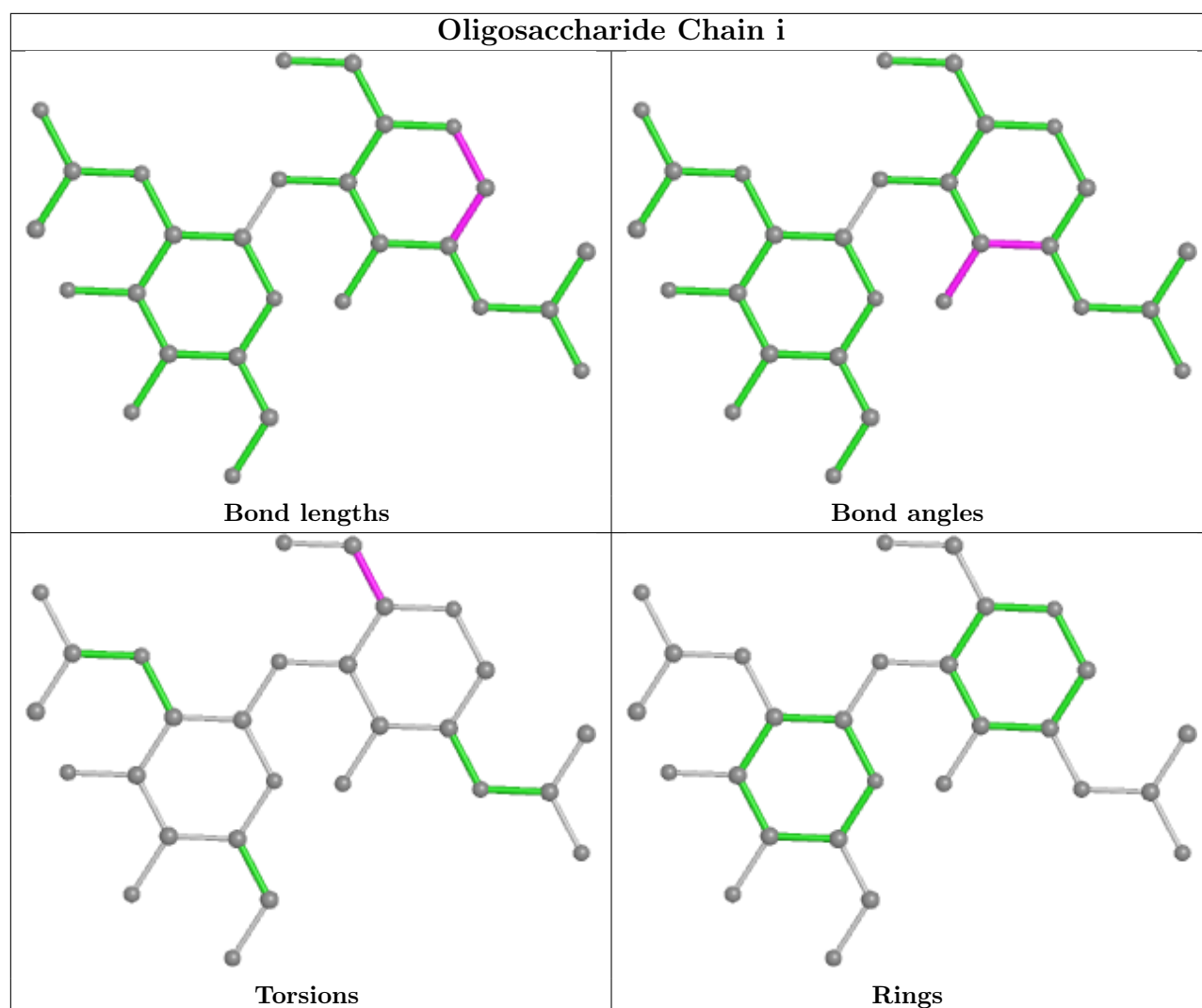


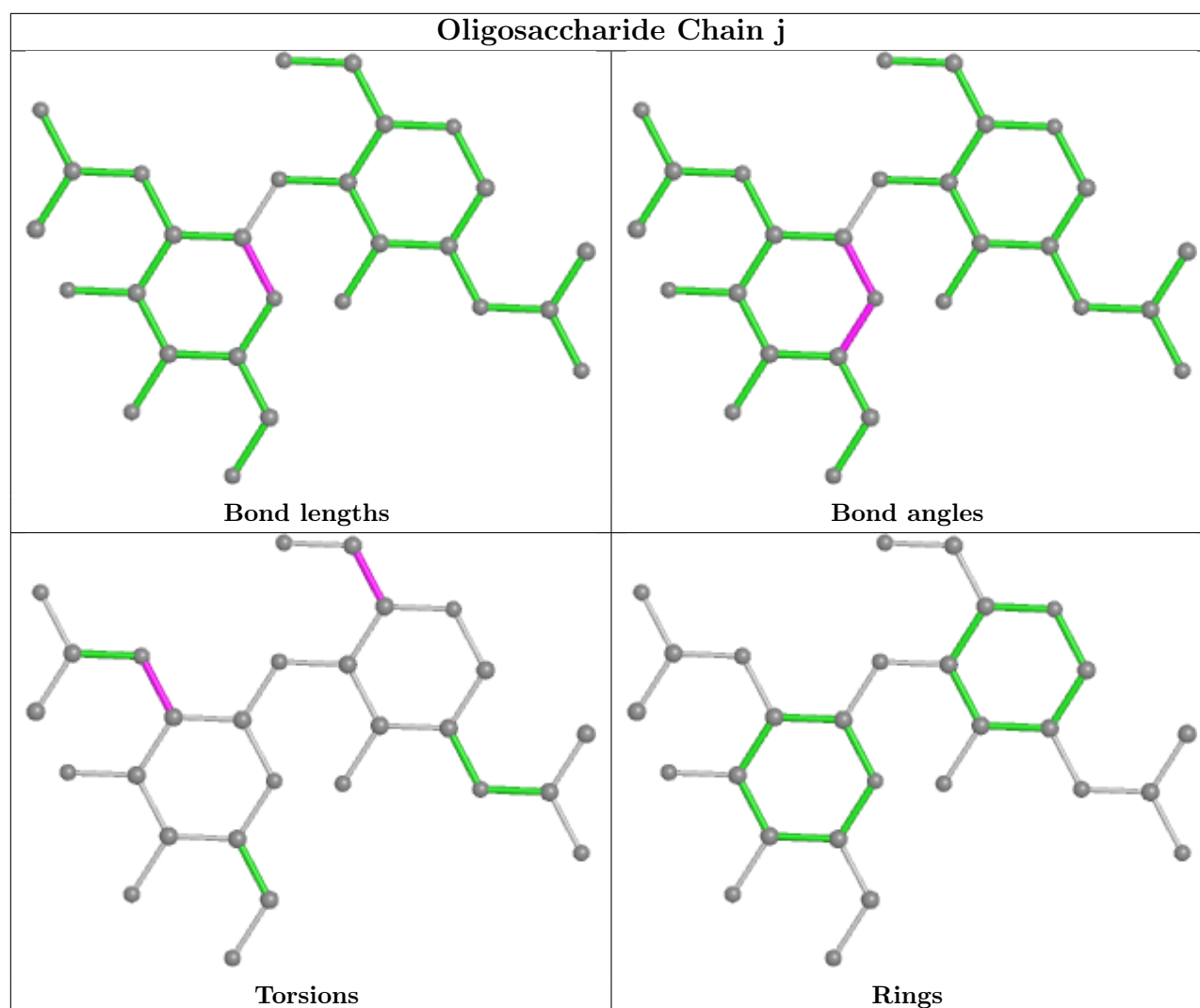












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	NAG	B	1304	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	B	1301	1	14,14,15	0.70	1 (7%)	17,19,21	0.59	0
5	NAG	C	1304	1	14,14,15	0.26	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1302	1	14,14,15	0.90	1 (7%)	17,19,21	1.20	1 (5%)
5	NAG	B	1303	1	14,14,15	0.45	0	17,19,21	1.32	1 (5%)
5	NAG	C	1305	1	14,14,15	0.30	0	17,19,21	0.34	0
5	NAG	C	1301	1	14,14,15	0.35	0	17,19,21	0.40	0
5	NAG	A	1304	1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
5	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	B	1306	1	14,14,15	1.07	1 (7%)	17,19,21	1.12	1 (5%)
5	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	1.24	1 (5%)
5	NAG	C	1302	1	14,14,15	0.93	1 (7%)	17,19,21	1.09	1 (5%)
5	NAG	B	1307	1	14,14,15	0.82	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	B	1305	1	14,14,15	0.35	0	17,19,21	0.39	0
5	NAG	A	1302	1	14,14,15	0.60	0	17,19,21	0.69	0
5	NAG	C	1306	1	14,14,15	0.49	0	17,19,21	0.51	0
5	NAG	C	1303	1	14,14,15	0.33	0	17,19,21	0.37	0
5	NAG	A	1305	1	14,14,15	0.55	0	17,19,21	0.88	0
5	NAG	A	1306	-	14,14,15	0.24	0	17,19,21	0.52	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
5	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1306	-	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1306	NAG	O5-C1	3.84	1.49	1.43
5	C	1302	NAG	O5-C1	3.20	1.48	1.43
5	B	1302	NAG	O5-C1	3.17	1.48	1.43
5	B	1301	NAG	C1-C2	2.47	1.56	1.52
5	B	1307	NAG	O5-C1	2.39	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1303	NAG	C1-O5-C5	4.92	118.86	112.19
5	A	1303	NAG	C1-O5-C5	4.71	118.57	112.19
5	B	1302	NAG	C1-O5-C5	4.70	118.56	112.19
5	B	1306	NAG	C1-O5-C5	4.21	117.90	112.19
5	C	1302	NAG	C1-O5-C5	4.20	117.89	112.19
5	B	1307	NAG	C1-O5-C5	3.80	117.34	112.19
5	A	1304	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1302	NAG	C4-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	B	1303	NAG	C8-C7-N2-C2
5	B	1303	NAG	O7-C7-N2-C2

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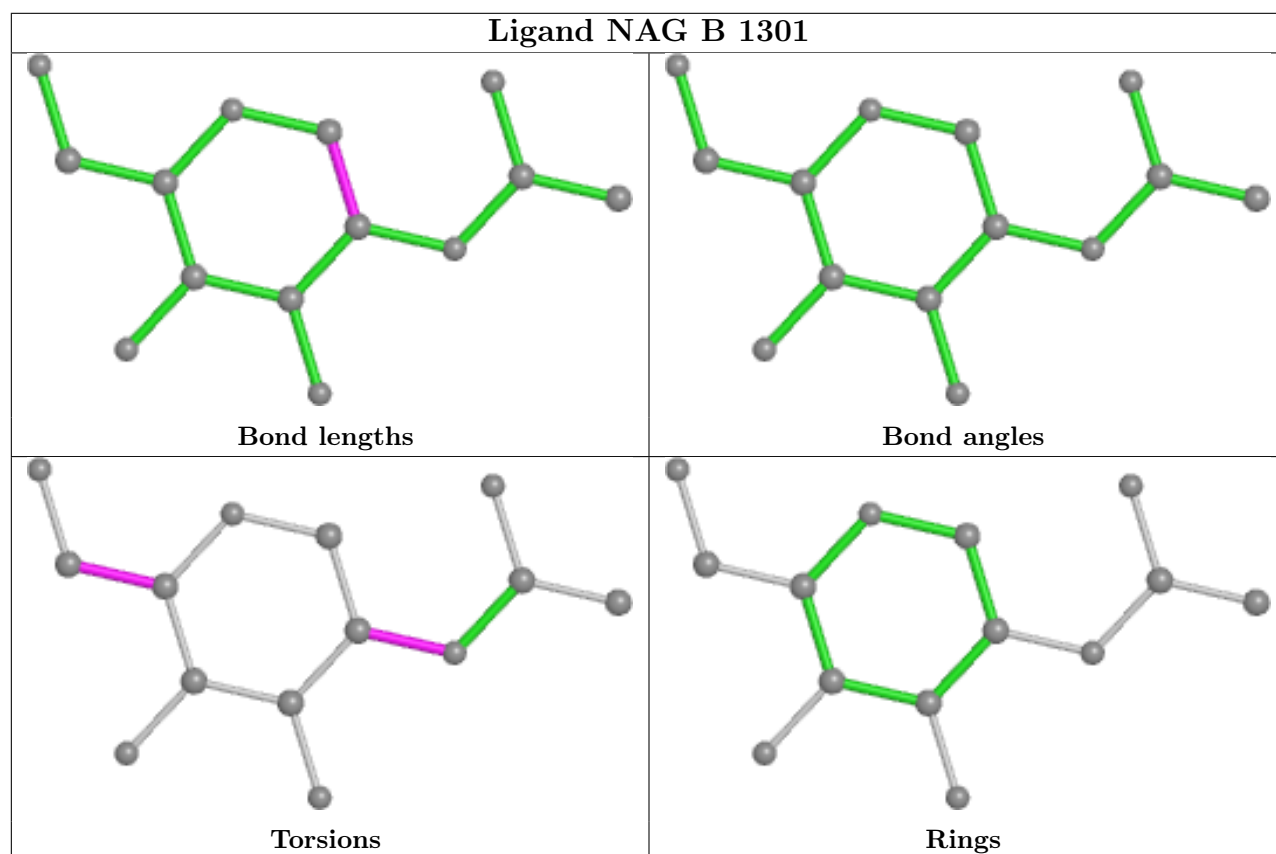
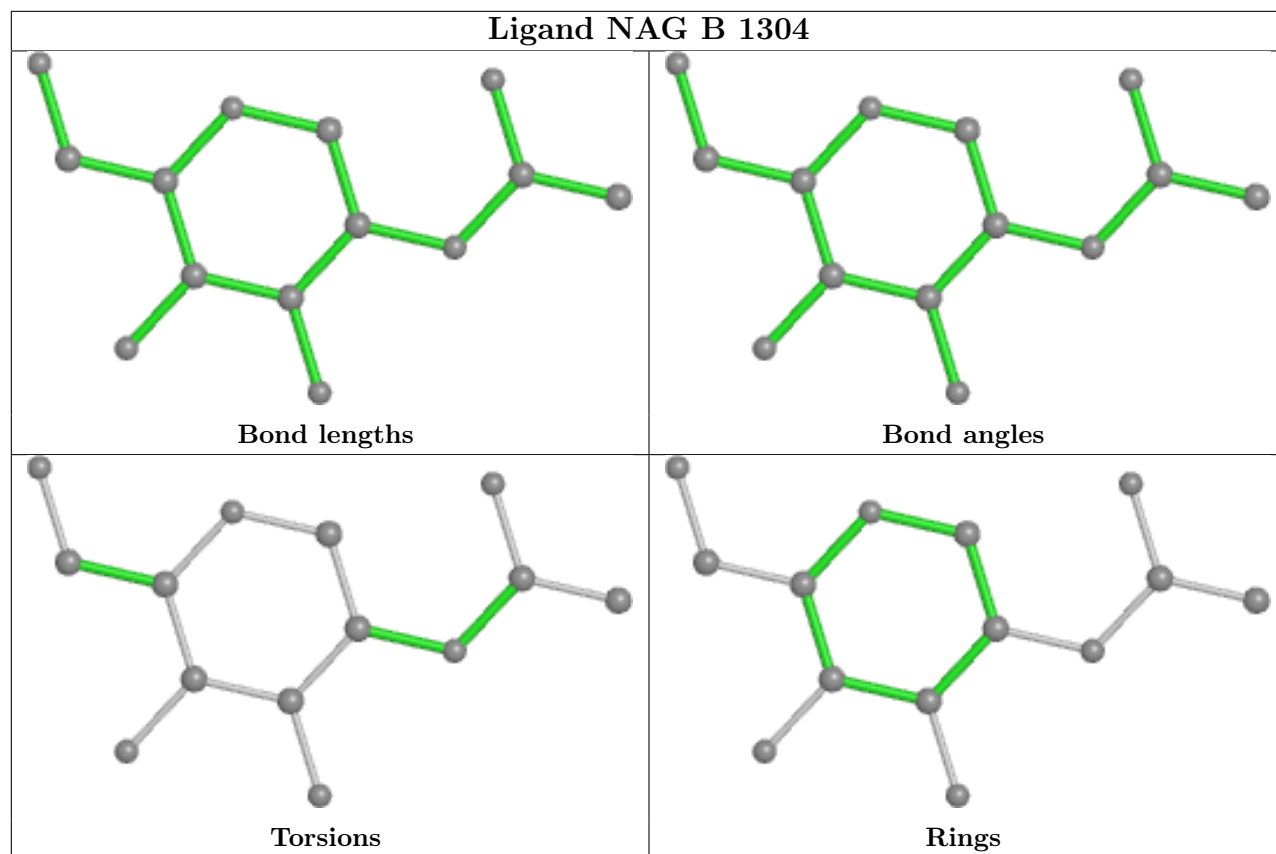
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Mol	Chain	Res	Type	Atoms
5	B	1307	NAG	C8-C7-N2-C2
5	B	1307	NAG	O7-C7-N2-C2
5	A	1302	NAG	C8-C7-N2-C2
5	A	1302	NAG	O7-C7-N2-C2
5	A	1305	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	B	1307	NAG	O5-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	A	1305	NAG	C1-C2-N2-C7
5	B	1303	NAG	O5-C5-C6-O6
5	B	1301	NAG	C1-C2-N2-C7
5	C	1303	NAG	C1-C2-N2-C7
5	B	1301	NAG	O5-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	C	1302	NAG	C1-C2-N2-C7
5	A	1301	NAG	C3-C2-N2-C7
5	A	1306	NAG	C3-C2-N2-C7
5	C	1304	NAG	C3-C2-N2-C7
5	C	1301	NAG	O5-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	B	1301	NAG	C3-C2-N2-C7
5	B	1302	NAG	C3-C2-N2-C7
5	C	1303	NAG	C3-C2-N2-C7
5	A	1304	NAG	O5-C5-C6-O6
5	B	1302	NAG	C1-C2-N2-C7

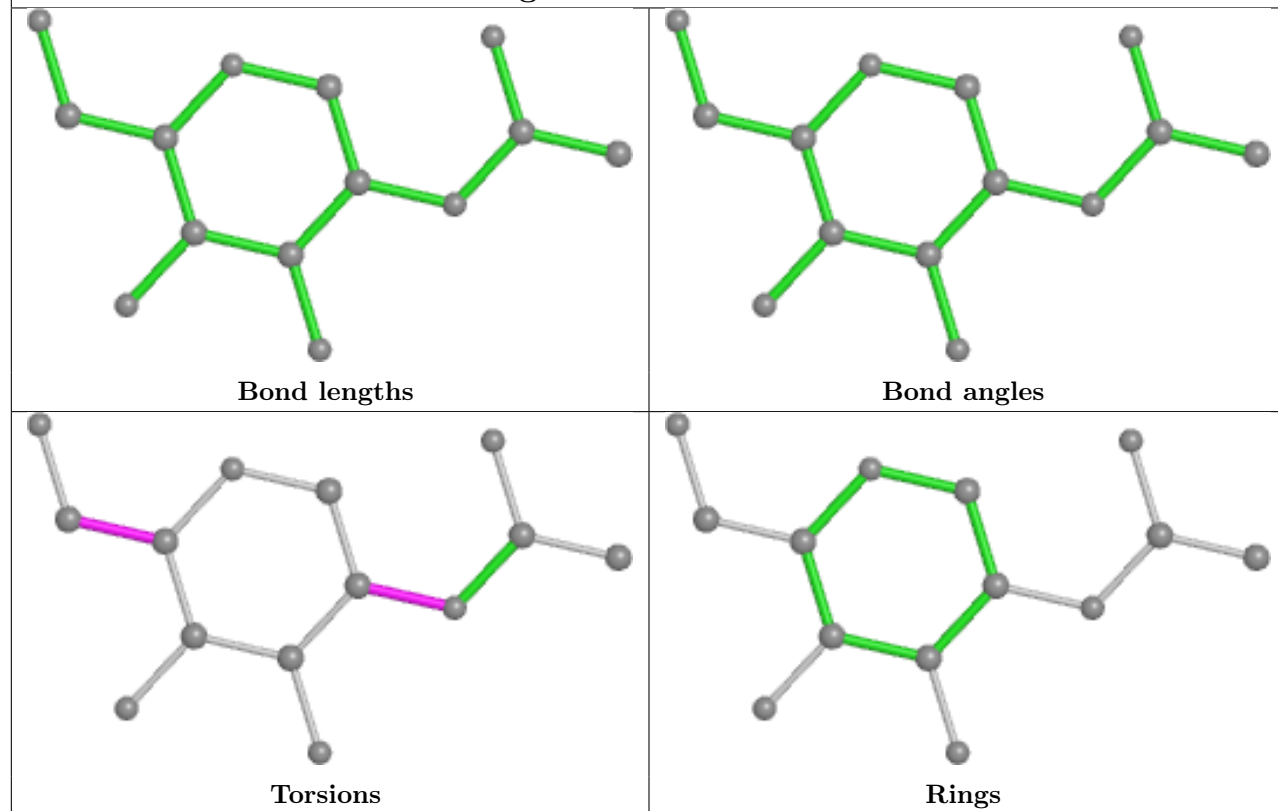
There are no ring outliers.

No monomer is involved in short contacts.

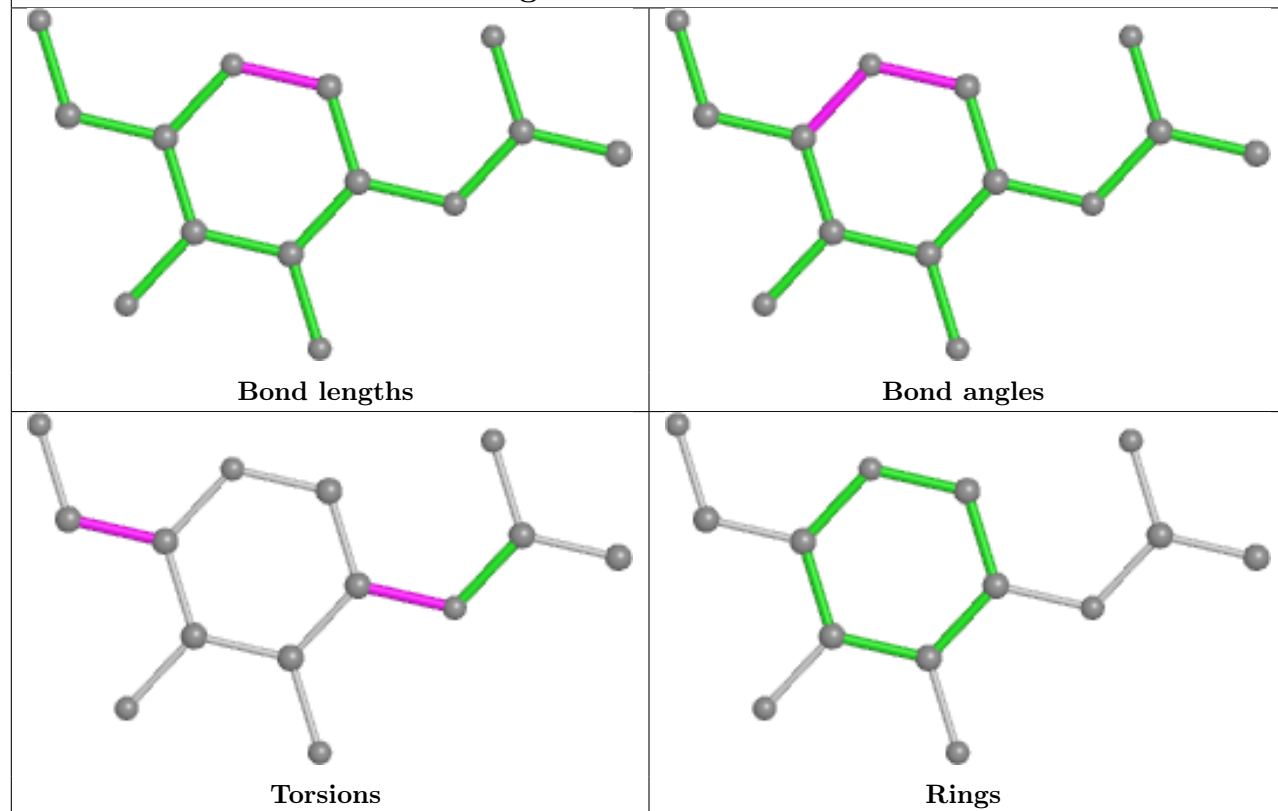
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



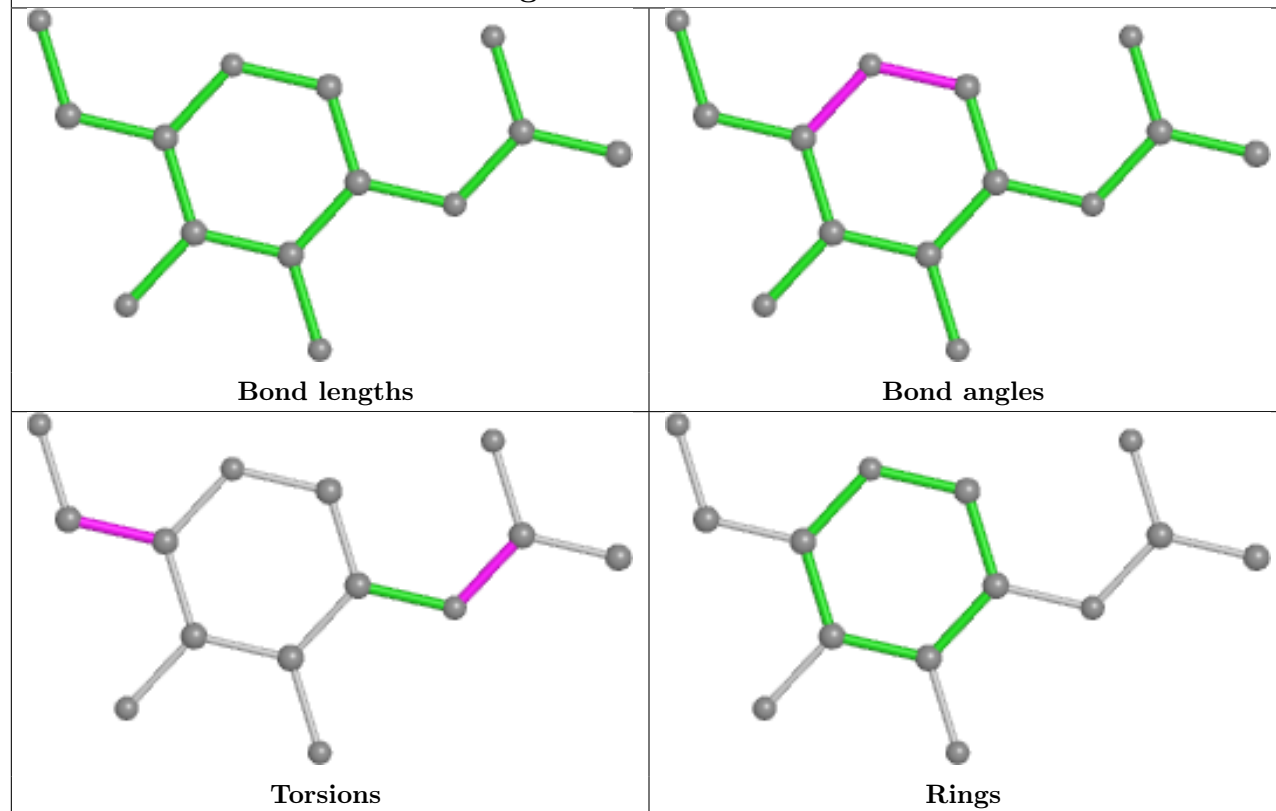
Ligand NAG C 1304



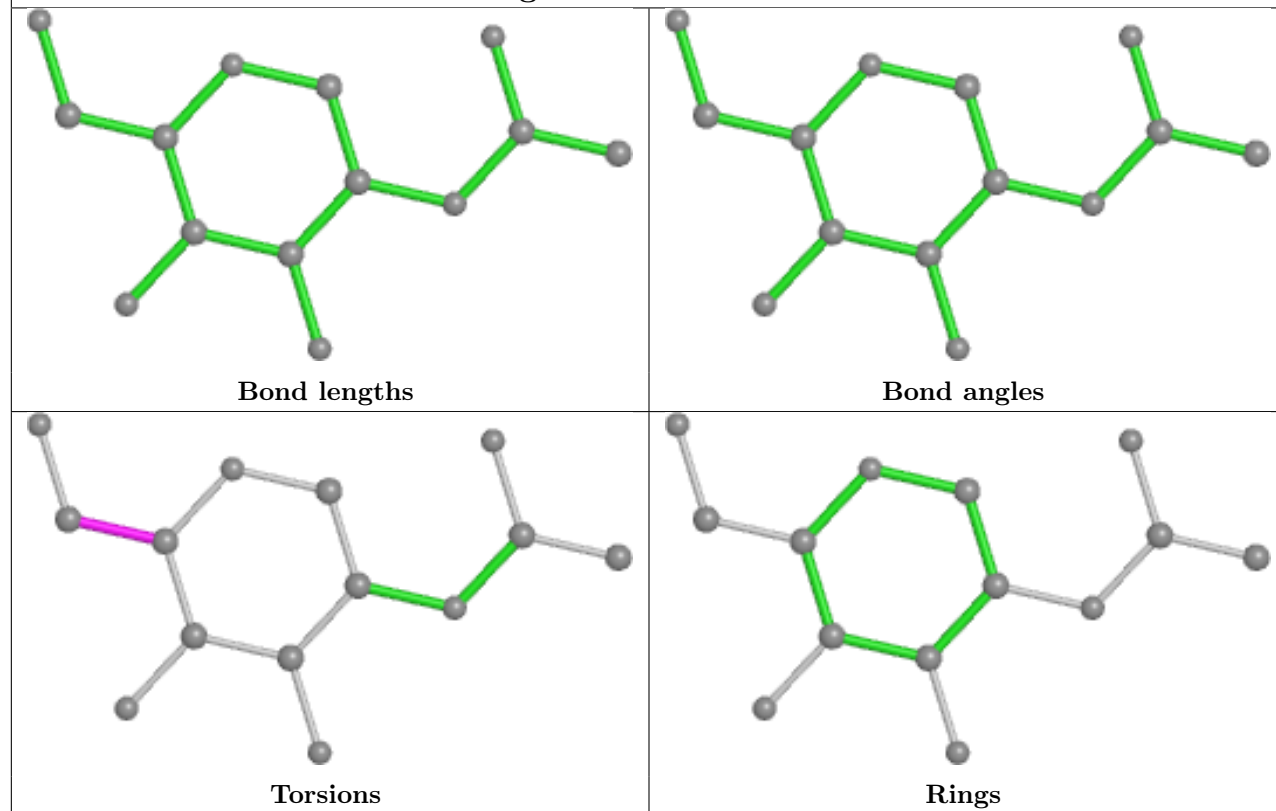
Ligand NAG B 1302



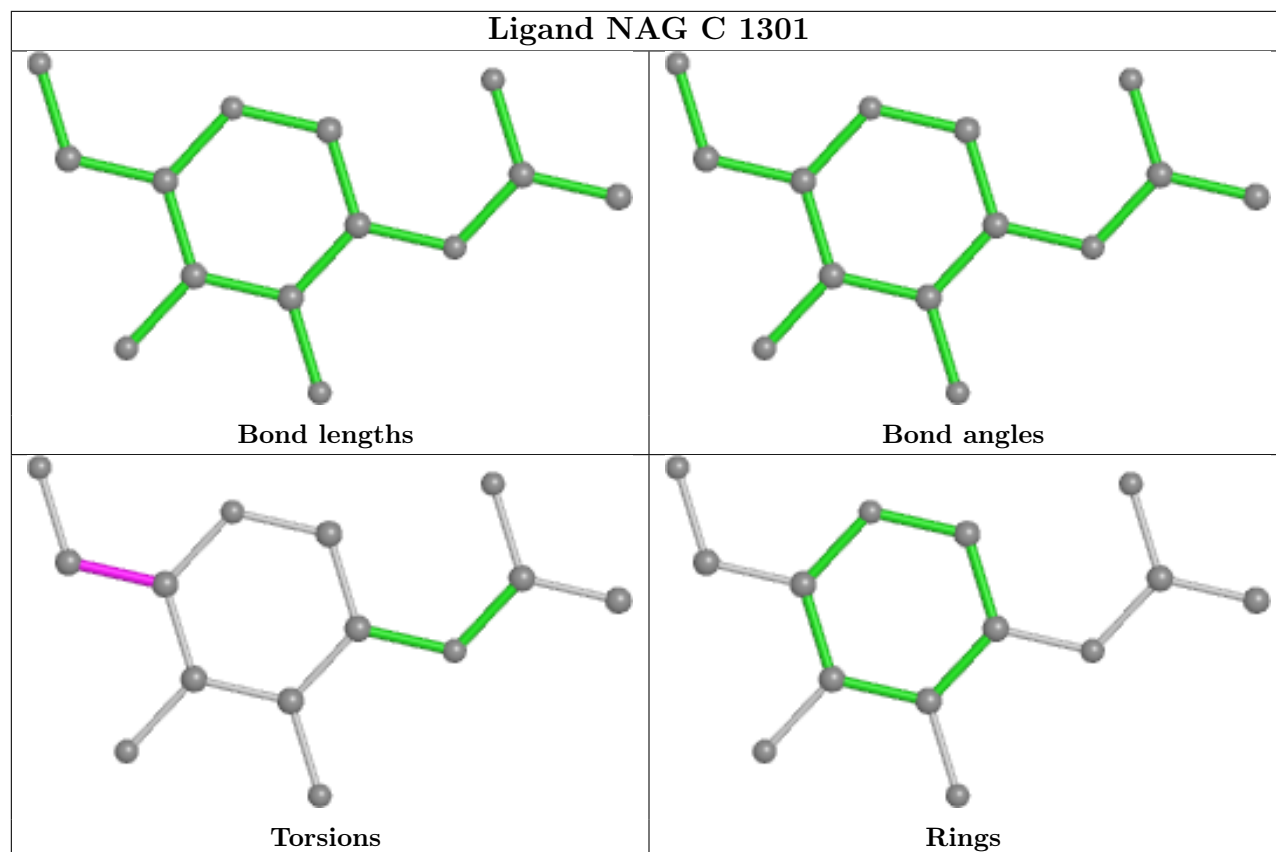
Ligand NAG B 1303



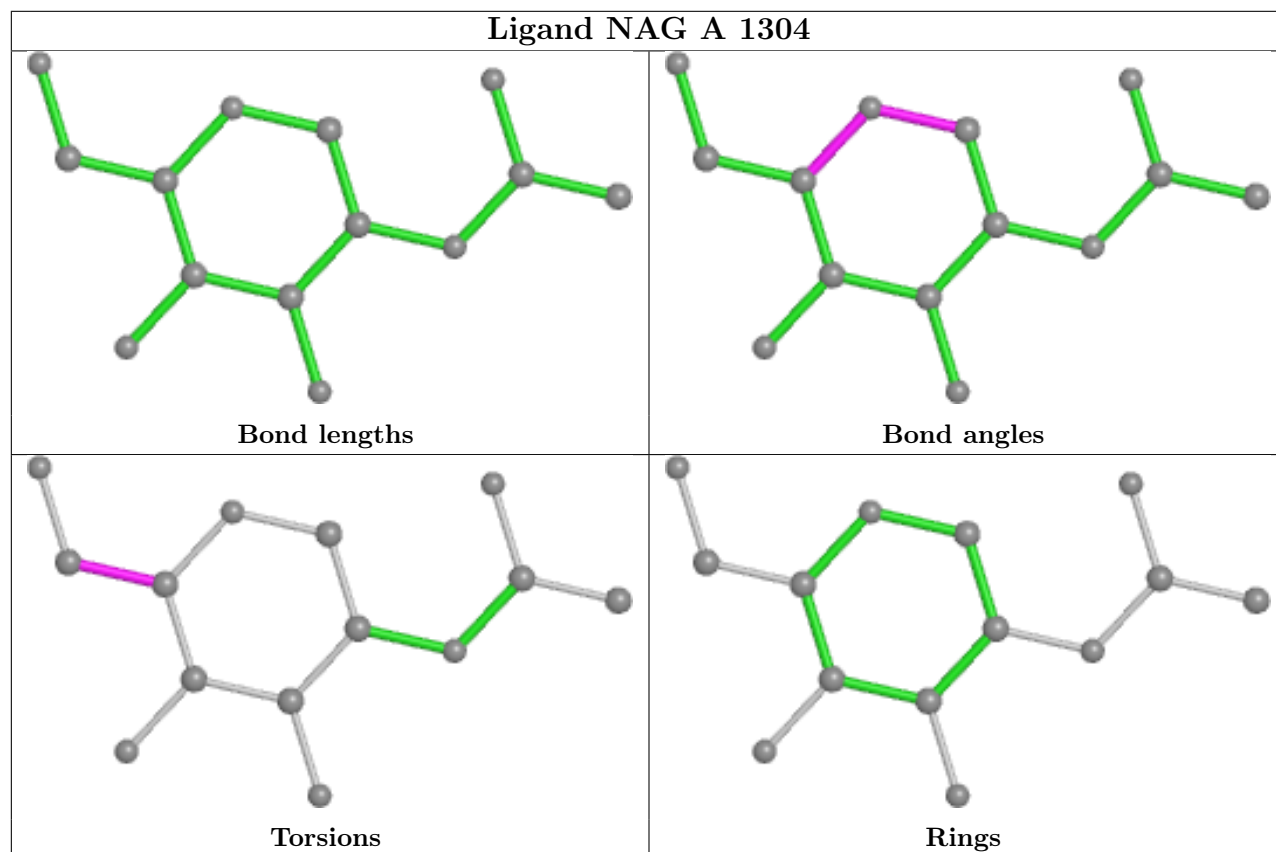
Ligand NAG C 1305



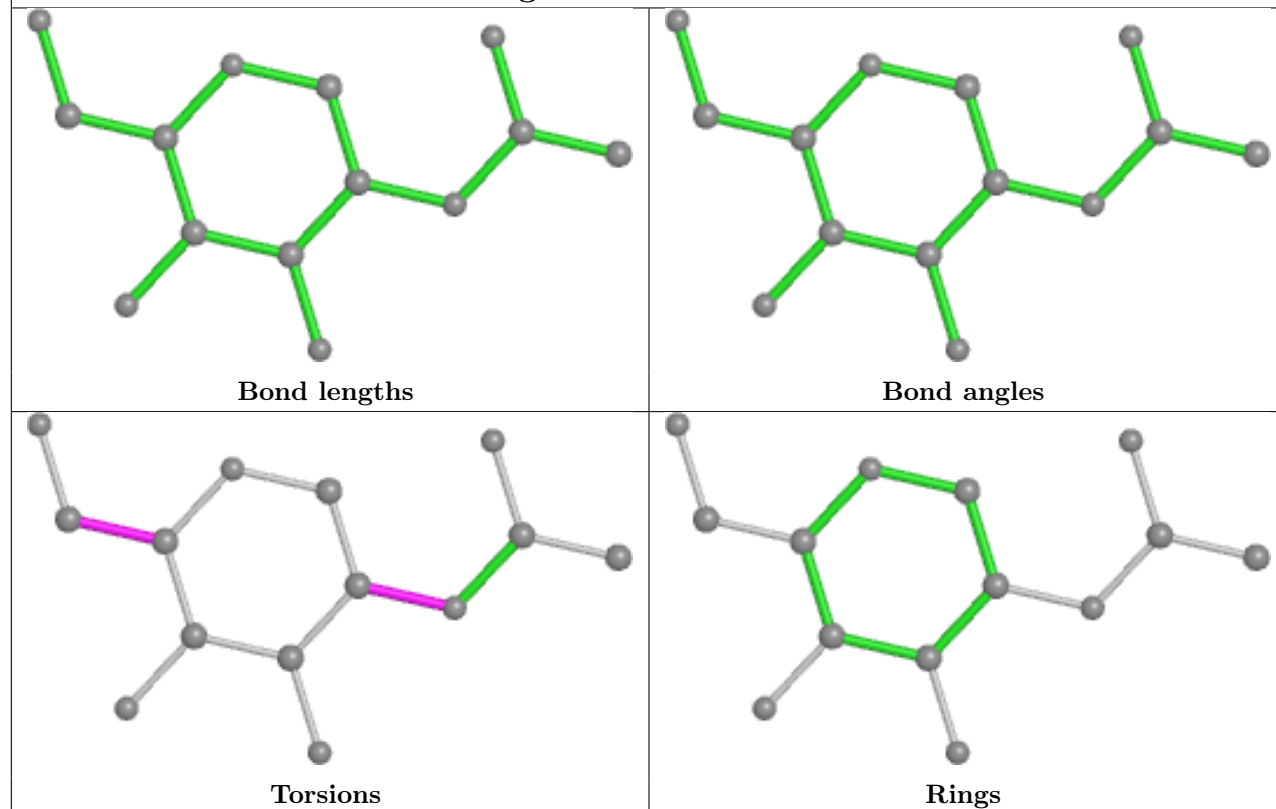
Ligand NAG C 1301



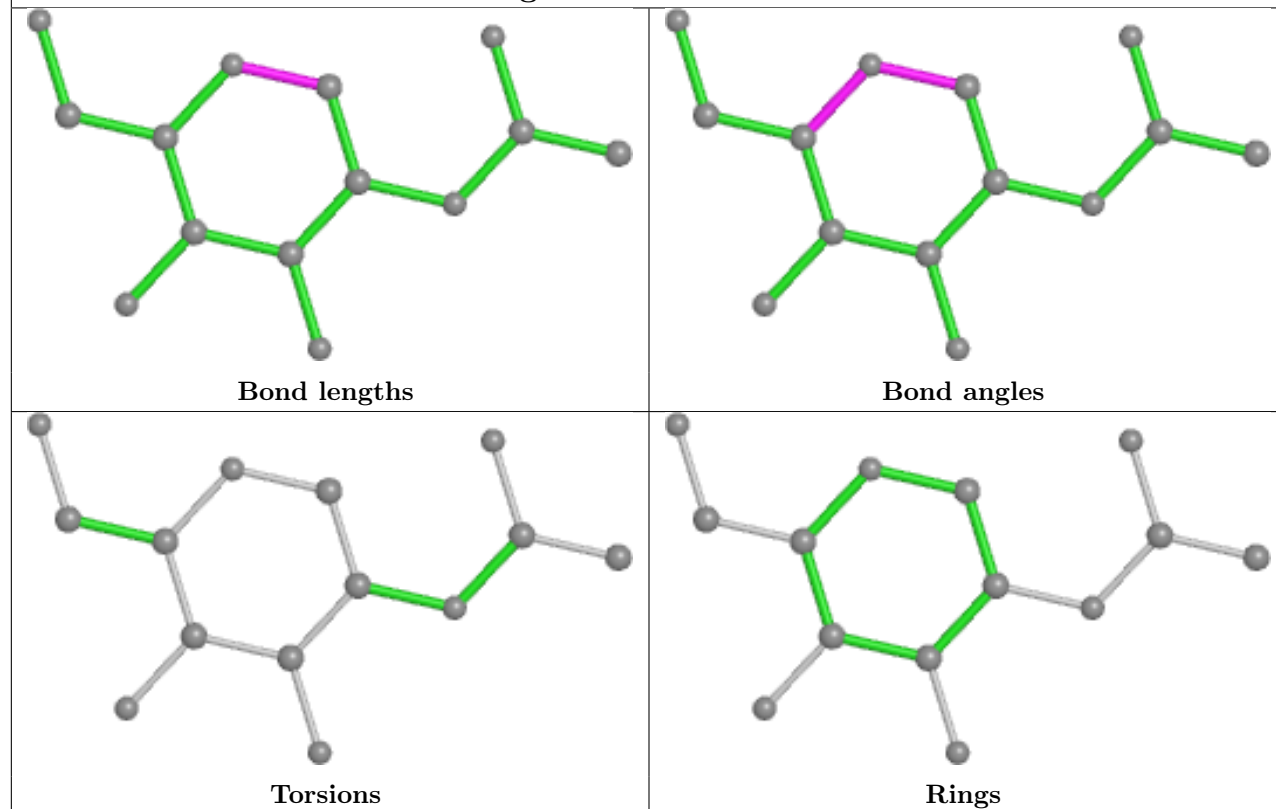
Ligand NAG A 1304



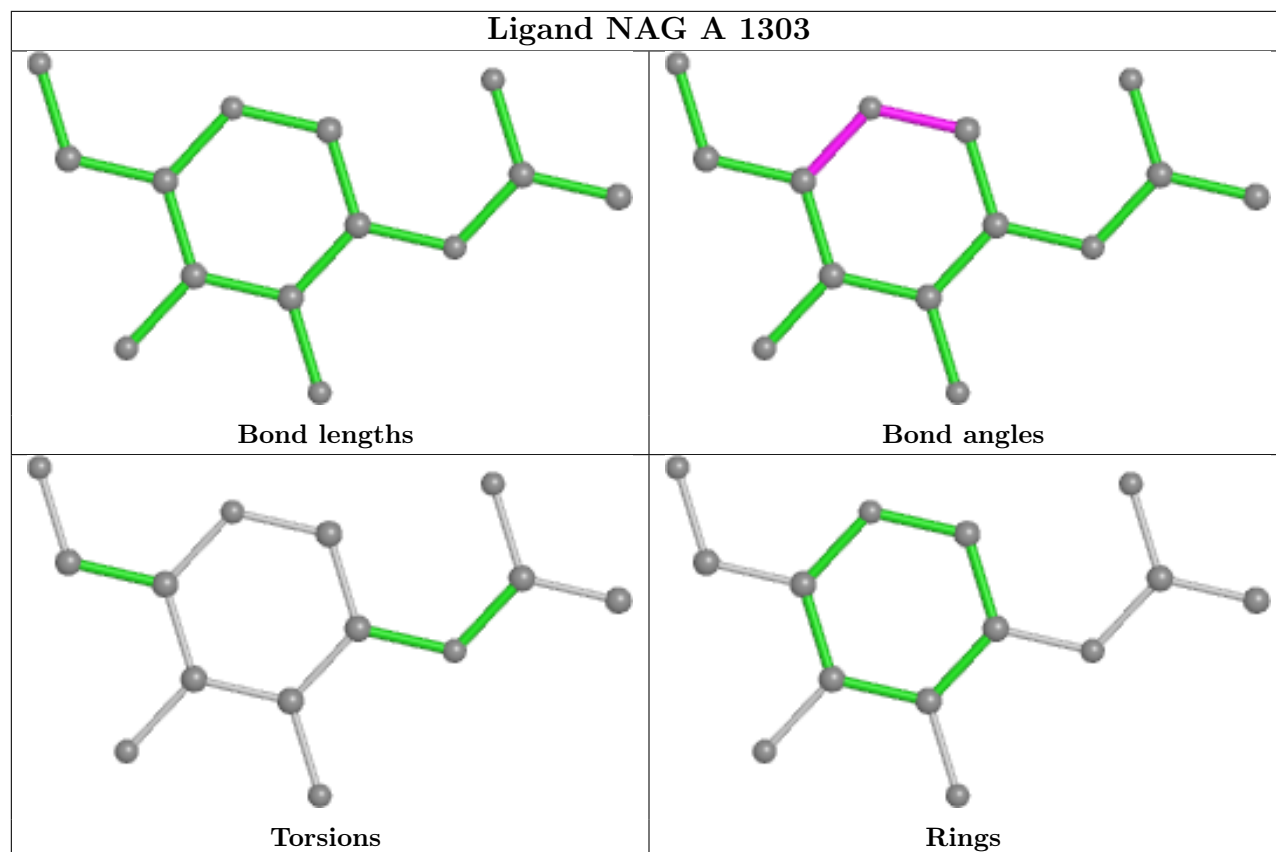
Ligand NAG A 1301



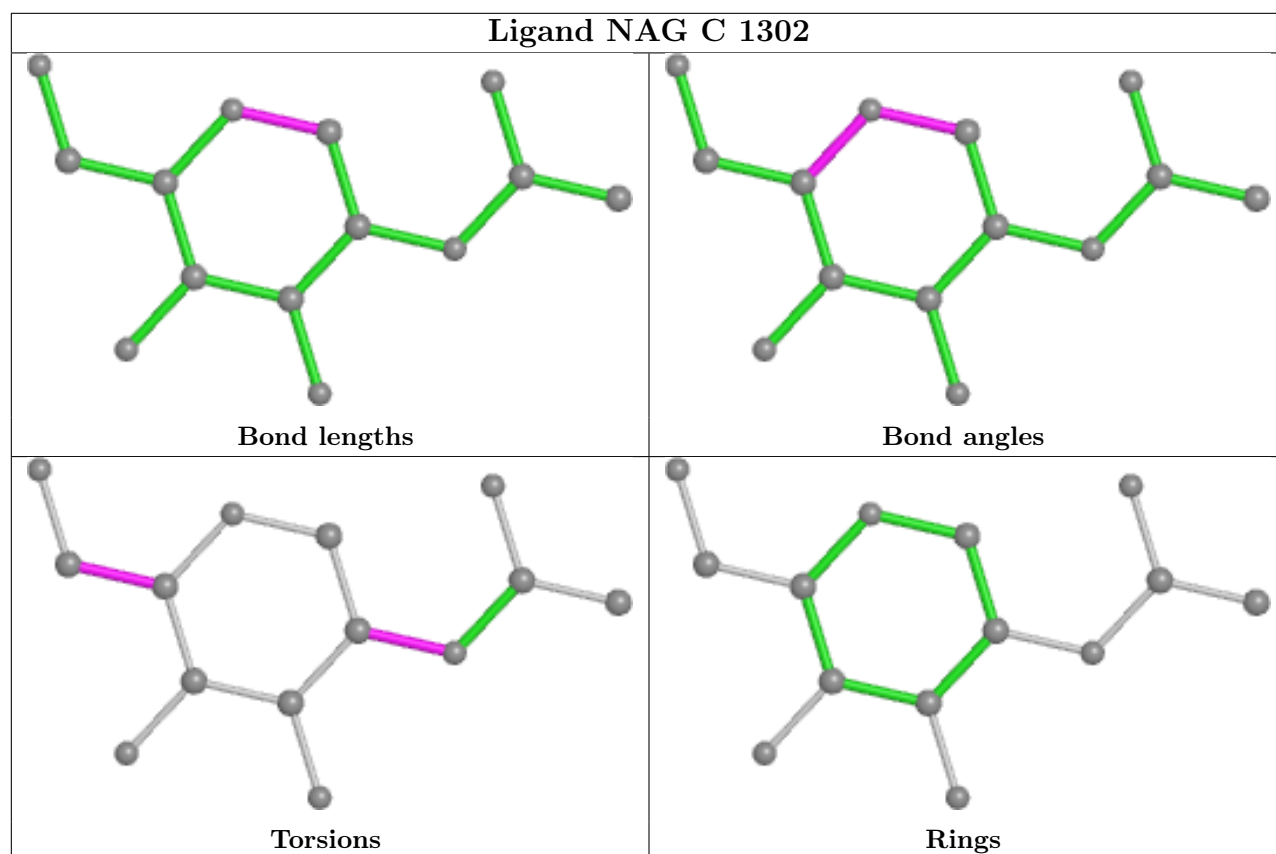
Ligand NAG B 1306



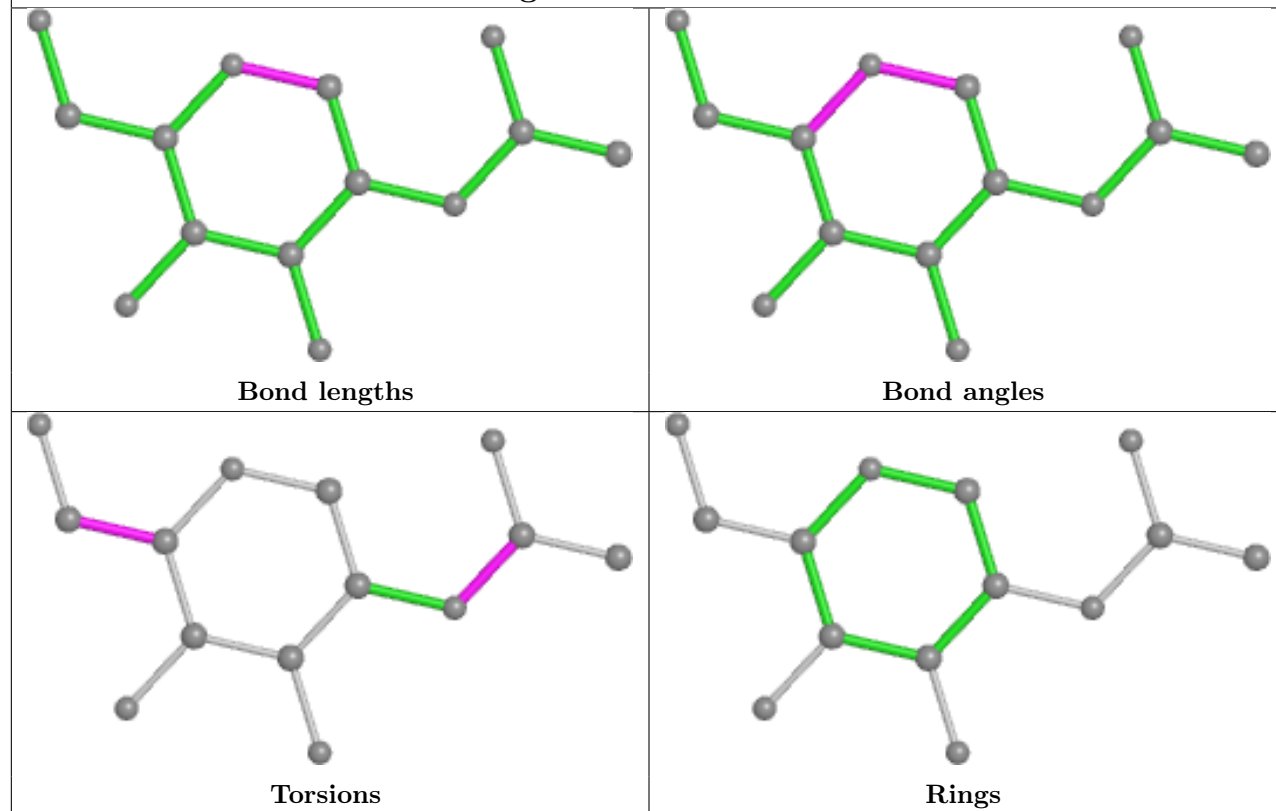
Ligand NAG A 1303



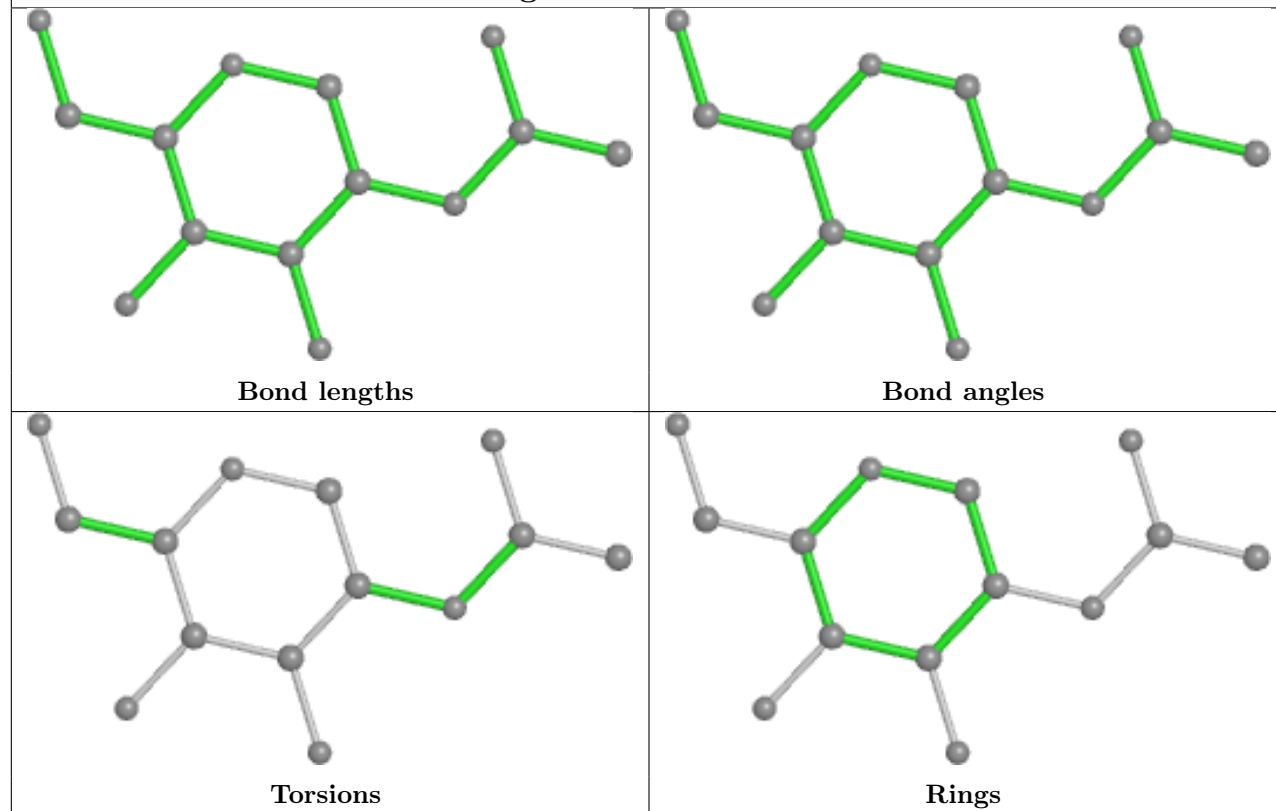
Ligand NAG C 1302



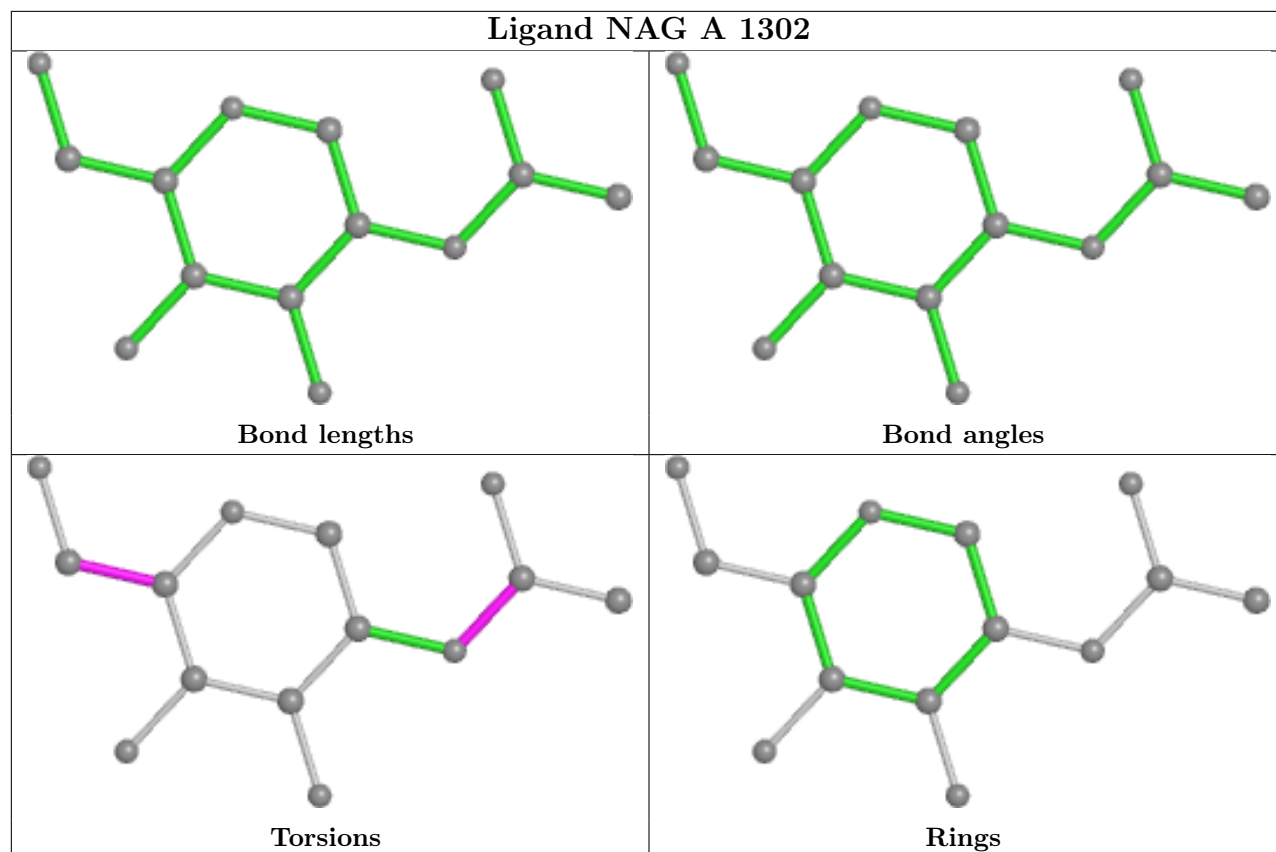
Ligand NAG B 1307



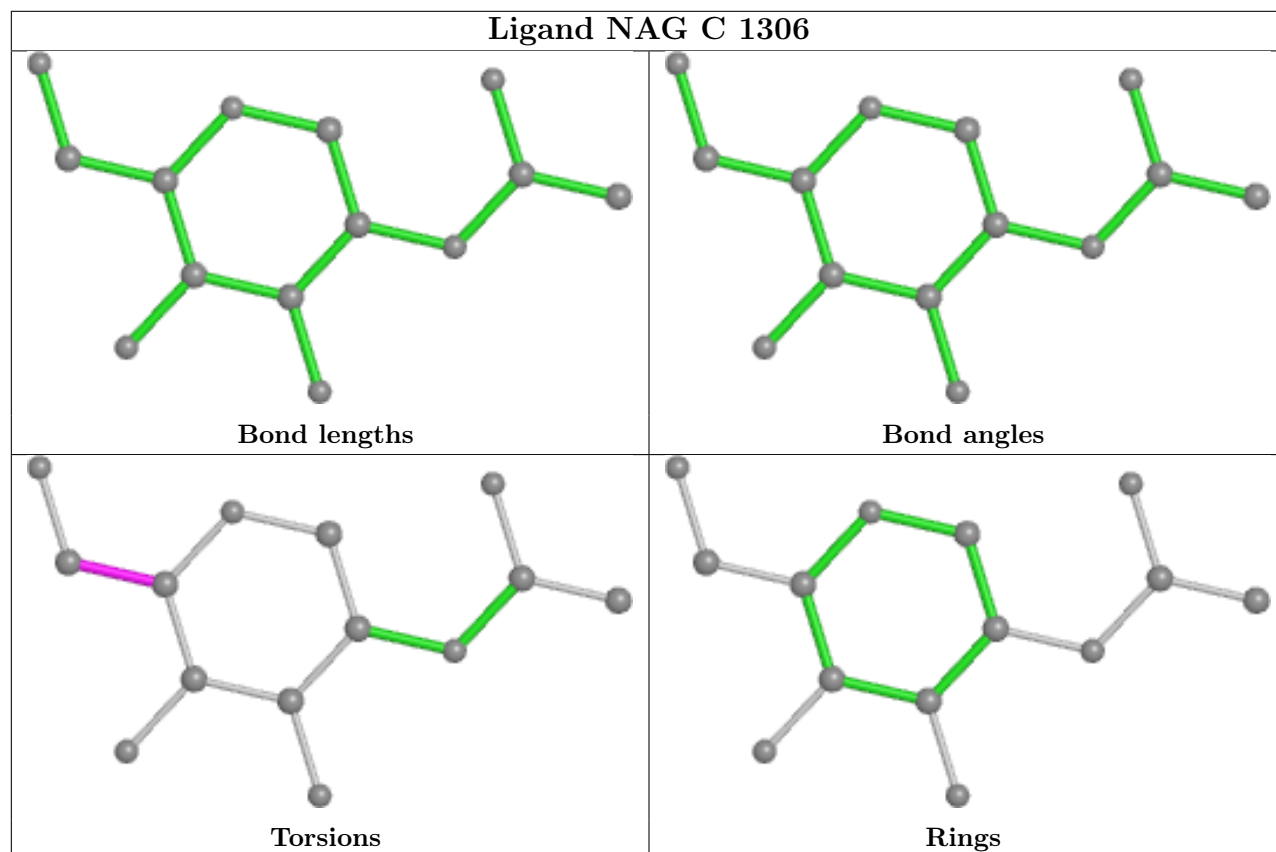
Ligand NAG B 1305



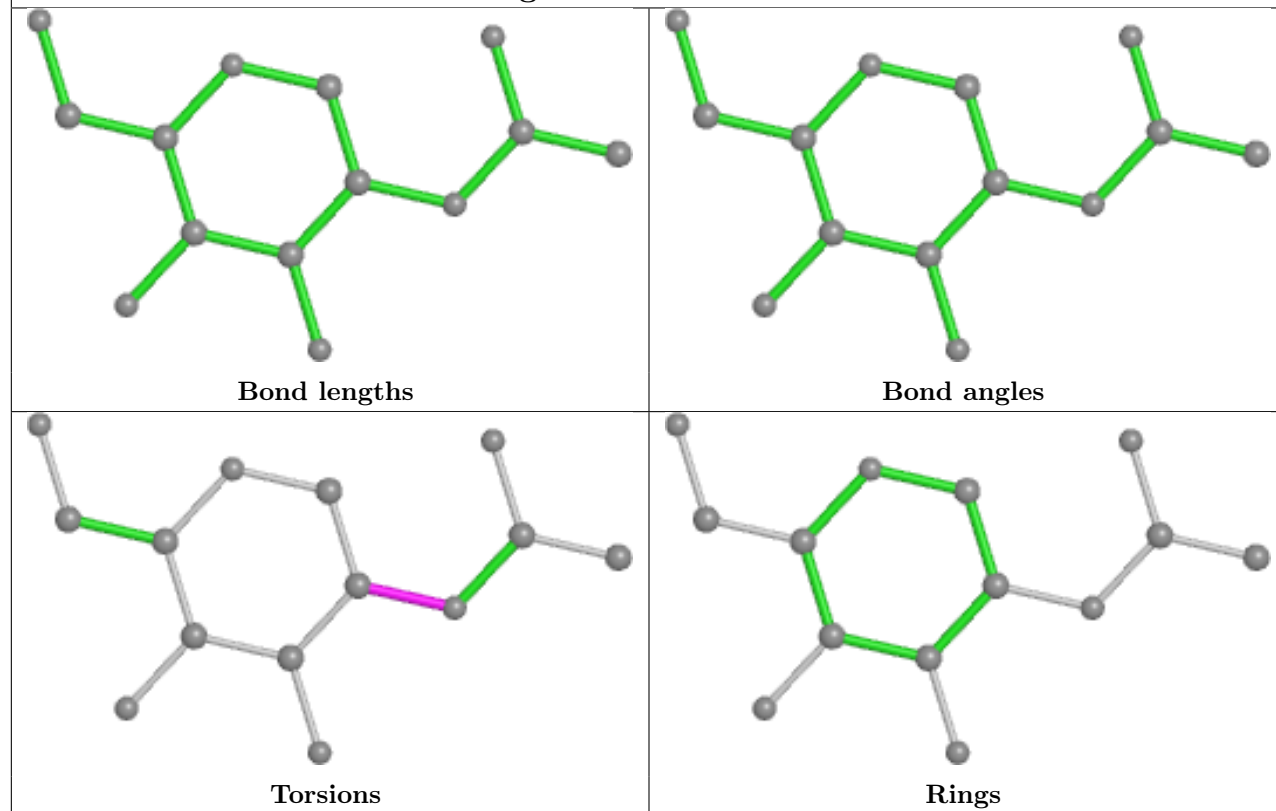
Ligand NAG A 1302



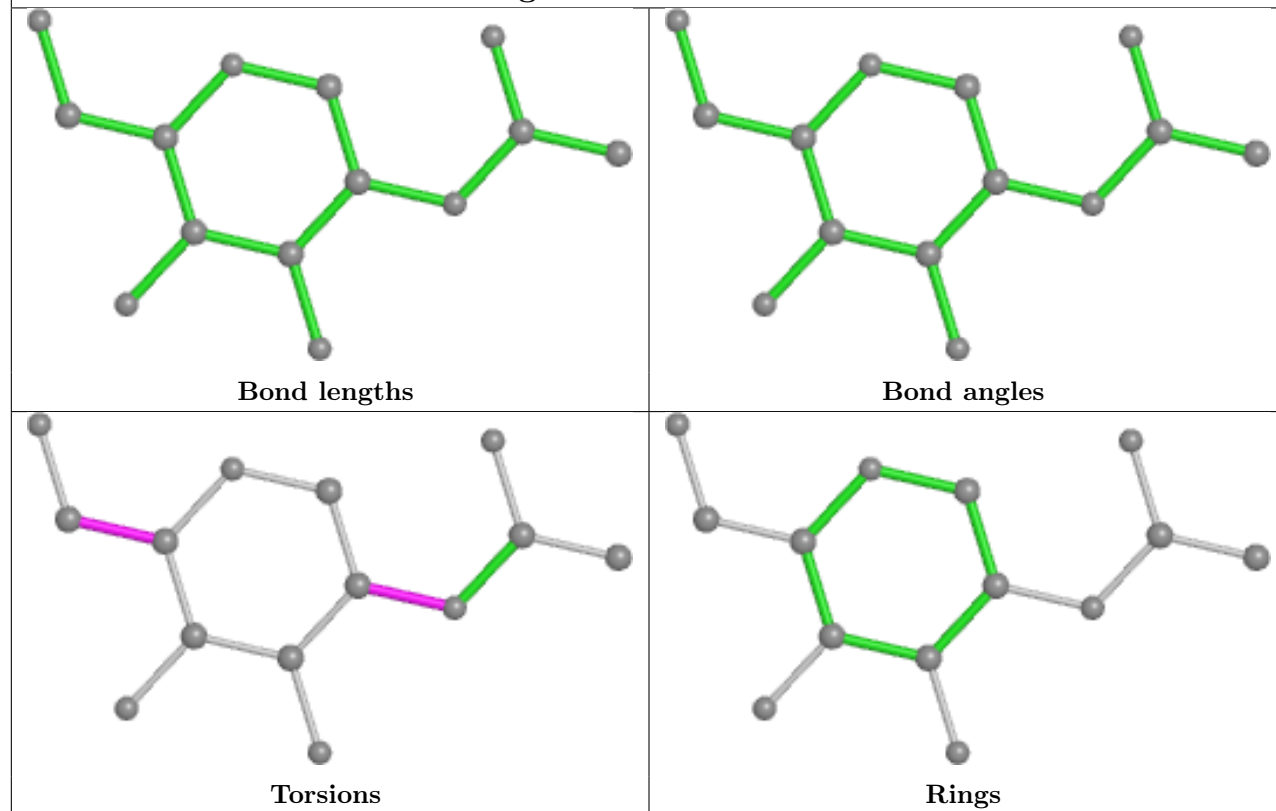
Ligand NAG C 1306

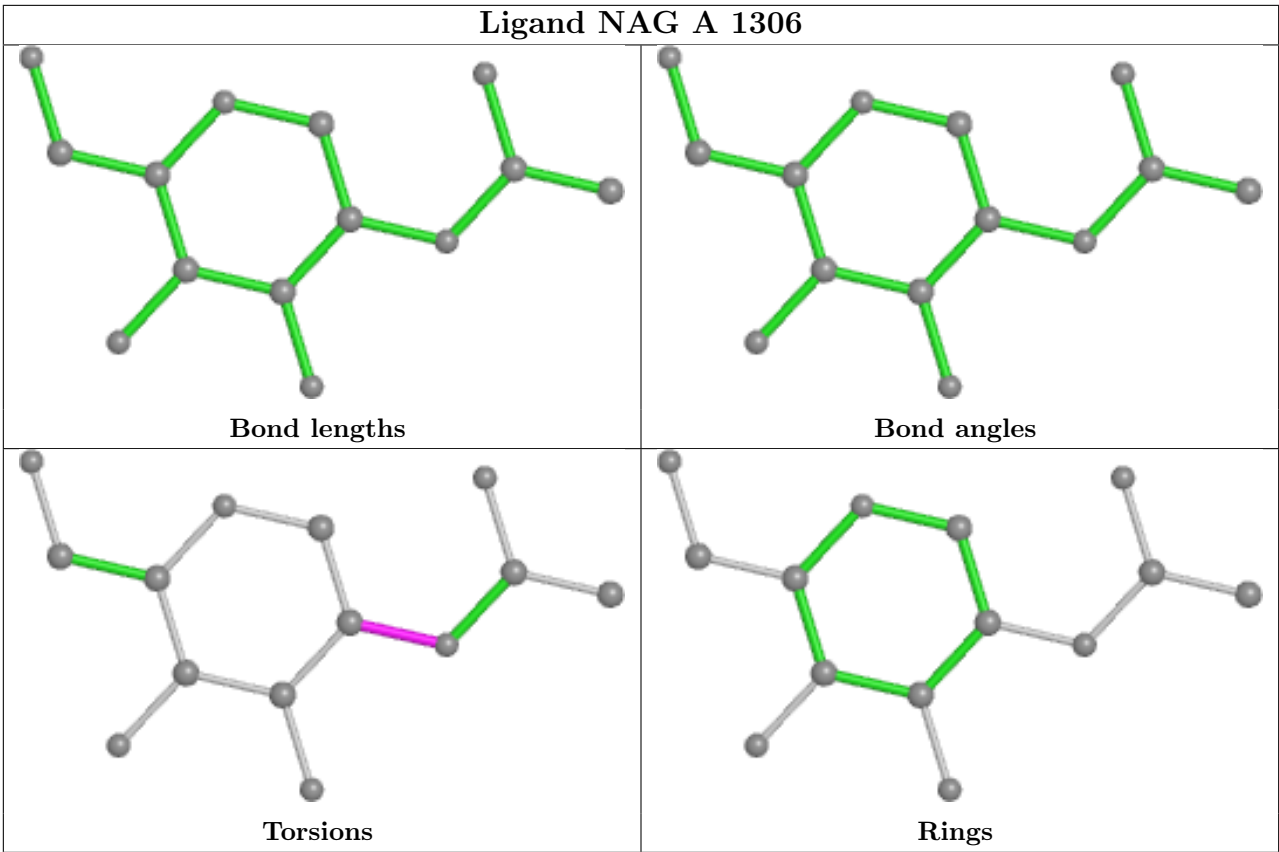


Ligand NAG C 1303



Ligand NAG A 1305





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	424:ASP	C	425:ASP	N	5.36
1	A	425:ASP	C	426:PHE	N	3.08

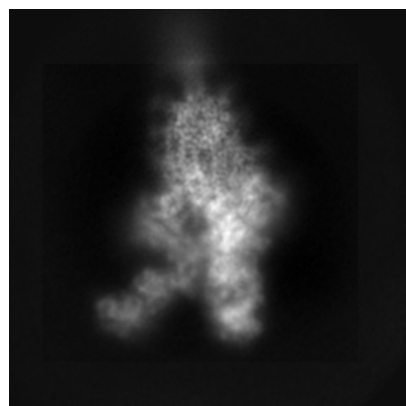
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27798. These allow visual inspection of the internal detail of the map and identification of artifacts.

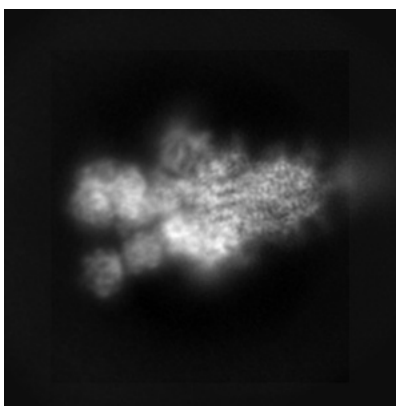
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

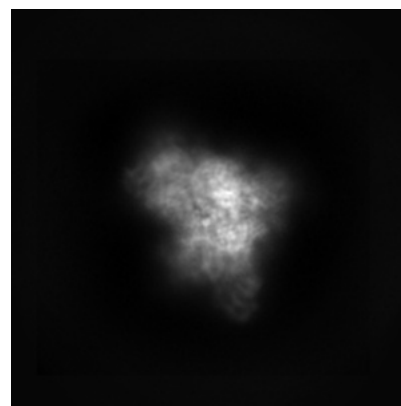
6.1.1 Primary map



X

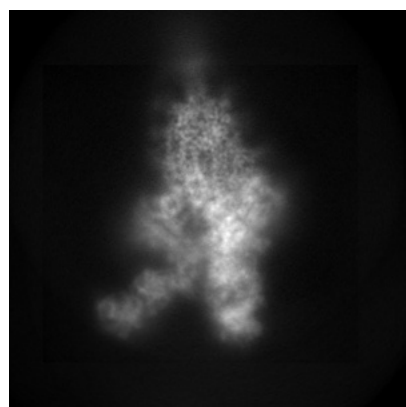


Y

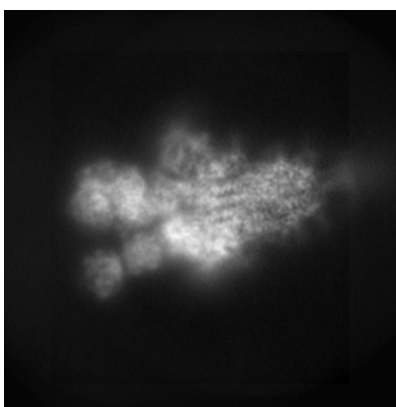


Z

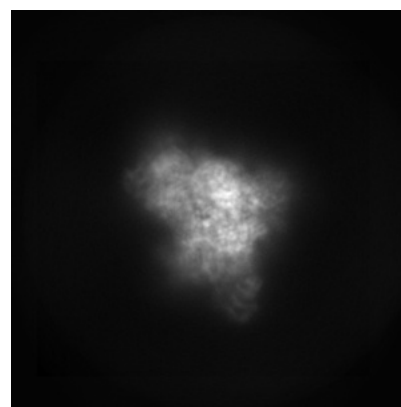
6.1.2 Raw map



X



Y

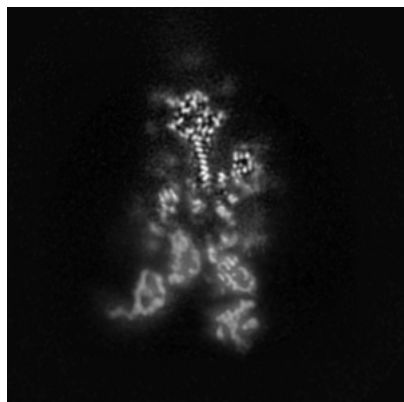


Z

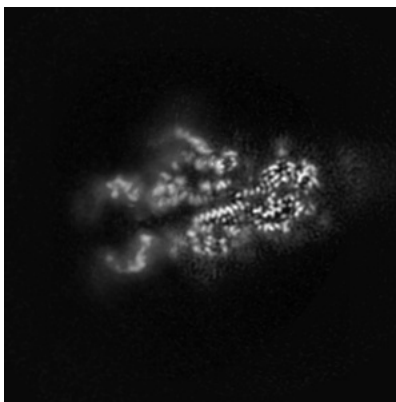
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

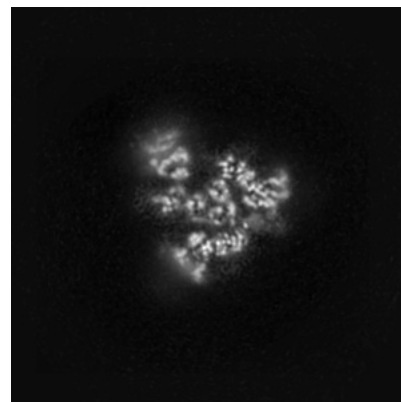
6.2.1 Primary map



X Index: 160

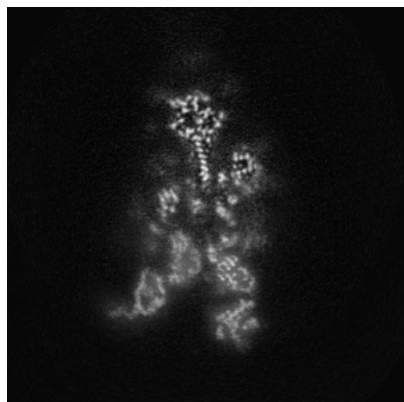


Y Index: 160

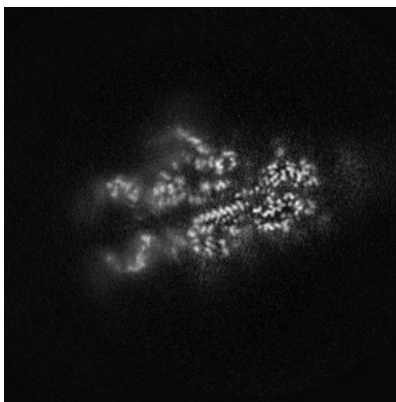


Z Index: 160

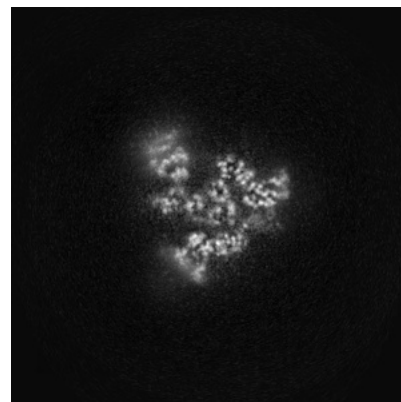
6.2.2 Raw map



X Index: 160



Y Index: 160

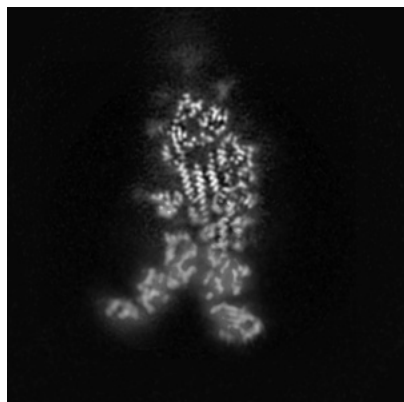


Z Index: 160

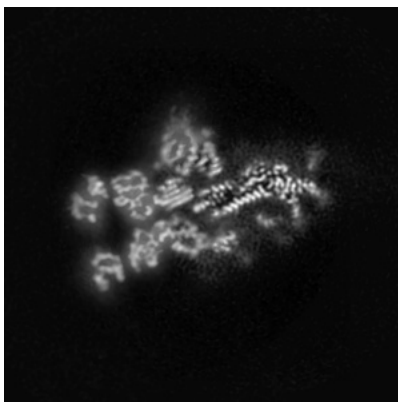
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

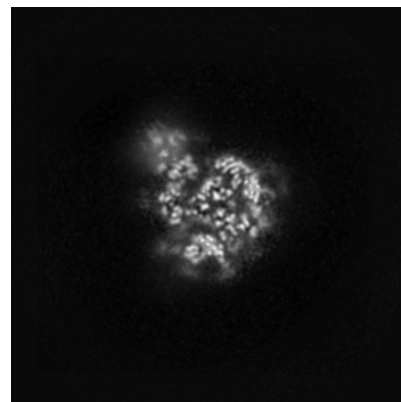
6.3.1 Primary map



X Index: 168

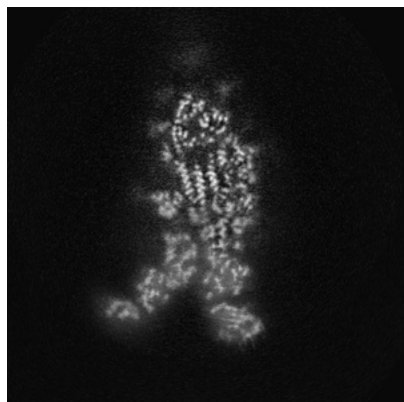


Y Index: 172

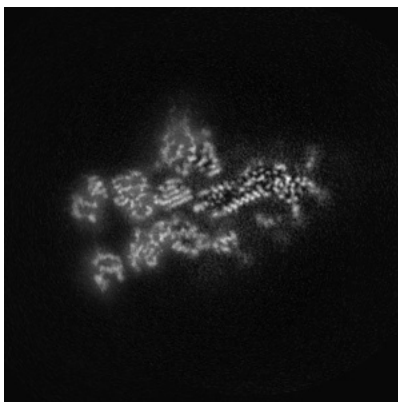


Z Index: 168

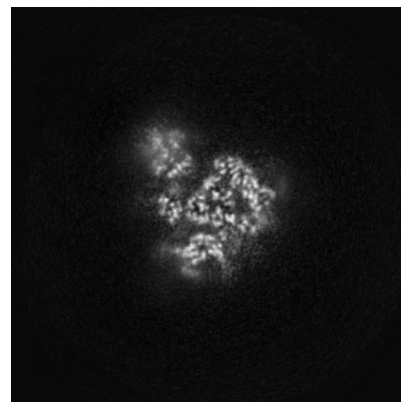
6.3.2 Raw map



X Index: 168



Y Index: 172



Z Index: 166

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

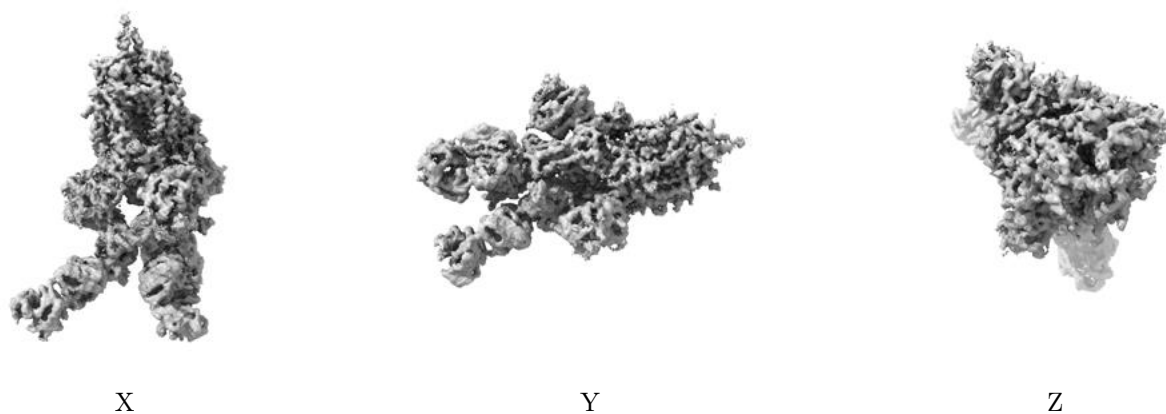
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

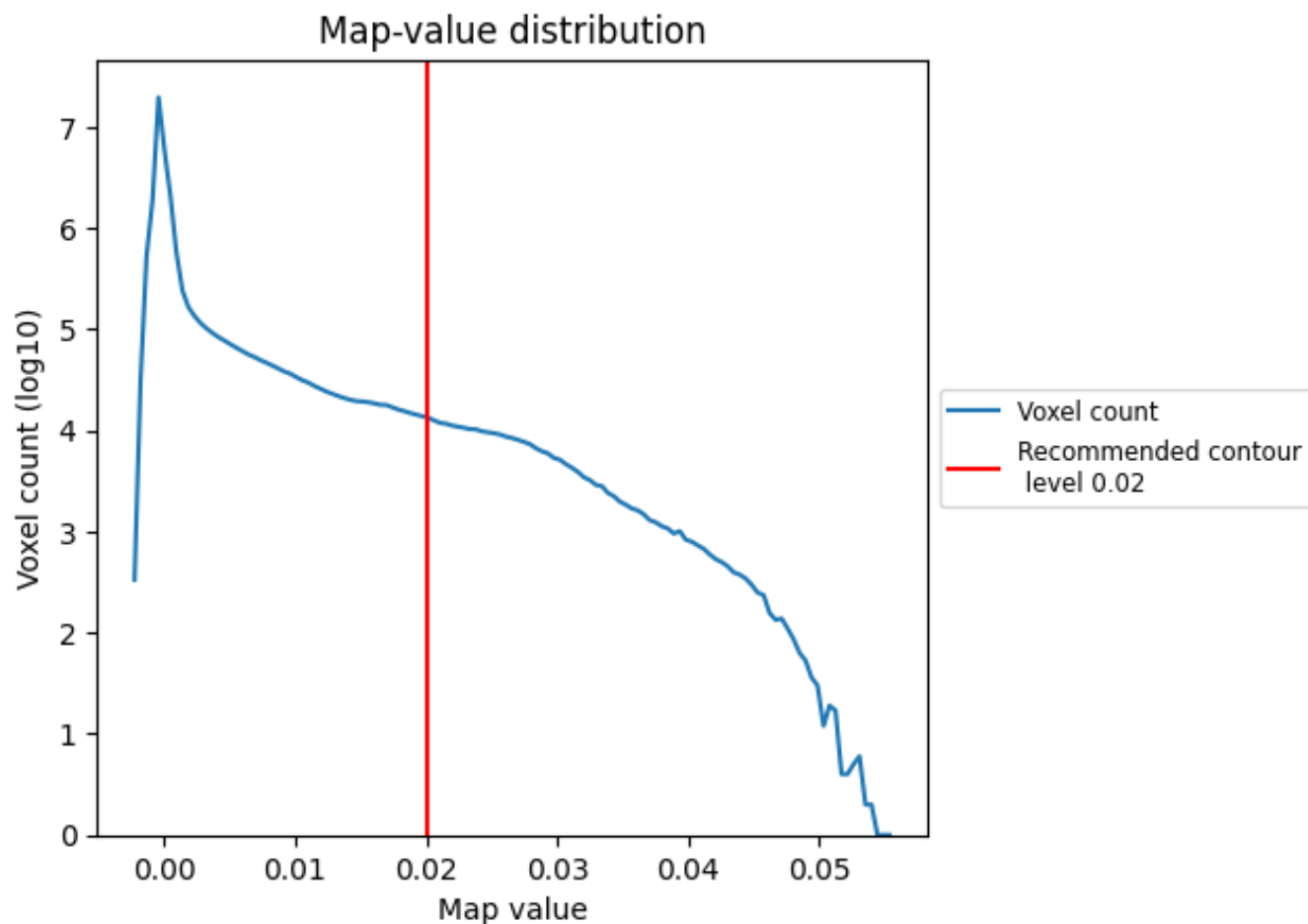
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

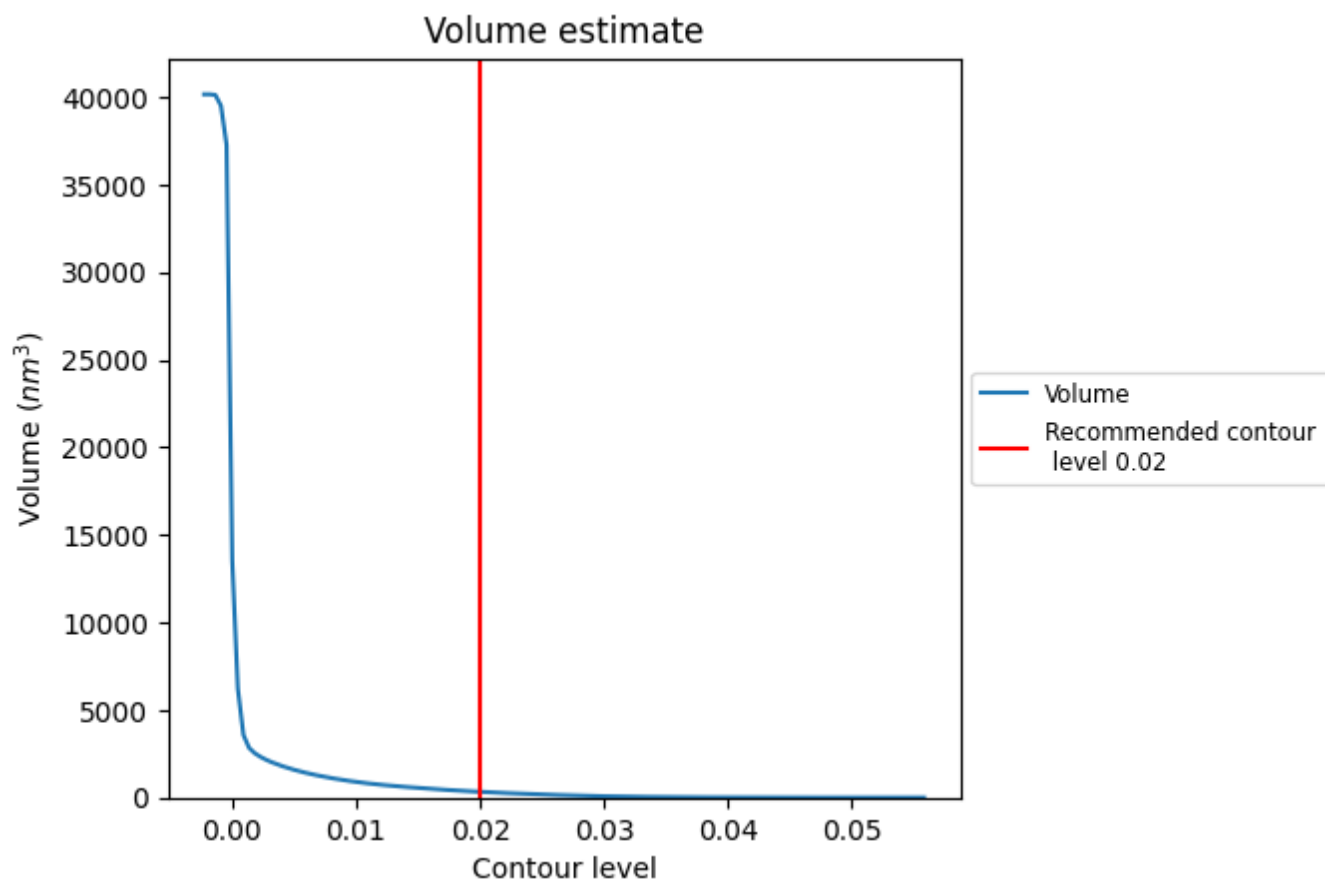
This section contains the results of statistical analysis of the map.

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.

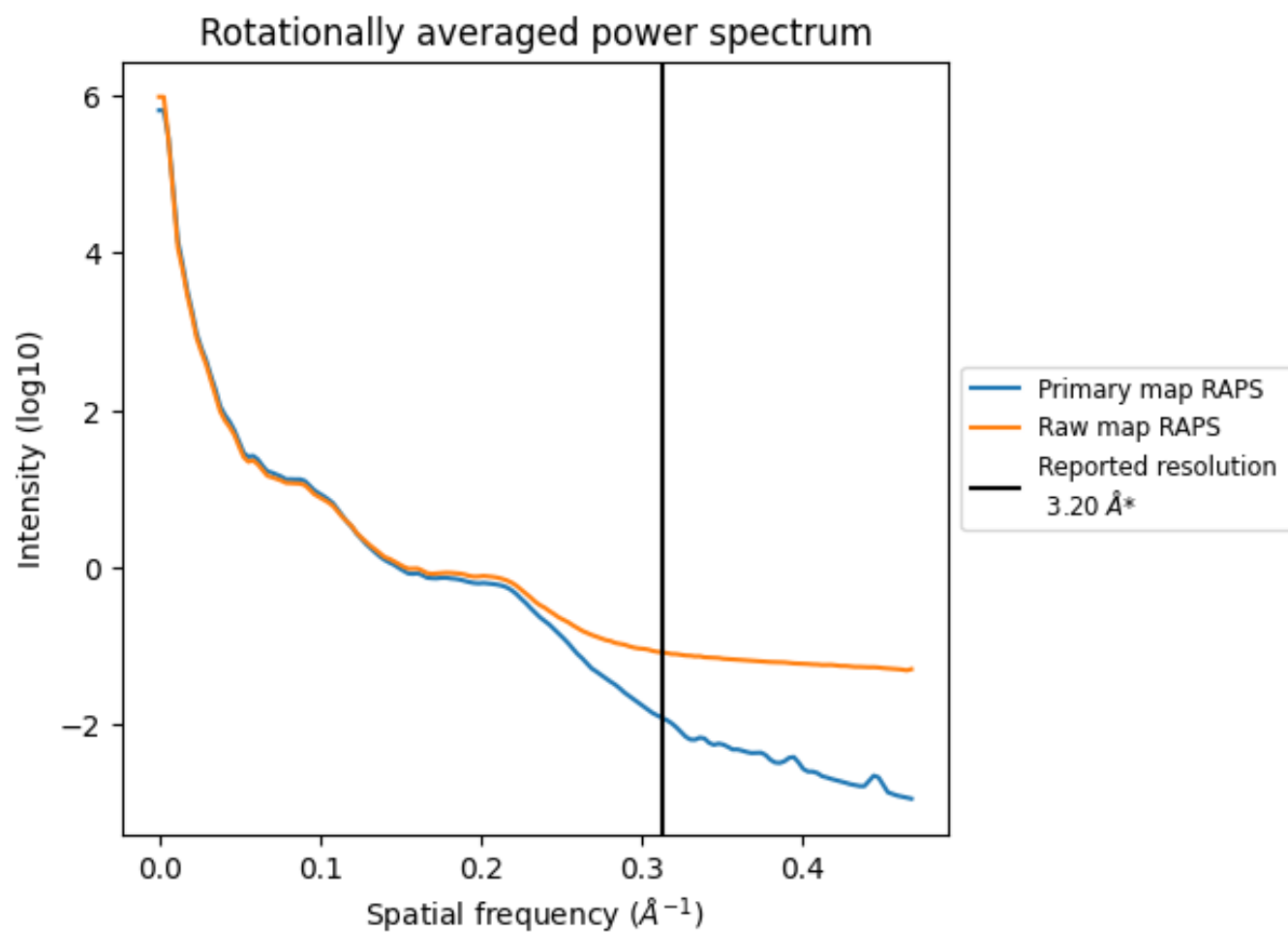
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327 nm³; this corresponds to an approximate mass of 296 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 ⓘ

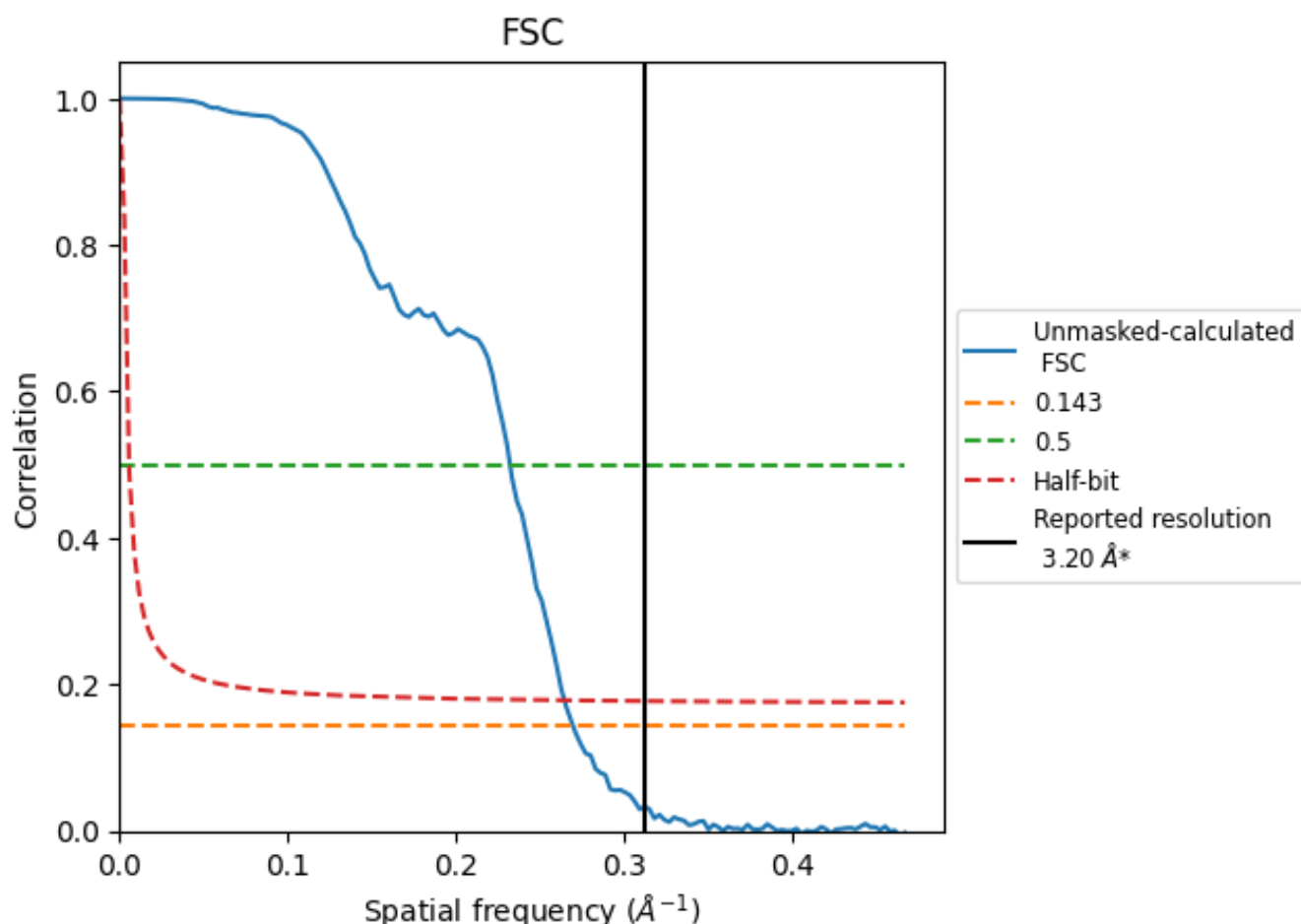


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

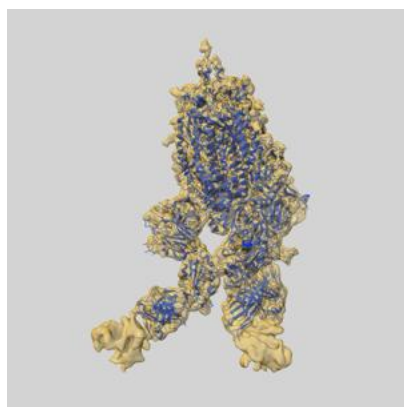
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.71	4.30	3.78

*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 3.71 differs from the reported value 3.2 by more than 10 %

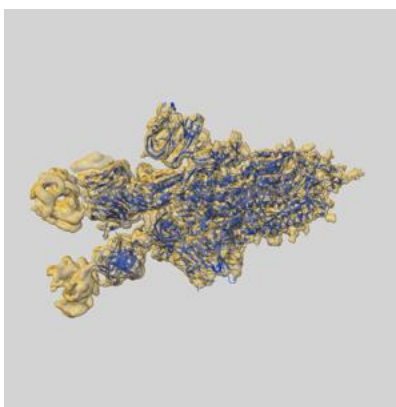
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27798 and PDB model 8DZH. Per-residue inclusion information can be found in section 3 on page 19.

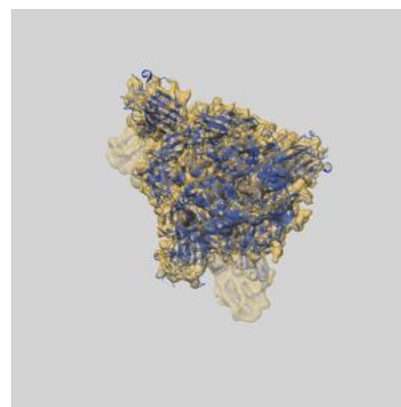
9.1 Map-model overlay [i](#)



X



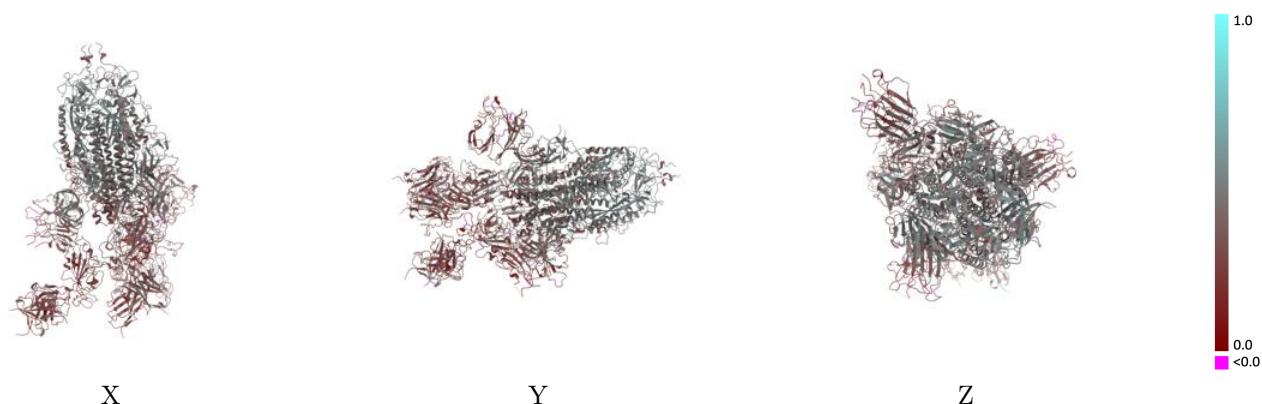
Y



Z

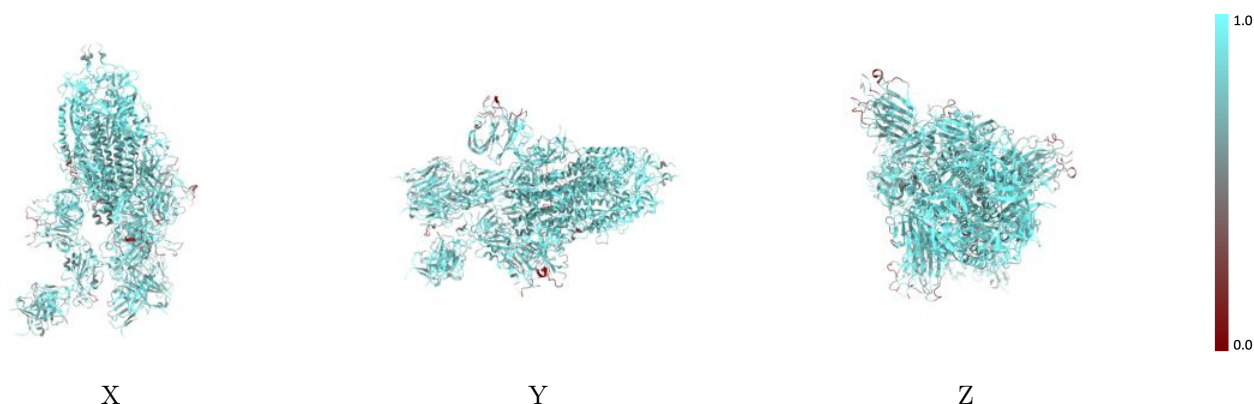
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



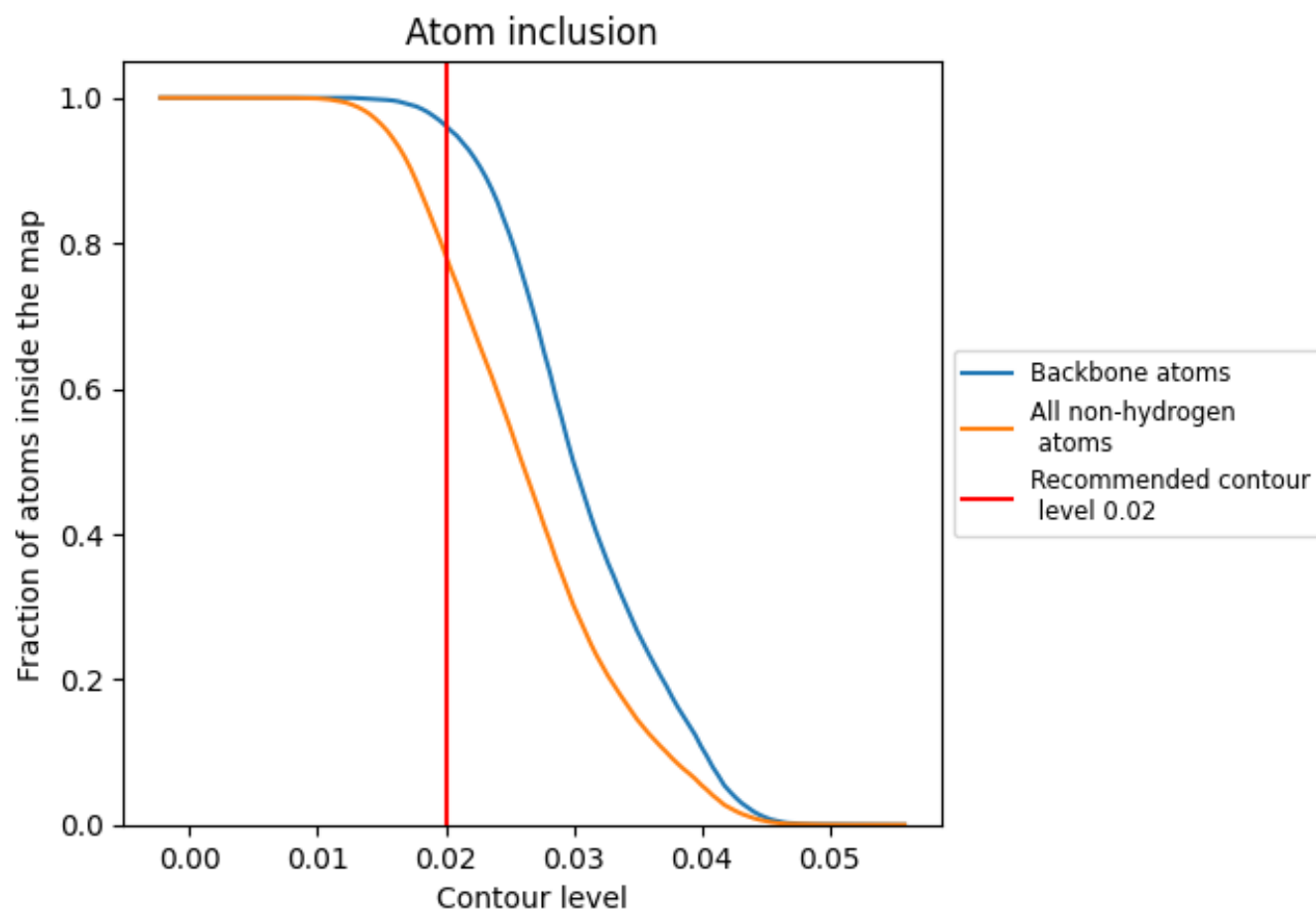
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 78% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7832	 0.3670
A	 0.8013	 0.3900
B	 0.7955	 0.3750
C	 0.7893	 0.3790
D	 0.7556	 0.2990
E	 0.8031	 0.3120
F	 0.8214	 0.3850
G	 0.7857	 0.4700
H	 0.7260	 0.2800
I	 0.8132	 0.2960
J	 0.7693	 0.2940
K	 0.6071	 0.4420
L	 0.7157	 0.2660
M	 0.3571	 0.3600
N	 0.5357	 0.3570
O	 0.6071	 0.4360
P	 0.3929	 0.3930
Q	 0.1786	 0.3140
R	 0.6071	 0.3550
S	 0.5357	 0.2030
T	 0.0714	 0.2410
U	 0.3571	 0.4030
V	 0.3214	 0.3490
W	 0.5357	 0.4030
X	 0.6071	 0.4240
Y	 0.6071	 0.4270
Z	 0.7143	 0.4680
a	 0.5714	 0.3860
b	 0.6786	 0.4200
c	 0.5000	 0.4090
d	 0.2857	 0.3030
e	 0.6786	 0.4460
f	 0.5714	 0.4250
g	 0.2500	 0.3390
h	 0.1786	 0.3170



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.5000	 0.3160
j	 0.5357	 0.3270