



wwPDB EM Validation Summary Report i

Nov 19, 2022 – 09:30 PM EST

PDB ID : 7N0G
EMDB ID : EMD-24105
Title : CryoEm structure of SARS-CoV-2 spike protein (S-6P, 1-up) in complex with
 sybodies (Sb45)
Authors : Jiang, J.; Huang, R.; Margulies, D.
Deposited on : 2021-05-25
Resolution : 3.02 Å(reported)
Based on initial models : 7B32, 7KGJ, 6XKL

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the i 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](#) ①) were used in the production of this report:

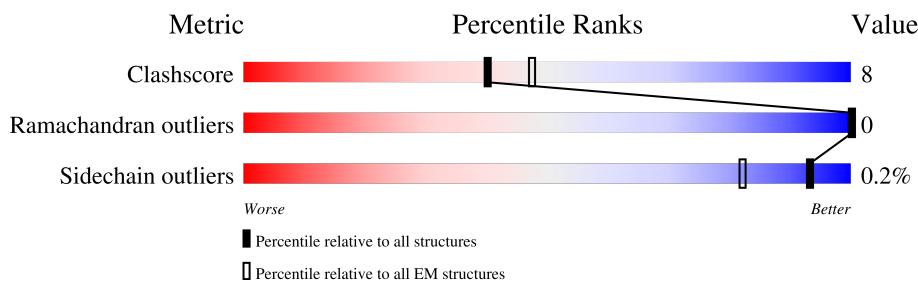
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

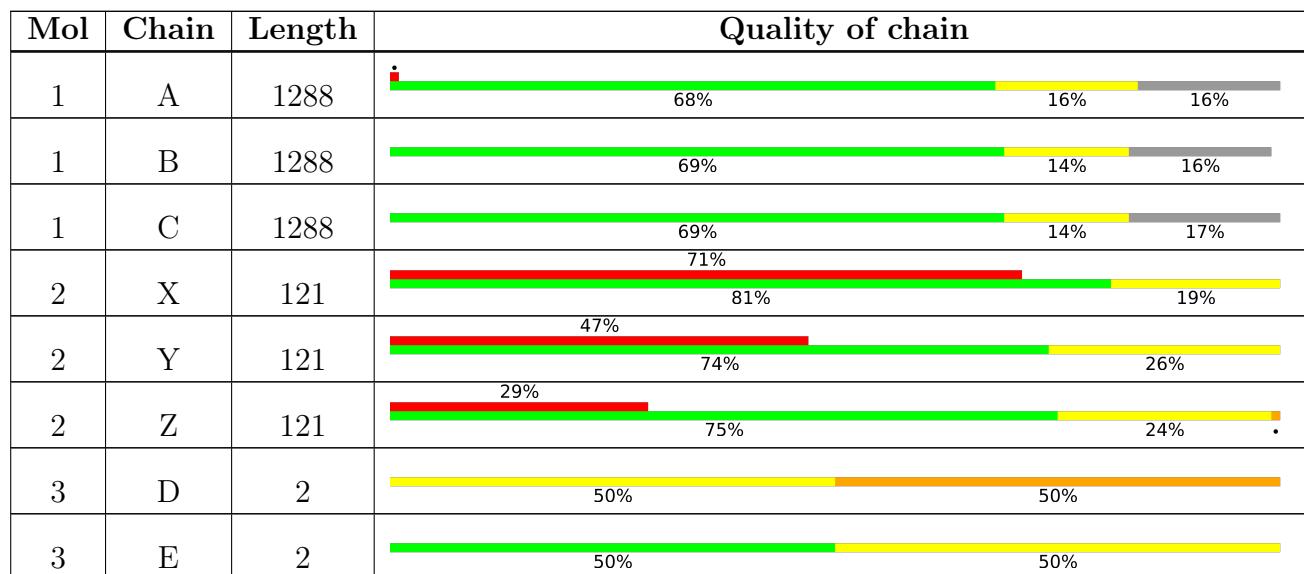
The reported resolution of this entry is 3.02 Å.

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.



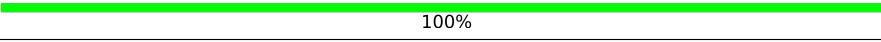
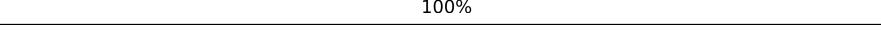
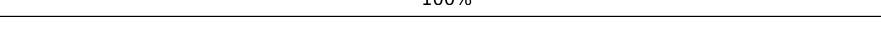
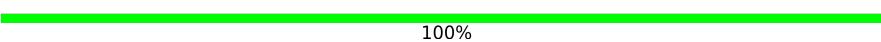
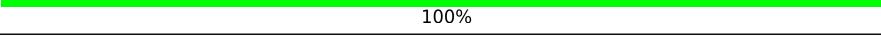
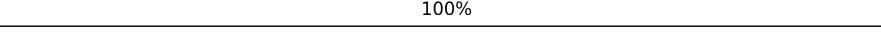
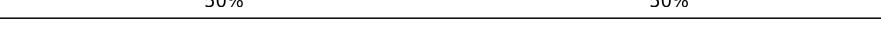
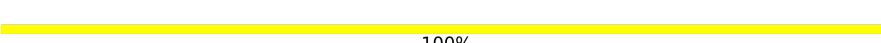
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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.



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Mol	Chain	Length	Quality of chain
3	F	2	 100%
3	G	2	 50%  50%
3	H	2	 100%
3	I	2	 100%
3	J	2	 100%
3	K	2	 100%
3	L	2	 50%  50%
3	M	2	 50%  50%
3	N	2	 100%
3	O	2	 50%  50%
3	P	2	 100%
3	Q	2	 100%
3	R	2	 50%  50%
3	S	2	 100%
3	U	2	 100%
3	V	2	 50%  50%
3	W	2	 100%

2 Entry composition [\(i\)](#)

There are 4 unique types of molecules in this entry. The entry contains 29062 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	1076	Total	C 8395	N 5352	O 1402	S 1603	38	0
1	B	1078	Total	C 8405	N 5357	O 1405	S 1605	38	0
1	C	1075	Total	C 8384	N 5345	O 1401	S 1600	38	0

There are 267 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 a protein called Synthetic nanobody (sybody), Sb45.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	121	Total	C	N	O	S	0	0
			952	598	169	181	4		
2	Y	121	Total	C	N	O	S	0	0
			952	598	169	181	4		
2	Z	121	Total	C	N	O	S	0	0
			952	598	169	181	4		

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



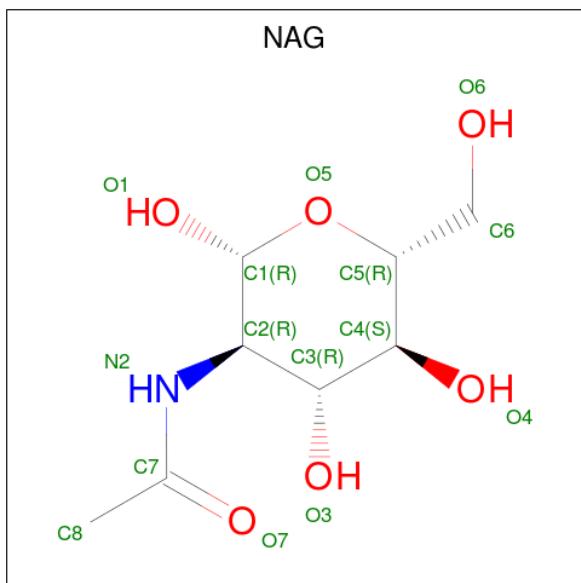
Mol	Chain	Residues	Atoms	AltConf	Trace
3	D	2	Total C N O 28 16 2 10	0	0
3	E	2	Total C N O 28 16 2 10	0	0
3	F	2	Total C N O 28 16 2 10	0	0
3	G	2	Total C N O 28 16 2 10	0	0
3	H	2	Total C N O 28 16 2 10	0	0
3	I	2	Total C N O 28 16 2 10	0	0
3	J	2	Total C N O 28 16 2 10	0	0
3	K	2	Total C N O 28 16 2 10	0	0
3	L	2	Total C N O 28 16 2 10	0	0
3	M	2	Total C N O 28 16 2 10	0	0
3	N	2	Total C N O 28 16 2 10	0	0
3	O	2	Total C N O 28 16 2 10	0	0
3	P	2	Total C N O 28 16 2 10	0	0
3	Q	2	Total C N O 28 16 2 10	0	0
3	R	2	Total C N O 28 16 2 10	0	0
3	S	2	Total C N O 28 16 2 10	0	0
3	U	2	Total C N O 28 16 2 10	0	0
3	V	2	Total C N O 28 16 2 10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	W	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 112	C 64	N 8	O 40	0
4	A	1	Total 112	C 64	N 8	O 40	0
4	A	1	Total 112	C 64	N 8	O 40	0
4	A	1	Total 112	C 64	N 8	O 40	0
4	A	1	Total 112	C 64	N 8	O 40	0
4	A	1	Total 112	C 64	N 8	O 40	0
4	A	1	Total 112	C 64	N 8	O 40	0
4	B	1	Total 210	C 120	N 15	O 75	0
4	B	1	Total 210	C 120	N 15	O 75	0

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	B	1	Total	C	N	O	0
			210	120	15	75	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	

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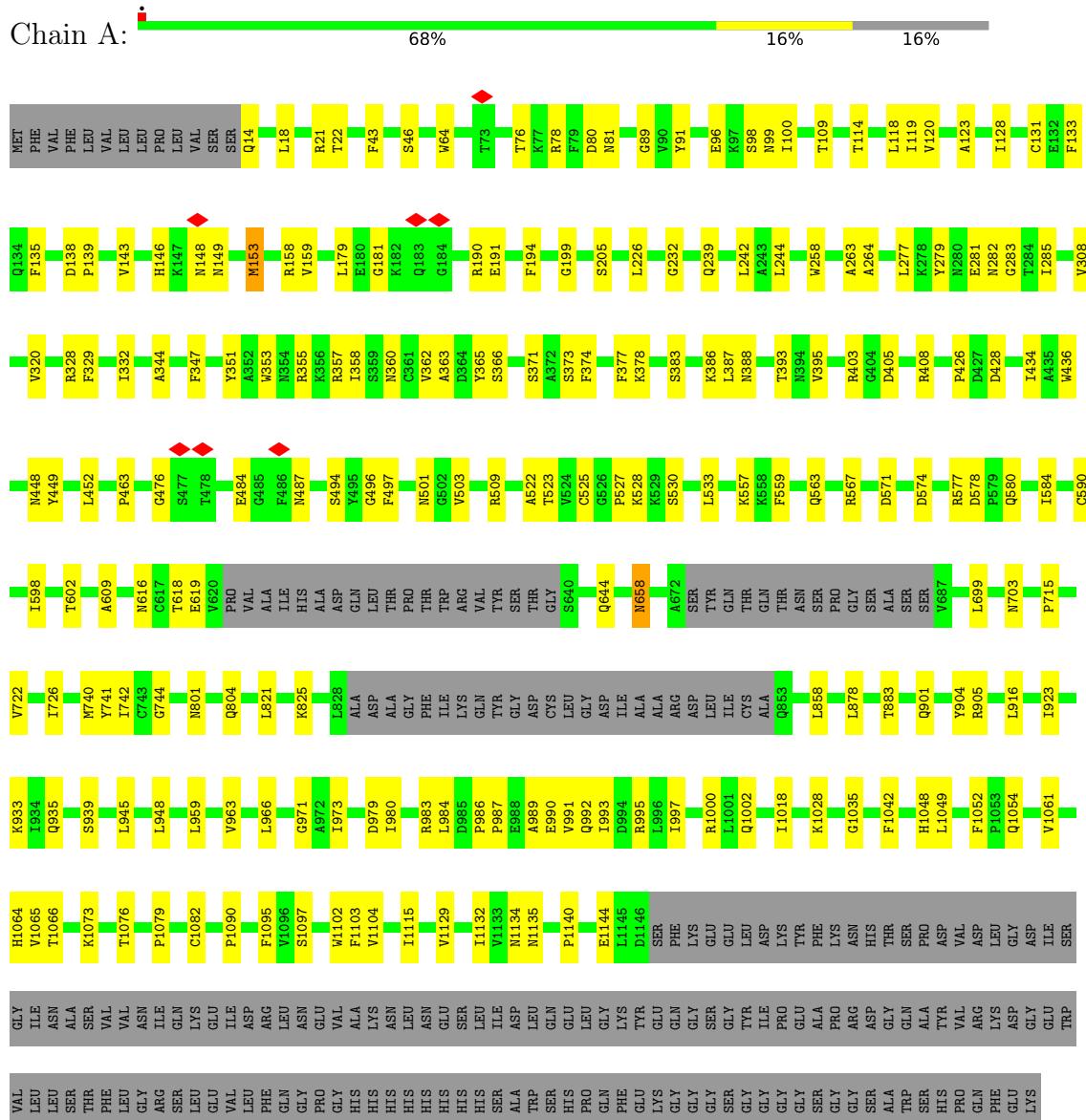
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	
4	C	1	Total	C	N	O	0
			168	96	12	60	

3 Residue-property plots [\(i\)](#)

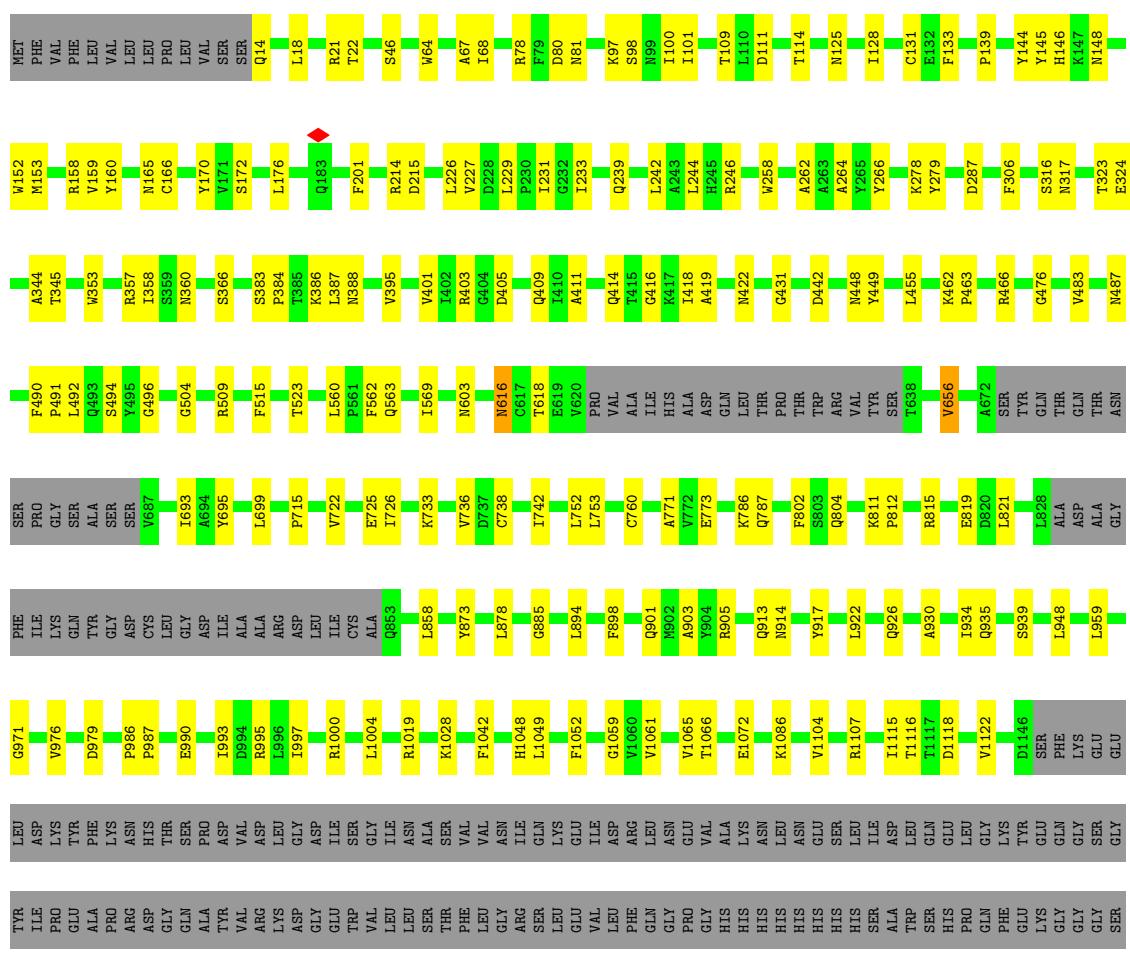
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



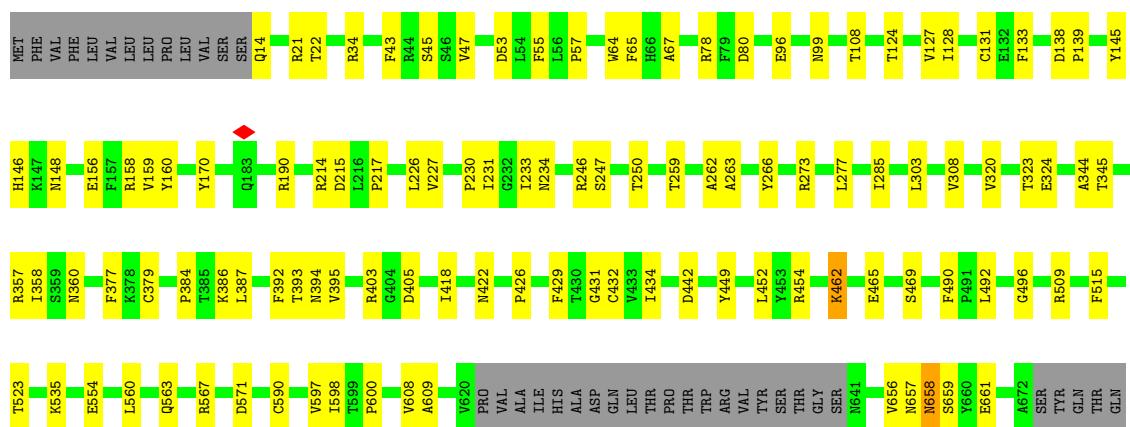
- Molecule 1: Spike glycoprotein

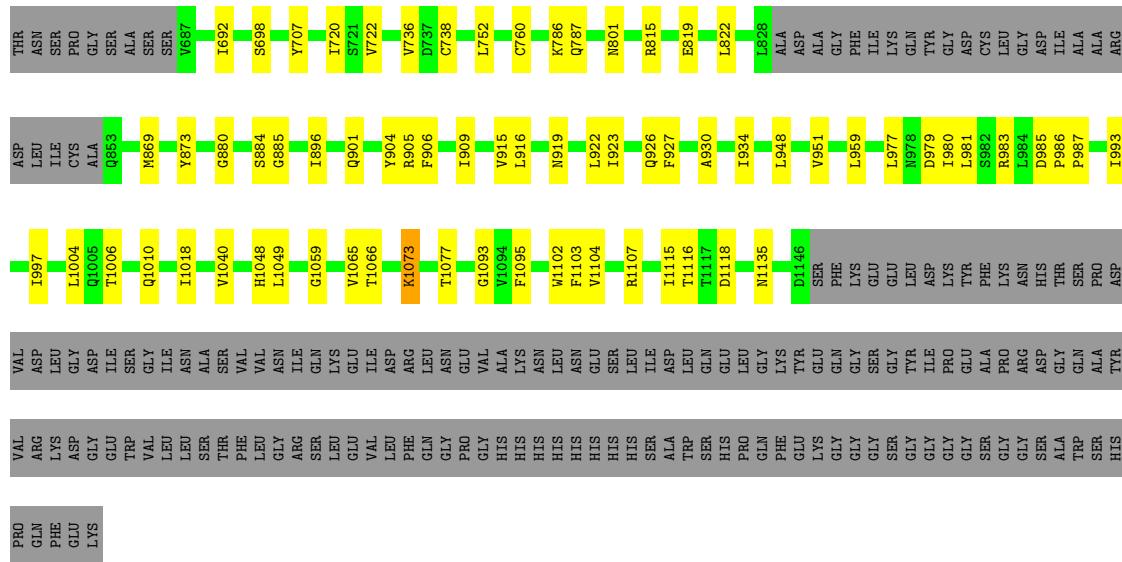
Chain B:



- Molecule 1: Spike glycoprotein

Chain C:

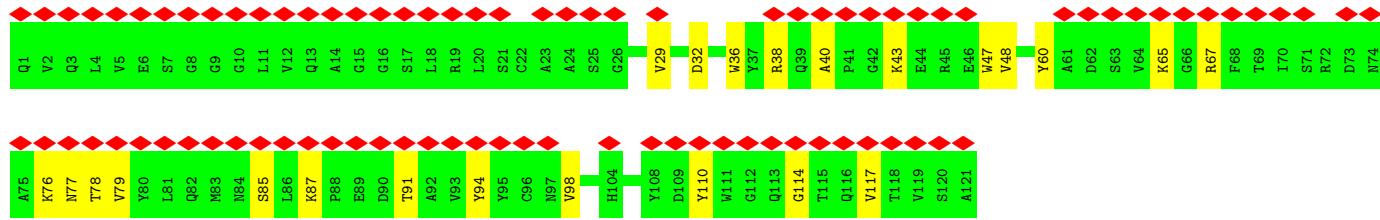




- Molecule 2: Synthetic nanobody (sybody), Sb45

Chain X: 81% 71% 19%

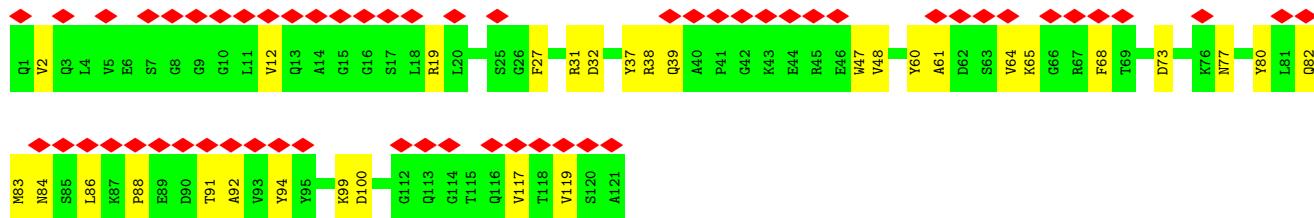
A horizontal progress bar for 'Chain X' is shown. The bar is mostly green, with a yellow segment at the end. The total length is labeled as 100%. The green part is labeled '81%' below it, and the yellow part is labeled '19%' to its right. Above the bar, the text 'Chain X:' is written.



- Molecule 2: Synthetic nanobody (sybody), Sb45

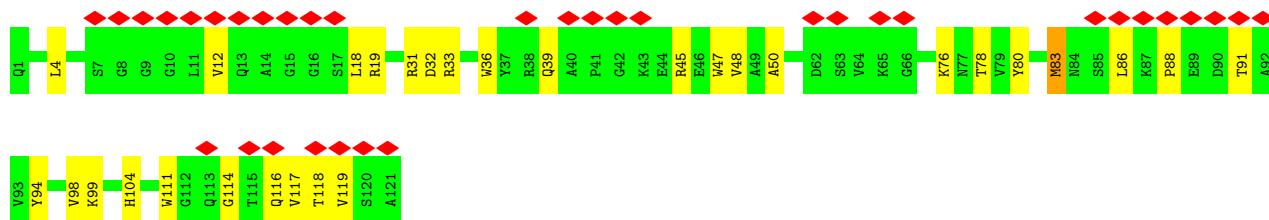
A horizontal bar chart illustrating the distribution of Chain Y across three categories. The x-axis represents the total length of the bar, which is divided into three segments. The first segment is red and labeled '47%'. The second segment is green and labeled '74%'. The third segment is yellow and labeled '26%'. The label 'Chain Y:' is positioned to the left of the first segment.

Category	Percentage
Red	47%
Green	74%
Yellow	26%



- Molecule 2: Synthetic nanobody (sybody), Sb45

A horizontal progress bar for 'Chain Z' is shown, consisting of three colored segments: red, green, and yellow. The red segment is labeled '29%' above it. The green segment is labeled '75%' below it. The yellow segment is labeled '24%' above it. The total length of the bar is indicated by a vertical line at the far right.



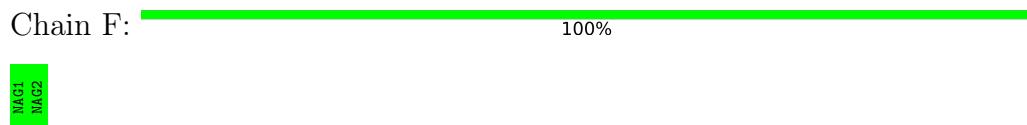
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



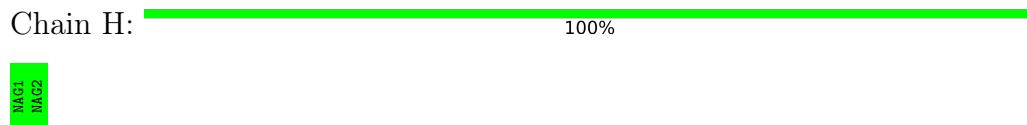
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



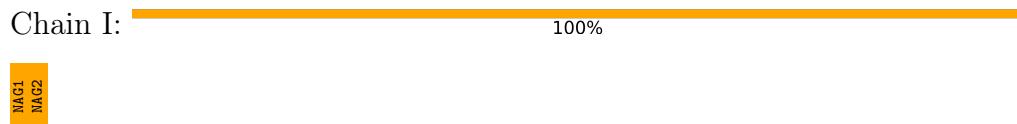
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





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

Chain K:  100%



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

Chain L:  50% 50%



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

Chain M:  50% 50%



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

Chain N:  100%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain Q:  100%

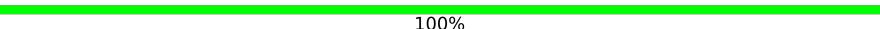


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50%  50%

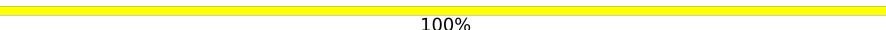


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



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

Chain U:  100%

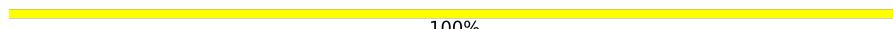


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50%  50%



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

Chain W:  100%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	214171	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; patch CTF estimation	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	535	Depositor
Maximum defocus (nm)	2431	Depositor
Magnification	47529	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.977	Depositor
Minimum map value	-0.329	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0429	Depositor
Map size (Å)	420.80002, 420.80002, 420.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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	0.26	0/8593	0.48	0/11704
1	B	0.26	0/8603	0.49	0/11716
1	C	0.26	0/8582	0.48	0/11689
2	X	0.25	0/975	0.51	0/1322
2	Y	0.25	0/975	0.50	0/1322
2	Z	0.24	0/975	0.51	0/1322
All	All	0.26	0/28703	0.49	0/39075

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	B	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	616	ASN	Peptide
1	B	656	VAL	Peptide
1	C	1073	LYS	Peptide

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	8395	0	8163	144	0
1	B	8405	0	8167	134	0
1	C	8384	0	8143	122	0
2	X	952	0	902	16	0
2	Y	952	0	902	24	0
2	Z	952	0	902	20	0
3	D	28	0	25	1	0
3	E	28	0	25	2	0
3	F	28	0	25	0	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	3	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	1	0
3	N	28	0	25	0	0
3	O	28	0	25	1	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	U	28	0	25	1	0
3	V	28	0	25	2	0
3	W	28	0	25	2	0
4	A	112	0	104	3	0
4	B	210	0	194	2	0
4	C	168	0	155	3	0
All	All	29062	0	28107	436	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 8.

The worst 5 of 436 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)
2:Y:91:THR:HA	2:Y:117:VAL:O	1.67	0.95
1:A:139:PRO:HA	1:A:158:ARG:O	1.76	0.84
1:B:462:LYS:HD2	1:B:463:PRO:HD2	1.64	0.78
1:C:139:PRO:HA	1:C:158:ARG:O	1.85	0.76
1:A:973:ILE:HD12	1:A:983:ARG:HH21	1.49	0.75

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	1068/1288 (83%)	1036 (97%)	32 (3%)	0	100 100
1	B	1070/1288 (83%)	1035 (97%)	35 (3%)	0	100 100
1	C	1067/1288 (83%)	1031 (97%)	36 (3%)	0	100 100
2	X	119/121 (98%)	116 (98%)	3 (2%)	0	100 100
2	Y	119/121 (98%)	116 (98%)	3 (2%)	0	100 100
2	Z	119/121 (98%)	114 (96%)	5 (4%)	0	100 100
All	All	3562/4227 (84%)	3448 (97%)	114 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [\(i\)](#)

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	940/1116 (84%)	937 (100%)	3 (0%)	92 97
1	B	940/1116 (84%)	940 (100%)	0	100 100
1	C	937/1116 (84%)	935 (100%)	2 (0%)	93 98
2	X	96/97 (99%)	96 (100%)	0	100 100
2	Y	96/97 (99%)	96 (100%)	0	100 100
2	Z	96/97 (99%)	95 (99%)	1 (1%)	76 91
All	All	3105/3639 (85%)	3099 (100%)	6 (0%)	93 98

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

Mol	Chain	Res	Type
1	C	462	LYS
1	C	658	ASN
2	Z	83	MET
1	A	658	ASN
1	A	153	MET

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

Mol	Chain	Res	Type
1	C	658	ASN
1	C	901	GLN
1	A	935	GLN
1	B	409	GLN
1	B	901	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

38 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
3	NAG	D	1	3,1	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
3	NAG	D	2	3	14,14,15	0.51	0	17,19,21	1.27	2 (11%)
3	NAG	E	1	3,1	14,14,15	0.33	0	17,19,21	0.58	0
3	NAG	E	2	3	14,14,15	0.35	0	17,19,21	0.55	0
3	NAG	F	1	3,1	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	G	1	3,1	14,14,15	0.47	0	17,19,21	0.49	0
3	NAG	G	2	3	14,14,15	0.18	0	17,19,21	0.56	0
3	NAG	H	1	3,1	14,14,15	0.28	0	17,19,21	0.42	0
3	NAG	H	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	I	1	3,1	14,14,15	0.35	0	17,19,21	1.26	2 (11%)
3	NAG	I	2	3	14,14,15	0.42	0	17,19,21	1.26	1 (5%)
3	NAG	J	1	3,1	14,14,15	0.42	0	17,19,21	0.39	0
3	NAG	J	2	3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	K	1	3,1	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	K	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	L	1	3,1	14,14,15	1.03	1 (7%)	17,19,21	1.53	1 (5%)
3	NAG	L	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	M	1	3,1	14,14,15	0.38	0	17,19,21	0.57	0
3	NAG	M	2	3	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	N	1	3,1	14,14,15	0.32	0	17,19,21	0.69	0
3	NAG	N	2	3	14,14,15	0.46	0	17,19,21	0.46	0
3	NAG	O	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	1.61	4 (23%)
3	NAG	O	2	3	14,14,15	0.20	0	17,19,21	0.59	0
3	NAG	P	1	3,1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	P	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	Q	1	3,1	14,14,15	0.19	0	17,19,21	0.53	0
3	NAG	Q	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	R	1	3,1	14,14,15	0.90	1 (7%)	17,19,21	1.32	1 (5%)
3	NAG	R	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	S	1	3,1	14,14,15	0.53	0	17,19,21	0.46	0
3	NAG	S	2	3	14,14,15	0.38	0	17,19,21	0.35	0
3	NAG	U	1	3,1	14,14,15	0.29	0	17,19,21	0.55	0
3	NAG	U	2	3	14,14,15	0.37	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	V	1	3,1	14,14,15	0.41	0	17,19,21	0.41	0
3	NAG	V	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	W	1	3,1	14,14,15	0.35	0	17,19,21	0.40	0
3	NAG	W	2	3	14,14,15	0.27	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
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	5/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	3/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1	NAG	O5-C1	3.74	1.49	1.43
3	R	1	NAG	O5-C1	3.24	1.48	1.43
3	O	1	NAG	O5-C1	-2.59	1.39	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	C1-O5-C5	6.03	120.36	112.19
3	R	1	NAG	C1-O5-C5	5.01	118.98	112.19
3	O	1	NAG	C2-N2-C7	4.66	129.54	122.90
3	I	1	NAG	C2-N2-C7	4.35	129.09	122.90
3	D	2	NAG	C2-N2-C7	4.31	129.03	122.90

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

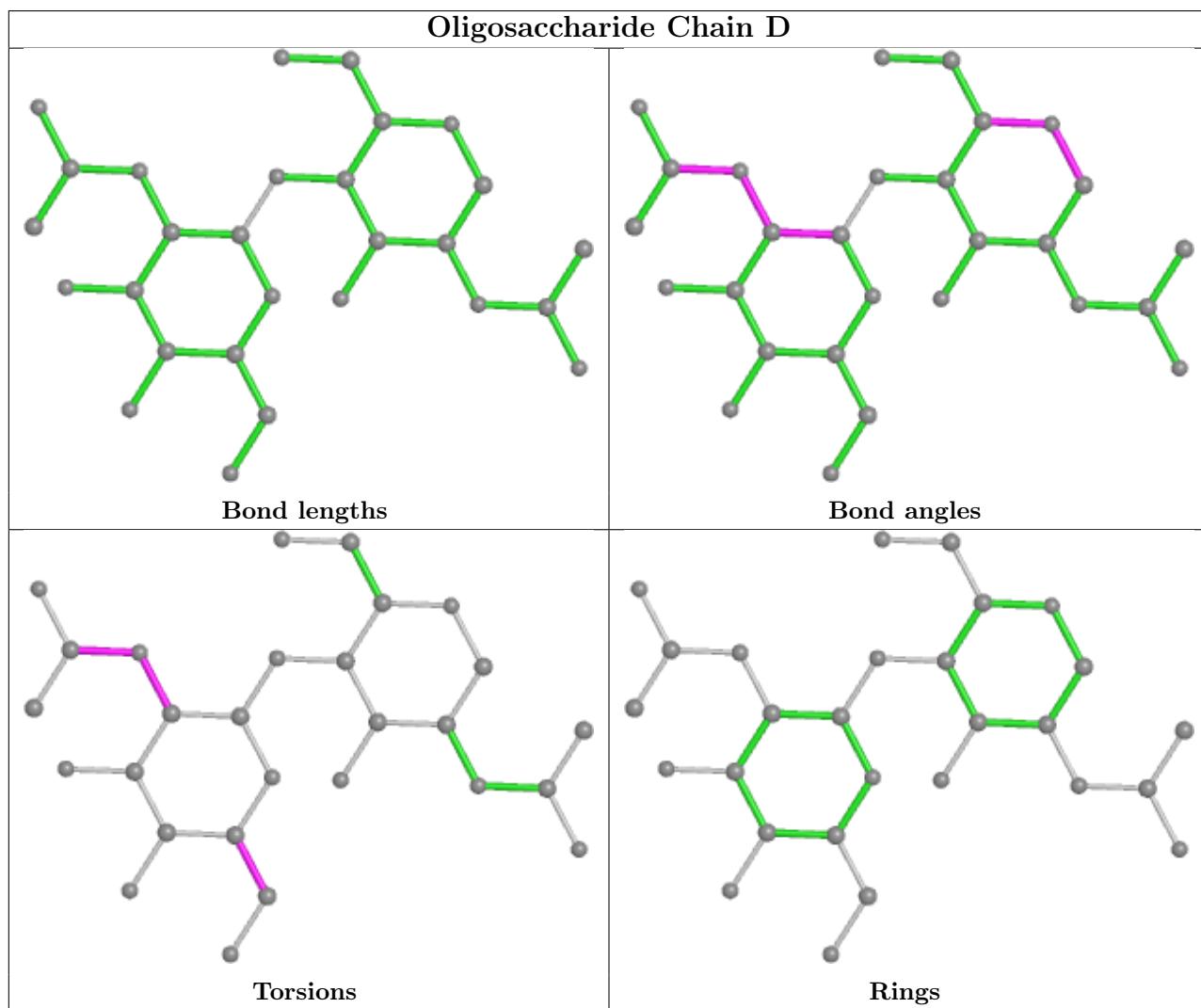
Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6

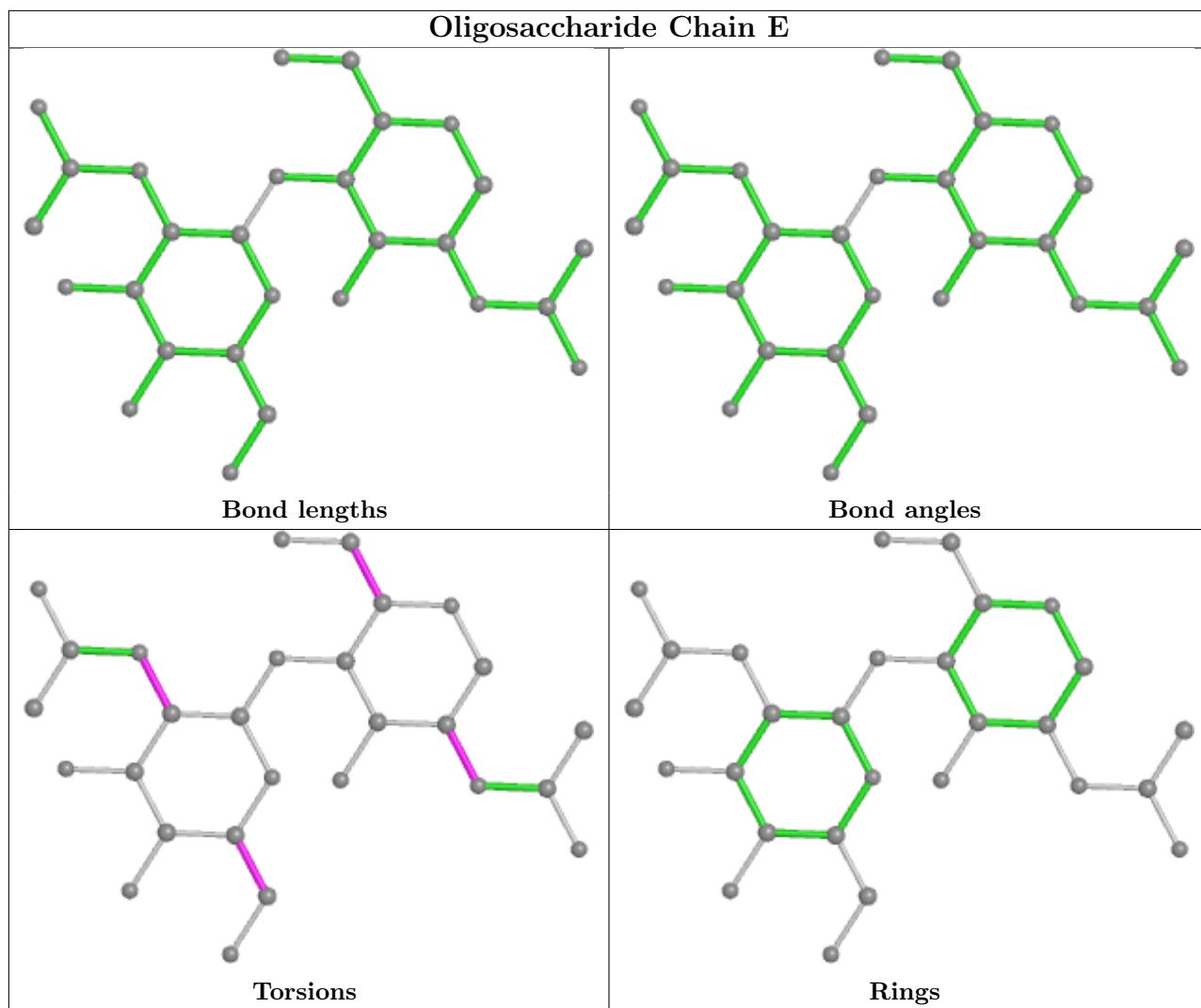
There are no ring outliers.

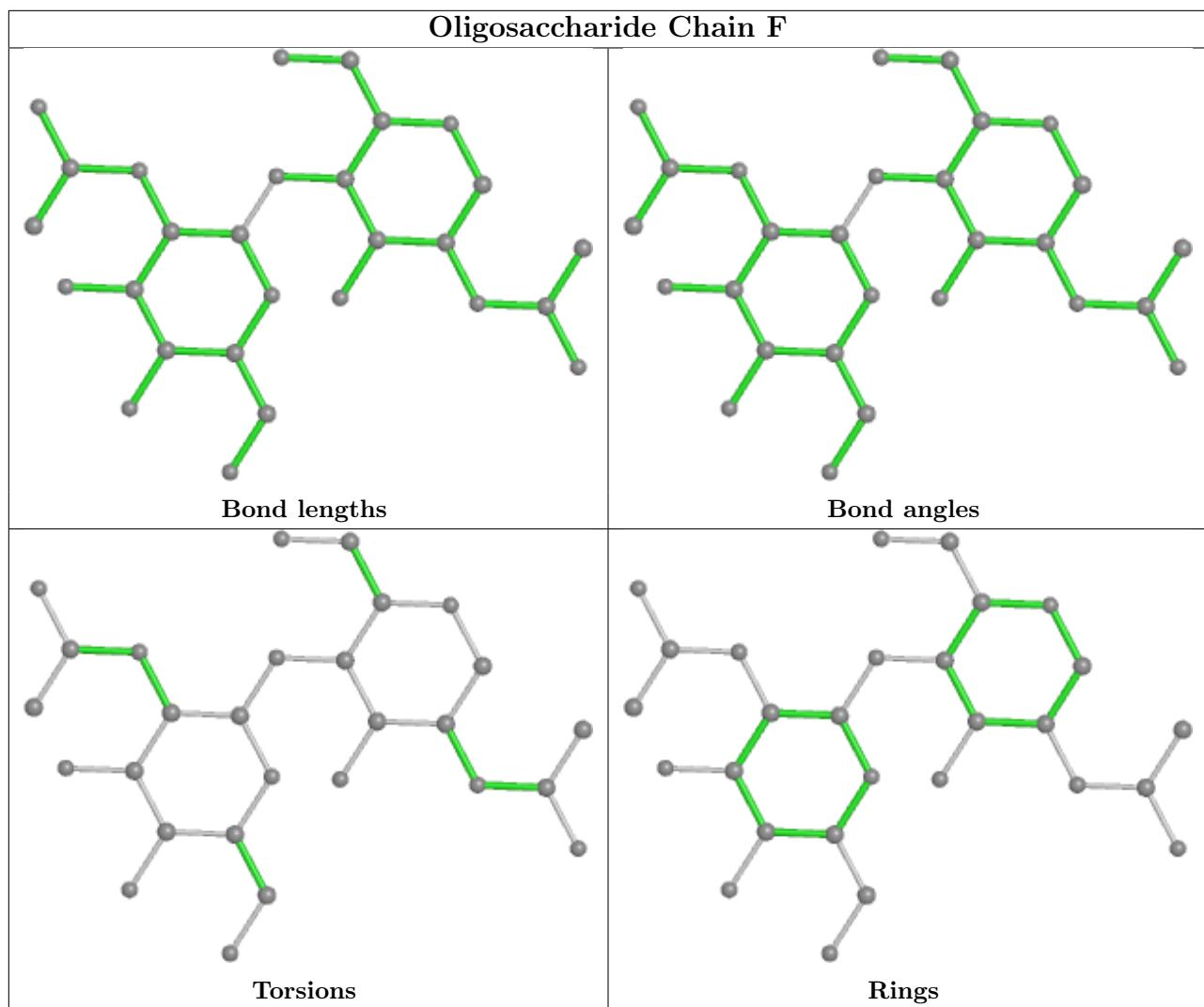
12 monomers are involved in 14 short contacts:

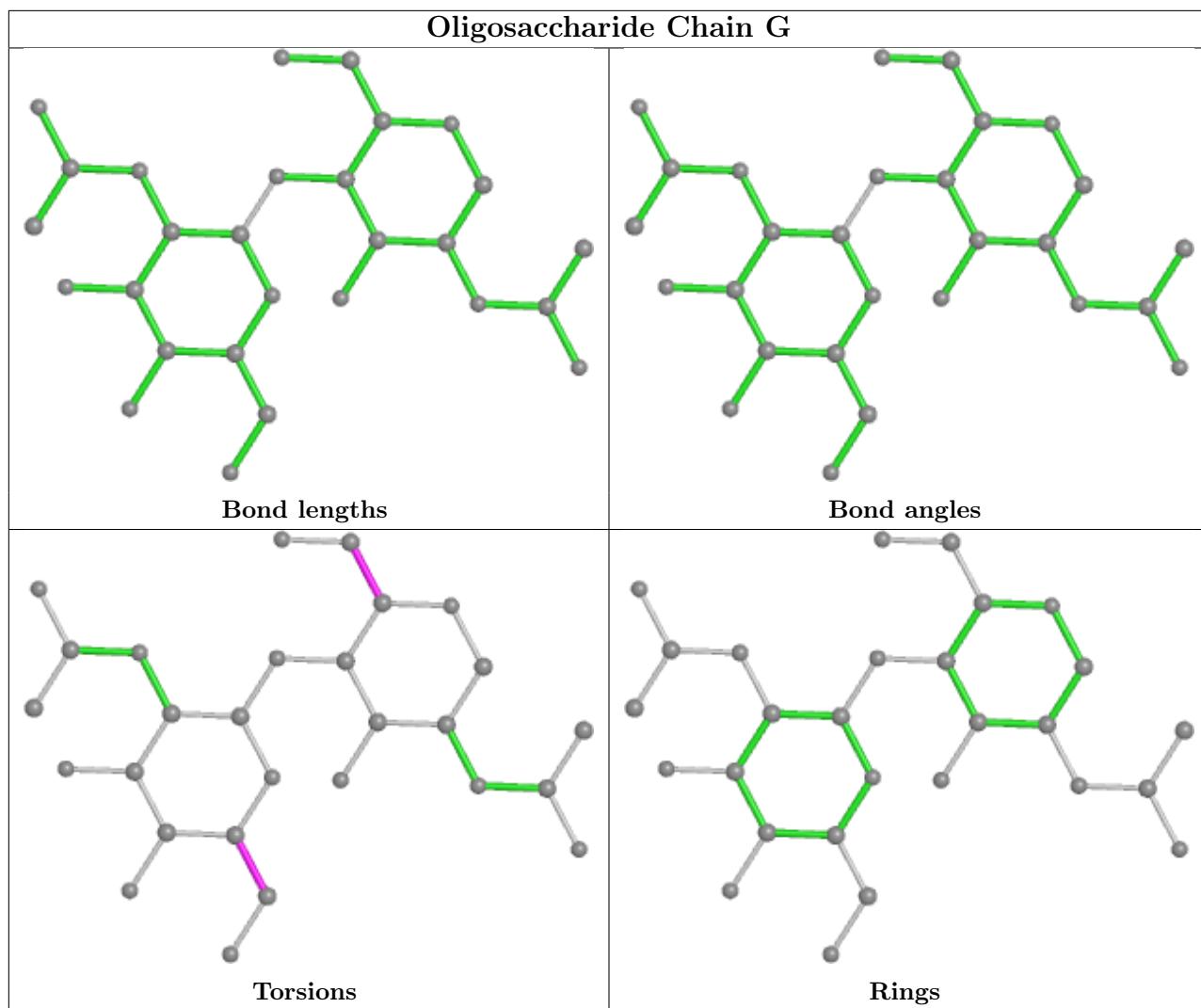
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	1	NAG	2	0
3	O	1	NAG	1	0
3	V	1	NAG	2	0
3	G	1	NAG	1	0
3	U	1	NAG	1	0
3	U	2	NAG	1	0
3	D	2	NAG	1	0
3	M	1	NAG	1	0
3	I	2	NAG	1	0
3	E	2	NAG	2	0
3	I	1	NAG	2	0
3	W	2	NAG	1	0

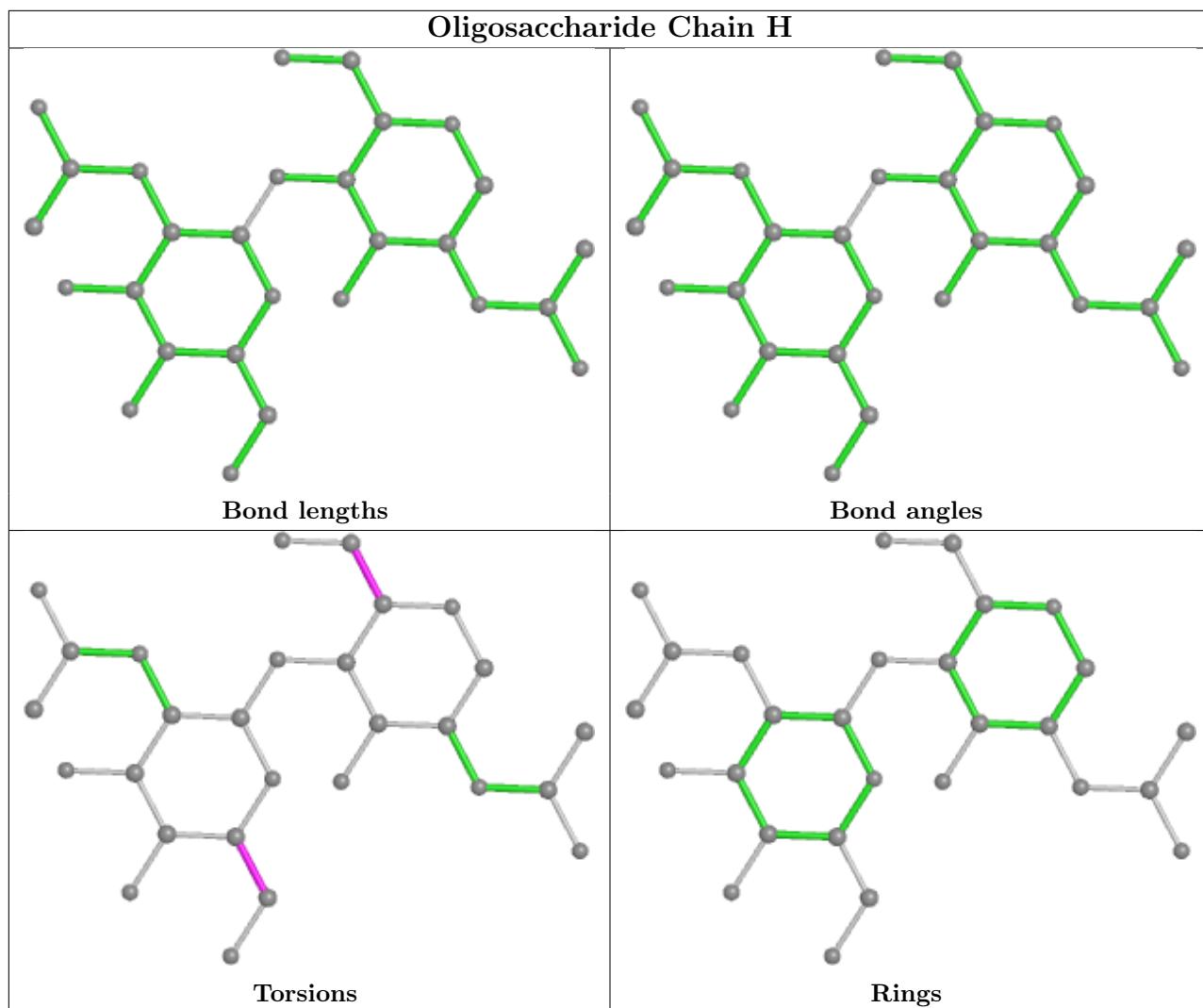
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

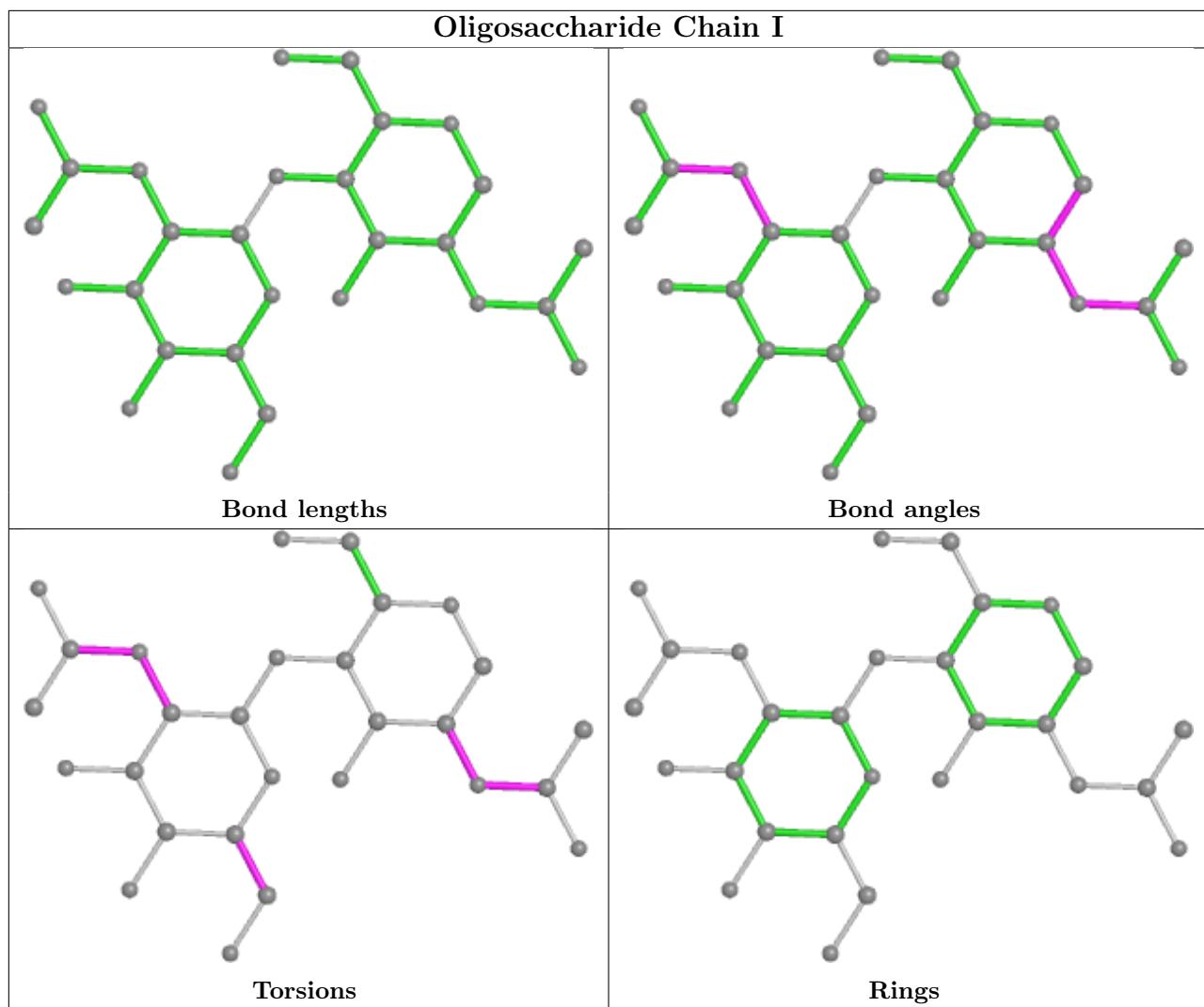


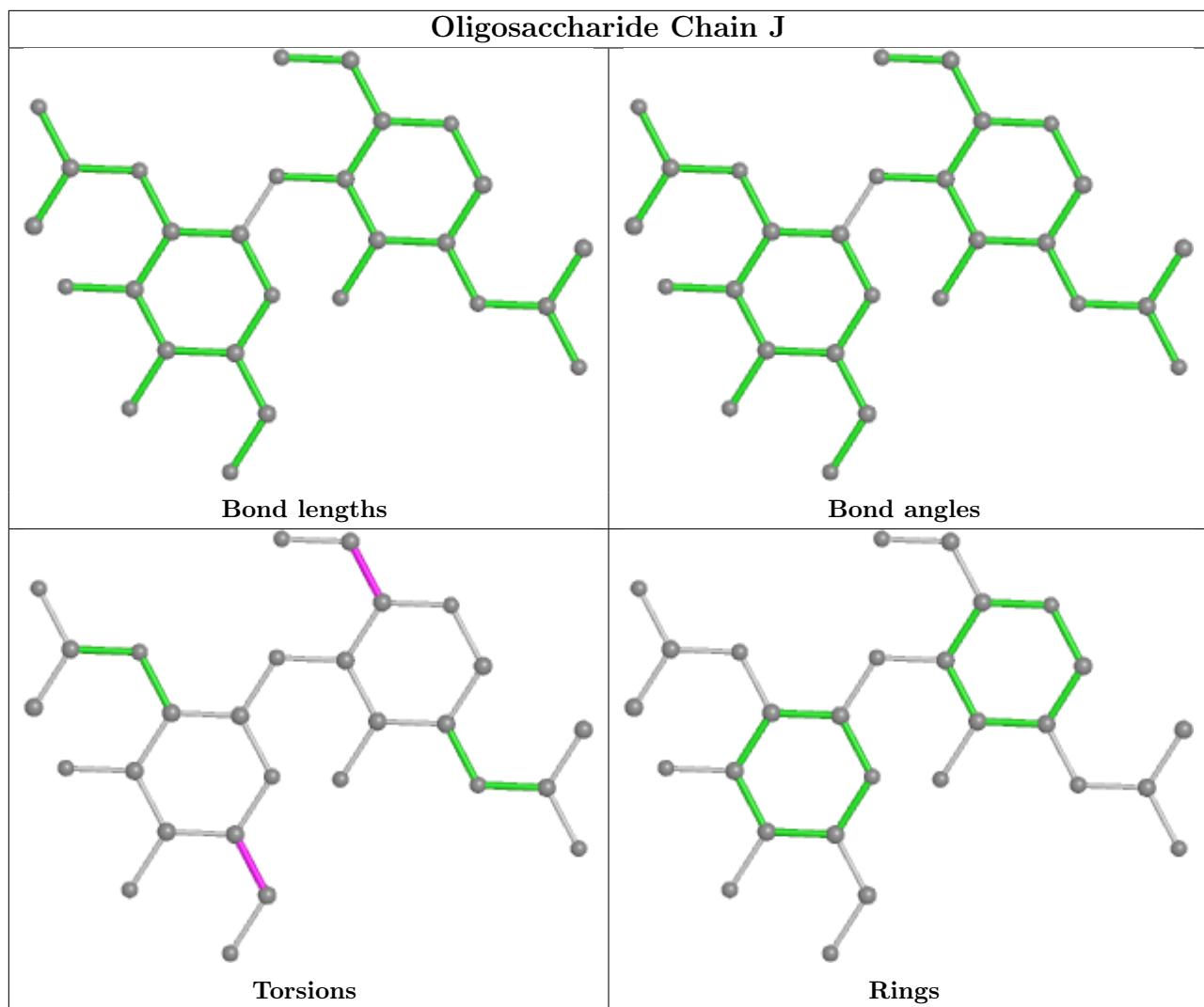


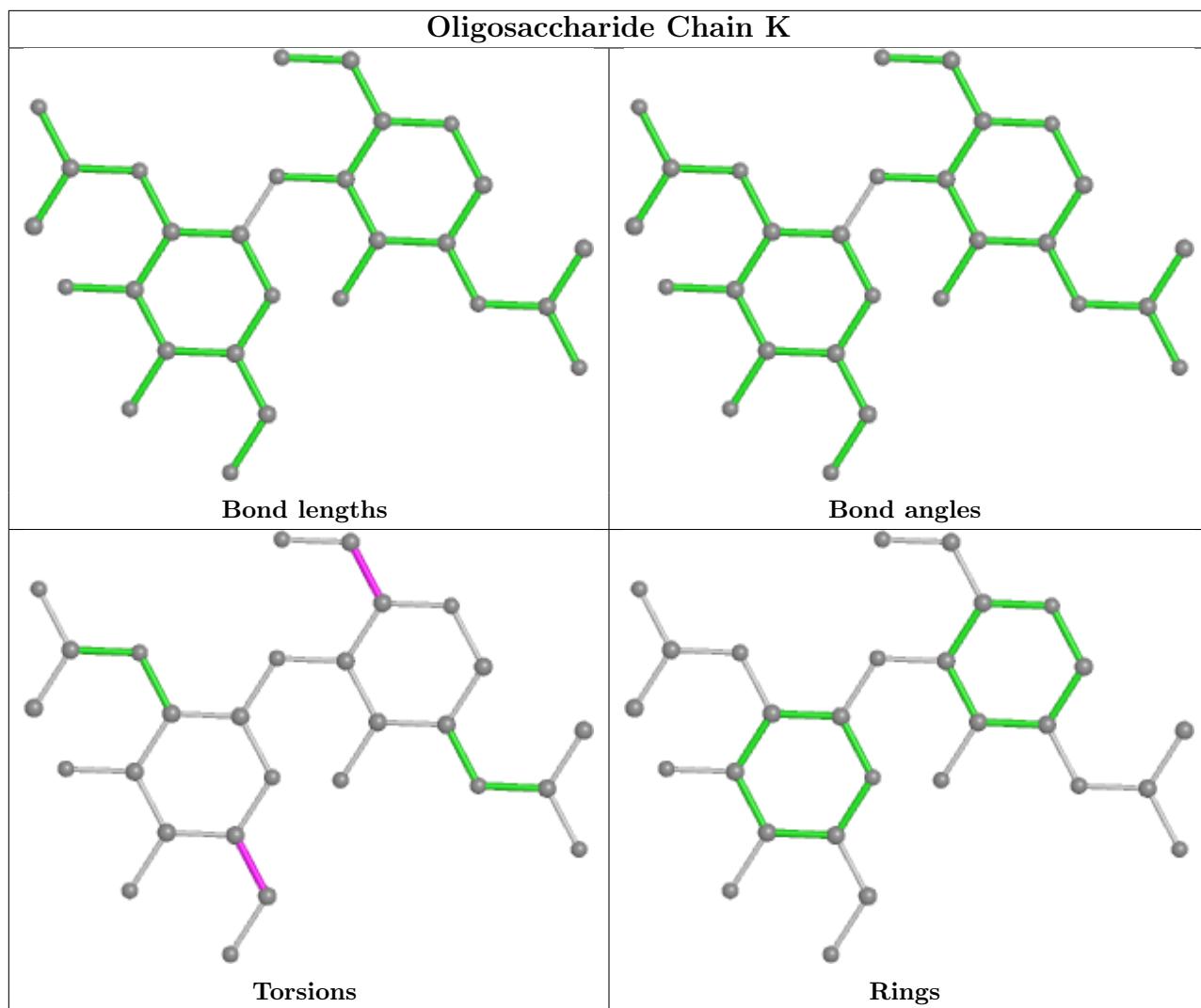


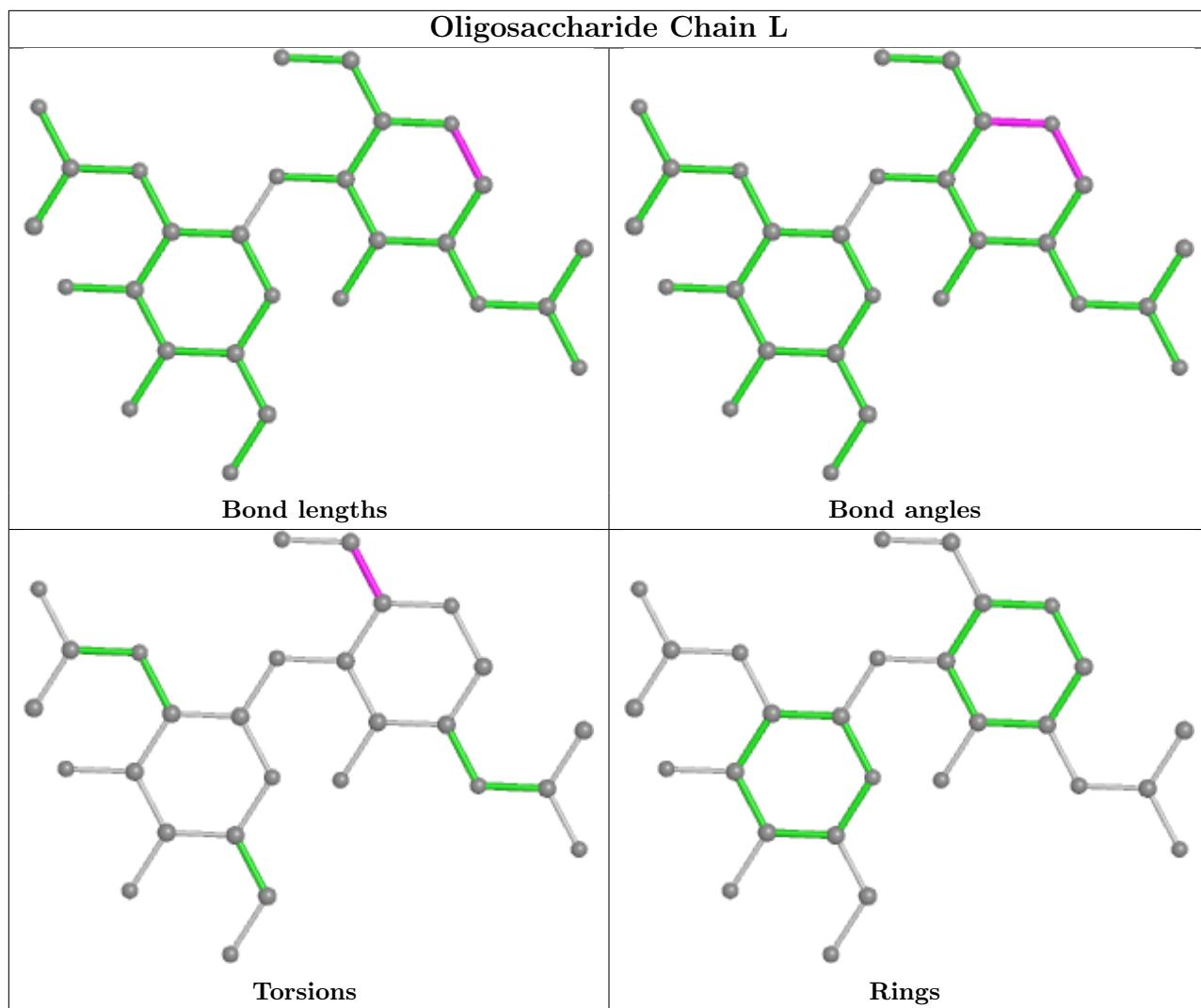


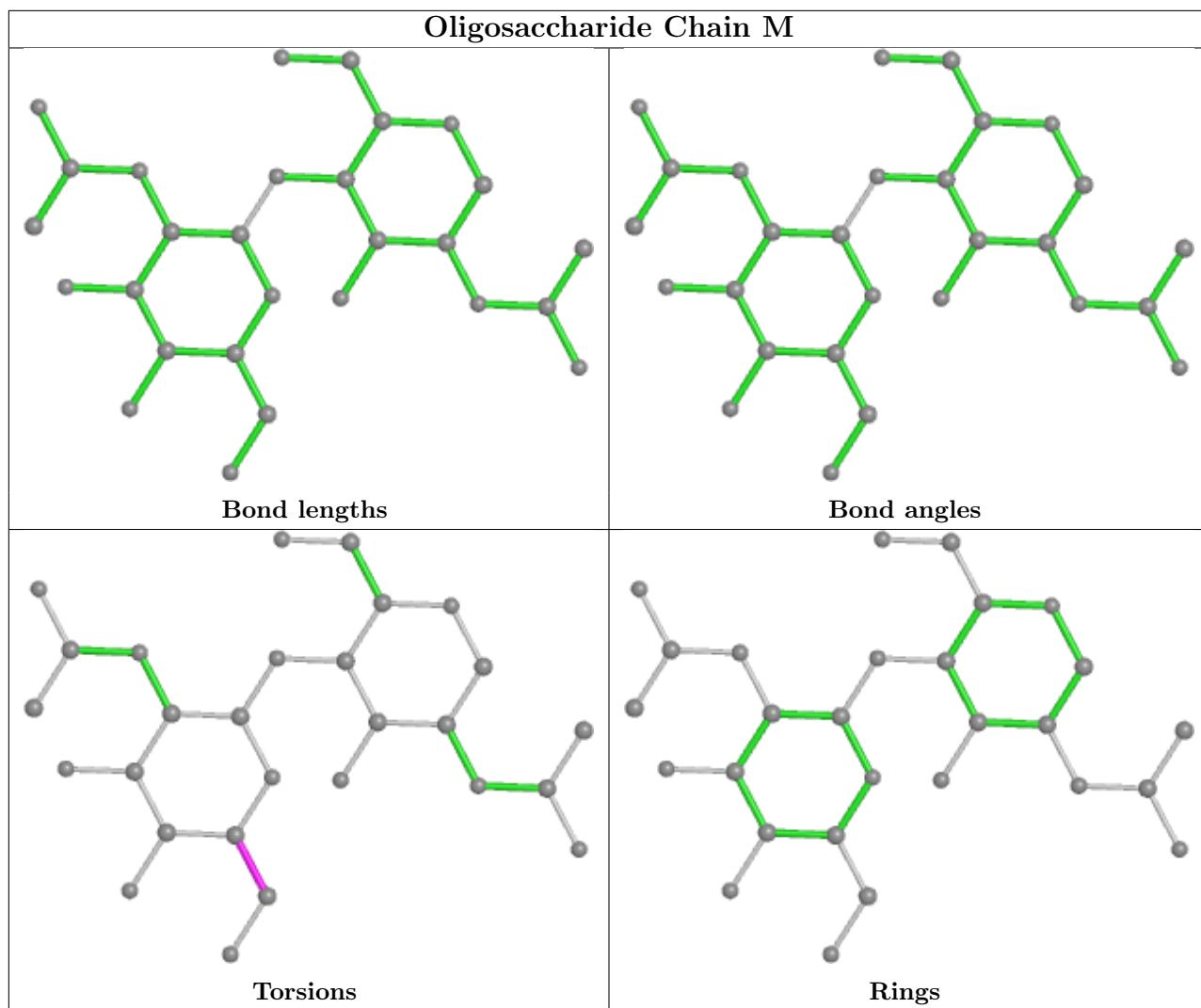


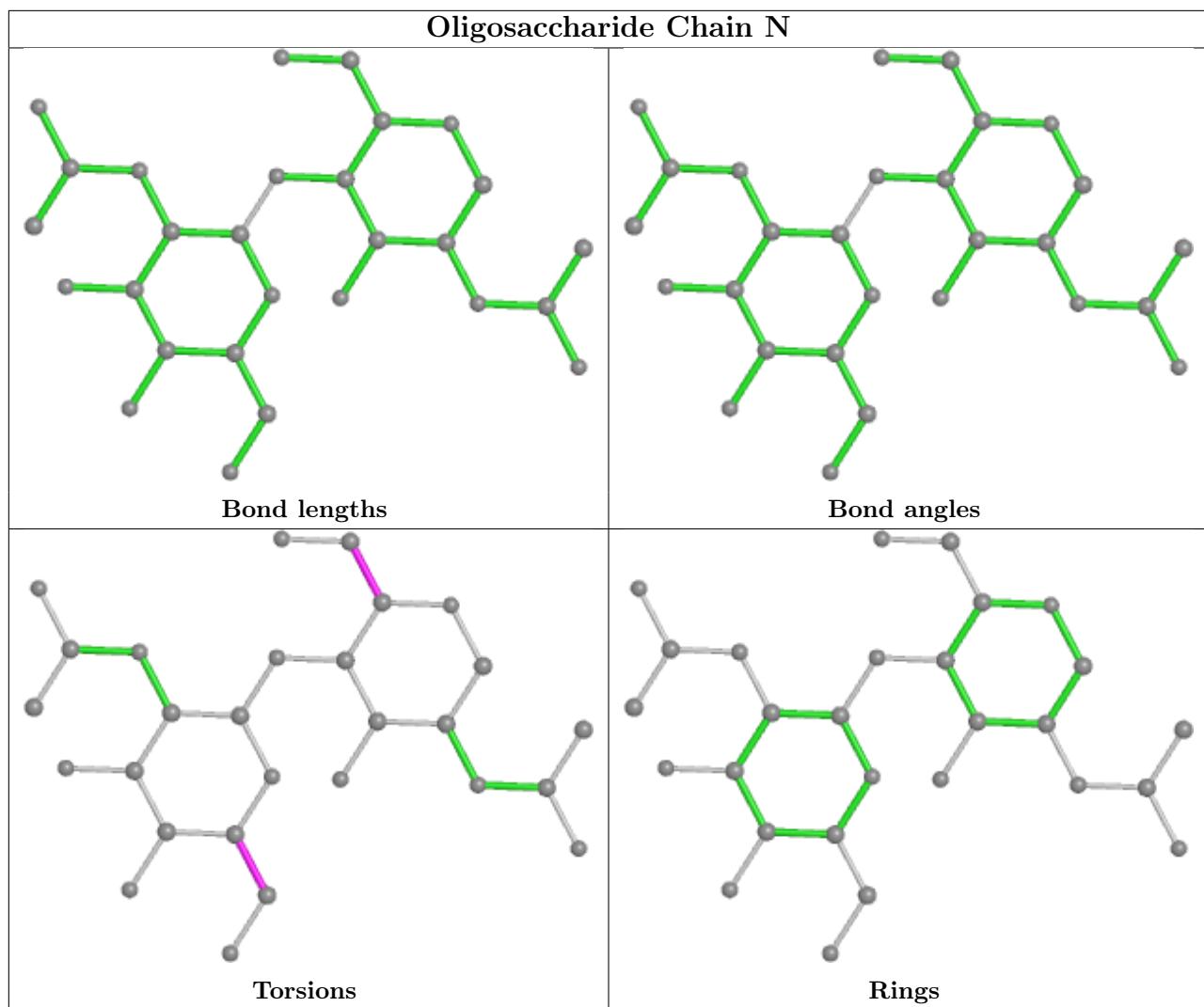


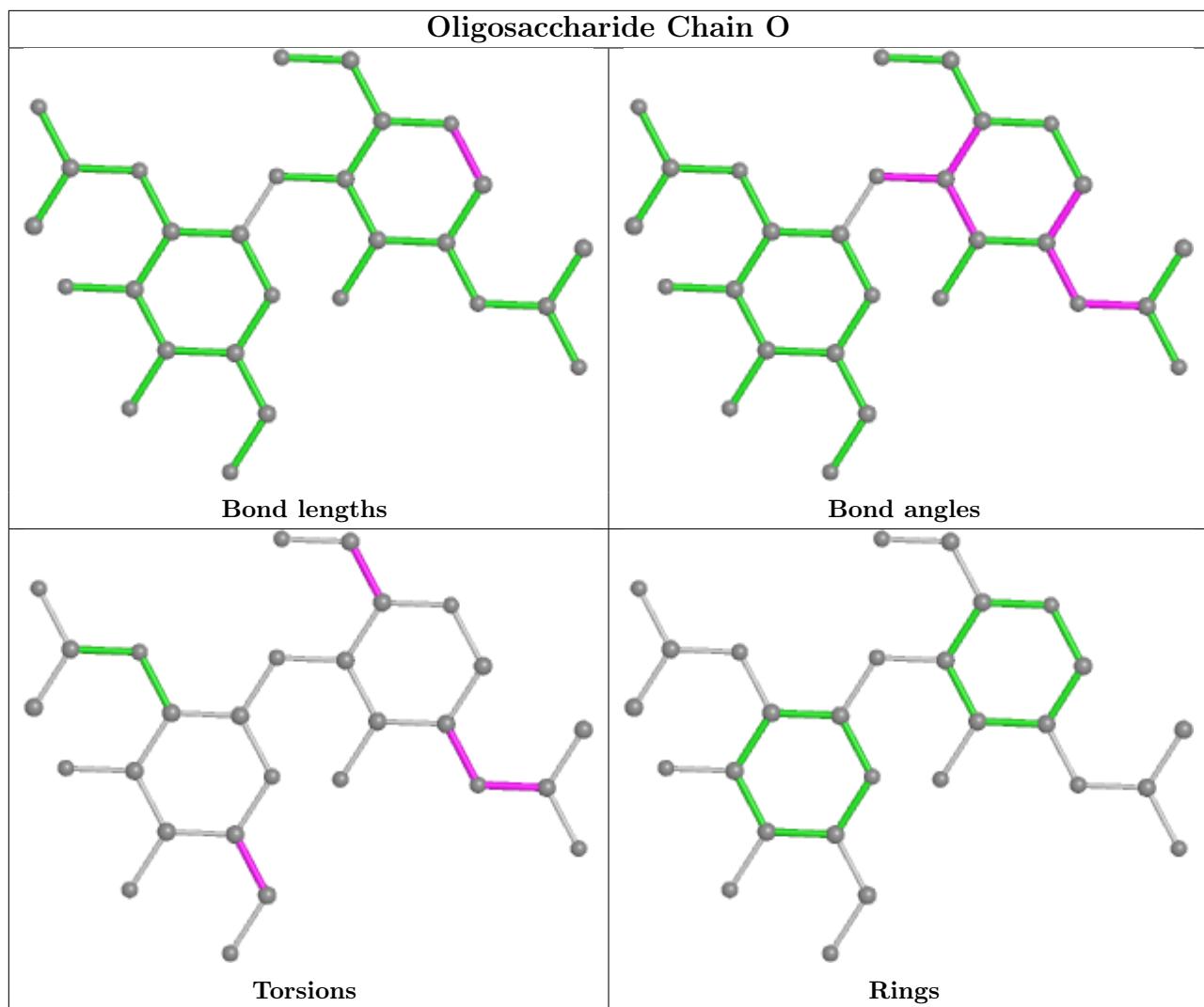


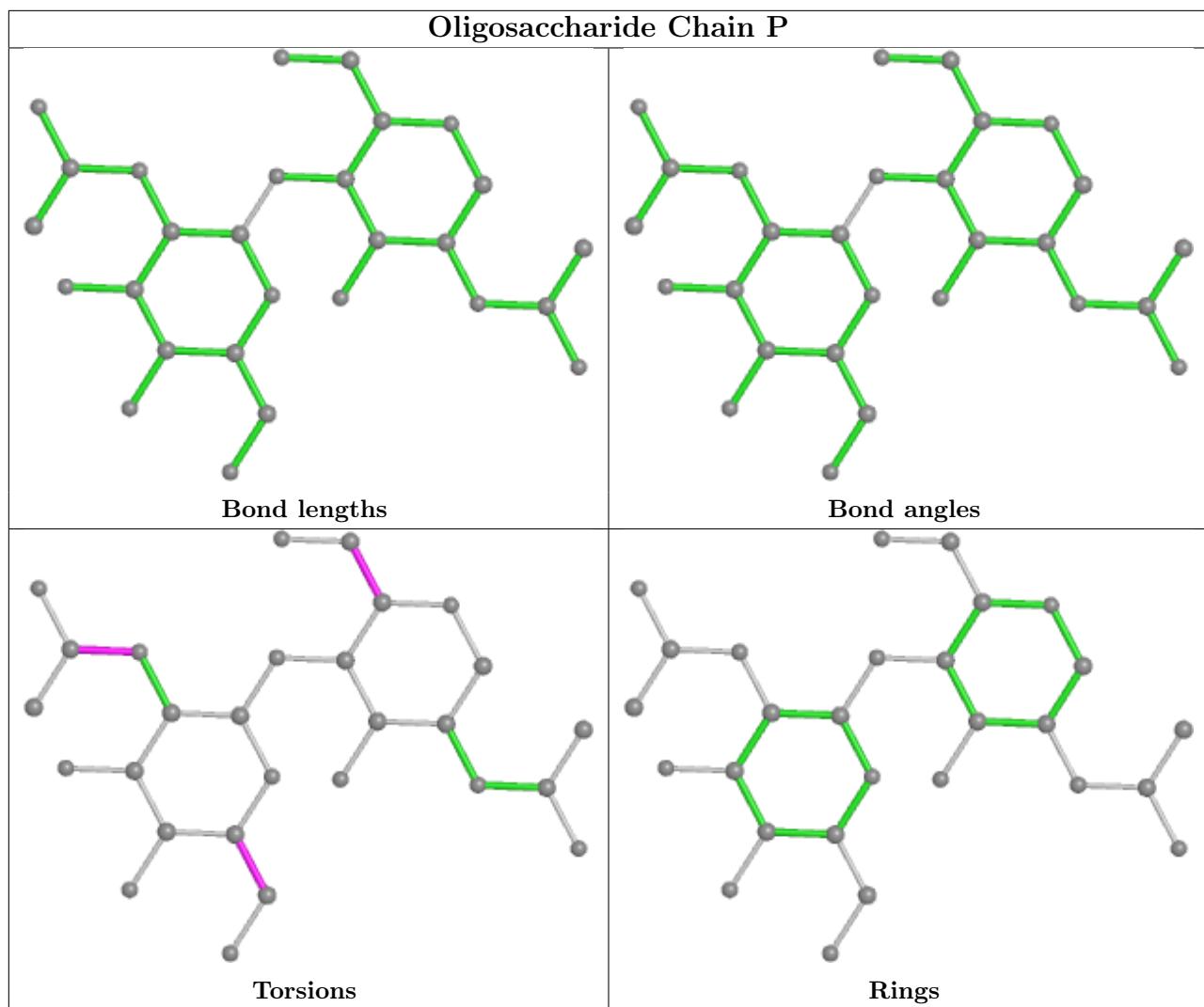


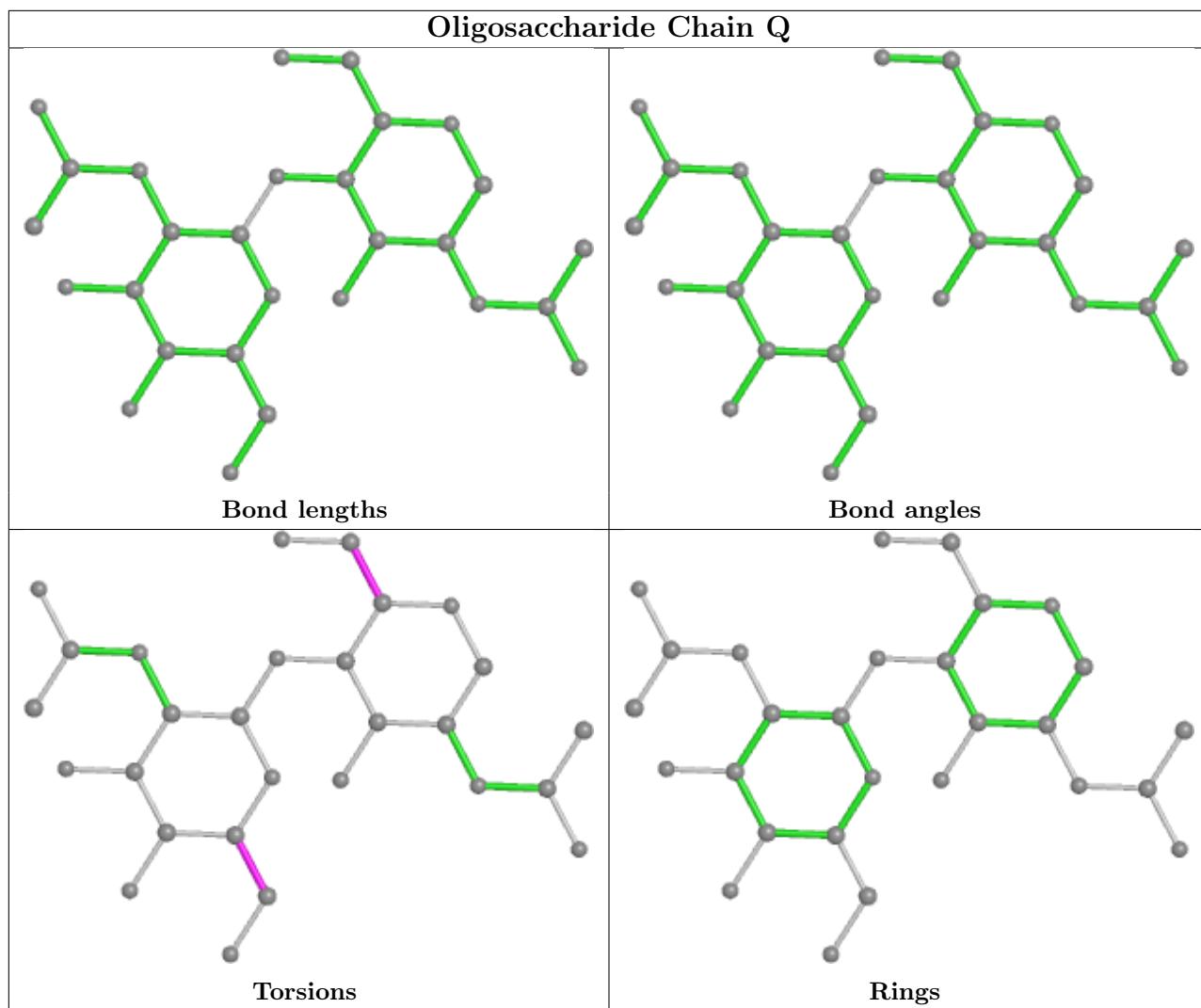


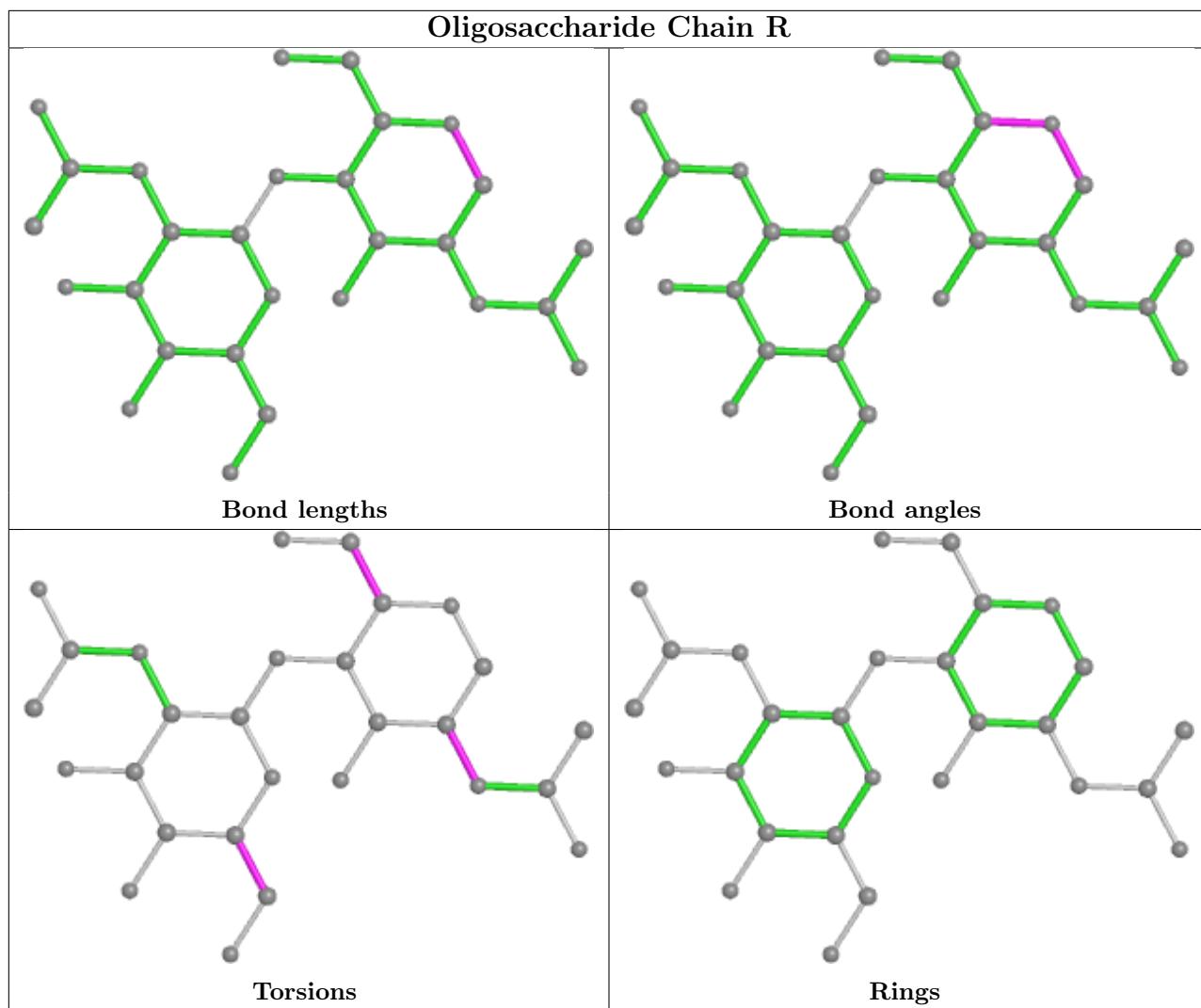


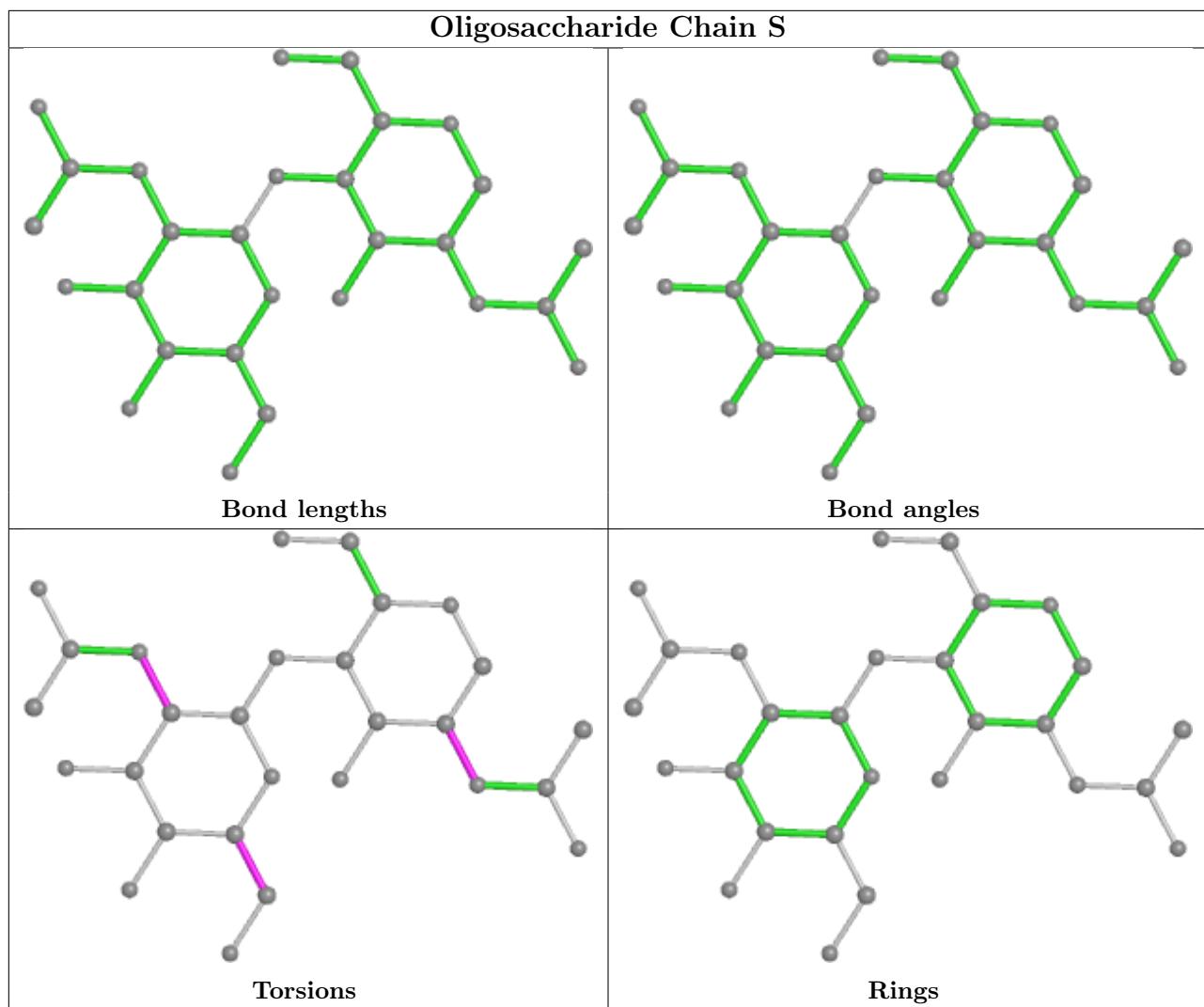


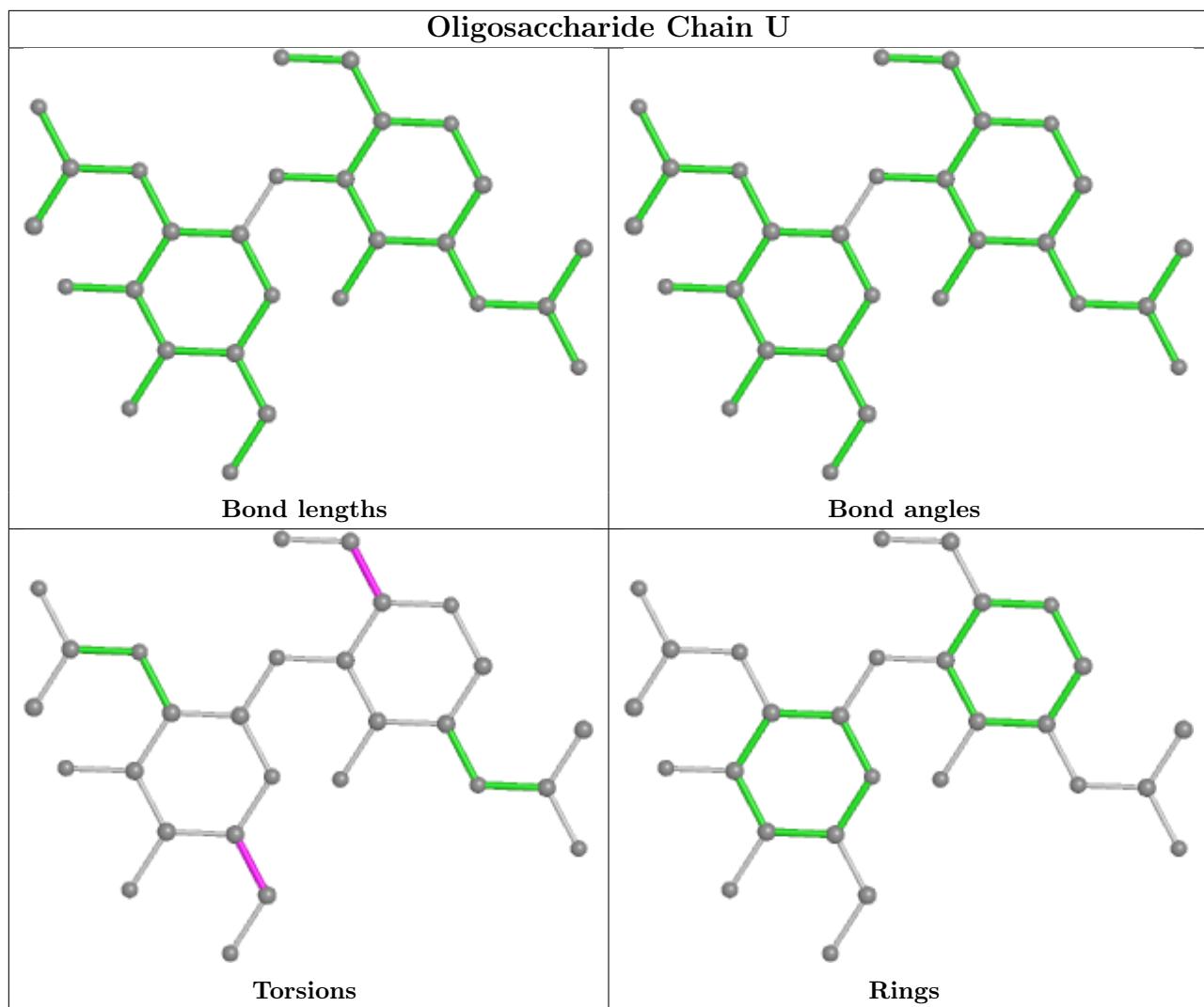


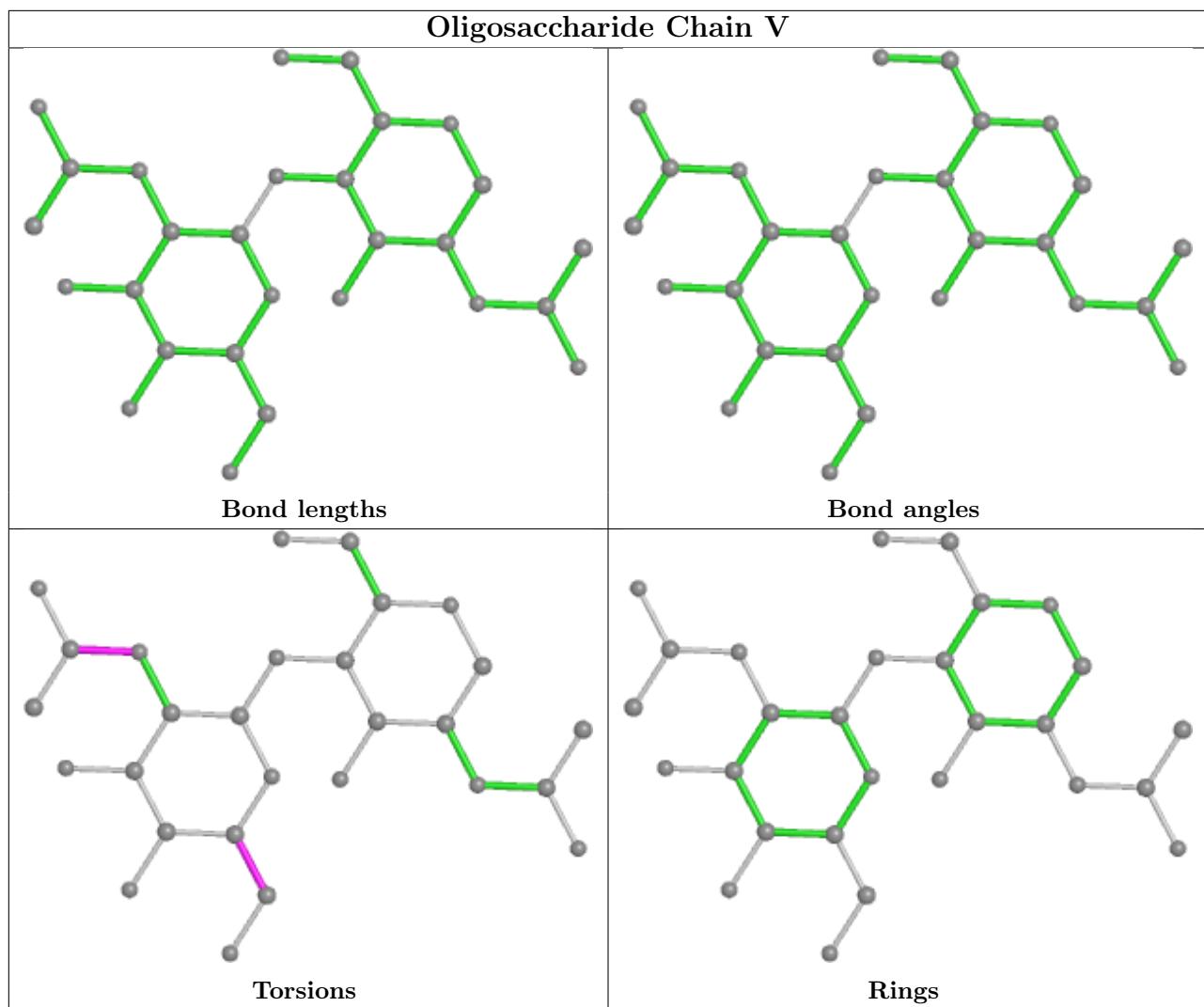


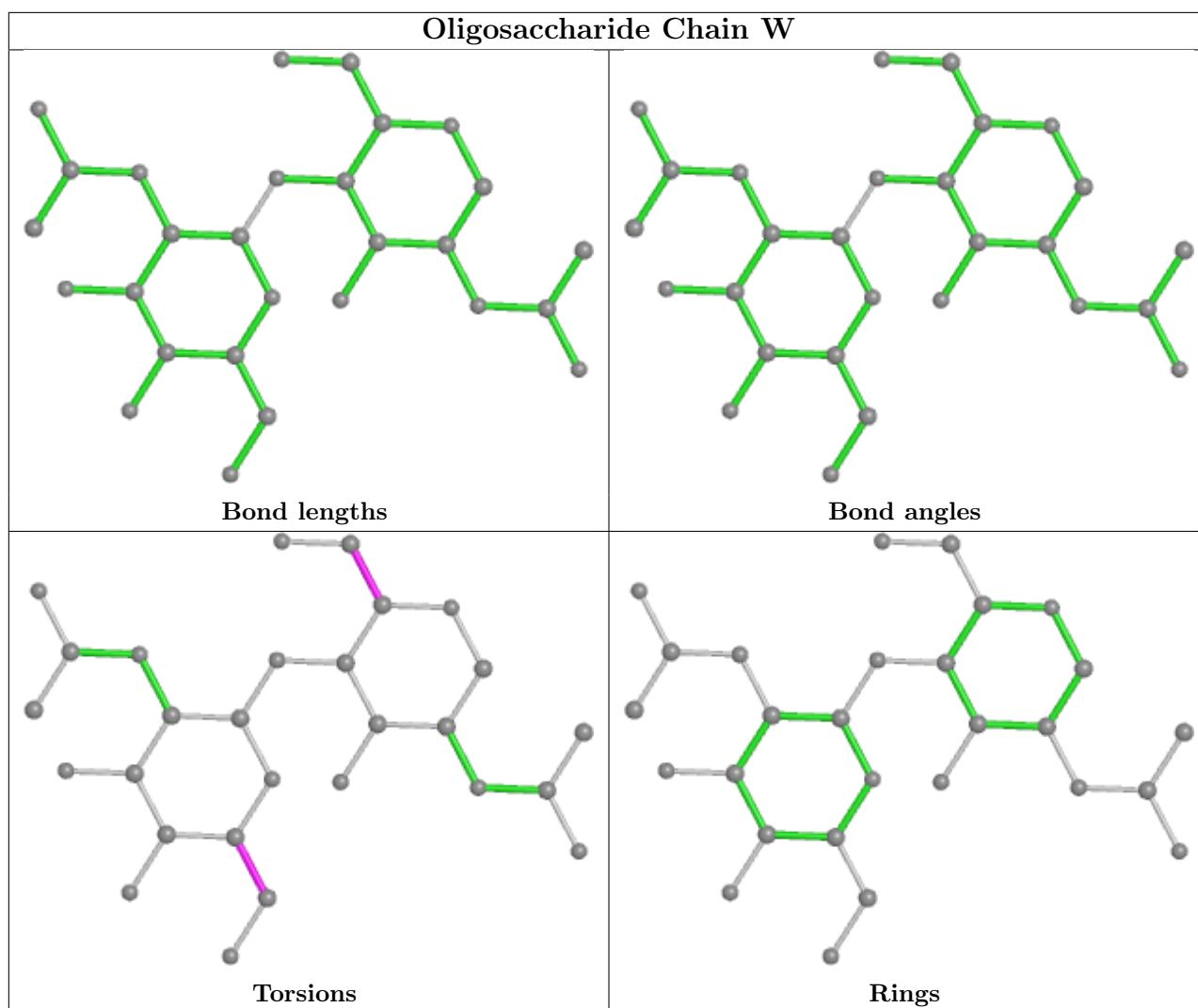












5.6 Ligand geometry (i)

35 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
4	NAG	B	1310	1	14,14,15	0.85	1 (7%)	17,19,21	0.65	0
4	NAG	A	1302	1	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	B	1302	1	14,14,15	1.30	2 (14%)	17,19,21	1.34	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1301	1	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	B	1305	1	14,14,15	1.03	1 (7%)	17,19,21	1.67	2 (11%)
4	NAG	A	1306	1	14,14,15	0.24	0	17,19,21	0.67	0
4	NAG	B	1308	1	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	B	1309	1	14,14,15	0.54	0	17,19,21	0.59	0
4	NAG	C	1312	1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	C	1307	1	14,14,15	0.34	0	17,19,21	0.58	0
4	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	C	1302	1	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	A	1305	1	14,14,15	0.42	0	17,19,21	0.58	0
4	NAG	B	1312	1	14,14,15	0.21	0	17,19,21	0.49	0
4	NAG	A	1307	1	14,14,15	0.49	0	17,19,21	1.32	2 (11%)
4	NAG	C	1311	1	14,14,15	0.38	0	17,19,21	0.59	0
4	NAG	B	1303	1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	B	1307	1	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	C	1308	1	14,14,15	0.24	0	17,19,21	0.55	0
4	NAG	B	1314	1	14,14,15	0.42	0	17,19,21	0.43	0
4	NAG	C	1303	1	14,14,15	0.72	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	C	1309	1	14,14,15	0.34	0	17,19,21	0.42	0
4	NAG	B	1311	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	C	1306	1	14,14,15	2.31	2 (14%)	17,19,21	1.97	2 (11%)
4	NAG	A	1303	1	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	C	1304	1	14,14,15	0.33	0	17,19,21	0.47	0
4	NAG	C	1301	1	14,14,15	0.92	1 (7%)	17,19,21	1.22	1 (5%)
4	NAG	A	1308	1	14,14,15	0.49	0	17,19,21	0.48	0
4	NAG	B	1306	1	14,14,15	0.91	1 (7%)	17,19,21	1.15	1 (5%)
4	NAG	B	1313	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	A	1304	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	C	1310	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	B	1315	1	14,14,15	0.35	0	17,19,21	0.40	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
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1315	1	-	2/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1306	NAG	O5-C1	6.32	1.53	1.43
4	C	1306	NAG	C1-C2	5.67	1.60	1.52
4	B	1302	NAG	O5-C1	4.33	1.50	1.43
4	C	1301	NAG	O5-C1	3.31	1.49	1.43
4	B	1305	NAG	O5-C1	3.29	1.49	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1306	NAG	C1-O5-C5	7.44	122.28	112.19
4	B	1302	NAG	C1-O5-C5	5.24	119.29	112.19
4	C	1301	NAG	C1-O5-C5	4.78	118.67	112.19
4	A	1307	NAG	C2-N2-C7	4.54	129.37	122.90
4	B	1305	NAG	C1-O5-C5	4.49	118.28	112.19

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1304	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	B	1313	NAG	C4-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6

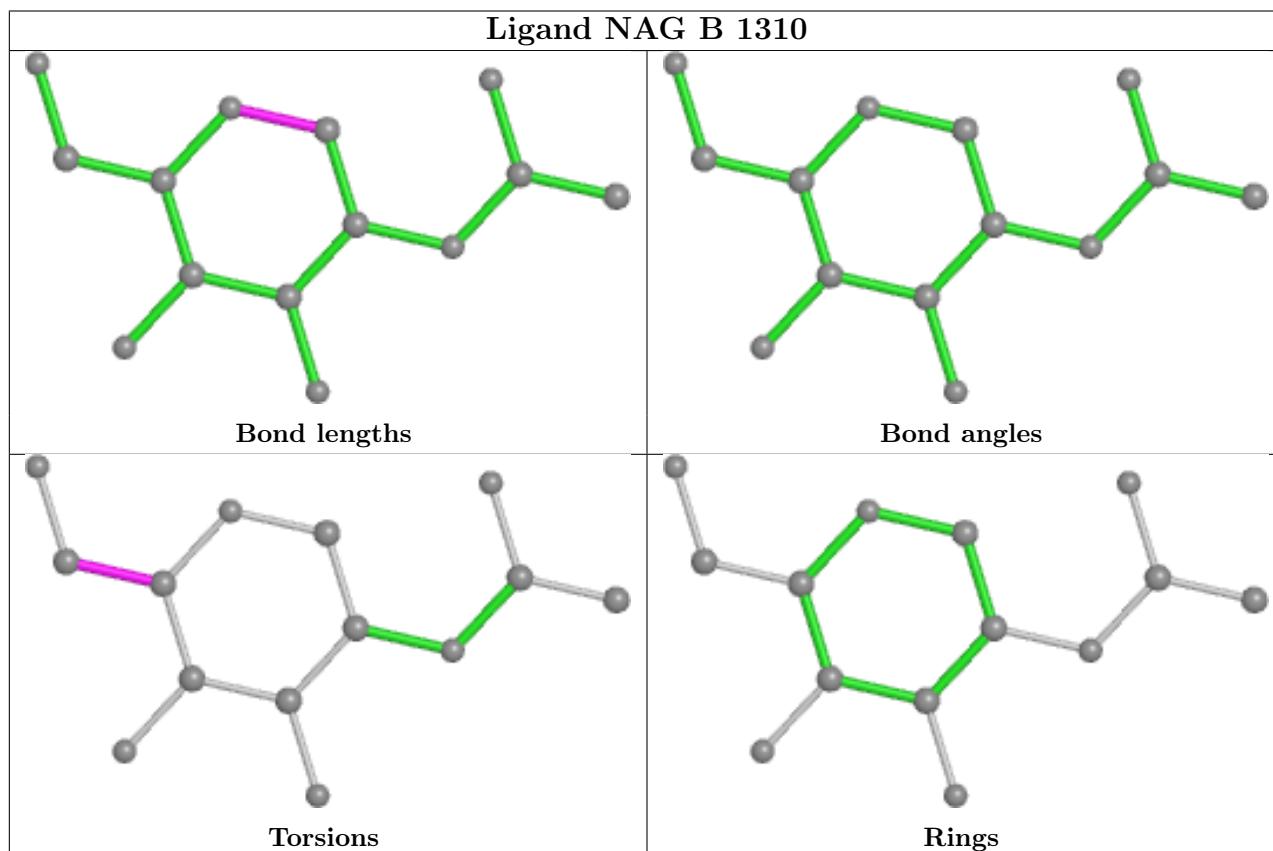
There are no ring outliers.

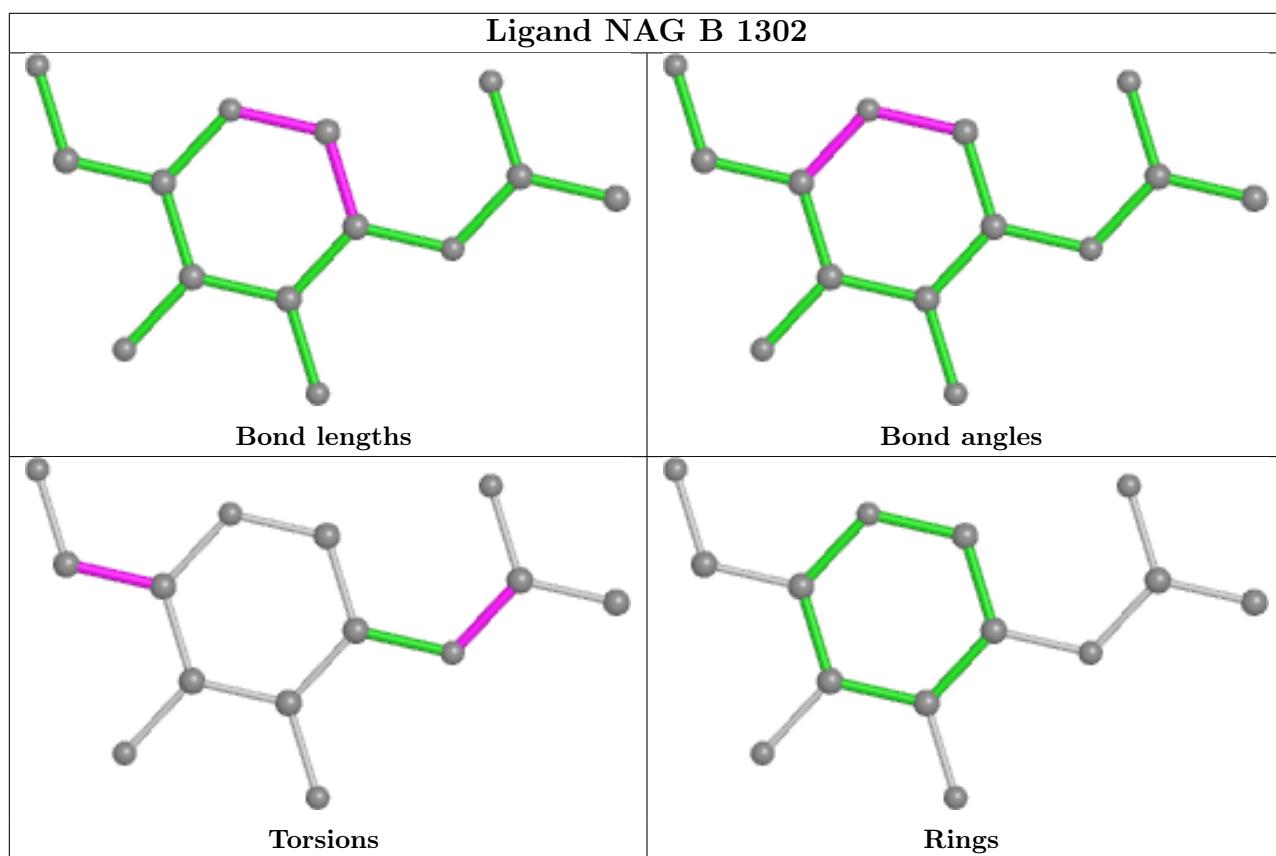
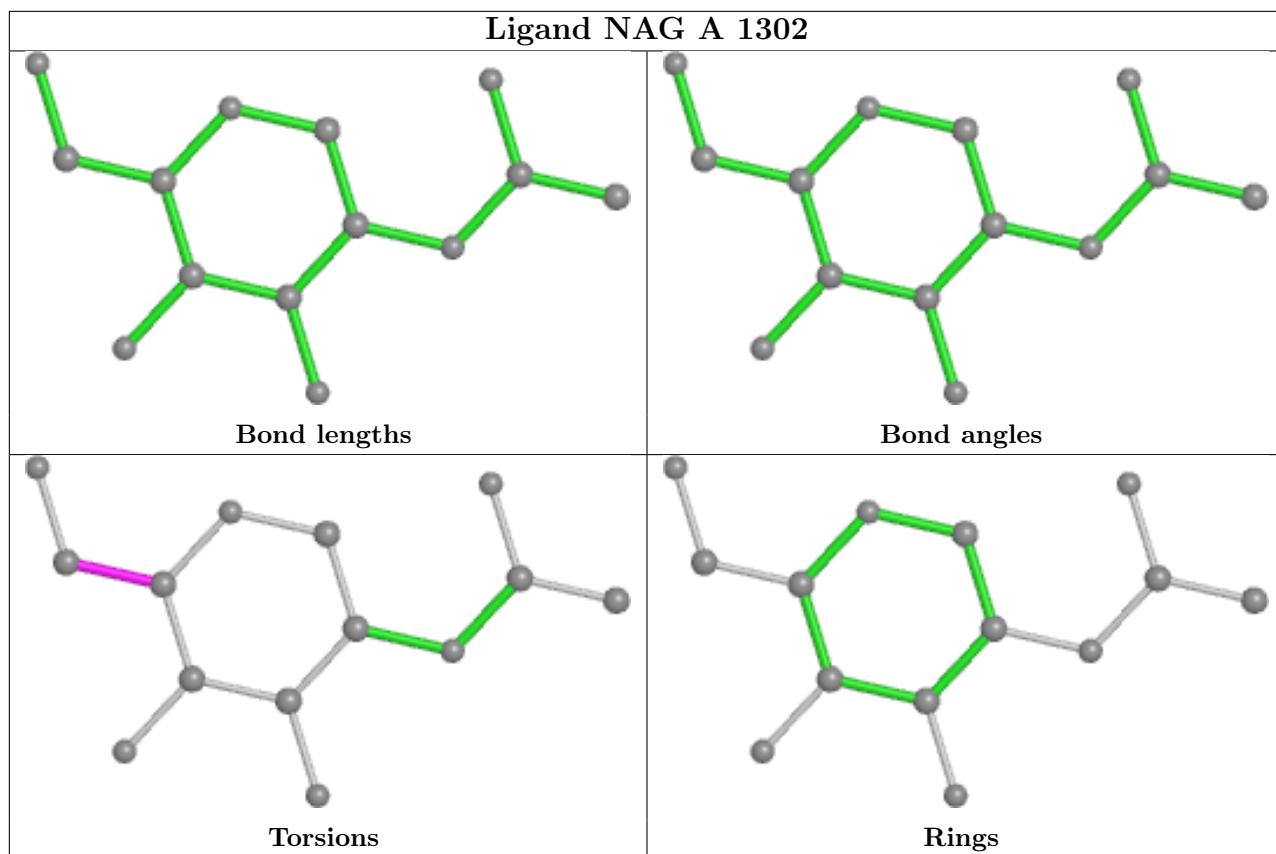
8 monomers are involved in 8 short contacts:

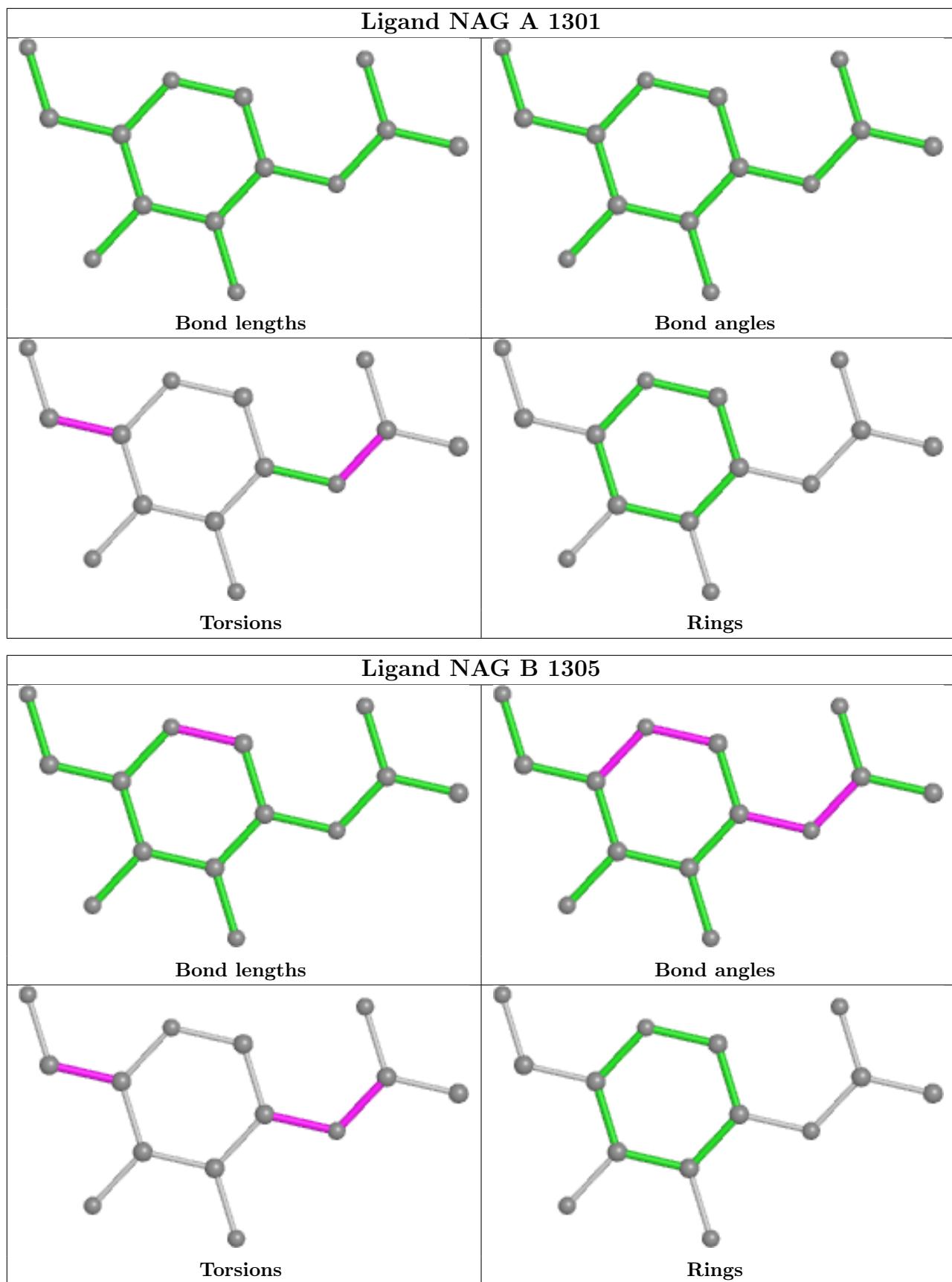
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1305	NAG	1	0
4	B	1308	NAG	1	0
4	A	1307	NAG	1	0
4	C	1311	NAG	1	0
4	C	1305	NAG	1	0
4	C	1309	NAG	1	0
4	A	1303	NAG	1	0
4	A	1308	NAG	1	0

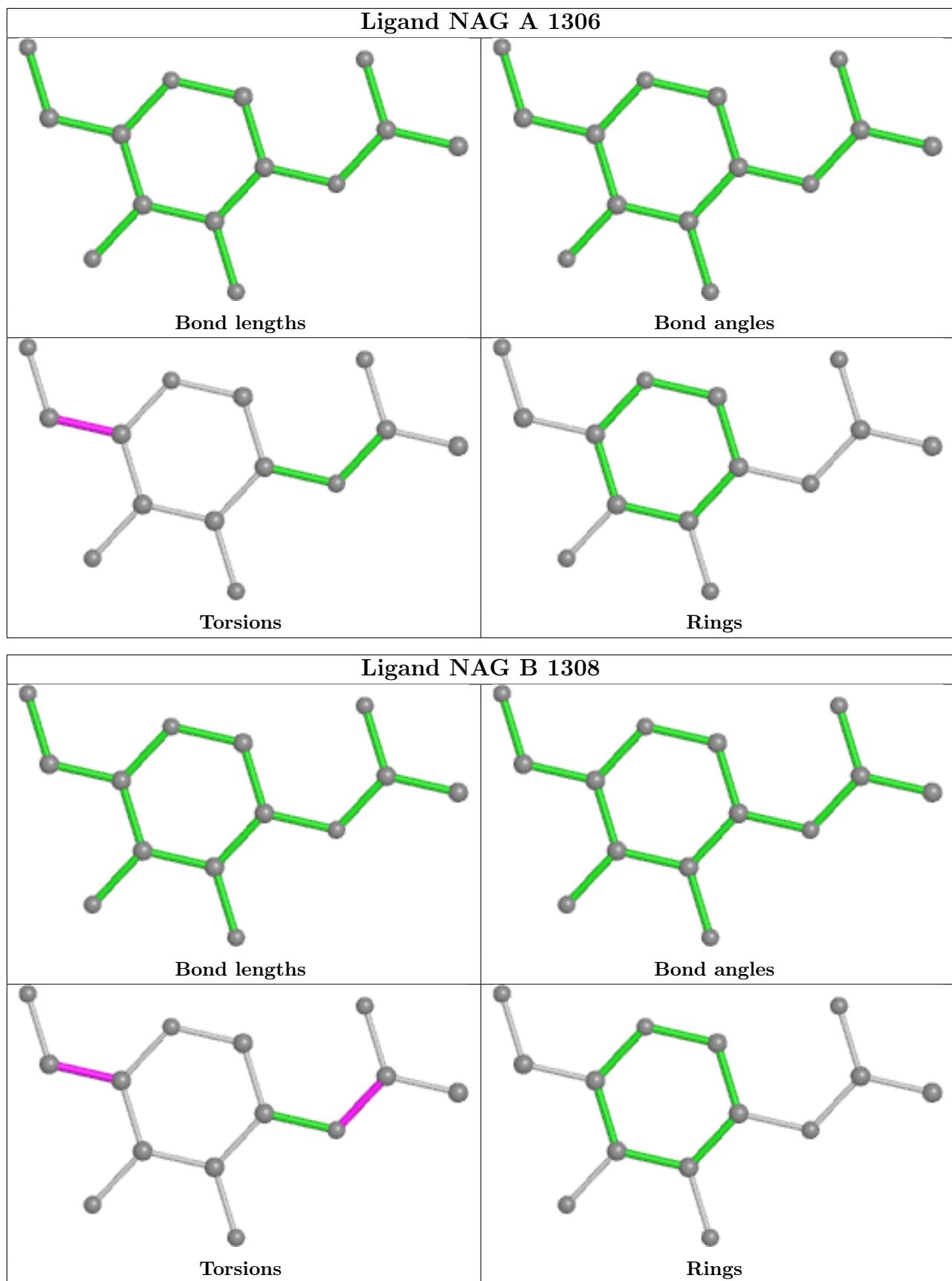
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

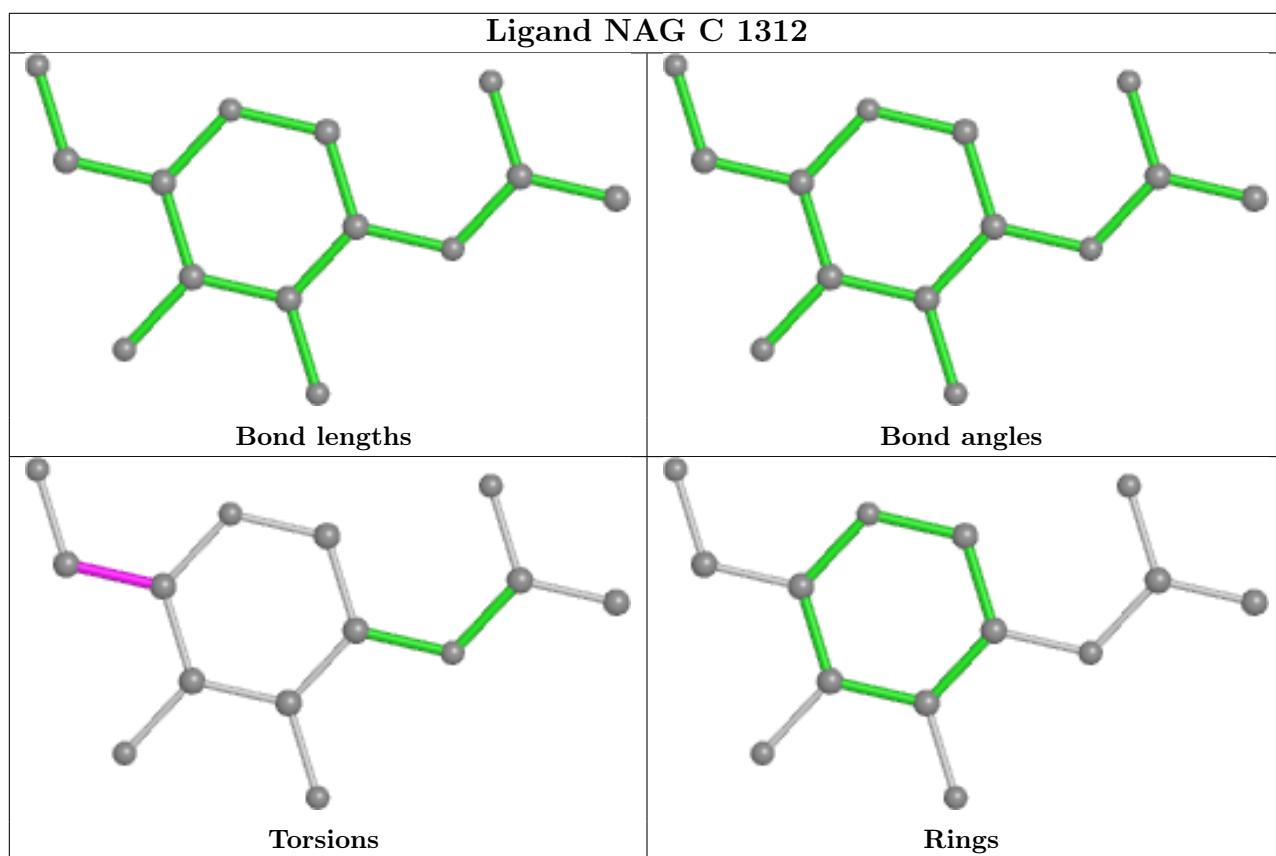
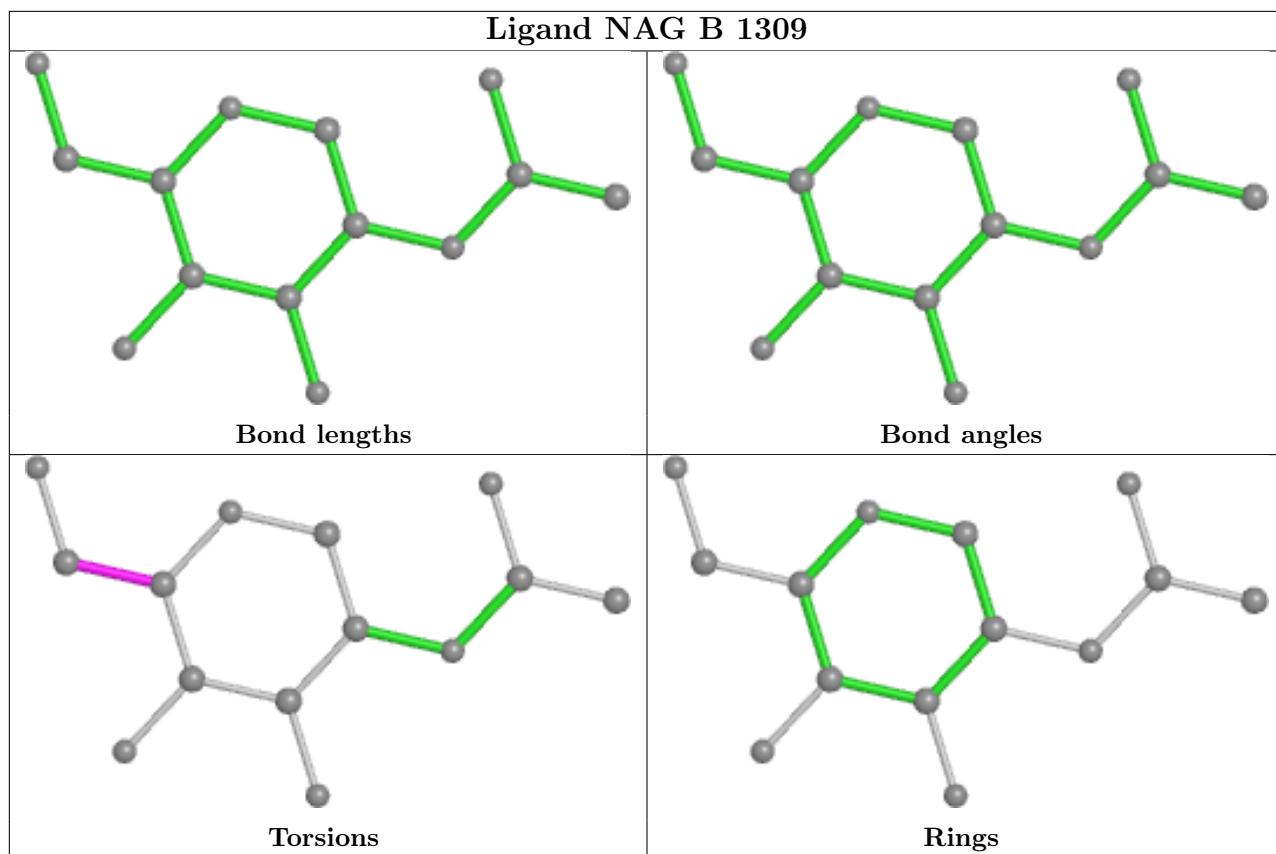
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

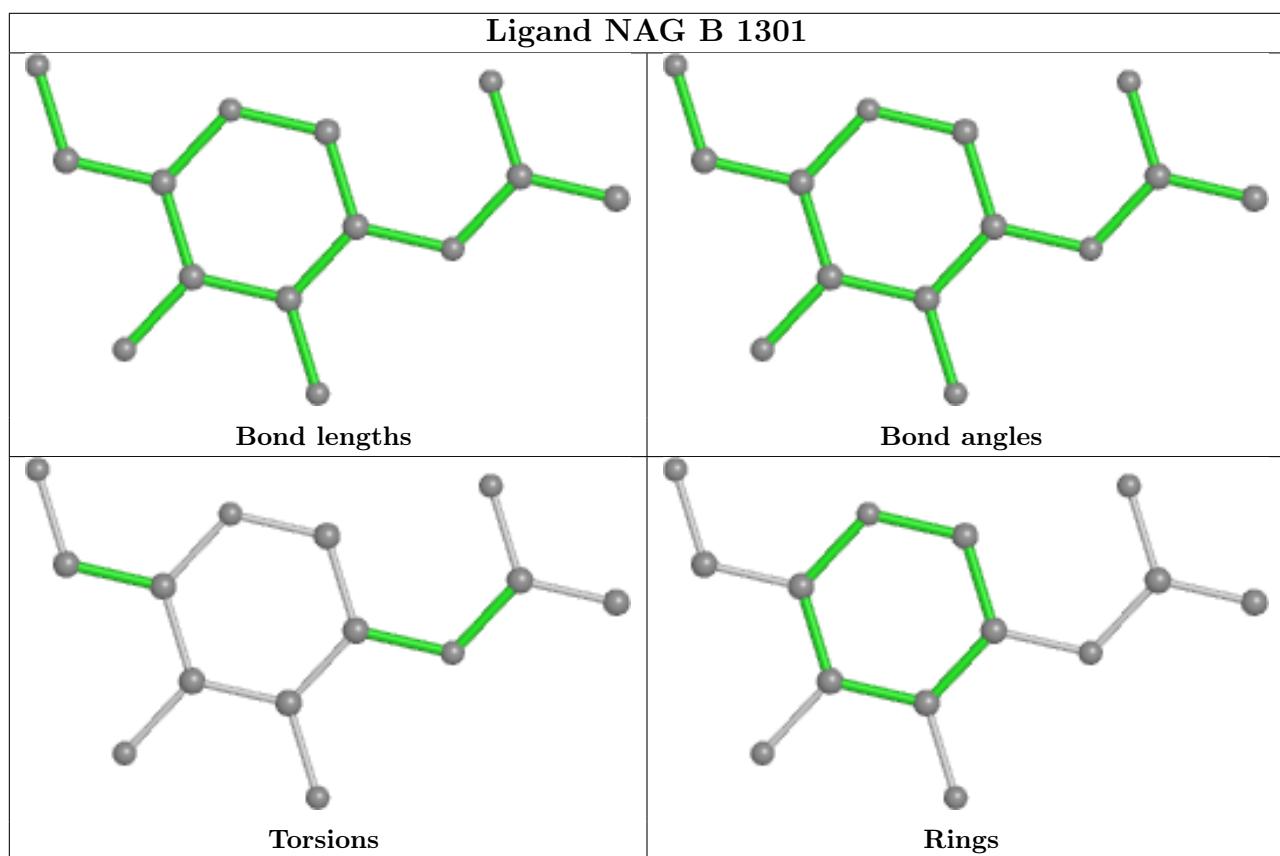
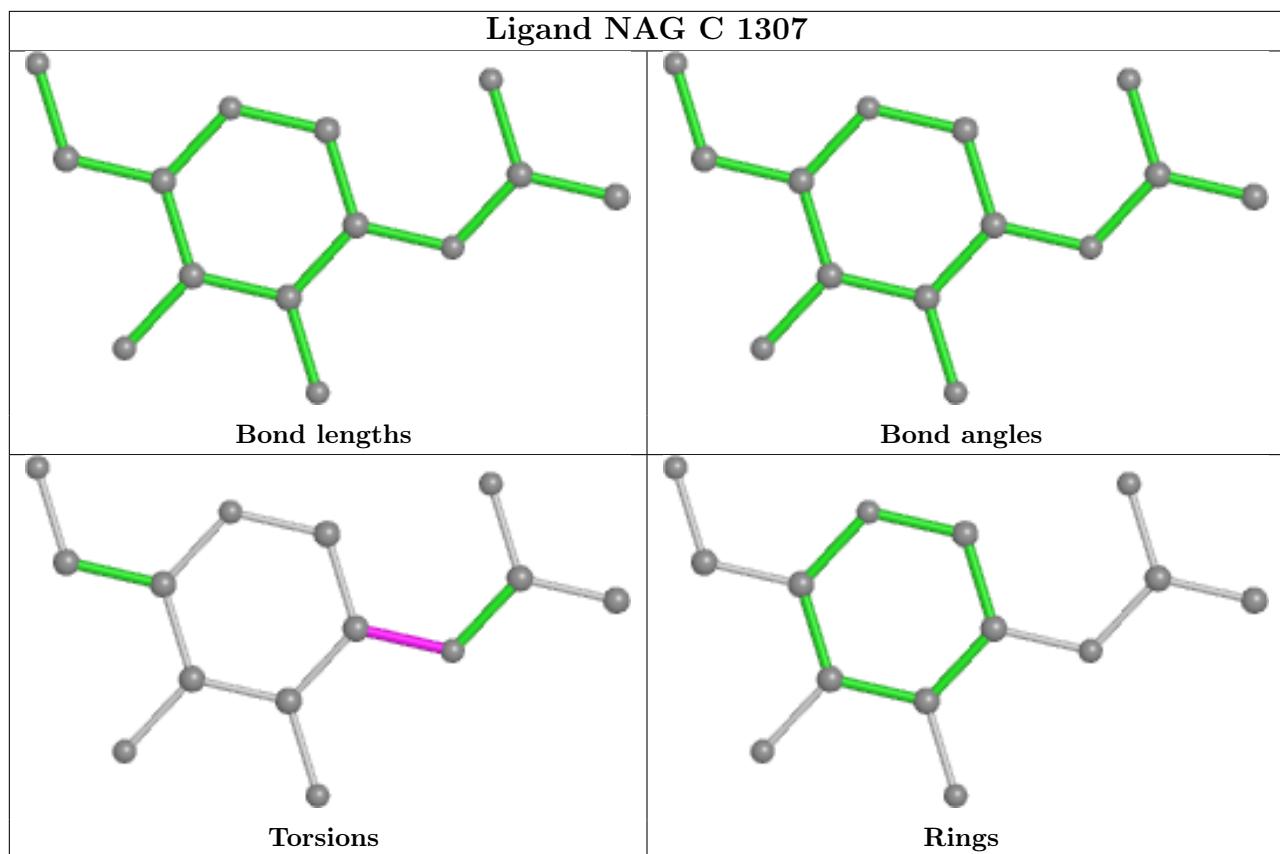


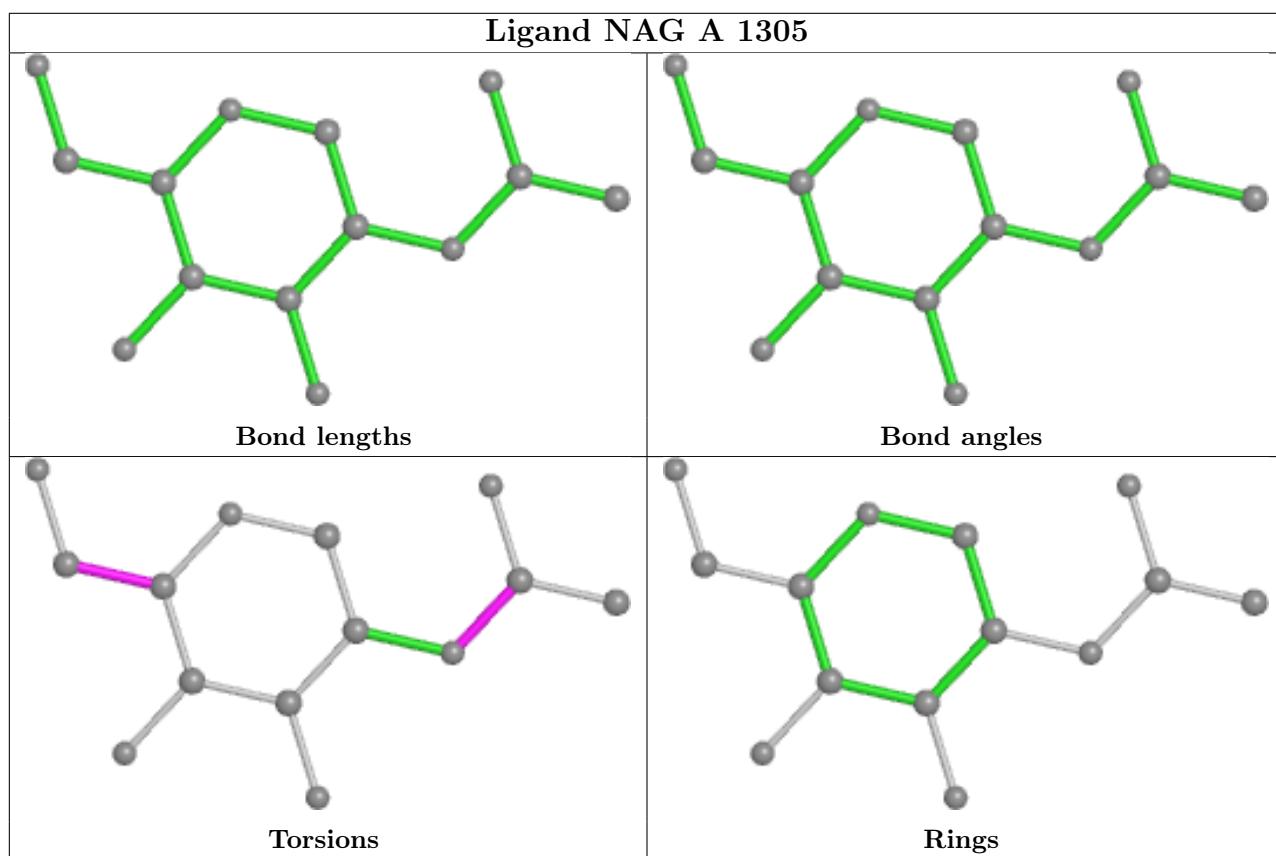
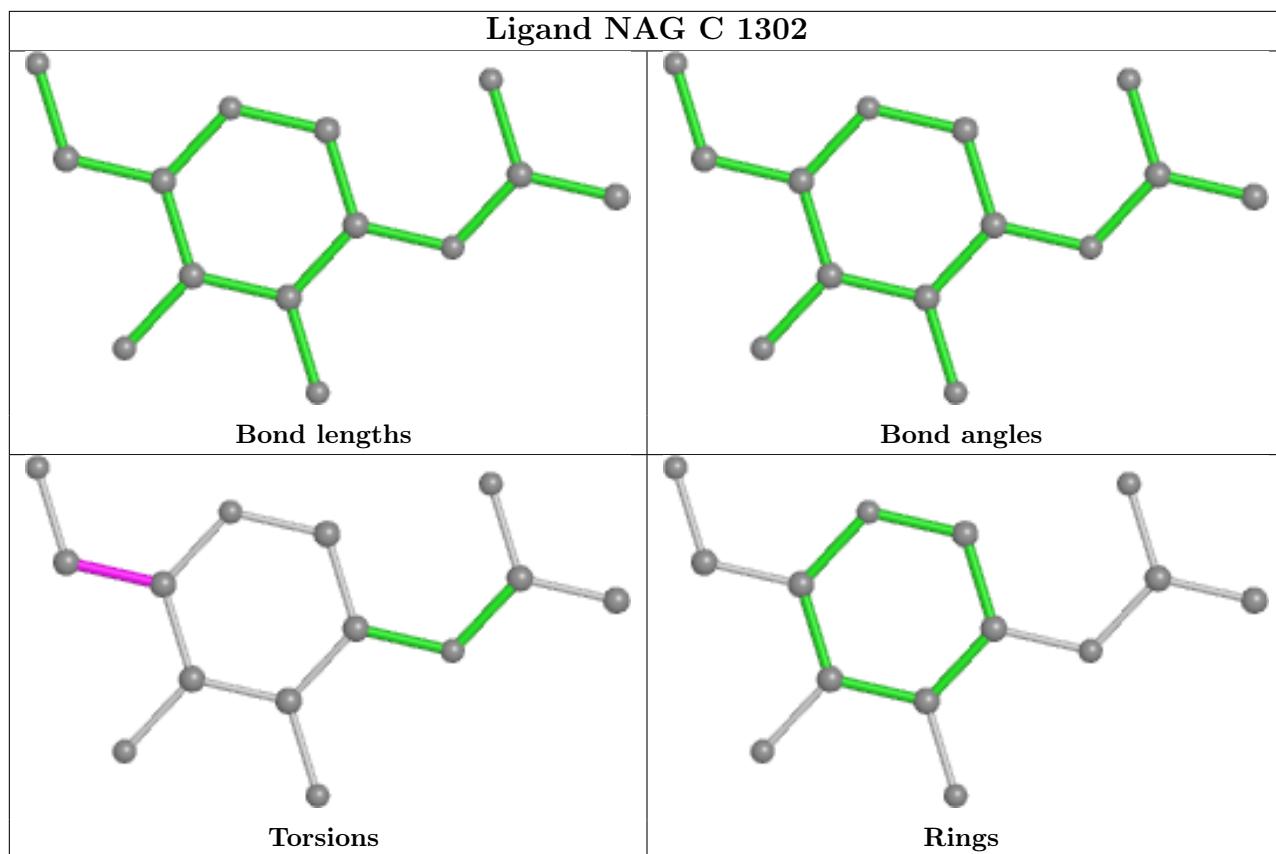


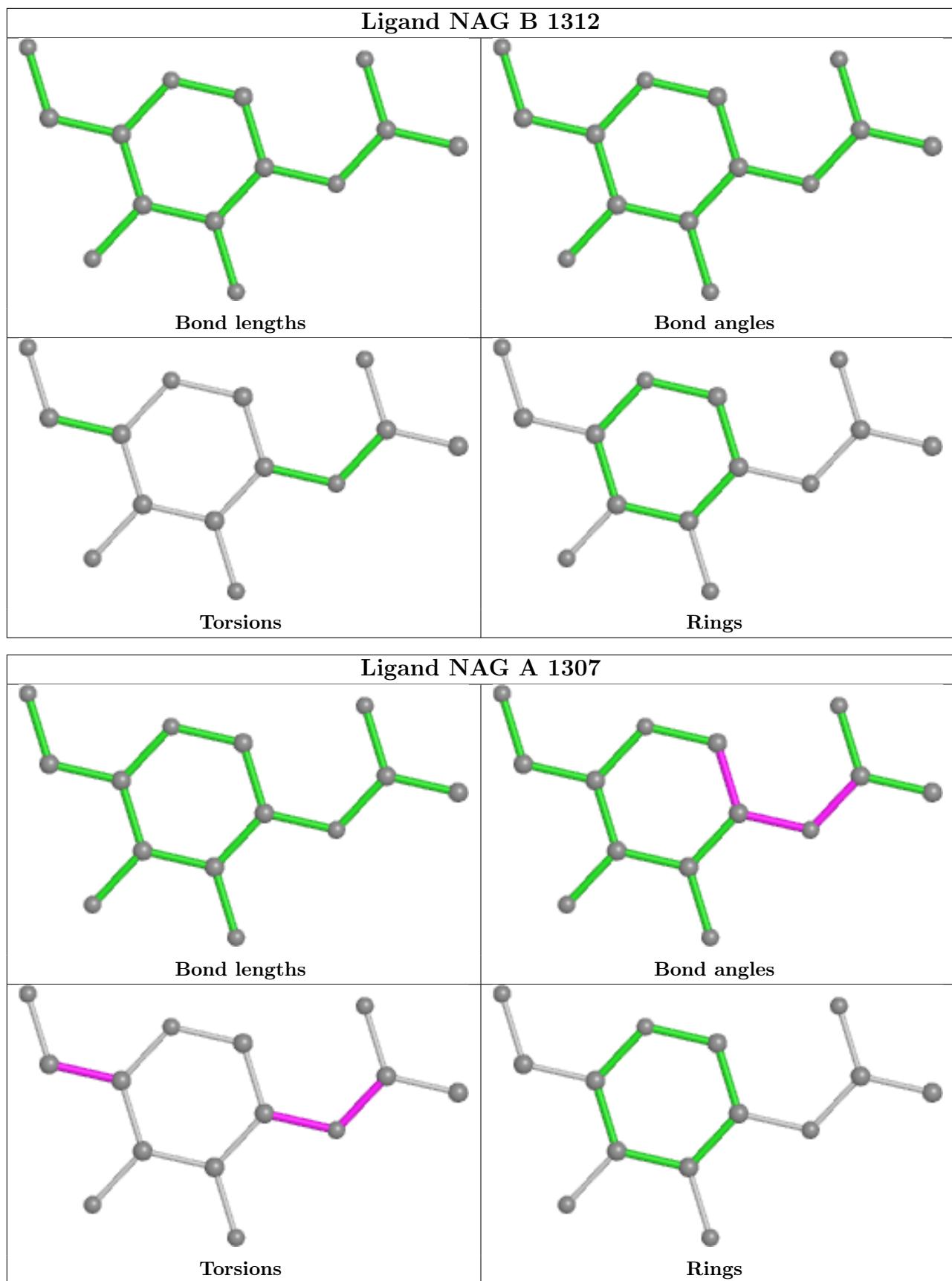


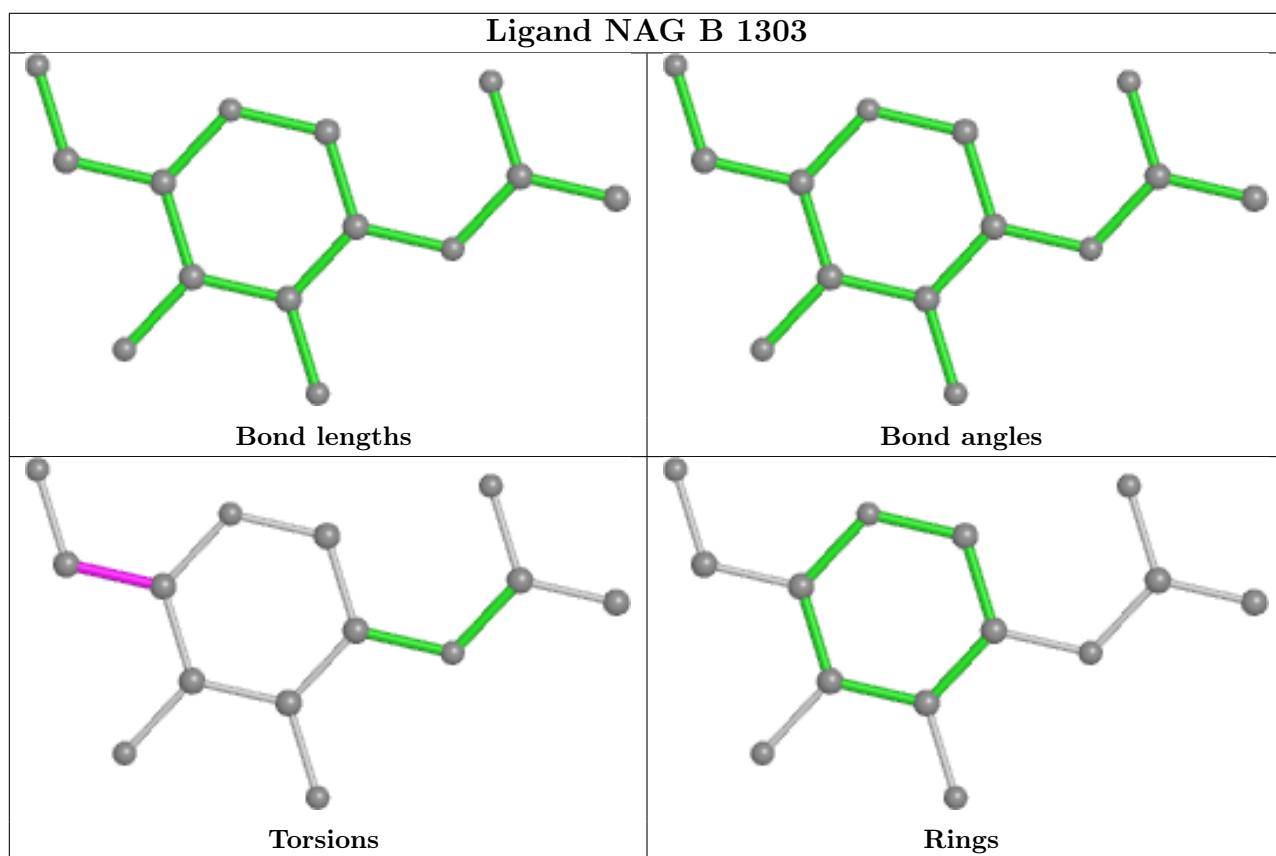
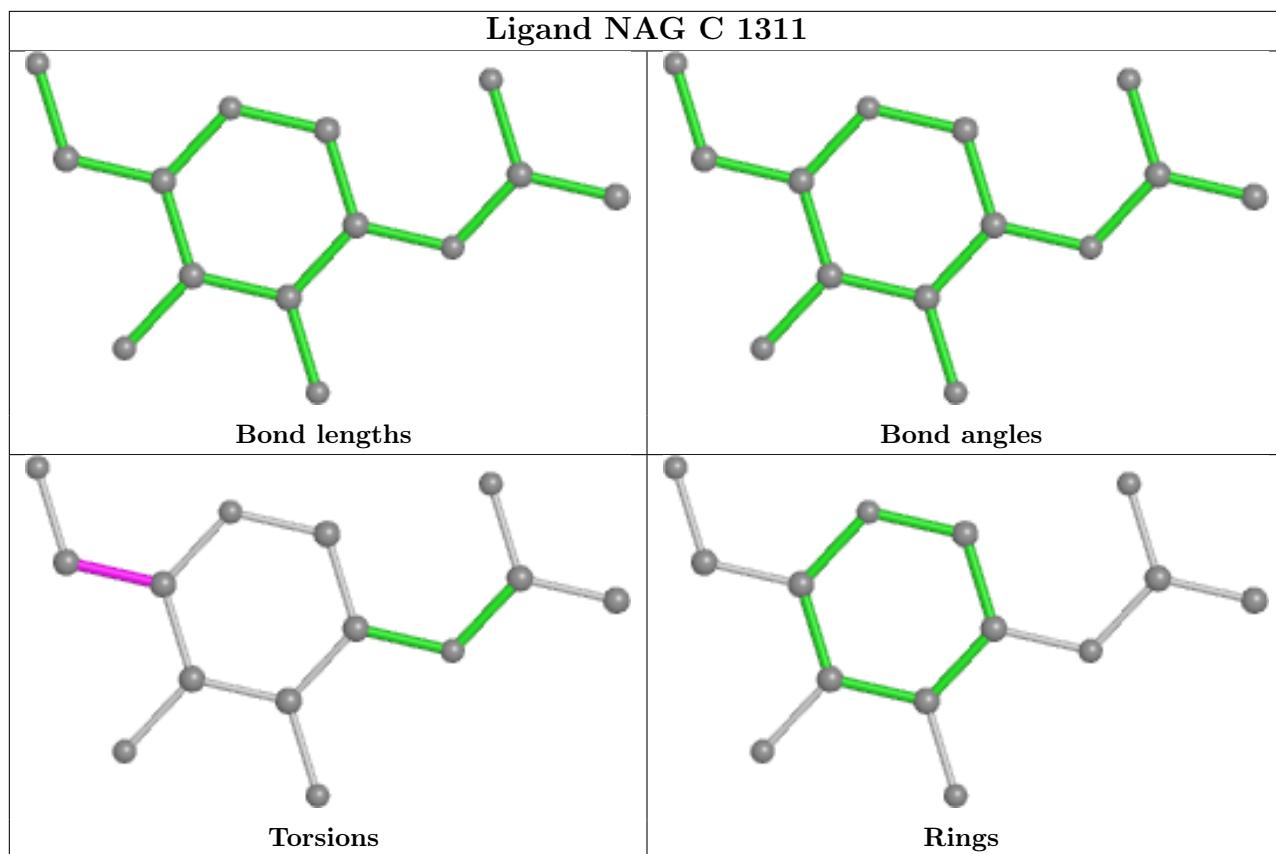


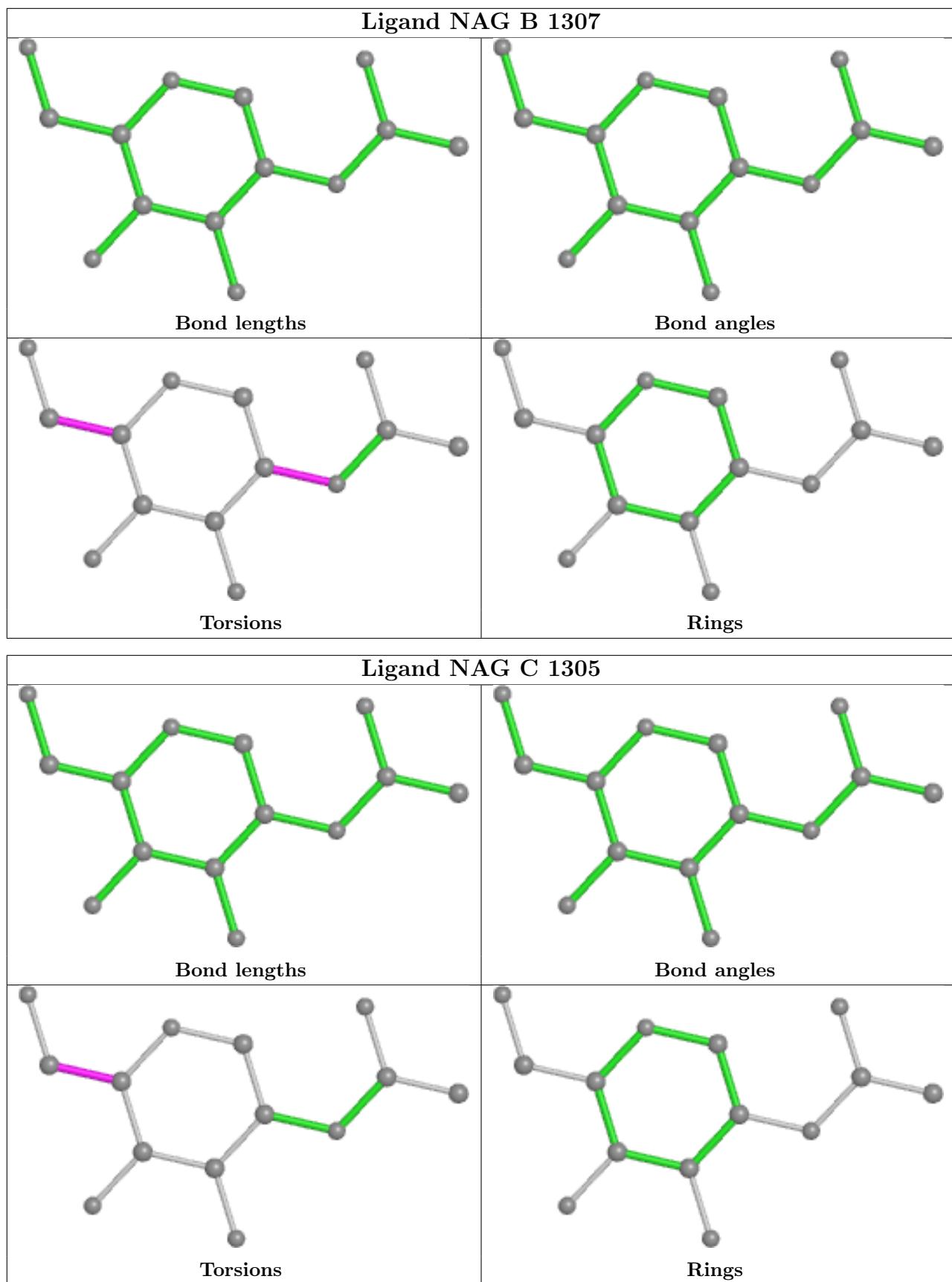


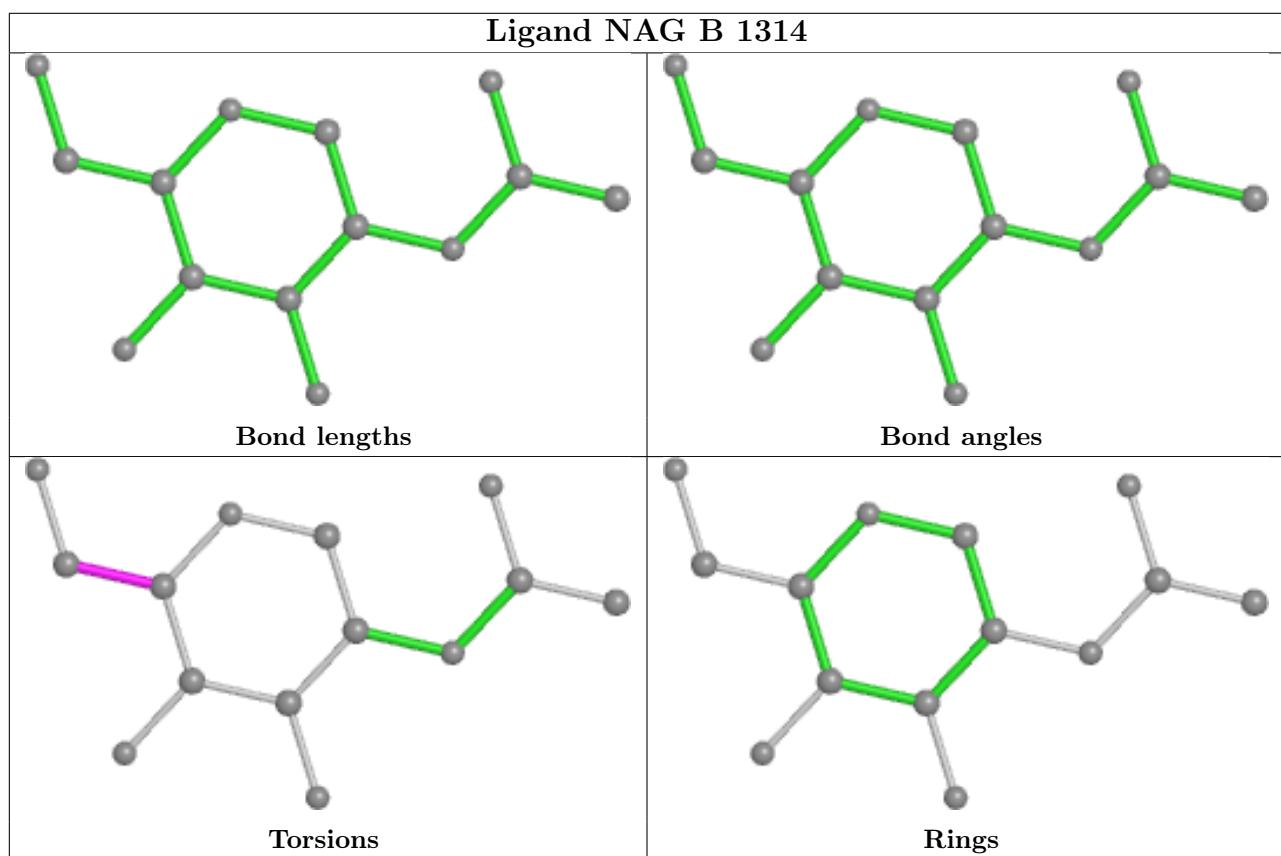
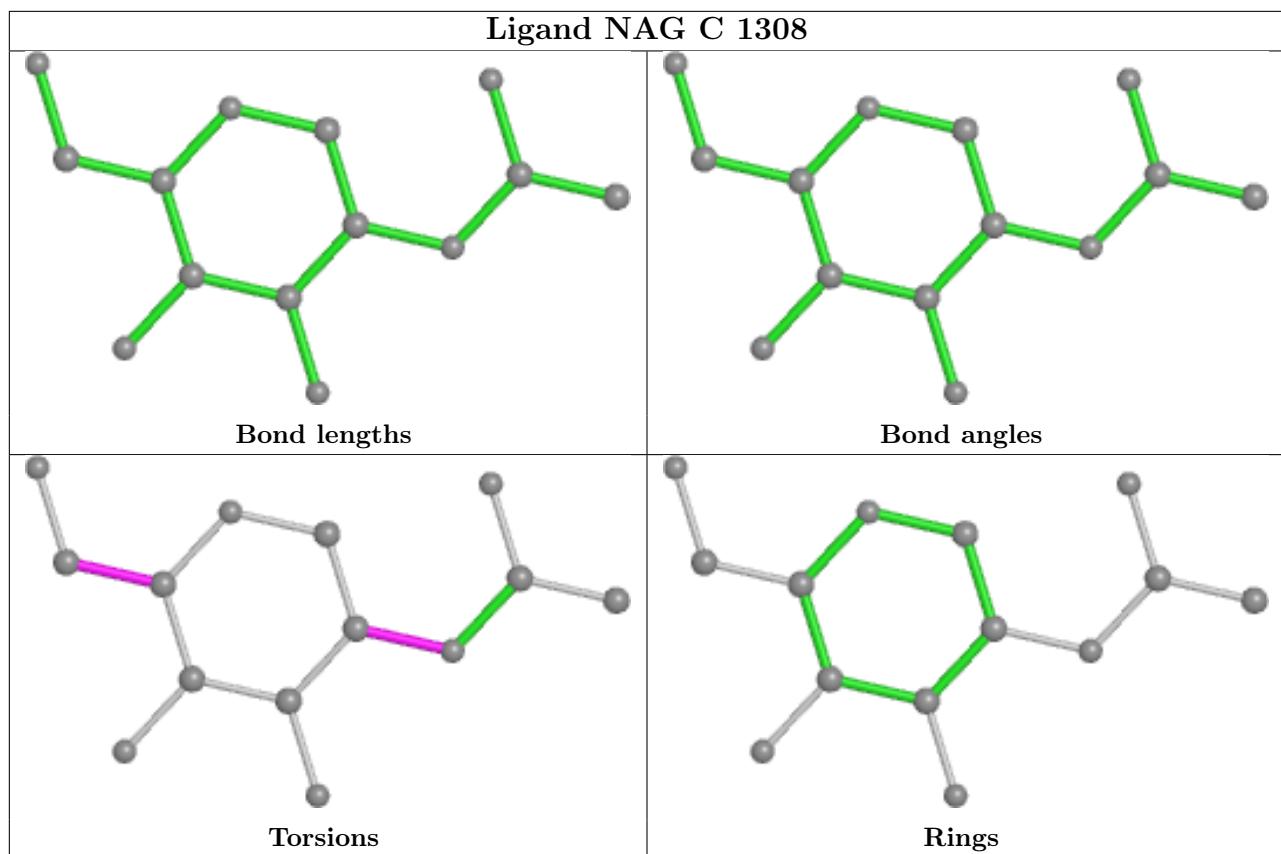


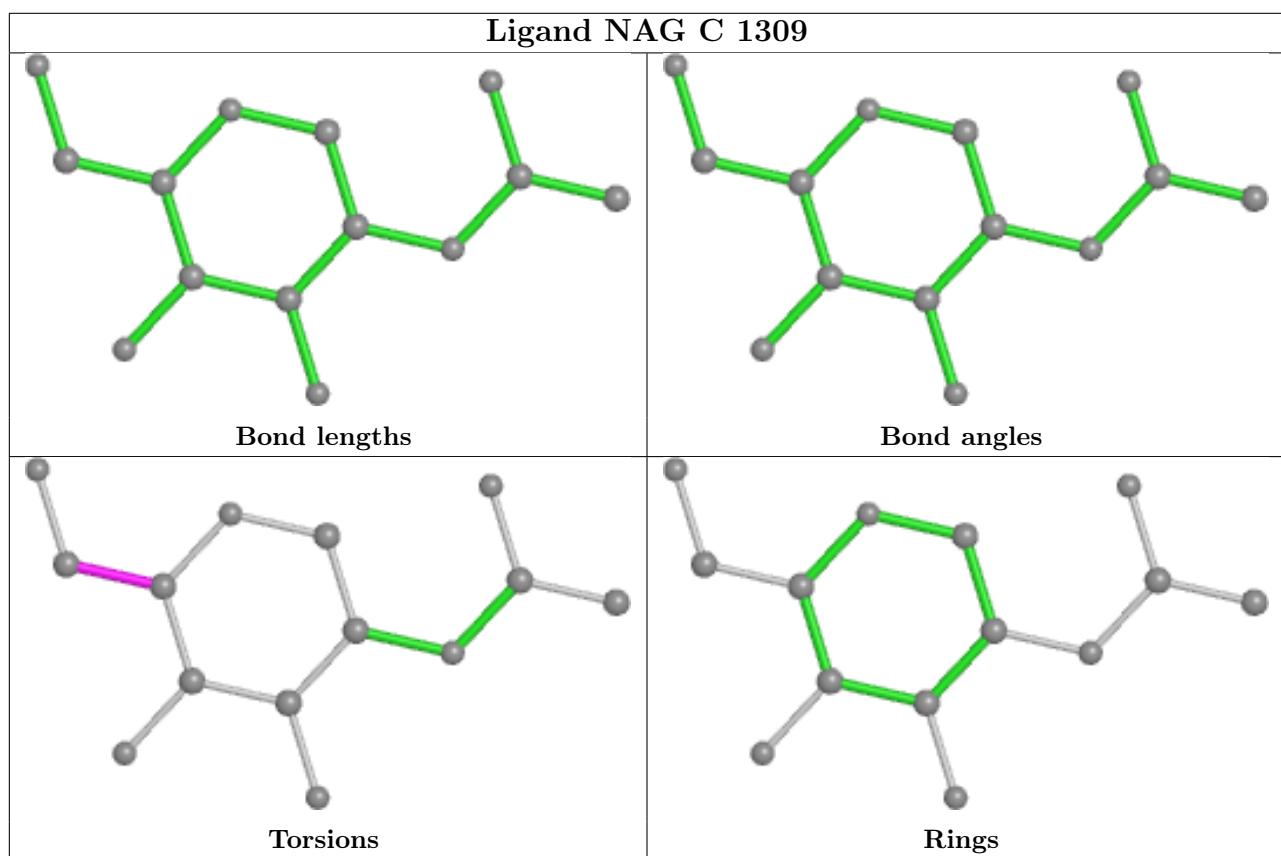
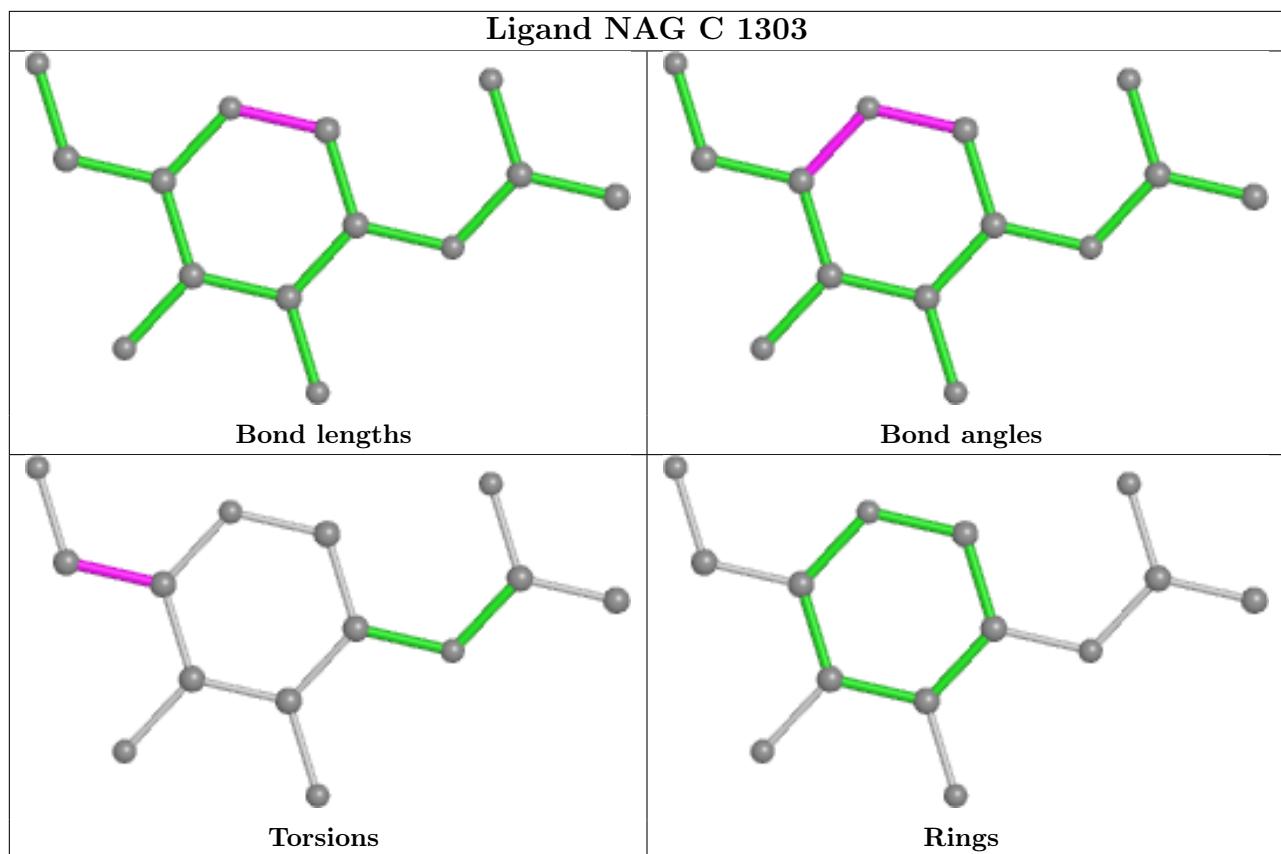


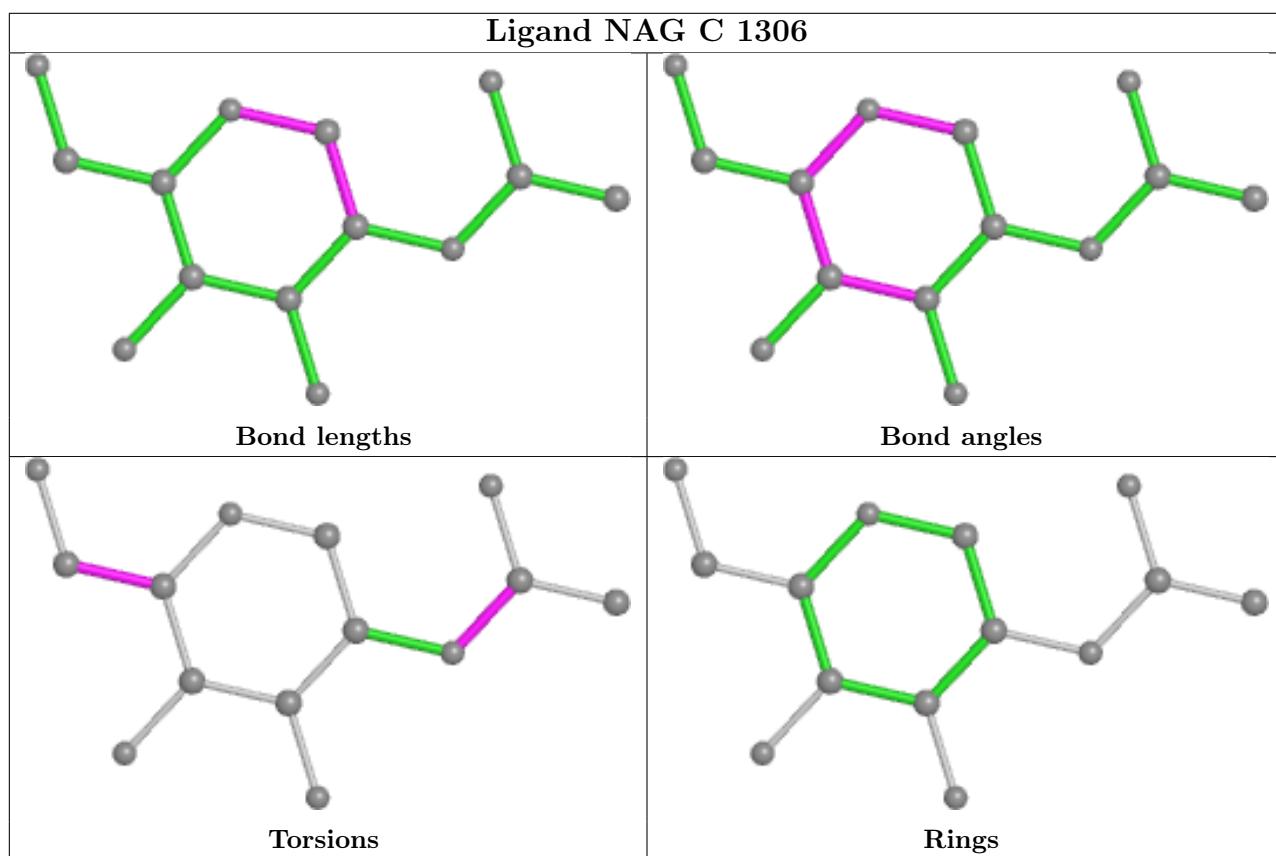
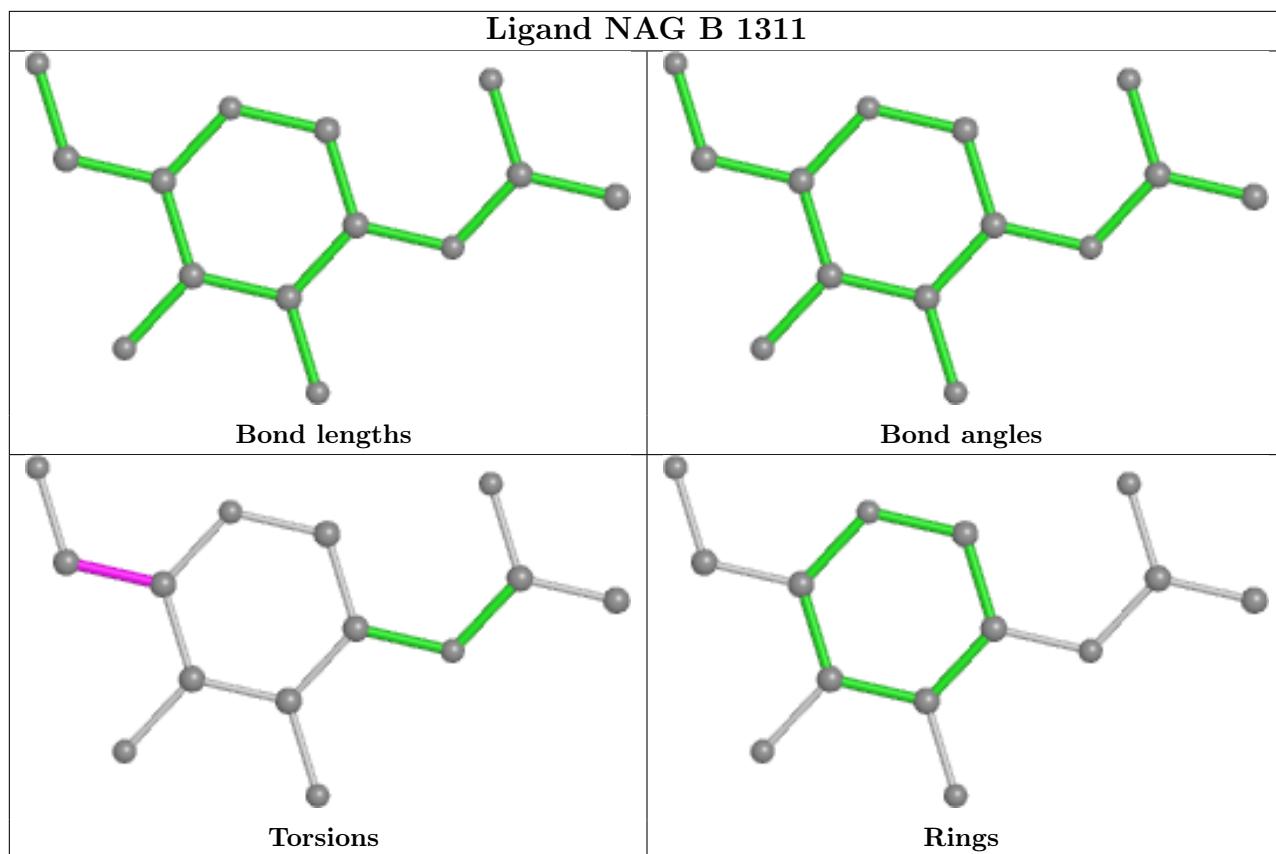


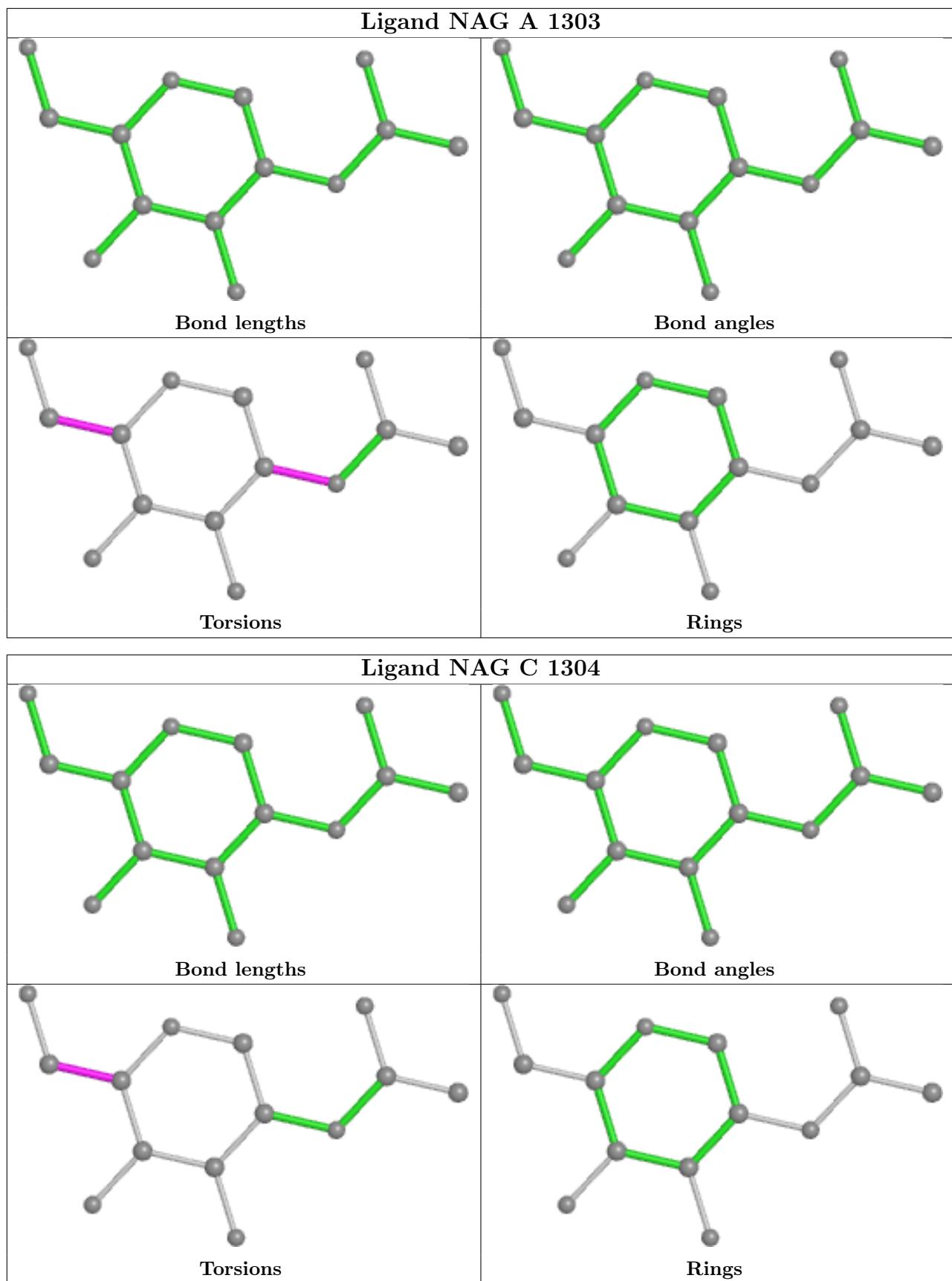


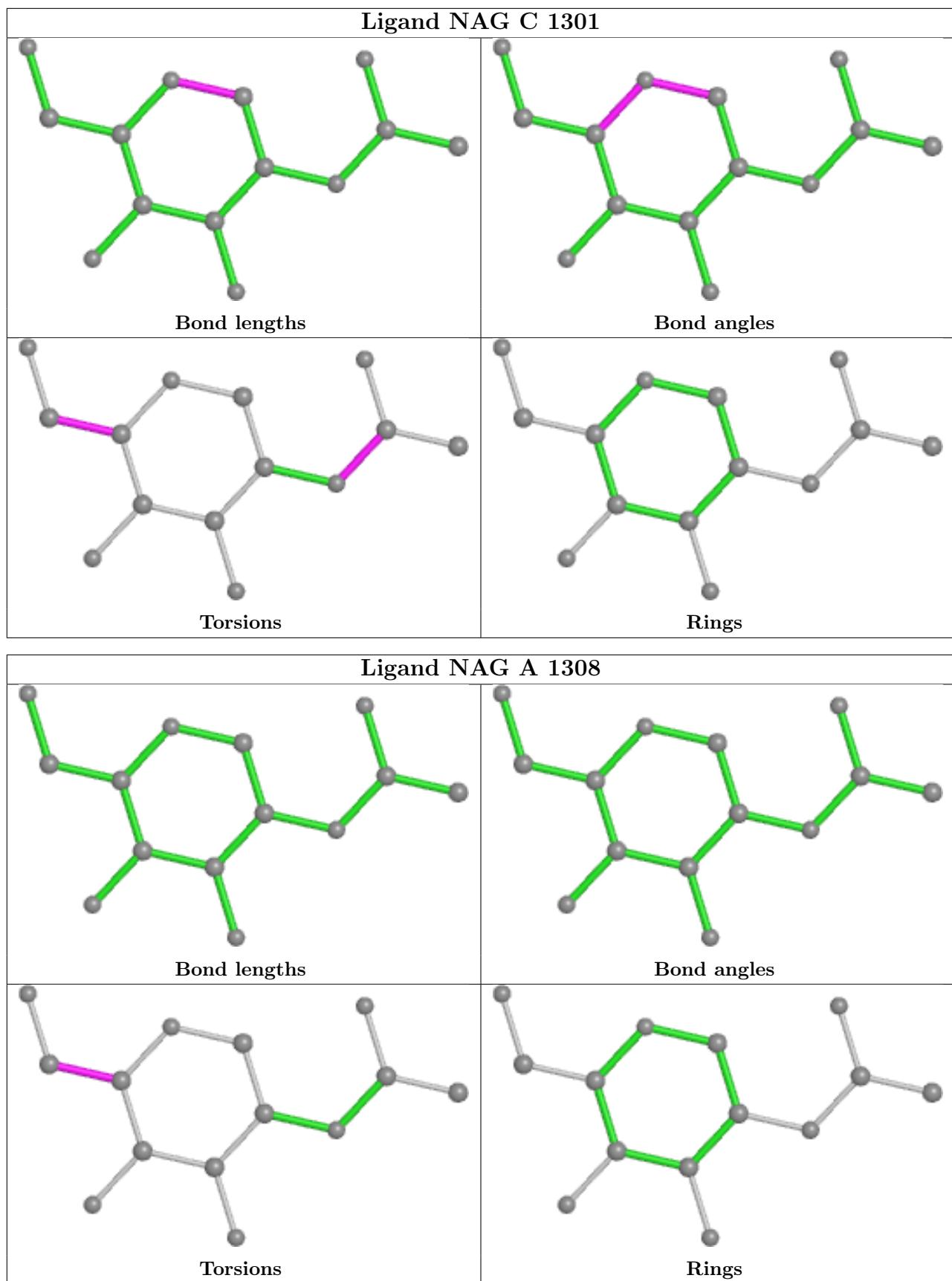


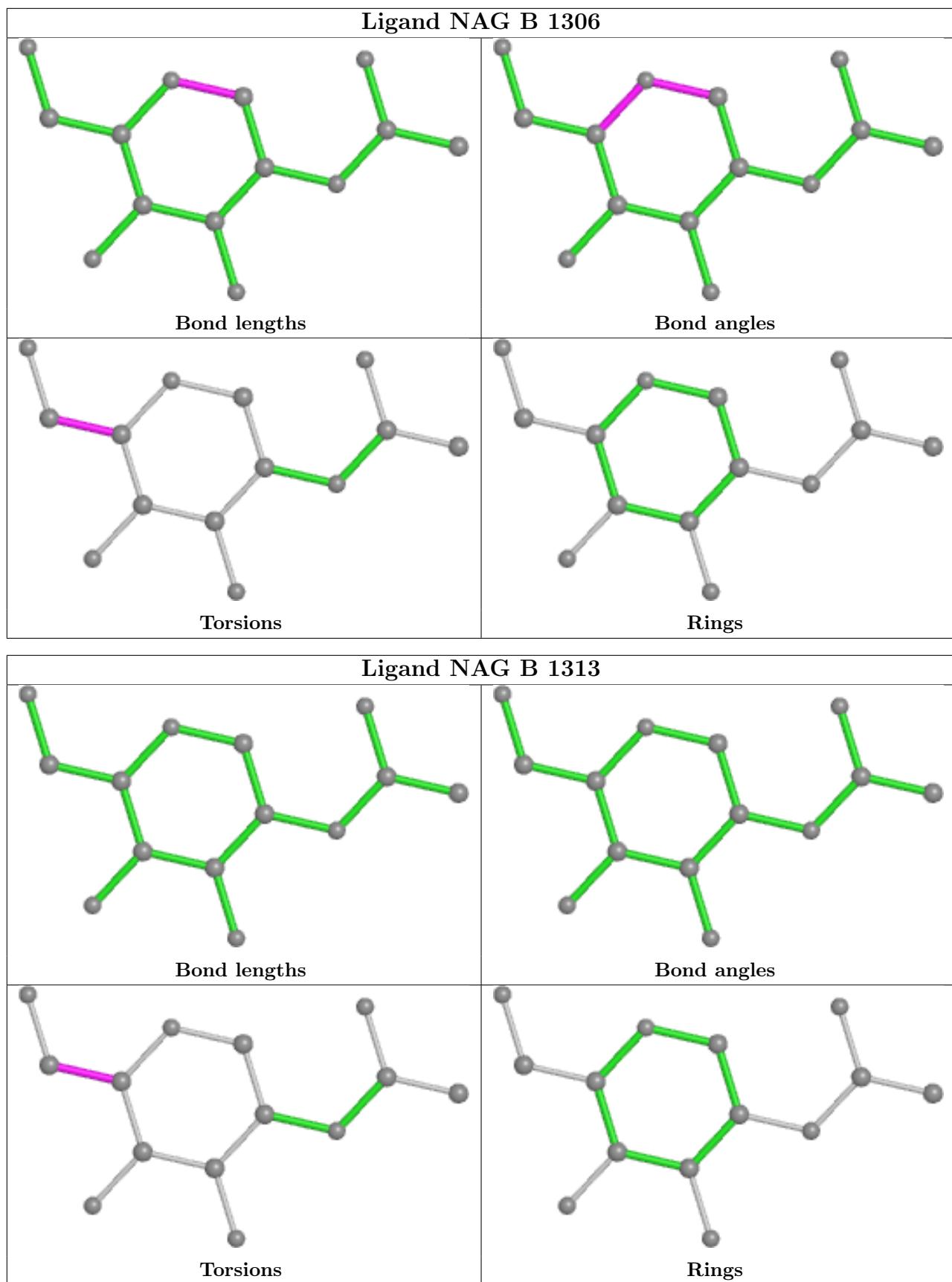


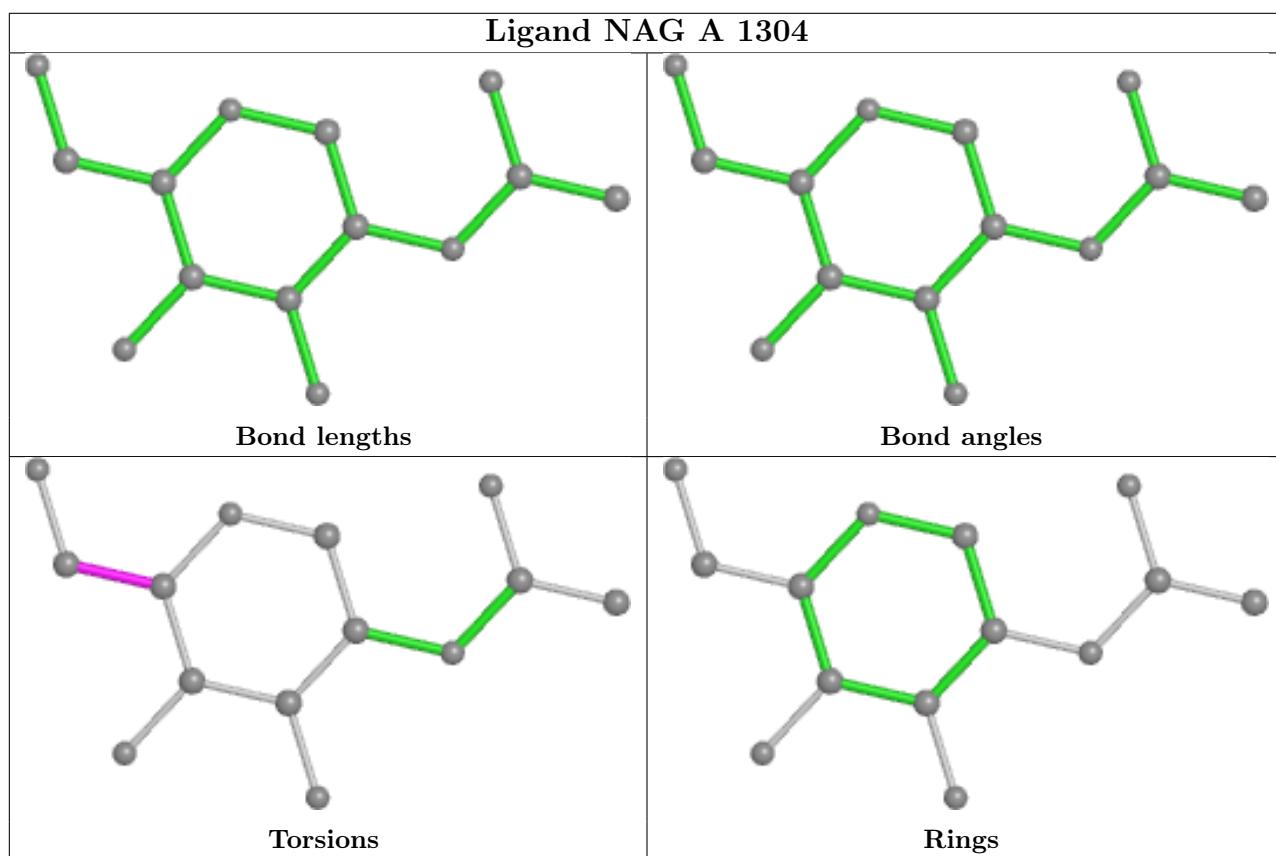
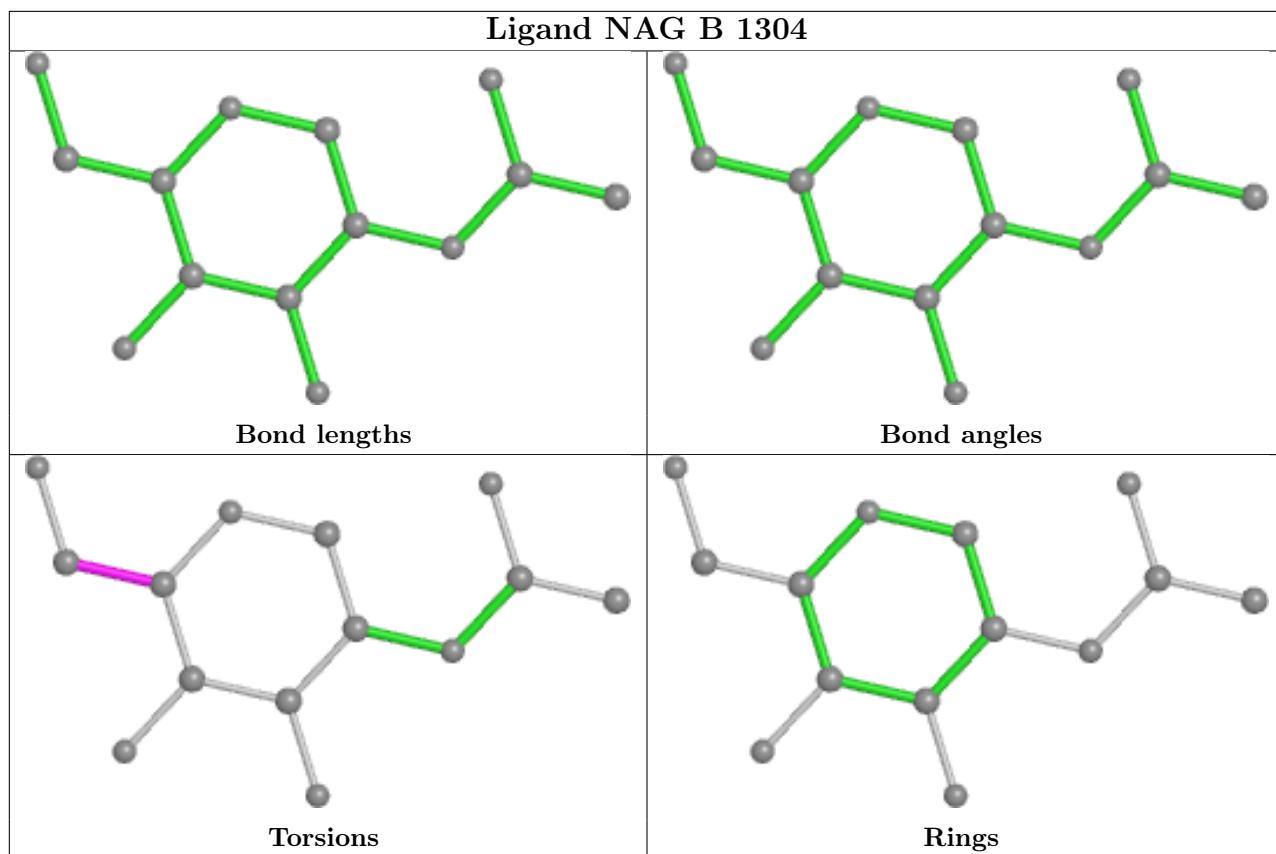


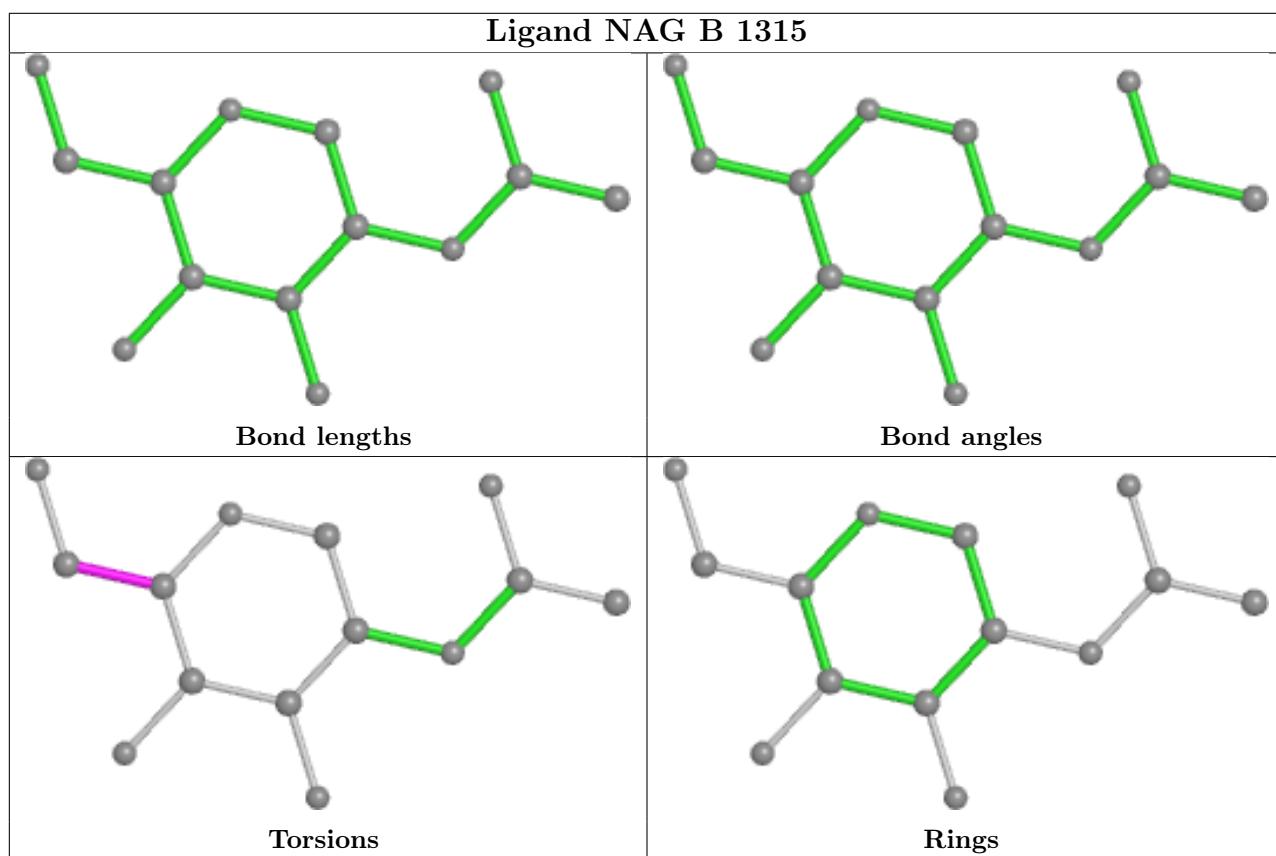
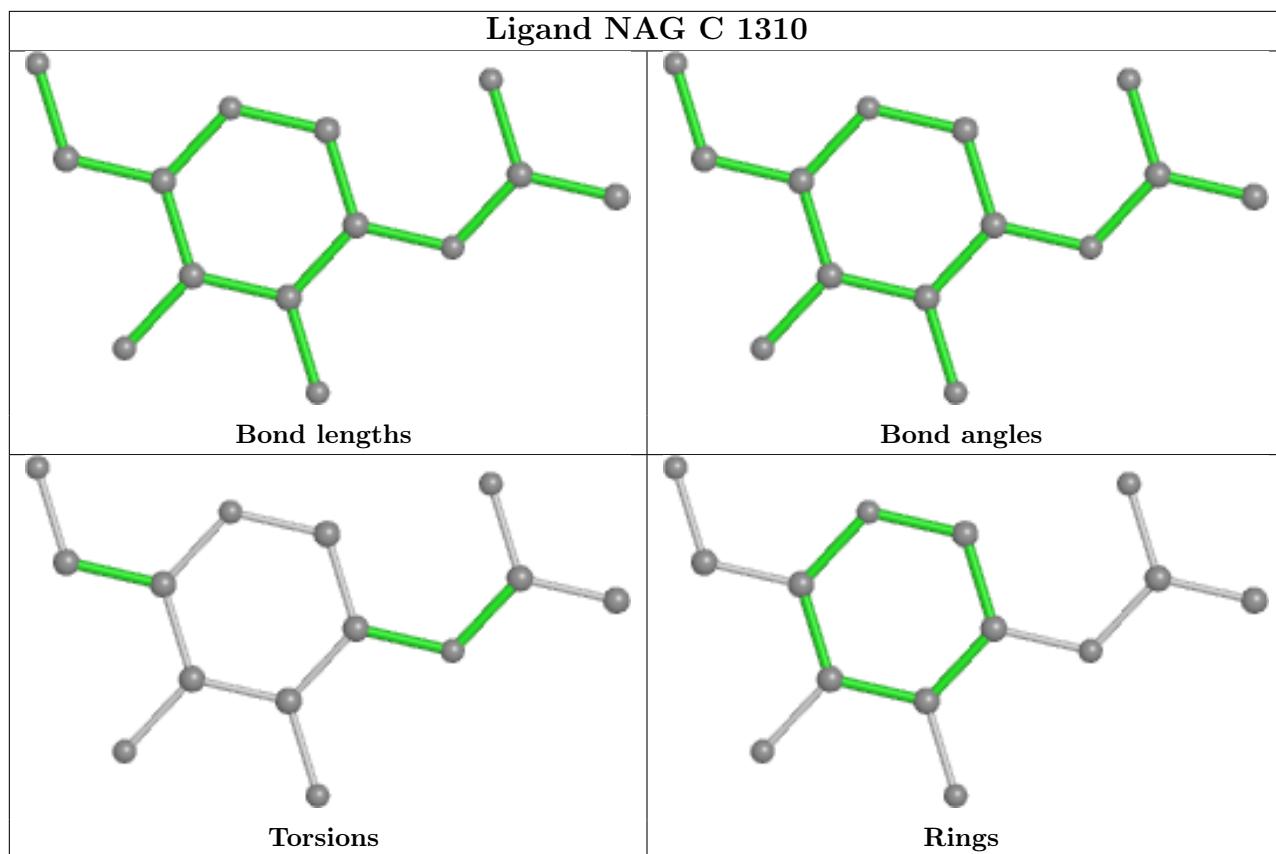












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

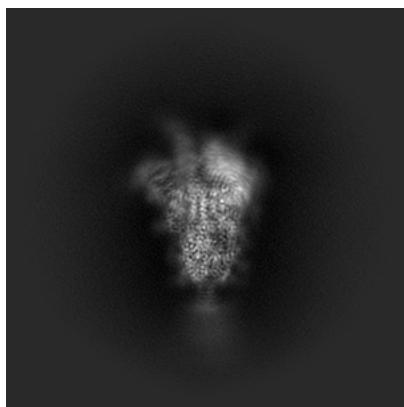
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24105. These allow visual inspection of the internal detail of the map and identification of artifacts.

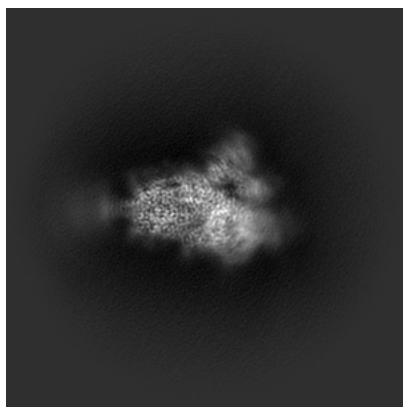
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

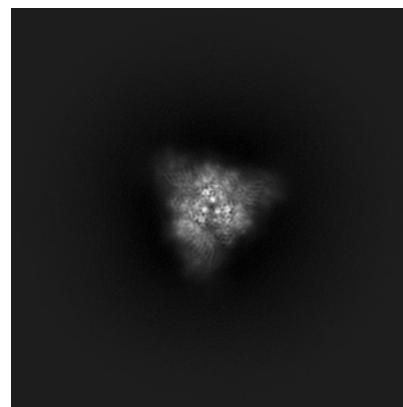
6.1.1 Primary map



X



Y

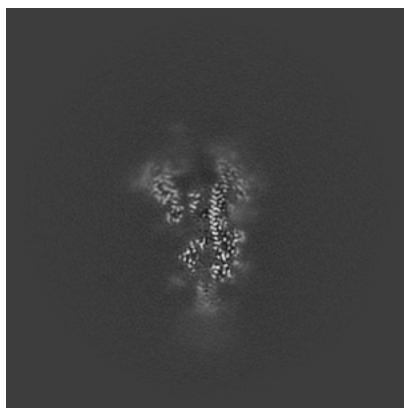


Z

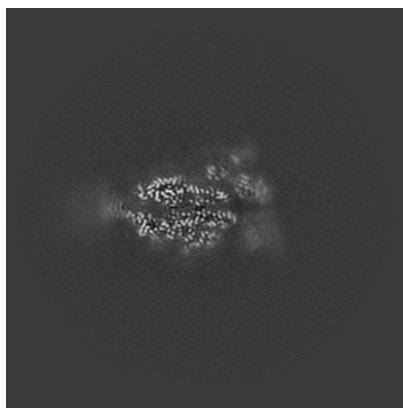
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

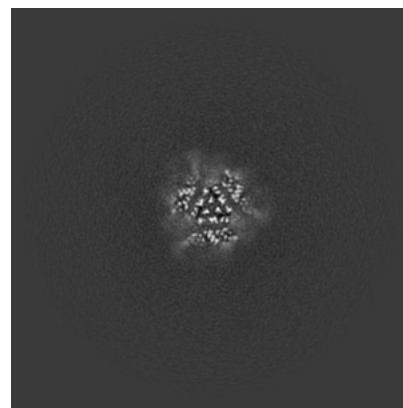
6.2.1 Primary map



X Index: 200



Y Index: 200

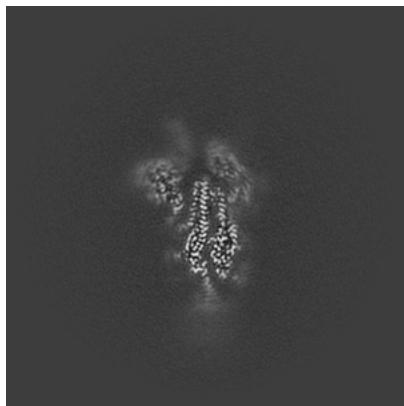


Z Index: 200

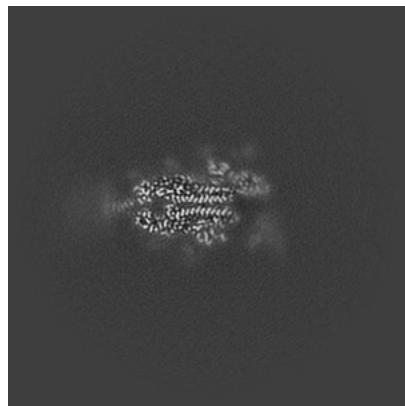
The images above show central slices of the map in three orthogonal directions.

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

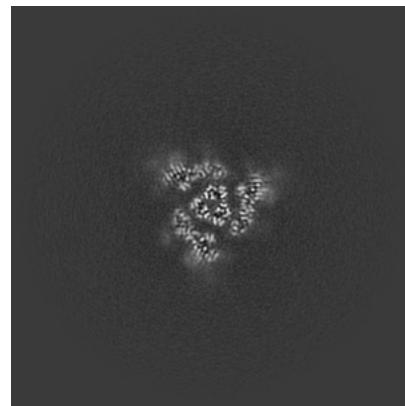
6.3.1 Primary map



X Index: 193



Y Index: 196



Z Index: 216

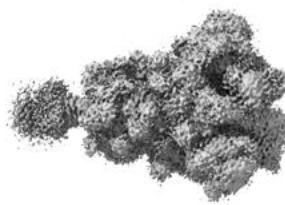
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [\(i\)](#)

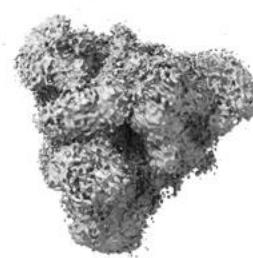
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0429. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

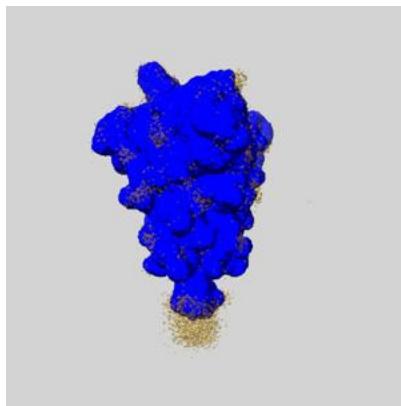
6.5 Mask visualisation [\(i\)](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

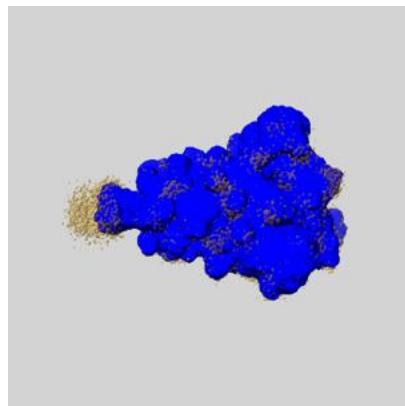
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

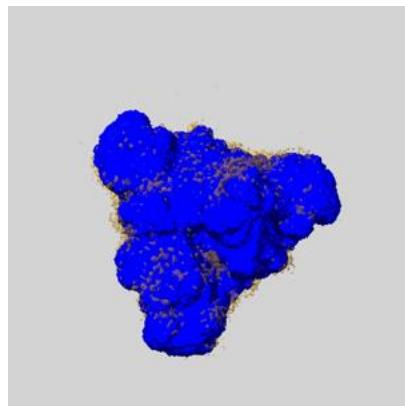
6.5.1 emd_24105_msk_1.map [\(i\)](#)



X



Y

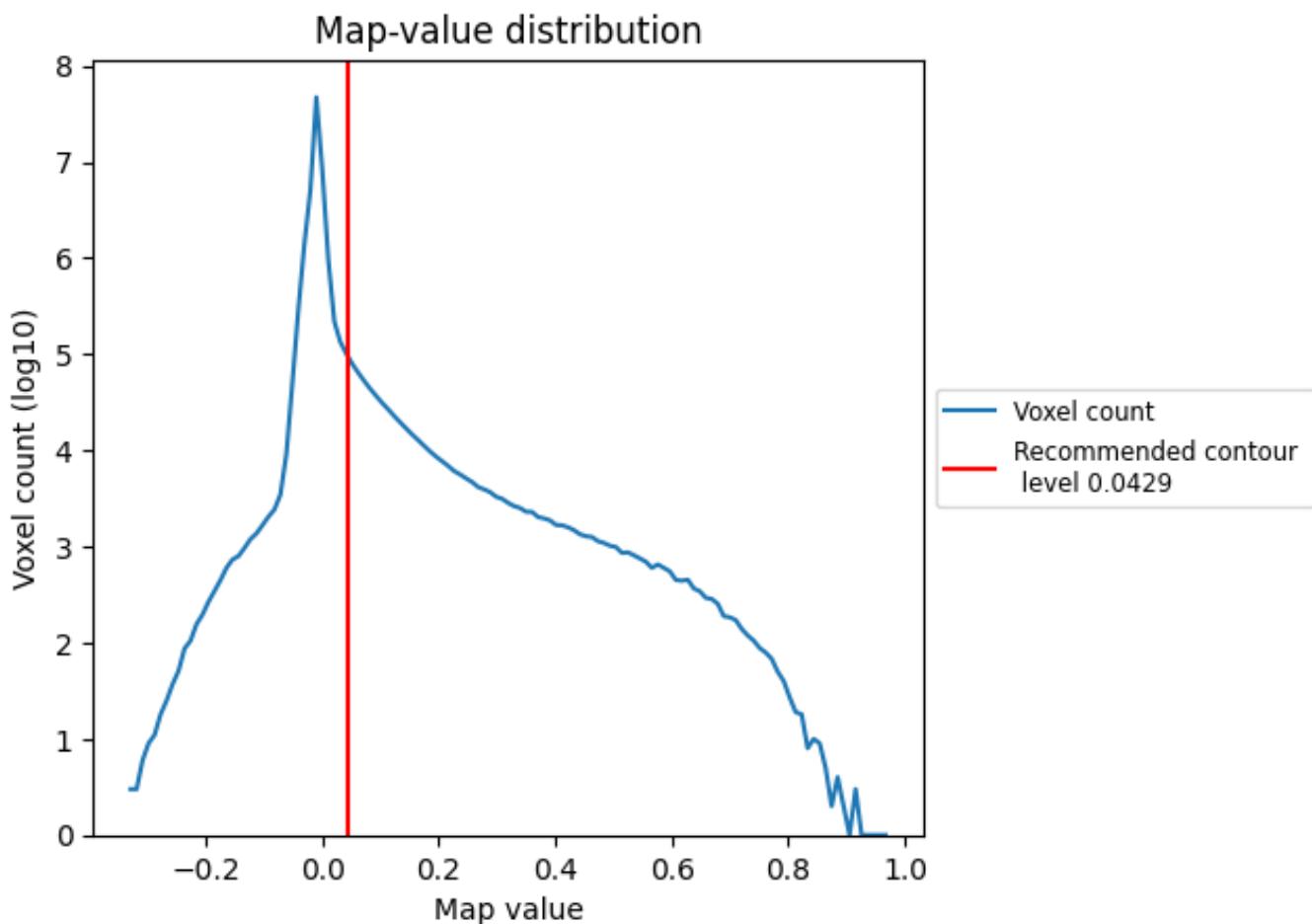


Z

7 Map analysis (i)

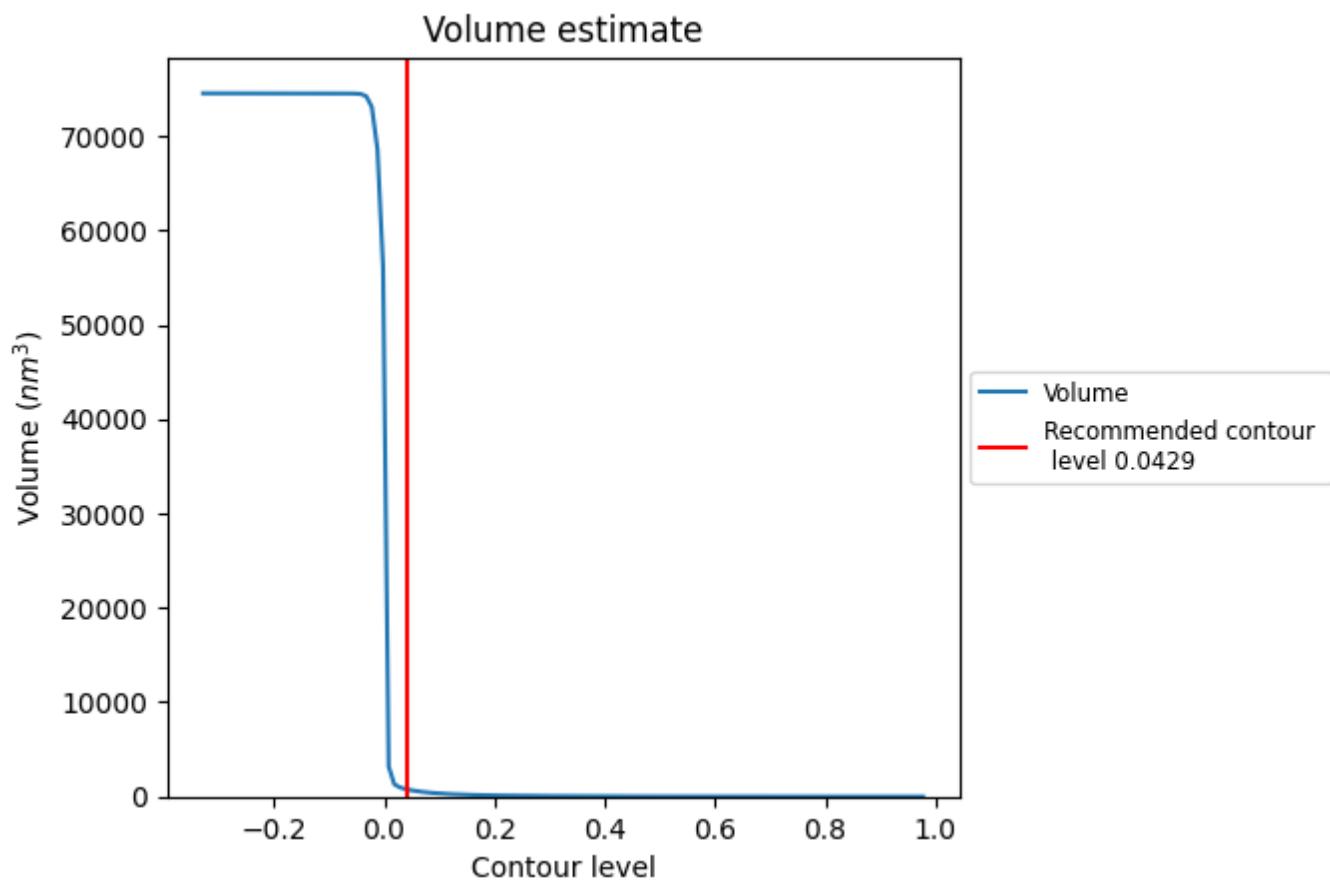
This section contains the results of statistical analysis of the map.

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.

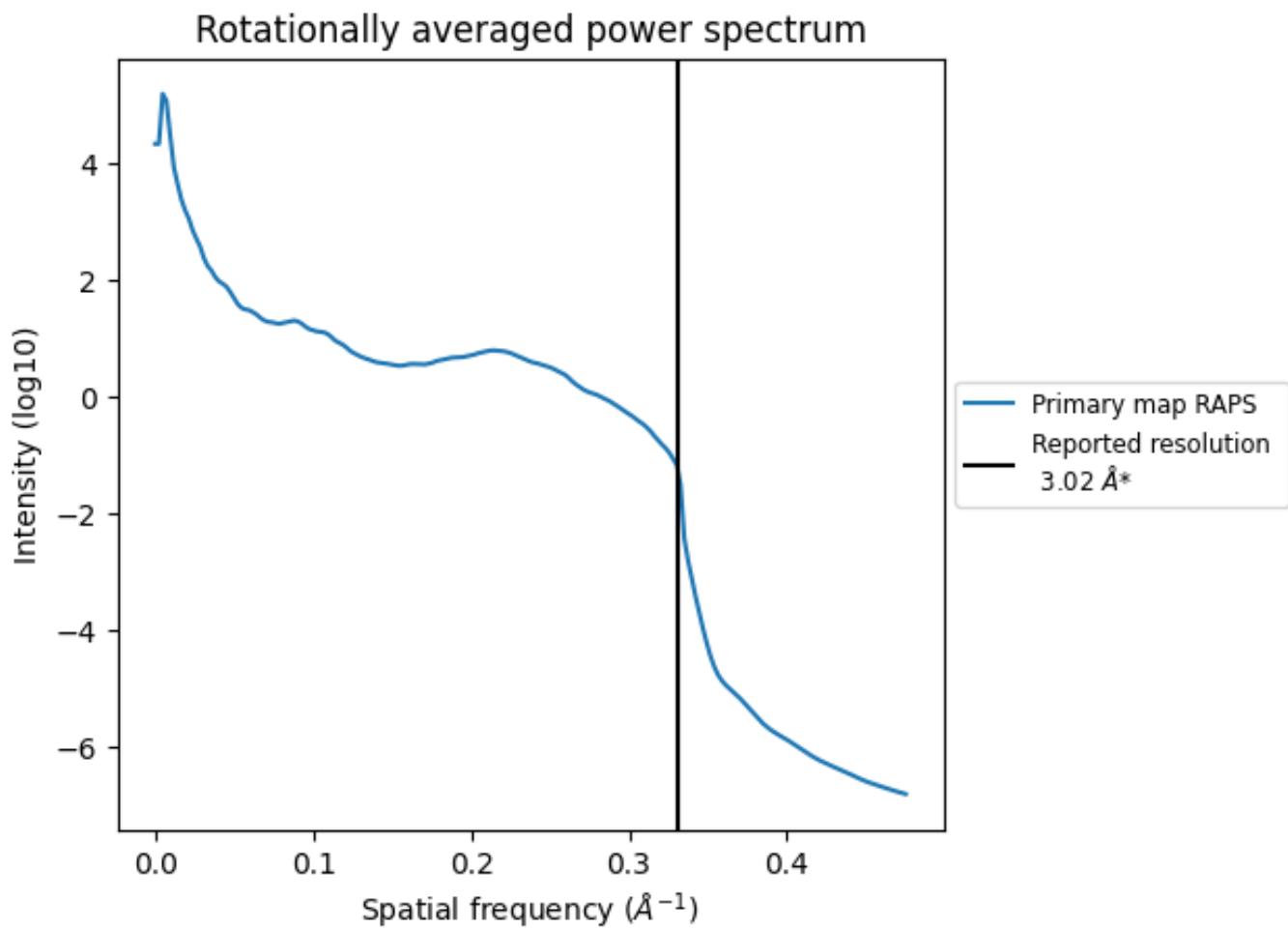
7.2 Volume estimate (i)



The volume at the recommended contour level is 744 nm^3 ; this corresponds to an approximate mass of 672 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 [\(i\)](#)

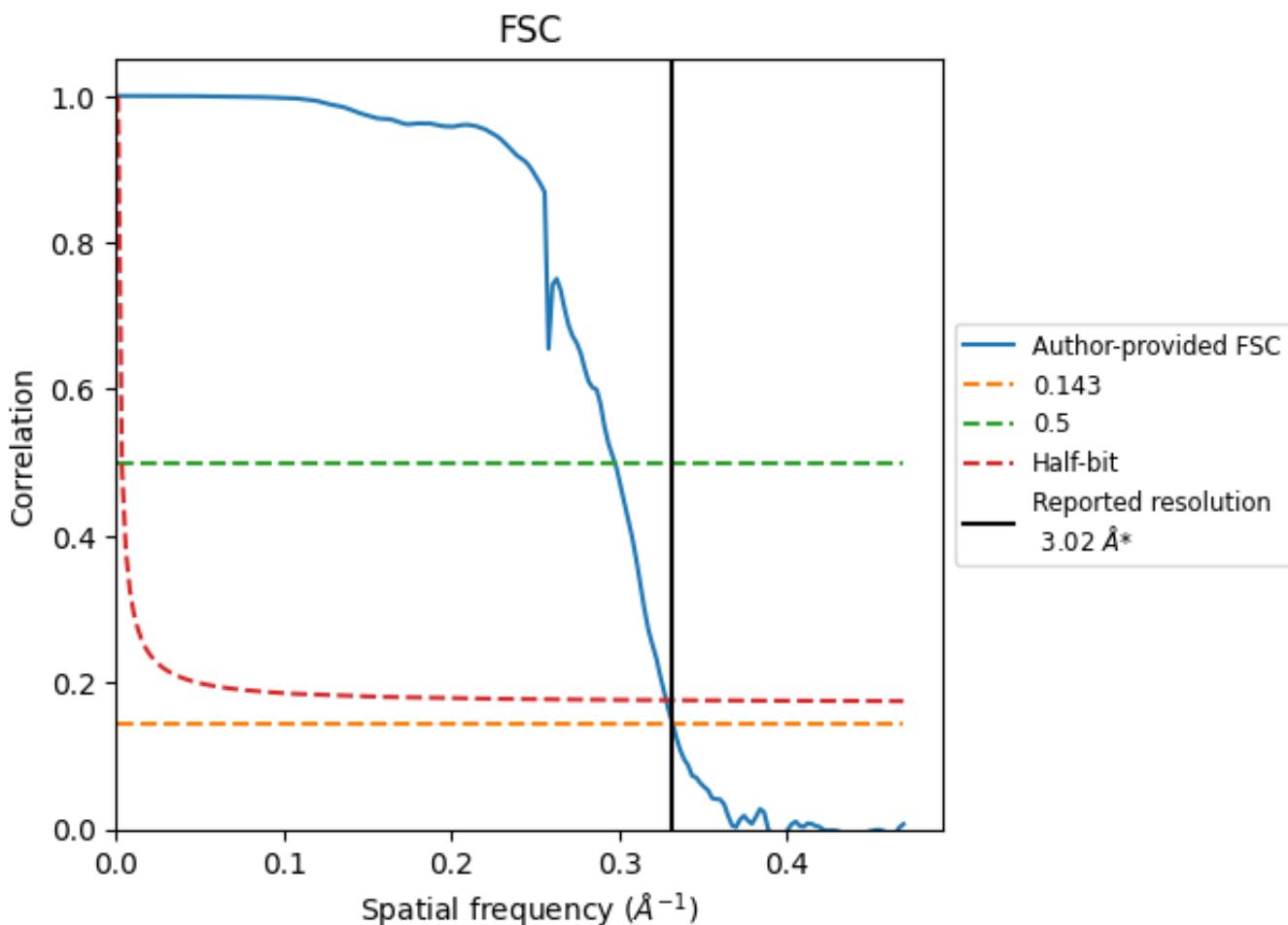


*Reported resolution corresponds to spatial frequency of 0.331\AA^{-1}

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 0.331 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

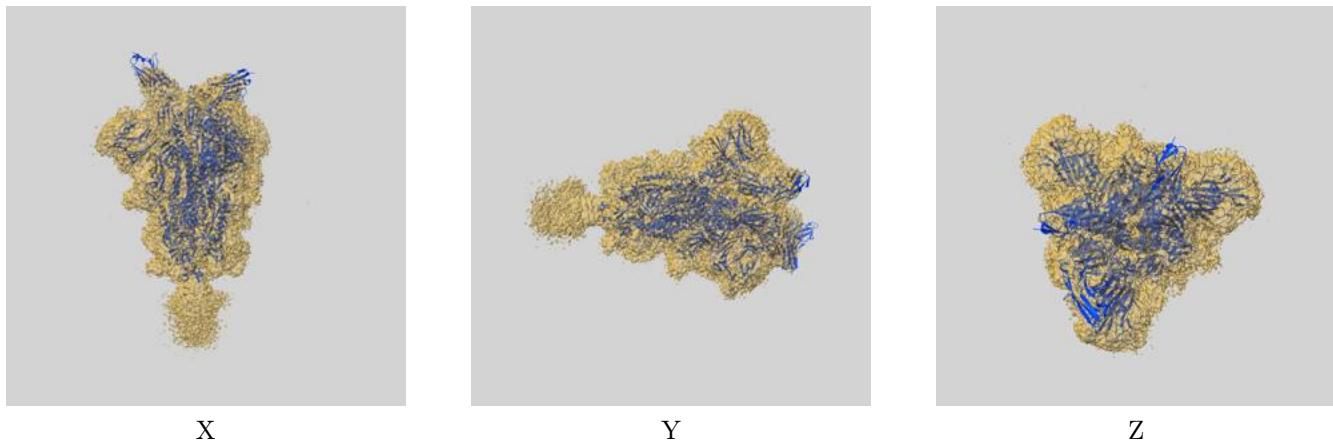
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.01	3.36	3.05
Unmasked-calculated*	-	-	-

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

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

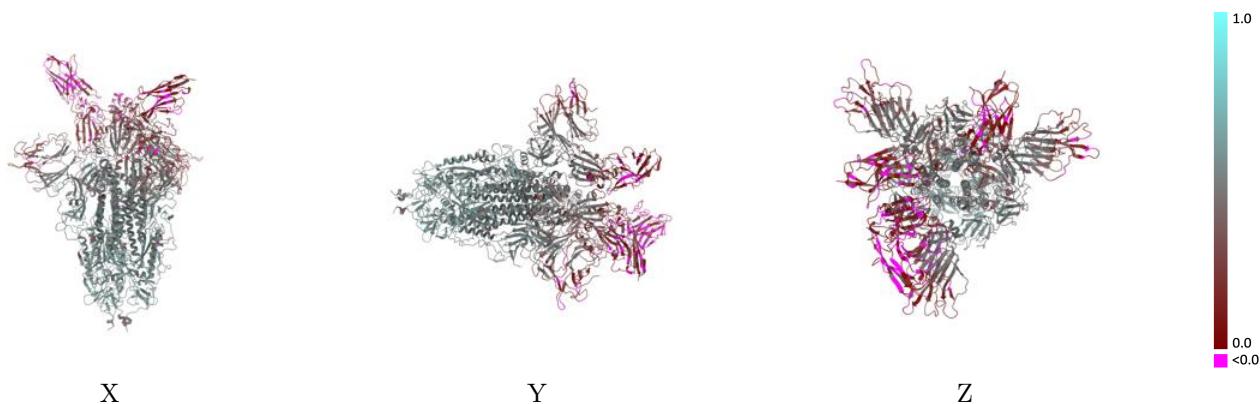
This section contains information regarding the fit between EMDB map EMD-24105 and PDB model 7N0G. Per-residue inclusion information can be found in section 3 on page 15.

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



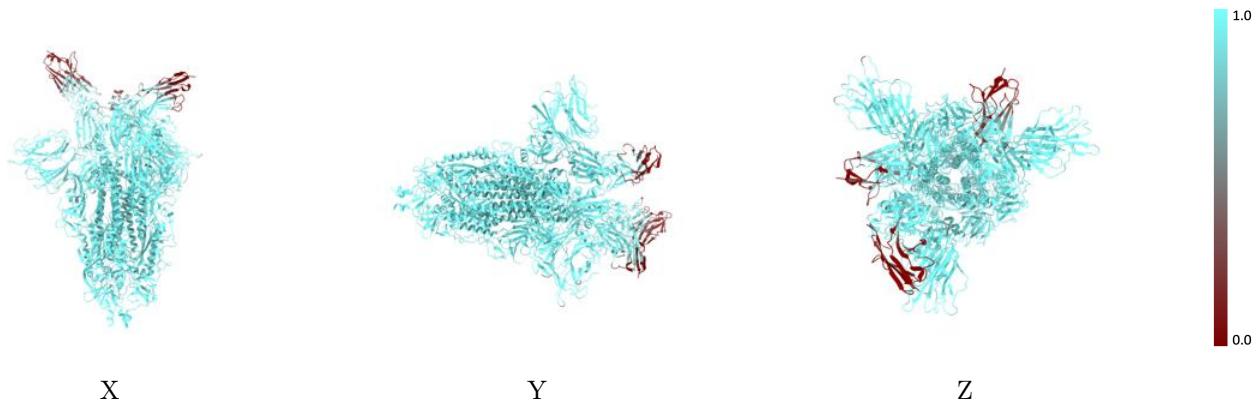
The images above show the 3D surface view of the map at the recommended contour level 0.0429 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



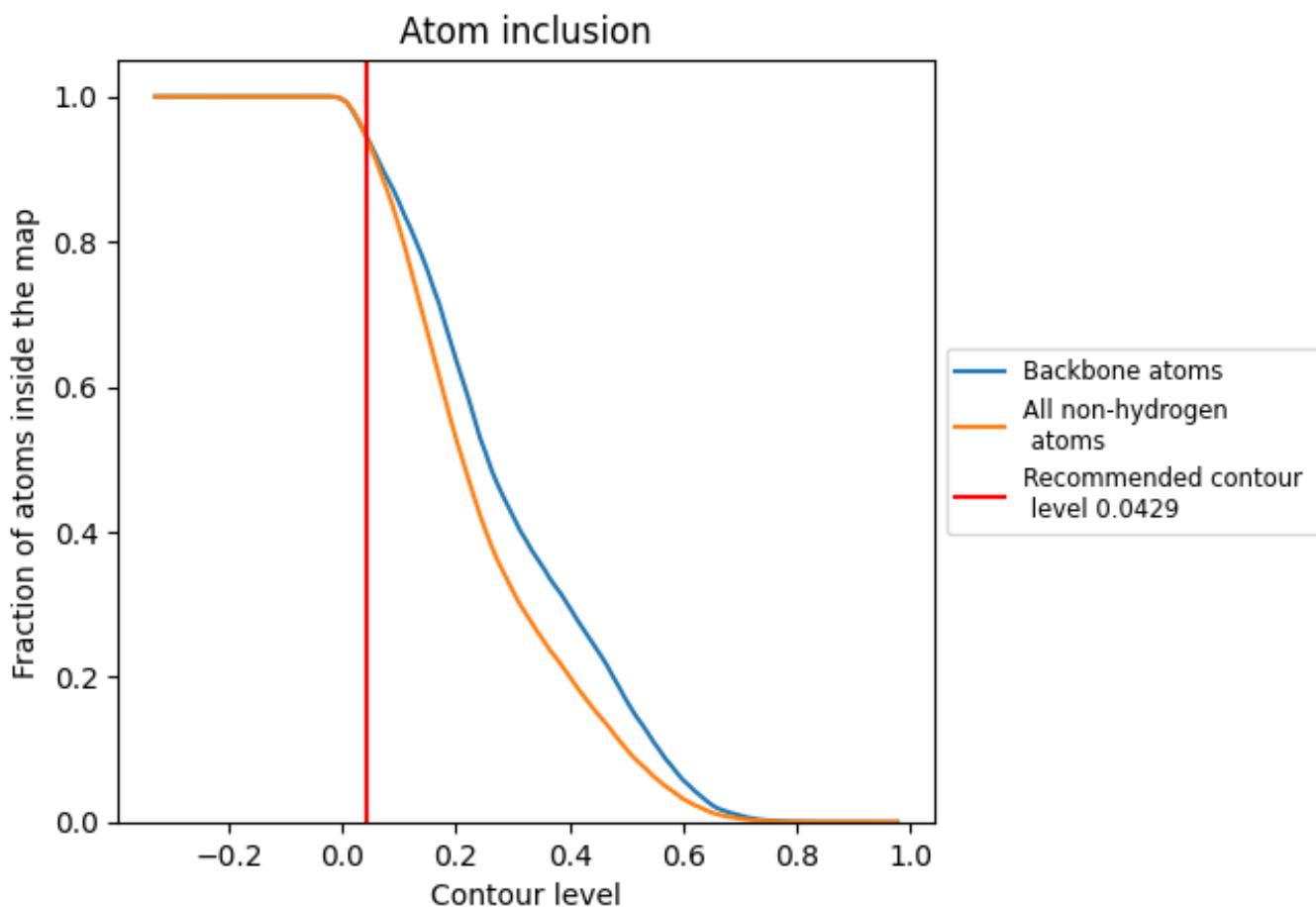
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0429).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0429) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9437	0.3970
A	0.9858	0.3990
B	0.9954	0.4510
C	0.9949	0.4430
D	1.0000	0.3190
E	1.0000	0.2760
F	1.0000	0.5080
G	1.0000	0.4660
H	1.0000	0.4790
I	1.0000	0.4330
J	1.0000	0.4360
K	1.0000	0.5170
L	1.0000	0.4560
M	1.0000	0.4290
N	1.0000	0.4760
O	1.0000	0.2340
P	1.0000	0.2940
Q	0.9286	0.2740
R	0.9286	0.2120
S	0.9643	0.1160
U	1.0000	0.2600
V	1.0000	0.2000
W	1.0000	0.1940
X	0.2701	0.0490
Y	0.5293	0.1060
Z	0.6768	0.1560

