



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 04:19 AM EST

PDB ID : 7SC1
EMDB ID : EMD-25008
Title : Structure of the SARS-CoV-2 S 6P trimer in complex with the human neutralizing antibody Fab fragment, R40-1G8
Authors : Fan, C.; Bjorkman, P.J.
Deposited on : 2021-09-26
Resolution : 3.20 Å (reported)
Based on initial models : 7K8O, 7K8T

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 : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

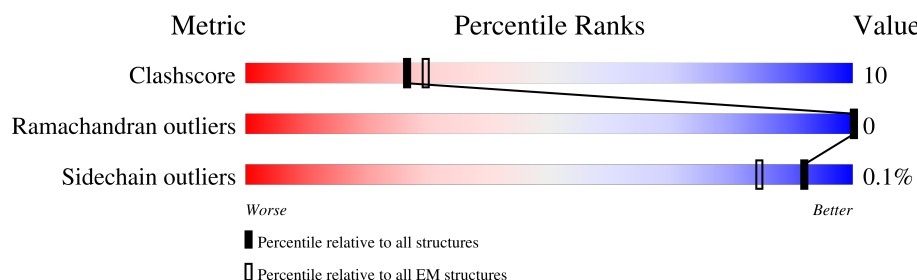
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1256	<div> <div>10%</div> <div>61%</div> <div>20%</div> <div>20%</div> </div>
1	B	1256	<div> <div>9%</div> <div>61%</div> <div>19%</div> <div>20%</div> </div>
1	C	1256	<div> <div>9%</div> <div>62%</div> <div>19%</div> <div>20%</div> </div>
2	H	224	<div> <div>50%</div> <div>36%</div> <div>16%</div> <div>48%</div> </div>
2	M	224	<div> <div>50%</div> <div>36%</div> <div>17%</div> <div>48%</div> </div>
2	P	224	<div> <div>50%</div> <div>34%</div> <div>18%</div> <div>48%</div> </div>
3	L	214	<div> <div>50%</div> <div>43%</div> <div>7%</div> <div>50%</div> </div>
3	N	214	<div> <div>50%</div> <div>41%</div> <div>9%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	214	<p>50% 41% 9% 50%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29415 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	1011	Total	C	N	O	S	0	0
			7896	5044	1312	1505	35		
1	B	1011	Total	C	N	O	S	0	0
			7896	5044	1312	1505	35		
1	C	1011	Total	C	N	O	S	0	0
			7896	5044	1312	1505	35		

There are 165 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	SER	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	ILE	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	PRO	-	expression tag	UNP P0DTC2
C	1233	ARG	-	expression tag	UNP P0DTC2
C	1234	ASP	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	GLN	-	expression tag	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP P0DTC2
C	1238	TYR	-	expression tag	UNP P0DTC2
C	1239	VAL	-	expression tag	UNP P0DTC2
C	1240	ARG	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	THR	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	LEU	-	expression tag	UNP P0DTC2
C	1253	GLY	-	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
C	1259	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called R40-1G8 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	117	Total	C	N	O	S	0	0
			890	564	155	166	5		
2	M	117	Total	C	N	O	S	0	0
			890	564	155	166	5		
2	P	117	Total	C	N	O	S	0	0
			890	564	155	166	5		

- Molecule 3 is a protein called R40-1G8 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			809	509	135	163	2		
3	N	107	Total	C	N	O	S	0	0
			809	509	135	163	2		
3	Q	107	Total	C	N	O	S	0	0
			809	509	135	163	2		

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



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

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

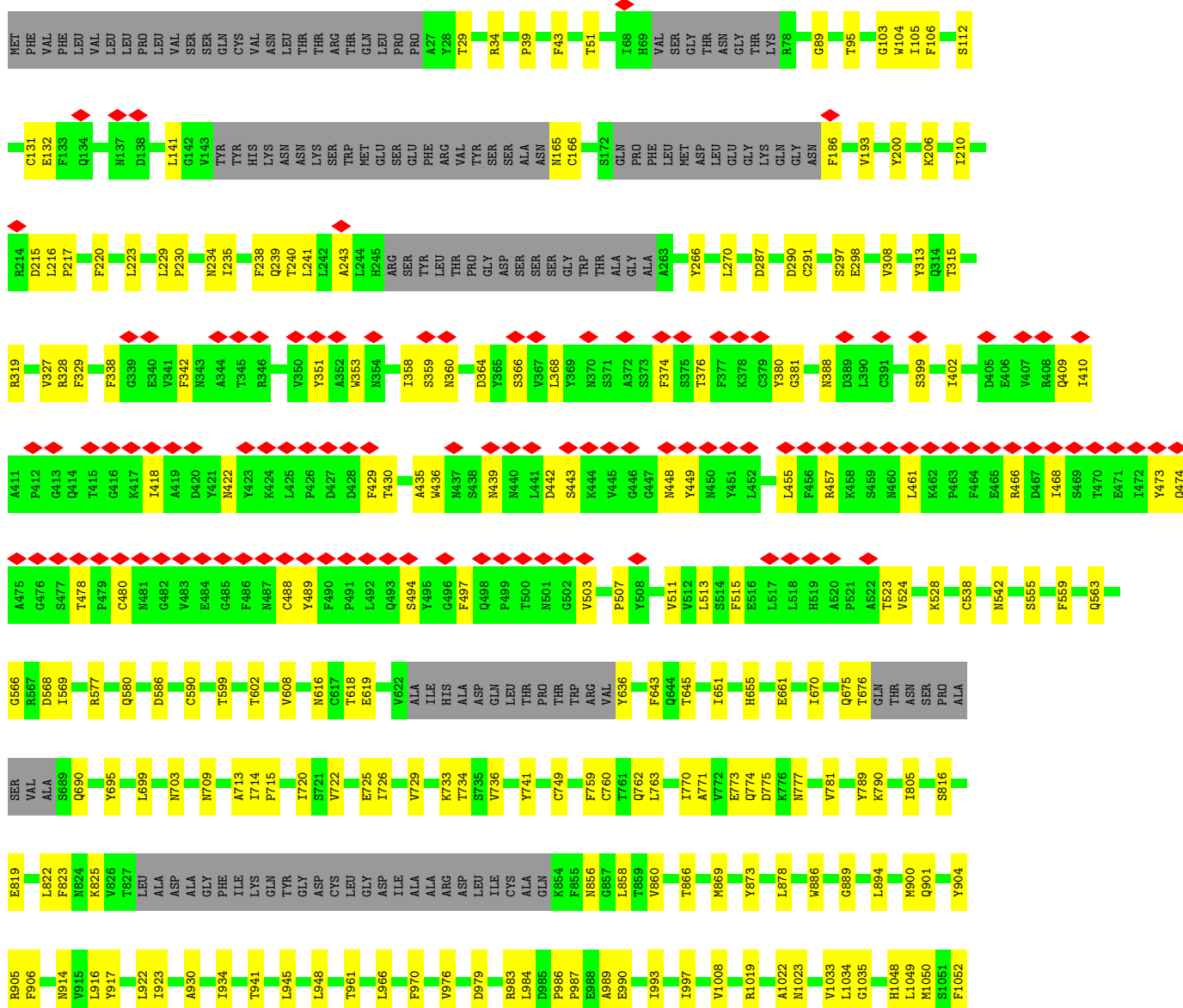
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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



- Molecule 1: Spike glycoprotein



SER	LEU	SER	SER	VAL	VAL	THR	VAL	PRO	SER	SER	SER	LEU	GLY	THR	THR	GLN	THR	THR	TYR	ILE	CYS	ASN	ASN	HIS	LYS	PRO	SER	SER	ASN	THR	THR	LYS	VAL	ASP	ASP	LYS	ARG	VAL	VAL	GLU	PRO	PRO	PRO	LYS	SER	SER	CYS	ASP	LYS	THR	HIS								
D61	S62	V63	K64	G65	R66	F67	I68	I69	S70	R71	H72	N73	S74	K75	N76	I77	L78	Y79	L80	Q81	M82	S82A	S82B	L82C	R83	A84	E85	D86	T87	A88	V89	Y90	F91	C92	A93	R94	D95	L96	Y97	V98	F99	G100	M100A	D101	V102	W103	G104	Q105	G106	T107	A108	V109	T110	V111	S112	A113	ALA	SER	THR
LYS	GLY	PRO	SER	VAL	PHE	PRO	LEU	ALA	PRO	SER	SER	LYS	THR	THR	SER	GLN	GLY	GLY	THR	CYS	LEU	VAL	LYS	ASP	TYR	PHE	GLU	GLU	VAL	THR	VAL	SER	TRP	ASN	SER	GLY	ALA	LEU	THR	SER	GLY	VAL	HIS	THR	PHE	PRO	ALA	VAL	LEU	GLN	SER	SER	GLY	LEU	TYR				

• Molecule 3: R40-1G8 Fab light chain



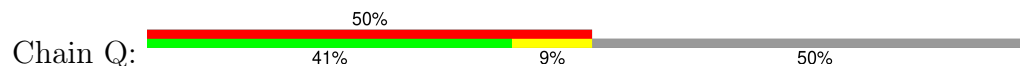
D1	I2	Q3	L4	T5	Q6	P7	S8	S9	F10	L11	S12	A13	S14	V15	G16	D17	R18	V19	T20	I21	T22	C23	R24	A25	S26	Q27	G28	I29	S30	S31	Y32	L33	A34	W35	Y36	Q37	Q38	K39	P40	G41	R42	A43	P44	K45	L46	L47	I48	Y49	A50	A51	S52	T53	L54	Q55	S56	G57	V58	P59	S60
R61	F62	S63	G64	S65	G66	S67	G68	T69	V70	F71	T72	L73	T74	I75	S76	S77	L78	Q79	P80	E81	D82	F83	A84	T85	Y86	Y87	C88	Q89	Q90	L91	N92	S93	D94	S95	S96	T97	F98	G99	Q100	G101	T102	K103	L104	E105	I106	K107	ARG	THR	VAL	ALA	ALA	PRO	SER	VAL	PHE	ILE	PHE	PRO	PRO
SER	ASP	GLU	GLN	LEU	LYS	SER	GLY	THR	ALA	SER	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA	VAL	GLN	SER	TRP	LYS	VAL	ASP	ASN	GLN	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	THR	TYR	SER	LEU	SER	SER	THR	LEU	THR							
LEU	SER	LYS	ALA	ASP	TYR	GLU	LYS	HIS	VAL	TYR	VAL	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS																										

• Molecule 3: R40-1G8 Fab light chain



LEU	SER	LYS	ALA	ASP	TYR	GLU	LYS	HIS	VAL	THR	VAL	ALA	CYS	GLY	VAL	THR	HIS	GLN	GLY	LEU	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	VAL	ASP	GLY	GLU	CYS																										
SER	ASP	GLN	LEU	LYS	SER	GLY	THR	ALA	SER	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA	VAL	GLN	TRP	LYS	VAL	ASP	ASN	GLY	GLU	CYS																											
D1	I2	Q3	L4	T5	Q6	S7	P8	S9	F10	L11	S12	A13	S14	V15	G16	D17	R18	V19	T20	I21	T22	C23	R24	A25	S26	Q27	G28	I29	S30	S31	Y32	L33	A34	W35	Y36	Q37	Q38	K39	P40	G41	R42	A43	P44	K45	L46	L47	I48	Y49	A50	A51	S52	T53	L54	Q55	S56	G57	V58	P59	S60
R61	F62	S63	G64	S65	G66	S67	G68	T69	V70	F71	T72	L73	T74	I75	S76	S77	L78	Q79	P80	E81	D82	F83	A84	T85	Y86	Y87	C88	Q89	Q90	L91	N92	S93	D94	S95	S96	T97	F98	G99	Q100	G101	T102	K103	L104	E105	I106	K107	ARG	THR	VAL	ALA	ALA	PRO	SER	VAL	PHE	ILE	PHE	PRO	PRO

• Molecule 3: R40-1G8 Fab light chain



D1	I2	Q3	L4	T5	Q6	S7	P8	S9	F10	L11	S12	A13	S14	V15	G16	D17	R18	V19	T20	I21	T22	C23	R24	A25	S26	Q27	G28	I29	S30	S31	Y32	L33	A34	W35	Y36	Q37	Q38	K39	P40	G41	R42	A43	P44	K45	L46	L47	I48	Y49	A50	A51	S52	T53	L54	Q55	S56	G57	V58	P59	S60
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[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	178597	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)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.090	Depositor
Minimum map value	-0.662	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	299.52002, 299.52002, 299.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8320001, 0.8320001, 0.8320001	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	0.36	0/8078	0.50	0/10997
1	B	0.36	1/8078 (0.0%)	0.50	0/10997
1	C	0.36	1/8078 (0.0%)	0.50	0/10997
2	H	0.24	0/908	0.50	0/1229
2	M	0.25	0/908	0.50	0/1229
2	P	0.25	0/908	0.53	0/1229
3	L	0.25	0/825	0.50	0/1119
3	N	0.25	0/825	0.50	0/1119
3	Q	0.25	0/825	0.50	0/1119
All	All	0.34	2/29433 (0.0%)	0.50	0/40035

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	760	CYS	CB-SG	-5.09	1.73	1.81
1	C	760	CYS	CB-SG	-5.08	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7896	0	7700	176	0
1	B	7896	0	7700	166	0
1	C	7896	0	7700	166	0
2	H	890	0	877	22	0
2	M	890	0	877	25	0
2	P	890	0	877	29	0
3	L	809	0	797	12	0
3	N	809	0	797	15	0
3	Q	809	0	797	17	0
4	A	210	0	195	5	0
4	B	210	0	195	5	0
4	C	210	0	195	6	0
All	All	29415	0	28707	570	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 10.

The worst 5 of 570 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:43:PHE:HB3	1:B:566:GLY:HA2	1.61	0.82
1:B:376:THR:HB	1:B:435:ALA:HB3	1.67	0.76
1:A:376:THR:HB	1:A:435:ALA:HB3	1.67	0.75
1:C:376:THR:HB	1:C:435:ALA:HB3	1.67	0.75
2:M:96:LEU:HD22	2:M:99:PHE:HB2	1.70	0.74

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	995/1256 (79%)	954 (96%)	41 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	995/1256 (79%)	953 (96%)	42 (4%)	0	100	100
1	C	995/1256 (79%)	955 (96%)	40 (4%)	0	100	100
2	H	115/224 (51%)	114 (99%)	1 (1%)	0	100	100
2	M	115/224 (51%)	112 (97%)	3 (3%)	0	100	100
2	P	115/224 (51%)	112 (97%)	3 (3%)	0	100	100
3	L	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
3	N	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
3	Q	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
All	All	3645/5082 (72%)	3500 (96%)	145 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	887/1096 (81%)	886 (100%)	1 (0%)	92	98
1	B	887/1096 (81%)	887 (100%)	0	100	100
1	C	887/1096 (81%)	886 (100%)	1 (0%)	92	98
2	H	93/186 (50%)	93 (100%)	0	100	100
2	M	93/186 (50%)	93 (100%)	0	100	100
2	P	93/186 (50%)	93 (100%)	0	100	100
3	L	91/187 (49%)	91 (100%)	0	100	100
3	N	91/187 (49%)	91 (100%)	0	100	100
3	Q	91/187 (49%)	91 (100%)	0	100	100
All	All	3213/4407 (73%)	3211 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	675	GLN
1	C	675	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	804	GLN
1	C	856	ASN
3	Q	37	GLN
1	C	935	GLN
1	B	935	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](#)

There are no oligosaccharides in this entry.

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	A	1315	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	A	1302	1	14,14,15	0.36	0	17,19,21	0.50	0
4	NAG	B	1308	1	14,14,15	0.19	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1312	1	14,14,15	0.35	0	17,19,21	0.52	0
4	NAG	B	1302	1	14,14,15	0.34	0	17,19,21	0.49	0
4	NAG	B	1303	1	14,14,15	0.35	0	17,19,21	1.25	1 (5%)
4	NAG	A	1307	1	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	B	1310	1	14,14,15	0.47	0	17,19,21	0.38	0
4	NAG	A	1309	1	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	A	1301	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	A	1312	1	14,14,15	0.33	0	17,19,21	0.56	0
4	NAG	B	1309	1	14,14,15	0.32	0	17,19,21	0.46	0
4	NAG	B	1312	1	14,14,15	0.32	0	17,19,21	0.55	0
4	NAG	B	1315	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	A	1305	1	14,14,15	0.79	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	C	1314	1	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	A	1306	1	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	B	1306	1	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	A	1314	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	1305	1	14,14,15	0.78	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	B	1314	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	C	1313	1	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	C	1306	1	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	1.24	1 (5%)
4	NAG	C	1315	1	14,14,15	0.17	0	17,19,21	0.43	0
4	NAG	A	1310	1	14,14,15	0.46	0	17,19,21	0.39	0
4	NAG	C	1304	1	14,14,15	0.28	0	17,19,21	0.37	0
4	NAG	C	1305	1	14,14,15	0.78	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	C	1307	1	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	B	1313	1	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	A	1311	1	14,14,15	0.25	0	17,19,21	0.54	0
4	NAG	C	1311	1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	C	1302	1	14,14,15	0.35	0	17,19,21	0.49	0
4	NAG	A	1304	1	14,14,15	0.29	0	17,19,21	0.37	0
4	NAG	C	1301	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	B	1307	1	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	C	1309	1	14,14,15	0.36	0	17,19,21	1.35	1 (5%)
4	NAG	B	1311	1	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	C	1303	1	14,14,15	0.35	0	17,19,21	1.25	1 (5%)
4	NAG	B	1304	1	14,14,15	0.29	0	17,19,21	0.36	0
4	NAG	C	1310	1	14,14,15	0.48	0	17,19,21	0.38	0
4	NAG	A	1313	1	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	B	1301	1	14,14,15	0.20	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1308	1	14,14,15	0.19	0	17,19,21	0.42	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	A	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1305	NAG	O5-C1	2.62	1.48	1.43
4	B	1305	NAG	O5-C1	2.61	1.48	1.43
4	C	1305	NAG	O5-C1	2.56	1.48	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1309	NAG	C1-O5-C5	4.96	118.84	112.19
4	B	1303	NAG	C1-O5-C5	4.71	118.50	112.19
4	C	1303	NAG	C1-O5-C5	4.71	118.49	112.19
4	A	1303	NAG	C1-O5-C5	4.67	118.44	112.19
4	B	1305	NAG	C1-O5-C5	4.08	117.66	112.19

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1309	NAG	C4-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1308	NAG	O5-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6

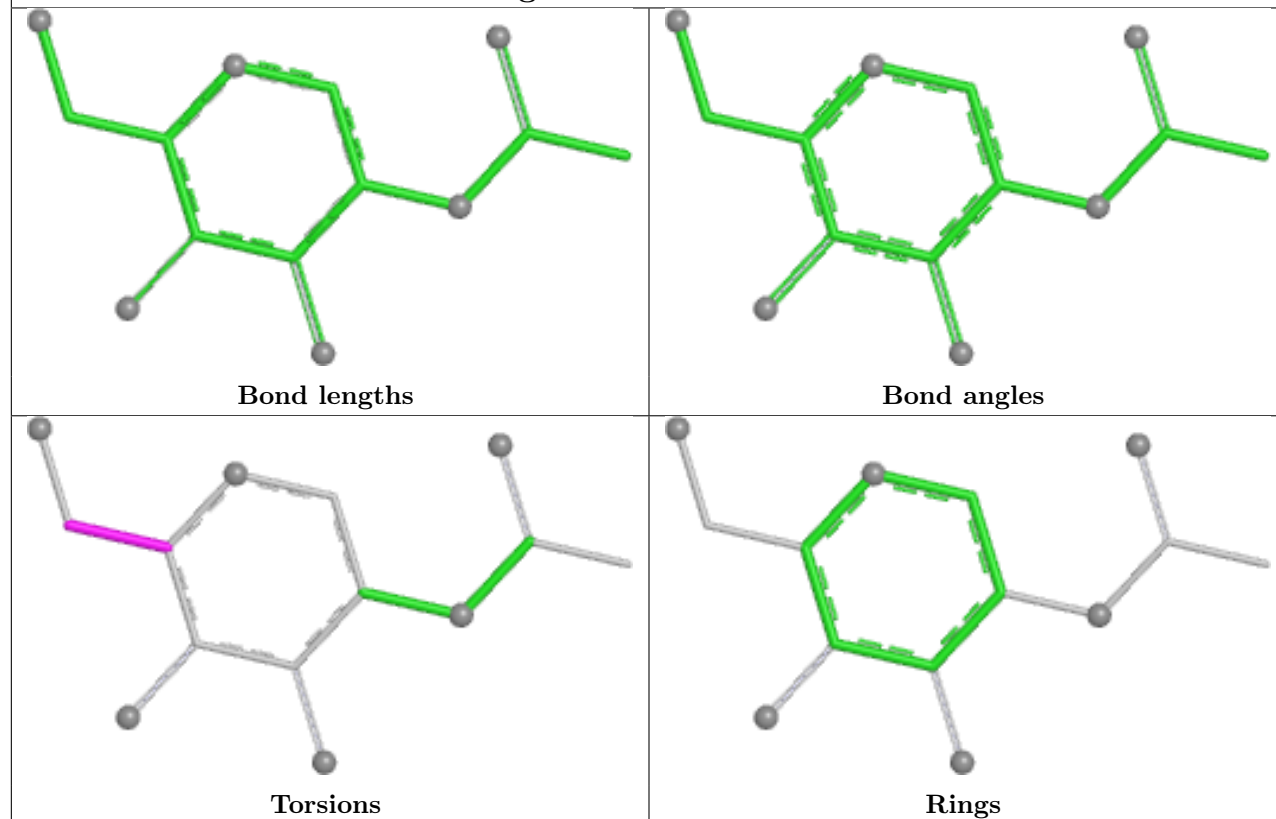
There are no ring outliers.

15 monomers are involved in 16 short contacts:

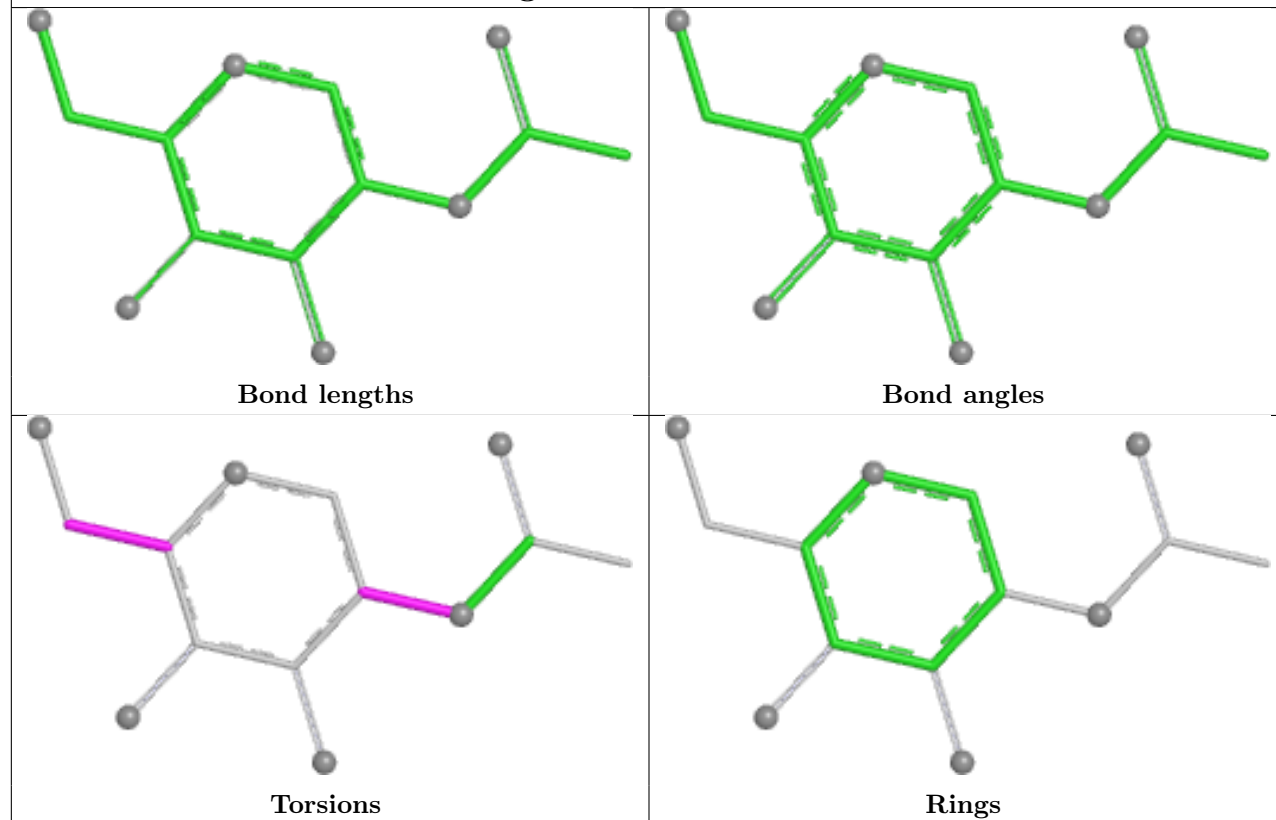
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1312	NAG	1	0
4	B	1303	NAG	1	0
4	A	1312	NAG	1	0
4	B	1312	NAG	1	0
4	A	1305	NAG	1	0
4	B	1314	NAG	1	0
4	A	1303	NAG	1	0
4	C	1304	NAG	1	0
4	A	1311	NAG	1	0
4	C	1311	NAG	1	0
4	A	1304	NAG	1	0
4	C	1309	NAG	1	0
4	B	1311	NAG	1	0
4	C	1303	NAG	2	0
4	B	1304	NAG	1	0

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

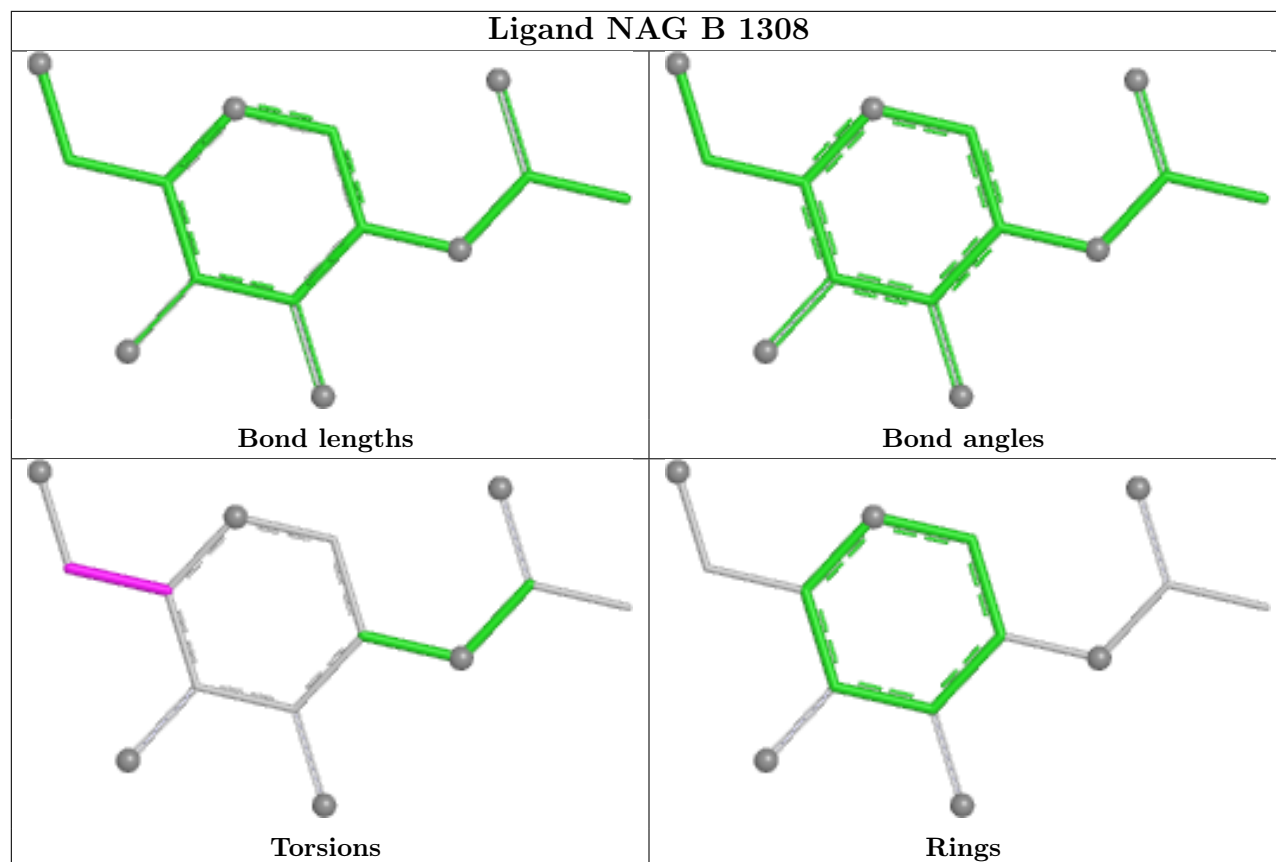
Ligand NAG A 1315



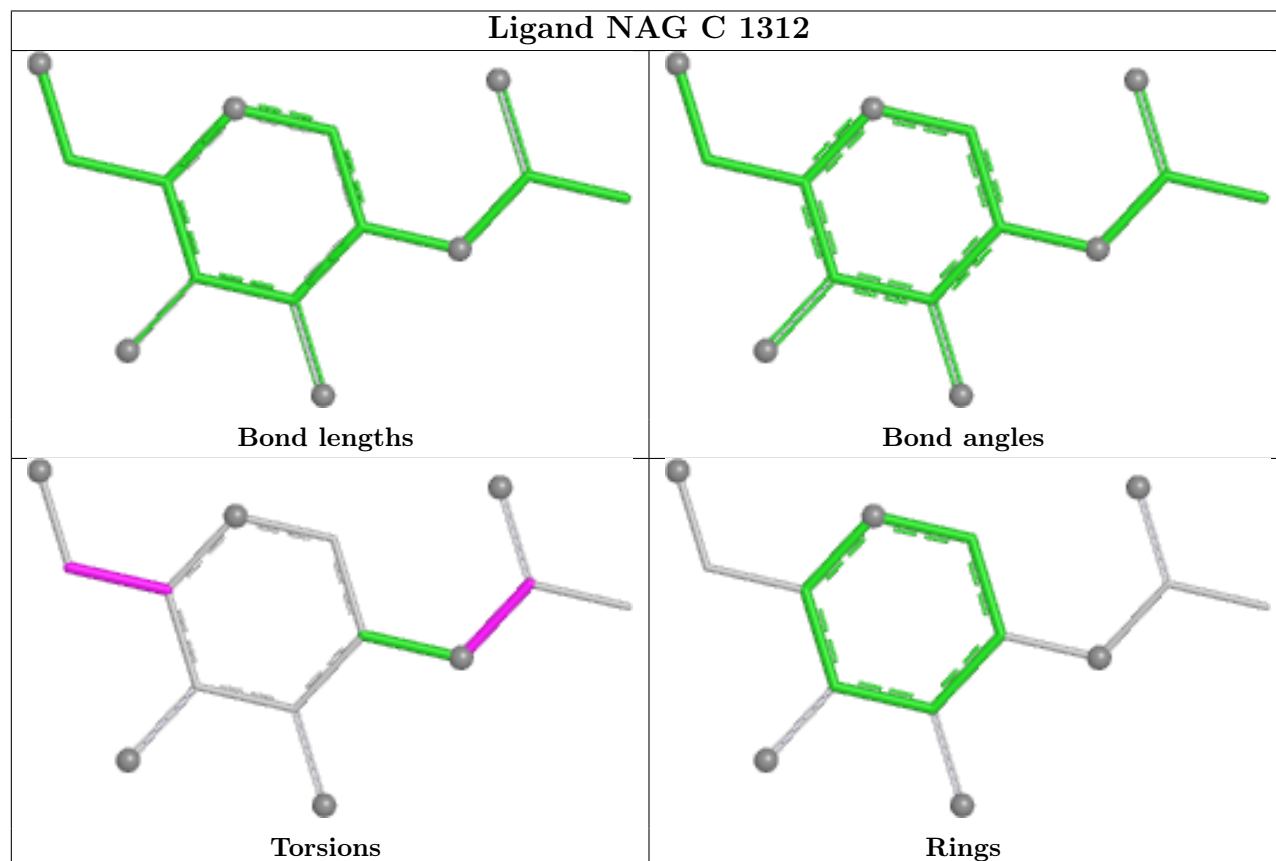
Ligand NAG A 1302

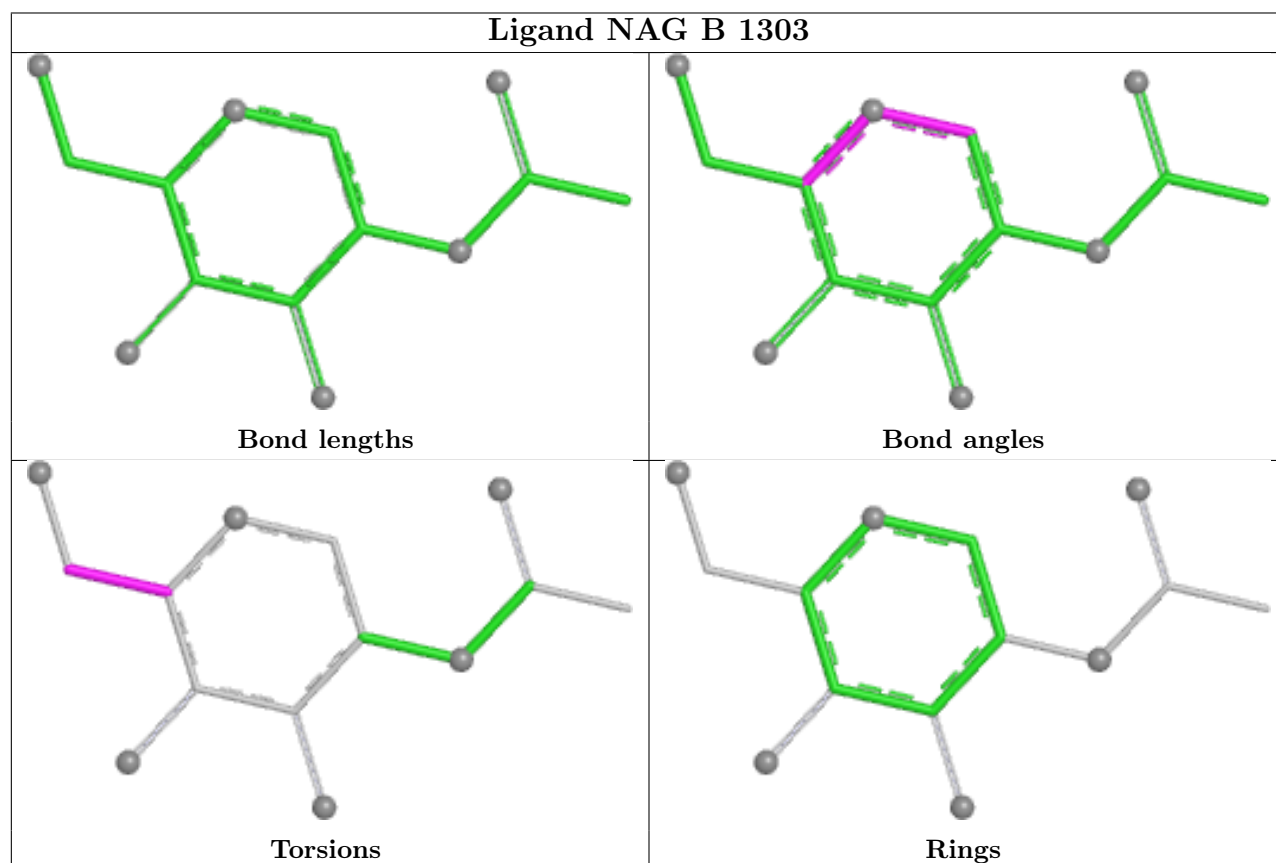
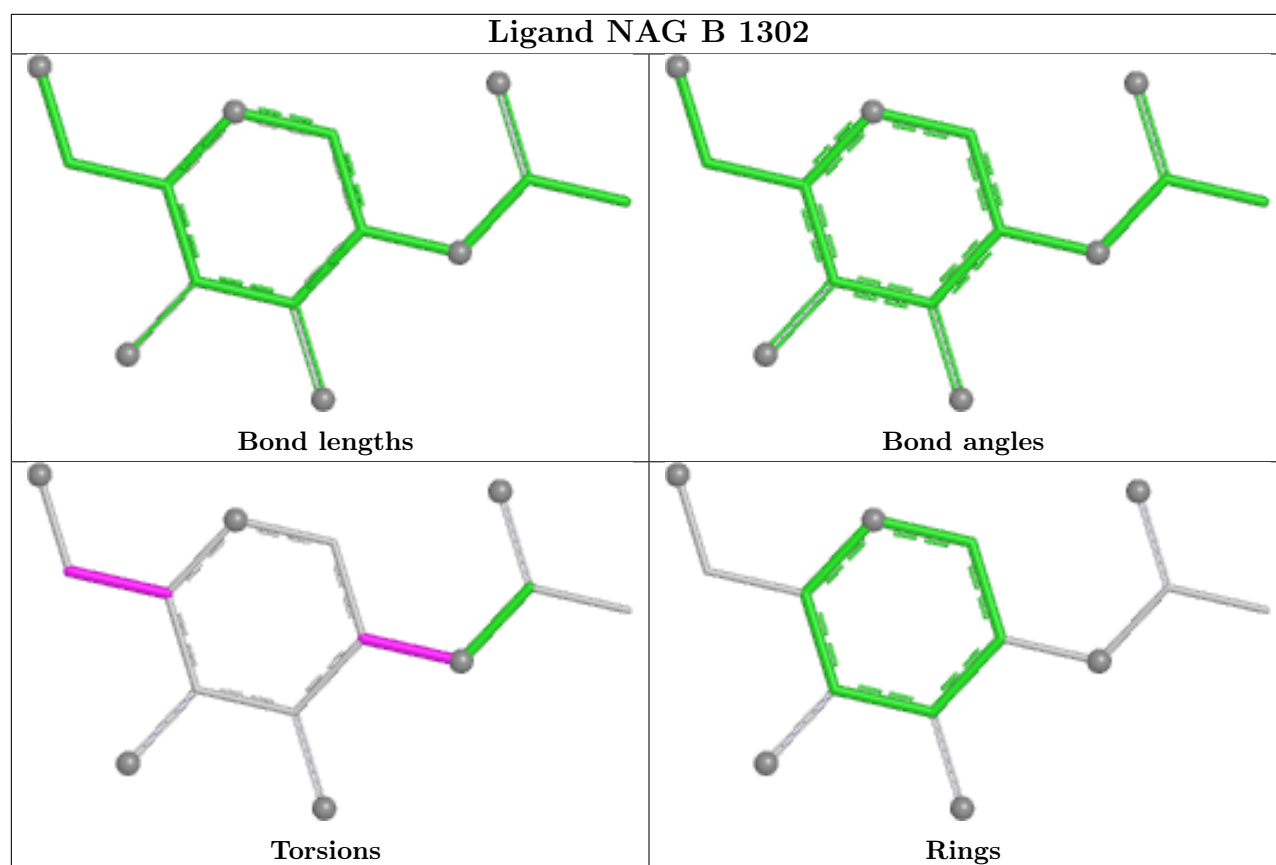


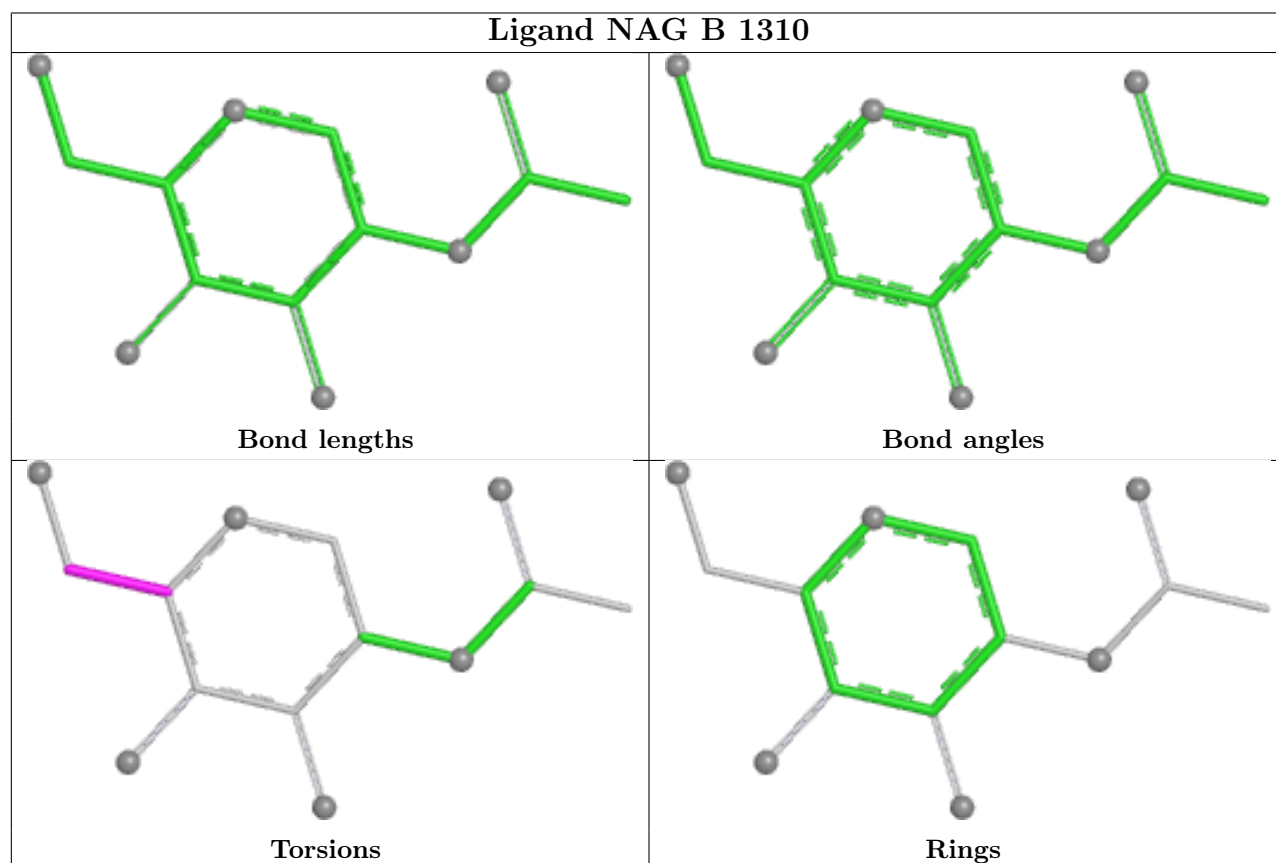
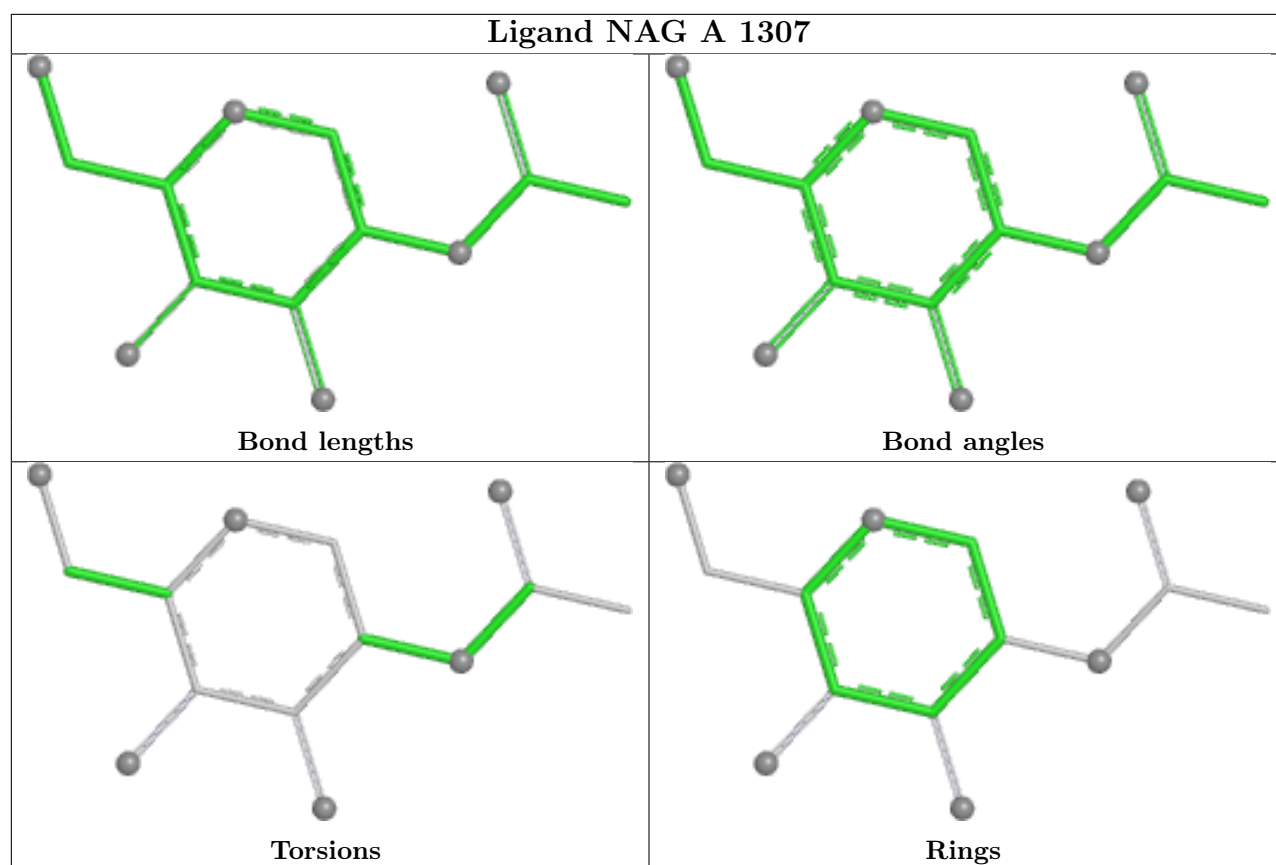
Ligand NAG B 1308

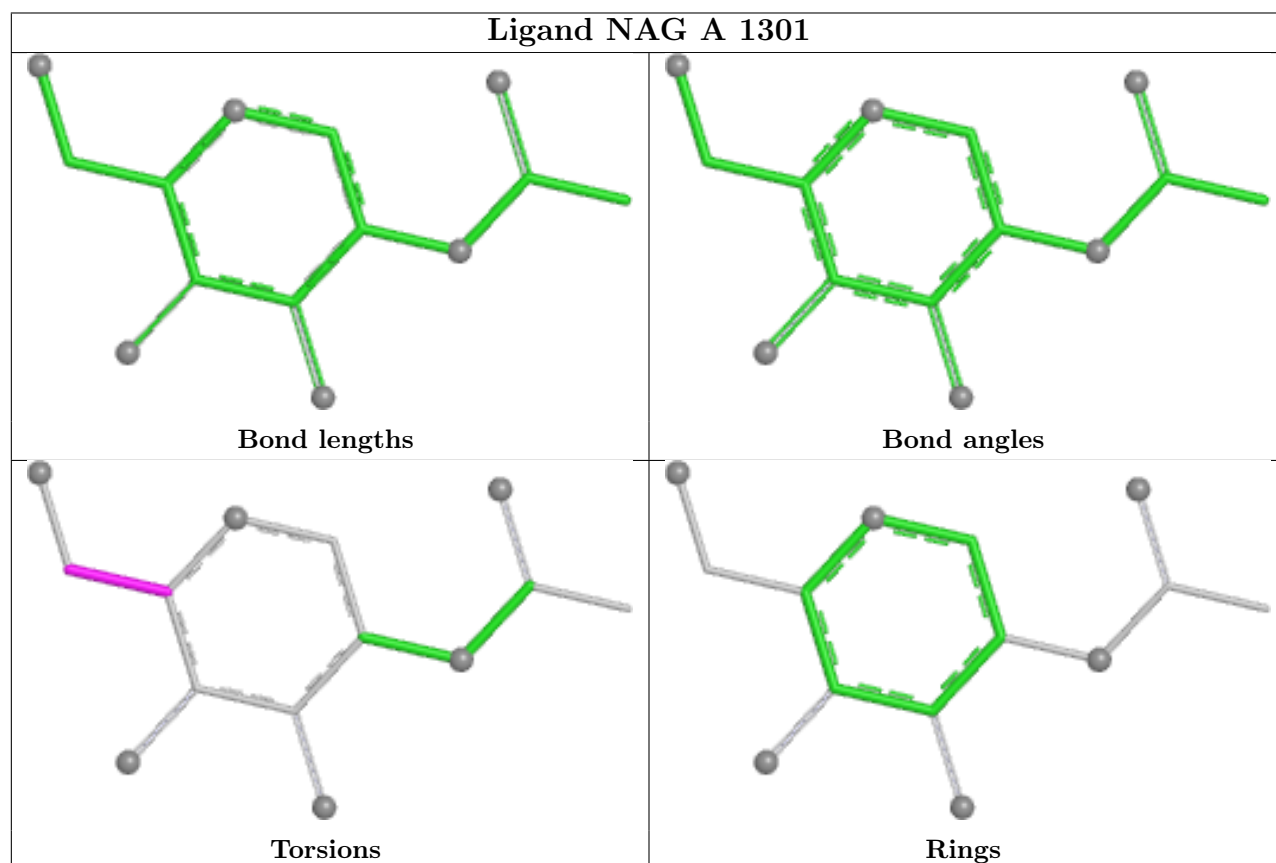
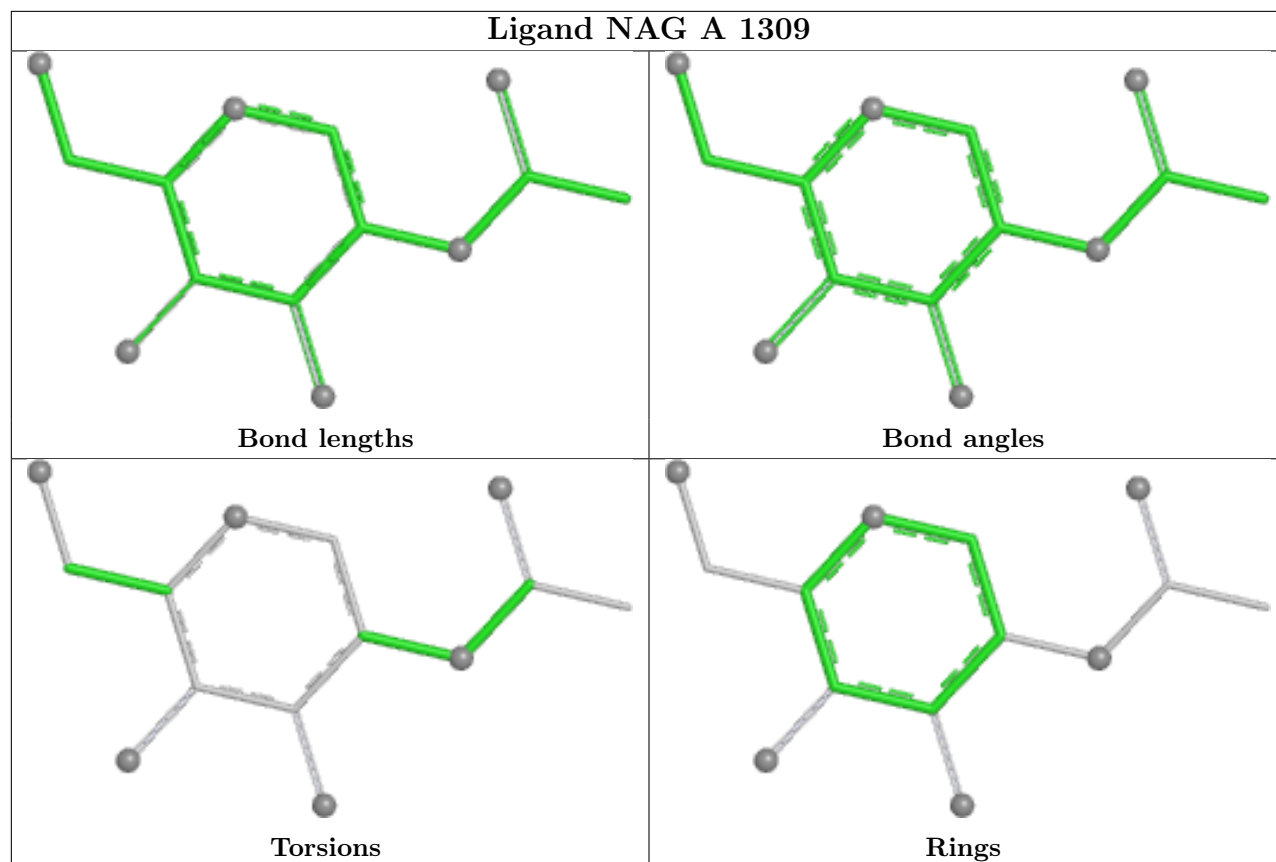


Ligand NAG C 1312

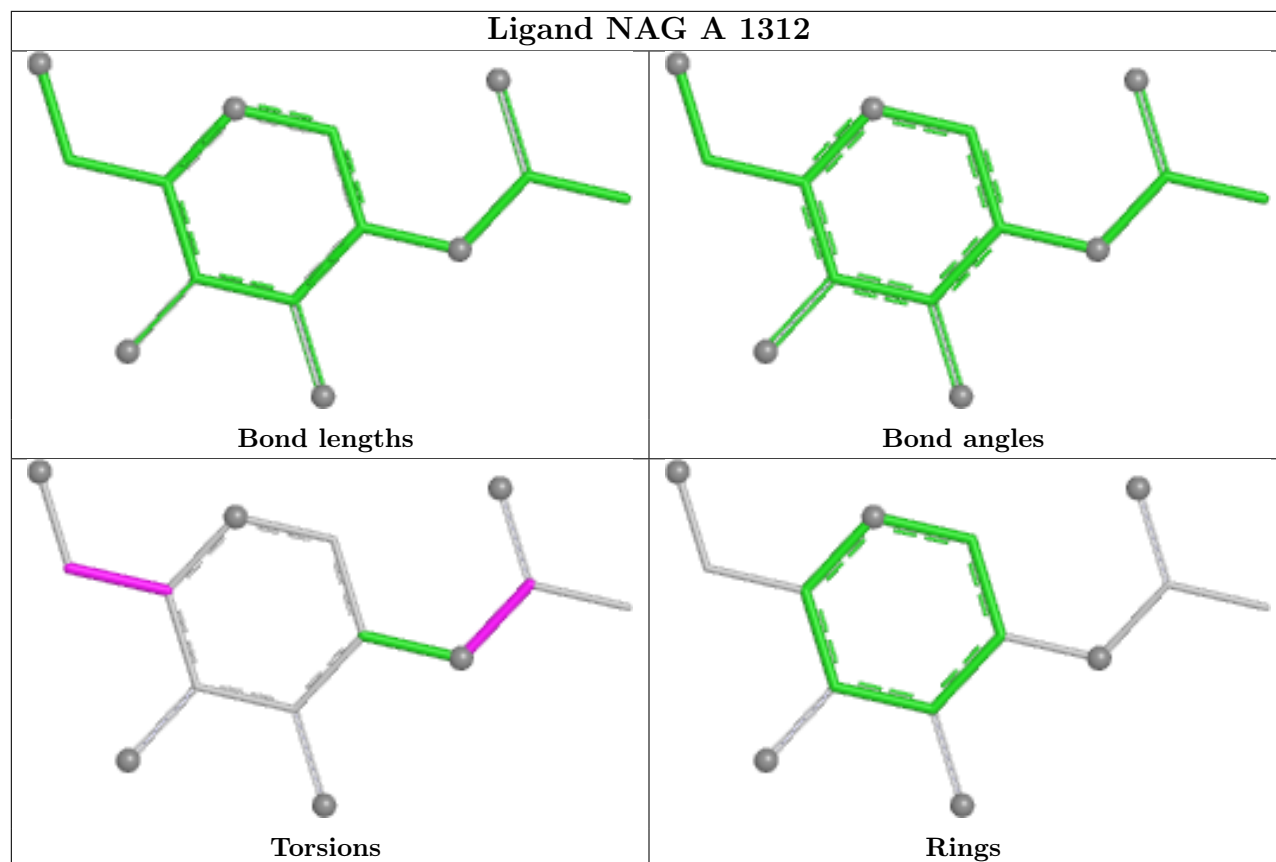




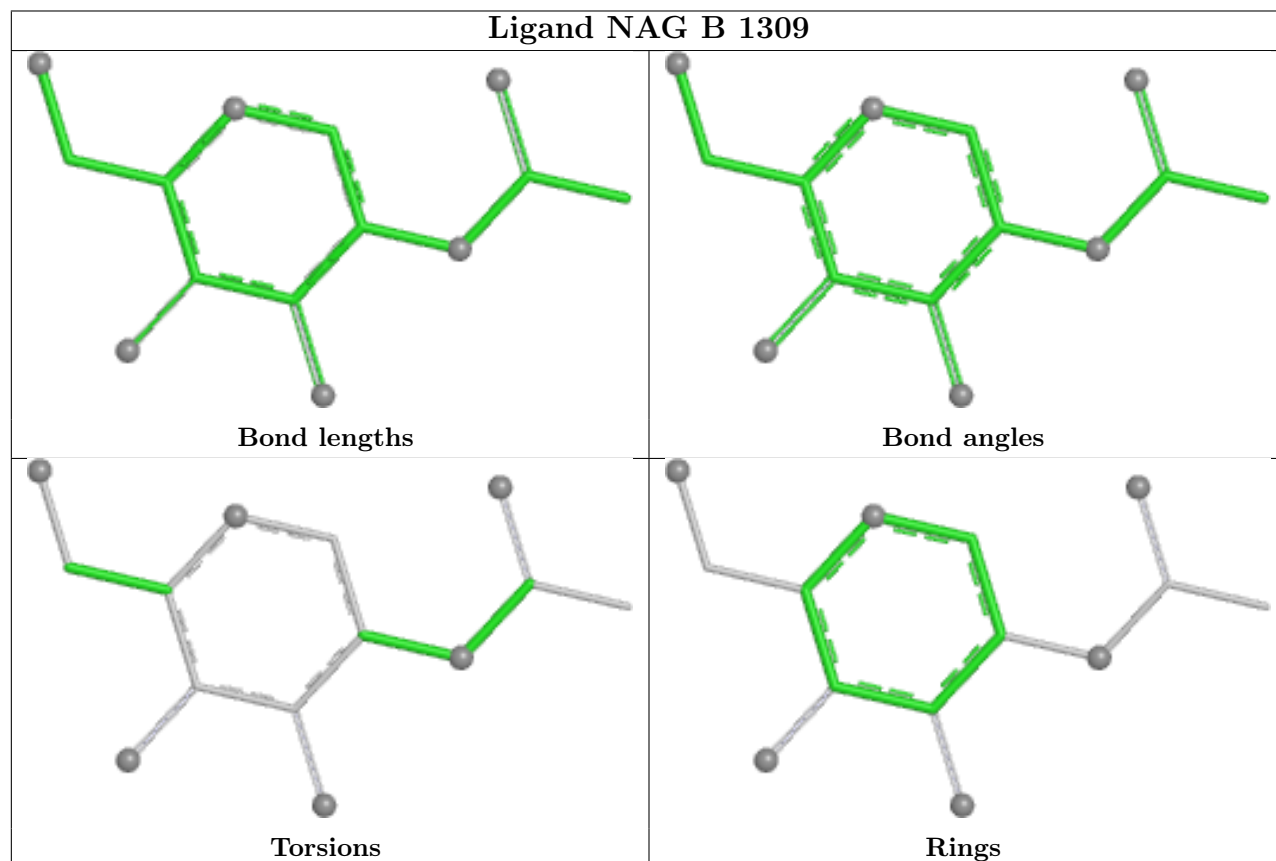


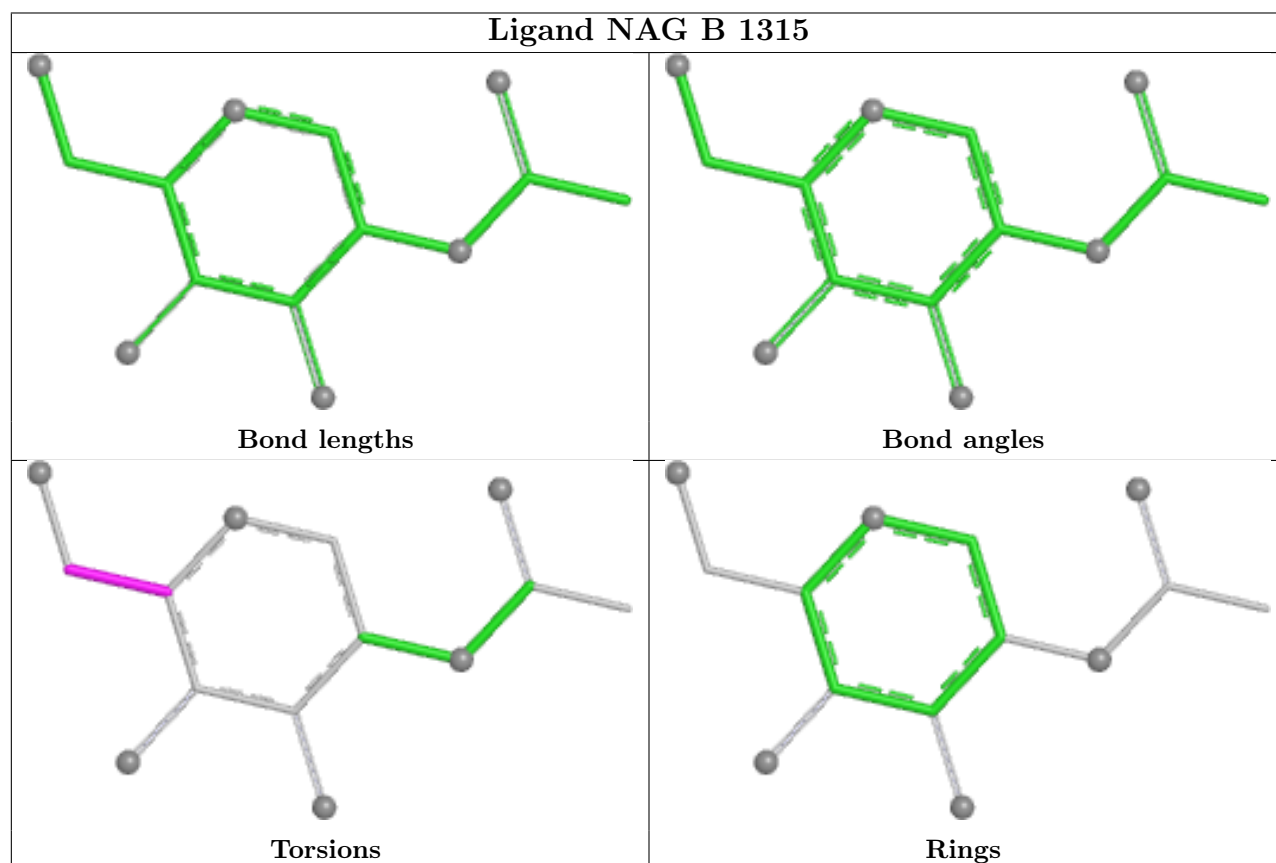
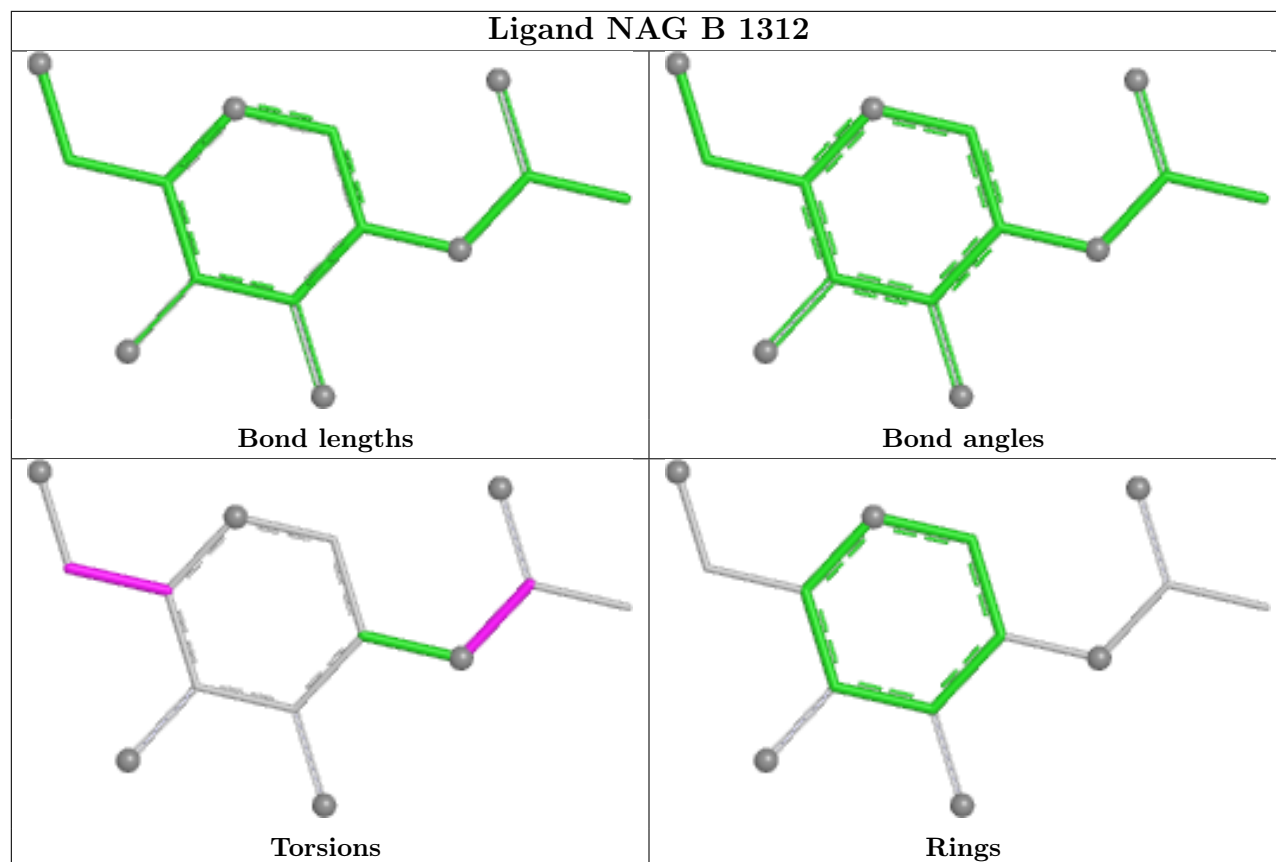


Ligand NAG A 1312

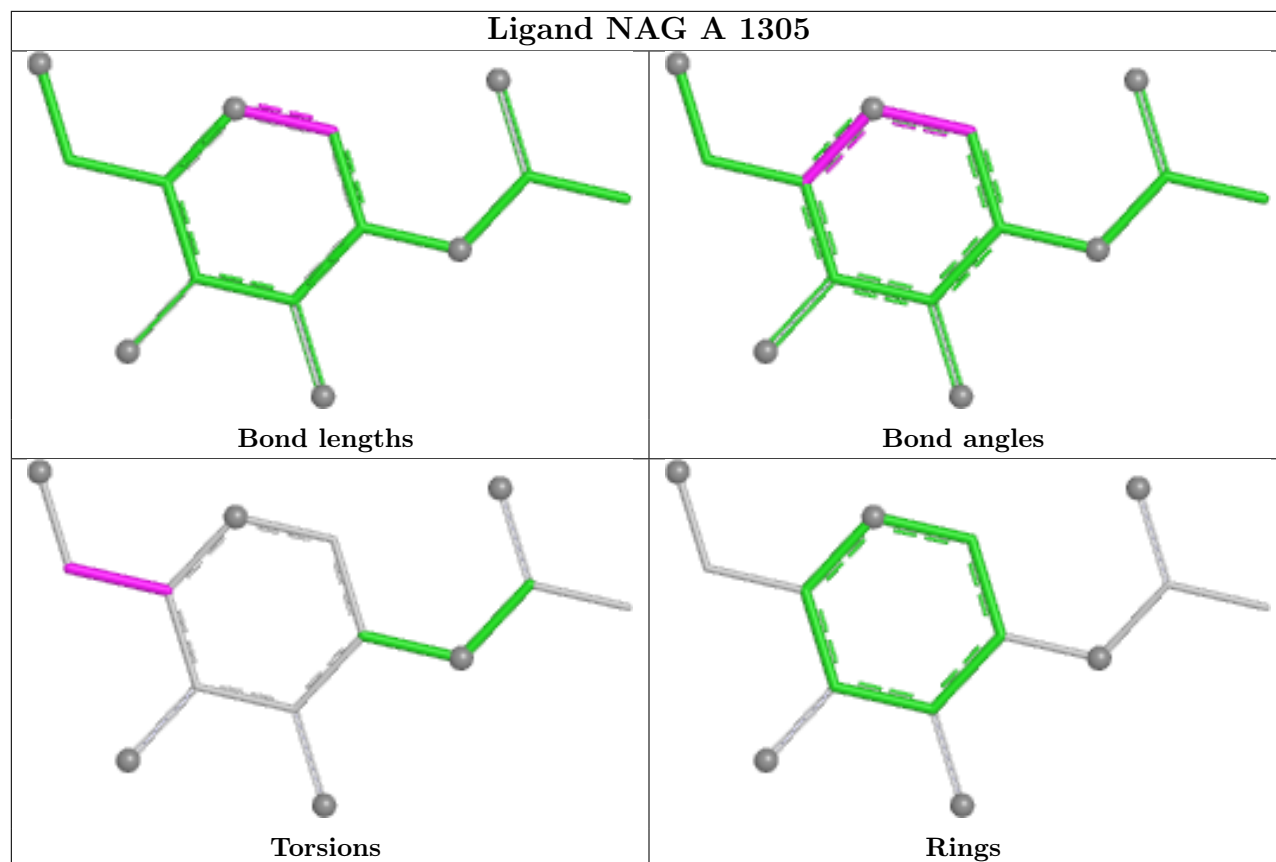


Ligand NAG B 1309

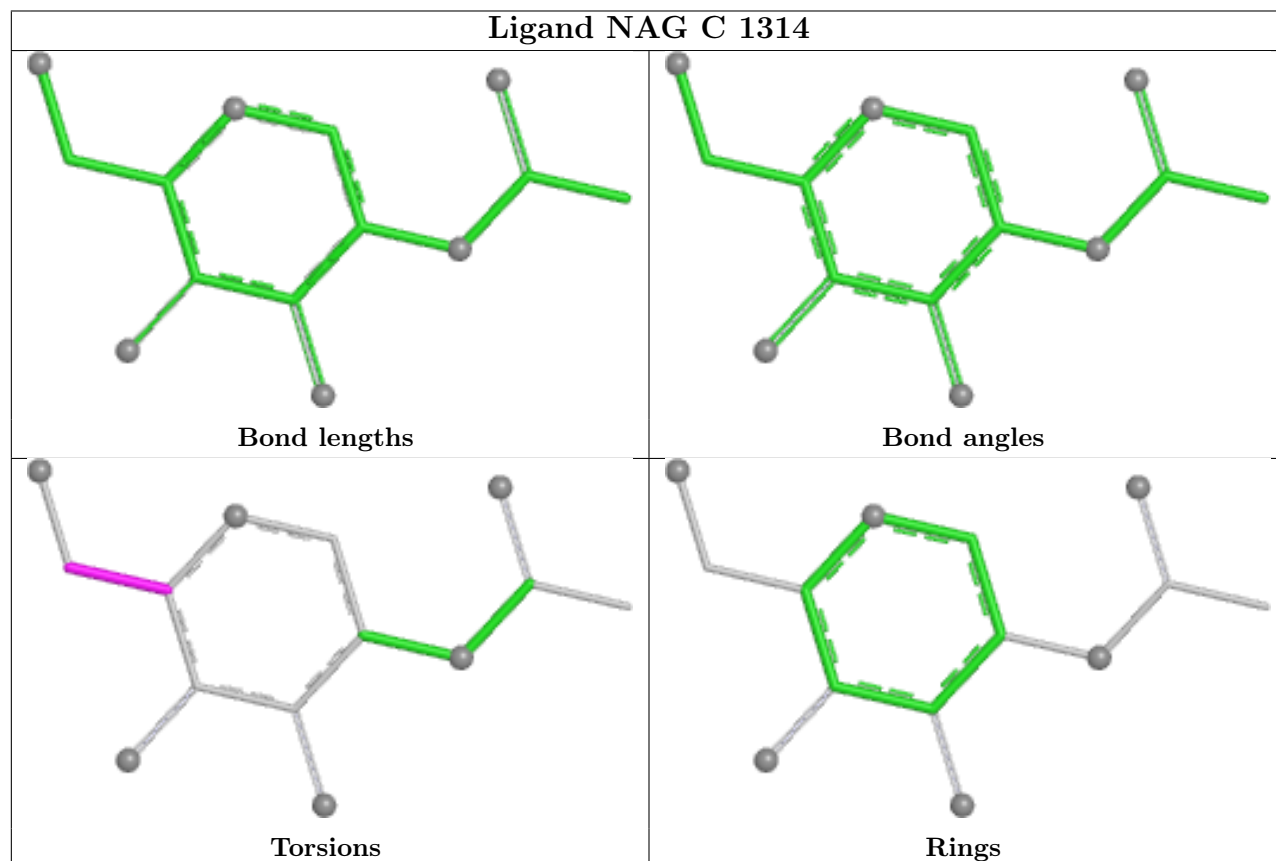




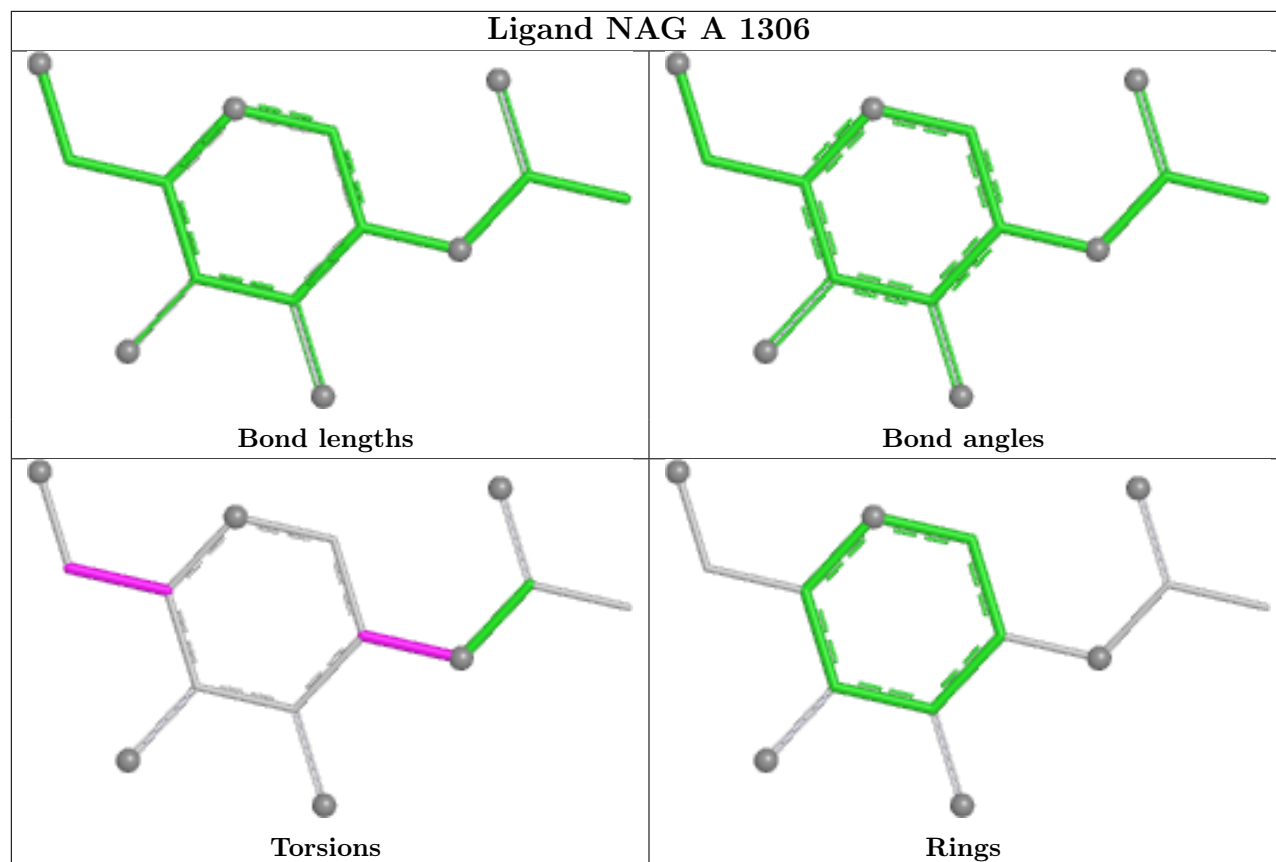
Ligand NAG A 1305



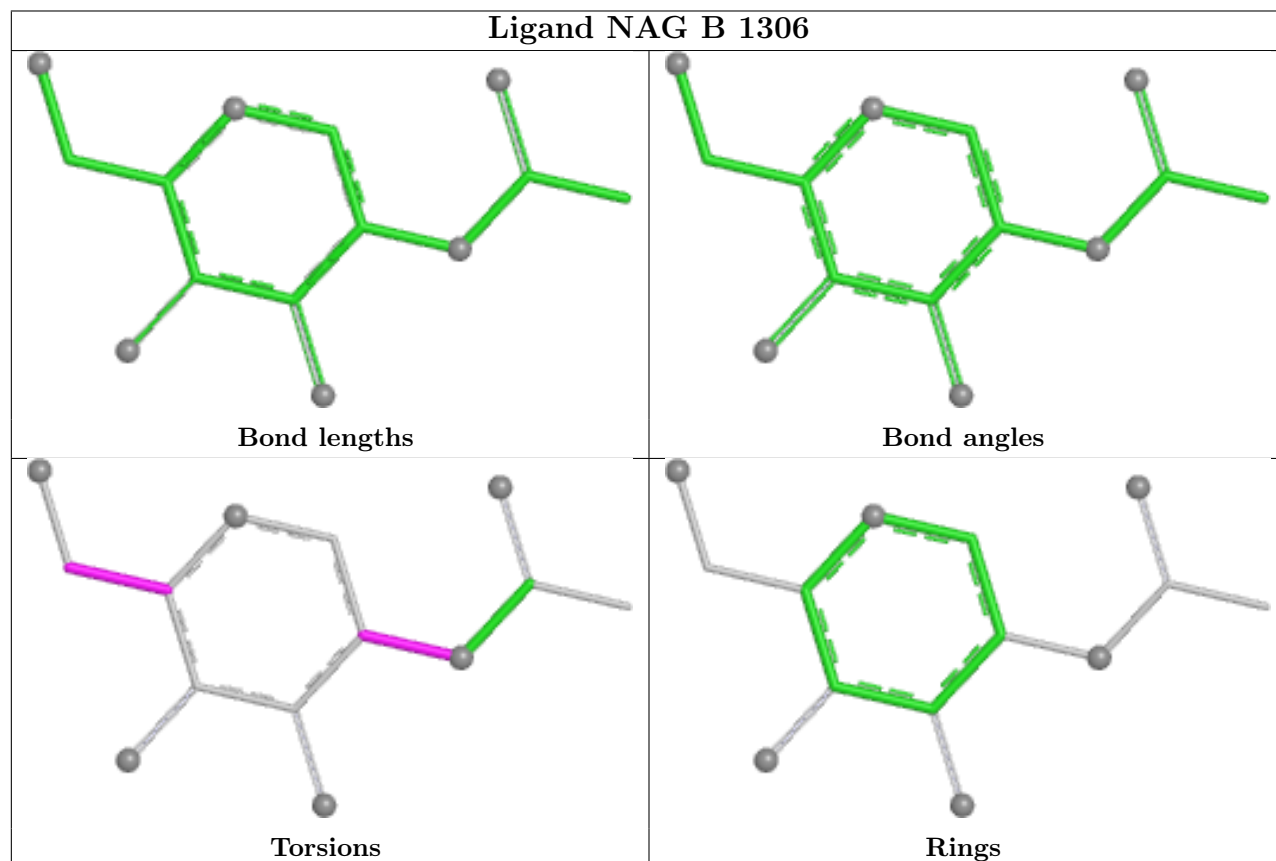
Ligand NAG C 1314



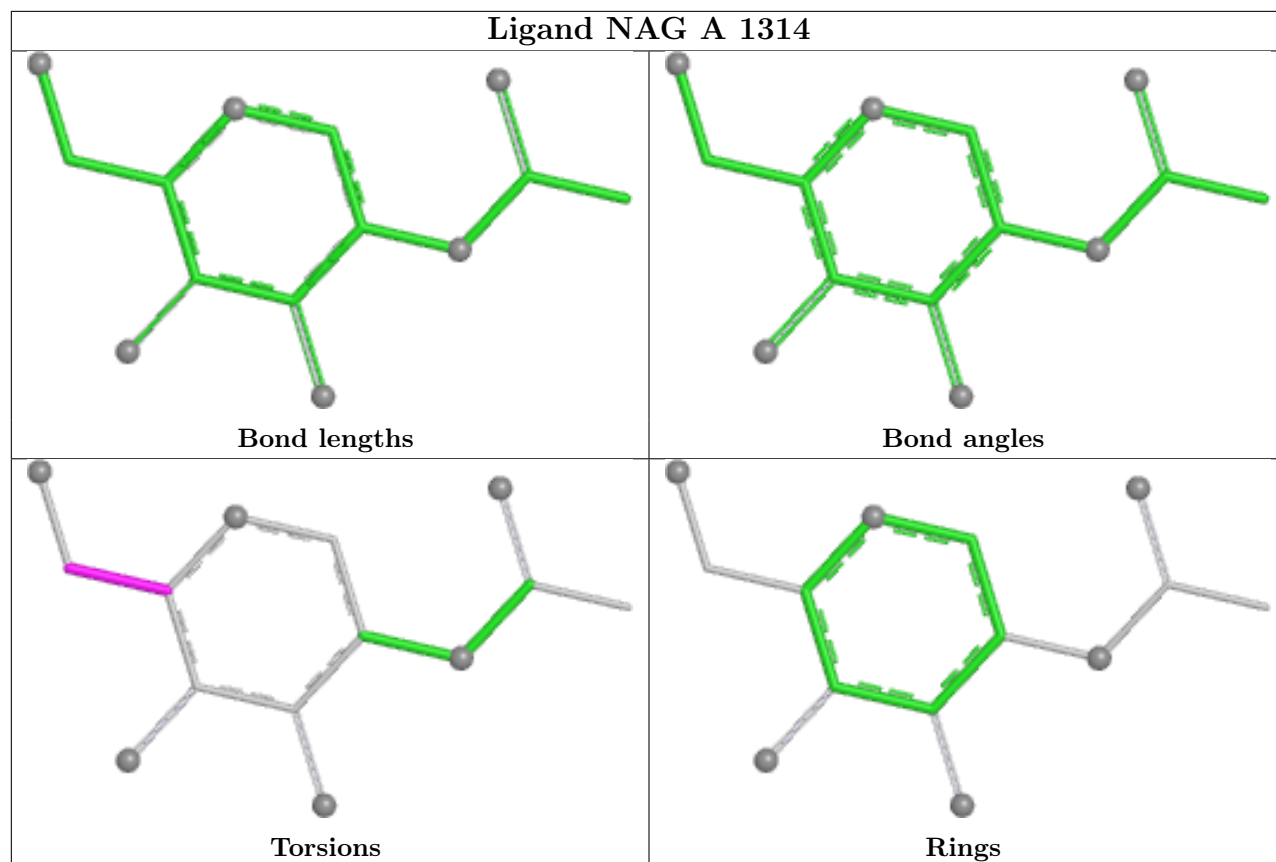
Ligand NAG A 1306



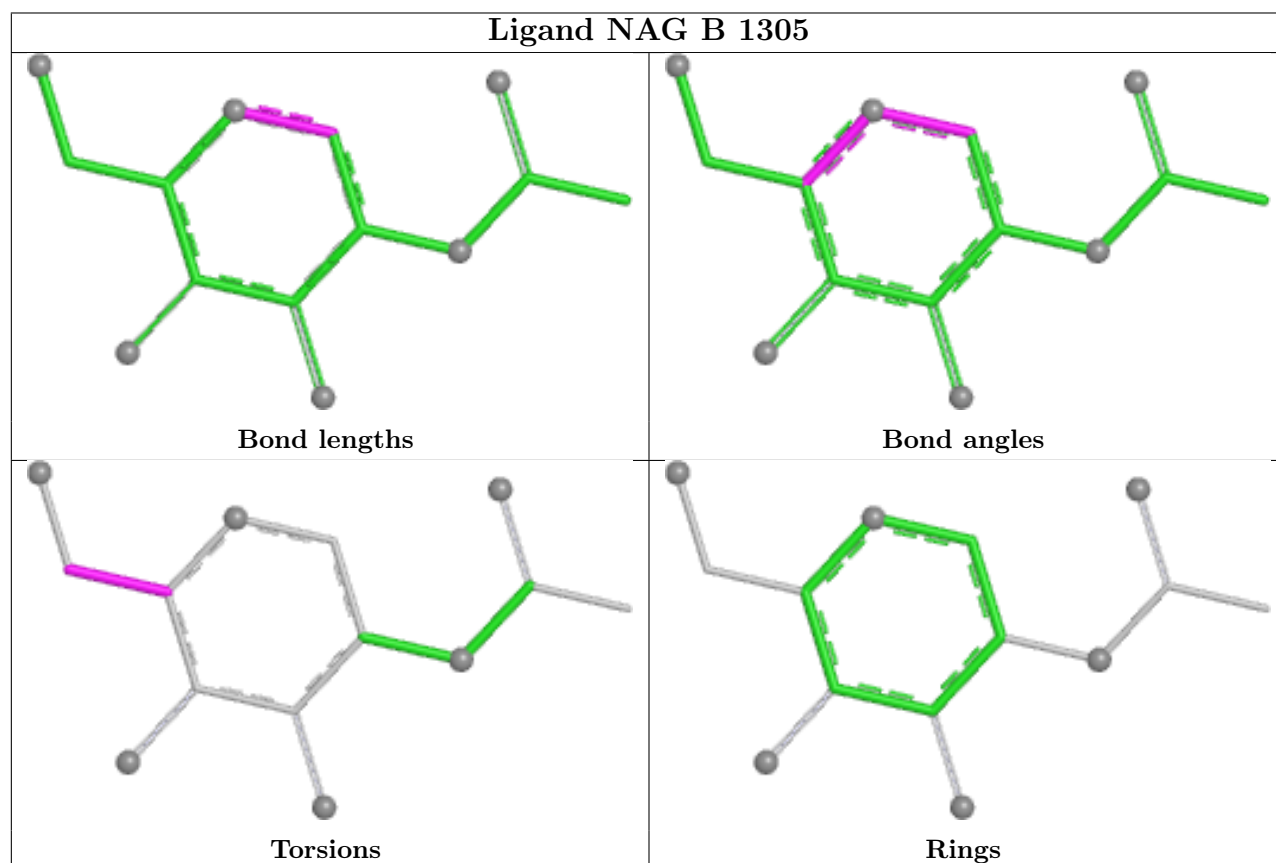
Ligand NAG B 1306



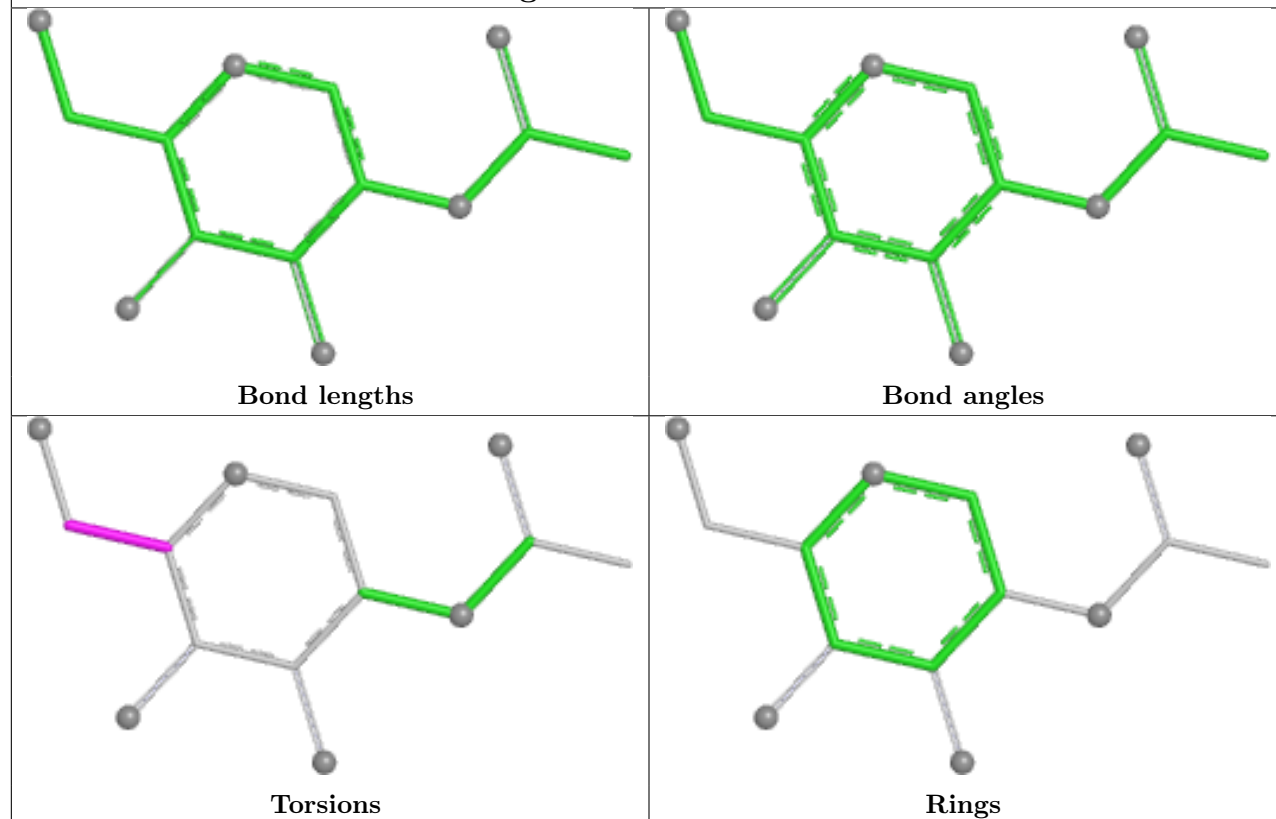
Ligand NAG A 1314



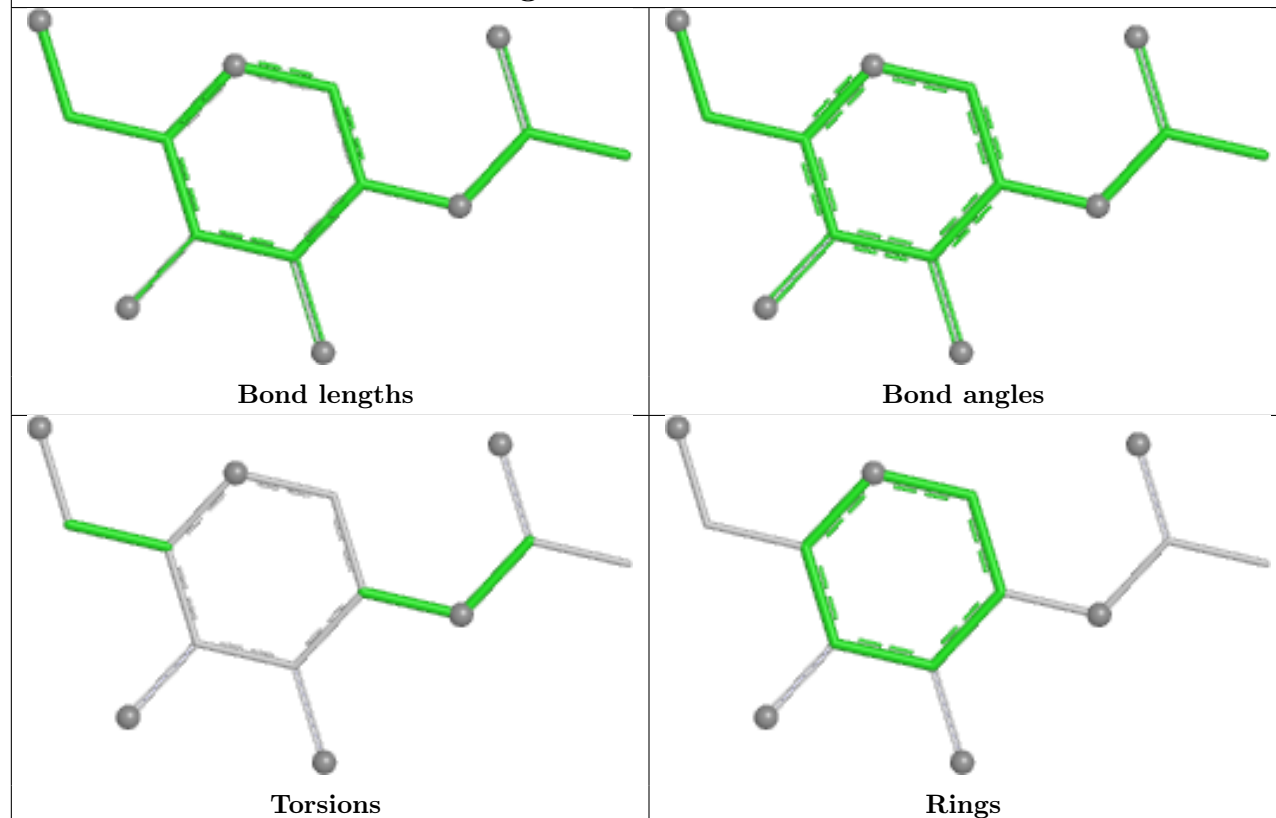
Ligand NAG B 1305



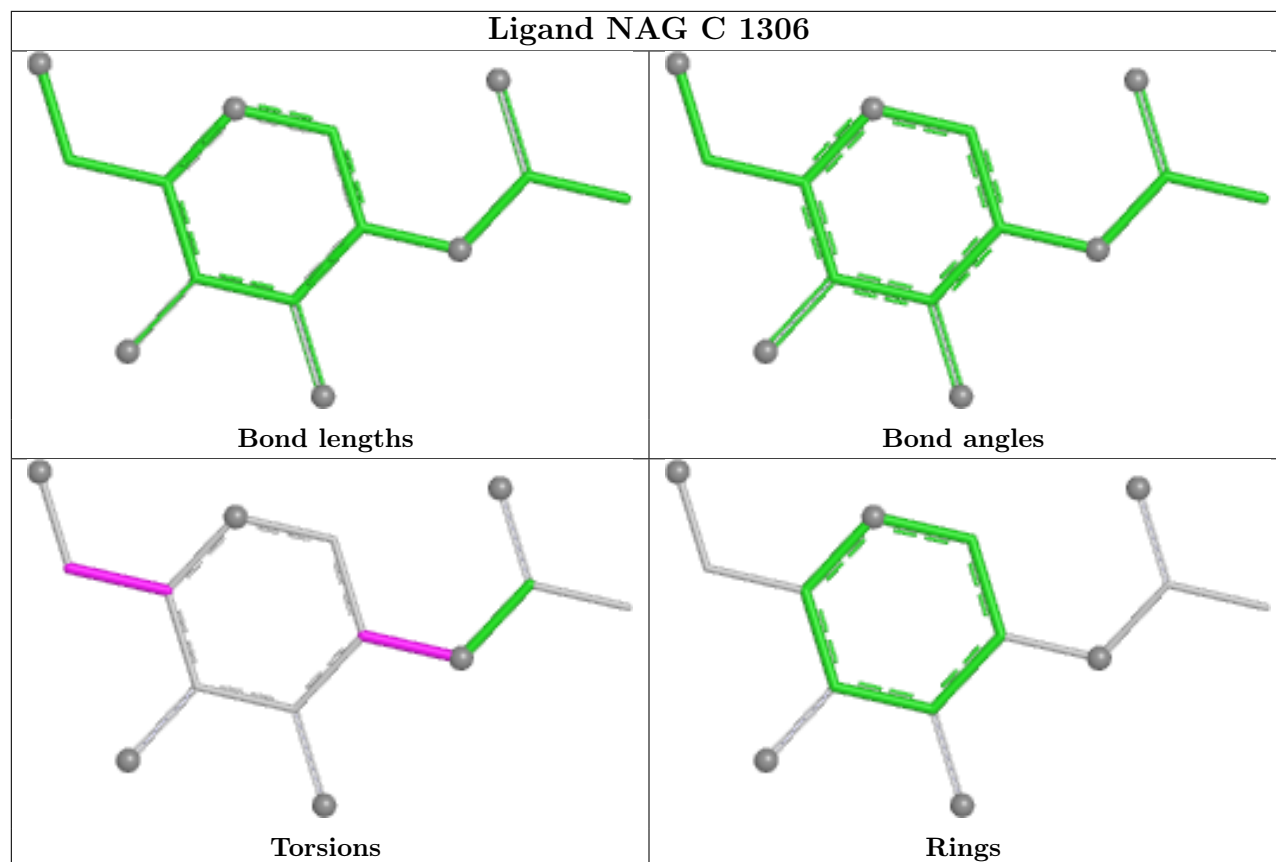
Ligand NAG B 1314



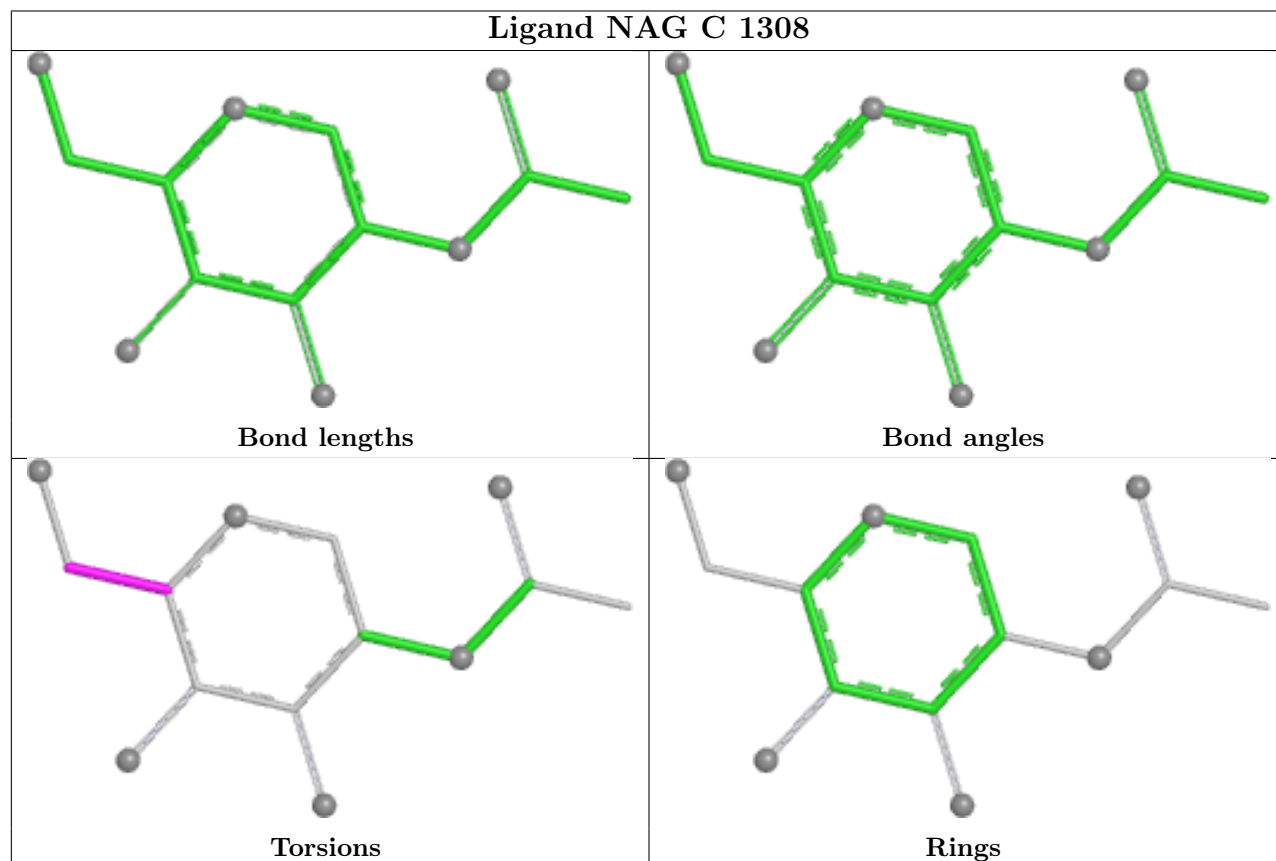
Ligand NAG C 1313

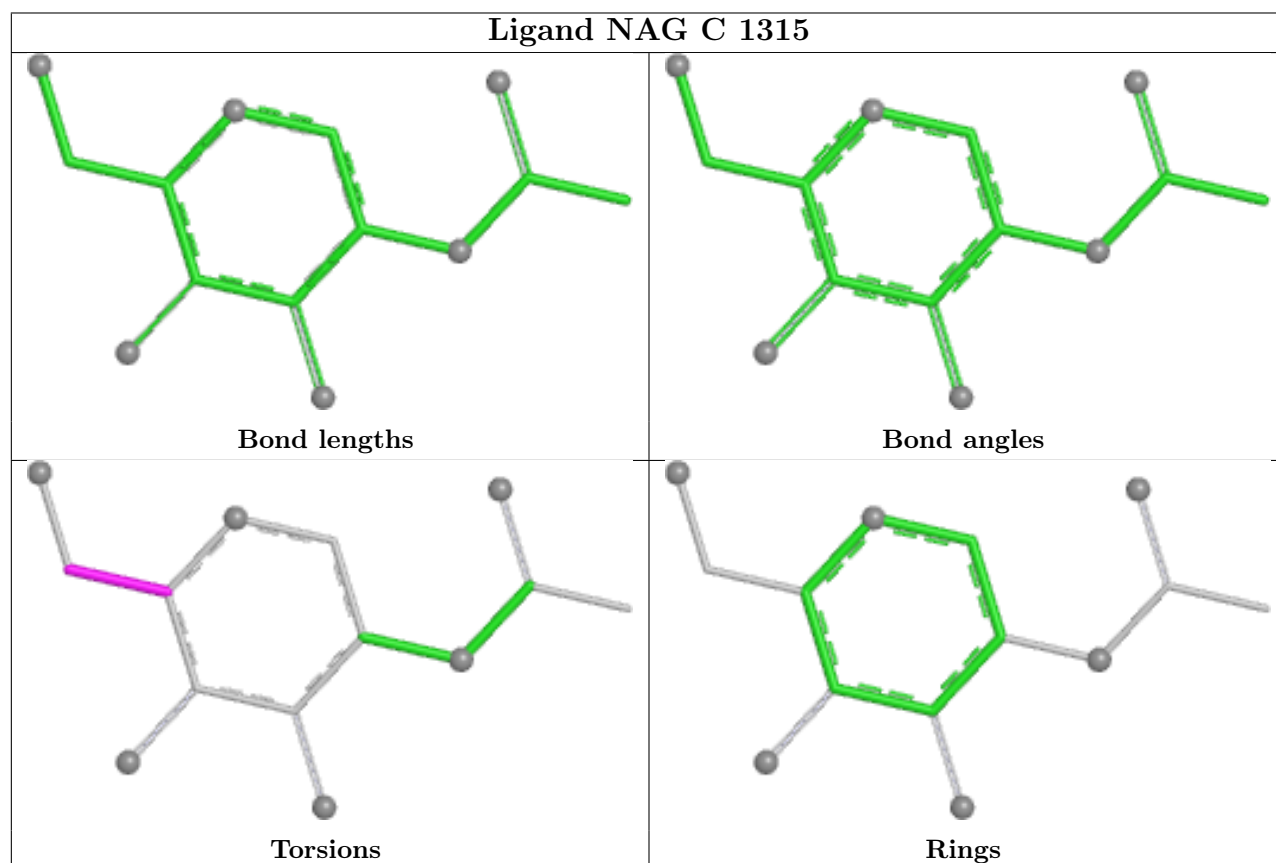
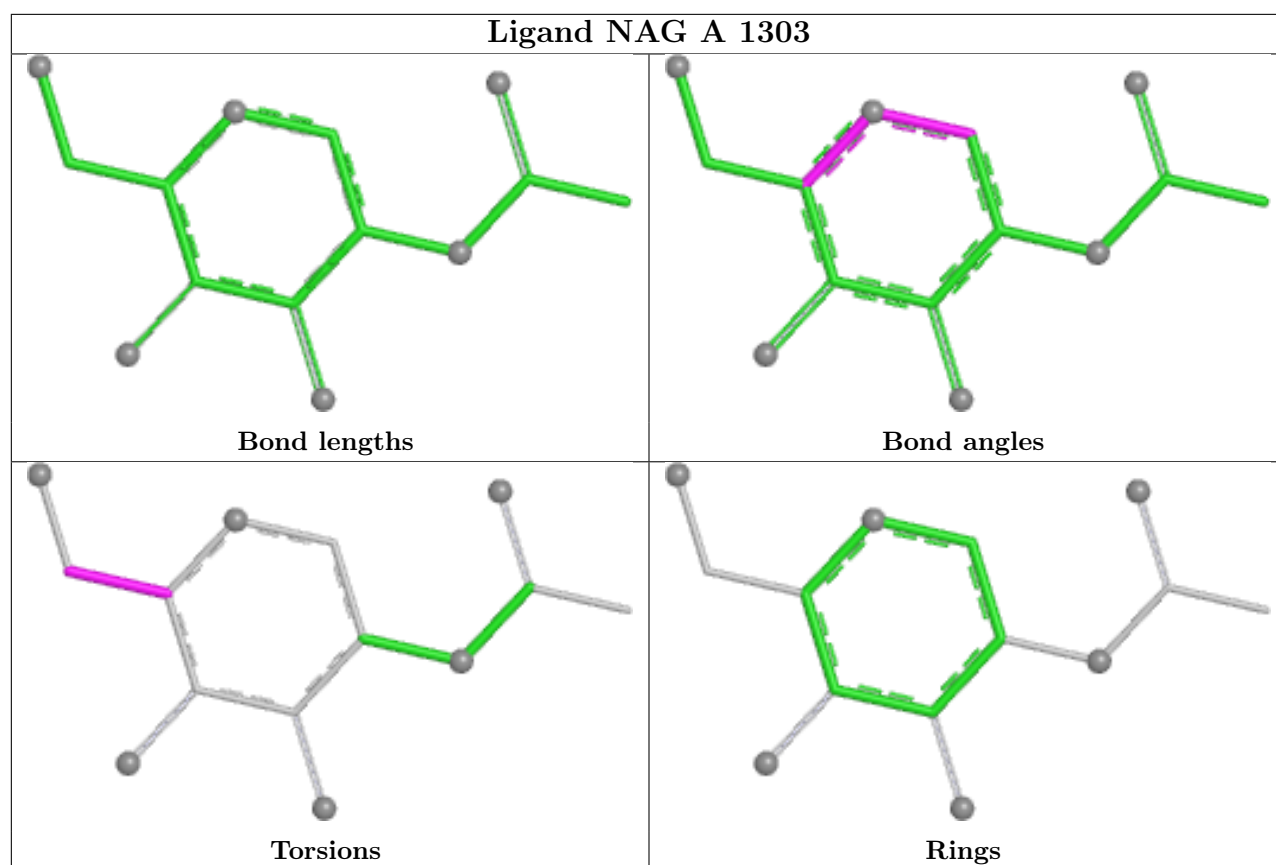


Ligand NAG C 1306

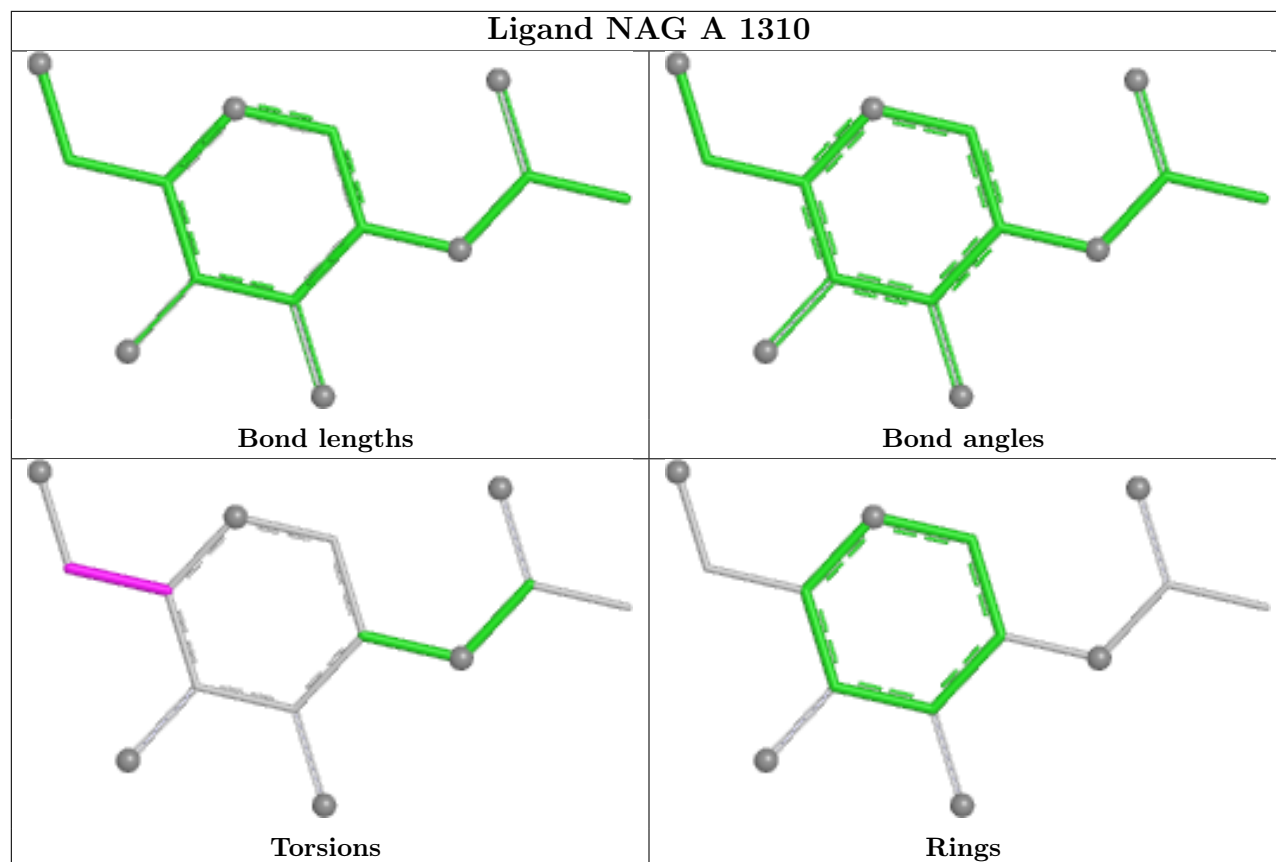


Ligand NAG C 1308

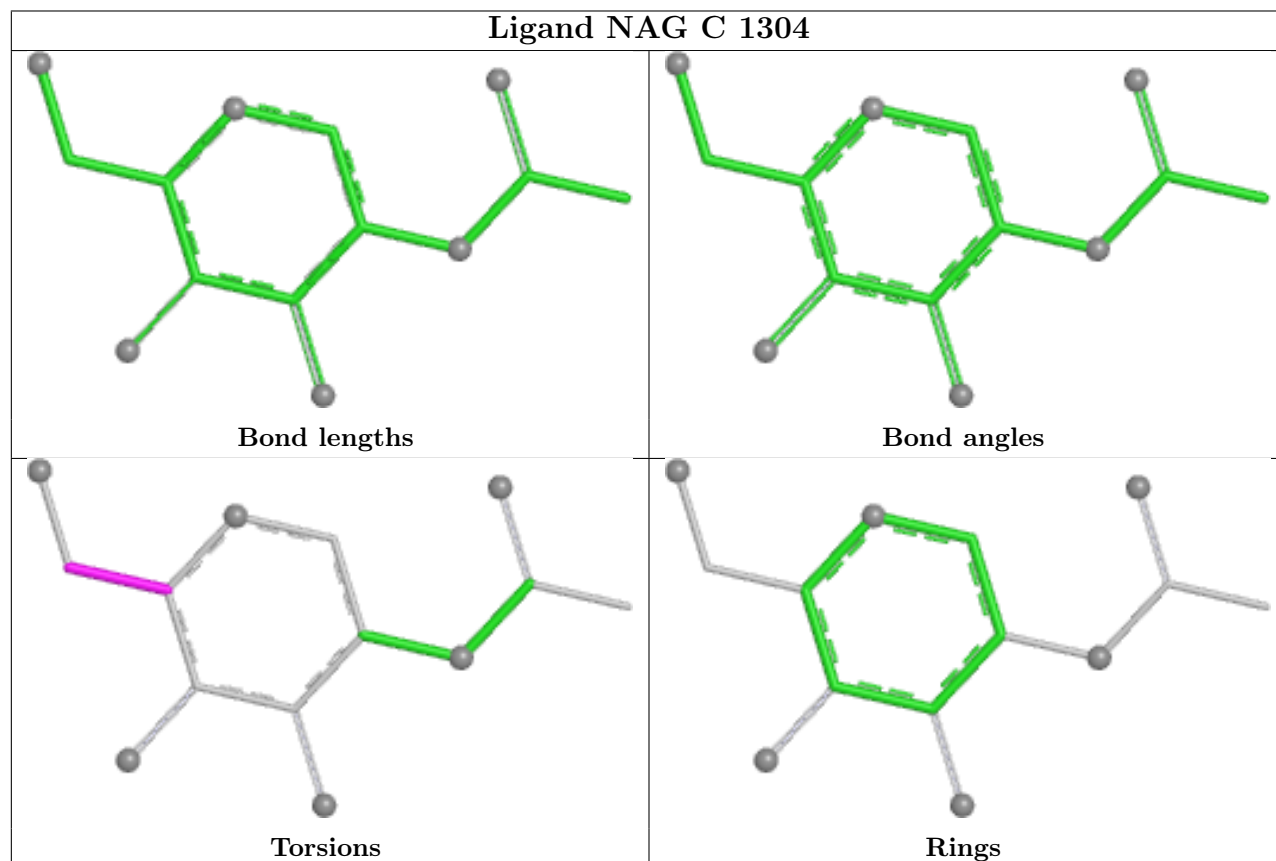


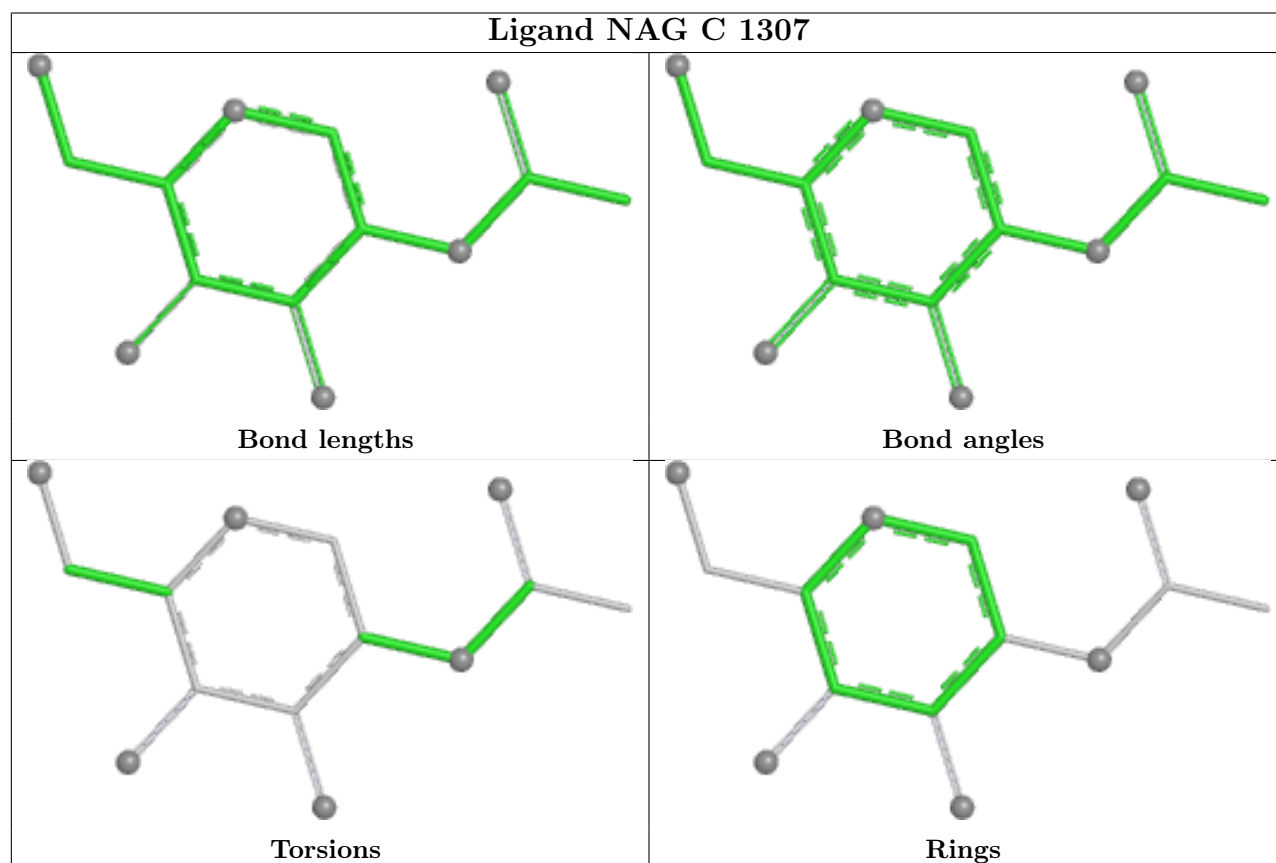
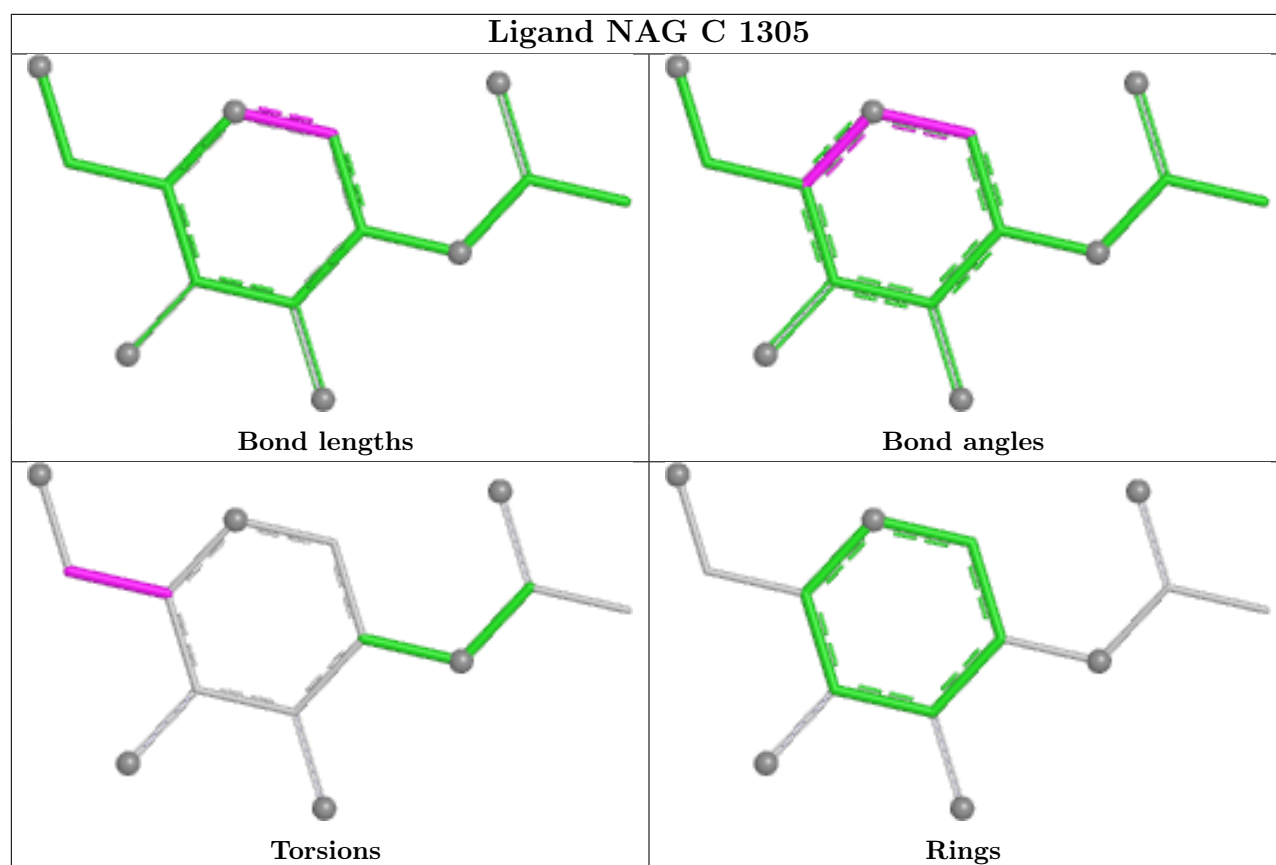


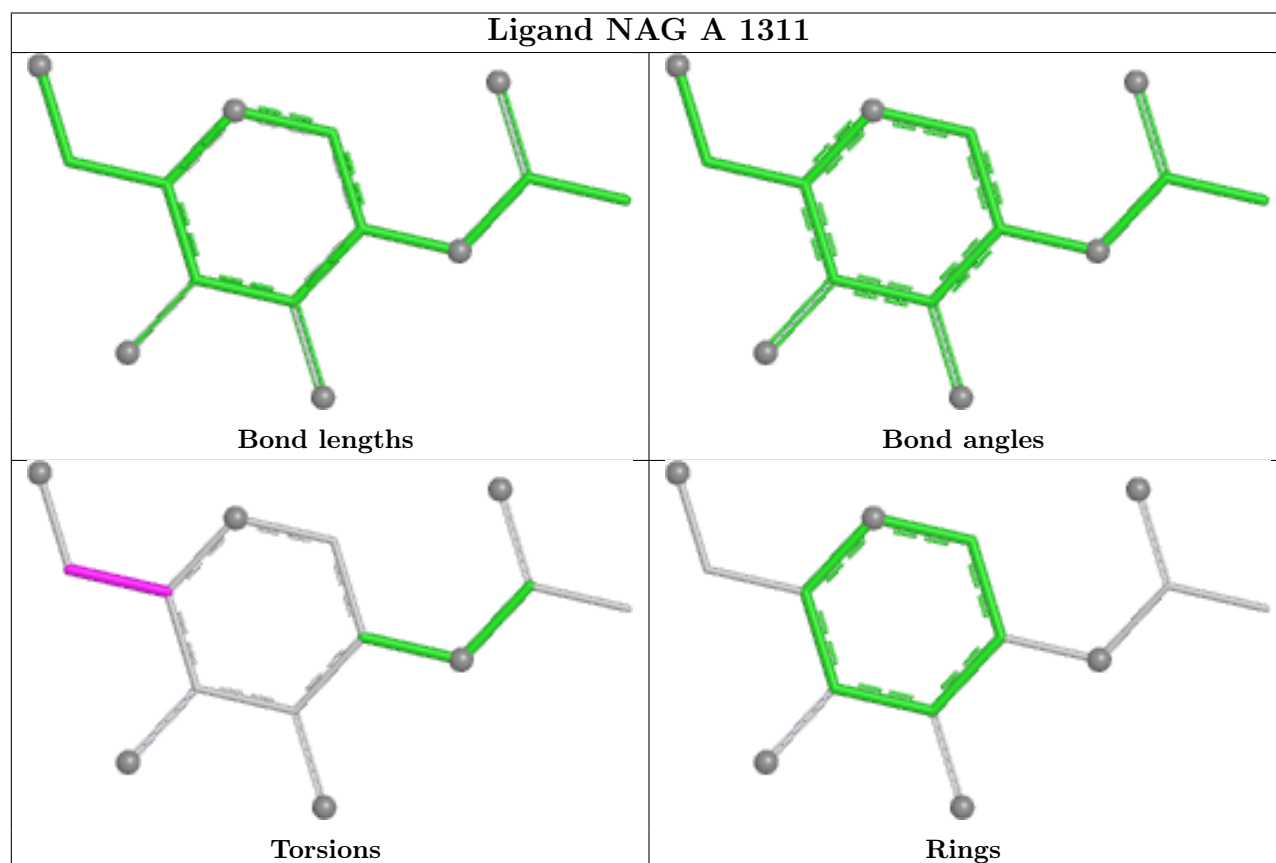
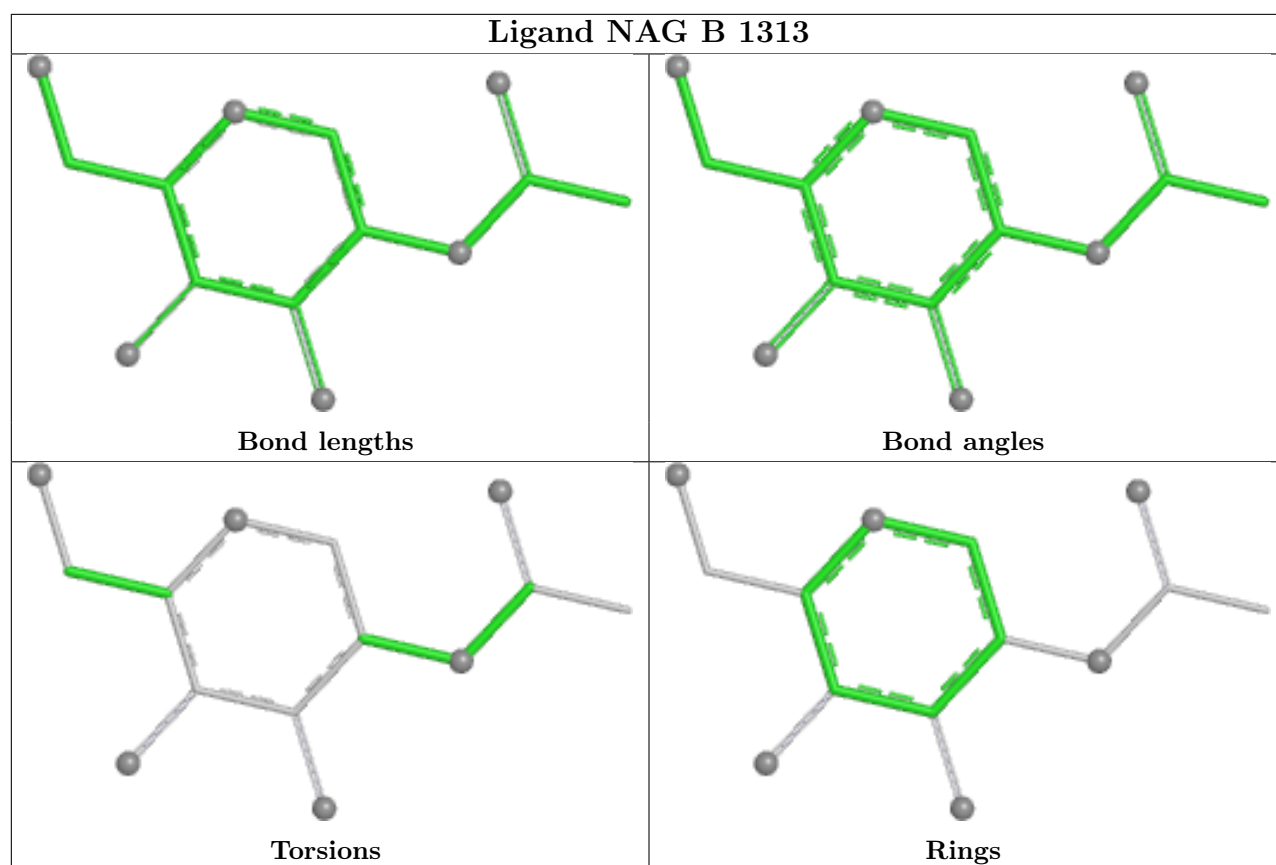
Ligand NAG A 1310

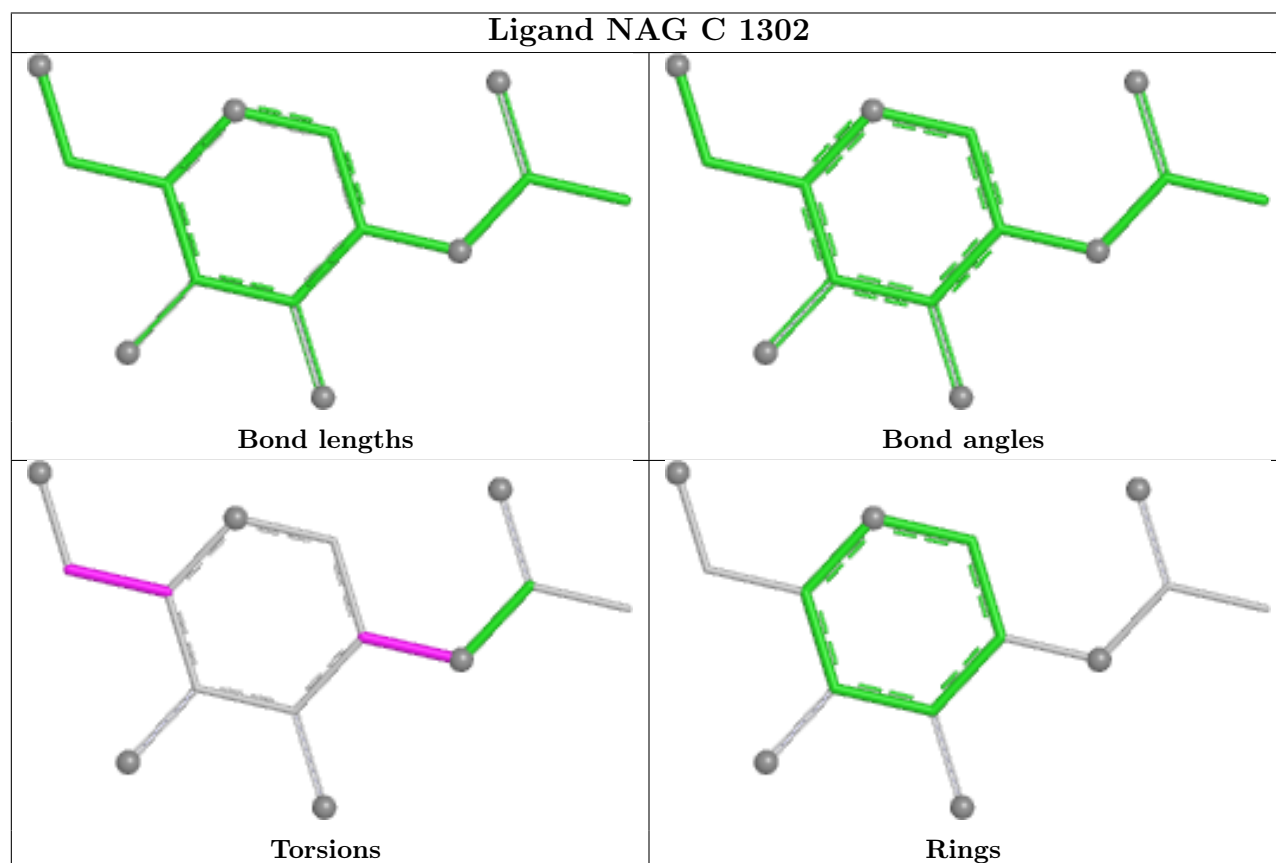
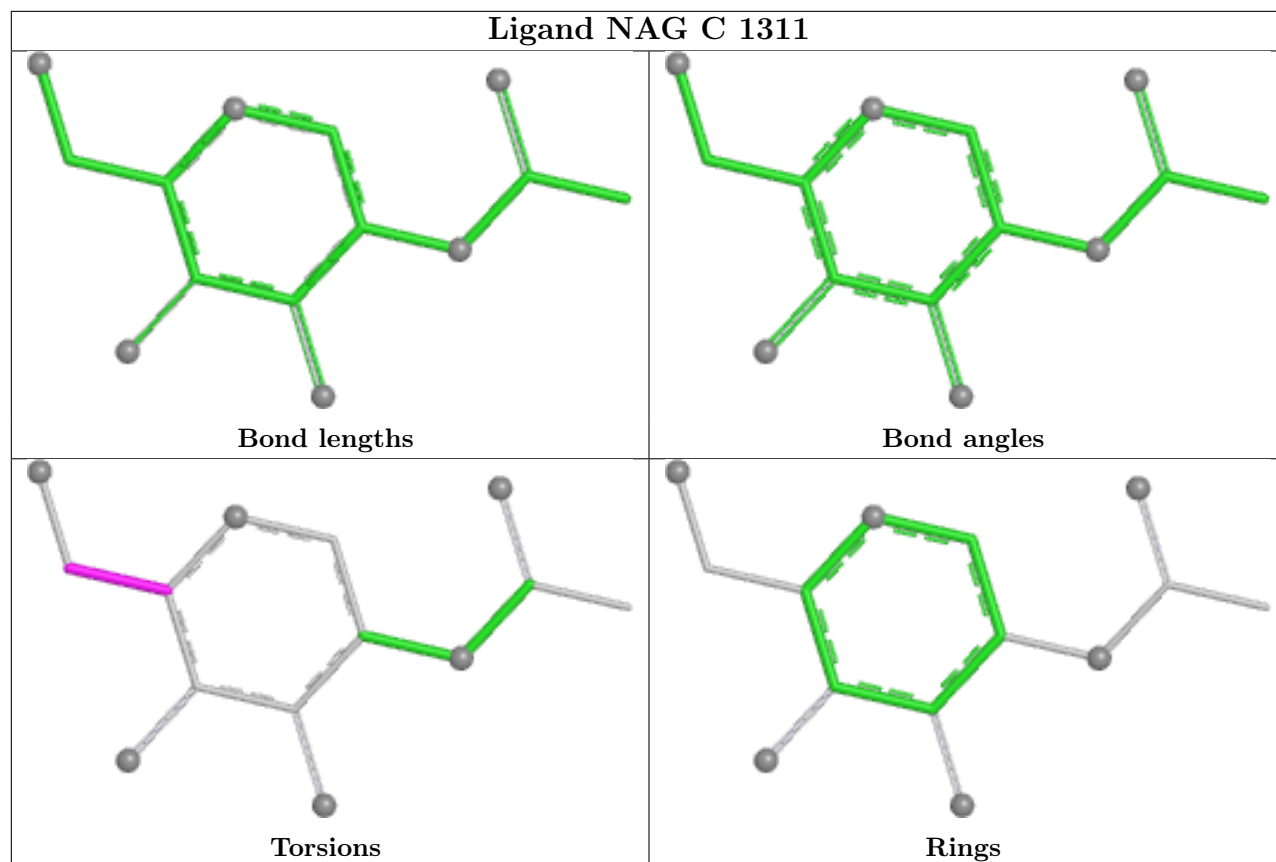


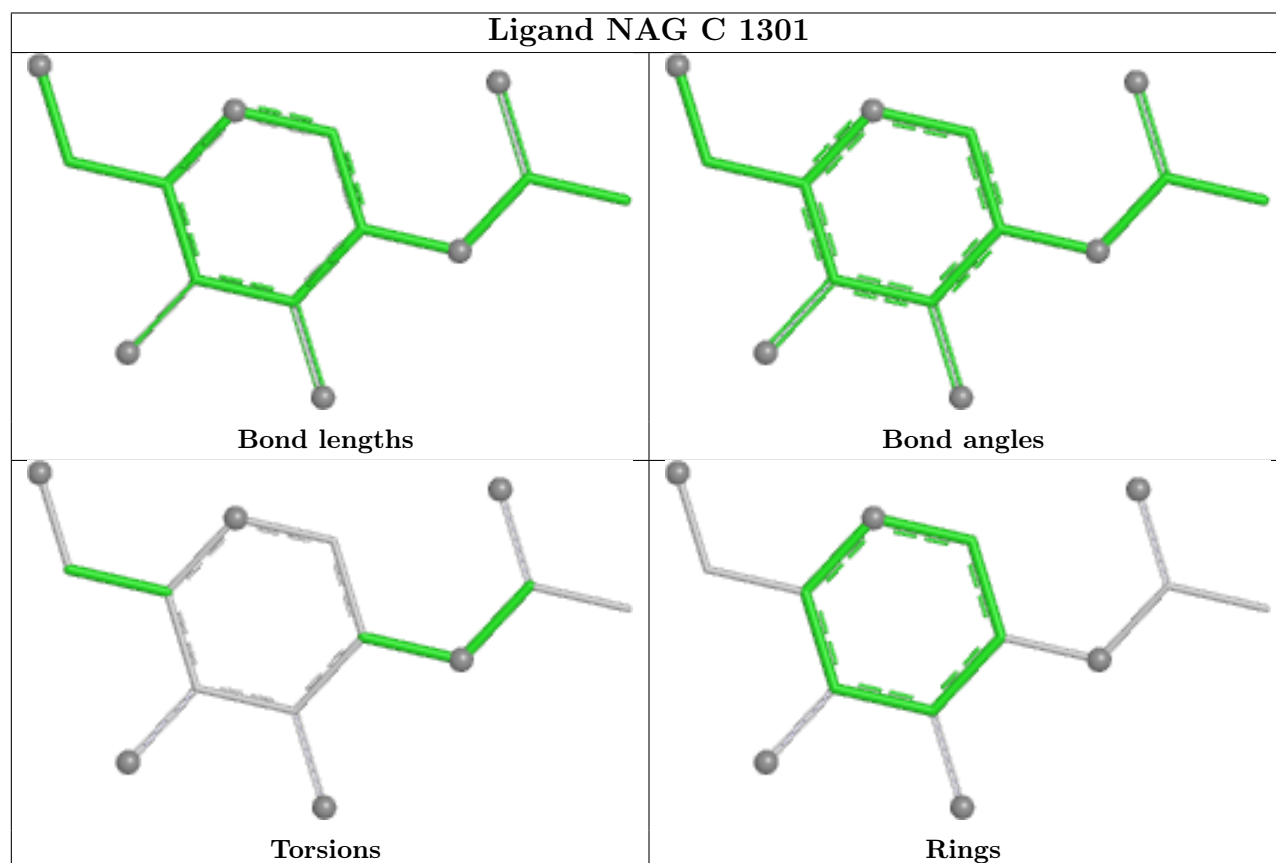
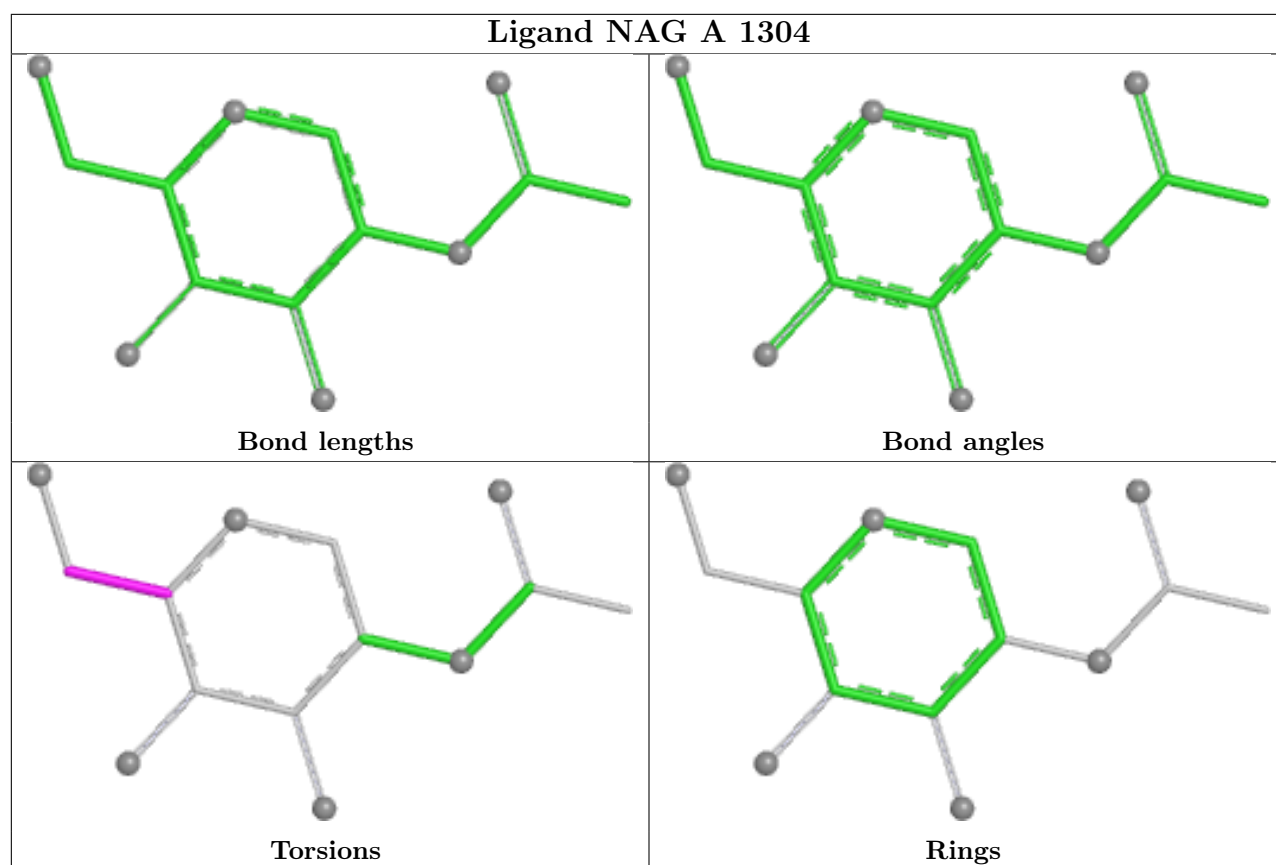
Ligand NAG C 1304



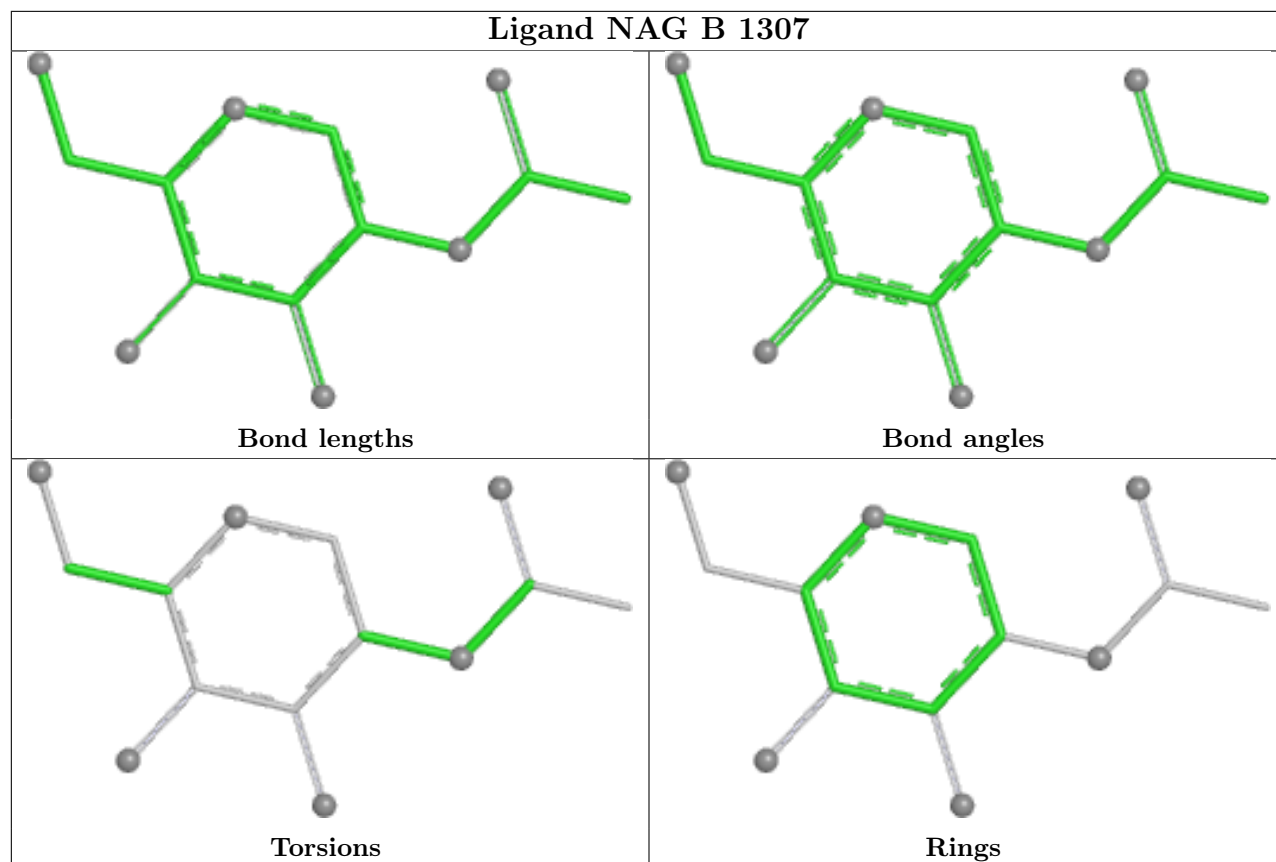




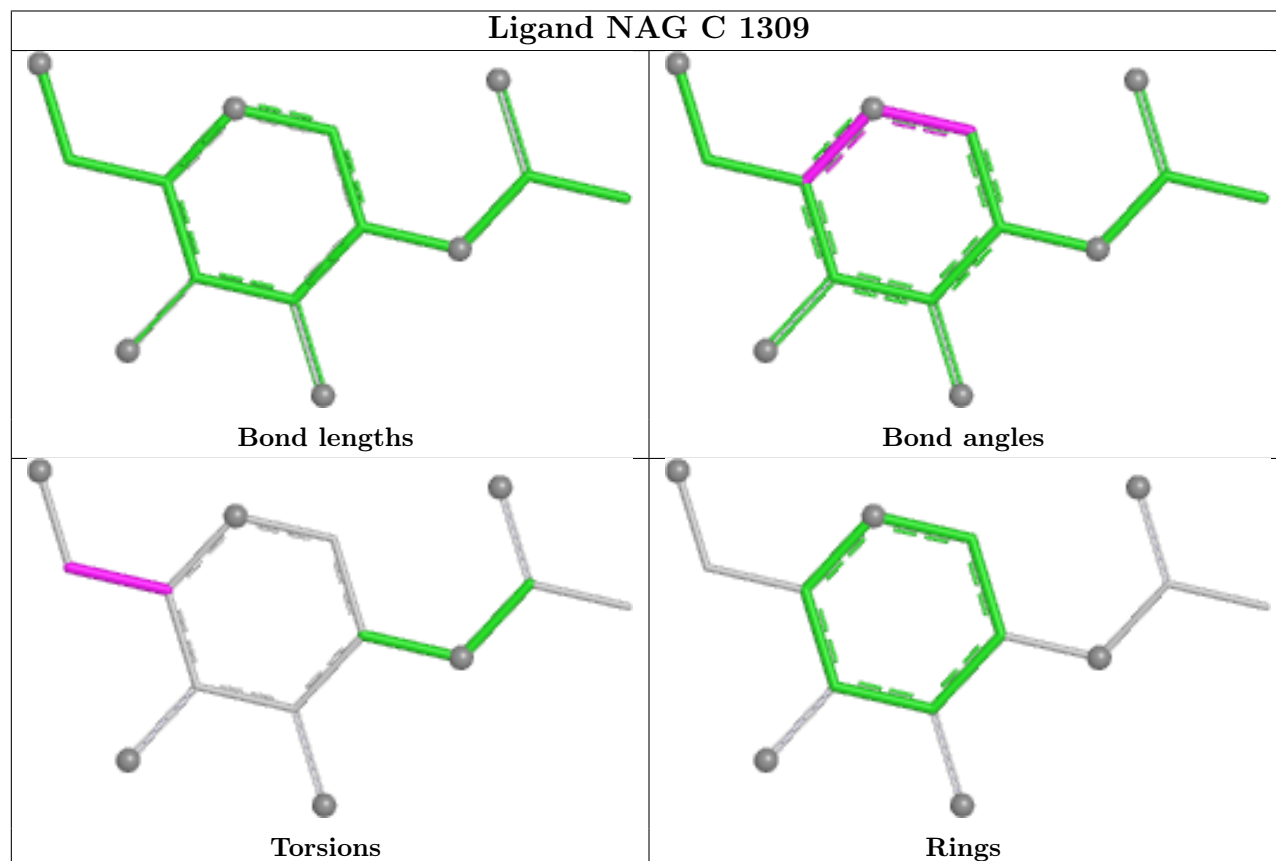




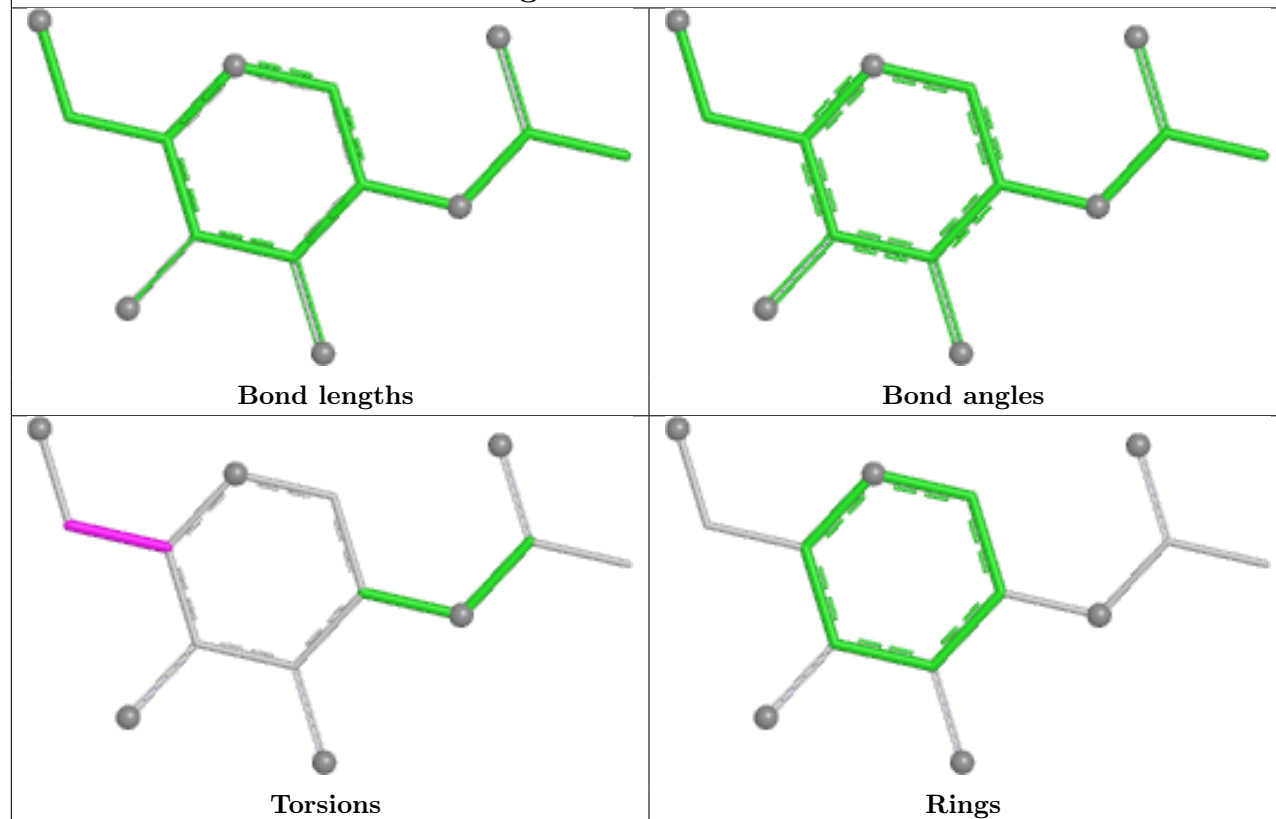
Ligand NAG B 1307



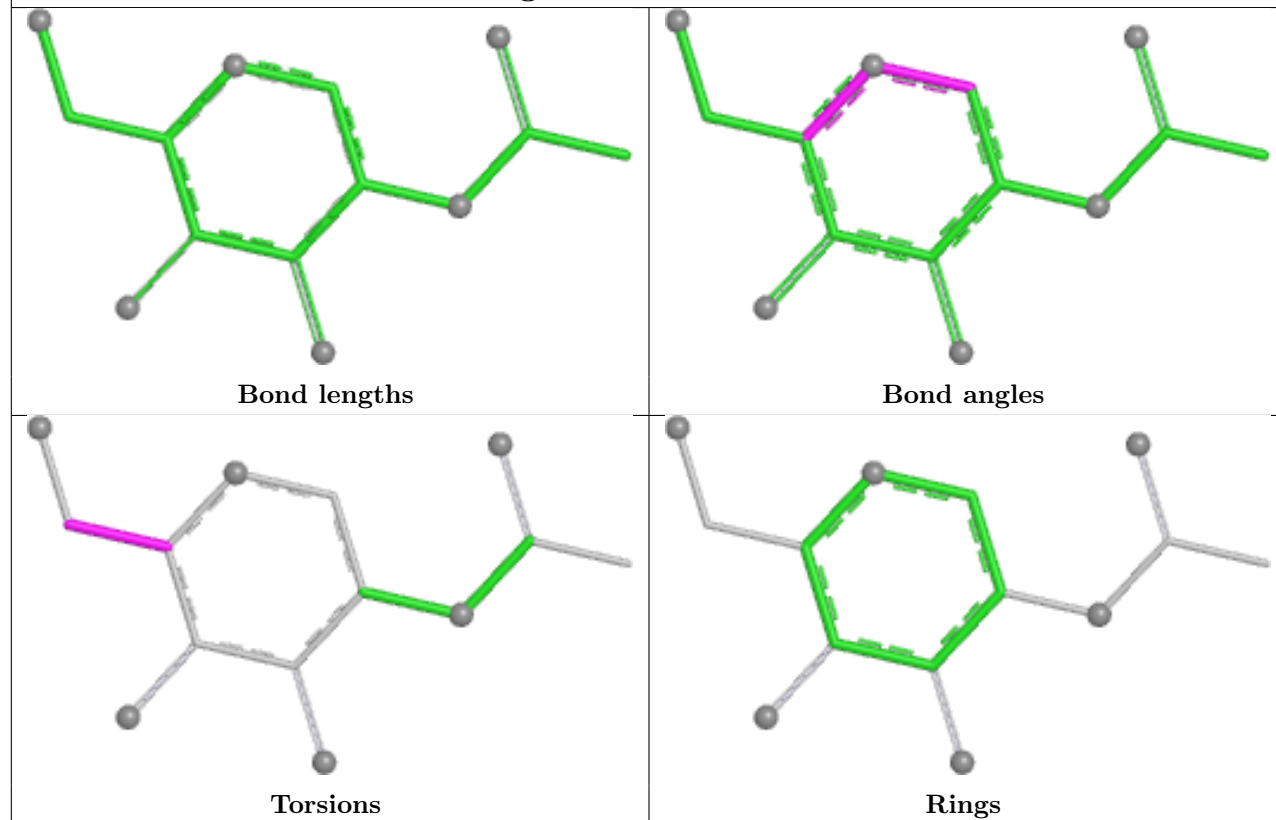
Ligand NAG C 1309

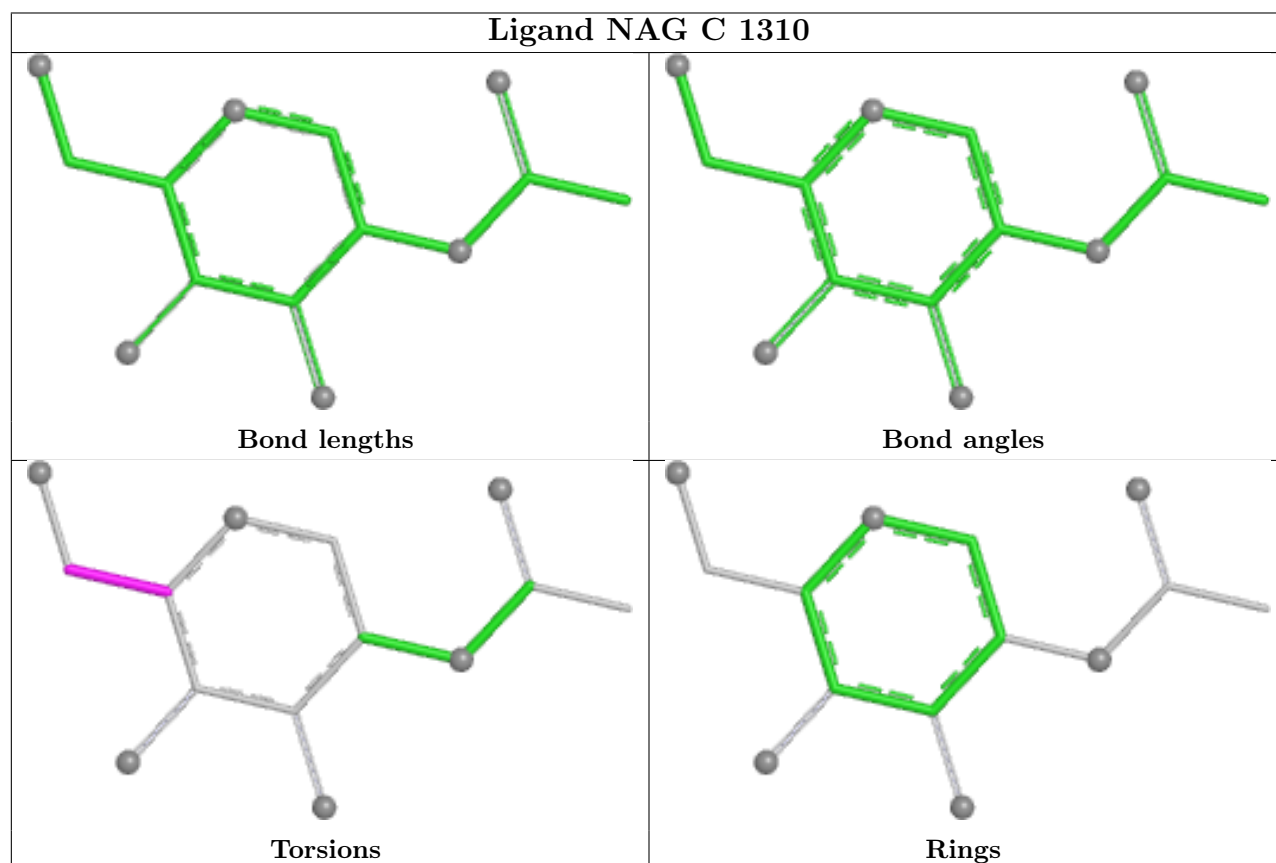
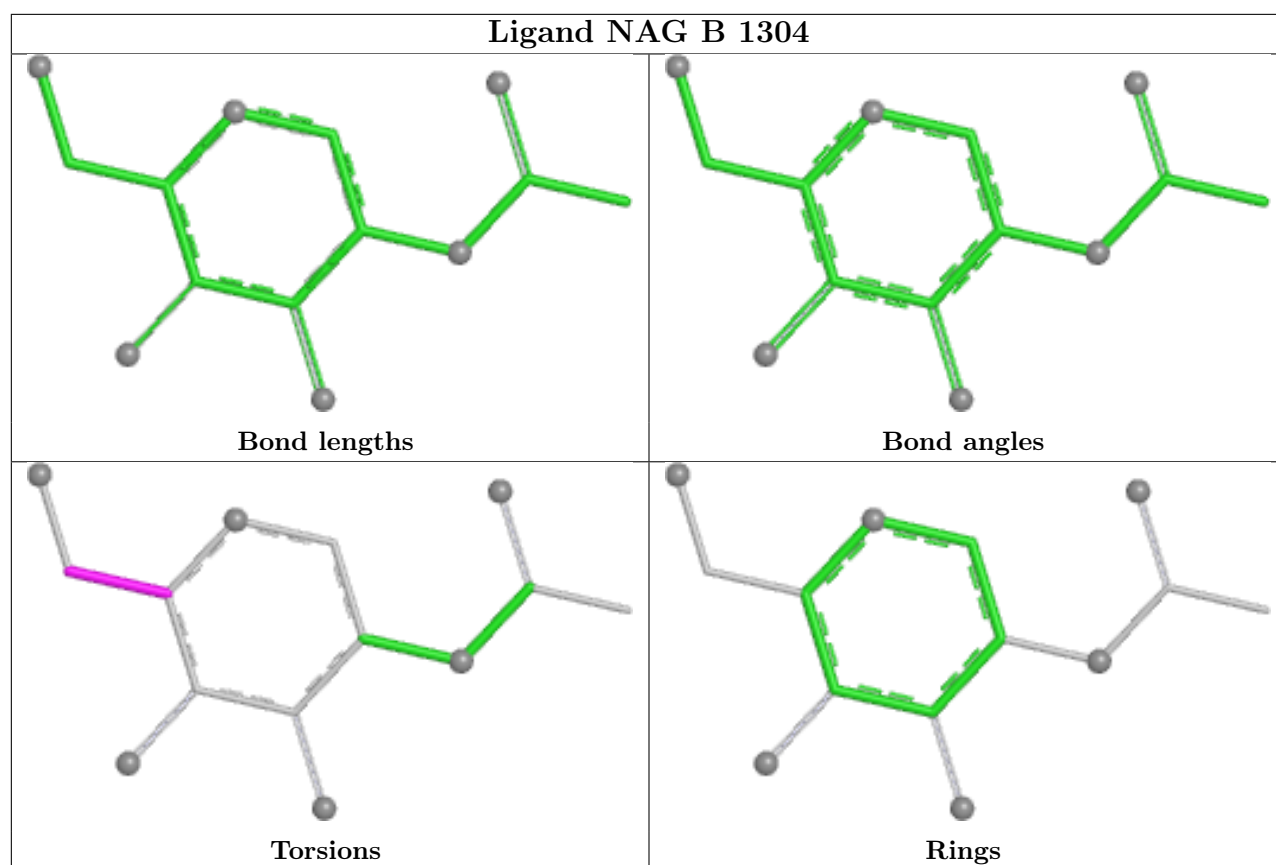


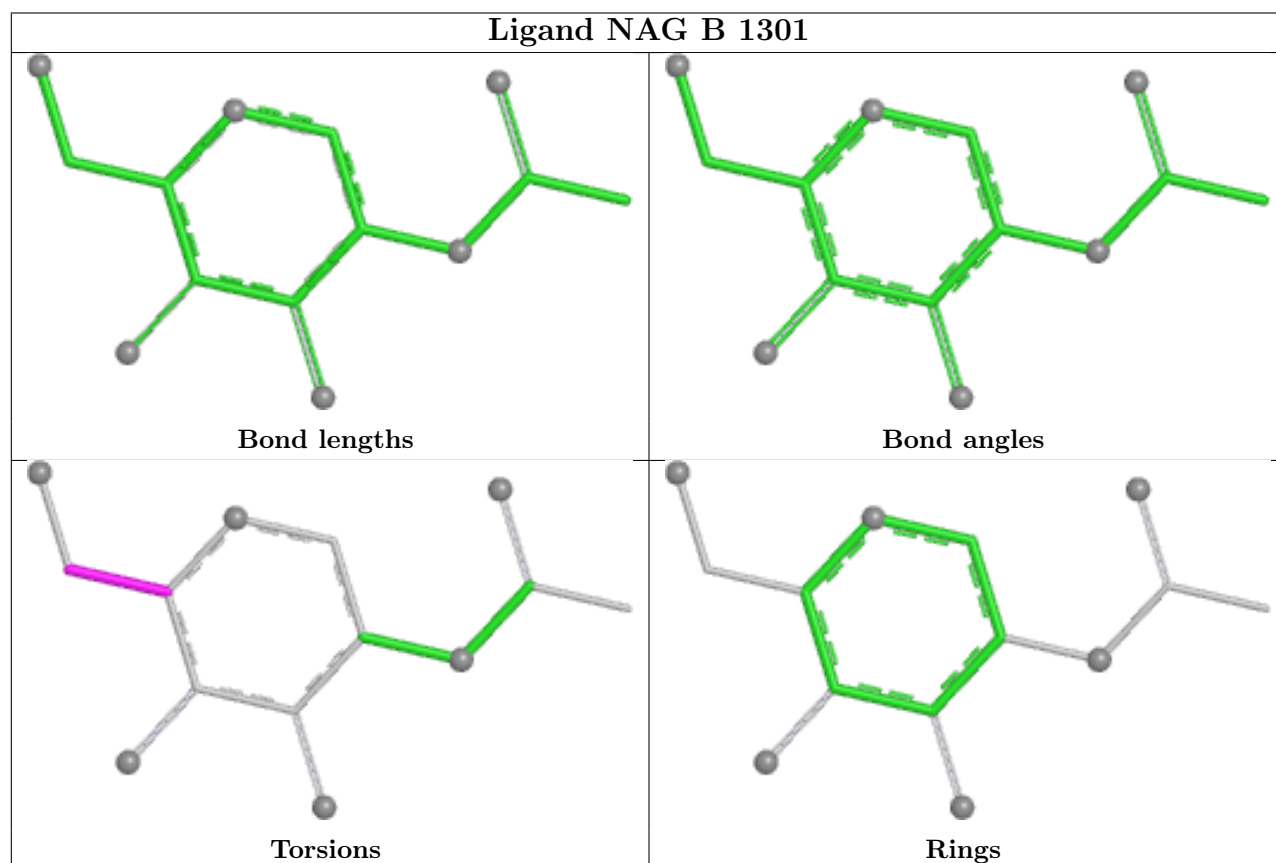
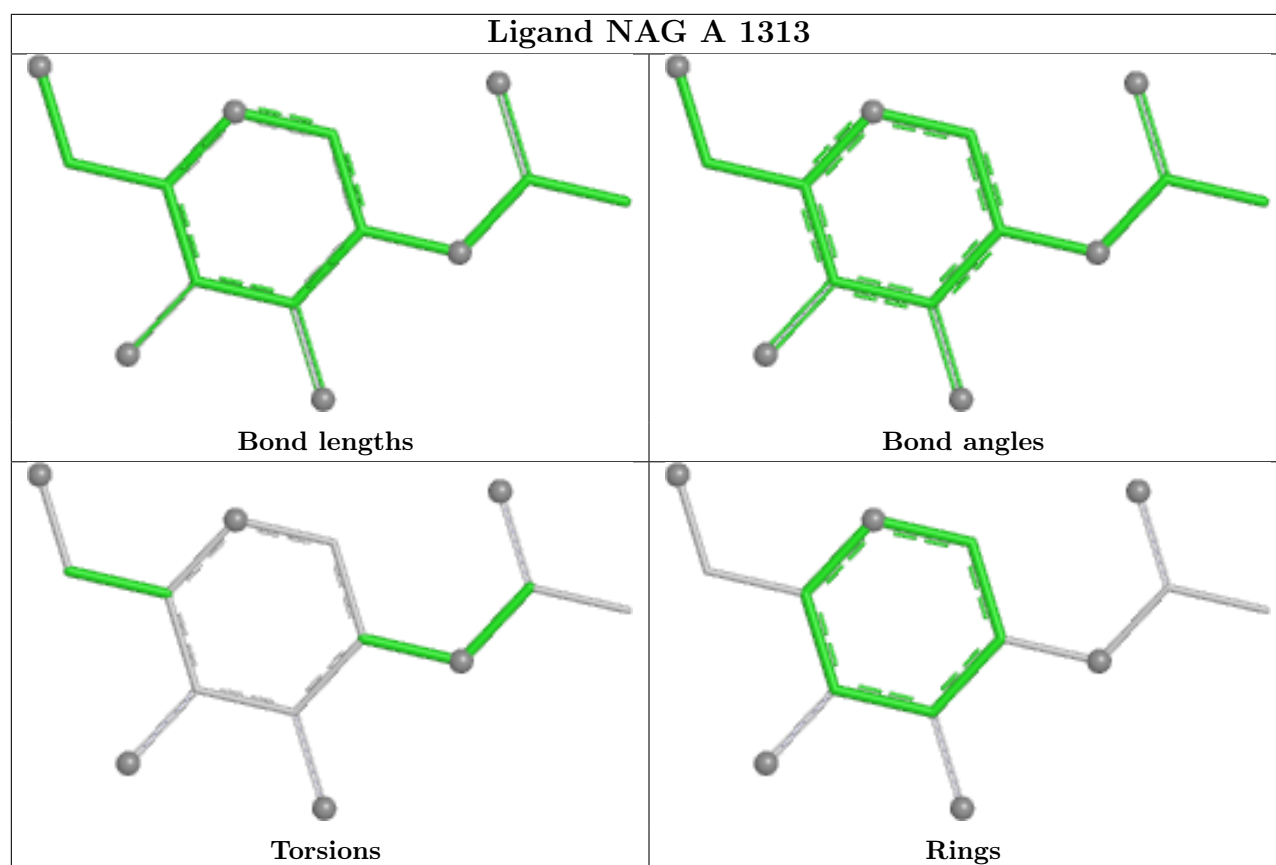
Ligand NAG B 1311

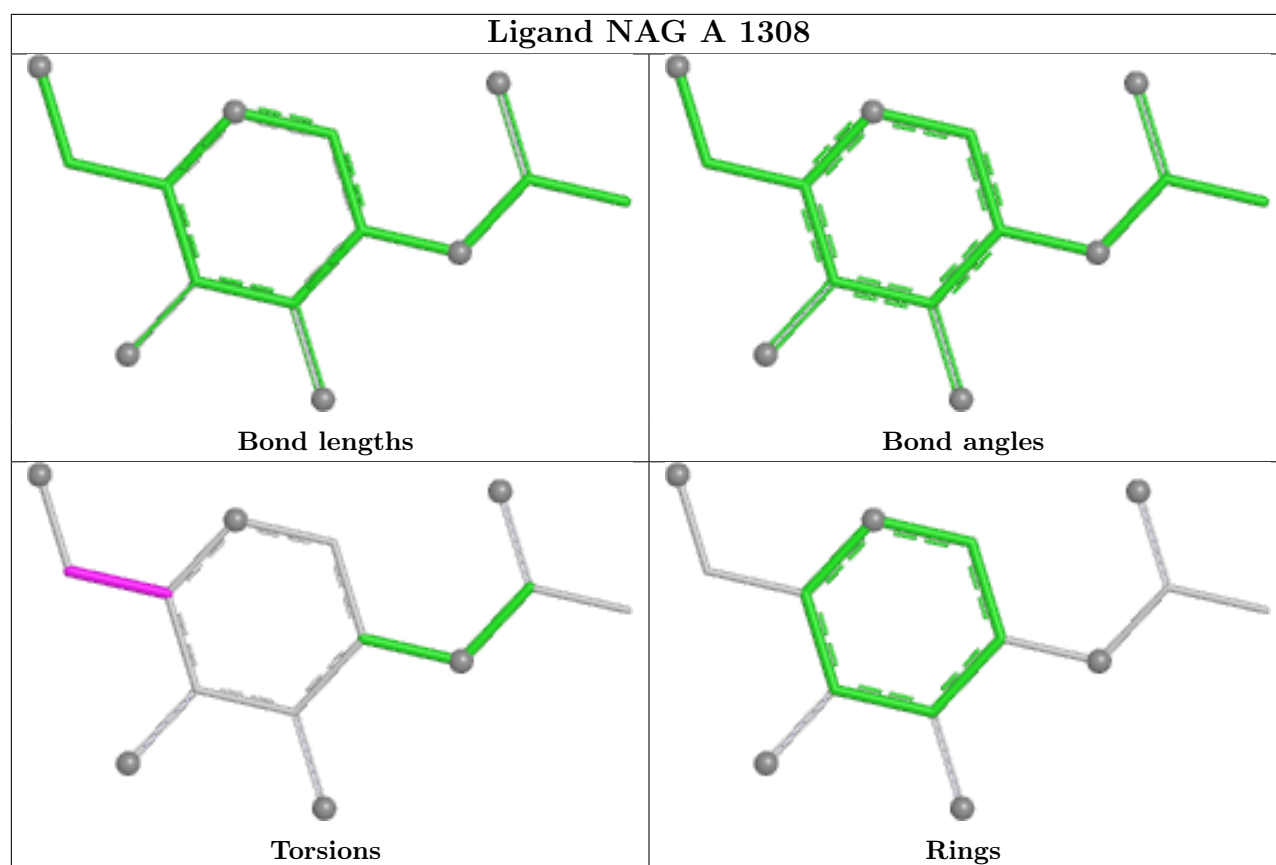


Ligand NAG C 1303









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.

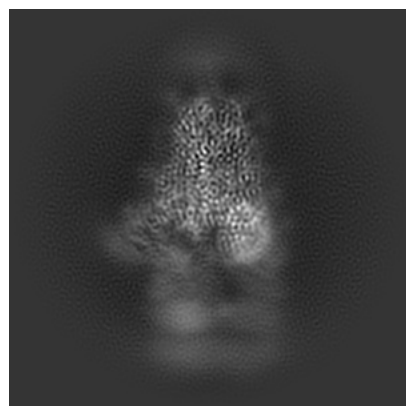
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25008. These allow visual inspection of the internal detail of the map and identification of artifacts.

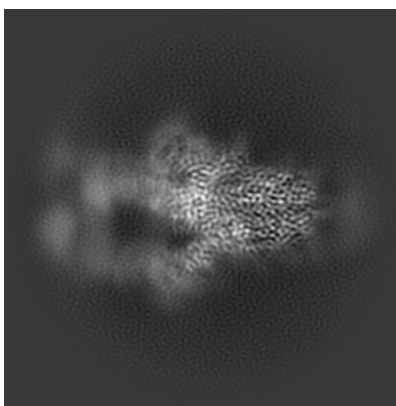
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

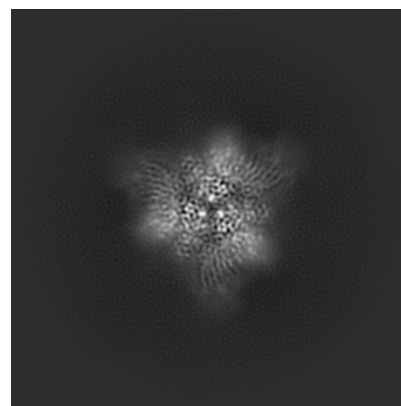
6.1.1 Primary map



X

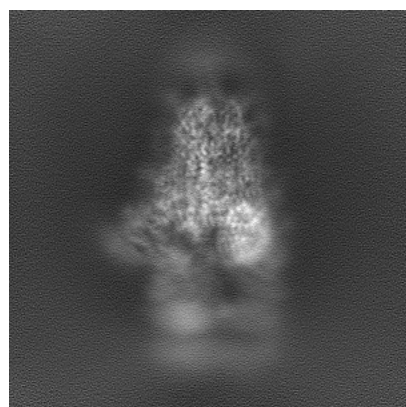


Y

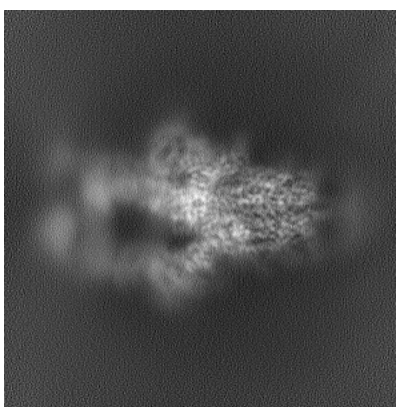


Z

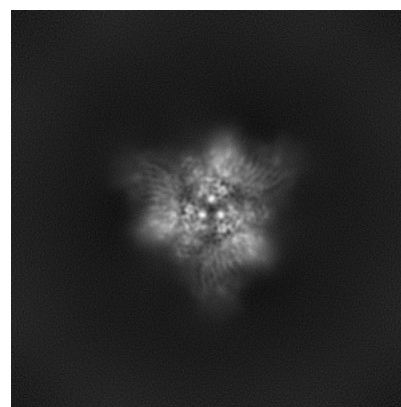
6.1.2 Raw map



X



Y

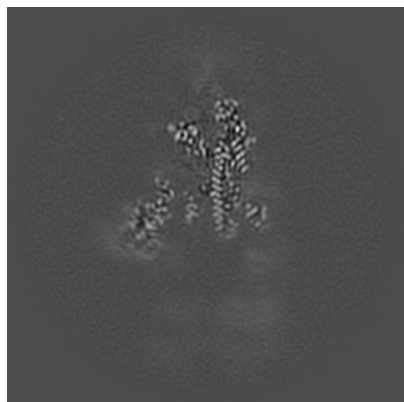


Z

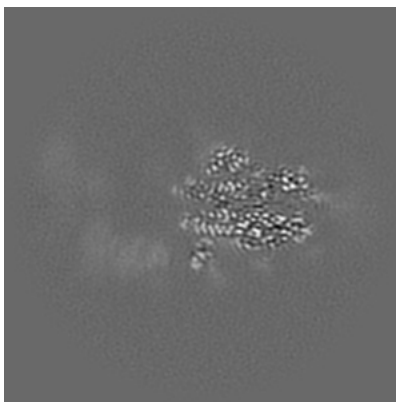
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

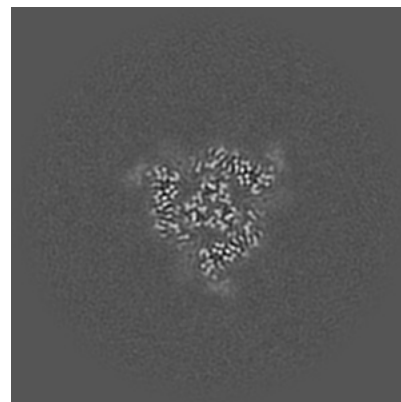
6.2.1 Primary map



X Index: 180

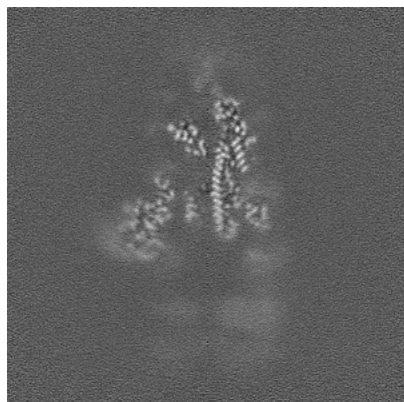


Y Index: 180

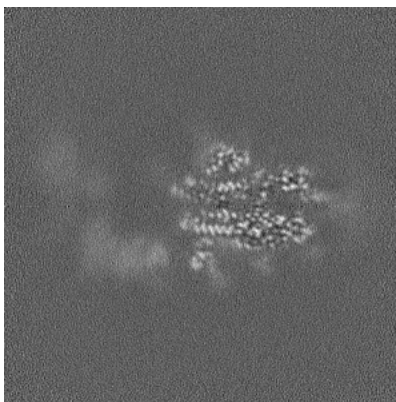


Z Index: 180

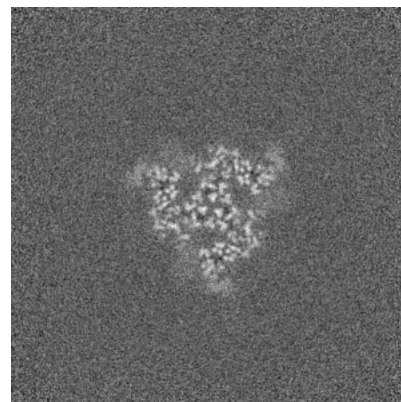
6.2.2 Raw map



X Index: 180



Y Index: 180

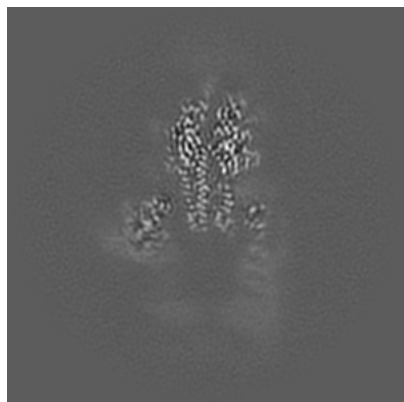


Z Index: 180

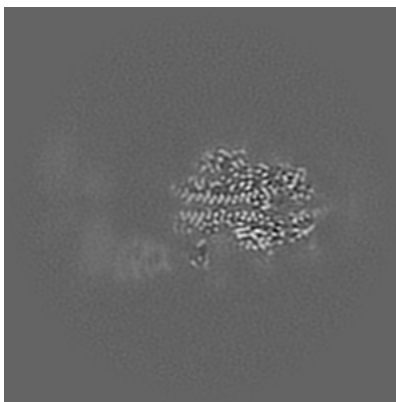
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

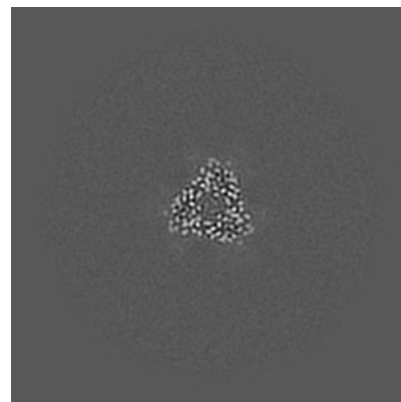
6.3.1 Primary map



X Index: 187

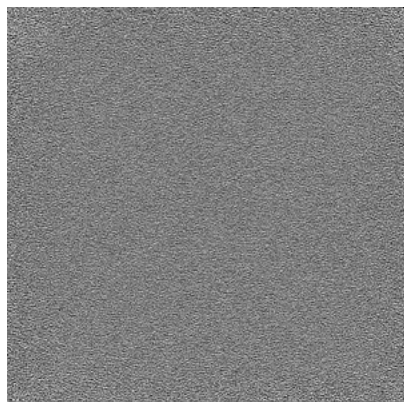


Y Index: 174

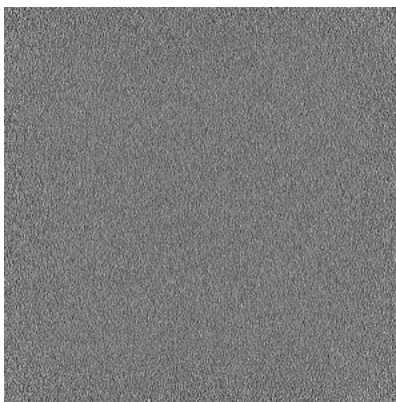


Z Index: 241

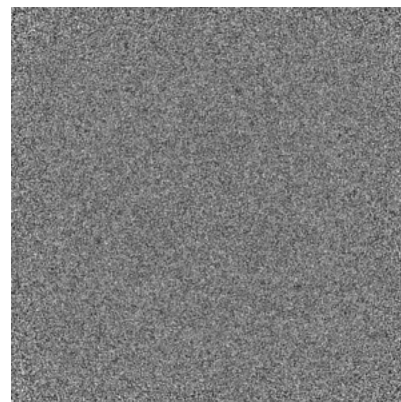
6.3.2 Raw map



X Index: 0



Y Index: 0

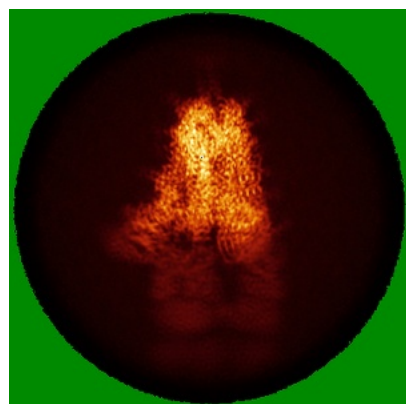


Z Index: 0

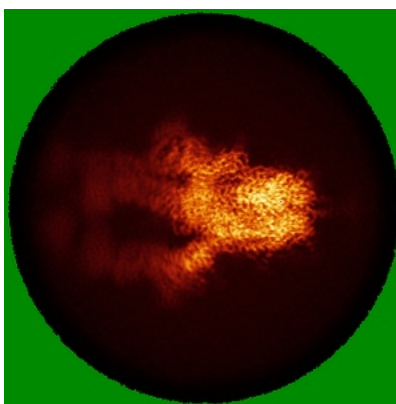
The images above show the largest variance slices of the map in three orthogonal directions.

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

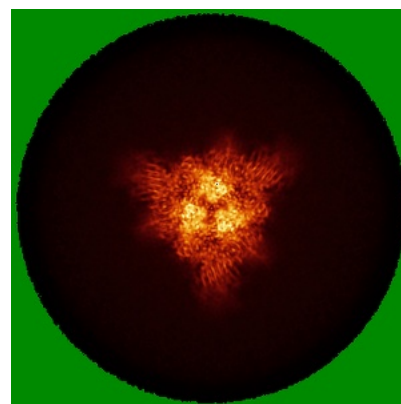
6.4.1 Primary map



X

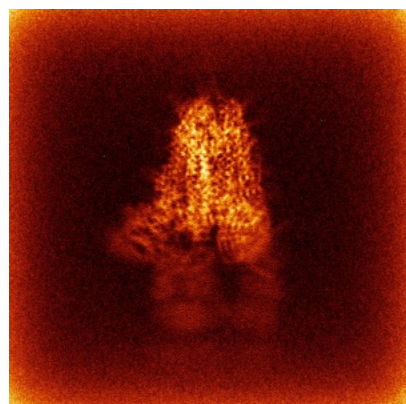


Y

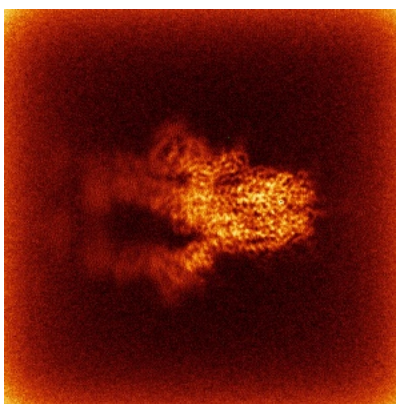


Z

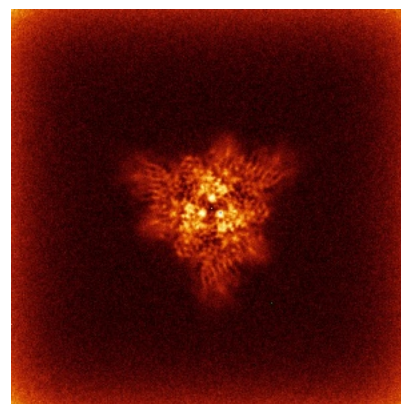
6.4.2 Raw map



X



Y

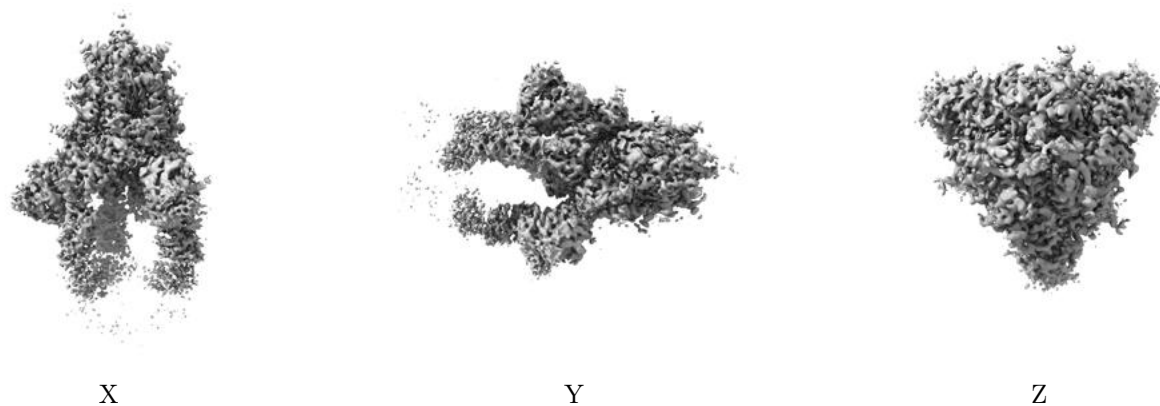


Z

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.

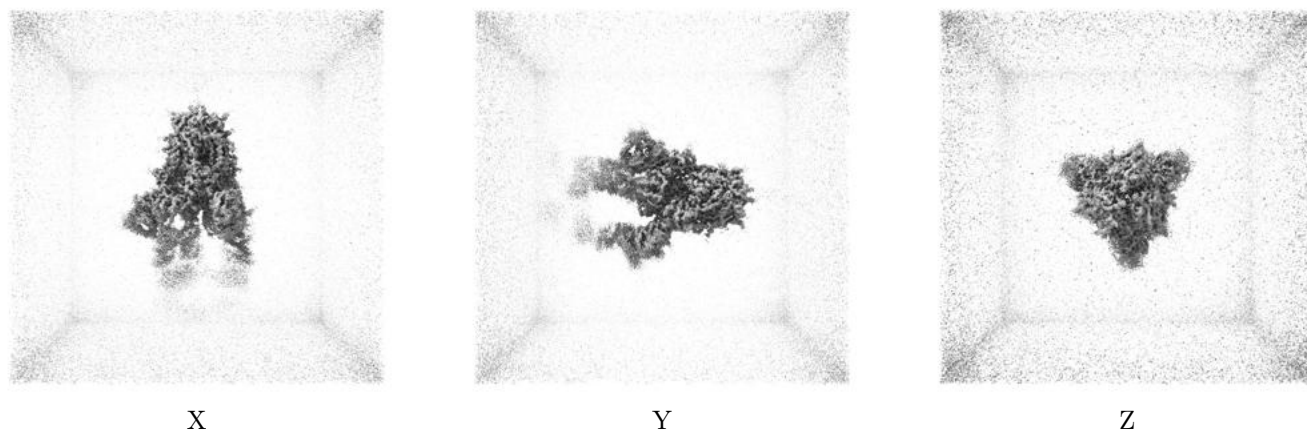
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

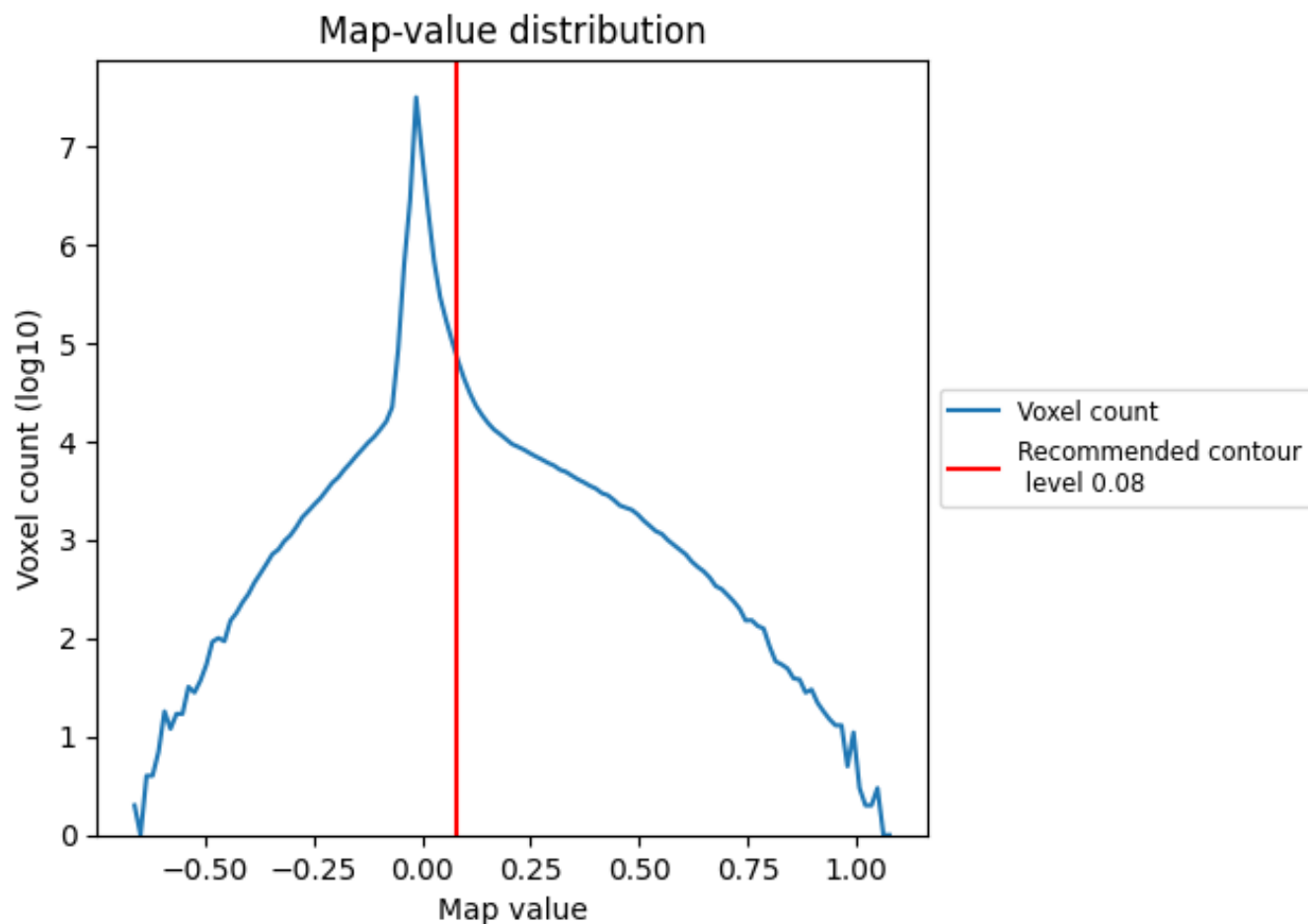
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

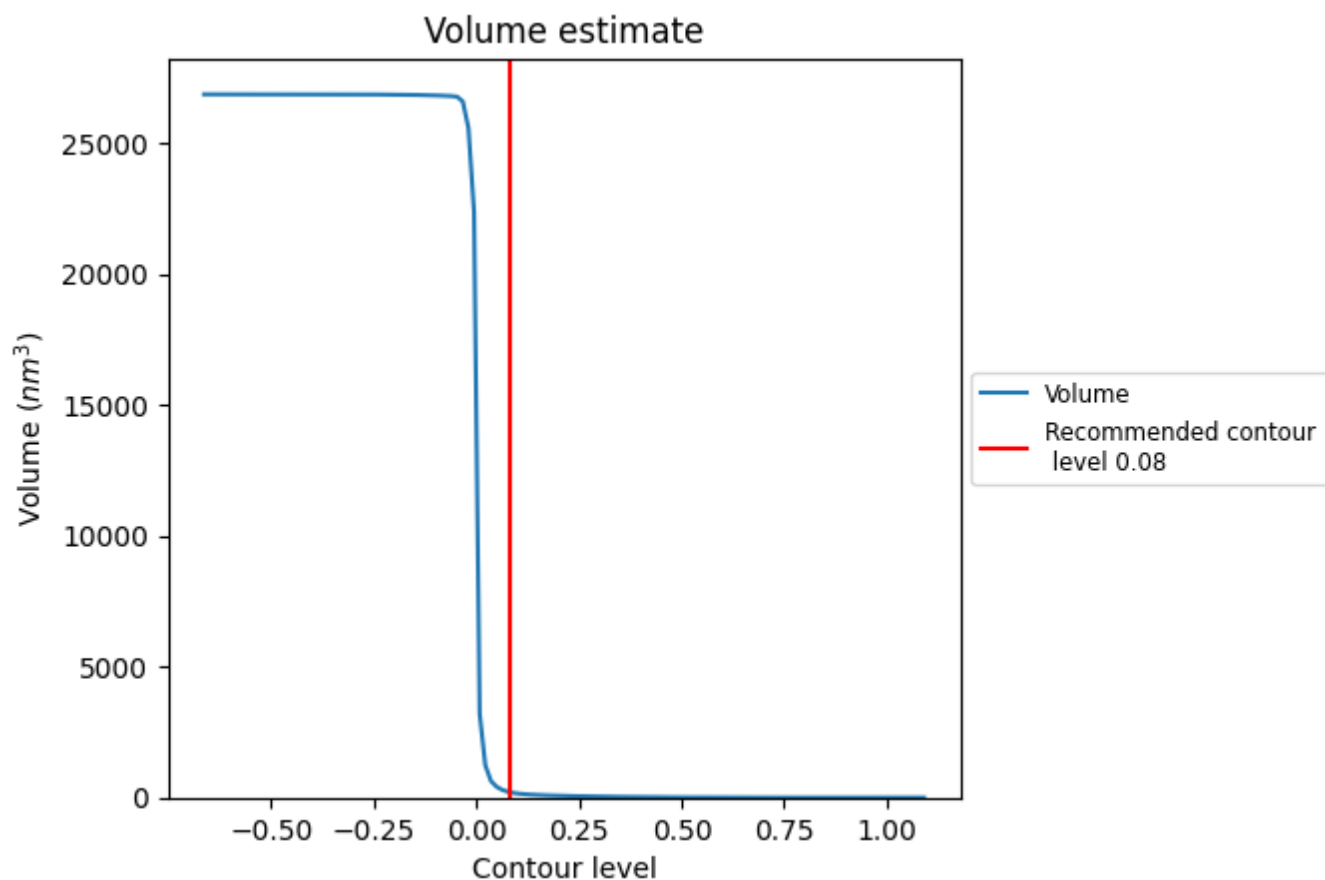
This section contains the results of statistical analysis of the map.

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.

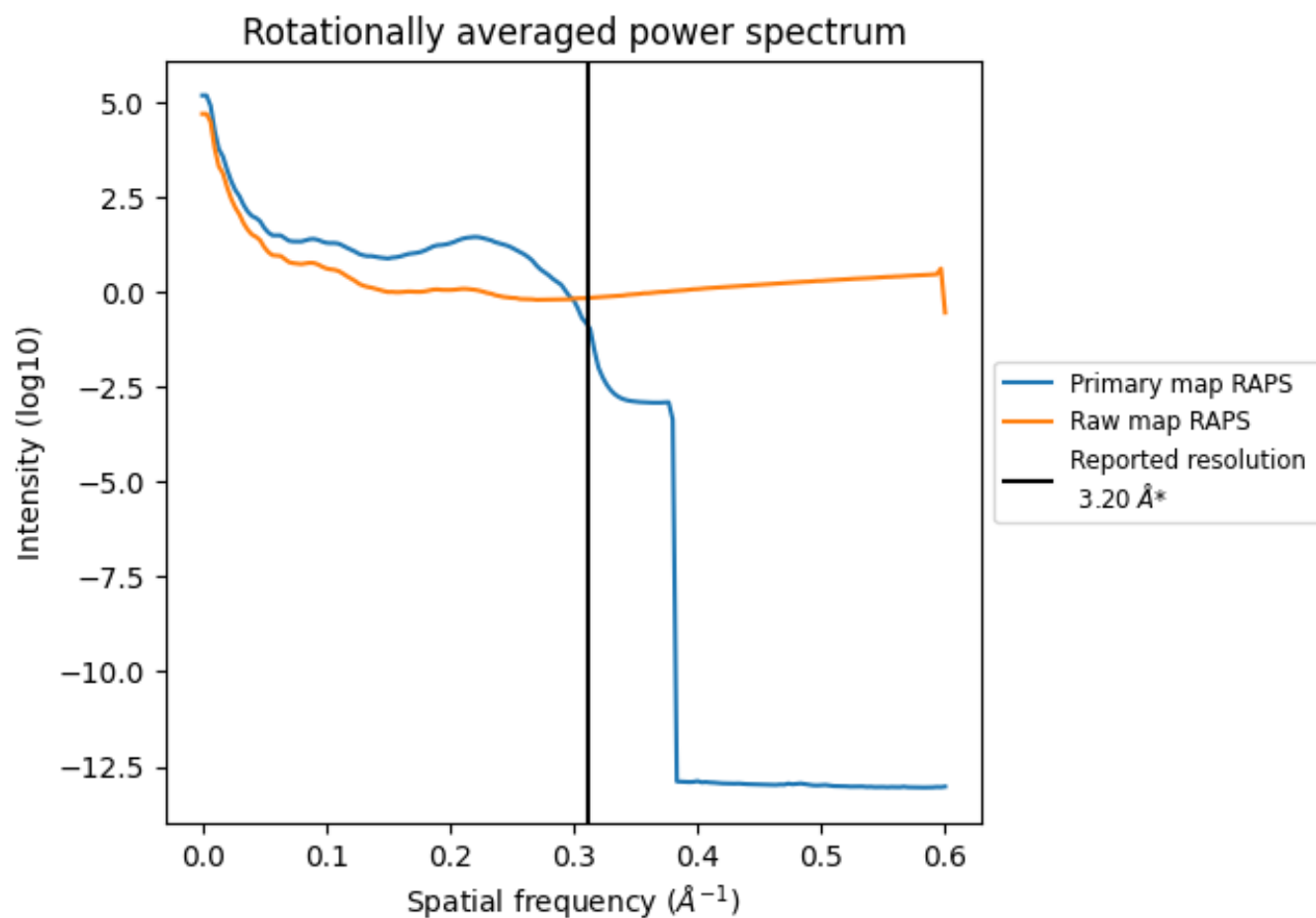
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm³; this corresponds to an approximate mass of 193 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

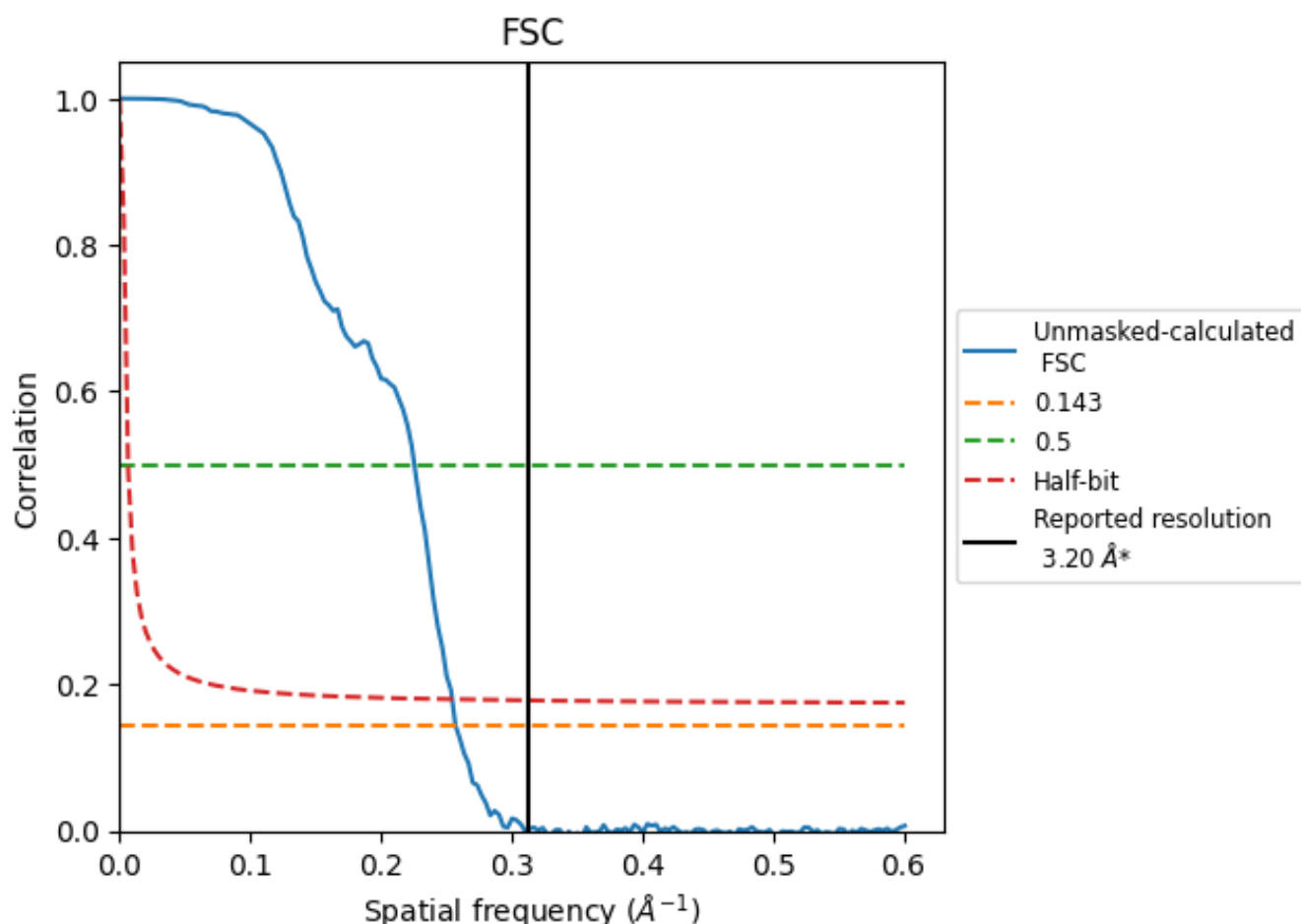


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

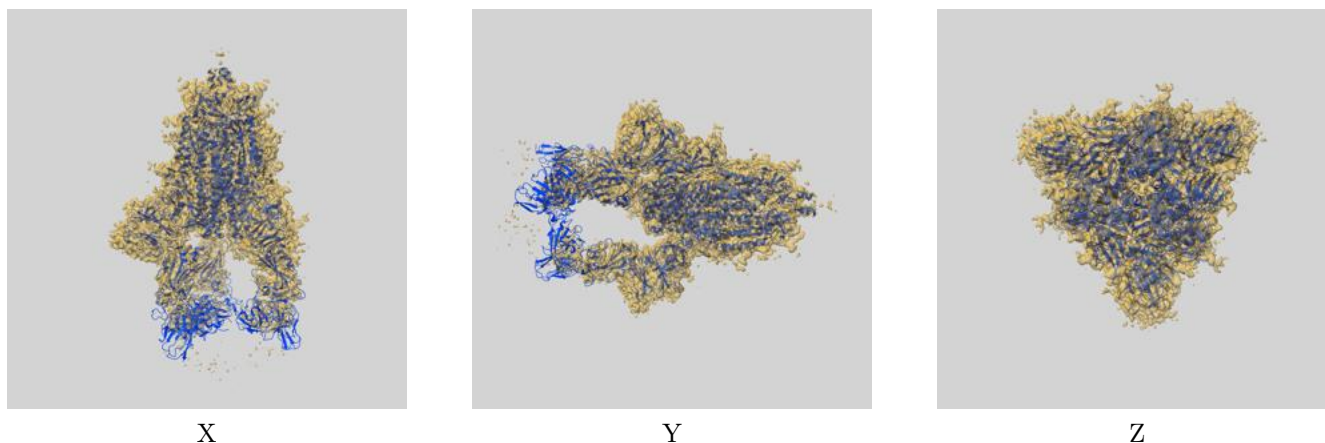
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	4.43	3.93

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

9 Map-model fit [i](#)

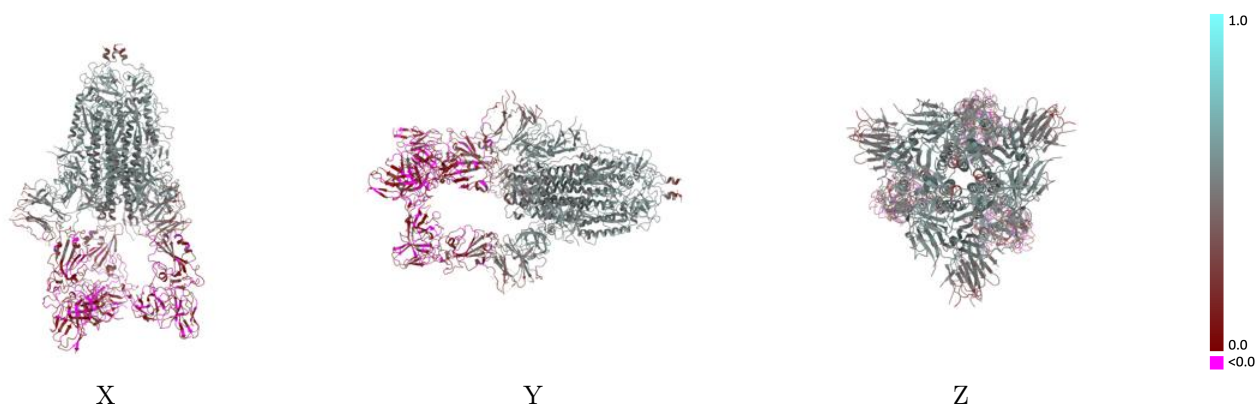
This section contains information regarding the fit between EMDB map EMD-25008 and PDB model 7SC1. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



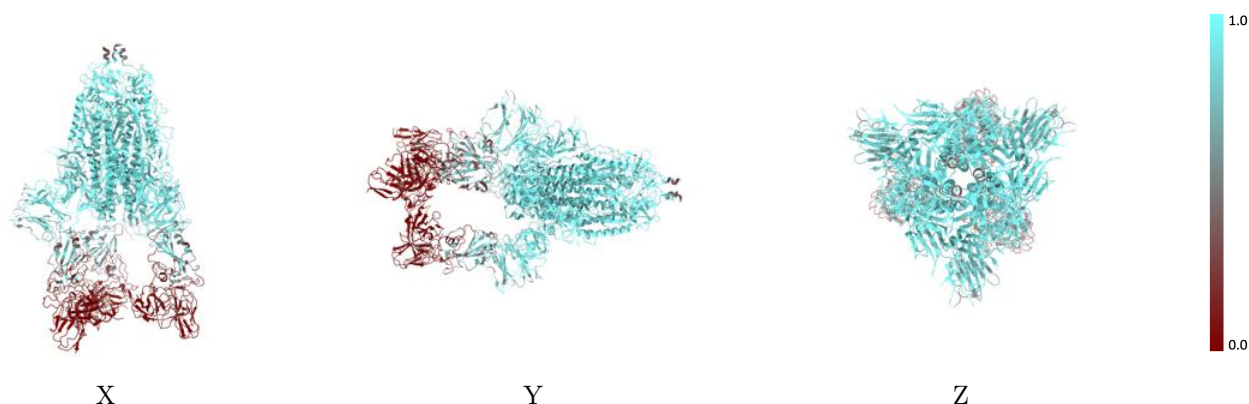
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



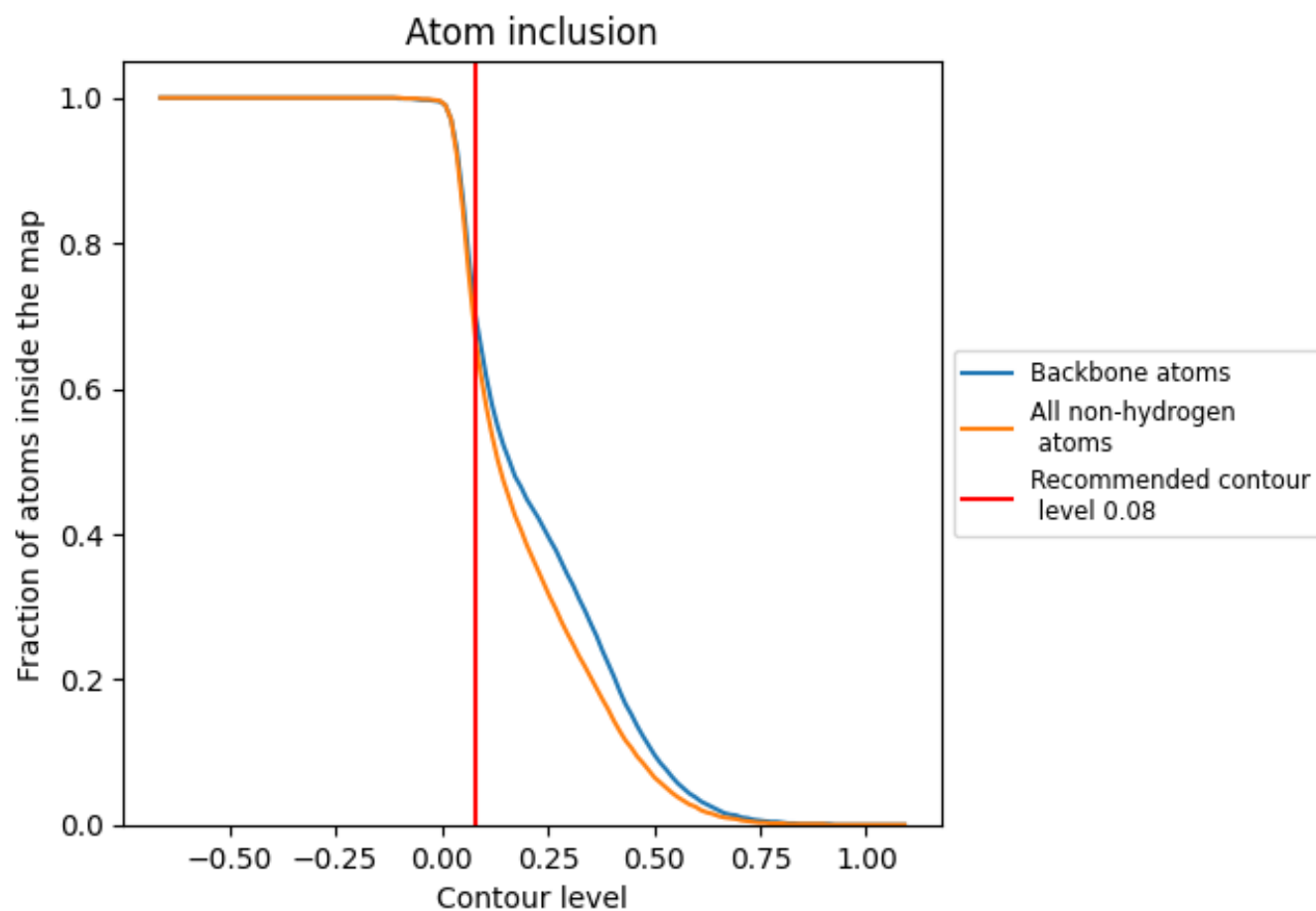
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 67% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6680	<div></div> 0.3640
A	<div></div> 0.7970	<div></div> 0.4230
B	<div></div> 0.7990	<div></div> 0.4250
C	<div></div> 0.7980	<div></div> 0.4240
H	<div></div> 0.0330	<div></div> 0.0610
L	<div></div> 0.0620	<div></div> 0.0990
M	<div></div> 0.0320	<div></div> 0.0530
N	<div></div> 0.0570	<div></div> 0.0980
P	<div></div> 0.0300	<div></div> 0.0470
Q	<div></div> 0.0550	<div></div> 0.0950

