



## Full wwPDB EM Validation Report ⓘ

May 27, 2024 – 08:23 PM JST

PDB ID : 8HLC  
EMDB ID : EMD-34872  
Title : S protein of SARS-CoV-2 in complex with 3711  
Authors : Zhang, Y.Y.; Guo, Y.Y.; Zhou, Q.  
Deposited on : 2022-11-29  
Resolution : 2.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

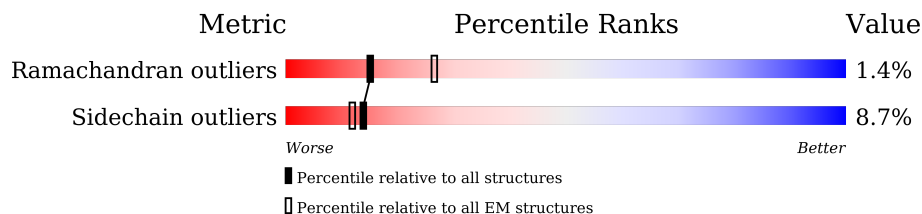
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1283	76% 8% 16%
1	B	1283	76% 7% 16%
1	C	1283	77% 7% 16%
2	H	267	65% 79% 6% 15%
2	I	267	73% 79% 6% 15%
2	J	267	81% 79% 6% 15%
3	L	257	57% 79% 6% 17%
3	M	257	64% 79% 6% 17%
3	N	257	76% 79% 6% 17%


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Mol	Chain	Length	Quality of chain
4	D	2	50% 100%
4	F	2	50% 100%
4	G	2	50% 100%
4	K	2	50% 50%
4	O	2	50% 100%
4	P	2	50% 100%
4	Q	2	100%
4	R	2	50% 100%
4	S	2	50% 50%
4	T	2	50% 100%
4	V	2	50% 100%
4	W	2	50% 100%
4	X	2	50% 50%
4	Y	2	50% 100%
4	Z	2	100%
4	a	2	50% 50%
4	b	2	50% 100%
4	d	2	100% 50%
4	e	2	50% 100%
4	f	2	50% 50%
4	g	2	50% 100%
4	h	2	100%
4	i	2	50% 50%
5	E	3	67% 33%
5	U	3	67% 33%

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Mol	Chain	Length	Quality of chain
5	c	3	 67% 33%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 36780 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1081	8451	5395	1409	1607	40	0	0
1	B	1081	8451	5395	1409	1607	40	0	0
1	C	1081	8451	5395	1409	1607	40	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called heavy chain of 3711.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	228	Total	C	N	O	S	0	0
			1708	1077	288	336	7		
2	I	228	Total	C	N	O	S	0	0
			1708	1077	288	336	7		
2	J	228	Total	C	N	O	S	0	0
			1708	1077	288	336	7		

- Molecule 3 is a protein called light chain of 3711.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	214	Total	C	N	O	S	0	0
			1647	1034	277	329	7		
3	M	214	Total	C	N	O	S	0	0
			1647	1034	277	329	7		
3	N	214	Total	C	N	O	S	0	0
			1647	1034	277	329	7		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		

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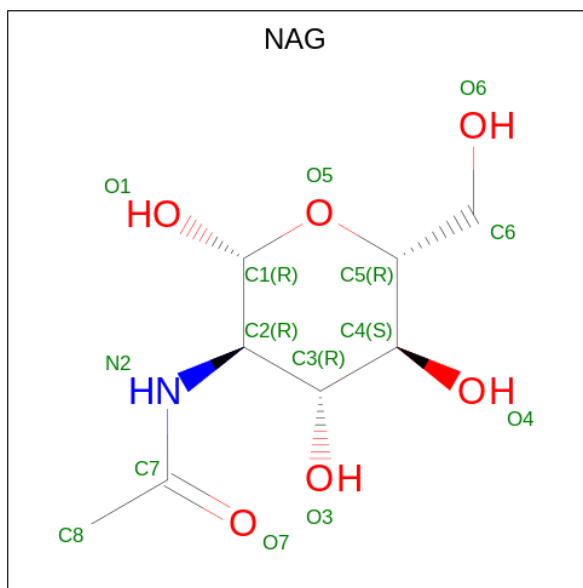
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	i	2	28	16	2	10	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	3	42	24	3	15	0	0
5	U	3	42	24	3	15	0	0
5	c	3	42	24	3	15	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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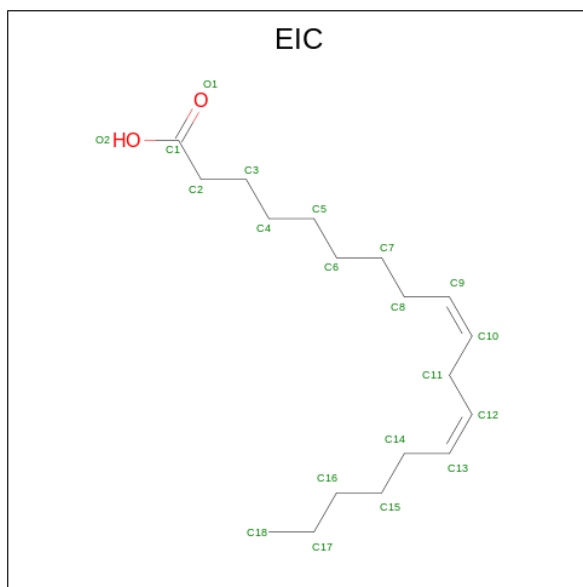
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	A	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8	1	5	0
6	B	1	14	8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

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

- Molecule 7 is LINOLEIC ACID (three-letter code: EIC) (formula:  $C_{18}H_{32}O_2$ ) (labeled as "Ligand of Interest" by depositor).

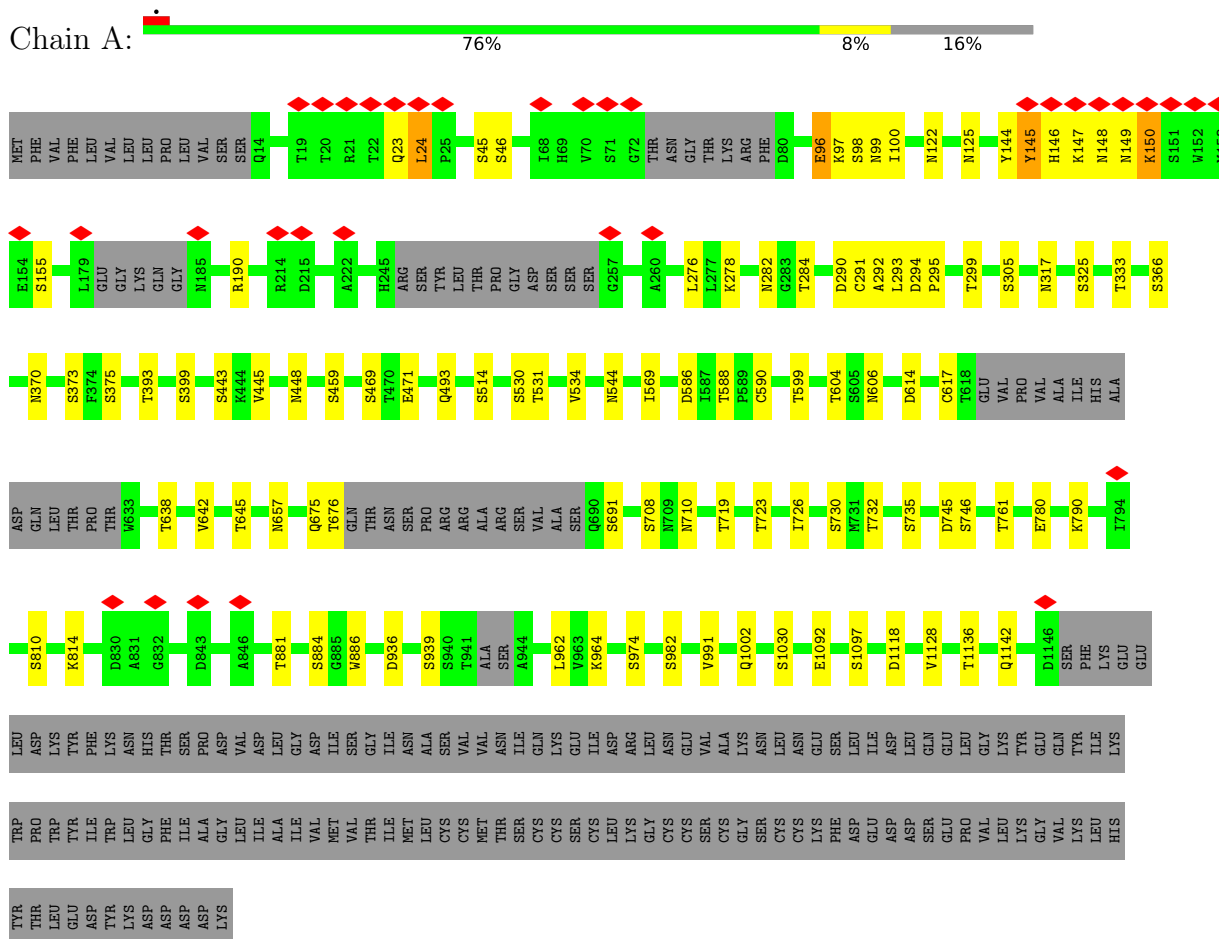


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			20	18	2	
7	B	1	Total	C	O	0
			20	18	2	
7	C	1	Total	C	O	0
			20	18	2	

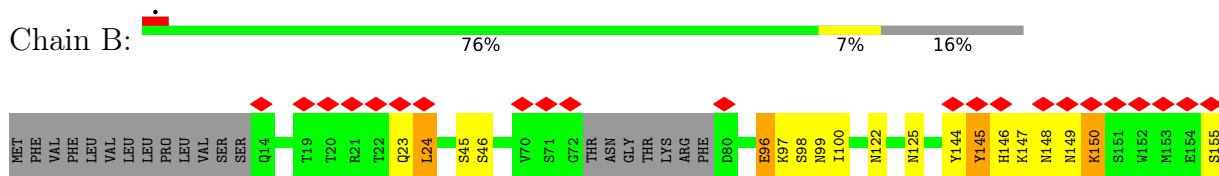
### 3 Residue-property plots

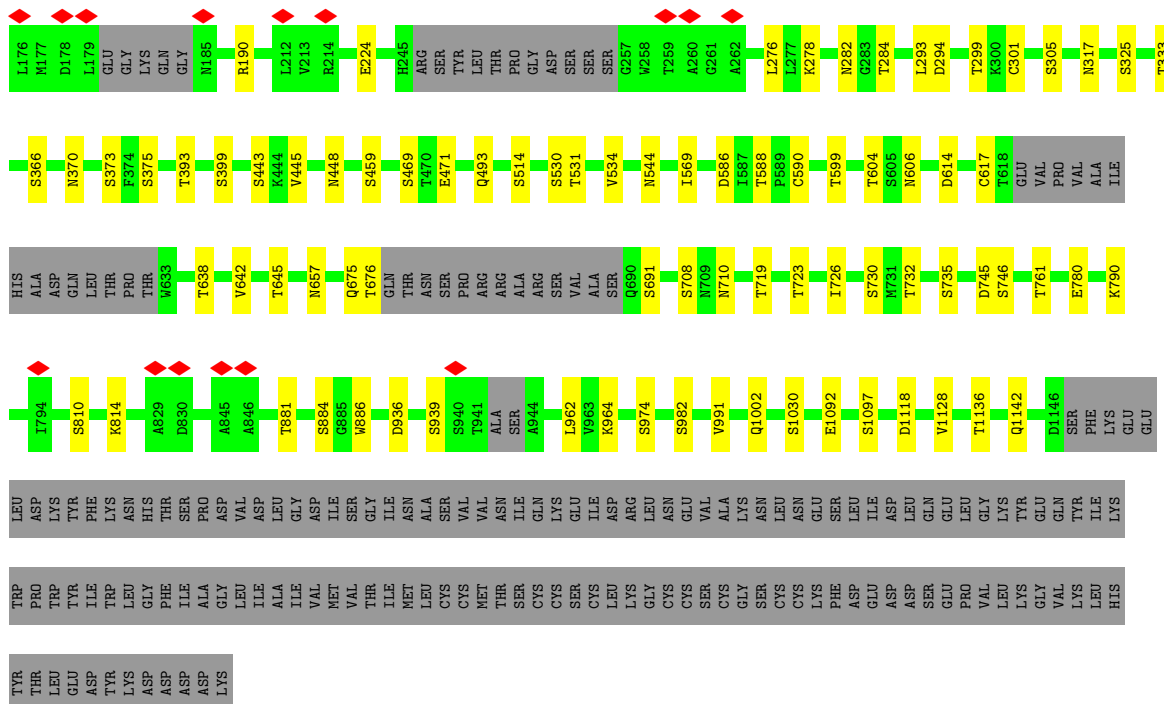
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Spike glycoprotein

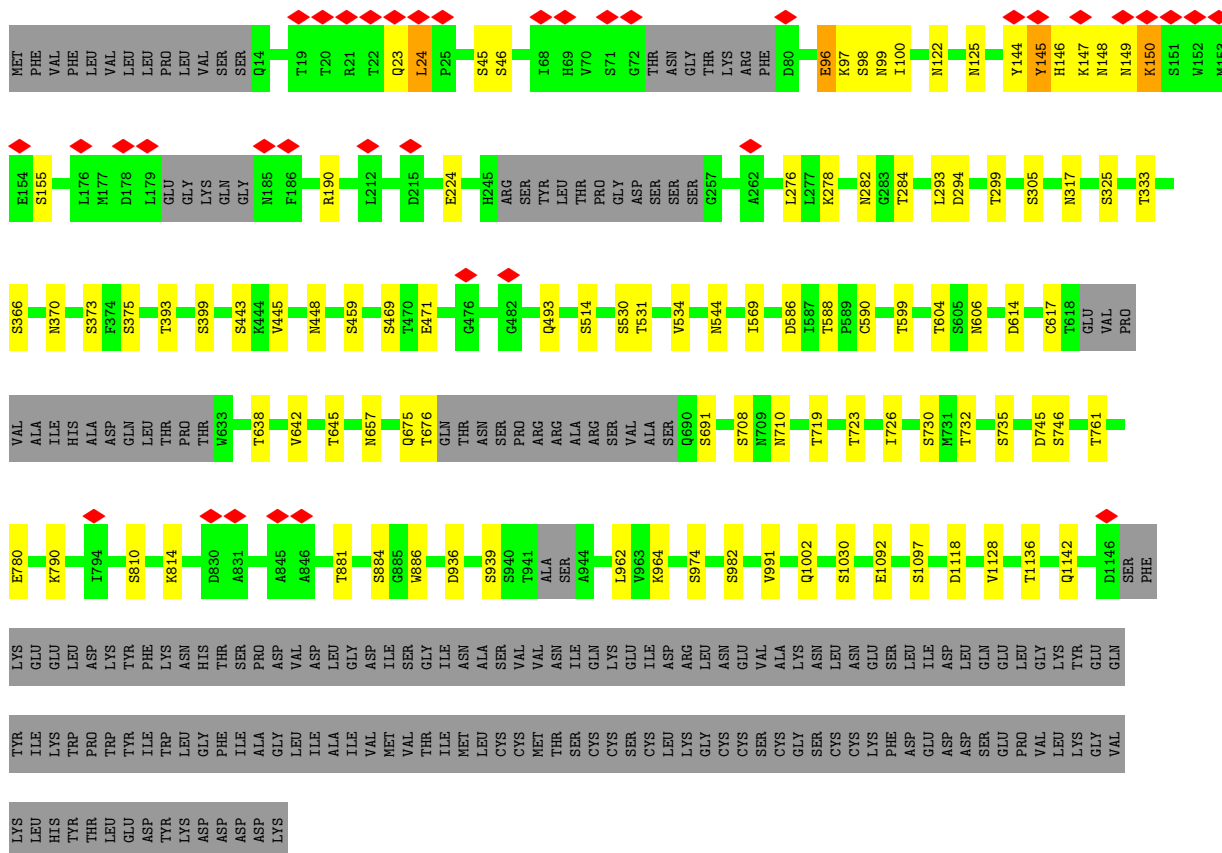
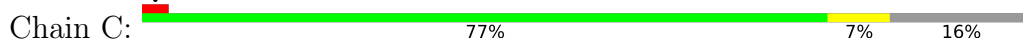


- Molecule 1: Spike glycoprotein

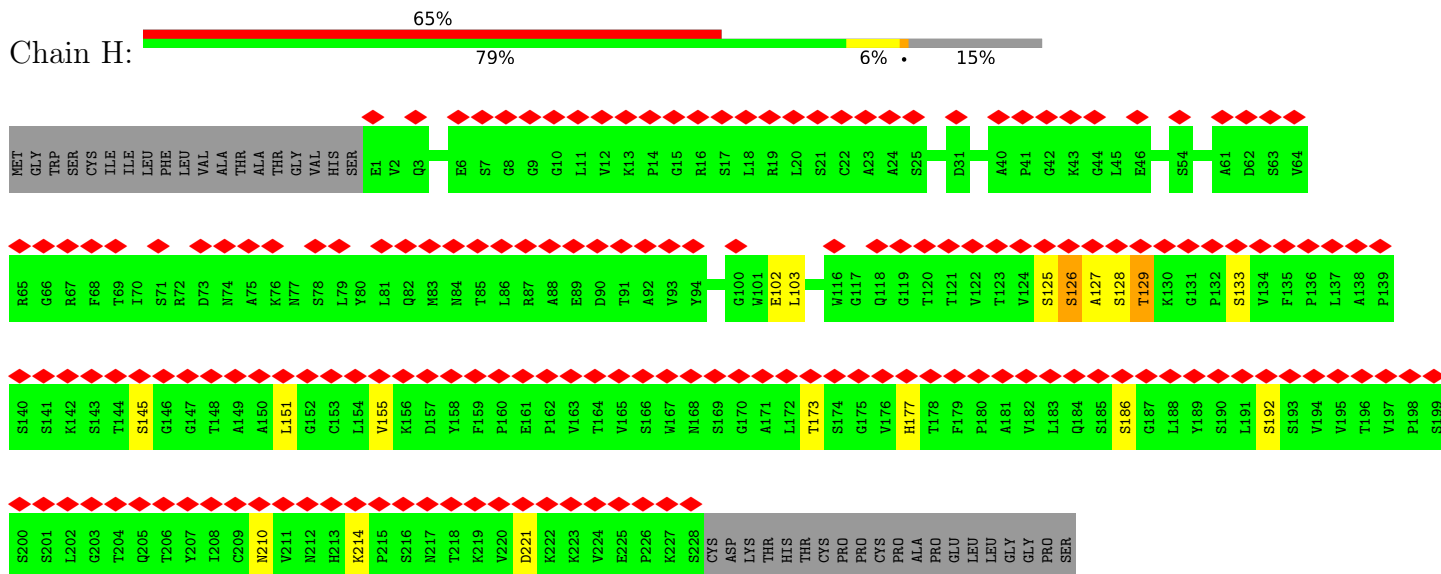




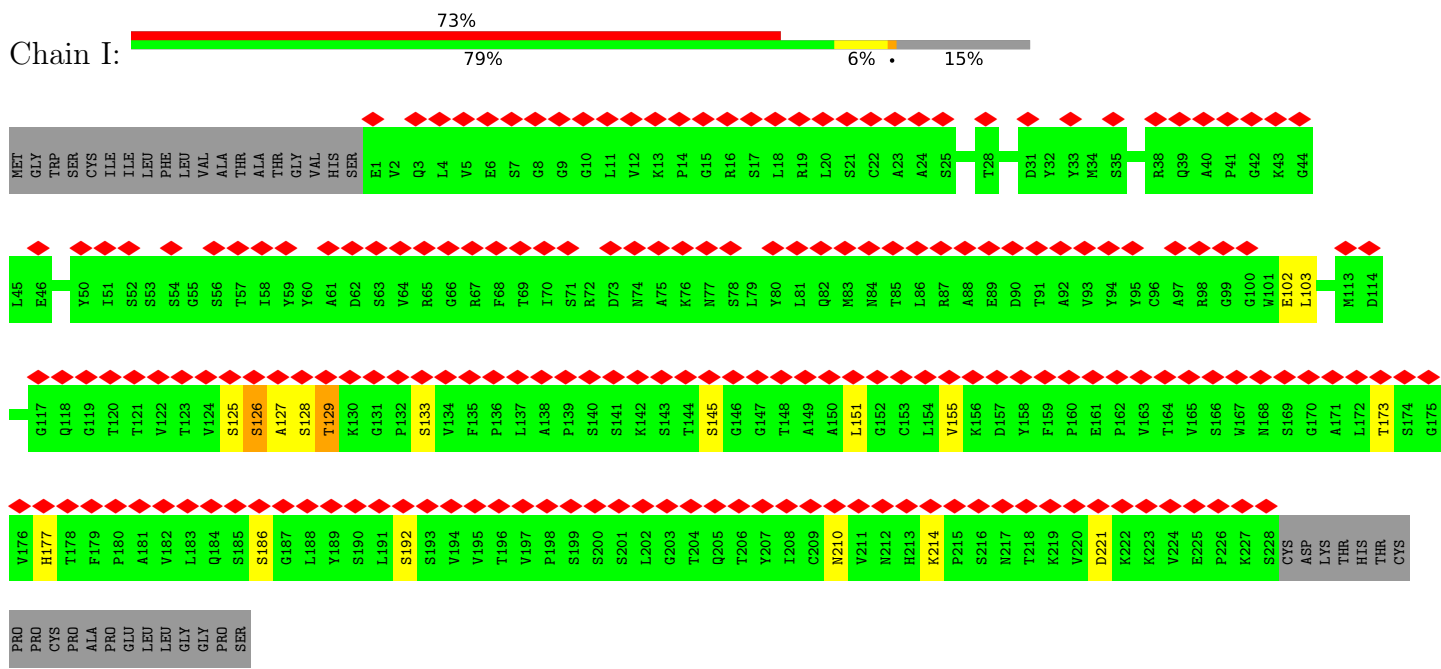
● Molecule 1: Spike glycoprotein



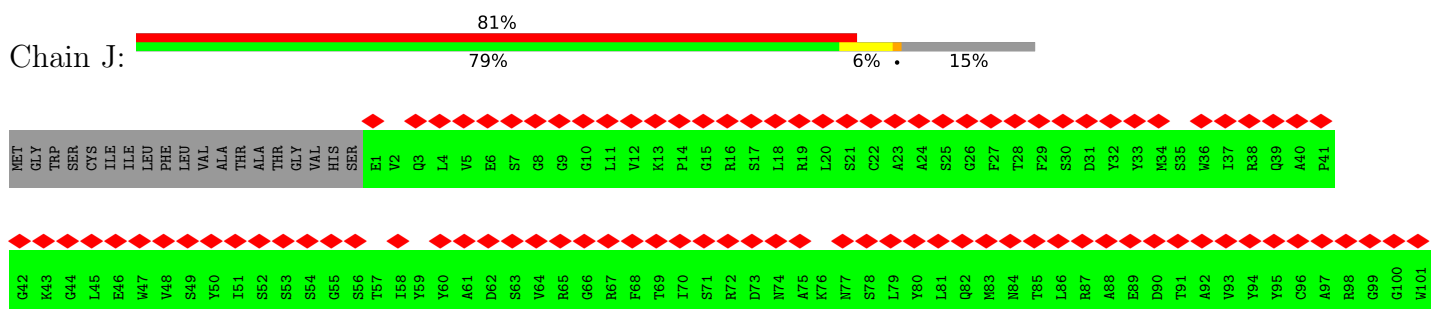
• Molecule 2: heavy chain of 3711

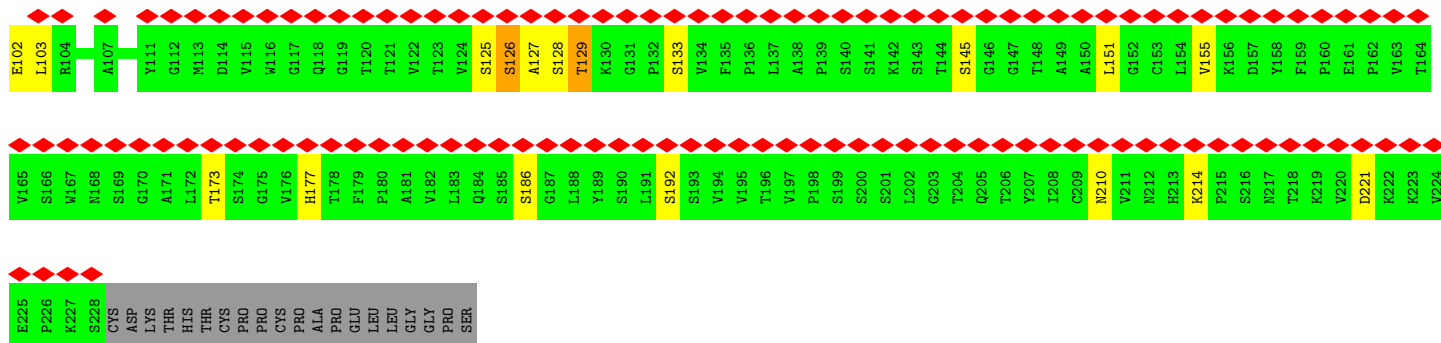


• Molecule 2: heavy chain of 3711

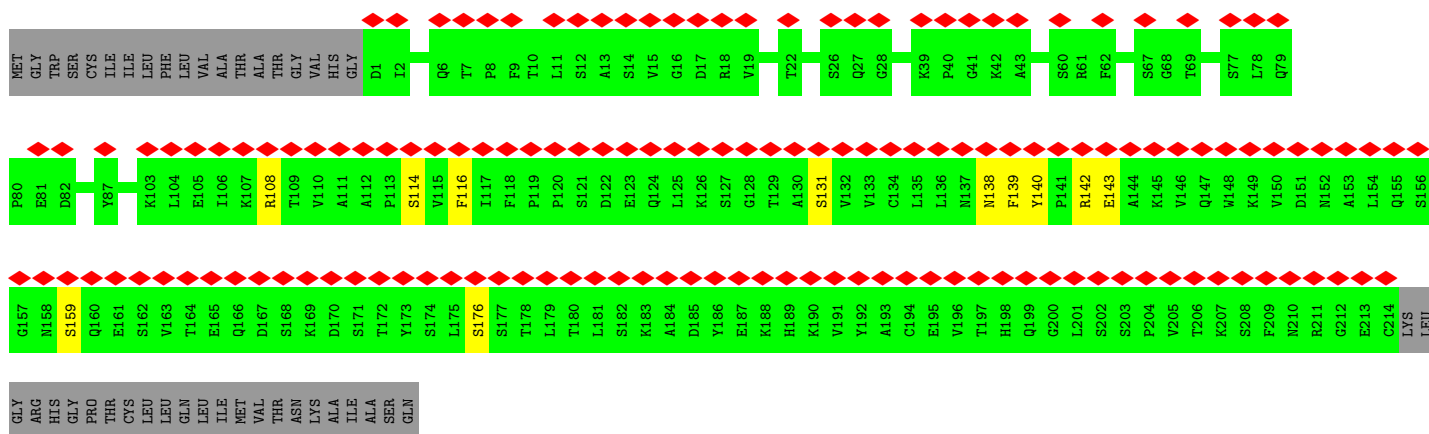


• Molecule 2: heavy chain of 3711

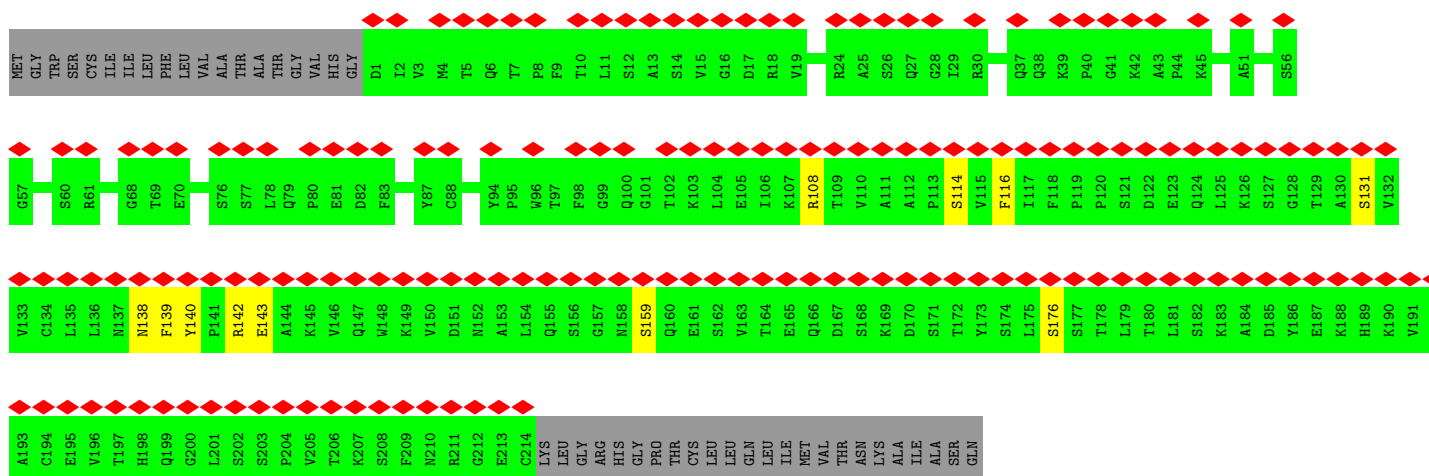
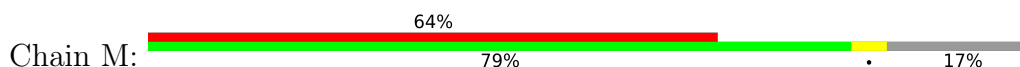




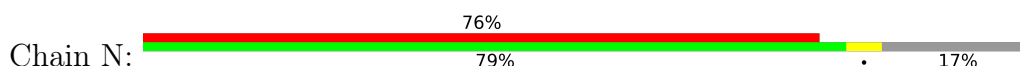
• Molecule 3: light chain of 3711

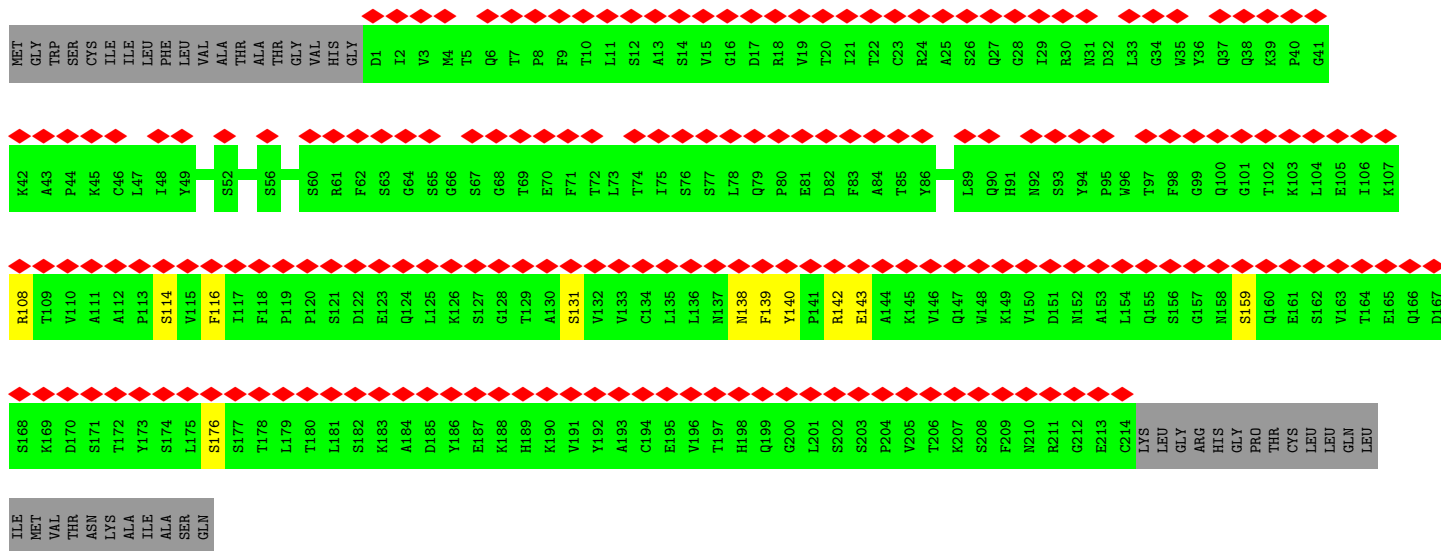


• Molecule 3: light chain of 3711



• Molecule 3: light chain of 3711





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



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





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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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

Chain i:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  67% 33%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  67% 33%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175006	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/8646	0.51	0/11767
1	B	0.42	0/8646	0.51	0/11767
1	C	0.42	0/8646	0.51	0/11767
2	H	0.35	0/1749	0.59	0/2379
2	I	0.35	0/1749	0.58	0/2379
2	J	0.35	0/1749	0.58	0/2379
3	L	0.43	0/1684	0.60	0/2287
3	M	0.43	0/1684	0.61	0/2287
3	N	0.43	0/1684	0.60	0/2287
All	All	0.41	0/36237	0.53	0/49299

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1067/1283 (83%)	977 (92%)	77 (7%)	13 (1%)	13	39
1	B	1067/1283 (83%)	977 (92%)	80 (8%)	10 (1%)	17	46
1	C	1067/1283 (83%)	978 (92%)	79 (7%)	10 (1%)	17	46
2	H	226/267 (85%)	206 (91%)	14 (6%)	6 (3%)	5	17
2	I	226/267 (85%)	206 (91%)	14 (6%)	6 (3%)	5	17
2	J	226/267 (85%)	206 (91%)	14 (6%)	6 (3%)	5	17
3	L	212/257 (82%)	187 (88%)	21 (10%)	4 (2%)	8	26
3	M	212/257 (82%)	187 (88%)	21 (10%)	4 (2%)	8	26
3	N	212/257 (82%)	187 (88%)	21 (10%)	4 (2%)	8	26
All	All	4515/5421 (83%)	4111 (91%)	341 (8%)	63 (1%)	15	34

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	LEU
1	A	145	TYR
1	B	23	GLN
1	B	24	LEU
1	B	145	TYR
1	C	23	GLN
1	C	24	LEU
1	C	145	TYR
2	H	127	ALA
2	H	128	SER
2	H	129	THR
3	L	138	ASN
2	I	127	ALA
2	I	128	SER
2	I	129	THR
3	M	138	ASN
2	J	127	ALA
2	J	128	SER
2	J	129	THR
3	N	138	ASN
1	A	122	ASN
1	A	292	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	122	ASN
1	C	122	ASN
1	A	939	SER
1	B	939	SER
1	C	939	SER
1	A	96	GLU
1	A	150	LYS
1	A	284	THR
1	B	96	GLU
1	B	150	LYS
1	B	284	THR
1	C	96	GLU
1	C	150	LYS
1	C	284	THR
2	H	102	GLU
2	I	102	GLU
2	J	102	GLU
1	A	291	CYS
1	A	936	ASP
1	B	294	ASP
1	B	936	ASP
1	C	936	ASP
2	H	126	SER
3	L	139	PHE
3	L	140	TYR
3	L	143	GLU
2	I	126	SER
3	M	139	PHE
3	M	140	TYR
3	M	143	GLU
2	J	126	SER
3	N	139	PHE
3	N	140	TYR
3	N	143	GLU
2	H	103	LEU
2	I	103	LEU
2	J	103	LEU
1	A	294	ASP
1	C	294	ASP
1	A	295	PRO



### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	941/1122 (84%)	848 (90%)	93 (10%)	8	23
1	B	941/1122 (84%)	847 (90%)	94 (10%)	7	22
1	C	941/1122 (84%)	848 (90%)	93 (10%)	8	23
2	H	189/221 (86%)	175 (93%)	14 (7%)	13	37
2	I	189/221 (86%)	175 (93%)	14 (7%)	13	37
2	J	189/221 (86%)	175 (93%)	14 (7%)	13	37
3	L	187/221 (85%)	180 (96%)	7 (4%)	34	68
3	M	187/221 (85%)	180 (96%)	7 (4%)	34	68
3	N	187/221 (85%)	180 (96%)	7 (4%)	34	68
All	All	3951/4692 (84%)	3608 (91%)	343 (9%)	14	30

All (343) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	45	SER
1	A	46	SER
1	A	96	GLU
1	A	97	LYS
1	A	98	SER
1	A	99	ASN
1	A	100	ILE
1	A	125	ASN
1	A	144	TYR
1	A	145	TYR
1	A	146	HIS
1	A	147	LYS
1	A	148	ASN
1	A	149	ASN
1	A	150	LYS
1	A	155	SER
1	A	190	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	276	LEU
1	A	278	LYS
1	A	282	ASN
1	A	290	ASP
1	A	293	LEU
1	A	299	THR
1	A	305	SER
1	A	317	ASN
1	A	325	SER
1	A	333	THR
1	A	366	SER
1	A	370	ASN
1	A	373	SER
1	A	375	SER
1	A	393	THR
1	A	399	SER
1	A	443	SER
1	A	445	VAL
1	A	448	ASN
1	A	459	SER
1	A	469	SER
1	A	471	GLU
1	A	493	GLN
1	A	514	SER
1	A	530	SER
1	A	531	THR
1	A	534	VAL
1	A	544	ASN
1	A	569	ILE
1	A	586	ASP
1	A	588	THR
1	A	590	CYS
1	A	599	THR
1	A	604	THR
1	A	606	ASN
1	A	614	ASP
1	A	617	CYS
1	A	638	THR
1	A	642	VAL
1	A	645	THR
1	A	657	ASN
1	A	675	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	676	THR
1	A	691	SER
1	A	708	SER
1	A	710	ASN
1	A	719	THR
1	A	723	THR
1	A	726	ILE
1	A	730	SER
1	A	732	THR
1	A	735	SER
1	A	745	ASP
1	A	746	SER
1	A	761	THR
1	A	780	GLU
1	A	790	LYS
1	A	810	SER
1	A	814	LYS
1	A	881	THR
1	A	884	SER
1	A	886	TRP
1	A	962	LEU
1	A	964	LYS
1	A	974	SER
1	A	982	SER
1	A	991	VAL
1	A	1002	GLN
1	A	1030	SER
1	A	1092	GLU
1	A	1097	SER
1	A	1118	ASP
1	A	1128	VAL
1	A	1136	THR
1	A	1142	GLN
1	B	24	LEU
1	B	45	SER
1	B	46	SER
1	B	96	GLU
1	B	97	LYS
1	B	98	SER
1	B	99	ASN
1	B	100	ILE
1	B	125	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	144	TYR
1	B	145	TYR
1	B	146	HIS
1	B	147	LYS
1	B	148	ASN
1	B	149	ASN
1	B	150	LYS
1	B	155	SER
1	B	190	ARG
1	B	224	GLU
1	B	276	LEU
1	B	278	LYS
1	B	282	ASN
1	B	293	LEU
1	B	299	THR
1	B	301	CYS
1	B	305	SER
1	B	317	ASN
1	B	325	SER
1	B	333	THR
1	B	366	SER
1	B	370	ASN
1	B	373	SER
1	B	375	SER
1	B	393	THR
1	B	399	SER
1	B	443	SER
1	B	445	VAL
1	B	448	ASN
1	B	459	SER
1	B	469	SER
1	B	471	GLU
1	B	493	GLN
1	B	514	SER
1	B	530	SER
1	B	531	THR
1	B	534	VAL
1	B	544	ASN
1	B	569	ILE
1	B	586	ASP
1	B	588	THR
1	B	590	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	599	THR
1	B	604	THR
1	B	606	ASN
1	B	614	ASP
1	B	617	CYS
1	B	638	THR
1	B	642	VAL
1	B	645	THR
1	B	657	ASN
1	B	675	GLN
1	B	676	THR
1	B	691	SER
1	B	708	SER
1	B	710	ASN
1	B	719	THR
1	B	723	THR
1	B	726	ILE
1	B	730	SER
1	B	732	THR
1	B	735	SER
1	B	745	ASP
1	B	746	SER
1	B	761	THR
1	B	780	GLU
1	B	790	LYS
1	B	810	SER
1	B	814	LYS
1	B	881	THR
1	B	884	SER
1	B	886	TRP
1	B	962	LEU
1	B	964	LYS
1	B	974	SER
1	B	982	SER
1	B	991	VAL
1	B	1002	GLN
1	B	1030	SER
1	B	1092	GLU
1	B	1097	SER
1	B	1118	ASP
1	B	1128	VAL
1	B	1136	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	1142	GLN
1	C	24	LEU
1	C	45	SER
1	C	46	SER
1	C	96	GLU
1	C	97	LYS
1	C	98	SER
1	C	99	ASN
1	C	100	ILE
1	C	125	ASN
1	C	144	TYR
1	C	145	TYR
1	C	146	HIS
1	C	147	LYS
1	C	148	ASN
1	C	149	ASN
1	C	150	LYS
1	C	155	SER
1	C	190	ARG
1	C	224	GLU
1	C	276	LEU
1	C	278	LYS
1	C	282	ASN
1	C	293	LEU
1	C	299	THR
1	C	305	SER
1	C	317	ASN
1	C	325	SER
1	C	333	THR
1	C	366	SER
1	C	370	ASN
1	C	373	SER
1	C	375	SER
1	C	393	THR
1	C	399	SER
1	C	443	SER
1	C	445	VAL
1	C	448	ASN
1	C	459	SER
1	C	469	SER
1	C	471	GLU
1	C	493	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	514	SER
1	C	530	SER
1	C	531	THR
1	C	534	VAL
1	C	544	ASN
1	C	569	ILE
1	C	586	ASP
1	C	588	THR
1	C	590	CYS
1	C	599	THR
1	C	604	THR
1	C	606	ASN
1	C	614	ASP
1	C	617	CYS
1	C	638	THR
1	C	642	VAL
1	C	645	THR
1	C	657	ASN
1	C	675	GLN
1	C	676	THR
1	C	691	SER
1	C	708	SER
1	C	710	ASN
1	C	719	THR
1	C	723	THR
1	C	726	ILE
1	C	730	SER
1	C	732	THR
1	C	735	SER
1	C	745	ASP
1	C	746	SER
1	C	761	THR
1	C	780	GLU
1	C	790	LYS
1	C	810	SER
1	C	814	LYS
1	C	881	THR
1	C	884	SER
1	C	886	TRP
1	C	962	LEU
1	C	964	LYS
1	C	974	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	982	SER
1	C	991	VAL
1	C	1002	GLN
1	C	1030	SER
1	C	1092	GLU
1	C	1097	SER
1	C	1118	ASP
1	C	1128	VAL
1	C	1136	THR
1	C	1142	GLN
2	H	125	SER
2	H	126	SER
2	H	129	THR
2	H	133	SER
2	H	145	SER
2	H	151	LEU
2	H	155	VAL
2	H	173	THR
2	H	177	HIS
2	H	186	SER
2	H	192	SER
2	H	210	ASN
2	H	214	LYS
2	H	221	ASP
3	L	108	ARG
3	L	114	SER
3	L	116	PHE
3	L	131	SER
3	L	142	ARG
3	L	159	SER
3	L	176	SER
2	I	125	SER
2	I	126	SER
2	I	129	THR
2	I	133	SER
2	I	145	SER
2	I	151	LEU
2	I	155	VAL
2	I	173	THR
2	I	177	HIS
2	I	186	SER
2	I	192	SER

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Mol	Chain	Res	Type
2	I	210	ASN
2	I	214	LYS
2	I	221	ASP
3	M	108	ARG
3	M	114	SER
3	M	116	PHE
3	M	131	SER
3	M	142	ARG
3	M	159	SER
3	M	176	SER
2	J	125	SER
2	J	126	SER
2	J	129	THR
2	J	133	SER
2	J	145	SER
2	J	151	LEU
2	J	155	VAL
2	J	173	THR
2	J	177	HIS
2	J	186	SER
2	J	192	SER
2	J	210	ASN
2	J	214	LYS
2	J	221	ASP
3	N	108	ARG
3	N	114	SER
3	N	116	PHE
3	N	131	SER
3	N	142	ARG
3	N	159	SER
3	N	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	69	HIS
1	A	87	ASN
1	A	99	ASN
1	A	148	ASN
1	A	149	ASN
1	A	188	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	271	GLN
1	A	314	GLN
1	A	317	ASN
1	A	448	ASN
1	A	450	ASN
1	A	493	GLN
1	A	498	GLN
1	A	532	ASN
1	A	544	ASN
1	A	556	ASN
1	A	564	GLN
1	A	606	ASN
1	A	613	GLN
1	A	675	GLN
1	A	710	ASN
1	A	751	ASN
1	A	804	GLN
1	A	856	ASN
1	A	919	ASN
1	A	925	ASN
1	A	1023	ASN
1	A	1036	GLN
1	A	1054	GLN
1	A	1064	HIS
1	A	1125	ASN
1	B	14	GLN
1	B	69	HIS
1	B	87	ASN
1	B	99	ASN
1	B	148	ASN
1	B	149	ASN
1	B	188	ASN
1	B	271	GLN
1	B	314	GLN
1	B	317	ASN
1	B	448	ASN
1	B	450	ASN
1	B	493	GLN
1	B	498	GLN
1	B	532	ASN
1	B	544	ASN
1	B	556	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	564	GLN
1	B	606	ASN
1	B	613	GLN
1	B	675	GLN
1	B	710	ASN
1	B	751	ASN
1	B	804	GLN
1	B	856	ASN
1	B	919	ASN
1	B	925	ASN
1	B	1023	ASN
1	B	1036	GLN
1	B	1054	GLN
1	B	1064	HIS
1	B	1125	ASN
1	C	14	GLN
1	C	69	HIS
1	C	87	ASN
1	C	99	ASN
1	C	148	ASN
1	C	149	ASN
1	C	188	ASN
1	C	271	GLN
1	C	314	GLN
1	C	317	ASN
1	C	448	ASN
1	C	450	ASN
1	C	493	GLN
1	C	498	GLN
1	C	532	ASN
1	C	544	ASN
1	C	556	ASN
1	C	564	GLN
1	C	606	ASN
1	C	613	GLN
1	C	675	GLN
1	C	710	ASN
1	C	751	ASN
1	C	804	GLN
1	C	856	ASN
1	C	919	ASN
1	C	925	ASN

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Mol	Chain	Res	Type
1	C	1023	ASN
1	C	1036	GLN
1	C	1054	GLN
1	C	1064	HIS
1	C	1125	ASN
2	H	77	ASN
3	L	6	GLN
2	I	77	ASN
3	M	6	GLN
2	J	77	ASN
3	N	6	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

55 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	D	1	4,1	14,14,15	0.80	1 (7%)	17,19,21	1.08	2 (11%)
4	NAG	D	2	4	14,14,15	0.66	1 (7%)	17,19,21	0.61	0
5	NAG	E	1	1,5	14,14,15	0.52	0	17,19,21	0.57	0
5	NAG	E	2	5	14,14,15	0.27	0	17,19,21	0.51	0
5	NAG	E	3	5	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
4	NAG	F	1	4,1	14,14,15	0.25	0	17,19,21	0.57	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	G	1	4,1	14,14,15	0.46	0	17,19,21	0.80	1 (5%)
4	NAG	G	2	4	14,14,15	0.80	1 (7%)	17,19,21	0.58	0
4	NAG	K	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	2.23	3 (17%)
4	NAG	K	2	4	14,14,15	0.40	0	17,19,21	0.50	0
4	NAG	O	1	4,1	14,14,15	1.15	1 (7%)	17,19,21	0.61	0
4	NAG	O	2	4	14,14,15	2.26	2 (14%)	17,19,21	0.98	2 (11%)
4	NAG	P	1	4,1	14,14,15	0.86	1 (7%)	17,19,21	0.56	0
4	NAG	P	2	4	14,14,15	2.92	2 (14%)	17,19,21	1.53	4 (23%)
4	NAG	Q	1	4,1	14,14,15	0.30	0	17,19,21	0.61	0
4	NAG	Q	2	4	14,14,15	0.53	0	17,19,21	0.47	0
4	NAG	R	1	4,1	14,14,15	0.71	1 (7%)	17,19,21	0.70	0
4	NAG	R	2	4	14,14,15	0.39	0	17,19,21	1.40	3 (17%)
4	NAG	S	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	0.67	0
4	NAG	S	2	4	14,14,15	0.29	0	17,19,21	0.65	0
4	NAG	T	1	4,1	14,14,15	0.79	1 (7%)	17,19,21	1.08	2 (11%)
4	NAG	T	2	4	14,14,15	0.68	1 (7%)	17,19,21	0.60	0
5	NAG	U	1	1,5	14,14,15	0.50	0	17,19,21	0.58	0
5	NAG	U	2	5	14,14,15	0.29	0	17,19,21	0.51	0
5	NAG	U	3	5	14,14,15	0.29	0	17,19,21	0.63	1 (5%)
4	NAG	V	1	4,1	14,14,15	0.25	0	17,19,21	0.57	0
4	NAG	V	2	4	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	W	1	4,1	14,14,15	0.45	0	17,19,21	0.81	1 (5%)
4	NAG	W	2	4	14,14,15	0.80	1 (7%)	17,19,21	0.57	0
4	NAG	X	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	2.23	3 (17%)
4	NAG	X	2	4	14,14,15	0.40	0	17,19,21	0.50	0
4	NAG	Y	1	4,1	14,14,15	1.16	1 (7%)	17,19,21	0.61	0
4	NAG	Y	2	4	14,14,15	2.27	2 (14%)	17,19,21	0.96	2 (11%)
4	NAG	Z	1	4,1	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	Z	2	4	14,14,15	0.51	0	17,19,21	0.46	0
4	NAG	a	1	4,1	14,14,15	0.72	1 (7%)	17,19,21	0.67	0
4	NAG	a	2	4	14,14,15	0.29	0	17,19,21	0.65	0
4	NAG	b	1	4,1	14,14,15	0.81	1 (7%)	17,19,21	1.08	2 (11%)
4	NAG	b	2	4	14,14,15	0.66	1 (7%)	17,19,21	0.60	0
5	NAG	c	1	1,5	14,14,15	0.53	0	17,19,21	0.57	0
5	NAG	c	2	5	14,14,15	0.29	0	17,19,21	0.51	0
5	NAG	c	3	5	14,14,15	0.29	0	17,19,21	0.63	1 (5%)
4	NAG	d	1	4,1	14,14,15	0.25	0	17,19,21	0.58	0
4	NAG	d	2	4	14,14,15	0.27	0	17,19,21	0.62	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	e	1	4,1	14,14,15	0.45	0	17,19,21	0.80	1 (5%)
4	NAG	e	2	4	14,14,15	0.80	1 (7%)	17,19,21	0.58	0
4	NAG	f	1	4,1	14,14,15	0.83	1 (7%)	17,19,21	2.22	3 (17%)
4	NAG	f	2	4	14,14,15	0.39	0	17,19,21	0.50	0
4	NAG	g	1	4,1	14,14,15	1.16	1 (7%)	17,19,21	0.60	0
4	NAG	g	2	4	14,14,15	2.26	2 (14%)	17,19,21	0.96	2 (11%)
4	NAG	h	1	4,1	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	h	2	4	14,14,15	0.52	0	17,19,21	0.47	0
4	NAG	i	1	4,1	14,14,15	0.72	1 (7%)	17,19,21	0.67	0
4	NAG	i	2	4	14,14,15	0.30	0	17,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	E	3	5	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	5/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	3	5	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	3/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	NAG	c	3	5	-	2/6/23/26	0/1/1/1
4	NAG	d	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	NAG	e	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
4	NAG	f	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	NAG	h	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	2/6/23/26	0/1/1/1
4	NAG	i	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	i	2	4	-	3/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	2	NAG	O5-C1	-8.06	1.30	1.43
4	Y	2	NAG	O5-C1	-7.15	1.32	1.43
4	O	2	NAG	O5-C1	-7.12	1.32	1.43
4	g	2	NAG	O5-C1	-7.11	1.32	1.43
4	P	2	NAG	C1-C2	-6.81	1.42	1.52
4	Y	2	NAG	C1-C2	-4.48	1.45	1.52
4	g	2	NAG	C1-C2	-4.46	1.45	1.52
4	O	2	NAG	C1-C2	-4.42	1.45	1.52
4	Y	1	NAG	O5-C1	-4.24	1.36	1.43
4	g	1	NAG	O5-C1	-4.23	1.37	1.43
4	O	1	NAG	O5-C1	-4.22	1.37	1.43
4	P	1	NAG	O5-C1	-2.83	1.39	1.43
4	b	1	NAG	O5-C1	-2.80	1.39	1.43
4	D	1	NAG	O5-C1	-2.80	1.39	1.43
4	T	1	NAG	O5-C1	-2.75	1.39	1.43
4	i	1	NAG	O5-C1	-2.64	1.39	1.43
4	a	1	NAG	O5-C1	-2.64	1.39	1.43
4	S	1	NAG	O5-C1	-2.55	1.39	1.43
4	f	1	NAG	C1-C2	2.49	1.56	1.52
4	X	1	NAG	C1-C2	2.47	1.56	1.52
4	K	1	NAG	C1-C2	2.44	1.56	1.52
4	R	1	NAG	O5-C1	-2.41	1.39	1.43
4	W	2	NAG	C1-C2	2.40	1.55	1.52
4	e	2	NAG	C1-C2	2.39	1.55	1.52
4	G	2	NAG	C1-C2	2.35	1.55	1.52
4	T	2	NAG	C1-C2	2.17	1.55	1.52
4	D	2	NAG	C1-C2	2.12	1.55	1.52
4	b	2	NAG	C1-C2	2.11	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1	NAG	C2-N2-C7	7.78	133.99	122.90
4	X	1	NAG	C2-N2-C7	7.77	133.96	122.90
4	f	1	NAG	C2-N2-C7	7.74	133.92	122.90
4	R	2	NAG	C2-N2-C7	4.43	129.21	122.90
4	f	1	NAG	C1-C2-N2	3.64	116.70	110.49
4	X	1	NAG	C1-C2-N2	3.62	116.67	110.49
4	K	1	NAG	C1-C2-N2	3.61	116.65	110.49
4	P	2	NAG	O5-C1-C2	3.25	116.43	111.29
4	P	2	NAG	C1-O5-C5	3.23	116.57	112.19
4	P	2	NAG	C1-C2-N2	3.22	115.99	110.49
4	Y	2	NAG	C1-C2-N2	2.54	114.83	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	2	NAG	C1-O5-C5	2.54	115.63	112.19
4	O	2	NAG	C1-C2-N2	2.50	114.76	110.49
4	g	2	NAG	C1-O5-C5	2.48	115.56	112.19
4	g	2	NAG	C1-C2-N2	2.45	114.68	110.49
4	T	1	NAG	O4-C4-C3	-2.43	104.73	110.35
4	b	1	NAG	O4-C4-C3	-2.42	104.75	110.35
4	D	1	NAG	O4-C4-C3	-2.40	104.79	110.35
4	R	2	NAG	C1-C2-N2	2.37	114.54	110.49
4	Y	2	NAG	C1-O5-C5	2.37	115.40	112.19
4	G	1	NAG	C1-O5-C5	2.30	115.30	112.19
4	W	1	NAG	C1-O5-C5	2.29	115.29	112.19
4	e	1	NAG	C1-O5-C5	2.28	115.28	112.19
5	U	3	NAG	C1-O5-C5	2.21	115.18	112.19
4	f	1	NAG	C8-C7-N2	2.18	119.80	116.10
4	X	1	NAG	C8-C7-N2	2.18	119.80	116.10
5	c	3	NAG	C1-O5-C5	2.18	115.14	112.19
5	E	3	NAG	C1-O5-C5	2.16	115.12	112.19
4	T	1	NAG	C3-C4-C5	2.16	114.09	110.24
4	b	1	NAG	C3-C4-C5	2.16	114.08	110.24
4	D	1	NAG	C3-C4-C5	2.14	114.05	110.24
4	K	1	NAG	C8-C7-N2	2.14	119.72	116.10
4	P	2	NAG	C2-N2-C7	2.13	125.93	122.90
4	R	2	NAG	C1-O5-C5	2.04	114.95	112.19
4	d	2	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	K	1	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
5	E	3	NAG	C4-C5-C6-O6
5	U	3	NAG	C4-C5-C6-O6
5	c	3	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
5	E	3	NAG	O5-C5-C6-O6
5	U	3	NAG	O5-C5-C6-O6
5	c	3	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
4	f	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	f	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
4	S	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7
4	i	2	NAG	C3-C2-N2-C7
4	T	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6

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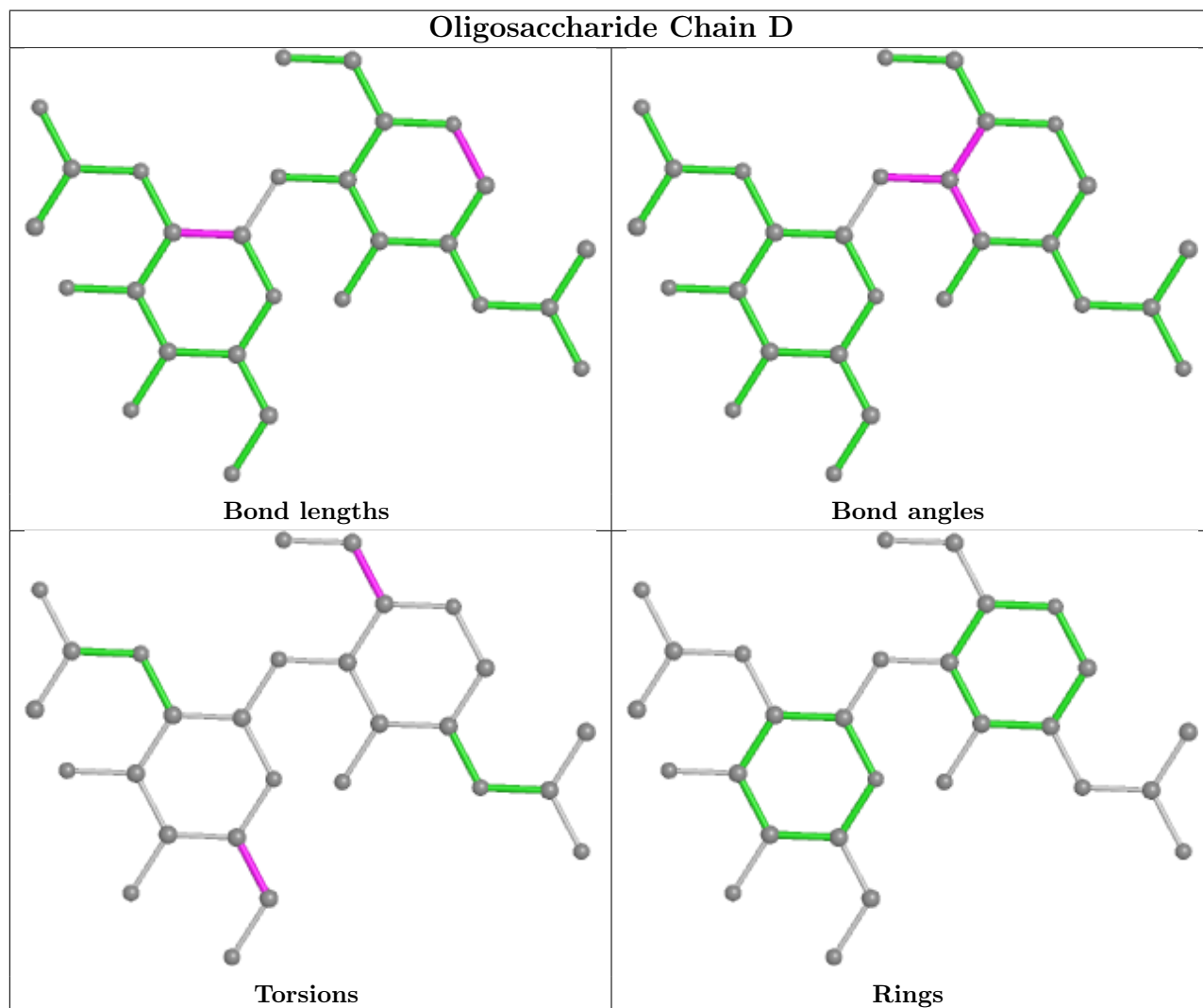
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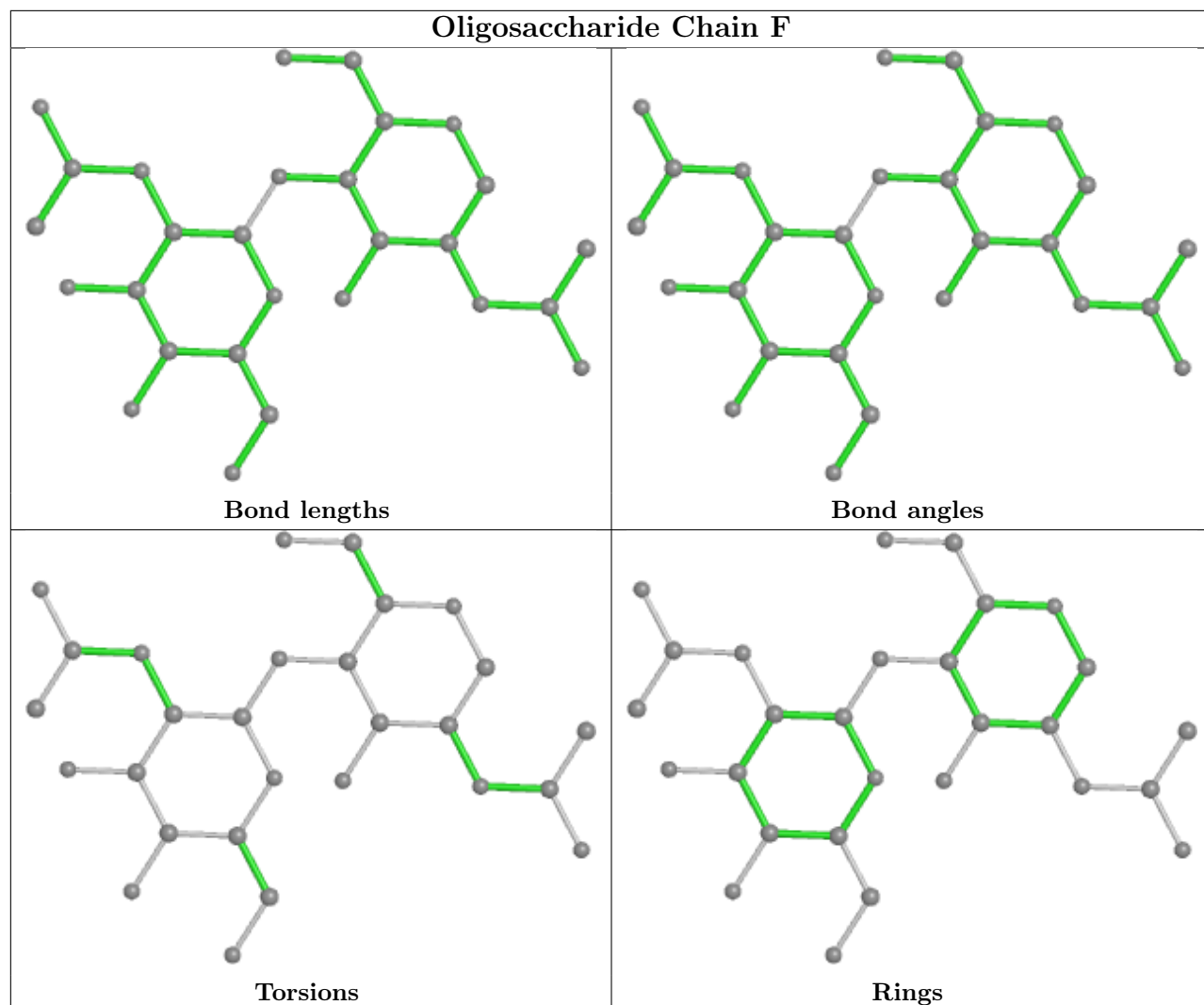
Mol	Chain	Res	Type	Atoms
4	g	1	NAG	C1-C2-N2-C7
4	O	1	NAG	C1-C2-N2-C7
4	Y	1	NAG	C1-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	f	1	NAG	C3-C2-N2-C7

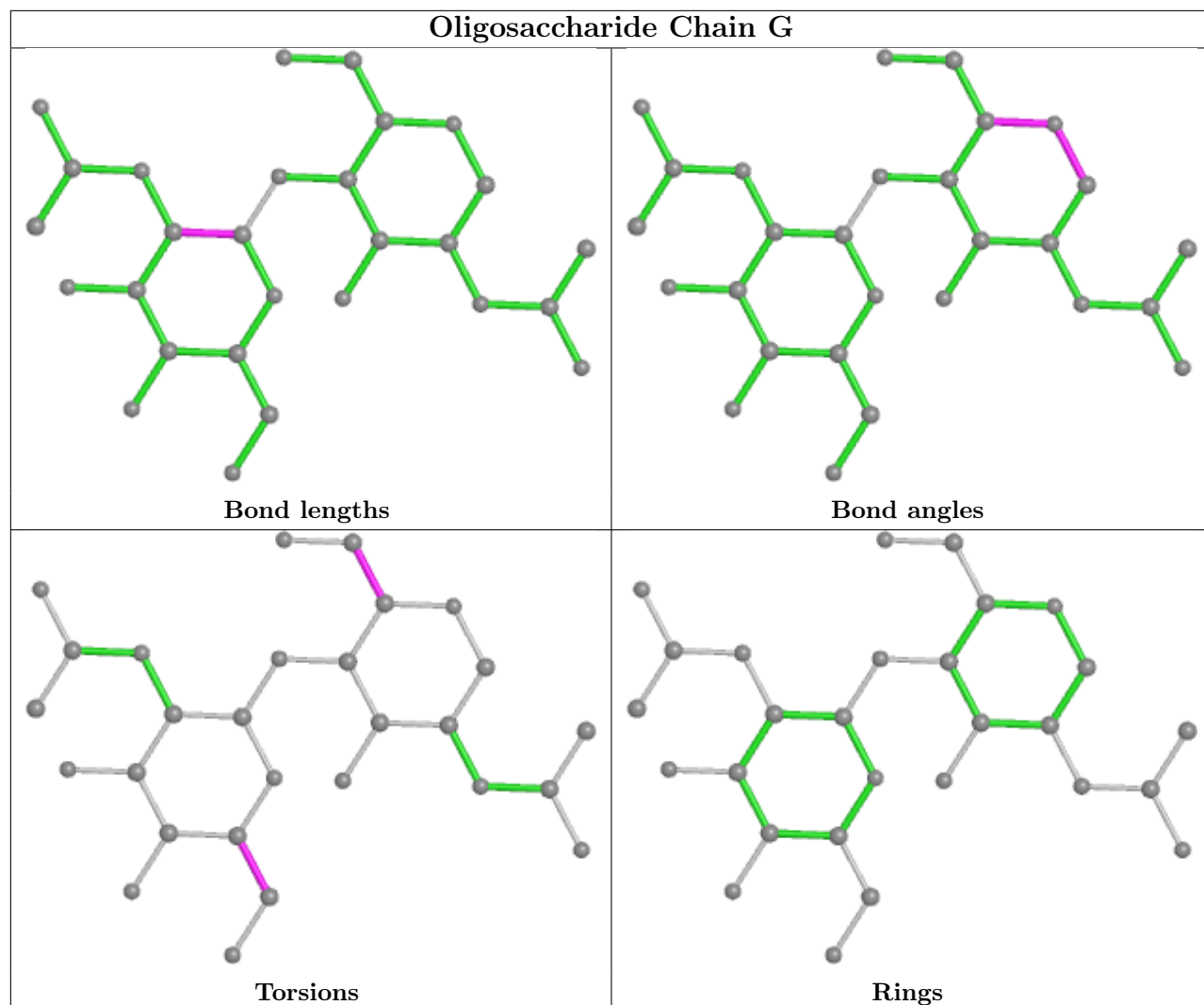
There are no ring outliers.

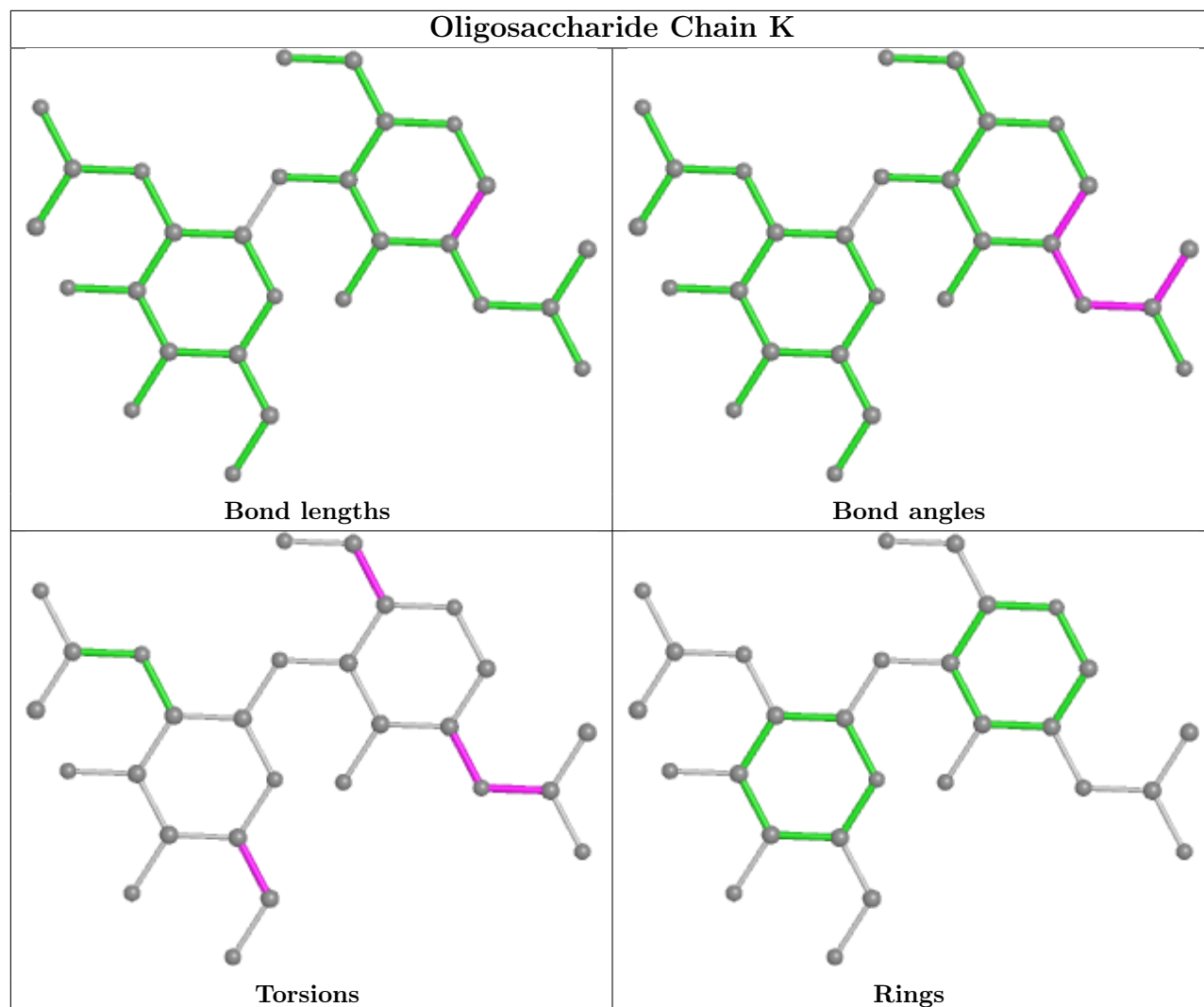
No monomer is involved in short contacts.

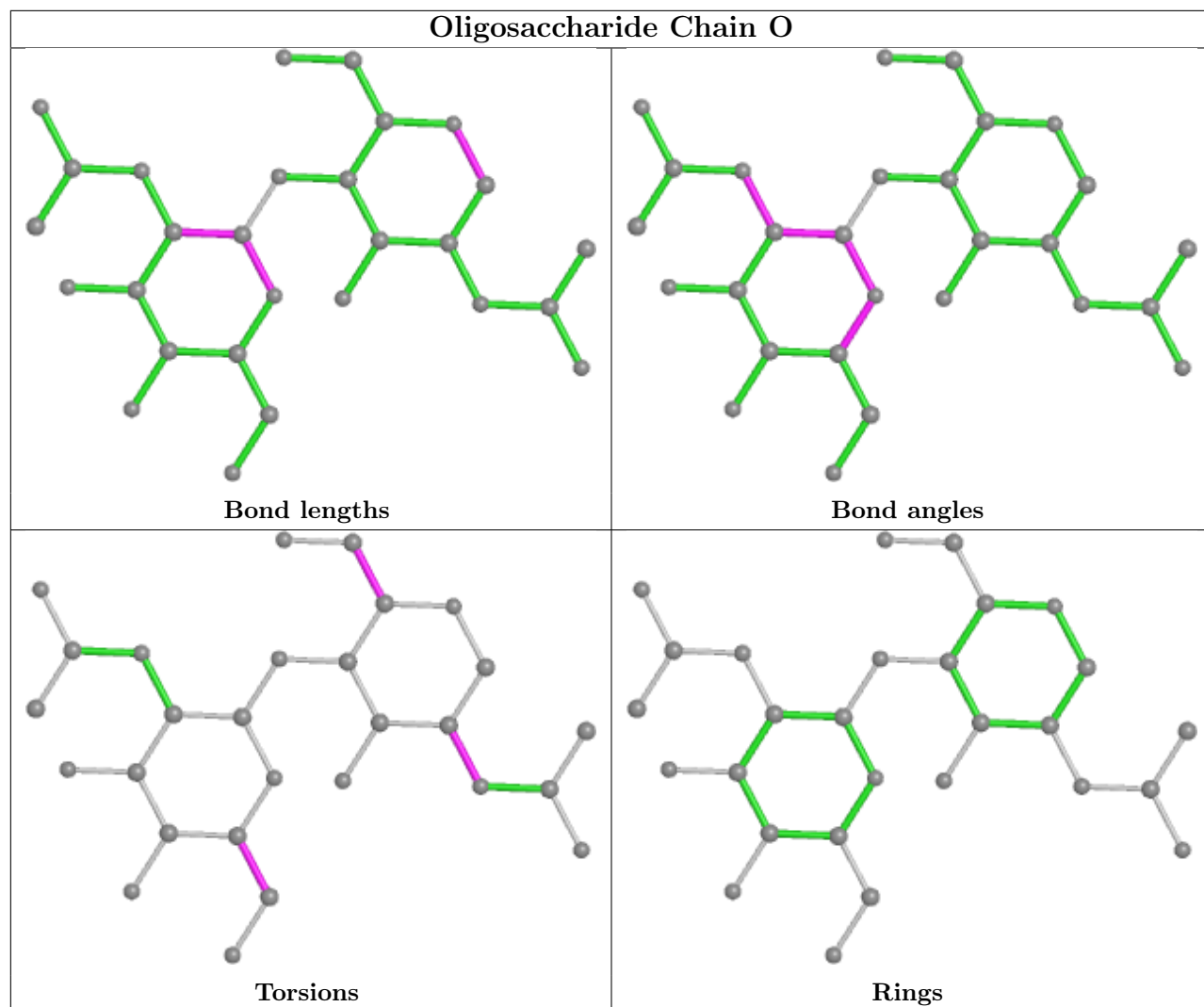
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



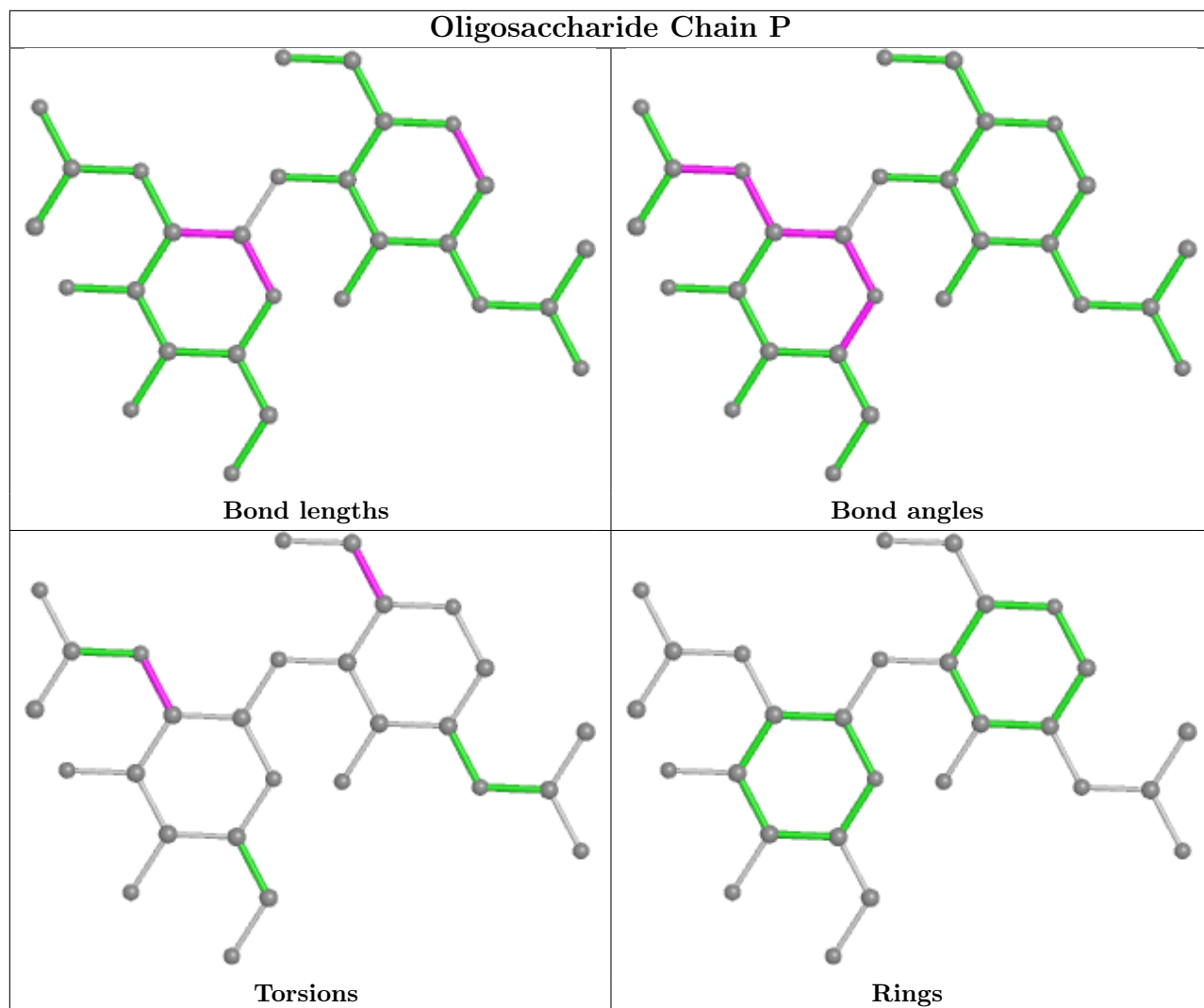


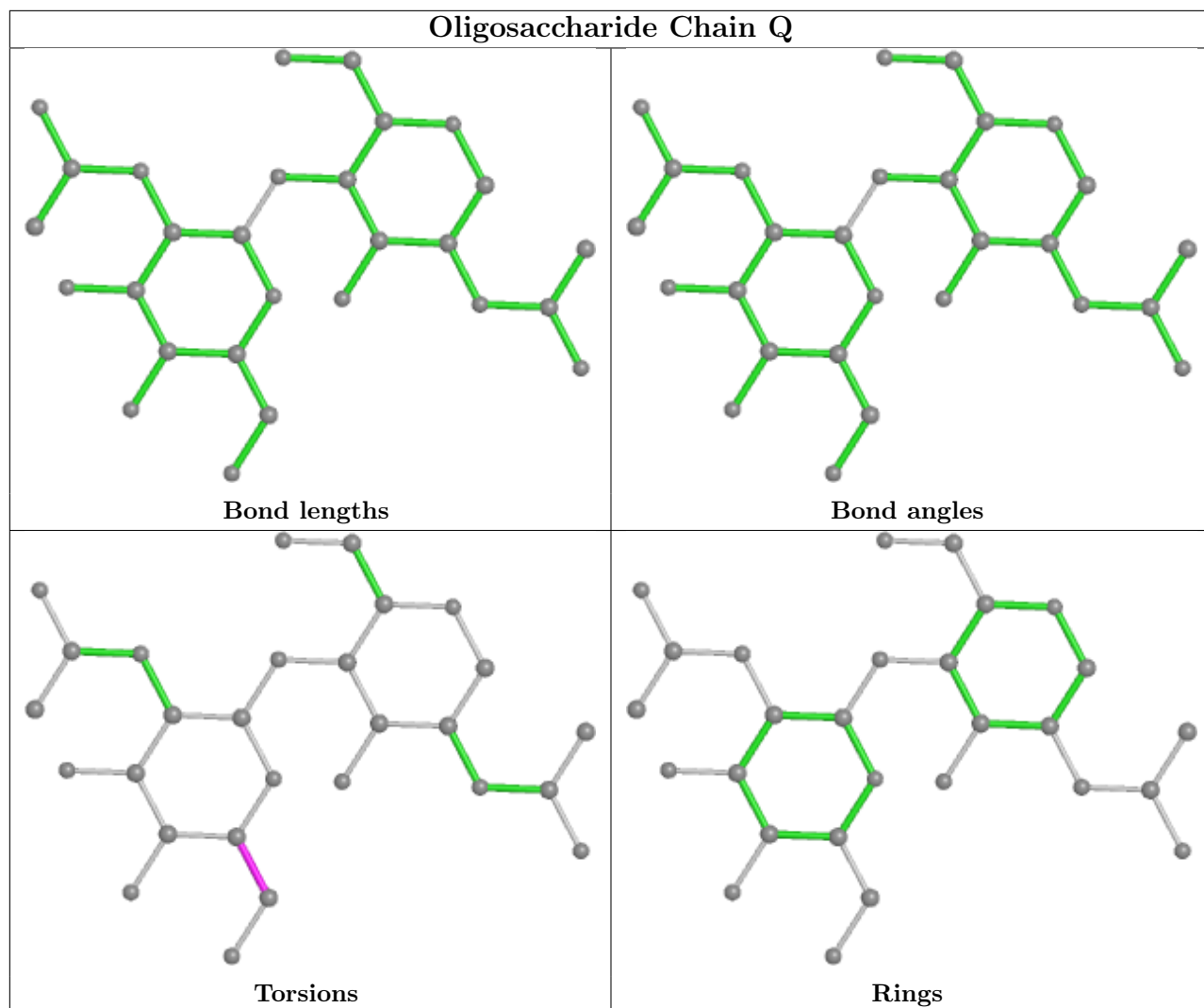


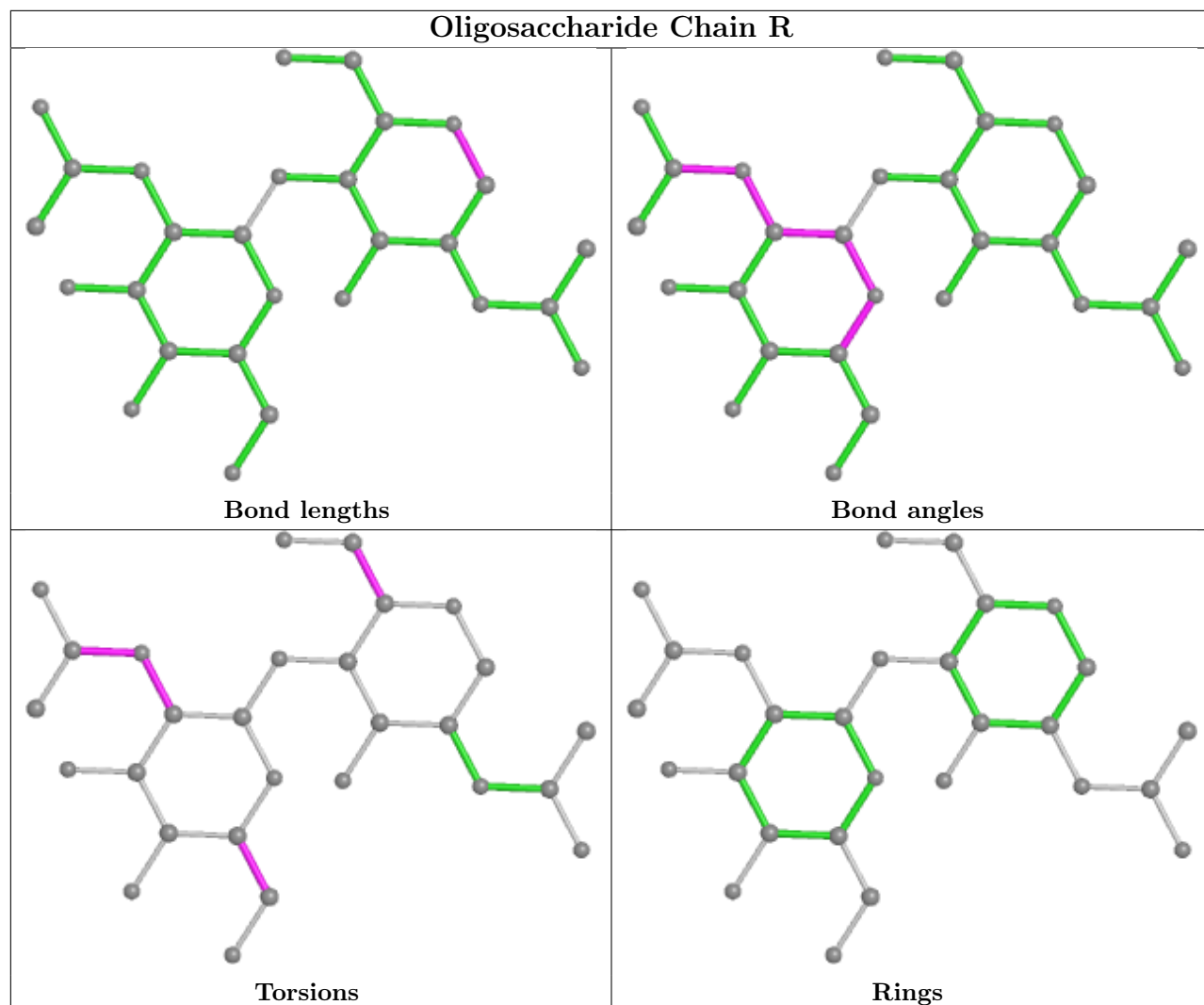


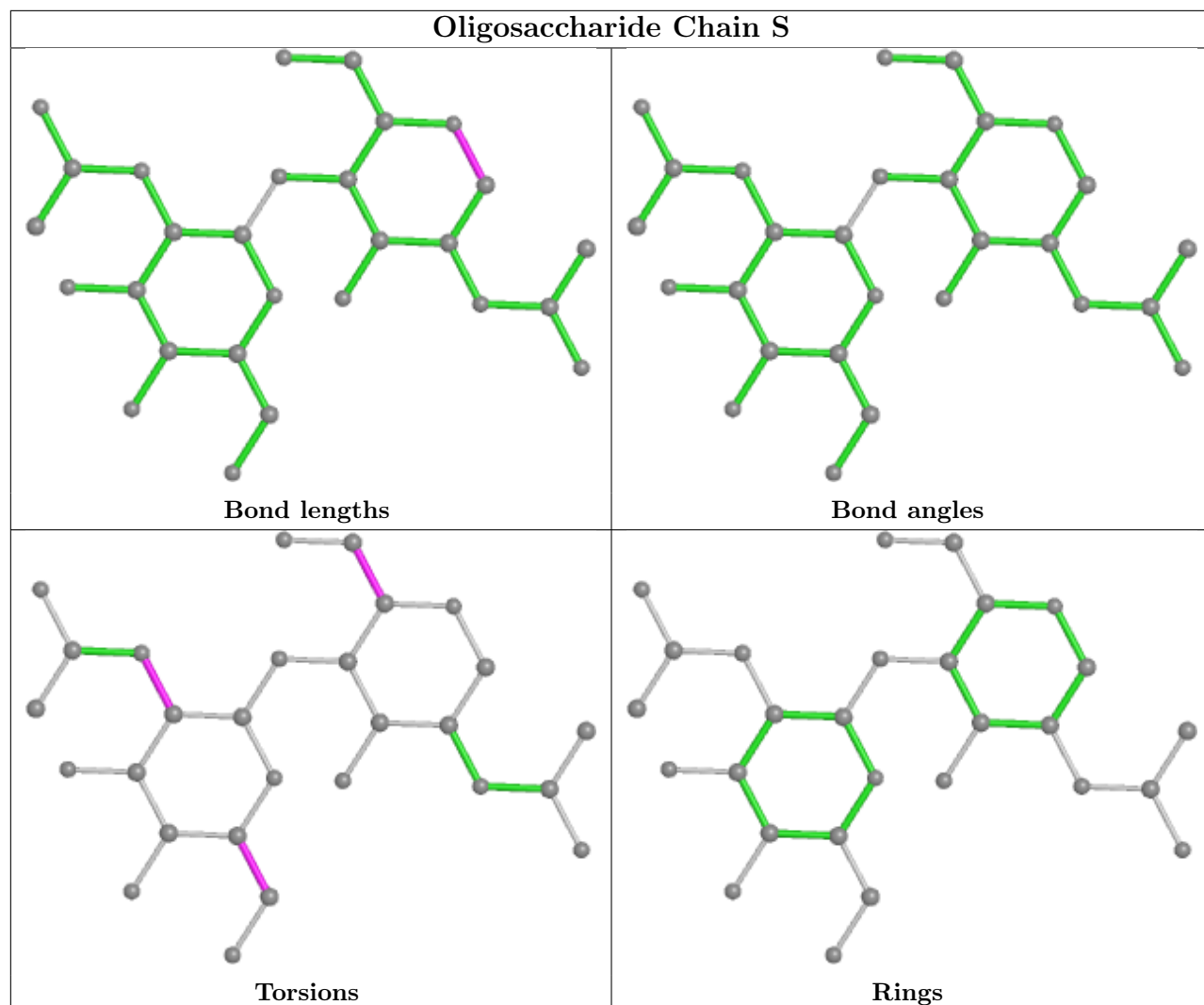


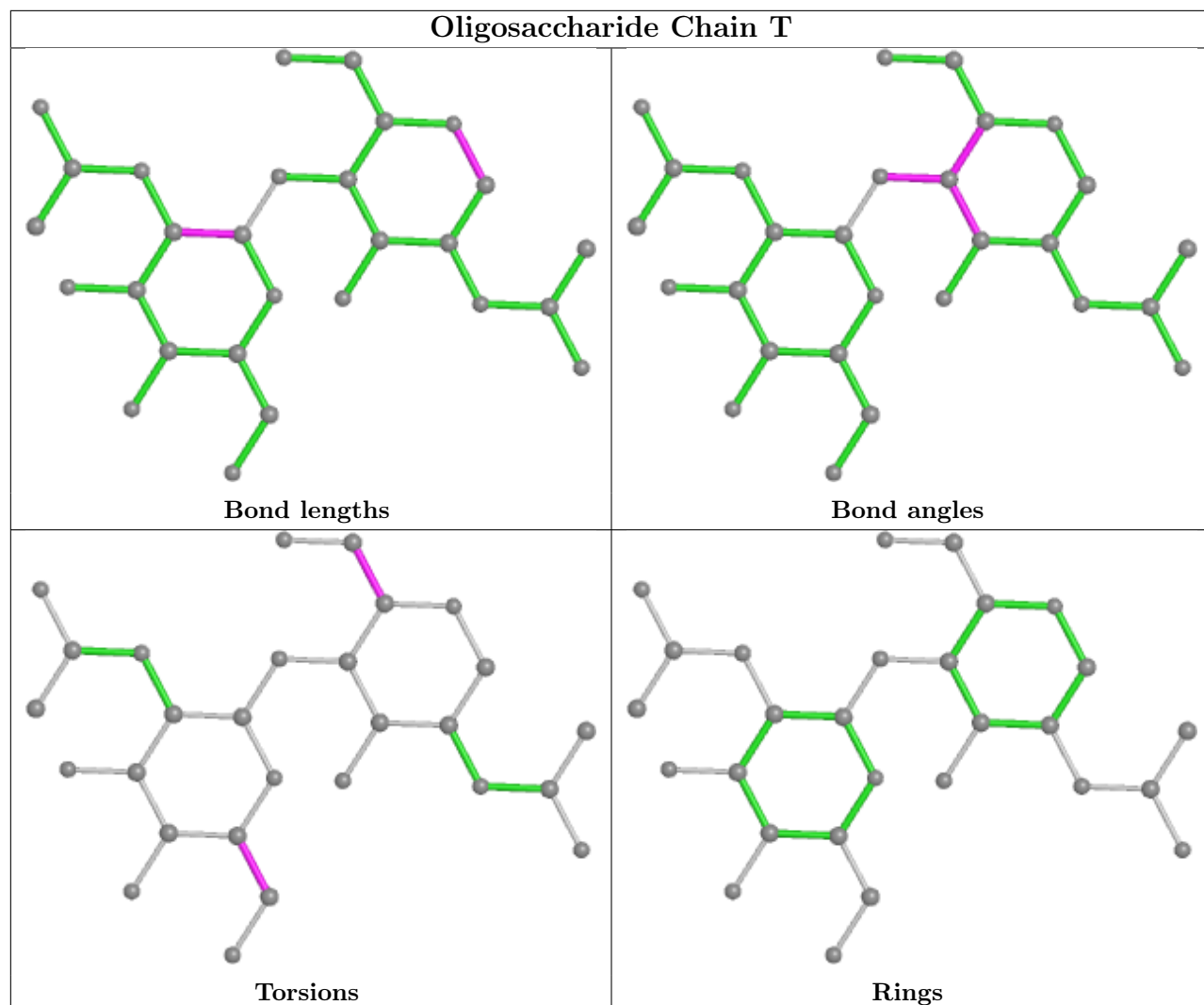


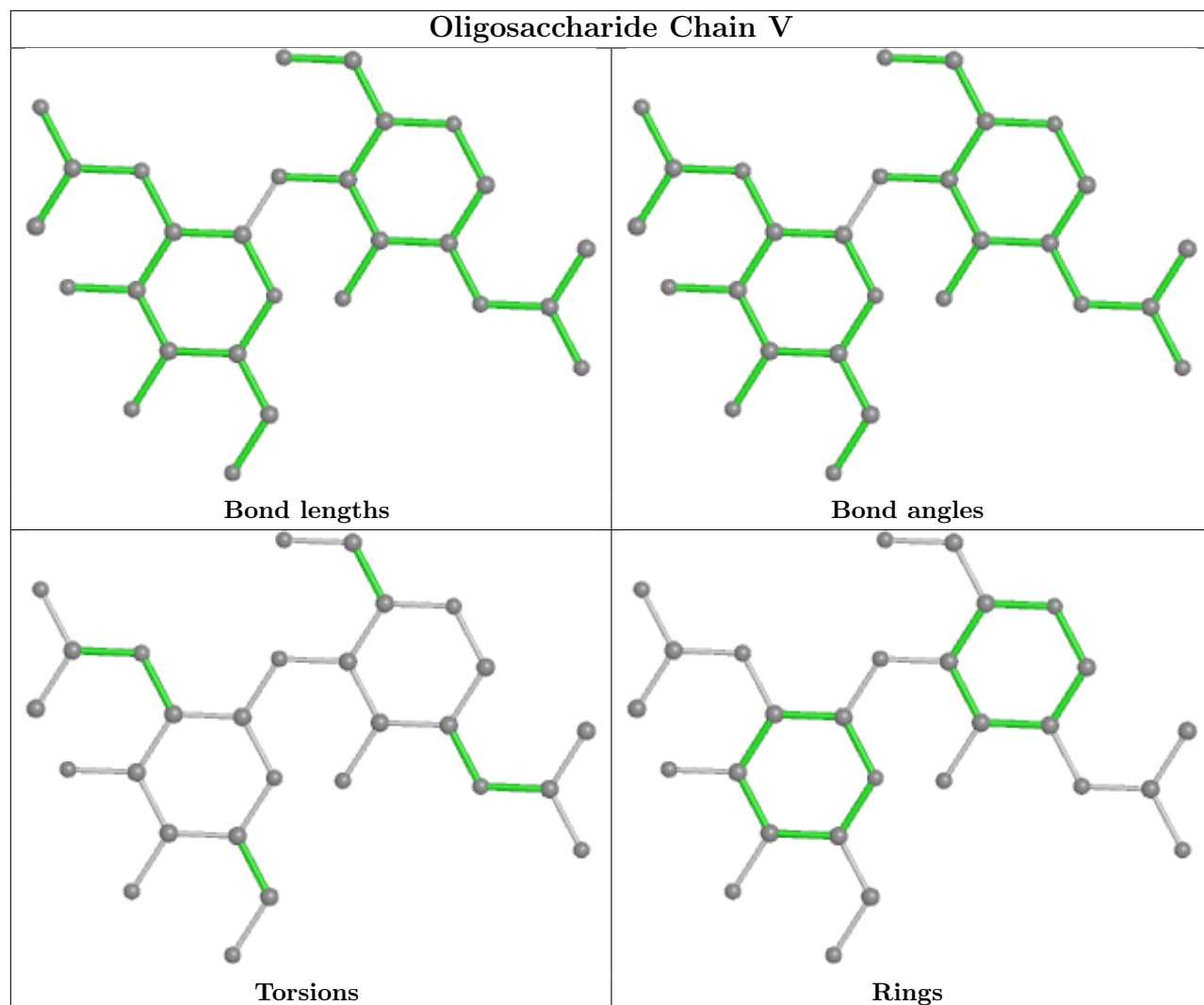


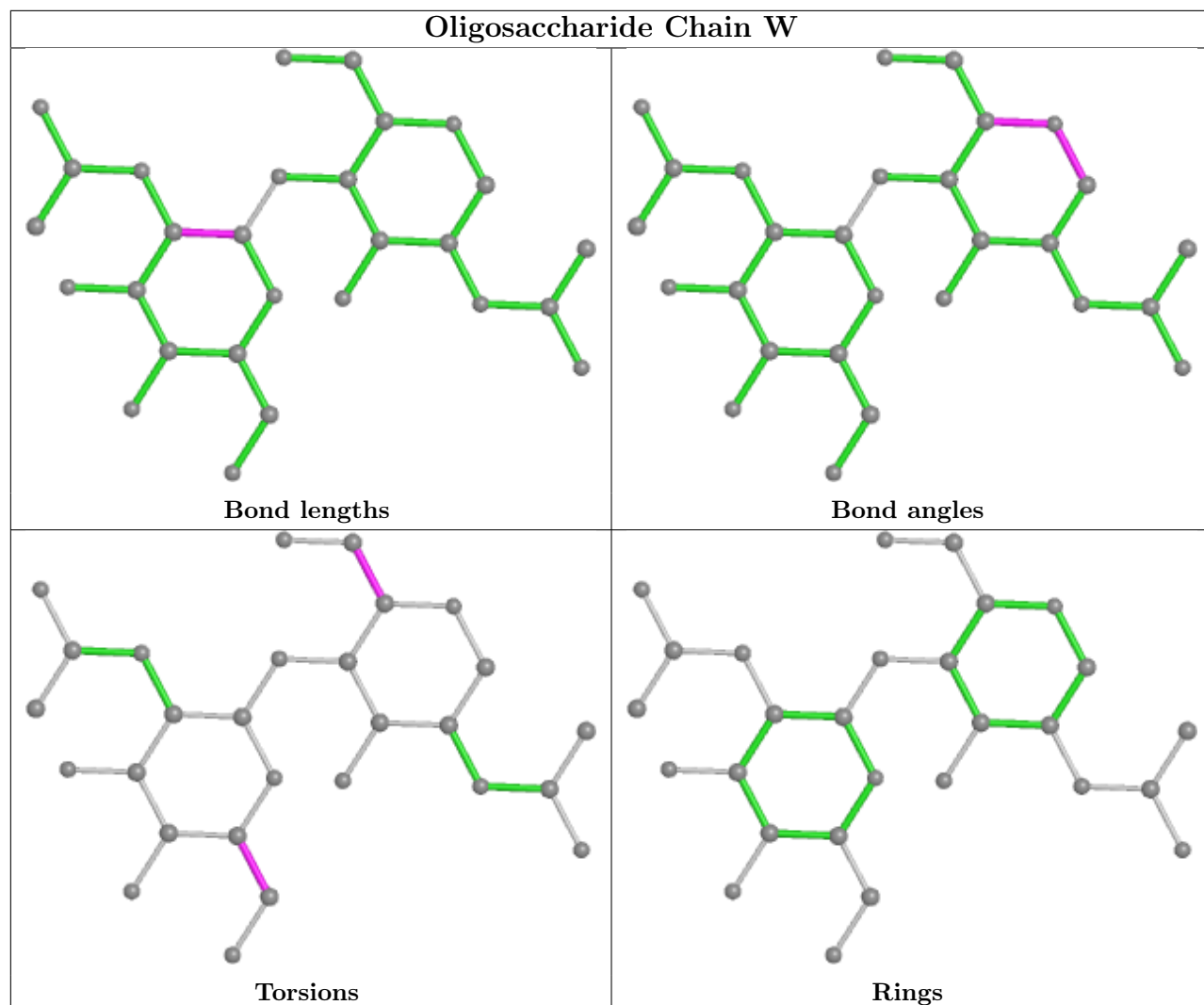


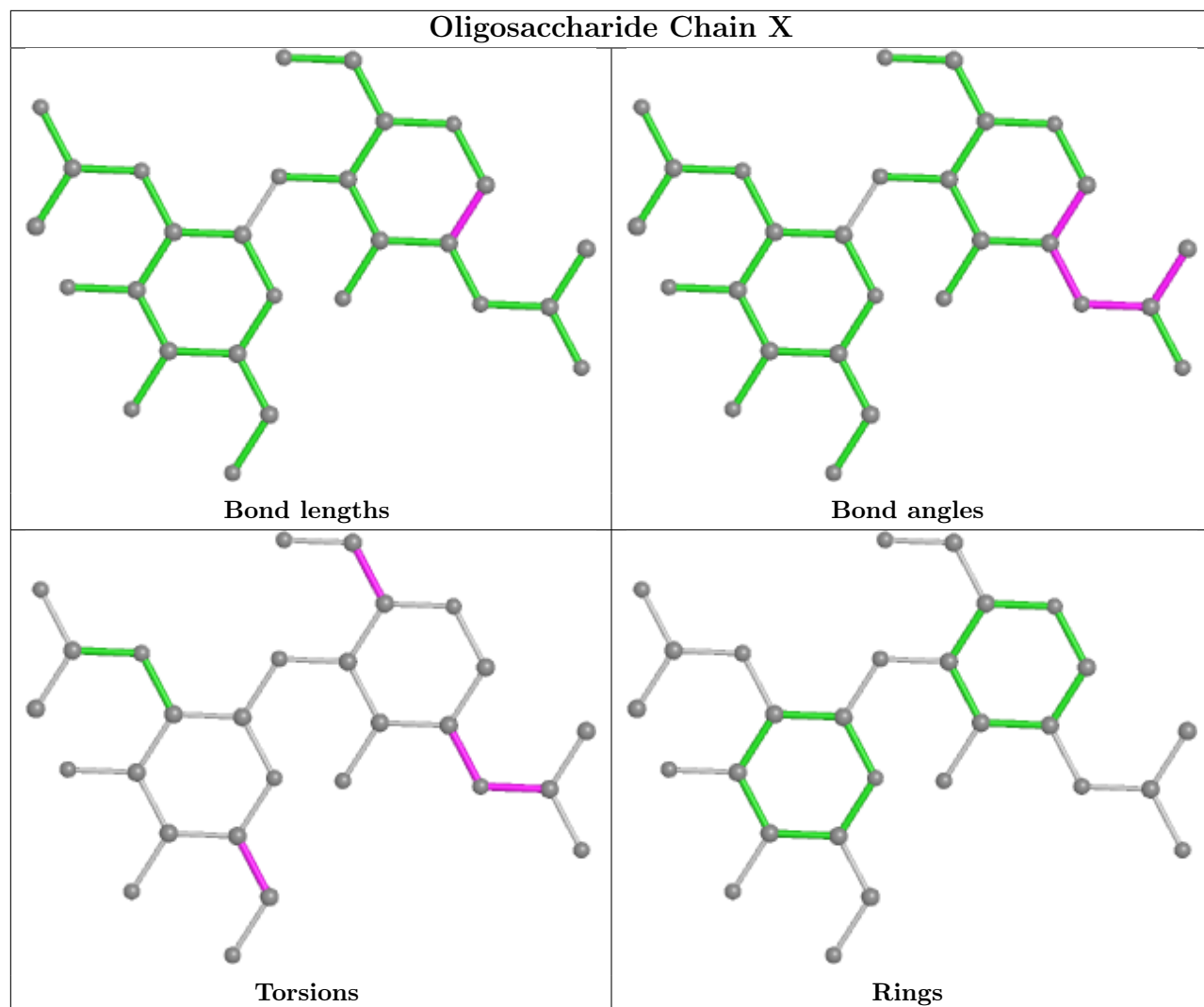




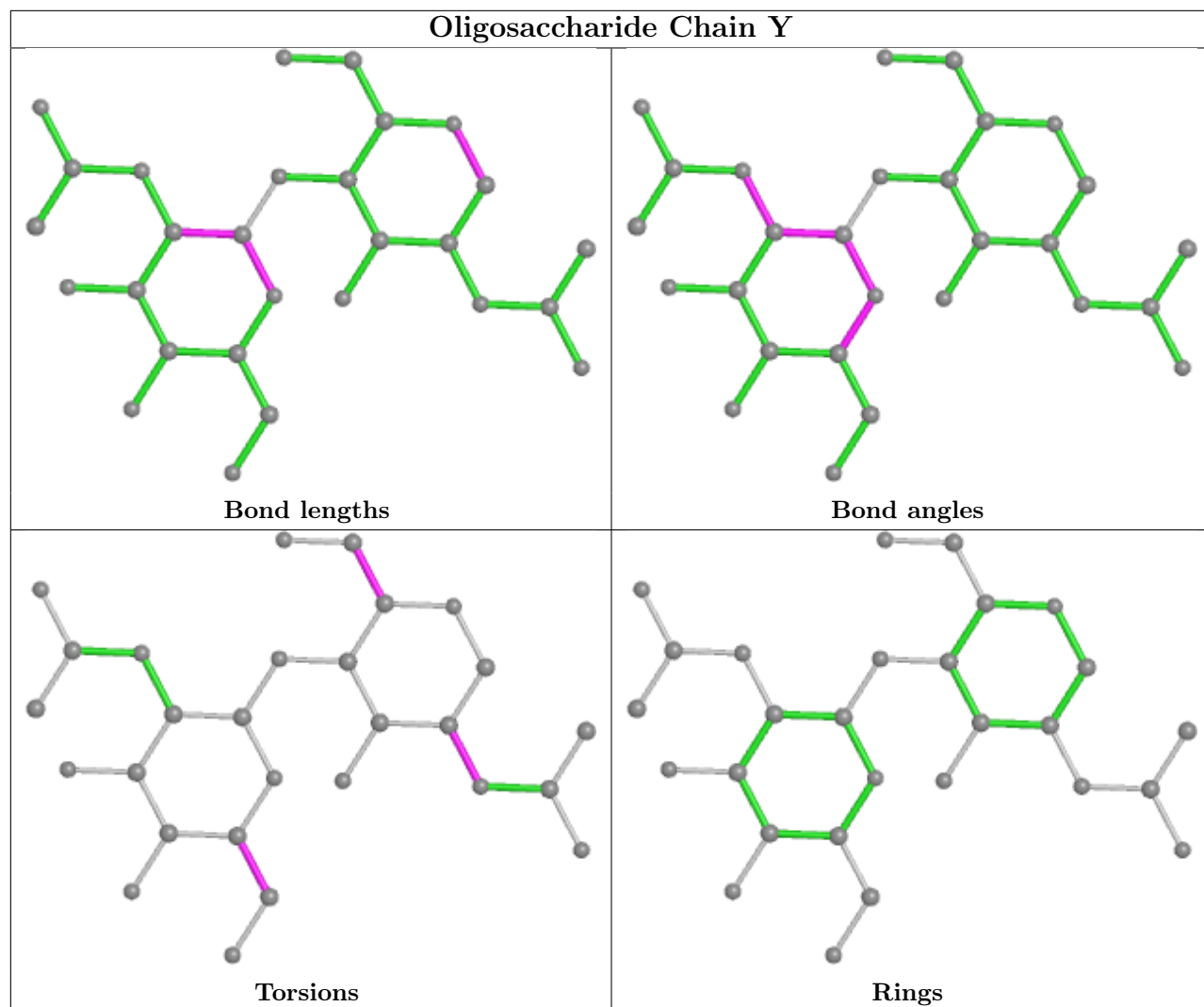


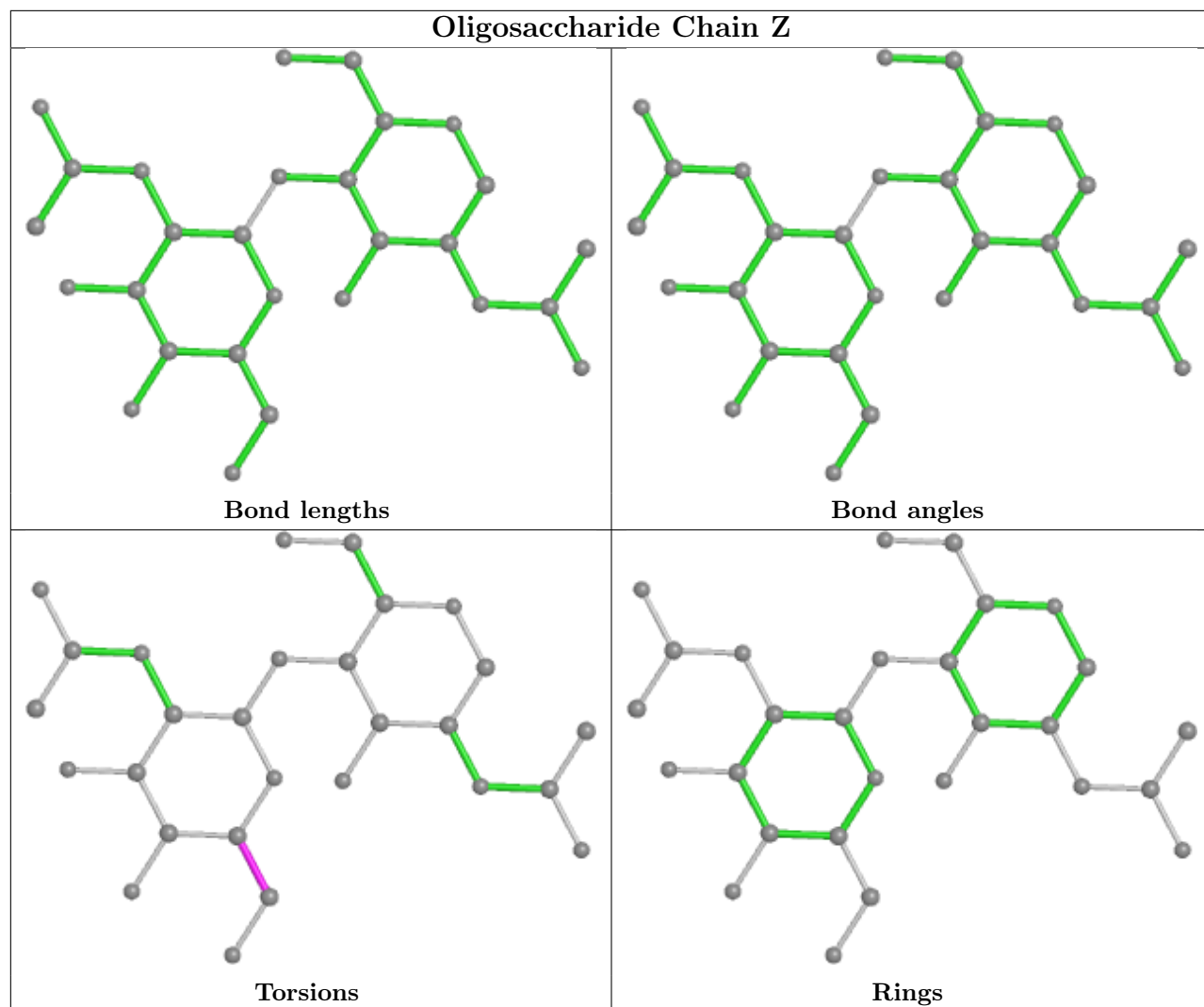


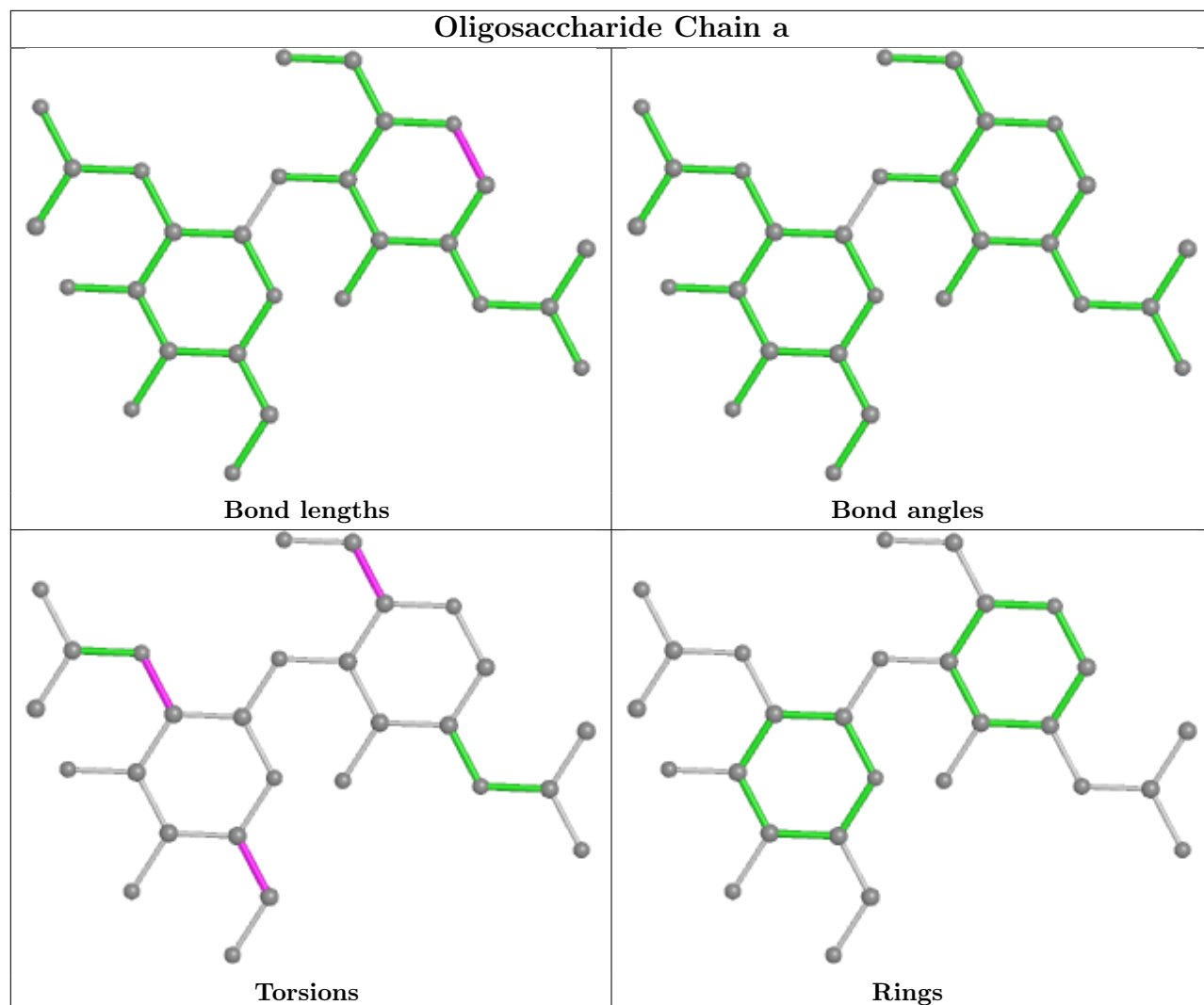


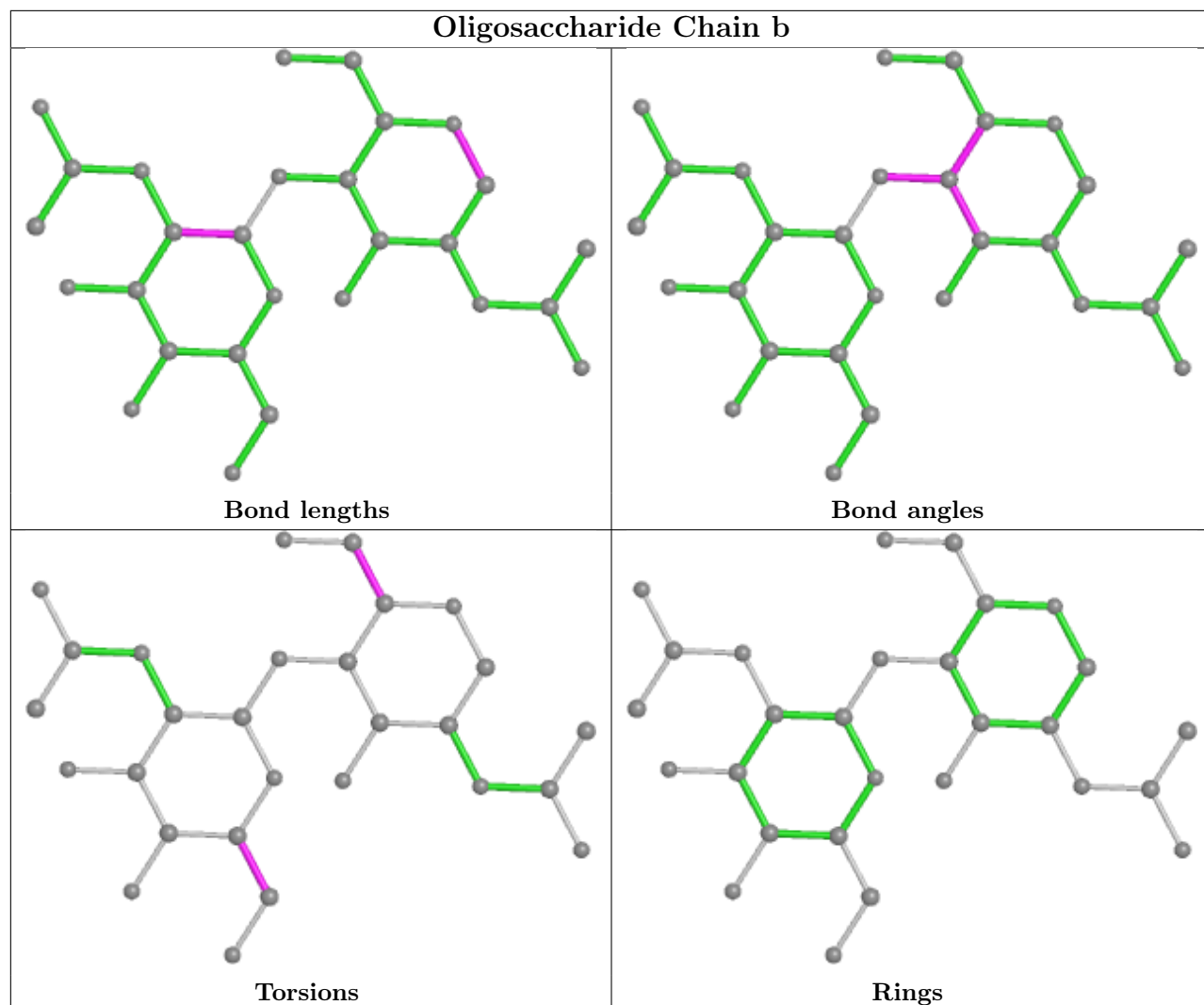


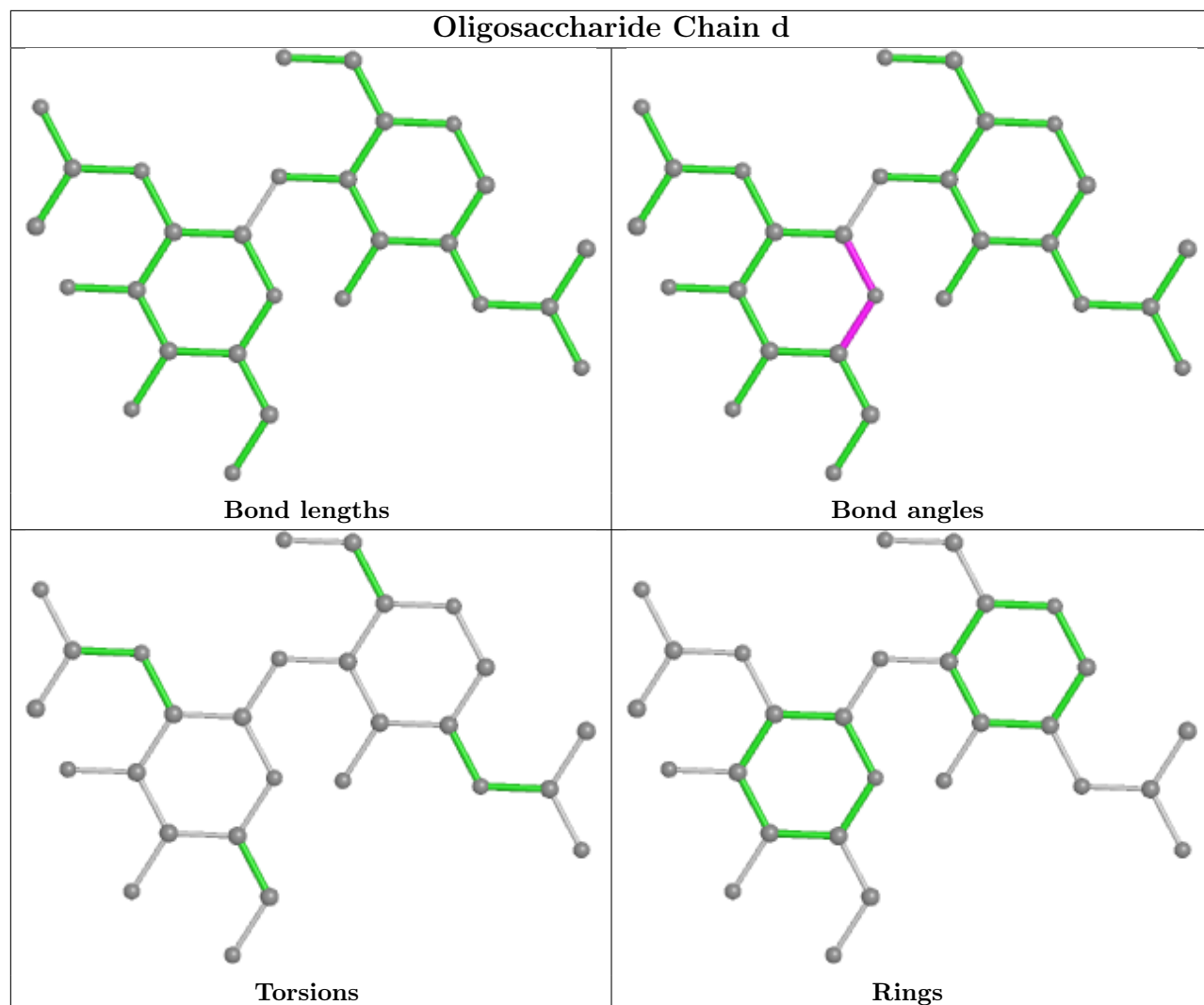


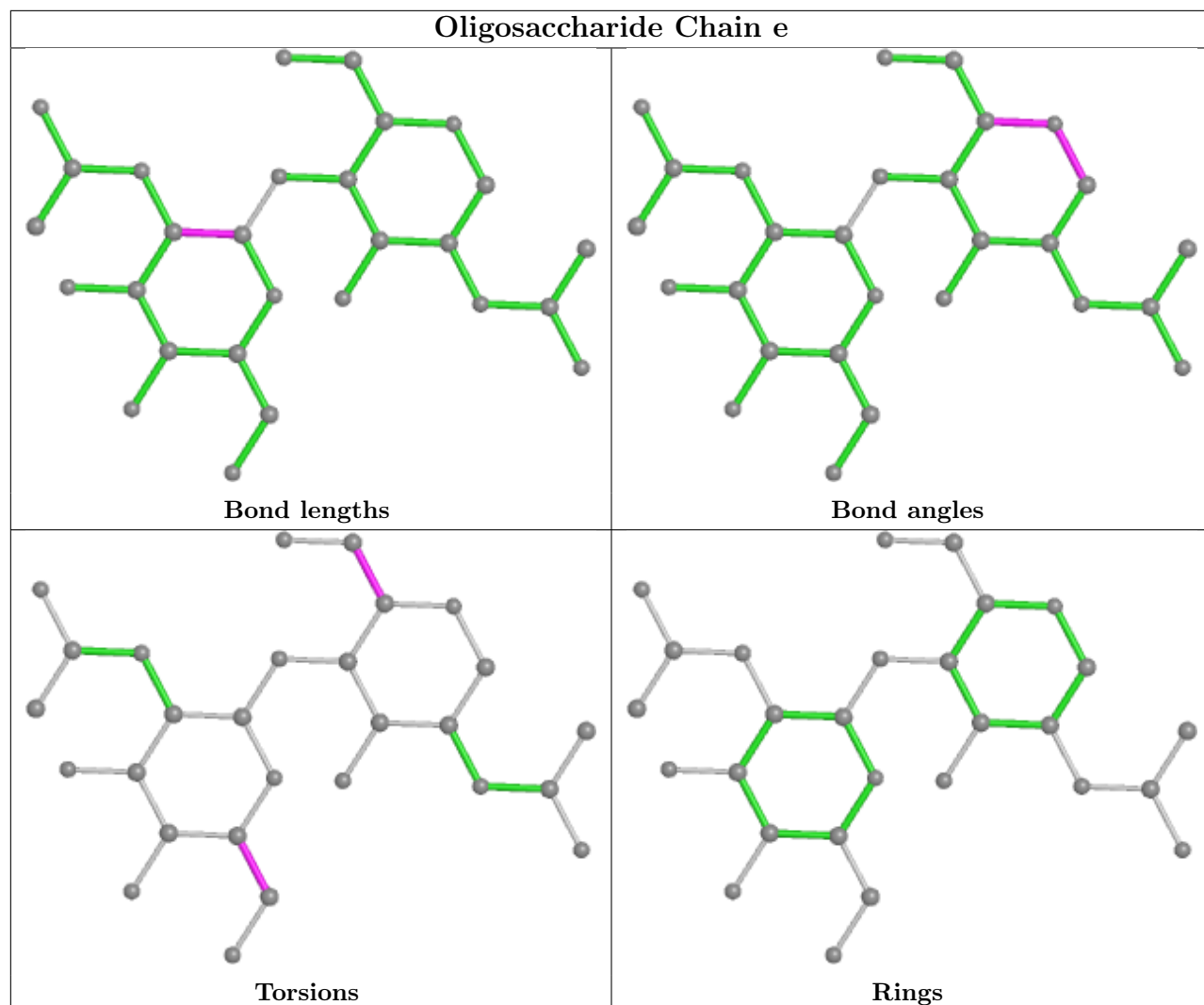


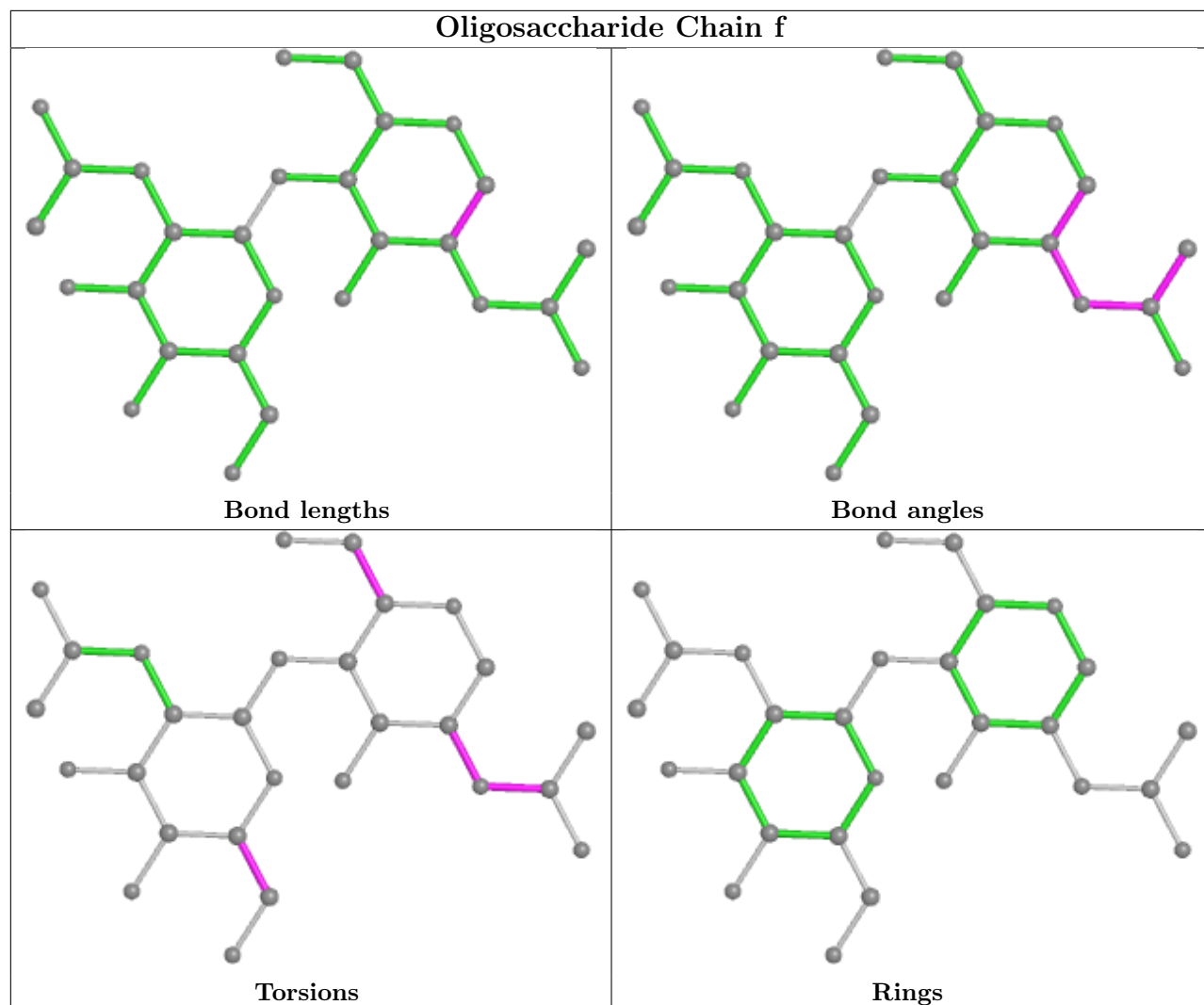


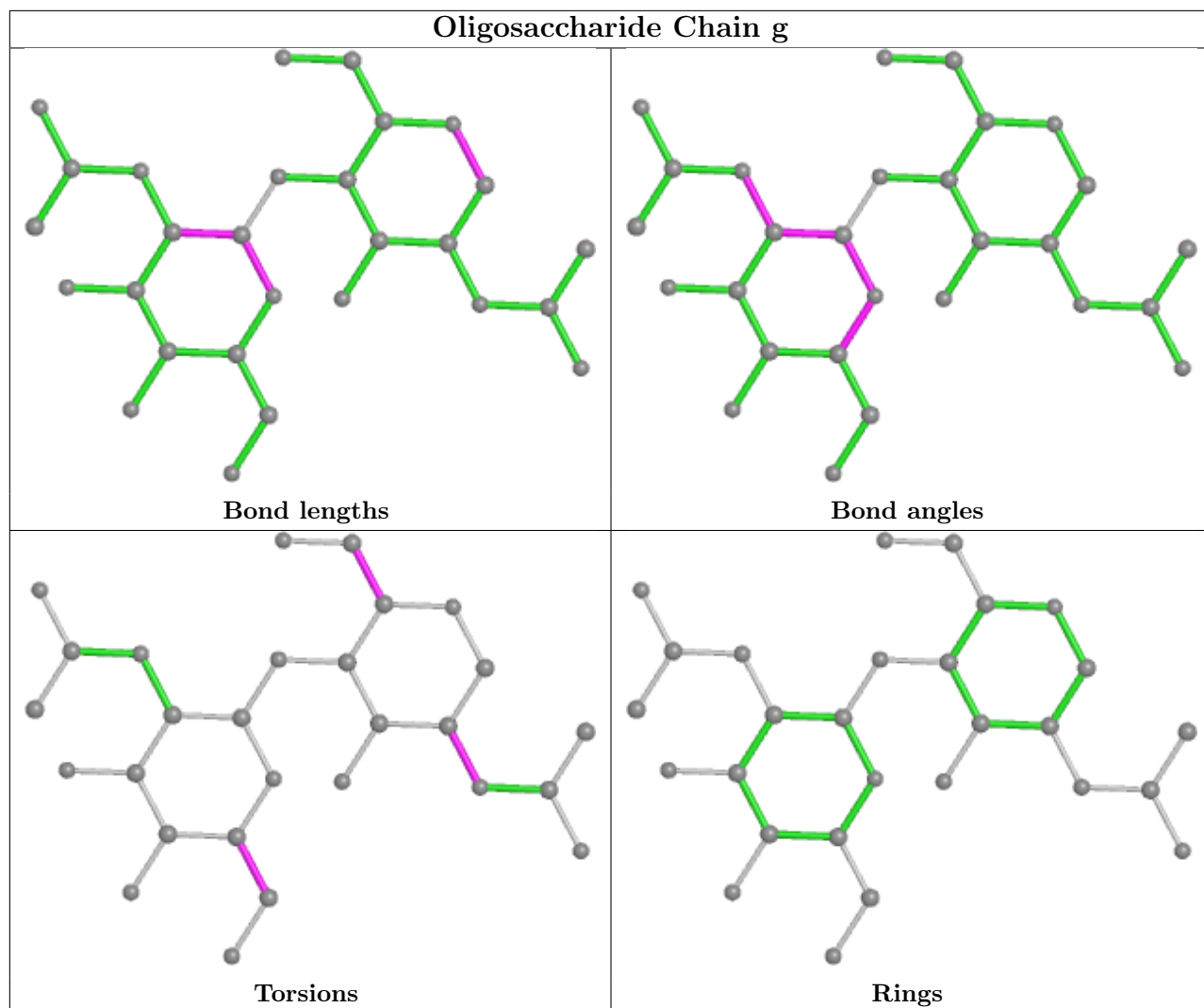




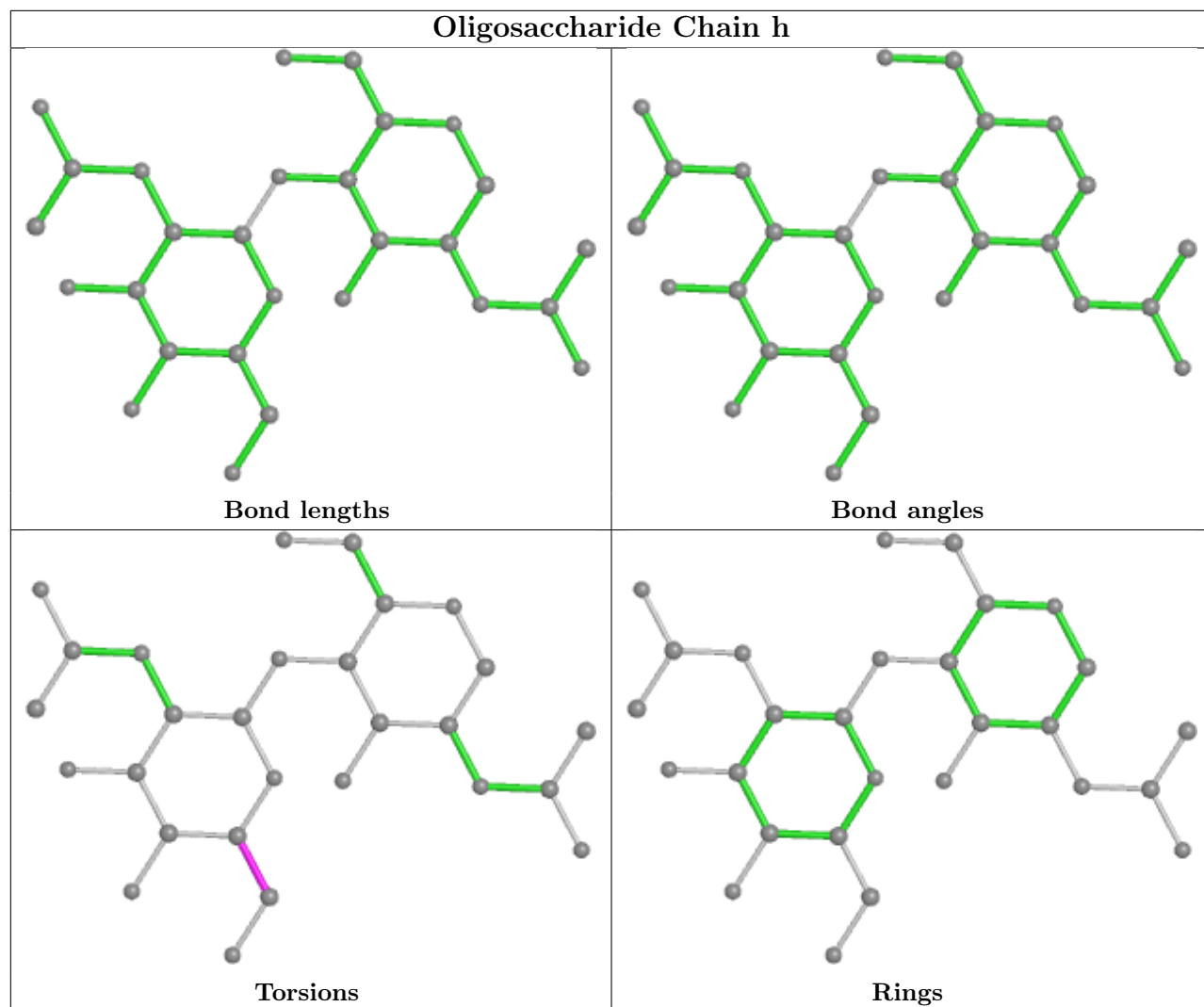


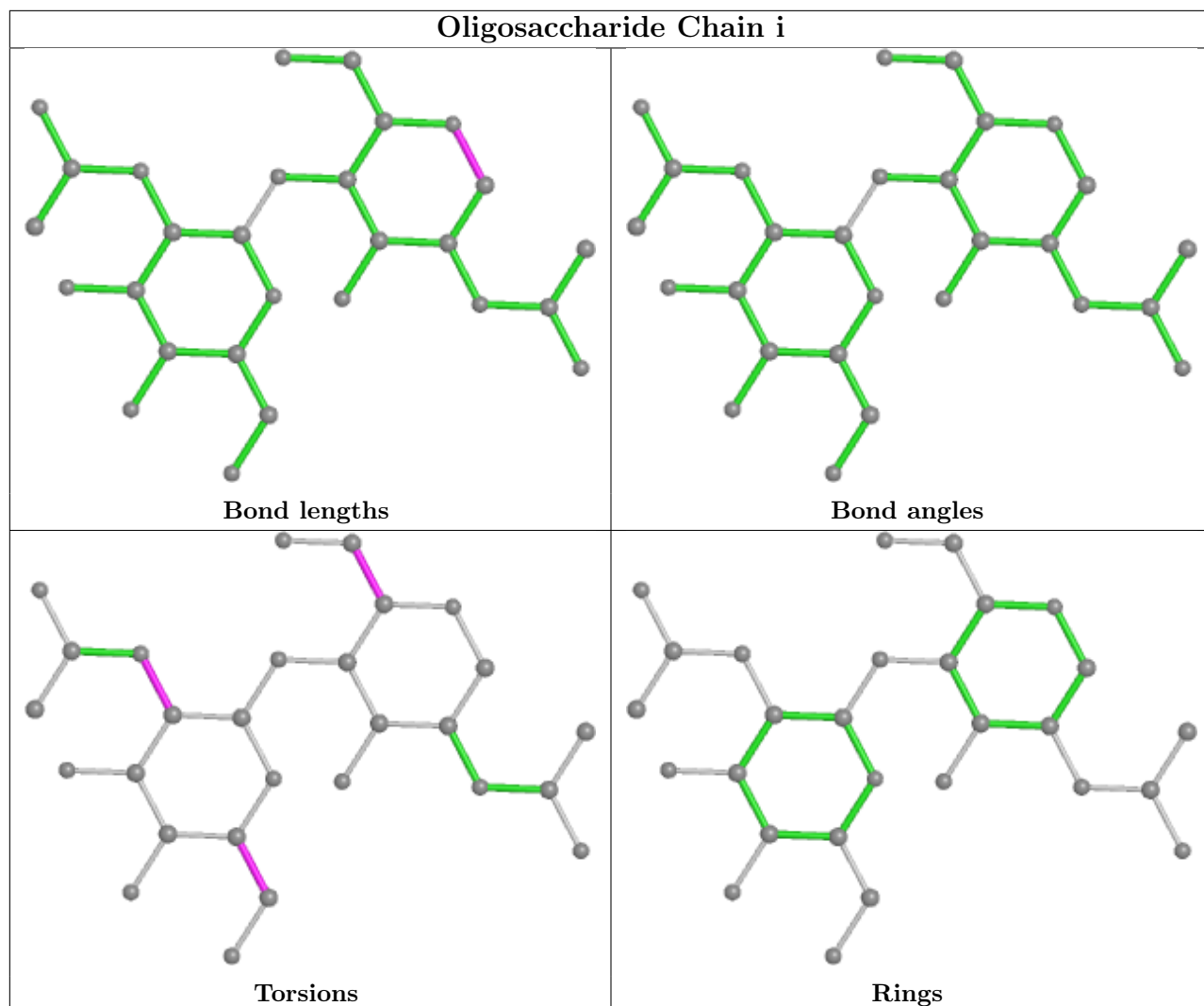


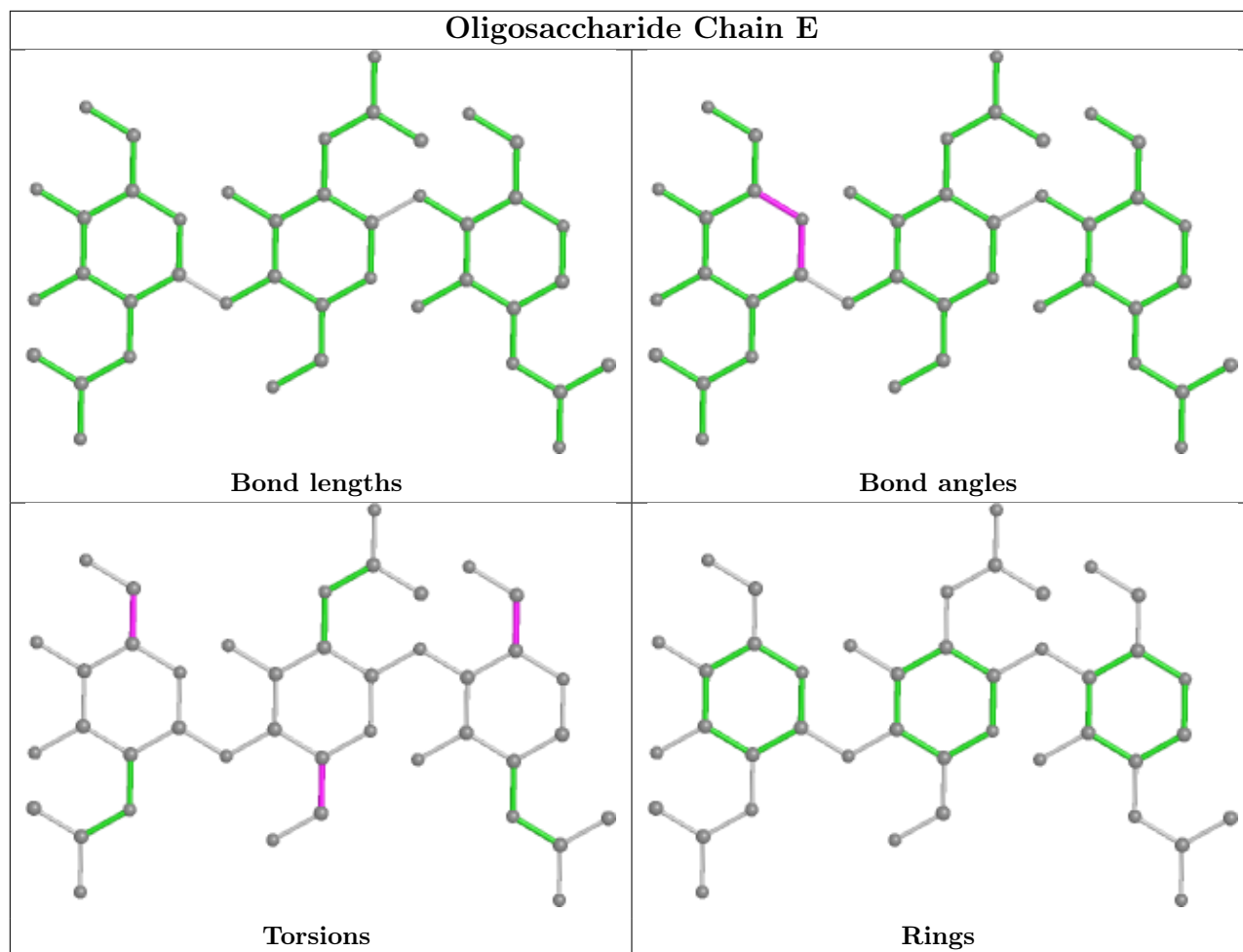


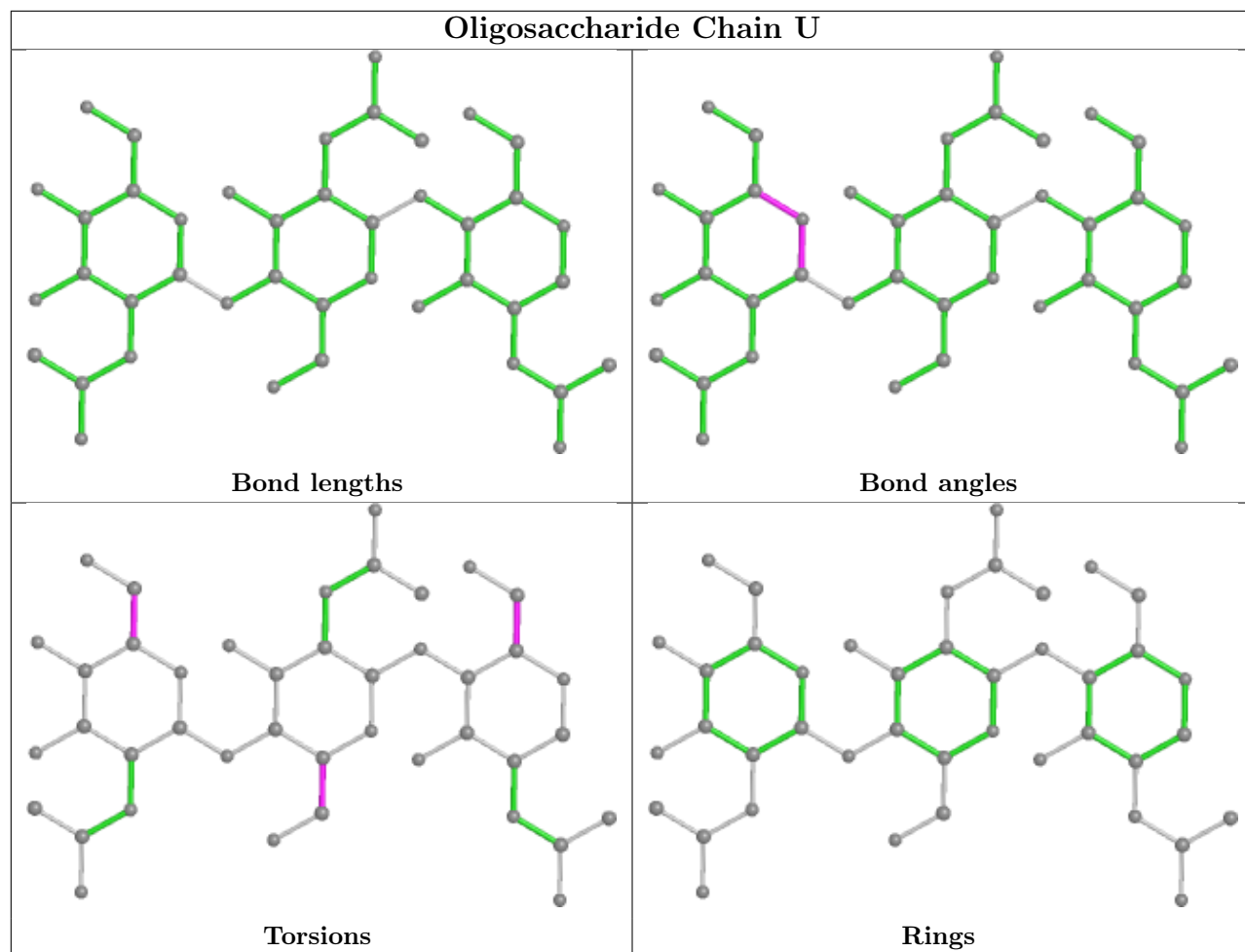


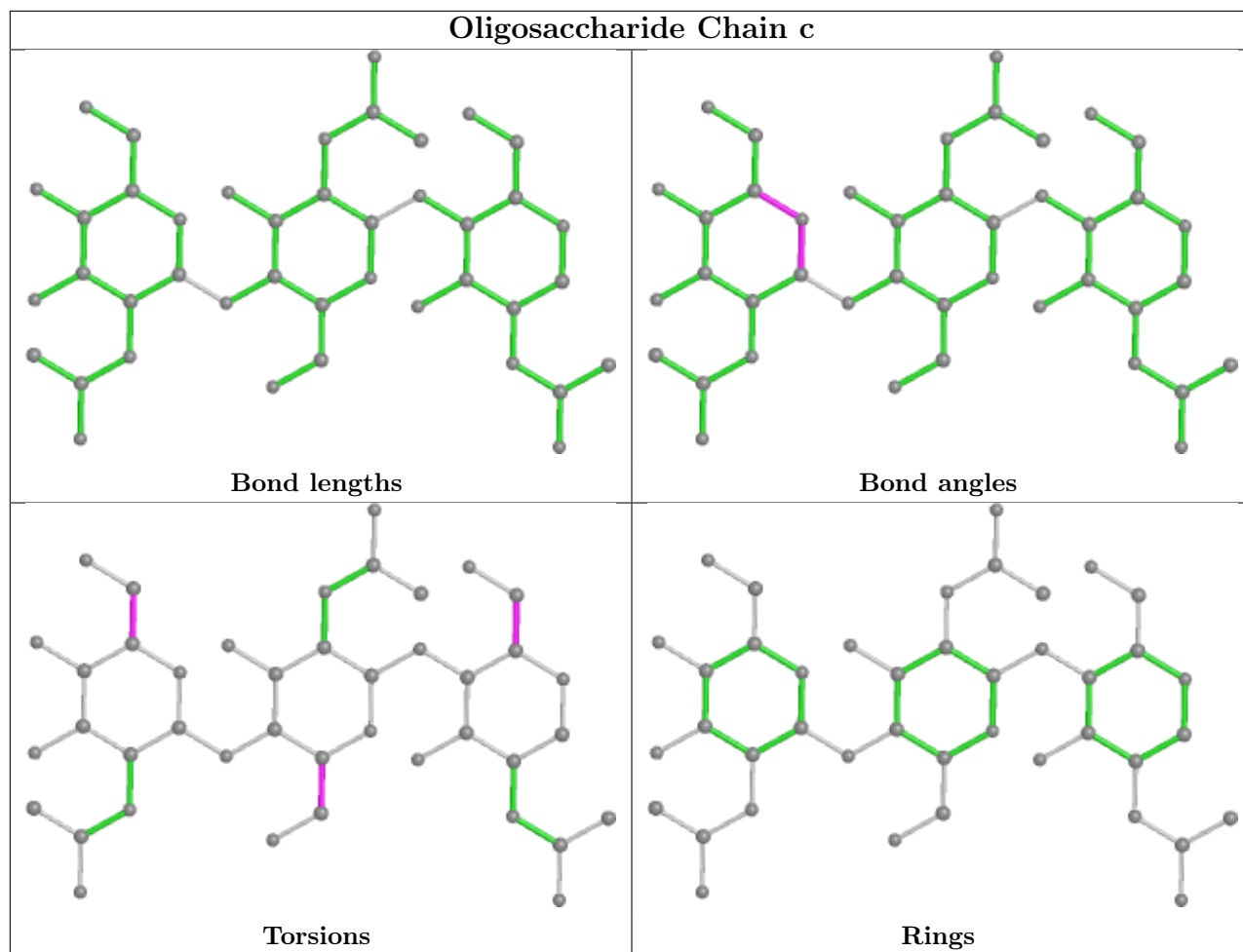












## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
6	NAG	B	1309	1	14,14,15	0.36	0	17,19,21	0.73	0
6	NAG	C	1310	-	14,14,15	0.30	0	17,19,21	1.32	2 (11%)
6	NAG	A	1309	1	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
6	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.63	0
6	NAG	B	1301	1	14,14,15	0.38	0	17,19,21	0.60	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	1307	1	14,14,15	0.38	0	17,19,21	0.72	0
6	NAG	B	1312	-	14,14,15	0.40	0	17,19,21	1.41	3 (17%)
6	NAG	C	1302	1	14,14,15	0.85	1 (7%)	17,19,21	0.56	0
6	NAG	C	1308	1	14,14,15	0.51	0	17,19,21	0.35	0
6	NAG	B	1304	1	14,14,15	0.62	0	17,19,21	0.75	1 (5%)
6	NAG	A	1308	-	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
6	NAG	B	1303	-	14,14,15	2.93	2 (14%)	17,19,21	1.52	4 (23%)
6	NAG	B	1302	1	14,14,15	0.86	1 (7%)	17,19,21	0.55	0
6	NAG	B	1308	1	14,14,15	0.52	0	17,19,21	0.36	0
6	NAG	A	1306	1	14,14,15	0.53	0	17,19,21	0.35	0
6	NAG	C	1312	-	14,14,15	0.42	0	17,19,21	1.41	3 (17%)
6	NAG	B	1306	-	14,14,15	0.42	0	17,19,21	1.16	1 (5%)
6	NAG	B	1314	-	14,14,15	0.16	0	17,19,21	0.47	0
6	NAG	C	1305	1	14,14,15	0.27	0	17,19,21	0.64	0
6	NAG	B	1313	1	14,14,15	0.24	0	17,19,21	0.68	1 (5%)
6	NAG	C	1306	-	14,14,15	0.42	0	17,19,21	1.17	2 (11%)
7	EIC	A	1311	-	19,19,19	0.55	0	19,19,19	0.99	0
6	NAG	C	1311	1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
6	NAG	C	1309	1	14,14,15	0.38	0	17,19,21	0.72	0
6	NAG	B	1307	1	14,14,15	0.26	0	17,19,21	0.63	0
6	NAG	C	1313	1	14,14,15	0.25	0	17,19,21	0.67	1 (5%)
6	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.62	0
6	NAG	A	1302	1	14,14,15	0.62	0	17,19,21	0.74	1 (5%)
6	NAG	A	1304	-	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
6	NAG	B	1311	1	14,14,15	0.71	1 (7%)	17,19,21	0.69	0
6	NAG	A	1310	-	14,14,15	0.16	0	17,19,21	0.47	0
6	NAG	C	1314	-	14,14,15	0.17	0	17,19,21	0.47	0
6	NAG	C	1301	1	14,14,15	0.38	0	17,19,21	0.61	1 (5%)
6	NAG	C	1303	-	14,14,15	2.95	3 (21%)	17,19,21	1.55	4 (23%)
6	NAG	A	1301	1	14,14,15	0.37	0	17,19,21	0.61	1 (5%)
6	NAG	C	1307	1	14,14,15	0.29	0	17,19,21	0.62	0
6	NAG	C	1304	1	14,14,15	0.62	0	17,19,21	0.73	1 (5%)
6	NAG	B	1310	-	14,14,15	0.29	0	17,19,21	1.32	2 (11%)
7	EIC	B	1315	-	19,19,19	0.57	0	19,19,19	0.97	0
7	EIC	C	1315	-	19,19,19	0.58	0	19,19,19	0.95	0
6	NAG	B	1305	1	14,14,15	0.29	0	17,19,21	0.62	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1310	-	-	3/6/23/26	0/1/1/1
6	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	6/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1312	-	-	5/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1308	-	-	3/6/23/26	0/1/1/1
6	NAG	B	1303	-	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1312	-	-	5/6/23/26	0/1/1/1
6	NAG	B	1306	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1314	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	6/6/23/26	0/1/1/1
6	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1306	-	-	0/6/23/26	0/1/1/1
7	EIC	A	1311	-	-	11/17/17/17	-
6	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1310	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1314	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1303	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1310	-	-	3/6/23/26	0/1/1/1
7	EIC	B	1315	-	-	7/17/17/17	-
7	EIC	C	1315	-	-	6/17/17/17	-
6	NAG	B	1305	1	-	6/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1303	NAG	O5-C1	-8.16	1.30	1.43
6	B	1303	NAG	O5-C1	-8.13	1.30	1.43
6	B	1303	NAG	C1-C2	-6.81	1.42	1.52
6	C	1303	NAG	C1-C2	-6.81	1.42	1.52
6	B	1302	NAG	O5-C1	-2.82	1.39	1.43
6	C	1302	NAG	O5-C1	-2.78	1.39	1.43
6	B	1311	NAG	O5-C1	-2.36	1.40	1.43
6	C	1311	NAG	O5-C1	-2.33	1.40	1.43
6	C	1303	NAG	C2-N2	-2.07	1.42	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1312	NAG	C2-N2-C7	4.48	129.29	122.90
6	C	1312	NAG	C2-N2-C7	4.44	129.23	122.90
6	B	1310	NAG	C2-N2-C7	4.30	129.03	122.90
6	C	1310	NAG	C2-N2-C7	4.30	129.03	122.90
6	A	1308	NAG	C2-N2-C7	4.30	129.03	122.90
6	C	1303	NAG	C1-C2-N2	3.32	116.16	110.49
6	C	1303	NAG	O5-C1-C2	3.29	116.48	111.29
6	B	1303	NAG	O5-C1-C2	3.28	116.47	111.29
6	B	1303	NAG	C1-C2-N2	3.27	116.08	110.49
6	C	1303	NAG	C1-O5-C5	3.23	116.57	112.19
6	B	1303	NAG	C1-O5-C5	3.11	116.41	112.19
6	C	1310	NAG	C1-C2-N2	2.37	114.53	110.49
6	B	1312	NAG	C1-C2-N2	2.37	114.53	110.49
6	C	1312	NAG	C1-C2-N2	2.36	114.52	110.49
6	A	1308	NAG	C1-C2-N2	2.35	114.50	110.49
6	A	1304	NAG	C8-C7-N2	2.34	120.06	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1310	NAG	C1-C2-N2	2.33	114.47	110.49
6	C	1306	NAG	C8-C7-N2	2.33	120.04	116.10
6	B	1306	NAG	C8-C7-N2	2.30	120.00	116.10
6	C	1303	NAG	C2-N2-C7	2.24	126.09	122.90
6	B	1304	NAG	C1-O5-C5	2.24	115.23	112.19
6	A	1302	NAG	C1-O5-C5	2.22	115.21	112.19
6	C	1304	NAG	C1-O5-C5	2.17	115.13	112.19
6	B	1303	NAG	C2-N2-C7	2.14	125.94	122.90
6	C	1301	NAG	C1-O5-C5	2.12	115.06	112.19
6	C	1312	NAG	C1-O5-C5	2.11	115.05	112.19
6	B	1312	NAG	C1-O5-C5	2.11	115.05	112.19
6	A	1301	NAG	C1-O5-C5	2.10	115.04	112.19
6	B	1313	NAG	C1-O5-C5	2.09	115.02	112.19
6	B	1301	NAG	C1-O5-C5	2.08	115.01	112.19
6	A	1309	NAG	C1-O5-C5	2.07	115.00	112.19
6	C	1313	NAG	C1-O5-C5	2.01	114.92	112.19
6	C	1306	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1305	NAG	C8-C7-N2-C2
6	A	1305	NAG	O7-C7-N2-C2
6	B	1307	NAG	C8-C7-N2-C2
6	B	1307	NAG	O7-C7-N2-C2
6	C	1307	NAG	C8-C7-N2-C2
6	C	1307	NAG	O7-C7-N2-C2
6	A	1303	NAG	O5-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	C	1305	NAG	O5-C5-C6-O6
6	A	1303	NAG	C8-C7-N2-C2
6	B	1305	NAG	C8-C7-N2-C2
6	C	1305	NAG	C8-C7-N2-C2
6	A	1301	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	A	1303	NAG	C4-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	1301	NAG	C4-C5-C6-O6
6	A	1303	NAG	C1-C2-N2-C7
6	B	1305	NAG	C1-C2-N2-C7
6	C	1305	NAG	C1-C2-N2-C7
6	A	1306	NAG	C4-C5-C6-O6
6	B	1308	NAG	C4-C5-C6-O6
6	C	1308	NAG	C4-C5-C6-O6
6	A	1303	NAG	O7-C7-N2-C2
6	A	1308	NAG	C8-C7-N2-C2
6	A	1308	NAG	O7-C7-N2-C2
6	B	1305	NAG	O7-C7-N2-C2
6	B	1310	NAG	C8-C7-N2-C2
6	B	1310	NAG	O7-C7-N2-C2
6	B	1312	NAG	C8-C7-N2-C2
6	B	1312	NAG	O7-C7-N2-C2
6	C	1305	NAG	O7-C7-N2-C2
6	C	1310	NAG	C8-C7-N2-C2
6	C	1310	NAG	O7-C7-N2-C2
6	C	1312	NAG	C8-C7-N2-C2
6	C	1312	NAG	O7-C7-N2-C2
6	B	1311	NAG	C4-C5-C6-O6
6	C	1311	NAG	C4-C5-C6-O6
6	A	1306	NAG	O5-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	B	1309	NAG	C4-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	A	1302	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
7	A	1311	EIC	C1-C2-C3-C4
6	A	1305	NAG	O5-C5-C6-O6
6	B	1307	NAG	O5-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	C	1304	NAG	C4-C5-C6-O6
6	B	1307	NAG	C1-C2-N2-C7
6	A	1307	NAG	O5-C5-C6-O6
6	B	1309	NAG	O5-C5-C6-O6
6	C	1309	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	B	1311	NAG	O5-C5-C6-O6
6	C	1311	NAG	O5-C5-C6-O6
7	C	1315	EIC	C4-C5-C6-C7
6	A	1305	NAG	C1-C2-N2-C7
6	C	1307	NAG	C1-C2-N2-C7
7	A	1311	EIC	C5-C6-C7-C8
7	A	1311	EIC	C13-C14-C15-C16
6	A	1309	NAG	C4-C5-C6-O6
6	C	1313	NAG	C4-C5-C6-O6
6	B	1313	NAG	C4-C5-C6-O6
6	C	1313	NAG	O5-C5-C6-O6
6	A	1309	NAG	O5-C5-C6-O6
6	B	1313	NAG	O5-C5-C6-O6
7	A	1311	EIC	C14-C15-C16-C17
7	A	1311	EIC	C15-C16-C17-C18
7	A	1311	EIC	C6-C7-C8-C9
6	A	1303	NAG	C3-C2-N2-C7
6	B	1305	NAG	C3-C2-N2-C7
6	C	1305	NAG	C3-C2-N2-C7
7	C	1315	EIC	C2-C3-C4-C5
7	B	1315	EIC	C4-C5-C6-C7
7	A	1311	EIC	C10-C11-C12-C13
7	B	1315	EIC	C10-C11-C12-C13
7	C	1315	EIC	C5-C6-C7-C8
7	B	1315	EIC	C15-C16-C17-C18
6	B	1312	NAG	C4-C5-C6-O6
6	C	1312	NAG	C4-C5-C6-O6
7	C	1315	EIC	O1-C1-C2-C3
7	A	1311	EIC	C9-C10-C11-C12
6	B	1312	NAG	O5-C5-C6-O6
7	B	1315	EIC	C7-C8-C9-C10
7	C	1315	EIC	O2-C1-C2-C3
6	C	1312	NAG	O5-C5-C6-O6
7	A	1311	EIC	C4-C5-C6-C7
6	C	1302	NAG	C4-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
7	B	1315	EIC	O1-C1-C2-C3
7	B	1315	EIC	O2-C1-C2-C3
7	C	1315	EIC	C7-C8-C9-C10
7	B	1315	EIC	C14-C15-C16-C17
6	A	1308	NAG	C3-C2-N2-C7
6	B	1303	NAG	C3-C2-N2-C7

*Continued on next page...*

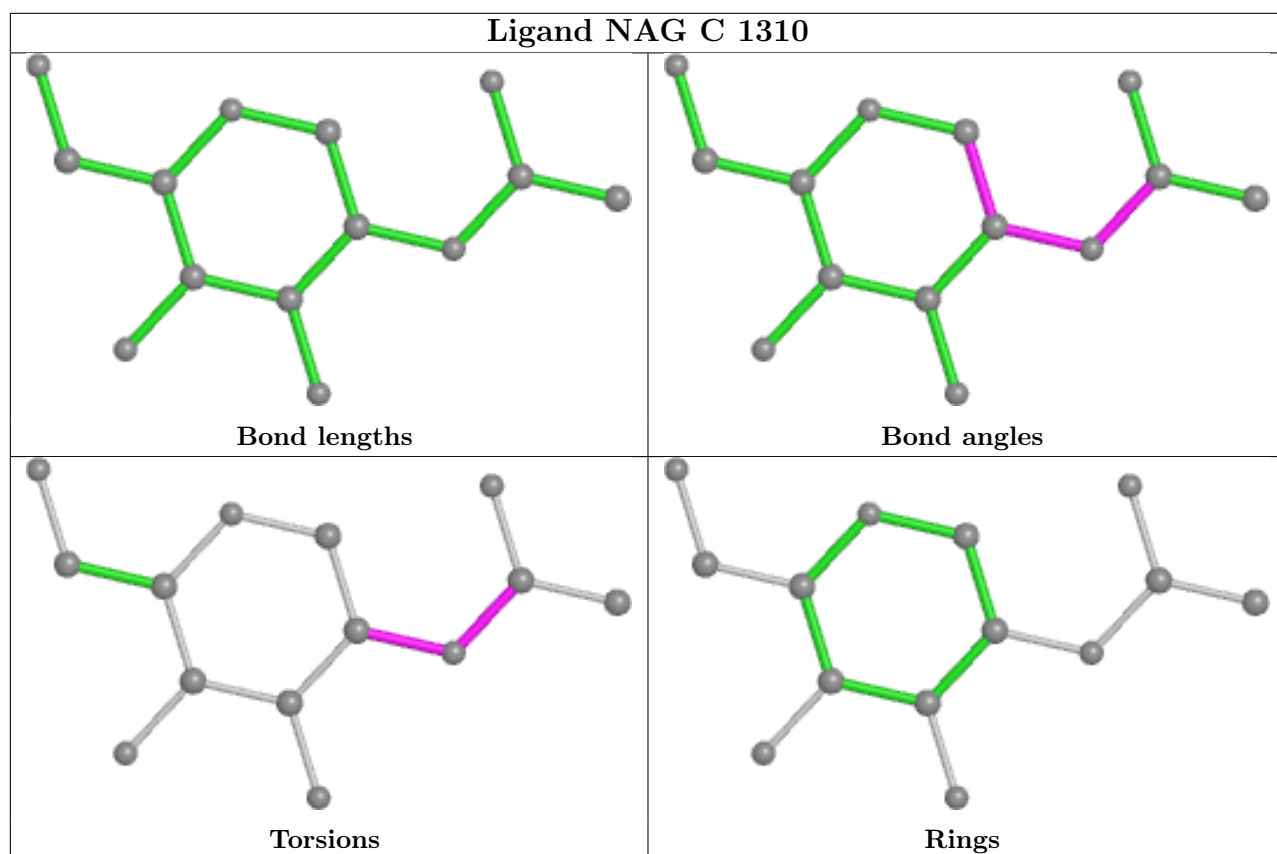
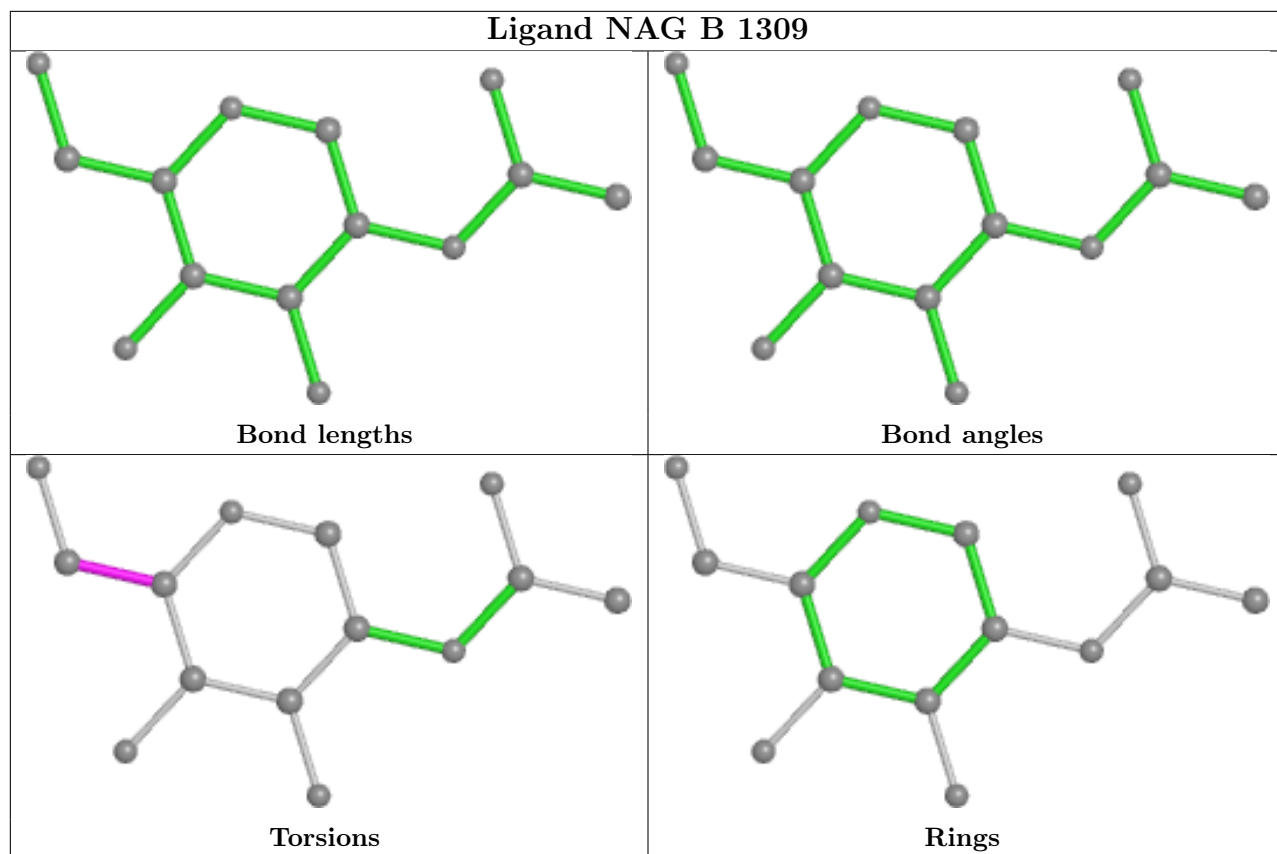
*Continued from previous page...*

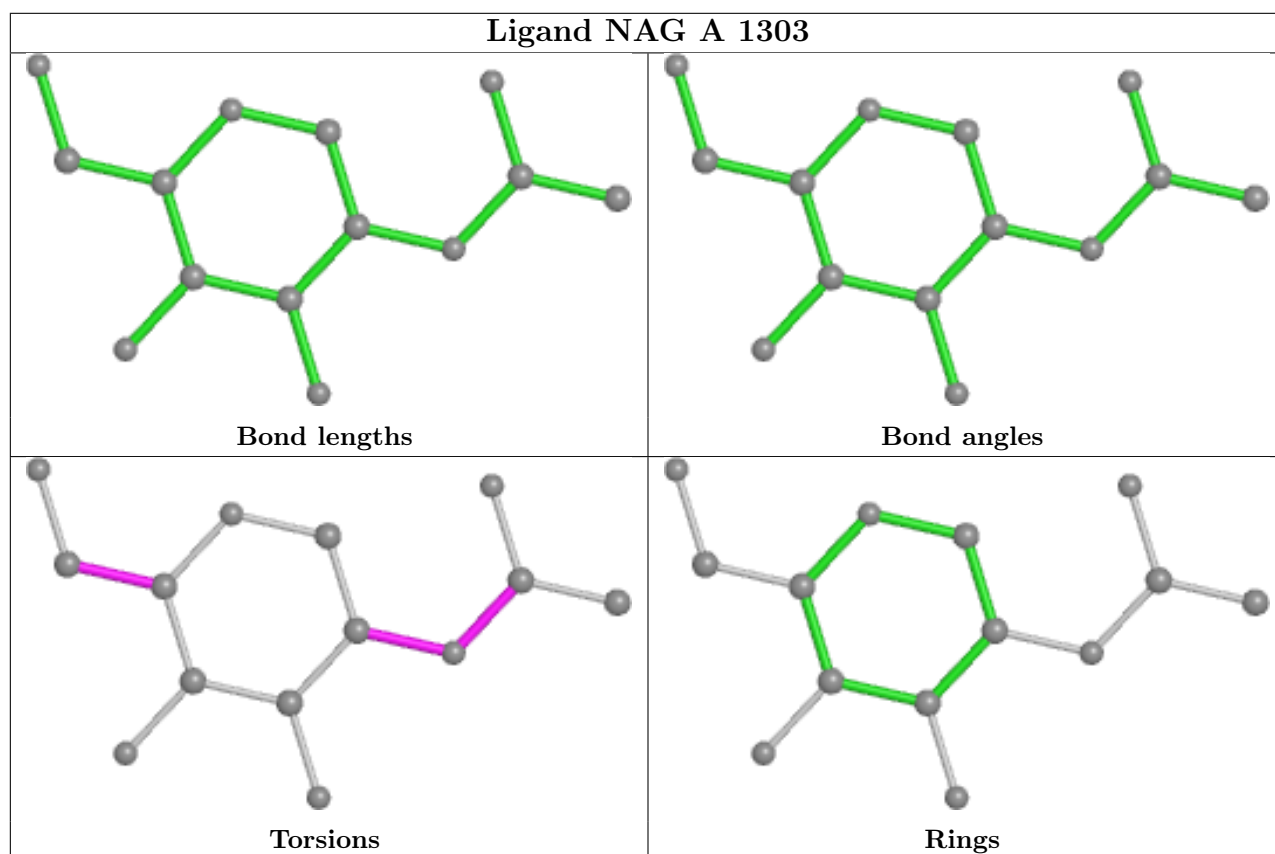
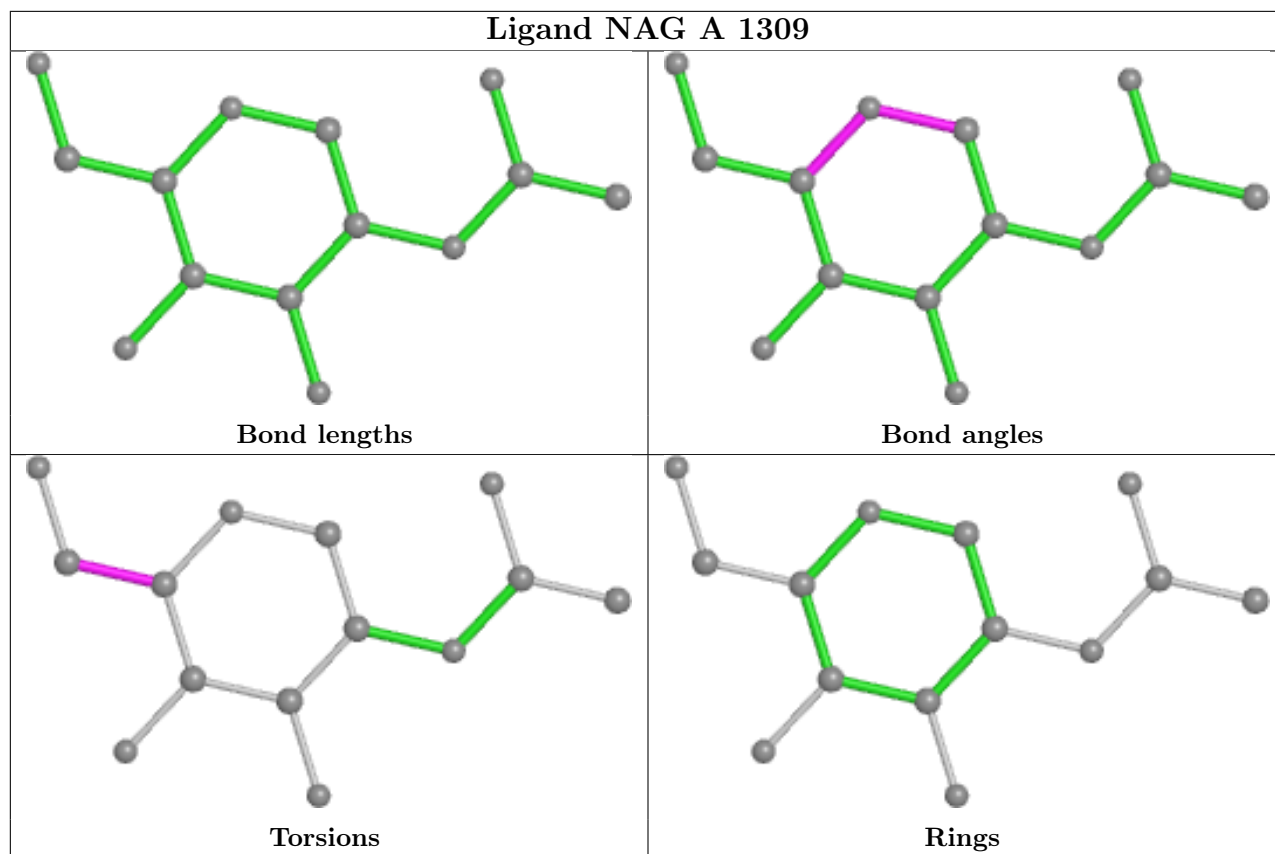
Mol	Chain	Res	Type	Atoms
6	B	1310	NAG	C3-C2-N2-C7
6	B	1312	NAG	C3-C2-N2-C7
6	C	1303	NAG	C3-C2-N2-C7
6	C	1310	NAG	C3-C2-N2-C7
6	C	1312	NAG	C3-C2-N2-C7
7	A	1311	EIC	C7-C8-C9-C10
6	B	1303	NAG	C1-C2-N2-C7
6	C	1303	NAG	C1-C2-N2-C7
7	A	1311	EIC	C12-C13-C14-C15

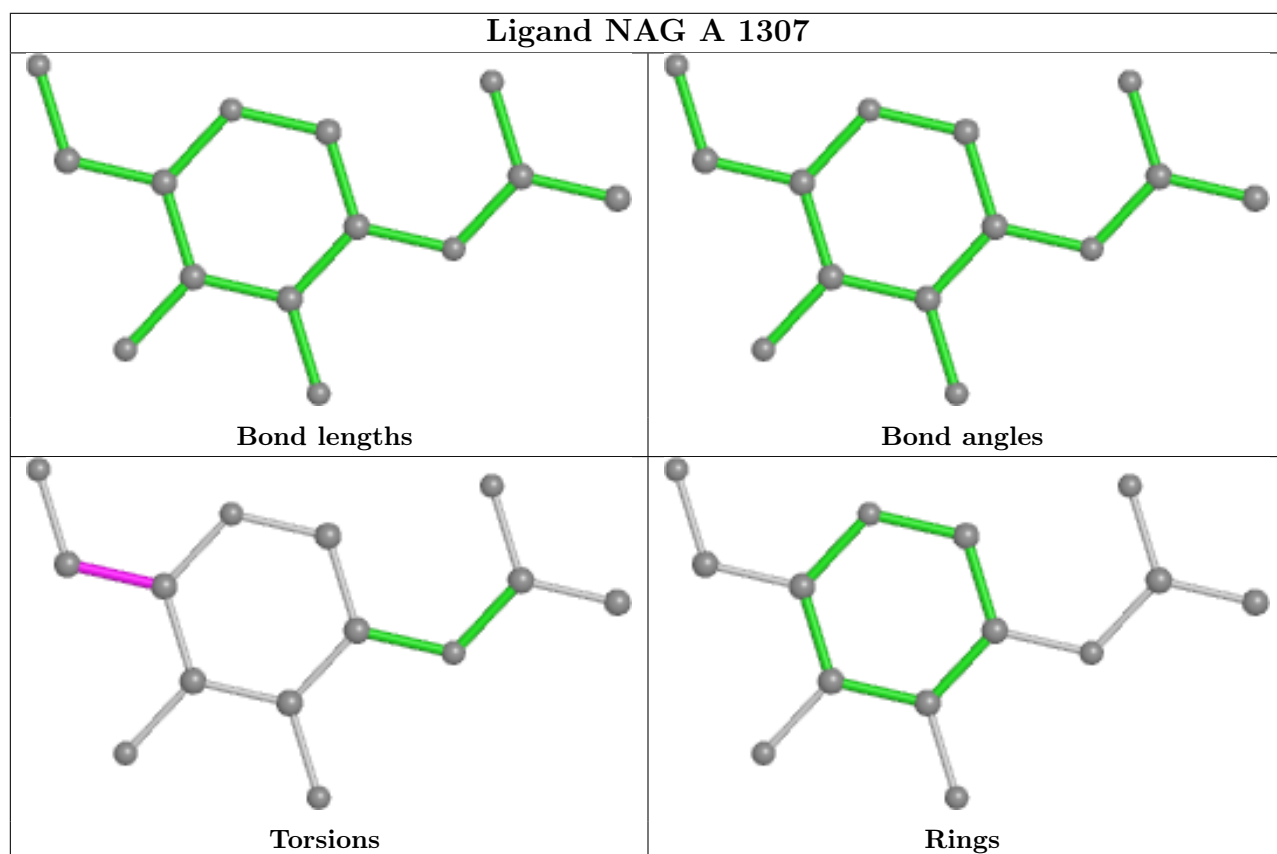
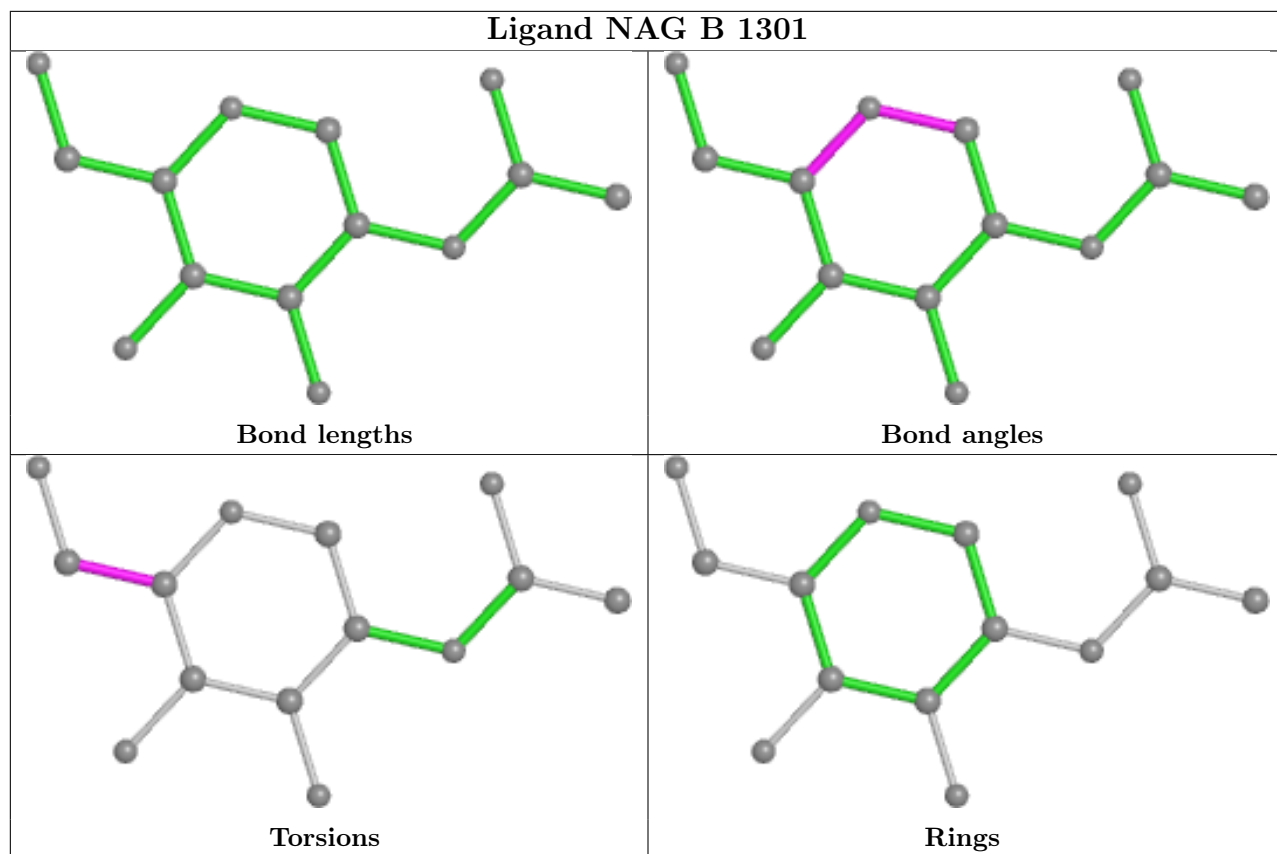
There are no ring outliers.

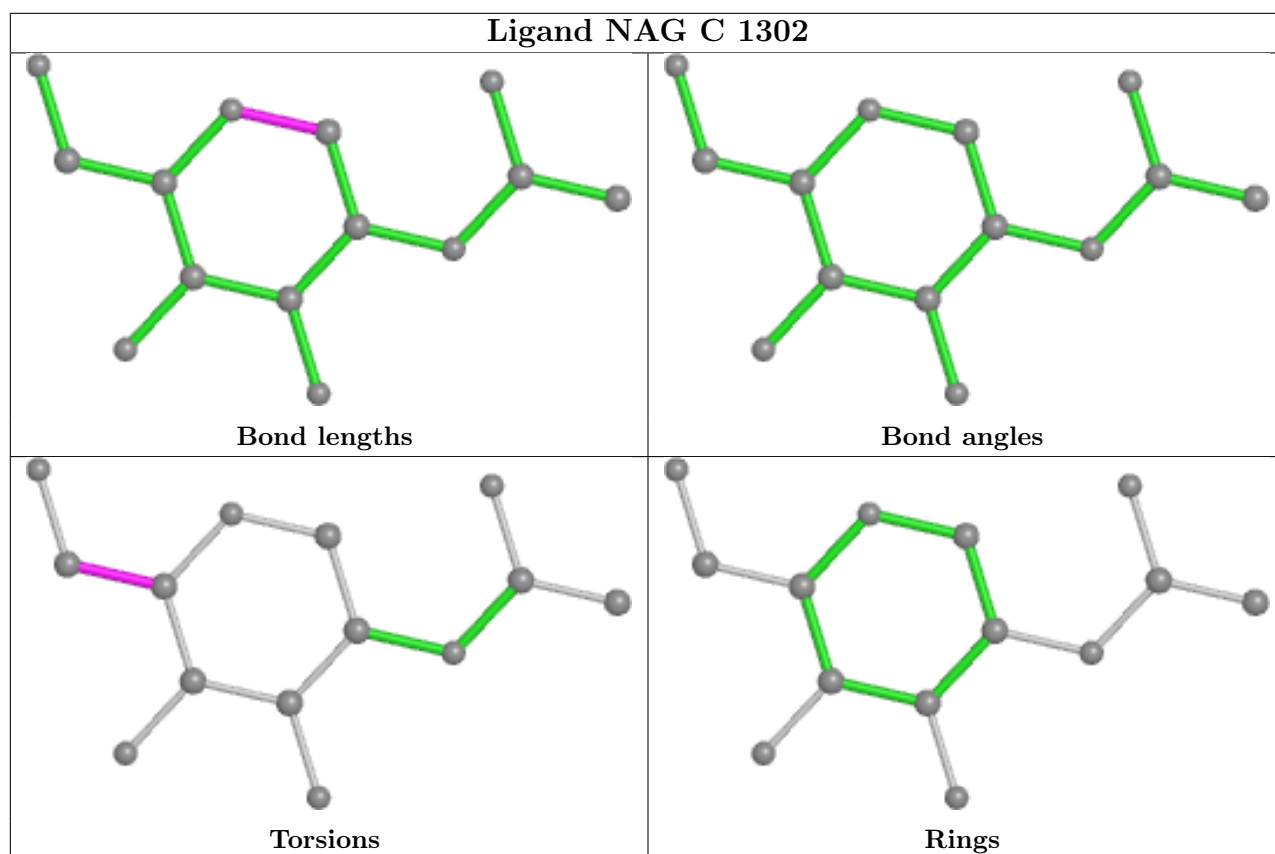
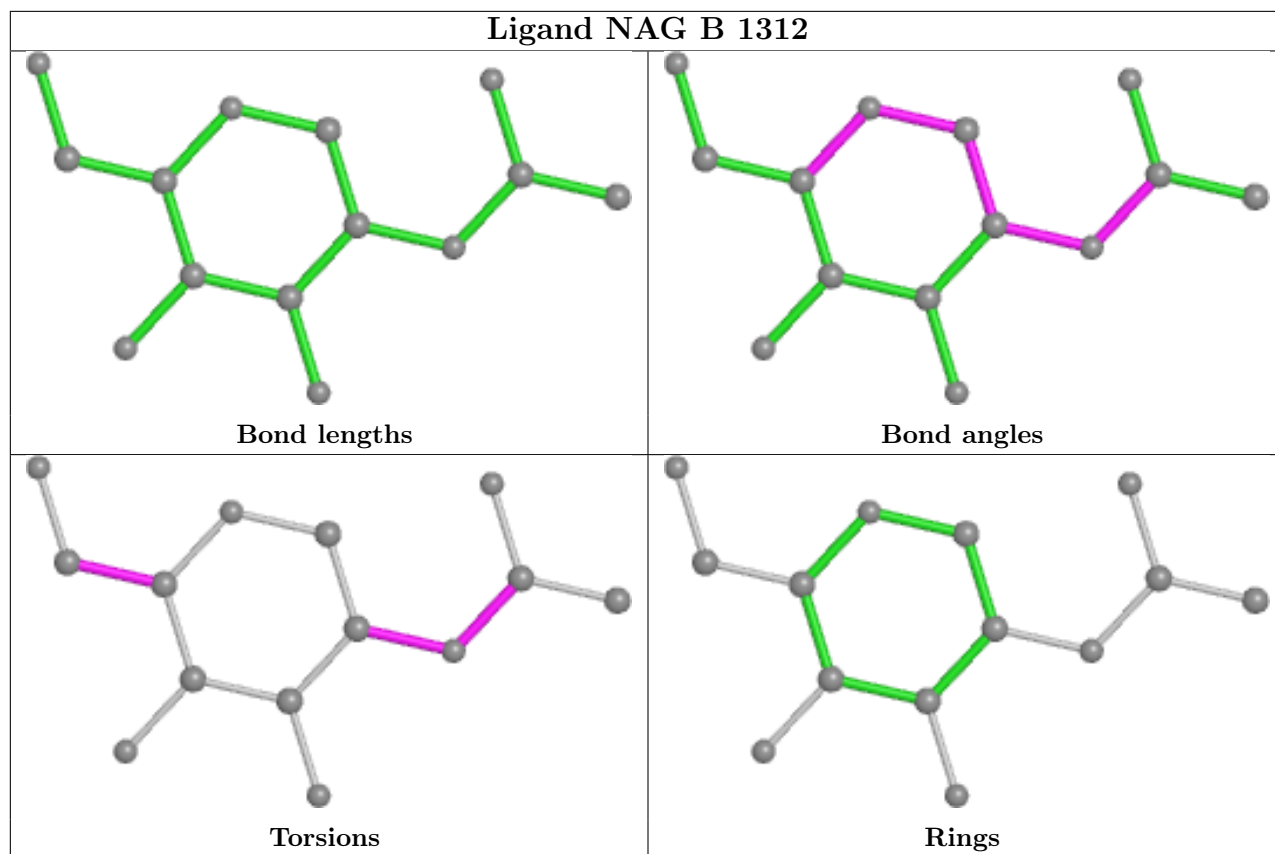
No monomer is involved in short contacts.

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.

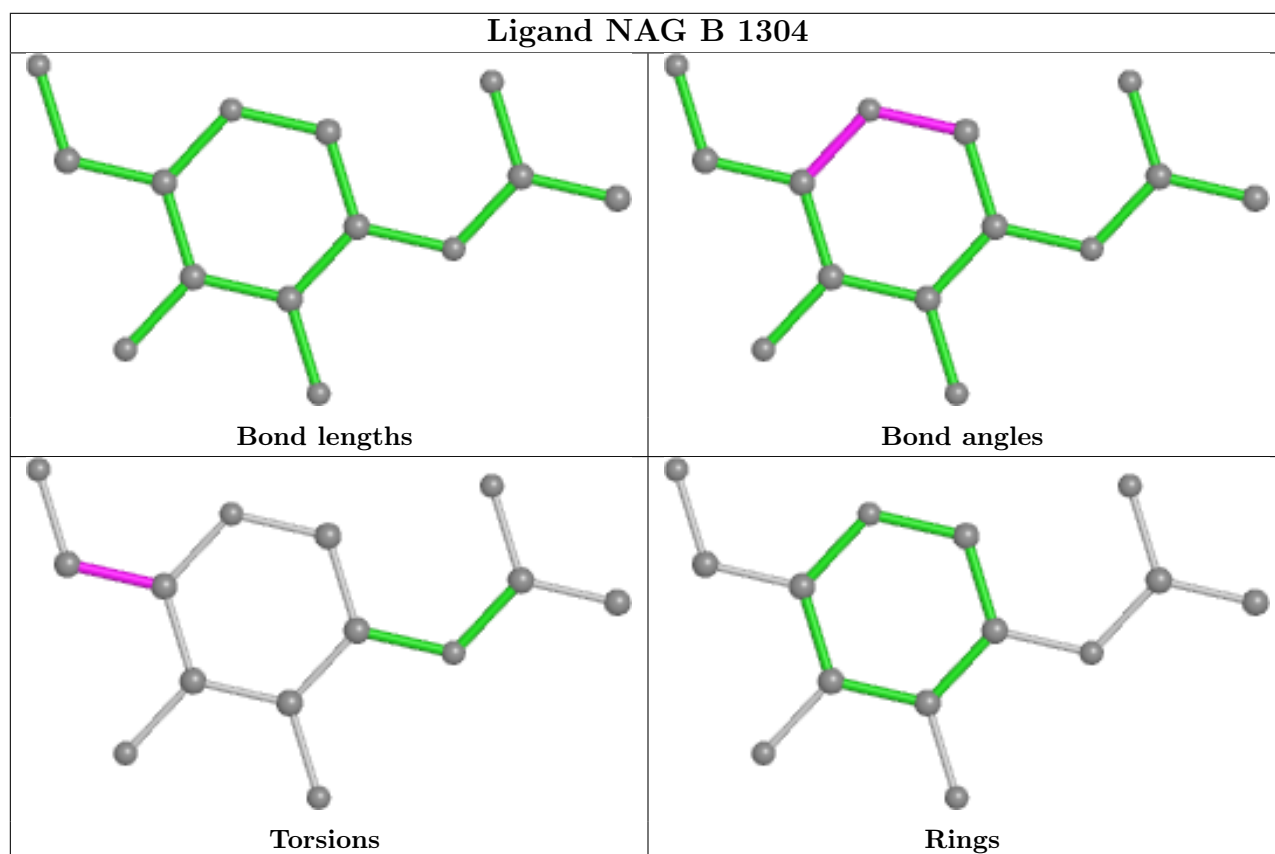
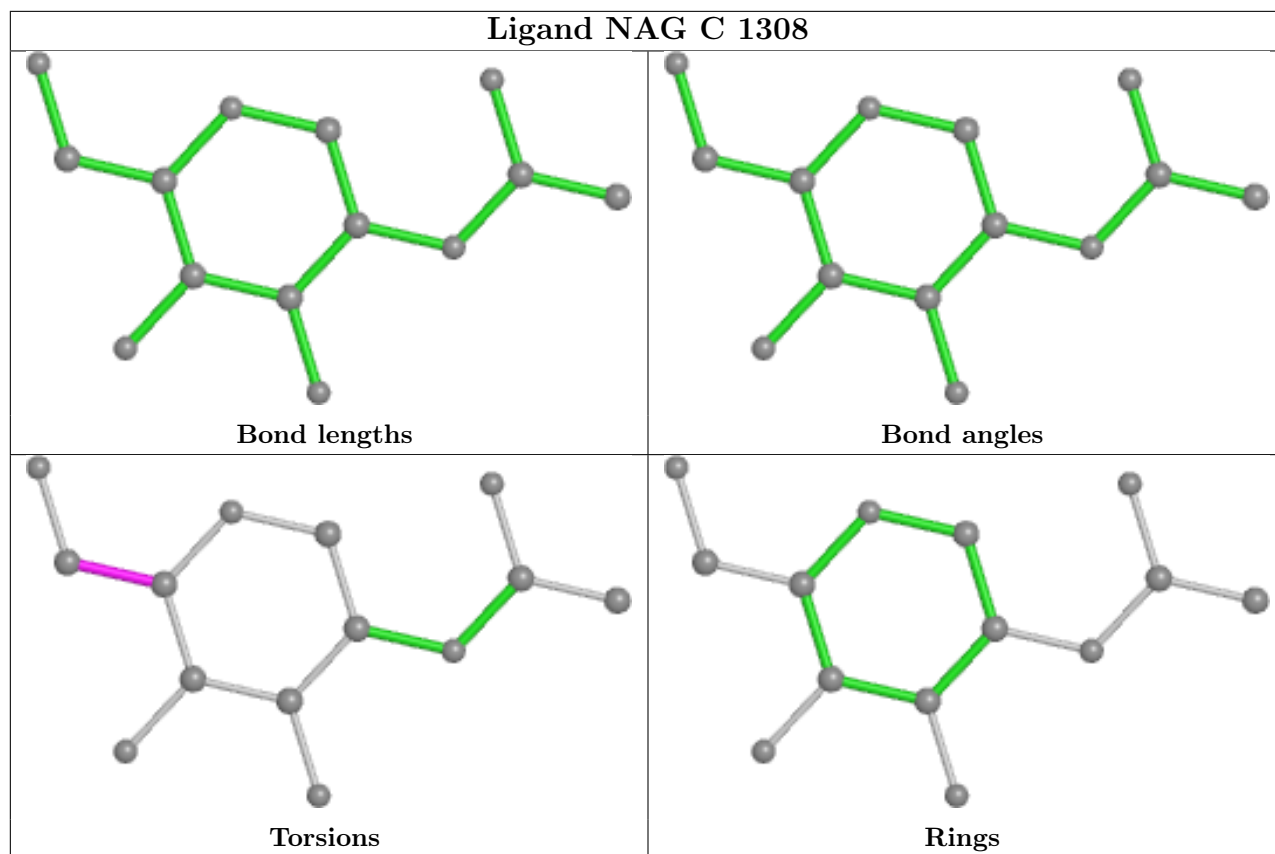


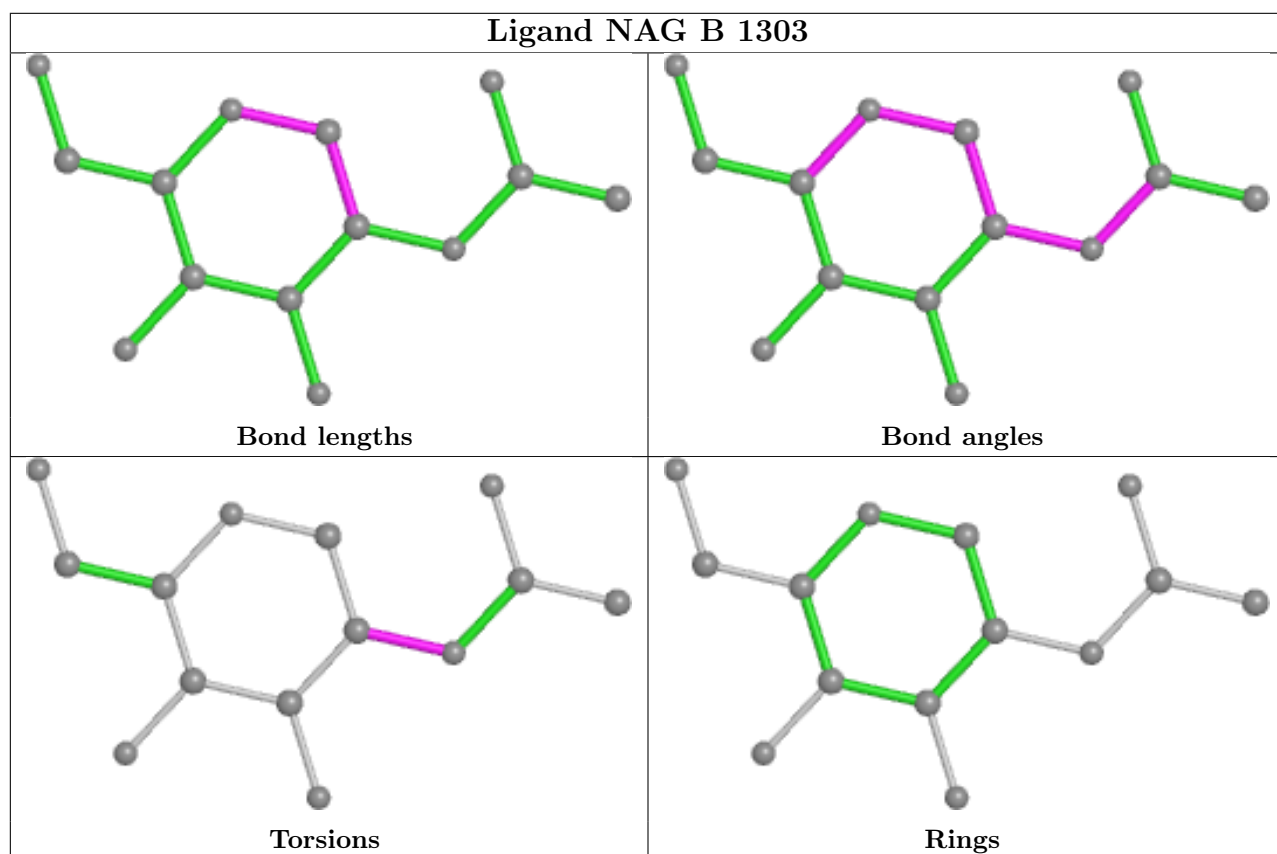
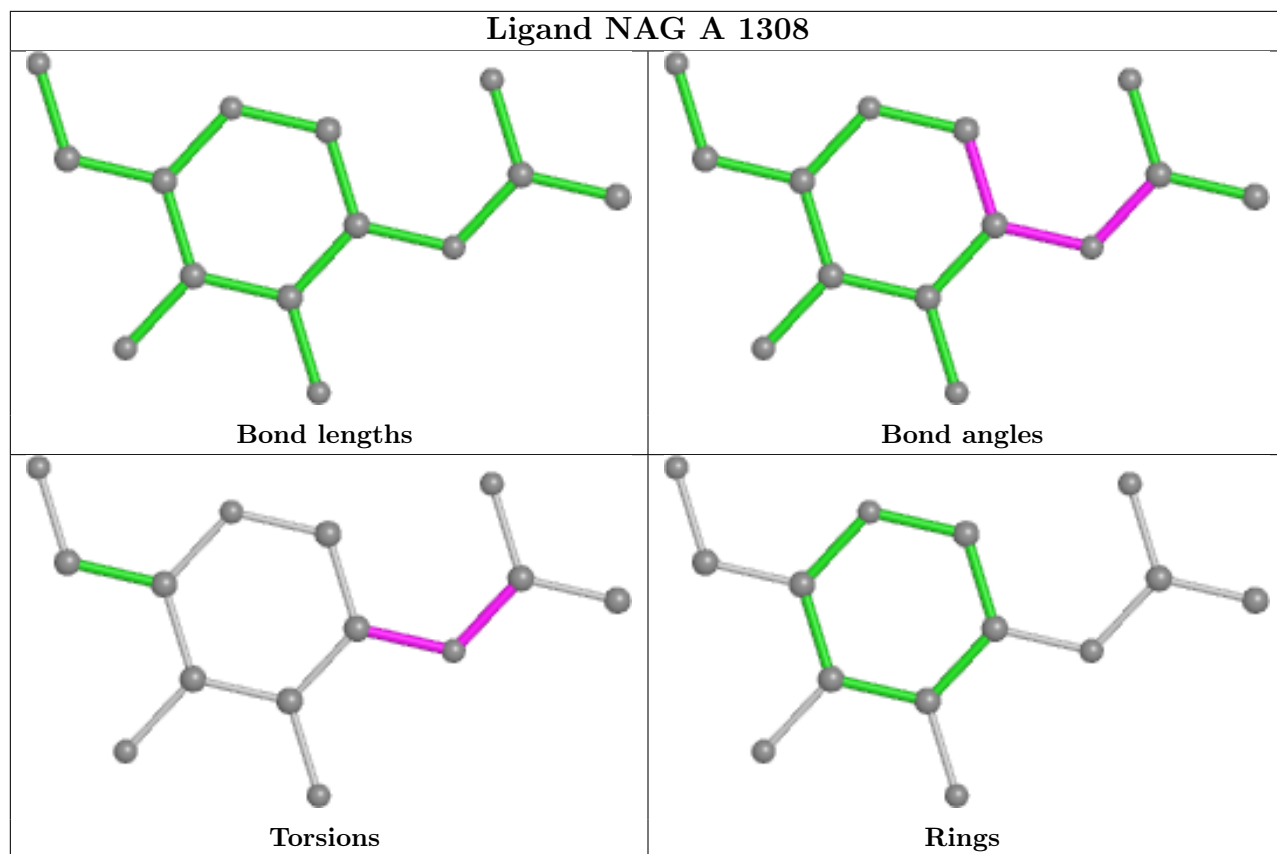


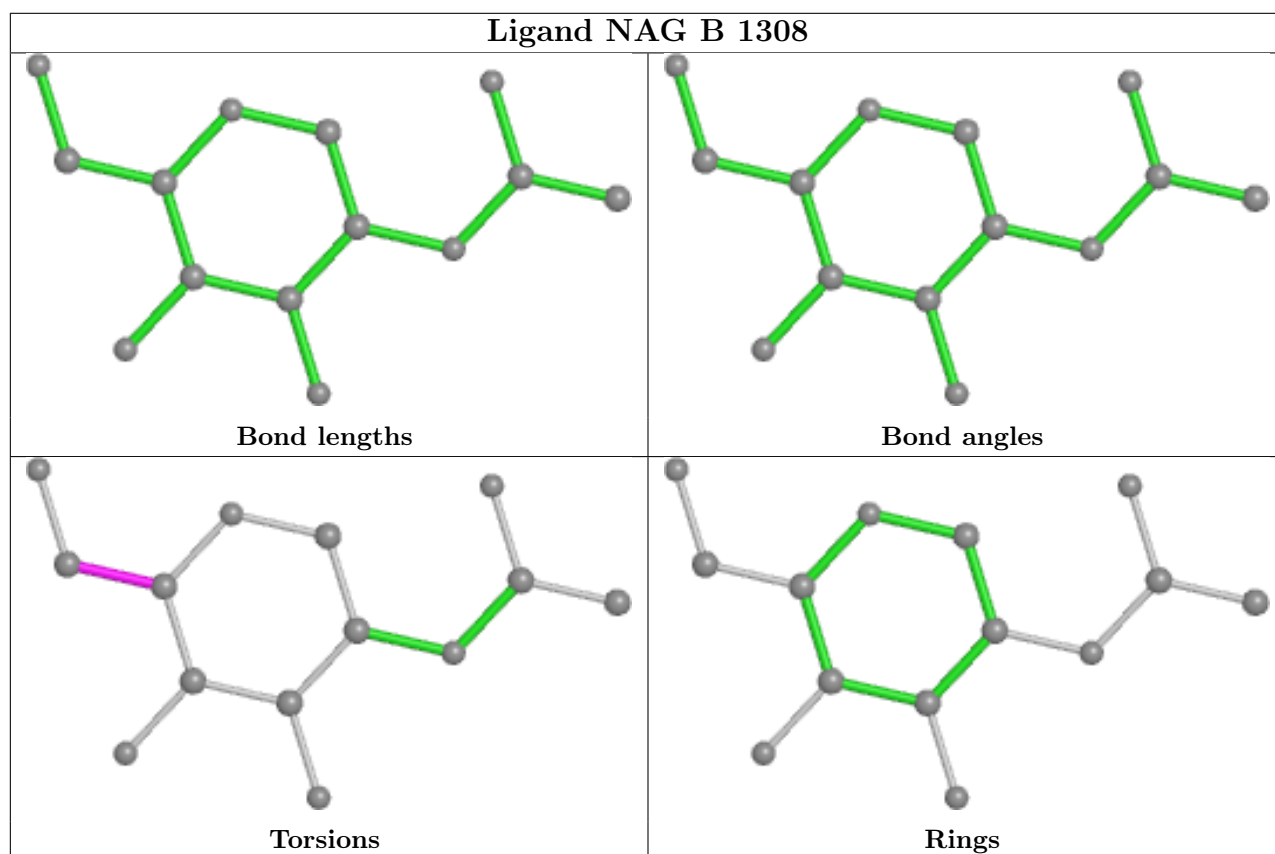
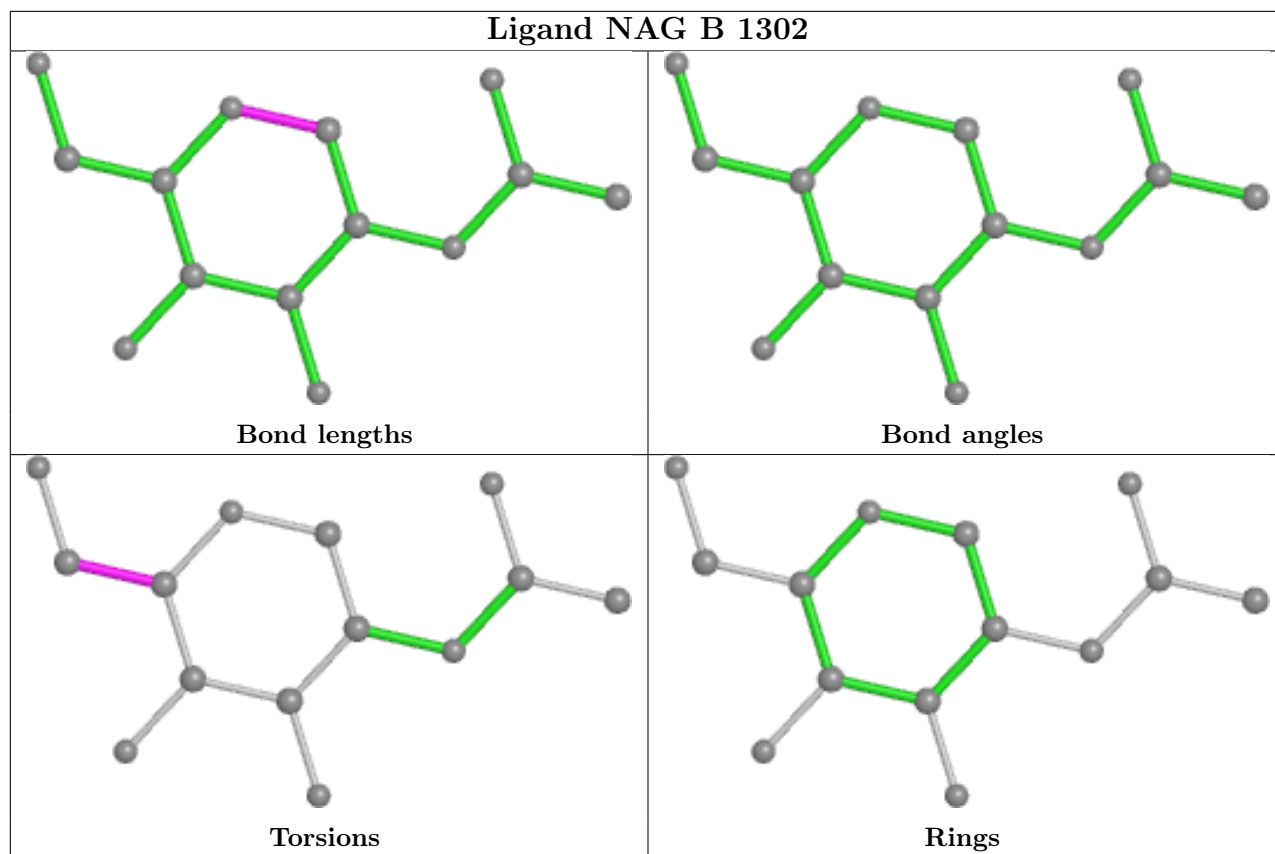


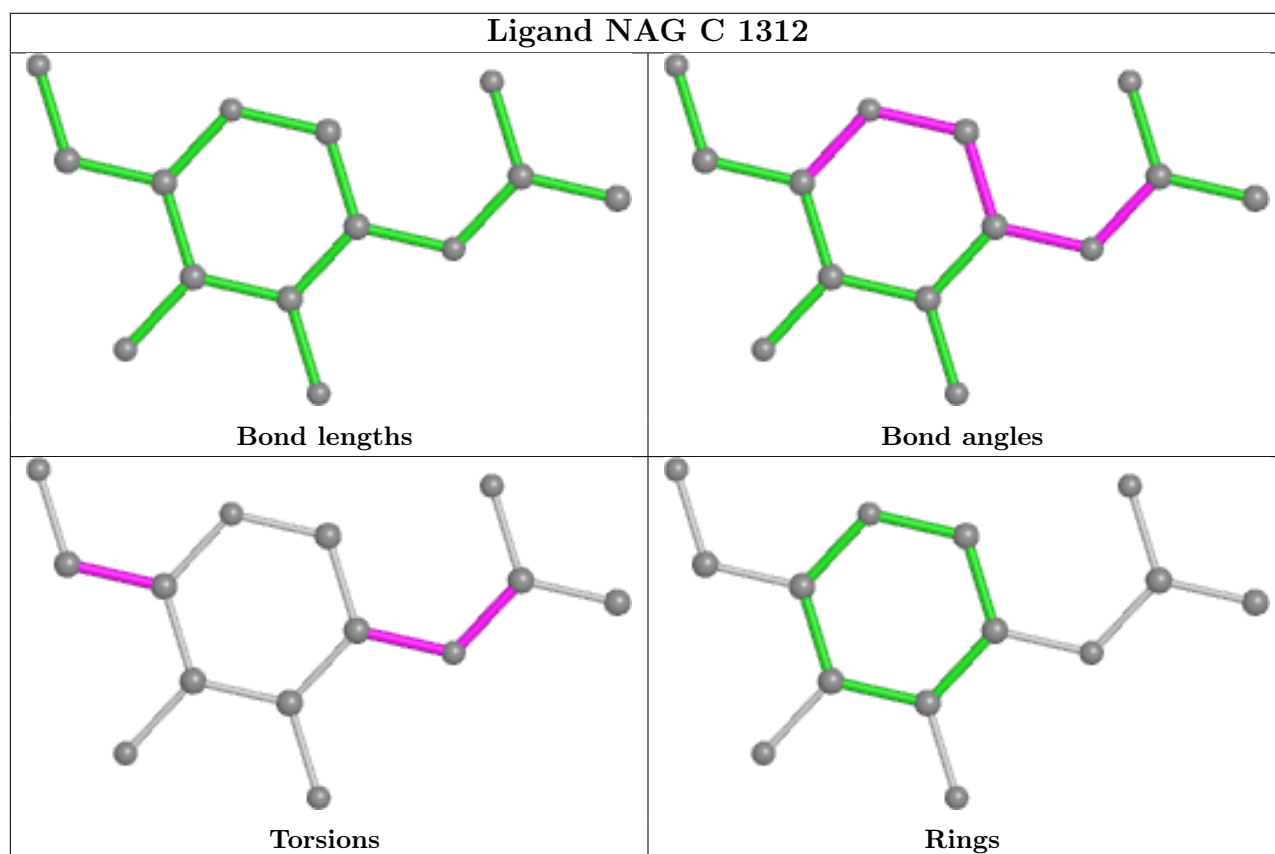
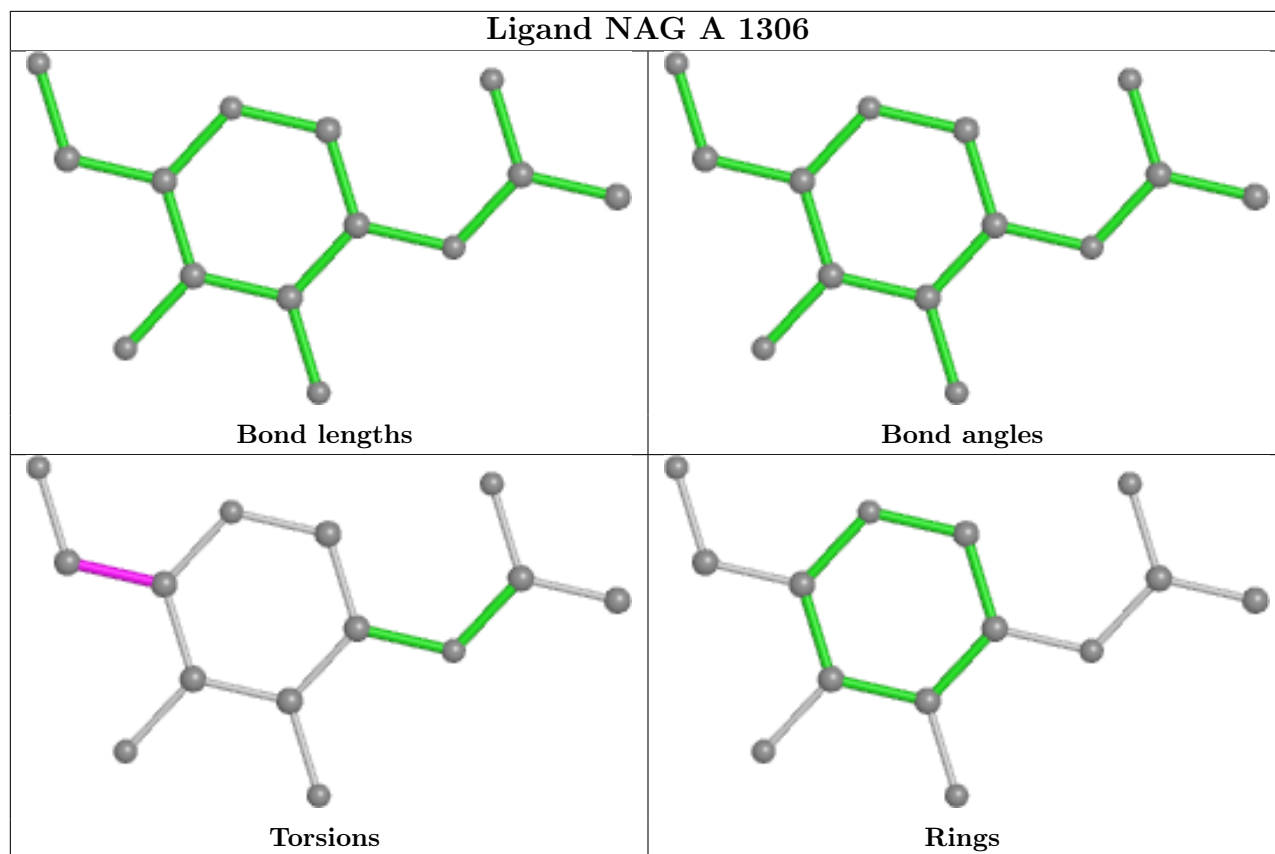


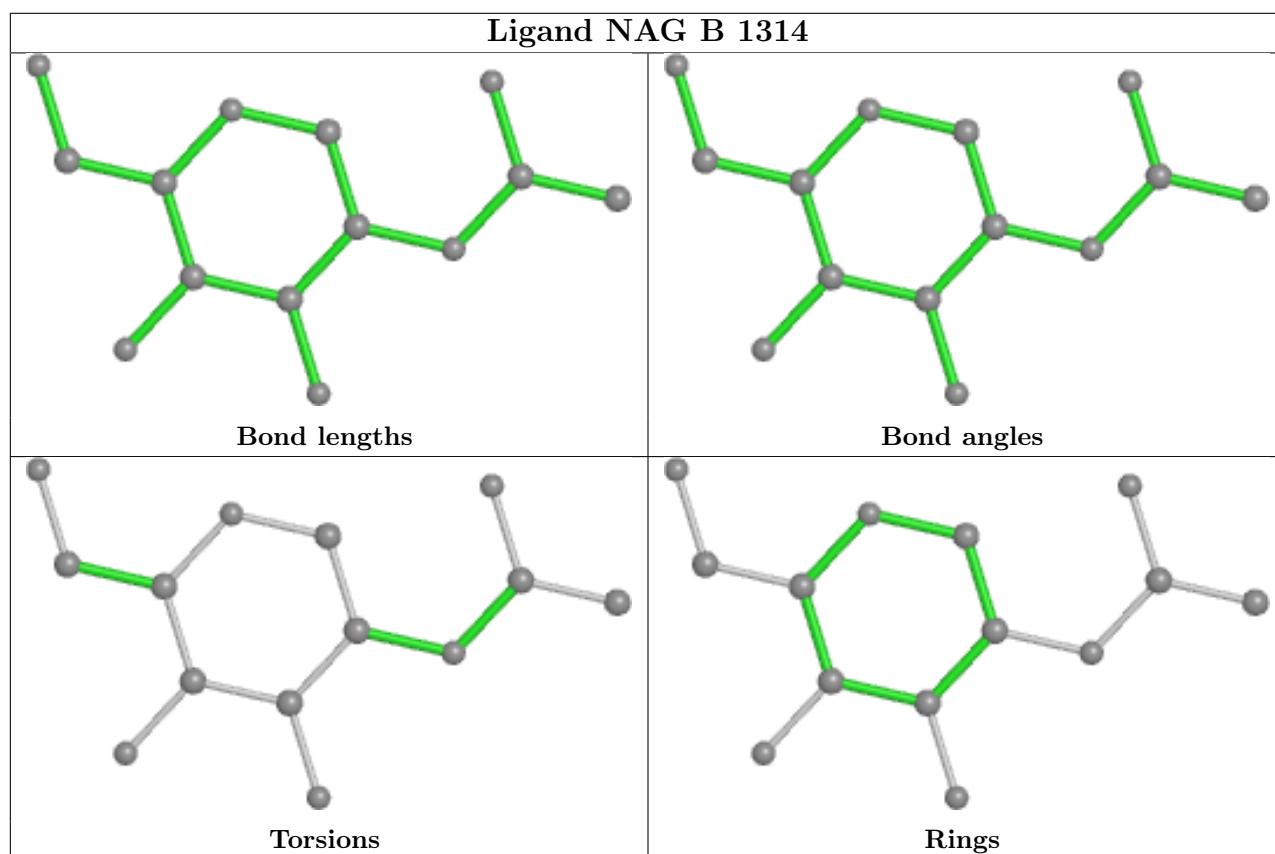
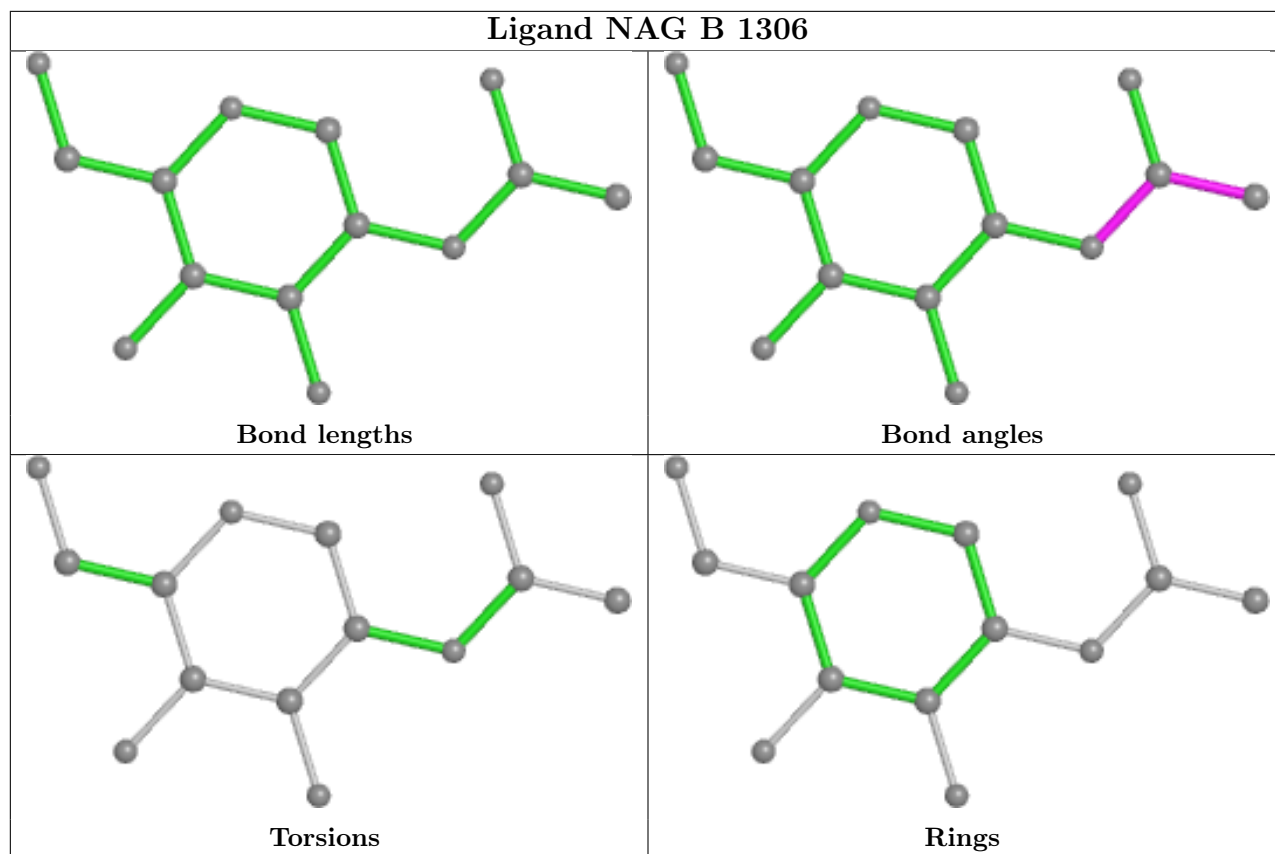


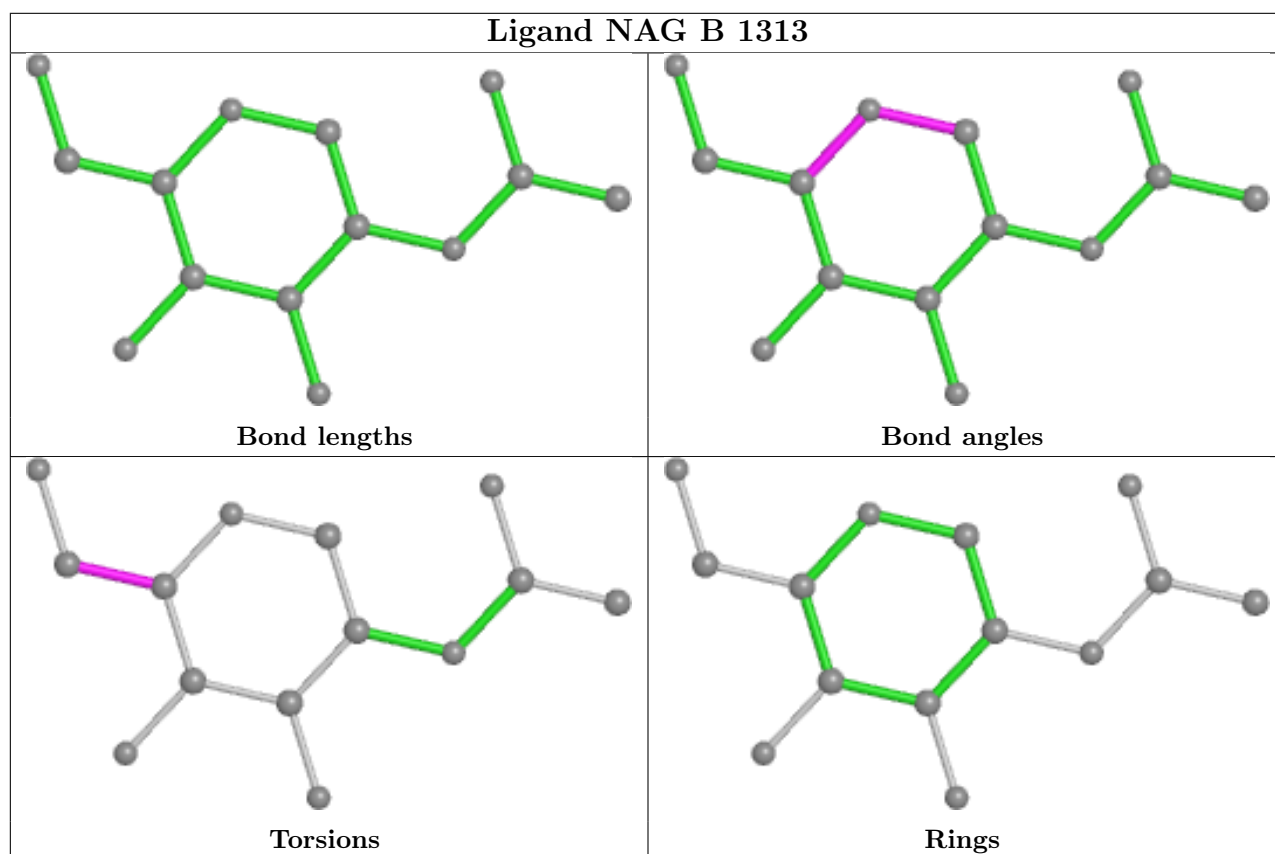
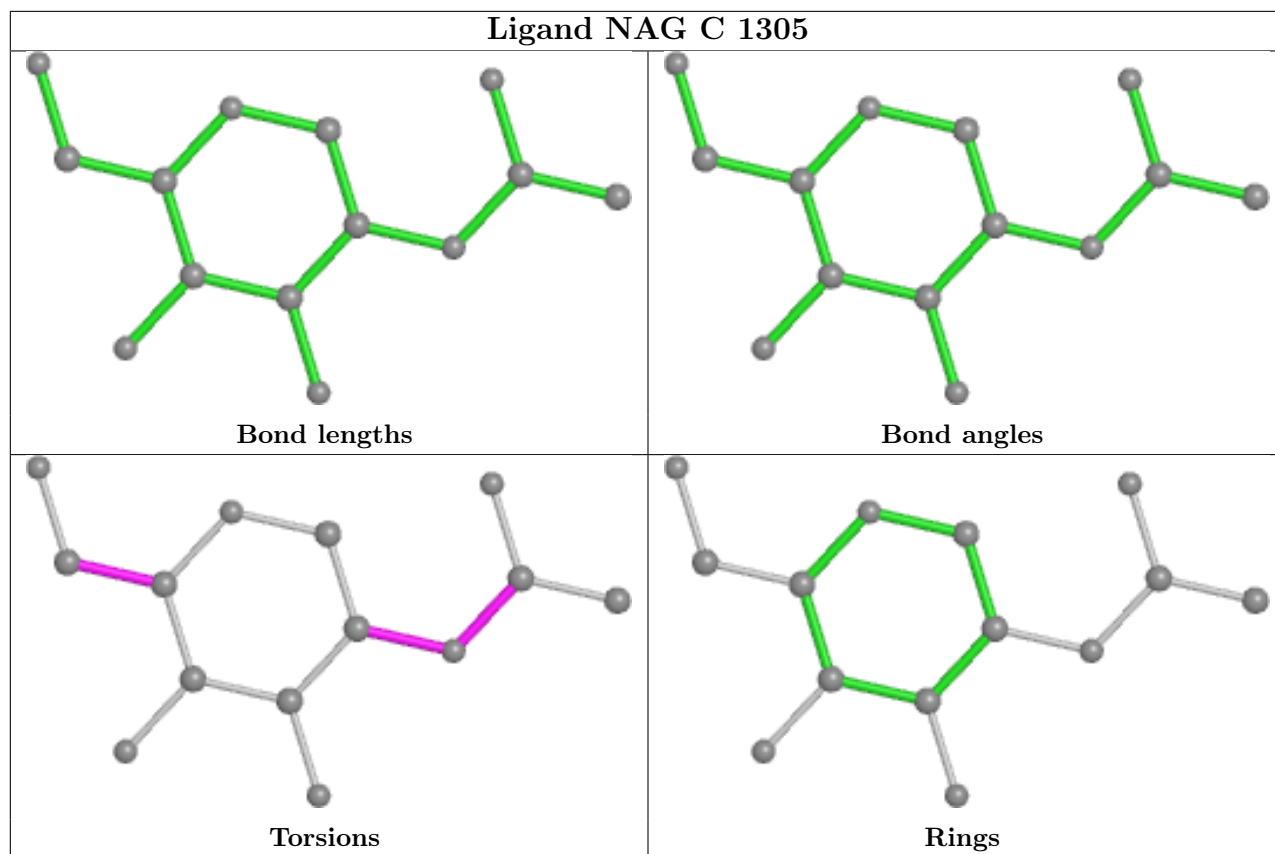


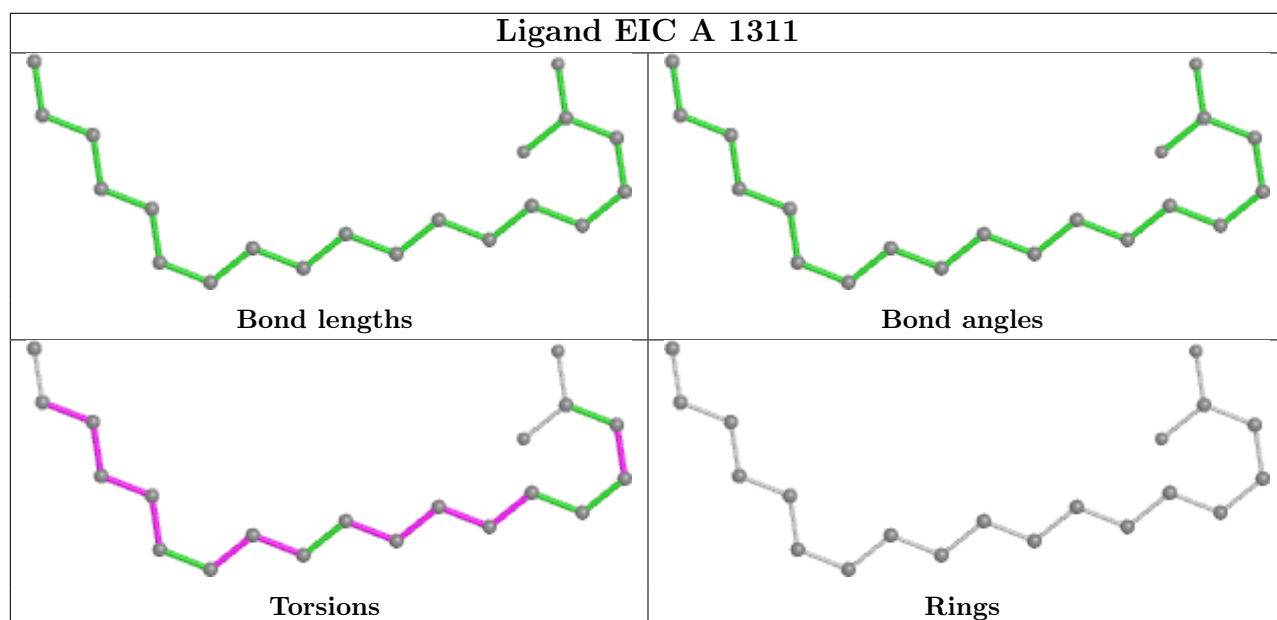
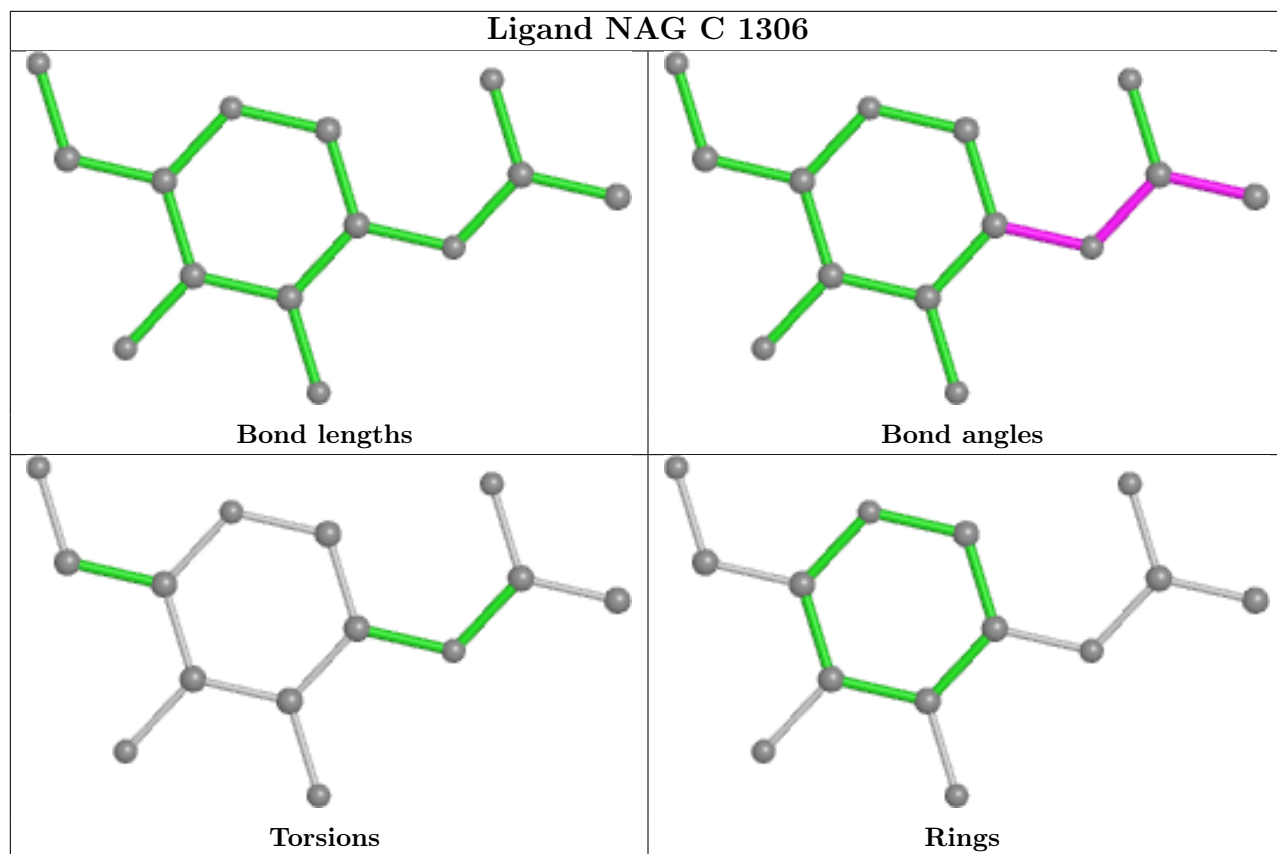


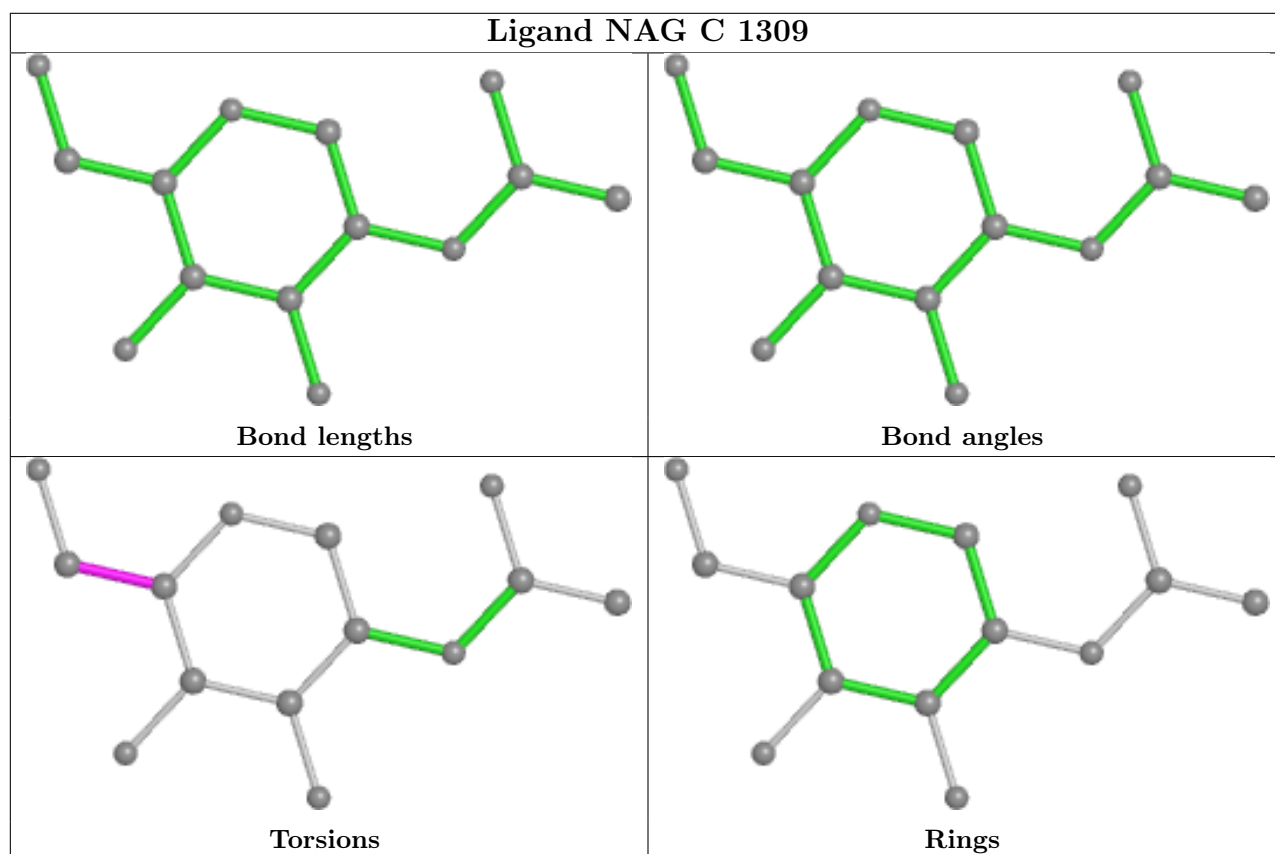
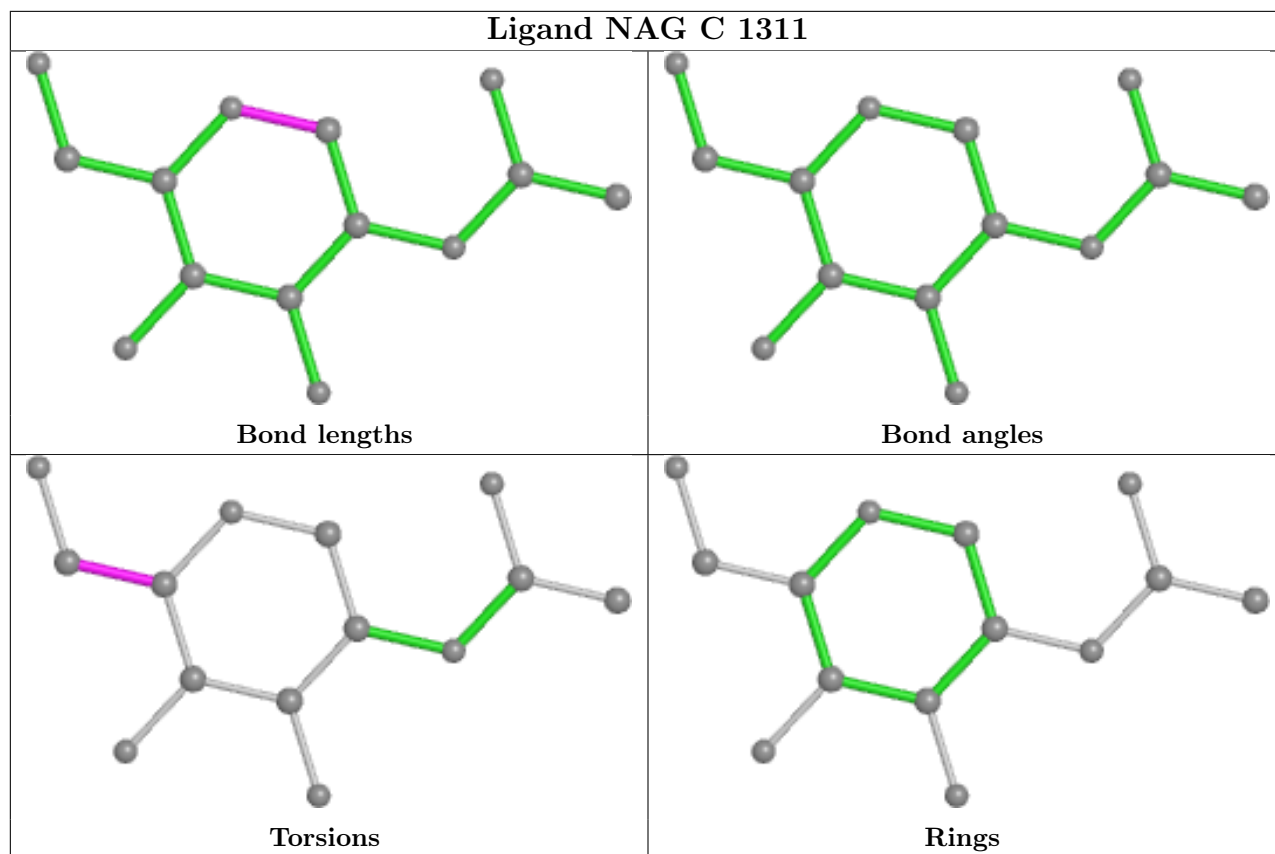




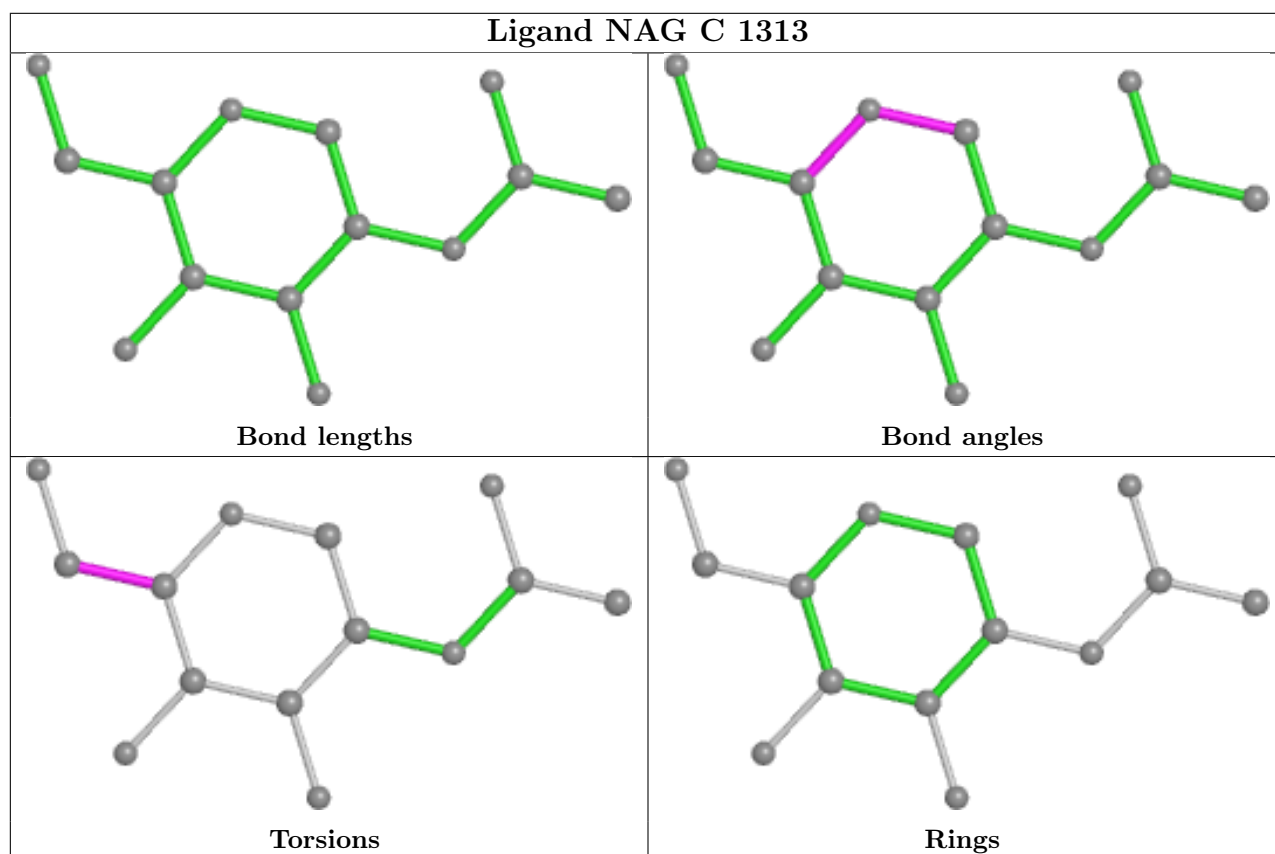
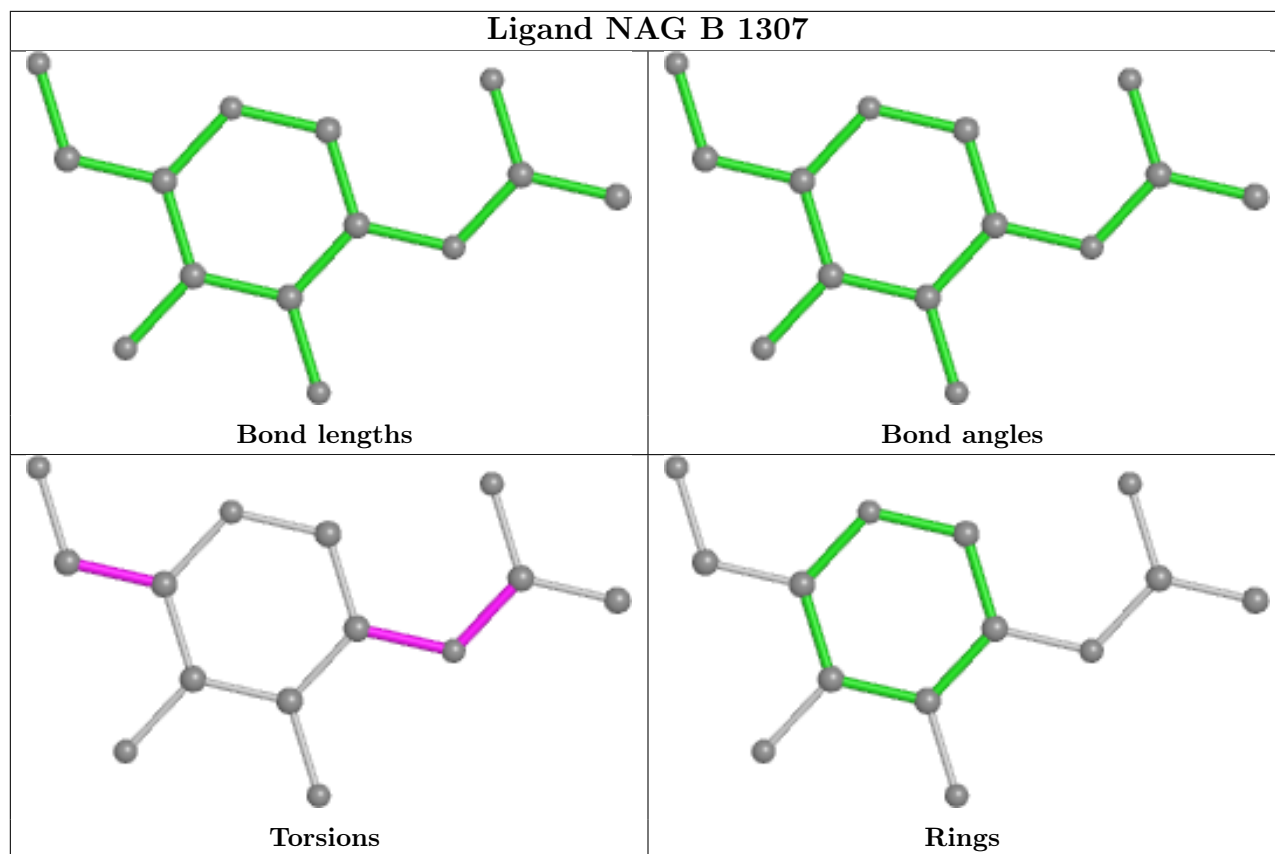


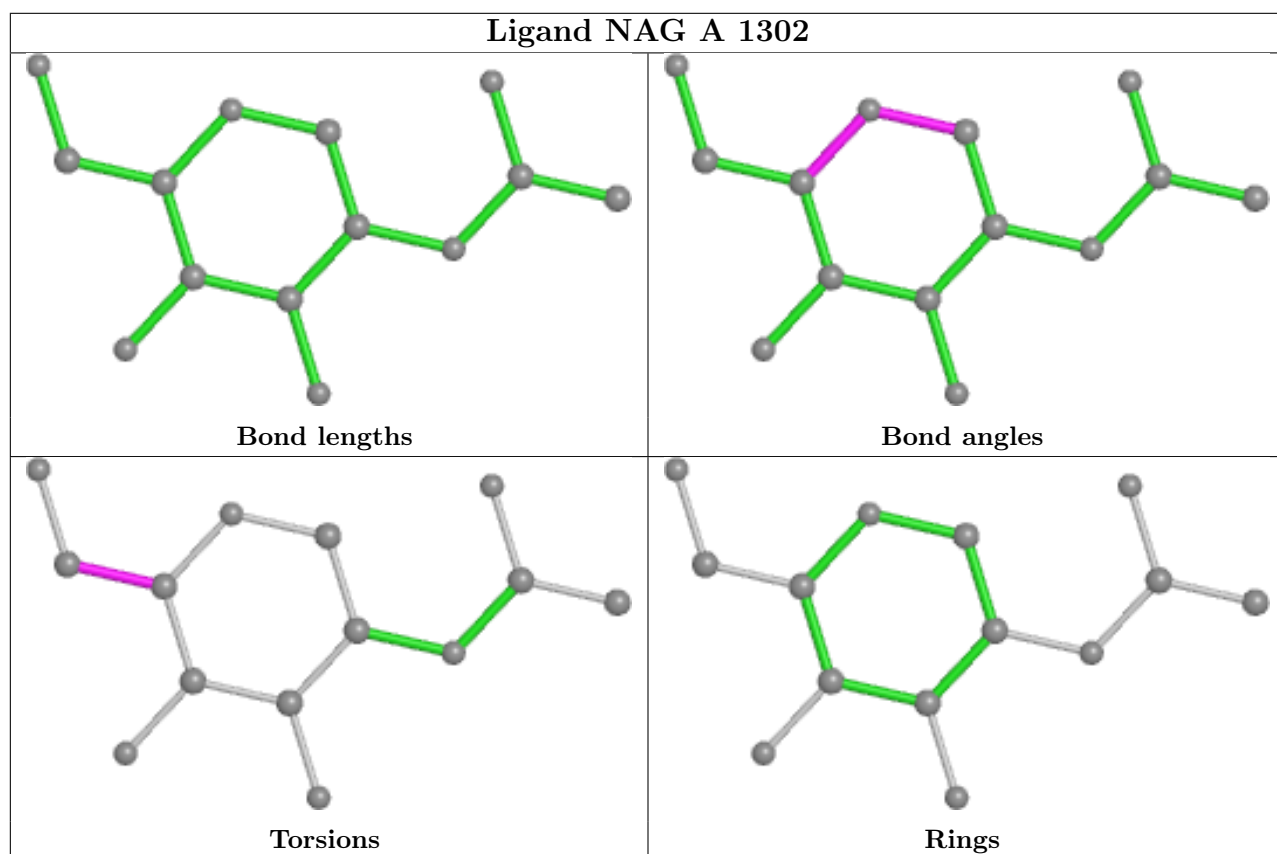
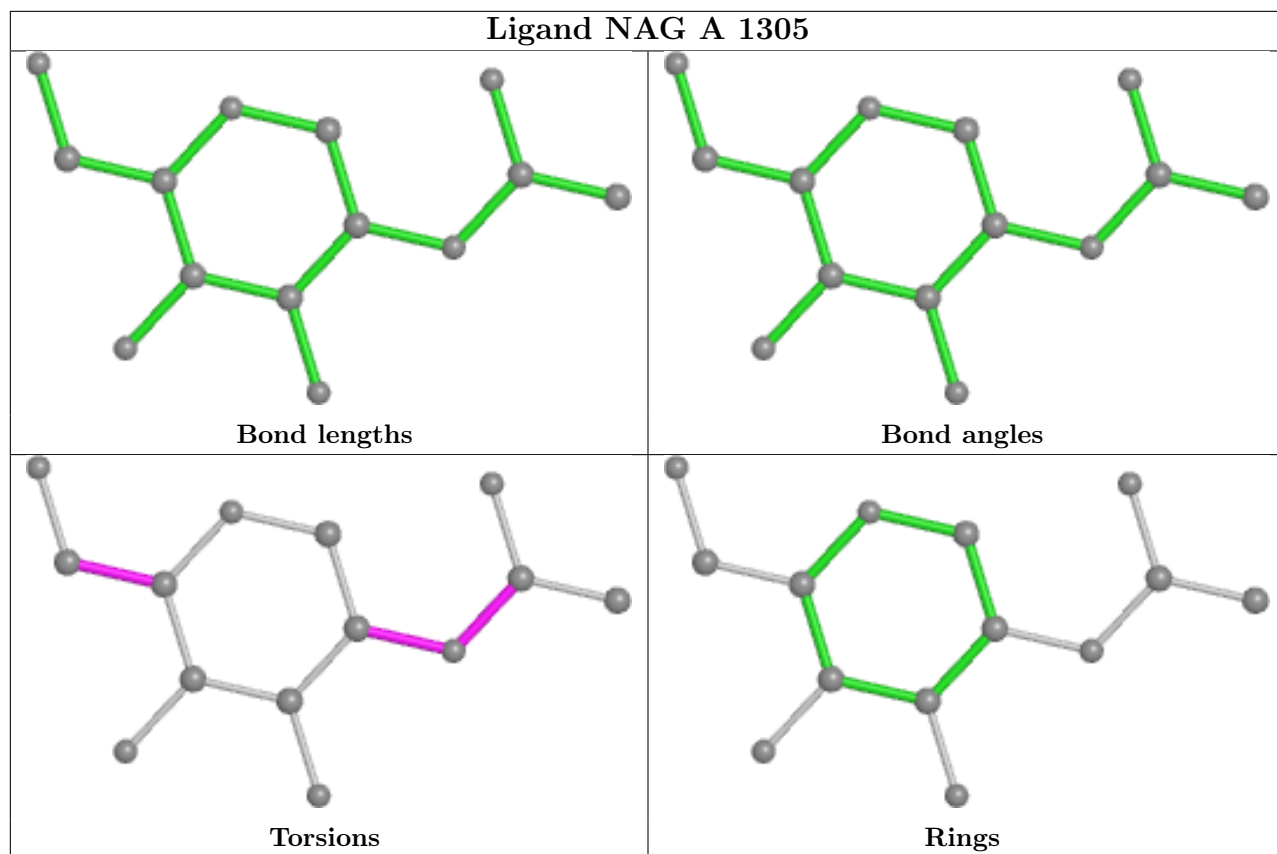


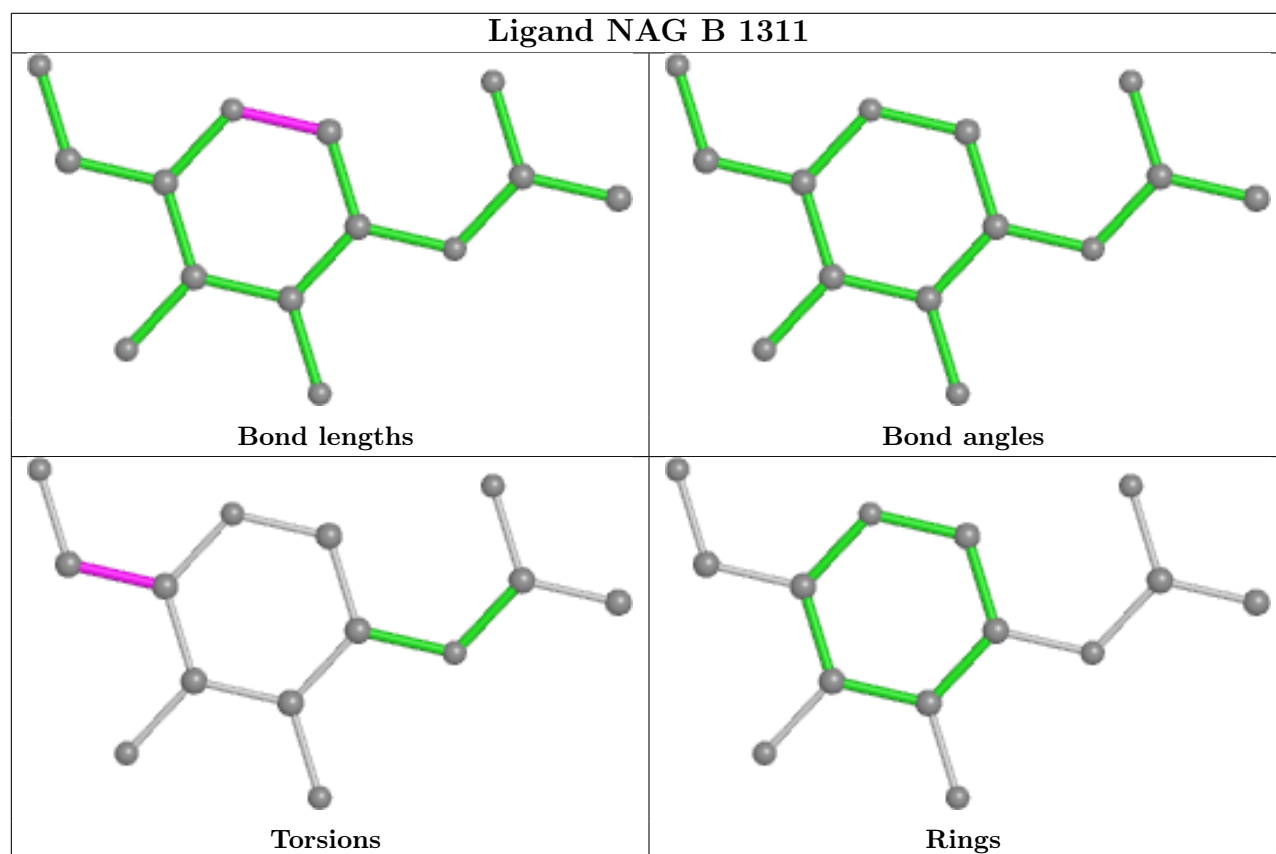
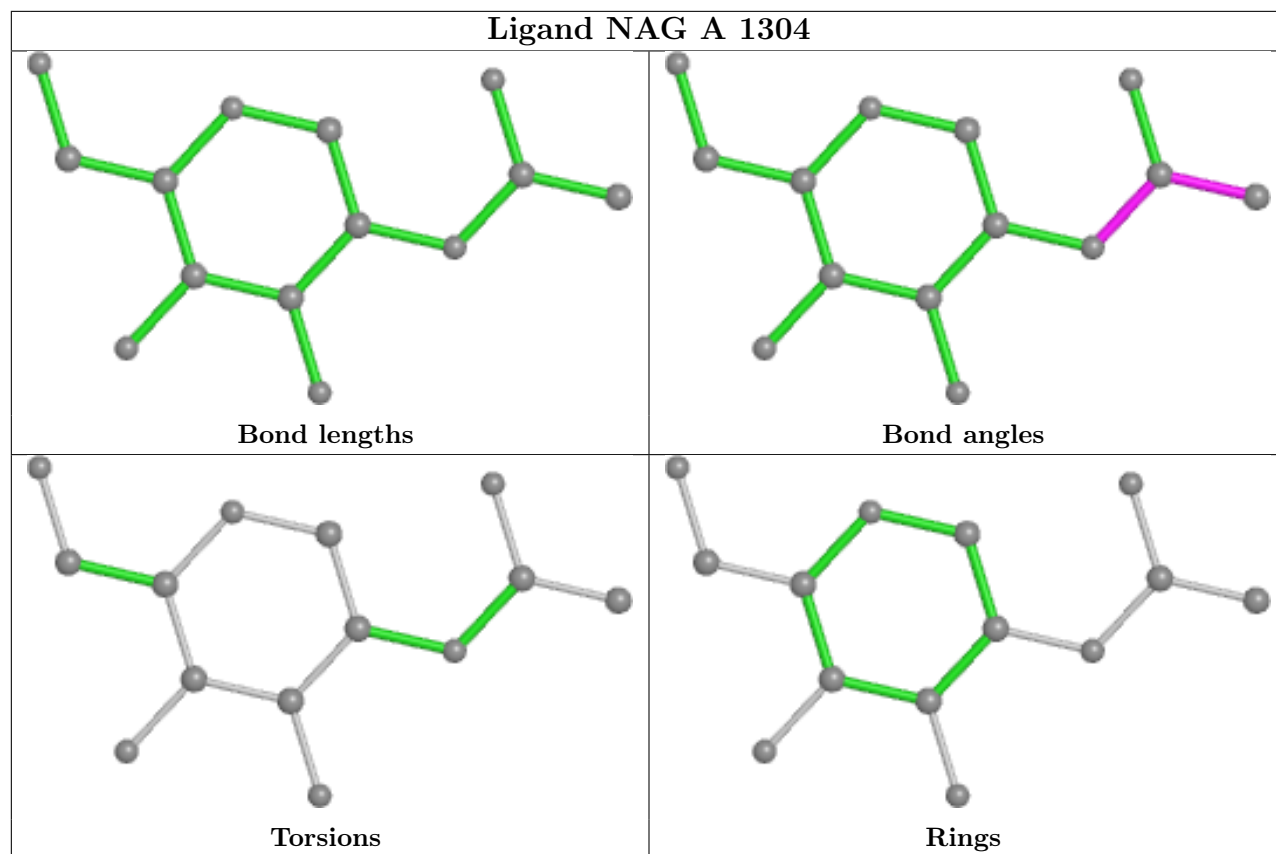


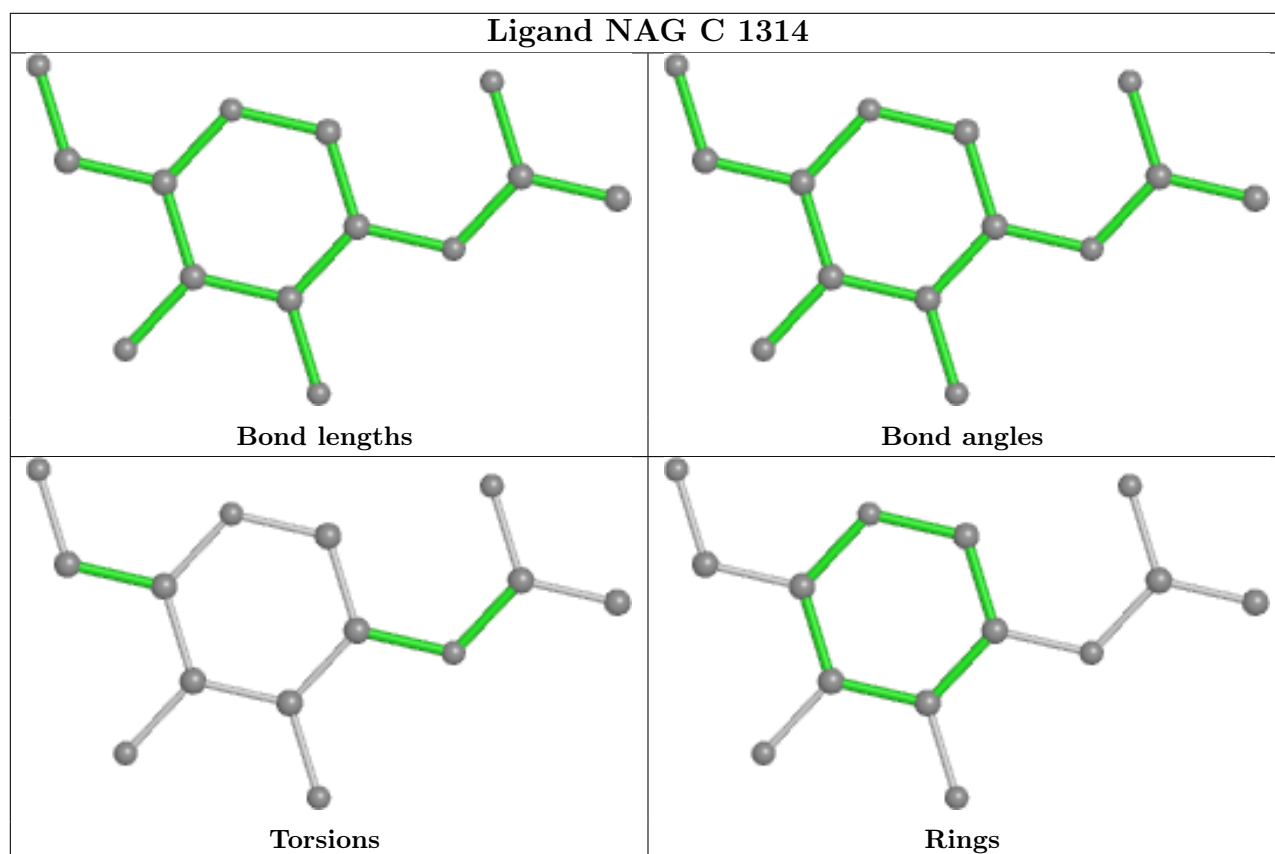
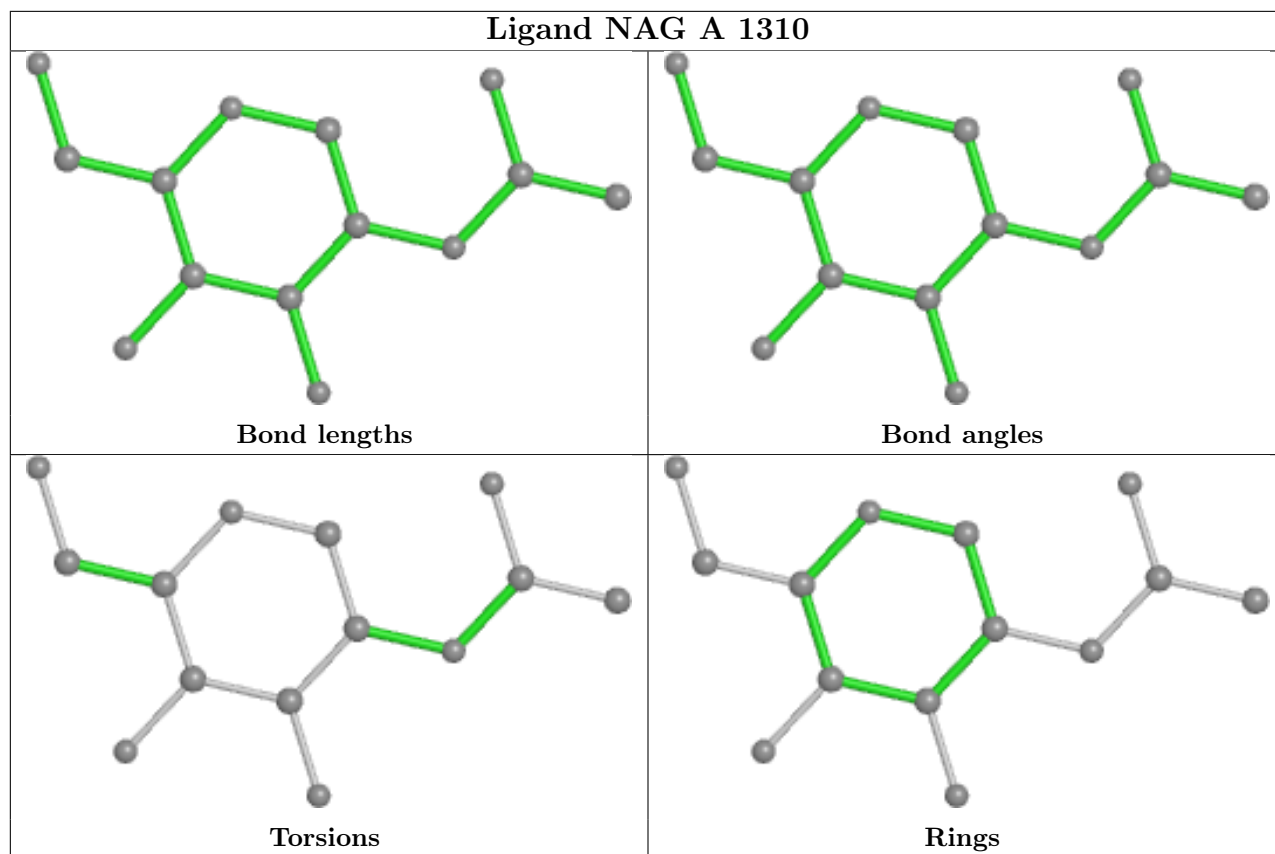


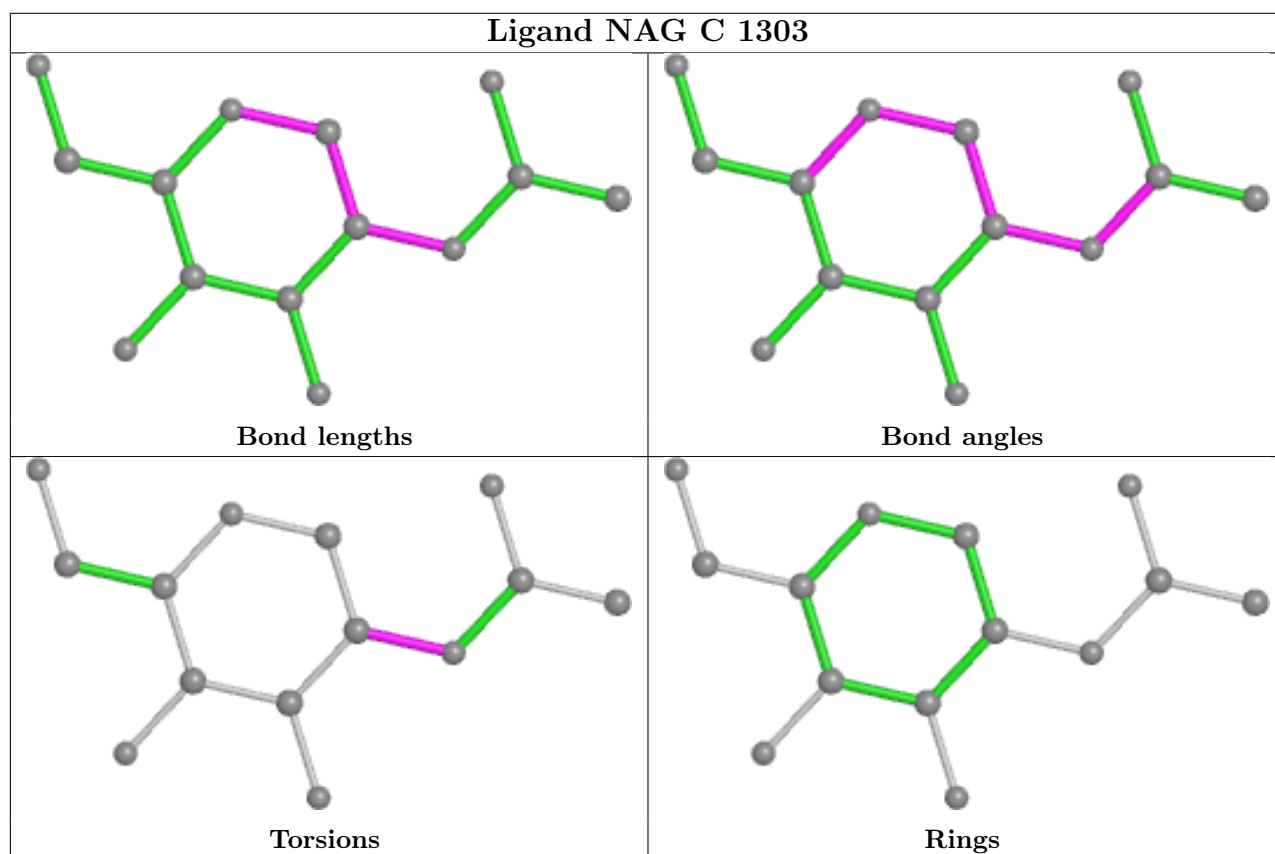
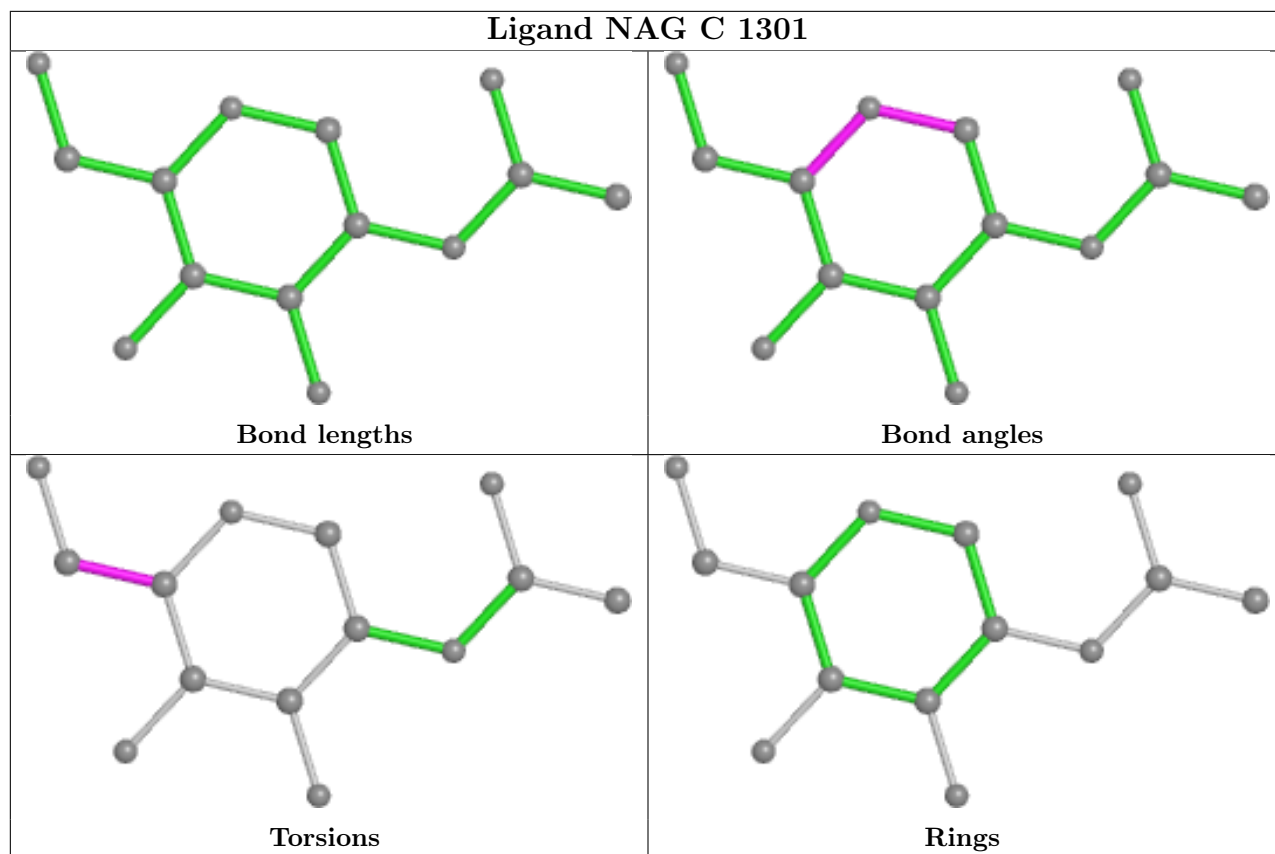


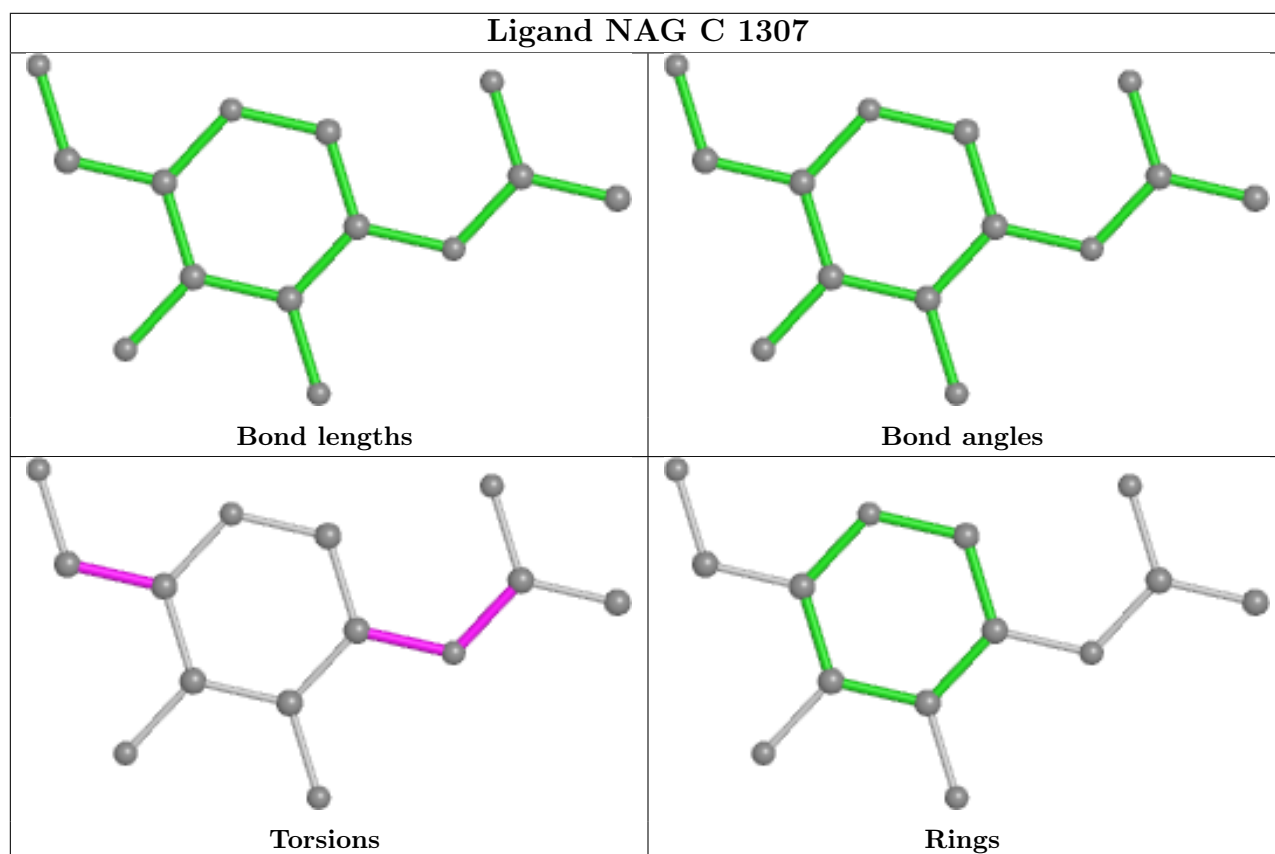
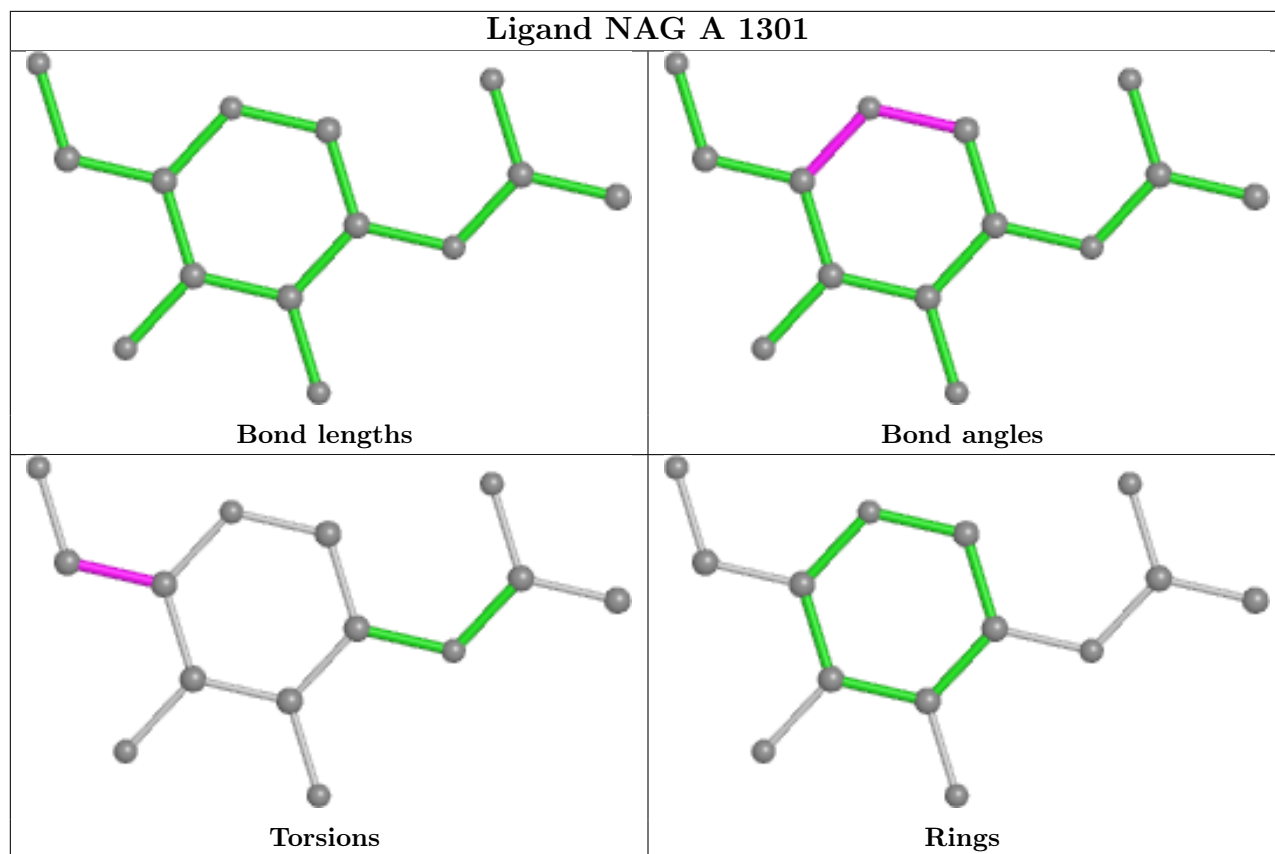


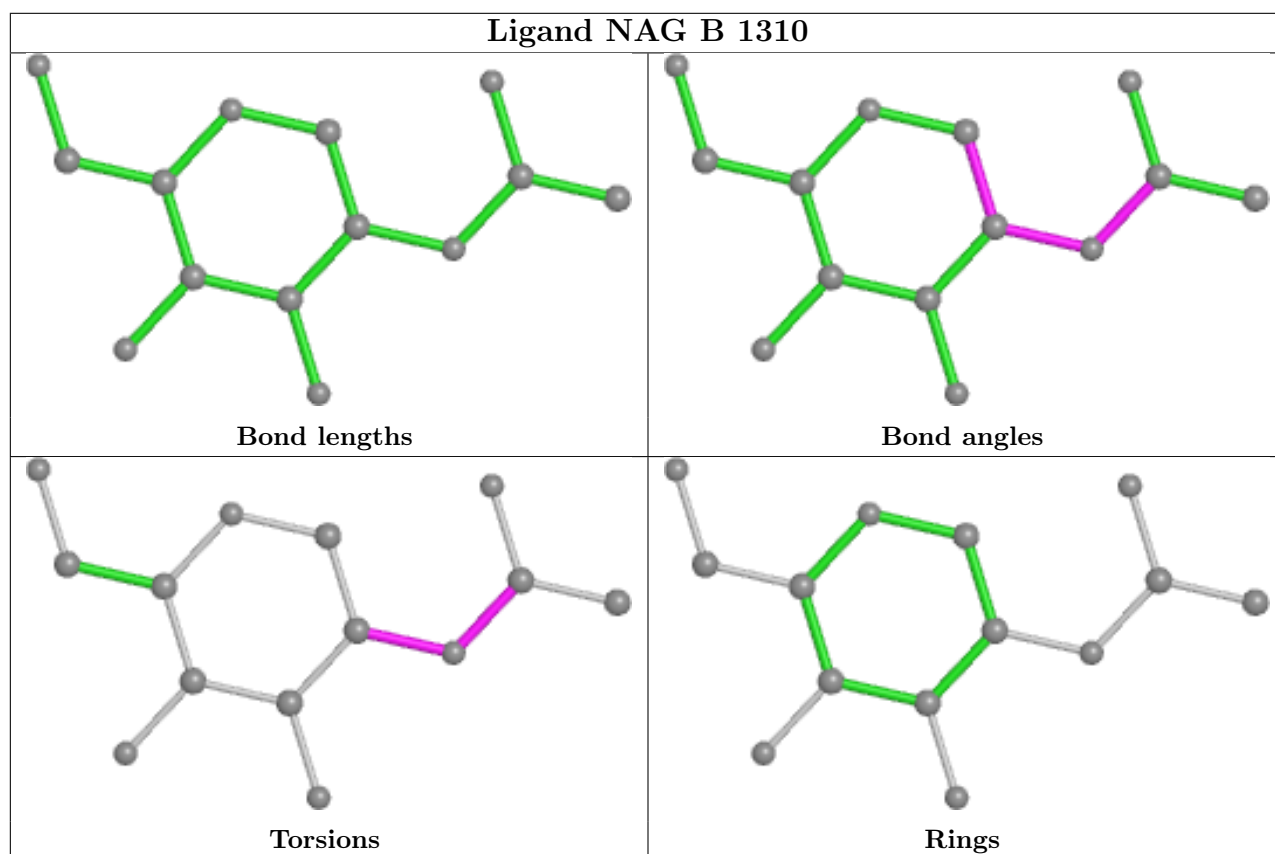
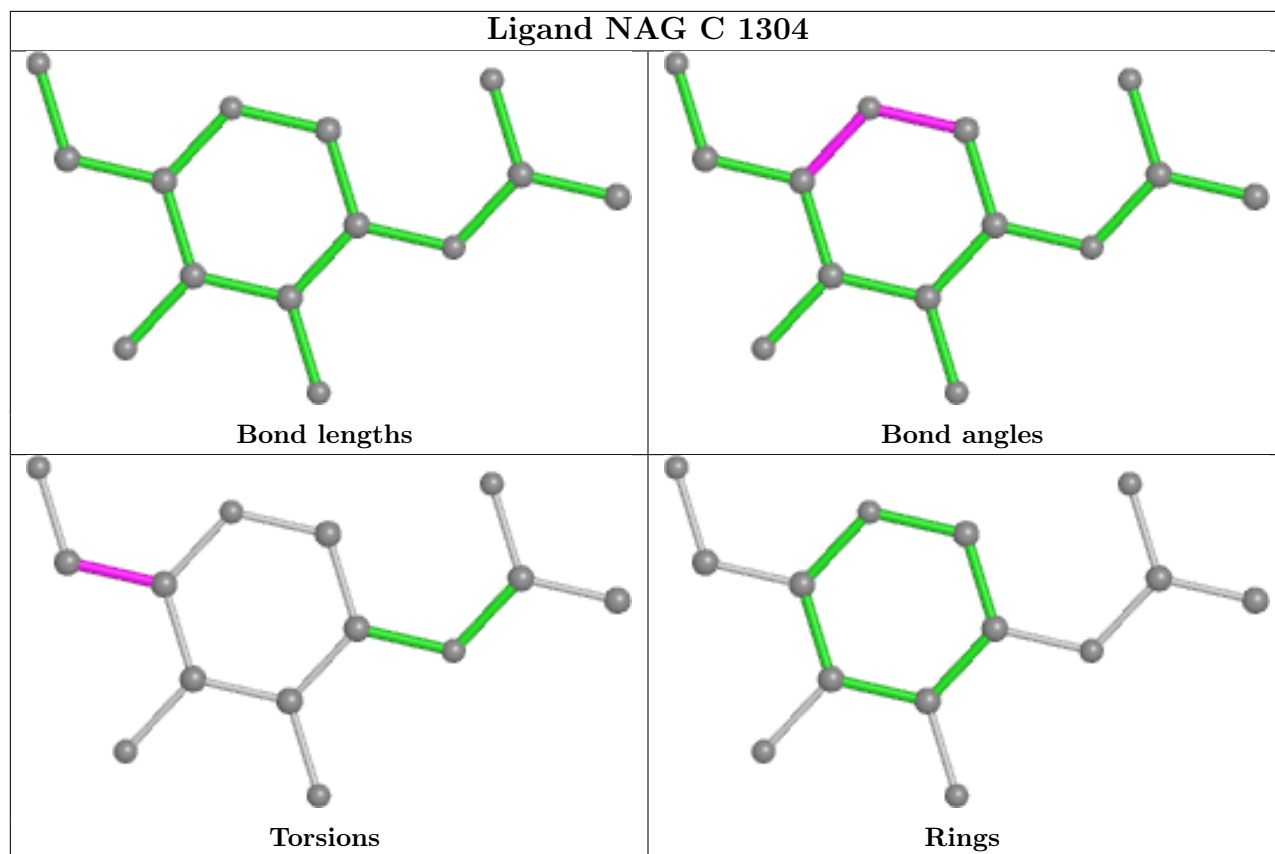


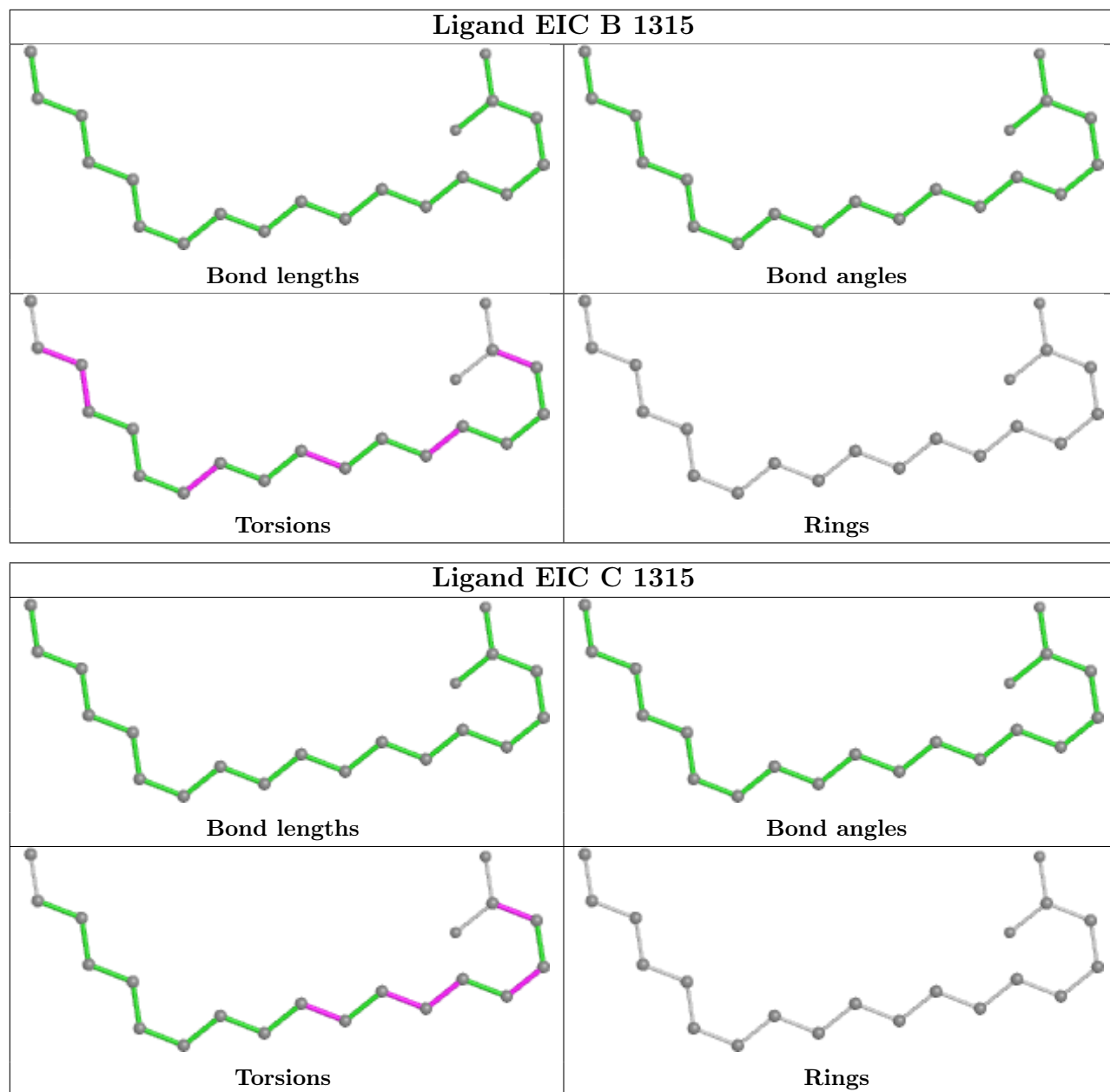




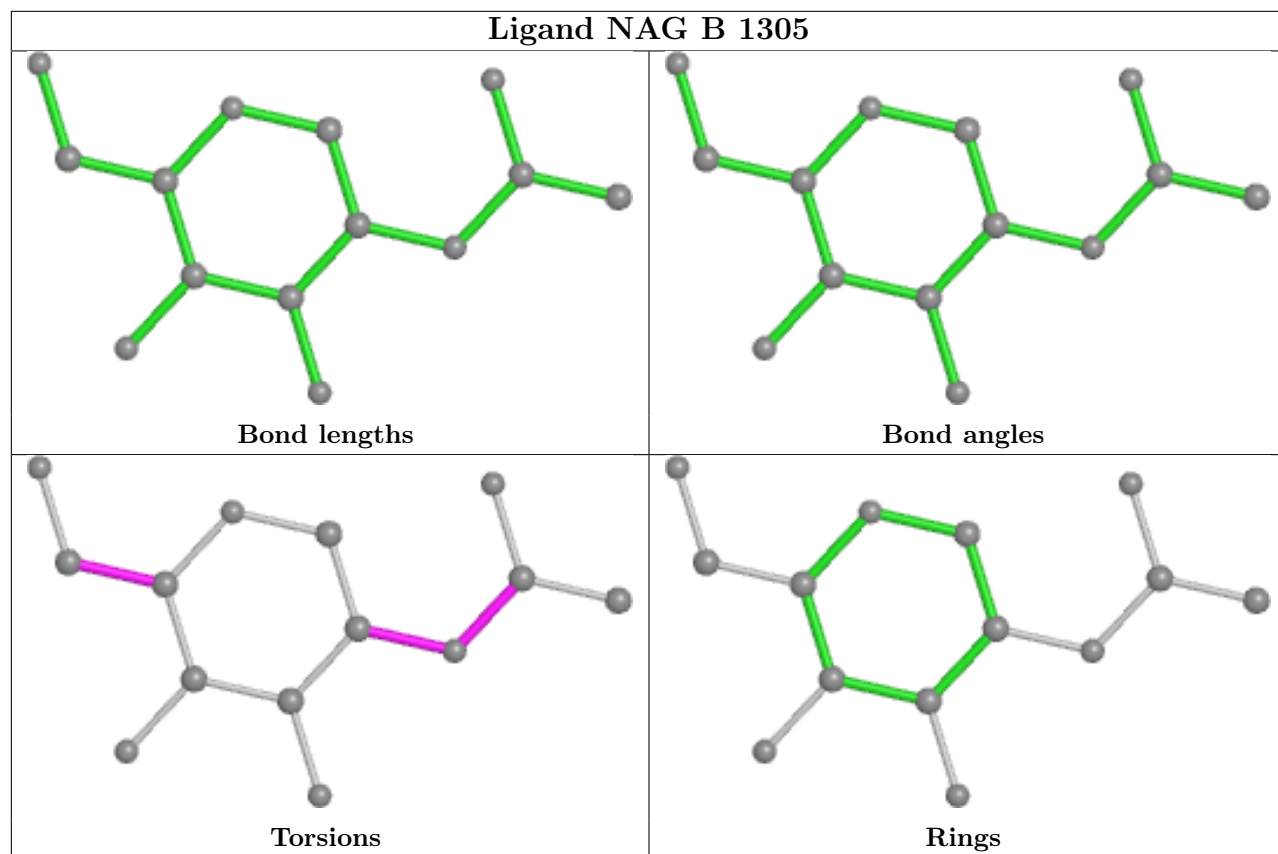












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

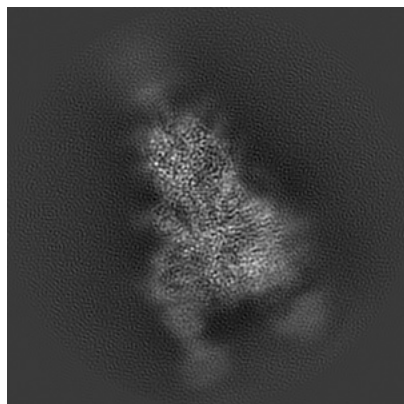
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34872. These allow visual inspection of the internal detail of the map and identification of artifacts.

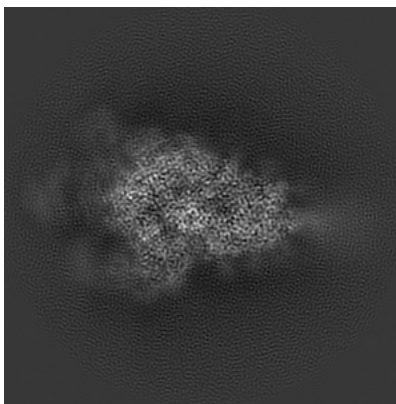
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

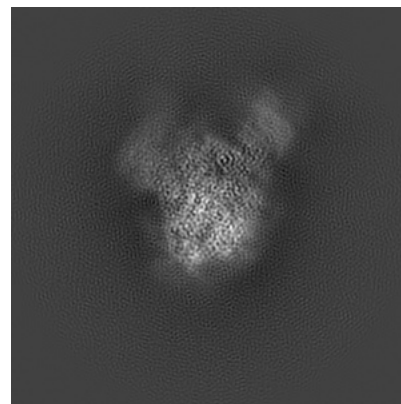
#### 6.1.1 Primary map



X

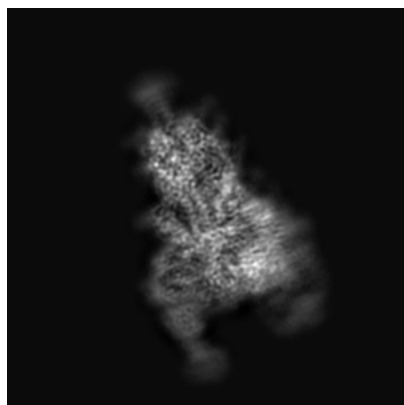


Y

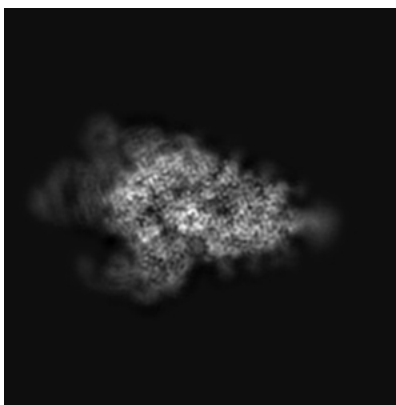


Z

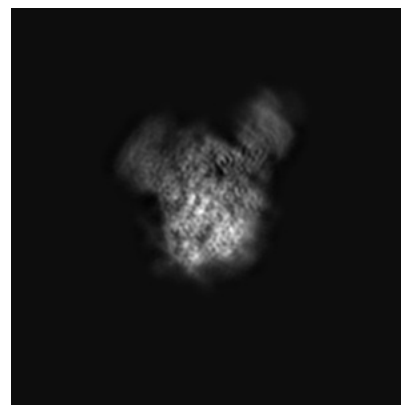
#### 6.1.2 Raw map



X



Y

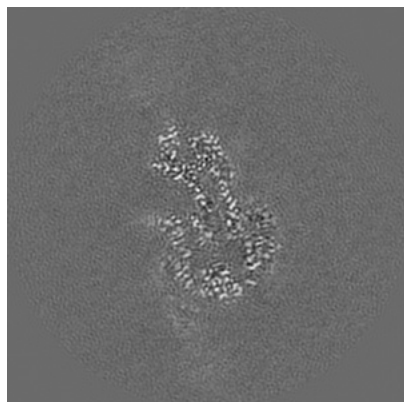


Z

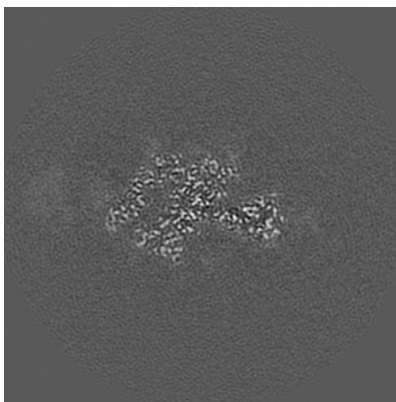
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

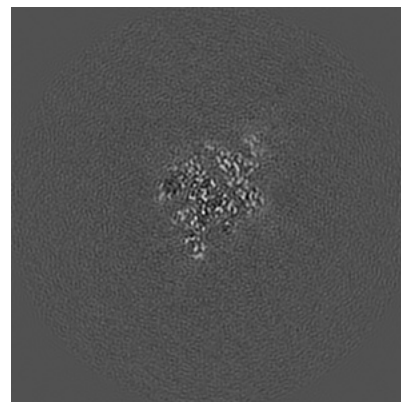
### 6.2.1 Primary map



X Index: 144

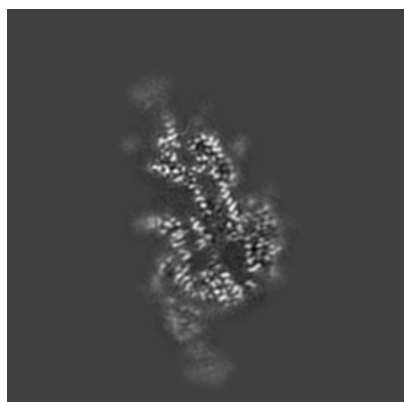


Y Index: 144

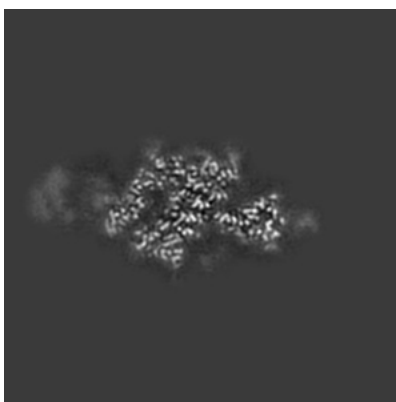


Z Index: 144

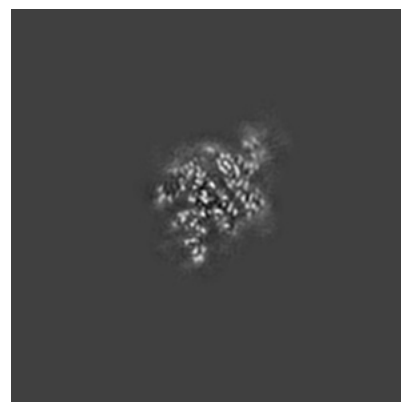
### 6.2.2 Raw map



X Index: 144



Y Index: 144

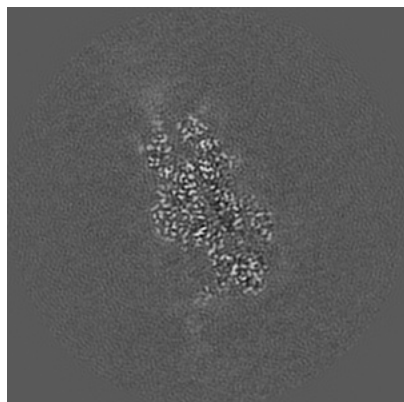


Z Index: 144

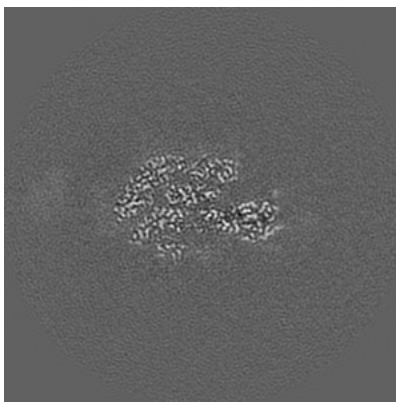
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

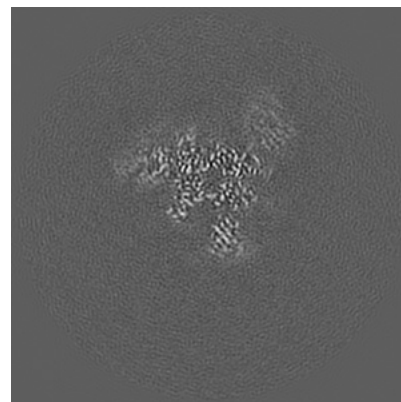
### 6.3.1 Primary map



X Index: 133

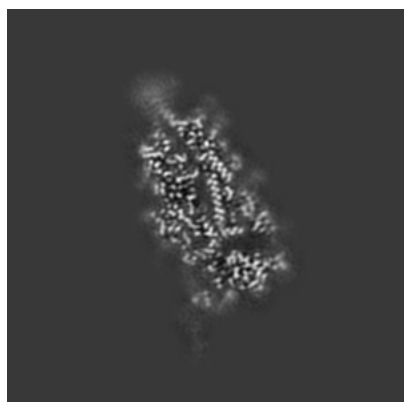


Y Index: 148

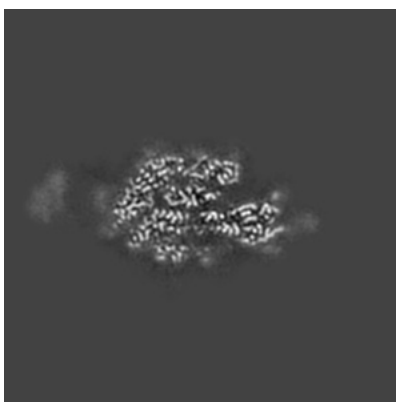


Z Index: 102

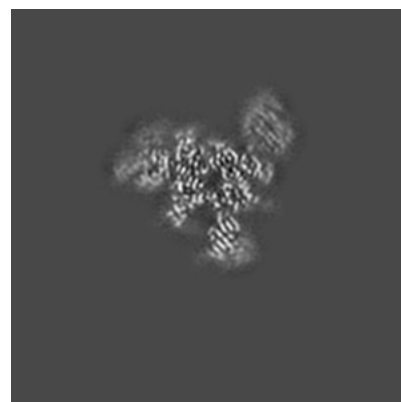
### 6.3.2 Raw map



X Index: 129



Y Index: 148

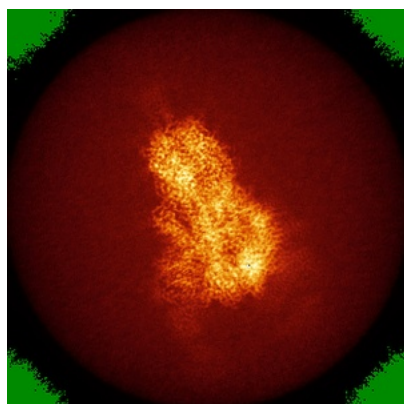


Z Index: 101

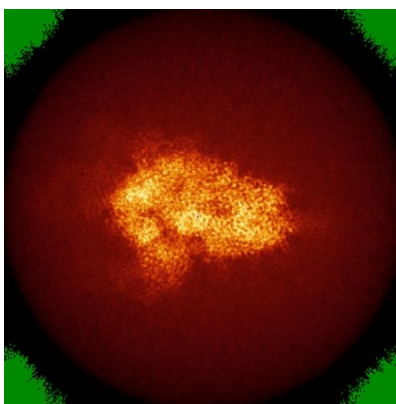
The images above show the largest variance slices of the map in three orthogonal directions.

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

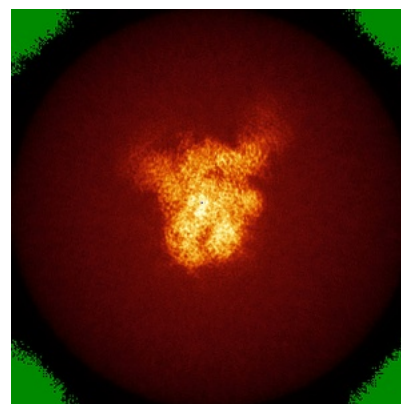
### 6.4.1 Primary map



X

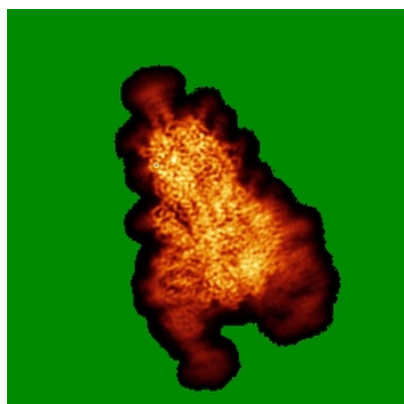


Y

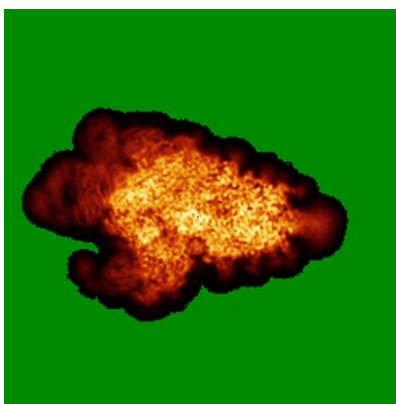


Z

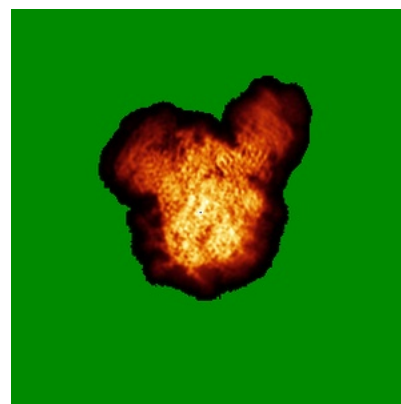
### 6.4.2 Raw map



X



Y

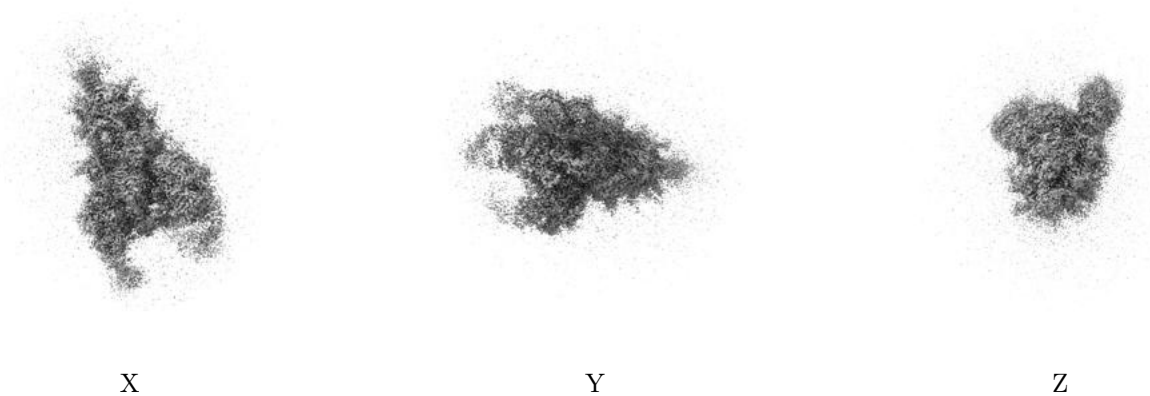


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

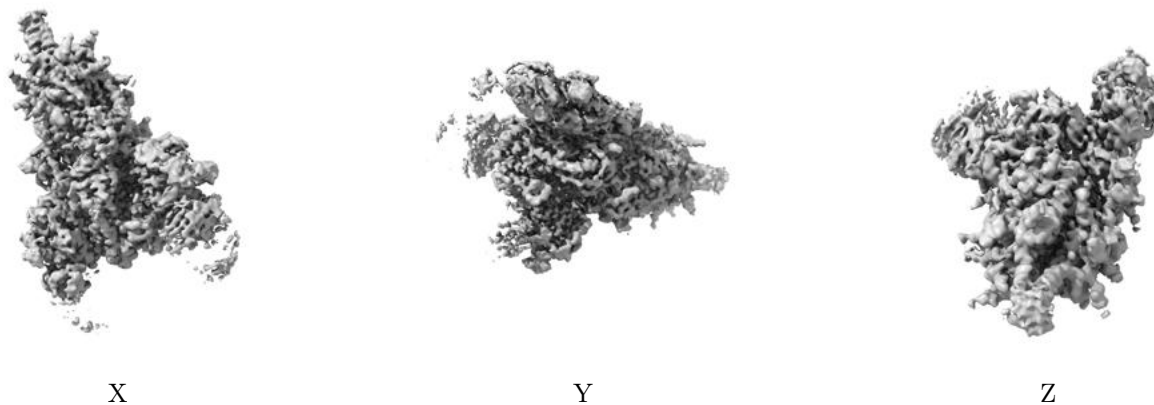
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

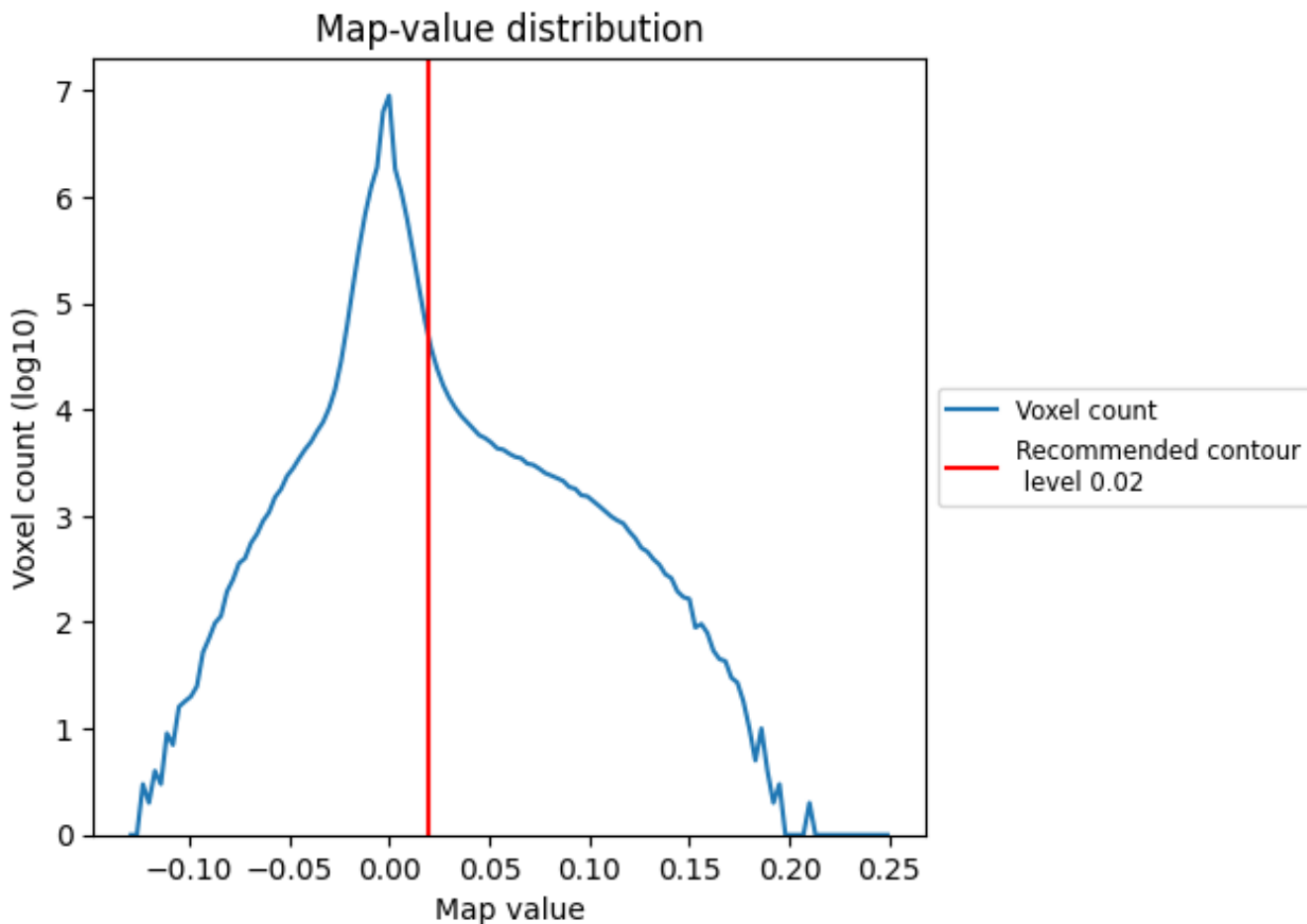
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

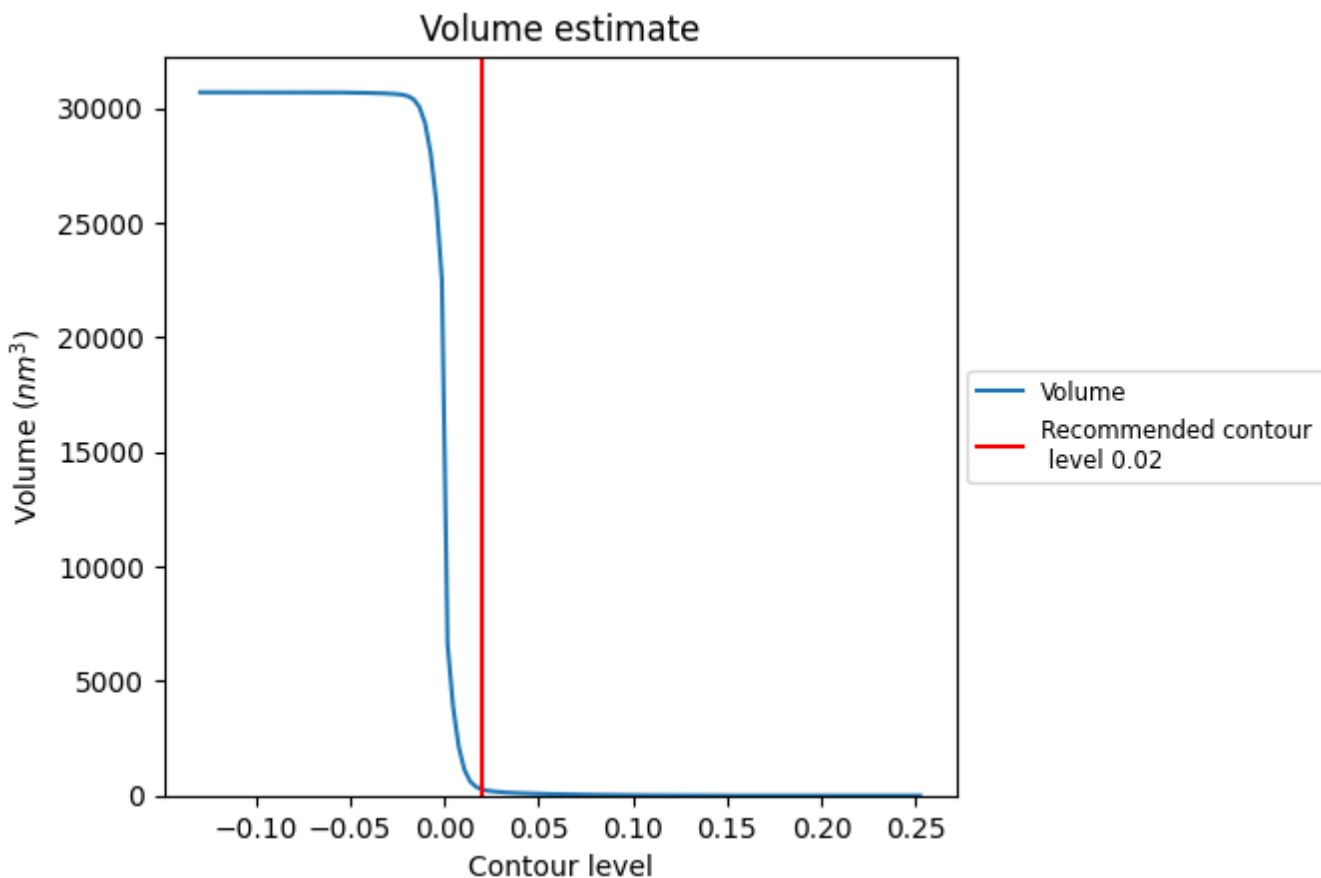
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

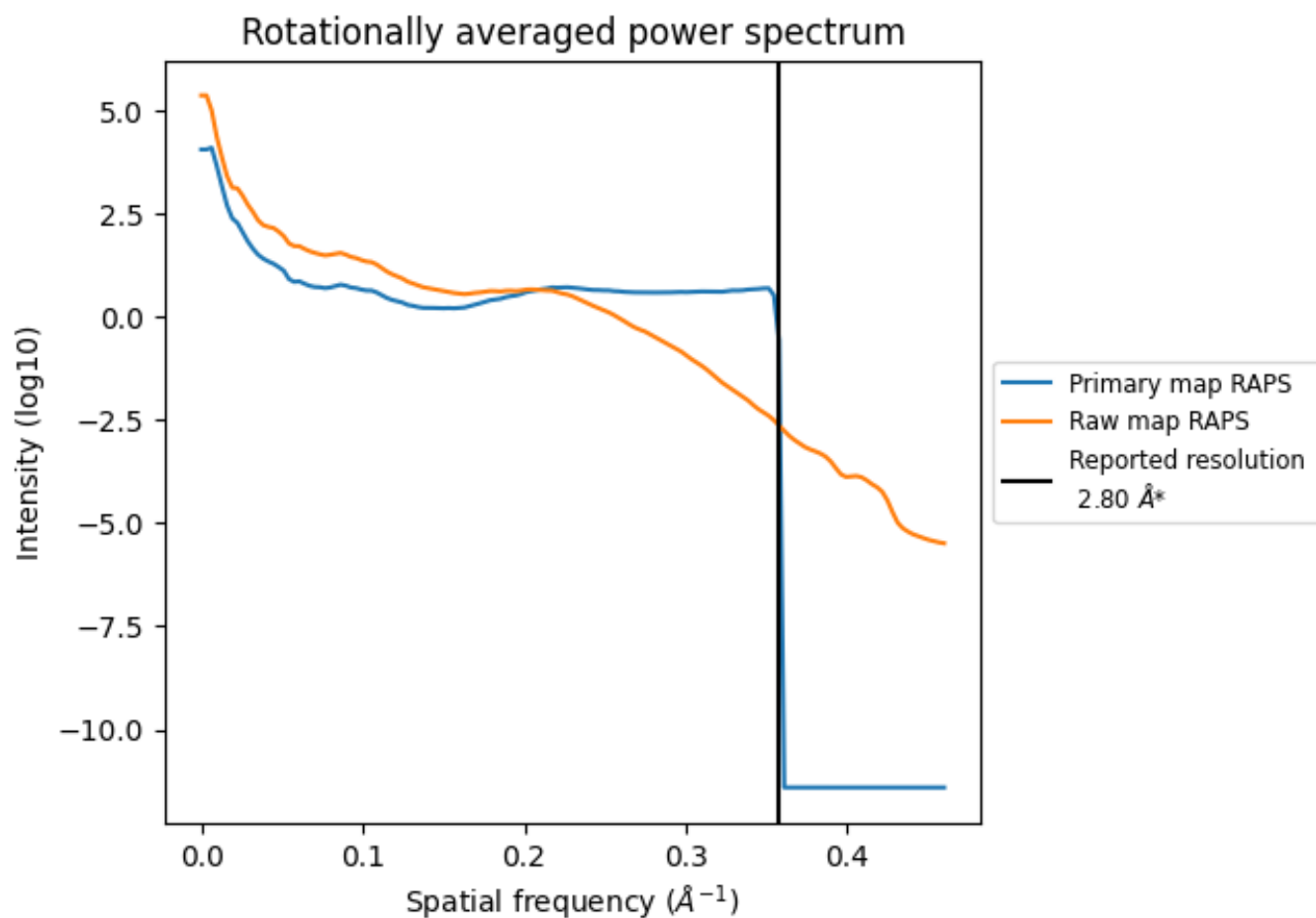


The volume at the recommended contour level is 273  $\text{nm}^3$ ; this corresponds to an approximate mass of 247 kDa.

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

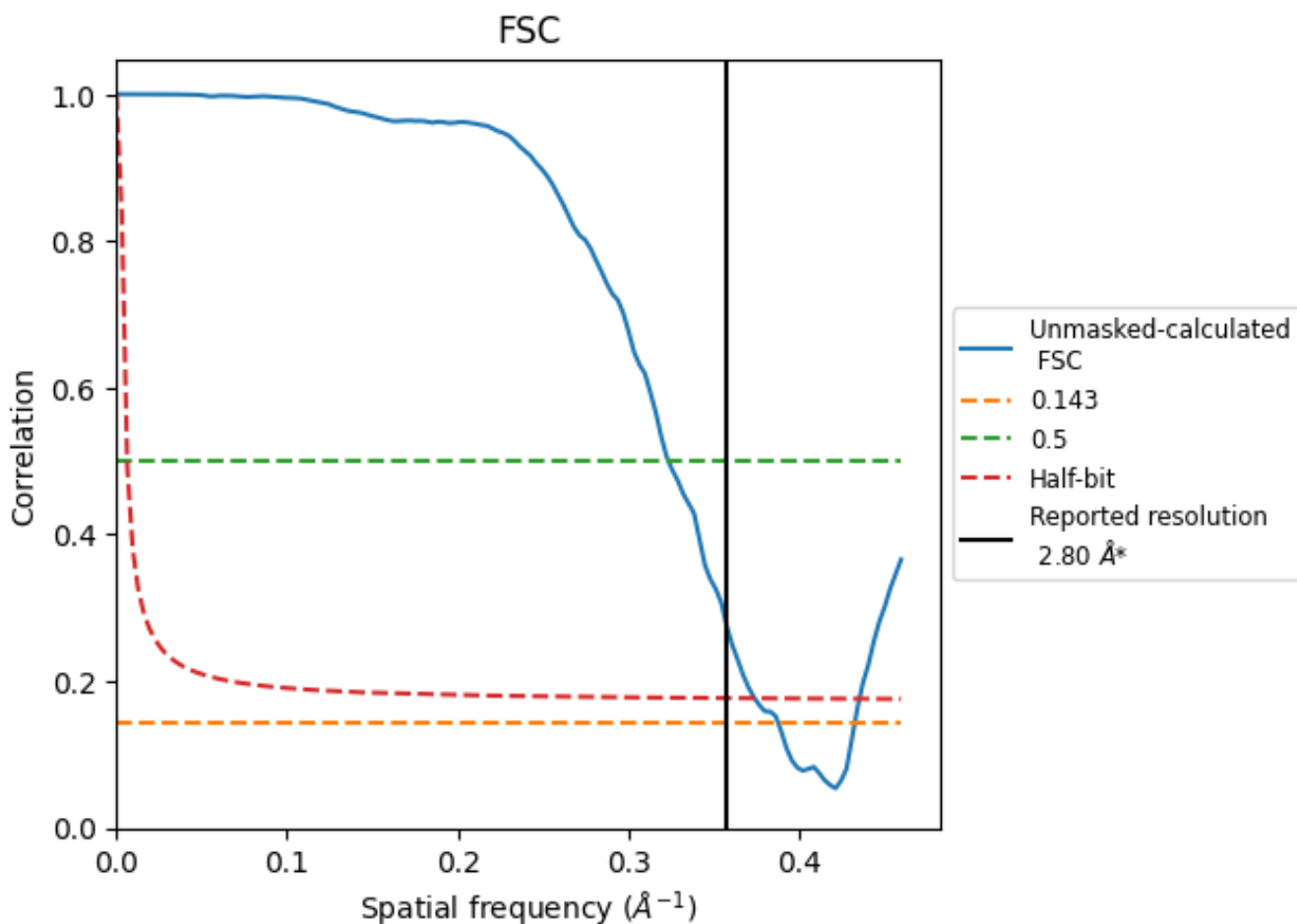


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 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 0.357 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

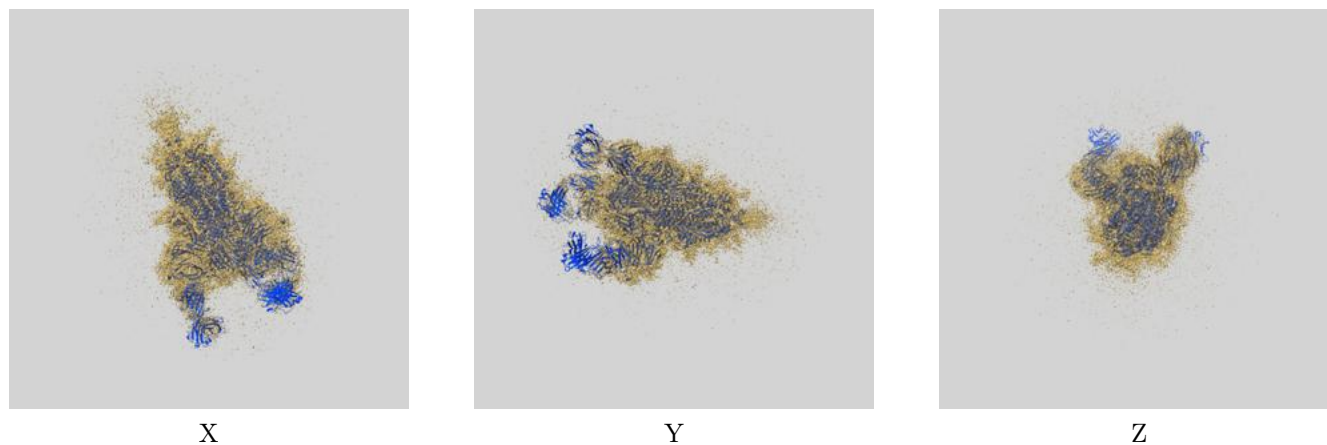
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.58	3.09	2.67

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

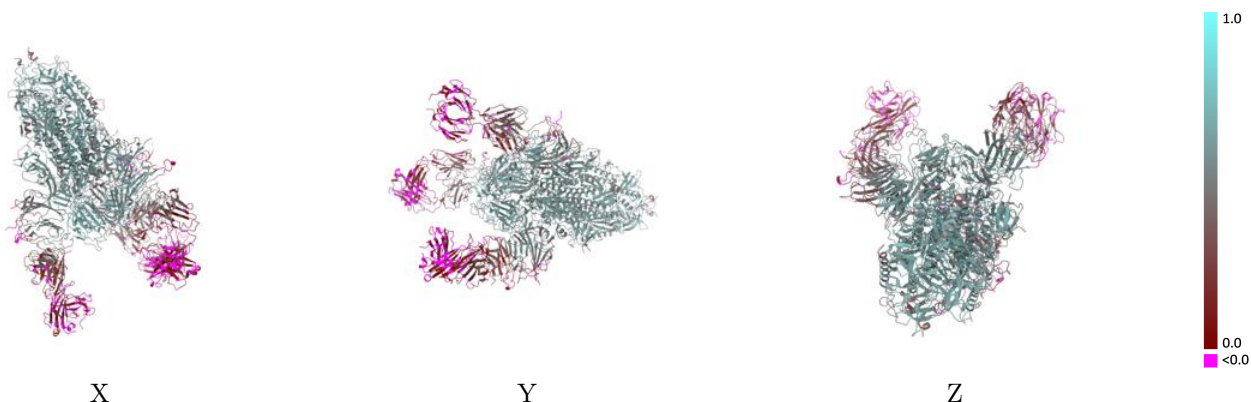
This section contains information regarding the fit between EMDB map EMD-34872 and PDB model 8HLC. Per-residue inclusion information can be found in section 3 on page 12.

### 9.1 Map-model overlay [i](#)



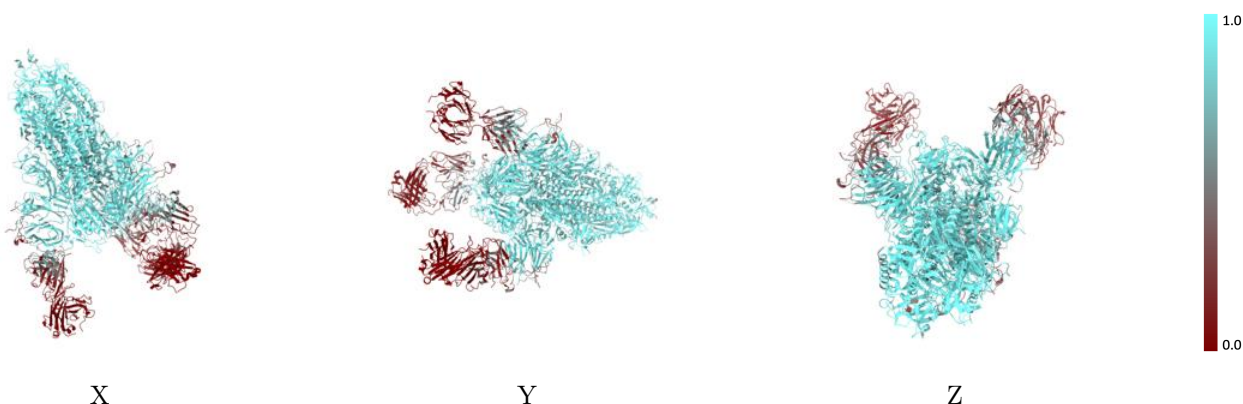
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



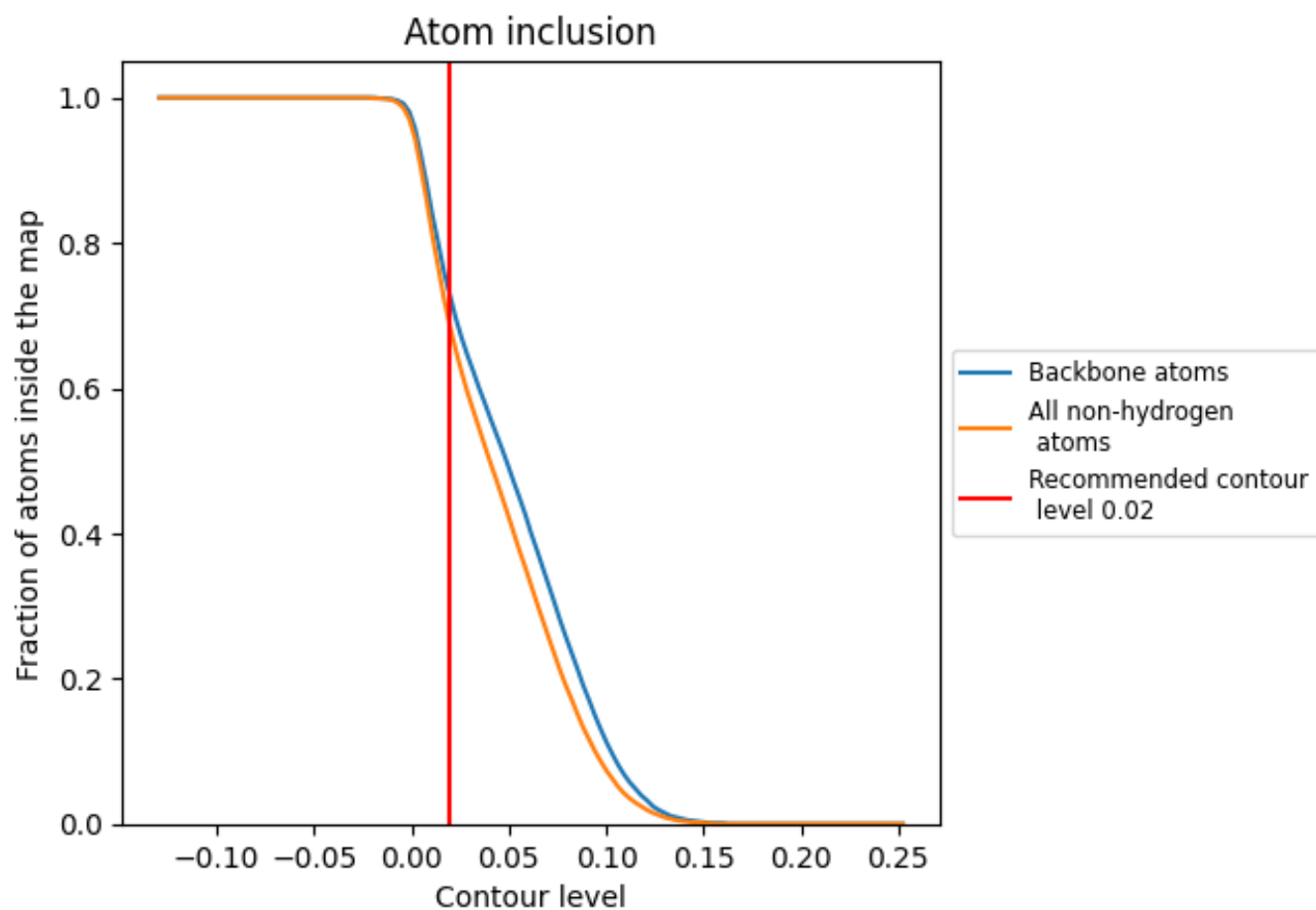
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.4310
A	 0.8930	 0.5480
B	 0.8870	 0.5420
C	 0.8740	 0.5270
D	 0.6070	 0.3990
E	 0.3090	 0.2320
F	 0.3570	 0.2730
G	 0.5360	 0.2820
H	 0.2550	 0.1820
I	 0.1770	 0.1590
J	 0.0920	 0.1240
K	 0.3210	 0.2010
L	 0.2550	 0.2020
M	 0.2000	 0.1850
N	 0.0950	 0.1320
O	 0.3570	 0.1460
P	 0.4290	 0.2080
Q	 0.7860	 0.5000
R	 0.5000	 0.3880
S	 0.8210	 0.3980
T	 0.4290	 0.2680
U	 0.3330	 0.2760
V	 0.3930	 0.1750
W	 0.6430	 0.3600
X	 0.3930	 0.1720
Y	 0.2500	 0.2620
Z	 0.8210	 0.4660
a	 0.8570	 0.4060
b	 0.5710	 0.2490
c	 0.2380	 0.1330
d	 0.2140	 0.0110
e	 0.5000	 0.2050
f	 0.2140	 0.1880
g	 0.2860	 0.0910
h	 0.7140	 0.4500
i	 0.7500	 0.3000

