



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 03:04 AM UTC

PDB ID : 9ML5 / pdb_00009ml5
EMDB ID : EMD-48348
Title : Structure of the SARS-CoV-2 Spike 6P in complex with the rabbit M8b-B8 Fab
Authors : Fan, C.; Bjorkman, P.J.
Deposited on : 2024-12-18
Resolution : 3.40 Å (reported)
Based on initial models : 7UZD, 7SC1

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

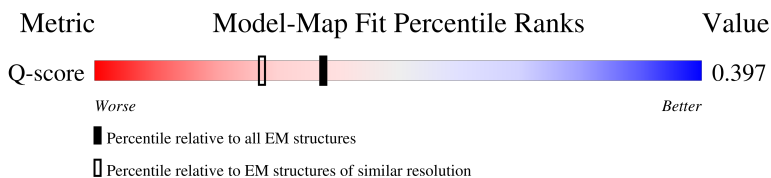
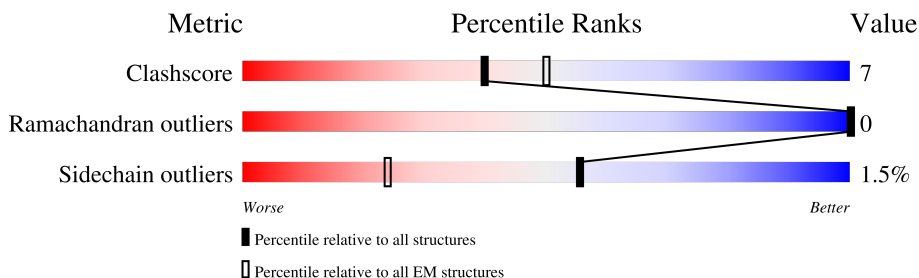
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	<p>6% (red), 64% (green), 16% (yellow), 20% (grey)</p>
1	B	1256	<p>8% (red), 66% (green), 14% (yellow), 20% (grey)</p>
1	C	1256	<p>10% (red), 67% (green), 13% (yellow), 20% (grey)</p>
2	H	223	<p>42% (red), 42% (green), 11% (yellow), 47% (grey)</p>

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Mol	Chain	Length	Quality of chain
2	M	223	<p>46% 38% 15% 47%</p>
3	L	219	<p>44% 41% 10% 49%</p>
3	N	219	<p>45% 39% 11% 49%</p>
4	D	2	<p>100%</p>
4	E	2	<p>100%</p>
4	F	2	<p>50% 50%</p>
4	G	2	<p>100%</p>
4	I	2	<p>100%</p>
4	J	2	<p>100%</p>
4	K	2	<p>50% 50%</p>
4	O	2	<p>50% 50%</p>
4	P	2	<p>100%</p>

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 27822 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
			Total	C	N	O	S		
1	A	1011	7896	5044	1312	1505	35	0	0
1	B	1011	7896	5044	1312	1505	35	0	0
1	C	1011	7896	5044	1312	1505	35	0	0

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	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	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	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	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	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	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 M8b-B8 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	118	894	569	142	178	5	0	0
2	M	118	894	569	142	178	5	0	0

- Molecule 3 is a protein called M8b-B8 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	111	830	516	139	171	4	0	0
3	N	111	830	516	139	171	4	0	0

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



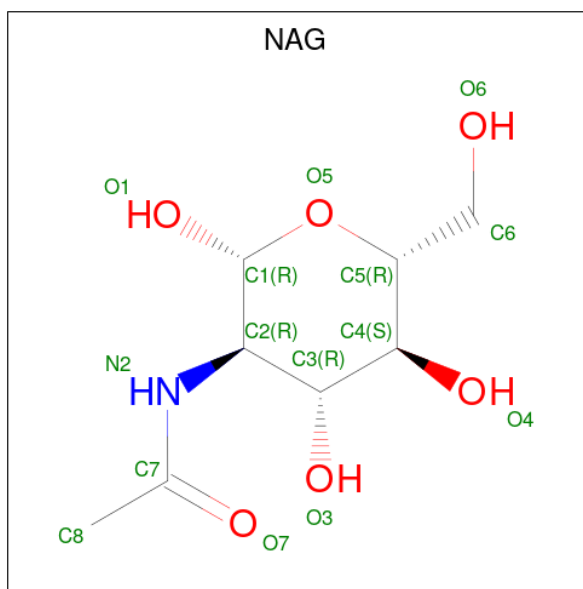
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	2	Total 28	C 16	N 2	O 10	0	0
4	F	2	Total 28	C 16	N 2	O 10	0	0
4	G	2	Total 28	C 16	N 2	O 10	0	0
4	I	2	Total 28	C 16	N 2	O 10	0	0
4	J	2	Total 28	C 16	N 2	O 10	0	0
4	K	2	Total 28	C 16	N 2	O 10	0	0
4	O	2	Total 28	C 16	N 2	O 10	0	0
4	P	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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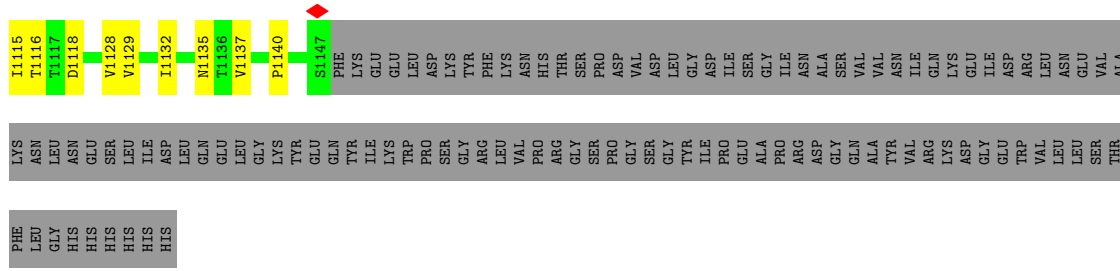
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	Total 14	8	1	5	0
5	A	1	Total 14	8	1	5	0
5	A	1	Total 14	8	1	5	0
5	A	1	Total 14	8	1	5	0
5	A	1	Total 14	8	1	5	0
5	A	1	Total 14	8	1	5	0
5	A	1	Total 14	8	1	5	0
5	A	1	Total 14	8	1	5	0
5	A	1	Total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

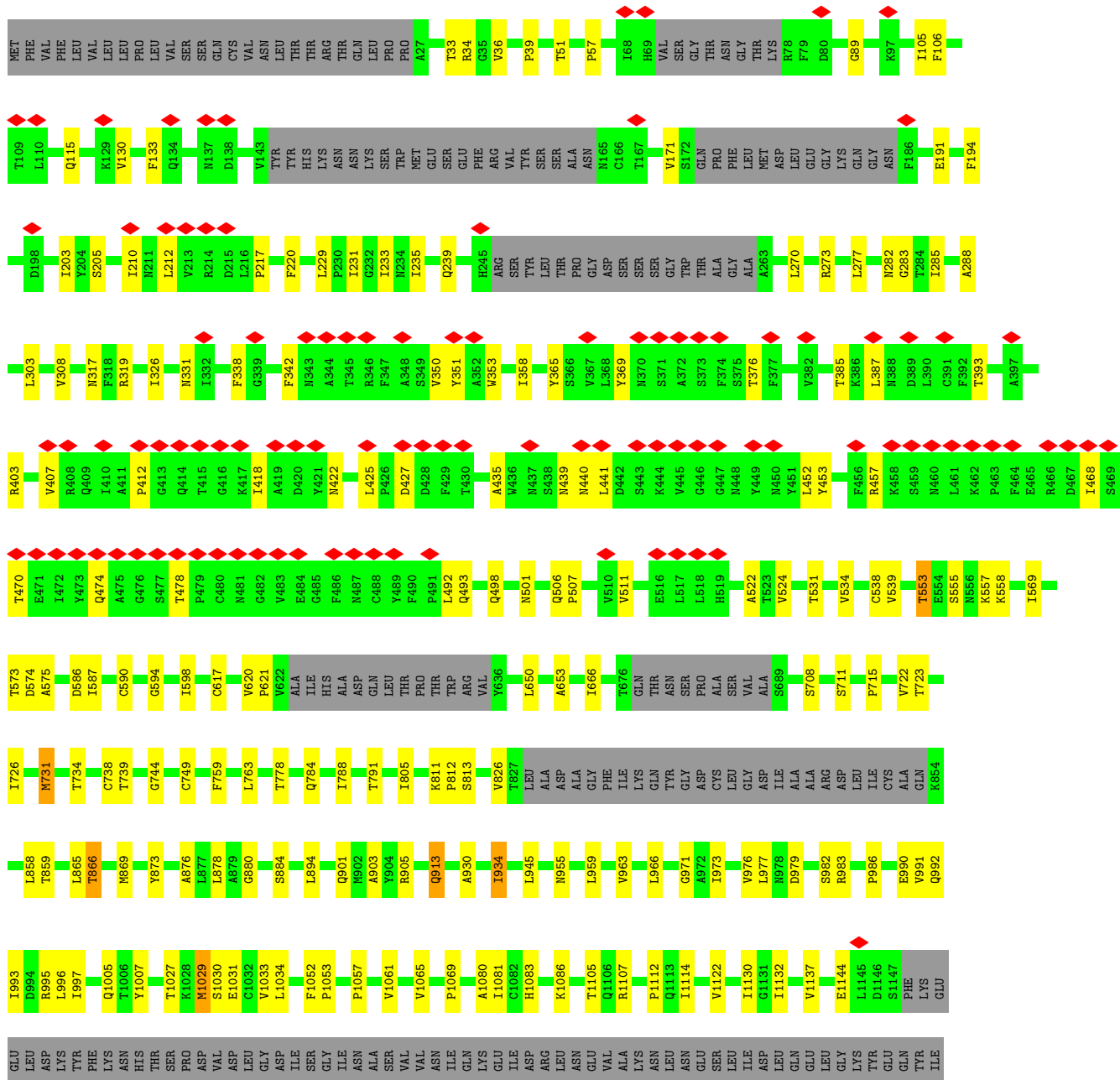
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0



• Molecule 1: Spike glycoprotein



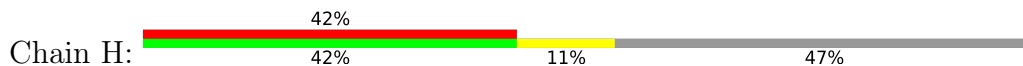
LYS	TRP	PHE	PRO	SER	GLY	ARG	LEU	VAL	PRO	PRO	ARG	GLY	TYR	PRO	GLY	PRO	GLY	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	LEU	SER	THR	THR	PHE	LEU	GLY	LEU	GLY	HIS	HIS	HIS	HIS	HIS	HIS
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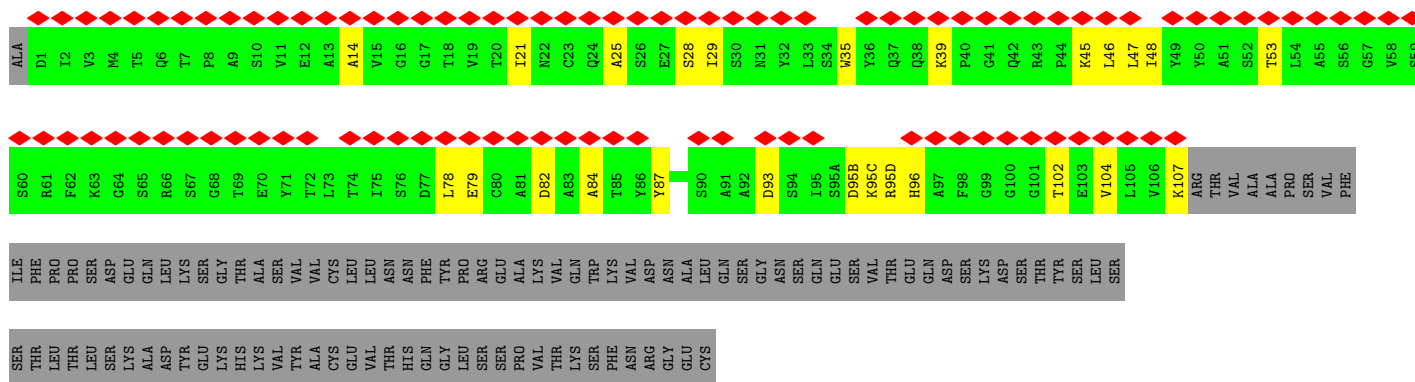
• Molecule 1: Spike glycoprotein



MET	PHE	VAL	PHE	LEU	VAL	LEU	VAL	LEU	PRO	PRO	LEU	VAL	VAL	SER	SER	PRO	GLY	SER	GLY	ILE	ASN	TYR	THR	THR	GLU	ALA	ARG	PRO	PRO	GLY	ALA	ALA	ALA	ASP	GLN	VAL	SER	GLY	LEU	LEU	SER	THR	THR	PHE	LEU	GLY	LEU	GLY	HIS	HIS	HIS	HIS	HIS																																										
K129	V130	C131	E132	V143	TYR	TYR	HIS	LYS	ASN	ASN	C361	LYS	SER	TRP	MET	GLU	SER	GLU	THR	PHE	ARG	VAL	VAL	TYR	THR	LEU	SER	SER	ALA	ASN	N165	F168	E169	Y170	V171	S172	GLN	PRO	PHE	LEU	LEU	MET	ASP	GLY	LEU	GLY	LYS	GLN	GLY	ASN	F186	V193	I197	F206	T210	N211	L212	V213	R214																																				
D215	L216	P217	S221	A222	L223	T231	G232	L233	R237	F238	Q239	T240	A243	L244	H245	ARG	SER	TYR	LEU	THR	THR	PRO	GLY	ASP	SER	SER	GLY	SER	GLY	A263	V267	T274	V289	D290	C291	S297	F306	V327	R328	F338	F342	T345	R346	V350	N354	R355	K356	R357	N360	V362	L368	F369	N370	S371	A372	S373	F374	S375	T376	F377	K378	C379	Y380	G382	S383	P384	T385	K386	L387	N388	D389	L390	C391	F392	T393	A397	D398	S399	F400	R403	G404	D405	E406	V407	R408	Q409	I410	A411	P412	G413	Q414	T415	G416	K417	I418
A419	D420	K424	L425	F426	D427	D428	C432	V433	I434	A435	A436	N437	S438	N439	N440	L441	D442	S443	K444	V445	G446	G447	N448	Y449	N450	Y451	L452	Y453	R454	L455	F456	R457	K458	S459	N460	L461	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	S477	T478	P479	C480	N481	G482	V483	E484	G485																																							
F486	N487	C488	Y489	F490	P491	L492	Q493	S494	Y495	G496	F497	Q498	P499	T500	N501	G502	V503	G504	Y505	G506	P507	Y508	R509	V512	E516	L517	L518	H519	A520	P521	A522	T523	Y524	C525	G526	P527	K528	N542	T547	S469	T553	E471	L560	R567	D571	T572	A575	P579	T584																																														
I598	V622	ALA	ILE	HIS	ASP	ALA	LEU	THR	PRO	THR	TRP	ARG	VAL	Y636	L650	A653	I664	A668	A672	T676	GLN	THR	ASN	SER	ALA	PRO	ALA	ALA	SER	VAL	ALA	S689	M697	S698	L699	F715	T723	I726	I742	C749	L752	F759	L763																																																				
I770	Q774	P792	S816	E819	L822	F823	N824	K825	W826	LEU	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ILE	ALA	ALA	ARG	ASP	LEU	ALA	S689	M697	S698	L699	F715	T723	I726	I742	C749	L752	F759	L763																																																				
A930	I934	P942	L945	L948	Q949	L977	E988	A989	E990	V991	I993	I997	V1008	V1033	L1034	K1038	R1039	V1040	D1041	M1050	P1053	P1057	V1061	H1083	R1091	S1097	W1102	F1103	I1114	F1121	V1122	V1128	M1135	T1136	V1137																																																												
Q1142	F1143	E1144	L1145	D1146	S1147	PHE	LYS	GLU	GLU	GLU	LEU	ASP	LYS	TYR	PHE	ARG	LEU	VAL	ASN	HIS	THR	SER	PRO	PRO	ASP	GLY	VAL	ASP	GLY	LEU	GLY	ASP	ILE	ALA	VAL	VAL	ASN	ILE	GLN	LYS	CYS	ALA	GLN	GLY	ILE	ASP	ARG	TRP	VAL	LEU	LEU	ASN	VAL	VAL	ALA	LYS	ASN	GLY	LEU	HIS	HIS	HIS	HIS	HIS	HIS	GLN																													
GLU	LEU	GLY	LYS	TYR	GLU	GLN	TYR	LYS	ILE	LEU	TRP	PRO	SER	SER	GLY	ARG	VAL	VAL	ASN	PRO	ARG	GLY	SER	PRO	PRO	GLY	GLY	TYR	ILE	ILE	ASP	ILE	ALA	VAL	VAL	ASN	ILE	GLN	ARG	LYS	ASP	GLY	GLY	TRP	VAL	VAL	LEU	LEU	ASN	VAL	THR	PHE	LEU	GLY	HIS	HIS	HIS	HIS	HIS	HIS	GLN																																		

• Molecule 2: M8b-B8 heavy chain





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

Chain D:  100%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain F:  50% 50%


MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain O:  50% 50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.070	Depositor
Minimum map value	-0.700	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	312.84, 312.84, 312.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.869, 0.869, 0.869	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	0.13	0/8078	0.32	0/10997
1	B	0.13	0/8078	0.30	0/10997
1	C	0.13	0/8078	0.29	1/10997 (0.0%)
2	H	0.12	0/918	0.38	0/1252
2	M	0.10	0/918	0.34	0/1252
3	L	0.08	0/844	0.24	0/1145
3	N	0.09	0/844	0.25	0/1145
All	All	0.13	0/27758	0.30	1/37785 (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	C	130	VAL	N-CA-C	-6.00	105.90	112.80

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	7697	125	0
1	B	7896	0	7702	118	0
1	C	7896	0	7700	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	894	0	850	17	0
2	M	894	0	850	21	0
3	L	830	0	808	15	0
3	N	830	0	808	18	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	1	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	O	28	0	25	2	0
4	P	28	0	25	0	0
5	A	196	0	182	1	0
5	B	98	0	91	0	0
5	C	140	0	130	0	0
All	All	27822	0	27043	392	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 7.

The worst 5 of 392 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:ILE:HG23	2:H:62:TRP:HB3	1.47	0.96
1:A:1116:THR:HG22	1:A:1118:ASP:H	1.47	0.79
1:B:498:GLN:HB3	1:B:501:ASN:HB2	1.68	0.75
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.69	0.74
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.70	0.74

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	995/1256 (79%)	962 (97%)	33 (3%)	0	100	100
1	B	995/1256 (79%)	960 (96%)	35 (4%)	0	100	100
1	C	995/1256 (79%)	955 (96%)	40 (4%)	0	100	100
2	H	116/223 (52%)	108 (93%)	8 (7%)	0	100	100
2	M	116/223 (52%)	110 (95%)	6 (5%)	0	100	100
3	L	109/219 (50%)	104 (95%)	5 (5%)	0	100	100
3	N	109/219 (50%)	104 (95%)	5 (5%)	0	100	100
All	All	3435/4652 (74%)	3303 (96%)	132 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	887/1096 (81%)	876 (99%)	11 (1%)	63	72
1	B	887/1096 (81%)	869 (98%)	18 (2%)	48	65
1	C	887/1096 (81%)	874 (98%)	13 (2%)	57	69
2	H	95/186 (51%)	95 (100%)	0	100	100
2	M	95/186 (51%)	93 (98%)	2 (2%)	47	64
3	L	90/186 (48%)	90 (100%)	0	100	100
3	N	90/186 (48%)	90 (100%)	0	100	100
All	All	3031/4032 (75%)	2987 (98%)	44 (2%)	55	69

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1130	ILE
1	C	949	GLN

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Mol	Chain	Res	Type
1	C	33	THR
1	C	723	THR
1	C	1033	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	957	GLN
1	C	211	ASN
1	C	188	ASN
1	C	370	ASN
1	A	675	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](#)

18 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
4	NAG	D	1	1,4	14,14,15	0.79	0	17,19,21	2.45	4 (23%)
4	NAG	D	2	4	14,14,15	0.71	0	17,19,21	0.96	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.79	0	17,19,21	1.38	3 (17%)
4	NAG	E	2	4	14,14,15	0.81	1 (7%)	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1	1,4	14,14,15	0.77	1 (7%)	17,19,21	2.19	3 (17%)
4	NAG	F	2	4	14,14,15	0.74	0	17,19,21	1.33	2 (11%)
4	NAG	G	1	1,4	14,14,15	0.77	0	17,19,21	1.13	1 (5%)
4	NAG	G	2	4	14,14,15	0.71	0	17,19,21	0.90	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
4	NAG	I	2	4	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.76	0	17,19,21	0.81	0
4	NAG	J	2	4	14,14,15	0.71	0	17,19,21	0.80	0
4	NAG	K	1	1,4	14,14,15	0.76	0	17,19,21	1.09	1 (5%)
4	NAG	K	2	4	14,14,15	0.72	0	17,19,21	0.88	0
4	NAG	O	1	1,4	14,14,15	0.72	0	17,19,21	0.89	0
4	NAG	O	2	4	14,14,15	0.71	0	17,19,21	0.88	0
4	NAG	P	1	1,4	14,14,15	0.73	0	17,19,21	0.80	0
4	NAG	P	2	4	14,14,15	0.73	0	17,19,21	0.79	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	D	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	C1-C2	2.08	1.55	1.52
4	E	2	NAG	C1-C2	2.01	1.55	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C2-N2-C7	8.27	133.99	122.90
4	F	1	NAG	C1-O5-C5	6.76	121.24	112.19
4	G	1	NAG	C1-O5-C5	3.41	116.75	112.19
4	F	1	NAG	O4-C4-C5	3.36	117.61	109.32
4	D	1	NAG	C1-O5-C5	3.25	116.54	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

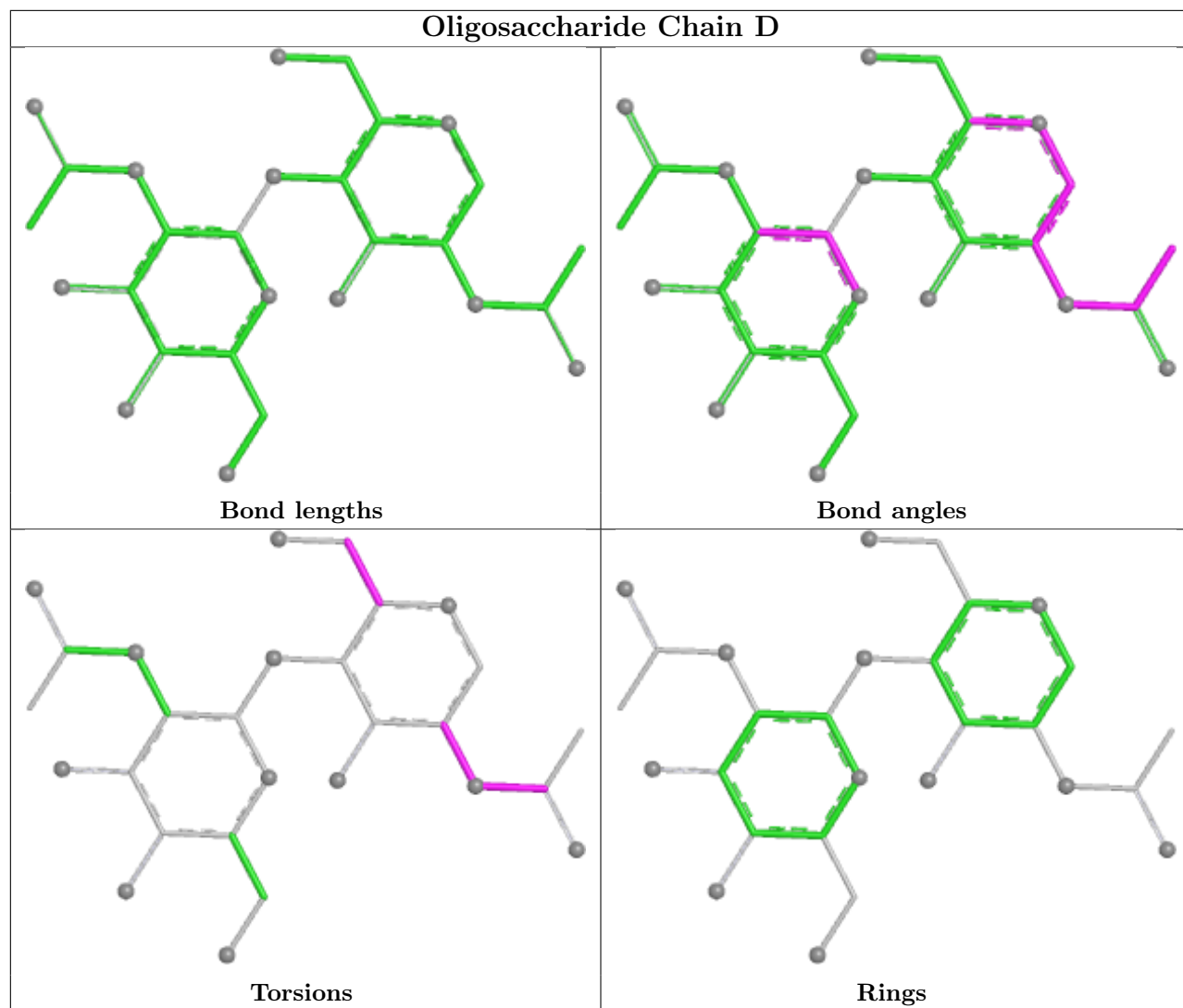
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2

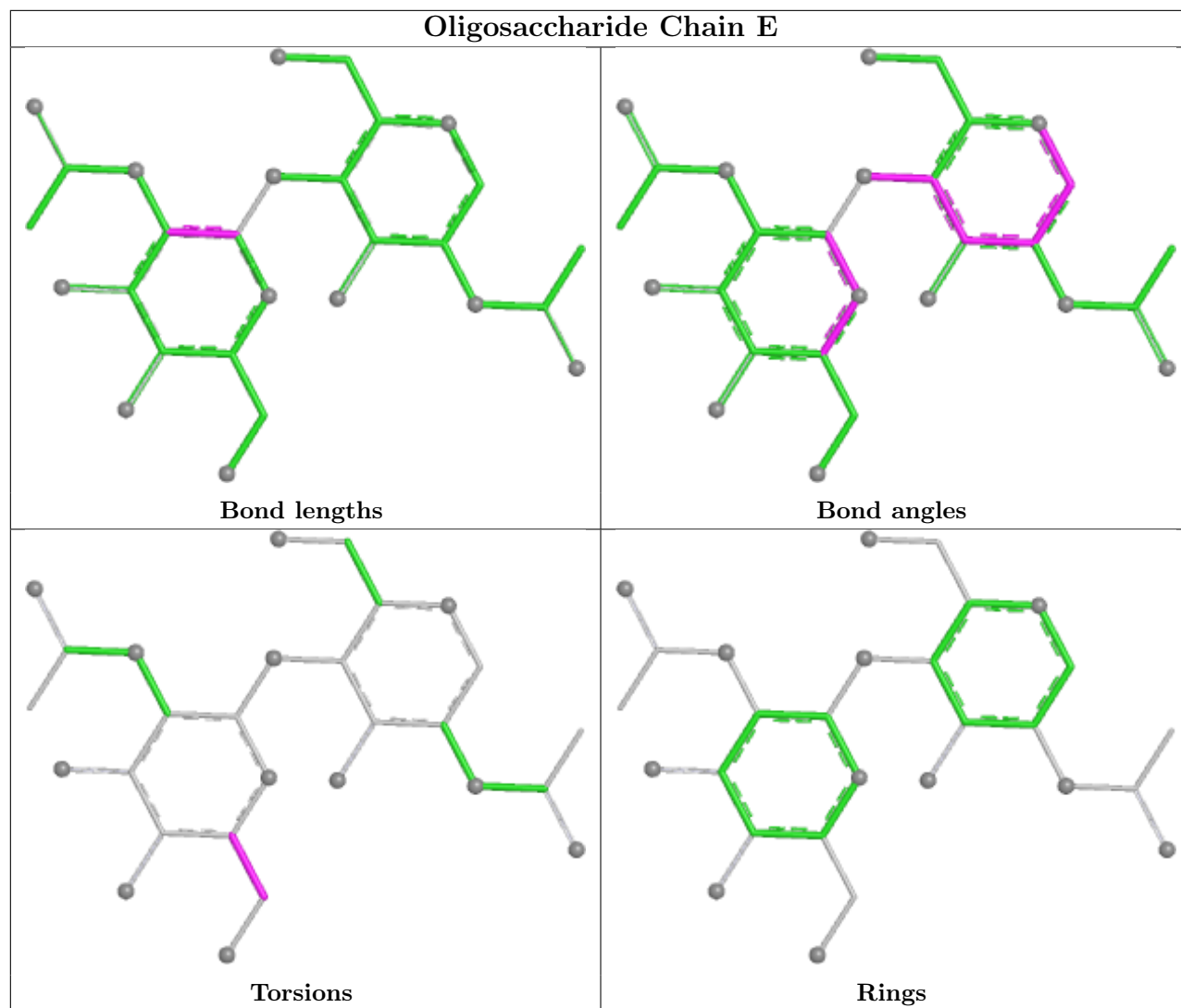
There are no ring outliers.

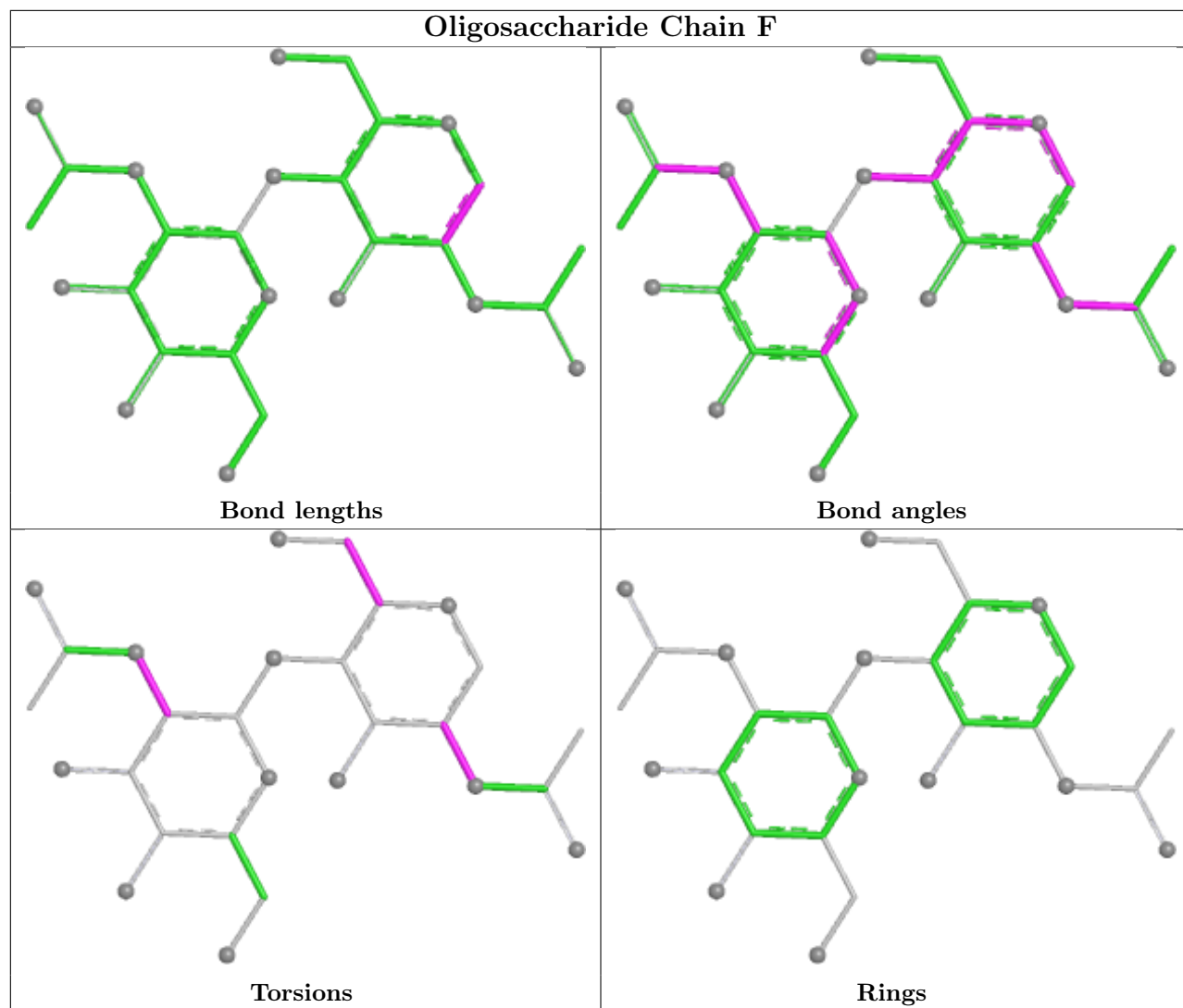
2 monomers are involved in 3 short contacts:

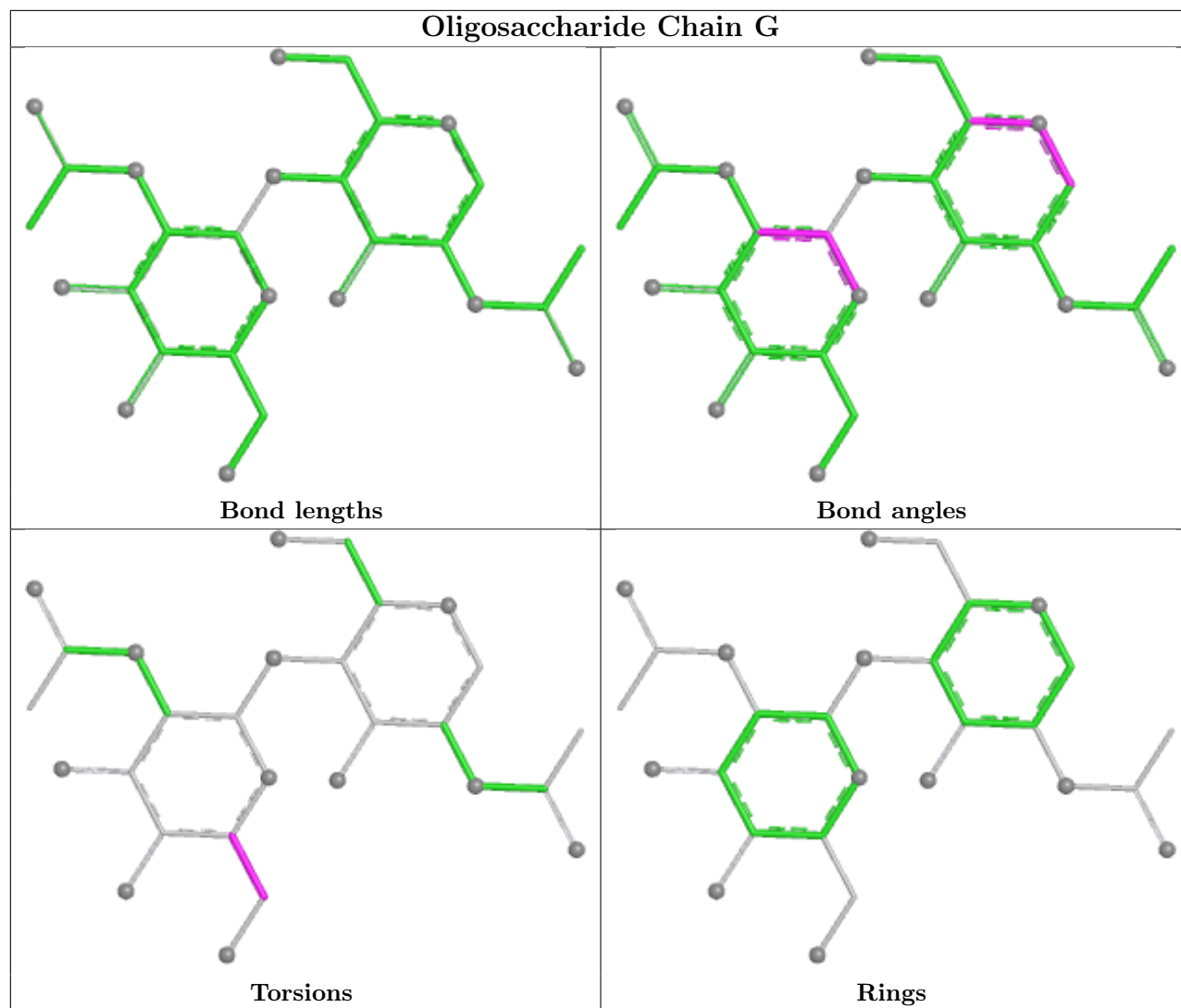
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	1	NAG	2	0
4	F	1	NAG	1	0

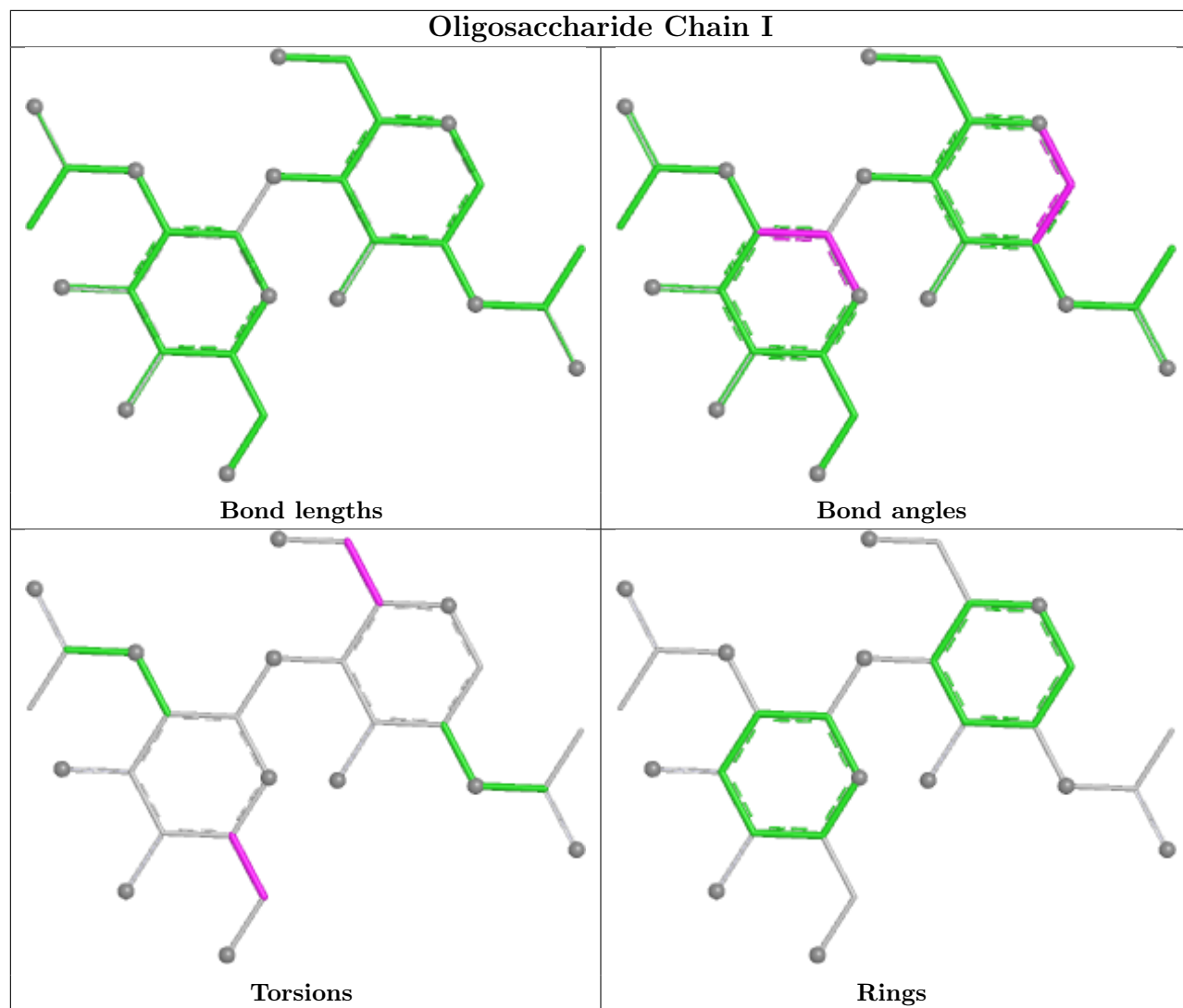
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

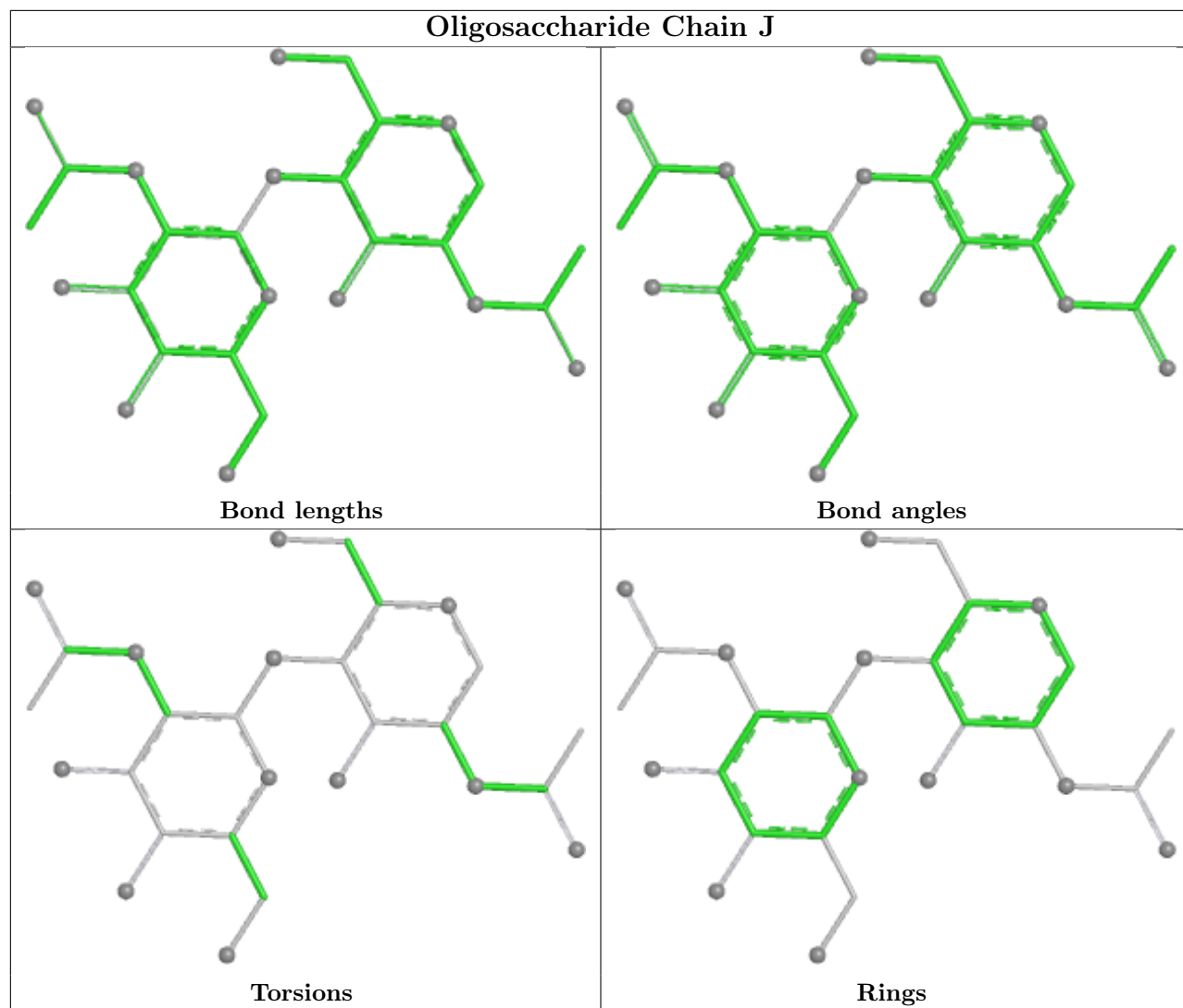


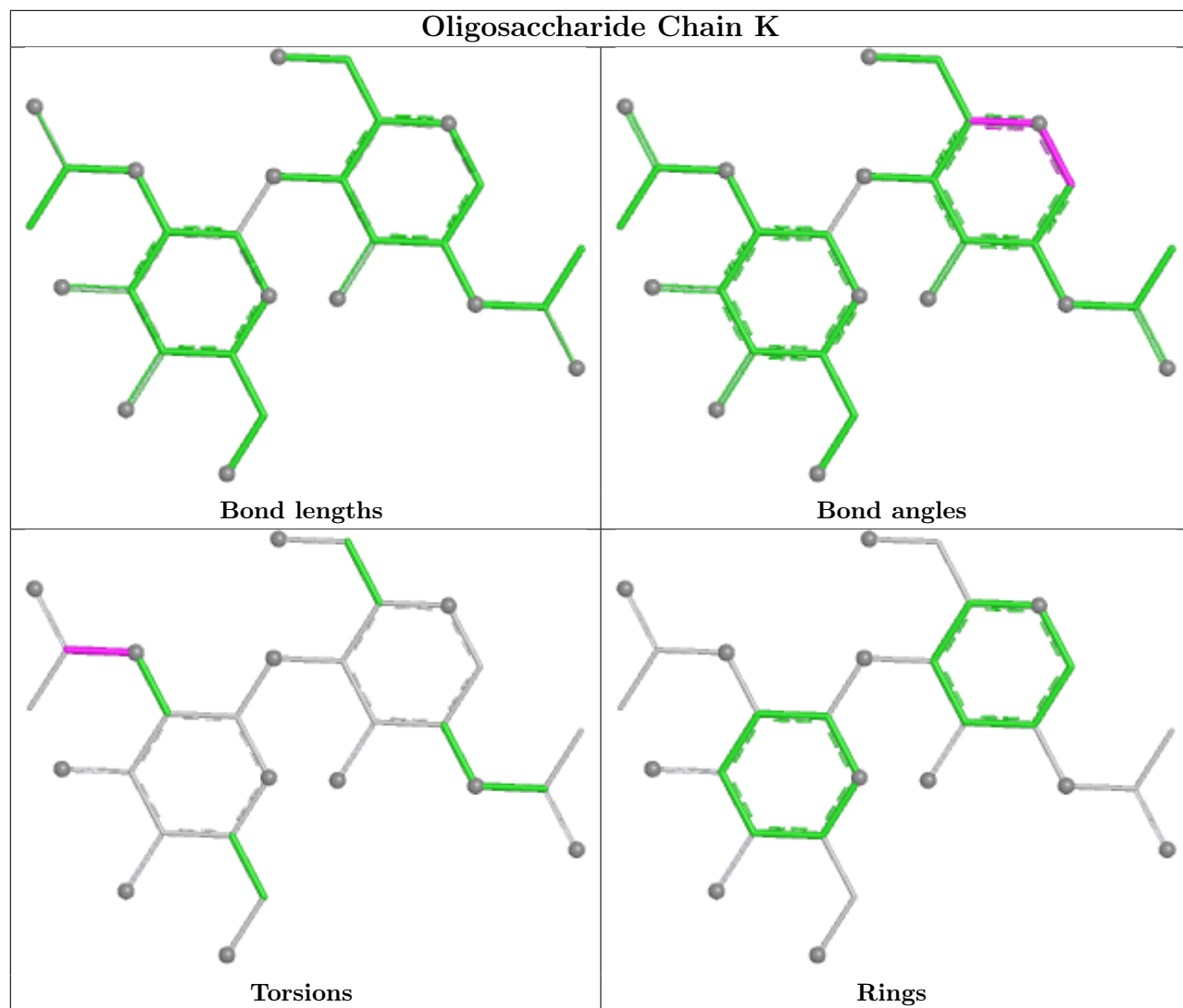


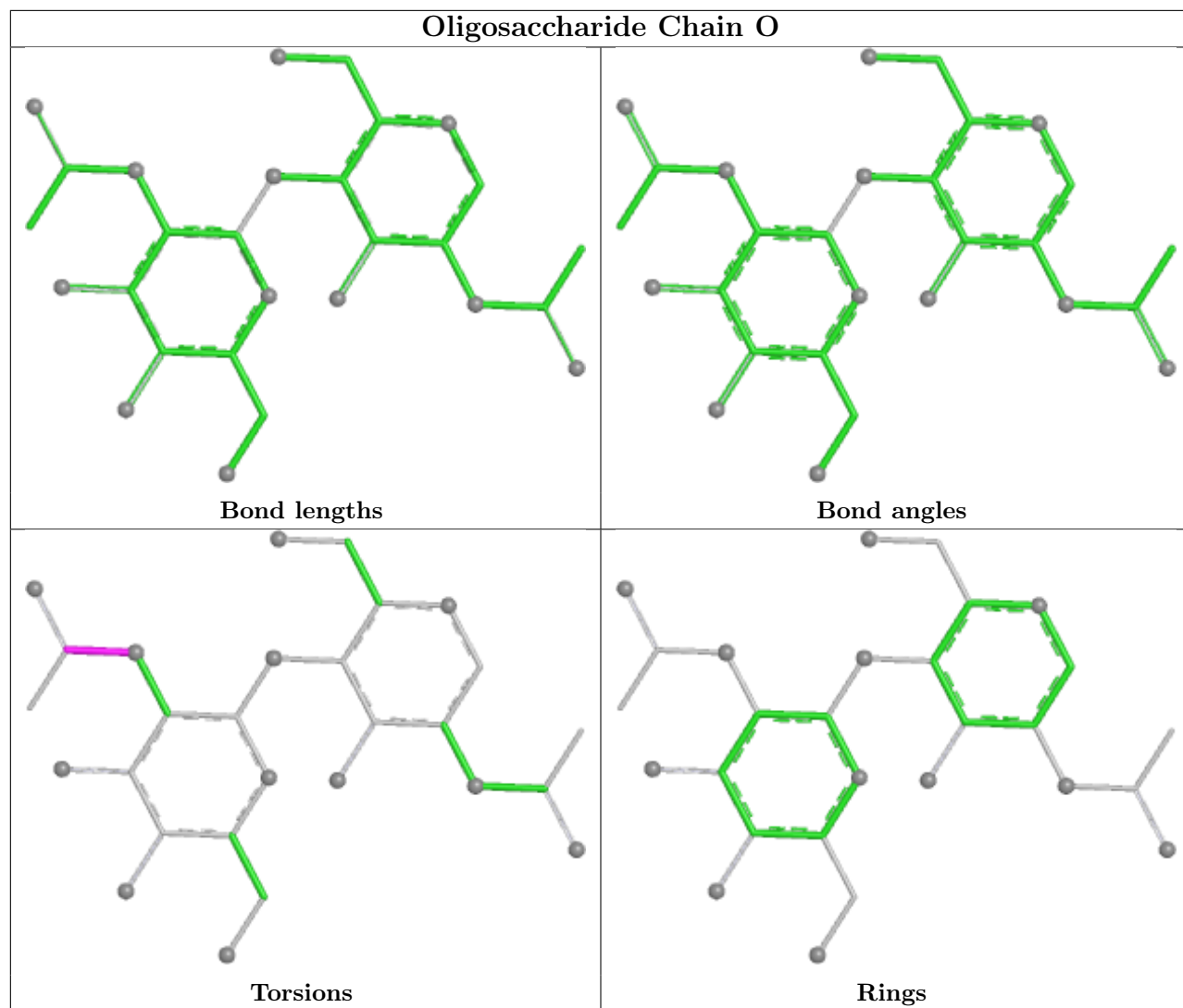


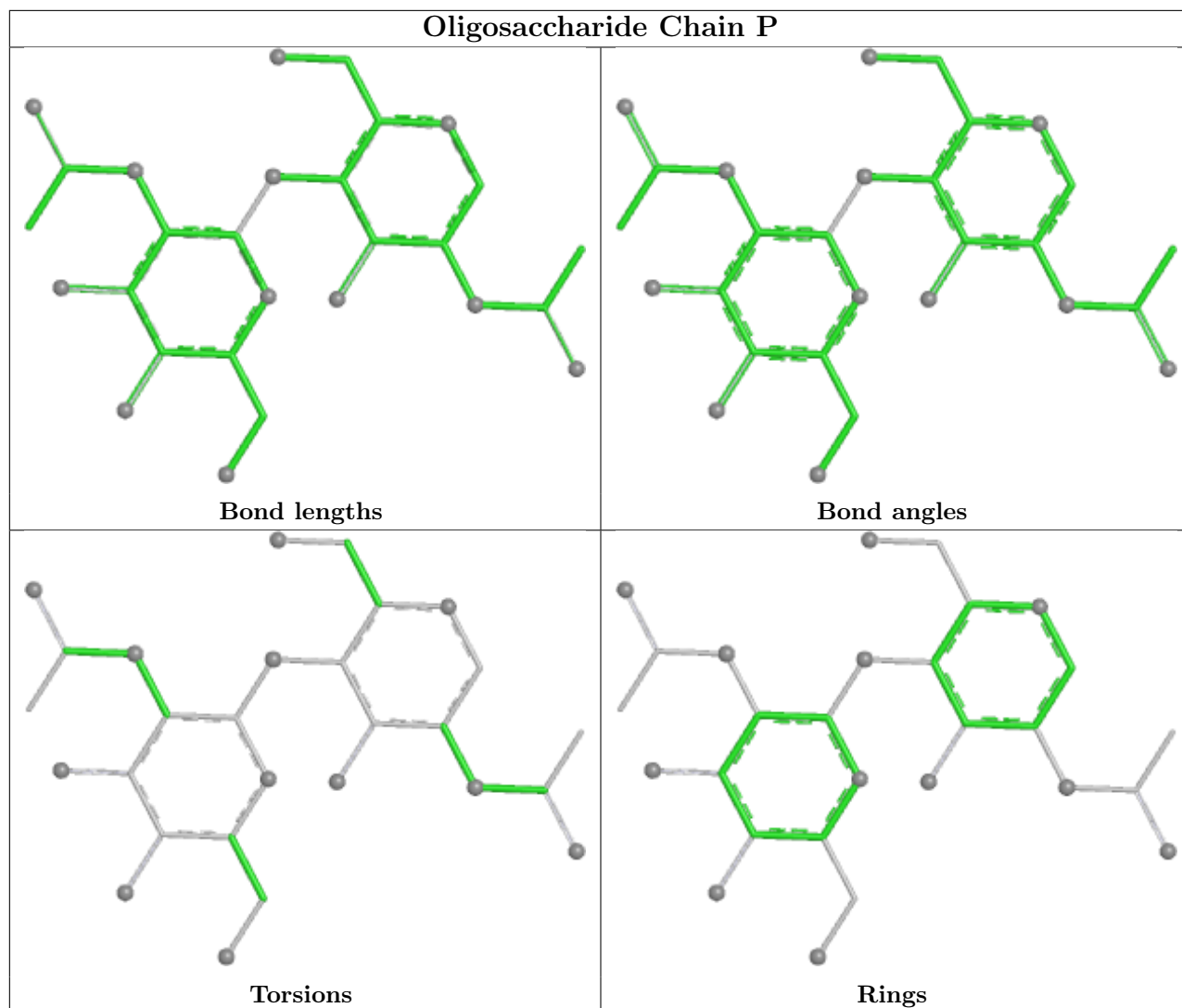












5.6 Ligand geometry [i](#)

31 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	$\# Z > 2$
5	NAG	A	1312	1	14,14,15	0.73	0	17,19,21	0.78	0
5	NAG	A	1308	1	14,14,15	0.78	0	17,19,21	0.95	1 (5%)
5	NAG	A	1307	1	14,14,15	0.69	0	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1305	1	14,14,15	0.68	0	17,19,21	2.24	3 (17%)
5	NAG	A	1309	1	14,14,15	0.72	0	17,19,21	0.78	0
5	NAG	A	1303	1	14,14,15	0.71	0	17,19,21	0.86	0
5	NAG	B	1303	1	14,14,15	0.74	0	17,19,21	0.96	1 (5%)
5	NAG	A	1311	1	14,14,15	0.71	0	17,19,21	0.79	0
5	NAG	A	1313	1	14,14,15	0.76	0	17,19,21	2.34	2 (11%)
5	NAG	C	1307	1	14,14,15	0.72	0	17,19,21	0.83	0
5	NAG	A	1304	1	14,14,15	0.77	0	17,19,21	1.12	1 (5%)
5	NAG	C	1309	1	14,14,15	0.75	0	17,19,21	2.32	3 (17%)
5	NAG	C	1302	1	14,14,15	0.71	0	17,19,21	0.85	0
5	NAG	A	1306	1	14,14,15	0.73	0	17,19,21	0.77	0
5	NAG	B	1306	1	14,14,15	0.78	0	17,19,21	2.36	3 (17%)
5	NAG	C	1301	1	14,14,15	0.75	0	17,19,21	0.85	0
5	NAG	B	1302	1	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
5	NAG	B	1307	1	14,14,15	0.74	0	17,19,21	0.82	0
5	NAG	B	1301	1	14,14,15	0.72	0	17,19,21	0.81	0
5	NAG	B	1305	1	14,14,15	0.83	1 (7%)	17,19,21	1.49	2 (11%)
5	NAG	C	1304	1	14,14,15	0.72	0	17,19,21	0.82	0
5	NAG	C	1303	1	14,14,15	0.72	0	17,19,21	0.89	0
5	NAG	A	1302	1	14,14,15	0.71	0	17,19,21	0.95	0
5	NAG	A	1301	1	14,14,15	0.71	0	17,19,21	0.83	0
5	NAG	C	1306	1	14,14,15	0.75	0	17,19,21	0.87	0
5	NAG	C	1310	1	14,14,15	0.72	0	17,19,21	0.81	0
5	NAG	C	1308	1	14,14,15	0.76	0	17,19,21	2.38	4 (23%)
5	NAG	B	1304	1	14,14,15	0.74	0	17,19,21	0.90	0
5	NAG	A	1310	1	14,14,15	0.75	0	17,19,21	0.90	0
5	NAG	A	1314	1	14,14,15	0.73	0	17,19,21	2.33	3 (17%)
5	NAG	C	1305	1	14,14,15	0.74	0	17,19,21	0.90	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
5	NAG	A	1312	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	1/6/23/26	0/1/1/1

Continued on next page...

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1305	NAG	C1-C2	2.03	1.55	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1313	NAG	C2-N2-C7	8.43	134.20	122.90
5	C	1308	NAG	C2-N2-C7	8.34	134.08	122.90
5	A	1314	NAG	C2-N2-C7	8.34	134.07	122.90
5	B	1306	NAG	C2-N2-C7	8.30	134.02	122.90
5	C	1309	NAG	C2-N2-C7	8.24	133.94	122.90

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

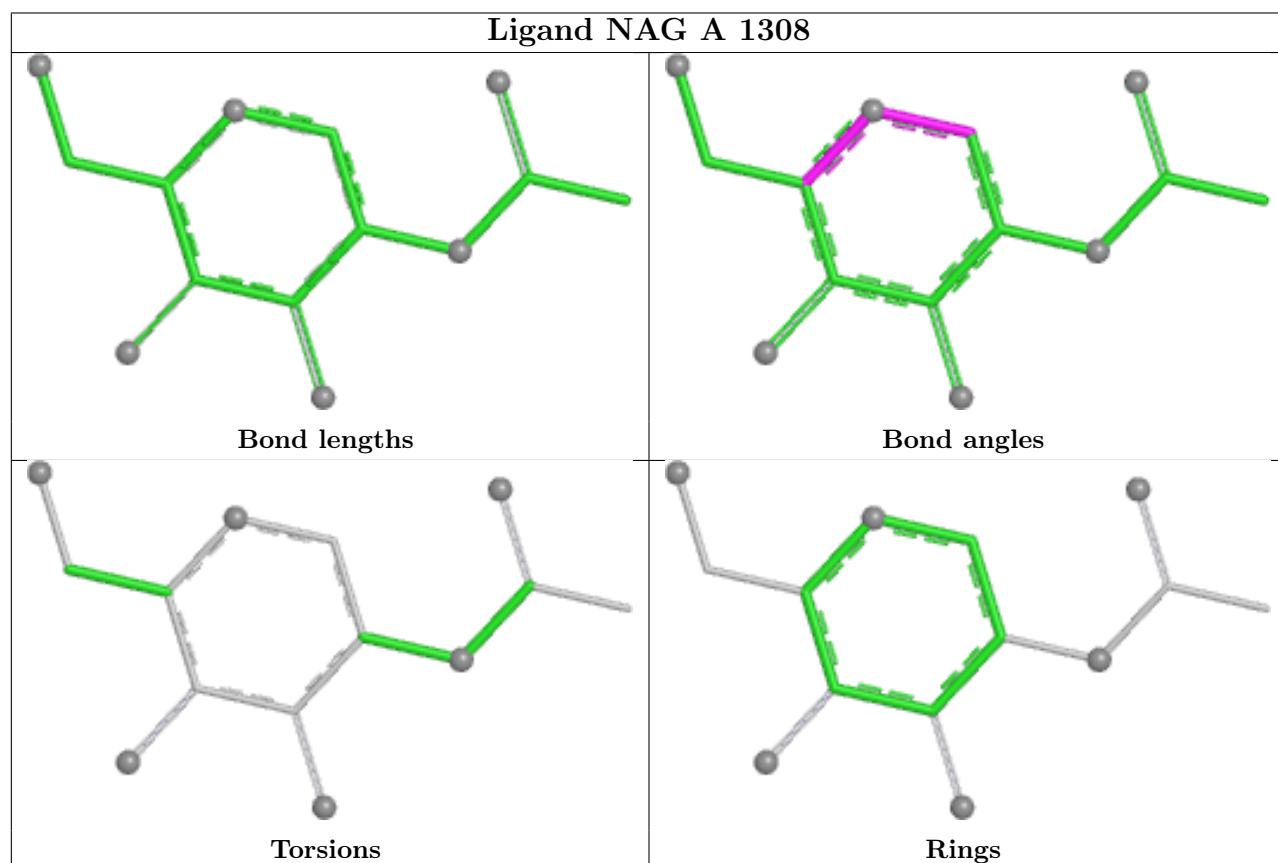
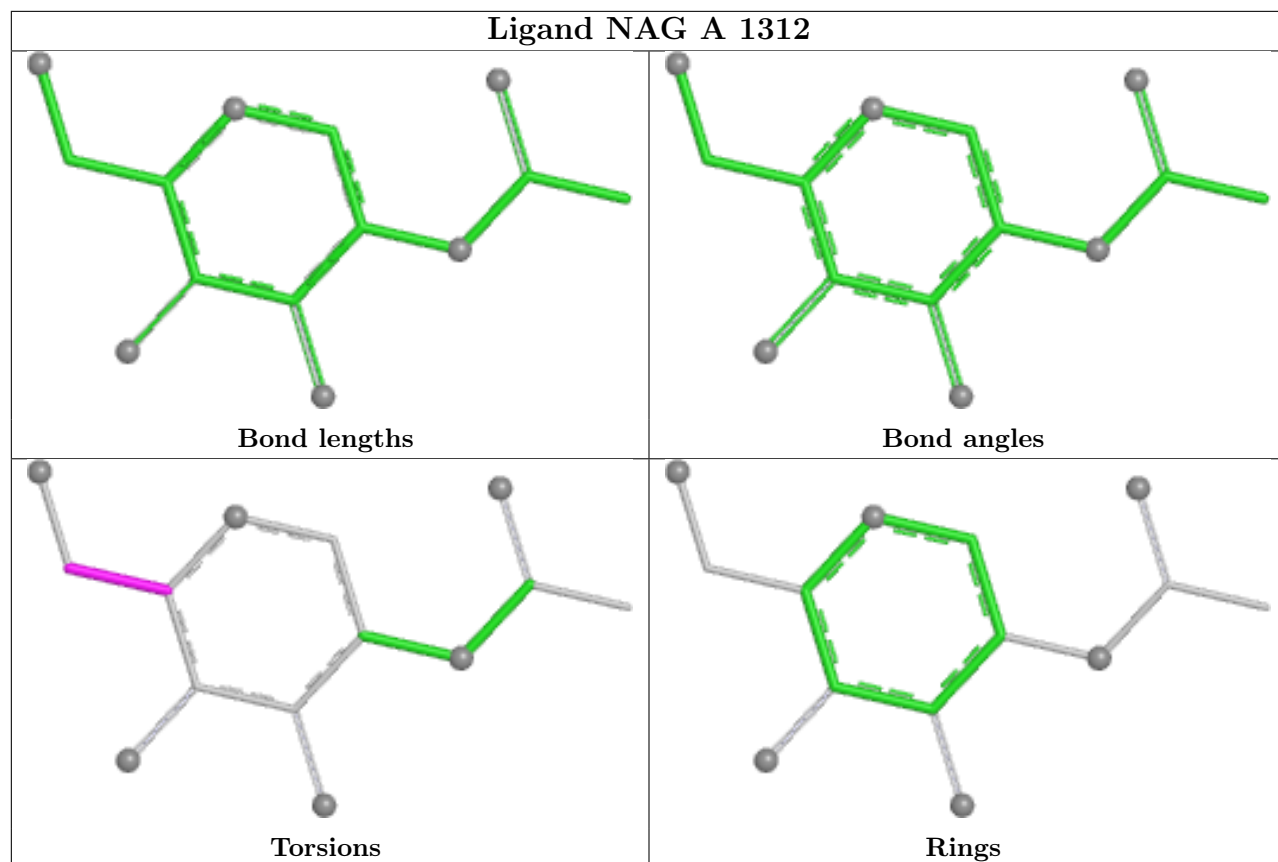
Mol	Chain	Res	Type	Atoms
5	A	1305	NAG	C3-C2-N2-C7
5	A	1302	NAG	C8-C7-N2-C2
5	A	1302	NAG	O7-C7-N2-C2
5	A	1313	NAG	C8-C7-N2-C2
5	A	1313	NAG	O7-C7-N2-C2

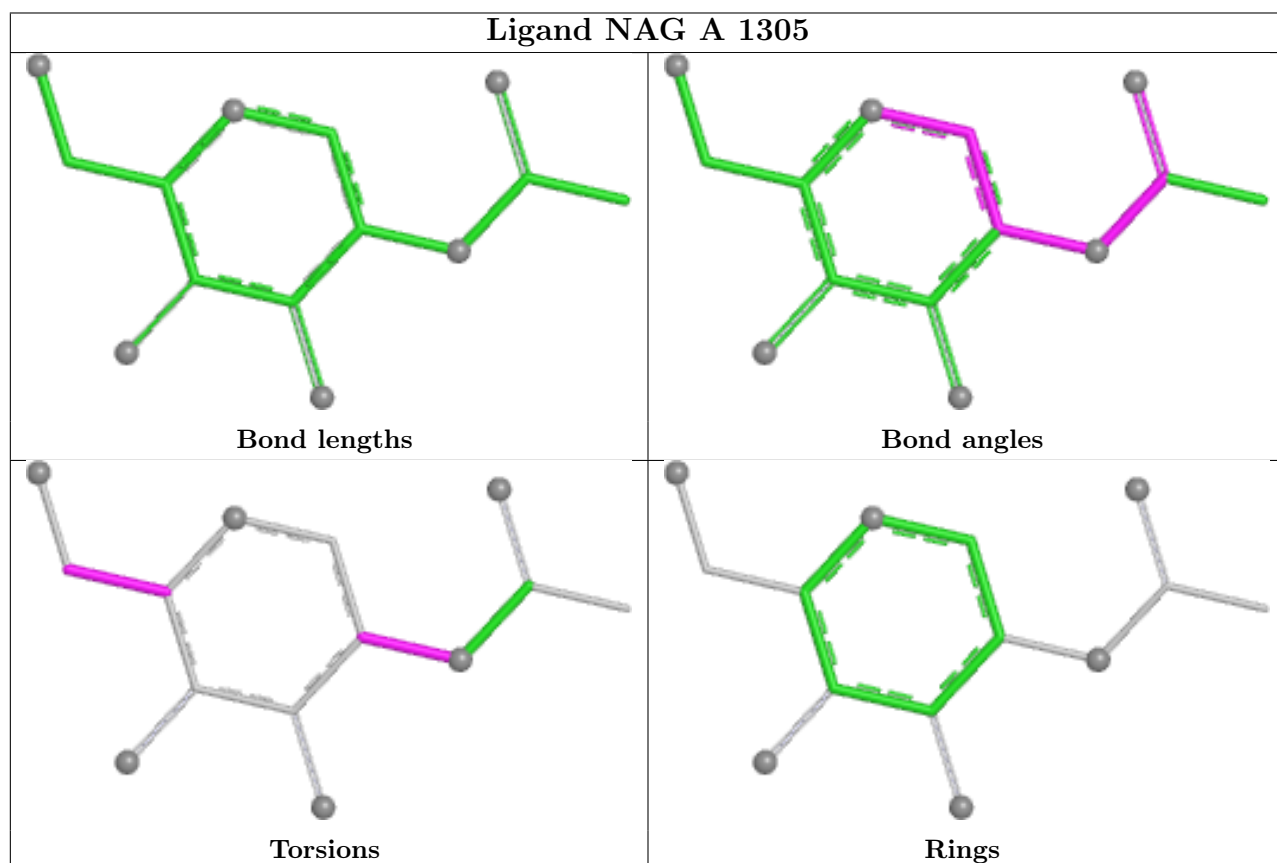
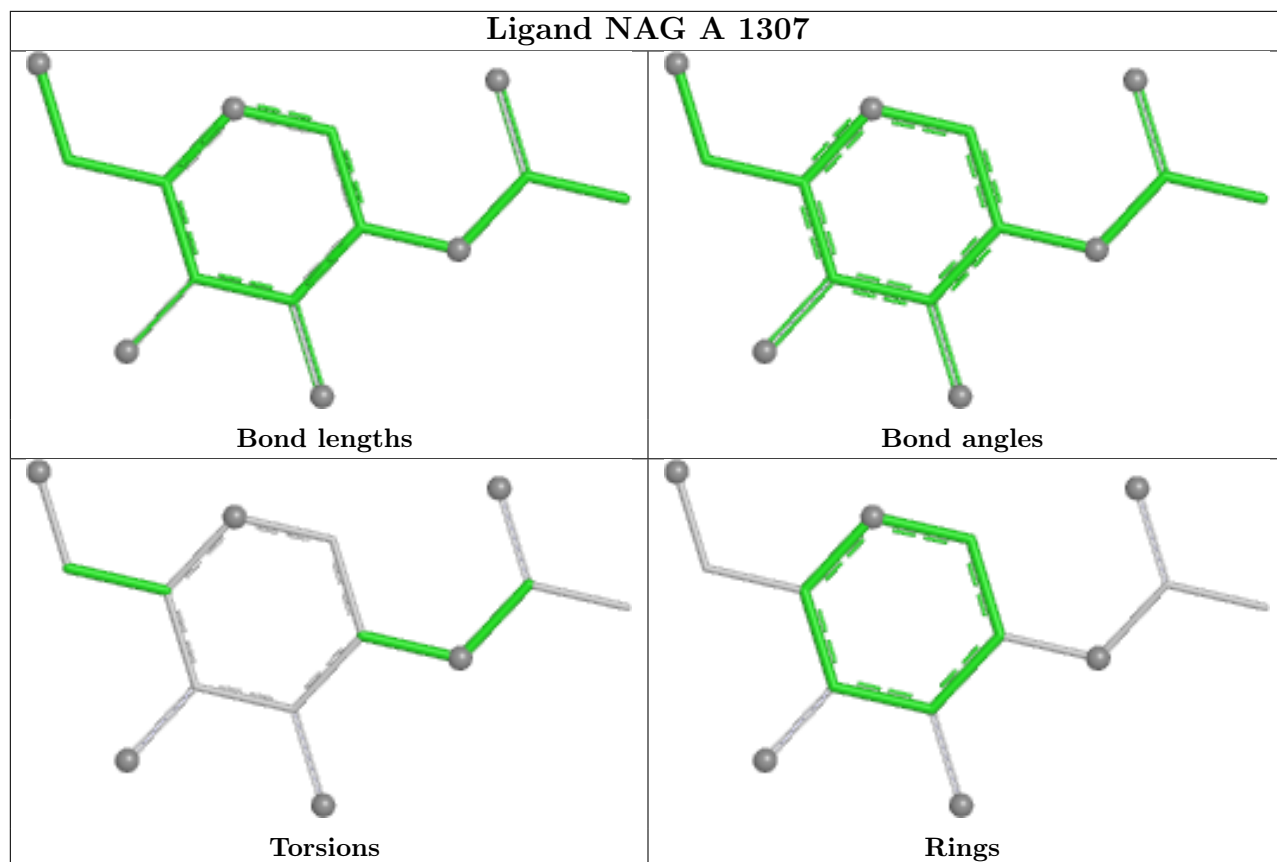
There are no ring outliers.

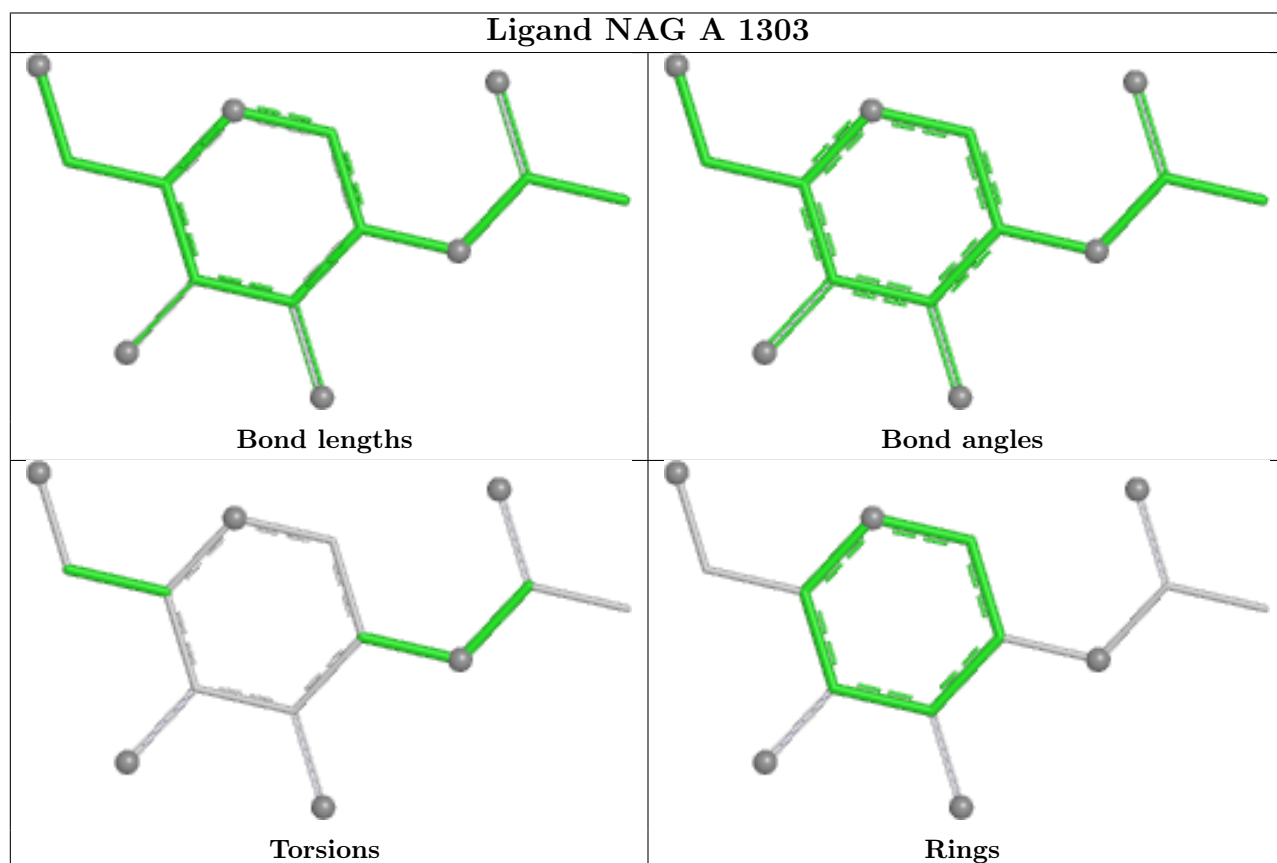
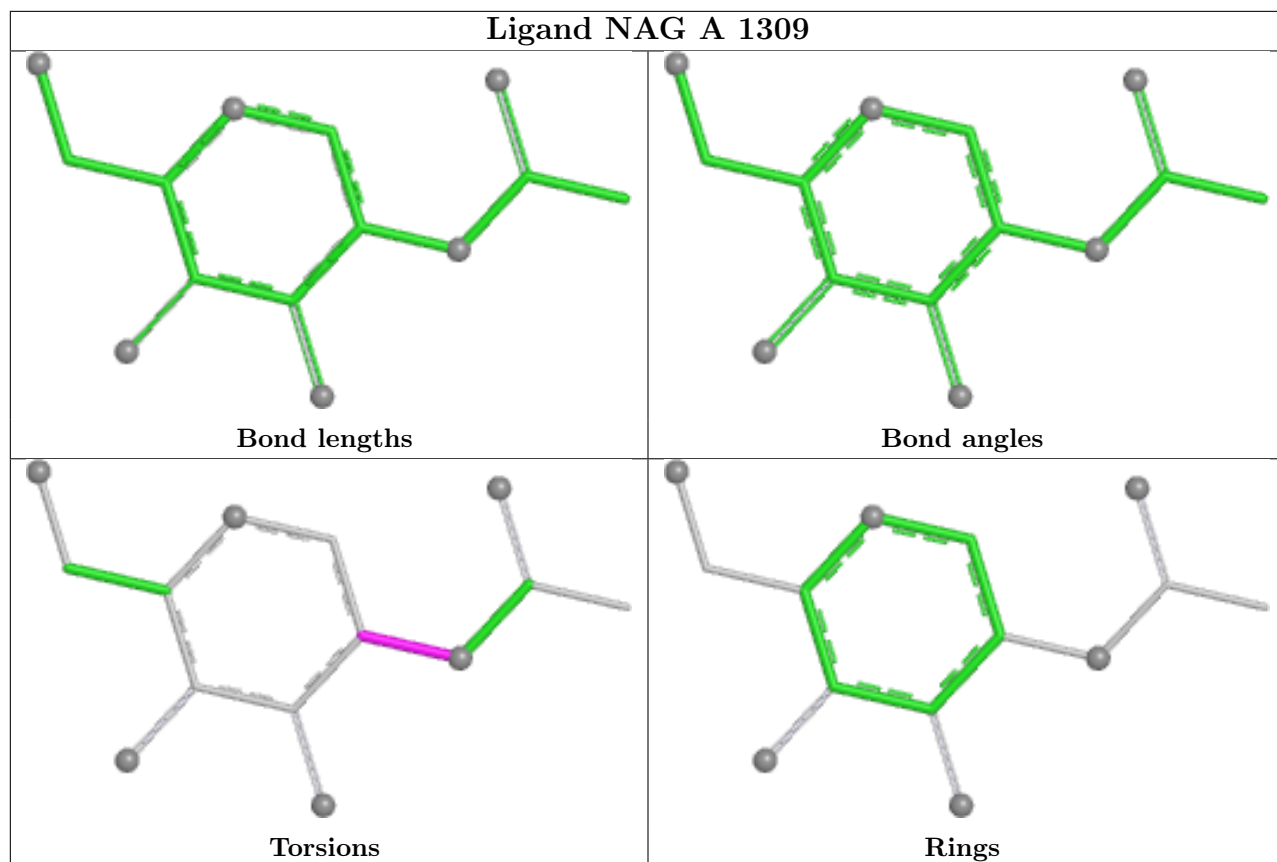
1 monomer is involved in 1 short contact:

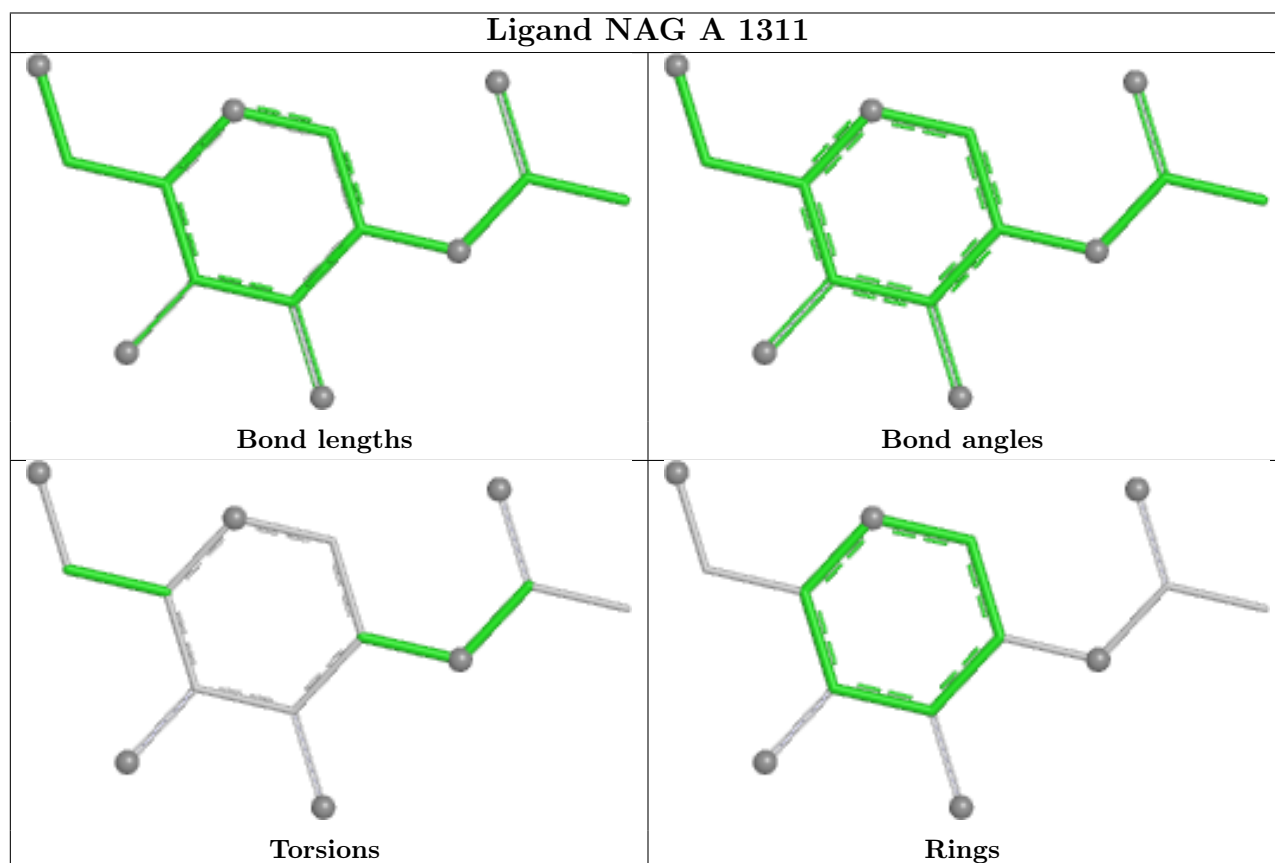
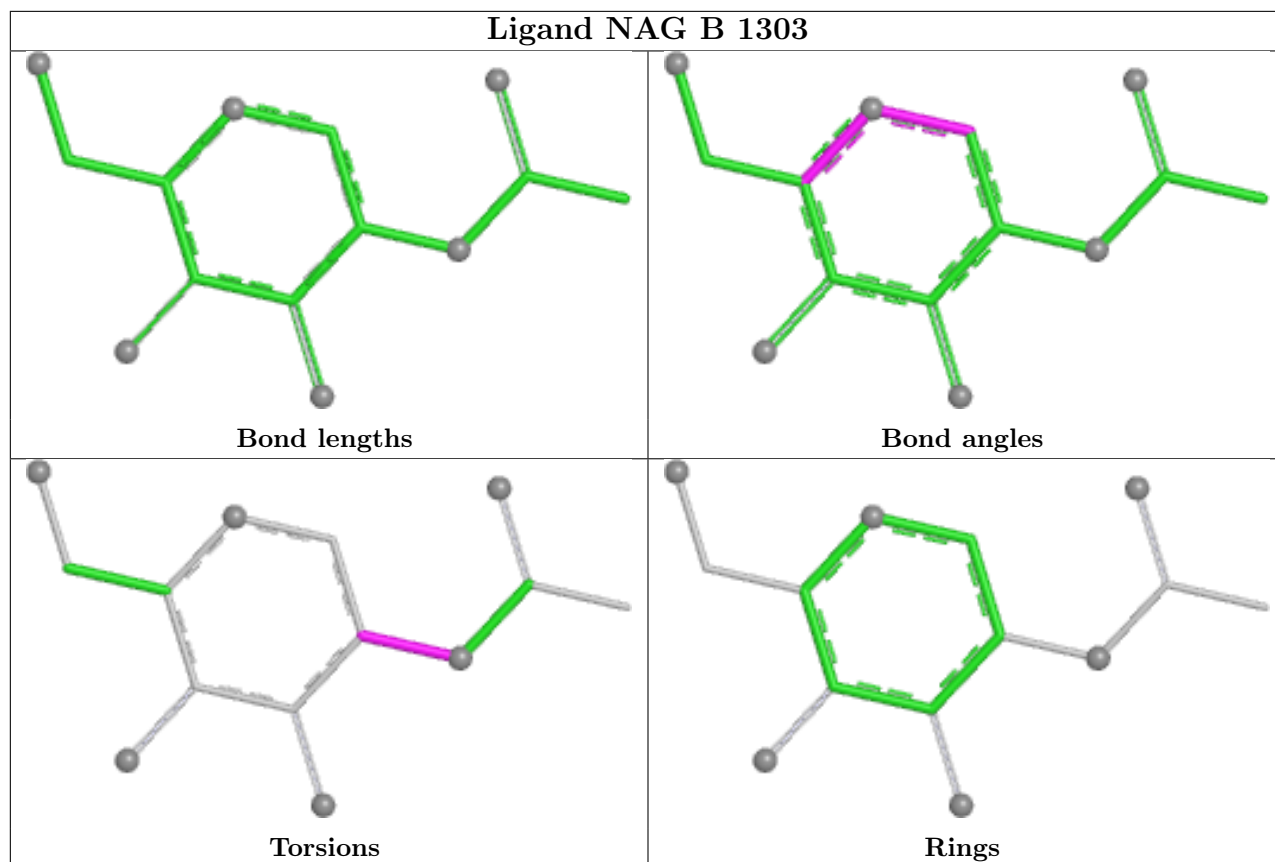
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1314	NAG	1	0

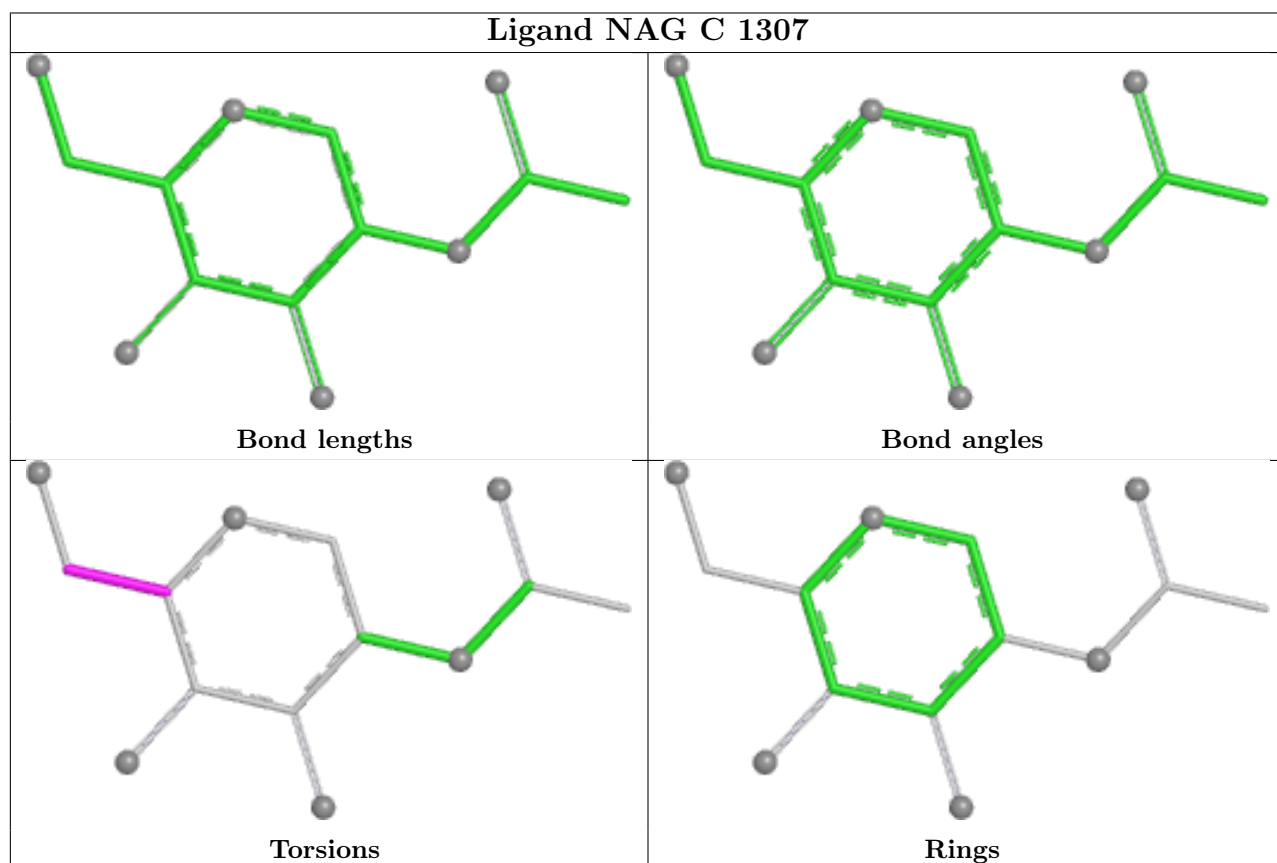
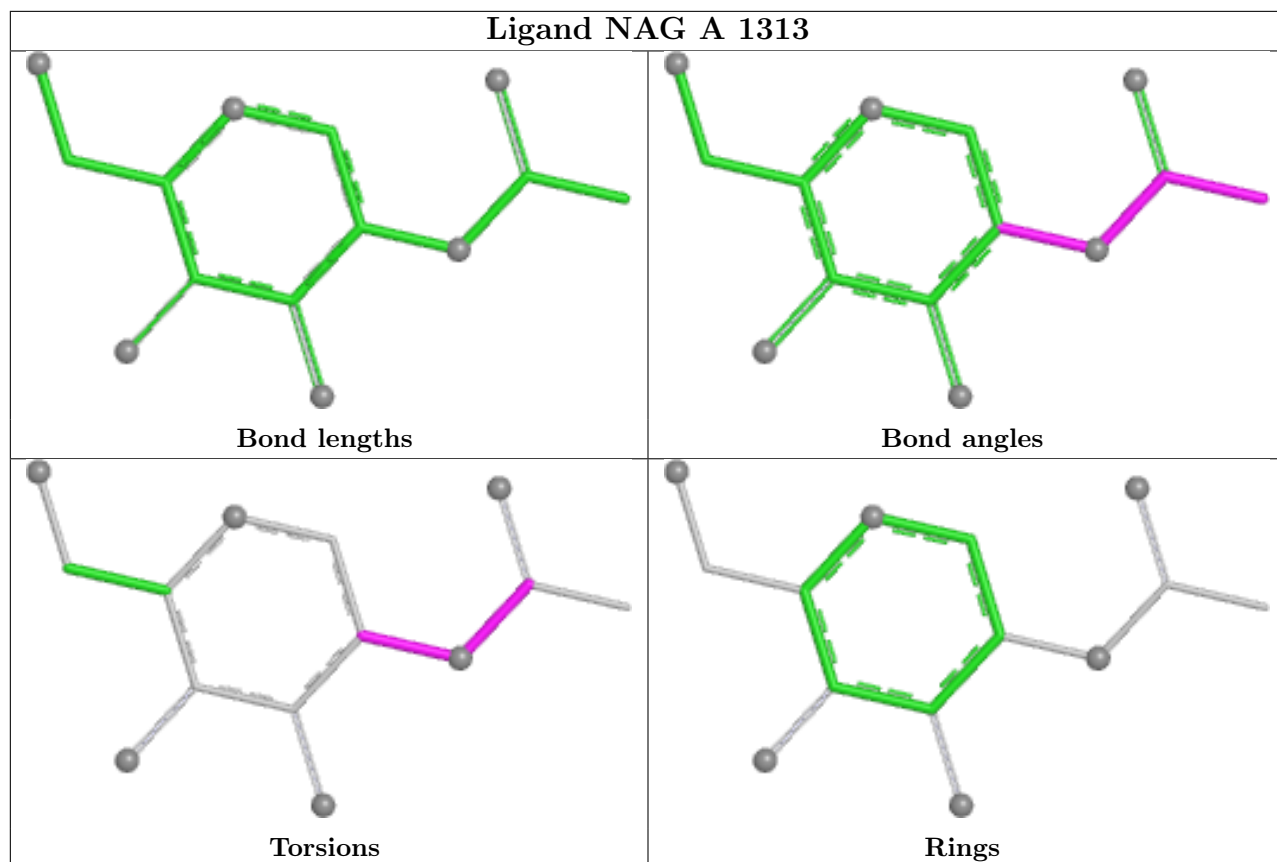
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

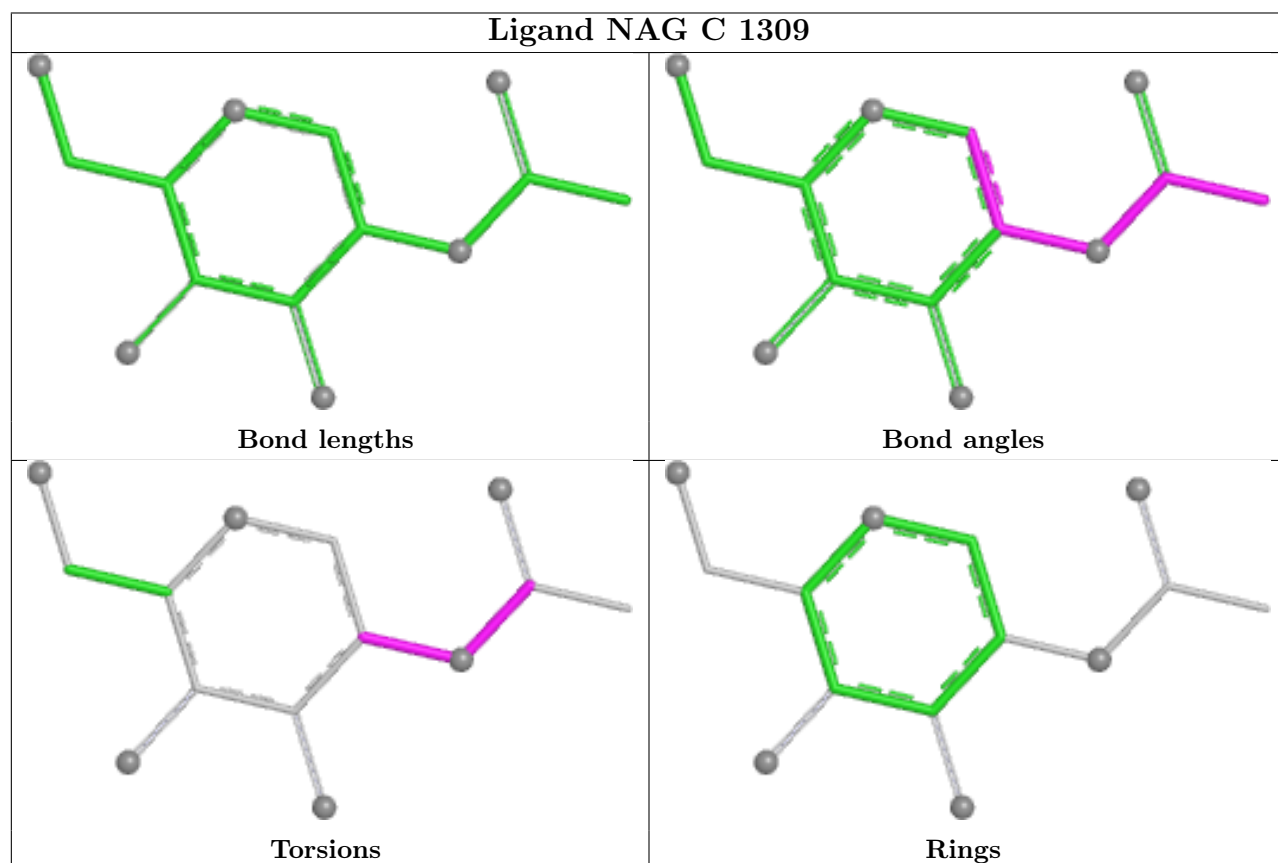
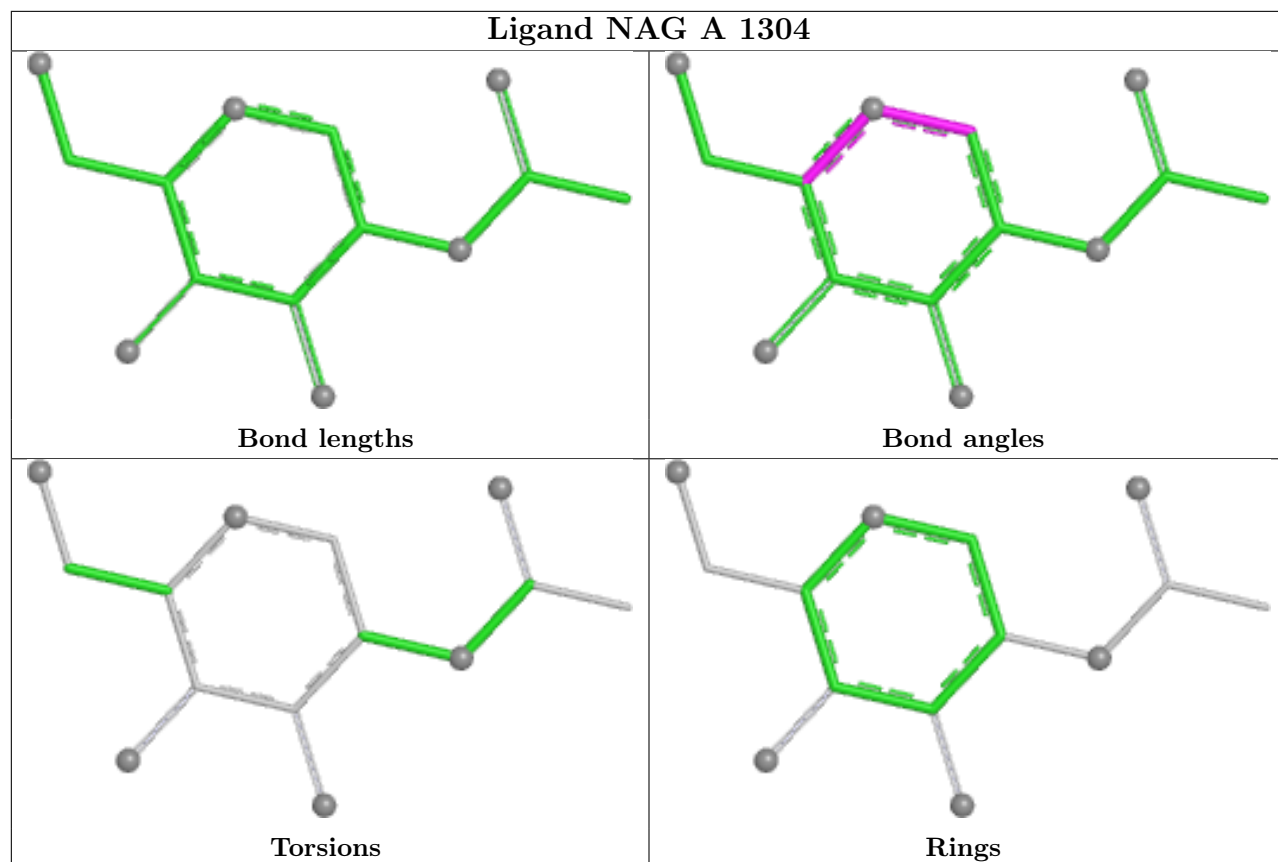


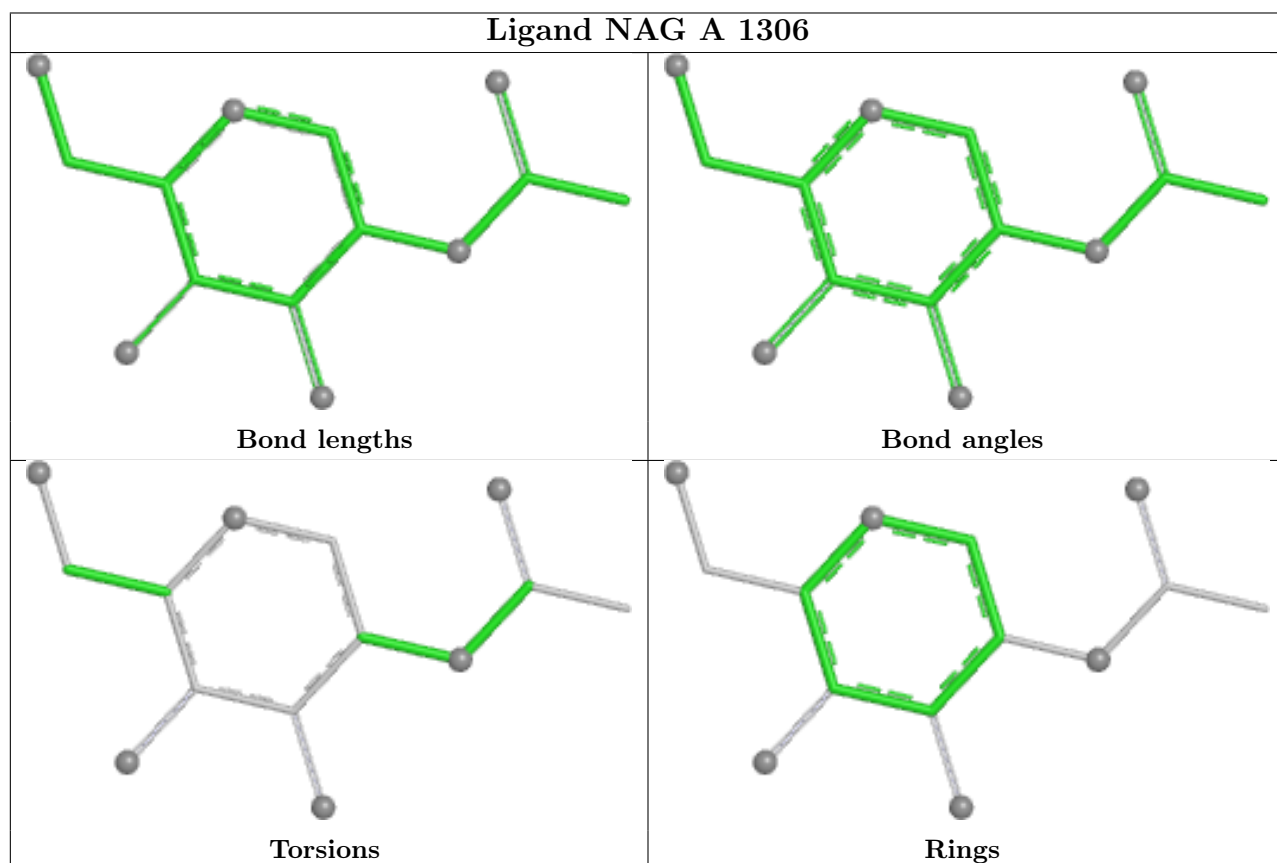
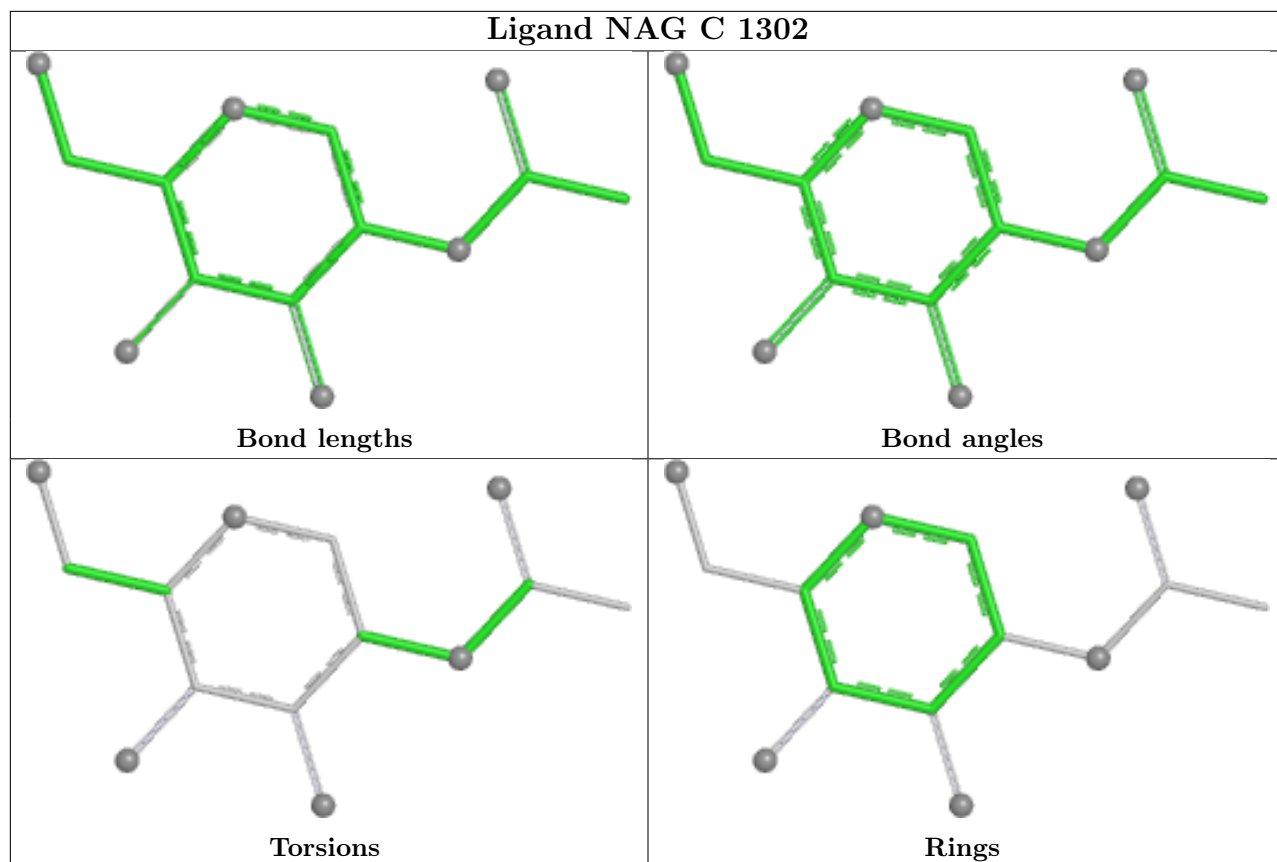


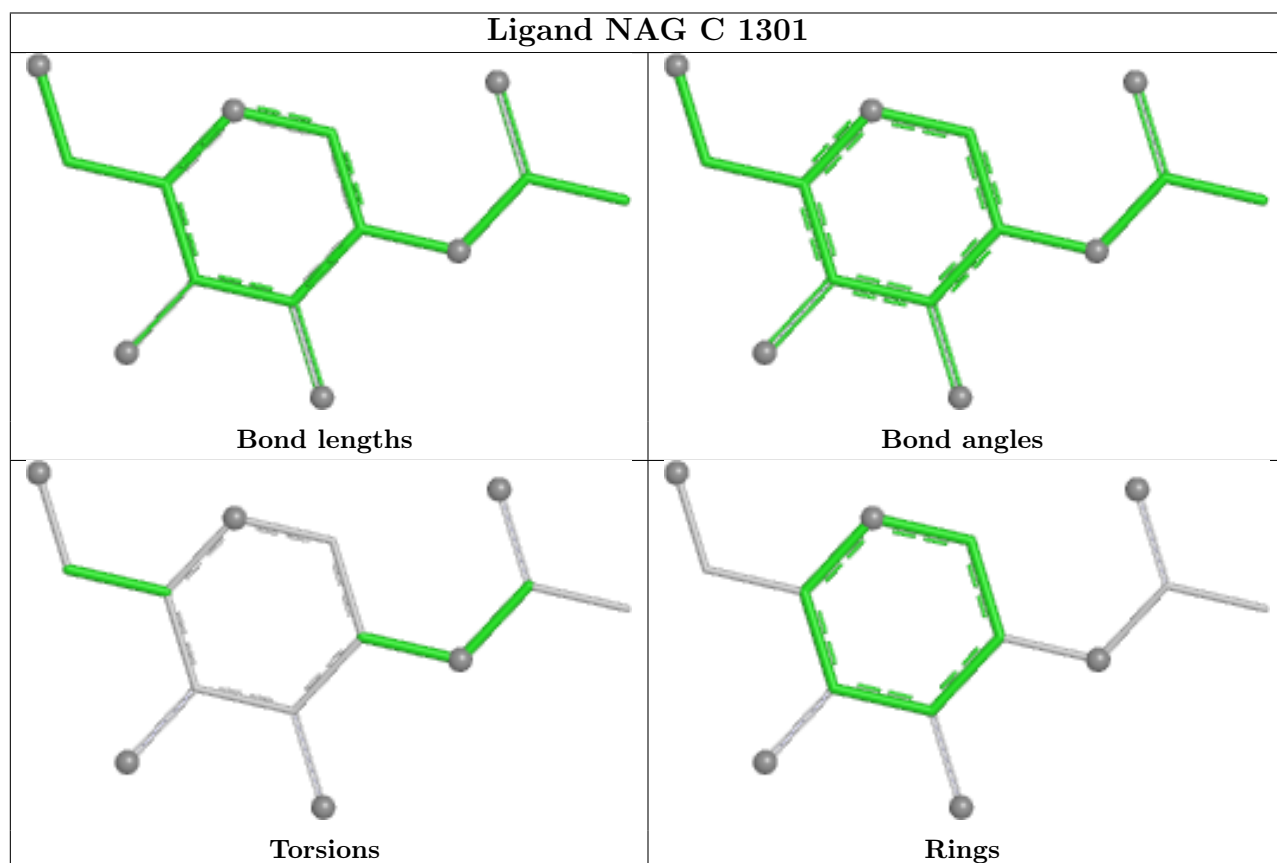
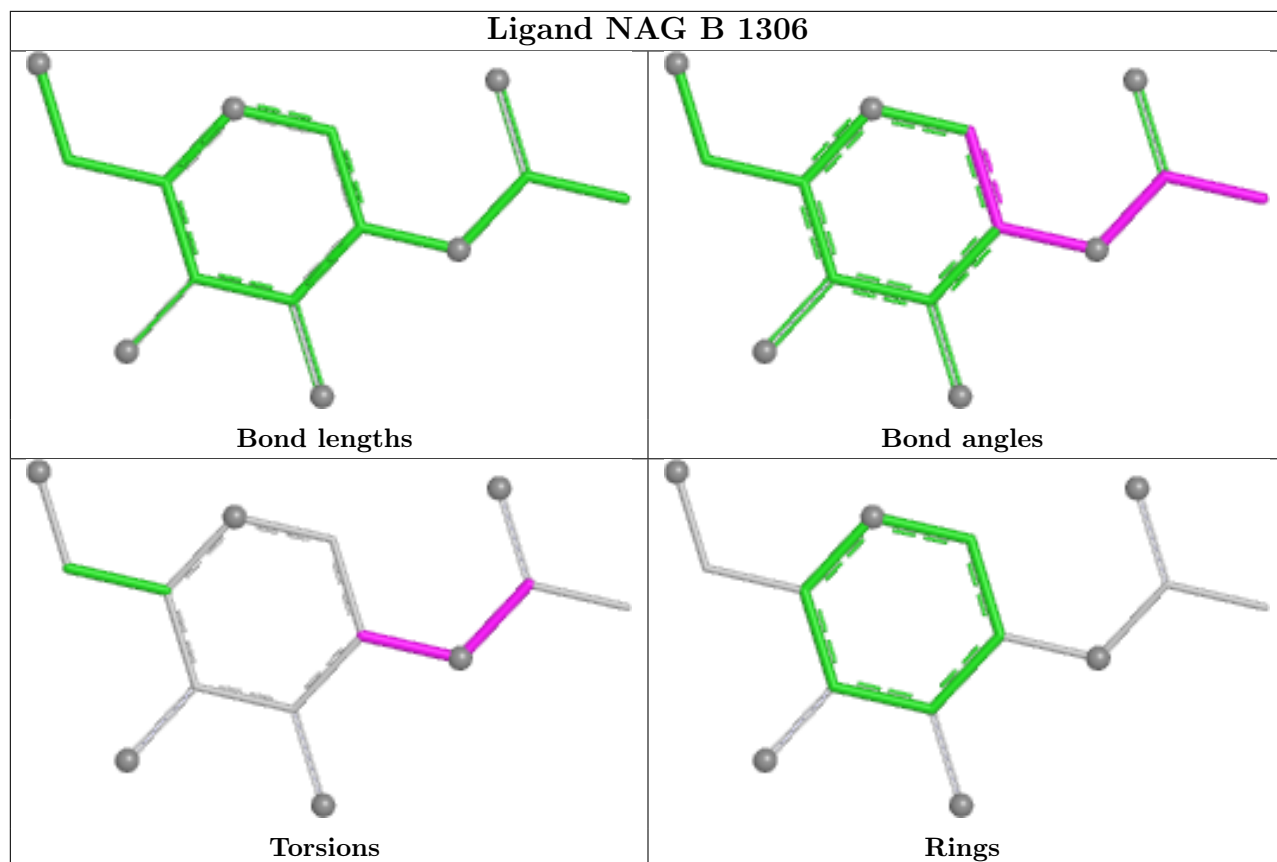


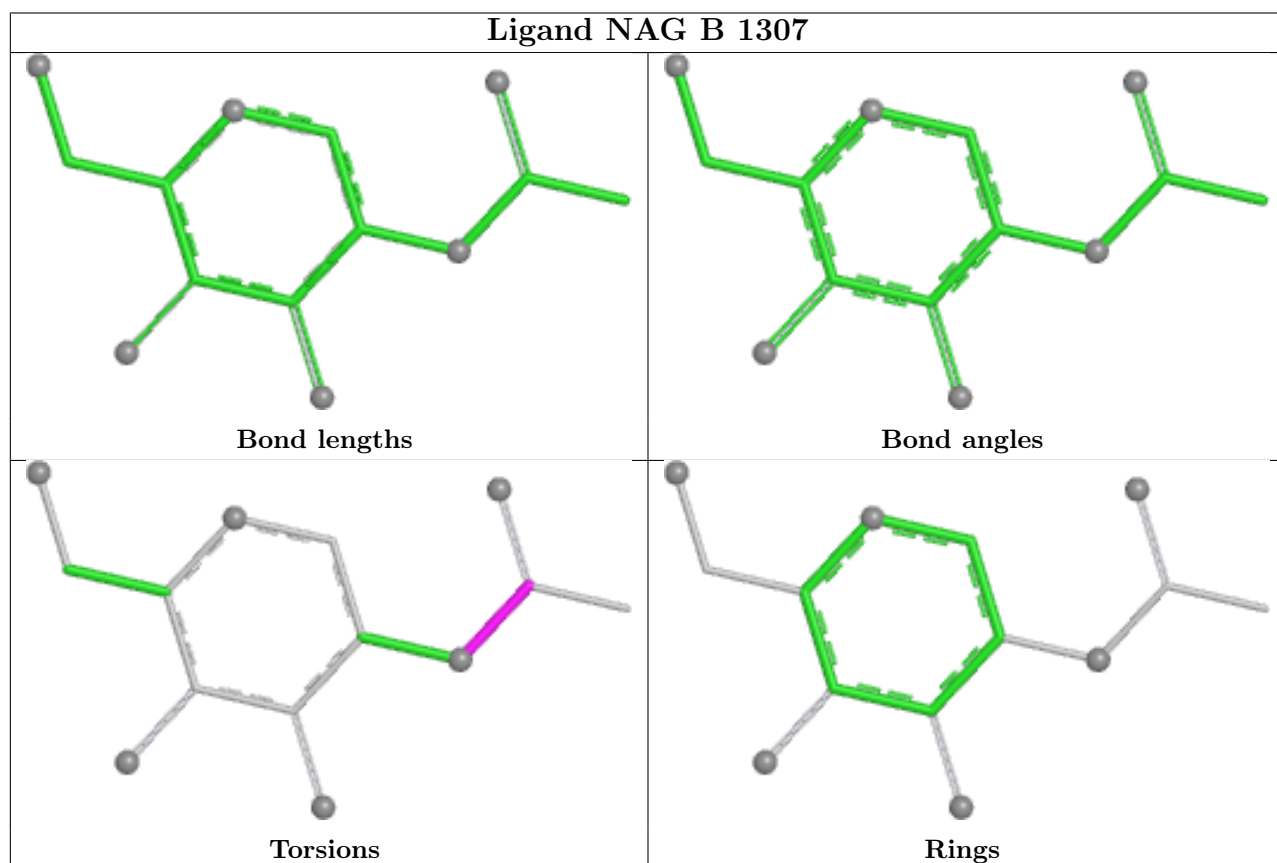
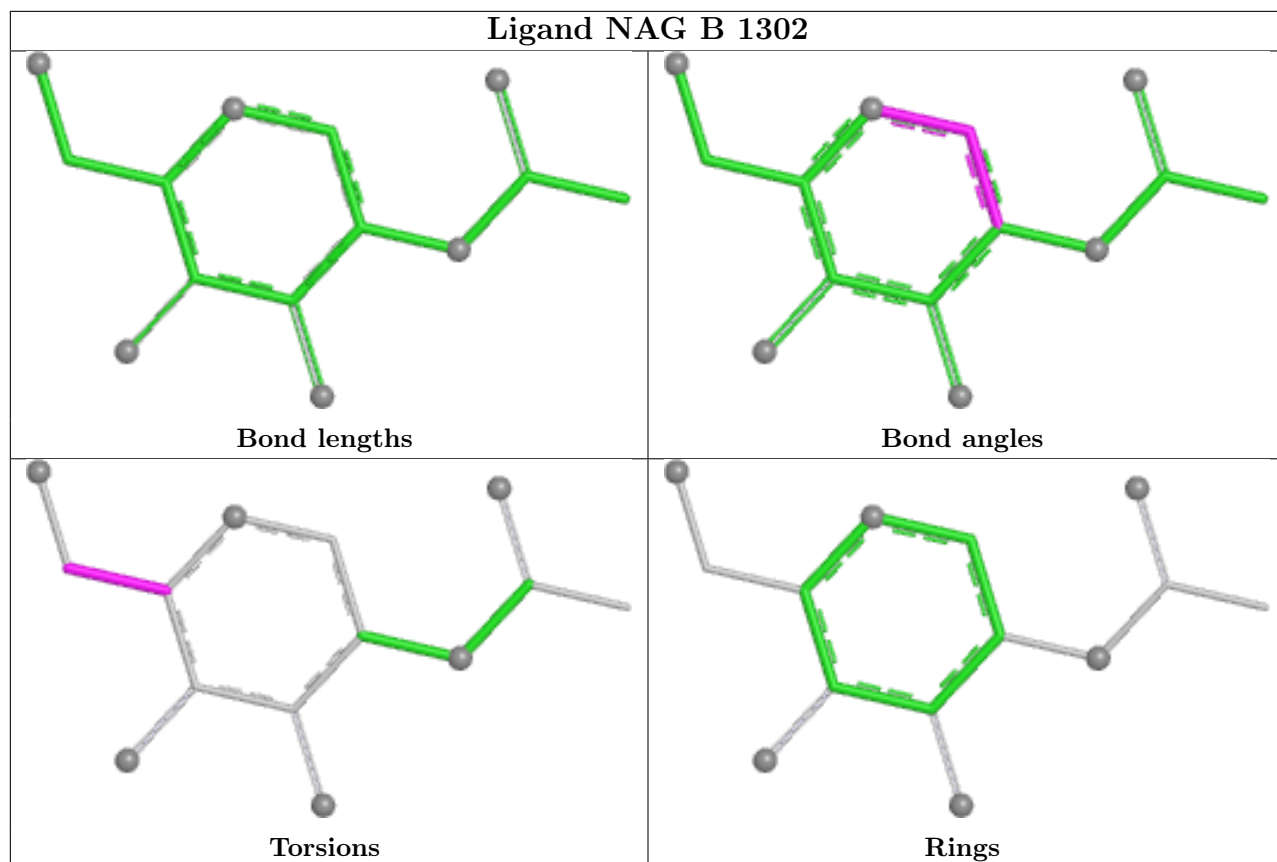


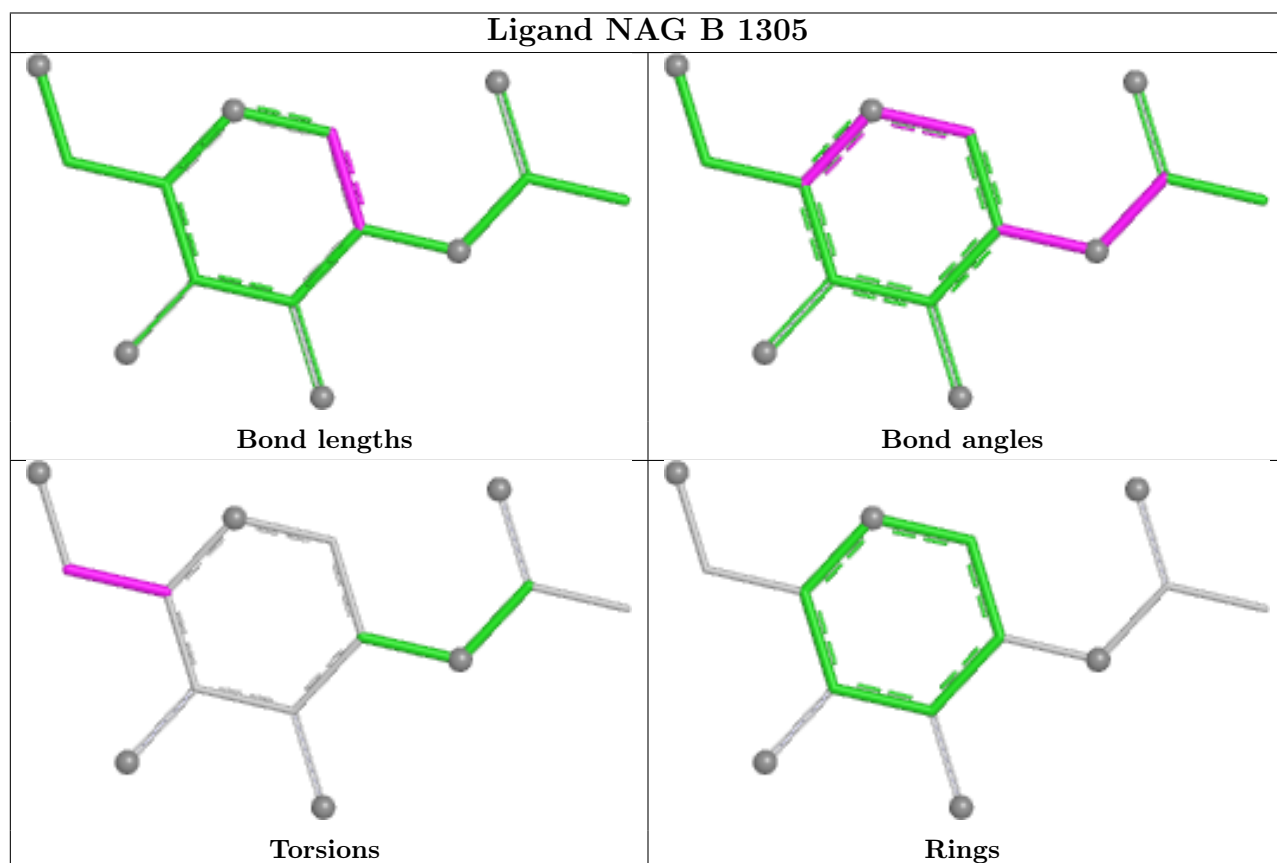
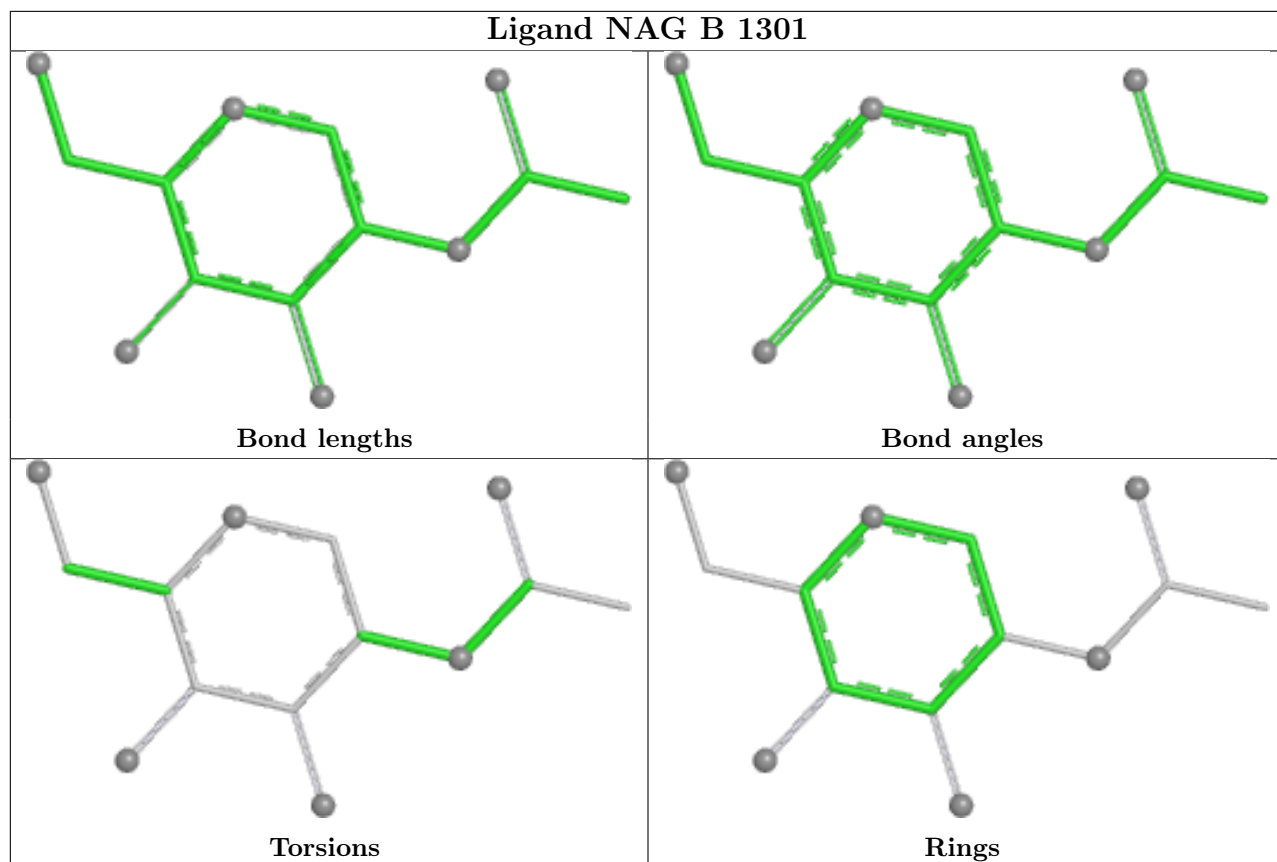


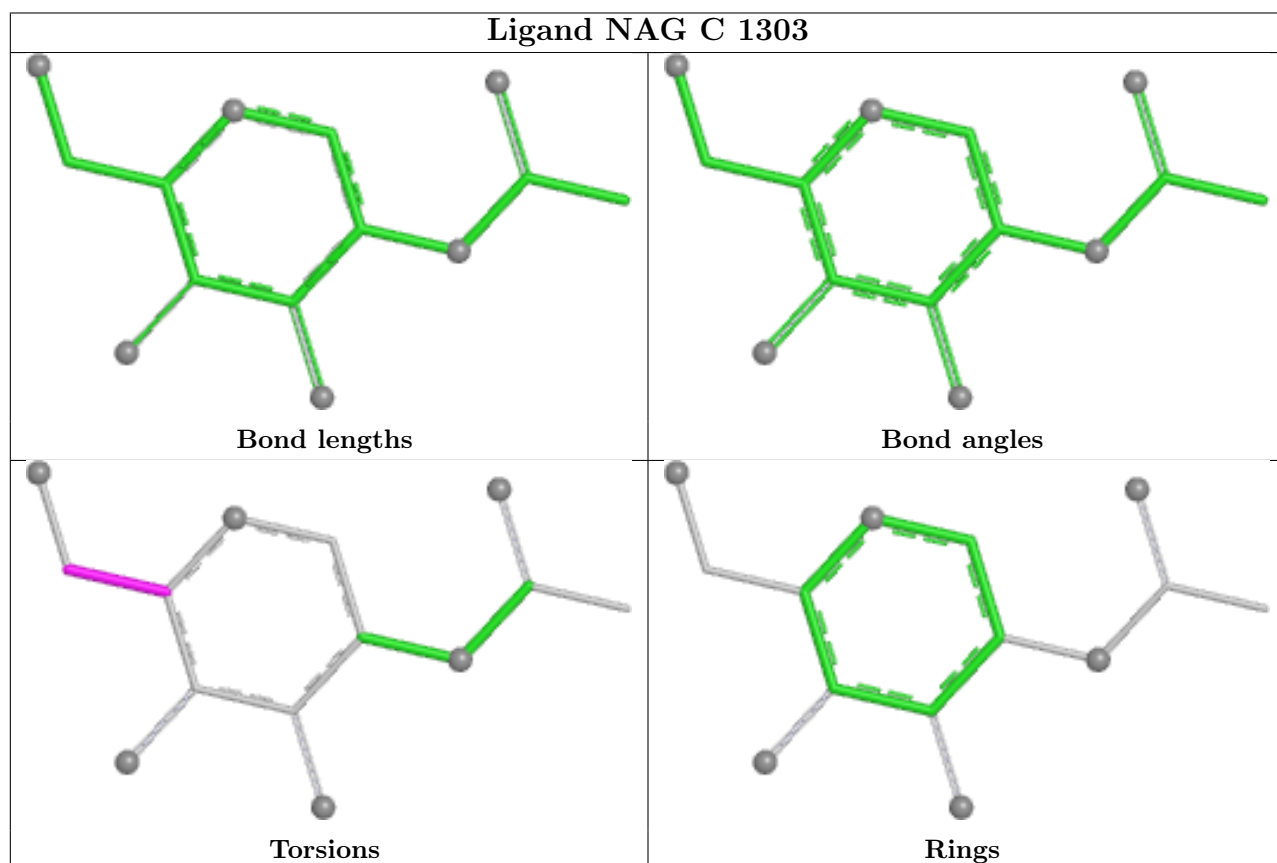
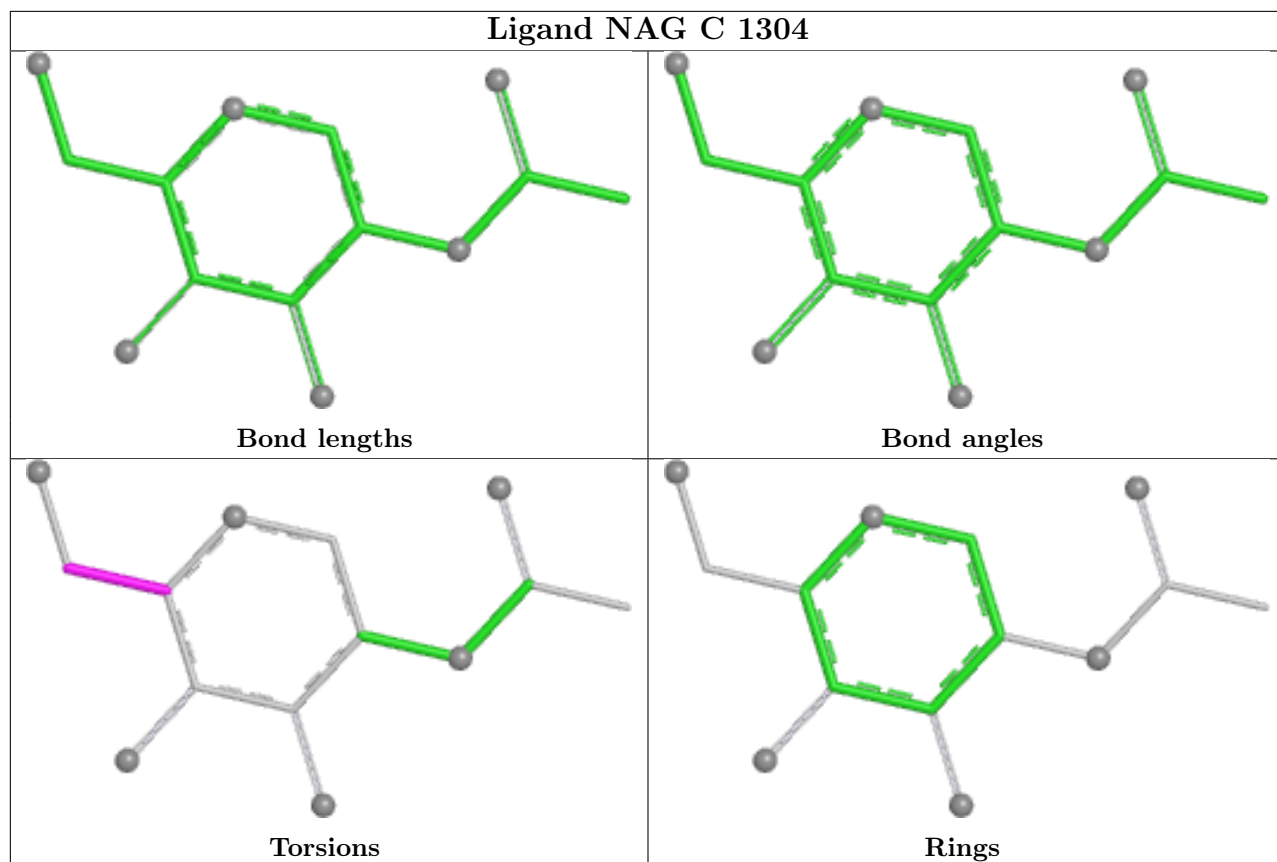


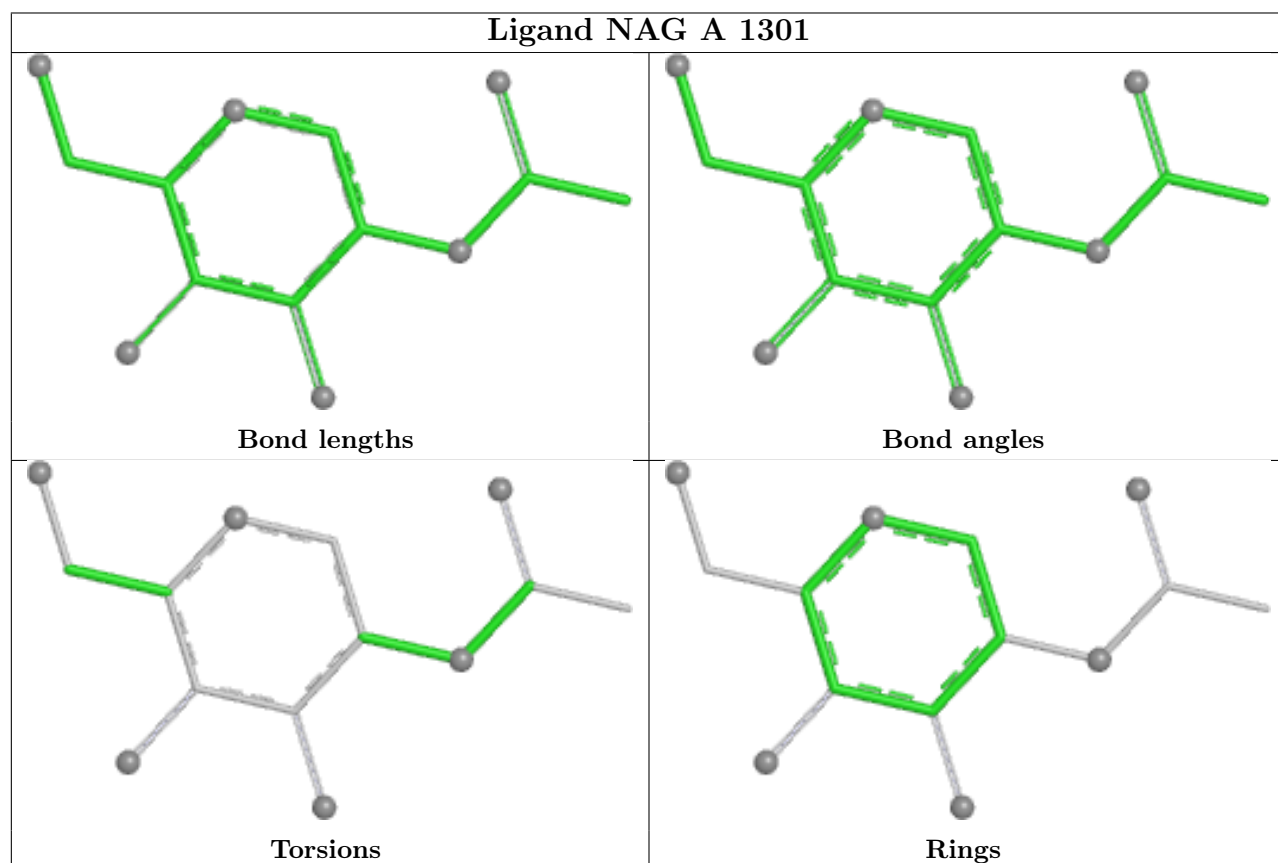
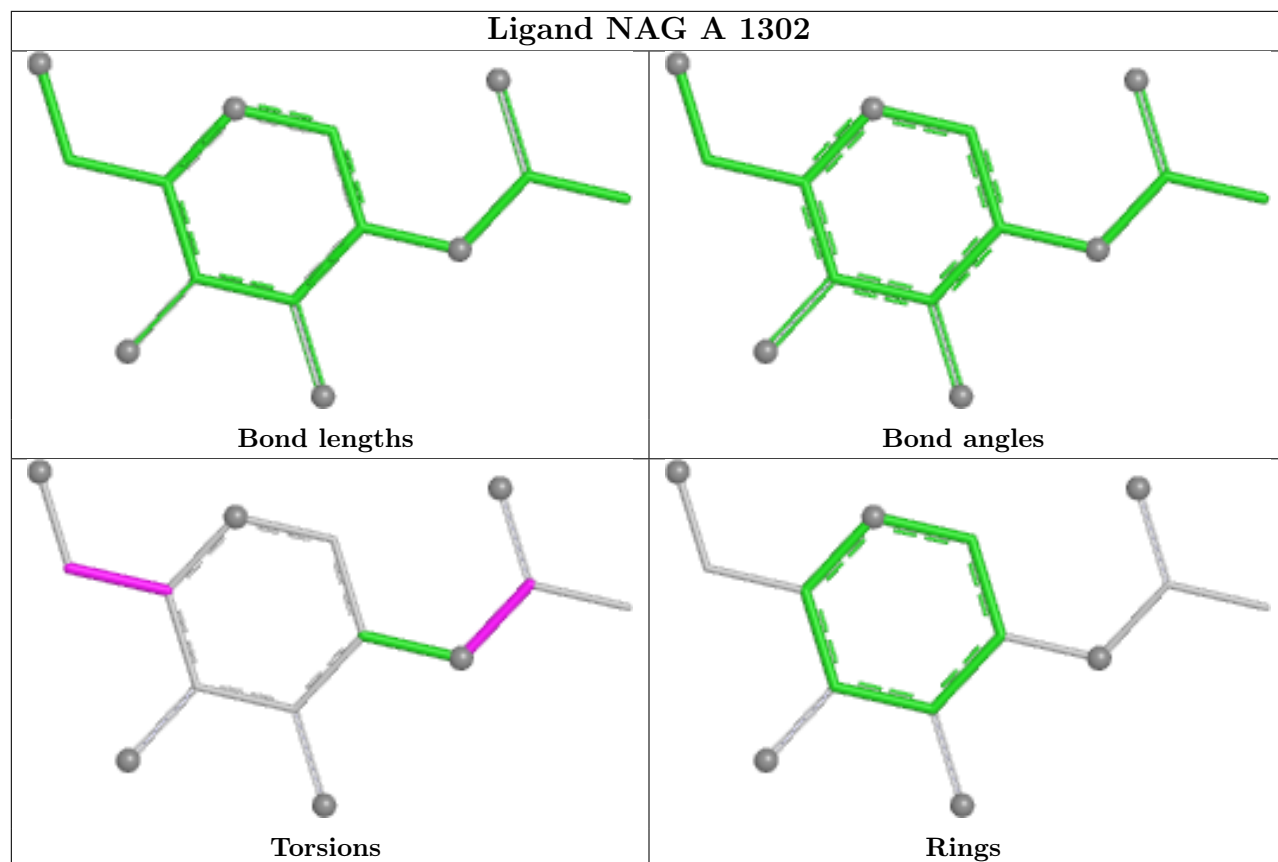


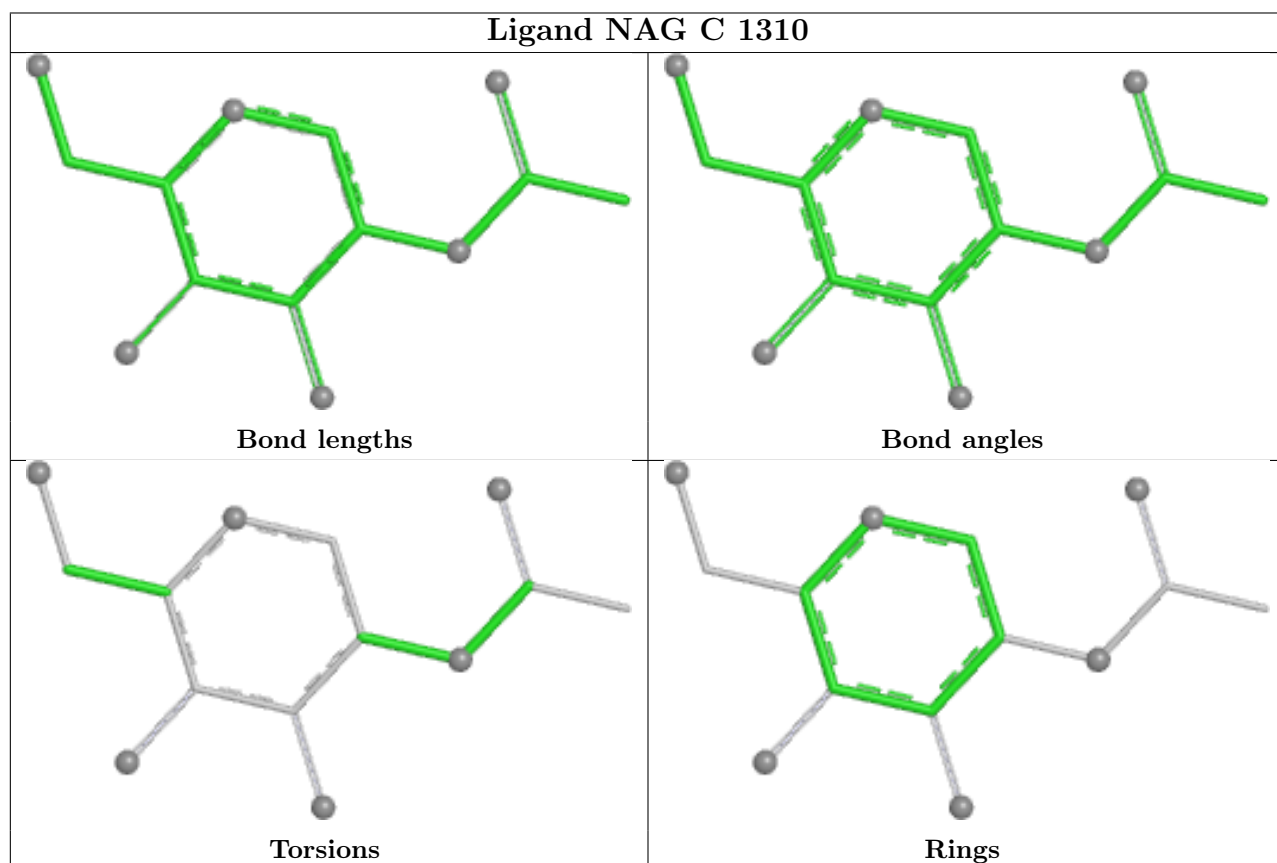
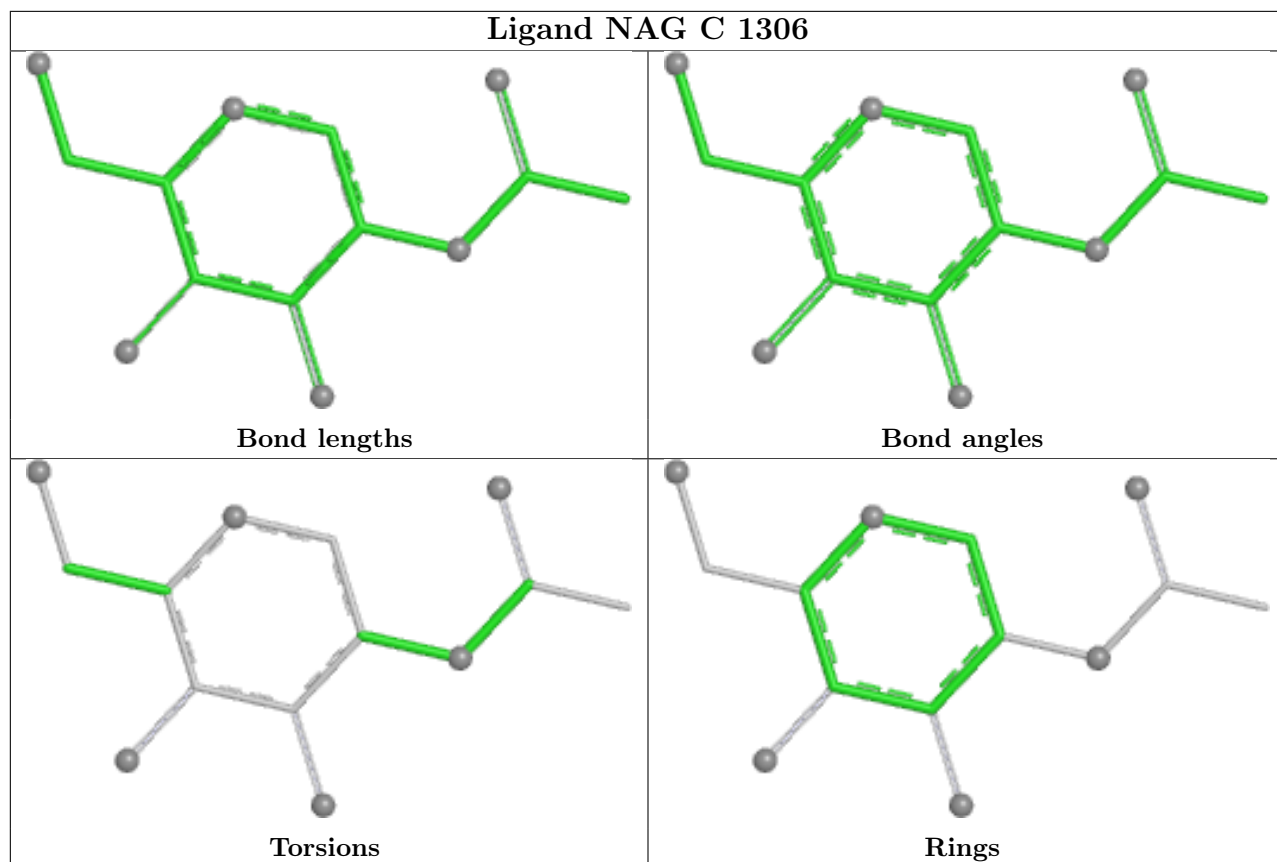


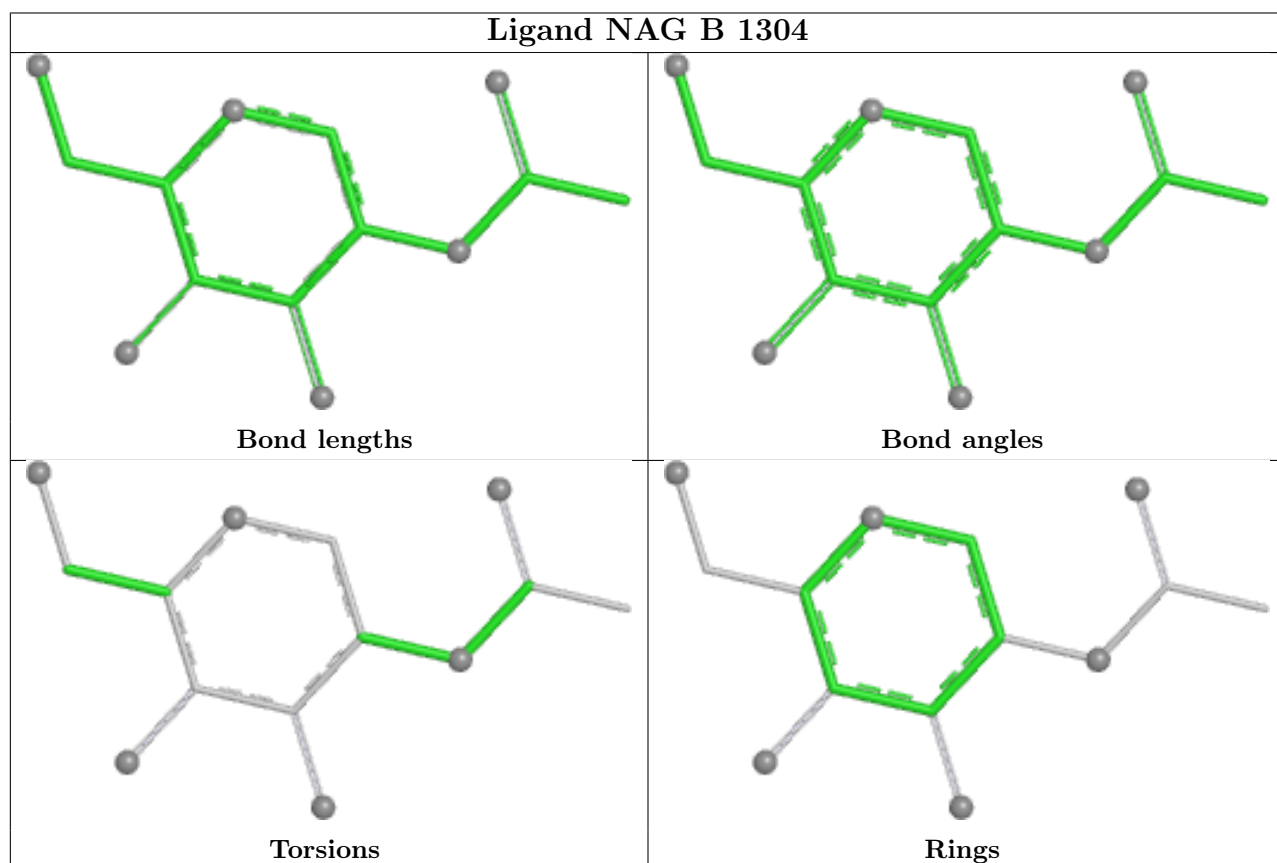
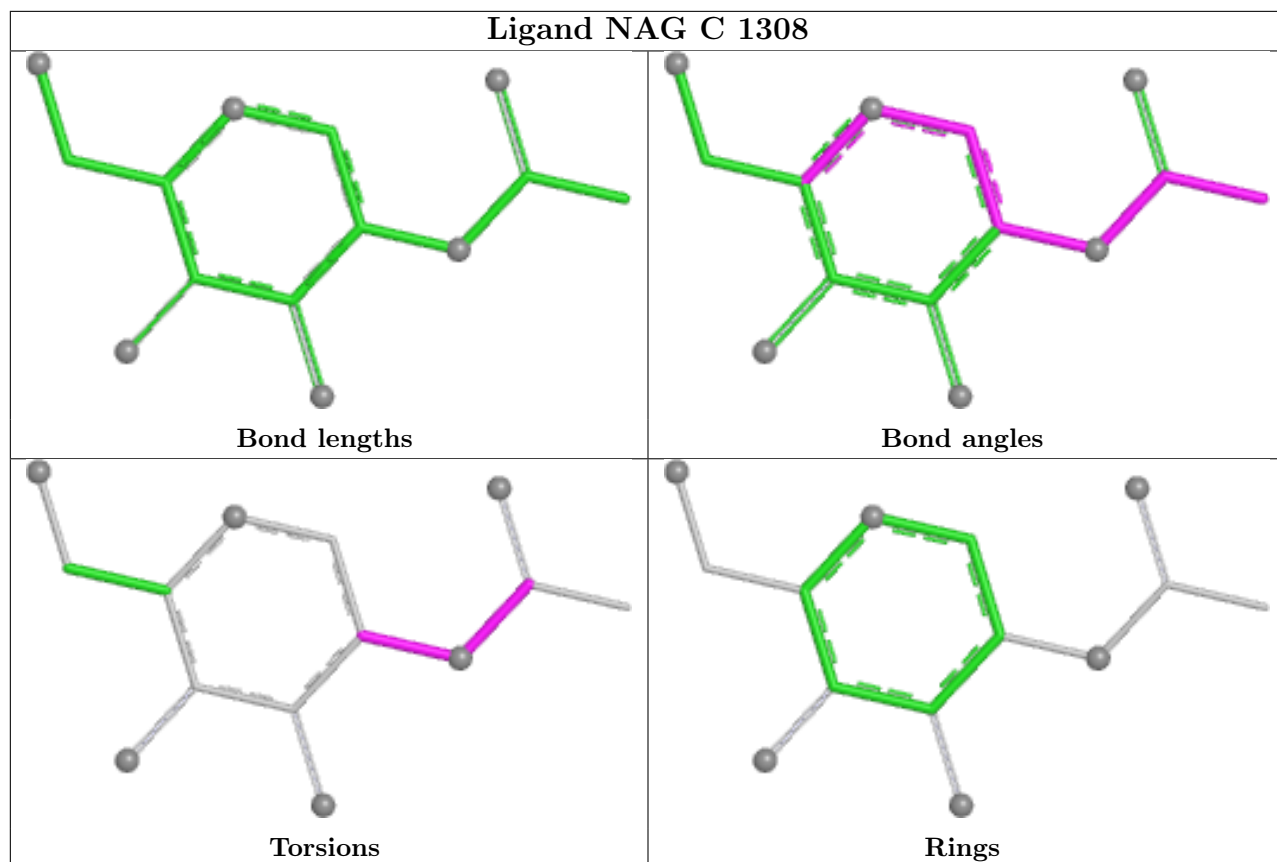


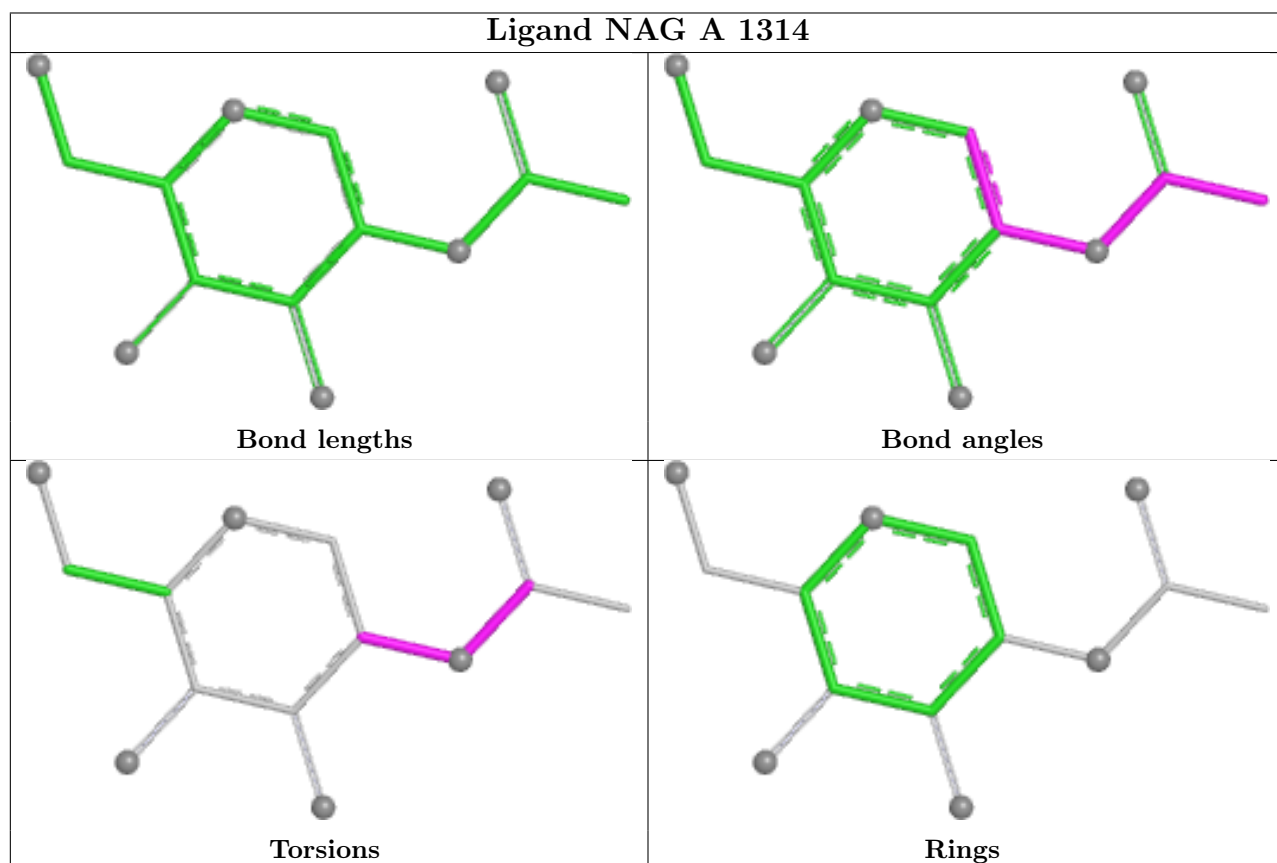
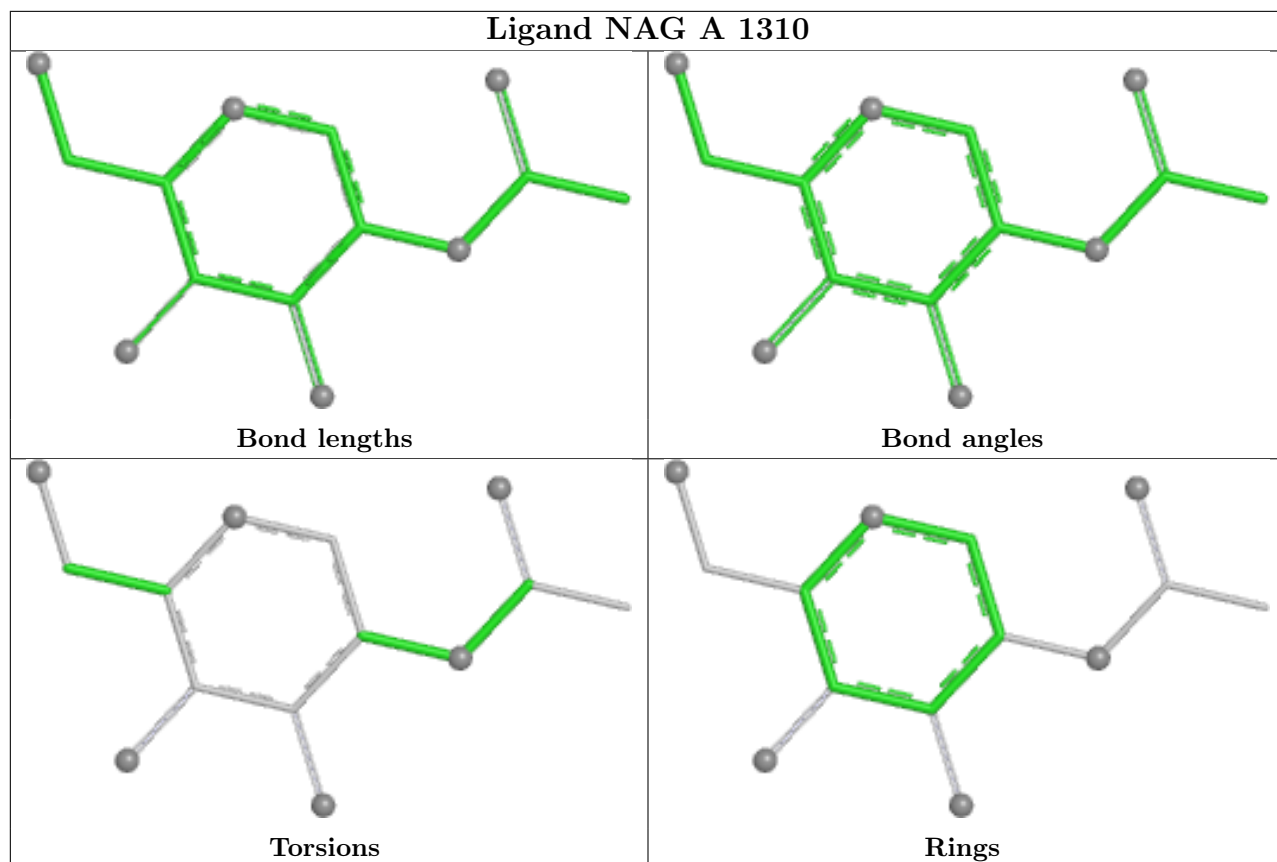


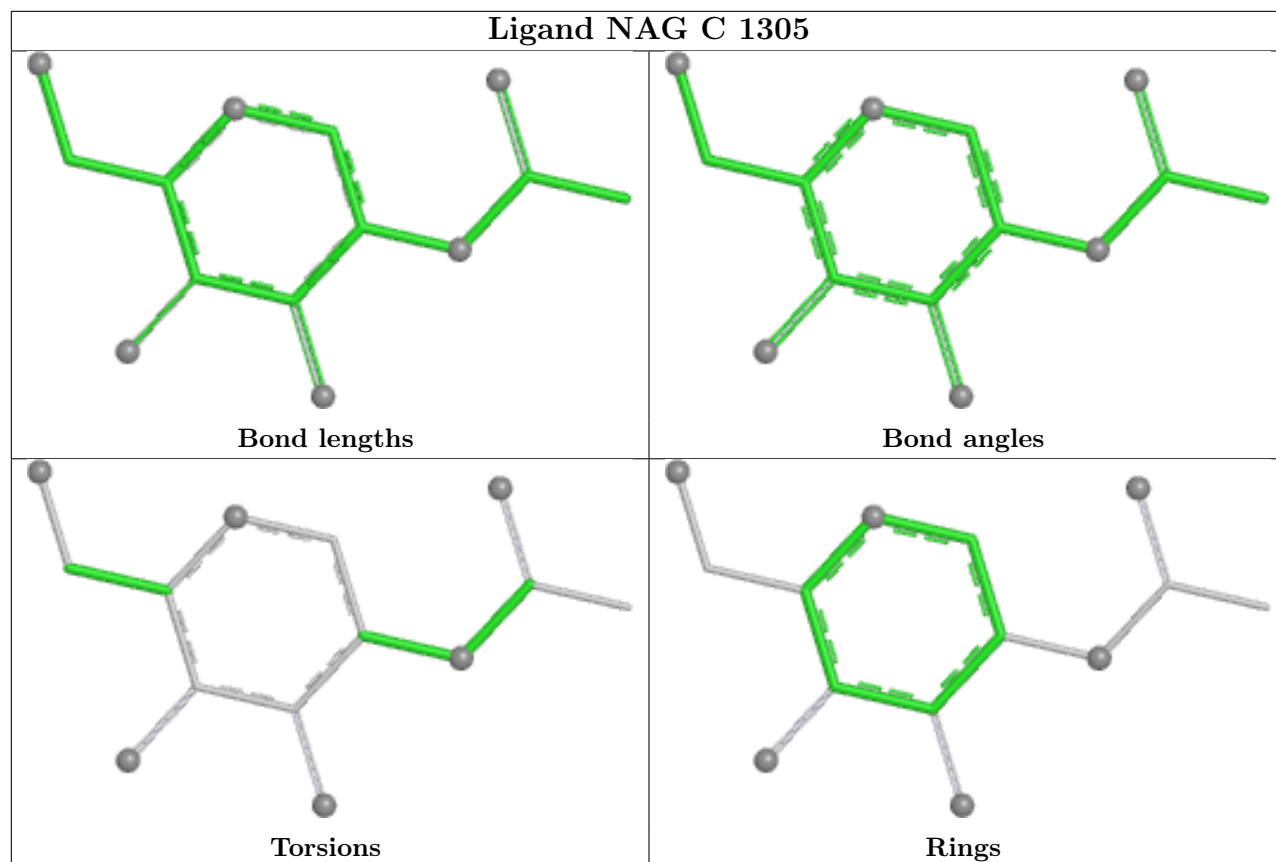












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

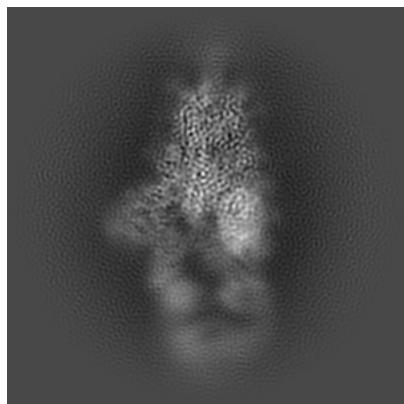
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48348. These allow visual inspection of the internal detail of the map and identification of artifacts.

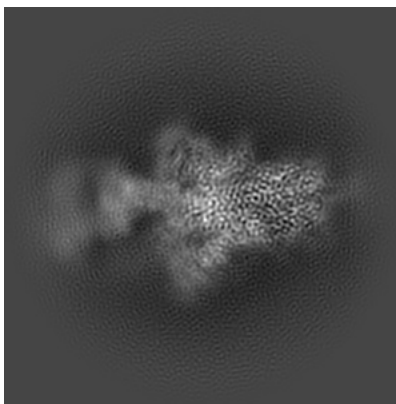
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

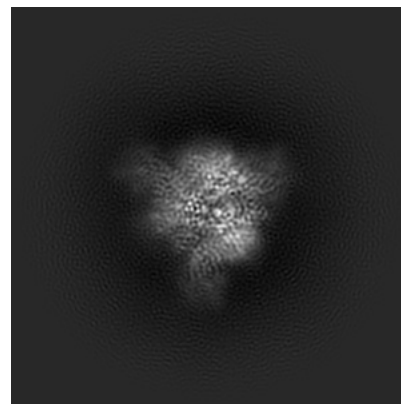
6.1.1 Primary map



X

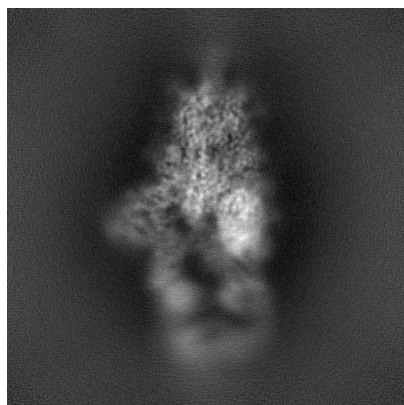


Y

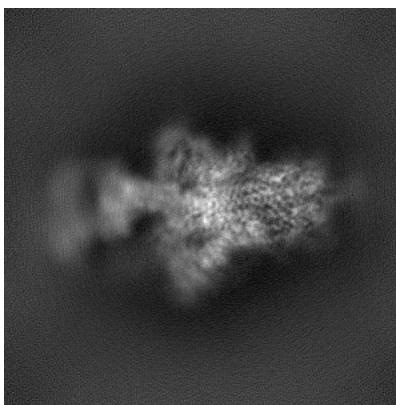


Z

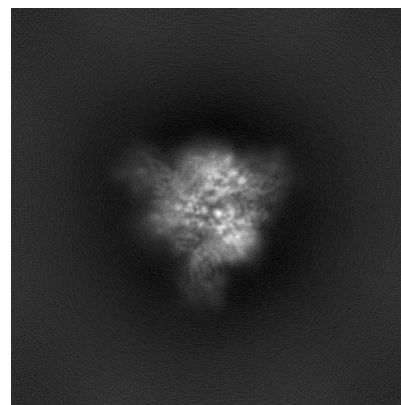
6.1.2 Raw map



X



Y

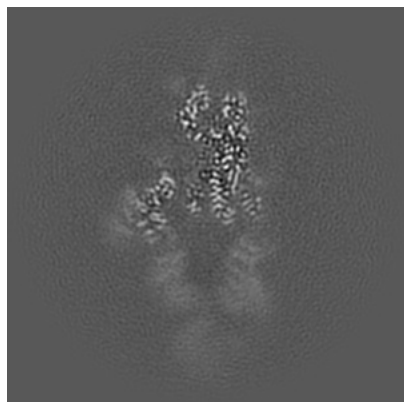


Z

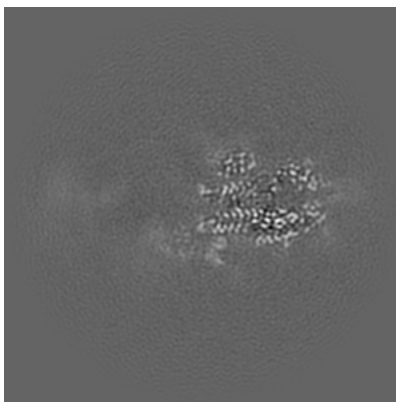
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

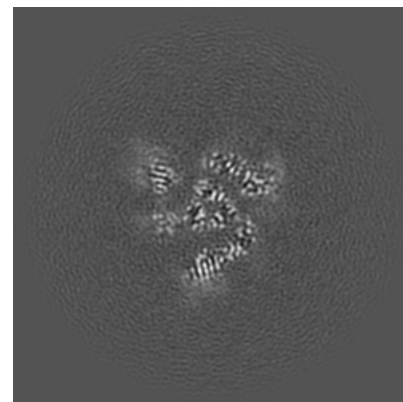
6.2.1 Primary map



X Index: 180

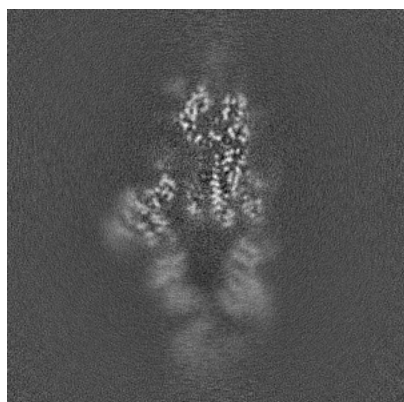


Y Index: 180

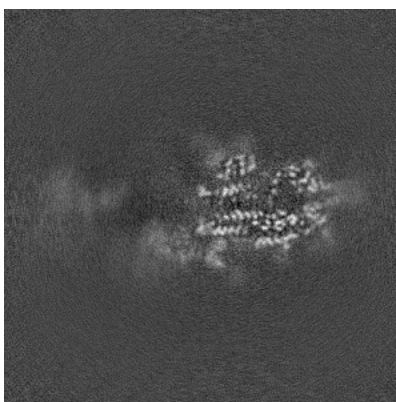


Z Index: 180

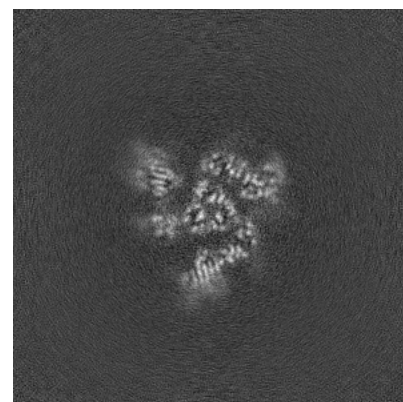
6.2.2 Raw map



X Index: 180



Y Index: 180

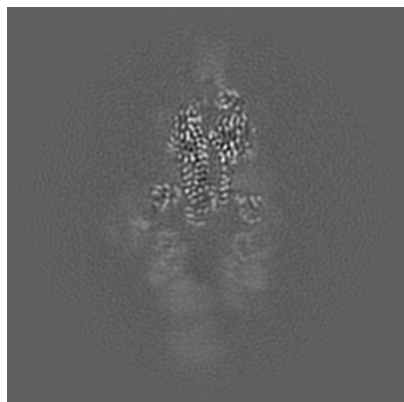


Z Index: 180

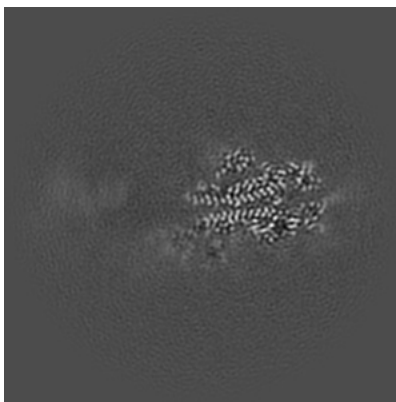
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

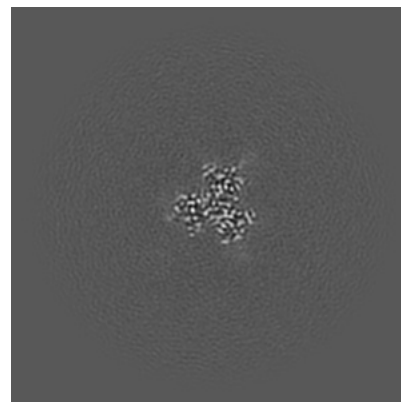
6.3.1 Primary map



X Index: 191

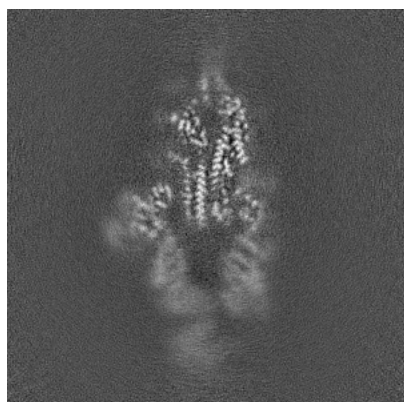


Y Index: 176

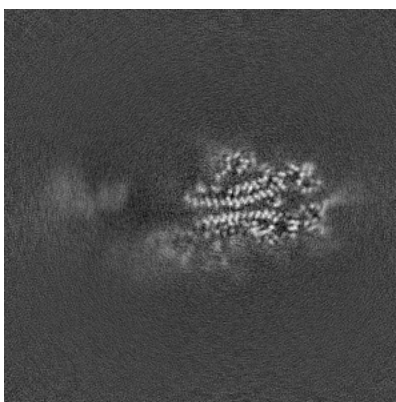


Z Index: 241

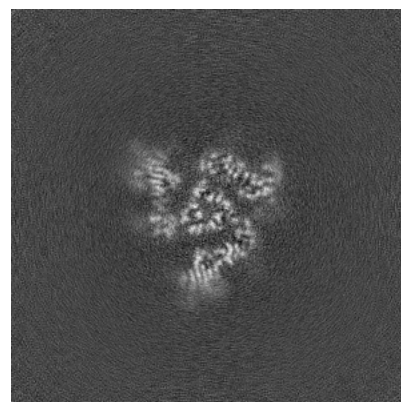
6.3.2 Raw map



X Index: 185



Y Index: 176

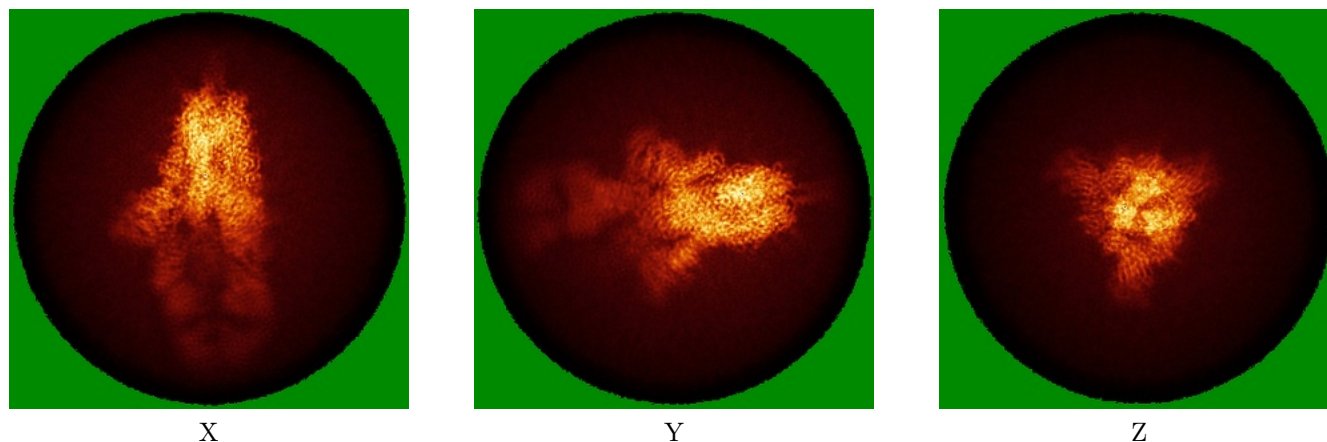


Z Index: 181

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

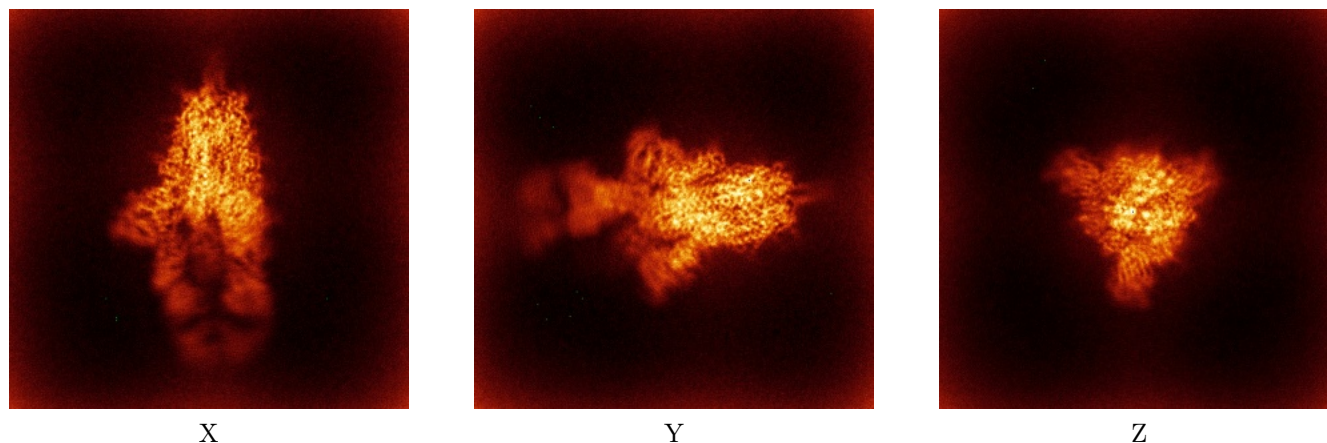


X

Y

Z

6.4.2 Raw map



X

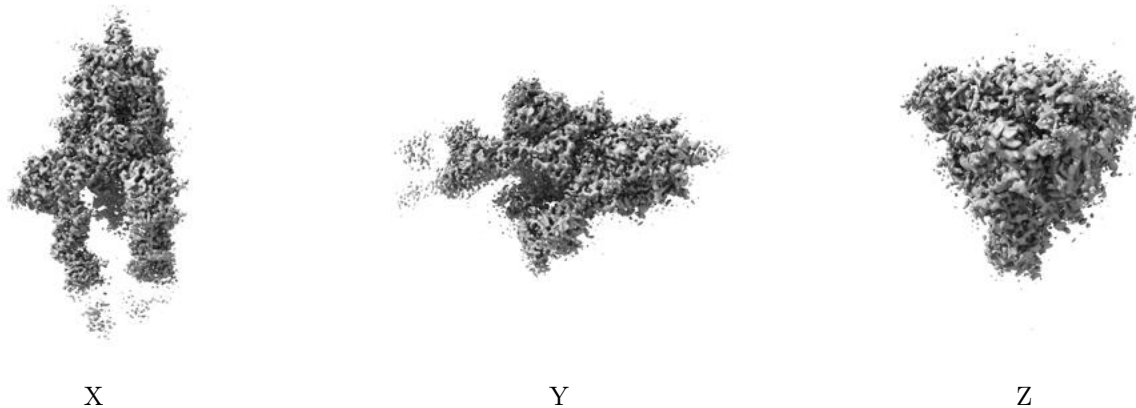
Y

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.

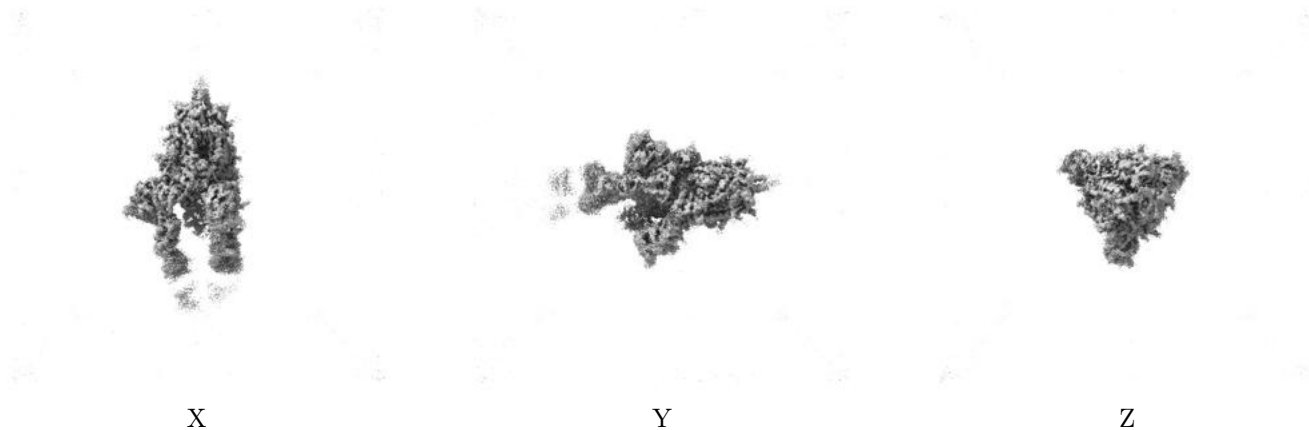
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

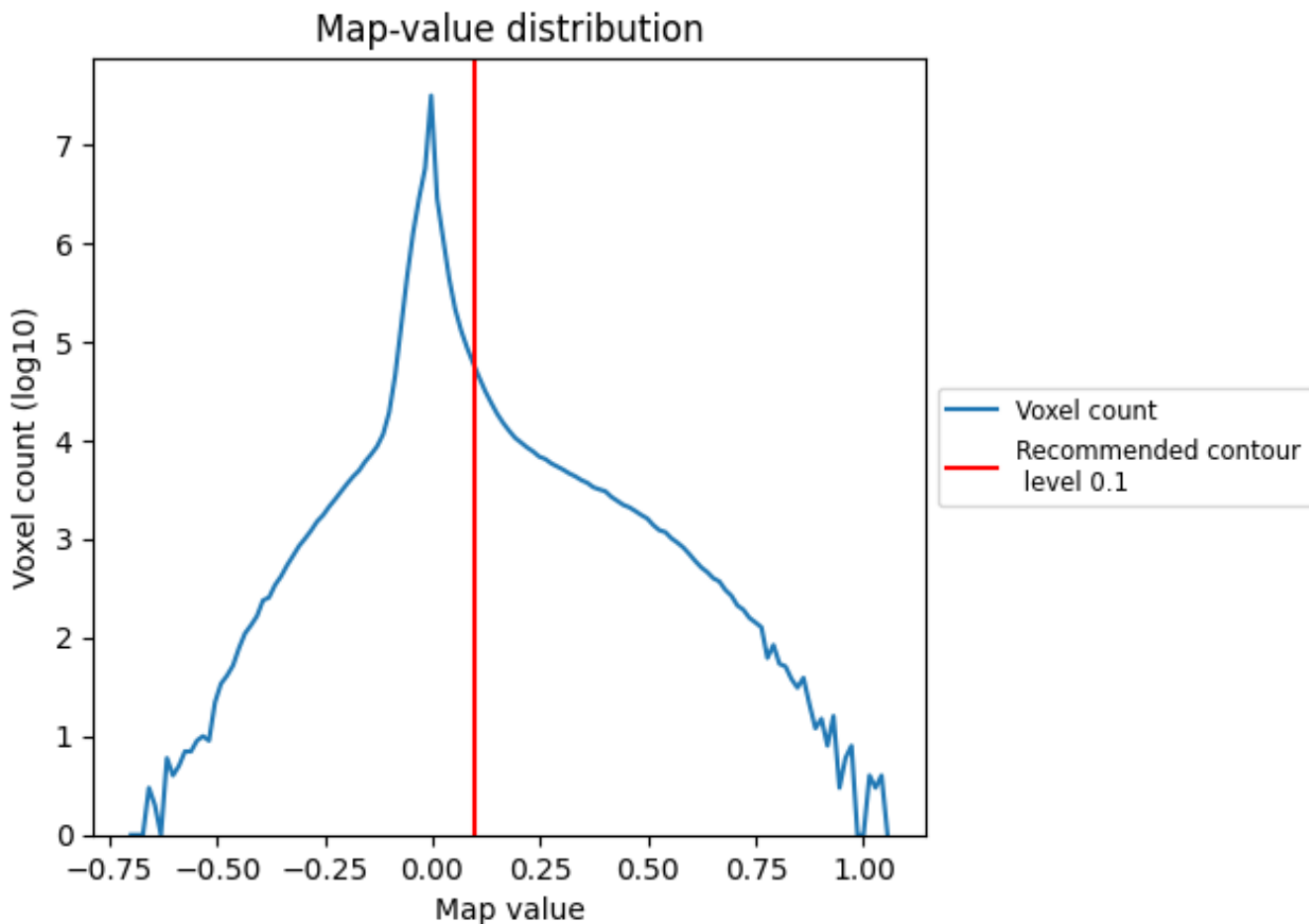
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

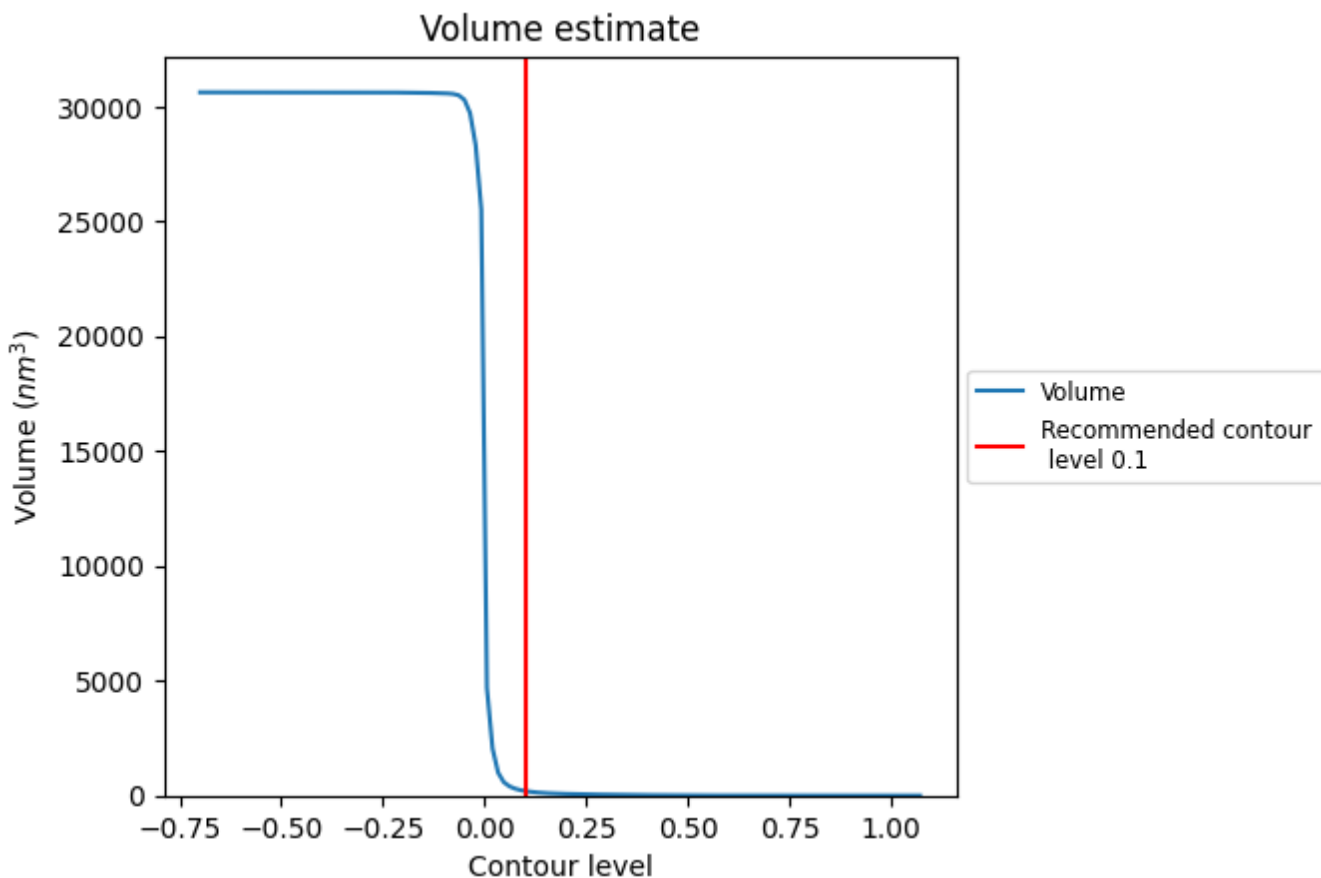
This section contains the results of statistical analysis of the map.

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.

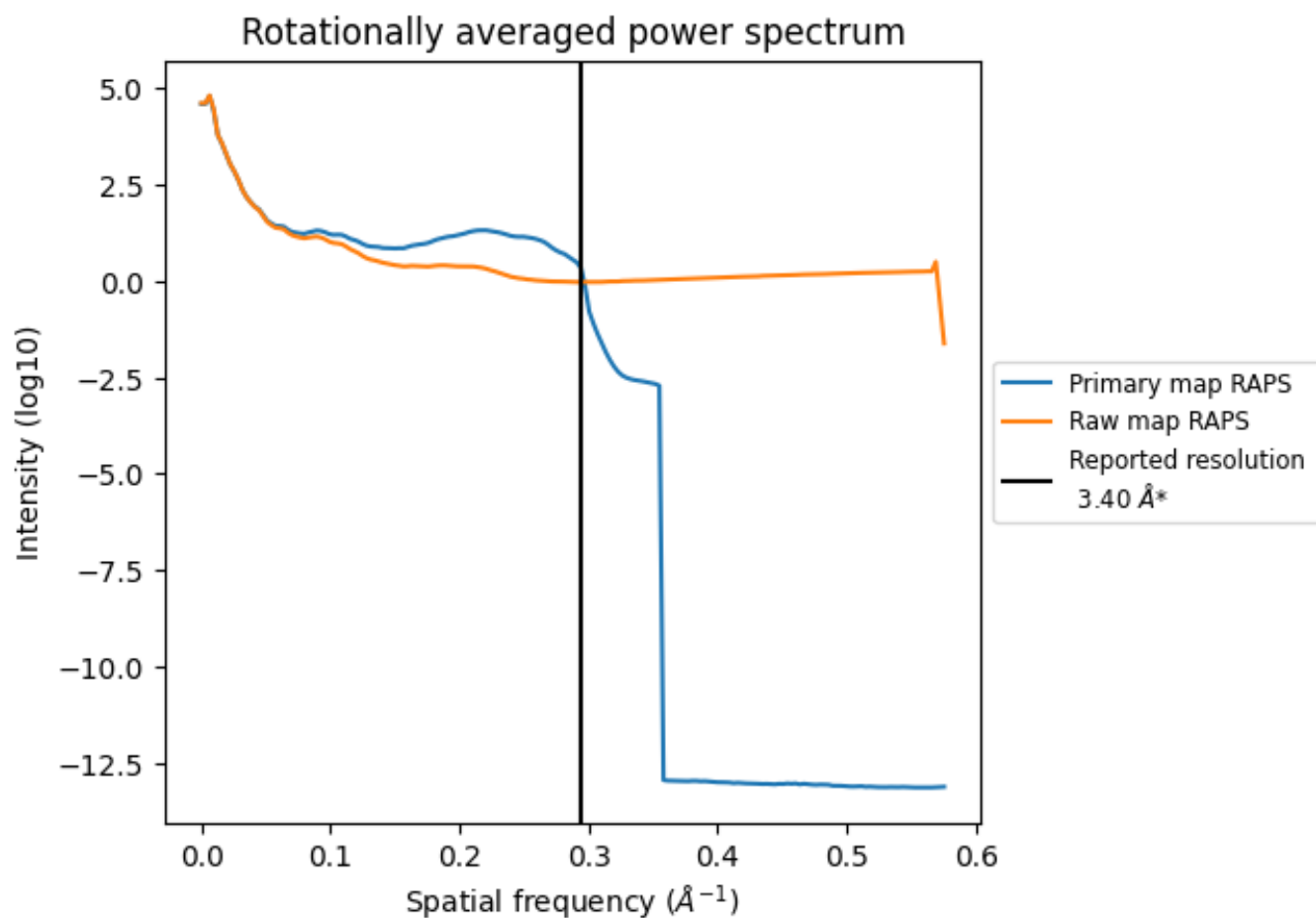
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm³; this corresponds to an approximate mass of 177 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](#)

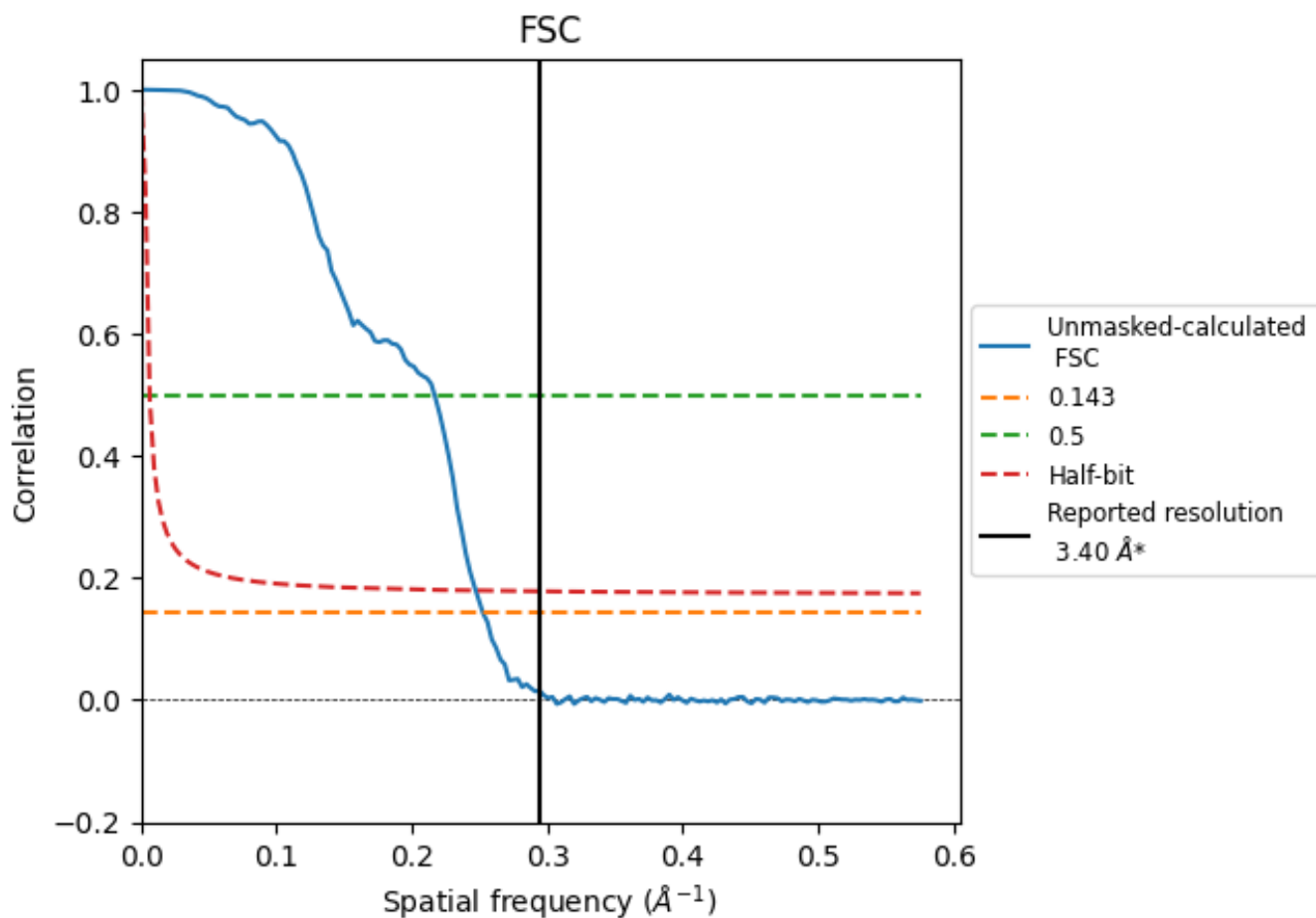


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

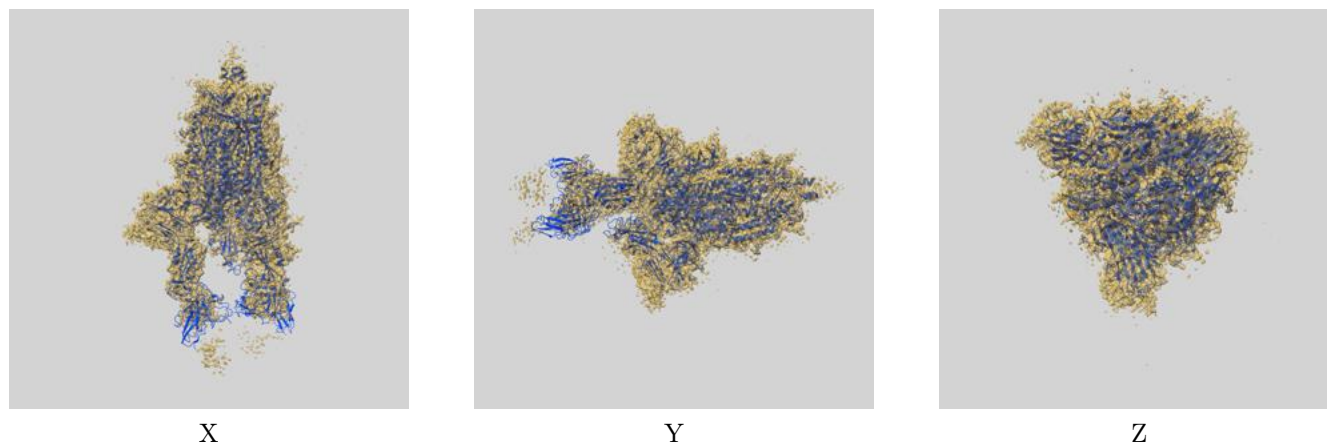
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	4.62	4.05

*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 3.96 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

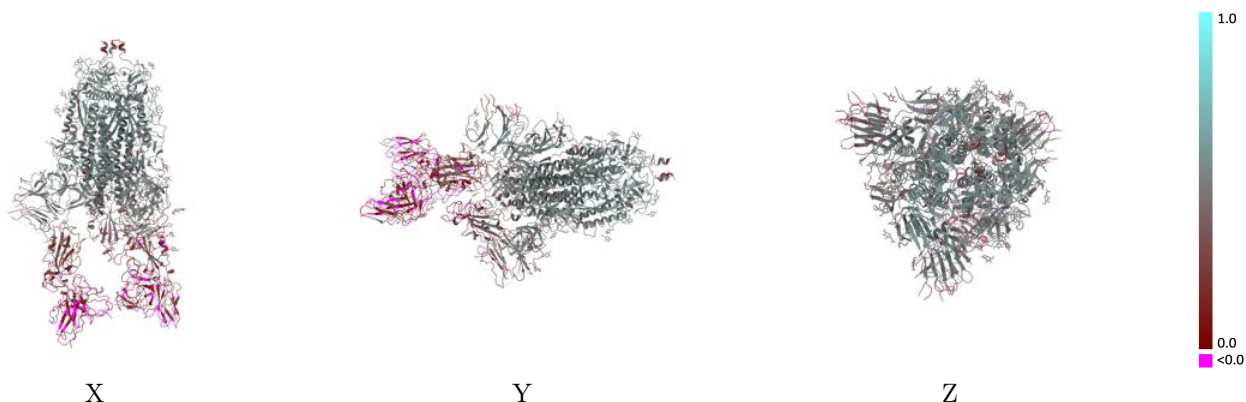
This section contains information regarding the fit between EMDB map EMD-48348 and PDB model 9ML5. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



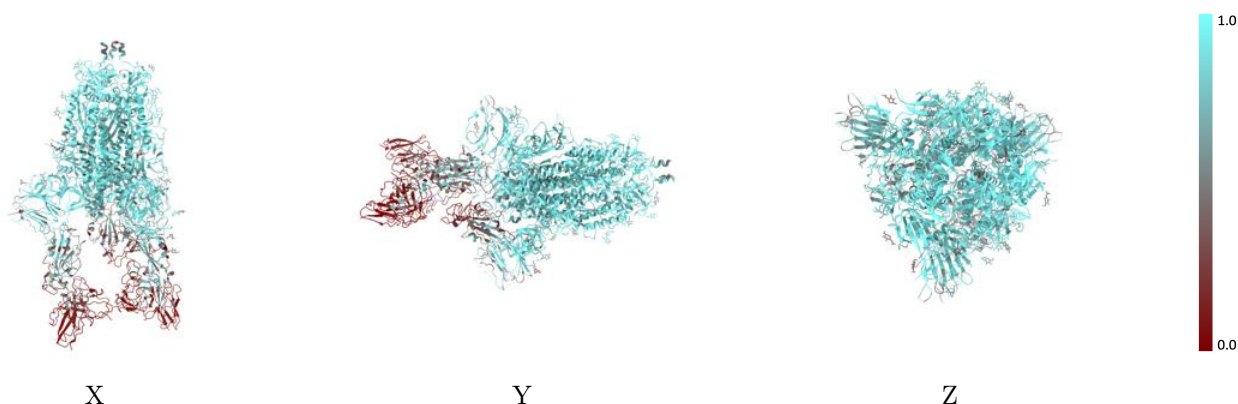
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



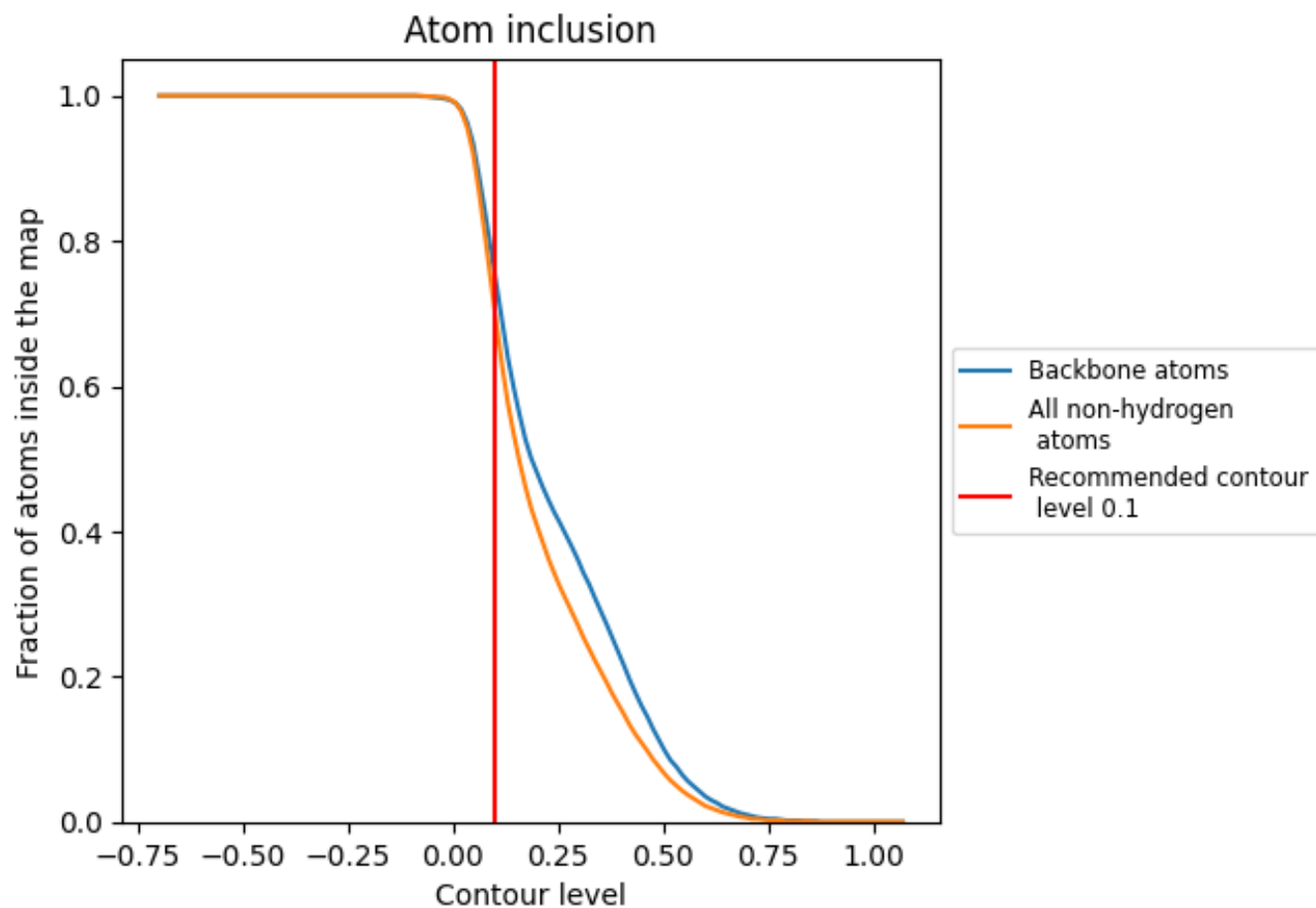
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.3970
A	 0.7950	 0.4370
B	 0.7700	 0.4270
C	 0.7620	 0.4490
D	 0.8570	 0.4500
E	 0.7500	 0.4430
F	 0.7140	 0.3830
G	 0.8210	 0.4530
H	 0.1680	 0.0900
I	 0.7140	 0.4570
J	 0.8570	 0.4410
K	 0.8210	 0.4500
L	 0.1180	 0.1040
M	 0.1340	 0.1120
N	 0.1220	 0.1230
O	 0.7500	 0.4680
P	 0.7140	 0.4100

