



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 11:49 PM UTC

PDB ID : 7SBS / pdb_00007sbs
EMDB ID : EMD-24987
Title : One RBD-up 1 of pre-fusion SARS-CoV-2 Gamma variant spike protein
Authors : Zhang, J.; Xiao, T.S.; Cai, Y.F.; Peng, H.Q.; Volloch, S.R.; Chen, B.
Deposited on : 2021-09-25
Resolution : 3.80 Å(reported)
Based on initial model : 7KRR

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:

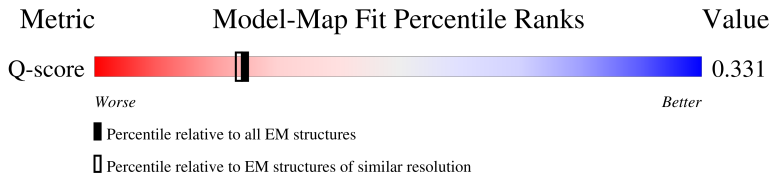
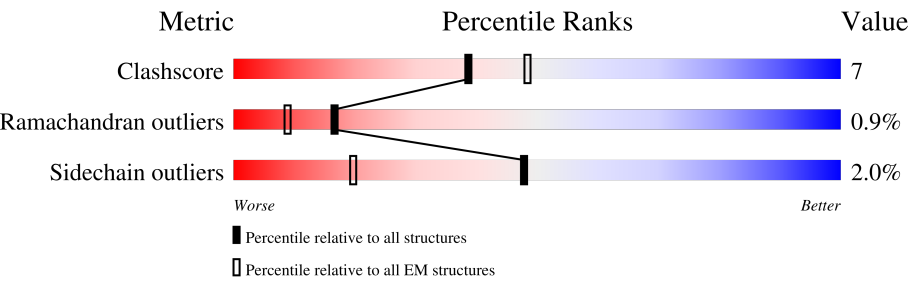
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	1310	75% 9% 15%
1	B	1310	75% 8% 16%
1	C	1310	77% 7% 15%
2	D	2	100%

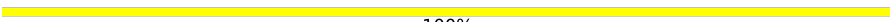
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Mol	Chain	Length	Quality of chain
2	E	2	100%
2	F	2	100%
2	G	2	100%
2	K	2	50% 50% 50%
2	L	2	100%
2	M	2	50% 50%
2	N	2	100%
2	O	2	100%
2	P	2	100%
2	T	2	50% 50% 50%
2	U	2	100%
2	V	2	50% 50%
2	W	2	50% 50%
2	X	2	100%
2	Y	2	50% 50%
2	Z	2	100%
2	a	2	100%
2	e	2	50% 50% 50%
3	H	3	33% 67%
3	Q	3	100%
3	b	3	33% 67%
4	I	3	67% 33%
4	J	3	100%
4	R	3	100%
4	S	3	100%

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Mol	Chain	Length	Quality of chain
4	c	3	 100%
4	d	3	 100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27327 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	1116	Total	C	N	O	S	0	0
			8715	5564	1447	1664	40		
1	B	1097	Total	C	N	O	S	0	0
			8589	5488	1427	1636	38		
1	C	1117	Total	C	N	O	S	0	0
			8737	5581	1452	1665	39		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	conflict	UNP P0DTC2
A	20	ASN	THR	conflict	UNP P0DTC2
A	26	SER	PRO	conflict	UNP P0DTC2
A	138	TYR	ASP	conflict	UNP P0DTC2
A	190	SER	ARG	conflict	UNP P0DTC2
A	417	THR	LYS	conflict	UNP P0DTC2
A	484	LYS	GLU	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	1027	ILE	THR	conflict	UNP P0DTC2
A	1176	PHE	VAL	conflict	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	ALA	-	expression tag	UNP P0DTC2
A	1282	TRP	-	expression tag	UNP P0DTC2
A	1283	SER	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1286	GLN	-	expression tag	UNP P0DTC2
A	1287	PHE	-	expression tag	UNP P0DTC2
A	1288	GLU	-	expression tag	UNP P0DTC2
A	1289	LYS	-	expression tag	UNP P0DTC2
A	1290	GLY	-	expression tag	UNP P0DTC2
A	1291	GLY	-	expression tag	UNP P0DTC2
A	1292	GLY	-	expression tag	UNP P0DTC2
A	1293	SER	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	GLY	-	expression tag	UNP P0DTC2
A	1296	GLY	-	expression tag	UNP P0DTC2
A	1297	SER	-	expression tag	UNP P0DTC2
A	1298	GLY	-	expression tag	UNP P0DTC2
A	1299	GLY	-	expression tag	UNP P0DTC2
A	1300	SER	-	expression tag	UNP P0DTC2
A	1301	SER	-	expression tag	UNP P0DTC2
A	1302	ALA	-	expression tag	UNP P0DTC2
A	1303	TRP	-	expression tag	UNP P0DTC2
A	1304	SER	-	expression tag	UNP P0DTC2
A	1305	HIS	-	expression tag	UNP P0DTC2
A	1306	PRO	-	expression tag	UNP P0DTC2
A	1307	GLN	-	expression tag	UNP P0DTC2
A	1308	PHE	-	expression tag	UNP P0DTC2
A	1309	GLU	-	expression tag	UNP P0DTC2
A	1310	LYS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	conflict	UNP P0DTC2
B	20	ASN	THR	conflict	UNP P0DTC2
B	26	SER	PRO	conflict	UNP P0DTC2
B	138	TYR	ASP	conflict	UNP P0DTC2
B	190	SER	ARG	conflict	UNP P0DTC2
B	417	THR	LYS	conflict	UNP P0DTC2
B	484	LYS	GLU	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	1027	ILE	THR	conflict	UNP P0DTC2
B	1176	PHE	VAL	conflict	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2

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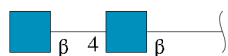
Chain	Residue	Modelled	Actual	Comment	Reference
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	ALA	-	expression tag	UNP P0DTC2
B	1282	TRP	-	expression tag	UNP P0DTC2
B	1283	SER	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	PRO	-	expression tag	UNP P0DTC2
B	1286	GLN	-	expression tag	UNP P0DTC2
B	1287	PHE	-	expression tag	UNP P0DTC2
B	1288	GLU	-	expression tag	UNP P0DTC2
B	1289	LYS	-	expression tag	UNP P0DTC2
B	1290	GLY	-	expression tag	UNP P0DTC2
B	1291	GLY	-	expression tag	UNP P0DTC2
B	1292	GLY	-	expression tag	UNP P0DTC2
B	1293	SER	-	expression tag	UNP P0DTC2
B	1294	GLY	-	expression tag	UNP P0DTC2
B	1295	GLY	-	expression tag	UNP P0DTC2
B	1296	GLY	-	expression tag	UNP P0DTC2
B	1297	SER	-	expression tag	UNP P0DTC2
B	1298	GLY	-	expression tag	UNP P0DTC2
B	1299	GLY	-	expression tag	UNP P0DTC2
B	1300	SER	-	expression tag	UNP P0DTC2
B	1301	SER	-	expression tag	UNP P0DTC2
B	1302	ALA	-	expression tag	UNP P0DTC2
B	1303	TRP	-	expression tag	UNP P0DTC2
B	1304	SER	-	expression tag	UNP P0DTC2
B	1305	HIS	-	expression tag	UNP P0DTC2
B	1306	PRO	-	expression tag	UNP P0DTC2
B	1307	GLN	-	expression tag	UNP P0DTC2
B	1308	PHE	-	expression tag	UNP P0DTC2
B	1309	GLU	-	expression tag	UNP P0DTC2
B	1310	LYS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	conflict	UNP P0DTC2
C	20	ASN	THR	conflict	UNP P0DTC2
C	26	SER	PRO	conflict	UNP P0DTC2
C	138	TYR	ASP	conflict	UNP P0DTC2
C	190	SER	ARG	conflict	UNP P0DTC2
C	417	THR	LYS	conflict	UNP P0DTC2
C	484	LYS	GLU	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1027	ILE	THR	conflict	UNP P0DTC2
C	1176	PHE	VAL	conflict	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	ALA	-	expression tag	UNP P0DTC2
C	1282	TRP	-	expression tag	UNP P0DTC2
C	1283	SER	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	PRO	-	expression tag	UNP P0DTC2
C	1286	GLN	-	expression tag	UNP P0DTC2
C	1287	PHE	-	expression tag	UNP P0DTC2
C	1288	GLU	-	expression tag	UNP P0DTC2
C	1289	LYS	-	expression tag	UNP P0DTC2
C	1290	GLY	-	expression tag	UNP P0DTC2
C	1291	GLY	-	expression tag	UNP P0DTC2
C	1292	GLY	-	expression tag	UNP P0DTC2
C	1293	SER	-	expression tag	UNP P0DTC2
C	1294	GLY	-	expression tag	UNP P0DTC2
C	1295	GLY	-	expression tag	UNP P0DTC2
C	1296	GLY	-	expression tag	UNP P0DTC2
C	1297	SER	-	expression tag	UNP P0DTC2
C	1298	GLY	-	expression tag	UNP P0DTC2
C	1299	GLY	-	expression tag	UNP P0DTC2
C	1300	SER	-	expression tag	UNP P0DTC2
C	1301	SER	-	expression tag	UNP P0DTC2
C	1302	ALA	-	expression tag	UNP P0DTC2
C	1303	TRP	-	expression tag	UNP P0DTC2
C	1304	SER	-	expression tag	UNP P0DTC2
C	1305	HIS	-	expression tag	UNP P0DTC2
C	1306	PRO	-	expression tag	UNP P0DTC2
C	1307	GLN	-	expression tag	UNP P0DTC2
C	1308	PHE	-	expression tag	UNP P0DTC2
C	1309	GLU	-	expression tag	UNP P0DTC2
C	1310	LYS	-	expression tag	UNP P0DTC2

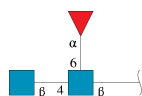
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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		
2	G	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		
2	P	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	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	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	e	2	Total	C	N	O	0	0
			28	16	2	10		

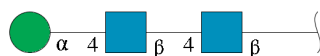
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al

pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	3	Total	C	N	O	0	0
			38	22	2	14		
3	Q	3	Total	C	N	O	0	0
			38	22	2	14		
3	b	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	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		
4	R	3	Total	C	N	O	0	0
			39	22	2	15		
4	S	3	Total	C	N	O	0	0
			39	22	2	15		
4	c	3	Total	C	N	O	0	0
			39	22	2	15		
4	d	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	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	

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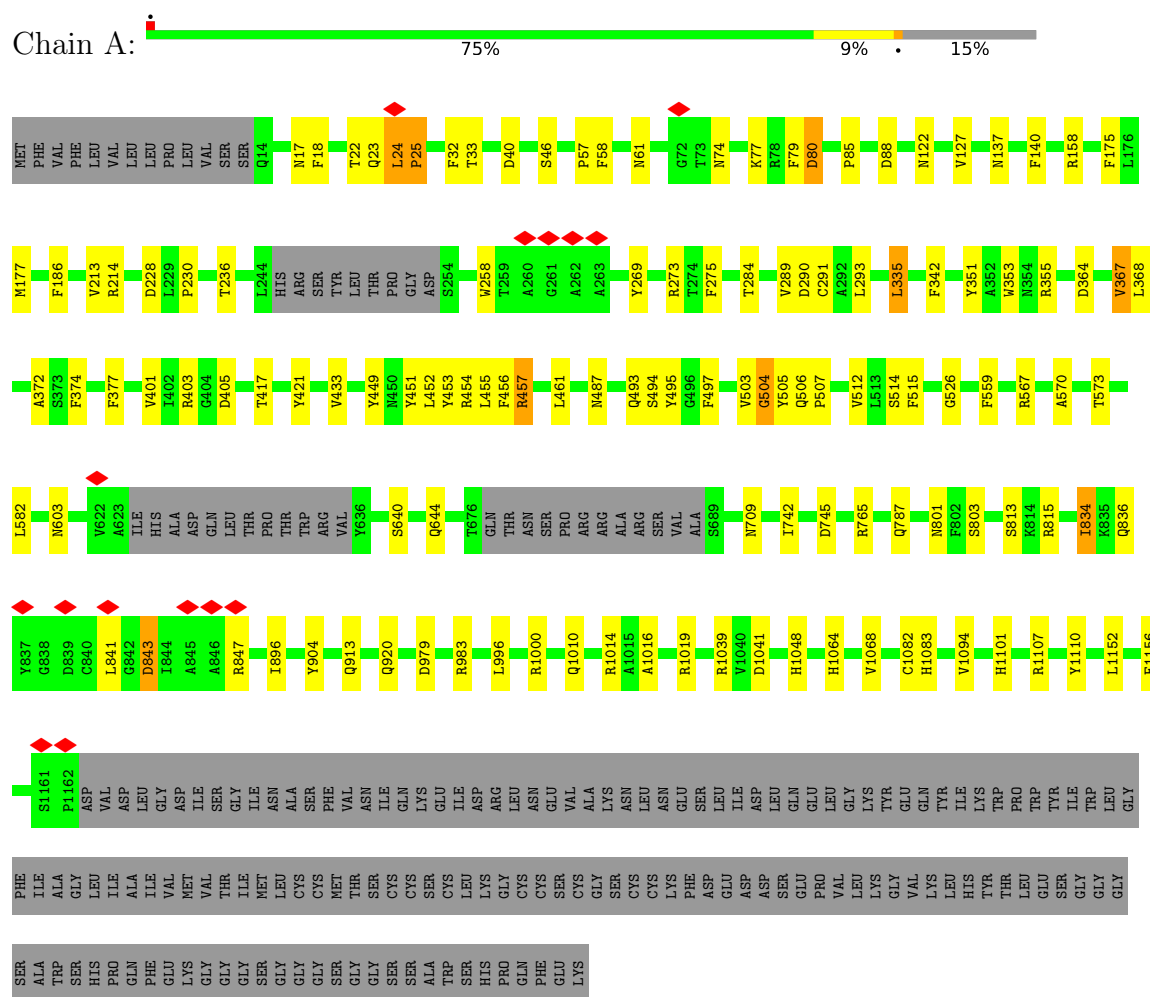
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C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

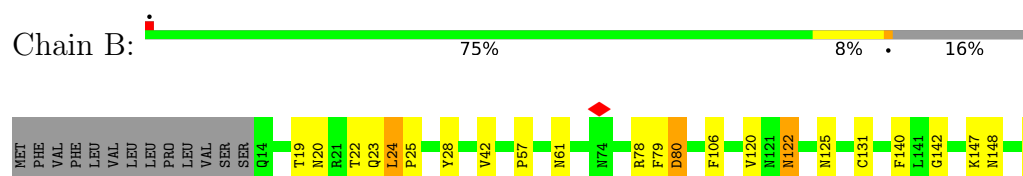
3 Residue-property plots

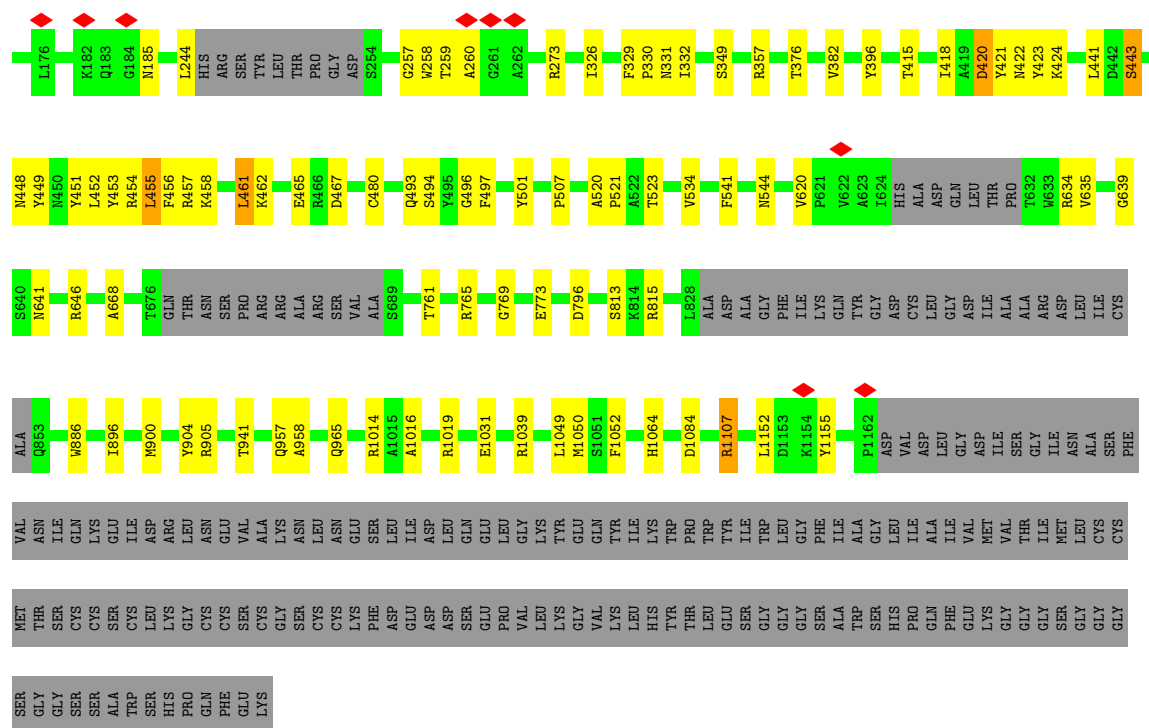
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein



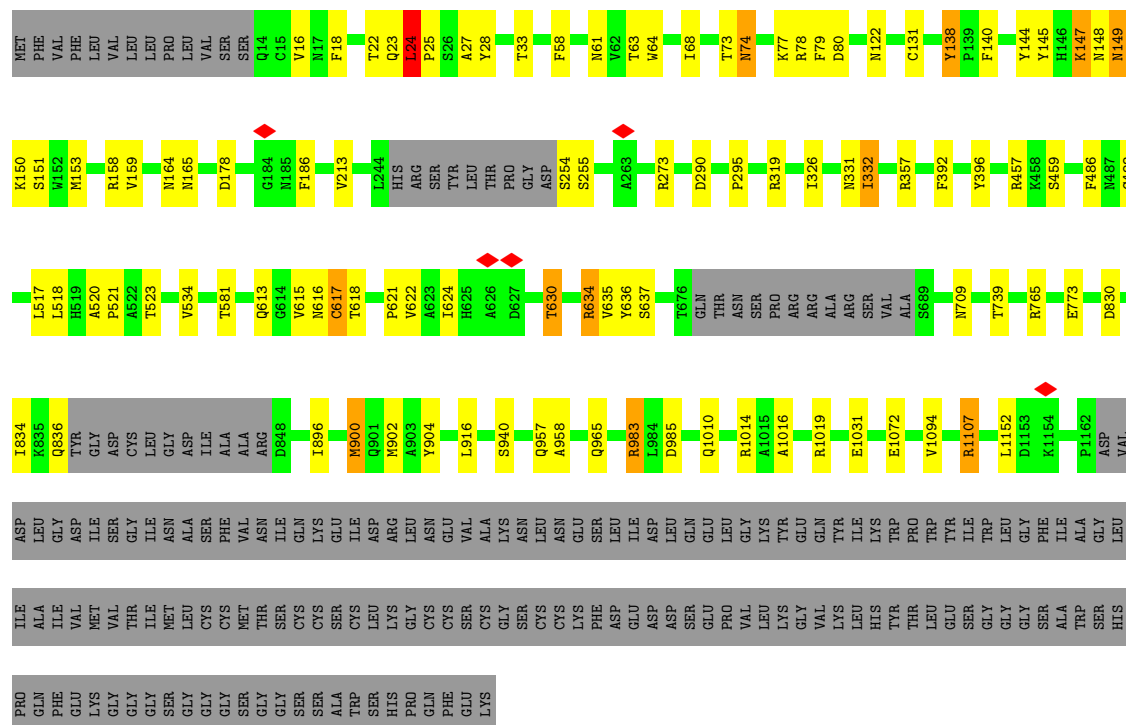
• Molecule 1: Spike glycoprotein



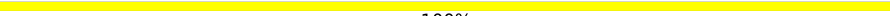


• Molecule 1: Spike glycoprotein

Chain C: 77% 7% 15%



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

Chain D:  100%

NAG1
NAG2

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

Chain E:  100%

NAG1
NAG2

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

Chain F:  100%

NAG1
NAG2

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

Chain G:  100%

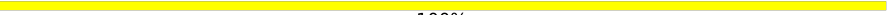
NAG1
NAG2

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

Chain K:  50% 50% 50%

NAG1
NAG2

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

Chain L:  100%

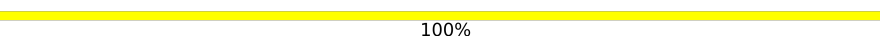
NAG1
NAG2

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

Chain M:  50% 50%

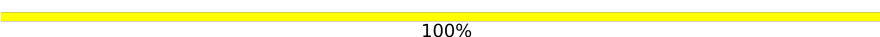


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%

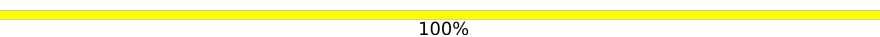


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 100%



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

Chain P: 100%

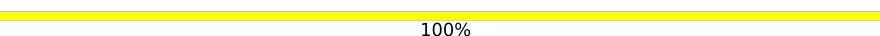


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 50%
50% 50%



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

Chain U: 100%



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

Chain V: 50% 50%

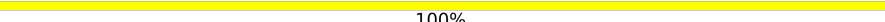


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 50%

MAG1
MAG2

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

Chain X:  100%

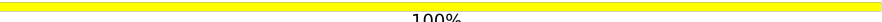
MAG1
MAG2

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

Chain Y:  50% 50%

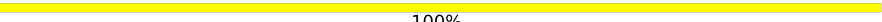
MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain a:  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% 50%

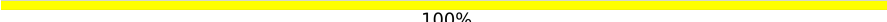
MAG1
MAG2

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

Chain H:  33% 67%

NAG1
NAG2
FUC3

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

Chain Q:  100%

NAG1
NAG2
FUC3

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

Chain b:  33% 67%

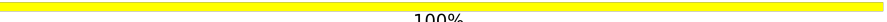
NAG1
NAG2
FUC3

- 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:  67% 33%

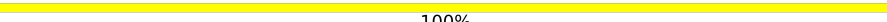
NAG1
NAG2
MAN3

- 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%

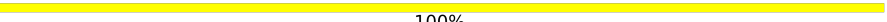
NAG1
NAG2
MAN3

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

Chain R:  100%

NAG1
NAG2
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 S:  100%

NAG1
NAG2
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 c:  100%

MAG1
MAG2
MAM3

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

Chain d:  100%

MAG1
MAG2
MAM3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69302	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 ($e^-/\text{\AA}^2$)	54.72	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	2.315	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.1	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, FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/8917	1.25	23/12130 (0.2%)
1	B	0.68	0/8790	1.23	11/11959 (0.1%)
1	C	0.68	0/8942	1.24	9/12168 (0.1%)
All	All	0.68	0/26649	1.24	43/36257 (0.1%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASN	N-CA-C	9.31	121.50	111.36
1	B	19	THR	N-CA-C	8.03	119.66	111.07
1	C	1107	ARG	N-CA-C	7.53	122.13	112.34
1	A	61	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	A	843	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	122	ASN	CA-CB-CG	6.89	119.49	112.60
1	B	122	ASN	CA-CB-CG	6.67	119.27	112.60
1	C	900	MET	N-CA-C	-6.48	104.30	111.36
1	A	61	ASN	CB-CG-ND2	6.40	126.00	116.40
1	B	80	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	214	ARG	N-CA-C	6.03	123.65	110.80
1	A	559	PHE	CA-CB-CG	5.96	119.76	113.80
1	C	615	VAL	CA-C-O	-5.95	113.69	120.66
1	B	458	LYS	N-CA-C	5.87	117.54	111.03
1	A	80	ASP	CA-CB-CG	5.66	118.25	112.60
1	A	40	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	106	PHE	CA-CB-CG	5.57	119.37	113.80
1	B	329	PHE	CA-C-N	5.48	126.69	119.84
1	B	329	PHE	C-N-CA	5.48	126.69	119.84
1	C	213	VAL	N-CA-C	5.46	116.11	110.82
1	C	178	ASP	CA-CB-CG	5.45	118.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1110	TYR	CA-C-N	5.44	127.87	122.00
1	A	1110	TYR	C-N-CA	5.44	127.87	122.00
1	A	342	PHE	O-C-N	5.39	130.02	122.36
1	B	1084	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	620	VAL	CA-C-N	5.34	125.01	119.56
1	B	620	VAL	C-N-CA	5.34	125.01	119.56
1	A	377	PHE	CA-CB-CG	5.31	119.11	113.80
1	C	332	ILE	CA-CB-CG1	5.22	119.27	110.40
1	B	1064	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	1083	HIS	CB-CG-CD2	-5.19	124.46	131.20
1	A	213	VAL	N-CA-C	5.16	115.93	110.72
1	A	1068	VAL	CA-C-N	5.14	125.38	119.83
1	A	1068	VAL	C-N-CA	5.14	125.38	119.83
1	A	228	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	1064	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	A	291	CYS	N-CA-C	5.09	116.83	111.28
1	C	634	ARG	CB-CA-C	5.08	117.97	109.80
1	A	526	GLY	CA-C-N	5.07	124.83	119.76
1	A	526	GLY	C-N-CA	5.07	124.83	119.76
1	A	913	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	C	983	ARG	N-CA-C	5.04	119.58	113.38
1	A	1048	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	8715	0	8474	178	0
1	B	8589	0	8356	161	0
1	C	8737	0	8498	118	0
2	D	28	0	25	0	0
2	E	28	0	25	6	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	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	T	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	6	0
2	X	28	0	25	0	0
2	Y	28	0	25	4	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	e	28	0	25	1	0
3	H	38	0	34	4	0
3	Q	38	0	34	0	0
3	b	38	0	34	3	0
4	I	39	0	34	1	0
4	J	39	0	34	0	0
4	R	39	0	34	0	0
4	S	39	0	34	0	0
4	c	39	0	34	0	0
4	d	39	0	34	0	0
5	A	154	0	143	2	0
5	B	140	0	130	4	0
5	C	112	0	104	2	0
All	All	27327	0	26486	394	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 (394) 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:497:PHE:CE1	1:B:507:PRO:HB3	1.33	1.59
1:A:372:ALA:HA	1:C:486:PHE:CZ	1.38	1.53
1:C:18:PHE:HE2	1:C:138:TYR:CE2	1.25	1.51
1:C:18:PHE:CE2	1:C:138:TYR:CE2	2.04	1.45
1:A:1010:GLN:HB3	1:A:1014:ARG:NH2	1.33	1.38
1:A:904:TYR:CE2	1:C:1107:ARG:HD3	1.61	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:LEU:HB3	1:C:25:PRO:CD	1.60	1.30
1:B:24:LEU:HB3	1:B:25:PRO:CD	1.62	1.29
1:A:904:TYR:HE2	1:C:1107:ARG:CD	1.49	1.26
1:B:497:PHE:CD1	1:B:507:PRO:HB3	1.77	1.19
1:B:497:PHE:CE1	1:B:507:PRO:CB	2.24	1.19
1:A:904:TYR:CE2	1:C:1107:ARG:CD	2.22	1.19
1:C:24:LEU:CB	1:C:25:PRO:HD3	1.73	1.17
1:A:567:ARG:HG2	1:B:42:VAL:CG1	1.75	1.16
1:B:24:LEU:CB	1:B:25:PRO:HD3	1.75	1.15
1:B:28:TYR:HD1	1:B:61:ASN:OD1	1.27	1.14
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.28	1.14
1:A:1010:GLN:CB	1:A:1014:ARG:HH22	1.63	1.11
1:A:372:ALA:CA	1:C:486:PHE:CZ	2.33	1.10
1:B:418:ILE:O	1:B:422:ASN:HB2	1.54	1.08
1:C:18:PHE:CE2	1:C:138:TYR:CD2	2.42	1.08
1:A:1094:VAL:HB	1:B:904:TYR:OH	1.54	1.07
1:A:567:ARG:CG	1:B:42:VAL:HG11	1.84	1.07
1:C:18:PHE:CE2	1:C:138:TYR:HE2	1.50	1.07
1:A:1107:ARG:NE	1:B:904:TYR:CE2	2.24	1.06
1:A:904:TYR:CD2	1:C:1107:ARG:HD3	1.90	1.06
1:C:902:MET:HB2	1:C:916:LEU:HD21	1.37	1.05
1:B:1016:ALA:HA	1:B:1019:ARG:NH1	1.75	1.01
1:A:1016:ALA:HA	1:A:1019:ARG:NH2	1.75	1.01
1:A:372:ALA:HA	1:C:486:PHE:HZ	1.22	0.99
1:C:23:GLN:HA	1:C:80:ASP:HB3	1.44	0.99
1:A:57:PRO:HB3	1:A:273:ARG:NH1	1.76	0.98
1:C:1016:ALA:HA	1:C:1019:ARG:NH1	1.78	0.98
1:A:405:ASP:OD2	1:A:504:GLY:HA3	1.64	0.96
1:B:57:PRO:HB3	1:B:273:ARG:NH1	1.79	0.96
1:A:18:PHE:CE1	1:A:258:TRP:NE1	2.32	0.96
1:A:567:ARG:HG2	1:B:42:VAL:HG11	1.40	0.96
1:B:24:LEU:HD13	1:B:78:ARG:HD3	1.48	0.96
1:A:904:TYR:CD2	1:C:1107:ARG:NH1	2.34	0.95
1:A:1016:ALA:HA	1:A:1019:ARG:HH22	1.31	0.95
1:A:1107:ARG:CD	1:B:904:TYR:CE2	2.49	0.95
1:B:497:PHE:HE1	1:B:507:PRO:HB3	1.23	0.95
1:A:1010:GLN:CB	1:A:1014:ARG:NH2	2.22	0.95
1:C:902:MET:HB2	1:C:916:LEU:CD2	1.96	0.95
1:A:904:TYR:CE2	1:C:1107:ARG:NE	2.33	0.95
1:C:18:PHE:CD2	1:C:138:TYR:CD2	2.55	0.95
1:A:979:ASP:O	1:A:983:ARG:HD3	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:TYR:HD2	1:C:1107:ARG:NH1	1.66	0.94
1:B:28:TYR:CD1	1:B:61:ASN:OD1	2.20	0.93
1:A:421:TYR:O	1:A:454:ARG:HD2	1.68	0.93
1:A:18:PHE:CZ	1:A:258:TRP:NE1	2.37	0.92
1:A:1107:ARG:HD3	1:B:904:TYR:CD2	2.04	0.91
1:A:421:TYR:CE2	1:A:455:LEU:O	2.23	0.91
1:A:1010:GLN:HB3	1:A:1014:ARG:HH22	0.85	0.91
1:C:18:PHE:CD2	1:C:138:TYR:CE2	2.58	0.91
1:A:451:TYR:O	1:A:495:TYR:HB2	1.70	0.91
1:A:1107:ARG:NE	1:B:904:TYR:CD2	2.39	0.91
2:Y:1:NAG:H62	2:Y:2:NAG:C7	2.01	0.90
1:B:1016:ALA:HA	1:B:1019:ARG:HH12	1.33	0.90
1:A:644:GLN:NE2	2:E:1:NAG:H82	1.85	0.89
1:B:422:ASN:HD21	1:B:454:ARG:HB3	1.36	0.89
1:A:765:ARG:NH1	1:C:957:GLN:HG2	1.90	0.86
1:A:644:GLN:CD	2:E:1:NAG:H82	2.01	0.86
1:A:904:TYR:CD2	1:C:1107:ARG:CZ	2.59	0.86
1:C:1016:ALA:HA	1:C:1019:ARG:HH12	1.39	0.85
1:A:1107:ARG:CZ	1:B:904:TYR:CD2	2.60	0.85
1:A:567:ARG:HG3	1:B:42:VAL:HG11	1.57	0.84
1:A:567:ARG:CG	1:B:42:VAL:CG1	2.48	0.84
1:A:1107:ARG:CD	1:B:904:TYR:CD2	2.60	0.83
1:B:497:PHE:CD1	1:B:507:PRO:CB	2.55	0.83
1:C:958:ALA:HB2	1:C:1014:ARG:HH12	1.43	0.82
1:A:1107:ARG:NE	1:B:904:TYR:HE2	1.71	0.82
1:C:140:PHE:CZ	1:C:158:ARG:HD2	2.15	0.81
1:A:17:ASN:HD22	1:A:137:ASN:HD22	1.28	0.81
1:C:1010:GLN:O	1:C:1014:ARG:HG3	1.80	0.81
1:A:24:LEU:H	1:A:25:PRO:CD	1.93	0.81
1:B:418:ILE:O	1:B:422:ASN:CB	2.29	0.81
1:A:230:PRO:HG3	1:C:357:ARG:NH1	1.94	0.81
1:A:140:PHE:CE2	1:A:158:ARG:HD2	2.16	0.81
1:A:1094:VAL:CB	1:B:904:TYR:OH	2.28	0.81
1:C:18:PHE:CD2	1:C:138:TYR:HD2	1.99	0.81
1:A:904:TYR:HD2	1:C:1107:ARG:HH11	1.25	0.80
1:A:497:PHE:HD1	1:A:507:PRO:HD3	1.44	0.80
1:A:405:ASP:OD2	1:A:504:GLY:CA	2.29	0.80
1:A:372:ALA:HA	1:C:486:PHE:CE2	2.16	0.79
1:C:896:ILE:HD11	1:C:900:MET:HG3	1.65	0.78
1:B:140:PHE:CZ	1:B:158:ARG:HD2	2.18	0.78
1:B:418:ILE:C	1:B:422:ASN:HB2	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:ARG:CD	1:B:904:TYR:HE2	1.95	0.77
1:A:904:TYR:CD2	1:C:1107:ARG:CD	2.62	0.77
1:B:496:GLY:O	1:B:501:TYR:HE2	1.67	0.77
1:A:230:PRO:HG3	1:C:357:ARG:HH11	1.48	0.77
1:A:453:TYR:OH	1:A:493:GLN:CD	2.27	0.77
1:C:24:LEU:HB3	1:C:25:PRO:HD3	0.81	0.77
1:B:462:LYS:HG3	2:W:1:NAG:C8	2.14	0.77
1:A:709:ASN:HB3	1:B:796:ASP:OD2	1.85	0.77
1:B:24:LEU:HB3	1:B:25:PRO:HD3	0.82	0.77
1:B:147:LYS:HB3	5:B:1402:NAG:H81	1.65	0.77
1:C:23:GLN:HA	1:C:80:ASP:CB	2.14	0.76
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.67	0.76
1:A:275:PHE:CZ	1:A:290:ASP:HB3	2.20	0.76
1:A:405:ASP:CG	1:A:504:GLY:CA	2.58	0.76
1:A:1152:LEU:HD21	1:B:1152:LEU:HD13	1.67	0.76
1:B:900:MET:HG3	1:B:904:TYR:HE1	1.51	0.76
1:A:421:TYR:HE2	1:A:455:LEU:O	1.69	0.76
1:A:25:PRO:HD2	1:A:80:ASP:OD2	1.85	0.75
1:C:617:CYS:O	1:C:621:PRO:CD	2.34	0.75
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	2.20	0.74
1:C:902:MET:CB	1:C:916:LEU:CD2	2.65	0.74
1:A:765:ARG:NH1	1:C:957:GLN:CG	2.50	0.74
1:B:497:PHE:HE1	1:B:507:PRO:CB	1.84	0.74
1:A:33:THR:HA	1:A:58:PHE:CE1	2.22	0.73
1:B:424:LYS:HB2	1:B:461:LEU:HD11	1.70	0.73
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.21	0.73
1:B:900:MET:HG3	1:B:904:TYR:CE1	2.25	0.72
1:A:497:PHE:CE1	1:A:507:PRO:CA	2.72	0.72
1:C:295:PRO:HG2	1:C:636:TYR:CE1	2.24	0.72
1:B:497:PHE:HE1	1:B:507:PRO:CA	2.03	0.71
1:A:1107:ARG:CZ	1:B:904:TYR:HD2	2.03	0.71
1:B:465:GLU:OE1	2:W:1:NAG:H81	1.90	0.71
1:A:497:PHE:CE1	1:A:507:PRO:N	2.59	0.71
1:A:24:LEU:H	1:A:25:PRO:HD3	1.54	0.71
1:A:1152:LEU:CD2	1:B:1152:LEU:HD13	2.22	0.70
1:A:644:GLN:NE2	2:E:1:NAG:C8	2.55	0.70
1:A:453:TYR:CE1	1:A:493:GLN:HB3	2.27	0.70
1:B:24:LEU:CD1	1:B:78:ARG:HD3	2.19	0.70
1:A:372:ALA:HA	1:C:486:PHE:CE1	2.20	0.70
1:A:417:THR:HG21	1:A:455:LEU:HD12	1.72	0.70
1:B:418:ILE:HD13	1:B:422:ASN:OD1	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ARG:HG2	1:B:42:VAL:HG13	1.72	0.69
1:A:834:ILE:HG21	2:Y:1:NAG:O7	1.92	0.69
1:C:902:MET:CB	1:C:916:LEU:HD22	2.22	0.69
1:A:904:TYR:HE2	1:C:1107:ARG:CG	2.04	0.69
1:B:1016:ALA:CA	1:B:1019:ARG:HH12	2.06	0.69
1:B:418:ILE:CA	1:B:422:ASN:HB2	2.22	0.69
1:A:765:ARG:HH12	1:C:957:GLN:HG2	1.56	0.69
1:A:421:TYR:CD2	1:A:455:LEU:O	2.46	0.69
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.25	0.69
1:A:497:PHE:HE1	1:A:506:GLN:C	2.01	0.68
1:B:422:ASN:ND2	1:B:454:ARG:HB3	2.06	0.68
1:C:295:PRO:HD2	1:C:636:TYR:HE1	1.58	0.68
1:A:1016:ALA:CA	1:A:1019:ARG:HH22	2.06	0.68
1:B:465:GLU:OE1	2:W:1:NAG:C8	2.42	0.67
1:A:497:PHE:CD1	1:A:507:PRO:CD	2.77	0.67
1:C:23:GLN:CA	1:C:80:ASP:HB3	2.23	0.67
1:B:457:ARG:HH22	1:B:467:ASP:HB2	1.59	0.67
1:B:453:TYR:CE2	1:B:455:LEU:HD23	2.30	0.67
1:C:1016:ALA:CA	1:C:1019:ARG:HH12	2.08	0.66
1:B:769:GLY:O	1:B:773:GLU:HG3	1.94	0.66
1:C:617:CYS:O	1:C:621:PRO:HD2	1.93	0.66
1:B:455:LEU:HD13	1:B:455:LEU:O	1.96	0.65
1:A:58:PHE:HD2	1:A:290:ASP:OD1	1.80	0.65
1:A:236:THR:OG1	5:A:1405:NAG:H5	1.96	0.65
1:A:497:PHE:CD1	1:A:507:PRO:HD3	2.29	0.65
1:A:497:PHE:HD1	1:A:507:PRO:CD	2.10	0.65
1:A:813:SER:OG	1:A:815:ARG:NH1	2.29	0.65
1:B:24:LEU:CD1	1:B:78:ARG:CD	2.75	0.65
1:B:457:ARG:NH2	1:B:467:ASP:CB	2.59	0.64
1:C:18:PHE:CD2	1:C:138:TYR:HE2	2.06	0.64
3:H:1:NAG:H62	3:H:2:NAG:O7	1.97	0.64
1:B:131:CYS:HA	1:B:165:ASN:O	1.97	0.64
1:B:244:LEU:HD23	1:B:244:LEU:C	2.23	0.64
1:C:331:ASN:OD1	1:C:331:ASN:O	2.16	0.64
1:B:28:TYR:HD1	1:B:61:ASN:CG	2.06	0.63
1:B:646:ARG:HB2	1:B:668:ALA:CB	2.29	0.63
1:B:497:PHE:CD1	1:B:507:PRO:CG	2.82	0.63
1:A:765:ARG:HH11	1:C:957:GLN:CD	2.07	0.62
1:C:22:THR:HB	1:C:79:PHE:H	1.64	0.62
1:A:421:TYR:CD1	1:A:457:ARG:CB	2.82	0.62
1:A:497:PHE:CE1	1:A:507:PRO:HA	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ARG:NH2	1:B:467:ASP:HB2	2.15	0.62
1:B:24:LEU:HD13	1:B:78:ARG:CD	2.27	0.62
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.80	0.62
1:C:28:TYR:HD1	1:C:61:ASN:OD1	1.82	0.62
1:B:1152:LEU:HD21	1:C:1152:LEU:HD13	1.82	0.62
1:A:289:VAL:HG12	1:A:289:VAL:O	2.00	0.62
1:A:644:GLN:HE22	2:E:1:NAG:C8	2.11	0.62
1:B:1039:ARG:NH2	1:C:1031:GLU:OE2	2.31	0.62
1:A:405:ASP:CG	1:A:504:GLY:HA2	2.24	0.61
1:A:405:ASP:CG	1:A:504:GLY:HA3	2.23	0.61
1:B:357:ARG:HB2	1:B:396:TYR:HE1	1.66	0.61
1:B:357:ARG:HB2	1:B:396:TYR:CE1	2.35	0.61
1:B:496:GLY:O	1:B:501:TYR:CE2	2.52	0.61
1:A:33:THR:HA	1:A:58:PHE:CD1	2.35	0.61
1:B:23:GLN:HA	1:B:80:ASP:HB3	1.83	0.61
1:C:147:LYS:HB3	5:C:1402:NAG:H81	1.83	0.61
3:b:1:NAG:H62	3:b:2:NAG:C7	2.30	0.61
1:B:451:TYR:HB2	1:B:497:PHE:HE2	1.65	0.60
1:B:813:SER:OG	1:B:815:ARG:NH1	2.34	0.60
1:C:131:CYS:HA	1:C:165:ASN:O	2.02	0.60
1:A:58:PHE:HB2	1:A:293:LEU:HD22	1.82	0.60
1:B:424:LYS:HB2	1:B:461:LEU:CD1	2.32	0.60
1:C:24:LEU:CB	1:C:25:PRO:CD	2.47	0.60
1:B:424:LYS:CB	1:B:461:LEU:HD11	2.31	0.60
1:B:646:ARG:HD2	1:B:668:ALA:HB1	1.83	0.60
1:A:403:ARG:HD2	1:A:505:TYR:HA	1.84	0.60
1:A:22:THR:HG22	1:A:77:LYS:O	2.02	0.60
1:B:382:VAL:HG12	1:C:983:ARG:HB3	1.84	0.60
1:A:22:THR:O	1:A:80:ASP:HB3	2.02	0.60
1:A:421:TYR:CD1	1:A:457:ARG:HB2	2.37	0.60
1:B:418:ILE:HA	1:B:422:ASN:CB	2.32	0.59
1:A:403:ARG:CG	1:A:504:GLY:O	2.51	0.59
1:A:497:PHE:CE1	1:A:506:GLN:C	2.79	0.59
1:A:497:PHE:CD1	1:A:507:PRO:N	2.71	0.59
1:B:896:ILE:HD11	1:B:904:TYR:CE1	2.37	0.59
1:A:372:ALA:CA	1:C:486:PHE:HZ	1.95	0.59
1:A:405:ASP:OD1	1:A:504:GLY:HA2	2.03	0.59
1:A:1094:VAL:CG2	1:B:904:TYR:OH	2.51	0.59
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.02	0.59
1:B:24:LEU:HD12	1:B:78:ARG:HG2	1.85	0.59
1:A:979:ASP:O	1:A:983:ARG:CD	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:PRO:O	1:B:332:ILE:N	2.35	0.58
1:B:147:LYS:O	5:B:1402:NAG:H82	2.04	0.58
1:A:503:VAL:HG12	1:A:503:VAL:O	2.03	0.58
1:B:421:TYR:HB3	1:B:454:ARG:HD2	1.85	0.58
1:C:16:VAL:HG21	1:C:255:SER:HB2	1.85	0.58
1:A:140:PHE:CZ	1:A:158:ARG:HD2	2.38	0.58
1:A:567:ARG:HD3	1:A:573:THR:HA	1.86	0.58
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.39	0.58
1:A:85:PRO:HG2	1:A:269:TYR:OH	2.03	0.58
1:A:1107:ARG:HE	1:B:904:TYR:HE2	1.52	0.57
1:C:958:ALA:HB2	1:C:1014:ARG:NH1	2.17	0.57
2:Y:1:NAG:O4	2:Y:2:NAG:O7	2.21	0.57
1:A:33:THR:HG22	1:A:58:PHE:CE1	2.39	0.57
1:A:904:TYR:CE2	1:C:1107:ARG:CZ	2.85	0.57
1:A:275:PHE:CE1	1:A:290:ASP:HB3	2.39	0.57
1:A:46:SER:HB2	1:A:847:ARG:HB3	1.87	0.57
1:C:18:PHE:HD2	1:C:138:TYR:CD2	2.20	0.57
1:A:1156:PHE:CE2	1:B:1155:TYR:HB3	2.40	0.57
1:C:773:GLU:OE2	1:C:1019:ARG:NH2	2.39	0.56
1:A:1107:ARG:CD	1:B:904:TYR:HD2	2.17	0.56
1:A:403:ARG:HG2	1:A:504:GLY:O	2.06	0.56
3:H:1:NAG:C6	3:H:2:NAG:O7	2.53	0.56
3:H:1:NAG:H61	3:H:2:NAG:C7	2.35	0.56
1:A:1107:ARG:HG2	1:B:904:TYR:HE2	1.71	0.55
1:C:616:ASN:O	1:C:618:THR:N	2.40	0.55
1:B:418:ILE:O	1:B:422:ASN:C	2.50	0.55
3:b:1:NAG:H62	3:b:2:NAG:C8	2.37	0.55
1:A:33:THR:HA	1:A:58:PHE:HE1	1.70	0.54
1:B:497:PHE:HD1	1:B:507:PRO:HD3	1.71	0.54
1:A:1107:ARG:CG	1:B:904:TYR:HE2	2.18	0.54
1:A:497:PHE:CD1	1:A:507:PRO:HB3	2.43	0.54
1:C:617:CYS:O	1:C:621:PRO:CG	2.56	0.54
1:C:902:MET:HB3	1:C:916:LEU:HD22	1.89	0.54
1:B:140:PHE:HE2	1:B:158:ARG:HH11	1.56	0.54
1:A:765:ARG:NH1	1:C:957:GLN:CD	2.64	0.54
1:A:46:SER:CB	1:A:847:ARG:HB3	2.38	0.54
1:B:415:THR:HA	1:B:420:ASP:OD1	2.08	0.54
1:B:457:ARG:NH1	1:B:461:LEU:HB3	2.22	0.54
1:C:68:ILE:HD12	1:C:78:ARG:HH11	1.73	0.53
1:B:457:ARG:HH22	1:B:467:ASP:CB	2.22	0.53
1:A:1152:LEU:HD11	1:B:1152:LEU:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:TYR:HB2	1:B:497:PHE:CE2	2.43	0.53
1:C:22:THR:HB	1:C:79:PHE:C	2.34	0.53
1:A:24:LEU:N	1:A:25:PRO:HD3	2.21	0.53
1:A:896:ILE:HD11	1:A:904:TYR:CE1	2.44	0.52
1:B:147:LYS:CB	5:B:1402:NAG:H81	2.38	0.52
1:B:497:PHE:HD1	1:B:507:PRO:CD	2.22	0.52
1:B:147:LYS:O	5:B:1402:NAG:C8	2.58	0.52
1:C:22:THR:HB	1:C:79:PHE:N	2.24	0.52
1:C:144:TYR:HB3	1:C:147:LYS:HG3	1.92	0.52
1:A:644:GLN:OE1	2:E:1:NAG:H82	2.10	0.52
1:C:896:ILE:HD11	1:C:900:MET:CG	2.39	0.52
1:B:497:PHE:HE1	1:B:507:PRO:HA	1.74	0.52
1:B:497:PHE:CE1	1:B:507:PRO:CA	2.86	0.52
1:B:424:LYS:CB	1:B:461:LEU:CD1	2.88	0.51
1:A:421:TYR:CG	1:A:457:ARG:HB2	2.45	0.51
1:A:1039:ARG:NH2	1:B:1031:GLU:OE2	2.42	0.51
1:C:153:MET:HE1	5:C:1402:NAG:O7	2.11	0.51
1:A:18:PHE:CZ	1:A:258:TRP:CD1	2.98	0.51
1:A:449:TYR:HA	1:A:495:TYR:O	2.11	0.51
1:B:886:TRP:CZ3	1:B:905:ARG:NH1	2.79	0.51
1:C:74:ASN:N	1:C:74:ASN:OD1	2.43	0.51
1:B:453:TYR:CZ	1:B:455:LEU:HD23	2.45	0.51
1:C:148:ASN:C	1:C:150:LYS:H	2.19	0.51
1:B:957:GLN:CD	1:C:765:ARG:NH2	2.68	0.51
1:A:904:TYR:CD2	1:C:1107:ARG:NE	2.68	0.50
3:H:1:NAG:C6	3:H:2:NAG:C7	2.90	0.50
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.94	0.50
3:b:1:NAG:C6	3:b:2:NAG:C7	2.89	0.50
1:C:617:CYS:O	1:C:621:PRO:HG2	2.10	0.50
1:A:57:PRO:HB3	1:A:273:ARG:HH11	1.72	0.50
1:A:644:GLN:HE22	2:E:1:NAG:H81	1.75	0.49
1:A:801:ASN:OD1	1:A:803:SER:OG	2.26	0.49
1:C:486:PHE:O	1:C:488:CYS:SG	2.71	0.49
1:C:295:PRO:CD	1:C:636:TYR:HE1	2.24	0.49
1:B:244:LEU:C	1:B:244:LEU:CD2	2.86	0.49
1:C:27:ALA:O	1:C:63:THR:HA	2.12	0.49
1:B:900:MET:O	1:B:904:TYR:HD1	1.95	0.49
1:C:319:ARG:O	1:C:319:ARG:HG3	2.12	0.49
1:A:453:TYR:OH	1:A:493:GLN:CG	2.60	0.49
1:A:996:LEU:O	1:A:1000:ARG:HG3	2.13	0.49
1:B:886:TRP:CE3	1:B:905:ARG:NH1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:PRO:HB3	1:B:273:ARG:HH11	1.69	0.49
1:A:904:TYR:HE2	1:C:1107:ARG:NE	1.82	0.49
1:A:1107:ARG:HG2	1:B:904:TYR:CE2	2.48	0.49
1:B:461:LEU:CD1	1:B:461:LEU:C	2.85	0.49
1:B:900:MET:O	1:B:904:TYR:CD1	2.66	0.49
1:B:453:TYR:CD1	1:B:493:GLN:O	2.66	0.49
1:B:497:PHE:HD1	1:B:507:PRO:CG	2.24	0.49
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.48	0.48
1:A:904:TYR:OH	1:C:1094:VAL:HB	2.13	0.48
1:B:451:TYR:CB	1:B:497:PHE:HE2	2.26	0.48
1:A:33:THR:HG22	1:A:58:PHE:CD1	2.48	0.48
1:A:23:GLN:HA	1:A:80:ASP:HB3	1.94	0.48
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.95	0.48
1:B:1107:ARG:HD3	1:C:904:TYR:CZ	2.49	0.48
1:A:497:PHE:CD1	1:A:507:PRO:CB	2.96	0.47
1:A:1107:ARG:CG	1:B:904:TYR:CE2	2.96	0.47
1:A:455:LEU:HD23	1:A:456:PHE:CE2	2.50	0.47
1:A:374:PHE:CZ	5:A:1407:NAG:H81	2.50	0.47
1:A:1010:GLN:O	1:A:1014:ARG:HG3	2.15	0.47
1:A:1101:HIS:CE1	4:I:1:NAG:H3	2.49	0.47
1:B:1039:ARG:CZ	1:C:1031:GLU:OE2	2.63	0.47
1:B:462:LYS:HG3	2:W:1:NAG:H83	1.94	0.47
2:W:1:NAG:O4	2:W:2:NAG:O7	2.33	0.47
1:A:452:LEU:HD23	1:A:494:SER:HB3	1.97	0.47
1:A:1107:ARG:NH1	1:B:904:TYR:HD2	2.13	0.46
1:C:295:PRO:CG	1:C:636:TYR:CE1	2.98	0.46
1:A:85:PRO:O	1:A:269:TYR:HE1	1.98	0.46
1:A:453:TYR:OH	1:A:493:GLN:HG2	2.14	0.46
1:A:765:ARG:HH12	1:C:957:GLN:CG	2.23	0.46
1:A:23:GLN:O	1:A:23:GLN:HG3	2.15	0.46
1:A:452:LEU:HD23	1:A:494:SER:HA	1.98	0.46
1:B:258:TRP:CZ3	1:B:260:ALA:HB2	2.50	0.46
1:A:453:TYR:OH	1:A:493:GLN:NE2	2.48	0.46
1:C:77:LYS:HG3	2:e:1:NAG:C8	2.46	0.46
1:A:18:PHE:CE1	1:A:258:TRP:CD1	3.03	0.46
1:A:1039:ARG:HE	1:B:1031:GLU:CD	2.24	0.46
1:C:33:THR:HG22	1:C:58:PHE:HE1	1.81	0.46
1:C:357:ARG:HB2	1:C:396:TYR:CE2	2.51	0.46
1:C:896:ILE:CD1	1:C:904:TYR:CZ	2.99	0.46
1:A:275:PHE:CE2	1:A:290:ASP:HB3	2.51	0.46
1:A:433:VAL:HG22	1:A:512:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:900:MET:CG	1:B:904:TYR:HE1	2.26	0.45
1:C:457:ARG:HD2	1:C:459:SER:O	2.15	0.45
1:B:22:THR:HB	1:B:79:PHE:H	1.80	0.45
1:C:295:PRO:HG2	1:C:636:TYR:CD1	2.51	0.45
1:B:761:THR:O	1:B:765:ARG:HG3	2.16	0.45
1:C:149:ASN:HB2	1:C:151:SER:OG	2.17	0.45
1:A:353:TRP:CZ3	1:A:355:ARG:HB2	2.51	0.45
1:C:319:ARG:HG2	1:C:630:THR:OG1	2.16	0.45
1:B:164:ASN:ND2	1:B:165:ASN:ND2	2.65	0.45
1:C:958:ALA:CB	1:C:1014:ARG:HH12	2.24	0.45
1:A:335:LEU:HD11	1:A:364:ASP:HB3	1.99	0.45
1:B:326:ILE:HD12	1:B:534:VAL:H	1.81	0.45
1:B:452:LEU:HD13	1:B:494:SER:HB3	1.99	0.45
1:A:1152:LEU:HD21	1:B:1152:LEU:CD1	2.44	0.44
1:B:639:GLY:C	1:B:641:ASN:H	2.25	0.44
1:C:140:PHE:HZ	1:C:158:ARG:HH11	1.66	0.44
1:A:401:VAL:HG21	1:A:451:TYR:CE1	2.53	0.44
1:A:1156:PHE:CZ	1:B:1155:TYR:HB3	2.52	0.44
1:A:405:ASP:OD1	1:A:504:GLY:CA	2.65	0.44
1:C:896:ILE:HD11	1:C:904:TYR:CE2	2.53	0.44
1:A:983:ARG:HD2	1:C:518:LEU:HD12	1.99	0.44
1:B:164:ASN:ND2	1:B:165:ASN:CG	2.75	0.44
1:C:896:ILE:HG12	1:C:900:MET:HB3	1.99	0.44
2:Y:1:NAG:C6	2:Y:2:NAG:C7	2.87	0.44
1:B:455:LEU:HD12	1:B:456:PHE:CE2	2.53	0.43
1:A:290:ASP:OD1	1:A:290:ASP:N	2.48	0.43
1:B:461:LEU:C	1:B:461:LEU:HD12	2.43	0.43
1:B:461:LEU:HD12	1:B:461:LEU:O	2.19	0.43
1:A:453:TYR:CD2	1:A:493:GLN:O	2.72	0.43
1:A:453:TYR:CE2	1:A:493:GLN:O	2.71	0.43
1:B:449:TYR:CE1	1:B:496:GLY:HA2	2.54	0.43
1:B:455:LEU:HD12	1:B:456:PHE:CD2	2.54	0.43
1:B:958:ALA:HB2	1:B:1014:ARG:HH12	1.84	0.42
1:C:158:ARG:NH2	1:C:254:SER:HA	2.34	0.42
1:A:1107:ARG:HD3	1:B:904:TYR:HD2	1.69	0.42
1:B:1107:ARG:HD3	1:C:904:TYR:CE2	2.54	0.42
1:A:175:PHE:CE1	1:A:177:MET:HE2	2.54	0.42
1:C:145:TYR:C	1:C:147:LYS:H	2.27	0.42
1:C:634:ARG:HG2	1:C:637:SER:OG	2.19	0.42
1:A:453:TYR:CZ	1:A:493:GLN:CG	3.03	0.42
1:C:148:ASN:O	1:C:150:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:TYR:HB3	1:A:454:ARG:HG2	2.02	0.42
1:A:452:LEU:HD23	1:A:494:SER:CA	2.50	0.41
1:B:497:PHE:CD1	1:B:507:PRO:HG3	2.55	0.41
2:W:1:NAG:H61	2:W:2:NAG:C7	2.51	0.41
1:B:57:PRO:HB3	1:B:273:ARG:HH12	1.75	0.41
1:B:244:LEU:HG	1:B:259:THR:O	2.21	0.41
1:C:58:PHE:HB2	1:C:290:ASP:CB	2.51	0.41
1:C:140:PHE:CE2	1:C:158:ARG:HD2	2.54	0.41
1:C:295:PRO:CD	1:C:636:TYR:CE1	3.04	0.41
1:A:1152:LEU:HD11	1:B:1152:LEU:HD11	2.02	0.41
1:B:326:ILE:HG23	1:B:541:PHE:HA	2.03	0.41
1:B:1050:MET:HE2	1:B:1052:PHE:CE1	2.56	0.41
1:C:326:ILE:HD11	1:C:534:VAL:HG22	2.02	0.41
1:B:28:TYR:CD1	1:B:61:ASN:CG	2.91	0.40
1:B:453:TYR:CE2	1:B:455:LEU:CD2	3.02	0.40
1:C:319:ARG:HB2	1:C:319:ARG:CZ	2.52	0.40
1:B:142:GLY:CA	1:B:156:GLU:HB2	2.52	0.40
1:B:357:ARG:CB	1:B:396:TYR:CE1	3.05	0.40
1:B:443:SER:HA	1:B:497:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1108/1310 (85%)	1008 (91%)	87 (8%)	13 (1%)	10	40
1	B	1087/1310 (83%)	998 (92%)	82 (8%)	7 (1%)	21	54
1	C	1109/1310 (85%)	1025 (92%)	75 (7%)	9 (1%)	16	48
All	All	3304/3930 (84%)	3031 (92%)	244 (7%)	29 (1%)	16	45

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	582	LEU
1	A	834	ILE
1	A	920	GLN
1	B	24	LEU
1	B	331	ASN
1	C	24	LEU
1	C	147	LYS
1	C	617	CYS
1	C	834	ILE
1	A	79	PHE
1	A	1041	ASP
1	C	149	ASN
1	C	830	ASP
1	C	940	SER
1	B	420	ASP
1	A	88	ASP
1	A	487	ASN
1	B	1107	ARG
1	A	570	ALA
1	B	148	ASN
1	B	423	TYR
1	A	25	PRO
1	A	32	PHE
1	C	709	ASN
1	A	504	GLY
1	C	159	VAL
1	A	367	VAL
1	B	257	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	970/1135 (86%)	950 (98%)	20 (2%)	47	64
1	B	959/1135 (84%)	941 (98%)	18 (2%)	50	66
1	C	974/1135 (86%)	954 (98%)	20 (2%)	47	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2903/3405 (85%)	2845 (98%)	58 (2%)	48 65

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	127	VAL
1	A	186	PHE
1	A	284	THR
1	A	335	LEU
1	A	351	TYR
1	A	367	VAL
1	A	368	LEU
1	A	457	ARG
1	A	461	LEU
1	A	514	SER
1	A	515	PHE
1	A	603	ASN
1	A	640	SER
1	A	745	ASP
1	A	787	GLN
1	A	836	GLN
1	A	841	LEU
1	A	843	ASP
1	A	1082	CYS
1	B	20	ASN
1	B	120	VAL
1	B	122	ASN
1	B	125	ASN
1	B	185	ASN
1	B	349	SER
1	B	376	THR
1	B	441	LEU
1	B	443	SER
1	B	455	LEU
1	B	461	LEU
1	B	480	CYS
1	B	523	THR
1	B	544	ASN
1	B	634	ARG
1	B	635	VAL
1	B	941	THR

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Mol	Chain	Res	Type
1	B	965	GLN
1	C	24	LEU
1	C	73	THR
1	C	74	ASN
1	C	122	ASN
1	C	138	TYR
1	C	186	PHE
1	C	273	ARG
1	C	332	ILE
1	C	523	THR
1	C	581	THR
1	C	613	GLN
1	C	622	VAL
1	C	624	ILE
1	C	630	THR
1	C	635	VAL
1	C	739	THR
1	C	836	GLN
1	C	965	GLN
1	C	985	ASP
1	C	1072	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	87	ASN
1	A	115	GLN
1	A	121	ASN
1	A	125	ASN
1	A	137	ASN
1	A	185	ASN
1	A	334	ASN
1	A	354	ASN
1	A	360	ASN
1	A	370	ASN
1	A	409	GLN
1	A	422	ASN
1	A	644	GLN
1	A	914	ASN
1	A	920	GLN
1	A	935	GLN

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Mol	Chain	Res	Type
1	A	1002	GLN
1	A	1054	GLN
1	A	1058	HIS
1	A	1119	ASN
1	A	1135	ASN
1	B	23	GLN
1	B	121	ASN
1	B	146	HIS
1	B	164	ASN
1	B	544	ASN
1	B	564	GLN
1	B	580	GLN
1	B	606	ASN
1	B	762	GLN
1	B	935	GLN
1	B	978	ASN
1	B	1002	GLN
1	B	1054	GLN
1	B	1058	HIS
1	C	23	GLN
1	C	121	ASN
1	C	137	ASN
1	C	146	HIS
1	C	196	ASN
1	C	314	GLN
1	C	613	GLN
1	C	690	GLN
1	C	762	GLN
1	C	764	ASN
1	C	787	GLN
1	C	901	GLN
1	C	907	ASN
1	C	919	ASN
1	C	935	GLN
1	C	949	GLN
1	C	953	ASN
1	C	957	GLN
1	C	1002	GLN
1	C	1119	ASN
1	C	1159	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 ⓘ

65 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	1.24	2 (14%)	17,19,21	1.40	2 (11%)
2	NAG	D	2	2	14,14,15	1.28	1 (7%)	17,19,21	0.59	0
2	NAG	E	1	1,2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	E	2	2	14,14,15	1.05	1 (7%)	17,19,21	0.98	1 (5%)
2	NAG	F	1	1,2	14,14,15	1.24	2 (14%)	17,19,21	0.79	0
2	NAG	F	2	2	14,14,15	1.16	1 (7%)	17,19,21	0.77	0
2	NAG	G	1	1,2	14,14,15	1.20	1 (7%)	17,19,21	0.91	0
2	NAG	G	2	2	14,14,15	1.16	1 (7%)	17,19,21	0.71	0
3	NAG	H	1	1,3	14,14,15	1.29	1 (7%)	17,19,21	0.98	2 (11%)
3	NAG	H	2	3	14,14,15	1.29	2 (14%)	17,19,21	1.05	1 (5%)
3	FUC	H	3	3	10,10,11	1.71	2 (20%)	14,14,16	1.08	1 (7%)
4	NAG	I	1	1,4	14,14,15	1.34	2 (14%)	17,19,21	1.20	3 (17%)
4	NAG	I	2	4	14,14,15	1.45	4 (28%)	17,19,21	1.32	2 (11%)
4	MAN	I	3	4	11,11,12	1.51	2 (18%)	15,15,17	0.77	0
4	NAG	J	1	1,4	14,14,15	1.22	2 (14%)	17,19,21	0.64	0
4	NAG	J	2	4	14,14,15	1.33	2 (14%)	17,19,21	0.64	0
4	MAN	J	3	4	11,11,12	1.47	2 (18%)	15,15,17	0.99	1 (6%)
2	NAG	K	1	1,2	14,14,15	0.24	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	K	2	2	14,14,15	1.18	2 (14%)	17,19,21	1.42	2 (11%)
2	NAG	L	1	1,2	14,14,15	1.27	1 (7%)	17,19,21	0.94	0
2	NAG	L	2	2	14,14,15	1.30	2 (14%)	17,19,21	0.80	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.27	0	17,19,21	0.46	0
2	NAG	M	2	2	14,14,15	1.17	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	N	1	1,2	14,14,15	1.27	2 (14%)	17,19,21	0.95	0
2	NAG	N	2	2	14,14,15	1.33	2 (14%)	17,19,21	0.73	1 (5%)
2	NAG	O	1	1,2	14,14,15	1.10	1 (7%)	17,19,21	0.88	0
2	NAG	O	2	2	14,14,15	1.21	1 (7%)	17,19,21	0.73	0
2	NAG	P	1	1,2	14,14,15	1.15	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	P	2	2	14,14,15	1.39	2 (14%)	17,19,21	0.58	0
3	NAG	Q	1	1,3	14,14,15	1.48	4 (28%)	17,19,21	0.89	1 (5%)
3	NAG	Q	2	3	14,14,15	1.30	1 (7%)	17,19,21	0.66	0
3	FUC	Q	3	3	10,10,11	1.79	2 (20%)	14,14,16	1.19	2 (14%)
4	NAG	R	1	1,4	14,14,15	1.17	2 (14%)	17,19,21	0.98	0
4	NAG	R	2	4	14,14,15	1.38	2 (14%)	17,19,21	0.78	1 (5%)
4	MAN	R	3	4	11,11,12	1.48	2 (18%)	15,15,17	0.89	0
4	NAG	S	1	1,4	14,14,15	1.56	2 (14%)	17,19,21	1.01	1 (5%)
4	NAG	S	2	4	14,14,15	1.36	2 (14%)	17,19,21	0.89	0
4	MAN	S	3	4	11,11,12	1.46	2 (18%)	15,15,17	0.87	0
2	NAG	T	1	1,2	14,14,15	0.23	0	17,19,21	0.50	0
2	NAG	T	2	2	14,14,15	1.18	3 (21%)	17,19,21	1.42	2 (11%)
2	NAG	U	1	1,2	14,14,15	1.30	2 (14%)	17,19,21	1.22	3 (17%)
2	NAG	U	2	2	14,14,15	1.25	1 (7%)	17,19,21	0.71	0
2	NAG	V	1	1,2	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	V	2	2	14,14,15	1.01	1 (7%)	17,19,21	0.73	0
2	NAG	W	1	1,2	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	W	2	2	14,14,15	1.07	1 (7%)	17,19,21	1.39	1 (5%)
2	NAG	X	1	1,2	14,14,15	1.22	1 (7%)	17,19,21	0.81	0
2	NAG	X	2	2	14,14,15	1.31	3 (21%)	17,19,21	0.95	1 (5%)
2	NAG	Y	1	1,2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	Y	2	2	14,14,15	1.09	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	Z	1	1,2	14,14,15	1.21	1 (7%)	17,19,21	0.76	0
2	NAG	Z	2	2	14,14,15	1.12	1 (7%)	17,19,21	0.73	0
2	NAG	a	1	1,2	14,14,15	1.10	1 (7%)	17,19,21	0.72	0
2	NAG	a	2	2	14,14,15	1.26	1 (7%)	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	b	1	1,3	14,14,15	0.20	0	17,19,21	0.84	1 (5%)
3	NAG	b	2	3	14,14,15	1.05	1 (7%)	17,19,21	0.86	1 (5%)
3	FUC	b	3	3	10,10,11	1.61	2 (20%)	14,14,16	1.20	2 (14%)
4	NAG	c	1	1,4	14,14,15	1.08	1 (7%)	17,19,21	1.01	2 (11%)
4	NAG	c	2	4	14,14,15	1.37	2 (14%)	17,19,21	0.71	0
4	MAN	c	3	4	11,11,12	1.44	2 (18%)	15,15,17	0.84	0
4	NAG	d	1	1,4	14,14,15	1.22	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	d	2	4	14,14,15	1.35	2 (14%)	17,19,21	0.62	0
4	MAN	d	3	4	11,11,12	1.57	2 (18%)	15,15,17	1.12	1 (6%)
2	NAG	e	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	1.26	1 (5%)
2	NAG	e	2	2	14,14,15	1.35	2 (14%)	17,19,21	0.86	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	-	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	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	-	1/2/19/22	1/1/1/1
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
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	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	1/6/23/26	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	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	FUC	Q	3	3	-	-	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	MAN	R	3	4	-	1/2/19/22	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	MAN	S	3	4	-	0/2/19/22	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	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
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	3/6/23/26	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	0/6/23/26	0/1/1/1
3	FUC	b	3	3	-	-	0/1/1/1
4	NAG	c	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
4	MAN	c	3	4	-	1/2/19/22	0/1/1/1
4	NAG	d	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	d	3	4	-	0/2/19/22	1/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	O5-C5	3.94	1.51	1.43
4	d	3	MAN	O5-C5	3.35	1.50	1.43
2	M	2	NAG	O5-C5	3.24	1.49	1.43
4	S	3	MAN	O5-C5	3.15	1.49	1.43
3	Q	3	FUC	O5-C1	3.11	1.48	1.43
4	I	1	NAG	O5-C5	3.09	1.49	1.43
2	U	1	NAG	O5-C5	3.06	1.49	1.43
4	c	2	NAG	O5-C5	3.05	1.49	1.43
3	b	3	FUC	C1-C2	3.04	1.59	1.52
3	H	3	FUC	O5-C1	3.03	1.48	1.43
4	J	3	MAN	O5-C5	3.02	1.49	1.43
3	Q	3	FUC	O5-C5	3.02	1.49	1.43
4	c	3	MAN	O5-C5	3.00	1.49	1.43
2	P	2	NAG	O5-C1	2.98	1.48	1.43
4	I	3	MAN	O5-C5	2.94	1.49	1.43
4	R	3	MAN	O5-C5	2.94	1.49	1.43
2	N	2	NAG	O5-C5	2.92	1.49	1.43
3	H	3	FUC	O5-C5	2.90	1.49	1.43
2	L	2	NAG	O5-C5	2.89	1.49	1.43
2	G	2	NAG	O5-C5	2.88	1.49	1.43
3	b	3	FUC	O5-C5	2.84	1.49	1.43
4	R	1	NAG	O5-C5	2.84	1.49	1.43
2	a	2	NAG	O5-C5	2.84	1.49	1.43
2	O	2	NAG	O5-C5	2.83	1.48	1.43
3	Q	2	NAG	O5-C5	2.82	1.48	1.43
4	R	2	NAG	O5-C5	2.80	1.48	1.43
2	D	1	NAG	O5-C5	2.80	1.48	1.43
2	W	2	NAG	O5-C5	2.79	1.48	1.43
3	Q	1	NAG	O5-C5	2.77	1.48	1.43
3	H	1	NAG	C1-C2	2.76	1.56	1.52
4	d	2	NAG	O5-C5	2.76	1.48	1.43
2	E	2	NAG	O5-C5	2.75	1.48	1.43
2	Z	2	NAG	O5-C5	2.74	1.48	1.43
3	H	2	NAG	O5-C5	2.73	1.48	1.43
3	b	2	NAG	O5-C5	2.72	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	O5-C5	2.71	1.48	1.43
2	X	1	NAG	O5-C5	2.71	1.48	1.43
2	X	2	NAG	O5-C5	2.70	1.48	1.43
3	Q	1	NAG	C1-C2	2.70	1.56	1.52
2	P	1	NAG	O5-C5	2.70	1.48	1.43
2	F	1	NAG	O5-C5	2.68	1.48	1.43
4	J	2	NAG	O5-C5	2.66	1.48	1.43
2	Z	1	NAG	O5-C5	2.65	1.48	1.43
2	U	2	NAG	O5-C5	2.64	1.48	1.43
2	L	1	NAG	O5-C5	2.61	1.48	1.43
4	I	3	MAN	O5-C1	2.61	1.48	1.43
2	N	1	NAG	O5-C5	2.60	1.48	1.43
2	V	2	NAG	O5-C5	2.60	1.48	1.43
2	e	2	NAG	O5-C5	2.60	1.48	1.43
4	d	1	NAG	O5-C5	2.59	1.48	1.43
4	S	2	NAG	O5-C5	2.58	1.48	1.43
2	Y	2	NAG	O5-C5	2.56	1.48	1.43
4	d	3	MAN	O5-C1	2.56	1.48	1.43
4	R	2	NAG	O4-C4	2.53	1.49	1.43
2	P	2	NAG	O5-C5	2.53	1.48	1.43
2	e	1	NAG	O5-C5	2.52	1.48	1.43
4	J	1	NAG	O5-C5	2.52	1.48	1.43
4	d	2	NAG	O4-C4	2.48	1.49	1.43
2	D	2	NAG	O5-C5	2.47	1.48	1.43
4	S	1	NAG	C1-C2	2.47	1.55	1.52
2	e	2	NAG	O4-C4	2.46	1.49	1.43
4	R	3	MAN	O5-C1	2.41	1.47	1.43
4	J	2	NAG	O4-C4	2.37	1.48	1.43
4	I	2	NAG	O4-C4	2.32	1.48	1.43
4	I	2	NAG	C1-C2	2.32	1.55	1.52
2	N	2	NAG	O5-C1	2.30	1.47	1.43
3	Q	1	NAG	O5-C1	2.30	1.47	1.43
4	J	3	MAN	O5-C1	2.29	1.47	1.43
3	H	2	NAG	C1-C2	2.29	1.55	1.52
4	I	2	NAG	O5-C5	2.29	1.47	1.43
4	S	3	MAN	O5-C1	2.28	1.47	1.43
2	L	2	NAG	O5-C1	2.28	1.47	1.43
4	S	2	NAG	O4-C4	2.28	1.48	1.43
2	O	1	NAG	O5-C5	2.26	1.47	1.43
2	T	2	NAG	O5-C5	2.25	1.47	1.43
2	K	2	NAG	O5-C5	2.24	1.47	1.43
4	I	2	NAG	O5-C1	2.21	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	3	MAN	O5-C1	2.19	1.47	1.43
2	a	1	NAG	O5-C5	2.19	1.47	1.43
2	K	2	NAG	O4-C4	2.19	1.48	1.43
4	c	1	NAG	O5-C5	2.19	1.47	1.43
2	T	2	NAG	O4-C4	2.17	1.48	1.43
2	D	1	NAG	O4-C4	2.16	1.48	1.43
4	c	2	NAG	O4-C4	2.14	1.48	1.43
3	Q	1	NAG	O4-C4	2.11	1.48	1.43
2	X	2	NAG	C1-C2	2.09	1.55	1.52
2	X	2	NAG	O5-C1	2.09	1.47	1.43
2	F	1	NAG	C1-C2	2.08	1.55	1.52
2	G	1	NAG	O4-C4	2.08	1.48	1.43
2	N	1	NAG	O5-C1	2.05	1.47	1.43
2	U	1	NAG	O4-C4	2.04	1.48	1.43
4	I	1	NAG	O5-C1	2.04	1.47	1.43
4	R	1	NAG	O4-C4	2.02	1.48	1.43
4	J	1	NAG	C1-C2	2.02	1.55	1.52
2	T	2	NAG	C8-C7	2.00	1.54	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	2	NAG	C1-O5-C5	4.88	118.73	112.19
2	K	2	NAG	C1-O5-C5	4.71	118.50	112.19
2	T	2	NAG	C1-O5-C5	4.71	118.50	112.19
2	e	1	NAG	C1-O5-C5	4.32	117.98	112.19
2	D	1	NAG	C1-O5-C5	4.30	117.95	112.19
4	I	2	NAG	C1-O5-C5	4.08	117.66	112.19
2	X	2	NAG	C1-O5-C5	3.43	116.79	112.19
3	H	2	NAG	C1-O5-C5	3.23	116.52	112.19
2	E	2	NAG	C1-O5-C5	3.03	116.24	112.19
4	d	3	MAN	C1-O5-C5	3.02	116.23	112.19
3	Q	1	NAG	O5-C5-C6	2.98	113.46	107.66
2	Y	2	NAG	C1-O5-C5	2.82	115.96	112.19
3	b	1	NAG	C1-O5-C5	2.77	115.89	112.19
2	M	2	NAG	C1-O5-C5	2.77	115.89	112.19
4	J	3	MAN	C1-O5-C5	2.66	115.76	112.19
2	L	2	NAG	C1-O5-C5	2.66	115.75	112.19
4	I	1	NAG	C1-O5-C5	2.60	115.67	112.19
3	b	3	FUC	C1-O5-C5	2.55	118.99	112.97
3	b	3	FUC	C1-C2-C3	2.49	113.27	109.64
2	D	1	NAG	C3-C4-C5	2.46	114.68	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	3	FUC	C1-C2-C3	2.44	113.19	109.64
3	b	2	NAG	C1-O5-C5	2.43	115.44	112.19
3	Q	3	FUC	C1-O5-C5	2.36	118.54	112.97
3	H	1	NAG	O5-C5-C6	2.34	112.22	107.66
2	U	1	NAG	O5-C1-C2	-2.31	107.72	111.29
3	H	3	FUC	C1-C2-C3	2.30	112.99	109.64
2	N	2	NAG	C1-O5-C5	2.25	115.20	112.19
2	U	1	NAG	C4-C3-C2	-2.24	107.74	111.02
4	d	1	NAG	C1-O5-C5	2.20	115.14	112.19
2	a	2	NAG	C1-O5-C5	2.18	115.10	112.19
3	H	1	NAG	C1-O5-C5	2.16	115.08	112.19
4	I	2	NAG	O5-C1-C2	-2.13	107.99	111.29
4	S	1	NAG	C4-C3-C2	-2.13	107.89	111.02
2	U	1	NAG	C1-C2-N2	2.12	113.78	110.43
4	R	2	NAG	O5-C1-C2	-2.09	108.06	111.29
4	c	1	NAG	C1-O5-C5	2.08	114.97	112.19
2	P	1	NAG	C1-O5-C5	-2.05	109.43	112.19
4	c	1	NAG	O4-C4-C3	-2.03	105.58	110.38
4	I	1	NAG	O5-C1-C2	-2.02	108.17	111.29
2	T	2	NAG	C1-C2-N2	2.02	113.61	110.43
2	K	2	NAG	C1-C2-N2	2.01	113.60	110.43
4	I	1	NAG	O4-C4-C3	-2.01	105.65	110.38

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C8-C7-N2-C2
2	T	2	NAG	C8-C7-N2-C2
2	K	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	K	2	NAG	O7-C7-N2-C2
2	T	2	NAG	O7-C7-N2-C2
4	I	3	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	c	3	MAN	O5-C5-C6-O6
4	R	3	MAN	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
2	N	1	NAG	C1-C2-N2-C7
2	Y	2	NAG	C1-C2-N2-C7
3	Q	1	NAG	C1-C2-N2-C7
2	Y	2	NAG	C3-C2-N2-C7
2	Y	2	NAG	C4-C5-C6-O6

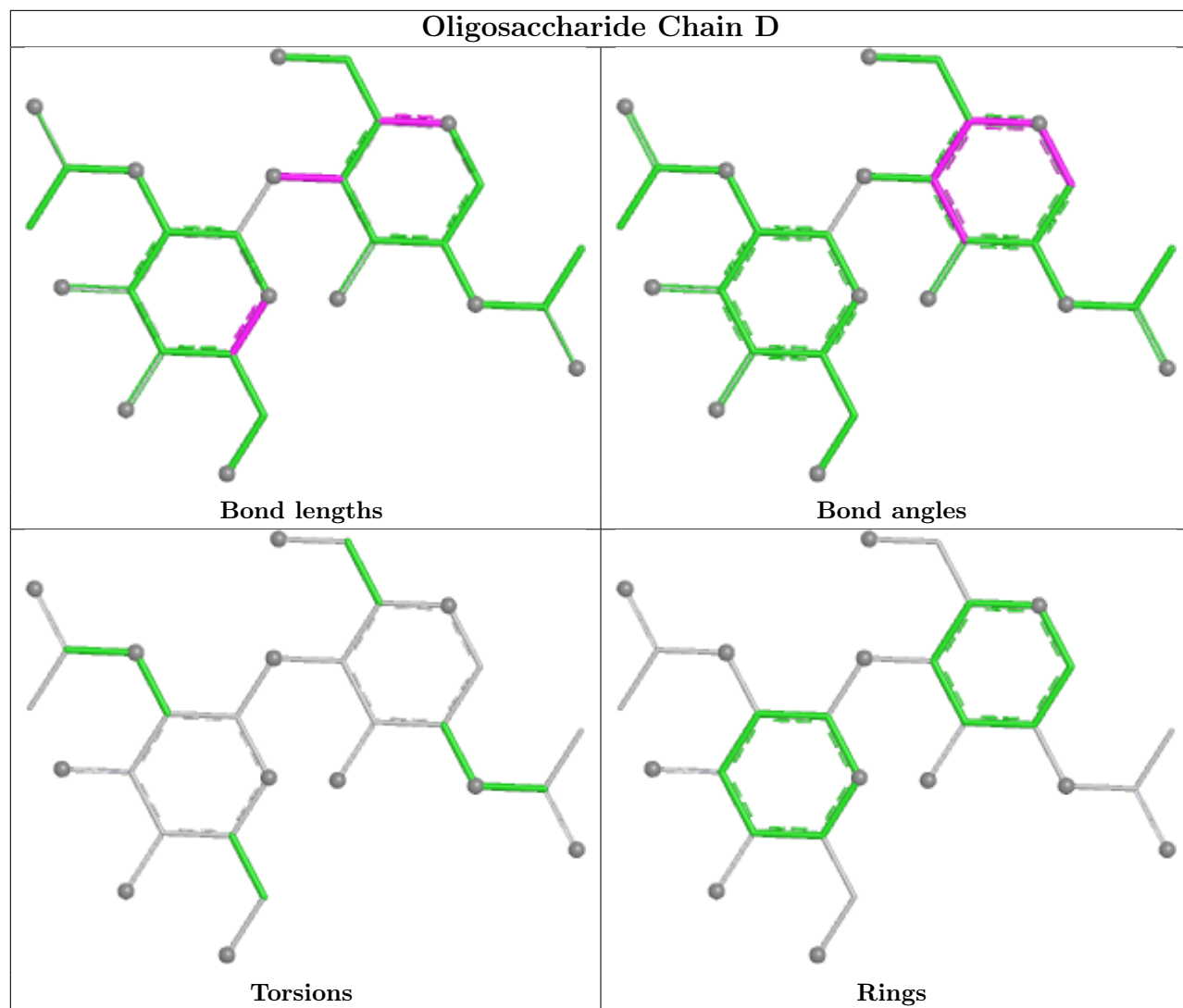
All (3) ring outliers are listed below:

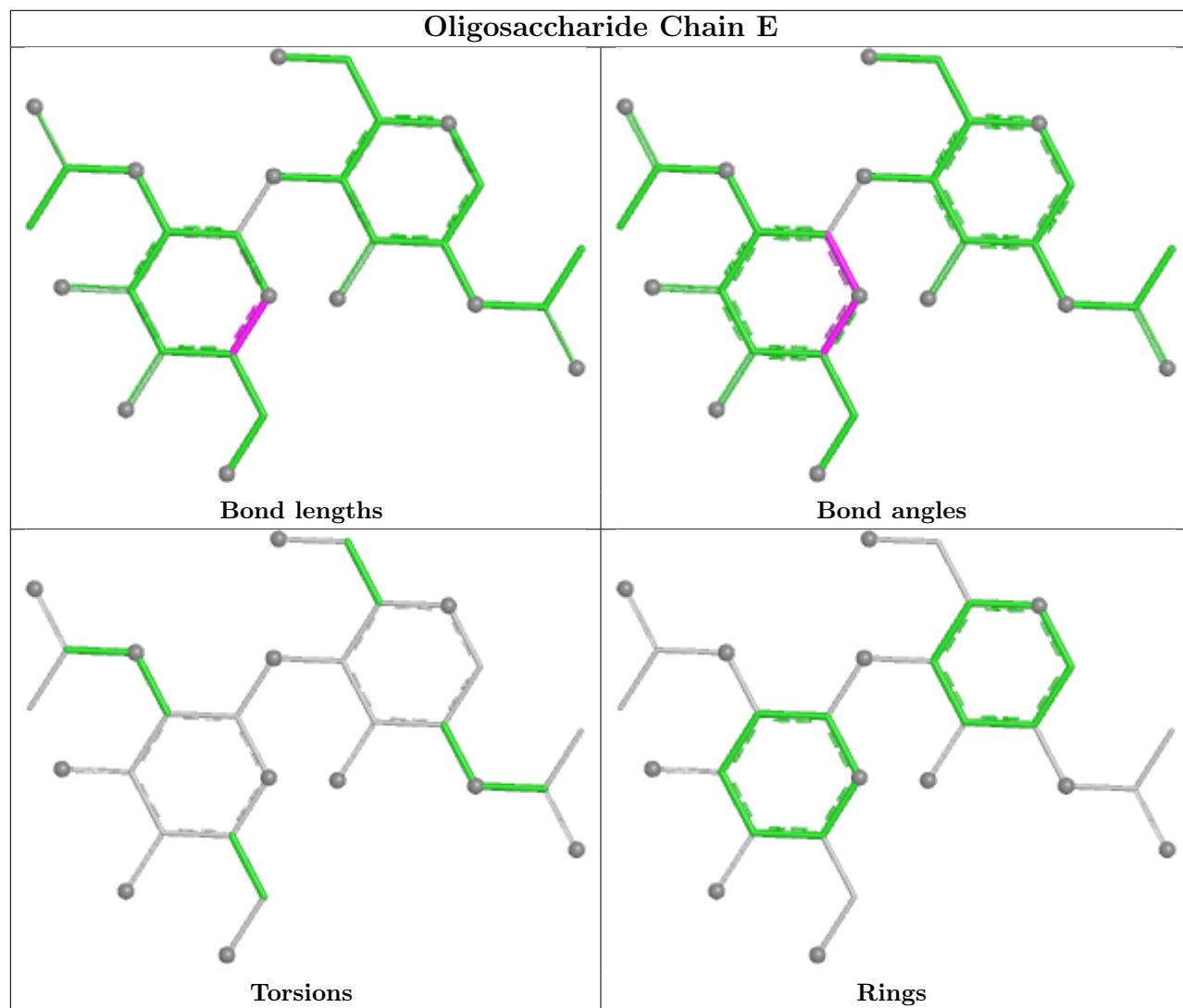
Mol	Chain	Res	Type	Atoms
4	I	3	MAN	C1-C2-C3-C4-C5-O5
4	J	3	MAN	C1-C2-C3-C4-C5-O5
4	d	3	MAN	C1-C2-C3-C4-C5-O5

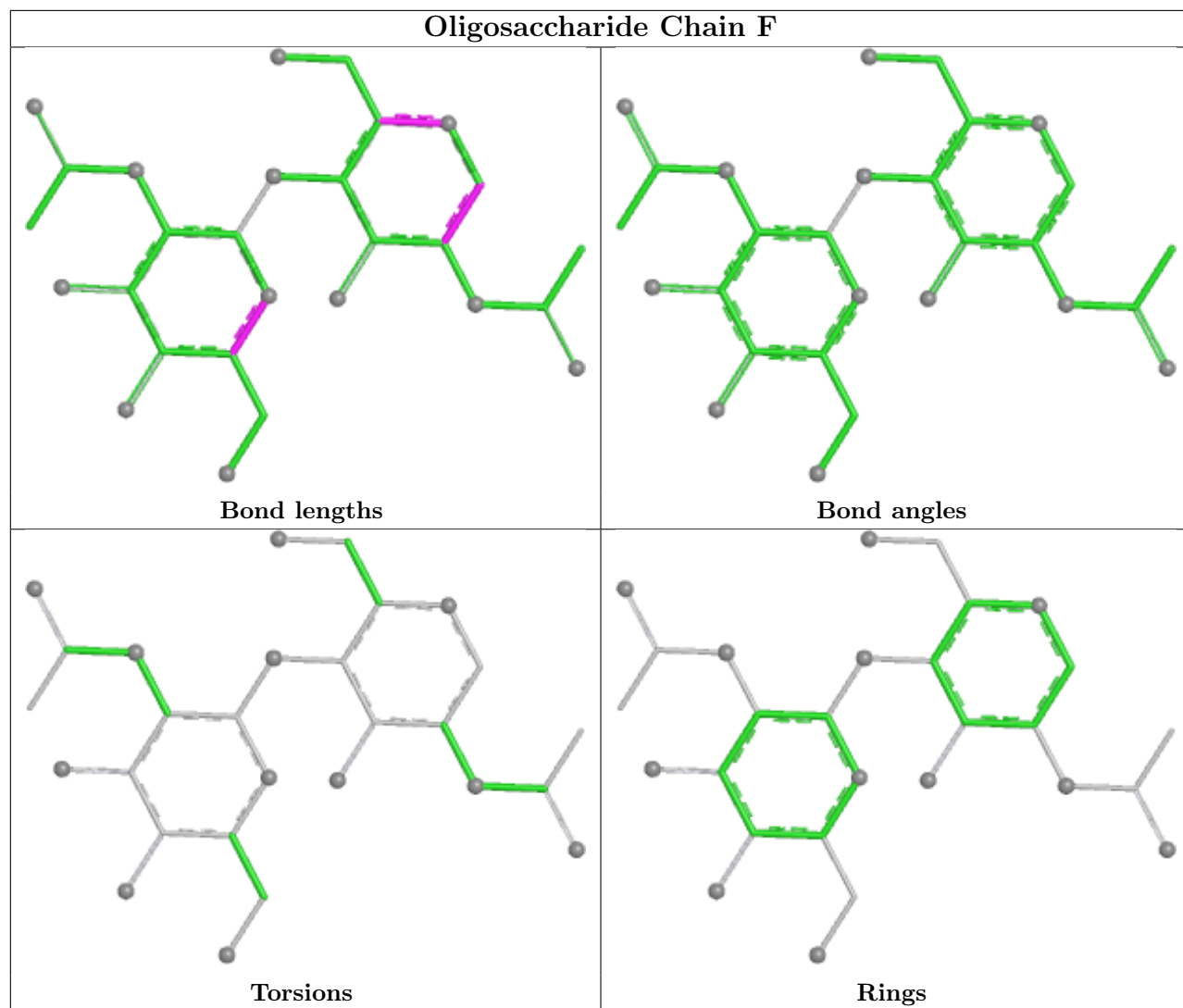
11 monomers are involved in 25 short contacts:

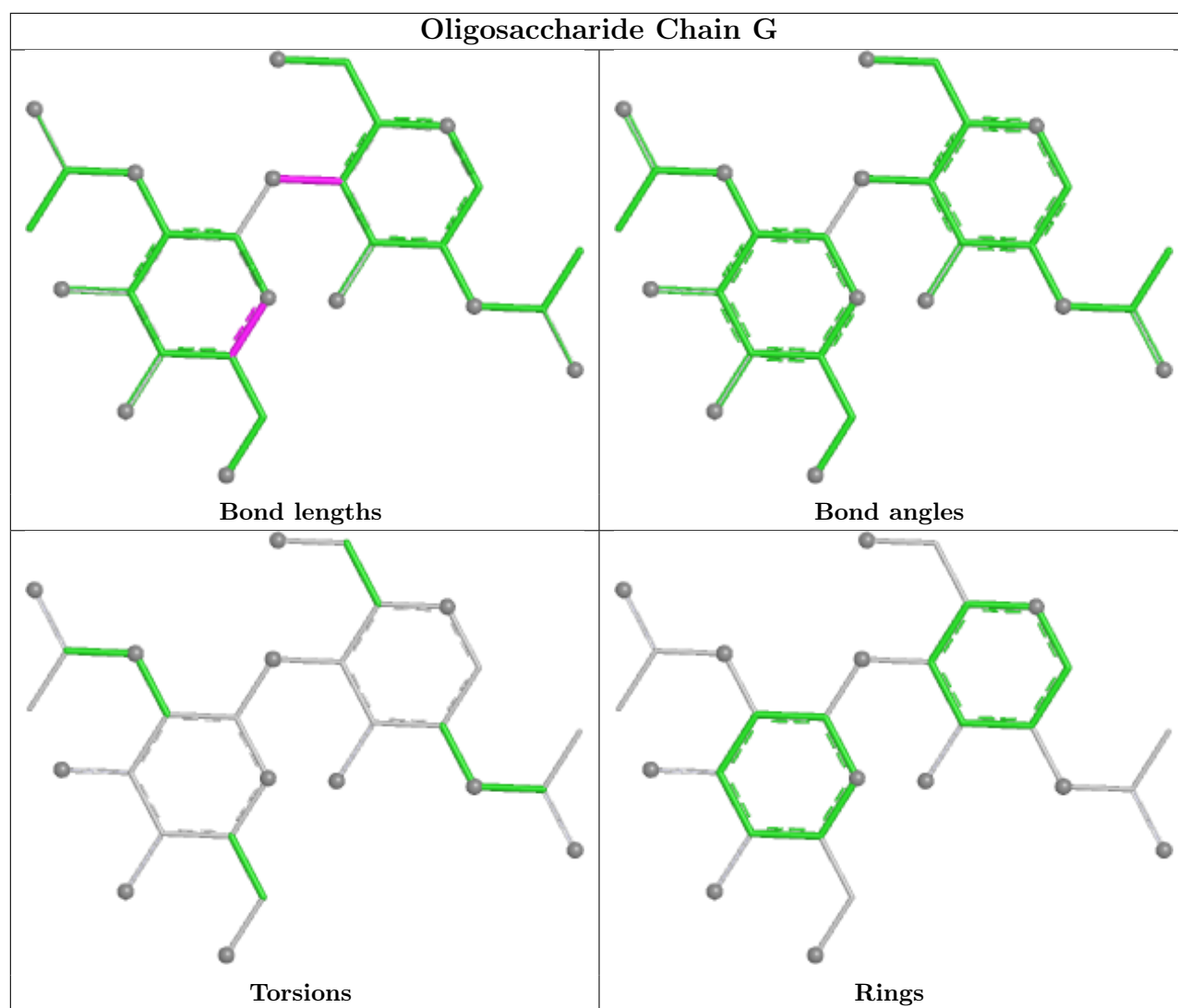
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	e	1	NAG	1	0
3	H	1	NAG	4	0
2	E	1	NAG	6	0
2	W	2	NAG	2	0
3	H	2	NAG	4	0
2	Y	1	NAG	4	0
2	W	1	NAG	6	0
2	Y	2	NAG	3	0
3	b	2	NAG	3	0
3	b	1	NAG	3	0
4	I	1	NAG	1	0

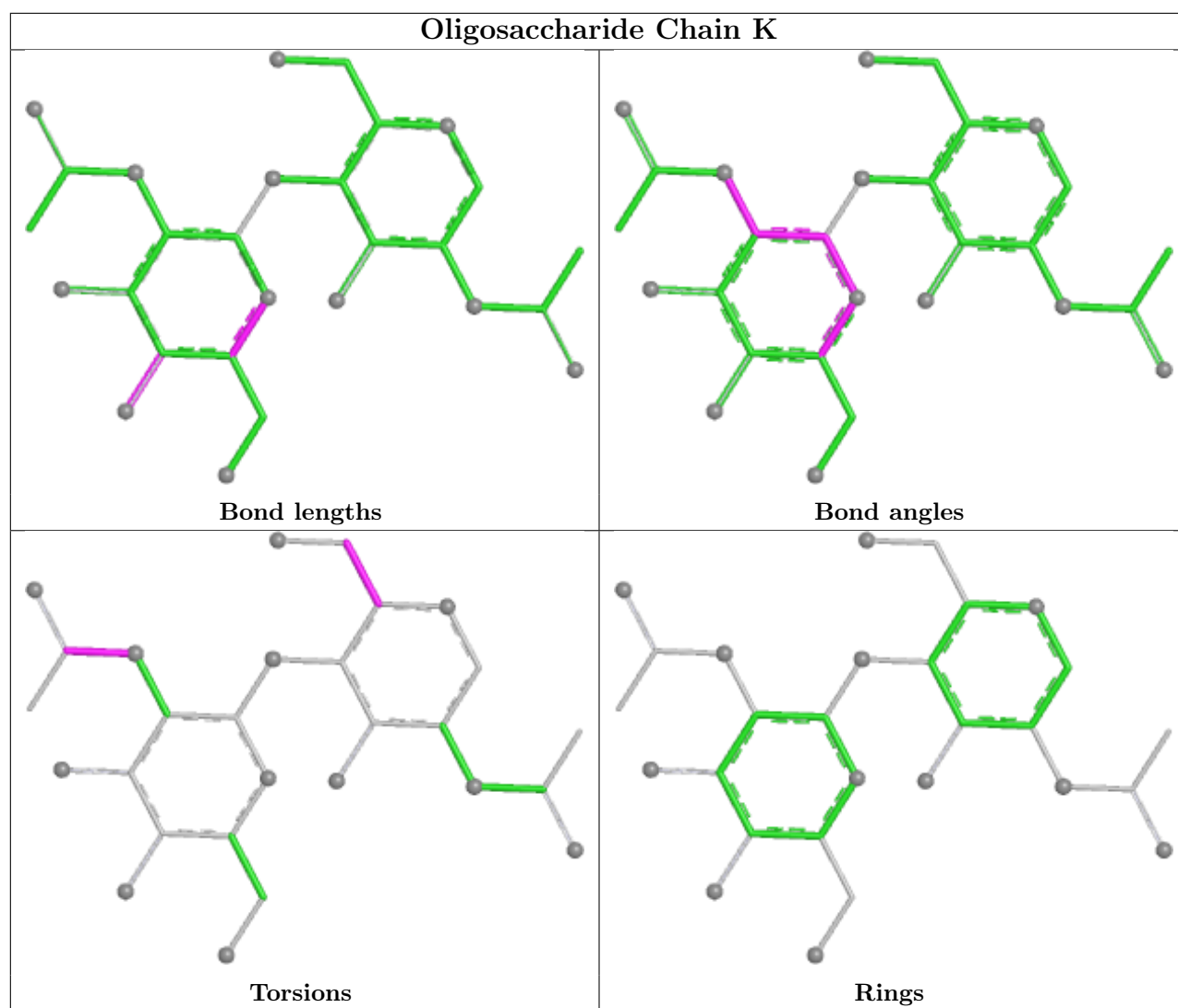
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

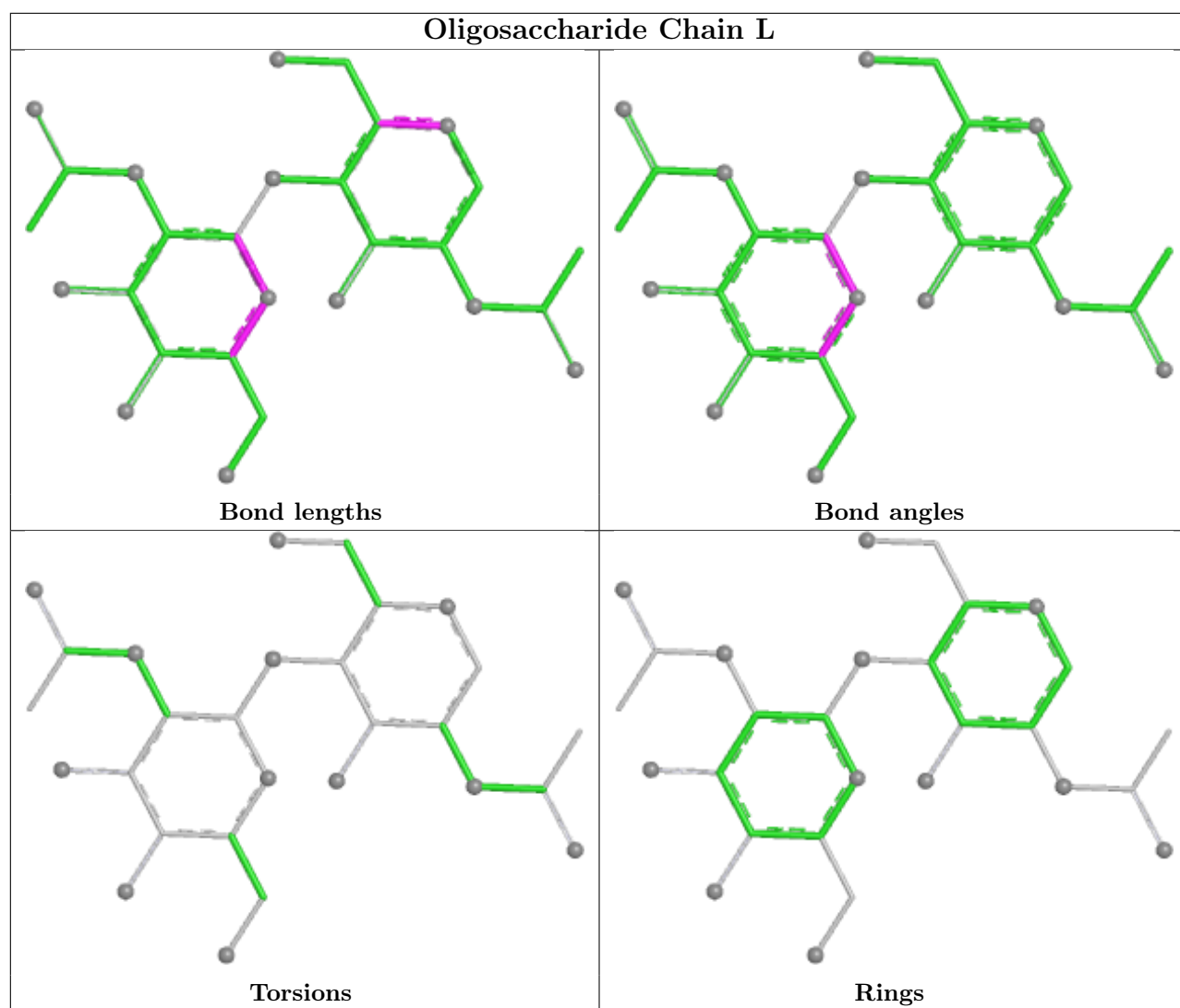


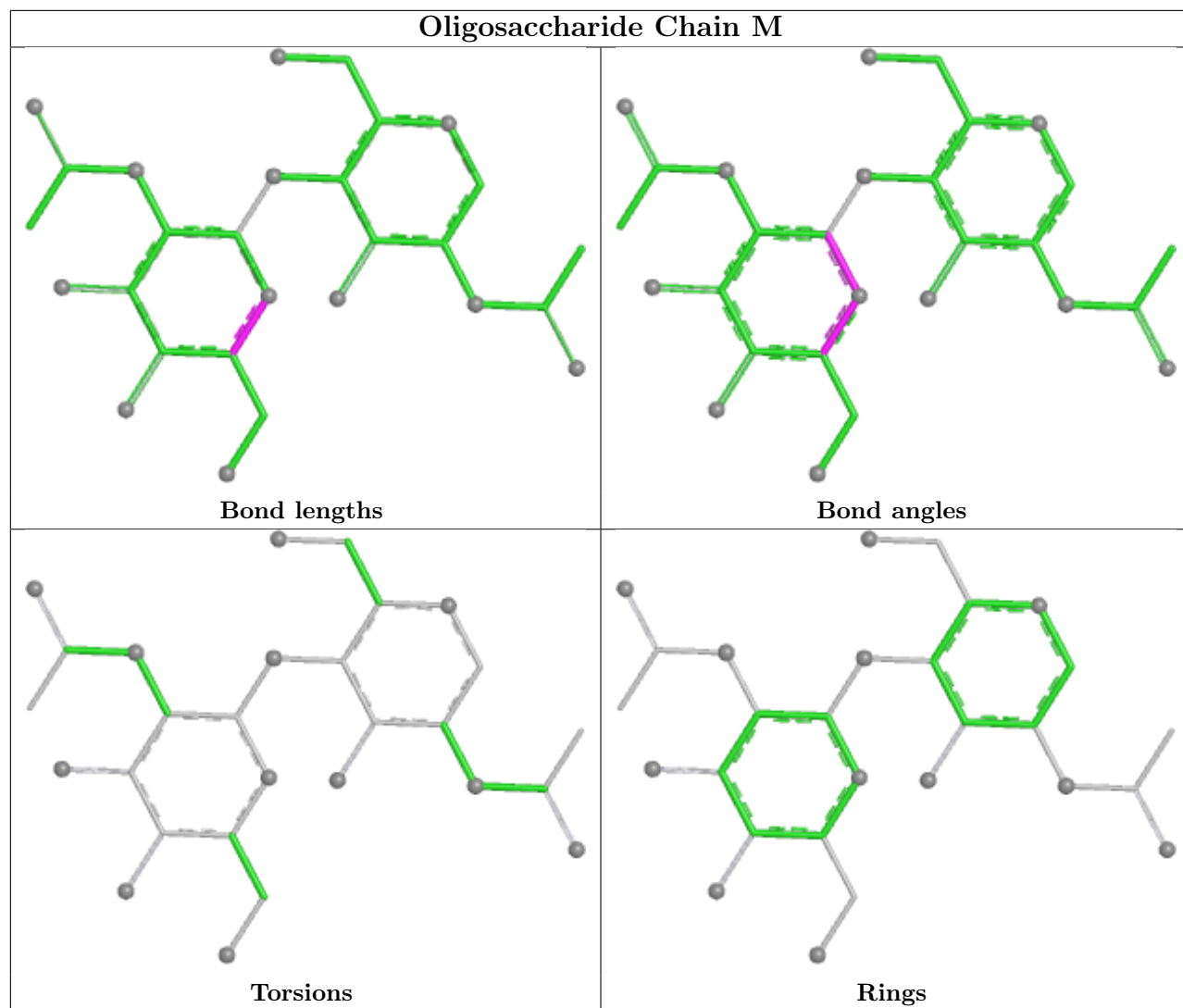


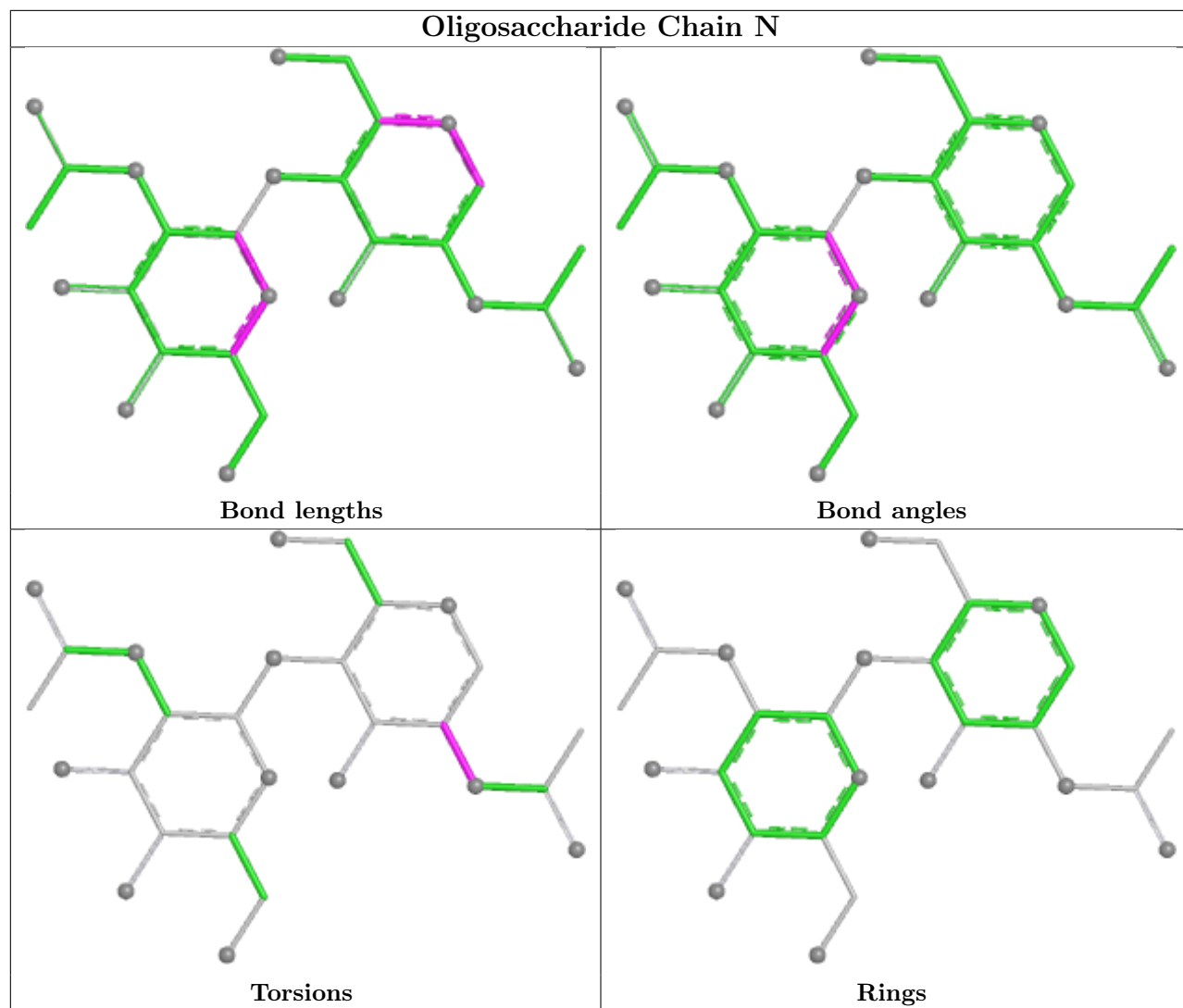


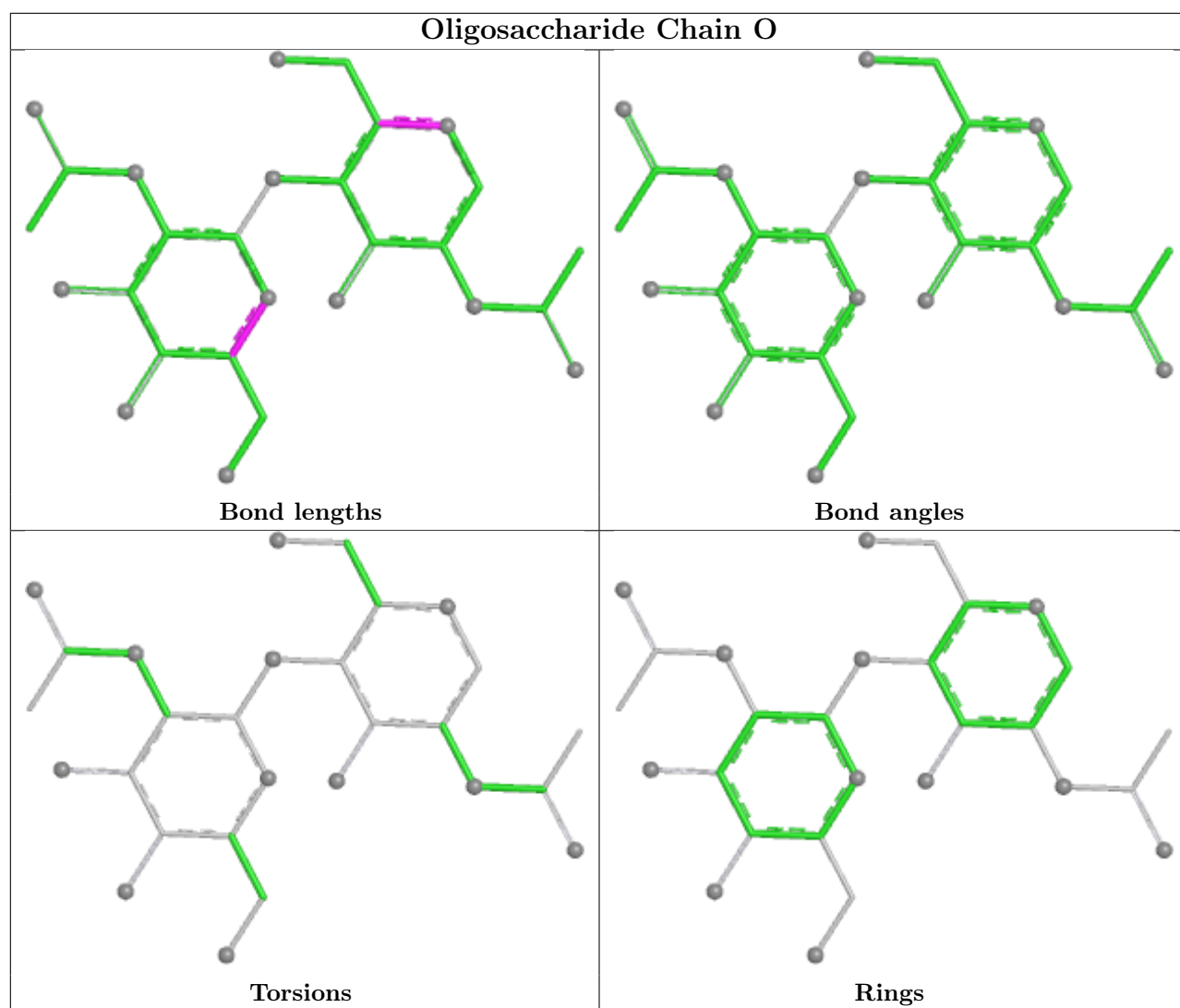


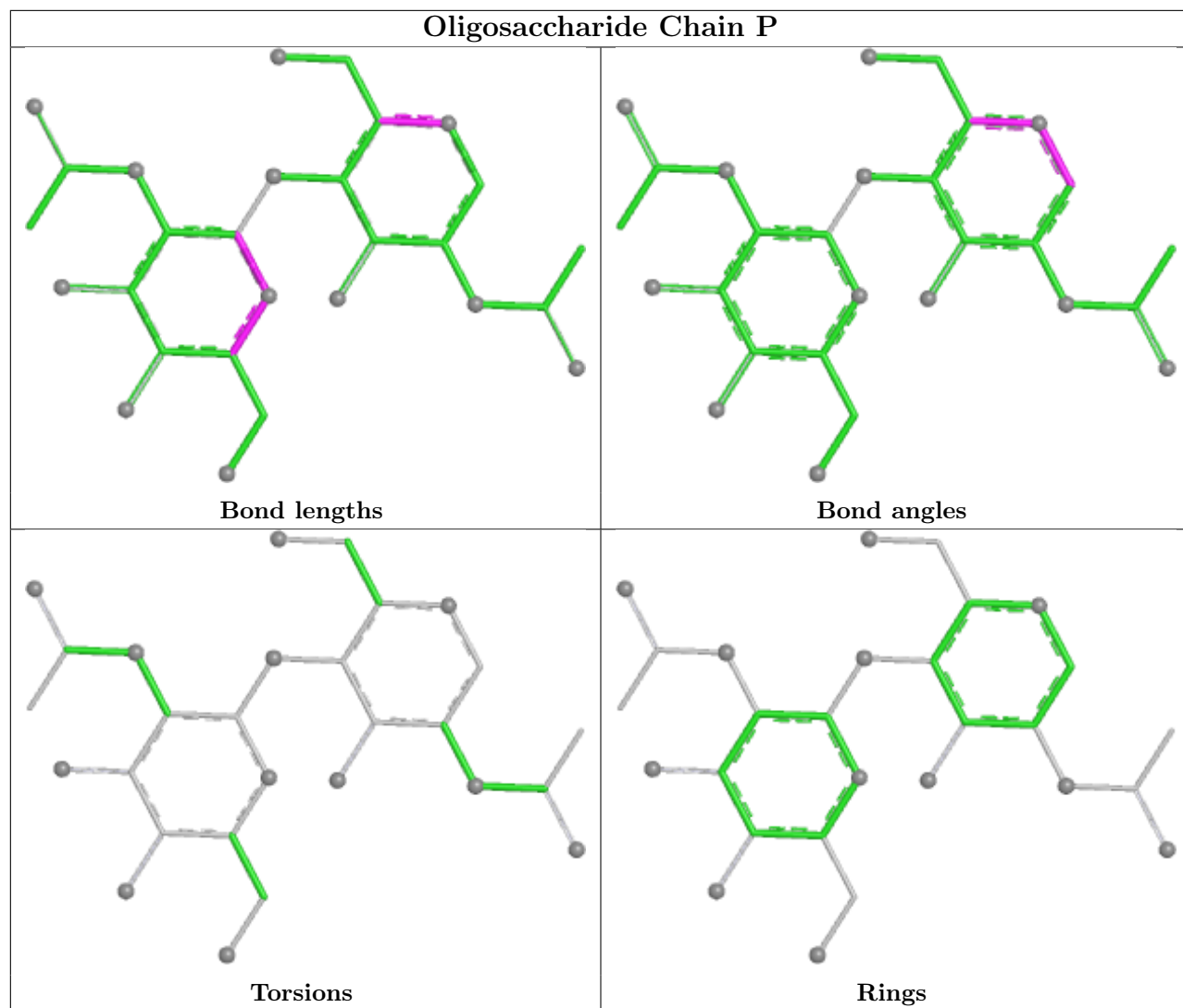


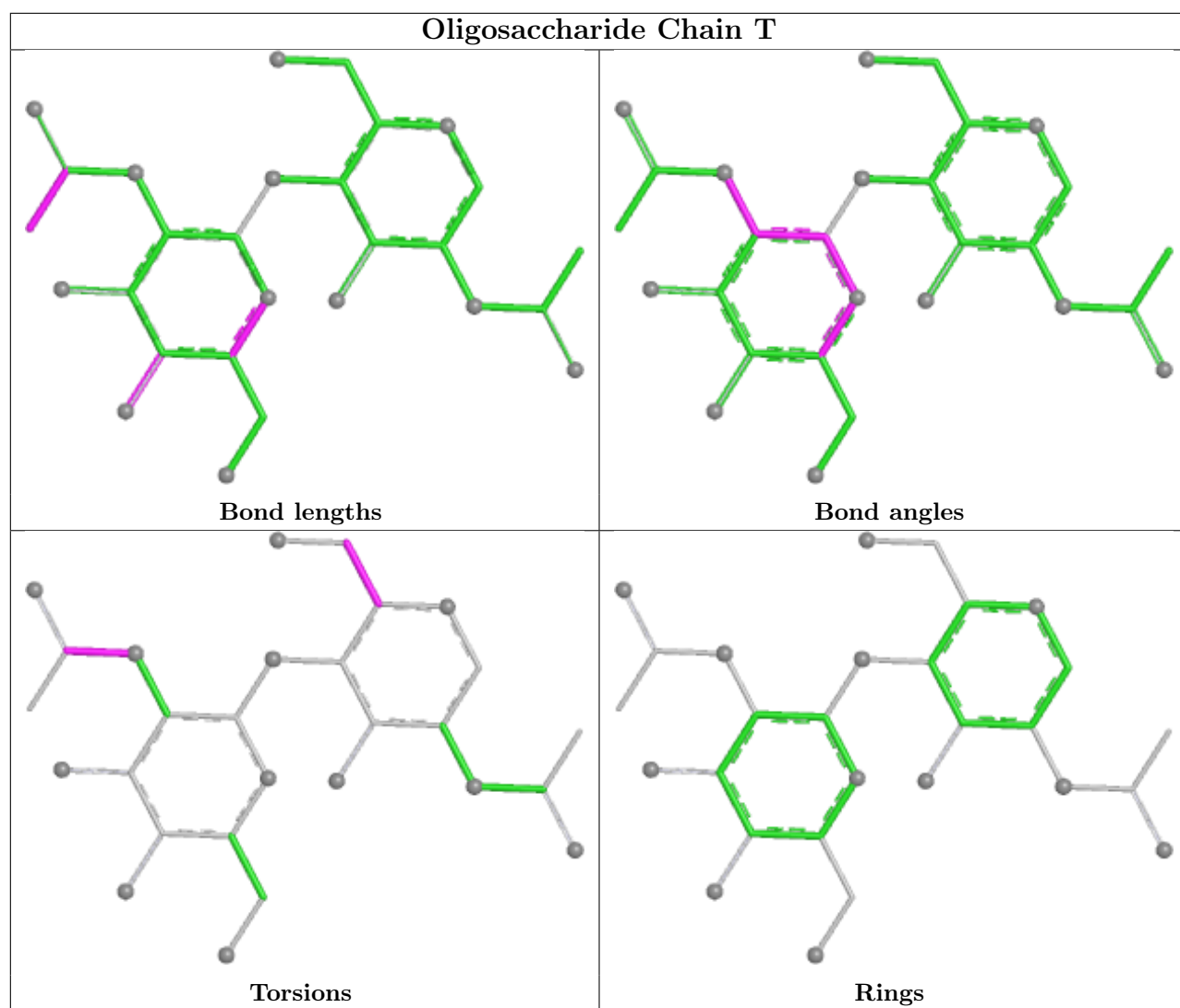


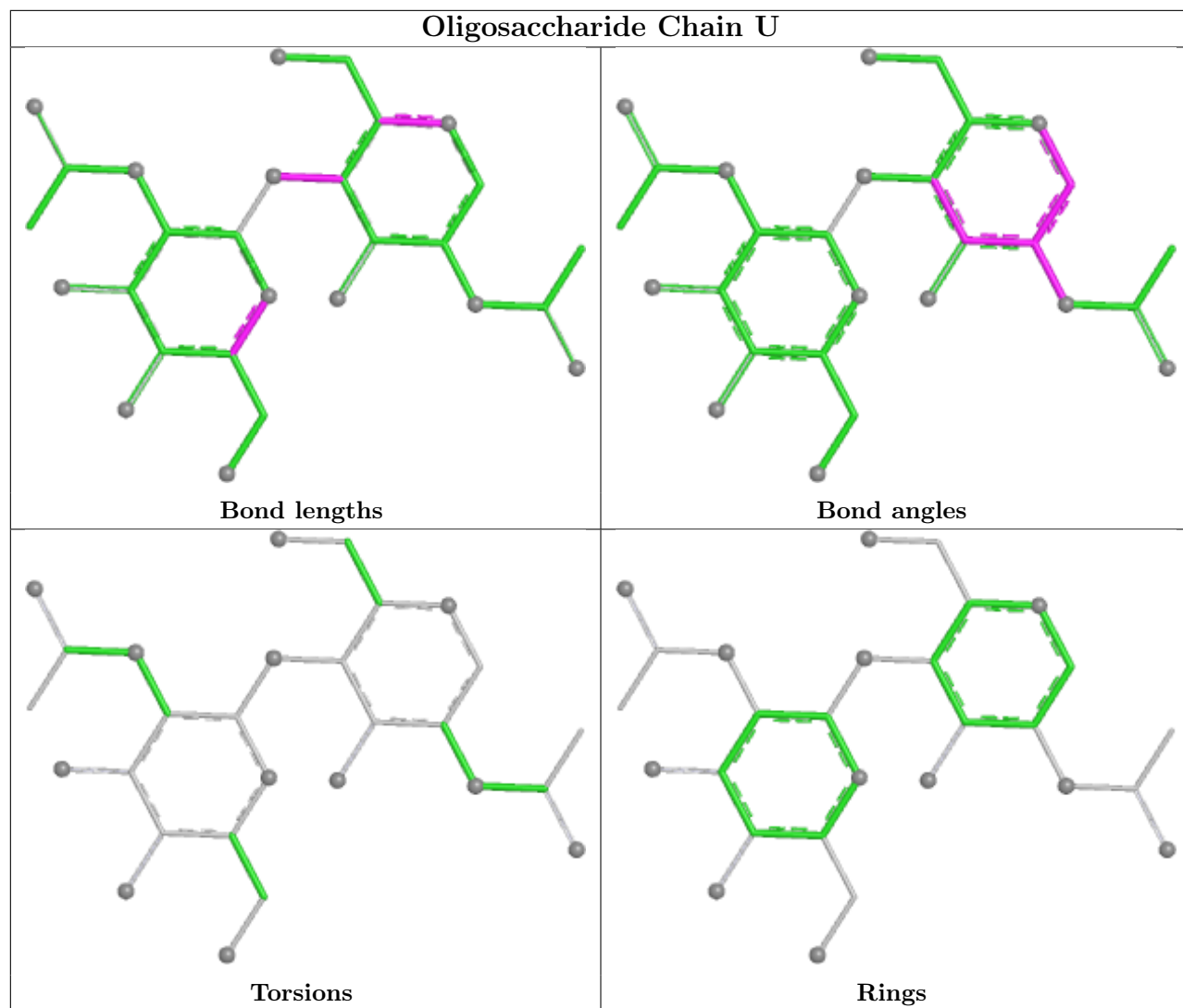


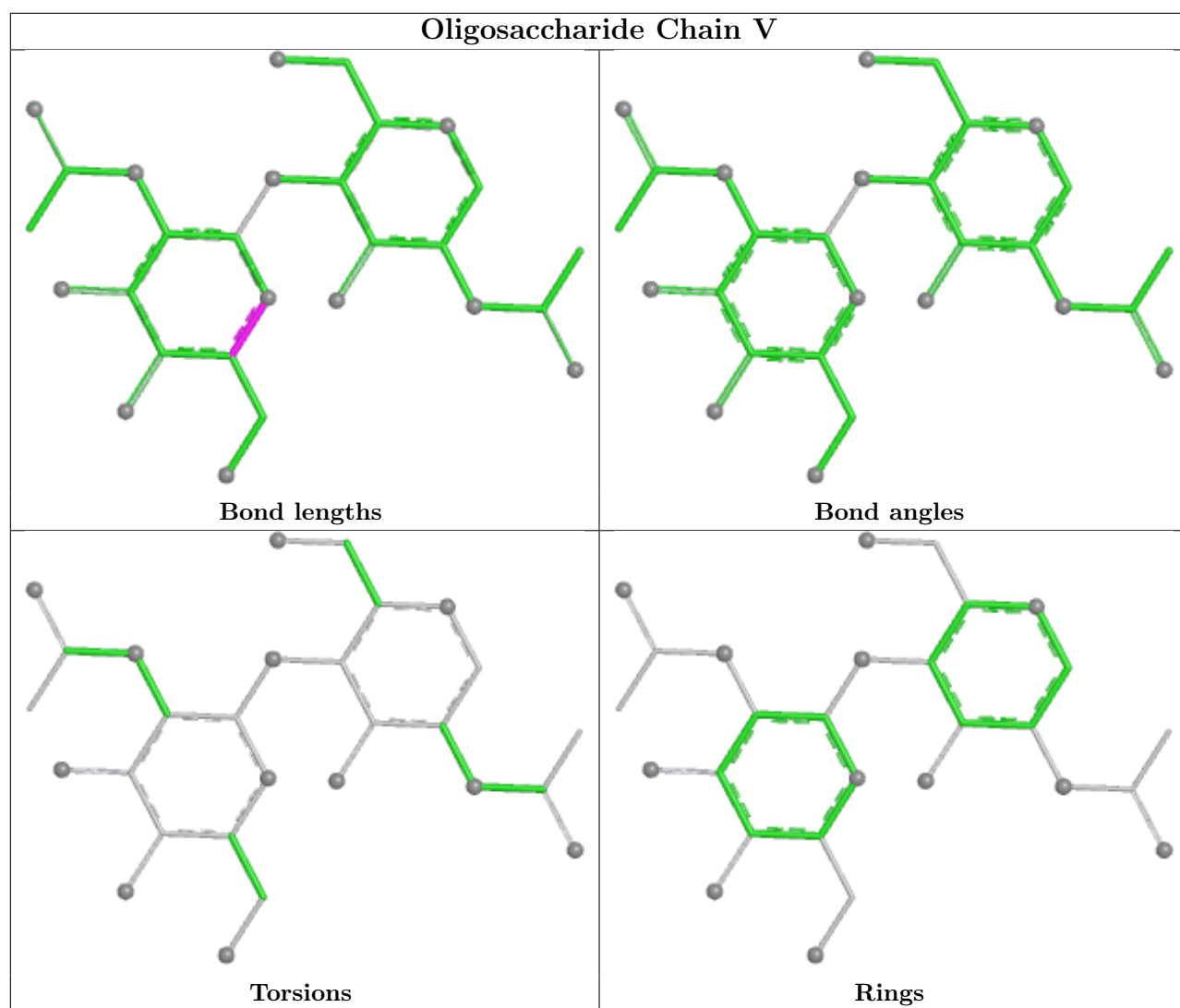


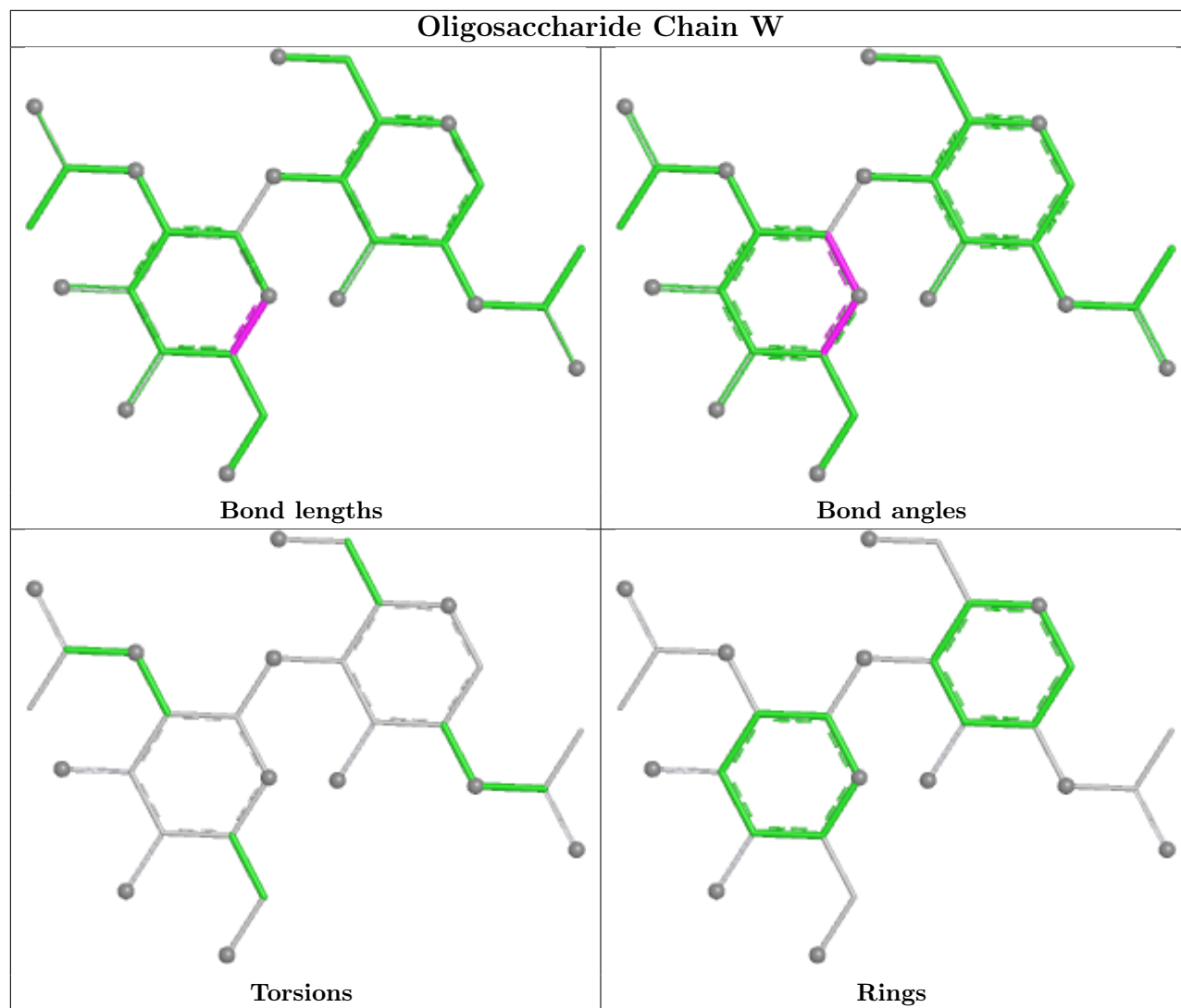


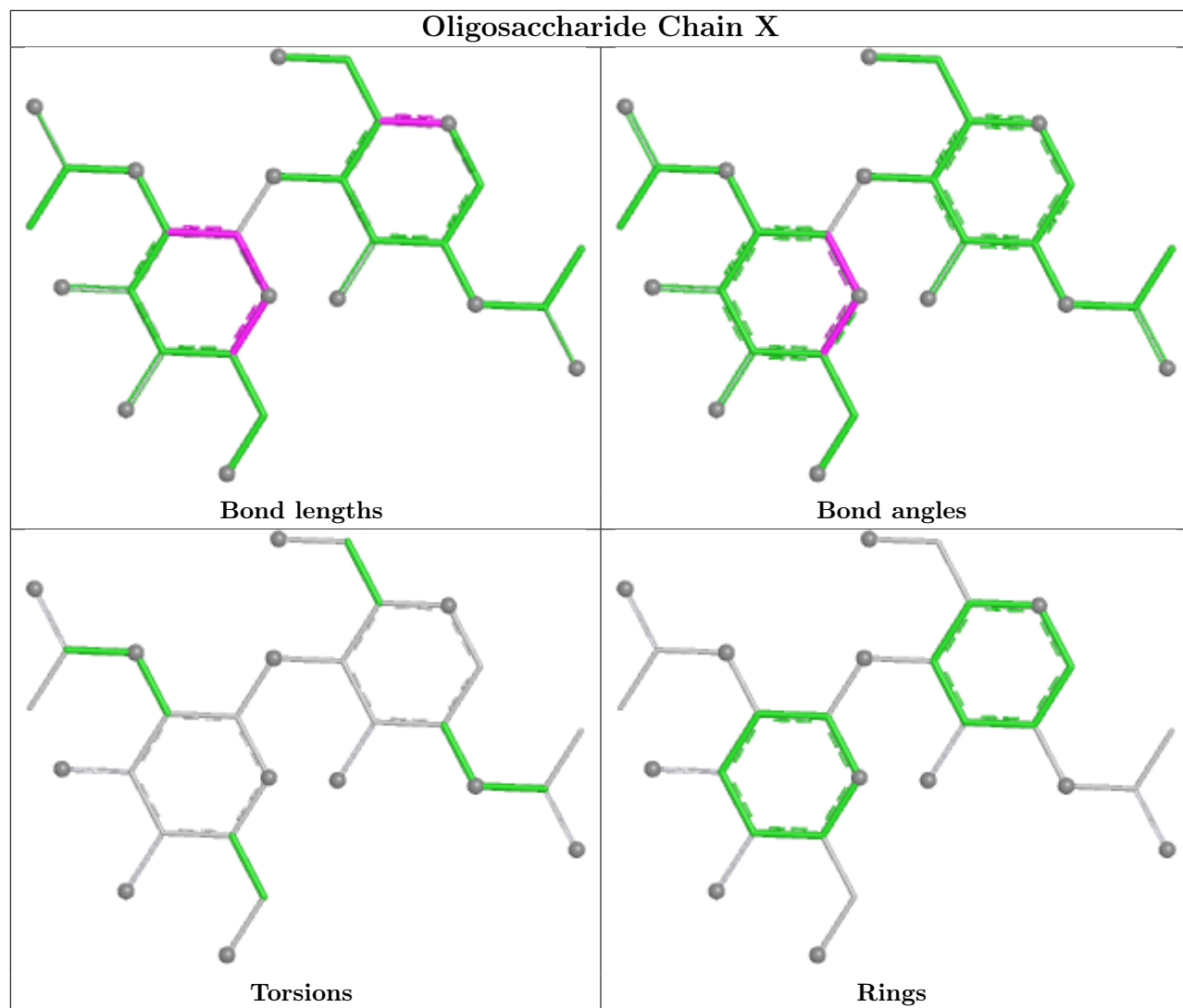


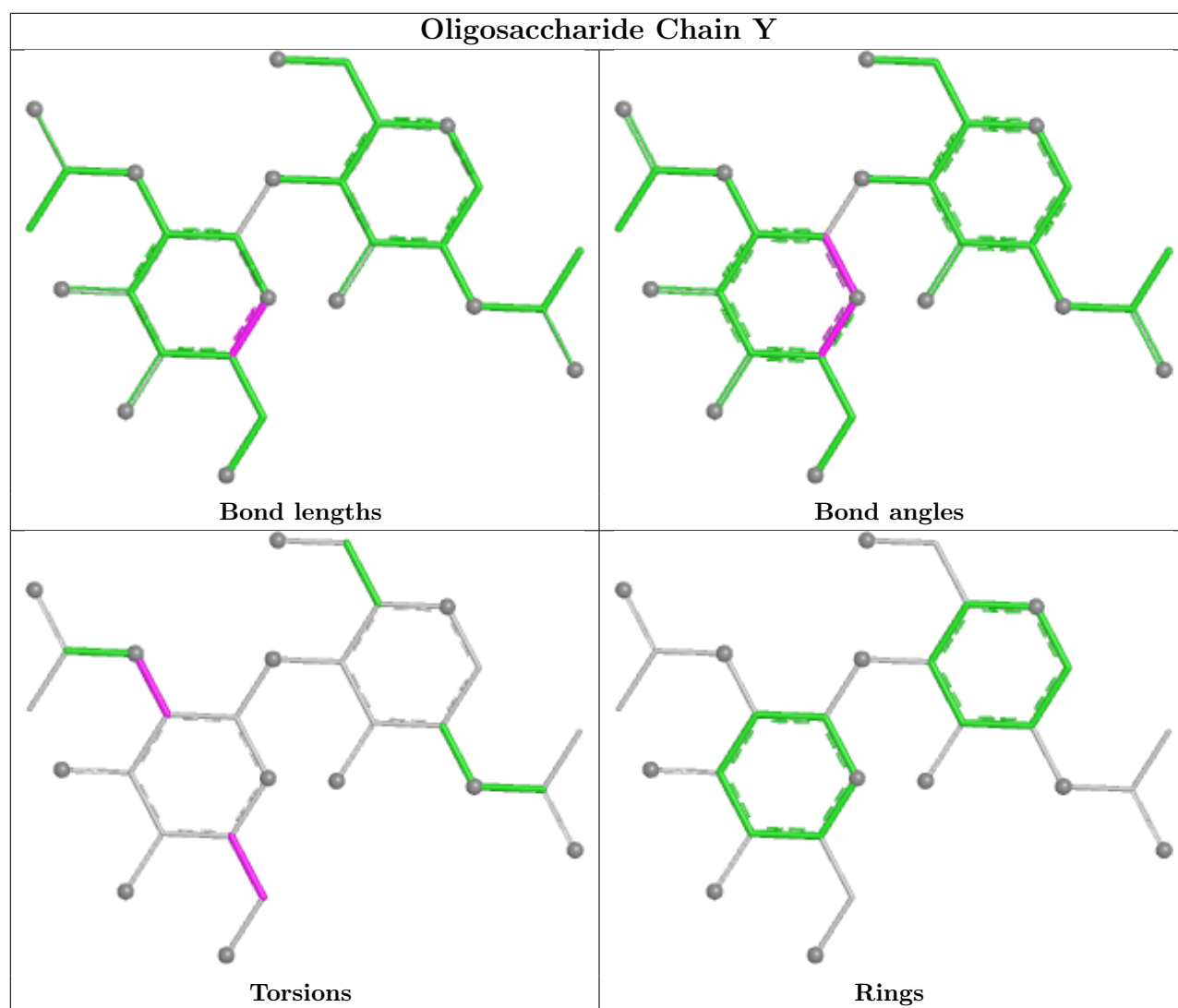


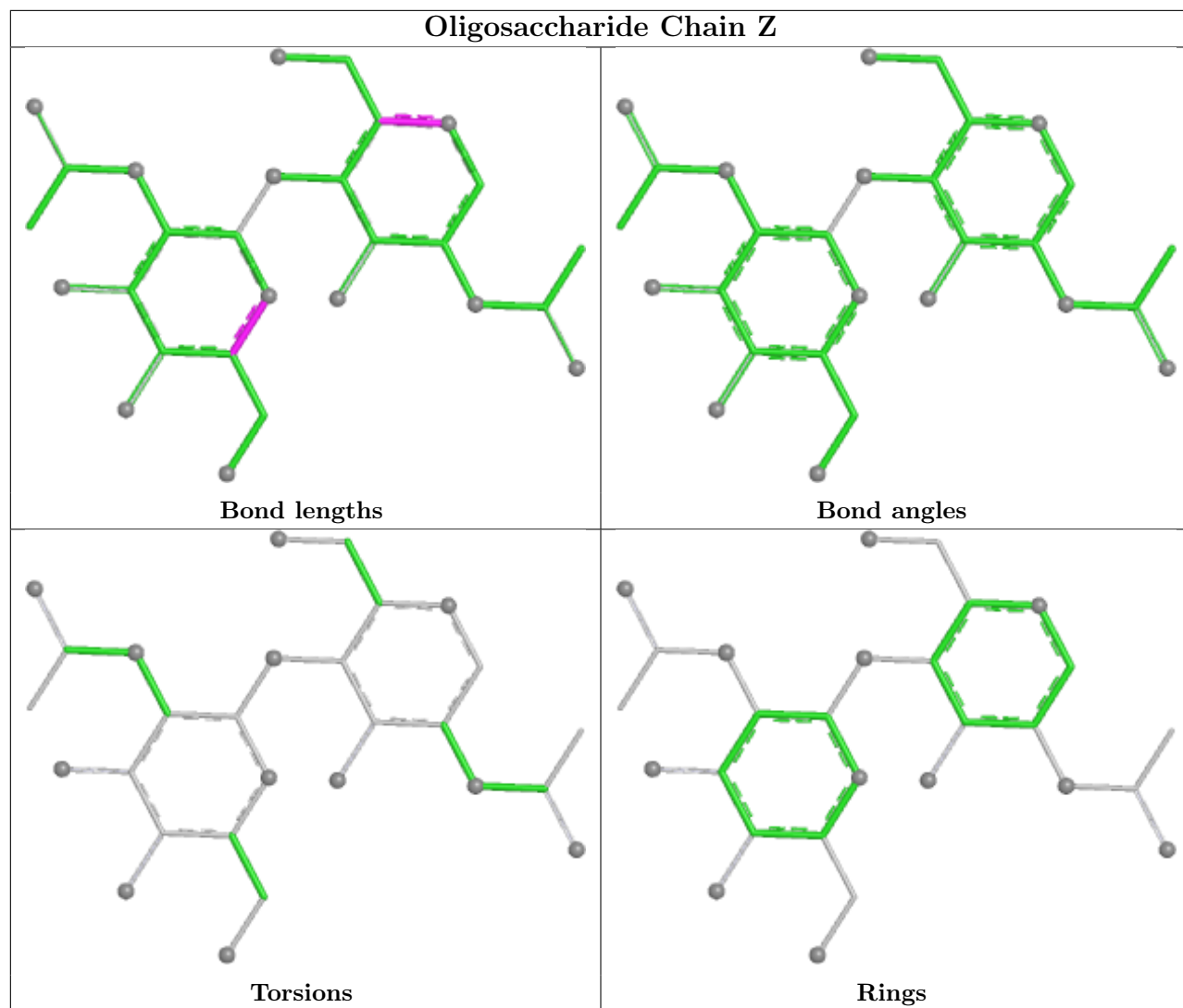


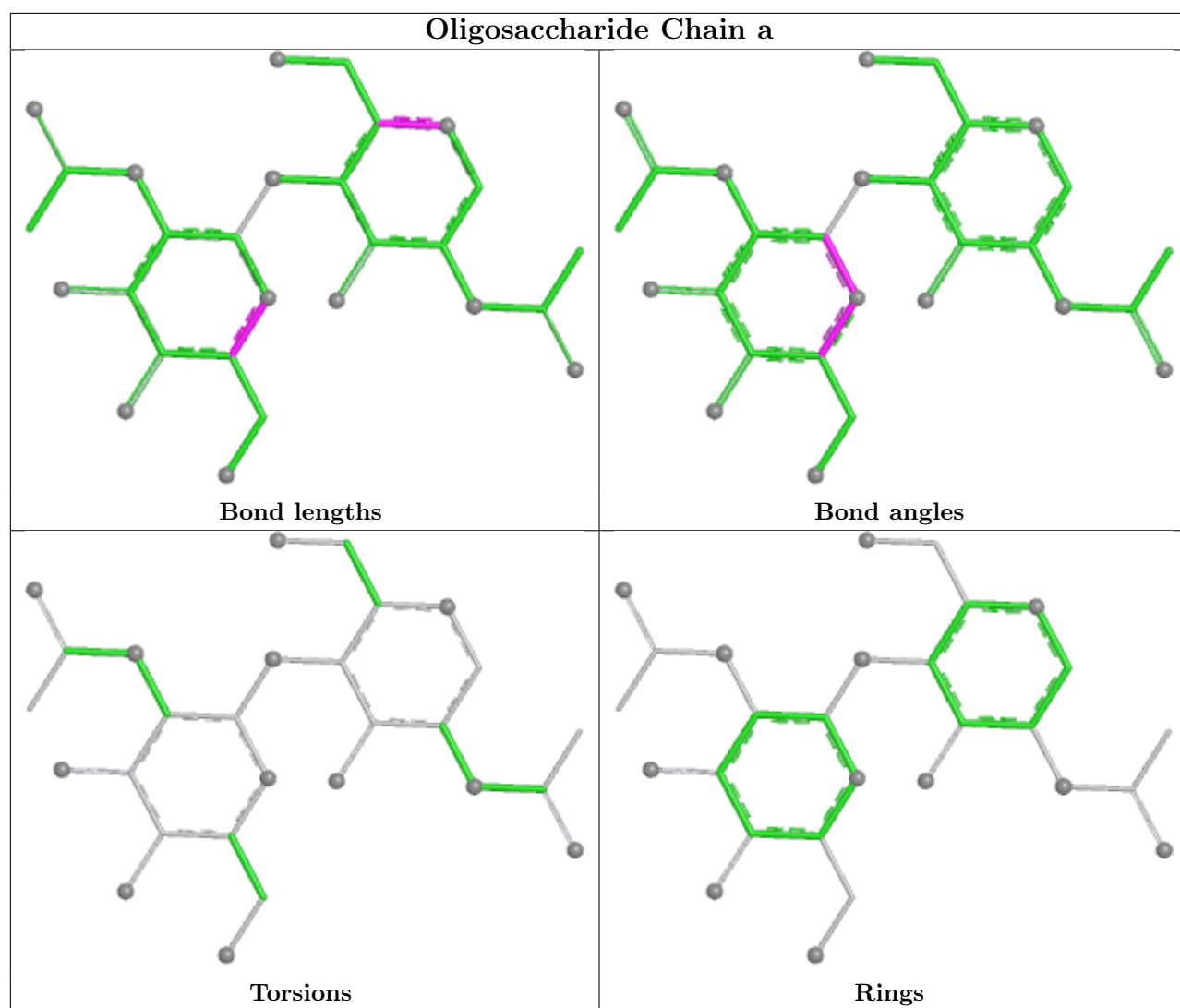


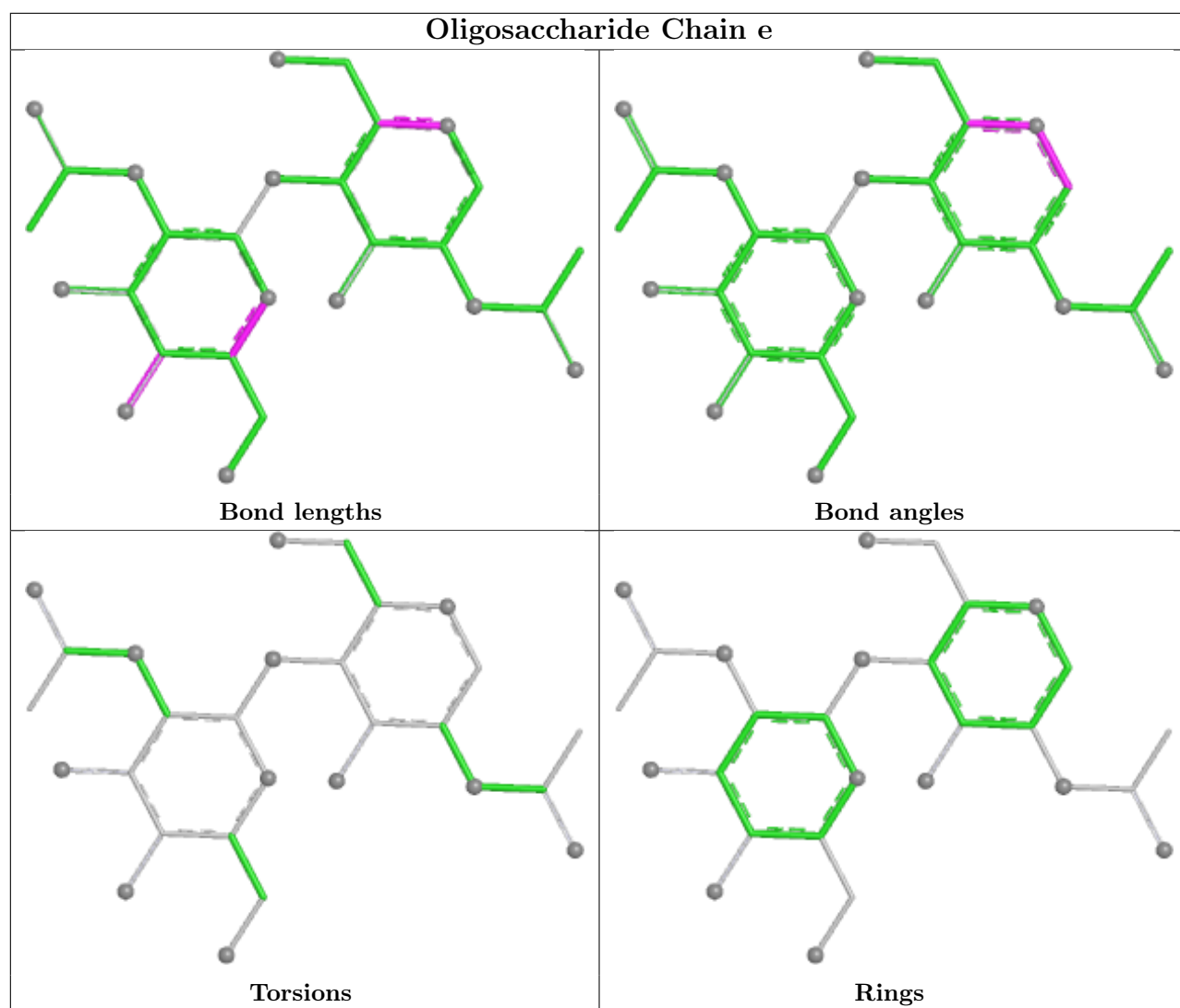


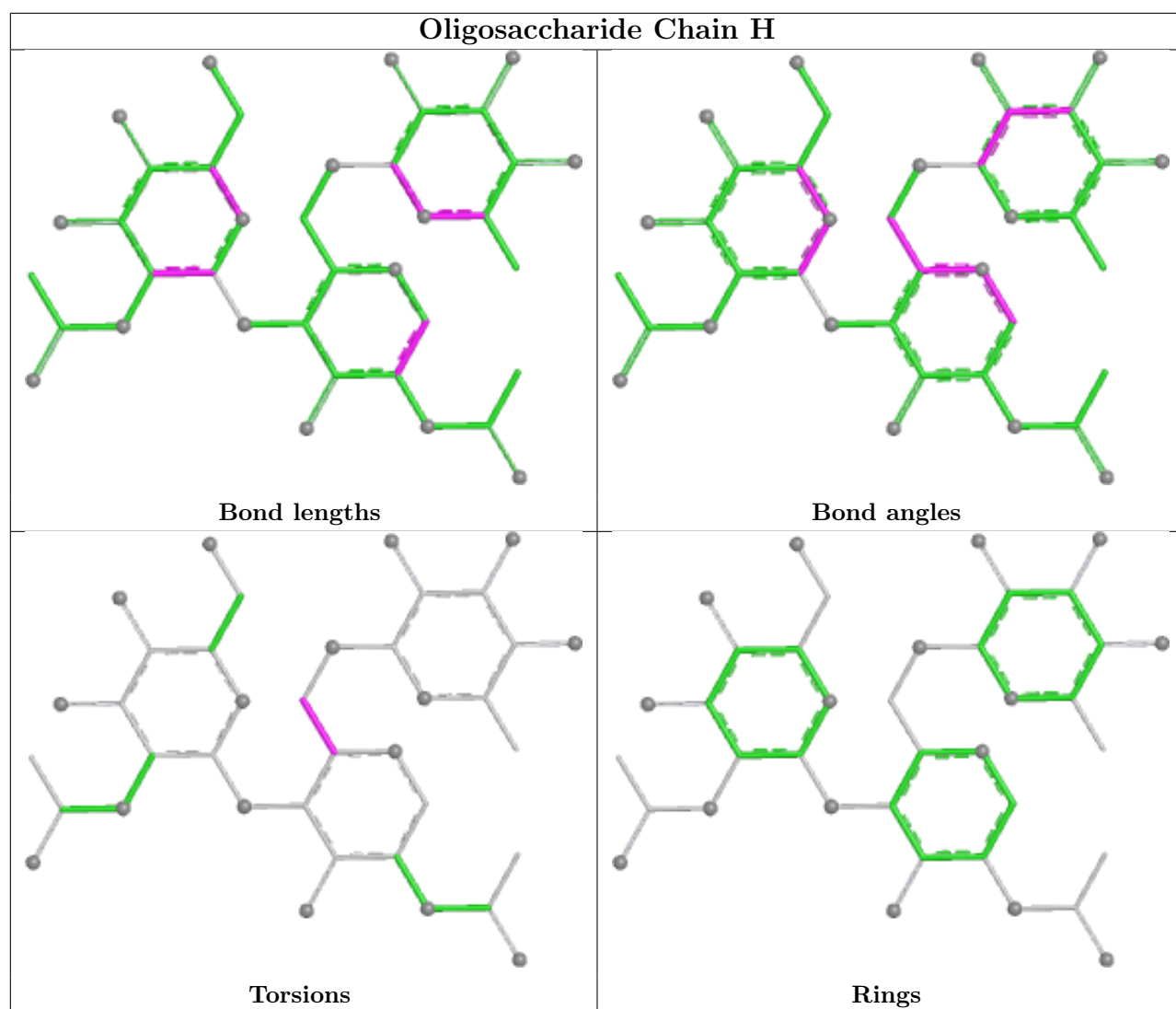


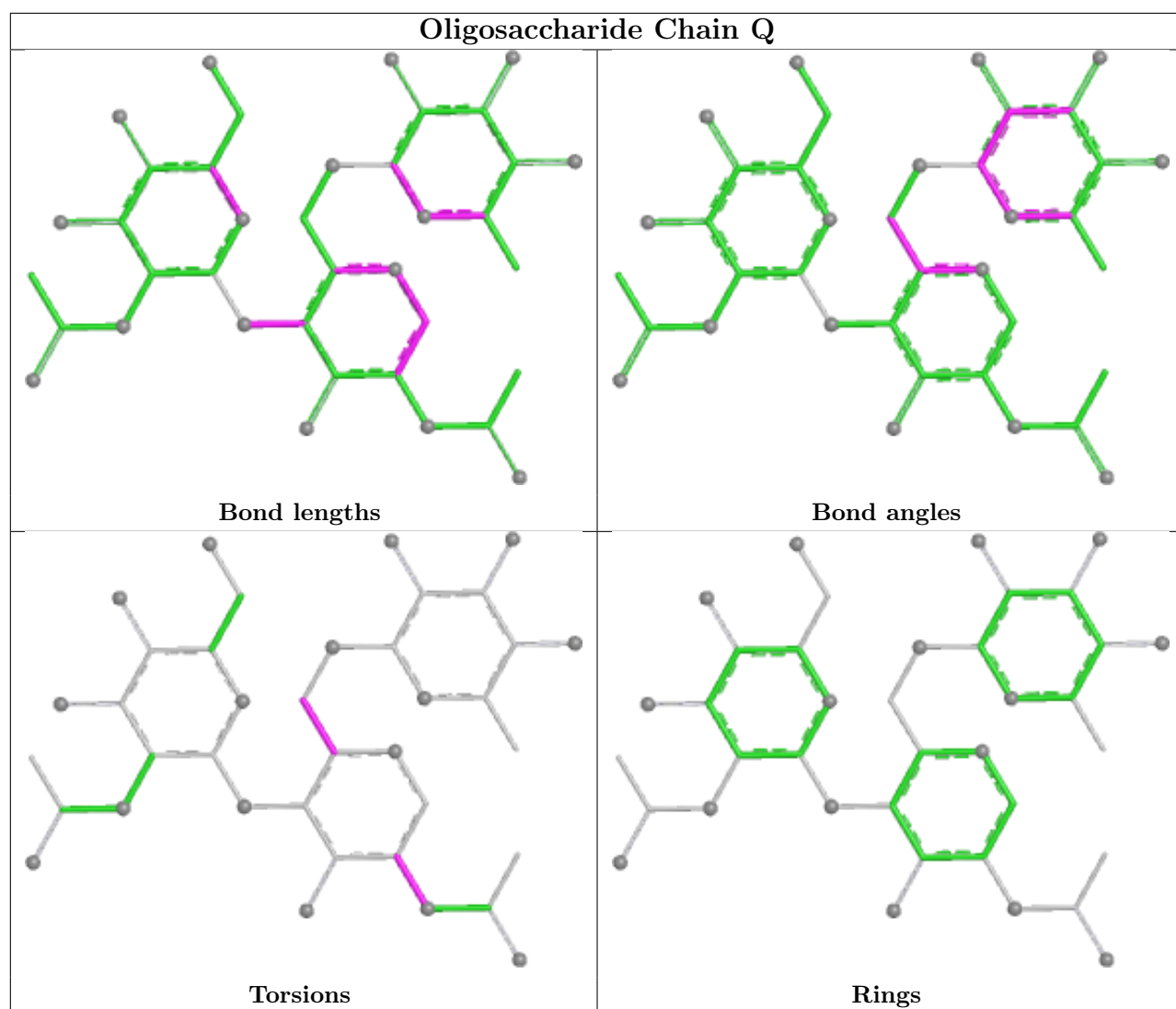


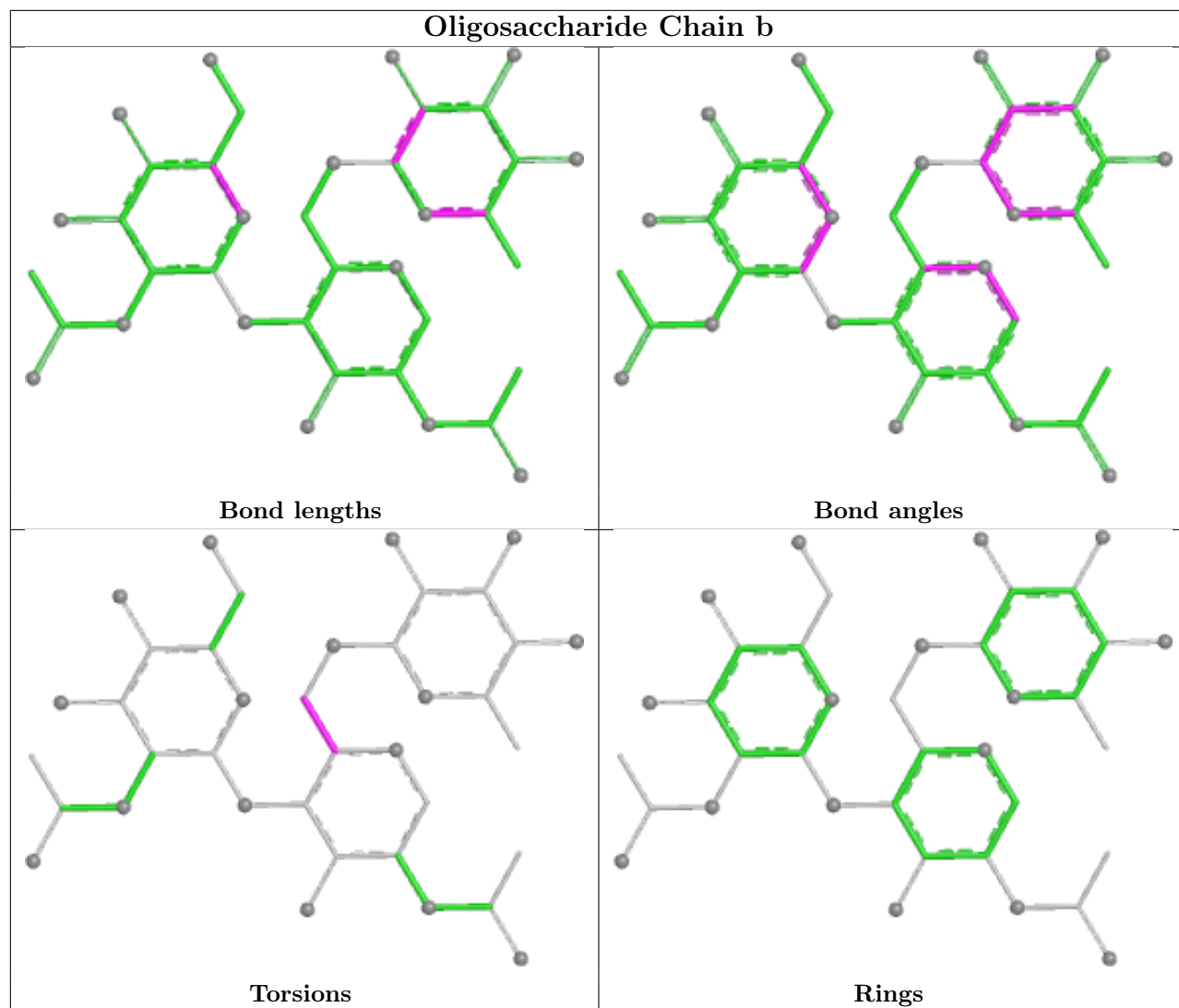


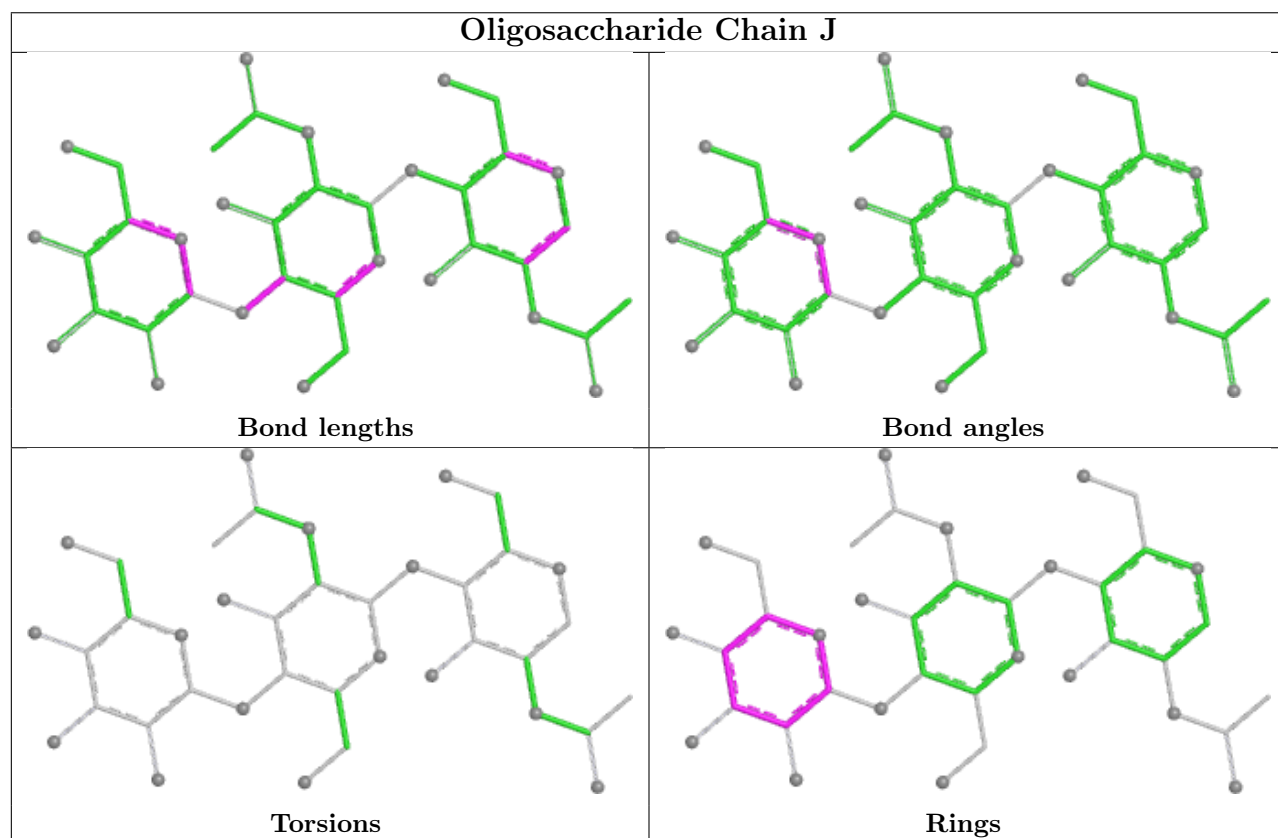
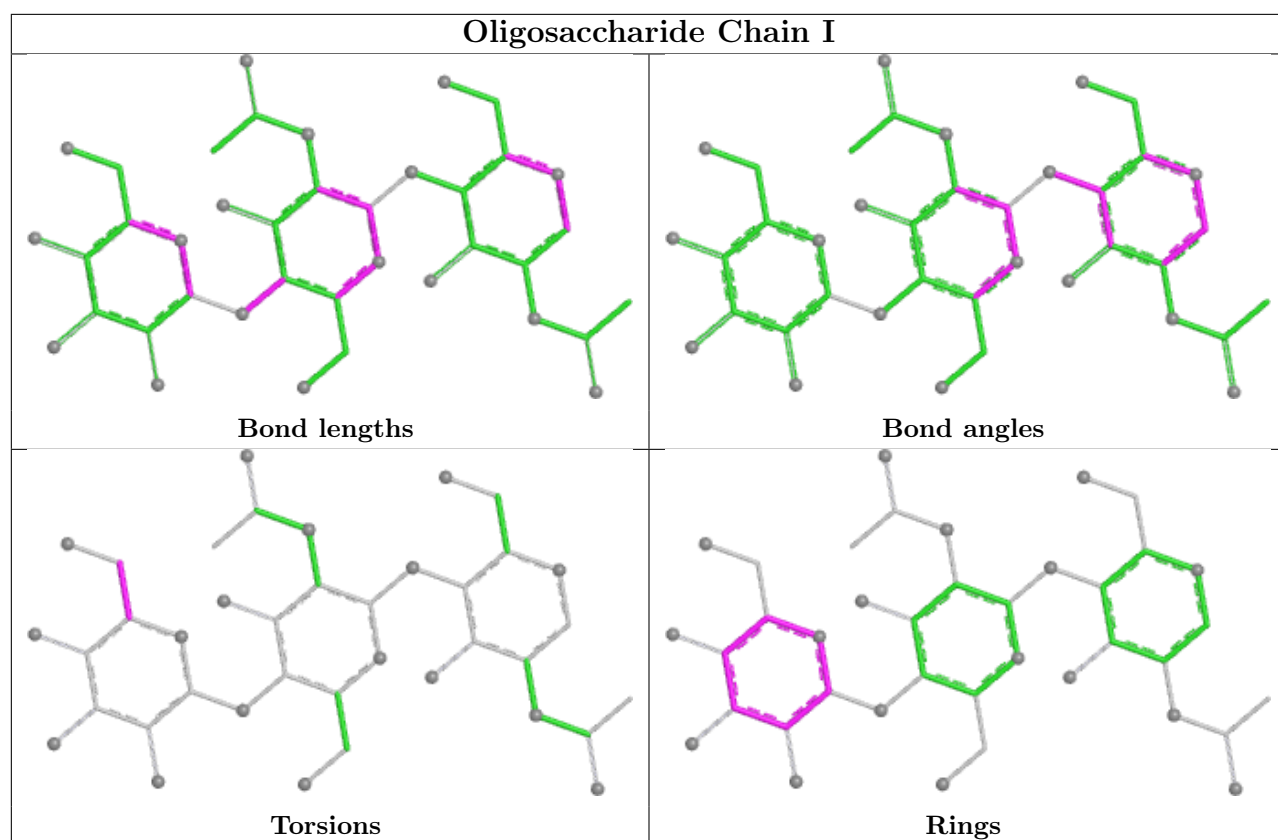


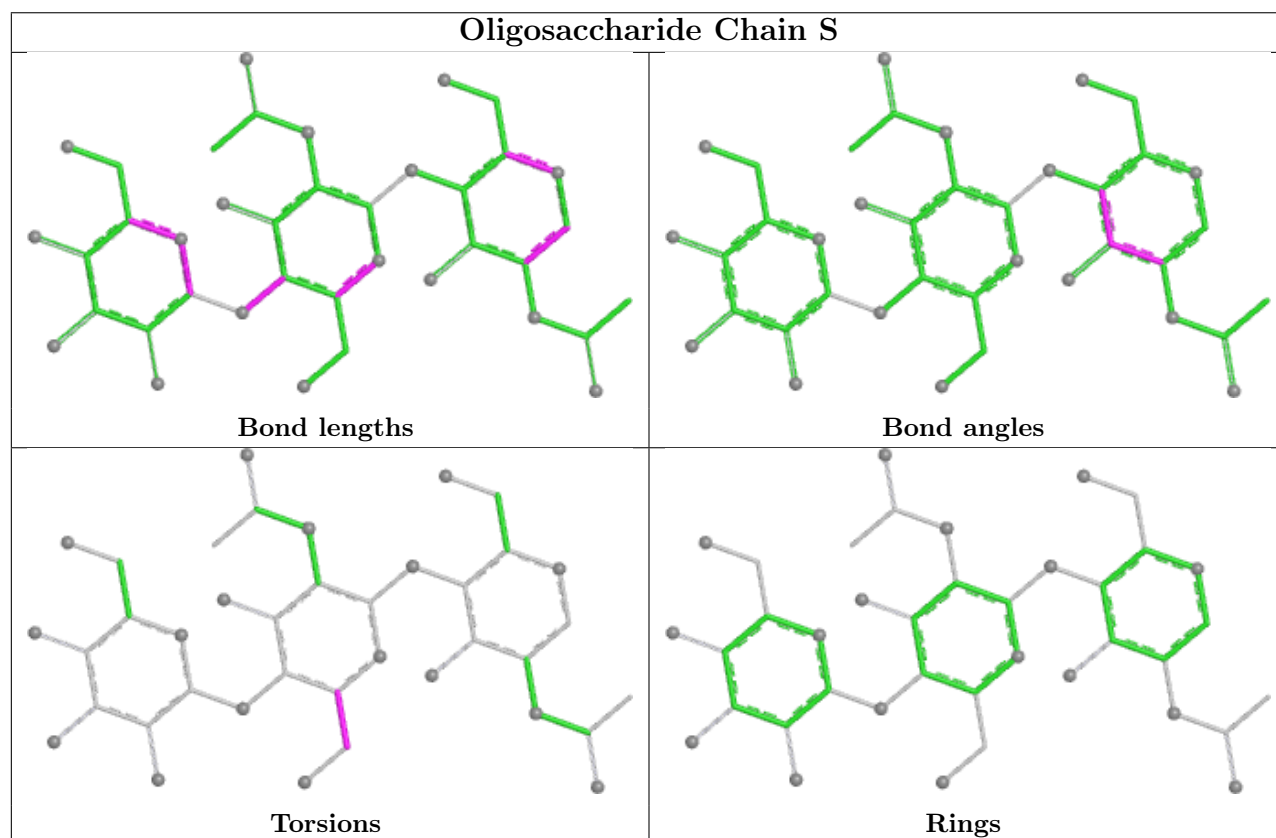
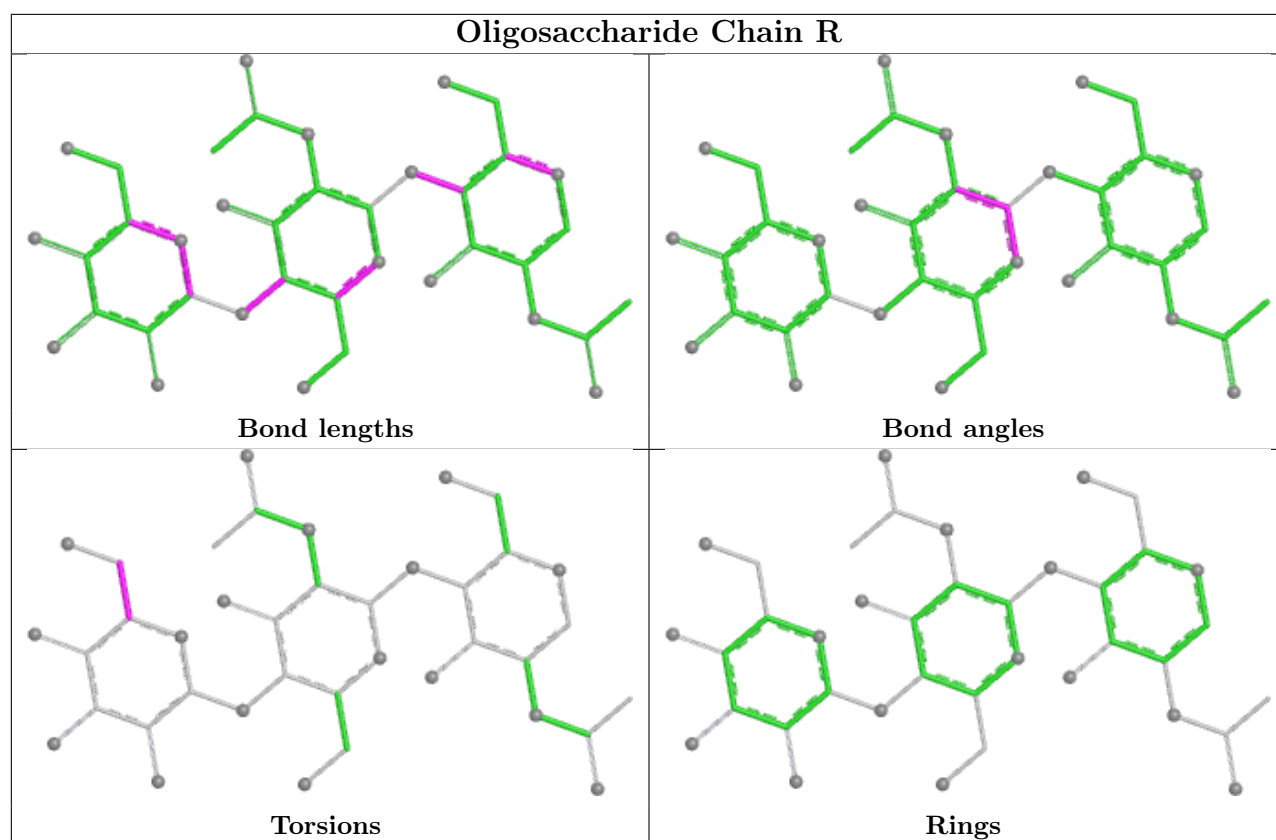


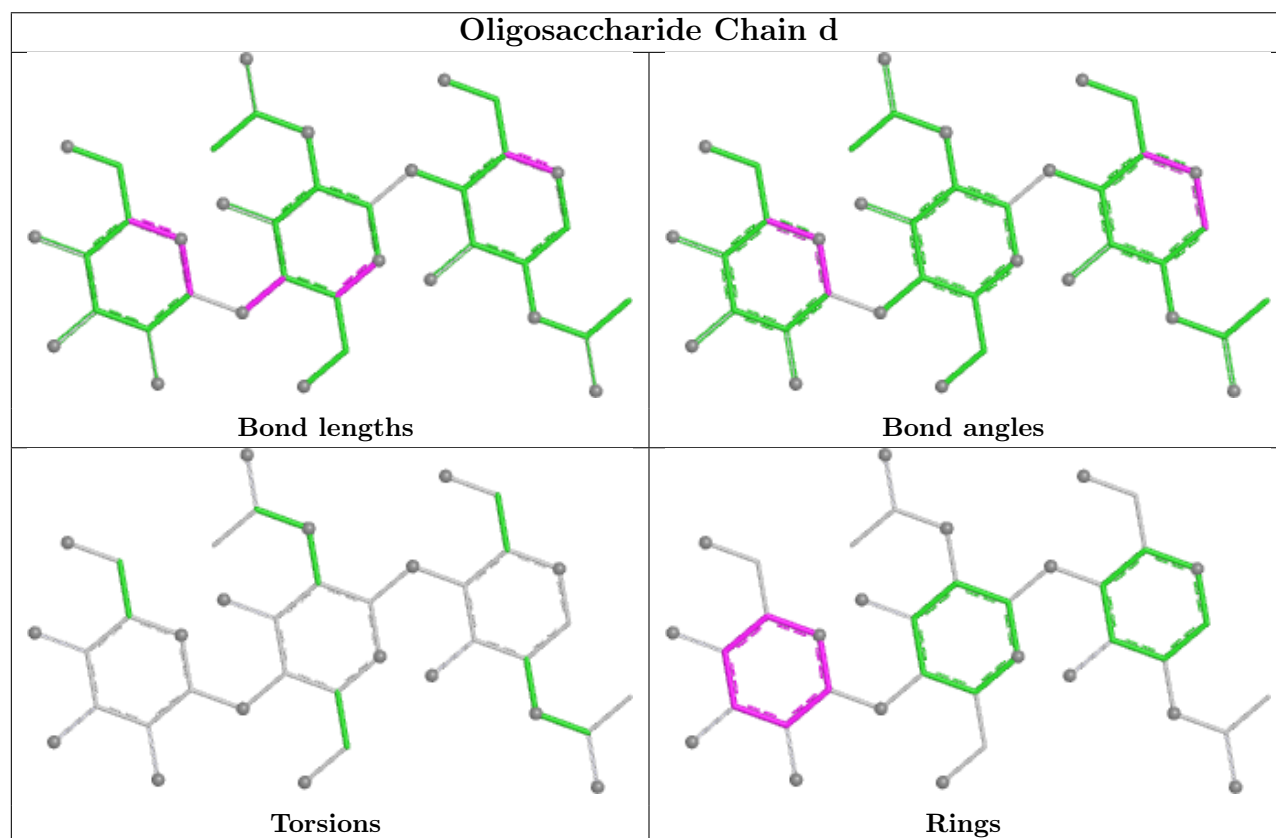
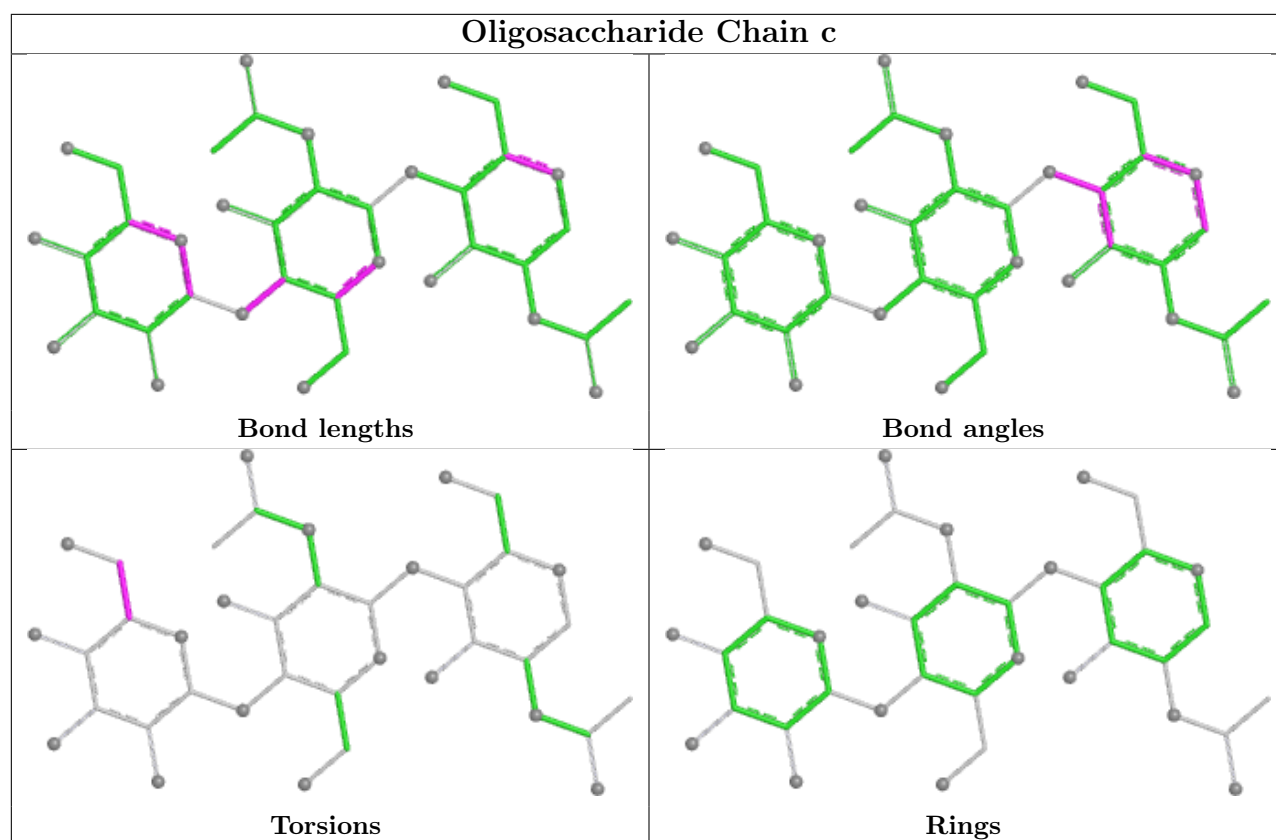












5.6 Ligand geometry

29 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	1403	1	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	A	1404	1	14,14,15	1.17	1 (7%)	17,19,21	0.84	1 (5%)
5	NAG	A	1402	1	14,14,15	1.27	2 (14%)	17,19,21	1.33	2 (11%)
5	NAG	C	1404	1	14,14,15	1.29	3 (21%)	17,19,21	1.01	1 (5%)
5	NAG	A	1407	1	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	C	1403	1	14,14,15	1.10	1 (7%)	17,19,21	1.10	1 (5%)
5	NAG	B	1410	1	14,14,15	1.26	1 (7%)	17,19,21	0.52	0
5	NAG	C	1401	1	14,14,15	0.60	0	17,19,21	0.44	0
5	NAG	A	1410	1	14,14,15	1.32	2 (14%)	17,19,21	0.92	1 (5%)
5	NAG	A	1403	1	14,14,15	1.23	1 (7%)	17,19,21	0.83	1 (5%)
5	NAG	C	1406	1	14,14,15	1.25	1 (7%)	17,19,21	0.81	1 (5%)
5	NAG	B	1401	1	14,14,15	0.50	0	17,19,21	0.45	0
5	NAG	A	1408	1	14,14,15	1.24	1 (7%)	17,19,21	0.62	0
5	NAG	A	1409	1	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	B	1406	1	14,14,15	1.40	3 (21%)	17,19,21	0.89	1 (5%)
5	NAG	B	1408	1	14,14,15	1.34	3 (21%)	17,19,21	0.78	0
5	NAG	A	1406	1	14,14,15	1.25	1 (7%)	17,19,21	0.65	0
5	NAG	C	1407	1	14,14,15	1.50	3 (21%)	17,19,21	0.65	0
5	NAG	A	1411	1	14,14,15	1.26	1 (7%)	17,19,21	0.52	0
5	NAG	C	1405	1	14,14,15	1.29	2 (14%)	17,19,21	0.64	0
5	NAG	B	1402	1	14,14,15	0.50	0	17,19,21	0.69	1 (5%)
5	NAG	C	1408	1	14,14,15	1.38	1 (7%)	17,19,21	0.62	0
5	NAG	B	1404	1	14,14,15	1.15	1 (7%)	17,19,21	0.92	0
5	NAG	C	1402	1	14,14,15	0.47	0	17,19,21	0.67	1 (5%)
5	NAG	A	1405	1	14,14,15	2.30	1 (7%)	17,19,21	1.90	1 (5%)
5	NAG	A	1401	1	14,14,15	1.48	3 (21%)	17,19,21	1.53	1 (5%)
5	NAG	B	1407	1	14,14,15	1.14	1 (7%)	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1405	1	14,14,15	1.53	2 (14%)	17,19,21	1.12	1 (5%)
5	NAG	B	1409	1	14,14,15	1.28	2 (14%)	17,19,21	0.82	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1410	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	1406	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	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1411	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	0/6/23/26	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1405	NAG	C1-C2	8.56	1.64	1.52
5	B	1405	NAG	O5-C1	-4.20	1.36	1.43
5	C	1403	NAG	O5-C1	-4.05	1.36	1.43
5	C	1408	NAG	O5-C5	3.19	1.49	1.43
5	A	1401	NAG	O5-C5	3.03	1.49	1.43
5	C	1406	NAG	O5-C5	3.01	1.49	1.43
5	A	1402	NAG	O5-C5	3.01	1.49	1.43
5	B	1408	NAG	O5-C5	2.97	1.49	1.43
5	C	1407	NAG	C8-C7	2.95	1.56	1.50
5	A	1406	NAG	O5-C5	2.94	1.49	1.43
5	C	1407	NAG	O5-C5	2.94	1.49	1.43
5	A	1401	NAG	C1-C2	2.91	1.56	1.52
5	B	1409	NAG	O5-C5	2.86	1.49	1.43
5	C	1404	NAG	O5-C5	2.83	1.48	1.43
5	B	1406	NAG	C1-C2	2.82	1.56	1.52
5	A	1403	NAG	O5-C5	2.76	1.48	1.43
5	A	1410	NAG	C1-C2	2.76	1.56	1.52
5	B	1406	NAG	O5-C5	2.68	1.48	1.43
5	A	1408	NAG	O5-C5	2.65	1.48	1.43
5	B	1410	NAG	O5-C5	2.62	1.48	1.43
5	A	1411	NAG	O5-C5	2.61	1.48	1.43
5	C	1405	NAG	O5-C5	2.61	1.48	1.43
5	A	1401	NAG	O5-C1	2.52	1.47	1.43
5	C	1405	NAG	C1-C2	2.50	1.55	1.52
5	A	1410	NAG	O5-C1	2.46	1.47	1.43
5	B	1404	NAG	O5-C5	2.43	1.48	1.43
5	A	1404	NAG	O5-C5	2.34	1.48	1.43
5	B	1405	NAG	O5-C5	2.32	1.47	1.43
5	B	1407	NAG	O5-C5	2.30	1.47	1.43
5	B	1406	NAG	O5-C1	2.28	1.47	1.43
5	B	1408	NAG	C1-C2	2.18	1.55	1.52
5	B	1409	NAG	C1-C2	2.15	1.55	1.52
5	C	1407	NAG	C1-C2	2.15	1.55	1.52
5	C	1404	NAG	O5-C1	2.08	1.47	1.43
5	A	1402	NAG	C1-C2	2.07	1.55	1.52
5	B	1408	NAG	O5-C1	2.07	1.47	1.43
5	C	1404	NAG	C1-C2	2.05	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1405	NAG	O5-C1-C2	-7.52	99.66	111.29
5	A	1401	NAG	C1-O5-C5	5.58	119.66	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1402	NAG	C1-O5-C5	3.75	117.21	112.19
5	B	1405	NAG	C1-O5-C5	3.08	116.32	112.19
5	C	1403	NAG	C1-O5-C5	3.01	116.22	112.19
5	B	1407	NAG	C3-C4-C5	2.98	115.63	110.23
5	C	1404	NAG	C1-O5-C5	2.93	116.12	112.19
5	B	1409	NAG	C1-O5-C5	2.47	115.50	112.19
5	A	1404	NAG	C1-O5-C5	2.40	115.40	112.19
5	B	1406	NAG	C1-O5-C5	2.36	115.35	112.19
5	B	1402	NAG	C1-O5-C5	2.35	115.33	112.19
5	C	1402	NAG	C1-O5-C5	2.35	115.33	112.19
5	C	1406	NAG	C1-O5-C5	2.30	115.27	112.19
5	A	1402	NAG	C4-C3-C2	-2.27	107.69	111.02
5	A	1410	NAG	C1-O5-C5	2.25	115.21	112.19
5	A	1403	NAG	O5-C1-C2	-2.11	108.03	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1401	NAG	O5-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	A	1406	NAG	C1-C2-N2-C7
5	C	1403	NAG	C3-C2-N2-C7
5	B	1402	NAG	C4-C5-C6-O6

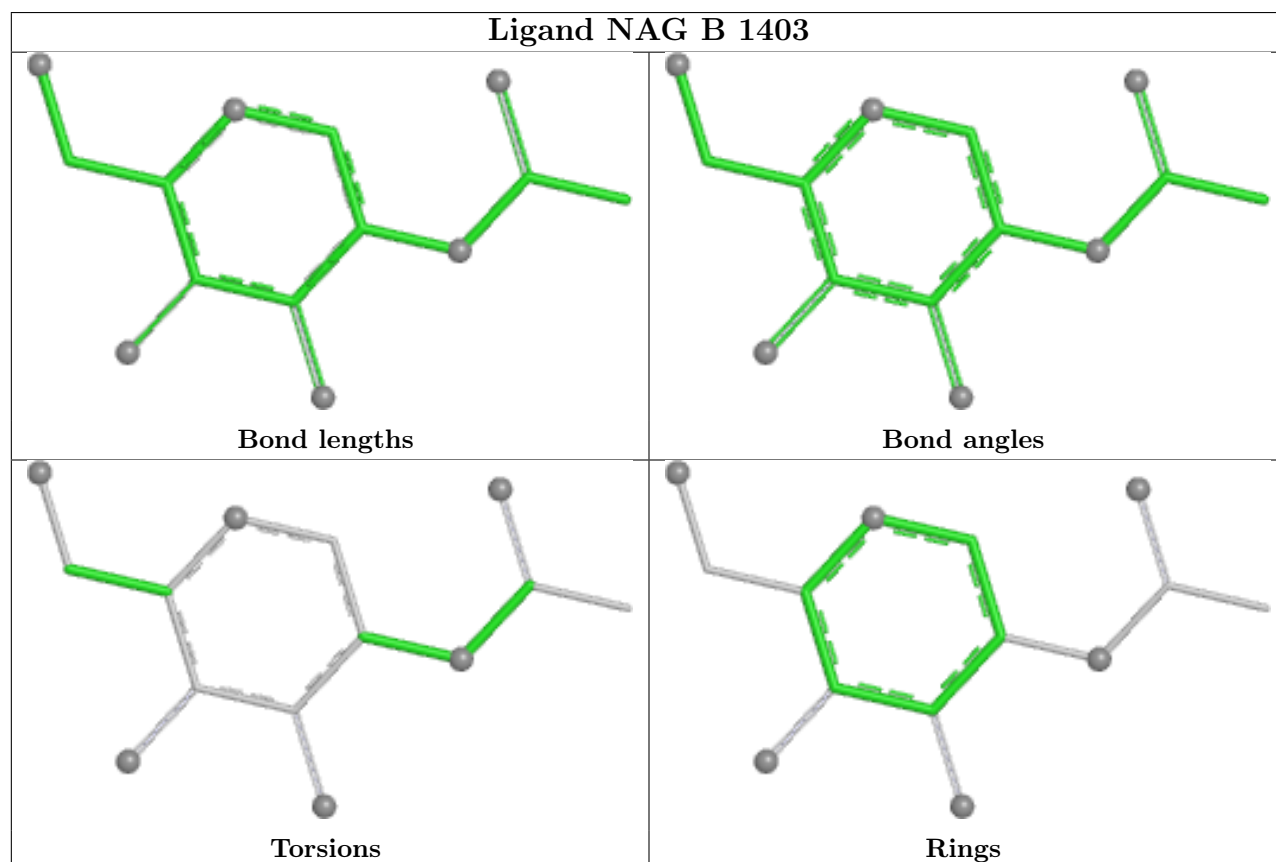
There are no ring outliers.

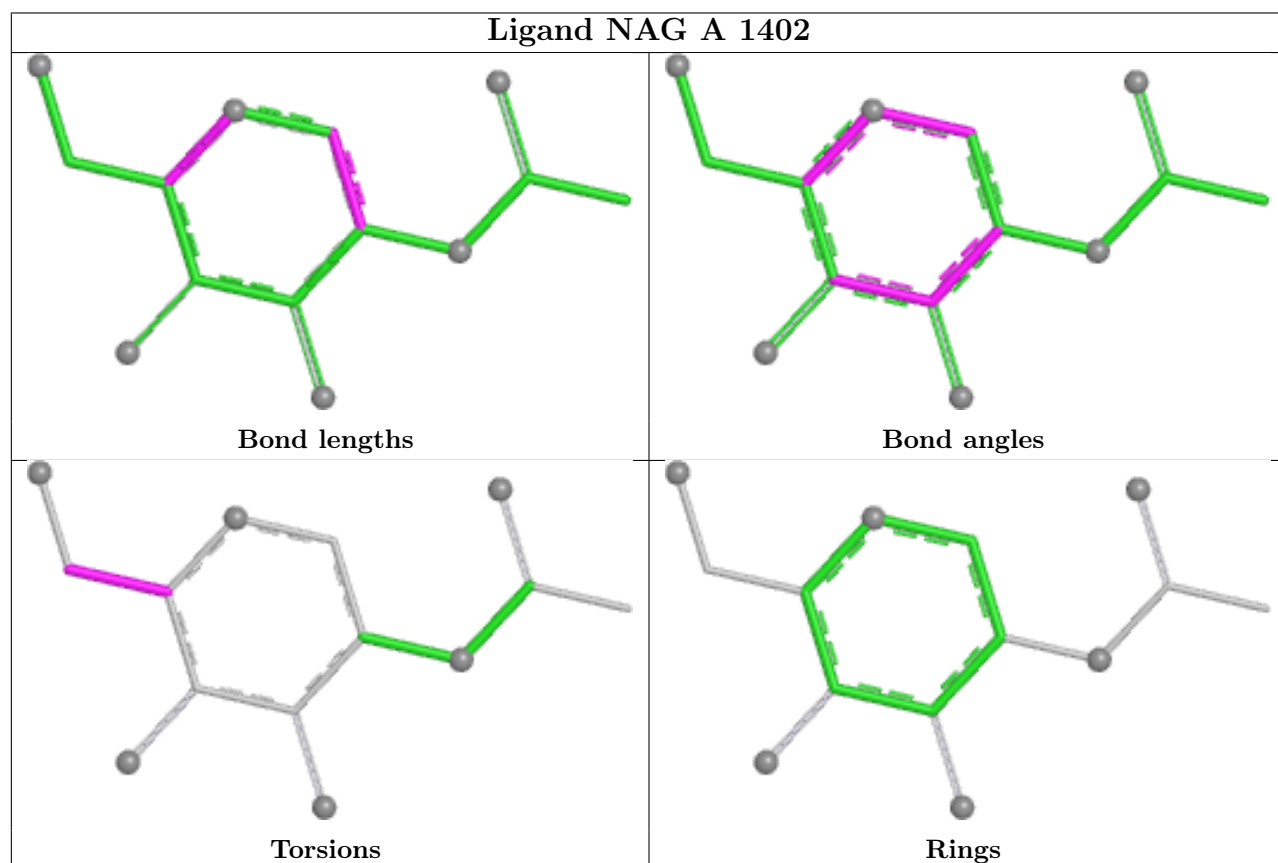
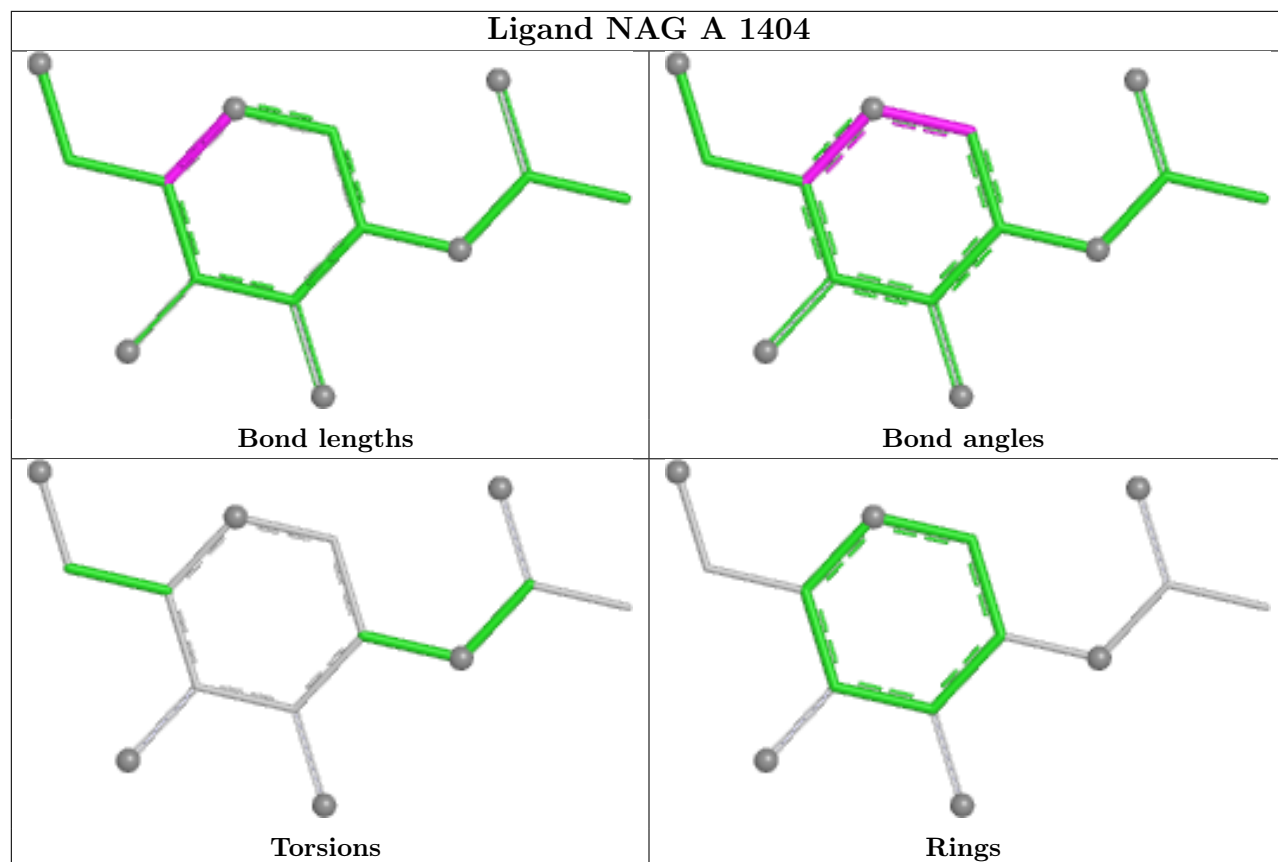
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1407	NAG	1	0
5	B	1402	NAG	4	0
5	C	1402	NAG	2	0
5	A	1405	NAG	1	0

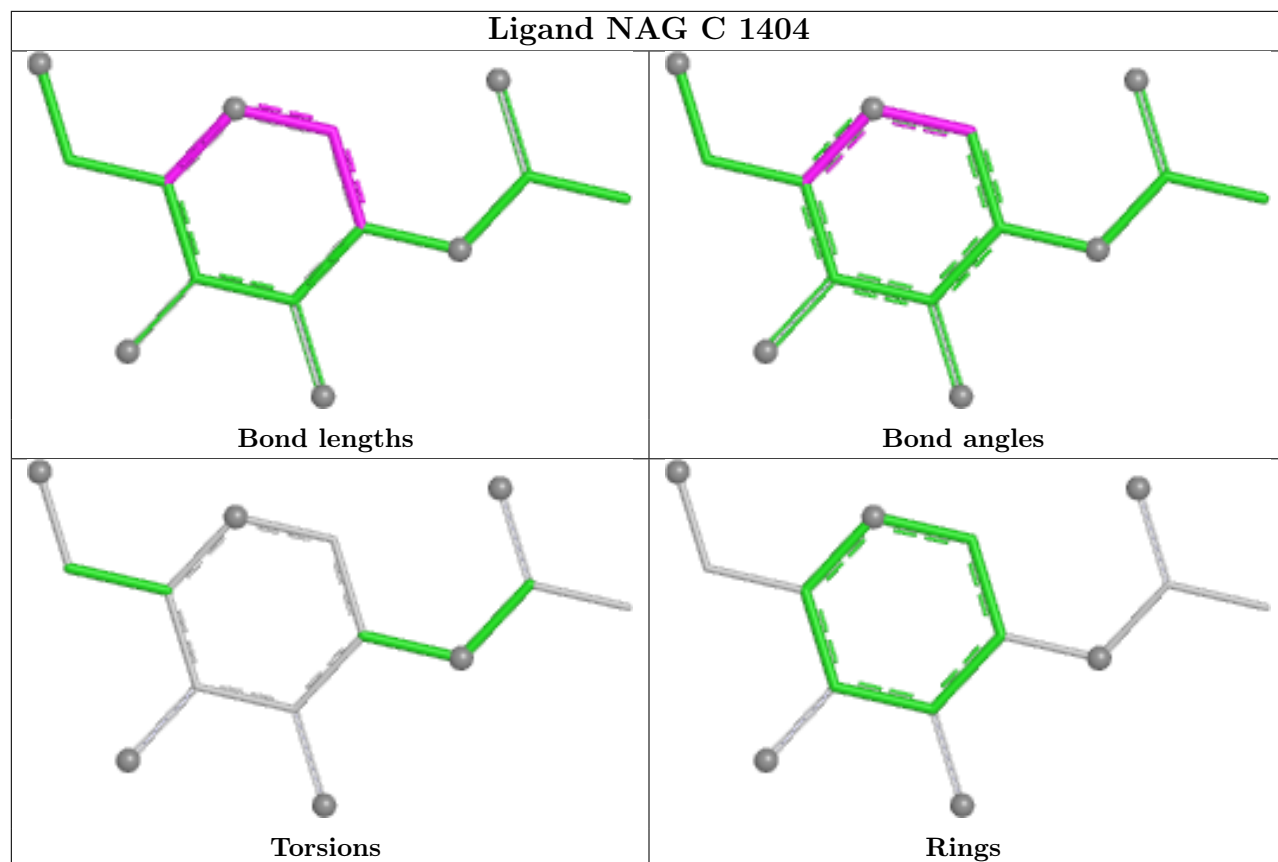
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for 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.

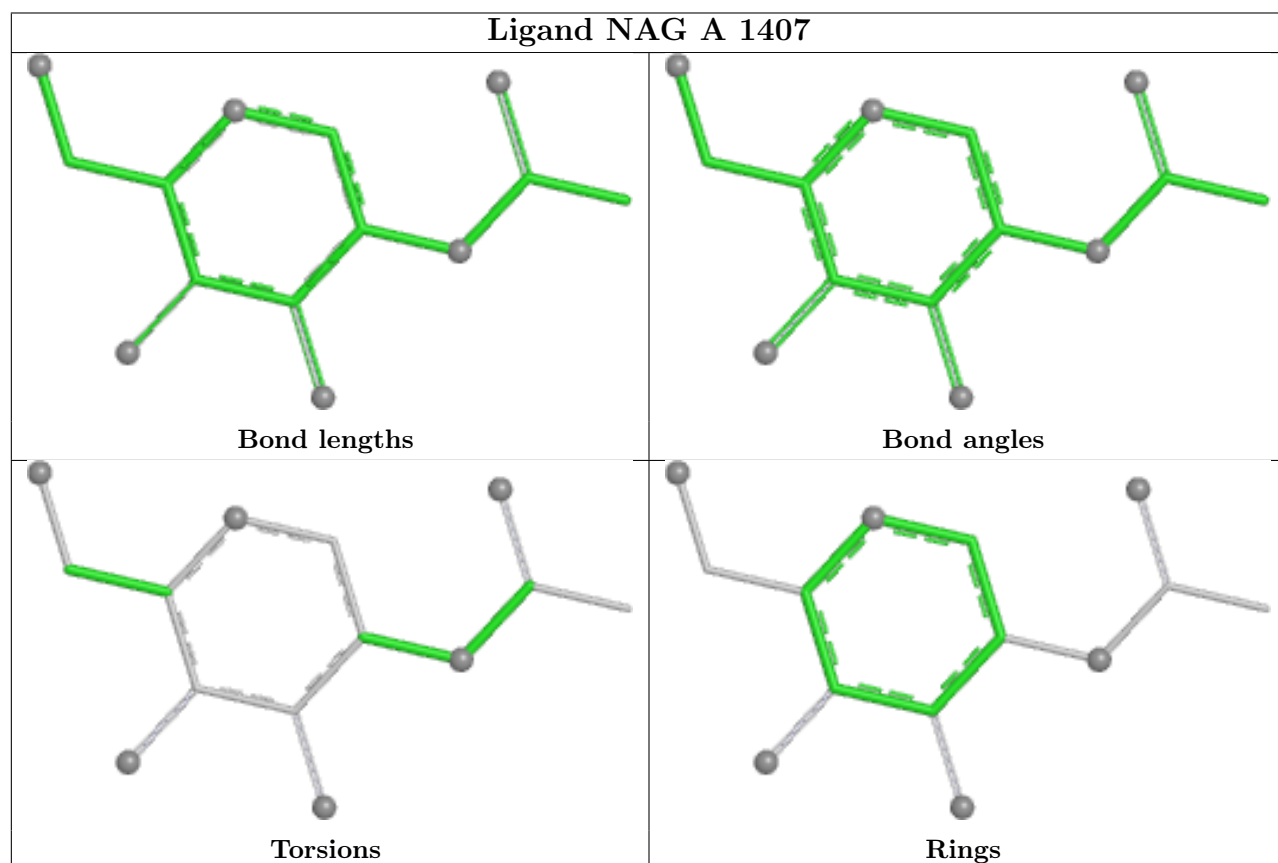




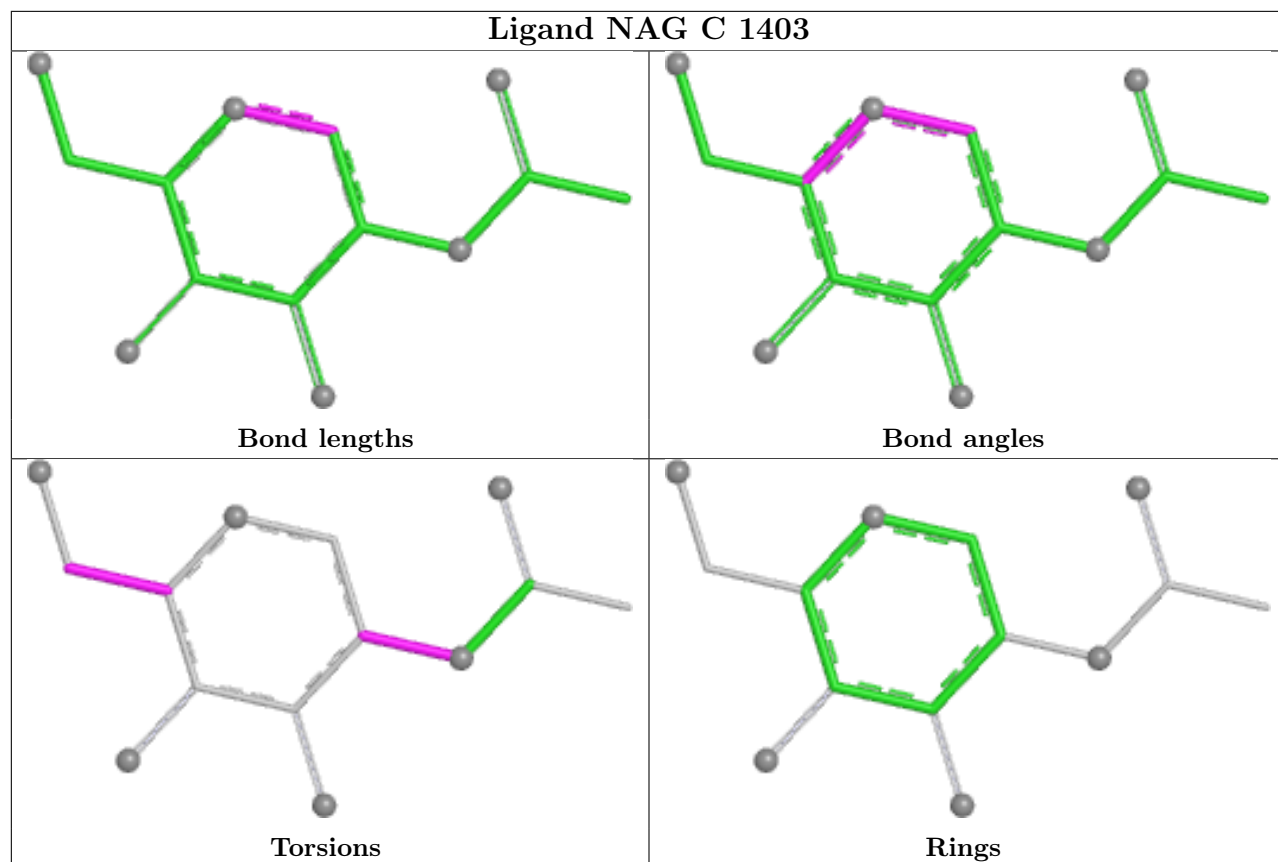
Ligand NAG C 1404



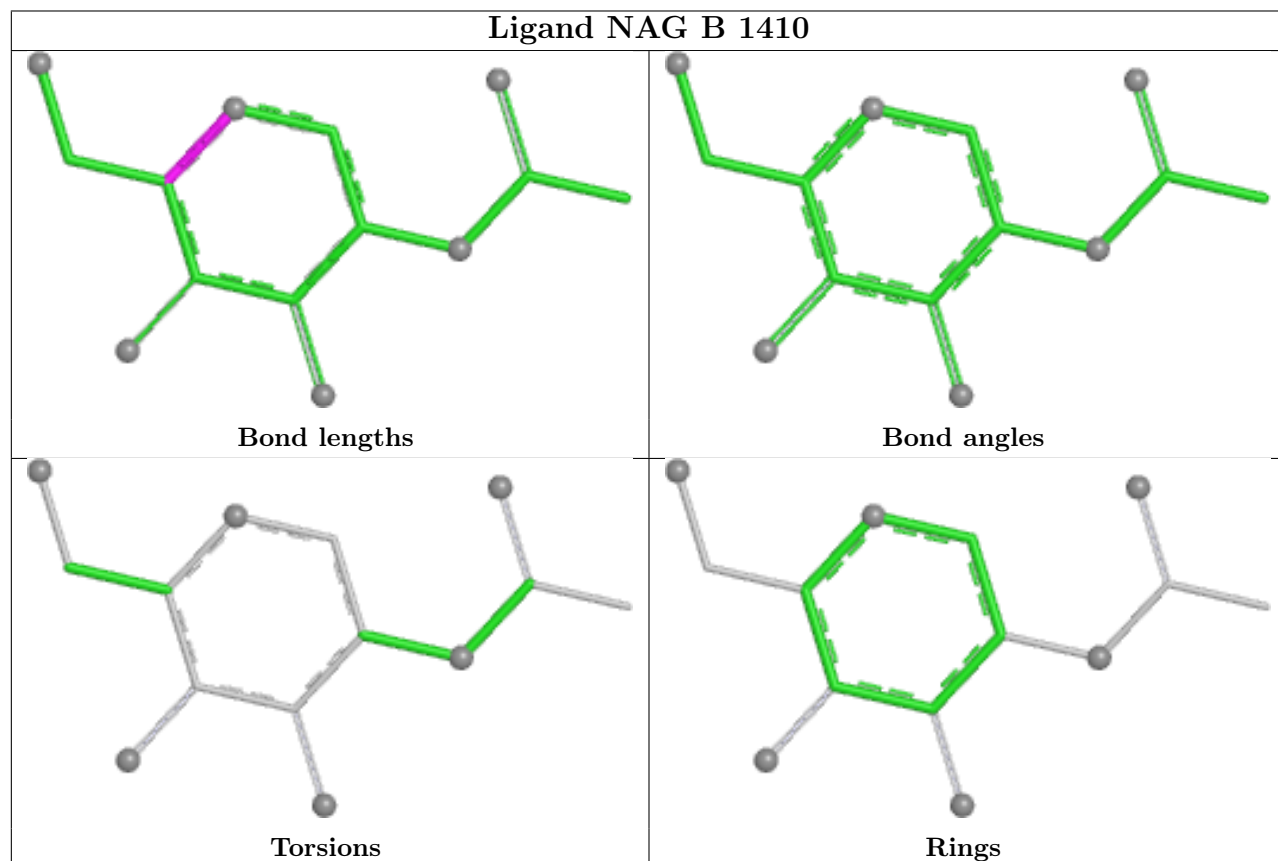
Ligand NAG A 1407

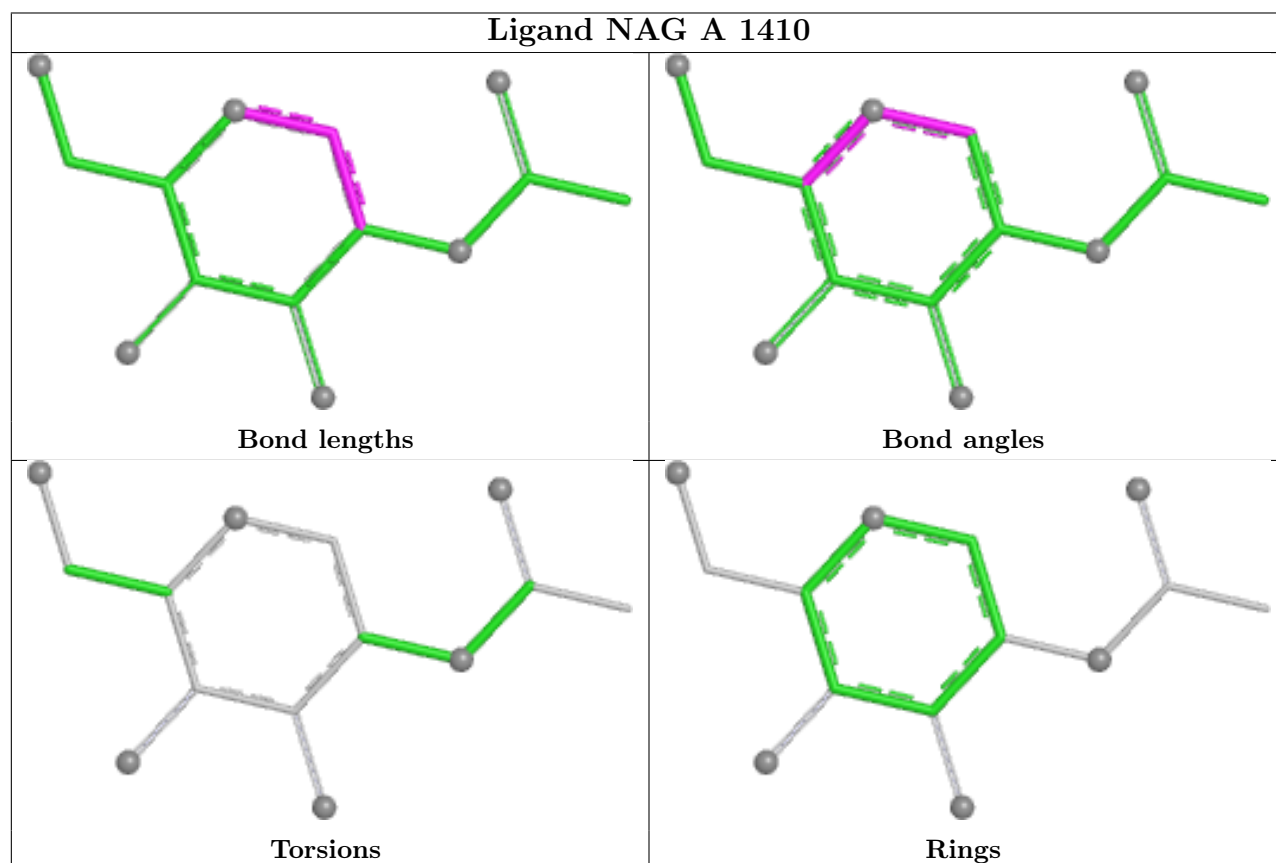
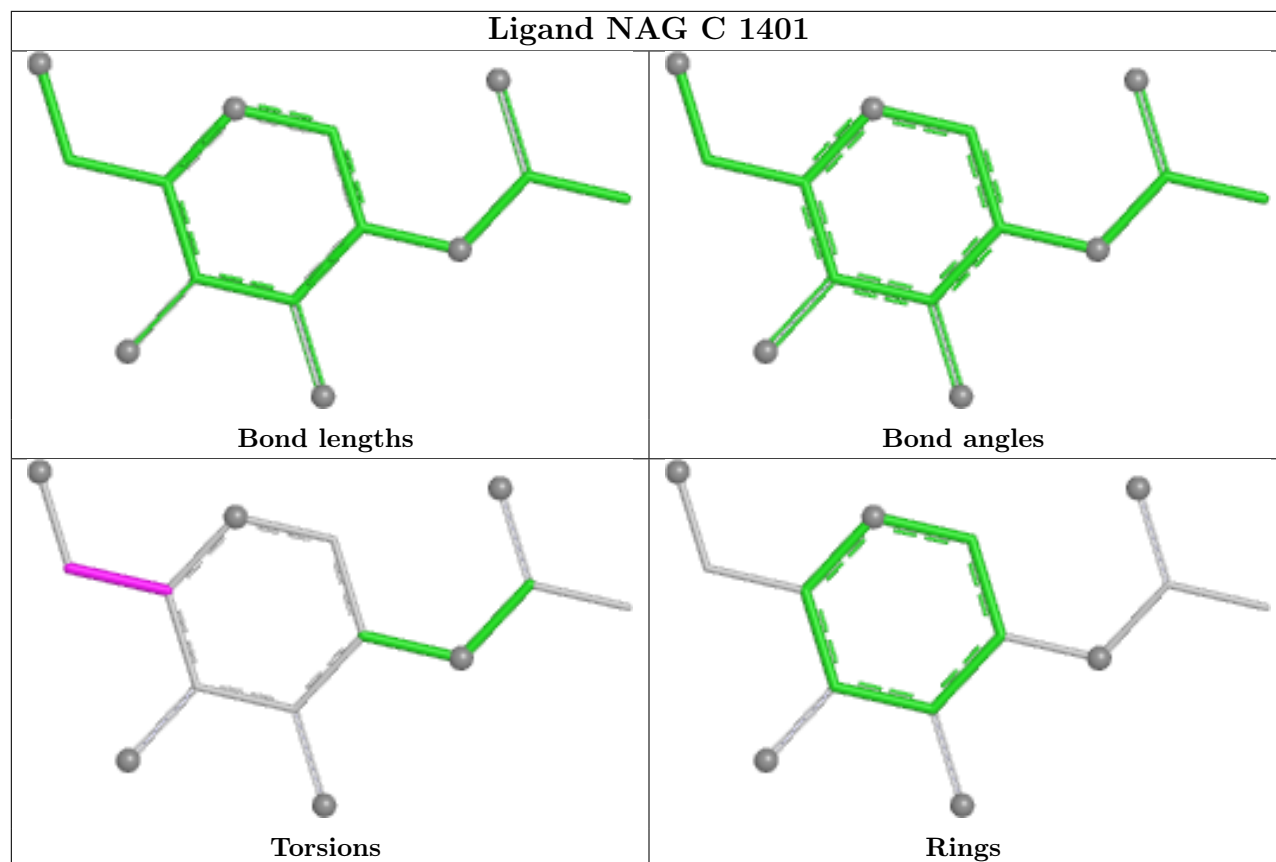


Ligand NAG C 1403

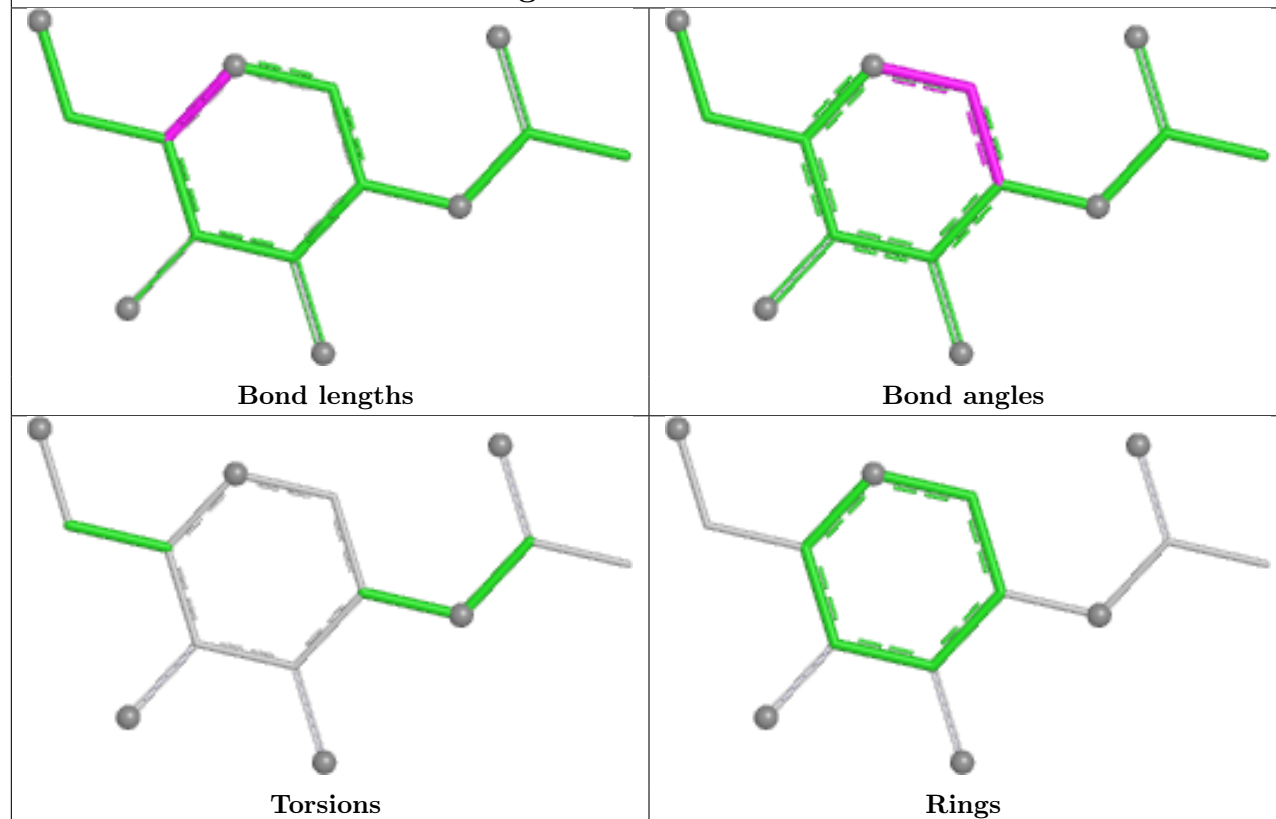


Ligand NAG B 1410

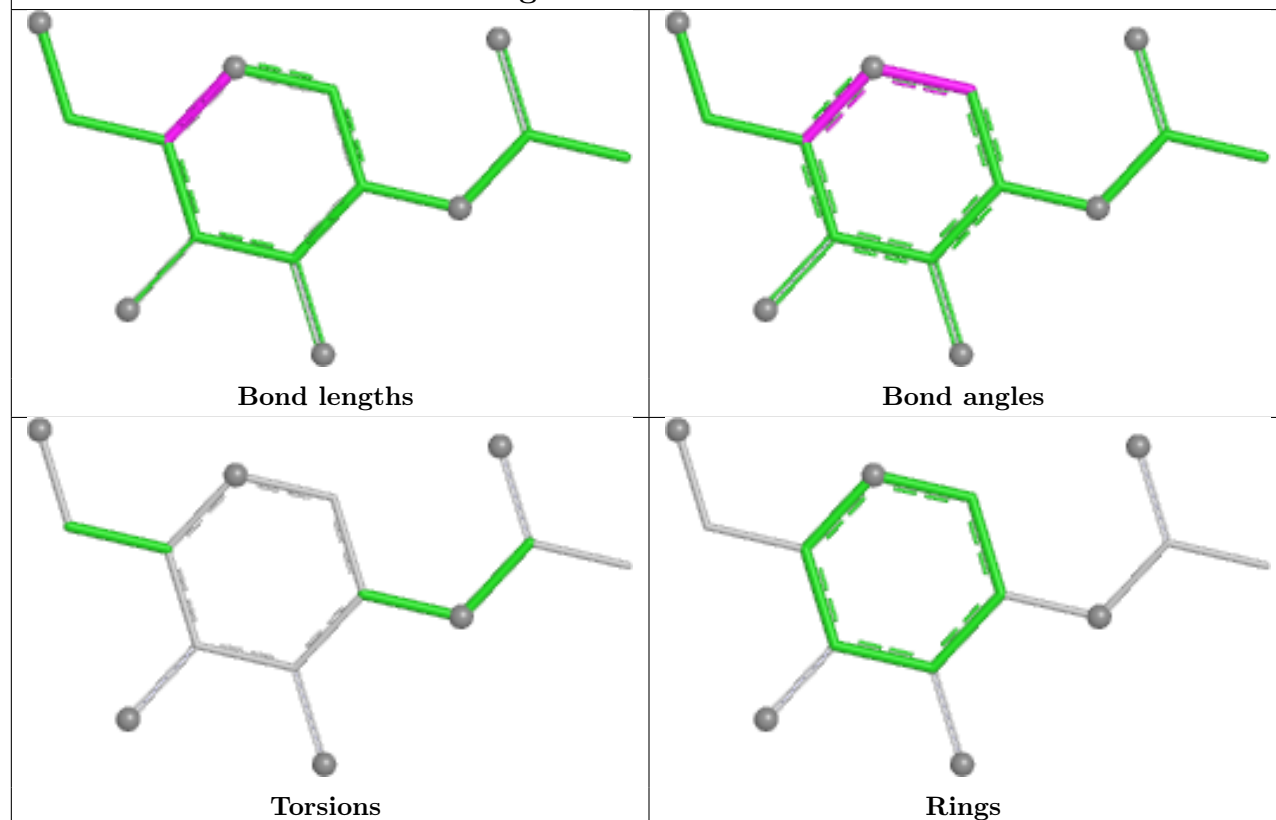




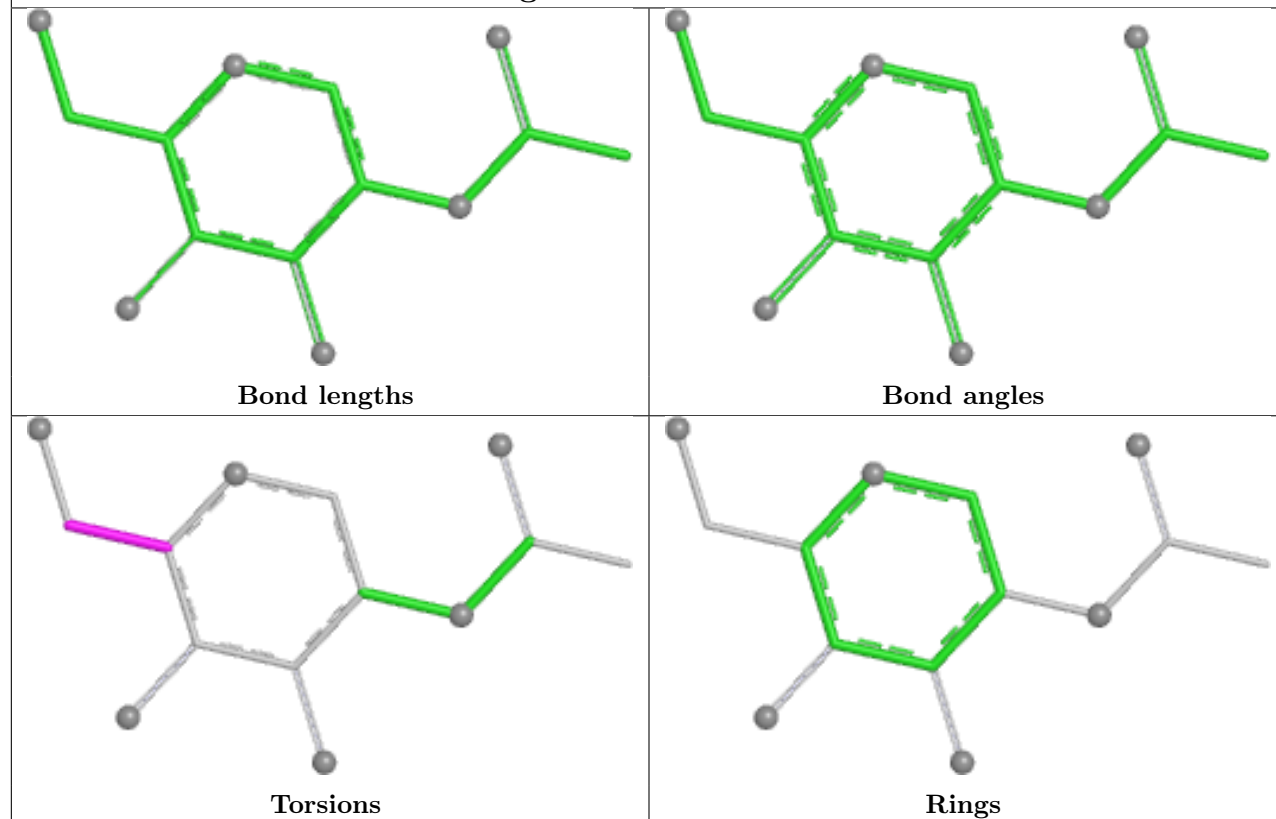
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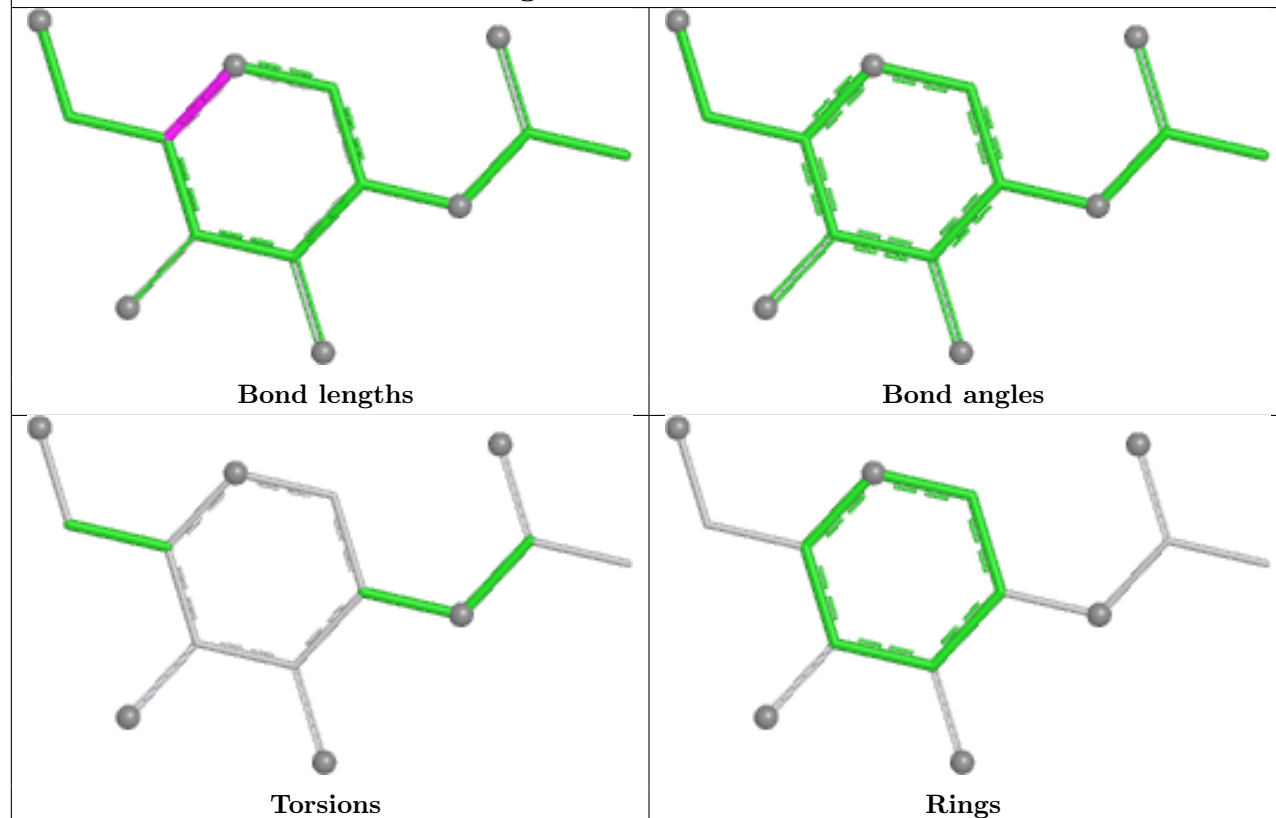
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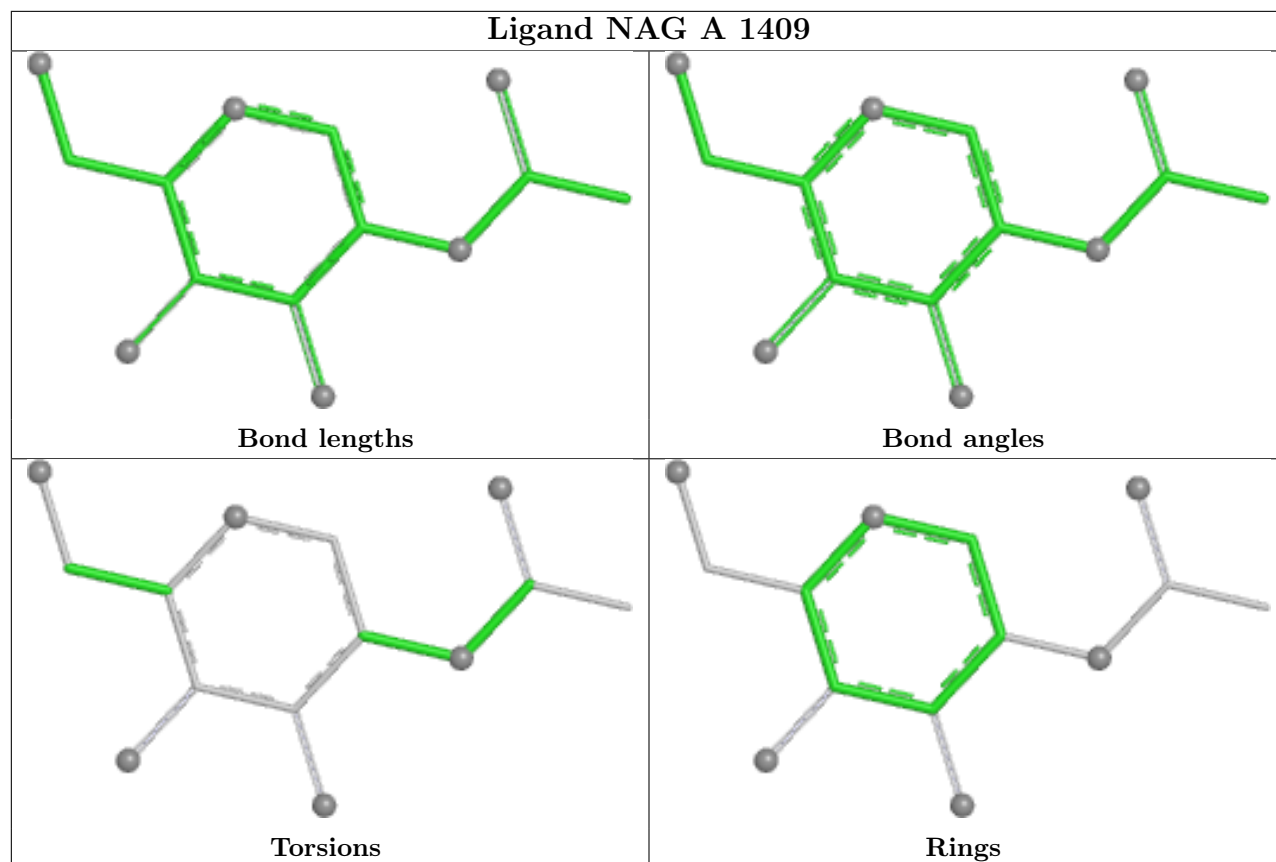
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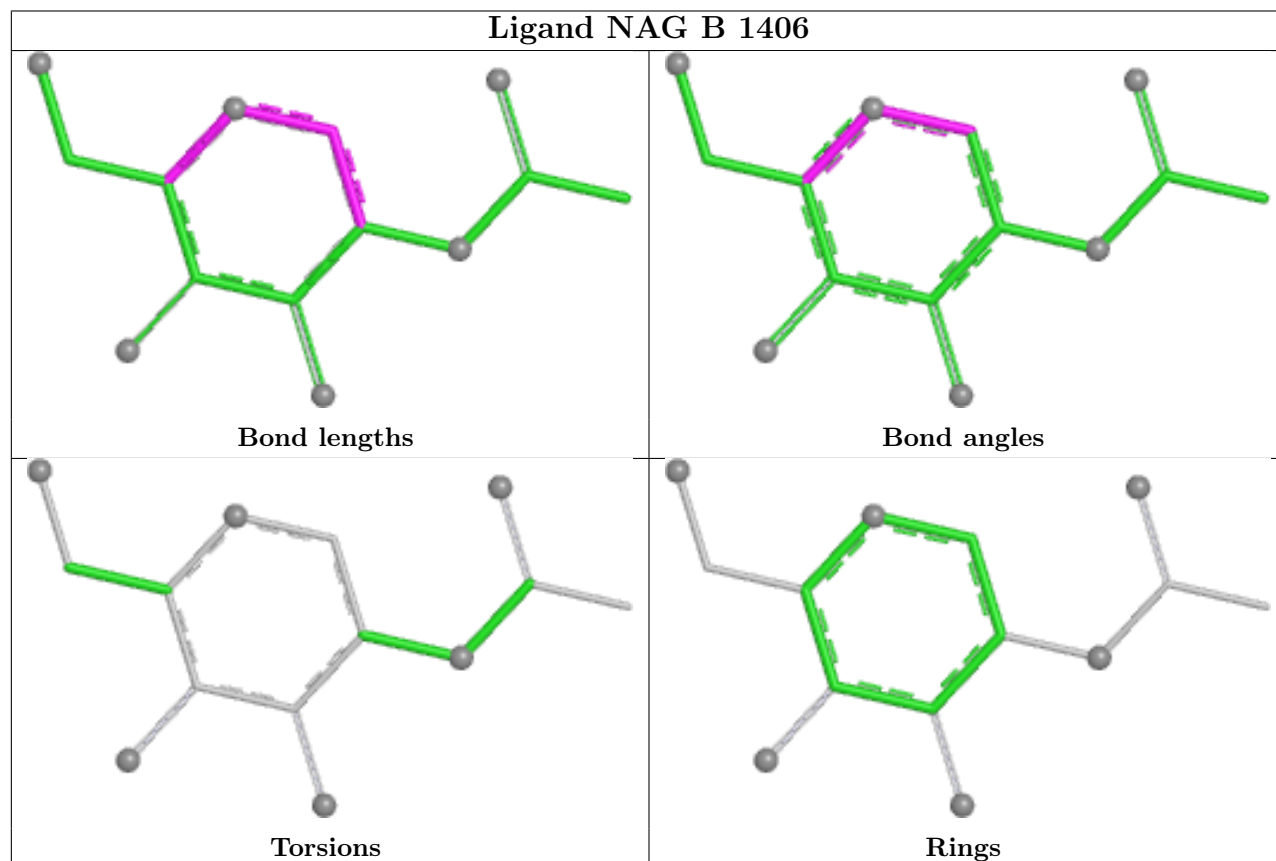
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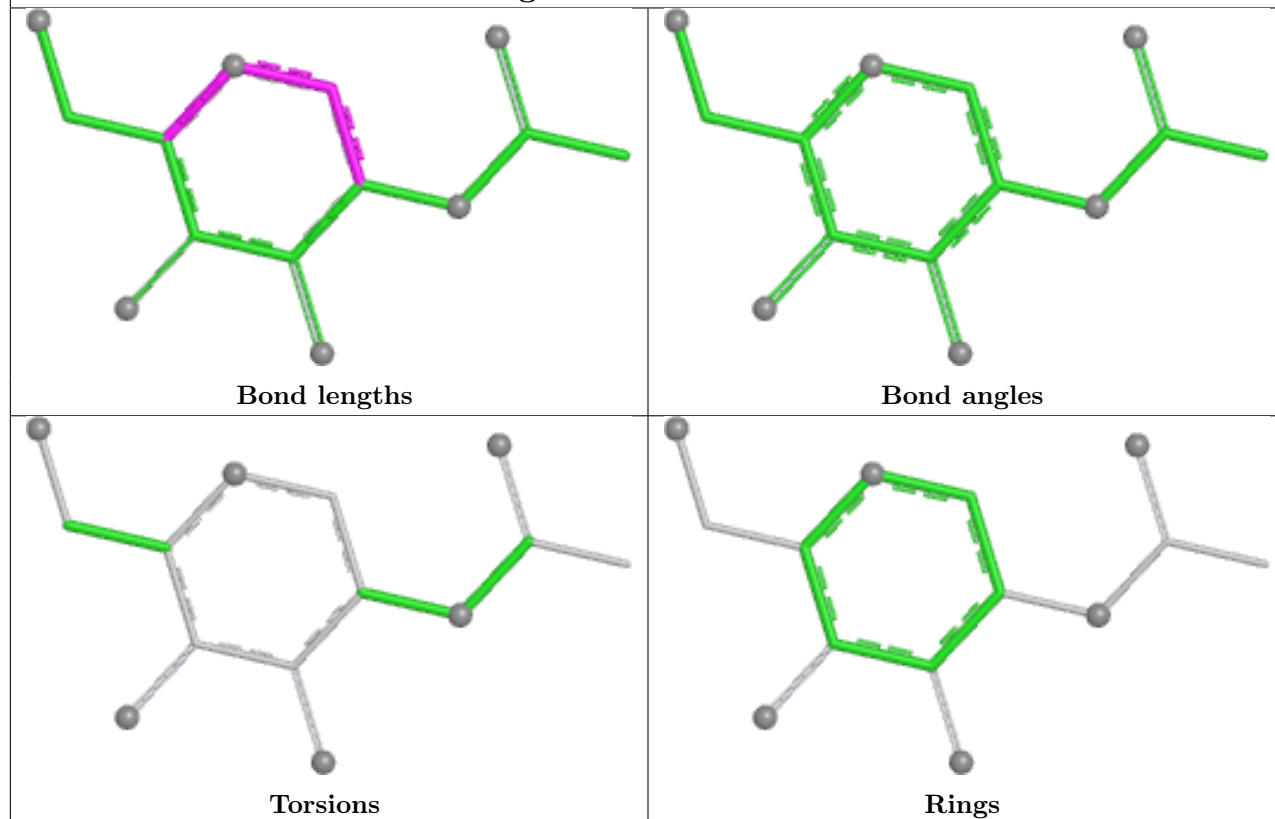
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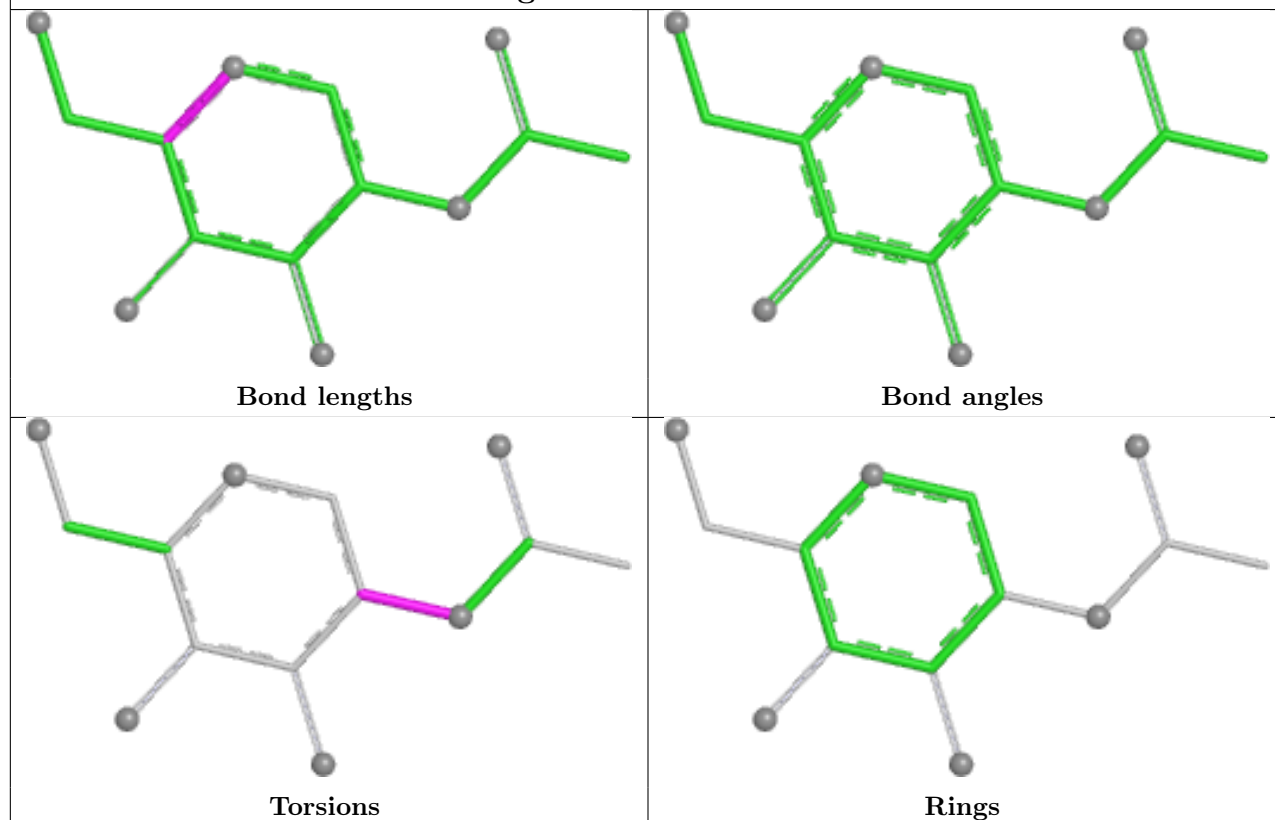
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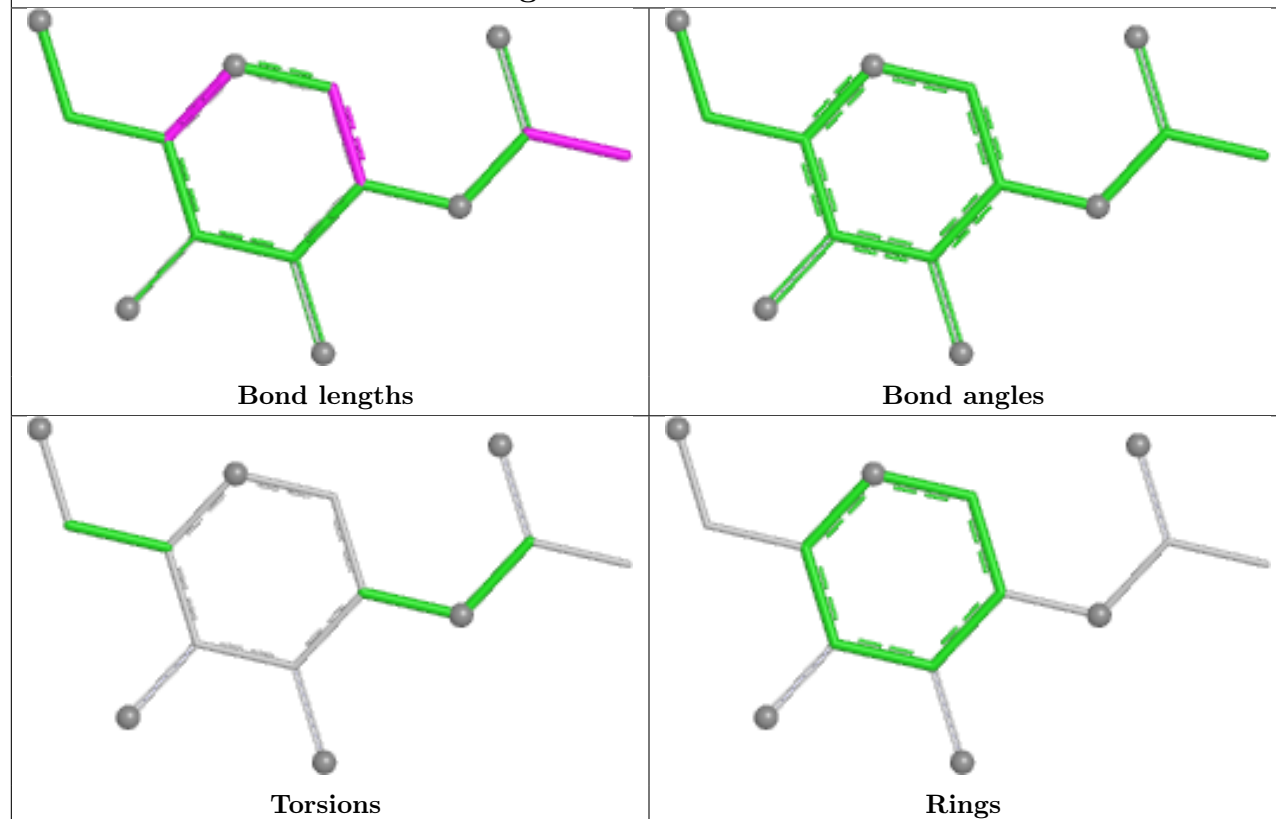
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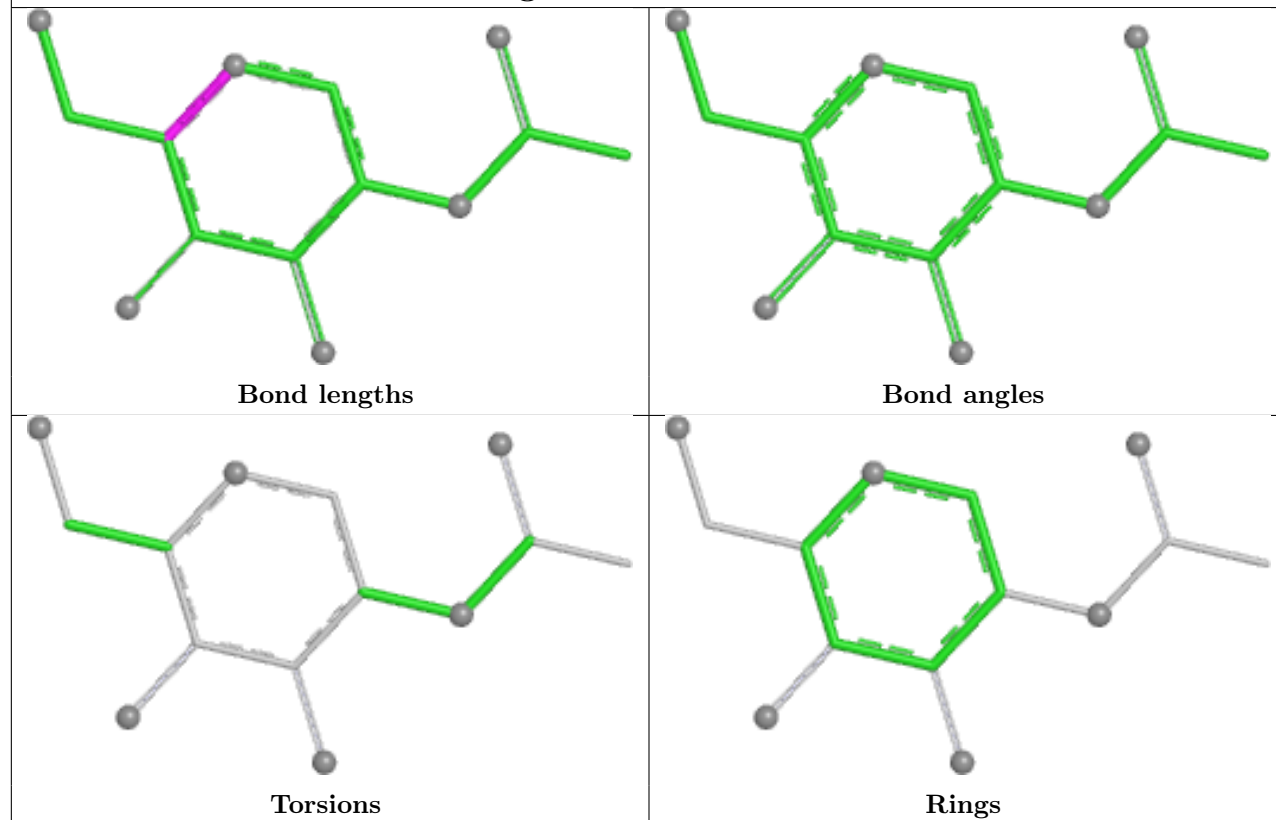
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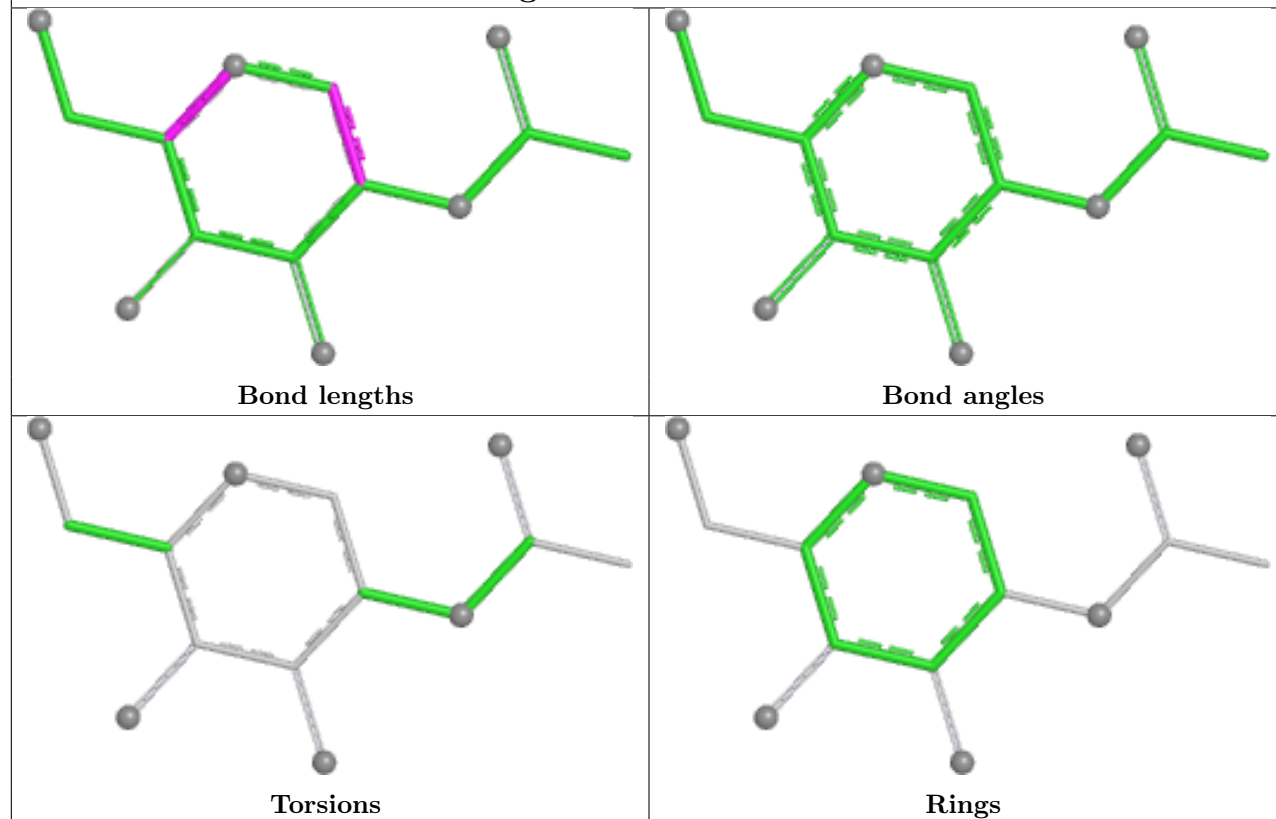
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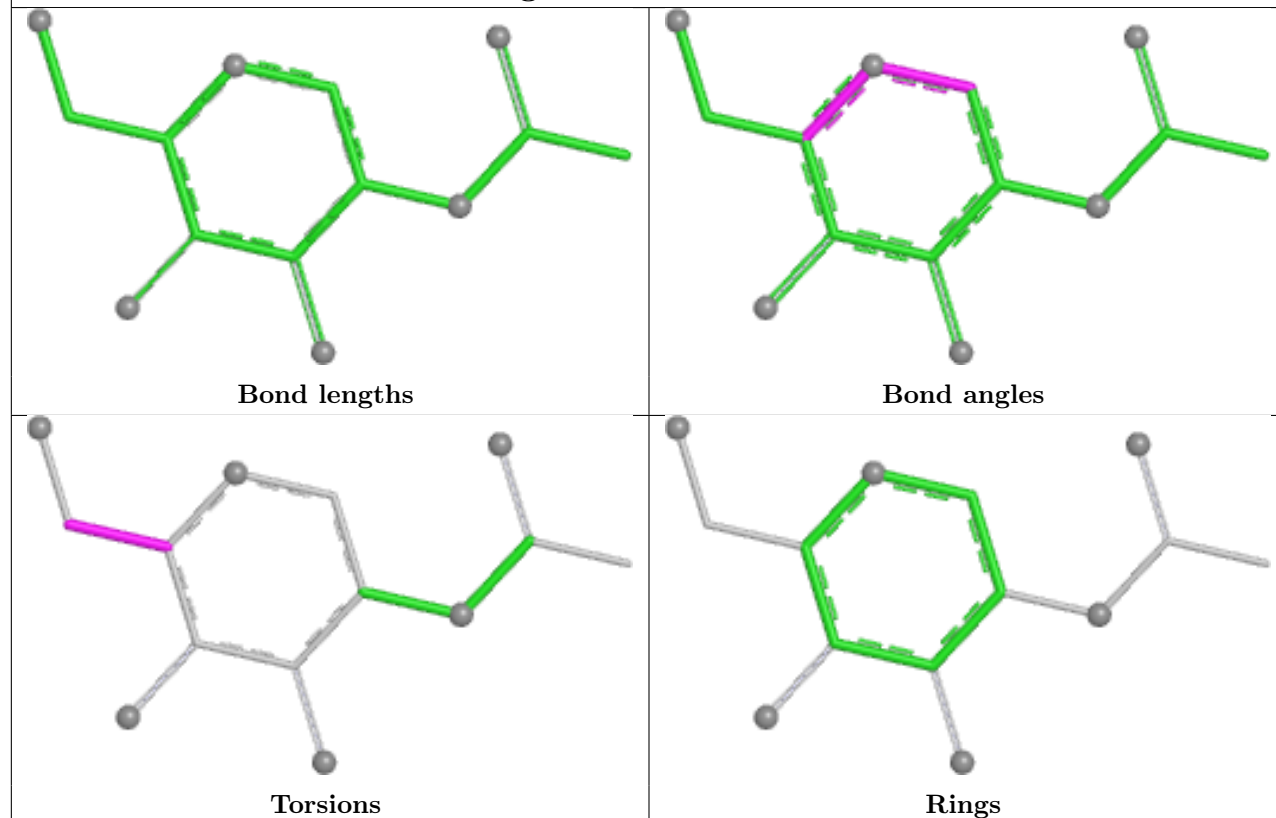
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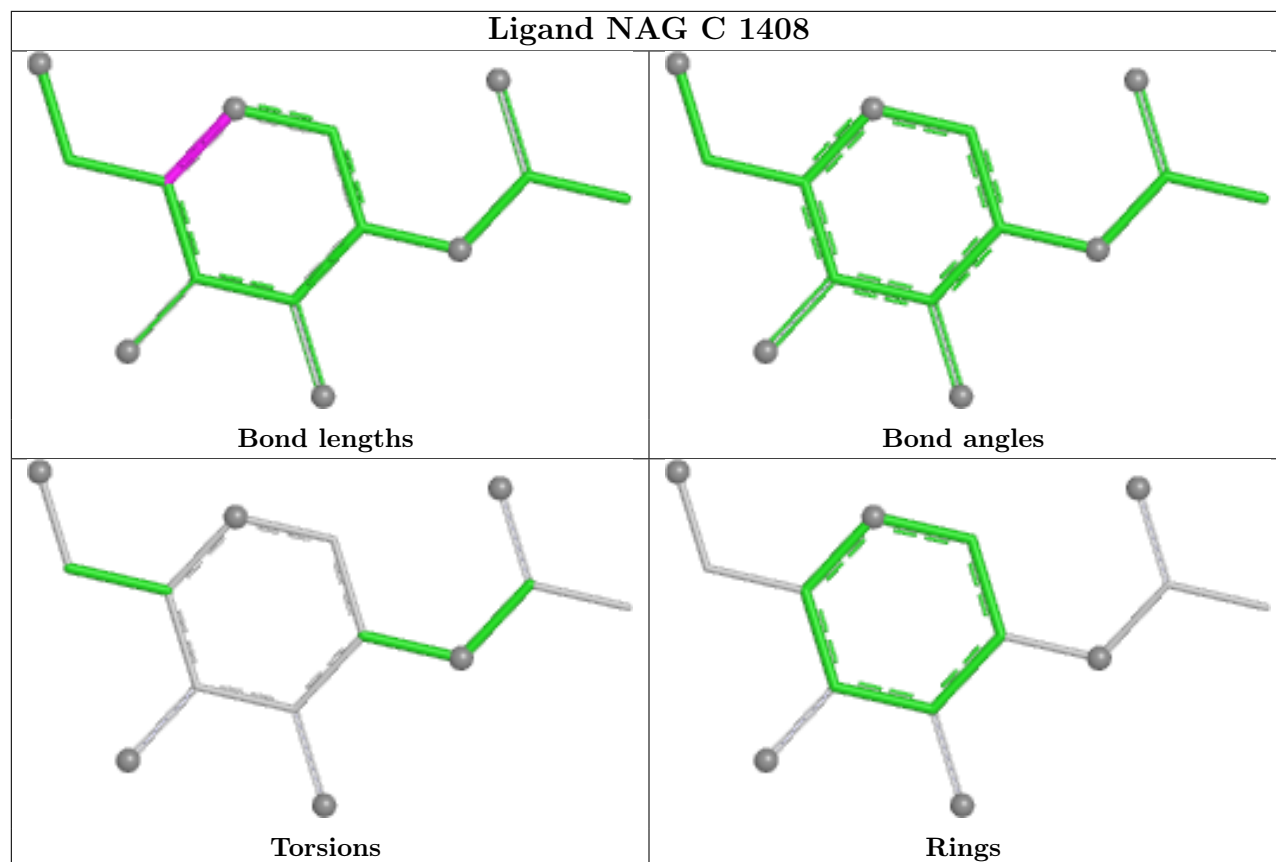
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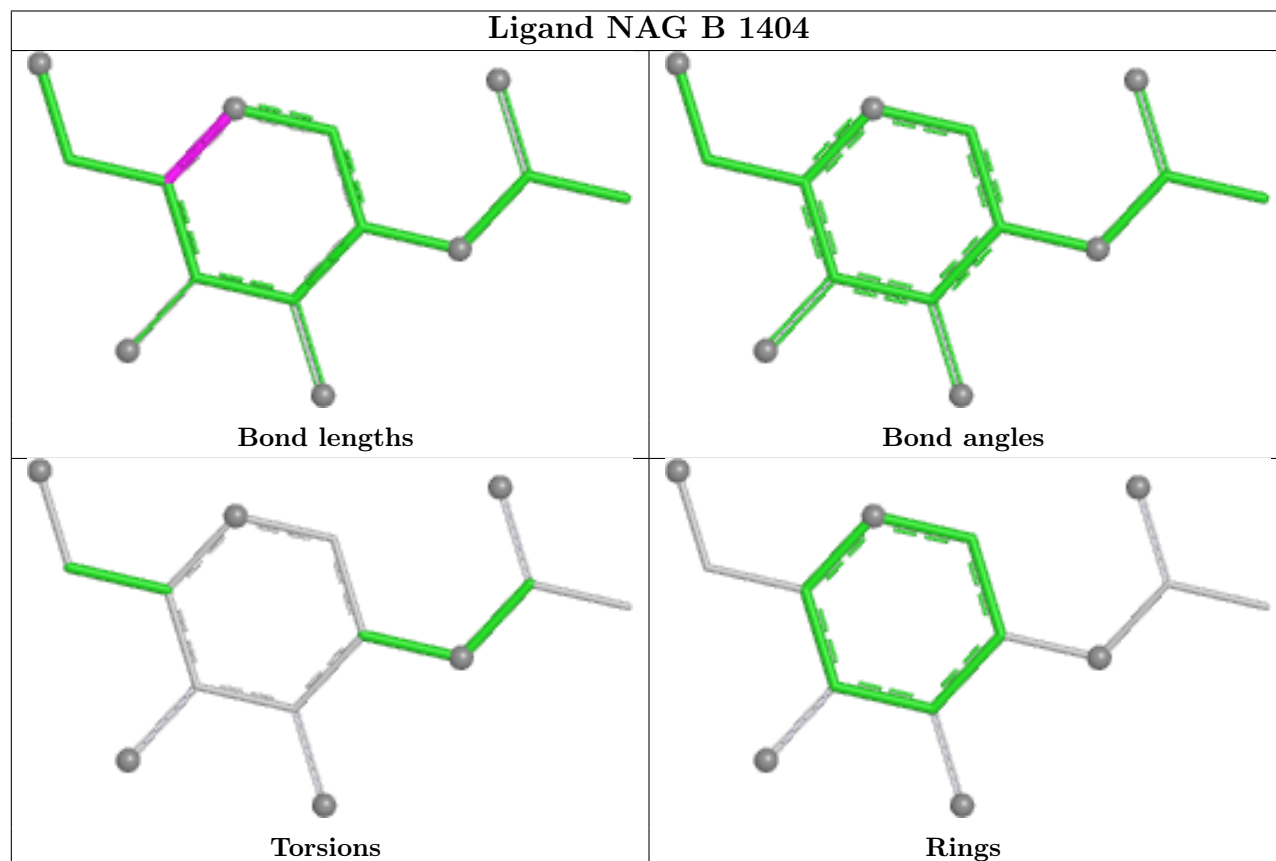
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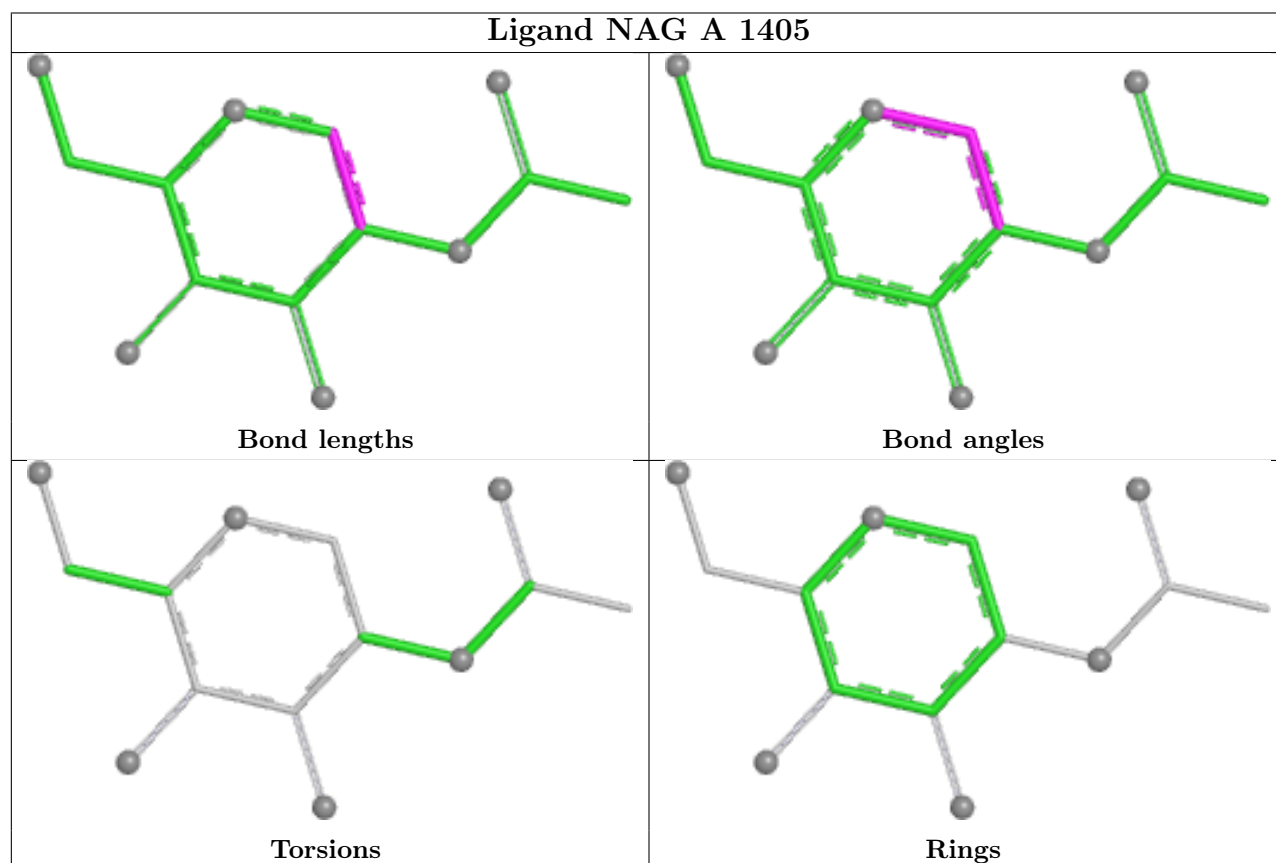
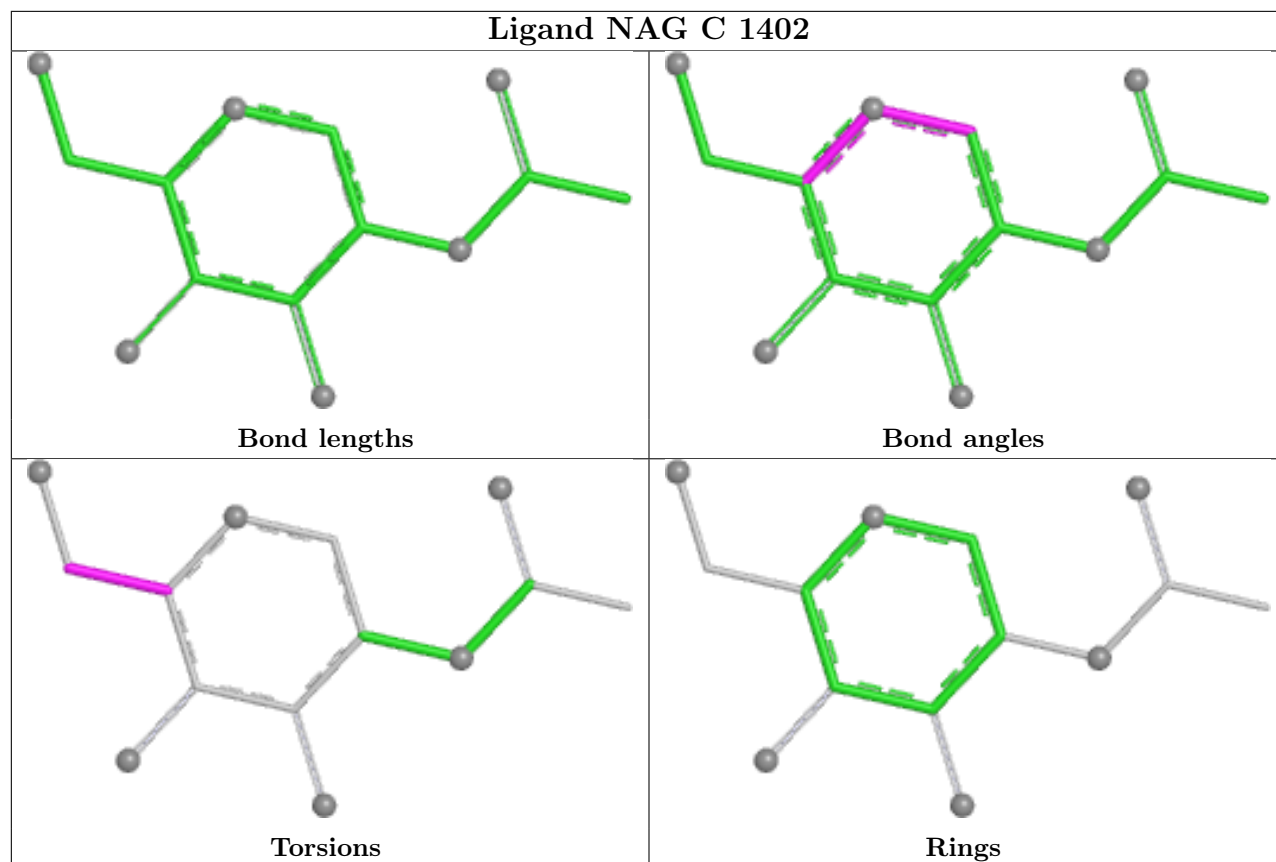


Ligand NAG C 1408

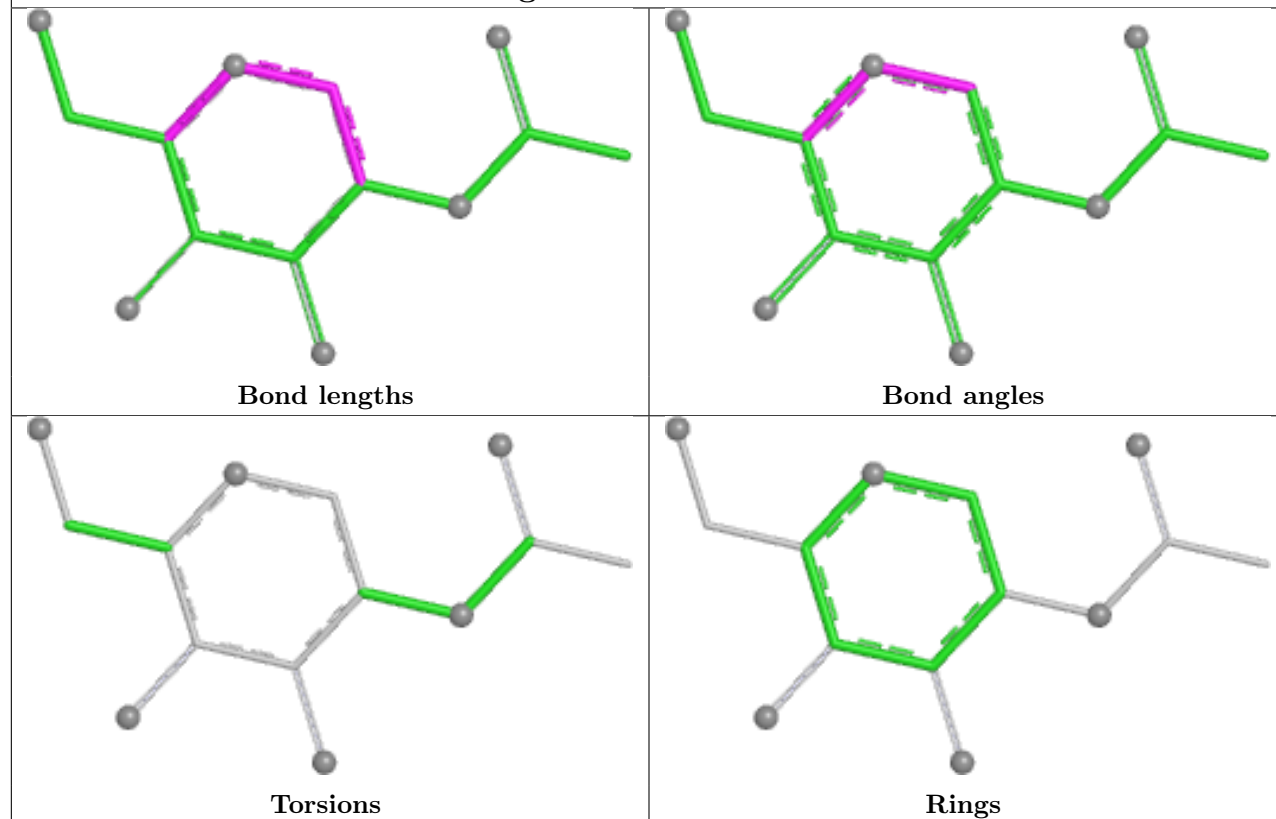


Ligand NAG B 1404

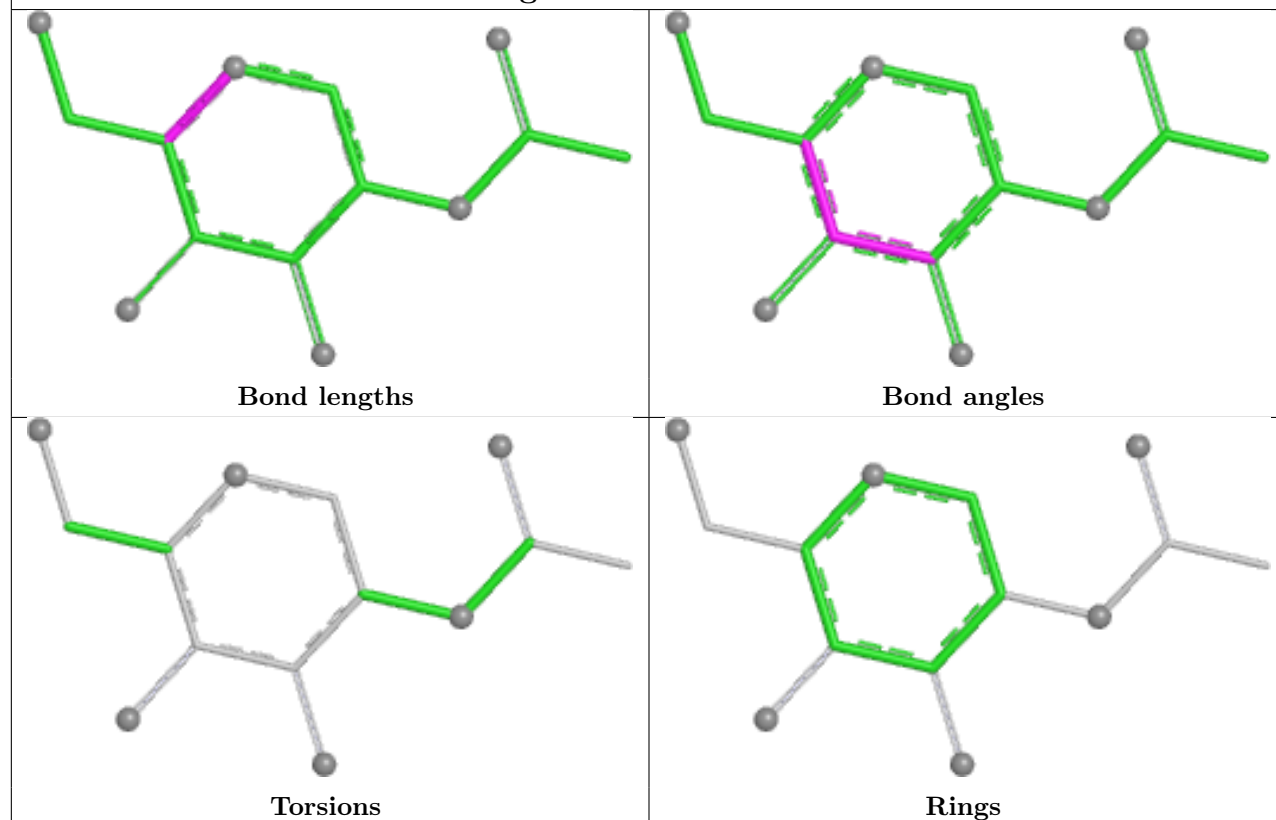




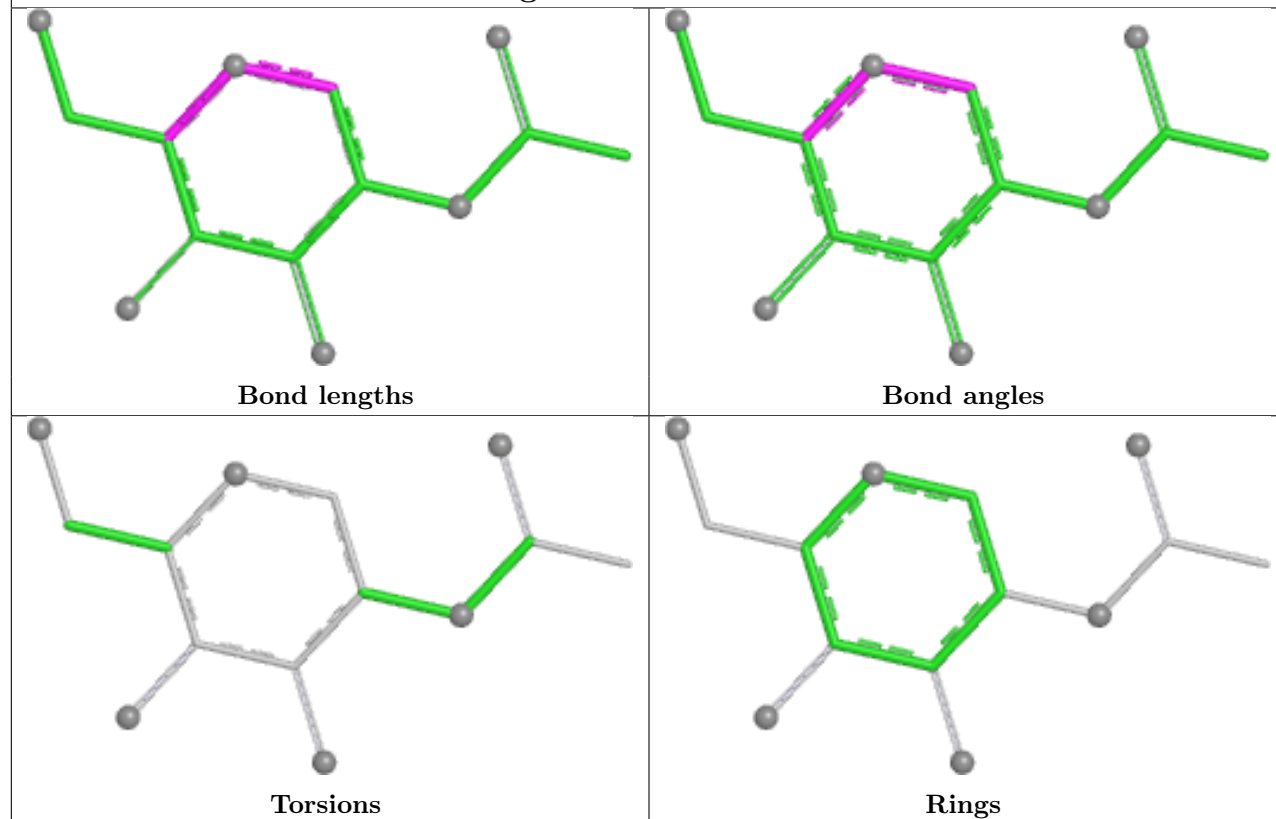
Ligand NAG A 1401



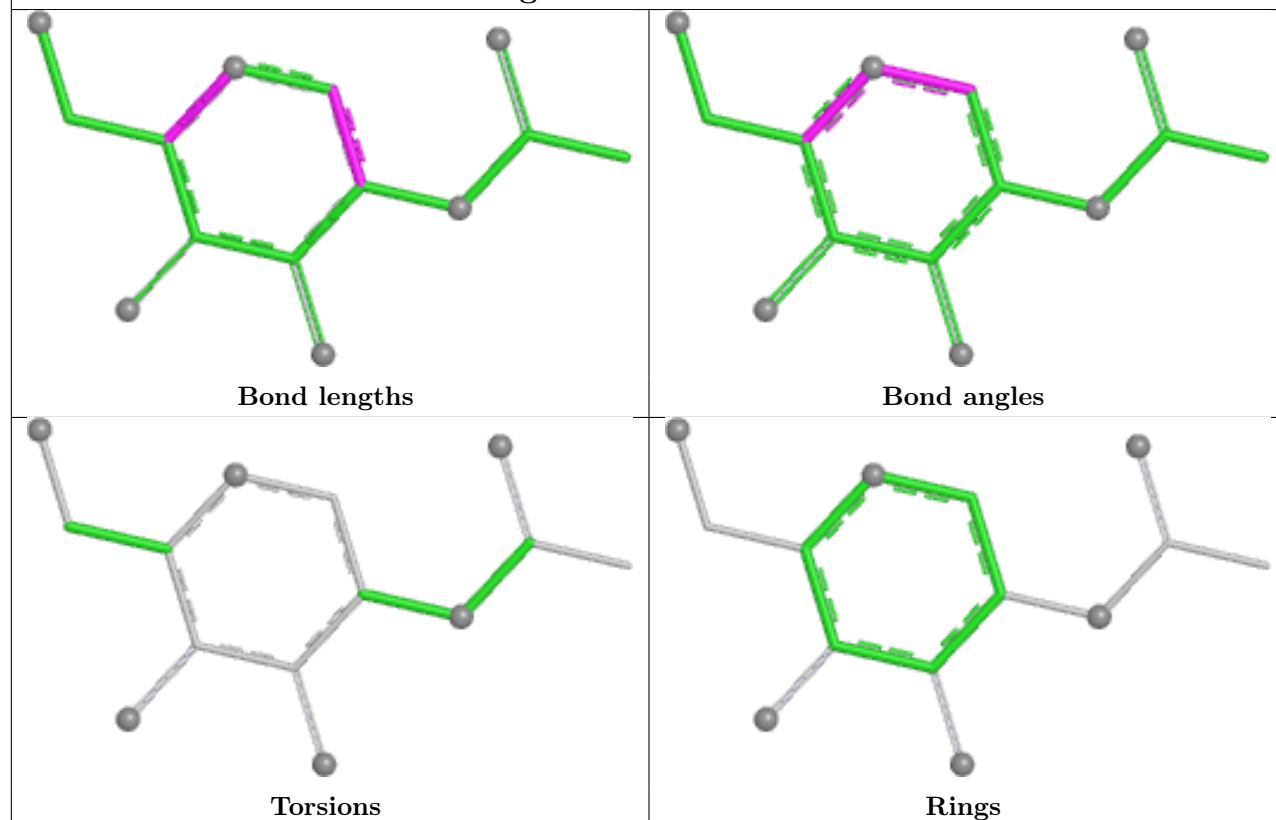
Ligand NAG B 1407



Ligand NAG B 1405



Ligand NAG B 1409



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.

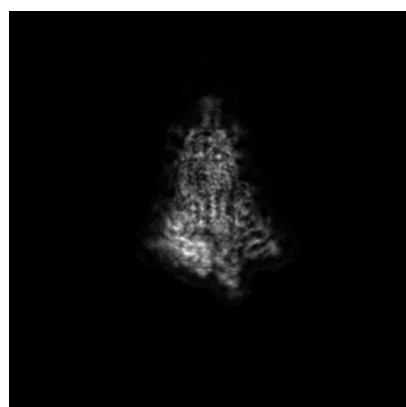
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24987. These allow visual inspection of the internal detail of the map and identification of artifacts.

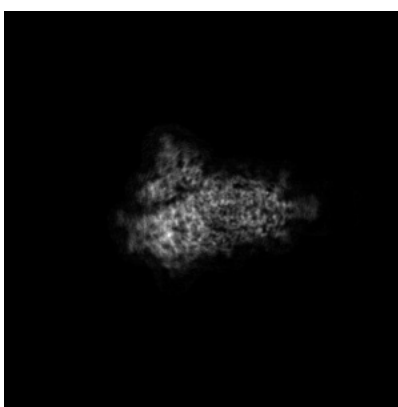
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

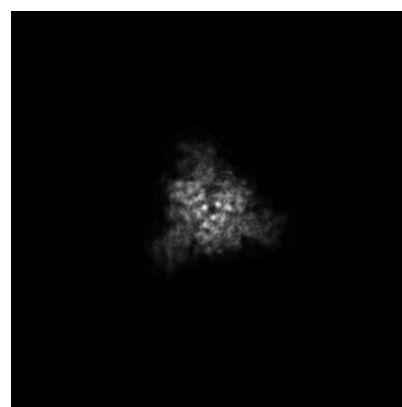
6.1.1 Primary map



X



Y



Z

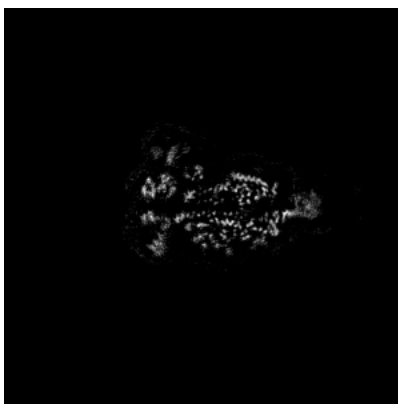
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

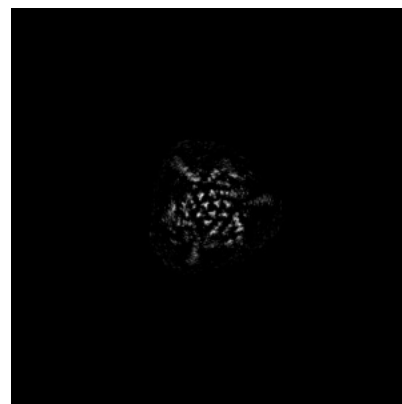
6.2.1 Primary map



X Index: 240



Y Index: 240

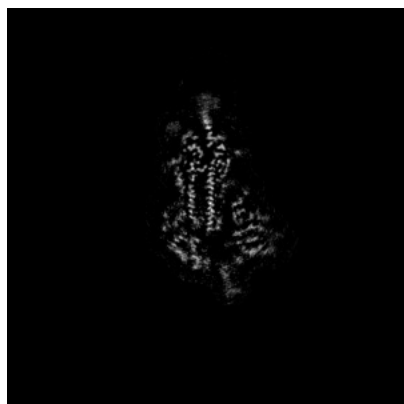


Z Index: 240

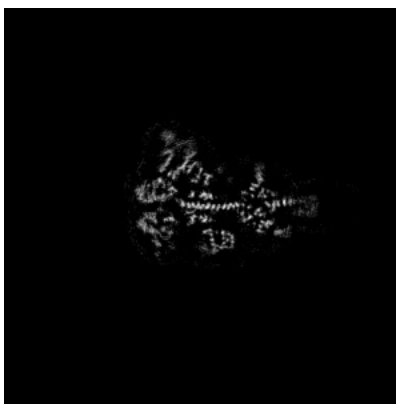
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 232



Y Index: 231

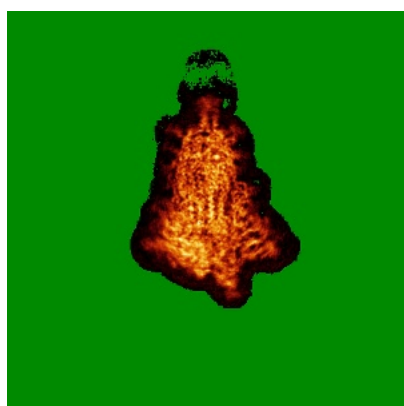


Z Index: 200

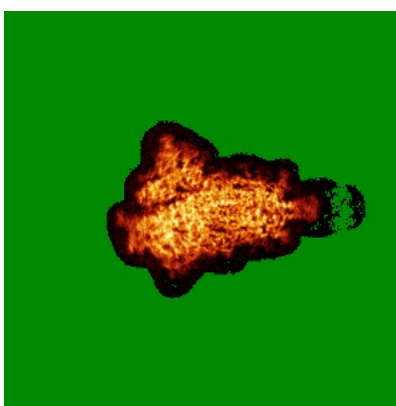
The images above show the largest variance slices of the map in three orthogonal directions.

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

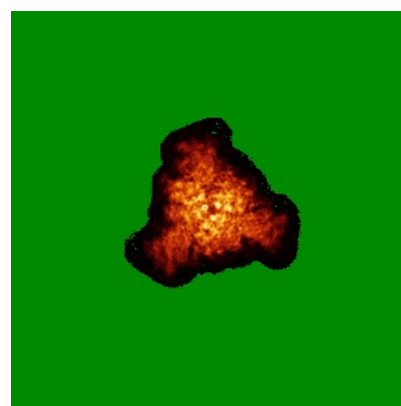
6.4.1 Primary map



X



Y

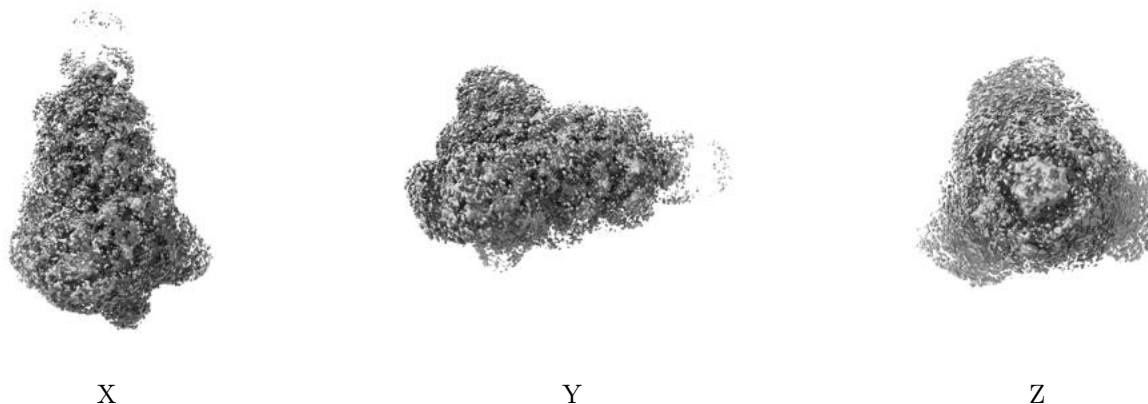


Z

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

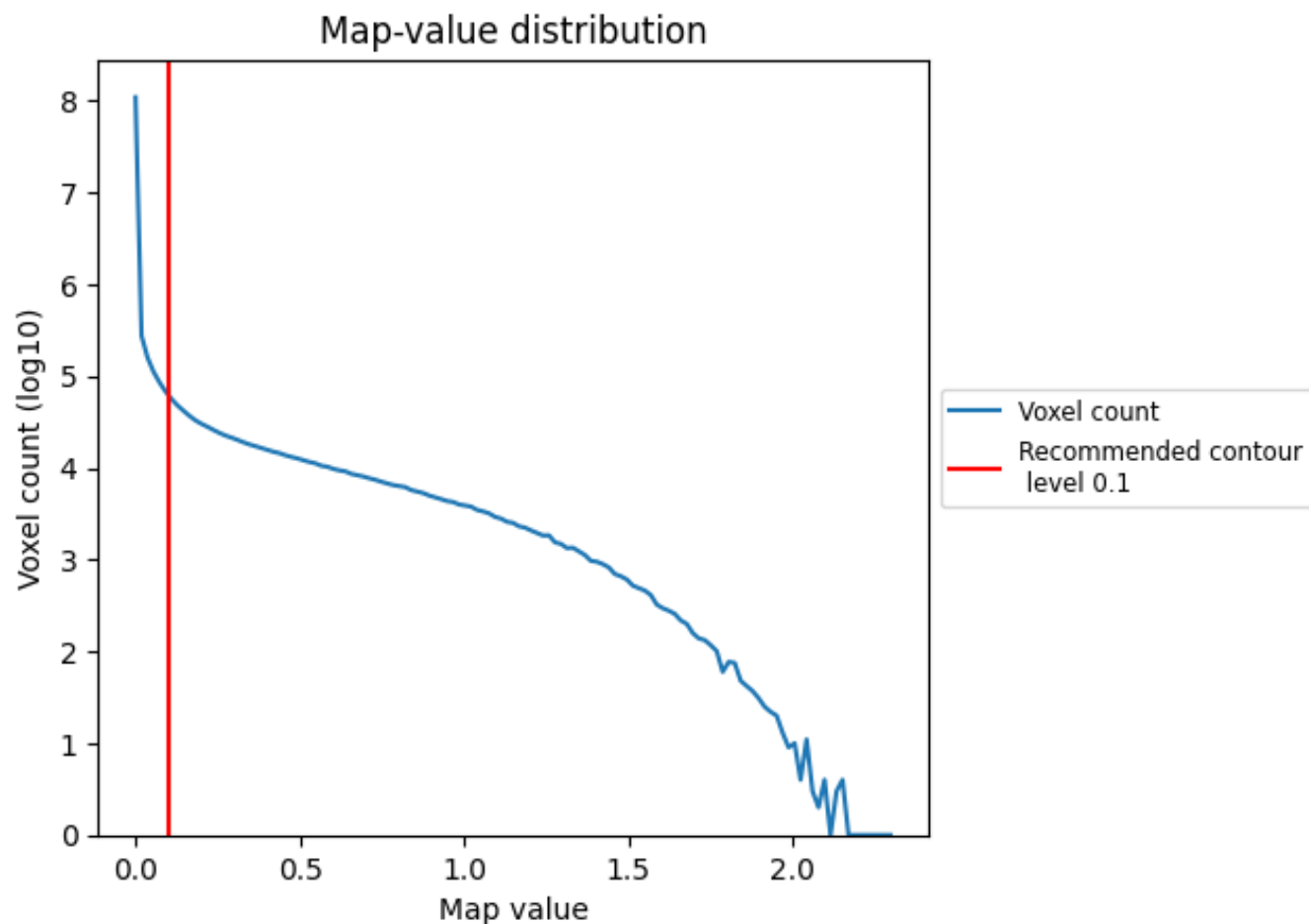
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

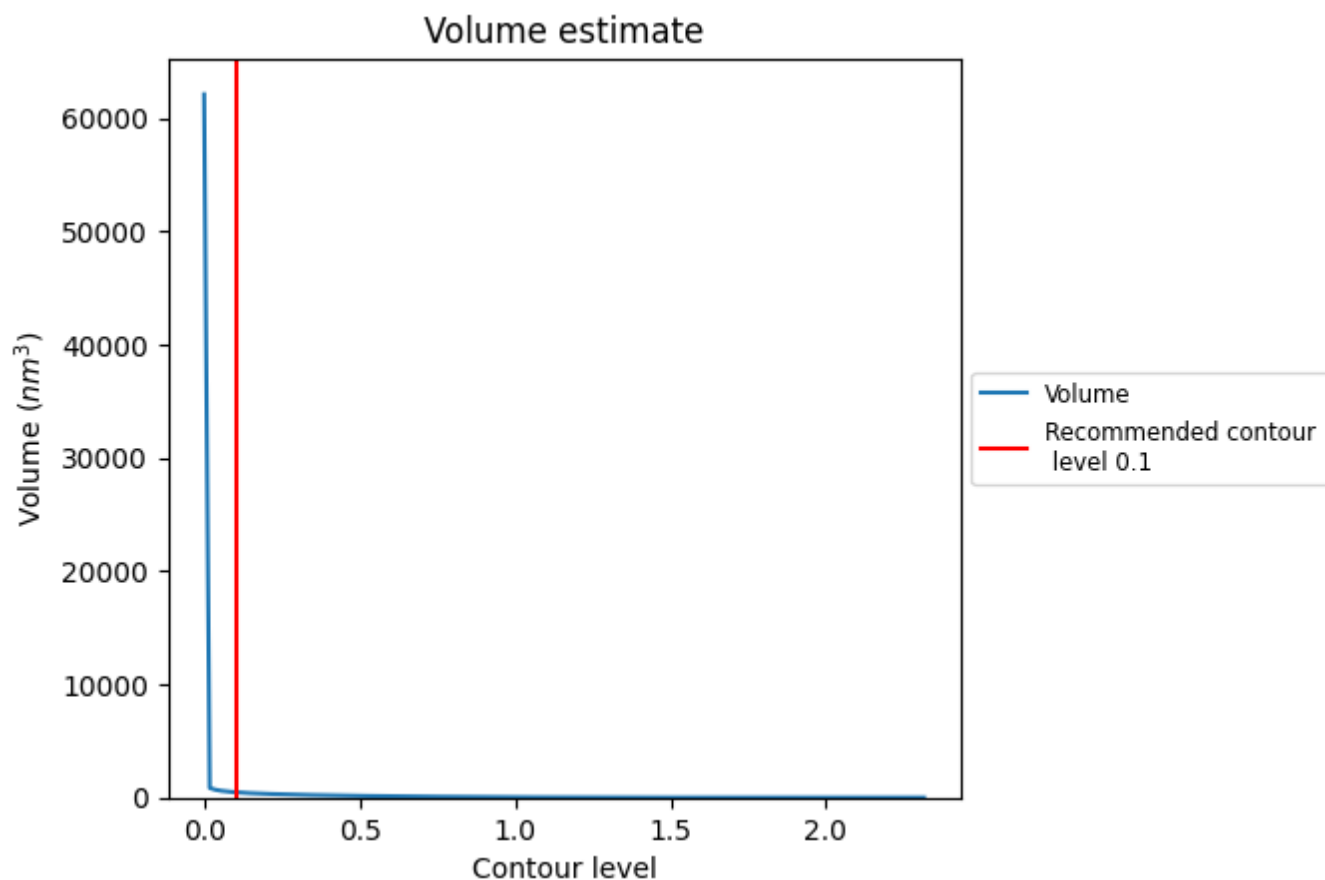
This section contains the results of statistical analysis of the map.

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.

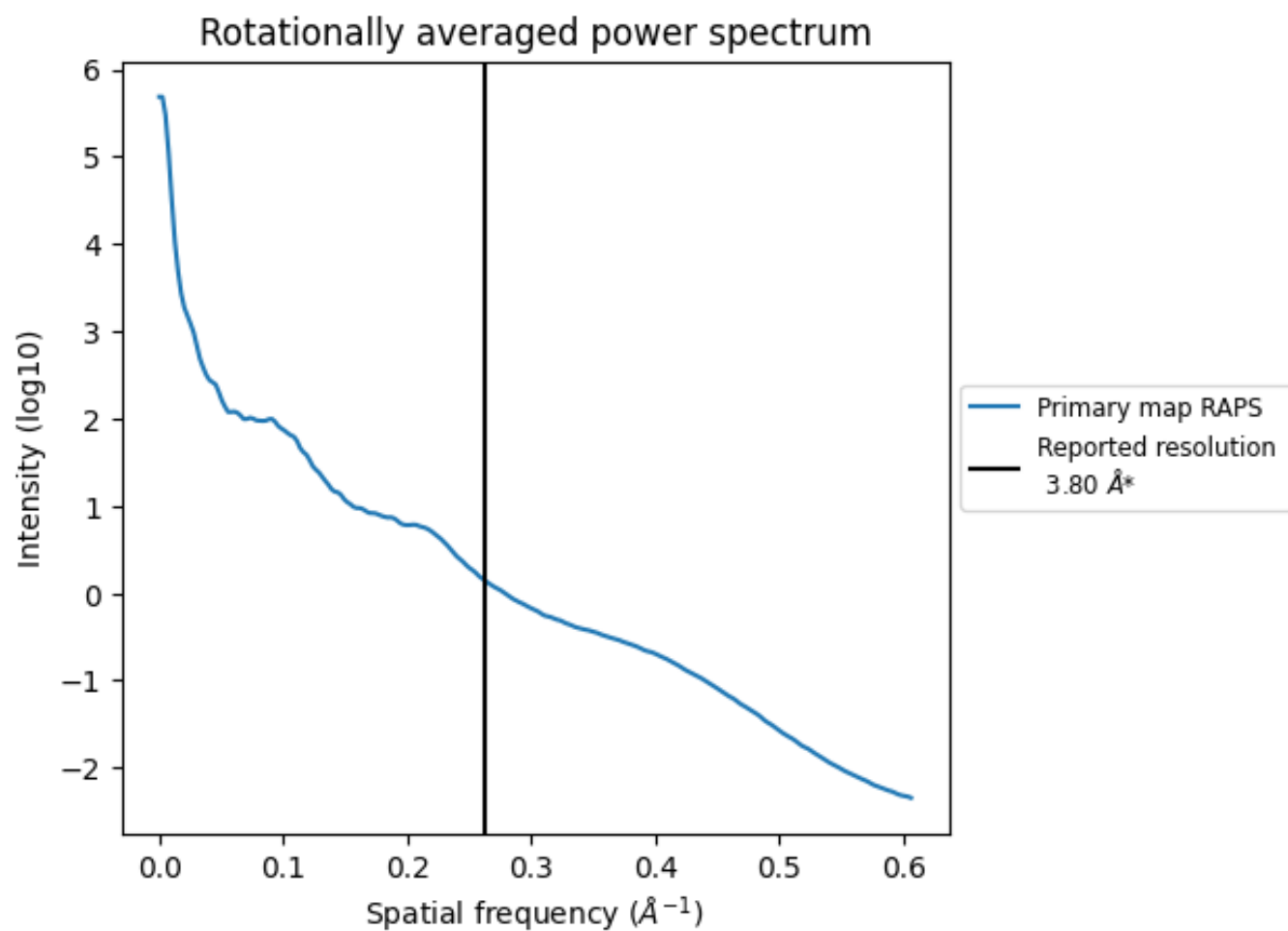
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 468 nm³; this corresponds to an approximate mass of 423 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 0.263 Å⁻¹

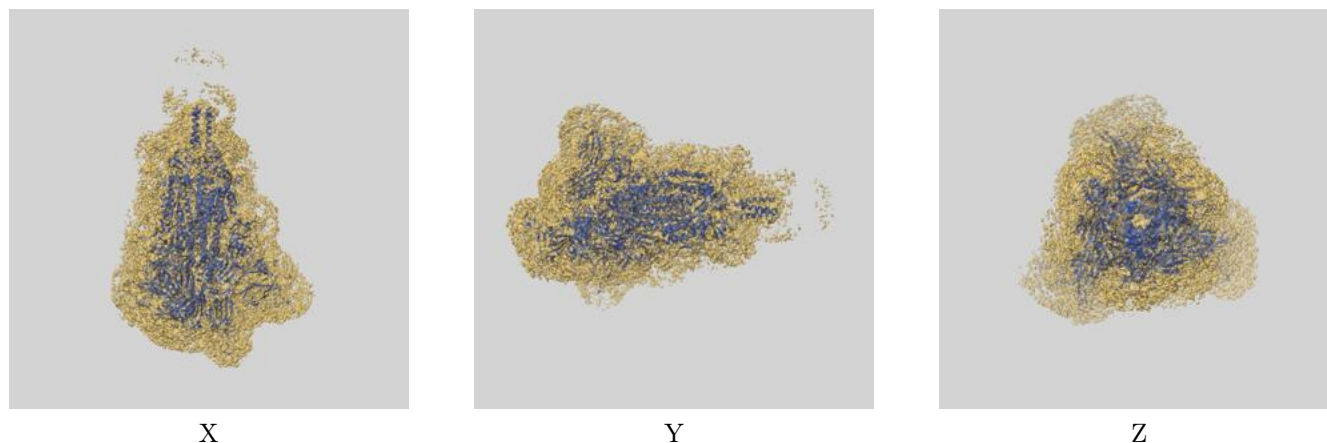
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

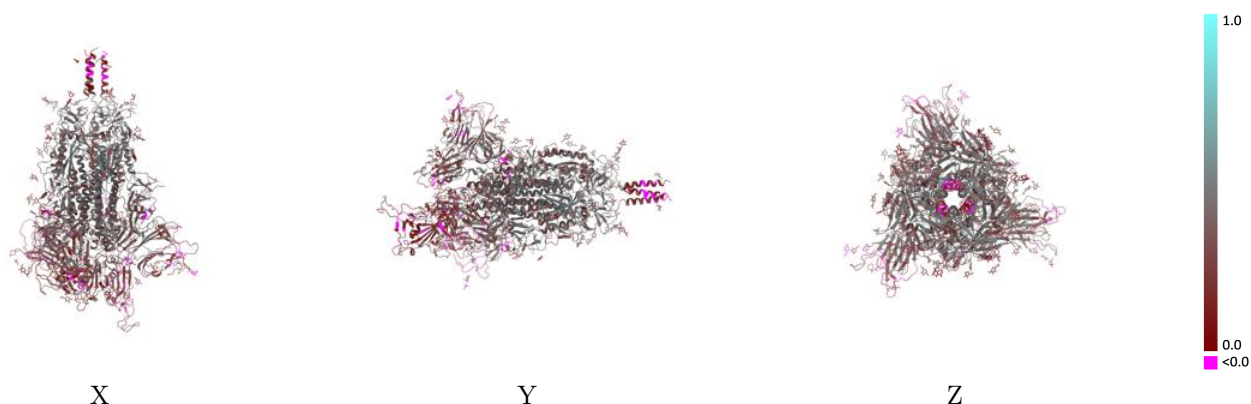
This section contains information regarding the fit between EMDB map EMD-24987 and PDB model 7SBS. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)



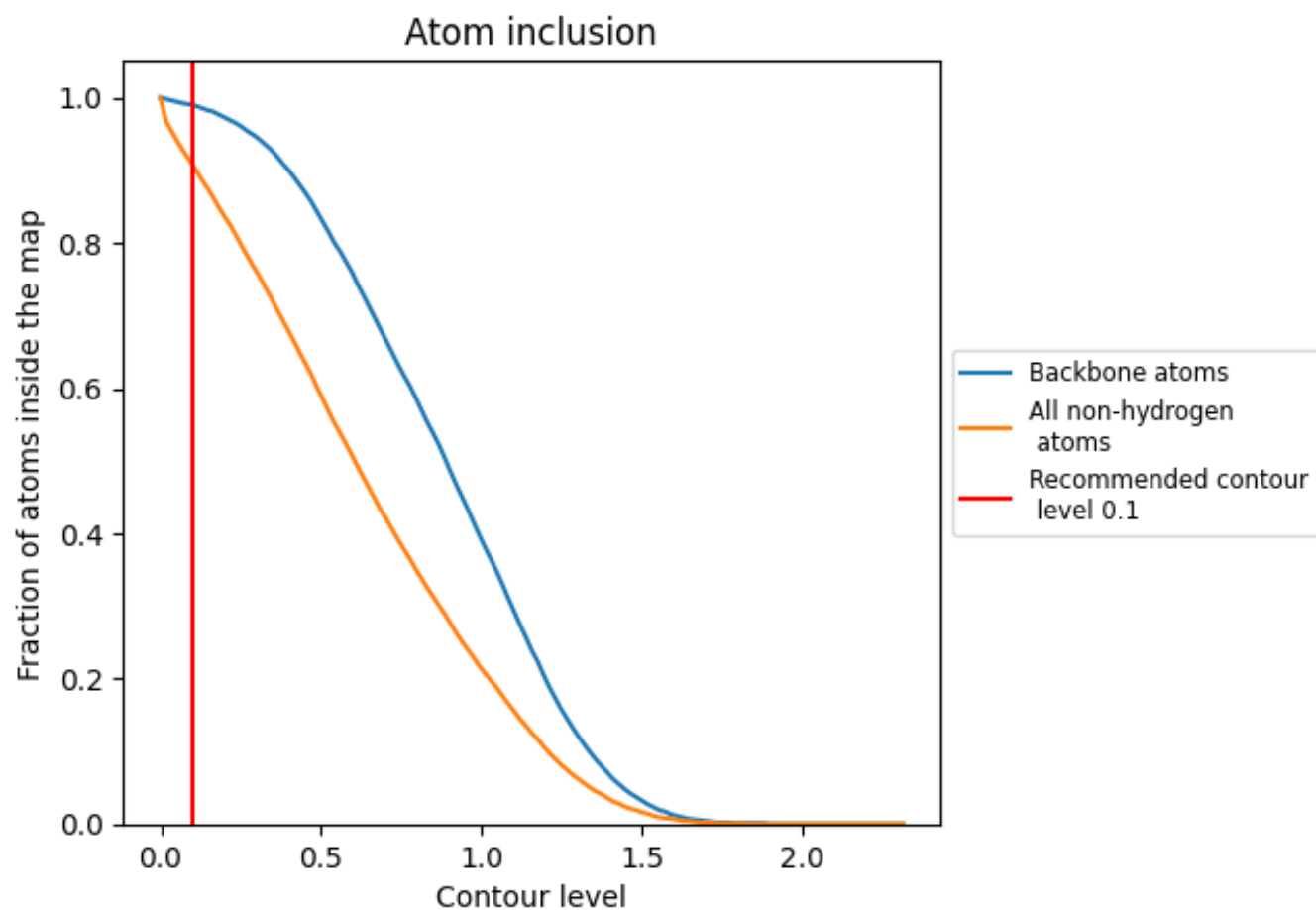
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 91% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.3310
A	 0.9010	 0.3100
B	 0.9090	 0.3420
C	 0.9120	 0.3500
D	 1.0000	 0.3960
E	 0.8930	 0.2470
F	 0.9290	 0.3210
G	 0.9640	 0.2830
H	 0.9210	 0.2940
I	 0.9740	 0.2920
J	 0.9740	 0.2370
K	 0.5000	 0.0080
L	 0.8930	 0.2340
M	 0.9640	 0.1410
N	 0.9290	 0.3200
O	 0.8570	 0.3900
P	 0.9290	 0.2860
Q	 0.8160	 0.2000
R	 0.9230	 0.3040
S	 0.9490	 0.2150
T	 0.5360	 0.0740
U	 0.9290	 0.2430
V	 0.9640	 0.2340
W	 0.8930	 0.3140
X	 0.9640	 0.2950
Y	 0.8570	 0.1890
Z	 0.8570	 0.2930
a	 0.9640	 0.3300
b	 0.8950	 0.2170
c	 0.9230	 0.2280
d	 0.9740	 0.3150
e	 0.5710	 0.1450

