



Full wwPDB EM Validation Report ⓘ

Jul 17, 2025 – 10:13 PM JST

PDB ID : 9JMH / pdb_00009jmh
EMDB ID : EMD-61602
Title : Cryo-EM structure of HKU25-BatCoV S-trimer stabilized with 2P and x1 disulfide bond
Authors : Yuan, H.; Xiong, X.
Deposited on : 2024-09-20
Resolution : 3.00 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

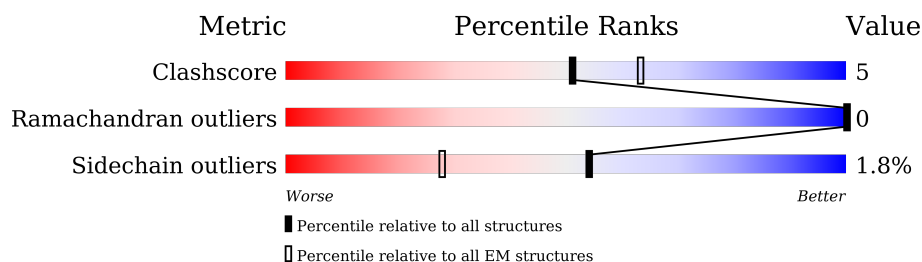
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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











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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1368	71% 10% • 18%
1	B	1368	69% 11% • 18%
1	C	1368	69% 12% • 18%
2	D	2	50% 50%
2	F	2	100%
2	H	2	100%
2	I	2	100%
2	J	2	50% 50%
2	M	2	100%

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Mol	Chain	Length	Quality of chain
2	N	2	 100%
2	O	2	 100%
2	R	2	 100%
2	S	2	 100%
3	E	3	 67%33%
3	G	3	 100%
3	K	3	 100%
3	L	3	 67%33%
3	P	3	 100%
3	Q	3	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27452 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1121	Total	C	N	O	S	0	0
			8778	5568	1466	1696	48		
1	B	1121	Total	C	N	O	S	0	0
			8784	5571	1469	1696	48		
1	C	1121	Total	C	N	O	S	0	0
			8784	5571	1469	1696	48		

There are 171 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	CYS	SER	engineered mutation	UNP A0A2I4R888
A	1051	CYS	ASP	engineered mutation	UNP A0A2I4R888
A	1052	PRO	ALA	engineered mutation	UNP A0A2I4R888
A	1053	PRO	VAL	engineered mutation	UNP A0A2I4R888
A	1290	GLY	-	linker	UNP A0A2I4R888
A	1291	SER	-	linker	UNP A0A2I4R888
A	1313	LEU	PHE	conflict	UNP P10104
A	1319	LEU	-	expression tag	UNP P10104
A	1320	GLU	-	expression tag	UNP P10104
A	1321	VAL	-	expression tag	UNP P10104
A	1322	LEU	-	expression tag	UNP P10104
A	1323	PHE	-	expression tag	UNP P10104
A	1324	GLN	-	expression tag	UNP P10104
A	1325	GLY	-	expression tag	UNP P10104
A	1326	PRO	-	expression tag	UNP P10104
A	1327	GLY	-	expression tag	UNP P10104
A	1328	HIS	-	expression tag	UNP P10104
A	1329	HIS	-	expression tag	UNP P10104
A	1330	HIS	-	expression tag	UNP P10104
A	1331	HIS	-	expression tag	UNP P10104
A	1332	HIS	-	expression tag	UNP P10104
A	1333	HIS	-	expression tag	UNP P10104
A	1334	HIS	-	expression tag	UNP P10104
A	1335	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1336	SER	-	expression tag	UNP P10104
A	1337	ALA	-	expression tag	UNP P10104
A	1338	TRP	-	expression tag	UNP P10104
A	1339	SER	-	expression tag	UNP P10104
A	1340	HIS	-	expression tag	UNP P10104
A	1341	PRO	-	expression tag	UNP P10104
A	1342	GLN	-	expression tag	UNP P10104
A	1343	PHE	-	expression tag	UNP P10104
A	1344	GLU	-	expression tag	UNP P10104
A	1345	LYS	-	expression tag	UNP P10104
A	1346	GLY	-	expression tag	UNP P10104
A	1347	GLY	-	expression tag	UNP P10104
A	1348	GLY	-	expression tag	UNP P10104
A	1349	SER	-	expression tag	UNP P10104
A	1350	GLY	-	expression tag	UNP P10104
A	1351	GLY	-	expression tag	UNP P10104
A	1352	GLY	-	expression tag	UNP P10104
A	1353	GLY	-	expression tag	UNP P10104
A	1354	SER	-	expression tag	UNP P10104
A	1355	GLY	-	expression tag	UNP P10104
A	1356	GLY	-	expression tag	UNP P10104
A	1357	SER	-	expression tag	UNP P10104
A	1358	ALA	-	expression tag	UNP P10104
A	1359	TRP	-	expression tag	UNP P10104
A	1360	SER	-	expression tag	UNP P10104
A	1361	HIS	-	expression tag	UNP P10104
A	1362	PRO	-	expression tag	UNP P10104
A	1363	GLN	-	expression tag	UNP P10104
A	1364	PHE	-	expression tag	UNP P10104
A	1365	GLU	-	expression tag	UNP P10104
A	1366	LYS	-	expression tag	UNP P10104
A	1367	SER	-	expression tag	UNP P10104
A	1368	ALA	-	expression tag	UNP P10104
B	437	CYS	SER	engineered mutation	UNP A0A2I4R888
B	1051	CYS	ASP	engineered mutation	UNP A0A2I4R888
B	1052	PRO	ALA	engineered mutation	UNP A0A2I4R888
B	1053	PRO	VAL	engineered mutation	UNP A0A2I4R888
B	1290	GLY	-	linker	UNP A0A2I4R888
B	1291	SER	-	linker	UNP A0A2I4R888
B	1313	LEU	PHE	conflict	UNP P10104
B	1319	LEU	-	expression tag	UNP P10104
B	1320	GLU	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1321	VAL	-	expression tag	UNP P10104
B	1322	LEU	-	expression tag	UNP P10104
B	1323	PHE	-	expression tag	UNP P10104
B	1324	GLN	-	expression tag	UNP P10104
B	1325	GLY	-	expression tag	UNP P10104
B	1326	PRO	-	expression tag	UNP P10104
B	1327	GLY	-	expression tag	UNP P10104
B	1328	HIS	-	expression tag	UNP P10104
B	1329	HIS	-	expression tag	UNP P10104
B	1330	HIS	-	expression tag	UNP P10104
B	1331	HIS	-	expression tag	UNP P10104
B	1332	HIS	-	expression tag	UNP P10104
B	1333	HIS	-	expression tag	UNP P10104
B	1334	HIS	-	expression tag	UNP P10104
B	1335	HIS	-	expression tag	UNP P10104
B	1336	SER	-	expression tag	UNP P10104
B	1337	ALA	-	expression tag	UNP P10104
B	1338	TRP	-	expression tag	UNP P10104
B	1339	SER	-	expression tag	UNP P10104
B	1340	HIS	-	expression tag	UNP P10104
B	1341	PRO	-	expression tag	UNP P10104
B	1342	GLN	-	expression tag	UNP P10104
B	1343	PHE	-	expression tag	UNP P10104
B	1344	GLU	-	expression tag	UNP P10104
B	1345	LYS	-	expression tag	UNP P10104
B	1346	GLY	-	expression tag	UNP P10104
B	1347	GLY	-	expression tag	UNP P10104
B	1348	GLY	-	expression tag	UNP P10104
B	1349	SER	-	expression tag	UNP P10104
B	1350	GLY	-	expression tag	UNP P10104
B	1351	GLY	-	expression tag	UNP P10104
B	1352	GLY	-	expression tag	UNP P10104
B	1353	GLY	-	expression tag	UNP P10104
B	1354	SER	-	expression tag	UNP P10104
B	1355	GLY	-	expression tag	UNP P10104
B	1356	GLY	-	expression tag	UNP P10104
B	1357	SER	-	expression tag	UNP P10104
B	1358	ALA	-	expression tag	UNP P10104
B	1359	TRP	-	expression tag	UNP P10104
B	1360	SER	-	expression tag	UNP P10104
B	1361	HIS	-	expression tag	UNP P10104
B	1362	PRO	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1363	GLN	-	expression tag	UNP P10104
B	1364	PHE	-	expression tag	UNP P10104
B	1365	GLU	-	expression tag	UNP P10104
B	1366	LYS	-	expression tag	UNP P10104
B	1367	SER	-	expression tag	UNP P10104
B	1368	ALA	-	expression tag	UNP P10104
C	437	CYS	SER	engineered mutation	UNP A0A2I4R888
C	1051	CYS	ASP	engineered mutation	UNP A0A2I4R888
C	1052	PRO	ALA	engineered mutation	UNP A0A2I4R888
C	1053	PRO	VAL	engineered mutation	UNP A0A2I4R888
C	1290	GLY	-	linker	UNP A0A2I4R888
C	1291	SER	-	linker	UNP A0A2I4R888
C	1313	LEU	PHE	conflict	UNP P10104
C	1319	LEU	-	expression tag	UNP P10104
C	1320	GLU	-	expression tag	UNP P10104
C	1321	VAL	-	expression tag	UNP P10104
C	1322	LEU	-	expression tag	UNP P10104
C	1323	PHE	-	expression tag	UNP P10104
C	1324	GLN	-	expression tag	UNP P10104
C	1325	GLY	-	expression tag	UNP P10104
C	1326	PRO	-	expression tag	UNP P10104
C	1327	GLY	-	expression tag	UNP P10104
C	1328	HIS	-	expression tag	UNP P10104
C	1329	HIS	-	expression tag	UNP P10104
C	1330	HIS	-	expression tag	UNP P10104
C	1331	HIS	-	expression tag	UNP P10104
C	1332	HIS	-	expression tag	UNP P10104
C	1333	HIS	-	expression tag	UNP P10104
C	1334	HIS	-	expression tag	UNP P10104
C	1335	HIS	-	expression tag	UNP P10104
C	1336	SER	-	expression tag	UNP P10104
C	1337	ALA	-	expression tag	UNP P10104
C	1338	TRP	-	expression tag	UNP P10104
C	1339	SER	-	expression tag	UNP P10104
C	1340	HIS	-	expression tag	UNP P10104
C	1341	PRO	-	expression tag	UNP P10104
C	1342	GLN	-	expression tag	UNP P10104
C	1343	PHE	-	expression tag	UNP P10104
C	1344	GLU	-	expression tag	UNP P10104
C	1345	LYS	-	expression tag	UNP P10104
C	1346	GLY	-	expression tag	UNP P10104
C	1347	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1348	GLY	-	expression tag	UNP P10104
C	1349	SER	-	expression tag	UNP P10104
C	1350	GLY	-	expression tag	UNP P10104
C	1351	GLY	-	expression tag	UNP P10104
C	1352	GLY	-	expression tag	UNP P10104
C	1353	GLY	-	expression tag	UNP P10104
C	1354	SER	-	expression tag	UNP P10104
C	1355	GLY	-	expression tag	UNP P10104
C	1356	GLY	-	expression tag	UNP P10104
C	1357	SER	-	expression tag	UNP P10104
C	1358	ALA	-	expression tag	UNP P10104
C	1359	TRP	-	expression tag	UNP P10104
C	1360	SER	-	expression tag	UNP P10104
C	1361	HIS	-	expression tag	UNP P10104
C	1362	PRO	-	expression tag	UNP P10104
C	1363	GLN	-	expression tag	UNP P10104
C	1364	PHE	-	expression tag	UNP P10104
C	1365	GLU	-	expression tag	UNP P10104
C	1366	LYS	-	expression tag	UNP P10104
C	1367	SER	-	expression tag	UNP P10104
C	1368	ALA	-	expression tag	UNP P10104

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		

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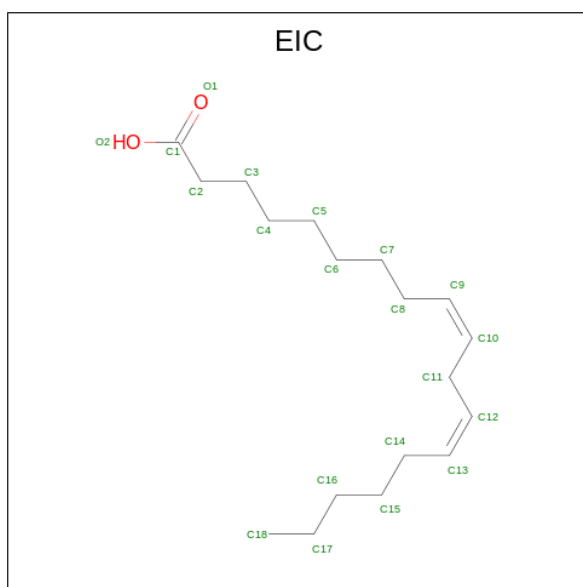
Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		

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



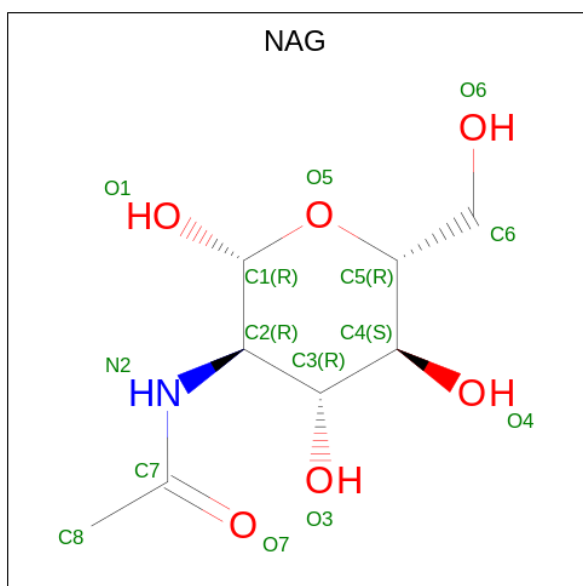
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	P	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is LINOLEIC ACID (CCD ID: EIC) (formula: C₁₈H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 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
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

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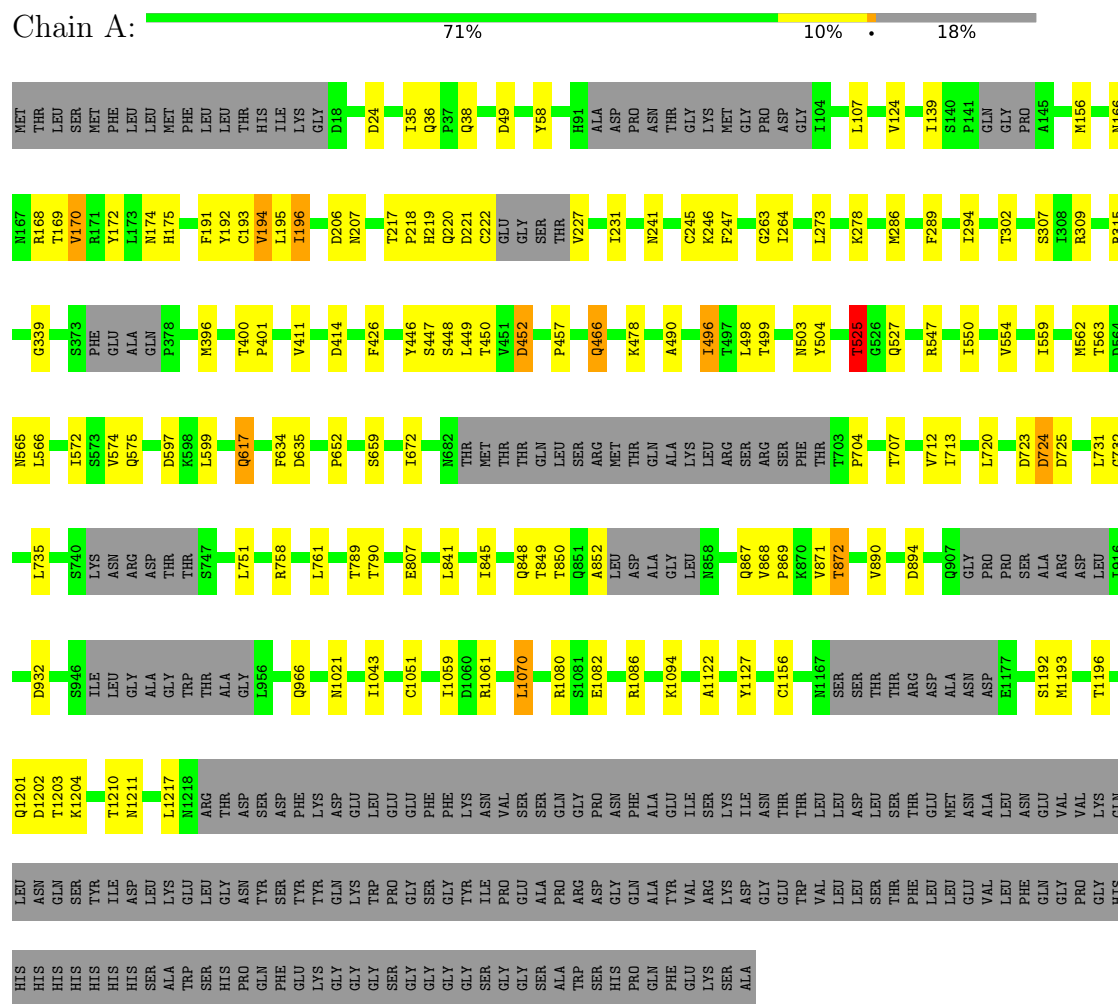
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C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

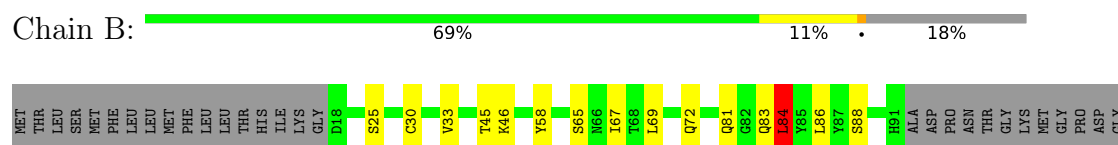
3 Residue-property plots

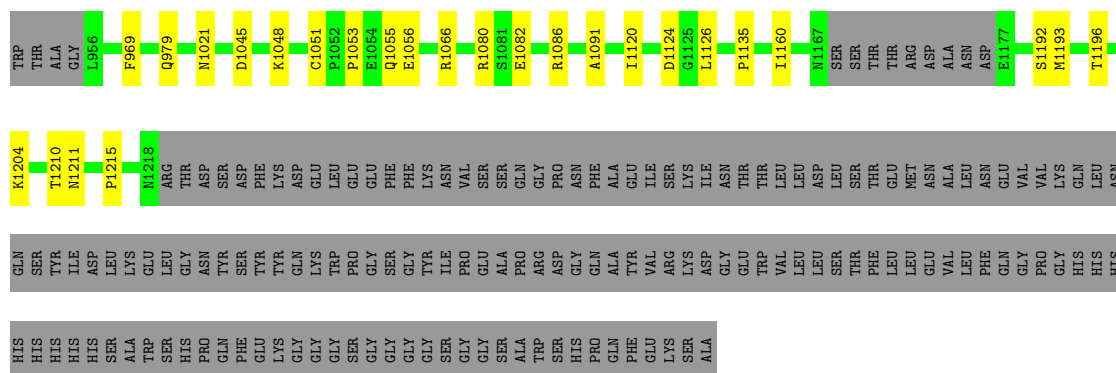
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

• Molecule 1: Spike glycoprotein,Fibrinin



• Molecule 1: Spike glycoprotein,Fibrinin





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

Chain D: 50% 50%



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

Chain F: 100%



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

Chain H: 100%



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

Chain I: 100%



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

Chain J: 50% 50%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain R:  100%



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

Chain S:  100%



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

Chain E:  67% 33%



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

Chain G:  100%



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

Chain K:  100%



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

Chain L:  67% 33%



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

Chain P:  100%



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

Chain Q:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110266	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)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, EIC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.61	8/8981 (0.1%)	0.58	12/12219 (0.1%)
1	B	0.65	14/8987 (0.2%)	0.62	24/12226 (0.2%)
1	C	0.55	4/8987 (0.0%)	0.58	15/12226 (0.1%)
All	All	0.61	26/26955 (0.1%)	0.59	51/36671 (0.1%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	245	CYS	CA-C	-7.00	1.43	1.52
1	B	84	LEU	CA-C	-6.77	1.44	1.52
1	B	512	LYS	CA-C	-6.50	1.44	1.52
1	B	465	GLN	CA-C	-6.30	1.44	1.52
1	A	894	ASP	CA-C	-6.10	1.45	1.52
1	B	919	GLN	CA-C	-6.08	1.45	1.52
1	C	629	PHE	CA-C	-5.83	1.45	1.52
1	A	1061	ARG	CA-C	-5.83	1.45	1.52
1	A	263	GLY	CA-C	-5.82	1.46	1.51
1	A	1070	LEU	C-O	-5.69	1.17	1.24
1	A	192	TYR	CA-C	-5.67	1.45	1.52
1	A	192	TYR	CA-CB	-5.60	1.45	1.53
1	B	288	LEU	CA-C	-5.55	1.45	1.52
1	B	448	SER	C-O	-5.54	1.17	1.23
1	B	278	LYS	CA-C	-5.49	1.46	1.53
1	C	723	ASP	CA-C	-5.37	1.45	1.52
1	B	1091	ALA	CA-C	-5.33	1.45	1.52
1	B	280	ASP	CA-C	-5.30	1.46	1.52
1	B	471	GLU	N-CA	-5.24	1.39	1.46
1	B	451	VAL	C-O	-5.21	1.18	1.24
1	A	723	ASP	CA-C	-5.16	1.46	1.52
1	B	449	LEU	C-O	-5.14	1.17	1.24
1	B	1090	LEU	CA-C	-5.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	370	SER	CA-C	-5.07	1.46	1.52
1	A	890	VAL	CA-C	-5.06	1.46	1.52
1	B	1088	ALA	CA-CB	-5.03	1.45	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	642	SER	N-CA-C	10.10	123.86	110.53
1	C	348	GLY	N-CA-C	9.65	124.31	112.73
1	B	209	TYR	N-CA-C	8.47	122.51	110.23
1	B	920	PHE	N-CA-C	8.46	120.50	111.28
1	A	466	GLN	N-CA-C	7.56	123.84	111.37
1	B	900	GLY	N-CA-C	7.05	121.19	112.73
1	C	288	LEU	N-CA-C	7.01	121.14	108.17
1	C	88	SER	N-CA-C	6.97	120.32	109.52
1	B	1088	ALA	N-CA-C	-6.79	104.01	112.90
1	C	289	PHE	N-CA-C	6.71	118.68	111.36
1	C	724	ASP	N-CA-C	-6.56	100.72	110.23
1	A	871	VAL	N-CA-C	-6.46	99.07	108.11
1	A	848	GLN	N-CA-C	6.33	118.18	111.28
1	C	89	VAL	N-CA-C	6.31	119.56	110.09
1	C	349	HIS	N-CA-C	6.31	118.16	111.28
1	A	1196	THR	N-CA-C	6.30	119.45	109.50
1	B	512	LYS	CA-C-N	-6.27	116.90	122.73
1	B	512	LYS	C-N-CA	-6.27	116.90	122.73
1	C	1196	THR	N-CA-C	6.25	119.20	109.52
1	A	194	VAL	N-CA-C	-6.21	99.48	108.17
1	A	525	THR	N-CA-C	6.20	119.34	110.10
1	A	872	THR	N-CA-C	5.99	118.72	109.07
1	B	394	SER	CA-C-N	-5.96	112.44	119.05
1	B	394	SER	C-N-CA	-5.96	112.44	119.05
1	C	27	ALA	N-CA-C	5.96	118.98	110.10
1	B	922	ALA	N-CA-C	5.93	117.83	111.36
1	B	1094	LYS	N-CA-C	-5.83	105.06	111.82
1	B	512	LYS	N-CA-C	-5.65	100.18	109.40
1	A	867	GLN	N-CA-C	5.58	117.89	110.53
1	C	291	SER	N-CA-C	-5.55	99.86	108.90
1	B	283	GLY	N-CA-C	-5.53	103.06	112.51
1	C	312	TYR	N-CA-C	-5.50	105.28	111.28
1	B	919	GLN	N-CA-C	-5.49	105.21	111.14
1	B	594	SER	N-CA-C	5.46	117.74	110.53
1	C	22	GLY	N-CA-C	5.44	123.43	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	SER	N-CA-C	5.39	118.97	109.80
1	B	1205	PHE	N-CA-C	5.38	117.82	110.24
1	C	721	VAL	N-CA-C	5.38	115.70	108.17
1	A	447	SER	N-CA-C	5.29	117.05	111.28
1	A	724	ASP	N-CA-C	-5.27	103.07	110.50
1	B	72	GLN	N-CA-C	-5.27	100.59	109.07
1	B	393	PHE	N-CA-C	-5.26	106.63	113.16
1	A	191	PHE	N-CA-C	5.25	117.23	108.99
1	B	660	VAL	N-CA-C	5.20	115.61	108.12
1	B	473	THR	N-CA-C	5.19	117.02	111.36
1	B	205	GLU	N-CA-C	-5.14	99.85	110.80
1	B	218	PRO	N-CA-C	-5.12	106.42	113.53
1	B	83	GLN	N-CA-C	-5.09	100.74	109.24
1	B	88	SER	CB-CA-C	-5.09	105.18	113.37
1	A	414	ASP	N-CA-C	5.04	118.55	111.74
1	C	635	ASP	N-CA-C	5.01	118.51	111.74

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	8778	0	8404	88	0
1	B	8784	0	8415	99	0
1	C	8784	0	8415	111	0
2	D	28	0	25	1	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	39	0	34	1	0
3	G	39	0	34	0	0
3	K	39	0	34	0	0
3	L	39	0	34	0	0
3	P	39	0	34	0	0
3	Q	39	0	34	0	0
4	A	40	0	62	5	0
4	B	20	0	31	1	0
5	A	182	0	169	0	0
5	B	168	0	156	0	0
5	C	182	0	169	0	0
All	All	27452	0	26275	283	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 5.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASN:HD21	1:B:341:ILE:H	1.05	0.98
1:A:170:VAL:HG21	1:A:302:THR:HG21	1.52	0.91
1:B:285:ASN:ND2	1:B:341:ILE:H	1.69	0.90
1:A:869:PRO:HG2	1:A:872:THR:HG22	1.60	0.83
1:A:401:PRO:HG3	1:A:498:LEU:HD22	1.61	0.83
1:B:657:PRO:HB2	1:B:674:GLY:HA3	1.60	0.83
1:B:467:GLY:O	1:C:438:PRO:HD2	1.84	0.78
1:C:137:ILE:HD11	1:C:317:GLY:HA2	1.69	0.73
1:A:496:ILE:HG22	1:A:498:LEU:H	1.55	0.72
1:A:411:VAL:HG22	1:A:450:THR:HG23	1.72	0.72
1:A:219:HIS:O	1:A:220:GLN:HB3	1.89	0.71
1:C:135:TYR:CZ	1:C:148:ILE:HG13	2.26	0.70
1:A:196:ILE:HG13	1:A:241:ASN:HB2	1.72	0.70
1:C:148:ILE:CD1	1:C:317:GLY:HA3	2.22	0.69
1:B:285:ASN:HD21	1:B:341:ILE:N	1.84	0.69
1:A:634:PHE:O	1:A:635:ASP:HB2	1.92	0.68
1:B:168:ARG:NH2	1:B:207:ASN:O	2.28	0.67
1:B:704:PRO:HB3	1:B:713:ILE:HG12	1.78	0.66
1:A:572:ILE:HD11	4:A:1401:EIC:H141	1.78	0.65
1:B:472:ILE:HA	1:B:476:ASN:HD22	1.60	0.65
1:A:496:ILE:HG22	1:A:498:LEU:N	2.11	0.64
1:A:724:ASP:O	1:A:725:ASP:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:PHE:CE2	1:C:293:PRO:HG2	2.35	0.62
1:C:500:LYS:HB3	1:C:562:MET:HE2	1.82	0.62
1:C:659:SER:HB2	1:C:672:ILE:HB	1.81	0.61
1:B:1162:GLY:HA2	1:B:1183:SER:HB3	1.83	0.61
1:C:883:GLU:HG3	1:C:1120:ILE:HB	1.84	0.60
1:A:1043:ILE:HG23	1:A:1059:ILE:HD12	1.82	0.60
1:C:343:ARG:HG2	1:C:362:PHE:CE2	2.37	0.60
1:B:86:LEU:HD13	1:B:320:ALA:HB2	1.84	0.59
1:B:148:ILE:HG12	1:B:317:GLY:HA3	1.84	0.59
1:C:148:ILE:HD13	1:C:317:GLY:HA3	1.83	0.59
1:A:218:PRO:HD2	1:A:309:ARG:O	2.03	0.59
1:C:135:TYR:HB2	1:C:136:PRO:HD2	1.84	0.58
1:C:148:ILE:HD12	1:C:317:GLY:HA3	1.85	0.57
1:C:807:GLU:OE2	1:C:807:GLU:N	2.35	0.57
1:C:628:ARG:HG2	1:C:628:ARG:O	2.03	0.57
1:C:190:VAL:HG11	1:C:292:LEU:HD11	1.87	0.57
1:C:496:ILE:HG23	1:C:498:LEU:H	1.69	0.57
1:C:113:THR:HG22	1:C:114:ASN:H	1.70	0.57
1:B:368:VAL:HG22	1:B:661:VAL:HG13	1.86	0.56
1:A:841:LEU:O	1:A:845:ILE:HG23	2.06	0.56
1:C:135:TYR:OH	1:C:148:ILE:HG21	2.05	0.56
1:A:466:GLN:HB3	1:C:1053:PRO:HG3	1.87	0.55
1:B:401:PRO:HG3	1:B:498:LEU:HD22	1.87	0.55
1:B:595:VAL:HG13	1:B:595:VAL:O	2.05	0.55
1:B:279:GLY:HA3	1:B:287:PHE:CD1	2.42	0.55
1:B:221:ASP:O	1:B:222:CYS:SG	2.65	0.55
1:A:217:THR:O	1:A:221:ASP:HB2	2.06	0.55
1:A:849:THR:CG2	1:C:762:VAL:HG23	2.37	0.54
1:B:217:THR:O	1:B:221:ASP:HB2	2.08	0.54
1:A:247:PHE:HZ	1:A:294:ILE:HD11	1.72	0.54
1:B:65:SER:O	1:B:67:ILE:HG23	2.08	0.54
1:A:170:VAL:CG2	1:A:302:THR:HG21	2.33	0.54
1:C:351:ASP:OD1	1:C:351:ASP:N	2.41	0.54
1:A:449:LEU:HD12	1:A:574:VAL:HG12	1.90	0.54
1:C:1021:ASN:OD1	1:C:1080:ARG:NH2	2.41	0.53
1:C:213:VAL:HG12	1:C:305:PRO:HB2	1.89	0.53
1:C:504:TYR:HB2	1:C:560:ALA:HB3	1.89	0.53
1:B:932:ASP:OD1	1:B:932:ASP:N	2.42	0.53
1:B:1058:GLN:OE1	1:B:1061:ARG:NH2	2.41	0.53
1:C:353:ALA:O	1:C:354:GLN:C	2.50	0.53
1:C:627:GLN:O	1:C:628:ARG:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:906:GLN:HG2	1:C:907:GLN:HG2	1.91	0.53
1:B:33:VAL:HG12	1:B:107:LEU:HB2	1.91	0.53
1:B:46:LYS:NZ	1:B:129:ASP:OD1	2.39	0.52
1:C:280:ASP:N	1:C:280:ASP:OD1	2.41	0.52
1:C:150:LYS:NZ	1:C:260:GLU:OE2	2.42	0.52
1:A:174:ASN:C	1:A:194:VAL:HG22	2.35	0.52
1:C:722:VAL:HG23	1:C:726:LYS:HB2	1.90	0.52
1:C:638:THR:O	1:C:650:VAL:N	2.43	0.52
1:C:192:TYR:CZ	1:C:294:ILE:HG23	2.45	0.51
1:C:1091:ALA:HB1	1:C:1126:LEU:HD12	1.92	0.51
1:C:21:LEU:HG	1:C:245:CYS:SG	2.50	0.51
1:C:124:VAL:HG12	1:C:286:MET:HE1	1.93	0.51
1:C:619:CYS:HB3	1:C:647:TYR:HD2	1.74	0.51
1:B:1053:PRO:HG3	1:C:466:GLN:HB3	1.92	0.51
1:C:28:GLN:O	1:C:200:GLN:HG3	2.10	0.51
1:C:228:ASN:OD1	1:C:228:ASN:N	2.44	0.51
1:B:1192:SER:OG	1:B:1193:MET:N	2.44	0.51
1:C:77:ARG:HG2	1:C:329:LEU:HD11	1.91	0.51
1:A:220:GLN:O	1:A:220:GLN:HG2	2.11	0.51
1:B:1077:GLN:OE1	1:B:1080:ARG:NH1	2.44	0.51
1:B:218:PRO:HD2	1:B:309:ARG:O	2.10	0.50
1:C:353:ALA:O	1:C:356:ARG:N	2.44	0.50
1:B:736:CYS:HB3	1:B:752:ALA:HB3	1.93	0.50
1:B:205:GLU:OE1	1:B:205:GLU:HA	2.11	0.50
1:C:1192:SER:OG	1:C:1193:MET:N	2.43	0.50
1:A:401:PRO:HG2	1:A:566:LEU:HD21	1.93	0.50
1:B:197:PRO:HB2	1:B:205:GLU:HG2	1.92	0.50
1:C:812:LEU:HD11	1:C:1056:GLU:HG3	1.93	0.50
1:C:1051:CYS:O	1:C:1055:GLN:N	2.45	0.50
1:A:478:LYS:HG2	1:A:525:THR:HG23	1.94	0.50
1:B:30:CYS:O	1:B:202:ARG:NH1	2.44	0.50
1:C:110:SER:OG	1:C:111:ASN:N	2.44	0.50
4:A:1415:EIC:H52	1:B:438:PRO:HB3	1.94	0.49
1:C:133:SER:O	1:C:148:ILE:HG12	2.11	0.49
1:C:1193:MET:HE3	1:C:1215:PRO:HA	1.94	0.49
1:A:1051:CYS:SG	1:B:467:GLY:HA2	2.52	0.49
1:C:411:VAL:HG22	1:C:450:THR:HG23	1.94	0.49
1:C:812:LEU:HD21	1:C:1056:GLU:HB3	1.95	0.49
1:A:166:ASN:ND2	1:A:206:ASP:O	2.46	0.49
1:B:107:LEU:HD21	1:B:309:ARG:HE	1.77	0.49
1:B:278:LYS:HD3	1:B:289:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:PRO:HG2	1:B:921:VAL:CG2	2.43	0.49
1:B:659:SER:HB3	1:B:672:ILE:HB	1.94	0.49
1:B:84:LEU:HD13	1:B:322:TYR:CE2	2.48	0.48
1:A:139:ILE:HD11	1:A:315:ARG:CZ	2.42	0.48
1:A:704:PRO:HB3	1:A:713:ILE:HG12	1.94	0.48
1:B:1205:PHE:CD1	1:B:1205:PHE:N	2.81	0.48
1:C:724:ASP:O	1:C:725:ASP:CB	2.61	0.48
1:B:672:ILE:HA	1:B:712:VAL:HG12	1.95	0.48
1:C:84:LEU:HD13	1:C:322:TYR:CE2	2.48	0.48
1:B:707:THR:OG1	1:B:710:GLY:O	2.30	0.48
1:C:512:LYS:HG2	1:C:521:HIS:NE2	2.29	0.48
1:A:1202:ASP:OD2	1:A:1204:LYS:HE2	2.13	0.48
1:B:210:SER:O	1:B:211:SER:HB2	2.12	0.48
1:C:260:GLU:OE2	1:C:277:ARG:NH1	2.41	0.48
1:A:1021:ASN:OD1	1:A:1080:ARG:NH2	2.43	0.48
1:C:36:GLN:OE1	1:C:38:GLN:NE2	2.44	0.47
1:C:1056:GLU:OE1	1:C:1056:GLU:N	2.46	0.47
1:A:217:THR:OG1	1:A:309:ARG:NH1	2.47	0.47
1:C:722:VAL:CG2	1:C:726:LYS:HB2	2.44	0.47
1:A:932:ASP:OD1	1:C:734:SER:OG	2.28	0.47
1:B:724:ASP:OD1	1:B:724:ASP:N	2.47	0.47
1:A:849:THR:HG21	1:C:762:VAL:HG23	1.96	0.47
1:A:789:THR:HG22	1:A:790:THR:HG23	1.96	0.47
1:C:709:VAL:HG11	1:C:732:GLY:HA3	1.96	0.47
1:A:1192:SER:OG	1:A:1193:MET:N	2.48	0.47
1:A:724:ASP:O	1:A:725:ASP:CB	2.63	0.47
1:B:219:HIS:O	1:B:220:GLN:HB3	2.15	0.47
1:A:1122:ALA:HB2	1:A:1127:TYR:HB2	1.97	0.47
1:B:723:ASP:OD1	1:B:723:ASP:N	2.45	0.47
1:A:35:ILE:HG21	2:D:1:NAG:H81	1.97	0.46
1:B:201:HIS:O	1:B:208:ALA:HB3	2.15	0.46
1:C:197:PRO:HB2	1:C:205:GLU:HG2	1.97	0.46
1:C:802:VAL:O	1:C:1066:ARG:NH1	2.43	0.46
1:A:452:ASP:N	1:A:452:ASP:OD1	2.46	0.46
1:C:490:ALA:HB3	1:C:570:PHE:HE2	1.80	0.46
1:C:622:VAL:O	1:C:641:HIS:NE2	2.48	0.46
1:B:411:VAL:HG22	1:B:450:THR:HG23	1.96	0.46
1:C:204:PRO:HA	1:C:209:TYR:CG	2.51	0.46
1:B:402:PRO:HG3	1:B:408:ARG:HD3	1.97	0.46
1:A:503:ASN:HD22	1:A:559:ILE:HG23	1.80	0.46
1:B:260:GLU:CD	1:B:277:ARG:HD2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASP:OD1	1:C:353:ALA:HB2	2.16	0.46
1:C:262:PHE:HE1	1:C:289:PHE:HZ	1.62	0.45
1:A:807:GLU:H	1:A:807:GLU:CD	2.24	0.45
1:A:868:VAL:HG23	1:A:869:PRO:HD2	1.98	0.45
1:C:137:ILE:HD11	1:C:317:GLY:CA	2.42	0.45
1:C:724:ASP:OD1	1:C:724:ASP:N	2.49	0.45
1:A:1086:ARG:HH21	1:B:1086:ARG:NH2	2.13	0.45
1:B:219:HIS:O	1:B:220:GLN:CB	2.63	0.45
1:A:175:HIS:CE1	1:A:246:LYS:HE3	2.51	0.45
1:A:1202:ASP:OD1	1:A:1203:THR:N	2.49	0.45
1:A:572:ILE:HD11	4:A:1401:EIC:C14	2.46	0.45
1:A:758:ARG:HA	1:A:758:ARG:HD3	1.76	0.45
1:C:906:GLN:CG	1:C:907:GLN:HG2	2.47	0.45
1:A:168:ARG:O	1:A:169:THR:OG1	2.31	0.45
1:A:222:CYS:HA	1:A:227:VAL:HG22	1.98	0.45
1:A:659:SER:HB2	1:A:672:ILE:HB	1.98	0.45
1:B:45:THR:OG1	1:B:81:GLN:OE1	2.34	0.45
1:A:525:THR:O	1:A:527:GLN:HG3	2.17	0.45
1:B:116:THR:O	1:B:116:THR:OG1	2.35	0.45
1:B:761:LEU:HD21	1:C:852:ALA:HB2	1.99	0.45
1:A:547:ARG:HG2	1:A:554:VAL:HG22	1.98	0.45
1:B:898:MET:HE3	1:B:899:GLN:CD	2.41	0.45
1:C:644:ASP:OD1	1:C:644:ASP:N	2.46	0.45
1:C:610:LEU:HD23	1:C:610:LEU:HA	1.85	0.44
1:A:156:MET:HE2	1:A:172:TYR:HD2	1.82	0.44
1:A:264:ILE:HG13	1:A:273:LEU:CD2	2.48	0.44
1:A:597:ASP:OD1	1:A:597:ASP:N	2.48	0.44
1:C:311:LYS:O	1:C:314:SER:N	2.47	0.44
1:C:563:THR:OG1	1:C:565:ASN:O	2.34	0.44
1:A:672:ILE:HD11	1:A:731:LEU:HD22	1.97	0.44
1:B:278:LYS:O	1:B:287:PHE:HB2	2.17	0.44
1:B:870:LYS:HD2	1:B:870:LYS:HA	1.59	0.44
1:A:1082:GLU:O	1:A:1086:ARG:HG3	2.17	0.44
1:B:196:ILE:HB	1:B:241:ASN:HB2	1.99	0.44
1:A:852:ALA:HB2	1:C:761:LEU:HD21	2.00	0.44
1:B:661:VAL:HG12	1:B:729:LEU:HD13	1.99	0.44
1:C:140:SER:O	1:C:140:SER:OG	2.32	0.44
1:A:1210:THR:OG1	1:A:1211:ASN:N	2.50	0.44
1:B:436:VAL:HB	1:B:484:PRO:HB3	1.99	0.44
1:B:619:CYS:HB2	1:B:649:CYS:HB2	1.30	0.44
1:C:166:ASN:ND2	1:C:206:ASP:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LYS:HD3	1:B:289:PHE:CB	2.47	0.44
1:C:273:LEU:HB3	1:C:289:PHE:CZ	2.53	0.44
1:B:284:GLY:O	1:B:285:ASN:C	2.59	0.43
1:A:707:THR:O	1:B:898:MET:HG3	2.18	0.43
1:A:732:GLY:HA3	1:B:928:PRO:HG2	2.00	0.43
1:B:25:SER:OG	1:B:198:ARG:NH1	2.51	0.43
1:B:168:ARG:NH1	2:J:2:NAG:O7	2.51	0.43
1:C:198:ARG:NE	1:C:238:HIS:O	2.52	0.43
1:A:221:ASP:O	1:A:222:CYS:HB2	2.18	0.43
1:A:1156:CYS:SG	1:A:1201:GLN:HB2	2.58	0.43
4:A:1401:EIC:H141	4:A:1401:EIC:H112	1.71	0.43
1:B:1094:LYS:HE3	1:B:1094:LYS:HB2	1.86	0.43
1:C:715:LEU:HD23	1:C:749:LEU:HB3	1.99	0.43
1:C:137:ILE:HD13	1:C:137:ILE:HA	1.65	0.43
1:B:547:ARG:HG2	1:B:554:VAL:HG22	2.00	0.43
1:C:775:PRO:HB3	1:C:1135:PRO:HB3	2.01	0.43
1:A:563:THR:OG1	1:A:565:ASN:O	2.36	0.43
4:B:1413:EIC:H52	1:C:438:PRO:HB3	2.00	0.43
1:C:43:ASP:OD1	1:C:43:ASP:N	2.51	0.43
1:B:454:PHE:CE2	1:B:569:ALA:HB3	2.54	0.43
1:B:466:GLN:H	1:B:466:GLN:HG3	1.42	0.43
1:B:1202:ASP:OD2	1:B:1204:LYS:NZ	2.50	0.43
1:A:107:LEU:HD22	1:A:307:SER:HB3	2.01	0.43
1:B:267:ASP:OD1	1:B:272:HIS:NE2	2.51	0.43
1:B:394:SER:O	1:B:395:PRO:C	2.58	0.43
1:B:972:MET:HA	1:B:975:ILE:HG12	2.01	0.43
1:C:598:LYS:HG3	1:C:603:ILE:HD13	2.01	0.43
1:C:724:ASP:O	1:C:725:ASP:HB2	2.18	0.43
1:A:49:ASP:OD1	1:A:49:ASP:N	2.52	0.43
1:B:972:MET:HG2	1:B:1115:ILE:HD12	2.01	0.43
1:C:932:ASP:OD1	1:C:932:ASP:N	2.52	0.43
1:A:457:PRO:HD3	1:A:504:TYR:CG	2.54	0.43
1:B:464:LEU:HB3	1:B:487:ARG:HD3	2.00	0.43
1:B:552:LYS:HA	1:B:552:LYS:HD3	1.89	0.43
1:A:426:PHE:HB3	1:A:490:ALA:HB1	2.00	0.42
1:B:465:GLN:O	1:B:468:SER:HB2	2.19	0.42
1:A:735:LEU:HD22	1:A:751:LEU:HD11	2.01	0.42
1:A:966:GLN:HG3	1:C:1204:LYS:NZ	2.35	0.42
1:C:634:PHE:O	1:C:635:ASP:HB2	2.20	0.42
1:A:124:VAL:HG12	1:A:286:MET:HE1	2.01	0.42
1:B:234:ASN:O	1:B:238:HIS:ND1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLU:OE2	1:B:277:ARG:NH1	2.48	0.42
1:B:273:LEU:O	1:B:288:LEU:HD12	2.18	0.42
1:B:969:PHE:HZ	1:B:979:GLN:HG2	1.85	0.42
1:A:562:MET:HE2	1:A:562:MET:HB2	1.85	0.42
1:A:36:GLN:OE1	1:A:38:GLN:NE2	2.44	0.42
1:B:221:ASP:HB3	1:B:231:ILE:CD1	2.50	0.42
1:A:672:ILE:HG12	1:A:712:VAL:HG12	2.02	0.42
1:B:496:ILE:HG23	1:B:498:LEU:H	1.85	0.42
1:C:273:LEU:O	1:C:288:LEU:HD12	2.20	0.42
1:C:794:VAL:HG22	1:C:926:VAL:HG22	2.02	0.42
1:B:168:ARG:HH22	1:B:207:ASN:ND2	2.18	0.41
1:B:272:HIS:HB3	1:B:288:LEU:CD1	2.50	0.41
1:C:969:PHE:HZ	1:C:979:GLN:HG2	1.85	0.41
1:A:652:PRO:HG2	1:B:921:VAL:HG21	2.02	0.41
1:B:149:LYS:HB3	1:B:149:LYS:HE3	1.73	0.41
1:C:233:LEU:HD12	1:C:233:LEU:HA	1.88	0.41
1:C:350:ASP:OD1	1:C:353:ALA:CB	2.68	0.41
1:C:1210:THR:OG1	1:C:1211:ASN:N	2.53	0.41
1:A:278:LYS:HG3	1:A:289:PHE:HB3	2.01	0.41
1:C:1082:GLU:HG3	1:C:1086:ARG:HH21	1.85	0.41
1:A:1193:MET:HE2	1:A:1193:MET:HB2	1.97	0.41
1:B:1021:ASN:OD1	1:B:1080:ARG:NH2	2.52	0.41
1:C:463:TYR:HD2	1:C:470:GLY:HA3	1.86	0.41
1:C:846:LYS:HD3	1:C:939:TYR:HE1	1.84	0.41
1:C:1045:ASP:HA	1:C:1048:LYS:HG2	2.03	0.41
1:A:966:GLN:HE21	1:C:1204:LYS:HD3	1.86	0.41
1:B:602:CYS:HB2	1:B:653:CYS:HB2	1.74	0.41
1:C:135:TYR:C	1:C:145:ALA:N	2.79	0.41
1:C:738:VAL:HA	1:C:739:PRO:HD3	1.92	0.41
1:A:396:MET:HE1	4:A:1401:EIC:H151	2.03	0.41
1:C:151:ILE:HD12	1:C:151:ILE:HA	1.92	0.41
1:C:672:ILE:HD11	1:C:731:LEU:HG	2.02	0.41
1:A:448:SER:OG	1:A:575:GLN:HB2	2.21	0.41
1:B:807:GLU:OE2	1:B:807:GLU:N	2.46	0.41
1:A:264:ILE:HG13	1:A:273:LEU:HD23	2.03	0.41
1:B:58:TYR:OH	1:B:339:GLY:O	2.35	0.41
1:B:191:PHE:HD2	1:B:193:CYS:HB2	1.85	0.41
1:C:180:LEU:HD22	1:C:214:ILE:HD13	2.02	0.41
1:C:312:TYR:HD1	1:C:312:TYR:O	2.04	0.41
1:C:371:VAL:HG11	1:C:660:VAL:HG21	2.03	0.41
1:C:537:GLN:HB3	3:E:2:NAG:H61	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:LYS:HE3	1:A:1094:LYS:HB2	1.93	0.41
1:C:194:VAL:HB	1:C:243:THR:O	2.21	0.41
1:C:712:VAL:HG21	1:C:715:LEU:HD12	2.03	0.40
1:A:400:THR:HG22	1:A:499:THR:HB	2.03	0.40
1:A:1070:LEU:HD23	1:A:1070:LEU:HA	1.84	0.40
1:B:313:ASN:OD1	1:B:314:SER:N	2.54	0.40
1:B:417:TYR:HH	1:B:446:TYR:HH	1.56	0.40
1:B:452:ASP:OD1	1:B:571:ILE:O	2.39	0.40
1:A:599:LEU:HD22	1:A:617:GLN:HA	2.03	0.40
1:B:1140:ASN:OD1	1:B:1140:ASN:N	2.52	0.40
1:C:1021:ASN:ND2	1:C:1124:ASP:OD2	2.54	0.40
1:A:58:TYR:OH	1:A:339:GLY:O	2.34	0.40
1:A:849:THR:HG22	1:A:850:THR:N	2.37	0.40
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.89	0.40
1:B:706:GLN:HA	1:B:711:CYS:HB2	2.03	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	1099/1368 (80%)	1067 (97%)	32 (3%)	0	100	100
1	B	1099/1368 (80%)	1058 (96%)	41 (4%)	0	100	100
1	C	1099/1368 (80%)	1067 (97%)	32 (3%)	0	100	100
All	All	3297/4104 (80%)	3192 (97%)	105 (3%)	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	973/1178 (83%)	956 (98%)	17 (2%)	56	81
1	B	974/1178 (83%)	954 (98%)	20 (2%)	48	77
1	C	974/1178 (83%)	959 (98%)	15 (2%)	60	83
All	All	2921/3534 (83%)	2869 (98%)	52 (2%)	54	80

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	170	VAL
1	A	193	CYS
1	A	195	LEU
1	A	196	ILE
1	A	207	ASN
1	A	231	ILE
1	A	245	CYS
1	A	446	TYR
1	A	452	ASP
1	A	496	ILE
1	A	525	THR
1	A	550	ILE
1	A	617	GLN
1	A	720	LEU
1	A	761	LEU
1	A	1217	LEU
1	B	69	LEU
1	B	84	LEU
1	B	193	CYS
1	B	213	VAL
1	B	217	THR
1	B	220	GLN
1	B	254	THR
1	B	408	ARG
1	B	437	CYS

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Mol	Chain	Res	Type
1	B	446	TYR
1	B	466	GLN
1	B	488	ILE
1	B	497	THR
1	B	658	LEU
1	B	661	VAL
1	B	711	CYS
1	B	761	LEU
1	B	863	LEU
1	B	1007	THR
1	B	1203	THR
1	C	41	GLN
1	C	137	ILE
1	C	245	CYS
1	C	291	SER
1	C	351	ASP
1	C	404	VAL
1	C	446	TYR
1	C	559	ILE
1	C	619	CYS
1	C	626	GLN
1	C	644	ASP
1	C	649	CYS
1	C	812	LEU
1	C	916	ILE
1	C	1160	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	175	HIS
1	A	349	HIS
1	A	465	GLN
1	A	466	GLN
1	A	483	ASN
1	A	524	GLN
1	A	575	GLN
1	A	668	ASN
1	A	733	GLN
1	A	825	GLN
1	A	828	HIS

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Mol	Chain	Res	Type
1	A	848	GLN
1	A	851	GLN
1	A	875	GLN
1	A	966	GLN
1	A	988	GLN
1	A	998	ASN
1	A	1015	GLN
1	A	1121	ASN
1	A	1130	HIS
1	A	1218	ASN
1	B	175	HIS
1	B	207	ASN
1	B	220	GLN
1	B	285	ASN
1	B	434	HIS
1	B	682	ASN
1	B	733	GLN
1	B	828	HIS
1	B	899	GLN
1	B	934	ASN
1	B	1015	GLN
1	B	1064	ASN
1	B	1076	GLN
1	B	1130	HIS
1	B	1187	ASN
1	C	427	GLN
1	C	434	HIS
1	C	465	GLN
1	C	575	GLN
1	C	581	ASN
1	C	667	ASN
1	C	750	GLN
1	C	766	ASN
1	C	828	HIS
1	C	851	GLN
1	C	906	GLN
1	C	907	GLN
1	C	919	GLN
1	C	973	ASN
1	C	1001	GLN
1	C	1102	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 ⓘ

38 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.21	0	17,19,21	0.47	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.52	0
3	NAG	E	1	3,1	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.39	0
3	BMA	E	3	3	11,11,12	0.61	0	15,15,17	0.88	0
2	NAG	F	1	2,1	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	F	2	2	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	G	1	3,1	14,14,15	0.31	0	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.24	0	17,19,21	0.47	0
3	BMA	G	3	3	11,11,12	0.67	0	15,15,17	0.86	0
2	NAG	H	1	2,1	14,14,15	0.25	0	17,19,21	0.50	0
2	NAG	H	2	2	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	I	1	2,1	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	I	2	2	14,14,15	0.28	0	17,19,21	0.47	0
2	NAG	J	1	2,1	14,14,15	0.19	0	17,19,21	0.50	0
2	NAG	J	2	2	14,14,15	0.23	0	17,19,21	0.55	0
3	NAG	K	1	3,1	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.46	0
3	BMA	K	3	3	11,11,12	0.65	0	15,15,17	0.83	0
3	NAG	L	1	3,1	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	L	2	3	14,14,15	0.27	0	17,19,21	0.80	1 (5%)
3	BMA	L	3	3	11,11,12	0.61	0	15,15,17	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	M	1	2,1	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	M	2	2	14,14,15	0.25	0	17,19,21	0.52	0
2	NAG	N	1	2,1	14,14,15	0.22	0	17,19,21	0.50	0
2	NAG	N	2	2	14,14,15	0.27	0	17,19,21	0.45	0
2	NAG	O	1	2,1	14,14,15	0.22	0	17,19,21	0.48	0
2	NAG	O	2	2	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	P	1	3,1	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	P	2	3	14,14,15	0.26	0	17,19,21	0.46	0
3	BMA	P	3	3	11,11,12	0.68	0	15,15,17	0.89	0
3	NAG	Q	1	3,1	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	Q	2	3	14,14,15	0.28	0	17,19,21	0.40	0
3	BMA	Q	3	3	11,11,12	0.63	0	15,15,17	0.86	0
2	NAG	R	1	2,1	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	R	2	2	14,14,15	0.27	0	17,19,21	0.54	0
2	NAG	S	1	2,1	14,14,15	0.24	0	17,19,21	0.54	0
2	NAG	S	2	2	14,14,15	0.26	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	K	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2	NAG	C2-N2-C7	2.47	126.42	122.90

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6

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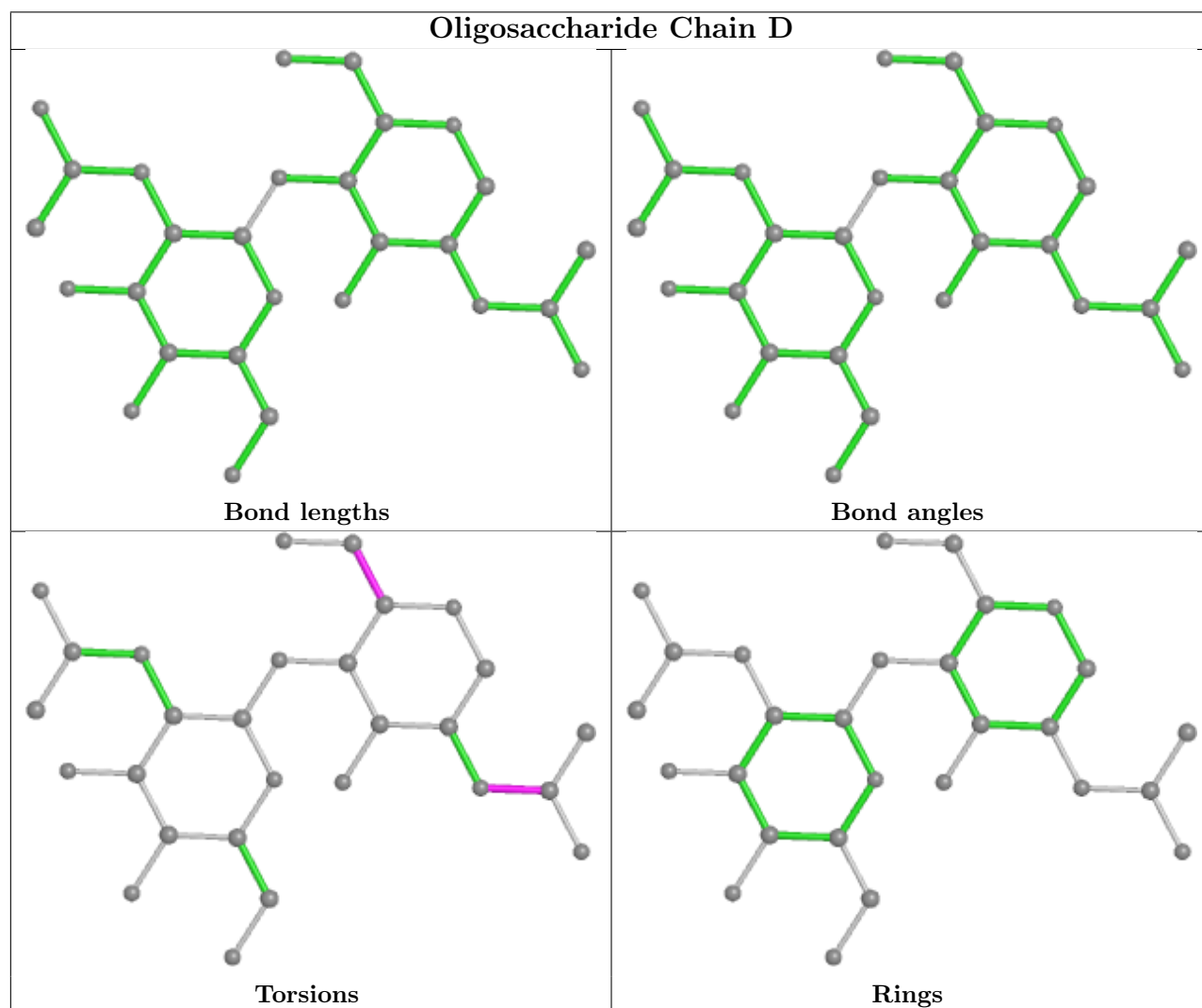
Mol	Chain	Res	Type	Atoms
3	L	2	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
2	I	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7

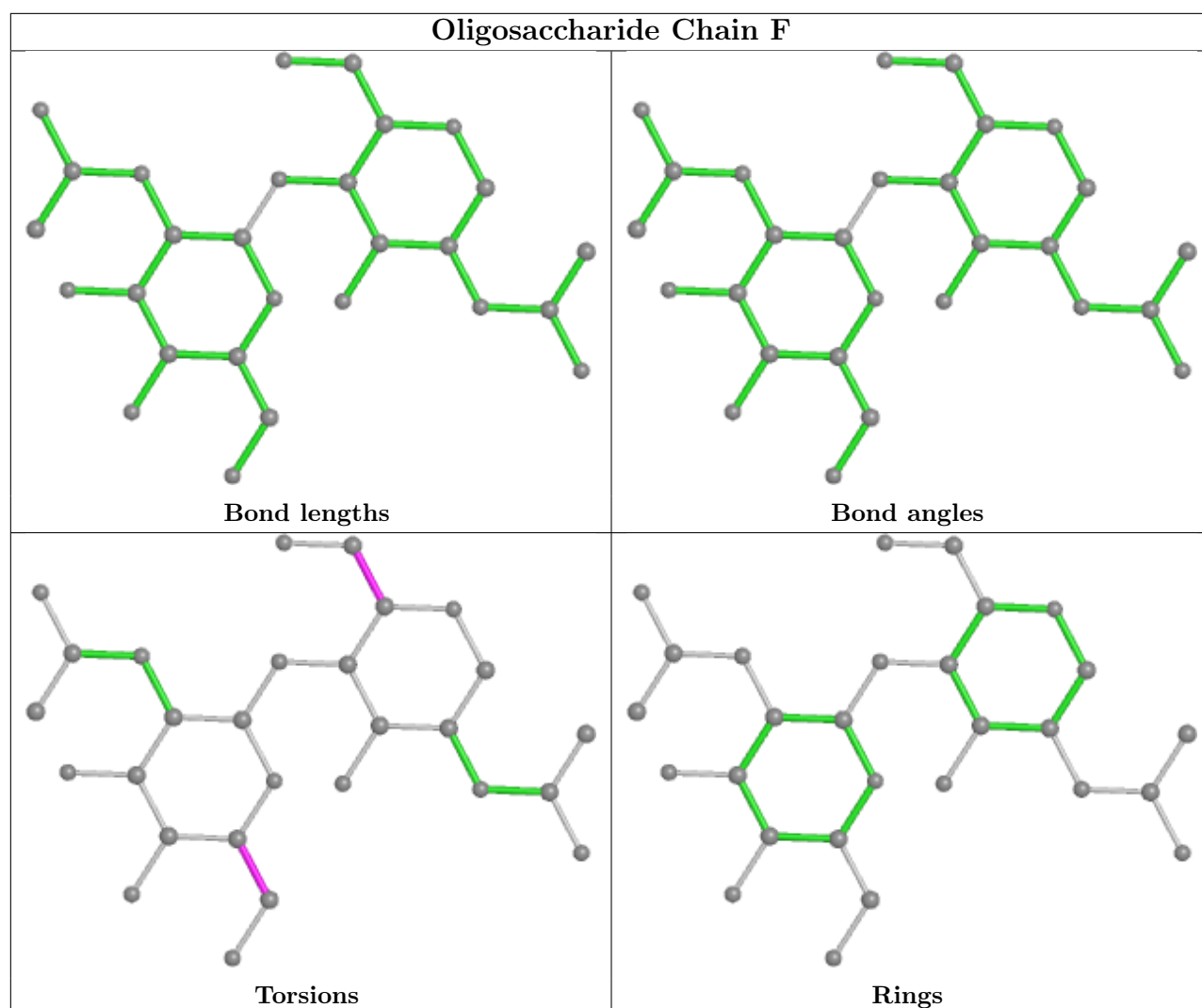
There are no ring outliers.

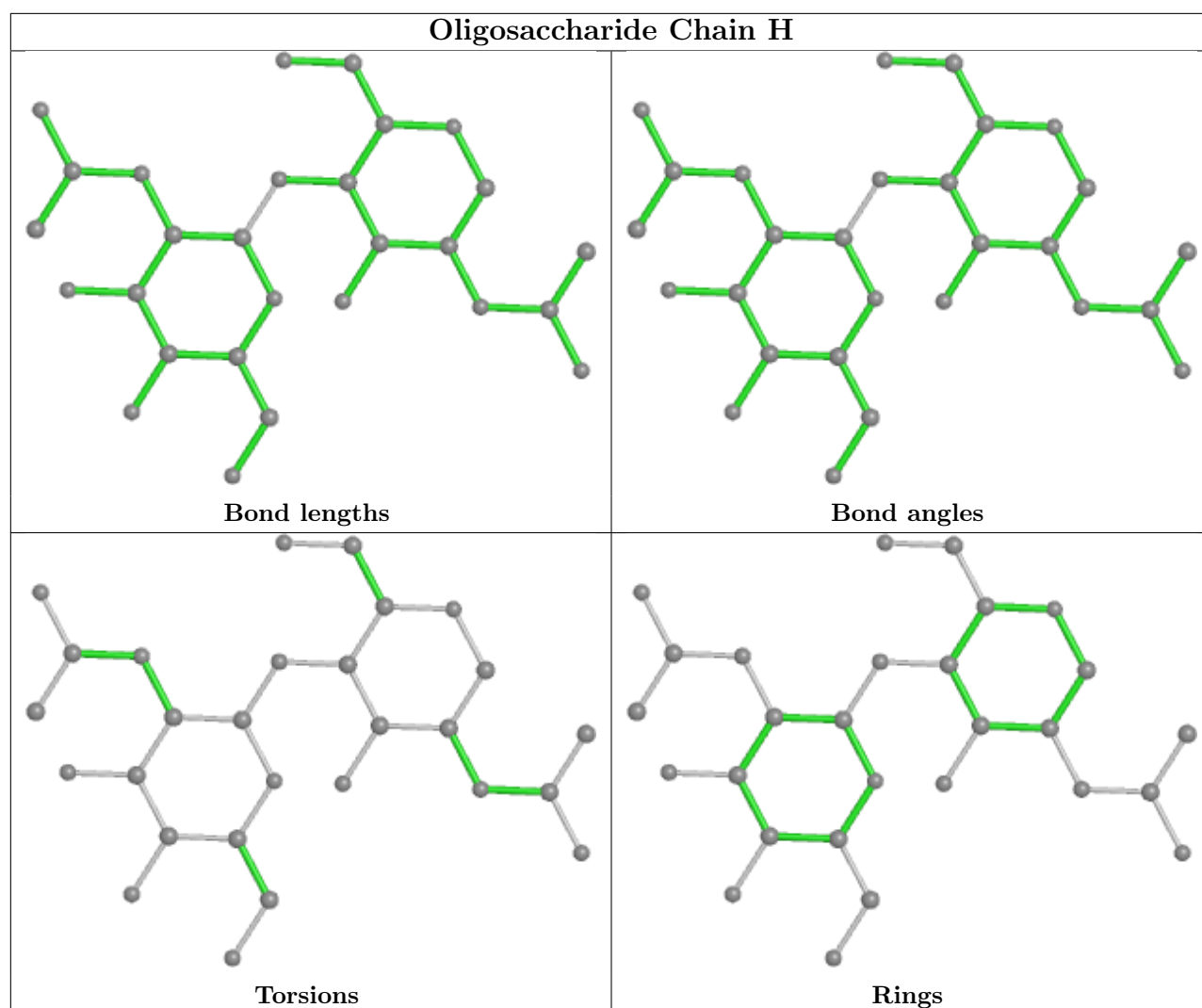
3 monomers are involved in 3 short contacts:

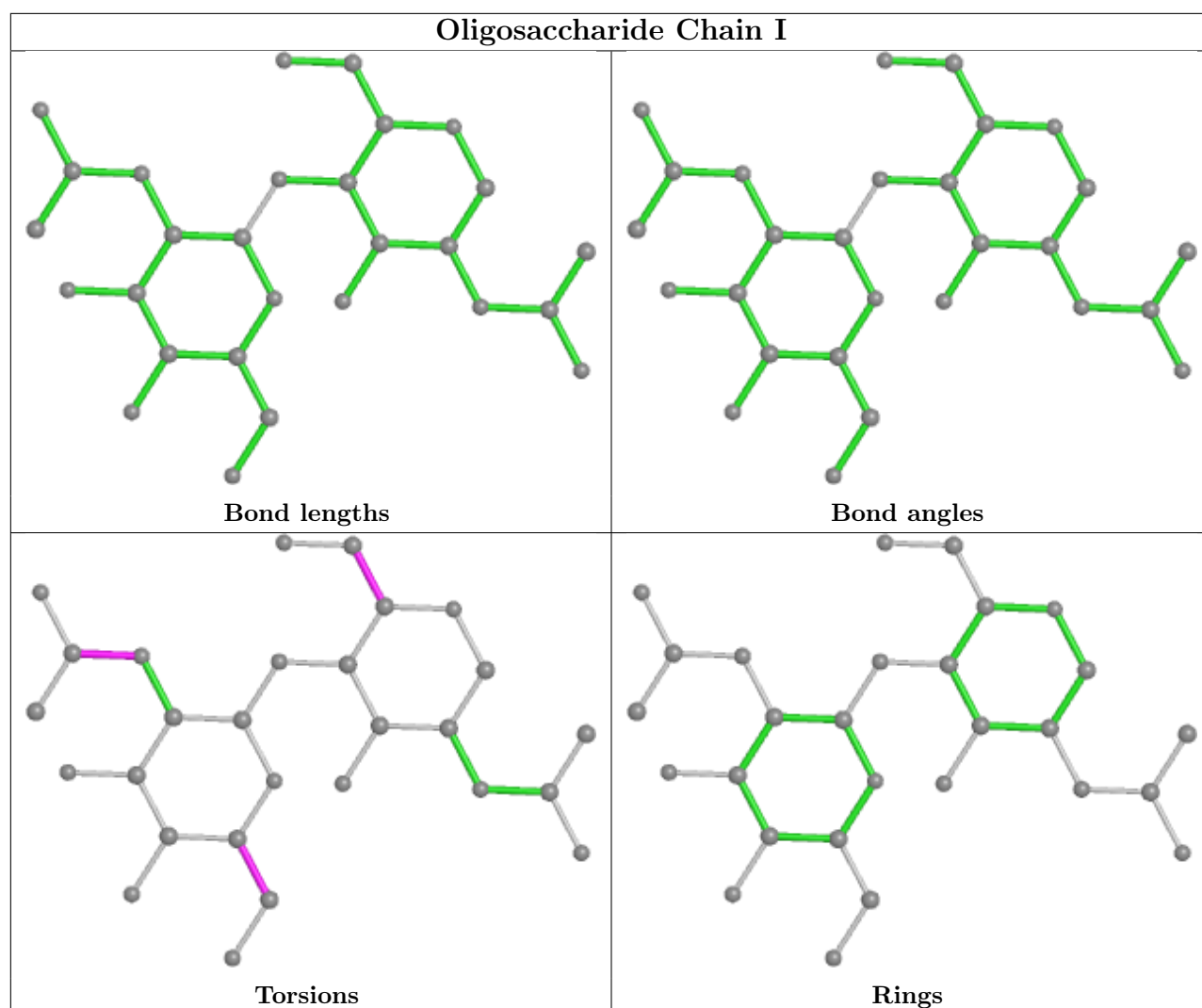
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
2	D	1	NAG	1	0
2	J	2	NAG	1	0

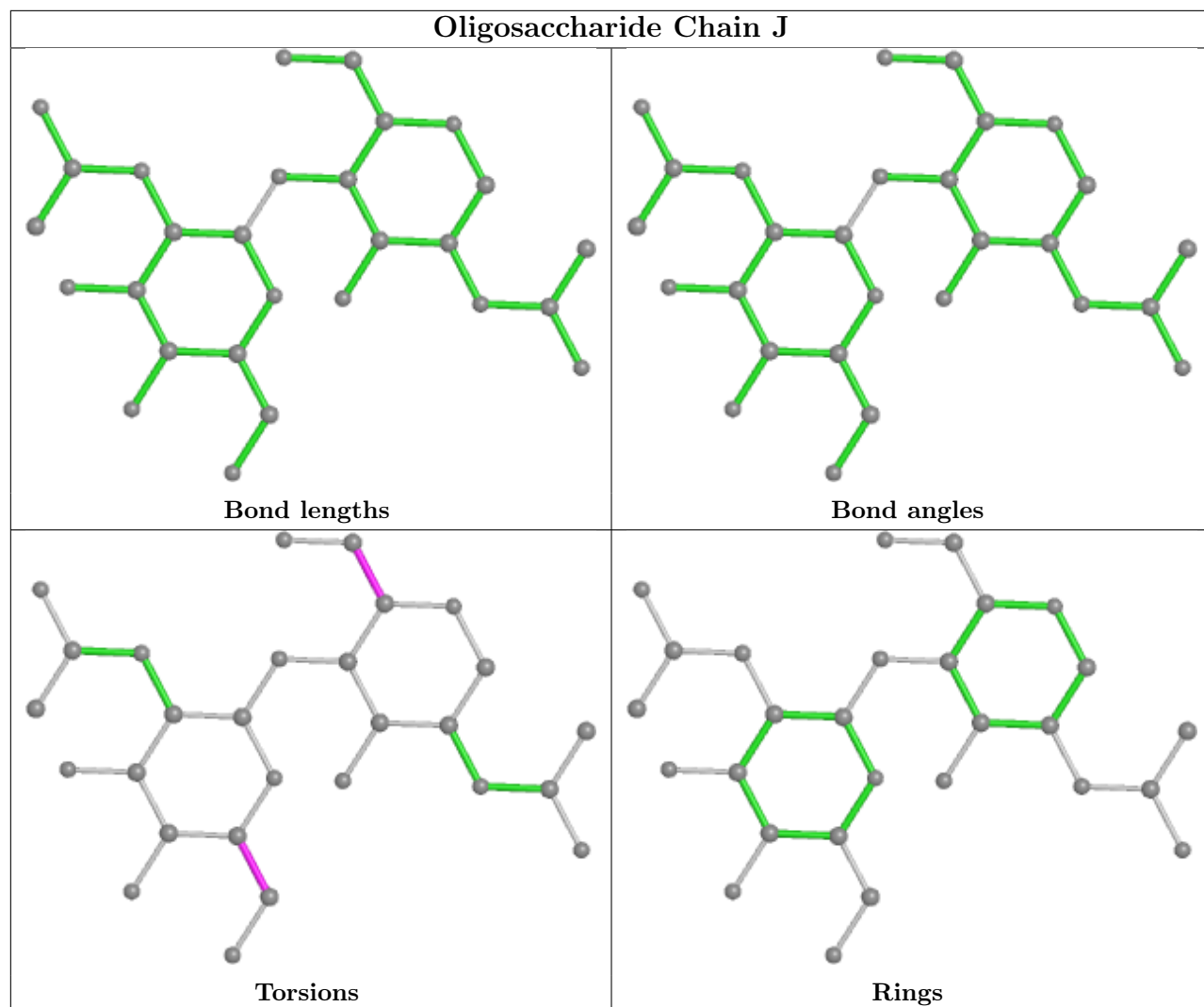
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

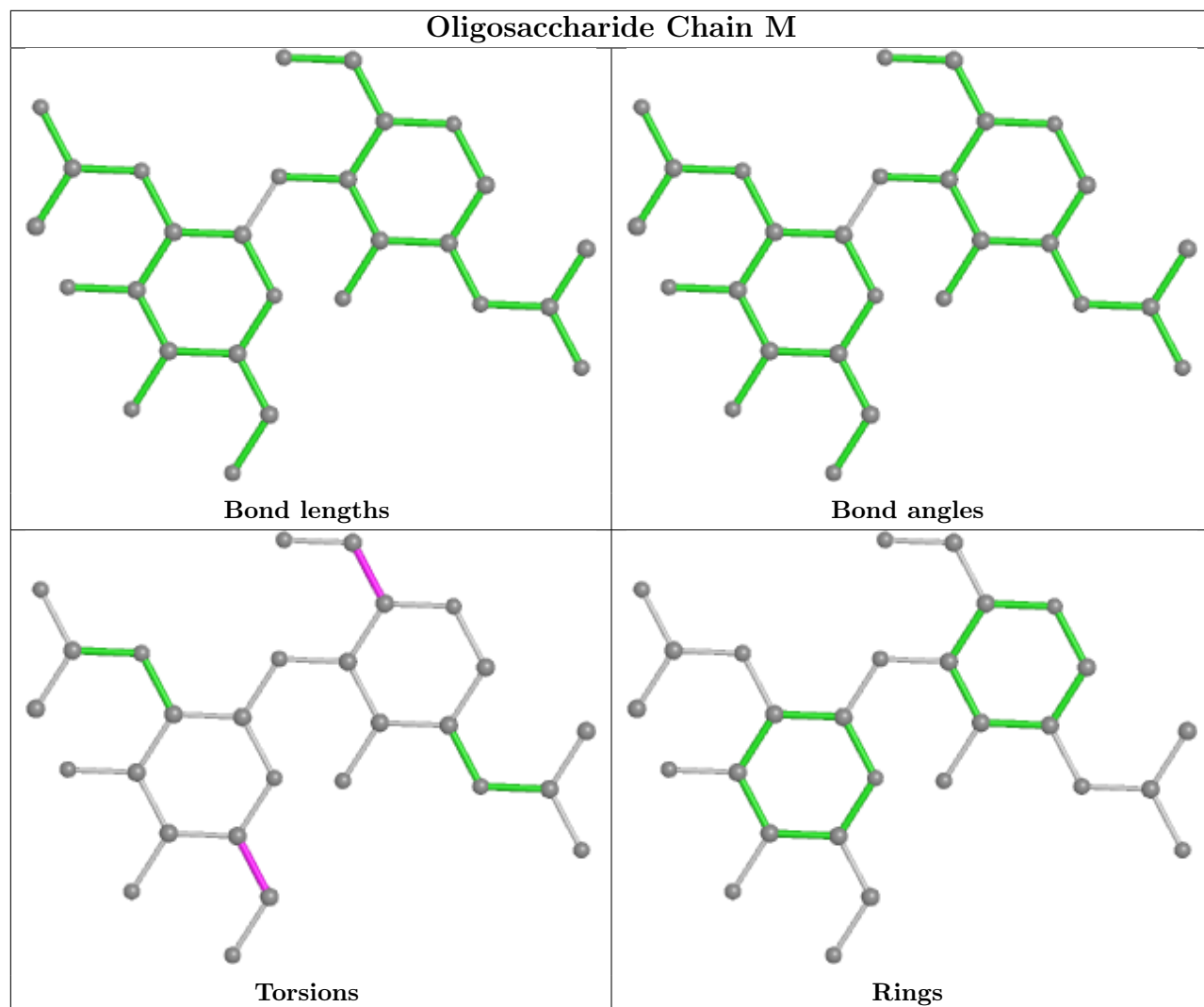


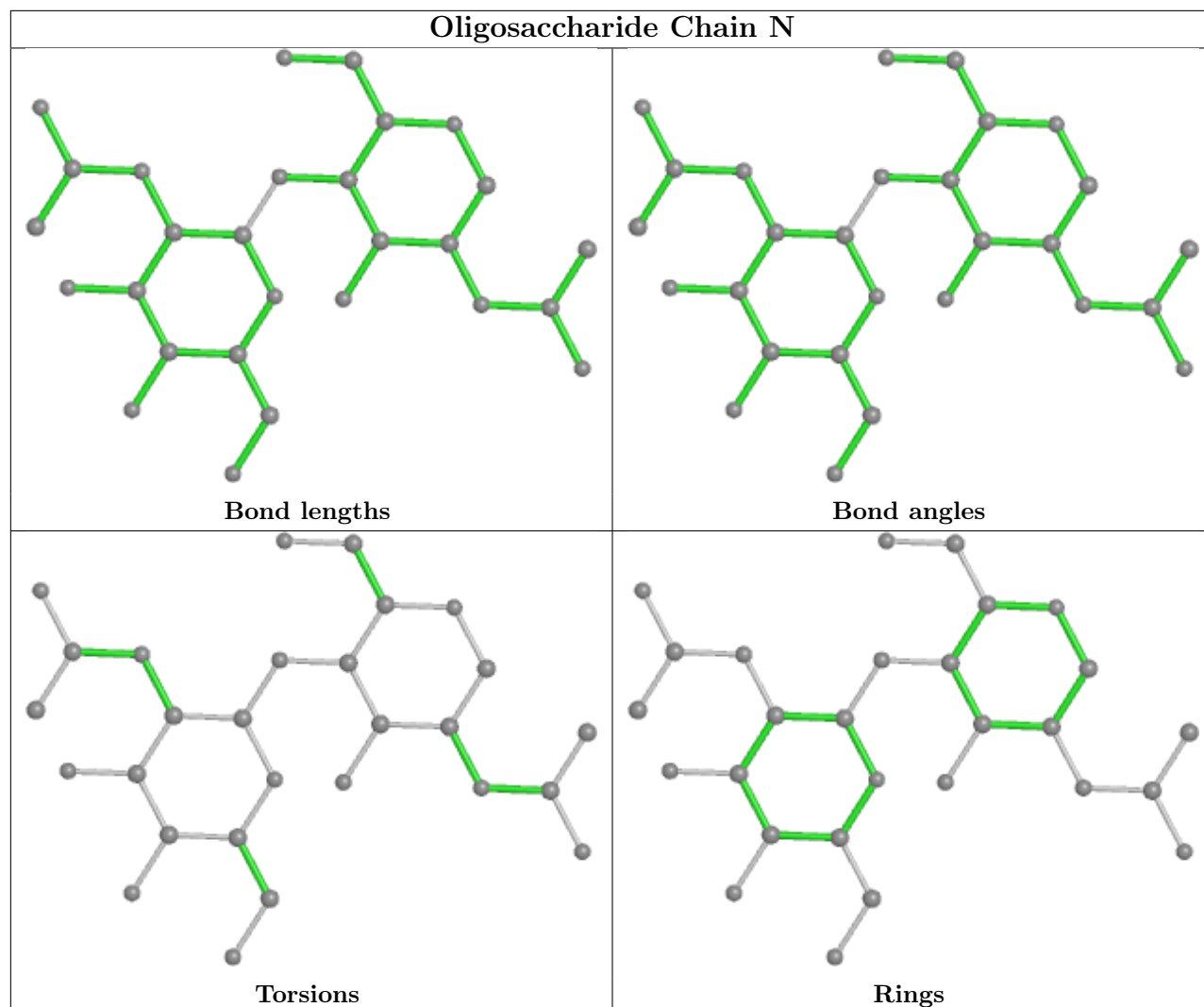


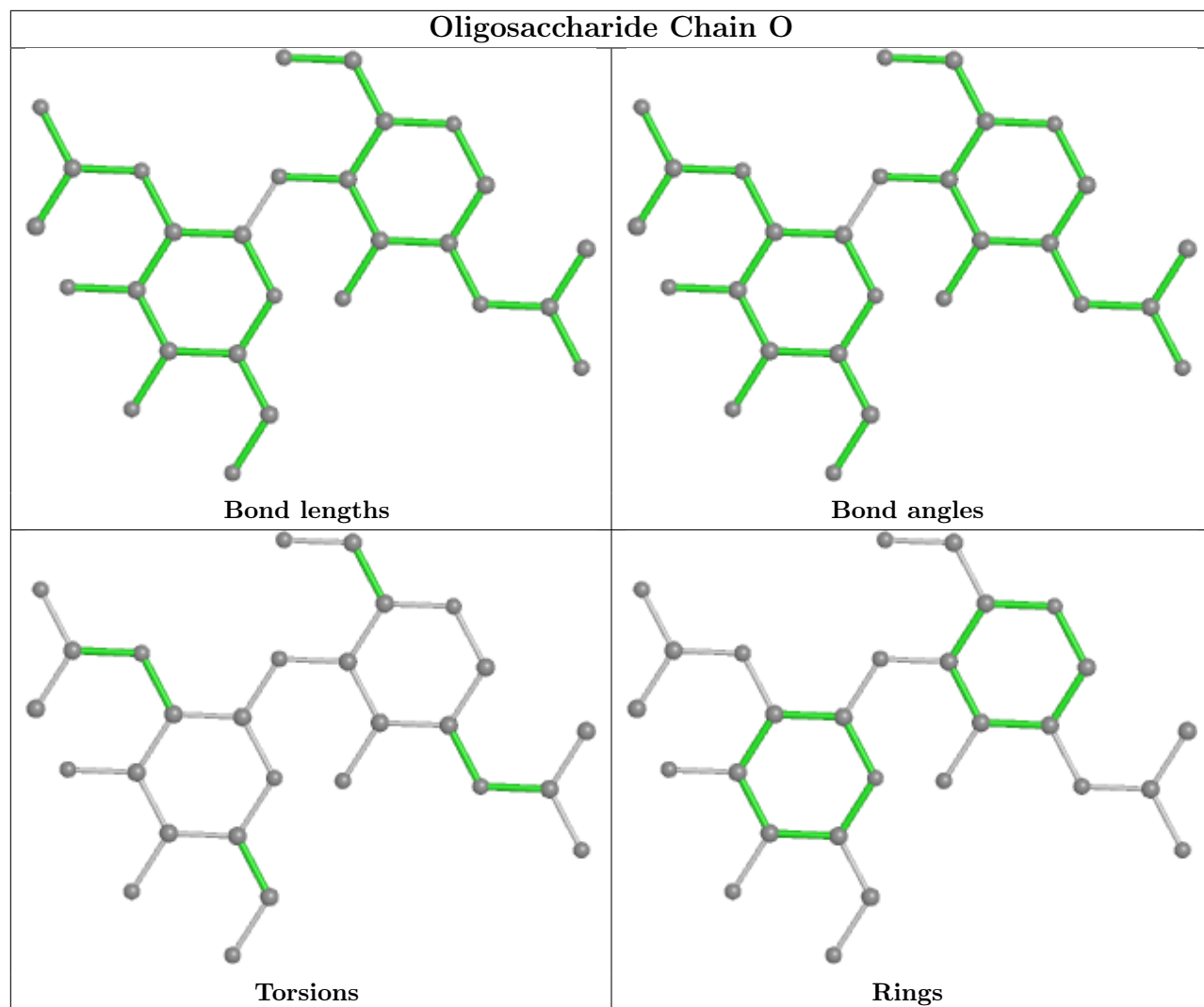


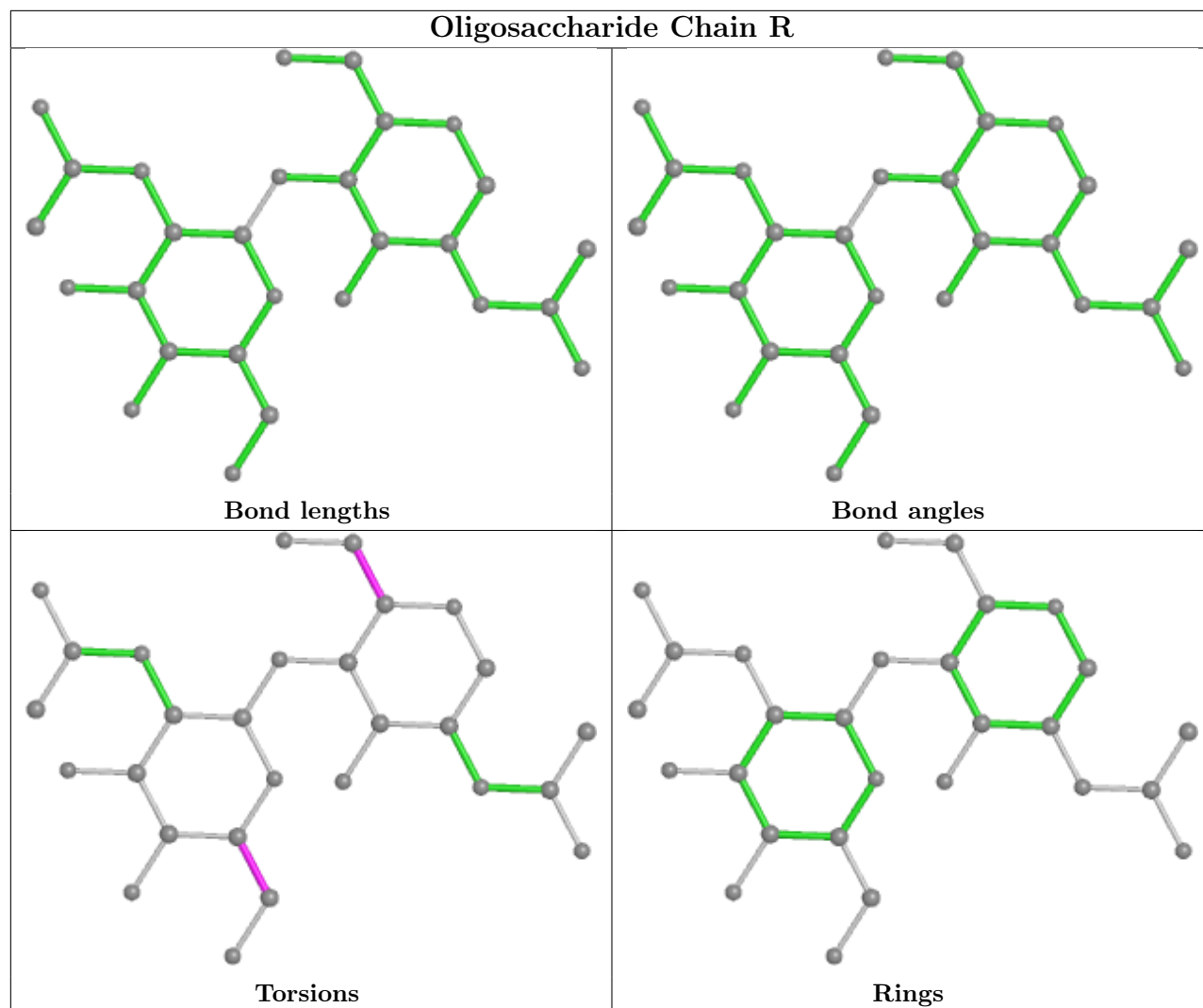


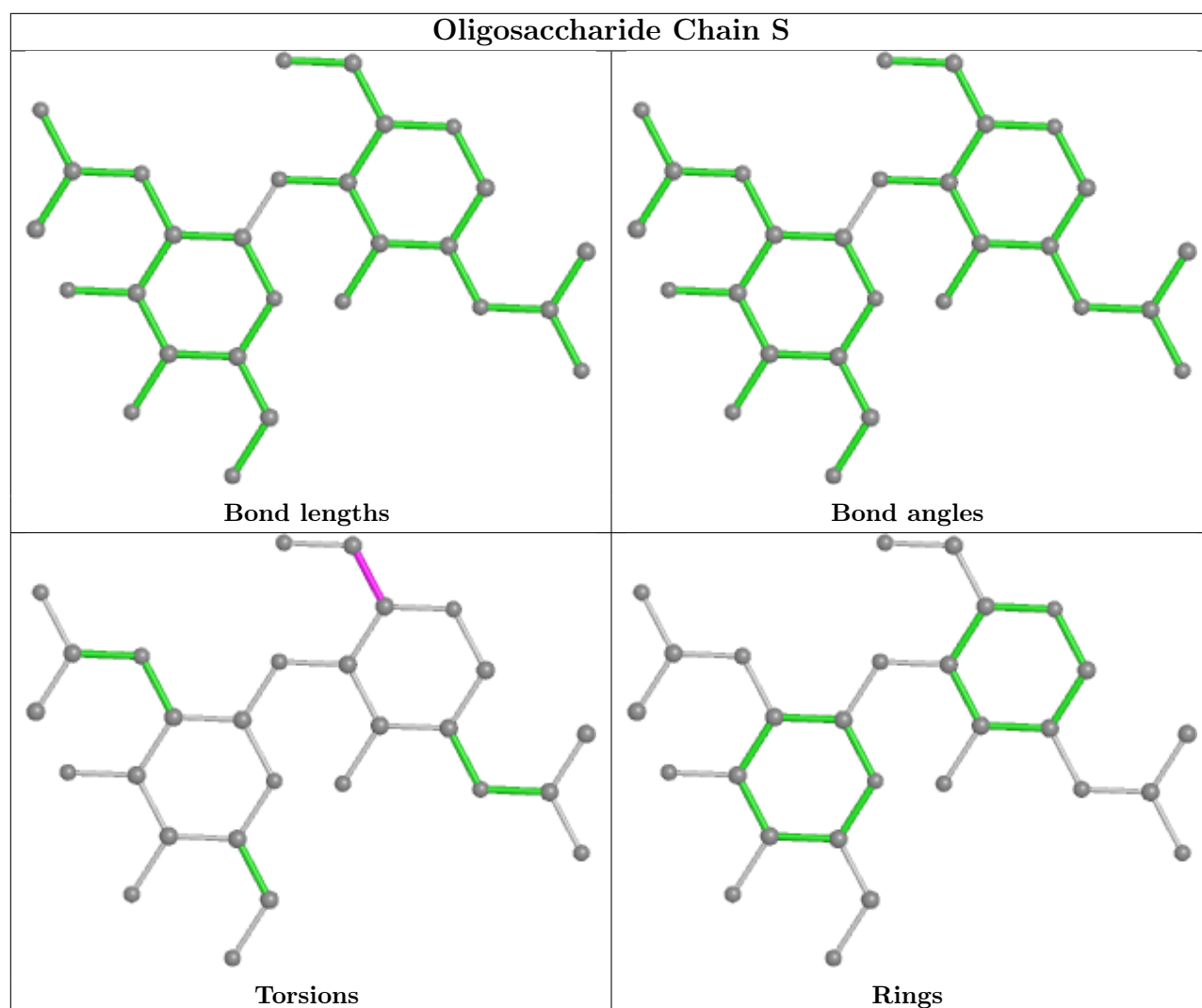


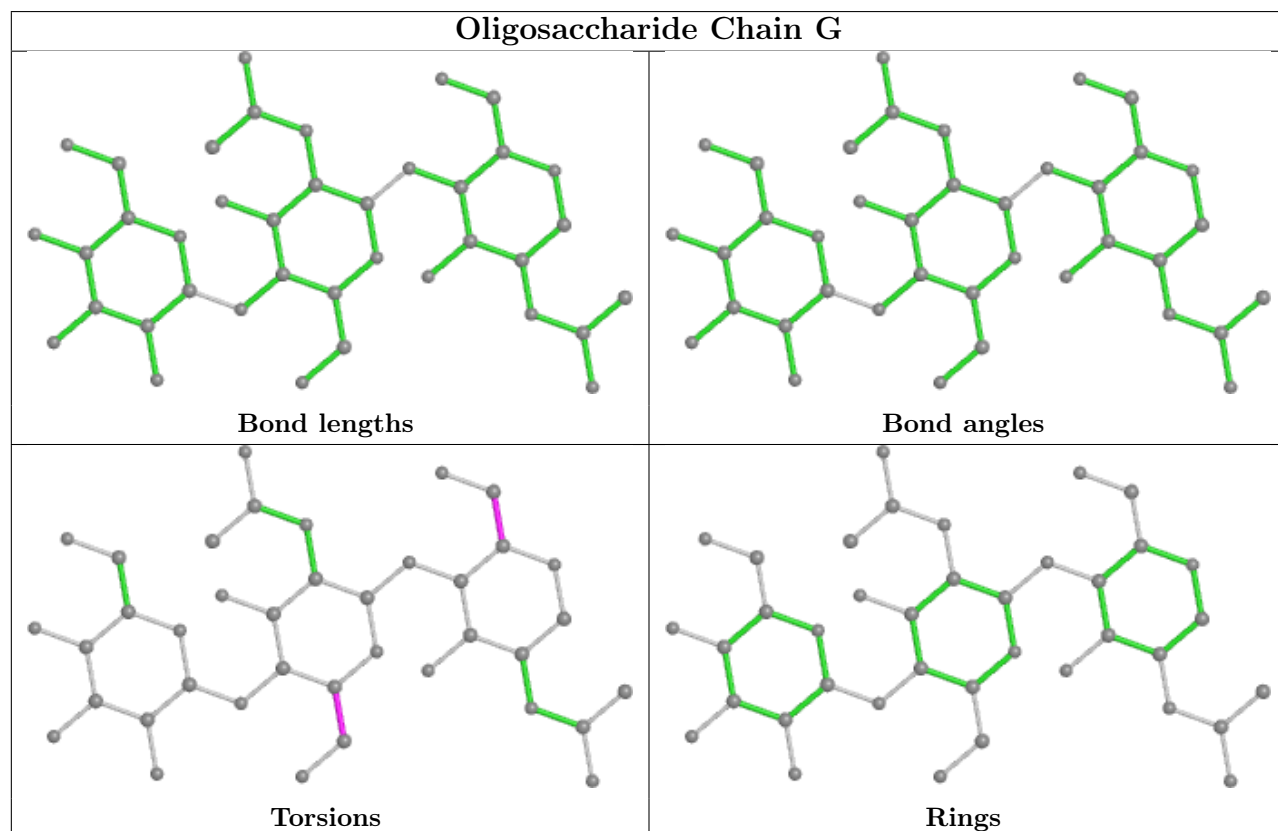
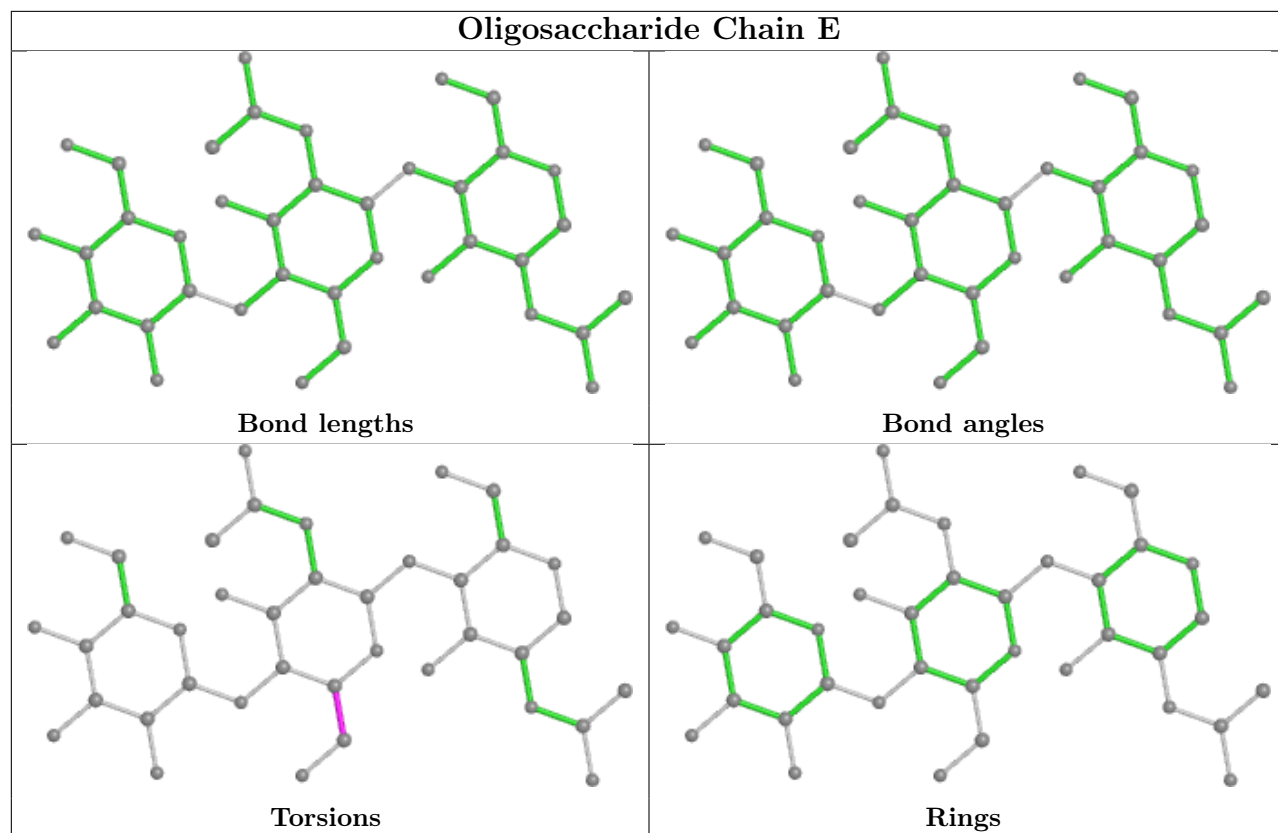


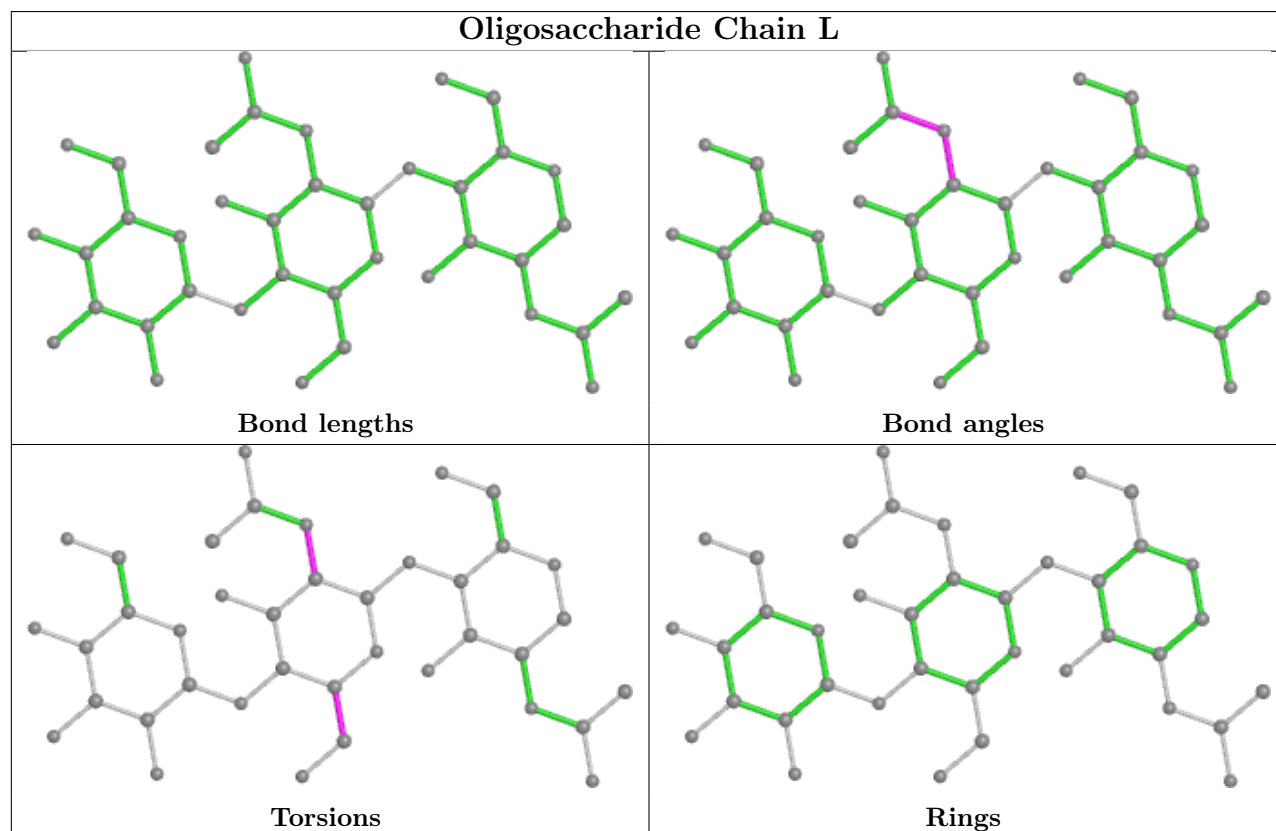
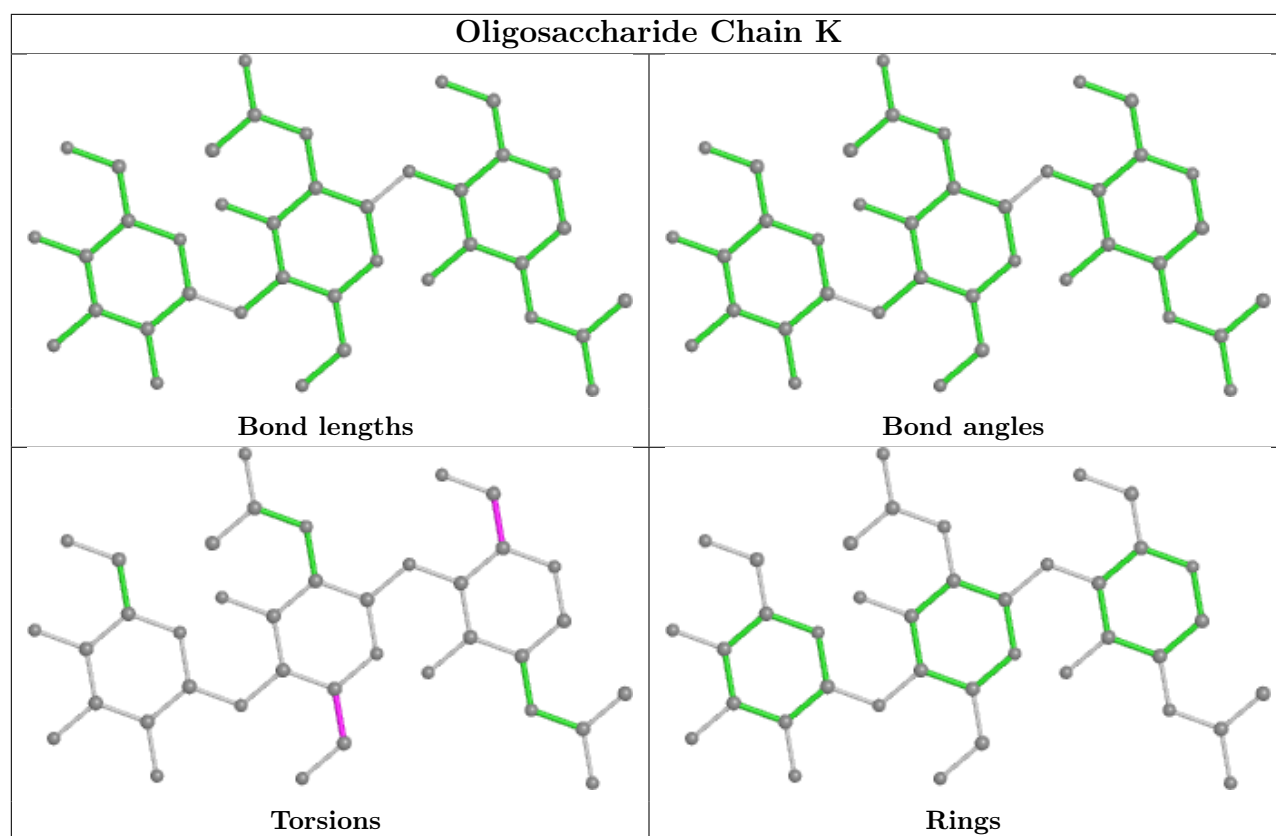


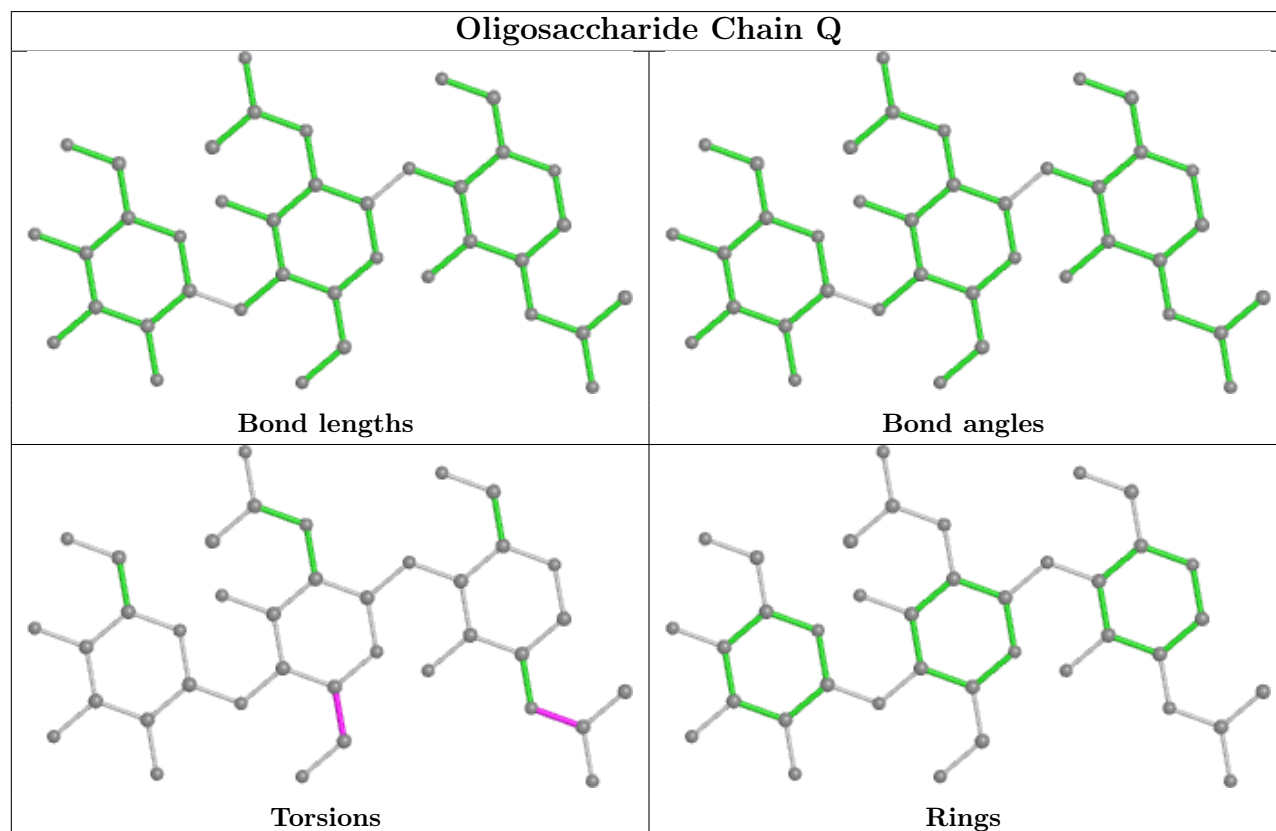
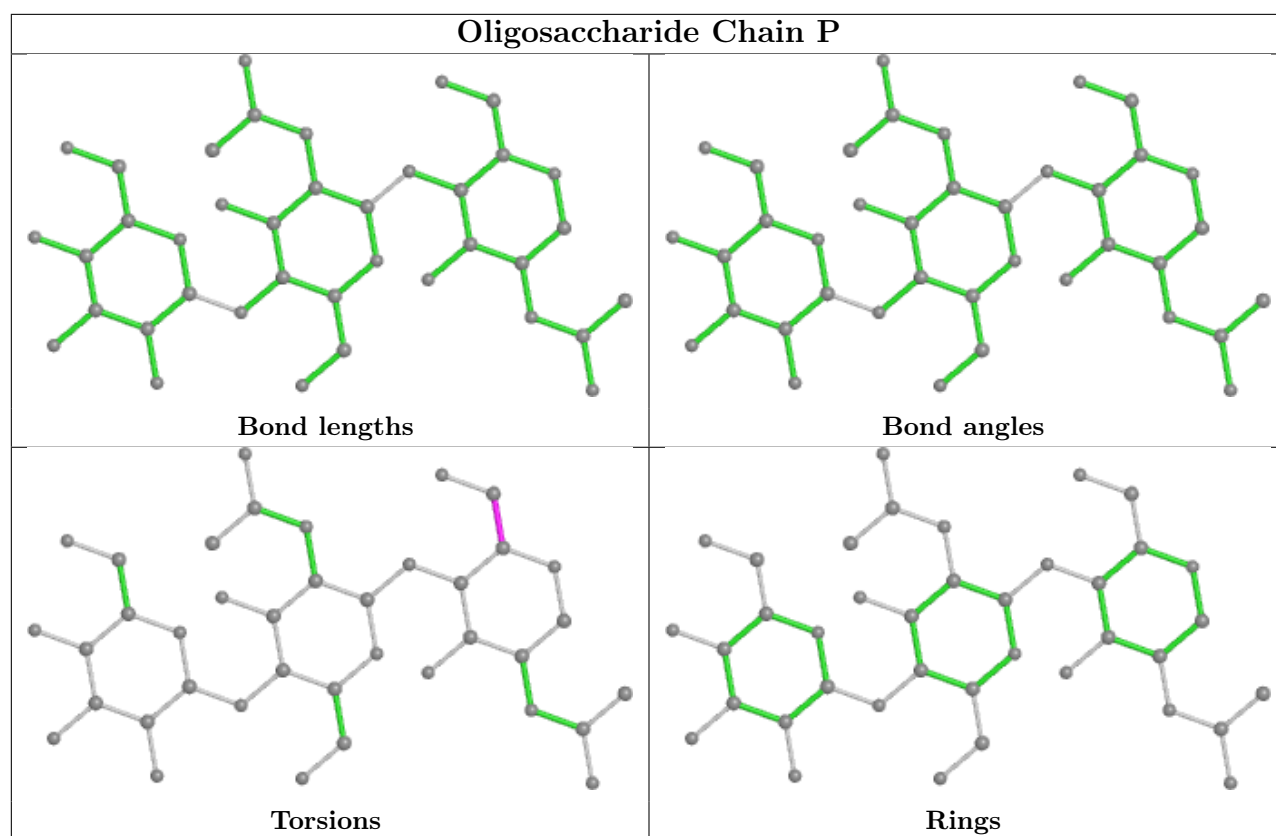












5.6 Ligand geometry

41 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	1404	1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	A	1412	1	14,14,15	0.26	0	17,19,21	0.47	0
5	NAG	B	1402	1	14,14,15	0.35	0	17,19,21	0.83	1 (5%)
5	NAG	A	1410	1	14,14,15	0.34	0	17,19,21	0.49	0
5	NAG	A	1402	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	A	1407	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	C	1407	1	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	B	1411	1	14,14,15	0.26	0	17,19,21	0.52	0
4	EIC	A	1415	-	19,19,19	0.58	0	19,19,19	0.56	0
5	NAG	B	1408	1	14,14,15	0.33	0	17,19,21	0.49	0
5	NAG	B	1407	1	14,14,15	0.32	0	17,19,21	0.47	0
4	EIC	A	1401	-	19,19,19	0.50	1 (5%)	19,19,19	0.89	0
5	NAG	C	1403	1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	A	1403	1	14,14,15	0.22	0	17,19,21	0.53	0
5	NAG	B	1401	1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	B	1403	1	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	B	1410	1	14,14,15	0.27	0	17,19,21	0.49	0
5	NAG	C	1409	1	14,14,15	0.31	0	17,19,21	0.50	0
5	NAG	C	1408	1	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	A	1408	1	14,14,15	0.33	0	17,19,21	0.46	0
5	NAG	A	1411	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	C	1406	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	C	1410	1	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	A	1405	1	14,14,15	0.28	0	17,19,21	0.47	0
5	NAG	B	1405	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	C	1405	1	14,14,15	0.41	0	17,19,21	0.85	1 (5%)
5	NAG	C	1401	1	14,14,15	0.31	0	17,19,21	0.84	1 (5%)
5	NAG	C	1404	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	B	1404	1	14,14,15	0.29	0	17,19,21	0.49	0
5	NAG	B	1409	1	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	C	1413	1	14,14,15	0.47	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1414	1	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	C	1412	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	A	1409	1	14,14,15	0.29	0	17,19,21	0.46	0
5	NAG	A	1413	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	B	1412	1	14,14,15	0.34	0	17,19,21	0.51	0
4	EIC	B	1413	-	19,19,19	0.58	0	19,19,19	0.56	0
5	NAG	B	1406	1	14,14,15	0.31	0	17,19,21	0.51	0
5	NAG	C	1411	1	14,14,15	0.25	0	17,19,21	0.48	0
5	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.50	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	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1412	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1411	1	-	4/6/23/26	0/1/1/1
4	EIC	A	1415	-	-	4/17/17/17	-
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
4	EIC	A	1401	-	-	6/17/17/17	-
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1411	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1414	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1412	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1412	1	-	2/6/23/26	0/1/1/1
4	EIC	B	1413	-	-	6/17/17/17	-
5	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1411	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1401	EIC	O2-C1	-2.03	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1401	NAG	C2-N2-C7	2.48	126.44	122.90
5	C	1405	NAG	C2-N2-C7	2.47	126.41	122.90
5	C	1413	NAG	C2-N2-C7	2.46	126.41	122.90
5	B	1402	NAG	C2-N2-C7	2.44	126.38	122.90

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1402	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1405	NAG	C4-C5-C6-O6
5	C	1408	NAG	O5-C5-C6-O6
5	B	1412	NAG	C4-C5-C6-O6
5	A	1411	NAG	O5-C5-C6-O6
5	A	1412	NAG	O5-C5-C6-O6
5	A	1413	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	B	1407	NAG	O5-C5-C6-O6
5	B	1409	NAG	O5-C5-C6-O6
5	B	1411	NAG	O5-C5-C6-O6
5	C	1411	NAG	O5-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	B	1410	NAG	O5-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	B	1407	NAG	C4-C5-C6-O6
5	B	1409	NAG	C4-C5-C6-O6
5	A	1406	NAG	O5-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	B	1411	NAG	C4-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6
5	A	1411	NAG	C4-C5-C6-O6
5	C	1411	NAG	C4-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
5	A	1410	NAG	C4-C5-C6-O6
5	C	1410	NAG	O5-C5-C6-O6
5	C	1407	NAG	C4-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	A	1413	NAG	C4-C5-C6-O6
5	B	1412	NAG	O5-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	A	1412	NAG	C4-C5-C6-O6
5	B	1410	NAG	C4-C5-C6-O6
5	B	1406	NAG	C8-C7-N2-C2
5	B	1406	NAG	O7-C7-N2-C2
5	B	1411	NAG	C8-C7-N2-C2
5	B	1411	NAG	O7-C7-N2-C2
5	A	1410	NAG	O5-C5-C6-O6

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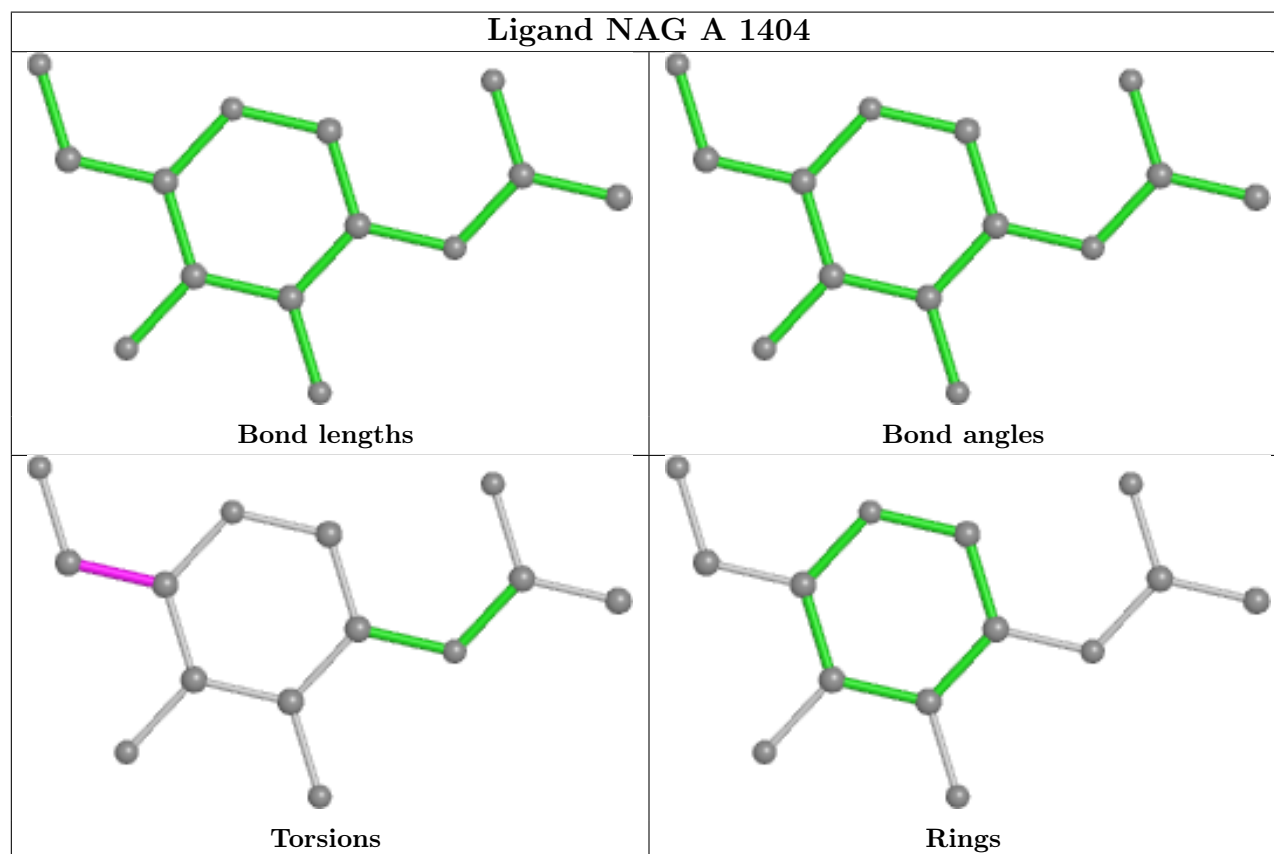
Mol	Chain	Res	Type	Atoms
5	A	1408	NAG	C4-C5-C6-O6
5	C	1412	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	C	1410	NAG	C4-C5-C6-O6
5	C	1407	NAG	O5-C5-C6-O6
5	A	1414	NAG	C4-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
4	A	1401	EIC	C1-C2-C3-C4
5	A	1406	NAG	C4-C5-C6-O6
5	C	1413	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	A	1414	NAG	O5-C5-C6-O6
4	A	1415	EIC	C6-C7-C8-C9
4	A	1415	EIC	C2-C3-C4-C5
5	A	1409	NAG	O5-C5-C6-O6
5	B	1408	NAG	O5-C5-C6-O6
5	B	1408	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
4	B	1413	EIC	C2-C3-C4-C5
4	A	1401	EIC	C9-C10-C11-C12
4	A	1415	EIC	C3-C4-C5-C6
4	B	1413	EIC	C3-C4-C5-C6
5	C	1405	NAG	C4-C5-C6-O6
5	C	1401	NAG	C3-C2-N2-C7
5	C	1413	NAG	C3-C2-N2-C7
4	B	1413	EIC	C5-C6-C7-C8
4	B	1413	EIC	C6-C7-C8-C9
4	A	1401	EIC	C10-C11-C12-C13
4	A	1415	EIC	C10-C11-C12-C13
4	B	1413	EIC	C10-C11-C12-C13
4	A	1401	EIC	O1-C1-C2-C3
5	C	1405	NAG	O5-C5-C6-O6
4	A	1401	EIC	C5-C6-C7-C8
5	B	1406	NAG	C4-C5-C6-O6
4	A	1401	EIC	O2-C1-C2-C3
5	B	1402	NAG	C3-C2-N2-C7
5	C	1405	NAG	C3-C2-N2-C7
5	C	1412	NAG	C4-C5-C6-O6
4	B	1413	EIC	O2-C1-C2-C3

There are no ring outliers.

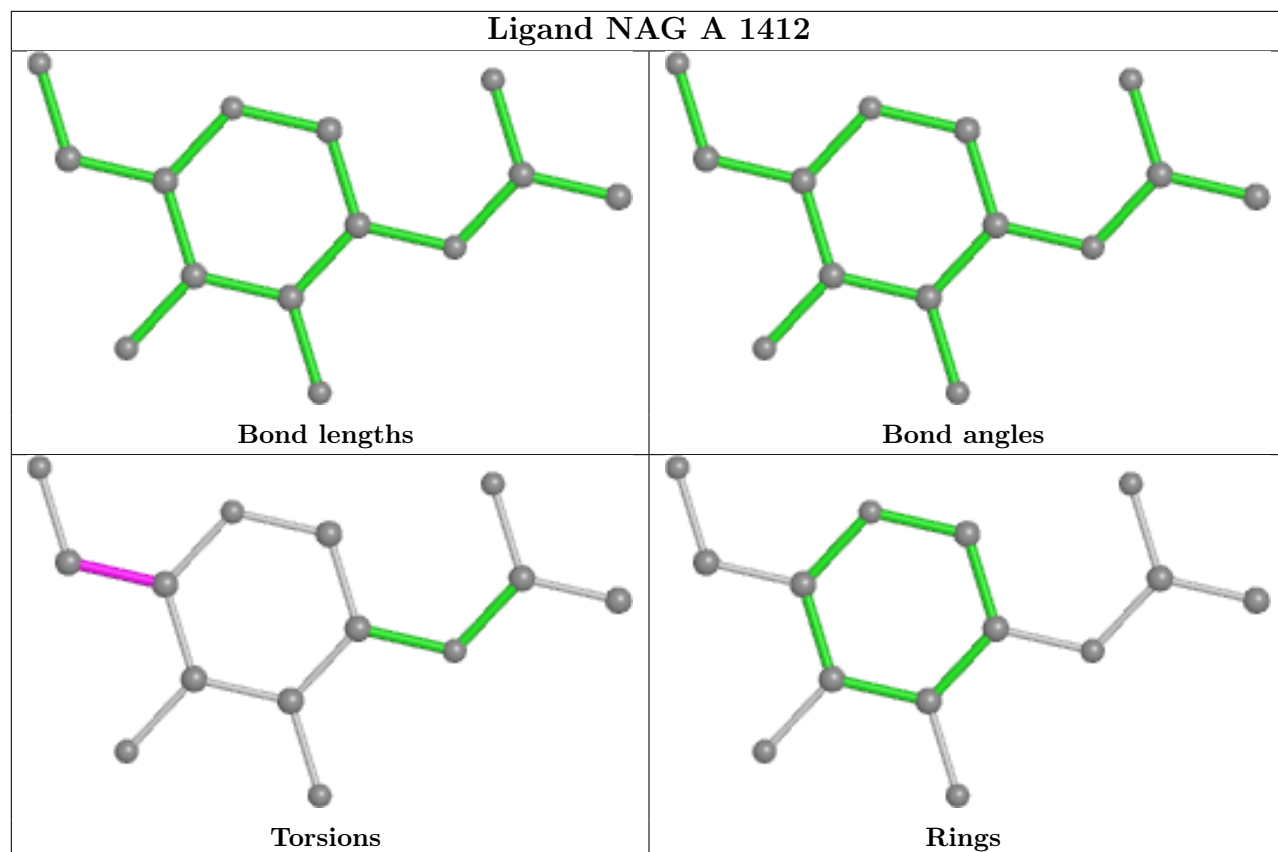
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1415	EIC	1	0
4	A	1401	EIC	4	0
4	B	1413	EIC	1	0

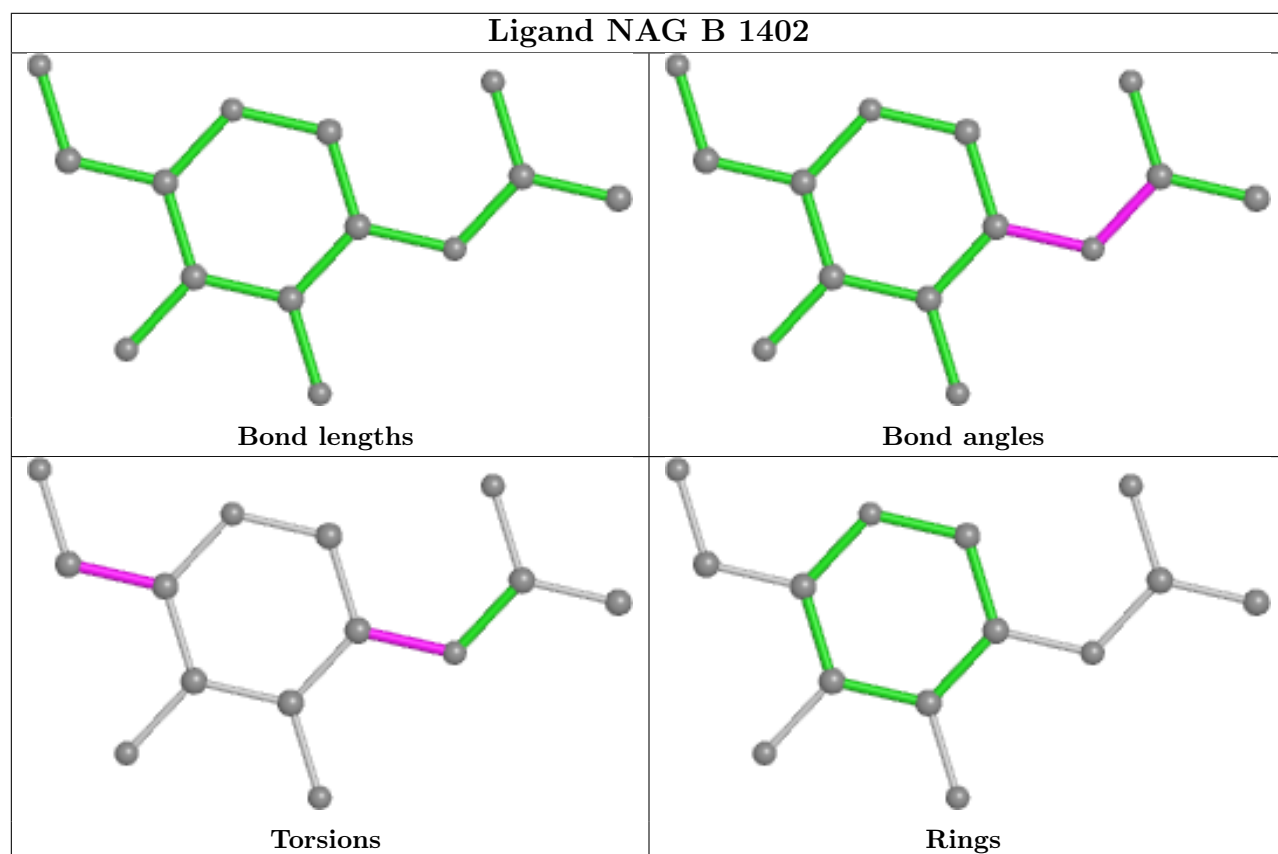
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



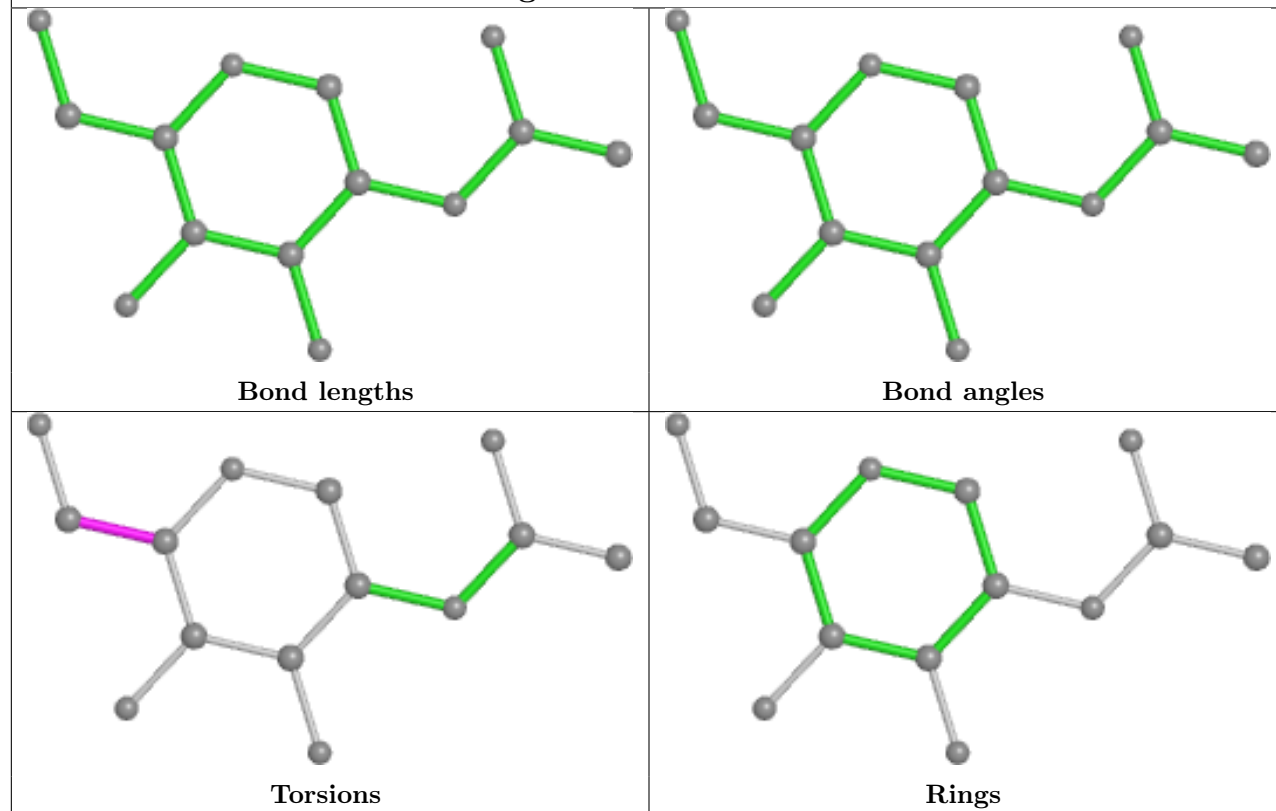
Ligand NAG A 1412



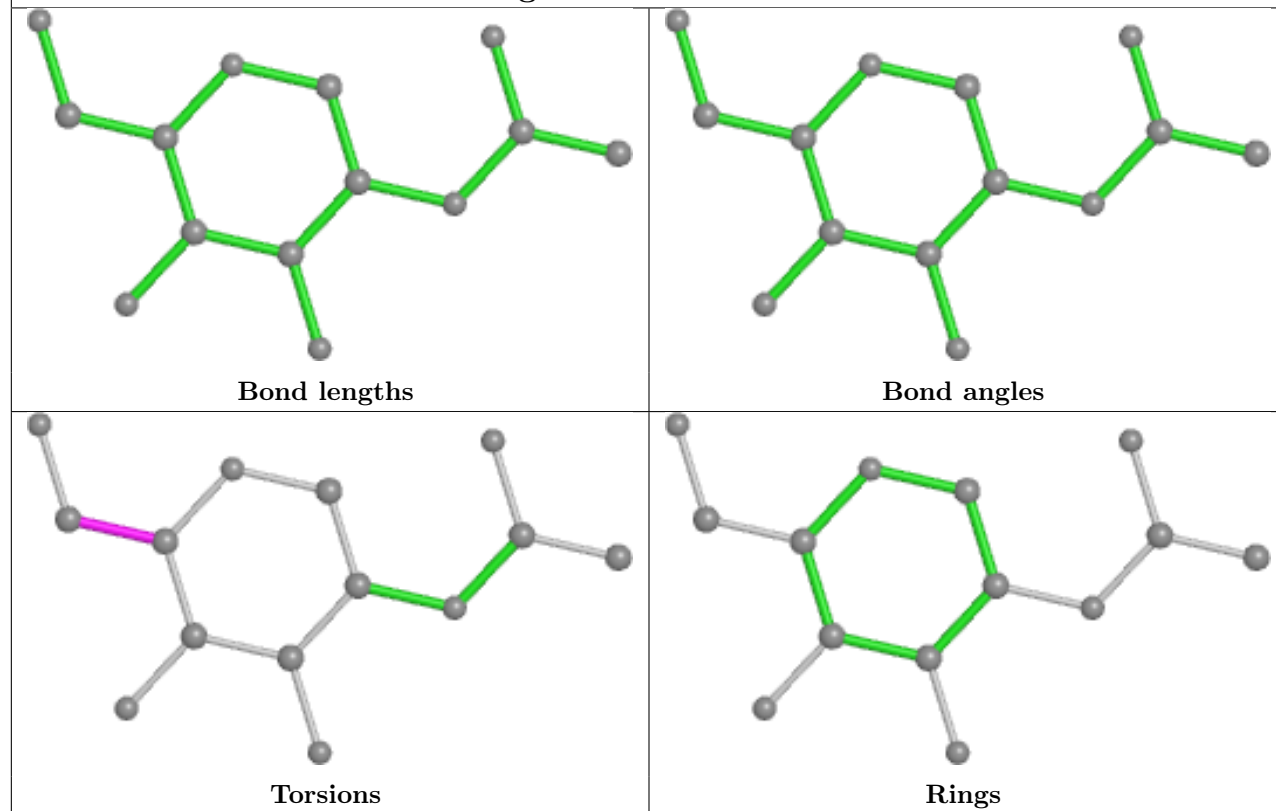
Ligand NAG B 1402

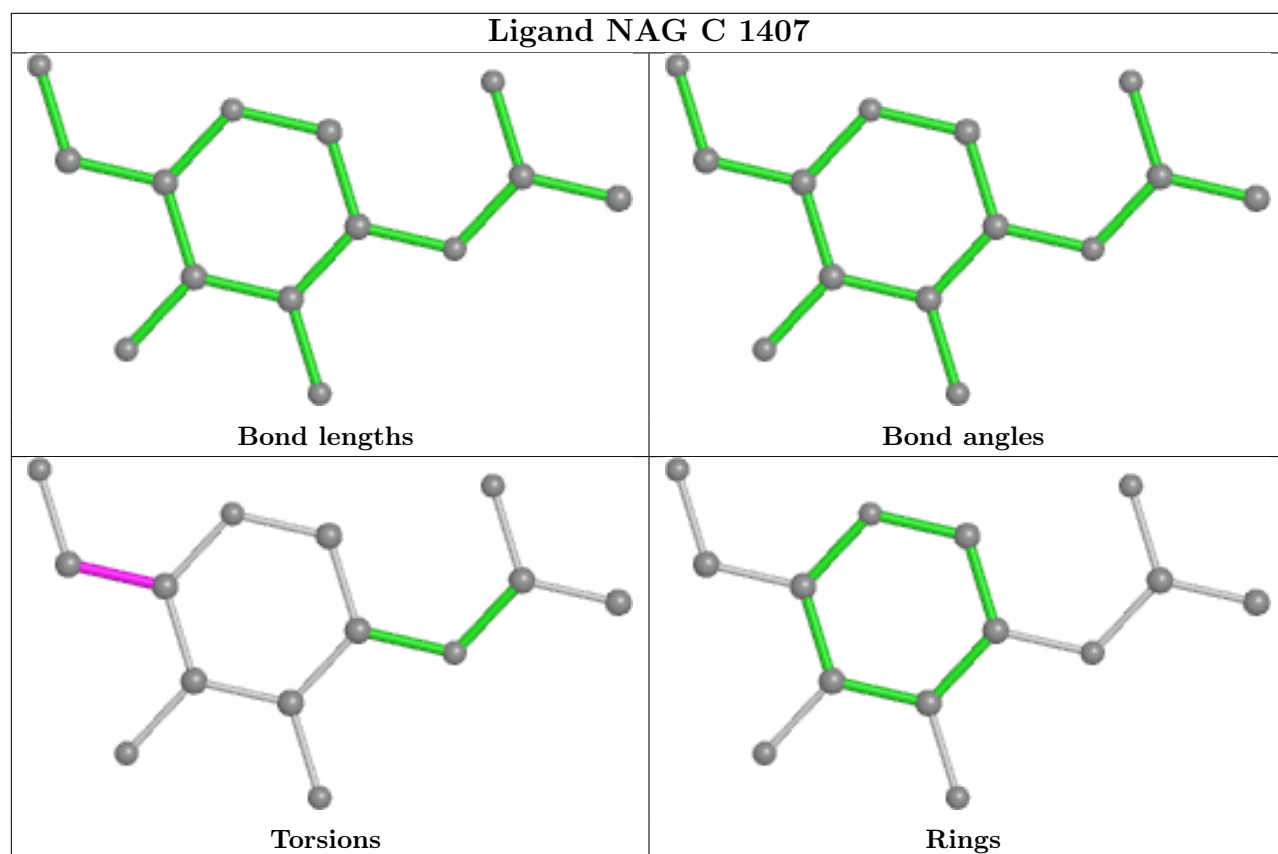
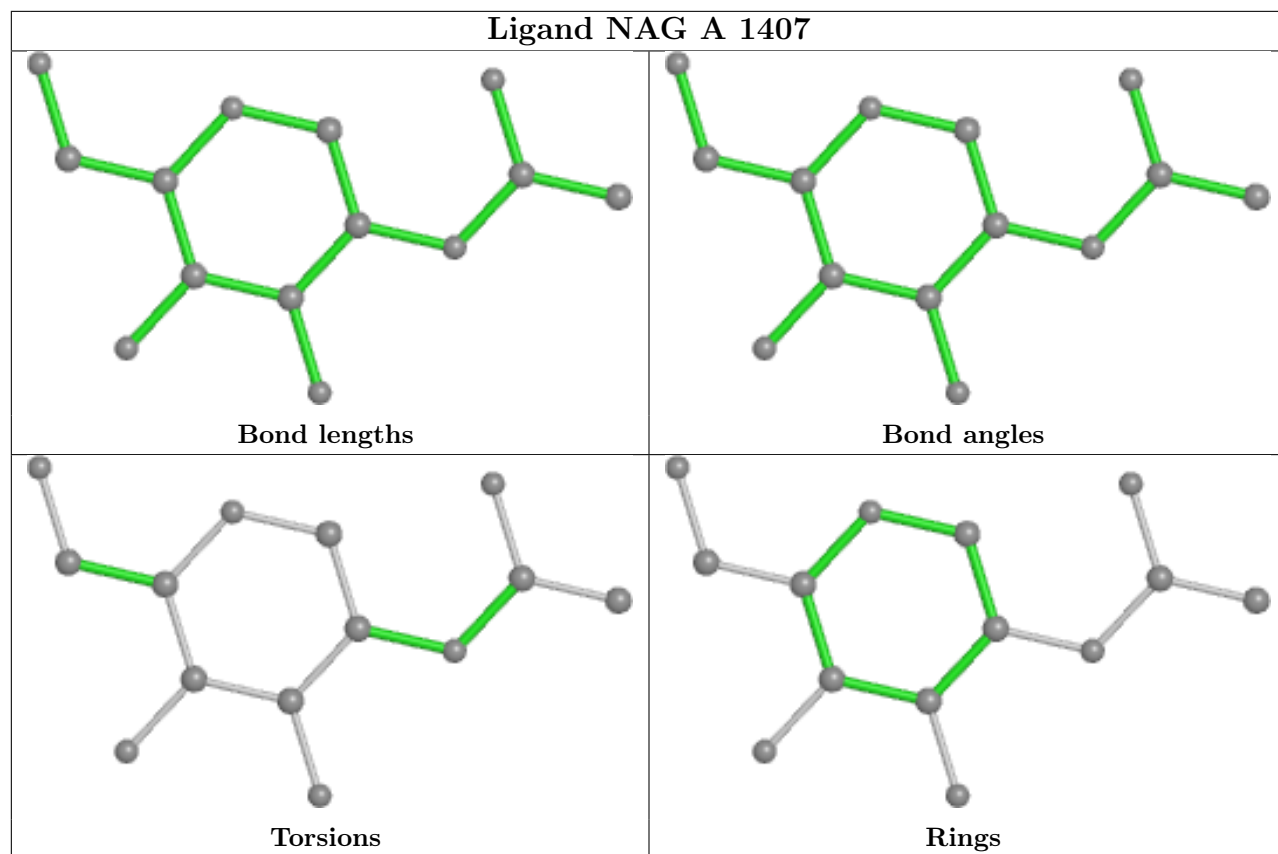


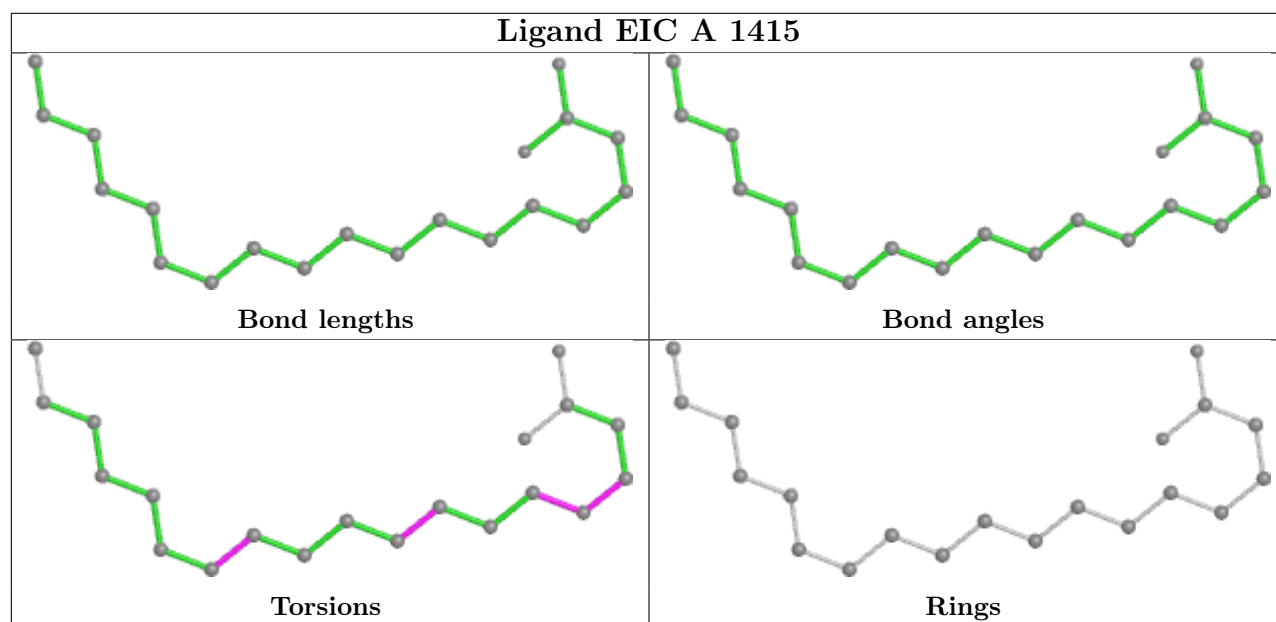
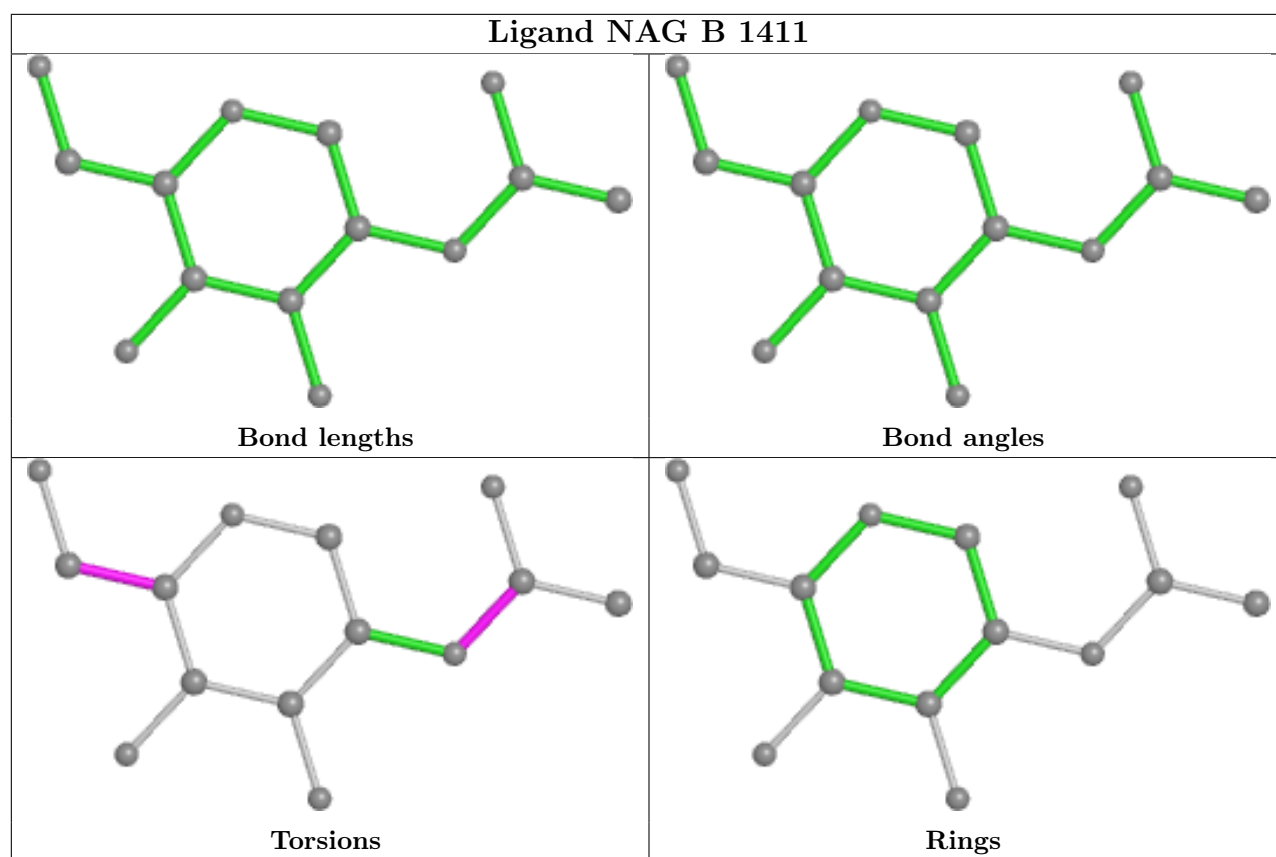
Ligand NAG A 1410



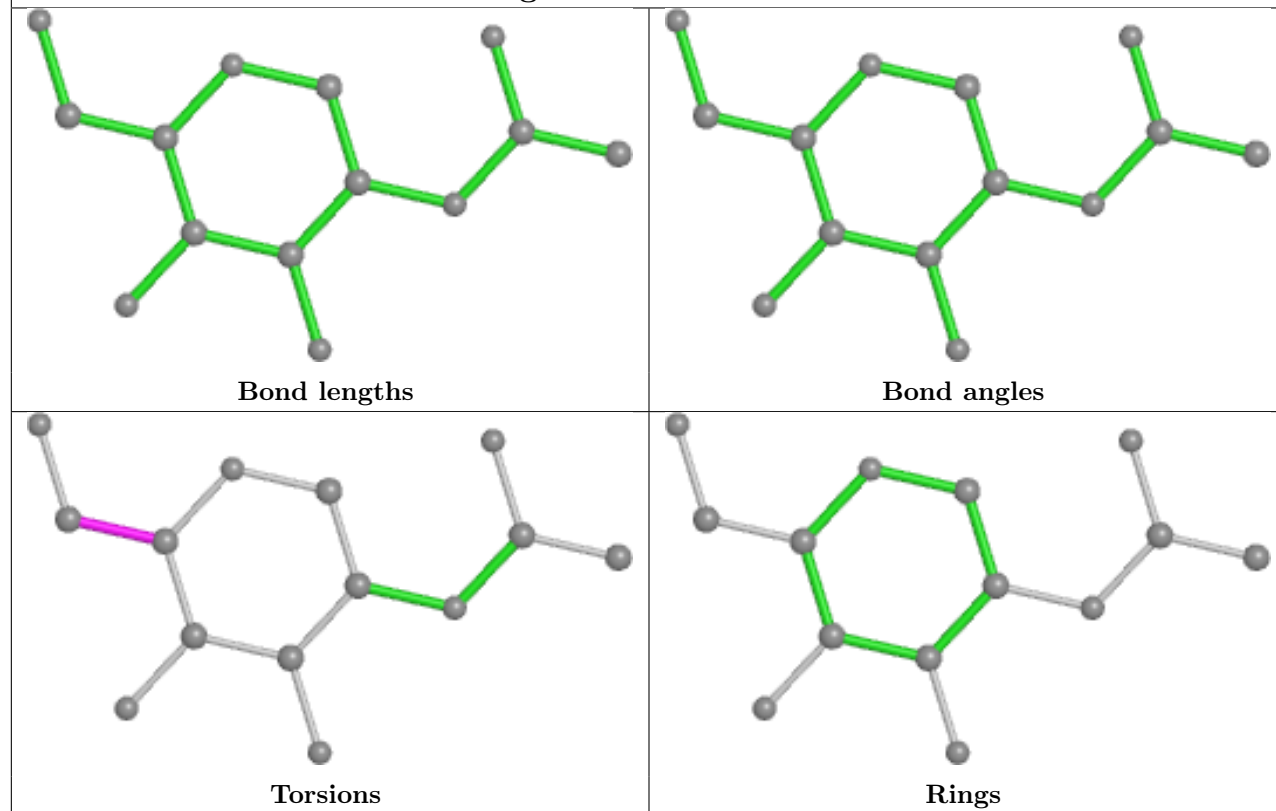
Ligand NAG A 1402



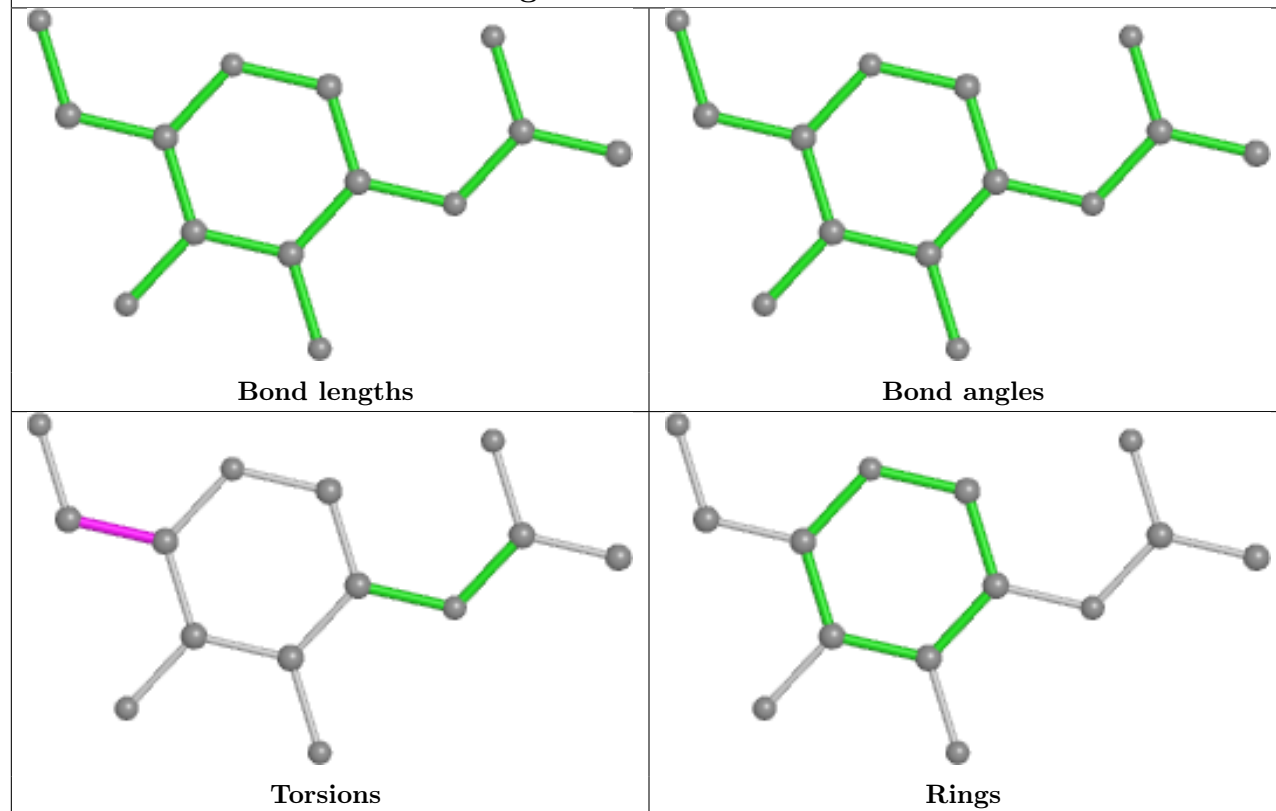


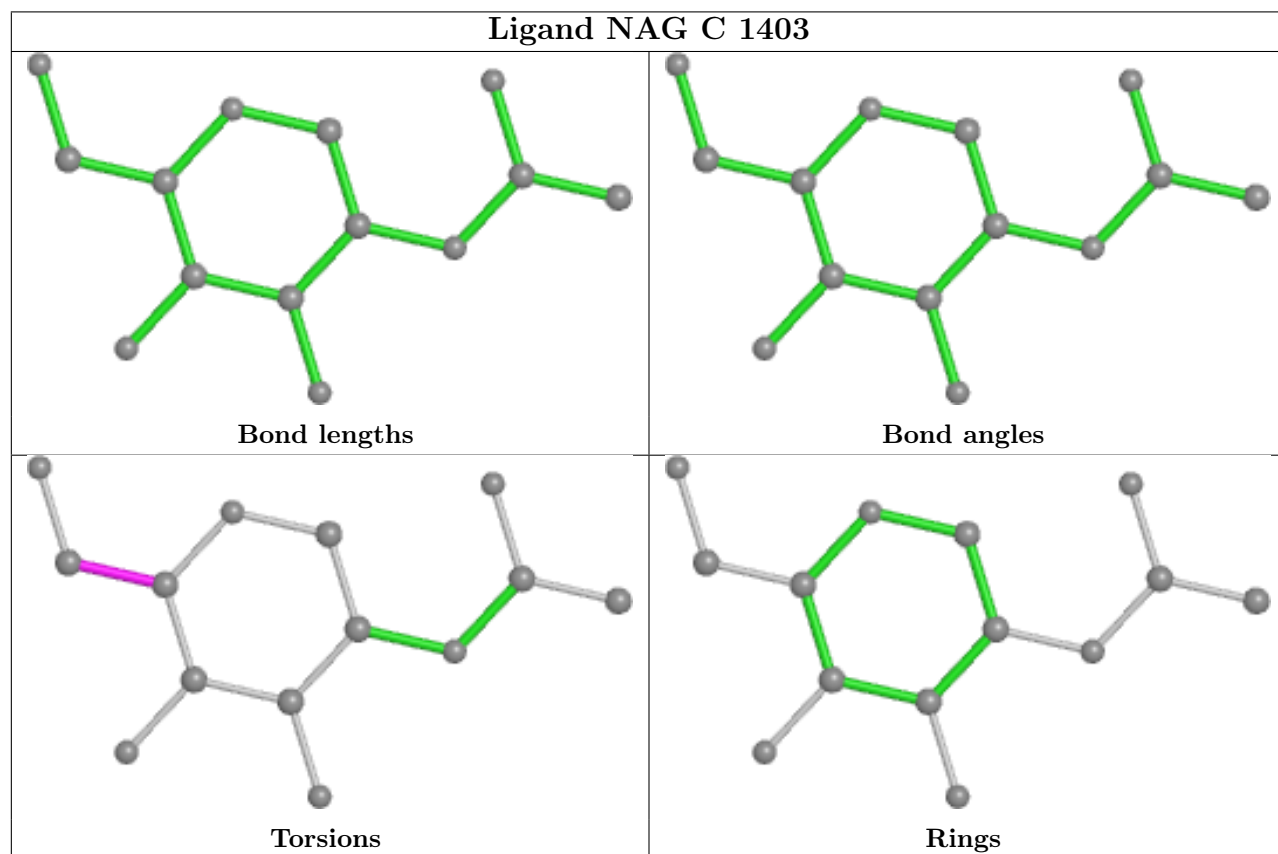
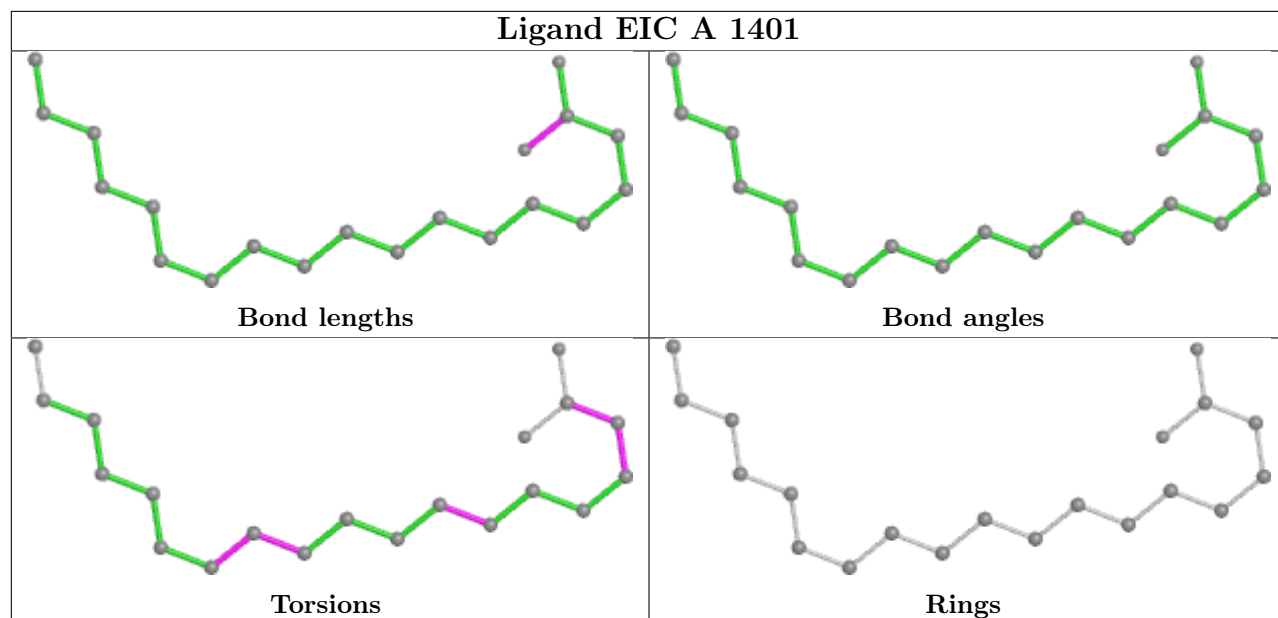


Ligand NAG B 1408



Ligand NAG B 1407

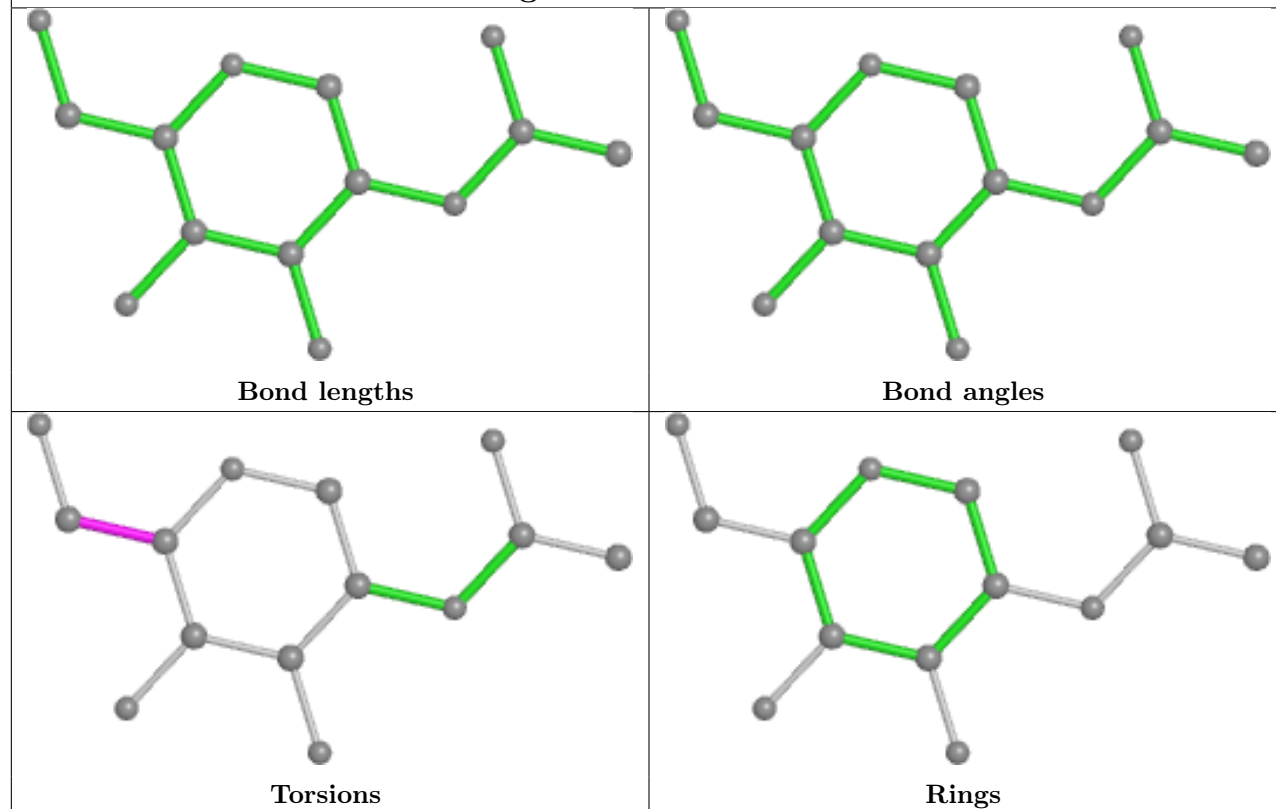


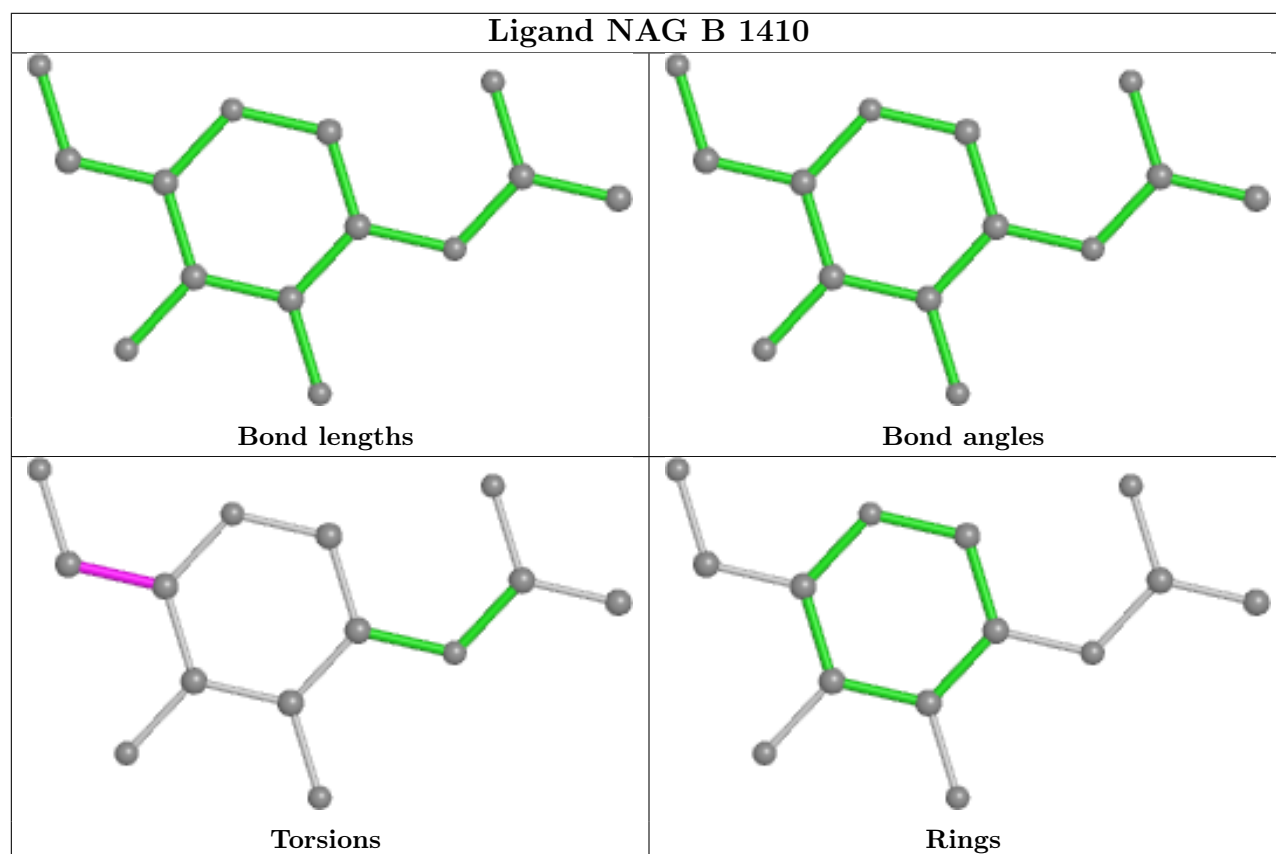
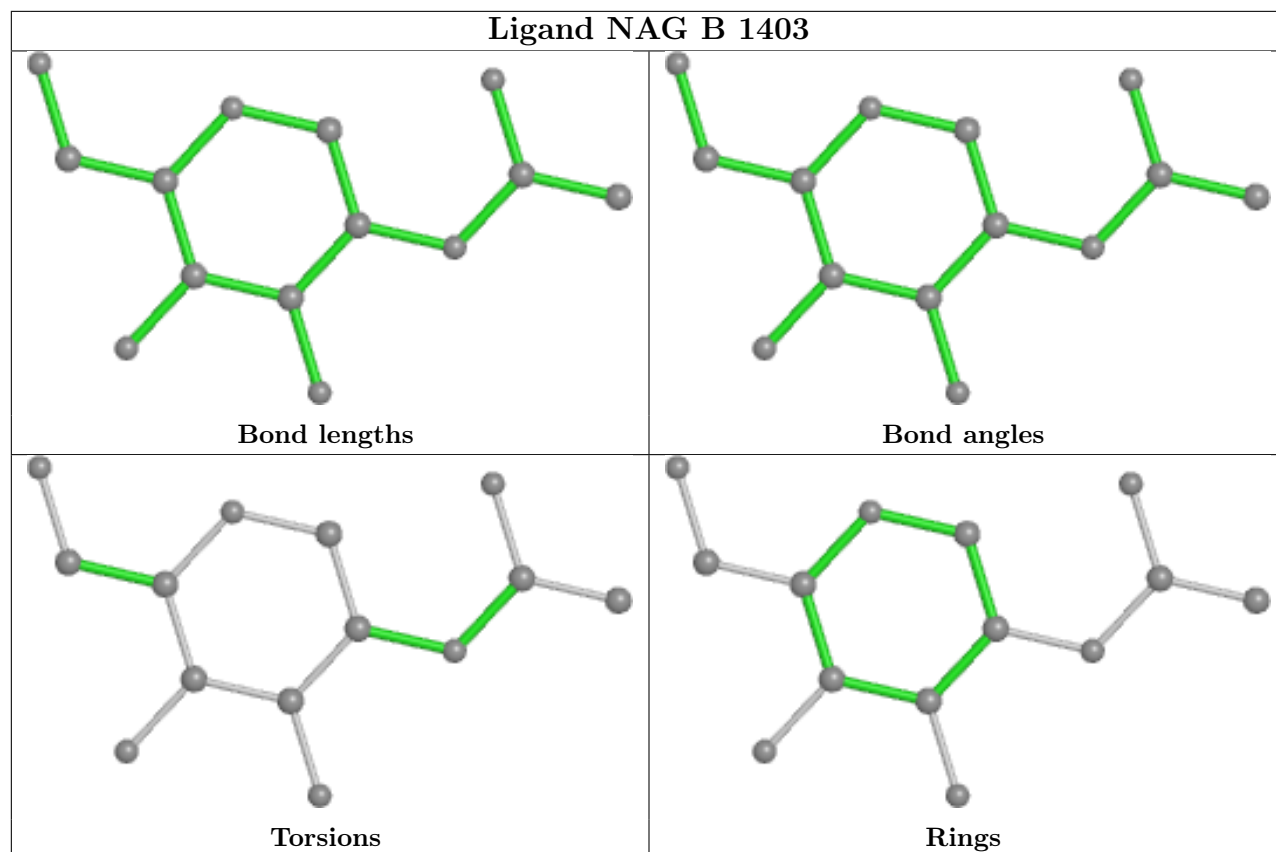


Ligand NAG A 1403

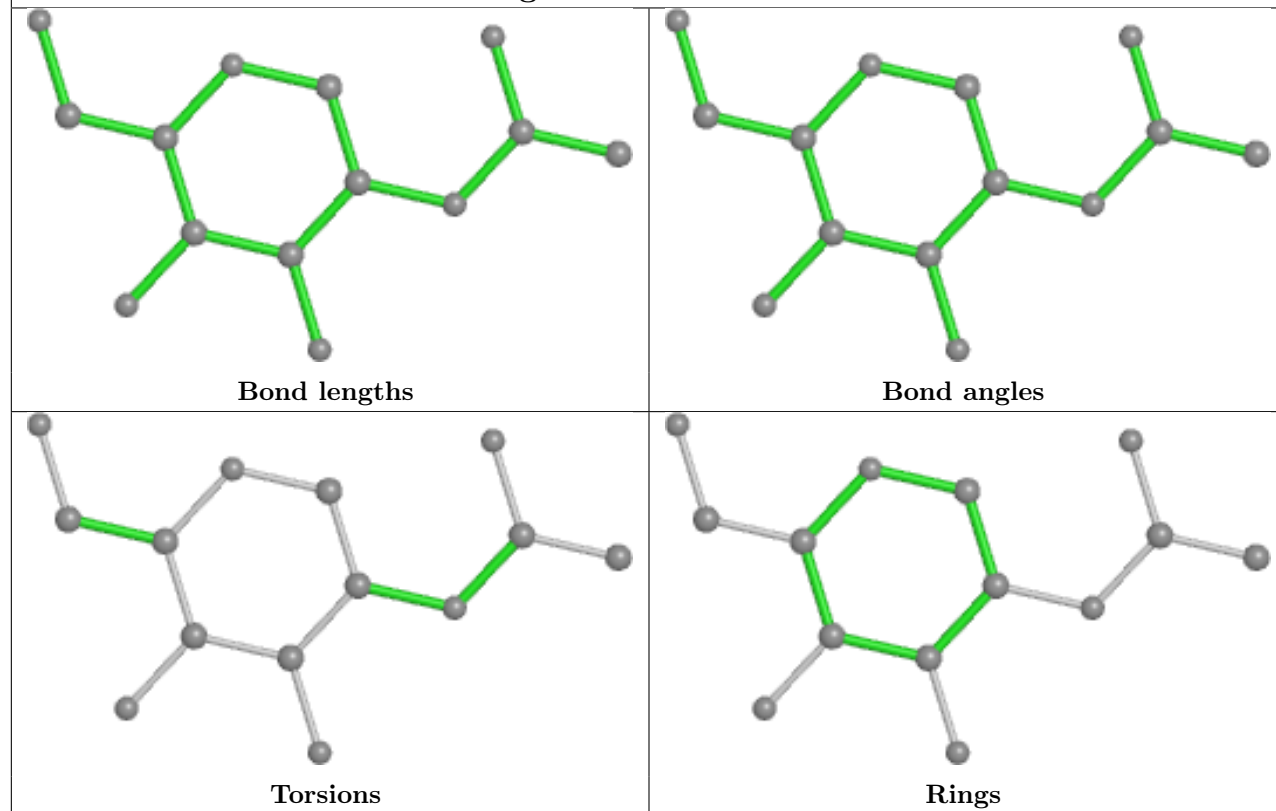


Ligand NAG B 1401

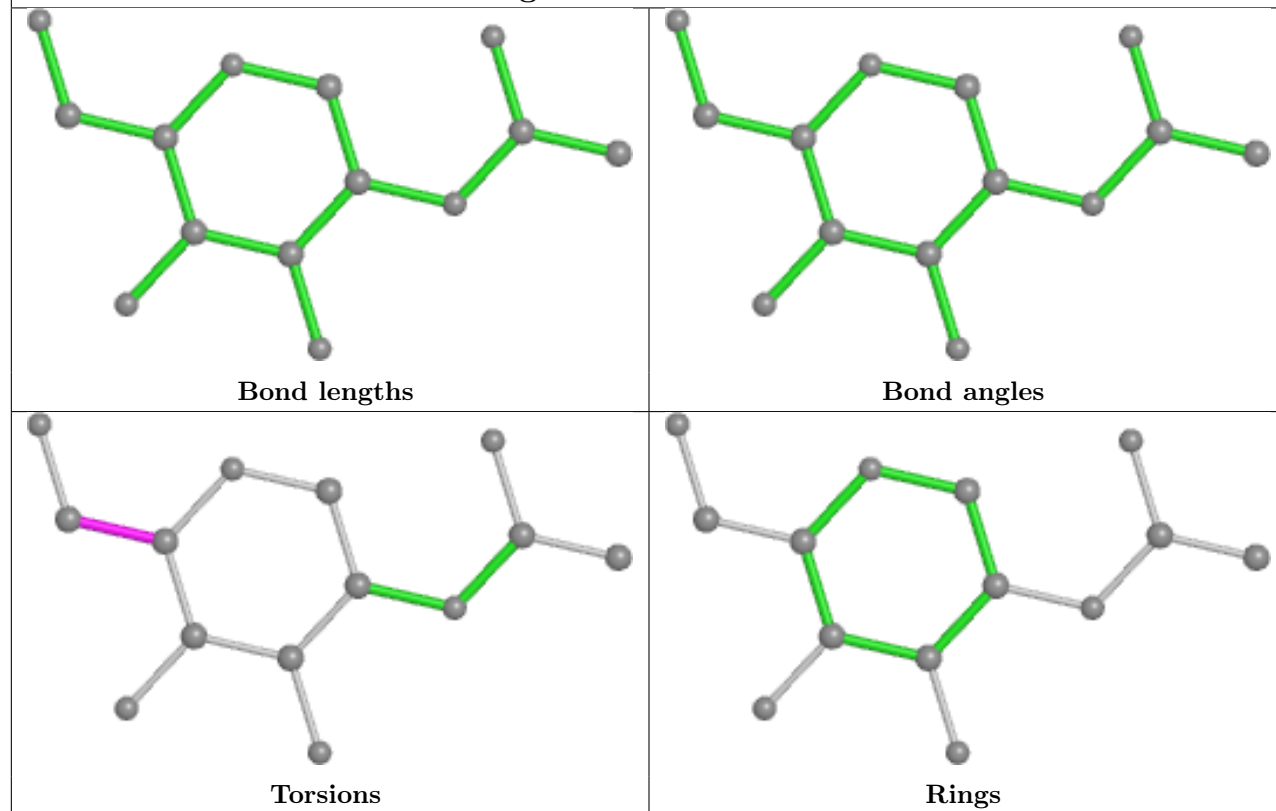




Ligand NAG C 1409



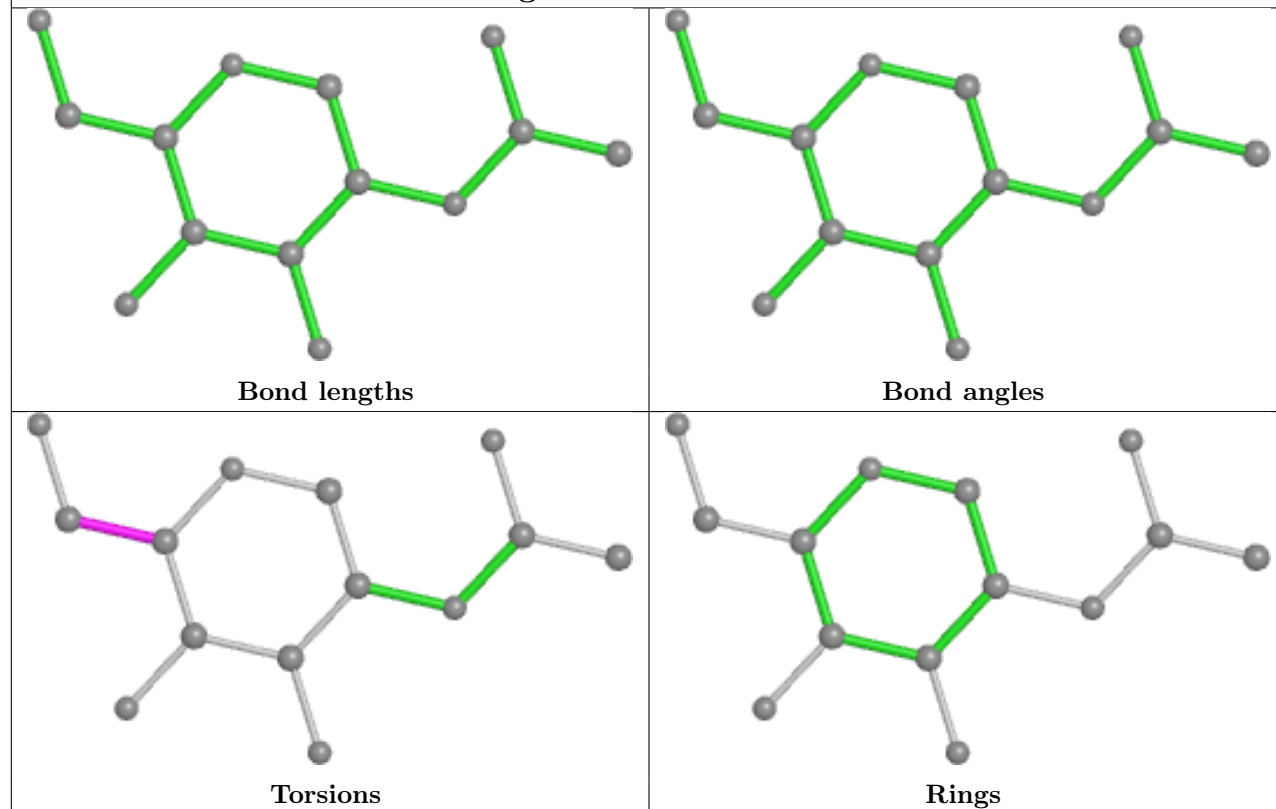
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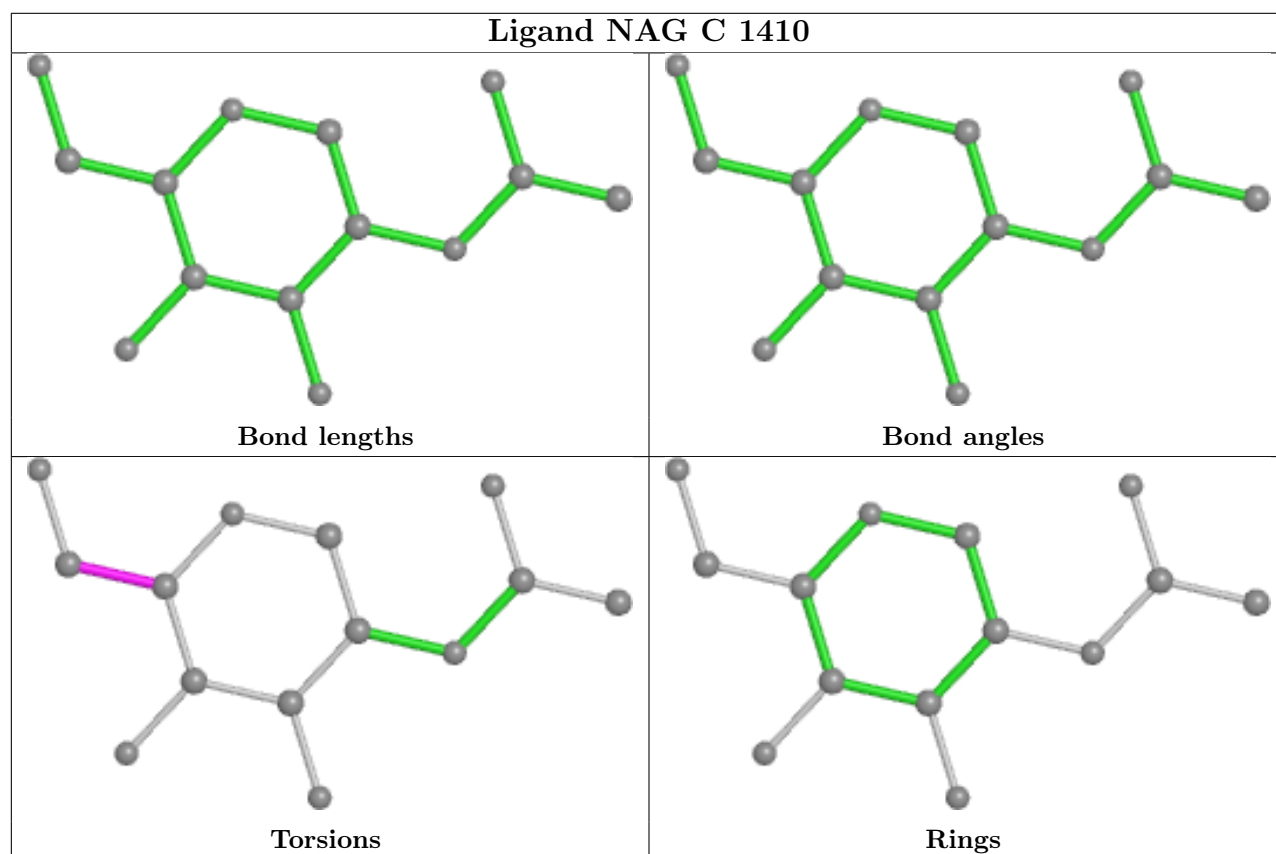
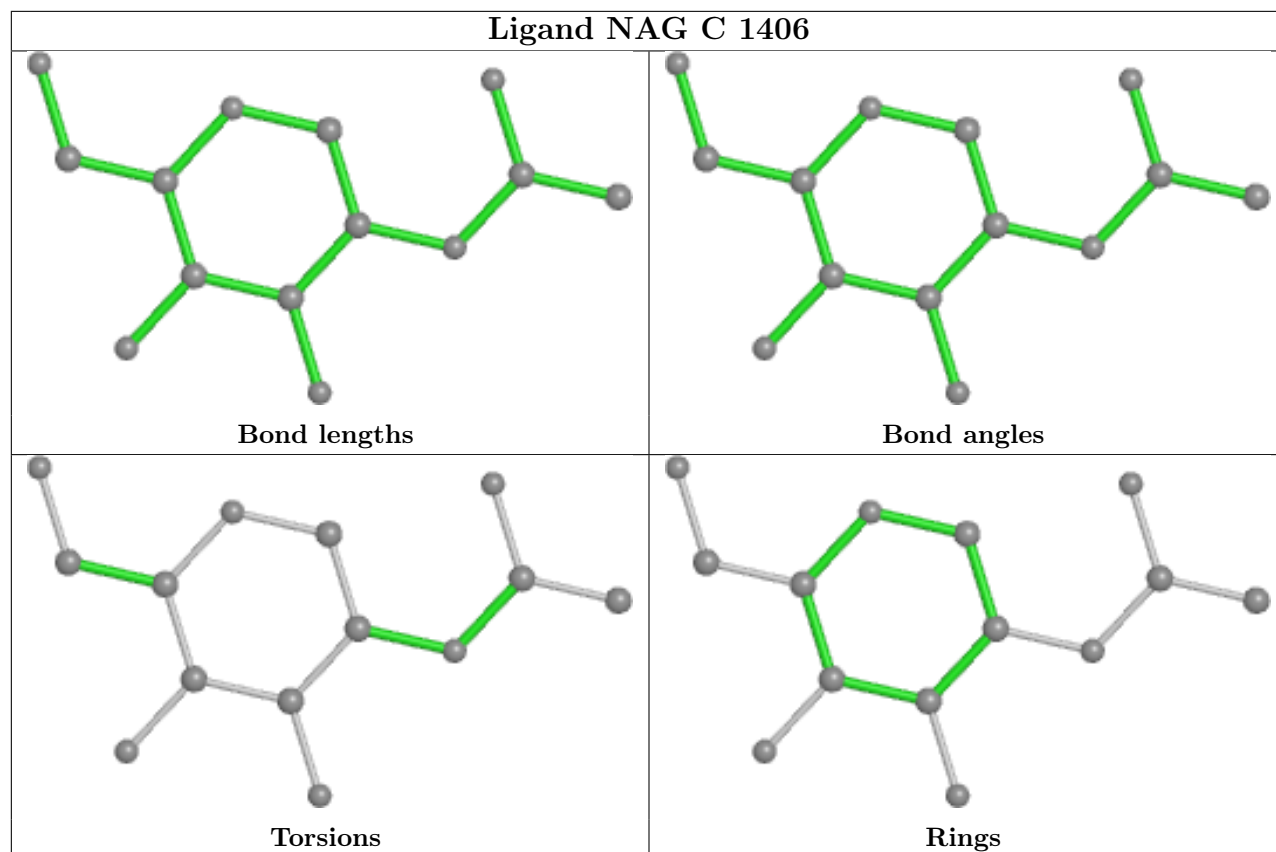


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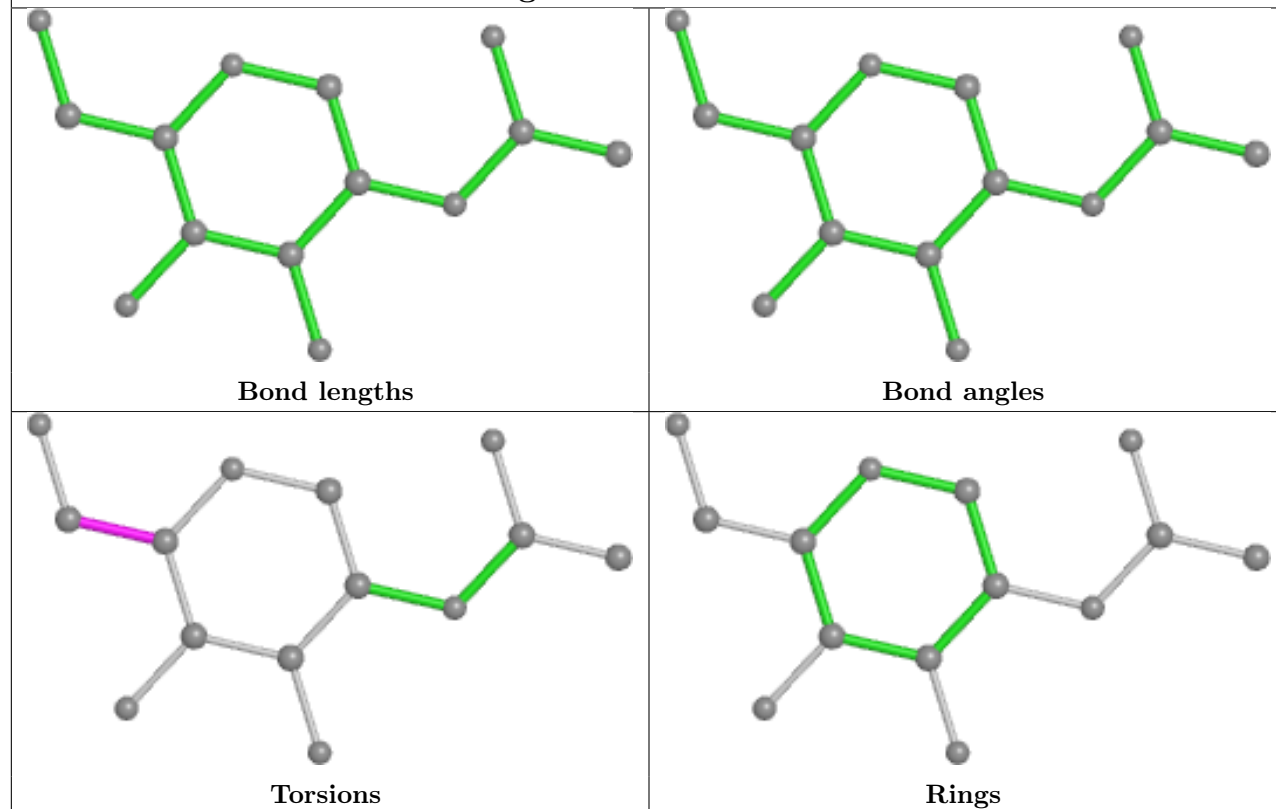


Ligand NAG A 1411

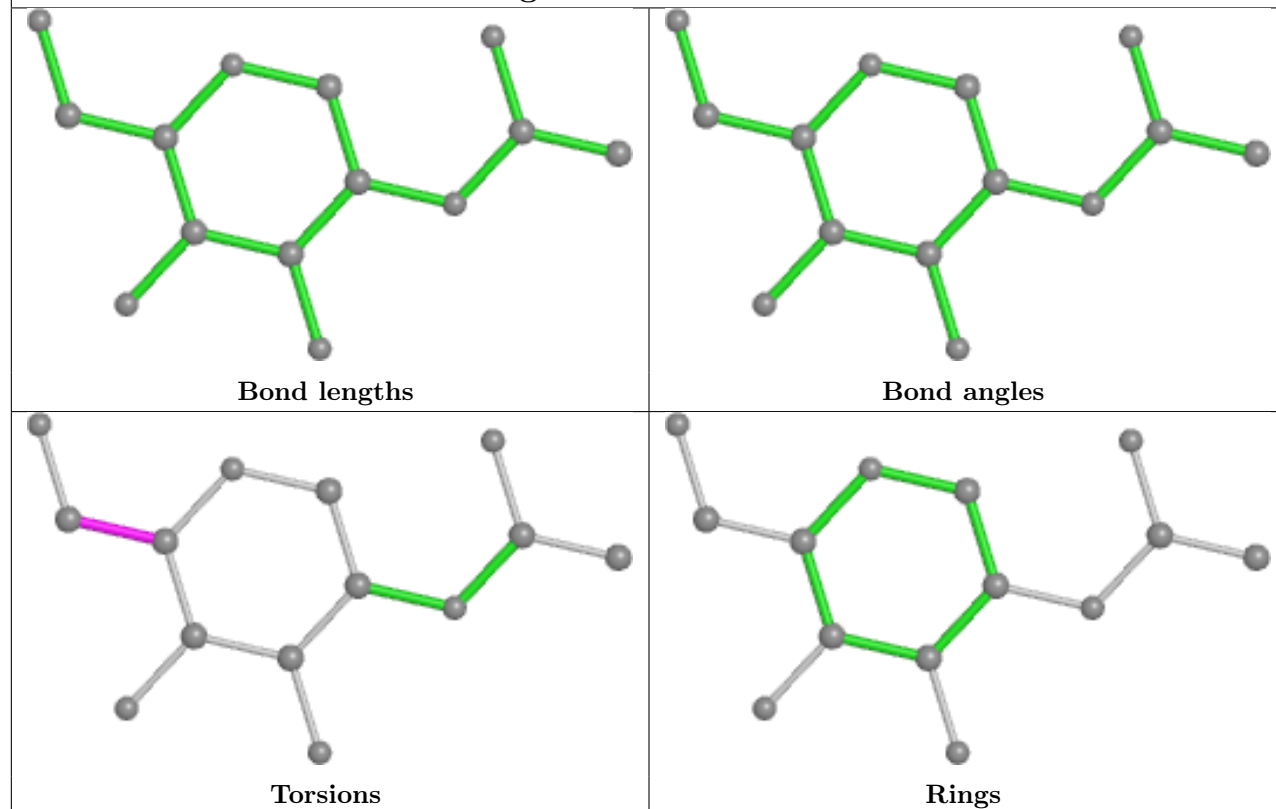




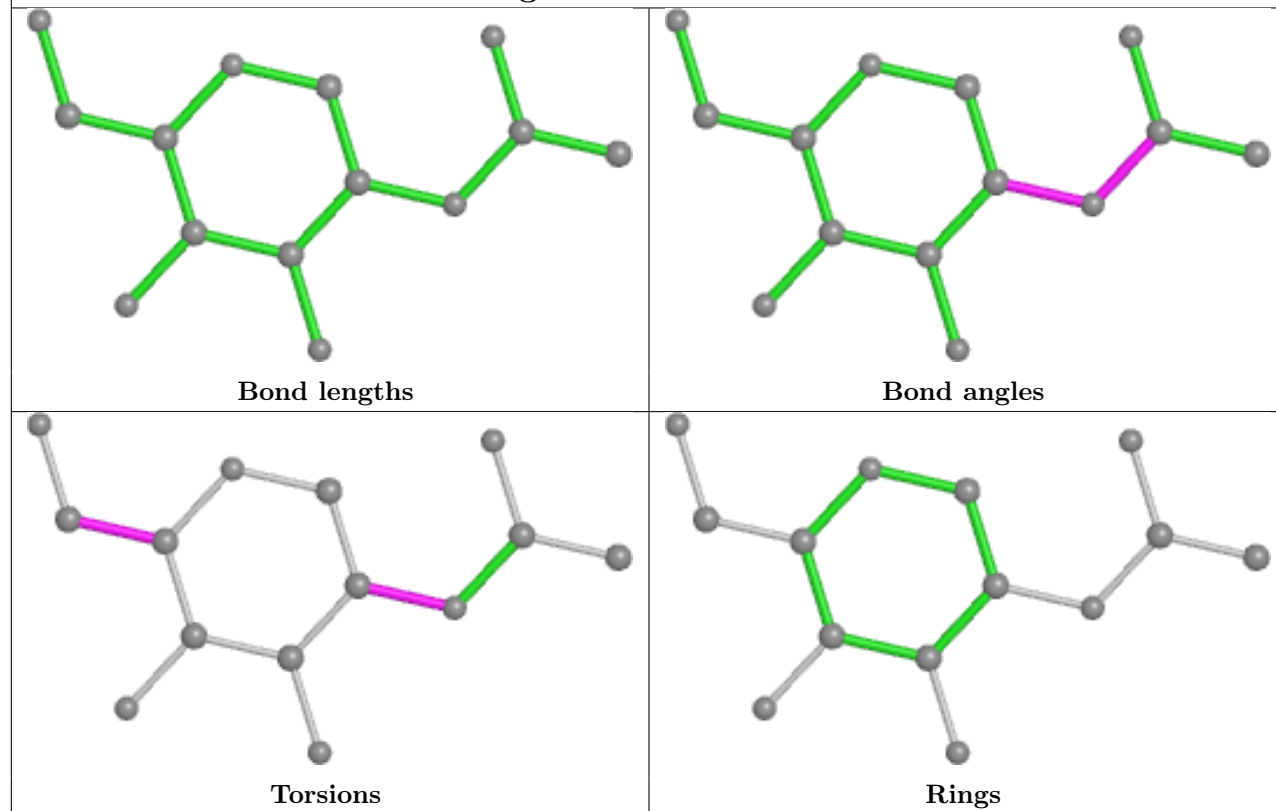
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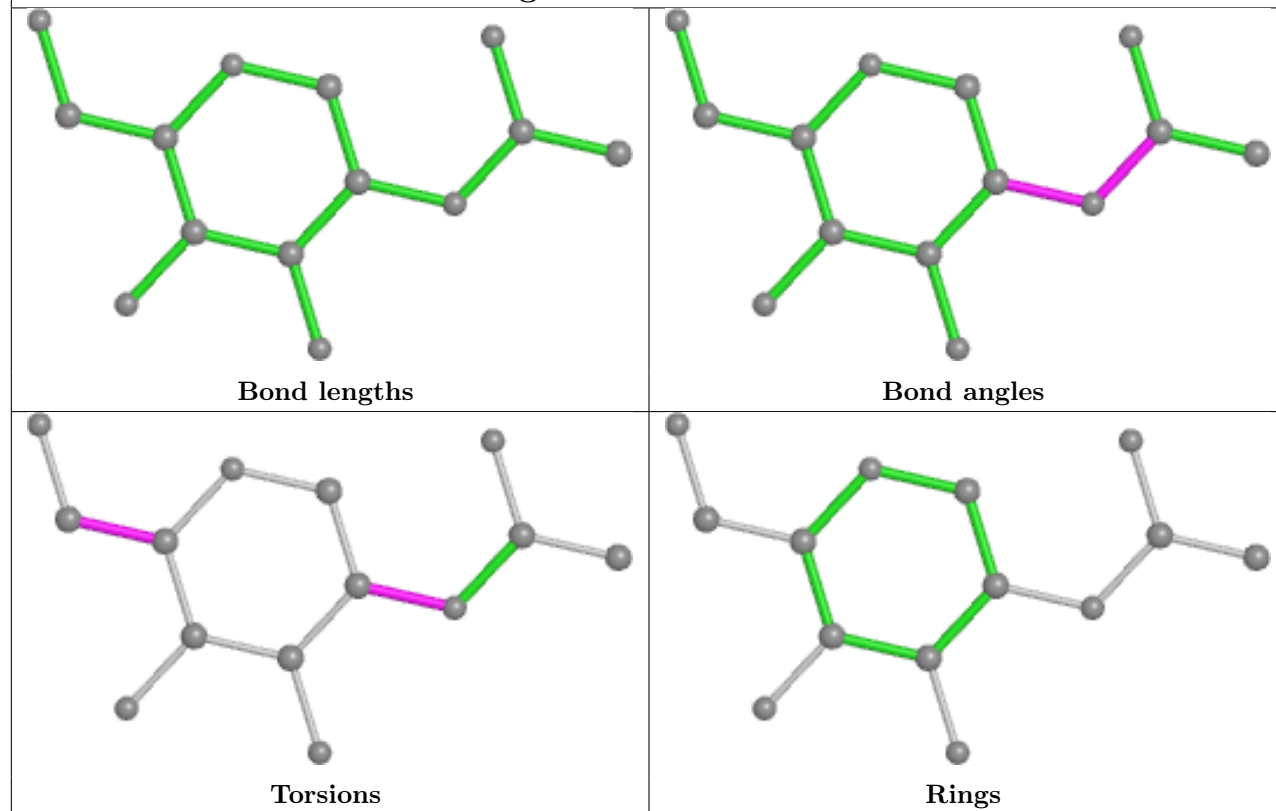
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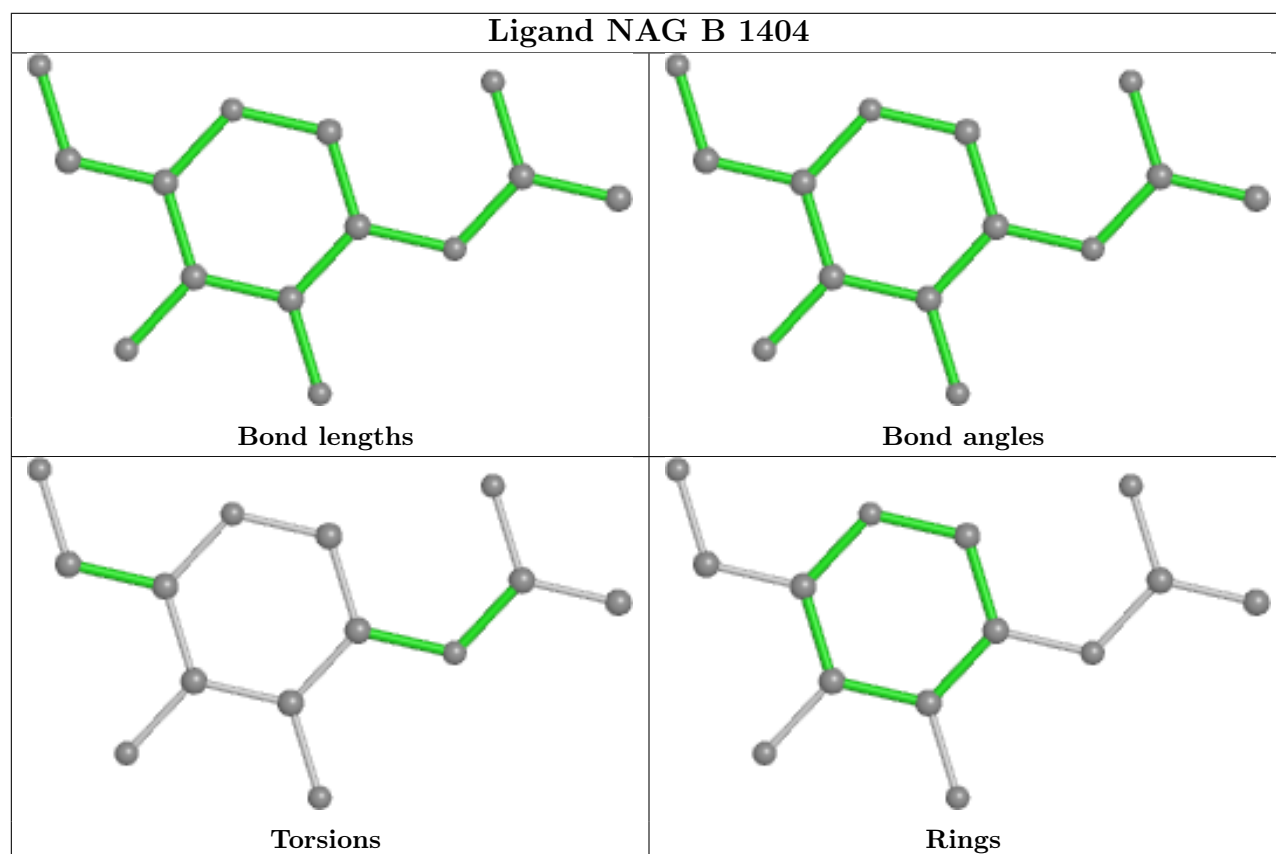
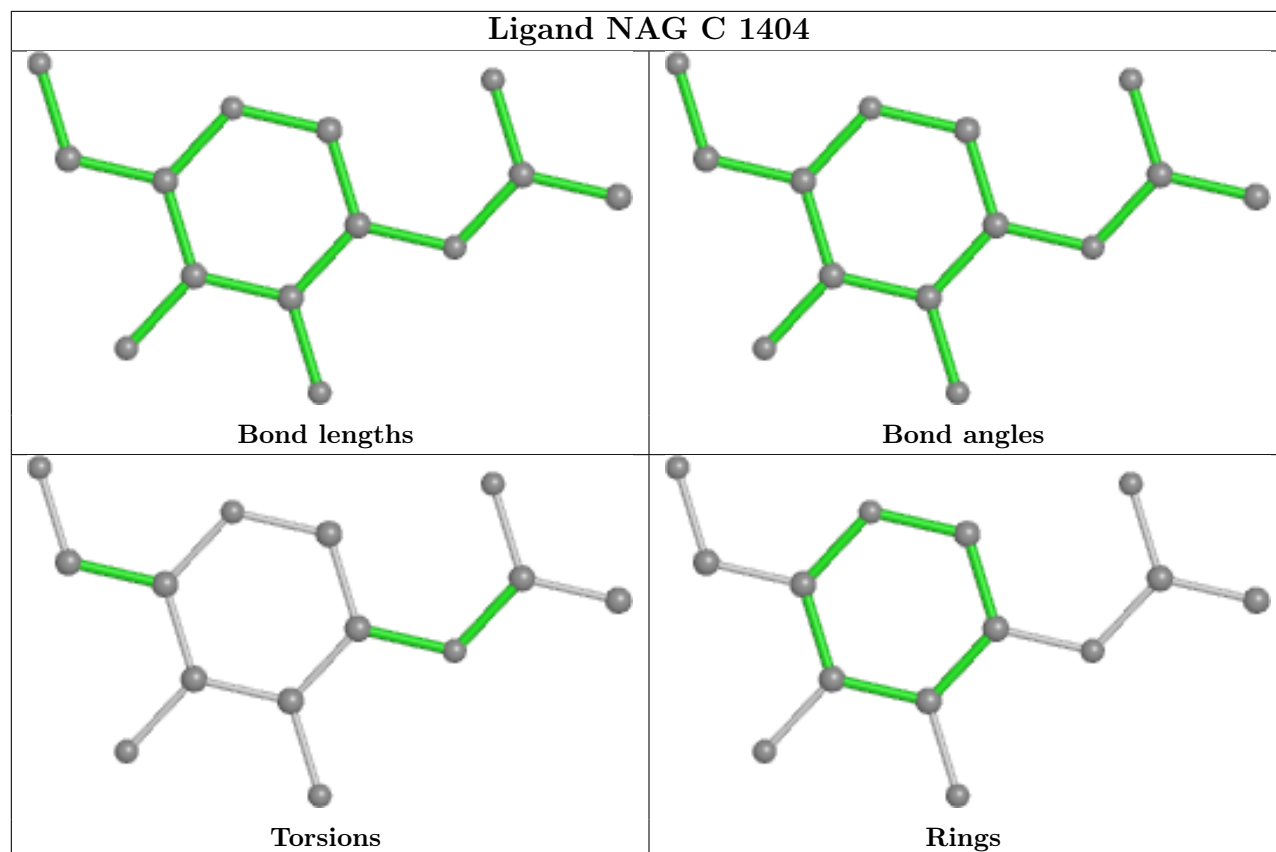


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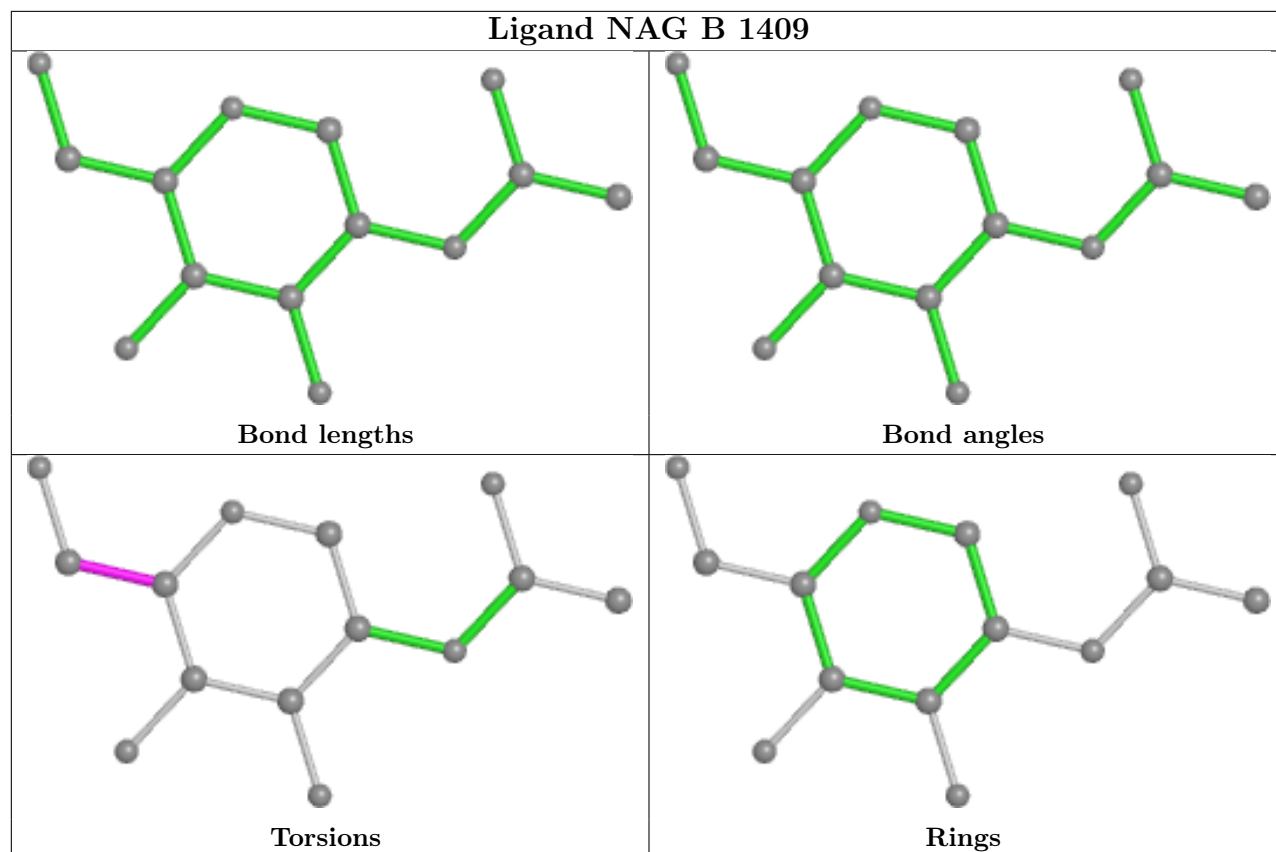


Ligand NAG C 1401

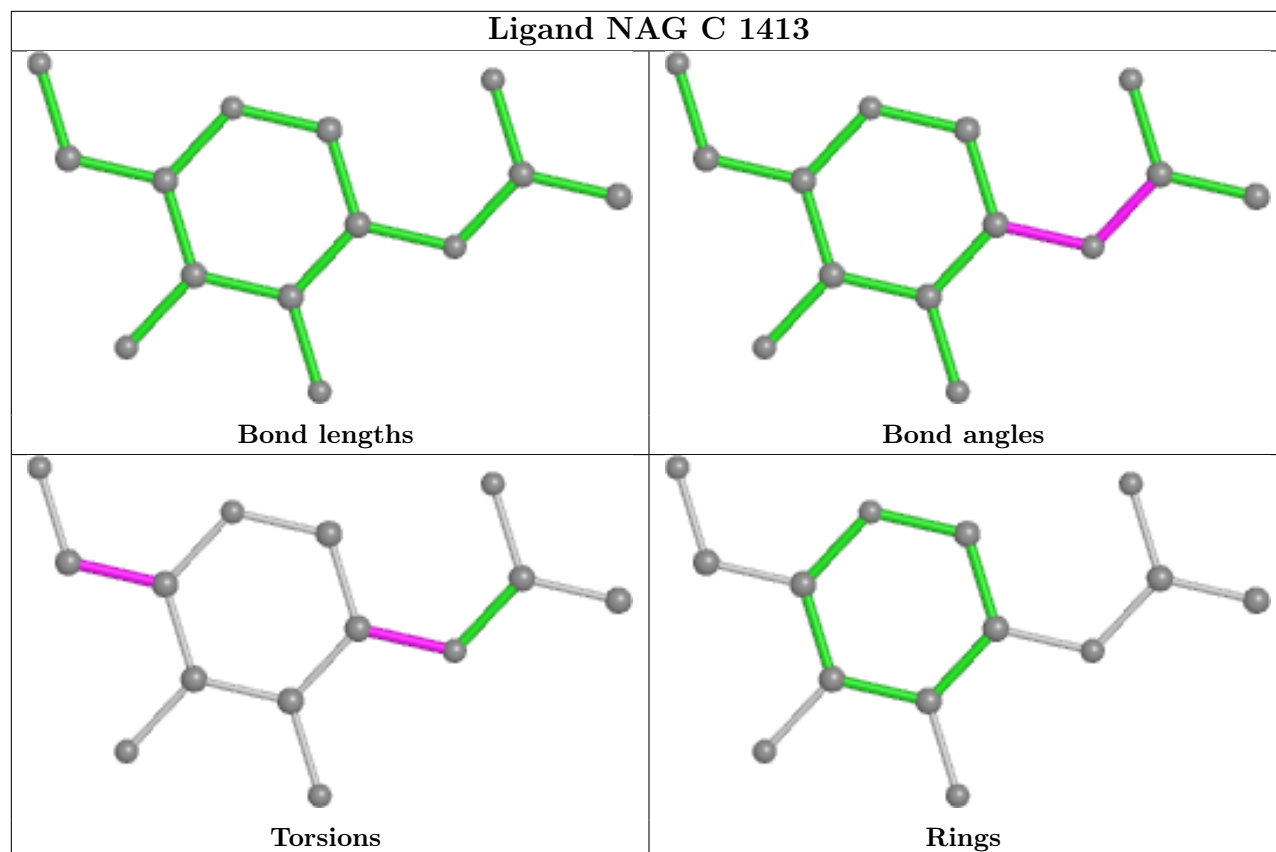




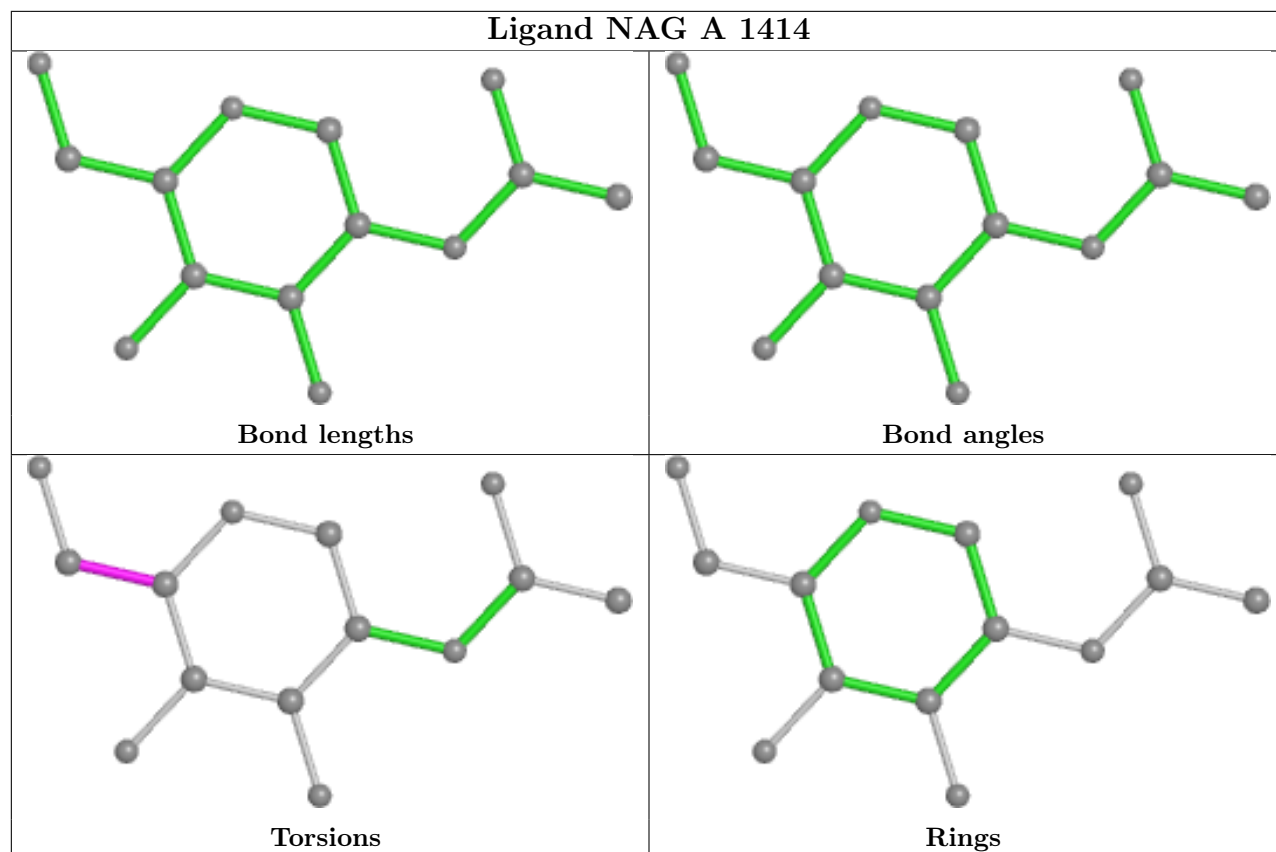
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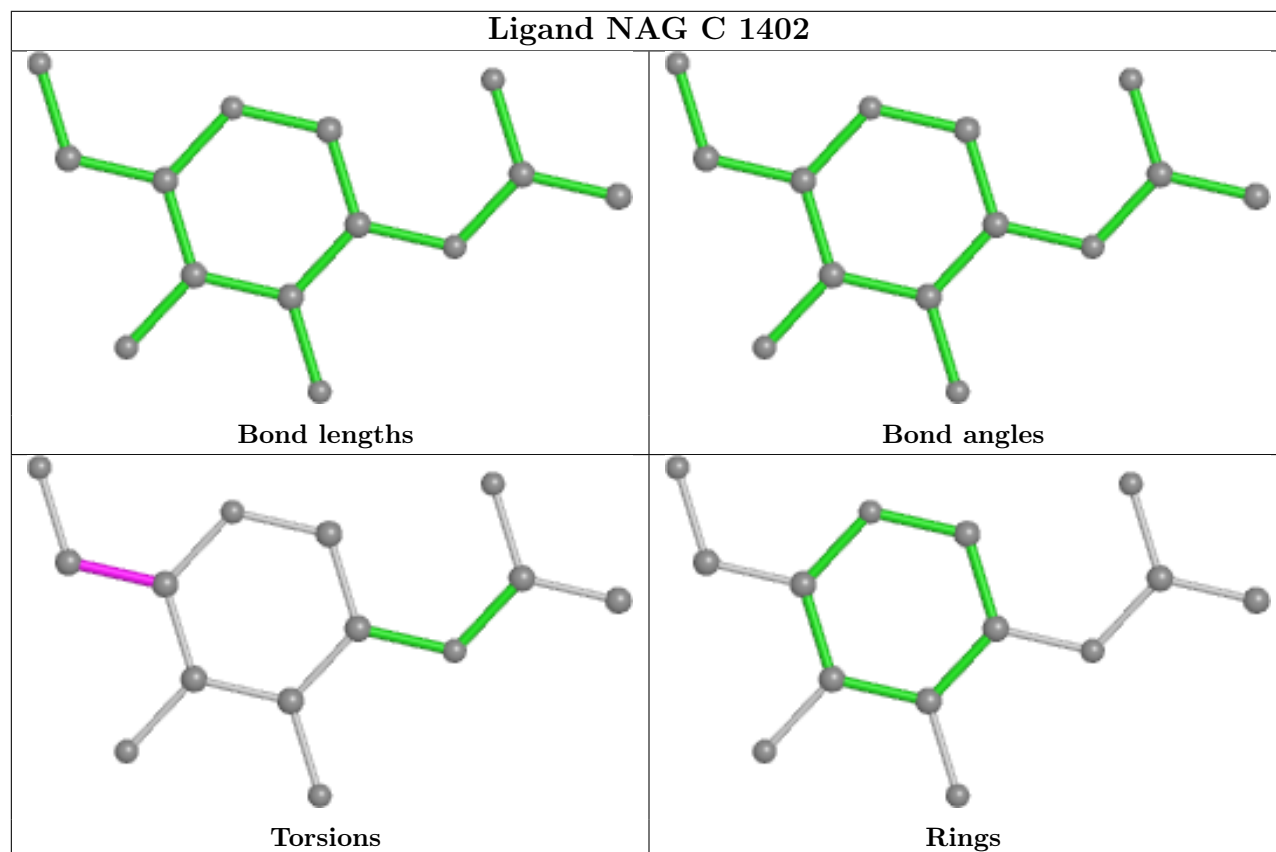
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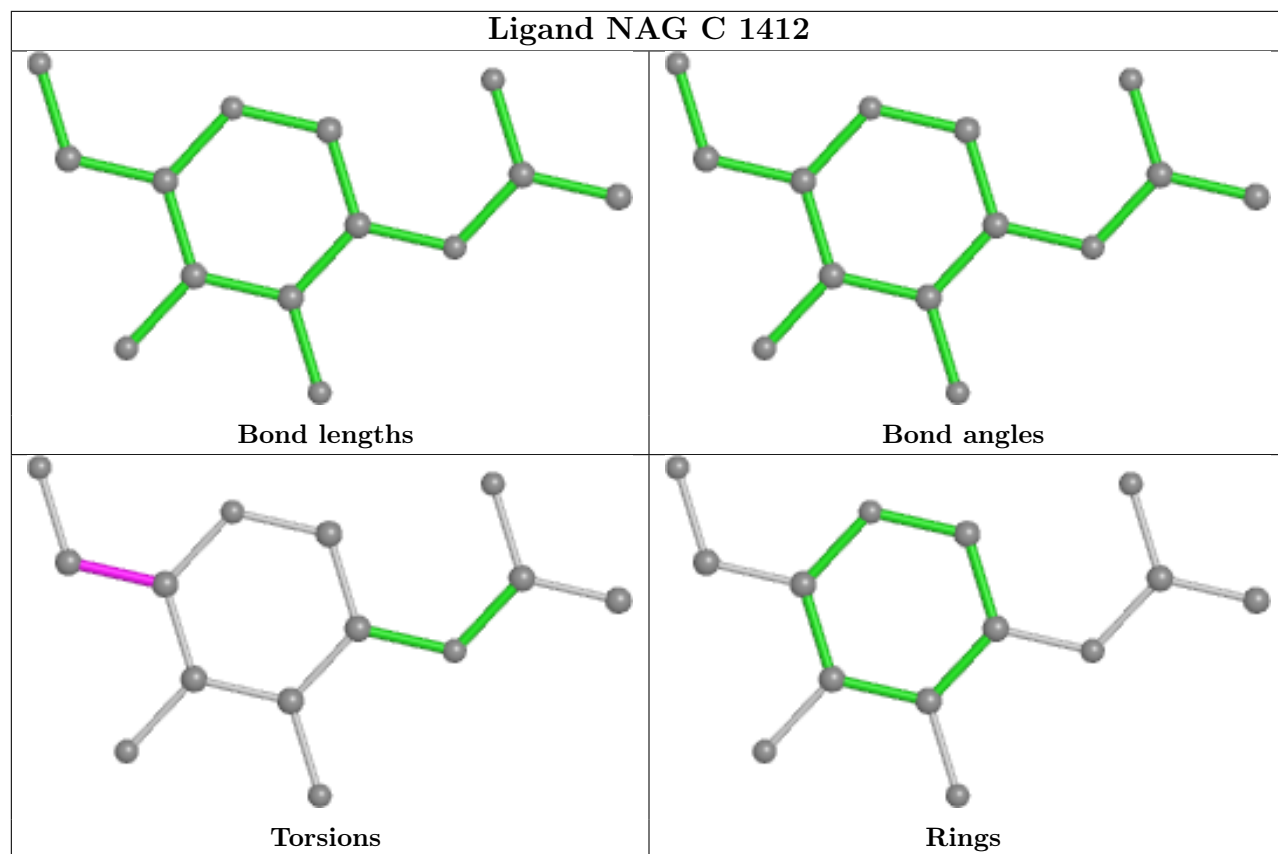
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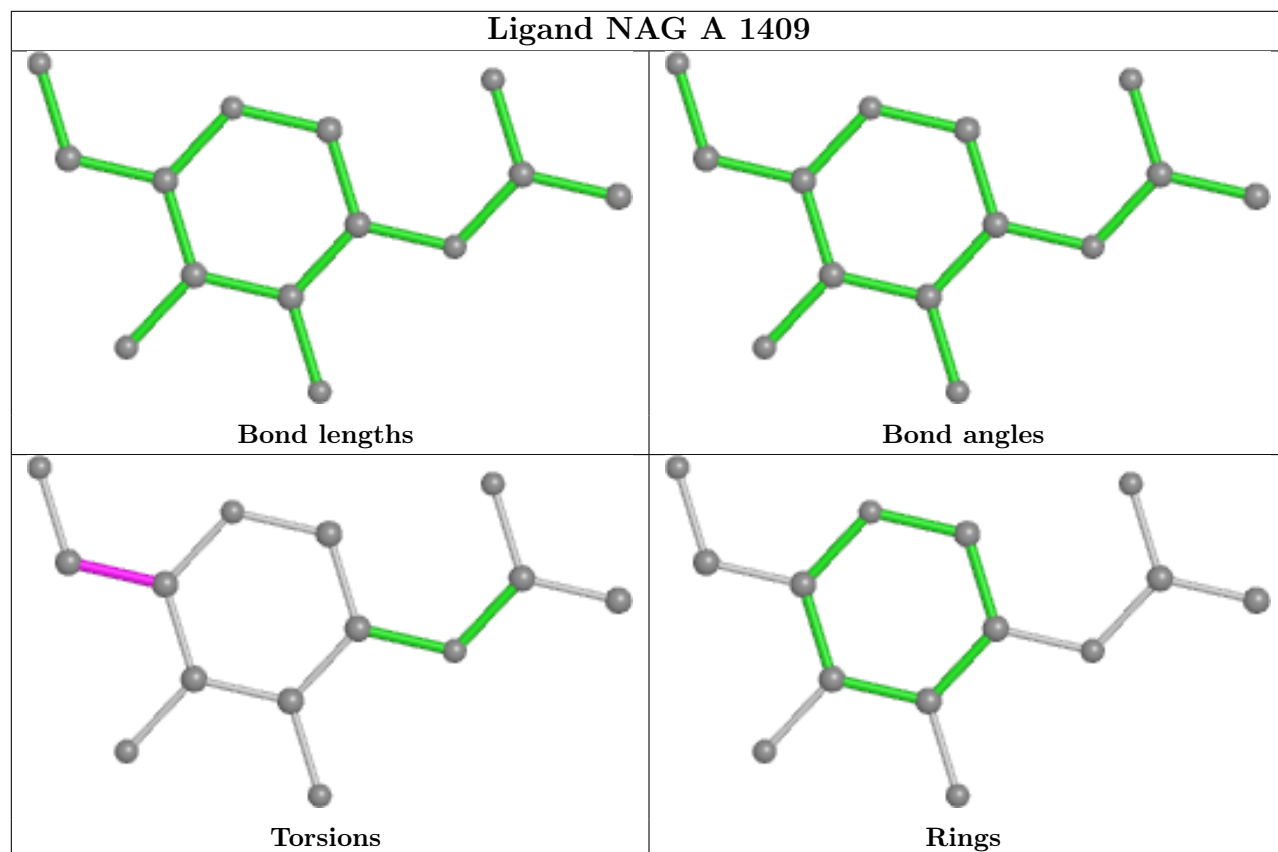
Ligand NAG C 1402



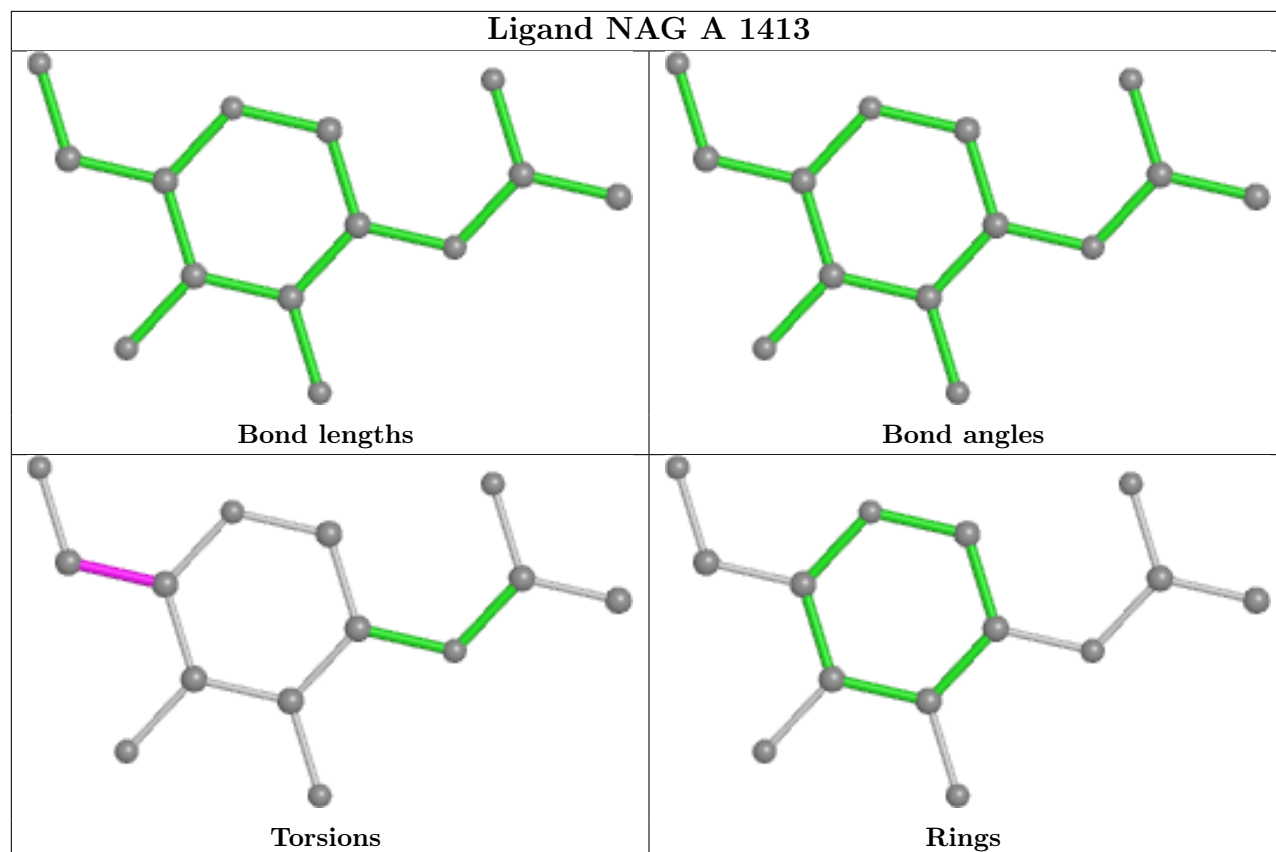
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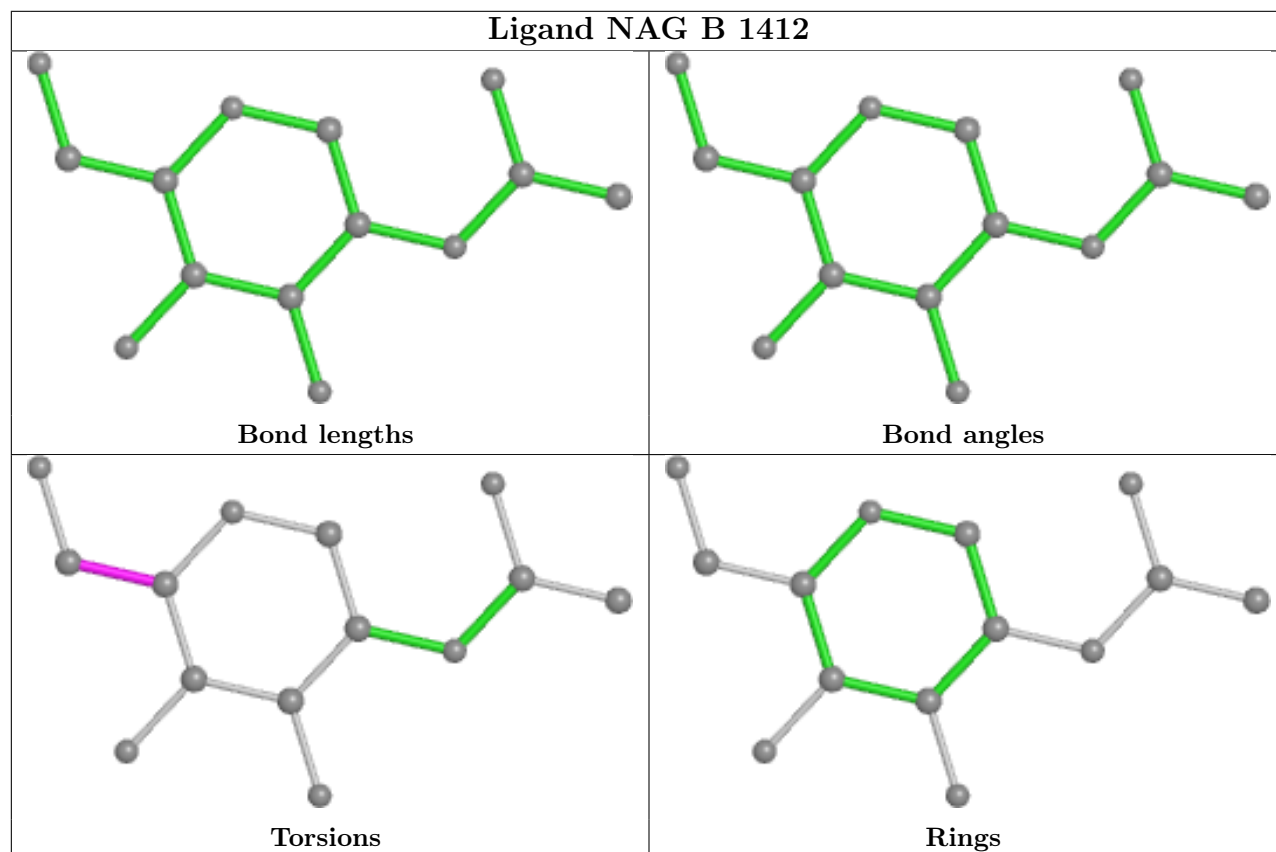
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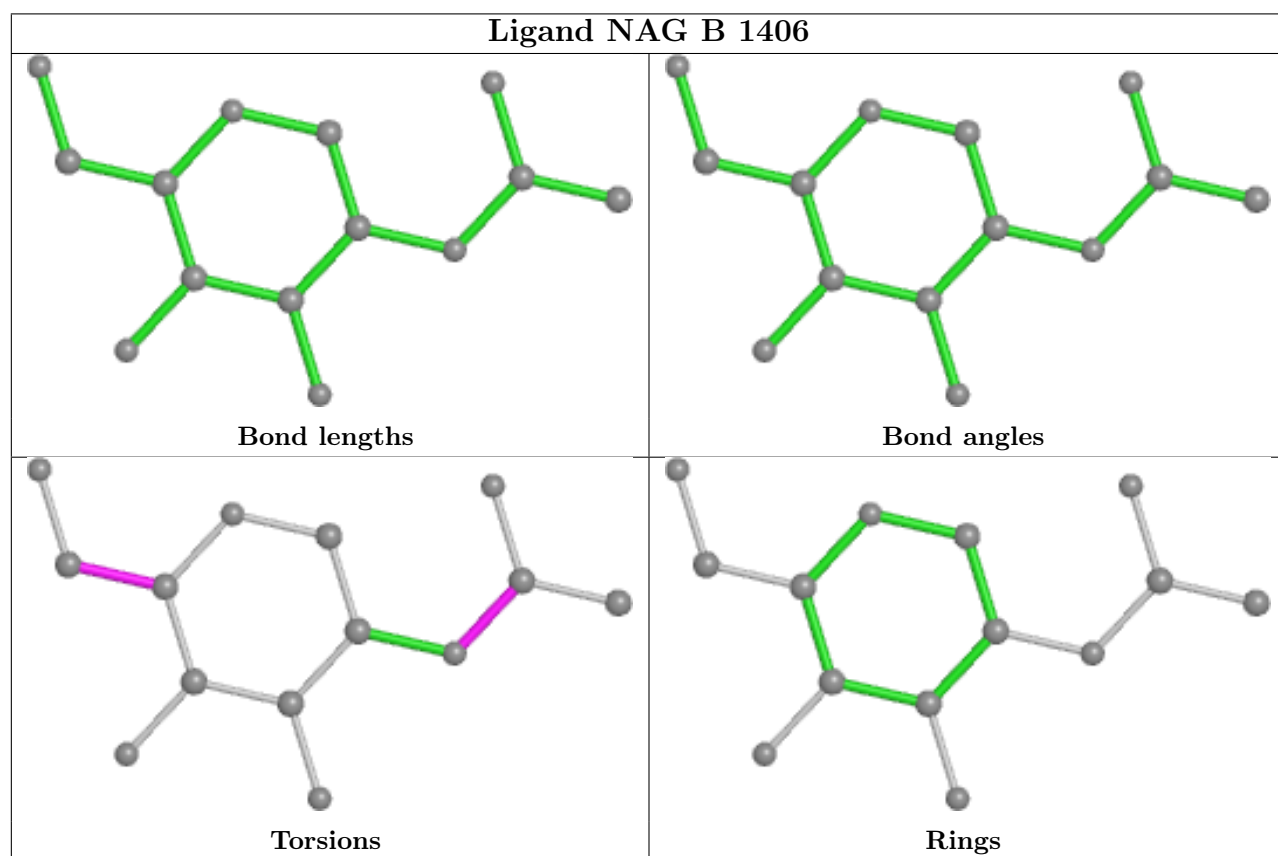
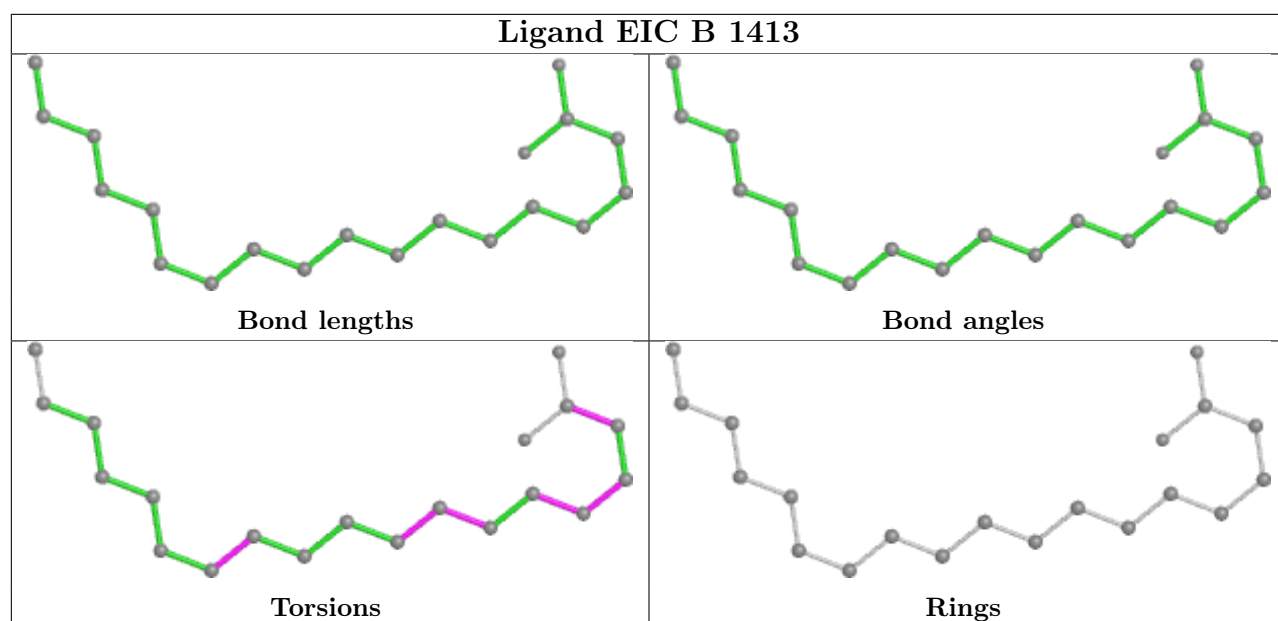


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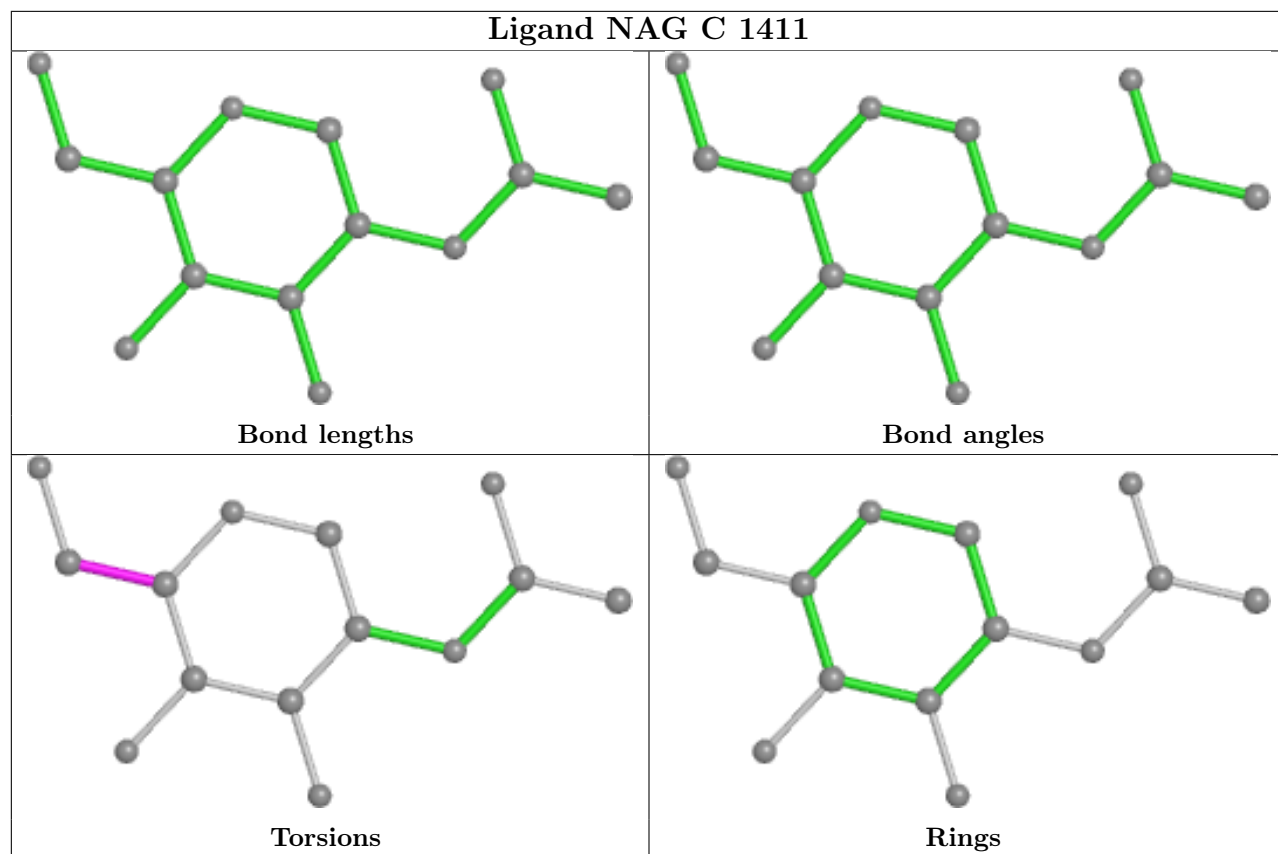


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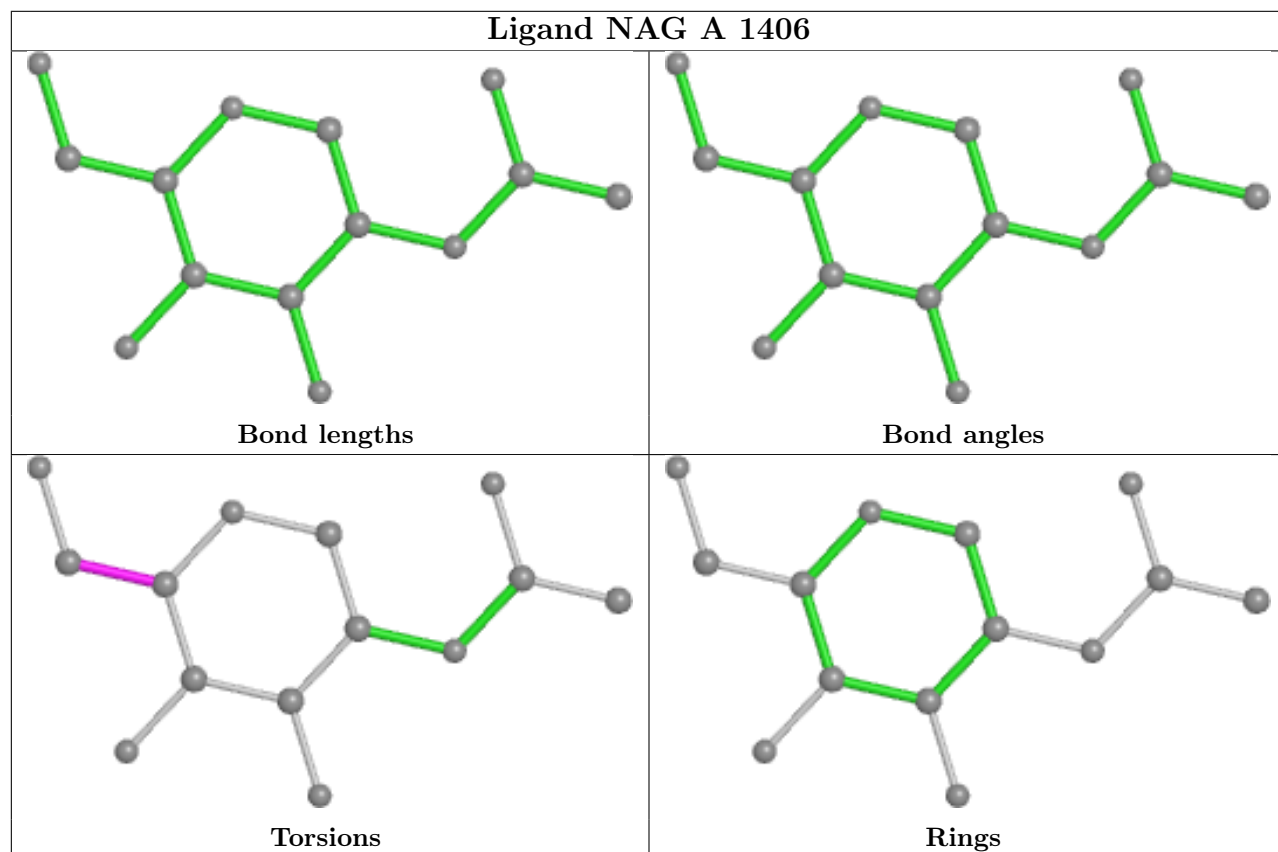




Ligand NAG C 1411



Ligand NAG A 1406



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.