



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:27 PM UTC

PDB ID : 7N1U / pdb_00007n1u
EMDB ID : EMD-24123
Title : Structural basis for enhanced infectivity and immune evasion of SARS-CoV-2 variants
Authors : Zhang, J.; Cai, Y.F.; Xiao, T.S.; Rawson, S.; Peng, H.Q.; Sterling, S.M.; Walsh Jr, R.M.; Volloch, S.R.; Chen, B.
Deposited on : 2021-05-28
Resolution : 3.14 Å (reported)
Based on initial model : 7KRQ

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

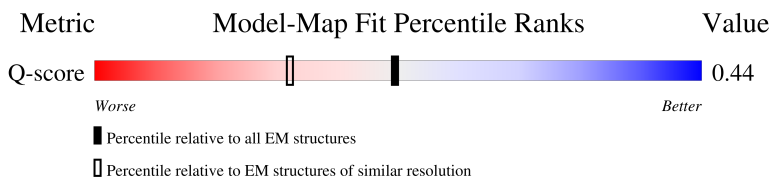
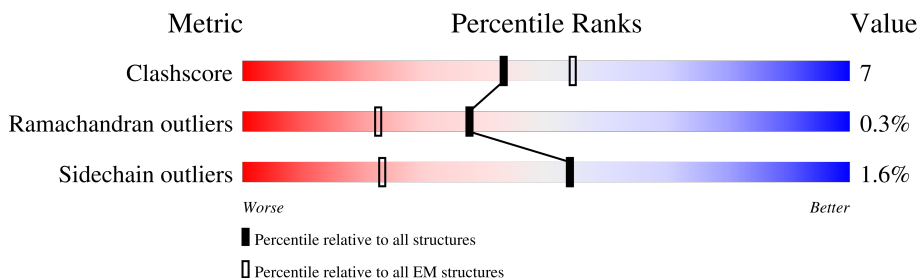
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.14 Å.

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



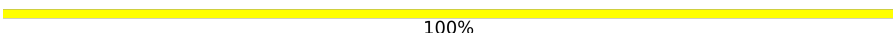
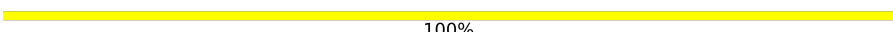
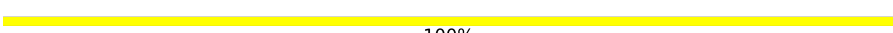
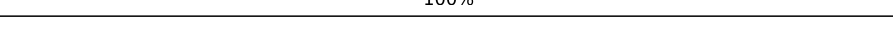
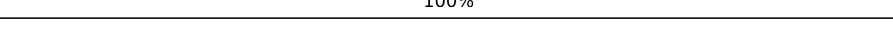
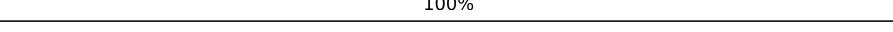
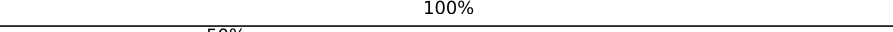
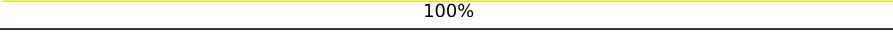
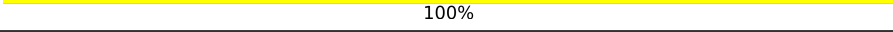
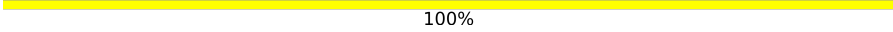
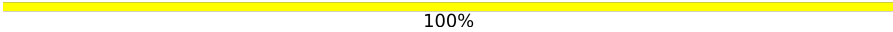
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14483 (2.64 - 3.64)

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

Mol	Chain	Length	Quality of chain
1	A	1305	
1	B	1305	
1	C	1305	

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Mol	Chain	Length	Quality of chain
2	D	2	 50%50%
2	E	2	 100%
2	F	2	 100%
2	G	2	 50%50%
2	H	2	 100%
2	I	2	 50%50%
2	J	2	 100%
2	K	2	 100%
2	O	2	 100%
2	P	2	 50%50%
2	Q	2	 100%
2	R	2	 50%100%
2	S	2	 50%100%
2	T	2	 50%50%
2	U	2	 100%
2	V	2	 100%
2	Z	2	 100%
2	a	2	 50%50%
2	b	2	 100%
2	c	2	 50%100%
2	d	2	 100%
2	e	2	 50%50%
2	f	2	 100%
2	g	2	 100%
3	L	3	 33%100%

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Mol	Chain	Length	Quality of chain
3	W	3	33% 100%
3	h	3	33% 100%
4	M	3	100%
4	N	3	100%
4	X	3	100%
4	Y	3	100%
4	i	3	100%
4	j	3	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26619 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1075	Total	C	N	O	S	0	0
			8421	5378	1403	1602	38		
1	B	1075	Total	C	N	O	S	0	0
			8421	5378	1403	1602	38		
1	C	1075	Total	C	N	O	S	0	0
			8421	5378	1403	1602	38		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	570	ASP	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	716	ILE	THR	conflict	UNP P0DTC2
A	982	ALA	SER	conflict	UNP P0DTC2
A	1118	HIS	ASP	conflict	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	GLY	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	SER	-	expression tag	UNP P0DTC2
A	1279	ALA	-	expression tag	UNP P0DTC2
A	1280	TRP	-	expression tag	UNP P0DTC2
A	1281	SER	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	PRO	-	expression tag	UNP P0DTC2
A	1284	GLN	-	expression tag	UNP P0DTC2
A	1285	PHE	-	expression tag	UNP P0DTC2
A	1286	GLU	-	expression tag	UNP P0DTC2
A	1287	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1288	GLY	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	GLY	-	expression tag	UNP P0DTC2
A	1291	SER	-	expression tag	UNP P0DTC2
A	1292	GLY	-	expression tag	UNP P0DTC2
A	1293	GLY	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	SER	-	expression tag	UNP P0DTC2
A	1296	GLY	-	expression tag	UNP P0DTC2
A	1297	GLY	-	expression tag	UNP P0DTC2
A	1298	SER	-	expression tag	UNP P0DTC2
A	1299	SER	-	expression tag	UNP P0DTC2
A	1300	ALA	-	expression tag	UNP P0DTC2
A	1301	TRP	-	expression tag	UNP P0DTC2
A	1302	SER	-	expression tag	UNP P0DTC2
A	1303	HIS	-	expression tag	UNP P0DTC2
A	1304	PRO	-	expression tag	UNP P0DTC2
A	1305	GLN	-	expression tag	UNP P0DTC2
A	1306	PHE	-	expression tag	UNP P0DTC2
A	1307	GLU	-	expression tag	UNP P0DTC2
A	1308	LYS	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	570	ASP	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	716	ILE	THR	conflict	UNP P0DTC2
B	982	ALA	SER	conflict	UNP P0DTC2
B	1118	HIS	ASP	conflict	UNP P0DTC2
B	1274	SER	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	GLY	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	SER	-	expression tag	UNP P0DTC2
B	1279	ALA	-	expression tag	UNP P0DTC2
B	1280	TRP	-	expression tag	UNP P0DTC2
B	1281	SER	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	PRO	-	expression tag	UNP P0DTC2
B	1284	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1285	PHE	-	expression tag	UNP P0DTC2
B	1286	GLU	-	expression tag	UNP P0DTC2
B	1287	LYS	-	expression tag	UNP P0DTC2
B	1288	GLY	-	expression tag	UNP P0DTC2
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	GLY	-	expression tag	UNP P0DTC2
B	1291	SER	-	expression tag	UNP P0DTC2
B	1292	GLY	-	expression tag	UNP P0DTC2
B	1293	GLY	-	expression tag	UNP P0DTC2
B	1294	GLY	-	expression tag	UNP P0DTC2
B	1295	SER	-	expression tag	UNP P0DTC2
B	1296	GLY	-	expression tag	UNP P0DTC2
B	1297	GLY	-	expression tag	UNP P0DTC2
B	1298	SER	-	expression tag	UNP P0DTC2
B	1299	SER	-	expression tag	UNP P0DTC2
B	1300	ALA	-	expression tag	UNP P0DTC2
B	1301	TRP	-	expression tag	UNP P0DTC2
B	1302	SER	-	expression tag	UNP P0DTC2
B	1303	HIS	-	expression tag	UNP P0DTC2
B	1304	PRO	-	expression tag	UNP P0DTC2
B	1305	GLN	-	expression tag	UNP P0DTC2
B	1306	PHE	-	expression tag	UNP P0DTC2
B	1307	GLU	-	expression tag	UNP P0DTC2
B	1308	LYS	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	570	ASP	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	716	ILE	THR	conflict	UNP P0DTC2
C	982	ALA	SER	conflict	UNP P0DTC2
C	1118	HIS	ASP	conflict	UNP P0DTC2
C	1274	SER	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	GLY	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	SER	-	expression tag	UNP P0DTC2
C	1279	ALA	-	expression tag	UNP P0DTC2
C	1280	TRP	-	expression tag	UNP P0DTC2
C	1281	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	PRO	-	expression tag	UNP P0DTC2
C	1284	GLN	-	expression tag	UNP P0DTC2
C	1285	PHE	-	expression tag	UNP P0DTC2
C	1286	GLU	-	expression tag	UNP P0DTC2
C	1287	LYS	-	expression tag	UNP P0DTC2
C	1288	GLY	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2
C	1290	GLY	-	expression tag	UNP P0DTC2
C	1291	SER	-	expression tag	UNP P0DTC2
C	1292	GLY	-	expression tag	UNP P0DTC2
C	1293	GLY	-	expression tag	UNP P0DTC2
C	1294	GLY	-	expression tag	UNP P0DTC2
C	1295	SER	-	expression tag	UNP P0DTC2
C	1296	GLY	-	expression tag	UNP P0DTC2
C	1297	GLY	-	expression tag	UNP P0DTC2
C	1298	SER	-	expression tag	UNP P0DTC2
C	1299	SER	-	expression tag	UNP P0DTC2
C	1300	ALA	-	expression tag	UNP P0DTC2
C	1301	TRP	-	expression tag	UNP P0DTC2
C	1302	SER	-	expression tag	UNP P0DTC2
C	1303	HIS	-	expression tag	UNP P0DTC2
C	1304	PRO	-	expression tag	UNP P0DTC2
C	1305	GLN	-	expression tag	UNP P0DTC2
C	1306	PHE	-	expression tag	UNP P0DTC2
C	1307	GLU	-	expression tag	UNP P0DTC2
C	1308	LYS	-	expression tag	UNP P0DTC2

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



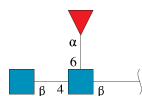
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		

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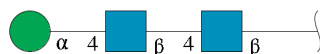
Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	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		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
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		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



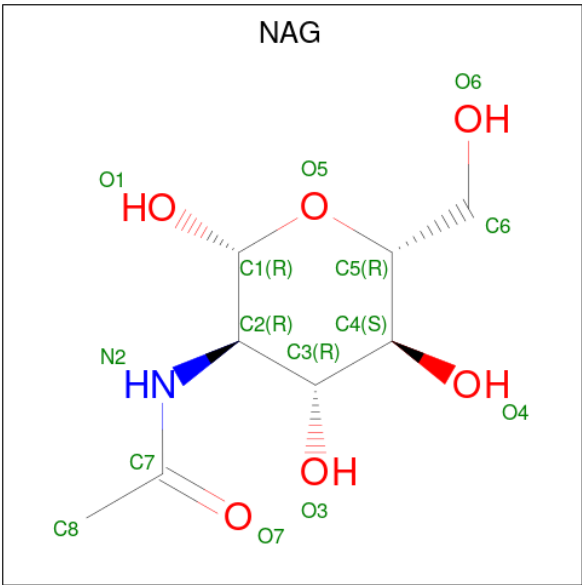
Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	3	Total	C	N	O	0	0
			38	22	2	14		
3	W	3	Total	C	N	O	0	0
			38	22	2	14		
3	h	3	Total	C	N	O	0	0
			38	22	2	14		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	3	Total	C	N	O	0	0
			39	22	2	15		
4	N	3	Total	C	N	O	0	0
			39	22	2	15		
4	X	3	Total	C	N	O	0	0
			39	22	2	15		
4	Y	3	Total	C	N	O	0	0
			39	22	2	15		
4	i	3	Total	C	N	O	0	0
			39	22	2	15		
4	j	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

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

GLU GLN TYR ILE LYS TRP PRO TRP TYR ILE TRP LEU GLY PHE ILE ILE GLY PRO GLN PHE ILE ILE VAL MET VAL THR ILE MET GLY LEU CYS CYS MET THR SER CYS TRP SER CYS LEU LYS GLY CYS SER CYS GLY SER CYS LYS PHE ASP GLU ASP ASP SER GLU PRO VAL LEU LYS

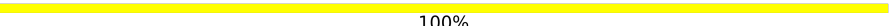
GLY VAL LYS LEU HIS TRP THR SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY VAL GLY VAL SER GLY GLY SER GLY SER SER ALA TRP SER HIS PRO GLN PHE GLU LYS

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

Chain D:  50% 50%

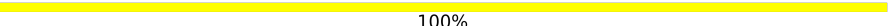
MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

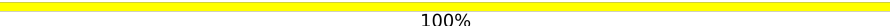
MAG1
MAG2

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

Chain G:  50% 50% 50%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

- 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 O:  100%



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

Chain P:  50% 50%



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

Chain Q:  100%



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

Chain R:  50% 100%



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



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



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



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



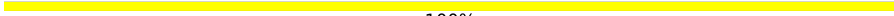
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain b:  100%

MAG1
MAG2

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

Chain c:  50% 100%

MAG1
MAG2

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

Chain d:  100%

MAG1
MAG2

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

Chain e:  50% 50%

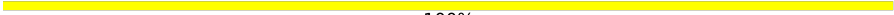
MAG1
MAG2

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

Chain f:  100%

MAG1
MAG2

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

Chain g:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33% 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



MAG1
MAG2
MAN3

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

Chain i:  100%

MAG1
MAG2
MAN3

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

Chain j:  100%

MAG1
MAG2
MAN3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41138	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 ($e^-/\text{\AA}^2$)	53.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.279	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	396.03217, 396.03217, 396.03217	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825067, 0.825067, 0.825067	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.67	0/8616	1.23	17/11718 (0.1%)
1	B	0.68	0/8616	1.23	17/11718 (0.1%)
1	C	0.68	1/8616 (0.0%)	1.23	23/11718 (0.2%)
All	All	0.68	1/25848 (0.0%)	1.23	57/35154 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	792	PRO	CA-C	5.15	1.54	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1107	ARG	N-CA-C	8.66	123.59	112.34
1	C	1074	ASN	OD1-CG-ND2	-8.39	114.21	122.60
1	B	1074	ASN	OD1-CG-ND2	-8.37	114.23	122.60
1	C	1107	ARG	N-CA-C	8.29	123.12	112.34
1	B	214	ARG	N-CA-C	8.10	122.64	112.03
1	C	96	GLU	N-CA-C	8.03	121.25	109.69
1	A	1074	ASN	OD1-CG-ND2	-7.67	114.93	122.60
1	B	1126	CYS	N-CA-C	7.46	121.80	113.21
1	C	1074	ASN	CB-CG-ND2	7.40	127.50	116.40
1	B	745	ASP	CA-CB-CG	7.31	119.91	112.60
1	B	1074	ASN	CB-CG-ND2	7.21	127.21	116.40
1	B	983	ARG	N-CA-C	6.94	121.58	113.18
1	A	1074	ASN	CB-CG-ND2	6.74	126.51	116.40
1	B	488	CYS	N-CA-C	-6.69	98.34	109.24
1	C	336	CYS	CA-C-N	6.55	128.03	119.84
1	C	336	CYS	C-N-CA	6.55	128.03	119.84
1	A	125	ASN	CA-CB-CG	6.42	119.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ASN	CA-CB-CG	6.42	119.02	112.60
1	C	1126	CYS	N-CA-C	6.38	120.79	113.19
1	C	979	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	559	PHE	CA-CB-CG	6.33	120.13	113.80
1	B	80	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	743	CYS	N-CA-C	6.25	120.95	112.88
1	C	32	PHE	CA-CB-CG	6.05	119.85	113.80
1	C	331	ASN	CB-CG-ND2	-5.96	107.47	116.40
1	C	125	ASN	CA-CB-CG	5.87	118.47	112.60
1	C	122	ASN	CA-CB-CG	5.50	118.10	112.60
1	C	80	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	159	VAL	N-CA-C	-5.45	108.53	113.71
1	A	159	VAL	N-CA-C	-5.45	108.54	113.71
1	C	985	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	40	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	1146	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	1091	ARG	N-CA-C	-5.39	105.10	110.97
1	C	559	PHE	CA-CB-CG	5.38	119.19	113.80
1	A	80	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	559	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	1126	CYS	N-CA-C	5.29	122.07	110.80
1	C	438	SER	CA-C-N	5.26	127.59	120.38
1	C	438	SER	C-N-CA	5.26	127.59	120.38
1	C	291	CYS	N-CA-C	5.25	119.17	112.34
1	A	66	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	C	449	TYR	CA-C-N	5.21	128.24	120.31
1	C	449	TYR	C-N-CA	5.21	128.24	120.31
1	C	617	CYS	N-CA-C	5.17	118.37	111.75
1	A	1054	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	C	331	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	B	138	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	138	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	291	CYS	N-CA-C	5.10	118.97	112.34
1	B	438	SER	CA-C-N	5.08	128.44	120.82
1	B	438	SER	C-N-CA	5.08	128.44	120.82
1	A	480	CYS	N-CA-C	5.04	116.27	107.49
1	A	185	ASN	CA-C-N	5.04	128.48	121.02
1	A	185	ASN	C-N-CA	5.04	128.48	121.02
1	C	1113	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	B	17	ASN	CA-CB-CG	5.03	117.63	112.60

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	8421	0	8222	115	0
1	B	8421	0	8228	113	0
1	C	8421	0	8222	113	0
2	D	28	0	25	6	0
2	E	28	0	25	4	0
2	F	28	0	25	2	0
2	G	28	0	25	5	0
2	H	28	0	25	0	0
2	I	28	0	25	2	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	O	28	0	25	2	0
2	P	28	0	25	4	0
2	Q	28	0	25	2	0
2	R	28	0	25	4	0
2	S	28	0	25	0	0
2	T	28	0	25	1	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	6	0
2	b	28	0	25	2	0
2	c	28	0	25	3	0
2	d	28	0	25	0	0
2	e	28	0	25	5	0
2	f	28	0	25	0	0
2	g	28	0	25	0	0
3	L	38	0	34	0	0
3	W	38	0	34	0	0
3	h	38	0	34	0	0
4	M	39	0	34	0	0
4	N	39	0	34	0	0
4	X	39	0	34	0	0
4	Y	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	i	39	0	34	0	0
4	j	39	0	34	0	0
5	A	112	0	104	8	0
5	B	112	0	104	12	0
5	C	112	0	104	7	0
All	All	26619	0	25890	325	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (325) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASN:HD21	2:Q:1:NAG:C1	0.98	1.58
1:B:17:ASN:ND2	2:O:1:NAG:C1	1.68	1.56
1:B:331:ASN:HD21	5:B:1403:NAG:C1	1.14	1.55
1:C:616:ASN:HD21	2:e:1:NAG:C1	1.20	1.53
1:A:165:ASN:HD21	2:F:1:NAG:C1	1.15	1.52
1:B:454:ARG:HD3	1:B:492:LEU:CD1	1.38	1.50
1:A:17:ASN:HD21	2:D:1:NAG:C1	1.24	1.48
1:B:149:ASN:ND2	5:B:1402:NAG:C1	1.74	1.48
1:C:616:ASN:ND2	2:e:1:NAG:C1	1.75	1.48
1:B:331:ASN:ND2	5:B:1403:NAG:C1	1.73	1.45
1:B:234:ASN:HD21	2:R:1:NAG:C1	1.25	1.45
1:B:165:ASN:ND2	2:Q:1:NAG:C1	1.82	1.37
1:A:234:ASN:HD21	2:G:1:NAG:C1	1.36	1.36
1:B:454:ARG:CD	1:B:492:LEU:CD1	2.04	1.35
1:B:1158:ASN:HD21	5:B:1408:NAG:C1	1.38	1.34
1:A:1158:ASN:HD21	5:A:1408:NAG:C1	1.39	1.33
1:C:122:ASN:ND2	2:a:1:NAG:C1	1.94	1.30
1:C:149:ASN:HD21	5:C:1402:NAG:C1	1.45	1.29
1:A:17:ASN:ND2	2:D:1:NAG:C1	1.92	1.28
1:A:122:ASN:ND2	2:E:1:NAG:C1	1.97	1.27
1:B:343:ASN:ND2	5:B:1404:NAG:C1	1.98	1.26
1:C:343:ASN:ND2	5:C:1404:NAG:C1	1.98	1.26
1:A:165:ASN:ND2	2:F:1:NAG:C1	1.96	1.26
1:B:234:ASN:ND2	2:R:1:NAG:C1	2.00	1.24
1:C:15:CYS:SG	1:C:136:CYS:HA	1.78	1.23
1:C:343:ASN:HD21	5:C:1404:NAG:C1	1.48	1.23
1:A:140:PHE:CE2	1:A:244:LEU:CD1	2.22	1.22
1:B:149:ASN:HD22	5:B:1402:NAG:C1	1.42	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASN:HD21	5:B:1404:NAG:C1	1.51	1.21
1:C:149:ASN:ND2	5:C:1402:NAG:C1	2.02	1.20
1:A:149:ASN:ND2	5:A:1402:NAG:C1	2.04	1.20
1:A:122:ASN:HD21	2:E:1:NAG:C1	1.53	1.19
1:B:1158:ASN:ND2	5:B:1408:NAG:C1	2.05	1.19
1:B:454:ARG:CD	1:B:492:LEU:HD11	1.69	1.17
1:A:234:ASN:ND2	2:G:1:NAG:C1	2.05	1.17
1:B:453:TYR:CD2	1:B:495:TYR:CZ	2.33	1.17
1:A:343:ASN:HD21	5:A:1404:NAG:C1	1.59	1.14
1:B:454:ARG:CD	1:B:492:LEU:HD13	1.69	1.14
1:C:15:CYS:HA	1:C:136:CYS:SG	1.87	1.13
1:B:122:ASN:ND2	2:P:1:NAG:C1	2.12	1.13
1:A:15:CYS:HA	1:A:136:CYS:SG	1.89	1.12
1:C:472:ILE:HG21	1:C:488:CYS:SG	1.89	1.11
1:A:141:LEU:CD1	1:A:241:LEU:CD1	2.29	1.11
1:A:662:CYS:SG	1:A:697:MET:HE3	1.92	1.09
1:B:454:ARG:HD2	1:B:492:LEU:HD13	1.27	1.08
1:A:1158:ASN:ND2	5:A:1408:NAG:C1	2.17	1.07
1:A:343:ASN:ND2	5:A:1404:NAG:C1	2.15	1.07
1:A:129:LYS:HE2	1:A:169:GLU:HB3	1.34	1.07
1:A:149:ASN:HD22	5:A:1402:NAG:C1	1.63	1.07
1:A:140:PHE:CE2	1:A:244:LEU:HD11	1.86	1.06
1:B:454:ARG:NE	1:B:492:LEU:HD21	1.72	1.03
1:C:122:ASN:HD21	2:a:1:NAG:C1	1.61	1.03
1:A:140:PHE:CE2	1:A:244:LEU:HD12	1.91	1.03
1:C:165:ASN:HD21	2:b:1:NAG:C1	1.72	1.02
1:C:472:ILE:CG2	1:C:488:CYS:SG	2.48	1.00
1:A:662:CYS:SG	1:A:697:MET:CE	2.51	0.98
1:A:662:CYS:SG	1:A:697:MET:SD	2.61	0.98
1:C:19:THR:O	1:C:21:ARG:HD3	1.65	0.97
1:C:165:ASN:ND2	2:b:1:NAG:C1	2.28	0.97
1:A:904:TYR:OH	1:B:1094:VAL:HB	1.66	0.96
1:B:149:ASN:HD21	5:B:1402:NAG:C1	1.62	0.95
1:B:351:TYR:HB2	1:B:454:ARG:HH21	1.32	0.95
1:B:454:ARG:NE	1:B:492:LEU:CD2	2.31	0.94
1:B:453:TYR:HD2	1:B:495:TYR:CE1	1.87	0.92
1:A:141:LEU:HD12	1:A:241:LEU:HD13	1.49	0.92
1:A:140:PHE:CD2	1:A:244:LEU:CD1	2.54	0.91
1:C:396:TYR:HB2	1:C:514:SER:OG	1.71	0.91
1:A:17:ASN:CG	2:D:1:NAG:C1	2.43	0.90
1:A:140:PHE:CD2	1:A:244:LEU:HG	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASN:CG	5:B:1403:NAG:C1	2.44	0.90
1:A:1107:ARG:HD3	1:C:904:TYR:CZ	2.07	0.89
1:B:351:TYR:CD2	1:B:454:ARG:NH2	2.41	0.89
1:A:141:LEU:HD13	1:A:241:LEU:CD1	2.01	0.88
1:B:904:TYR:OH	1:C:1094:VAL:HB	1.74	0.88
1:B:122:ASN:HD21	2:P:1:NAG:C1	1.87	0.88
1:A:141:LEU:CD1	1:A:241:LEU:HD13	1.99	0.88
1:B:357:ARG:HG2	1:B:357:ARG:HH11	1.37	0.86
1:C:122:ASN:HD22	2:a:1:NAG:C1	1.83	0.86
1:A:662:CYS:SG	1:A:697:MET:CB	2.63	0.86
1:B:454:ARG:CZ	1:B:492:LEU:HD21	2.05	0.86
1:C:140:PHE:CE2	1:C:158:ARG:HD2	2.11	0.84
1:A:140:PHE:CD2	1:A:244:LEU:CG	2.59	0.84
1:A:140:PHE:HD2	1:A:244:LEU:HG	1.42	0.84
1:B:453:TYR:CD2	1:B:495:TYR:CE1	2.64	0.84
1:C:149:ASN:ND2	5:C:1402:NAG:O5	2.03	0.83
1:B:122:ASN:HD22	2:P:1:NAG:C1	1.89	0.83
1:C:140:PHE:CZ	1:C:158:ARG:HD2	2.12	0.83
1:A:15:CYS:CA	1:A:136:CYS:SG	2.67	0.82
2:P:1:NAG:H61	2:P:2:NAG:C7	2.09	0.82
1:B:17:ASN:HD22	2:O:1:NAG:C1	1.90	0.81
1:A:97:LYS:NZ	1:A:183:GLN:O	2.12	0.81
1:A:140:PHE:CD2	1:A:244:LEU:HD11	2.13	0.81
1:B:453:TYR:HD2	1:B:495:TYR:CZ	1.96	0.81
1:C:743:CYS:O	1:C:977:LEU:CD2	2.29	0.80
1:A:149:ASN:HD21	5:A:1402:NAG:C1	1.93	0.80
1:A:17:ASN:OD1	2:D:1:NAG:C1	2.29	0.80
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.15	0.79
1:A:122:ASN:HD22	2:E:1:NAG:C1	1.93	0.79
1:B:454:ARG:HD3	1:B:492:LEU:HD11	0.81	0.79
1:A:141:LEU:CD1	1:A:241:LEU:HD11	2.13	0.78
1:A:1107:ARG:HD3	1:C:904:TYR:CE1	2.18	0.77
1:A:140:PHE:HE2	1:A:244:LEU:HD12	1.47	0.77
1:C:140:PHE:CZ	1:C:158:ARG:CD	2.68	0.77
1:B:234:ASN:HD21	2:R:1:NAG:C2	1.98	0.77
1:C:28:TYR:CE2	5:C:1401:NAG:H5	2.19	0.77
1:A:1107:ARG:CD	1:C:904:TYR:CE1	2.67	0.76
1:A:129:LYS:HE2	1:A:169:GLU:CB	2.13	0.76
1:A:662:CYS:SG	1:A:697:MET:HB2	2.24	0.76
1:C:617:CYS:HG	1:C:649:CYS:HG	0.76	0.75
1:C:34:ARG:HH11	1:C:191:GLU:CD	1.95	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:ILE:HD11	1:C:904:TYR:HE2	1.51	0.74
1:A:17:ASN:HD21	2:D:1:NAG:C2	1.97	0.74
1:C:1082:CYS:HG	1:C:1126:CYS:HG	0.89	0.74
1:C:15:CYS:HA	1:C:136:CYS:HG	1.45	0.74
1:B:129:LYS:HE2	1:B:169:GLU:CG	2.17	0.74
1:A:141:LEU:HD12	1:A:241:LEU:CD1	2.07	0.73
1:B:453:TYR:CE2	1:B:495:TYR:CE2	2.78	0.72
1:B:357:ARG:HG2	1:B:357:ARG:NH1	1.98	0.71
1:C:472:ILE:HG22	1:C:488:CYS:SG	2.29	0.71
1:A:45:SER:O	1:A:47:VAL:HG23	1.91	0.71
1:C:15:CYS:CA	1:C:136:CYS:HG	2.04	0.70
1:B:453:TYR:CE2	1:B:495:TYR:CZ	2.80	0.70
1:A:669:GLY:HA2	1:C:869:MET:HE1	1.73	0.70
1:B:391:CYS:HB2	1:B:544:ASN:O	1.92	0.70
1:A:141:LEU:HD13	1:A:241:LEU:HD11	1.72	0.70
1:C:200:TYR:HB2	1:C:202:LYS:HZ3	1.56	0.69
1:C:329:PHE:CE1	1:C:525:CYS:SG	2.86	0.69
1:A:662:CYS:SG	1:A:697:MET:HB3	2.32	0.69
1:C:474:GLN:NE2	1:C:480:CYS:SG	2.65	0.69
1:B:351:TYR:HD2	1:B:454:ARG:NH2	1.91	0.69
1:B:1082:CYS:HG	1:B:1126:CYS:HG	0.97	0.69
1:B:322:PRO:HA	1:B:538:CYS:SG	2.33	0.68
1:B:351:TYR:CB	1:B:454:ARG:HH21	2.04	0.68
1:C:15:CYS:HG	1:C:136:CYS:HA	1.58	0.68
1:C:353:TRP:CE2	1:C:466:ARG:HG3	2.28	0.68
1:B:1082:CYS:CB	1:B:1126:CYS:HG	2.07	0.67
1:B:854:LYS:O	1:B:856:ASN:N	2.25	0.66
1:C:19:THR:C	1:C:21:ARG:HD3	2.20	0.66
1:B:351:TYR:HB2	1:B:454:ARG:NH2	2.10	0.66
1:A:869:MET:HE1	1:B:669:GLY:HA2	1.76	0.65
1:C:336:CYS:HB3	1:C:337:PRO:HD2	1.77	0.65
1:C:616:ASN:HD22	2:e:1:NAG:C1	2.00	0.65
1:C:15:CYS:CB	1:C:136:CYS:HG	2.08	0.65
1:C:742:ILE:HA	1:C:1000:ARG:HD3	1.78	0.65
1:B:480:CYS:HG	1:B:488:CYS:HG	1.44	0.65
1:C:322:PRO:HA	1:C:538:CYS:SG	2.36	0.65
1:B:351:TYR:HD2	1:B:454:ARG:HH22	1.45	0.64
1:C:15:CYS:SG	1:C:136:CYS:CA	2.71	0.64
1:A:1094:VAL:HB	1:C:904:TYR:OH	1.97	0.64
1:A:403:ARG:NH2	1:A:505:TYR:CE1	2.65	0.64
1:B:454:ARG:NH1	1:B:469:SER:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:CYS:O	1:C:977:LEU:HD23	1.97	0.63
1:A:14:GLN:O	1:A:136:CYS:SG	2.56	0.63
1:A:617:CYS:SG	1:A:642:VAL:HG12	2.39	0.63
1:B:357:ARG:HB2	1:B:396:TYR:HE2	1.63	0.63
1:B:453:TYR:CD2	1:B:495:TYR:OH	2.51	0.63
1:C:1082:CYS:CB	1:C:1126:CYS:HG	2.11	0.63
1:A:1156:PHE:CZ	1:C:1155:TYR:HB3	2.34	0.62
1:C:147:LYS:C	1:C:149:ASN:H	2.07	0.62
1:B:983:ARG:O	1:C:382:VAL:HA	2.00	0.62
1:A:391:CYS:SG	1:A:525:CYS:HB2	2.39	0.61
1:A:462:LYS:HZ1	2:c:1:NAG:H83	1.65	0.61
1:A:1082:CYS:HG	1:A:1126:CYS:HG	0.61	0.61
1:C:395:VAL:HG12	1:C:395:VAL:O	2.00	0.61
1:C:353:TRP:NE1	1:C:466:ARG:HG3	2.16	0.61
1:C:15:CYS:CA	1:C:136:CYS:SG	2.77	0.60
1:A:15:CYS:CB	1:A:136:CYS:SG	2.90	0.60
1:A:129:LYS:CD	1:A:169:GLU:HG3	2.32	0.60
1:B:454:ARG:HD2	1:B:492:LEU:CD1	1.99	0.60
1:B:869:MET:HE1	1:C:669:GLY:CA	2.32	0.60
1:B:866:THR:H	1:B:869:MET:HE3	1.67	0.59
1:C:21:ARG:HH11	1:C:21:ARG:CG	2.15	0.59
1:A:108:THR:O	1:A:108:THR:HG23	2.03	0.59
1:A:617:CYS:SG	1:A:642:VAL:CG1	2.91	0.59
1:B:454:ARG:HE	1:B:492:LEU:CD2	2.16	0.59
1:A:140:PHE:CZ	1:A:244:LEU:HD11	2.36	0.59
1:C:471:GLU:N	1:C:471:GLU:OE1	2.34	0.58
1:C:196:ASN:HD21	1:C:235:ILE:HD12	1.67	0.58
1:C:140:PHE:CZ	1:C:158:ARG:HD3	2.37	0.58
1:B:78:ARG:HH11	1:B:78:ARG:HG2	1.69	0.58
1:A:329:PHE:CE2	1:A:525:CYS:SG	2.96	0.57
1:B:336:CYS:HG	1:B:361:CYS:CB	2.16	0.57
1:B:336:CYS:HG	1:B:361:CYS:HG	0.85	0.57
1:B:454:ARG:NE	1:B:492:LEU:HD22	2.18	0.57
1:C:329:PHE:HD1	1:C:525:CYS:HG	1.41	0.57
1:C:391:CYS:SG	1:C:525:CYS:CB	2.92	0.57
1:B:331:ASN:ND2	5:B:1403:NAG:O5	2.37	0.57
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.87	0.57
1:C:854:LYS:O	1:C:856:ASN:N	2.32	0.57
1:A:109:THR:OG1	1:A:114:THR:OG1	2.18	0.57
1:B:129:LYS:HE2	1:B:169:GLU:HG2	1.86	0.56
1:C:431:GLY:HA2	1:C:515:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:TYR:CE2	1:B:1107:ARG:NH1	2.73	0.56
1:B:454:ARG:CD	1:B:492:LEU:CD2	2.81	0.56
1:B:462:LYS:NZ	2:G:1:NAG:H83	2.21	0.56
1:C:329:PHE:CD1	1:C:525:CYS:SG	2.87	0.56
1:C:738:CYS:SG	1:C:760:CYS:O	2.64	0.55
1:A:129:LYS:HD3	1:A:169:GLU:HG3	1.88	0.55
1:C:96:GLU:OE2	1:C:101:ILE:HG12	2.07	0.55
1:C:34:ARG:O	1:C:56:LEU:HD23	2.07	0.55
1:C:34:ARG:NH1	1:C:191:GLU:CD	2.63	0.55
1:B:480:CYS:CB	1:B:488:CYS:SG	2.95	0.55
1:A:1107:ARG:NE	1:C:904:TYR:CE1	2.75	0.55
1:A:854:LYS:C	1:B:589:PRO:HG3	2.32	0.54
1:A:1156:PHE:CE2	1:C:1155:TYR:HB3	2.42	0.54
1:C:332:ILE:HG21	1:C:361:CYS:HA	1.88	0.54
1:A:336:CYS:HB3	1:A:337:PRO:HD2	1.89	0.54
1:C:743:CYS:O	1:C:977:LEU:HD22	2.08	0.54
1:B:15:CYS:SG	1:B:136:CYS:CB	2.96	0.53
1:C:569:ILE:H	1:C:569:ILE:HD12	1.74	0.53
1:C:129:LYS:HE2	2:a:1:NAG:H62	1.90	0.53
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.09	0.53
2:D:1:NAG:H62	2:D:2:NAG:C7	2.39	0.52
1:C:140:PHE:HZ	1:C:158:ARG:CD	2.20	0.52
1:A:854:LYS:O	1:B:589:PRO:HG3	2.10	0.52
1:A:45:SER:O	1:A:47:VAL:CG2	2.58	0.52
1:C:391:CYS:SG	1:C:525:CYS:HB2	2.50	0.52
1:B:357:ARG:NH1	1:B:359:SER:HB3	2.25	0.52
1:B:357:ARG:HB2	1:B:396:TYR:CE2	2.43	0.52
1:C:480:CYS:HG	1:C:488:CYS:HG	1.24	0.51
1:A:404:GLY:HA3	1:A:508:TYR:CD1	2.45	0.51
1:A:391:CYS:HG	1:A:525:CYS:CB	2.24	0.51
1:C:102:ARG:HA	1:C:102:ARG:NE	2.26	0.51
1:C:200:TYR:HD2	1:C:228:ASP:OD1	1.95	0.50
1:B:748:GLU:CD	1:B:748:GLU:H	2.20	0.50
1:B:904:TYR:HH	1:C:1094:VAL:HB	1.76	0.50
1:C:343:ASN:CG	5:C:1404:NAG:C1	2.80	0.50
1:B:357:ARG:HH11	1:B:357:ARG:CG	2.14	0.49
1:B:480:CYS:CB	1:B:488:CYS:HG	2.25	0.49
1:B:129:LYS:HE2	1:B:169:GLU:HB3	1.94	0.49
1:C:149:ASN:C	1:C:151:SER:H	2.19	0.49
1:C:156:GLU:HB3	1:C:158:ARG:HG3	1.94	0.49
1:A:141:LEU:HD13	1:A:241:LEU:HD12	1.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:CYS:SG	1:A:526:GLY:N	2.85	0.49
1:A:343:ASN:CG	5:A:1404:NAG:C1	2.84	0.49
1:A:865:LEU:HA	1:A:869:MET:HE3	1.94	0.49
1:B:129:LYS:CE	1:B:169:GLU:HG2	2.42	0.49
1:A:903:ALA:HB1	1:A:913:GLN:HB2	1.95	0.49
1:B:129:LYS:HE2	1:B:169:GLU:CB	2.43	0.48
1:C:865:LEU:HA	1:C:869:MET:HE3	1.95	0.48
1:A:904:TYR:CE1	1:B:1107:ARG:HD3	2.48	0.48
1:C:21:ARG:CG	1:C:21:ARG:NH1	2.74	0.48
1:A:437:ASN:HB2	1:A:508:TYR:CZ	2.49	0.48
1:B:34:ARG:O	1:B:56:LEU:HD23	2.14	0.48
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.13	0.48
1:B:738:CYS:SG	1:B:760:CYS:O	2.72	0.48
1:C:21:ARG:HH11	1:C:21:ARG:HG2	1.78	0.48
1:A:129:LYS:CE	1:A:169:GLU:HB3	2.25	0.48
1:A:408:ARG:O	1:A:414:GLN:NE2	2.44	0.48
1:B:343:ASN:CG	5:B:1404:NAG:C1	2.80	0.48
1:B:869:MET:HE1	1:C:669:GLY:HA2	1.97	0.47
1:C:149:ASN:C	1:C:151:SER:N	2.70	0.47
1:B:129:LYS:HZ3	1:B:169:GLU:HG2	1.79	0.47
1:C:322:PRO:CA	1:C:538:CYS:SG	3.02	0.47
1:A:404:GLY:CA	1:A:508:TYR:CD1	2.98	0.46
2:e:1:NAG:H62	2:e:2:NAG:C7	2.45	0.46
1:A:901:GLN:O	1:A:905:ARG:HG2	2.15	0.46
1:C:336:CYS:CB	1:C:337:PRO:HD2	2.45	0.46
1:A:141:LEU:CD1	1:A:241:LEU:HD12	2.40	0.46
2:I:1:NAG:H62	2:I:2:NAG:C7	2.45	0.46
1:B:281:GLU:CD	1:B:281:GLU:H	2.24	0.45
1:C:395:VAL:CG2	1:C:524:VAL:HG11	2.45	0.45
1:A:1050:MET:HE2	1:A:1052:PHE:CE1	2.52	0.45
1:A:1107:ARG:CD	1:C:904:TYR:CZ	2.87	0.45
1:A:462:LYS:NZ	2:c:1:NAG:H83	2.29	0.45
1:A:669:GLY:CA	1:C:869:MET:HE1	2.43	0.45
1:B:380:TYR:CE2	1:B:412:PRO:HD3	2.51	0.45
1:B:462:LYS:HZ3	2:G:1:NAG:H83	1.80	0.45
1:B:332:ILE:HG21	1:B:361:CYS:HA	1.98	0.45
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.66	0.45
1:C:21:ARG:NH1	1:C:23:GLN:HE22	2.15	0.44
1:A:391:CYS:HB2	1:A:544:ASN:O	2.18	0.44
1:A:592:PHE:CD2	1:C:740:MET:HE1	2.53	0.44
1:A:403:ARG:CZ	1:A:505:TYR:CD1	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LYS:HD3	2:a:2:NAG:C8	2.47	0.44
2:G:1:NAG:H62	2:G:2:NAG:H82	1.99	0.44
1:A:129:LYS:CD	1:A:169:GLU:CG	2.96	0.44
1:C:95:THR:O	1:C:186:PHE:CD1	2.71	0.44
1:A:124:THR:HB	2:E:1:NAG:H82	1.99	0.44
1:C:15:CYS:HG	1:C:136:CYS:CA	2.25	0.43
1:C:15:CYS:HG	1:C:136:CYS:CB	2.31	0.43
2:I:1:NAG:H62	2:I:2:NAG:H82	2.00	0.43
1:A:391:CYS:SG	1:A:525:CYS:CB	3.04	0.43
2:e:1:NAG:H62	2:e:2:NAG:H82	2.00	0.43
1:C:21:ARG:HH11	1:C:23:GLN:HE22	1.66	0.43
1:C:129:LYS:HD3	2:a:2:NAG:H81	2.01	0.43
1:C:395:VAL:HG23	1:C:524:VAL:CG1	2.46	0.43
1:A:403:ARG:CZ	1:A:505:TYR:CE1	3.01	0.43
1:B:453:TYR:HE2	1:B:495:TYR:CE2	2.33	0.43
1:B:351:TYR:CG	1:B:454:ARG:NH2	2.86	0.43
1:B:78:ARG:HG2	1:B:78:ARG:NH1	2.33	0.43
1:A:159:VAL:HG23	1:A:160:TYR:CD1	2.54	0.43
1:A:1082:CYS:CB	1:A:1126:CYS:HG	2.25	0.43
1:B:157:PHE:O	1:B:157:PHE:CD1	2.72	0.43
1:B:216:LEU:C	1:B:216:LEU:HD23	2.44	0.43
1:A:157:PHE:O	1:A:157:PHE:CD1	2.72	0.42
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.59	0.42
1:B:454:ARG:HE	1:B:492:LEU:HD22	1.78	0.42
1:B:404:GLY:HA3	1:B:508:TYR:CE1	2.54	0.42
1:C:140:PHE:HZ	1:C:158:ARG:HD3	1.79	0.42
2:T:1:NAG:H62	2:T:2:NAG:H82	2.01	0.42
1:C:858:LEU:HD13	1:C:959:LEU:HD22	2.01	0.42
1:A:662:CYS:HG	1:A:671:CYS:HG	1.61	0.42
1:A:858:LEU:HD13	1:A:959:LEU:HD22	2.01	0.42
1:B:129:LYS:NZ	1:B:169:GLU:HG2	2.35	0.42
1:B:234:ASN:CG	2:R:1:NAG:C1	2.86	0.42
1:C:742:ILE:HG12	1:C:1000:ARG:HB3	2.00	0.42
1:A:156:GLU:C	1:A:158:ARG:H	2.28	0.42
1:B:159:VAL:HG23	1:B:160:TYR:CD1	2.54	0.42
1:B:156:GLU:C	1:B:158:ARG:H	2.28	0.41
1:C:391:CYS:HB2	1:C:544:ASN:O	2.19	0.41
1:A:44:ARG:O	1:A:283:GLY:CA	2.69	0.41
1:B:379:CYS:SG	1:B:384:PRO:HD3	2.61	0.41
1:A:462:LYS:NZ	2:c:1:NAG:C8	2.83	0.41
1:B:36:VAL:HG21	1:B:220:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:MET:HE1	1:C:592:PHE:CG	2.56	0.41
1:B:742:ILE:HA	1:B:1000:ARG:HD3	2.03	0.41
1:C:474:GLN:HE22	1:C:480:CYS:HG	1.68	0.41
1:A:274:THR:HG22	1:A:291:CYS:SG	2.60	0.40
1:B:129:LYS:CE	1:B:169:GLU:CG	2.92	0.40
1:B:453:TYR:CD2	1:B:495:TYR:CE2	2.94	0.40
1:A:474:GLN:NE2	1:A:480:CYS:H	2.19	0.40
1:A:904:TYR:CD1	1:B:1107:ARG:HD3	2.55	0.40
1:A:117:LEU:HD12	1:A:231:ILE:HD12	2.04	0.40
1:C:147:LYS:C	1:C:149:ASN:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1063/1305 (82%)	992 (93%)	69 (6%)	2 (0%)	43	70
1	B	1063/1305 (82%)	992 (93%)	67 (6%)	4 (0%)	30	59
1	C	1063/1305 (82%)	1004 (94%)	57 (5%)	2 (0%)	43	70
All	All	3189/3915 (82%)	2988 (94%)	193 (6%)	8 (0%)	37	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	744	GLY
1	B	855	PHE
1	C	148	ASN
1	C	855	PHE
1	B	744	GLY
1	A	381	GLY
1	B	32	PHE

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Mol	Chain	Res	Type
1	B	381	GLY

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	903/1130 (80%)	890 (99%)	13 (1%)	59	72
1	B	941/1130 (83%)	925 (98%)	16 (2%)	53	70
1	C	941/1130 (83%)	926 (98%)	15 (2%)	55	71
All	All	2785/3390 (82%)	2741 (98%)	44 (2%)	54	71

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	87	ASN
1	A	109	THR
1	A	125	ASN
1	A	136	CYS
1	A	137	ASN
1	A	159	VAL
1	A	241	LEU
1	A	289	VAL
1	A	318	PHE
1	A	391	CYS
1	A	646	ARG
1	A	1107	ARG
1	B	15	CYS
1	B	21	ARG
1	B	24	LEU
1	B	87	ASN
1	B	108	THR
1	B	125	ASN
1	B	137	ASN
1	B	159	VAL

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Mol	Chain	Res	Type
1	B	166	CYS
1	B	289	VAL
1	B	318	PHE
1	B	357	ARG
1	B	396	TYR
1	B	546	LEU
1	B	745	ASP
1	B	854	LYS
1	C	15	CYS
1	C	21	ARG
1	C	24	LEU
1	C	125	ASN
1	C	129	LYS
1	C	136	CYS
1	C	166	CYS
1	C	316	SER
1	C	318	PHE
1	C	319	ARG
1	C	326	ILE
1	C	391	CYS
1	C	466	ARG
1	C	547	THR
1	C	854	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	137	ASN
1	A	149	ASN
1	A	164	ASN
1	A	165	ASN
1	A	234	ASN
1	A	271	GLN
1	A	460	ASN
1	A	474	GLN
1	A	536	ASN
1	A	606	ASN
1	A	751	ASN
1	A	762	GLN
1	A	913	GLN
1	A	1002	GLN

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Mol	Chain	Res	Type
1	A	1010	GLN
1	A	1036	GLN
1	A	1158	ASN
1	B	14	GLN
1	B	23	GLN
1	B	81	ASN
1	B	137	ASN
1	B	149	ASN
1	B	165	ASN
1	B	188	ASN
1	B	234	ASN
1	B	239	GLN
1	B	331	ASN
1	B	343	ASN
1	B	493	GLN
1	B	536	ASN
1	B	544	ASN
1	B	564	GLN
1	B	606	ASN
1	B	675	GLN
1	B	690	GLN
1	B	762	GLN
1	B	1002	GLN
1	B	1058	HIS
1	B	1158	ASN
1	C	23	GLN
1	C	121	ASN
1	C	137	ASN
1	C	165	ASN
1	C	196	ASN
1	C	343	ASN
1	C	474	GLN
1	C	493	GLN
1	C	536	ASN
1	C	540	ASN
1	C	544	ASN
1	C	606	ASN
1	C	616	ASN
1	C	762	GLN
1	C	764	ASN
1	C	804	GLN
1	C	957	GLN

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Mol	Chain	Res	Type
1	C	969	ASN
1	C	1002	GLN
1	C	1058	HIS
1	C	1088	HIS

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 ⓘ

75 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	D	2	2	14,14,15	1.08	1 (7%)	17,19,21	1.00	1 (5%)
2	NAG	E	1	2	14,14,15	0.20	0	17,19,21	0.49	0
2	NAG	E	2	2	14,14,15	1.08	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	F	1	2	14,14,15	0.21	0	17,19,21	0.45	0
2	NAG	F	2	2	14,14,15	1.08	1 (7%)	17,19,21	1.23	1 (5%)
2	NAG	G	1	2	14,14,15	0.29	0	17,19,21	0.42	0
2	NAG	G	2	2	14,14,15	1.06	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	H	1	1,2	14,14,15	1.21	1 (7%)	17,19,21	0.81	1 (5%)
2	NAG	H	2	2	14,14,15	1.30	2 (14%)	17,19,21	0.94	1 (5%)
2	NAG	I	1	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	I	2	2	14,14,15	1.13	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	J	1	1,2	14,14,15	1.22	1 (7%)	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	J	2	2	14,14,15	1.17	1 (7%)	17,19,21	0.81	1 (5%)
2	NAG	K	1	1,2	14,14,15	1.16	1 (7%)	17,19,21	0.85	1 (5%)
2	NAG	K	2	2	14,14,15	1.28	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	L	1	1,3	14,14,15	1.33	3 (21%)	17,19,21	1.01	1 (5%)
3	NAG	L	2	3	14,14,15	1.34	3 (21%)	17,19,21	0.87	1 (5%)
3	FUC	L	3	3	10,10,11	1.65	2 (20%)	14,14,16	1.12	1 (7%)
4	NAG	M	1	1,4	14,14,15	1.19	1 (7%)	17,19,21	0.88	0
4	NAG	M	2	4	14,14,15	1.29	2 (14%)	17,19,21	0.81	1 (5%)
4	MAN	M	3	4	11,11,12	1.39	2 (18%)	15,15,17	0.83	0
4	NAG	N	1	1,4	14,14,15	1.28	2 (14%)	17,19,21	0.92	1 (5%)
4	NAG	N	2	4	14,14,15	1.46	3 (21%)	17,19,21	0.82	0
4	MAN	N	3	4	11,11,12	1.55	2 (18%)	15,15,17	0.78	0
2	NAG	O	1	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	O	2	2	14,14,15	1.11	1 (7%)	17,19,21	0.73	0
2	NAG	P	1	2	14,14,15	0.19	0	17,19,21	0.47	0
2	NAG	P	2	2	14,14,15	1.06	1 (7%)	17,19,21	1.14	1 (5%)
2	NAG	Q	1	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	Q	2	2	14,14,15	1.21	1 (7%)	17,19,21	1.05	1 (5%)
2	NAG	R	1	2	14,14,15	0.29	0	17,19,21	0.42	0
2	NAG	R	2	2	14,14,15	1.11	1 (7%)	17,19,21	1.06	2 (11%)
2	NAG	S	1	1,2	14,14,15	1.32	2 (14%)	17,19,21	0.66	0
2	NAG	S	2	2	14,14,15	1.24	1 (7%)	17,19,21	0.94	1 (5%)
2	NAG	T	1	2	14,14,15	0.24	0	17,19,21	0.43	0
2	NAG	T	2	2	14,14,15	1.16	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	U	1	1,2	14,14,15	1.21	1 (7%)	17,19,21	0.75	0
2	NAG	U	2	2	14,14,15	1.26	1 (7%)	17,19,21	0.78	0
2	NAG	V	1	1,2	14,14,15	1.05	1 (7%)	17,19,21	0.74	0
2	NAG	V	2	2	14,14,15	1.22	1 (7%)	17,19,21	0.70	0
3	NAG	W	1	1,3	14,14,15	1.31	1 (7%)	17,19,21	1.09	1 (5%)
3	NAG	W	2	3	14,14,15	1.31	2 (14%)	17,19,21	0.92	1 (5%)
3	FUC	W	3	3	10,10,11	1.55	2 (20%)	14,14,16	1.09	1 (7%)
4	NAG	X	1	1,4	14,14,15	1.17	1 (7%)	17,19,21	0.87	0
4	NAG	X	2	4	14,14,15	1.25	2 (14%)	17,19,21	0.81	0
4	MAN	X	3	4	11,11,12	1.40	2 (18%)	15,15,17	0.71	0
4	NAG	Y	1	1,4	14,14,15	1.28	2 (14%)	17,19,21	1.09	1 (5%)
4	NAG	Y	2	4	14,14,15	1.38	2 (14%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	Y	3	4	11,11,12	1.50	2 (18%)	15,15,17	0.78	0
2	NAG	Z	1	1,2	14,14,15	1.32	2 (14%)	17,19,21	0.65	0
2	NAG	Z	2	2	14,14,15	1.24	2 (14%)	17,19,21	1.03	2 (11%)
2	NAG	a	1	2	14,14,15	0.18	0	17,19,21	0.49	0
2	NAG	a	2	2	14,14,15	1.08	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	b	1	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	b	2	2	14,14,15	1.07	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	c	1	1,2	14,14,15	0.35	0	17,19,21	0.43	0
2	NAG	c	2	2	14,14,15	1.12	1 (7%)	17,19,21	0.81	0
2	NAG	d	1	1,2	14,14,15	1.30	2 (14%)	17,19,21	1.11	1 (5%)
2	NAG	d	2	2	14,14,15	1.24	2 (14%)	17,19,21	1.01	1 (5%)
2	NAG	e	1	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	e	2	2	14,14,15	1.13	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	f	1	1,2	14,14,15	1.19	1 (7%)	17,19,21	0.58	0
2	NAG	f	2	2	14,14,15	1.20	1 (7%)	17,19,21	0.80	0
2	NAG	g	1	1,2	14,14,15	1.06	1 (7%)	17,19,21	0.63	0
2	NAG	g	2	2	14,14,15	1.17	1 (7%)	17,19,21	1.22	1 (5%)
3	NAG	h	1	1,3	14,14,15	1.23	1 (7%)	17,19,21	0.89	0
3	NAG	h	2	3	14,14,15	1.26	1 (7%)	17,19,21	0.84	1 (5%)
3	FUC	h	3	3	10,10,11	1.59	2 (20%)	14,14,16	1.08	1 (7%)
4	NAG	i	1	1,4	14,14,15	1.15	1 (7%)	17,19,21	0.93	0
4	NAG	i	2	4	14,14,15	1.18	1 (7%)	17,19,21	0.96	0
4	MAN	i	3	4	11,11,12	1.34	1 (9%)	15,15,17	0.84	0
4	NAG	j	1	1,4	14,14,15	1.25	2 (14%)	17,19,21	1.04	2 (11%)
4	NAG	j	2	4	14,14,15	1.45	2 (14%)	17,19,21	0.77	0
4	MAN	j	3	4	11,11,12	1.47	2 (18%)	15,15,17	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2	-	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	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	FUC	L	3	3	-	-	0/1/1/1
4	NAG	M	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	MAN	M	3	4	-	1/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	MAN	N	3	4	-	0/2/19/22	1/1/1/1
2	NAG	O	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	2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	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	2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	FUC	W	3	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	X	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	MAN	X	3	4	-	1/2/19/22	1/1/1/1
4	NAG	Y	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	MAN	Y	3	4	-	0/2/19/22	0/1/1/1
2	NAG	Z	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	NAG	a	1	2	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	NAG	b	1	2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
2	NAG	e	1	2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	NAG	f	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1
2	NAG	g	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
3	NAG	h	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	0/6/23/26	0/1/1/1
3	FUC	h	3	3	-	-	0/1/1/1
4	NAG	i	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1
4	MAN	i	3	4	-	2/2/19/22	0/1/1/1
4	NAG	j	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	j	2	4	-	0/6/23/26	0/1/1/1
4	MAN	j	3	4	-	0/2/19/22	1/1/1/1

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	2	NAG	O5-C5	3.51	1.50	1.43
2	T	2	NAG	O5-C5	3.40	1.50	1.43
4	N	3	MAN	O5-C5	3.30	1.49	1.43
4	Y	3	MAN	O5-C5	3.29	1.49	1.43
4	j	3	MAN	O5-C5	3.23	1.49	1.43
2	R	2	NAG	O5-C5	3.21	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	2	NAG	O5-C5	3.19	1.49	1.43
2	I	2	NAG	O5-C5	3.19	1.49	1.43
2	e	2	NAG	O5-C5	3.17	1.49	1.43
4	j	2	NAG	O5-C5	3.16	1.49	1.43
2	c	2	NAG	O5-C5	3.12	1.49	1.43
2	K	2	NAG	O5-C5	3.11	1.49	1.43
2	O	2	NAG	O5-C5	3.08	1.49	1.43
4	Y	2	NAG	O5-C5	3.03	1.49	1.43
2	V	2	NAG	O5-C5	2.97	1.49	1.43
4	X	3	MAN	O5-C5	2.95	1.49	1.43
2	Z	2	NAG	O5-C5	2.93	1.49	1.43
4	M	3	MAN	O5-C5	2.90	1.49	1.43
2	G	2	NAG	O5-C5	2.90	1.49	1.43
2	g	2	NAG	O5-C5	2.88	1.49	1.43
2	U	2	NAG	O5-C5	2.88	1.49	1.43
3	W	2	NAG	O5-C5	2.87	1.49	1.43
3	h	3	FUC	O5-C5	2.85	1.49	1.43
2	D	2	NAG	O5-C5	2.84	1.49	1.43
4	j	1	NAG	O5-C5	2.83	1.49	1.43
3	L	2	NAG	O5-C5	2.82	1.48	1.43
4	Y	1	NAG	O5-C5	2.81	1.48	1.43
2	F	2	NAG	O5-C5	2.80	1.48	1.43
2	S	1	NAG	O5-C5	2.80	1.48	1.43
3	W	3	FUC	O5-C5	2.78	1.49	1.43
3	L	3	FUC	O5-C5	2.78	1.49	1.43
2	b	2	NAG	O5-C5	2.78	1.48	1.43
4	i	3	MAN	O5-C5	2.77	1.48	1.43
4	N	1	NAG	O5-C5	2.77	1.48	1.43
2	Z	1	NAG	O5-C5	2.77	1.48	1.43
2	S	2	NAG	O5-C5	2.73	1.48	1.43
4	M	2	NAG	O5-C5	2.73	1.48	1.43
3	h	2	NAG	O5-C5	2.72	1.48	1.43
2	H	1	NAG	O5-C5	2.71	1.48	1.43
2	f	2	NAG	O5-C5	2.70	1.48	1.43
2	a	2	NAG	O5-C5	2.67	1.48	1.43
2	E	2	NAG	O5-C5	2.67	1.48	1.43
2	H	2	NAG	O5-C5	2.67	1.48	1.43
3	W	1	NAG	O5-C5	2.65	1.48	1.43
2	d	2	NAG	O5-C5	2.65	1.48	1.43
2	P	2	NAG	O5-C5	2.62	1.48	1.43
4	i	2	NAG	O5-C5	2.60	1.48	1.43
4	M	1	NAG	O5-C5	2.60	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	NAG	O5-C5	2.59	1.48	1.43
3	L	3	FUC	O5-C1	2.59	1.48	1.43
2	K	1	NAG	O5-C5	2.57	1.48	1.43
4	i	1	NAG	O5-C5	2.57	1.48	1.43
3	L	1	NAG	O5-C5	2.56	1.48	1.43
4	j	2	NAG	O5-C1	2.55	1.48	1.43
4	X	2	NAG	O5-C5	2.55	1.48	1.43
4	N	3	MAN	O5-C1	2.53	1.47	1.43
2	U	1	NAG	O5-C5	2.53	1.48	1.43
2	J	2	NAG	O5-C5	2.52	1.48	1.43
4	X	1	NAG	O5-C5	2.49	1.48	1.43
3	h	1	NAG	O5-C5	2.47	1.48	1.43
3	h	3	FUC	O5-C1	2.45	1.47	1.43
2	d	1	NAG	O5-C5	2.45	1.48	1.43
2	f	1	NAG	O5-C5	2.44	1.48	1.43
4	Y	3	MAN	O5-C1	2.34	1.47	1.43
4	N	2	NAG	O5-C1	2.31	1.47	1.43
2	S	1	NAG	O4-C4	2.30	1.48	1.43
2	d	1	NAG	C1-C2	2.29	1.55	1.52
4	Y	2	NAG	O5-C1	2.28	1.47	1.43
3	W	3	FUC	O5-C1	2.27	1.47	1.43
4	M	2	NAG	O4-C4	2.23	1.48	1.43
2	Z	2	NAG	O5-C1	2.22	1.47	1.43
2	g	1	NAG	O5-C5	2.21	1.47	1.43
2	Z	1	NAG	O4-C4	2.18	1.48	1.43
4	N	1	NAG	O4-C4	2.18	1.48	1.43
4	N	2	NAG	O4-C4	2.18	1.48	1.43
4	j	3	MAN	O5-C1	2.17	1.47	1.43
3	W	2	NAG	O5-C1	2.16	1.47	1.43
3	L	2	NAG	O5-C1	2.15	1.47	1.43
4	j	1	NAG	O4-C4	2.14	1.48	1.43
4	X	3	MAN	O5-C1	2.14	1.47	1.43
3	L	2	NAG	C1-C2	2.13	1.55	1.52
2	H	2	NAG	O5-C1	2.13	1.47	1.43
2	V	1	NAG	O5-C5	2.10	1.47	1.43
4	Y	1	NAG	O4-C4	2.10	1.48	1.43
3	L	1	NAG	C1-C2	2.09	1.55	1.52
4	M	3	MAN	O5-C1	2.05	1.47	1.43
4	X	2	NAG	O4-C4	2.05	1.48	1.43
2	d	2	NAG	O5-C1	2.01	1.47	1.43
3	L	1	NAG	O4-C4	2.01	1.47	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	4.64	118.40	112.19
2	P	2	NAG	C1-O5-C5	4.04	117.59	112.19
2	g	2	NAG	C1-O5-C5	3.98	117.51	112.19
2	E	2	NAG	C1-O5-C5	3.88	117.38	112.19
2	a	2	NAG	C1-O5-C5	3.87	117.37	112.19
2	G	2	NAG	C1-O5-C5	3.46	116.83	112.19
2	Q	2	NAG	C1-O5-C5	3.45	116.81	112.19
3	W	1	NAG	C1-O5-C5	3.43	116.78	112.19
2	D	2	NAG	C1-O5-C5	3.20	116.48	112.19
3	L	1	NAG	C1-O5-C5	3.17	116.44	112.19
2	d	2	NAG	C1-O5-C5	3.09	116.33	112.19
2	R	2	NAG	C1-O5-C5	3.07	116.30	112.19
2	I	2	NAG	C1-O5-C5	3.06	116.29	112.19
2	e	2	NAG	C1-O5-C5	3.05	116.28	112.19
2	S	2	NAG	C1-O5-C5	2.96	116.15	112.19
2	b	2	NAG	C1-O5-C5	2.95	116.14	112.19
4	Y	1	NAG	C1-O5-C5	2.85	116.01	112.19
2	K	1	NAG	C1-O5-C5	2.79	115.92	112.19
3	W	2	NAG	C1-O5-C5	2.75	115.87	112.19
2	H	2	NAG	C1-O5-C5	2.74	115.86	112.19
3	L	2	NAG	C1-O5-C5	2.68	115.78	112.19
2	T	2	NAG	C1-O5-C5	2.64	115.72	112.19
4	j	1	NAG	C1-O5-C5	2.59	115.66	112.19
3	h	2	NAG	C1-O5-C5	2.51	115.55	112.19
2	Z	2	NAG	O5-C1-C2	-2.39	107.59	111.29
4	N	1	NAG	C1-O5-C5	2.30	115.26	112.19
2	d	1	NAG	C3-C4-C5	2.29	114.39	110.23
3	W	3	FUC	C1-C2-C3	2.29	112.97	109.64
2	K	2	NAG	C1-O5-C5	2.28	115.25	112.19
3	h	3	FUC	C1-C2-C3	2.25	112.91	109.64
4	M	2	NAG	C1-O5-C5	2.14	115.06	112.19
2	J	2	NAG	C1-O5-C5	2.13	115.05	112.19
2	H	1	NAG	C3-C4-C5	2.13	114.10	110.23
4	j	1	NAG	O5-C1-C2	-2.09	108.05	111.29
2	Z	2	NAG	C1-O5-C5	2.02	114.89	112.19
2	R	2	NAG	O4-C4-C3	-2.00	105.65	110.38
3	L	3	FUC	C1-C2-C3	2.00	112.56	109.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	h	1	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
4	i	3	MAN	O5-C5-C6-O6
2	S	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
4	M	3	MAN	O5-C5-C6-O6
4	X	3	MAN	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
4	i	3	MAN	C4-C5-C6-O6
2	S	1	NAG	C8-C7-N2-C2
2	F	1	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
4	M	1	NAG	C1-C2-N2-C7

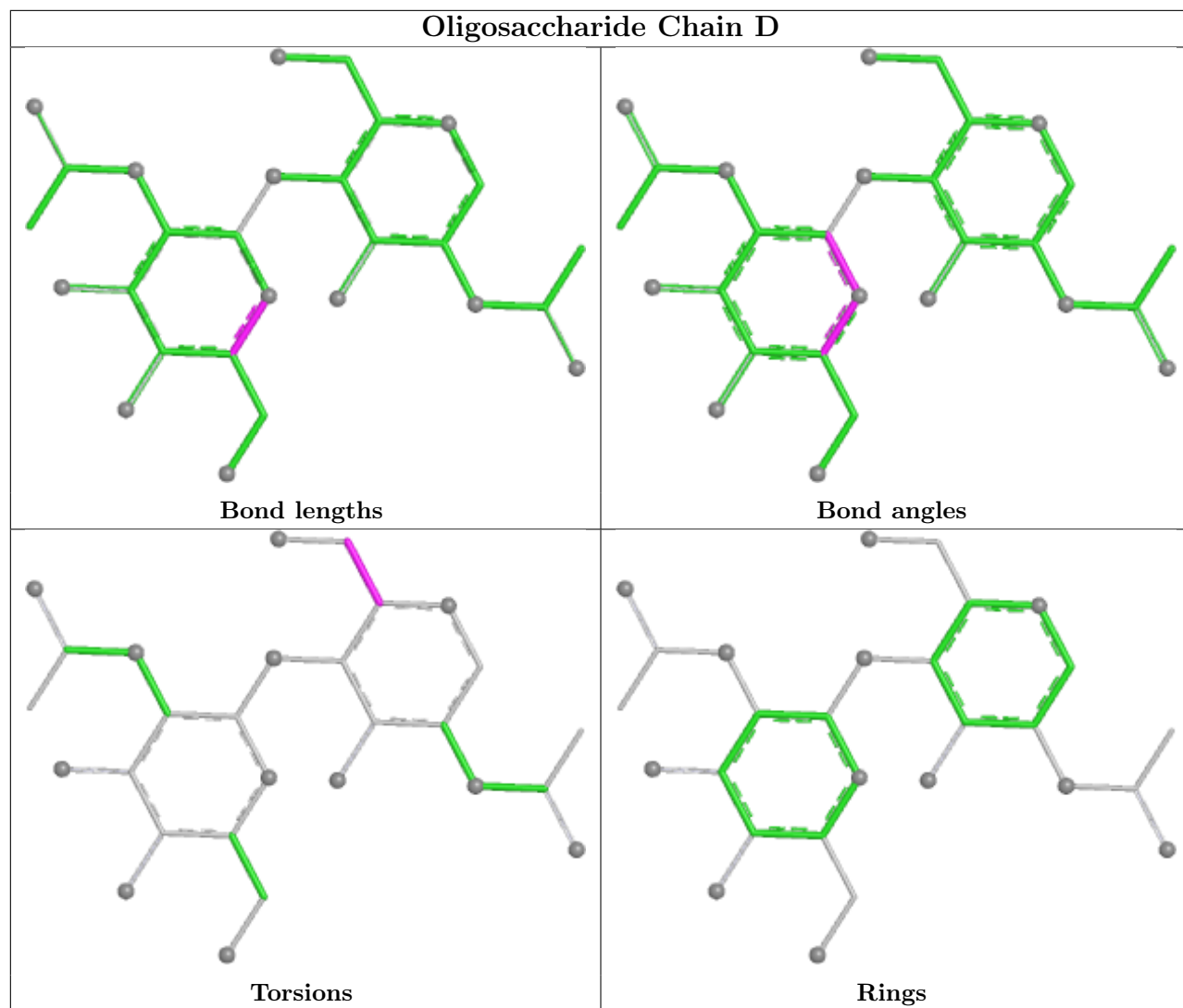
All (3) ring outliers are listed below:

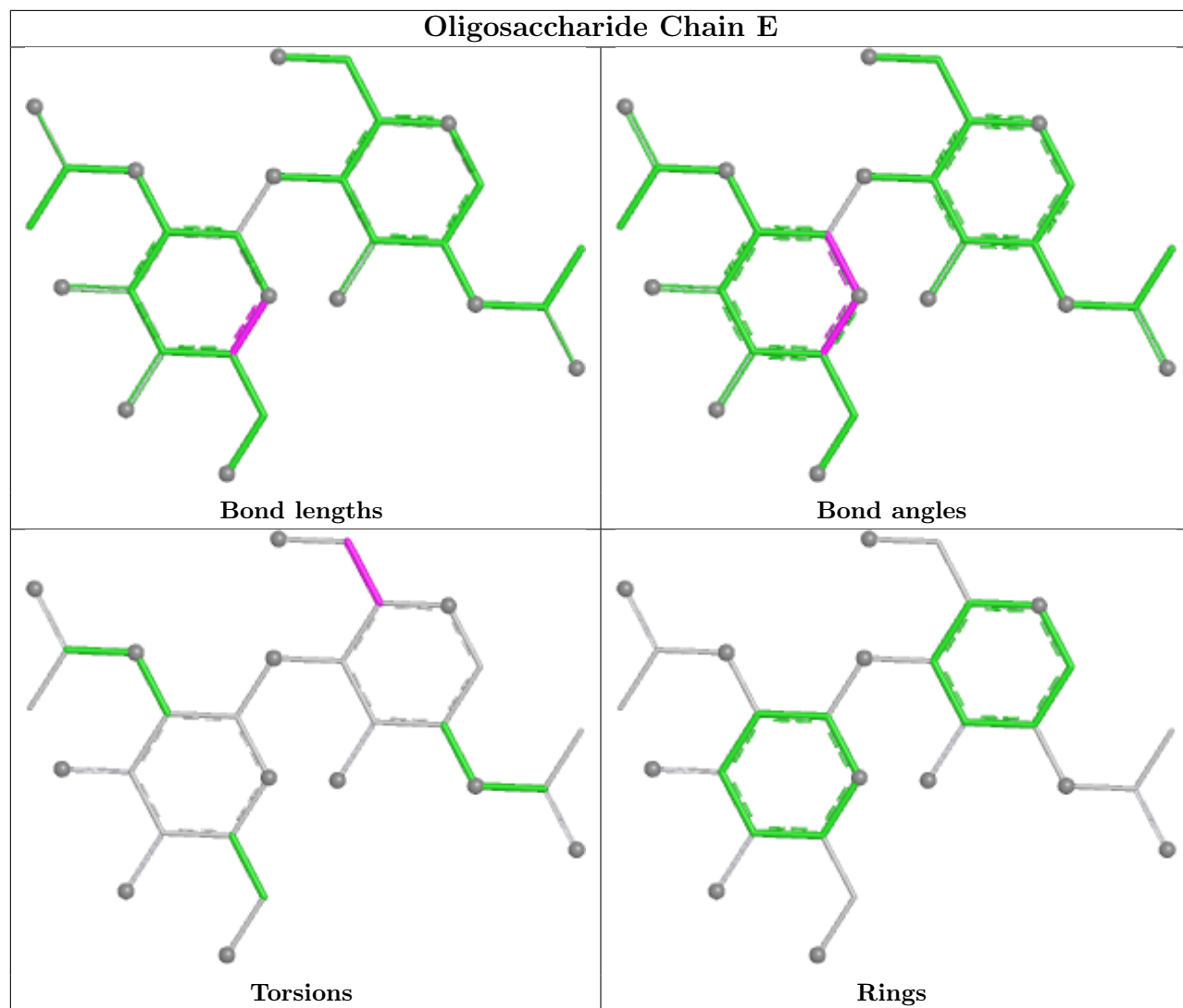
Mol	Chain	Res	Type	Atoms
4	j	3	MAN	C1-C2-C3-C4-C5-O5
4	X	3	MAN	C1-C2-C3-C4-C5-O5
4	N	3	MAN	C1-C2-C3-C4-C5-O5

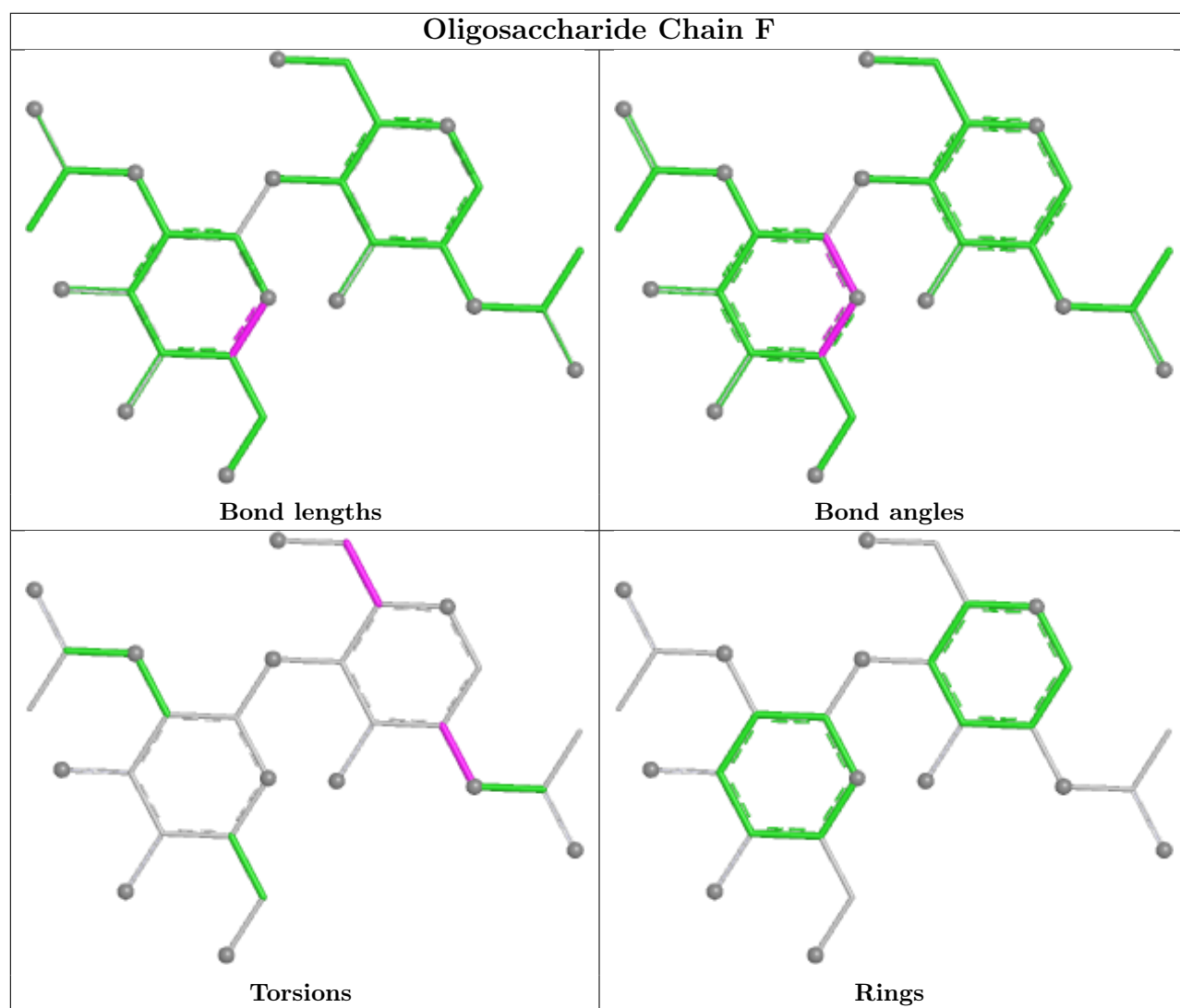
21 monomers are involved in 48 short contacts:

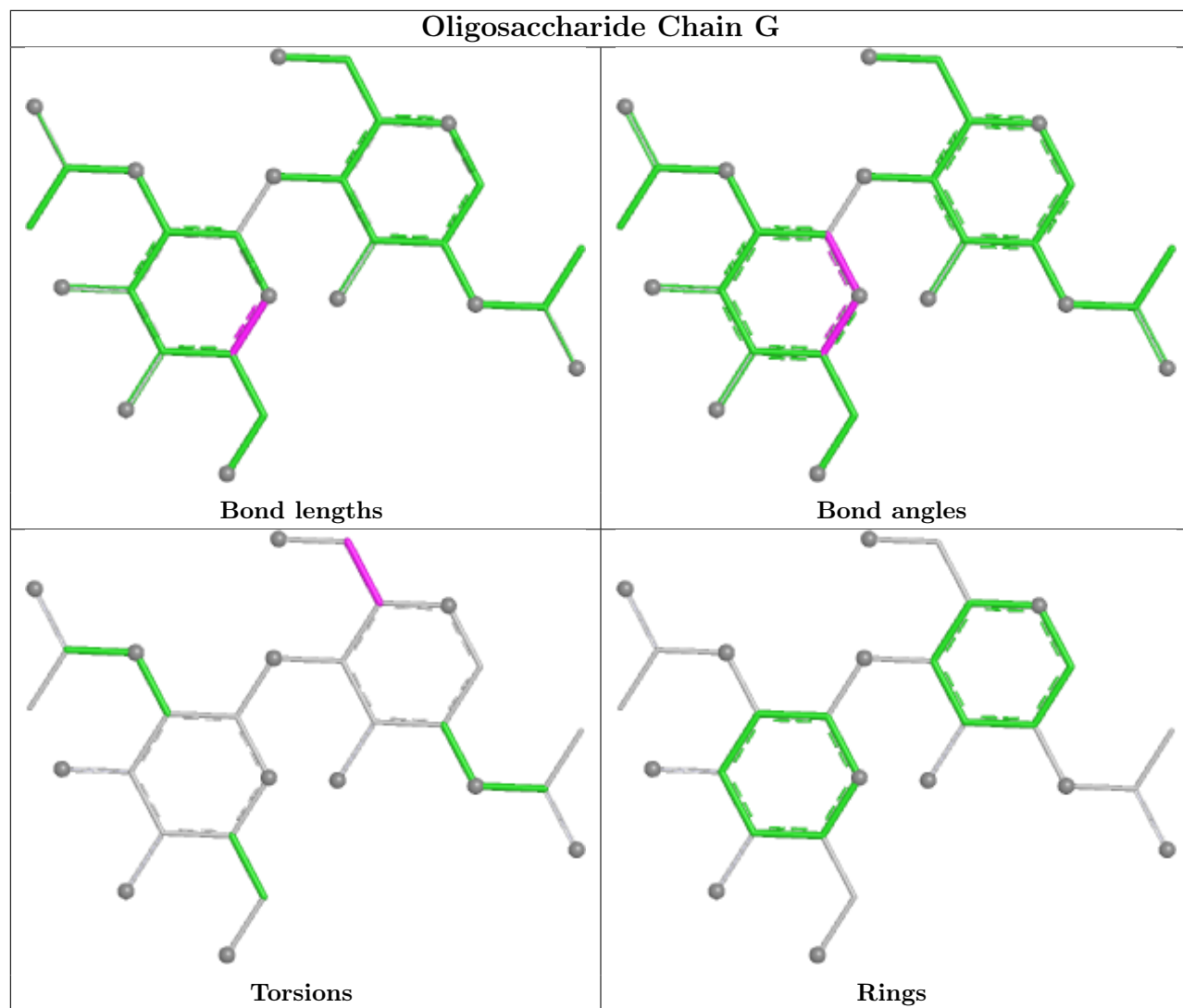
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	G	1	NAG	5	0
2	T	2	NAG	1	0
2	c	1	NAG	3	0
2	O	1	NAG	2	0
2	R	1	NAG	4	0
2	T	1	NAG	1	0
2	b	1	NAG	2	0
2	Q	1	NAG	2	0
2	D	1	NAG	6	0
2	E	1	NAG	4	0
2	D	2	NAG	1	0
2	a	1	NAG	4	0
2	e	2	NAG	2	0
2	F	1	NAG	2	0
2	P	2	NAG	1	0
2	P	1	NAG	4	0
2	I	1	NAG	2	0
2	a	2	NAG	2	0
2	e	1	NAG	5	0
2	I	2	NAG	2	0

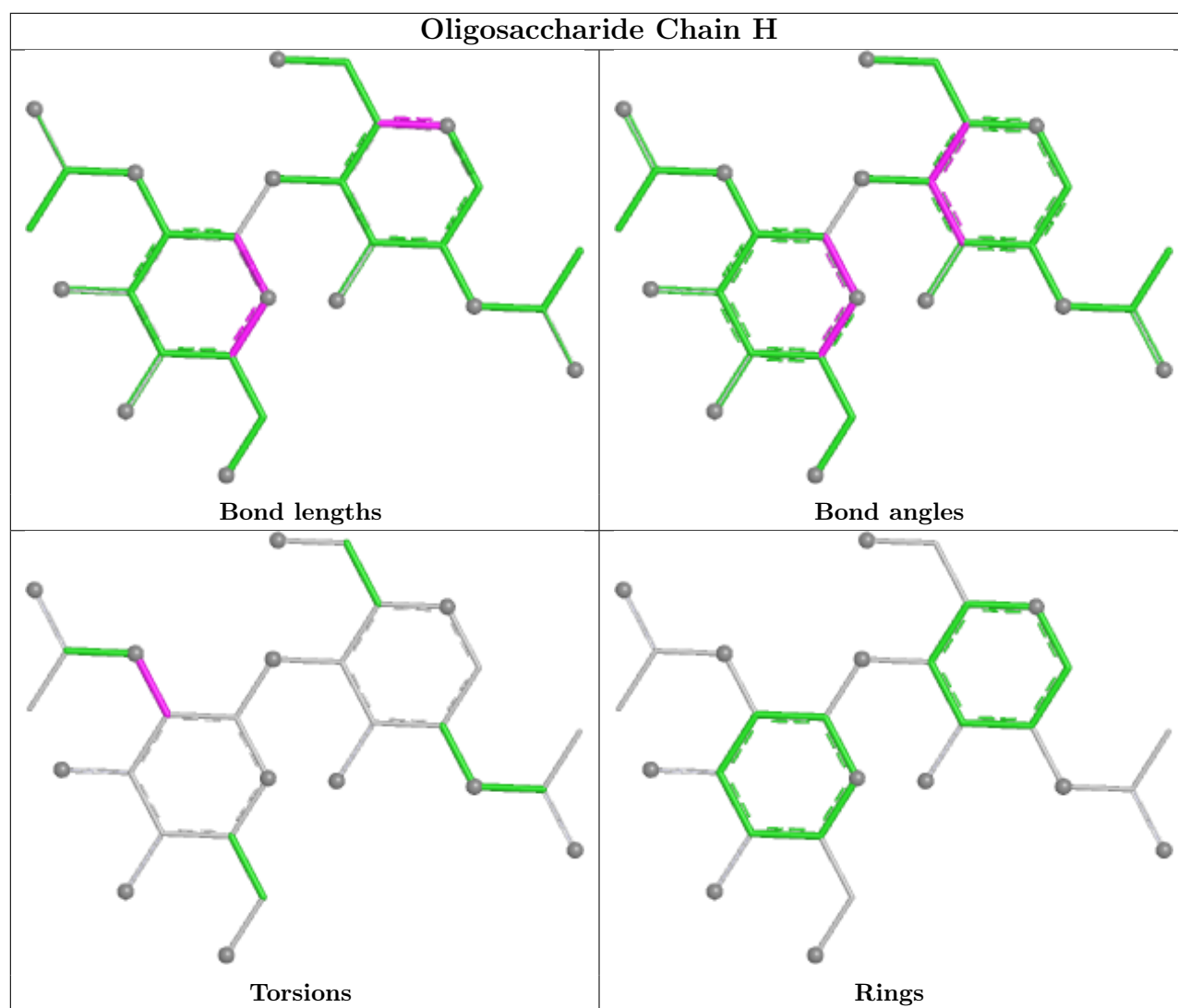
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

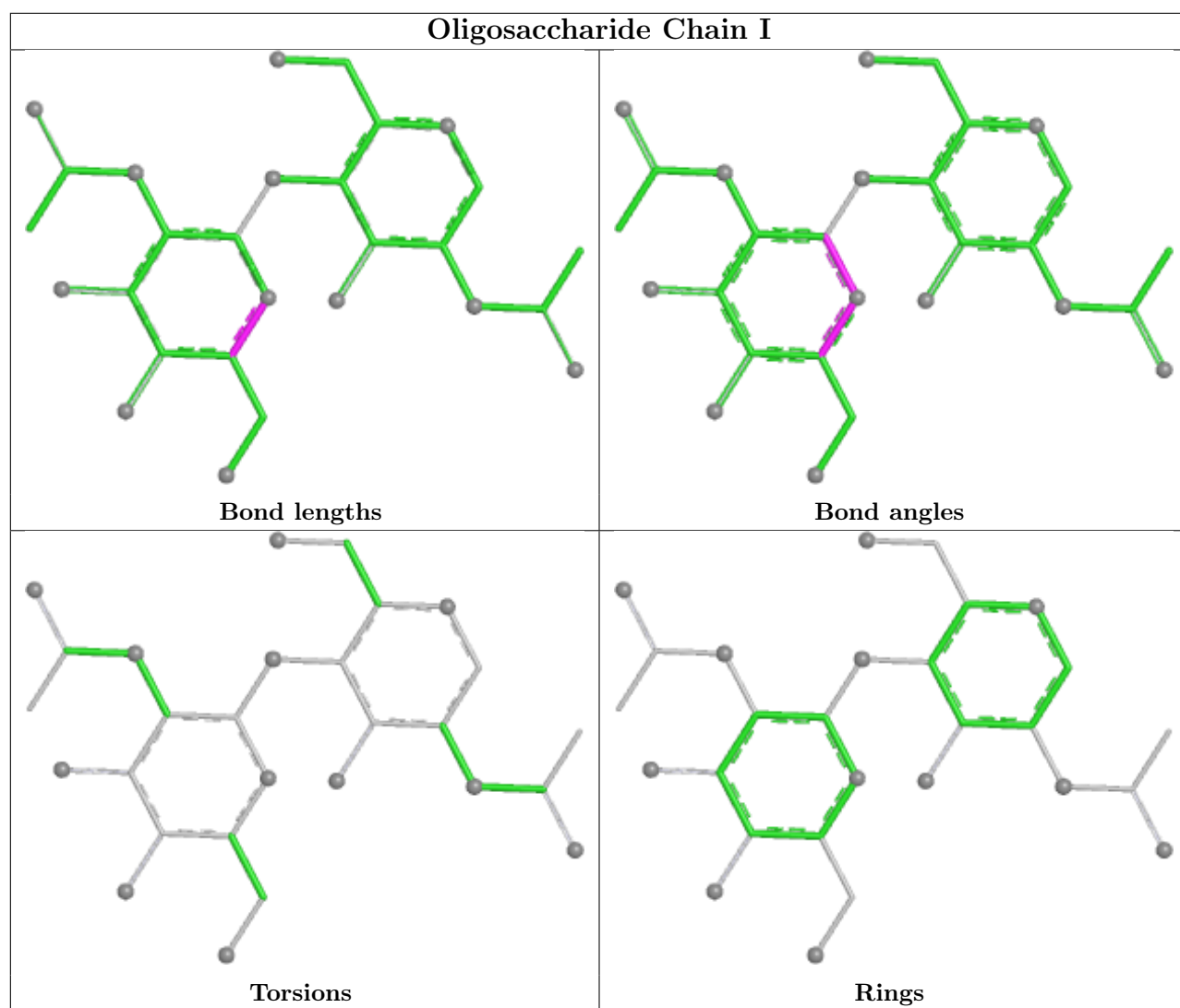


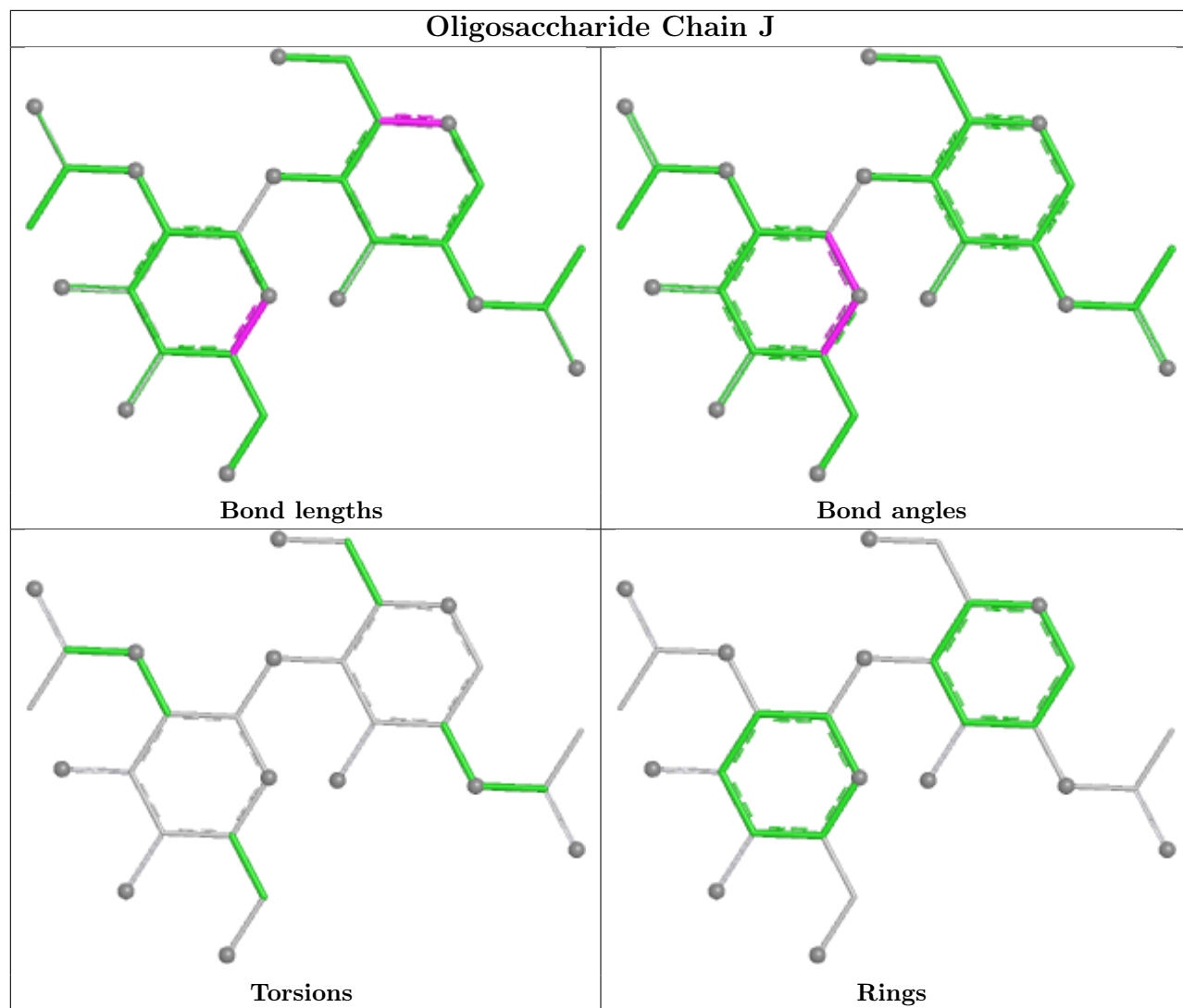


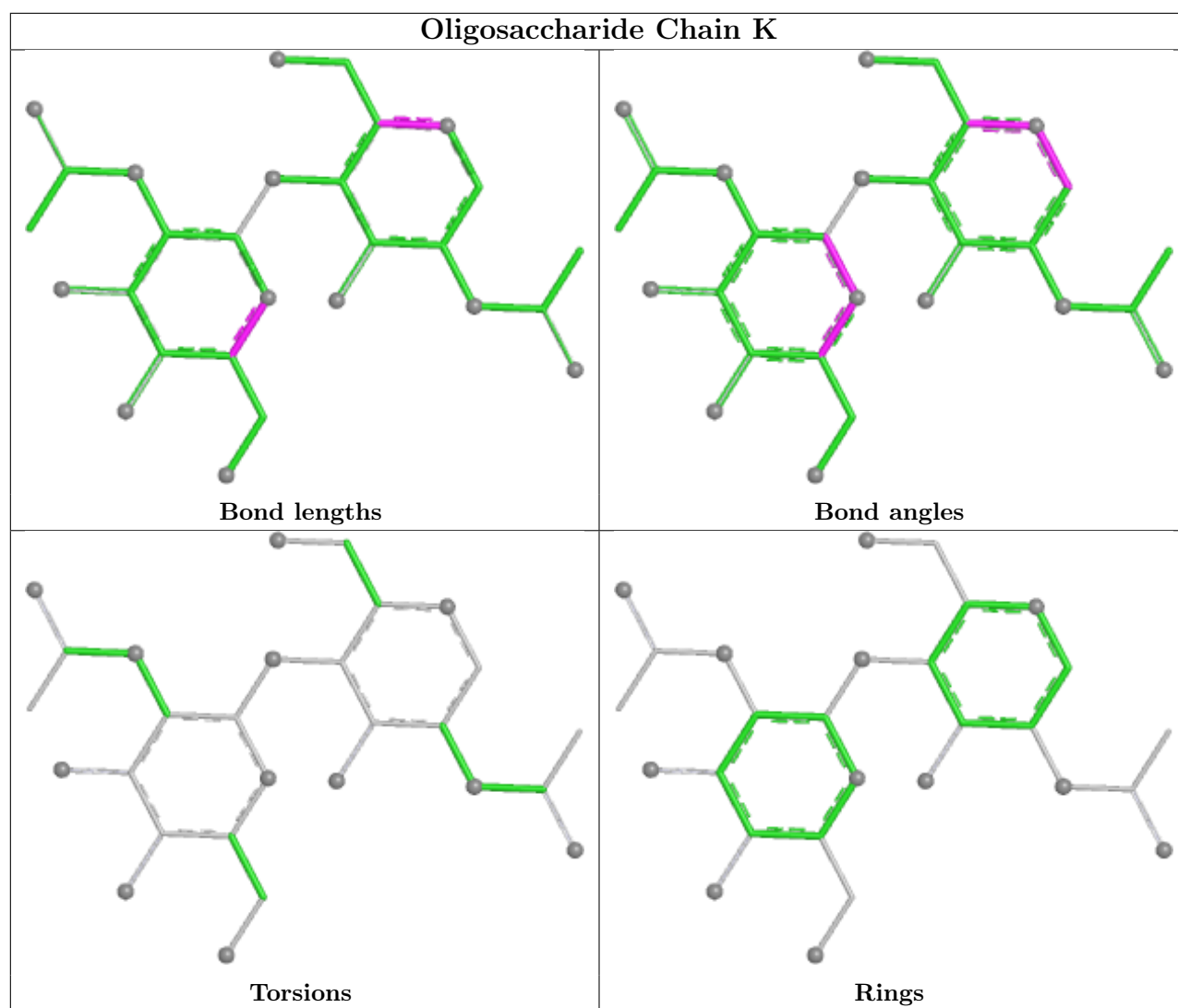


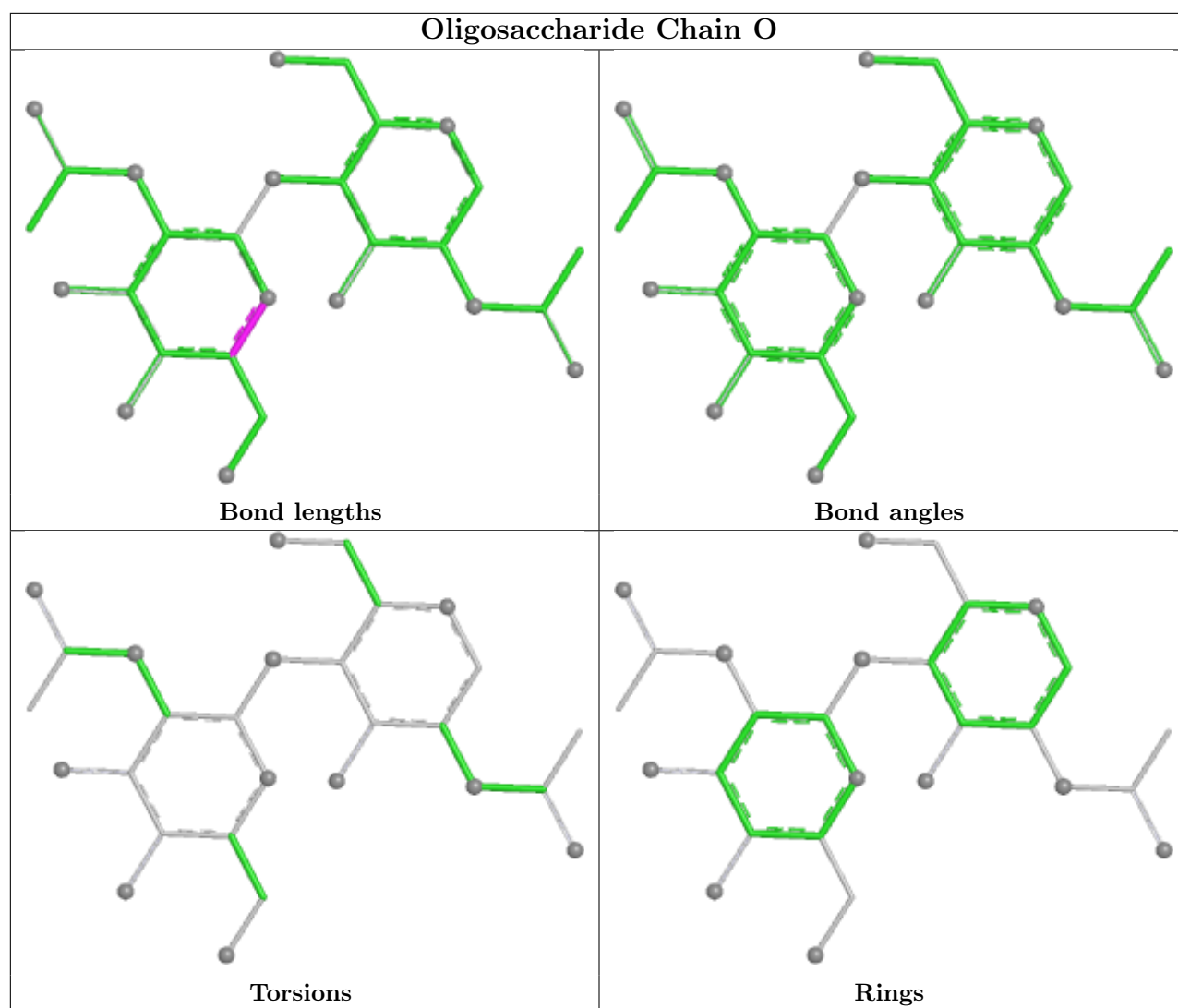


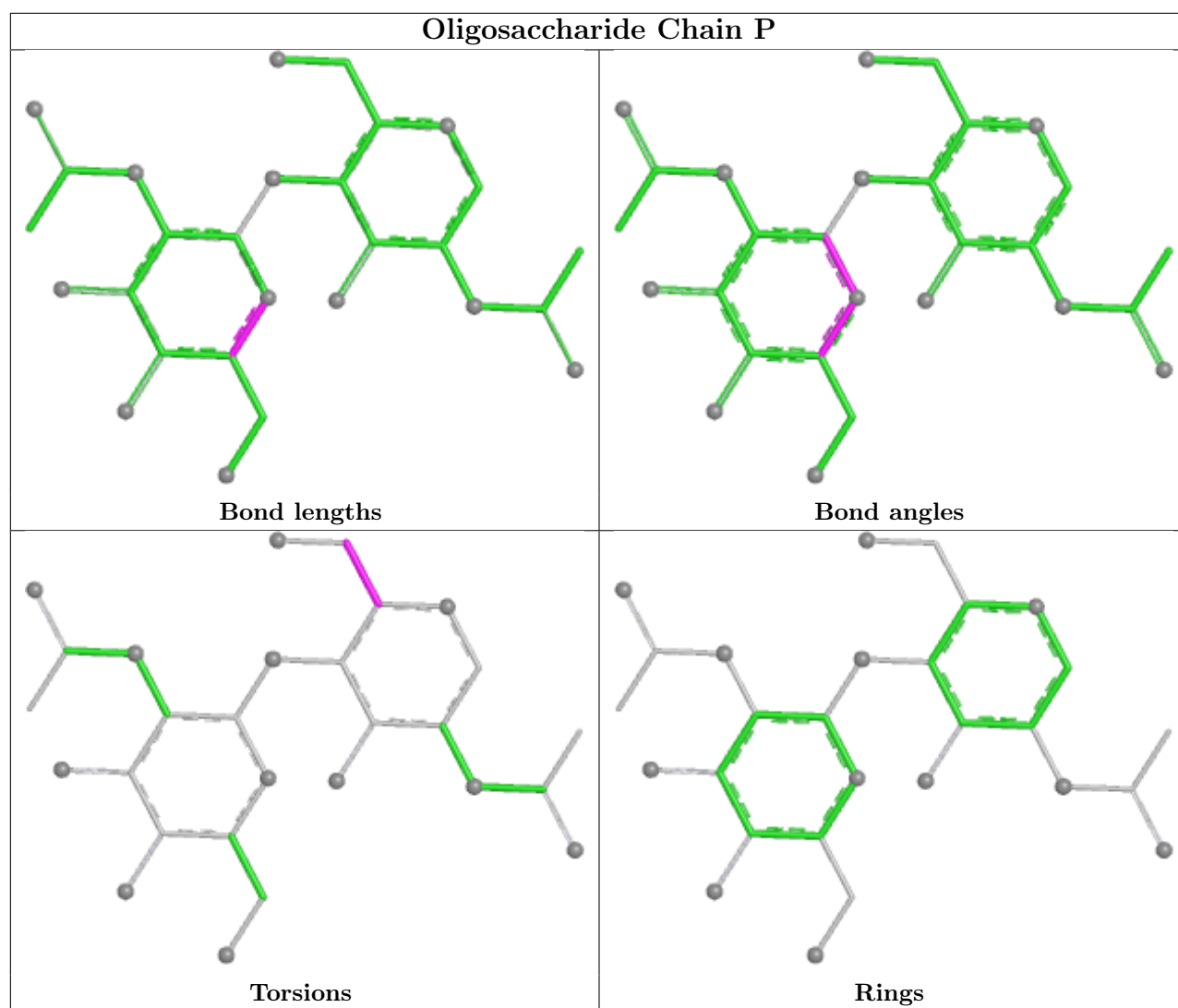


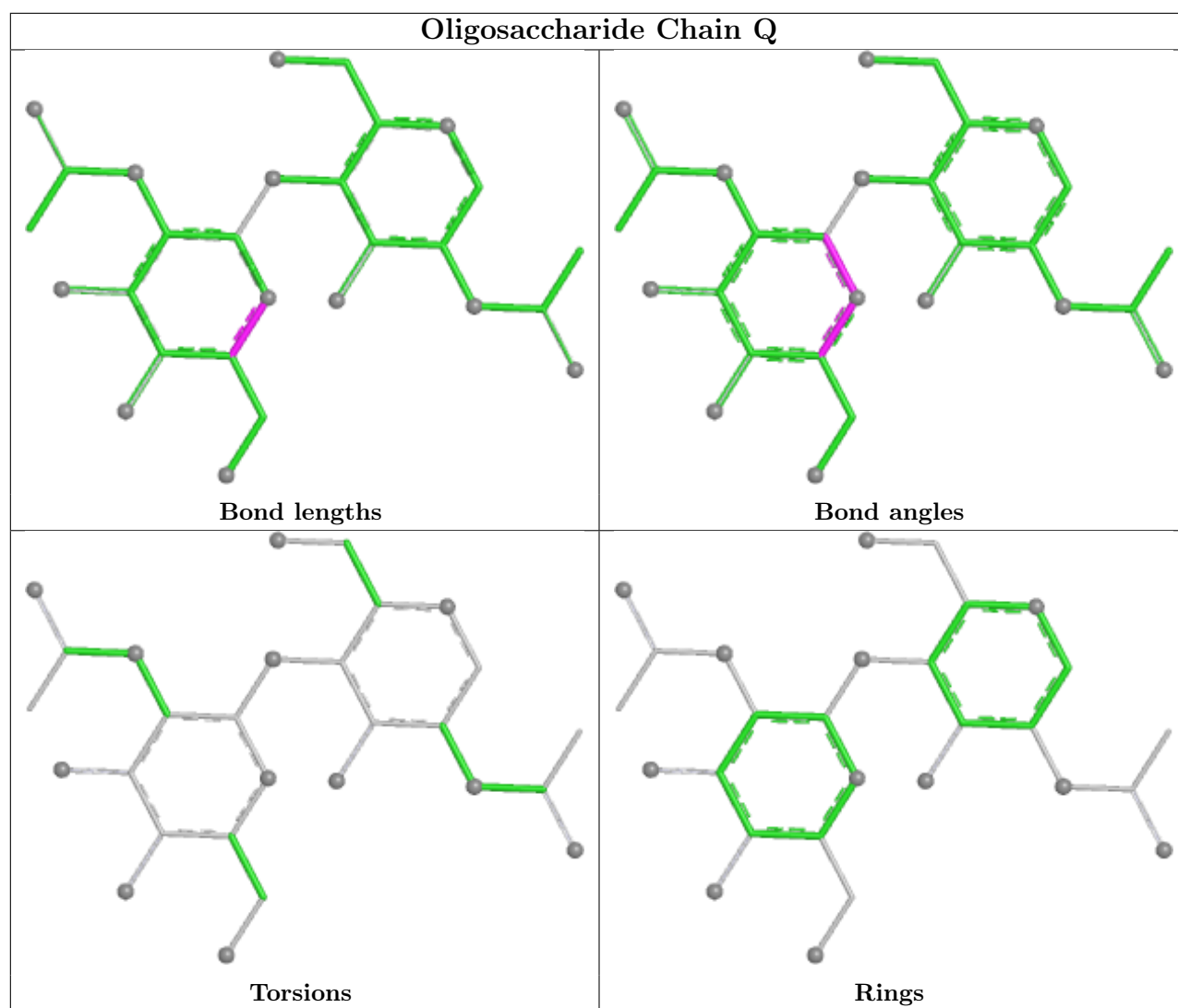


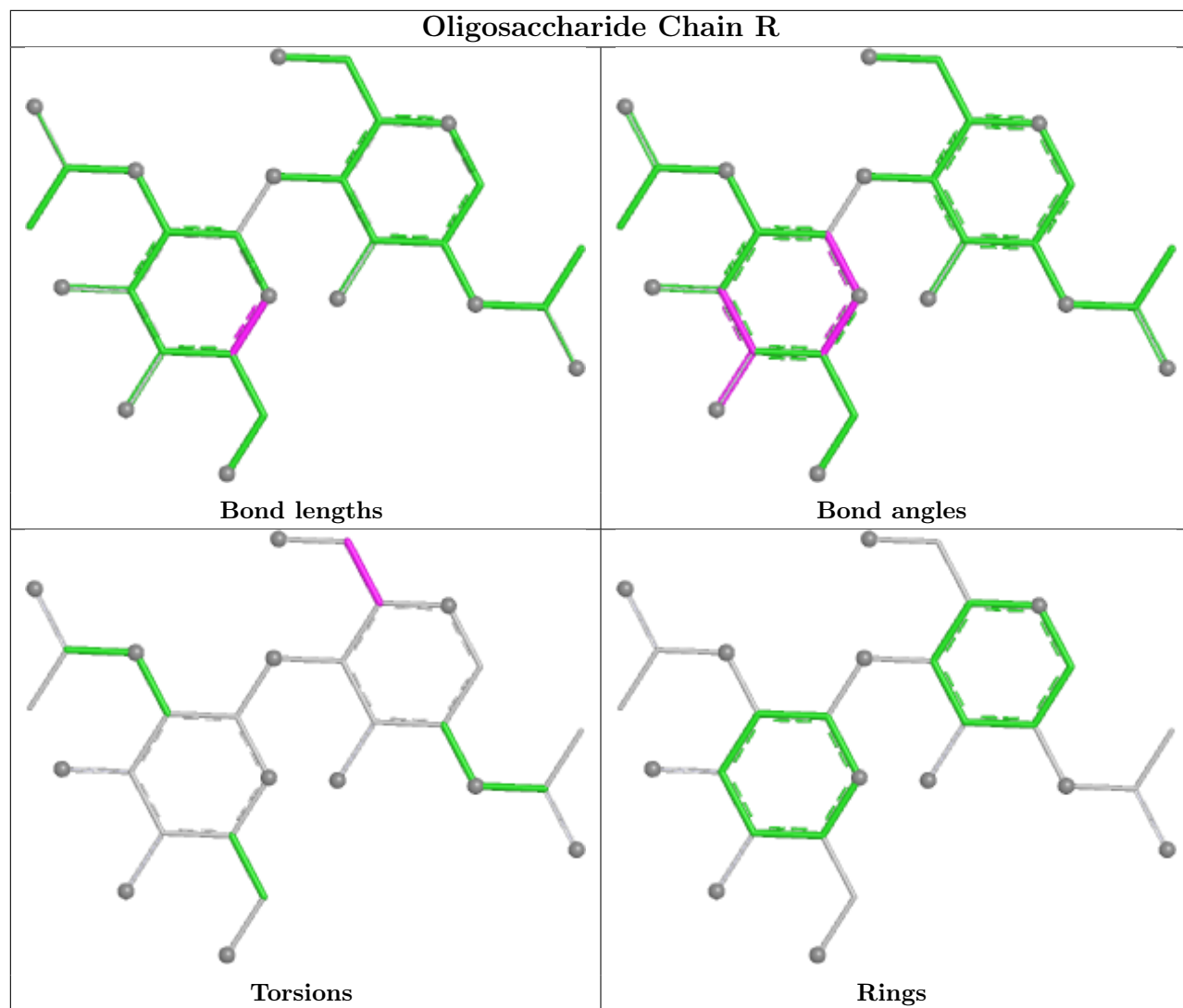


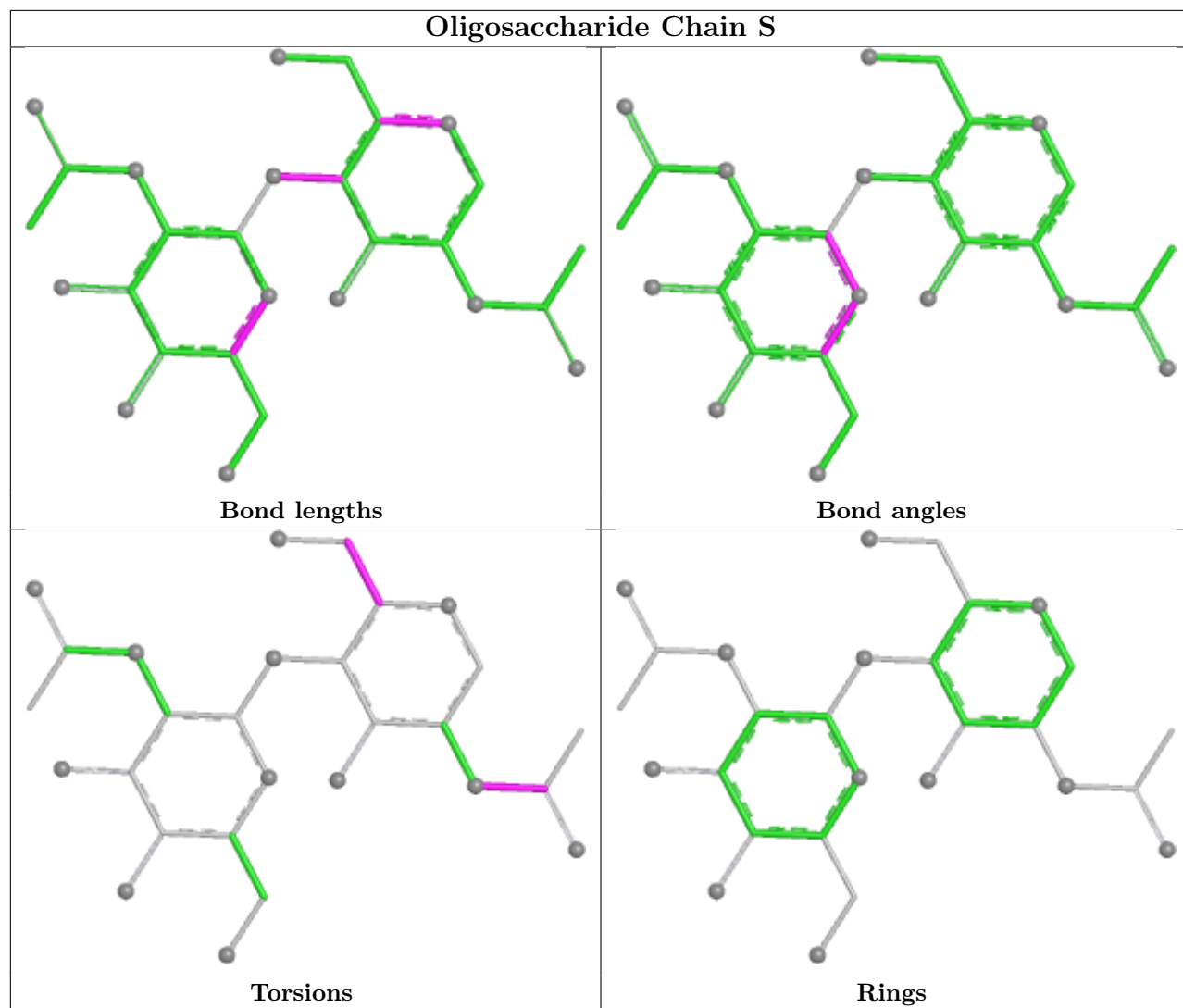


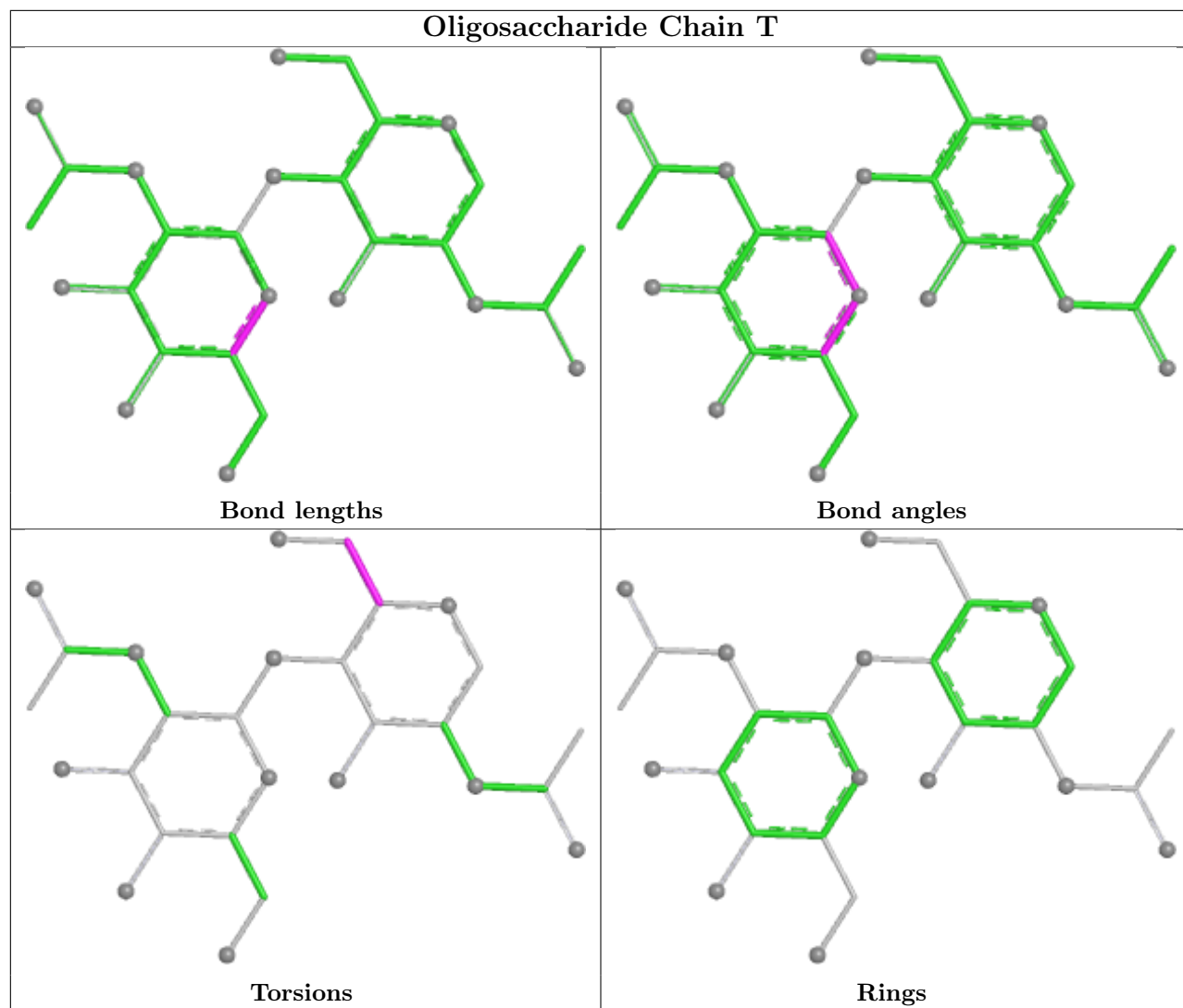


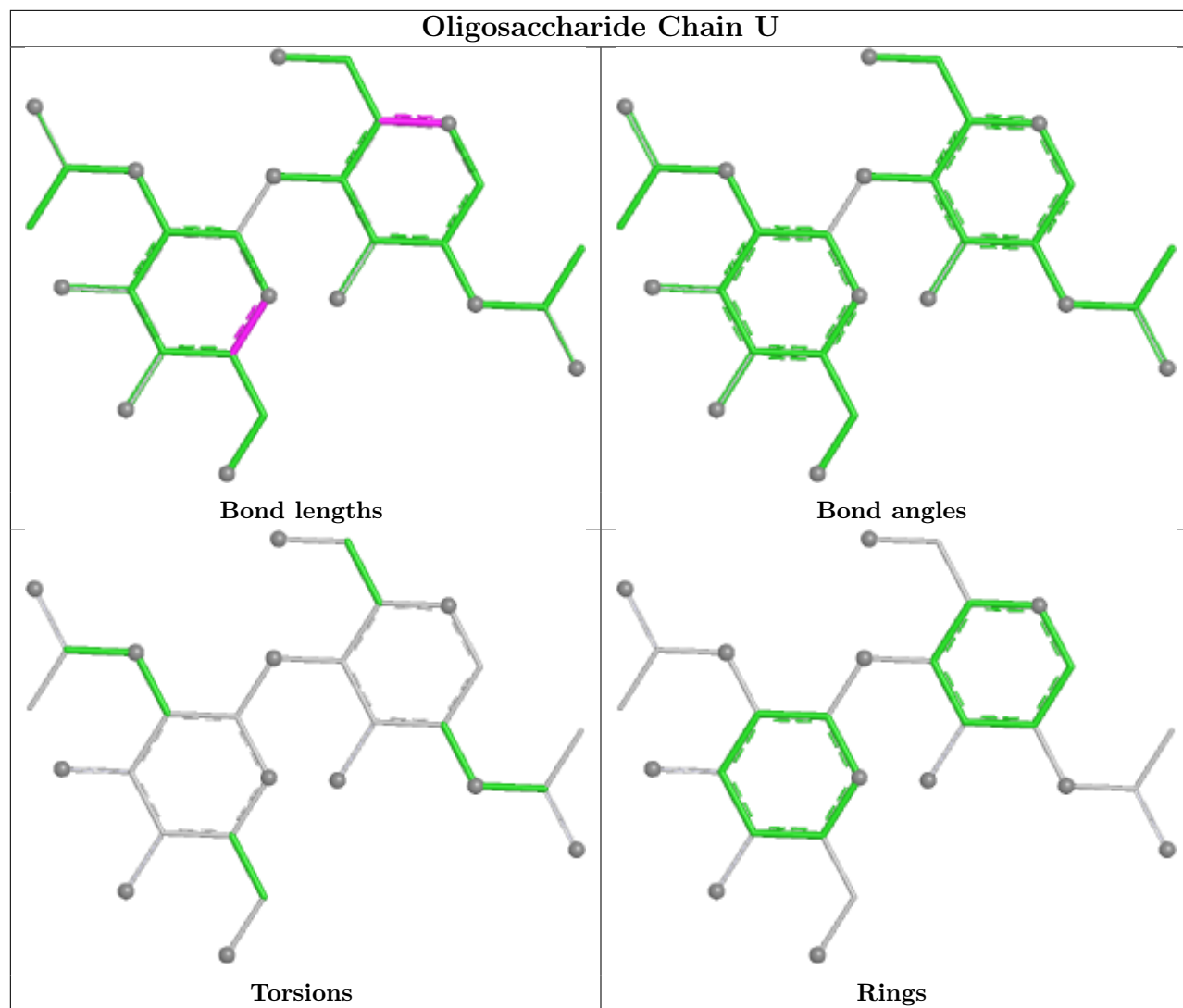


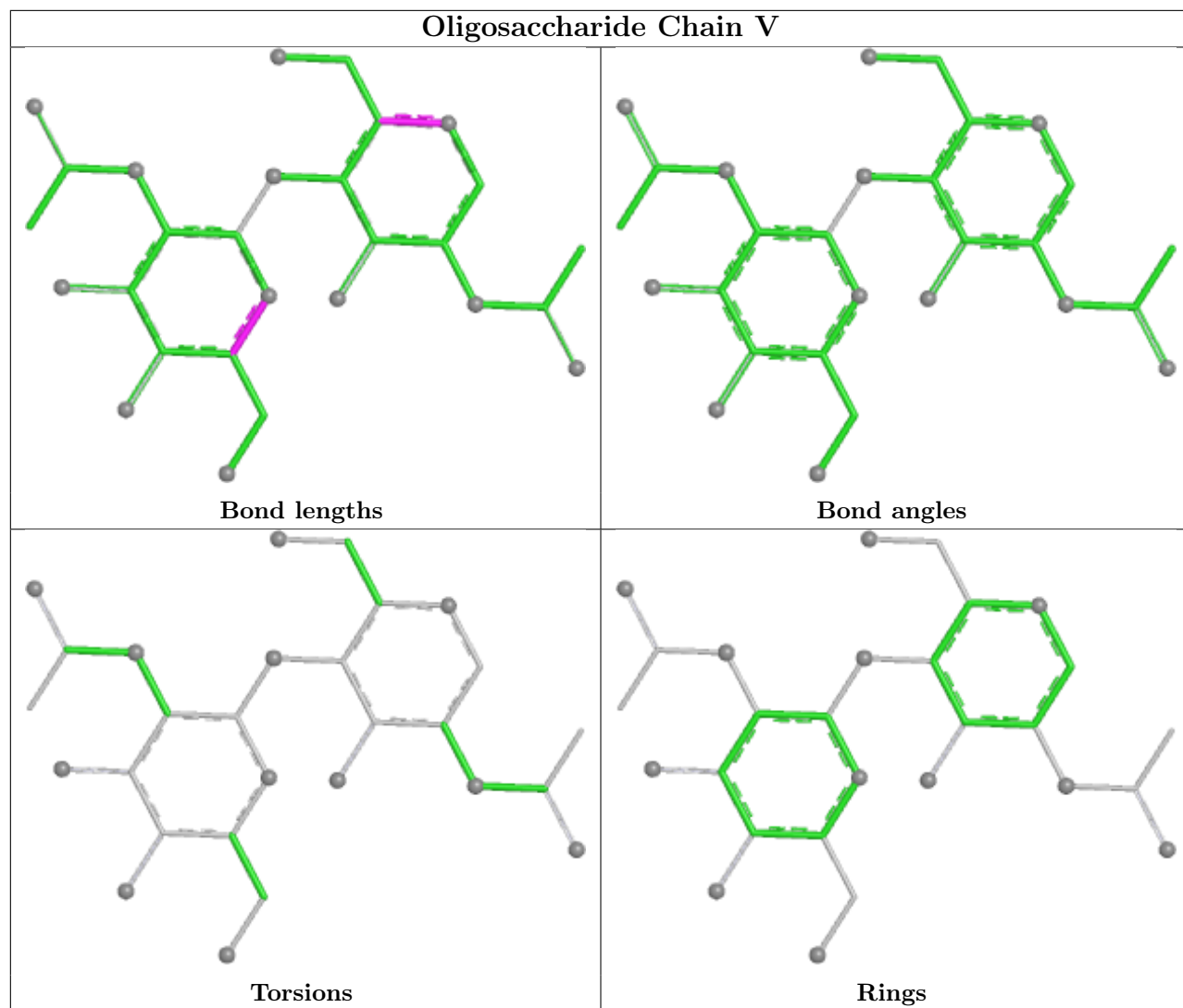


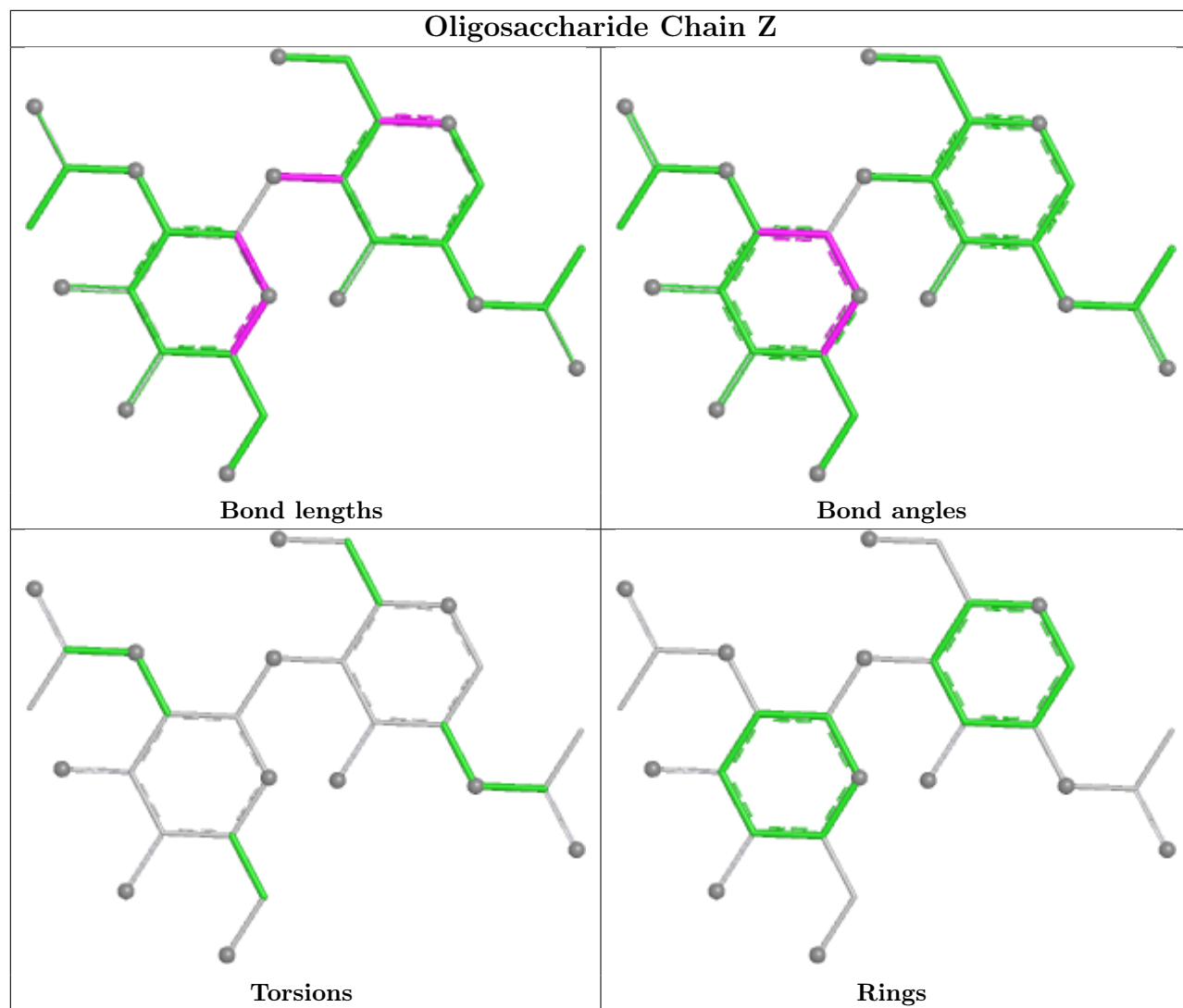


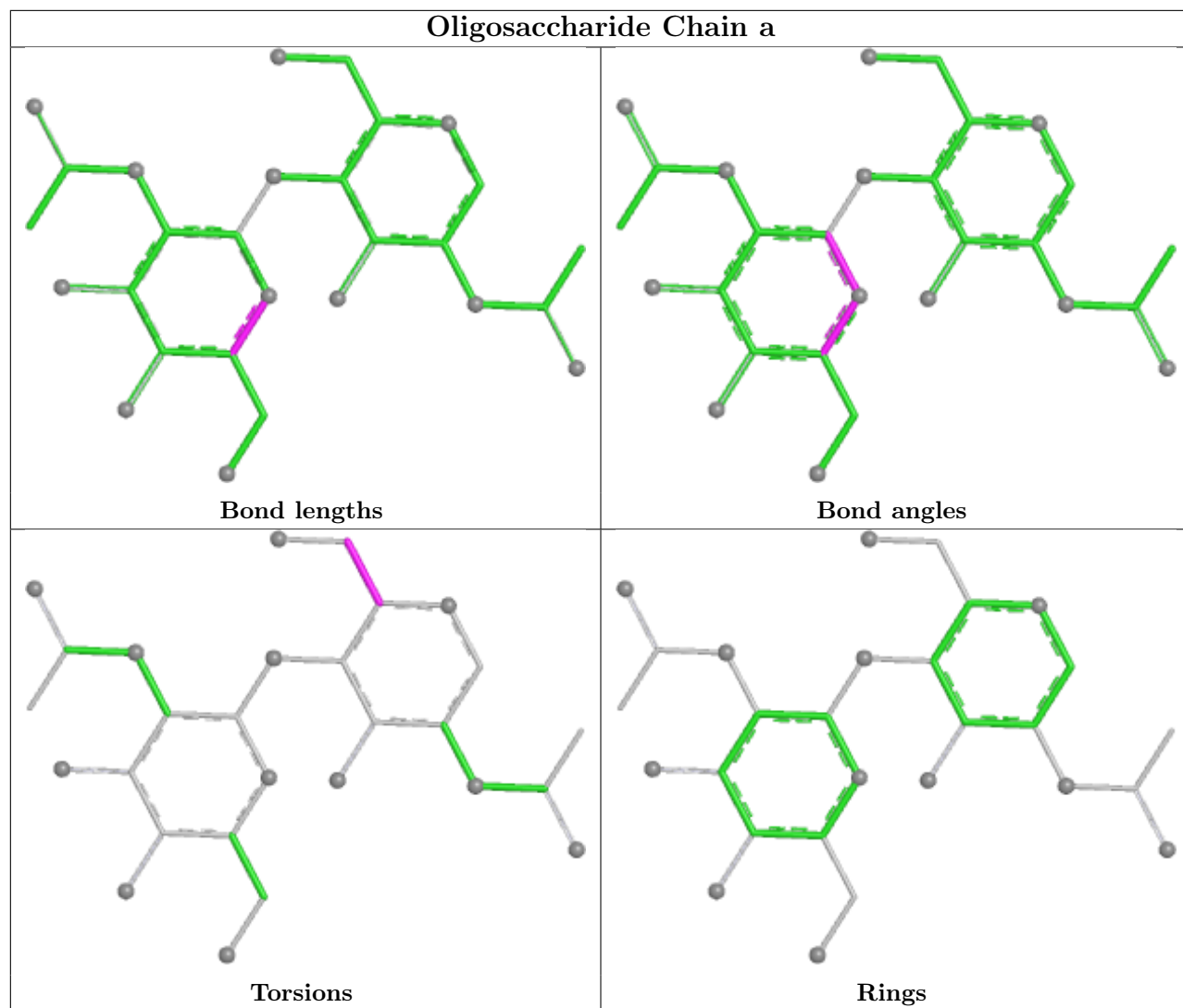


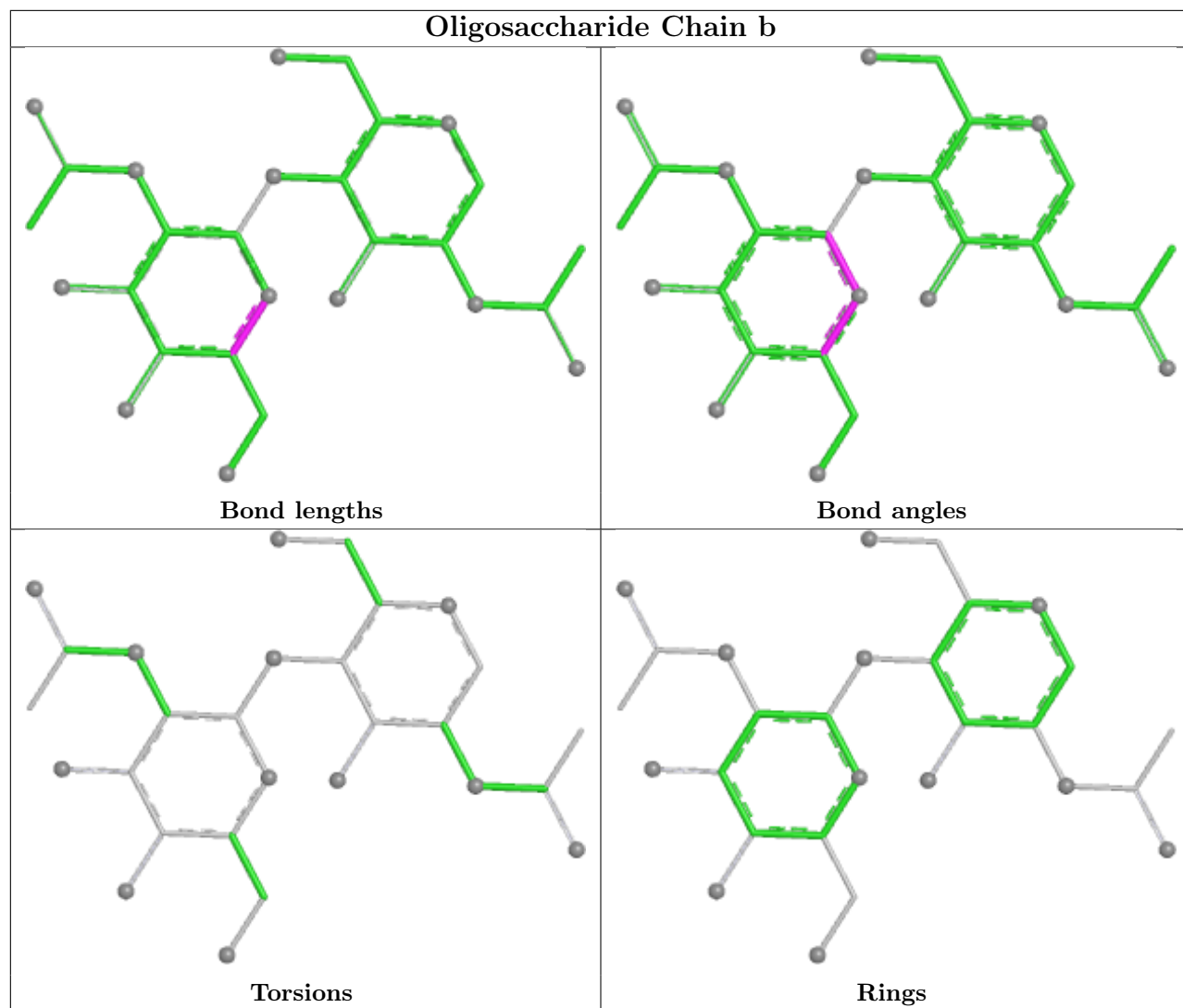


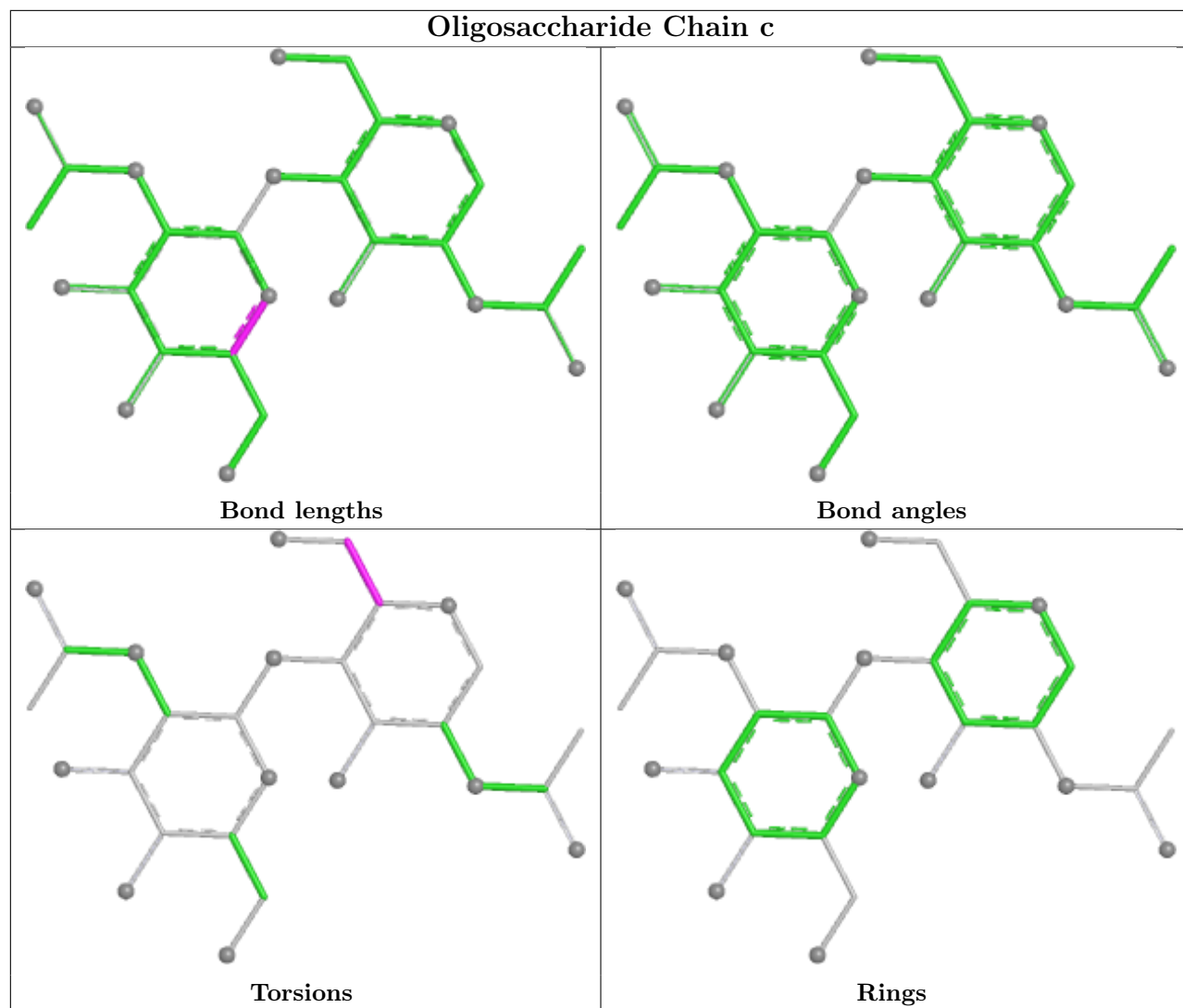


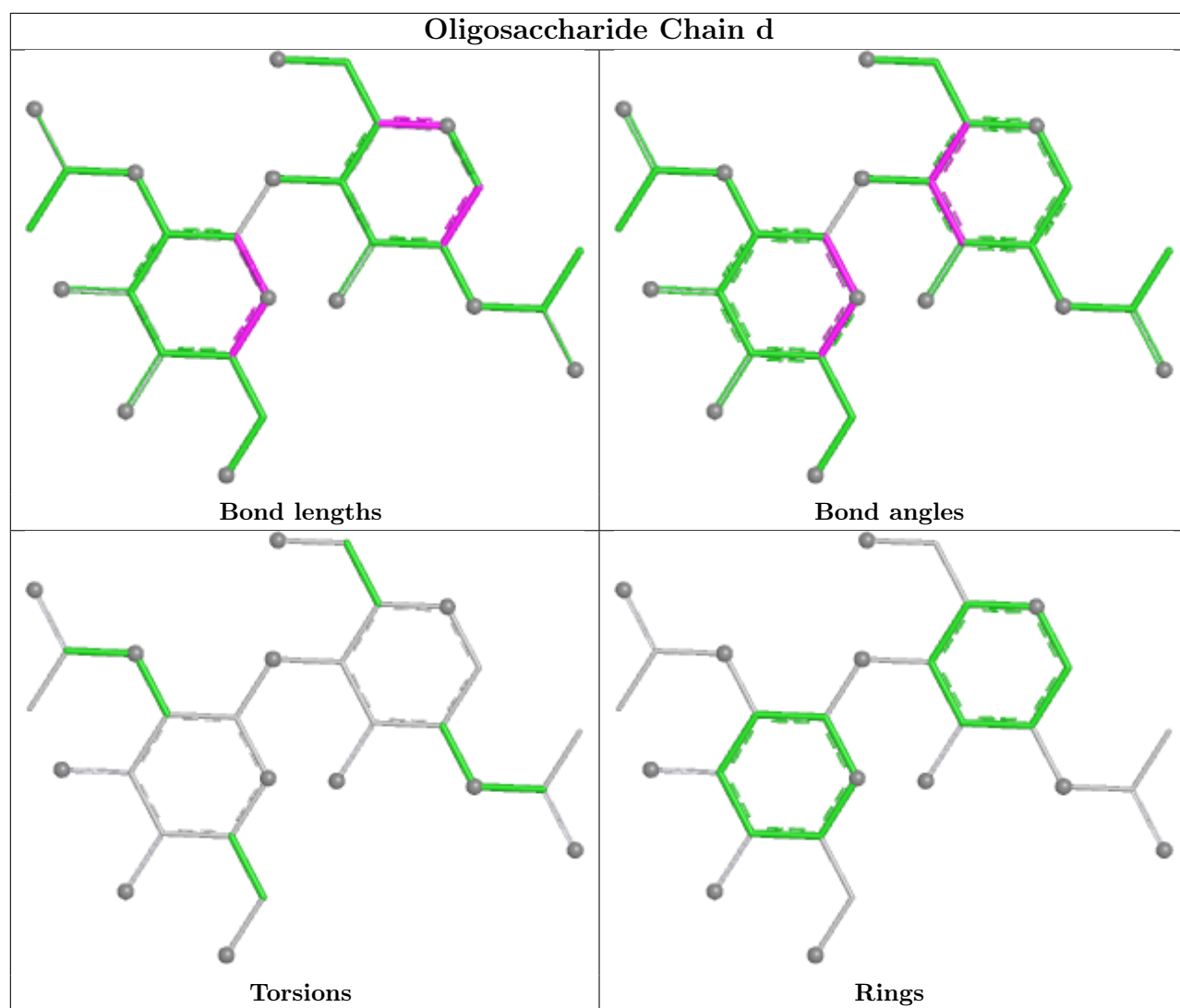


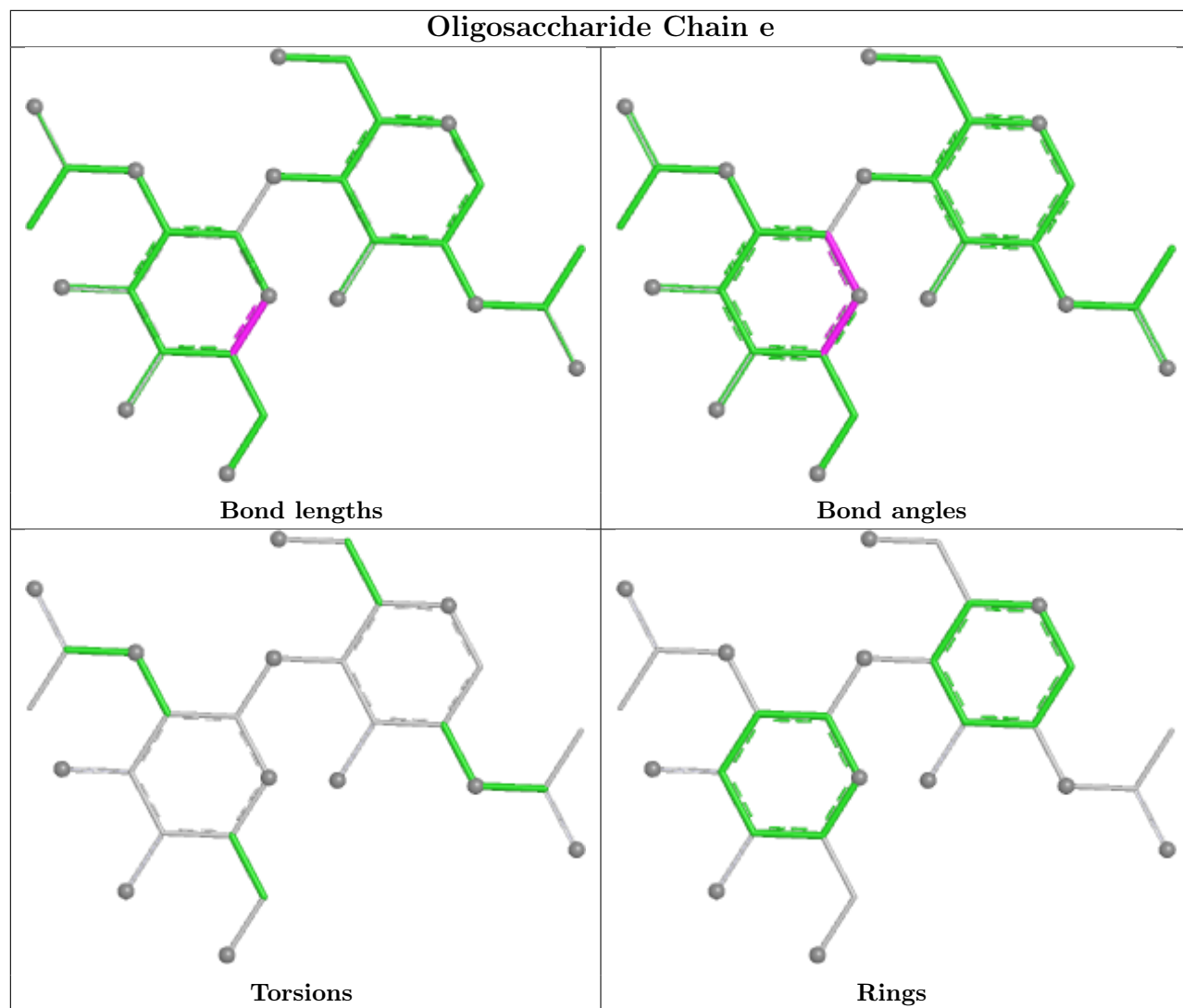


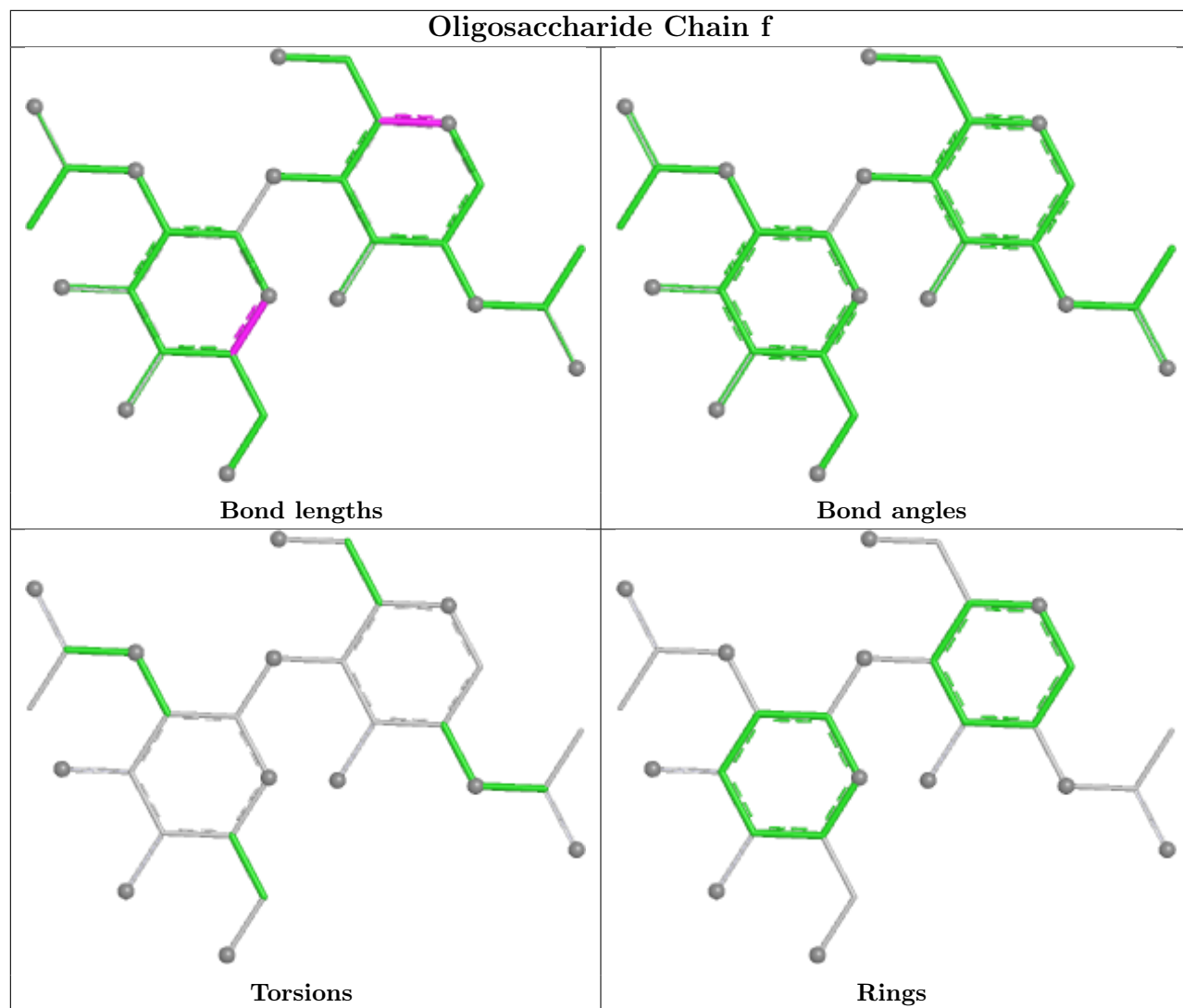


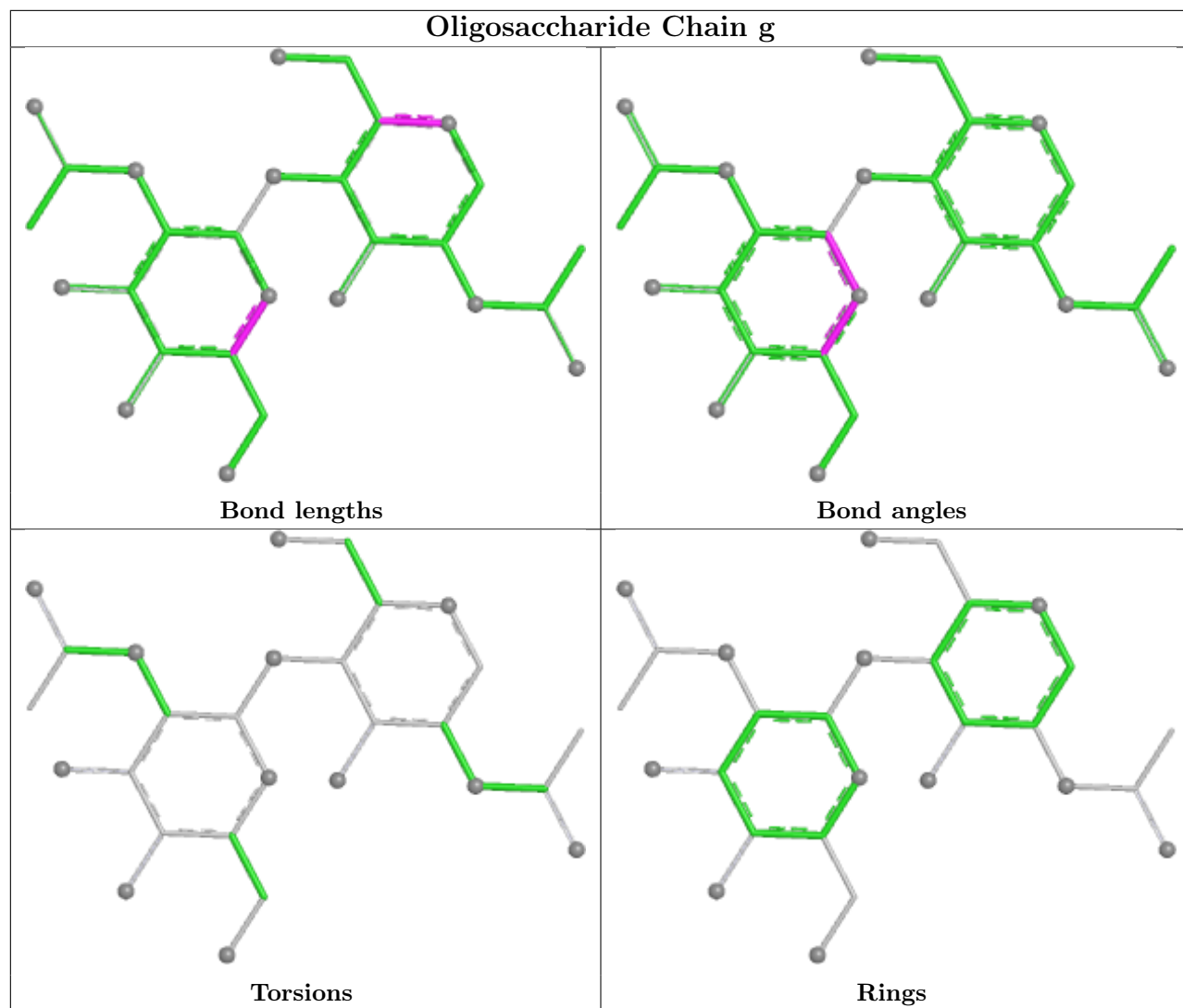


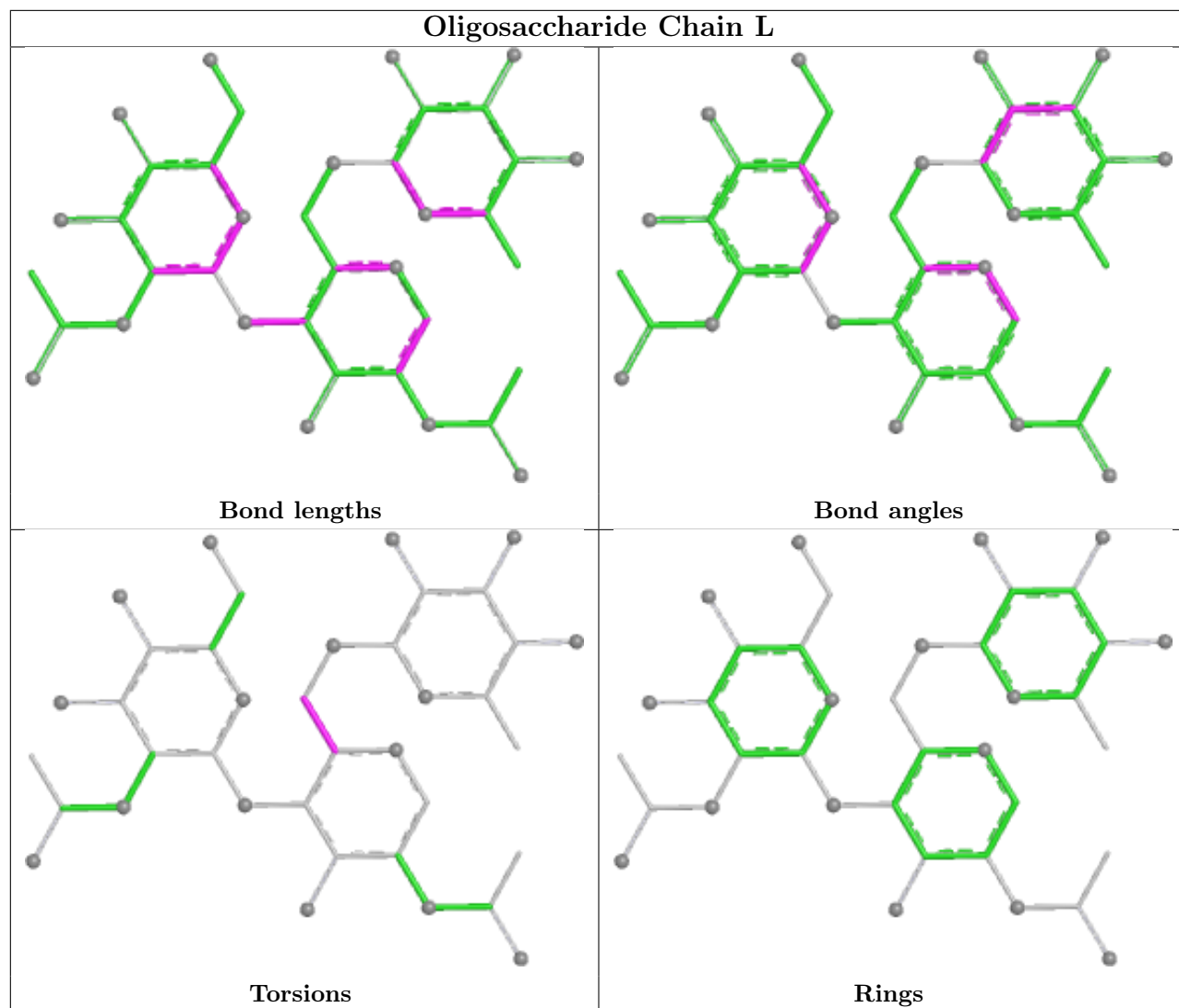


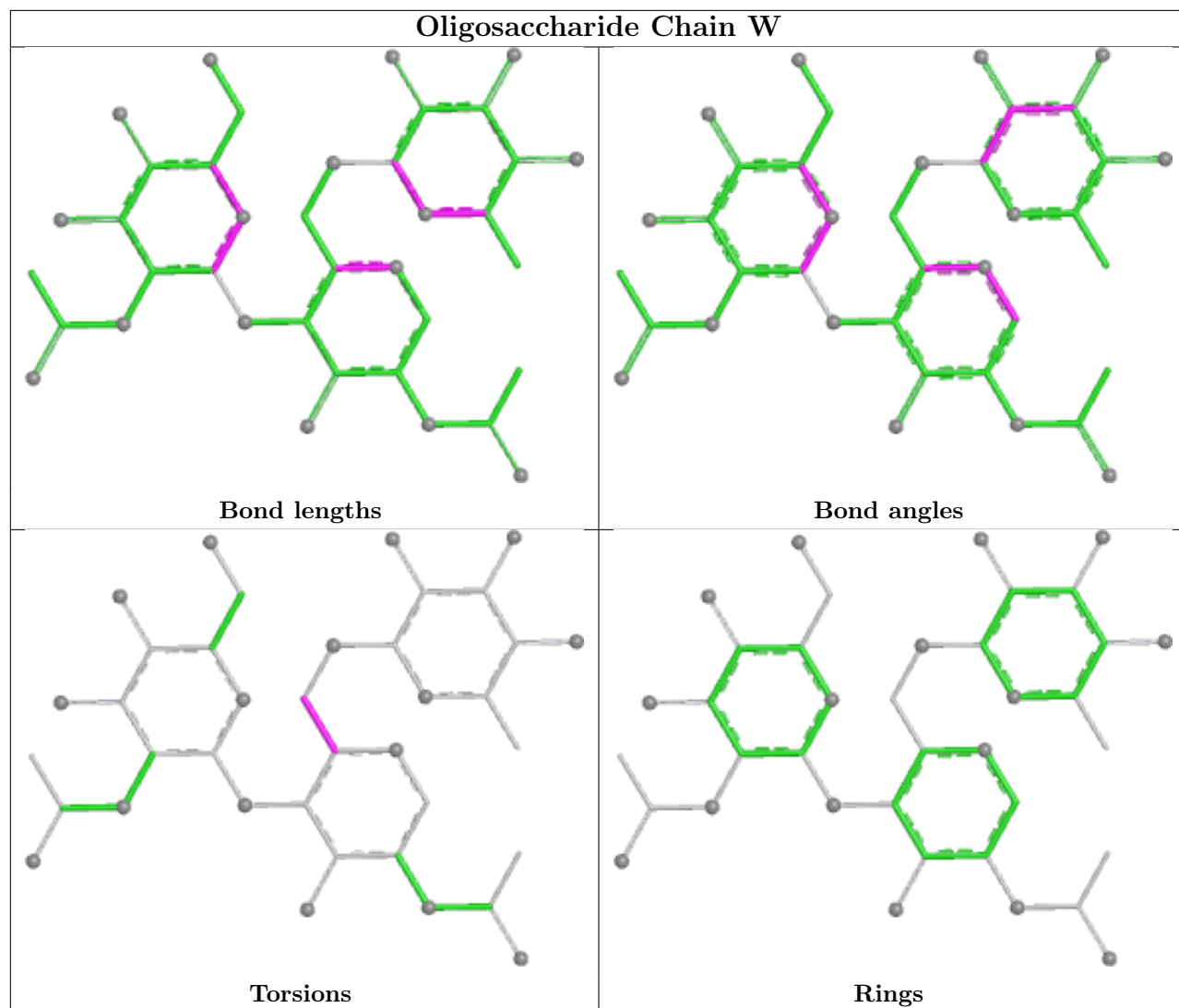


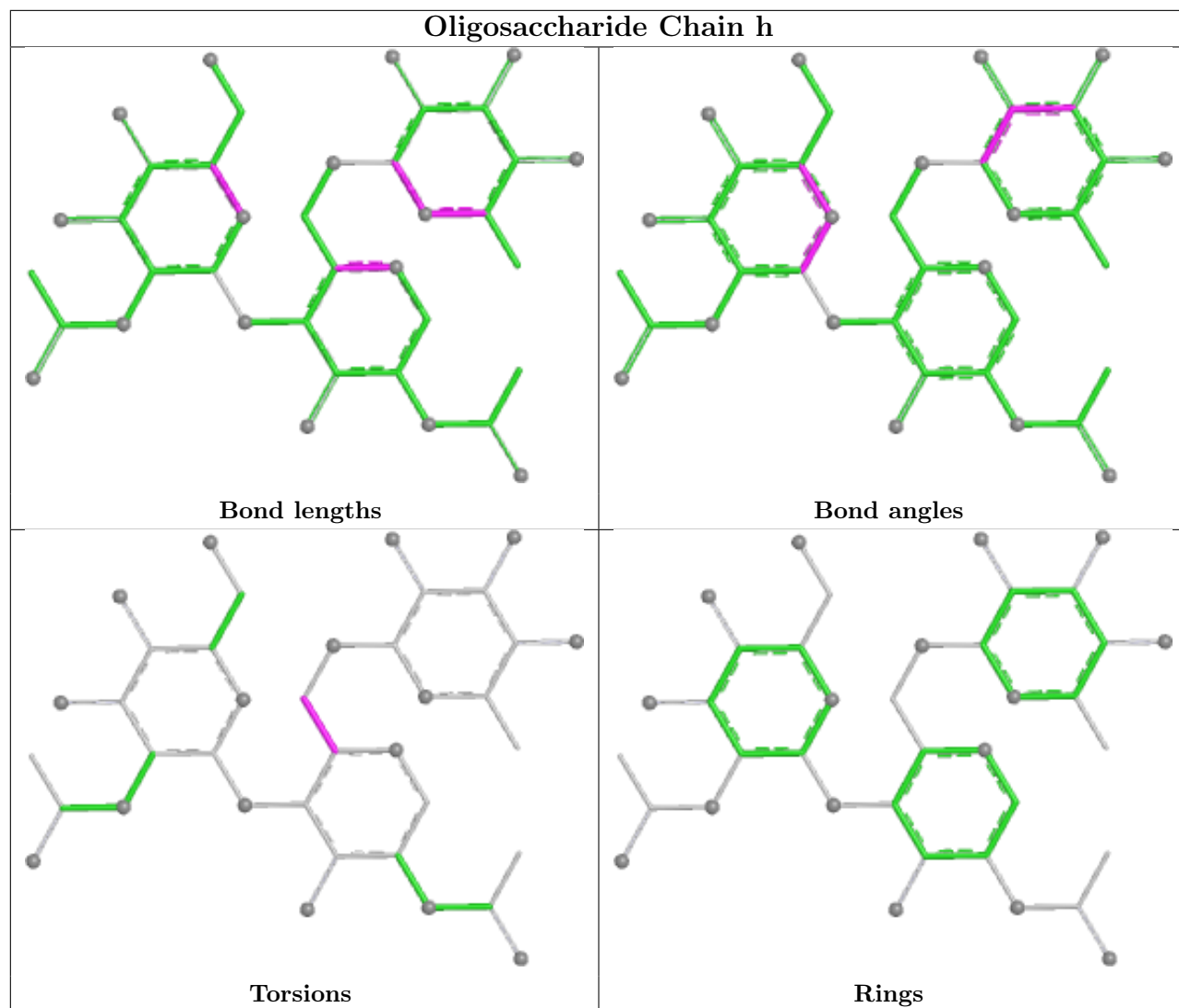


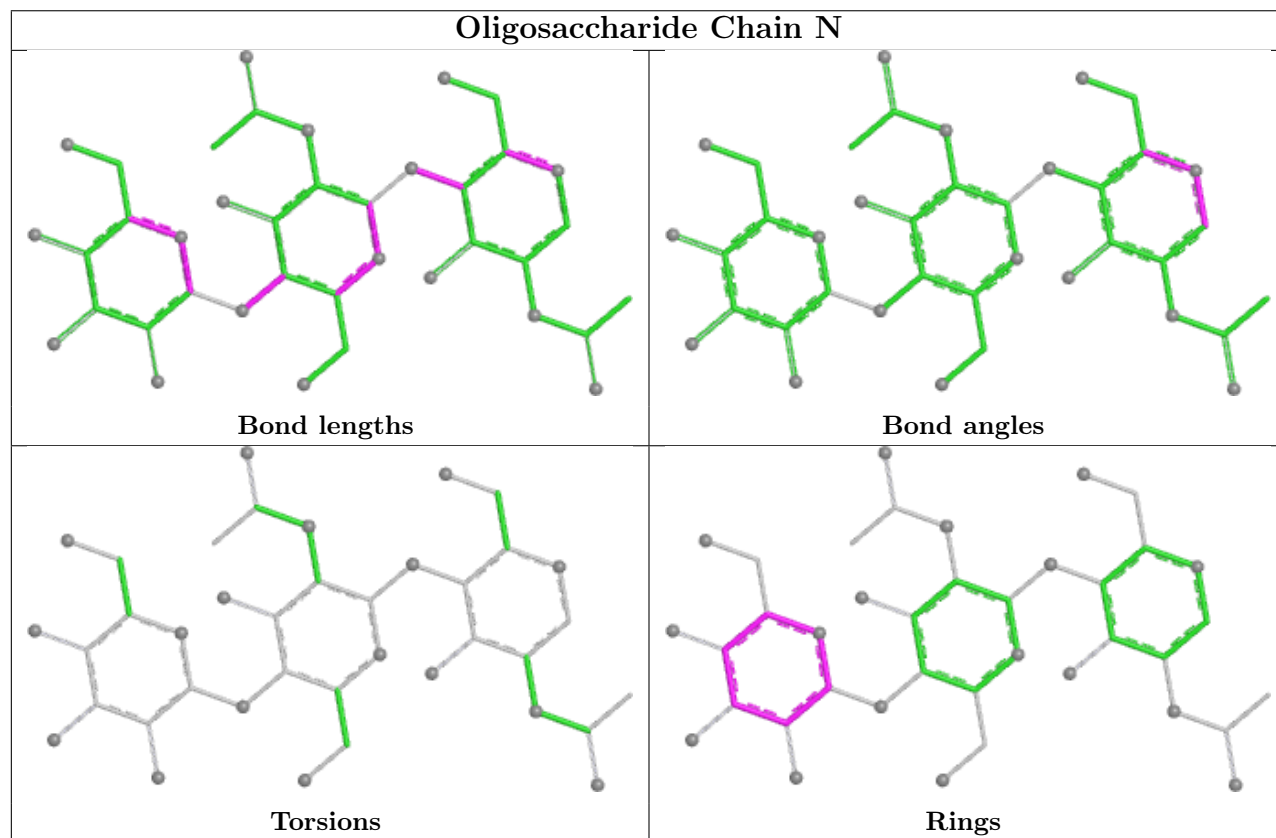
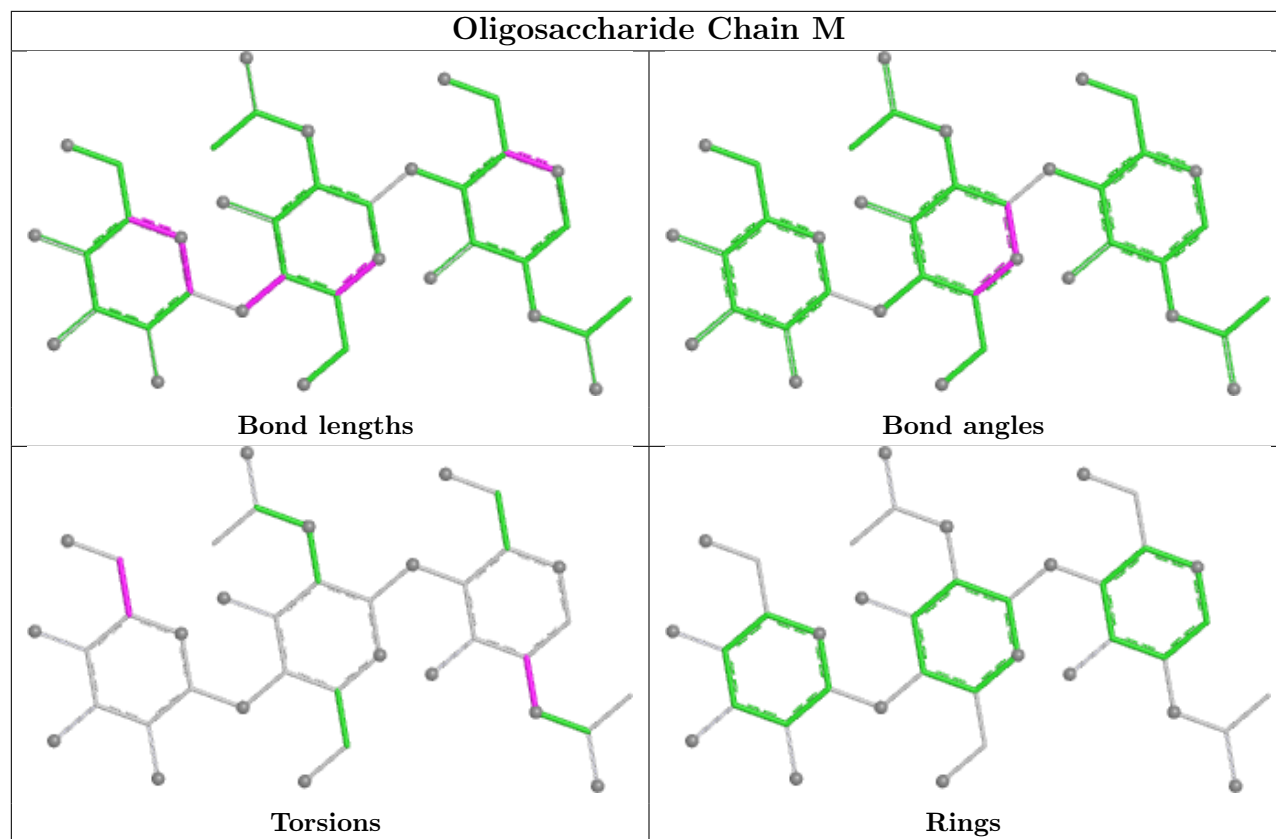


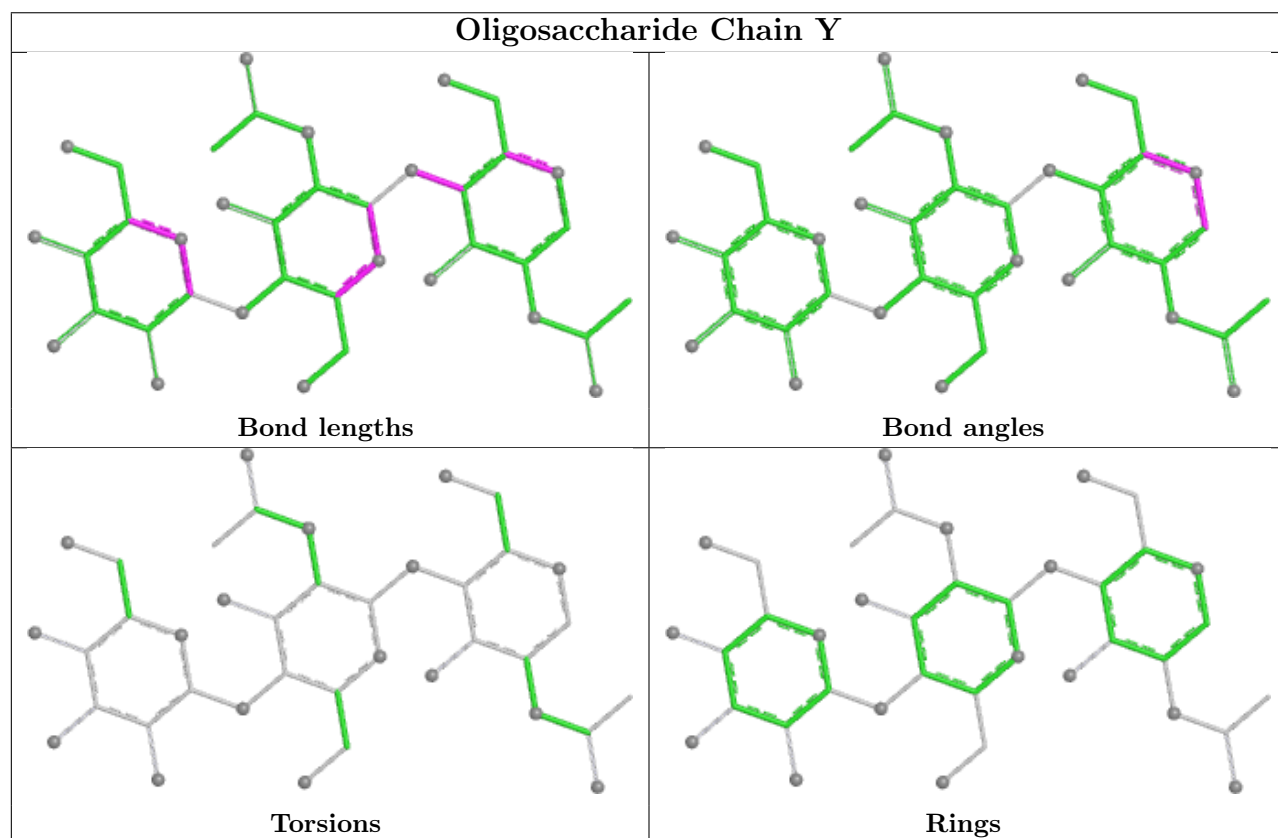
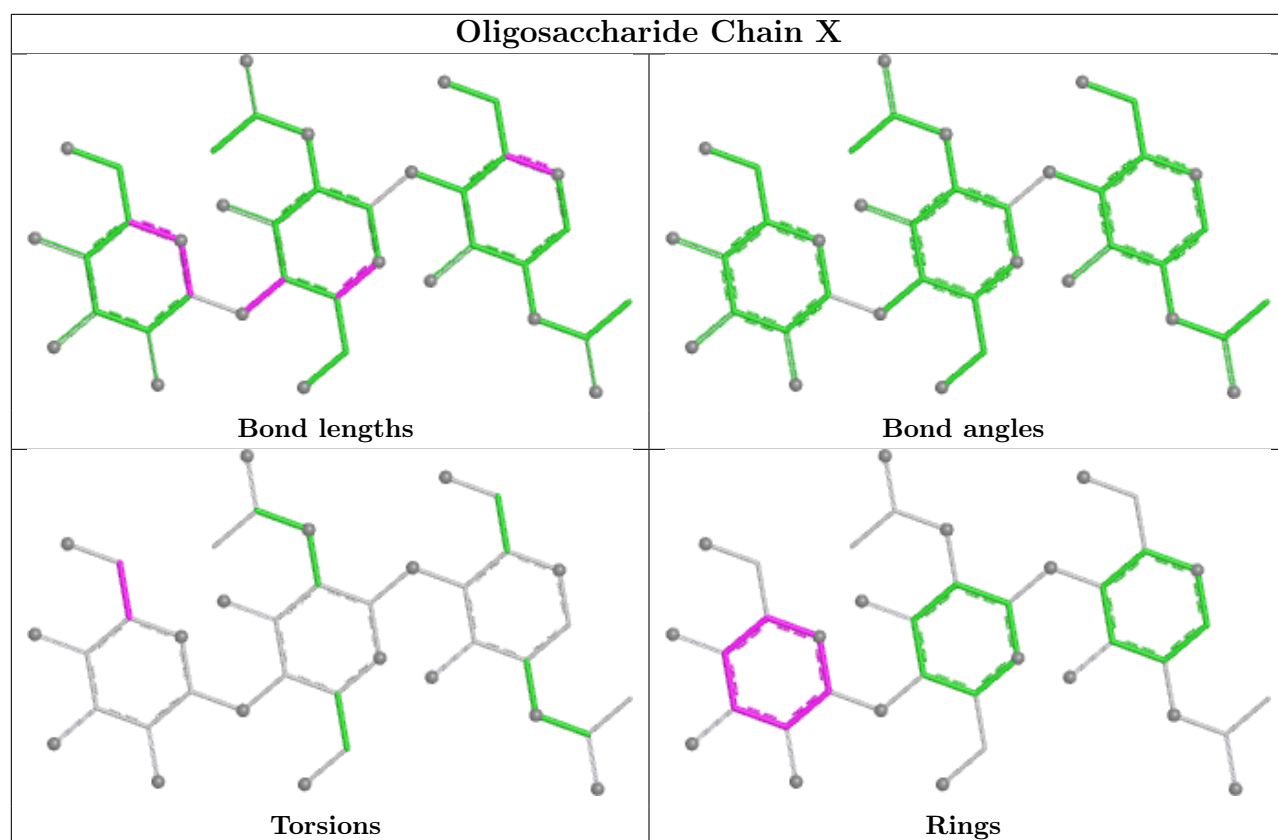


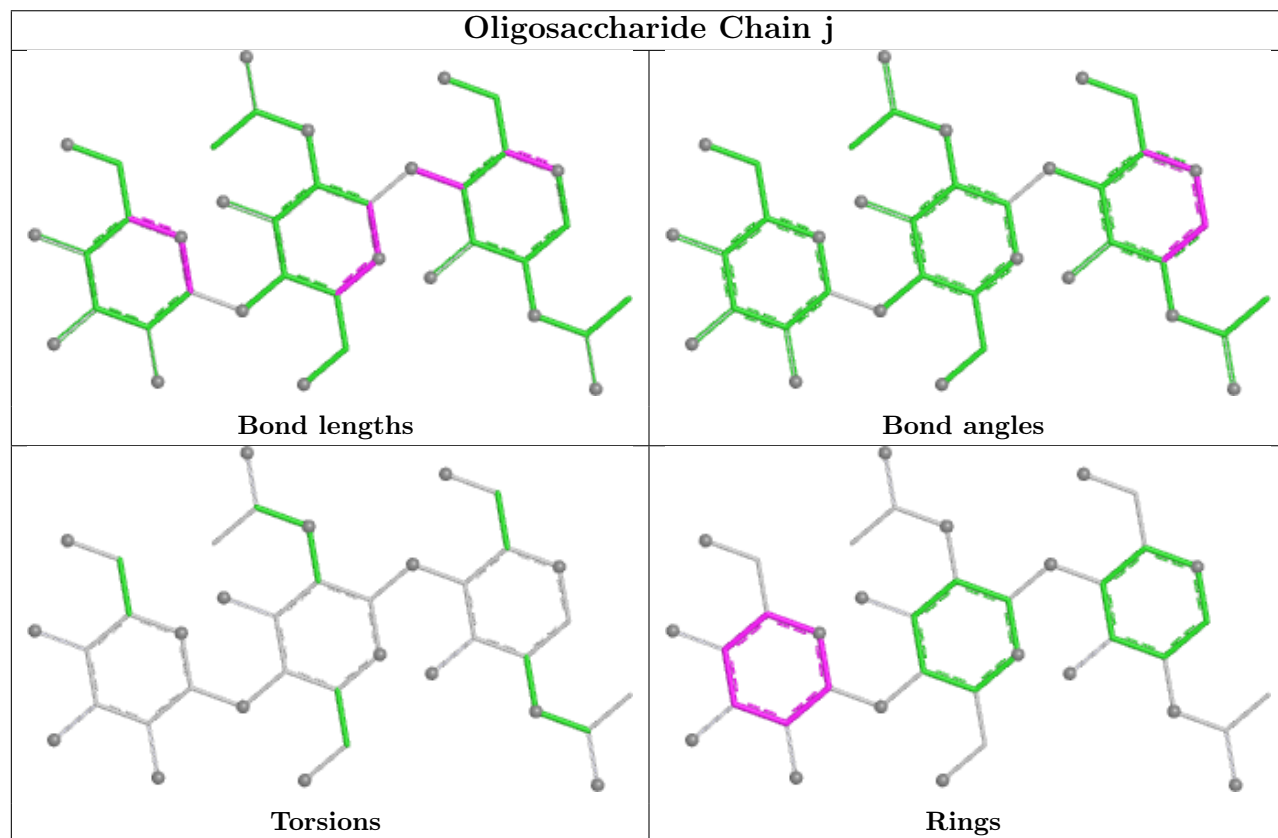
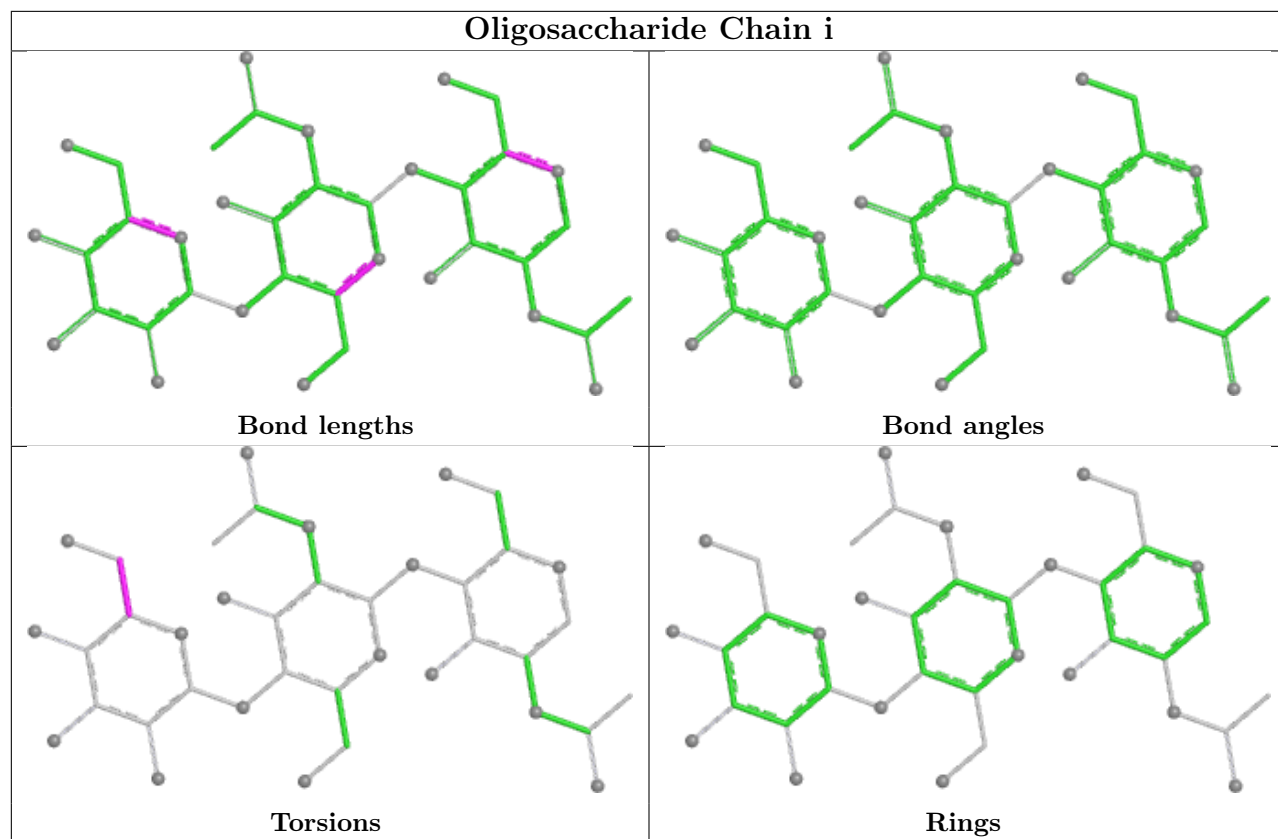












5.6 Ligand geometry

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1406	1	14,14,15	1.31	2 (14%)	17,19,21	0.78	0
5	NAG	C	1404	-	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	A	1407	1	14,14,15	1.23	1 (7%)	17,19,21	0.71	0
5	NAG	B	1403	-	14,14,15	1.22	2 (14%)	17,19,21	1.11	1 (5%)
5	NAG	A	1402	-	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	A	1406	1	14,14,15	1.30	2 (14%)	17,19,21	0.70	0
5	NAG	C	1407	1	14,14,15	1.19	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	A	1403	1	14,14,15	1.26	2 (14%)	17,19,21	1.08	1 (5%)
5	NAG	C	1403	1	14,14,15	1.27	2 (14%)	17,19,21	1.00	1 (5%)
5	NAG	A	1405	1	14,14,15	1.38	2 (14%)	17,19,21	0.91	1 (5%)
5	NAG	B	1408	-	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	C	1408	1	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	C	1406	1	14,14,15	1.30	1 (7%)	17,19,21	0.61	0
5	NAG	B	1404	-	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	A	1404	-	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	B	1402	-	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	B	1405	1	14,14,15	1.29	2 (14%)	17,19,21	1.00	1 (5%)
5	NAG	C	1401	1	14,14,15	1.30	1 (7%)	17,19,21	0.80	0
5	NAG	B	1401	1	14,14,15	1.22	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	A	1408	-	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	A	1401	1	14,14,15	1.21	1 (7%)	17,19,21	0.86	1 (5%)
5	NAG	C	1405	-	14,14,15	0.18	0	17,19,21	0.44	0
5	NAG	B	1407	1	14,14,15	1.23	2 (14%)	17,19,21	0.72	1 (5%)
5	NAG	C	1402	-	14,14,15	0.23	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1404	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1403	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1408	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1404	-	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	-	-	1/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1408	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	-	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	-	-	2/6/23/26	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1405	NAG	O5-C5	3.07	1.49	1.43
5	B	1406	NAG	O5-C5	3.03	1.49	1.43
5	A	1406	NAG	O5-C5	3.02	1.49	1.43
5	A	1405	NAG	O5-C5	2.92	1.49	1.43
5	C	1406	NAG	O5-C5	2.92	1.49	1.43
5	C	1401	NAG	O5-C5	2.82	1.48	1.43
5	A	1407	NAG	O5-C5	2.76	1.48	1.43
5	C	1407	NAG	O5-C5	2.68	1.48	1.43
5	B	1401	NAG	O5-C5	2.65	1.48	1.43
5	A	1403	NAG	O5-C5	2.59	1.48	1.43
5	A	1401	NAG	O5-C5	2.58	1.48	1.43
5	B	1407	NAG	O5-C5	2.53	1.48	1.43
5	B	1403	NAG	O5-C5	2.52	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1403	NAG	O5-C5	2.48	1.48	1.43
5	A	1403	NAG	C1-C2	2.41	1.55	1.52
5	A	1405	NAG	C1-C2	2.38	1.55	1.52
5	B	1403	NAG	C1-C2	2.37	1.55	1.52
5	C	1403	NAG	C1-C2	2.36	1.55	1.52
5	B	1407	NAG	C1-C2	2.12	1.55	1.52
5	B	1406	NAG	C1-C2	2.06	1.55	1.52
5	A	1406	NAG	C1-C2	2.04	1.55	1.52
5	B	1405	NAG	C1-C2	2.00	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1403	NAG	C1-O5-C5	3.07	116.30	112.19
5	B	1403	NAG	C1-O5-C5	2.89	116.06	112.19
5	B	1405	NAG	C1-O5-C5	2.85	116.00	112.19
5	B	1401	NAG	C1-O5-C5	2.81	115.95	112.19
5	A	1401	NAG	C1-O5-C5	2.71	115.82	112.19
5	C	1407	NAG	C1-O5-C5	2.66	115.75	112.19
5	A	1405	NAG	C1-O5-C5	2.33	115.31	112.19
5	C	1403	NAG	C1-O5-C5	2.26	115.22	112.19
5	B	1407	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1404	NAG	O5-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	C	1408	NAG	O5-C5-C6-O6
5	B	1408	NAG	O5-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6
5	C	1405	NAG	O5-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	C	1405	NAG	C4-C5-C6-O6
5	B	1408	NAG	C4-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1401	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	A	1401	NAG	C1-C2-N2-C7

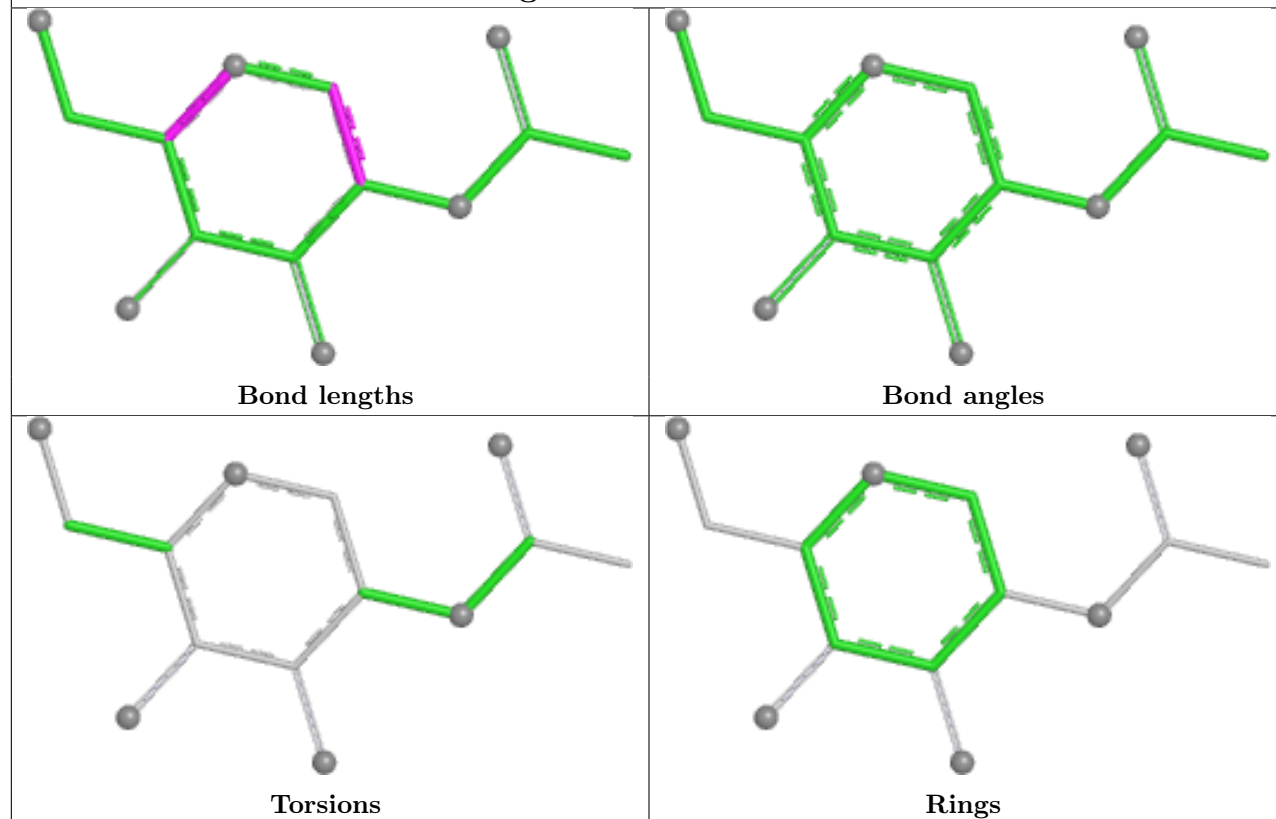
There are no ring outliers.

10 monomers are involved in 27 short contacts:

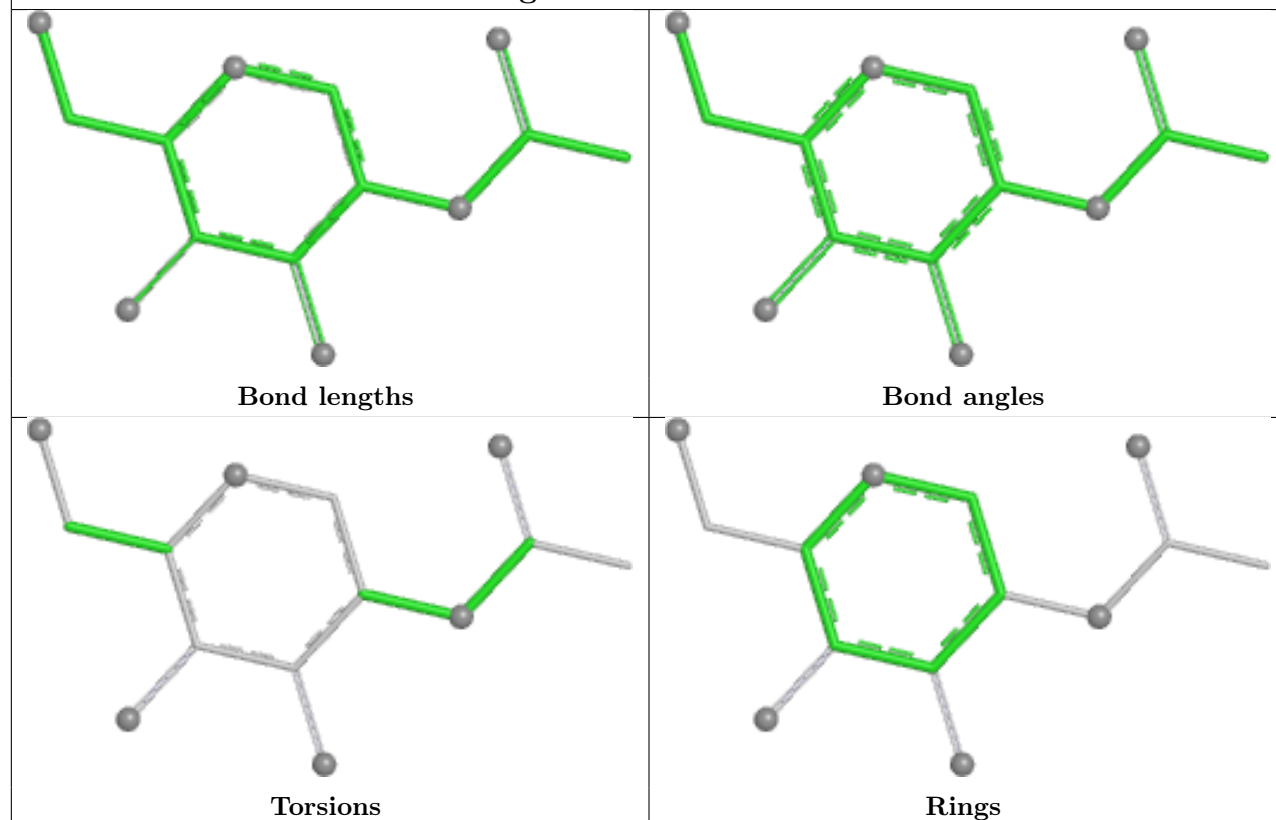
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1404	NAG	3	0
5	B	1403	NAG	4	0
5	A	1402	NAG	3	0
5	B	1408	NAG	2	0
5	B	1404	NAG	3	0
5	A	1404	NAG	3	0
5	B	1402	NAG	3	0
5	C	1401	NAG	1	0
5	A	1408	NAG	2	0
5	C	1402	NAG	3	0

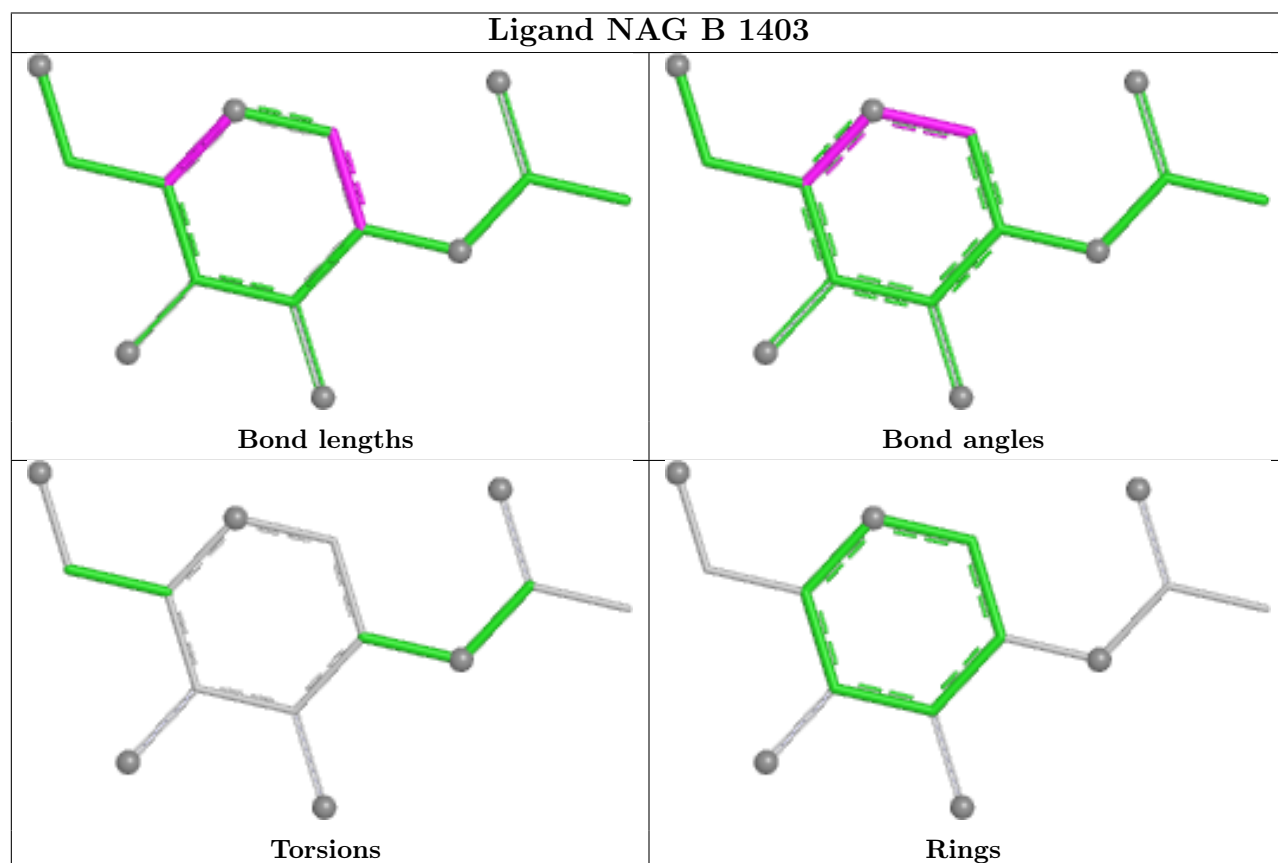
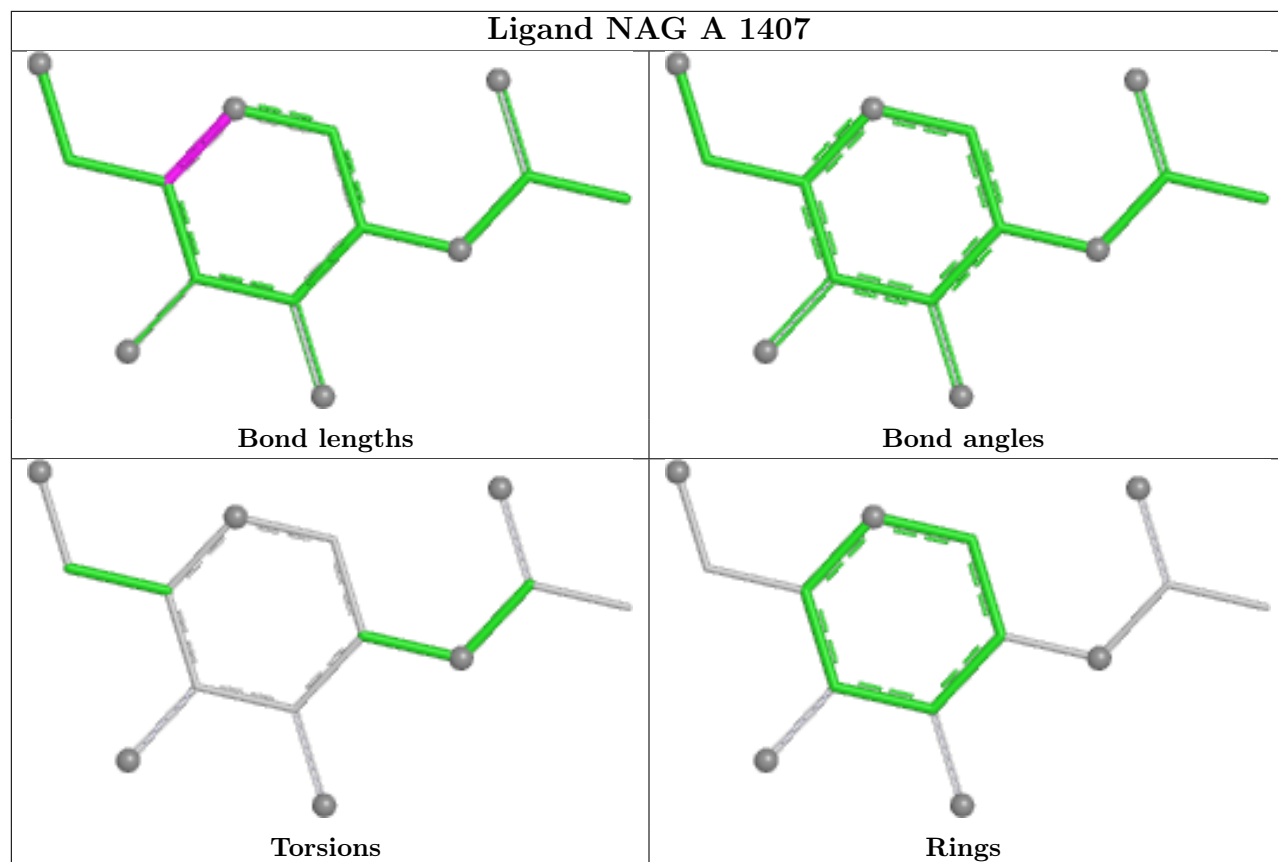
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

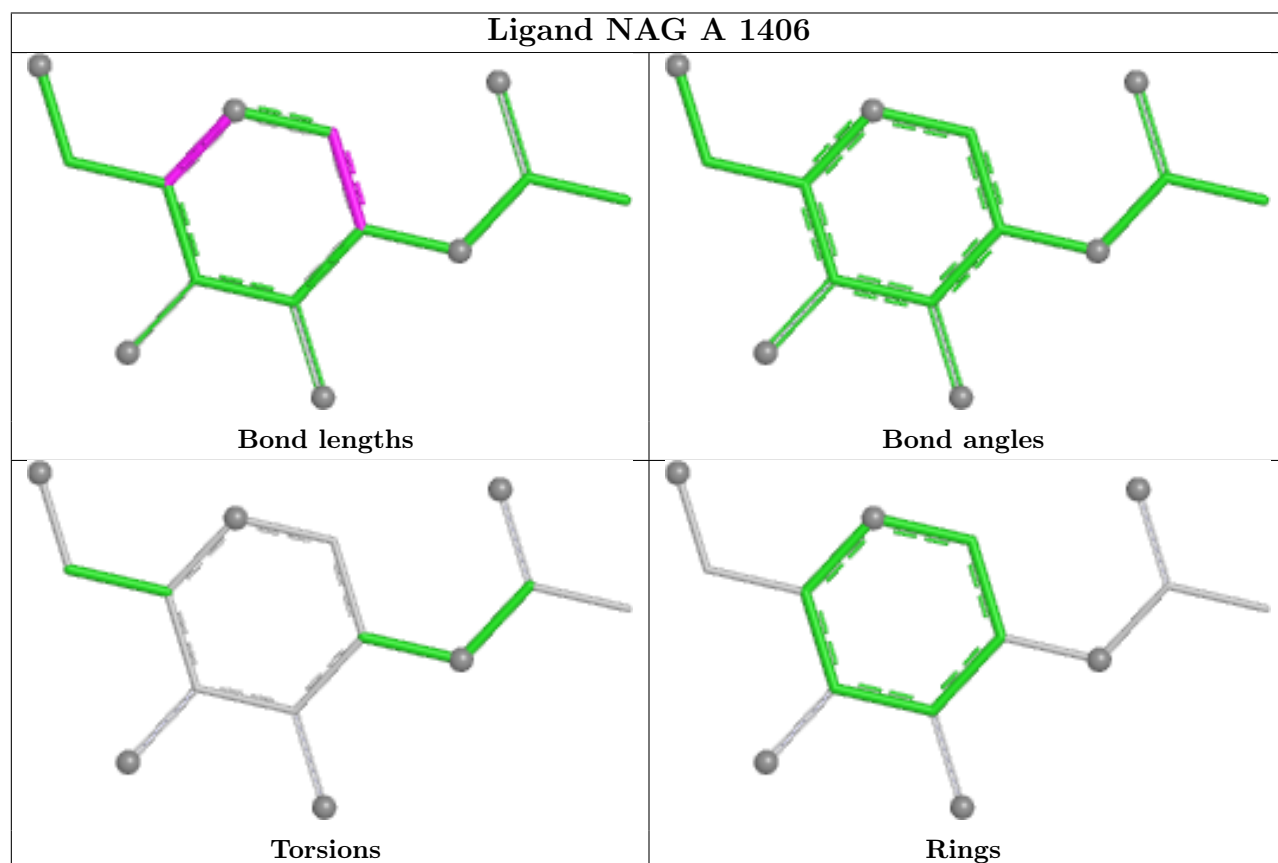
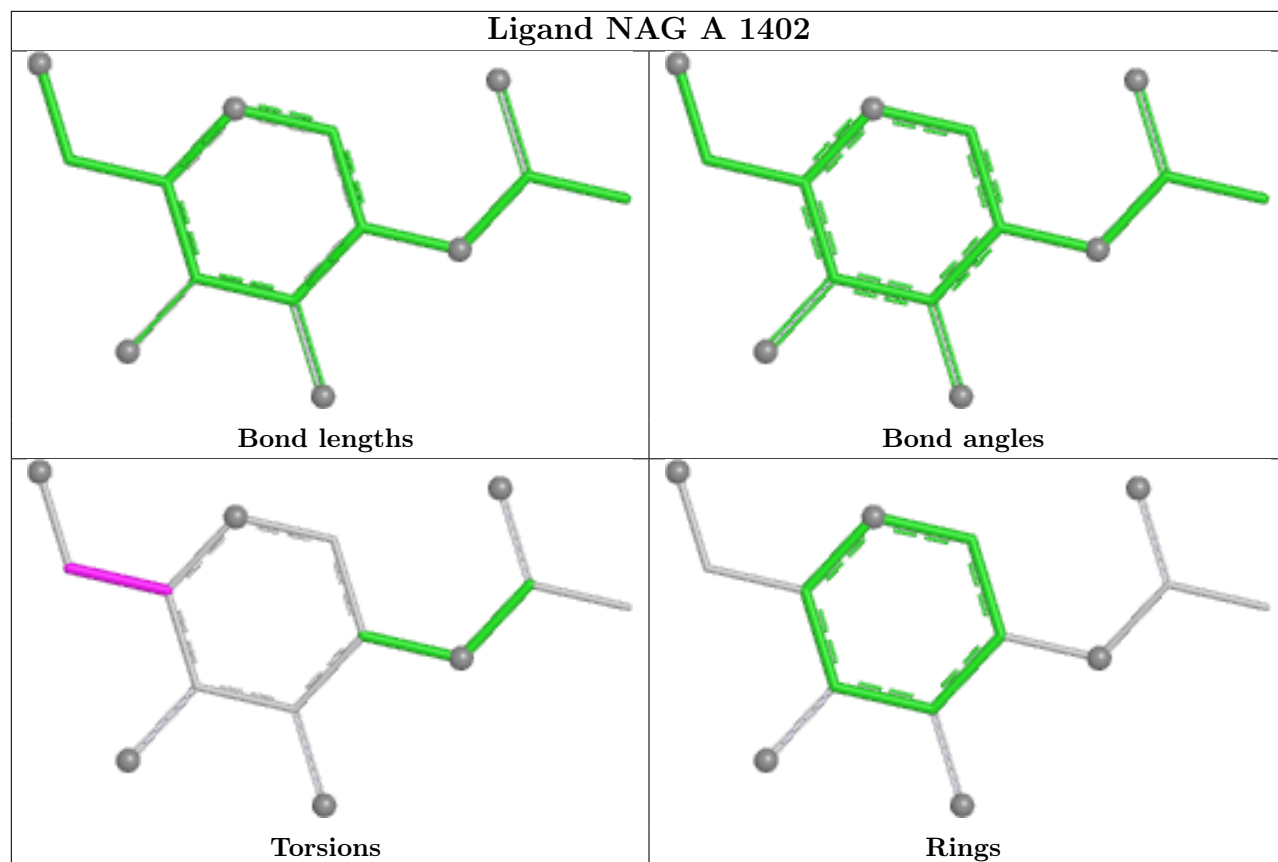
Ligand NAG B 1406



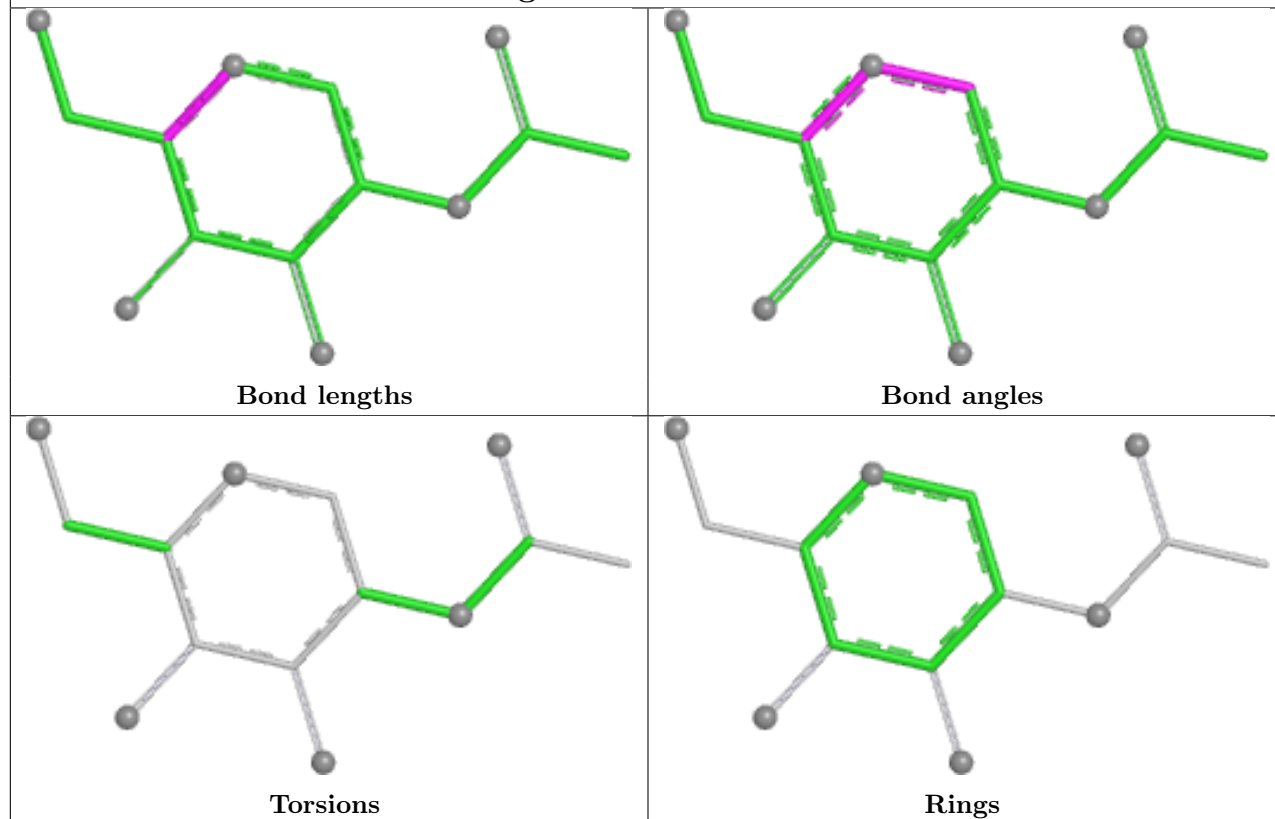
Ligand NAG C 1404



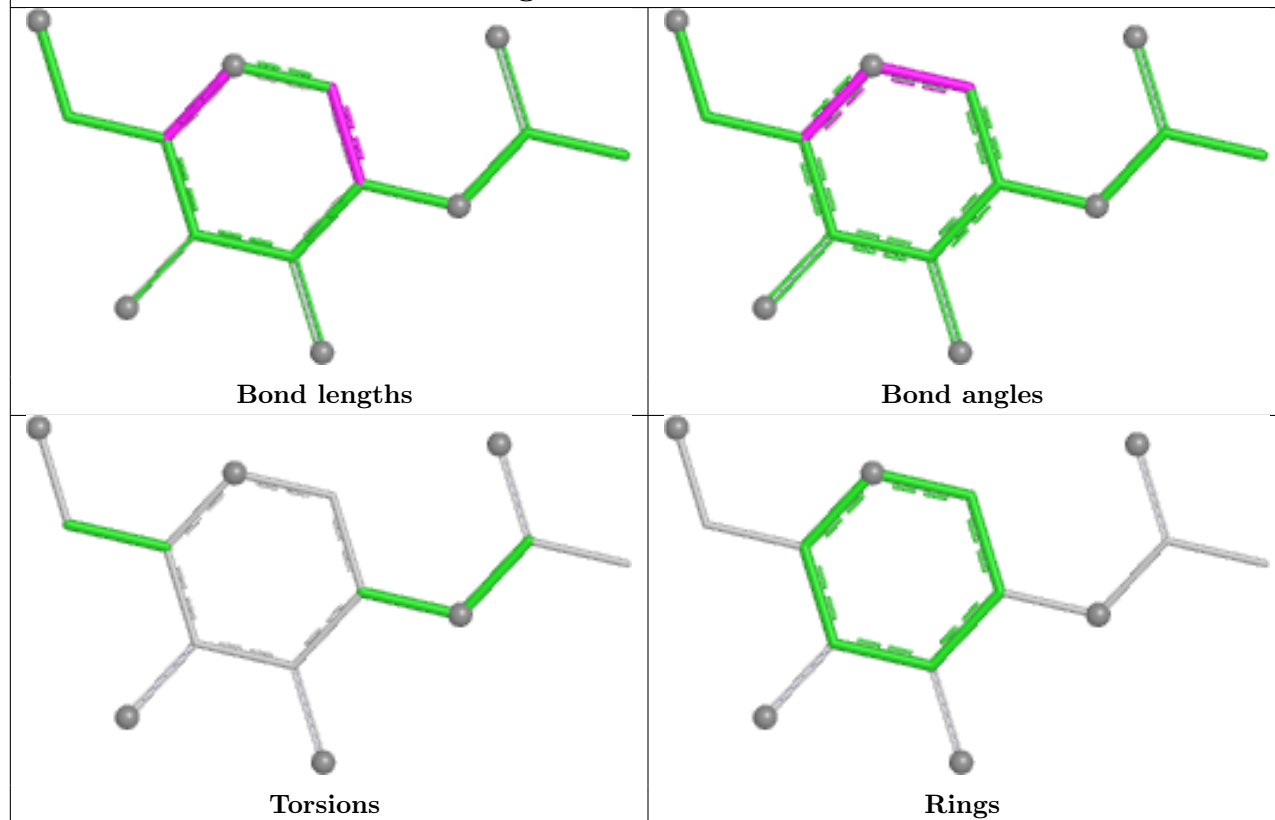




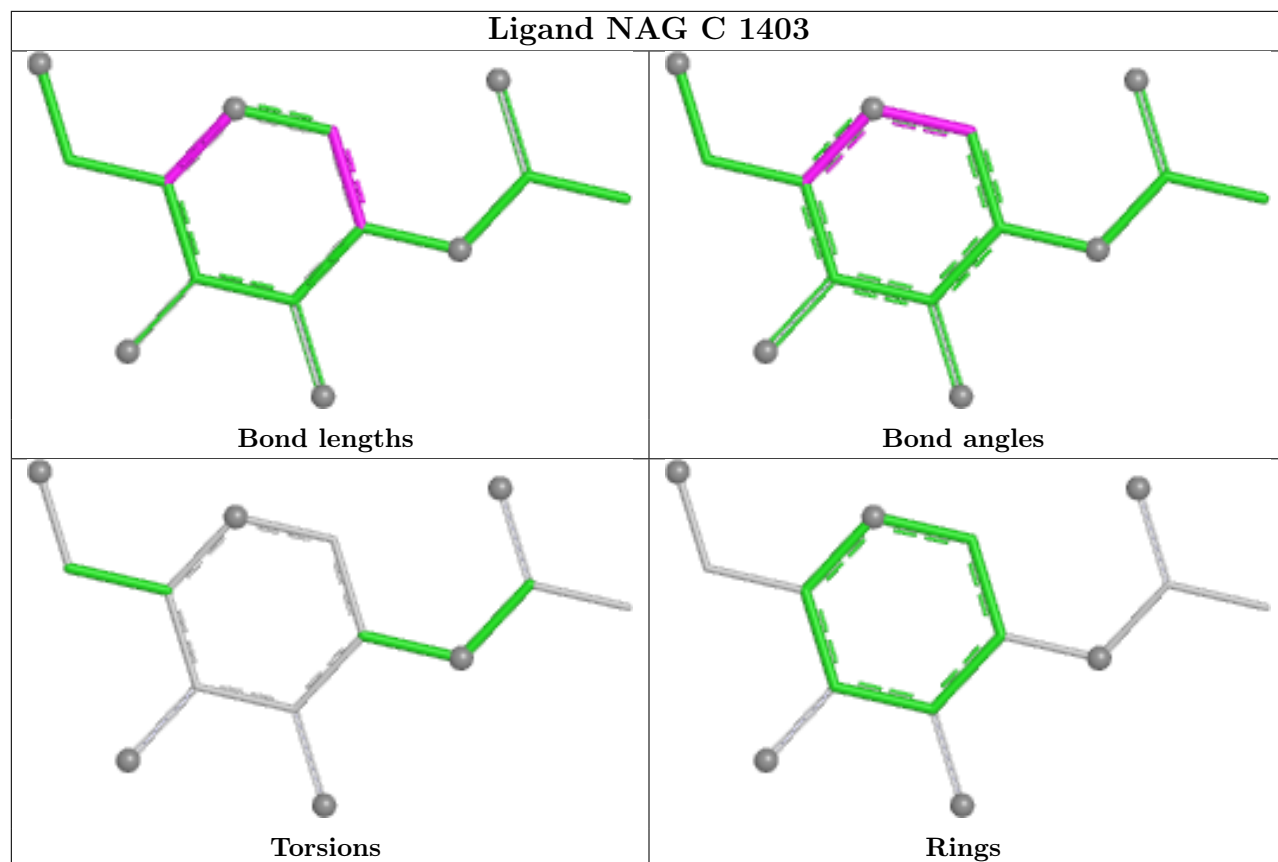
Ligand NAG C 1407



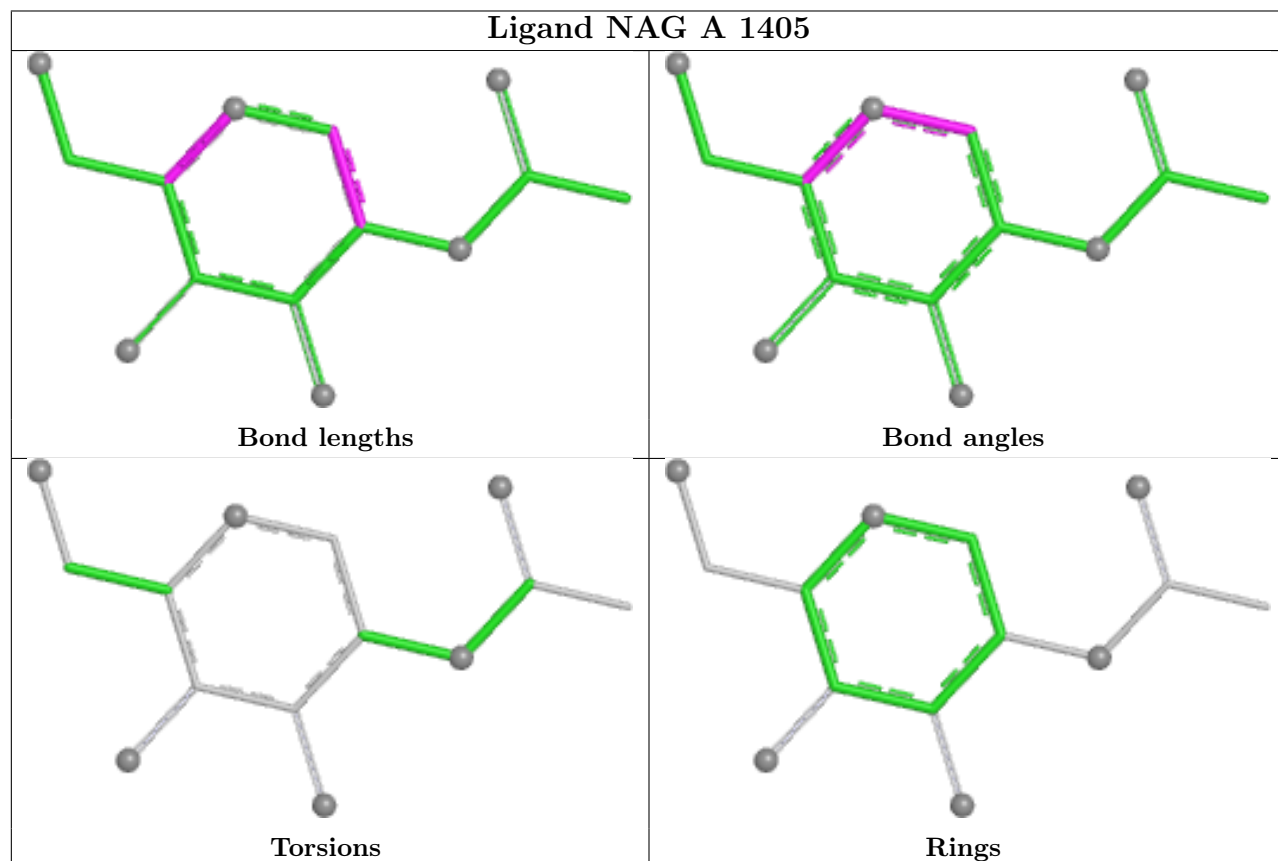
Ligand NAG A 1403



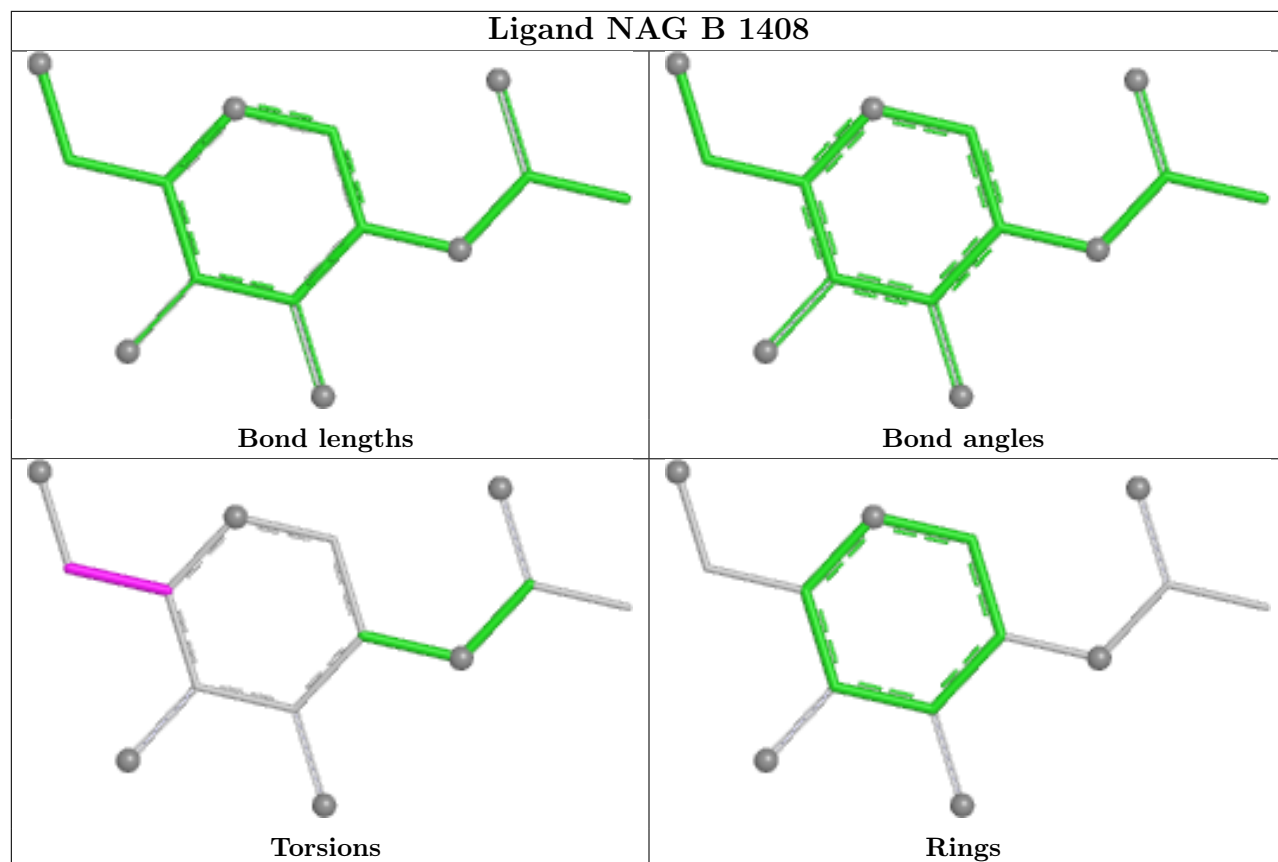
Ligand NAG C 1403



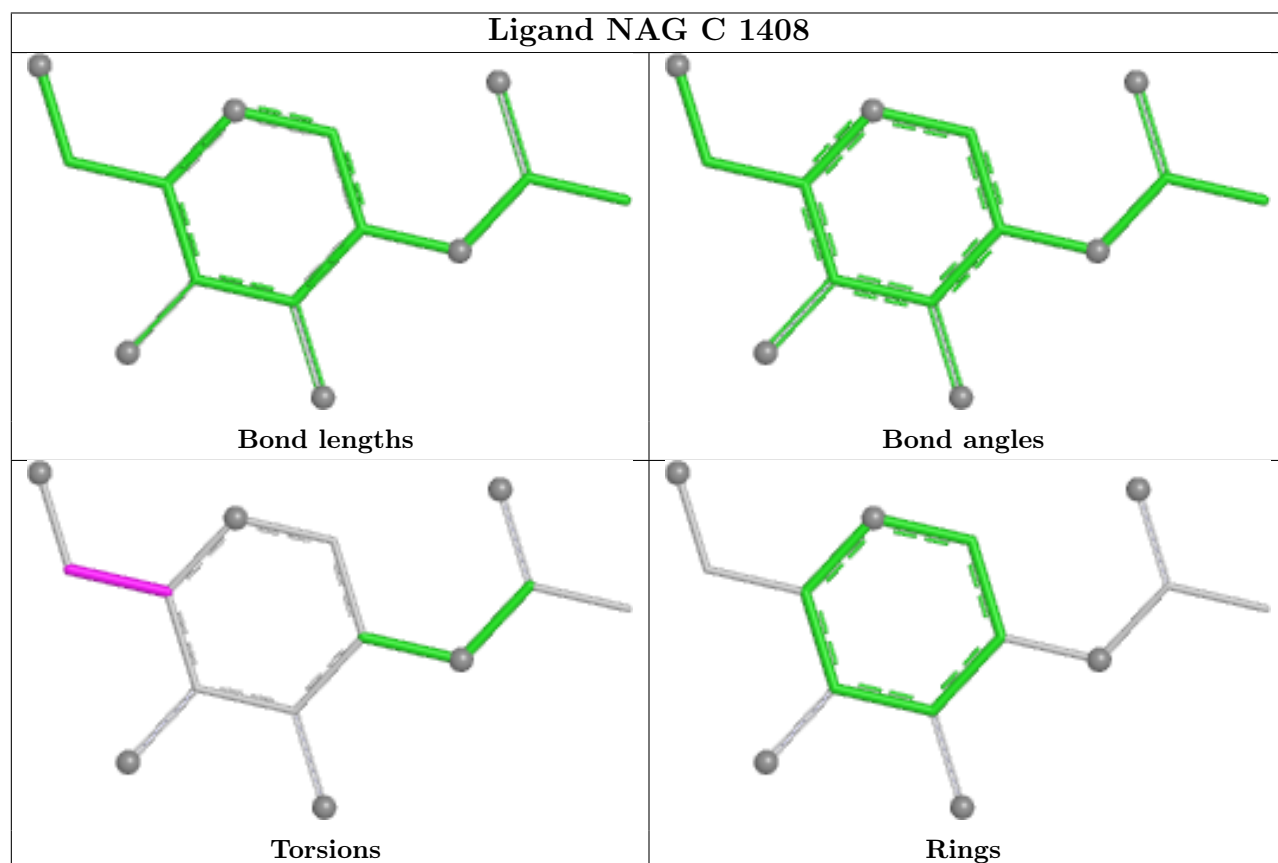
Ligand NAG A 1405



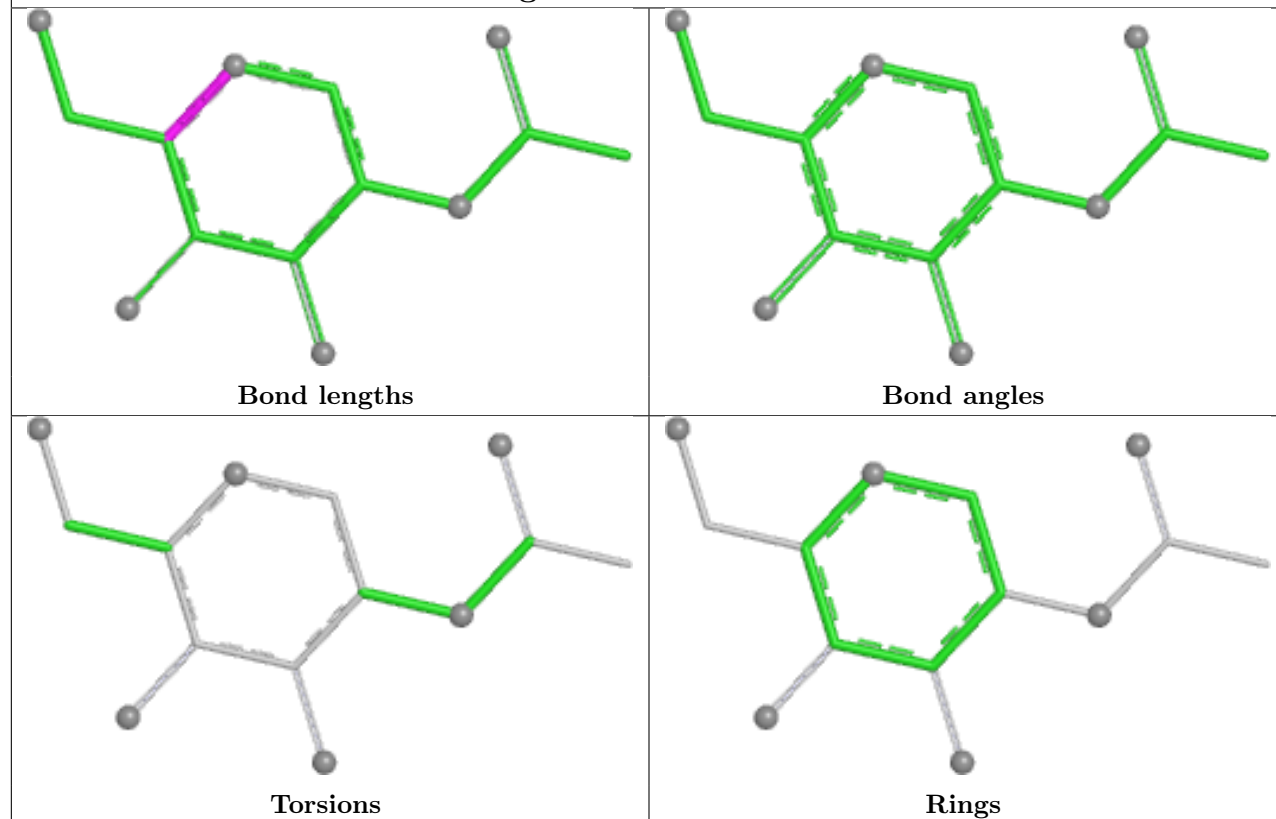
Ligand NAG B 1408



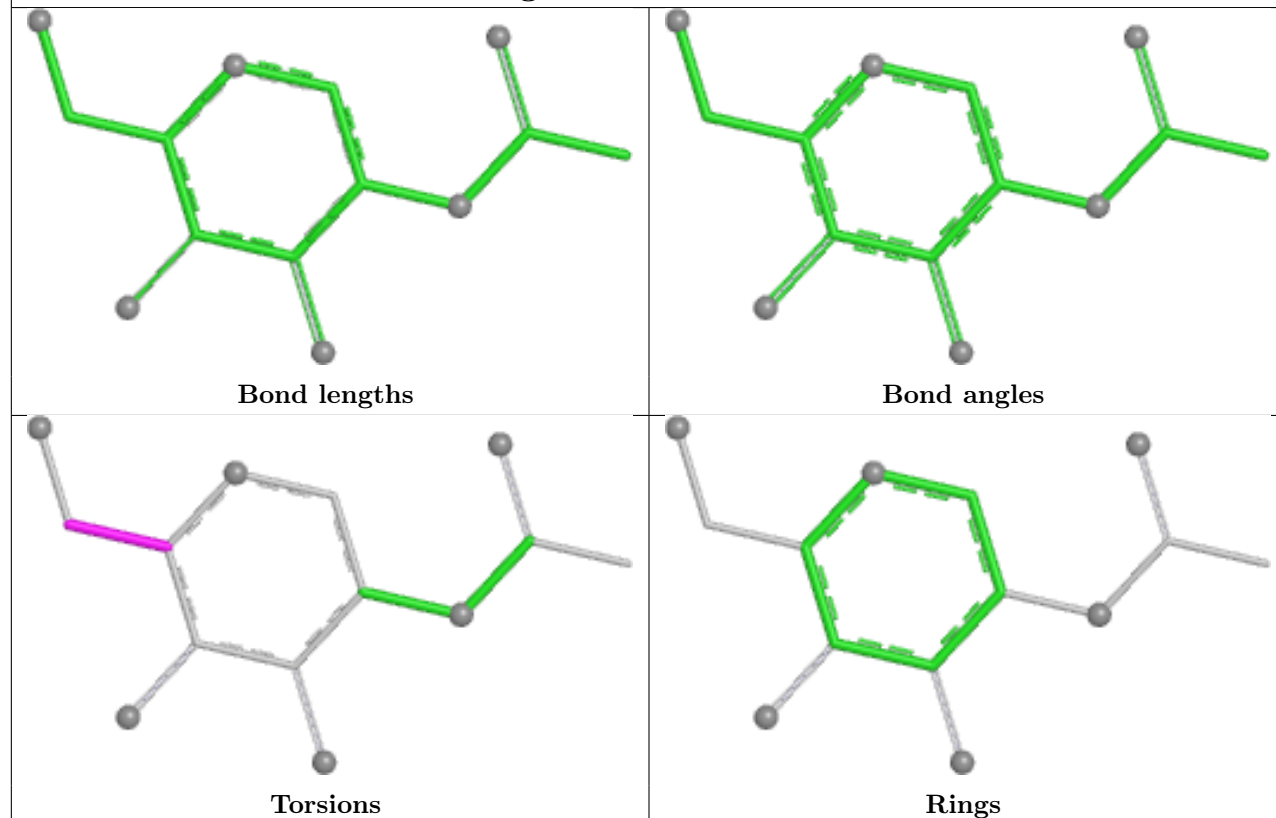
Ligand NAG C 1408



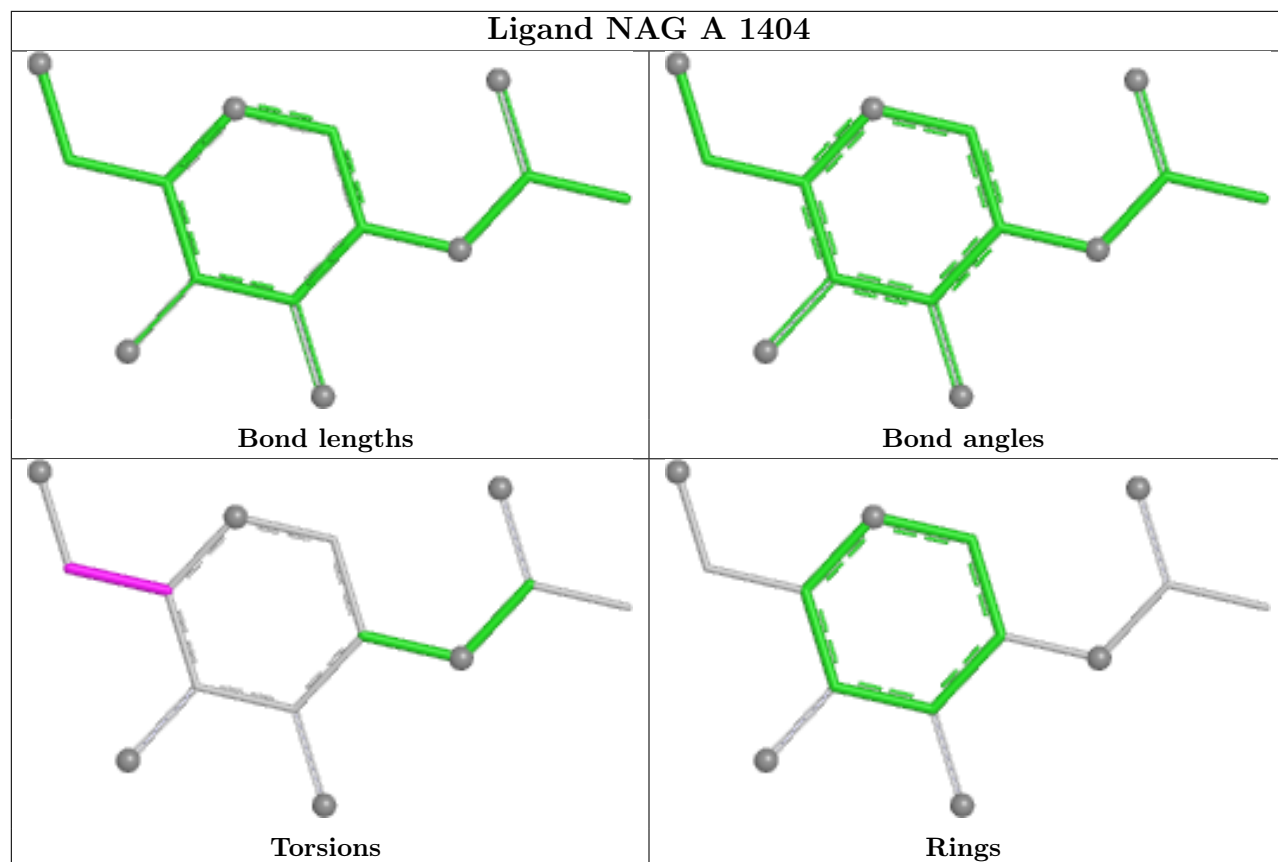
Ligand NAG C 1406



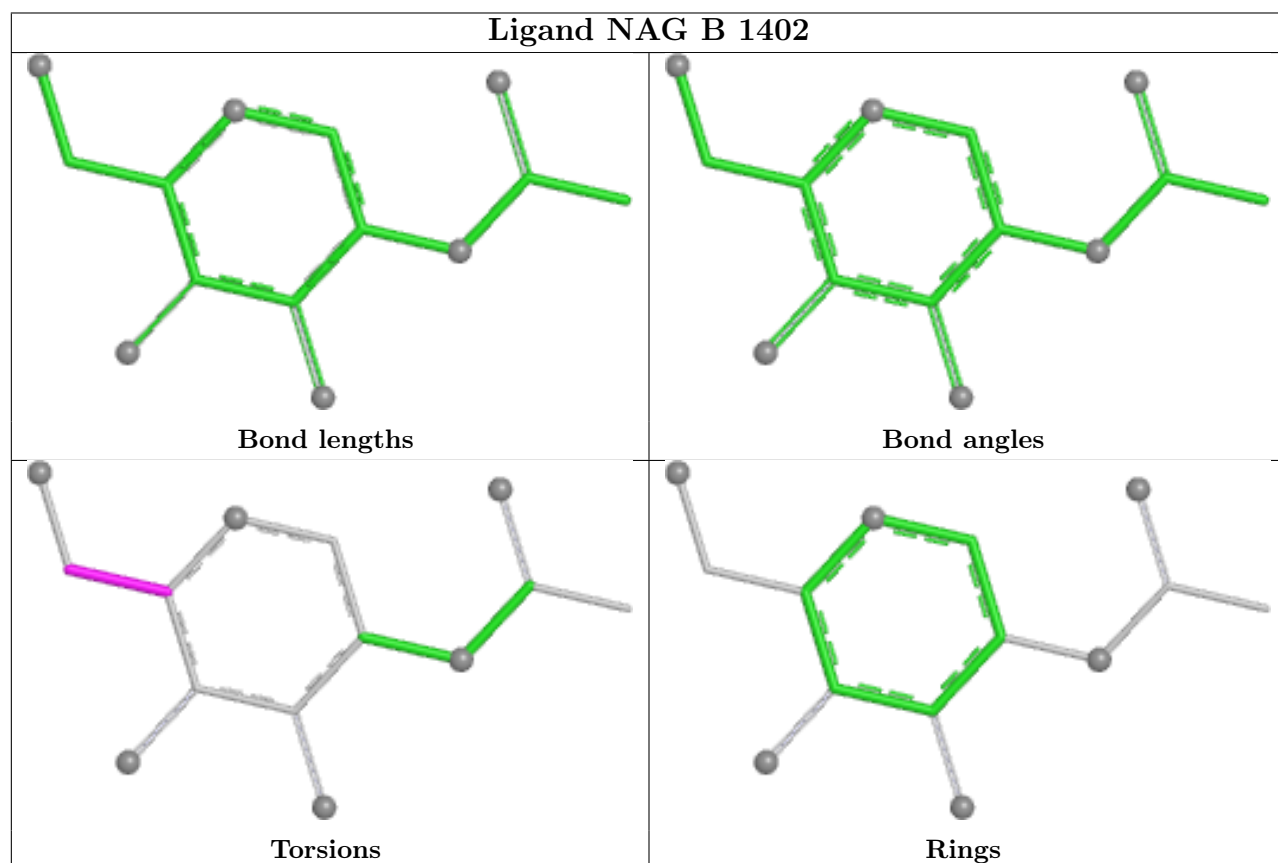
Ligand NAG B 1404



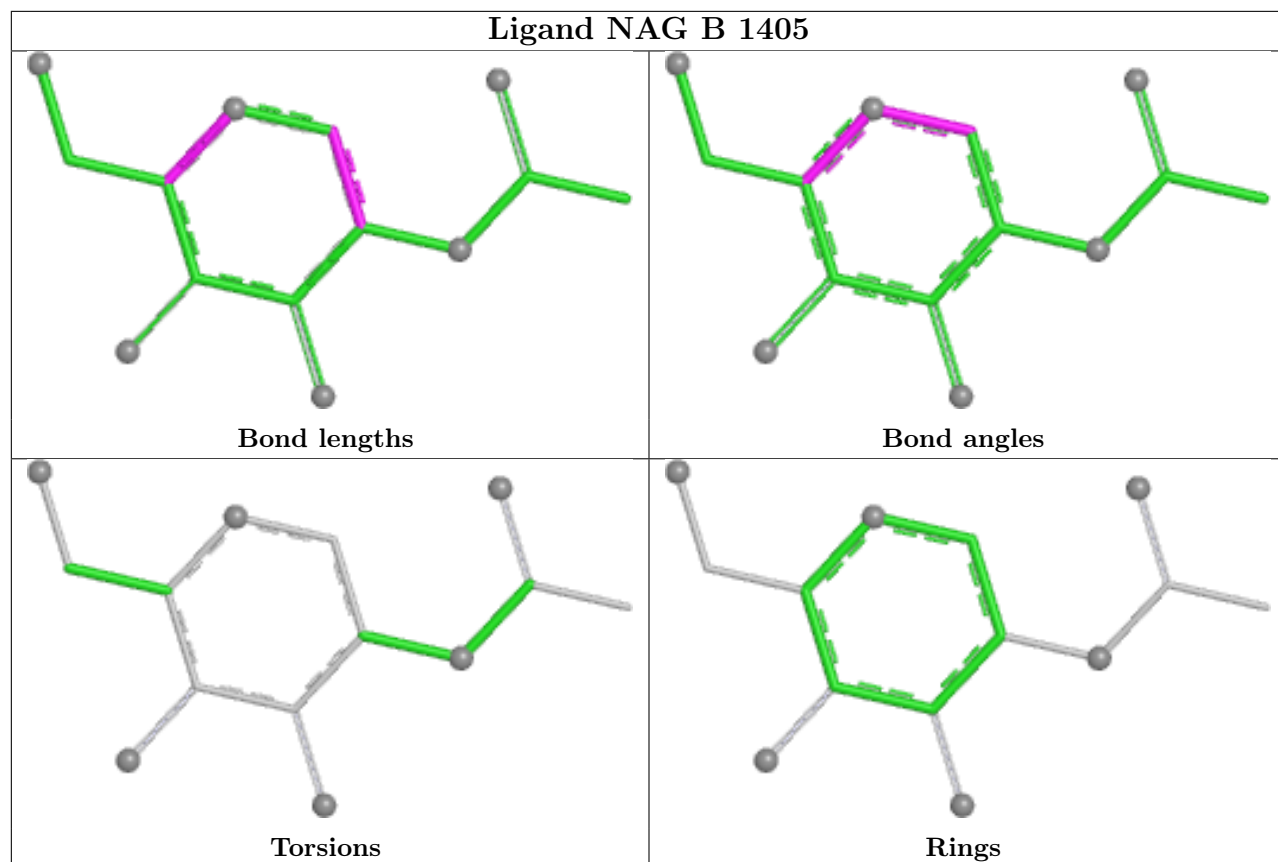
Ligand NAG A 1404



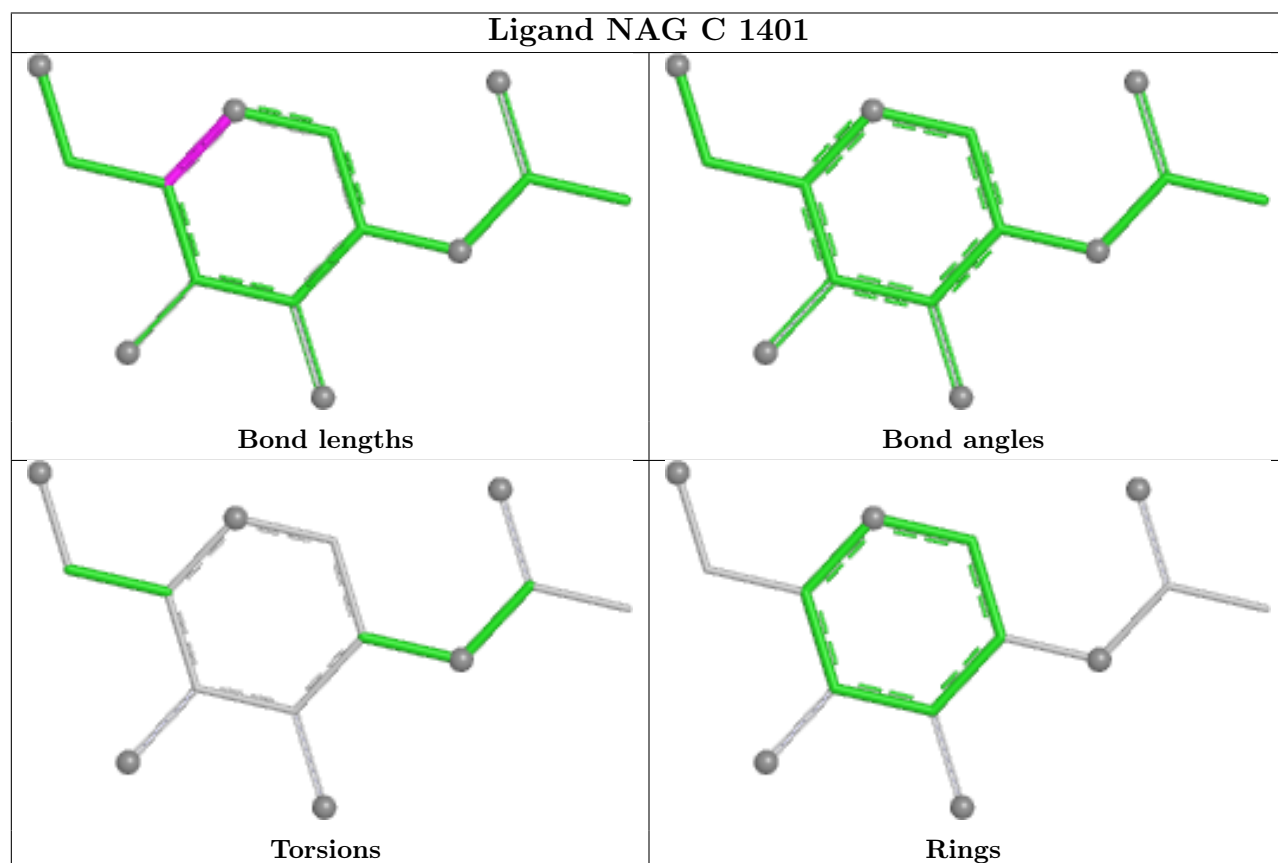
Ligand NAG B 1402



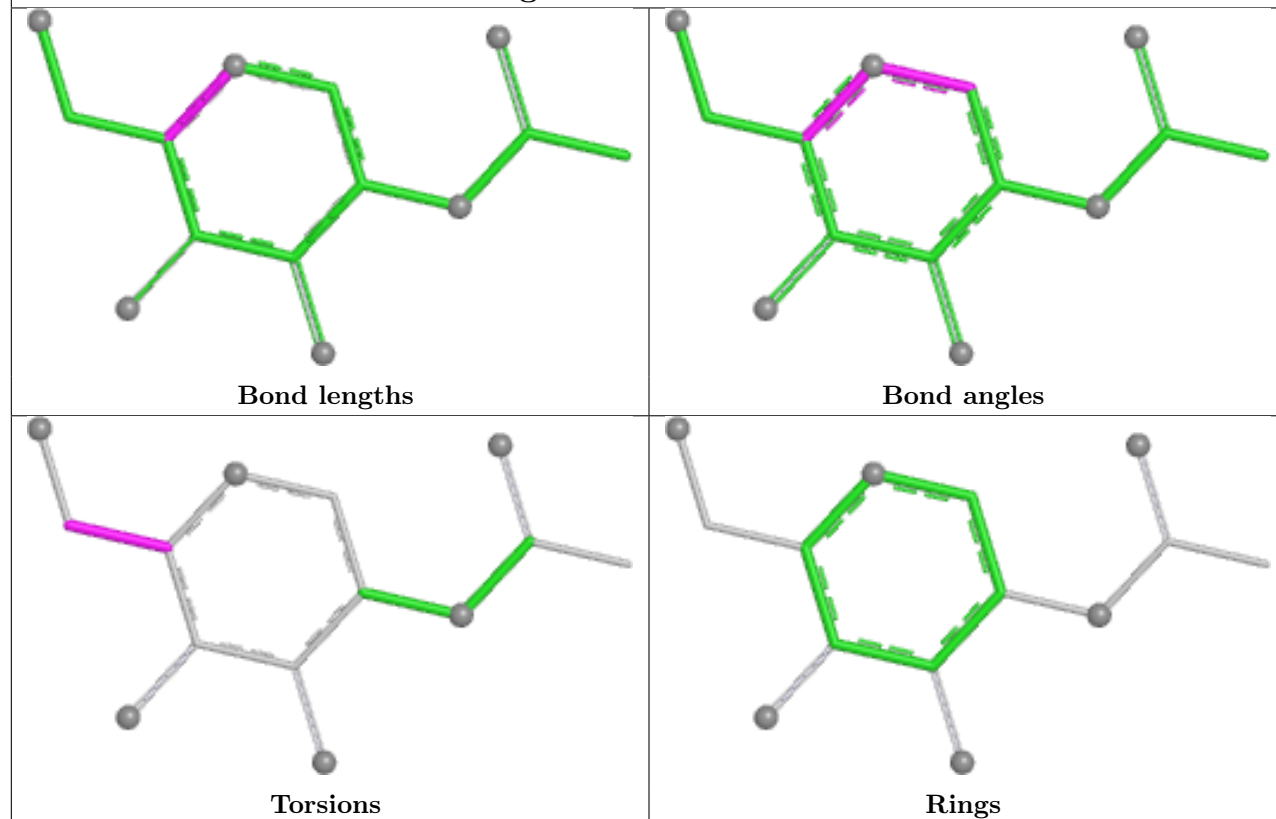
Ligand NAG B 1405



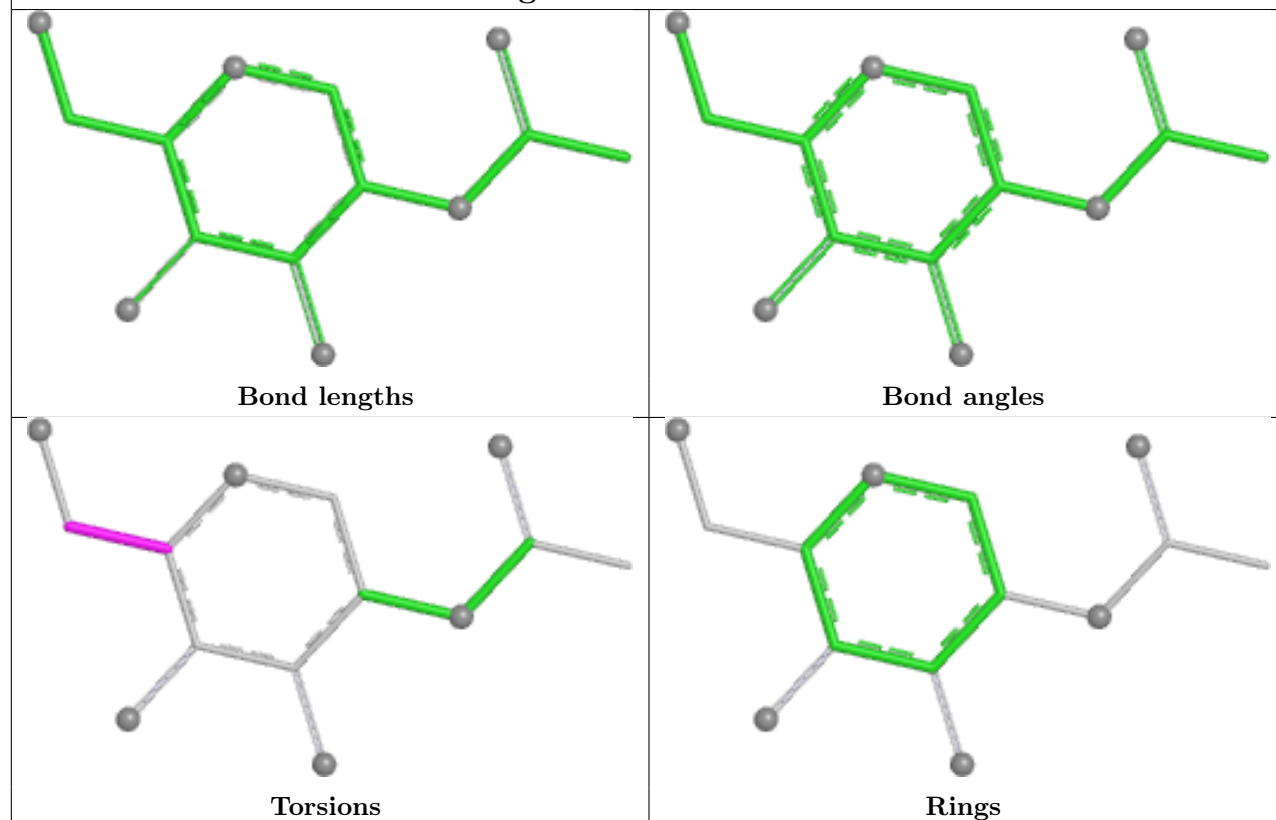
Ligand NAG C 1401



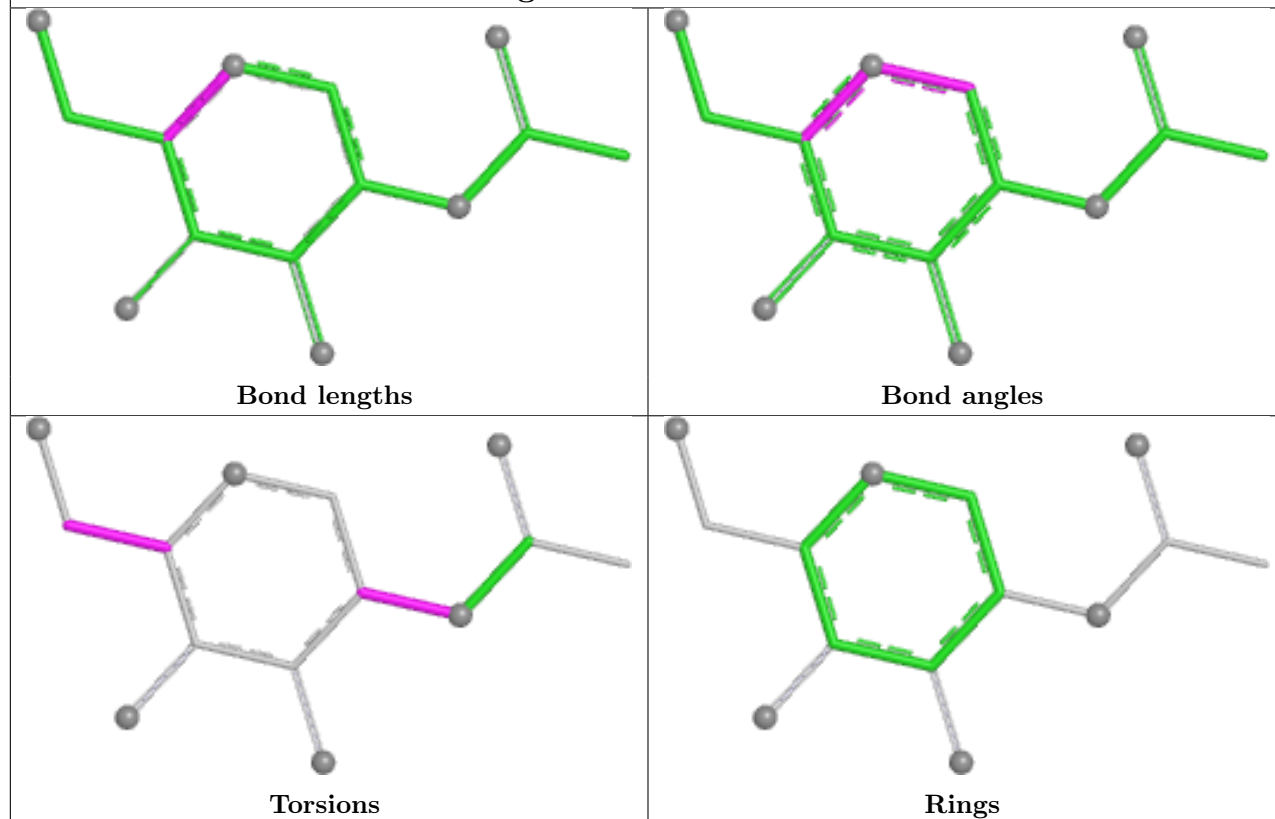
Ligand NAG B 1401



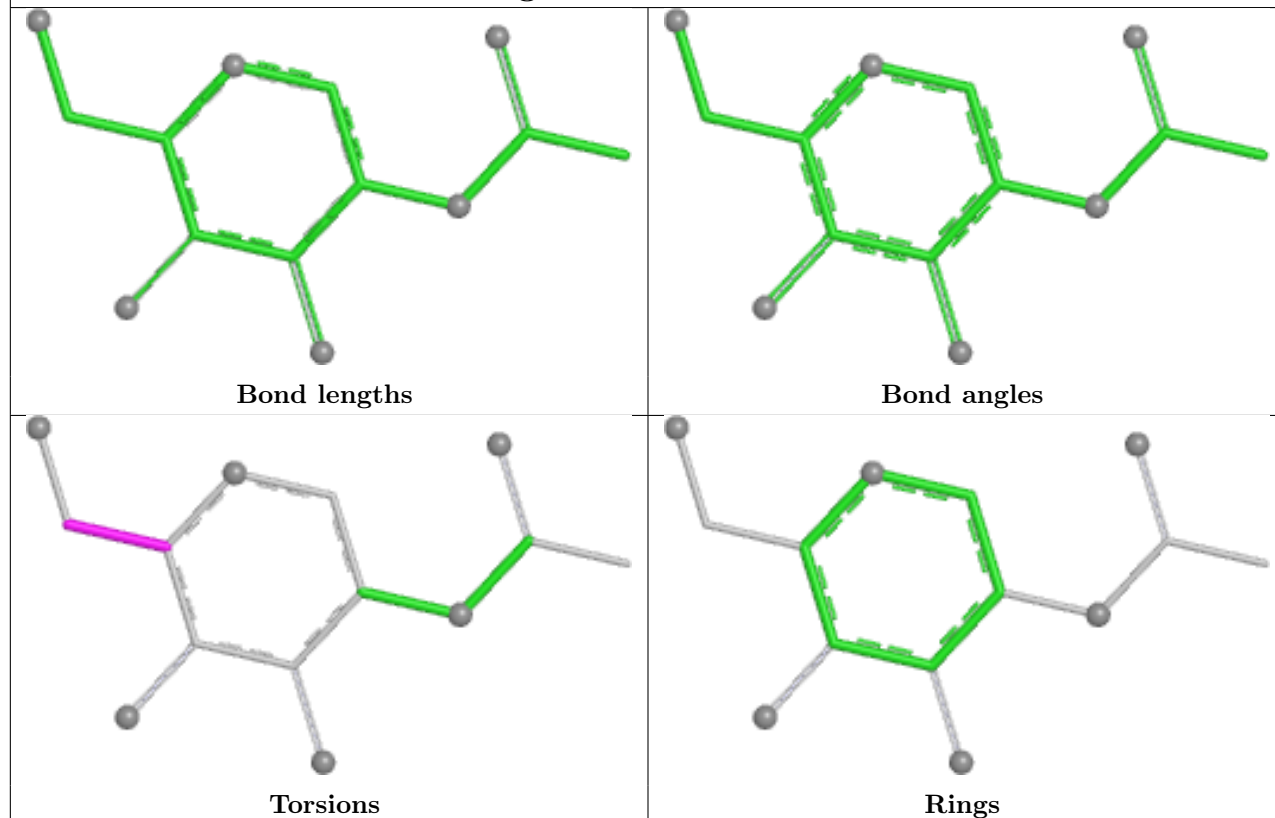
Ligand NAG A 1408

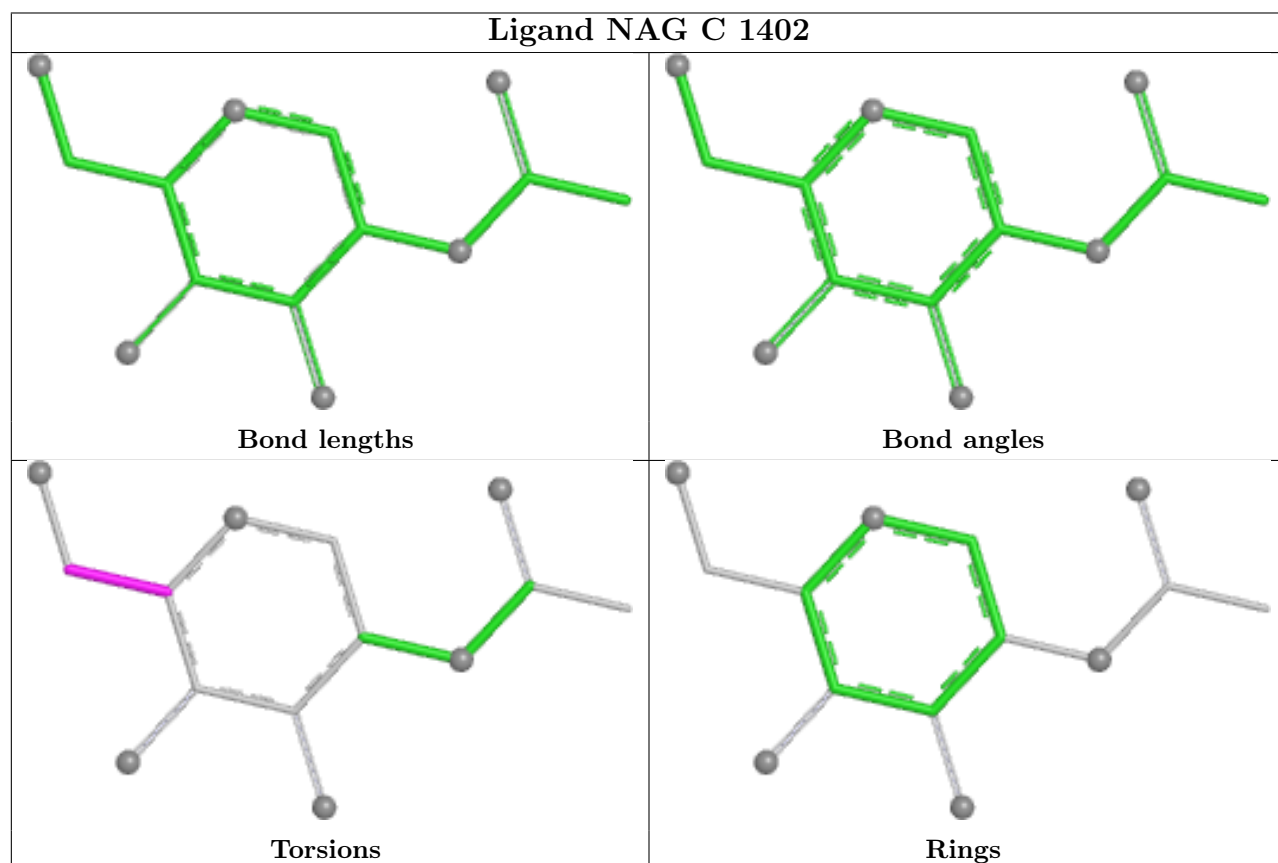
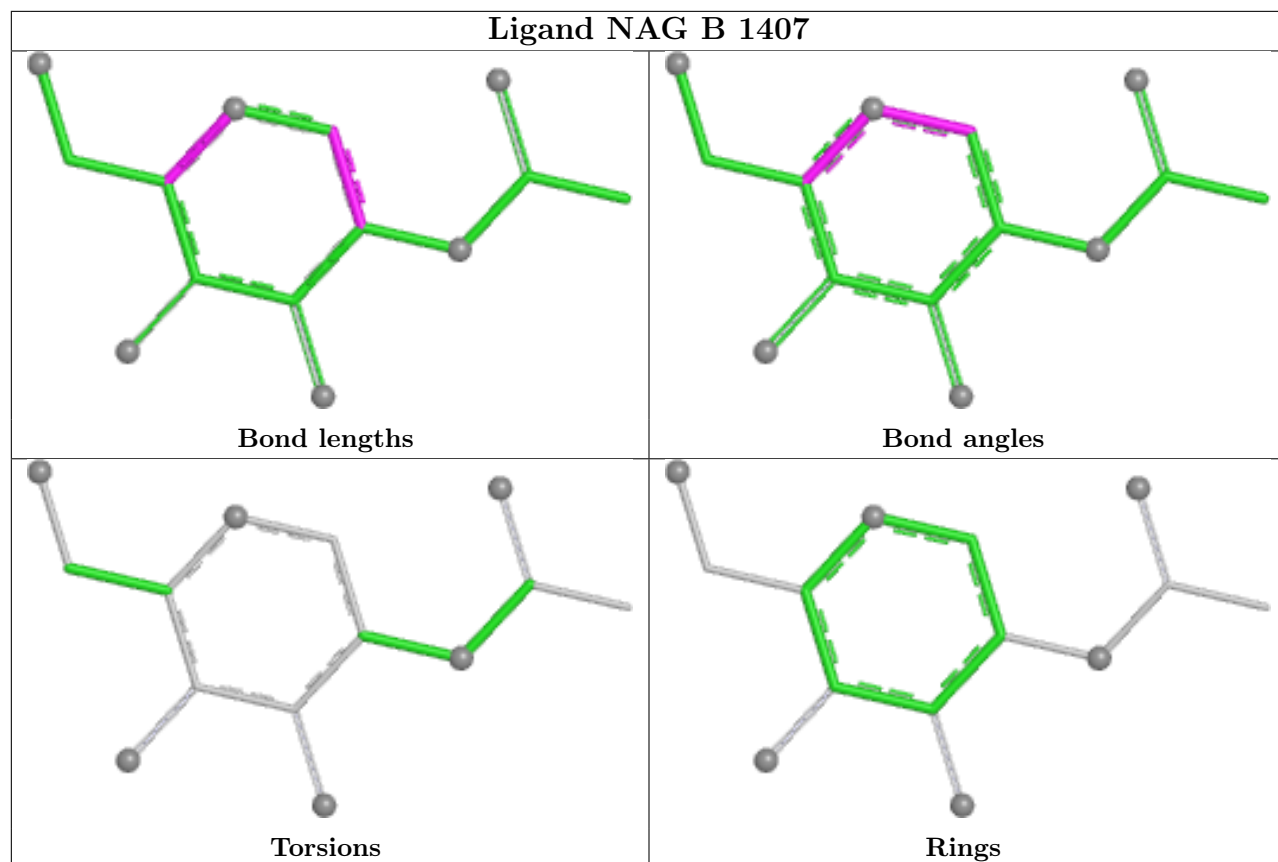


Ligand NAG A 1401



Ligand NAG C 1405





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

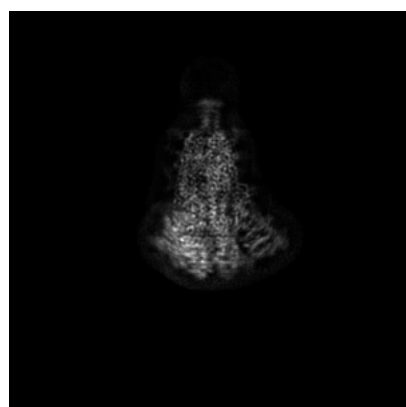
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24123. These allow visual inspection of the internal detail of the map and identification of artifacts.

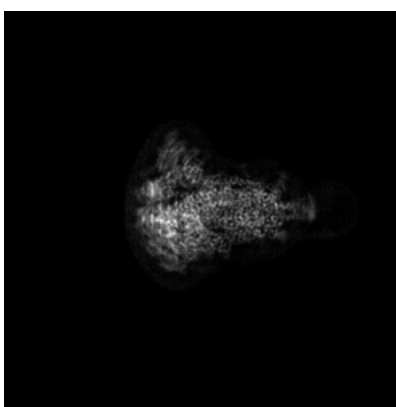
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

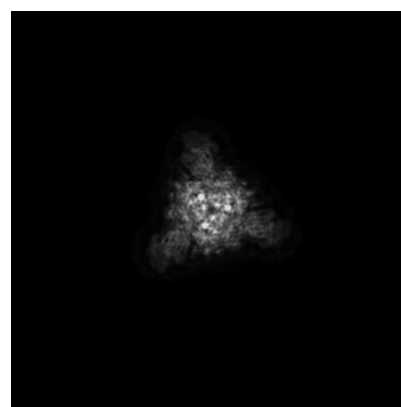
6.1.1 Primary map



X



Y



Z

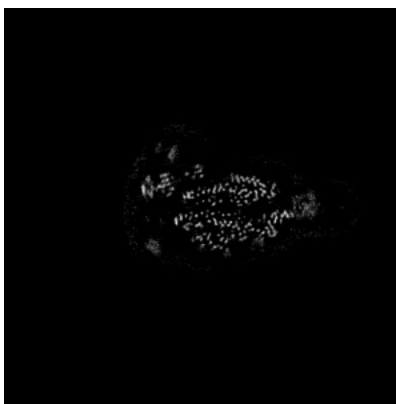
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240



Z Index: 240

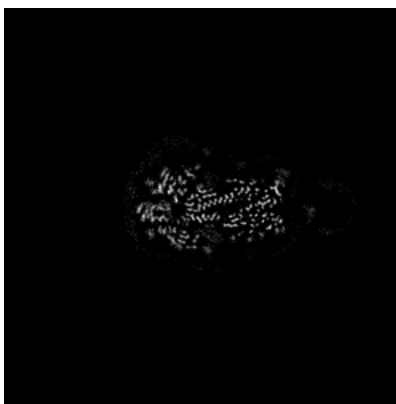
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 231



Y Index: 256

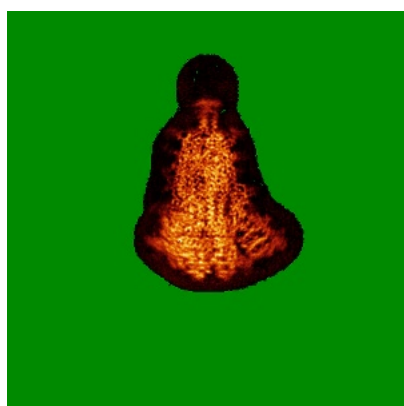


Z Index: 198

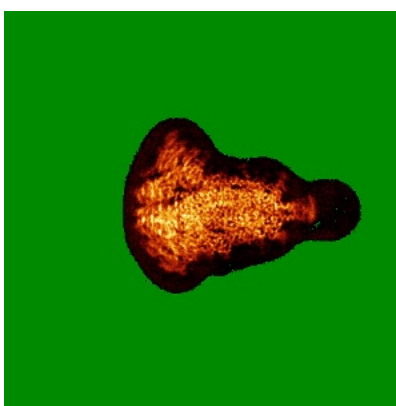
The images above show the largest variance slices of the map in three orthogonal directions.

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

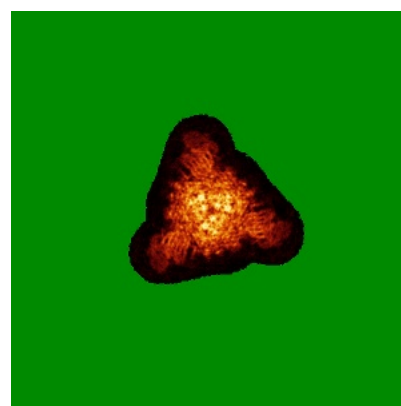
6.4.1 Primary map



X



Y



Z

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 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

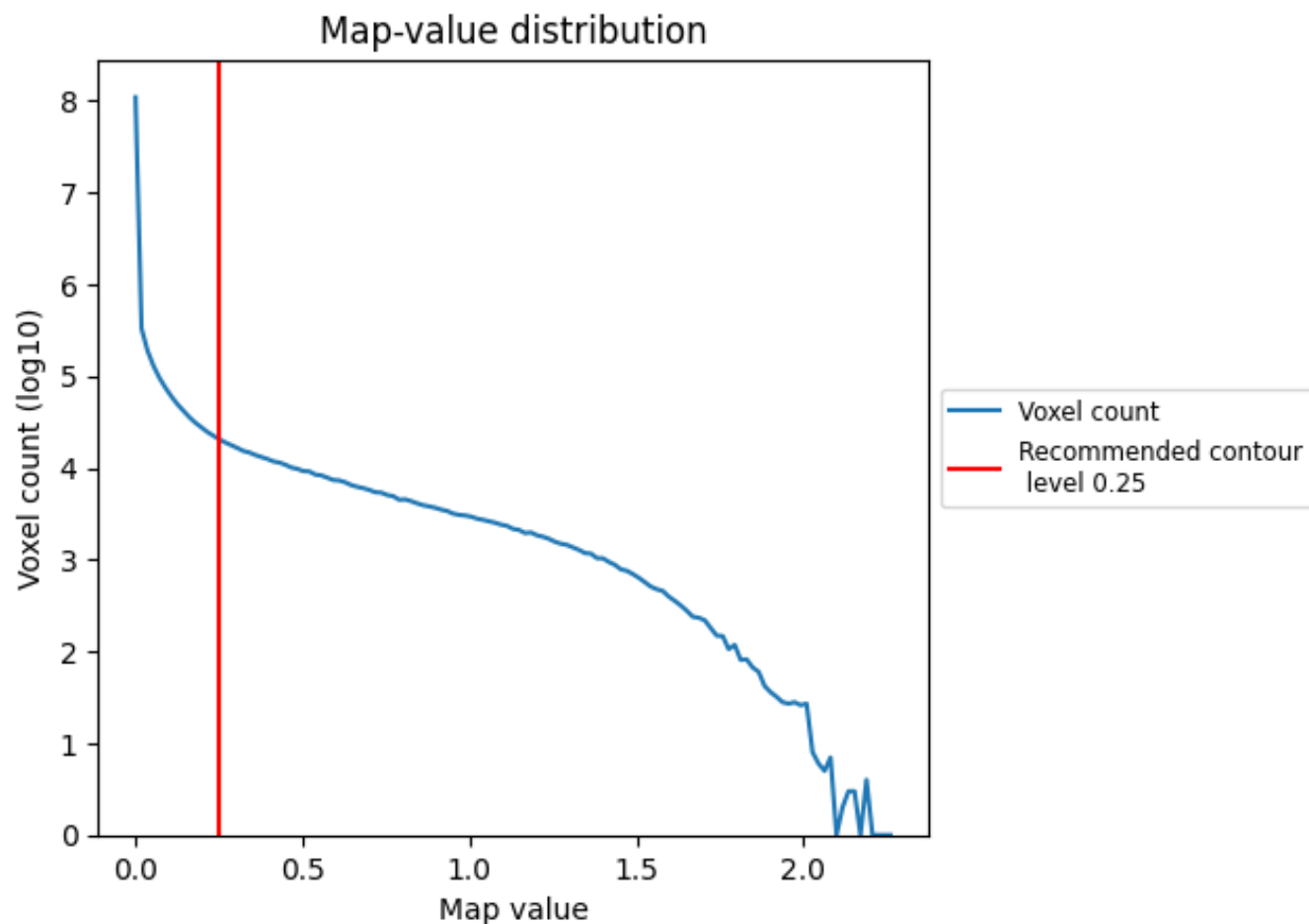
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

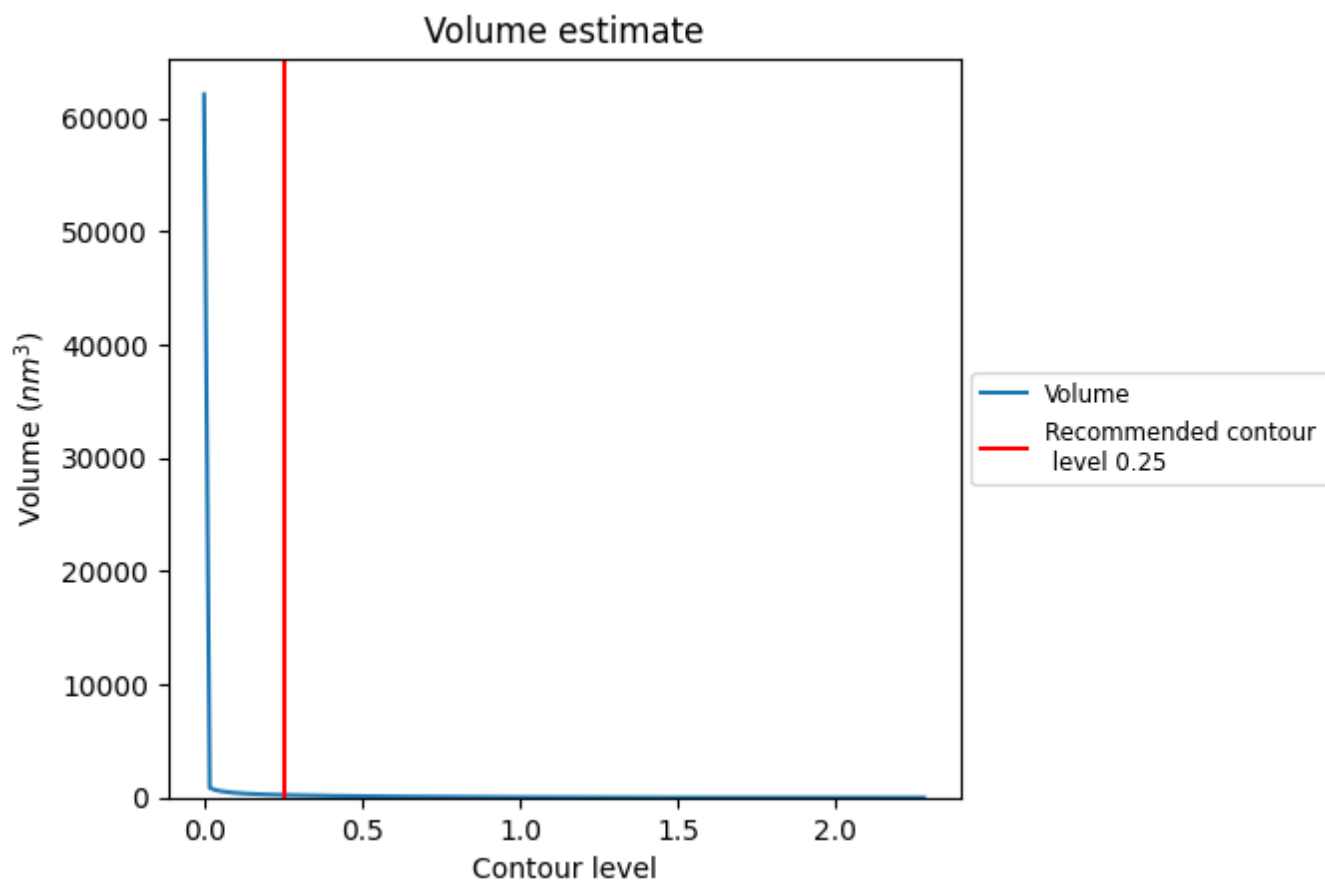
This section contains the results of statistical analysis of the map.

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.

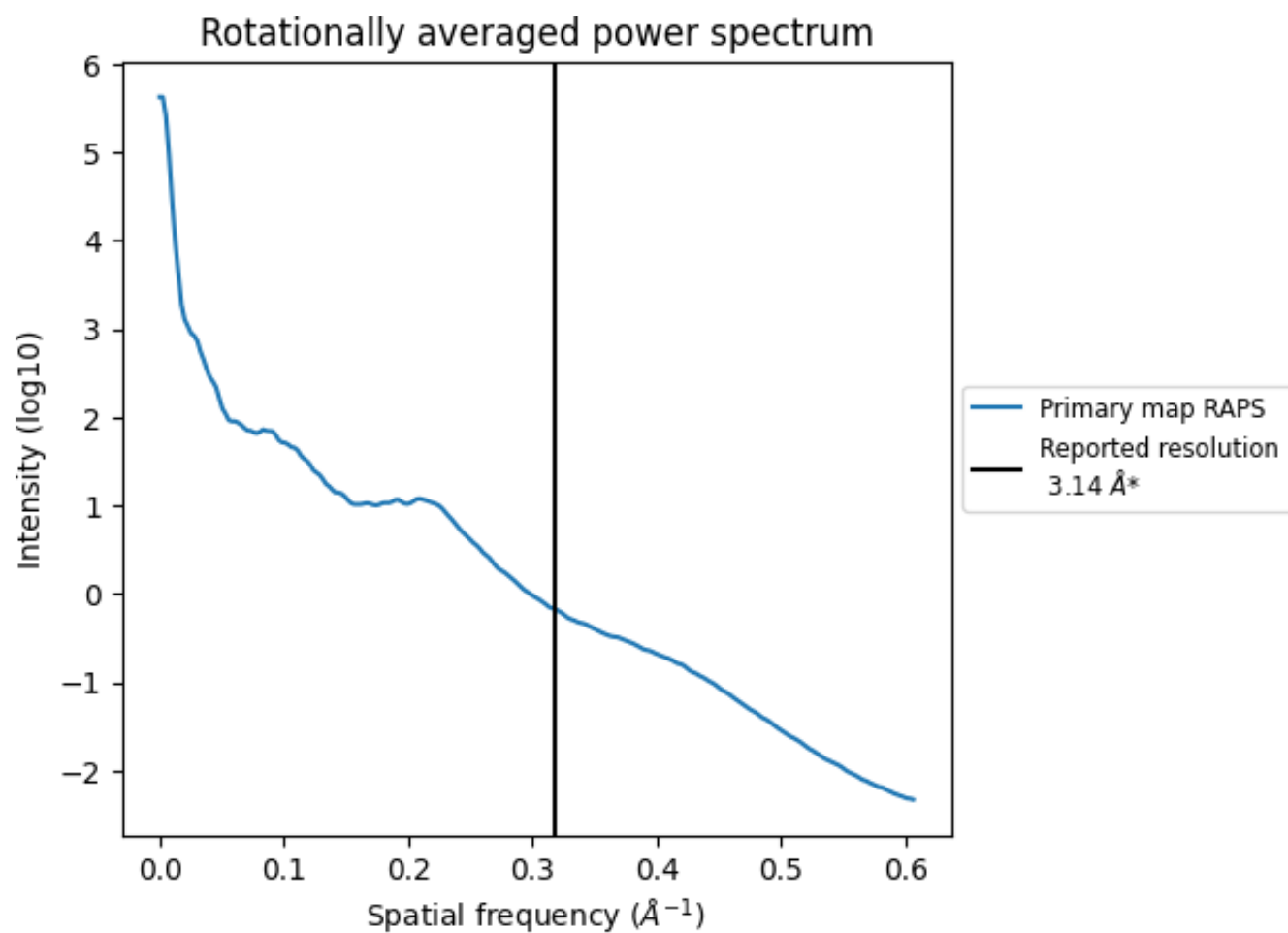
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm³; this corresponds to an approximate mass of 206 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 0.318 Å⁻¹

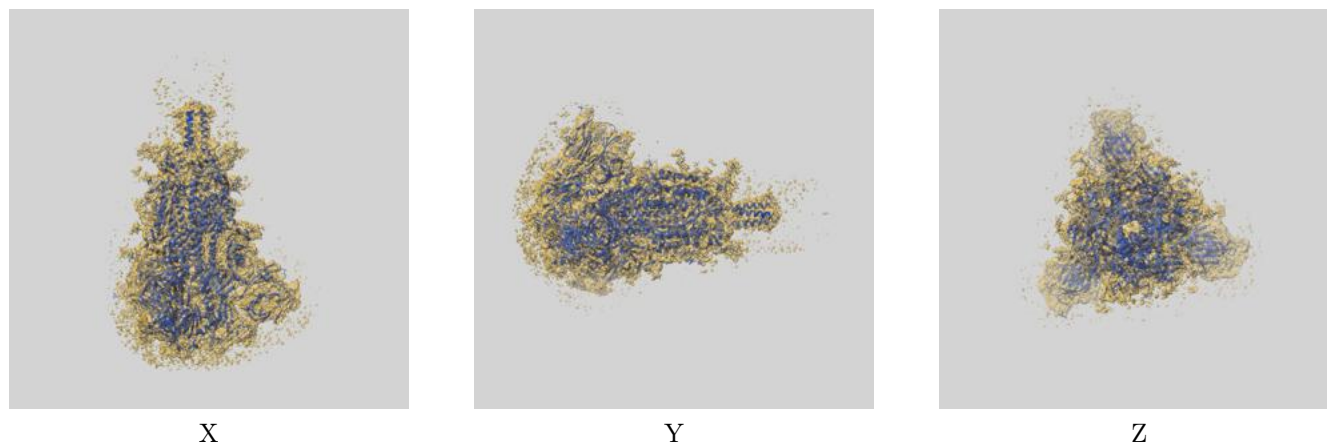
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

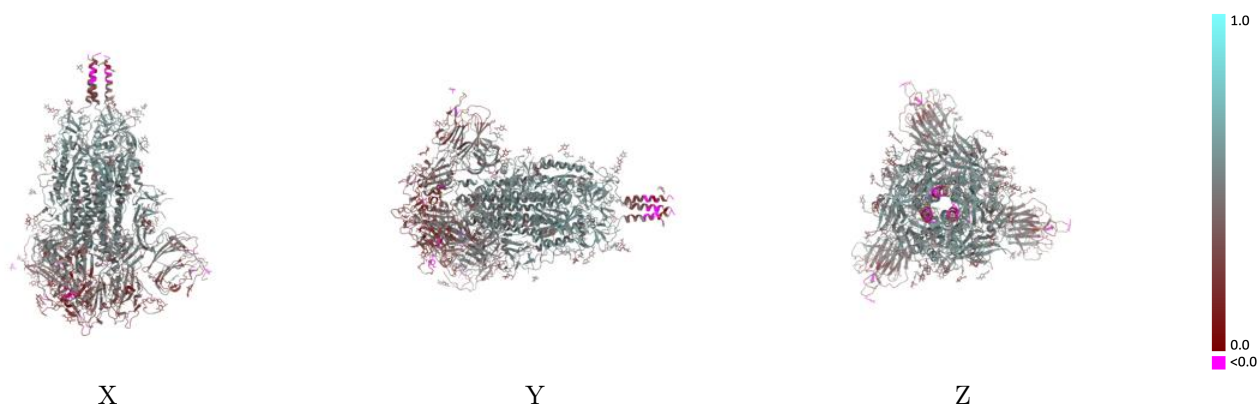
This section contains information regarding the fit between EMDB map EMD-24123 and PDB model 7N1U. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



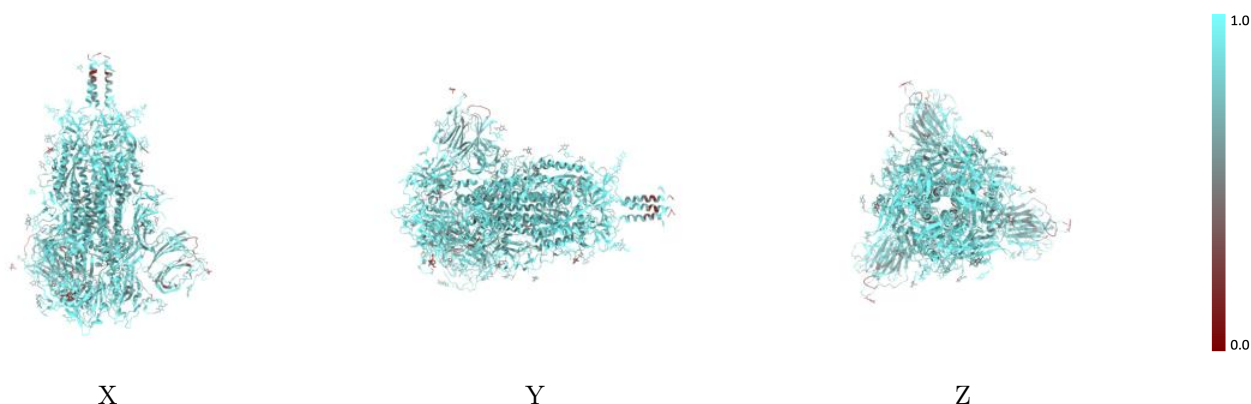
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



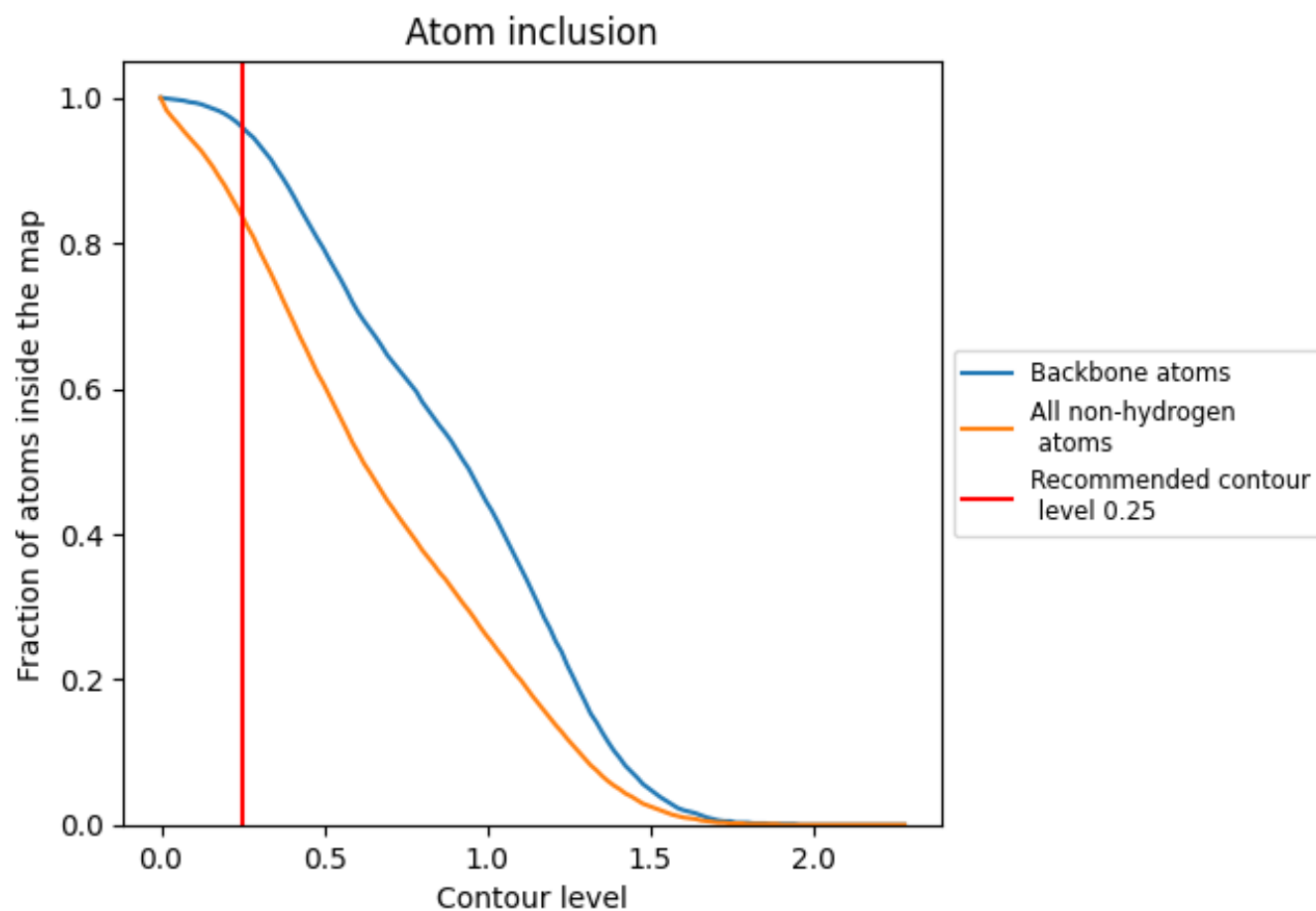
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.4400
A	 0.8390	 0.4430
B	 0.8390	 0.4450
C	 0.8400	 0.4440
D	 0.6430	 0.2910
E	 0.7500	 0.2960
F	 0.8570	 0.1230
G	 0.6070	 0.2790
H	 0.7140	 0.3880
I	 0.7140	 0.3080
J	 0.7500	 0.5000
K	 0.7500	 0.3680
L	 0.5260	 0.3720
M	 0.8970	 0.4360
N	 0.8970	 0.3540
O	 0.7500	 0.1700
P	 0.7860	 0.2720
Q	 0.7140	 0.2070
R	 0.6430	 0.1830
S	 0.6430	 0.2860
T	 0.6430	 0.2410
U	 0.8570	 0.5110
V	 0.8570	 0.4570
W	 0.6320	 0.3950
X	 0.9230	 0.4840
Y	 0.8970	 0.3600
Z	 0.7500	 0.3740
a	 0.7140	 0.2410
b	 0.8210	 0.2060
c	 0.6430	 0.2700
d	 0.7140	 0.3530
e	 0.7500	 0.3230
f	 0.7500	 0.5100
g	 0.7860	 0.4340
h	 0.4740	 0.2820



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Chain	Atom inclusion	Q-score
i	 0.9740	 0.4570
j	 0.8210	 0.3620