



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 05:50 PM UTC

PDB ID : 7N8H / pdb_00007n8h
EMDB ID : EMD-24236
Title : SARS-CoV-2 S (B.1.429 / epsilon variant) + S2M11 + S2L20 Global Refinement
Authors : McCallum, M.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-06-14
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

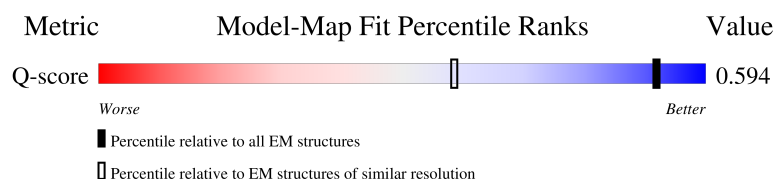
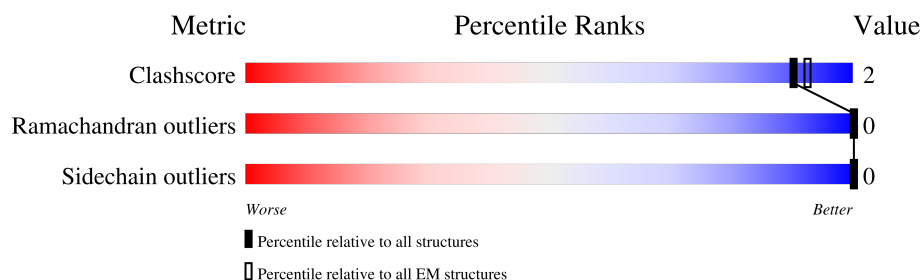
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1277	14% 72% 6% 22%
1	F	1277	14% 72% 6% 22%
1	K	1277	14% 72% 6% 22%
2	D	104	40% 94% 5%

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Mol	Chain	Length	Quality of chain
2	G	104	39% 95% 5%
2	L	104	40% 94% 5%
3	E	122	30% 96% .
3	H	122	30% 96% .
3	M	122	30% 96% .
4	B	106	99% 92% 6%
4	I	106	99% 94% 6%
4	N	106	99% 94% 6%
5	C	121	98% 98% .
5	J	121	98% 98% .
5	O	121	98% 98% .
6	P	3	100% 33% 67%
6	S	3	100% 33% 67%
6	V	3	100% 33% 67%
7	Q	2	50% 100%
7	R	2	50% 100%
7	T	2	50% 100%
7	U	2	50% 100%
7	W	2	50% 100%
7	X	2	50% 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 32921 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	999	Total	C	N	O	S	0	0
			7603	4851	1266	1452	34		
1	F	999	Total	C	N	O	S	0	0
			7603	4851	1266	1452	34		
1	K	999	Total	C	N	O	S	0	0
			7603	4851	1266	1452	34		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ILE	SER	conflict	UNP P0DTC2
A	152	CYS	TRP	conflict	UNP P0DTC2
A	452	ARG	LEU	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	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	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	ASN	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	ILE	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	TRP	-	expression tag	UNP P0DTC2
A	1265	HIS	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	HIS	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	HIS	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
F	13	ILE	SER	conflict	UNP P0DTC2
F	152	CYS	TRP	conflict	UNP P0DTC2
F	452	ARG	LEU	conflict	UNP P0DTC2
F	682	GLY	ARG	conflict	UNP P0DTC2
F	683	SER	ARG	conflict	UNP P0DTC2
F	685	SER	ARG	conflict	UNP P0DTC2
F	817	PRO	PHE	conflict	UNP P0DTC2
F	892	PRO	ALA	conflict	UNP P0DTC2
F	899	PRO	ALA	conflict	UNP P0DTC2
F	942	PRO	ALA	conflict	UNP P0DTC2
F	986	PRO	LYS	conflict	UNP P0DTC2
F	987	PRO	VAL	conflict	UNP P0DTC2
F	1209	GLY	-	expression tag	UNP P0DTC2
F	1210	SER	-	expression tag	UNP P0DTC2
F	1211	GLY	-	expression tag	UNP P0DTC2
F	1212	TYR	-	expression tag	UNP P0DTC2
F	1213	ILE	-	expression tag	UNP P0DTC2
F	1214	PRO	-	expression tag	UNP P0DTC2
F	1215	GLU	-	expression tag	UNP P0DTC2
F	1216	ALA	-	expression tag	UNP P0DTC2
F	1217	PRO	-	expression tag	UNP P0DTC2
F	1218	ARG	-	expression tag	UNP P0DTC2
F	1219	ASP	-	expression tag	UNP P0DTC2
F	1220	GLY	-	expression tag	UNP P0DTC2
F	1221	GLN	-	expression tag	UNP P0DTC2
F	1222	ALA	-	expression tag	UNP P0DTC2
F	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1224	VAL	-	expression tag	UNP P0DTC2
F	1225	ARG	-	expression tag	UNP P0DTC2
F	1226	LYS	-	expression tag	UNP P0DTC2
F	1227	ASP	-	expression tag	UNP P0DTC2
F	1228	GLY	-	expression tag	UNP P0DTC2
F	1229	GLU	-	expression tag	UNP P0DTC2
F	1230	TRP	-	expression tag	UNP P0DTC2
F	1231	VAL	-	expression tag	UNP P0DTC2
F	1232	LEU	-	expression tag	UNP P0DTC2
F	1233	LEU	-	expression tag	UNP P0DTC2
F	1234	SER	-	expression tag	UNP P0DTC2
F	1235	THR	-	expression tag	UNP P0DTC2
F	1236	PHE	-	expression tag	UNP P0DTC2
F	1237	LEU	-	expression tag	UNP P0DTC2
F	1238	GLY	-	expression tag	UNP P0DTC2
F	1239	ARG	-	expression tag	UNP P0DTC2
F	1240	SER	-	expression tag	UNP P0DTC2
F	1241	LEU	-	expression tag	UNP P0DTC2
F	1242	GLU	-	expression tag	UNP P0DTC2
F	1243	VAL	-	expression tag	UNP P0DTC2
F	1244	LEU	-	expression tag	UNP P0DTC2
F	1245	PHE	-	expression tag	UNP P0DTC2
F	1246	GLN	-	expression tag	UNP P0DTC2
F	1247	GLY	-	expression tag	UNP P0DTC2
F	1248	PRO	-	expression tag	UNP P0DTC2
F	1249	GLY	-	expression tag	UNP P0DTC2
F	1250	SER	-	expression tag	UNP P0DTC2
F	1251	GLY	-	expression tag	UNP P0DTC2
F	1252	GLY	-	expression tag	UNP P0DTC2
F	1253	LEU	-	expression tag	UNP P0DTC2
F	1254	ASN	-	expression tag	UNP P0DTC2
F	1255	ASP	-	expression tag	UNP P0DTC2
F	1256	ILE	-	expression tag	UNP P0DTC2
F	1257	PHE	-	expression tag	UNP P0DTC2
F	1258	GLU	-	expression tag	UNP P0DTC2
F	1259	ALA	-	expression tag	UNP P0DTC2
F	1260	GLN	-	expression tag	UNP P0DTC2
F	1261	LYS	-	expression tag	UNP P0DTC2
F	1262	ILE	-	expression tag	UNP P0DTC2
F	1263	GLU	-	expression tag	UNP P0DTC2
F	1264	TRP	-	expression tag	UNP P0DTC2
F	1265	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1266	GLU	-	expression tag	UNP P0DTC2
F	1267	GLY	-	expression tag	UNP P0DTC2
F	1268	SER	-	expression tag	UNP P0DTC2
F	1269	GLY	-	expression tag	UNP P0DTC2
F	1270	HIS	-	expression tag	UNP P0DTC2
F	1271	HIS	-	expression tag	UNP P0DTC2
F	1272	HIS	-	expression tag	UNP P0DTC2
F	1273	HIS	-	expression tag	UNP P0DTC2
F	1274	HIS	-	expression tag	UNP P0DTC2
F	1275	HIS	-	expression tag	UNP P0DTC2
F	1276	HIS	-	expression tag	UNP P0DTC2
F	1277	HIS	-	expression tag	UNP P0DTC2
K	13	ILE	SER	conflict	UNP P0DTC2
K	152	CYS	TRP	conflict	UNP P0DTC2
K	452	ARG	LEU	conflict	UNP P0DTC2
K	682	GLY	ARG	conflict	UNP P0DTC2
K	683	SER	ARG	conflict	UNP P0DTC2
K	685	SER	ARG	conflict	UNP P0DTC2
K	817	PRO	PHE	conflict	UNP P0DTC2
K	892	PRO	ALA	conflict	UNP P0DTC2
K	899	PRO	ALA	conflict	UNP P0DTC2
K	942	PRO	ALA	conflict	UNP P0DTC2
K	986	PRO	LYS	conflict	UNP P0DTC2
K	987	PRO	VAL	conflict	UNP P0DTC2
K	1209	GLY	-	expression tag	UNP P0DTC2
K	1210	SER	-	expression tag	UNP P0DTC2
K	1211	GLY	-	expression tag	UNP P0DTC2
K	1212	TYR	-	expression tag	UNP P0DTC2
K	1213	ILE	-	expression tag	UNP P0DTC2
K	1214	PRO	-	expression tag	UNP P0DTC2
K	1215	GLU	-	expression tag	UNP P0DTC2
K	1216	ALA	-	expression tag	UNP P0DTC2
K	1217	PRO	-	expression tag	UNP P0DTC2
K	1218	ARG	-	expression tag	UNP P0DTC2
K	1219	ASP	-	expression tag	UNP P0DTC2
K	1220	GLY	-	expression tag	UNP P0DTC2
K	1221	GLN	-	expression tag	UNP P0DTC2
K	1222	ALA	-	expression tag	UNP P0DTC2
K	1223	TYR	-	expression tag	UNP P0DTC2
K	1224	VAL	-	expression tag	UNP P0DTC2
K	1225	ARG	-	expression tag	UNP P0DTC2
K	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1227	ASP	-	expression tag	UNP P0DTC2
K	1228	GLY	-	expression tag	UNP P0DTC2
K	1229	GLU	-	expression tag	UNP P0DTC2
K	1230	TRP	-	expression tag	UNP P0DTC2
K	1231	VAL	-	expression tag	UNP P0DTC2
K	1232	LEU	-	expression tag	UNP P0DTC2
K	1233	LEU	-	expression tag	UNP P0DTC2
K	1234	SER	-	expression tag	UNP P0DTC2
K	1235	THR	-	expression tag	UNP P0DTC2
K	1236	PHE	-	expression tag	UNP P0DTC2
K	1237	LEU	-	expression tag	UNP P0DTC2
K	1238	GLY	-	expression tag	UNP P0DTC2
K	1239	ARG	-	expression tag	UNP P0DTC2
K	1240	SER	-	expression tag	UNP P0DTC2
K	1241	LEU	-	expression tag	UNP P0DTC2
K	1242	GLU	-	expression tag	UNP P0DTC2
K	1243	VAL	-	expression tag	UNP P0DTC2
K	1244	LEU	-	expression tag	UNP P0DTC2
K	1245	PHE	-	expression tag	UNP P0DTC2
K	1246	GLN	-	expression tag	UNP P0DTC2
K	1247	GLY	-	expression tag	UNP P0DTC2
K	1248	PRO	-	expression tag	UNP P0DTC2
K	1249	GLY	-	expression tag	UNP P0DTC2
K	1250	SER	-	expression tag	UNP P0DTC2
K	1251	GLY	-	expression tag	UNP P0DTC2
K	1252	GLY	-	expression tag	UNP P0DTC2
K	1253	LEU	-	expression tag	UNP P0DTC2
K	1254	ASN	-	expression tag	UNP P0DTC2
K	1255	ASP	-	expression tag	UNP P0DTC2
K	1256	ILE	-	expression tag	UNP P0DTC2
K	1257	PHE	-	expression tag	UNP P0DTC2
K	1258	GLU	-	expression tag	UNP P0DTC2
K	1259	ALA	-	expression tag	UNP P0DTC2
K	1260	GLN	-	expression tag	UNP P0DTC2
K	1261	LYS	-	expression tag	UNP P0DTC2
K	1262	ILE	-	expression tag	UNP P0DTC2
K	1263	GLU	-	expression tag	UNP P0DTC2
K	1264	TRP	-	expression tag	UNP P0DTC2
K	1265	HIS	-	expression tag	UNP P0DTC2
K	1266	GLU	-	expression tag	UNP P0DTC2
K	1267	GLY	-	expression tag	UNP P0DTC2
K	1268	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1269	GLY	-	expression tag	UNP P0DTC2
K	1270	HIS	-	expression tag	UNP P0DTC2
K	1271	HIS	-	expression tag	UNP P0DTC2
K	1272	HIS	-	expression tag	UNP P0DTC2
K	1273	HIS	-	expression tag	UNP P0DTC2
K	1274	HIS	-	expression tag	UNP P0DTC2
K	1275	HIS	-	expression tag	UNP P0DTC2
K	1276	HIS	-	expression tag	UNP P0DTC2
K	1277	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called S2M11 Fab Light Chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	104	Total	C	N	O	S	0	0
			751	475	127	145	4		
2	G	104	Total	C	N	O	S	0	0
			751	475	127	145	4		
2	L	104	Total	C	N	O	S	0	0
			751	475	127	145	4		

- Molecule 3 is a protein called S2M11 Fab Heavy Chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	122	Total	C	N	O	S	0	0
			953	613	155	179	6		
3	H	122	Total	C	N	O	S	0	0
			953	613	155	179	6		
3	M	122	Total	C	N	O	S	0	0
			953	613	155	179	6		

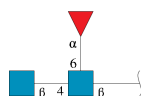
- Molecule 4 is a protein called S2L20 Fab Light Chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	106	Total	C	N	O	S	0	0
			538	324	106	106	2		
4	I	106	Total	C	N	O	S	0	0
			538	324	106	106	2		
4	N	106	Total	C	N	O	S	0	0
			538	324	106	106	2		

- Molecule 5 is a protein called S2L20 Fab Heavy Chain variable region.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	121	Total	C	N	O	S	0	0
			596	352	121	121	2		
5	J	121	Total	C	N	O	S	0	0
			596	352	121	121	2		
5	O	121	Total	C	N	O	S	0	0
			596	352	121	121	2		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



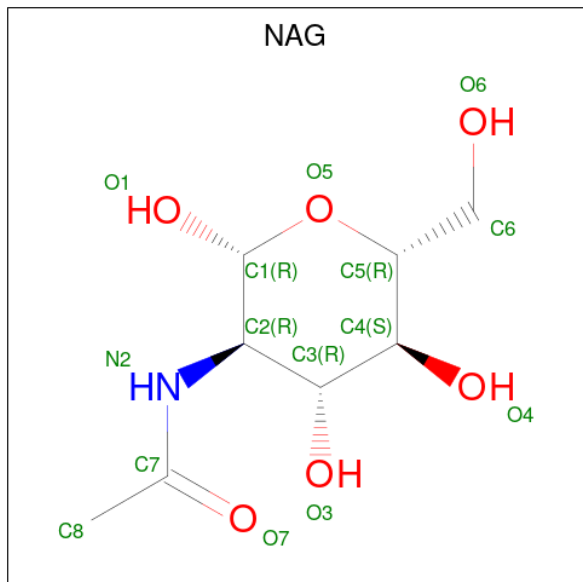
Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	3	Total	C	N	O	0	0
			38	22	2	14		
6	S	3	Total	C	N	O	0	0
			38	22	2	14		
6	V	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 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
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	R	2	Total	C	N	O	0	0
			28	16	2	10		
7	T	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

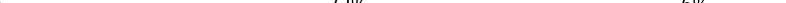
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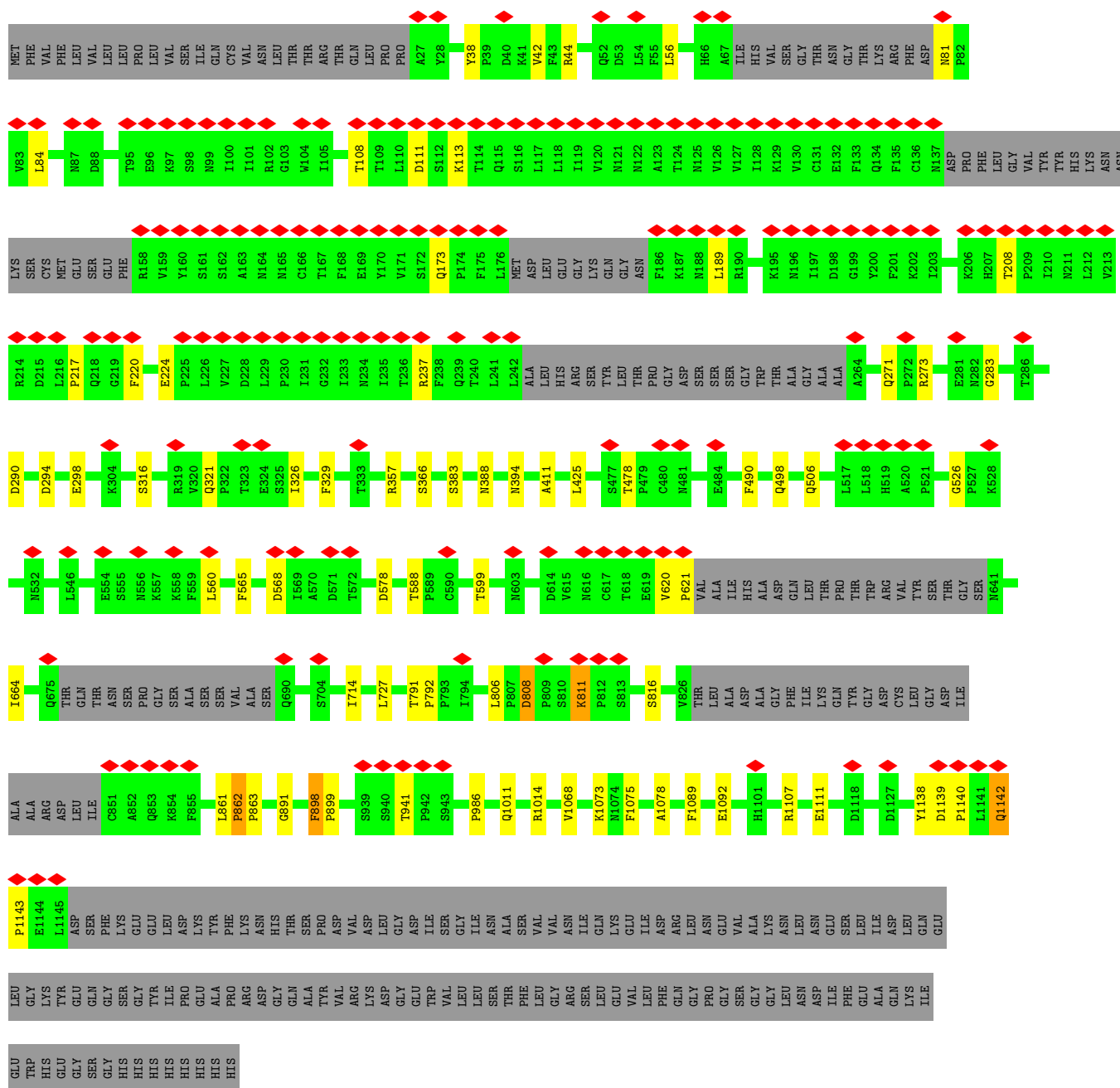
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Mol	Chain	Residues	Atoms				AltConf
8	K	1	Total	C	N	O	0
			14	8	1	5	
8	K	1	Total	C	N	O	0
			14	8	1	5	
8	K	1	Total	C	N	O	0
			14	8	1	5	
8	K	1	Total	C	N	O	0
			14	8	1	5	
8	K	1	Total	C	N	O	0
			14	8	1	5	
8	K	1	Total	C	N	O	0
			13	8	1	4	

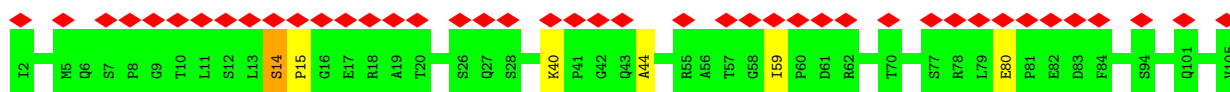
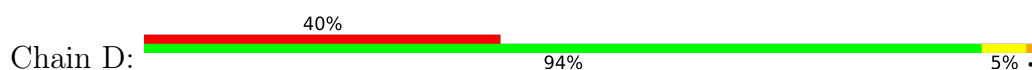
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	240	Total	O	0
			240	240	
9	D	2	Total	O	0
			2	2	
9	E	15	Total	O	0
			15	15	
9	F	240	Total	O	0
			240	240	
9	G	2	Total	O	0
			2	2	
9	H	15	Total	O	0
			15	15	
9	K	240	Total	O	0
			240	240	
9	L	2	Total	O	0
			2	2	
9	M	15	Total	O	0
			15	15	

Chain K: 

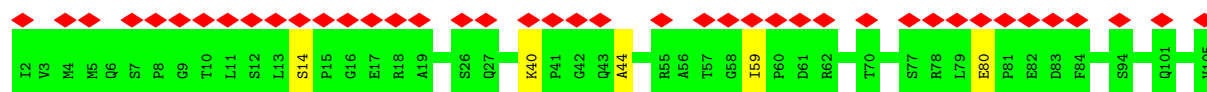


• Molecule 2: S2M11 Fab Light Chain variable region

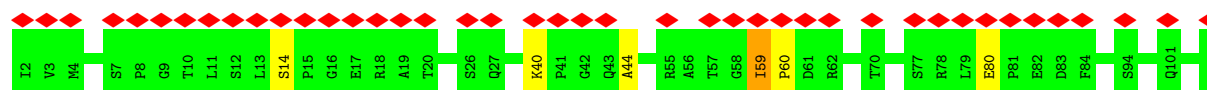
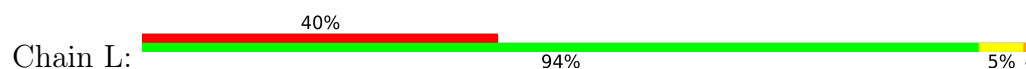


• Molecule 2: S2M11 Fab Light Chain variable region

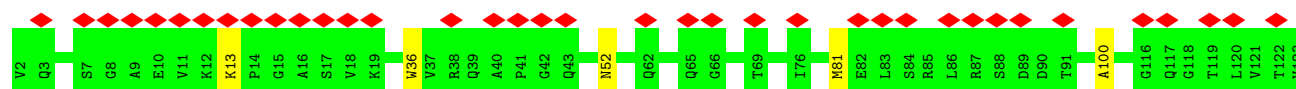




- Molecule 2: S2M11 Fab Light Chain variable region



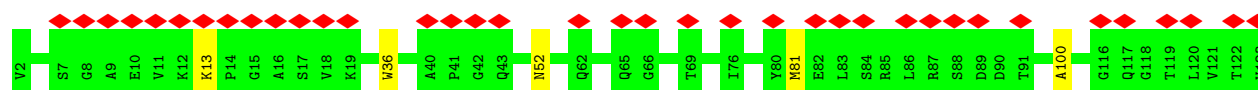
- Molecule 3: S2M11 Fab Heavy Chain variable region



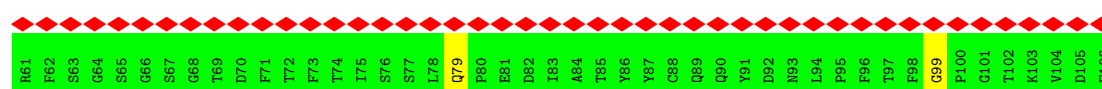
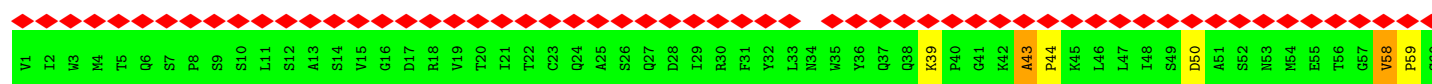
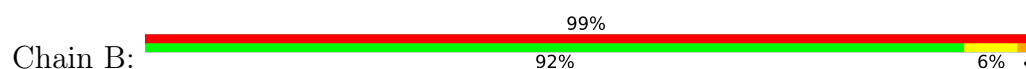
- Molecule 3: S2M11 Fab Heavy Chain variable region



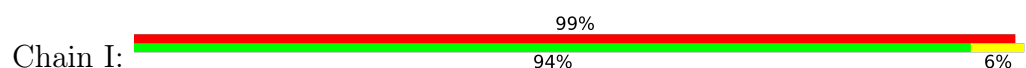
- Molecule 3: S2M11 Fab Heavy Chain variable region



- Molecule 4: S2L20 Fab Light Chain variable region



- Molecule 4: S2L20 Fab Light Chain variable region





• Molecule 4: S2L20 Fab Light Chain variable region



• Molecule 5: S2L20 Fab Heavy Chain variable region

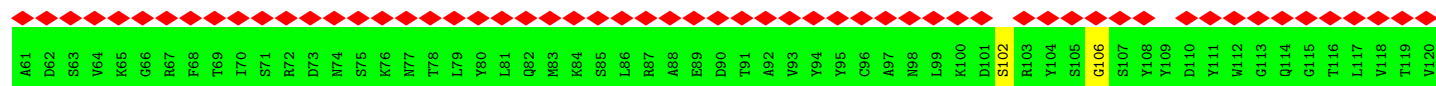
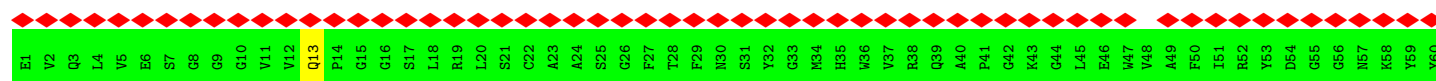


• Molecule 5: S2L20 Fab Heavy Chain variable region



• Molecule 5: S2L20 Fab Heavy Chain variable region





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	330083	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 ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.347	Depositor
Minimum map value	-6.580	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	431.616, 431.616, 431.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.843, 0.843, 0.843	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: FUC, 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	0.67	0/7776	0.95	87/10610 (0.8%)
1	F	0.68	0/7776	0.95	87/10610 (0.8%)
1	K	0.68	0/7776	0.95	87/10610 (0.8%)
2	D	0.55	0/770	0.94	10/1050 (1.0%)
2	G	0.55	0/770	0.94	10/1050 (1.0%)
2	L	0.55	0/770	0.94	10/1050 (1.0%)
3	E	0.58	0/983	0.85	6/1341 (0.4%)
3	H	0.59	0/983	0.85	6/1341 (0.4%)
3	M	0.59	0/983	0.85	6/1341 (0.4%)
4	B	0.52	0/544	1.09	10/760 (1.3%)
4	I	0.52	0/544	1.09	10/760 (1.3%)
4	N	0.52	0/544	1.09	10/760 (1.3%)
5	C	0.51	0/597	0.95	2/826 (0.2%)
5	J	0.51	0/597	0.95	2/826 (0.2%)
5	O	0.51	0/597	0.95	2/826 (0.2%)
All	All	0.64	0/32010	0.95	345/43761 (0.8%)

There are no bond length outliers.

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	791	THR	CA-C-N	9.08	126.20	119.66
1	A	791	THR	C-N-CA	9.08	126.20	119.66
1	K	791	THR	CA-C-N	9.04	126.17	119.66
1	K	791	THR	C-N-CA	9.04	126.17	119.66
1	F	791	THR	CA-C-N	9.02	126.16	119.66
1	F	791	THR	C-N-CA	9.02	126.16	119.66
1	A	861	LEU	CA-C-N	8.18	125.55	119.66
1	A	861	LEU	C-N-CA	8.18	125.55	119.66
1	K	861	LEU	CA-C-N	8.18	125.55	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	861	LEU	C-N-CA	8.18	125.55	119.66
1	K	986	PRO	N-CA-C	8.17	120.66	110.70
1	A	986	PRO	N-CA-C	8.16	120.66	110.70
1	F	986	PRO	N-CA-C	8.15	120.65	110.70
1	F	861	LEU	CA-C-N	8.14	125.52	119.66
1	F	861	LEU	C-N-CA	8.14	125.52	119.66
1	F	490	PHE	CA-C-N	7.88	127.52	119.56
1	F	490	PHE	C-N-CA	7.88	127.52	119.56
1	A	490	PHE	CA-C-N	7.84	127.48	119.56
1	A	490	PHE	C-N-CA	7.84	127.48	119.56
1	K	490	PHE	CA-C-N	7.82	127.46	119.56
1	K	490	PHE	C-N-CA	7.82	127.46	119.56
1	A	941	THR	CA-C-N	7.54	127.25	119.56
1	A	941	THR	C-N-CA	7.54	127.25	119.56
1	F	941	THR	CA-C-N	7.53	127.24	119.56
1	F	941	THR	C-N-CA	7.53	127.24	119.56
1	K	941	THR	CA-C-N	7.53	127.24	119.56
1	K	941	THR	C-N-CA	7.53	127.24	119.56
1	F	498	GLN	CA-C-N	7.21	126.91	119.56
1	F	498	GLN	C-N-CA	7.21	126.91	119.56
1	K	498	GLN	CA-C-N	7.20	126.91	119.56
1	K	498	GLN	C-N-CA	7.20	126.91	119.56
4	N	99	GLY	CA-C-N	7.20	127.53	119.32
4	N	99	GLY	C-N-CA	7.20	127.53	119.32
1	A	498	GLN	CA-C-N	7.20	126.90	119.56
1	A	498	GLN	C-N-CA	7.20	126.90	119.56
4	I	99	GLY	CA-C-N	7.18	127.51	119.32
4	I	99	GLY	C-N-CA	7.18	127.51	119.32
4	B	99	GLY	CA-C-N	7.17	127.50	119.32
4	B	99	GLY	C-N-CA	7.17	127.50	119.32
3	H	100	ALA	CA-C-N	7.11	127.07	120.03
3	H	100	ALA	C-N-CA	7.11	127.07	120.03
1	F	578	ASP	CA-C-N	7.11	126.81	119.56
1	F	578	ASP	C-N-CA	7.11	126.81	119.56
3	M	100	ALA	CA-C-N	7.09	127.05	120.03
3	M	100	ALA	C-N-CA	7.09	127.05	120.03
3	E	100	ALA	CA-C-N	7.08	127.04	120.03
3	E	100	ALA	C-N-CA	7.08	127.04	120.03
1	K	578	ASP	CA-C-N	7.07	126.77	119.56
1	K	578	ASP	C-N-CA	7.07	126.77	119.56
1	F	478	THR	CA-C-N	7.05	127.09	119.89
1	F	478	THR	C-N-CA	7.05	127.09	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	ASP	CA-C-N	7.05	126.75	119.56
1	A	578	ASP	C-N-CA	7.05	126.75	119.56
1	A	478	THR	CA-C-N	7.05	127.08	119.89
1	A	478	THR	C-N-CA	7.05	127.08	119.89
1	K	1078	ALA	CA-C-N	7.04	126.67	119.56
1	K	1078	ALA	C-N-CA	7.04	126.67	119.56
1	K	478	THR	CA-C-N	7.03	127.06	119.89
1	K	478	THR	C-N-CA	7.03	127.06	119.89
1	K	38	TYR	CA-C-N	7.02	126.65	119.56
1	K	38	TYR	C-N-CA	7.02	126.65	119.56
1	A	38	TYR	CA-C-N	7.02	126.65	119.56
1	A	38	TYR	C-N-CA	7.02	126.65	119.56
1	F	38	TYR	CA-C-N	7.01	126.64	119.56
1	F	38	TYR	C-N-CA	7.01	126.64	119.56
1	F	1078	ALA	CA-C-N	7.00	126.63	119.56
1	F	1078	ALA	C-N-CA	7.00	126.63	119.56
1	F	811	LYS	CA-C-N	6.99	126.97	119.28
1	F	811	LYS	C-N-CA	6.99	126.97	119.28
1	A	811	LYS	CA-C-N	6.99	126.97	119.28
1	A	811	LYS	C-N-CA	6.99	126.97	119.28
1	A	1078	ALA	CA-C-N	6.98	126.61	119.56
1	A	1078	ALA	C-N-CA	6.98	126.61	119.56
1	K	811	LYS	CA-C-N	6.97	126.95	119.28
1	K	811	LYS	C-N-CA	6.97	126.95	119.28
1	F	1068	VAL	CA-C-N	6.92	126.89	119.76
1	F	1068	VAL	C-N-CA	6.92	126.89	119.76
1	A	1068	VAL	CA-C-N	6.91	126.88	119.76
1	A	1068	VAL	C-N-CA	6.91	126.88	119.76
1	K	1068	VAL	CA-C-N	6.91	126.88	119.76
1	K	1068	VAL	C-N-CA	6.91	126.88	119.76
1	A	81	ASN	CA-C-N	6.89	126.85	120.03
1	A	81	ASN	C-N-CA	6.89	126.85	120.03
1	F	81	ASN	CA-C-N	6.88	126.84	120.03
1	F	81	ASN	C-N-CA	6.88	126.84	120.03
1	K	81	ASN	CA-C-N	6.87	126.83	120.03
1	K	81	ASN	C-N-CA	6.87	126.83	120.03
2	D	59	ILE	CA-C-N	6.84	126.87	119.89
2	D	59	ILE	C-N-CA	6.84	126.87	119.89
2	L	59	ILE	CA-C-N	6.83	126.86	119.89
2	L	59	ILE	C-N-CA	6.83	126.86	119.89
2	G	59	ILE	CA-C-N	6.82	126.85	119.89
2	G	59	ILE	C-N-CA	6.82	126.85	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	792	PRO	CA-C-N	6.82	127.10	119.32
1	A	792	PRO	C-N-CA	6.82	127.10	119.32
1	K	792	PRO	CA-C-N	6.82	127.09	119.32
1	K	792	PRO	C-N-CA	6.82	127.09	119.32
1	F	792	PRO	CA-C-N	6.82	127.09	119.32
1	F	792	PRO	C-N-CA	6.82	127.09	119.32
1	F	727	LEU	CA-C-N	6.76	126.72	119.76
1	F	727	LEU	C-N-CA	6.76	126.72	119.76
1	A	727	LEU	CA-C-N	6.74	126.70	119.76
1	A	727	LEU	C-N-CA	6.74	126.70	119.76
3	E	52	ASN	CA-C-N	6.73	127.28	119.47
3	E	52	ASN	C-N-CA	6.73	127.28	119.47
3	M	52	ASN	CA-C-N	6.73	127.28	119.47
3	M	52	ASN	C-N-CA	6.73	127.28	119.47
1	K	727	LEU	CA-C-N	6.72	126.69	119.76
1	K	727	LEU	C-N-CA	6.72	126.69	119.76
1	A	808	ASP	CA-C-N	6.71	126.41	119.56
1	A	808	ASP	C-N-CA	6.71	126.41	119.56
1	F	808	ASP	CA-C-N	6.71	126.40	119.56
1	F	808	ASP	C-N-CA	6.71	126.40	119.56
1	K	808	ASP	CA-C-N	6.71	126.40	119.56
1	K	808	ASP	C-N-CA	6.71	126.40	119.56
3	H	52	ASN	CA-C-N	6.70	127.25	119.47
3	H	52	ASN	C-N-CA	6.70	127.25	119.47
1	F	383	SER	CA-C-N	6.69	126.64	119.28
1	F	383	SER	C-N-CA	6.69	126.64	119.28
4	I	43	ALA	CA-C-N	6.68	126.64	119.76
4	I	43	ALA	C-N-CA	6.68	126.64	119.76
1	K	383	SER	CA-C-N	6.68	126.62	119.28
1	K	383	SER	C-N-CA	6.68	126.62	119.28
4	N	43	ALA	CA-C-N	6.65	126.61	119.76
4	N	43	ALA	C-N-CA	6.65	126.61	119.76
4	I	58	VAL	CA-C-N	6.65	126.68	119.90
4	I	58	VAL	C-N-CA	6.65	126.68	119.90
4	B	43	ALA	CA-C-N	6.65	126.61	119.76
4	B	43	ALA	C-N-CA	6.65	126.61	119.76
1	A	383	SER	CA-C-N	6.64	126.59	119.28
1	A	383	SER	C-N-CA	6.64	126.59	119.28
4	N	58	VAL	CA-C-N	6.62	126.66	119.90
4	N	58	VAL	C-N-CA	6.62	126.66	119.90
4	B	58	VAL	CA-C-N	6.60	126.63	119.90
4	B	58	VAL	C-N-CA	6.60	126.63	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	816	SER	CA-C-N	6.60	126.84	119.32
1	K	816	SER	C-N-CA	6.60	126.84	119.32
1	K	208	THR	CA-C-N	6.59	126.35	119.76
1	K	208	THR	C-N-CA	6.59	126.35	119.76
1	A	208	THR	CA-C-N	6.59	126.35	119.76
1	A	208	THR	C-N-CA	6.59	126.35	119.76
1	F	208	THR	CA-C-N	6.59	126.35	119.76
1	F	208	THR	C-N-CA	6.59	126.35	119.76
1	F	425	LEU	CA-C-N	6.59	126.55	120.03
1	F	425	LEU	C-N-CA	6.59	126.55	120.03
1	K	425	LEU	CA-C-N	6.58	126.55	120.03
1	K	425	LEU	C-N-CA	6.58	126.55	120.03
1	A	816	SER	CA-C-N	6.58	126.81	119.32
1	A	816	SER	C-N-CA	6.58	126.81	119.32
1	F	816	SER	CA-C-N	6.58	126.82	119.32
1	F	816	SER	C-N-CA	6.58	126.82	119.32
1	A	425	LEU	CA-C-N	6.56	126.53	120.03
1	A	425	LEU	C-N-CA	6.56	126.53	120.03
1	A	1139	ASP	CA-C-N	6.55	128.03	119.84
1	A	1139	ASP	C-N-CA	6.55	128.03	119.84
1	F	1139	ASP	CA-C-N	6.54	128.02	119.84
1	F	1139	ASP	C-N-CA	6.54	128.02	119.84
1	K	1139	ASP	CA-C-N	6.54	128.02	119.84
1	K	1139	ASP	C-N-CA	6.54	128.02	119.84
2	L	80	GLU	CA-C-N	6.45	126.14	119.56
2	L	80	GLU	C-N-CA	6.45	126.14	119.56
2	D	80	GLU	CA-C-N	6.44	126.13	119.56
2	D	80	GLU	C-N-CA	6.44	126.13	119.56
2	G	80	GLU	CA-C-N	6.42	126.11	119.56
2	G	80	GLU	C-N-CA	6.42	126.11	119.56
1	F	294	ASP	CA-C-N	6.41	126.63	119.32
1	F	294	ASP	C-N-CA	6.41	126.63	119.32
1	K	329	PHE	CA-C-N	6.40	126.37	119.78
1	K	329	PHE	C-N-CA	6.40	126.37	119.78
1	A	294	ASP	CA-C-N	6.38	126.60	119.32
1	A	294	ASP	C-N-CA	6.38	126.60	119.32
1	K	294	ASP	CA-C-N	6.37	126.58	119.32
1	K	294	ASP	C-N-CA	6.37	126.58	119.32
1	F	329	PHE	CA-C-N	6.37	126.34	119.78
1	F	329	PHE	C-N-CA	6.37	126.34	119.78
1	K	526	GLY	CA-C-N	6.37	127.80	119.84
1	K	526	GLY	C-N-CA	6.37	127.80	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	13	LYS	CA-C-N	6.36	126.31	119.76
3	E	13	LYS	C-N-CA	6.36	126.31	119.76
1	K	862	PRO	CA-C-N	6.36	126.33	119.78
1	K	862	PRO	C-N-CA	6.36	126.33	119.78
1	A	329	PHE	CA-C-N	6.36	126.33	119.78
1	A	329	PHE	C-N-CA	6.36	126.33	119.78
3	M	13	LYS	CA-C-N	6.35	126.31	119.76
3	M	13	LYS	C-N-CA	6.35	126.31	119.76
1	F	862	PRO	CA-C-N	6.35	126.32	119.78
1	F	862	PRO	C-N-CA	6.35	126.32	119.78
3	H	13	LYS	CA-C-N	6.35	126.30	119.76
3	H	13	LYS	C-N-CA	6.35	126.30	119.76
1	A	526	GLY	CA-C-N	6.35	127.78	119.84
1	A	526	GLY	C-N-CA	6.35	127.78	119.84
1	F	526	GLY	CA-C-N	6.35	127.77	119.84
1	F	526	GLY	C-N-CA	6.35	127.77	119.84
1	A	506	GLN	CA-C-N	6.35	126.11	119.76
1	A	506	GLN	C-N-CA	6.35	126.11	119.76
1	K	506	GLN	CA-C-N	6.34	126.10	119.76
1	K	506	GLN	C-N-CA	6.34	126.10	119.76
1	F	506	GLN	CA-C-N	6.34	126.10	119.76
1	F	506	GLN	C-N-CA	6.34	126.10	119.76
1	A	862	PRO	CA-C-N	6.32	126.29	119.78
1	A	862	PRO	C-N-CA	6.32	126.29	119.78
1	F	560	LEU	CA-C-N	6.30	126.78	119.47
1	F	560	LEU	C-N-CA	6.30	126.78	119.47
2	D	14	SER	CA-C-N	6.28	126.23	119.76
2	D	14	SER	C-N-CA	6.28	126.23	119.76
1	A	560	LEU	CA-C-N	6.28	126.75	119.47
1	A	560	LEU	C-N-CA	6.28	126.75	119.47
2	L	14	SER	CA-C-N	6.28	126.22	119.76
2	L	14	SER	C-N-CA	6.28	126.22	119.76
2	G	14	SER	CA-C-N	6.27	126.22	119.76
2	G	14	SER	C-N-CA	6.27	126.22	119.76
1	K	560	LEU	CA-C-N	6.26	126.73	119.47
1	K	560	LEU	C-N-CA	6.26	126.73	119.47
1	K	714	ILE	CA-C-N	6.25	126.20	119.76
1	K	714	ILE	C-N-CA	6.25	126.20	119.76
1	A	714	ILE	CA-C-N	6.24	126.19	119.76
1	A	714	ILE	C-N-CA	6.24	126.19	119.76
1	F	714	ILE	CA-C-N	6.23	126.17	119.76
1	F	714	ILE	C-N-CA	6.23	126.17	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLN	CA-C-N	6.20	126.22	119.90
1	A	173	GLN	C-N-CA	6.20	126.22	119.90
1	K	173	GLN	CA-C-N	6.19	126.22	119.90
1	K	173	GLN	C-N-CA	6.19	126.22	119.90
1	F	1111	GLU	CA-C-N	6.16	126.37	119.90
1	F	1111	GLU	C-N-CA	6.16	126.37	119.90
1	A	1111	GLU	CA-C-N	6.15	126.36	119.90
1	A	1111	GLU	C-N-CA	6.15	126.36	119.90
1	F	173	GLN	CA-C-N	6.15	126.17	119.90
1	F	173	GLN	C-N-CA	6.15	126.17	119.90
1	K	1111	GLU	CA-C-N	6.14	126.35	119.90
1	K	1111	GLU	C-N-CA	6.14	126.35	119.90
1	A	84	LEU	CA-C-N	6.09	126.00	119.85
1	A	84	LEU	C-N-CA	6.09	126.00	119.85
2	G	44	ALA	CA-C-N	6.07	126.04	119.78
2	G	44	ALA	C-N-CA	6.07	126.04	119.78
1	F	84	LEU	CA-C-N	6.07	125.98	119.85
1	F	84	LEU	C-N-CA	6.07	125.98	119.85
2	L	44	ALA	CA-C-N	6.05	126.02	119.78
2	L	44	ALA	C-N-CA	6.05	126.02	119.78
2	D	44	ALA	CA-C-N	6.05	126.01	119.78
2	D	44	ALA	C-N-CA	6.05	126.01	119.78
1	K	84	LEU	CA-C-N	6.04	125.95	119.85
1	K	84	LEU	C-N-CA	6.04	125.95	119.85
1	F	588	THR	CA-C-N	6.04	125.95	119.85
1	F	588	THR	C-N-CA	6.04	125.95	119.85
1	K	588	THR	CA-C-N	6.04	125.95	119.85
1	K	588	THR	C-N-CA	6.04	125.95	119.85
1	A	588	THR	CA-C-N	6.02	125.93	119.85
1	A	588	THR	C-N-CA	6.02	125.93	119.85
1	K	806	LEU	CA-C-N	5.94	125.88	119.76
1	K	806	LEU	C-N-CA	5.94	125.88	119.76
1	F	806	LEU	CA-C-N	5.93	125.87	119.76
1	F	806	LEU	C-N-CA	5.93	125.87	119.76
1	A	806	LEU	CA-C-N	5.92	125.86	119.76
1	A	806	LEU	C-N-CA	5.92	125.86	119.76
1	K	1142	GLN	CA-C-N	5.86	125.47	119.56
1	K	1142	GLN	C-N-CA	5.86	125.47	119.56
1	F	1142	GLN	CA-C-N	5.85	125.46	119.56
1	F	1142	GLN	C-N-CA	5.85	125.46	119.56
1	A	1142	GLN	CA-C-N	5.84	125.46	119.56
1	A	1142	GLN	C-N-CA	5.84	125.46	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	599	THR	CA-C-N	5.76	125.73	120.03
1	K	599	THR	C-N-CA	5.76	125.73	120.03
1	A	898	PHE	CA-C-N	5.75	125.44	119.05
1	A	898	PHE	C-N-CA	5.75	125.44	119.05
1	A	599	THR	CA-C-N	5.75	125.72	120.03
1	A	599	THR	C-N-CA	5.75	125.72	120.03
1	F	898	PHE	CA-C-N	5.75	125.43	119.05
1	F	898	PHE	C-N-CA	5.75	125.43	119.05
1	F	599	THR	CA-C-N	5.74	125.72	120.03
1	F	599	THR	C-N-CA	5.74	125.72	120.03
1	K	898	PHE	CA-C-N	5.72	125.39	119.05
1	K	898	PHE	C-N-CA	5.72	125.39	119.05
1	A	224	GLU	CA-C-N	5.71	126.05	119.93
1	A	224	GLU	C-N-CA	5.71	126.05	119.93
5	O	13	GLN	CA-C-N	5.70	126.03	119.93
5	O	13	GLN	C-N-CA	5.70	126.03	119.93
1	A	321	GLN	CA-C-N	5.69	125.97	119.83
1	A	321	GLN	C-N-CA	5.69	125.97	119.83
5	J	13	GLN	CA-C-N	5.69	126.02	119.93
5	J	13	GLN	C-N-CA	5.69	126.02	119.93
5	C	13	GLN	CA-C-N	5.68	126.01	119.93
5	C	13	GLN	C-N-CA	5.68	126.01	119.93
1	K	321	GLN	CA-C-N	5.68	125.97	119.83
1	K	321	GLN	C-N-CA	5.68	125.97	119.83
1	F	321	GLN	CA-C-N	5.68	125.96	119.83
1	F	321	GLN	C-N-CA	5.68	125.96	119.83
1	K	224	GLU	CA-C-N	5.67	126.00	119.93
1	K	224	GLU	C-N-CA	5.67	126.00	119.93
1	F	224	GLU	CA-C-N	5.66	125.99	119.93
1	F	224	GLU	C-N-CA	5.66	125.99	119.93
4	N	79	GLN	CA-C-N	5.53	125.88	119.47
4	N	79	GLN	C-N-CA	5.53	125.88	119.47
1	A	891	GLY	CA-C-N	5.52	125.28	119.76
1	A	891	GLY	C-N-CA	5.52	125.28	119.76
1	F	411	ALA	CA-C-N	5.52	125.45	119.76
1	F	411	ALA	C-N-CA	5.52	125.45	119.76
1	F	664	ILE	CA-C-N	5.52	125.69	119.90
1	F	664	ILE	C-N-CA	5.52	125.69	119.90
1	A	56	LEU	CA-C-N	5.51	125.44	119.76
1	A	56	LEU	C-N-CA	5.51	125.44	119.76
4	I	79	GLN	CA-C-N	5.51	125.86	119.47
4	I	79	GLN	C-N-CA	5.51	125.86	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	664	ILE	CA-C-N	5.51	125.69	119.90
1	K	664	ILE	C-N-CA	5.51	125.69	119.90
1	K	891	GLY	CA-C-N	5.51	125.27	119.76
1	K	891	GLY	C-N-CA	5.51	125.27	119.76
4	B	79	GLN	CA-C-N	5.50	125.85	119.47
4	B	79	GLN	C-N-CA	5.50	125.85	119.47
1	A	664	ILE	CA-C-N	5.50	125.68	119.90
1	A	664	ILE	C-N-CA	5.50	125.68	119.90
1	K	56	LEU	CA-C-N	5.50	125.42	119.76
1	K	56	LEU	C-N-CA	5.50	125.42	119.76
1	K	411	ALA	CA-C-N	5.50	125.42	119.76
1	K	411	ALA	C-N-CA	5.50	125.42	119.76
1	F	56	LEU	CA-C-N	5.49	125.41	119.76
1	F	56	LEU	C-N-CA	5.49	125.41	119.76
1	A	411	ALA	CA-C-N	5.49	125.41	119.76
1	A	411	ALA	C-N-CA	5.49	125.41	119.76
1	F	891	GLY	CA-C-N	5.47	125.23	119.76
1	F	891	GLY	C-N-CA	5.47	125.23	119.76
4	N	39	LYS	CA-C-N	5.34	125.65	119.93
4	N	39	LYS	C-N-CA	5.34	125.65	119.93
4	I	39	LYS	CA-C-N	5.34	125.64	119.93
4	I	39	LYS	C-N-CA	5.34	125.64	119.93
4	B	39	LYS	CA-C-N	5.34	125.64	119.93
4	B	39	LYS	C-N-CA	5.34	125.64	119.93
2	G	40	LYS	CA-C-N	5.32	125.63	119.93
2	G	40	LYS	C-N-CA	5.32	125.63	119.93
2	L	40	LYS	CA-C-N	5.30	125.61	119.93
2	L	40	LYS	C-N-CA	5.30	125.61	119.93
2	D	40	LYS	CA-C-N	5.29	125.59	119.93
2	D	40	LYS	C-N-CA	5.29	125.59	119.93
1	A	1089	PHE	CA-C-N	5.28	125.19	119.76
1	A	1089	PHE	C-N-CA	5.28	125.19	119.76
1	F	1089	PHE	CA-C-N	5.26	125.18	119.76
1	F	1089	PHE	C-N-CA	5.26	125.18	119.76
1	K	1089	PHE	CA-C-N	5.26	125.18	119.76
1	K	1089	PHE	C-N-CA	5.26	125.18	119.76
1	F	271	GLN	CA-C-N	5.06	126.17	119.84
1	F	271	GLN	C-N-CA	5.06	126.17	119.84
1	A	271	GLN	CA-C-N	5.04	126.15	119.84
1	A	271	GLN	C-N-CA	5.04	126.15	119.84
1	K	271	GLN	CA-C-N	5.04	126.14	119.84
1	K	271	GLN	C-N-CA	5.04	126.14	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7603	0	7212	24	0
1	F	7603	0	7212	24	0
1	K	7603	0	7212	26	0
2	D	751	0	695	1	0
2	G	751	0	695	0	0
2	L	751	0	695	1	0
3	E	953	0	884	1	0
3	H	953	0	884	1	0
3	M	953	0	884	1	0
4	B	538	0	276	3	0
4	I	538	0	276	1	0
4	N	538	0	276	1	0
5	C	596	0	297	2	0
5	J	596	0	297	2	0
5	O	596	0	297	2	0
6	P	38	0	34	2	0
6	S	38	0	34	2	0
6	V	38	0	34	2	0
7	Q	28	0	25	2	0
7	R	28	0	25	2	0
7	T	28	0	25	2	0
7	U	28	0	25	2	0
7	W	28	0	25	2	0
7	X	28	0	25	2	0
8	A	182	0	169	0	0
8	F	182	0	169	0	0
8	K	181	0	169	0	0
9	A	240	0	0	0	0
9	D	2	0	0	0	0
9	E	15	0	0	0	0
9	F	240	0	0	0	0
9	G	2	0	0	0	0
9	H	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	240	0	0	0	0
9	L	2	0	0	0	0
9	M	15	0	0	0	0
All	All	32921	0	28851	96	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 2.

All (96) 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)
7:X:1:NAG:C4	7:X:2:NAG:C1	2.38	1.02
7:T:1:NAG:C4	7:T:2:NAG:C1	2.38	1.02
7:R:1:NAG:C4	7:R:2:NAG:C1	2.38	1.01
7:U:1:NAG:C4	7:U:2:NAG:C1	2.38	1.01
7:W:1:NAG:C4	7:W:2:NAG:C1	2.38	1.00
7:Q:1:NAG:C4	7:Q:2:NAG:C1	2.38	1.00
6:V:1:NAG:C4	6:V:2:NAG:C1	2.42	0.97
6:S:1:NAG:C4	6:S:2:NAG:C1	2.42	0.97
6:P:1:NAG:C4	6:P:2:NAG:C1	2.42	0.96
7:R:1:NAG:H4	7:R:2:NAG:C1	2.27	0.65
7:W:1:NAG:H4	7:W:2:NAG:C1	2.28	0.63
7:U:1:NAG:H4	7:U:2:NAG:C1	2.27	0.62
7:X:1:NAG:H4	7:X:2:NAG:C1	2.27	0.61
7:T:1:NAG:H4	7:T:2:NAG:C1	2.28	0.60
7:Q:1:NAG:H4	7:Q:2:NAG:C1	2.28	0.58
1:A:808:ASP:OD2	1:A:811:LYS:NZ	2.43	0.52
1:F:808:ASP:OD2	1:F:811:LYS:NZ	2.43	0.52
1:A:298:GLU:OE2	1:A:316:SER:HB3	2.10	0.51
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.25	0.51
1:F:1142:GLN:N	1:F:1143:PRO:HD2	2.25	0.51
1:K:298:GLU:OE2	1:K:316:SER:HB3	2.10	0.51
1:K:1142:GLN:N	1:K:1143:PRO:HD2	2.25	0.51
1:F:298:GLU:OE2	1:F:316:SER:HB3	2.10	0.51
1:K:1092:GLU:O	1:K:1107:ARG:NH1	2.45	0.50
1:A:1092:GLU:O	1:A:1107:ARG:NH1	2.45	0.50
1:F:1092:GLU:O	1:F:1107:ARG:NH1	2.45	0.49
1:A:189:LEU:HD22	1:A:217:PRO:HG3	1.94	0.49
1:K:808:ASP:OD2	1:K:811:LYS:NZ	2.43	0.49
6:P:1:NAG:H4	6:P:2:NAG:C1	2.39	0.48
1:A:273:ARG:HH11	1:A:290:ASP:CG	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:LEU:HD22	1:F:217:PRO:HG3	1.94	0.48
1:F:273:ARG:HH11	1:F:290:ASP:CG	2.22	0.48
1:K:273:ARG:HH11	1:K:290:ASP:CG	2.22	0.48
1:K:898:PHE:N	1:K:899:PRO:CD	2.77	0.48
6:V:1:NAG:H4	6:V:2:NAG:C1	2.38	0.48
1:K:189:LEU:HD22	1:K:217:PRO:HG3	1.95	0.48
6:S:1:NAG:H4	6:S:2:NAG:C1	2.38	0.47
1:F:898:PHE:N	1:F:899:PRO:CD	2.77	0.47
1:A:898:PHE:N	1:A:899:PRO:CD	2.77	0.46
1:A:113:LYS:HE2	4:B:50:ASP:O	2.16	0.45
1:A:357:ARG:NH2	1:A:394:ASN:OD1	2.50	0.45
1:F:113:LYS:HE2	4:I:50:ASP:O	2.16	0.45
1:K:111:ASP:OD1	1:K:111:ASP:C	2.59	0.45
1:F:111:ASP:OD1	1:F:111:ASP:C	2.59	0.45
1:K:113:LYS:HE2	4:N:50:ASP:O	2.16	0.45
1:A:111:ASP:OD1	1:A:111:ASP:C	2.59	0.45
1:F:357:ARG:NH2	1:F:394:ASN:OD1	2.50	0.45
1:K:862:PRO:HA	1:K:863:PRO:HD3	1.86	0.45
1:A:620:VAL:N	1:A:621:PRO:HD2	2.33	0.45
1:K:357:ARG:NH2	1:K:394:ASN:OD1	2.50	0.45
1:A:189:LEU:CD2	1:A:217:PRO:HG3	2.48	0.44
1:K:620:VAL:N	1:K:621:PRO:HD2	2.32	0.44
1:K:898:PHE:HB3	1:K:899:PRO:HD3	2.00	0.44
1:K:1073:LYS:HG3	1:K:1075:PHE:CE2	2.53	0.43
1:F:189:LEU:CD2	1:F:217:PRO:HG3	2.48	0.43
1:F:620:VAL:N	1:F:621:PRO:HD2	2.32	0.43
1:F:898:PHE:HB3	1:F:899:PRO:HD3	2.00	0.43
1:A:366:SER:HB3	1:A:388:ASN:HD21	1.84	0.43
1:F:237:ARG:HG2	5:J:106:GLY:HA2	2.01	0.43
1:A:898:PHE:HB3	1:A:899:PRO:HD3	2.00	0.43
1:F:220:PHE:CD2	1:F:220:PHE:C	2.97	0.43
1:K:237:ARG:HG2	5:O:106:GLY:HA2	2.01	0.43
1:A:1073:LYS:HG3	1:A:1075:PHE:CE2	2.53	0.42
1:F:366:SER:HB3	1:F:388:ASN:HD21	1.84	0.42
1:K:189:LEU:CD2	1:K:217:PRO:HG3	2.48	0.42
1:A:220:PHE:CD2	1:A:220:PHE:C	2.97	0.42
1:F:1073:LYS:HG3	1:F:1075:PHE:CE2	2.54	0.42
1:A:237:ARG:HG2	5:C:106:GLY:HA2	2.01	0.42
1:K:366:SER:HB3	1:K:388:ASN:HD21	1.84	0.42
1:K:220:PHE:CD2	1:K:220:PHE:C	2.97	0.41
1:K:1138:TYR:CE2	1:K:1140:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:59:ILE:HA	2:L:60:PRO:HD3	1.88	0.41
1:A:1138:TYR:CE2	1:A:1140:PRO:HA	2.55	0.41
1:A:565:PHE:CE1	1:F:42:VAL:HG22	2.56	0.41
3:H:36:TRP:CE2	3:H:81:MET:HB2	2.56	0.41
1:A:326:ILE:O	1:A:326:ILE:HG13	2.21	0.41
1:F:565:PHE:CE1	1:K:42:VAL:HG22	2.56	0.41
1:F:1138:TYR:CE2	1:F:1140:PRO:HA	2.55	0.41
3:M:36:TRP:CE2	3:M:81:MET:HB2	2.56	0.41
1:A:108:THR:HB	5:C:102:SER:O	2.20	0.41
3:E:36:TRP:CE2	3:E:81:MET:HB2	2.56	0.41
1:K:108:THR:HB	5:O:102:SER:O	2.20	0.41
4:B:58:VAL:HA	4:B:59:PRO:HD3	1.90	0.40
1:F:108:THR:HB	5:J:102:SER:O	2.20	0.40
1:F:1011:GLN:OE1	1:F:1014:ARG:NH1	2.54	0.40
1:A:44:ARG:O	1:A:283:GLY:HA2	2.21	0.40
1:K:44:ARG:O	1:K:283:GLY:HA2	2.21	0.40
1:K:568:ASP:OD1	1:K:568:ASP:C	2.64	0.40
4:B:43:ALA:HA	4:B:44:PRO:HD3	1.90	0.40
1:A:568:ASP:OD1	1:A:568:ASP:C	2.64	0.40
2:D:14:SER:HA	2:D:15:PRO:HD3	1.96	0.40
1:K:326:ILE:O	1:K:326:ILE:HG13	2.21	0.40
1:K:1011:GLN:OE1	1:K:1014:ARG:NH1	2.54	0.40
1:A:42:VAL:HG22	1:K:565:PHE:CE1	2.56	0.40
1:F:44:ARG:O	1:F:283:GLY:HA2	2.21	0.40
1:F:326:ILE:O	1:F:326:ILE:HG13	2.21	0.40

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	983/1277 (77%)	964 (98%)	19 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	983/1277 (77%)	964 (98%)	19 (2%)	0	100	100
1	K	983/1277 (77%)	964 (98%)	19 (2%)	0	100	100
2	D	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
2	G	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
2	L	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
3	E	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
3	H	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
3	M	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
4	B	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
4	I	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
4	N	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
5	C	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
5	J	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
5	O	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
All	All	4284/5190 (82%)	4212 (98%)	72 (2%)	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	818/1111 (74%)	818 (100%)	0	100	100
1	F	818/1111 (74%)	818 (100%)	0	100	100
1	K	818/1111 (74%)	818 (100%)	0	100	100
2	D	75/85 (88%)	75 (100%)	0	100	100
2	G	75/85 (88%)	75 (100%)	0	100	100
2	L	75/85 (88%)	75 (100%)	0	100	100
3	E	97/100 (97%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	97/100 (97%)	97 (100%)	0	100	100
3	M	97/100 (97%)	97 (100%)	0	100	100
4	B	9/93 (10%)	9 (100%)	0	100	100
4	I	9/93 (10%)	9 (100%)	0	100	100
4	N	9/93 (10%)	9 (100%)	0	100	100
5	C	4/98 (4%)	4 (100%)	0	100	100
5	J	4/98 (4%)	4 (100%)	0	100	100
5	O	4/98 (4%)	4 (100%)	0	100	100
All	All	3009/4461 (68%)	3009 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	A	762	GLN
1	A	935	GLN
1	A	949	GLN
1	A	1010	GLN
1	F	450	ASN
1	F	762	GLN
1	F	935	GLN
1	F	949	GLN
1	F	1010	GLN
1	K	450	ASN
1	K	762	GLN
1	K	935	GLN
1	K	949	GLN
1	K	1010	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

21 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$
6	NAG	P	1	1,6	14,14,15	2.52	5 (35%)	17,19,21	2.22	4 (23%)
6	NAG	P	2	6	14,14,15	2.11	3 (21%)	17,19,21	1.59	4 (23%)
6	FUC	P	3	6	10,10,11	2.01	4 (40%)	14,14,16	0.85	0
7	NAG	Q	1	1,7	14,14,15	2.22	4 (28%)	17,19,21	1.87	6 (35%)
7	NAG	Q	2	7	14,14,15	1.23	1 (7%)	17,19,21	0.87	0
7	NAG	R	1	1,7	14,14,15	2.27	4 (28%)	17,19,21	1.91	6 (35%)
7	NAG	R	2	7	14,14,15	1.23	1 (7%)	17,19,21	0.93	1 (5%)
6	NAG	S	1	1,6	14,14,15	2.51	5 (35%)	17,19,21	2.22	4 (23%)
6	NAG	S	2	6	14,14,15	2.11	3 (21%)	17,19,21	1.60	4 (23%)
6	FUC	S	3	6	10,10,11	2.01	4 (40%)	14,14,16	0.85	0
7	NAG	T	1	1,7	14,14,15	2.22	4 (28%)	17,19,21	1.87	6 (35%)
7	NAG	T	2	7	14,14,15	1.23	1 (7%)	17,19,21	0.87	0
7	NAG	U	1	1,7	14,14,15	2.27	4 (28%)	17,19,21	1.90	6 (35%)
7	NAG	U	2	7	14,14,15	1.23	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	V	1	1,6	14,14,15	2.51	5 (35%)	17,19,21	2.22	4 (23%)
6	NAG	V	2	6	14,14,15	2.11	3 (21%)	17,19,21	1.59	4 (23%)
6	FUC	V	3	6	10,10,11	2.01	4 (40%)	14,14,16	0.85	0
7	NAG	W	1	1,7	14,14,15	2.22	4 (28%)	17,19,21	1.87	6 (35%)
7	NAG	W	2	7	14,14,15	1.23	1 (7%)	17,19,21	0.87	0
7	NAG	X	1	1,7	14,14,15	2.27	4 (28%)	17,19,21	1.90	6 (35%)
7	NAG	X	2	7	14,14,15	1.23	1 (7%)	17,19,21	0.92	1 (5%)

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
6	NAG	P	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	FUC	P	3	6	-	-	0/1/1/1
7	NAG	Q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	NAG	R	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	R	2	7	-	0/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	FUC	S	3	6	-	-	0/1/1/1
7	NAG	T	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	NAG	U	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
6	FUC	V	3	6	-	-	0/1/1/1
7	NAG	W	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	1	NAG	C2-N2	6.78	1.57	1.46
6	V	1	NAG	C2-N2	6.76	1.57	1.46
6	S	1	NAG	C2-N2	6.75	1.57	1.46
6	V	2	NAG	C1-C2	6.16	1.60	1.52
6	S	2	NAG	C1-C2	6.12	1.60	1.52
6	P	2	NAG	C1-C2	6.10	1.60	1.52
7	X	1	NAG	O4-C4	-5.11	1.30	1.43
7	R	1	NAG	O4-C4	-5.10	1.30	1.43
7	U	1	NAG	O4-C4	-5.09	1.30	1.43
7	T	1	NAG	O4-C4	-4.96	1.30	1.43
7	Q	1	NAG	O4-C4	-4.96	1.30	1.43
7	W	1	NAG	O4-C4	-4.95	1.30	1.43
6	P	3	FUC	C1-C2	4.32	1.62	1.52
6	V	3	FUC	C1-C2	4.30	1.62	1.52
6	S	3	FUC	C1-C2	4.30	1.62	1.52
7	T	1	NAG	C4-C3	4.23	1.63	1.52
7	Q	1	NAG	C4-C3	4.23	1.63	1.52
7	W	1	NAG	C4-C3	4.22	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	1	NAG	C4-C5	4.06	1.61	1.53
7	T	1	NAG	C4-C5	4.05	1.61	1.53
7	W	1	NAG	C4-C5	4.04	1.61	1.53
7	R	1	NAG	C4-C3	4.03	1.62	1.52
7	U	1	NAG	C4-C3	4.03	1.62	1.52
7	X	1	NAG	C4-C3	4.02	1.62	1.52
7	X	1	NAG	C4-C5	4.01	1.61	1.53
7	U	1	NAG	C4-C5	4.00	1.61	1.53
7	R	1	NAG	C4-C5	4.00	1.61	1.53
7	R	2	NAG	C1-C2	3.90	1.57	1.52
7	X	2	NAG	C1-C2	3.89	1.57	1.52
7	U	2	NAG	C1-C2	3.88	1.57	1.52
7	Q	2	NAG	C1-C2	3.88	1.57	1.52
7	T	2	NAG	C1-C2	3.87	1.57	1.52
7	W	2	NAG	C1-C2	3.84	1.57	1.52
6	P	1	NAG	O5-C5	3.71	1.50	1.43
6	S	1	NAG	O5-C5	3.71	1.50	1.43
6	V	1	NAG	O5-C5	3.70	1.50	1.43
6	P	2	NAG	O5-C1	3.66	1.49	1.43
6	S	2	NAG	O5-C1	3.66	1.49	1.43
6	V	2	NAG	O5-C1	3.64	1.49	1.43
6	S	1	NAG	C3-C2	-3.01	1.46	1.52
6	P	1	NAG	C3-C2	-3.00	1.46	1.52
6	V	1	NAG	C3-C2	-2.97	1.46	1.52
7	U	1	NAG	C1-C2	2.96	1.56	1.52
7	X	1	NAG	C1-C2	2.94	1.56	1.52
6	V	1	NAG	C1-C2	-2.93	1.48	1.52
7	R	1	NAG	C1-C2	2.93	1.56	1.52
6	S	1	NAG	C1-C2	-2.92	1.48	1.52
6	P	1	NAG	C1-C2	-2.91	1.48	1.52
6	P	2	NAG	C3-C2	2.76	1.58	1.52
6	S	3	FUC	O5-C1	2.75	1.48	1.43
6	V	3	FUC	O5-C1	2.74	1.48	1.43
6	P	3	FUC	O5-C1	2.74	1.48	1.43
6	V	2	NAG	C3-C2	2.73	1.58	1.52
6	S	2	NAG	C3-C2	2.71	1.58	1.52
6	P	3	FUC	O5-C5	2.43	1.48	1.43
6	S	3	FUC	O5-C5	2.43	1.48	1.43
6	V	3	FUC	O5-C5	2.41	1.48	1.43
7	W	1	NAG	C1-C2	2.21	1.55	1.52
7	T	1	NAG	C1-C2	2.21	1.55	1.52
6	S	3	FUC	C2-C3	2.19	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	1	NAG	C1-C2	2.19	1.55	1.52
6	P	3	FUC	C2-C3	2.17	1.55	1.52
6	V	3	FUC	C2-C3	2.17	1.55	1.52
6	V	1	NAG	C4-C3	-2.12	1.46	1.52
6	P	1	NAG	C4-C3	-2.11	1.46	1.52
6	S	1	NAG	C4-C3	-2.11	1.46	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	1	NAG	C1-C2-N2	5.18	118.60	110.43
6	S	1	NAG	C1-C2-N2	5.17	118.59	110.43
6	P	1	NAG	C1-C2-N2	5.15	118.55	110.43
6	S	1	NAG	O5-C1-C2	4.56	118.34	111.29
6	V	1	NAG	O5-C1-C2	4.56	118.34	111.29
6	P	1	NAG	O5-C1-C2	4.55	118.33	111.29
7	R	1	NAG	C3-C4-C5	-4.19	102.64	110.23
7	X	1	NAG	C3-C4-C5	-4.18	102.65	110.23
7	U	1	NAG	C3-C4-C5	-4.17	102.67	110.23
7	T	1	NAG	C3-C4-C5	-3.97	103.04	110.23
7	Q	1	NAG	C3-C4-C5	-3.96	103.05	110.23
7	W	1	NAG	C3-C4-C5	-3.95	103.06	110.23
6	P	1	NAG	O4-C4-C3	-3.54	102.04	110.38
6	S	1	NAG	O4-C4-C3	-3.54	102.04	110.38
6	V	1	NAG	O4-C4-C3	-3.53	102.05	110.38
7	W	1	NAG	O4-C4-C3	-3.42	102.32	110.38
7	T	1	NAG	O4-C4-C3	-3.41	102.33	110.38
7	Q	1	NAG	O4-C4-C3	-3.41	102.34	110.38
6	S	2	NAG	O5-C1-C2	-3.18	106.37	111.29
6	V	2	NAG	O5-C1-C2	-3.17	106.39	111.29
6	S	2	NAG	C1-O5-C5	3.16	116.42	112.19
6	P	2	NAG	O5-C1-C2	-3.16	106.41	111.29
6	P	2	NAG	C1-O5-C5	3.15	116.41	112.19
6	V	2	NAG	C1-O5-C5	3.15	116.41	112.19
7	R	1	NAG	O4-C4-C3	-3.01	103.28	110.38
7	U	1	NAG	O4-C4-C3	-3.01	103.28	110.38
7	X	1	NAG	O4-C4-C3	-3.00	103.31	110.38
6	S	1	NAG	C1-O5-C5	-2.95	108.23	112.19
6	P	1	NAG	C1-O5-C5	-2.95	108.24	112.19
6	V	1	NAG	C1-O5-C5	-2.95	108.24	112.19
6	S	2	NAG	C4-C3-C2	-2.62	107.18	111.02
6	P	2	NAG	C4-C3-C2	-2.61	107.19	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	2	NAG	C4-C3-C2	-2.61	107.20	111.02
7	R	1	NAG	O4-C4-C5	-2.54	103.07	109.32
7	X	1	NAG	O4-C4-C5	-2.54	103.08	109.32
7	U	1	NAG	O4-C4-C5	-2.53	103.09	109.32
7	W	1	NAG	C8-C7-N2	2.43	120.15	116.12
7	T	1	NAG	C8-C7-N2	2.43	120.15	116.12
7	Q	1	NAG	C8-C7-N2	2.41	120.11	116.12
7	T	1	NAG	O4-C4-C5	-2.40	103.40	109.32
7	W	1	NAG	O4-C4-C5	-2.40	103.42	109.32
7	Q	1	NAG	O4-C4-C5	-2.39	103.43	109.32
6	P	2	NAG	C2-N2-C7	-2.32	119.79	122.90
6	V	2	NAG	C2-N2-C7	-2.32	119.80	122.90
6	S	2	NAG	C2-N2-C7	-2.31	119.81	122.90
7	R	1	NAG	C8-C7-N2	2.30	119.92	116.12
7	U	1	NAG	C8-C7-N2	2.28	119.90	116.12
7	X	1	NAG	C8-C7-N2	2.28	119.89	116.12
7	Q	1	NAG	C2-N2-C7	-2.25	119.88	122.90
7	W	1	NAG	C2-N2-C7	-2.23	119.91	122.90
7	T	1	NAG	C2-N2-C7	-2.23	119.92	122.90
7	X	2	NAG	C8-C7-N2	2.13	119.65	116.12
7	R	2	NAG	C8-C7-N2	2.12	119.63	116.12
7	U	2	NAG	C8-C7-N2	2.10	119.61	116.12
7	X	1	NAG	C2-N2-C7	-2.06	120.14	122.90
7	U	1	NAG	C2-N2-C7	-2.05	120.15	122.90
7	R	1	NAG	C2-N2-C7	-2.03	120.17	122.90
7	T	1	NAG	O3-C3-C4	-2.03	105.59	110.38
7	Q	1	NAG	O3-C3-C4	-2.02	105.61	110.38
7	U	1	NAG	C6-C5-C4	-2.02	108.06	113.02
7	X	1	NAG	C6-C5-C4	-2.02	108.06	113.02
7	W	1	NAG	O3-C3-C4	-2.02	105.62	110.38
7	R	1	NAG	C6-C5-C4	-2.01	108.08	113.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	Q	1	NAG	C4-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6

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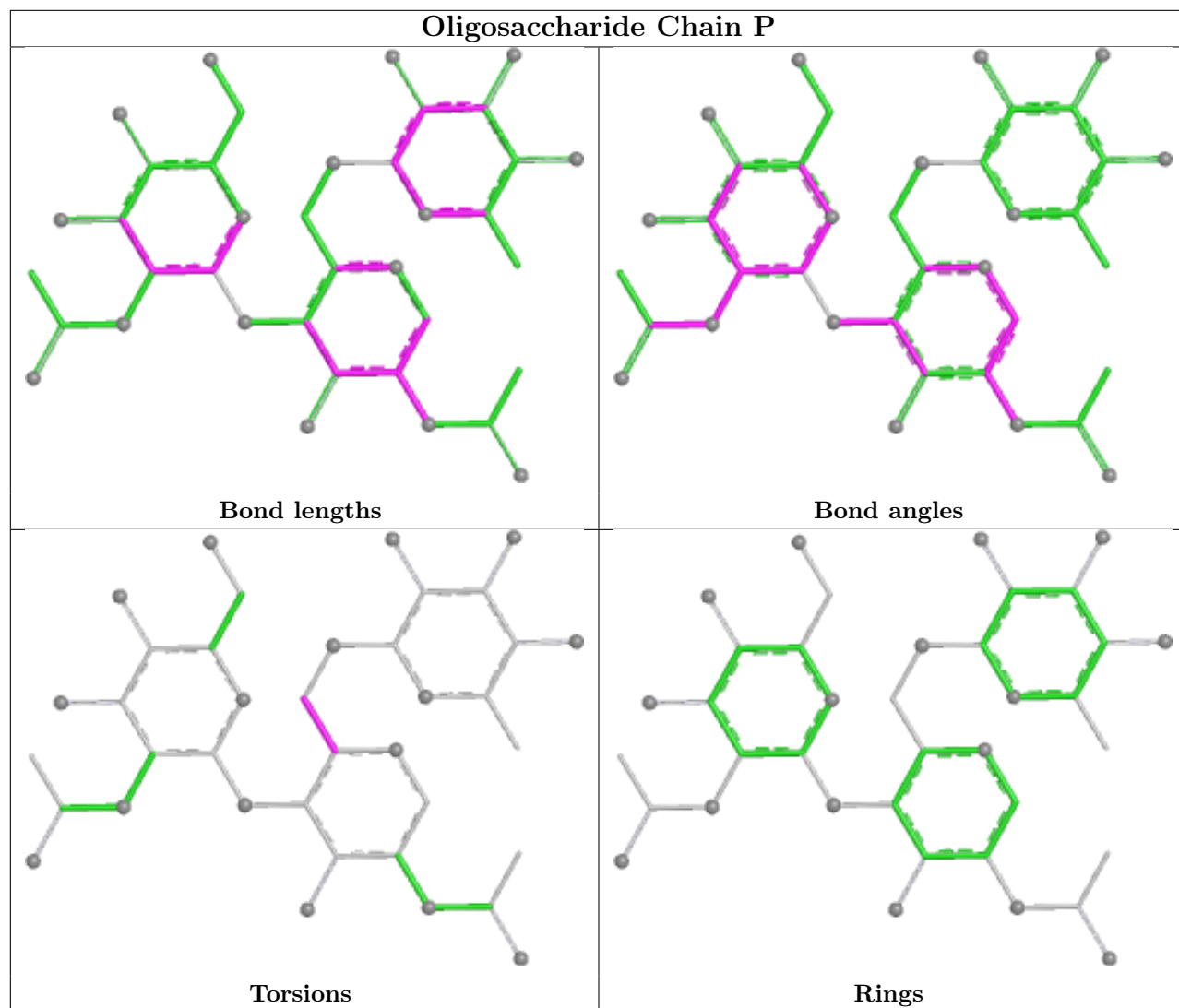
Mol	Chain	Res	Type	Atoms
7	T	1	NAG	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6

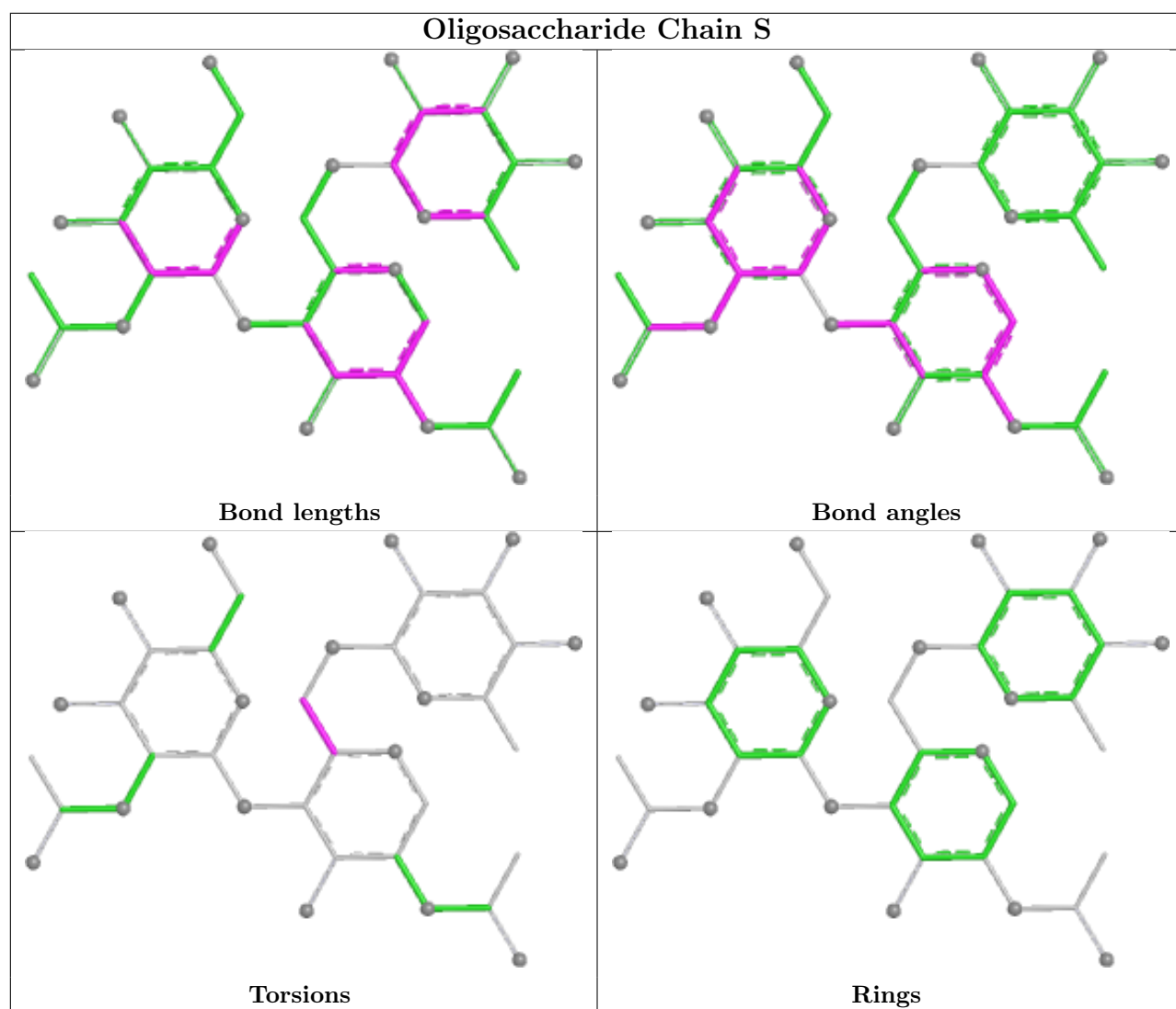
There are no ring outliers.

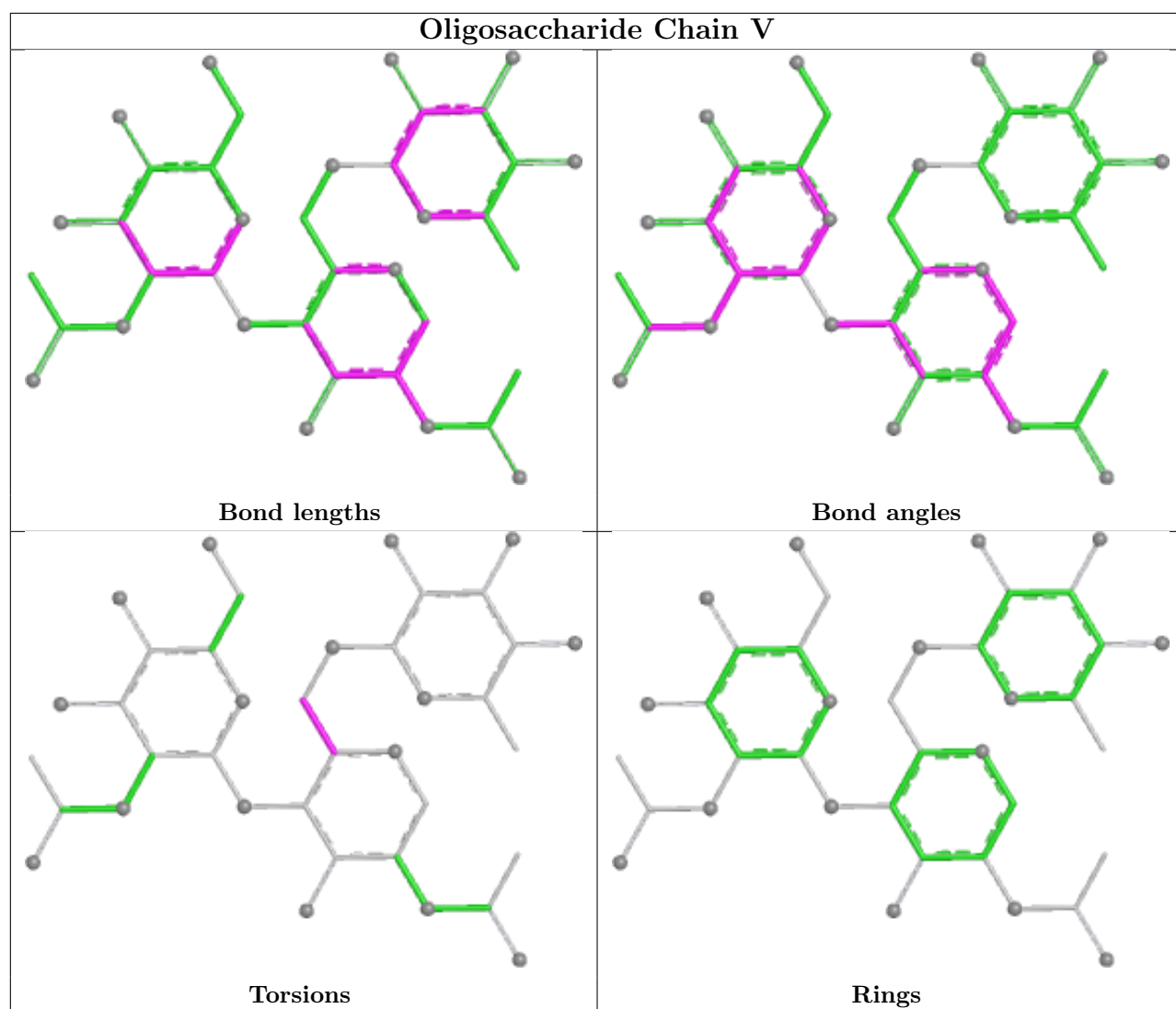
18 monomers are involved in 18 short contacts:

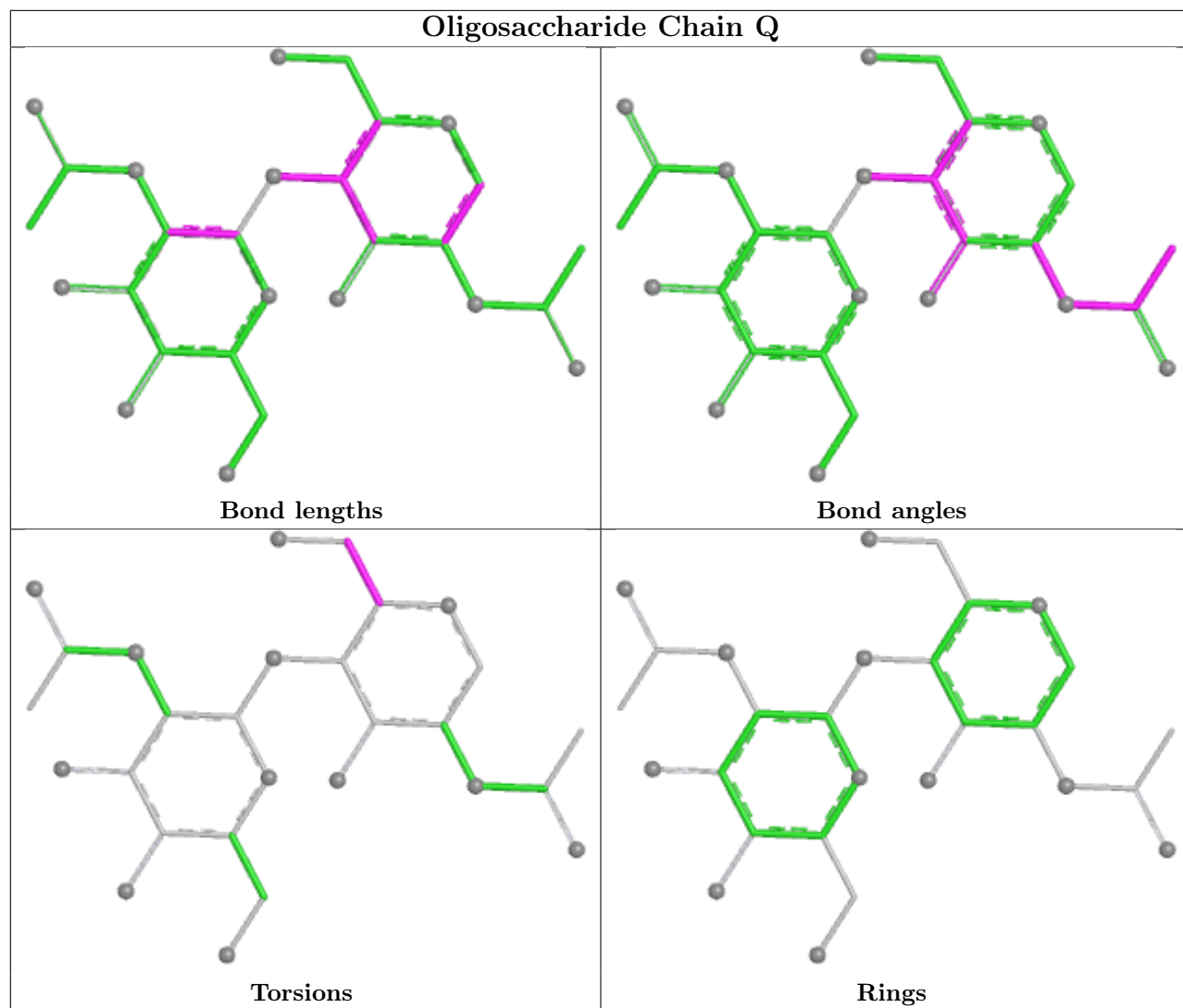
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	2	NAG	2	0
7	U	2	NAG	2	0
7	R	2	NAG	2	0
7	X	2	NAG	2	0
7	T	2	NAG	2	0
6	V	2	NAG	2	0
6	P	2	NAG	2	0
7	U	1	NAG	2	0
7	W	2	NAG	2	0
7	Q	2	NAG	2	0
7	X	1	NAG	2	0
7	R	1	NAG	2	0
6	S	1	NAG	2	0
6	V	1	NAG	2	0
7	T	1	NAG	2	0
6	P	1	NAG	2	0
7	Q	1	NAG	2	0
7	W	1	NAG	2	0

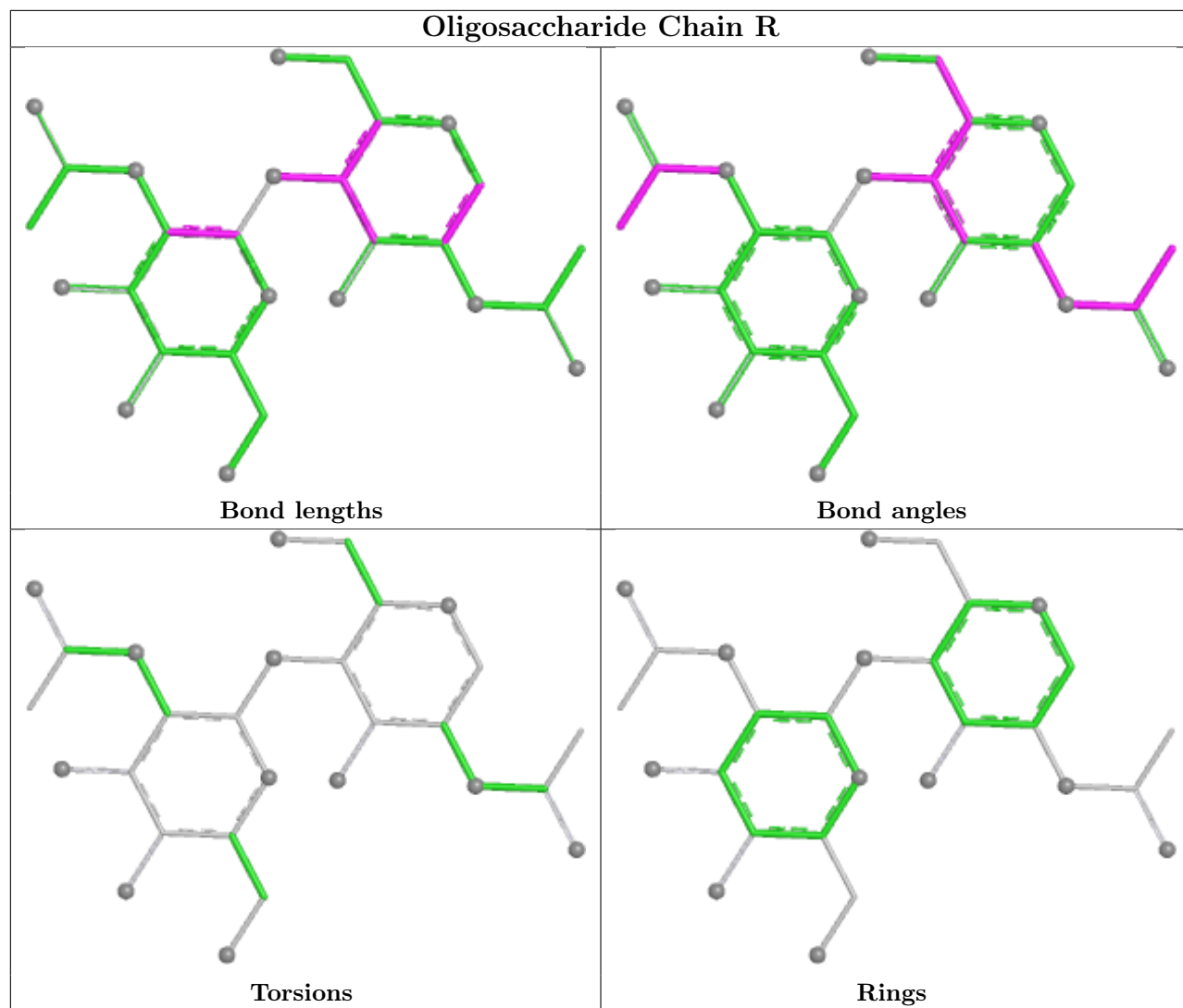
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

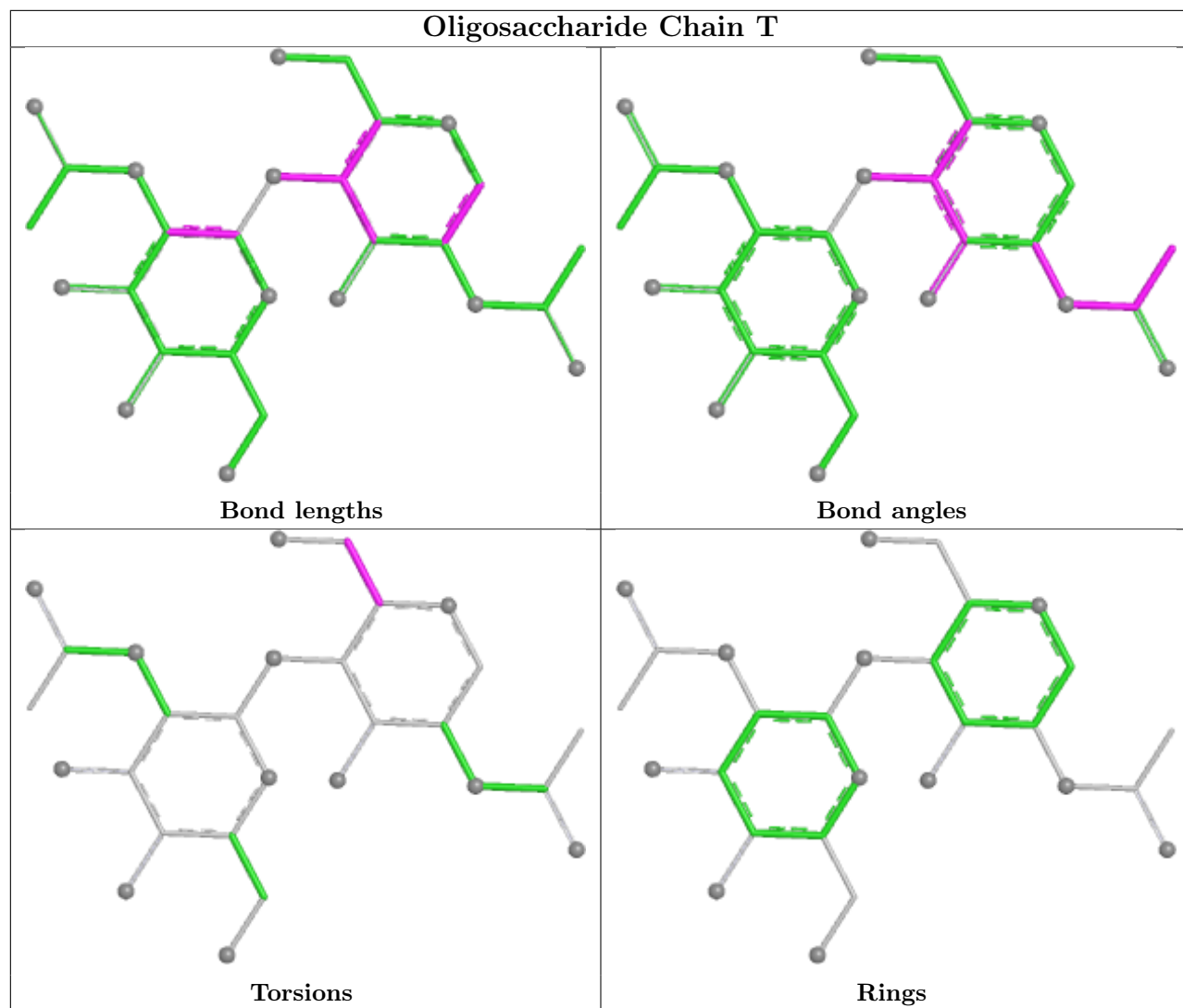


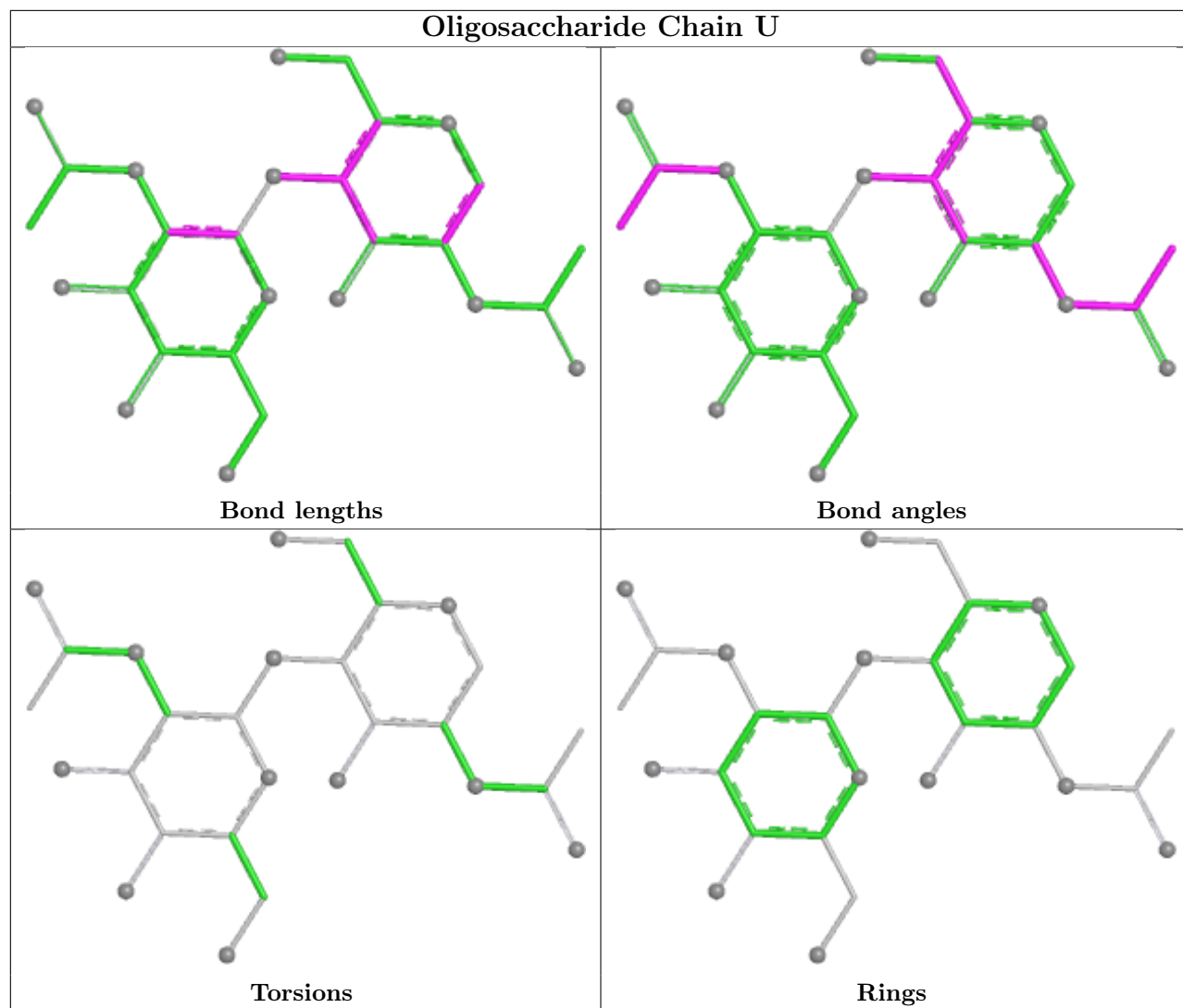


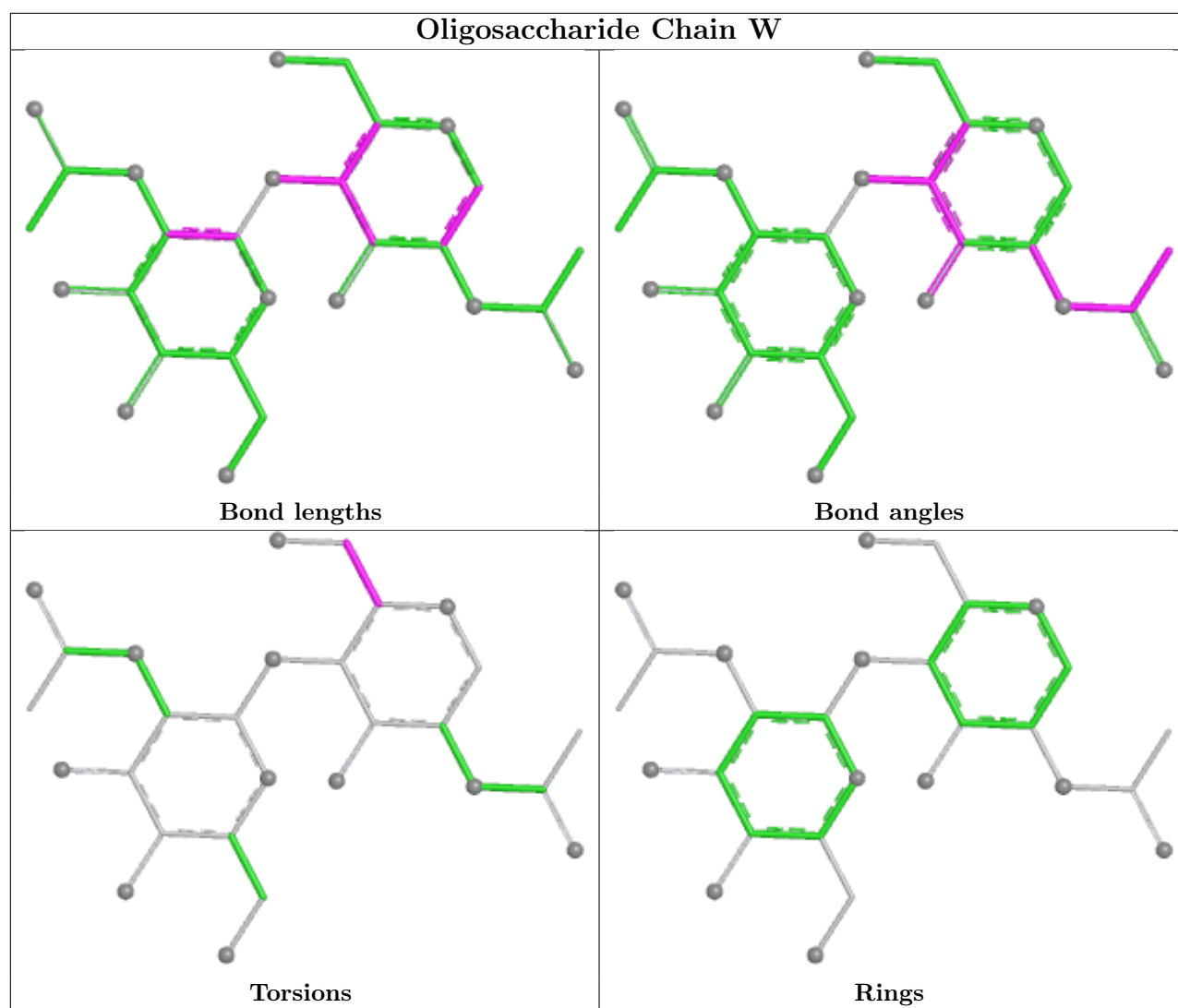


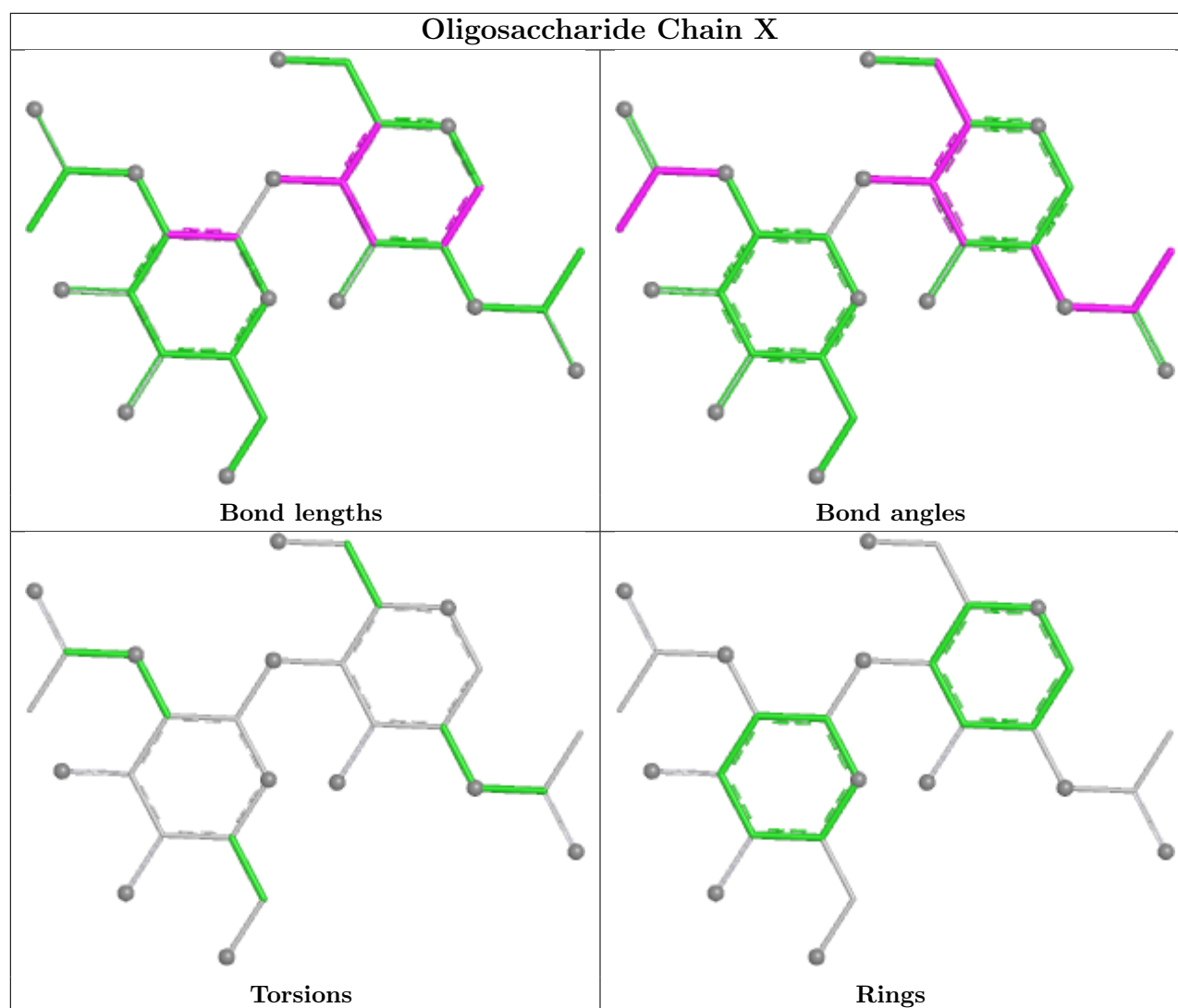












5.6 Ligand geometry [i](#)

39 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	$\# Z > 2$
8	NAG	A	1307	1	14,14,15	1.36	2 (14%)	17,19,21	1.23	2 (11%)
8	NAG	A	1305	1	14,14,15	1.31	1 (7%)	17,19,21	1.07	1 (5%)
8	NAG	K	1308	1	14,14,15	1.26	1 (7%)	17,19,21	1.12	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	F	1312	1	14,14,15	1.08	1 (7%)	17,19,21	1.19	3 (17%)
8	NAG	K	1317	1	14,14,15	1.29	1 (7%)	17,19,21	1.22	2 (11%)
8	NAG	F	1302	1	14,14,15	1.40	2 (14%)	17,19,21	1.20	2 (11%)
8	NAG	F	1308	1	14,14,15	1.60	1 (7%)	17,19,21	1.07	1 (5%)
8	NAG	A	1302	1	14,14,15	1.40	2 (14%)	17,19,21	1.19	2 (11%)
8	NAG	A	1310	1	14,14,15	1.34	2 (14%)	17,19,21	1.18	2 (11%)
8	NAG	K	1319	1	13,13,15	1.55	2 (15%)	16,17,21	1.51	2 (12%)
8	NAG	K	1309	1	14,14,15	1.37	2 (14%)	17,19,21	1.23	2 (11%)
8	NAG	K	1305	1	14,14,15	1.32	1 (7%)	17,19,21	1.07	1 (5%)
8	NAG	K	1318	1	14,14,15	1.09	1 (7%)	17,19,21	1.19	3 (17%)
8	NAG	F	1310	1	14,14,15	1.34	2 (14%)	17,19,21	1.18	2 (11%)
8	NAG	K	1303	1	14,14,15	1.38	2 (14%)	17,19,21	1.18	3 (17%)
8	NAG	A	1312	1	14,14,15	1.08	1 (7%)	17,19,21	1.19	3 (17%)
8	NAG	K	1316	1	14,14,15	1.34	2 (14%)	17,19,21	1.18	2 (11%)
8	NAG	F	1313	1	14,14,15	1.44	2 (14%)	17,19,21	1.23	2 (11%)
8	NAG	K	1314	1	14,14,15	1.59	1 (7%)	17,19,21	1.07	1 (5%)
8	NAG	A	1311	1	14,14,15	1.30	1 (7%)	17,19,21	1.21	2 (11%)
8	NAG	A	1303	1	14,14,15	1.38	2 (14%)	17,19,21	1.18	3 (17%)
8	NAG	A	1308	1	14,14,15	1.59	1 (7%)	17,19,21	1.07	1 (5%)
8	NAG	F	1303	1	14,14,15	1.38	2 (14%)	17,19,21	1.18	3 (17%)
8	NAG	A	1301	1	14,14,15	1.33	2 (14%)	17,19,21	1.14	2 (11%)
8	NAG	A	1306	1	14,14,15	1.26	1 (7%)	17,19,21	1.12	2 (11%)
8	NAG	F	1301	1	14,14,15	1.32	2 (14%)	17,19,21	1.15	1 (5%)
8	NAG	K	1302	1	14,14,15	1.40	2 (14%)	17,19,21	1.19	2 (11%)
8	NAG	K	1304	1	14,14,15	1.36	2 (14%)	17,19,21	1.33	3 (17%)
8	NAG	A	1309	1	14,14,15	1.42	2 (14%)	17,19,21	1.14	1 (5%)
8	NAG	F	1311	1	14,14,15	1.31	2 (14%)	17,19,21	1.22	2 (11%)
8	NAG	K	1301	1	14,14,15	1.32	2 (14%)	17,19,21	1.15	1 (5%)
8	NAG	F	1306	1	14,14,15	1.26	2 (14%)	17,19,21	1.12	2 (11%)
8	NAG	F	1307	1	14,14,15	1.36	2 (14%)	17,19,21	1.22	2 (11%)
8	NAG	A	1304	1	14,14,15	1.36	2 (14%)	17,19,21	1.33	3 (17%)
8	NAG	F	1309	1	14,14,15	1.42	2 (14%)	17,19,21	1.14	1 (5%)
8	NAG	A	1313	1	14,14,15	1.44	2 (14%)	17,19,21	1.22	2 (11%)
8	NAG	K	1315	1	14,14,15	1.42	2 (14%)	17,19,21	1.14	1 (5%)
8	NAG	F	1305	1	14,14,15	1.31	1 (7%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	F	1304	1	14,14,15	1.36	2 (14%)	17,19,21	1.33	3 (17%)

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
8	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1308	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1312	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1317	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1302	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1308	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1319	1	-	2/5/22/26	0/1/1/1
8	NAG	K	1309	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1305	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1318	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1310	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1303	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1316	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1313	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1314	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1303	1	-	1/6/23/26	0/1/1/1
8	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1302	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1304	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1311	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1301	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1306	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1307	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1304	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	F	1309	1	-	0/6/23/26	0/1/1/1
8	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
8	NAG	K	1315	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1305	1	-	0/6/23/26	0/1/1/1
8	NAG	F	1304	1	-	0/6/23/26	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1308	NAG	C1-C2	5.38	1.59	1.52
8	A	1308	NAG	C1-C2	5.34	1.59	1.52
8	K	1314	NAG	C1-C2	5.34	1.59	1.52
8	F	1313	NAG	C1-C2	4.53	1.58	1.52
8	A	1313	NAG	C1-C2	4.52	1.58	1.52
8	K	1319	NAG	C1-C2	4.50	1.58	1.52
8	A	1309	NAG	C1-C2	4.49	1.58	1.52
8	K	1315	NAG	C1-C2	4.48	1.58	1.52
8	F	1309	NAG	C1-C2	4.47	1.58	1.52
8	K	1302	NAG	C1-C2	4.35	1.58	1.52
8	F	1302	NAG	C1-C2	4.34	1.58	1.52
8	A	1302	NAG	C1-C2	4.33	1.58	1.52
8	F	1310	NAG	C1-C2	4.18	1.58	1.52
8	K	1309	NAG	C1-C2	4.17	1.58	1.52
8	K	1316	NAG	C1-C2	4.17	1.58	1.52
8	A	1310	NAG	C1-C2	4.14	1.58	1.52
8	F	1307	NAG	C1-C2	4.13	1.58	1.52
8	A	1307	NAG	C1-C2	4.11	1.57	1.52
8	A	1304	NAG	C1-C2	3.90	1.57	1.52
8	K	1304	NAG	C1-C2	3.88	1.57	1.52
8	F	1304	NAG	C1-C2	3.87	1.57	1.52
8	A	1301	NAG	C1-C2	3.87	1.57	1.52
8	K	1301	NAG	C1-C2	3.84	1.57	1.52
8	F	1303	NAG	C1-C2	3.84	1.57	1.52
8	K	1303	NAG	C1-C2	3.84	1.57	1.52
8	F	1301	NAG	C1-C2	3.83	1.57	1.52
8	K	1305	NAG	C1-C2	3.83	1.57	1.52
8	A	1303	NAG	C1-C2	3.82	1.57	1.52
8	A	1305	NAG	C1-C2	3.79	1.57	1.52
8	F	1305	NAG	C1-C2	3.79	1.57	1.52
8	F	1311	NAG	C1-C2	3.75	1.57	1.52
8	A	1311	NAG	C1-C2	3.72	1.57	1.52
8	K	1317	NAG	C1-C2	3.70	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1306	NAG	C1-C2	3.52	1.57	1.52
8	K	1308	NAG	C1-C2	3.52	1.57	1.52
8	F	1306	NAG	C1-C2	3.50	1.57	1.52
8	K	1318	NAG	C1-C2	2.86	1.56	1.52
8	A	1312	NAG	C1-C2	2.83	1.56	1.52
8	F	1312	NAG	C1-C2	2.83	1.56	1.52
8	K	1301	NAG	O5-C5	2.58	1.48	1.43
8	A	1301	NAG	O5-C5	2.58	1.48	1.43
8	F	1301	NAG	O5-C5	2.55	1.48	1.43
8	A	1313	NAG	O5-C1	2.23	1.47	1.43
8	F	1309	NAG	O5-C5	2.23	1.47	1.43
8	K	1315	NAG	O5-C5	2.23	1.47	1.43
8	A	1309	NAG	O5-C5	2.23	1.47	1.43
8	F	1313	NAG	O5-C1	2.22	1.47	1.43
8	K	1319	NAG	O5-C1	2.21	1.47	1.43
8	A	1304	NAG	O5-C5	2.14	1.47	1.43
8	K	1304	NAG	O5-C5	2.14	1.47	1.43
8	F	1304	NAG	O5-C5	2.13	1.47	1.43
8	K	1309	NAG	O5-C5	2.08	1.47	1.43
8	F	1307	NAG	O5-C5	2.08	1.47	1.43
8	A	1302	NAG	O5-C5	2.07	1.47	1.43
8	A	1307	NAG	O5-C5	2.07	1.47	1.43
8	F	1302	NAG	O5-C5	2.07	1.47	1.43
8	K	1316	NAG	O5-C5	2.07	1.47	1.43
8	K	1302	NAG	O5-C5	2.07	1.47	1.43
8	A	1303	NAG	O5-C5	2.06	1.47	1.43
8	F	1310	NAG	O5-C5	2.05	1.47	1.43
8	F	1303	NAG	O5-C5	2.05	1.47	1.43
8	A	1310	NAG	O5-C5	2.04	1.47	1.43
8	K	1303	NAG	O5-C5	2.04	1.47	1.43
8	F	1306	NAG	O5-C5	2.01	1.47	1.43
8	F	1311	NAG	O5-C5	2.01	1.47	1.43

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	1319	NAG	C7-N2-C2	4.77	121.70	114.43
8	F	1313	NAG	C8-C7-N2	2.80	120.76	116.12
8	A	1313	NAG	C8-C7-N2	2.78	120.74	116.12
8	K	1314	NAG	C1-O5-C5	2.73	115.85	112.19
8	A	1308	NAG	C1-O5-C5	2.72	115.84	112.19
8	F	1308	NAG	C1-O5-C5	2.71	115.82	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	1304	NAG	C8-C7-N2	2.71	120.61	116.12
8	A	1304	NAG	C8-C7-N2	2.70	120.60	116.12
8	K	1304	NAG	C8-C7-N2	2.69	120.58	116.12
8	A	1304	NAG	C2-N2-C7	-2.69	119.30	122.90
8	K	1304	NAG	C2-N2-C7	-2.69	119.30	122.90
8	F	1304	NAG	C2-N2-C7	-2.68	119.31	122.90
8	F	1312	NAG	C2-N2-C7	-2.52	119.52	122.90
8	K	1318	NAG	C2-N2-C7	-2.52	119.53	122.90
8	A	1312	NAG	C2-N2-C7	-2.51	119.54	122.90
8	A	1312	NAG	C8-C7-N2	2.50	120.26	116.12
8	K	1318	NAG	C8-C7-N2	2.48	120.23	116.12
8	F	1312	NAG	C8-C7-N2	2.48	120.23	116.12
8	K	1309	NAG	C8-C7-N2	2.47	120.21	116.12
8	A	1307	NAG	C8-C7-N2	2.46	120.20	116.12
8	F	1307	NAG	C8-C7-N2	2.46	120.20	116.12
8	F	1313	NAG	O5-C5-C6	-2.45	102.89	107.66
8	A	1313	NAG	O5-C5-C6	-2.45	102.90	107.66
8	K	1319	NAG	O5-C5-C6	-2.45	102.90	107.66
8	F	1302	NAG	C8-C7-N2	2.45	120.17	116.12
8	K	1302	NAG	C8-C7-N2	2.44	120.17	116.12
8	A	1302	NAG	C8-C7-N2	2.43	120.15	116.12
8	F	1307	NAG	C2-N2-C7	-2.42	119.65	122.90
8	K	1309	NAG	C2-N2-C7	-2.41	119.67	122.90
8	A	1307	NAG	C2-N2-C7	-2.41	119.67	122.90
8	A	1311	NAG	C8-C7-N2	2.40	120.10	116.12
8	F	1311	NAG	C8-C7-N2	2.40	120.09	116.12
8	K	1317	NAG	C8-C7-N2	2.40	120.09	116.12
8	F	1304	NAG	C4-C3-C2	-2.37	107.55	111.02
8	A	1304	NAG	C4-C3-C2	-2.36	107.56	111.02
8	K	1303	NAG	C8-C7-N2	2.36	120.03	116.12
8	A	1303	NAG	C8-C7-N2	2.35	120.02	116.12
8	K	1304	NAG	C4-C3-C2	-2.35	107.57	111.02
8	K	1302	NAG	C2-N2-C7	-2.35	119.75	122.90
8	F	1303	NAG	C8-C7-N2	2.34	120.00	116.12
8	F	1302	NAG	C2-N2-C7	-2.34	119.76	122.90
8	A	1302	NAG	C2-N2-C7	-2.34	119.76	122.90
8	K	1316	NAG	C8-C7-N2	2.28	119.89	116.12
8	F	1301	NAG	C2-N2-C7	-2.27	119.86	122.90
8	A	1310	NAG	C8-C7-N2	2.26	119.87	116.12
8	F	1310	NAG	C8-C7-N2	2.26	119.87	116.12
8	A	1306	NAG	C8-C7-N2	2.25	119.85	116.12
8	K	1308	NAG	C8-C7-N2	2.25	119.85	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1301	NAG	C2-N2-C7	-2.25	119.89	122.90
8	K	1301	NAG	C2-N2-C7	-2.24	119.89	122.90
8	F	1306	NAG	C8-C7-N2	2.24	119.83	116.12
8	F	1311	NAG	C2-N2-C7	-2.19	119.96	122.90
8	A	1311	NAG	C2-N2-C7	-2.19	119.97	122.90
8	F	1305	NAG	C8-C7-N2	2.19	119.74	116.12
8	K	1317	NAG	C2-N2-C7	-2.18	119.98	122.90
8	F	1310	NAG	C2-N2-C7	-2.17	119.99	122.90
8	A	1305	NAG	C8-C7-N2	2.17	119.72	116.12
8	K	1305	NAG	C8-C7-N2	2.17	119.71	116.12
8	A	1310	NAG	C2-N2-C7	-2.16	120.00	122.90
8	K	1316	NAG	C2-N2-C7	-2.15	120.02	122.90
8	F	1306	NAG	C2-N2-C7	-2.15	120.02	122.90
8	A	1306	NAG	C2-N2-C7	-2.14	120.03	122.90
8	F	1309	NAG	C1-O5-C5	2.14	115.06	112.19
8	K	1308	NAG	C2-N2-C7	-2.14	120.03	122.90
8	A	1309	NAG	C1-O5-C5	2.14	115.05	112.19
8	K	1315	NAG	C1-O5-C5	2.14	115.05	112.19
8	F	1303	NAG	C4-C3-C2	-2.08	107.97	111.02
8	K	1303	NAG	C4-C3-C2	-2.08	107.97	111.02
8	K	1303	NAG	C2-N2-C7	-2.06	120.14	122.90
8	F	1303	NAG	C2-N2-C7	-2.06	120.14	122.90
8	A	1303	NAG	C4-C3-C2	-2.06	108.01	111.02
8	A	1303	NAG	C2-N2-C7	-2.05	120.15	122.90
8	A	1301	NAG	C8-C7-N2	2.01	119.46	116.12
8	K	1318	NAG	C4-C3-C2	-2.01	108.07	111.02
8	F	1312	NAG	C4-C3-C2	-2.01	108.07	111.02
8	A	1312	NAG	C4-C3-C2	-2.01	108.08	111.02

There are no chirality outliers.

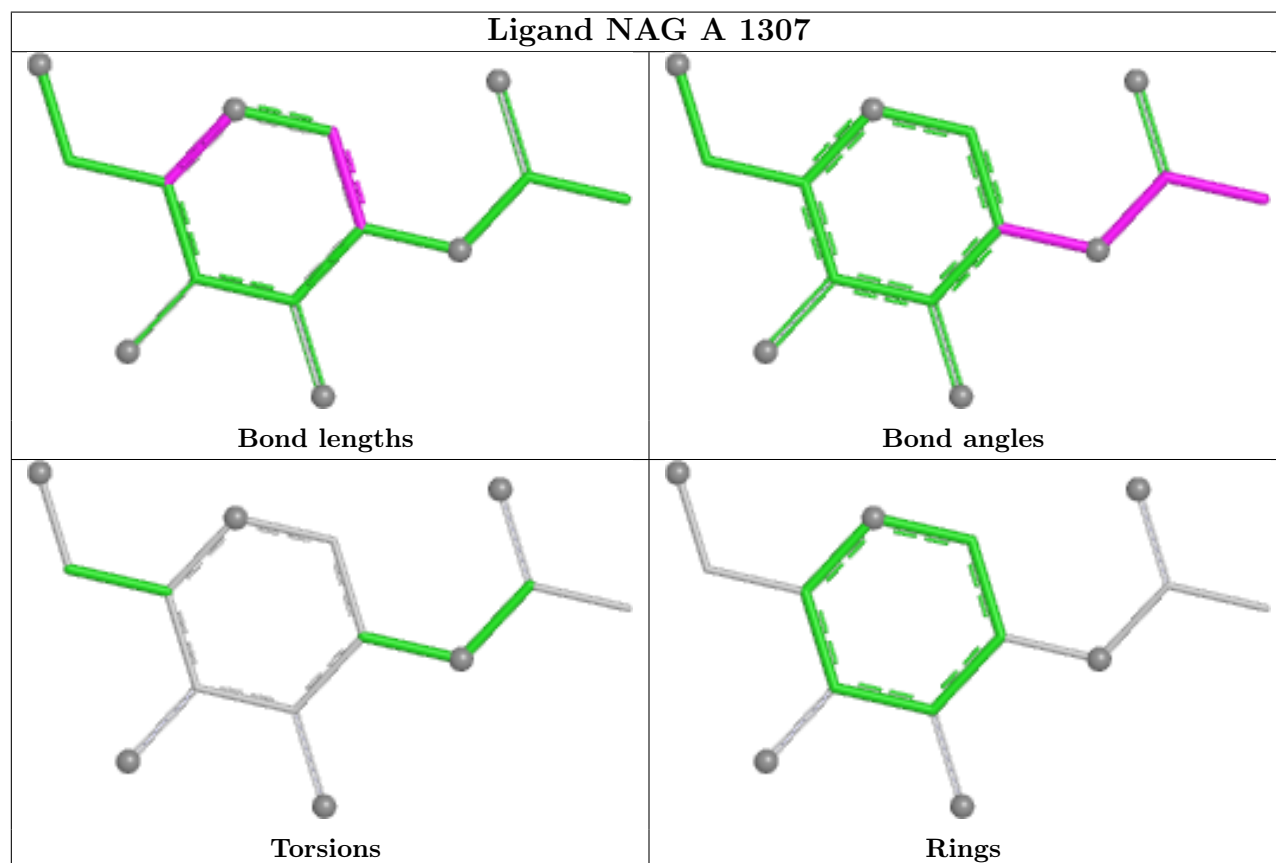
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	K	1319	NAG	C1-C2-N2-C7
8	K	1319	NAG	C3-C2-N2-C7
8	A	1303	NAG	O5-C5-C6-O6
8	F	1303	NAG	O5-C5-C6-O6
8	K	1303	NAG	O5-C5-C6-O6

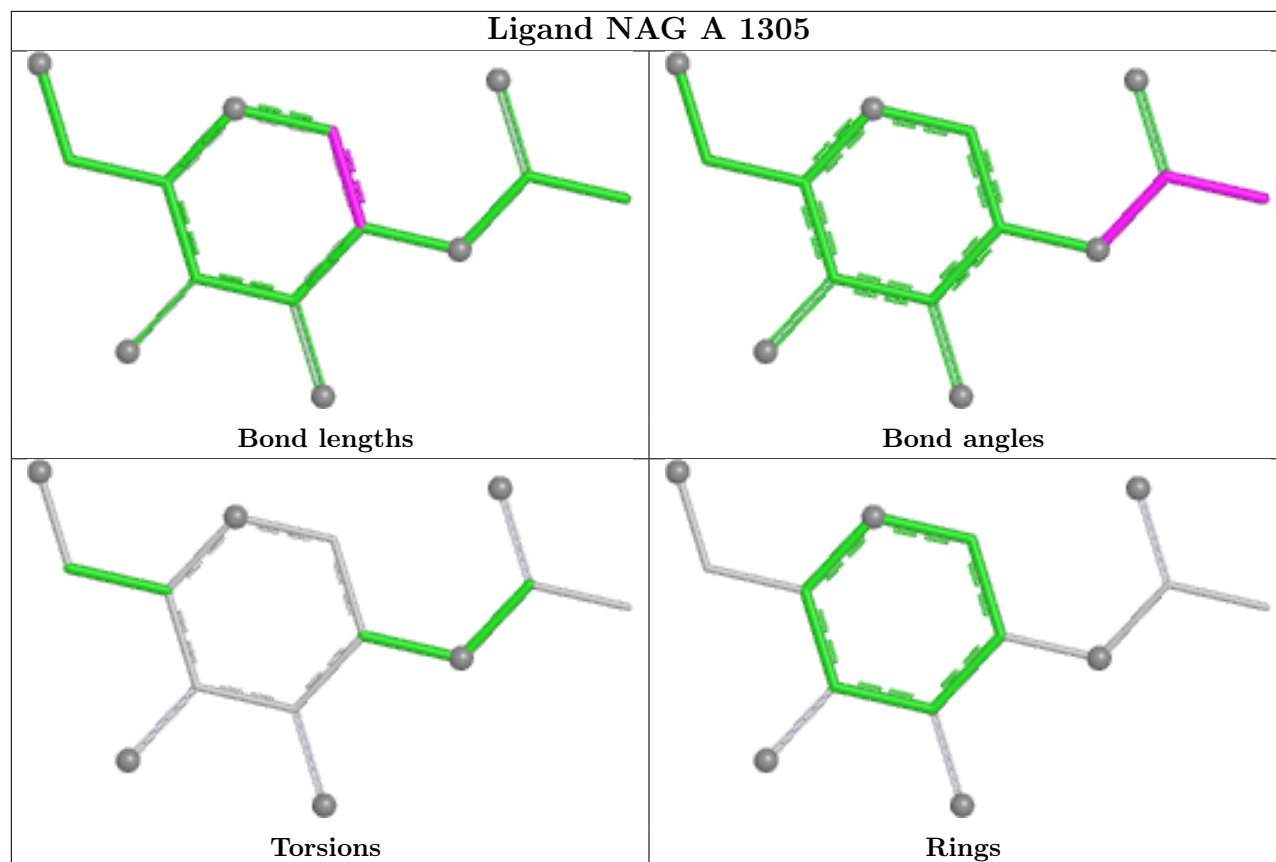
There are no ring outliers.

No monomer is involved in short contacts.

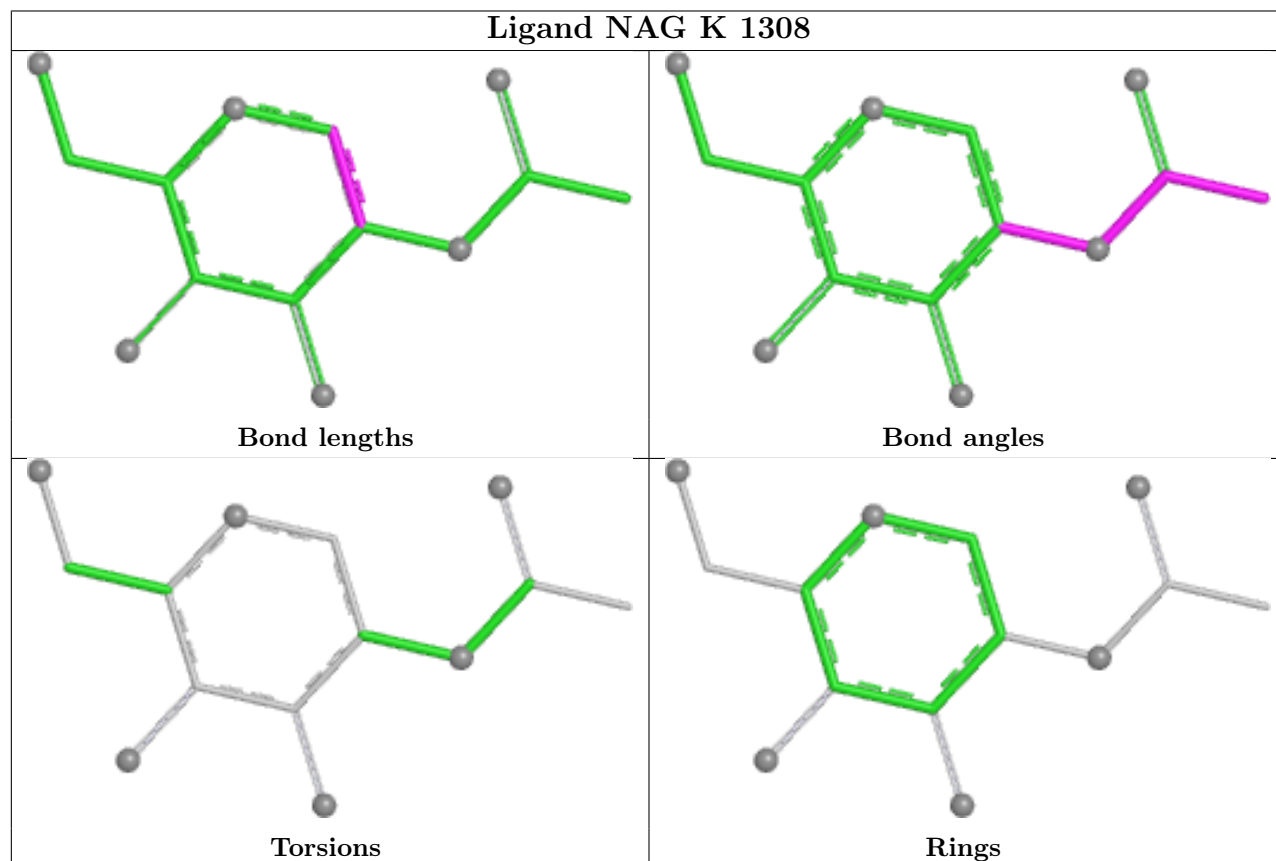
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

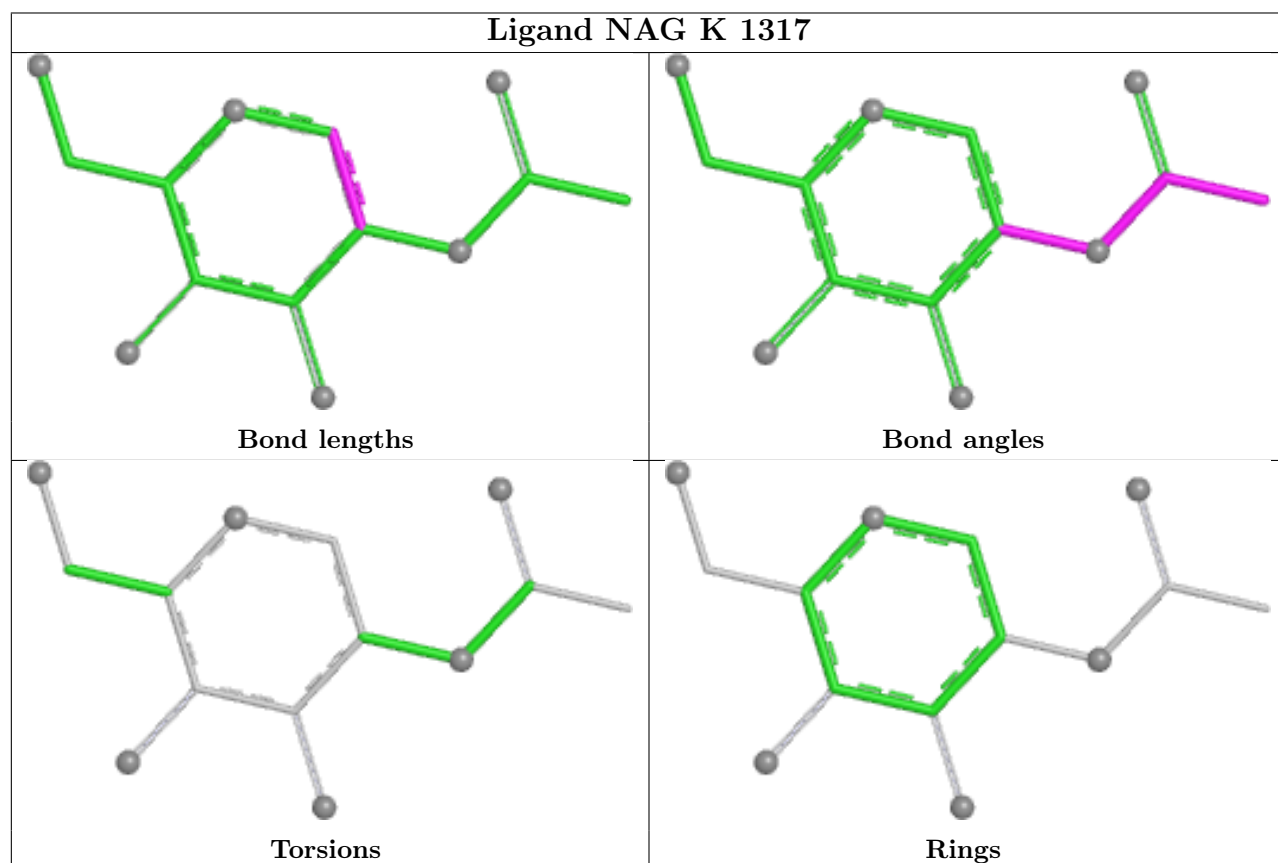
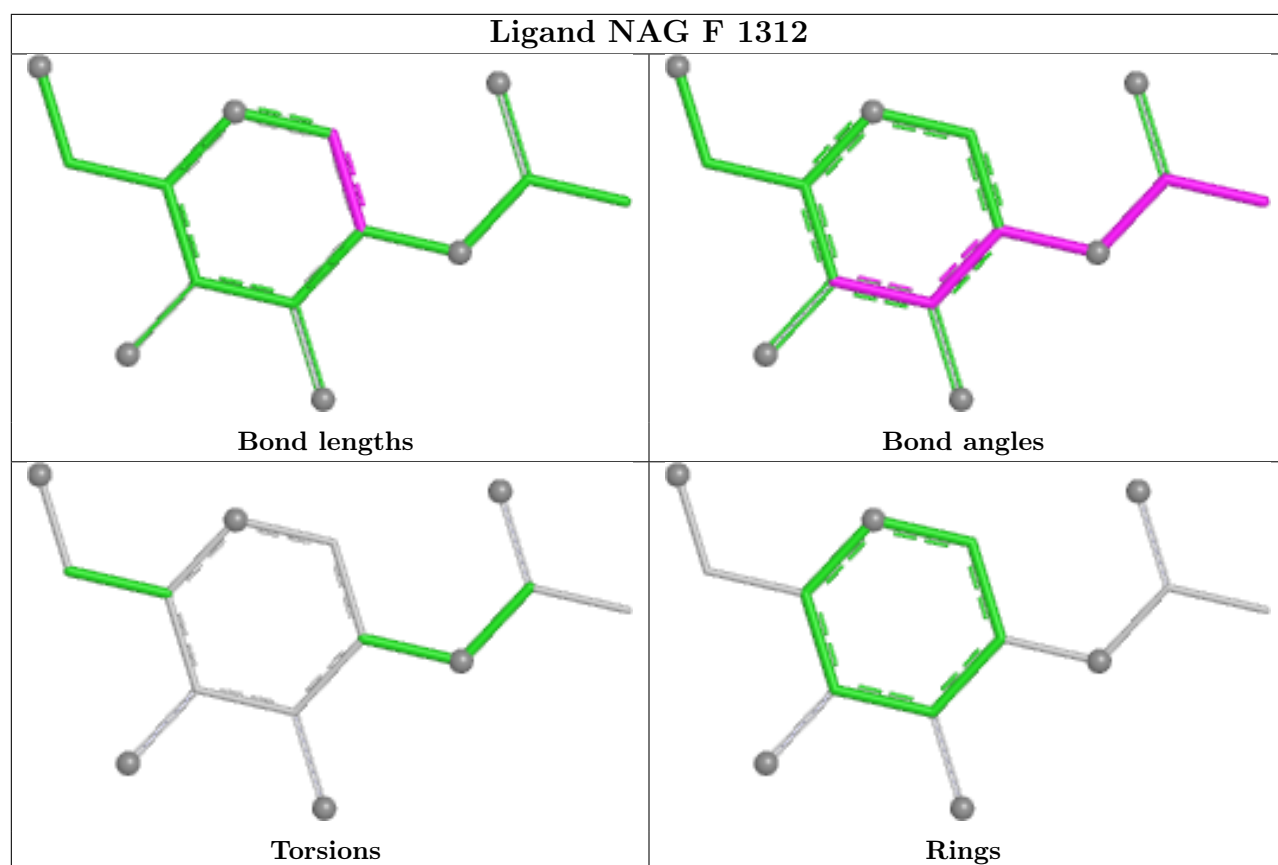


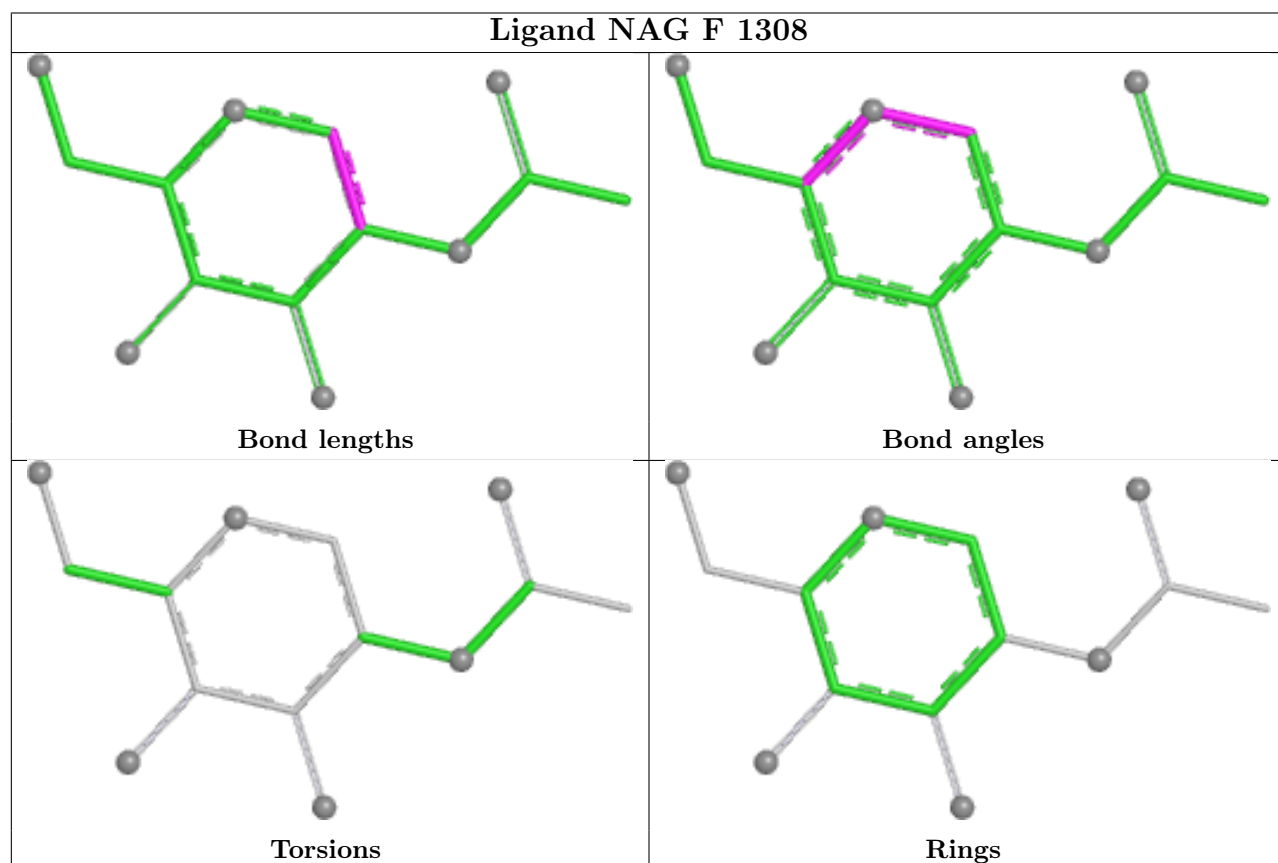
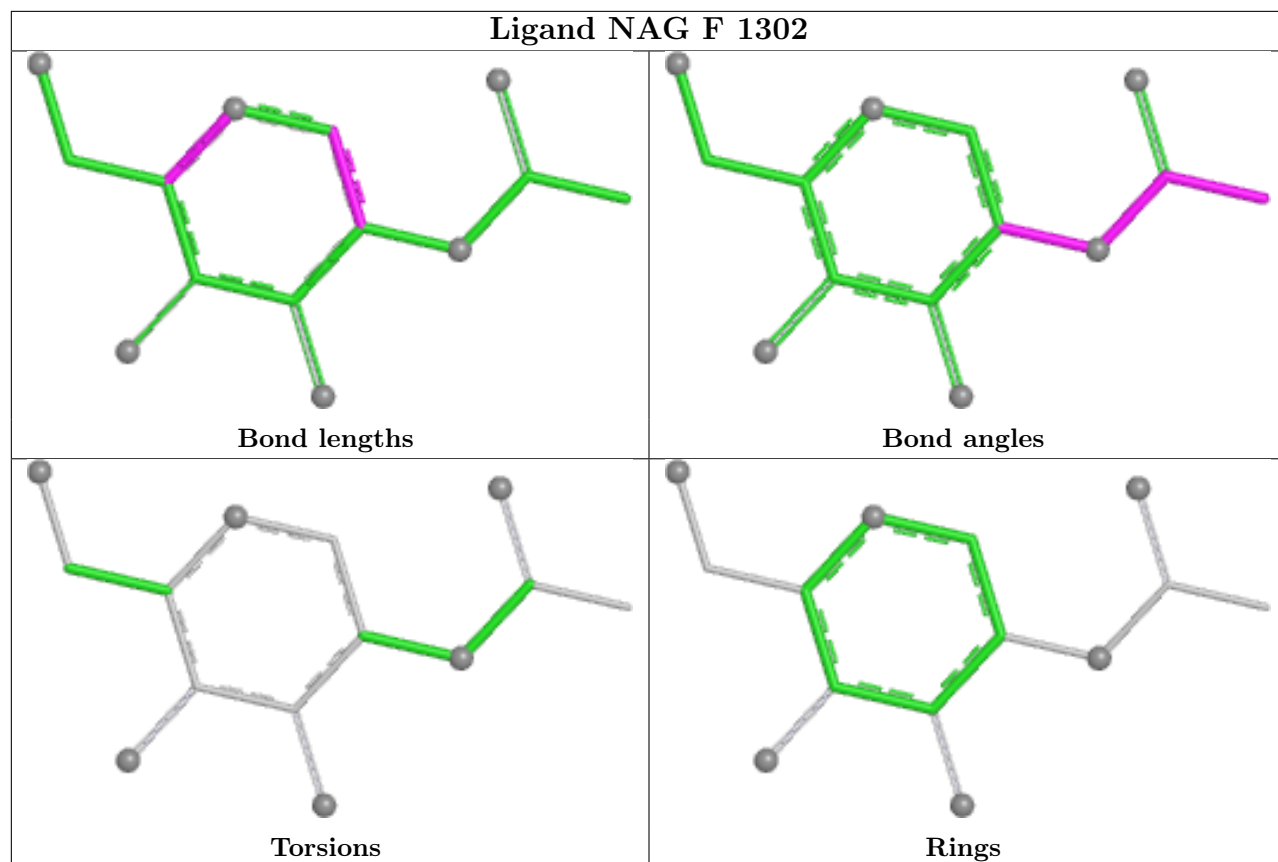
Ligand NAG A 1305



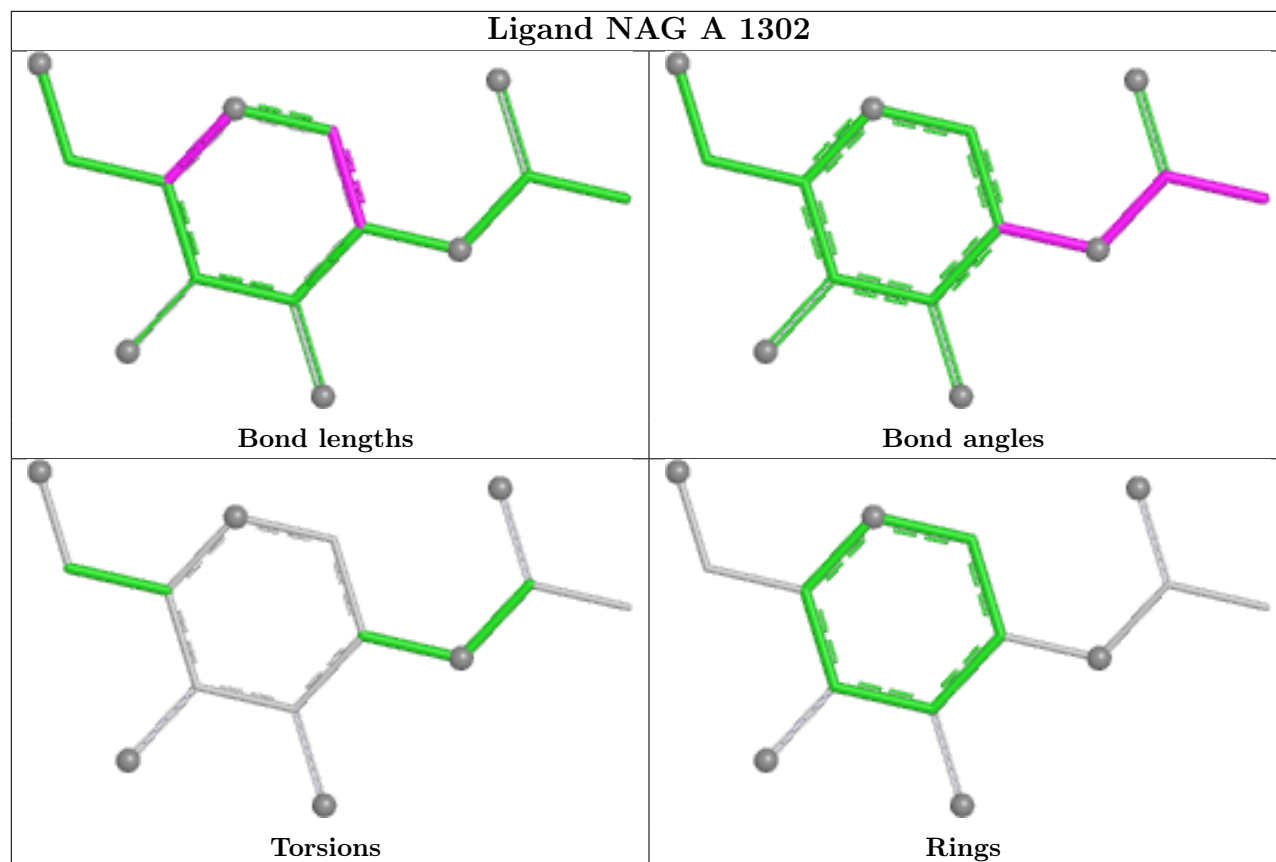
Ligand NAG K 1308



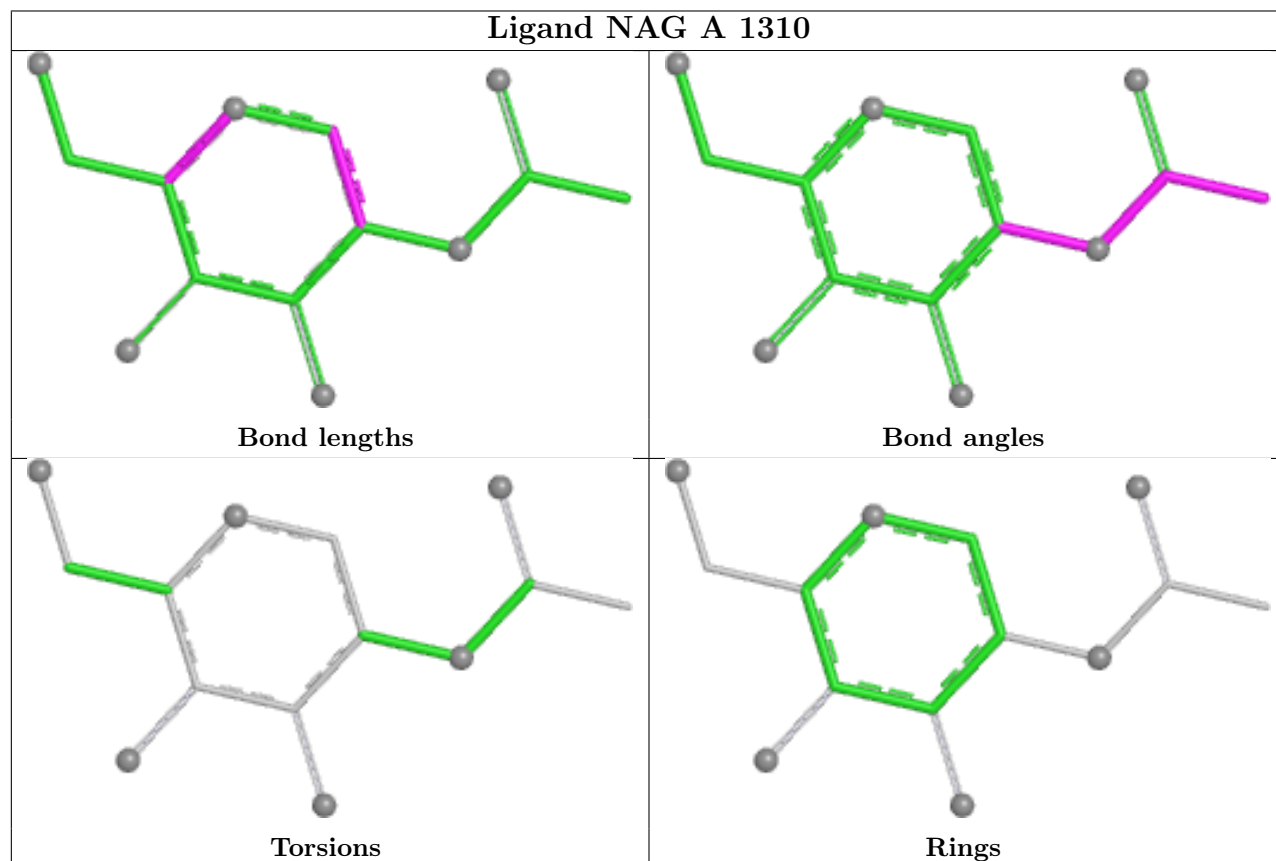




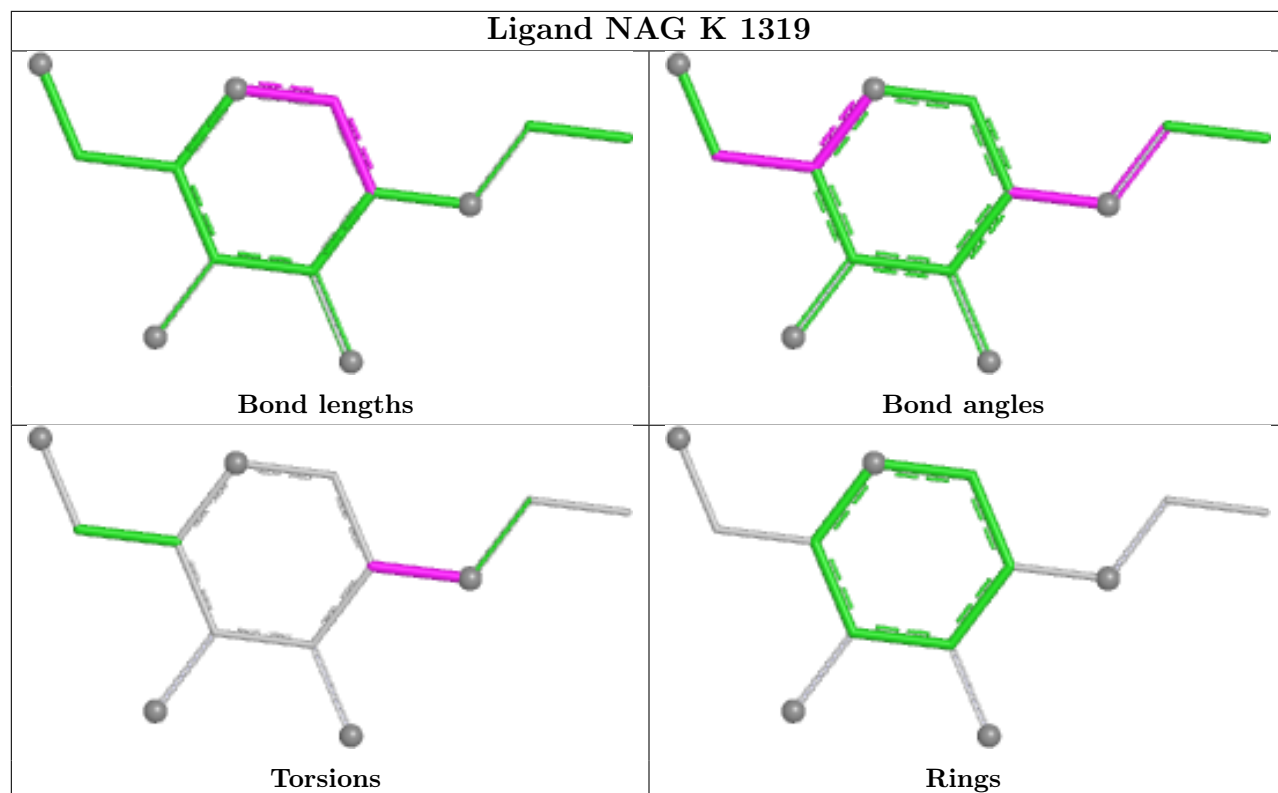
Ligand NAG A 1302



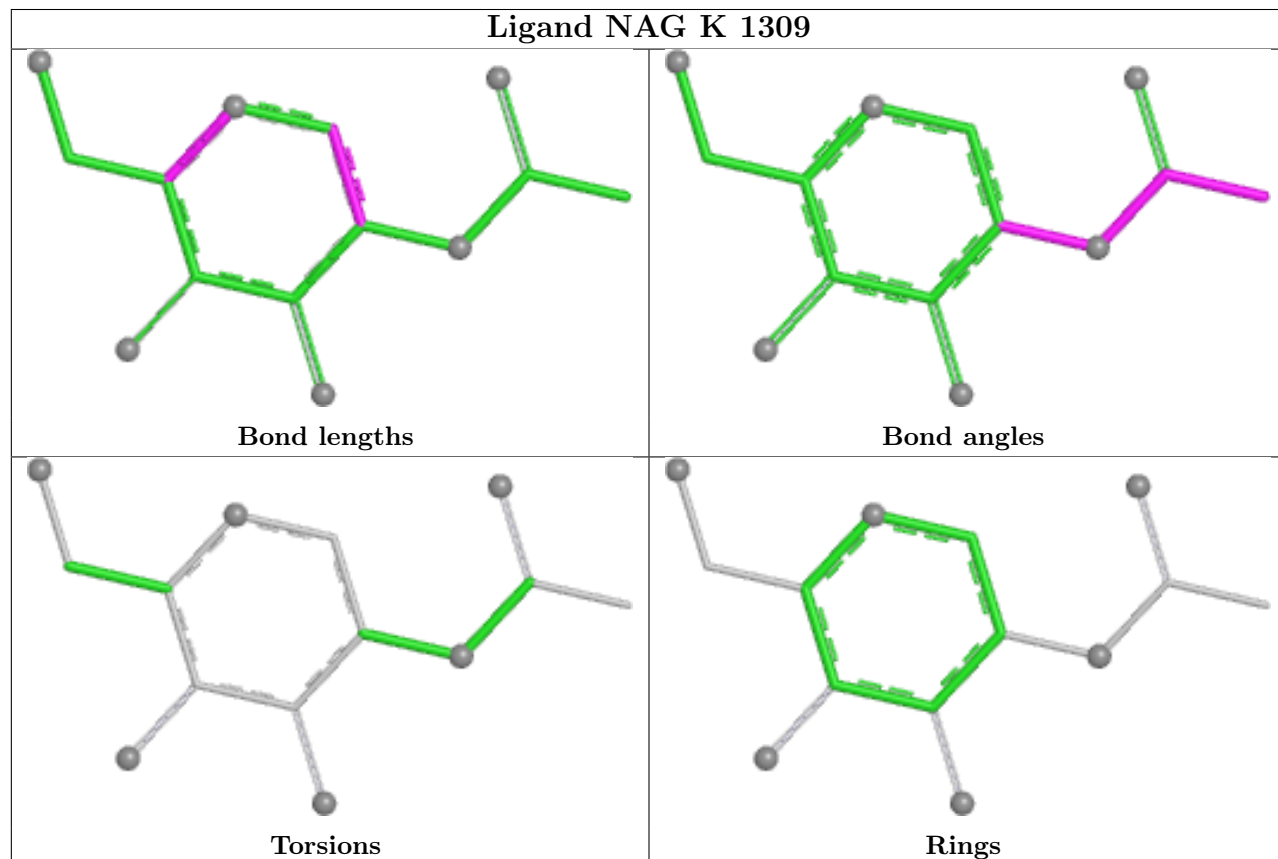
Ligand NAG A 1310

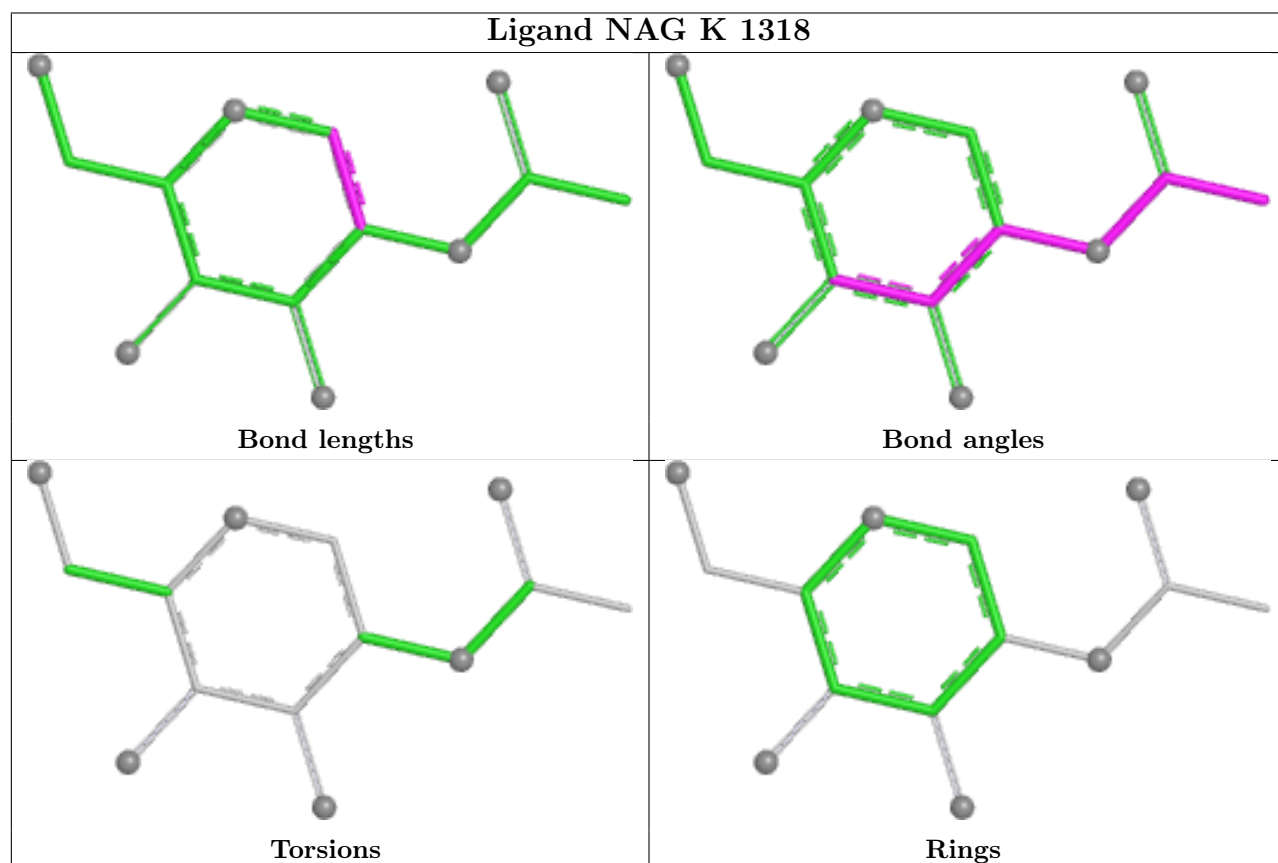
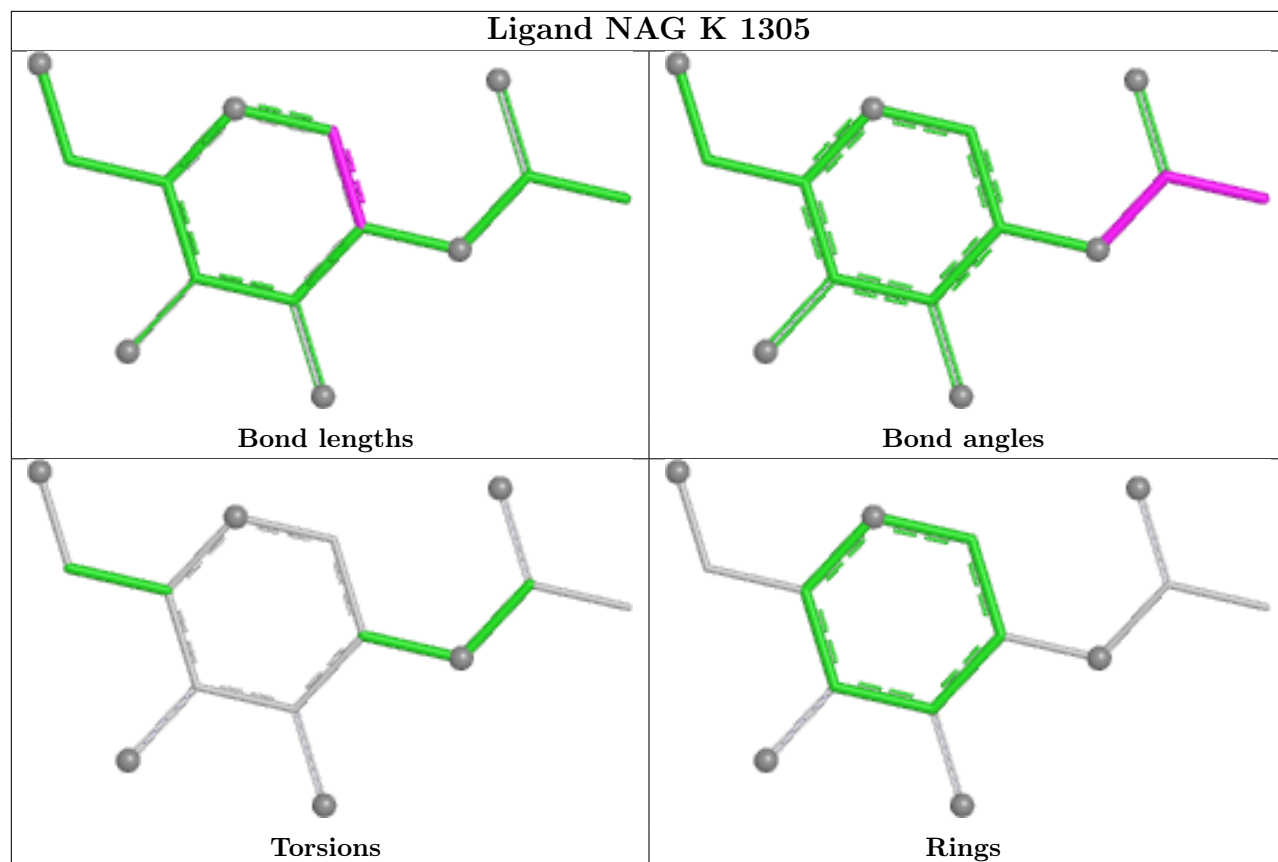


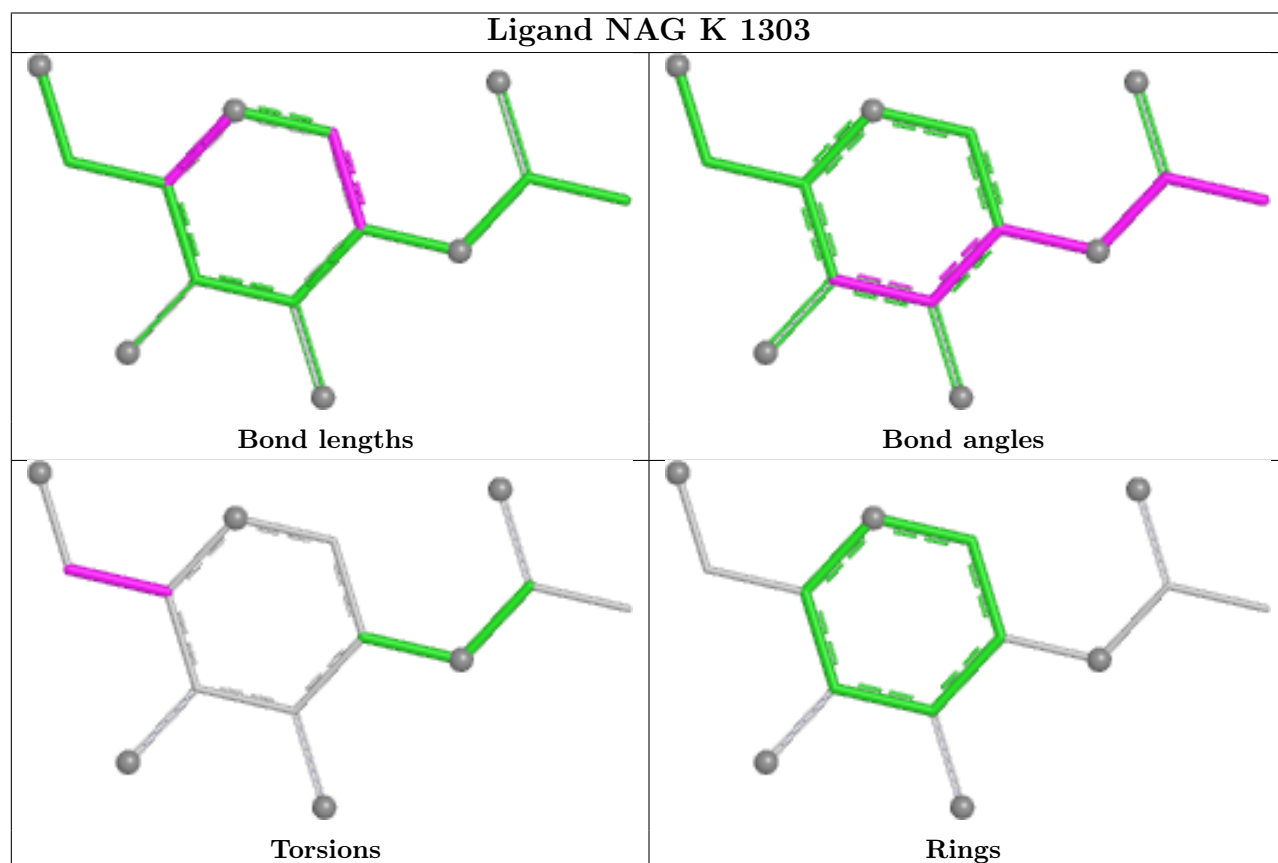
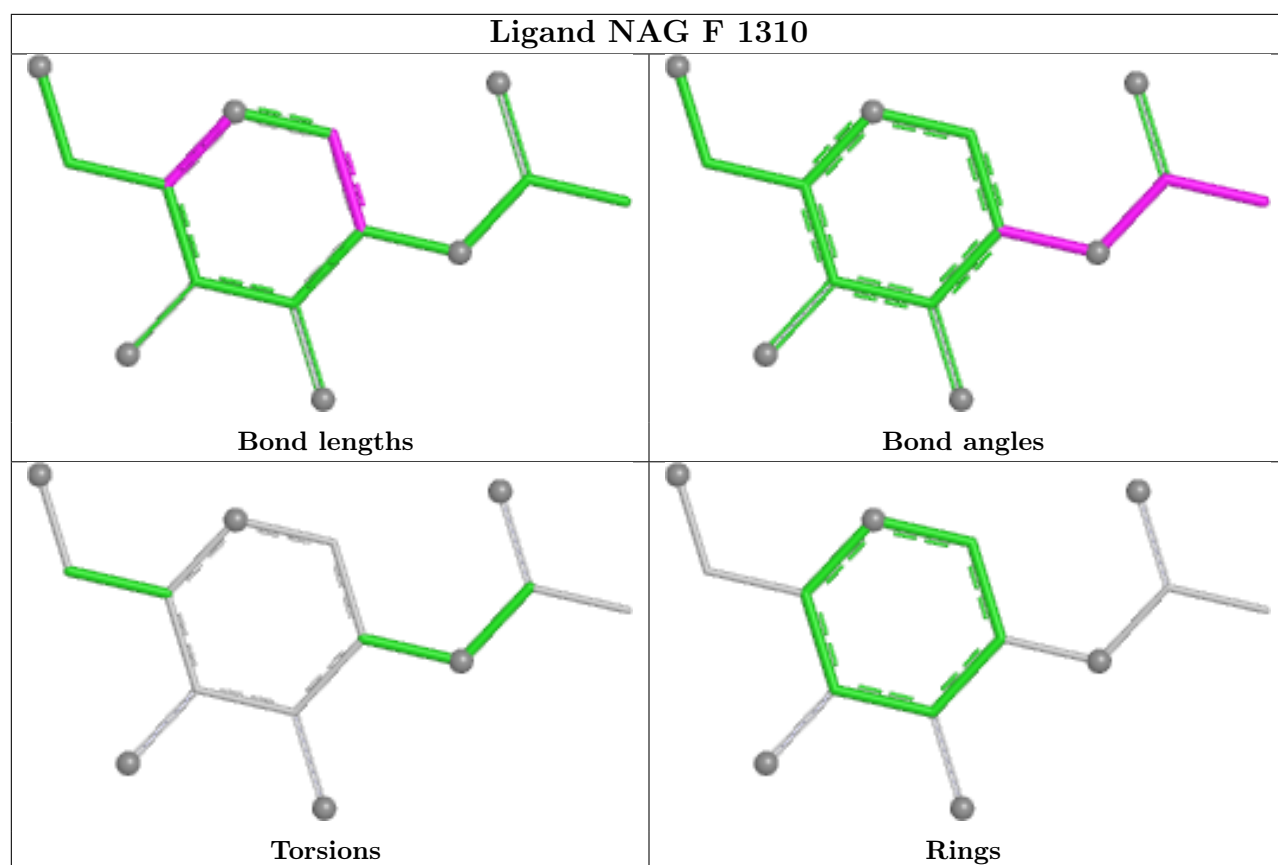
Ligand NAG K 1319



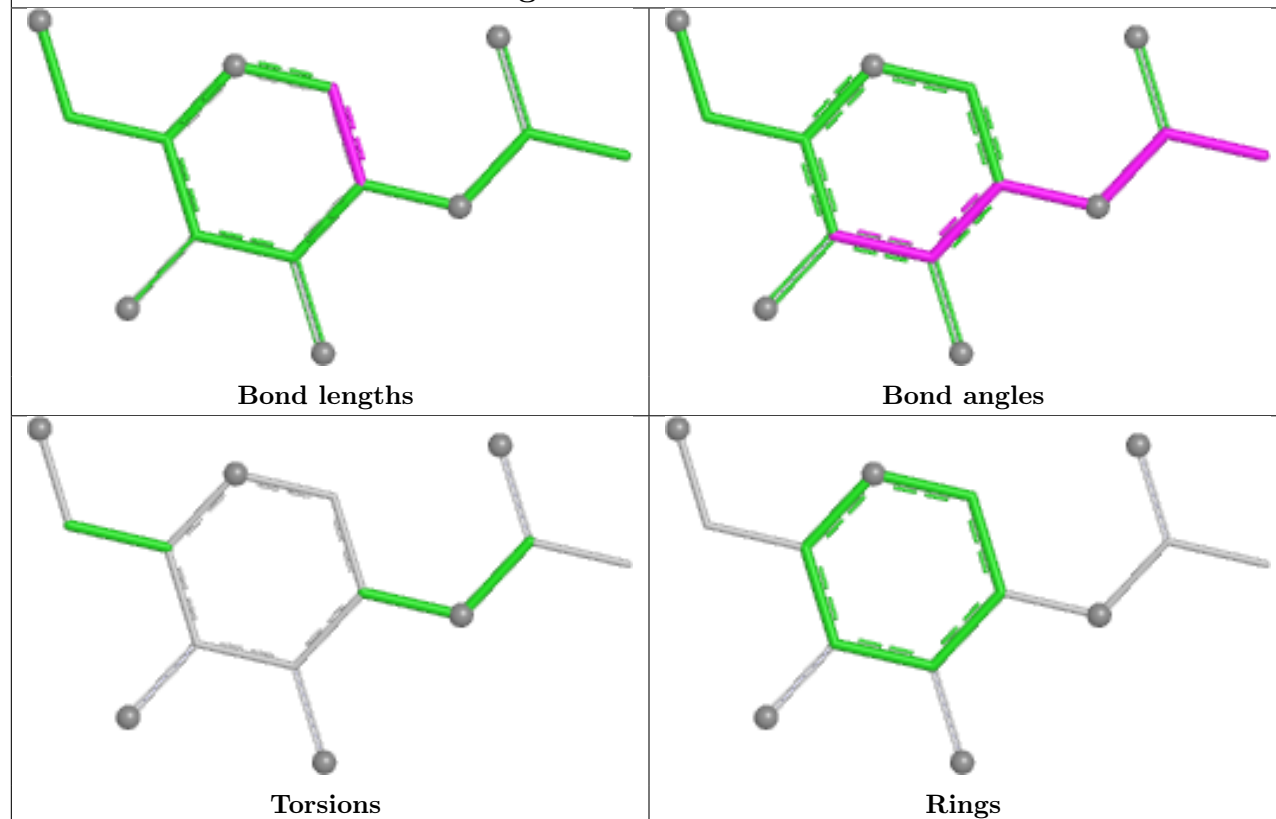
Ligand NAG K 1309



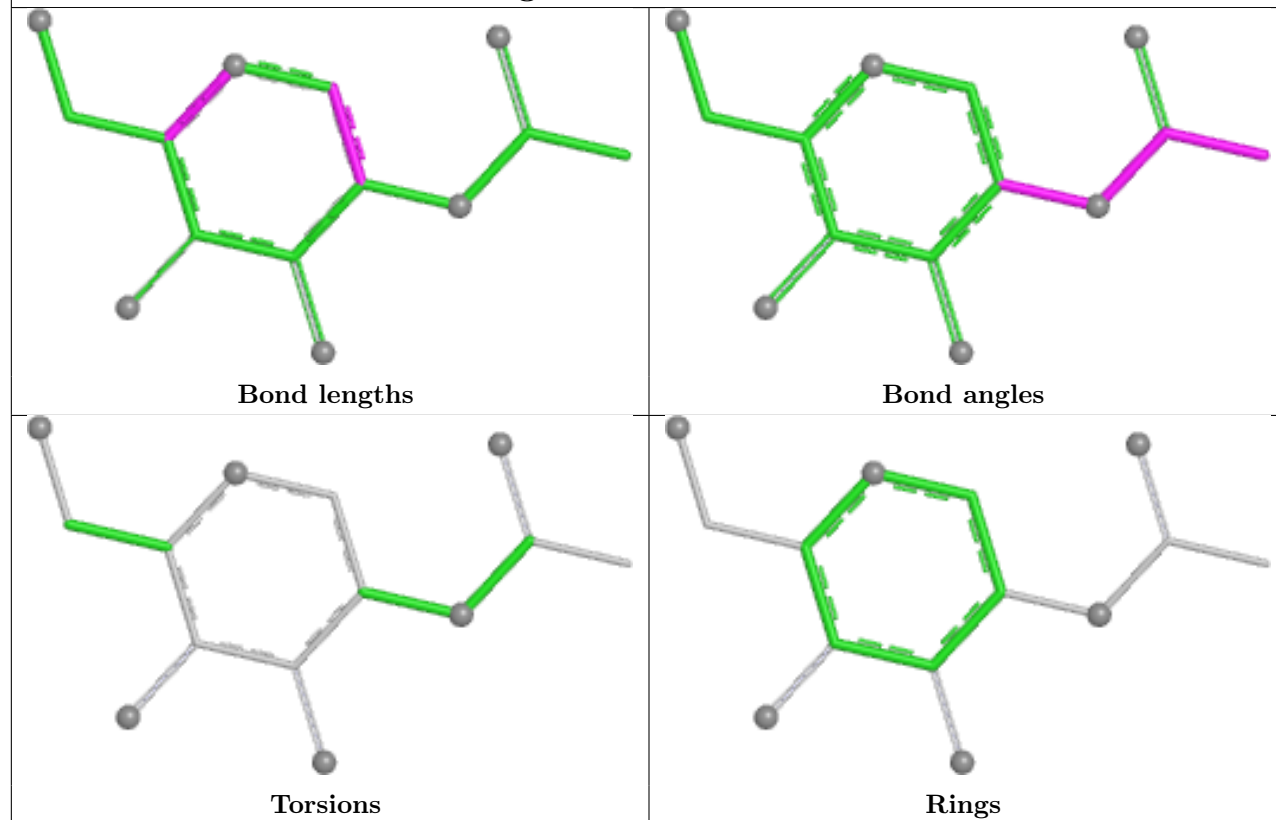


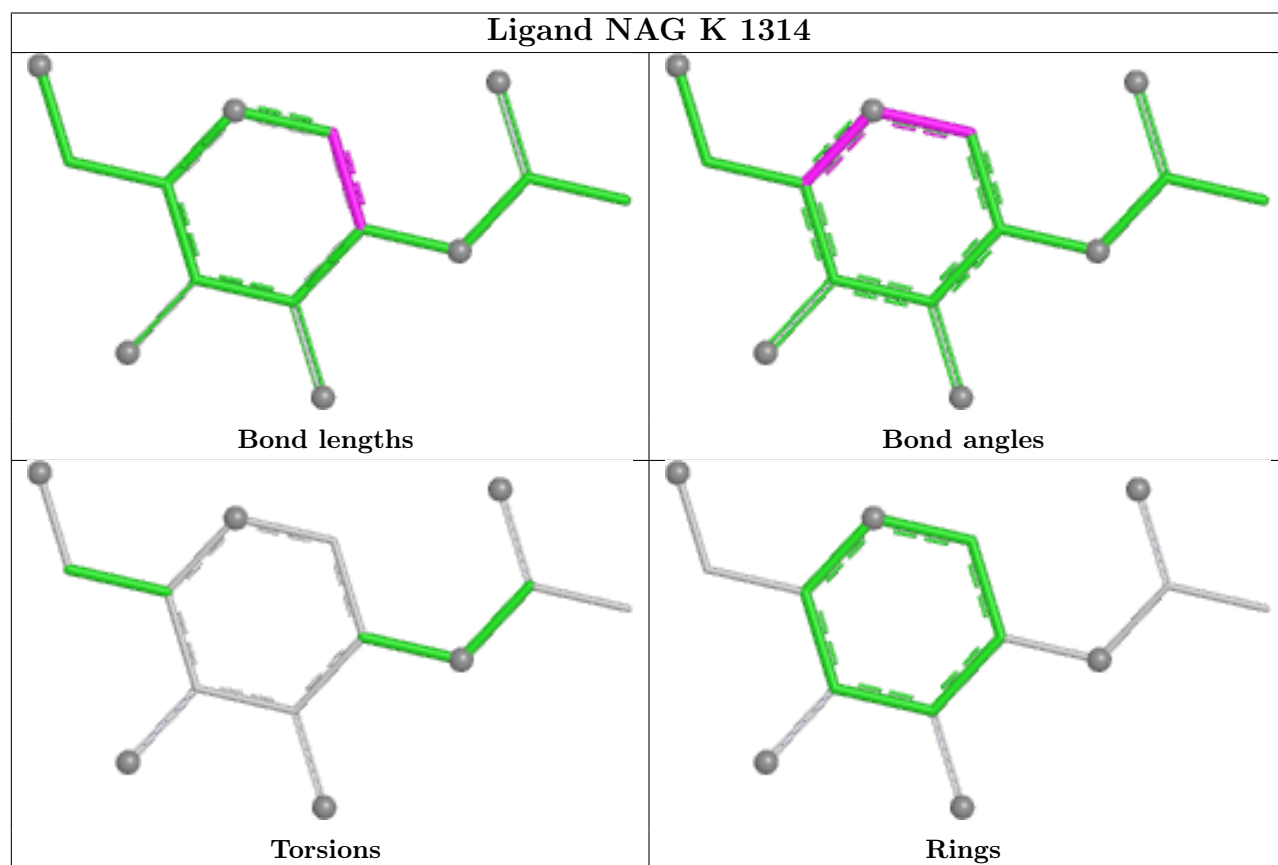
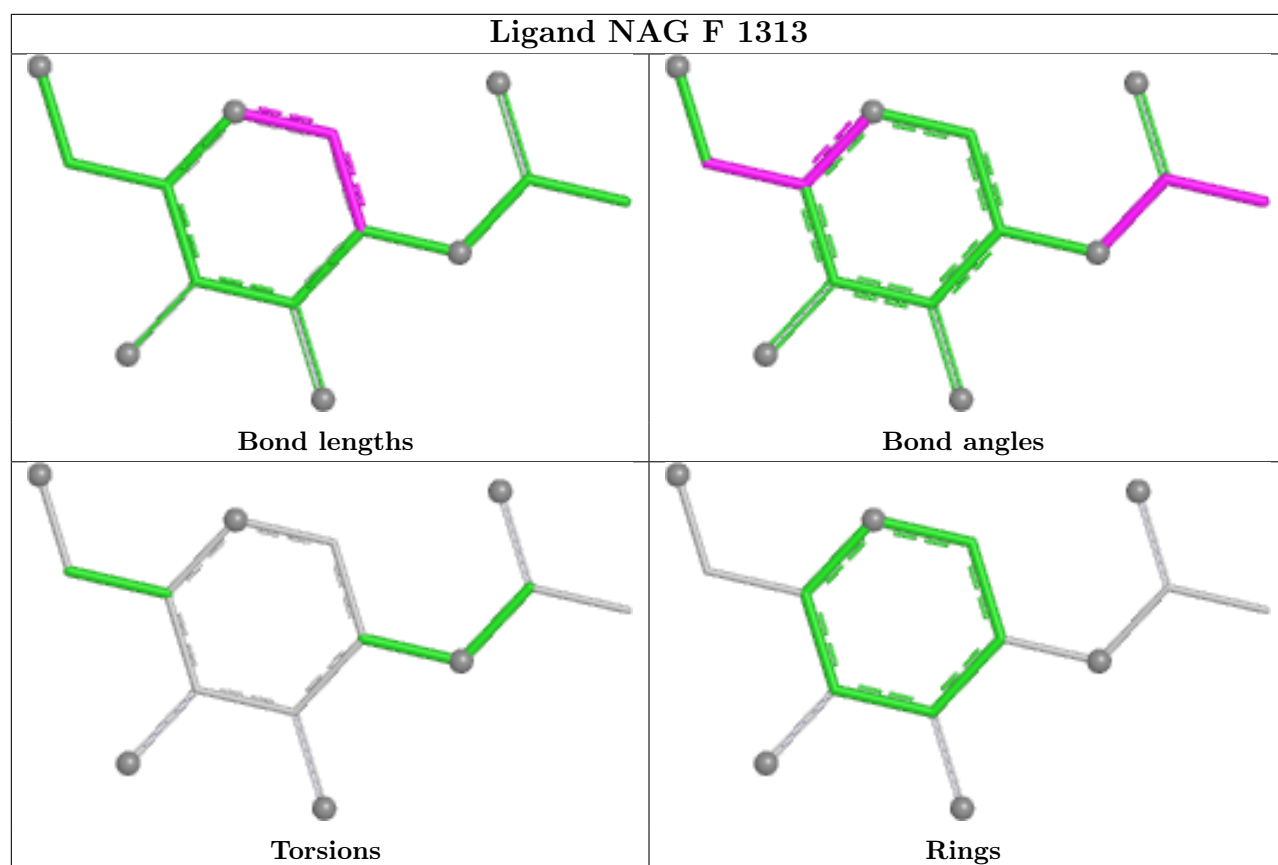


Ligand NAG A 1312

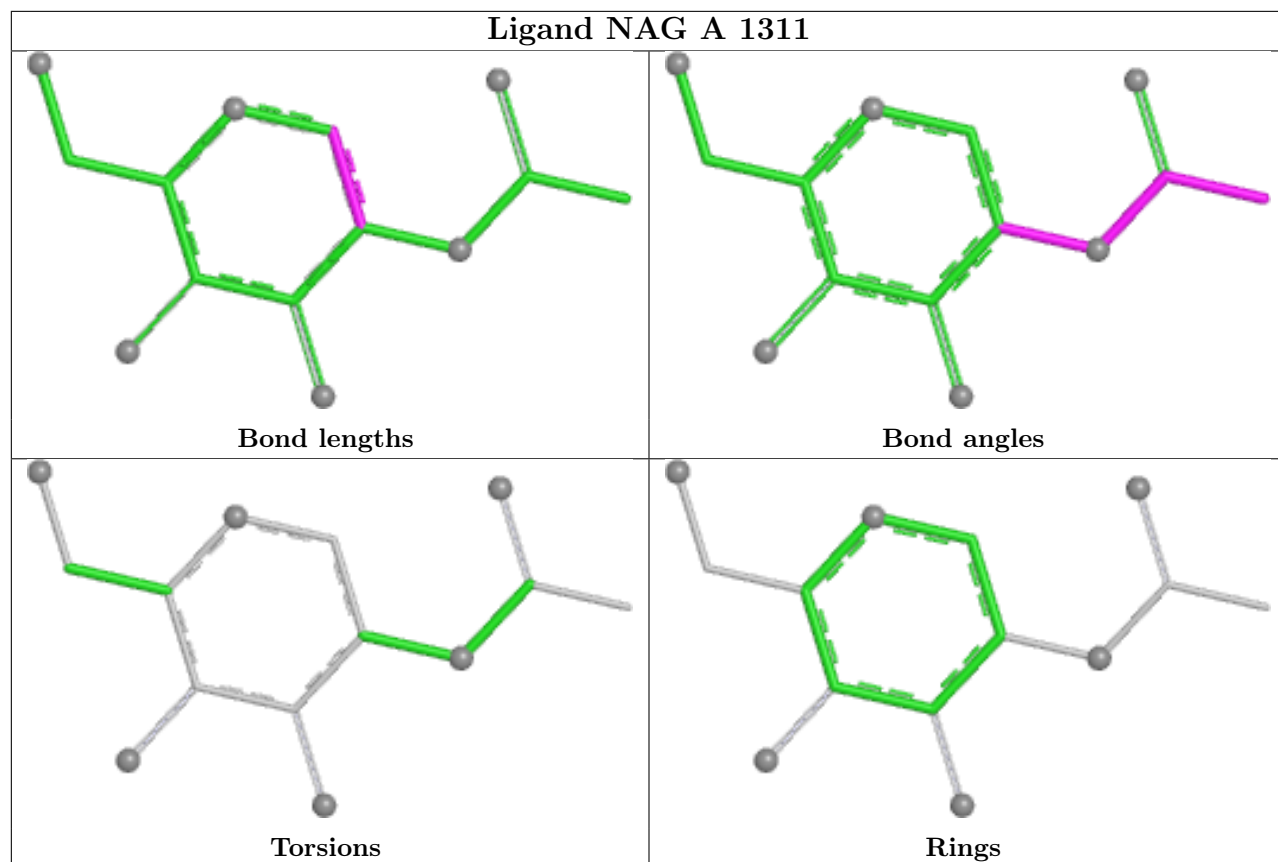


Ligand NAG K 1316

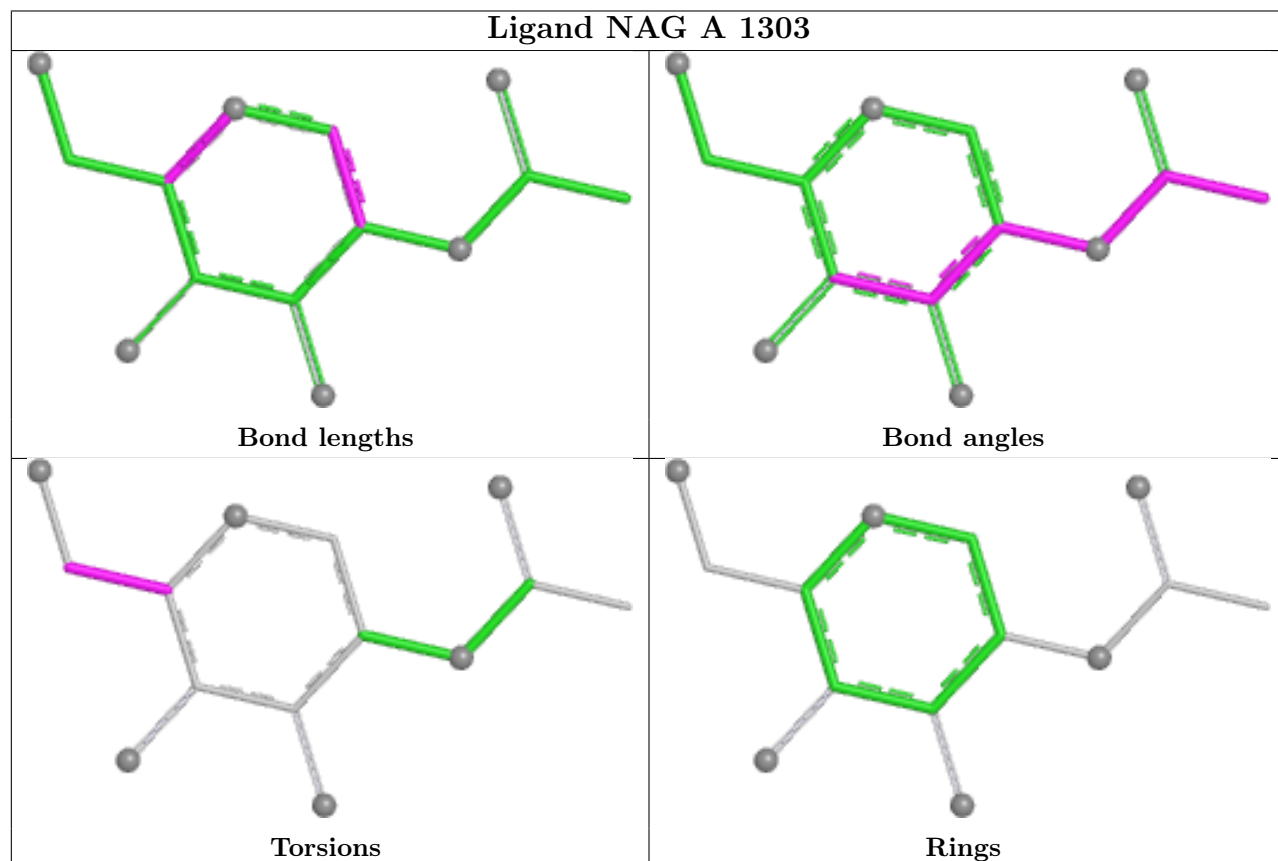




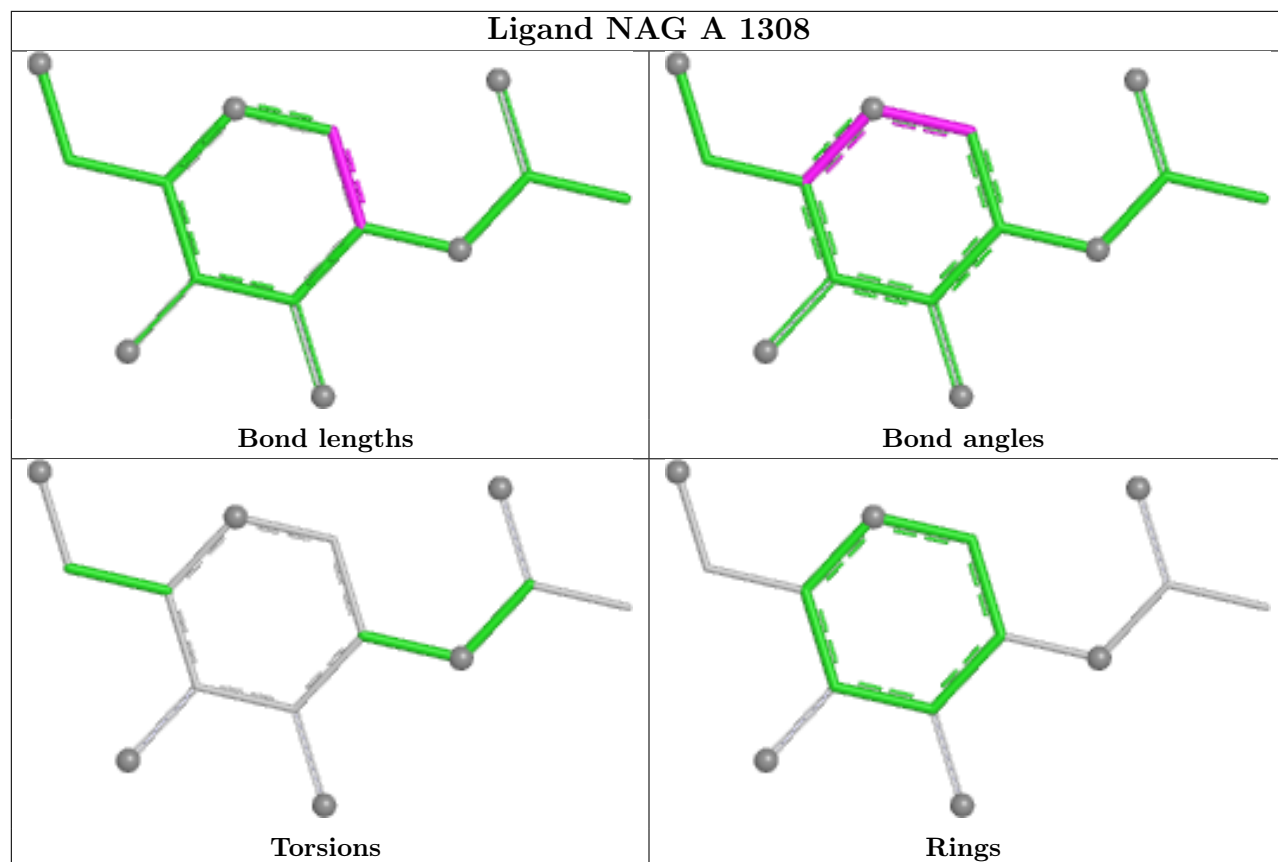
Ligand NAG A 1311



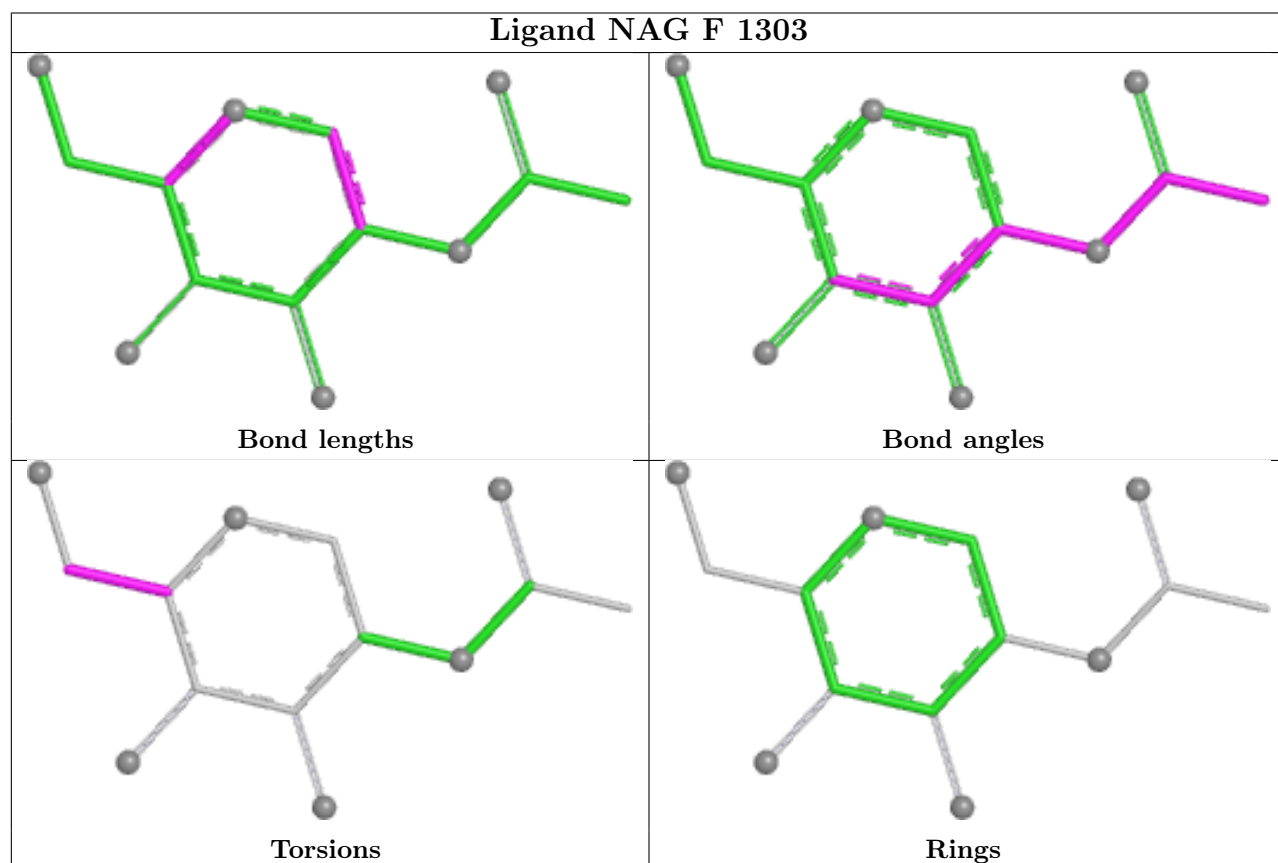
Ligand NAG A 1303

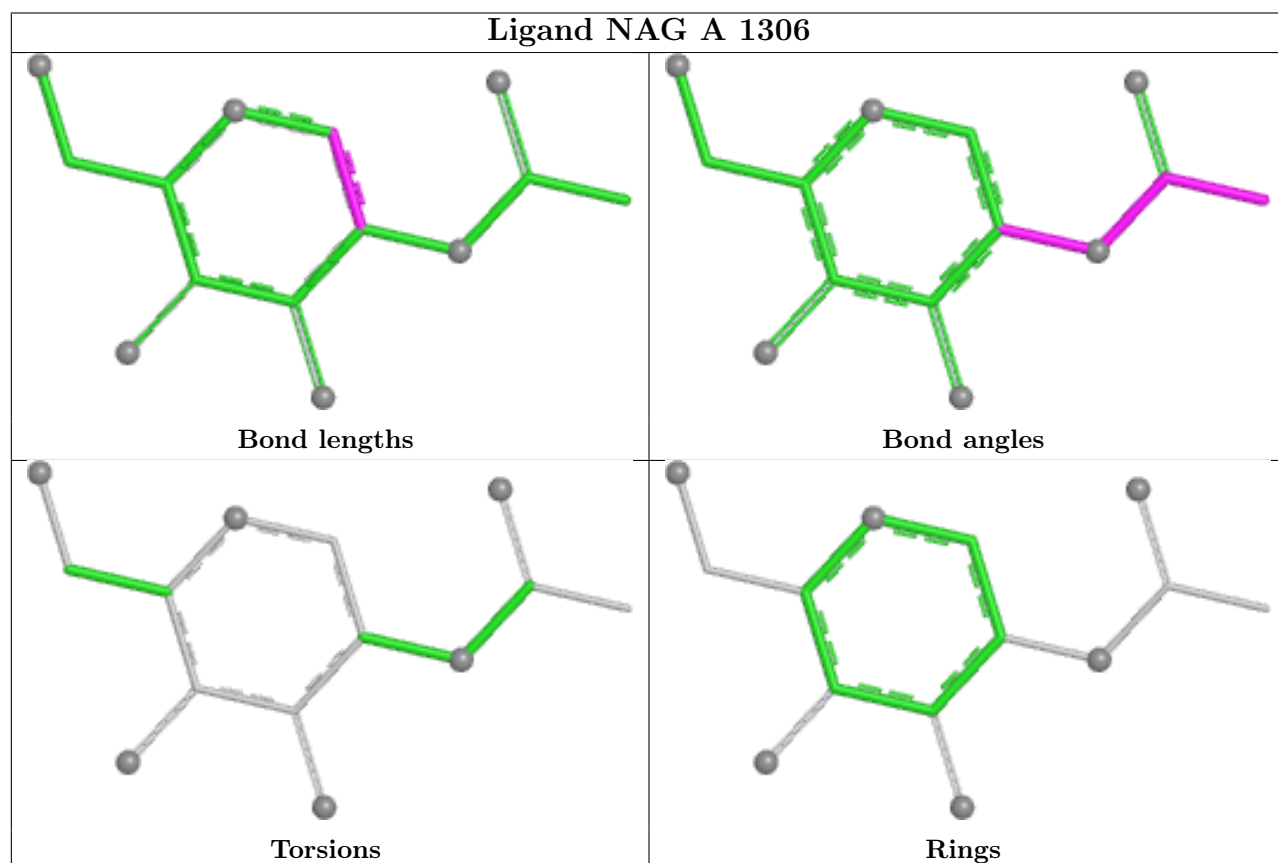
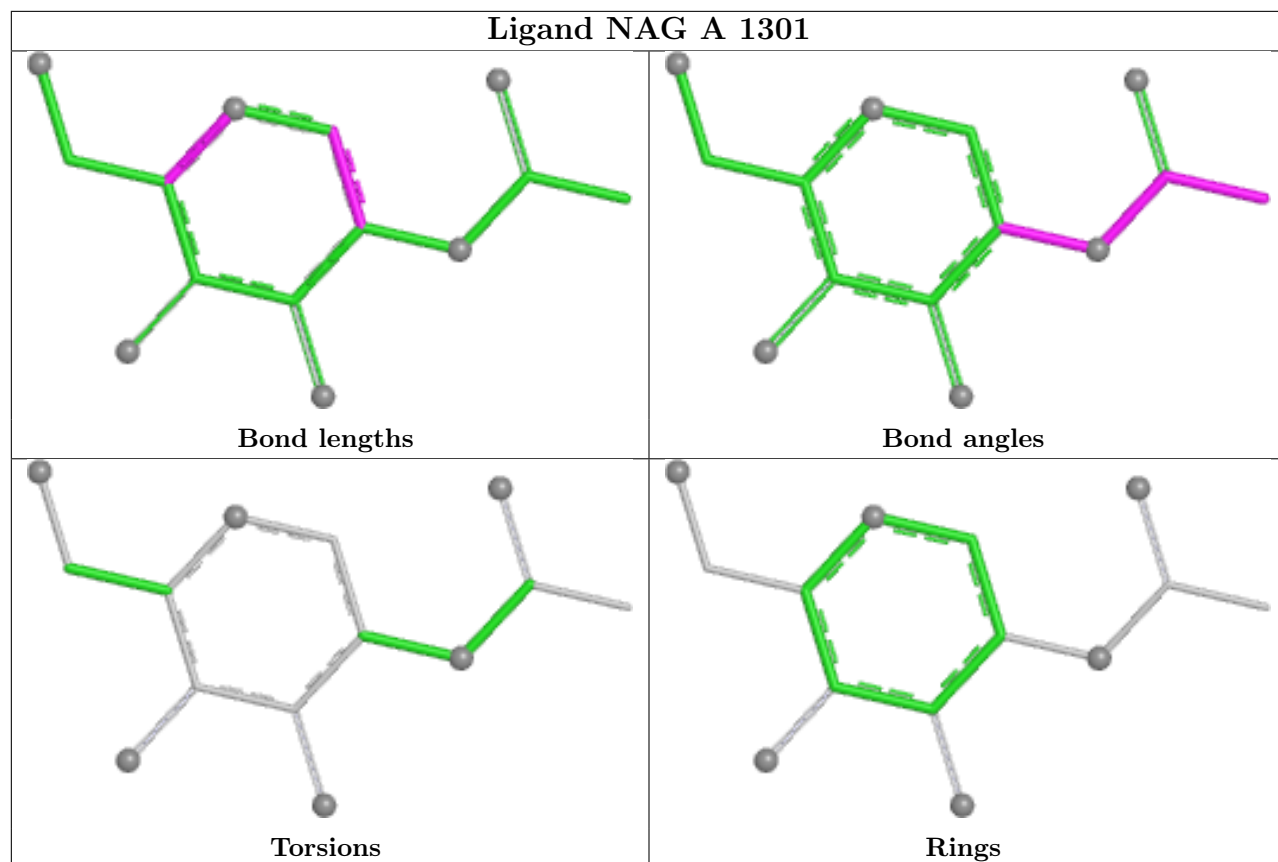


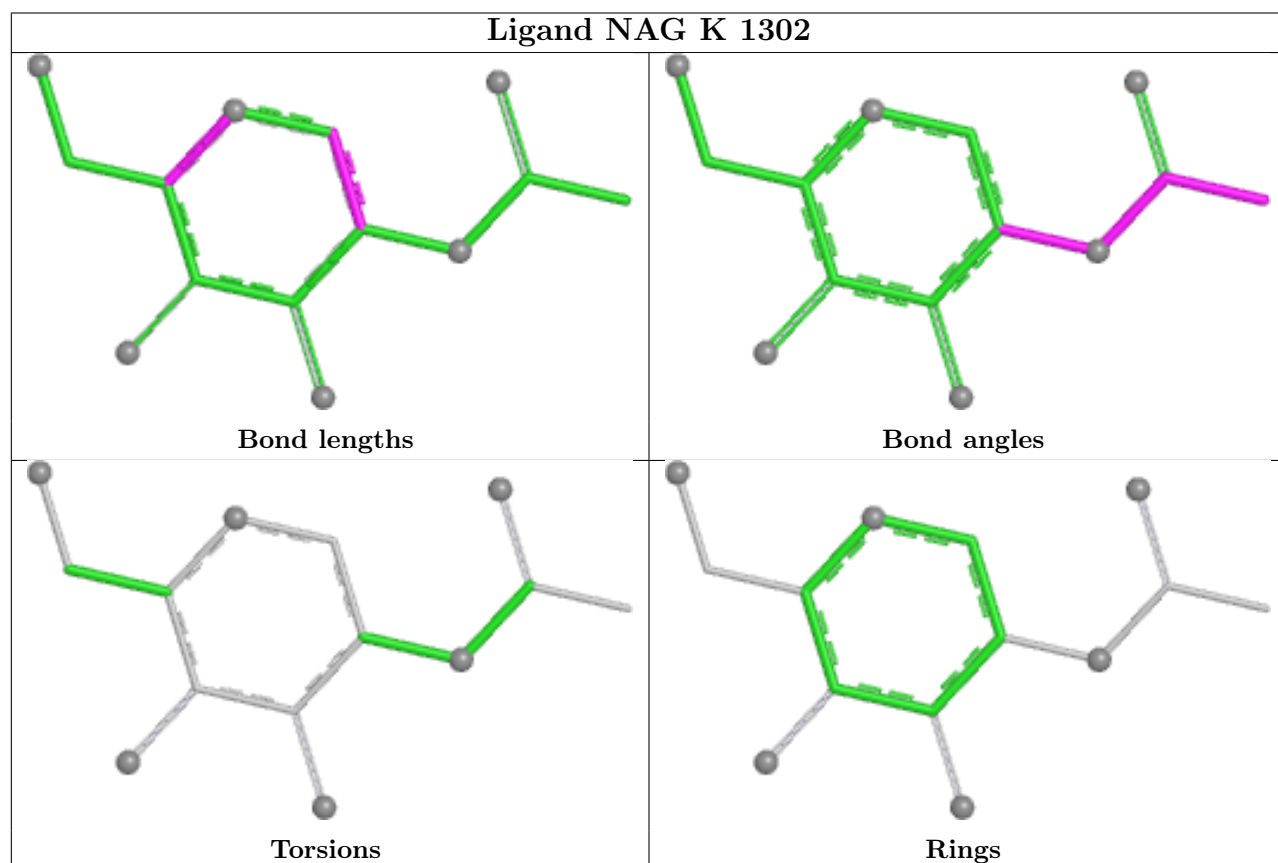
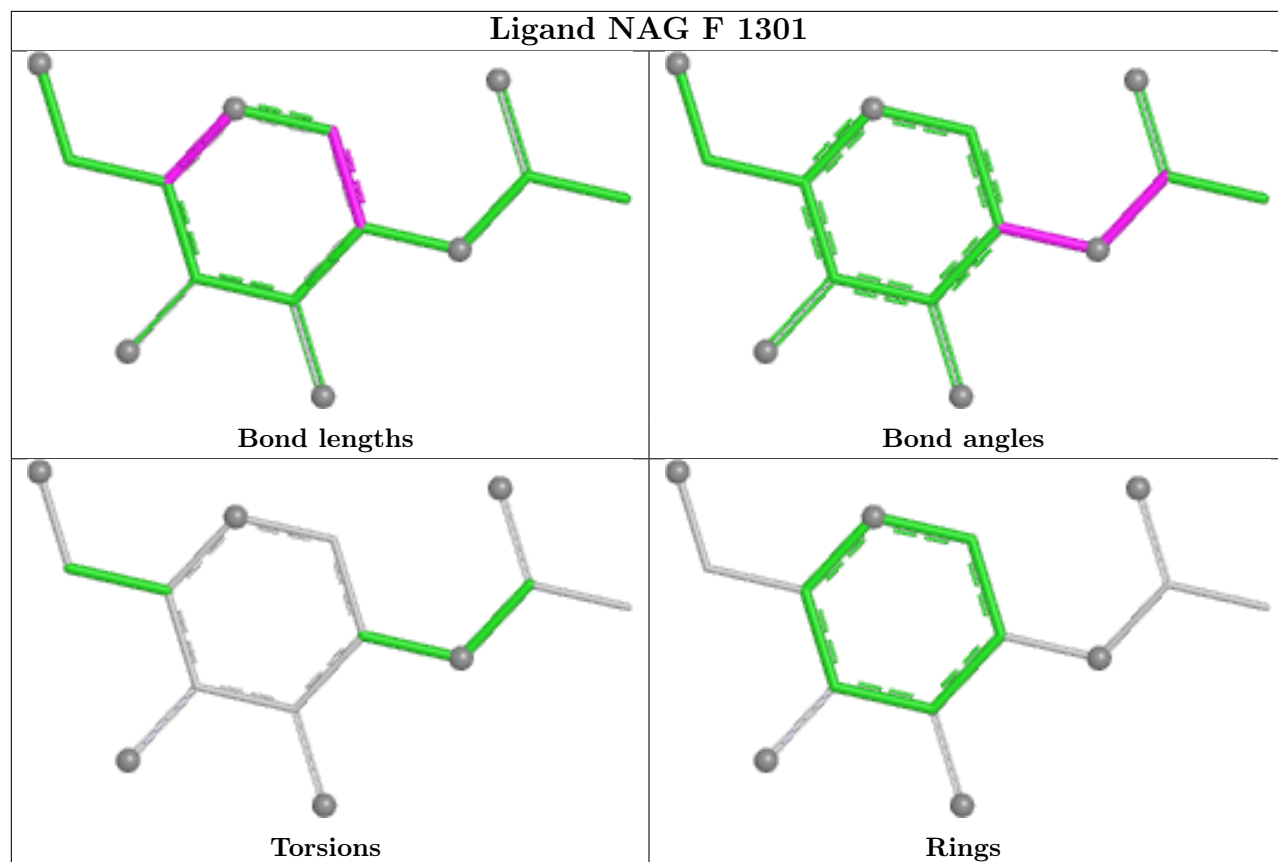
Ligand NAG A 1308

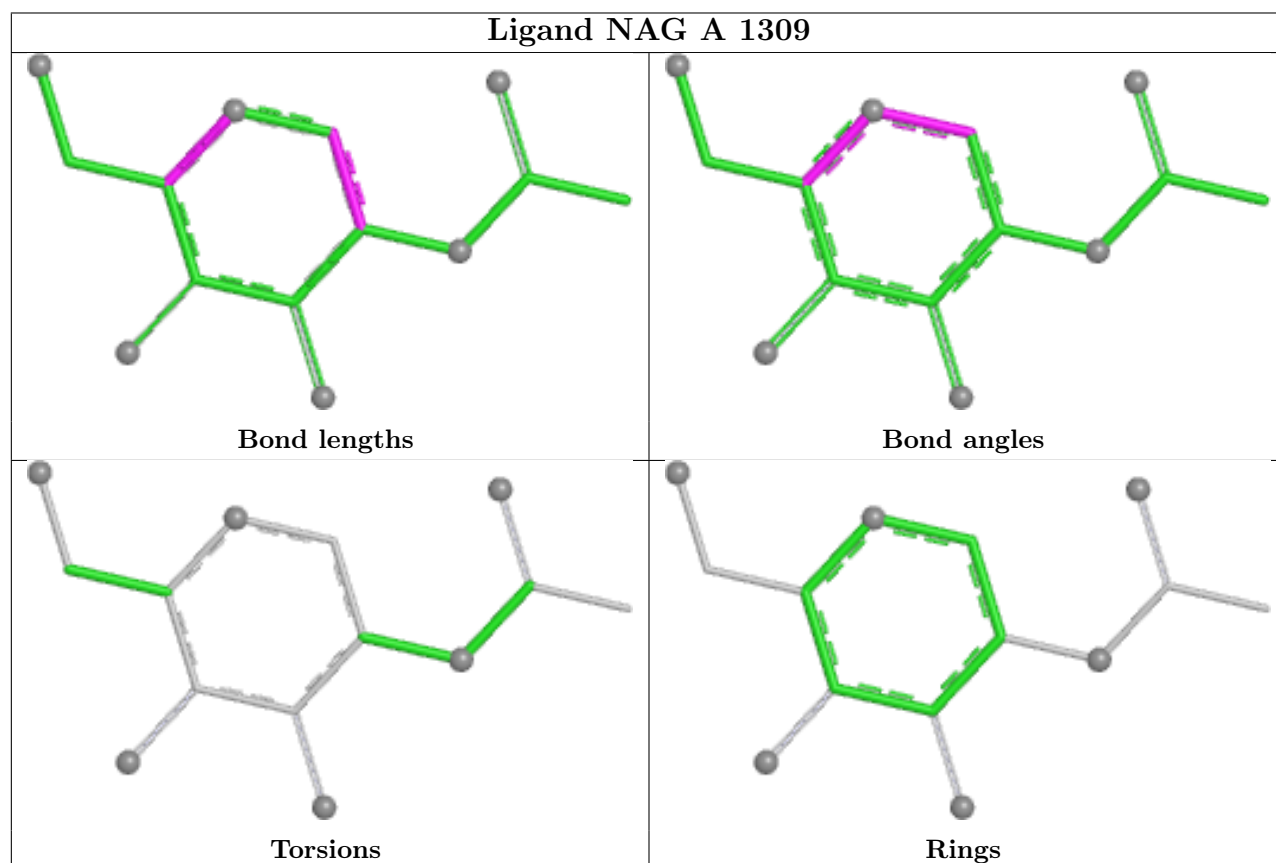
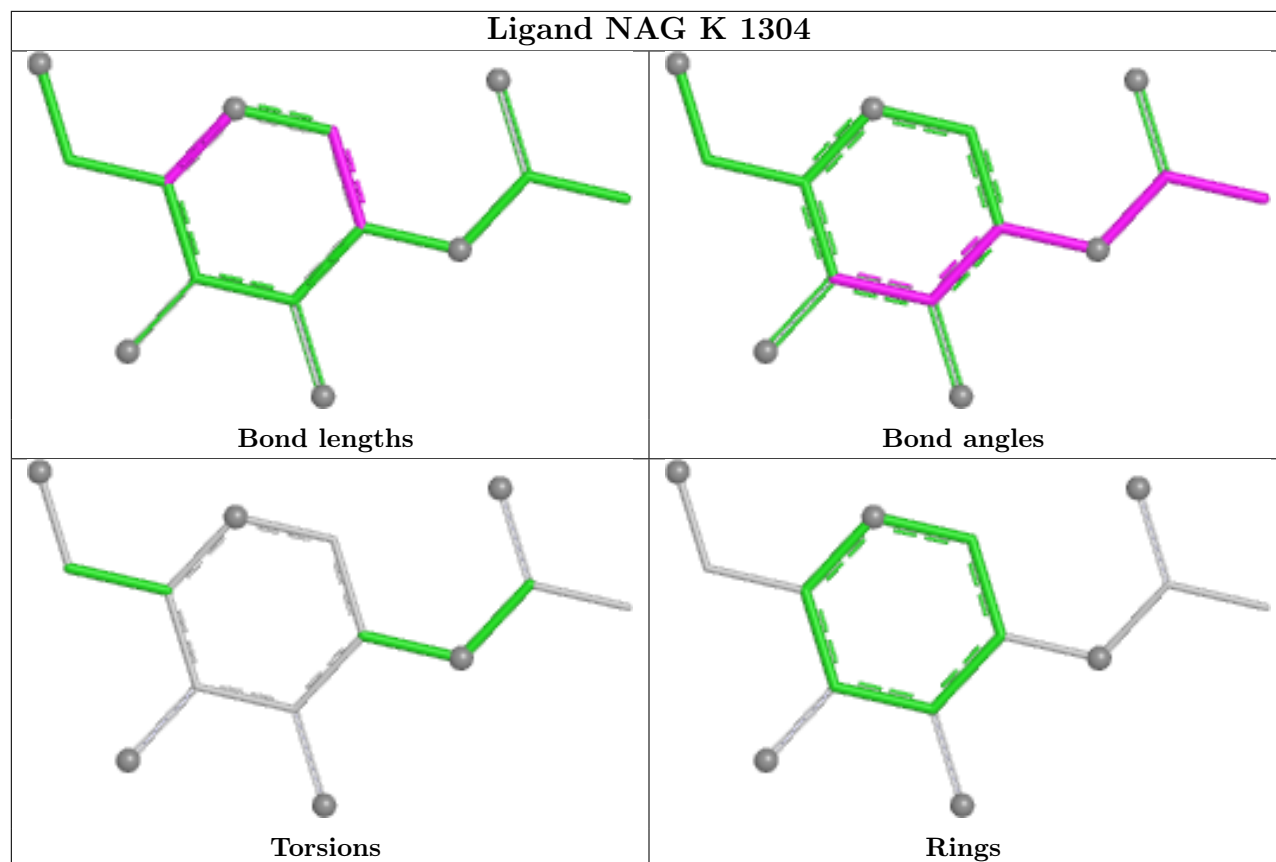


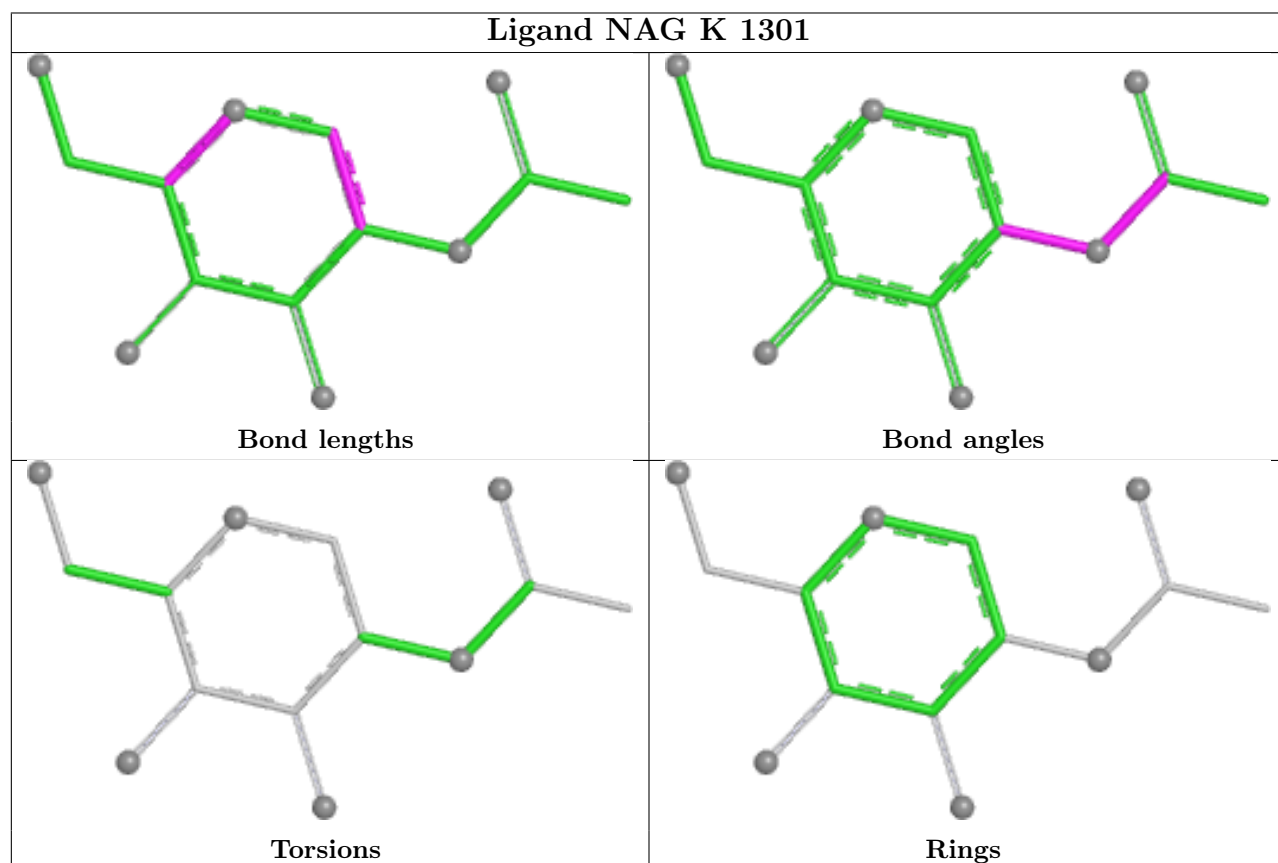
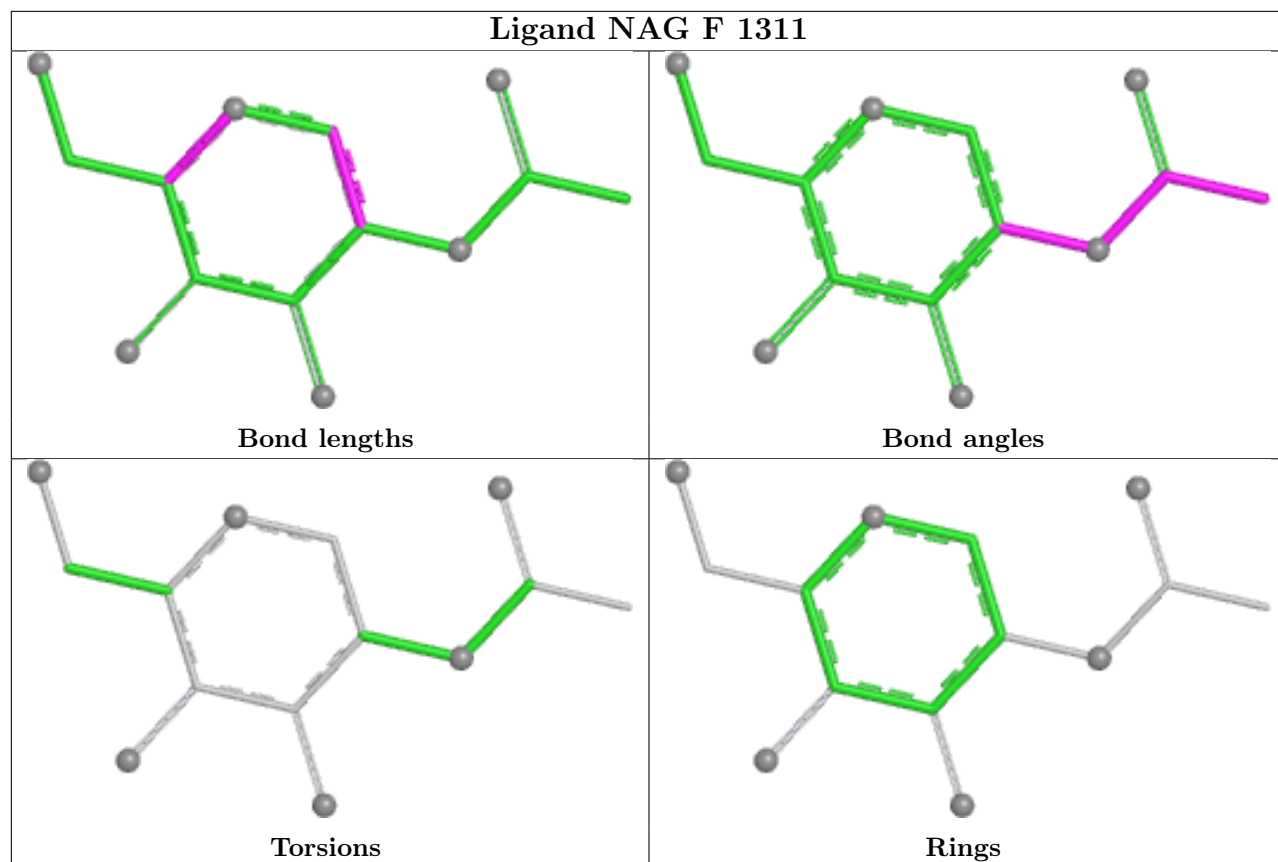
Ligand NAG F 1303

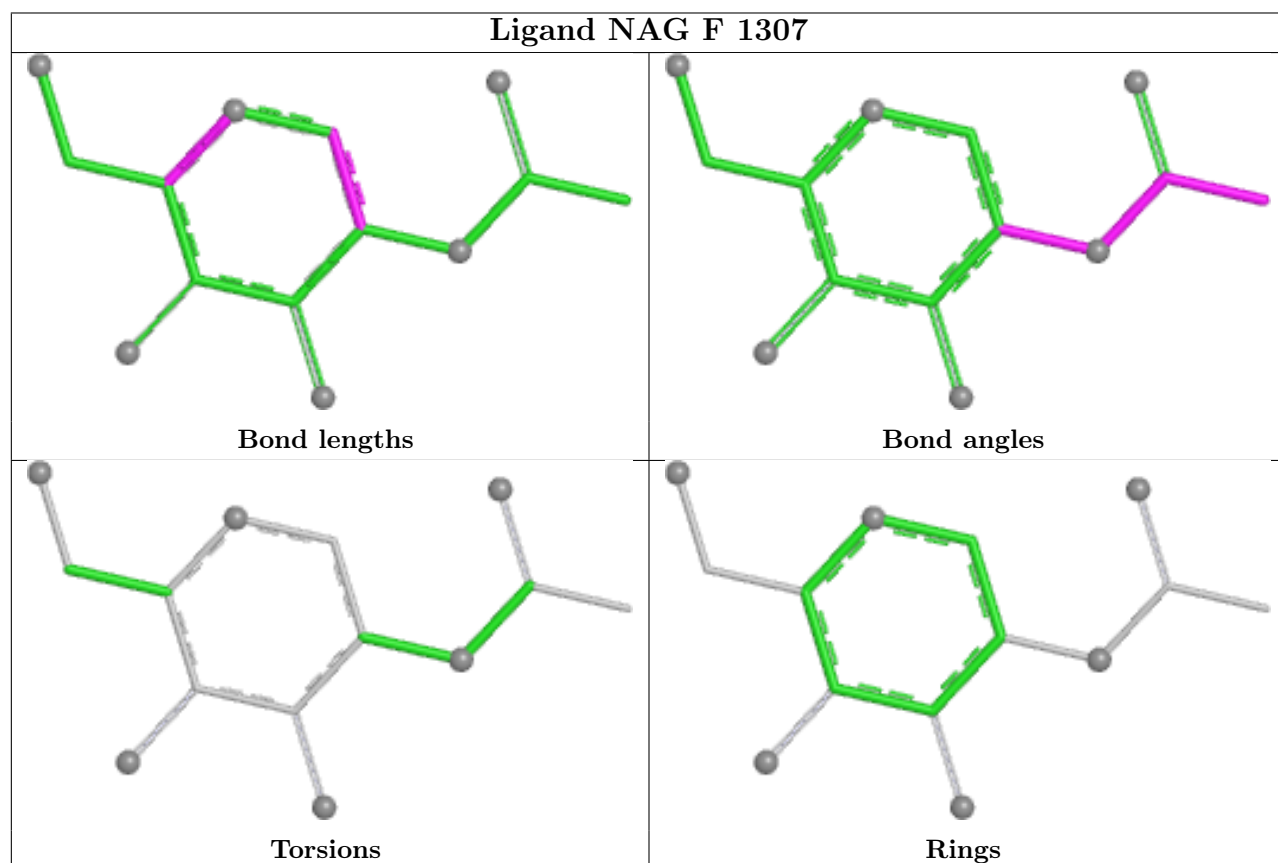
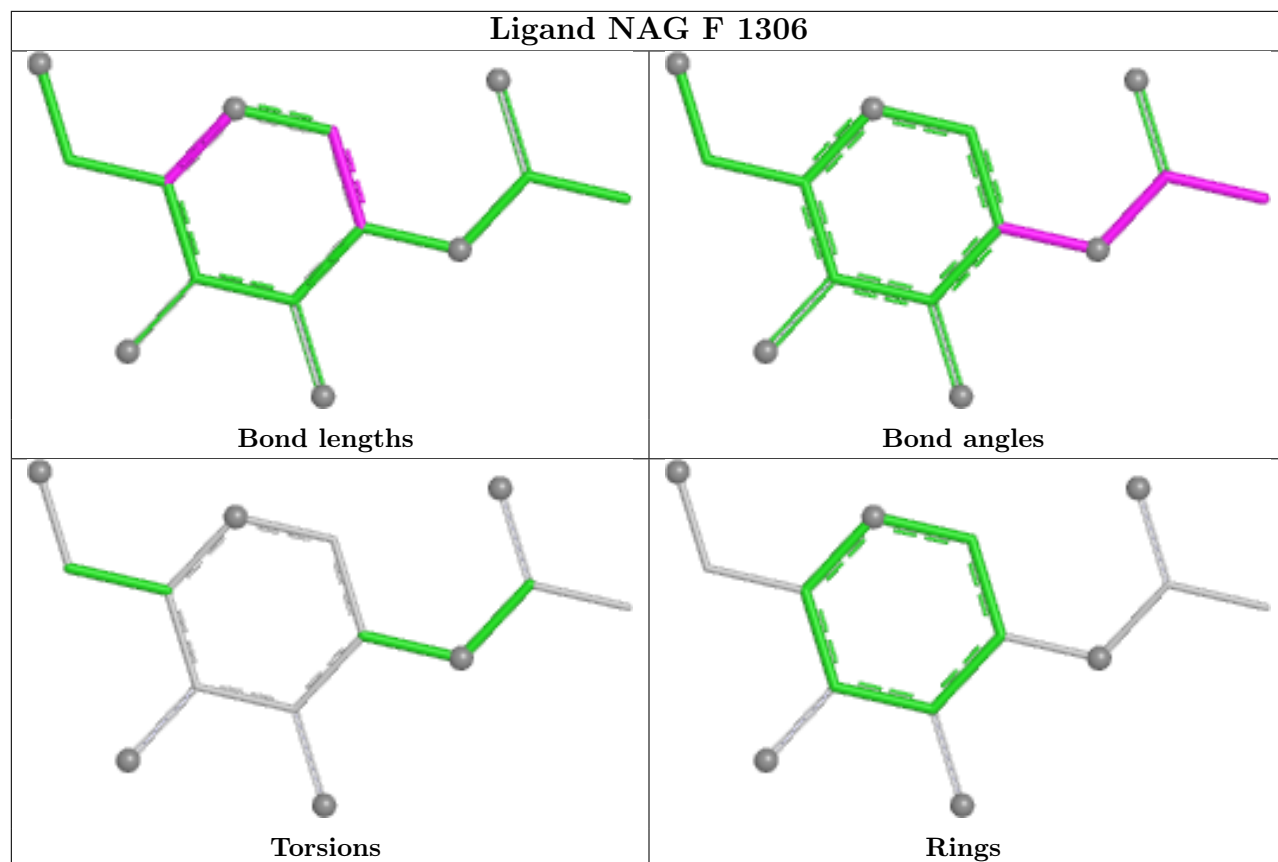




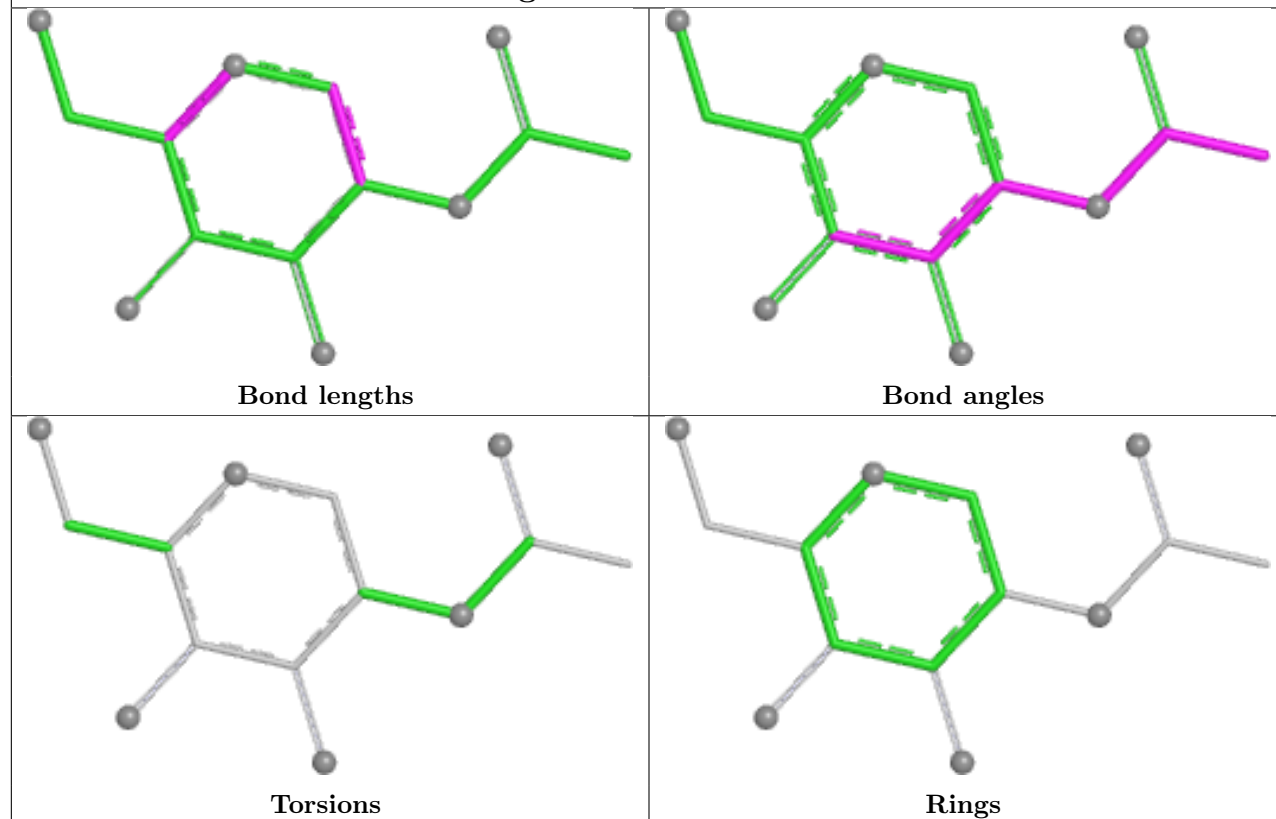




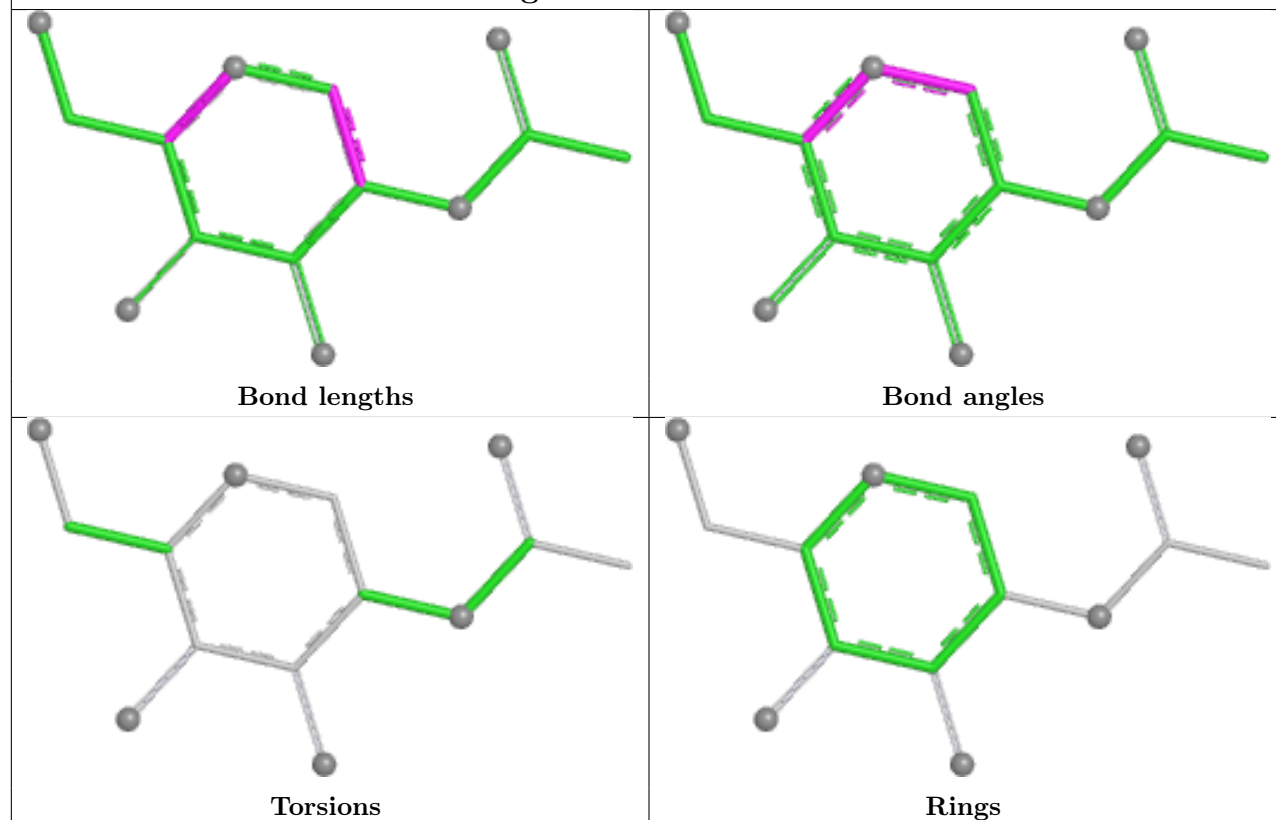




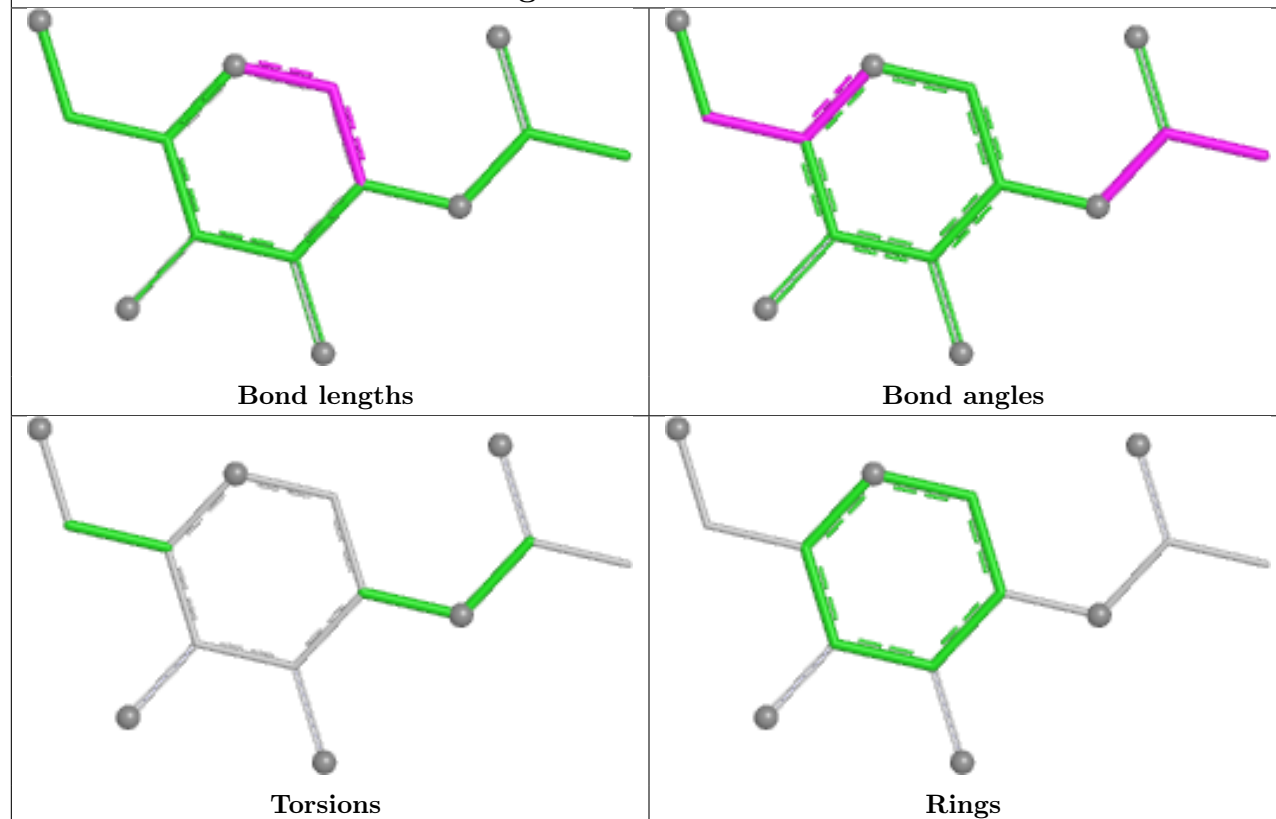
Ligand NAG A 1304



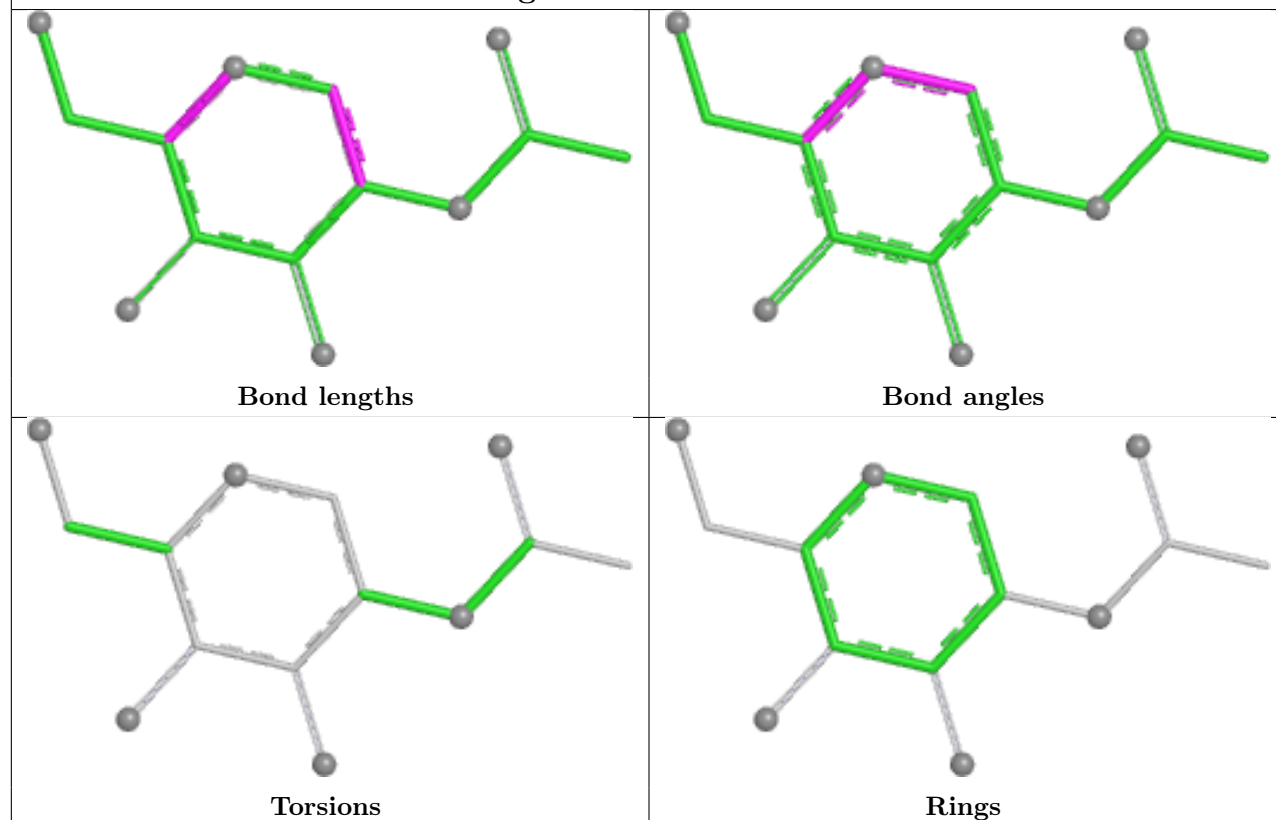
Ligand NAG F 1309

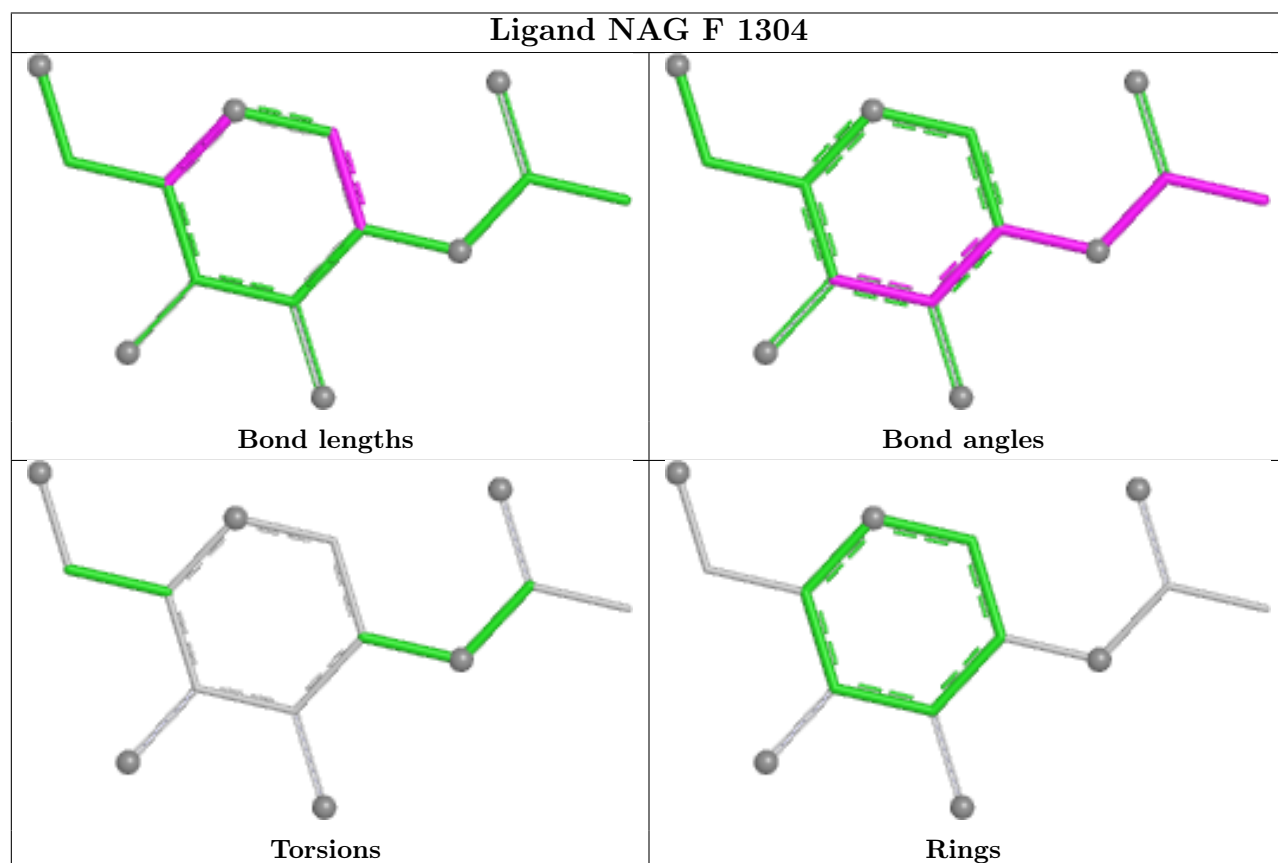
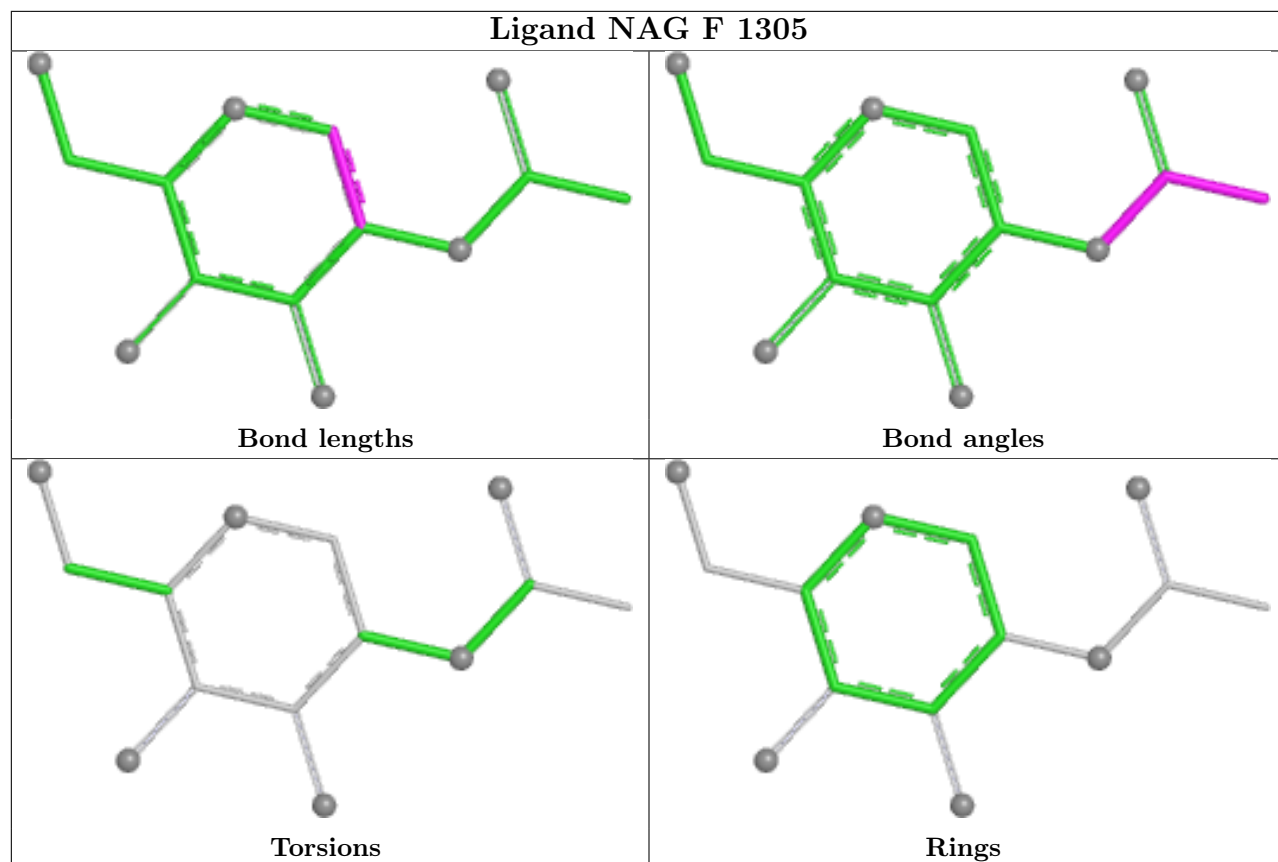


Ligand NAG A 1313



Ligand NAG K 1315





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

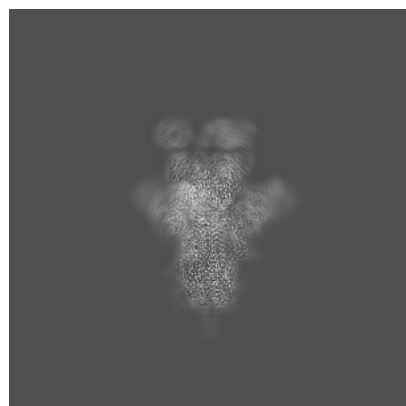
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24236. These allow visual inspection of the internal detail of the map and identification of artifacts.

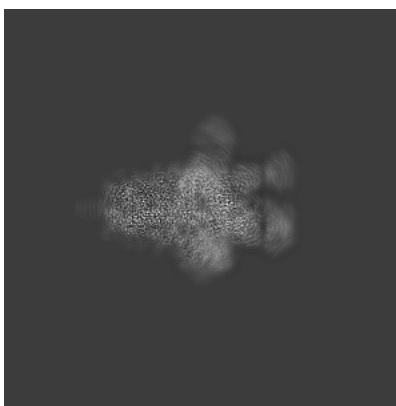
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

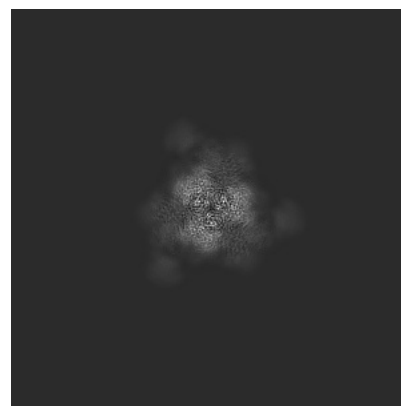
6.1.1 Primary map



X

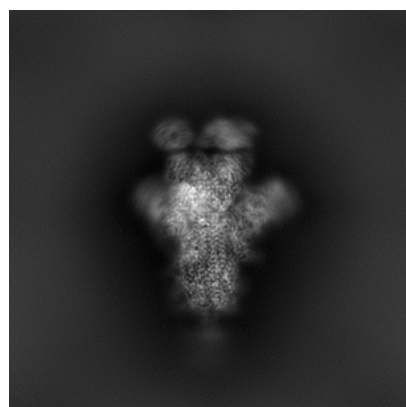


Y

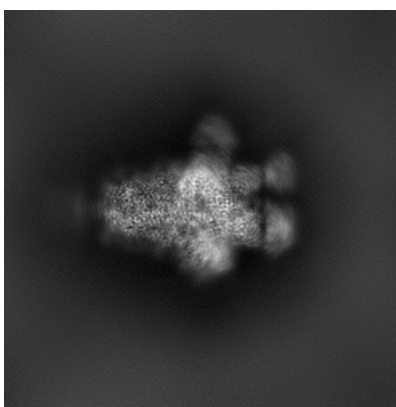


Z

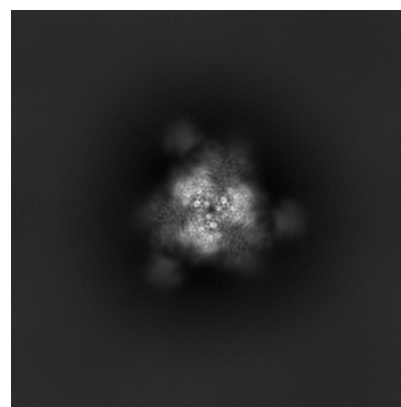
6.1.2 Raw map



X



Y



Z

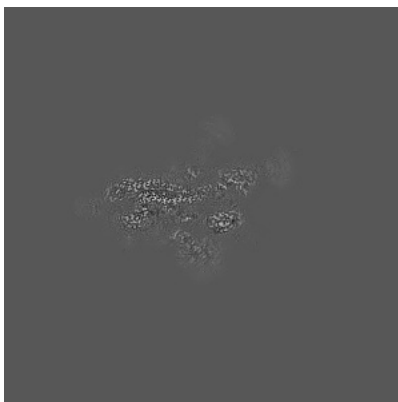
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

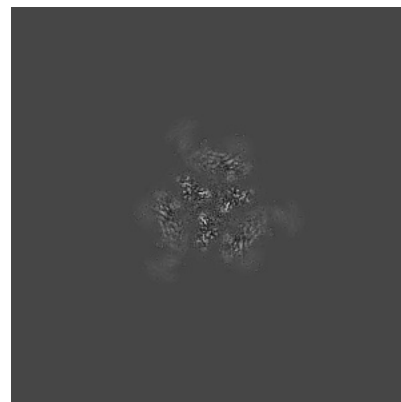
6.2.1 Primary map



X Index: 256

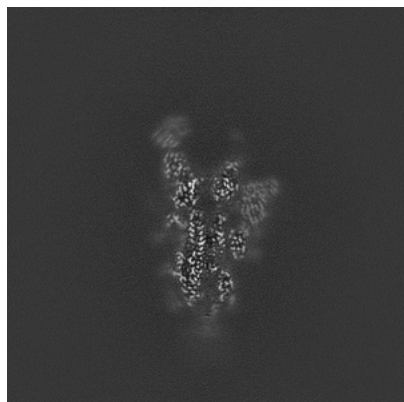


Y Index: 256

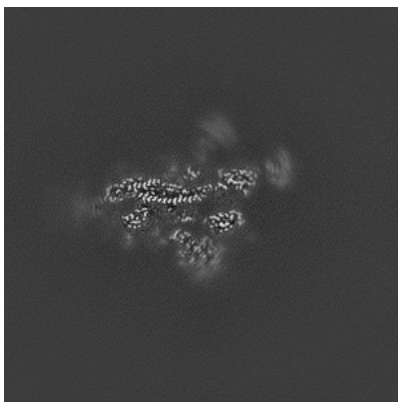


Z Index: 256

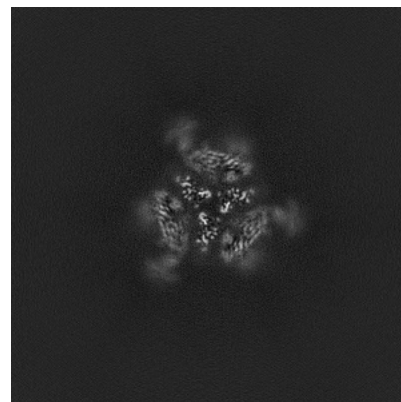
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

6.3 Largest variance slices [i](#)

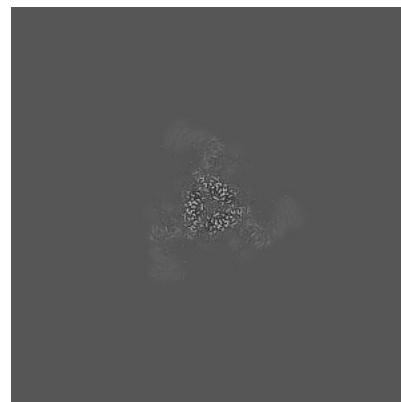
6.3.1 Primary map



X Index: 252

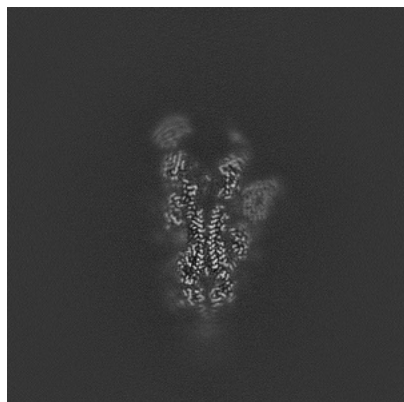


Y Index: 265

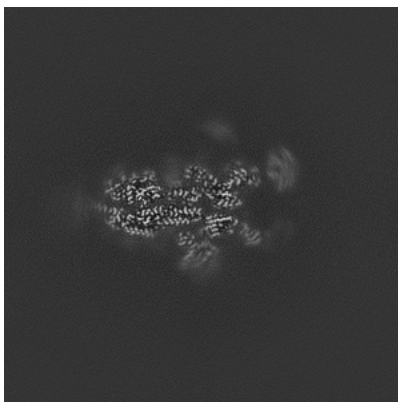


Z Index: 279

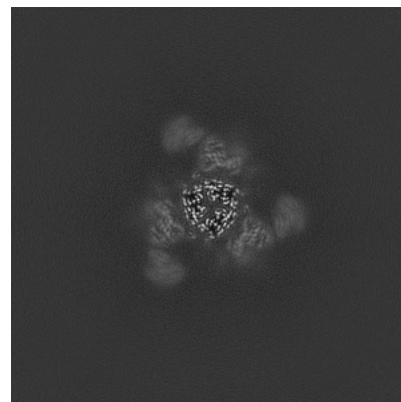
6.3.2 Raw map



X Index: 251



Y Index: 265

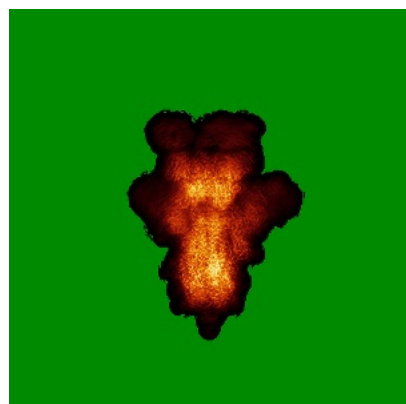


Z Index: 274

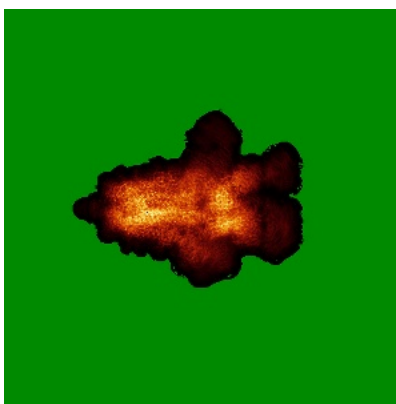
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

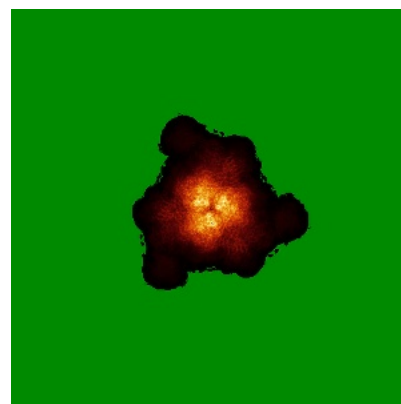
6.4.1 Primary map



X

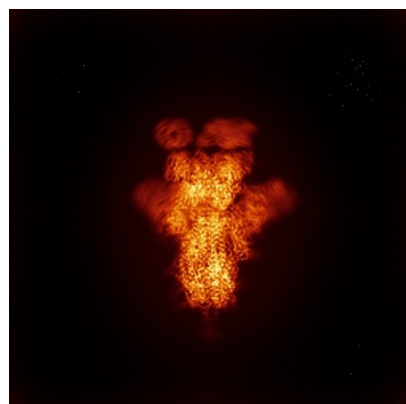


Y

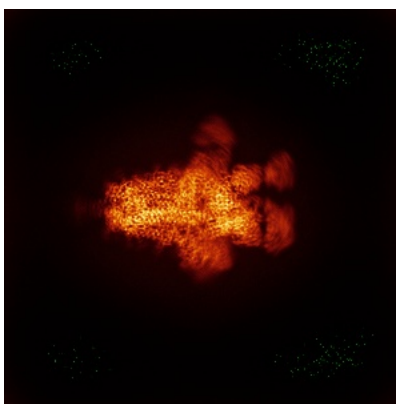


Z

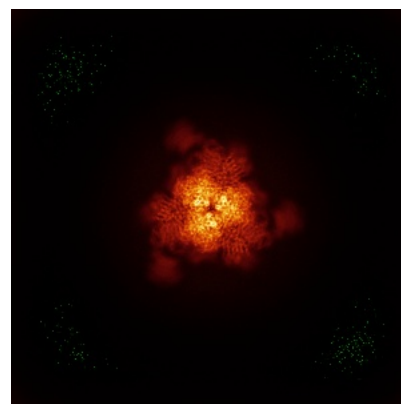
6.4.2 Raw map



X



Y

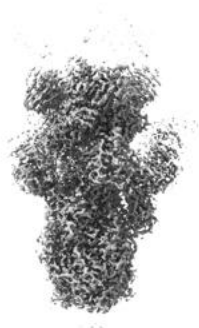


Z

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](#)

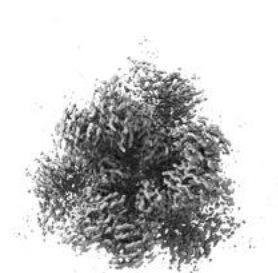
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

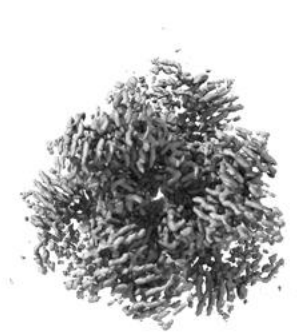
6.5.2 Raw map



X



Y



Z

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.

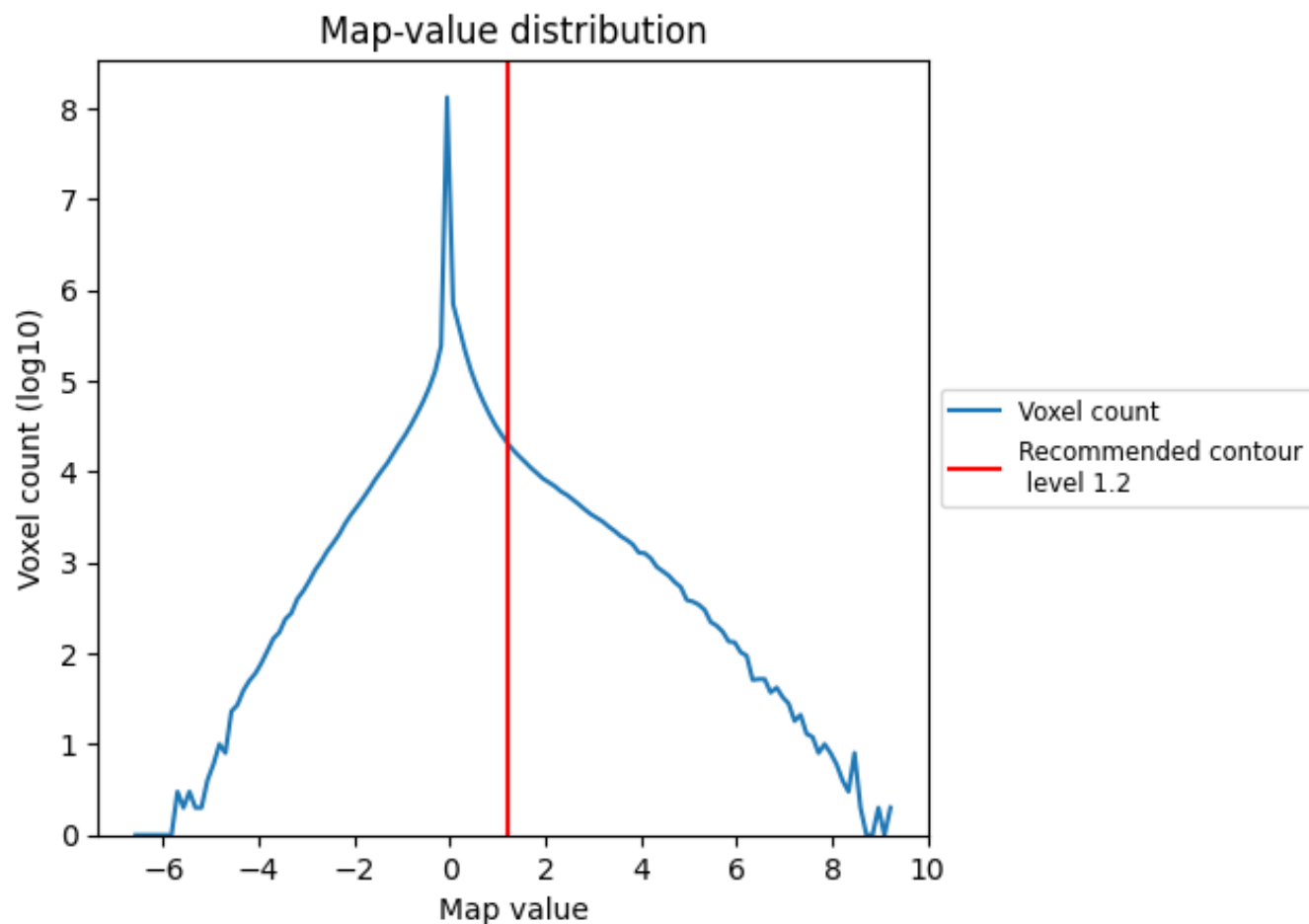
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

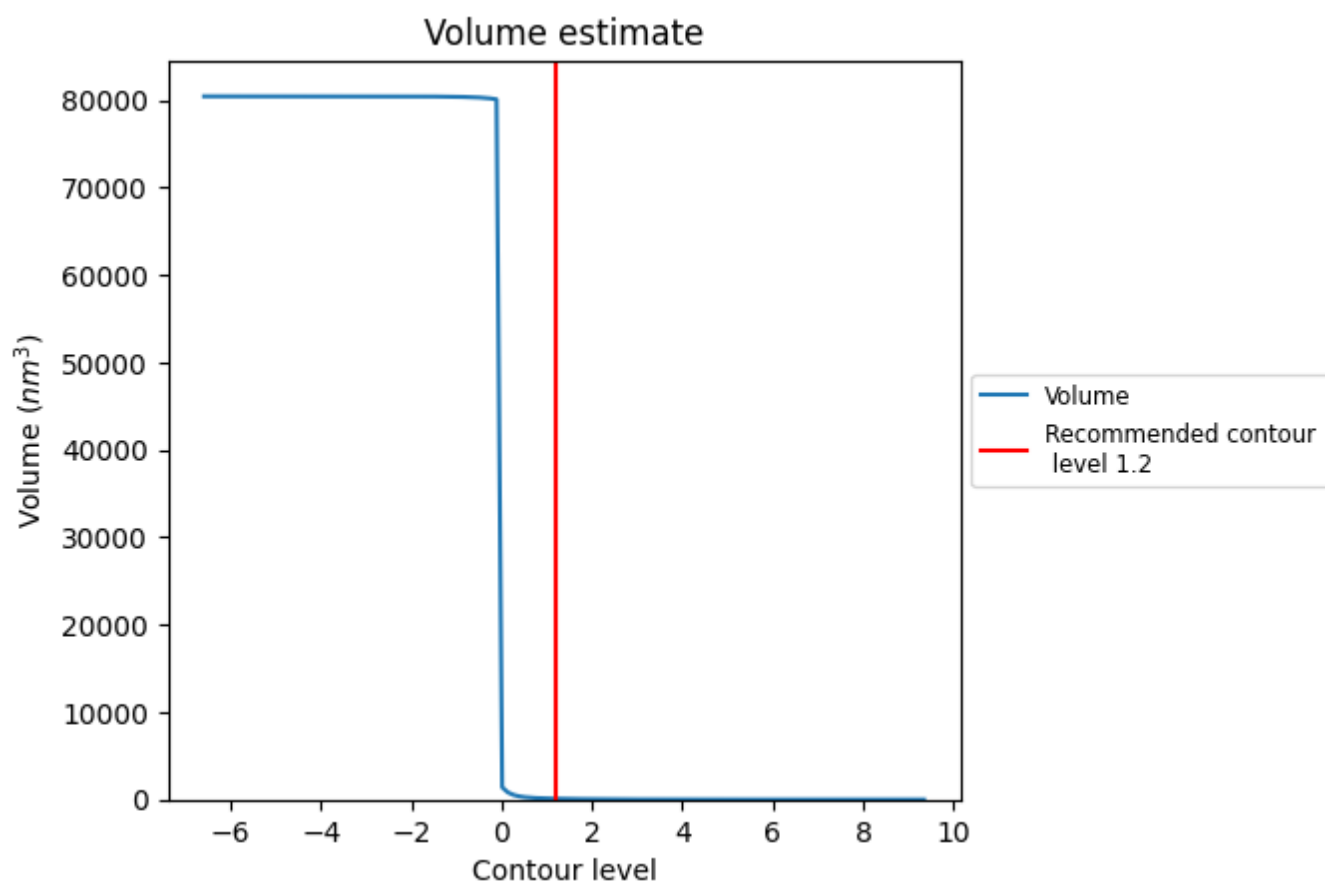
This section contains the results of statistical analysis of the map.

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.

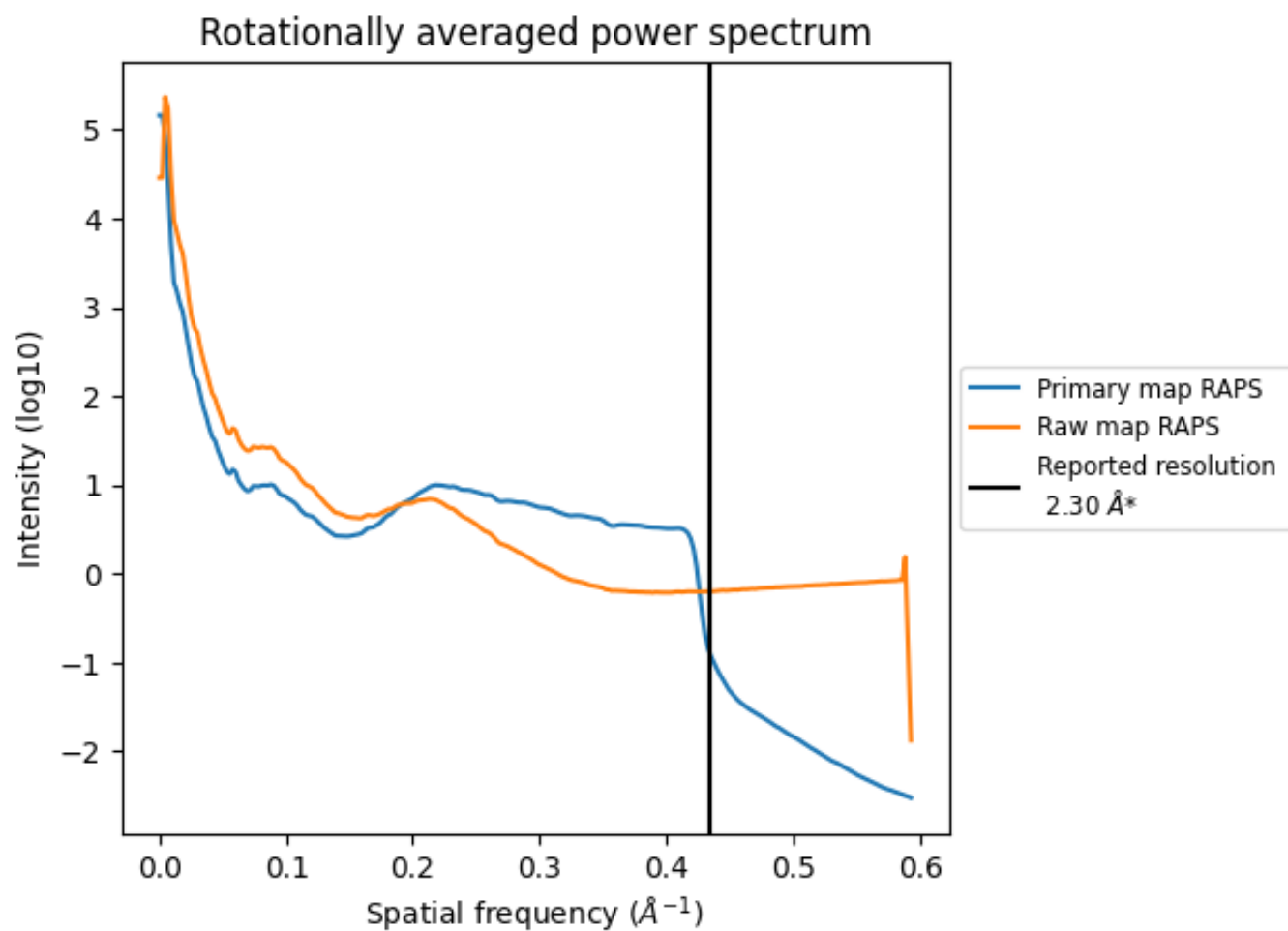
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 88 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 ⓘ

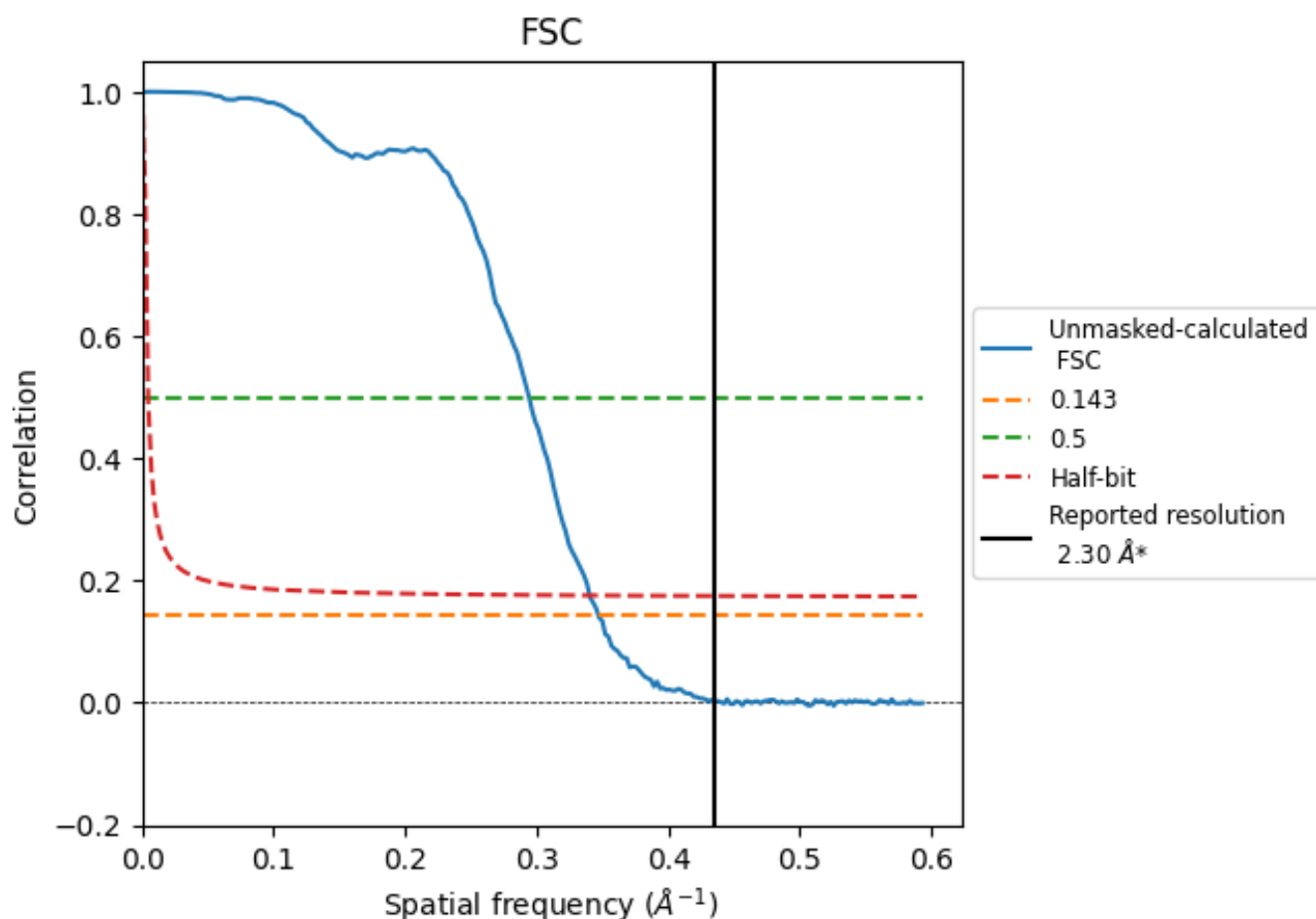


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

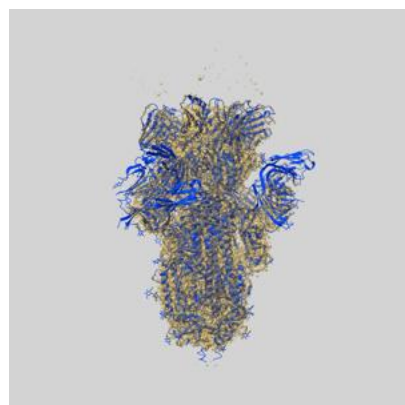
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.88	3.40	2.94

*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 2.88 differs from the reported value 2.3 by more than 10 %

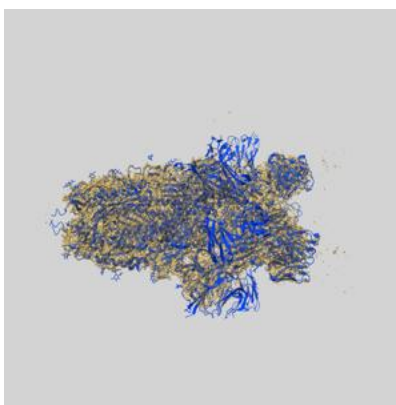
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24236 and PDB model 7N8H. Per-residue inclusion information can be found in section [3](#) on page [15](#).

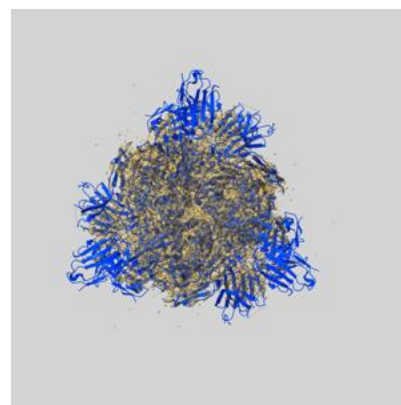
9.1 Map-model overlay [i](#)



X



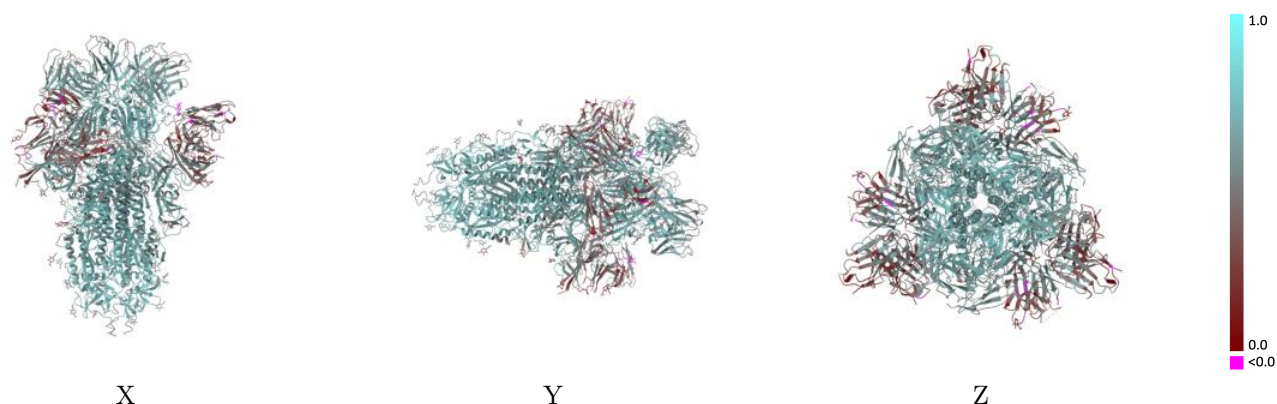
Y



Z

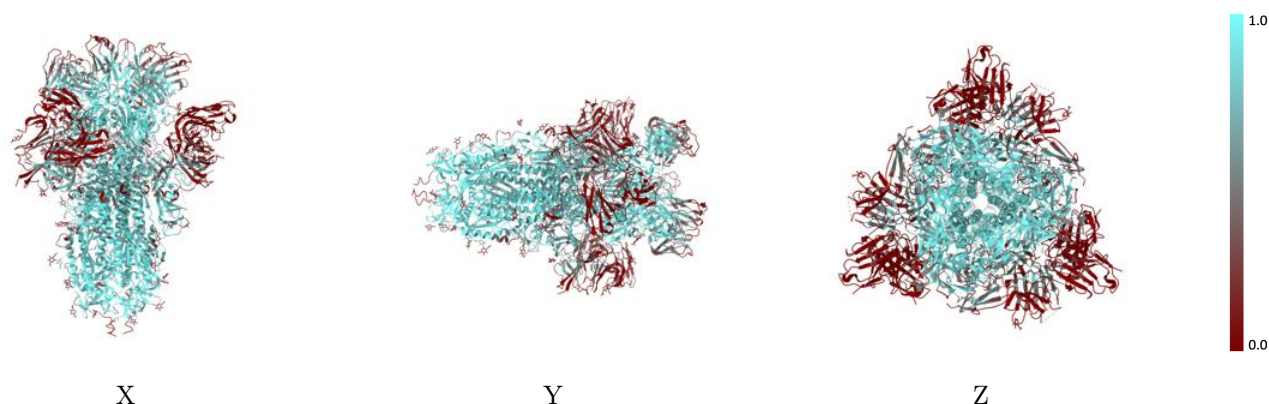
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



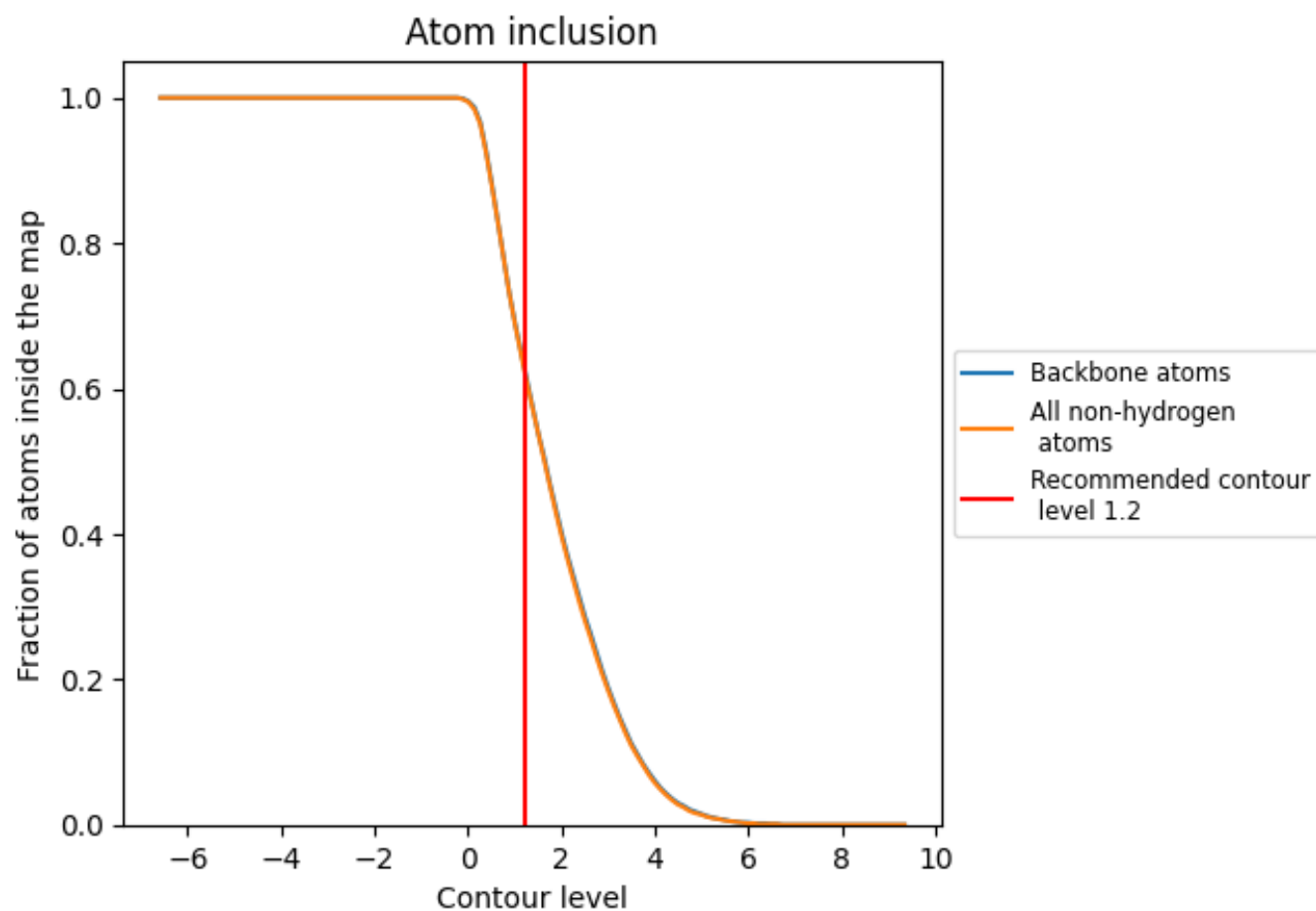
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6280	 0.5940
A	 0.7230	 0.6260
B	 0.0370	 0.4010
C	 0.0740	 0.3700
D	 0.5350	 0.5850
E	 0.6640	 0.6040
F	 0.7210	 0.6250
G	 0.5310	 0.5830
H	 0.6550	 0.6020
I	 0.0450	 0.4080
J	 0.0770	 0.3700
K	 0.7220	 0.6250
L	 0.5320	 0.5830
M	 0.6570	 0.6010
N	 0.0410	 0.3990
O	 0.0820	 0.3710
P	 0.1580	 0.4630
Q	 0.4290	 0.5620
R	 0.3930	 0.4790
S	 0.1320	 0.4580
T	 0.4290	 0.5810
U	 0.3570	 0.4670
V	 0.1320	 0.4540
W	 0.4640	 0.5710
X	 0.3570	 0.4750

