



wwPDB EM Validation Summary Report ⓘ

Jan 14, 2025 – 04:33 PM JST

PDB ID : 8XYH
EMDB ID : EMD-38773
Title : Cryo-EM structure of BANAL-20-52 spike protein (6P)
Authors : Xu, Z.P.; Li, L.J.; Gu, Y.H.; Qi, J.X.; Gao, G.F.
Deposited on : 2024-01-19
Resolution : 2.50 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

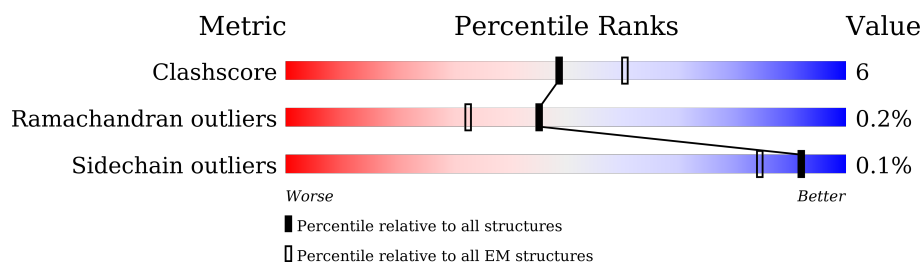
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1282	
1	B	1282	
1	C	1282	
2	D	2	
2	E	2	
2	F	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25878 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	1073	Total	C	N	O	S	0	0
			8368	5335	1400	1595	38		
1	B	1073	Total	C	N	O	S	0	0
			8368	5335	1400	1595	38		
1	C	1073	Total	C	N	O	S	0	0
			8368	5335	1400	1595	38		

There are 285 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	PHE	conflict	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	76	ILE	THR	variant	UNP P0DTC2
A	147	ARG	LYS	variant	UNP P0DTC2
A	218	PRO	GLN	conflict	UNP P0DTC2
A	292	SER	ALA	conflict	UNP P0DTC2
A	346	THR	ARG	conflict	UNP P0DTC2
A	372	THR	ALA	conflict	UNP P0DTC2
A	402	VAL	ILE	conflict	UNP P0DTC2
A	498	HIS	GLN	conflict	UNP P0DTC2
A	519	ASN	HIS	conflict	UNP P0DTC2
A	534	ILE	VAL	variant	UNP P0DTC2
A	604	ALA	THR	conflict	UNP P0DTC2
A	627	ASN	ASP	conflict	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	789	GLN	PRO	conflict	UNP P0DTC2
A	813	PRO	PHE	engineered mutation	UNP P0DTC2
A	888	PRO	ALA	engineered mutation	UNP P0DTC2
A	895	PRO	ALA	engineered mutation	UNP P0DTC2
A	938	PRO	ALA	engineered mutation	UNP P0DTC2
A	982	PRO	LYS	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	983	PRO	VAL	engineered mutation	UNP P0DTC2
A	1163	SER	GLY	conflict	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	GLY	-	expression tag	UNP P0DTC2
A	1217	SER	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	SER	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	ILE	-	expression tag	UNP P0DTC2
A	1225	PRO	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2
A	1227	ALA	-	expression tag	UNP P0DTC2
A	1228	PRO	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLN	-	expression tag	UNP P0DTC2
A	1233	ALA	-	expression tag	UNP P0DTC2
A	1234	TYR	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	LYS	-	expression tag	UNP P0DTC2
A	1238	ASP	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLU	-	expression tag	UNP P0DTC2
A	1241	TRP	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	THR	-	expression tag	UNP P0DTC2
A	1247	PHE	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	SER	-	expression tag	UNP P0DTC2
A	1253	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1254	TRP	-	expression tag	UNP P0DTC2
A	1255	SER	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	PRO	-	expression tag	UNP P0DTC2
A	1258	GLN	-	expression tag	UNP P0DTC2
A	1259	PHE	-	expression tag	UNP P0DTC2
A	1260	GLU	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	SER	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	SER	-	expression tag	UNP P0DTC2
A	1273	SER	-	expression tag	UNP P0DTC2
A	1274	ALA	-	expression tag	UNP P0DTC2
A	1275	TRP	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
A	1278	PRO	-	expression tag	UNP P0DTC2
A	1279	GLN	-	expression tag	UNP P0DTC2
A	1280	PHE	-	expression tag	UNP P0DTC2
A	1281	GLU	-	expression tag	UNP P0DTC2
A	1282	LYS	-	expression tag	UNP P0DTC2
B	32	SER	PHE	conflict	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	76	ILE	THR	variant	UNP P0DTC2
B	147	ARG	LYS	variant	UNP P0DTC2
B	218	PRO	GLN	conflict	UNP P0DTC2
B	292	SER	ALA	conflict	UNP P0DTC2
B	346	THR	ARG	conflict	UNP P0DTC2
B	372	THR	ALA	conflict	UNP P0DTC2
B	402	VAL	ILE	conflict	UNP P0DTC2
B	498	HIS	GLN	conflict	UNP P0DTC2
B	519	ASN	HIS	conflict	UNP P0DTC2
B	534	ILE	VAL	variant	UNP P0DTC2
B	604	ALA	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	627	ASN	ASP	conflict	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	789	GLN	PRO	conflict	UNP P0DTC2
B	813	PRO	PHE	engineered mutation	UNP P0DTC2
B	888	PRO	ALA	engineered mutation	UNP P0DTC2
B	895	PRO	ALA	engineered mutation	UNP P0DTC2
B	938	PRO	ALA	engineered mutation	UNP P0DTC2
B	982	PRO	LYS	engineered mutation	UNP P0DTC2
B	983	PRO	VAL	engineered mutation	UNP P0DTC2
B	1163	SER	GLY	conflict	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	GLY	-	expression tag	UNP P0DTC2
B	1217	SER	-	expression tag	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	SER	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	ILE	-	expression tag	UNP P0DTC2
B	1225	PRO	-	expression tag	UNP P0DTC2
B	1226	GLU	-	expression tag	UNP P0DTC2
B	1227	ALA	-	expression tag	UNP P0DTC2
B	1228	PRO	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLN	-	expression tag	UNP P0DTC2
B	1233	ALA	-	expression tag	UNP P0DTC2
B	1234	TYR	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	ARG	-	expression tag	UNP P0DTC2
B	1237	LYS	-	expression tag	UNP P0DTC2
B	1238	ASP	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	GLU	-	expression tag	UNP P0DTC2
B	1241	TRP	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	SER	-	expression tag	UNP P0DTC2
B	1246	THR	-	expression tag	UNP P0DTC2
B	1247	PHE	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	GLY	-	expression tag	UNP P0DTC2
B	1252	SER	-	expression tag	UNP P0DTC2
B	1253	ALA	-	expression tag	UNP P0DTC2
B	1254	TRP	-	expression tag	UNP P0DTC2
B	1255	SER	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	PRO	-	expression tag	UNP P0DTC2
B	1258	GLN	-	expression tag	UNP P0DTC2
B	1259	PHE	-	expression tag	UNP P0DTC2
B	1260	GLU	-	expression tag	UNP P0DTC2
B	1261	LYS	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	SER	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	GLY	-	expression tag	UNP P0DTC2
B	1272	SER	-	expression tag	UNP P0DTC2
B	1273	SER	-	expression tag	UNP P0DTC2
B	1274	ALA	-	expression tag	UNP P0DTC2
B	1275	TRP	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
B	1278	PRO	-	expression tag	UNP P0DTC2
B	1279	GLN	-	expression tag	UNP P0DTC2
B	1280	PHE	-	expression tag	UNP P0DTC2
B	1281	GLU	-	expression tag	UNP P0DTC2
B	1282	LYS	-	expression tag	UNP P0DTC2
C	32	SER	PHE	conflict	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	76	ILE	THR	variant	UNP P0DTC2
C	147	ARG	LYS	variant	UNP P0DTC2
C	218	PRO	GLN	conflict	UNP P0DTC2
C	292	SER	ALA	conflict	UNP P0DTC2
C	346	THR	ARG	conflict	UNP P0DTC2
C	372	THR	ALA	conflict	UNP P0DTC2
C	402	VAL	ILE	conflict	UNP P0DTC2
C	498	HIS	GLN	conflict	UNP P0DTC2
C	519	ASN	HIS	conflict	UNP P0DTC2
C	534	ILE	VAL	variant	UNP P0DTC2
C	604	ALA	THR	conflict	UNP P0DTC2
C	627	ASN	ASP	conflict	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	789	GLN	PRO	conflict	UNP P0DTC2
C	813	PRO	PHE	engineered mutation	UNP P0DTC2
C	888	PRO	ALA	engineered mutation	UNP P0DTC2
C	895	PRO	ALA	engineered mutation	UNP P0DTC2
C	938	PRO	ALA	engineered mutation	UNP P0DTC2
C	982	PRO	LYS	engineered mutation	UNP P0DTC2
C	983	PRO	VAL	engineered mutation	UNP P0DTC2
C	1163	SER	GLY	conflict	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	GLY	-	expression tag	UNP P0DTC2
C	1217	SER	-	expression tag	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	GLY	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	SER	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	ILE	-	expression tag	UNP P0DTC2
C	1225	PRO	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	ALA	-	expression tag	UNP P0DTC2
C	1228	PRO	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1232	GLN	-	expression tag	UNP P0DTC2
C	1233	ALA	-	expression tag	UNP P0DTC2
C	1234	TYR	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	LYS	-	expression tag	UNP P0DTC2
C	1238	ASP	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLU	-	expression tag	UNP P0DTC2
C	1241	TRP	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	SER	-	expression tag	UNP P0DTC2
C	1246	THR	-	expression tag	UNP P0DTC2
C	1247	PHE	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	SER	-	expression tag	UNP P0DTC2
C	1253	ALA	-	expression tag	UNP P0DTC2
C	1254	TRP	-	expression tag	UNP P0DTC2
C	1255	SER	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	PRO	-	expression tag	UNP P0DTC2
C	1258	GLN	-	expression tag	UNP P0DTC2
C	1259	PHE	-	expression tag	UNP P0DTC2
C	1260	GLU	-	expression tag	UNP P0DTC2
C	1261	LYS	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	SER	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	SER	-	expression tag	UNP P0DTC2
C	1273	SER	-	expression tag	UNP P0DTC2

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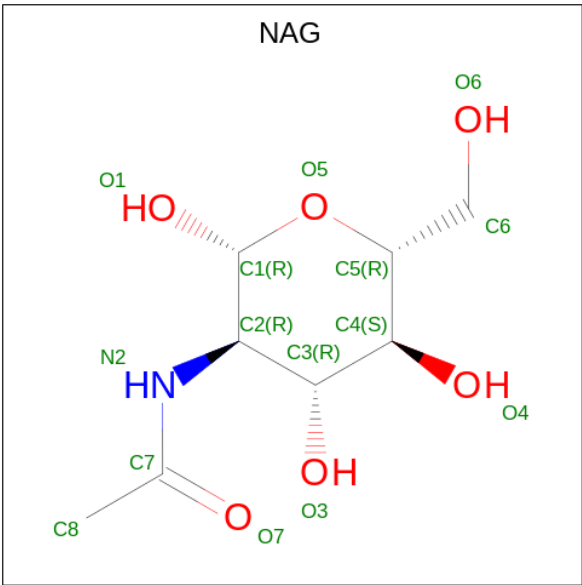
Chain	Residue	Modelled	Actual	Comment	Reference
C	1274	ALA	-	expression tag	UNP P0DTC2
C	1275	TRP	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	HIS	-	expression tag	UNP P0DTC2
C	1278	PRO	-	expression tag	UNP P0DTC2
C	1279	GLN	-	expression tag	UNP P0DTC2
C	1280	PHE	-	expression tag	UNP P0DTC2
C	1281	GLU	-	expression tag	UNP P0DTC2
C	1282	LYS	-	expression tag	UNP P0DTC2

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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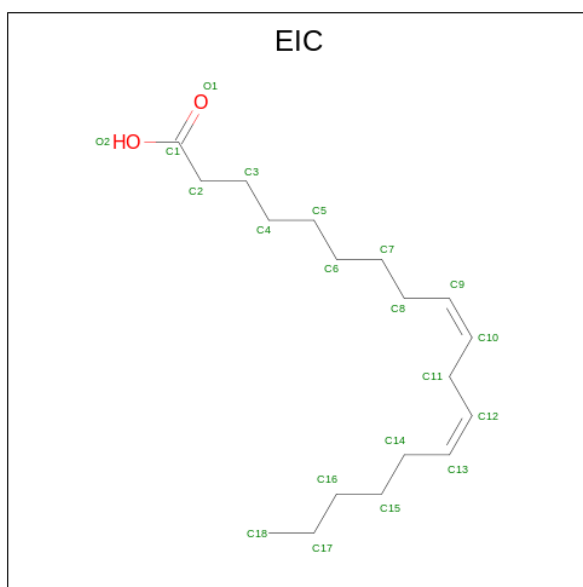
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B	1	Total 14	C 8	N 1	O 5	0
3	B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

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

- Molecule 4 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			20	18	2	

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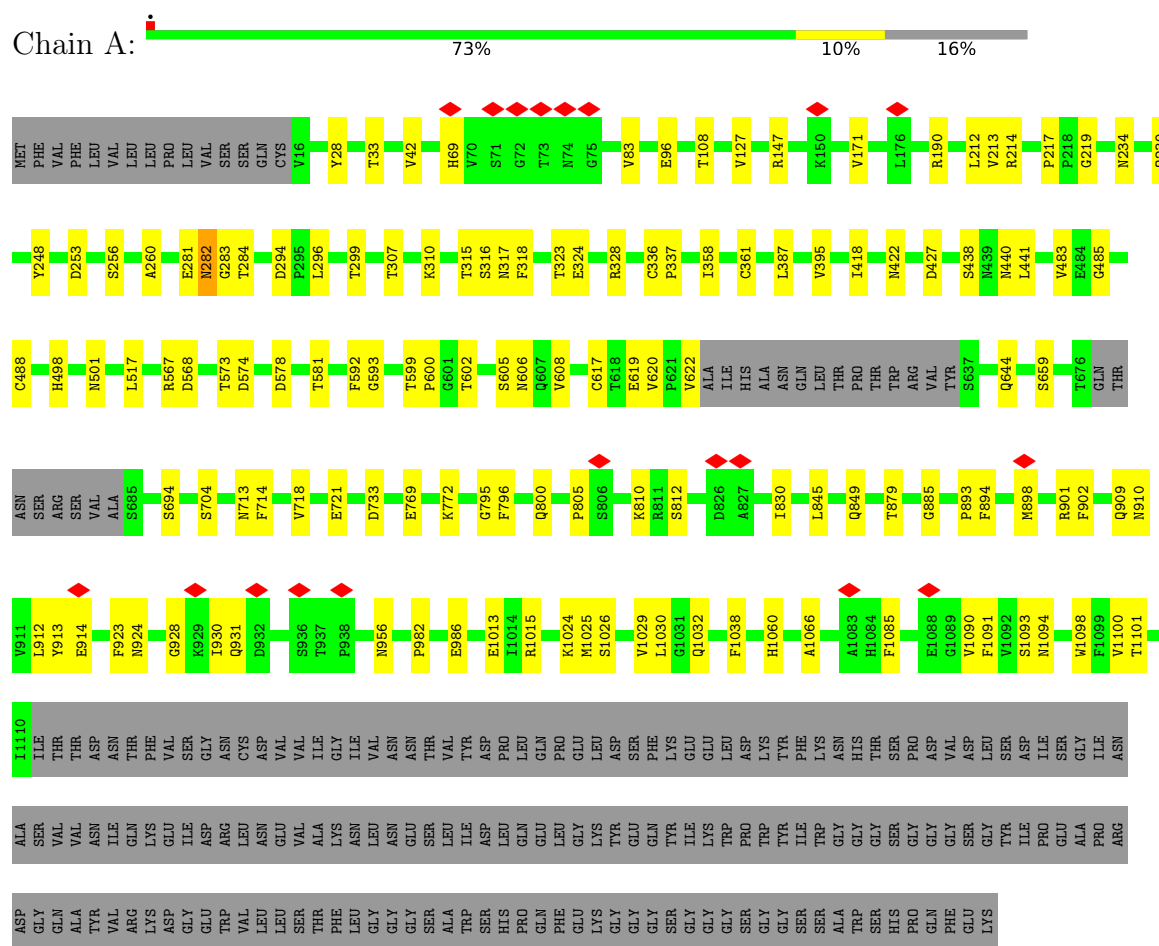
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Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			20	18	2	
4	C	1	Total	C	O	0
			20	18	2	

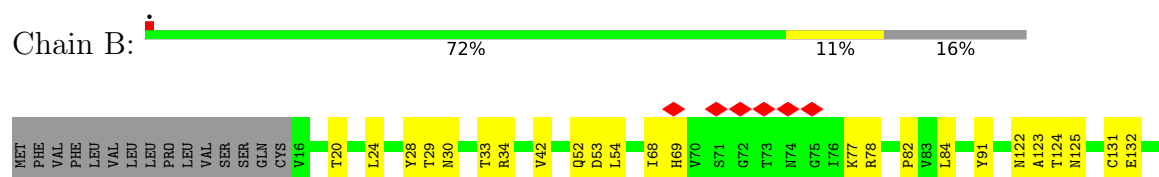
3 Residue-property plots

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

• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



ASP
ILE
SER
GLY
ILE
ASN
ALA
SER
VAL
ASN
ILE
GLN
LYS
GLU
ILE
ASP
ARG
LEU
ASN
GLU
VAL
ALA
THR
PHE
LYS
LEU
ASN
GLY
GLY
SER
SER
ALA
LEU
TRP
ILE
ASP
LEU
GLN
GLU
PHE
GLY
LYS
TYR
GLY
GLN
TYR
SER
ILE
LYS
TRP
GLY
GLY
SER
GLY
GLY
GLY
GLY
GLY
GLY
GLY
TYR

ILE
PRO
GLU
ALA
ARG
ASP
GLY
GLN
ALA
VAL
ARG
LYS
ASP
GLY
GLU
TRP
VAL
LEU
LEU
SER
THR
PHE
LEU
GLY
GLY
GLY
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLY
LYS
GLY
GLY
GLY
SER
GLY
GLY
GLY
GLY
SER
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
SER
LYS

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

Chain D: 100%

MAG1
MAG2

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

Chain E: 100%

MAG1
MAG2

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

Chain F: 50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	253926	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.987	Depositor
Minimum map value	-0.435	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.69, 0.69, 0.69	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, EIC

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	0.29	0/8566	0.52	0/11661
1	B	0.29	0/8566	0.52	1/11661 (0.0%)
1	C	0.29	0/8566	0.52	0/11661
All	All	0.29	0/25698	0.52	1/34983 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	618	THR	N-CA-C	-5.14	97.12	111.00

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	8368	0	8156	94	0
1	B	8368	0	8153	103	0
1	C	8368	0	8156	98	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	2	0
3	A	210	0	195	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	210	0	195	9	0
3	C	210	0	195	2	0
4	A	20	0	31	4	0
4	B	20	0	31	4	0
4	C	20	0	31	3	0
All	All	25878	0	25218	284	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 284 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:ARG:NH1	1:A:1032:GLN:HB2	1.79	0.97
1:C:102:ARG:HH12	1:C:177:MET:CE	1.85	0.90
1:A:617:CYS:SG	1:A:644:GLN:NE2	2.50	0.84
1:C:189:LEU:O	1:C:189:LEU:HG	1.77	0.83
1:C:318:PHE:H	1:C:593:GLY:HA2	1.45	0.82

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	1067/1282 (83%)	998 (94%)	67 (6%)	2 (0%)	44	64
1	B	1067/1282 (83%)	998 (94%)	68 (6%)	1 (0%)	48	69
1	C	1067/1282 (83%)	988 (93%)	77 (7%)	2 (0%)	44	64
All	All	3201/3846 (83%)	2984 (93%)	212 (7%)	5 (0%)	45	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	GLY
1	C	150	LYS
1	A	281	GLU
1	B	483	VAL
1	C	483	VAL

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	934/1110 (84%)	933 (100%)	1 (0%)	92	97
1	B	934/1110 (84%)	934 (100%)	0	100	100
1	C	934/1110 (84%)	932 (100%)	2 (0%)	92	97
All	All	2802/3330 (84%)	2799 (100%)	3 (0%)	92	97

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

Mol	Chain	Res	Type
1	A	282	ASN
1	C	149	ASN
1	C	331	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	644	GLN
1	B	909	GLN
1	C	1007	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](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.29	0	17,19,21	0.41	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	E	1	2,1	14,14,15	0.40	0	17,19,21	0.44	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.69	0
2	NAG	F	1	2,1	14,14,15	0.45	0	17,19,21	1.39	3 (17%)
2	NAG	F	2	2	14,14,15	0.42	0	17,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C4-C3-C2	-2.93	106.72	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	O4-C4-C5	2.49	115.47	109.30
2	F	1	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

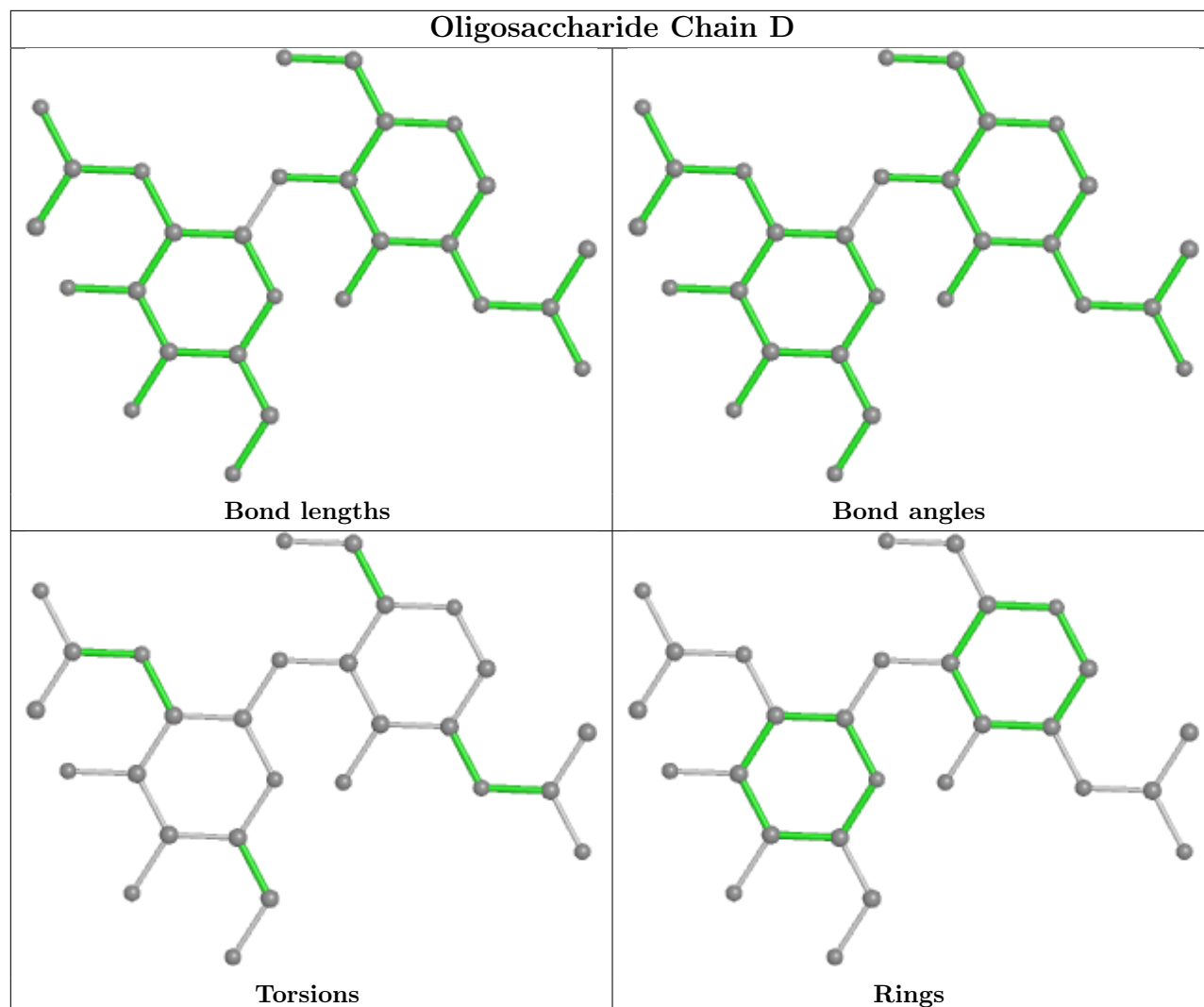
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

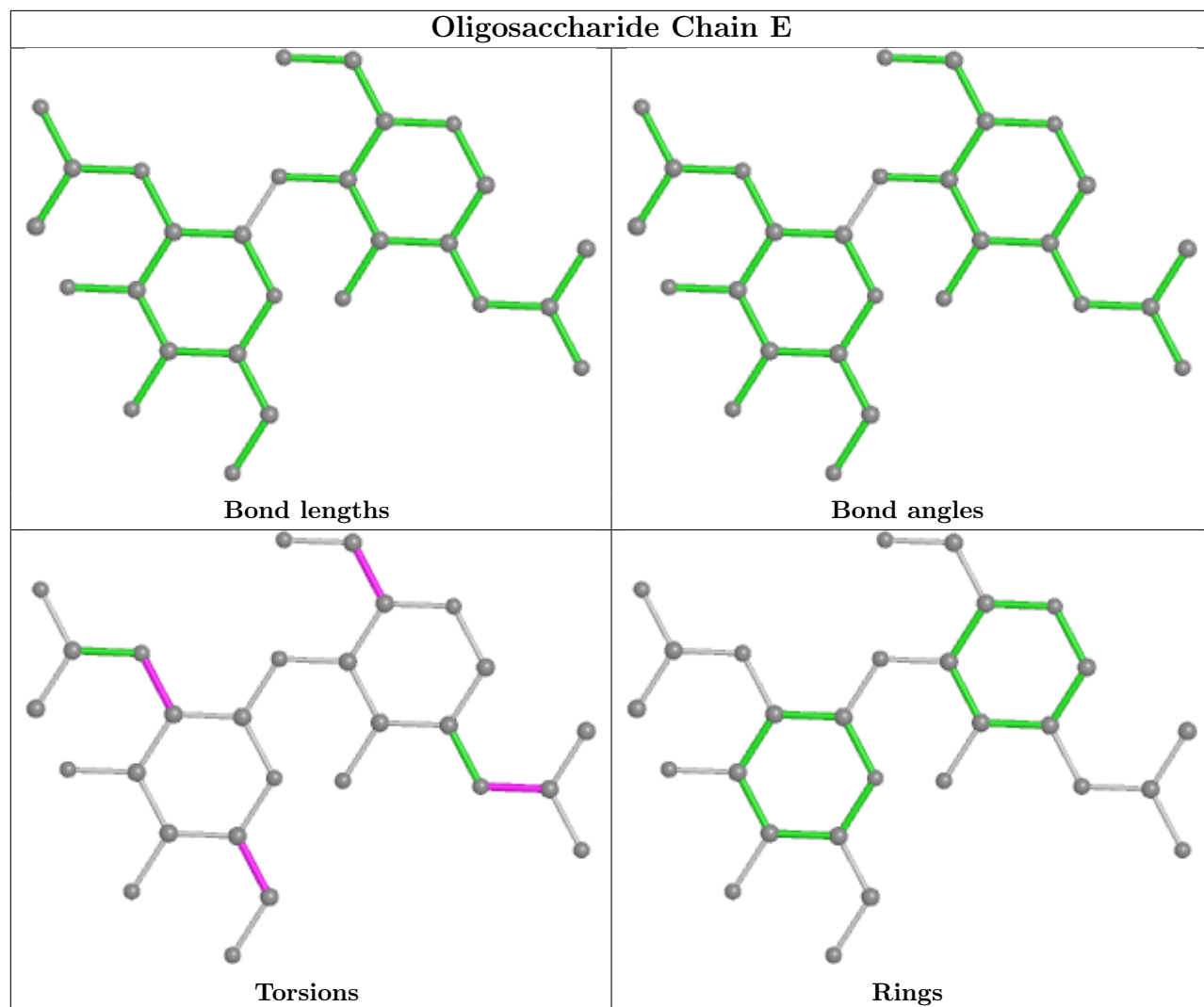
There are no ring outliers.

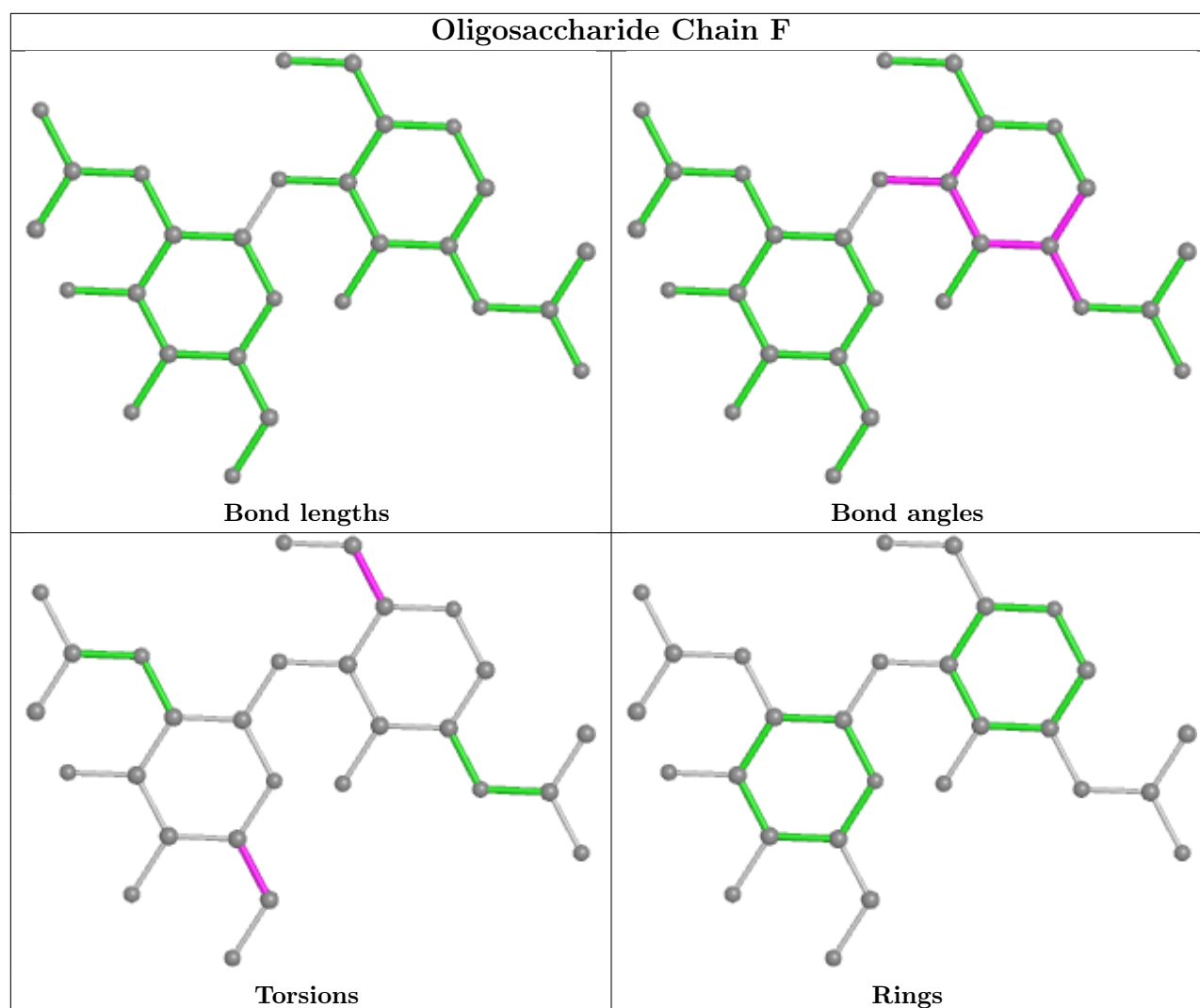
2 monomers are involved in 2 short contacts:

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

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







5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1312	1	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	B	1308	1	14,14,15	0.38	0	17,19,21	0.55	0
3	NAG	B	1313	1	14,14,15	0.37	0	17,19,21	0.63	0
3	NAG	A	1316	1	14,14,15	0.38	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1312	1	14,14,15	0.19	0	17,19,21	0.48	0
4	EIC	B	1316	-	19,19,19	0.57	0	19,19,19	0.58	0
3	NAG	C	1307	1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	C	1309	1	14,14,15	0.38	0	17,19,21	1.03	3 (17%)
3	NAG	C	1313	1	14,14,15	0.38	0	17,19,21	0.67	0
3	NAG	B	1305	1	14,14,15	0.46	0	17,19,21	0.56	0
3	NAG	B	1311	1	14,14,15	0.39	0	17,19,21	0.93	1 (5%)
3	NAG	B	1306	1	14,14,15	0.38	0	17,19,21	1.03	2 (11%)
3	NAG	C	1316	1	14,14,15	0.37	0	17,19,21	0.59	0
3	NAG	C	1311	1	14,14,15	0.39	0	17,19,21	0.60	0
3	NAG	A	1305	1	14,14,15	0.34	0	17,19,21	0.87	1 (5%)
3	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.38	0
3	NAG	A	1312	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	A	1303	1	14,14,15	0.28	0	17,19,21	0.49	0
3	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.60	0
3	NAG	A	1313	1	14,14,15	0.71	1 (7%)	17,19,21	0.67	0
3	NAG	C	1310	1	14,14,15	0.18	0	17,19,21	0.70	1 (5%)
3	NAG	B	1303	1	14,14,15	0.73	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	B	1309	1	14,14,15	0.39	0	17,19,21	0.48	0
3	NAG	C	1301	1	14,14,15	0.31	0	17,19,21	0.38	0
3	NAG	C	1314	1	14,14,15	0.37	0	17,19,21	0.89	1 (5%)
3	NAG	C	1303	1	14,14,15	0.40	0	17,19,21	1.12	2 (11%)
3	NAG	A	1311	1	14,14,15	0.25	0	17,19,21	0.48	0
4	EIC	C	1315	-	19,19,19	0.56	0	19,19,19	0.59	0
3	NAG	B	1314	1	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	A	1314	1	14,14,15	0.38	0	17,19,21	1.13	1 (5%)
3	NAG	B	1310	1	14,14,15	0.42	0	17,19,21	0.42	0
3	NAG	B	1302	1	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	A	1306	1	14,14,15	0.19	0	17,19,21	0.56	0
3	NAG	B	1315	1	14,14,15	0.38	0	17,19,21	0.67	1 (5%)
3	NAG	C	1305	1	14,14,15	0.38	0	17,19,21	0.72	0
4	EIC	A	1315	-	19,19,19	0.58	0	19,19,19	0.57	0
3	NAG	A	1304	1	14,14,15	0.15	0	17,19,21	0.69	1 (5%)
3	NAG	A	1310	1	14,14,15	0.36	0	17,19,21	0.36	0
3	NAG	B	1304	1	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	C	1306	1	14,14,15	0.41	0	17,19,21	0.43	0
3	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	C	1308	1	14,14,15	0.39	0	17,19,21	0.92	2 (11%)
3	NAG	A	1307	1	14,14,15	0.38	0	17,19,21	1.03	2 (11%)
3	NAG	A	1309	1	14,14,15	0.24	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	B	1301	1	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
3	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	B	1307	1	14,14,15	0.37	0	17,19,21	0.37	0
3	NAG	C	1302	1	14,14,15	0.41	0	17,19,21	0.47	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	B	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1313	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
4	EIC	B	1316	-	-	8/17/17/17	-
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1316	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1313	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1314	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
4	EIC	C	1315	-	-	6/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1314	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1315	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	EIC	A	1315	-	-	4/17/17/17	-
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1303	NAG	O5-C1	2.50	1.47	1.43
3	A	1313	NAG	O5-C1	2.28	1.47	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1314	NAG	C2-N2-C7	3.99	128.59	122.90
3	B	1303	NAG	C1-O5-C5	3.59	117.05	112.19
3	C	1303	NAG	C1-C2-N2	3.57	116.59	110.49
3	A	1305	NAG	C1-O5-C5	3.27	116.62	112.19
3	A	1307	NAG	C1-C2-N2	3.07	115.73	110.49

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1307	NAG	C3-C2-N2-C7
3	A	1314	NAG	C3-C2-N2-C7
3	A	1314	NAG	C8-C7-N2-C2
3	A	1314	NAG	O7-C7-N2-C2
3	A	1316	NAG	C8-C7-N2-C2

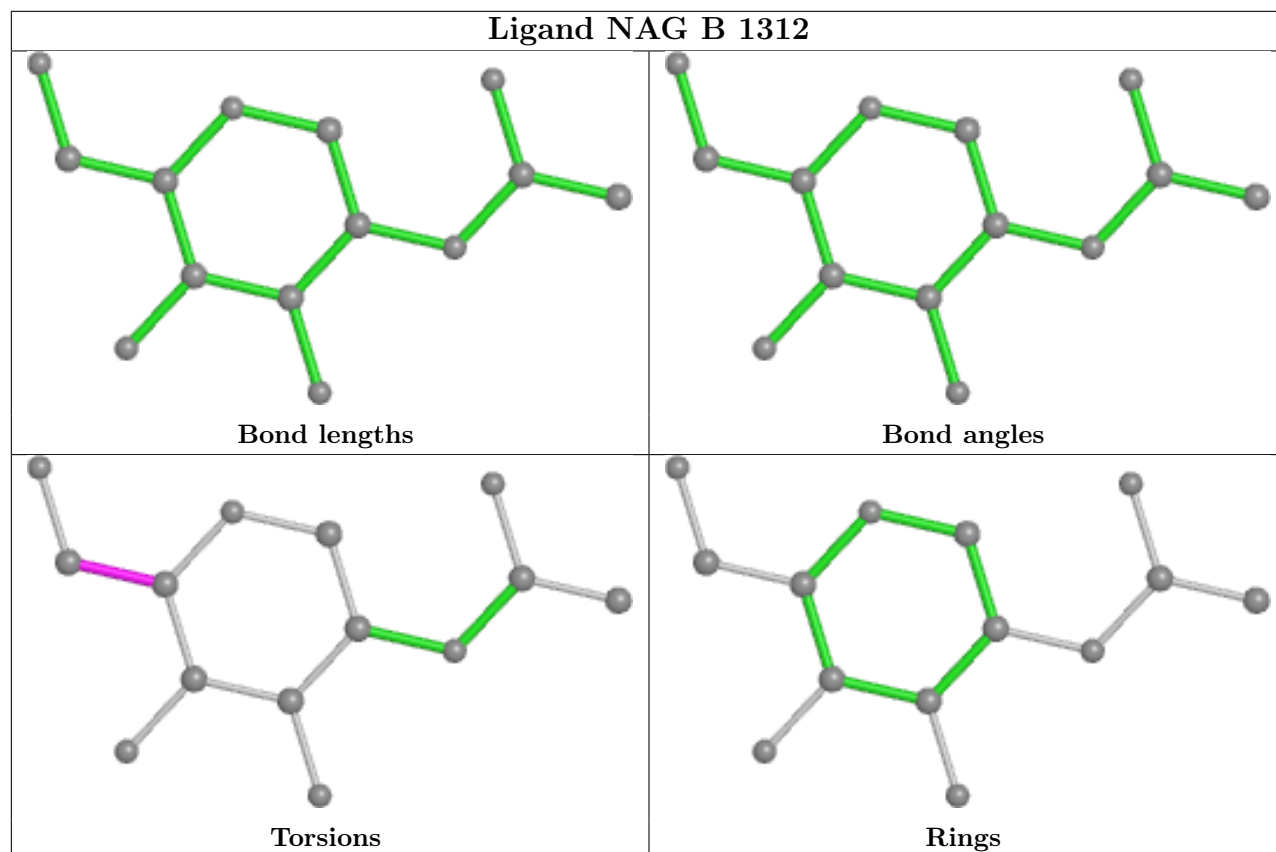
There are no ring outliers.

14 monomers are involved in 27 short contacts:

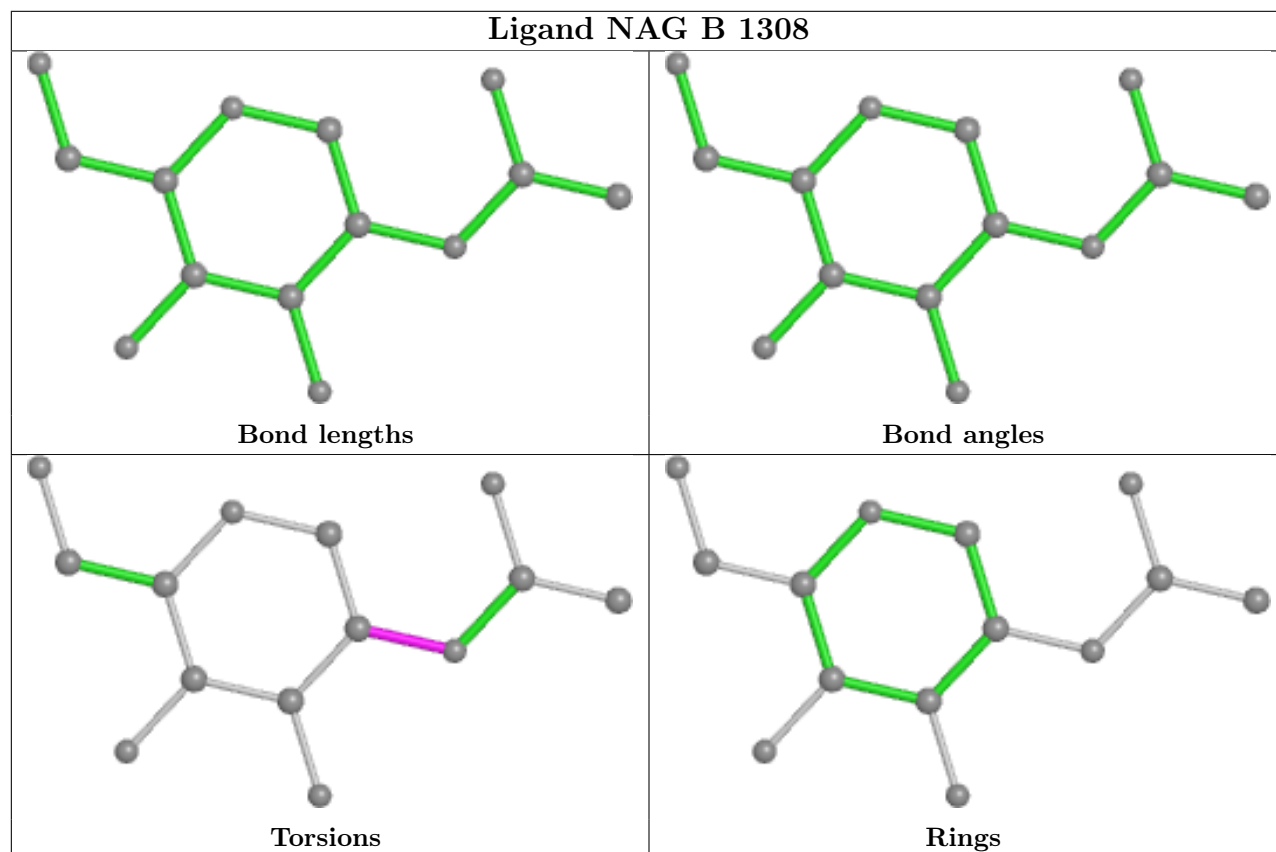
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1313	NAG	1	0
4	B	1316	EIC	4	0
3	B	1311	NAG	1	0
3	B	1306	NAG	1	0
3	C	1316	NAG	1	0
3	A	1305	NAG	1	0
3	A	1313	NAG	2	0
3	B	1303	NAG	4	0
3	C	1301	NAG	1	0
4	C	1315	EIC	3	0
3	B	1302	NAG	1	0
4	A	1315	EIC	4	0
3	A	1302	NAG	2	0
3	B	1307	NAG	1	0

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

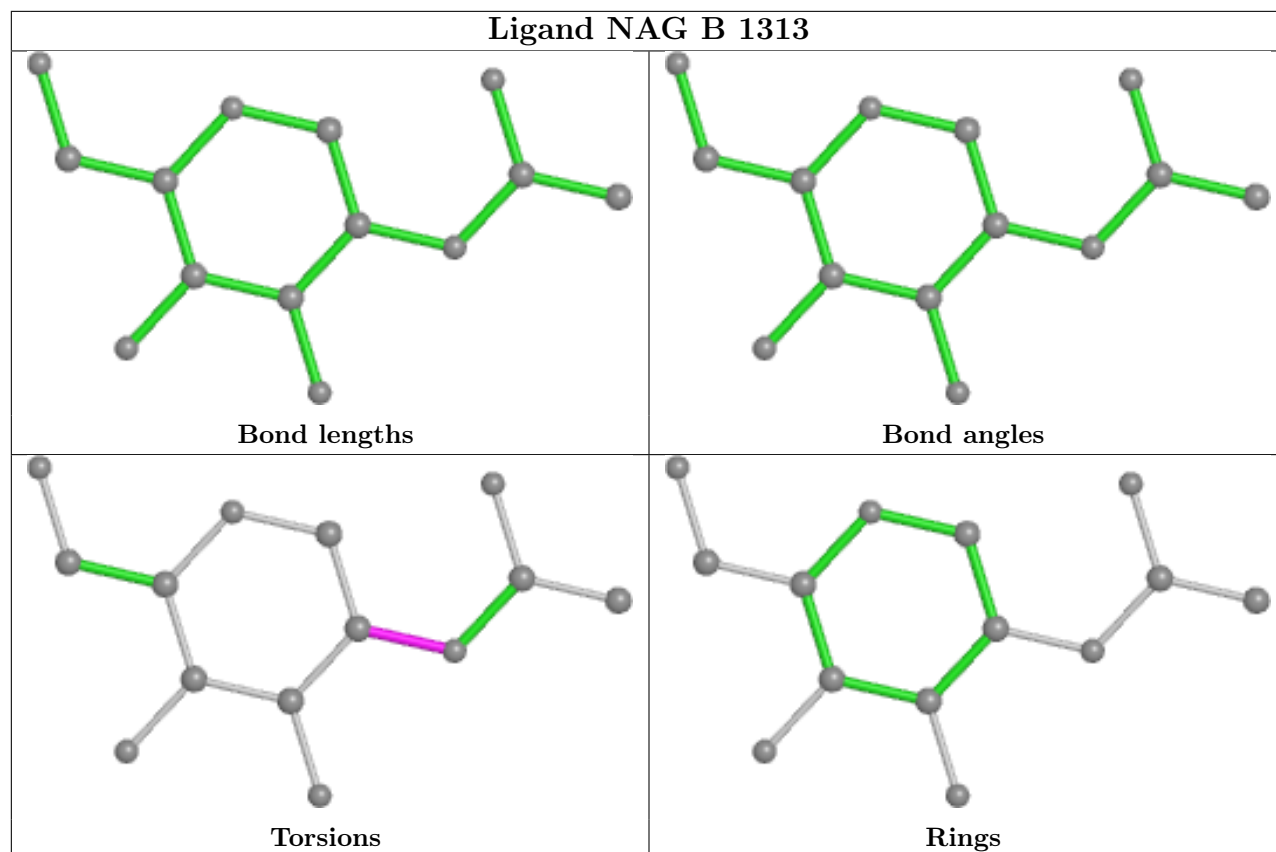
Ligand NAG B 1312



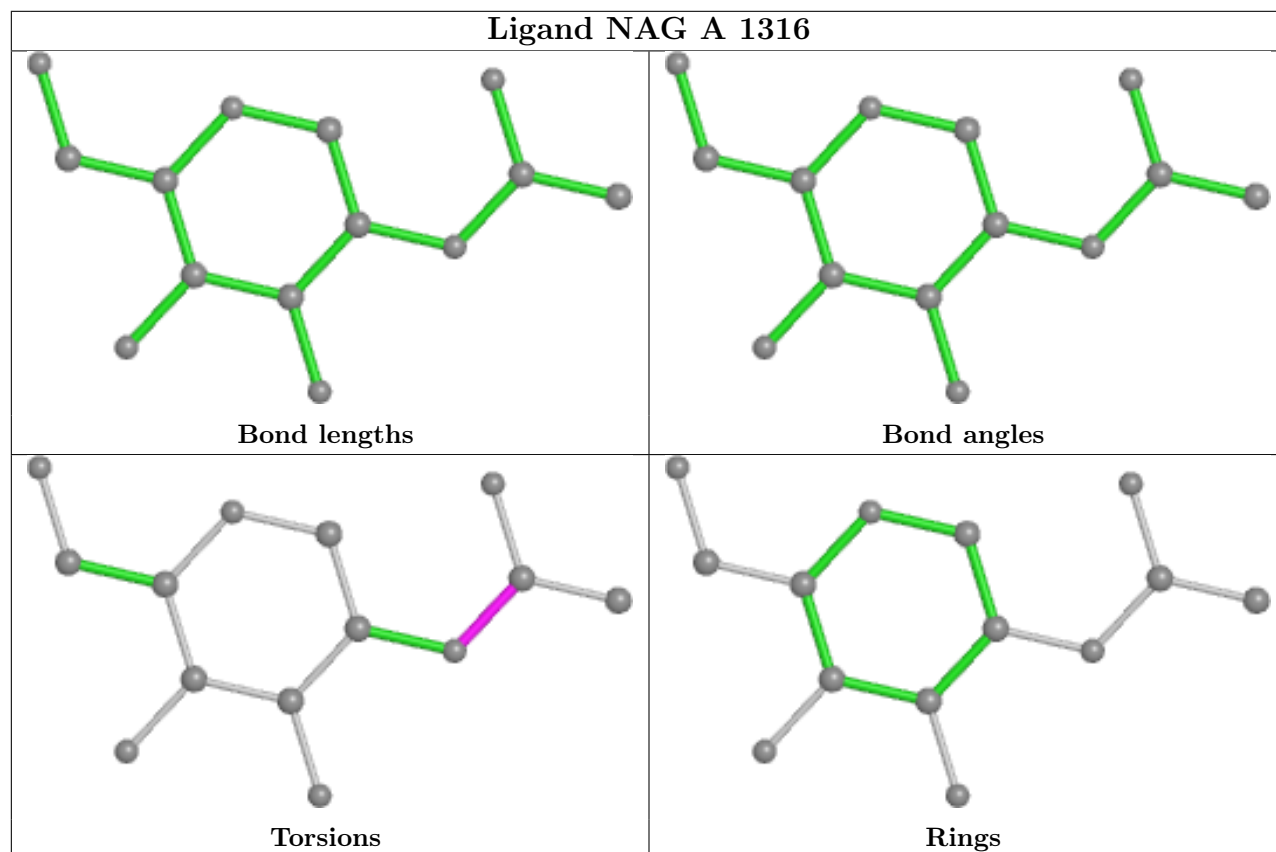
Ligand NAG B 1308

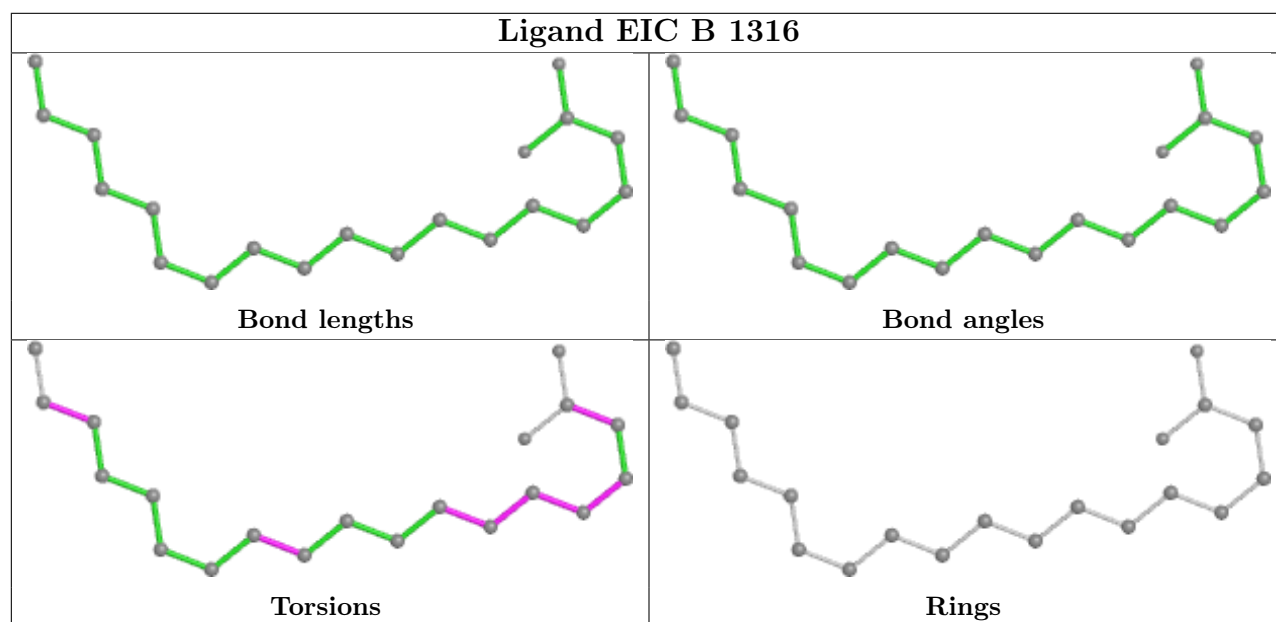
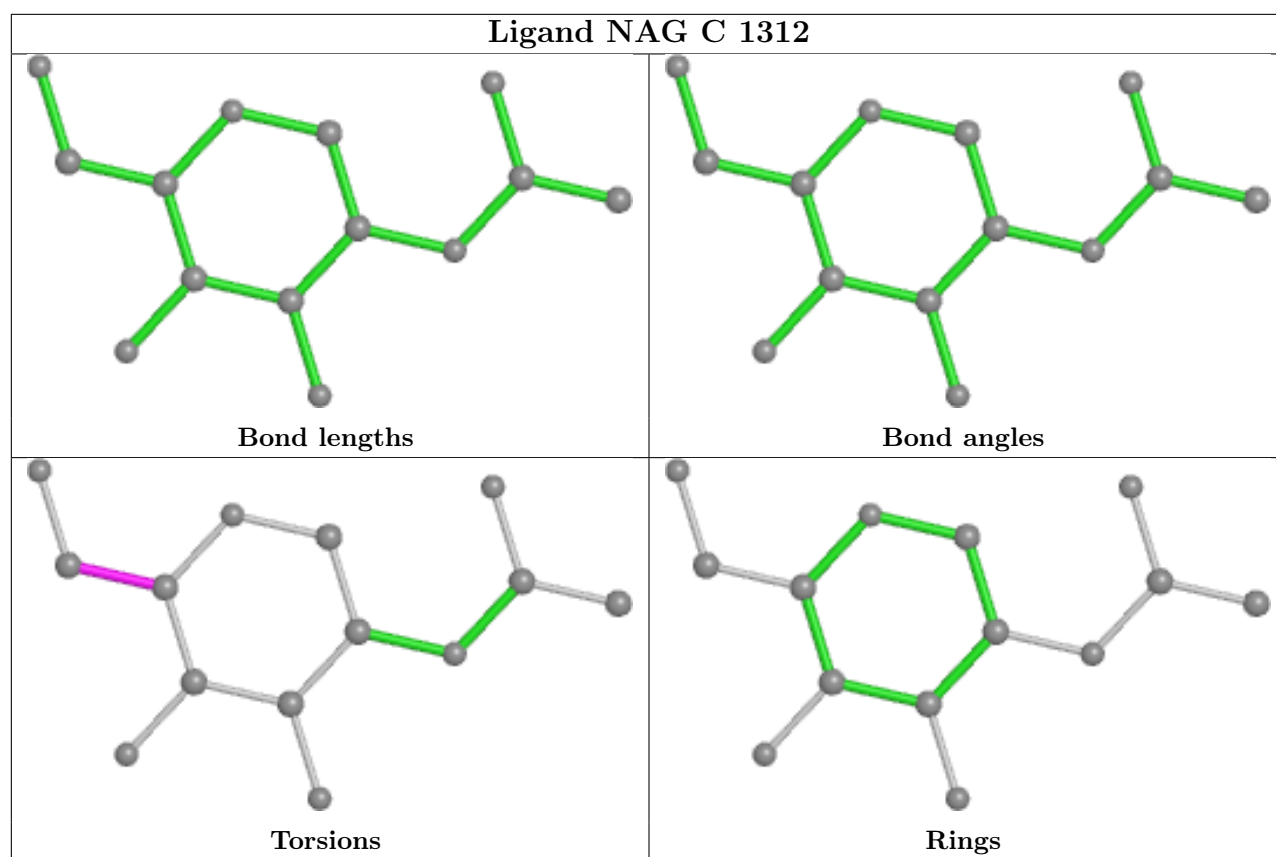


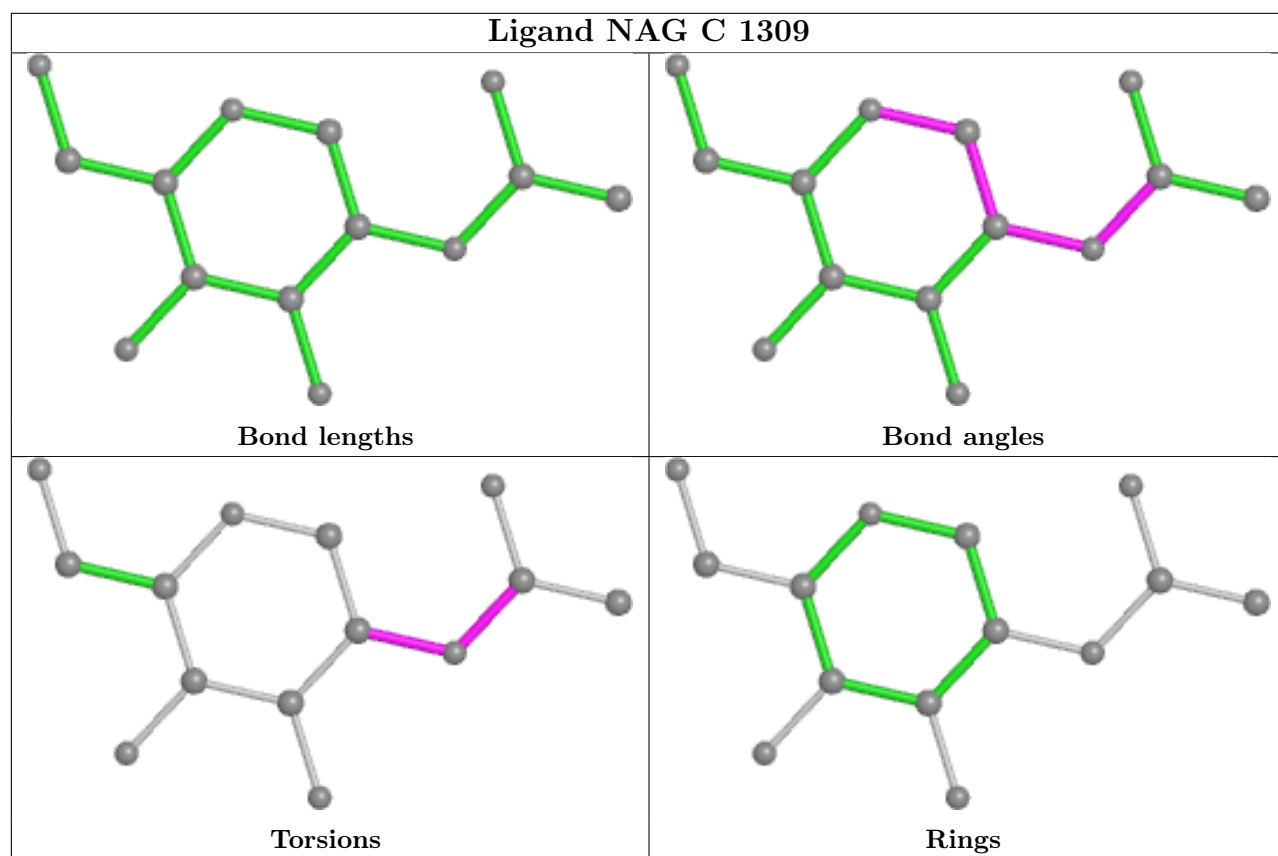
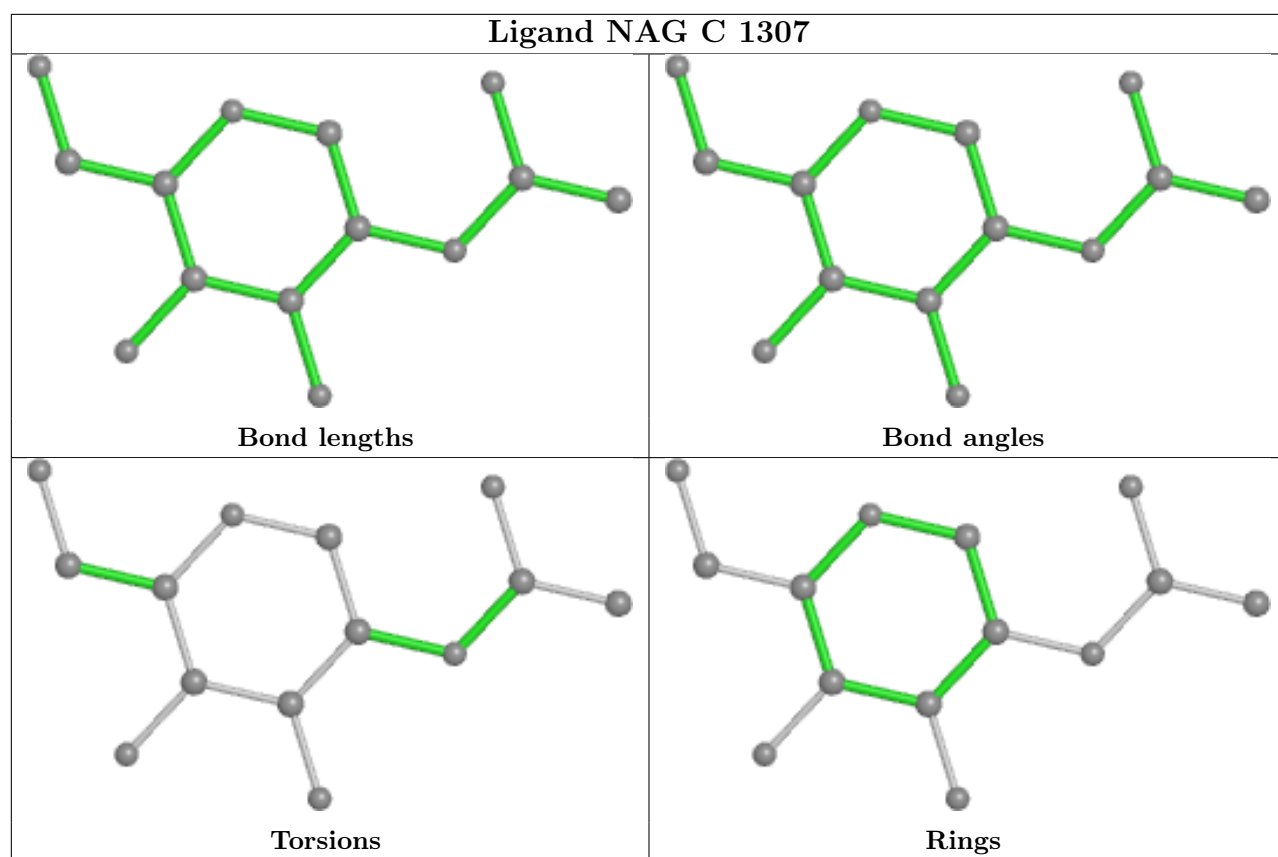
Ligand NAG B 1313



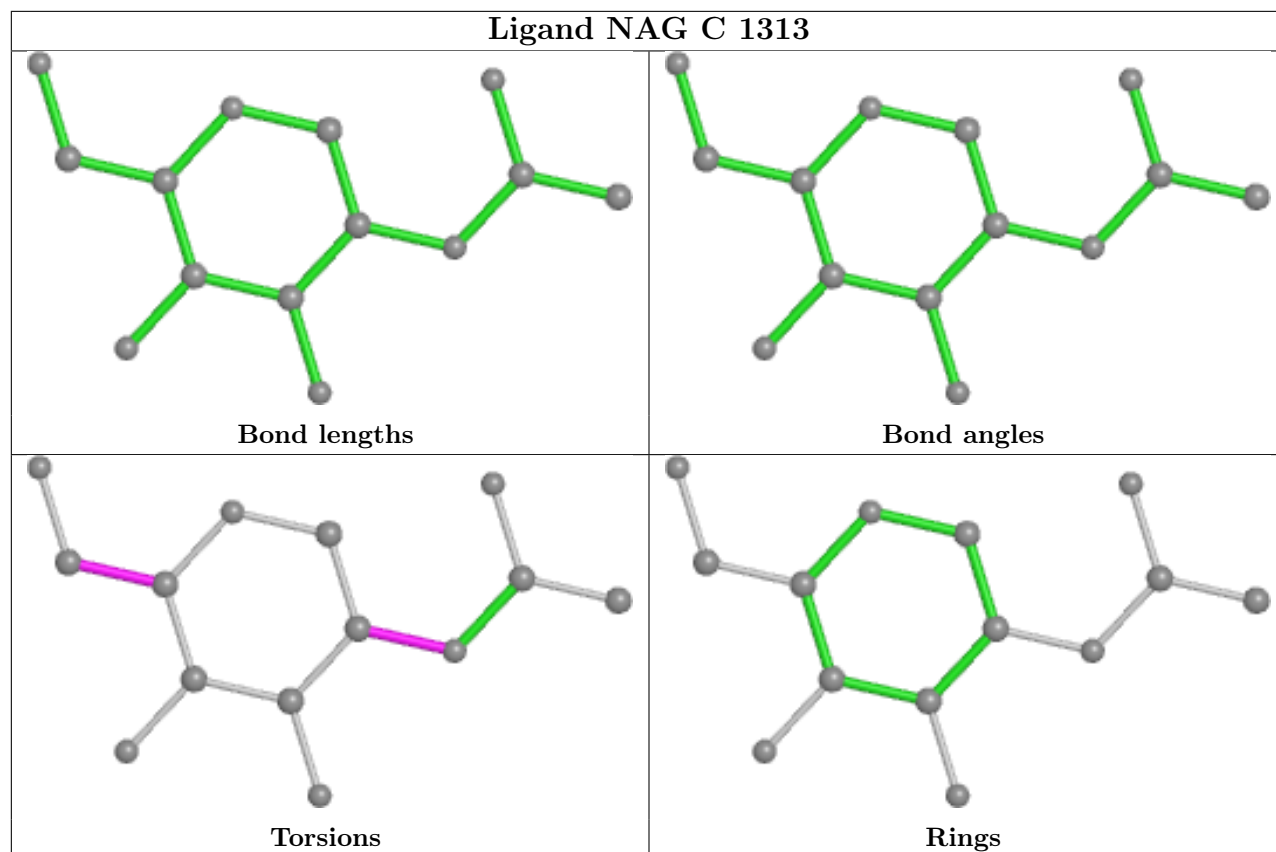
Ligand NAG A 1316



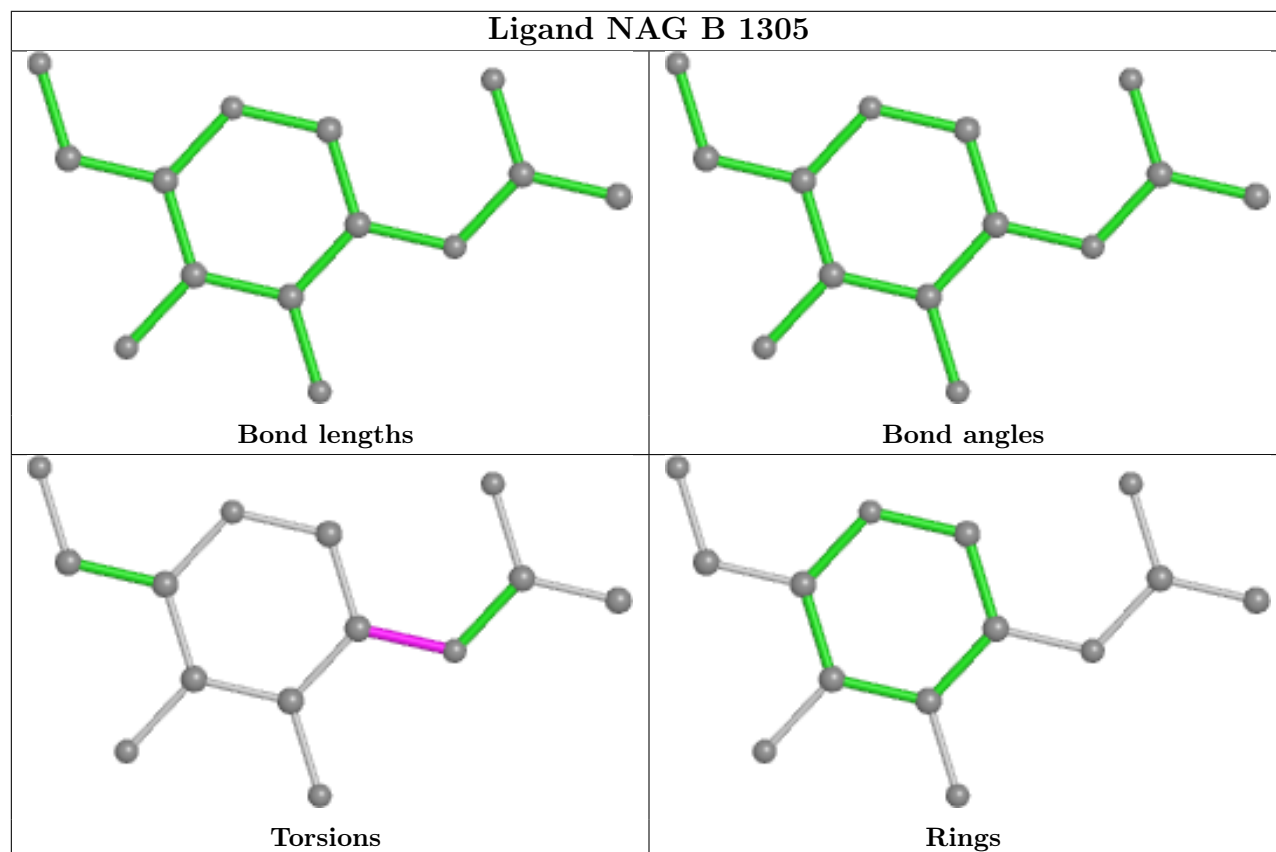




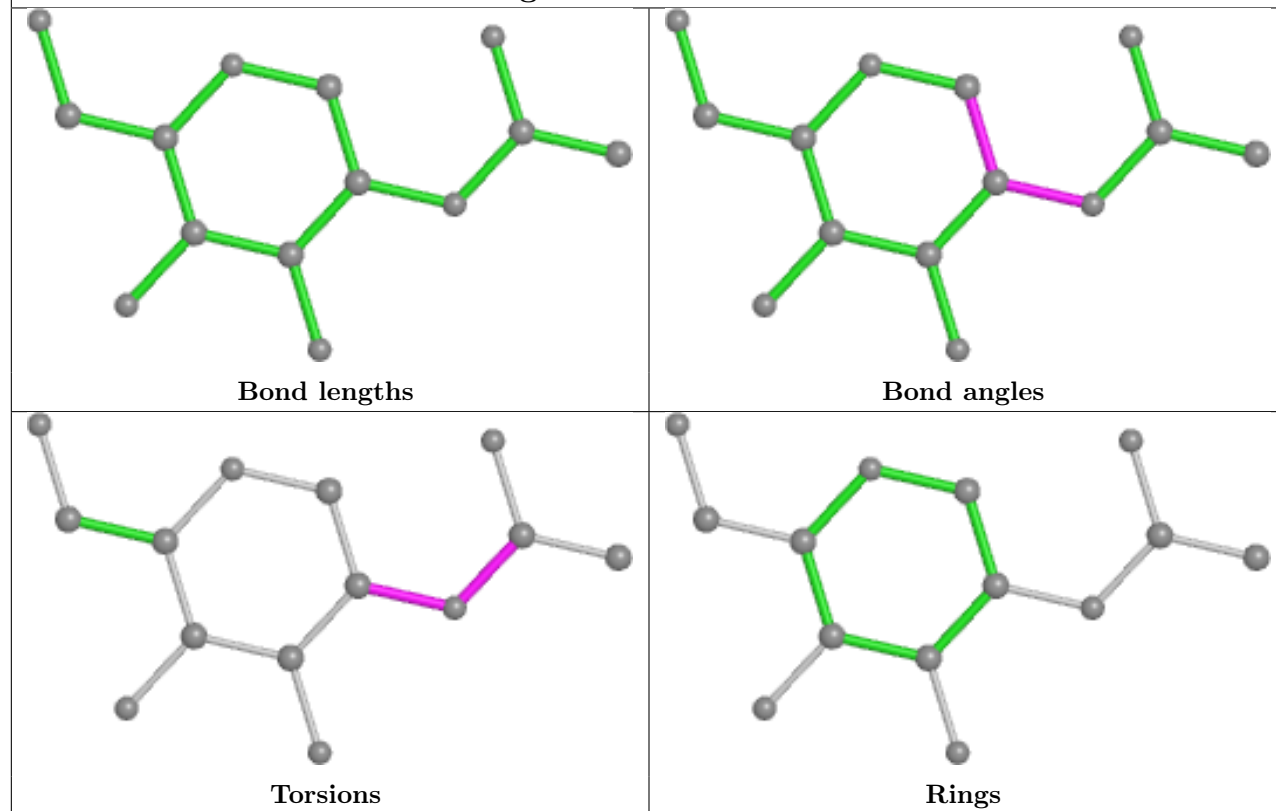
Ligand NAG C 1313



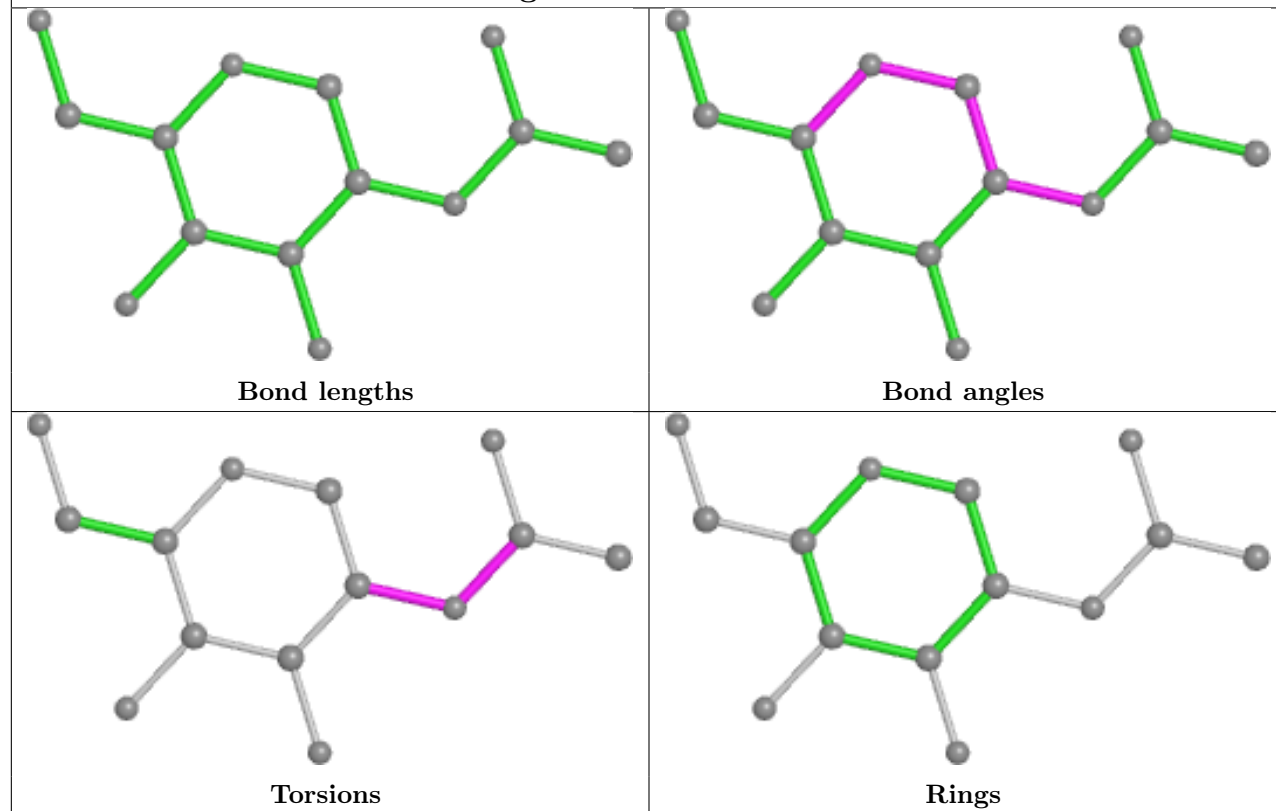
Ligand NAG B 1305



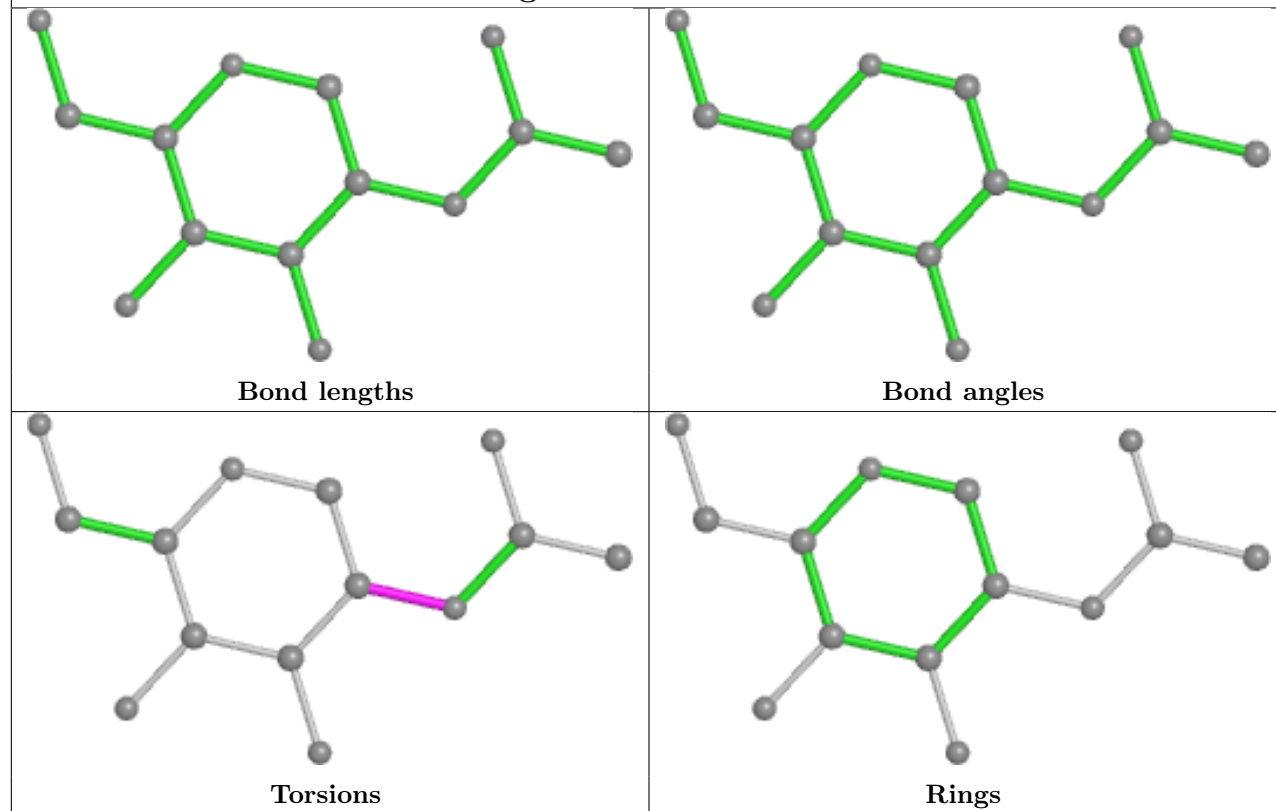
Ligand NAG B 1311



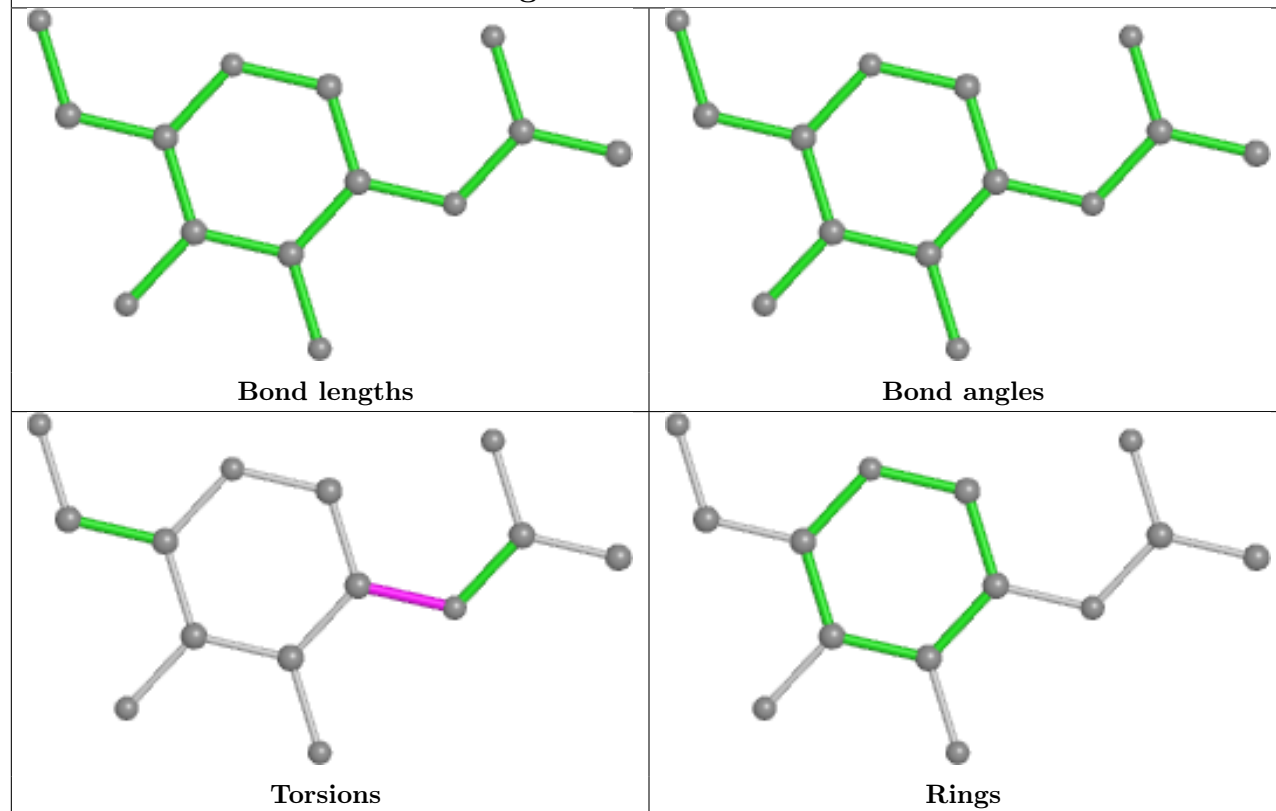
Ligand NAG B 1306



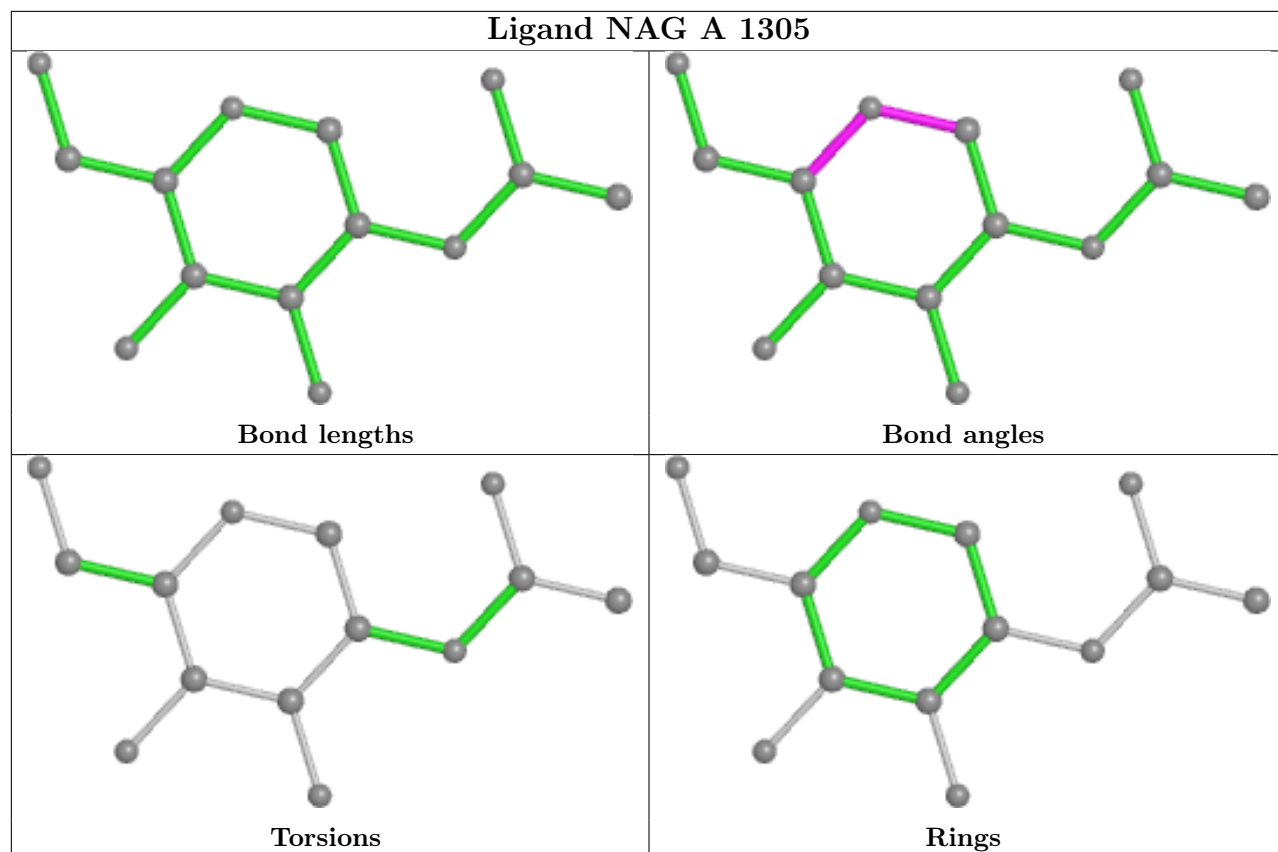
Ligand NAG C 1316



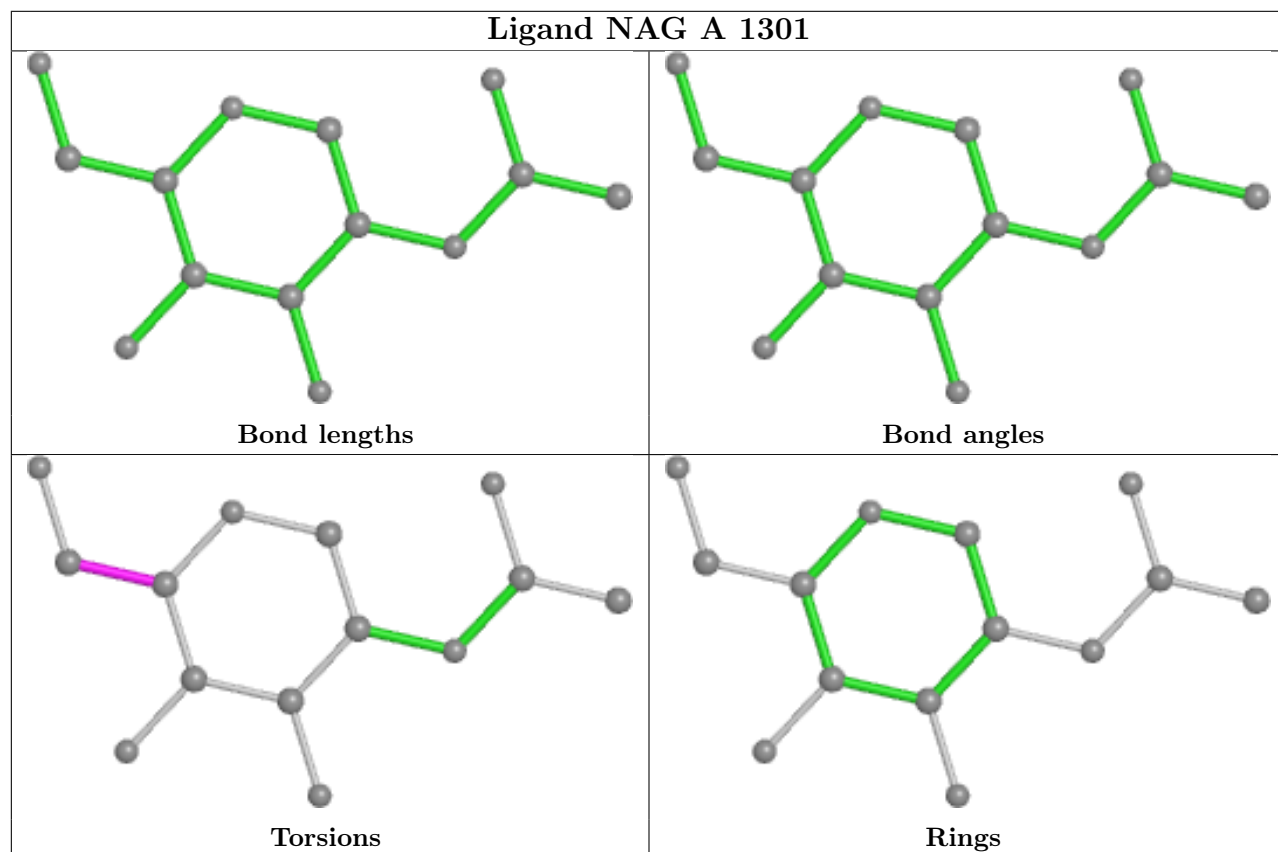
Ligand NAG C 1311



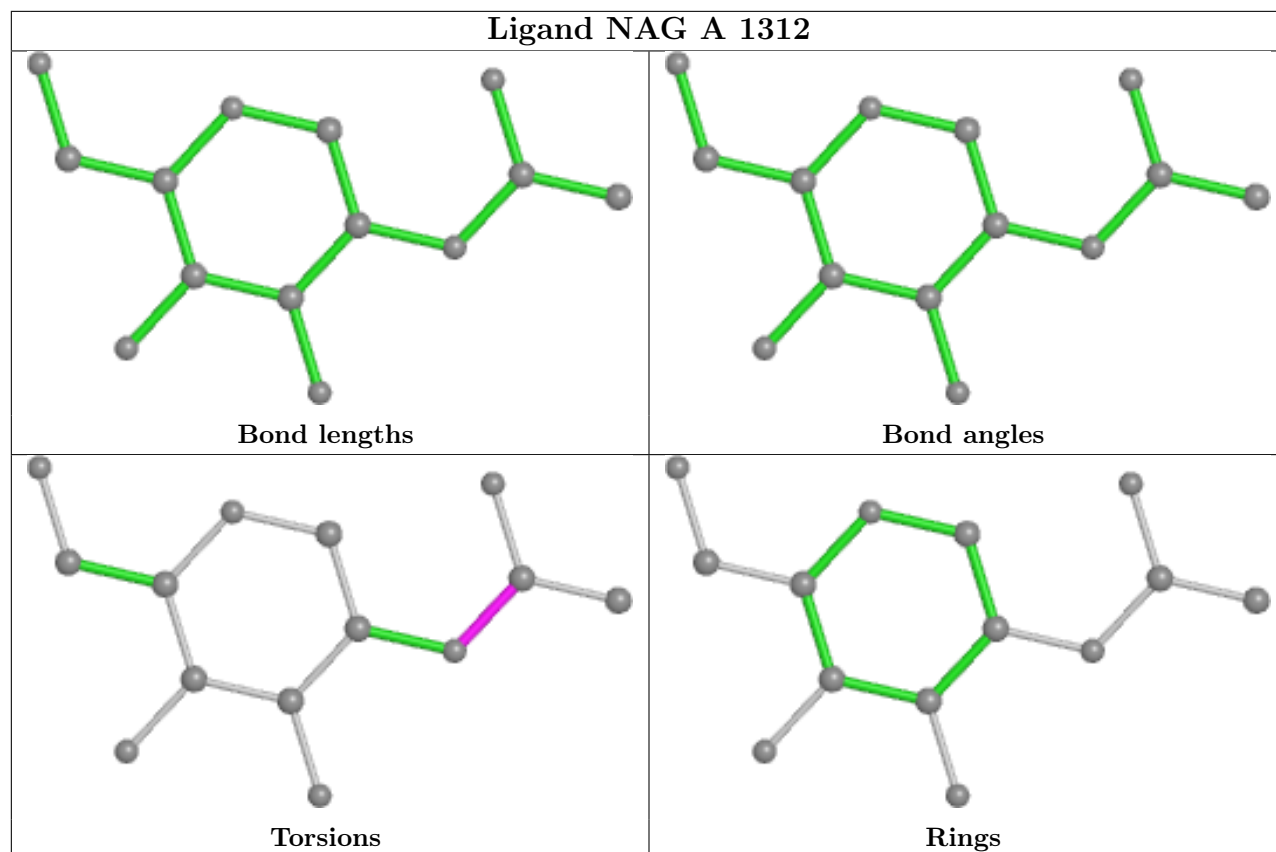
Ligand NAG A 1305



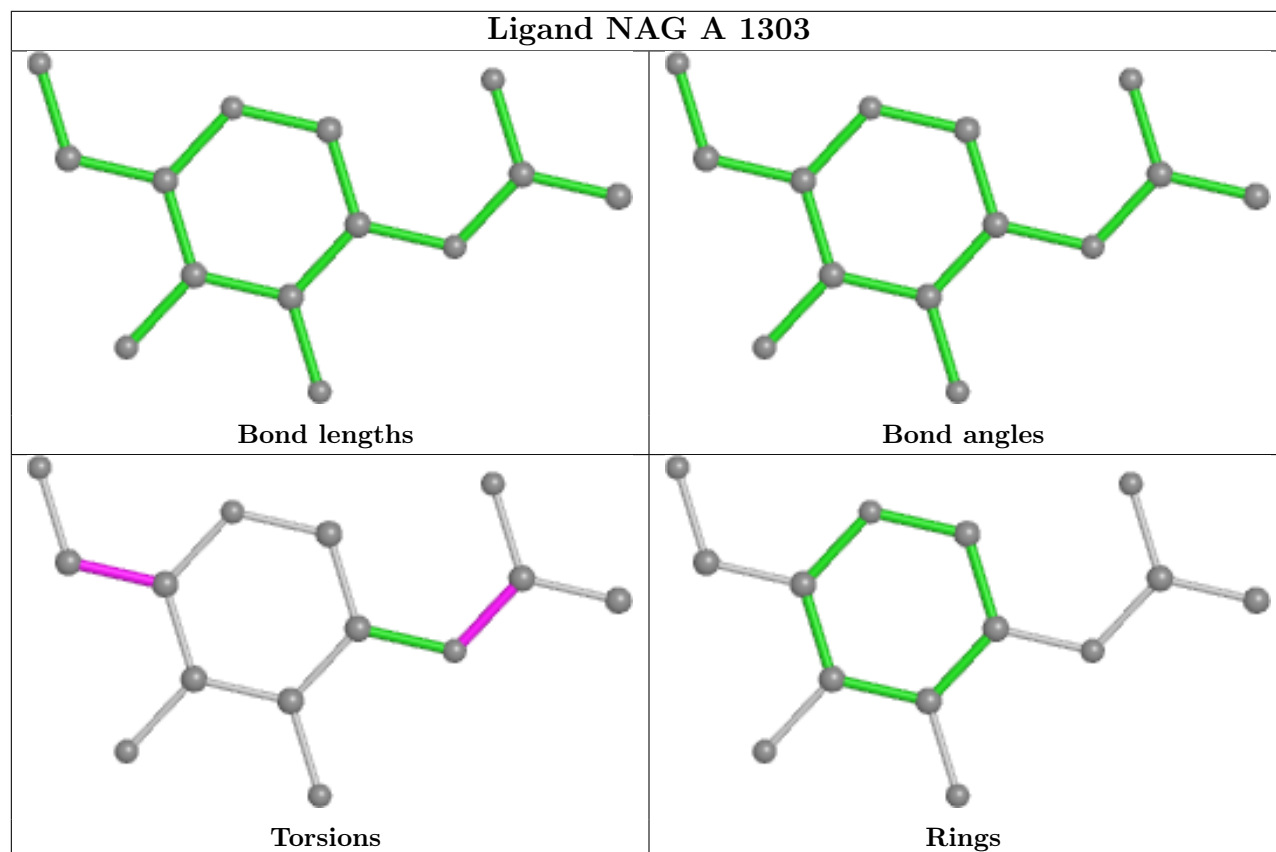
Ligand NAG A 1301

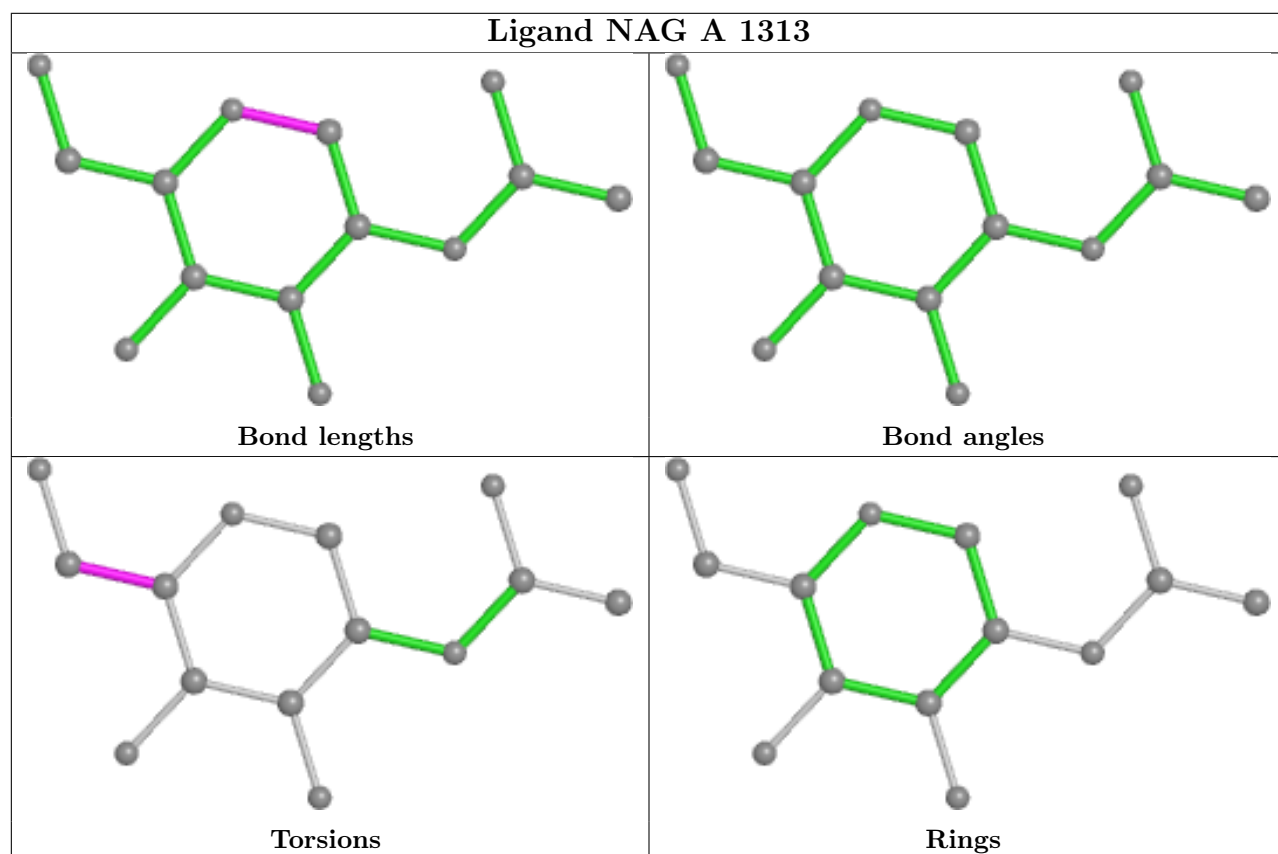
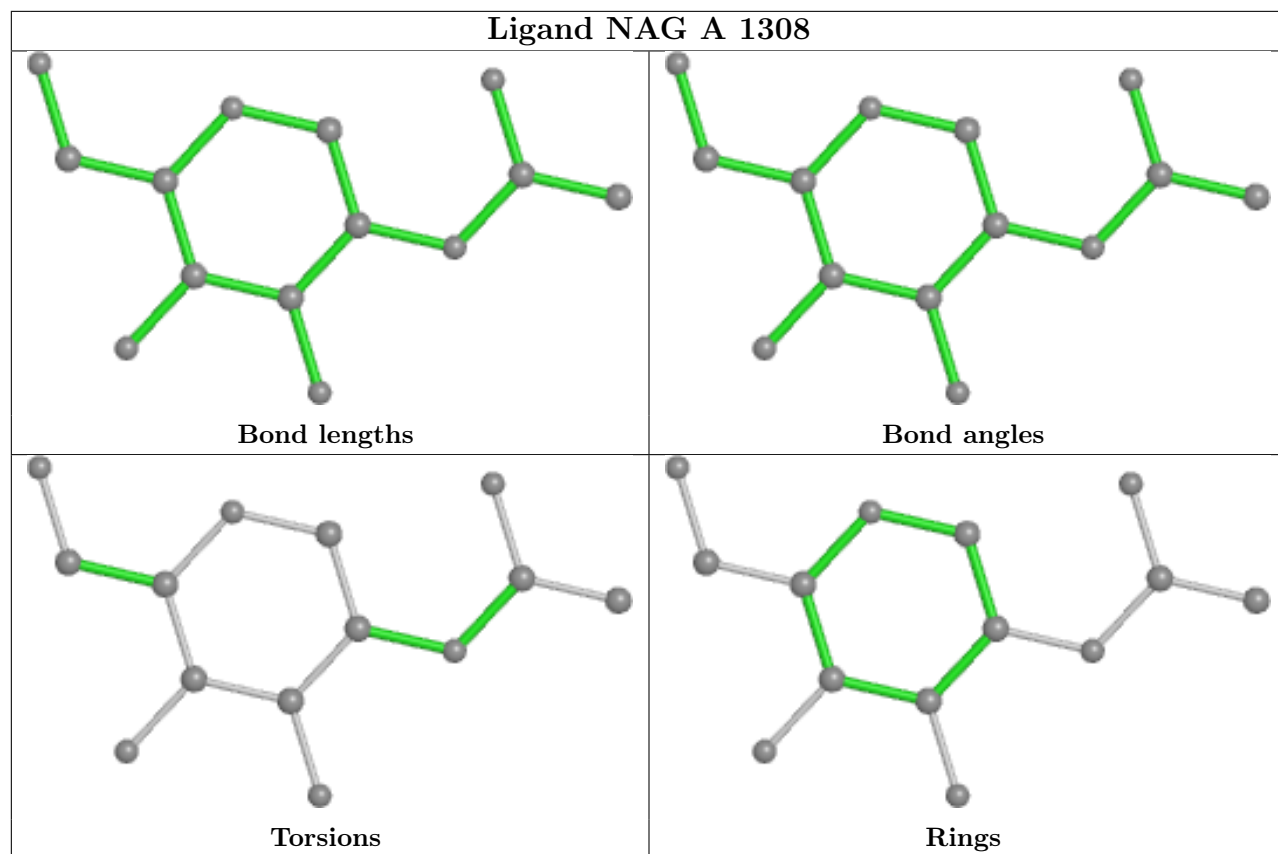


Ligand NAG A 1312

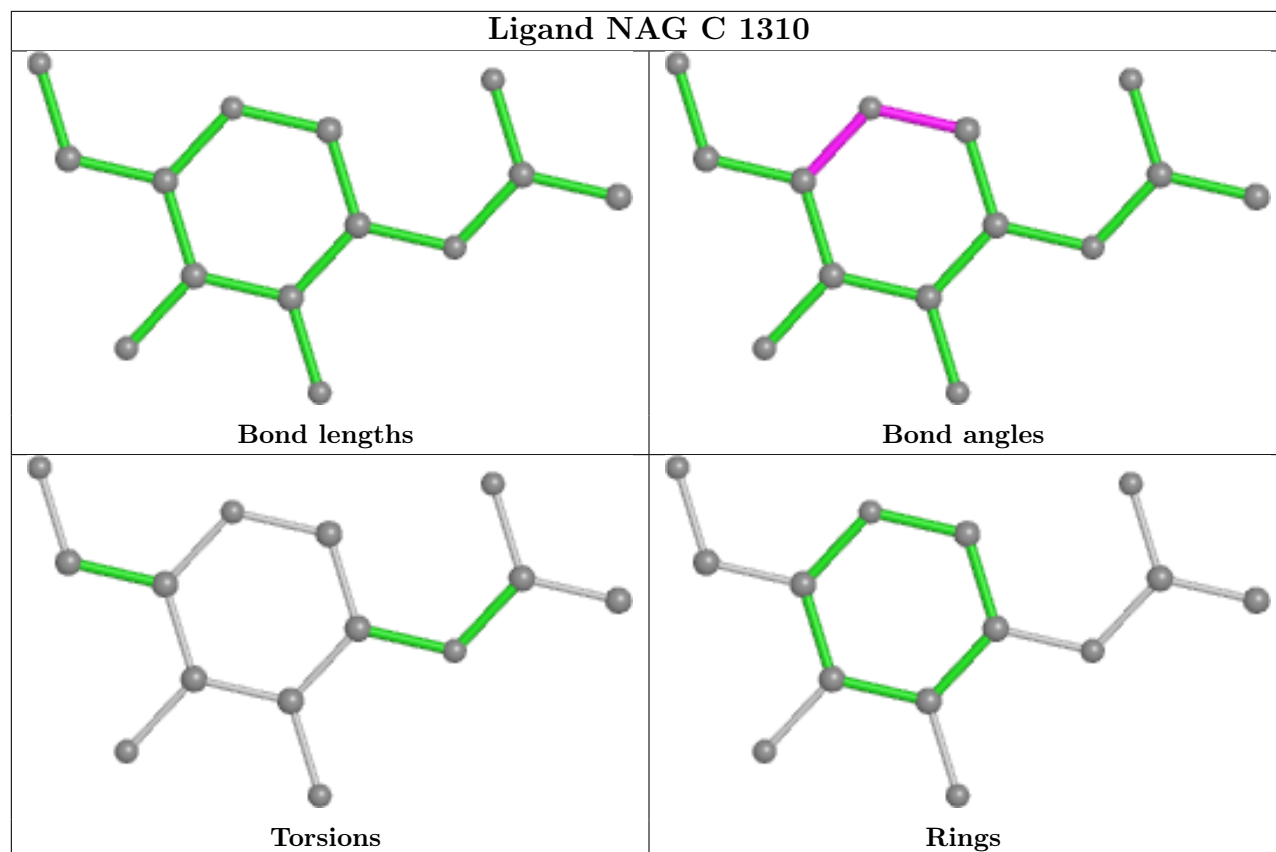


Ligand NAG A 1303

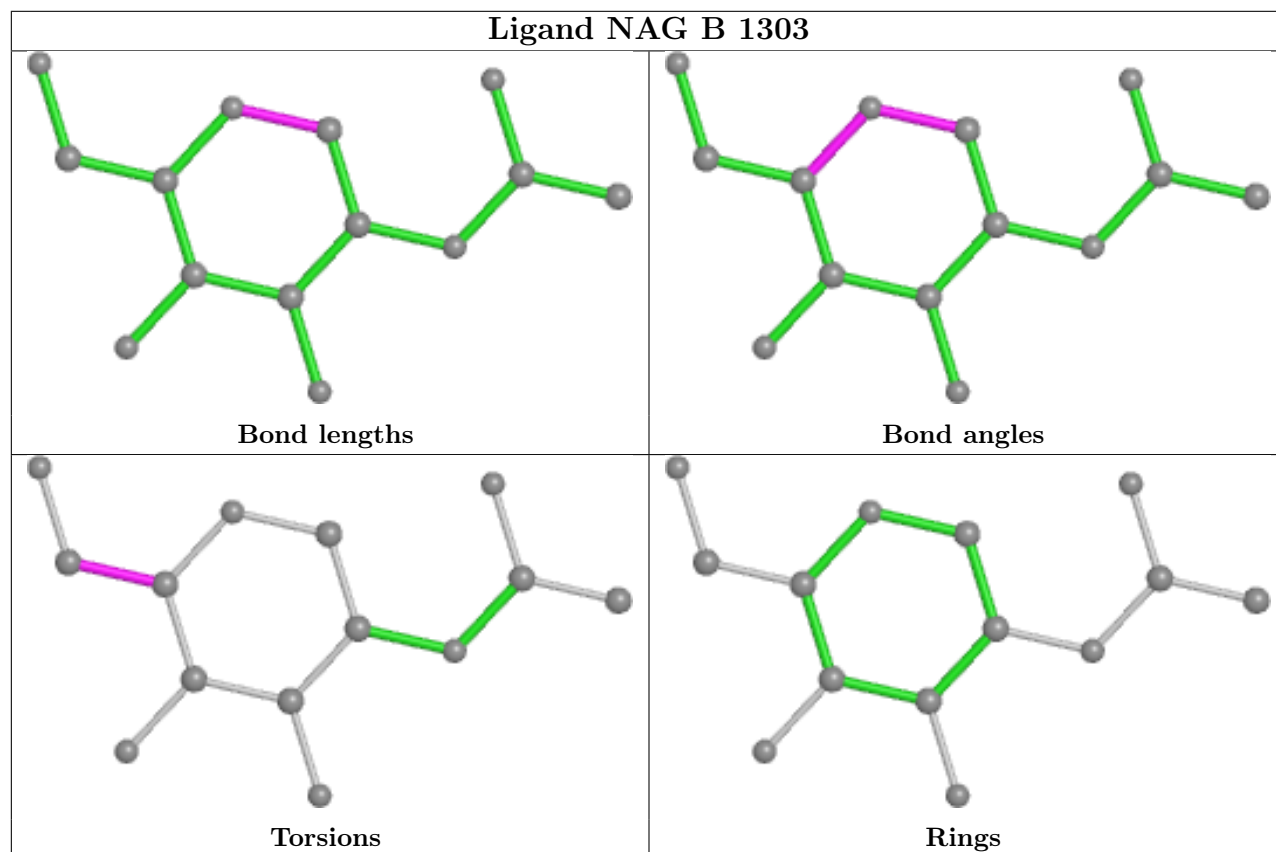


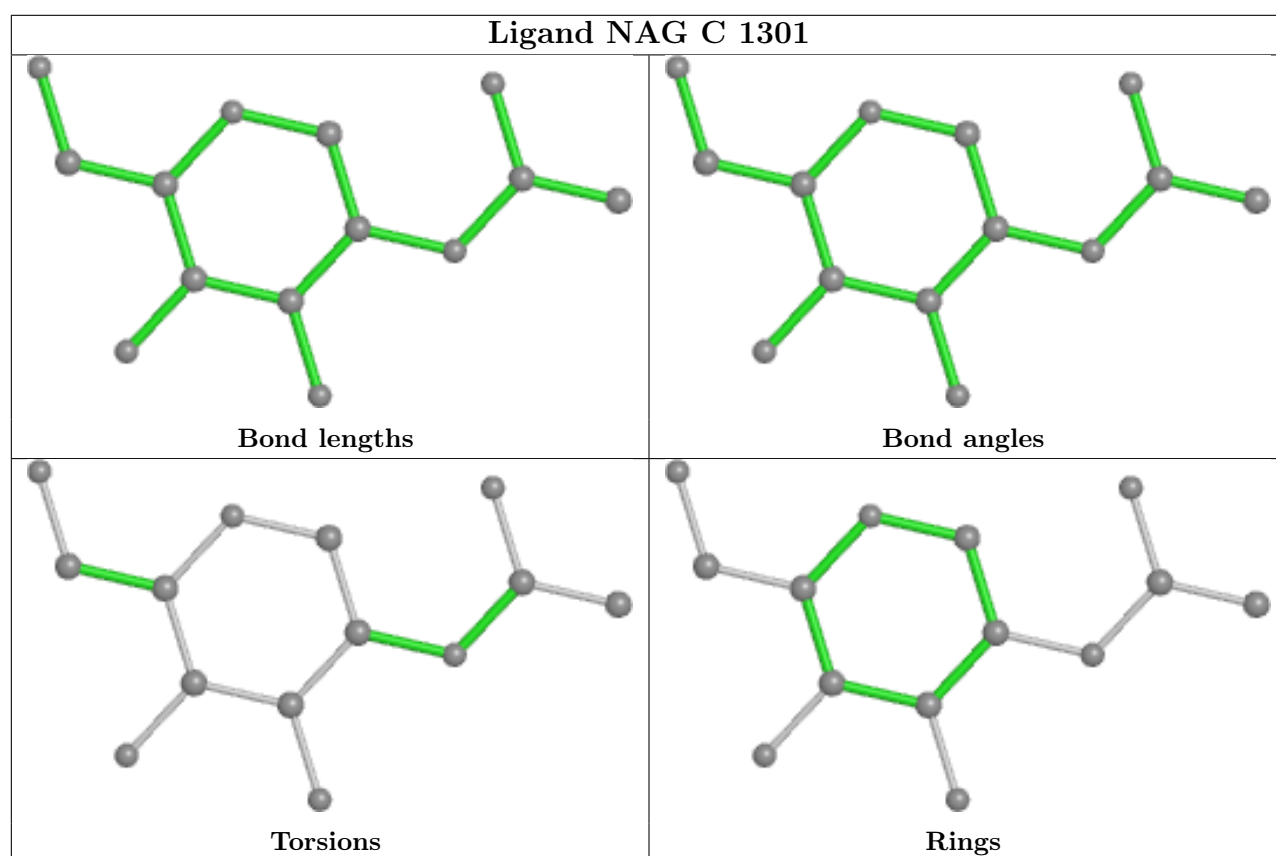
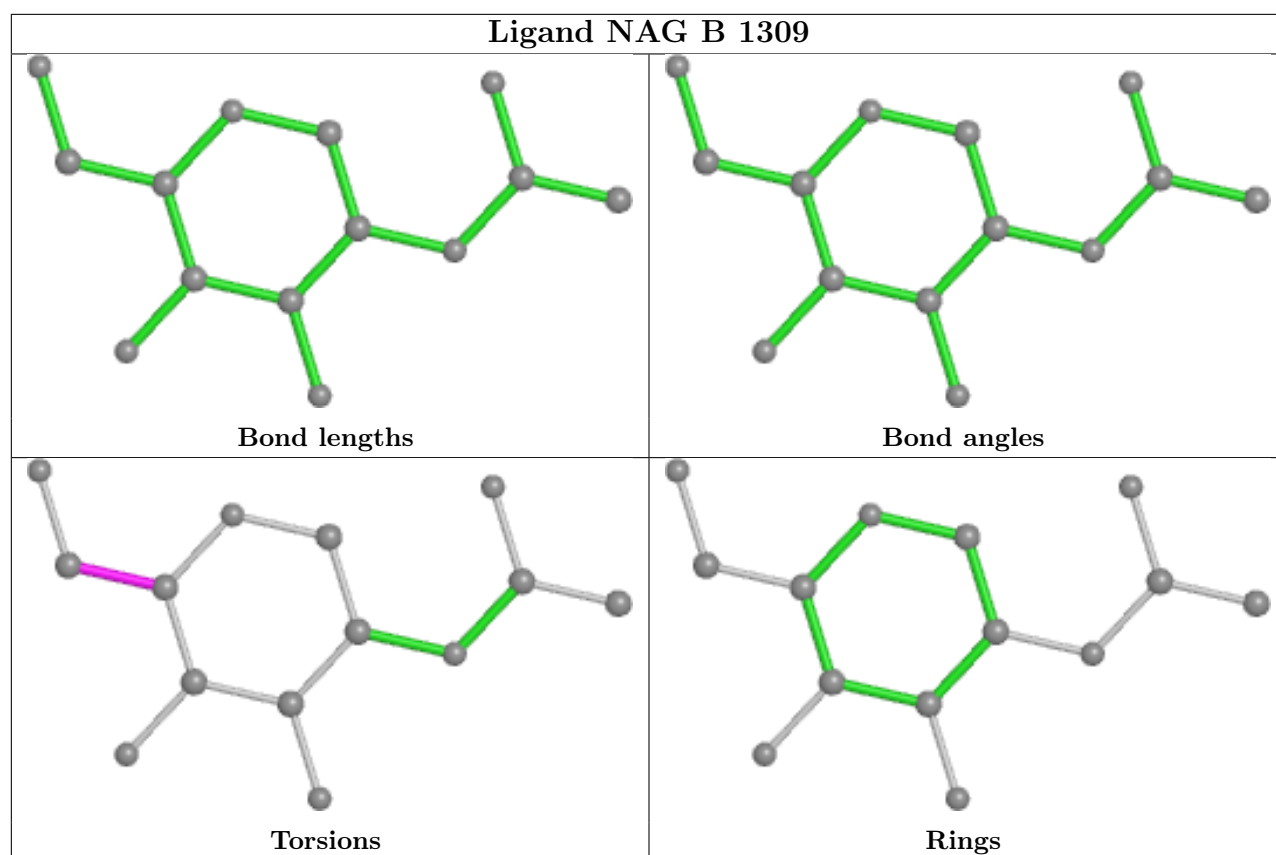


Ligand NAG C 1310

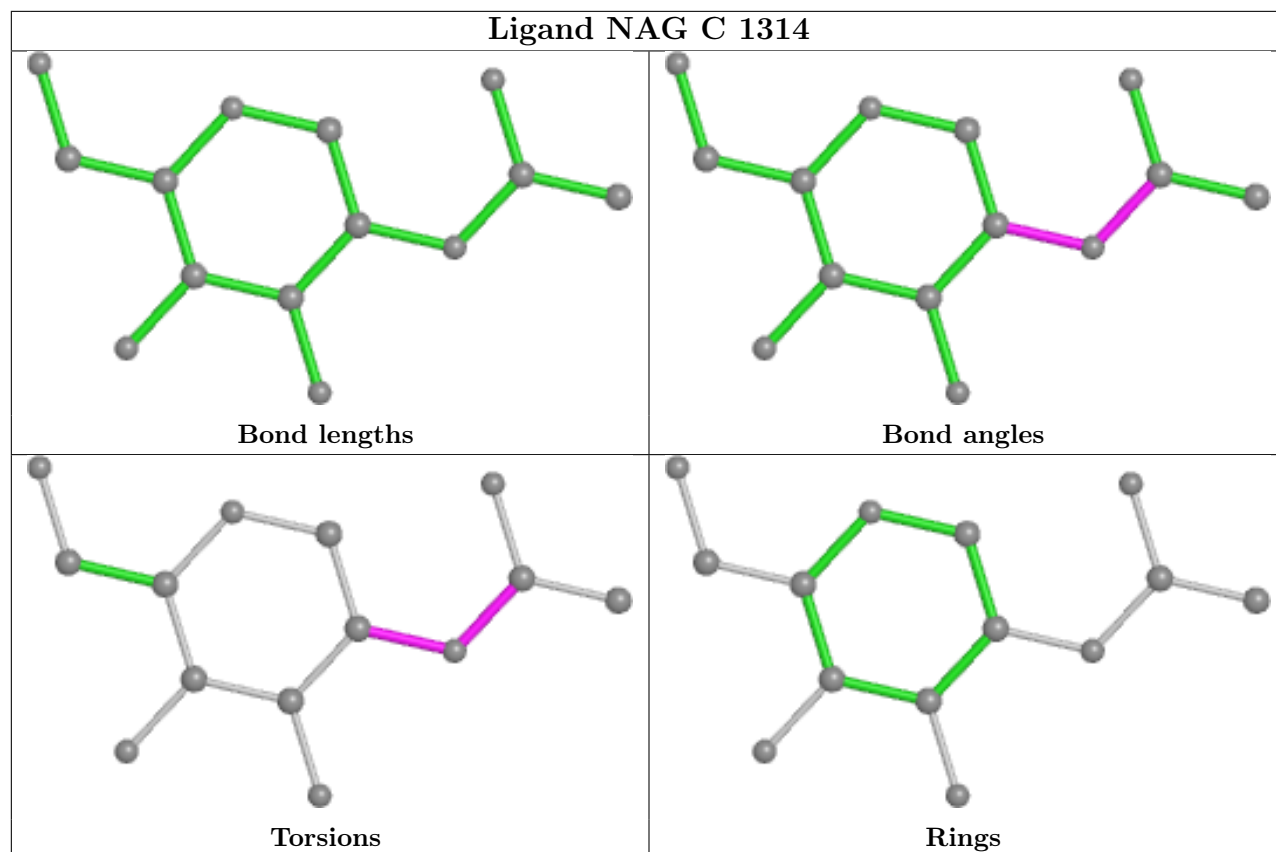


Ligand NAG B 1303

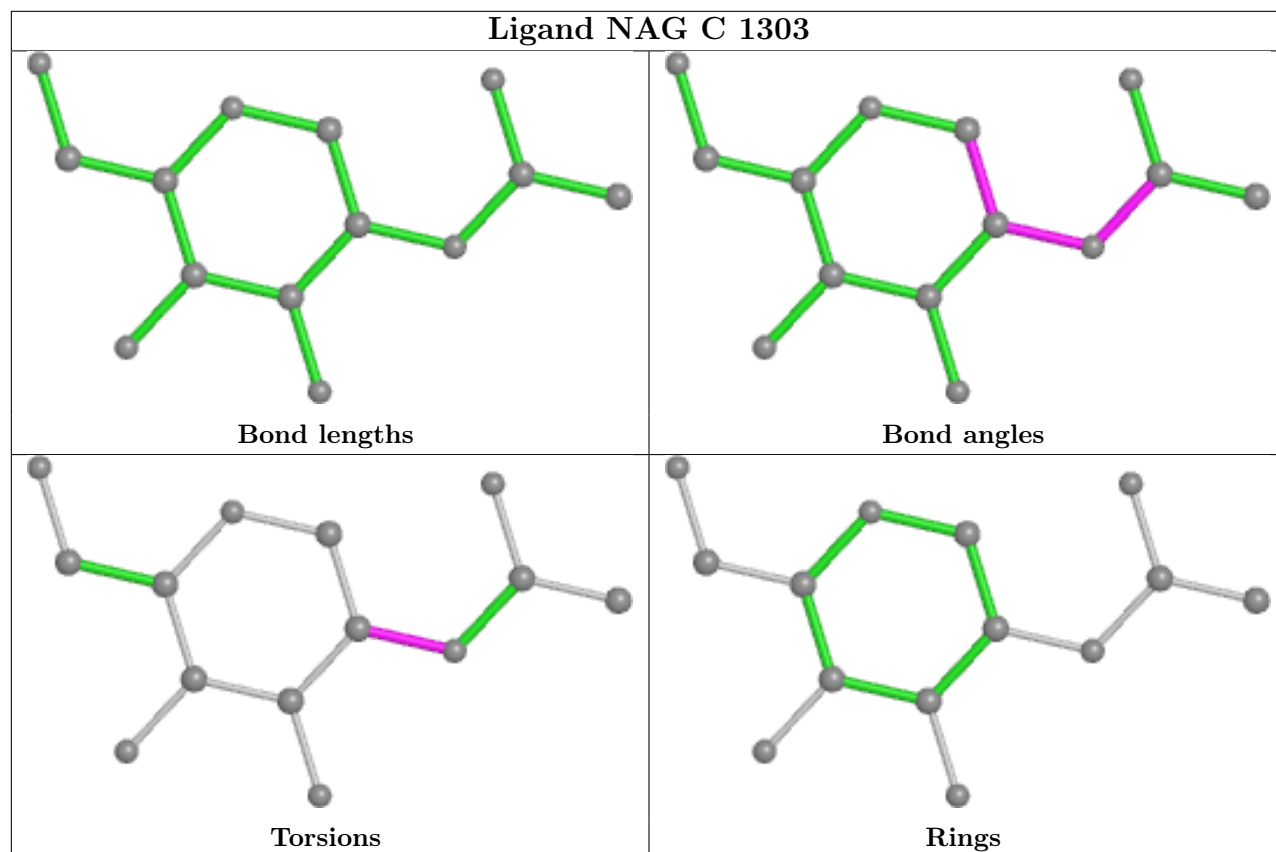


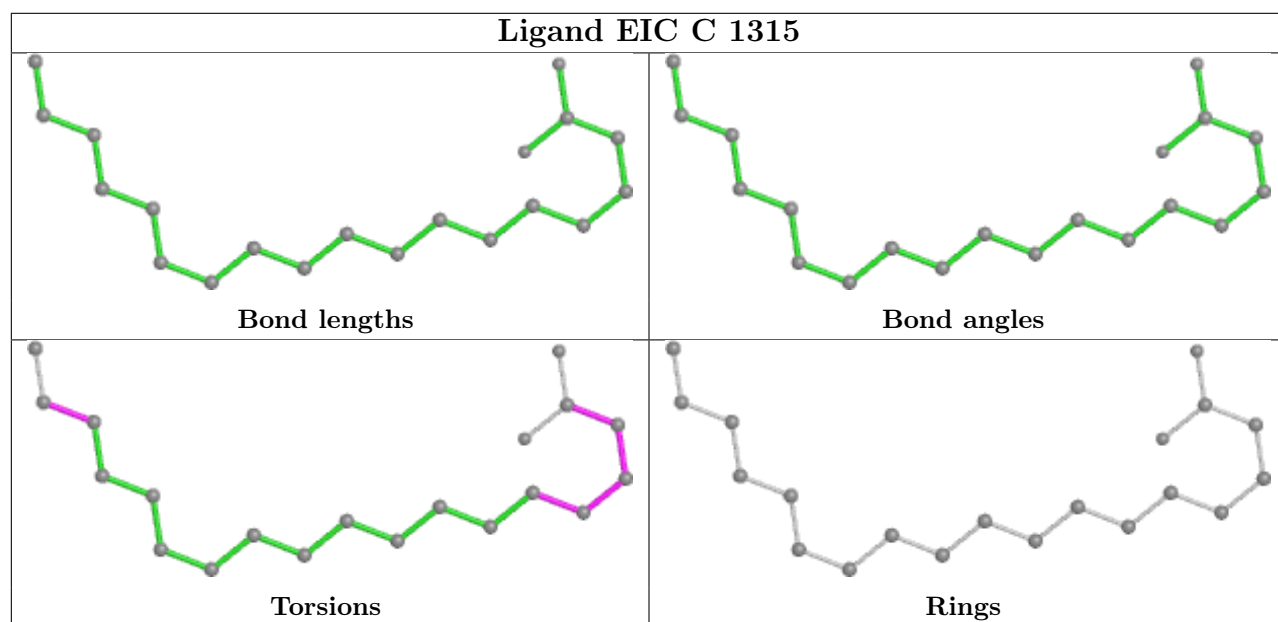
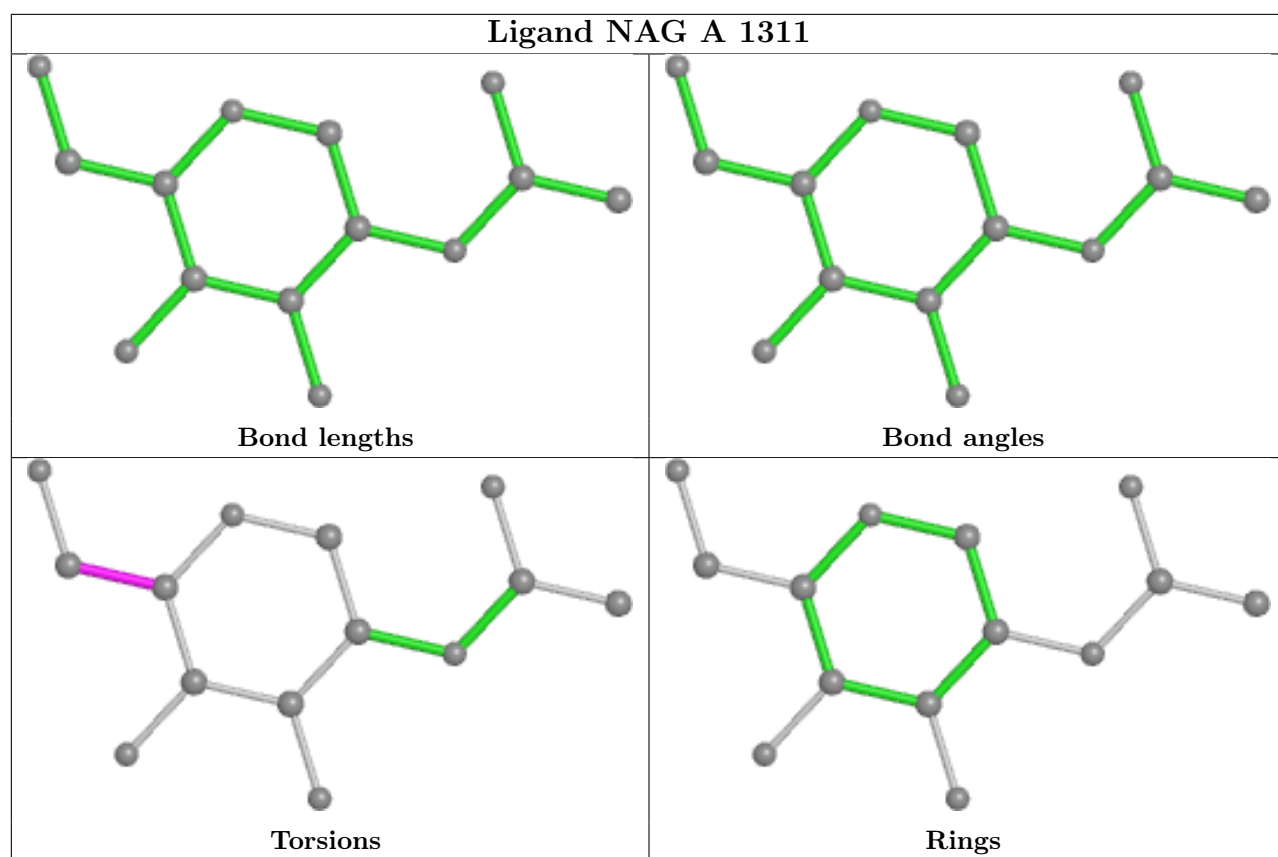


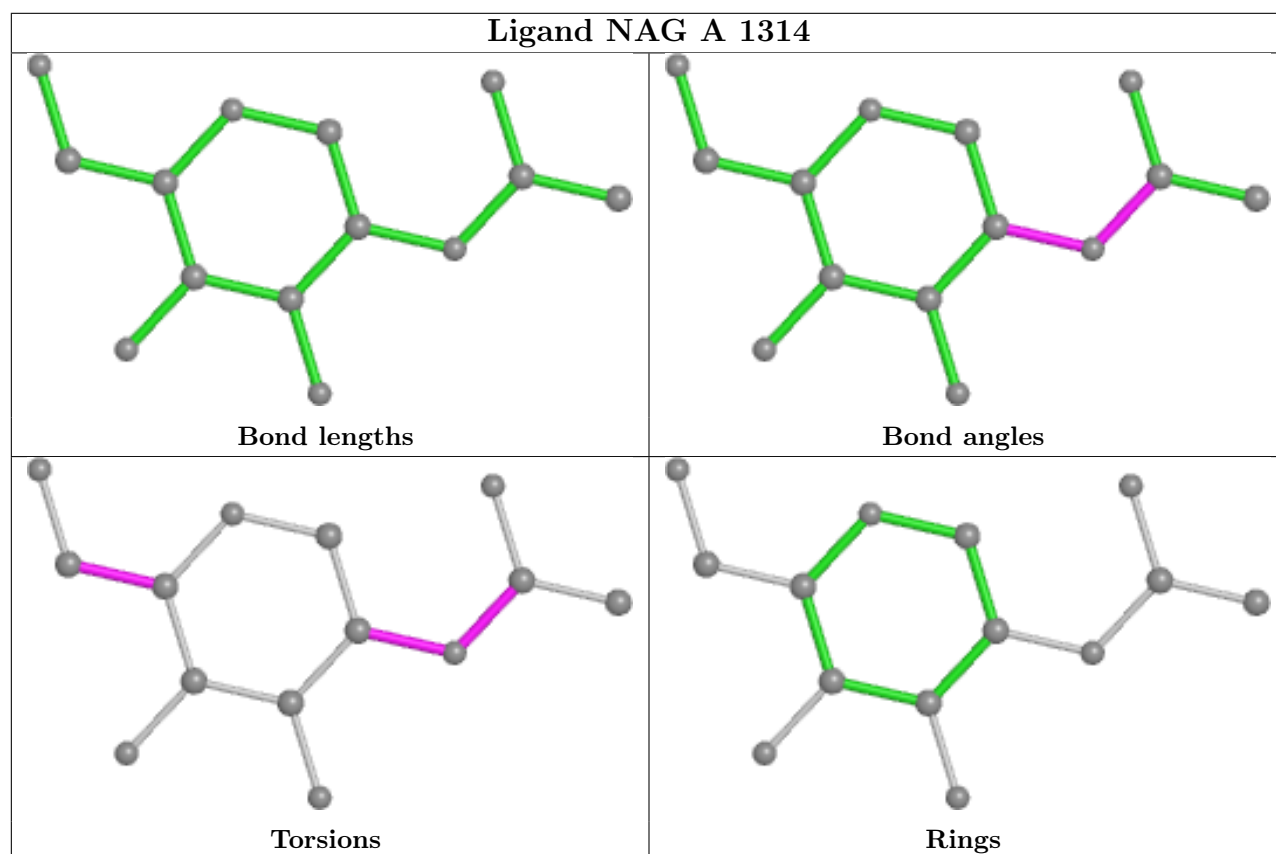
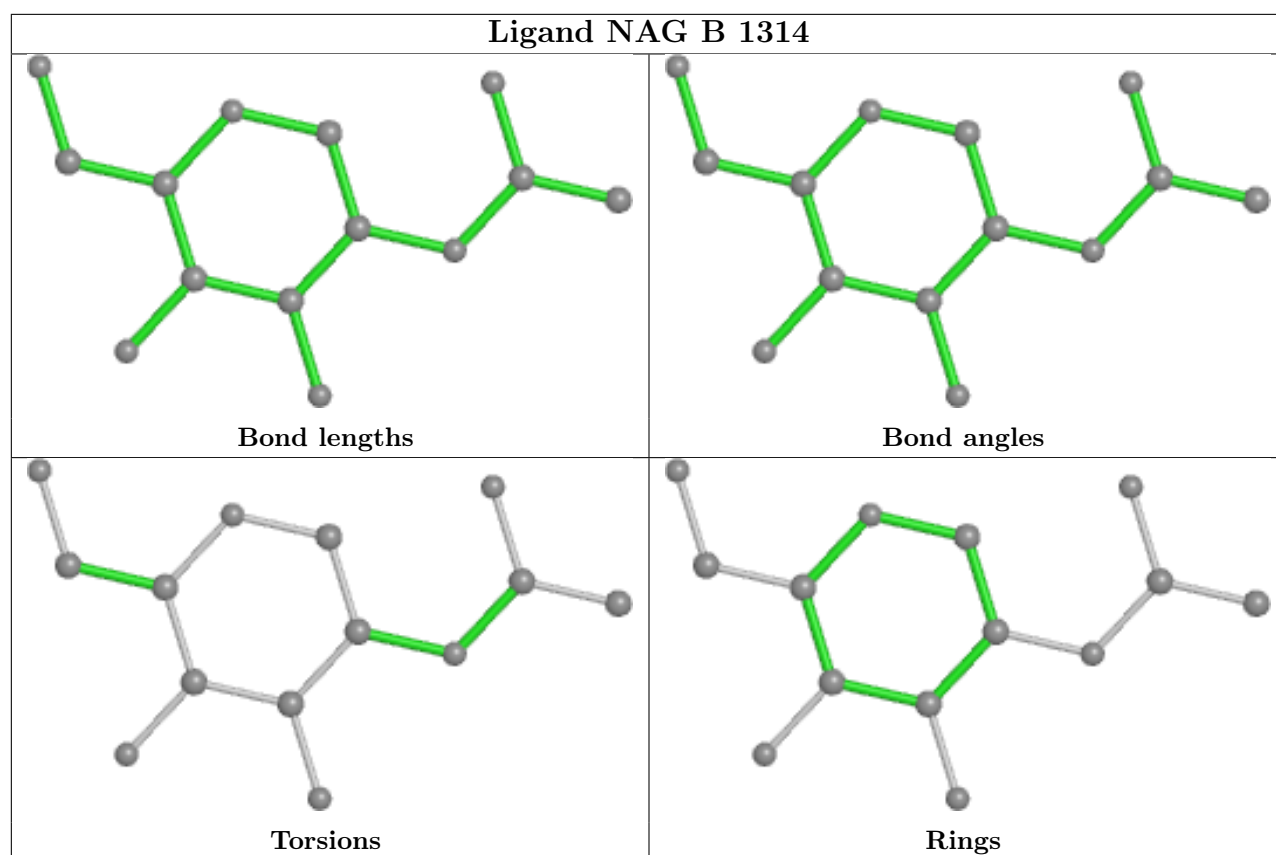
Ligand NAG C 1314



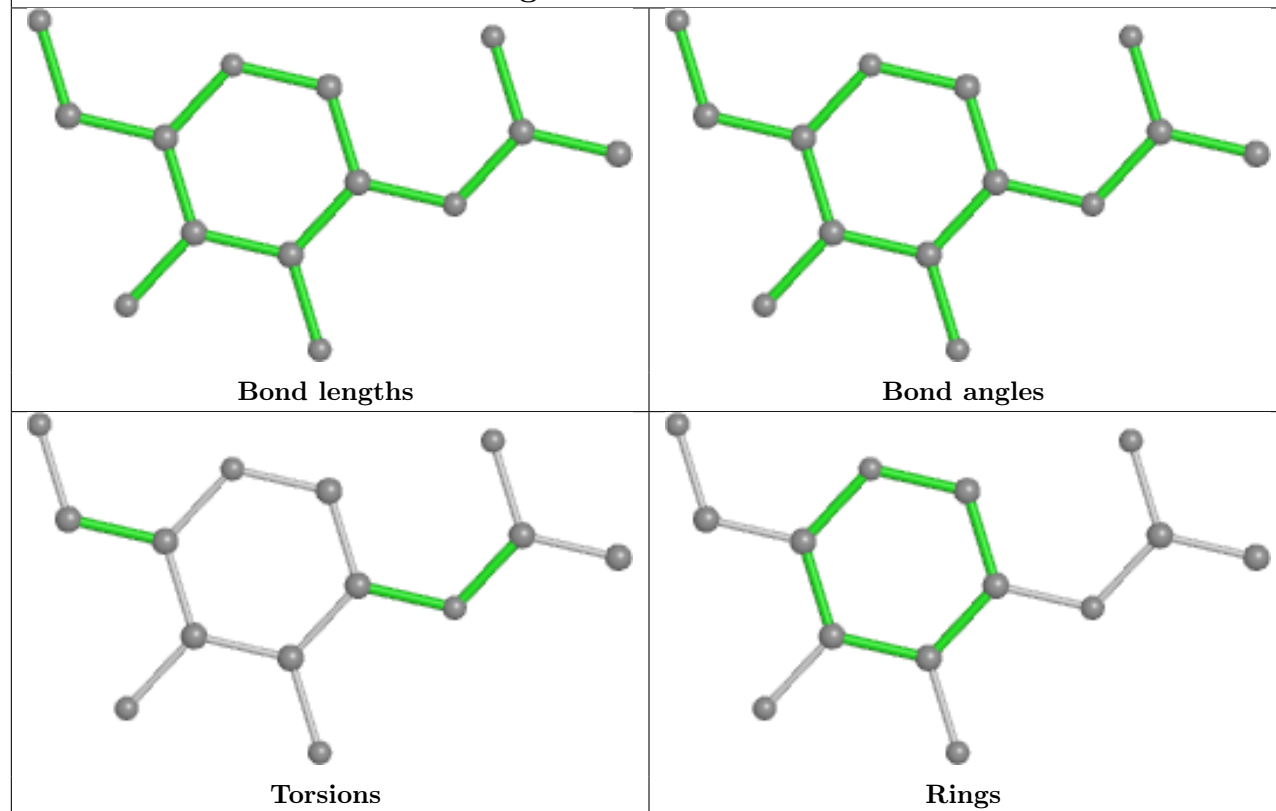
Ligand NAG C 1303



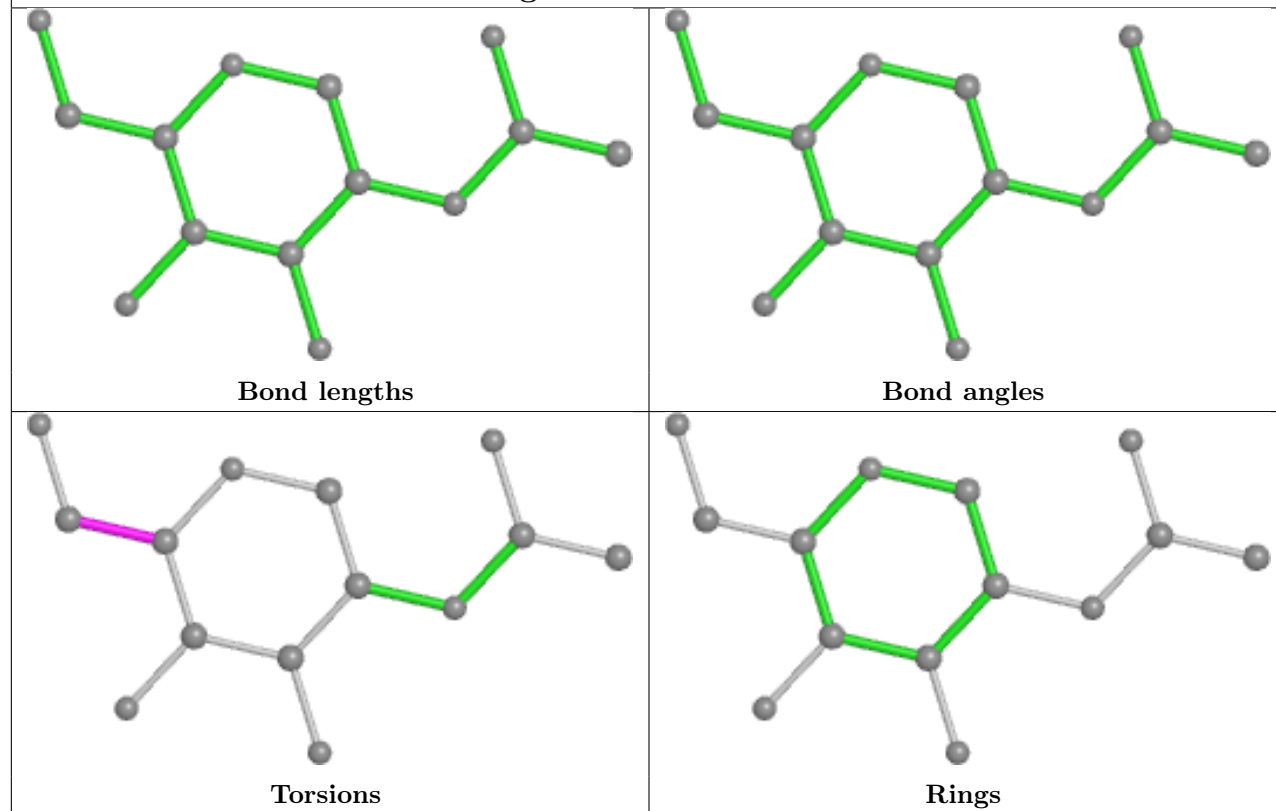




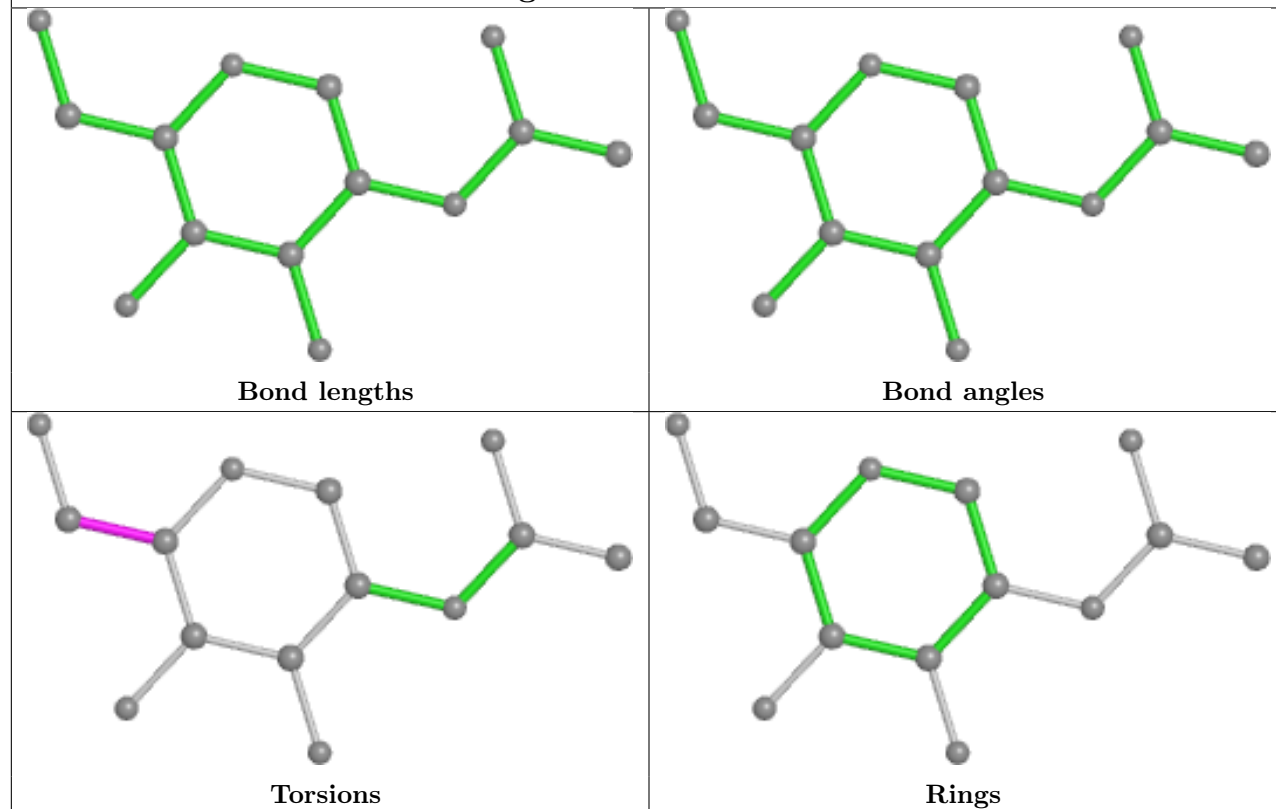
Ligand NAG B 1310



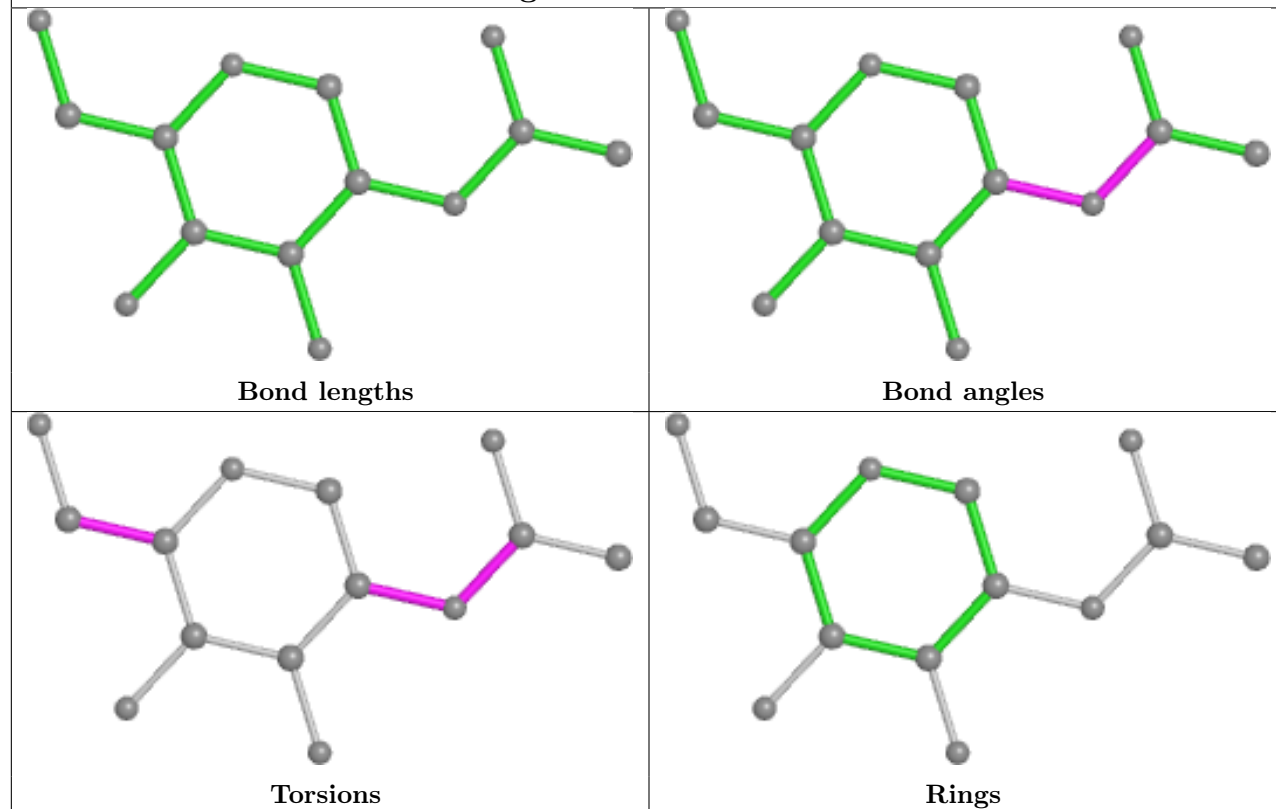
Ligand NAG B 1302

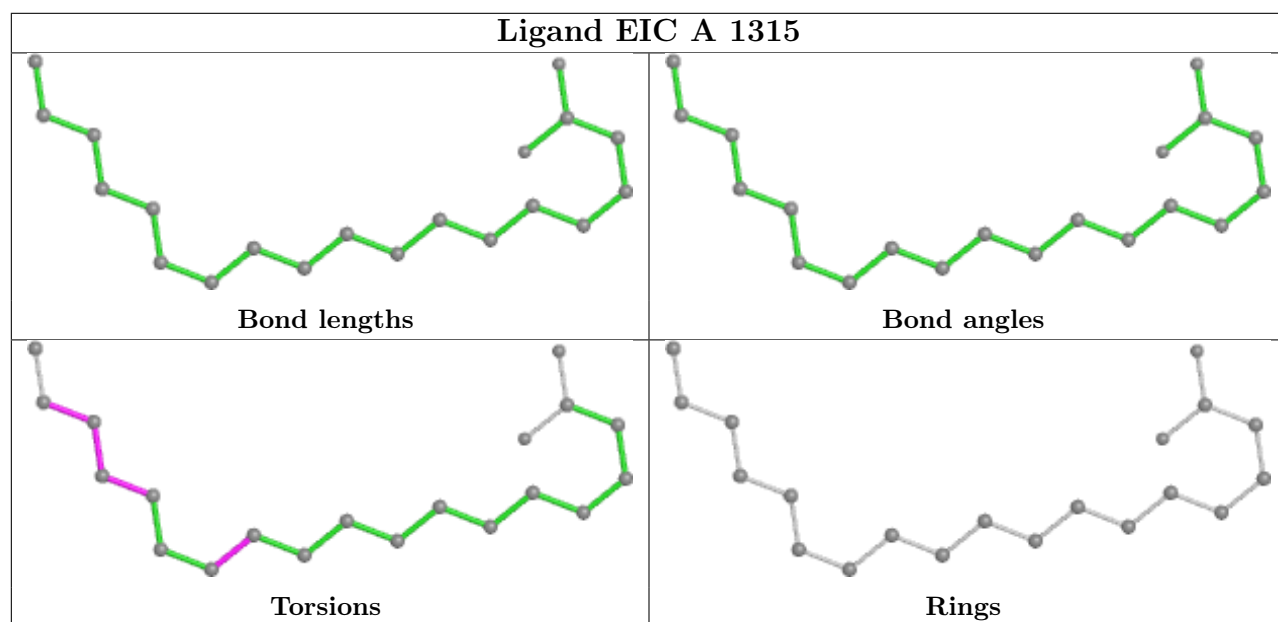
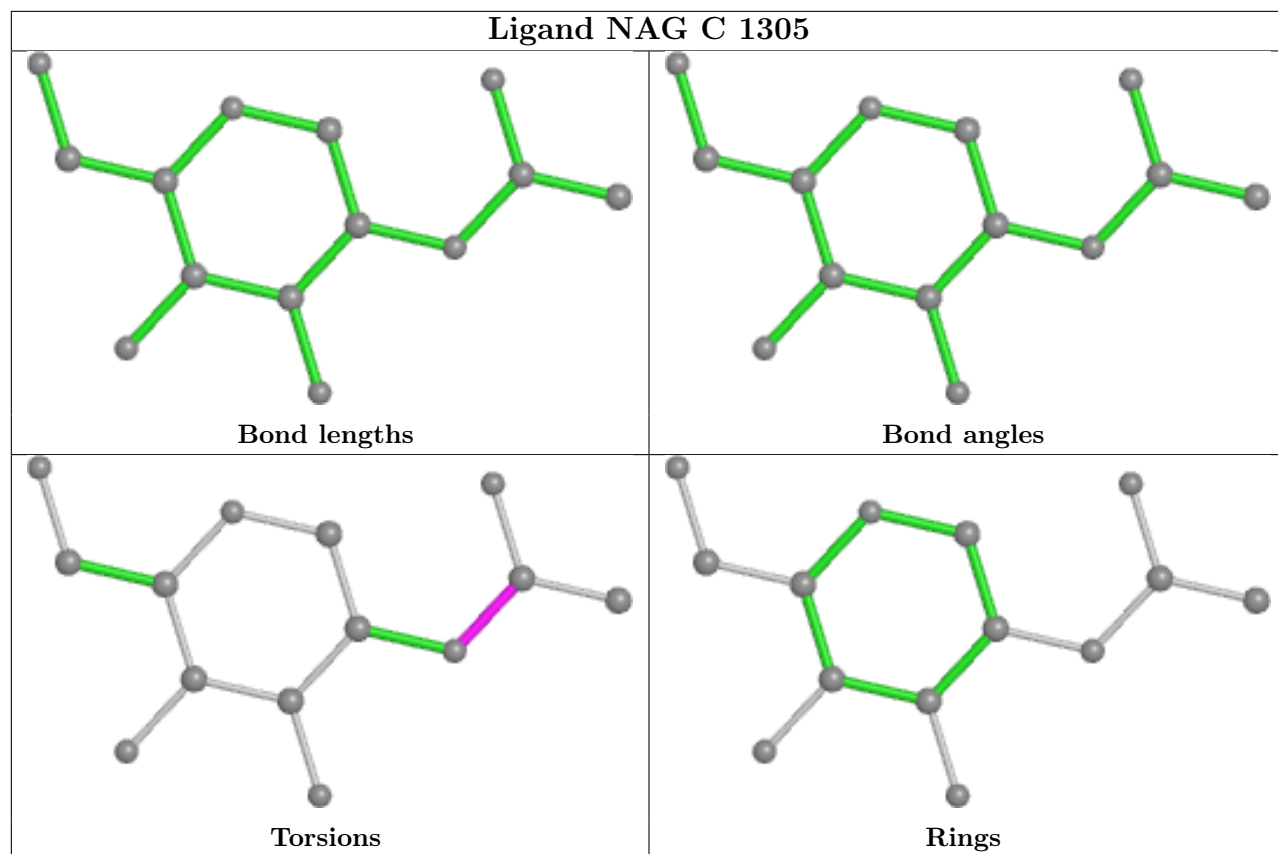


Ligand NAG A 1306

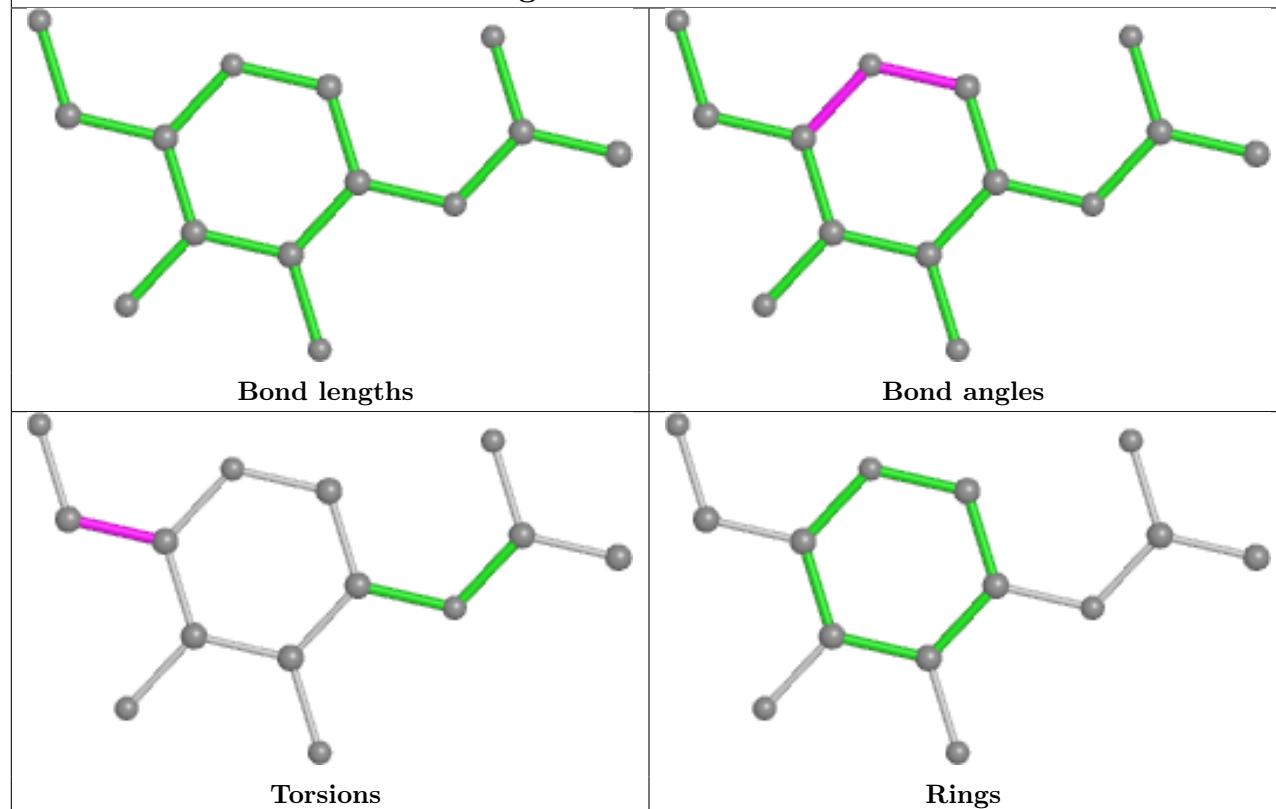


Ligand NAG B 1315

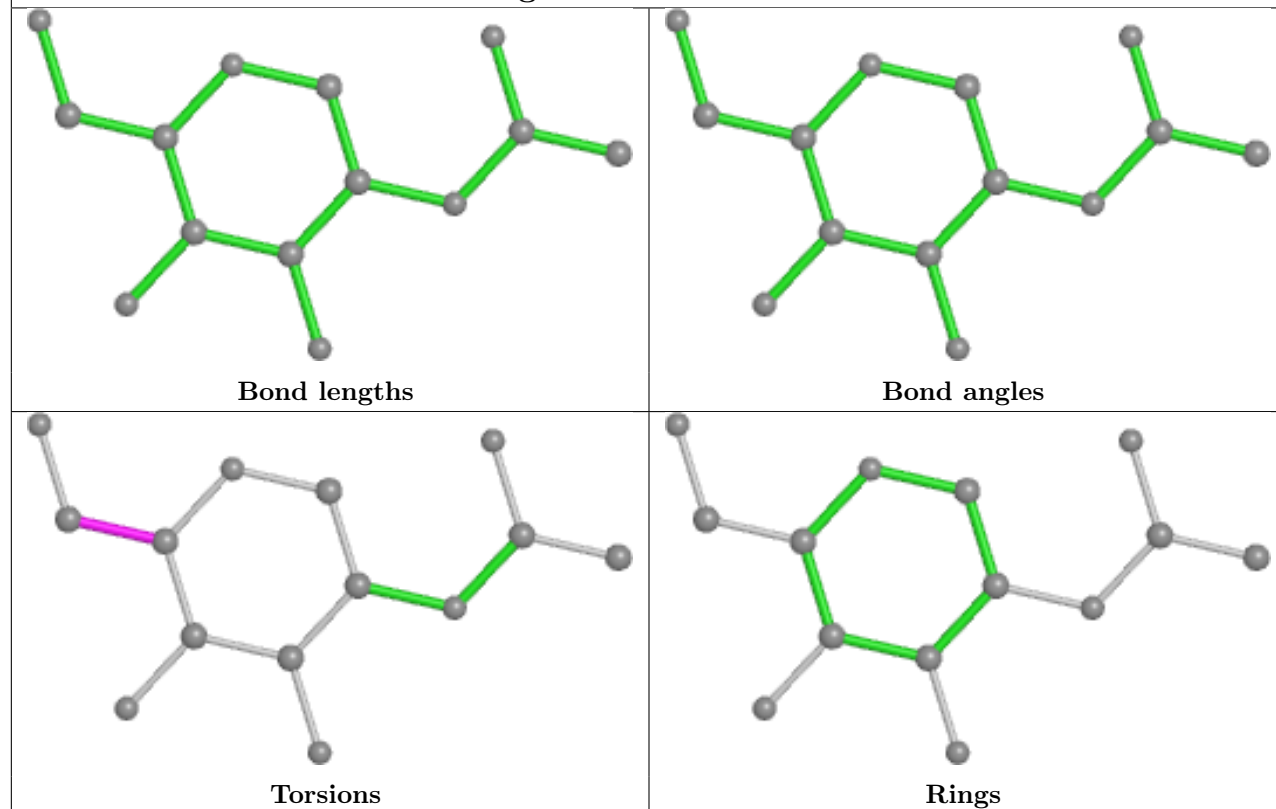




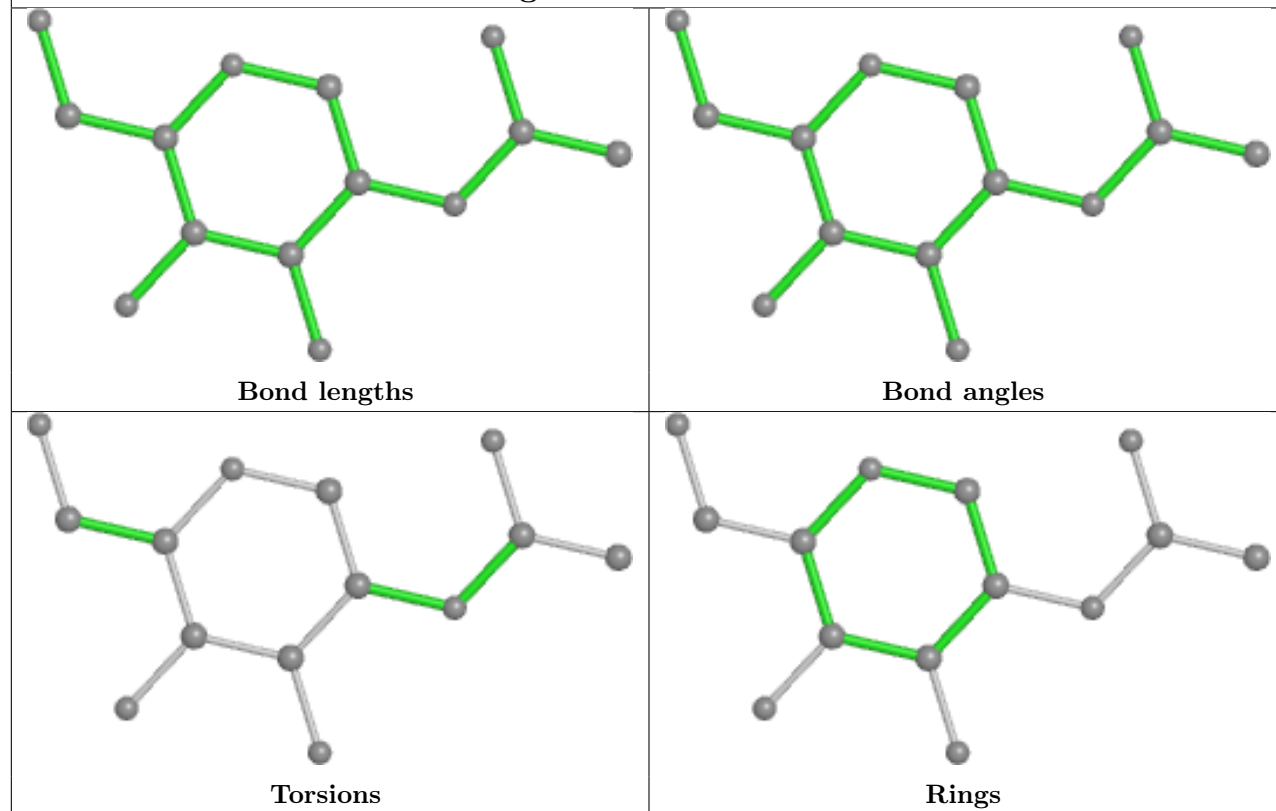
Ligand NAG A 1304



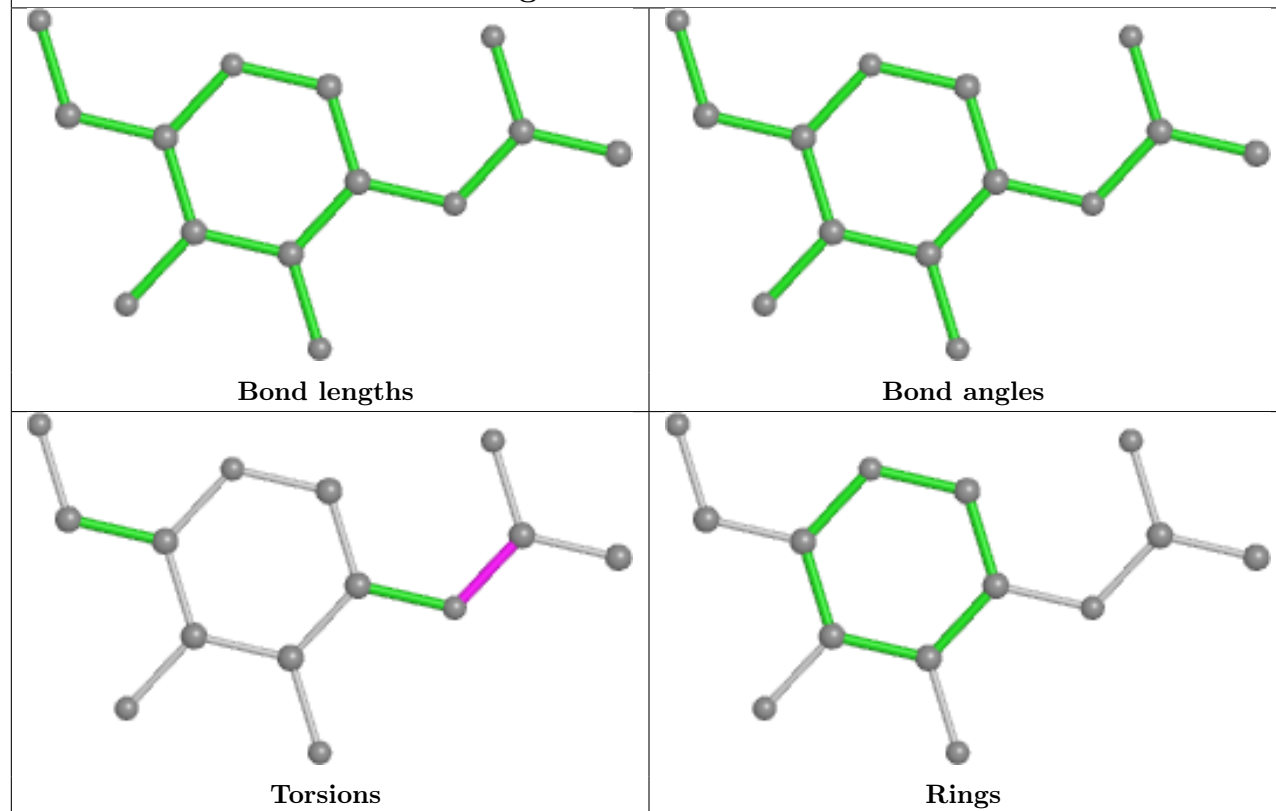
Ligand NAG A 1310



Ligand NAG B 1304



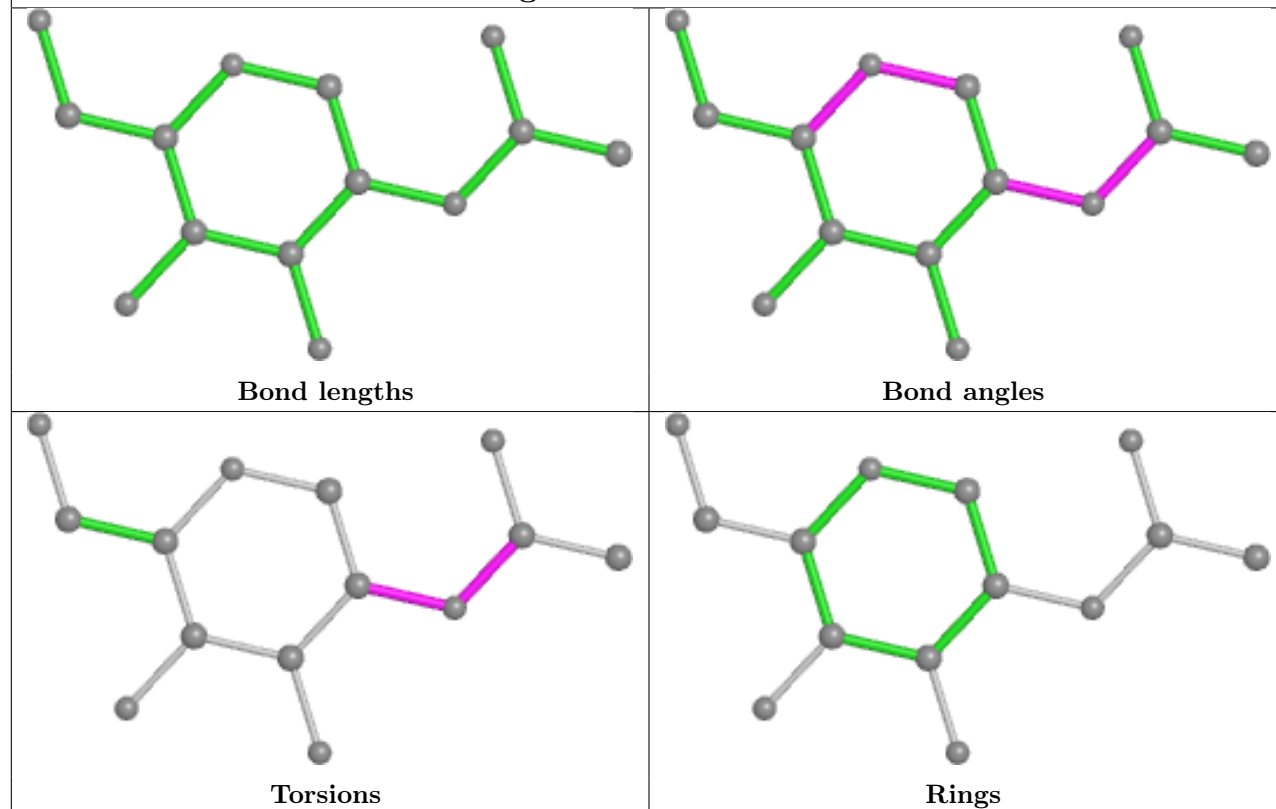
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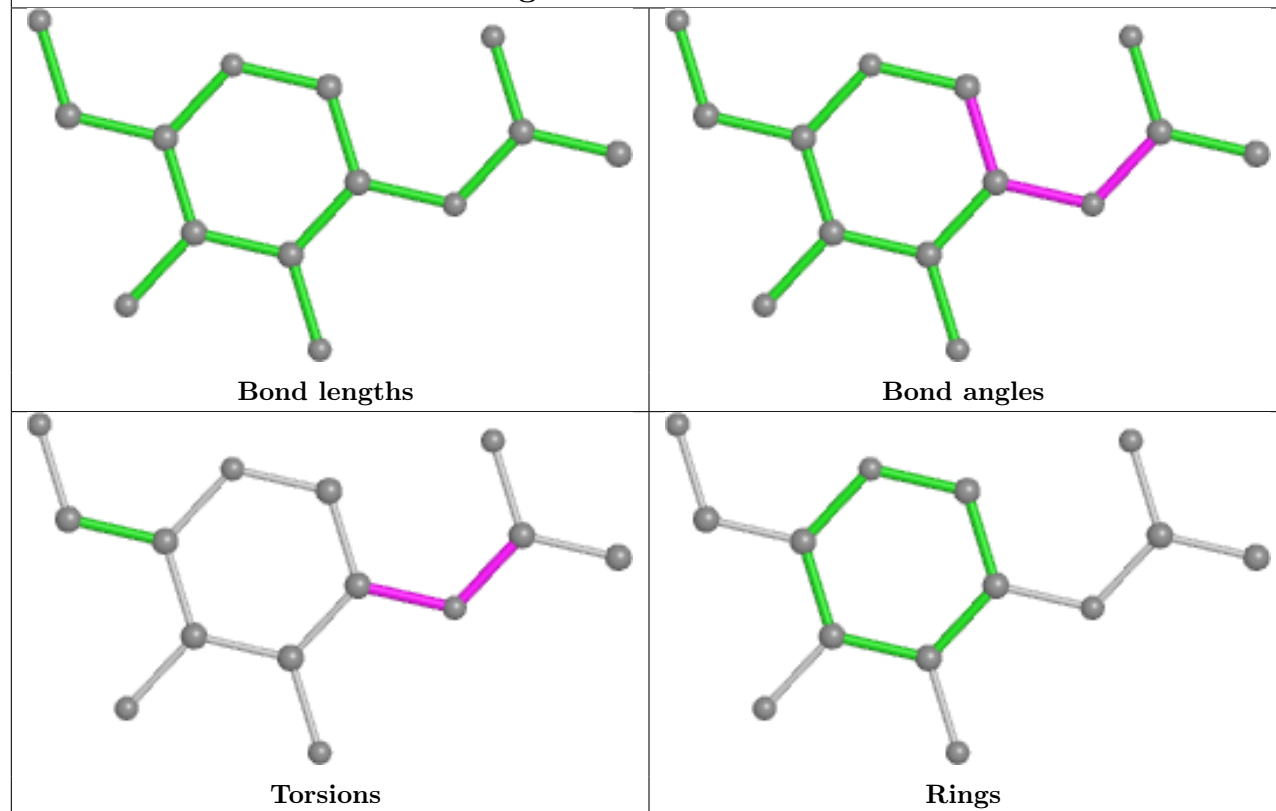
Ligand NAG A 1302



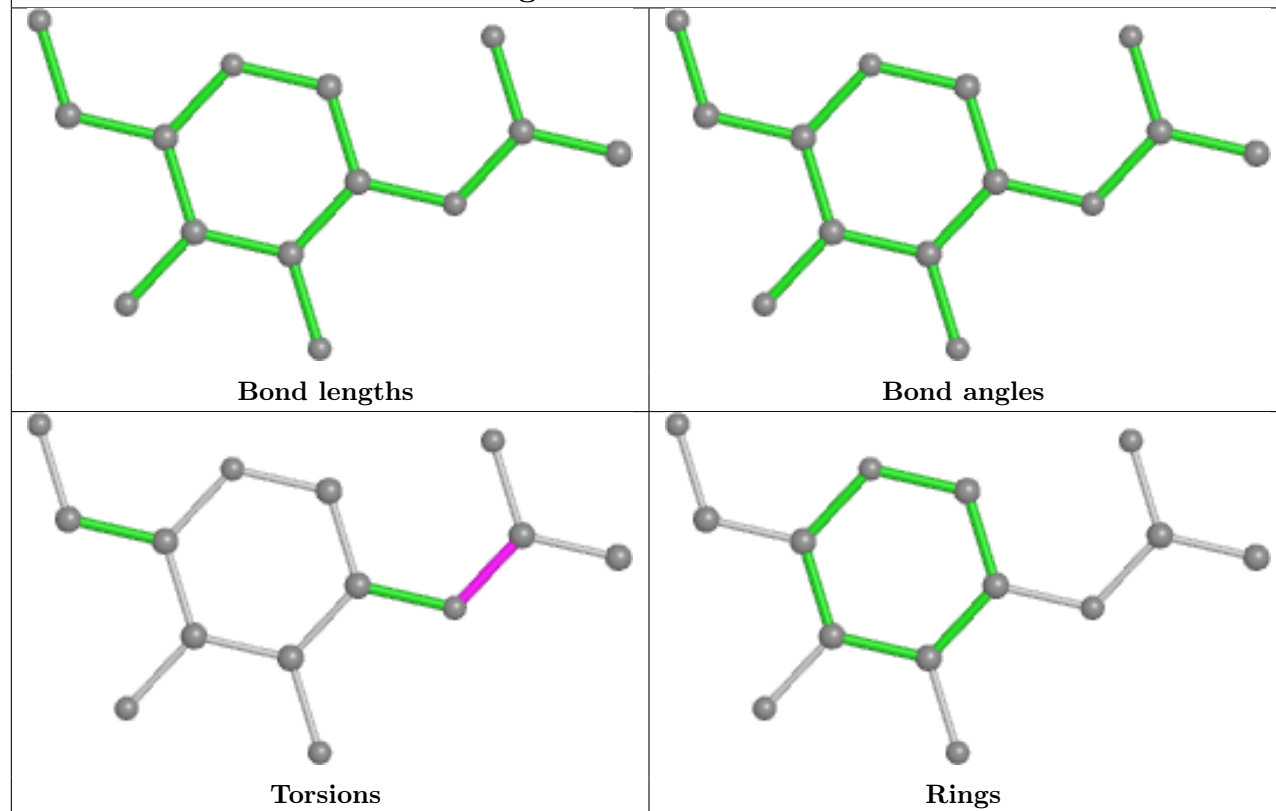
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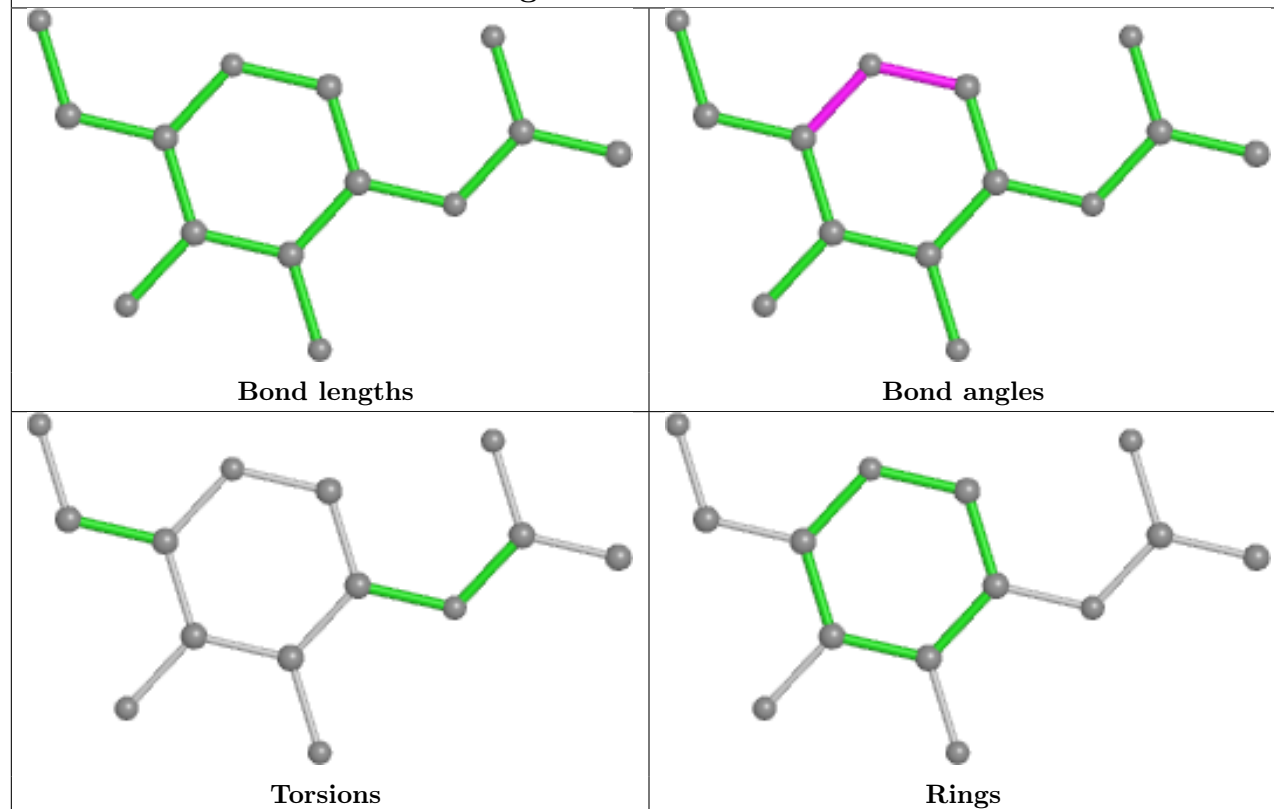
Ligand NAG A 1307



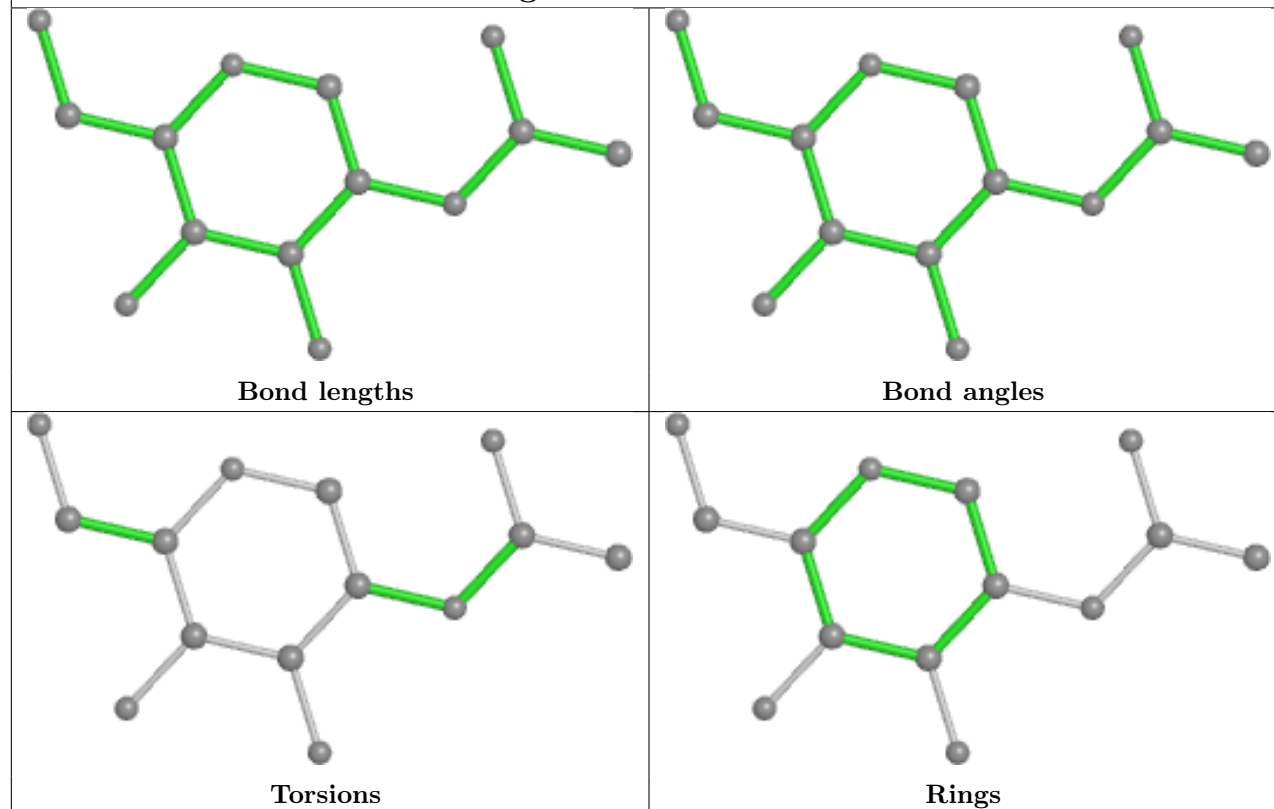
Ligand NAG A 1309



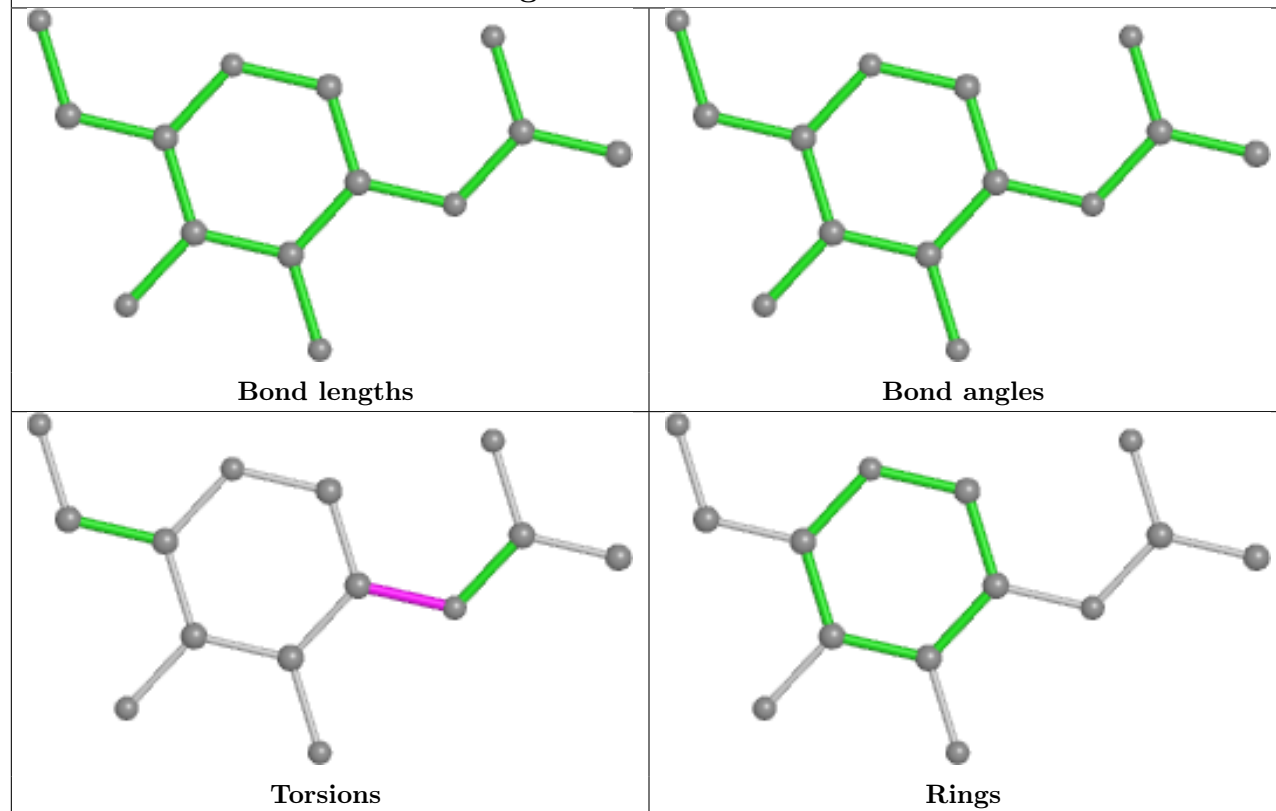
Ligand NAG B 1301



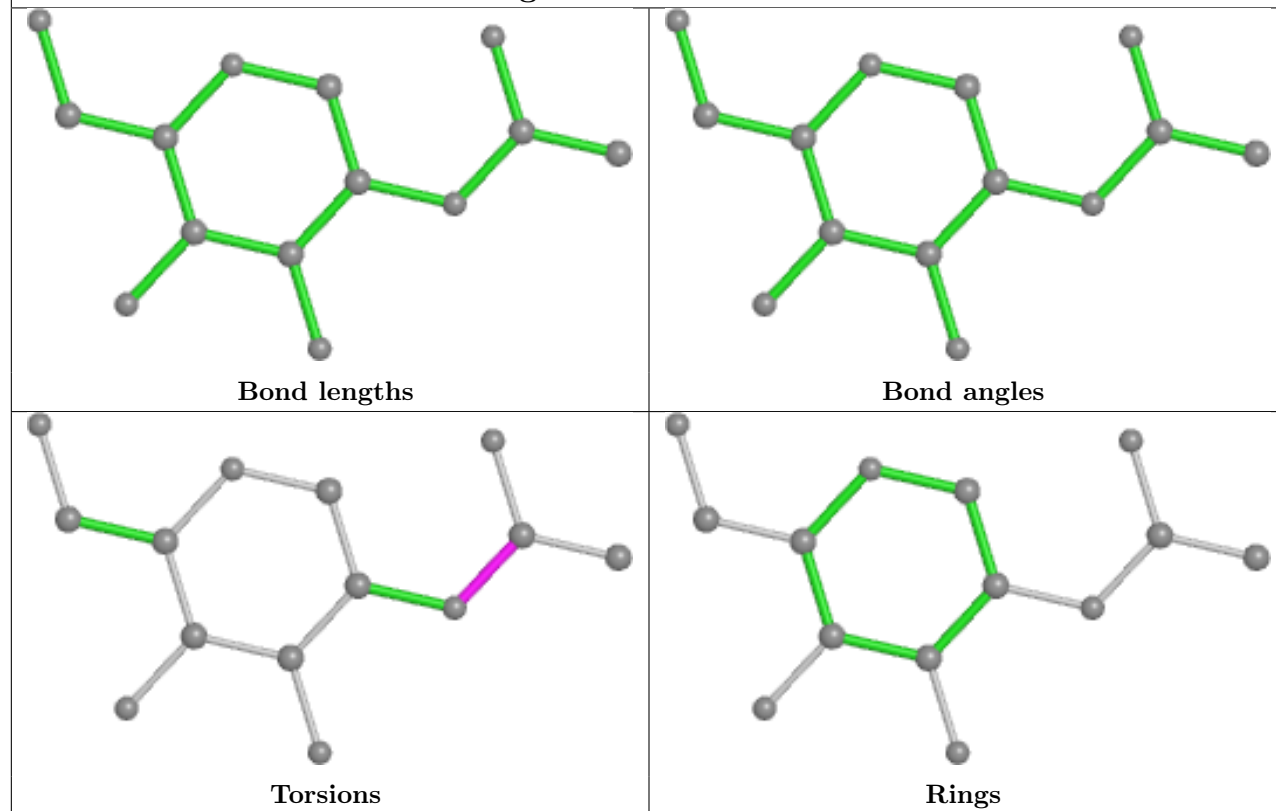
Ligand NAG C 1304



Ligand NAG B 1307



Ligand NAG C 1302



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.

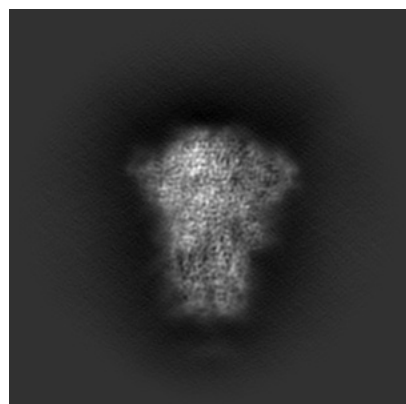
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38773. These allow visual inspection of the internal detail of the map and identification of artifacts.

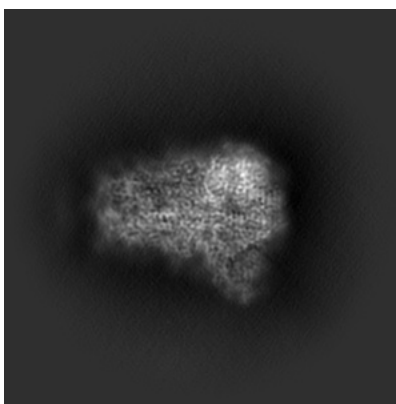
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

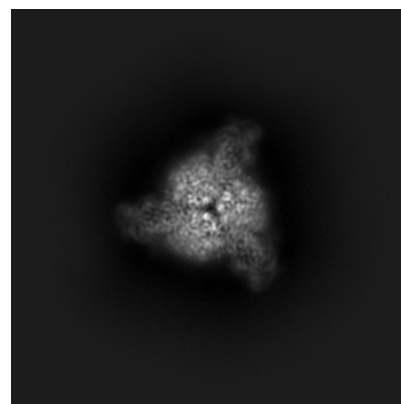
6.1.1 Primary map



X

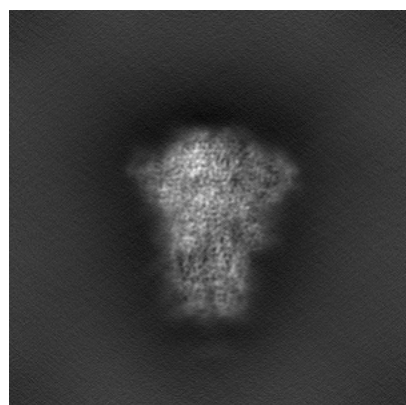


Y

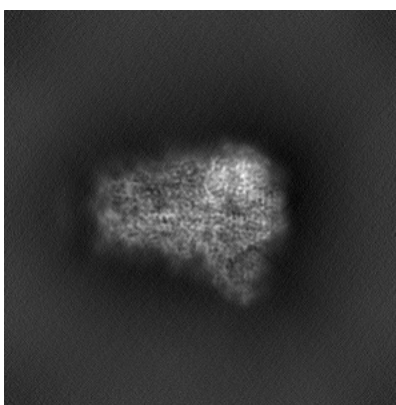


Z

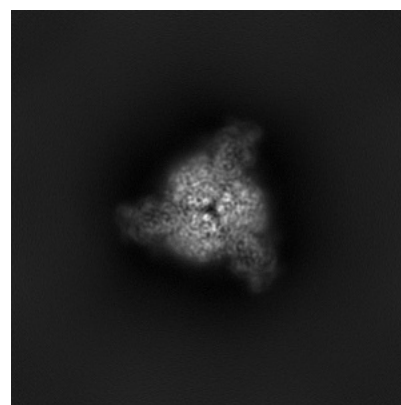
6.1.2 Raw map



X



Y

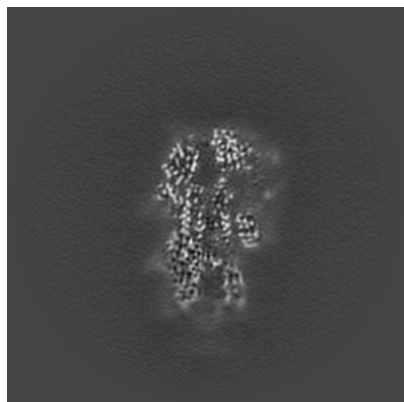


Z

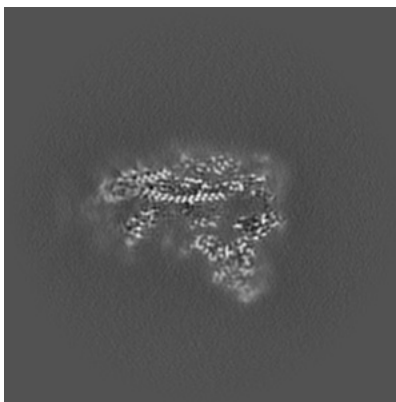
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

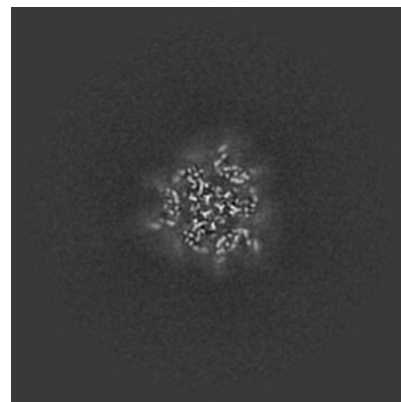
6.2.1 Primary map



X Index: 240

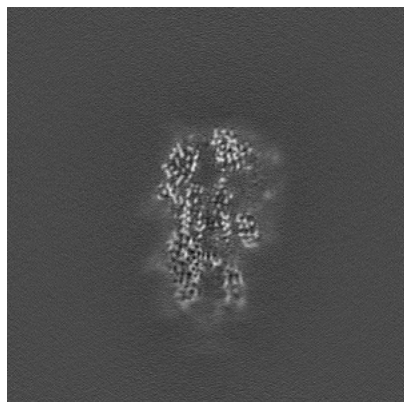


Y Index: 240

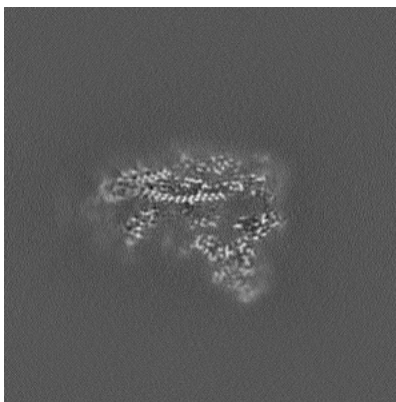


Z Index: 240

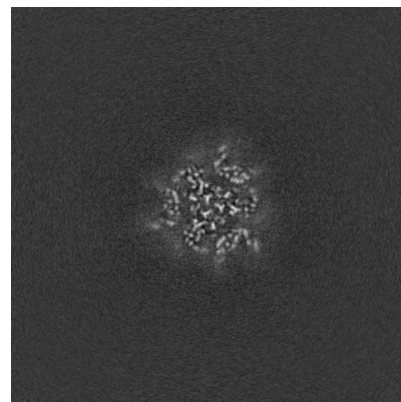
6.2.2 Raw map



X Index: 240



Y Index: 240

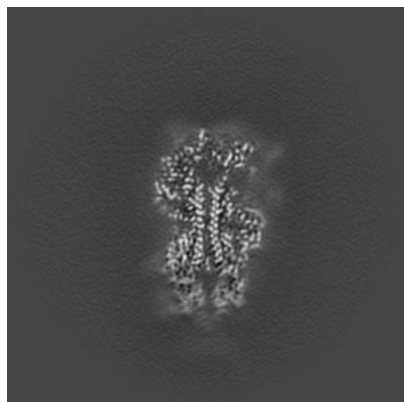


Z Index: 240

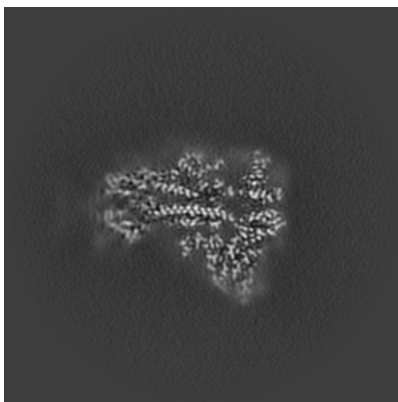
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

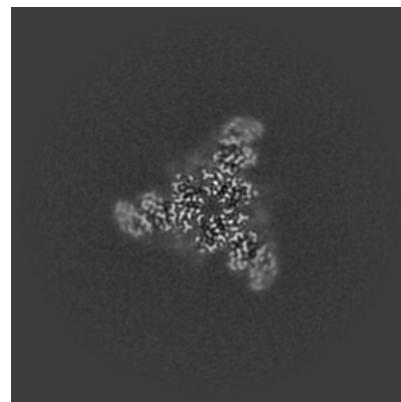
6.3.1 Primary map



X Index: 233

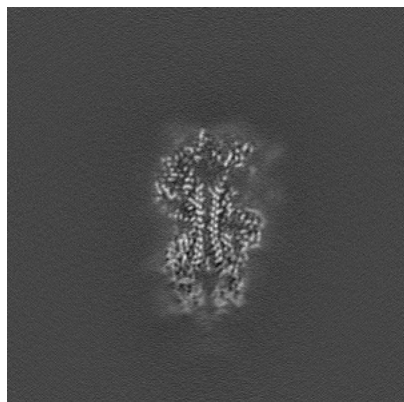


Y Index: 231

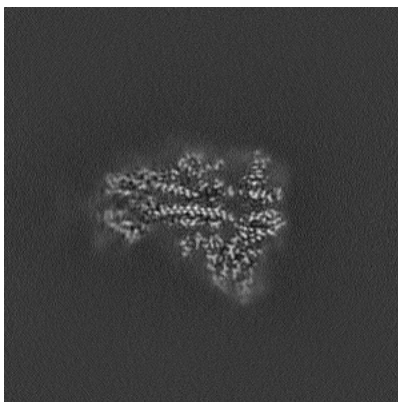


Z Index: 289

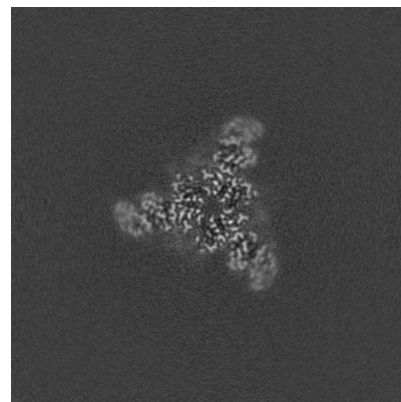
6.3.2 Raw map



X Index: 233



Y Index: 231

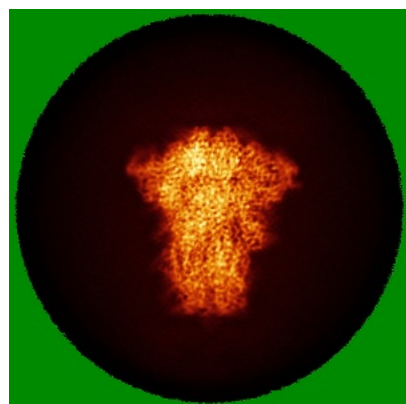


Z Index: 289

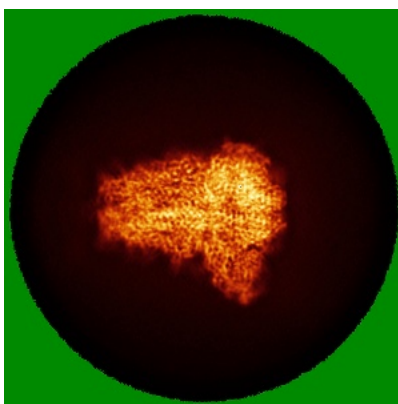
The images above show the largest variance slices of the map in three orthogonal directions.

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

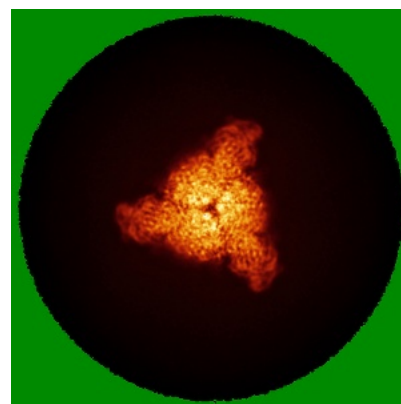
6.4.1 Primary map



X

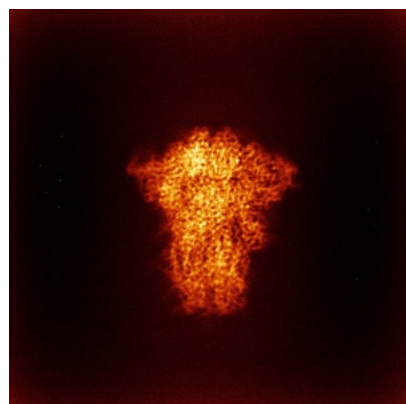


Y

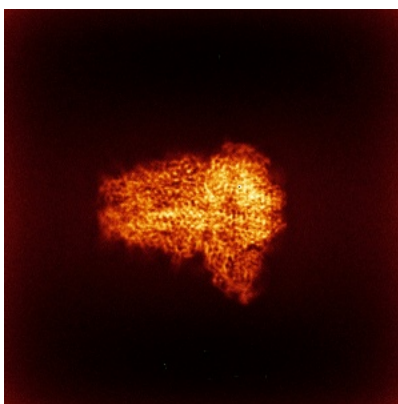


Z

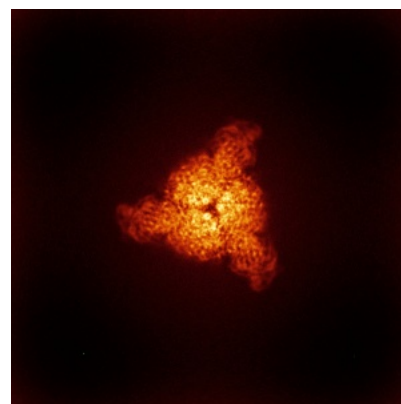
6.4.2 Raw map



X



Y

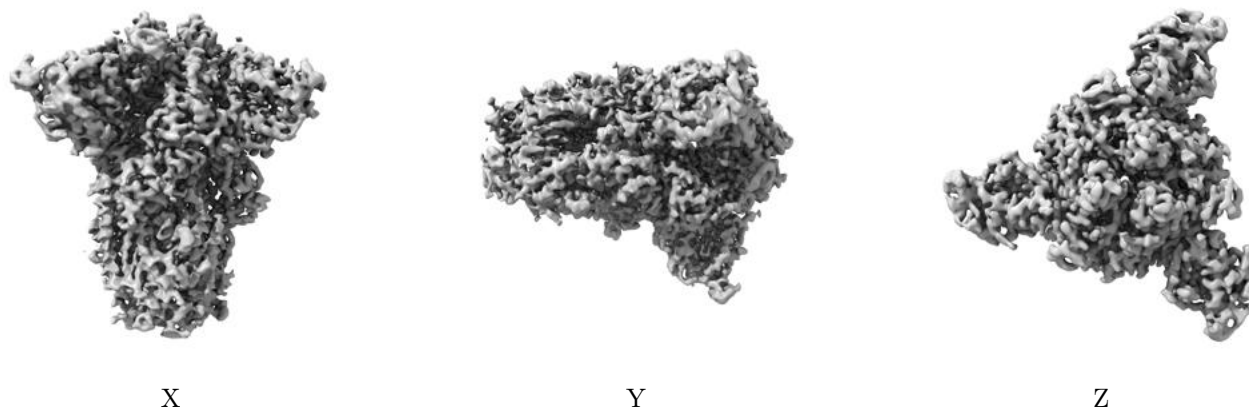


Z

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.

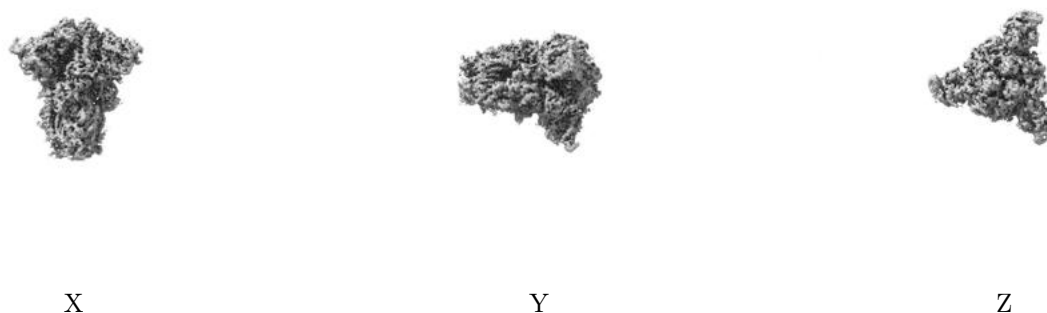
6.5 Orthogonal surface views [i](#)

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.

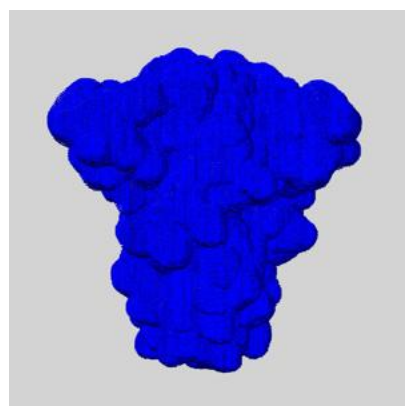
6.6 Mask visualisation [i](#)

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

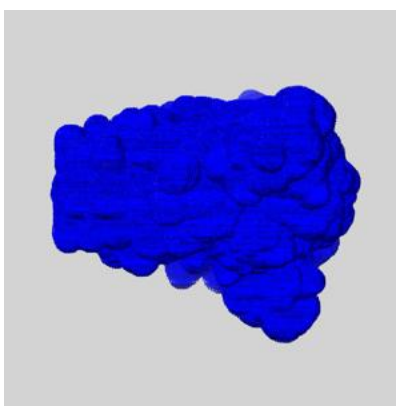
A mask typically either:

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

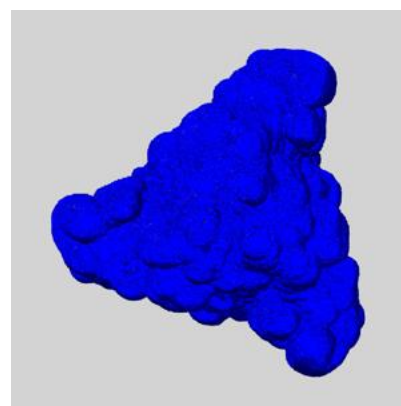
6.6.1 emd_38773_msk_1.map [i](#)



X



Y

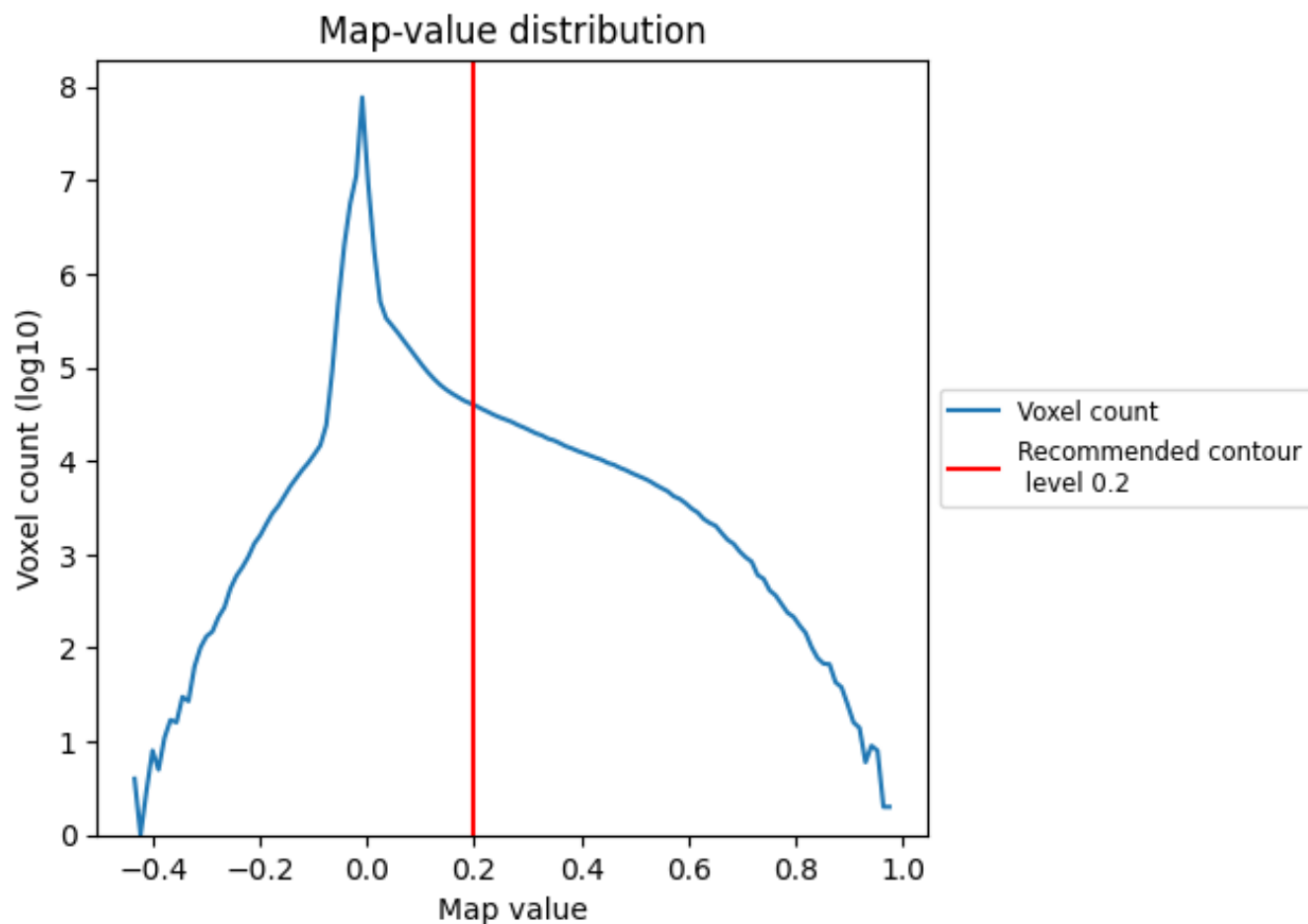


Z

7 Map analysis [i](#)

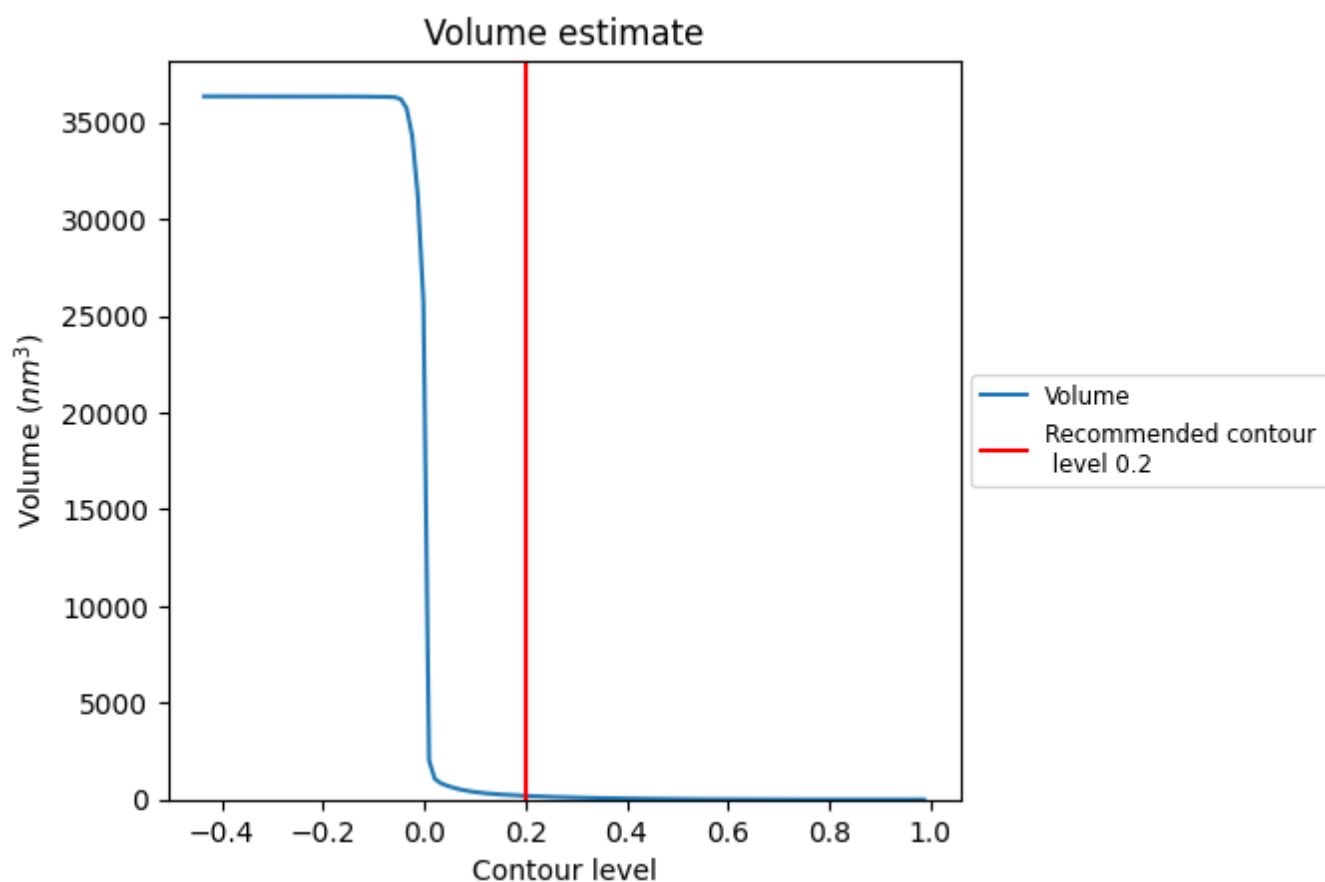
This section contains the results of statistical analysis of the map.

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.

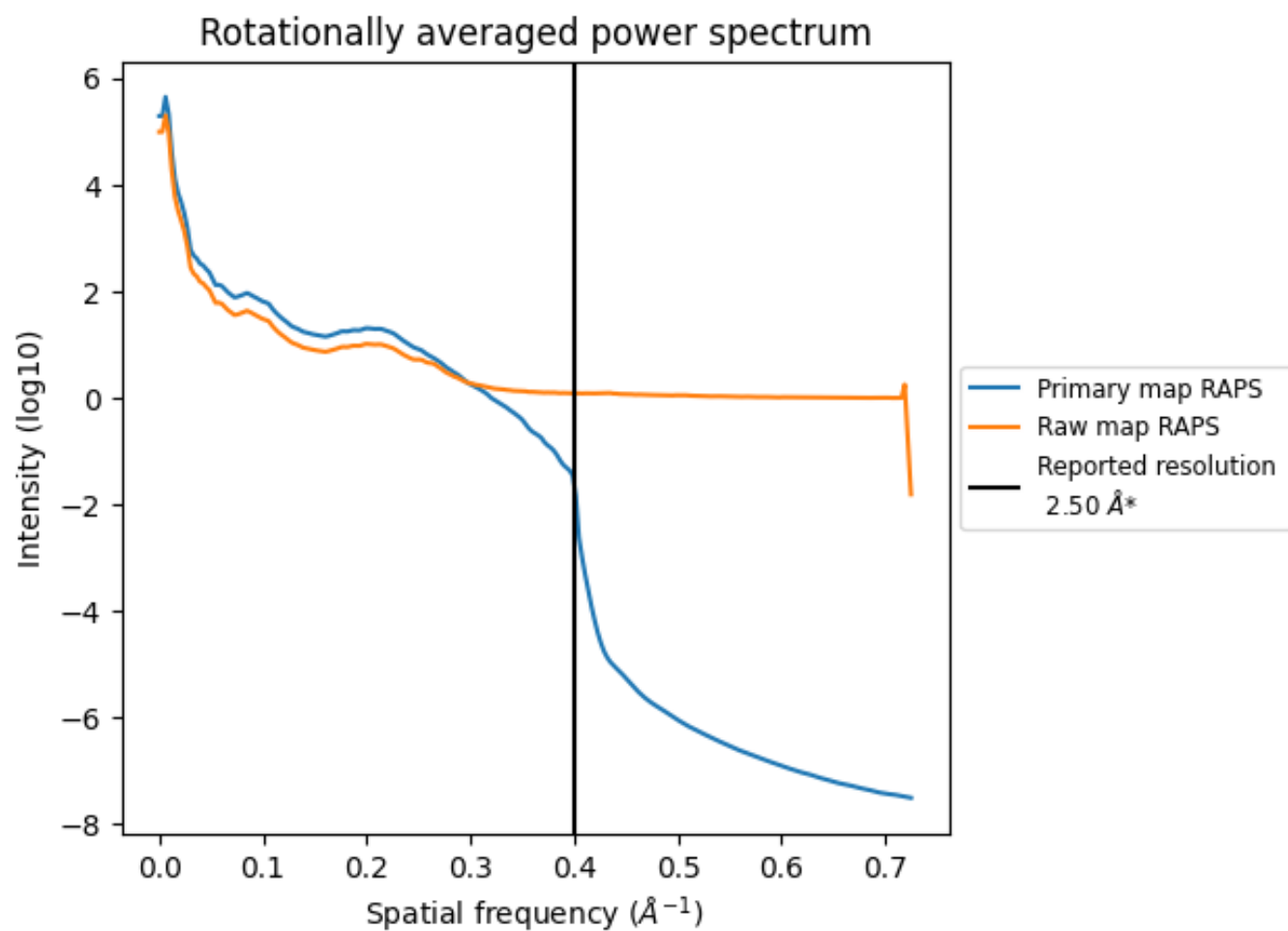
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm³; this corresponds to an approximate mass of 174 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](#)

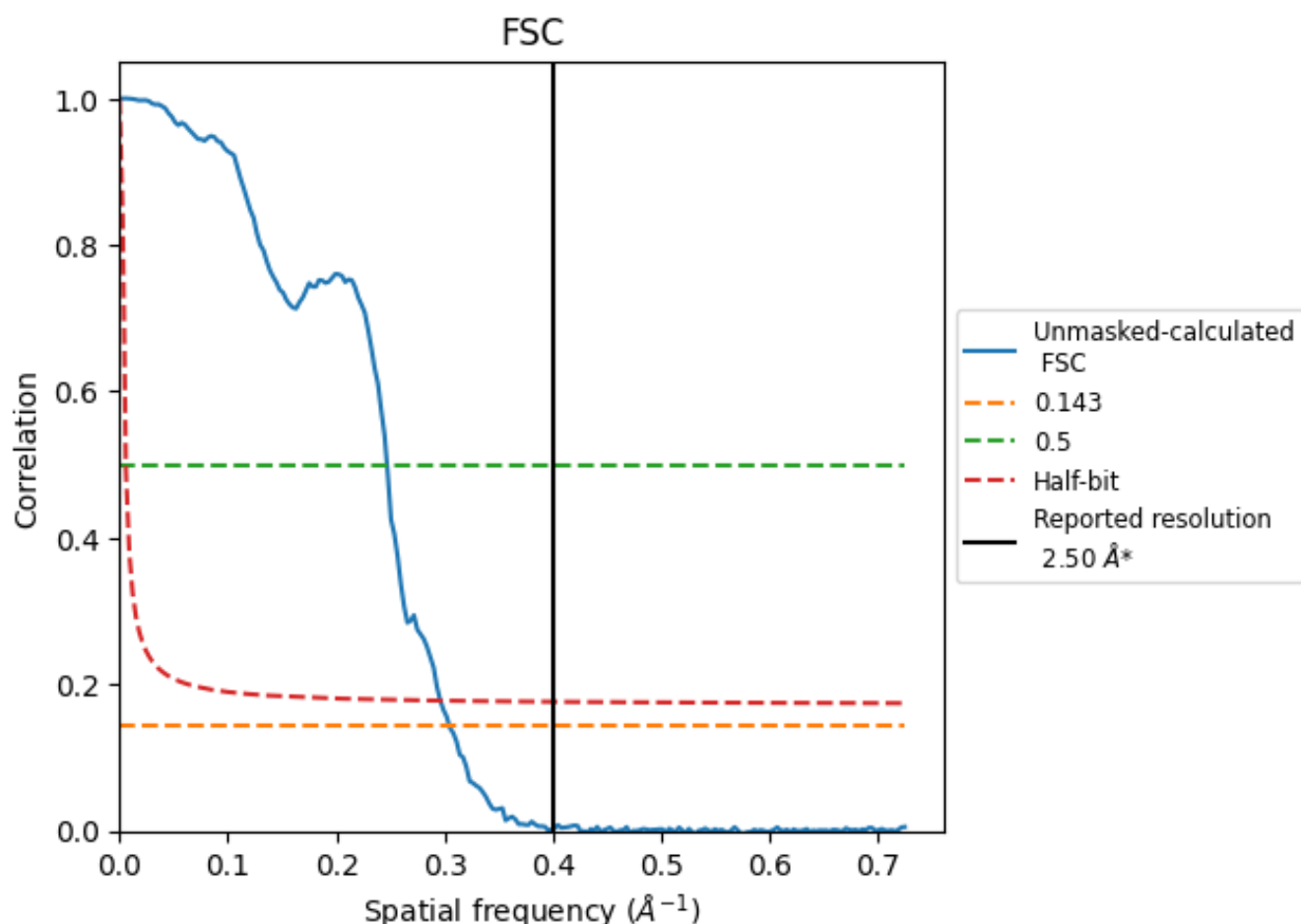


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

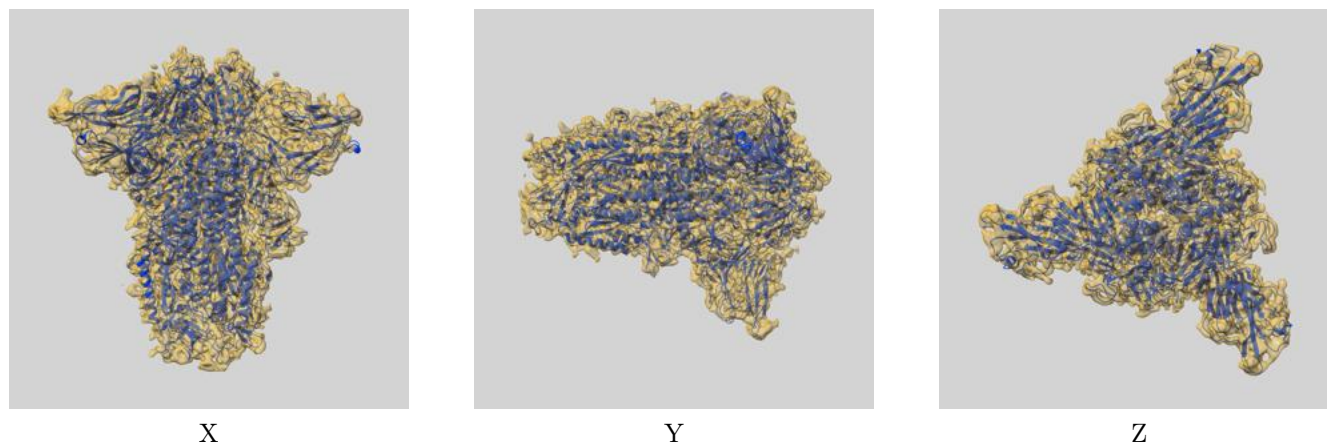
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.29	4.05	3.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

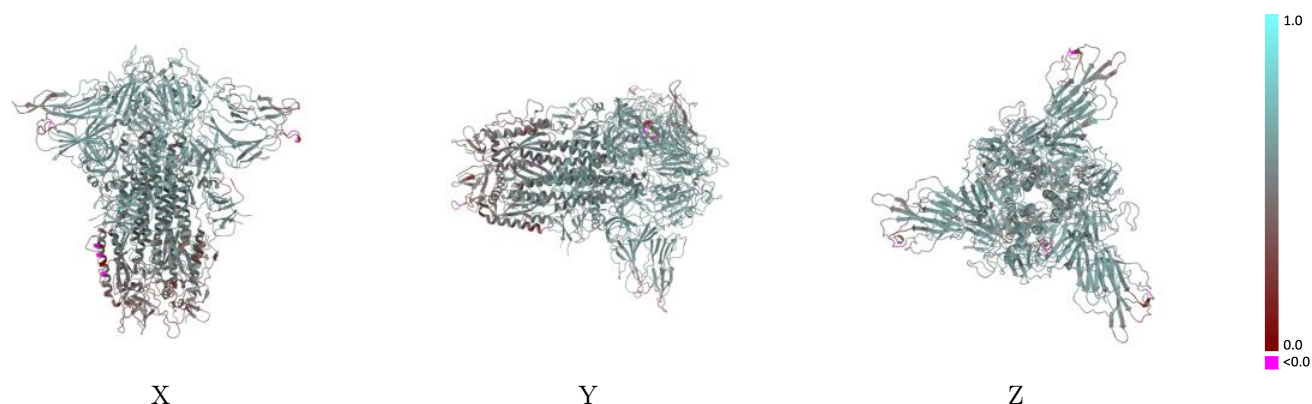
This section contains information regarding the fit between EMDB map EMD-38773 and PDB model 8XYH. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



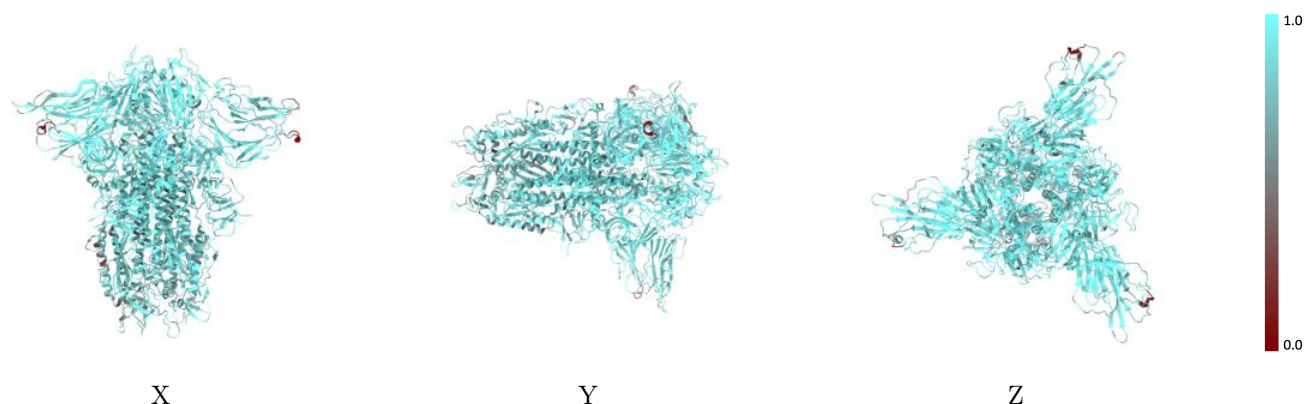
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



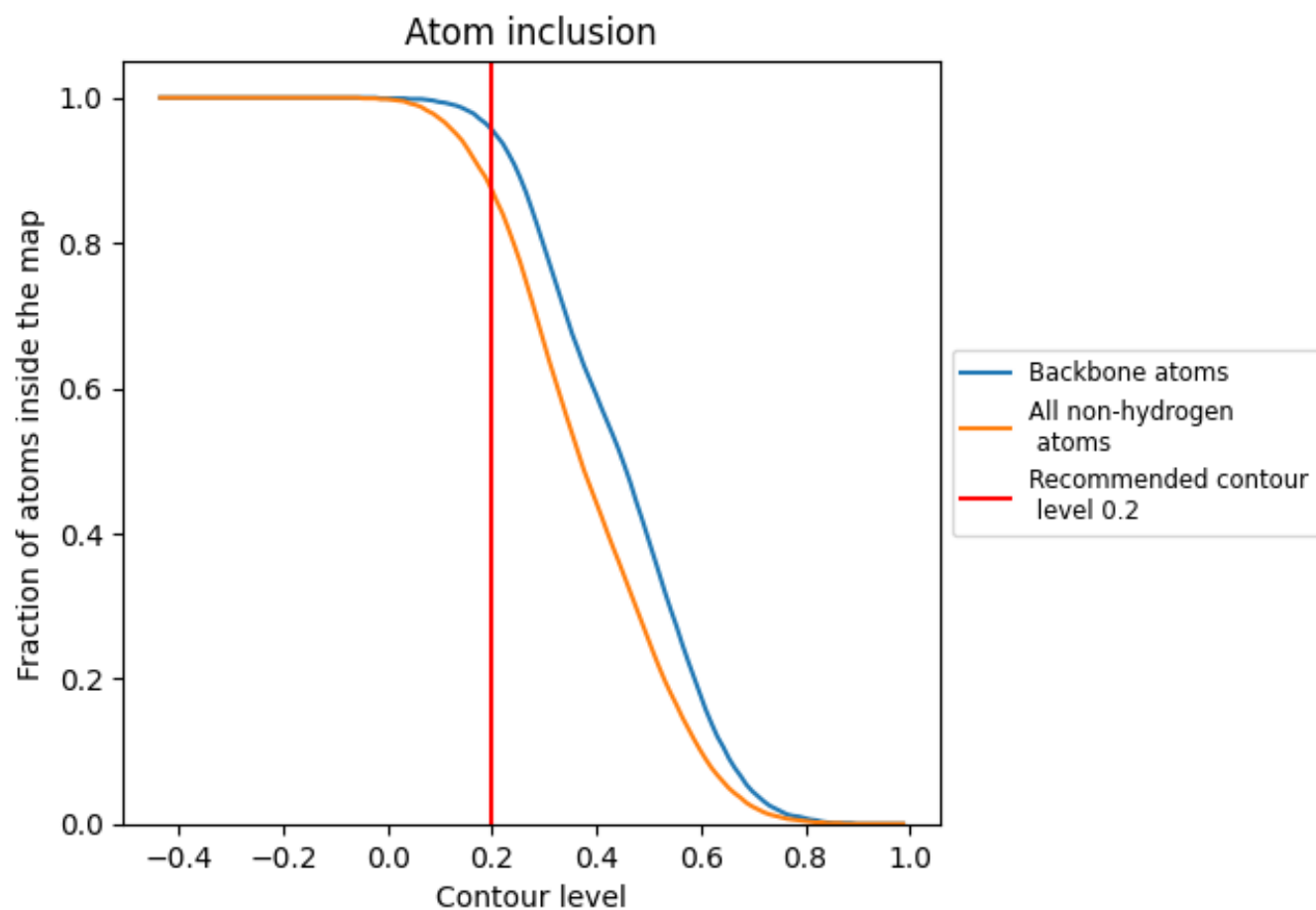
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 87% 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	<div><div></div></div> 0.8730	<div><div></div></div> 0.5310
A	<div><div></div></div> 0.8730	<div><div></div></div> 0.5290
B	<div><div></div></div> 0.8710	<div><div></div></div> 0.5300
C	<div><div></div></div> 0.8760	<div><div></div></div> 0.5360
D	<div><div></div></div> 0.7500	<div><div></div></div> 0.4710
E	<div><div></div></div> 0.6070	<div><div></div></div> 0.4000
F	<div><div></div></div> 0.7140	<div><div></div></div> 0.2920

1.0

0.0

<0.0