



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 07:22 PM UTC

PDB ID : 7XID / pdb_00007xid
EMDB ID : EMD-33203
Title : S-ECD (Omicron) in complex with PD of ACE2
Authors : Li, Y.N.; Shen, Y.P.; Zhang, Y.Y.; Yan, R.H.
Deposited on : 2022-04-12
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

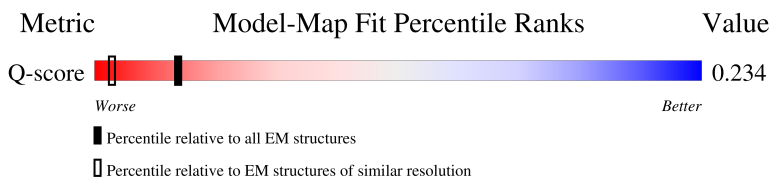
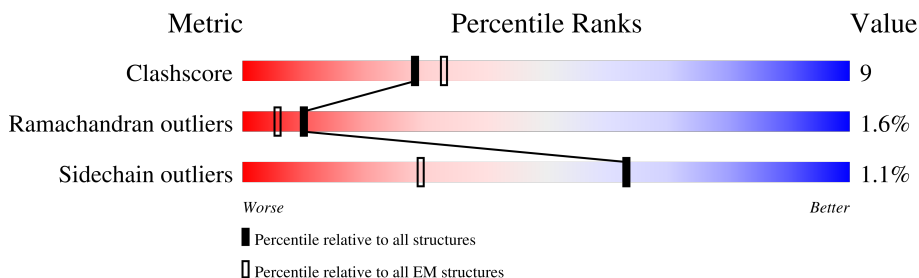
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	1267	9% 67% 7% 24%
1	B	1267	11% 66% 11% 21%
1	C	1267	7% 69% 9% 21%
2	D	817	63% 58% 14% 27%

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Mol	Chain	Length	Quality of chain
2	E	817	 72% 58% 14% 27%
3	F	2	 50% 100%
3	G	2	 100%
3	H	2	 50% 50%
3	I	2	 100%
3	J	2	 50% 50%
3	K	2	 50% 50%
3	L	2	 100%
3	M	2	 50% 100%
3	N	2	 50% 100%
3	O	2	 50% 50%
3	P	2	 50% 50%
3	Q	2	 100%
3	R	2	 100%
3	S	2	 100%
3	T	2	 100%
3	U	2	 50% 50%
3	V	2	 50% 50%
3	W	2	 100%
3	X	2	 50% 50%
3	Y	2	 100%
3	Z	2	 100%
3	a	2	 50% 50%
3	b	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	D	902	-	-	X	-
4	NAG	E	902	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34256 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	963	Total	C	N	O	S	0	0
			7558	4842	1255	1427	34		
1	B	998	Total	C	N	O	S	0	0
			7842	5025	1304	1477	36		
1	C	998	Total	C	N	O	S	0	0
			7842	5025	1304	1477	36		

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	145	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	211	ILE	LEU	variant	UNP P0DTC2
A	214	GLU	-	insertion	UNP P0DTC2
A	214A	PRO	-	insertion	UNP P0DTC2
A	214B	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	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
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	LEU	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	SER	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLU	-	expression tag	UNP P0DTC2
A	1244	VAL	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	ALA	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	SER	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	SER	-	expression tag	UNP P0DTC2
A	1261	VAL	-	expression tag	UNP P0DTC2
A	1262	GLU	-	expression tag	UNP P0DTC2
A	1263	ASP	-	expression tag	UNP P0DTC2
A	1264	TYR	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	ASP	-	expression tag	UNP P0DTC2
A	1267	ASP	-	expression tag	UNP P0DTC2
A	1268	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	ASP	-	expression tag	UNP P0DTC2
A	1270	LYS	-	expression tag	UNP P0DTC2
B	69	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	145	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	211	ILE	LEU	variant	UNP P0DTC2
B	214	GLU	-	insertion	UNP P0DTC2
B	214A	PRO	-	insertion	UNP P0DTC2
B	214B	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	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
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	LEU	-	expression tag	UNP P0DTC2
B	1239	GLU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	SER	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1243	GLU	-	expression tag	UNP P0DTC2
B	1244	VAL	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	ALA	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	SER	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	SER	-	expression tag	UNP P0DTC2
B	1261	VAL	-	expression tag	UNP P0DTC2
B	1262	GLU	-	expression tag	UNP P0DTC2
B	1263	ASP	-	expression tag	UNP P0DTC2
B	1264	TYR	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	ASP	-	expression tag	UNP P0DTC2
B	1267	ASP	-	expression tag	UNP P0DTC2
B	1268	ASP	-	expression tag	UNP P0DTC2
B	1269	ASP	-	expression tag	UNP P0DTC2
B	1270	LYS	-	expression tag	UNP P0DTC2
C	69	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	145	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	211	ILE	LEU	variant	UNP P0DTC2
C	214	GLU	-	insertion	UNP P0DTC2
C	214A	PRO	-	insertion	UNP P0DTC2
C	214B	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	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
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	SER	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLU	-	expression tag	UNP P0DTC2
C	1244	VAL	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	ALA	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	SER	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	SER	-	expression tag	UNP P0DTC2
C	1261	VAL	-	expression tag	UNP P0DTC2
C	1262	GLU	-	expression tag	UNP P0DTC2
C	1263	ASP	-	expression tag	UNP P0DTC2
C	1264	TYR	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	ASP	-	expression tag	UNP P0DTC2
C	1267	ASP	-	expression tag	UNP P0DTC2
C	1268	ASP	-	expression tag	UNP P0DTC2
C	1269	ASP	-	expression tag	UNP P0DTC2
C	1270	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	E	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP Q9BYF1
D	-10	ALA	-	expression tag	UNP Q9BYF1
D	-9	SER	-	expression tag	UNP Q9BYF1
D	-8	GLY	-	expression tag	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1
E	-11	MET	-	expression tag	UNP Q9BYF1
E	-10	ALA	-	expression tag	UNP Q9BYF1
E	-9	SER	-	expression tag	UNP Q9BYF1
E	-8	GLY	-	expression tag	UNP Q9BYF1
E	-7	ARG	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	TRP	-	insertion	UNP Q9BYF1
E	11	SER	-	insertion	UNP Q9BYF1
E	12	HIS	-	insertion	UNP Q9BYF1
E	13	PRO	-	insertion	UNP Q9BYF1
E	14	GLN	-	insertion	UNP Q9BYF1
E	15	PHE	-	insertion	UNP Q9BYF1
E	16	GLU	-	insertion	UNP Q9BYF1
E	17	LYS	-	insertion	UNP Q9BYF1

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



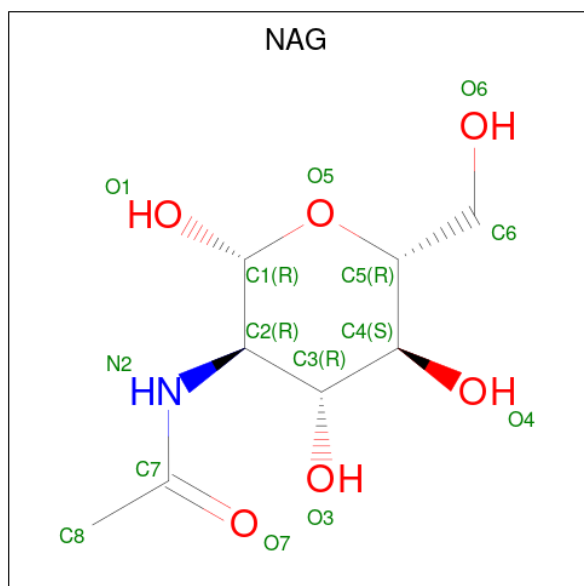
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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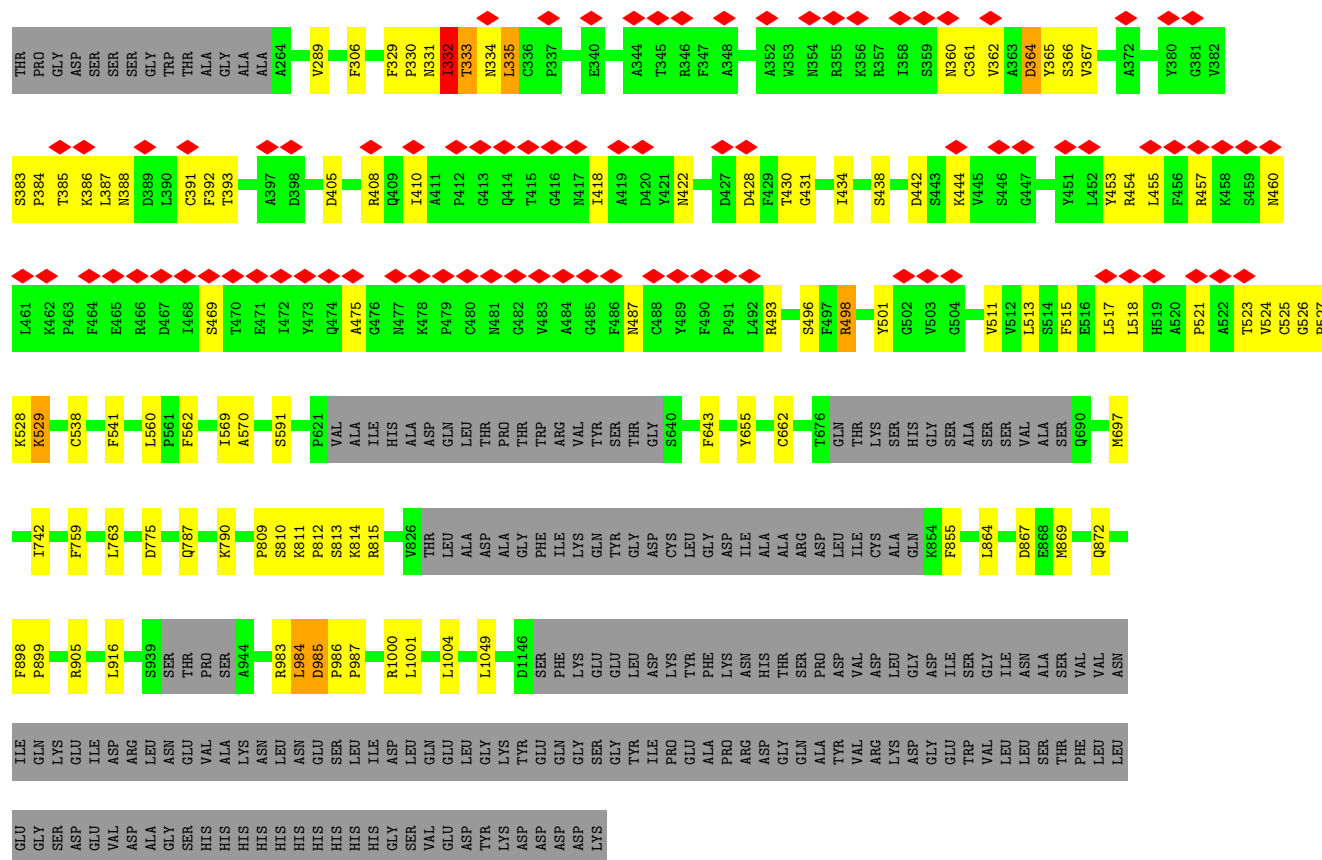
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total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

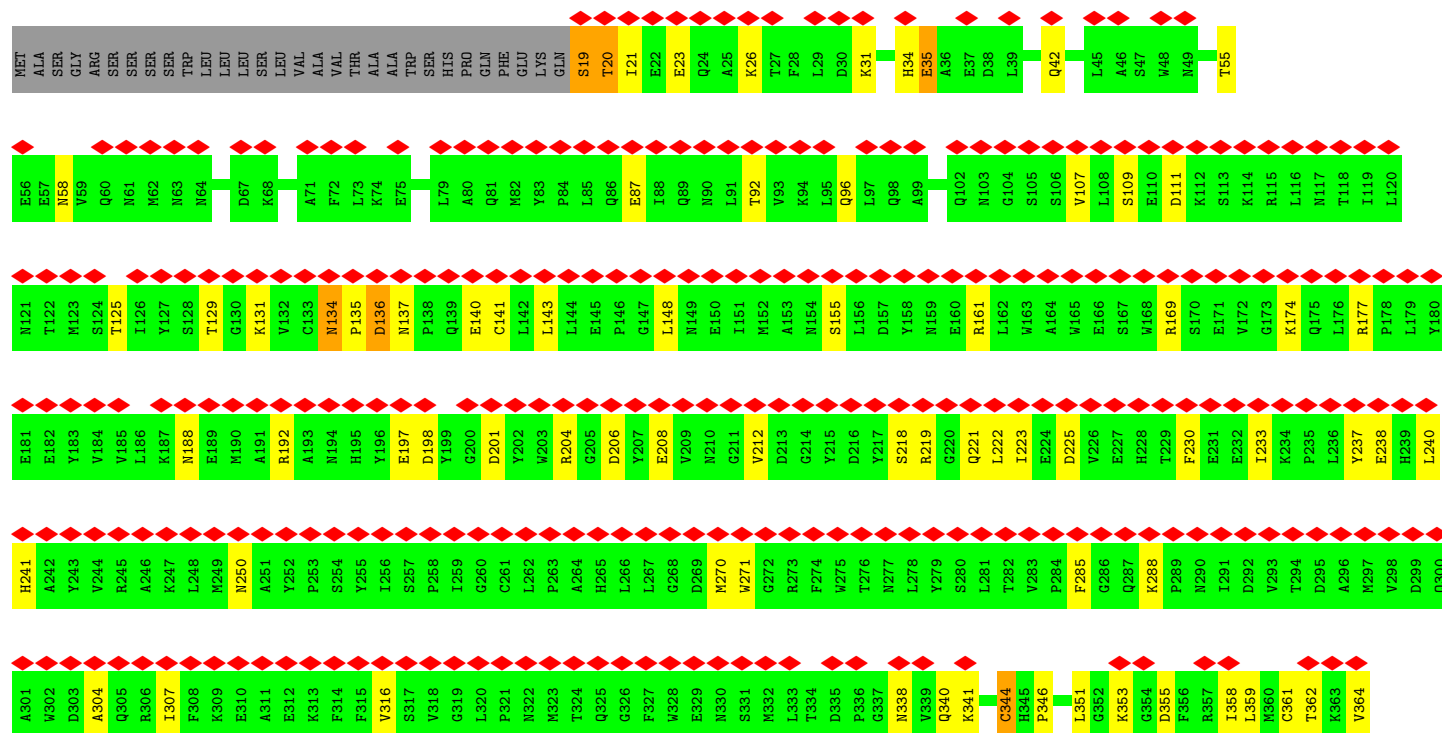
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Mol	Chain	Residues	Atoms				AltConf
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	



• Molecule 2: Angiotensin-converting enzyme 2



T365	M366	D367	D368	T371	A372	H373	H374	E375	M376	G377	I379	Q380	Y381	D382	M383	A384	Y385	A386	A387	Q388	P389	F390	L391	L392	R393	N394	G395	A396	G399	F400	H401	E402	A403	V404	G405	E406	I407	M408	S409	L410	S411	A412	T413	P415	K416	H417	L418	K419	S420	I421	G422	L423	L424	S425	P426																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
D427	F428	Q429	E430	M431	E433	T434	E435	I436	M437	F438	L439	L440	K441	Q442	A443	L444	T445	I446	V447	G448	T449	L450	P451	F452	T453	Y454	M455	L456	E457	K458	R460	W461	M462	V463	F464	K465	G466	E467	I468	P469	K470	D471	Q472	M473	M474	K475	K476	W477	W478	E479	M480	R482	E483	I484	V485	G486																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
V487	V488	E489	P490	V491	H493	D494	E495	T496	Y497	G498	D499	P500	A501	S502	L503	F504	H505	V506	S507	N508	D509	Y510	S511	F512	I513	R514	Y515	Y516	T517	R518	T519	L520	Y521	Q522	F523	Q524	F525	Q526	E527	A528	L529	C530	Q531	A532	A533	K534	H535	E536	G537	P538	L539	H540	K541	C542	D543	I544	S545	N546																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
S547	T548	E549	A550	G551	Q552	K553	L554	F555	N556	M557	K562	S563	E564	P565	M566	T567	L568	A569	L570	E571	N572	V573	V574	G575	A576	K577	N578	M579	N580	V581	E582	P583	L584	L585	N586	T587	F588	E589	P590	L591	F592	T593	M594	L595	K596	D597	Q598	N599	K600	M601	S602	F603	V604	G605	W606	S607	T608	D609																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
W610	S611	P612	Y613	A614	D615	G616	S617	E618	T619	N620	P621	L622	A623	M624	T625	K626	V627	L628	A629	P630	N631	D632	Y633	S634	E635	M636	L637	N638	V639	T640	P641	L642	A643	M644	T645	K646	V647	N648	D649	Y650	S651	L652	F653	H654	G655	P656	L657	M658	T659	K660	V661	L662	A663	M664	T665	K666	V667	N668	D669	Y670	S671	L672	F673	H674	G675	P676	L677	M678	T679	K680	V681	T682	P683	L684	A685	M686	T687	K688	V689	N690	D691	Y692	S693	L694	F695	H696	G697	P698	L699	M700	T701	K702	V703	N704	D705	Y706	S707	L708	F709	H710	G711	P712	L713	M714	T715	K716	V717	N718	D719	Y720	S721	L722	F723	H724	G725	P726	L727	M728	T729	K730	V731	N732	D733	Y734	S735	L736	F737	H738	G739	P740	L741	M742	T743	K744	V745	N746	D747	Y748	S749	L750	F751	H752	G753	P754	L755	M756	T757	K758	V759	N760	D761	Y762	S763	L764	F765	H766	G767	P768	L769	M770	T771	K772	V773	N774	D775	Y776	S777	L778	F779	H780	G781	P782	L783	M784	T785	K786	V787	N788	D789	Y790	S791	L792	F793	H794	G795	P796	L797	M798	T799	K800	V801	N802	D803	Y804	S805	L806	F807	H808	G809	P810	L811	M812	T813	K814	V815	N816	D817	Y818	S819	L820	F821	H822	G823	P824	L825	M826	T827	K828	V829	N830	D831	Y832	S833	L834	F835	H836	G837	P838	L839	M840	T841	K842	V843	N844	D845	Y846	S847	L848	F849	H850	G851	P852	L853	M854	T855	K856	V857	N858	D859	Y860	S861	L862	F863	H864	G865	P866	L867	M868	T869	K870	V871	N872	D873	Y874	S875	L876	F877	H878	G879	P880	L881	M882	T883	K884	V885	N886	D887	Y888	S889	L890	F891	H892	G893	P894	L895	M896	T897	K898	V899	N900	D901	Y902	S903	L904	F905	H906	G907	P908	L909	M910	T911	K912	V913	N914	D915	Y916	S917	L918	F919	H920	G921	P922	L923	M924	T925	K926	V927	N928	D929	Y930	S931	L932	F933	H934	G935	P936	L937	M938	T939	K940	V941	N942	D943	Y944	S945	L946	F947	H948	G949	P950	L951	M952	T953	K954	V955	N956	D957	Y958	S959	L960	F961	H962	G963	P964	L965	M966	T967	K968	V969	N970	D971	Y972	S973	L974	F975	H976	G977	P978	L979	M980	T981	K982	V983	N984	D985	Y986	S987	L988	F989	H990	G991	P992	L993	M994	T995	K996	V997	N998	D999	Y1000	S1001	L1002	F1003	H1004	G1005	P1006	L1007	M1008	T1009	K1010	V1011	N1012	D1013	Y1014	S1015	L1016	F1017	H1018	G1019	P1020	L1021	M1022	T1023	K1024	V1025	N1026	D1027	Y1028	S1029	L1030	F1031	H1032	G1033	P1034	L1035	M1036	T1037	K1038	V1039	N1040	D1041	Y1042	S1043	L1044	F1045	H1046	G1047	P1048	L1049	M1050	T1051	K1052	V1053	N1054	D1055	Y1056	S1057	L1058	F1059	H1060	G1061	P1062	L1063	M1064	T1065	K1066	V1067	N1068	D1069	Y1070	S1071	L1072	F1073	H1074	G1075	P1076	L1077	M1078	T1079	K1080	V1081	N1082	D1083	Y1084	S1085	L1086	F1087	H1088	G1089	P1090	L1091	M1092	T1093	K1094	V1095	N1096	D1097	Y1098	S1099	L1100	F1101	H1102	G1103	P1104	L1105	M1106	T1107	K1108	V1109	N1110	D1111	Y1112	S1113	L1114	F1115	H1116	G1117	P1118	L1119	M1120	T1121	K1122	V1123	N1124	D1125	Y1126	S1127	L1128	F1129	H1130	G1131	P1132	L1133	M1134	T1135	K1136	V1137	N1138	D1139	Y1140	S1141	L1142	F1143	H1144	G1145	P1146	L1147	M1148	T1149	K1150	V1151	N1152	D1153	Y1154	S1155	L1156	F1157	H1158	G1159	P1160	L1161	M1162	T1163	K1164	V1165	N1166	D1167	Y1168	S1169	L1170	F1171	H1172	G1173	P1174	L1175	M1176	T1177	K1178	V1179	N1180	D1181	Y1182	S1183	L1184	F1185	H1186	G1187	P1188	L1189	M1190	T1191	K1192	V1193	N1194	D1195	Y1196	S1197	L1198	F1199	H1200	G1201	P1202	L1203	M1204	T1205	K1206	V1207	N1208	D1209	Y1210	S1211	L1212	F1213	H1214	G1215	P1216	L1217	M1218	T1219	K1220	V1221	N1222	D1223	Y1224	S1225	L1226	F1227	H1228	G1229	P1230	L1231	M1232	T1233	K1234	V1235	N1236	D1237	Y1238	S1239	L1240	F1241	H1242	G1243	P1244	L1245	M1246	T1247	K1248	V1249	N1250	D1251	Y1252	S1253	L1254	F1255	H1256	G1257	P1258	L1259	M1260	T1261	K1262	V1263	N1264	D1265	Y1266	S1267	L1268	F1269	H1270	G1271	P1272	L1273	M1274	T1275	K1276	V1277	N1278	D1279	Y1280	S1281	L1282	F1283	H1284	G1285	P1286	L1287	M1288	T1289	K1290	V1291	N1292	D1293	Y1294	S1295	L1296	F1297	H1298	G1299	P1300	L1301	M1302	T1303	K1304	V1305	N1306	D1307	Y1308	S1309	L1310	F1311	H1312	G1313	P1314	L1315	M1316	T1317	K1318	V1319	N1320	D1321	Y1322	S1323	L1324	F1325	H1326	G1327	P1328	L1329	M1330	T1331	K1332	V1333	N1334	D1335	Y1336	S1337	L1338	F1339	H1340	G1341	P1342	L1343	M1344	T1345	K1346	V1347	N1348	D1349	Y1350	S1351	L1352	F1353	H1354	G1355	P1356	L1357	M1358	T1359	K1360	V1361	N1362	D1363	Y1364	S1365	L1366	F1367	H1368	G1369	P1370	L1371	M1372	T1373	K1374	V1375	N1376	D1377	Y1378	S1379	L1380	F1381	H1382	G1383	P1384	L1385	M1386	T1387	K1388	V1389	N1390	D1391	Y1392	S1393	L1394	F1395	H1396	G1397	P1398	L1399	M1400	T1401	K1402	V1403	N1404	D1405	Y1406	S1407	L1408	F1409	H1410	G1411	P1412	L1413	M1414	T1415	K1416	V1417	N1418	D1419	Y1420	S1421	L1422	F1423	H1424	G1425	P1426	L1427	M1428	T1429	K1430	V1431	N1432	D1433	Y1434	S1435	L1436	F1437	H1438	G1439	P1440	L1441	M1442	T1443	K1444	V1445	N1446	D1447	Y1448	S1449	L1450	F1451	H1452	G1453	P1454	L1455	M1456	T1457	K1458	V1459	N1460	D1461	Y1462	S1463	L1464	F1465	H1466	G1467	P1468	L1469	M1470	T1471	K1472	V1473	N1474	D1475	Y1476	S1477	L1478	F1479	H1480	G1481	P1482	L1483	M1484	T1485	K1486	V1487	N1488	D1489	Y1490	S1491	L1492	F1493	H1494	G1495	P1496	L1497	M1498	T1499	K1500	V1501	N1502	D1503	Y1504	S1505	L1506	F1507	H1508	G1509	P1510	L1511	M1512	T1513	K1514	V1515	N1516	D1517	Y1518	S1519	L1520	F1521	H1522	G1523	P1524	L1525	M1526	T1527	K1528	V1529	N1530	D1531	Y1532	S1533	L1534	F1535	H1536	G1537	P1538	L1539	M1540	T1541	K1542	V1543	N1544	D1545	Y1546	S1547	L1548	F1549	H1550	G1551	P1552	L1553	M1554	T1555	K1556	V1557	N1558	D1559	Y1560	S1561	L1562	F1563	H1564	G1565	P1566	L1567	M1568	T1569	K1570	V1571	N1572	D1573	Y1574	S1575	L1576	F1577	H1578	G1579	P1580	L1581	M1582	T1583	K1584	V1585	N1586	D1587	Y1588	S1589	L1590	F1591	H1592	G1593	P1594	L1595	M1596	T1597	K1598	V1599	N1600	D1601	Y1602	S1603	L1604	F1605	H1606	G1607	P1608	L1609	M1610	T1611	K1612	V1613	N1614	D1615	Y1616	S1617	L1618	F1619	H1620	G1621	P1622	L1623	M1624	T1625	K1626	V1627	N1628	D1629	Y1630	S1631	L1632	F1633	H1634	G1635	P1636	L1637	M1638	T1639	K1640	V1641	N1642	D1643	Y1644	S1645	L1646	F1647	H1648	G1649	P1650	L1651	M1652	T1653	K1654	V1655	N1656	D1657	Y1658	S1659	L1660	F1661	H1662	G1663	P1664	L1665	M1666	T1667	K1668	V1669	N1670	D1671	Y1672	S1673	L1674	F1675	H1676	G1677	P1678	L1679	M1680	T1681	K1682	V1683	N1684	D1685	Y1686	S1687	L1688	F1689	H1690	G1691	P1692	L1693	M1694	T1695	K1696	V1697	N1698	D1699	Y1700	S1701	L1702	F1703	H1704	G1705	P1706	L1707	M1708	T1709	K1710	V1711	N1712	D1713	Y1714	S1715	L1716	F1717	H1718	G1719	P1720	L1721	M1722	T1723	K1724	V1725	N1726	D1727	Y1728	S1729	L1730	F1731	H1732	G1733	P1734	L1735	M1736	T1737	K1738	V1739	N1740	D1741	Y1742	S1743	L1744	F1745	H1746	G1747	P1748	L1749	M1750	T1751	K1752	V1753	N1754	D1755	Y1756	S1757	L1758	F1759	H1760	G1761	P1762	L1763	M1764	T1765	K1766	V1767	N1768	D1769	Y1770	S1771	L1772	F1773	H1774	G1775	P1776	L1777	M1778	T1779	K1780	V1781	N1782	D1783	Y1784	S1785	L1786	F1787	H1788	G1789	P1790	L1791	M1792	T1793	K1794

LYS	LYS	ARG	TYR	E589	L529	P469	S409	W349
LYS	LYS	ARG	ALA	P590	C530	K470	L410	D350
LYS	ILE	ILE	MET	F590	Q531	D471	A411	L351
ASN	ASN	ARG	GLN	F592	A532	Q472	A412	G352
ALA	ALA	ASP	TYR	T593	A533	W473	A413	K353
ARG	PHE	PHE	PHE	W594	K534	W474	T414	G354
SER	ARG	LEU	LEU	L595	H535	K475	P415	D355
GLY	ASN	LYS	VAL	K596	E536	K476	K416	F356
ASN	ASN	LYS	ASN	D597	G537	W477	H417	R357
PRO	ASN	GLN	ASN	Q598	P538	W478	L418	I358
ALA	LEU	MET	GLN	N599	L539	E479	K419	L359
GLU	LEU	ILE	ILE	K600	H540	W480	S420	M360
PHE	LEU	LEU	PHE	N601	K541	K481	I421	C361
ASP	LEU	PHE	GLY	S602	C542	R482	G422	T362
ILE	GLY	GLY	GLU	F603	D543	E483	L423	K363
SER	ILE	GLN	GLU	V604	I544	I484	L424	V364
LYS	GLN	ASN	ASP	G605	S545	V485	S425	T365
GLY	THR	THR	VAL	W606	N546	G486	P426	M366
ASN	ASN	GLY	VAL	S607	S547	V487	P426	D367
PRO	PRO	ALA	ALA	T608	T548	V488	F428	D368
GLY	PRO	ASN	ASN	D609	E549	E489	Q429	F369
PHE	ASN	GLN	LEU	W610	A550	P490	E430	L370
GLN	GLN	ASN	LYS	S611	G551	V491	D431	T371
ASN	PRO	PRO	PRO	P612	Q552	P492	N432	A372
THR	THR	VAL	ILE	P612	Q552	P492	N432	A372
ASP	VAL	VAL	ILE	P613	K553	H493	E433	H373
ASN	ASN	ILE	PHE	A614	L554	D494	T434	H374
VAL	ILE	ASN	ASN	A614	L554	D494	T434	H374
THR	THR	LEU	PHE	D615	F555	E495	E435	E375
SER	ILE	ILE	PHE	D615	N556	T496	I436	K376
SER	VAL	VAL	VAL	SER	M557	Y497	N437	G377
PHE	PHE	THR	THR	ILE	M557	Y497	N437	G377
GLY	GLY	ALA	ALA	LYS	L558	C498	F438	H378
VAL	VAL	PRO	PRO	VAL	R559	D499	L439	I379
VAL	VAL	LYS	LYS	ARG	L560	P500	L440	Q380
MET	MET	ASN	ASN	ILE	G561	A501	K441	Y381
GLY	VAL	VAL	VAL	SER	S562	S502	Q442	D382
VAL	VAL	SER	SER	LEU	K562	L503	A443	M383
ILE	ILE	ASP	ASP	LYS	S563	F504	L444	A384
LYS	VAL	ILE	ILE	SER	E564	F504	L444	A384
VAL	VAL	ILE	ILE	ALA	P565	H505	T445	Y385
GLY	GLY	PRO	PRO	LEU	P565	H505	T445	Y385
ILE	ILE	ARG	ARG	GLY	W566	V506	I446	A386
VAL	VAL	THR	THR	ASP	T567	S507	V447	A387
ILE	ILE	GLU	GLU	LYS	L568	N508	G448	Q388
LEU	LEU	VAL	VAL	ALA	L568	N508	G448	Q388
ILE	ILE	VAL	VAL	TYR	A569	D509	T449	P389
PHE	PHE	LYS	LYS	GLU	L570	Y510	L450	F390
THR	THR	ALA	ALA	TRP	E571	S511	P451	L391
GLY	GLY	ILE	ILE	ASN	N572	F512	F452	L392
ILE	ILE	ARG	ARG	ASP	V573	I513	T453	R393
ARG	ARG	MET	MET	ASN	V574	R514	Y454	N394
ASP	ASP	SER	SER	GLU	G575	A514	Y454	N394
ARG	ARG	ARG	ARG	MET	G576	Y515	M455	G395
		LEU	LEU	TYR	A576	Y516	L456	A396
		PHE	PHE	THR	K577	T517	E457	N397
		ARG	ARG	ARG	N578	A518	K458	E398
		SER	SER	SER	W579	T519	W459	G399
		SER	SER	SER	N580	L520	R460	F400
		VAL	VAL	VAL	V581	Y521	W461	H401
		ALA	ALA	ALA	B582	Q522	M462	E402
				F583	L584	F523	V463	A403
				L585	L585	Q524	F464	V404
				N586	N586	F525	K465	G405
				Y587	Y587	Q526	G466	E406
				F588	F588	E527	E467	I407
						A528	T468	M408

- 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 I:  100%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain L:  100%



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

Chain M:  50% 100%



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

Chain N:  50% 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:  50% 50%



- 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:  100%



- 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 T:  100% 100%



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

Chain U:  50% 50% 50%



- 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%



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

Chain X: 50% 50%



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

Chain Y: 100%



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

Chain Z: 100%



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

Chain a: 50% 100% 50%



- Molecule 3: 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	97021	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.014	Depositor
Minimum map value	-1.616	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	0.53	1/7732 (0.0%)	0.66	11/10514 (0.1%)
1	B	0.50	0/8025	0.65	7/10911 (0.1%)
1	C	0.50	0/8025	0.65	8/10911 (0.1%)
2	D	0.32	0/5007	0.68	4/6803 (0.1%)
2	E	0.32	0/5007	0.68	4/6803 (0.1%)
All	All	0.46	1/33796 (0.0%)	0.66	34/45942 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	SER	CA-C	-6.63	1.44	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	432	ASN	N-CA-C	7.40	120.40	111.82
2	E	432	ASN	N-CA-C	7.39	120.39	111.82
1	A	794	ILE	N-CA-C	-6.29	103.19	110.05
1	C	208	THR	CA-C-N	-6.06	114.37	120.31
1	C	208	THR	C-N-CA	-6.06	114.37	120.31

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	7558	0	7394	129	0
1	B	7842	0	7665	205	0
1	C	7842	0	7665	137	0
2	D	4870	0	4633	116	0
2	E	4870	0	4633	116	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	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	24	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	1	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	24	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	2	0
3	b	28	0	25	2	0
4	A	154	0	142	0	0
4	B	154	0	142	6	0
4	C	126	0	117	0	0
4	D	98	0	89	12	0
4	E	98	0	89	12	0
All	All	34256	0	33142	637	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 9.

The worst 5 of 637 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)
4:B:1410:NAG:O4	4:B:1411:NAG:C1	1.63	1.43
4:D:905:NAG:O4	4:D:906:NAG:C1	1.65	1.43
4:E:905:NAG:O4	4:E:906:NAG:C1	1.65	1.42
1:A:230:PRO:HB3	1:C:521:PRO:CG	1.57	1.33
1:A:230:PRO:CB	1:C:521:PRO:HG2	1.59	1.32

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	941/1267 (74%)	868 (92%)	52 (6%)	21 (2%)	5	26
1	B	978/1267 (77%)	904 (92%)	61 (6%)	13 (1%)	9	35
1	C	978/1267 (77%)	899 (92%)	62 (6%)	17 (2%)	7	30
2	D	595/817 (73%)	553 (93%)	35 (6%)	7 (1%)	10	37
2	E	595/817 (73%)	553 (93%)	35 (6%)	7 (1%)	10	37
All	All	4087/5435 (75%)	3777 (92%)	245 (6%)	65 (2%)	10	31

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	46	SER
1	A	332	ILE
1	A	591	SER
1	A	855	PHE

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	848/1108 (76%)	836 (99%)	12 (1%)	59	73
1	B	878/1108 (79%)	870 (99%)	8 (1%)	70	78
1	C	878/1108 (79%)	871 (99%)	7 (1%)	73	79
2	D	527/721 (73%)	520 (99%)	7 (1%)	61	74
2	E	527/721 (73%)	520 (99%)	7 (1%)	61	74
All	All	3658/4766 (77%)	3617 (99%)	41 (1%)	63	76

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	35	GLU
2	E	35	GLU
2	D	223	ILE
2	D	499	ASP
2	E	344	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	992	GLN
2	D	241	HIS
2	E	586	ASN
2	E	508	ASN
2	D	49	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 ⓘ

46 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	F	1	3,1	14,14,15	0.52	0	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	G	1	3,1	14,14,15	0.30	0	17,19,21	0.63	0
3	NAG	G	2	3	14,14,15	0.54	0	17,19,21	0.49	0
3	NAG	H	1	3,1	14,14,15	0.36	0	17,19,21	0.74	0
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	1.39	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.71	0
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	1.49	3 (17%)
3	NAG	J	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.68	0
3	NAG	J	2	3	14,14,15	0.27	0	17,19,21	0.68	0
3	NAG	K	1	3,1	14,14,15	0.24	0	17,19,21	0.70	1 (5%)
3	NAG	K	2	3	14,14,15	0.17	0	17,19,21	0.49	0
3	NAG	L	1	3,1	14,14,15	0.51	0	17,19,21	0.52	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	M	1	3,1	14,14,15	0.57	0	17,19,21	0.59	0
3	NAG	M	2	3	14,14,15	0.29	0	17,19,21	0.46	0
3	NAG	N	1	3,1	14,14,15	0.29	0	17,19,21	0.41	0
3	NAG	N	2	3	14,14,15	0.38	0	17,19,21	0.38	0
3	NAG	O	1	3,1	14,14,15	0.35	0	17,19,21	1.17	1 (5%)
3	NAG	O	2	3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	P	1	3,1	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
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	0.71	1 (7%)	17,19,21	0.92	1 (5%)
3	NAG	Q	2	3	14,14,15	0.37	0	17,19,21	0.74	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	R	2	3	14,14,15	0.29	0	17,19,21	0.39	0
3	NAG	S	1	3,1	14,14,15	0.50	0	17,19,21	0.52	0
3	NAG	S	2	3	14,14,15	0.24	0	17,19,21	0.60	0
3	NAG	T	1	3,1	14,14,15	0.57	0	17,19,21	0.58	0
3	NAG	T	2	3	14,14,15	0.29	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	U	1	3,1	14,14,15	0.23	0	17,19,21	1.45	2 (11%)
3	NAG	U	2	3	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	V	1	3,1	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
3	NAG	V	2	3	14,14,15	0.40	0	17,19,21	0.49	0
3	NAG	W	1	3,1	14,14,15	0.41	0	17,19,21	0.41	0
3	NAG	W	2	3	14,14,15	0.21	0	17,19,21	0.77	0
3	NAG	X	1	3,1	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	X	2	3	14,14,15	0.61	1 (7%)	17,19,21	1.38	2 (11%)
3	NAG	Y	1	3,1	14,14,15	0.62	1 (7%)	17,19,21	0.43	0
3	NAG	Y	2	3	14,14,15	0.34	0	17,19,21	1.43	2 (11%)
3	NAG	Z	1	3,1	14,14,15	0.38	0	17,19,21	0.47	0
3	NAG	Z	2	3	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	a	1	2,3	14,14,15	0.57	0	17,19,21	0.74	0
3	NAG	a	2	3	14,14,15	0.55	0	17,19,21	0.39	0
3	NAG	b	1	2,3	14,14,15	0.59	1 (7%)	17,19,21	0.74	0
3	NAG	b	2	3	14,14,15	0.54	0	17,19,21	0.39	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	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	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	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	-	3/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	O5-C1	-2.58	1.39	1.43
3	J	1	NAG	O5-C1	-2.44	1.39	1.43
3	I	1	NAG	O5-C1	-2.18	1.40	1.43
3	X	2	NAG	C1-C2	2.07	1.55	1.52
3	b	1	NAG	O5-C1	-2.07	1.40	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1	NAG	C2-N2-C7	5.01	129.62	122.90
3	I	2	NAG	C2-N2-C7	4.73	129.24	122.90
3	Y	2	NAG	C2-N2-C7	4.59	129.06	122.90
3	X	2	NAG	C2-N2-C7	4.58	129.04	122.90
3	H	2	NAG	C2-N2-C7	4.52	128.96	122.90

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

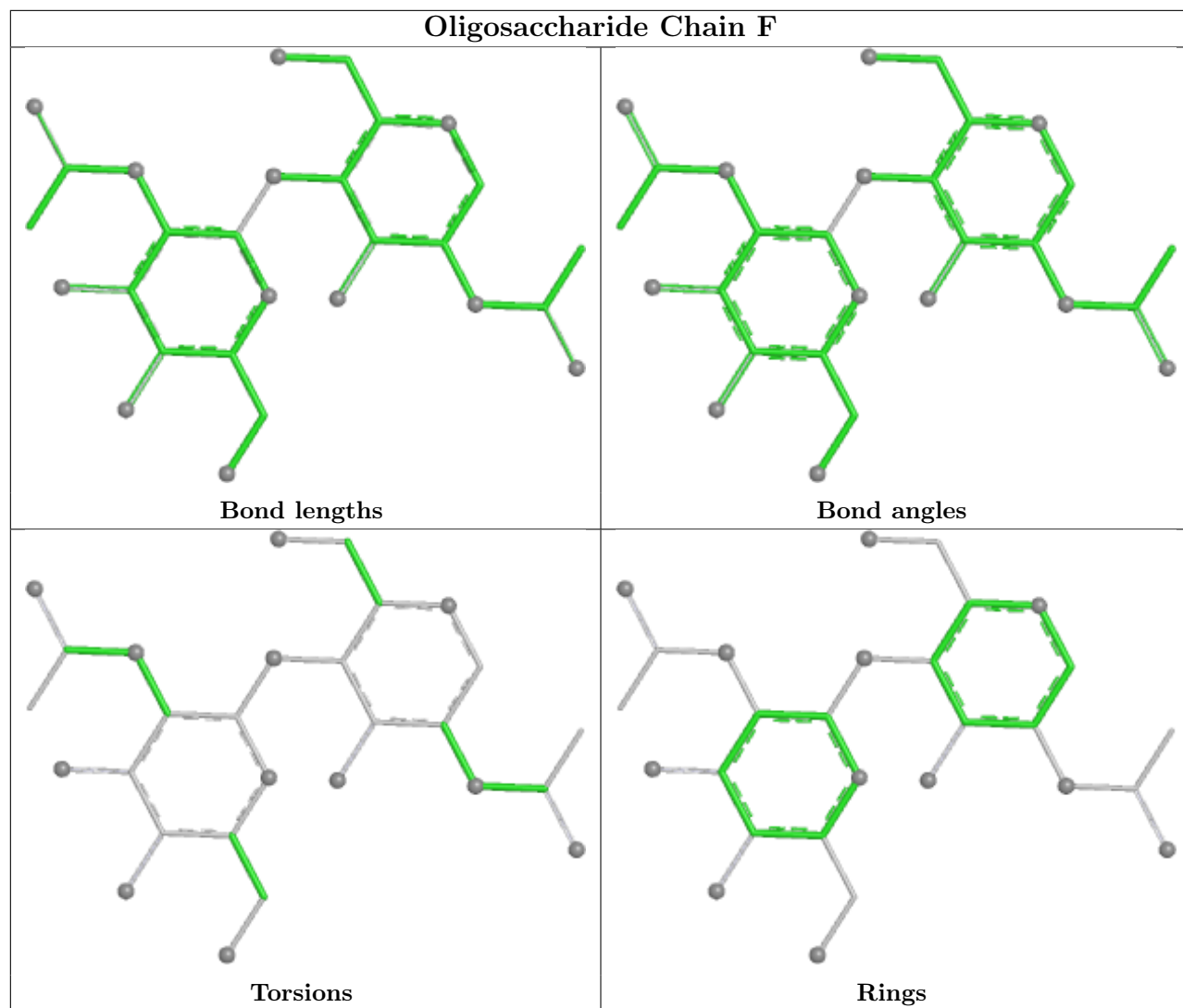
Mol	Chain	Res	Type	Atoms
3	a	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6

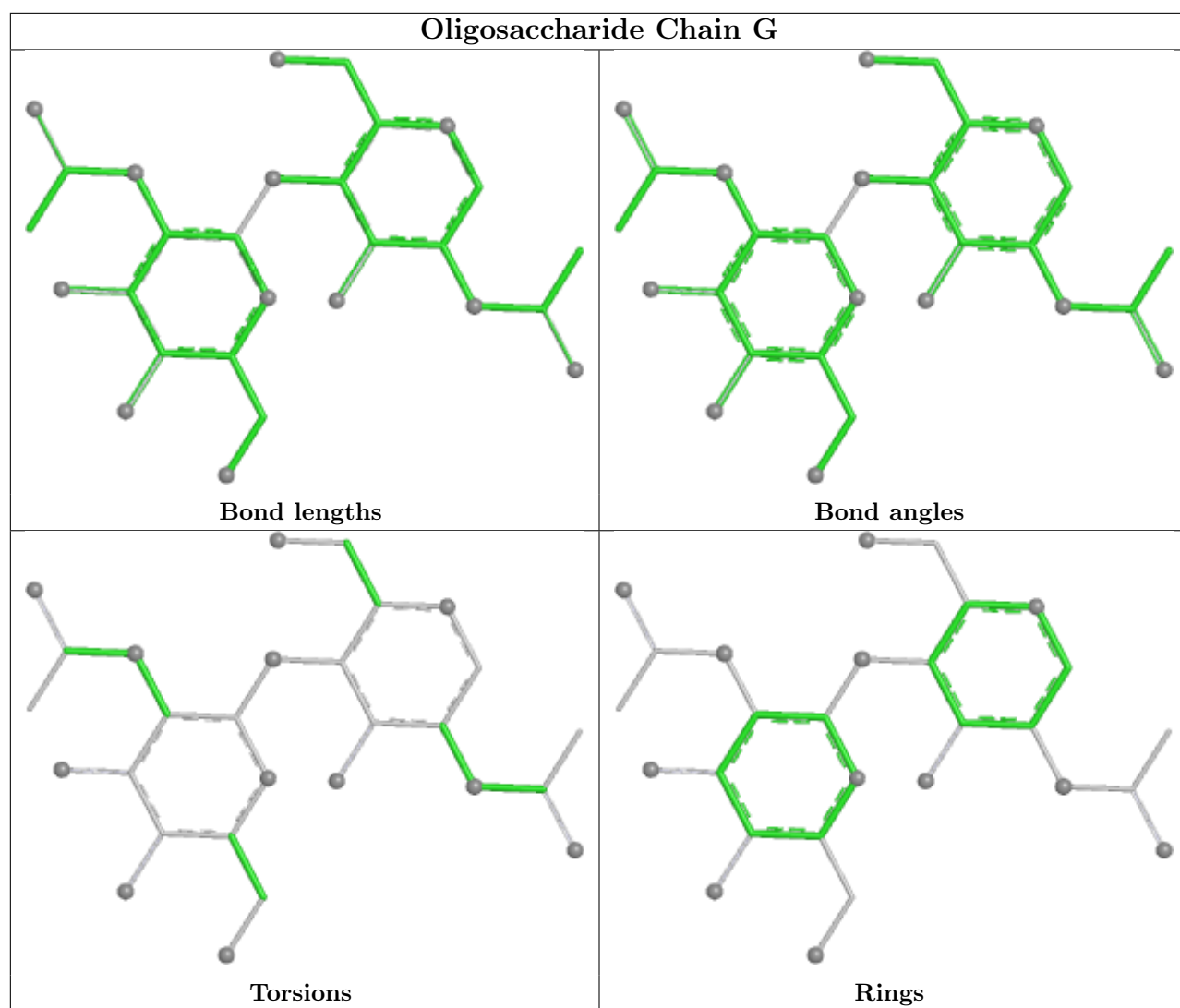
There are no ring outliers.

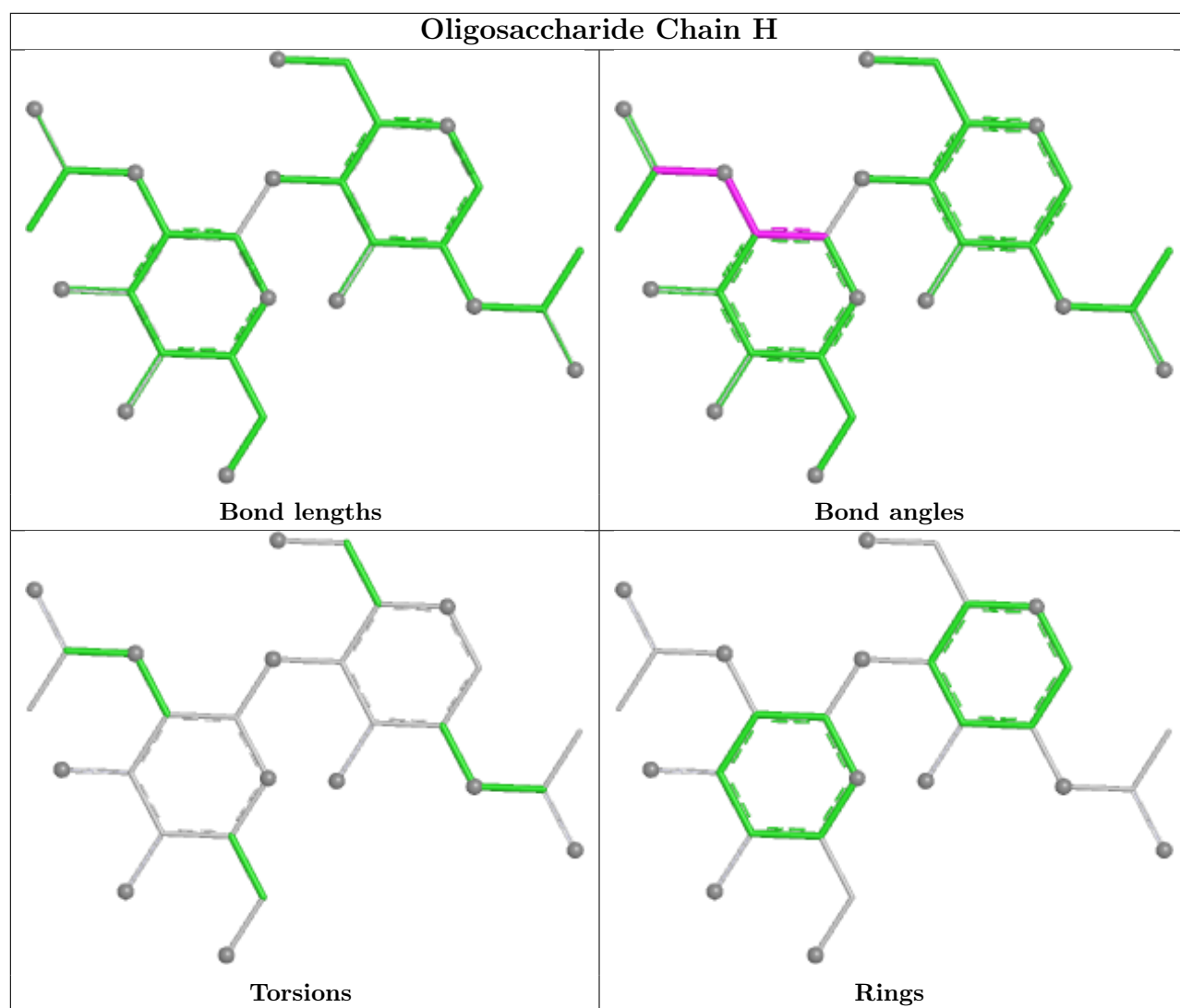
4 monomers are involved in 5 short contacts:

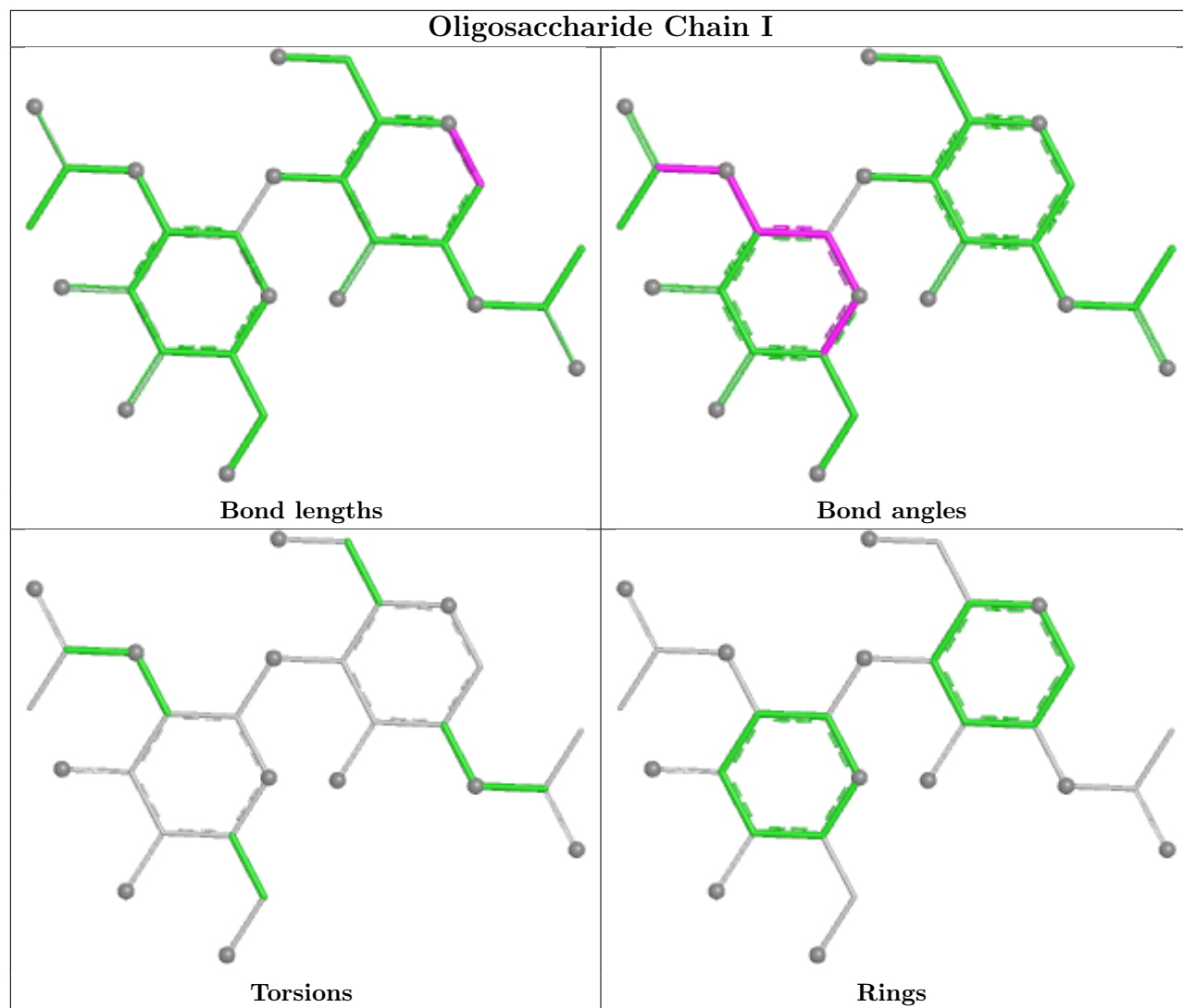
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	a	1	NAG	2	0
3	b	1	NAG	2	0
3	Q	1	NAG	1	0
3	Q	2	NAG	1	0

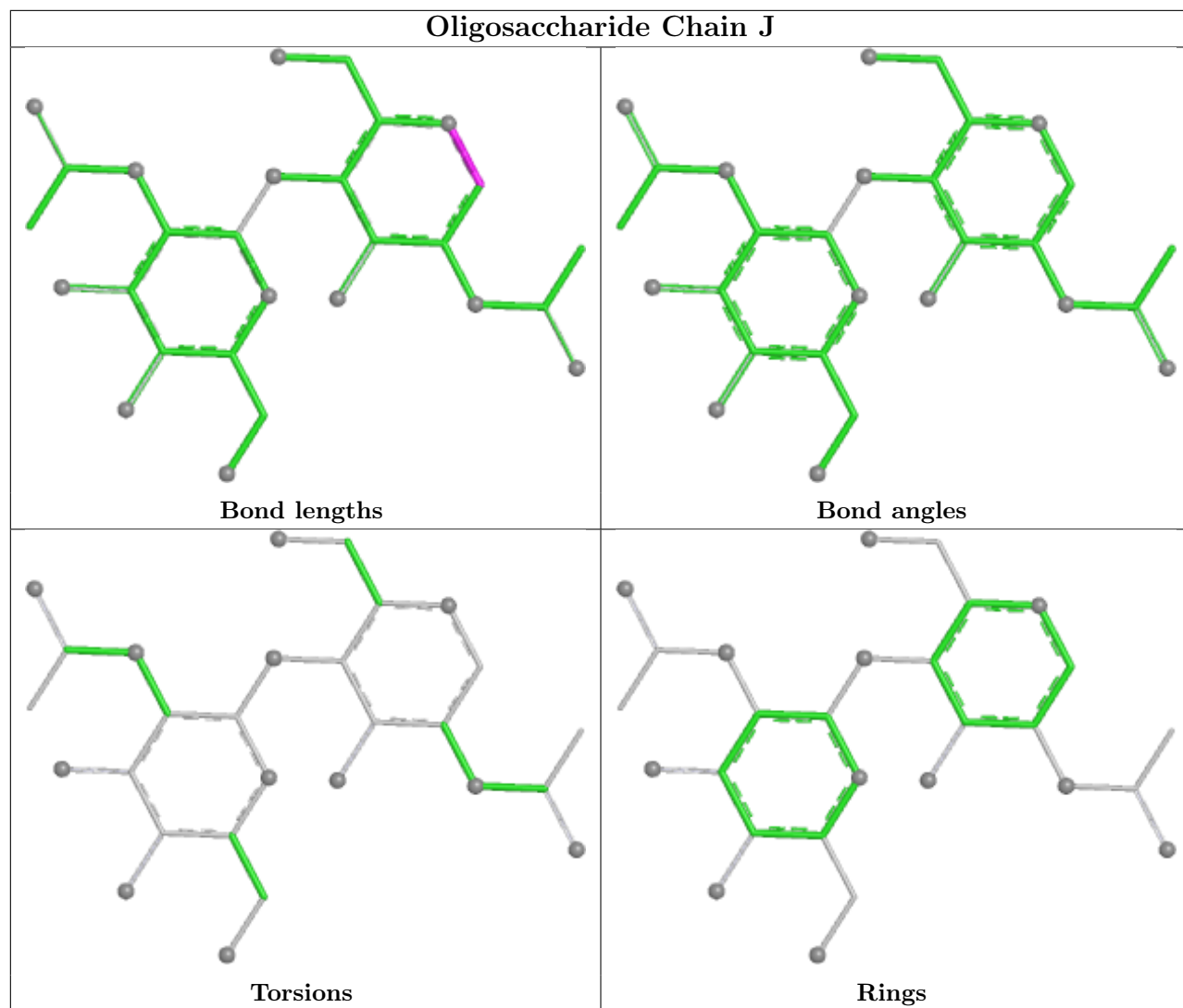
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

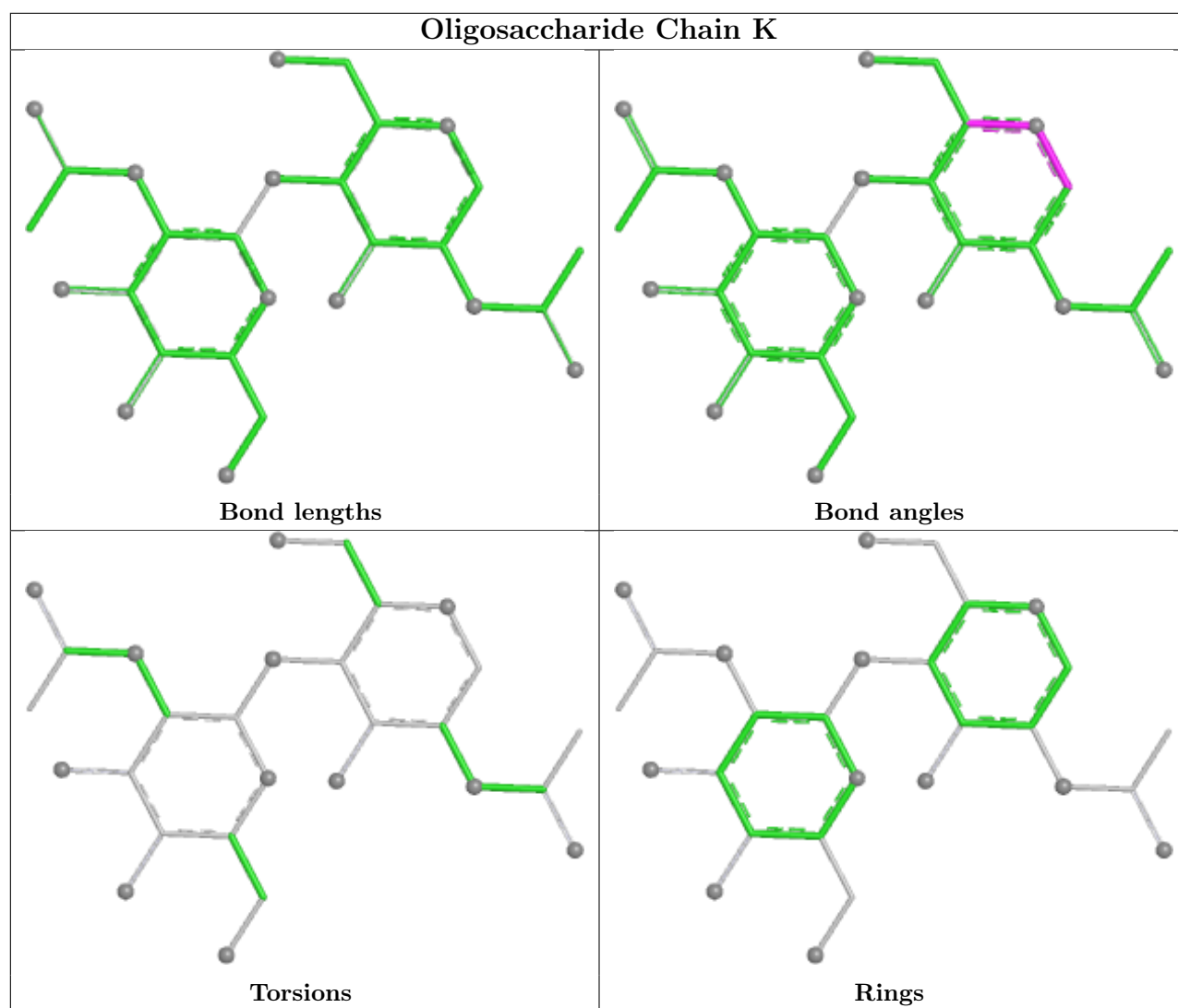


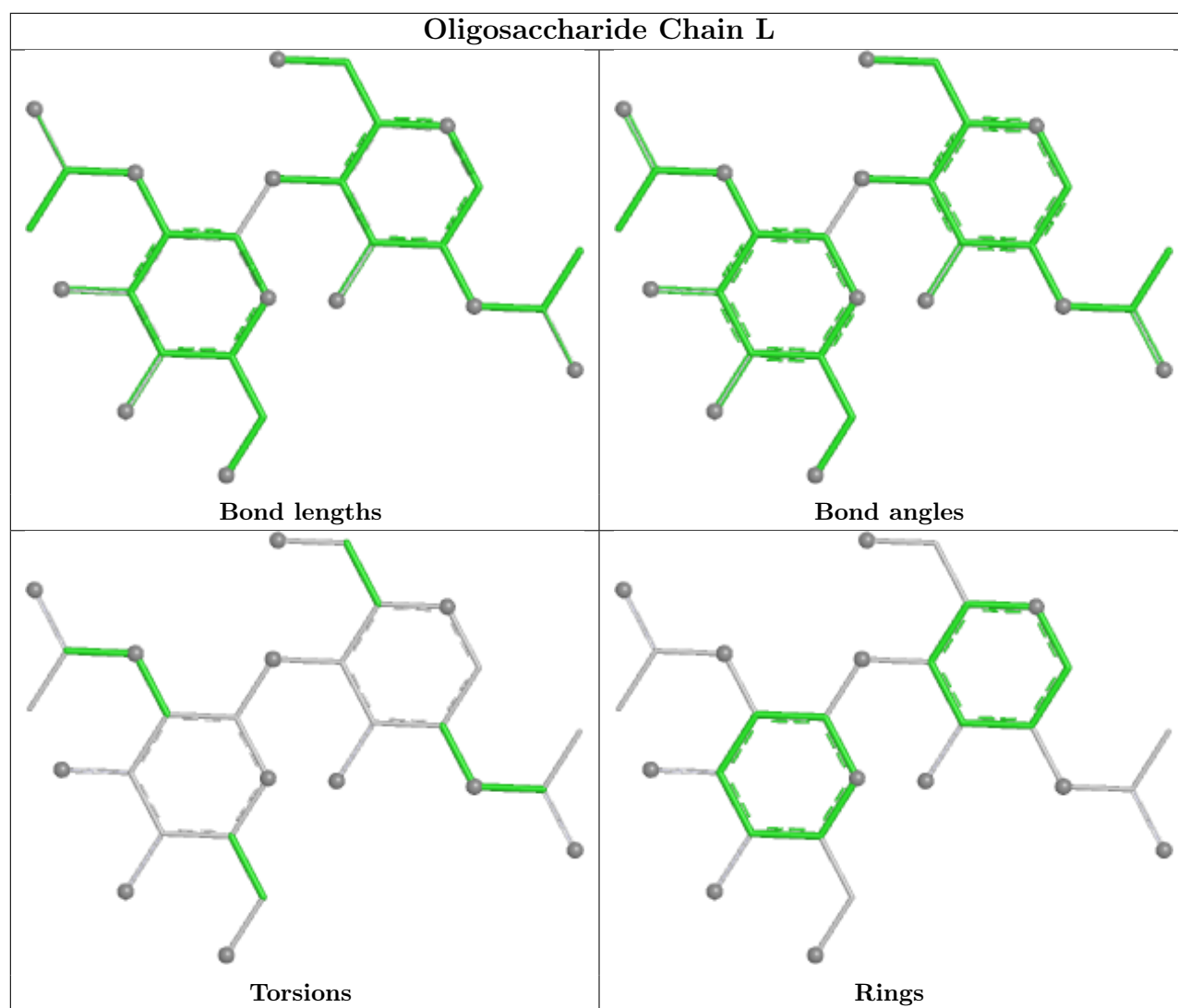


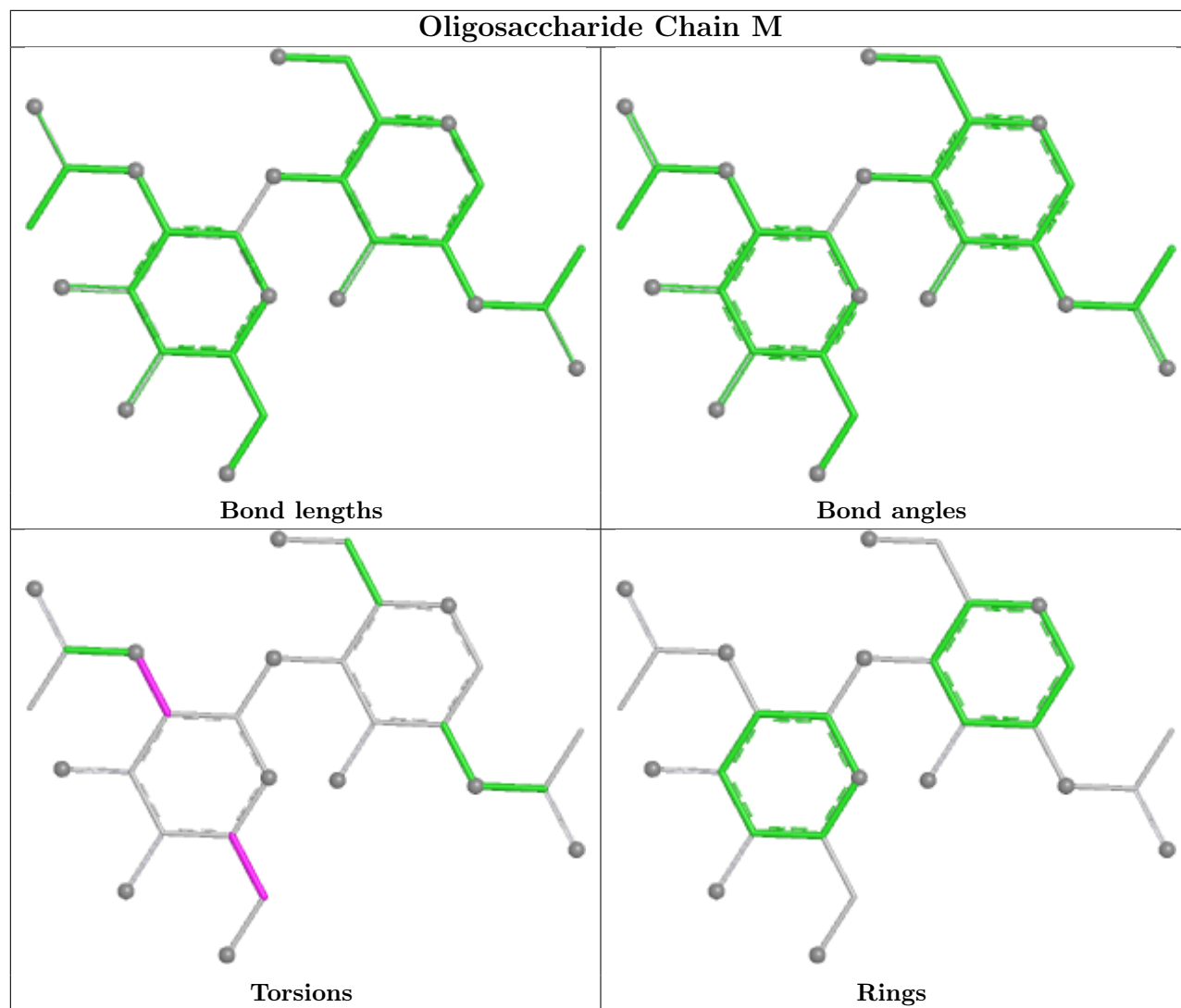


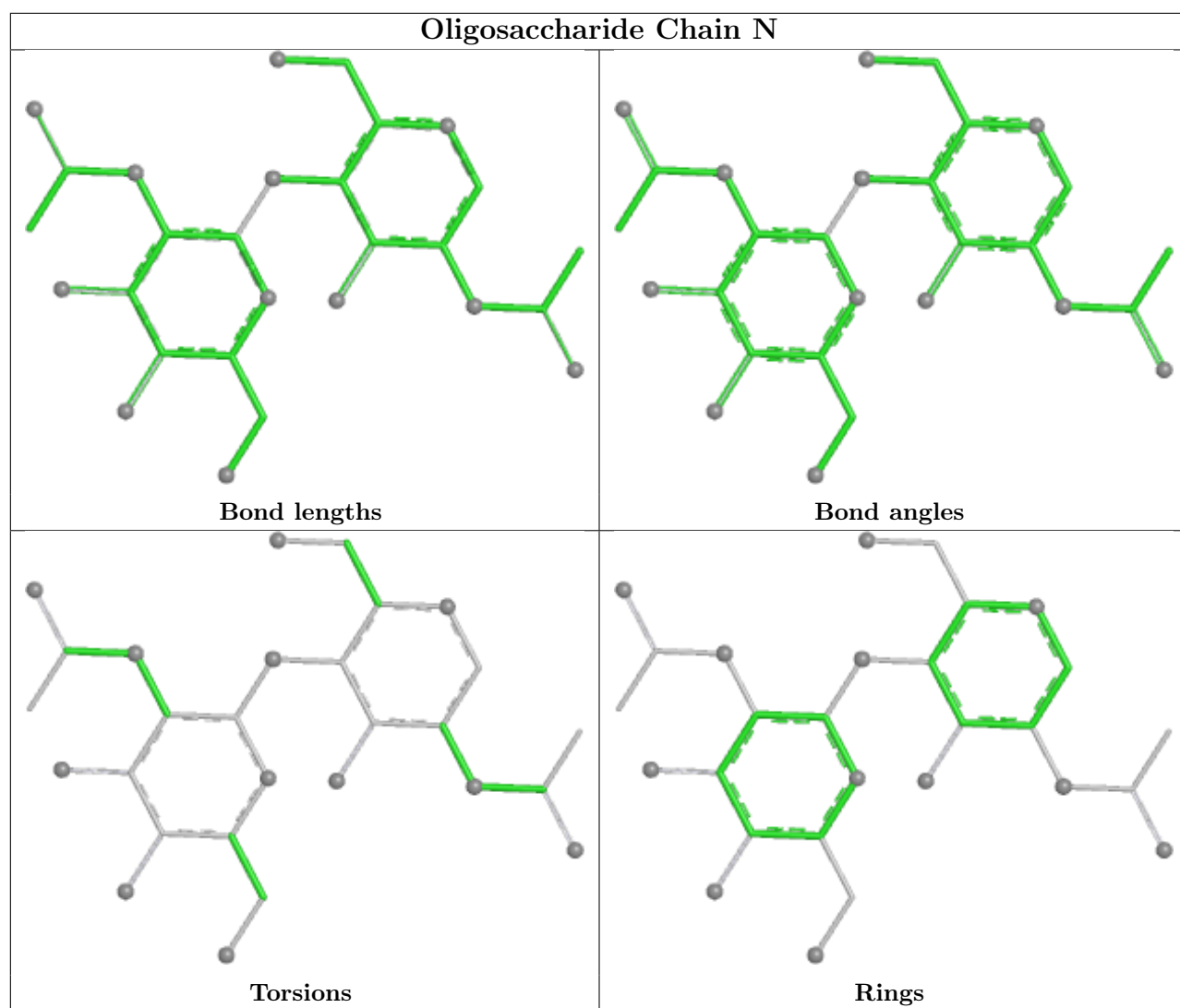


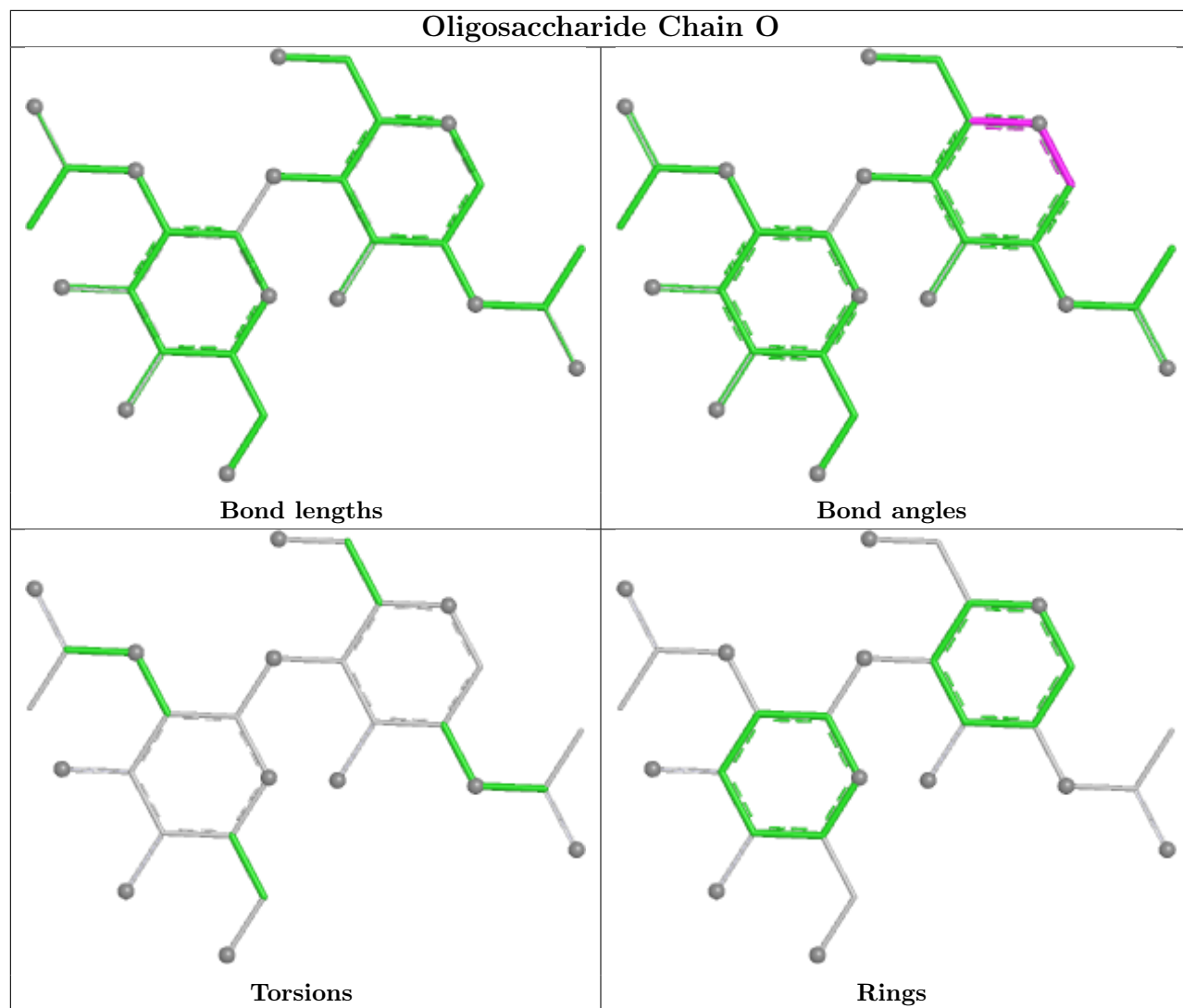


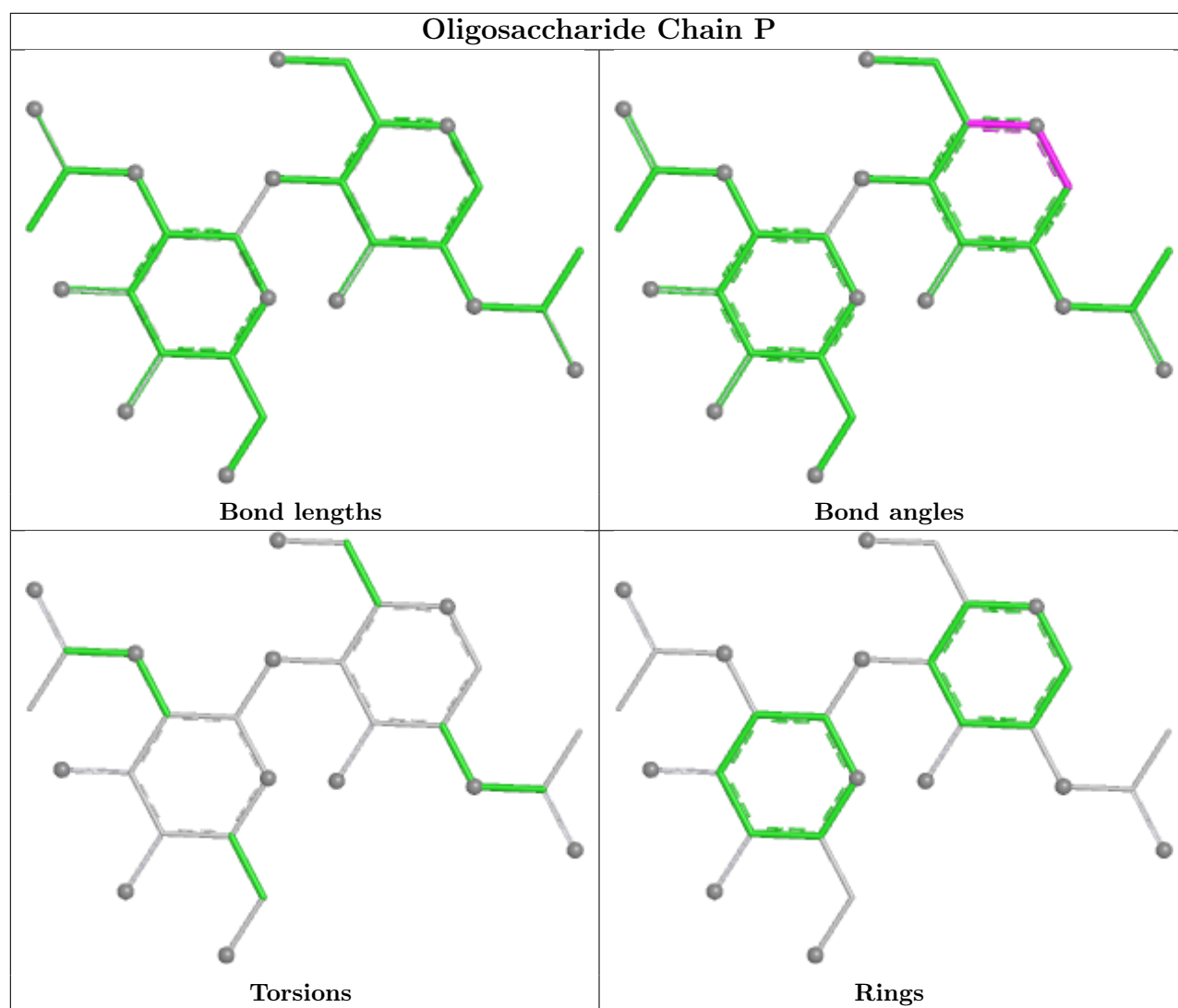


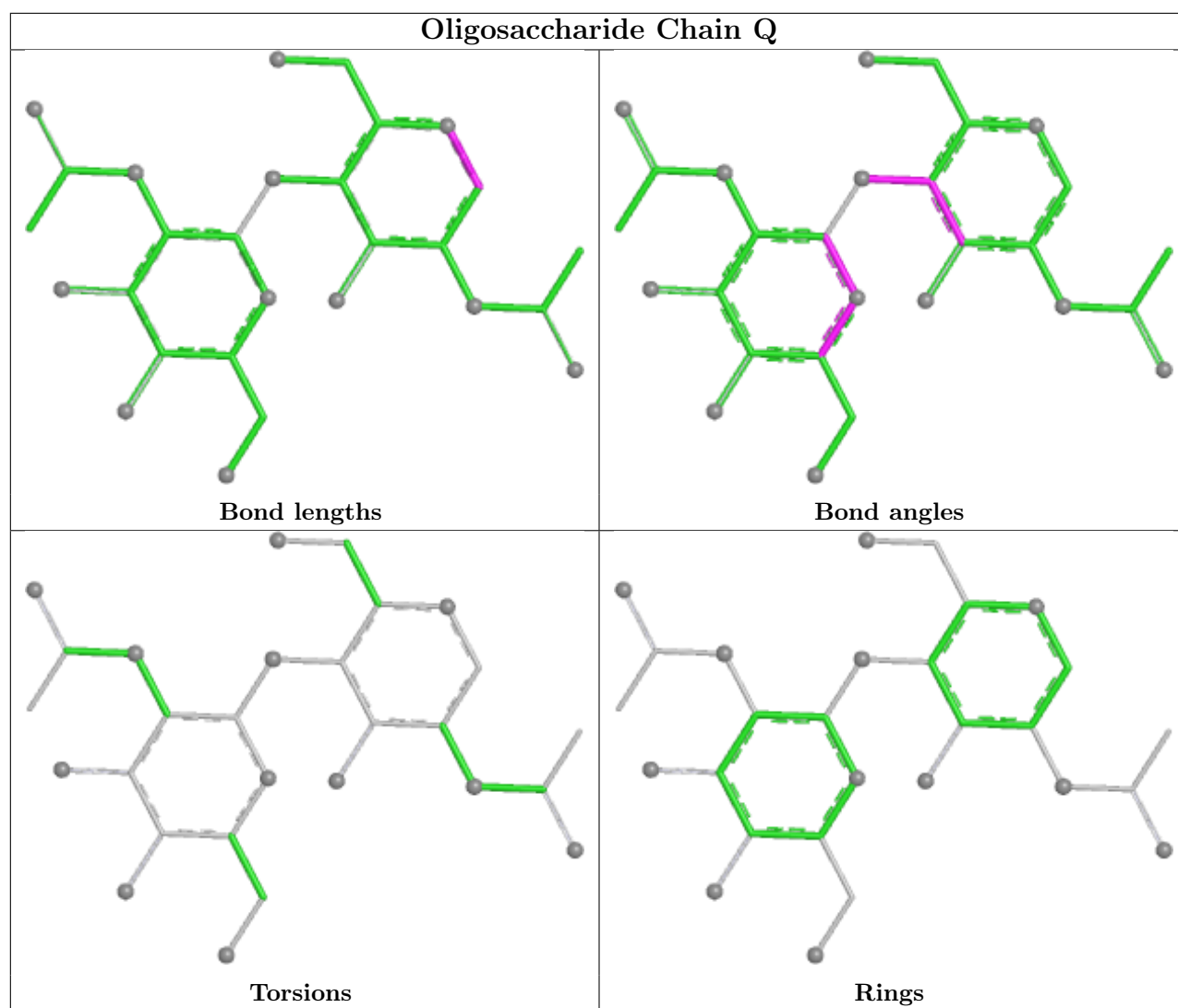


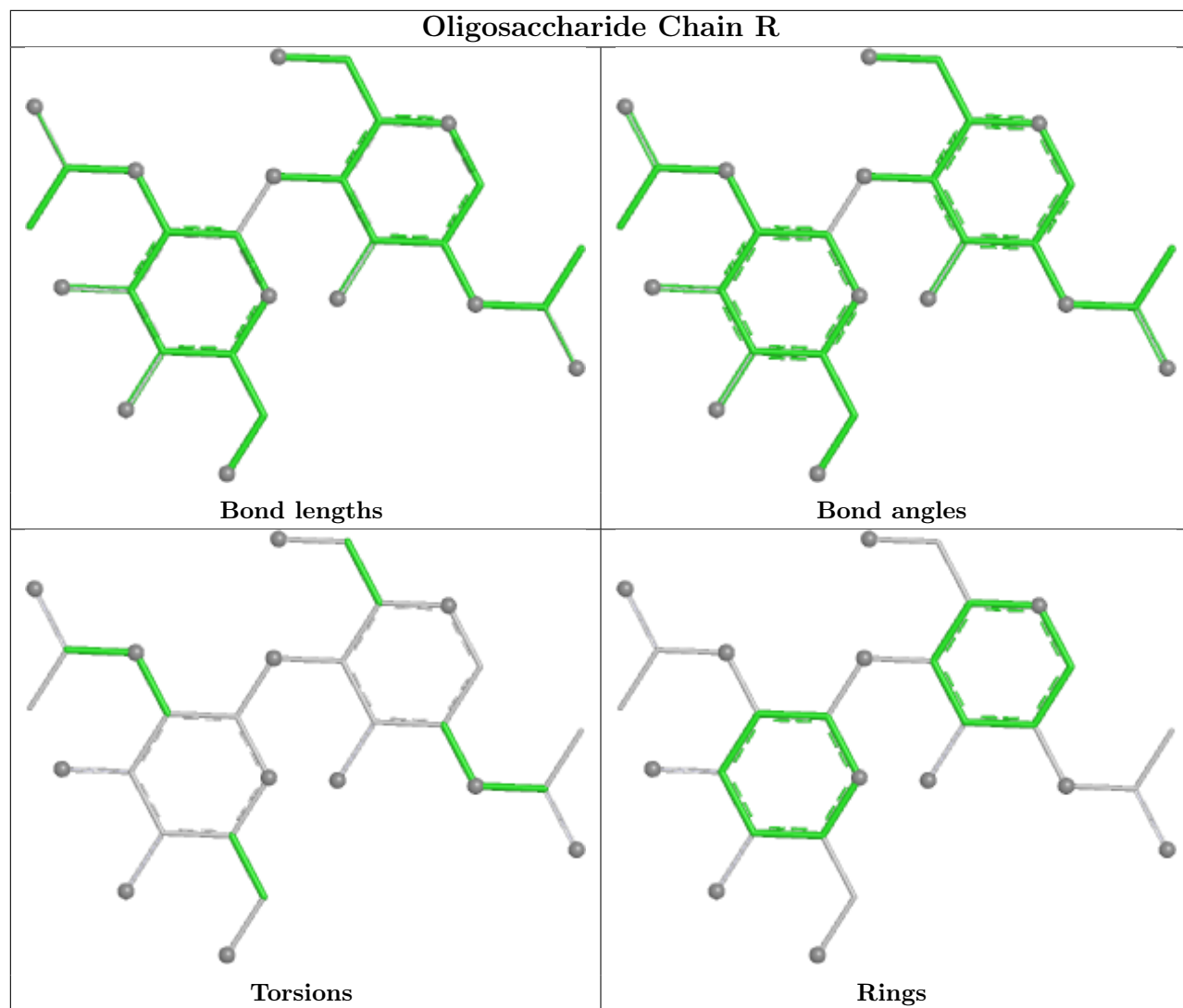


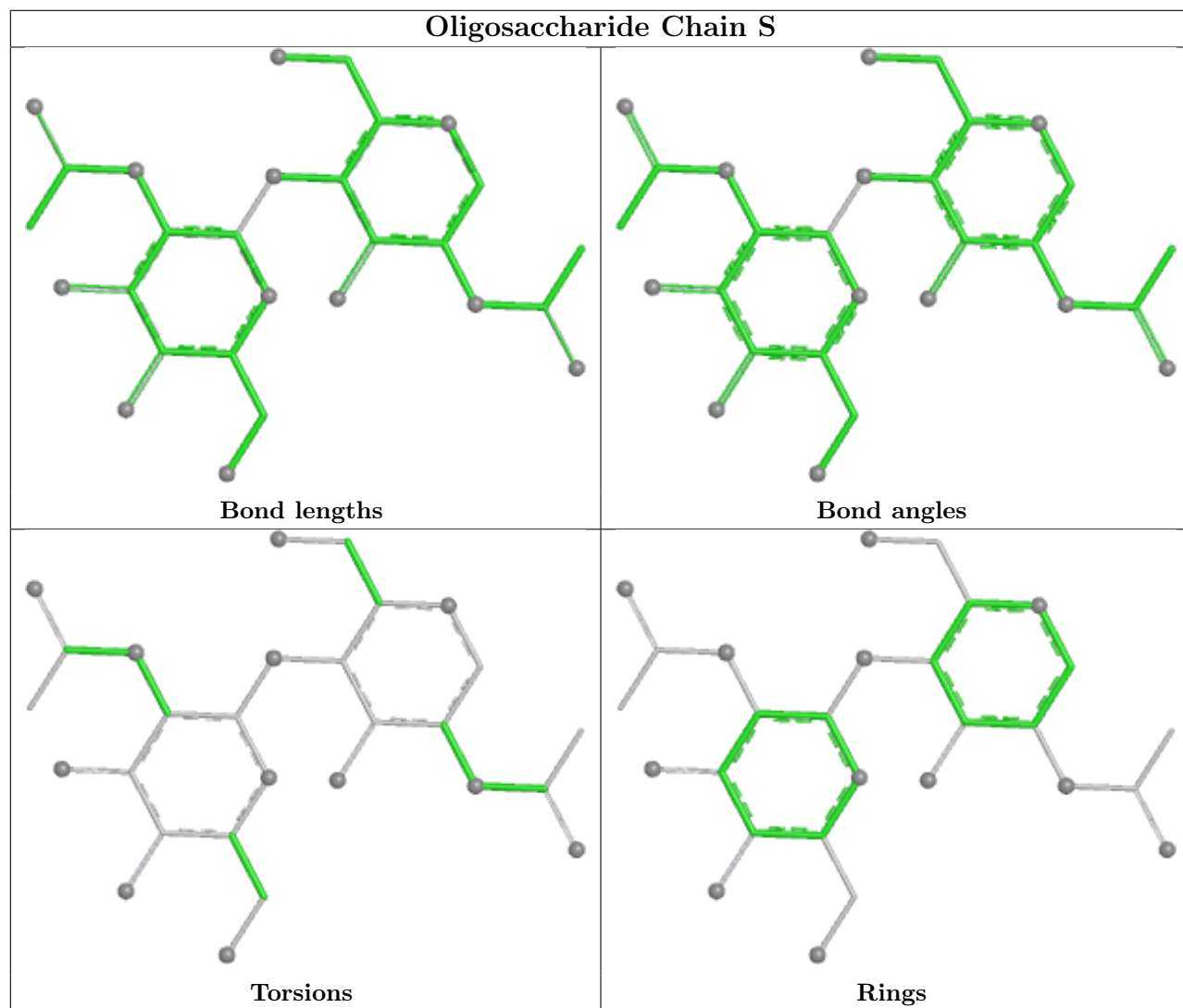


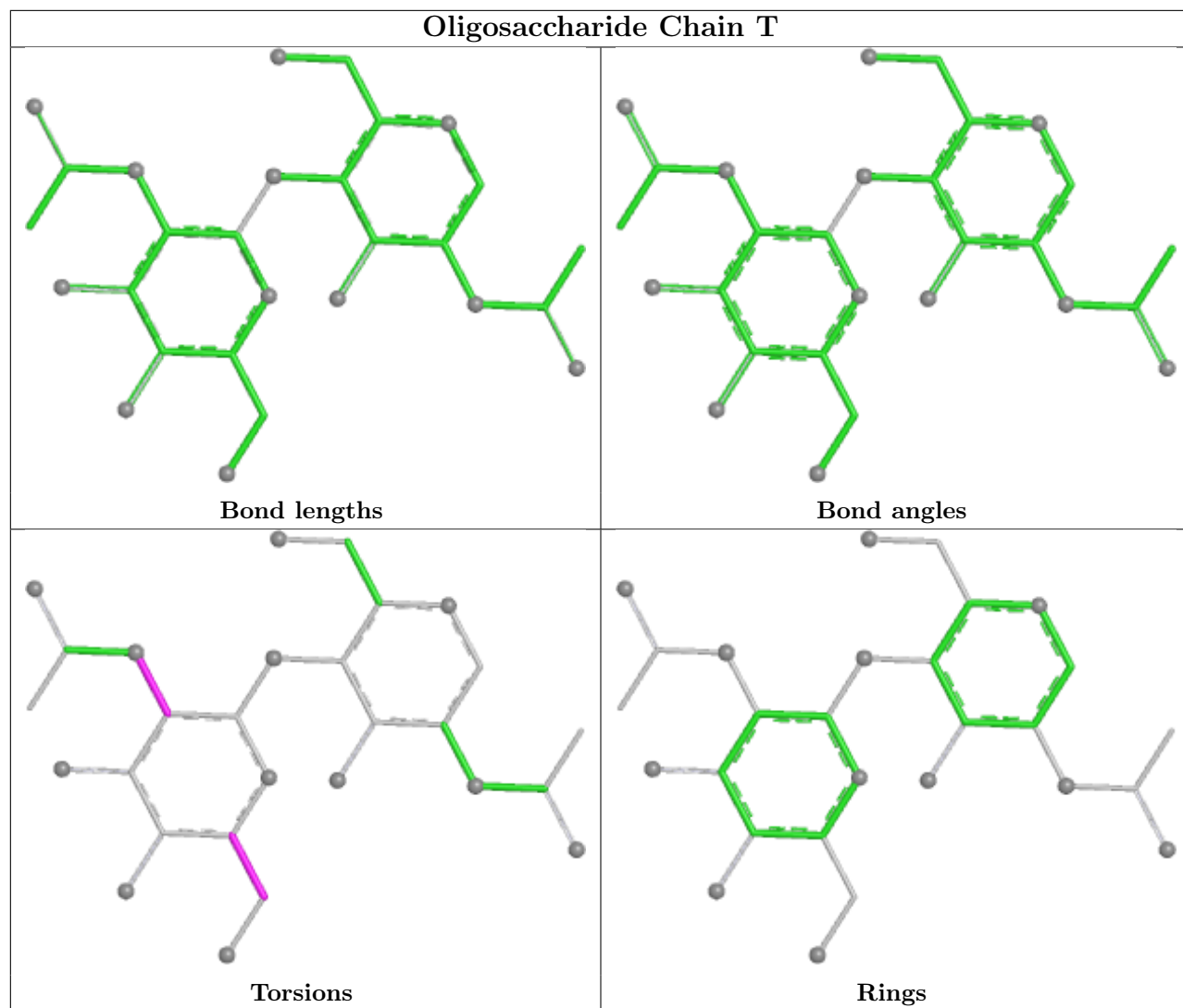


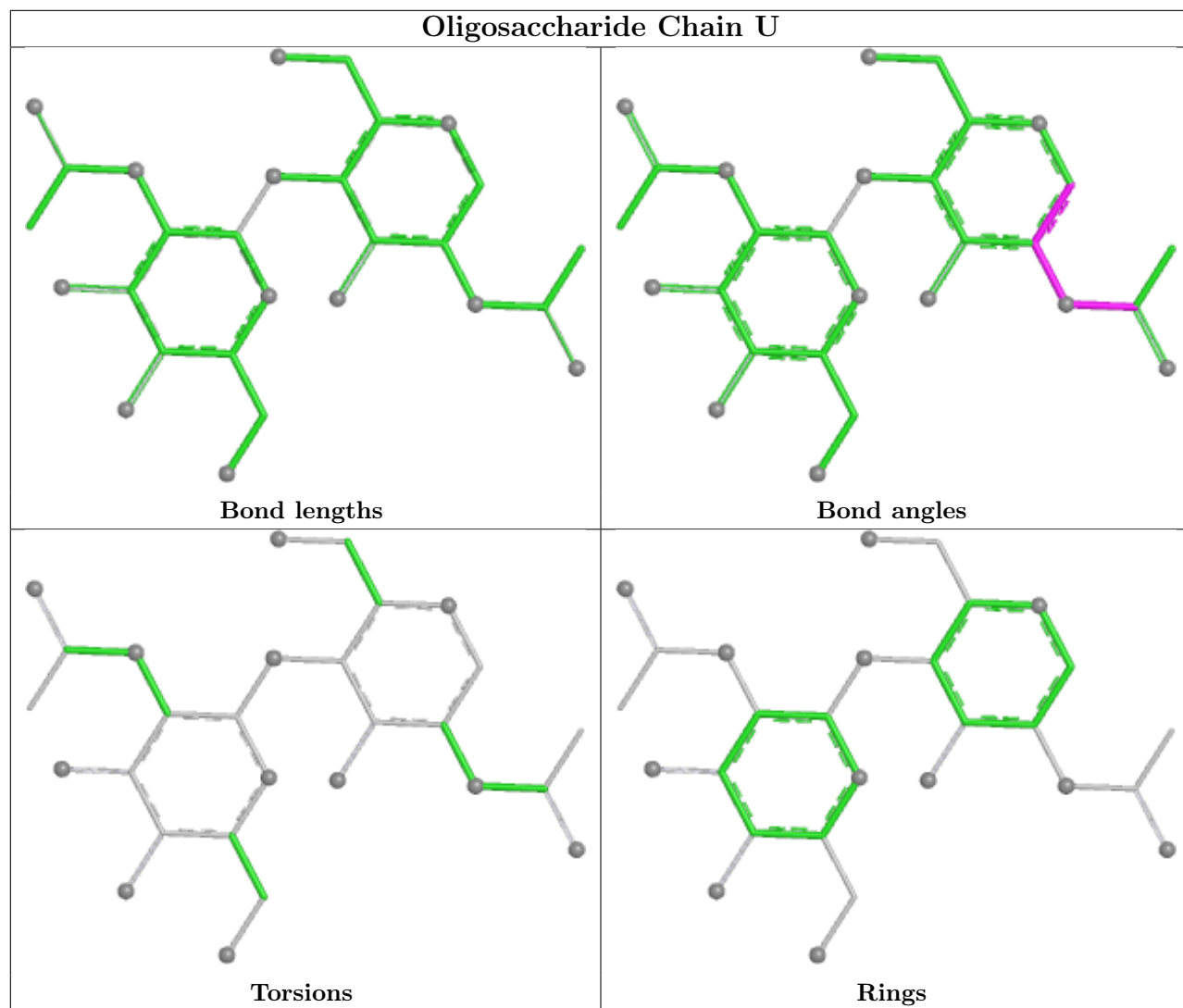


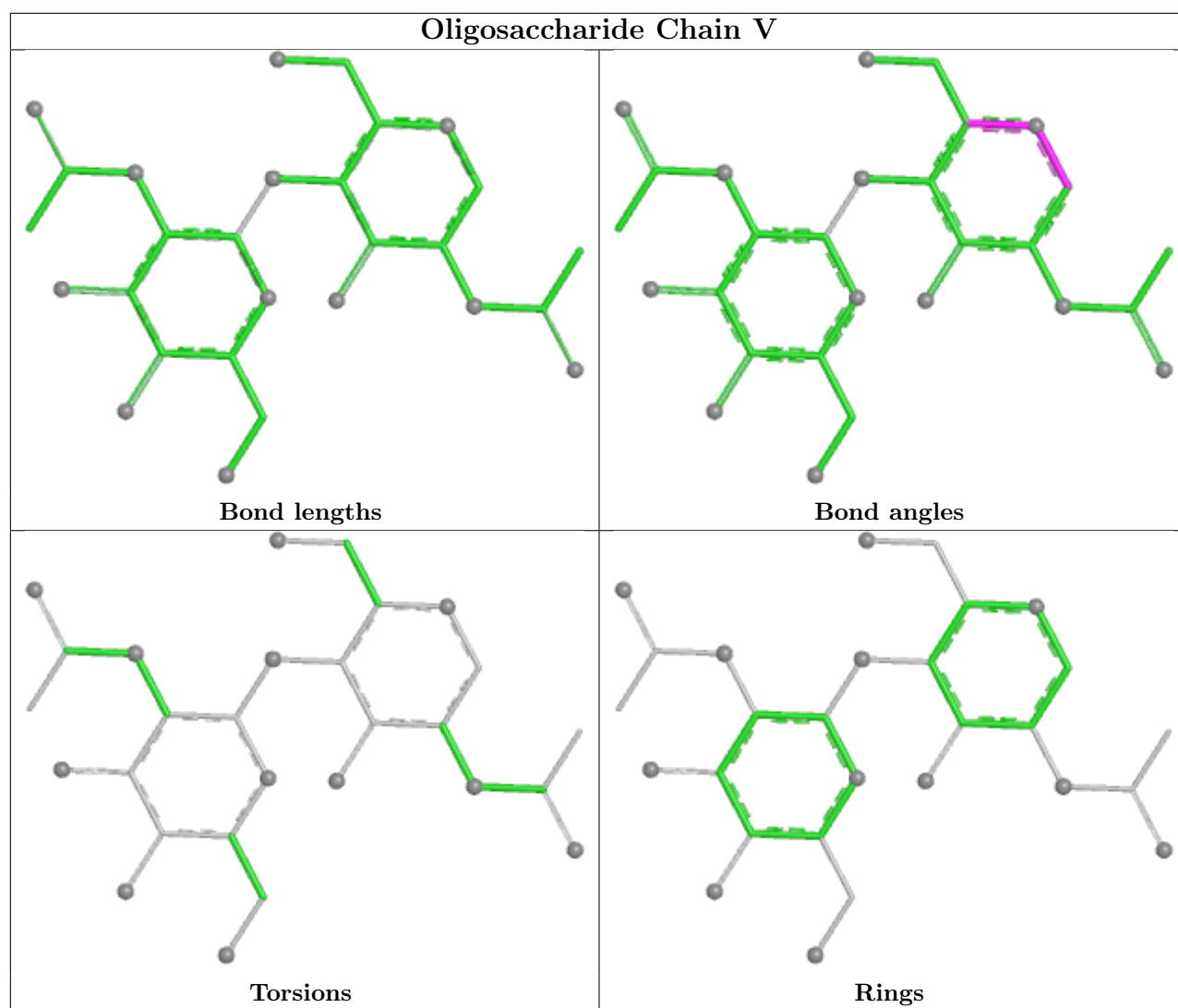


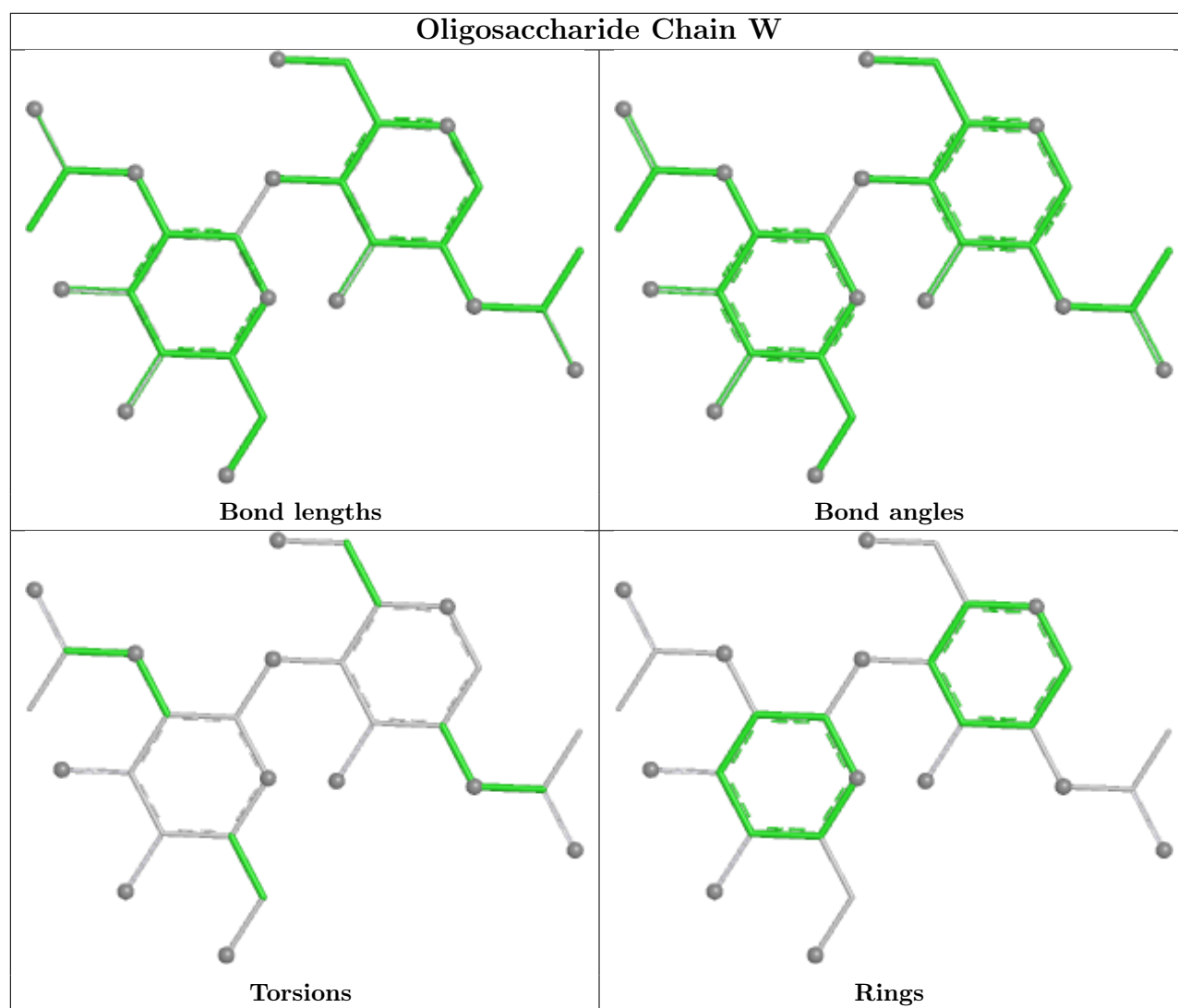


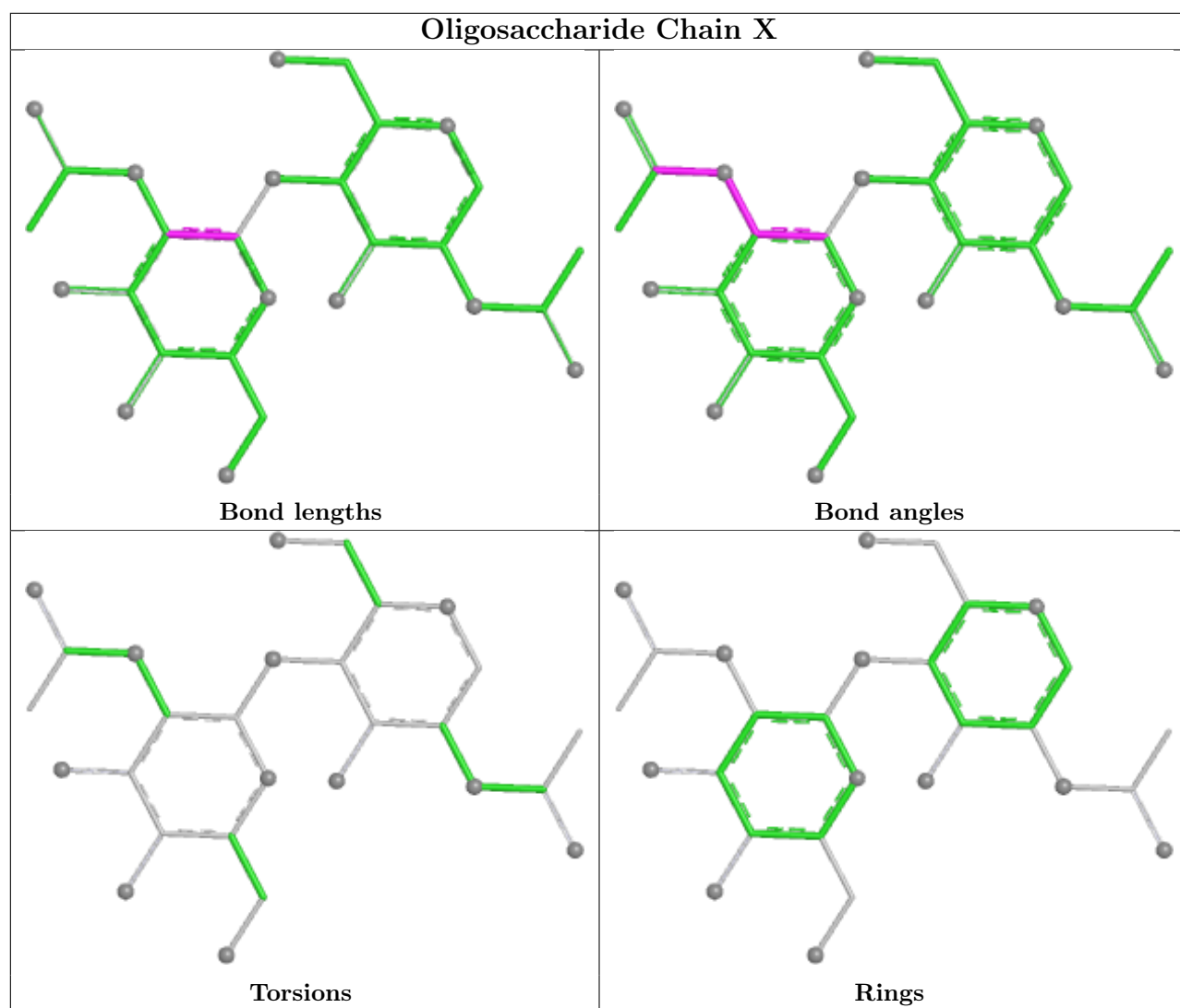


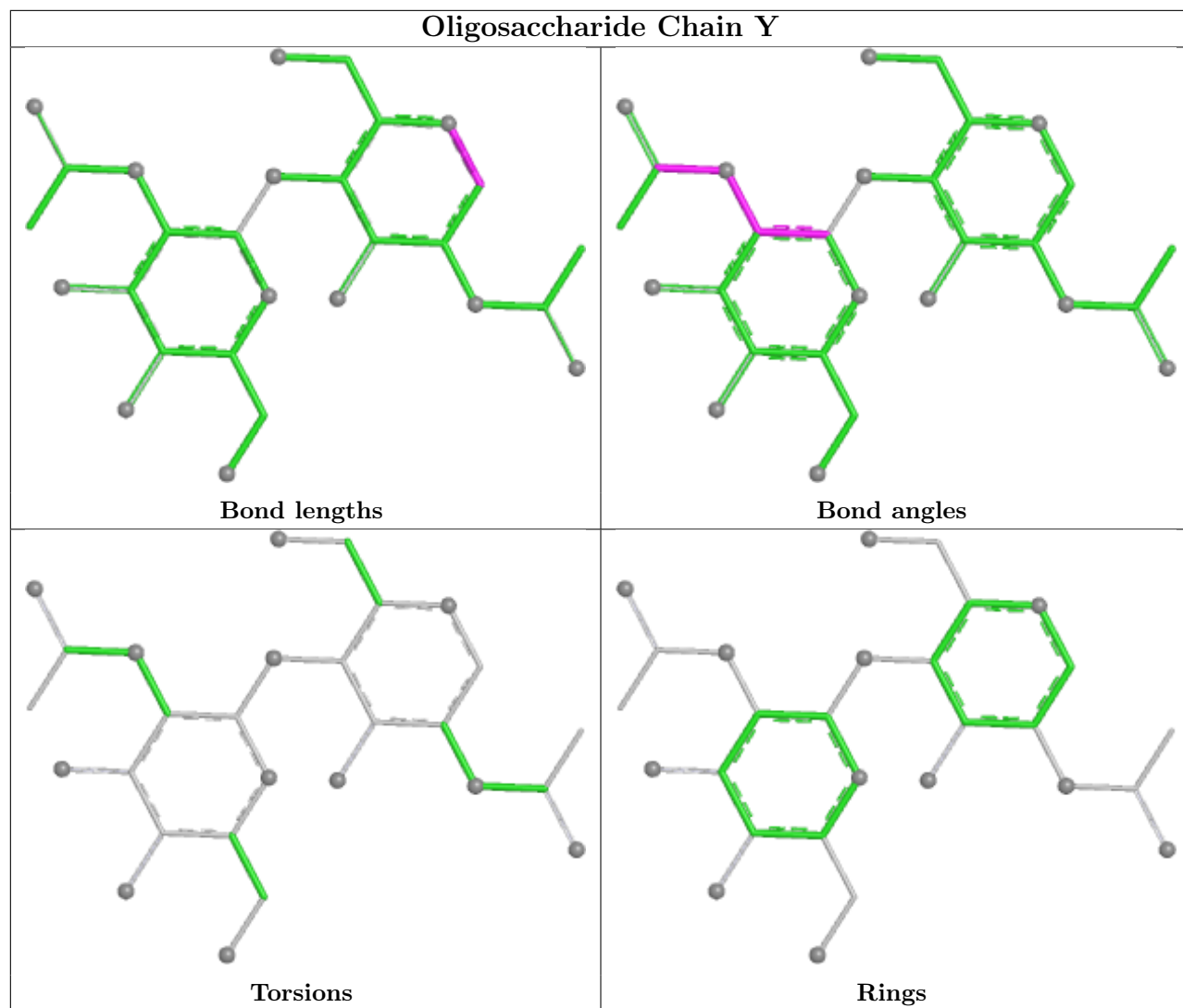


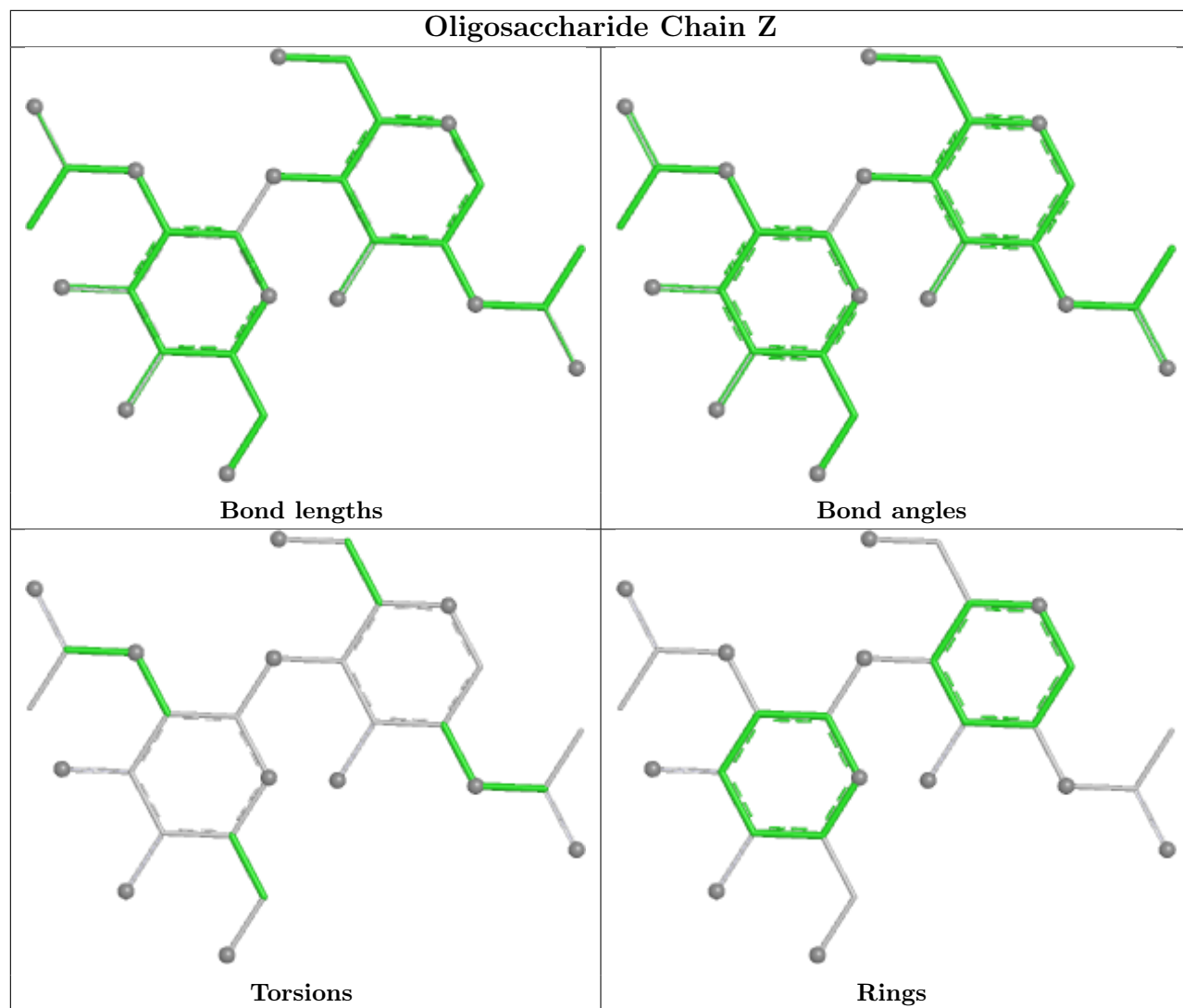


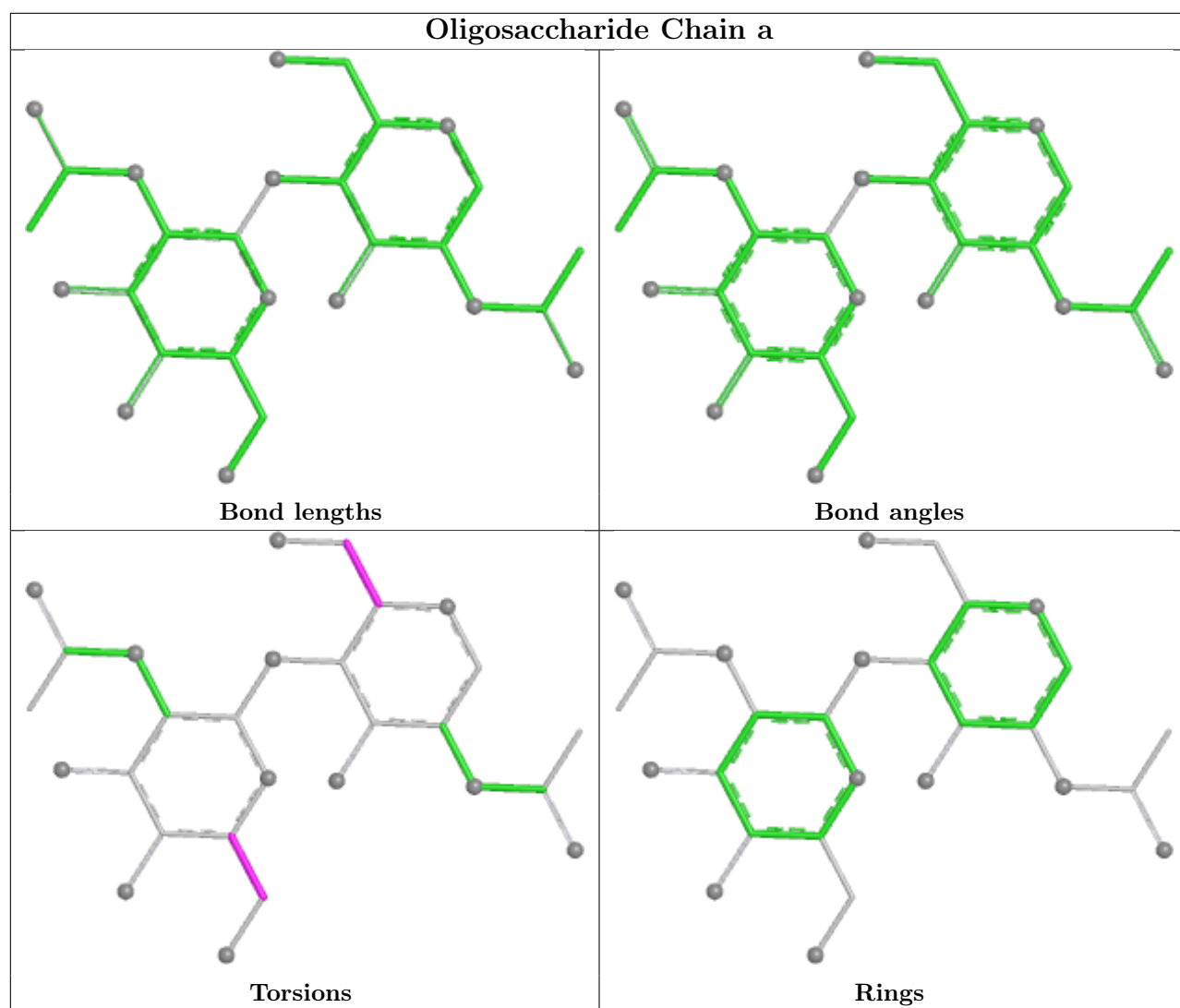


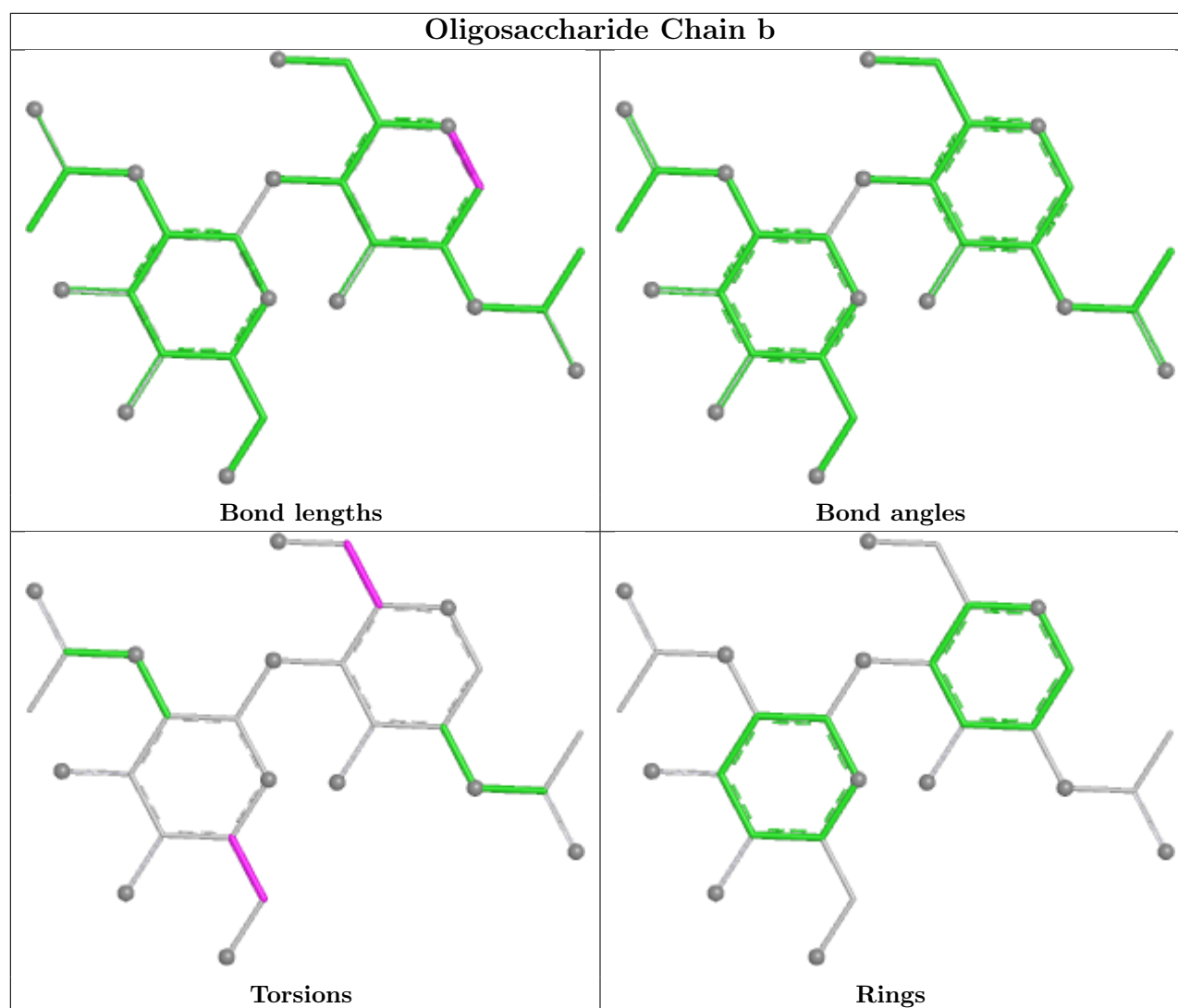












5.6 Ligand geometry [i](#)

45 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	E	905	-	14,14,15	0.34	0	17,19,21	0.50	0
4	NAG	A	1405	1	14,14,15	0.61	0	17,19,21	1.34	2 (11%)
4	NAG	B	1401	1	14,14,15	0.33	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1408	1	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	B	1407	1	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	E	902	-	14,14,15	0.27	0	17,19,21	0.58	0
4	NAG	A	1411	1	14,14,15	0.49	0	17,19,21	0.37	0
4	NAG	A	1409	1	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	E	903	2	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
4	NAG	C	1401	1	14,14,15	0.29	0	17,19,21	0.35	0
4	NAG	D	901	2	14,14,15	0.40	0	17,19,21	0.67	0
4	NAG	A	1404	1	14,14,15	0.50	0	17,19,21	0.55	0
4	NAG	E	906	-	14,14,15	0.23	0	17,19,21	0.64	0
4	NAG	B	1411	-	14,14,15	0.37	0	17,19,21	0.43	0
4	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	D	905	-	14,14,15	0.35	0	17,19,21	0.49	0
4	NAG	B	1404	1	14,14,15	0.49	0	17,19,21	0.55	0
4	NAG	B	1405	1	14,14,15	0.62	0	17,19,21	1.35	2 (11%)
4	NAG	C	1405	1	14,14,15	0.64	0	17,19,21	1.35	2 (11%)
4	NAG	E	904	2	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	C	1409	1	14,14,15	0.32	0	17,19,21	0.41	0
4	NAG	B	1409	1	14,14,15	0.32	0	17,19,21	0.41	0
4	NAG	A	1401	1	14,14,15	0.31	0	17,19,21	0.35	0
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	D	902	-	14,14,15	0.28	0	17,19,21	0.58	0
4	NAG	B	1410	1	14,14,15	0.42	0	17,19,21	1.13	2 (11%)
4	NAG	D	907	-	14,14,15	0.34	0	17,19,21	0.62	1 (5%)
4	NAG	C	1406	-	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	B	1406	-	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	D	906	-	14,14,15	0.23	0	17,19,21	0.63	0
4	NAG	A	1408	1	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	B	1403	1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.65	0
4	NAG	A	1407	-	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	C	1403	1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	A	1410	1	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	D	904	2	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	C	1407	1	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	E	907	-	14,14,15	0.34	0	17,19,21	0.61	1 (5%)
4	NAG	A	1406	1	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	B	1402	1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	E	901	2	14,14,15	0.39	0	17,19,21	0.67	0
4	NAG	C	1404	1	14,14,15	0.51	0	17,19,21	0.54	0
4	NAG	D	903	2	14,14,15	0.42	0	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1408	1	14,14,15	0.23	0	17,19,21	0.51	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	E	905	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	E	902	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1411	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	E	903	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	E	906	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1411	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
4	NAG	D	905	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	E	904	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	D	902	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	D	907	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1406	-	-	0/6/23/26	0/1/1/1
4	NAG	D	906	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	D	904	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	E	907	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	D	903	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1405	NAG	C2-N2-C7	4.67	129.16	122.90
4	C	1405	NAG	C2-N2-C7	4.65	129.14	122.90
4	A	1405	NAG	C2-N2-C7	4.62	129.09	122.90
4	C	1406	NAG	C8-C7-N2	2.40	120.09	116.12
4	B	1406	NAG	C8-C7-N2	2.39	120.08	116.12

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	902	NAG	O7-C7-N2-C2
4	E	902	NAG	O7-C7-N2-C2
4	D	902	NAG	C8-C7-N2-C2
4	E	902	NAG	C8-C7-N2-C2
4	D	907	NAG	O5-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 30 short contacts:

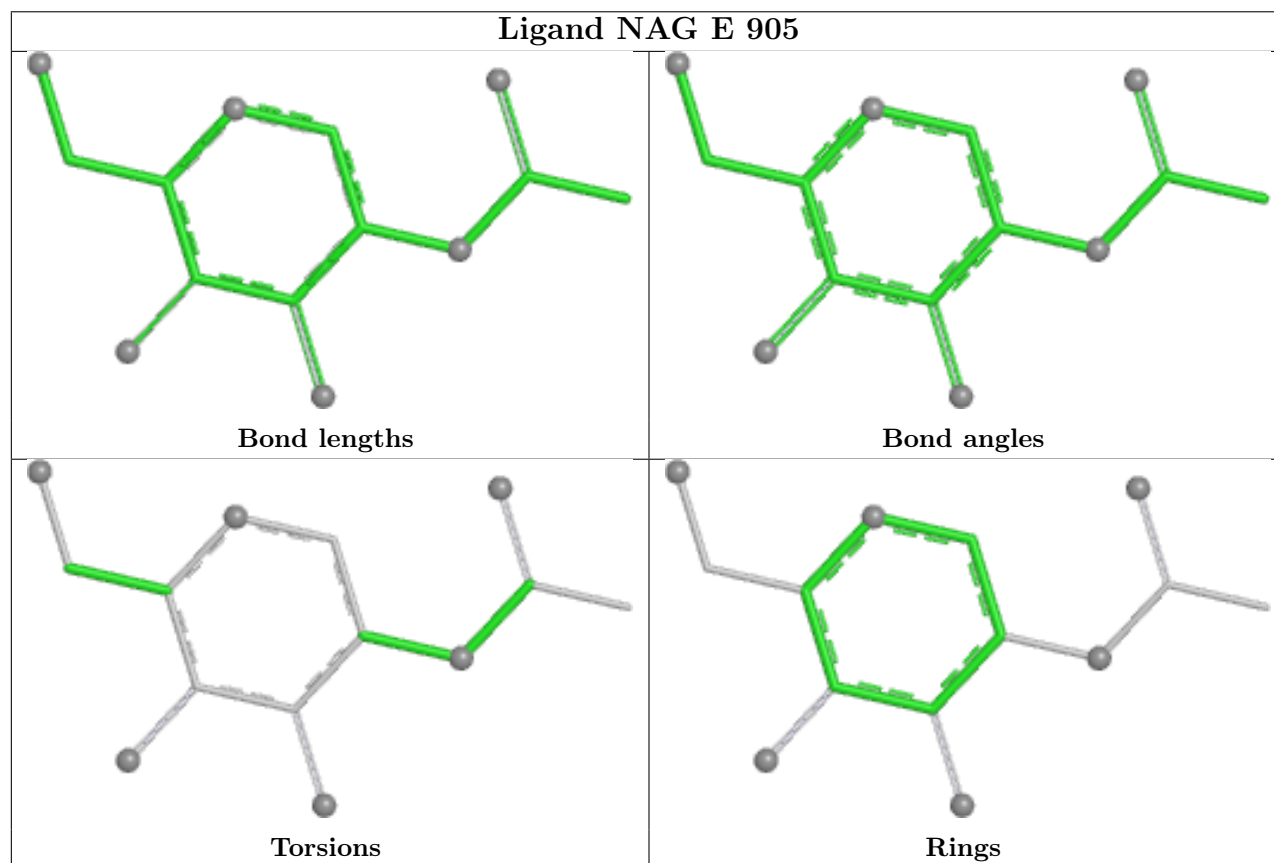
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	905	NAG	2	0
4	E	902	NAG	8	0
4	E	903	NAG	1	0
4	E	906	NAG	2	0

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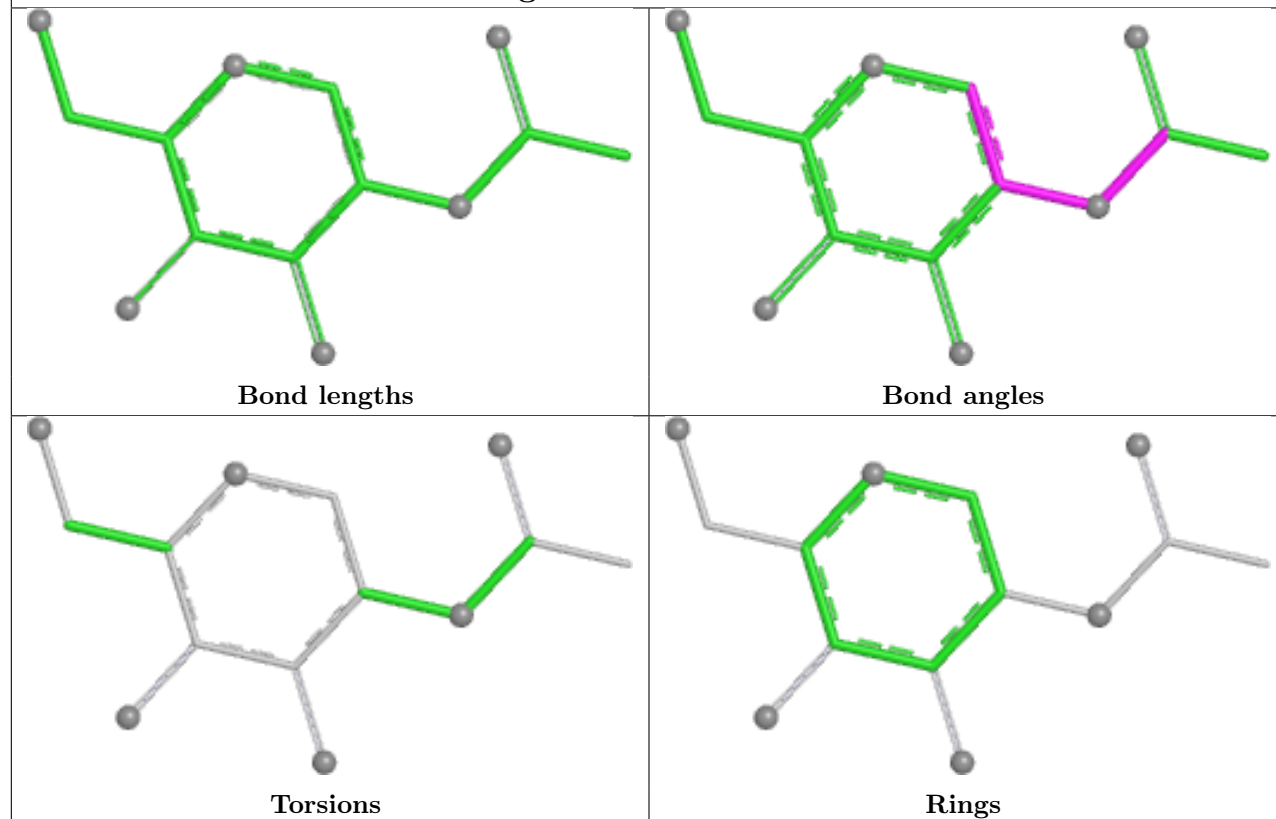
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1411	NAG	4	0
4	D	905	NAG	2	0
4	E	904	NAG	1	0
4	D	902	NAG	8	0
4	B	1410	NAG	6	0
4	D	906	NAG	2	0
4	D	904	NAG	1	0
4	D	903	NAG	1	0

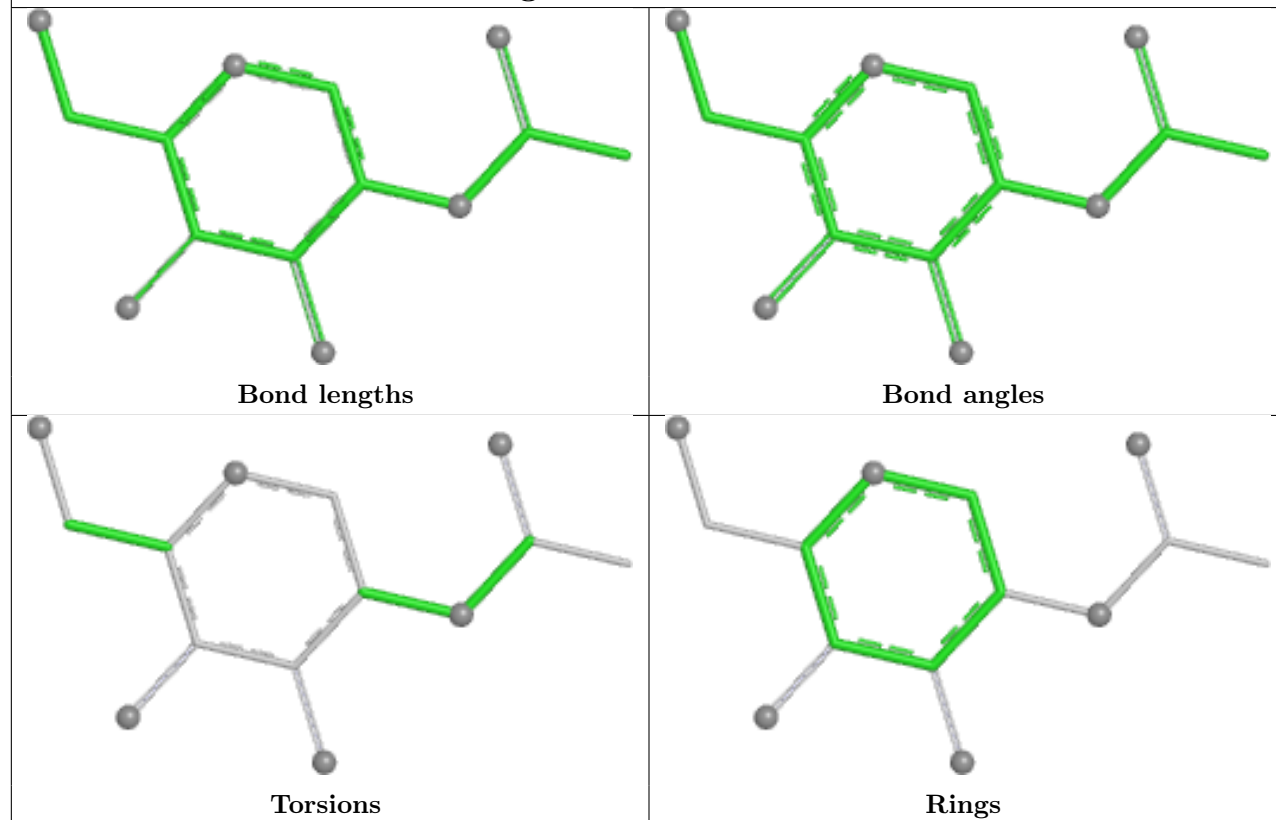
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



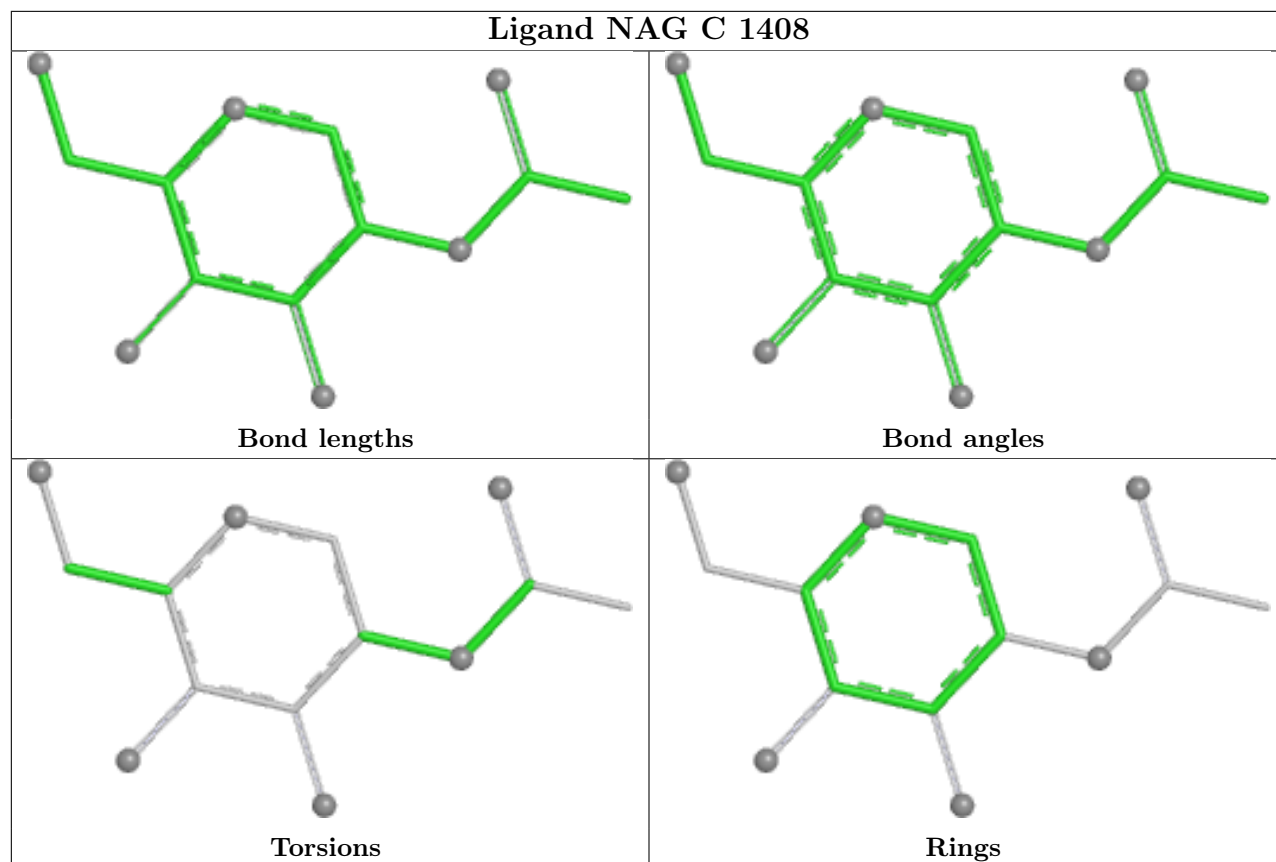
Ligand NAG A 1405



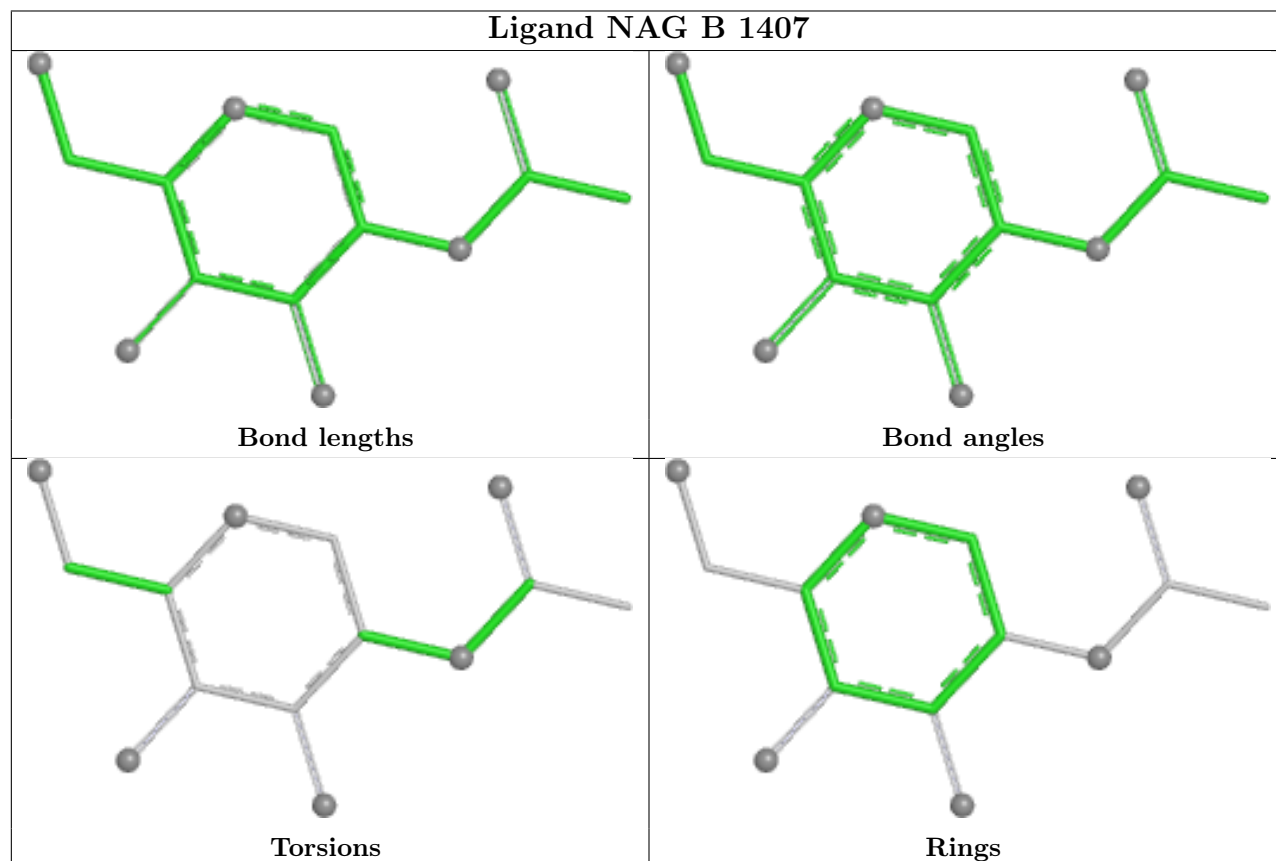
Ligand NAG B 1401

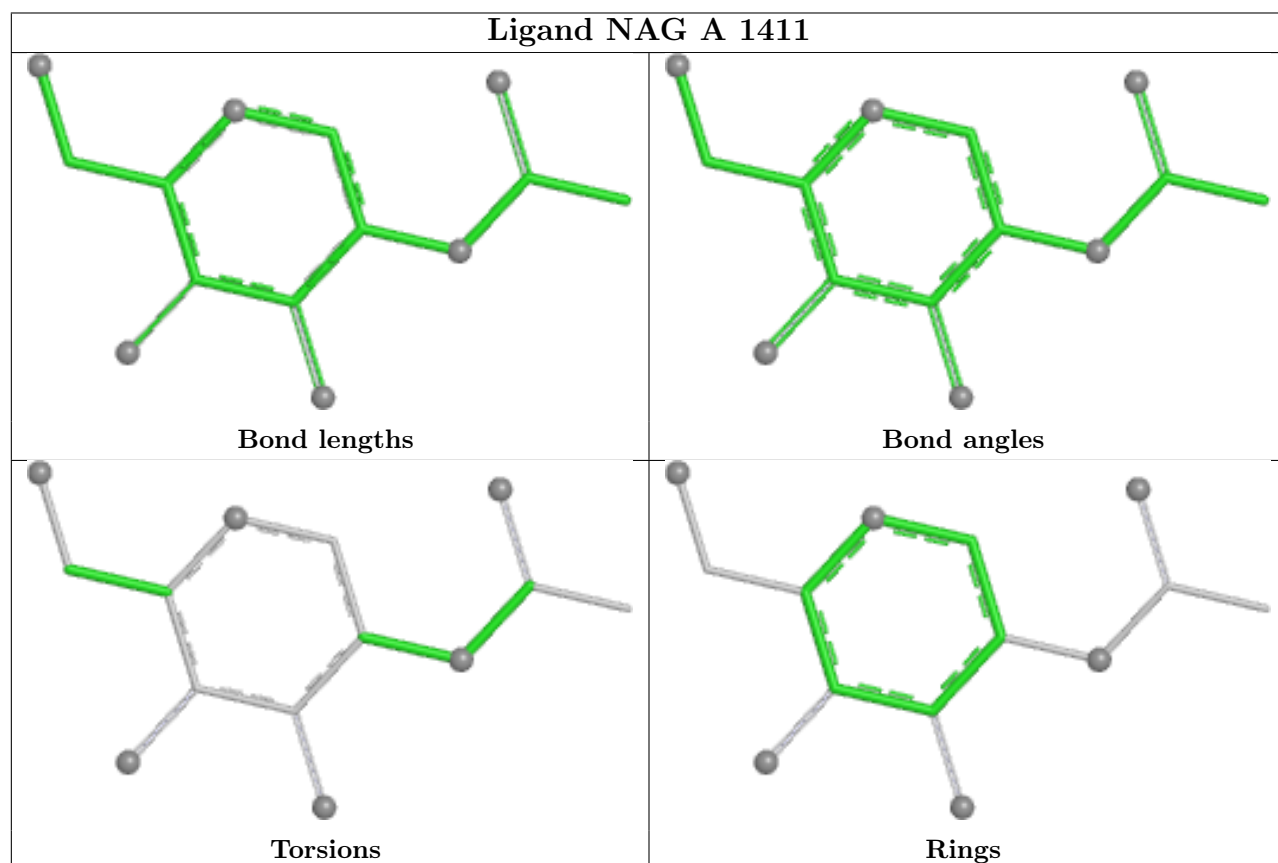
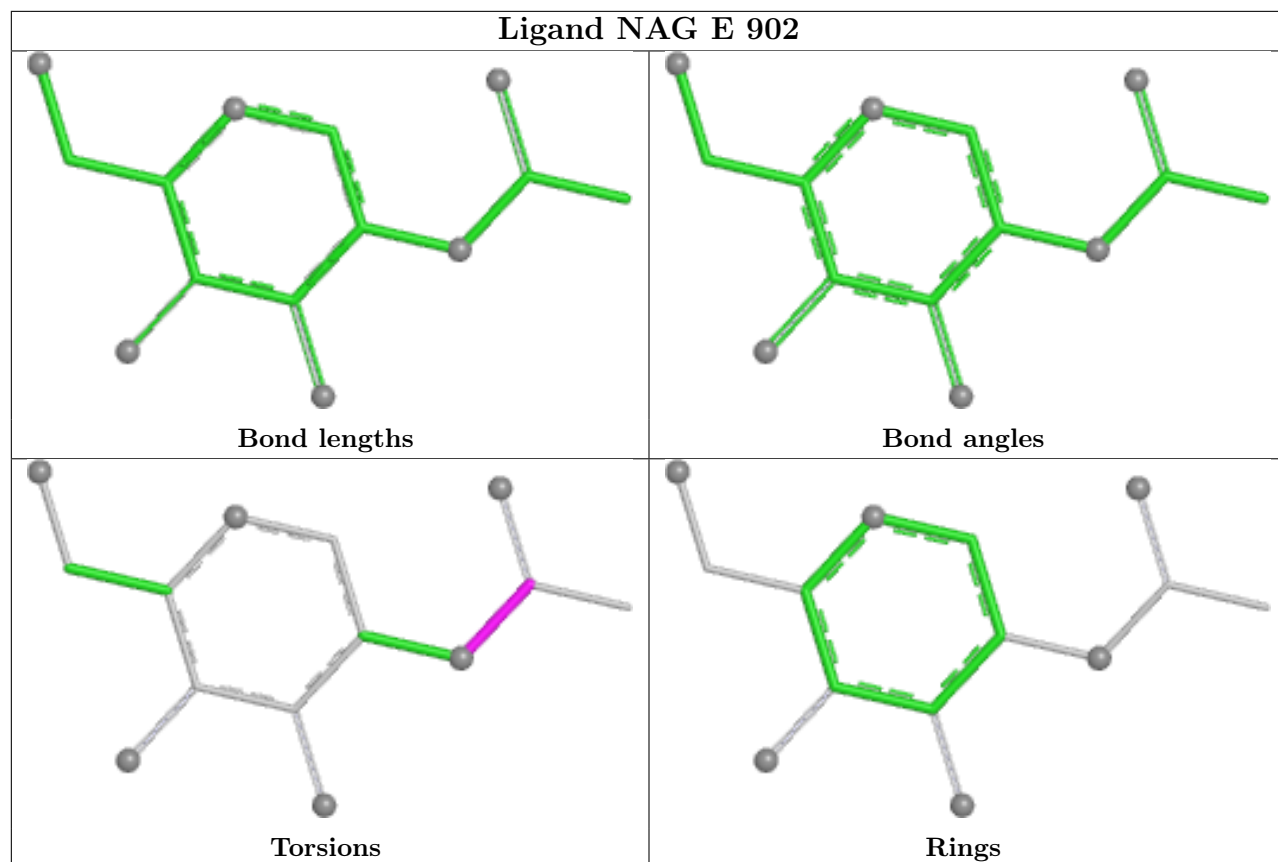


Ligand NAG C 1408

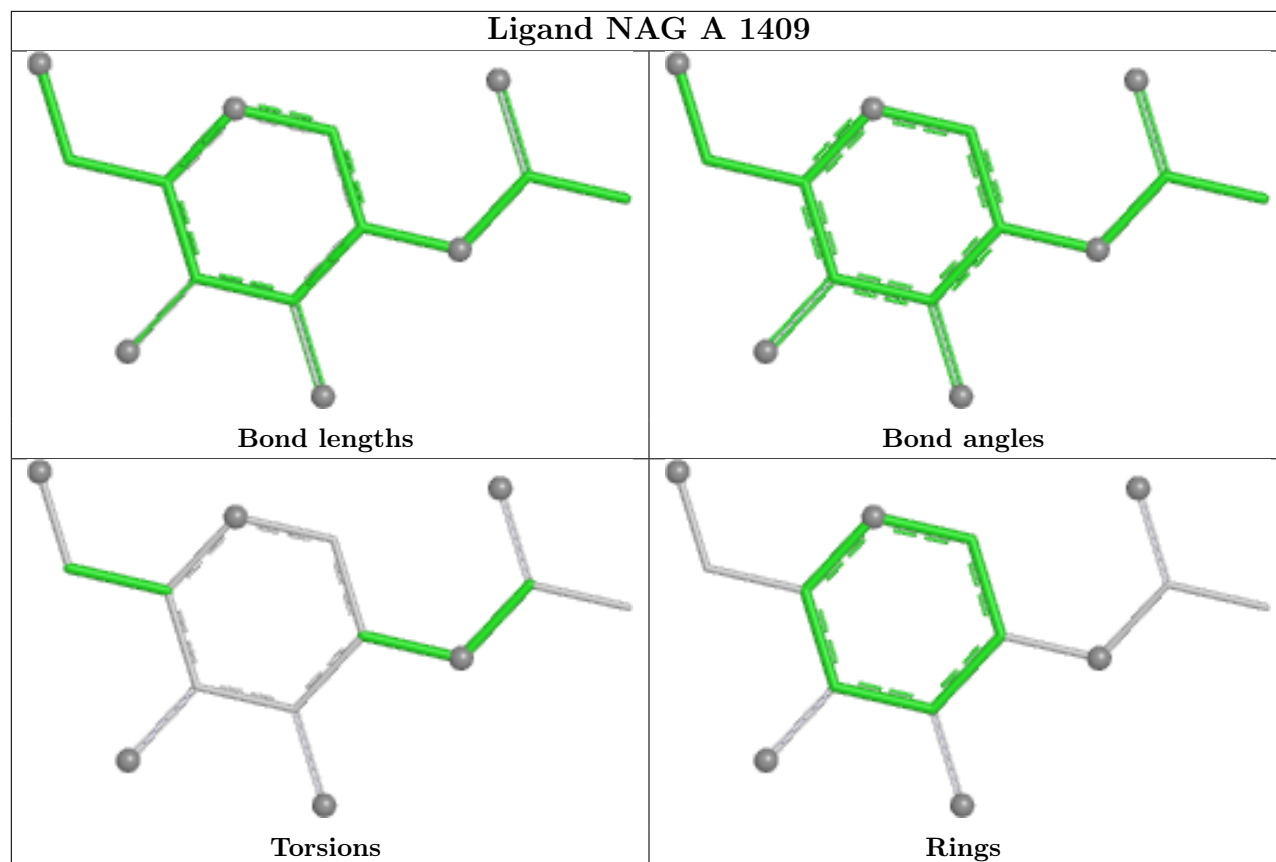


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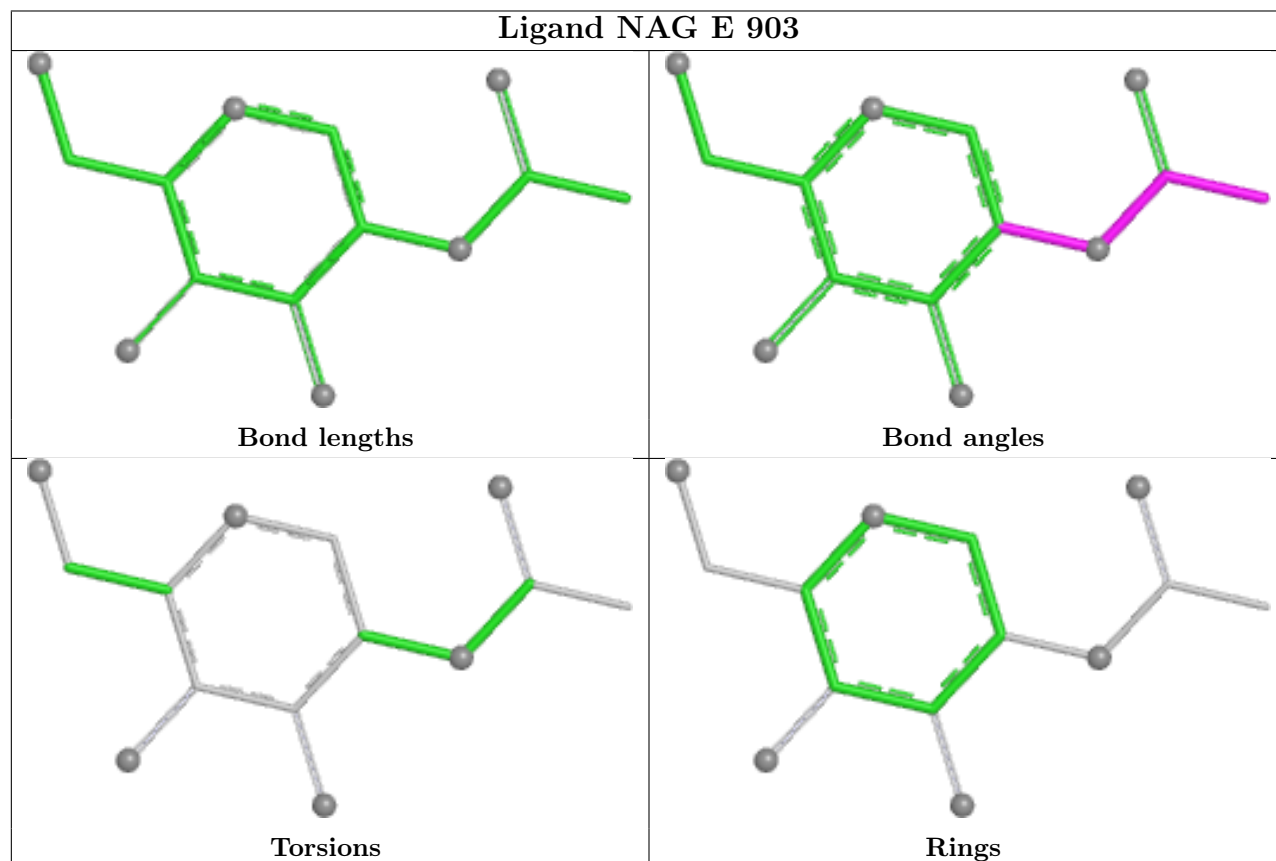


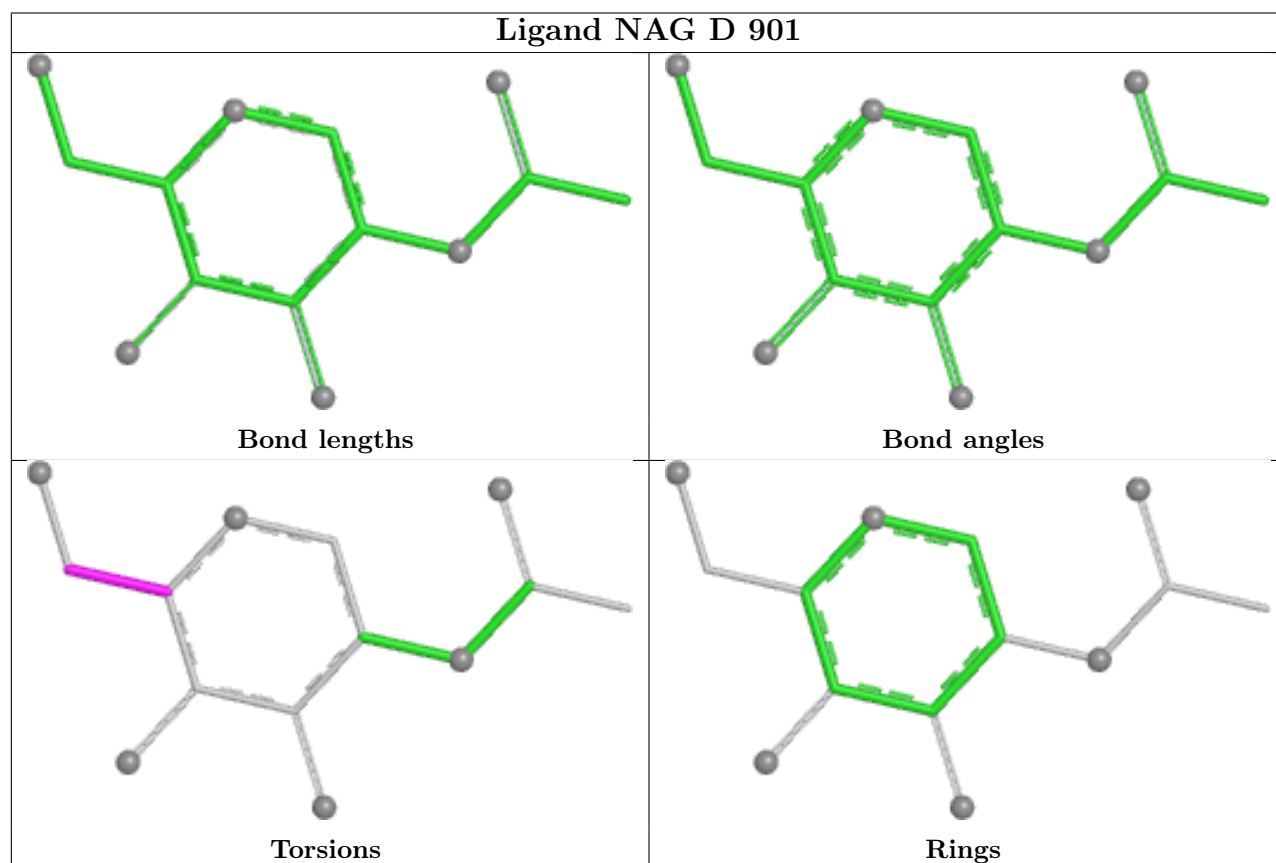
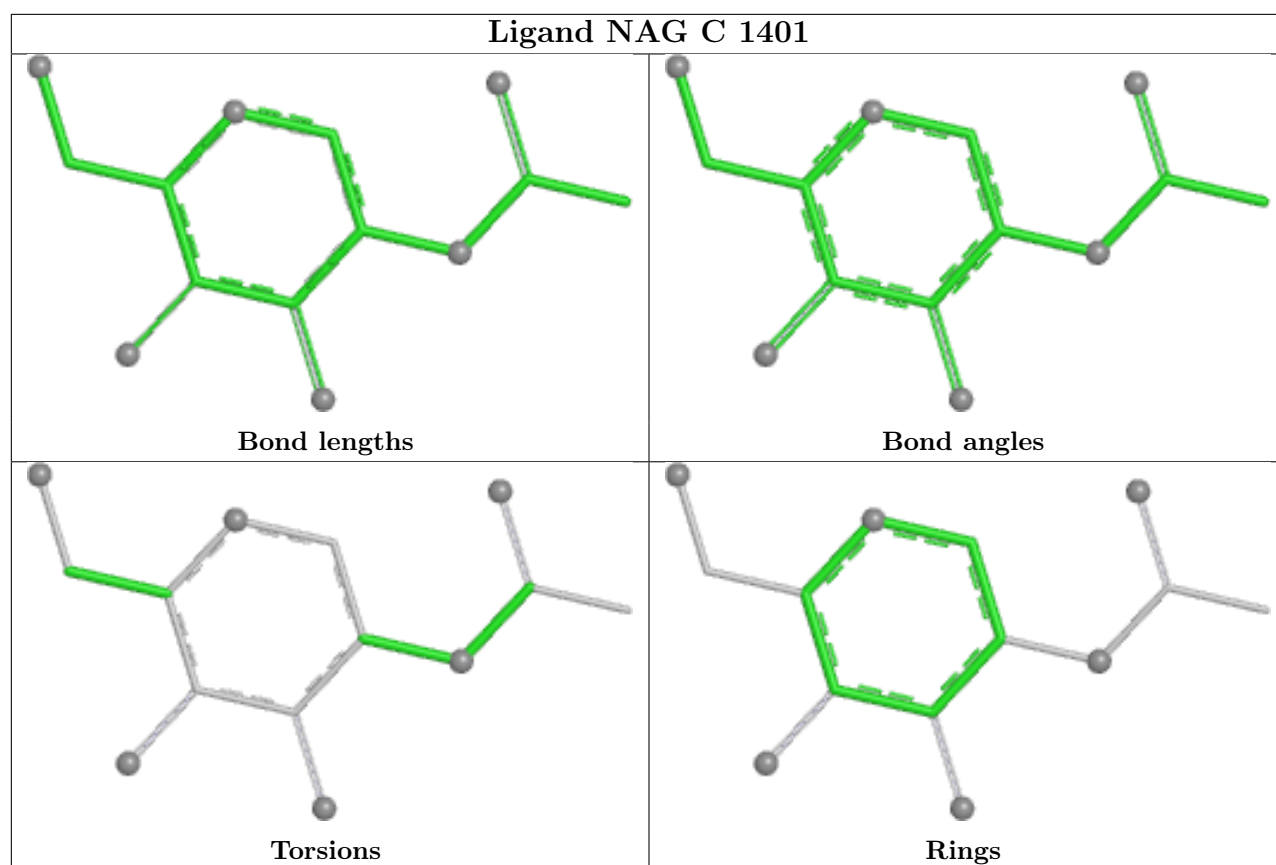


Ligand NAG A 1409

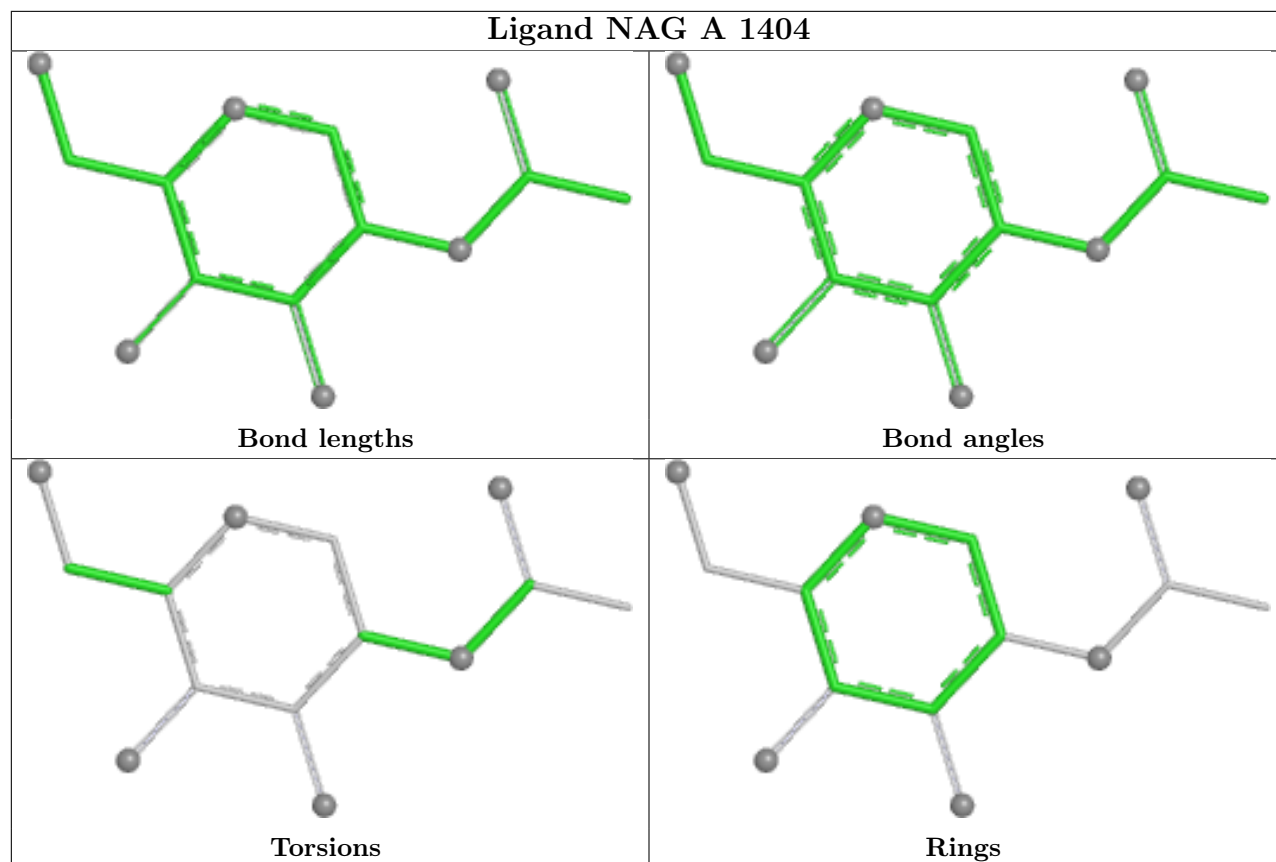


Ligand NAG E 903

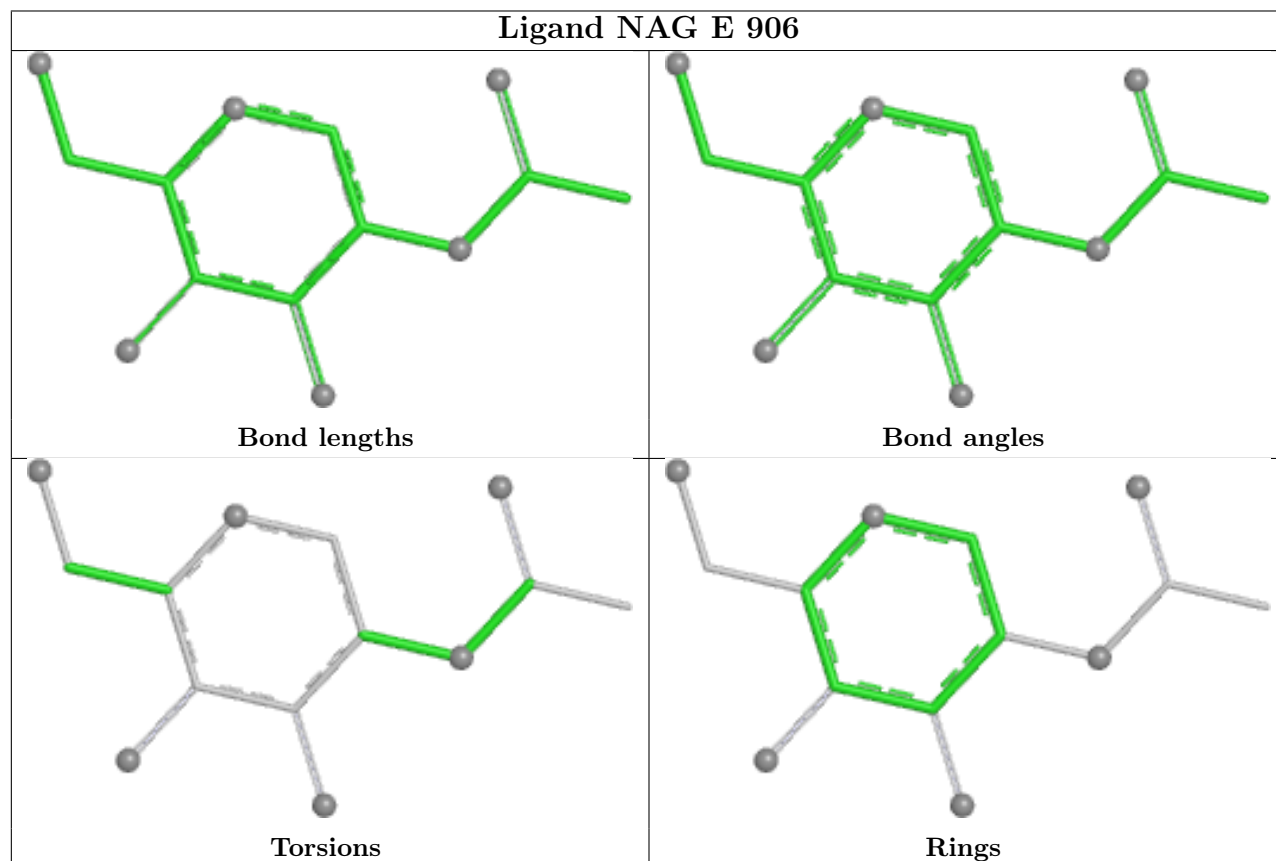


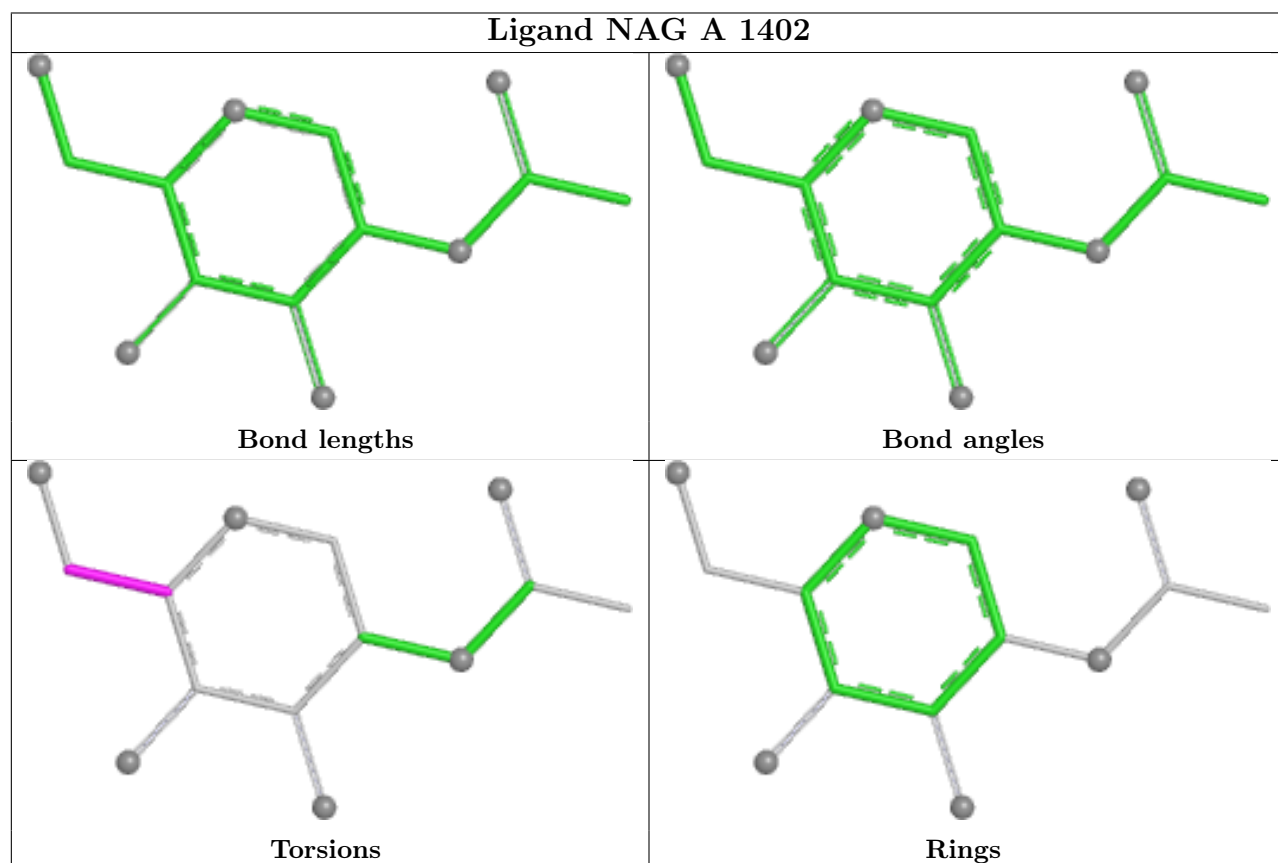
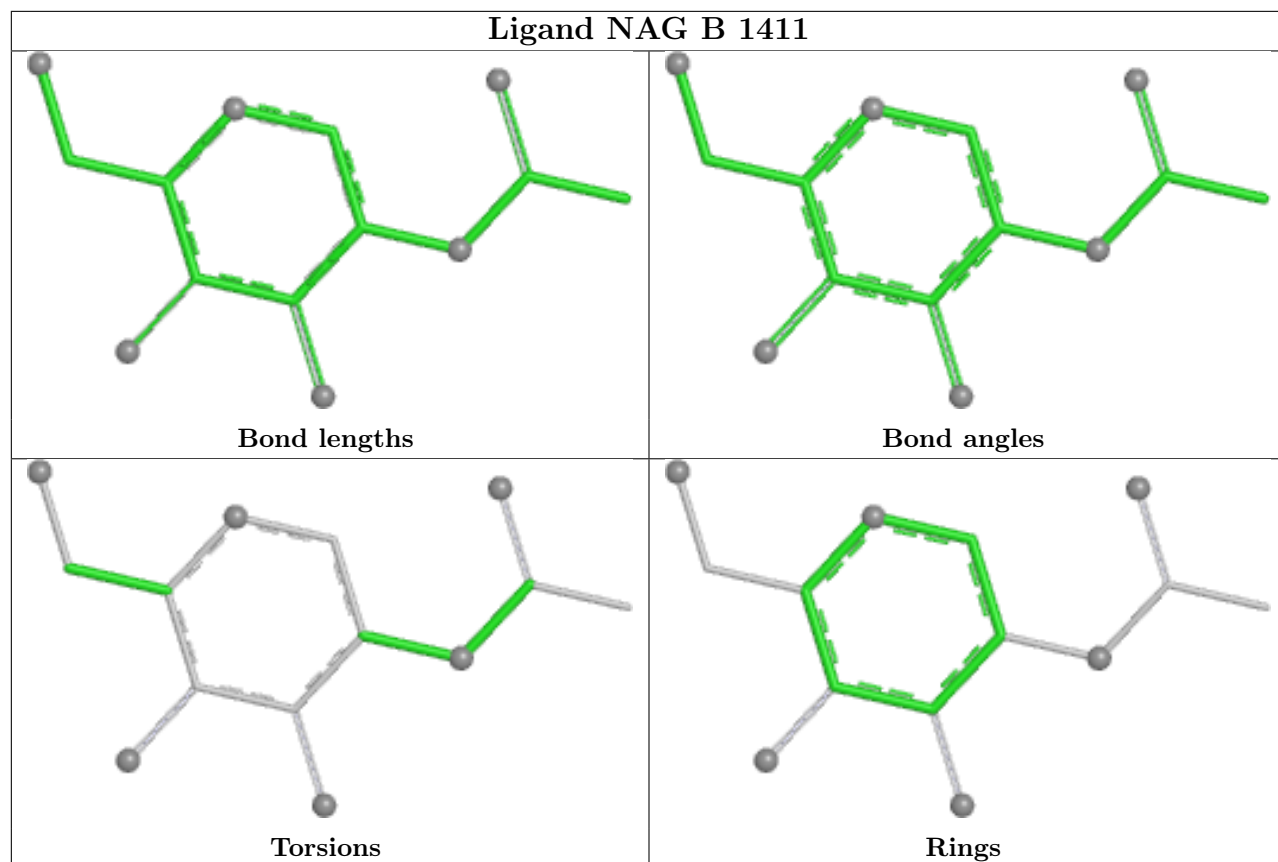


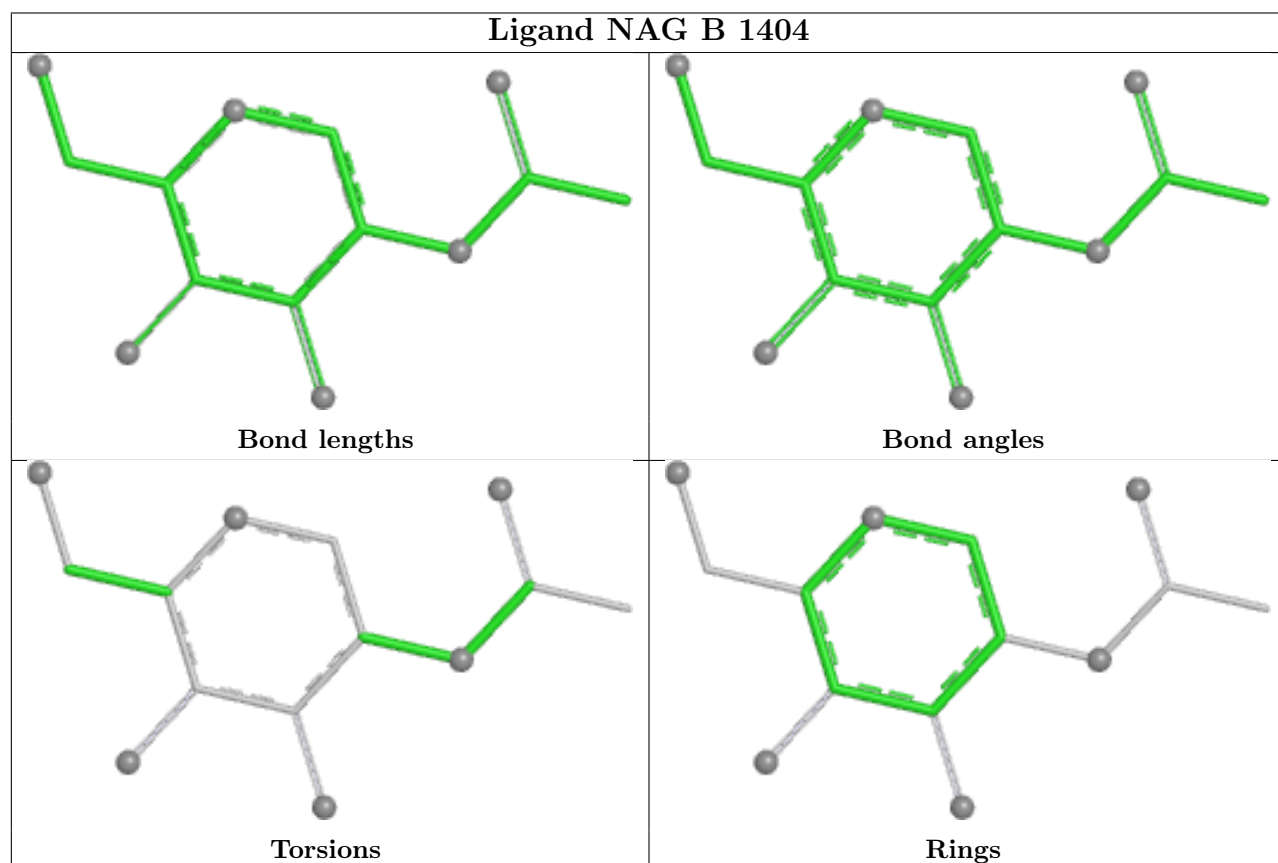
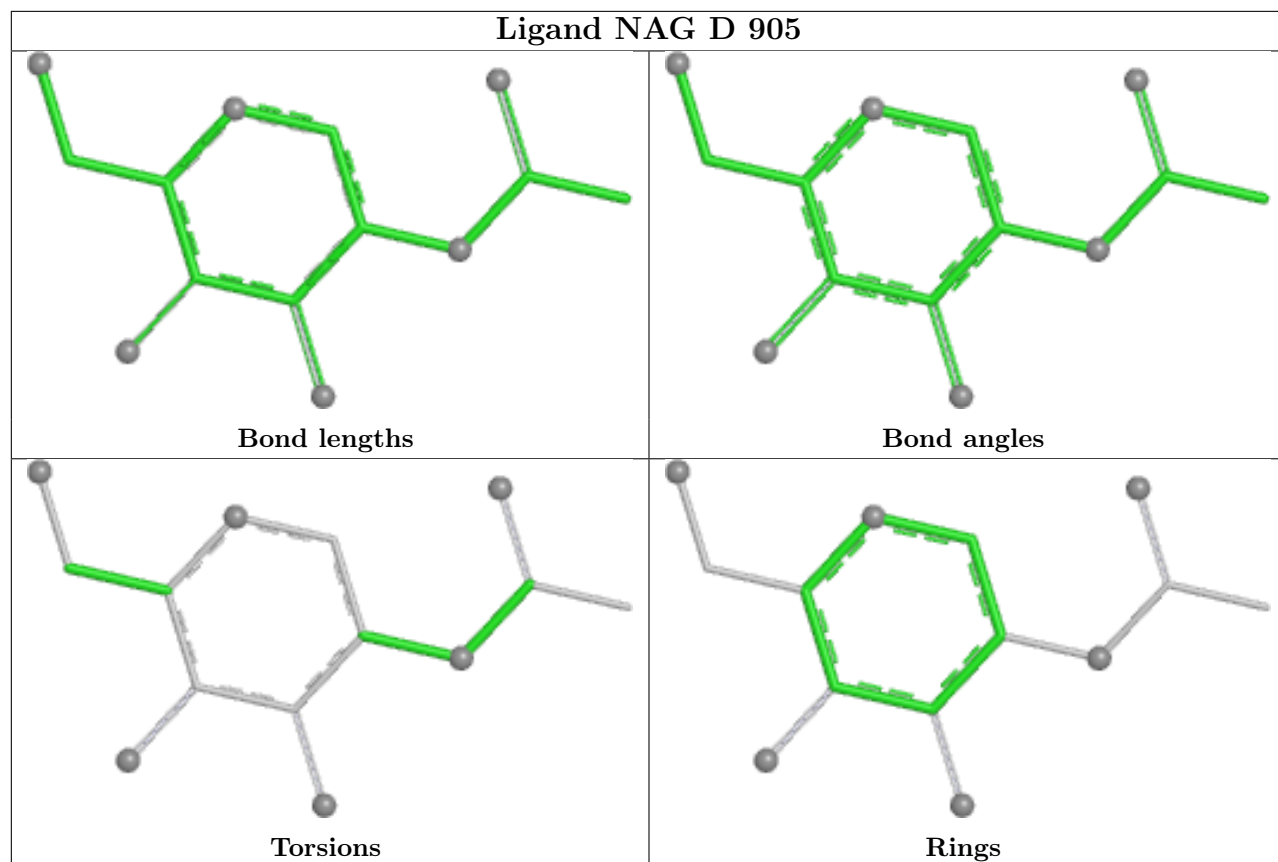
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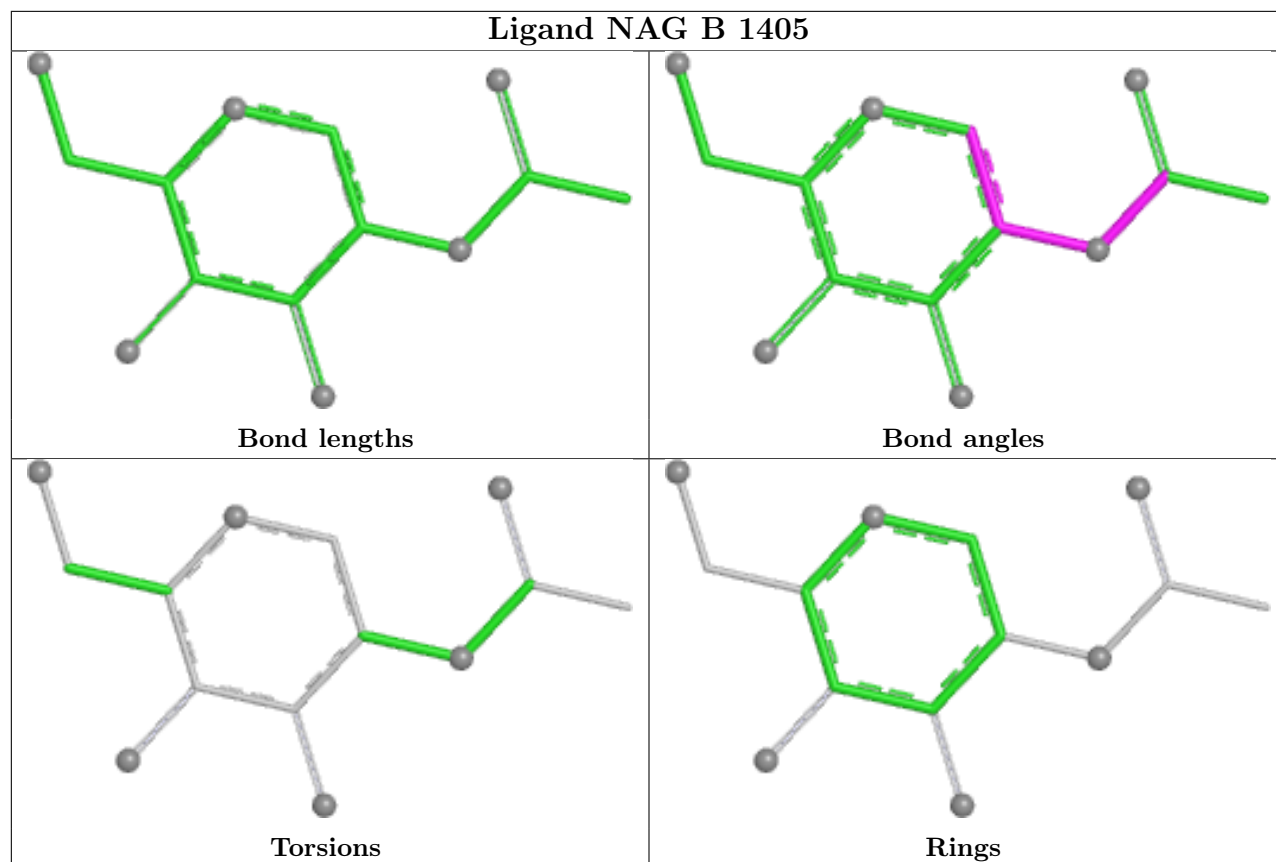
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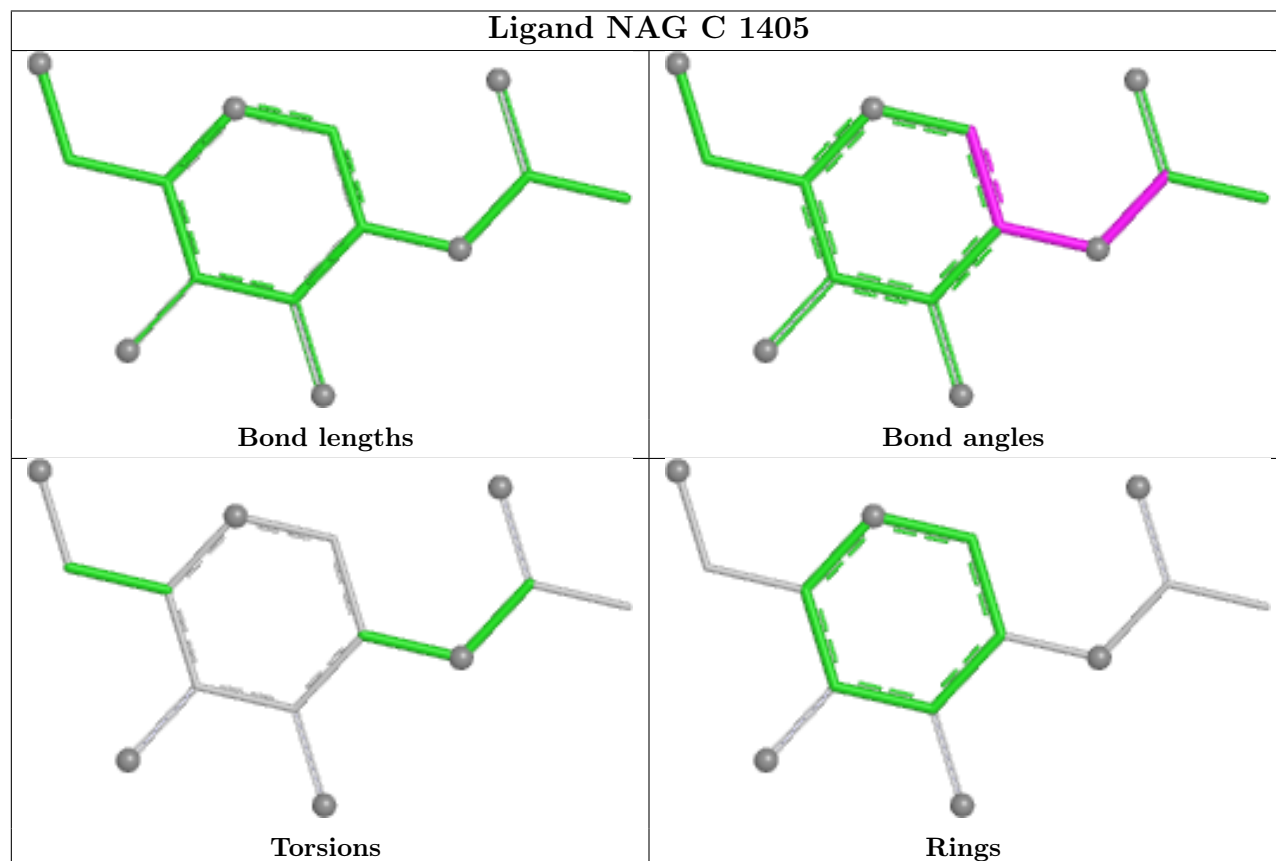


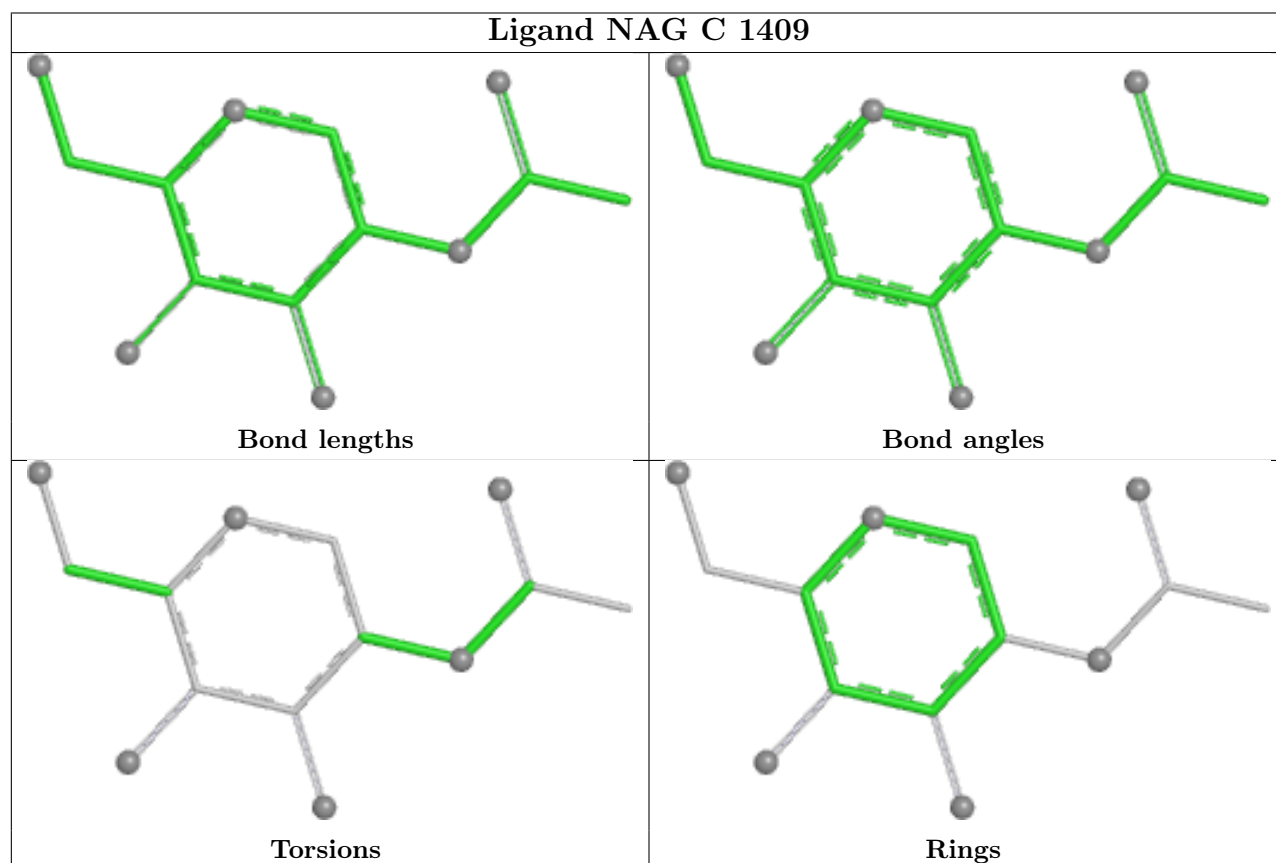
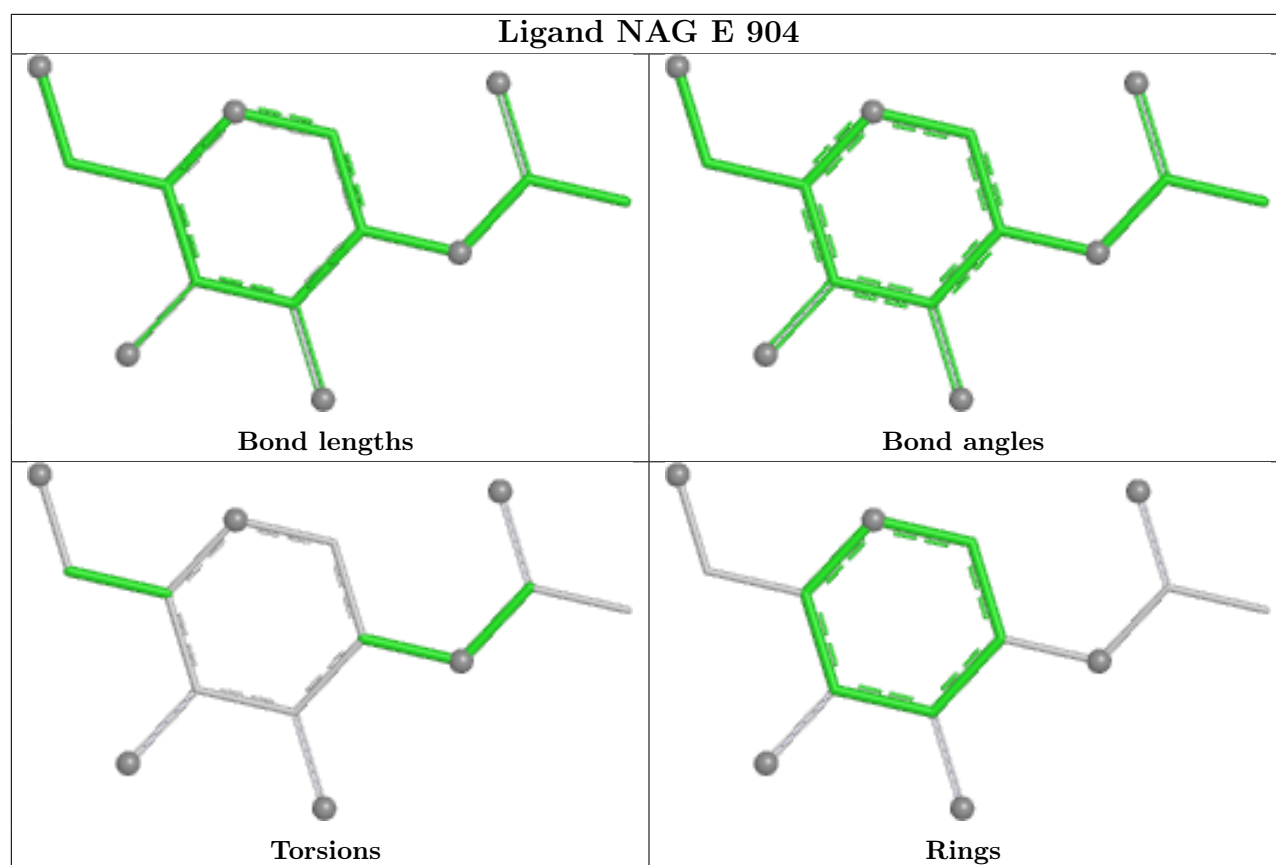


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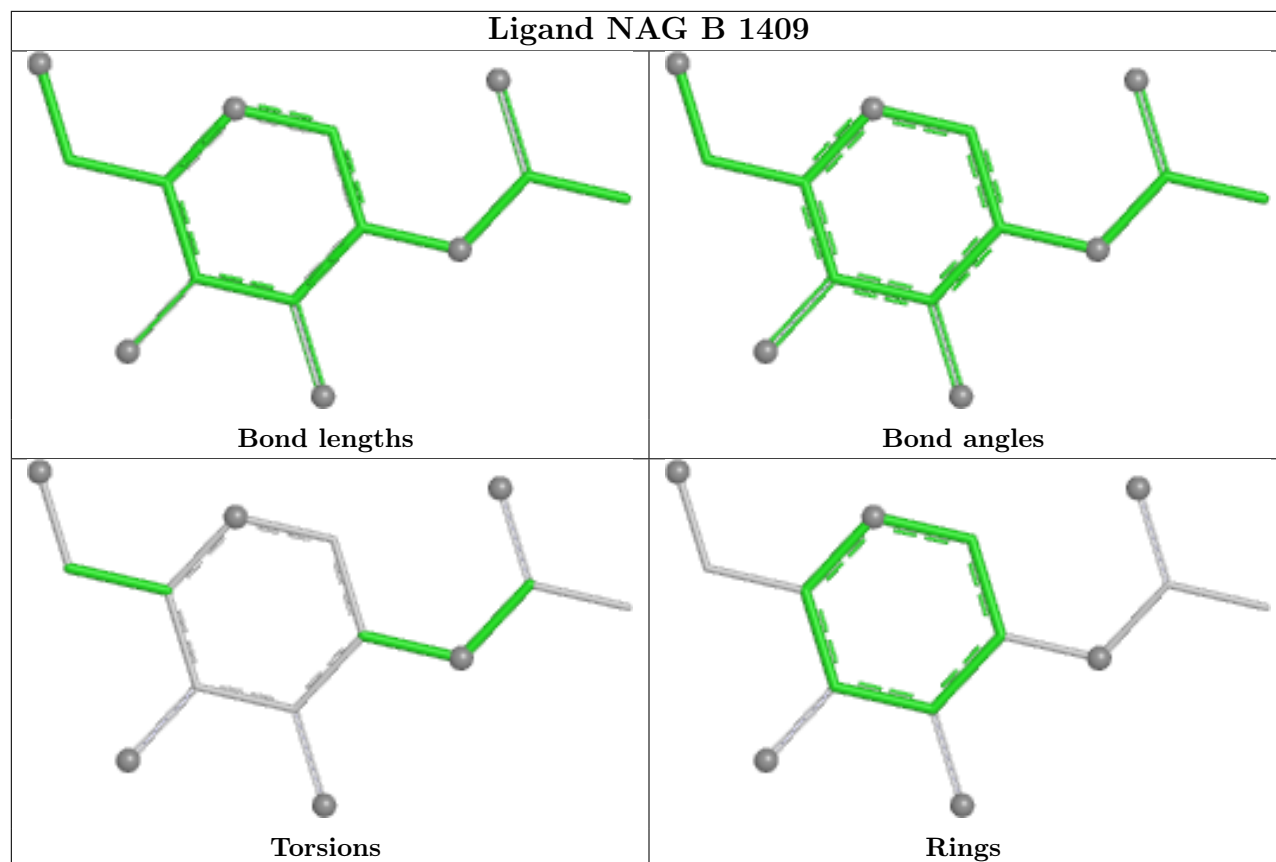


Ligand NAG C 1405

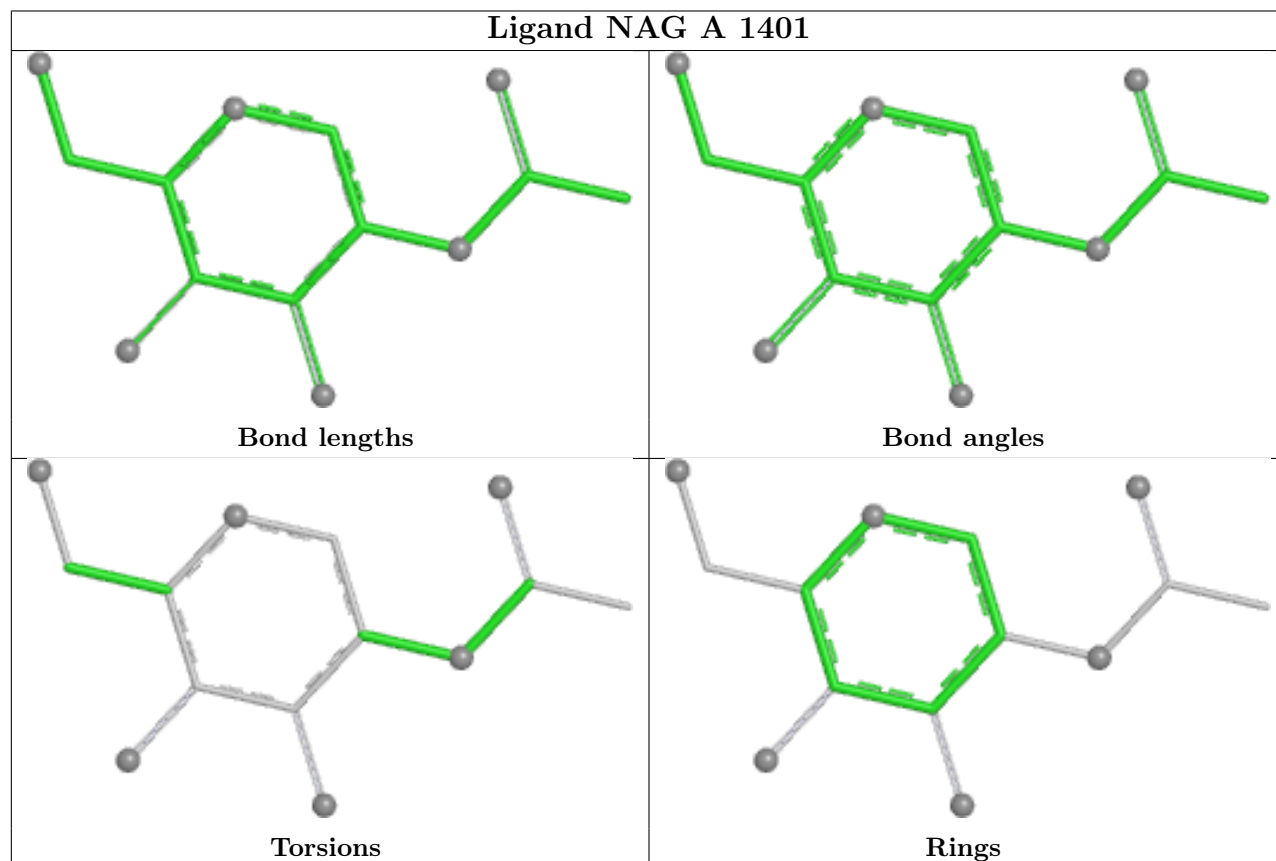




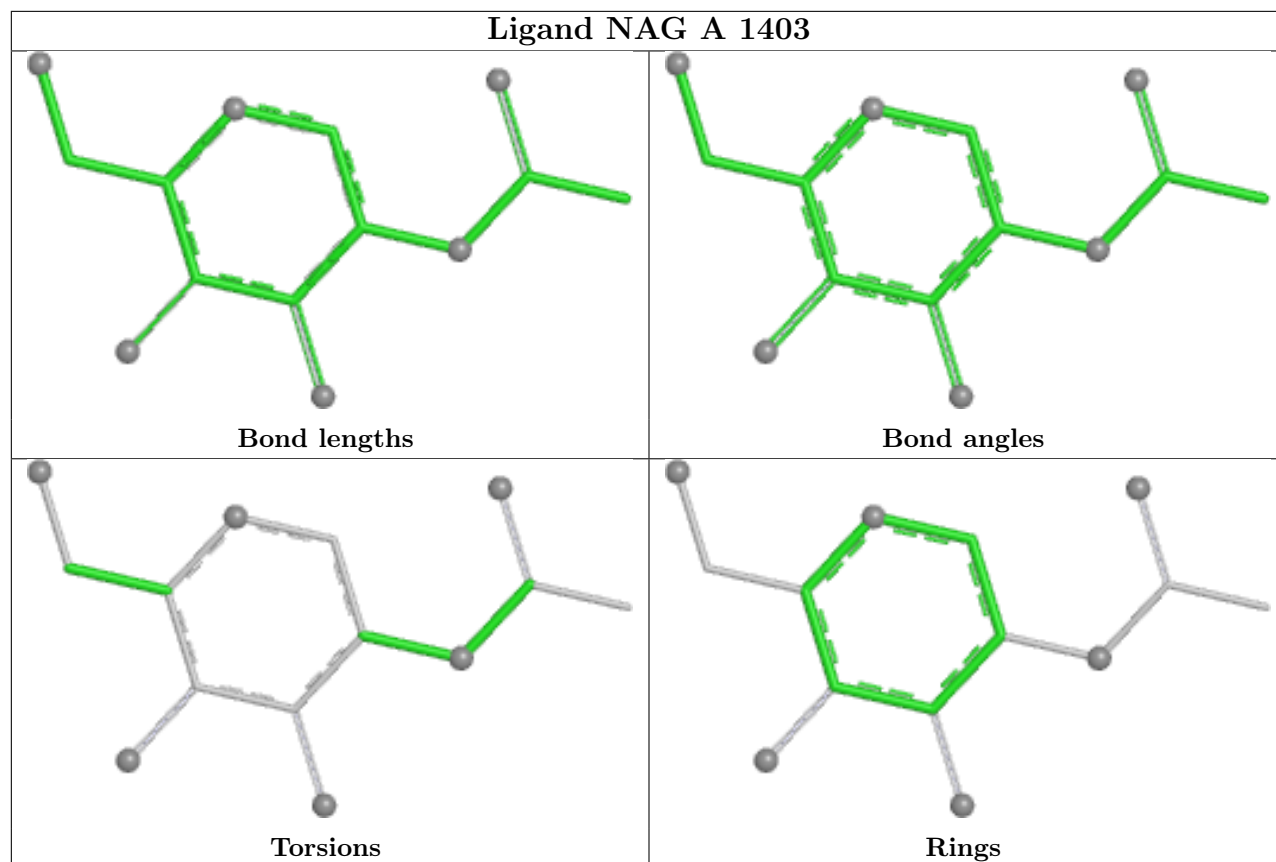
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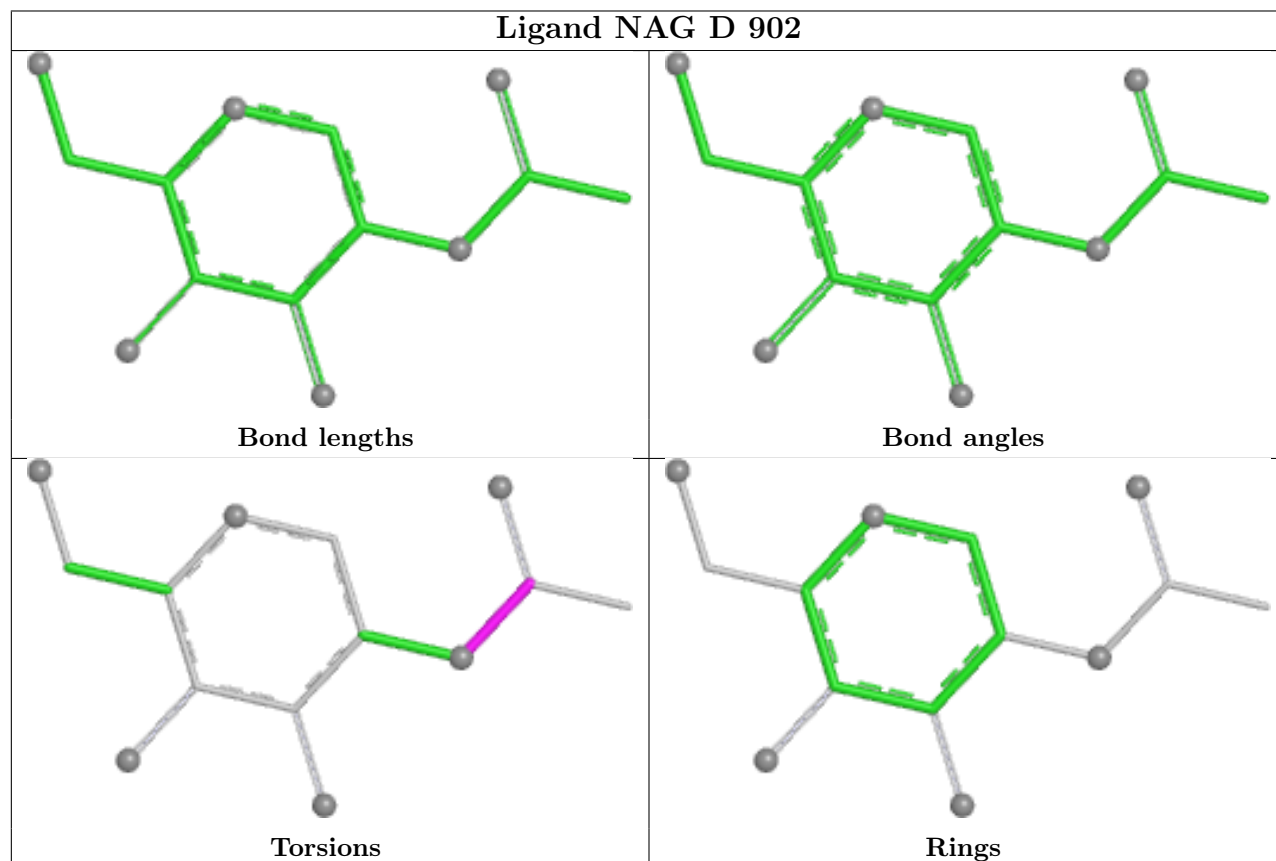
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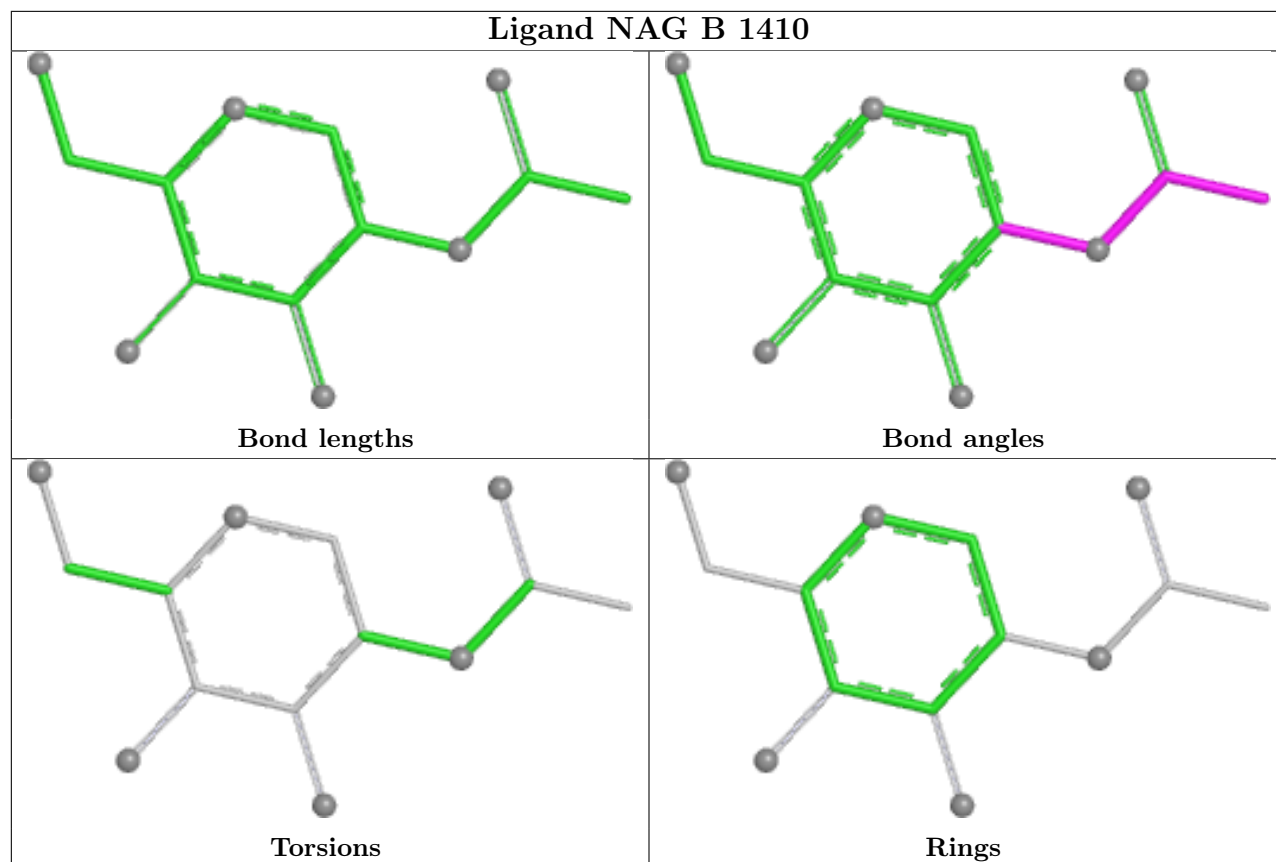
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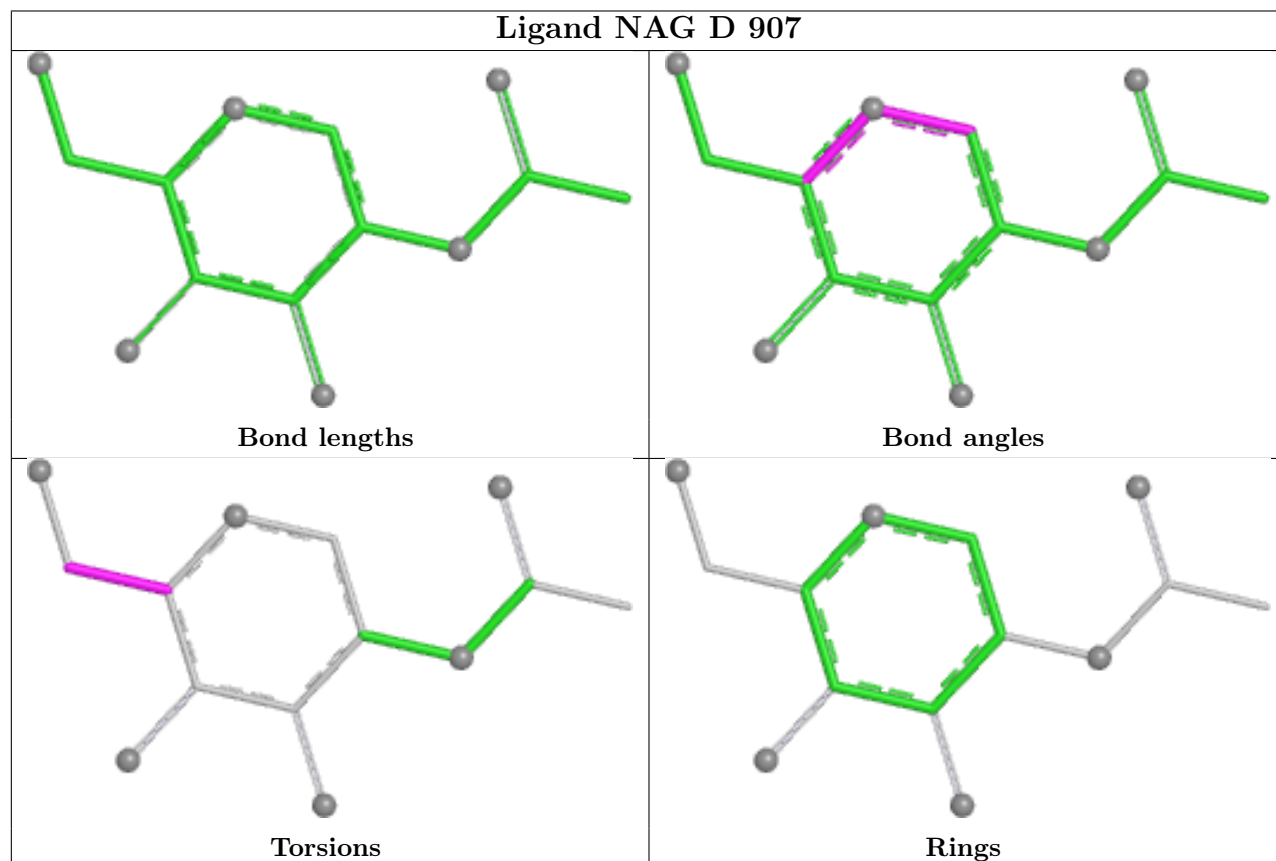
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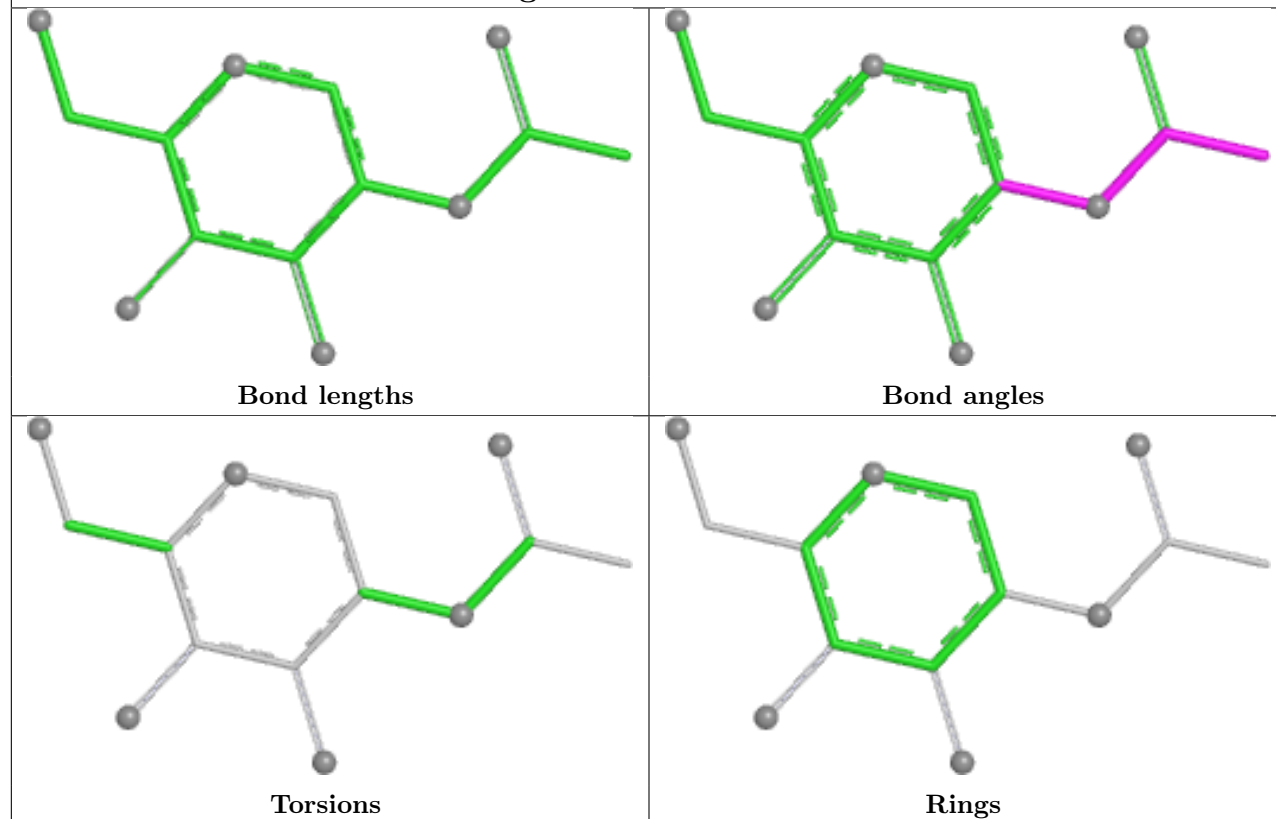
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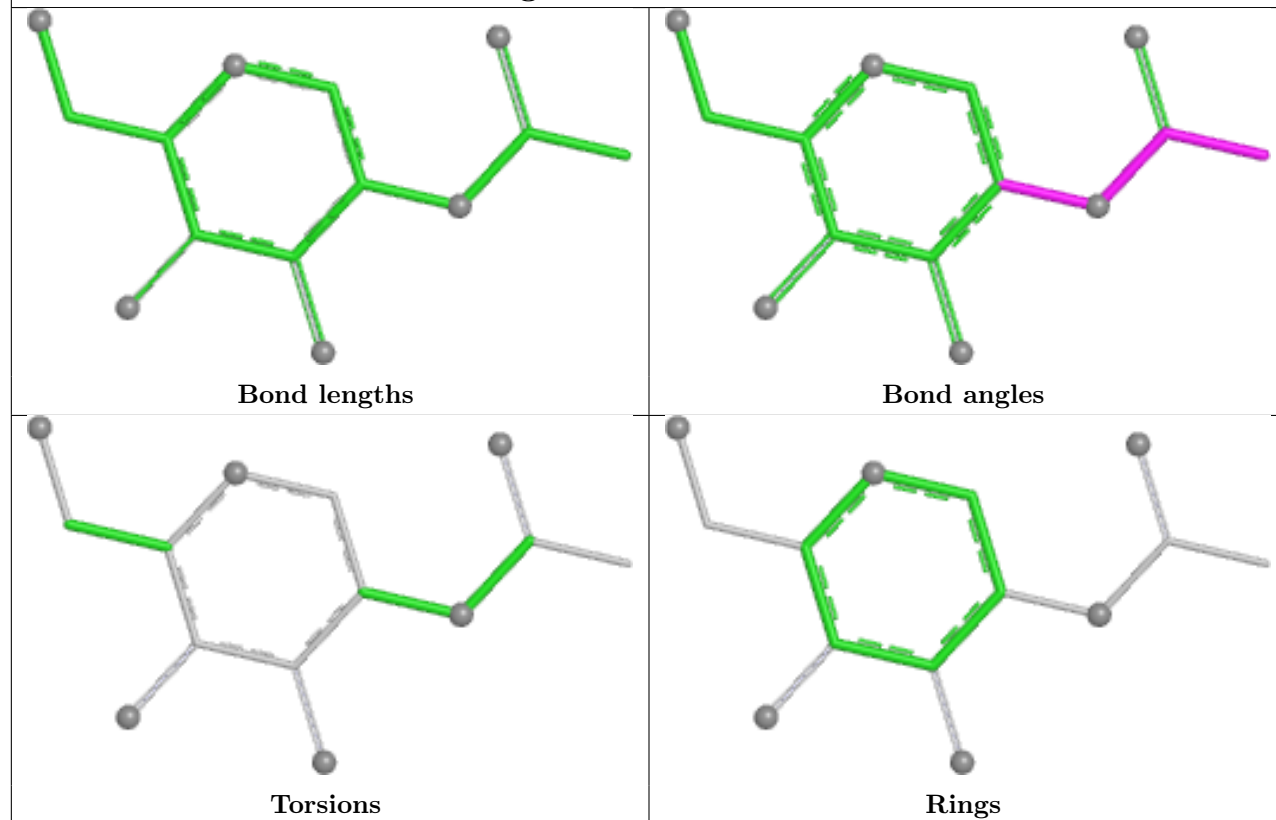
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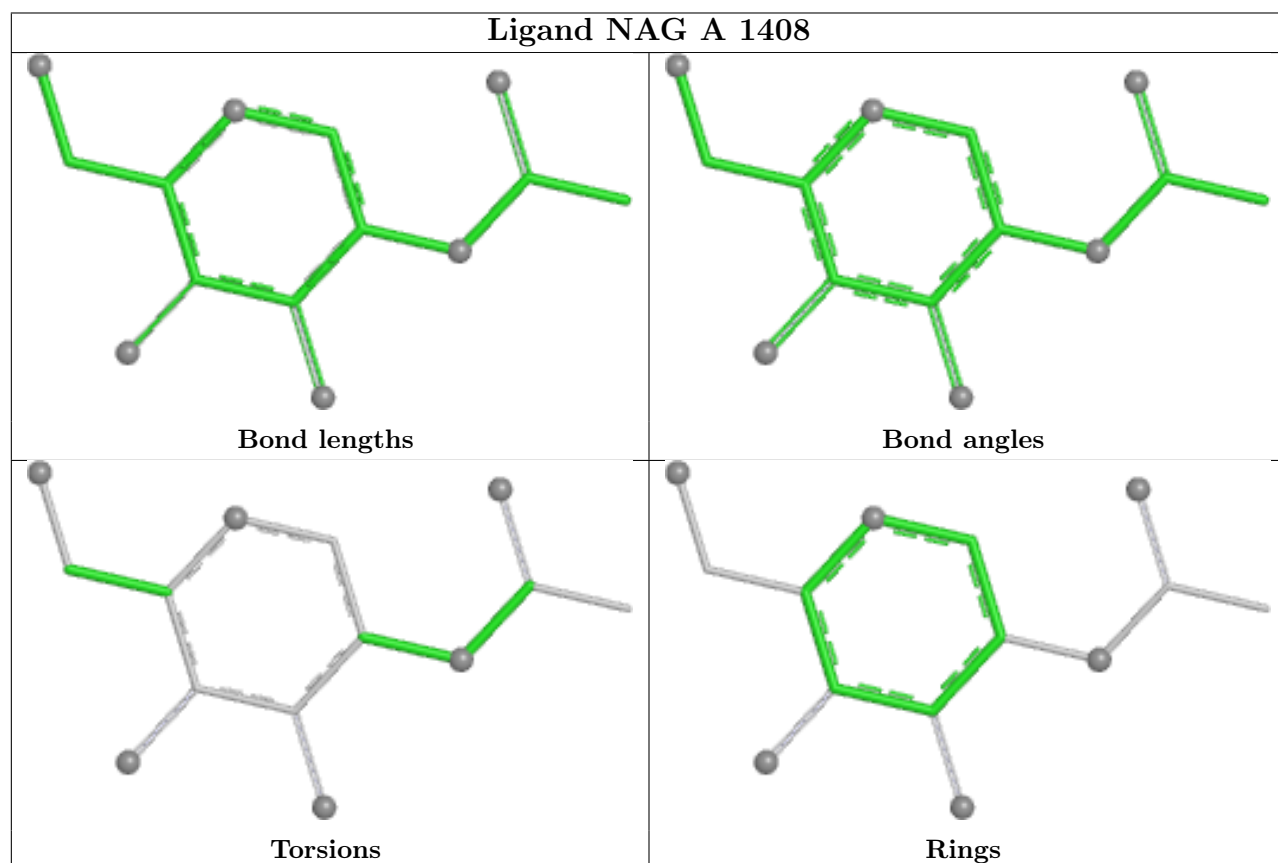
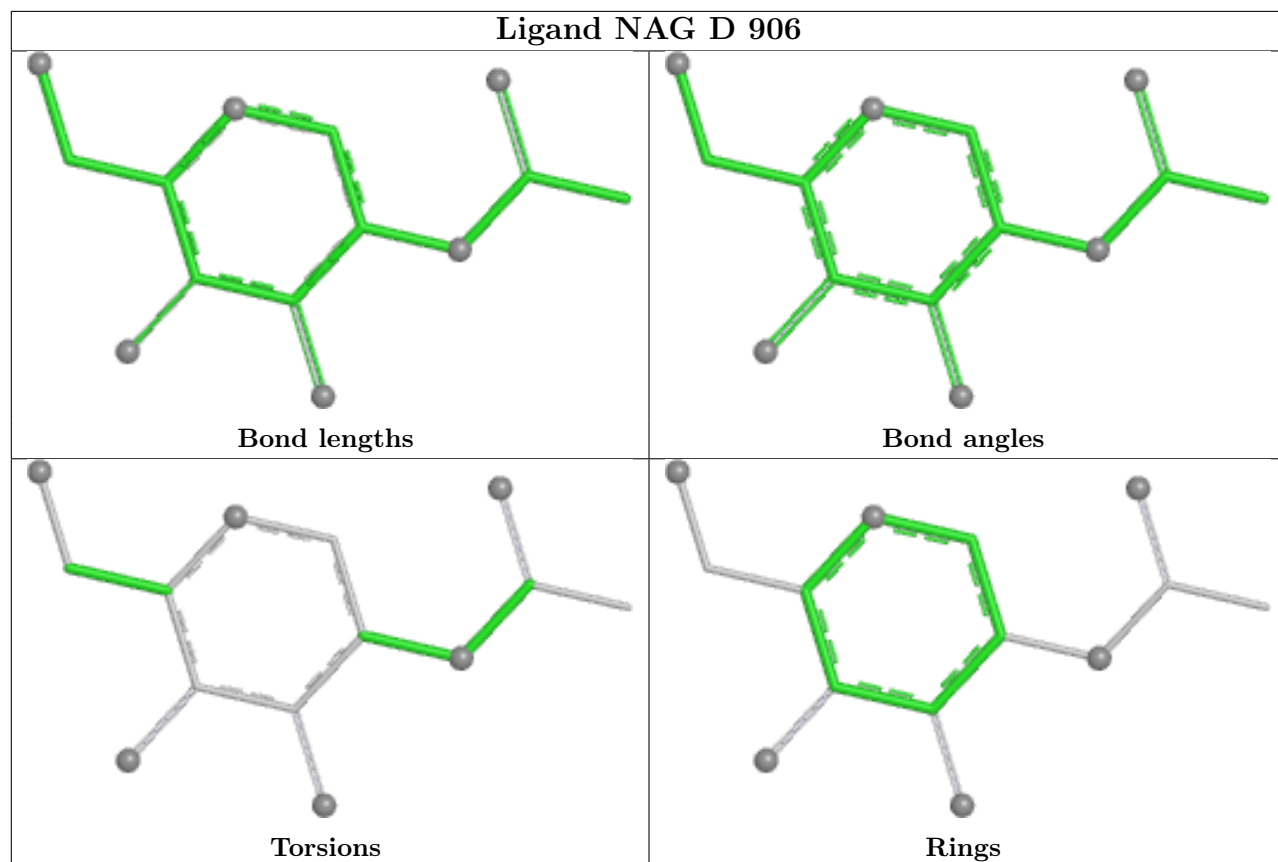


Ligand NAG C 1406

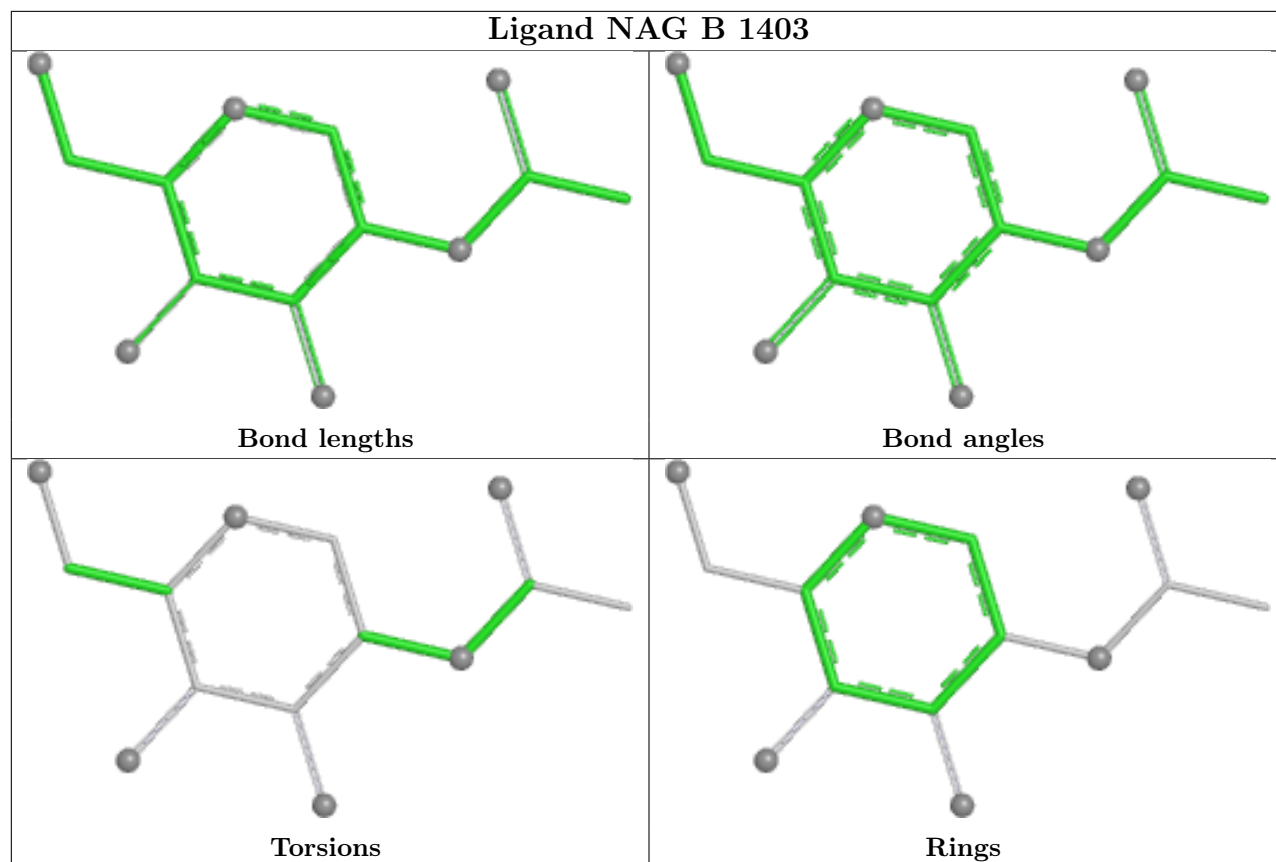


Ligand NAG B 1406

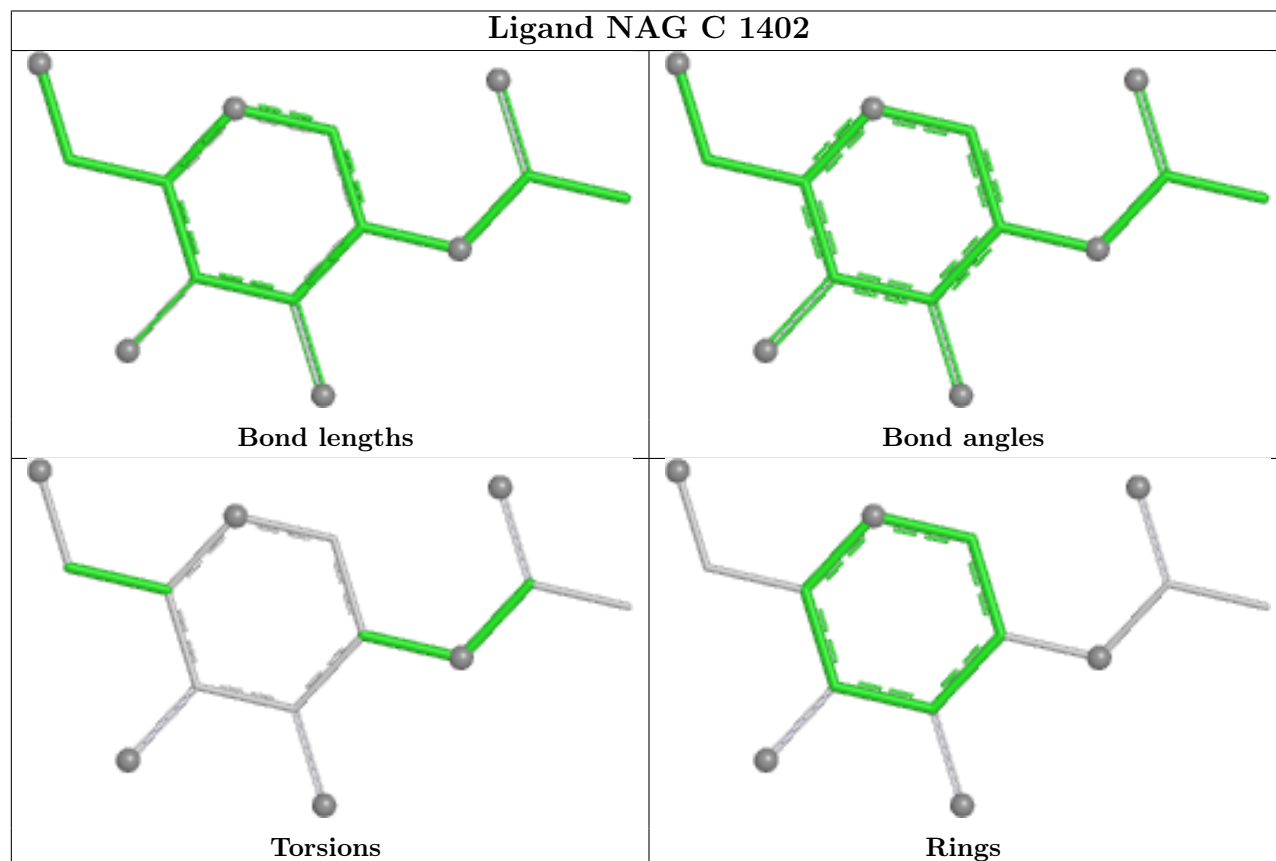




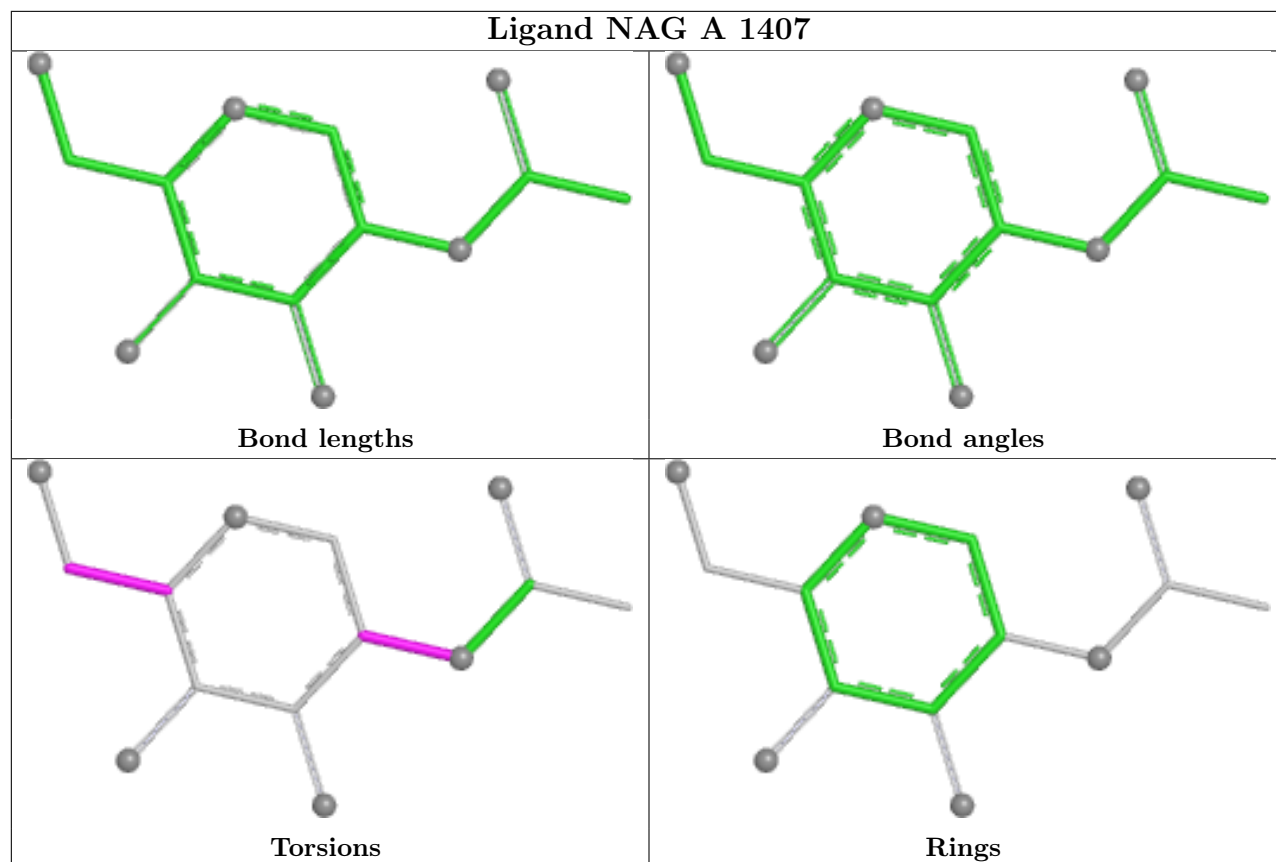
Ligand NAG B 1403



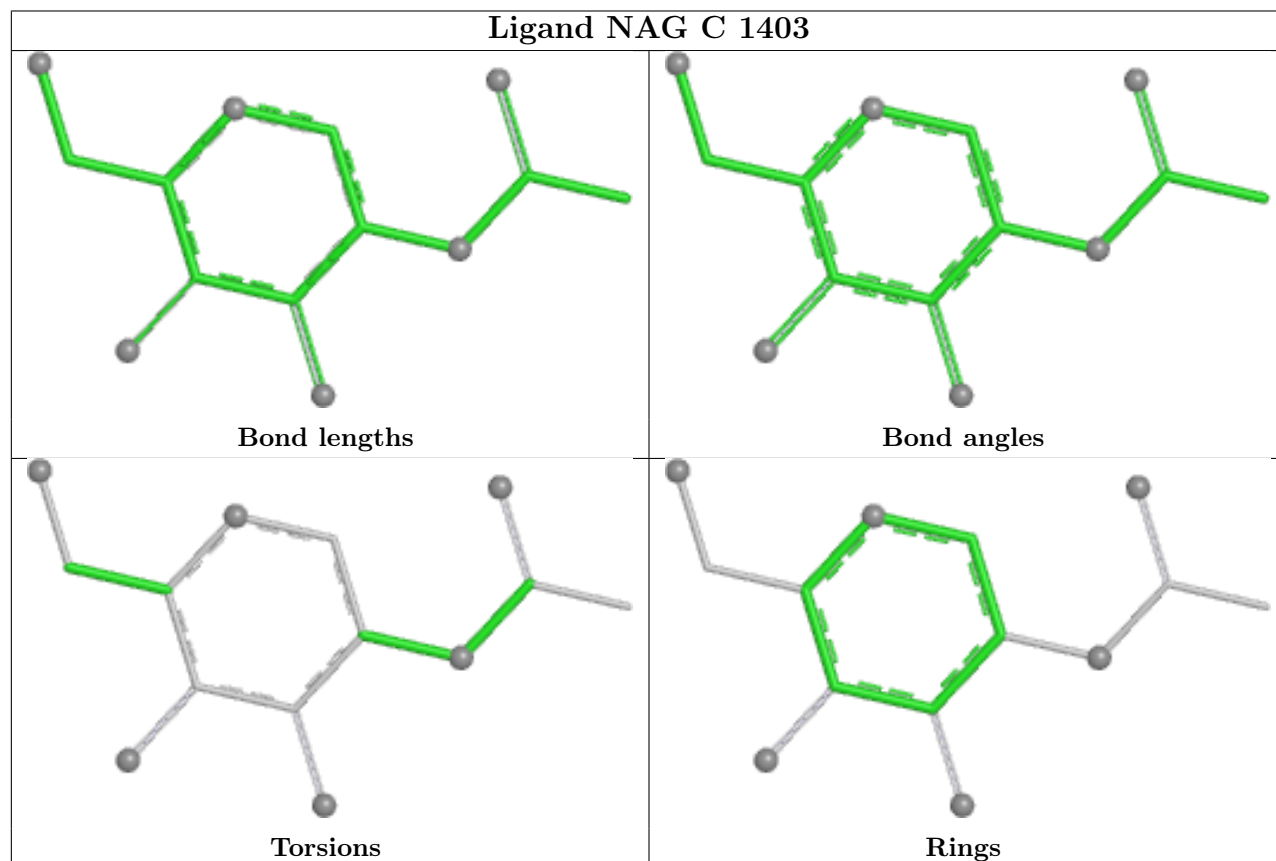
Ligand NAG C 1402



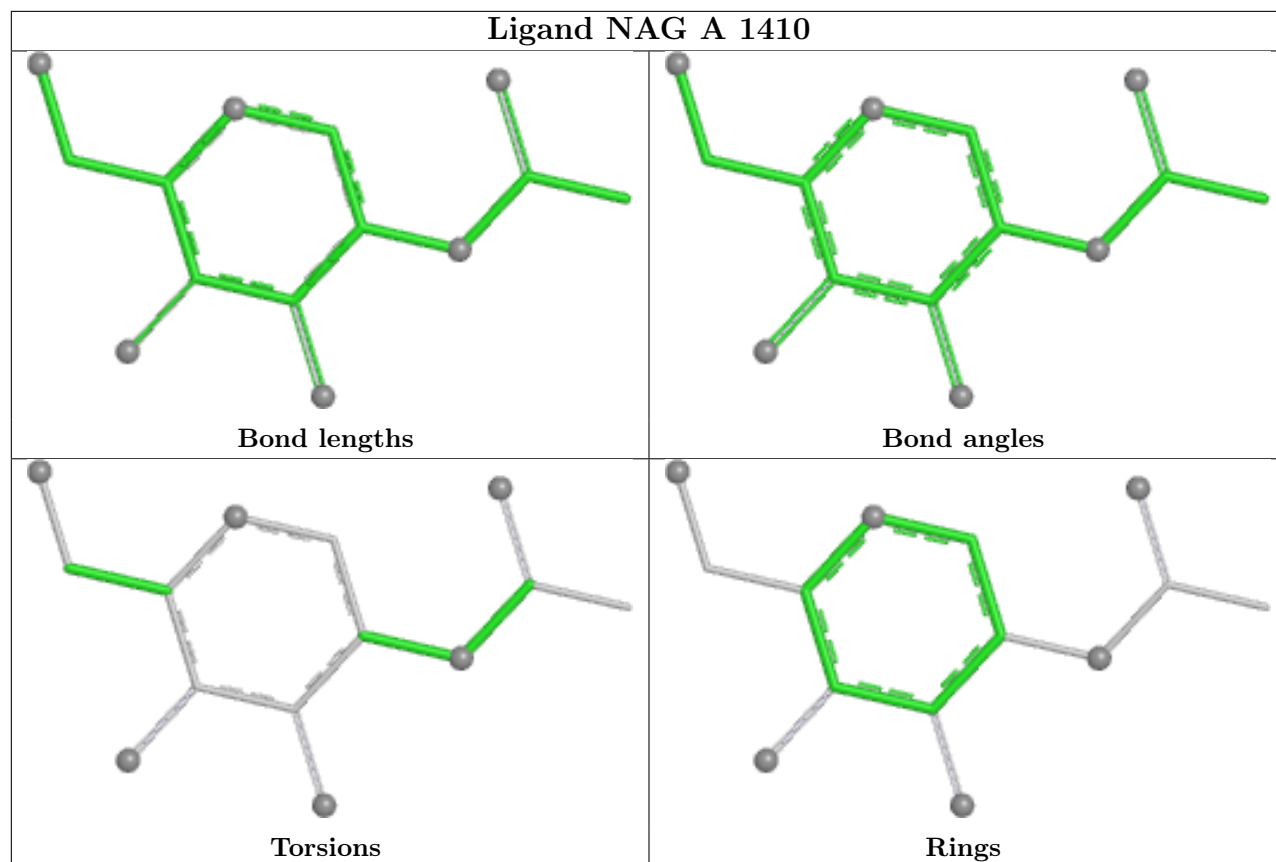
Ligand NAG A 1407



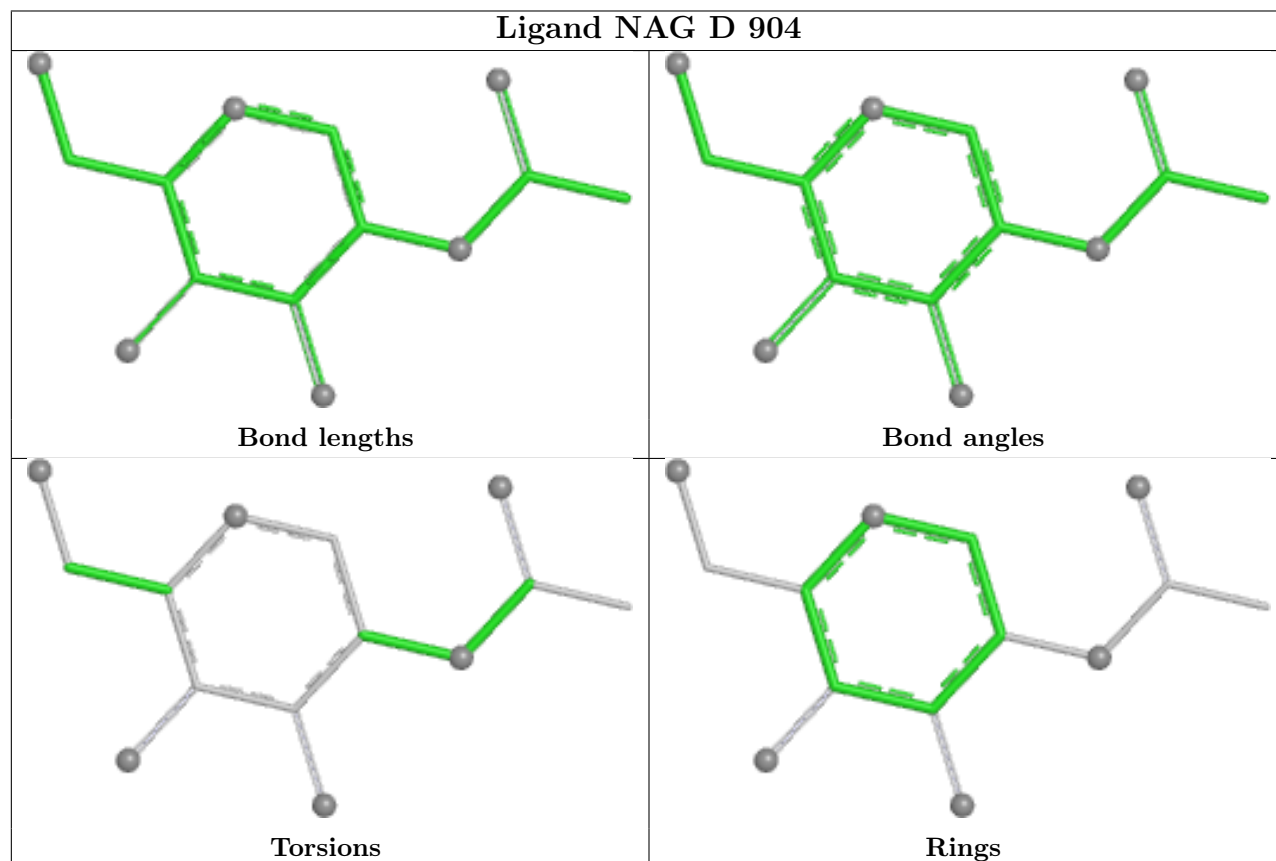
Ligand NAG C 1403

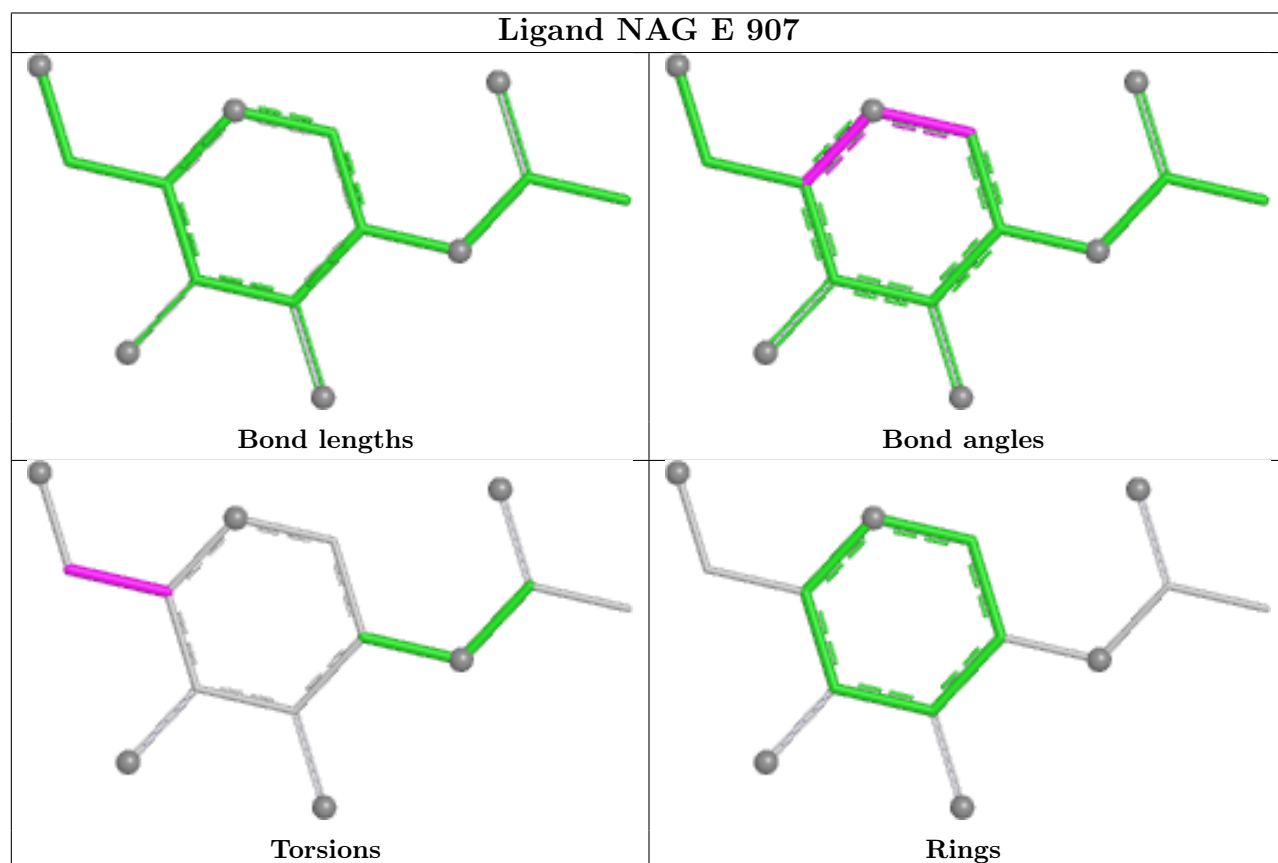
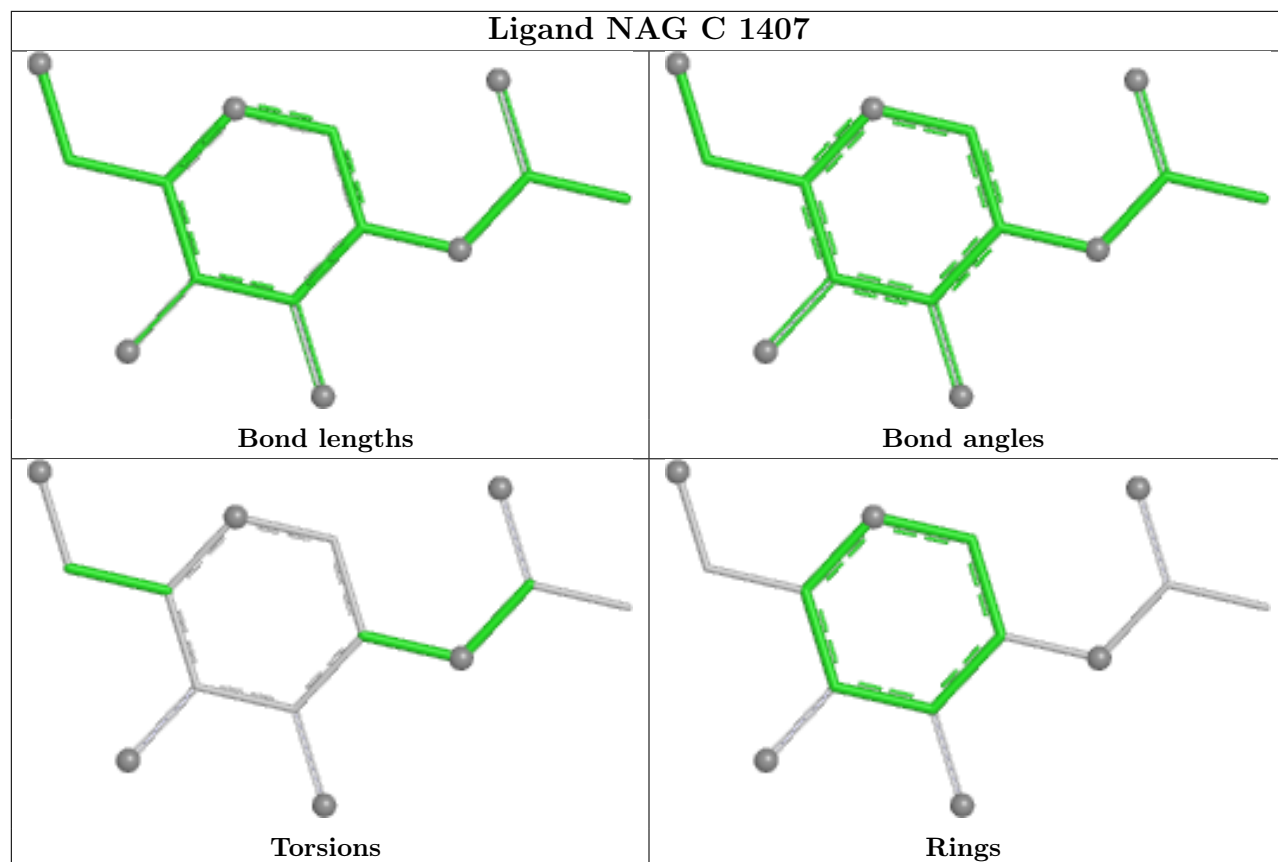


Ligand NAG A 1410

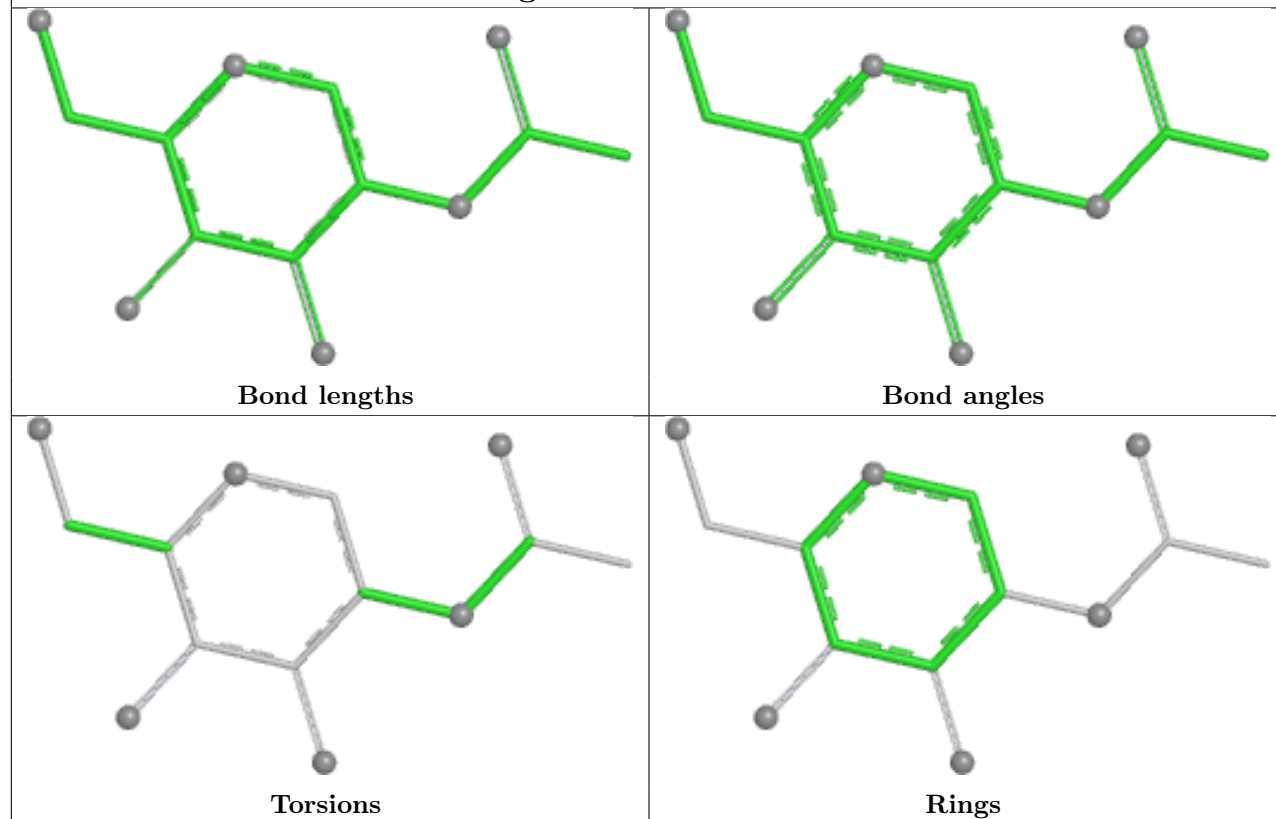


Ligand NAG D 904

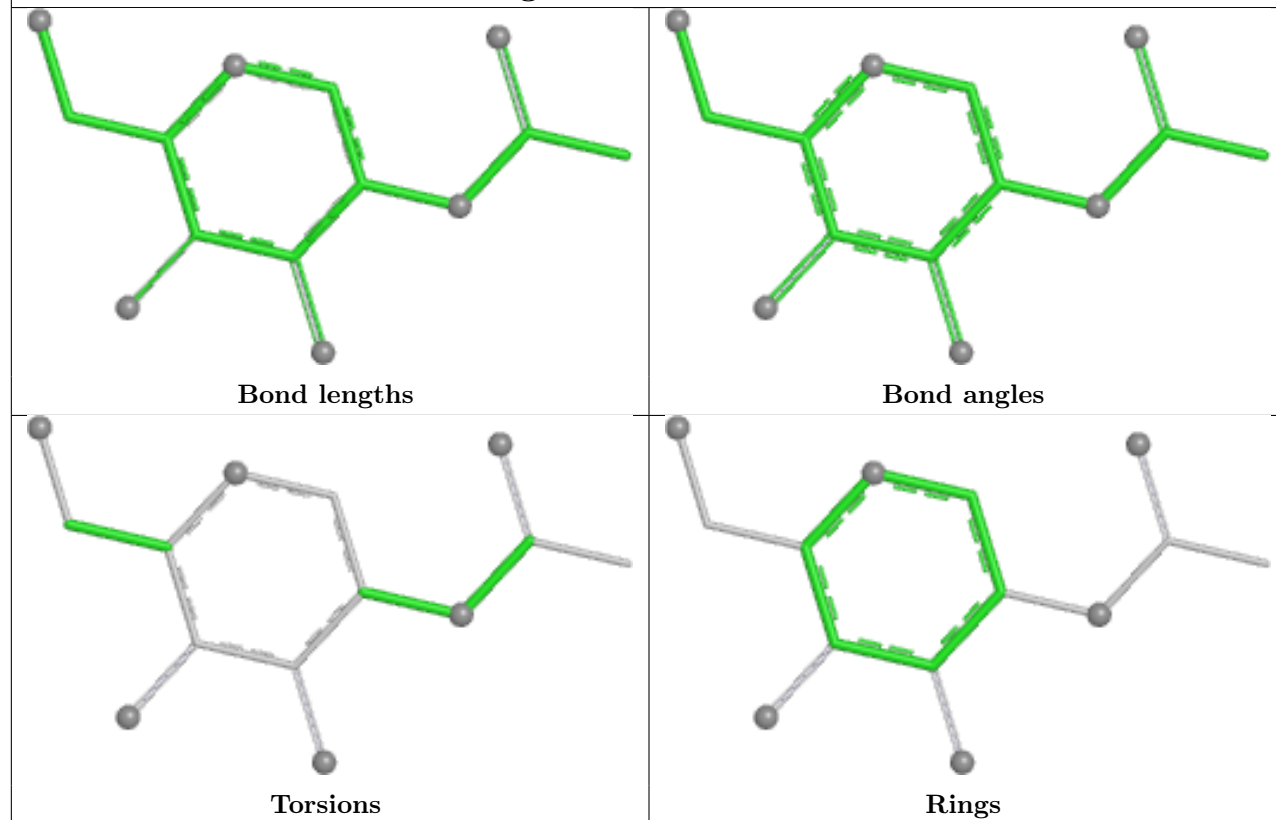


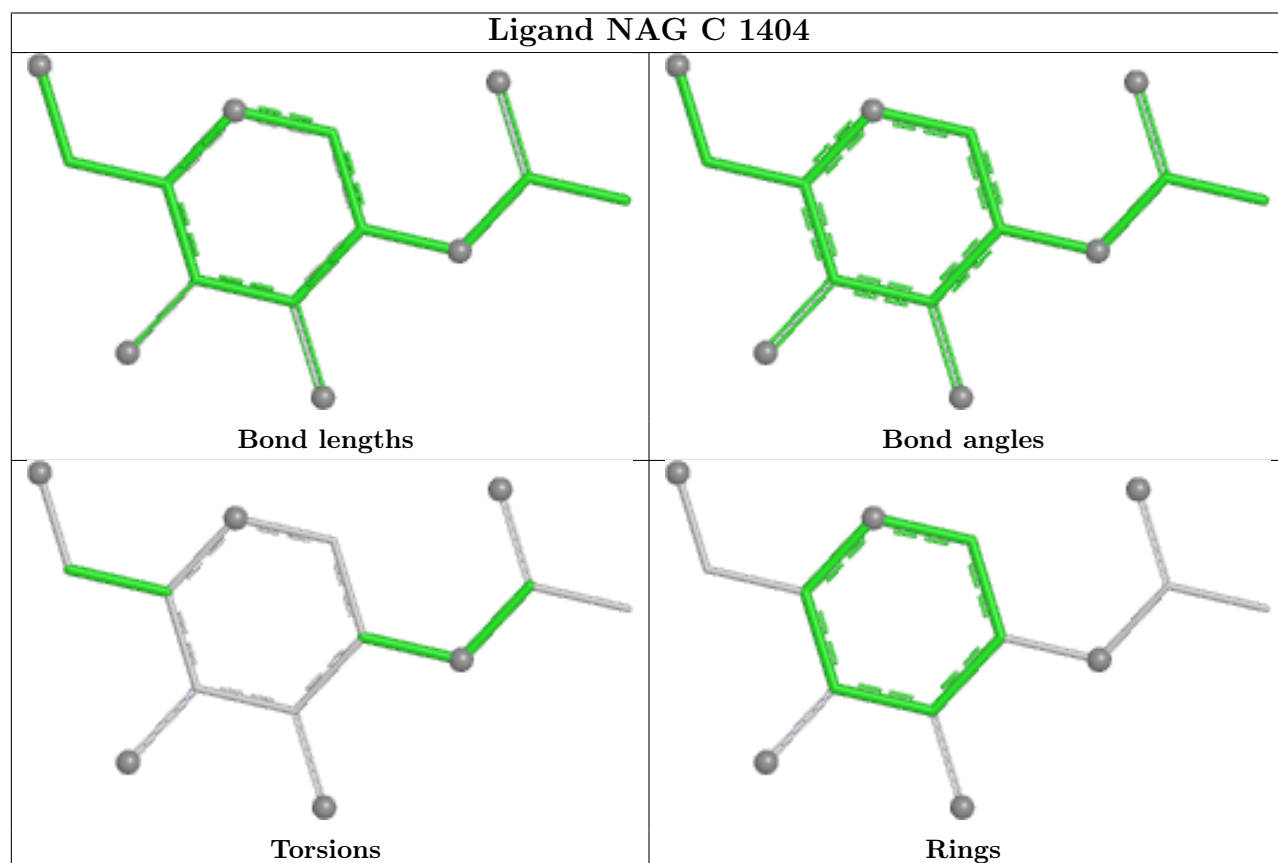
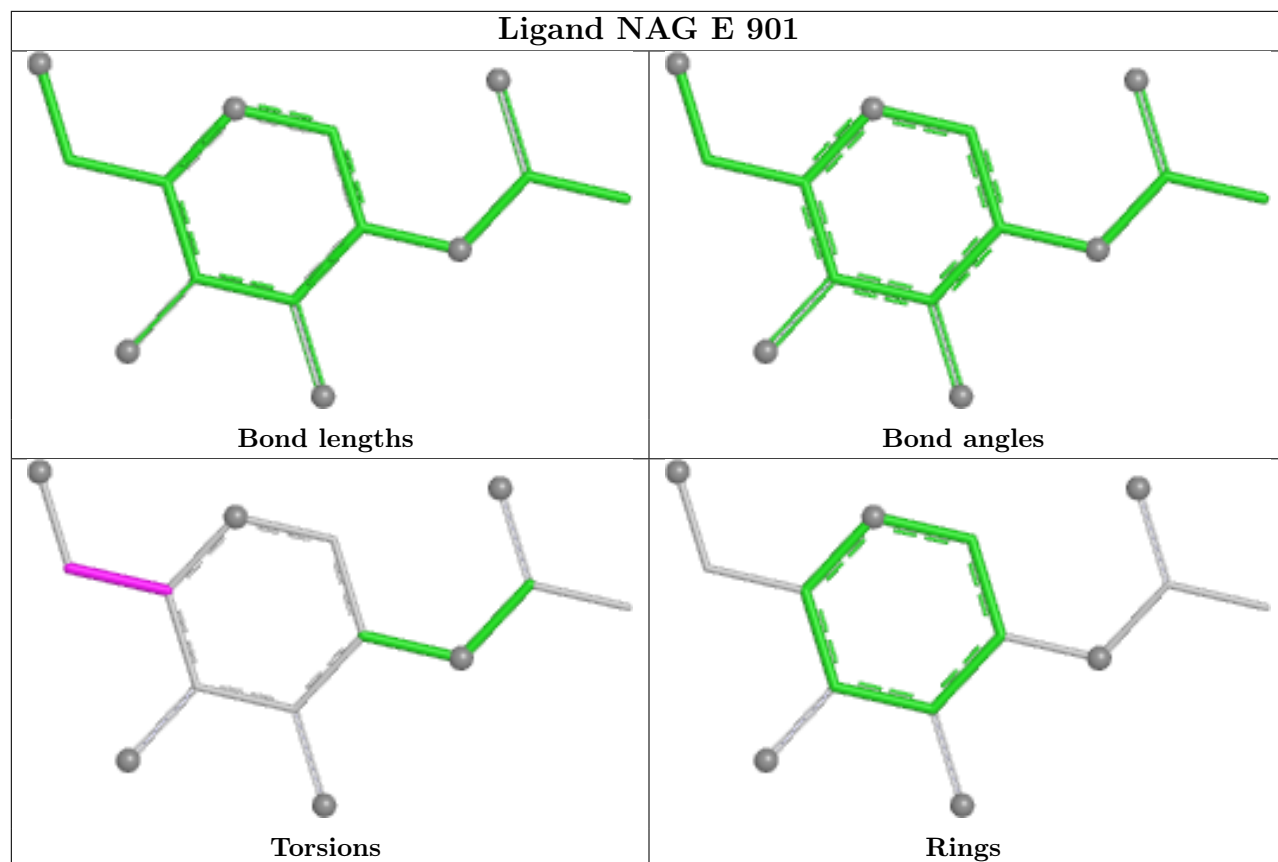


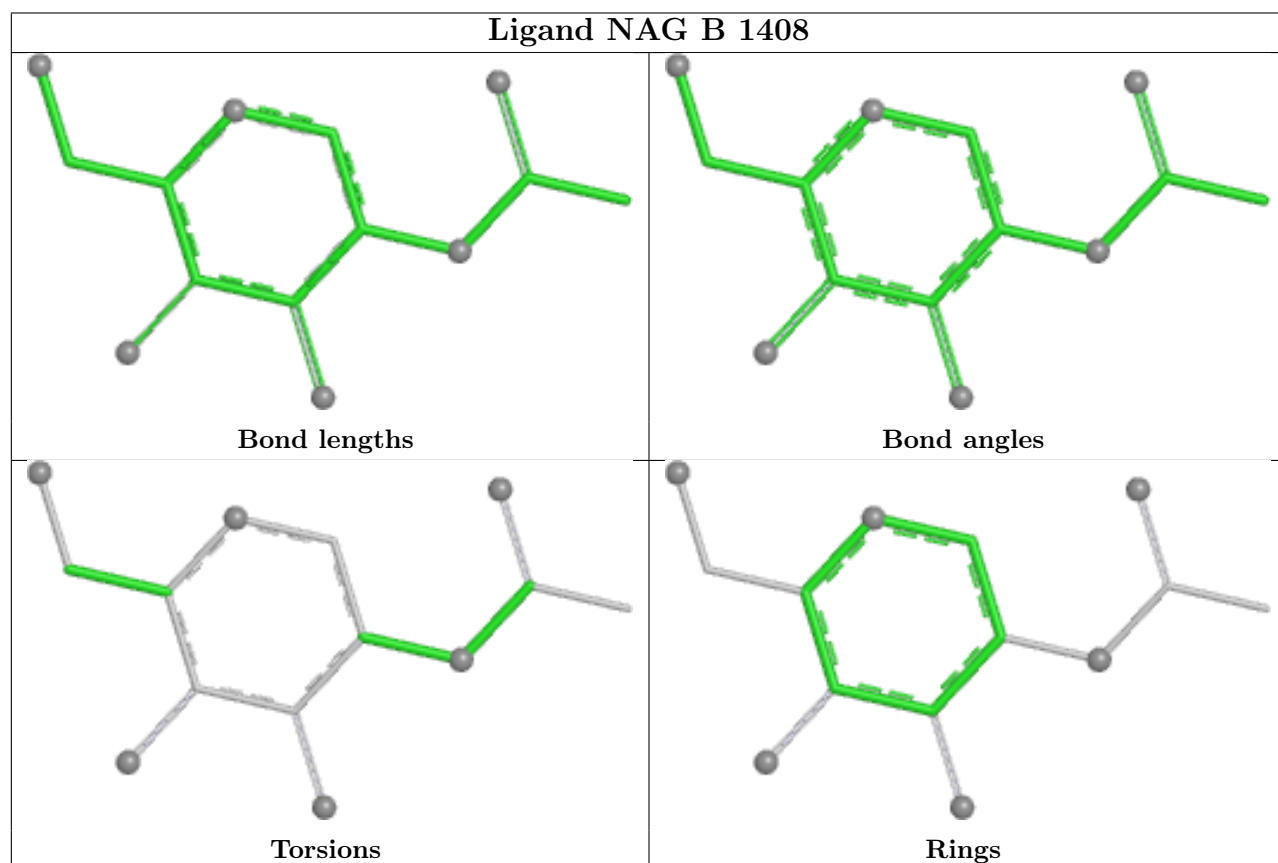
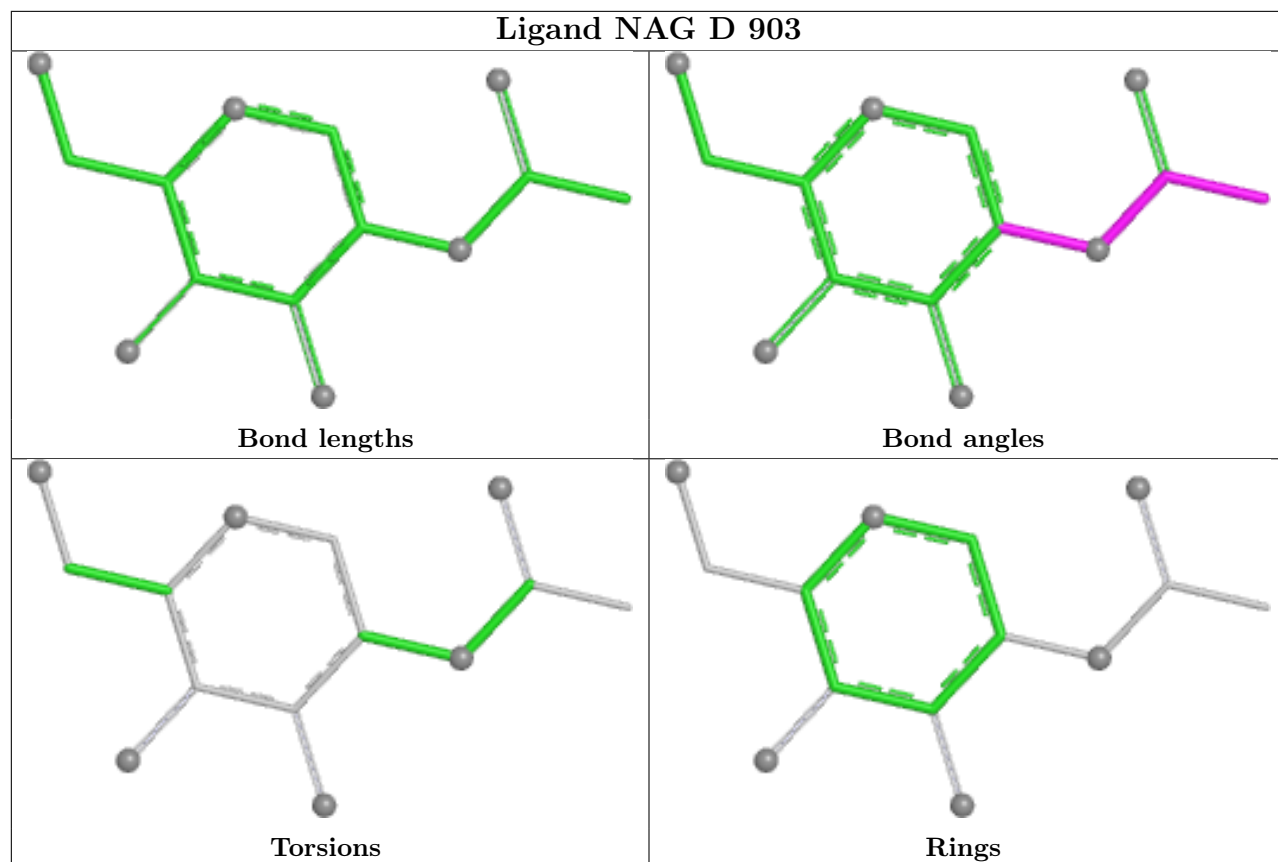
Ligand NAG A 1406



Ligand NAG B 1402







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.

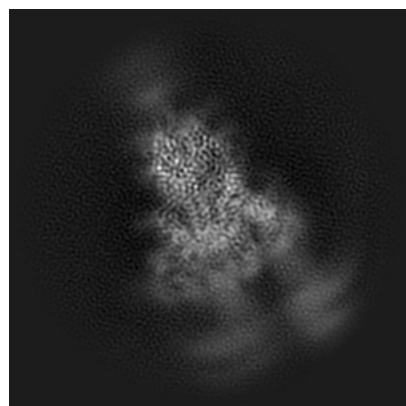
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33203. These allow visual inspection of the internal detail of the map and identification of artifacts.

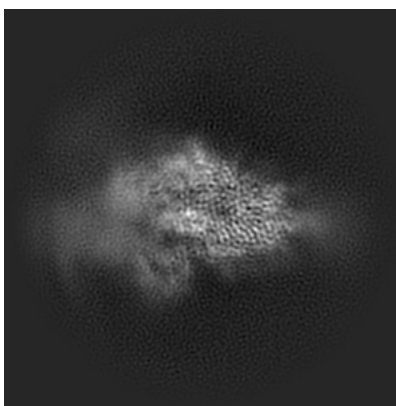
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

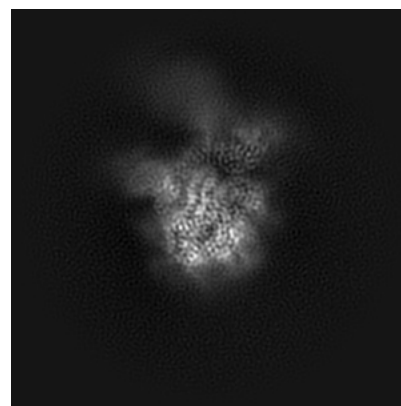
6.1.1 Primary map



X

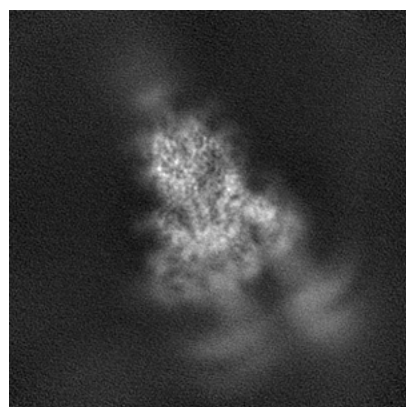


Y

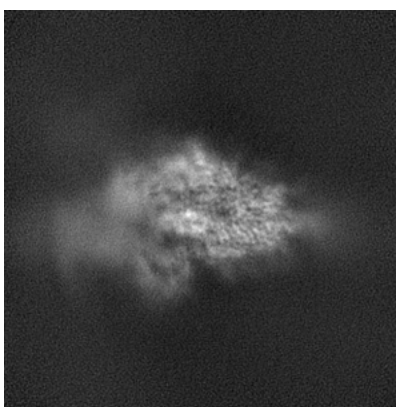


Z

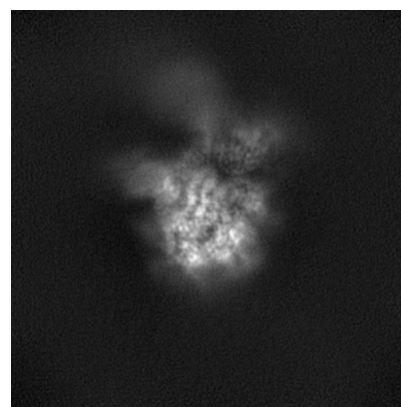
6.1.2 Raw map



X



Y

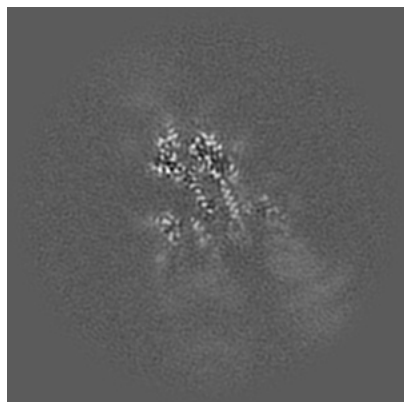


Z

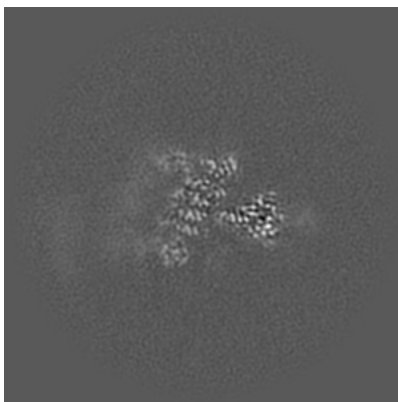
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

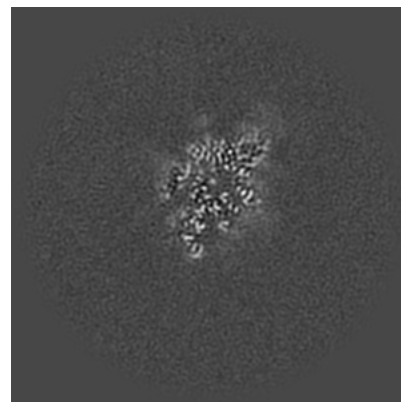
6.2.1 Primary map



X Index: 144

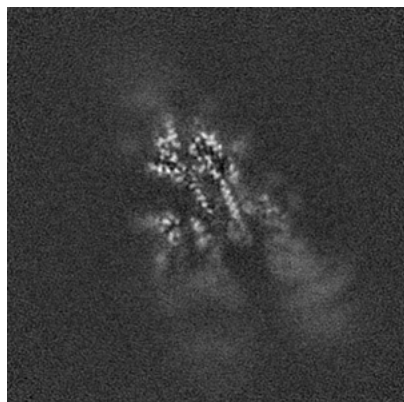


Y Index: 144

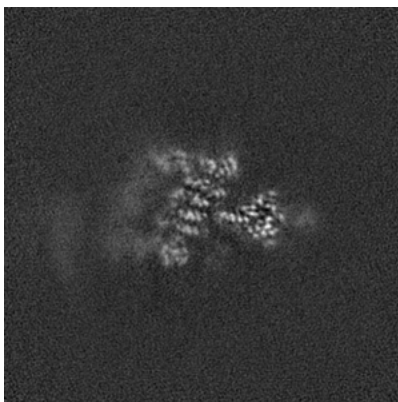


Z Index: 144

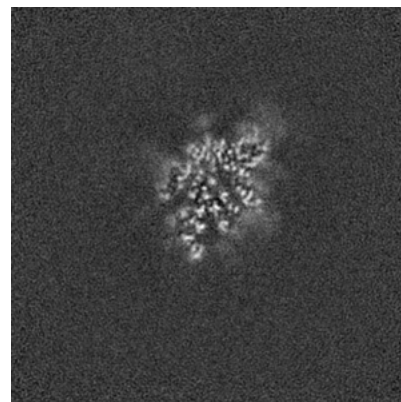
6.2.2 Raw map



X Index: 144



Y Index: 144

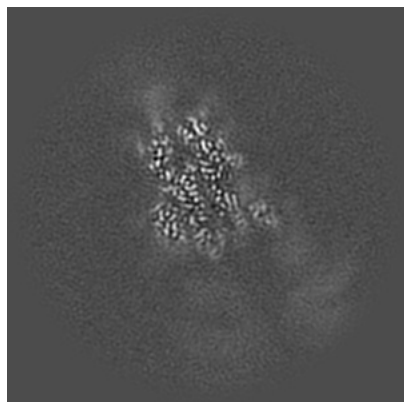


Z Index: 144

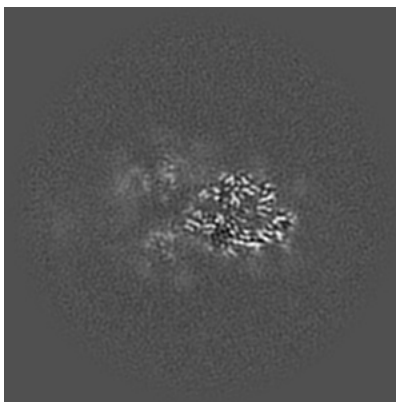
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

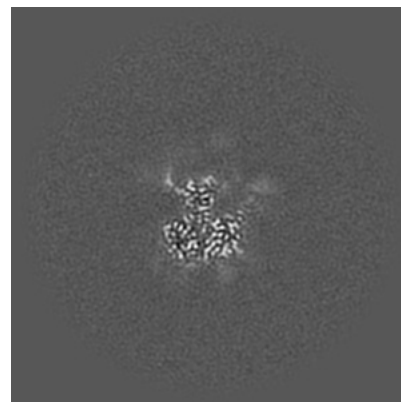
6.3.1 Primary map



X Index: 133

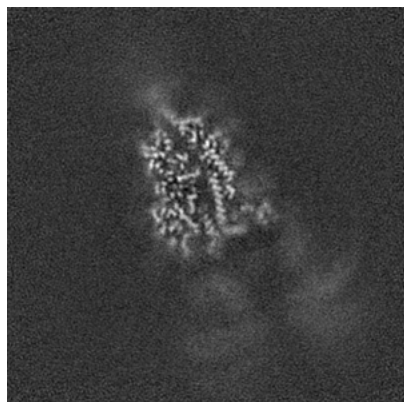


Y Index: 132

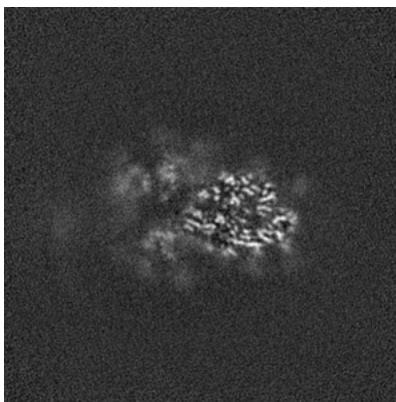


Z Index: 168

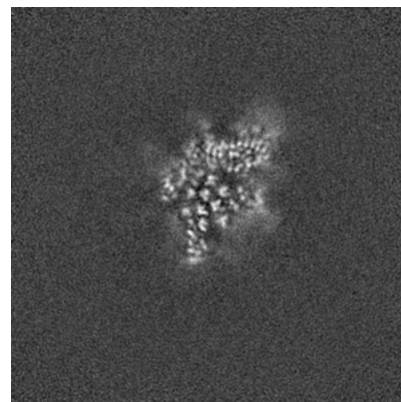
6.3.2 Raw map



X Index: 129



Y Index: 132

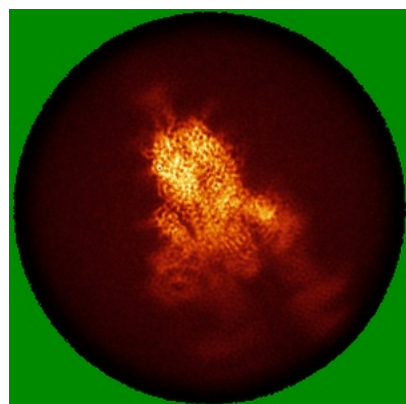


Z Index: 141

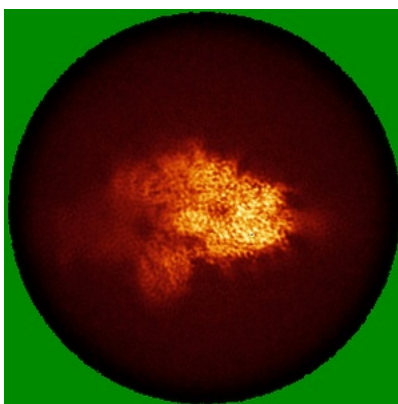
The images above show the largest variance slices of the map in three orthogonal directions.

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

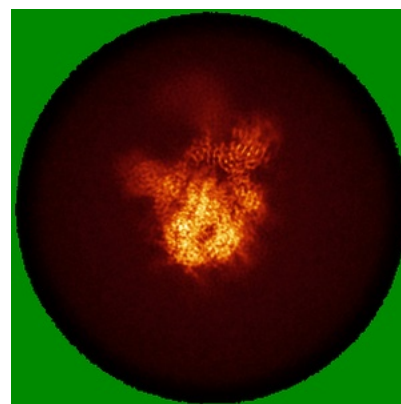
6.4.1 Primary map



X

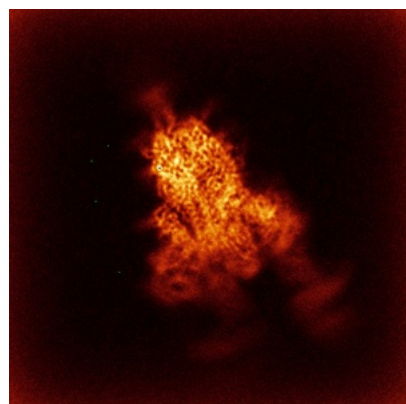


Y



Z

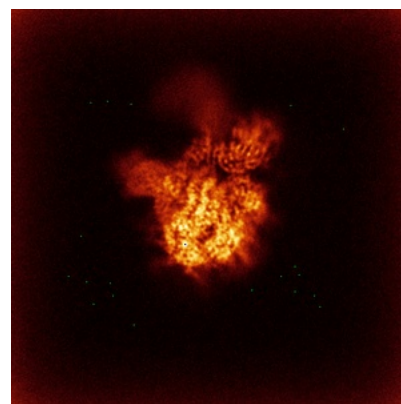
6.4.2 Raw map



X



Y

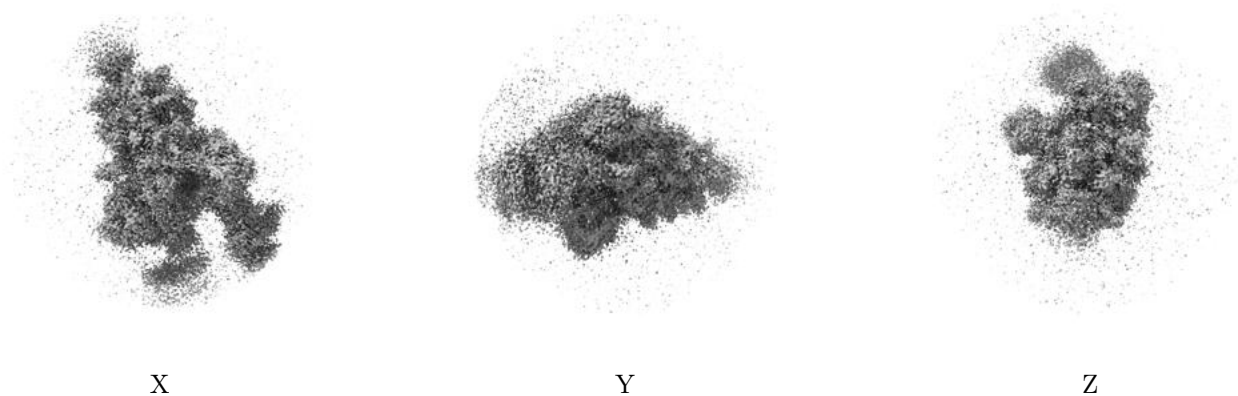


Z

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

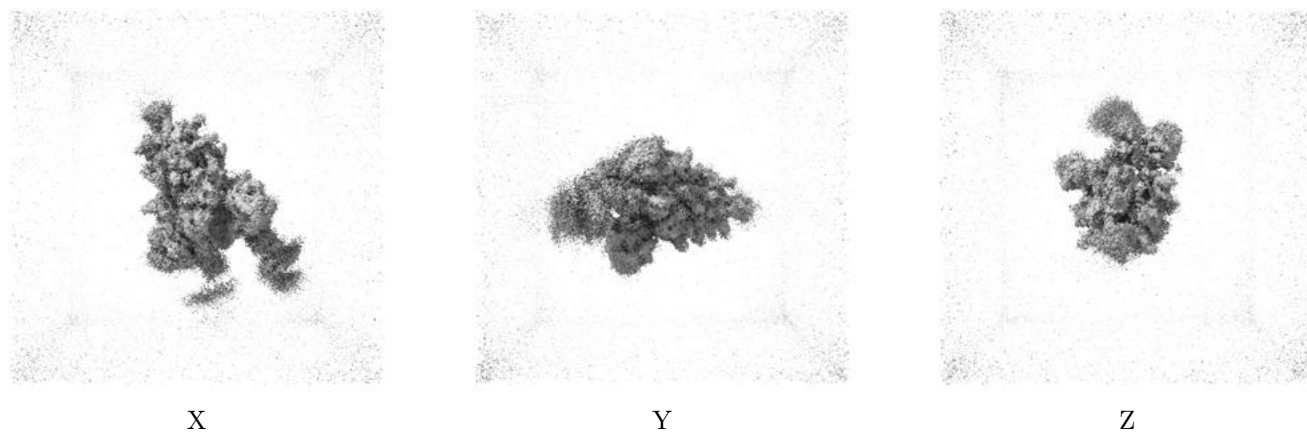
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

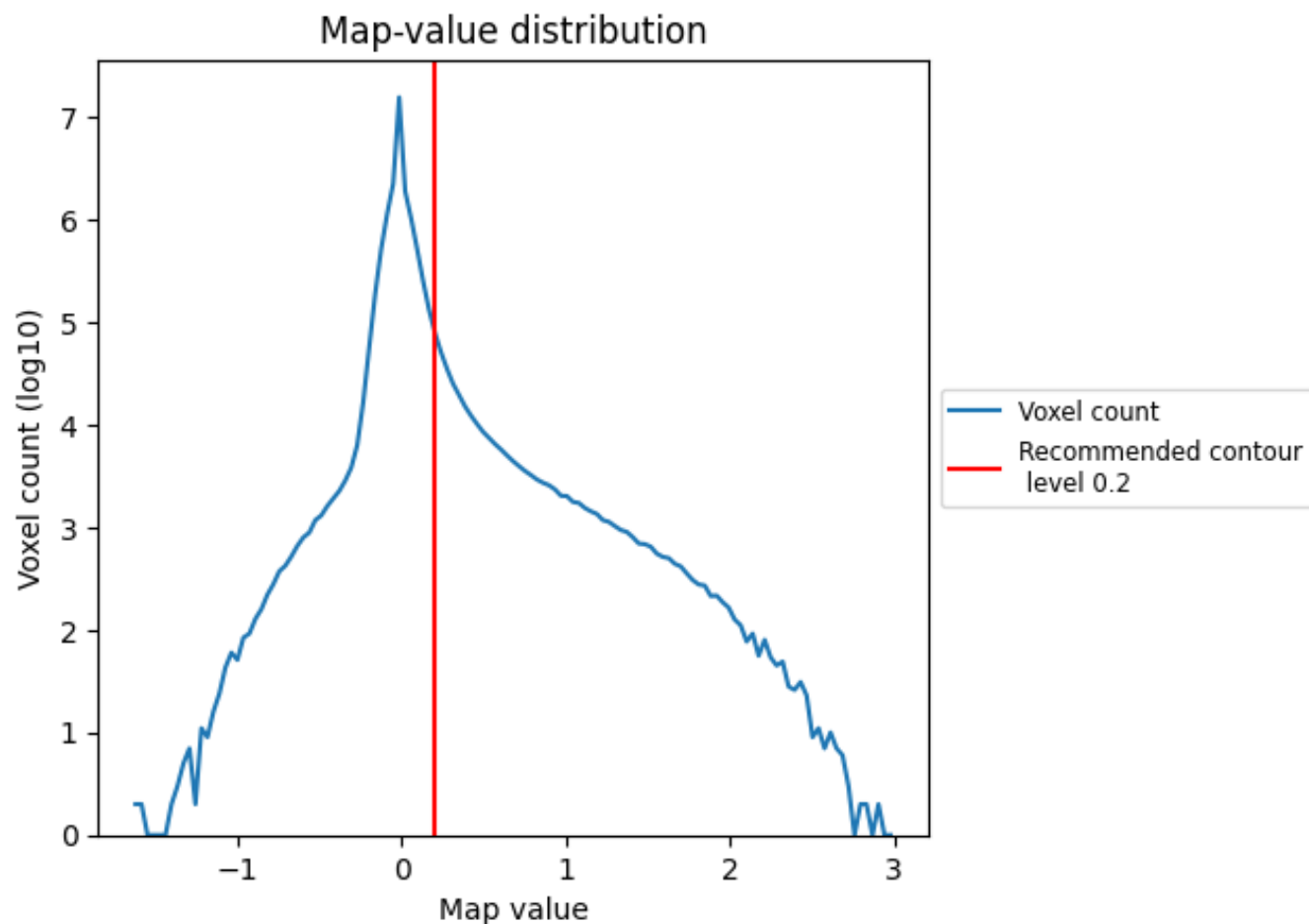
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

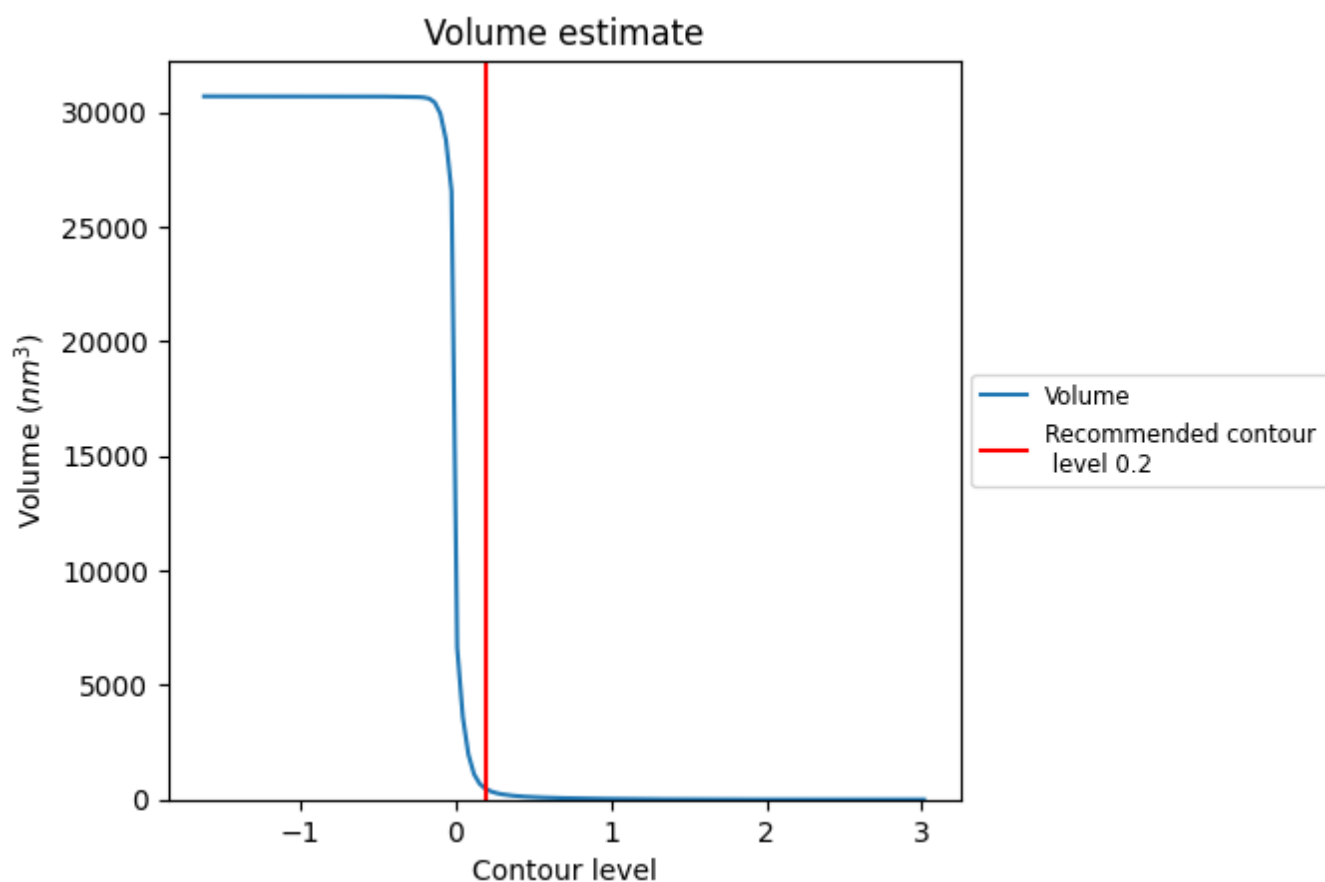
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

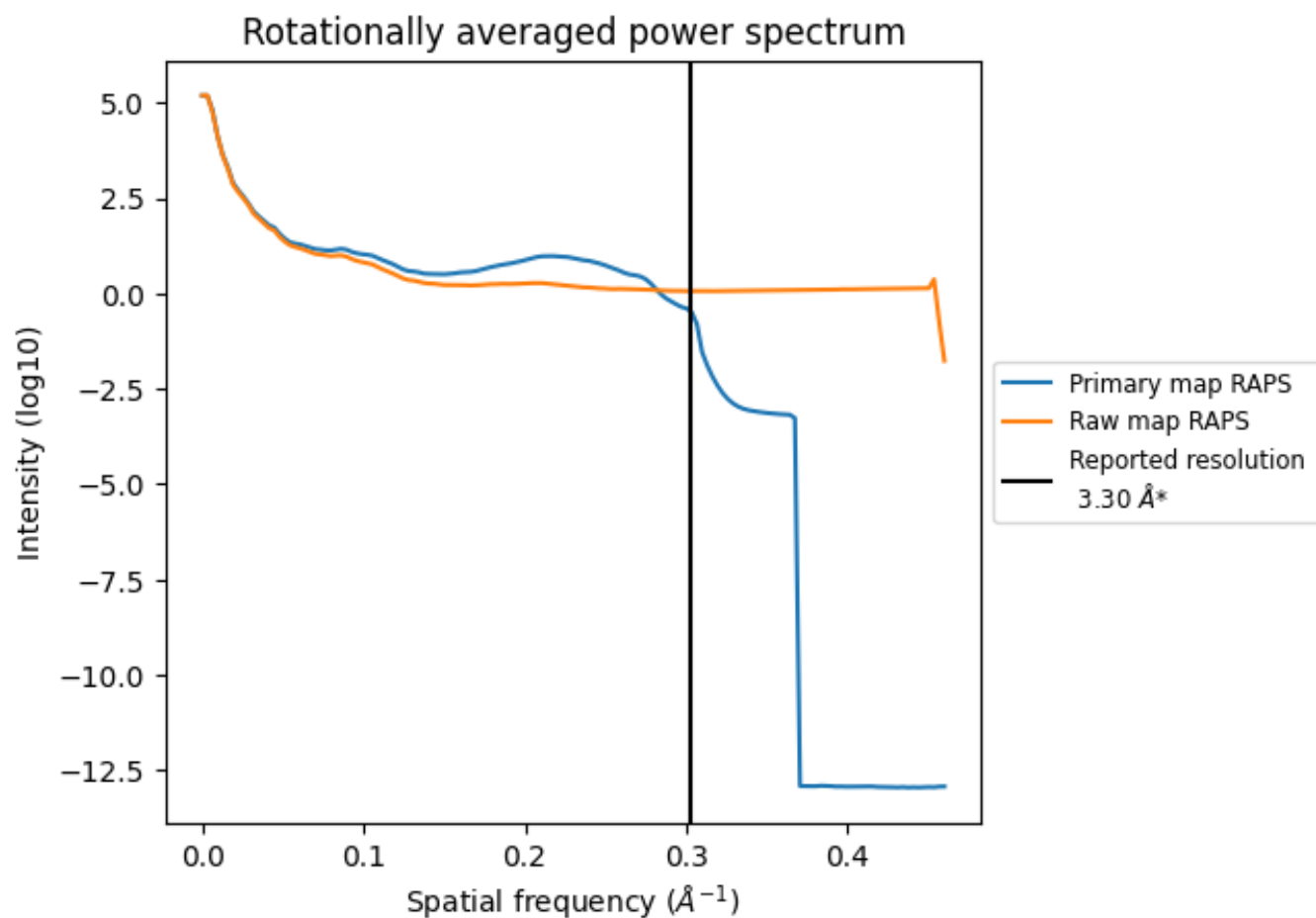
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 408 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 ⓘ

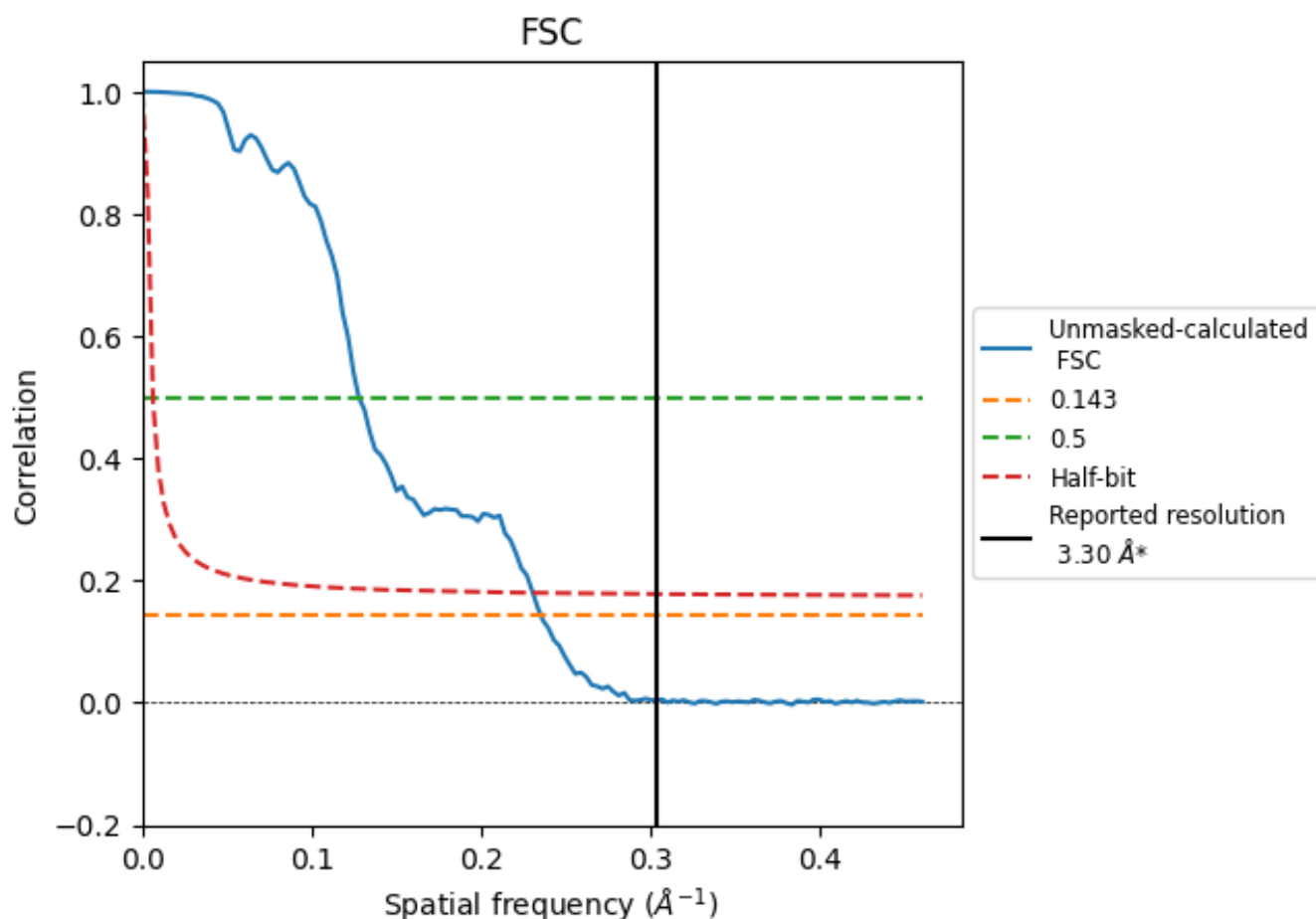


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

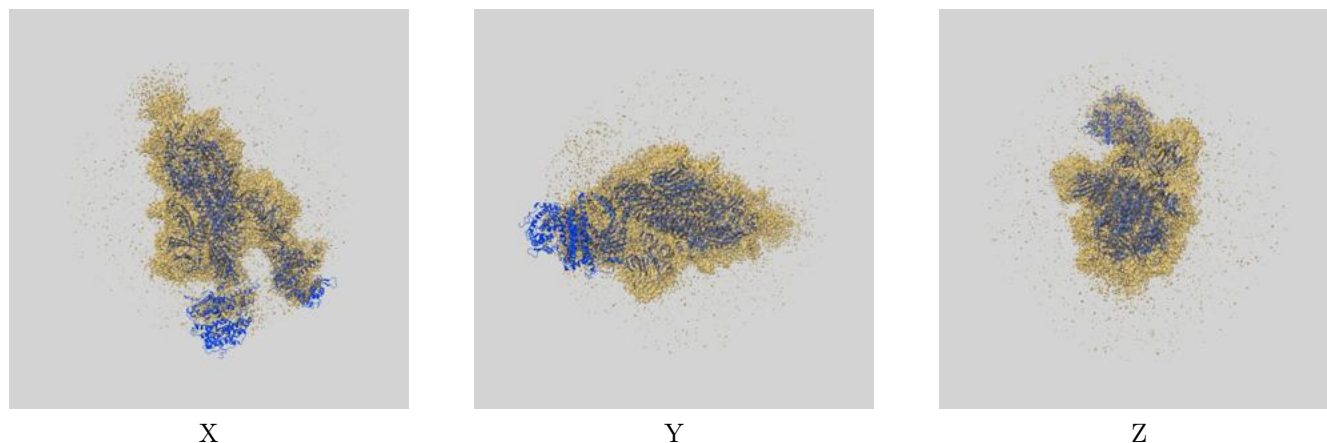
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.25	7.83	4.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

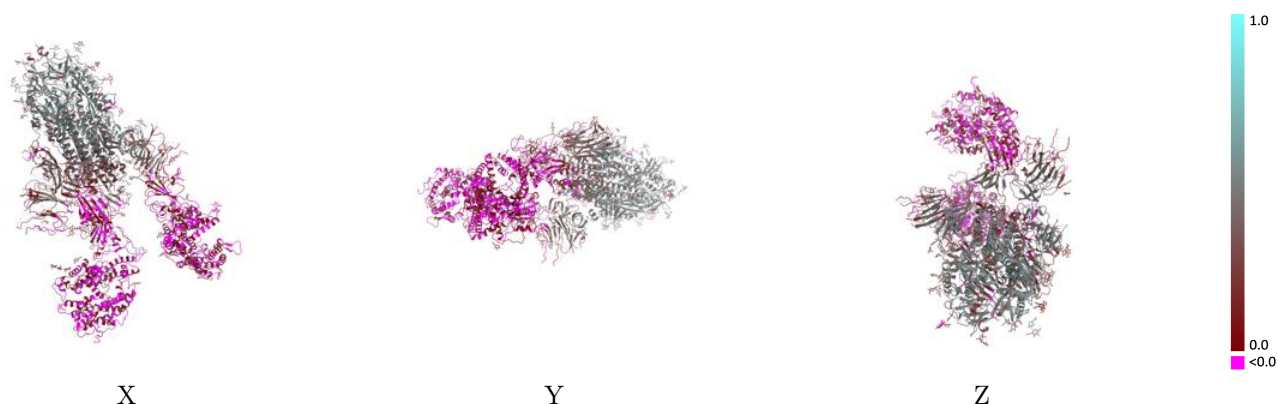
This section contains information regarding the fit between EMDB map EMD-33203 and PDB model 7XID. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



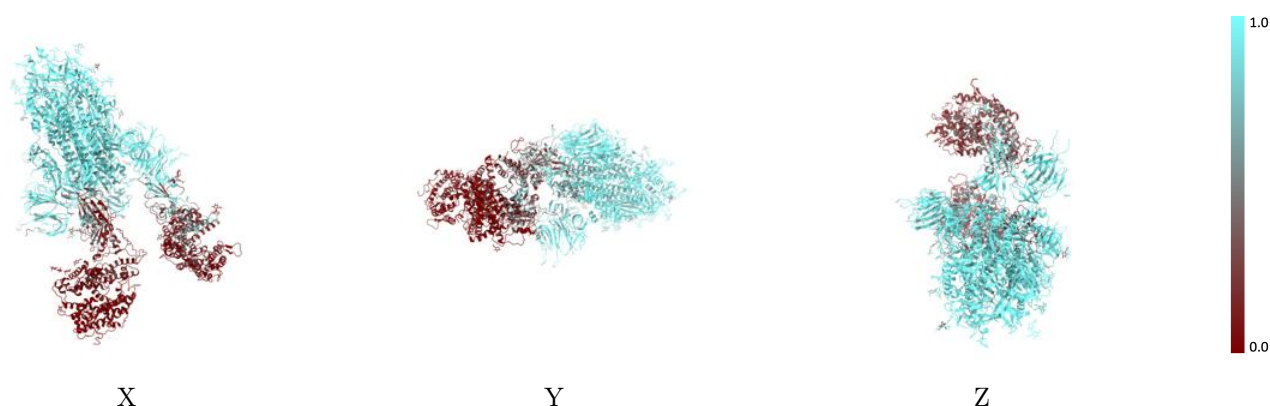
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



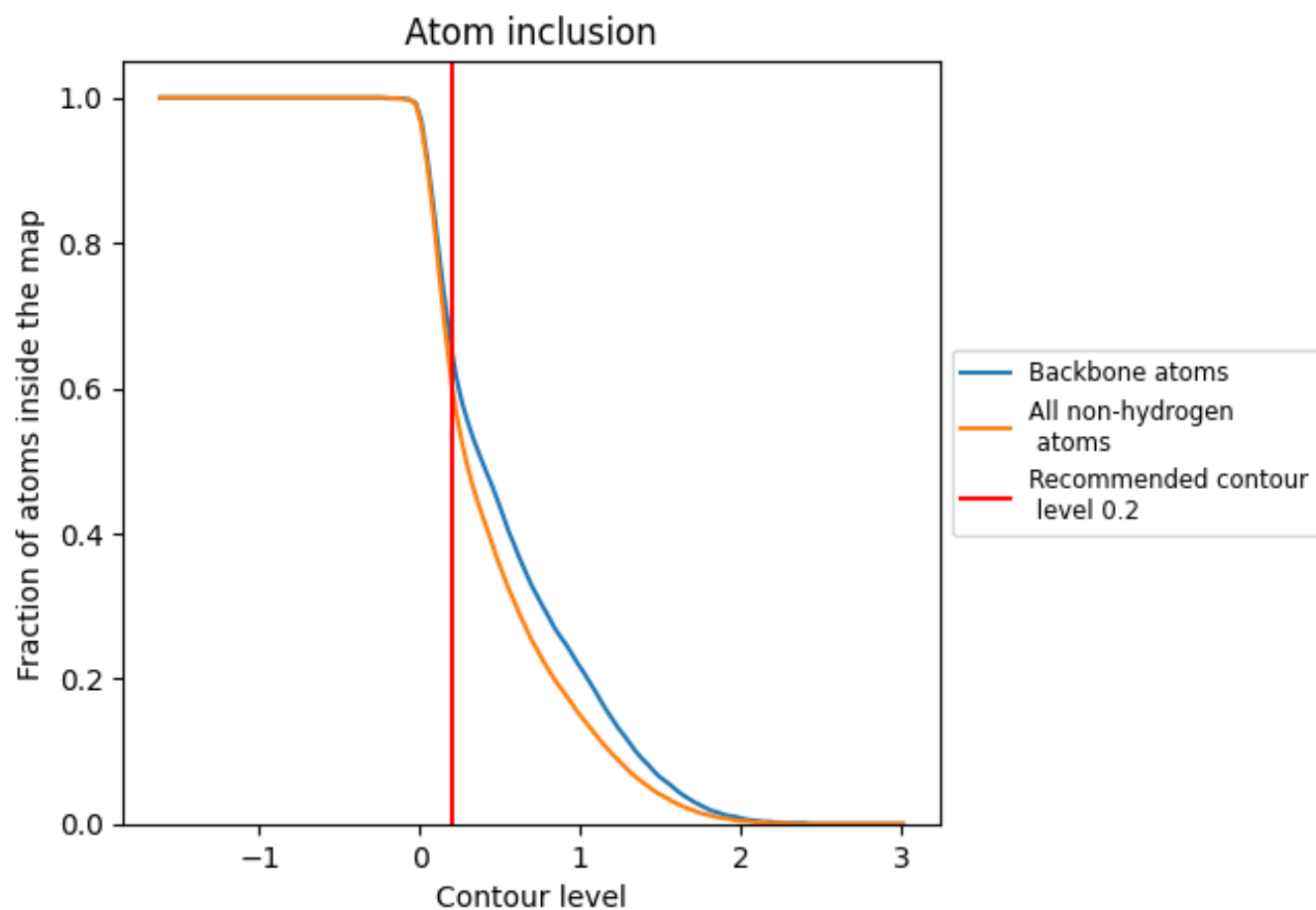
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.6050	 0.2340
A	 0.8250	 0.3430
B	 0.7820	 0.2950
C	 0.8350	 0.3350
D	 0.1560	 0.0170
E	 0.0400	 0.0150
F	 0.5000	 0.0540
G	 0.9640	 0.4330
H	 0.9290	 0.3310
I	 0.8570	 0.3310
J	 1.0000	 0.4650
K	 0.9640	 0.4130
L	 0.8570	 0.2420
M	 0.3930	 0.1630
N	 0.4290	 0.0570
O	 0.9290	 0.3700
P	 0.9290	 0.3030
Q	 0.9640	 0.3670
R	 0.8570	 0.3030
S	 0.8930	 0.3210
T	 0.3210	 -0.0170
U	 0.5360	 0.1110
V	 1.0000	 0.4560
W	 0.8210	 0.3020
X	 0.9290	 0.3490
Y	 0.8930	 0.3180
Z	 0.8930	 0.2670
a	 0.1070	 -0.0600
b	 0.0710	 0.0160

