



## Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 07:07 PM JST

PDB ID : 9JMF / pdb\_00009jmf  
EMDB ID : EMD-61600  
Title : Cryo-EM structure of SA-BatCoV (Neoromicia/PML-PHE1/RSA/2011)  
S-trimer  
Authors : Yuan, H.; Xiong, X.  
Deposited on : 2024-09-20  
Resolution : 3.10 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.dev118  
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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

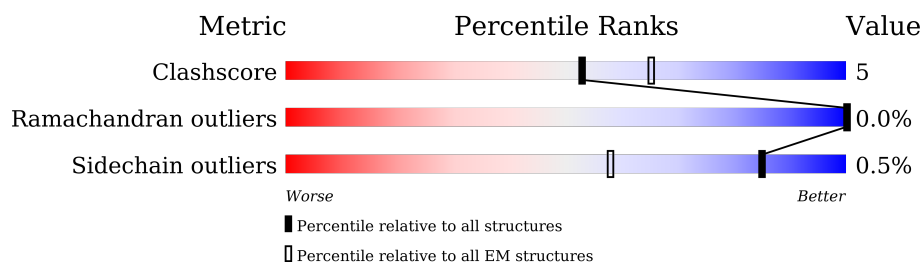
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.




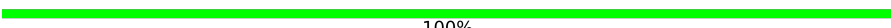
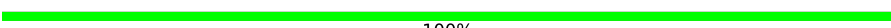
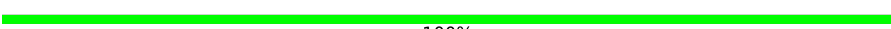




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1366	
1	B	1366	
1	C	1366	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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Mol	Chain	Length	Quality of chain
2	I	2	 50% 50%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 50% 50%
2	O	2	 100%
2	P	2	 100%
2	Q	2	 100%
2	R	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EIC	A	1412	-	-	X	-
4	EIC	B	1412	-	-	X	-
4	EIC	C	1412	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27750 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	1147	Total	C	N	O	S	0	0
			8936	5675	1490	1723	48		
1	B	1147	Total	C	N	O	S	0	0
			8936	5675	1490	1723	48		
1	C	1147	Total	C	N	O	S	0	0
			8936	5675	1490	1723	48		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1288	GLY	-	linker	UNP U5NJG5
A	1289	SER	-	linker	UNP U5NJG5
A	1311	LEU	PHE	conflict	UNP P10104
A	1317	LEU	-	expression tag	UNP P10104
A	1318	GLU	-	expression tag	UNP P10104
A	1319	VAL	-	expression tag	UNP P10104
A	1320	LEU	-	expression tag	UNP P10104
A	1321	PHE	-	expression tag	UNP P10104
A	1322	GLN	-	expression tag	UNP P10104
A	1323	GLY	-	expression tag	UNP P10104
A	1324	PRO	-	expression tag	UNP P10104
A	1325	GLY	-	expression tag	UNP P10104
A	1326	HIS	-	expression tag	UNP P10104
A	1327	HIS	-	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	SER	-	expression tag	UNP P10104
A	1335	ALA	-	expression tag	UNP P10104
A	1336	TRP	-	expression tag	UNP P10104
A	1337	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1338	HIS	-	expression tag	UNP P10104
A	1339	PRO	-	expression tag	UNP P10104
A	1340	GLN	-	expression tag	UNP P10104
A	1341	PHE	-	expression tag	UNP P10104
A	1342	GLU	-	expression tag	UNP P10104
A	1343	LYS	-	expression tag	UNP P10104
A	1344	GLY	-	expression tag	UNP P10104
A	1345	GLY	-	expression tag	UNP P10104
A	1346	GLY	-	expression tag	UNP P10104
A	1347	SER	-	expression tag	UNP P10104
A	1348	GLY	-	expression tag	UNP P10104
A	1349	GLY	-	expression tag	UNP P10104
A	1350	GLY	-	expression tag	UNP P10104
A	1351	GLY	-	expression tag	UNP P10104
A	1352	SER	-	expression tag	UNP P10104
A	1353	GLY	-	expression tag	UNP P10104
A	1354	GLY	-	expression tag	UNP P10104
A	1355	SER	-	expression tag	UNP P10104
A	1356	ALA	-	expression tag	UNP P10104
A	1357	TRP	-	expression tag	UNP P10104
A	1358	SER	-	expression tag	UNP P10104
A	1359	HIS	-	expression tag	UNP P10104
A	1360	PRO	-	expression tag	UNP P10104
A	1361	GLN	-	expression tag	UNP P10104
A	1362	PHE	-	expression tag	UNP P10104
A	1363	GLU	-	expression tag	UNP P10104
A	1364	LYS	-	expression tag	UNP P10104
A	1365	SER	-	expression tag	UNP P10104
A	1366	ALA	-	expression tag	UNP P10104
B	1288	GLY	-	linker	UNP U5NJB5
B	1289	SER	-	linker	UNP U5NJB5
B	1311	LEU	PHE	conflict	UNP P10104
B	1317	LEU	-	expression tag	UNP P10104
B	1318	GLU	-	expression tag	UNP P10104
B	1319	VAL	-	expression tag	UNP P10104
B	1320	LEU	-	expression tag	UNP P10104
B	1321	PHE	-	expression tag	UNP P10104
B	1322	GLN	-	expression tag	UNP P10104
B	1323	GLY	-	expression tag	UNP P10104
B	1324	PRO	-	expression tag	UNP P10104
B	1325	GLY	-	expression tag	UNP P10104
B	1326	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1327	HIS	-	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	SER	-	expression tag	UNP P10104
B	1335	ALA	-	expression tag	UNP P10104
B	1336	TRP	-	expression tag	UNP P10104
B	1337	SER	-	expression tag	UNP P10104
B	1338	HIS	-	expression tag	UNP P10104
B	1339	PRO	-	expression tag	UNP P10104
B	1340	GLN	-	expression tag	UNP P10104
B	1341	PHE	-	expression tag	UNP P10104
B	1342	GLU	-	expression tag	UNP P10104
B	1343	LYS	-	expression tag	UNP P10104
B	1344	GLY	-	expression tag	UNP P10104
B	1345	GLY	-	expression tag	UNP P10104
B	1346	GLY	-	expression tag	UNP P10104
B	1347	SER	-	expression tag	UNP P10104
B	1348	GLY	-	expression tag	UNP P10104
B	1349	GLY	-	expression tag	UNP P10104
B	1350	GLY	-	expression tag	UNP P10104
B	1351	GLY	-	expression tag	UNP P10104
B	1352	SER	-	expression tag	UNP P10104
B	1353	GLY	-	expression tag	UNP P10104
B	1354	GLY	-	expression tag	UNP P10104
B	1355	SER	-	expression tag	UNP P10104
B	1356	ALA	-	expression tag	UNP P10104
B	1357	TRP	-	expression tag	UNP P10104
B	1358	SER	-	expression tag	UNP P10104
B	1359	HIS	-	expression tag	UNP P10104
B	1360	PRO	-	expression tag	UNP P10104
B	1361	GLN	-	expression tag	UNP P10104
B	1362	PHE	-	expression tag	UNP P10104
B	1363	GLU	-	expression tag	UNP P10104
B	1364	LYS	-	expression tag	UNP P10104
B	1365	SER	-	expression tag	UNP P10104
B	1366	ALA	-	expression tag	UNP P10104
C	1288	GLY	-	linker	UNP U5NJB5
C	1289	SER	-	linker	UNP U5NJB5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1311	LEU	PHE	conflict	UNP P10104
C	1317	LEU	-	expression tag	UNP P10104
C	1318	GLU	-	expression tag	UNP P10104
C	1319	VAL	-	expression tag	UNP P10104
C	1320	LEU	-	expression tag	UNP P10104
C	1321	PHE	-	expression tag	UNP P10104
C	1322	GLN	-	expression tag	UNP P10104
C	1323	GLY	-	expression tag	UNP P10104
C	1324	PRO	-	expression tag	UNP P10104
C	1325	GLY	-	expression tag	UNP P10104
C	1326	HIS	-	expression tag	UNP P10104
C	1327	HIS	-	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	SER	-	expression tag	UNP P10104
C	1335	ALA	-	expression tag	UNP P10104
C	1336	TRP	-	expression tag	UNP P10104
C	1337	SER	-	expression tag	UNP P10104
C	1338	HIS	-	expression tag	UNP P10104
C	1339	PRO	-	expression tag	UNP P10104
C	1340	GLN	-	expression tag	UNP P10104
C	1341	PHE	-	expression tag	UNP P10104
C	1342	GLU	-	expression tag	UNP P10104
C	1343	LYS	-	expression tag	UNP P10104
C	1344	GLY	-	expression tag	UNP P10104
C	1345	GLY	-	expression tag	UNP P10104
C	1346	GLY	-	expression tag	UNP P10104
C	1347	SER	-	expression tag	UNP P10104
C	1348	GLY	-	expression tag	UNP P10104
C	1349	GLY	-	expression tag	UNP P10104
C	1350	GLY	-	expression tag	UNP P10104
C	1351	GLY	-	expression tag	UNP P10104
C	1352	SER	-	expression tag	UNP P10104
C	1353	GLY	-	expression tag	UNP P10104
C	1354	GLY	-	expression tag	UNP P10104
C	1355	SER	-	expression tag	UNP P10104
C	1356	ALA	-	expression tag	UNP P10104
C	1357	TRP	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1358	SER	-	expression tag	UNP P10104
C	1359	HIS	-	expression tag	UNP P10104
C	1360	PRO	-	expression tag	UNP P10104
C	1361	GLN	-	expression tag	UNP P10104
C	1362	PHE	-	expression tag	UNP P10104
C	1363	GLU	-	expression tag	UNP P10104
C	1364	LYS	-	expression tag	UNP P10104
C	1365	SER	-	expression tag	UNP P10104
C	1366	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	E	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	G	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	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
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		

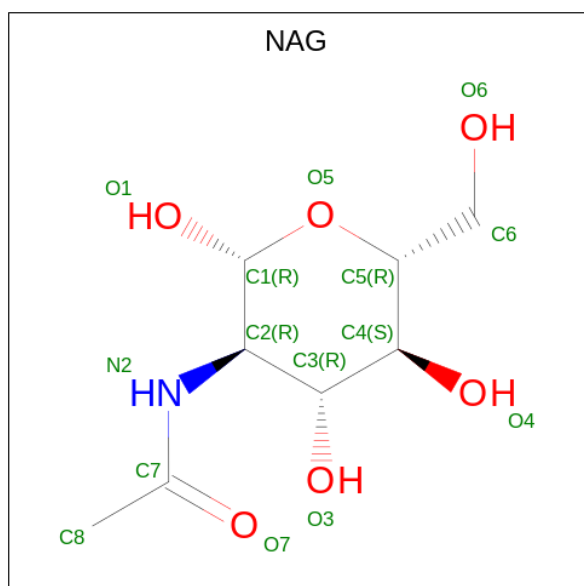
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Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

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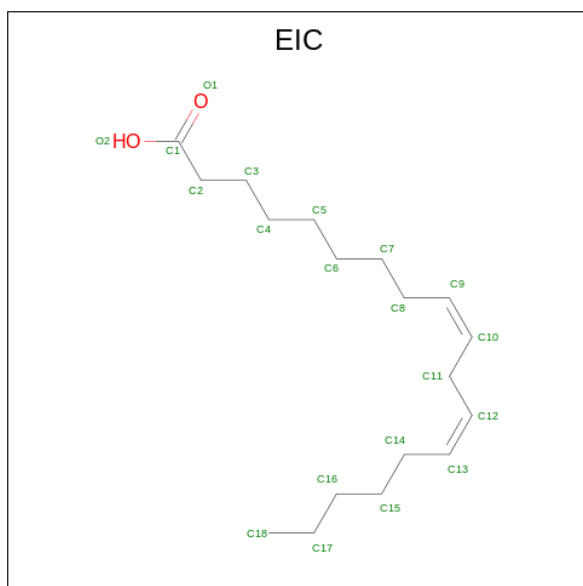
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3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

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

- Molecule 4 is LINOLEIC ACID (CCD ID: EIC) (formula:  $C_{18}H_{32}O_2$ ) (labeled as "Ligand of Interest" by depositor).

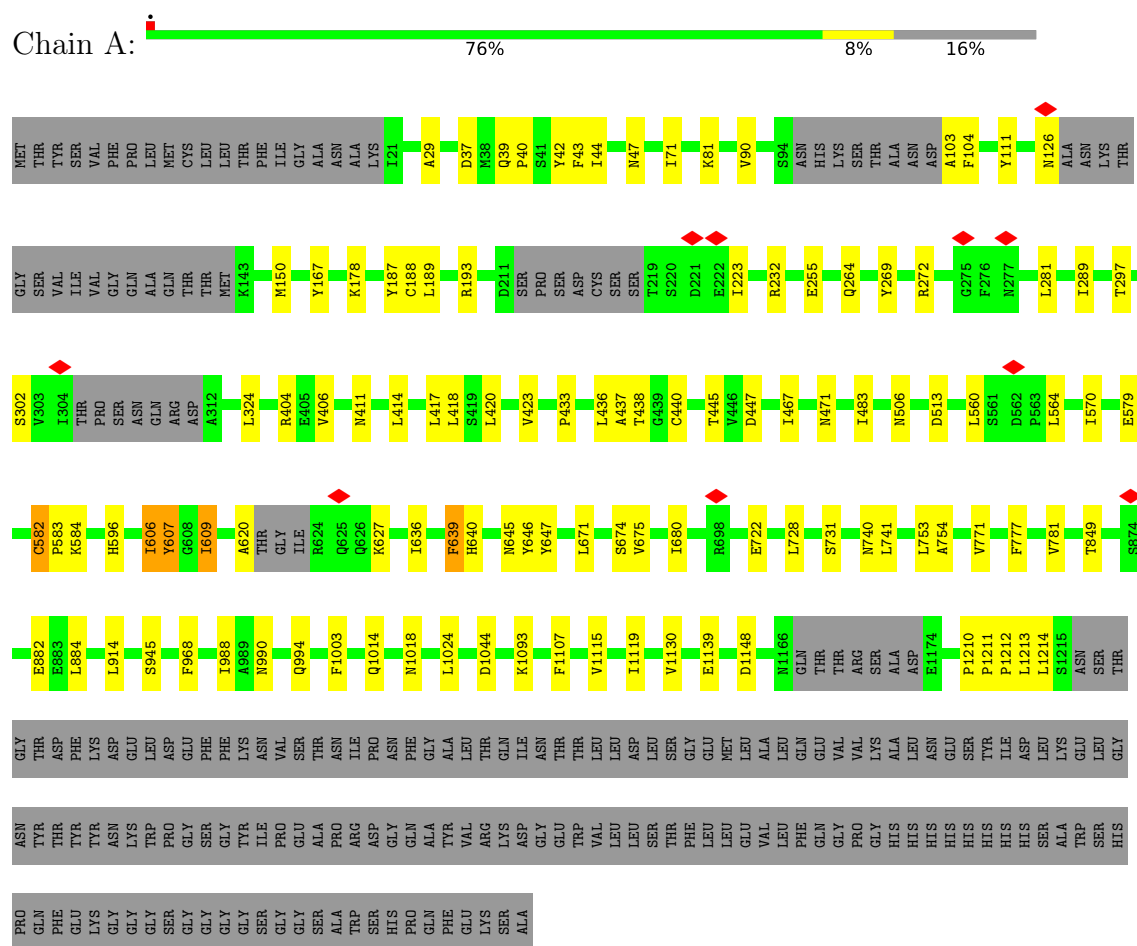


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			20	18	2	
4	B	1	Total	C	O	0
			20	18	2	
4	C	1	Total	C	O	0
			20	18	2	

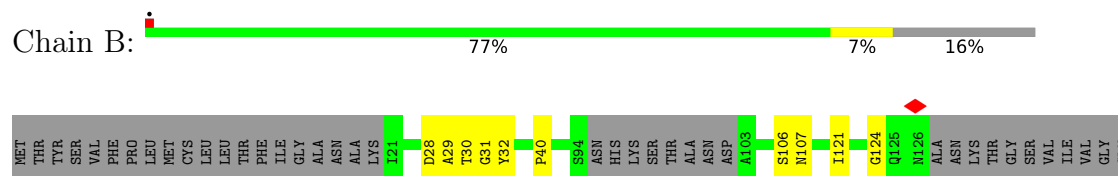
### 3 Residue-property plots

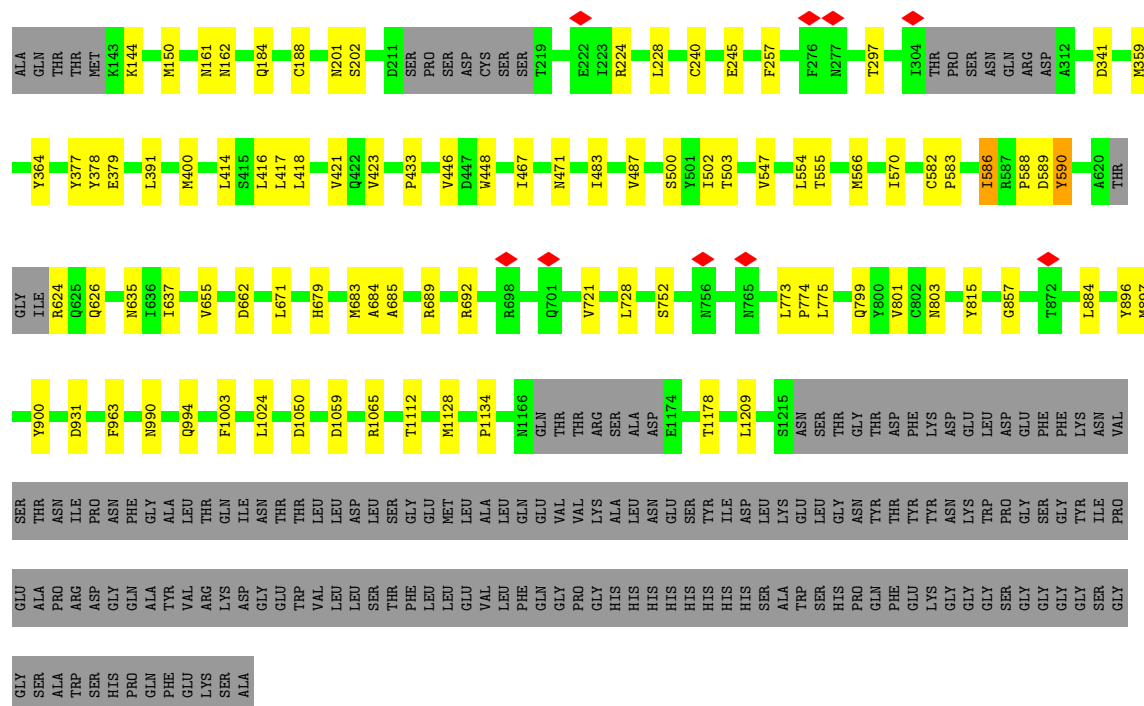
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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,Fibritin



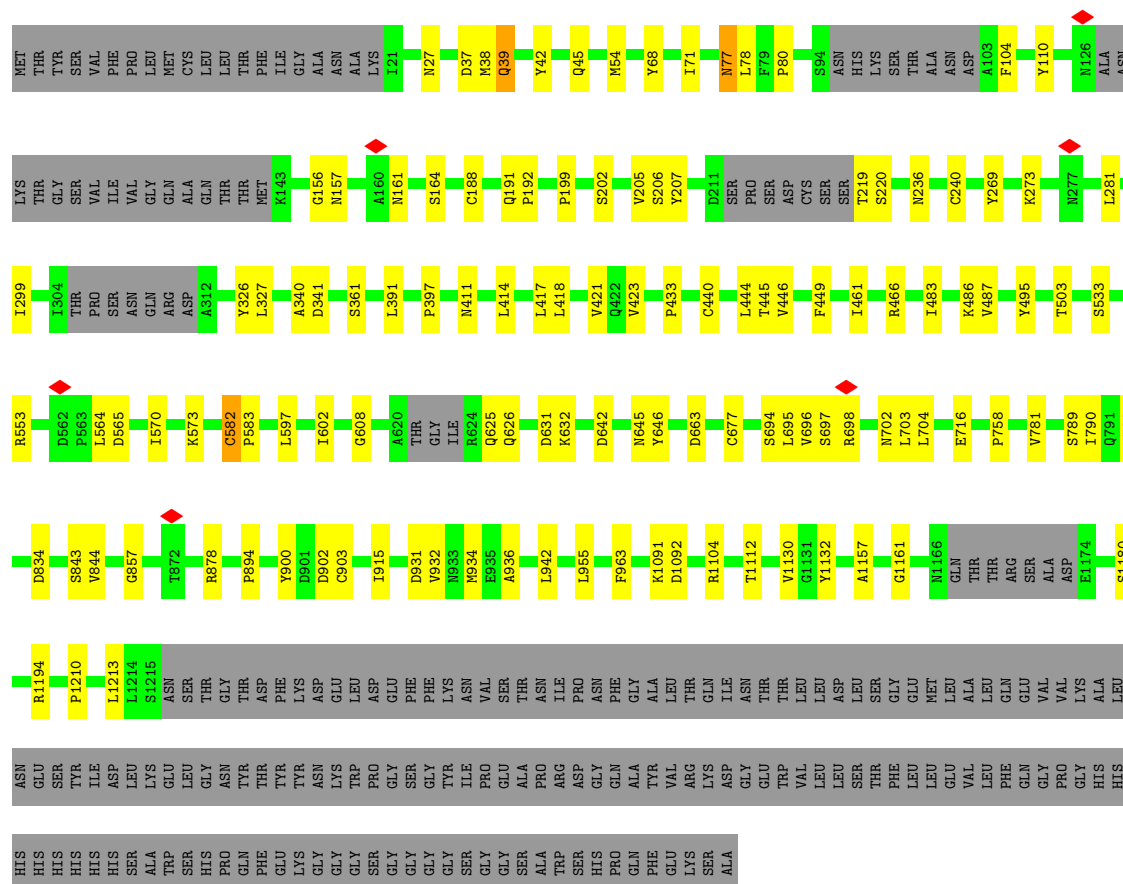
#### • Molecule 1: Spike glycoprotein,Fibritin





### ● Molecule 1: Spike glycoprotein,Fibritin

Chain C: 75% 9% 16%



- 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 E:  100%



- 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 G:  50% 50%



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

Chain H:  50% 50%



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

Chain I:  50% 50%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  100%



- 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:  50% 50%



- 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 P:  100%



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

Chain Q:  100%

MG1  
MG2

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

Chain R:  100%

MG1  
MG2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196103	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
Maximum map value	0.250	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.026	Depositor
Map size ( $\text{\AA}$ )	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.32, 1.32, 1.32	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	1/9146 (0.0%)	0.44	0/12446
1	B	0.34	2/9146 (0.0%)	0.49	7/12446 (0.1%)
1	C	0.36	3/9146 (0.0%)	0.46	6/12446 (0.0%)
All	All	0.34	6/27438 (0.0%)	0.46	13/37338 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	900	TYR	CA-C	-7.75	1.43	1.52
1	B	900	TYR	CA-C	-6.19	1.45	1.52
1	B	582	CYS	C-O	-6.09	1.18	1.24
1	A	607	TYR	CA-C	-5.90	1.47	1.53
1	C	1092	ASP	CA-C	-5.65	1.45	1.52
1	C	582	CYS	C-O	-5.59	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	694	SER	N-CA-C	10.00	122.18	111.28
1	B	590	TYR	N-CA-C	9.53	123.67	110.24
1	B	588	PRO	N-CA-C	7.54	123.50	113.40
1	C	789	SER	N-CA-C	7.08	119.62	108.79
1	B	31	GLY	N-CA-C	6.90	121.38	112.54
1	C	695	LEU	N-CA-C	-6.41	104.57	112.38
1	B	684	ALA	N-CA-C	6.35	119.01	111.33
1	B	897	MET	N-CA-C	6.08	117.91	111.28
1	B	589	ASP	N-CA-C	5.40	117.25	111.36
1	C	583	PRO	N-CA-C	5.29	119.80	111.38
1	B	583	PRO	CA-C-O	-5.16	115.37	121.67
1	C	39	GLN	CA-C-N	-5.11	114.71	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	GLN	C-N-CA	-5.11	114.71	120.89

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	8936	0	8572	100	0
1	B	8936	0	8575	75	0
1	C	8936	0	8575	98	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	24	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
3	A	154	0	143	1	0
3	B	154	0	143	2	0
3	C	154	0	143	2	0
4	A	20	0	31	33	0
4	B	20	0	31	22	0
4	C	20	0	31	33	0
All	All	27750	0	26618	275	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 (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:CD2	4:A:1412:EIC:H81	1.11	1.56
1:C:414:LEU:CD1	4:C:1412:EIC:H181	1.38	1.50
1:A:418:LEU:CD2	4:A:1412:EIC:C8	1.91	1.46
1:C:414:LEU:HD13	4:C:1412:EIC:C18	1.47	1.43
1:A:414:LEU:CD1	4:A:1412:EIC:H183	1.49	1.40
1:A:418:LEU:HD21	4:A:1412:EIC:C7	1.49	1.40
1:C:414:LEU:CD1	4:C:1412:EIC:C18	1.99	1.36
1:A:418:LEU:HD21	4:A:1412:EIC:C8	1.54	1.25
1:C:414:LEU:CD1	4:C:1412:EIC:C17	2.18	1.21
1:C:418:LEU:CD2	4:C:1412:EIC:H71	1.70	1.20
1:C:414:LEU:HD12	4:C:1412:EIC:C17	1.73	1.18
1:A:418:LEU:HD23	4:A:1412:EIC:C8	1.62	1.15
1:C:414:LEU:HD12	4:C:1412:EIC:H171	1.17	1.14
1:B:418:LEU:HD23	4:B:1412:EIC:H82	1.22	1.14
1:A:414:LEU:HD13	4:A:1412:EIC:H183	1.13	1.12
1:C:418:LEU:HD21	4:C:1412:EIC:H71	1.15	1.10
1:A:418:LEU:HD21	4:A:1412:EIC:H72	1.26	1.08
1:B:414:LEU:HD13	4:B:1412:EIC:H172	1.31	1.08
1:B:418:LEU:CD2	4:B:1412:EIC:H82	1.84	1.06
1:B:418:LEU:HD21	4:B:1412:EIC:H62	1.11	1.06
1:B:418:LEU:HD21	4:B:1412:EIC:C6	1.87	1.04
1:A:414:LEU:HD13	4:A:1412:EIC:C18	1.89	1.01
1:B:414:LEU:HD13	4:B:1412:EIC:C17	1.94	0.98
1:A:417:LEU:HD23	4:A:1412:EIC:H131	1.46	0.98
1:C:417:LEU:HD22	4:C:1412:EIC:C14	1.93	0.97
1:A:418:LEU:CD2	4:A:1412:EIC:C7	2.34	0.95
1:C:418:LEU:HD21	4:C:1412:EIC:C7	1.97	0.95
1:C:54:MET:HE1	1:C:341:ASP:HB2	1.45	0.94
1:C:417:LEU:HD22	4:C:1412:EIC:H141	1.48	0.93
1:A:414:LEU:HD12	4:A:1412:EIC:H183	1.48	0.92
1:C:414:LEU:CD1	4:C:1412:EIC:H171	1.91	0.89
1:A:414:LEU:CD1	4:A:1412:EIC:C18	2.45	0.88
1:A:609:ILE:HD12	1:A:636:ILE:HD13	1.55	0.88
1:C:417:LEU:CD2	4:C:1412:EIC:H142	2.03	0.88
1:A:39:GLN:HB2	1:A:104:PHE:CE1	2.09	0.88
1:C:417:LEU:CD2	4:C:1412:EIC:C14	2.52	0.87
1:C:414:LEU:HD11	4:C:1412:EIC:H181	1.54	0.87
1:A:418:LEU:HD23	4:A:1412:EIC:H81	0.87	0.86
1:C:414:LEU:HD11	4:C:1412:EIC:C18	2.03	0.85
1:A:39:GLN:HB2	1:A:104:PHE:HE1	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:MET:CE	1:C:341:ASP:HB2	2.11	0.80
1:A:423:VAL:HG21	4:A:1412:EIC:H21	1.61	0.79
1:C:414:LEU:HD13	4:C:1412:EIC:C17	2.01	0.78
1:A:417:LEU:CD2	4:A:1412:EIC:H151	2.14	0.78
1:A:417:LEU:HD23	4:A:1412:EIC:C13	2.14	0.77
1:A:418:LEU:HD22	4:A:1412:EIC:H81	1.54	0.76
1:A:418:LEU:HD23	4:A:1412:EIC:C9	2.16	0.75
1:C:418:LEU:CD2	4:C:1412:EIC:C7	2.59	0.73
1:B:483:ILE:HG21	4:B:1412:EIC:H42	1.71	0.73
1:B:418:LEU:CD2	4:B:1412:EIC:C8	2.65	0.72
1:C:414:LEU:HD13	4:C:1412:EIC:H181	0.73	0.72
1:C:188:CYS:HB3	1:C:240:CYS:HA	1.71	0.71
1:A:417:LEU:CD2	4:A:1412:EIC:H131	2.20	0.70
1:B:418:LEU:CD2	4:B:1412:EIC:H62	2.06	0.70
1:A:438:THR:HA	1:A:583:PRO:HG3	1.74	0.70
1:B:418:LEU:HD23	4:B:1412:EIC:C8	2.12	0.70
1:C:696:VAL:HG12	1:C:697:SER:H	1.56	0.69
1:C:77:ASN:HD22	1:C:78:LEU:H	1.41	0.68
4:A:1412:EIC:H72	4:A:1412:EIC:H32	1.76	0.68
1:C:570:ILE:HD13	4:C:1412:EIC:H152	1.77	0.67
1:C:433:PRO:HB3	4:C:1412:EIC:H51	1.78	0.66
1:B:418:LEU:HD21	4:B:1412:EIC:C7	2.26	0.65
1:C:696:VAL:HG12	1:C:697:SER:N	2.10	0.65
1:A:639:PHE:CE1	1:A:647:TYR:HD2	2.16	0.64
1:A:467:ILE:HA	1:A:471:ASN:HD22	1.62	0.63
1:B:570:ILE:HD11	4:B:1412:EIC:H111	1.78	0.63
1:B:433:PRO:HB3	4:B:1412:EIC:H52	1.80	0.63
1:C:417:LEU:HD21	4:C:1412:EIC:H142	1.81	0.63
1:A:417:LEU:HD23	4:A:1412:EIC:C15	2.28	0.63
1:C:417:LEU:HD22	4:C:1412:EIC:H142	1.66	0.63
1:A:417:LEU:HD23	4:A:1412:EIC:H151	1.80	0.62
1:A:433:PRO:HB3	4:A:1412:EIC:H31	1.82	0.62
1:C:1161:GLY:HA2	1:C:1180:SER:HB3	1.82	0.61
1:C:857:GLY:HA2	1:C:963:PHE:HB3	1.82	0.61
1:C:417:LEU:CD2	4:C:1412:EIC:H112	2.31	0.60
1:B:655:VAL:HG21	1:B:683:MET:HE1	1.84	0.60
1:C:790:ILE:HG13	1:C:790:ILE:O	2.00	0.60
1:A:1211:PRO:HA	1:A:1214:LEU:HD12	1.83	0.59
1:C:417:LEU:HD23	4:C:1412:EIC:H112	1.84	0.59
1:A:433:PRO:HB3	4:A:1412:EIC:H52	1.85	0.58
1:A:189:LEU:HD12	1:A:189:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:CYS:HB3	1:B:240:CYS:HA	1.85	0.58
1:B:184:GLN:HE22	1:B:228:LEU:HB2	1.68	0.58
1:B:590:TYR:CD1	1:B:590:TYR:N	2.71	0.58
1:C:844:VAL:HG13	1:C:942:LEU:HD22	1.86	0.58
1:B:590:TYR:H	1:B:590:TYR:HD1	1.49	0.57
1:C:54:MET:HE1	1:C:341:ASP:CB	2.25	0.57
1:A:29:ALA:O	1:A:193:ARG:NH1	2.37	0.57
1:A:40:PRO:HB2	3:A:1402:NAG:H62	1.86	0.57
1:A:483:ILE:CD1	4:A:1412:EIC:H61	2.35	0.56
1:A:483:ILE:HD11	4:A:1412:EIC:H51	1.86	0.56
1:A:570:ILE:HD13	4:A:1412:EIC:H161	1.88	0.56
1:A:582:CYS:SG	1:A:583:PRO:HD2	2.46	0.55
1:C:433:PRO:HB3	4:C:1412:EIC:C5	2.36	0.55
1:B:378:TYR:CE2	1:B:586:ILE:HG22	2.40	0.55
1:C:1157:ALA:O	1:C:1194:ARG:HG2	2.07	0.55
1:A:417:LEU:HD21	4:A:1412:EIC:H151	1.88	0.55
1:A:483:ILE:HD13	4:A:1412:EIC:H61	1.87	0.55
1:A:42:TYR:CD1	1:A:104:PHE:HZ	2.25	0.55
1:C:781:VAL:HG22	1:C:1130:VAL:HG12	1.88	0.55
1:C:533:SER:HB3	1:C:553:ARG:HD3	1.88	0.54
1:B:150:MET:HB3	1:B:297:THR:HG22	1.90	0.54
1:B:418:LEU:HD21	4:B:1412:EIC:C8	2.36	0.54
1:B:799:GLN:NE2	1:B:803:ASN:OD1	2.40	0.54
1:A:627:LYS:NZ	1:A:640:HIS:O	2.37	0.54
1:C:161:ASN:HB3	1:C:202:SER:HA	1.89	0.54
1:C:625:GLN:HG3	1:C:626:GLN:HG2	1.90	0.54
1:C:1210:PRO:HD2	1:C:1213:LEU:HD12	1.90	0.53
1:A:437:ALA:O	1:A:583:PRO:HB3	2.08	0.53
1:A:639:PHE:HE1	1:A:647:TYR:HD2	1.54	0.53
1:C:192:PRO:HB3	1:C:199:PRO:HB2	1.90	0.53
1:B:341:ASP:OD2	1:B:689:ARG:NH2	2.41	0.53
1:A:884:LEU:HD22	1:A:1003:PHE:HD2	1.74	0.53
1:A:1014:GLN:O	1:A:1018:ASN:ND2	2.42	0.53
1:A:44:ILE:O	1:A:47:ASN:ND2	2.42	0.53
1:C:495:TYR:HB3	1:C:564:LEU:HD11	1.91	0.53
1:A:39:GLN:CB	1:A:104:PHE:HE1	2.18	0.52
1:C:1112:THR:HB	1:C:1132:TYR:HB3	1.90	0.52
1:C:327:LEU:HB3	1:C:340:ALA:HB3	1.91	0.52
1:A:103:ALA:HB3	1:A:302:SER:CB	2.40	0.52
1:B:418:LEU:HD21	4:B:1412:EIC:H82	1.82	0.52
1:C:191:GLN:HB2	1:C:236:ASN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:LYS:NZ	1:A:1107:PHE:O	2.38	0.51
1:B:421:VAL:HG12	1:B:487:VAL:HG22	1.92	0.51
1:B:184:GLN:NE2	1:B:228:LEU:HB2	2.25	0.51
1:B:417:LEU:CD2	4:B:1412:EIC:H161	2.40	0.51
1:B:224:ARG:NH1	1:B:245:GLU:OE2	2.34	0.51
1:C:110:TYR:OH	1:C:205:VAL:O	2.26	0.51
1:C:645:ASN:OD1	1:C:646:TYR:N	2.44	0.51
1:B:662:ASP:N	1:B:662:ASP:OD1	2.44	0.51
1:C:486:LYS:NZ	1:C:565:ASP:OD2	2.43	0.51
1:C:631:ASP:OD1	1:C:632:LYS:N	2.44	0.50
1:C:704:LEU:HD13	1:C:716:GLU:HG2	1.93	0.50
1:A:1148:ASP:OD1	1:A:1148:ASP:N	2.34	0.50
1:C:38:MET:HE3	1:C:206:SER:HB2	1.93	0.50
1:C:207:TYR:HE1	1:C:299:ILE:HG12	1.76	0.50
1:B:500:SER:HB3	1:B:555:THR:HG22	1.93	0.50
1:A:740:ASN:OD1	1:A:741:LEU:N	2.44	0.50
1:A:1210:PRO:HB2	1:A:1212:PRO:HD2	1.94	0.50
4:A:1412:EIC:H41	4:A:1412:EIC:H82	1.94	0.50
1:C:27:ASN:OD1	1:C:27:ASN:N	2.44	0.50
1:C:219:THR:OG1	1:C:220:SER:N	2.44	0.50
1:A:37:ASP:OD1	1:A:37:ASP:N	2.43	0.50
1:A:849:THR:HG22	1:C:758:PRO:HB2	1.92	0.50
1:C:696:VAL:CG1	1:C:697:SER:H	2.24	0.50
1:C:42:TYR:O	1:C:45:GLN:NE2	2.45	0.50
1:A:269:TYR:HB3	1:A:281:LEU:HB3	1.92	0.49
1:A:570:ILE:CD1	4:A:1412:EIC:H142	2.42	0.49
1:A:560:LEU:HD13	1:A:564:LEU:HD11	1.94	0.49
1:A:722:GLU:HG2	1:A:754:ALA:HB3	1.93	0.49
1:B:418:LEU:CD2	4:B:1412:EIC:C7	2.89	0.49
1:B:774:PRO:HB3	1:B:1134:PRO:HB3	1.93	0.49
1:B:685:ALA:HA	1:B:692:ARG:HE	1.77	0.49
1:A:433:PRO:CB	4:A:1412:EIC:H31	2.42	0.49
1:B:448:TRP:HD1	1:B:566:MET:HE1	1.77	0.49
1:C:843:SER:OG	1:C:1091:LYS:NZ	2.40	0.49
1:A:777:PHE:HZ	1:A:988:ILE:HG22	1.78	0.49
1:B:161:ASN:ND2	1:B:201:ASN:O	2.41	0.49
1:A:1210:PRO:HD2	1:A:1213:LEU:HD12	1.94	0.49
1:A:671:LEU:HD22	1:A:728:LEU:HD22	1.94	0.48
1:A:255:GLU:OE1	1:A:272:ARG:HG2	2.11	0.48
1:A:189:LEU:HD12	1:A:189:LEU:N	2.28	0.48
1:A:639:PHE:HE1	1:A:647:TYR:CD2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ILE:HG22	1:A:607:TYR:H	1.78	0.48
1:C:361:SER:OG	1:C:663:ASP:OD1	2.31	0.48
1:C:269:TYR:HB3	1:C:281:LEU:HB3	1.96	0.48
1:C:696:VAL:CG1	1:C:697:SER:N	2.77	0.48
1:C:421:VAL:HG12	1:C:487:VAL:HG22	1.95	0.47
1:B:990:ASN:O	1:B:994:GLN:HG3	2.14	0.47
1:B:423:VAL:HG21	4:B:1412:EIC:H22	1.95	0.47
1:A:264:GLN:OE1	1:C:445:THR:OG1	2.32	0.47
1:A:81:LYS:HG2	1:A:324:LEU:HD11	1.97	0.47
1:B:40:PRO:HB2	3:B:1402:NAG:H62	1.96	0.47
1:B:391:LEU:HD21	1:B:446:VAL:HG11	1.96	0.47
4:C:1412:EIC:H81	4:C:1412:EIC:H111	1.51	0.47
1:A:103:ALA:HB3	1:A:302:SER:HB3	1.96	0.47
1:A:1044:ASP:OD1	1:A:1044:ASP:N	2.48	0.46
1:B:124:GLY:HA3	1:B:144:LYS:HG3	1.96	0.46
1:C:697:SER:OG	1:C:698:ARG:N	2.38	0.46
1:C:894:PRO:HB3	1:C:915:ILE:HD12	1.98	0.46
1:B:503:THR:HG21	1:B:554:LEU:HD12	1.97	0.46
1:C:68:TYR:HD2	1:C:71:ILE:HD11	1.80	0.46
1:C:642:ASP:OD1	1:C:642:ASP:N	2.49	0.46
1:A:433:PRO:HA	1:A:436:LEU:HD12	1.97	0.46
1:A:609:ILE:HD12	1:A:636:ILE:CD1	2.38	0.46
1:A:968:PHE:HE1	1:A:988:ILE:HD11	1.80	0.46
1:A:404:ARG:NH2	1:A:447:ASP:OD2	2.49	0.46
1:B:467:ILE:HA	1:B:471:ASN:HD22	1.81	0.46
1:B:378:TYR:HB2	1:B:590:TYR:CD2	2.51	0.45
1:B:400:MET:HG3	1:B:502:ILE:HG13	1.98	0.45
1:B:931:ASP:OD1	1:B:931:ASP:N	2.45	0.45
1:C:156:GLY:HA2	3:C:1403:NAG:H82	1.98	0.45
1:C:161:ASN:HA	3:C:1404:NAG:H82	1.97	0.45
1:C:573:LYS:HE3	1:C:573:LYS:HB3	1.72	0.45
1:C:483:ILE:HD13	4:C:1412:EIC:H72	1.97	0.45
1:A:43:PHE:HD2	1:A:90:VAL:HG13	1.82	0.45
1:A:406:VAL:HG22	1:A:445:THR:HG23	1.98	0.45
1:B:121:ILE:HD12	1:B:257:PHE:HD2	1.82	0.45
1:B:359:MET:HE2	1:B:364:TYR:CZ	2.51	0.45
1:C:792:LYS:NZ	1:C:834:ASP:OD1	2.43	0.45
1:A:1115:VAL:HG12	1:A:1130:VAL:HB	2.00	0.44
1:A:178:LYS:HG3	1:A:223:ILE:HG22	1.99	0.44
1:A:781:VAL:HG22	1:A:1130:VAL:HG22	2.00	0.44
1:B:590:TYR:N	1:B:590:TYR:HD1	2.12	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:ASP:O	1:C:903:CYS:C	2.60	0.44
1:C:423:VAL:HG11	4:C:1412:EIC:H31	1.99	0.44
1:A:506:ASN:ND2	1:A:513:ASP:OD1	2.51	0.44
1:A:596:HIS:H	1:A:596:HIS:CD2	2.36	0.44
1:B:1050:ASP:HB2	1:C:461:ILE:HG12	2.00	0.44
1:B:635:ASN:O	1:B:637:ILE:HG23	2.18	0.43
1:B:655:VAL:HG21	1:B:683:MET:CE	2.46	0.43
1:B:414:LEU:HD13	4:B:1412:EIC:H171	1.92	0.43
1:C:417:LEU:CD2	4:C:1412:EIC:H141	2.27	0.43
4:C:1412:EIC:H21	4:C:1412:EIC:H52	1.80	0.43
1:A:675:VAL:HG21	1:A:680:ILE:HD11	1.99	0.43
1:C:39:GLN:HB2	1:C:104:PHE:CE1	2.53	0.43
1:C:80:PRO:O	1:C:326:TYR:OH	2.25	0.43
1:C:440:CYS:HB2	1:C:608:GLY:HA3	2.00	0.43
1:A:411:ASN:HB3	1:A:584:LYS:HG2	2.01	0.43
1:B:416:LEU:HD12	1:B:416:LEU:HA	1.87	0.43
1:C:444:LEU:HD21	4:C:1412:EIC:H162	2.01	0.43
1:B:483:ILE:CG2	4:B:1412:EIC:H42	2.42	0.43
1:C:466:ARG:HD2	1:C:503:THR:HG23	2.01	0.43
1:A:882:GLU:HG2	1:A:1119:ILE:HB	2.01	0.43
1:B:377:TYR:OH	1:B:379:GLU:OE1	2.32	0.43
4:B:1412:EIC:H41	4:B:1412:EIC:H71	1.54	0.43
1:C:1104:ARG:H	1:C:1104:ARG:HG2	1.62	0.42
1:A:620:ALA:C	1:A:646:TYR:CD2	2.97	0.42
1:B:1024:LEU:HD23	1:B:1024:LEU:HA	1.80	0.42
1:C:411:ASN:HA	1:C:582:CYS:O	2.20	0.42
1:A:731:SER:HA	1:A:753:LEU:HD13	2.01	0.42
1:A:914:LEU:HD11	1:A:1024:LEU:HB3	2.00	0.42
4:B:1412:EIC:H112	4:B:1412:EIC:H81	1.73	0.42
1:C:931:ASP:OD1	1:C:932:VAL:N	2.51	0.42
1:B:721:VAL:HG22	1:B:752:SER:HB3	2.01	0.42
1:B:857:GLY:HA2	1:B:963:PHE:HB3	2.01	0.42
1:B:1209:LEU:HD23	1:B:1209:LEU:HA	1.92	0.42
1:A:1024:LEU:HD23	1:A:1024:LEU:HA	1.88	0.42
1:B:161:ASN:HB3	1:B:202:SER:HA	2.01	0.42
4:C:1412:EIC:H141	4:C:1412:EIC:H112	1.83	0.42
1:A:945:SER:O	1:A:945:SER:OG	2.38	0.42
1:C:597:LEU:HB3	1:C:602:ILE:HG21	2.02	0.42
1:C:677:CYS:HB3	1:C:703:LEU:HD13	2.02	0.42
1:A:111:TYR:O	1:A:297:THR:HG22	2.20	0.42
1:A:990:ASN:O	1:A:994:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASP:OD1	1:B:29:ALA:N	2.52	0.41
1:A:187:TYR:CE1	1:A:289:ILE:HD12	2.55	0.41
1:B:773:LEU:HA	1:B:774:PRO:HD3	1.94	0.41
1:B:815:TYR:OH	1:B:1059:ASP:OD1	2.29	0.41
1:C:702:ASN:OD1	1:C:702:ASN:N	2.53	0.41
1:A:150:MET:HG2	1:A:167:TYR:CD2	2.56	0.41
1:C:878:ARG:HG2	1:C:936:ALA:HB2	2.03	0.41
1:B:162:ASN:ND2	3:B:1404:NAG:O7	2.53	0.41
1:B:884:LEU:HD22	1:B:1003:PHE:HD2	1.84	0.41
1:C:934:MET:HE3	1:C:934:MET:HB2	1.86	0.41
1:A:674:SER:CB	1:B:896:TYR:O	2.69	0.41
1:A:777:PHE:CZ	1:A:988:ILE:HG22	2.56	0.41
1:B:1112:THR:HG22	1:C:955:LEU:H	1.85	0.41
1:C:157:ASN:HA	1:C:164:SER:HA	2.01	0.41
1:A:126:ASN:OD1	1:A:126:ASN:N	2.54	0.41
1:B:671:LEU:HD22	1:B:728:LEU:HD22	2.02	0.41
1:B:106:SER:OG	1:B:107:ASN:N	2.54	0.41
1:B:773:LEU:HD21	1:B:1178:THR:HG21	2.04	0.41
1:A:771:VAL:O	1:A:1139:GLU:HA	2.20	0.40
1:B:679:HIS:ND1	1:B:683:MET:HE2	2.36	0.40
1:B:801:VAL:O	1:B:1065:ARG:NH1	2.50	0.40
1:C:37:ASP:OD1	1:C:37:ASP:N	2.44	0.40
1:C:391:LEU:HD21	1:C:446:VAL:HG11	2.02	0.40
1:C:397:PRO:HG2	1:C:449:PHE:HA	2.03	0.40
1:A:440:CYS:HB3	1:A:579:GLU:HB3	2.03	0.40
1:A:968:PHE:CE1	1:A:988:ILE:HD11	2.57	0.40
1:B:624:ARG:HG3	1:B:626:GLN:O	2.21	0.40
1:B:655:VAL:CG2	1:B:683:MET:HE1	2.50	0.40
1:B:1128:MET:HE2	1:B:1128:MET:HB2	1.87	0.40
1:C:273:LYS:HE3	1:C:273:LYS:HB3	1.88	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	1133/1366 (83%)	1088 (96%)	44 (4%)	1 (0%)	48	79
1	B	1133/1366 (83%)	1082 (96%)	51 (4%)	0	100	100
1	C	1133/1366 (83%)	1091 (96%)	42 (4%)	0	100	100
All	All	3399/4098 (83%)	3261 (96%)	137 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	606	ILE

### 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	981/1163 (84%)	973 (99%)	8 (1%)	79	89
1	B	981/1163 (84%)	976 (100%)	5 (0%)	86	92
1	C	981/1163 (84%)	980 (100%)	1 (0%)	92	97
All	All	2943/3489 (84%)	2929 (100%)	14 (0%)	85	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ILE
1	A	188	CYS
1	A	232	ARG
1	A	420	LEU
1	A	582	CYS
1	A	609	ILE
1	A	639	PHE
1	A	645	ASN
1	B	30	THR

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Mol	Chain	Res	Type
1	B	32	TYR
1	B	547	VAL
1	B	586	ILE
1	B	775	LEU
1	C	77	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	702	ASN
1	A	730	GLN
1	A	783	GLN
1	A	839	ASN
1	A	918	GLN
1	A	972	ASN
1	A	1018	ASN
1	A	1095	ASN
1	A	1133	HIS
1	B	39	GLN
1	B	184	GLN
1	B	322	HIS
1	B	338	GLN
1	B	349	GLN
1	B	585	GLN
1	B	635	ASN
1	B	666	ASN
1	B	776	ASN
1	B	824	GLN
1	B	898	GLN
1	B	972	ASN
1	B	978	GLN
1	B	984	ASN
1	B	1011	GLN
1	B	1101	GLN
1	B	1154	ASN
1	B	1199	GLN
1	B	1203	GLN
1	C	39	GLN
1	C	77	ASN
1	C	201	ASN
1	C	478	ASN
1	C	506	ASN

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Mol	Chain	Res	Type
1	C	525	GLN
1	C	640	HIS
1	C	783	GLN
1	C	839	ASN
1	C	861	ASN
1	C	876	ASN
1	C	979	GLN
1	C	985	GLN
1	C	1014	GLN
1	C	1057	GLN
1	C	1070	ASN
1	C	1203	GLN
1	C	1208	ASN

### 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 ⓘ

30 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	1,2	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
2	NAG	D	2	2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	E	1	1,2	14,14,15	0.20	0	17,19,21	0.58	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	F	1	1,2	14,14,15	0.24	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	F	2	2	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	G	1	1,2	14,14,15	0.36	0	17,19,21	0.70	1 (5%)
2	NAG	G	2	2	14,14,15	0.39	0	17,19,21	0.52	0
2	NAG	H	1	1,2	14,14,15	0.50	0	17,19,21	0.90	1 (5%)
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.63	0
2	NAG	I	1	1,2	14,14,15	0.28	0	17,19,21	0.66	1 (5%)
2	NAG	I	2	2	14,14,15	0.26	0	17,19,21	0.46	0
2	NAG	J	1	1,2	14,14,15	0.19	0	17,19,21	0.60	0
2	NAG	J	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	K	1	1,2	14,14,15	0.32	0	17,19,21	0.51	0
2	NAG	K	2	2	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	L	1	1,2	14,14,15	0.28	0	17,19,21	0.58	0
2	NAG	L	2	2	14,14,15	0.29	0	17,19,21	0.45	0
2	NAG	M	1	1,2	14,14,15	0.43	0	17,19,21	0.59	0
2	NAG	M	2	2	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	N	1	1,2	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
2	NAG	N	2	2	14,14,15	0.26	0	17,19,21	0.48	0
2	NAG	O	1	1,2	14,14,15	0.23	0	17,19,21	0.54	0
2	NAG	O	2	2	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	P	1	1,2	14,14,15	0.22	0	17,19,21	0.47	0
2	NAG	P	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	Q	1	1,2	14,14,15	0.28	0	17,19,21	0.53	0
2	NAG	Q	2	2	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	R	1	1,2	14,14,15	0.40	0	17,19,21	0.62	0
2	NAG	R	2	2	14,14,15	0.29	0	17,19,21	0.36	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	2.32	115.33	112.19
2	I	1	NAG	C1-O5-C5	2.29	115.30	112.19
2	N	1	NAG	C1-O5-C5	2.26	115.26	112.19
2	G	1	NAG	C1-O5-C5	2.23	115.22	112.19
2	H	1	NAG	C1-O5-C5	2.05	114.98	112.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C8-C7-N2-C2

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

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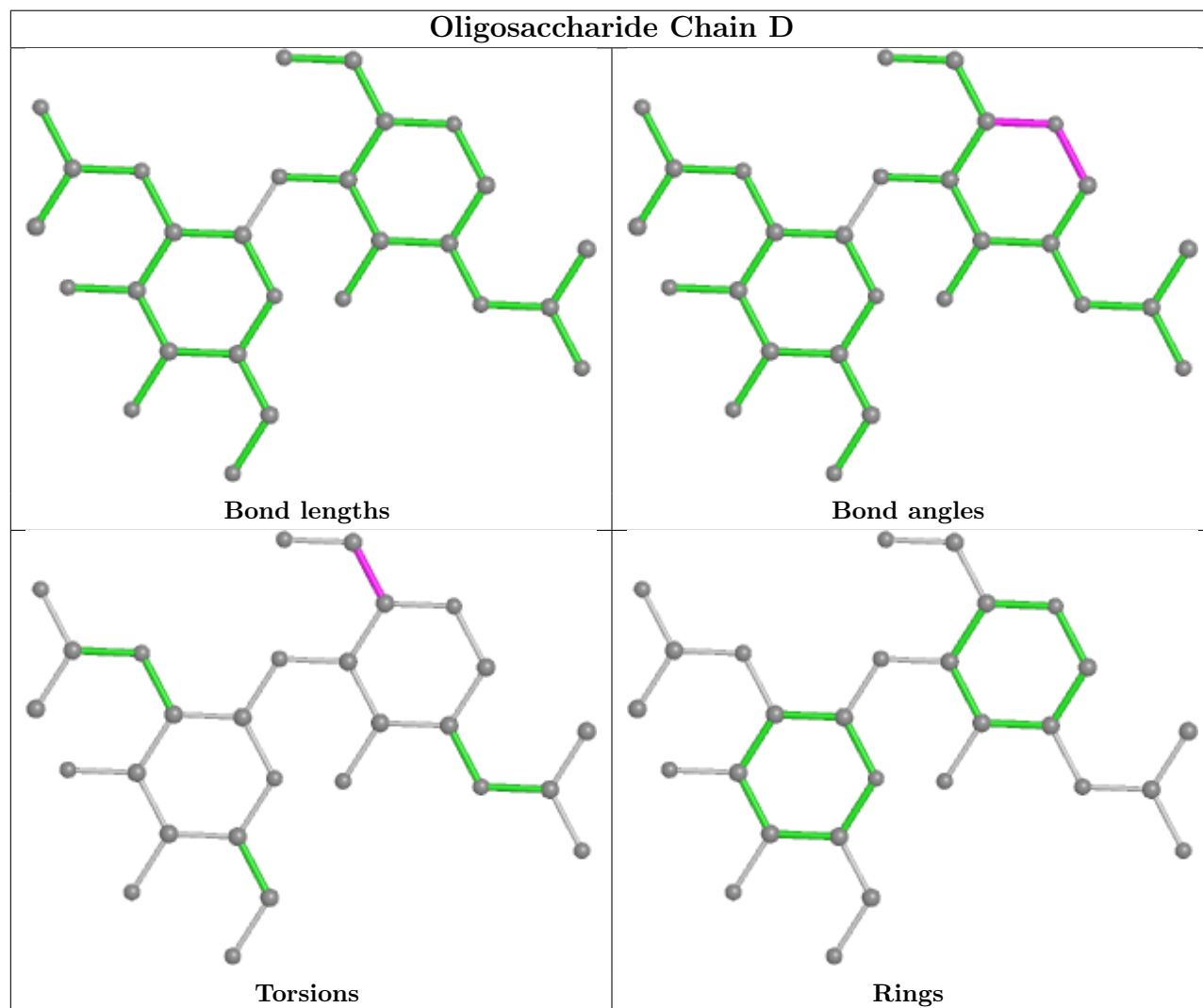
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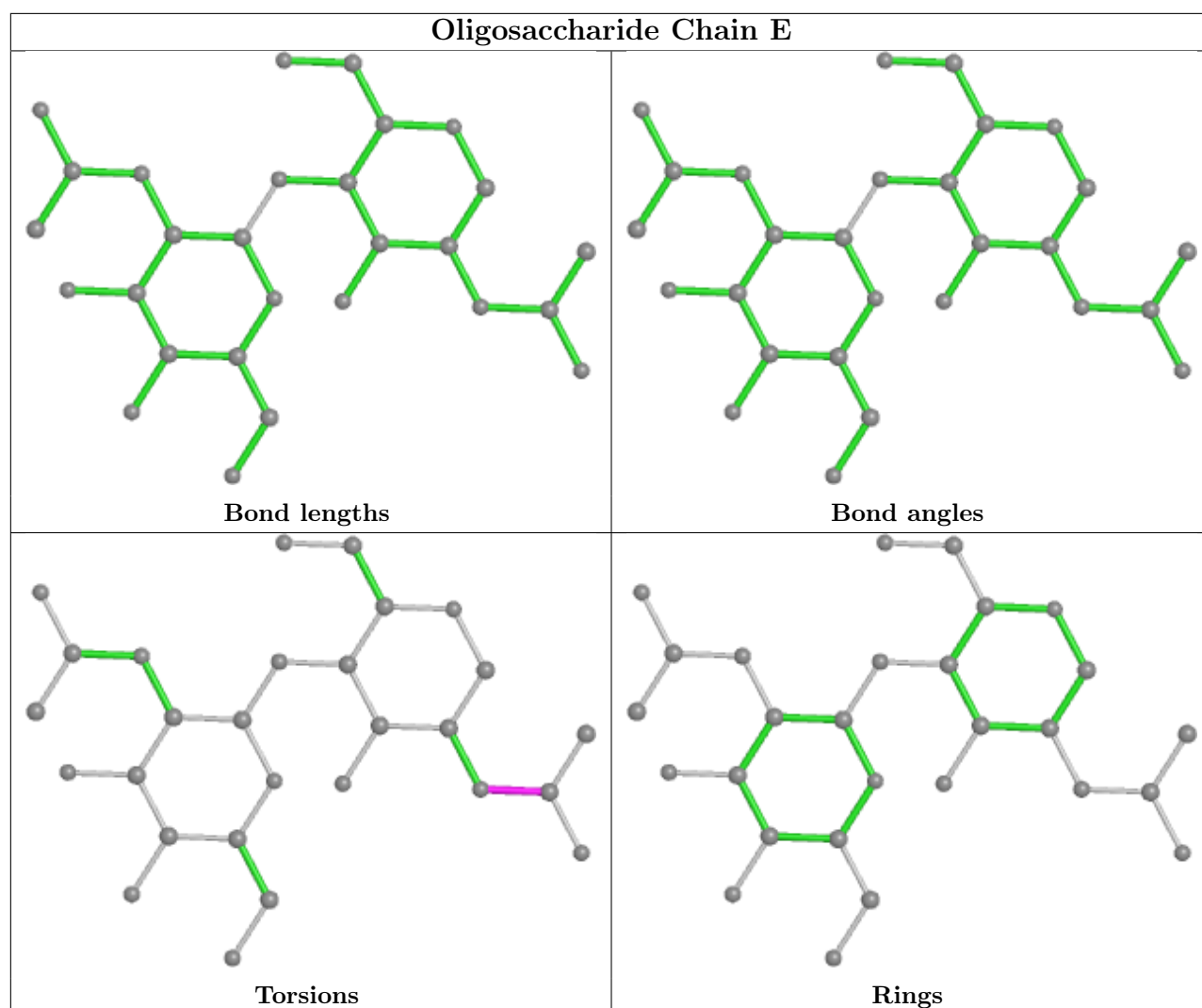
Mol	Chain	Res	Type	Atoms
2	J	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6

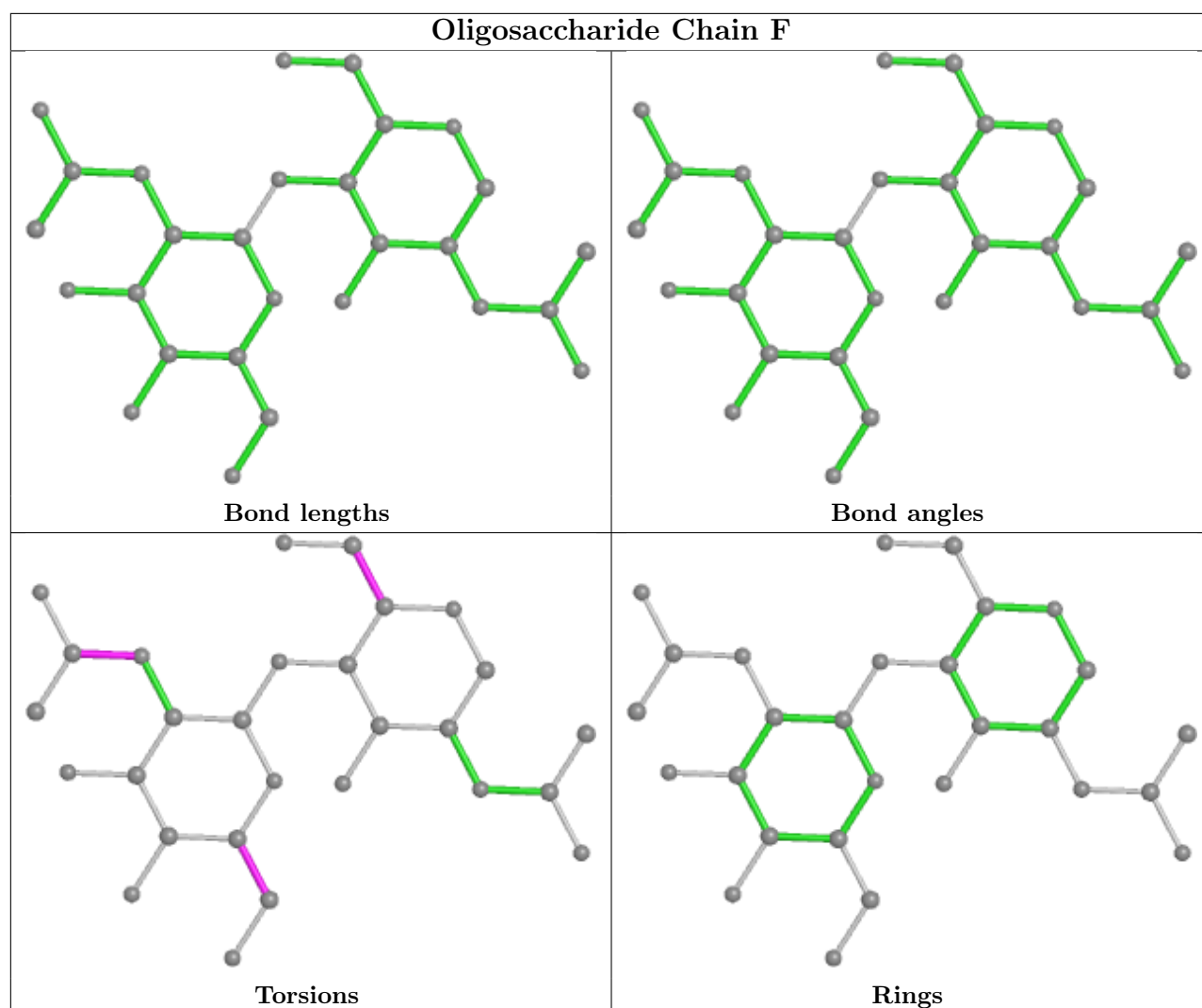
There are no ring outliers.

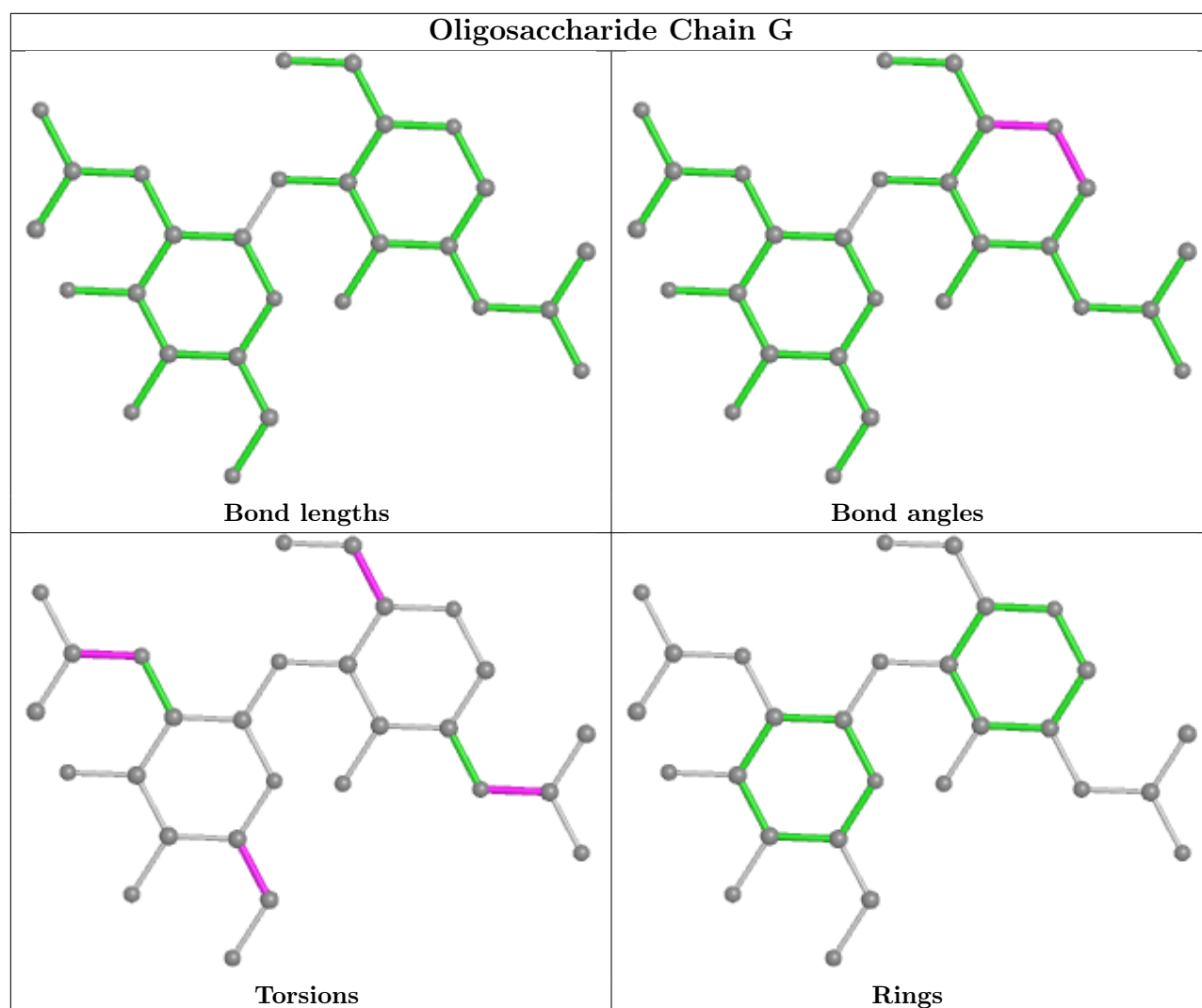
No monomer is involved in short contacts.

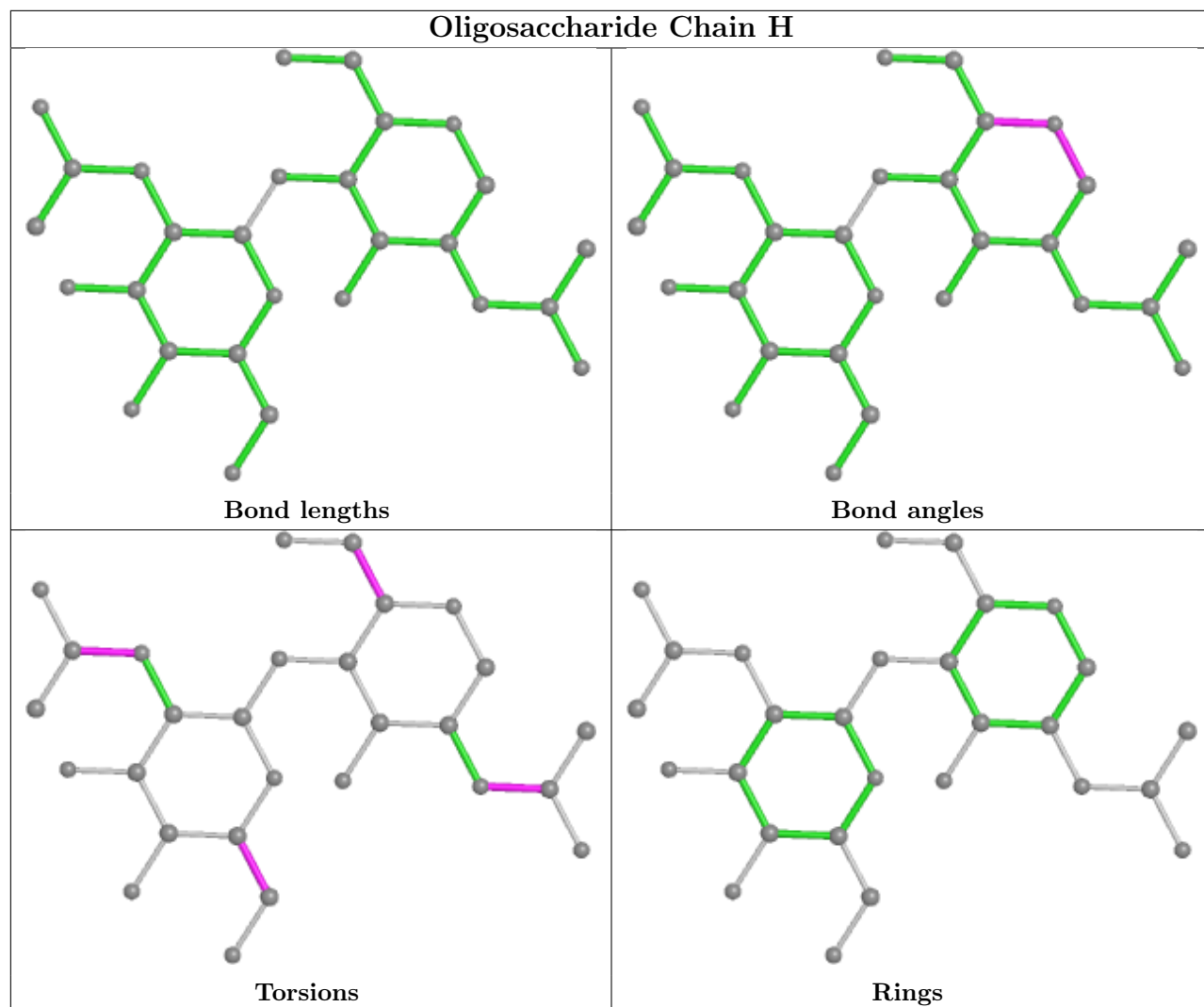
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

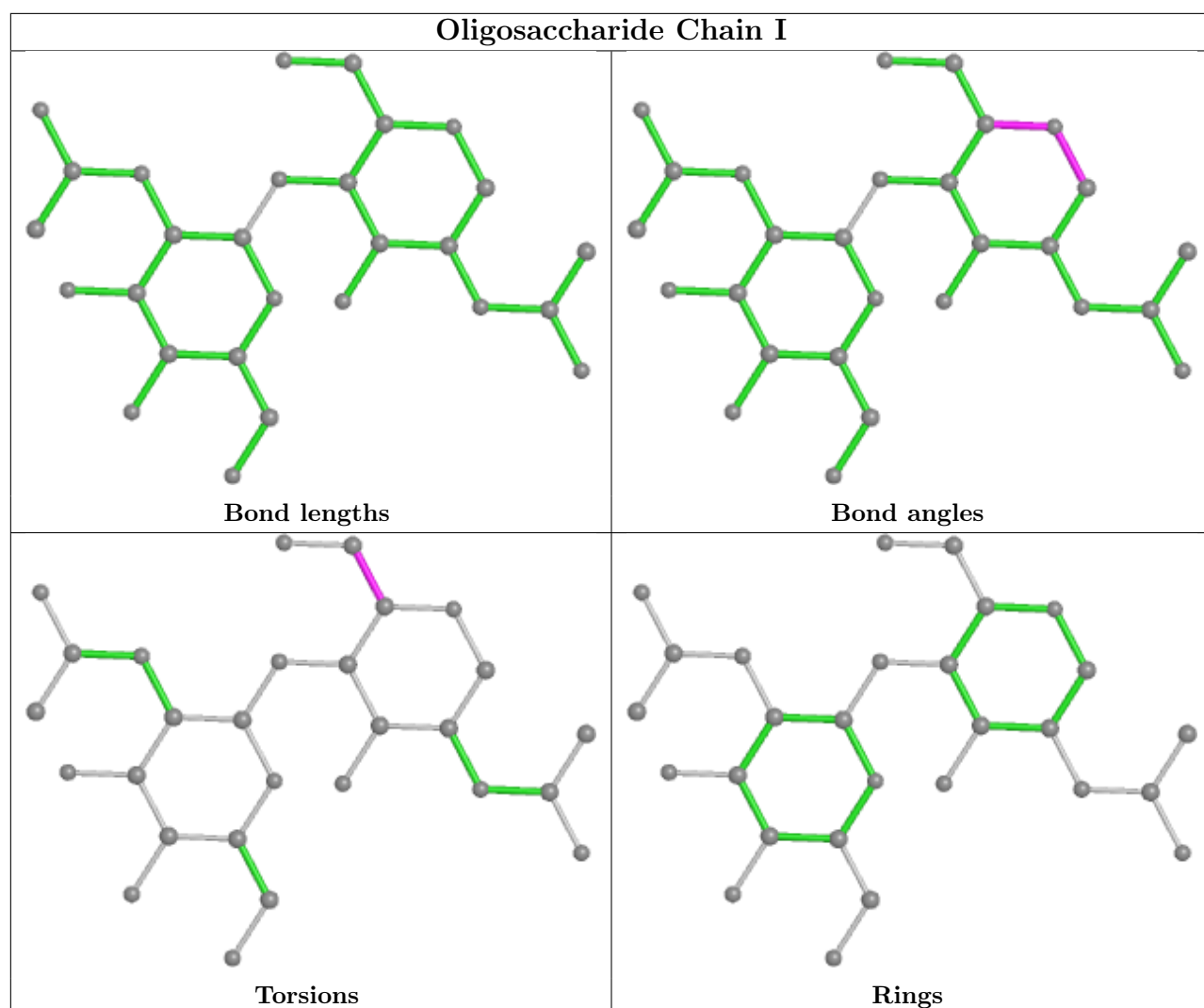


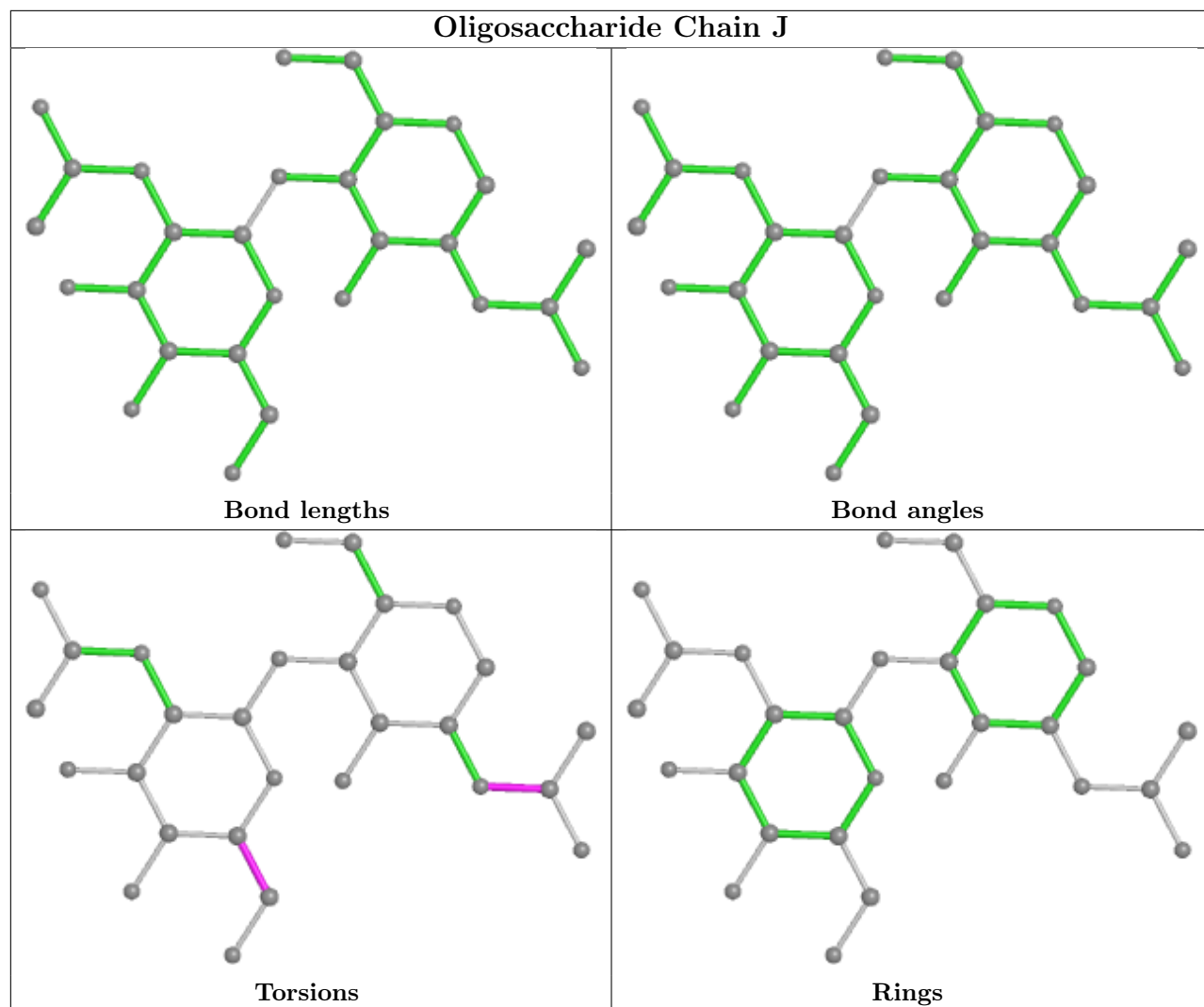


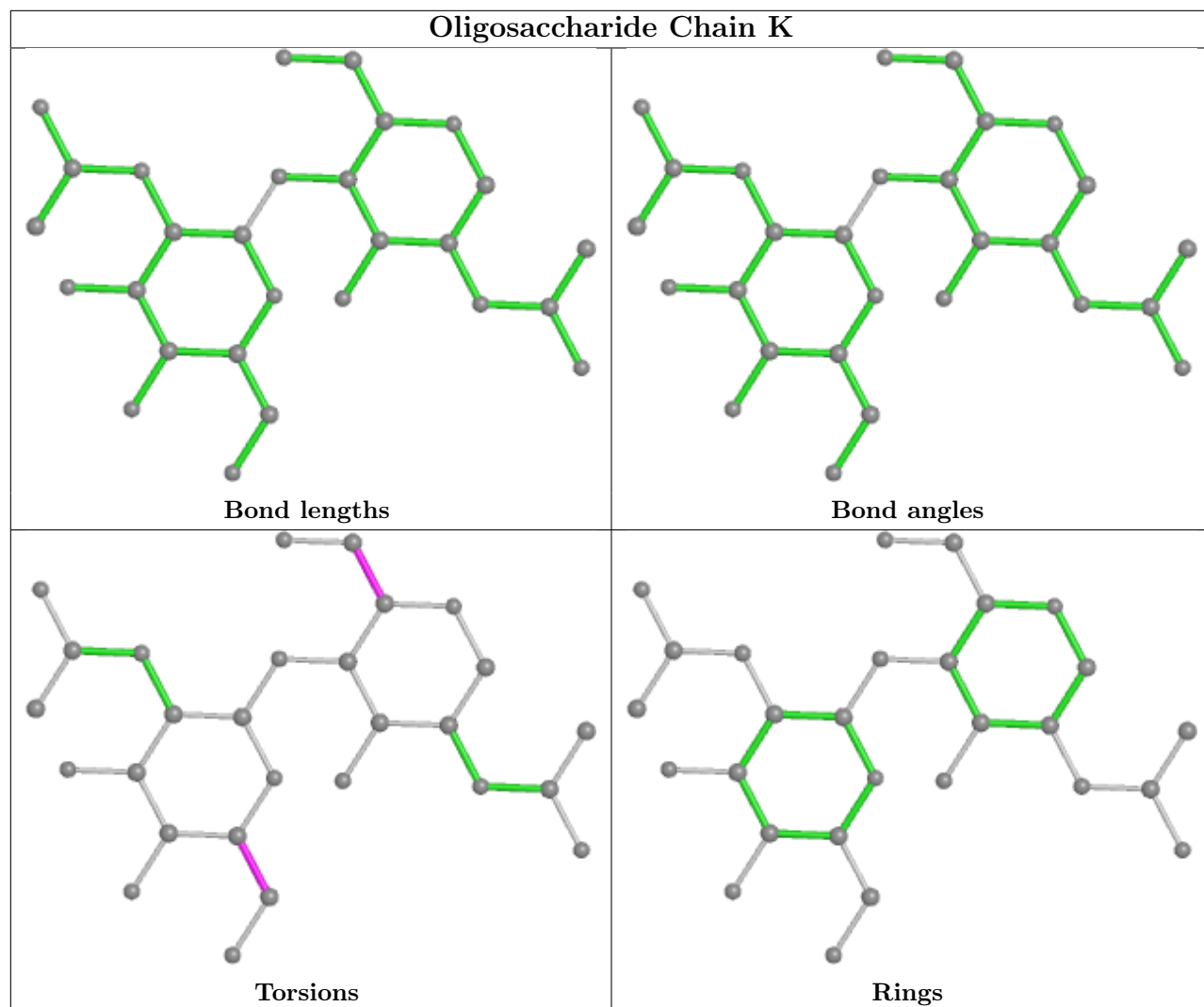




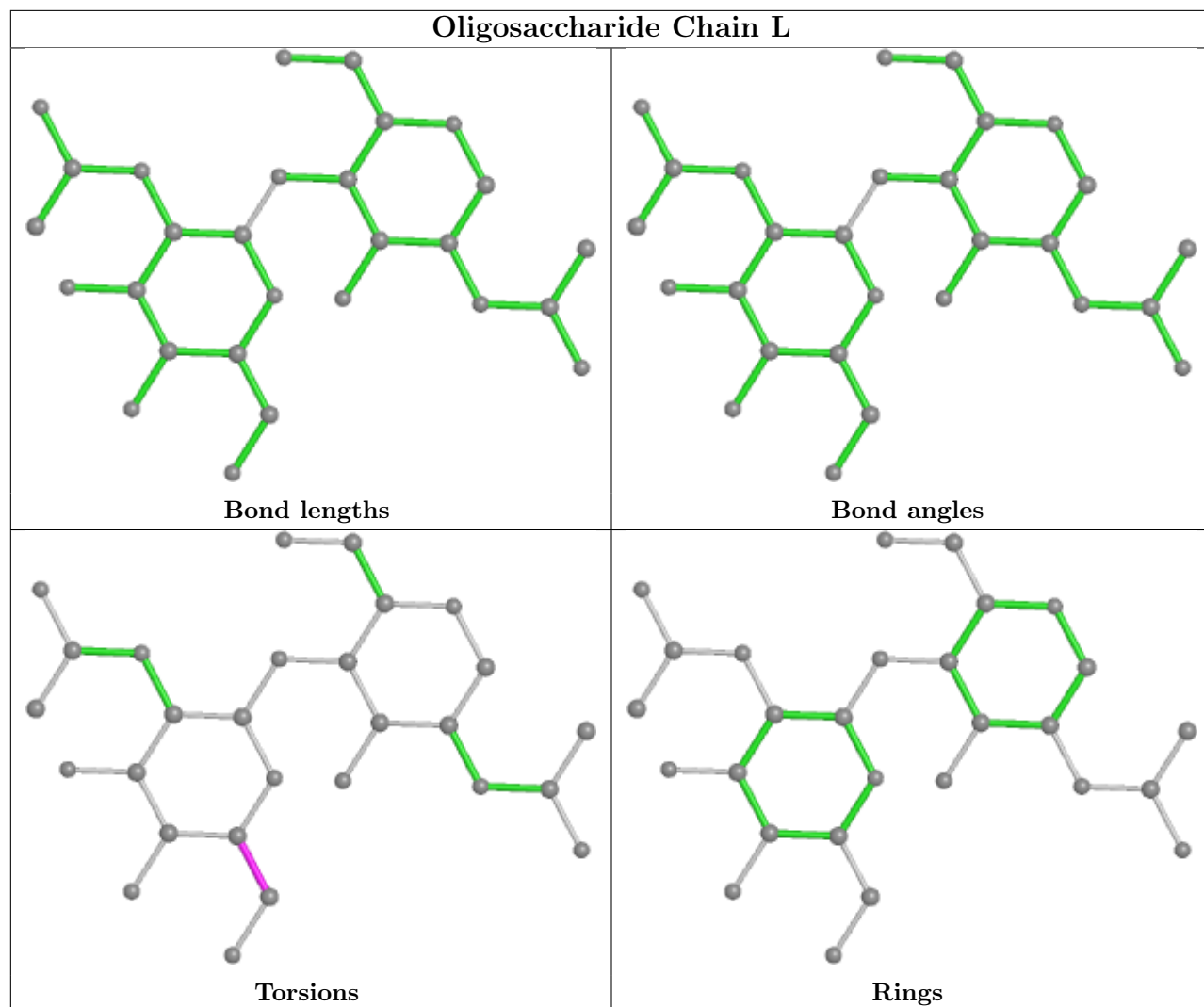


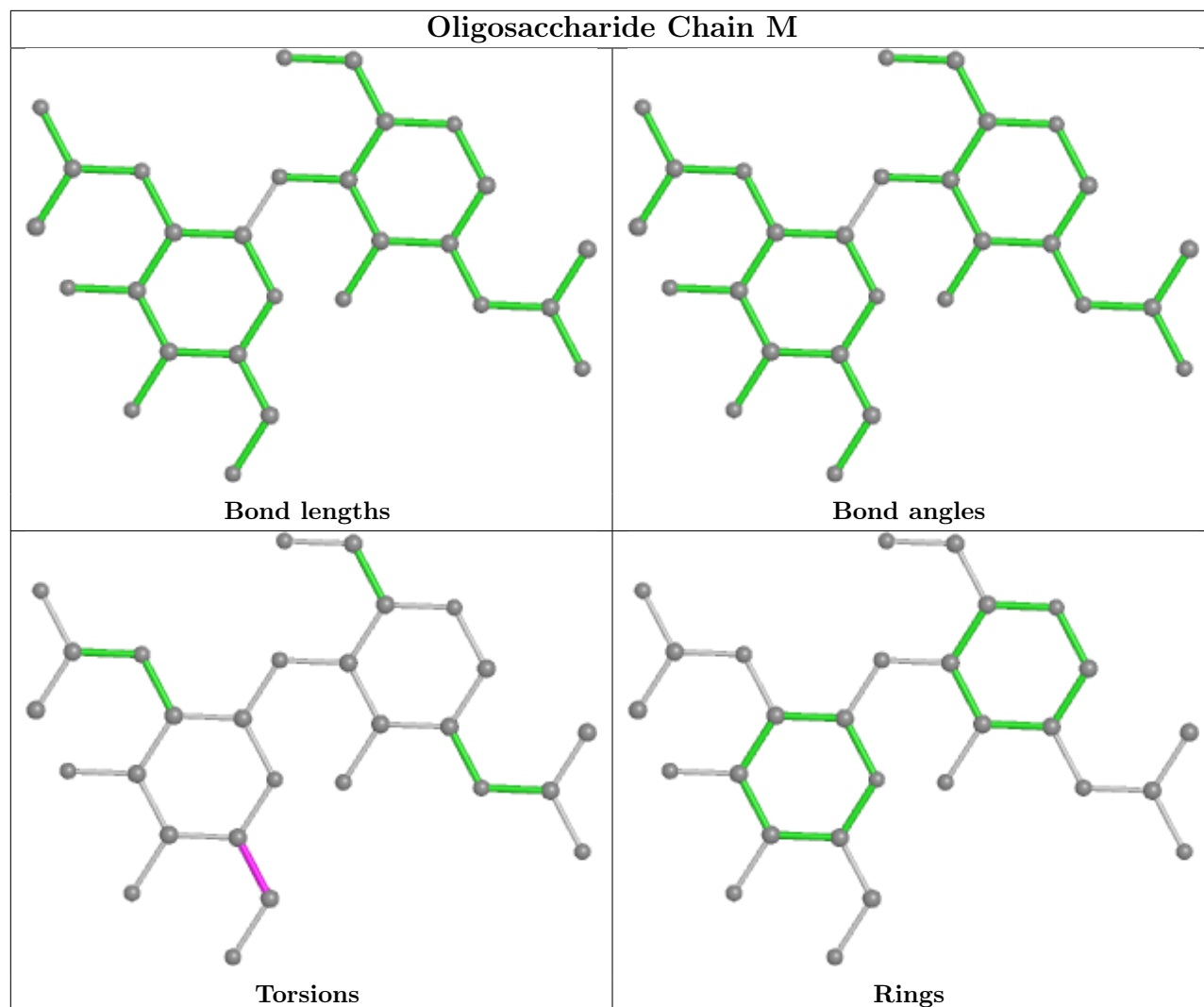


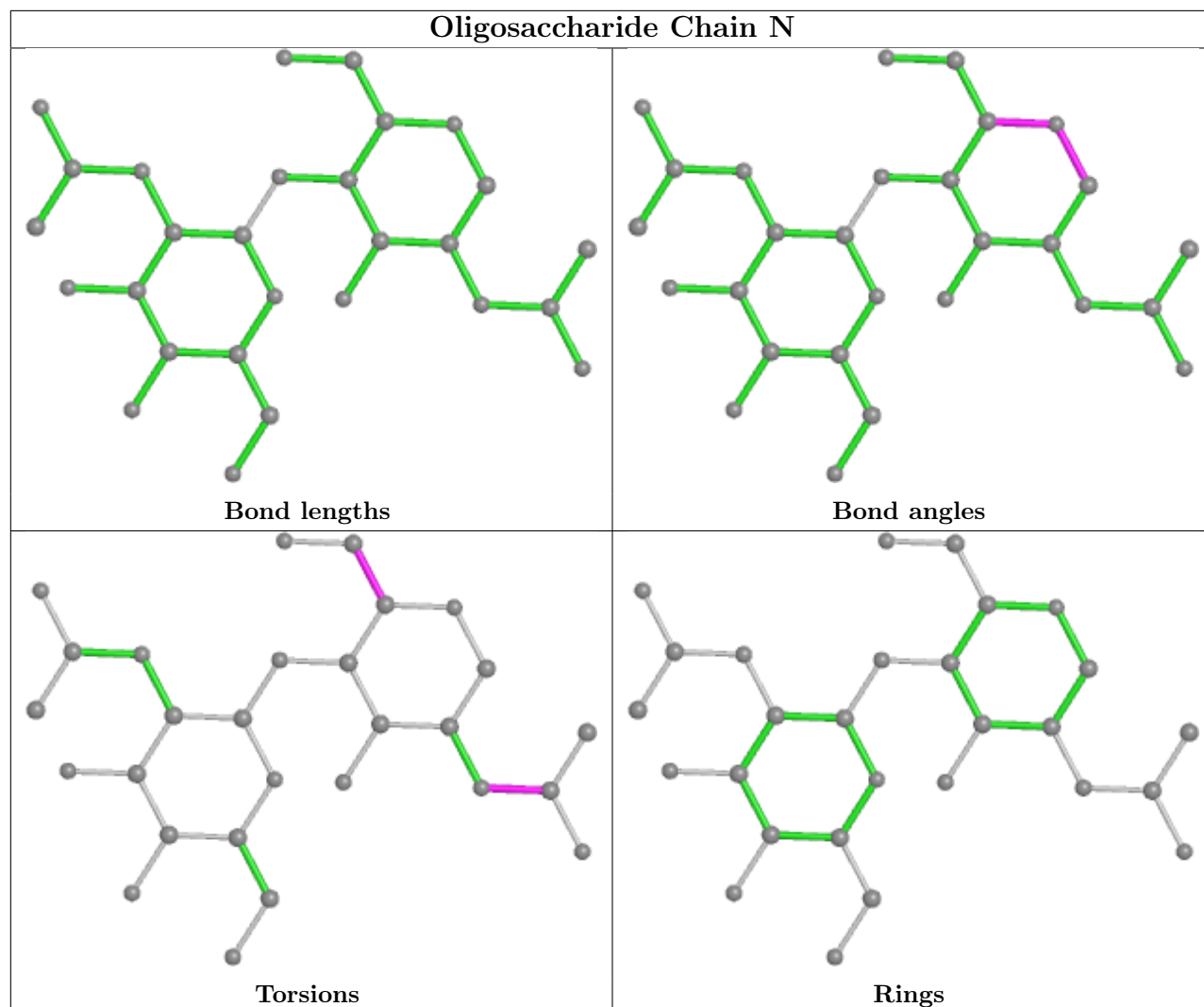


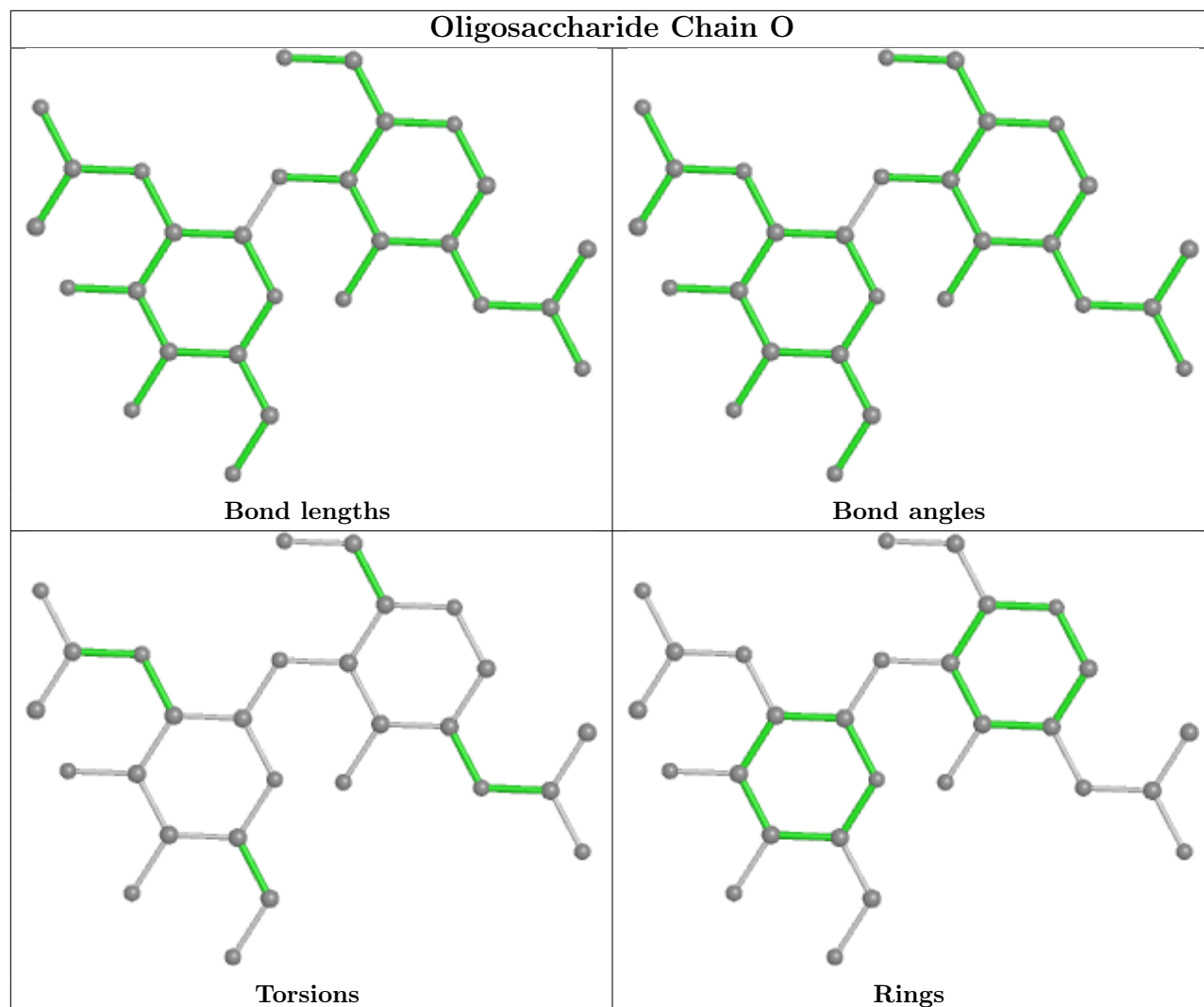


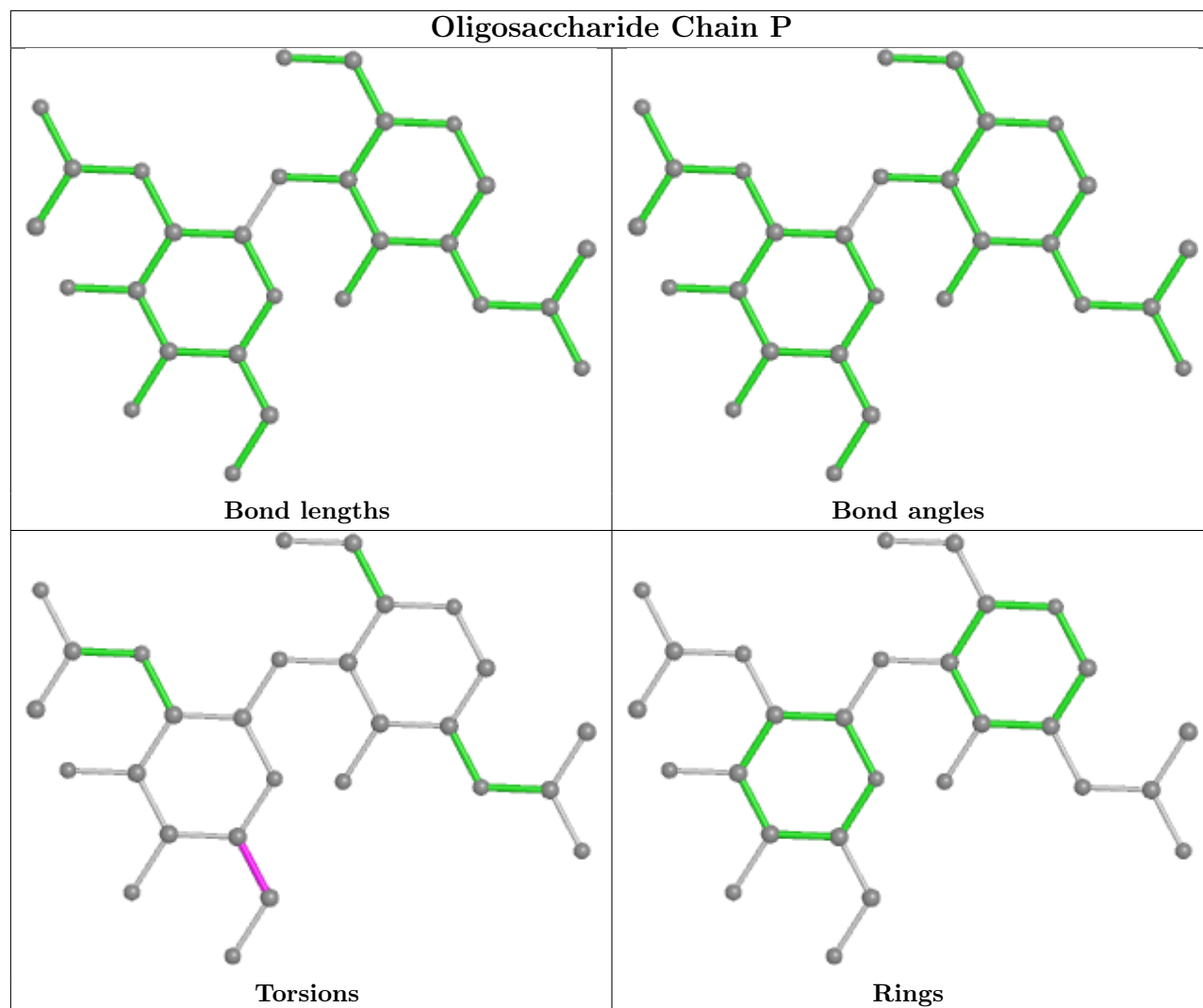


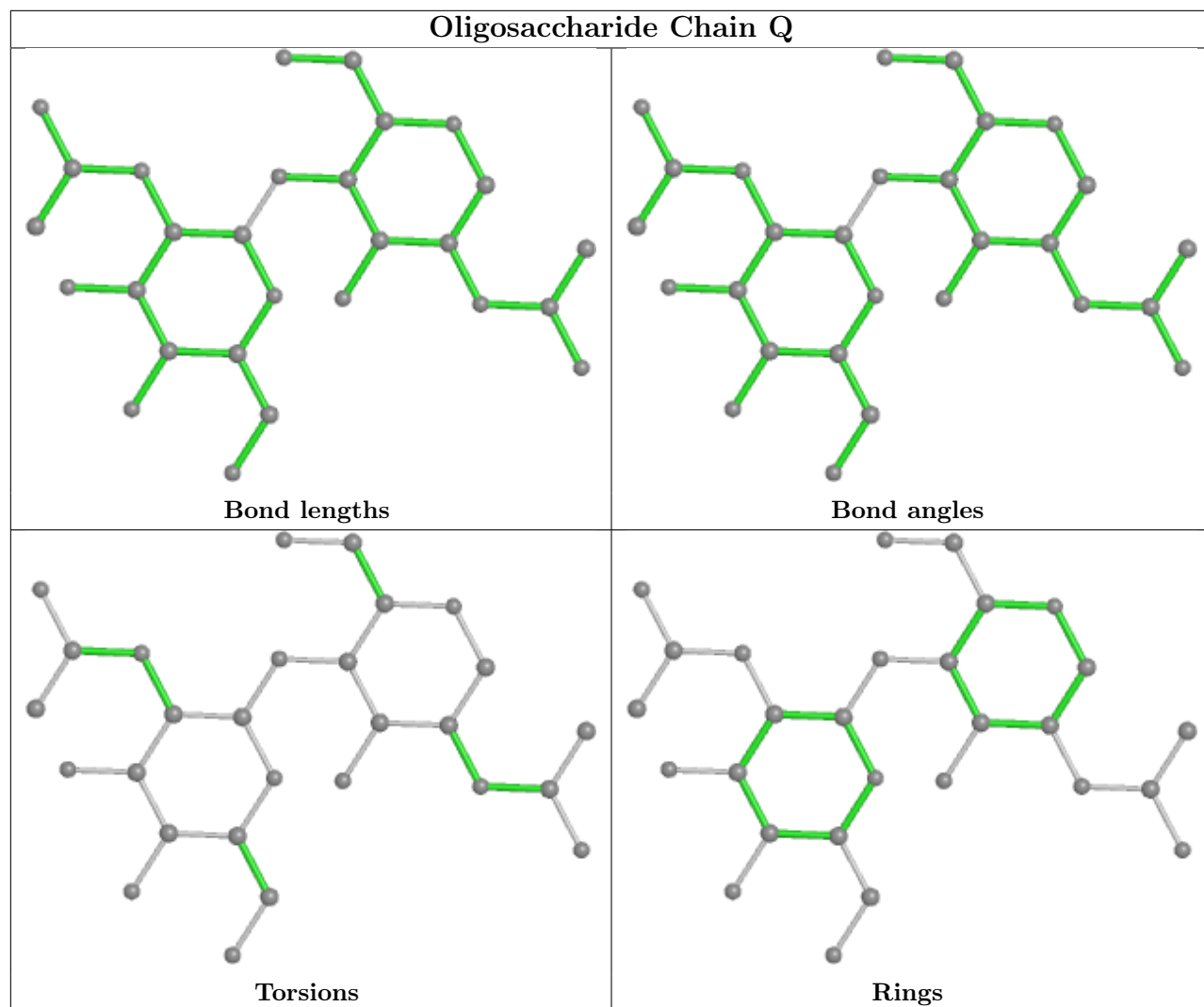


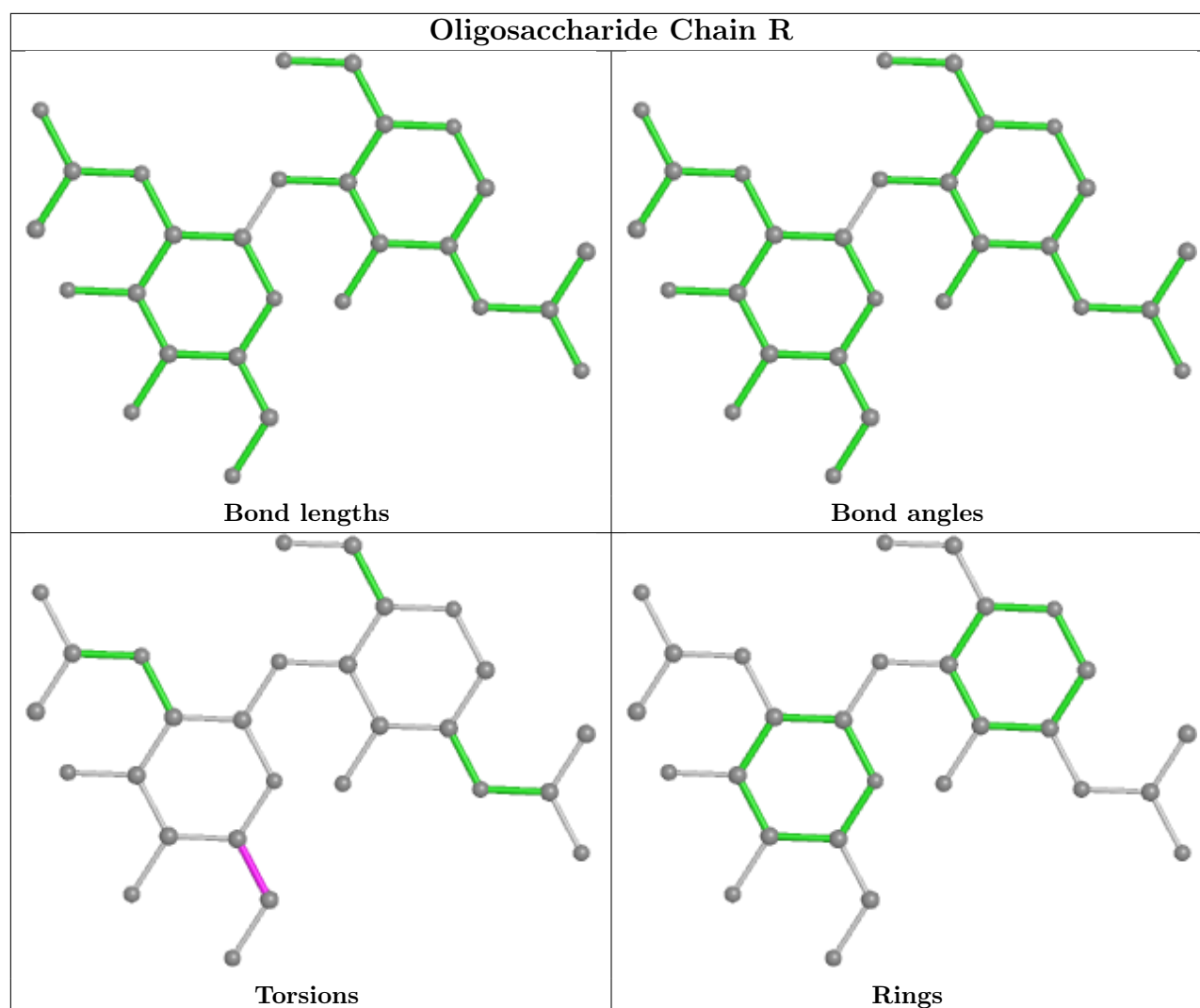












## 5.6 Ligand geometry [i](#)

36 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	$\# Z  > 2$
3	NAG	A	1402	1	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	A	1401	1	14,14,15	0.29	0	17,19,21	0.41	0
3	NAG	B	1402	1	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	A	1405	1	14,14,15	0.31	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1408	1	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	C	1404	1	14,14,15	0.41	0	17,19,21	0.45	0
3	NAG	C	1401	1	14,14,15	0.25	0	17,19,21	0.39	0
3	NAG	C	1409	1	14,14,15	0.27	0	17,19,21	0.47	0
3	NAG	C	1410	-	14,14,15	0.24	0	17,19,21	0.42	0
4	EIC	C	1412	-	19,19,19	0.44	0	19,19,19	0.95	0
3	NAG	B	1406	1	14,14,15	0.25	0	17,19,21	0.48	0
4	EIC	A	1412	-	19,19,19	0.47	0	19,19,19	0.88	1 (5%)
3	NAG	B	1403	1	14,14,15	0.22	0	17,19,21	0.52	0
3	NAG	C	1403	1	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	B	1404	-	14,14,15	0.19	0	17,19,21	0.48	0
3	NAG	B	1401	1	14,14,15	0.38	0	17,19,21	0.34	0
3	NAG	A	1404	1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	B	1410	-	14,14,15	0.23	0	17,19,21	0.45	0
4	EIC	B	1412	-	19,19,19	0.45	0	19,19,19	0.83	0
3	NAG	A	1411	1	14,14,15	0.34	0	17,19,21	0.51	0
3	NAG	A	1403	1	14,14,15	0.26	0	17,19,21	0.53	0
3	NAG	C	1408	1	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	A	1409	1	14,14,15	0.33	0	17,19,21	0.47	0
3	NAG	B	1411	1	14,14,15	0.31	0	17,19,21	0.50	0
3	NAG	C	1407	1	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	A	1410	1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	A	1407	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	B	1408	1	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	C	1405	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	C	1406	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	B	1407	1	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	C	1411	1	14,14,15	0.34	0	17,19,21	0.49	0
3	NAG	C	1402	1	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	A	1406	1	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	B	1405	1	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	B	1409	-	14,14,15	0.20	0	17,19,21	0.49	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
3	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1402	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1410	-	-	1/6/23/26	0/1/1/1
4	EIC	C	1412	-	-	7/17/17/17	-
3	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
4	EIC	A	1412	-	-	3/17/17/17	-
3	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1404	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1401	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
4	EIC	B	1412	-	-	7/17/17/17	-
3	NAG	A	1411	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1411	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1410	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1407	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1407	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1411	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1402	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1409	-	-	2/6/23/26	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(°)
4	A	1412	EIC	C3-C2-C1	-2.61	107.89	114.47

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1412	EIC	C10-C11-C12-C13
3	A	1409	NAG	O5-C5-C6-O6
3	A	1402	NAG	C4-C5-C6-O6
3	A	1403	NAG	O5-C5-C6-O6
3	A	1406	NAG	O5-C5-C6-O6
3	C	1409	NAG	O5-C5-C6-O6
3	A	1402	NAG	O5-C5-C6-O6
3	B	1402	NAG	C4-C5-C6-O6
3	B	1408	NAG	C4-C5-C6-O6
3	C	1402	NAG	C4-C5-C6-O6
3	C	1408	NAG	C4-C5-C6-O6
3	A	1410	NAG	O5-C5-C6-O6
3	B	1403	NAG	O5-C5-C6-O6
3	C	1403	NAG	O5-C5-C6-O6
3	C	1409	NAG	C4-C5-C6-O6
3	A	1403	NAG	C4-C5-C6-O6
3	C	1403	NAG	C4-C5-C6-O6
3	C	1401	NAG	O5-C5-C6-O6
3	A	1406	NAG	C4-C5-C6-O6
3	B	1403	NAG	C4-C5-C6-O6
3	B	1406	NAG	C4-C5-C6-O6
3	C	1408	NAG	O5-C5-C6-O6
3	A	1405	NAG	C4-C5-C6-O6
3	A	1404	NAG	O5-C5-C6-O6
3	B	1402	NAG	O5-C5-C6-O6
3	B	1408	NAG	O5-C5-C6-O6
3	B	1404	NAG	O5-C5-C6-O6
3	A	1409	NAG	C4-C5-C6-O6
3	A	1404	NAG	C4-C5-C6-O6
3	A	1410	NAG	C4-C5-C6-O6
3	A	1407	NAG	C8-C7-N2-C2
3	A	1407	NAG	O7-C7-N2-C2
3	A	1410	NAG	C8-C7-N2-C2
3	A	1410	NAG	O7-C7-N2-C2
3	B	1407	NAG	C8-C7-N2-C2
3	B	1407	NAG	O7-C7-N2-C2
3	B	1409	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	B	1409	NAG	O7-C7-N2-C2
3	C	1402	NAG	C8-C7-N2-C2
3	C	1402	NAG	O7-C7-N2-C2
3	C	1411	NAG	C8-C7-N2-C2
3	C	1411	NAG	O7-C7-N2-C2
3	B	1404	NAG	C4-C5-C6-O6
3	A	1401	NAG	O5-C5-C6-O6
3	C	1411	NAG	C4-C5-C6-O6
3	A	1407	NAG	O5-C5-C6-O6
3	A	1408	NAG	O5-C5-C6-O6
3	C	1402	NAG	O5-C5-C6-O6
3	C	1406	NAG	O5-C5-C6-O6
3	B	1407	NAG	O5-C5-C6-O6
3	A	1408	NAG	C4-C5-C6-O6
3	B	1406	NAG	O5-C5-C6-O6
4	B	1412	EIC	C3-C4-C5-C6
4	C	1412	EIC	C4-C5-C6-C7
3	C	1411	NAG	O5-C5-C6-O6
3	A	1405	NAG	O5-C5-C6-O6
4	B	1412	EIC	C4-C5-C6-C7
3	C	1401	NAG	C4-C5-C6-O6
4	A	1412	EIC	C5-C6-C7-C8
4	A	1412	EIC	C3-C4-C5-C6
3	C	1407	NAG	O5-C5-C6-O6
4	B	1412	EIC	C13-C14-C15-C16
3	B	1411	NAG	C4-C5-C6-O6
3	A	1407	NAG	C4-C5-C6-O6
3	B	1401	NAG	O5-C5-C6-O6
3	C	1406	NAG	C4-C5-C6-O6
4	A	1412	EIC	C4-C5-C6-C7
3	C	1410	NAG	O5-C5-C6-O6
3	A	1401	NAG	C4-C5-C6-O6
4	B	1412	EIC	C10-C11-C12-C13
4	C	1412	EIC	C6-C7-C8-C9
3	B	1411	NAG	O5-C5-C6-O6
4	B	1412	EIC	C9-C10-C11-C12
4	C	1412	EIC	C9-C10-C11-C12
4	B	1412	EIC	O2-C1-C2-C3
4	C	1412	EIC	O2-C1-C2-C3
3	C	1404	NAG	C4-C5-C6-O6
4	B	1412	EIC	O1-C1-C2-C3
3	A	1411	NAG	C4-C5-C6-O6

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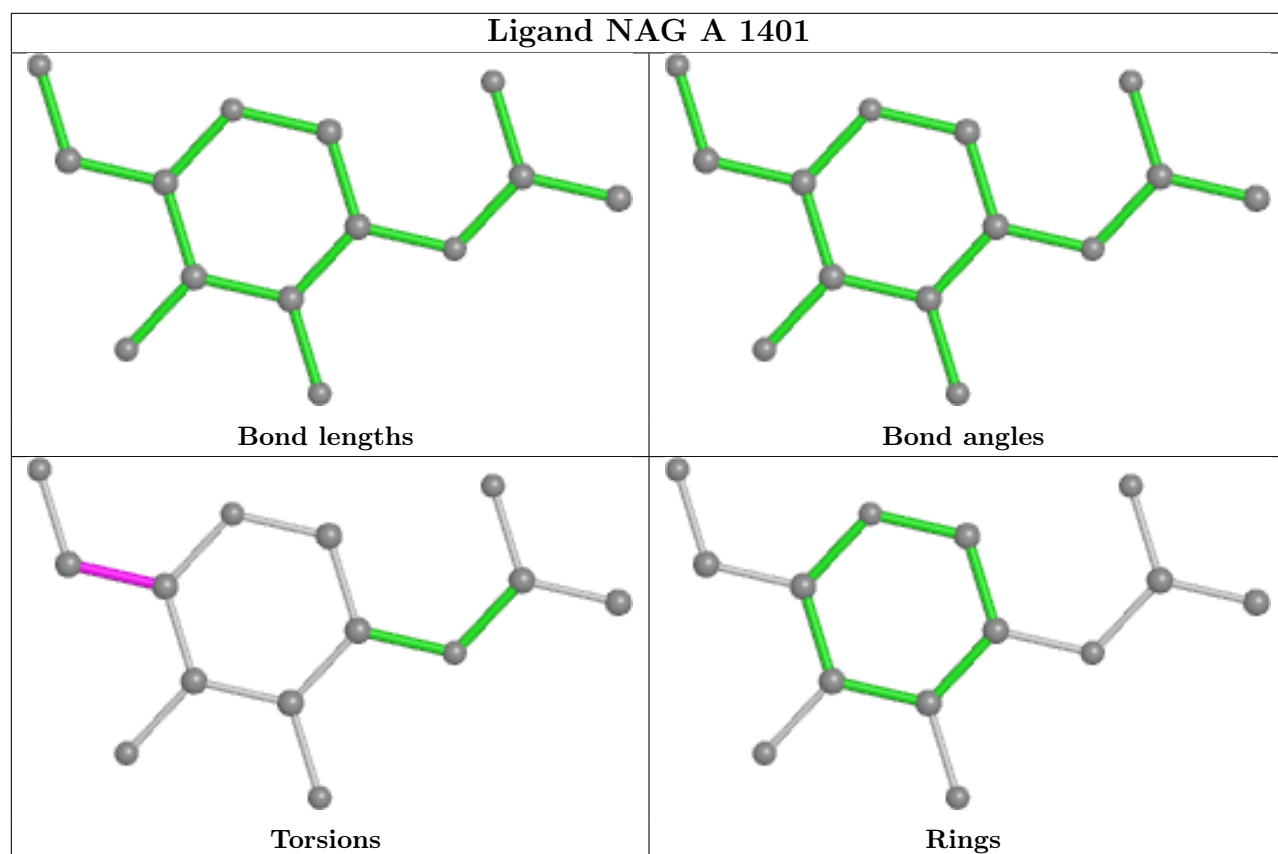
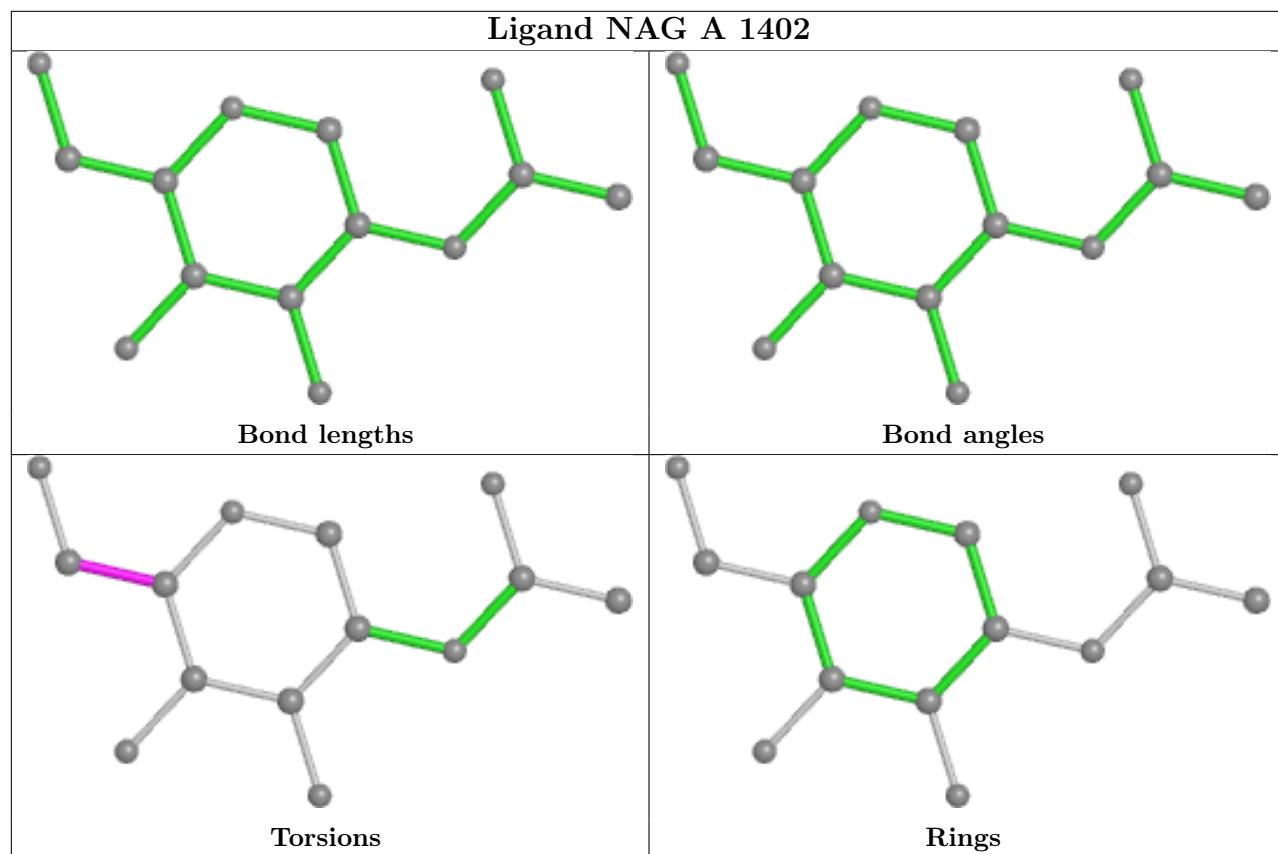
Mol	Chain	Res	Type	Atoms
4	C	1412	EIC	O1-C1-C2-C3
4	C	1412	EIC	C7-C8-C9-C10

There are no ring outliers.

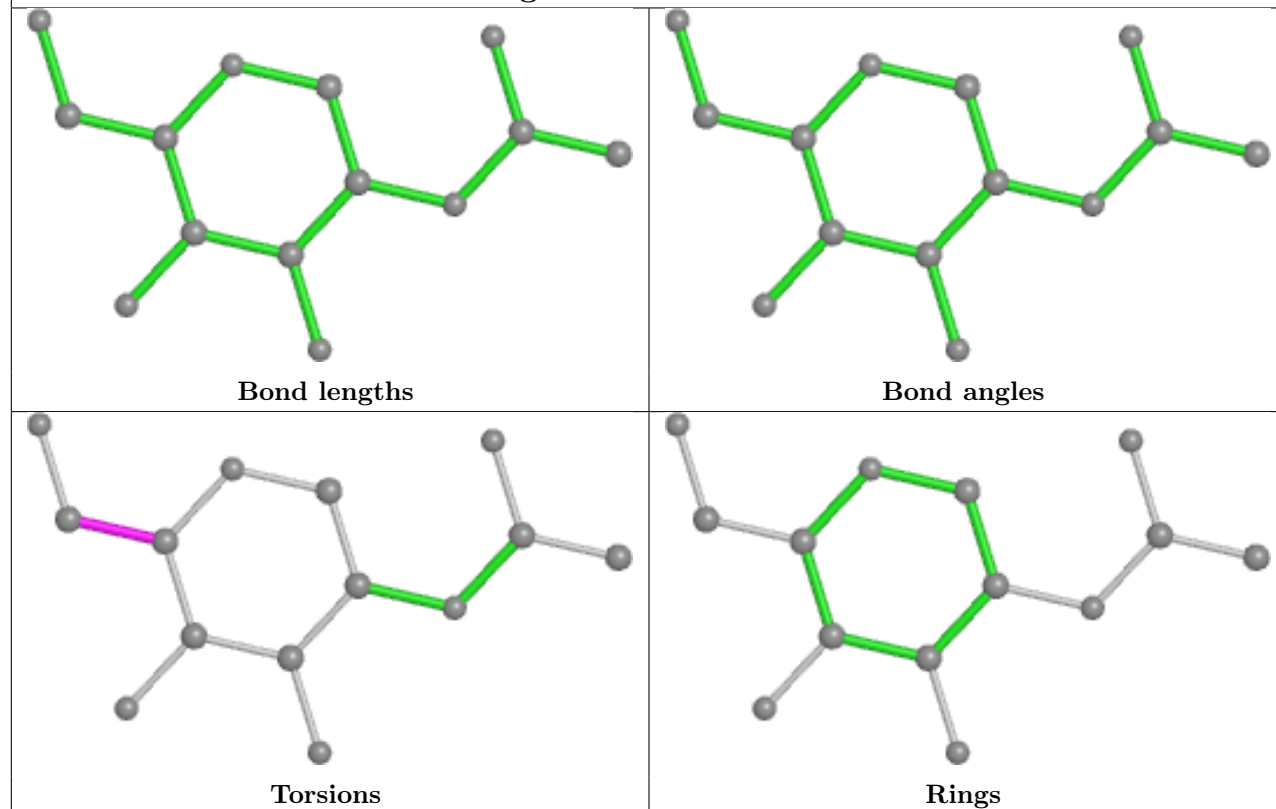
8 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1402	NAG	1	0
3	B	1402	NAG	1	0
3	C	1404	NAG	1	0
4	C	1412	EIC	33	0
4	A	1412	EIC	33	0
3	C	1403	NAG	1	0
3	B	1404	NAG	1	0
4	B	1412	EIC	22	0

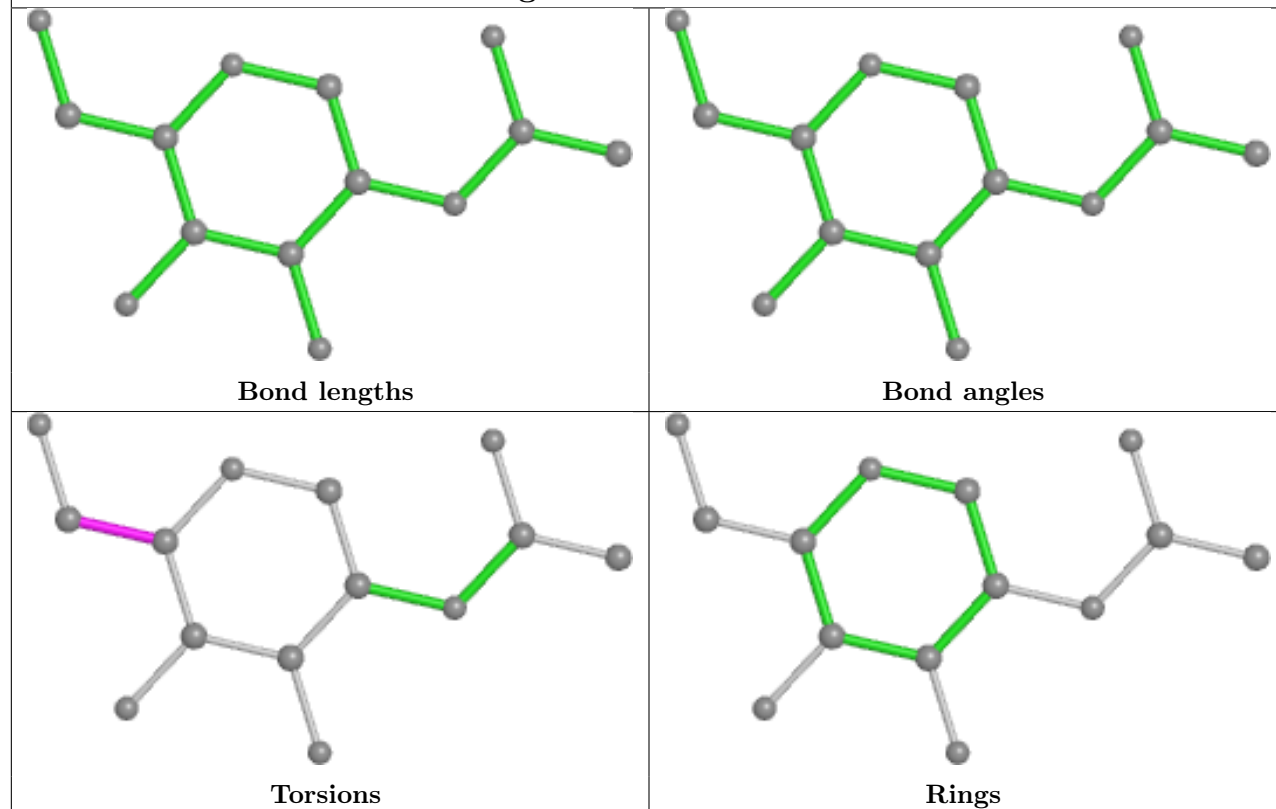
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



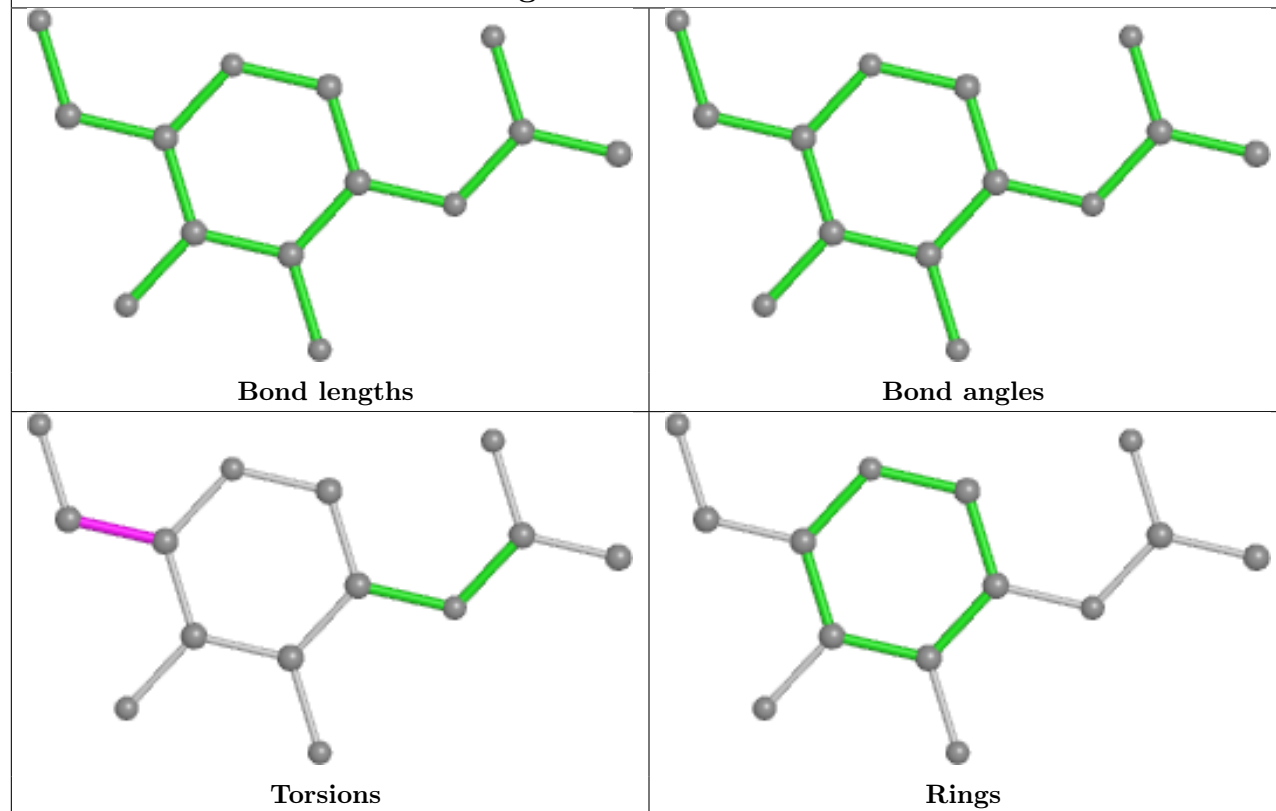
## Ligand NAG B 1402



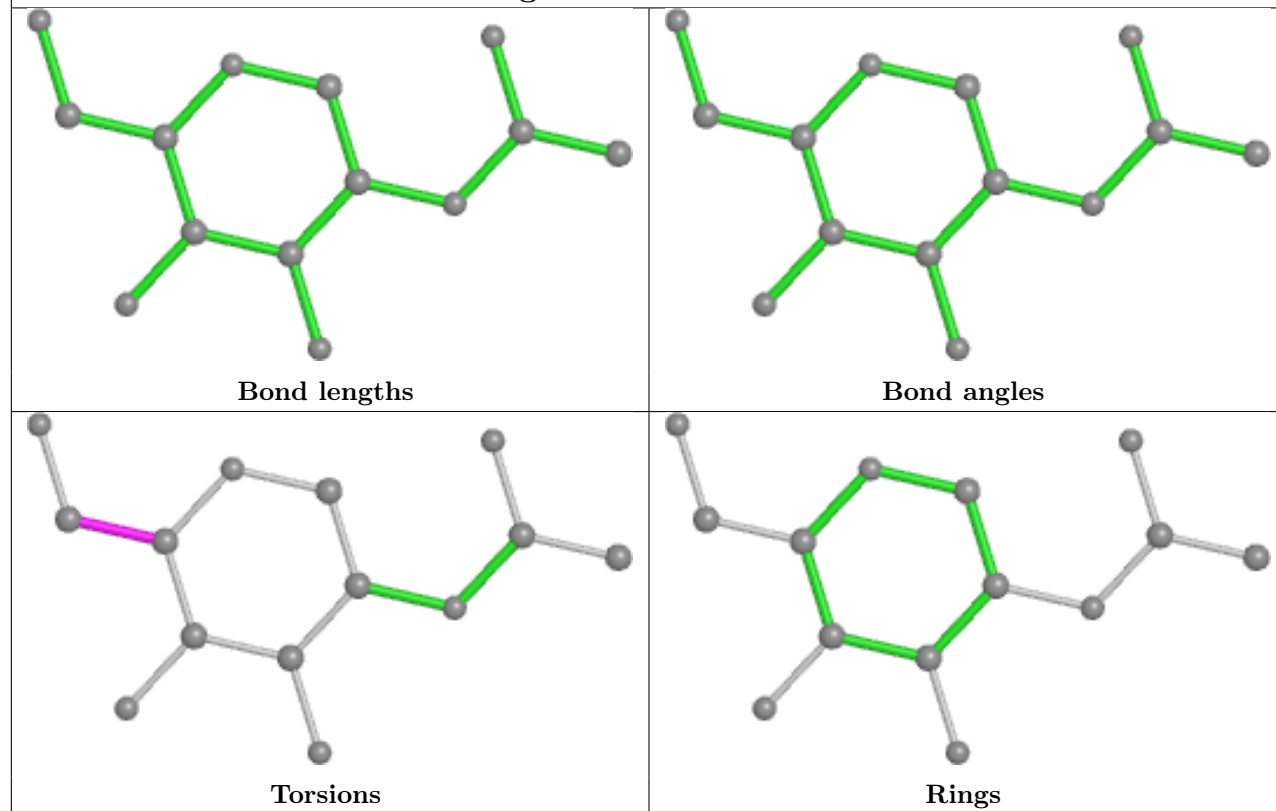
## Ligand NAG A 1405



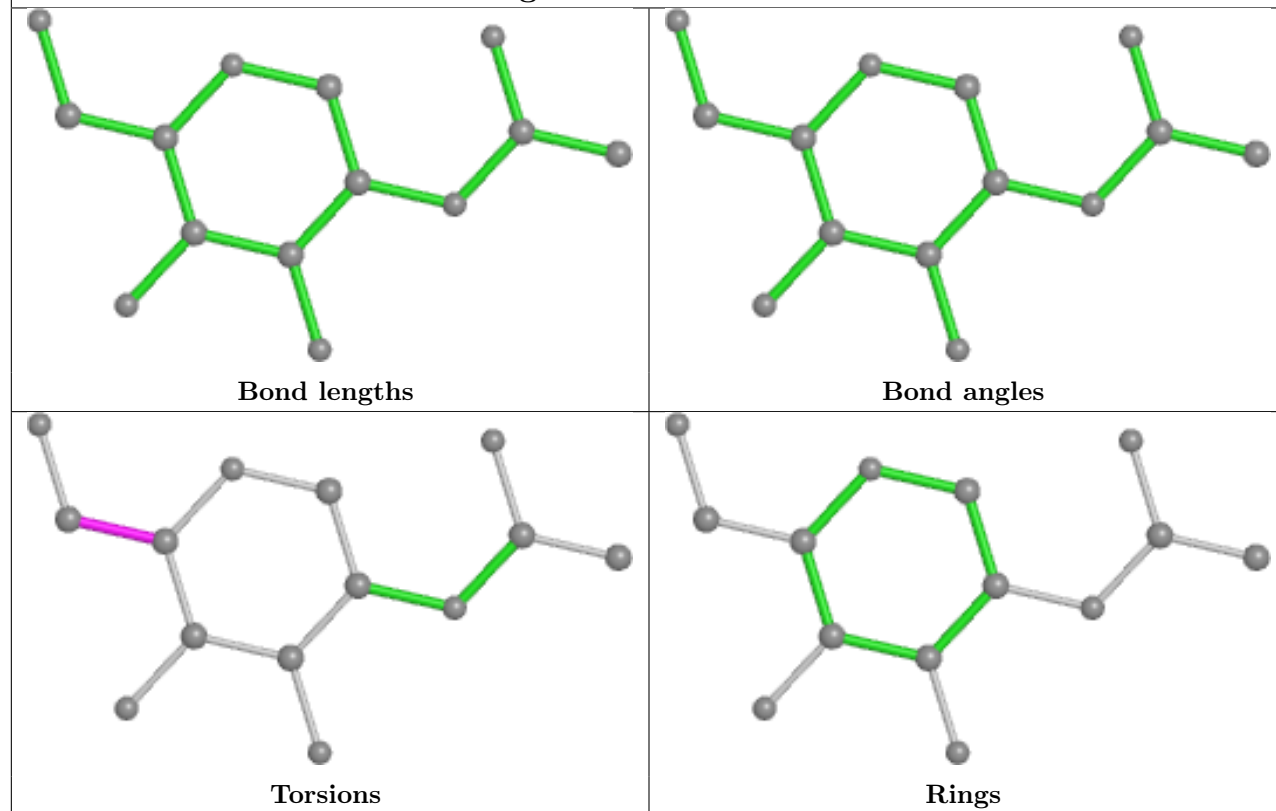
## Ligand NAG A 1408



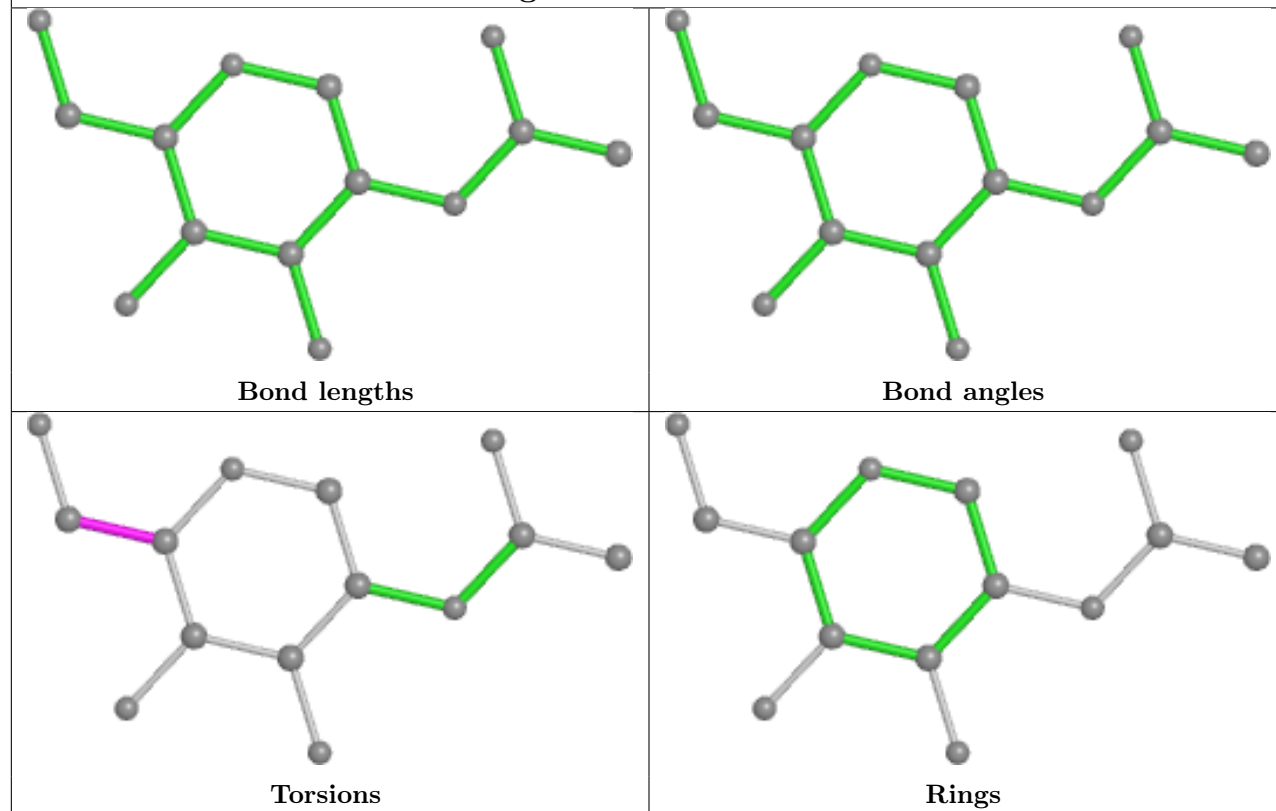
## Ligand NAG C 1404



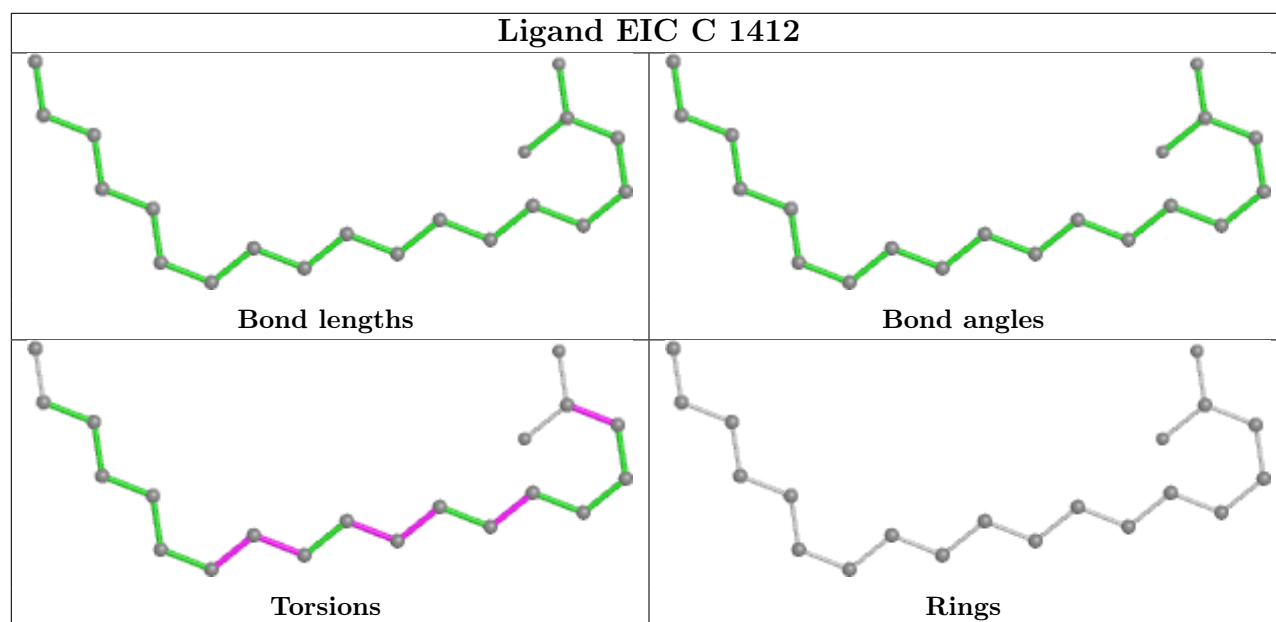
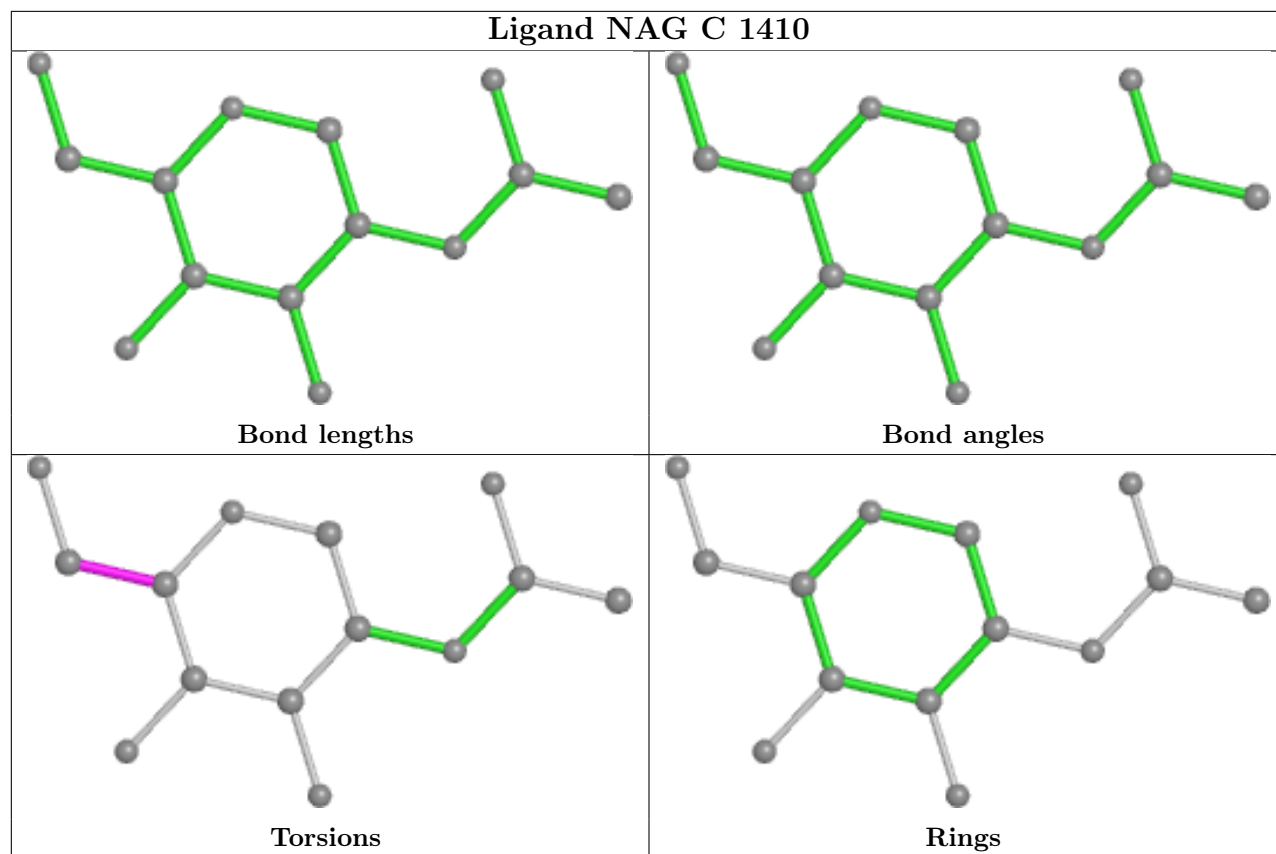
## Ligand NAG C 1401

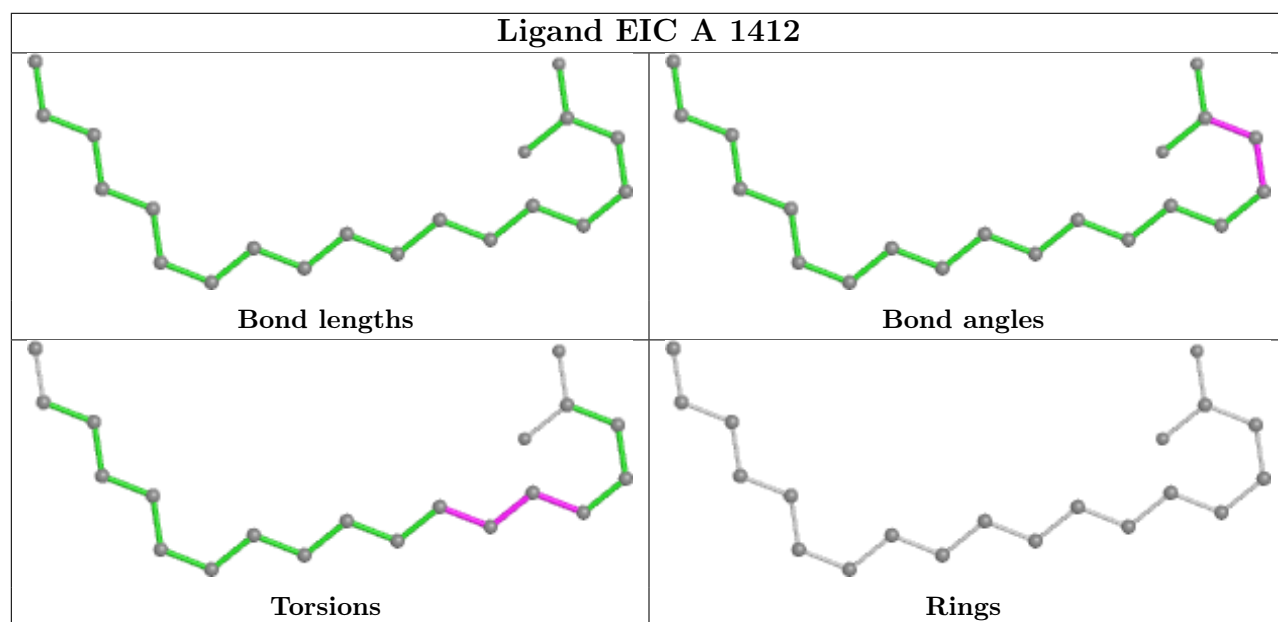
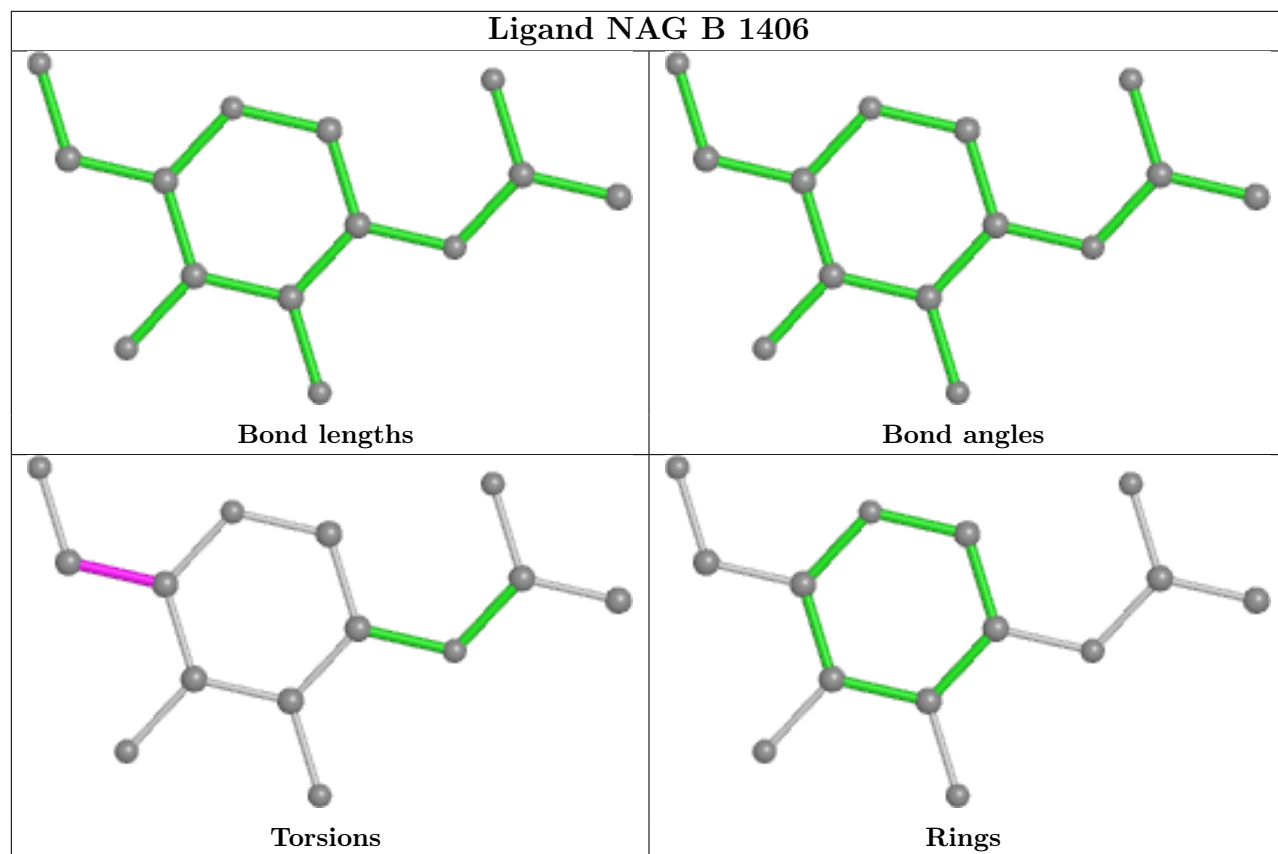


## Ligand NAG C 1409

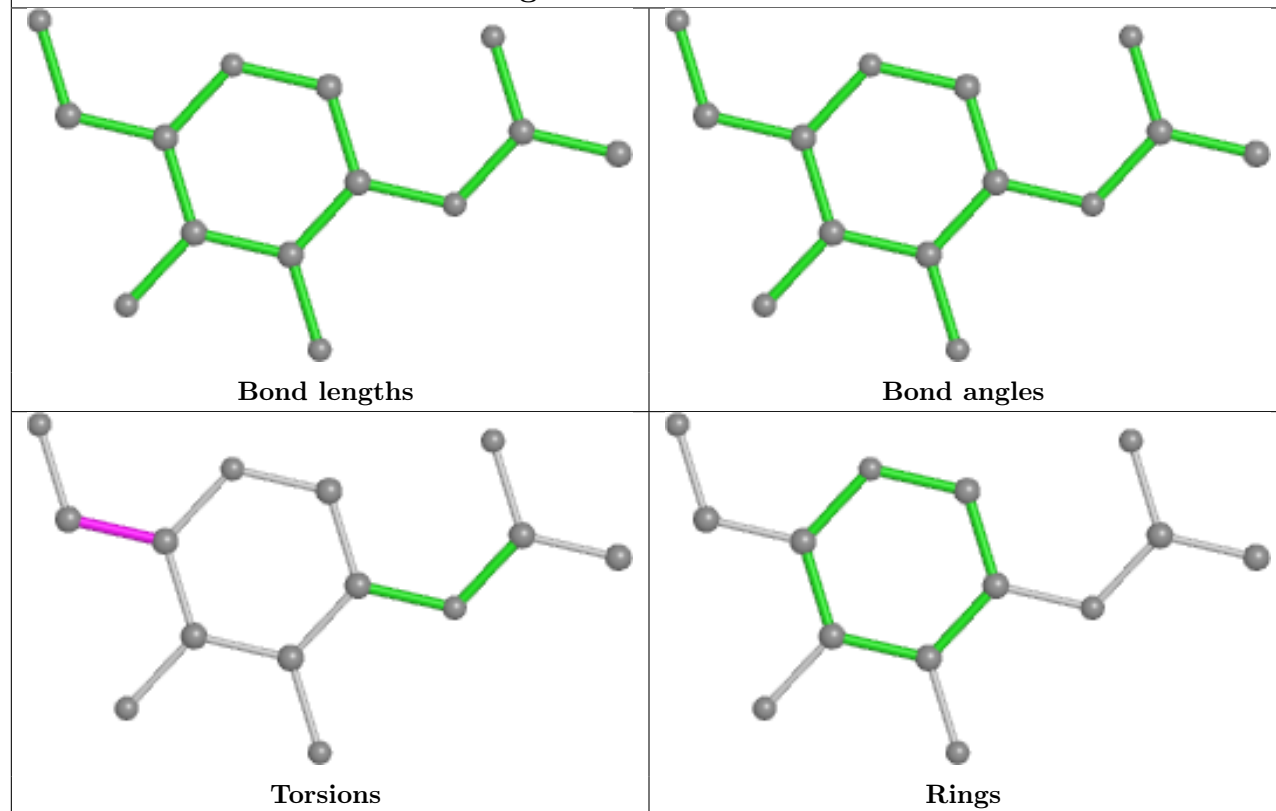






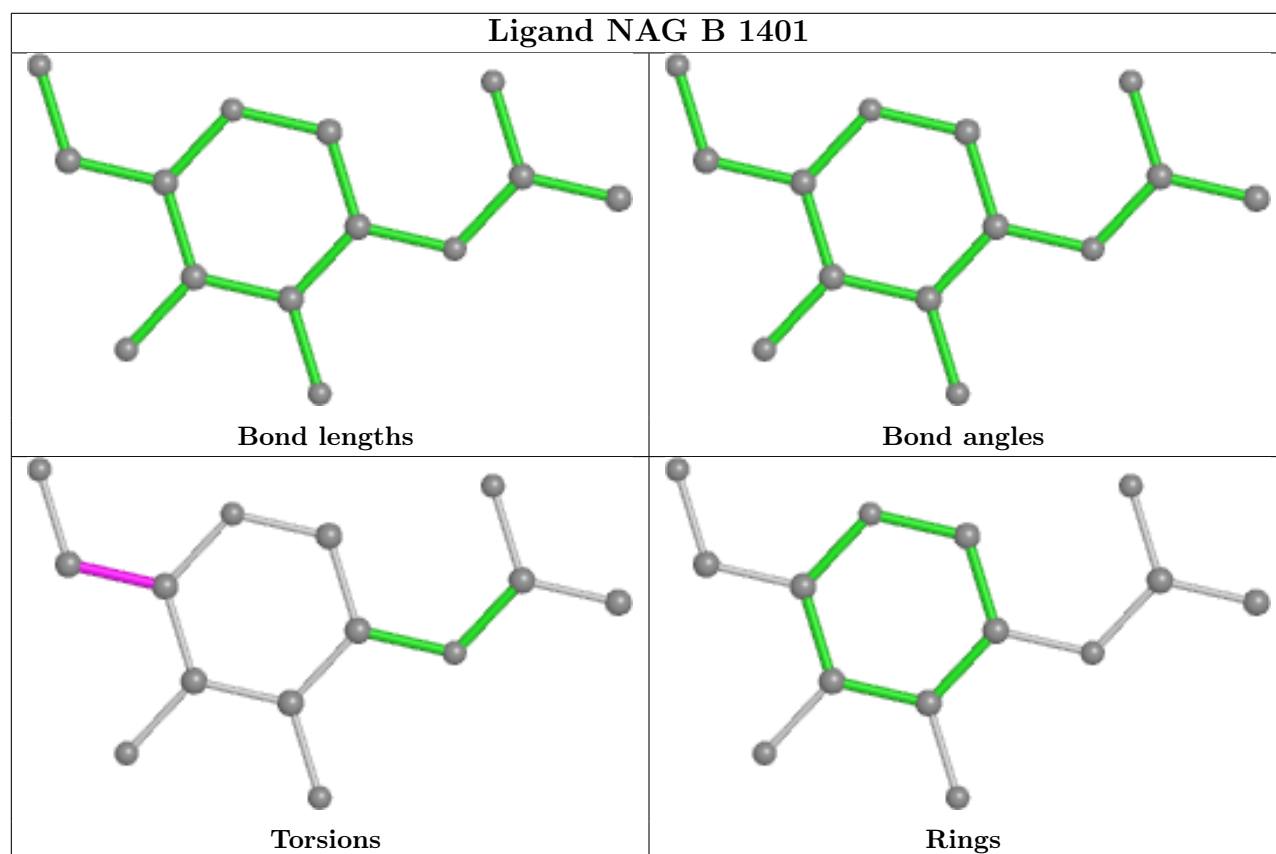
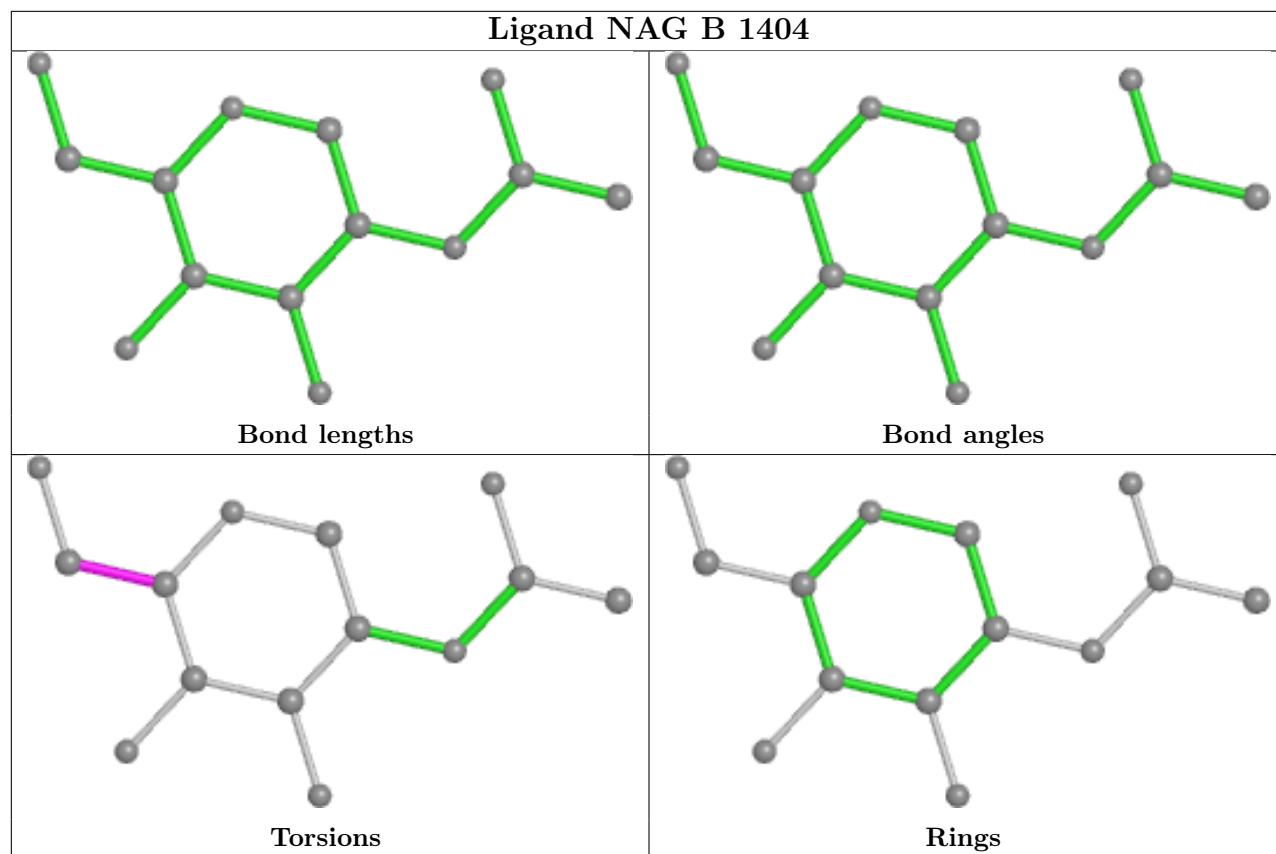


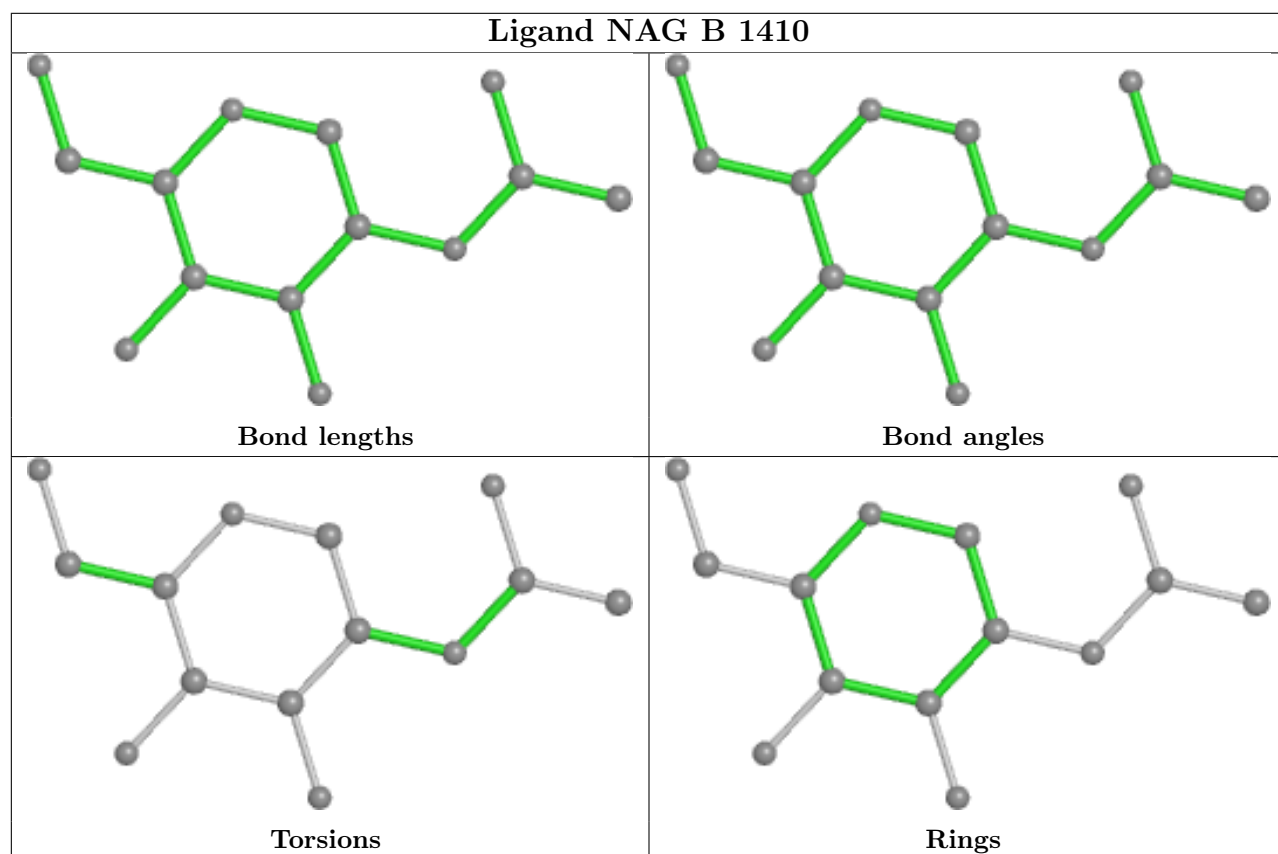
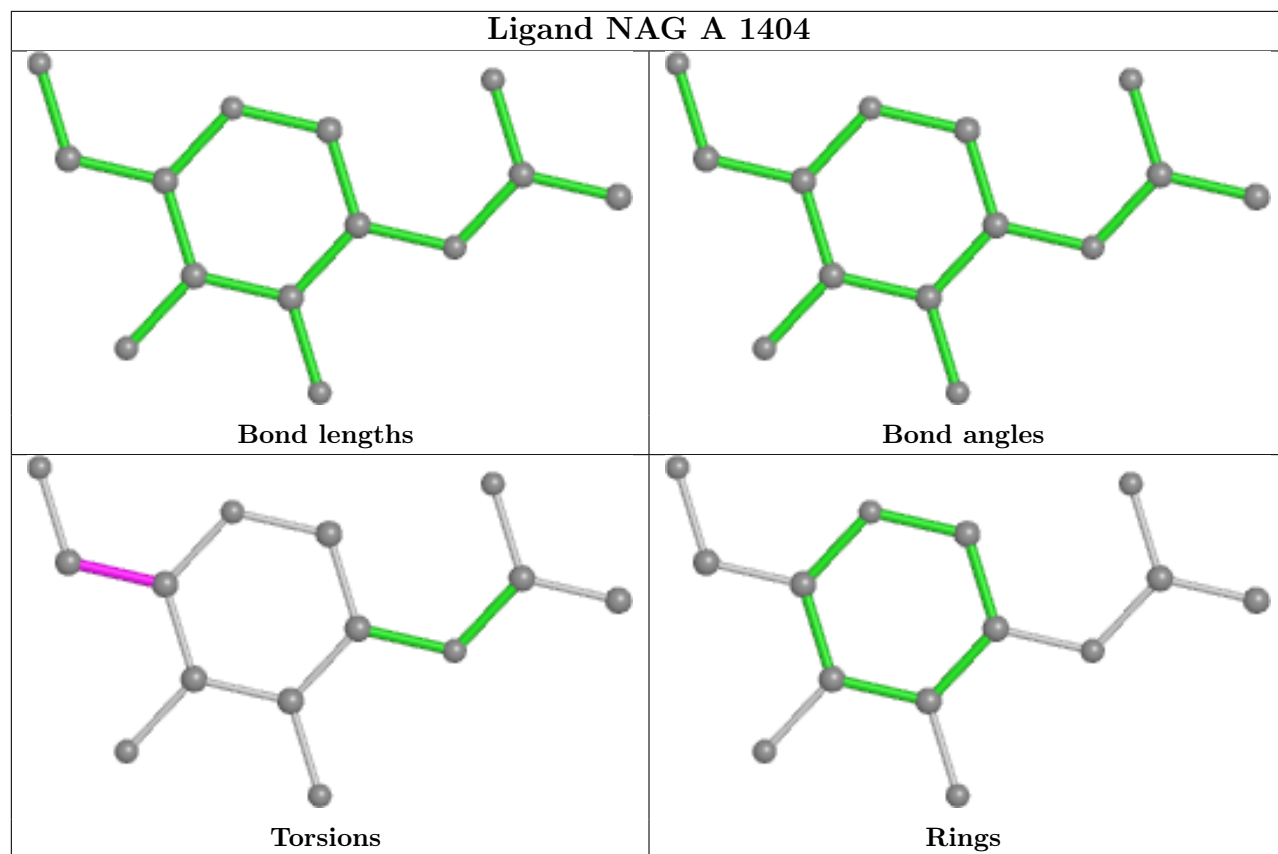
## Ligand NAG B 1403

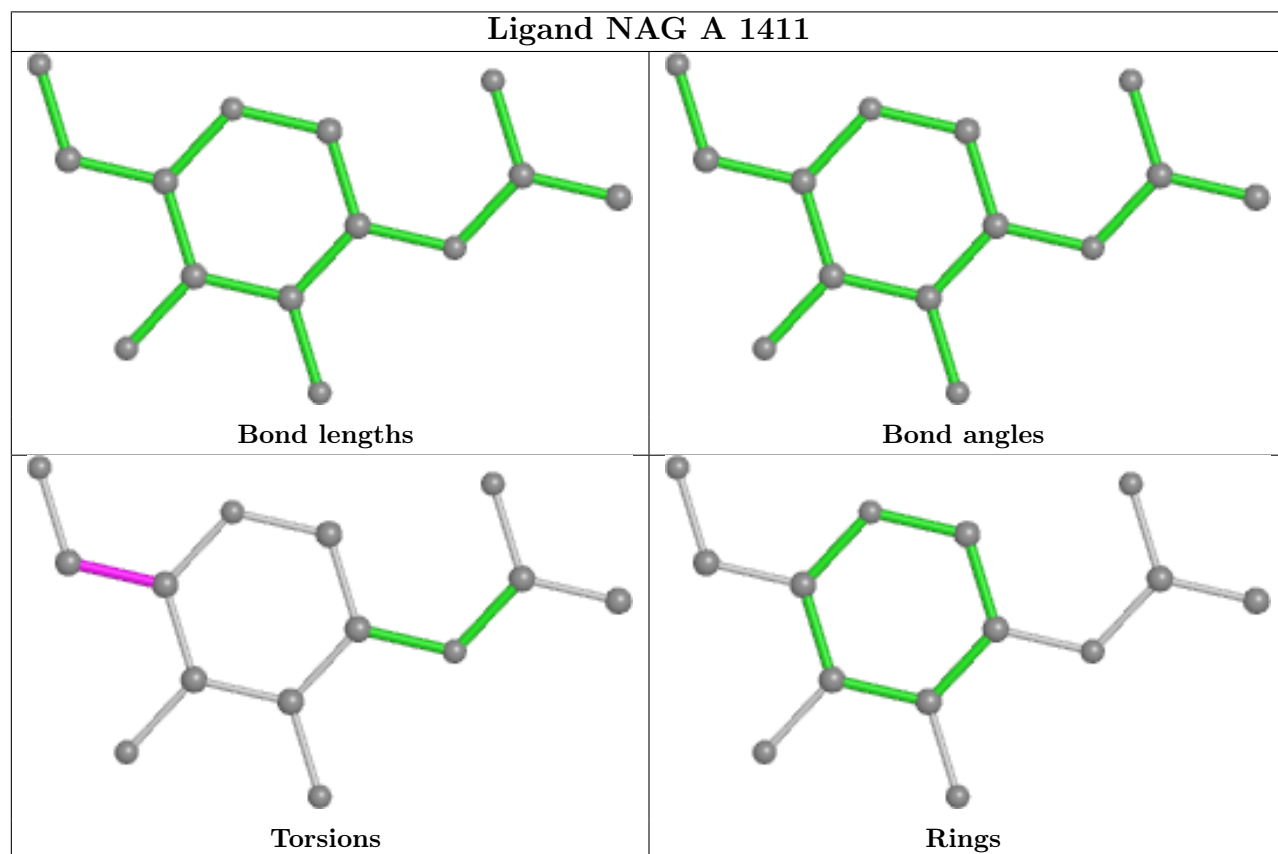
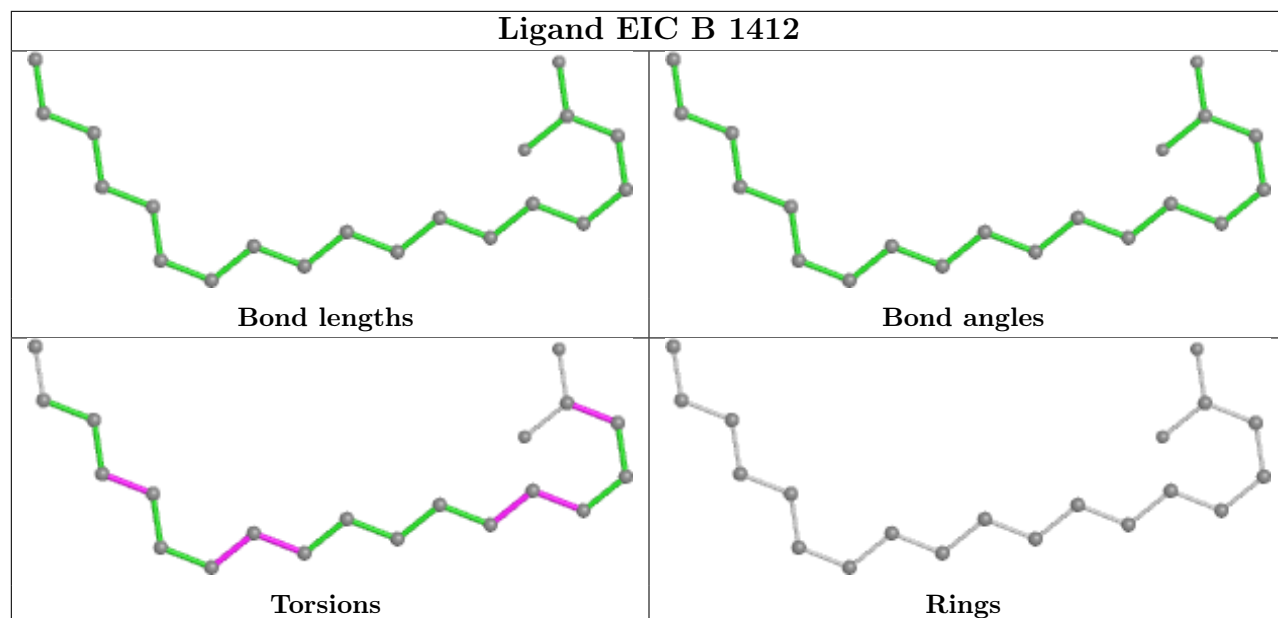


## Ligand NAG C 1403





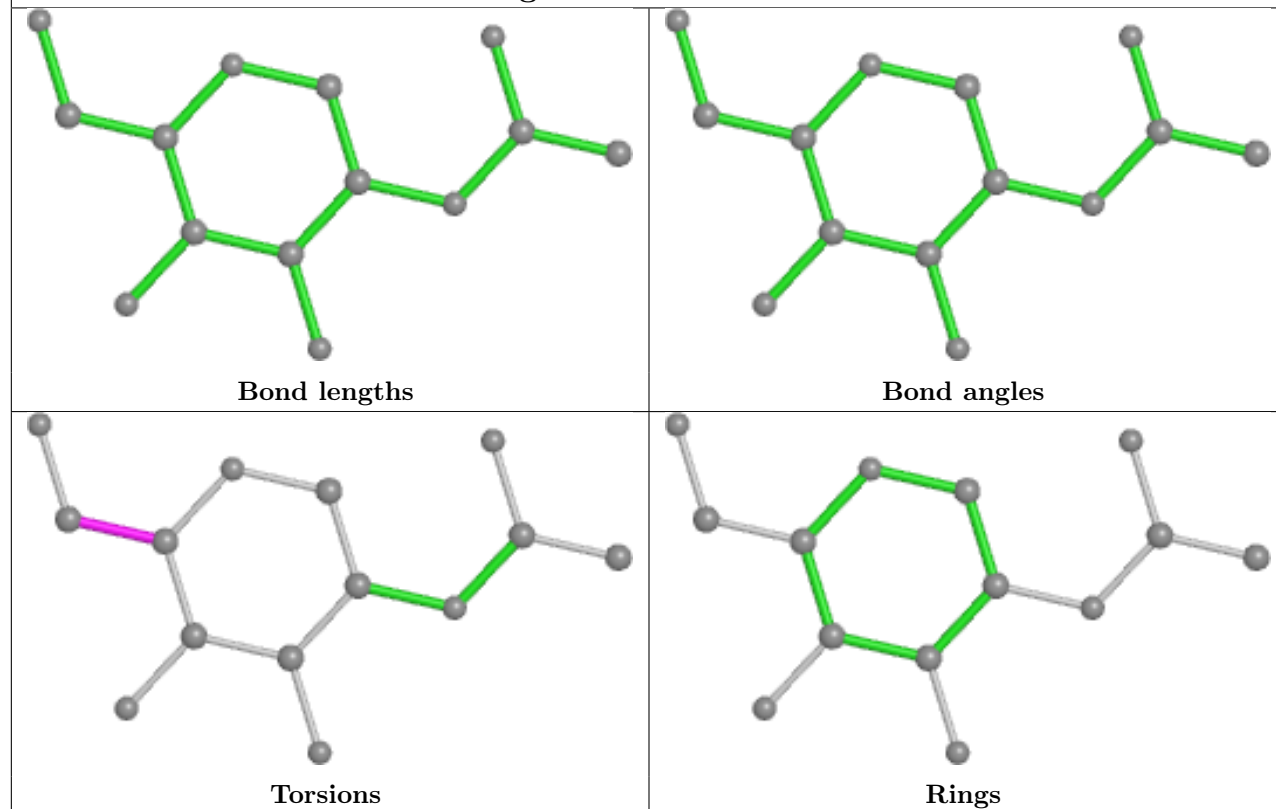




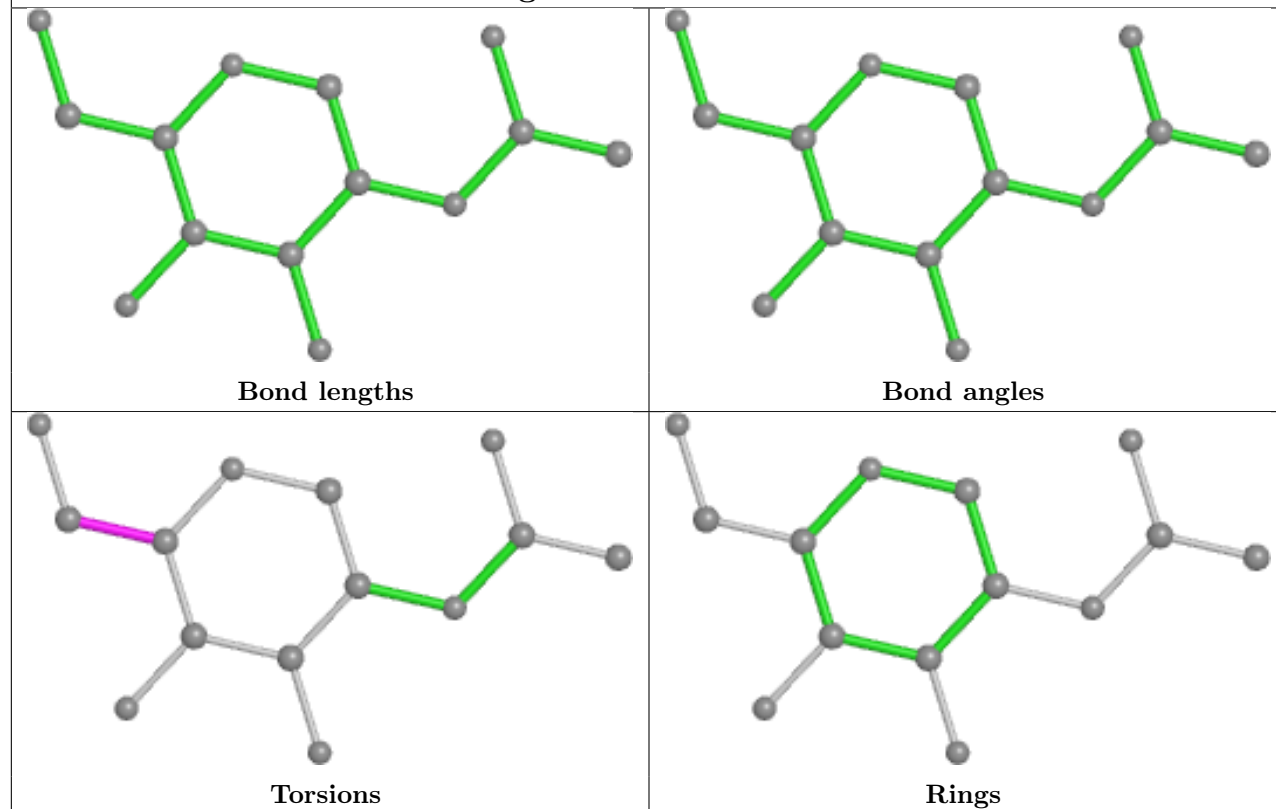
## Ligand NAG A 1403



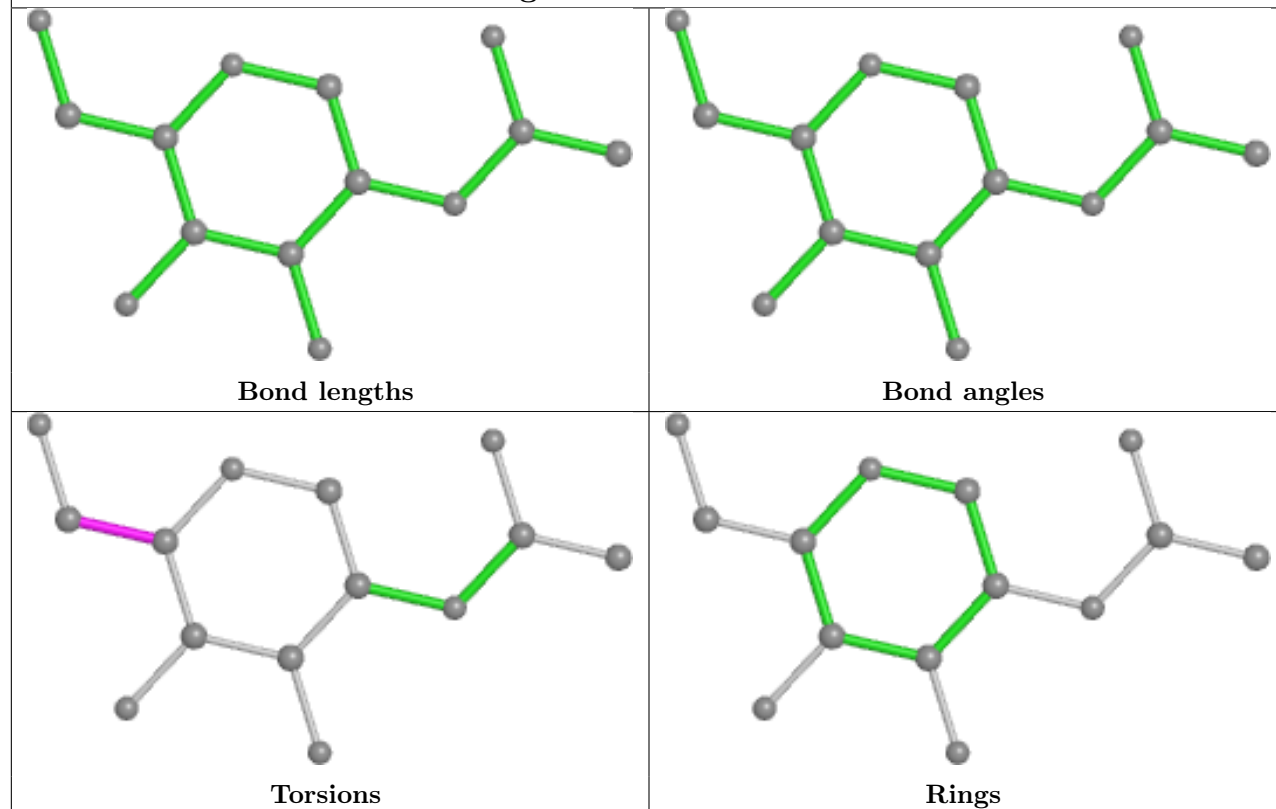
## Ligand NAG C 1408



## Ligand NAG A 1409



## Ligand NAG B 1411

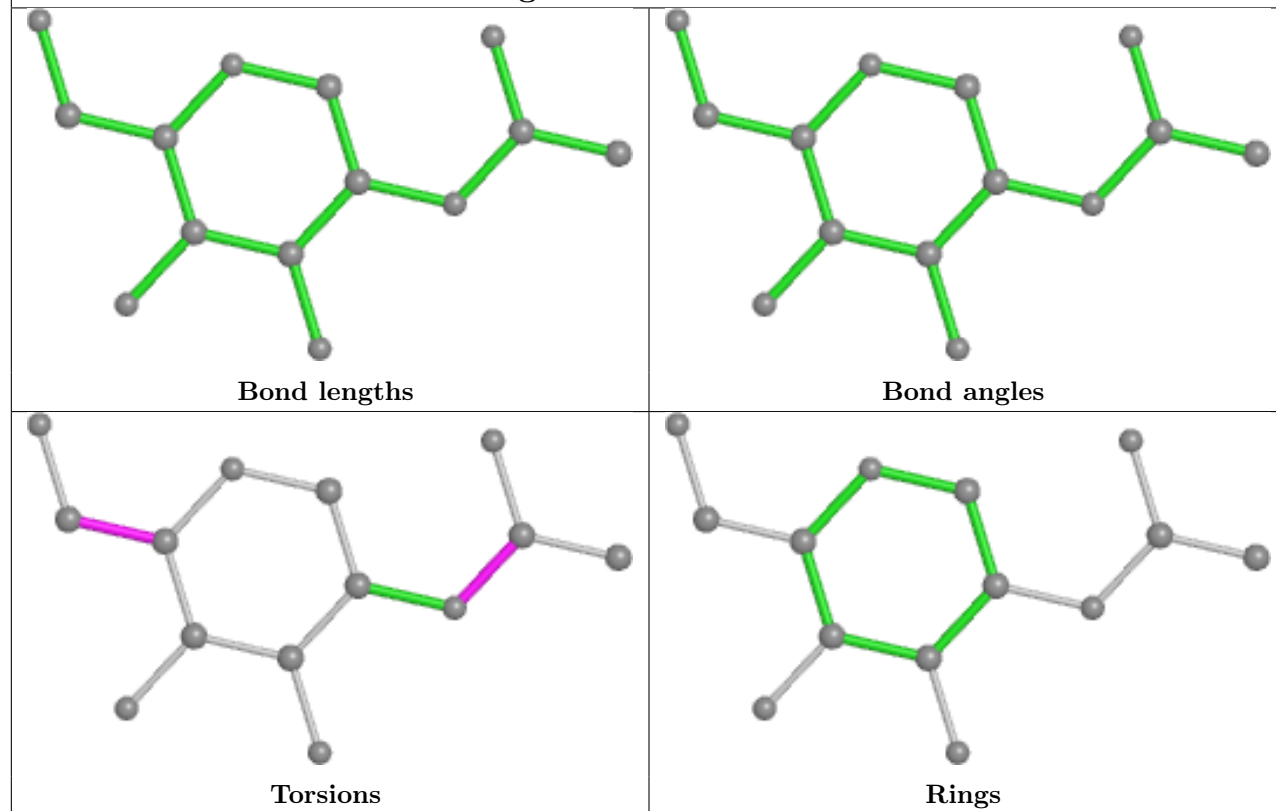




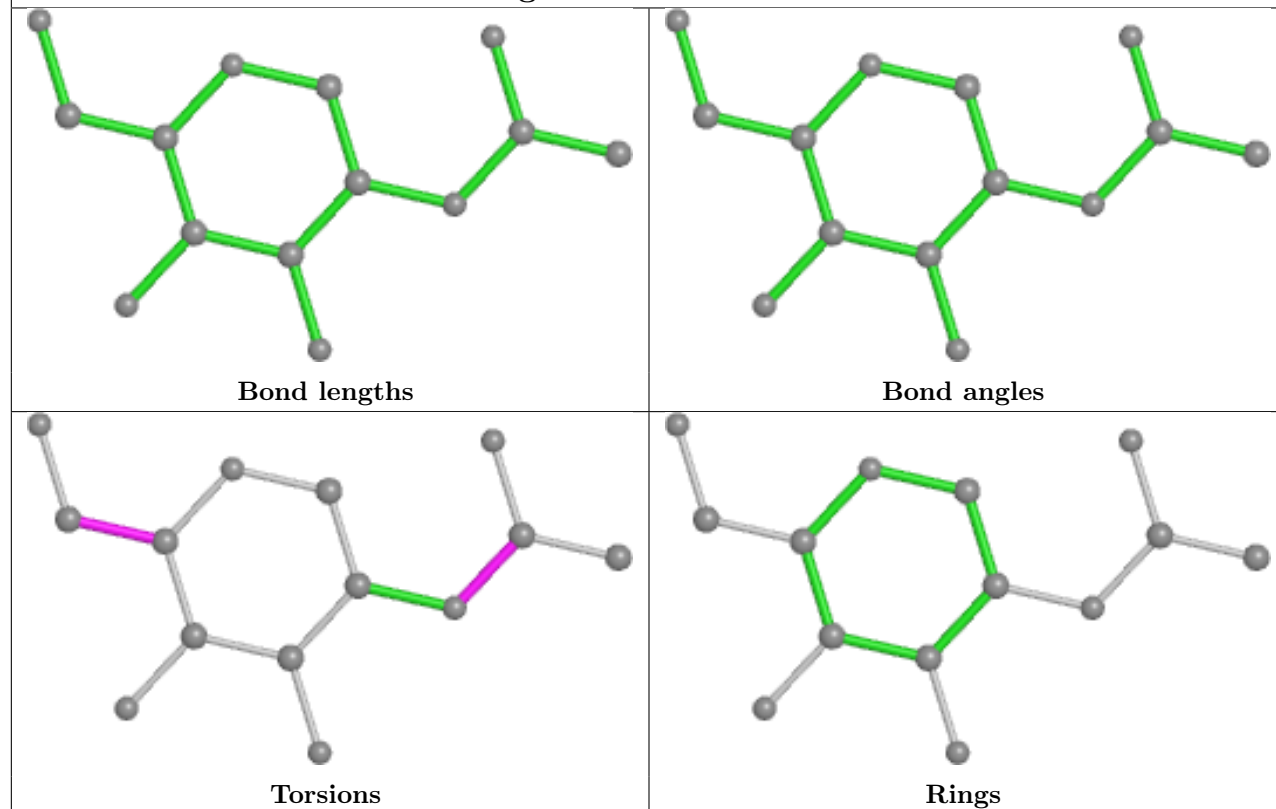
## Ligand NAG C 1407



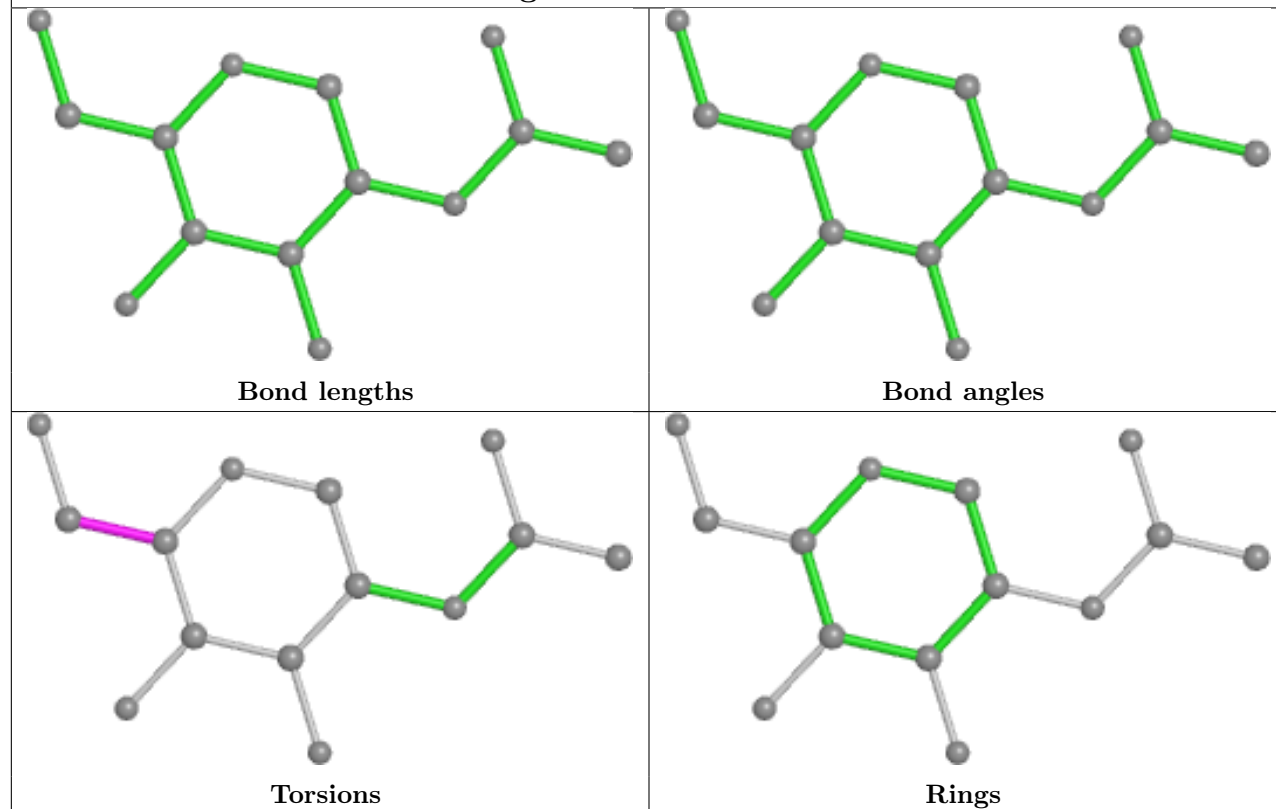
## Ligand NAG A 1410

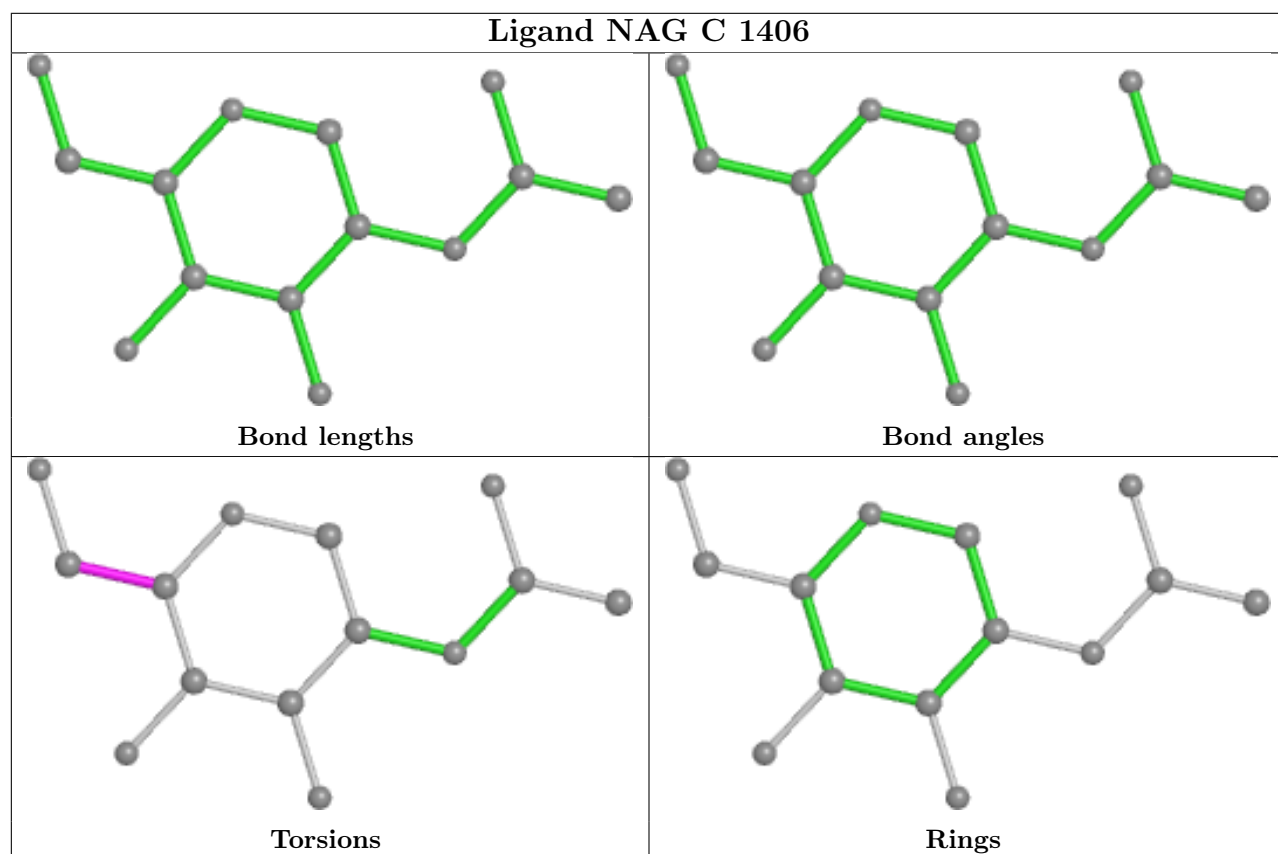
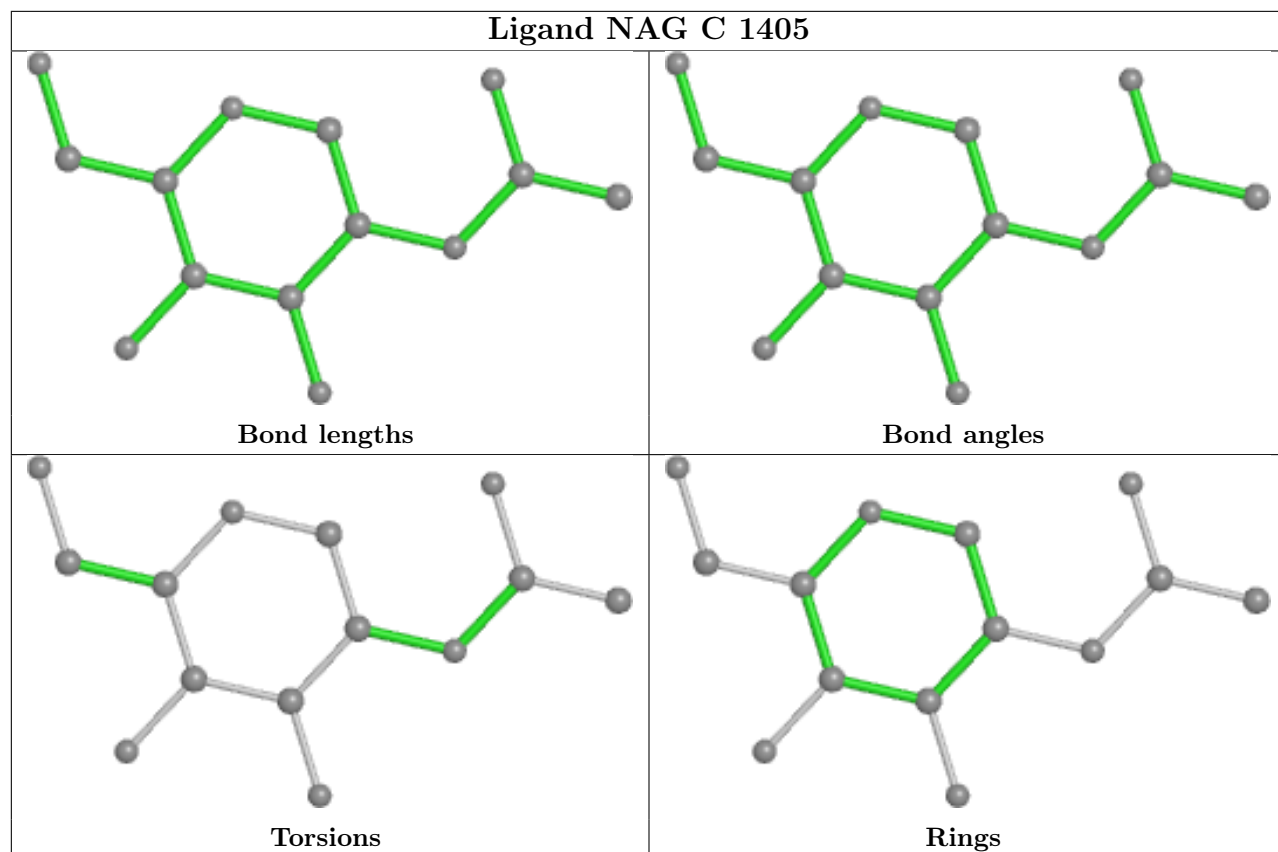


## Ligand NAG A 1407

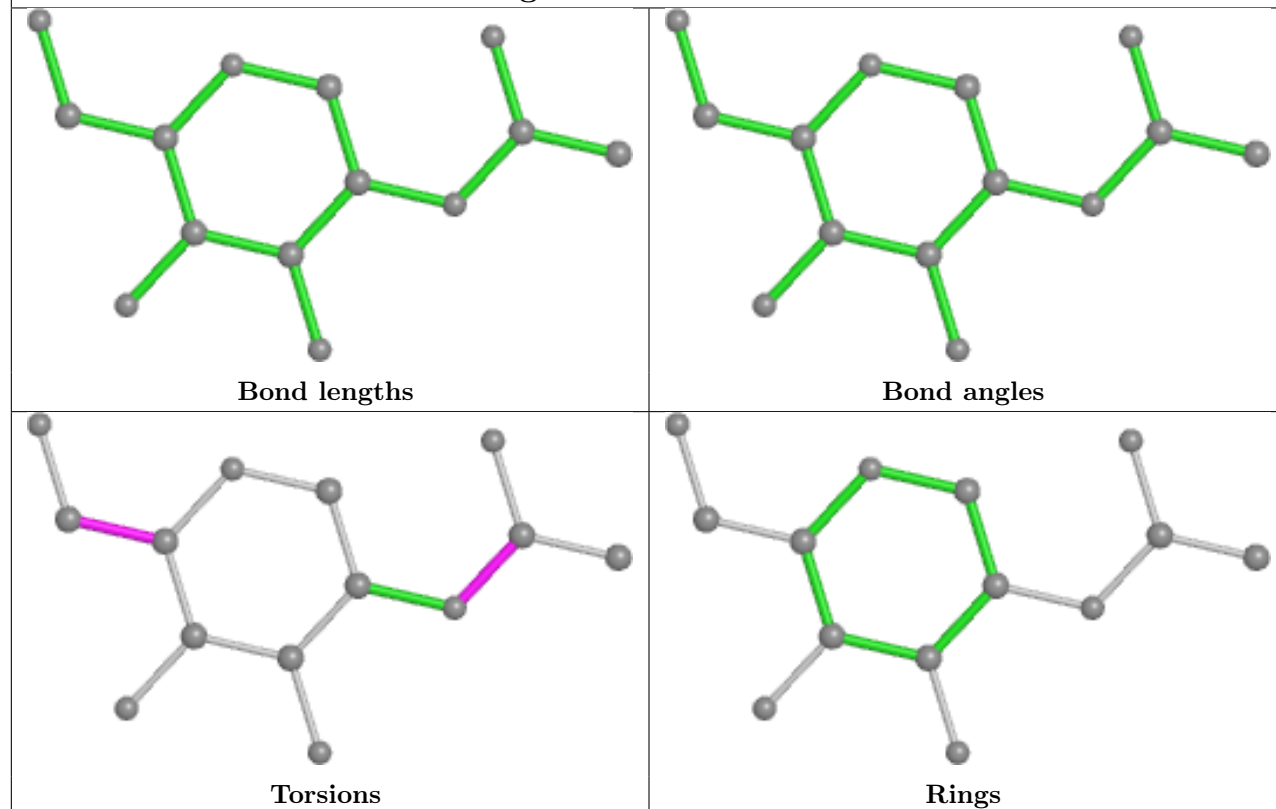


## Ligand NAG B 1408

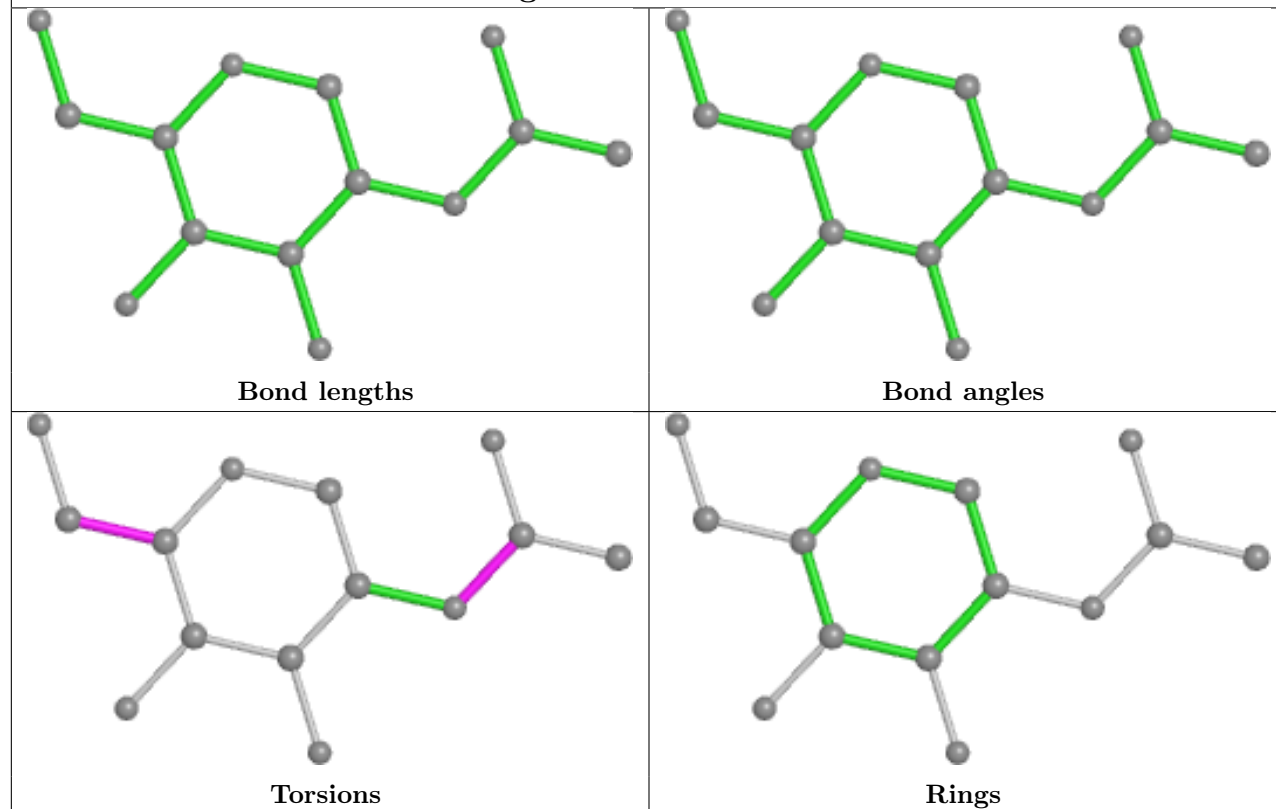




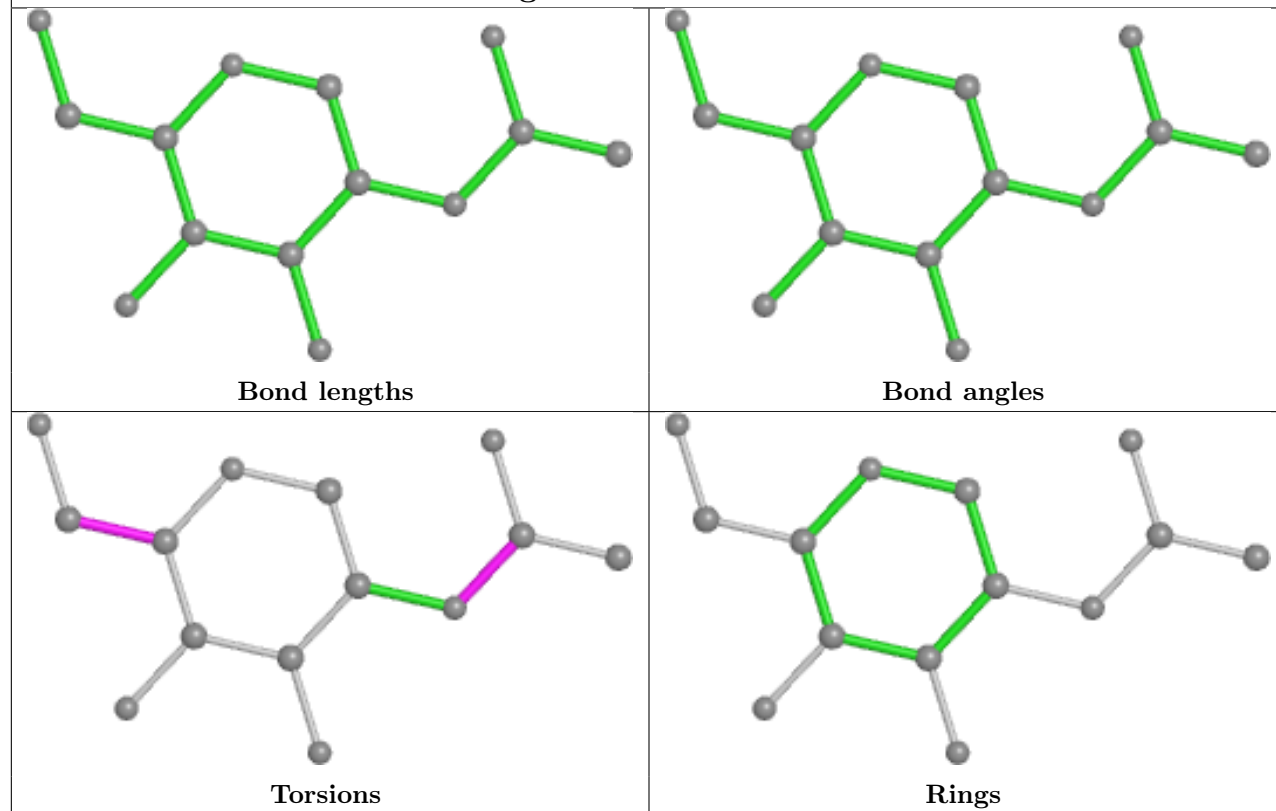
## Ligand NAG B 1407



## Ligand NAG C 1411

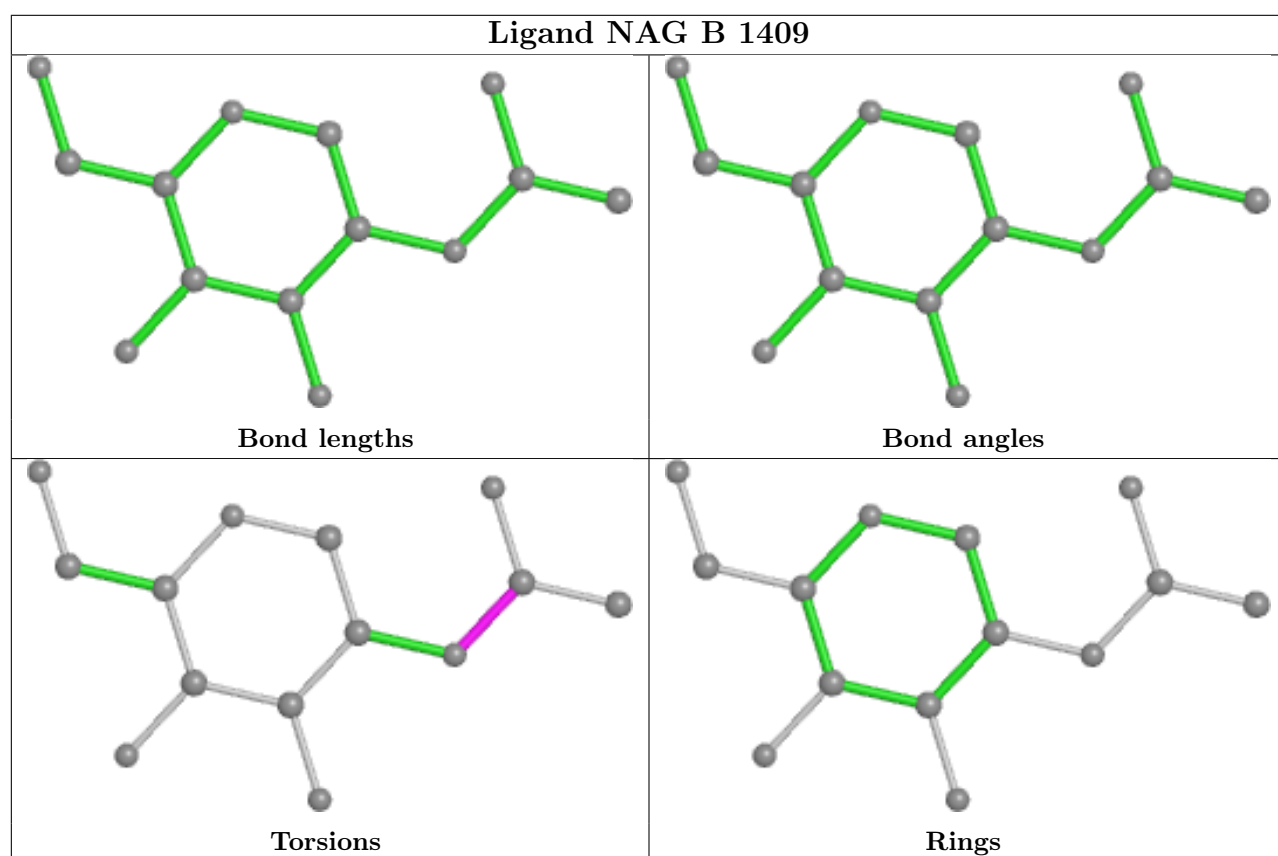
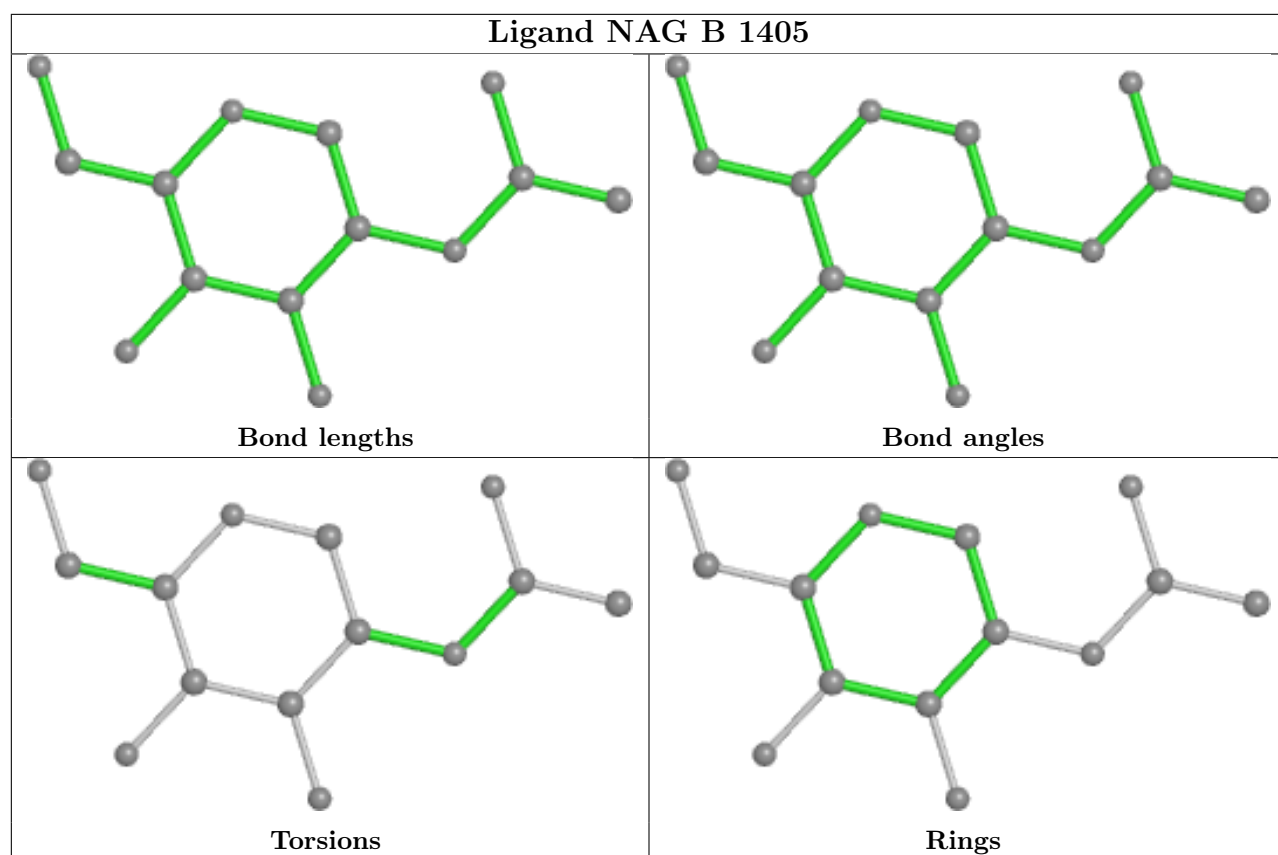


## Ligand NAG C 1402



## Ligand NAG A 1406





## 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.

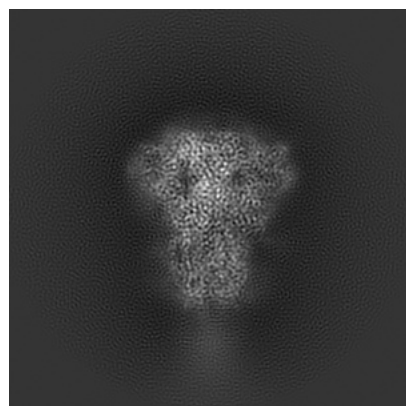
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61600. These allow visual inspection of the internal detail of the map and identification of artifacts.

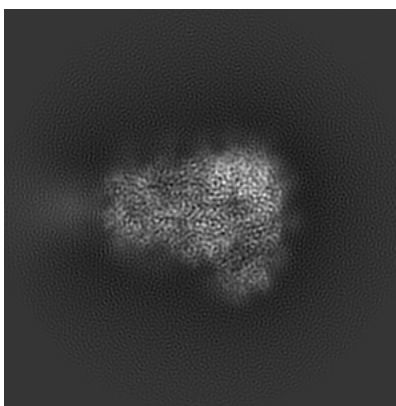
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

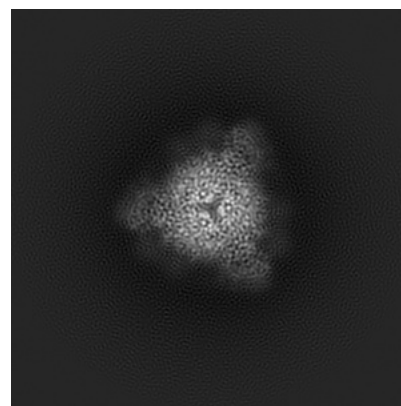
#### 6.1.1 Primary map



X

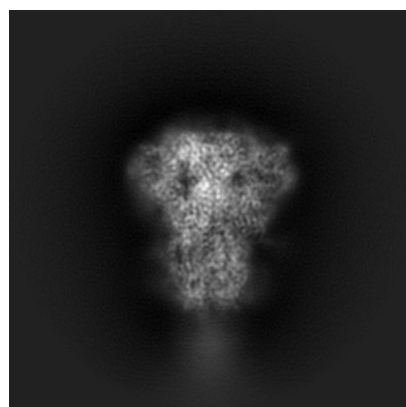


Y

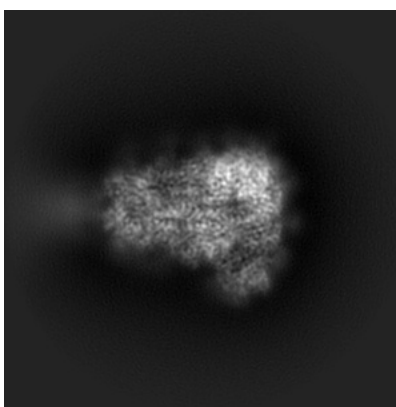


Z

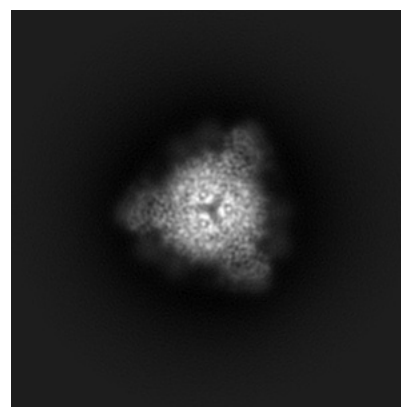
#### 6.1.2 Raw map



X



Y



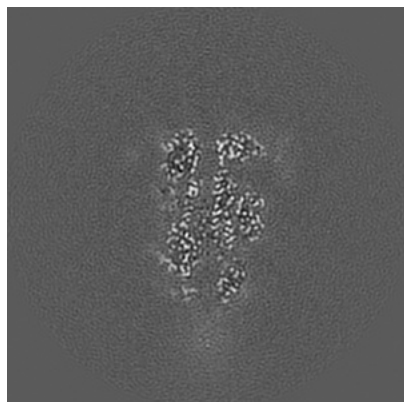
Z

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

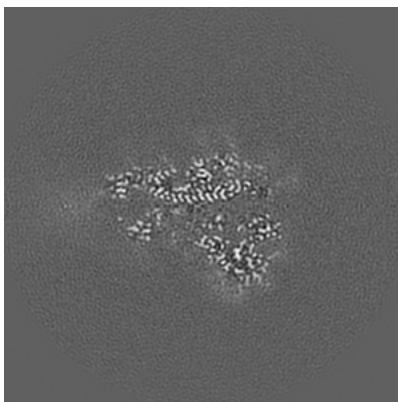


## 6.2 Central slices [i](#)

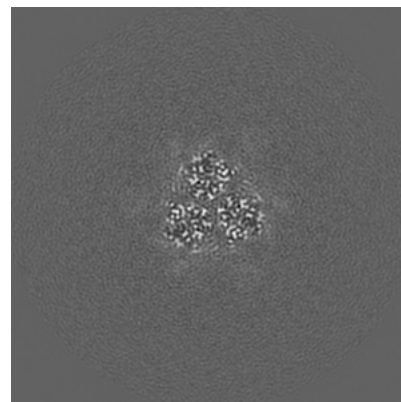
### 6.2.1 Primary map



X Index: 120

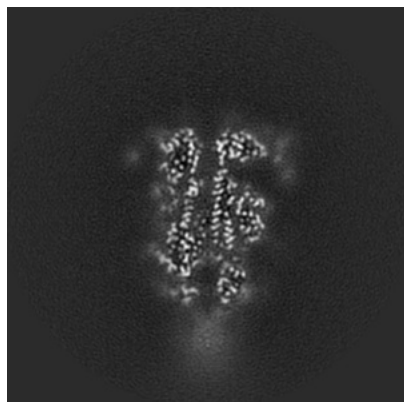


Y Index: 120

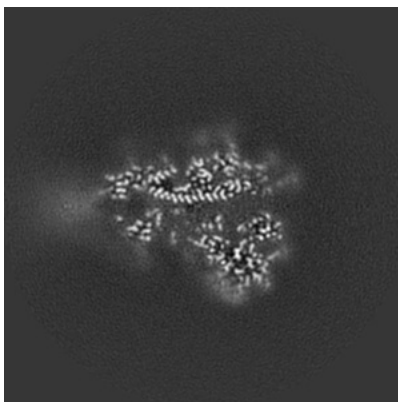


Z Index: 120

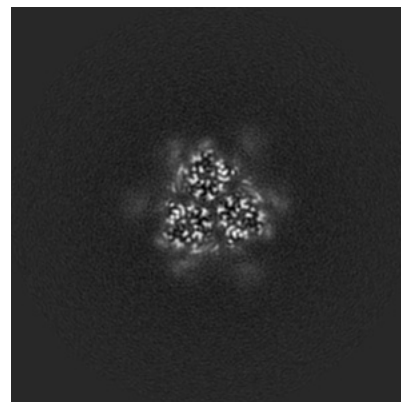
### 6.2.2 Raw map



X Index: 120



Y Index: 120

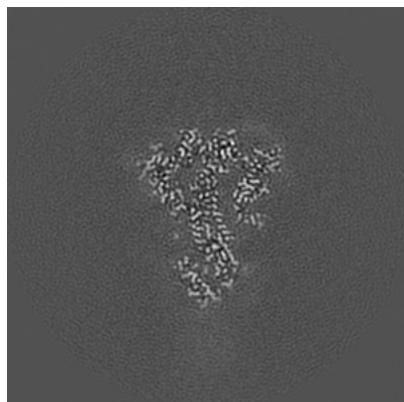


Z Index: 120

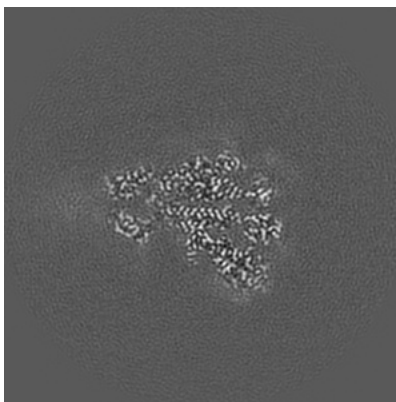
The images above show central slices of the map in three orthogonal directions.

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

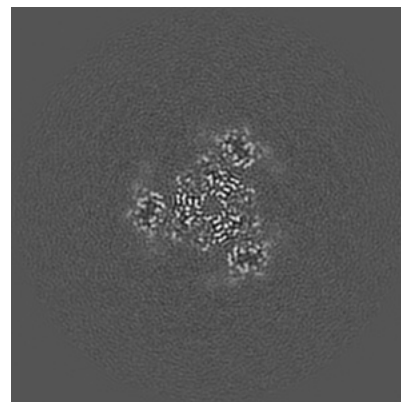
### 6.3.1 Primary map



X Index: 130

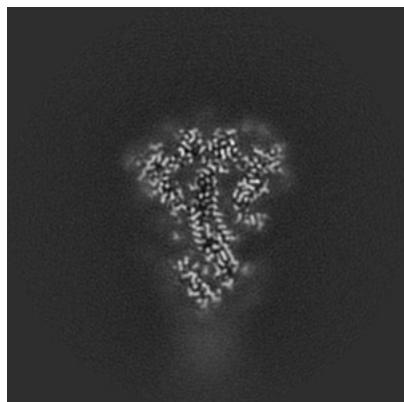


Y Index: 116

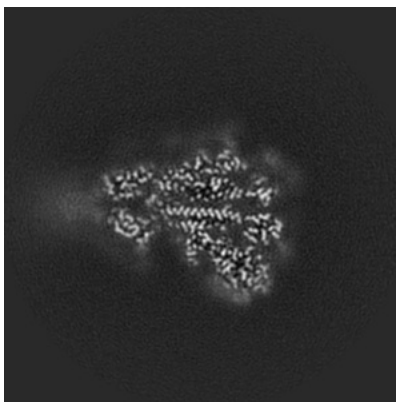


Z Index: 150

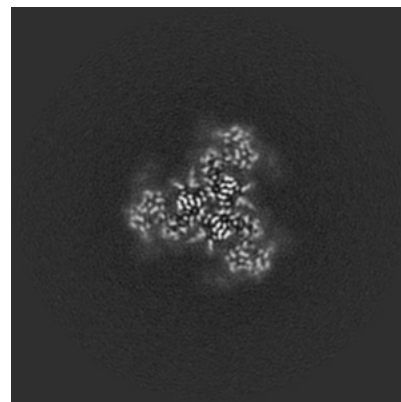
### 6.3.2 Raw map



X Index: 130



Y Index: 116

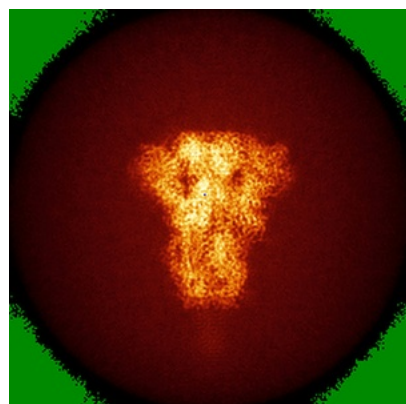


Z Index: 154

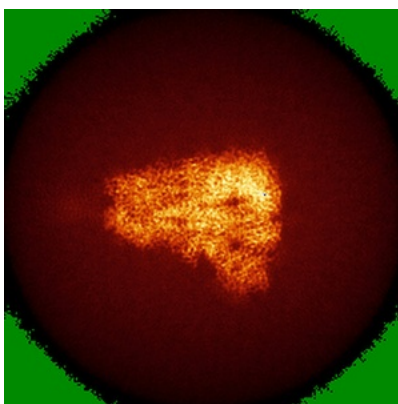
The images above show the largest variance slices of the map in three orthogonal directions.

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

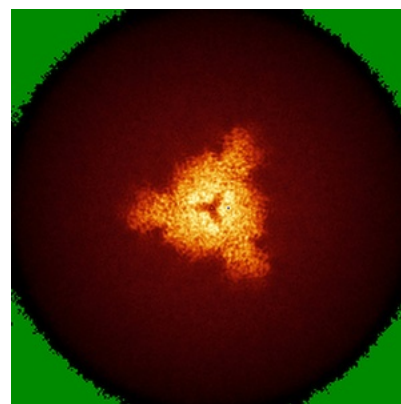
### 6.4.1 Primary map



X

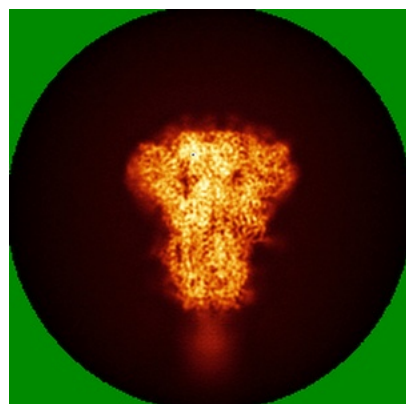


Y

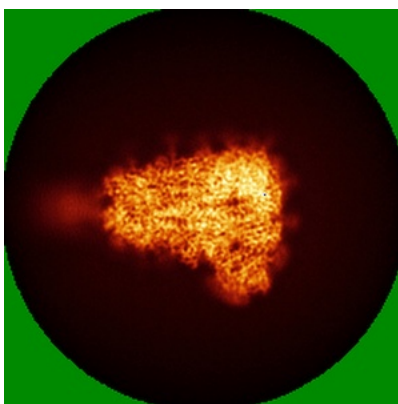


Z

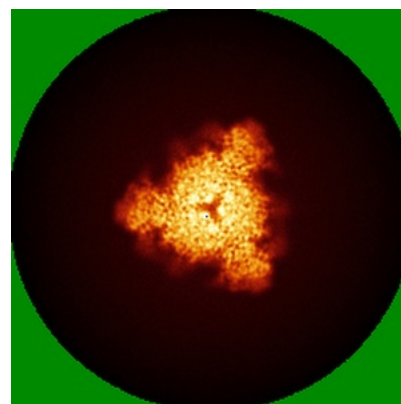
### 6.4.2 Raw map



X



Y

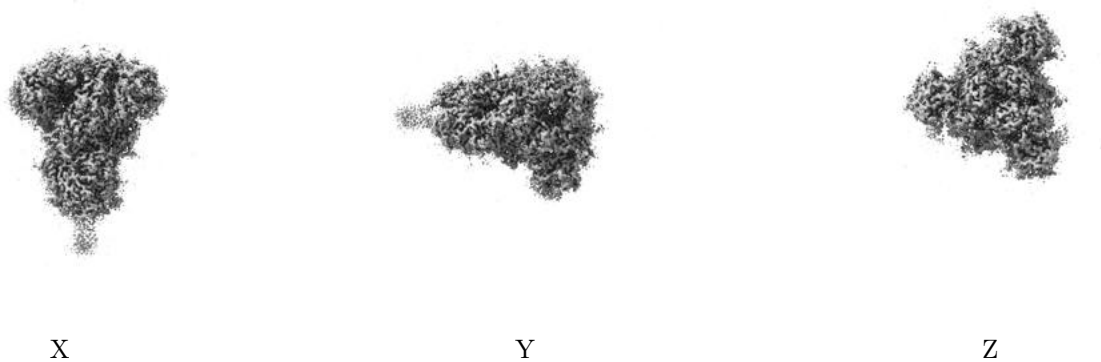


Z

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.

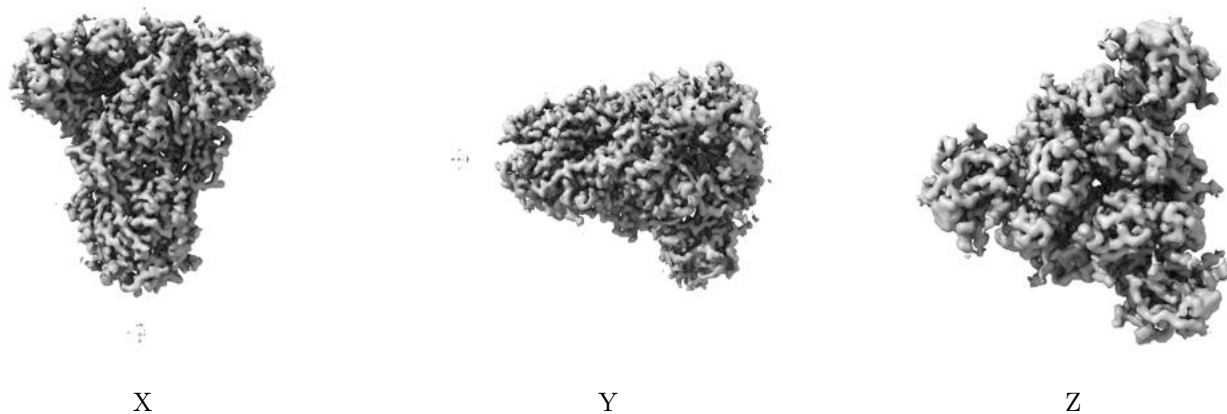
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.026. 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.

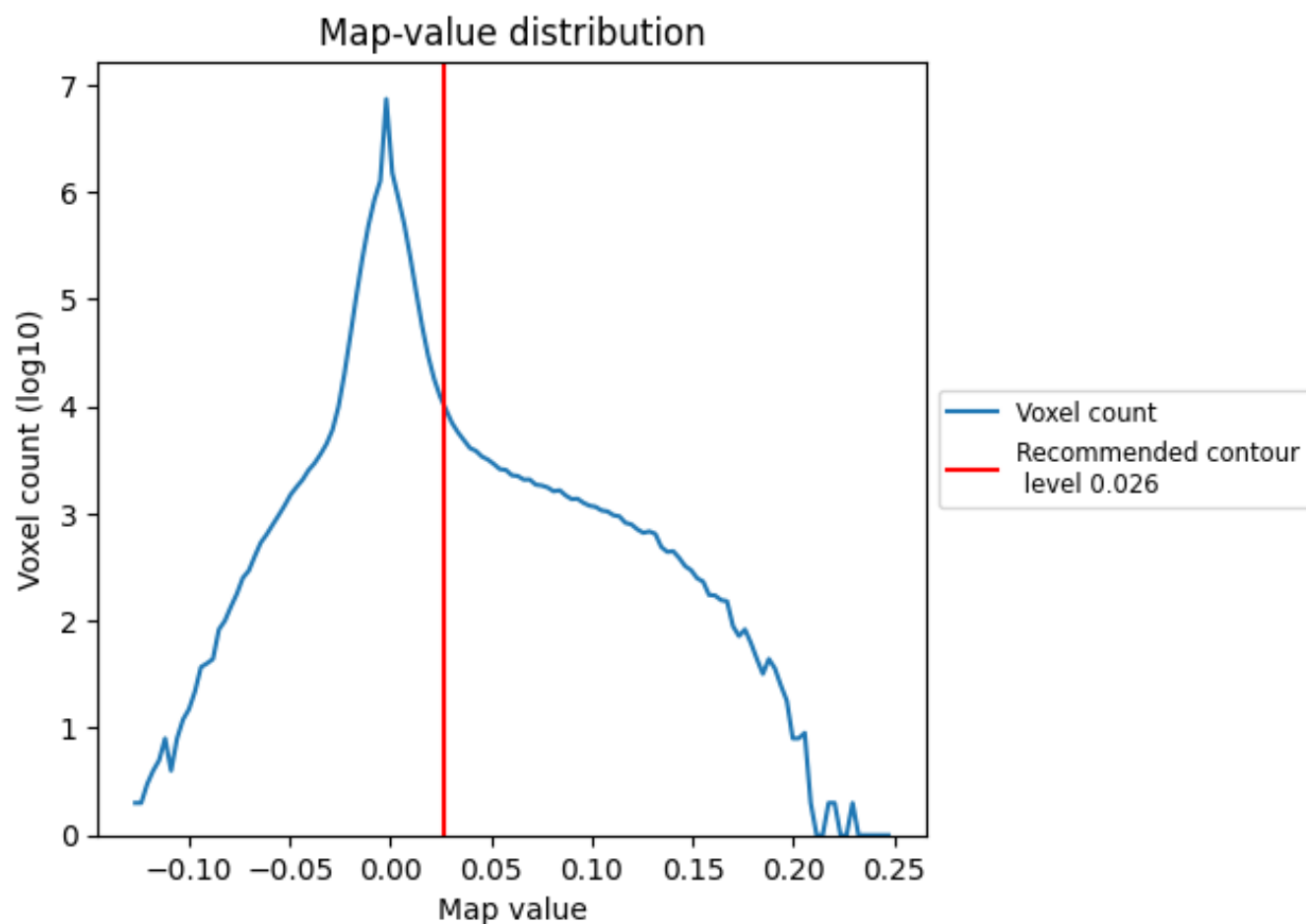
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

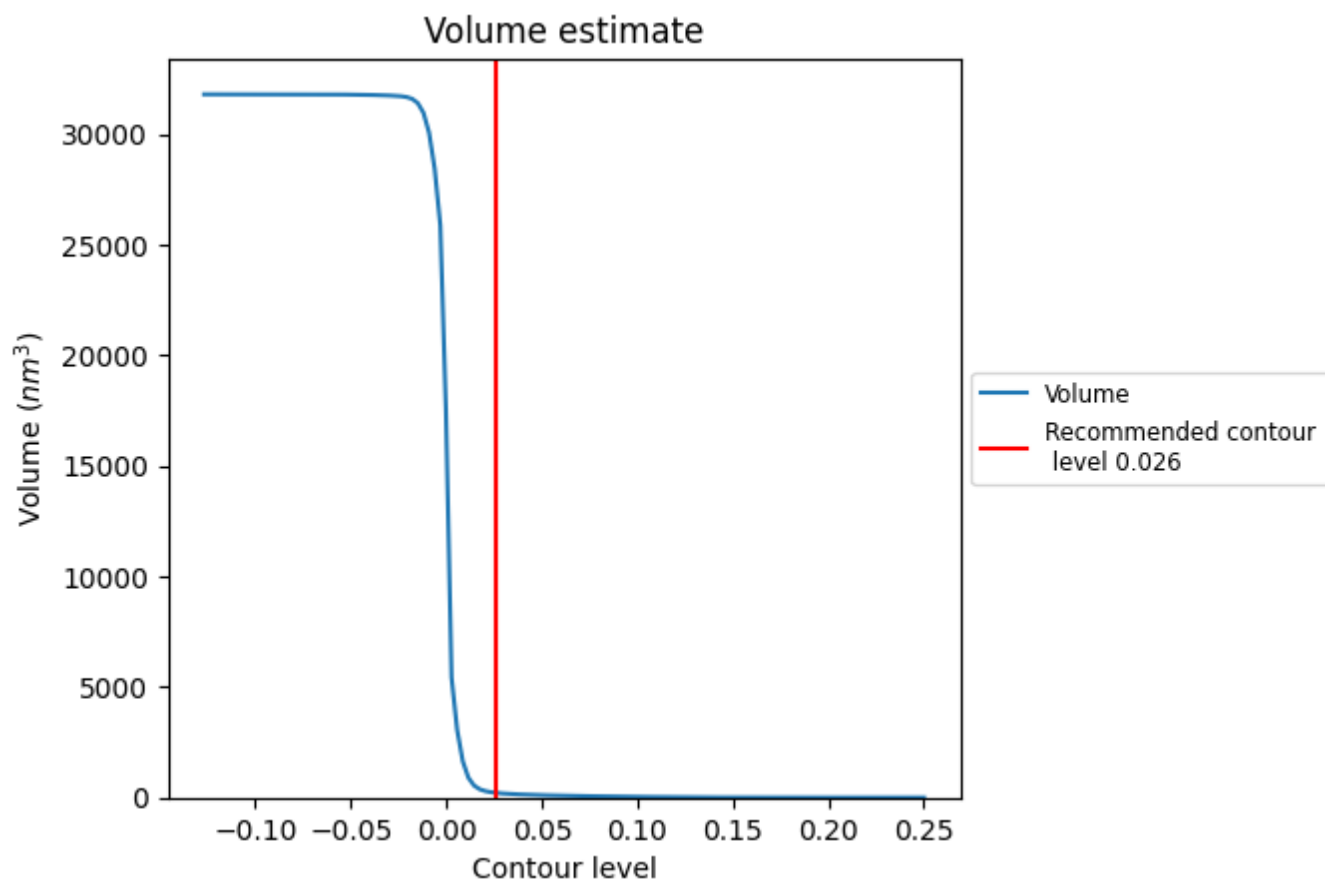
This section contains the results of statistical analysis of the map.

### 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.

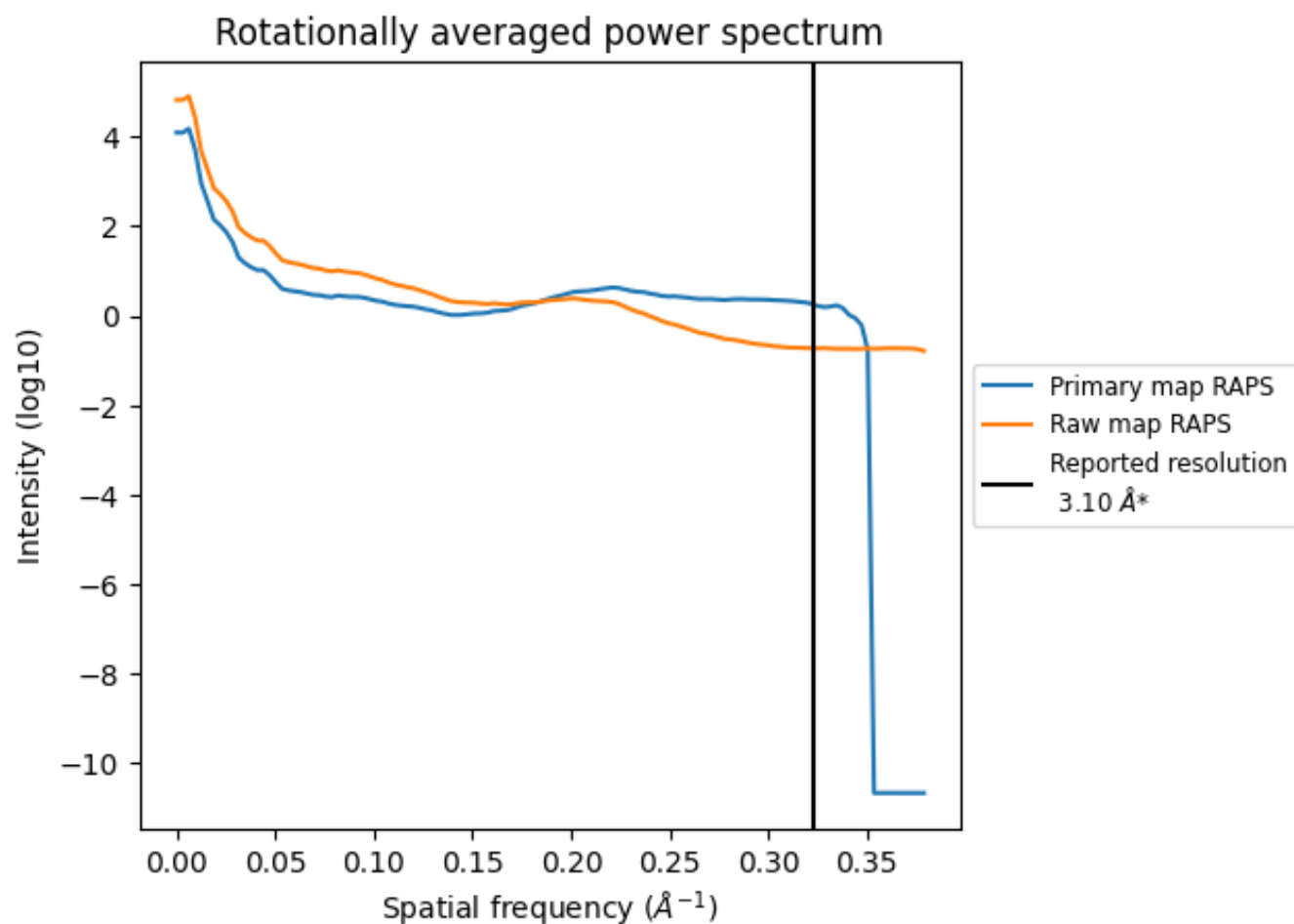
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214  $\text{nm}^3$ ; this corresponds to an approximate mass of 193 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

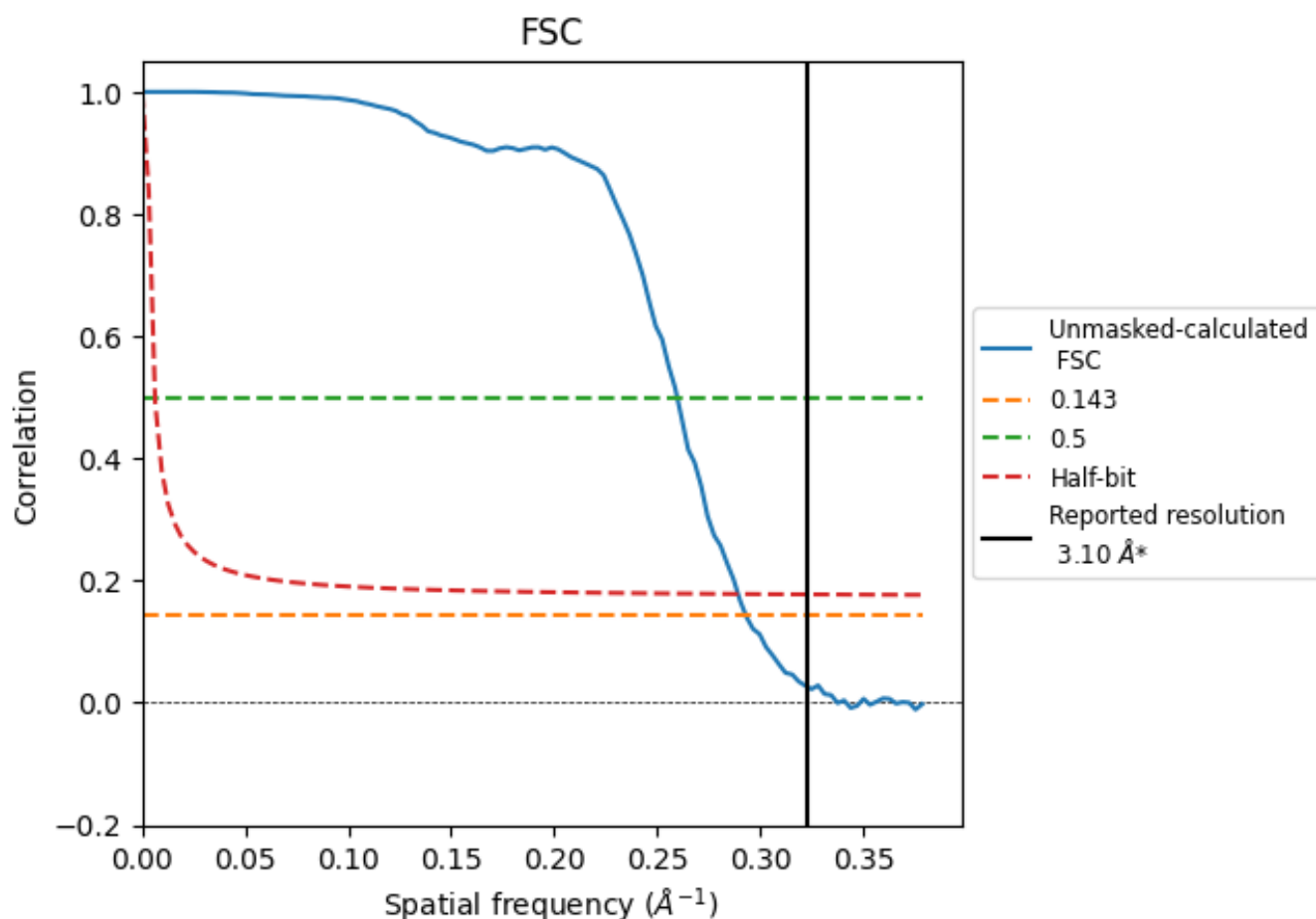


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

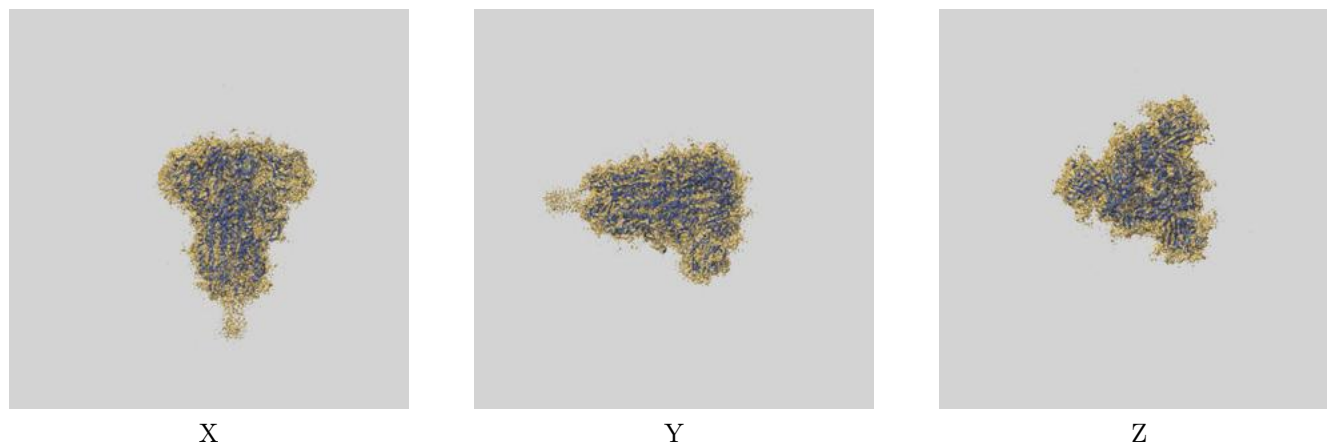
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.41	3.85	3.46

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 3.1 by more than 10 %

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

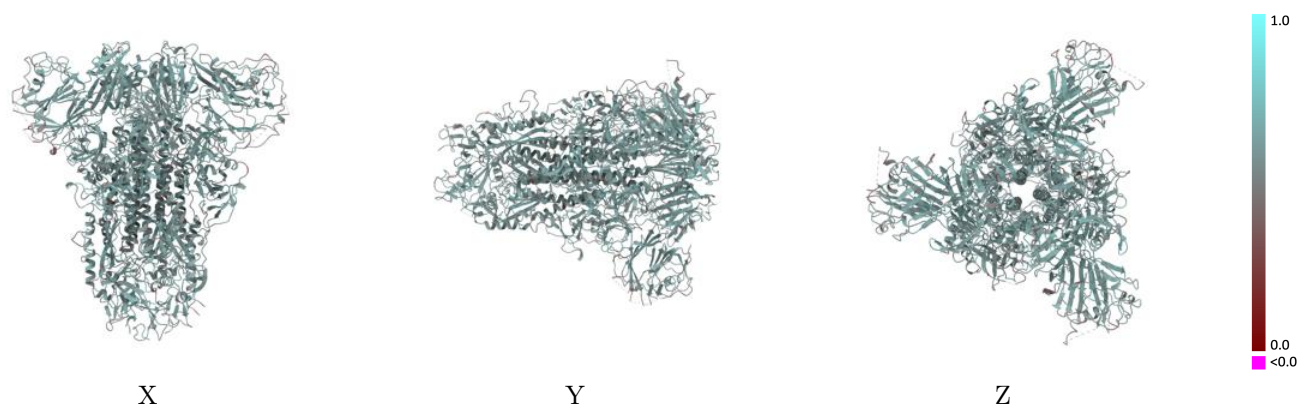
This section contains information regarding the fit between EMDB map EMD-61600 and PDB model 9JMF. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



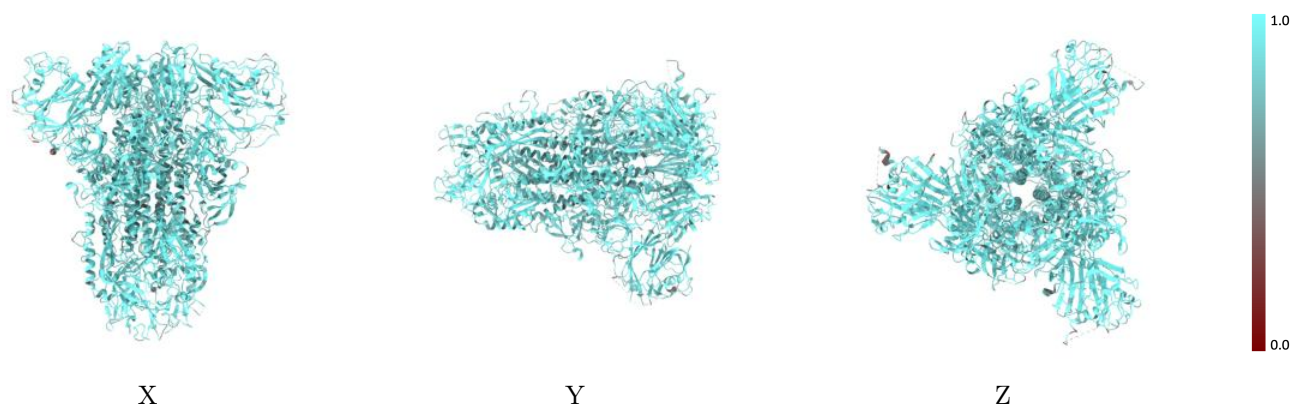
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



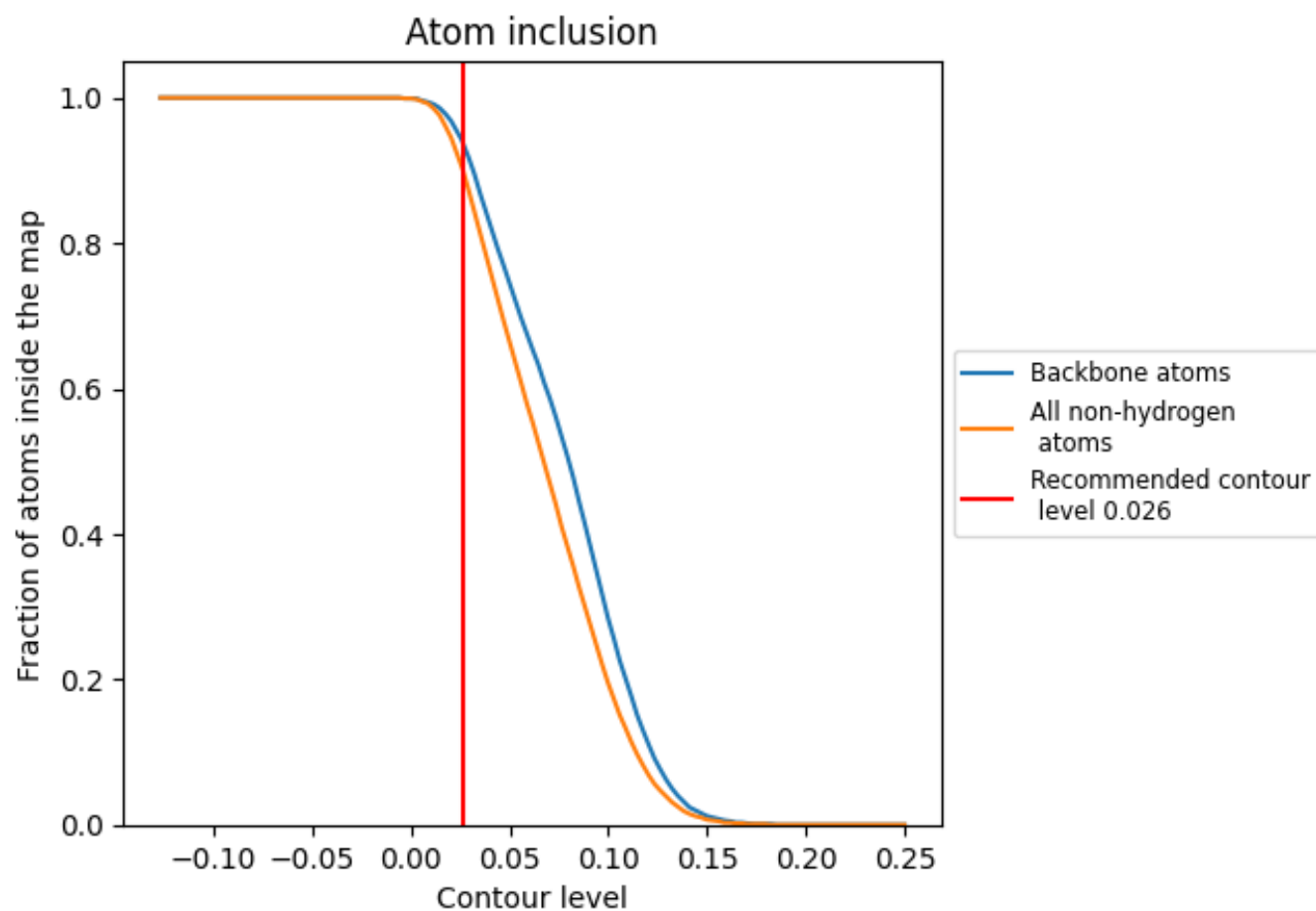
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.026).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.5700
A	 0.9070	 0.5720
B	 0.9070	 0.5710
C	 0.9050	 0.5720
D	 0.8210	 0.5280
E	 0.7140	 0.5240
F	 0.6790	 0.4480
G	 0.6070	 0.4240
H	 0.7500	 0.4960
I	 0.8210	 0.5470
J	 0.7500	 0.5270
K	 0.6790	 0.4810
L	 0.5710	 0.3790
M	 0.7140	 0.4580
N	 0.7860	 0.5400
O	 0.7860	 0.5260
P	 0.6430	 0.4540
Q	 0.6430	 0.3600
R	 0.6790	 0.4100

