



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 01:23 am GMT

PDB ID : 7Q1Z  
EMDB ID : EMD-13776  
Title : Structure of formaldehyde cross-linked SARS-CoV-2 S glycoprotein  
Authors : Sulbaran, G.; Effantin, G.; Schoehn, G.; Weissenhorn, W.  
Deposited on : 2021-10-22  
Resolution : 3.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

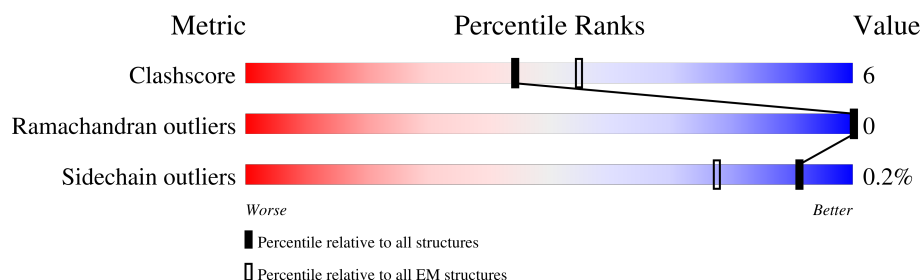
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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.








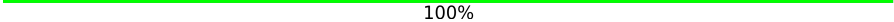
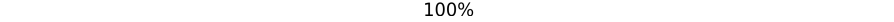
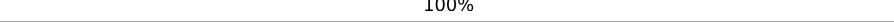
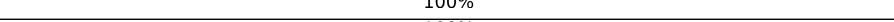
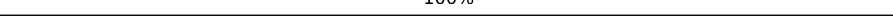
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1288	<div> <div>37%</div> <div>63%</div> <div>12%</div> <div>25%</div> </div>
1	B	1288	<div> <div>38%</div> <div>63%</div> <div>12%</div> <div>25%</div> </div>
1	C	1288	<div> <div>35%</div> <div>63%</div> <div>12%</div> <div>25%</div> </div>
2	D	2	<div> <div>100%</div> <div>100%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>100%</div> <div>50%</div> <div>50%</div> </div>
2	G	2	<div> <div>100%</div> <div>100%</div> </div>
2	H	2	<div> <div>50%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	2	100% 
2	J	2	50%  50%
2	K	2	100% 
2	L	2	50%  100%
2	M	2	100% 
2	N	2	100% 
2	O	2	100% 
2	P	2	50%  100%
2	Q	2	50%  100%
2	R	2	100% 

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23694 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	972	Total	C	N	O	S	0	0
			7604	4861	1262	1448	33		
1	B	972	Total	C	N	O	S	0	0
			7604	4861	1262	1448	33		
1	C	972	Total	C	N	O	S	0	0
			7604	4861	1262	1448	33		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2

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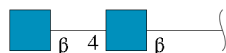
Chain	Residue	Modelled	Actual	Comment	Reference
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

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



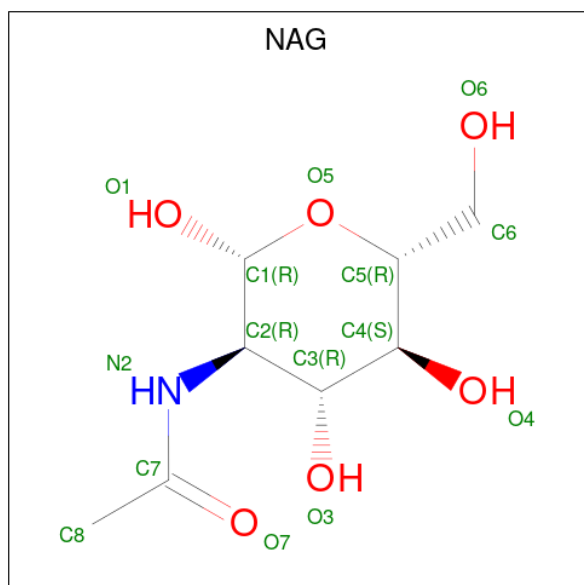
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

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

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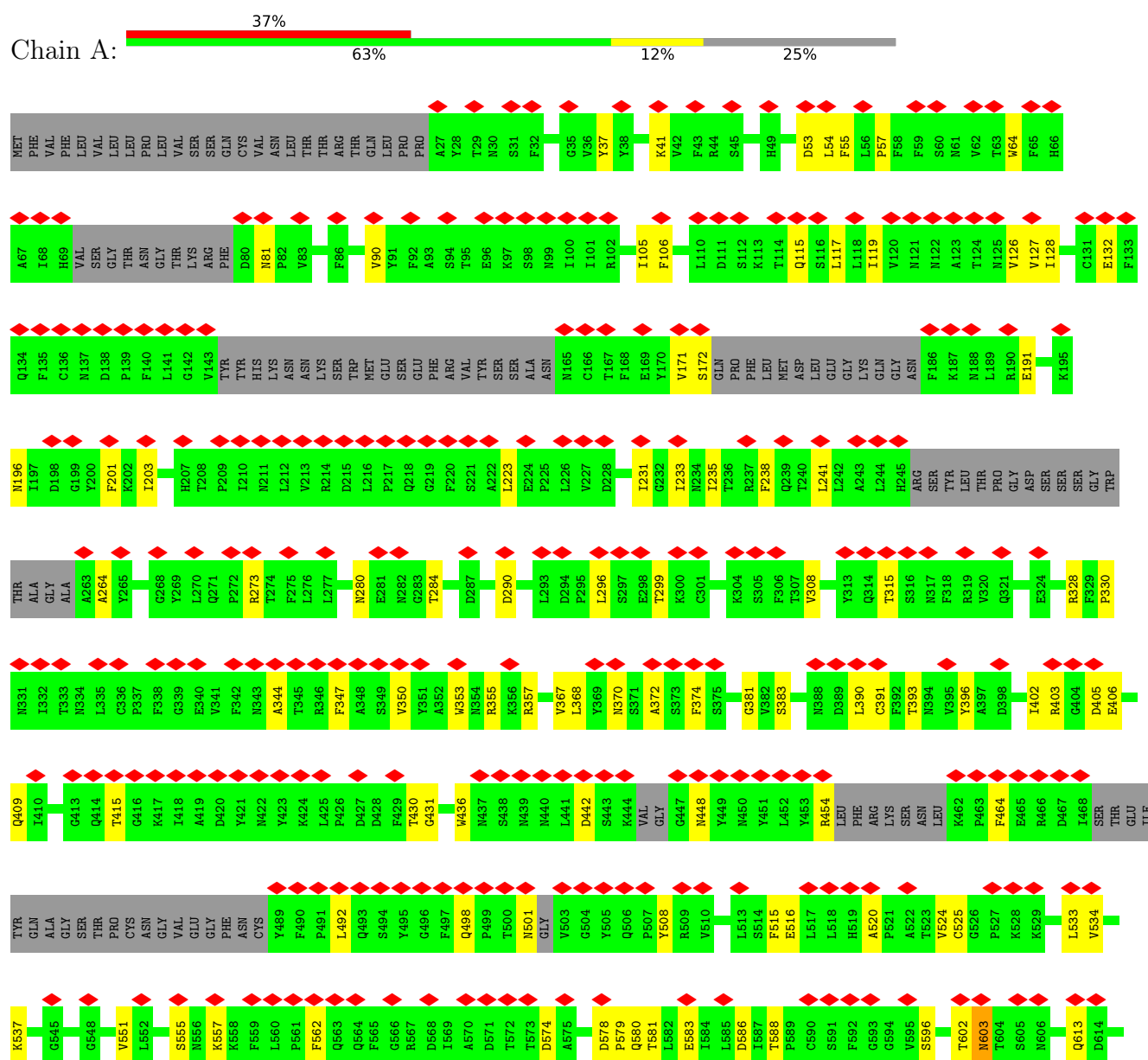
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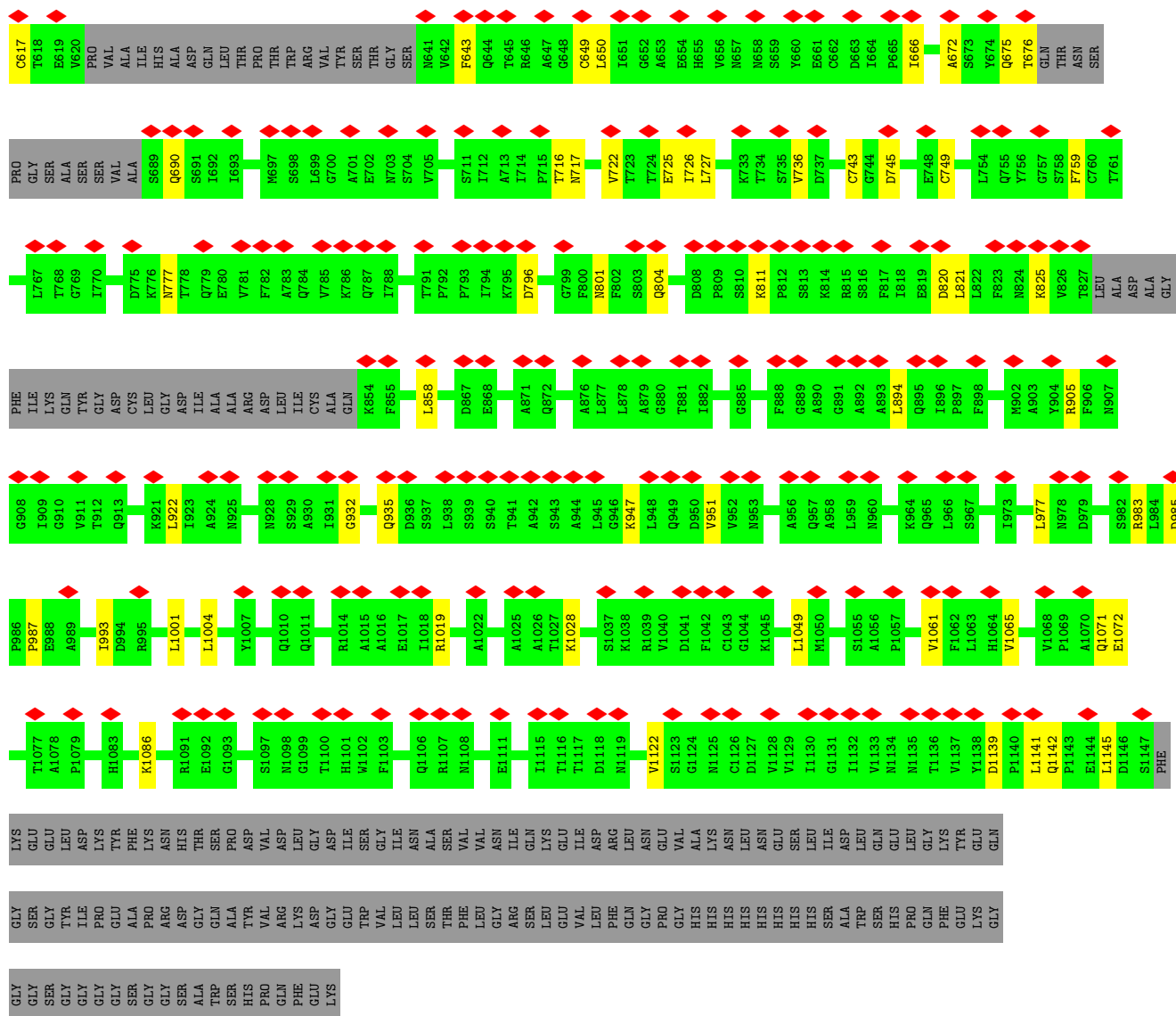
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

### 3 Residue-property plots

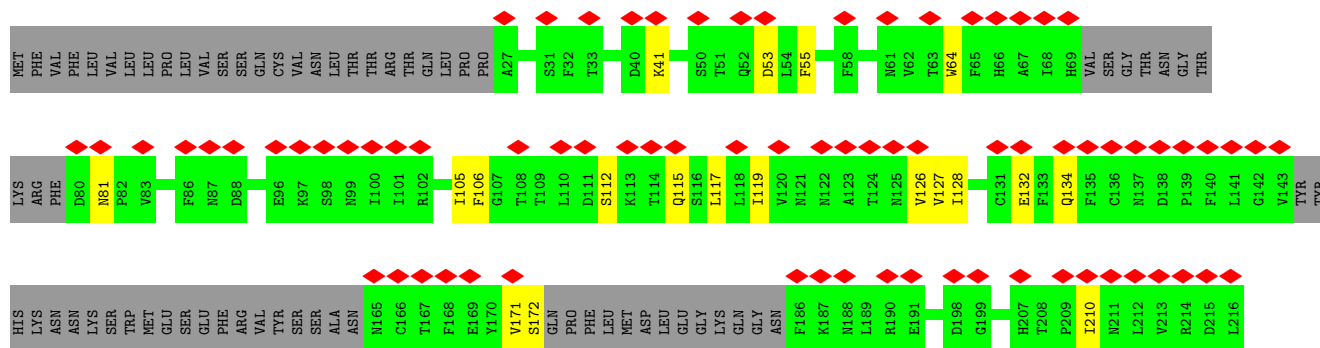
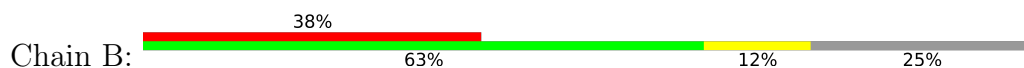
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Spike glycoprotein





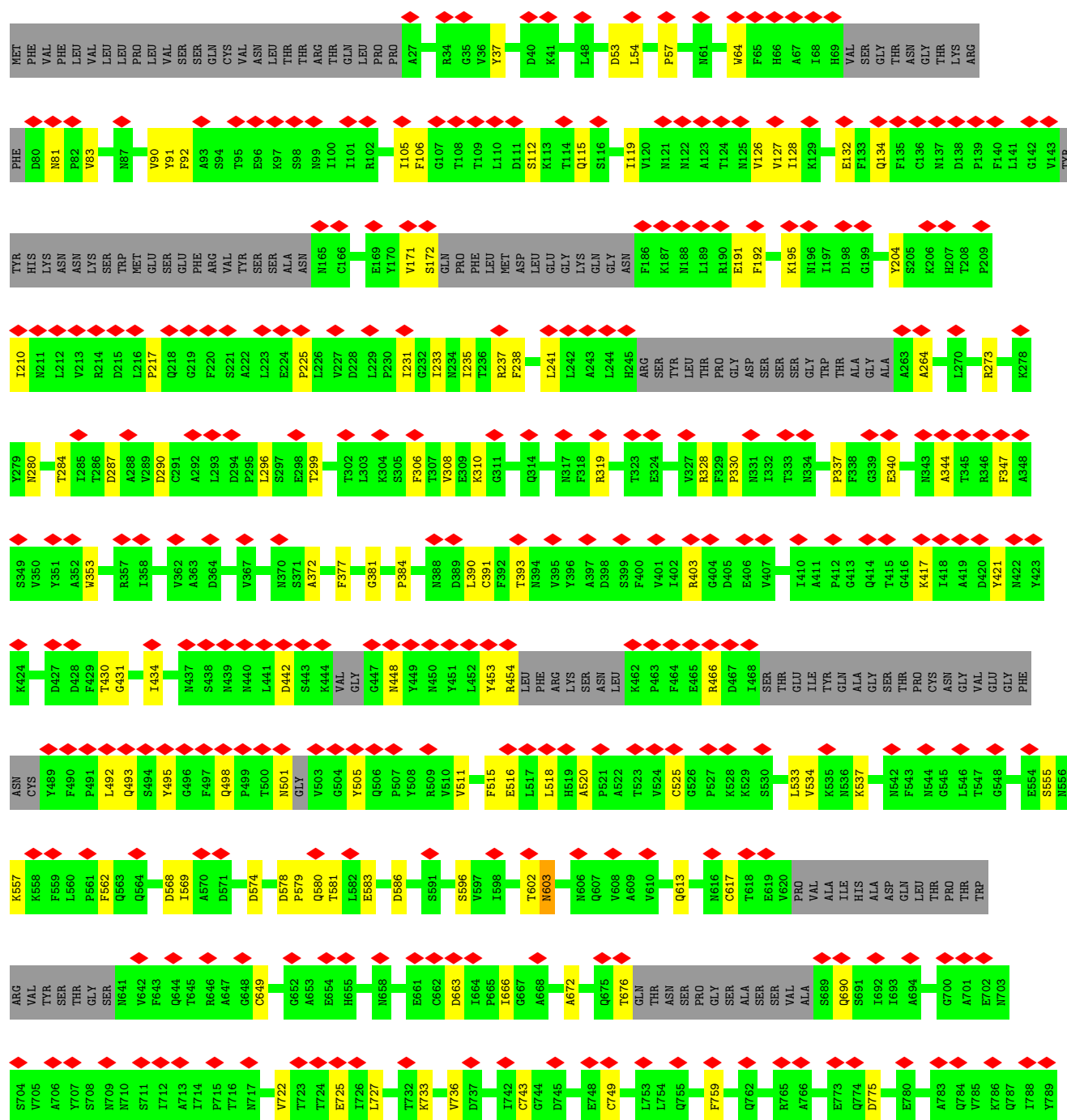
• Molecule 1: Spike glycoprotein

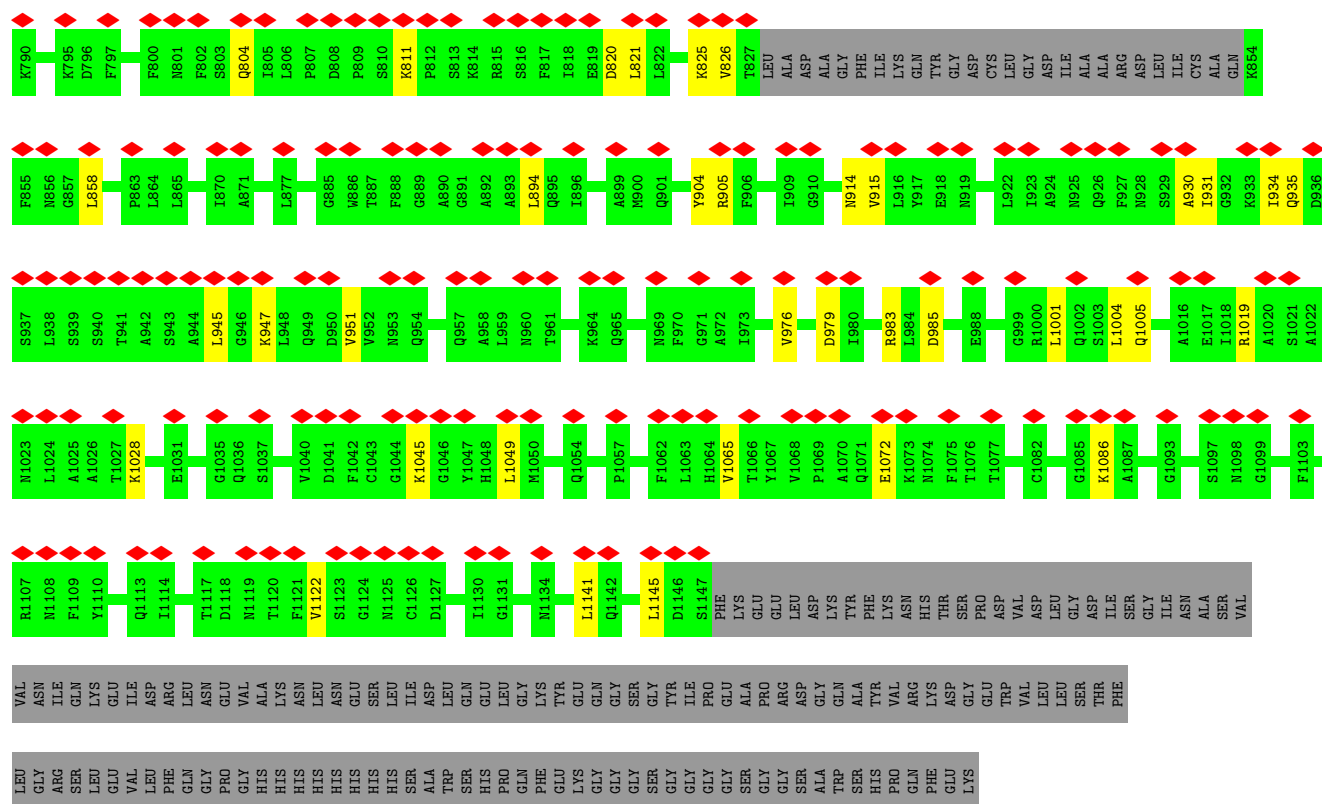


THR	SER	PRO	ASP	VAL	ASP	LEU	GLY	ASP	ILE	SER	GLY	ILE	ASN	ALA	SER	VAL	VAL	ASN	ILE	GLN	LYS	GLU	ILE	ASP	ARG	LEU	ASN	GLU	VAL	ALA	LYS	ASN	LEU	ASN	ILE	ASP	LEU	GLN	GLY	THR	THR	ALA	GLY	ALA	A263	A264	Y265	R273	L277	N280	E281	N282	G283	T284	I285	T286	D289	C291
F1089	P1090	R1091	E1092	G1093	V1094	F1095	G1099	W1102	R1107	E1111	P1112	Q1113	T1114	T1115	T1116	T1117	D1118	V1122	S1123	G1124	N1125	C1126	V1127	D1128	V1129	T1130	G1131	I1132	N1135	T1136	V1137	V1138	D1139	P1140	L1141	Q1142	P1143	E1144	L1145	D1146	PHE	LYS	GLU	LEU	ASP	LYS	TYR	PHE	ASN	HIS								
A1022	A1026	T1027	K1028	M1029	S1030	I1031	C1032	V1033	L1034	G1035	K1038	R1039	V1040	D1041	G1044	K1045	G1046	Y1047	L1049	M1050	S1051	F1052	P1053	A1056	P1057	H1058	G1059	V1060	V1061	F1062	L1063	H1064	V1065	T1066	Y1067	Q1071	E1072	K1073	N1074	F1075	T1076	T1077	A1078	P1079	C1082	H1083	L1084	G1085	K1086	A1087	H1088							
A930	I931	G932	K933	I934	Q935	L938	S939	S940	T941	A942	S943	A944	L945	G946	K947	L948	Q949	D950	V951	V952	N953	Q954	N955	A958	L962	L966	G971	A972	I973	S974	L977	L981	S982	L984	D985	E990	I993	D994	L1001	Q1002	S1003	L1004	A1016	R1019	A1020	S1021												
M856	G857	L858	T859	L864	M869	K872	A876	C880	T881	L882	T883	S884	C885	W886	C889	A890	C891	A892	A893	Q895	I896	F898	A899	Q901	N902	A903	Y904	R905	G908	I909	T912	Q913	N914	V915	L916	Y917	E918	N919	Q920	K921	L922	I923	A924	N925	Q926	F927	S929											
S704	V705	A706	V707	S708	N709	M710	S711	I712	A713	I714	P715	T716	N717	F718	T719	I720	S721	W722	E725	L726	L727	F728	K733	V736	D737	C738	T739	C743	E748	C749	S750	M751	L752	Q755	F759	Q762	A771	V772	Q773	Q774	D775	K776	Q779	E780	A783	K786												
T794	K795	D796	F800	H801	F802	S803	Q804	L805	L806	P807	D808	P809	S810	K811	P812	S813	K814	R815	S816	F817	L818	E819	D820	L821	L822	F823	P827	K825	W826	T827	LEU	ASP	ALA	GLY	PHE	ILE	GLN	TYR	GLY	ASP	CYS	GLY	ASP	ILE	CYS	ALA	K854	F855										
THR	GLY	SER	N641	V642	F643	R646	A647	G648	C649	L650	L651	G652	A653	E654	H655	V656	N657	N658	S659	C662	D663	L664	P665	A668	G669	L670	C671	A672	S673	Y674	Q675	G676	GLN	THR	ASN	SER	PRO	GLY	SER	ALA	SER	VAL	ALA	S689	Q690	S691	L692	T693	A694	V695	T696	N697	E702	N703				
I569	A570	D571	T572	T573	D574	A575	G576	R577	D578	Q580	T581	L582	E583	L584	L585	D586	L587	T588	P589	F592	G593	G601	T602	N603	T604	S605	P527	S630	L533	V534	K535	N536	K537	C538	V539	N544	G545	L546	G550	S555	K557	N558	P561	F562	Q563	Q564	F565	G566	D568									
F497	Q498	P499	T500	N501	GLY	V503	G504	Y505	Q506	P507	Y508	R509	V510	V511	S514	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	S530	L533	V534	K535	N536	K537	C538	V539	N544	G545	L546	G550	S555	K557	N558	P561	F562	Q563	Q564	F565	G566	D568									
M437	S438	N439	M440	L441	D442	S443	K444	VAL	GLY	G447	M448	M450	Y451	L452	Y453	R454	PHE	ARG	LYS	SER	ASN	LEU	K462	F463	F464	E465	R466	D467	I468	SER	THR	GLU	ILE	TYR	GLN	ALA	GLY	SER	THR	PRO	CYS	ASN	GLY	GLU	PHE	ASN	CYS	Y489	F490	L492	Q493	S494	Y495	G496				
A363	D364	V367	L368	Y369	A372	S375	T376	F377	K378	G381	V382	S383	P384	L390	C391	F392	T393	N394	D398	S399	F400	Y401	I402	R403	G404	D405	E406	Q409	G413	Q414	T415	G416	K417	I418	A419	D420	Y421	M422	Y423	K424	L425	P426	D427	F429	T430	G431	T434	A435	W436									
A392	L293	D294	P295	L296	S297	E298	T299	K300	C301	T302	L303	K304	V308	E309	K310	Q314	N317	F318	R319	V320	Q321	P322	T323	S325	I326	V327	R328	F329	P330	N331	I332	P337	E340	V341	F342	N343	A344	T345	R346	Y347	A348	S349	V350	Y351	A352	W353	N354	R355	K356	R357	N360							



- Molecule 1: Spike glycoprotein





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



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



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



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

Chain G: 



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

Chain H: 



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

Chain I: 



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

Chain J: 



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

Chain K: 



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

Chain L: 



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



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



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



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



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126719	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.770	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.28	0/7772	0.48	0/10572
1	B	0.28	0/7772	0.48	0/10572
1	C	0.27	0/7772	0.48	0/10572
All	All	0.28	0/23316	0.48	0/31716

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	7604	0	7419	105	0
1	B	7604	0	7419	107	0
1	C	7604	0	7417	102	0
2	D	28	0	25	0	0
2	E	28	0	25	3	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
3	A	154	0	142	1	0
3	B	154	0	142	1	0
3	C	154	0	142	1	0
All	All	23694	0	23056	289	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 6.

The worst 5 of 289 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:C:391:CYS:HB2	1:C:525:CYS:HA	1.53	0.90
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.54	0.89
1:A:196:ASN:HD21	1:A:235:ILE:HD12	1.54	0.72
1:A:393:THR:OG1	1:A:516:GLU:OE2	2.07	0.72
1:A:191:GLU:HG2	1:A:223:LEU:HD21	1.70	0.72

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	948/1288 (74%)	929 (98%)	19 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	948/1288 (74%)	923 (97%)	25 (3%)	0	100	100
1	C	948/1288 (74%)	930 (98%)	18 (2%)	0	100	100
All	All	2844/3864 (74%)	2782 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	852/1113 (76%)	850 (100%)	2 (0%)	92	96
1	B	852/1113 (76%)	849 (100%)	3 (0%)	89	93
1	C	852/1113 (76%)	851 (100%)	1 (0%)	92	97
All	All	2556/3339 (76%)	2550 (100%)	6 (0%)	91	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	603	ASN
1	B	675	GLN
1	C	603	ASN
1	A	675	GLN
1	A	603	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	804	GLN
1	C	935	GLN
1	C	1005	GLN
1	B	949	GLN
1	A	196	ASN

### 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 ⓘ

30 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	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.45	0
2	NAG	E	1	2	14,14,15	0.46	0	17,19,21	0.43	0
2	NAG	E	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	F	1	2	14,14,15	0.36	0	17,19,21	0.37	0
2	NAG	F	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	G	1	2,1	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	G	2	2	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	H	1	2,1	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	H	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	I	1	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	J	1	2	14,14,15	0.45	0	17,19,21	0.42	0
2	NAG	J	2	2	14,14,15	0.18	0	17,19,21	0.42	0
2	NAG	K	1	2	14,14,15	0.32	0	17,19,21	0.37	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	L	1	2,1	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	L	2	2	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	M	1	2,1	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	M	2	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	N	1	2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	N	2	2	14,14,15	0.19	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	O	1	2,1	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	O	2	2	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	P	1	2,1	14,14,15	0.24	0	17,19,21	0.39	0
2	NAG	P	2	2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	Q	1	2,1	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	Q	2	2	14,14,15	0.27	0	17,19,21	0.41	0
2	NAG	R	1	2,1	14,14,15	0.17	0	17,19,21	0.45	0
2	NAG	R	2	2	14,14,15	0.24	0	17,19,21	0.43	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
2	NAG	D	1	2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	1/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

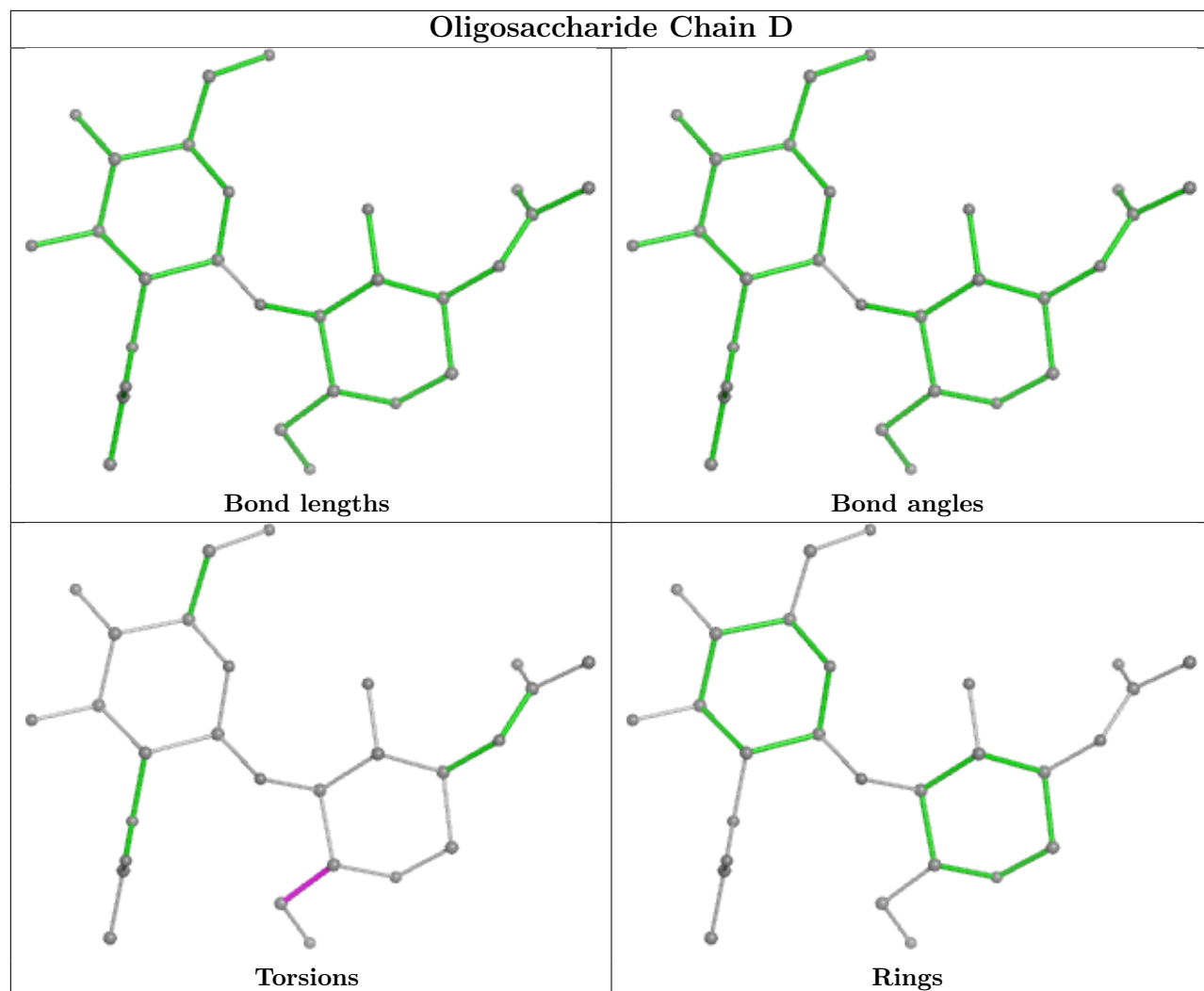
Mol	Chain	Res	Type	Atoms
2	N	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6

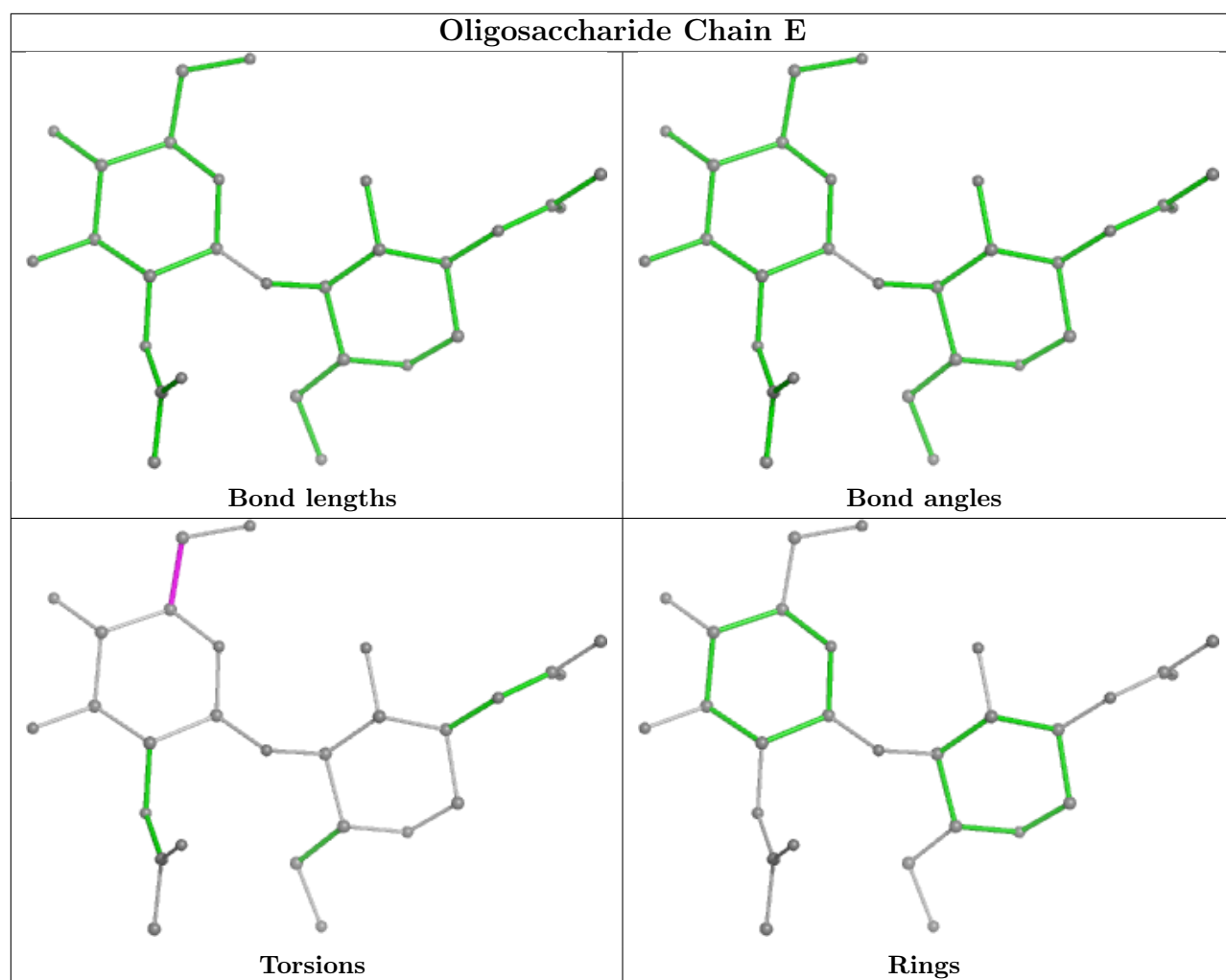
There are no ring outliers.

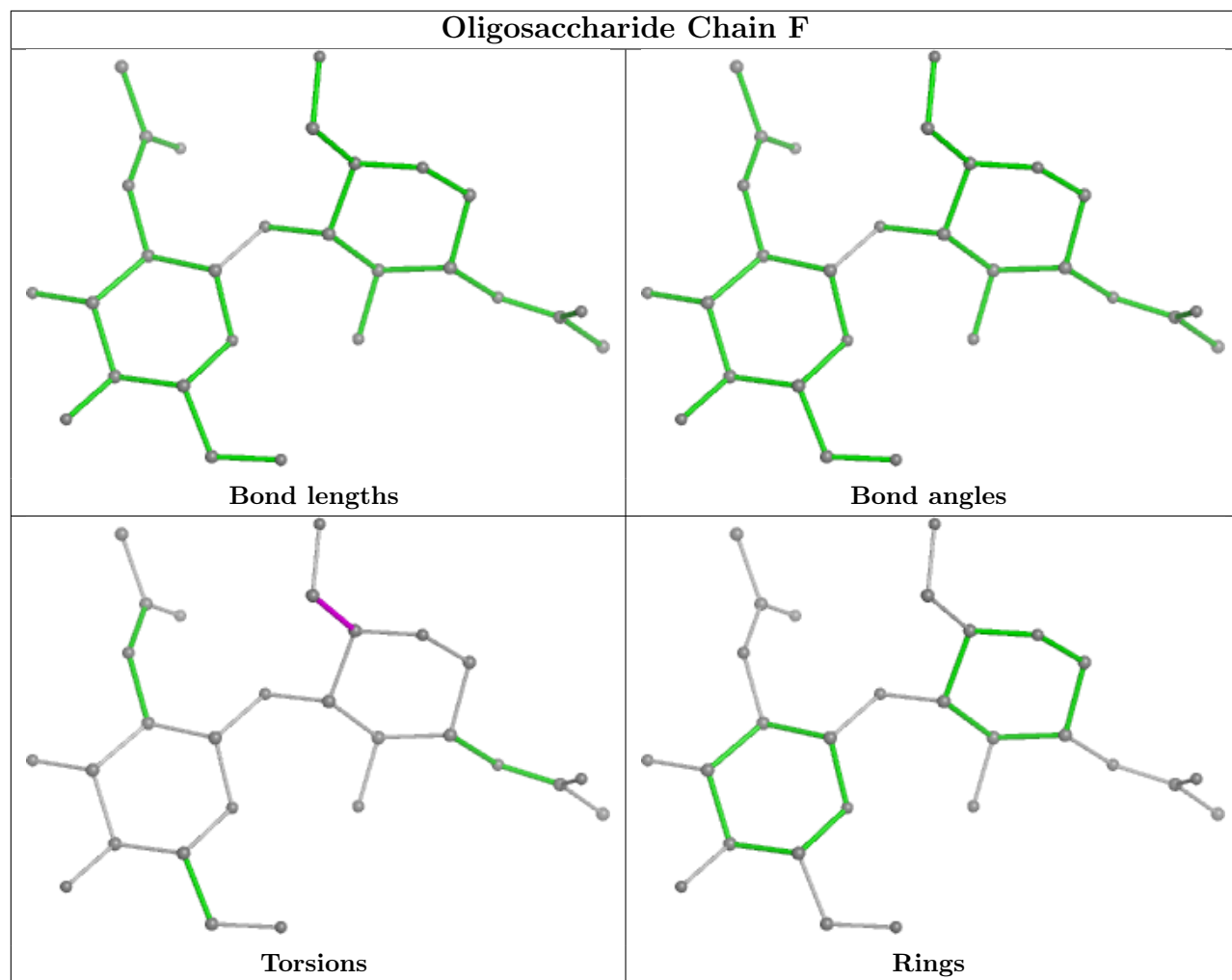
3 monomers are involved in 7 short contacts:

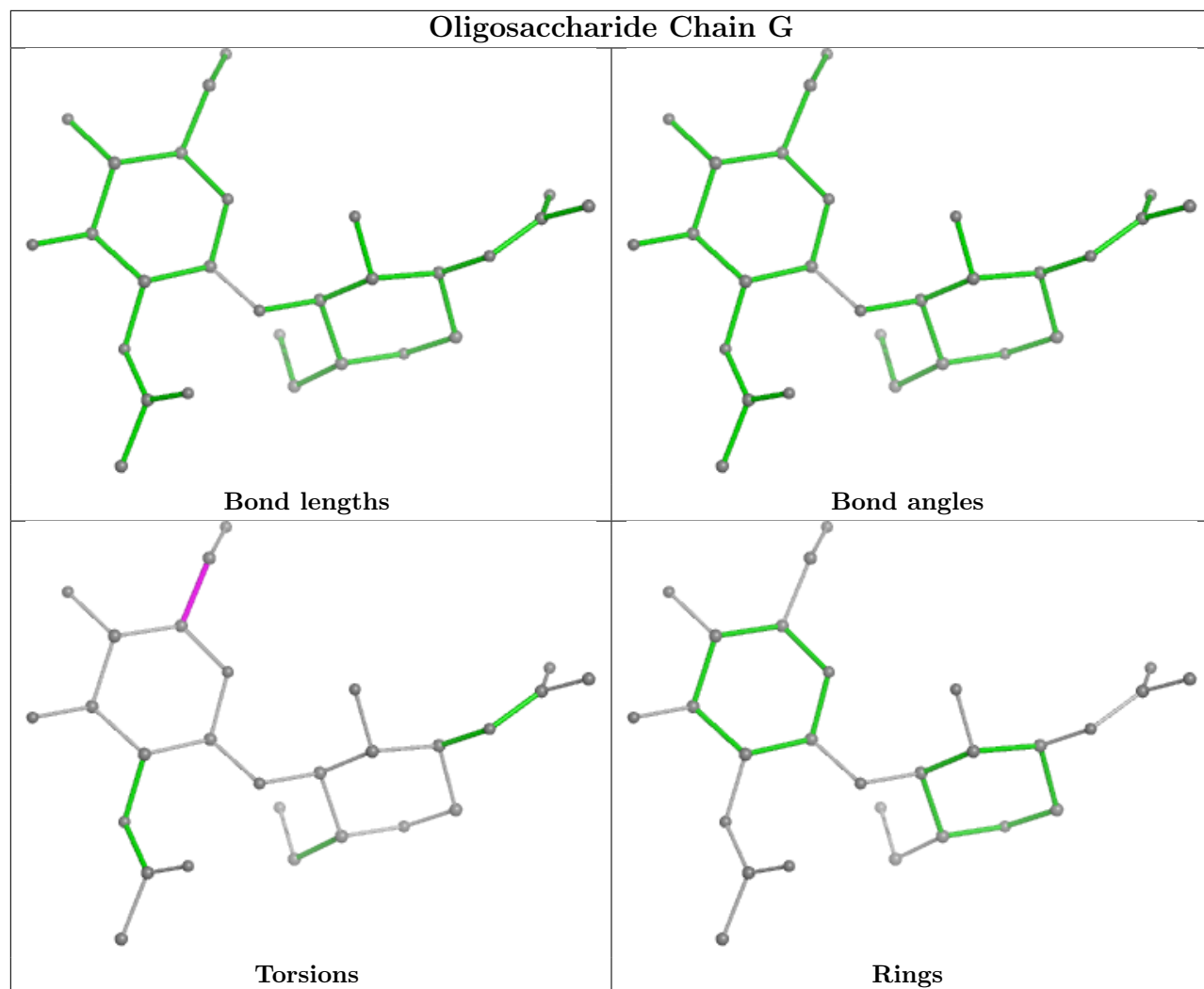
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	3	0
2	J	1	NAG	3	0
2	F	1	NAG	1	0

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

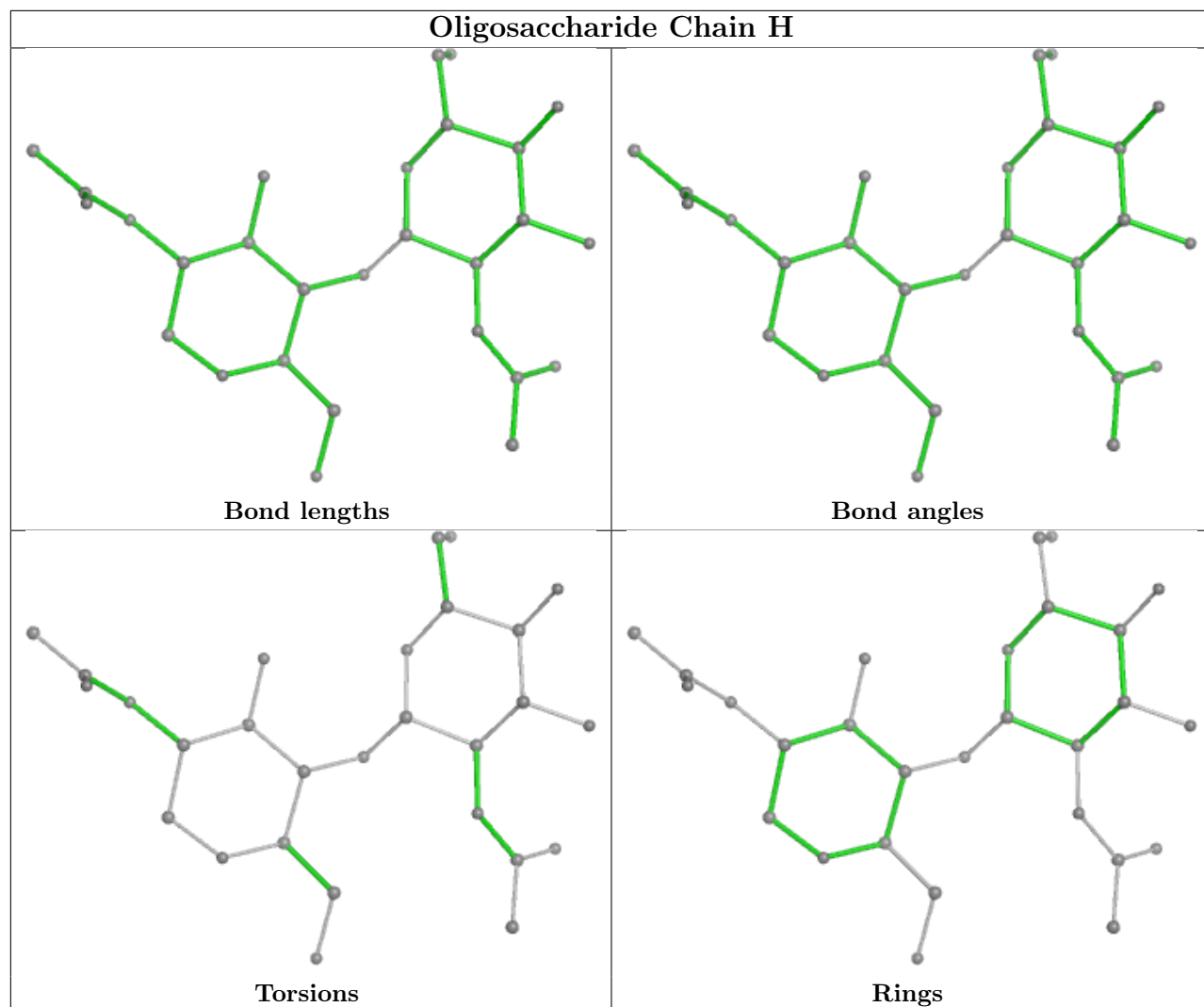


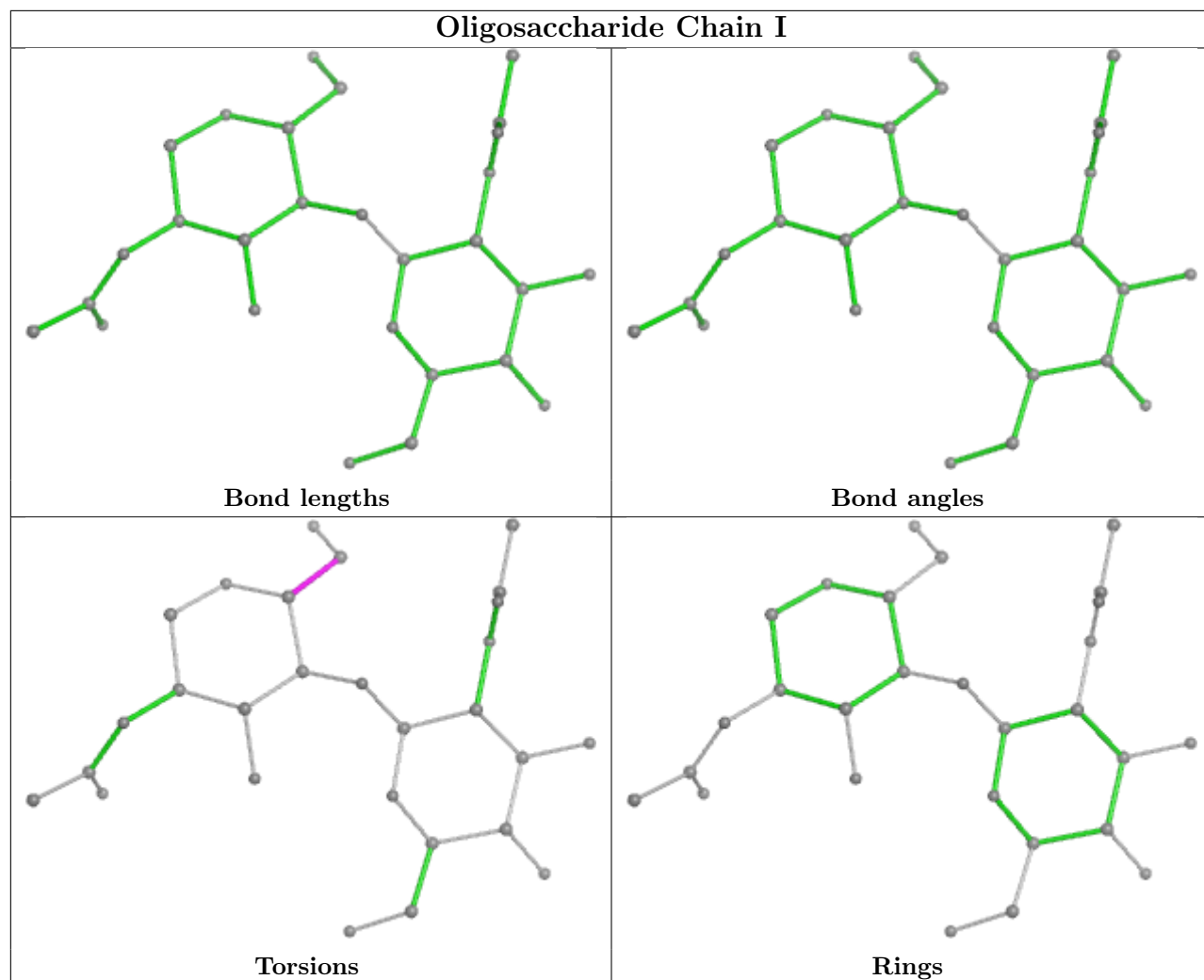


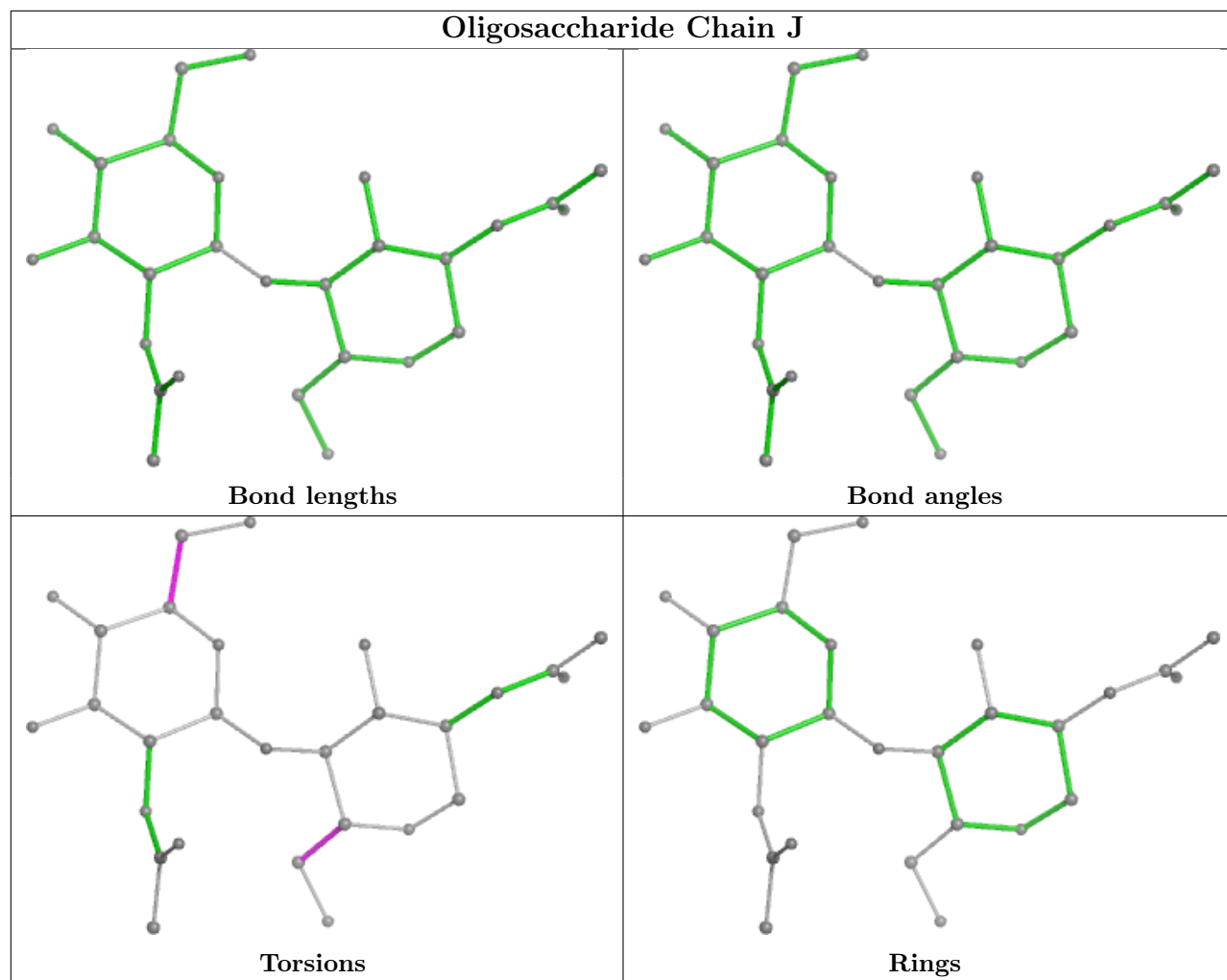


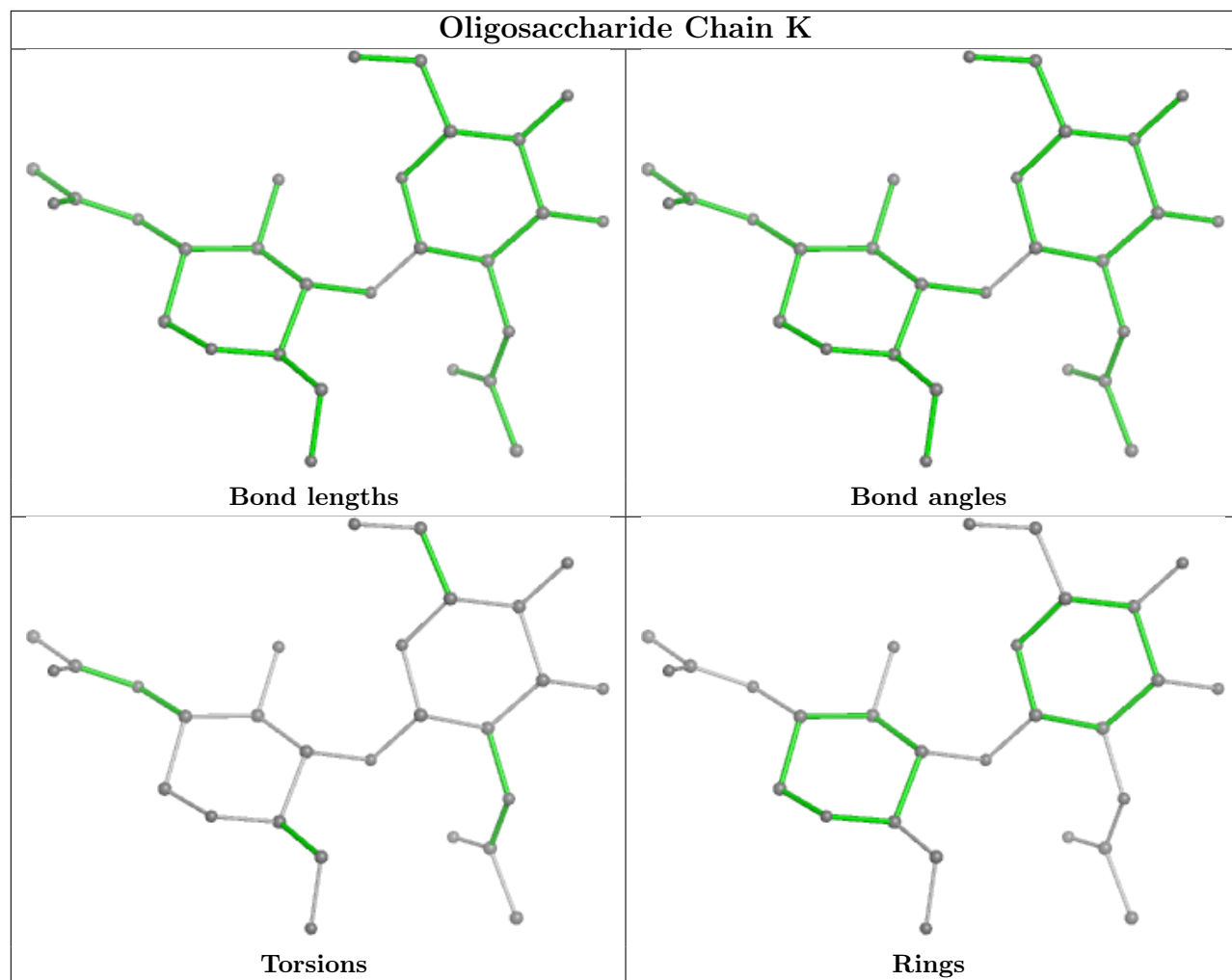




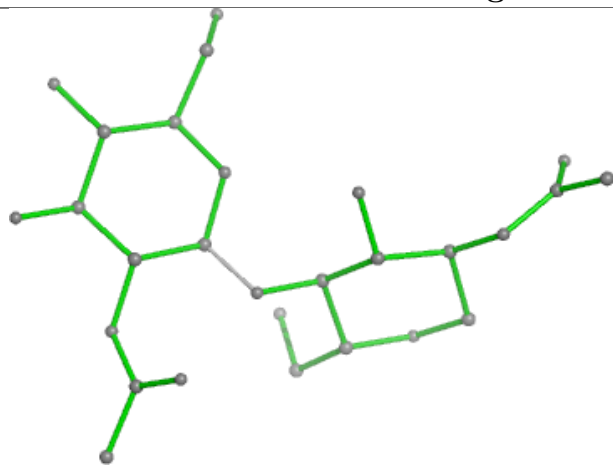




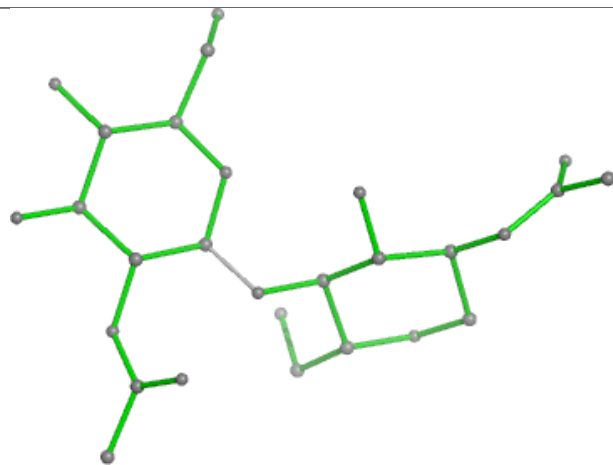




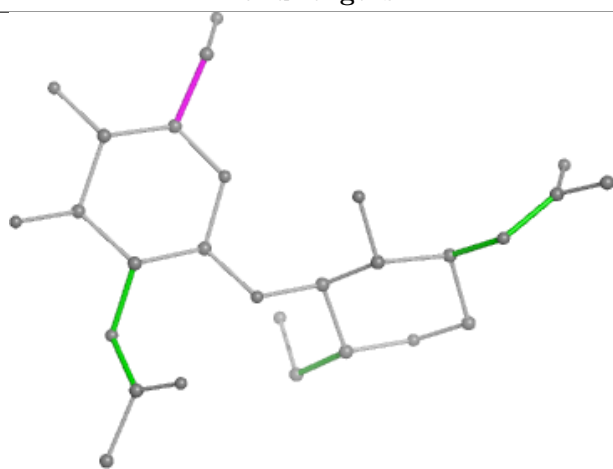
## Oligosaccharide Chain L



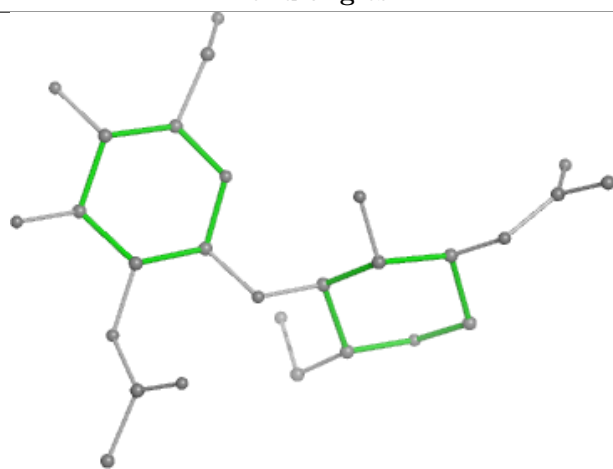
Bond lengths



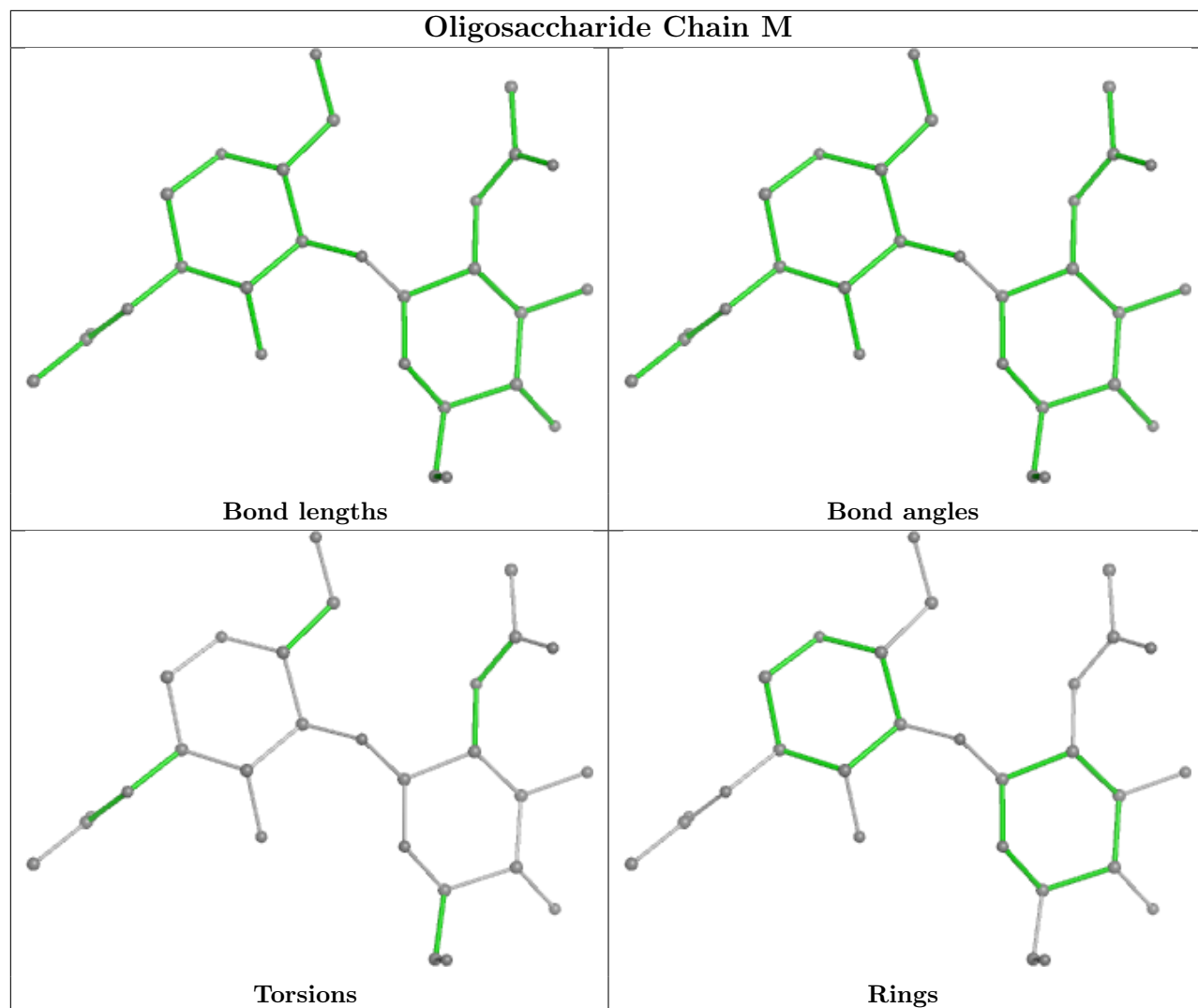
Bond angles

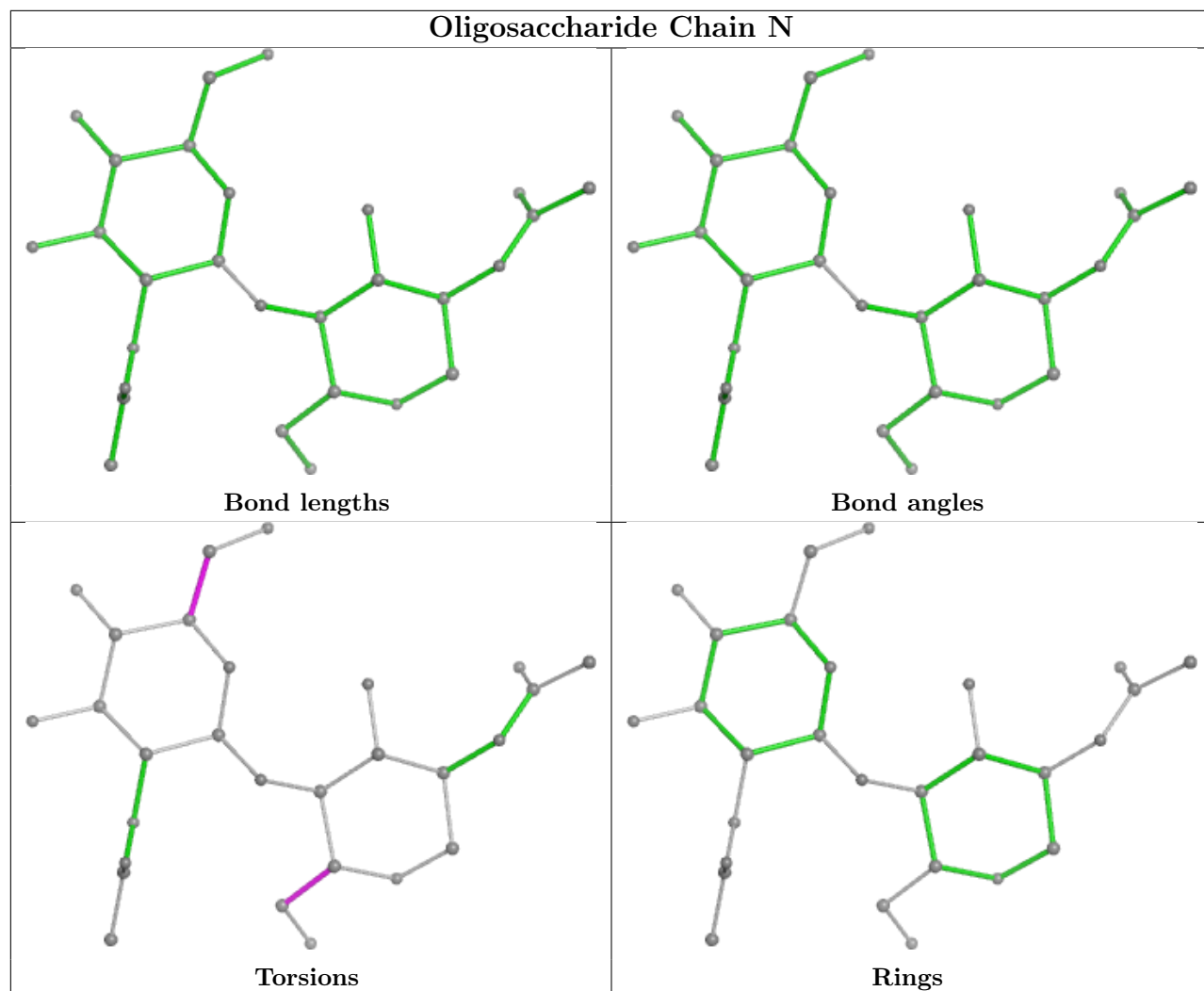


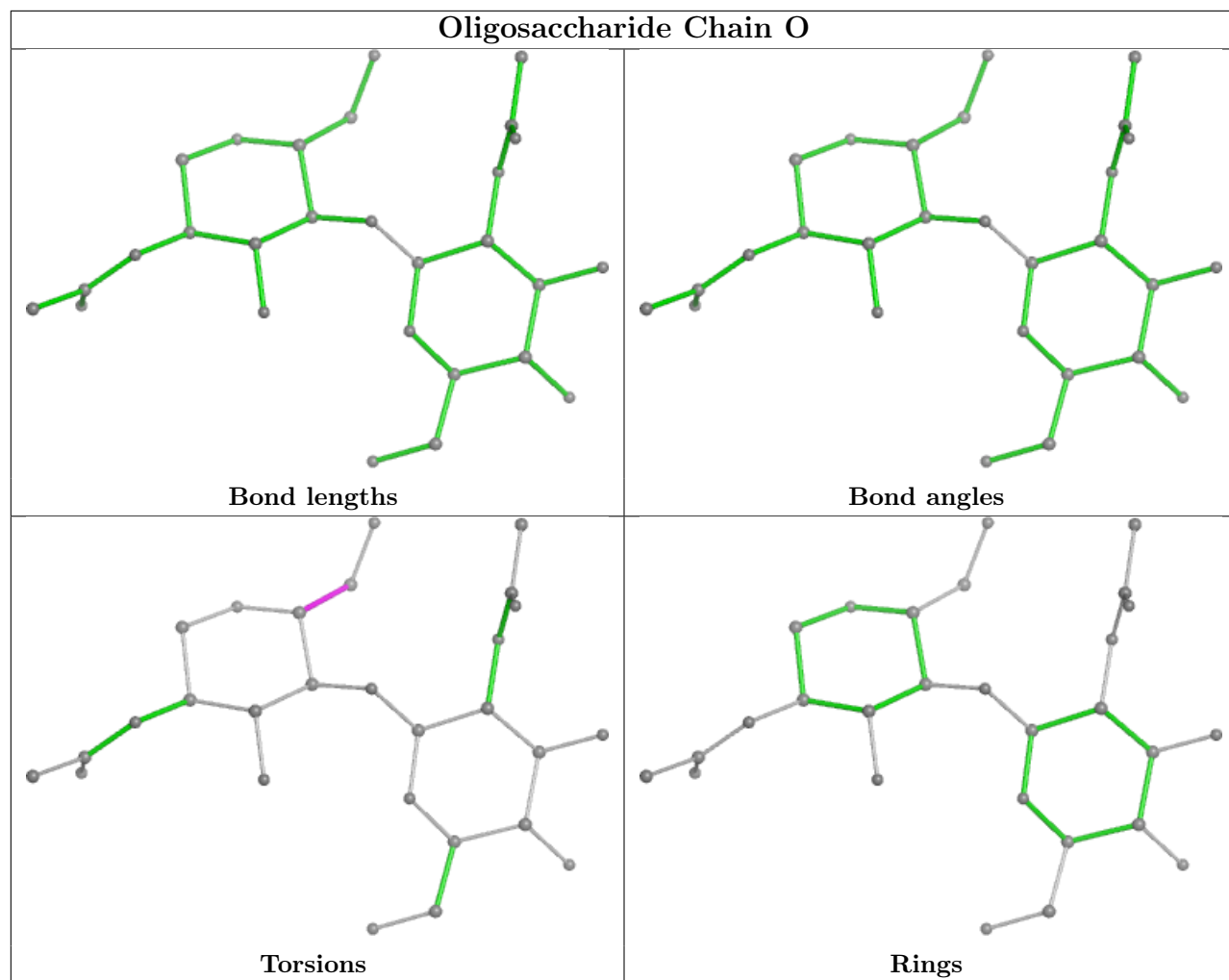
Torsions



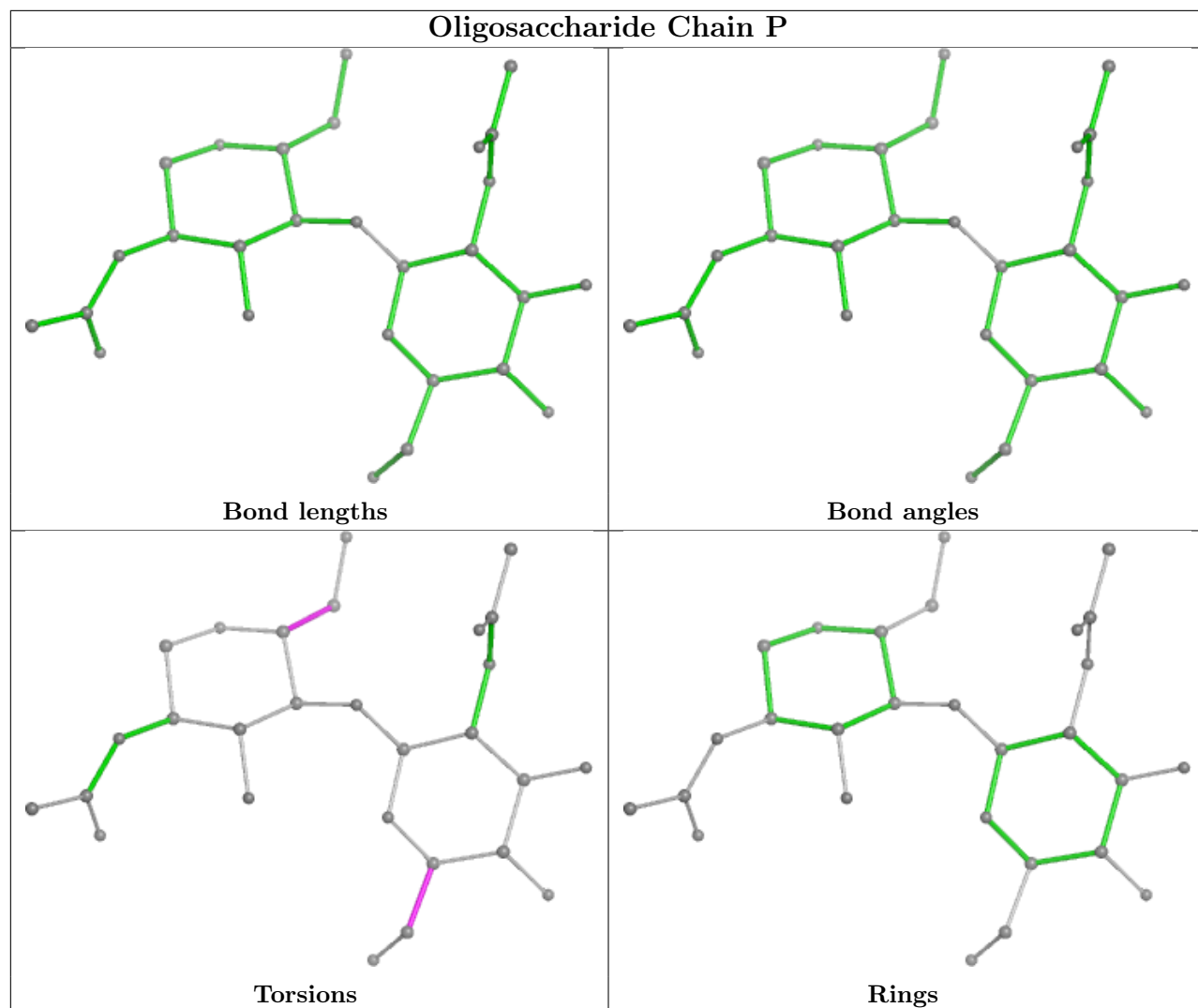
Rings

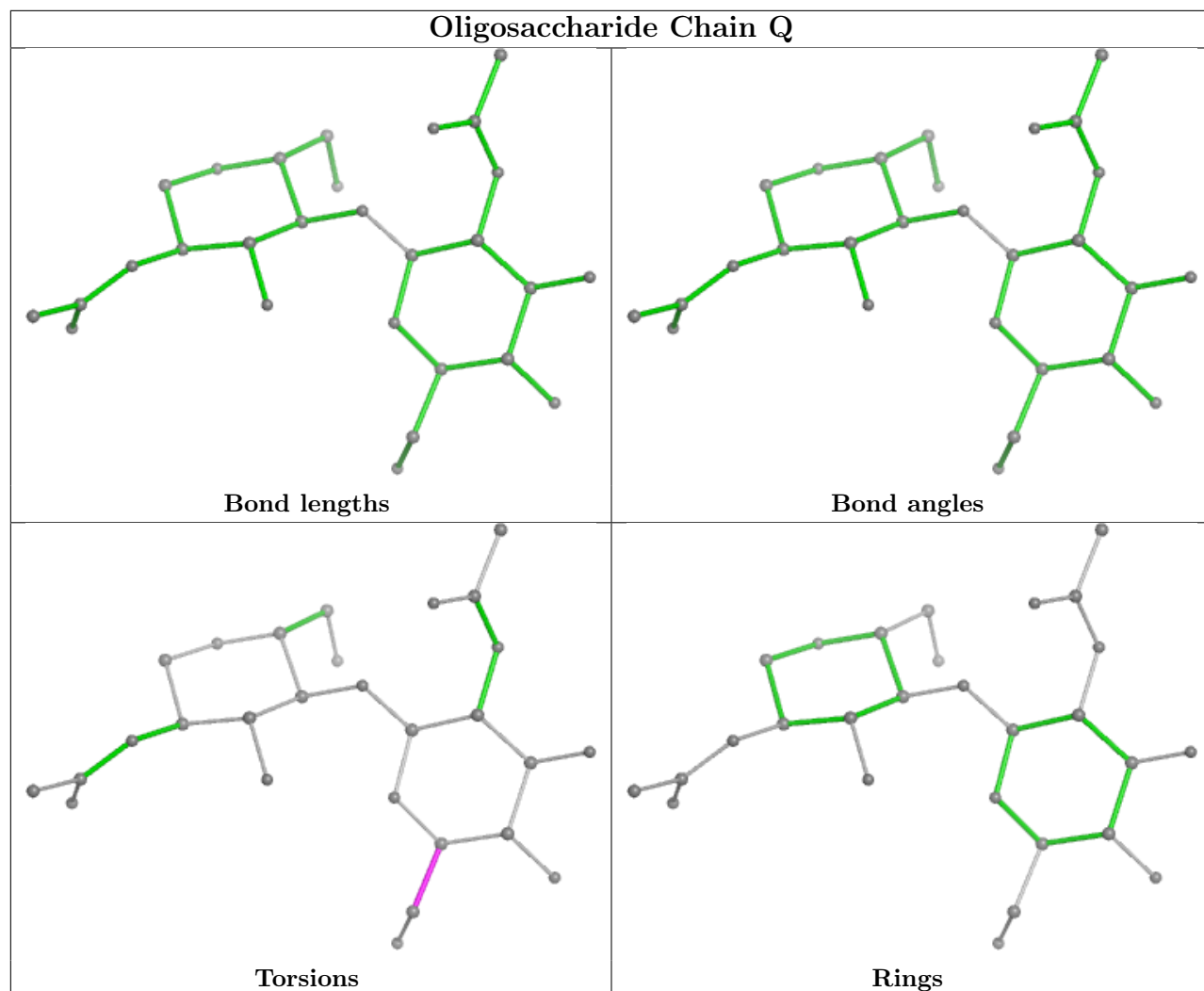


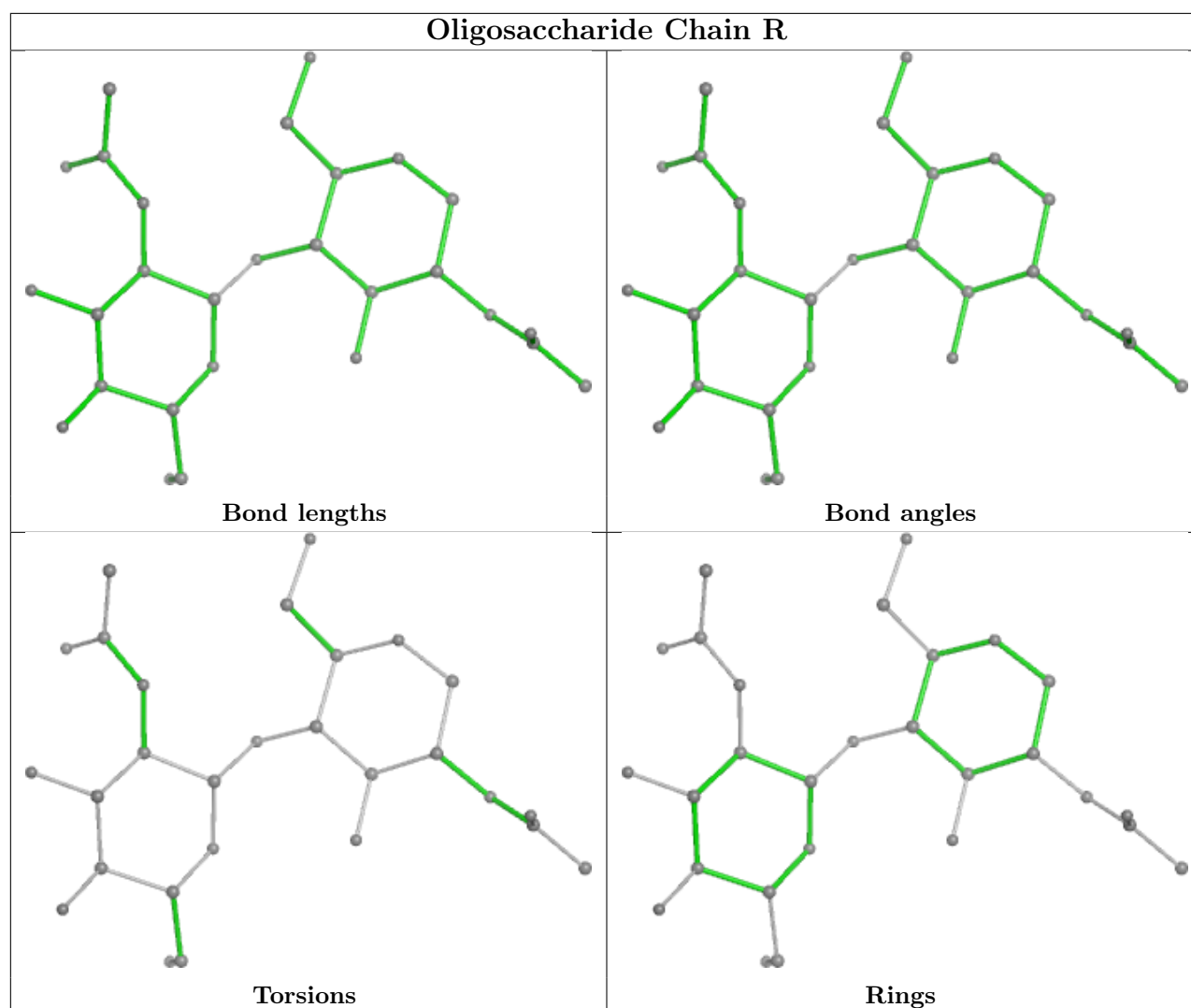












## 5.6 Ligand geometry [i](#)

33 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	$\# Z  > 2$
3	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	B	1310	1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1307	1	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	B	1303	1	14,14,15	0.30	0	17,19,21	0.43	0
3	NAG	C	1301	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.50	0
3	NAG	C	1311	-	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	B	1311	-	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	A	1302	-	14,14,15	0.25	0	17,19,21	0.53	0
3	NAG	C	1305	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	A	1309	1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	C	1303	1	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	B	1308	1	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	C	1309	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	A	1301	1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	B	1302	-	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	B	1306	-	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	A	1304	1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	C	1306	-	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	A	1310	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	B	1307	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	C	1307	1	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.44	0
3	NAG	B	1309	1	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	C	1302	-	14,14,15	0.24	0	17,19,21	0.53	0
3	NAG	A	1311	-	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	A	1306	-	14,14,15	0.20	0	17,19,21	0.43	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
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1311	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1311	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	-	-	1/6/23/26	0/1/1/1
3	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1302	-	-	1/6/23/26	0/1/1/1
3	NAG	A	1311	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1308	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6

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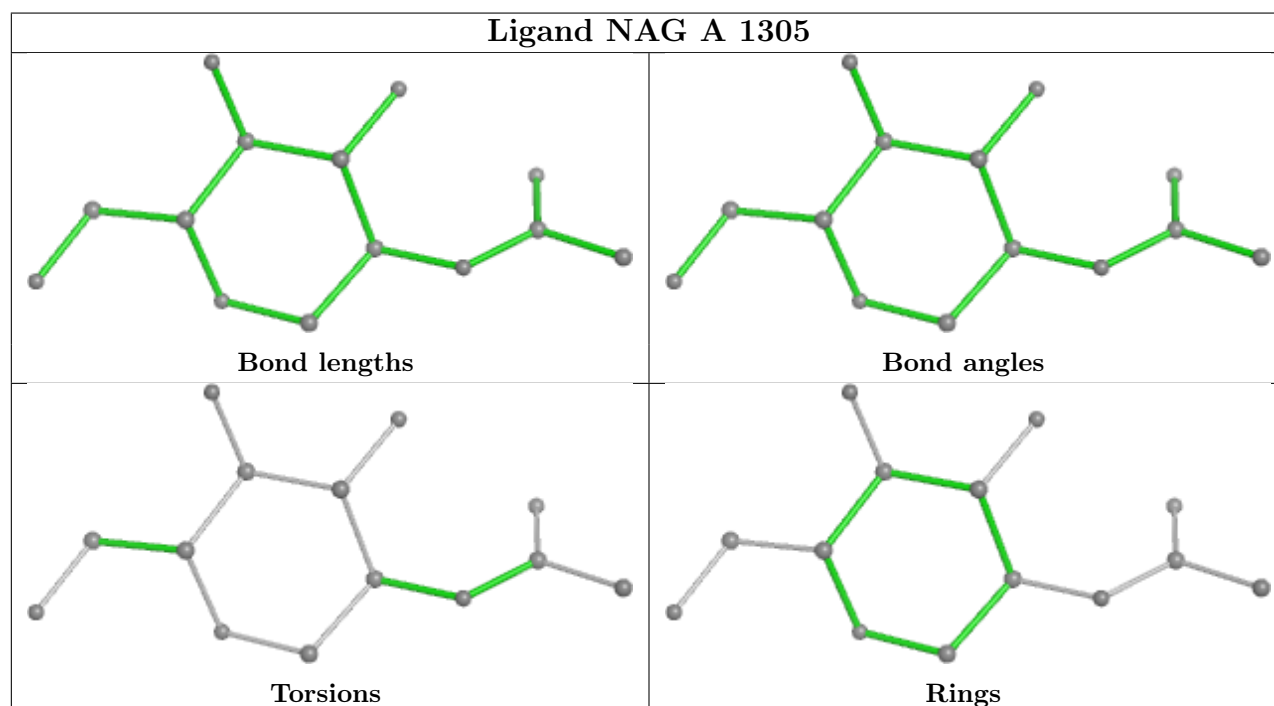
Mol	Chain	Res	Type	Atoms
3	A	1303	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6

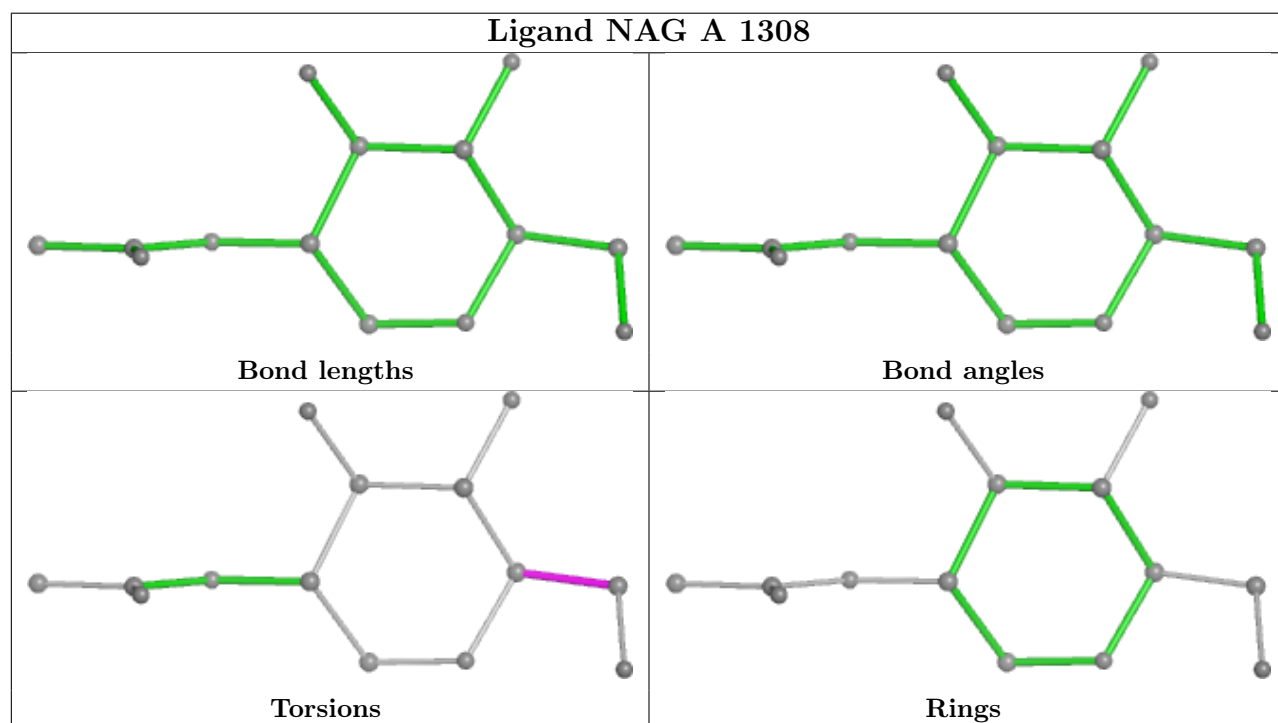
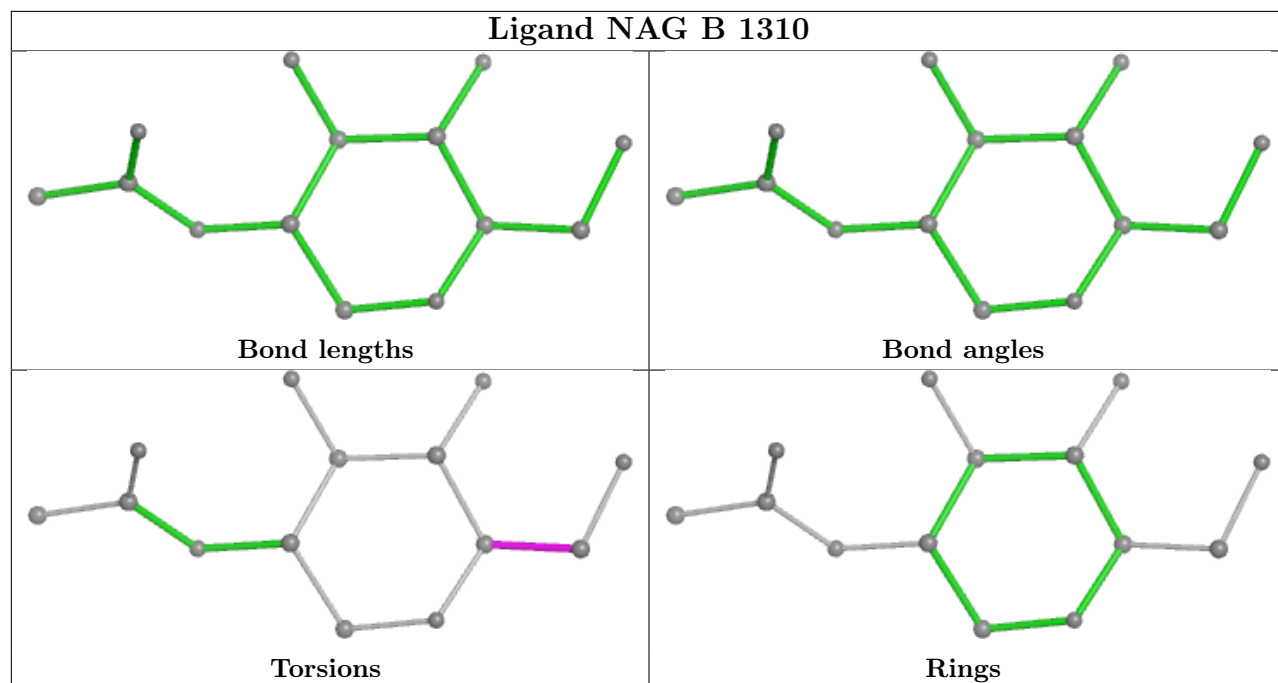
There are no ring outliers.

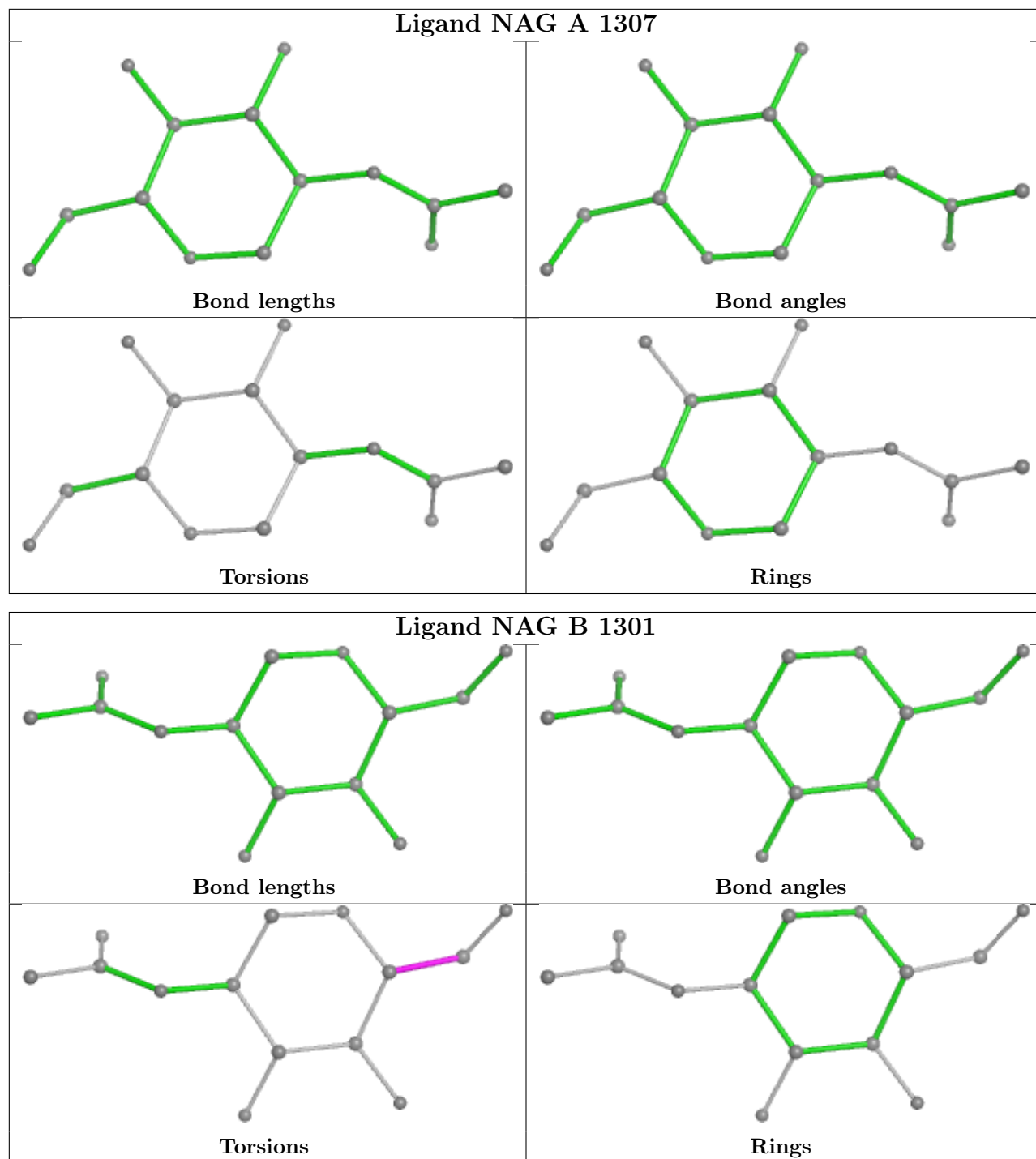
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1304	NAG	1	0
3	C	1304	NAG	1	0
3	A	1304	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.

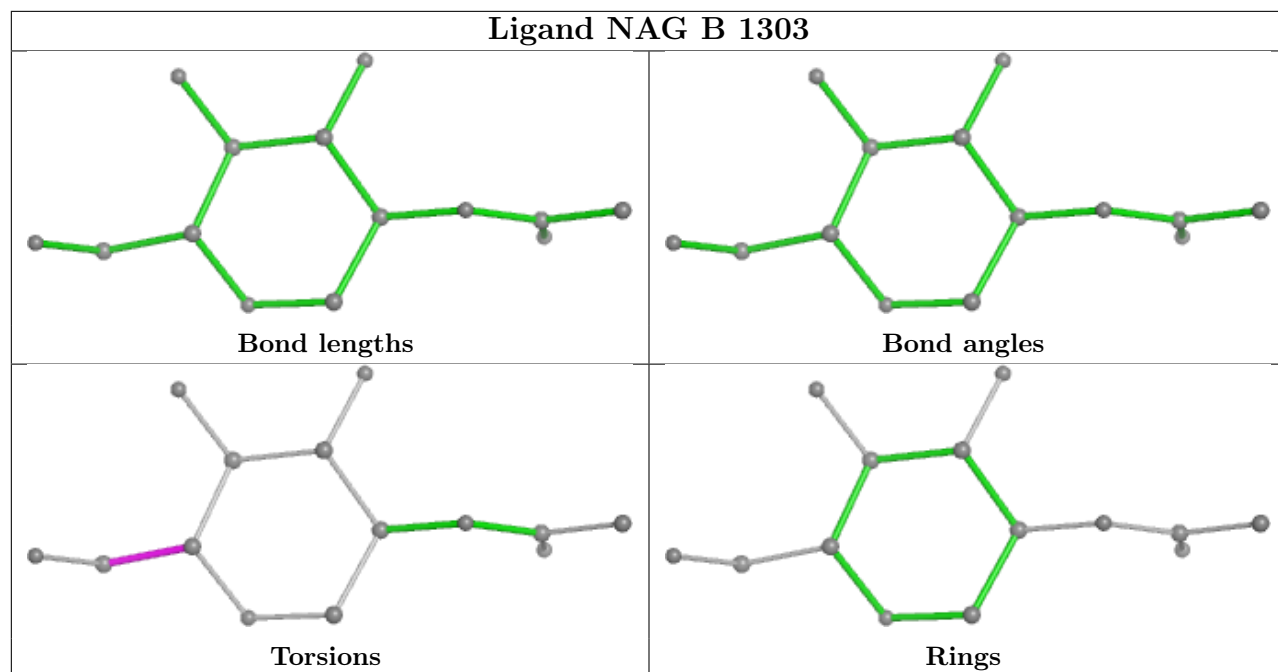




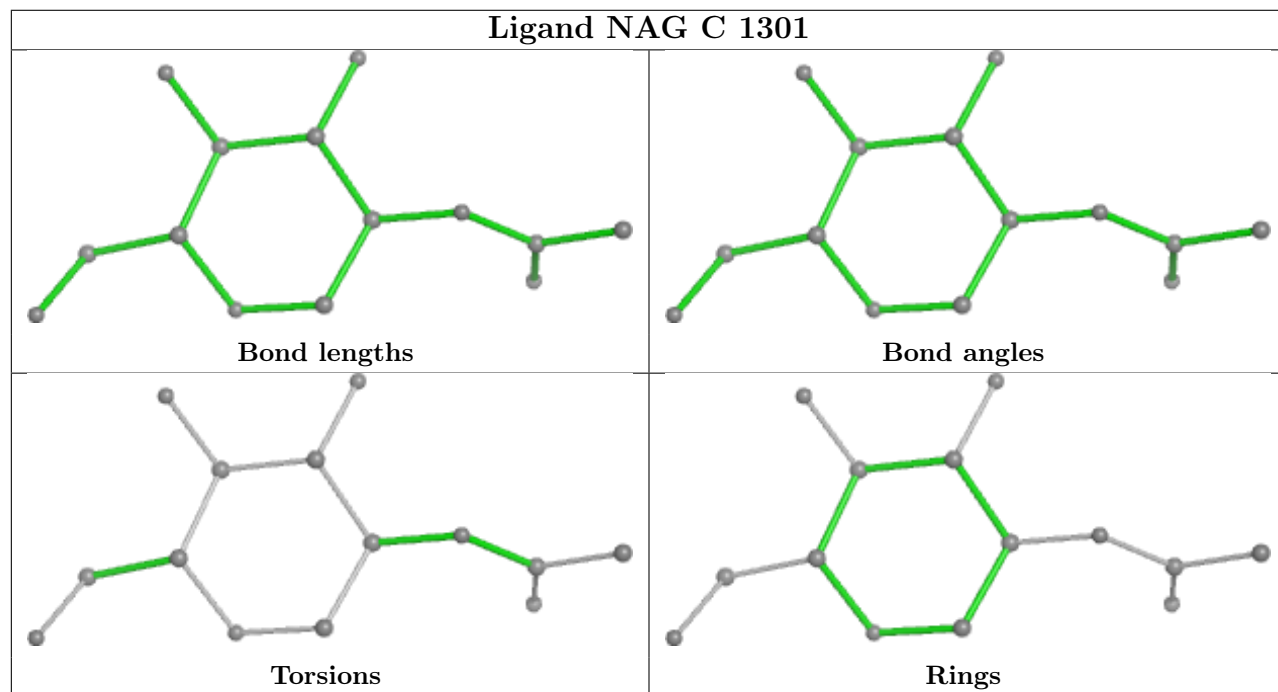




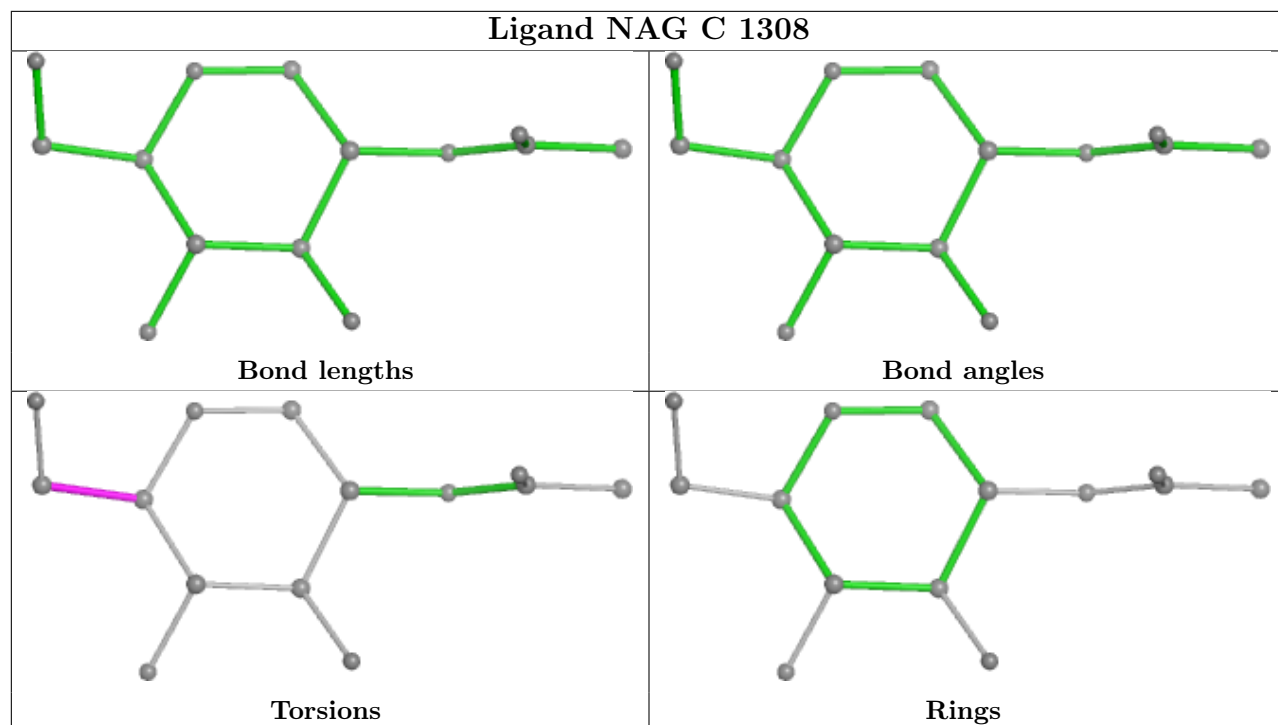
## Ligand NAG B 1303



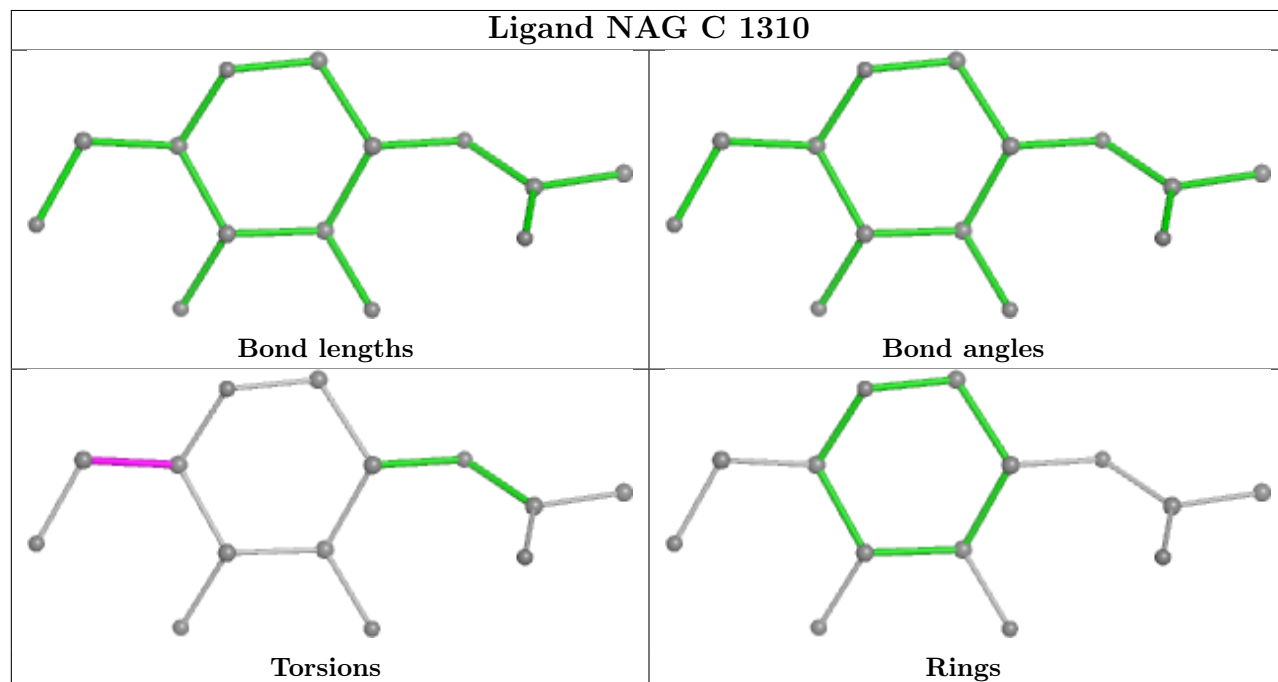
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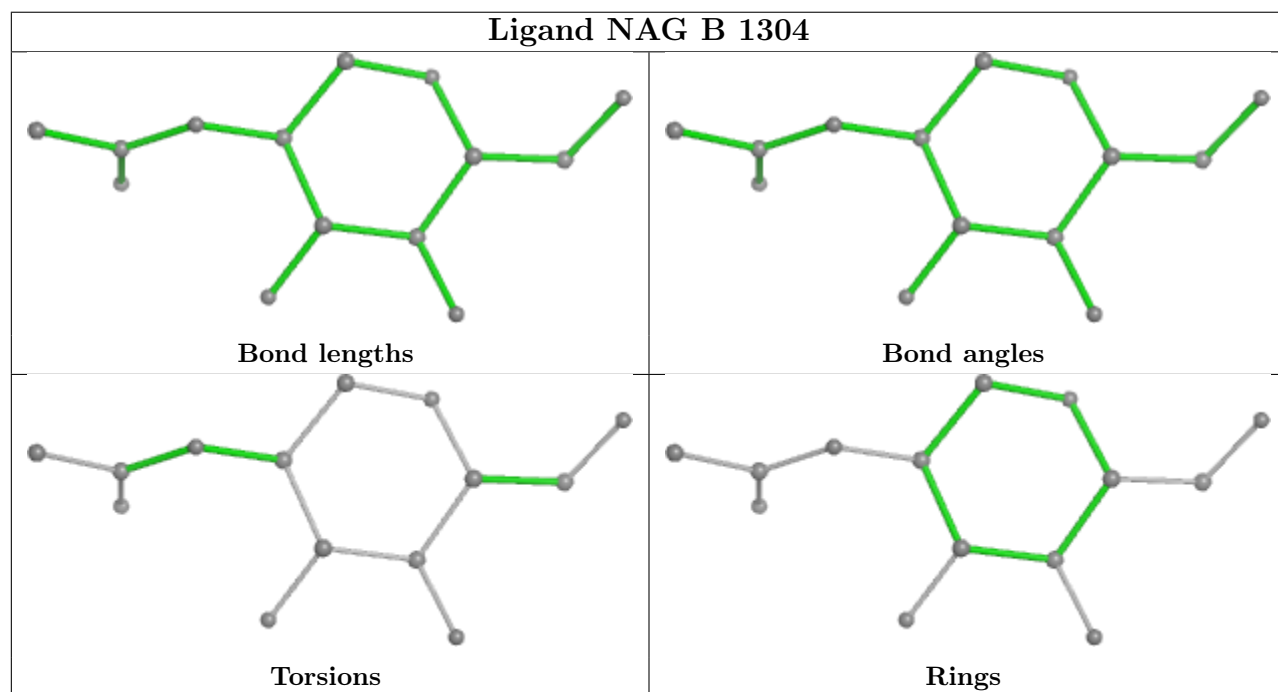
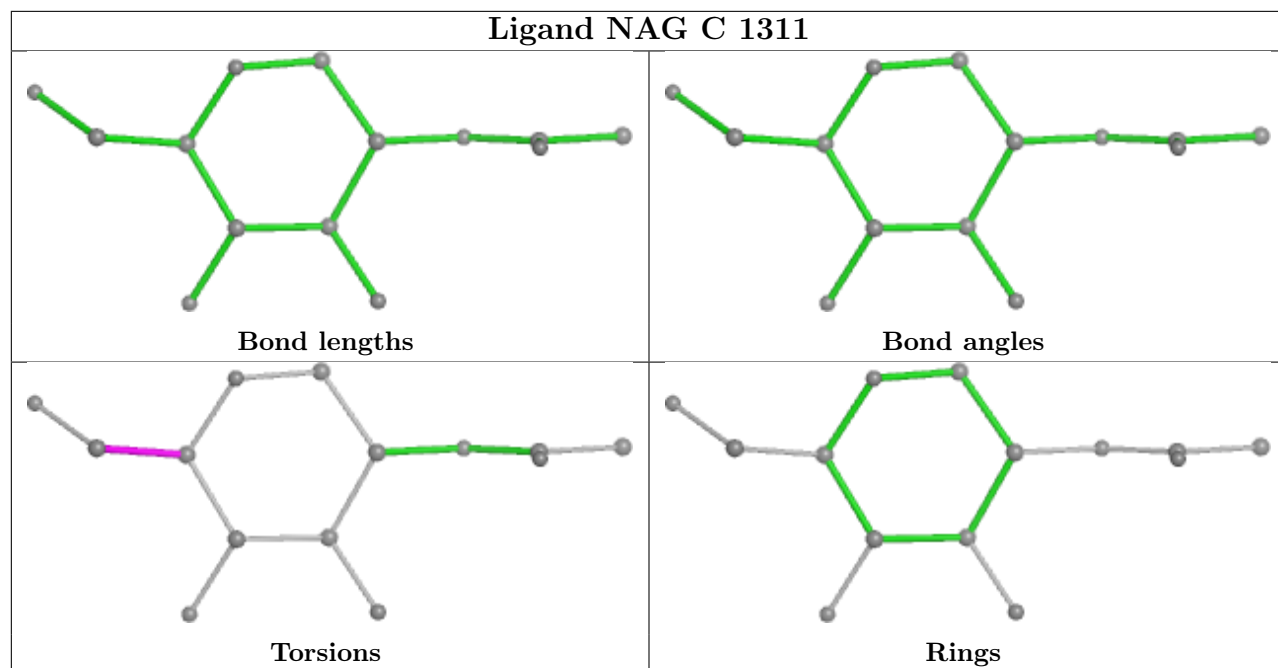


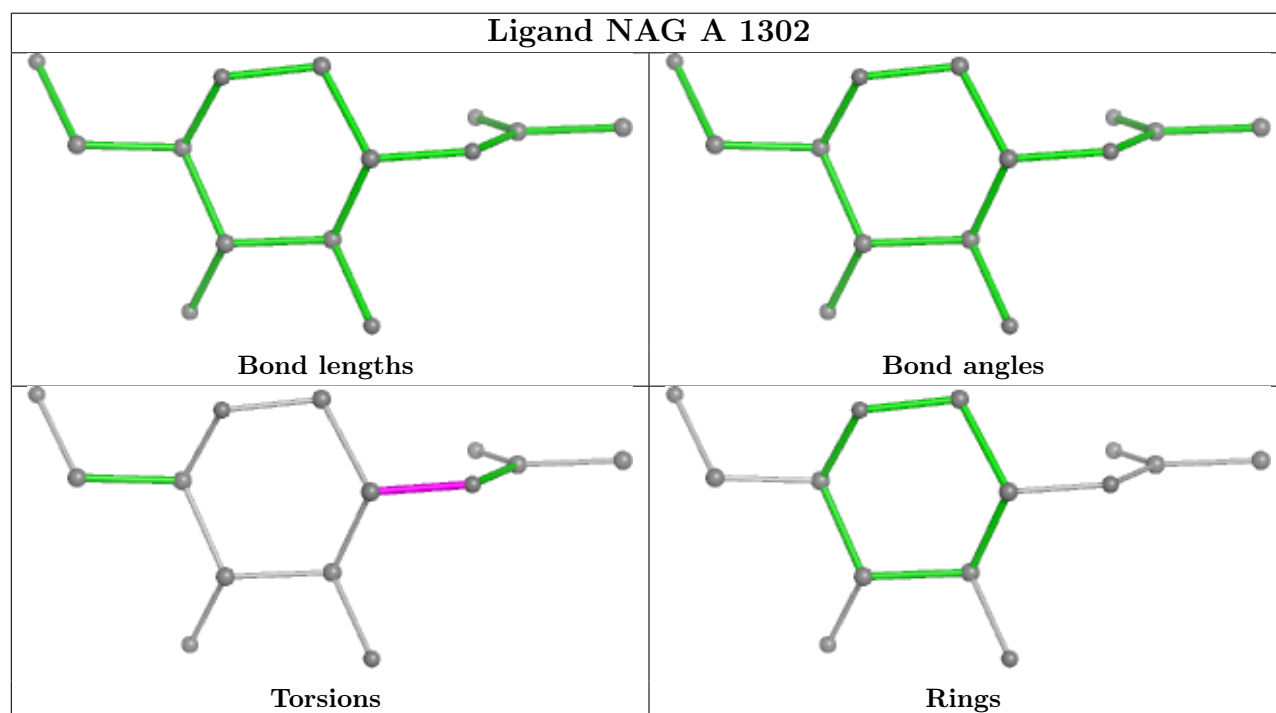
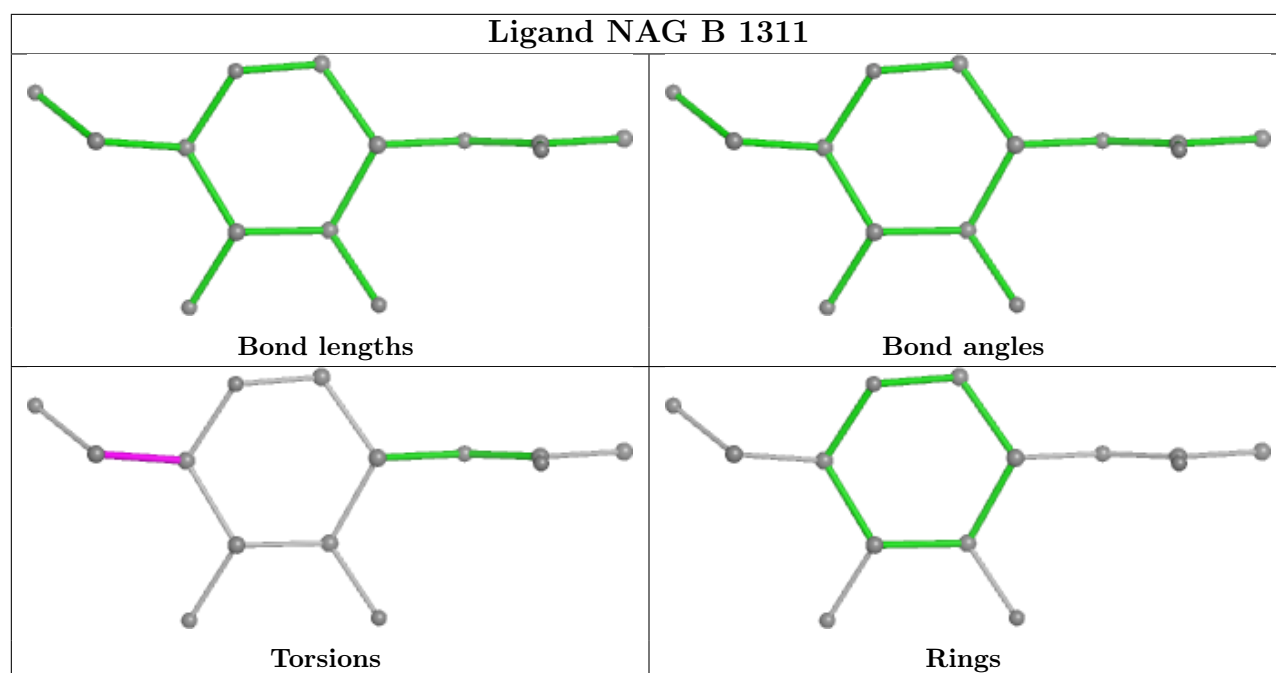
## Ligand NAG C 1308

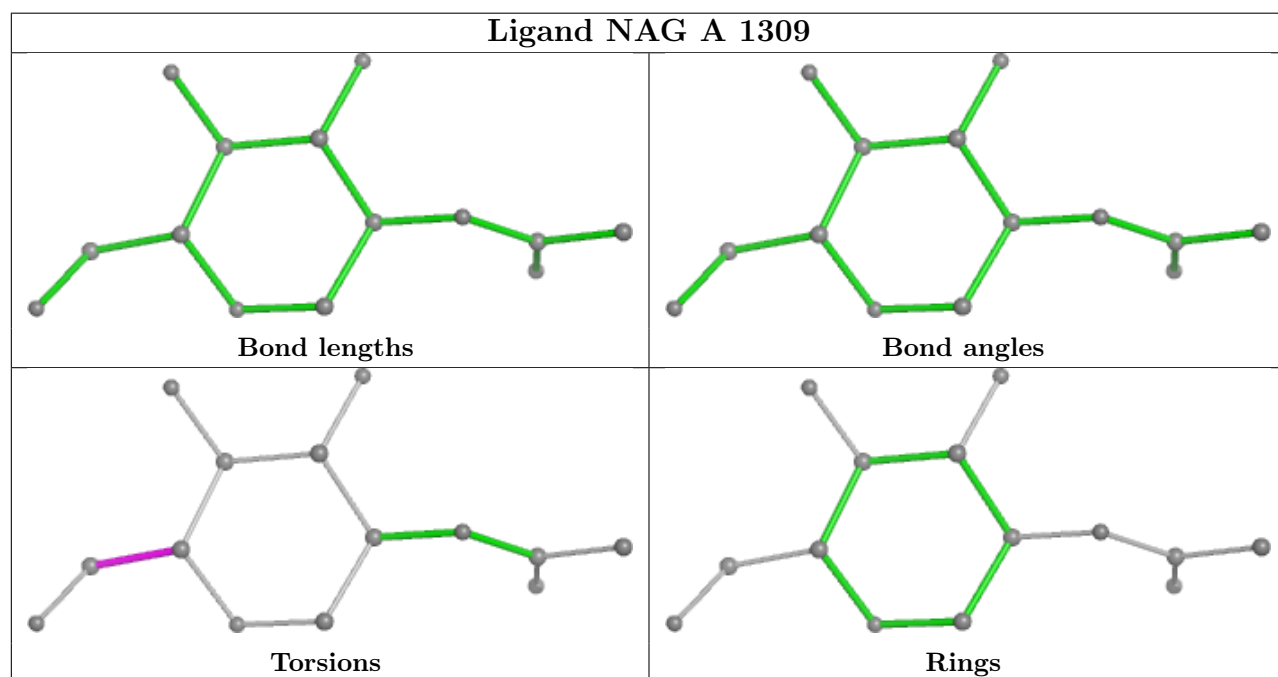
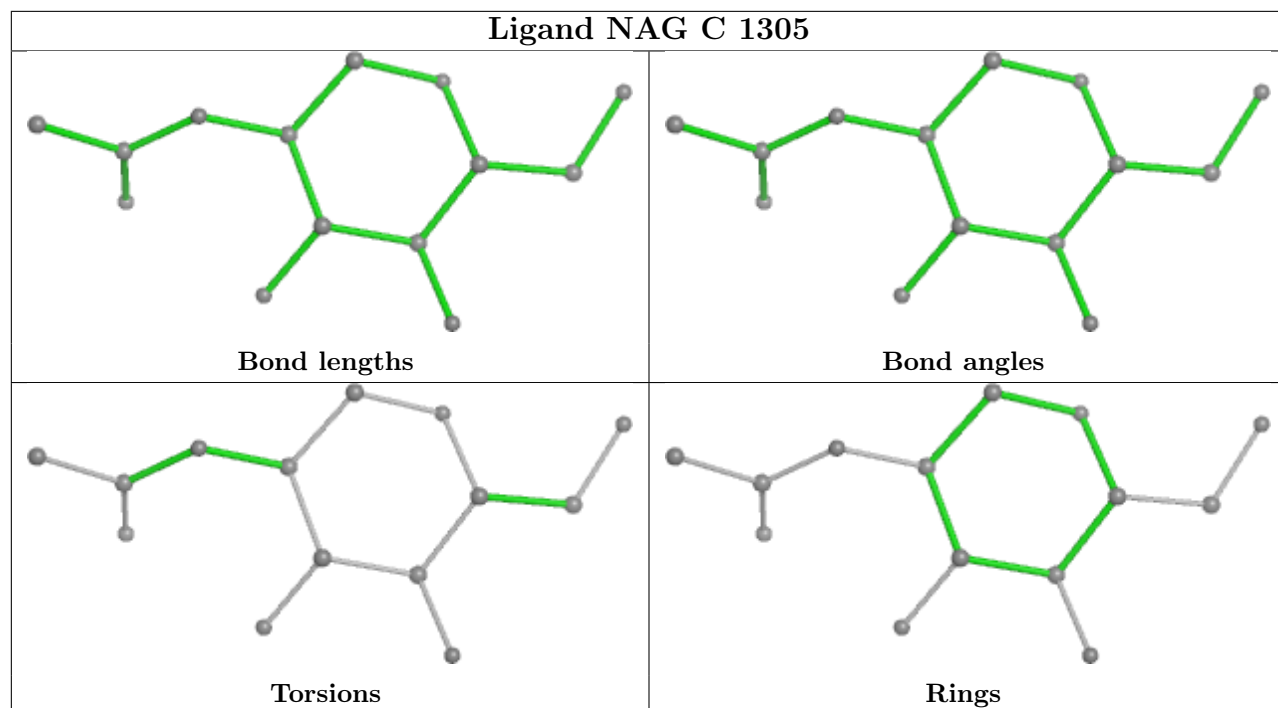


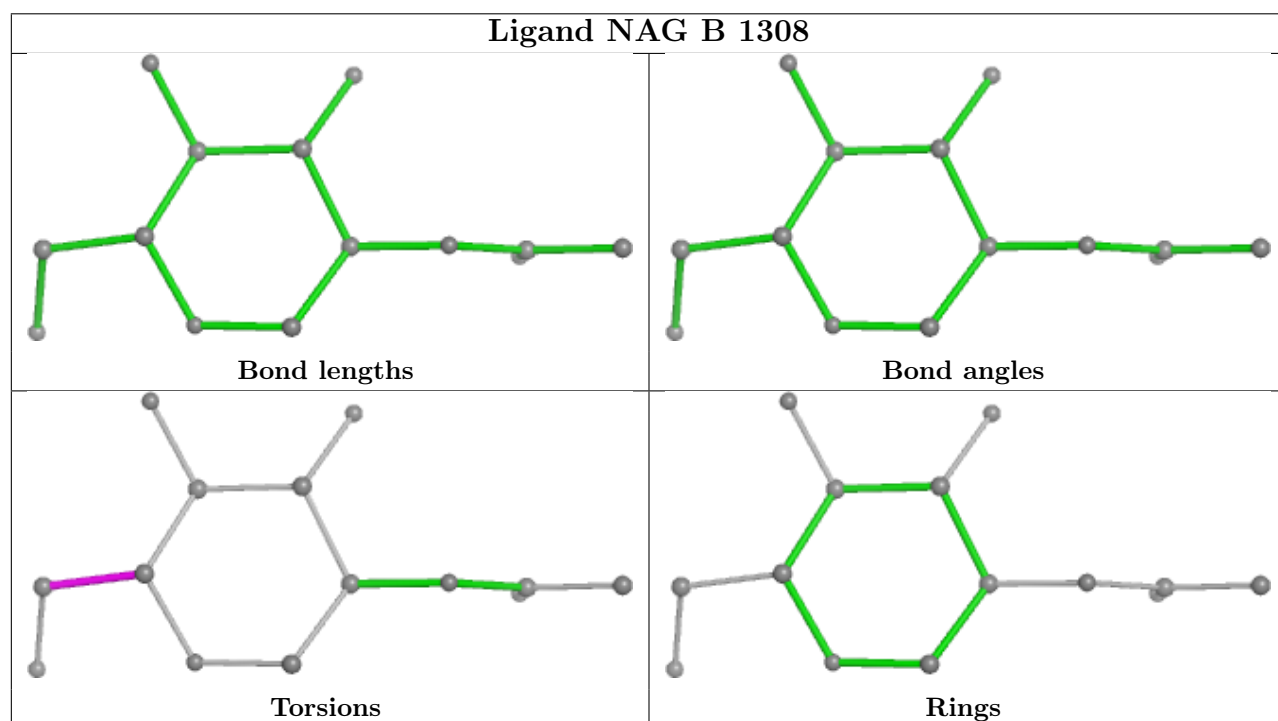
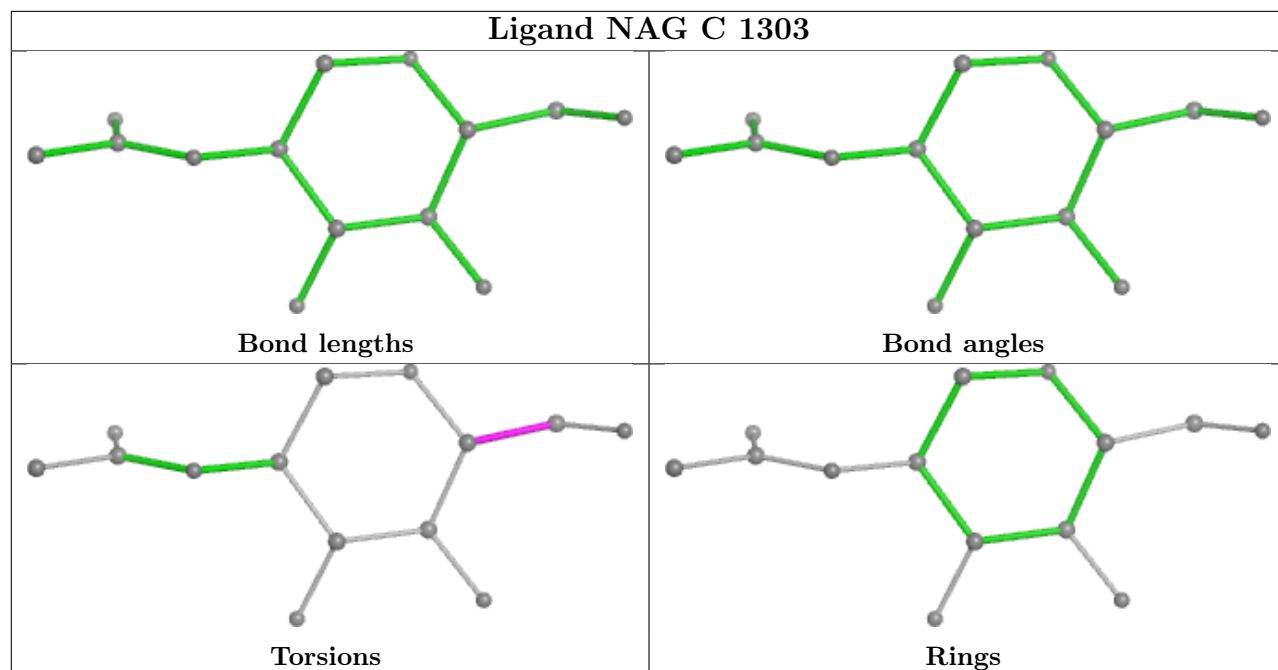
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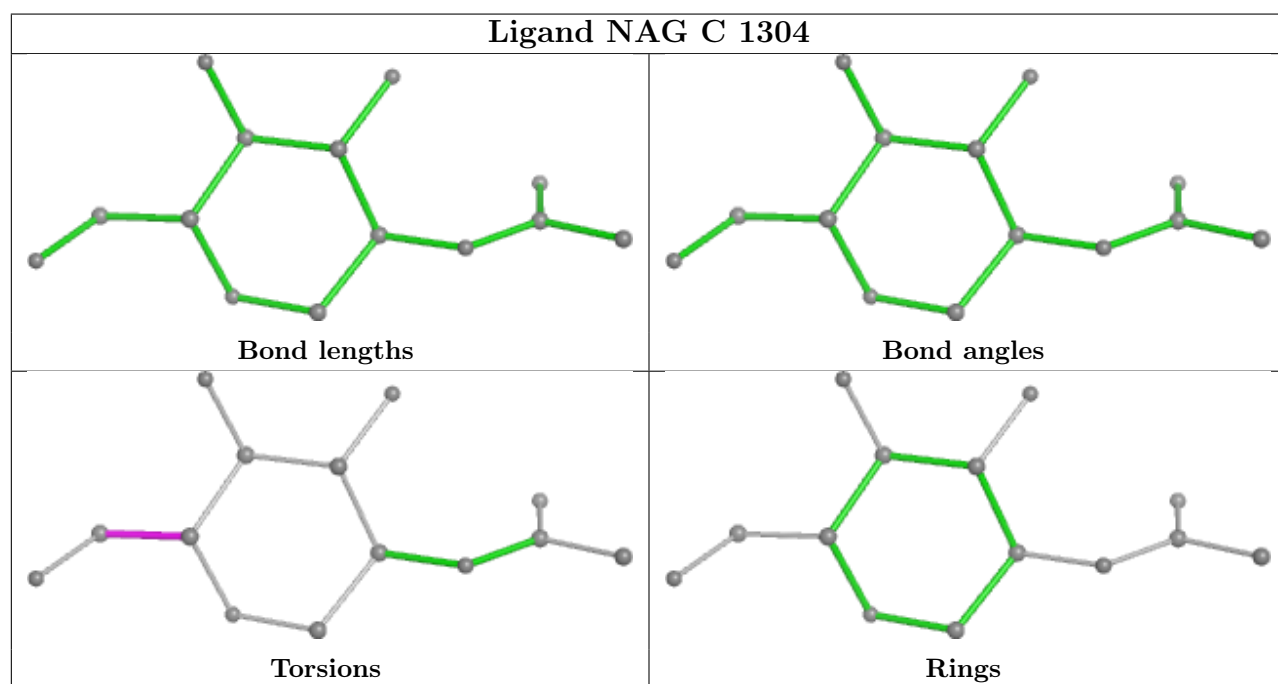
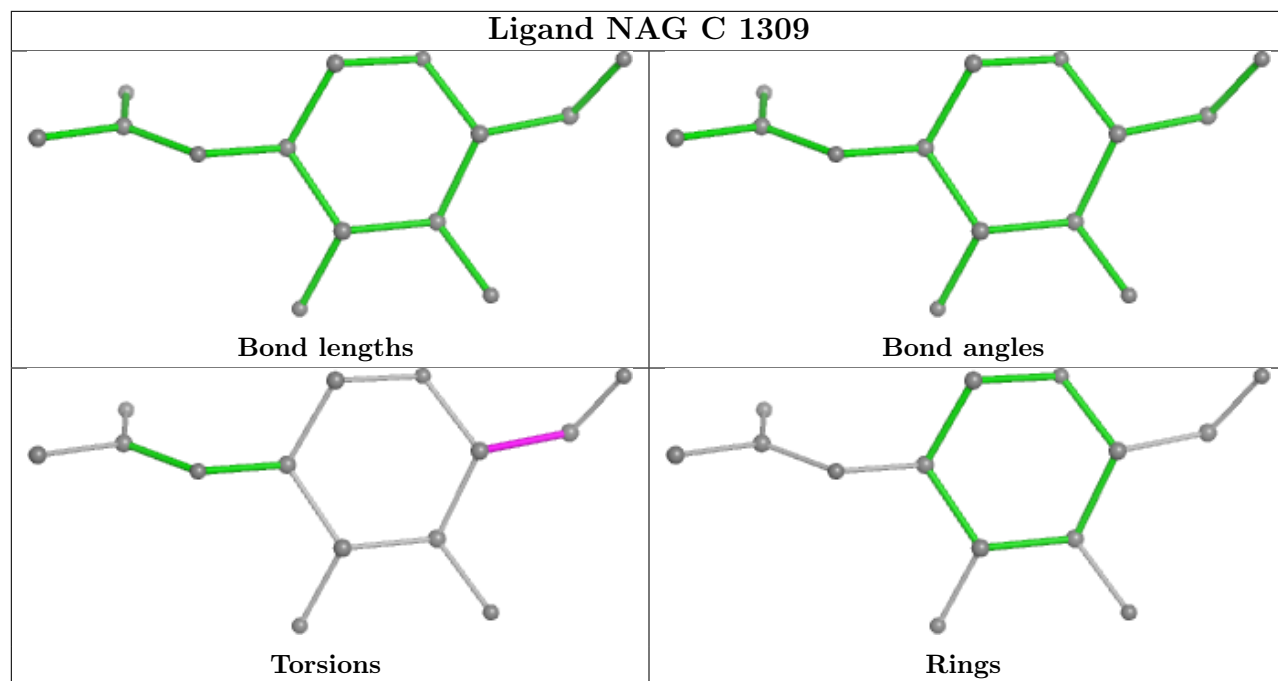




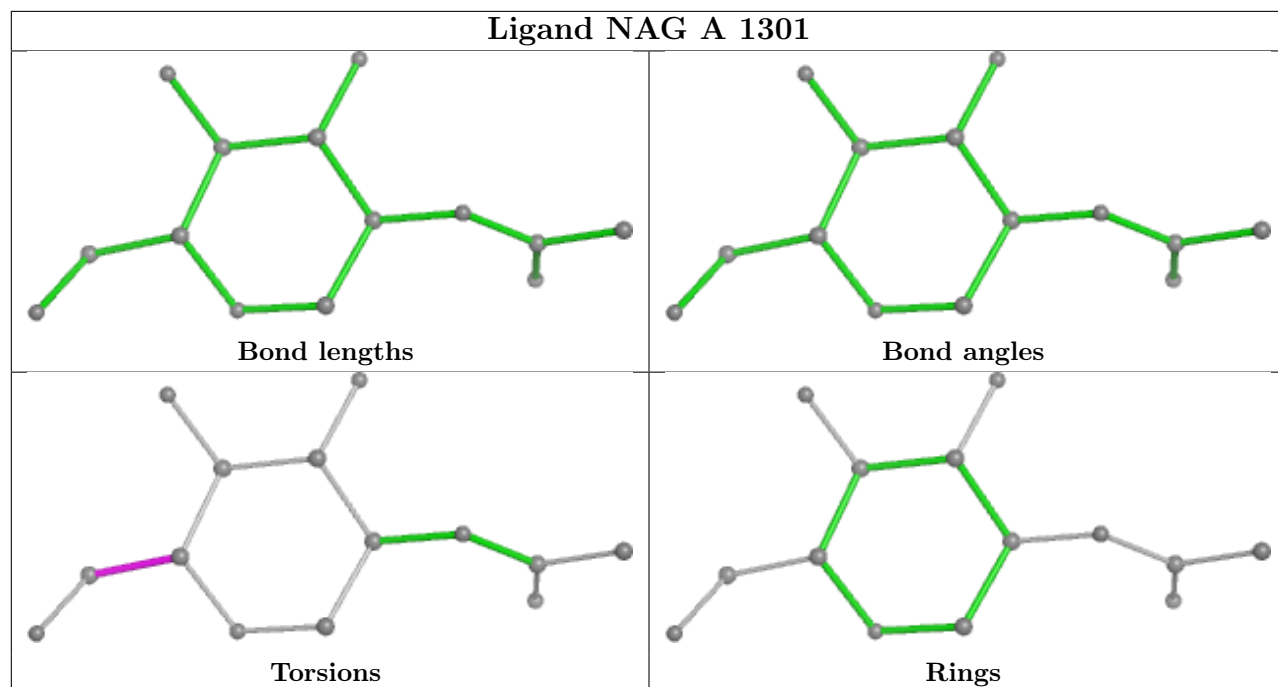




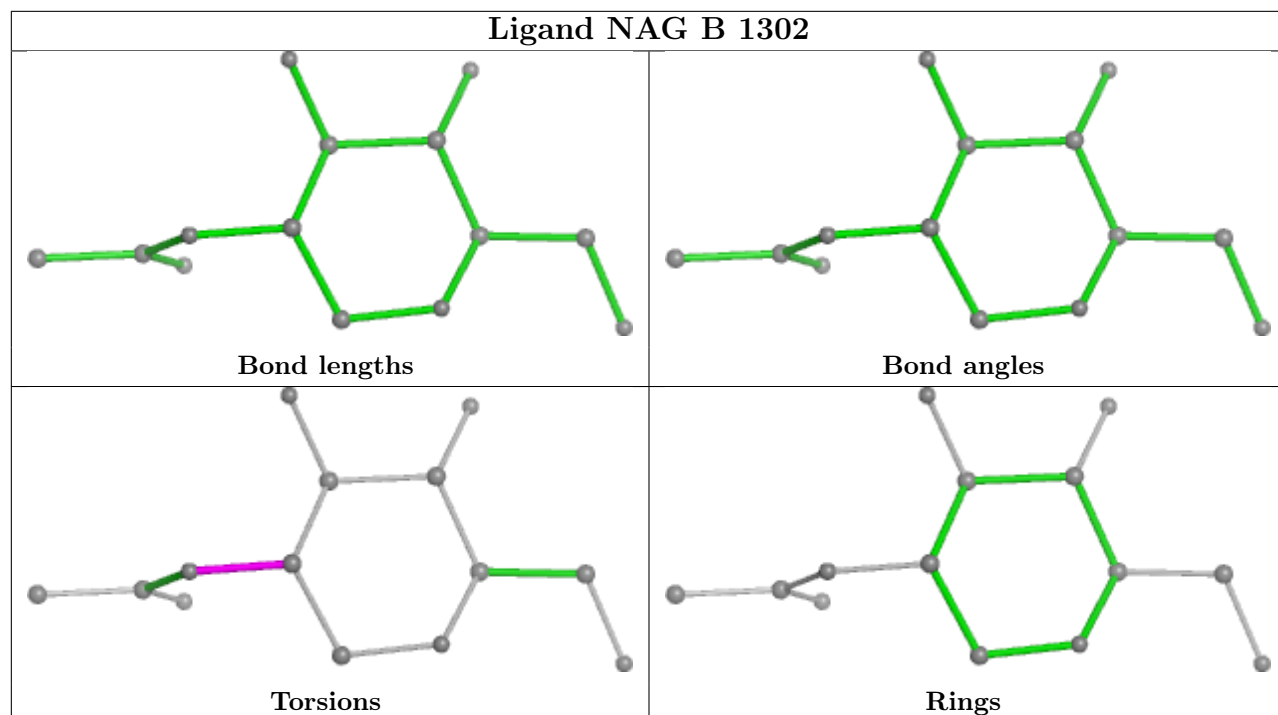




## Ligand NAG A 1301

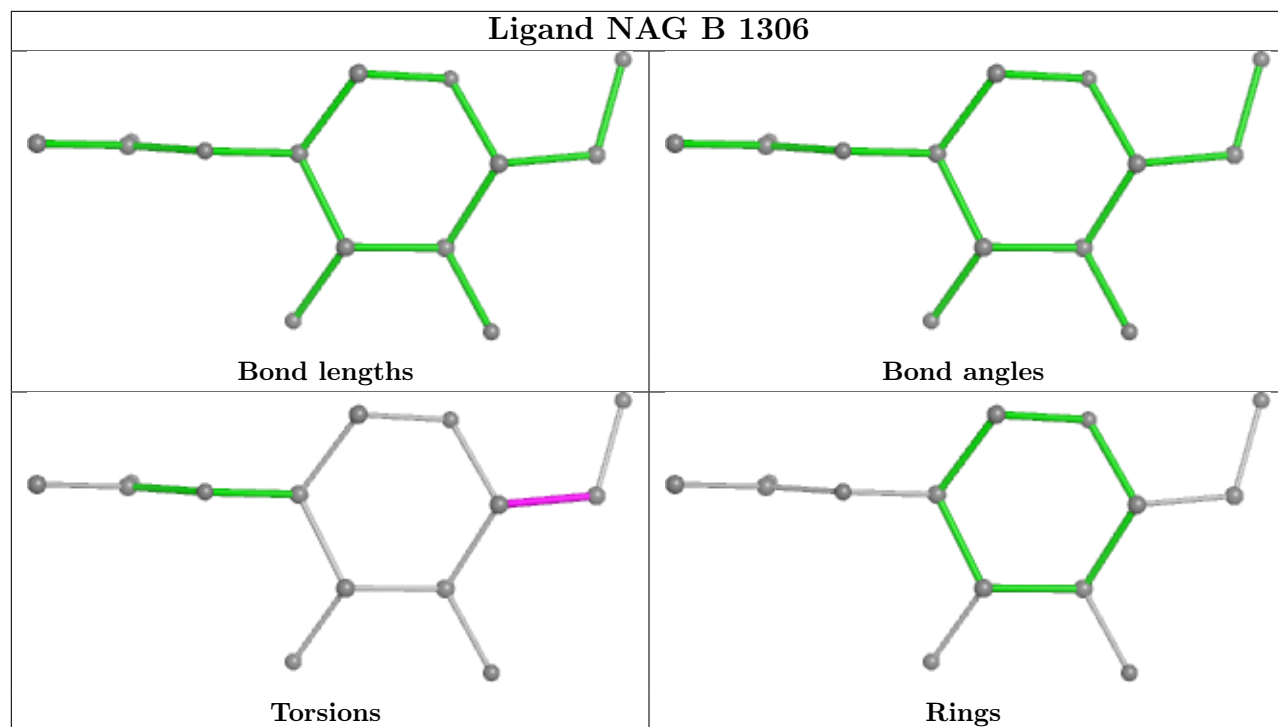


## Ligand NAG B 1302

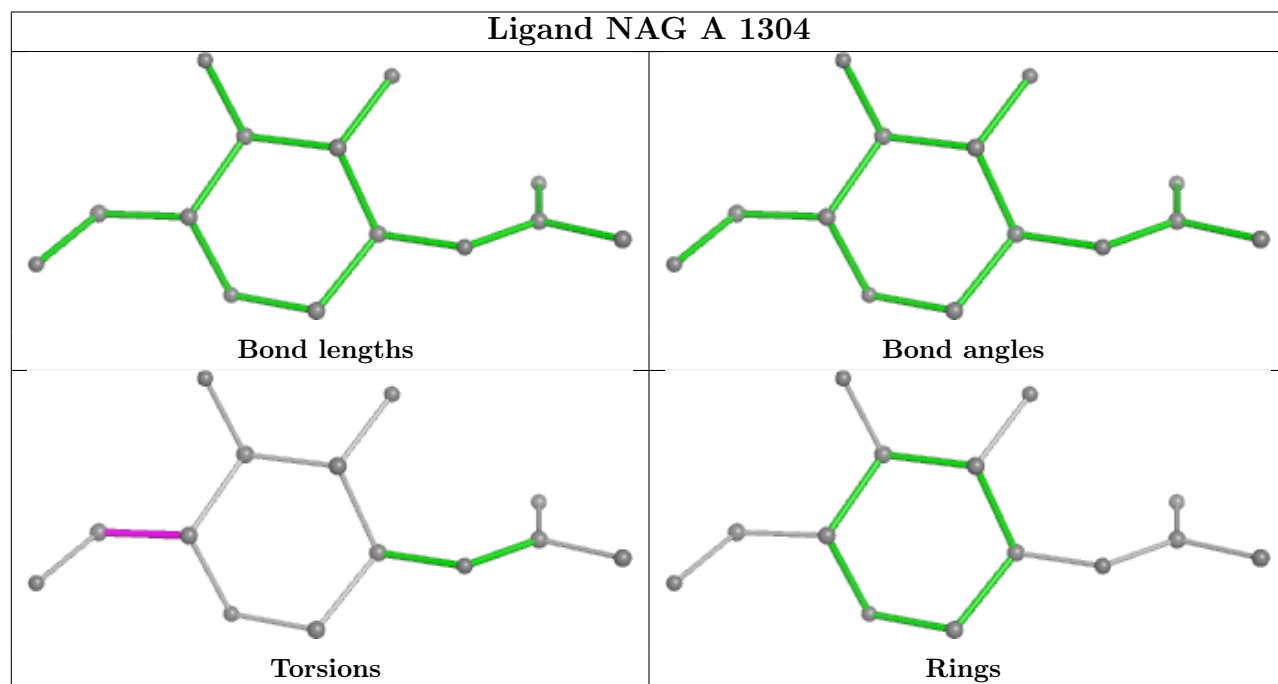




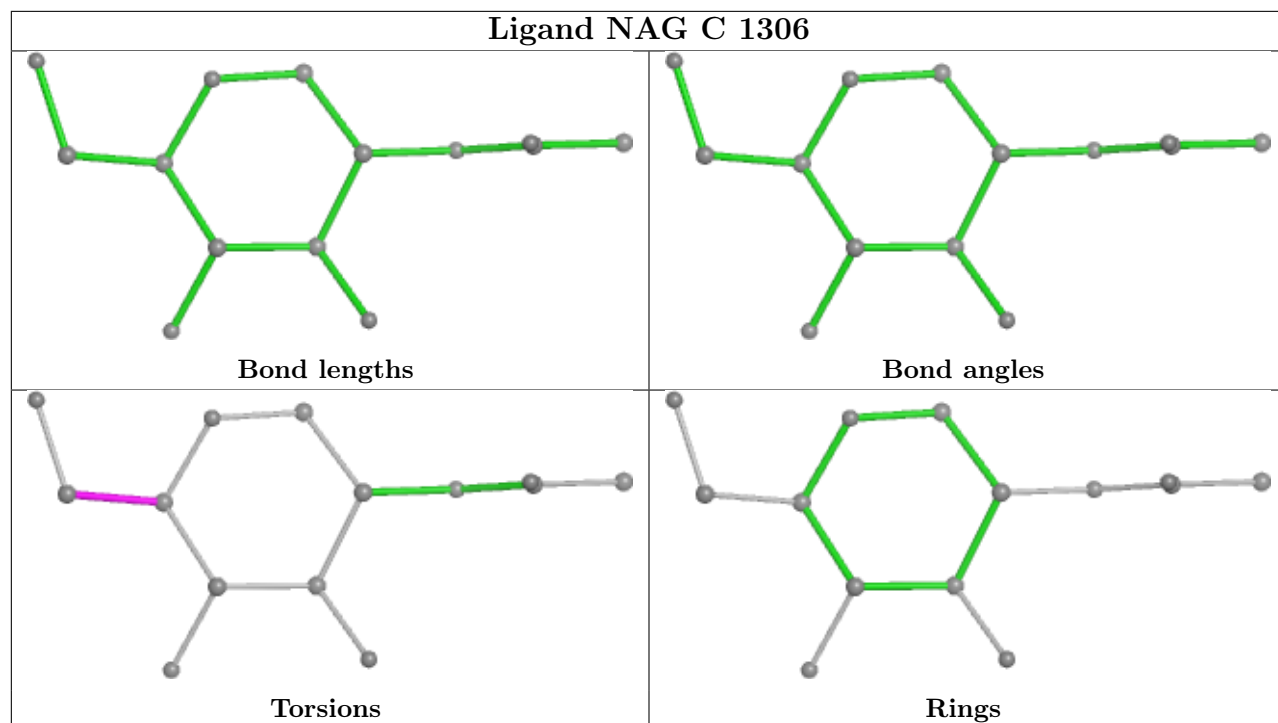
## Ligand NAG B 1306



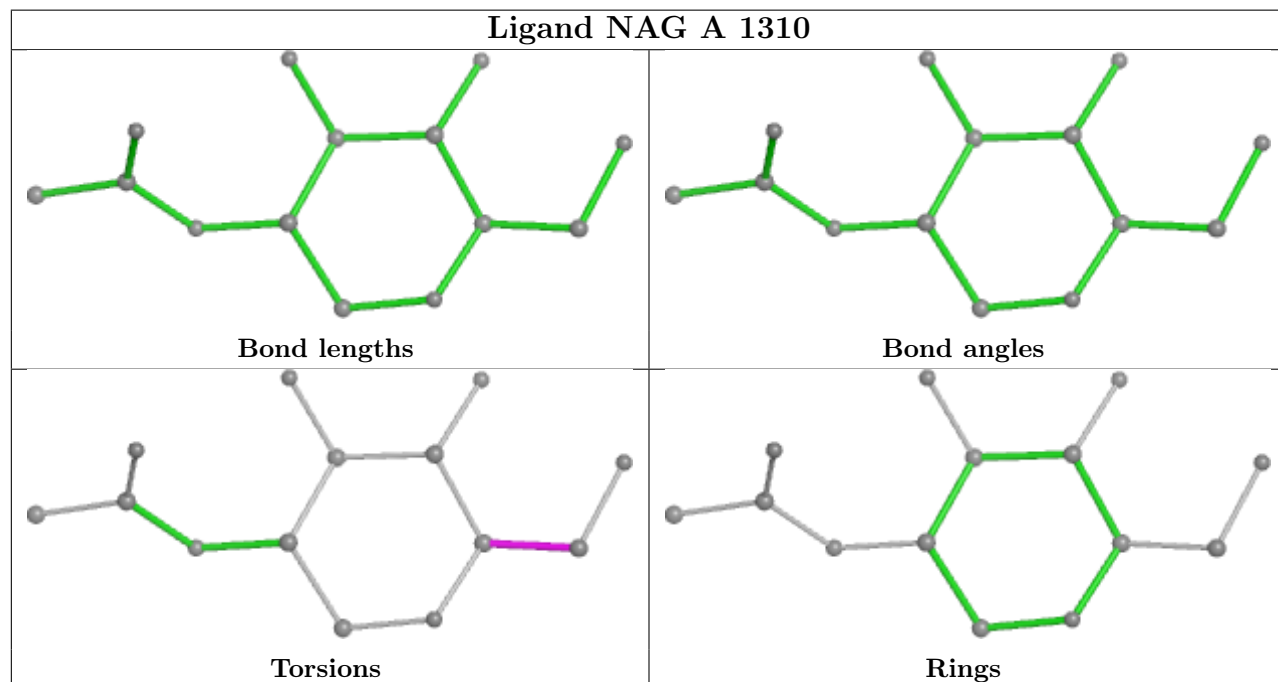
## Ligand NAG A 1304

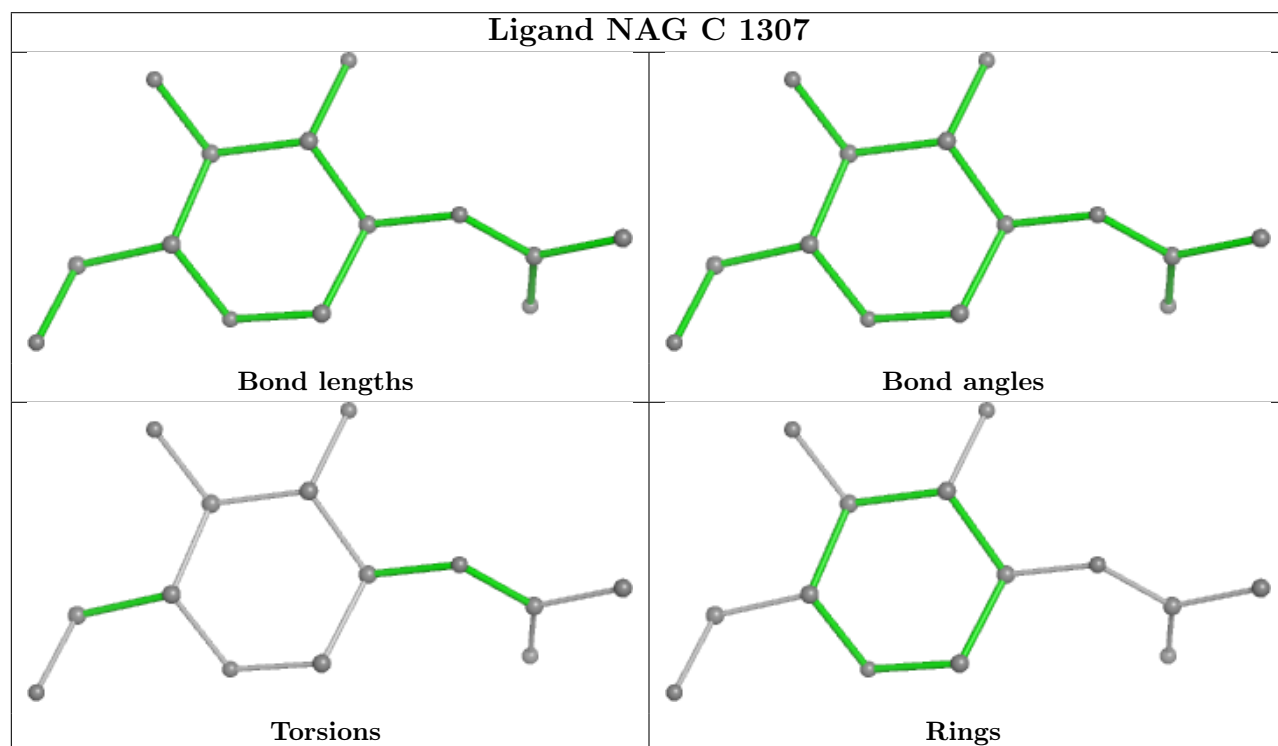
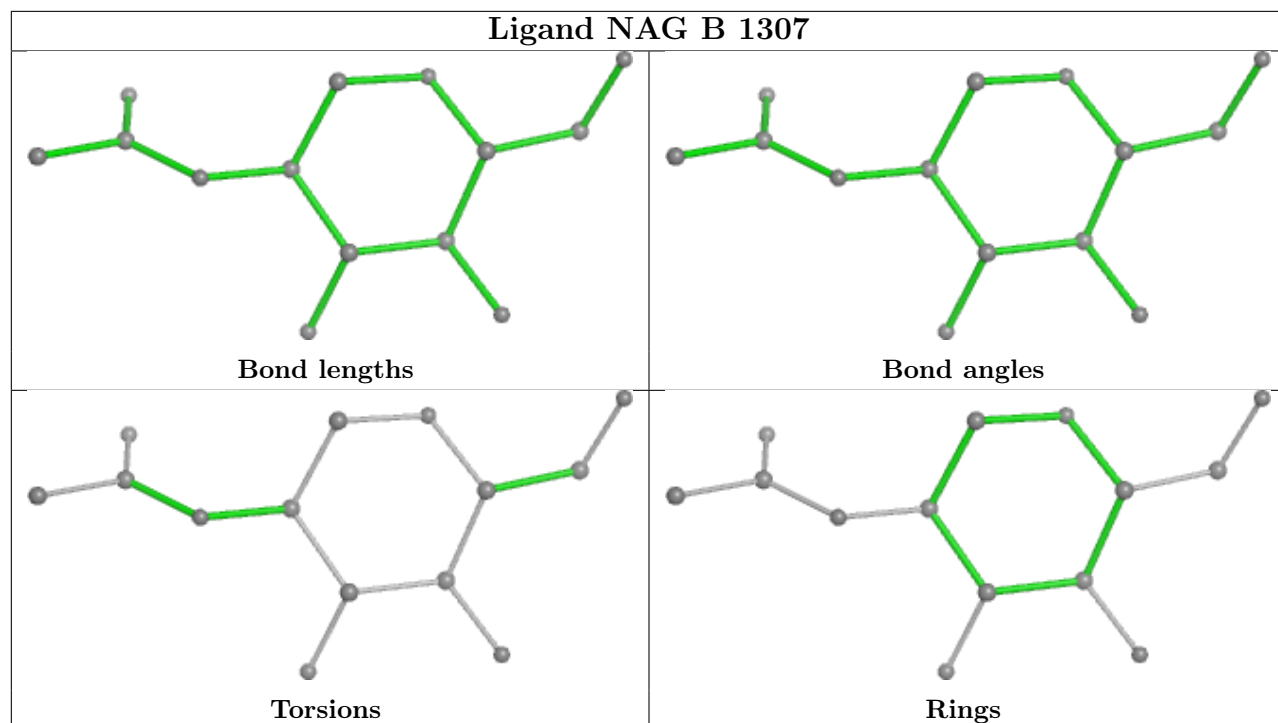


## Ligand NAG C 1306

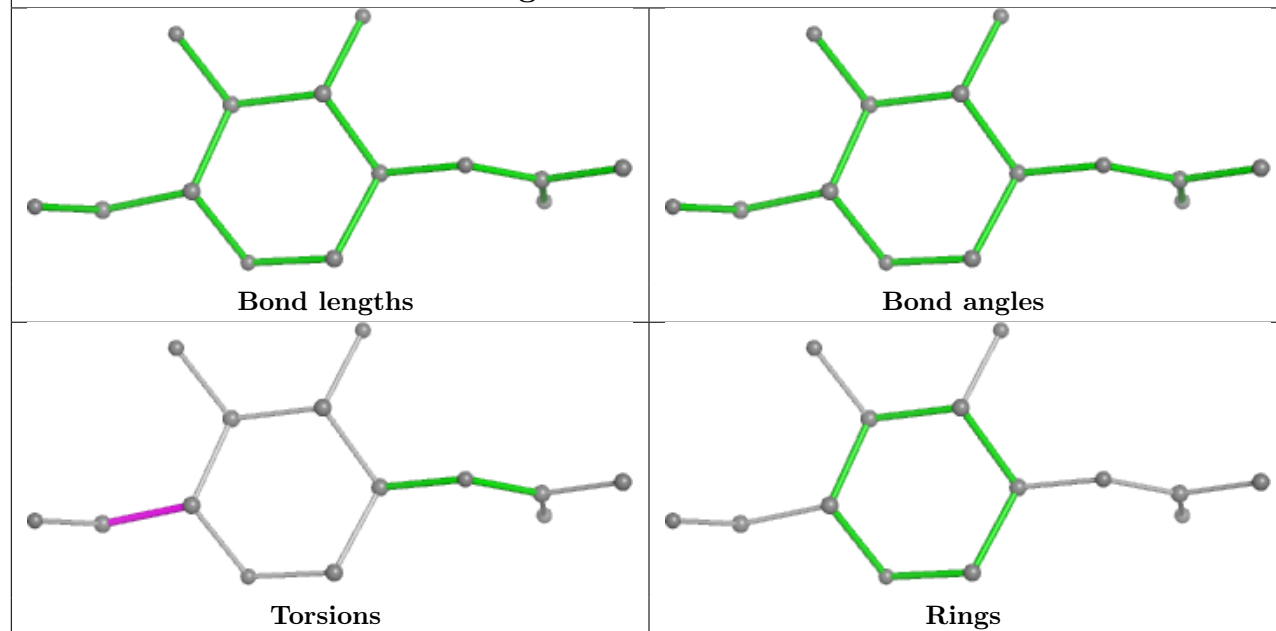


## Ligand NAG A 1310

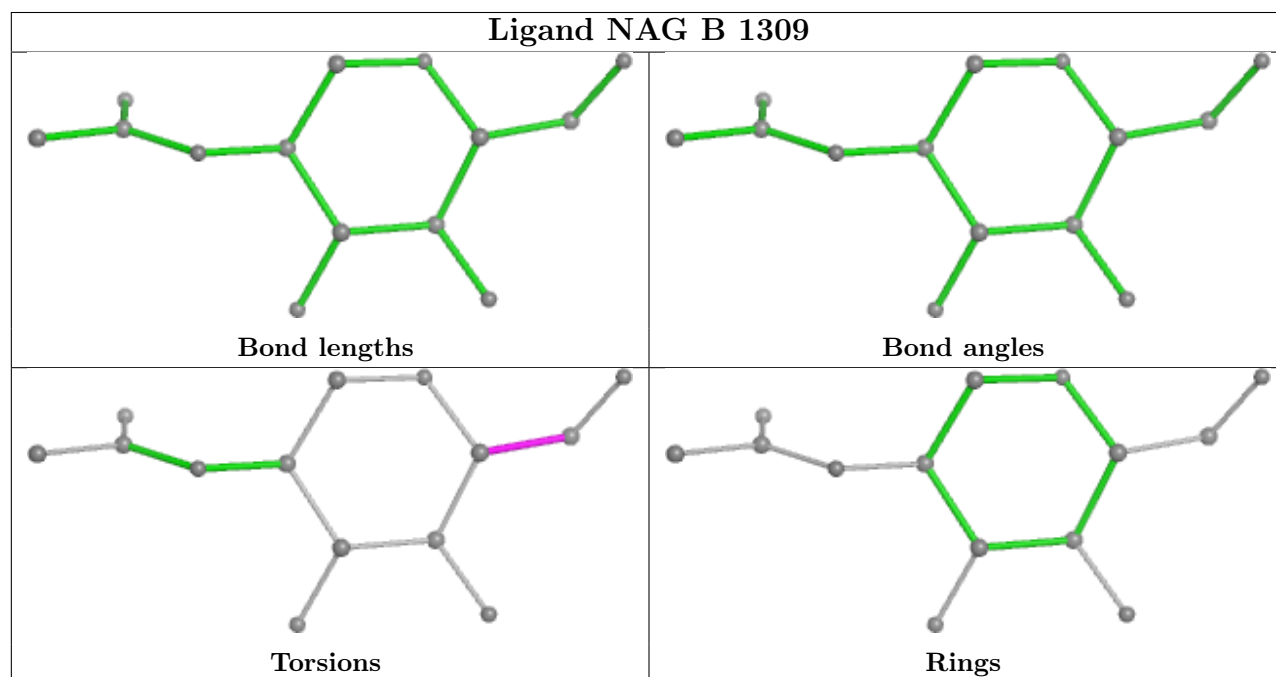


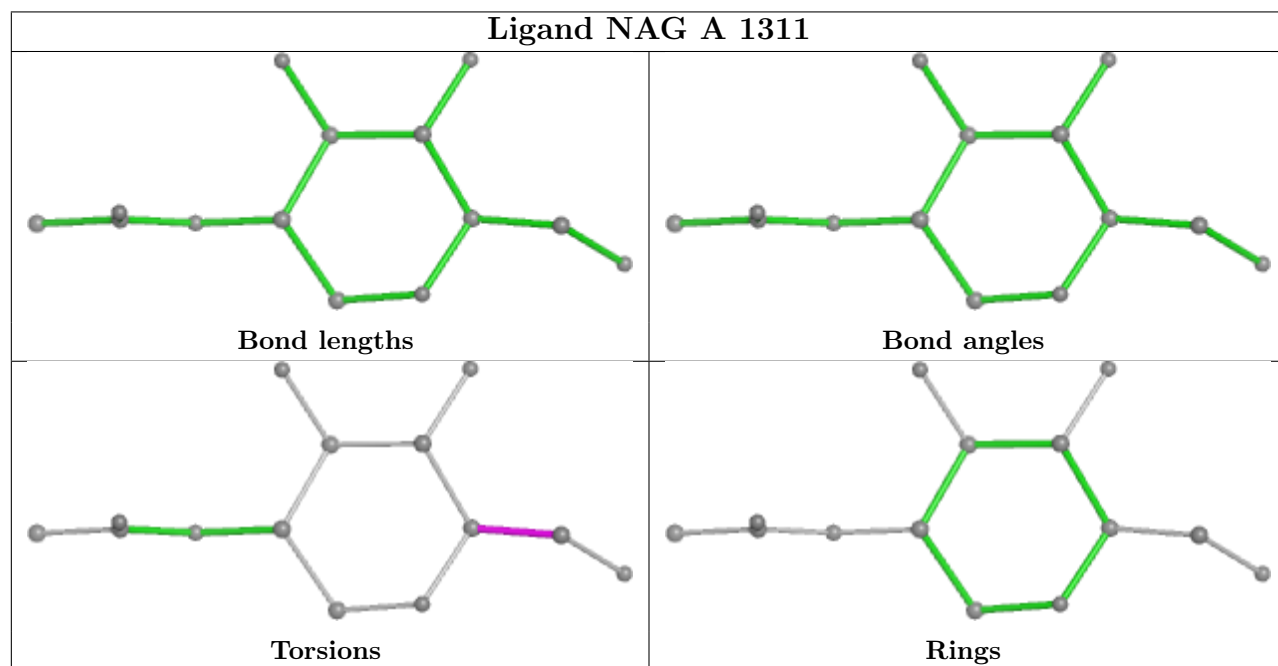
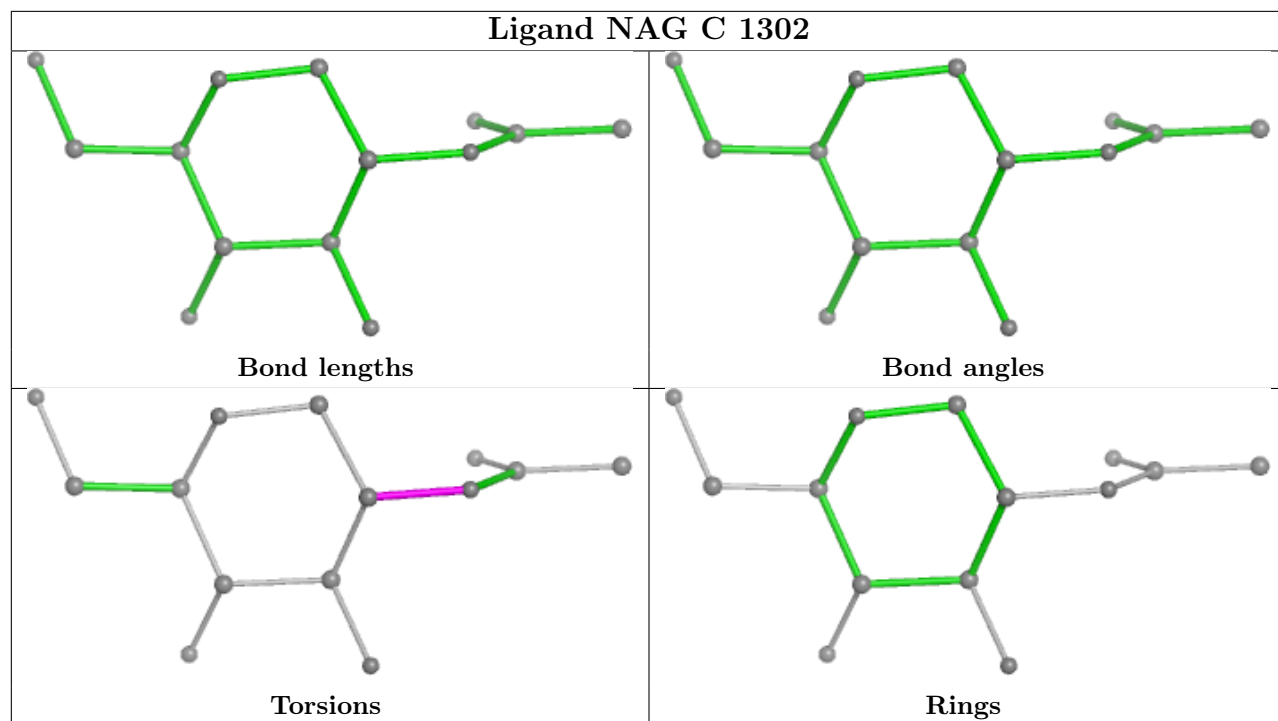


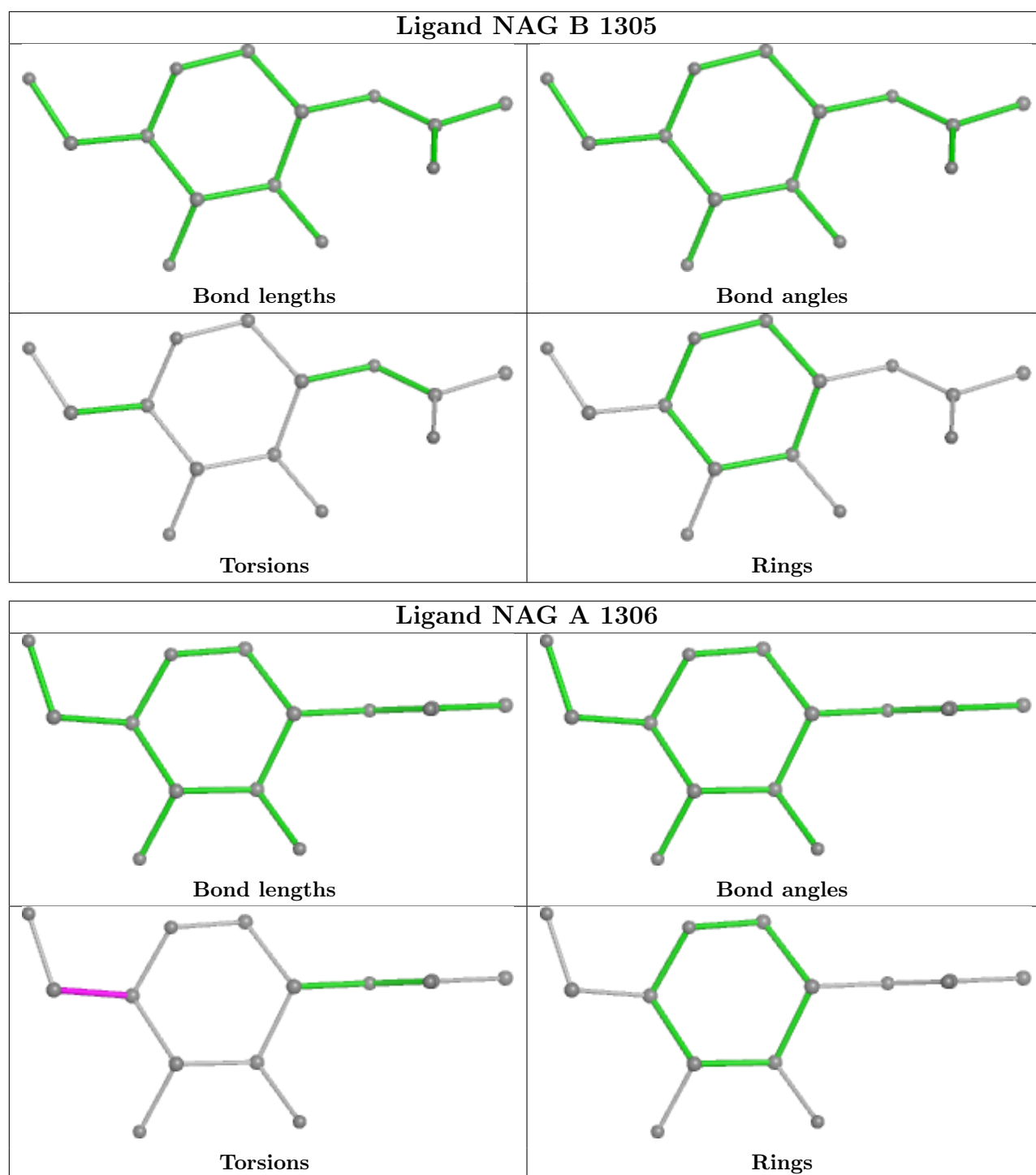
## Ligand NAG A 1303



## Ligand NAG B 1309







## 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.

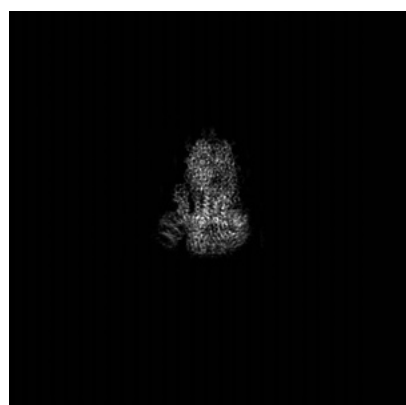
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13776. These allow visual inspection of the internal detail of the map and identification of artifacts.

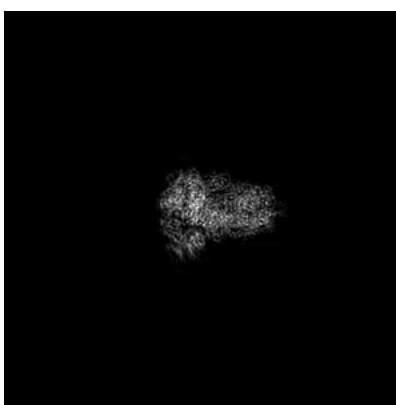
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

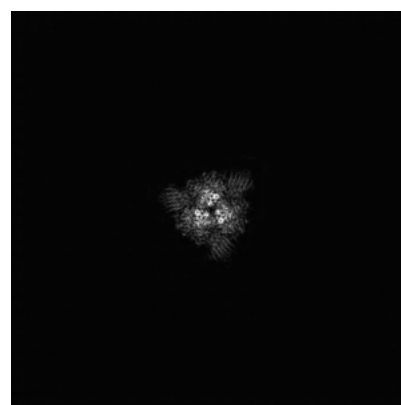
#### 6.1.1 Primary map



X



Y

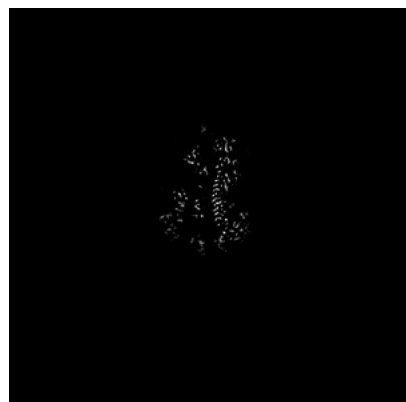


Z

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

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

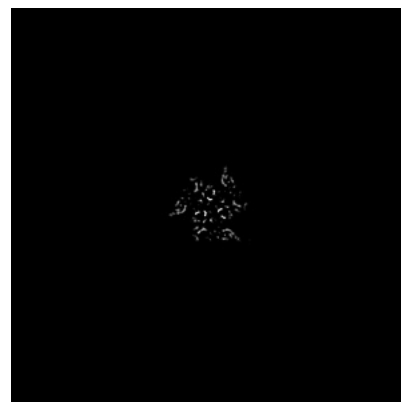
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

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: 194



Y Index: 195

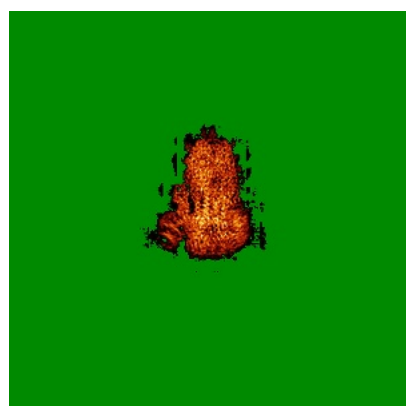


Z Index: 192

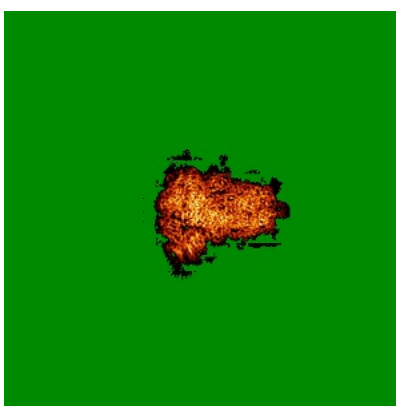
The images above show the largest variance slices of the map in three orthogonal directions.

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

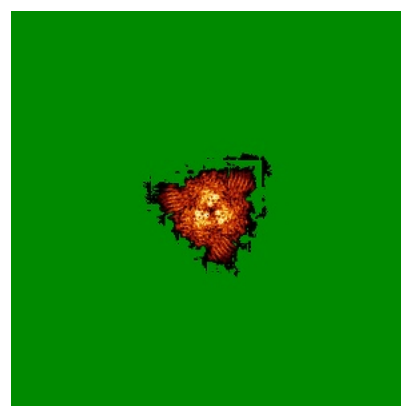
### 6.4.1 Primary map



X



Y



Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

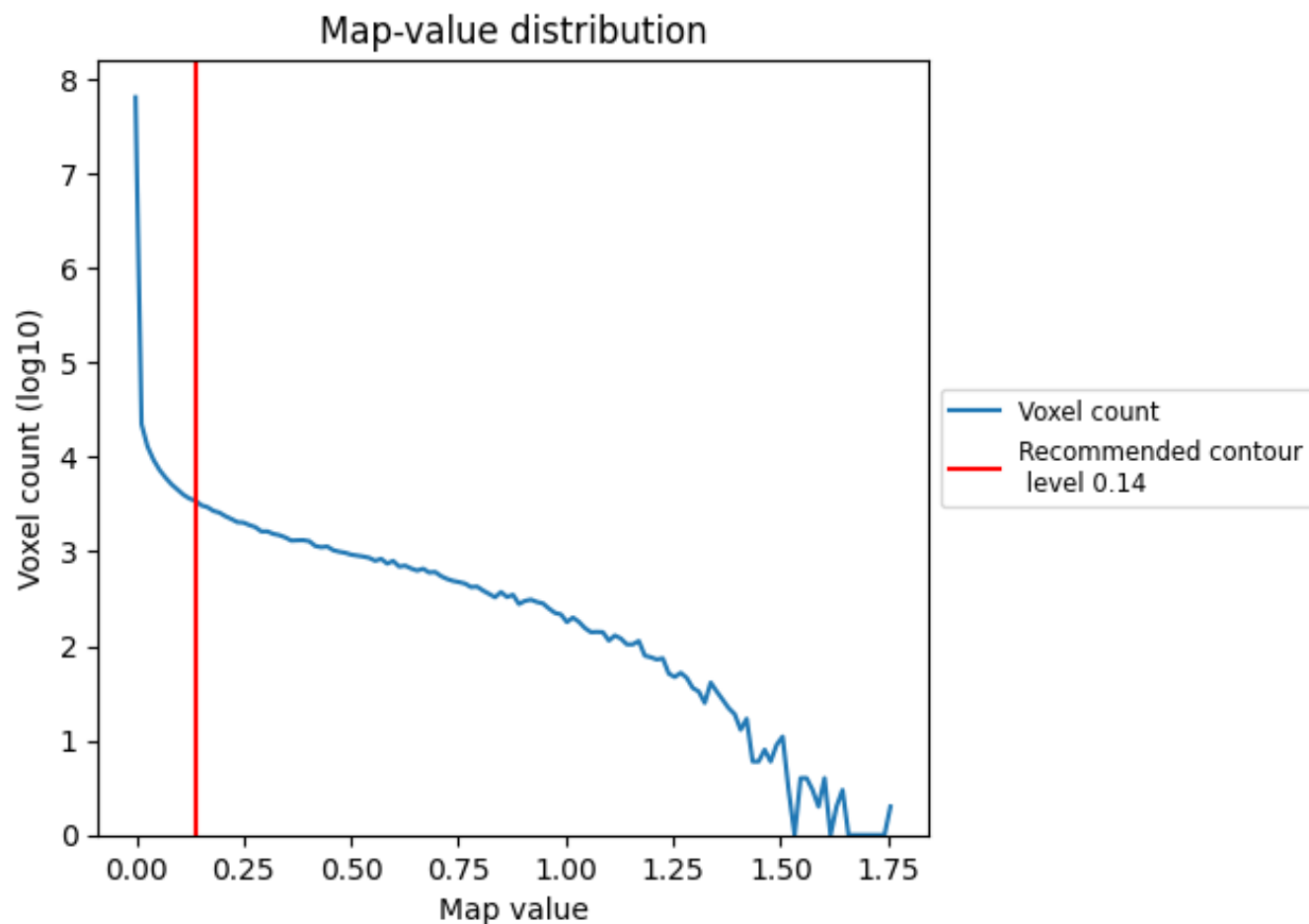
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

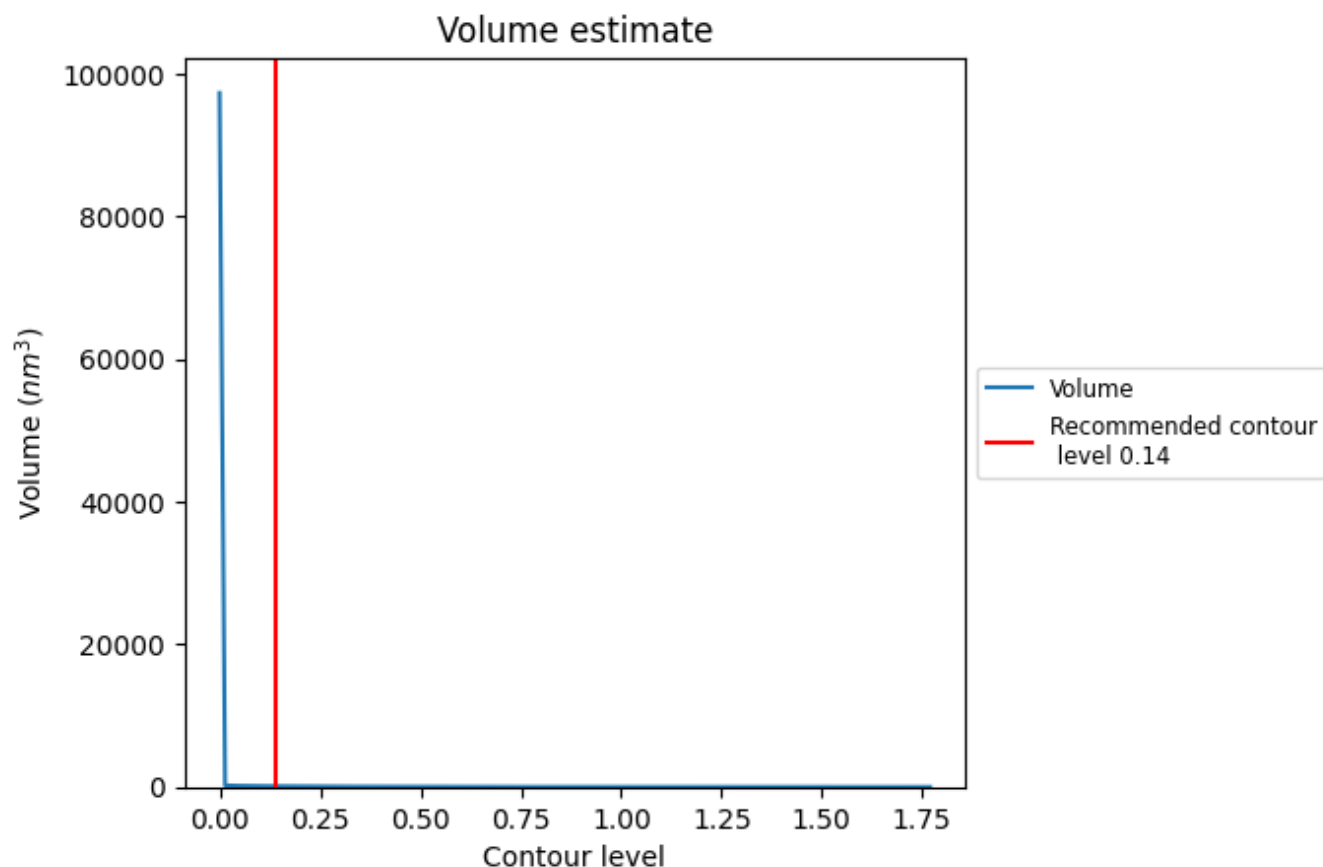
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

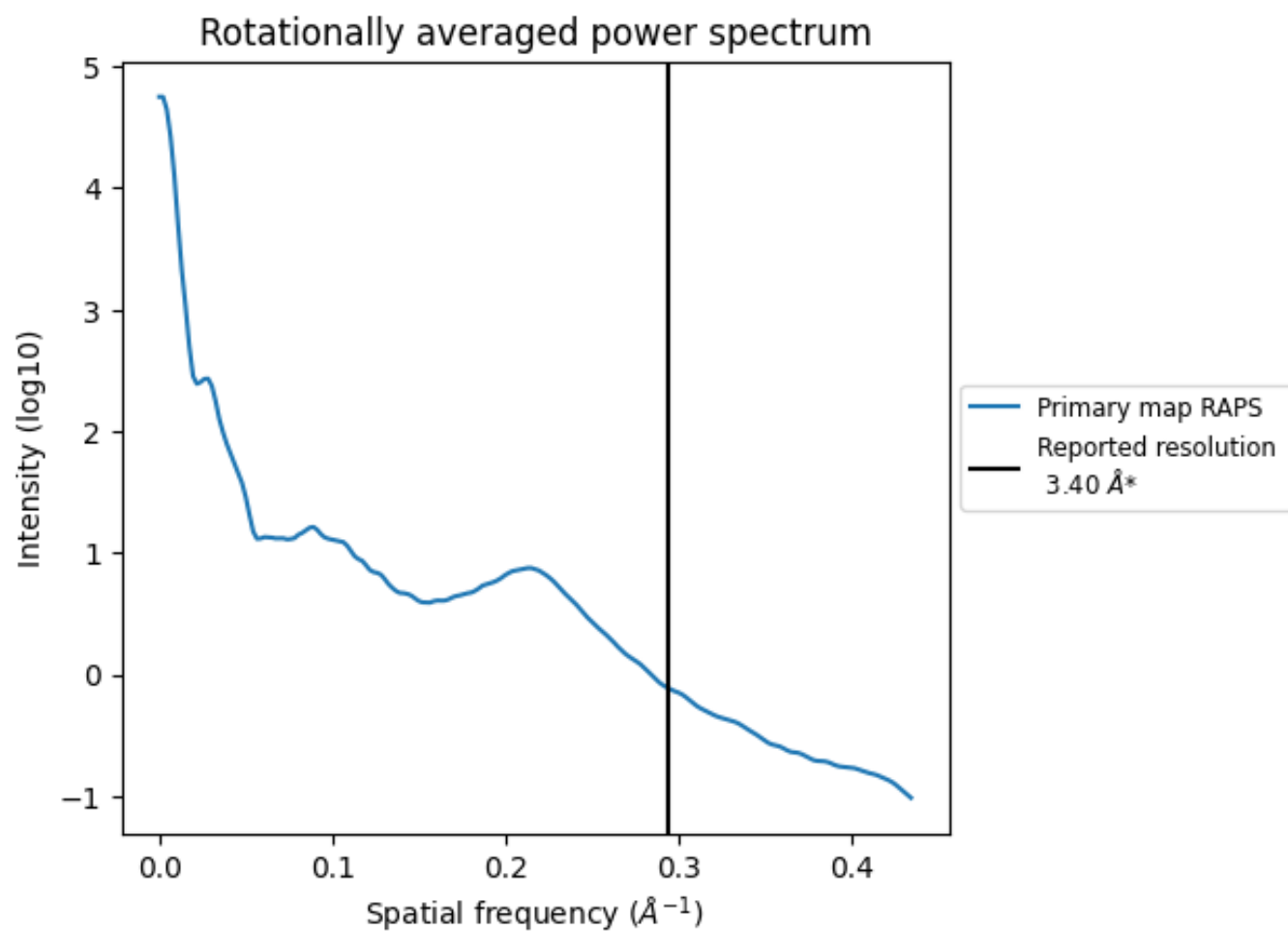
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102  $\text{nm}^3$ ; this corresponds to an approximate mass of 93 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 ⓘ

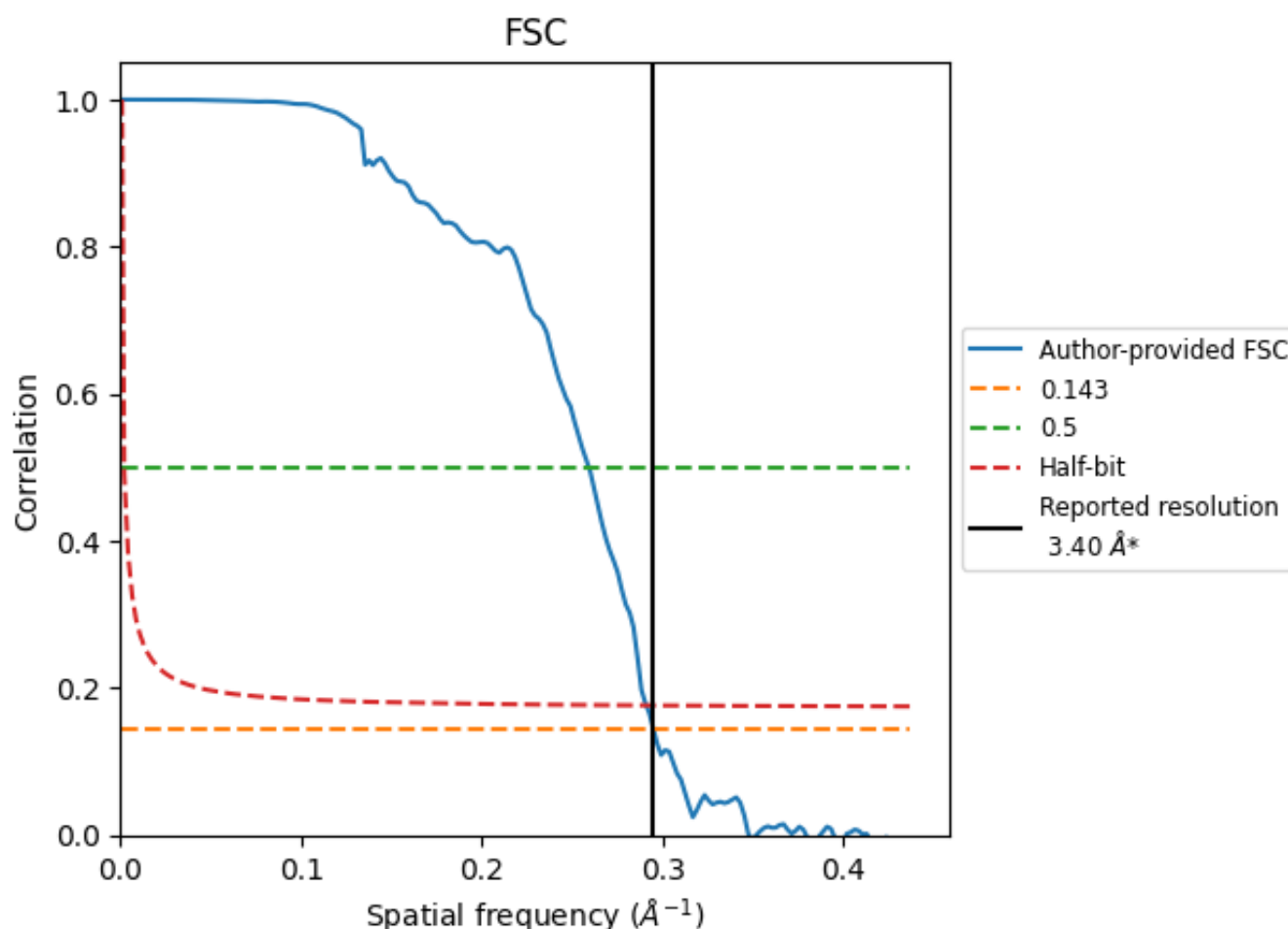


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

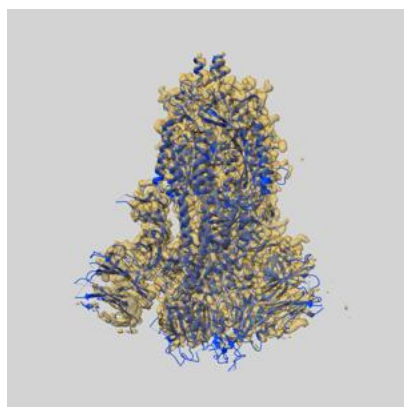
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.86	3.44
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

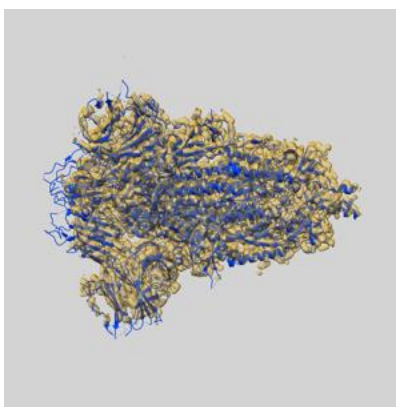
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13776 and PDB model 7Q1Z. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

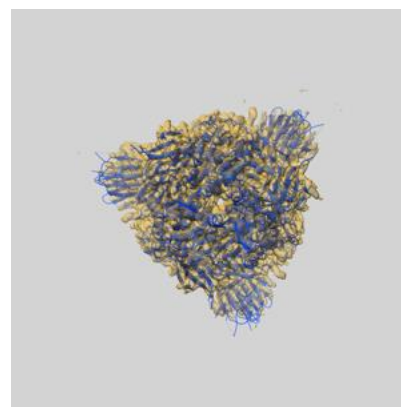
### 9.1 Map-model overlay [i](#)



X



Y



Z

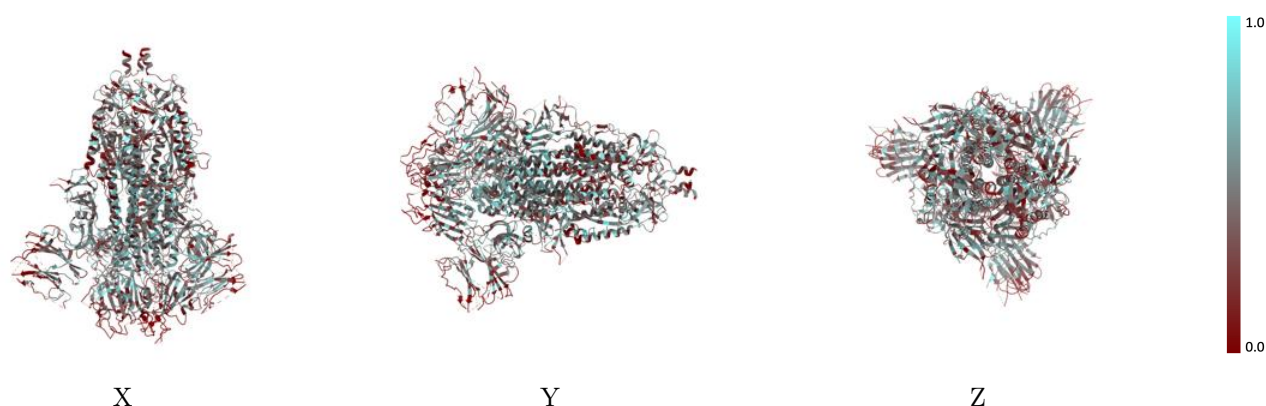
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

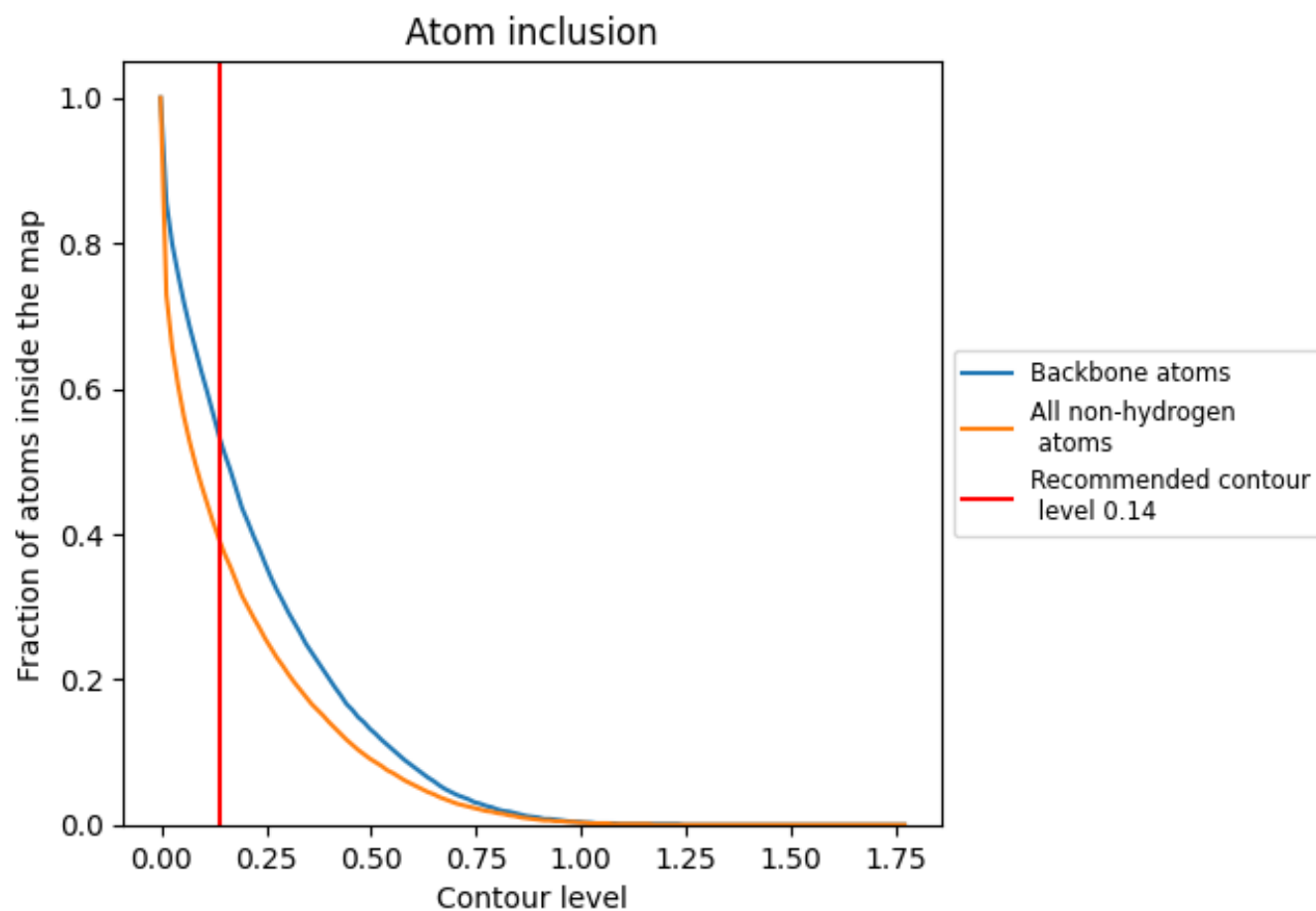
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.14).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 39% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3890	<div></div> 0.0340
A	<div></div> 0.3940	<div></div> 0.0330
B	<div></div> 0.3820	<div></div> 0.0300
C	<div></div> 0.4040	<div></div> 0.0420
D	<div></div> 0.0000	<div></div> -0.0450
E	<div></div> 0.2500	<div></div> 0.0310
F	<div></div> 0.0710	<div></div> -0.1210
G	<div></div> 0.0360	<div></div> -0.1120
H	<div></div> 0.2500	<div></div> 0.0320
I	<div></div> 0.0000	<div></div> -0.0530
J	<div></div> 0.2500	<div></div> 0.0960
K	<div></div> 0.0000	<div></div> -0.1110
L	<div></div> 0.2860	<div></div> -0.0380
M	<div></div> 0.0000	<div></div> -0.1550
N	<div></div> 0.0000	<div></div> -0.0520
O	<div></div> 0.1070	<div></div> -0.0250
P	<div></div> 0.2860	<div></div> 0.1820
Q	<div></div> 0.3930	<div></div> 0.1830
R	<div></div> 0.1790	<div></div> 0.1560

1.0  
0.0  
<0.0