



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:50 PM UTC

PDB ID : 7SBO / pdb_00007sbo
EMDB ID : EMD-24983
Title : One RBD-up 2 of pre-fusion SARS-CoV-2 Delta 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 : 4.30 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:

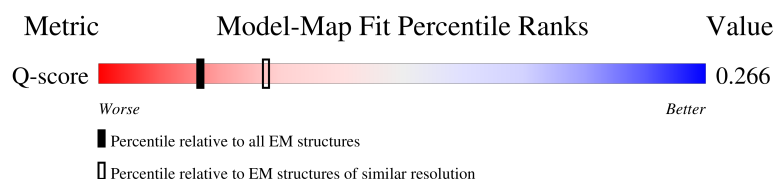
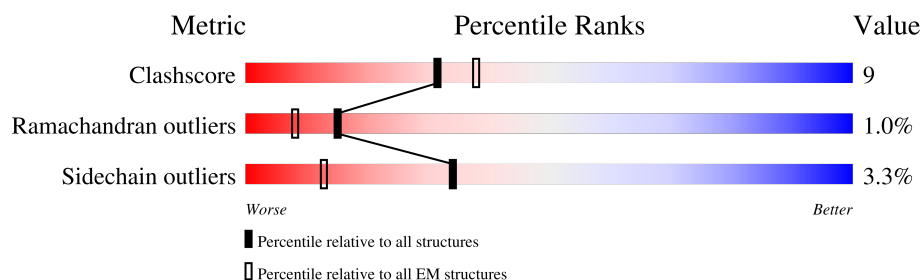
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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	1308	
1	B	1308	
1	C	1308	
2	D	3	

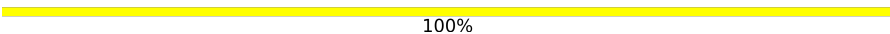
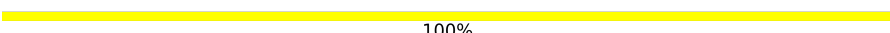
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Mol	Chain	Length	Quality of chain
2	J	3	100%
2	K	3	33% 67%
2	L	3	100%
2	T	3	100%
2	U	3	100%
2	V	3	100%
2	e	3	100%
2	f	3	33% 67%
2	g	3	67% 33%
3	E	2	100%
3	F	2	100%
3	G	2	100%
3	H	2	100%
3	M	2	50% 100%
3	N	2	100%
3	O	2	50% 50%
3	P	2	100%
3	Q	2	100%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

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Mol	Chain	Length	Quality of chain
3	c	2	 50% 50%
4	I	3	 100%
4	S	3	 33% 67%
4	d	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	M	1	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26900 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	1091	Total	C	N	O	S	0	0
			8536	5447	1426	1624	39		
1	B	1082	Total	C	N	O	S	0	0
			8480	5414	1418	1610	38		
1	C	1094	Total	C	N	O	S	0	0
			8568	5469	1433	1627	39		

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	156	GLY	ARG	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	950	ASN	ASP	variant	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
A	1286	GLN	-	expression tag	UNP P0DTC2
A	1287	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	19	ARG	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	GLU	deletion	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	156	GLY	ARG	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	950	ASN	ASP	variant	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
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

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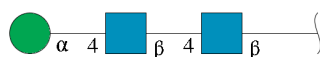
Chain	Residue	Modelled	Actual	Comment	Reference
B	1283	SER	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	PRO	-	expression tag	UNP P0DTC2
B	1286	GLN	-	expression tag	UNP P0DTC2
B	1287	PHE	-	expression tag	UNP P0DTC2
B	1288	GLU	-	expression tag	UNP P0DTC2
B	1289	LYS	-	expression 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	19	ARG	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	GLU	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	156	GLY	ARG	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	950	ASN	ASP	variant	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 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
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		
2	L	3	Total	C	N	O	0	0
			39	22	2	15		
2	T	3	Total	C	N	O	0	0
			39	22	2	15		
2	U	3	Total	C	N	O	0	0
			39	22	2	15		
2	V	3	Total	C	N	O	0	0
			39	22	2	15		
2	e	3	Total	C	N	O	0	0
			39	22	2	15		
2	f	3	Total	C	N	O	0	0
			39	22	2	15		
2	g	3	Total	C	N	O	0	0
			39	22	2	15		

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



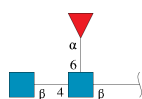
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		

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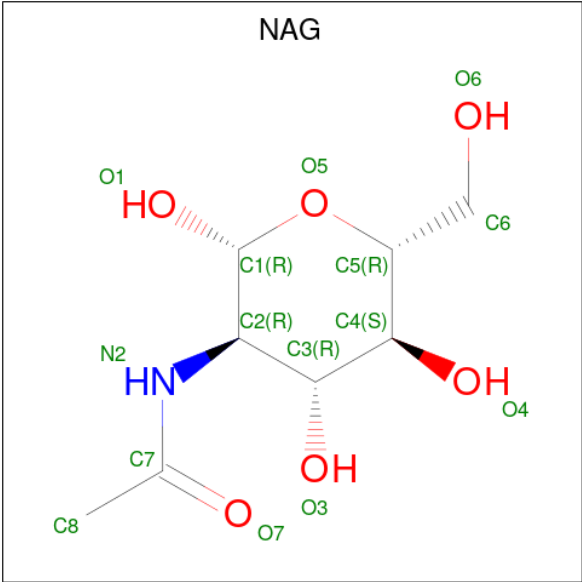
Mol	Chain	Residues	Atoms				AltConf	Trace
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	c	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	I	3	Total	C	N	O	0	0
			38	22	2	14		
4	S	3	Total	C	N	O	0	0
			38	22	2	14		
4	d	3	Total	C	N	O	0	0
			38	22	2	14		

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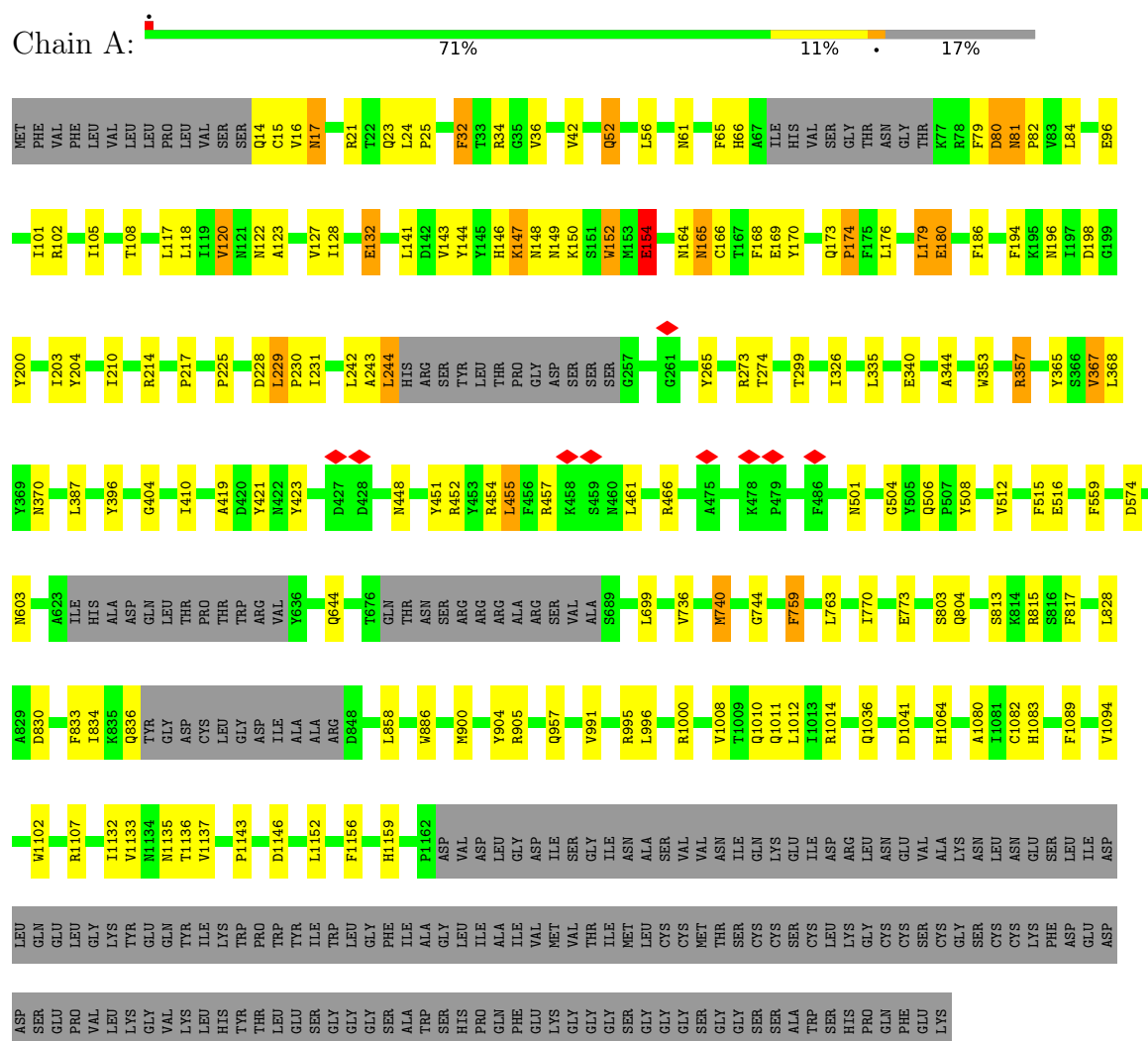
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C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

3 Residue-property plots

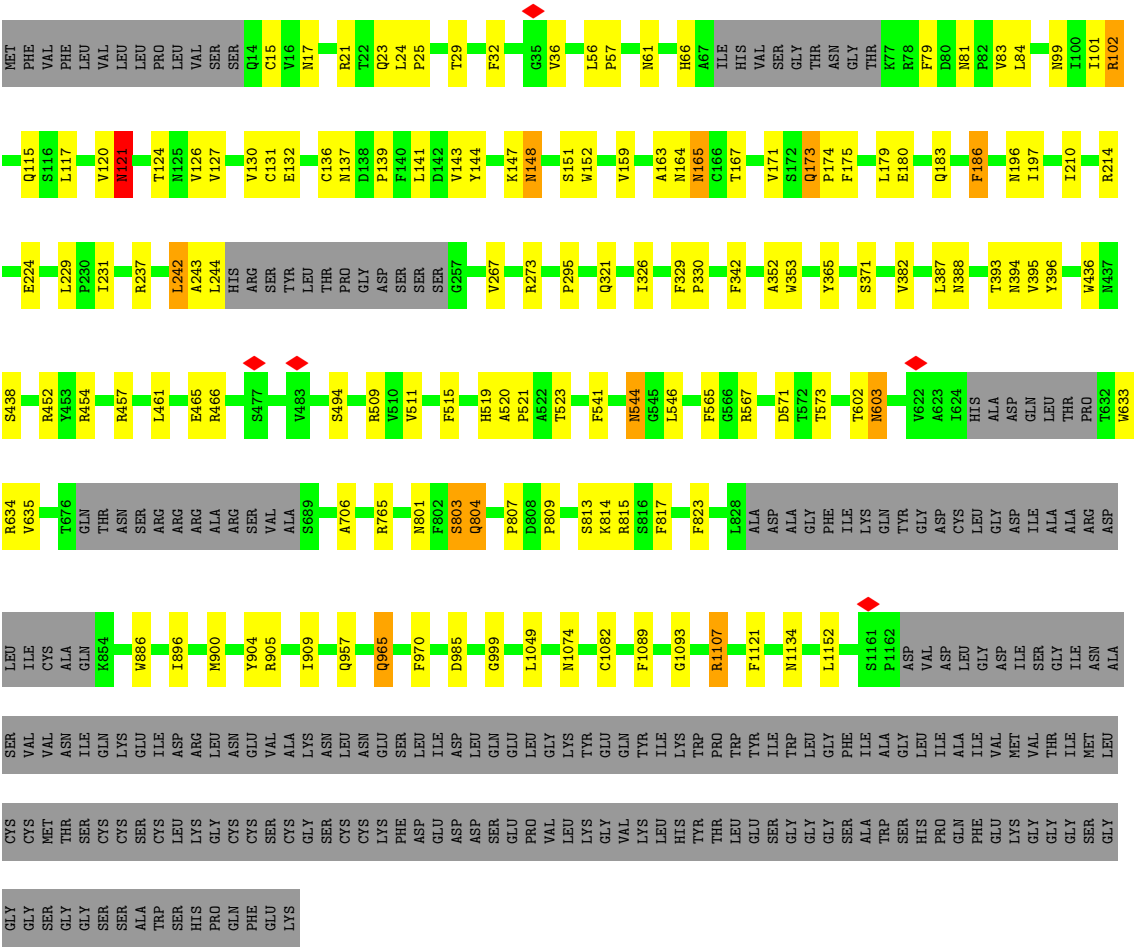
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

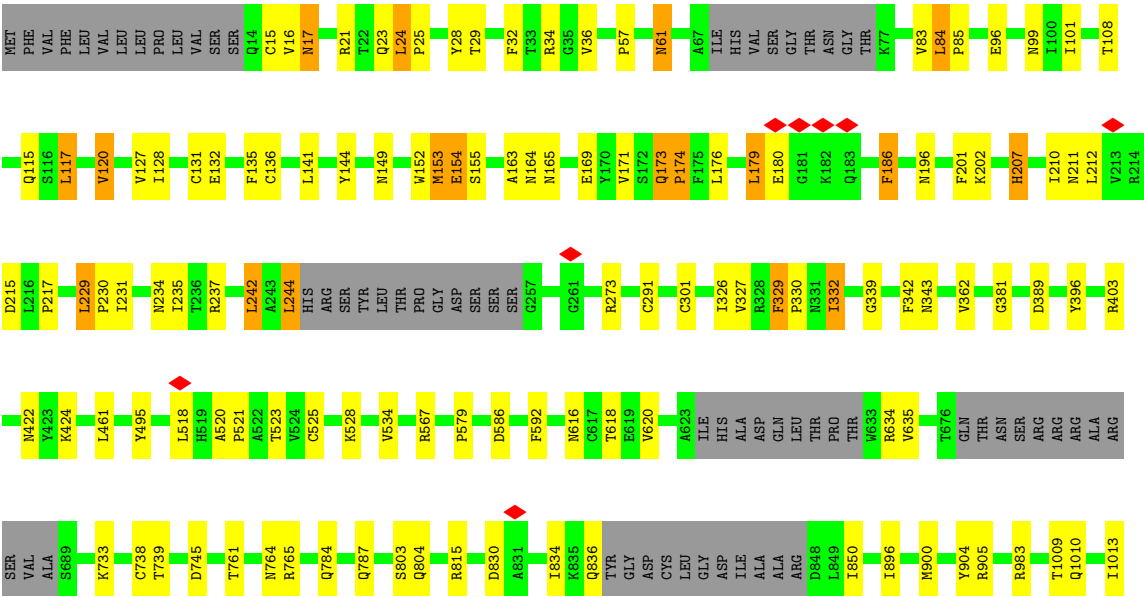


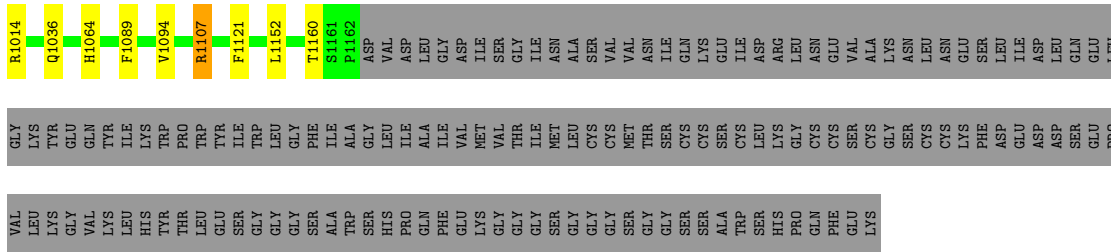
• Molecule 1: Spike glycoprotein





● Molecule 1: Spike glycoprotein





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



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



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



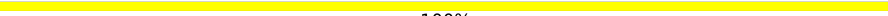
- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

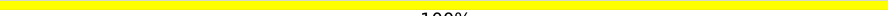


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

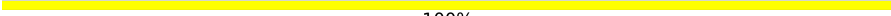
NAG1
NAG2
MAN3

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

Chain V:  100%

NAG1
NAG2
MAN3

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

Chain e:  100%

NAG1
NAG2
MAN3

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

Chain f:  33% 67%

NAG1
NAG2
MAN3

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

Chain g:  67% 33%

NAG1
NAG2
MAN3

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

Chain E:  100%

NAG1
NAG2

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

Chain F:  100%

NAG1
NAG2

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

Chain G:  100%

NAG1
NAG2

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

Chain H:  100%

NAG1
NAG2

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

Chain M:  50%
100%

♦
NAG1
NAG2

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

Chain N:  100%

NAG1
NAG2

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

Chain O:  50%  50%

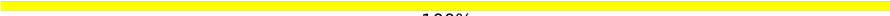
NAG1
NAG2

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

Chain P:  100%

NAG1
NAG2

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

Chain Q:  100%

NAG1
NAG2

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

Chain R:  100%

NAG1
NAG2

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

Chain W:  100%

NAG1
NAG2

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

Chain X:  100%

NAG1
NAG2

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

Chain Y:  50% 50%

NAG1
NAG2

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

Chain Z:  100%

NAG1
NAG2

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

Chain a:  100%

NAG1
NAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain c:  50% 50%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2
FUC3

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

Chain S:  33% 67%

MAG1
MAG2
FUC3

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

Chain d:  100%

MAG1
MAG2
FUC3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25370	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 ($e^-/\text{\AA}^2$)	51.48	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	2.412	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.047	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: NAG, MAN, 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	0.71	0/8731	1.28	23/11872 (0.2%)
1	B	0.73	3/8676 (0.0%)	1.30	26/11800 (0.2%)
1	C	0.72	0/8765	1.28	18/11919 (0.2%)
All	All	0.72	3/26172 (0.0%)	1.29	67/35591 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	330	PRO	C-N	-8.93	1.22	1.33
1	B	603	ASN	N-CA	-6.48	1.38	1.46
1	B	1074	ASN	C-N	5.44	1.41	1.33

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	ASN	N-CA-C	8.81	123.00	110.23
1	B	17	ASN	N-CA-C	8.79	122.97	110.23
1	A	17	ASN	N-CA-C	8.78	122.96	110.23
1	A	146	HIS	N-CA-C	8.47	124.19	112.93
1	B	214	ARG	N-CA-C	7.92	123.07	112.30
1	B	544	ASN	CA-CB-CG	7.67	120.27	112.60
1	A	759	PHE	CA-CB-CG	6.93	120.73	113.80
1	B	186	PHE	CA-CB-CG	6.83	120.63	113.80
1	B	137	ASN	N-CA-C	-6.78	103.58	110.97
1	B	602	THR	CA-C-N	6.73	129.97	120.28
1	B	602	THR	C-N-CA	6.73	129.97	120.28
1	B	137	ASN	CB-CA-C	-6.59	100.81	110.96
1	B	148	ASN	N-CA-C	-6.36	101.18	111.04
1	A	559	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	699	LEU	CA-C-N	6.07	129.29	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	LEU	C-N-CA	6.07	129.29	120.91
1	A	574	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	102	ARG	N-CA-C	5.96	121.42	114.62
1	B	519	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	C	1107	ARG	N-CA-C	5.86	119.96	112.34
1	A	1064	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	C	381	GLY	CA-C-N	5.83	128.63	122.11
1	C	381	GLY	C-N-CA	5.83	128.63	122.11
1	C	620	VAL	CA-C-N	5.75	126.14	119.47
1	C	620	VAL	C-N-CA	5.75	126.14	119.47
1	A	164	ASN	N-CA-C	5.73	119.75	112.87
1	A	830	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	815	ARG	N-CA-C	5.62	117.54	110.24
1	B	965	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	B	121	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	B	267	VAL	CA-C-N	5.55	125.42	121.65
1	B	267	VAL	C-N-CA	5.55	125.42	121.65
1	A	833	PHE	CA-CB-CG	5.54	119.33	113.80
1	B	321	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	B	329	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	66	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	B	985	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	1107	ARG	N-CA-C	5.46	119.42	112.87
1	B	15	CYS	N-CA-C	5.44	117.57	109.25
1	A	52	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	B	603	ASN	N-CA-CB	-5.37	101.95	110.22
1	A	452	ARG	N-CA-C	5.35	117.89	108.75
1	C	586	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	516	GLU	CB-CA-C	5.32	118.53	109.75
1	B	102	ARG	N-CA-C	5.32	120.68	114.62
1	A	80	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	66	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	C	207	HIS	CB-CG-CD2	-5.28	124.33	131.20
1	C	99	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	32	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	165	ASN	N-CA-C	-5.18	99.95	108.49
1	A	165	ASN	N-CA-C	-5.17	99.96	108.49
1	A	455	LEU	N-CA-C	5.17	116.99	111.36
1	C	389	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	544	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	A	1089	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	299	THR	N-CA-CB	5.11	117.40	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	ASN	N-CA-C	5.11	117.16	109.23
1	C	153	MET	CA-C-N	5.10	131.28	121.54
1	C	153	MET	C-N-CA	5.10	131.28	121.54
1	A	501	ASN	N-CA-C	5.07	117.25	110.35
1	C	787	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	137	ASN	CA-C-N	-5.04	116.84	123.34
1	B	137	ASN	C-N-CA	-5.04	116.84	123.34
1	C	745	ASP	CA-CB-CG	5.02	117.62	112.60
1	C	784	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	C	1064	HIS	CB-CG-CD2	-5.00	124.69	131.20

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	8536	0	8313	190	0
1	B	8480	0	8263	161	0
1	C	8568	0	8346	169	0
2	D	39	0	34	0	0
2	J	39	0	34	0	0
2	K	39	0	34	1	0
2	L	39	0	34	0	0
2	T	39	0	34	0	0
2	U	39	0	34	0	0
2	V	39	0	34	0	0
2	e	39	0	34	0	0
2	f	39	0	34	1	0
2	g	39	0	34	1	0
3	E	28	0	25	2	0
3	F	28	0	25	3	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	M	28	0	25	11	0
3	N	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	4	0
4	I	38	0	34	0	0
4	S	38	0	34	6	0
4	d	38	0	34	0	0
5	A	126	0	117	0	0
5	B	112	0	104	0	0
5	C	98	0	91	0	0
All	All	26900	0	26101	458	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 9.

All (458) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:LEU:HD21	1:B:1152:LEU:CD1	1.50	1.40
1:A:1152:LEU:CD2	1:B:1152:LEU:HD13	1.61	1.30
1:B:24:LEU:CG	1:B:25:PRO:HD2	1.65	1.26
1:C:34:ARG:NH2	1:C:217:PRO:HG2	1.50	1.24
1:A:423:TYR:OH	1:A:512:VAL:HG21	1.38	1.22
1:A:644:GLN:OE1	3:F:1:NAG:H82	1.36	1.20
1:A:904:TYR:CD1	1:C:1107:ARG:CZ	2.26	1.19
1:A:24:LEU:CD1	1:A:25:PRO:HD2	1.74	1.18
1:A:904:TYR:HD1	1:C:1107:ARG:CZ	1.60	1.15
1:C:804:GLN:NE2	3:c:1:NAG:H62	1.64	1.13
1:A:24:LEU:HD12	1:A:25:PRO:HD2	1.28	1.12
1:B:24:LEU:HG	1:B:25:PRO:CD	1.80	1.12
1:B:147:LYS:HE2	1:B:147:LYS:HA	1.29	1.12
1:B:57:PRO:HB3	1:B:273:ARG:NH1	1.63	1.12
1:B:342:PHE:CZ	1:B:511:VAL:HG11	1.86	1.09
1:A:1107:ARG:NE	1:B:904:TYR:CE2	2.23	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLN:CB	1:B:174:PRO:HD3	1.85	1.06
1:C:403:ARG:HG3	1:C:495:TYR:CE1	1.91	1.05
1:A:904:TYR:CD1	1:C:1107:ARG:NE	2.24	1.05
1:A:148:ASN:HB2	1:A:152:TRP:HE1	0.93	1.05
1:B:173:GLN:HB2	1:B:174:PRO:CD	1.86	1.04
1:A:1107:ARG:CD	1:B:904:TYR:CE2	2.40	1.04
1:C:1010:GLN:HB3	1:C:1014:ARG:NH2	1.74	1.03
1:B:173:GLN:CB	1:B:174:PRO:CD	2.37	1.02
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.38	1.02
1:A:173:GLN:HB2	1:A:174:PRO:HD3	1.41	1.01
1:C:57:PRO:HB3	1:C:273:ARG:NH1	1.76	1.01
1:A:357:ARG:HG3	1:A:396:TYR:CE1	1.95	1.01
1:A:200:TYR:HD2	1:A:228:ASP:OD1	1.44	1.00
1:C:329:PHE:HB3	1:C:330:PRO:CD	1.92	0.99
1:B:115:GLN:HE21	3:M:1:NAG:H83	1.23	0.98
1:A:24:LEU:CG	1:A:25:PRO:HD2	1.93	0.98
1:B:141:LEU:HD23	1:B:144:TYR:OH	1.62	0.98
1:A:148:ASN:HB2	1:A:152:TRP:NE1	1.78	0.98
1:A:904:TYR:CE1	1:C:1107:ARG:NE	2.32	0.98
1:A:900:MET:HG3	1:A:904:TYR:HE2	1.30	0.97
1:A:904:TYR:HD1	1:C:1107:ARG:NH1	1.61	0.97
1:A:194:PHE:CE1	1:A:203:ILE:HD13	1.99	0.97
1:A:904:TYR:CD1	1:C:1107:ARG:HD3	1.99	0.97
1:C:1010:GLN:HB3	1:C:1014:ARG:HH22	1.25	0.96
1:B:57:PRO:HB3	1:B:273:ARG:HH12	1.15	0.95
1:A:423:TYR:HH	1:A:512:VAL:HG21	1.28	0.94
1:B:115:GLN:NE2	3:M:1:NAG:H83	1.81	0.93
1:B:1152:LEU:HD21	1:C:1152:LEU:HD13	1.50	0.93
1:A:1107:ARG:NE	1:B:904:TYR:HE2	1.64	0.93
1:A:904:TYR:CD1	1:C:1107:ARG:CD	2.51	0.93
1:B:173:GLN:HB3	1:B:174:PRO:HD3	1.46	0.93
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	2.04	0.92
1:A:1107:ARG:CD	1:B:904:TYR:HE2	1.79	0.91
1:A:904:TYR:CE1	1:C:1107:ARG:CD	2.53	0.91
1:A:1107:ARG:HD3	1:B:904:TYR:CD2	2.06	0.91
1:C:173:GLN:HB2	1:C:174:PRO:HD3	1.52	0.91
1:B:896:ILE:HD11	1:B:904:TYR:CE1	2.07	0.90
1:A:24:LEU:HD12	1:A:25:PRO:CD	2.02	0.90
1:C:34:ARG:HH21	1:C:217:PRO:HG2	1.13	0.90
1:A:21:ARG:CG	1:A:79:PHE:CZ	2.53	0.90
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:900:MET:O	1:C:904:TYR:CD2	2.24	0.89
1:C:327:VAL:CG1	1:C:329:PHE:HE2	1.86	0.88
1:C:900:MET:HG3	1:C:904:TYR:HE2	1.38	0.88
1:B:342:PHE:CE2	1:B:511:VAL:HG11	2.08	0.88
1:B:115:GLN:CG	3:M:1:NAG:H82	2.04	0.88
1:C:327:VAL:CG1	1:C:329:PHE:CE2	2.58	0.86
1:A:194:PHE:CE1	1:A:203:ILE:CD1	2.58	0.86
3:E:1:NAG:H62	3:E:2:NAG:HN2	1.39	0.86
1:A:1152:LEU:HD13	1:C:1152:LEU:HD21	1.56	0.86
1:B:396:TYR:OH	1:C:230:PRO:HB3	1.76	0.85
1:A:1152:LEU:HD13	1:C:1152:LEU:CD2	2.07	0.85
1:A:1008:VAL:O	1:A:1012:LEU:HG	1.77	0.85
1:A:200:TYR:CD2	1:A:228:ASP:OD1	2.30	0.84
1:B:896:ILE:HD11	1:B:904:TYR:HE1	1.42	0.84
1:C:21:ARG:HE	1:C:21:ARG:HA	1.42	0.84
1:B:115:GLN:HG3	3:M:1:NAG:H82	1.60	0.84
1:A:900:MET:HG3	1:A:904:TYR:CE2	2.12	0.83
1:A:21:ARG:HG3	1:A:79:PHE:CZ	2.14	0.83
1:A:14:GLN:NE2	1:A:147:LYS:HE3	1.93	0.83
1:B:148:ASN:OD1	1:B:152:TRP:CE2	2.32	0.83
1:A:176:LEU:HD12	1:A:176:LEU:O	1.79	0.82
1:A:905:ARG:NH1	1:A:1036:GLN:HB2	1.94	0.82
1:A:904:TYR:CD1	1:C:1107:ARG:NH1	2.44	0.82
1:C:101:ILE:CD1	1:C:242:LEU:HD23	2.10	0.82
1:C:424:LYS:HB2	1:C:461:LEU:HD11	1.61	0.82
1:C:115:GLN:HA	1:C:132:GLU:HG3	1.61	0.81
1:B:886:TRP:CE3	1:B:905:ARG:NH1	2.49	0.81
1:C:461:LEU:HD12	1:C:461:LEU:O	1.80	0.81
1:A:1107:ARG:NE	1:B:904:TYR:CD2	2.48	0.81
1:C:291:CYS:HG	1:C:301:CYS:HG	1.18	0.81
1:B:395:VAL:HG22	1:B:515:PHE:HB3	1.61	0.81
1:A:24:LEU:HG	1:A:25:PRO:HD2	1.62	0.80
1:C:176:LEU:HD12	1:C:176:LEU:O	1.80	0.80
1:B:21:ARG:HE	1:B:21:ARG:HA	1.47	0.80
1:C:144:TYR:CD2	1:C:152:TRP:HB3	2.16	0.80
1:B:461:LEU:HD13	1:B:465:GLU:O	1.82	0.80
1:C:329:PHE:O	1:C:579:PRO:HG2	1.81	0.80
1:C:804:GLN:HE21	3:c:1:NAG:H62	1.40	0.80
1:B:141:LEU:CD2	1:B:144:TYR:OH	2.30	0.80
1:B:173:GLN:HB2	1:B:174:PRO:HD2	1.62	0.79
1:C:900:MET:HG3	1:C:904:TYR:CE2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:LEU:HD11	1:C:1152:LEU:HD11	1.64	0.79
1:B:886:TRP:CZ3	1:B:905:ARG:NH1	2.50	0.78
1:B:21:ARG:HA	1:B:21:ARG:NE	1.99	0.78
1:B:141:LEU:HD23	1:B:144:TYR:CZ	2.19	0.78
1:B:57:PRO:CB	1:B:273:ARG:NH1	2.45	0.77
1:C:34:ARG:NH2	1:C:217:PRO:CG	2.42	0.77
1:A:644:GLN:OE1	3:F:1:NAG:C8	2.27	0.77
1:A:1152:LEU:CD1	1:C:1152:LEU:HD11	2.15	0.76
1:C:905:ARG:NH1	1:C:1036:GLN:HB2	2.00	0.76
1:C:403:ARG:HE	1:C:495:TYR:HD1	1.33	0.76
1:A:34:ARG:NH2	1:A:217:PRO:HG2	2.01	0.76
1:C:424:LYS:HB2	1:C:461:LEU:CD1	2.15	0.76
1:B:173:GLN:HB2	1:B:174:PRO:HD3	1.54	0.76
1:C:24:LEU:HB3	1:C:25:PRO:HD2	1.68	0.76
1:C:201:PHE:CD1	1:C:229:LEU:HD21	2.20	0.76
1:B:167:THR:HB	3:M:1:NAG:H81	1.68	0.75
1:A:1107:ARG:CD	1:B:904:TYR:CD2	2.66	0.75
1:B:141:LEU:HD23	1:B:144:TYR:CE2	2.20	0.75
1:A:904:TYR:CE1	1:C:1107:ARG:HD3	2.19	0.75
1:A:194:PHE:HE1	1:A:203:ILE:HD13	1.50	0.75
1:B:24:LEU:HG	1:B:25:PRO:HD2	0.83	0.75
1:C:15:CYS:O	1:C:17:ASN:N	2.20	0.75
1:B:365:TYR:HB2	1:B:388:ASN:OD1	1.86	0.74
3:E:1:NAG:H62	3:E:2:NAG:N2	2.02	0.74
1:A:905:ARG:HH11	1:A:1036:GLN:HB2	1.50	0.74
1:A:173:GLN:CB	1:A:174:PRO:HD3	2.16	0.74
1:C:120:VAL:HG11	1:C:154:GLU:OE2	1.86	0.74
1:A:1156:PHE:HE2	1:B:1152:LEU:HD12	1.53	0.73
1:B:815:ARG:NH1	1:B:823:PHE:CG	2.56	0.73
1:B:454:ARG:HD3	1:B:457:ARG:HG2	1.69	0.73
1:B:23:GLN:OE1	1:B:23:GLN:N	2.19	0.73
1:C:896:ILE:HD11	1:C:904:TYR:CE2	2.24	0.73
1:C:900:MET:O	1:C:904:TYR:HD2	1.68	0.73
1:A:1010:GLN:O	1:A:1014:ARG:HG3	1.88	0.73
1:B:342:PHE:CE2	1:B:511:VAL:CG1	2.72	0.72
1:A:15:CYS:O	1:A:17:ASN:N	2.23	0.72
1:A:644:GLN:CD	3:F:1:NAG:H82	2.14	0.72
1:A:42:VAL:HG11	1:C:567:ARG:HG3	1.71	0.72
1:B:147:LYS:HE2	1:B:147:LYS:CA	2.13	0.72
1:C:23:GLN:OE1	1:C:23:GLN:N	2.18	0.71
1:A:423:TYR:CZ	1:A:512:VAL:HG21	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ILE:CD1	1:A:1012:LEU:HD23	2.19	0.71
1:B:1082:CYS:HB2	1:B:1134:ASN:OD1	1.90	0.71
1:A:21:ARG:HG2	1:A:79:PHE:CZ	2.26	0.71
1:C:186:PHE:HB3	1:C:211:ASN:OD1	1.90	0.71
1:A:506:GLN:O	1:A:508:TYR:CD2	2.44	0.71
1:B:342:PHE:HE2	1:B:511:VAL:HB	1.53	0.71
1:B:365:TYR:CG	1:B:387:LEU:HB3	2.26	0.70
1:A:143:VAL:HG13	1:A:243:ALA:HB1	1.72	0.70
1:B:342:PHE:CZ	1:B:511:VAL:CG1	2.69	0.70
1:A:1107:ARG:CZ	1:B:904:TYR:CD2	2.74	0.70
1:A:1156:PHE:CE2	1:B:1152:LEU:HD12	2.26	0.69
1:C:173:GLN:CB	1:C:174:PRO:HD3	2.21	0.69
1:A:23:GLN:OE1	1:A:23:GLN:N	2.21	0.69
1:B:342:PHE:CE2	1:B:511:VAL:CB	2.76	0.69
1:B:461:LEU:HB2	1:B:465:GLU:OE2	1.93	0.69
1:A:804:GLN:NE2	1:A:817:PHE:CB	2.56	0.68
1:A:230:PRO:HB2	1:C:396:TYR:OH	1.93	0.68
1:C:1009:THR:O	1:C:1013:ILE:HG13	1.93	0.68
1:C:21:ARG:HA	1:C:21:ARG:NE	2.09	0.68
1:A:423:TYR:OH	1:A:512:VAL:CG2	2.31	0.68
1:B:126:VAL:CG2	1:B:175:PHE:HB2	2.24	0.68
1:C:327:VAL:HG11	1:C:329:PHE:HE2	1.55	0.68
1:C:761:THR:O	1:C:765:ARG:HG3	1.94	0.68
1:A:1156:PHE:HE2	1:B:1152:LEU:CD1	2.05	0.67
1:B:139:PRO:HB2	1:B:159:VAL:HG23	1.74	0.67
1:A:904:TYR:HE1	1:C:1107:ARG:CD	2.07	0.67
1:B:438:SER:CB	1:B:509:ARG:HG3	2.25	0.67
1:C:327:VAL:HG12	1:C:329:PHE:CE2	2.28	0.67
1:A:904:TYR:HE1	1:C:1107:ARG:NE	1.91	0.67
1:C:905:ARG:HH11	1:C:1036:GLN:HB2	1.58	0.67
1:A:194:PHE:HE1	1:A:203:ILE:CD1	2.05	0.67
1:C:201:PHE:HD1	1:C:229:LEU:CD2	2.08	0.67
1:B:115:GLN:CG	3:M:1:NAG:C8	2.73	0.67
1:B:815:ARG:NH1	1:B:823:PHE:CD2	2.63	0.66
1:C:24:LEU:CB	1:C:25:PRO:HD2	2.25	0.66
1:B:813:SER:C	1:B:815:ARG:H	2.02	0.66
1:B:126:VAL:HG21	1:B:175:PHE:HB2	1.77	0.66
1:B:546:LEU:HD12	1:B:565:PHE:CE1	2.30	0.66
1:A:770:ILE:HD11	1:A:1012:LEU:CD2	2.20	0.66
1:A:42:VAL:CG1	1:C:567:ARG:HG3	2.26	0.65
1:C:29:THR:O	1:C:61:ASN:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASN:CB	1:A:152:TRP:HE1	1.88	0.65
1:B:342:PHE:CE2	1:B:511:VAL:HB	2.30	0.65
1:A:904:TYR:HD1	1:C:1107:ARG:NE	1.75	0.65
4:S:1:NAG:H62	4:S:2:NAG:C7	2.26	0.65
1:A:419:ALA:HA	1:A:423:TYR:O	1.97	0.65
1:C:84:LEU:O	1:C:237:ARG:HG2	1.97	0.64
1:A:14:GLN:HE22	1:A:147:LYS:HE3	1.61	0.64
1:A:900:MET:O	1:A:904:TYR:CD2	2.50	0.64
1:C:144:TYR:HD2	1:C:152:TRP:HB3	1.59	0.64
1:C:804:GLN:HE22	3:c:1:NAG:H62	1.60	0.64
1:C:101:ILE:HD12	1:C:242:LEU:HD23	1.80	0.64
1:A:506:GLN:O	1:A:508:TYR:CE2	2.51	0.63
1:A:904:TYR:HD1	1:C:1107:ARG:CD	2.02	0.63
1:B:126:VAL:CG2	1:B:175:PHE:CB	2.76	0.63
1:C:108:THR:HG21	1:C:234:ASN:HB3	1.80	0.63
1:A:194:PHE:CD1	1:A:203:ILE:CD1	2.82	0.63
1:B:24:LEU:CG	1:B:25:PRO:CD	2.54	0.63
1:A:200:TYR:CD2	1:A:228:ASP:CG	2.77	0.62
1:A:1152:LEU:HD21	1:B:1152:LEU:HD13	0.70	0.62
1:B:546:LEU:CD1	1:B:565:PHE:CE1	2.82	0.62
1:A:957:GLN:CD	1:B:765:ARG:NH1	2.57	0.62
1:A:1152:LEU:HD11	1:B:1152:LEU:HD11	1.81	0.62
1:A:1156:PHE:CE2	1:B:1152:LEU:CD1	2.81	0.62
1:B:801:ASN:OD1	1:B:803:SER:HB2	2.00	0.62
4:S:1:NAG:H62	4:S:2:NAG:C8	2.29	0.62
1:B:454:ARG:HD3	1:B:457:ARG:CG	2.29	0.62
1:A:886:TRP:HZ3	1:A:905:ARG:HD3	1.65	0.61
1:A:340:GLU:O	1:A:344:ALA:HB2	2.00	0.61
1:C:424:LYS:CB	1:C:461:LEU:CD1	2.79	0.61
1:C:634:ARG:HG2	1:C:634:ARG:O	2.00	0.61
1:B:163:ALA:O	1:B:165:ASN:N	2.33	0.61
1:C:403:ARG:HG3	1:C:495:TYR:HE1	1.58	0.61
4:S:1:NAG:C6	4:S:2:NAG:C7	2.78	0.60
1:C:131:CYS:HB3	1:C:163:ALA:CB	2.32	0.60
1:C:291:CYS:SG	1:C:301:CYS:CB	2.89	0.60
1:A:1107:ARG:HE	1:B:904:TYR:HE2	1.49	0.60
1:A:1152:LEU:CD2	1:B:1152:LEU:CD1	2.45	0.60
1:C:201:PHE:CD1	1:C:229:LEU:CD2	2.84	0.60
1:A:804:GLN:HE21	1:A:804:GLN:HA	1.67	0.59
1:B:382:VAL:HG12	1:C:983:ARG:HB3	1.84	0.59
1:B:126:VAL:HG21	1:B:175:PHE:CB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:O	1:A:143:VAL:HG23	2.01	0.59
1:A:804:GLN:NE2	1:A:817:PHE:HB2	2.18	0.59
1:A:1107:ARG:CG	1:B:904:TYR:HE2	2.14	0.59
1:B:143:VAL:HG23	1:B:143:VAL:O	2.03	0.59
1:C:201:PHE:HD1	1:C:229:LEU:HD21	1.63	0.59
1:A:813:SER:HB2	1:A:815:ARG:NH1	2.18	0.59
1:A:42:VAL:HG11	1:C:567:ARG:CG	2.32	0.59
1:A:1107:ARG:CZ	1:B:904:TYR:HD2	2.16	0.58
1:B:115:GLN:NE2	3:M:1:NAG:C8	2.63	0.58
1:B:147:LYS:HA	1:B:147:LYS:CE	2.16	0.58
1:C:424:LYS:CB	1:C:461:LEU:HD11	2.33	0.58
1:C:330:PRO:HG3	1:C:525:CYS:SG	2.44	0.58
1:C:1010:GLN:CB	1:C:1014:ARG:HH22	2.10	0.58
1:A:24:LEU:HG	1:A:25:PRO:CD	2.32	0.58
1:A:176:LEU:HD12	1:A:176:LEU:C	2.29	0.58
1:A:804:GLN:NE2	1:A:804:GLN:HA	2.19	0.57
1:A:230:PRO:CB	1:C:396:TYR:OH	2.52	0.57
1:A:410:ILE:HG23	1:A:423:TYR:CE2	2.39	0.57
1:A:1152:LEU:CD1	1:C:1152:LEU:HD21	2.32	0.57
1:C:212:LEU:HD23	1:C:215:ASP:O	2.04	0.57
1:A:828:LEU:H	1:A:828:LEU:HD12	1.69	0.57
1:C:34:ARG:CZ	1:C:217:PRO:HG2	2.29	0.57
1:C:84:LEU:O	1:C:237:ARG:CG	2.51	0.57
1:A:353:TRP:CZ3	1:A:466:ARG:NH2	2.73	0.57
1:A:357:ARG:HG3	1:A:396:TYR:CD1	2.39	0.57
1:B:144:TYR:HB2	1:B:151:SER:HA	1.87	0.57
1:C:422:ASN:C	1:C:461:LEU:HD21	2.28	0.57
1:A:804:GLN:HE21	1:A:817:PHE:CB	2.18	0.57
2:K:1:NAG:O4	2:K:2:NAG:O7	2.22	0.57
2:f:1:NAG:O4	2:f:2:NAG:O7	2.22	0.57
1:A:900:MET:O	1:A:904:TYR:HD2	1.87	0.57
1:C:461:LEU:HD12	1:C:461:LEU:C	2.30	0.57
1:B:144:TYR:CB	1:B:152:TRP:H	2.17	0.56
1:B:452:ARG:HG2	1:B:494:SER:HB3	1.86	0.56
1:C:804:GLN:NE2	3:c:1:NAG:C6	2.54	0.56
1:A:122:ASN:OD1	1:A:123:ALA:N	2.39	0.56
1:A:148:ASN:HD22	1:A:152:TRP:HZ2	1.54	0.56
1:B:957:GLN:HG2	1:C:765:ARG:HH12	1.69	0.56
1:C:291:CYS:SG	1:C:301:CYS:HB2	2.46	0.56
1:B:21:ARG:HE	1:B:21:ARG:CA	2.16	0.55
1:C:131:CYS:CB	1:C:163:ALA:CB	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ILE:CD1	1:B:904:TYR:CE1	2.85	0.55
1:A:957:GLN:HG2	1:B:765:ARG:HH12	1.71	0.55
1:C:900:MET:O	1:C:904:TYR:CE2	2.59	0.55
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.06	0.55
1:A:120:VAL:HG21	1:A:154:GLU:HG3	1.88	0.55
1:B:124:THR:O	1:B:173:GLN:O	2.24	0.55
1:A:128:ILE:HG21	1:A:229:LEU:HD13	1.89	0.54
1:A:804:GLN:NE2	1:A:817:PHE:CG	2.75	0.54
1:C:329:PHE:CB	1:C:330:PRO:CD	2.72	0.54
1:C:329:PHE:CZ	1:C:528:LYS:HB2	2.42	0.54
1:A:506:GLN:O	1:A:508:TYR:HD2	1.91	0.54
1:B:101:ILE:CD1	1:B:242:LEU:HD23	2.37	0.54
1:C:128:ILE:HG21	1:C:229:LEU:HD13	1.89	0.54
1:A:1094:VAL:HB	1:B:904:TYR:OH	2.07	0.54
1:B:173:GLN:HB3	1:B:174:PRO:CD	2.22	0.54
1:B:438:SER:HB3	1:B:509:ARG:HG3	1.89	0.53
1:C:34:ARG:HH21	1:C:217:PRO:CG	2.03	0.53
1:C:616:ASN:OD1	1:C:618:THR:HG23	2.08	0.53
1:A:42:VAL:HG11	1:C:567:ARG:CD	2.38	0.53
1:A:21:ARG:NE	1:A:21:ARG:HA	2.23	0.53
1:C:24:LEU:CB	1:C:25:PRO:CD	2.86	0.53
1:C:57:PRO:HB3	1:C:273:ARG:HH12	1.69	0.53
1:A:21:ARG:HG3	1:A:79:PHE:CE2	2.44	0.53
1:A:1152:LEU:CD1	1:C:1152:LEU:CD1	2.86	0.53
1:C:403:ARG:HG3	1:C:495:TYR:CD1	2.42	0.53
1:A:204:TYR:CD2	1:A:225:PRO:HA	2.43	0.53
1:B:396:TYR:OH	1:C:230:PRO:CB	2.53	0.53
1:B:148:ASN:OD1	1:B:152:TRP:NE1	2.42	0.52
1:A:421:TYR:CD1	1:A:457:ARG:HB2	2.45	0.52
1:A:454:ARG:HD3	1:A:457:ARG:HD3	1.90	0.52
1:B:970:PHE:CD1	1:B:999:GLY:HA3	2.45	0.52
1:C:850:ILE:HD12	1:C:850:ILE:H	1.74	0.52
1:A:423:TYR:HH	1:A:512:VAL:CG2	2.13	0.52
1:A:904:TYR:HE1	1:C:1107:ARG:HG2	1.75	0.52
1:B:24:LEU:CD1	1:B:25:PRO:HD2	2.36	0.52
1:C:179:LEU:HD23	1:C:180:GLU:H	1.75	0.52
1:C:201:PHE:CE1	1:C:229:LEU:HD21	2.45	0.52
1:B:148:ASN:OD1	1:B:152:TRP:CZ2	2.63	0.52
1:A:244:LEU:C	1:A:244:LEU:HD12	2.34	0.51
1:B:167:THR:CB	3:M:1:NAG:H81	2.38	0.51
1:A:141:LEU:HB3	1:A:144:TYR:HE2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:PRO:HB3	1:B:273:ARG:CZ	2.34	0.51
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.91	0.51
1:B:115:GLN:HG2	3:M:1:NAG:C8	2.39	0.51
1:B:546:LEU:C	1:B:546:LEU:HD23	2.36	0.51
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.92	0.51
1:A:194:PHE:CE1	1:A:203:ILE:HD11	2.41	0.51
1:A:759:PHE:O	1:A:763:LEU:HG	2.10	0.51
1:B:436:TRP:CE2	1:B:509:ARG:HB2	2.45	0.51
1:B:1093:GLY:H	1:B:1107:ARG:NH2	2.09	0.51
1:C:21:ARG:HE	1:C:21:ARG:CA	2.18	0.51
1:C:201:PHE:HB3	1:C:229:LEU:HG	1.92	0.51
4:S:1:NAG:C6	4:S:2:NAG:C8	2.88	0.51
1:C:141:LEU:CD2	1:C:154:GLU:HA	2.41	0.51
1:A:404:GLY:HA3	1:A:508:TYR:CE2	2.45	0.50
1:A:957:GLN:CD	1:B:765:ARG:HH11	2.17	0.50
1:B:342:PHE:CD2	1:B:511:VAL:HG21	2.45	0.50
1:C:403:ARG:CG	1:C:495:TYR:CE1	2.80	0.50
1:B:83:VAL:CG1	1:B:237:ARG:HD3	2.42	0.50
1:C:131:CYS:HB3	1:C:163:ALA:HB3	1.92	0.50
1:B:121:ASN:OD1	1:B:175:PHE:HB3	2.12	0.50
1:A:957:GLN:CG	1:B:765:ARG:HH12	2.24	0.50
1:A:991:VAL:O	1:A:995:ARG:HG3	2.12	0.50
1:C:131:CYS:HB3	1:C:163:ALA:HB1	1.93	0.50
1:C:186:PHE:CD1	1:C:211:ASN:OD1	2.64	0.49
1:A:1107:ARG:CG	1:B:904:TYR:CE2	2.93	0.49
1:B:634:ARG:NH1	1:B:634:ARG:HB3	2.28	0.49
1:A:194:PHE:CD1	1:A:203:ILE:HD11	2.47	0.49
1:A:214:ARG:HG3	1:A:214:ARG:O	2.12	0.49
1:B:143:VAL:HG13	1:B:243:ALA:HB1	1.94	0.49
1:B:130:VAL:HB	1:B:167:THR:HG23	1.94	0.49
1:A:23:GLN:H	1:A:23:GLN:CD	2.16	0.49
1:B:813:SER:C	1:B:815:ARG:N	2.70	0.49
1:C:326:ILE:HD11	1:C:534:VAL:HG22	1.94	0.49
1:A:21:ARG:HB2	1:A:79:PHE:CE1	2.47	0.49
1:A:421:TYR:CE2	1:A:455:LEU:O	2.65	0.49
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.95	0.49
1:A:1107:ARG:HG2	1:B:904:TYR:HE2	1.77	0.49
1:A:1107:ARG:NH1	1:B:904:TYR:HD2	2.11	0.49
1:C:329:PHE:CE2	1:C:528:LYS:CB	2.96	0.49
1:B:21:ARG:HB2	1:B:79:PHE:CZ	2.48	0.48
1:A:81:ASN:H	1:A:82:PRO:HD3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:HD23	1:A:180:GLU:H	1.77	0.48
1:C:132:GLU:N	1:C:163:ALA:HB1	2.29	0.48
1:A:904:TYR:HE1	1:C:1107:ARG:CG	2.25	0.48
1:C:131:CYS:CB	1:C:163:ALA:HB3	2.44	0.48
1:C:896:ILE:HD11	1:C:904:TYR:HE2	1.75	0.48
1:C:83:VAL:HG12	1:C:237:ARG:HD3	1.96	0.47
1:C:329:PHE:HB3	1:C:330:PRO:HD3	1.88	0.47
1:B:99:ASN:O	1:B:102:ARG:NE	2.44	0.47
1:C:330:PRO:CG	1:C:525:CYS:SG	3.03	0.47
1:A:904:TYR:OH	1:C:1094:VAL:CG2	2.62	0.47
1:C:329:PHE:CE2	1:C:528:LYS:HB3	2.49	0.47
1:B:352:ALA:HA	1:B:466:ARG:HD2	1.96	0.47
1:B:807:PRO:O	1:B:809:PRO:HD3	2.14	0.47
1:C:28:TYR:HD1	1:C:61:ASN:CB	2.27	0.47
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.97	0.47
1:C:131:CYS:CB	1:C:163:ALA:HB1	2.45	0.47
1:A:804:GLN:HE21	1:A:817:PHE:HB3	1.80	0.47
1:B:295:PRO:HG3	1:B:633:TRP:CE3	2.51	0.47
1:B:957:GLN:CG	1:C:765:ARG:HH12	2.28	0.47
1:A:34:ARG:CZ	1:A:217:PRO:HG2	2.45	0.46
1:A:1107:ARG:HG2	1:B:904:TYR:CE2	2.50	0.46
1:C:24:LEU:HB3	1:C:25:PRO:CD	2.38	0.46
1:B:957:GLN:CD	1:C:765:ARG:NH1	2.73	0.46
1:A:353:TRP:CE3	1:A:466:ARG:NH2	2.84	0.46
1:B:126:VAL:HG23	1:B:175:PHE:HB2	1.96	0.46
1:C:153:MET:C	1:C:155:SER:H	2.24	0.46
1:A:996:LEU:O	1:A:1000:ARG:HG3	2.16	0.45
1:B:342:PHE:CE2	1:B:511:VAL:HG21	2.52	0.45
1:C:23:GLN:H	1:C:23:GLN:CD	2.15	0.45
1:A:52:GLN:HG3	1:A:273:ARG:O	2.17	0.45
1:C:329:PHE:O	1:C:579:PRO:CG	2.58	0.45
1:A:1159:HIS:CD2	1:C:1160:THR:HG22	2.52	0.45
1:B:115:GLN:HA	1:B:132:GLU:HG2	1.97	0.45
1:C:332:ILE:HB	1:C:362:VAL:HG23	1.99	0.45
1:A:149:ASN:HB3	1:A:150:LYS:H	1.56	0.45
1:A:1082:CYS:SG	1:A:1132:ILE:CD1	3.05	0.45
1:A:1083:HIS:CG	1:A:1137:VAL:H	2.34	0.45
1:A:448:ASN:ND2	1:A:451:TYR:HE2	2.14	0.45
1:B:804:GLN:NE2	1:B:817:PHE:CD1	2.84	0.45
1:A:65:PHE:HB2	1:A:265:TYR:CE1	2.52	0.45
1:B:148:ASN:N	1:B:148:ASN:HD22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:GLN:NE2	1:B:804:GLN:HA	2.32	0.45
1:A:194:PHE:CD1	1:A:203:ILE:HG12	2.52	0.45
1:B:546:LEU:HD13	1:B:565:PHE:CE1	2.52	0.45
1:B:21:ARG:NE	1:B:21:ARG:CA	2.73	0.44
1:B:115:GLN:HG2	3:M:1:NAG:H82	1.92	0.44
1:A:736:VAL:HG13	1:A:858:LEU:HD23	1.98	0.44
1:A:1011:GLN:HA	1:A:1011:GLN:NE2	2.32	0.44
1:C:201:PHE:CD1	1:C:229:LEU:HG	2.51	0.44
1:C:117:LEU:HD23	1:C:235:ILE:HD11	1.99	0.44
1:B:24:LEU:CB	1:B:25:PRO:HD2	2.40	0.44
1:B:804:GLN:CA	1:B:804:GLN:HE21	2.29	0.44
1:C:201:PHE:CD1	1:C:229:LEU:CG	3.01	0.44
1:A:957:GLN:CG	1:B:765:ARG:NH1	2.81	0.43
1:B:900:MET:O	1:B:904:TYR:CD1	2.71	0.43
1:A:1152:LEU:HD13	1:C:1152:LEU:CD1	2.49	0.43
1:A:168:PHE:CE1	1:A:170:TYR:HB3	2.54	0.43
1:A:1136:THR:HG23	1:A:1136:THR:O	2.18	0.43
1:B:353:TRP:NE1	1:B:466:ARG:HG3	2.33	0.43
1:A:105:ILE:CD1	1:A:118:LEU:HD13	2.49	0.43
1:A:1102:TRP:HB2	1:A:1135:ASN:CG	2.44	0.43
1:C:738:CYS:SG	1:C:764:ASN:OD1	2.76	0.43
1:B:141:LEU:HD23	1:B:144:TYR:HE2	1.75	0.43
1:B:567:ARG:HD3	1:B:571:ASP:O	2.18	0.43
1:C:329:PHE:CE2	1:C:528:LYS:HB2	2.53	0.43
1:A:21:ARG:HG2	1:A:79:PHE:HZ	1.76	0.43
1:A:404:GLY:N	1:A:504:GLY:O	2.52	0.43
1:B:804:GLN:NE2	1:B:817:PHE:HB3	2.33	0.43
1:A:23:GLN:N	1:A:23:GLN:CD	2.76	0.42
1:A:132:GLU:OE1	1:A:165:ASN:HB2	2.19	0.42
4:S:1:NAG:H61	4:S:2:NAG:C7	2.48	0.42
1:B:634:ARG:HB3	1:B:634:ARG:CZ	2.49	0.42
1:A:176:LEU:C	1:A:176:LEU:CD1	2.93	0.42
1:B:115:GLN:CD	3:M:1:NAG:C8	2.93	0.42
1:B:1089:PHE:HB2	1:B:1121:PHE:CE2	2.53	0.42
1:A:1082:CYS:SG	1:A:1132:ILE:HD11	2.59	0.42
1:C:327:VAL:HG12	1:C:329:PHE:CD2	2.54	0.42
1:A:132:GLU:OE1	1:A:165:ASN:CB	2.68	0.42
1:B:126:VAL:HG23	1:B:175:PHE:CB	2.50	0.42
1:A:1152:LEU:HD11	1:C:1152:LEU:CD1	2.43	0.42
1:B:24:LEU:CD1	1:B:25:PRO:CD	2.96	0.42
1:A:144:TYR:HB2	1:A:152:TRP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:MET:CG	1:A:904:TYR:HE2	2.14	0.41
1:C:176:LEU:HD12	1:C:176:LEU:C	2.42	0.41
1:C:201:PHE:HB3	1:C:229:LEU:O	2.20	0.41
1:C:244:LEU:C	1:C:244:LEU:HD12	2.44	0.41
1:C:461:LEU:CD1	1:C:461:LEU:C	2.93	0.41
1:C:1089:PHE:HB2	1:C:1121:PHE:CE2	2.55	0.41
1:A:421:TYR:HE2	1:A:455:LEU:O	2.03	0.41
1:A:42:VAL:HG11	1:C:567:ARG:HD2	2.03	0.41
1:A:740:MET:HE1	1:C:592:PHE:CE2	2.56	0.41
1:A:1080:ALA:O	1:A:1133:VAL:HG22	2.21	0.41
1:C:101:ILE:HD13	1:C:242:LEU:HB3	2.02	0.41
4:S:1:NAG:H62	4:S:2:NAG:O7	2.21	0.41
1:A:204:TYR:CD2	1:A:225:PRO:CA	3.04	0.41
1:C:57:PRO:HB3	1:C:273:ARG:CZ	2.46	0.41
1:C:342:PHE:HB2	2:g:1:NAG:H81	2.03	0.41
1:A:1143:PRO:HA	1:A:1146:ASP:HB3	2.02	0.41
1:B:136:CYS:O	1:B:139:PRO:HD3	2.20	0.41
1:C:186:PHE:CB	1:C:211:ASN:OD1	2.65	0.41
1:A:24:LEU:CG	1:A:25:PRO:CD	2.81	0.41
1:B:147:LYS:CA	1:B:147:LYS:CE	2.86	0.41
1:B:326:ILE:HG23	1:B:541:PHE:HA	2.03	0.41
1:C:128:ILE:HG21	1:C:229:LEU:CD1	2.51	0.41
1:A:365:TYR:CE2	1:A:387:LEU:HB2	2.56	0.40
1:A:273:ARG:HB3	1:A:274:THR:H	1.73	0.40
1:C:24:LEU:HG	1:C:25:PRO:HD2	2.04	0.40
1:C:339:GLY:O	1:C:343:ASN:HB2	2.22	0.40
1:A:204:TYR:HE2	1:A:225:PRO:HG3	1.86	0.40
1:A:804:GLN:HE21	1:A:804:GLN:CA	2.26	0.40
1:C:85:PRO:HA	1:C:237:ARG:HG3	2.02	0.40
1:C:108:THR:CG2	1:C:234:ASN:HB3	2.49	0.40
1:C:163:ALA:O	1:C:165:ASN:N	2.54	0.40
1:C:403:ARG:CG	1:C:495:TYR:CD1	3.05	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	1079/1308 (82%)	985 (91%)	82 (8%)	12 (1%)	11	45
1	B	1070/1308 (82%)	984 (92%)	77 (7%)	9 (1%)	16	52
1	C	1082/1308 (83%)	985 (91%)	85 (8%)	12 (1%)	11	45
All	All	3231/3924 (82%)	2954 (91%)	244 (8%)	33 (1%)	15	47

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	147	LYS
1	A	154	GLU
1	A	174	PRO
1	B	32	PHE
1	B	164	ASN
1	B	173	GLN
1	C	16	VAL
1	C	154	GLU
1	C	164	ASN
1	C	174	PRO
1	C	834	ILE
1	A	744	GLY
1	B	180	GLU
1	B	635	VAL
1	B	814	LYS
1	C	733	LYS
1	A	834	ILE
1	A	1041	ASP
1	B	706	ALA
1	C	135	PHE
1	C	830	ASP
1	A	81	ASN
1	A	180	GLU
1	A	198	ASP
1	B	371	SER
1	C	518	LEU
1	A	32	PHE
1	C	32	PHE
1	C	329	PHE

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Mol	Chain	Res	Type
1	B	81	ASN
1	A	367	VAL
1	C	173	GLN

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	951/1133 (84%)	914 (96%)	37 (4%)	28	50
1	B	946/1133 (84%)	916 (97%)	30 (3%)	34	56
1	C	954/1133 (84%)	927 (97%)	27 (3%)	38	59
All	All	2851/3399 (84%)	2757 (97%)	94 (3%)	34	55

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	56	LEU
1	A	61	ASN
1	A	80	ASP
1	A	84	LEU
1	A	96	GLU
1	A	101	ILE
1	A	108	THR
1	A	117	LEU
1	A	120	VAL
1	A	127	VAL
1	A	132	GLU
1	A	152	TRP
1	A	154	GLU
1	A	166	CYS
1	A	169	GLU
1	A	179	LEU
1	A	186	PHE
1	A	196	ASN

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Mol	Chain	Res	Type
1	A	210	ILE
1	A	229	LEU
1	A	231	ILE
1	A	242	LEU
1	A	244	LEU
1	A	326	ILE
1	A	335	LEU
1	A	357	ARG
1	A	367	VAL
1	A	368	LEU
1	A	370	ASN
1	A	461	LEU
1	A	515	PHE
1	A	603	ASN
1	A	740	MET
1	A	773	GLU
1	A	803	SER
1	A	836	GLN
1	B	29	THR
1	B	36	VAL
1	B	56	LEU
1	B	61	ASN
1	B	84	LEU
1	B	117	LEU
1	B	120	VAL
1	B	121	ASN
1	B	127	VAL
1	B	131	CYS
1	B	171	VAL
1	B	179	LEU
1	B	183	GLN
1	B	186	PHE
1	B	196	ASN
1	B	197	ILE
1	B	210	ILE
1	B	224	GLU
1	B	229	LEU
1	B	231	ILE
1	B	242	LEU
1	B	244	LEU
1	B	394	ASN
1	B	523	THR

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Mol	Chain	Res	Type
1	B	544	ASN
1	B	603	ASN
1	B	803	SER
1	B	804	GLN
1	B	909	ILE
1	B	965	GLN
1	C	24	LEU
1	C	36	VAL
1	C	61	ASN
1	C	84	LEU
1	C	96	GLU
1	C	117	LEU
1	C	120	VAL
1	C	127	VAL
1	C	136	CYS
1	C	169	GLU
1	C	171	VAL
1	C	179	LEU
1	C	186	PHE
1	C	196	ASN
1	C	202	LYS
1	C	207	HIS
1	C	210	ILE
1	C	229	LEU
1	C	231	ILE
1	C	242	LEU
1	C	244	LEU
1	C	332	ILE
1	C	523	THR
1	C	635	VAL
1	C	739	THR
1	C	803	SER
1	C	836	GLN

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

Mol	Chain	Res	Type
1	A	14	GLN
1	A	66	HIS
1	A	148	ASN
1	A	460	ASN
1	A	519	HIS

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Mol	Chain	Res	Type
1	A	564	GLN
1	A	606	ASN
1	A	764	ASN
1	A	804	GLN
1	A	856	ASN
1	A	949	GLN
1	A	1005	GLN
1	A	1011	GLN
1	A	1088	HIS
1	A	1108	ASN
1	B	148	ASN
1	B	164	ASN
1	B	271	GLN
1	B	450	ASN
1	B	607	GLN
1	B	762	GLN
1	B	784	GLN
1	B	804	GLN
1	B	978	ASN
1	B	992	GLN
1	B	1002	GLN
1	B	1011	GLN
1	B	1108	ASN
1	B	1113	GLN
1	B	1119	ASN
1	C	121	ASN
1	C	188	ASN
1	C	388	ASN
1	C	460	ASN
1	C	501	ASN
1	C	655	HIS
1	C	690	GLN
1	C	755	GLN
1	C	787	GLN
1	C	804	GLN
1	C	836	GLN
1	C	856	ASN
1	C	919	ASN
1	C	920	GLN
1	C	935	GLN
1	C	949	GLN
1	C	960	ASN

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Mol	Chain	Res	Type
1	C	1010	GLN
1	C	1048	HIS
1	C	1054	GLN
1	C	1101	HIS
1	C	1113	GLN
1	C	1119	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

73 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	D	1	2,1	14,14,15	1.58	2 (14%)	17,19,21	1.01	1 (5%)
2	NAG	D	2	2	14,14,15	1.44	2 (14%)	17,19,21	0.91	1 (5%)
2	MAN	D	3	2	11,11,12	1.51	2 (18%)	15,15,17	0.87	0
3	NAG	E	1	3,1	14,14,15	1.21	1 (7%)	17,19,21	1.17	2 (11%)
3	NAG	E	2	3	14,14,15	1.19	1 (7%)	17,19,21	0.54	0
3	NAG	F	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	F	2	3	14,14,15	1.08	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	G	1	3,1	14,14,15	1.28	2 (14%)	17,19,21	0.96	0
3	NAG	G	2	3	14,14,15	1.32	2 (14%)	17,19,21	0.68	0
3	NAG	H	1	3,1	14,14,15	1.22	1 (7%)	17,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	H	2	3	14,14,15	1.18	1 (7%)	17,19,21	0.69	0
4	NAG	I	1	1,4	14,14,15	1.28	1 (7%)	17,19,21	0.99	2 (11%)
4	NAG	I	2	4	14,14,15	1.31	2 (14%)	17,19,21	1.23	1 (5%)
4	FUC	I	3	4	10,10,11	1.70	2 (20%)	14,14,16	1.21	1 (7%)
2	NAG	J	1	2,1	14,14,15	1.15	1 (7%)	17,19,21	1.06	2 (11%)
2	NAG	J	2	2	14,14,15	1.40	3 (21%)	17,19,21	0.67	0
2	MAN	J	3	2	11,11,12	1.43	2 (18%)	15,15,17	0.71	0
2	NAG	K	1	2,1	14,14,15	1.44	3 (21%)	17,19,21	0.98	0
2	NAG	K	2	2	14,14,15	1.42	3 (21%)	17,19,21	0.95	1 (5%)
2	MAN	K	3	2	11,11,12	1.52	2 (18%)	15,15,17	0.78	0
2	NAG	L	1	2,1	14,14,15	1.62	2 (14%)	17,19,21	0.99	1 (5%)
2	NAG	L	2	2	14,14,15	0.39	0	17,19,21	0.87	1 (5%)
2	MAN	L	3	2	11,11,12	1.47	2 (18%)	15,15,17	0.81	0
3	NAG	M	1	3,1	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	M	2	3	14,14,15	1.18	1 (7%)	17,19,21	0.68	0
3	NAG	N	1	3,1	14,14,15	1.15	2 (14%)	17,19,21	0.73	0
3	NAG	N	2	3	14,14,15	1.24	1 (7%)	17,19,21	1.10	1 (5%)
3	NAG	O	1	3,1	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	O	2	3	14,14,15	1.00	1 (7%)	17,19,21	0.74	0
3	NAG	P	1	3,1	14,14,15	1.35	2 (14%)	17,19,21	0.85	0
3	NAG	P	2	3	14,14,15	1.29	1 (7%)	17,19,21	0.67	0
3	NAG	Q	1	3,1	14,14,15	1.14	1 (7%)	17,19,21	1.07	2 (11%)
3	NAG	Q	2	3	14,14,15	1.23	1 (7%)	17,19,21	0.69	0
3	NAG	R	1	3,1	14,14,15	1.17	2 (14%)	17,19,21	1.04	1 (5%)
3	NAG	R	2	3	14,14,15	1.49	2 (14%)	17,19,21	0.75	0
4	NAG	S	1	1,4	14,14,15	0.28	0	17,19,21	0.93	1 (5%)
4	NAG	S	2	4	14,14,15	1.12	1 (7%)	17,19,21	0.89	1 (5%)
4	FUC	S	3	4	10,10,11	1.51	1 (10%)	14,14,16	1.85	2 (14%)
2	NAG	T	1	2,1	14,14,15	1.15	1 (7%)	17,19,21	1.06	2 (11%)
2	NAG	T	2	2	14,14,15	1.41	3 (21%)	17,19,21	0.67	0
2	MAN	T	3	2	11,11,12	1.42	2 (18%)	15,15,17	0.72	0
2	NAG	U	1	2,1	14,14,15	1.57	2 (14%)	17,19,21	1.02	1 (5%)
2	NAG	U	2	2	14,14,15	1.51	2 (14%)	17,19,21	0.89	1 (5%)
2	MAN	U	3	2	11,11,12	1.55	2 (18%)	15,15,17	0.95	0
2	NAG	V	1	2,1	14,14,15	1.34	2 (14%)	17,19,21	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	V	2	2	14,14,15	1.45	2 (14%)	17,19,21	0.84	1 (5%)
2	MAN	V	3	2	11,11,12	1.57	2 (18%)	15,15,17	0.85	0
3	NAG	W	1	3,1	14,14,15	1.44	4 (28%)	17,19,21	1.35	1 (5%)
3	NAG	W	2	3	14,14,15	1.12	2 (14%)	17,19,21	1.11	2 (11%)
3	NAG	X	1	3,1	14,14,15	1.15	1 (7%)	17,19,21	0.63	0
3	NAG	X	2	3	14,14,15	1.41	3 (21%)	17,19,21	1.04	1 (5%)
3	NAG	Y	1	3,1	14,14,15	0.27	0	17,19,21	0.56	0
3	NAG	Y	2	3	14,14,15	1.11	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	Z	1	3,1	14,14,15	1.31	1 (7%)	17,19,21	1.48	3 (17%)
3	NAG	Z	2	3	14,14,15	1.28	1 (7%)	17,19,21	1.07	1 (5%)
3	NAG	a	1	3,1	14,14,15	1.07	1 (7%)	17,19,21	1.52	1 (5%)
3	NAG	a	2	3	14,14,15	1.25	1 (7%)	17,19,21	0.79	0
3	NAG	b	1	3,1	14,14,15	1.27	2 (14%)	17,19,21	0.78	0
3	NAG	b	2	3	14,14,15	1.09	1 (7%)	17,19,21	1.02	1 (5%)
3	NAG	c	1	3,1	14,14,15	1.23	2 (14%)	17,19,21	0.91	0
3	NAG	c	2	3	14,14,15	1.35	2 (14%)	17,19,21	0.69	0
4	NAG	d	1	1,4	14,14,15	0.19	0	17,19,21	0.85	1 (5%)
4	NAG	d	2	4	14,14,15	1.12	1 (7%)	17,19,21	0.89	1 (5%)
4	FUC	d	3	4	10,10,11	1.67	2 (20%)	14,14,16	1.32	2 (14%)
2	NAG	e	1	2,1	14,14,15	1.15	1 (7%)	17,19,21	1.06	2 (11%)
2	NAG	e	2	2	14,14,15	1.40	3 (21%)	17,19,21	0.67	0
2	MAN	e	3	2	11,11,12	1.43	2 (18%)	15,15,17	0.72	0
2	NAG	f	1	2,1	14,14,15	1.44	3 (21%)	17,19,21	0.98	0
2	NAG	f	2	2	14,14,15	1.42	3 (21%)	17,19,21	0.94	1 (5%)
2	MAN	f	3	2	11,11,12	1.52	2 (18%)	15,15,17	0.79	0
2	NAG	g	1	2,1	14,14,15	1.59	2 (14%)	17,19,21	0.99	1 (5%)
2	NAG	g	2	2	14,14,15	1.34	2 (14%)	17,19,21	1.51	3 (17%)
2	MAN	g	3	2	11,11,12	1.48	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	2,1	-	0/6/23/26	0/1/1/1

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

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

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-4.43	1.36	1.43
2	L	1	NAG	O5-C5	4.15	1.51	1.43
2	g	1	NAG	O5-C5	4.05	1.51	1.43
2	U	1	NAG	O5-C5	4.01	1.51	1.43
2	D	1	NAG	O5-C5	4.00	1.51	1.43
2	U	2	NAG	O5-C5	3.56	1.50	1.43
2	V	3	MAN	O5-C5	3.50	1.50	1.43
2	U	3	MAN	O5-C5	3.41	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3	MAN	O5-C5	3.37	1.50	1.43
2	f	3	MAN	O5-C5	3.36	1.50	1.43
3	X	2	NAG	O5-C5	3.30	1.49	1.43
2	D	3	MAN	O5-C5	3.28	1.49	1.43
3	E	2	NAG	O5-C5	3.22	1.49	1.43
2	K	1	NAG	O5-C5	3.21	1.49	1.43
2	V	2	NAG	O5-C5	3.20	1.49	1.43
3	M	2	NAG	O5-C5	3.18	1.49	1.43
2	J	2	NAG	O5-C5	3.18	1.49	1.43
2	f	1	NAG	O5-C5	3.18	1.49	1.43
2	T	2	NAG	O5-C5	3.17	1.49	1.43
2	e	2	NAG	O5-C5	3.17	1.49	1.43
3	c	1	NAG	O5-C5	3.14	1.49	1.43
2	g	3	MAN	O5-C5	3.13	1.49	1.43
2	L	3	MAN	O5-C5	3.08	1.49	1.43
4	S	3	FUC	O5-C5	3.07	1.49	1.43
3	R	2	NAG	O5-C1	3.07	1.48	1.43
4	d	3	FUC	O5-C5	3.07	1.49	1.43
4	d	3	FUC	C1-C2	3.06	1.59	1.52
3	G	2	NAG	O5-C5	3.01	1.49	1.43
4	I	3	FUC	O5-C1	3.00	1.48	1.43
2	f	2	NAG	O5-C5	2.99	1.49	1.43
2	K	2	NAG	O5-C5	2.99	1.49	1.43
3	c	2	NAG	O5-C5	2.95	1.49	1.43
2	D	2	NAG	O5-C5	2.95	1.49	1.43
3	P	1	NAG	O5-C5	2.94	1.49	1.43
4	I	3	FUC	O5-C5	2.94	1.49	1.43
3	R	2	NAG	O5-C5	2.93	1.49	1.43
4	d	2	NAG	O5-C5	2.88	1.49	1.43
3	a	2	NAG	O5-C5	2.87	1.49	1.43
3	Y	2	NAG	O5-C5	2.87	1.49	1.43
3	F	2	NAG	O5-C5	2.86	1.49	1.43
2	e	3	MAN	O5-C5	2.86	1.49	1.43
2	J	3	MAN	O5-C5	2.85	1.49	1.43
3	Q	2	NAG	O5-C5	2.85	1.49	1.43
2	T	3	MAN	O5-C5	2.83	1.49	1.43
3	H	2	NAG	O5-C5	2.83	1.48	1.43
4	S	2	NAG	O5-C5	2.82	1.48	1.43
4	I	1	NAG	C1-C2	2.80	1.56	1.52
4	I	2	NAG	O5-C5	2.80	1.48	1.43
3	Z	1	NAG	O5-C5	2.79	1.48	1.43
3	P	2	NAG	O5-C5	2.77	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C5	2.73	1.48	1.43
3	Z	2	NAG	O5-C5	2.72	1.48	1.43
3	b	1	NAG	C1-C2	2.70	1.56	1.52
2	L	1	NAG	C1-C2	2.67	1.56	1.52
3	N	2	NAG	O5-C5	2.66	1.48	1.43
2	g	1	NAG	C1-C2	2.64	1.55	1.52
3	b	2	NAG	O5-C5	2.59	1.48	1.43
3	W	1	NAG	C1-C2	2.58	1.55	1.52
2	D	2	NAG	O4-C4	2.58	1.49	1.43
2	D	1	NAG	C1-C2	2.57	1.55	1.52
2	T	1	NAG	O5-C5	2.56	1.48	1.43
2	U	1	NAG	C1-C2	2.55	1.55	1.52
3	G	1	NAG	O5-C5	2.54	1.48	1.43
3	W	1	NAG	O5-C5	2.52	1.48	1.43
2	e	1	NAG	O5-C5	2.52	1.48	1.43
2	J	1	NAG	O5-C5	2.52	1.48	1.43
2	T	2	NAG	O4-C4	2.48	1.49	1.43
2	e	2	NAG	O4-C4	2.47	1.49	1.43
3	X	2	NAG	O5-C1	2.46	1.47	1.43
2	V	1	NAG	O5-C5	2.45	1.48	1.43
2	J	2	NAG	O4-C4	2.45	1.49	1.43
2	f	1	NAG	O5-C1	2.44	1.47	1.43
2	K	1	NAG	O5-C1	2.44	1.47	1.43
2	V	2	NAG	O4-C4	2.41	1.48	1.43
2	U	2	NAG	O4-C4	2.38	1.48	1.43
2	U	3	MAN	O5-C1	2.34	1.47	1.43
2	V	1	NAG	C1-C2	2.33	1.55	1.52
3	b	1	NAG	O5-C5	2.32	1.48	1.43
2	K	3	MAN	O5-C1	2.32	1.47	1.43
2	V	3	MAN	O5-C1	2.32	1.47	1.43
3	c	2	NAG	C1-C2	2.31	1.55	1.52
2	f	3	MAN	O5-C1	2.31	1.47	1.43
2	K	2	NAG	O5-C1	2.30	1.47	1.43
2	T	3	MAN	O5-C1	2.29	1.47	1.43
4	I	2	NAG	C1-C2	2.27	1.55	1.52
2	g	2	NAG	O5-C5	2.26	1.47	1.43
2	f	2	NAG	O5-C1	2.26	1.47	1.43
2	J	3	MAN	O5-C1	2.26	1.47	1.43
2	e	3	MAN	O5-C1	2.25	1.47	1.43
2	D	3	MAN	O5-C1	2.24	1.47	1.43
3	X	1	NAG	O5-C5	2.22	1.47	1.43
2	g	2	NAG	O4-C4	2.21	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	2	NAG	O4-C4	2.18	1.48	1.43
2	K	2	NAG	O4-C4	2.18	1.48	1.43
3	W	2	NAG	O5-C5	2.16	1.47	1.43
3	W	1	NAG	O4-C4	2.13	1.48	1.43
3	W	2	NAG	O5-C1	2.12	1.47	1.43
3	a	1	NAG	O5-C5	2.12	1.47	1.43
3	Q	1	NAG	O5-C5	2.12	1.47	1.43
3	O	2	NAG	O5-C5	2.11	1.47	1.43
2	K	1	NAG	C1-C2	2.11	1.55	1.52
3	G	2	NAG	O5-C1	2.10	1.47	1.43
3	H	1	NAG	O4-C4	2.10	1.48	1.43
3	N	1	NAG	C1-C2	2.10	1.55	1.52
2	g	3	MAN	O5-C1	2.09	1.47	1.43
2	f	1	NAG	C1-C2	2.09	1.55	1.52
2	L	3	MAN	O5-C1	2.06	1.47	1.43
3	W	1	NAG	C8-C7	2.06	1.54	1.50
2	T	2	NAG	O5-C1	2.05	1.47	1.43
3	c	1	NAG	C8-C7	2.03	1.54	1.50
2	J	2	NAG	O5-C1	2.03	1.47	1.43
3	X	2	NAG	C8-C7	2.03	1.54	1.50
2	e	2	NAG	O5-C1	2.02	1.47	1.43
3	G	1	NAG	O5-C1	2.01	1.47	1.43
3	N	1	NAG	O5-C5	2.00	1.47	1.43
3	R	1	NAG	C8-C7	2.00	1.54	1.50
3	P	1	NAG	O4-C4	2.00	1.47	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1	NAG	C1-O5-C5	5.10	119.02	112.19
2	g	2	NAG	C1-O5-C5	4.29	117.94	112.19
3	Y	2	NAG	C1-O5-C5	4.26	117.89	112.19
4	S	3	FUC	C1-C2-C3	4.24	115.82	109.64
4	I	2	NAG	C1-O5-C5	4.09	117.67	112.19
2	V	1	NAG	C1-O5-C5	4.05	117.61	112.19
3	W	1	NAG	C1-O5-C5	4.02	117.57	112.19
4	S	3	FUC	C1-O5-C5	4.01	122.42	112.97
3	N	2	NAG	C1-O5-C5	3.79	117.26	112.19
3	Z	1	NAG	C3-C4-C5	3.67	116.88	110.23
3	Z	2	NAG	C1-O5-C5	3.47	116.84	112.19
4	S	1	NAG	C1-O5-C5	3.21	116.48	112.19
3	Z	1	NAG	C1-O5-C5	3.16	116.43	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	3	FUC	C1-C2-C3	3.15	114.23	109.64
4	d	2	NAG	C1-O5-C5	3.02	116.23	112.19
3	E	1	NAG	C1-O5-C5	2.97	116.17	112.19
4	S	2	NAG	C1-O5-C5	2.92	116.09	112.19
3	W	2	NAG	C1-O5-C5	2.89	116.06	112.19
2	D	2	NAG	C1-O5-C5	2.89	116.05	112.19
4	d	1	NAG	C1-O5-C5	2.82	115.97	112.19
2	L	2	NAG	O5-C1-C2	-2.75	107.04	111.29
3	b	2	NAG	C1-O5-C5	2.70	115.81	112.19
2	K	2	NAG	O5-C1-C2	-2.65	107.19	111.29
3	X	2	NAG	C1-O5-C5	2.64	115.73	112.19
3	F	2	NAG	C1-O5-C5	2.63	115.70	112.19
2	f	2	NAG	O5-C1-C2	-2.62	107.24	111.29
4	I	3	FUC	C1-C2-C3	2.59	113.41	109.64
3	W	2	NAG	O5-C1-C2	-2.45	107.51	111.29
2	T	1	NAG	C1-O5-C5	2.37	115.36	112.19
4	I	1	NAG	O5-C5-C6	2.36	112.26	107.66
2	e	1	NAG	C1-O5-C5	2.36	115.35	112.19
2	V	1	NAG	C4-C3-C2	-2.35	107.57	111.02
2	J	1	NAG	C1-O5-C5	2.35	115.34	112.19
2	U	2	NAG	C4-C3-C2	-2.34	107.58	111.02
3	Q	1	NAG	C4-C3-C2	-2.32	107.62	111.02
2	g	2	NAG	C2-N2-C7	-2.27	119.86	122.90
3	Z	1	NAG	O5-C1-C2	-2.27	107.78	111.29
2	g	2	NAG	C4-C3-C2	-2.22	107.77	111.02
4	d	3	FUC	C1-O5-C5	2.20	118.16	112.97
4	I	1	NAG	C1-O5-C5	2.19	115.13	112.19
2	D	1	NAG	C4-C3-C2	-2.15	107.87	111.02
2	U	1	NAG	C4-C3-C2	-2.15	107.87	111.02
2	V	2	NAG	C1-O5-C5	2.13	115.05	112.19
2	T	1	NAG	O4-C4-C3	-2.13	105.36	110.38
2	L	1	NAG	C4-C3-C2	-2.11	107.92	111.02
2	e	1	NAG	O4-C4-C3	-2.11	105.40	110.38
3	E	1	NAG	C3-C4-C5	2.11	114.06	110.23
3	Q	1	NAG	C1-O5-C5	2.10	115.00	112.19
2	J	1	NAG	O4-C4-C3	-2.09	105.44	110.38
3	R	1	NAG	C1-O5-C5	-2.05	109.44	112.19
2	g	1	NAG	C4-C3-C2	-2.04	108.02	111.02

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	2	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
4	S	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	J	3	MAN	O5-C5-C6-O6
2	T	3	MAN	O5-C5-C6-O6
2	e	3	MAN	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C1-C2-N2-C7
2	f	2	NAG	C1-C2-N2-C7
3	G	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C3-C2-N2-C7
3	W	1	NAG	C4-C5-C6-O6

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	U	3	MAN	C1-C2-C3-C4-C5-O5
2	K	3	MAN	C1-C2-C3-C4-C5-O5
2	f	3	MAN	C1-C2-C3-C4-C5-O5
2	V	3	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 29 short contacts:

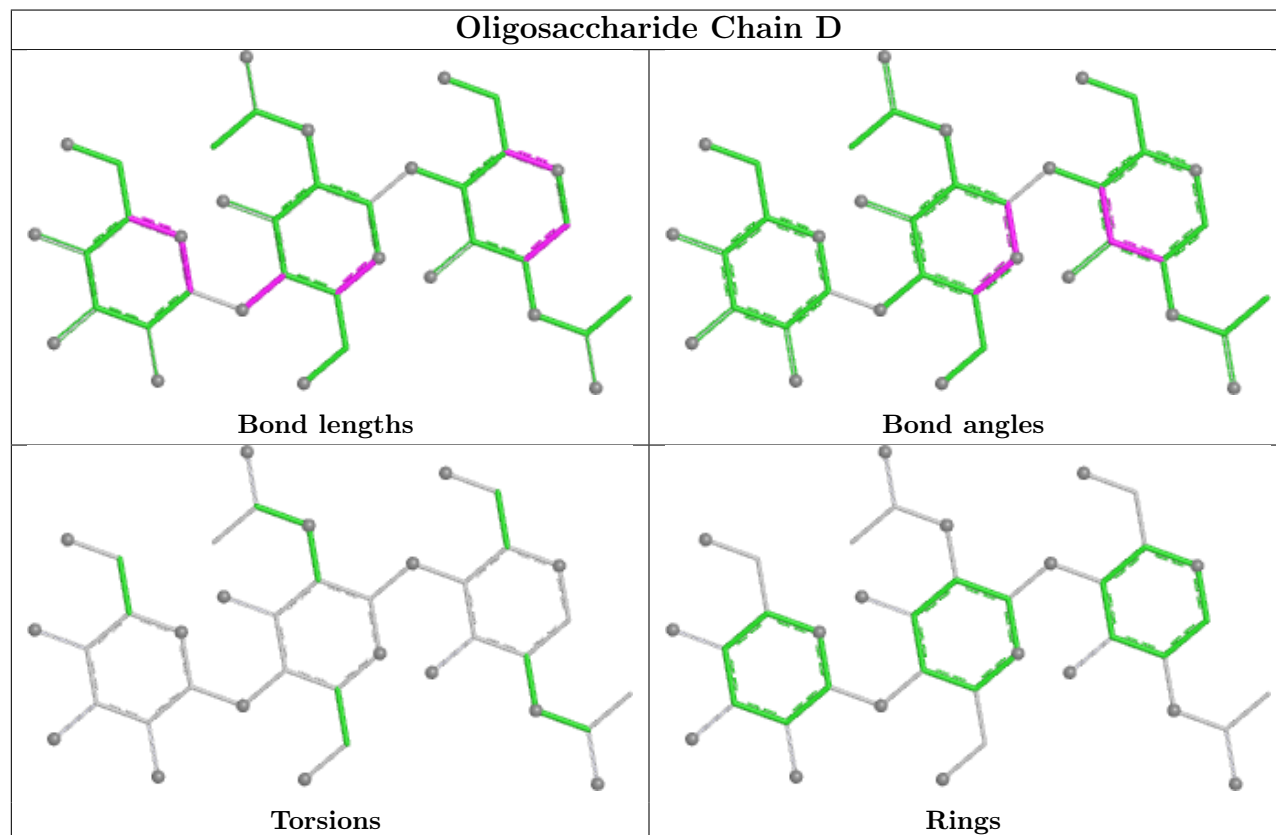
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	c	1	NAG	4	0
3	E	1	NAG	2	0
3	M	1	NAG	11	0
2	f	2	NAG	1	0
2	f	1	NAG	1	0
2	K	1	NAG	1	0
2	K	2	NAG	1	0
4	S	1	NAG	6	0
2	g	1	NAG	1	0
3	F	1	NAG	3	0

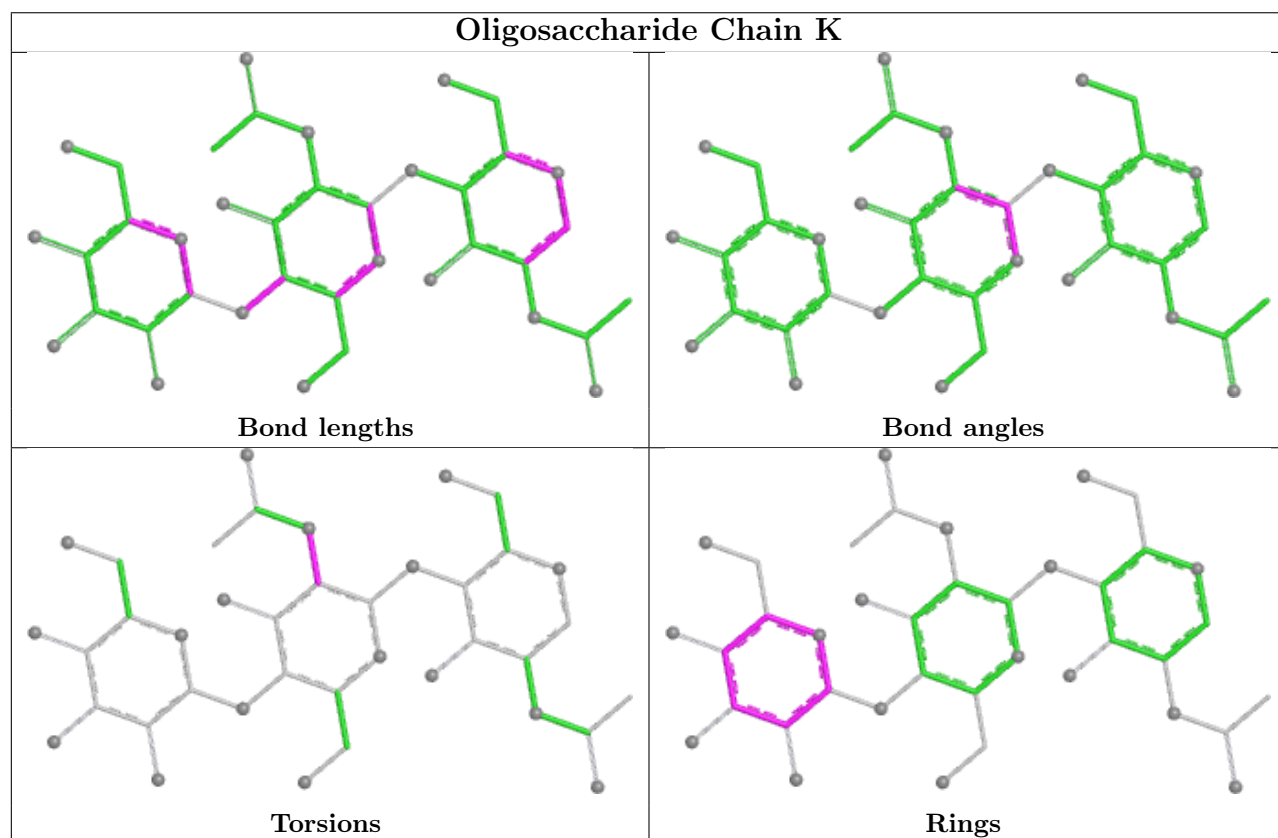
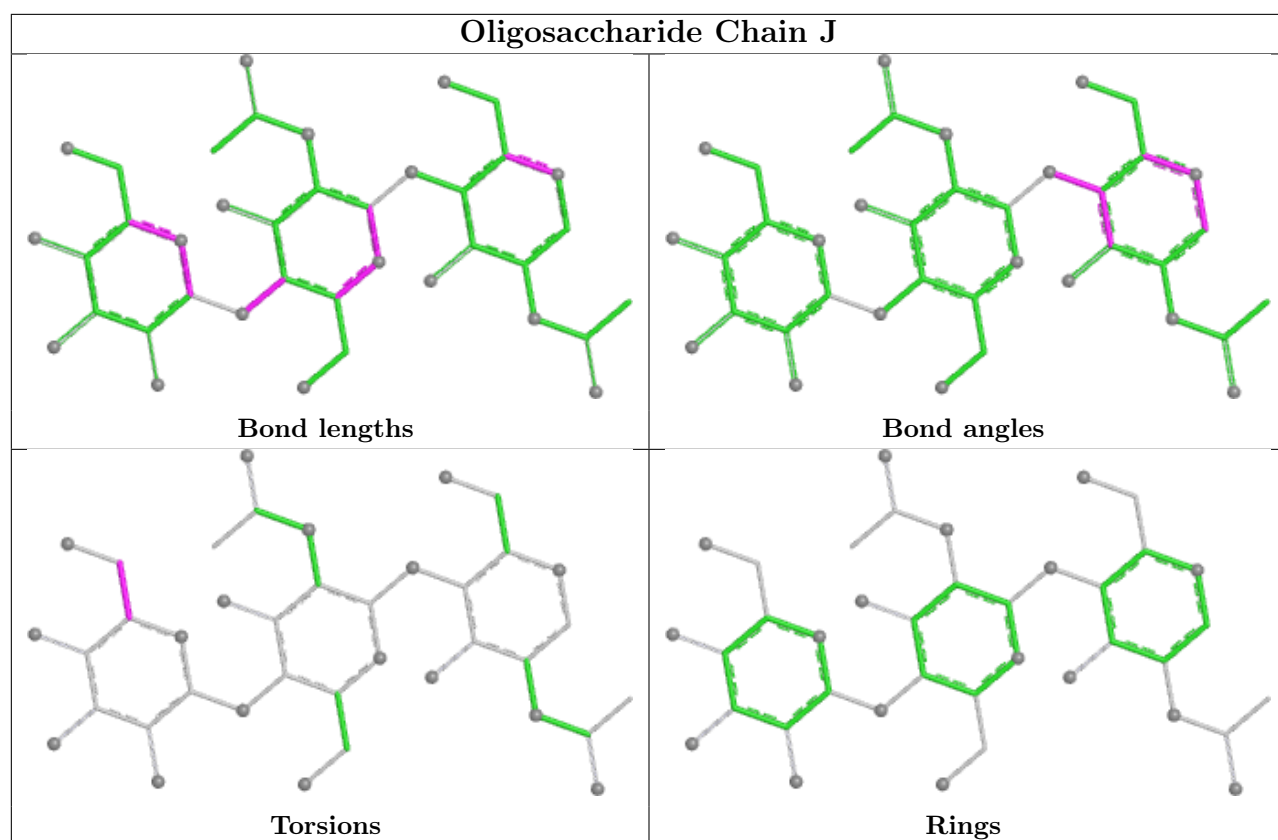
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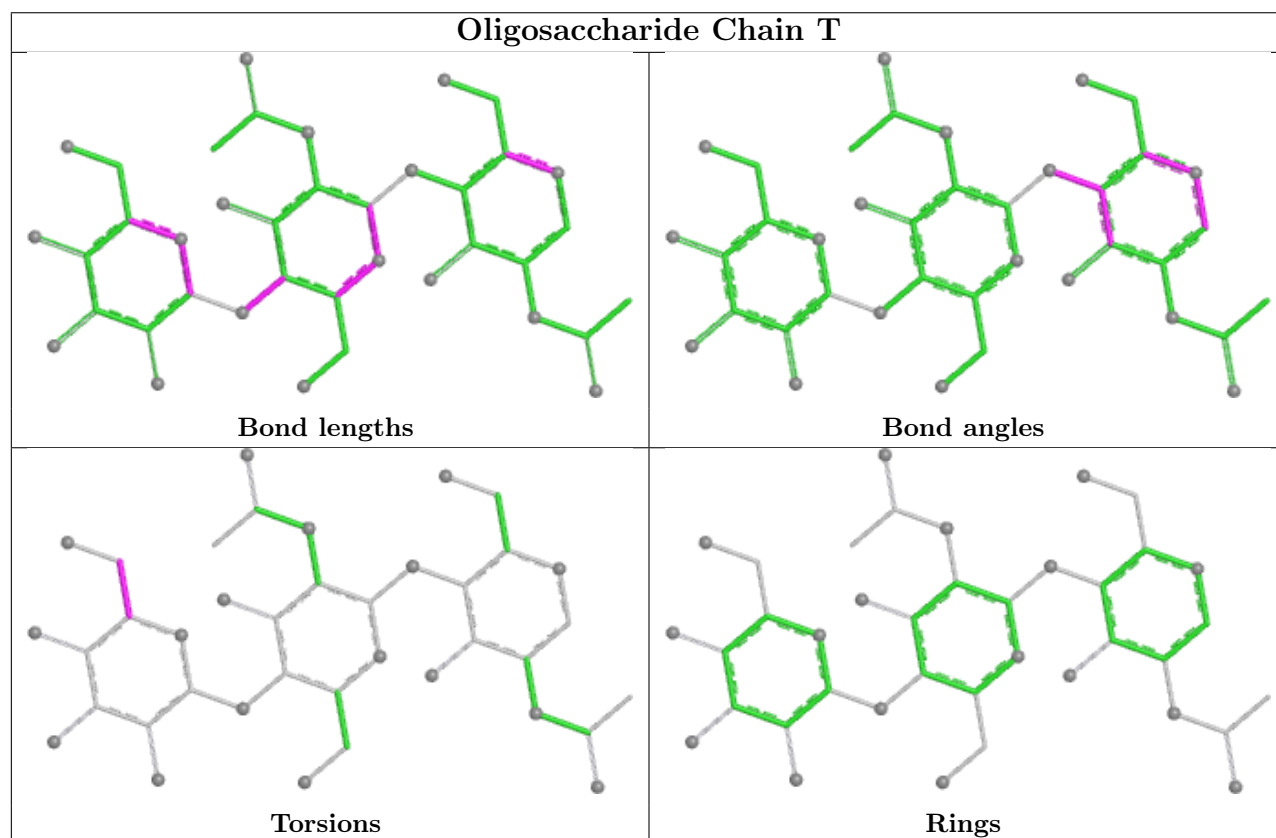
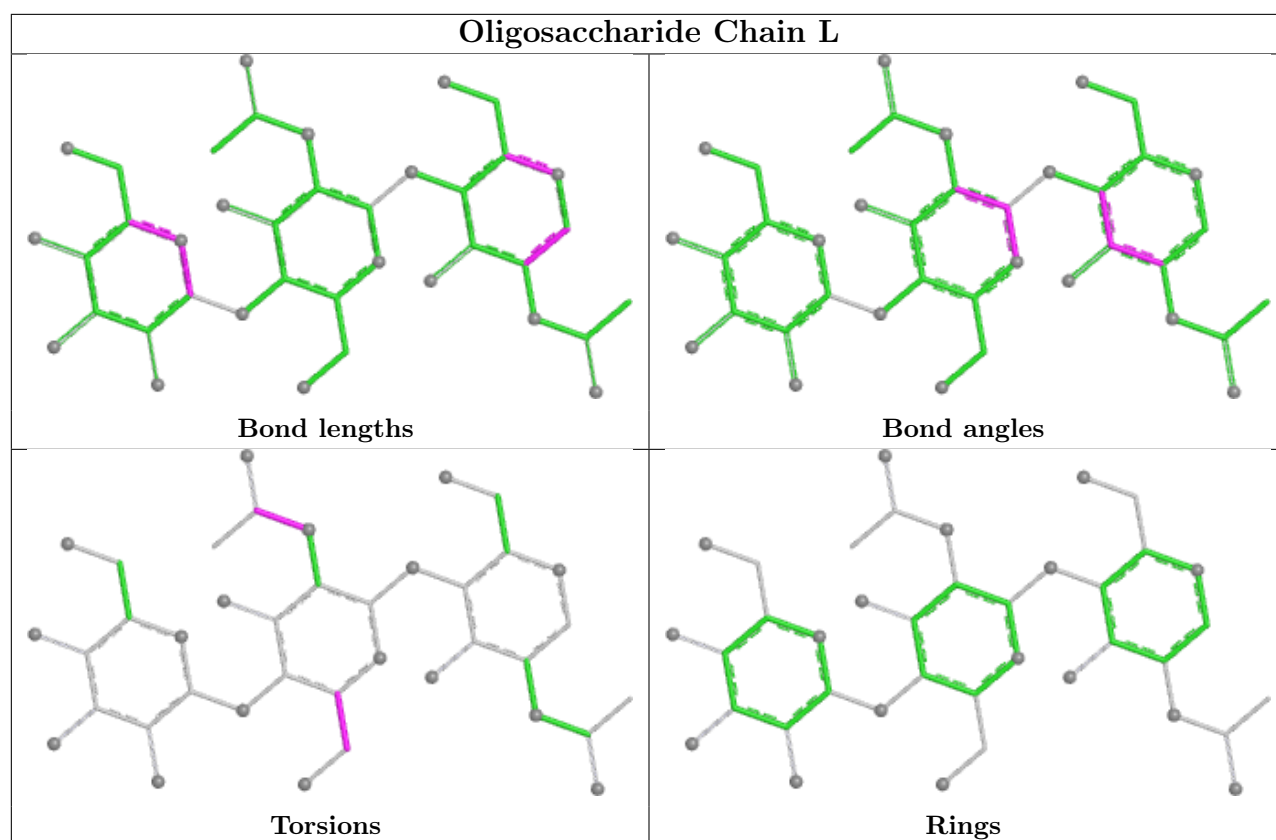
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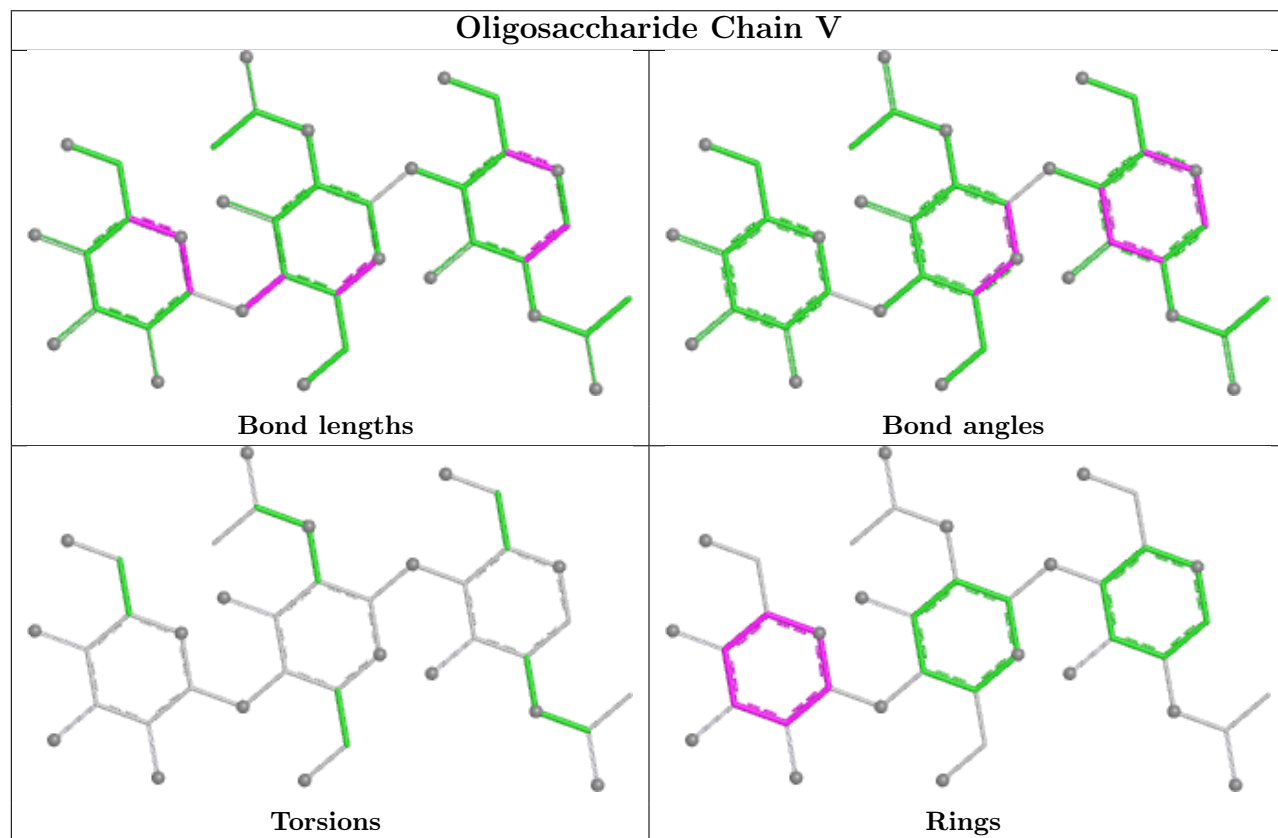
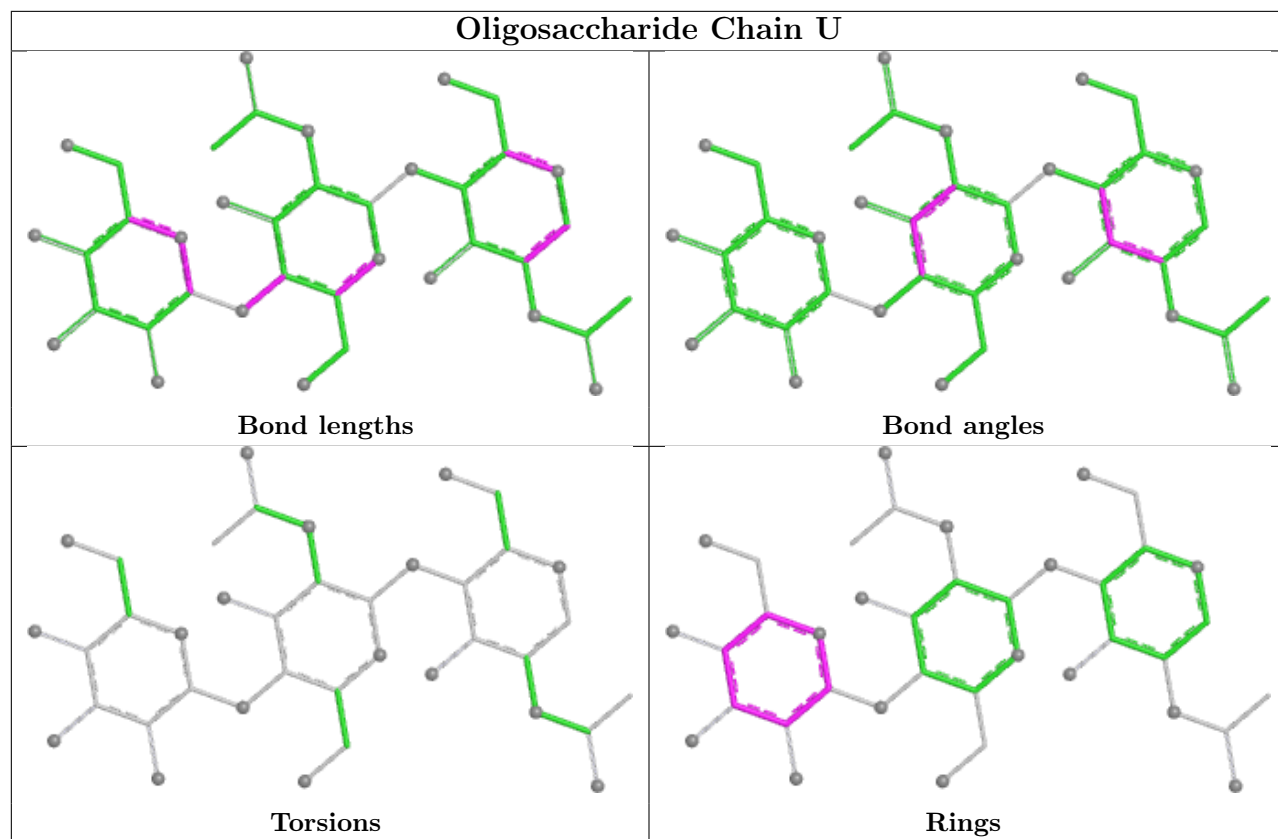
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	2	NAG	6	0
3	E	2	NAG	2	0

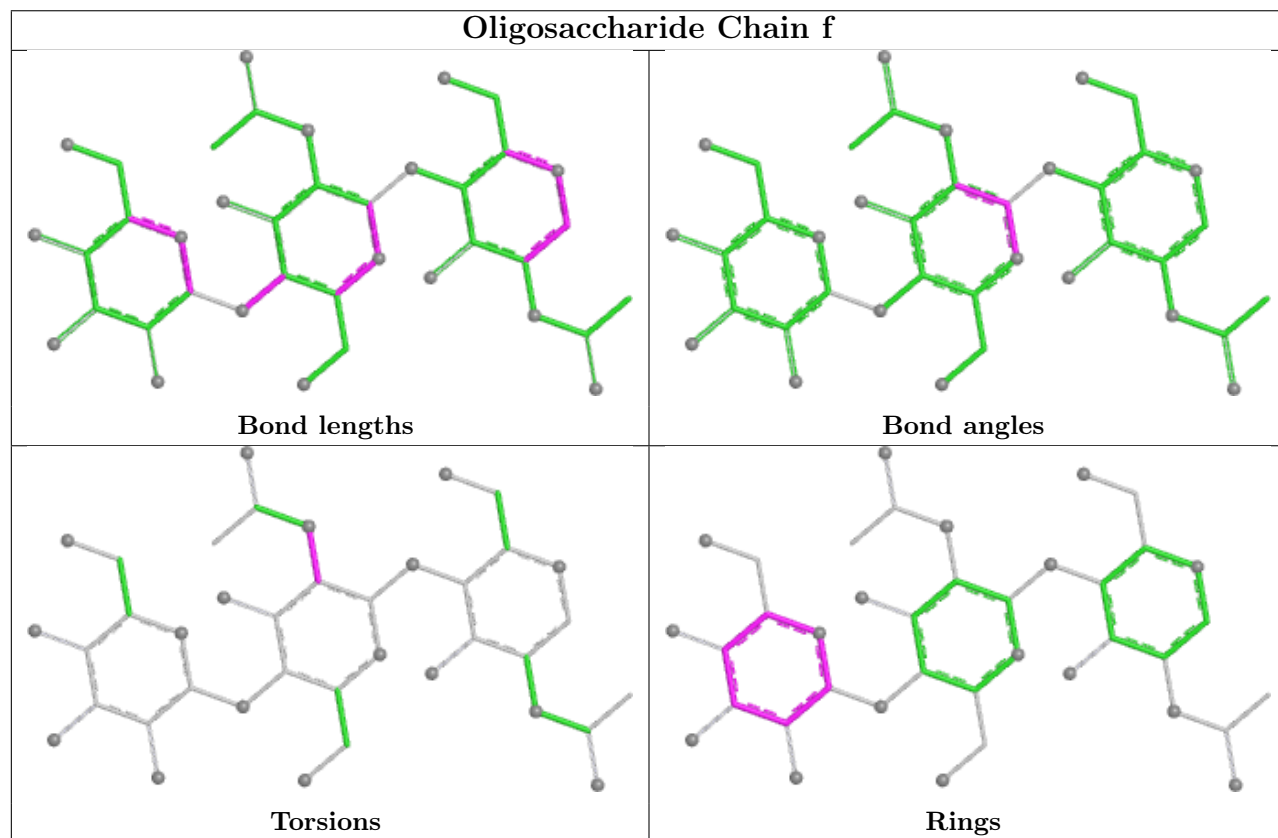
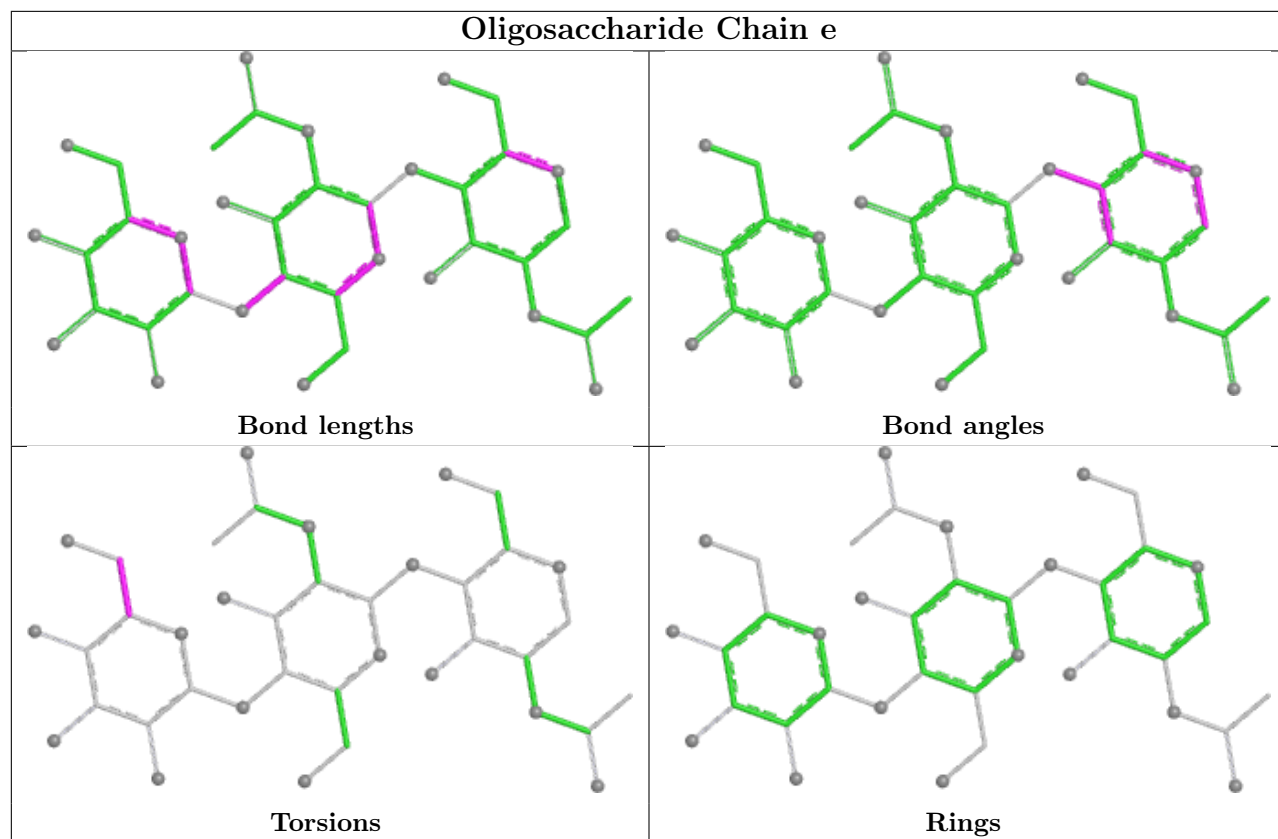
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

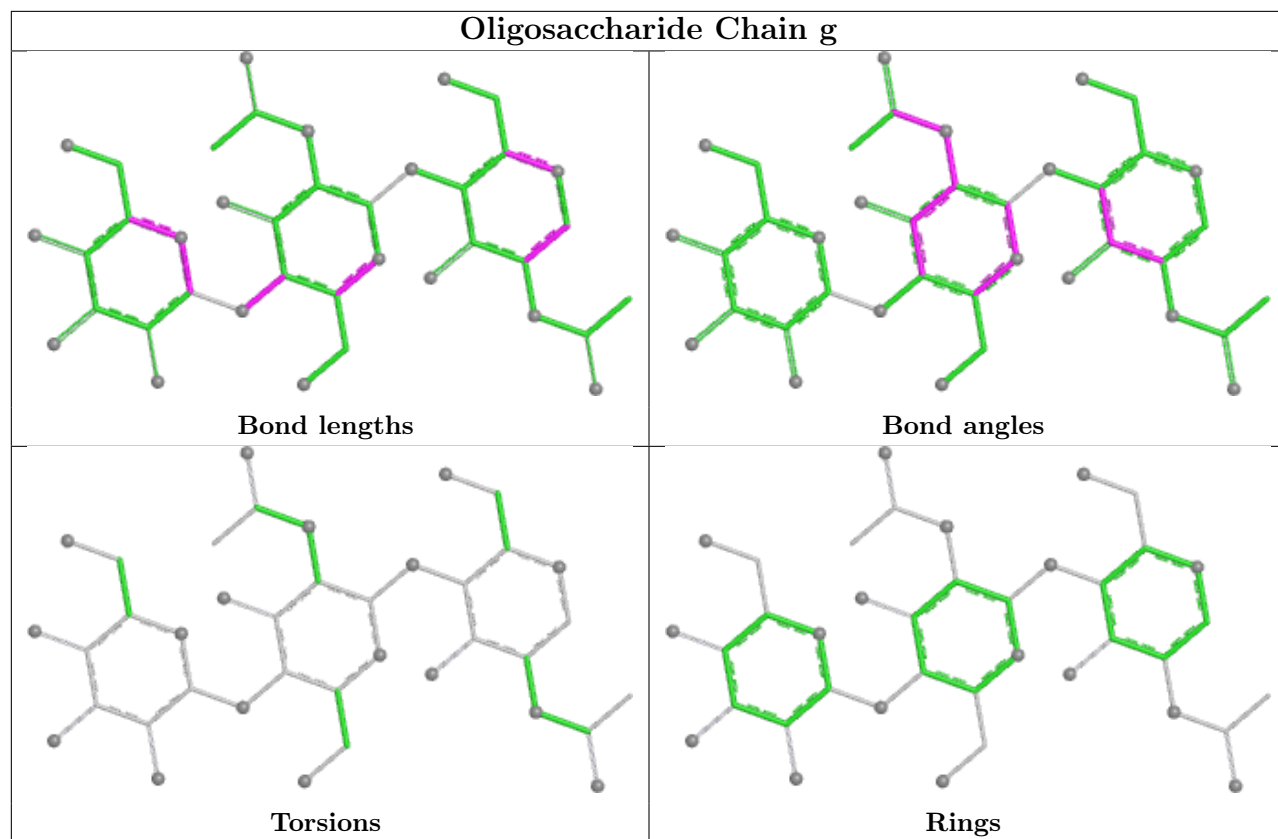


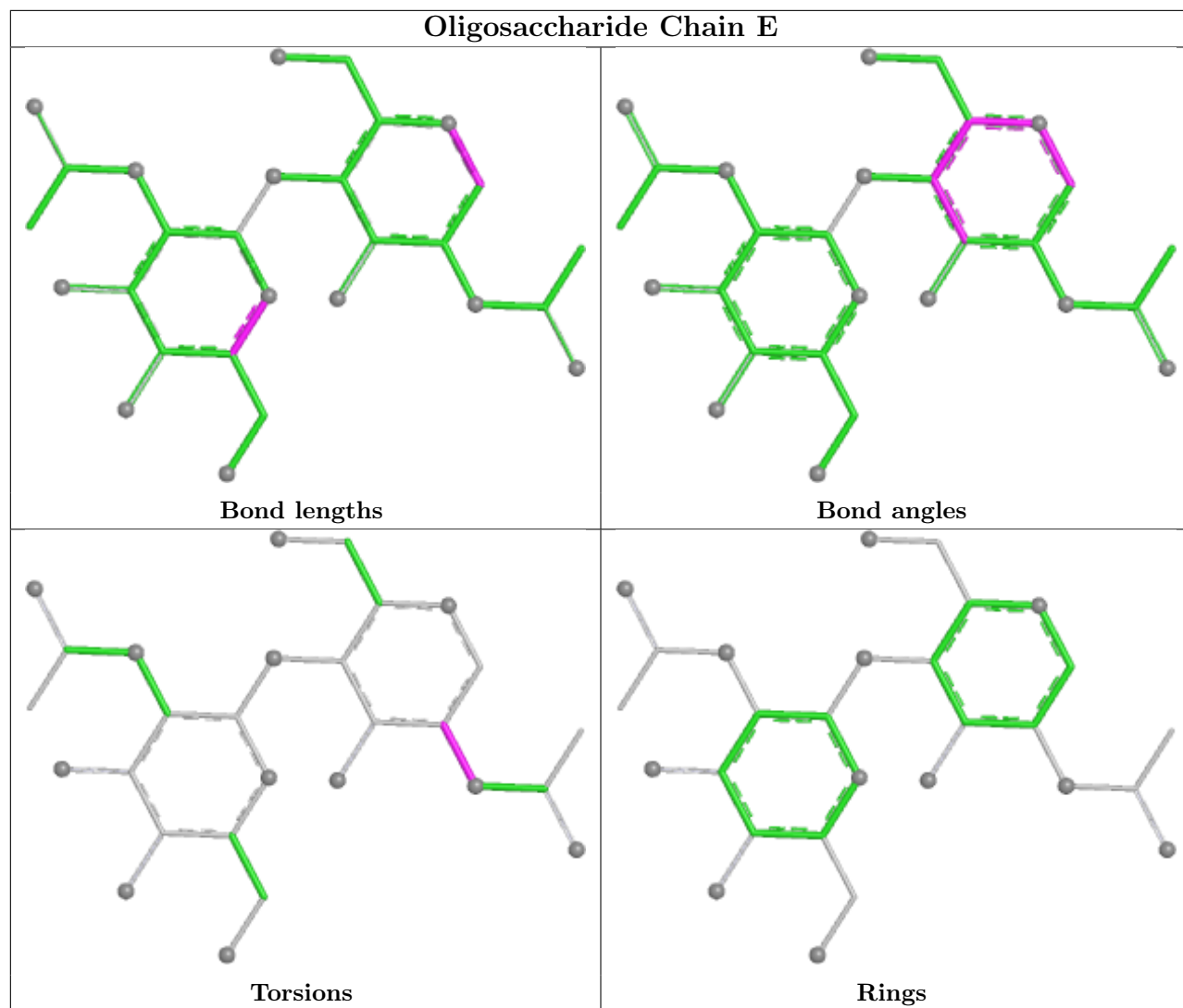


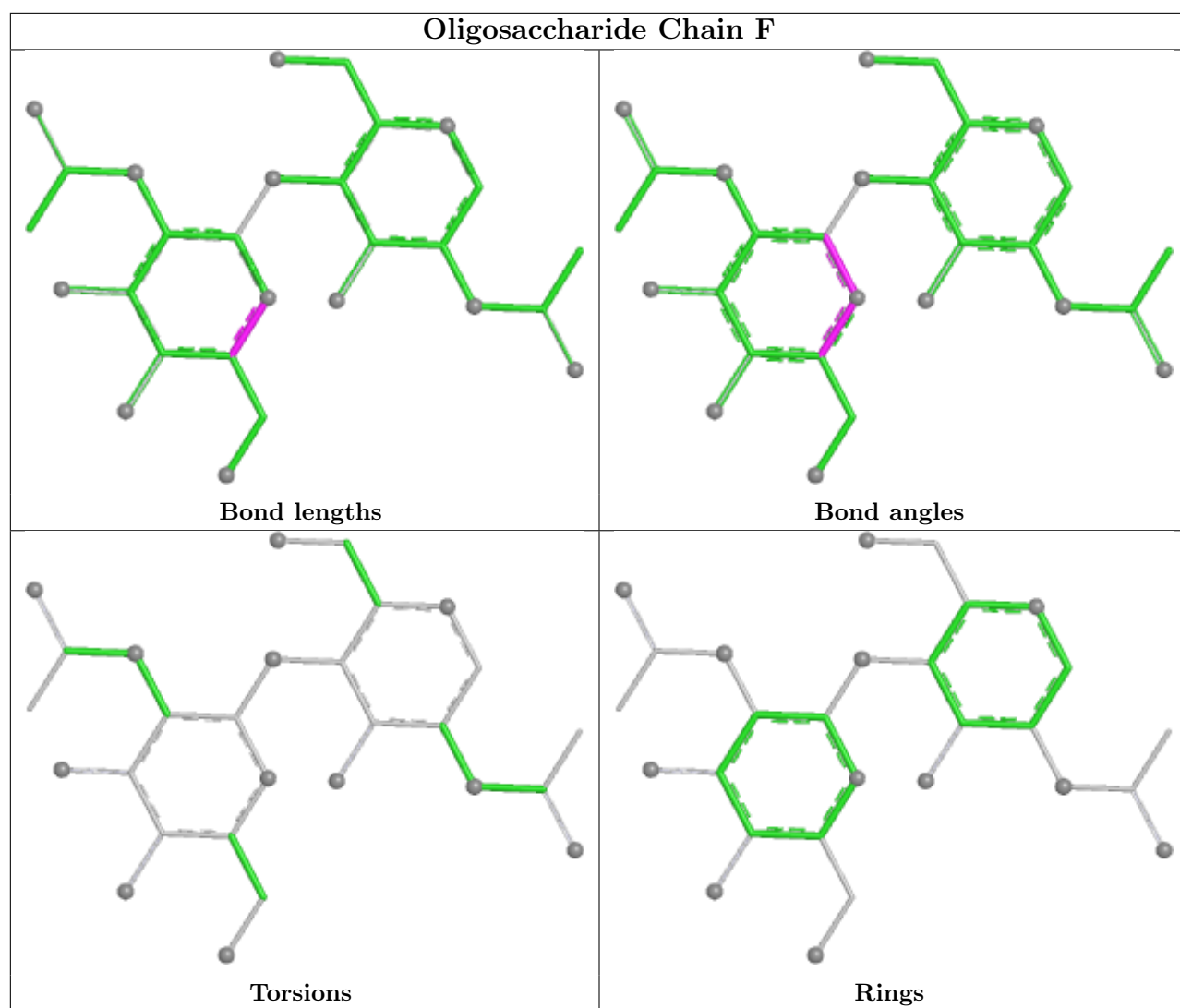


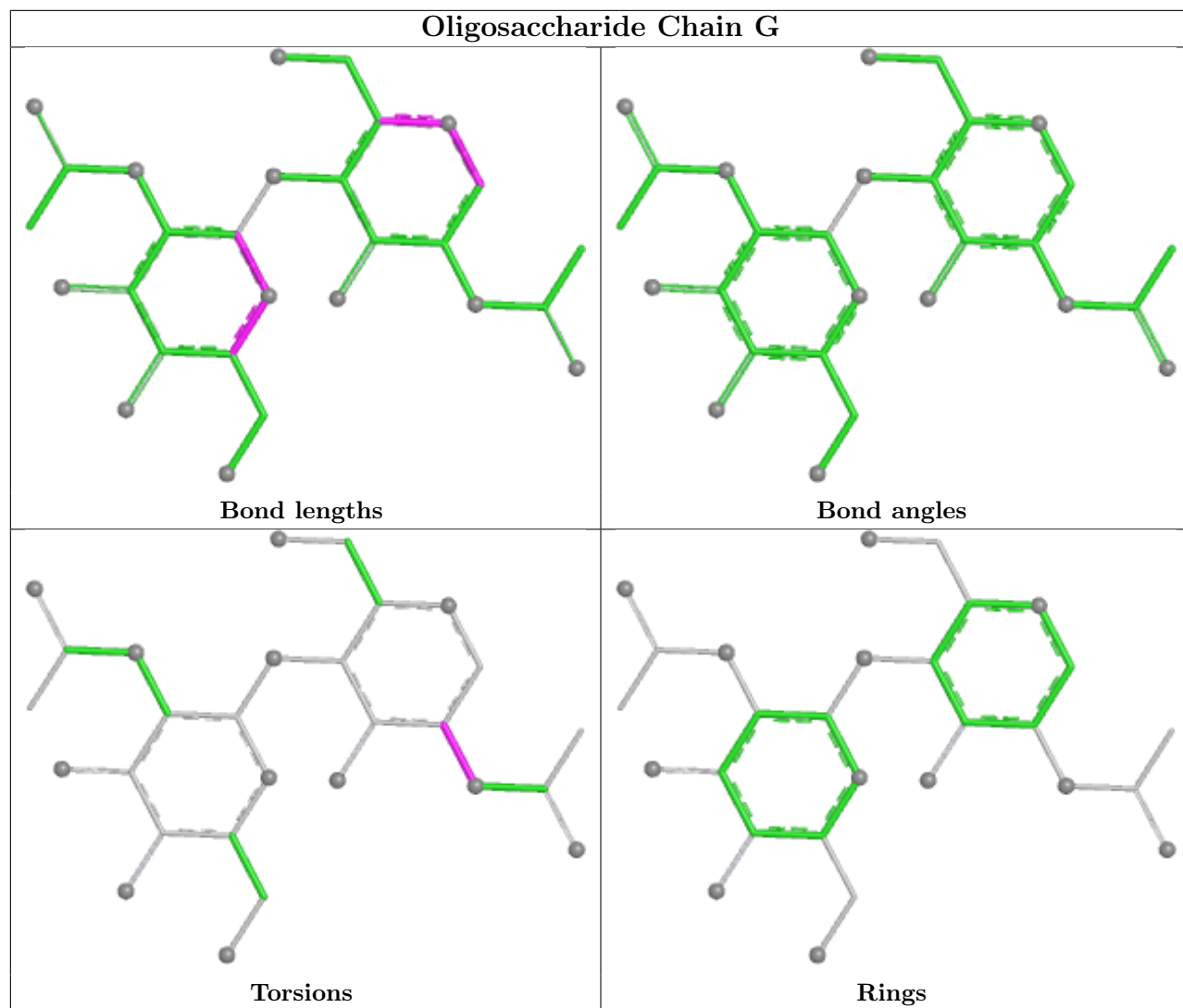


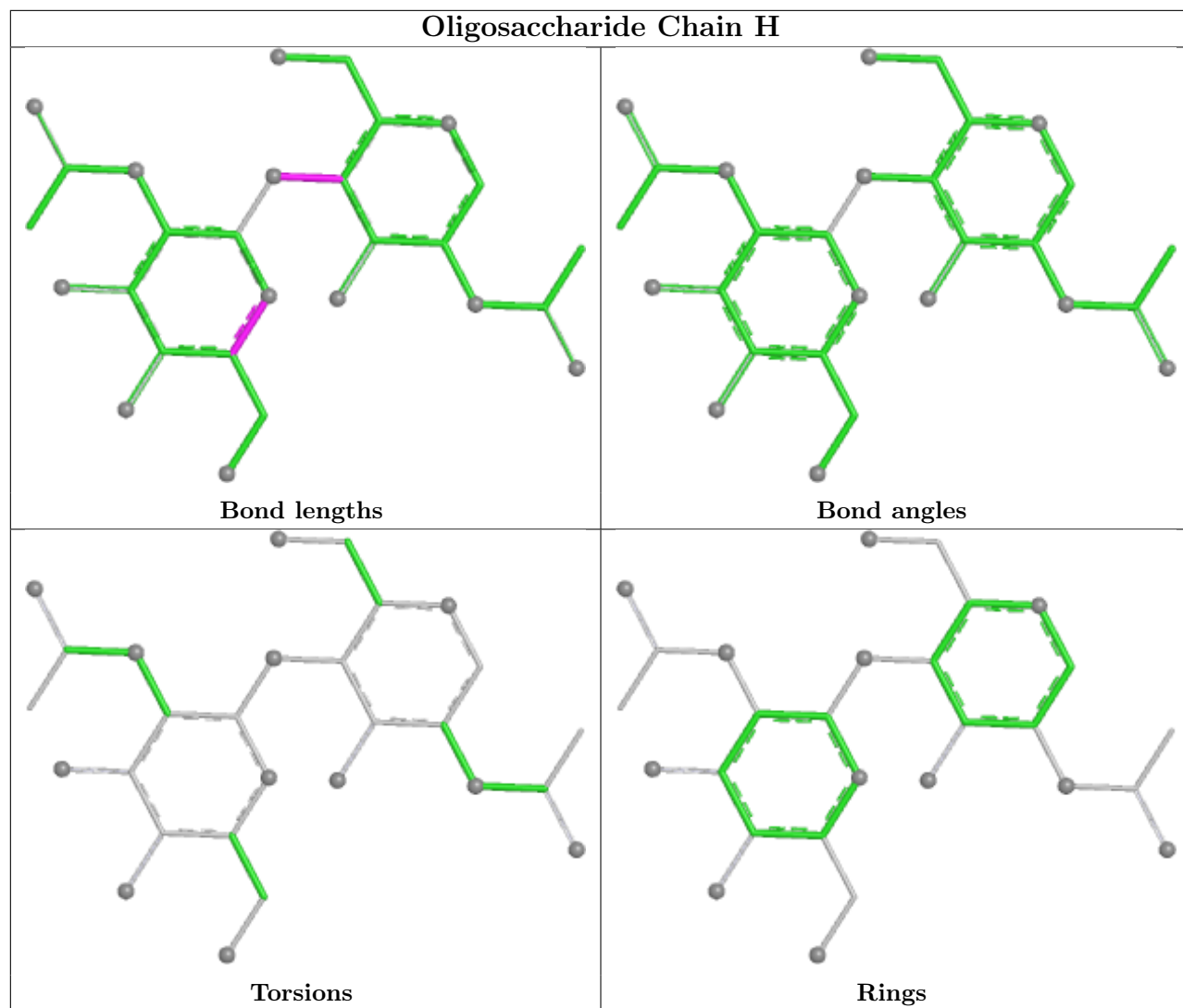


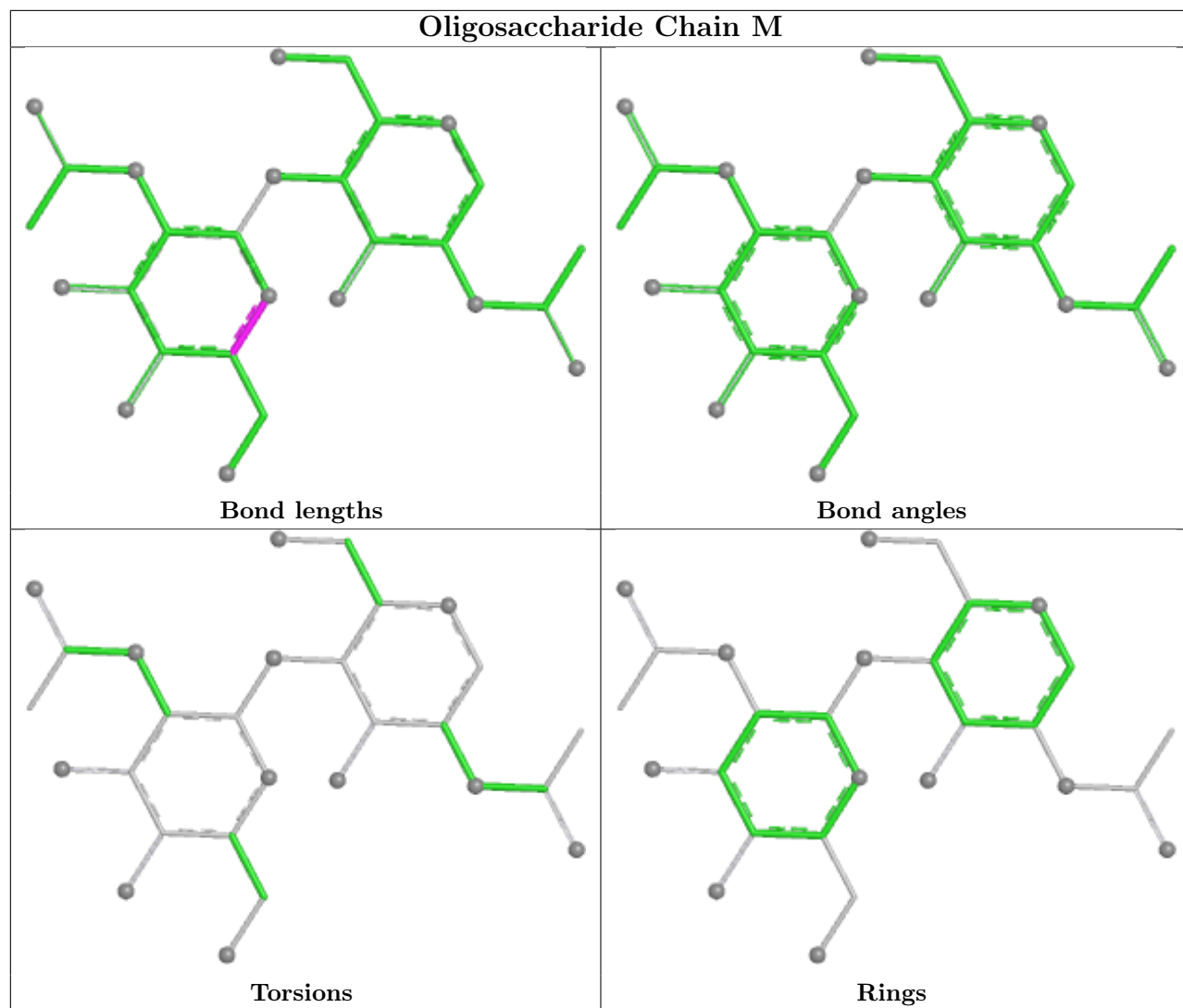


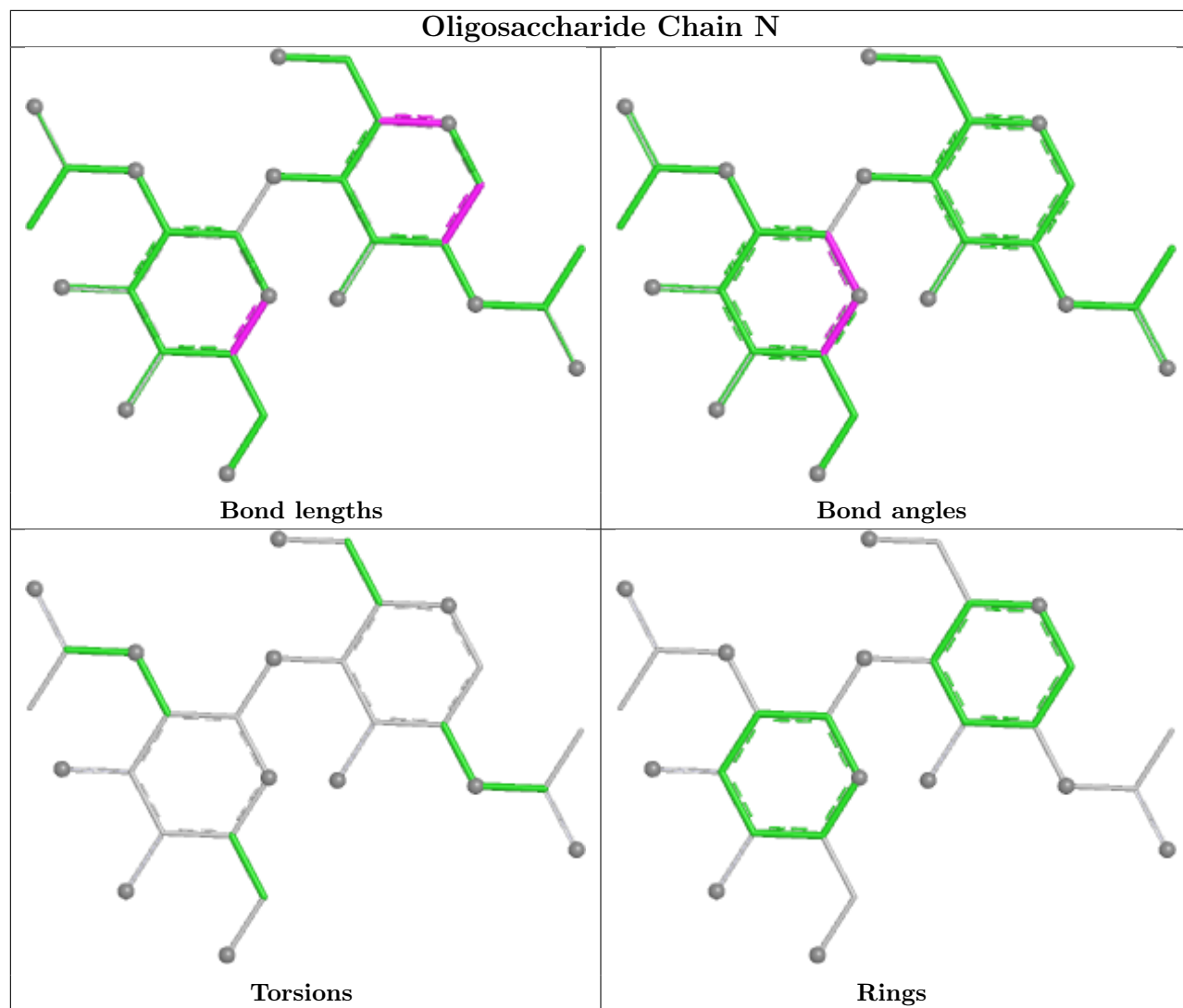


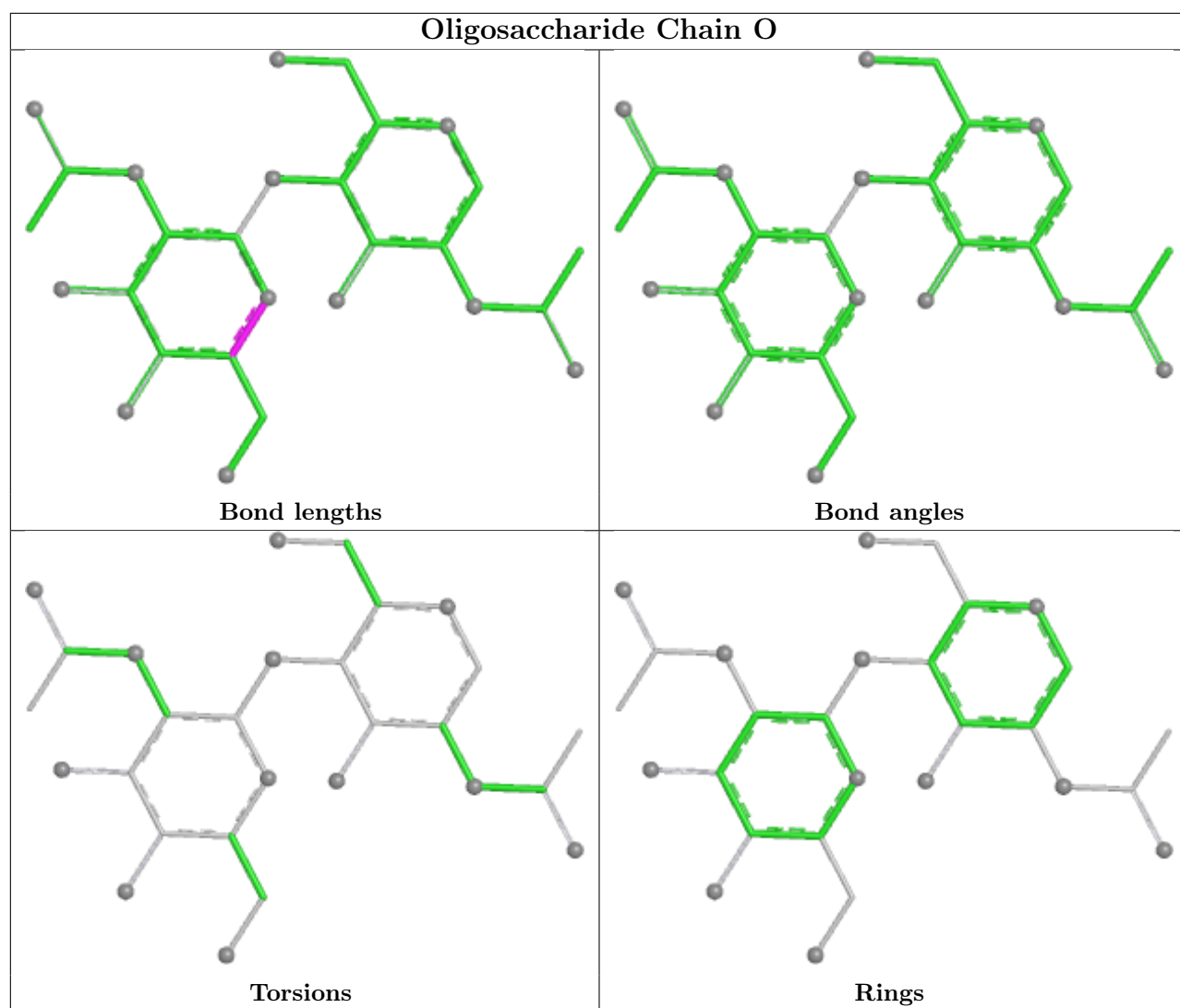


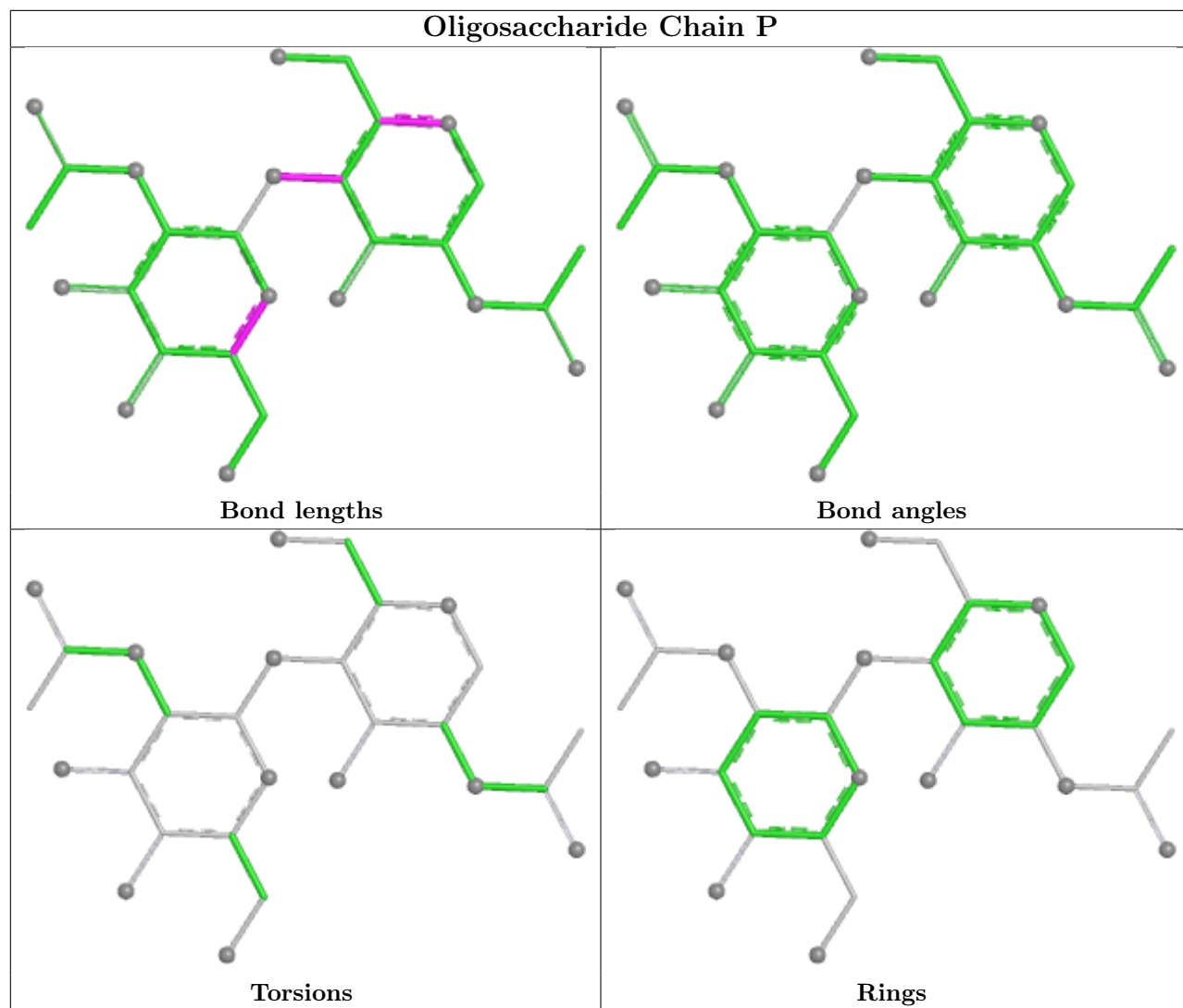


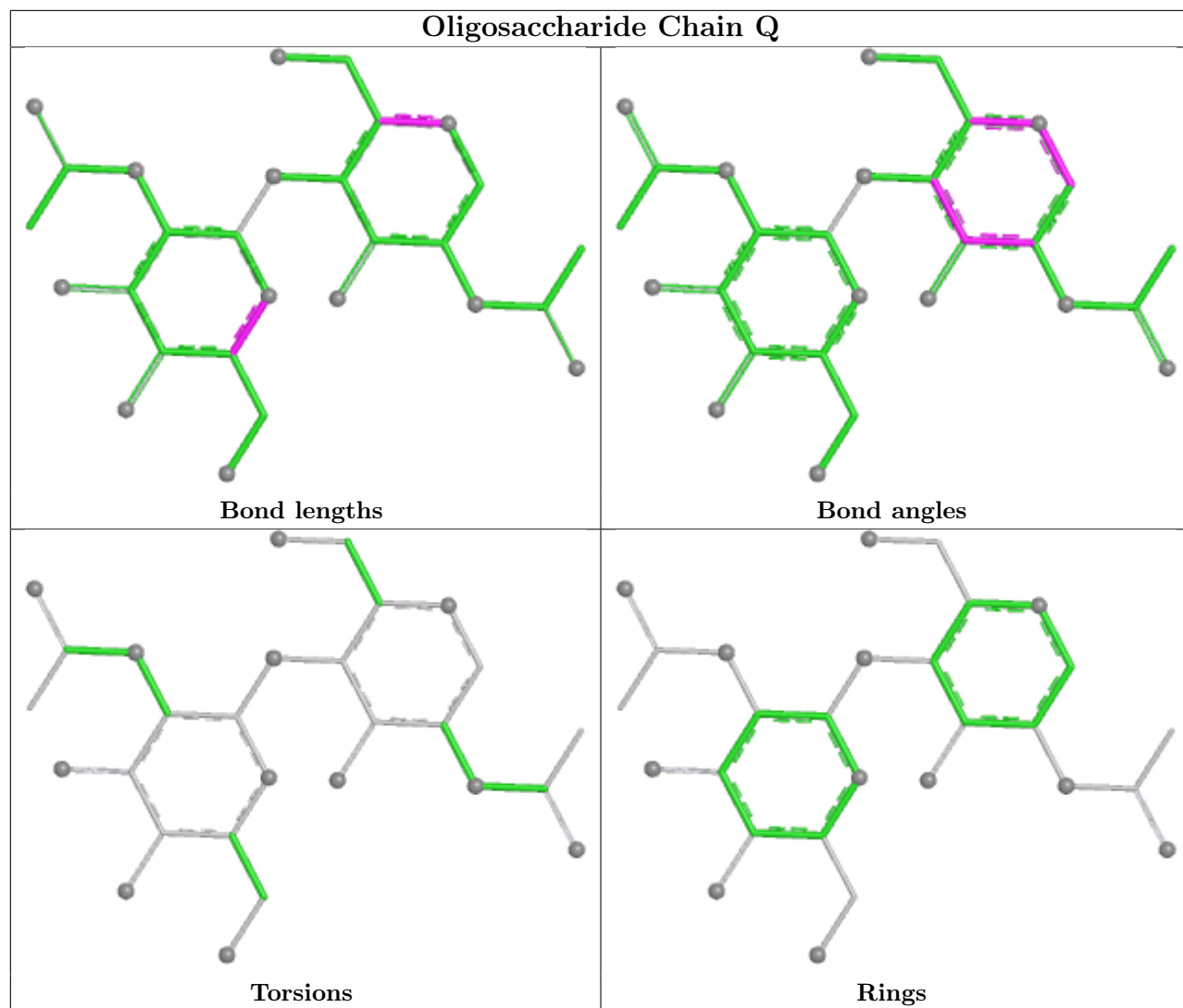


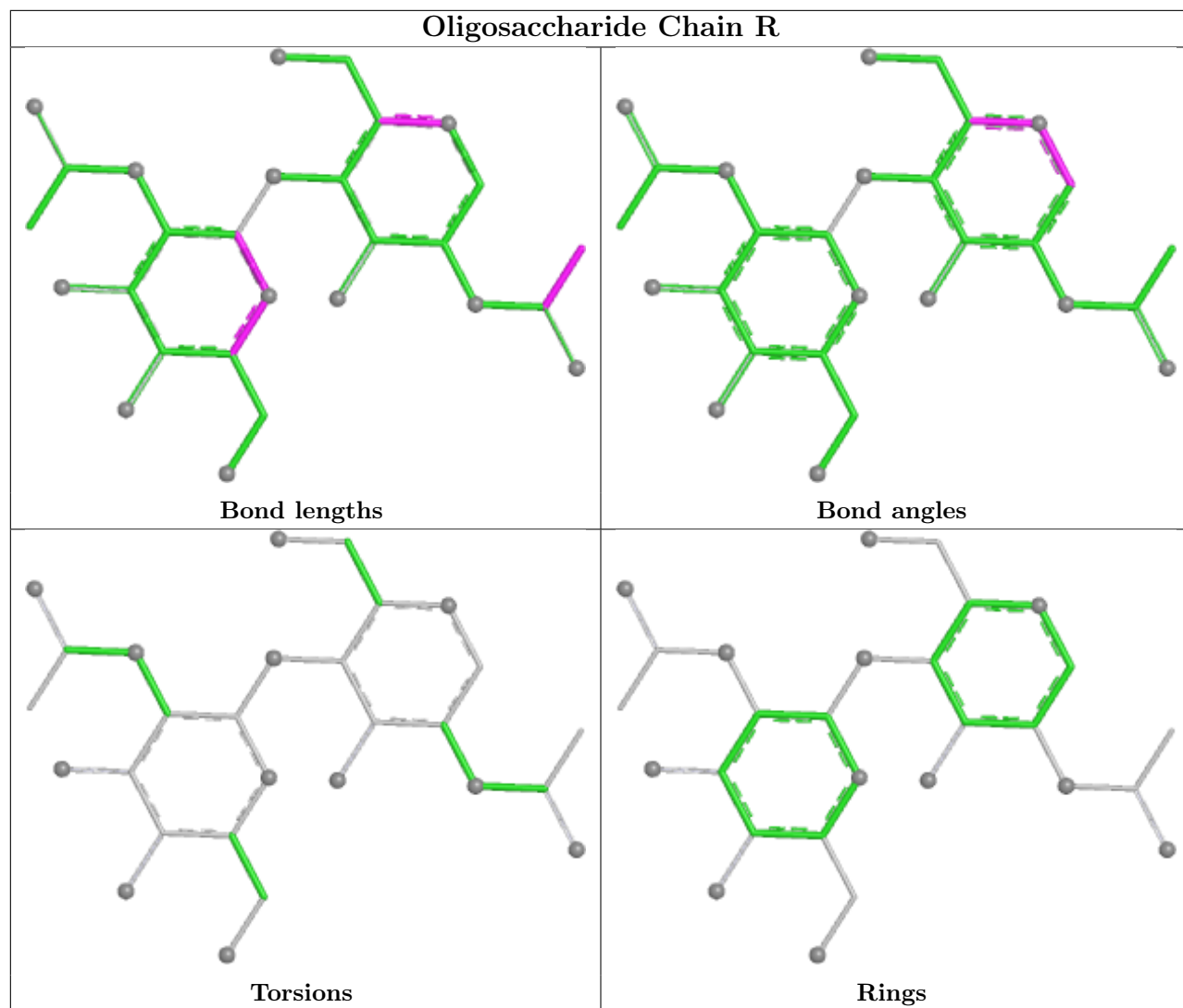


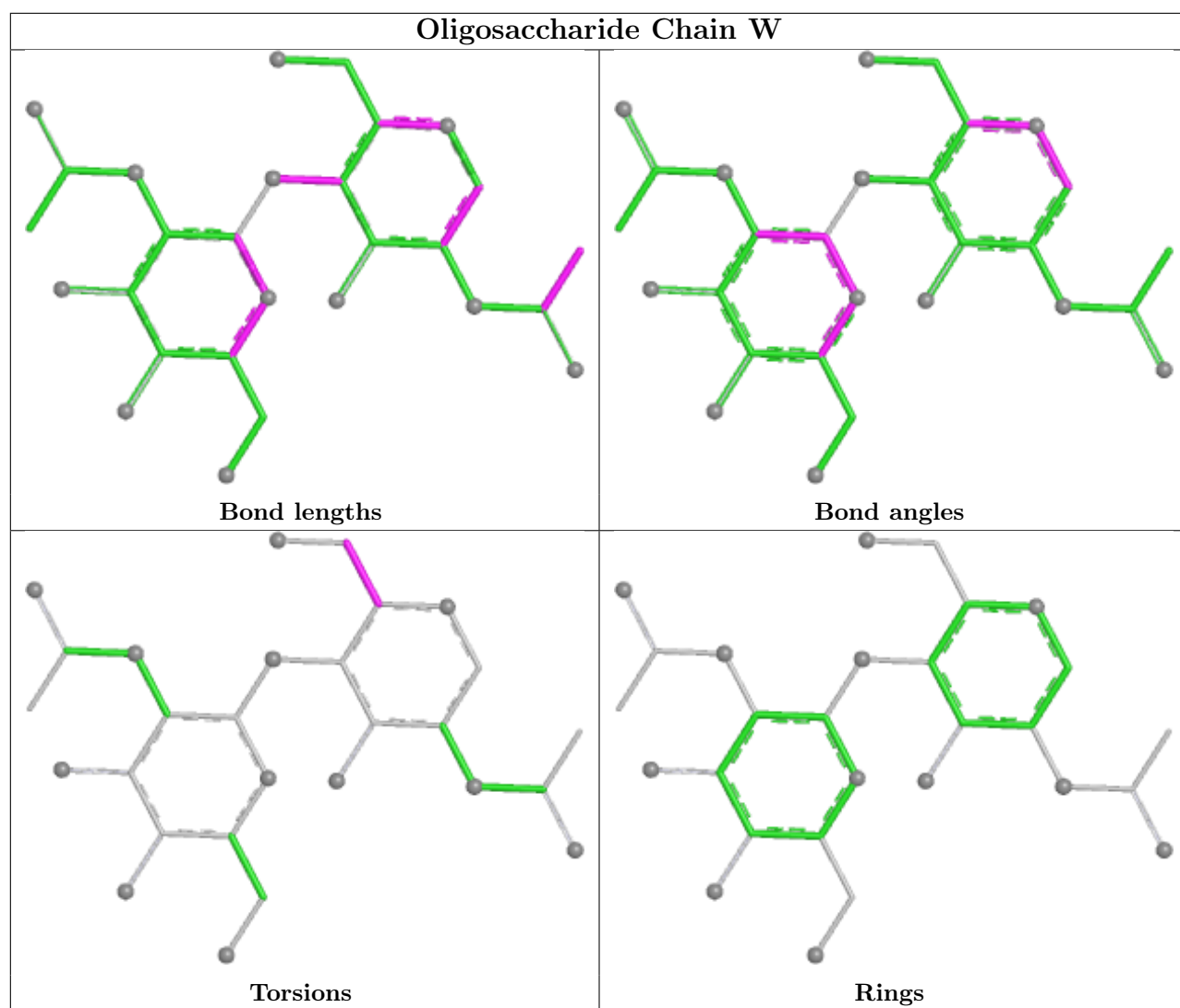


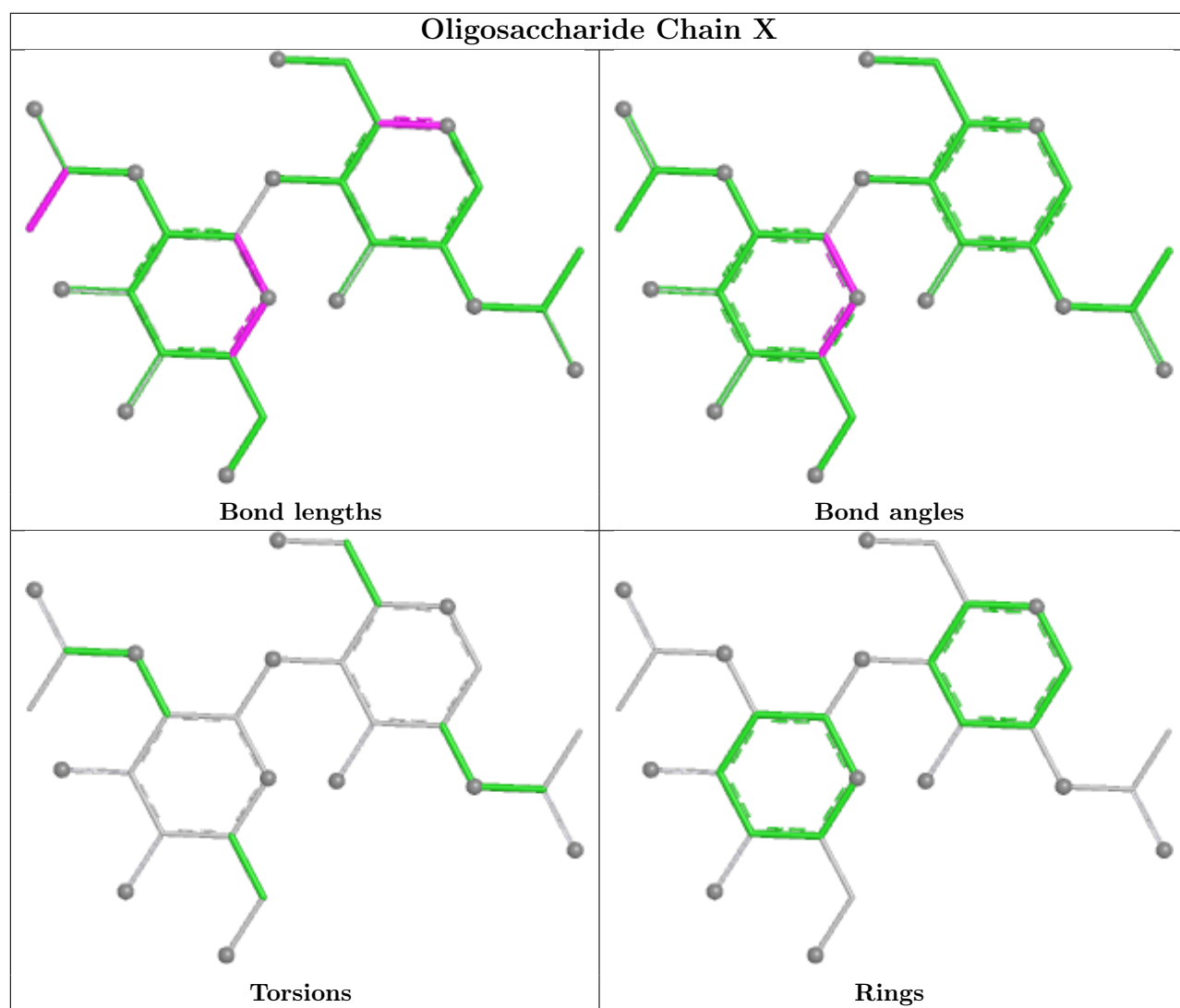


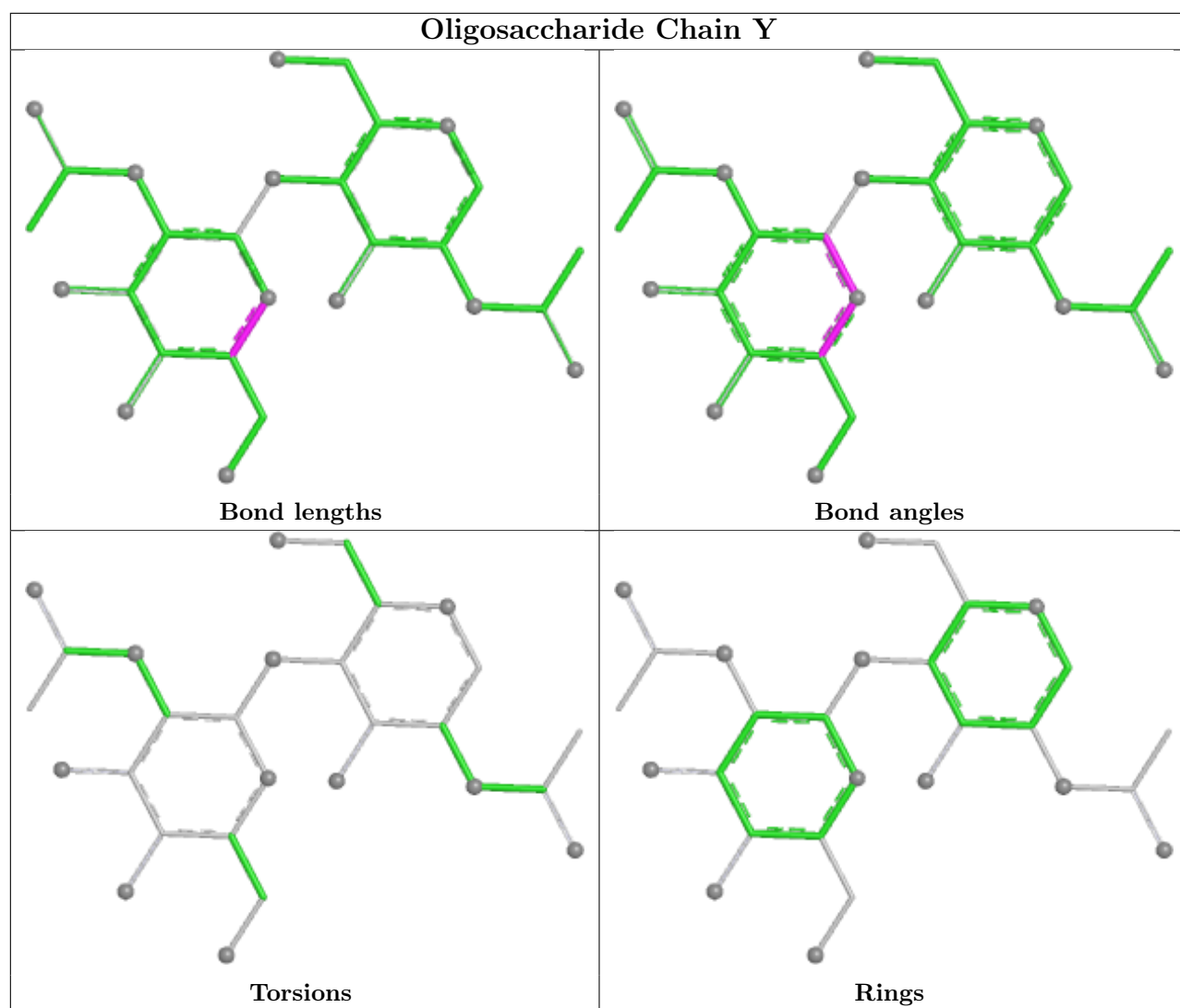


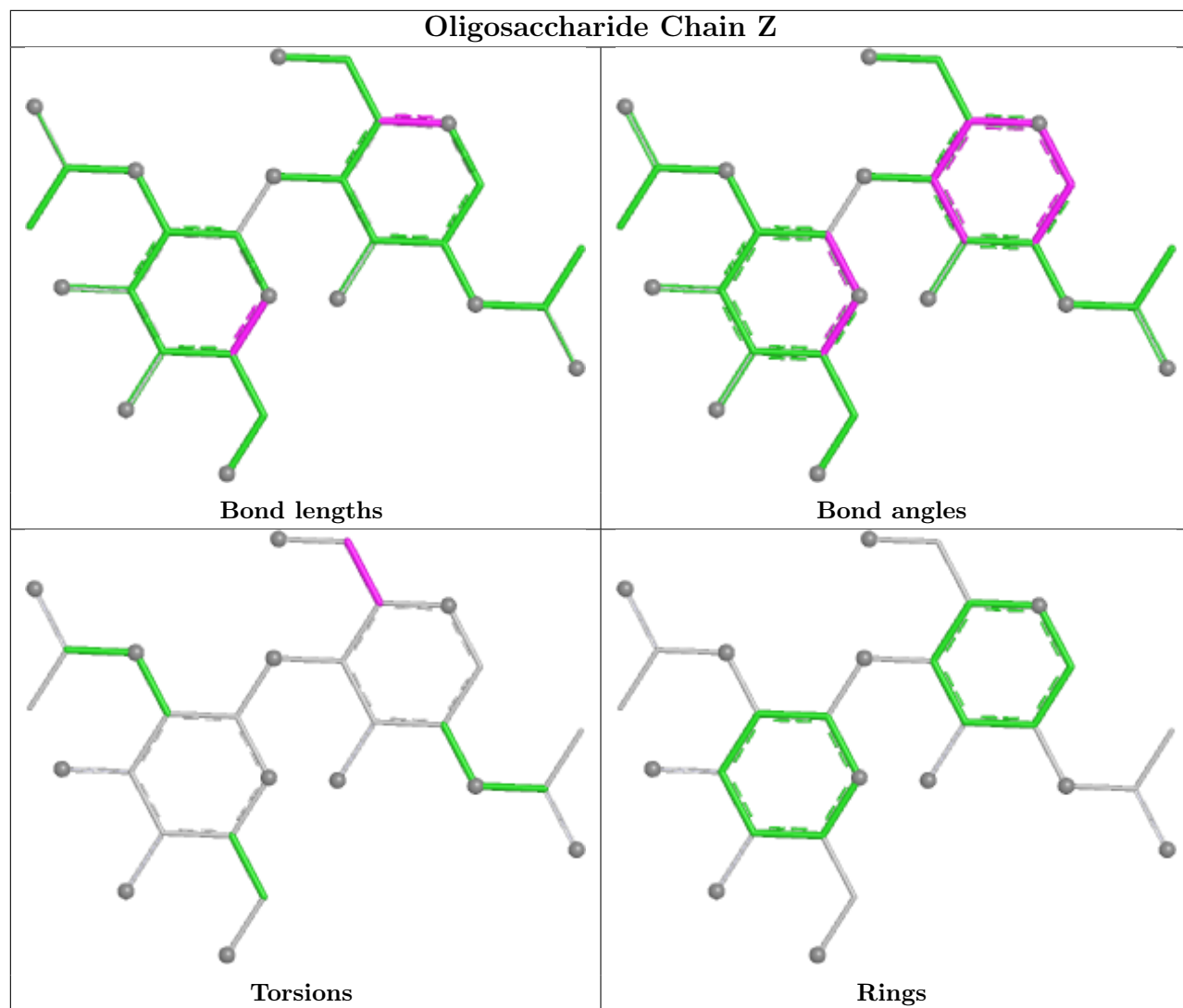


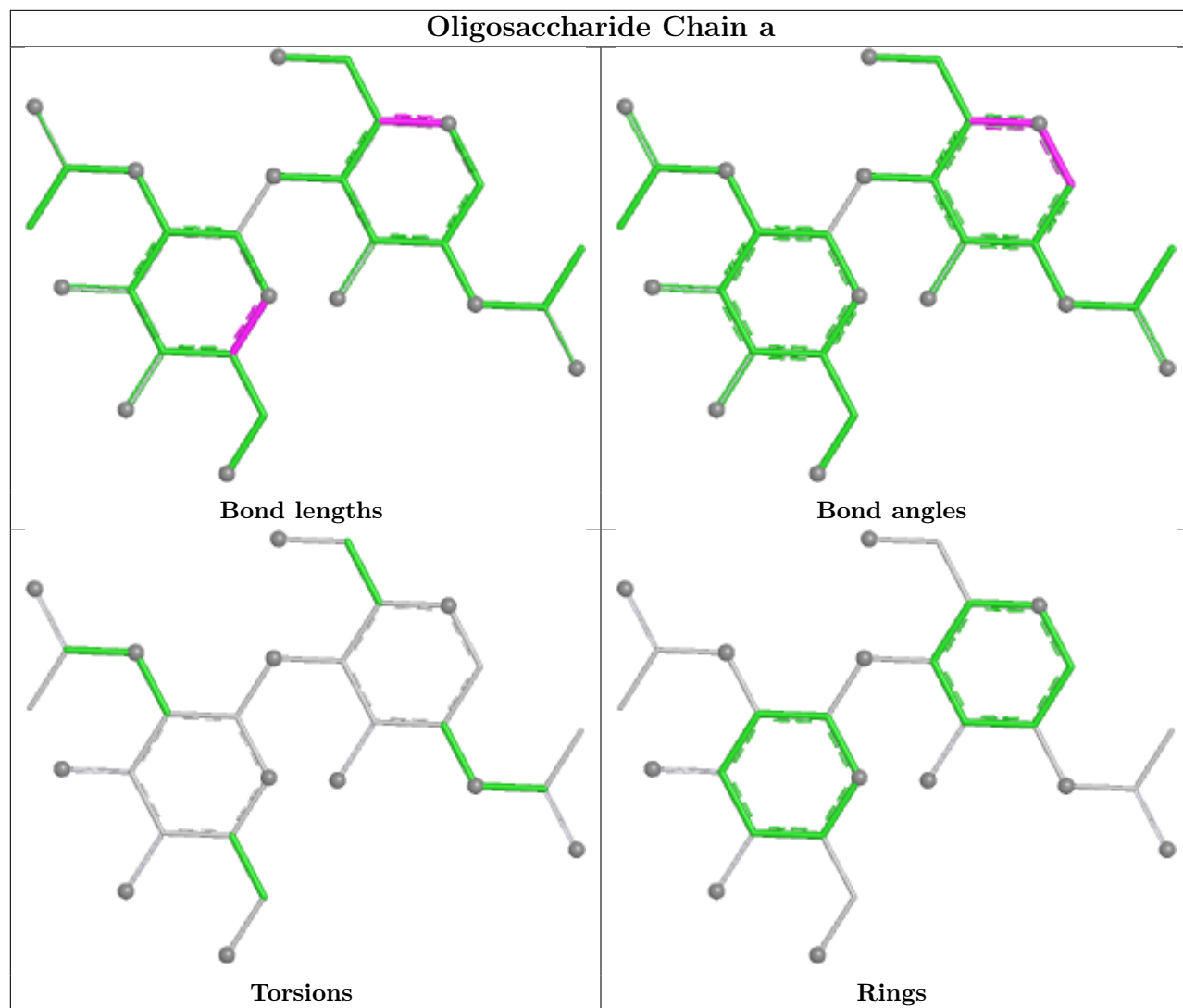


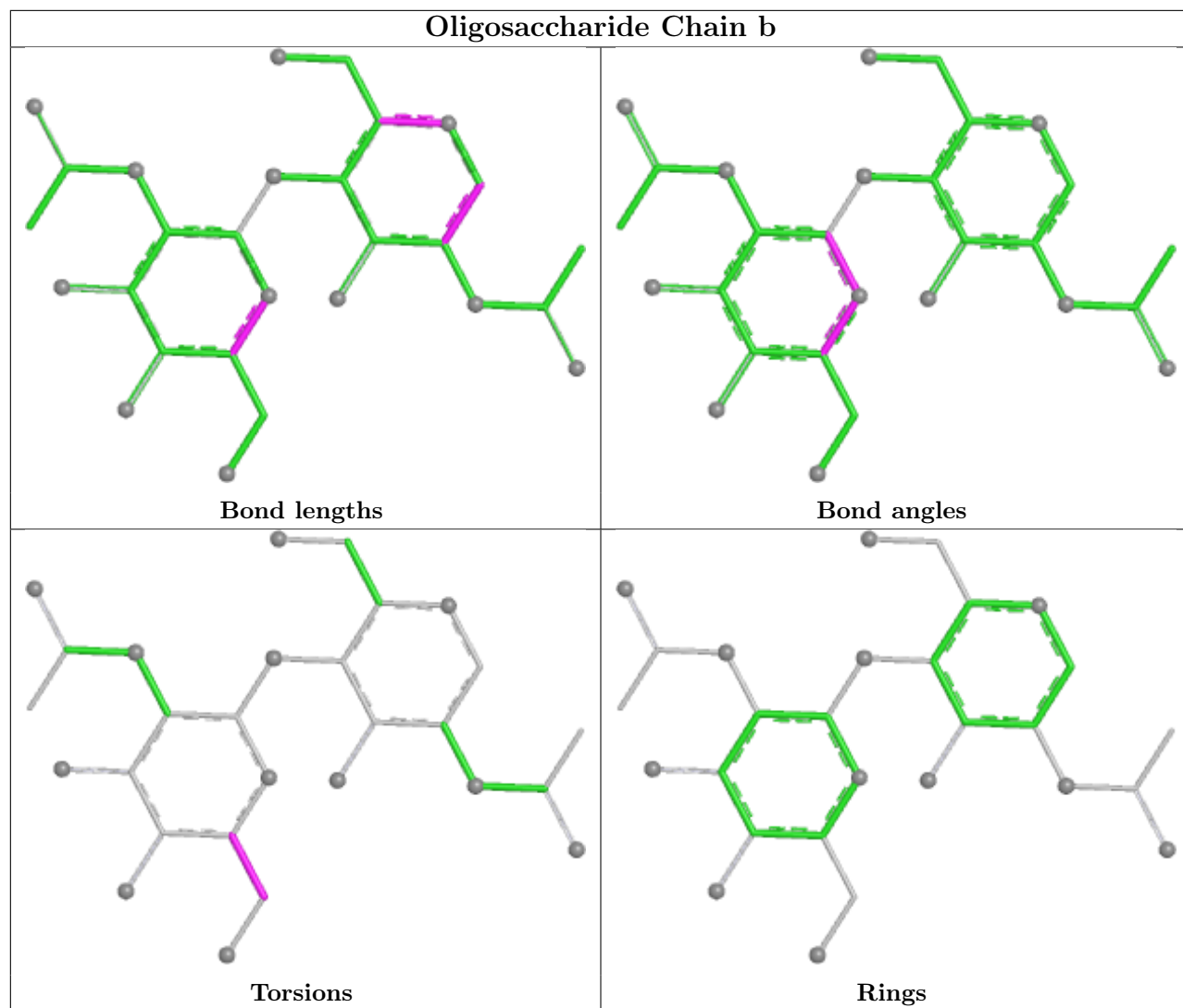


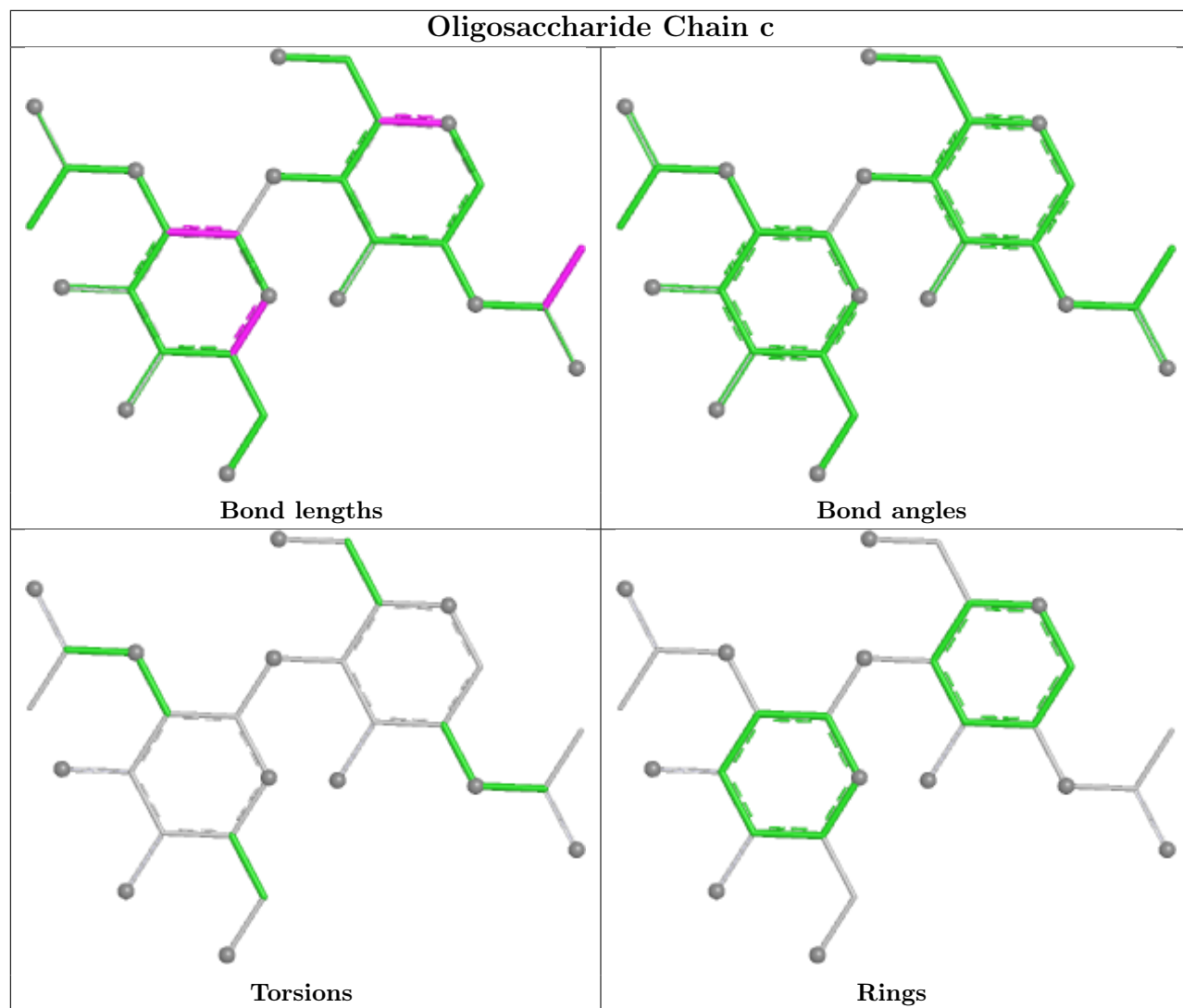


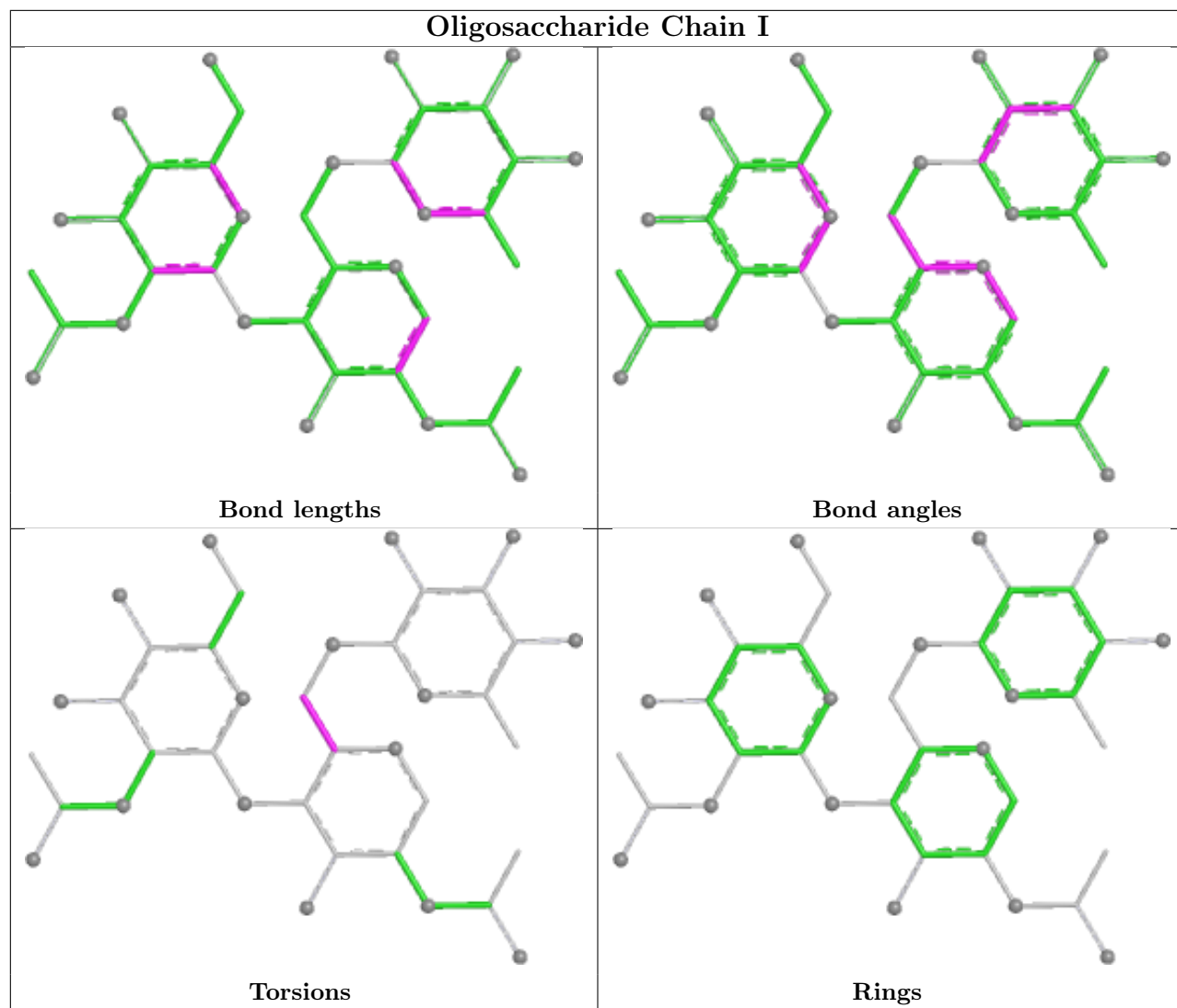


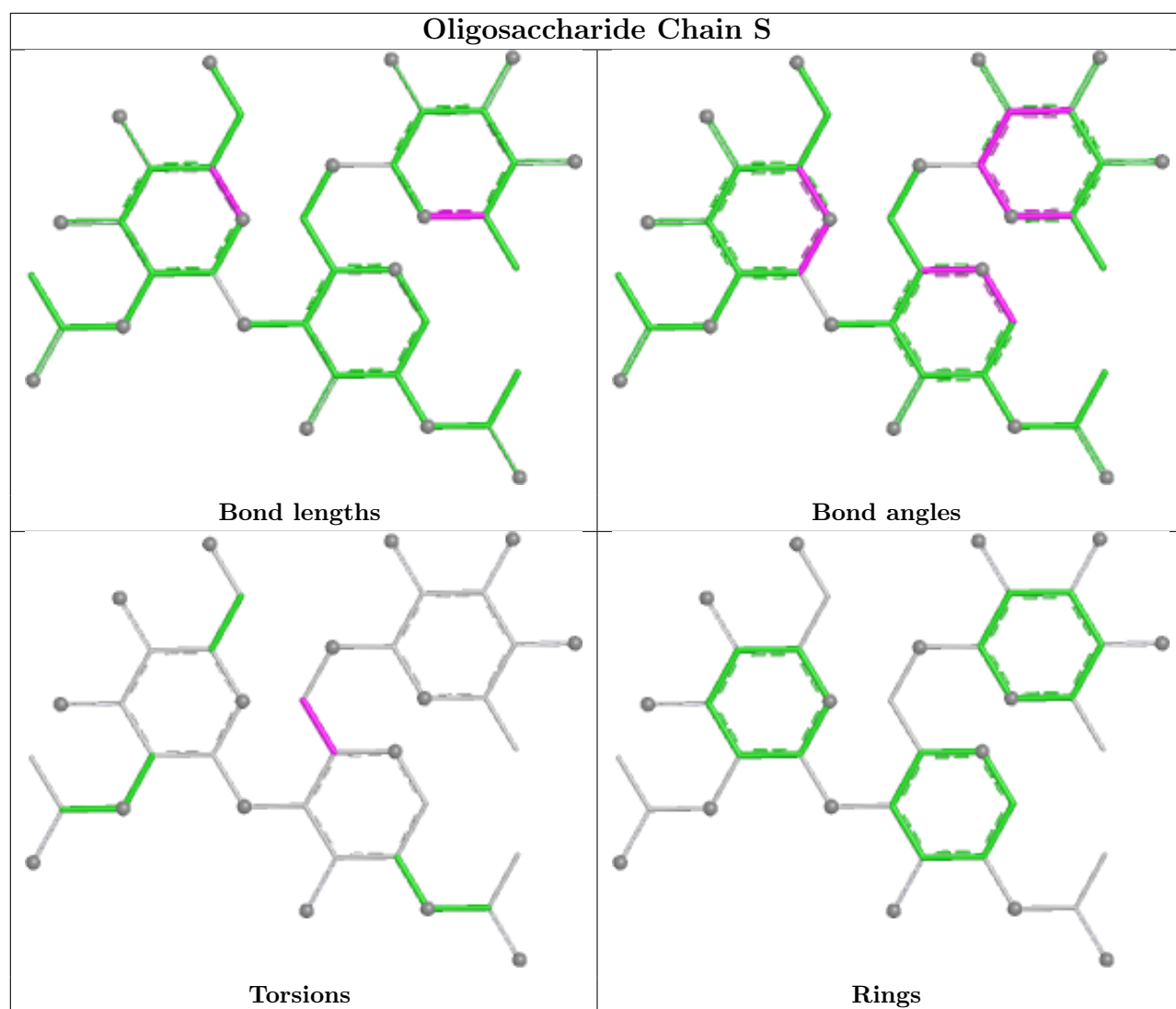


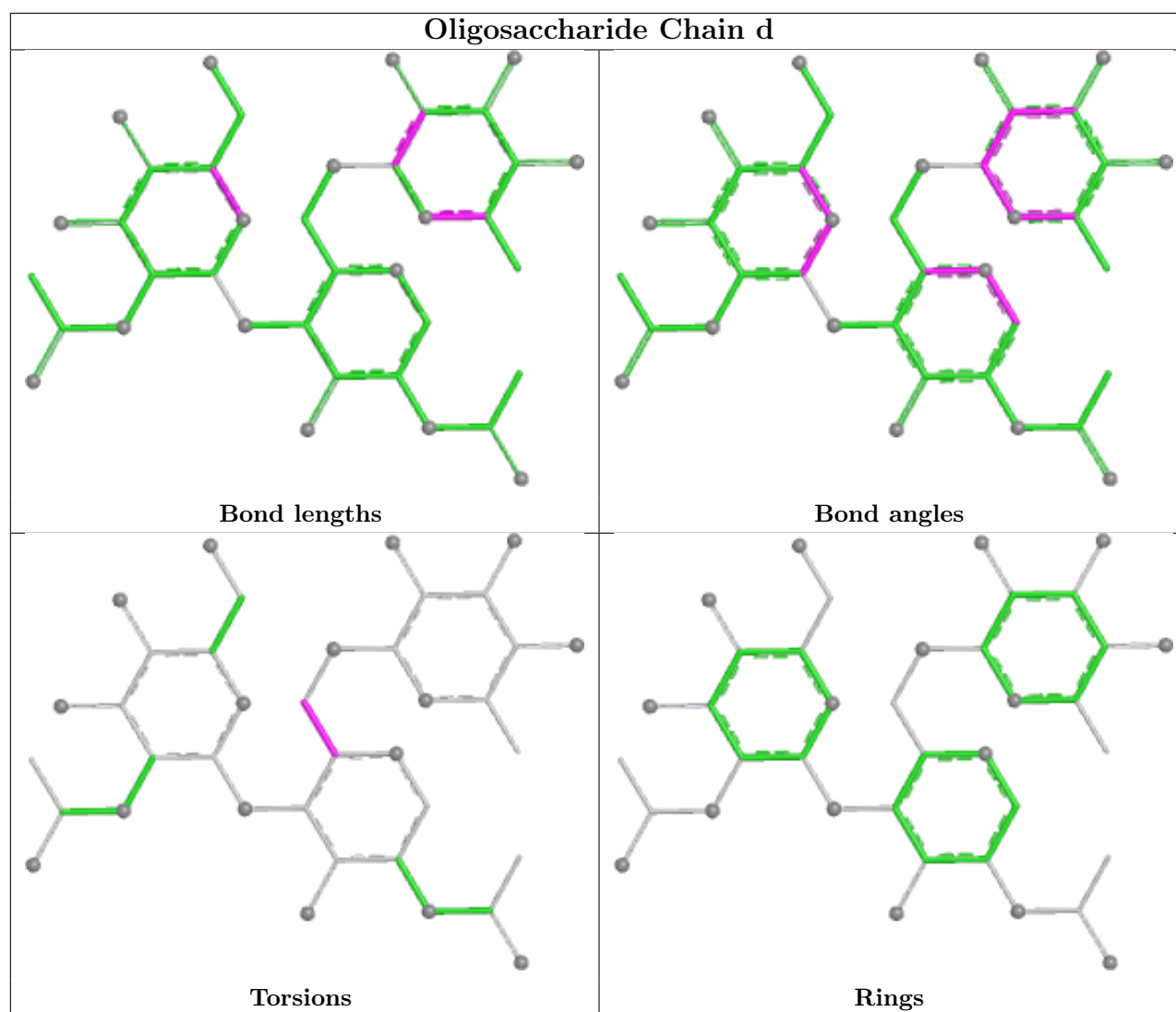












5.6 Ligand geometry [i](#)

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	A	1401	1	14,14,15	1.39	2 (14%)	17,19,21	1.40	1 (5%)
5	NAG	A	1403	1	14,14,15	0.54	0	17,19,21	0.63	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1405	1	14,14,15	1.15	1 (7%)	17,19,21	0.80	0
5	NAG	B	1408	1	14,14,15	1.33	3 (21%)	17,19,21	0.88	0
5	NAG	A	1408	1	14,14,15	1.29	2 (14%)	17,19,21	0.78	0
5	NAG	B	1406	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	C	1403	1	14,14,15	1.58	2 (14%)	17,19,21	0.73	0
5	NAG	A	1402	1	14,14,15	1.16	1 (7%)	17,19,21	1.32	2 (11%)
5	NAG	C	1404	1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	B	1403	1	14,14,15	0.27	0	17,19,21	0.56	0
5	NAG	A	1406	1	14,14,15	1.29	3 (21%)	17,19,21	0.73	0
5	NAG	C	1402	1	14,14,15	1.14	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	B	1404	1	14,14,15	1.57	2 (14%)	17,19,21	0.73	0
5	NAG	B	1405	1	14,14,15	1.58	2 (14%)	17,19,21	0.70	0
5	NAG	C	1406	1	14,14,15	1.49	3 (21%)	17,19,21	0.65	0
5	NAG	A	1404	1	14,14,15	0.33	0	17,19,21	0.60	0
5	NAG	A	1405	1	14,14,15	0.34	0	17,19,21	0.45	0
5	NAG	A	1409	1	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	B	1401	1	14,14,15	0.52	0	17,19,21	0.45	0
5	NAG	B	1402	1	14,14,15	1.17	1 (7%)	17,19,21	0.71	0
5	NAG	B	1407	1	14,14,15	1.15	2 (14%)	17,19,21	0.60	0
5	NAG	A	1407	1	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	C	1401	1	14,14,15	0.61	0	17,19,21	0.43	0
5	NAG	C	1407	1	14,14,15	1.23	1 (7%)	17,19,21	0.69	0

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

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

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1403	NAG	O5-C1	-4.29	1.36	1.43
5	B	1404	NAG	O5-C1	-4.23	1.36	1.43
5	B	1405	NAG	C1-C2	4.17	1.58	1.52
5	A	1402	NAG	O5-C5	3.43	1.50	1.43
5	C	1405	NAG	O5-C5	3.11	1.49	1.43
5	A	1401	NAG	C1-C2	3.03	1.56	1.52
5	A	1401	NAG	O5-C5	2.95	1.49	1.43
5	C	1406	NAG	O5-C5	2.95	1.49	1.43
5	C	1406	NAG	C8-C7	2.91	1.56	1.50
5	C	1402	NAG	O5-C5	2.81	1.48	1.43
5	B	1408	NAG	O5-C5	2.78	1.48	1.43
5	B	1404	NAG	O5-C5	2.77	1.48	1.43
5	C	1403	NAG	O5-C5	2.76	1.48	1.43
5	A	1408	NAG	O5-C5	2.74	1.48	1.43
5	C	1407	NAG	O5-C5	2.70	1.48	1.43
5	B	1402	NAG	O5-C5	2.65	1.48	1.43
5	B	1405	NAG	O5-C5	2.59	1.48	1.43
5	A	1408	NAG	C1-C2	2.42	1.55	1.52
5	A	1406	NAG	O5-C5	2.34	1.48	1.43
5	B	1407	NAG	O5-C5	2.19	1.47	1.43
5	B	1408	NAG	C1-C2	2.17	1.55	1.52
5	C	1406	NAG	C1-C2	2.16	1.55	1.52
5	A	1406	NAG	C1-C2	2.15	1.55	1.52
5	A	1406	NAG	O5-C1	2.13	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1408	NAG	O5-C1	2.12	1.47	1.43
5	B	1407	NAG	C1-C2	2.03	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1401	NAG	C1-O5-C5	4.96	118.83	112.19
5	C	1402	NAG	C1-O5-C5	3.08	116.31	112.19
5	A	1402	NAG	C1-O5-C5	2.95	116.14	112.19
5	A	1402	NAG	C4-C3-C2	-2.60	107.20	111.02
5	A	1403	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

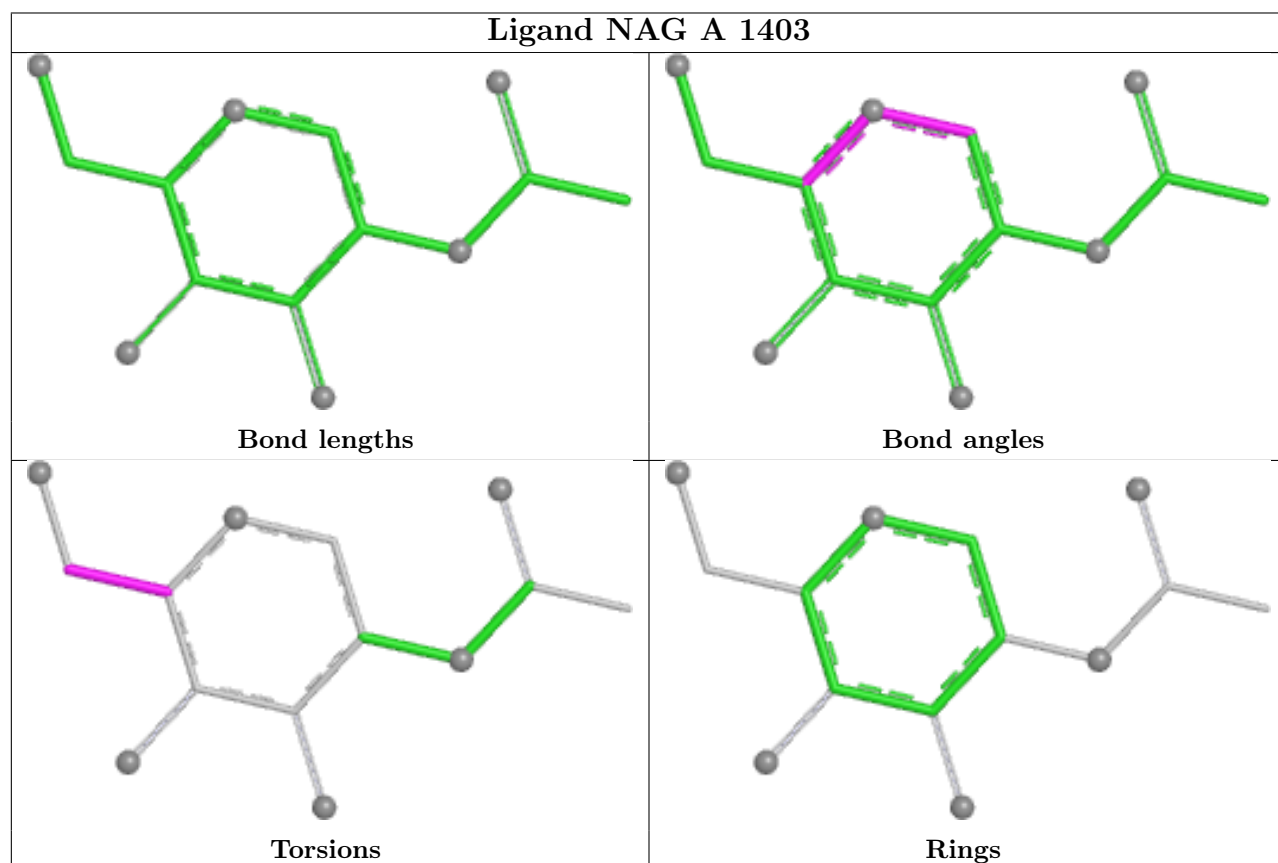
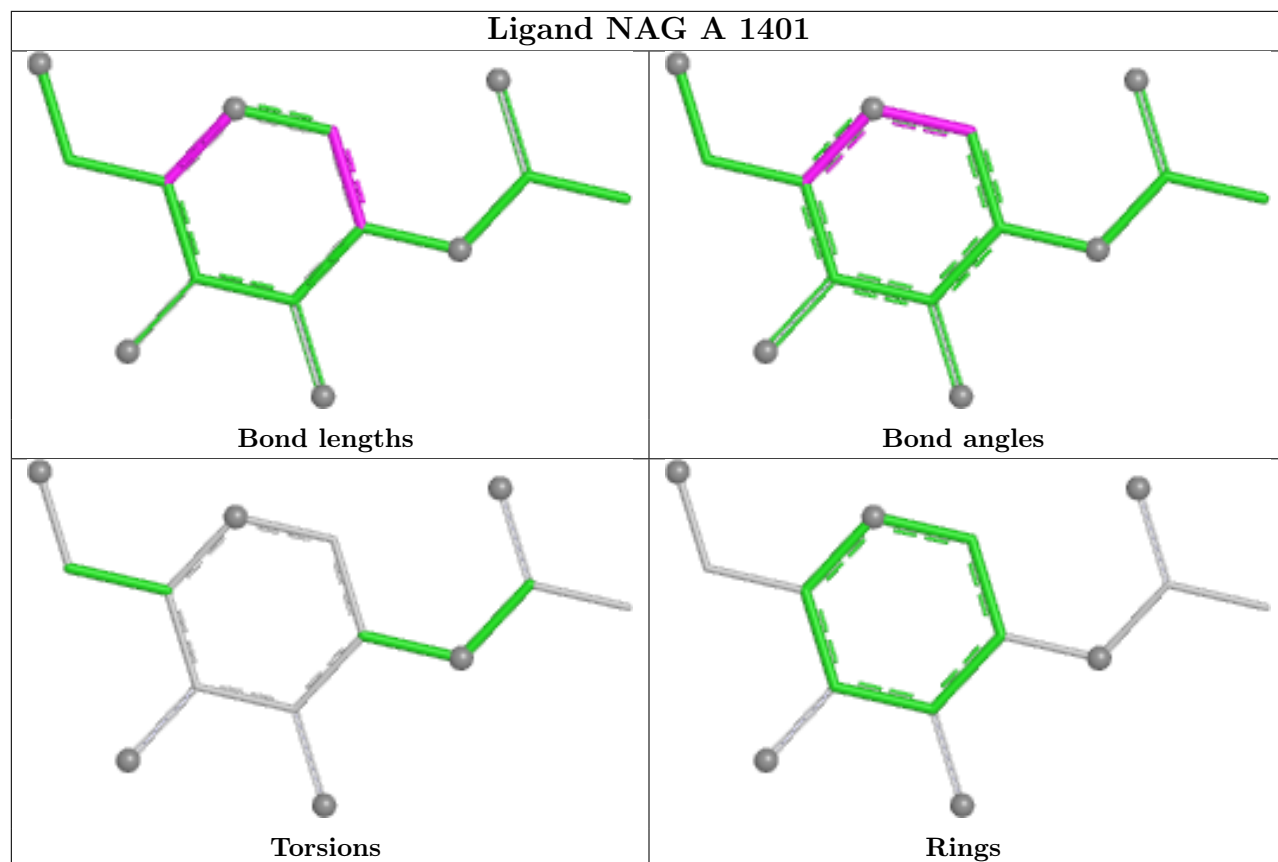
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1401	NAG	O5-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6

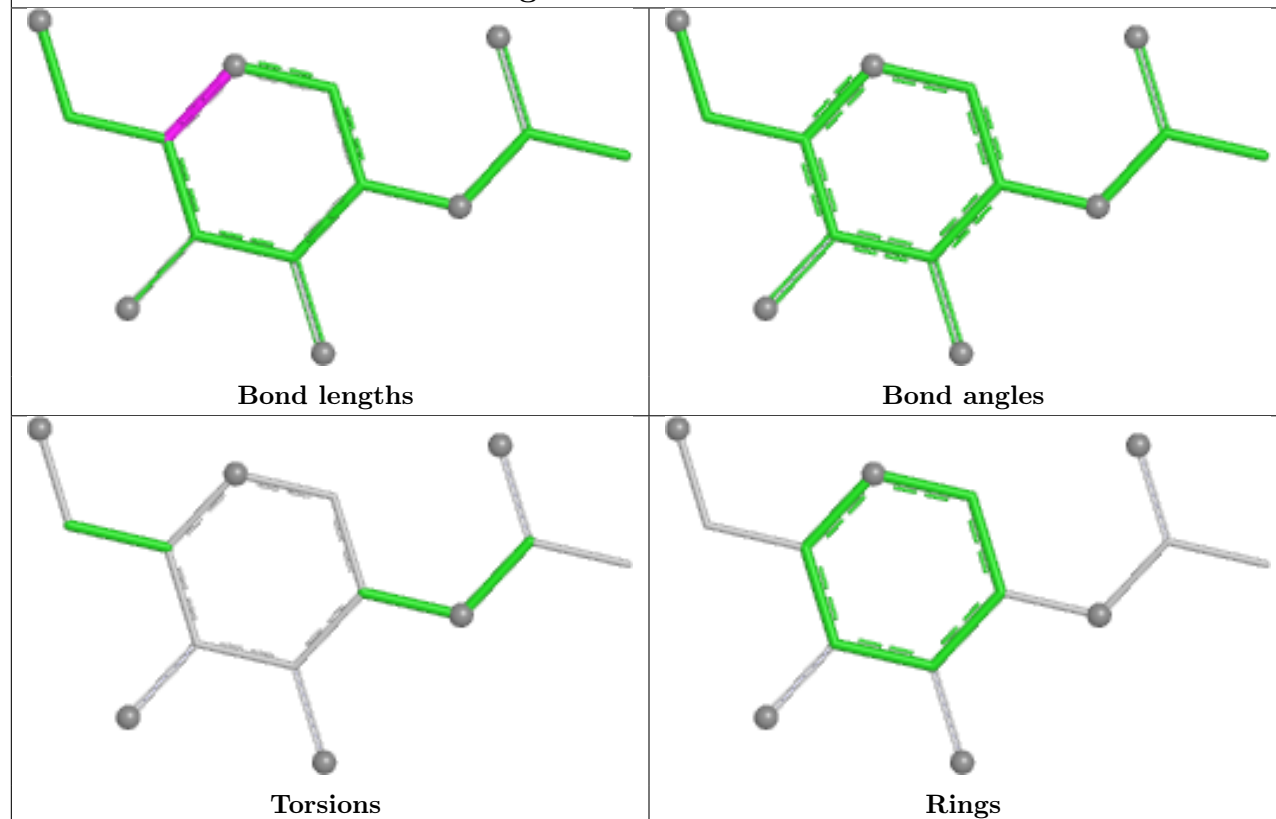
There are no ring outliers.

No monomer is involved in short contacts.

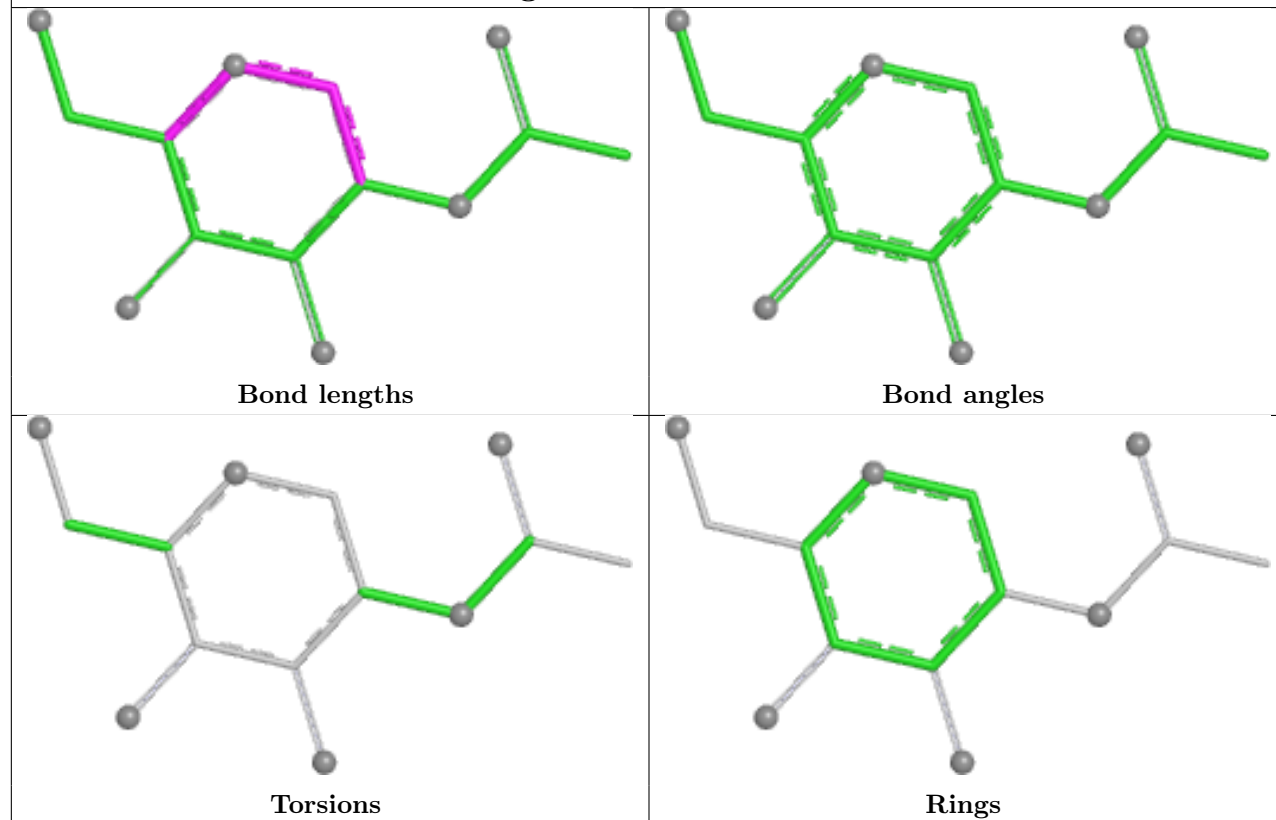
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

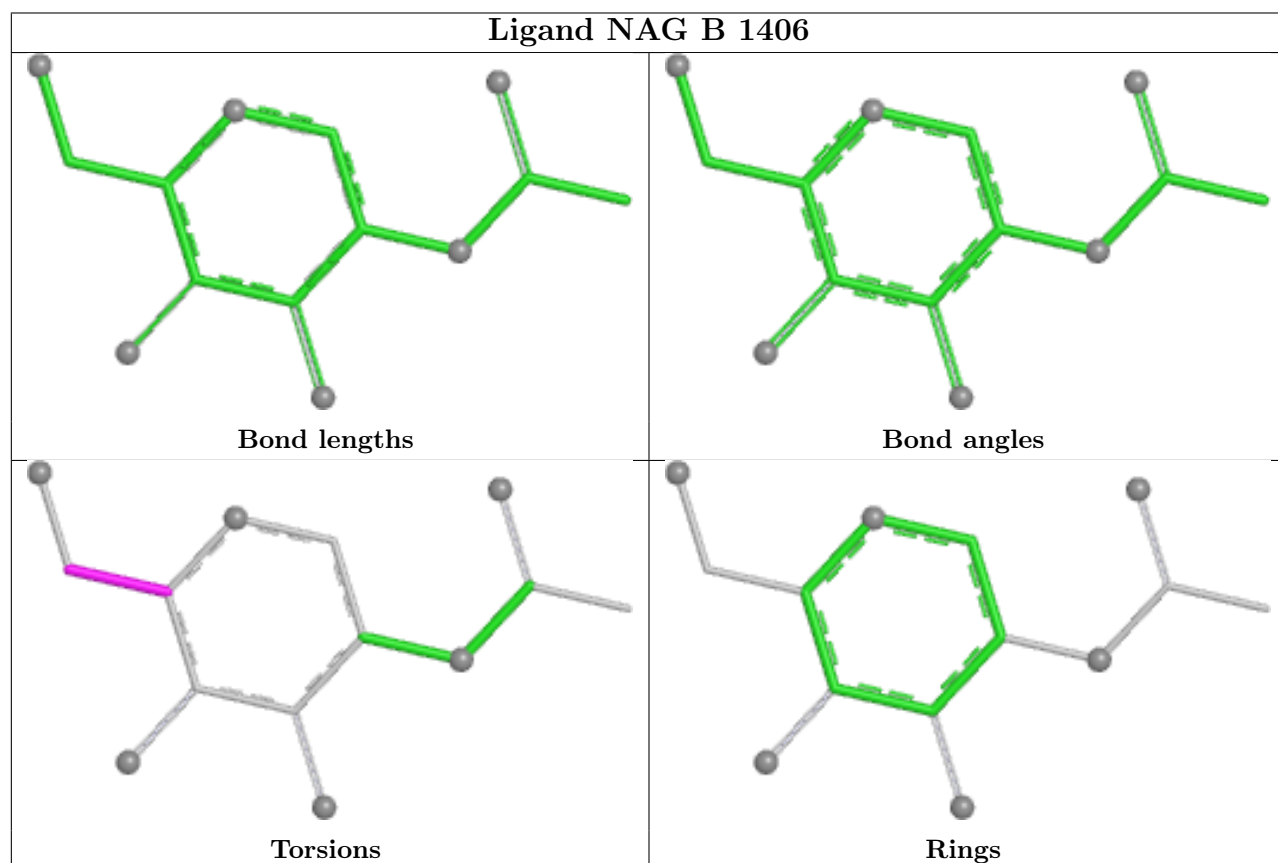
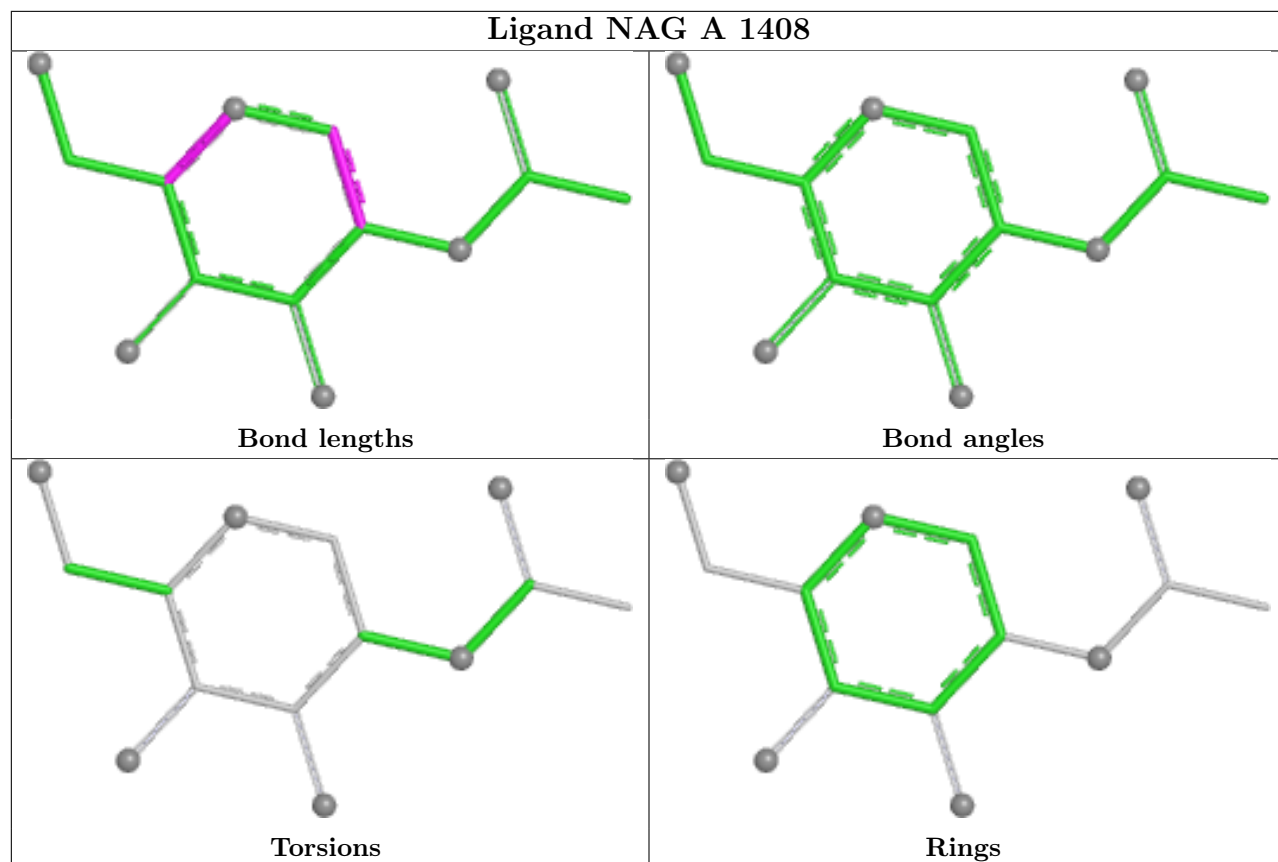


Ligand NAG C 1405

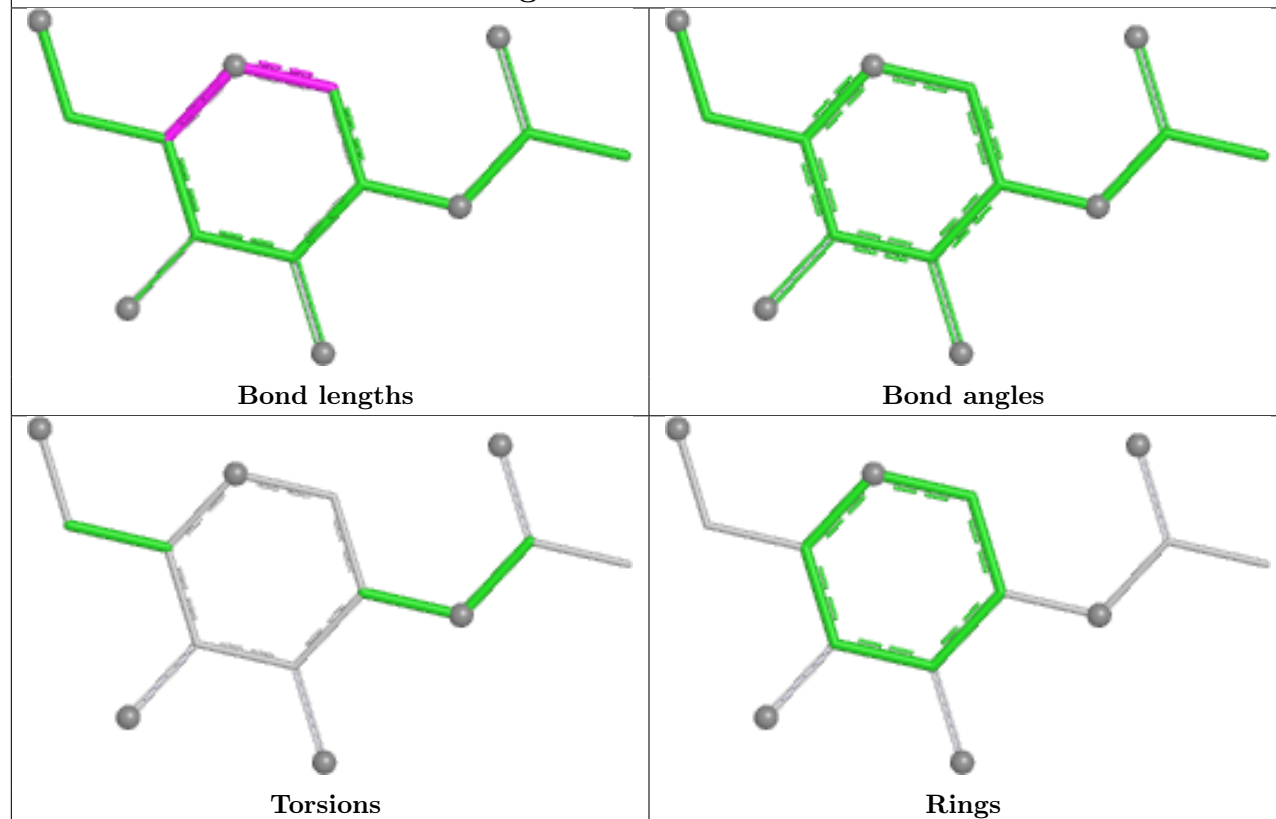


Ligand NAG B 1408

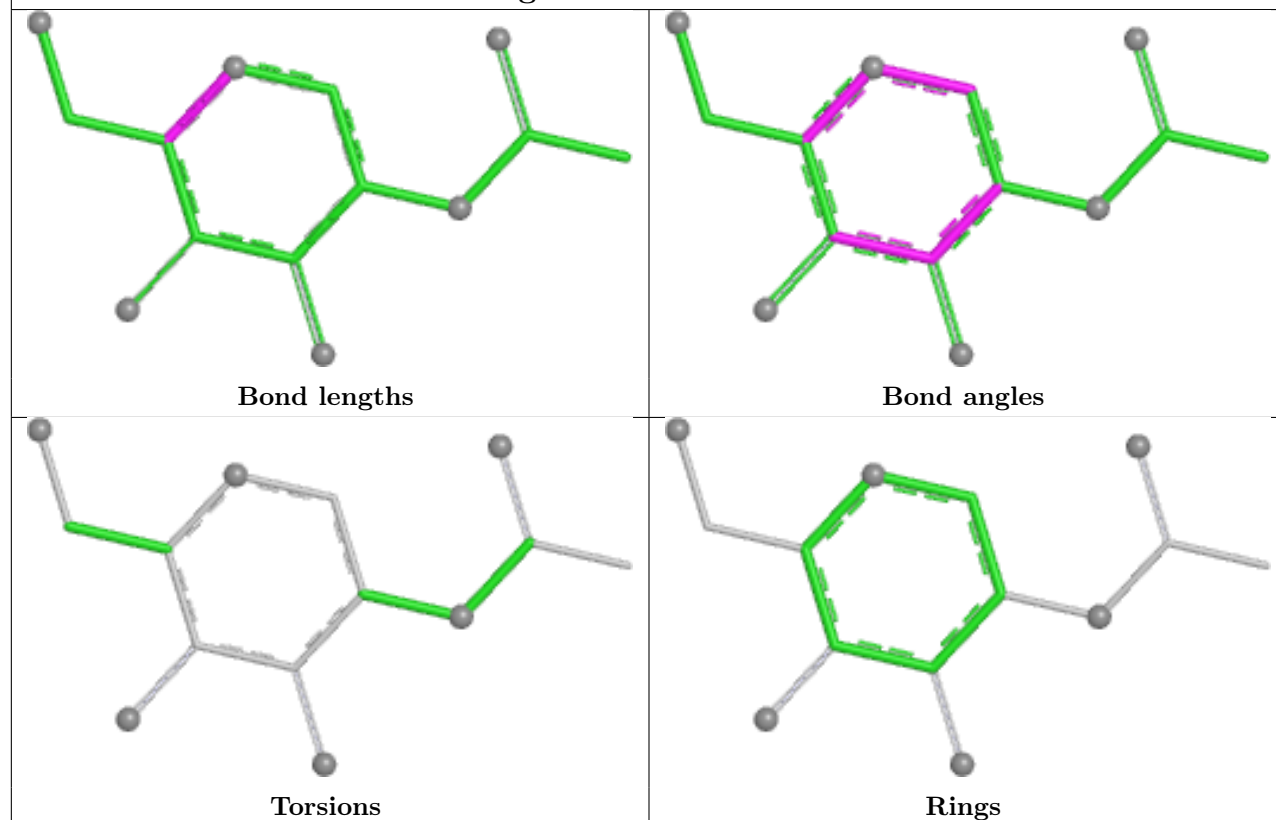


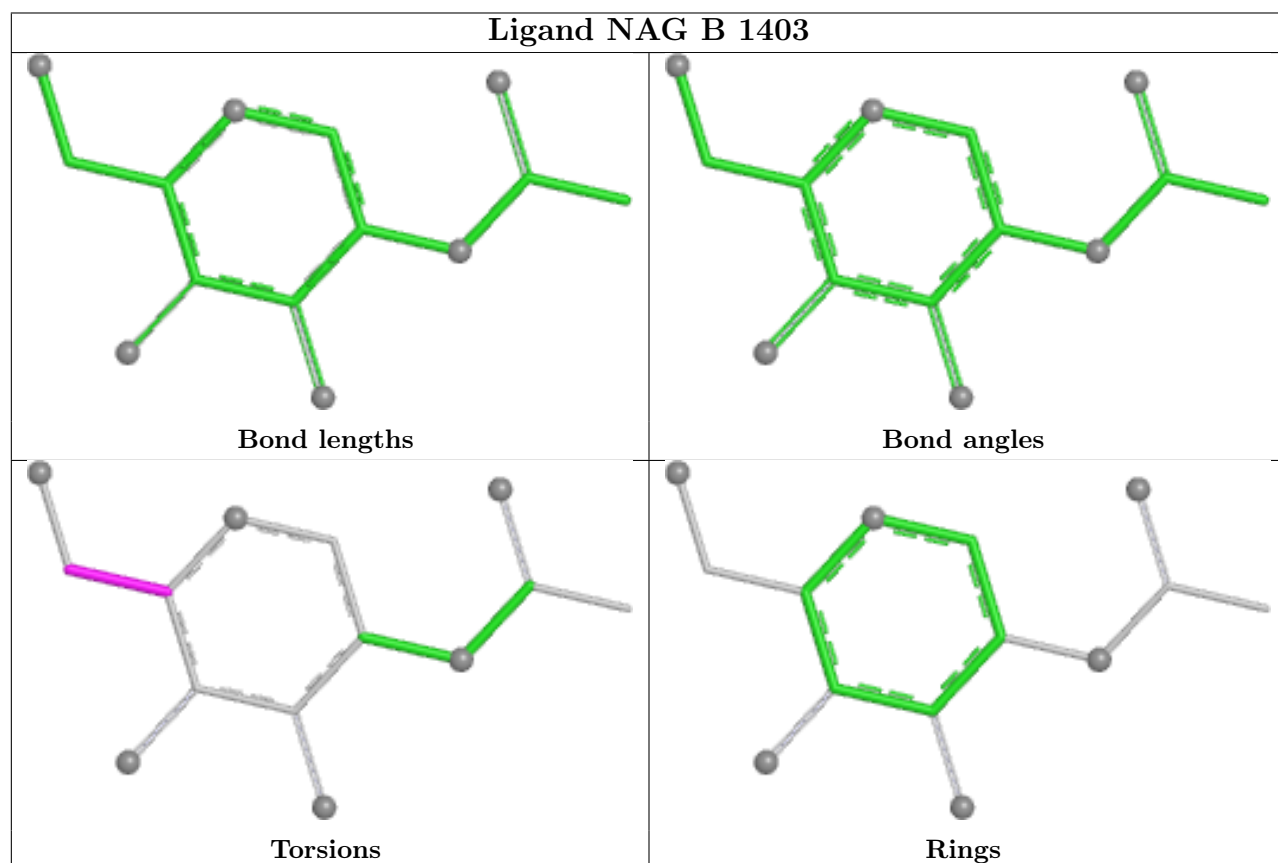
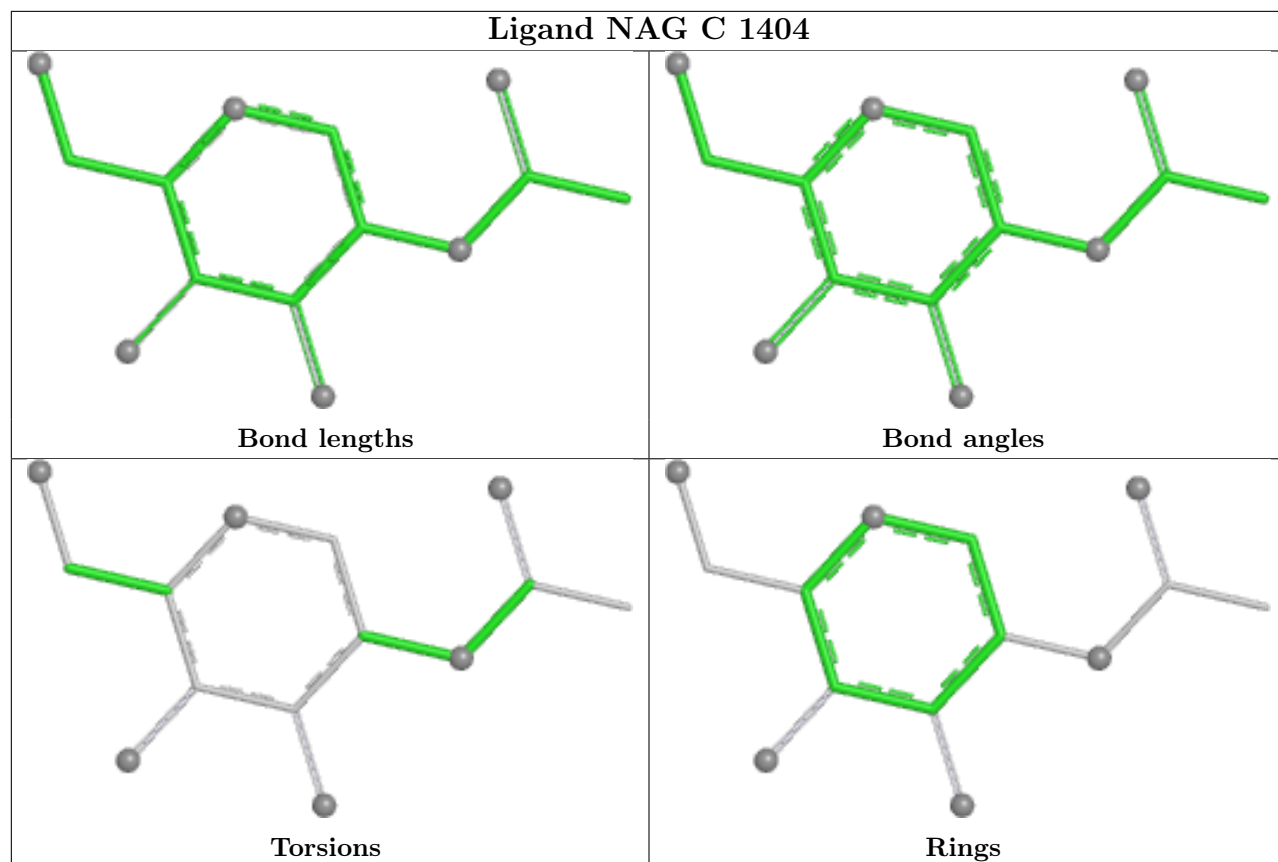


Ligand NAG C 1403

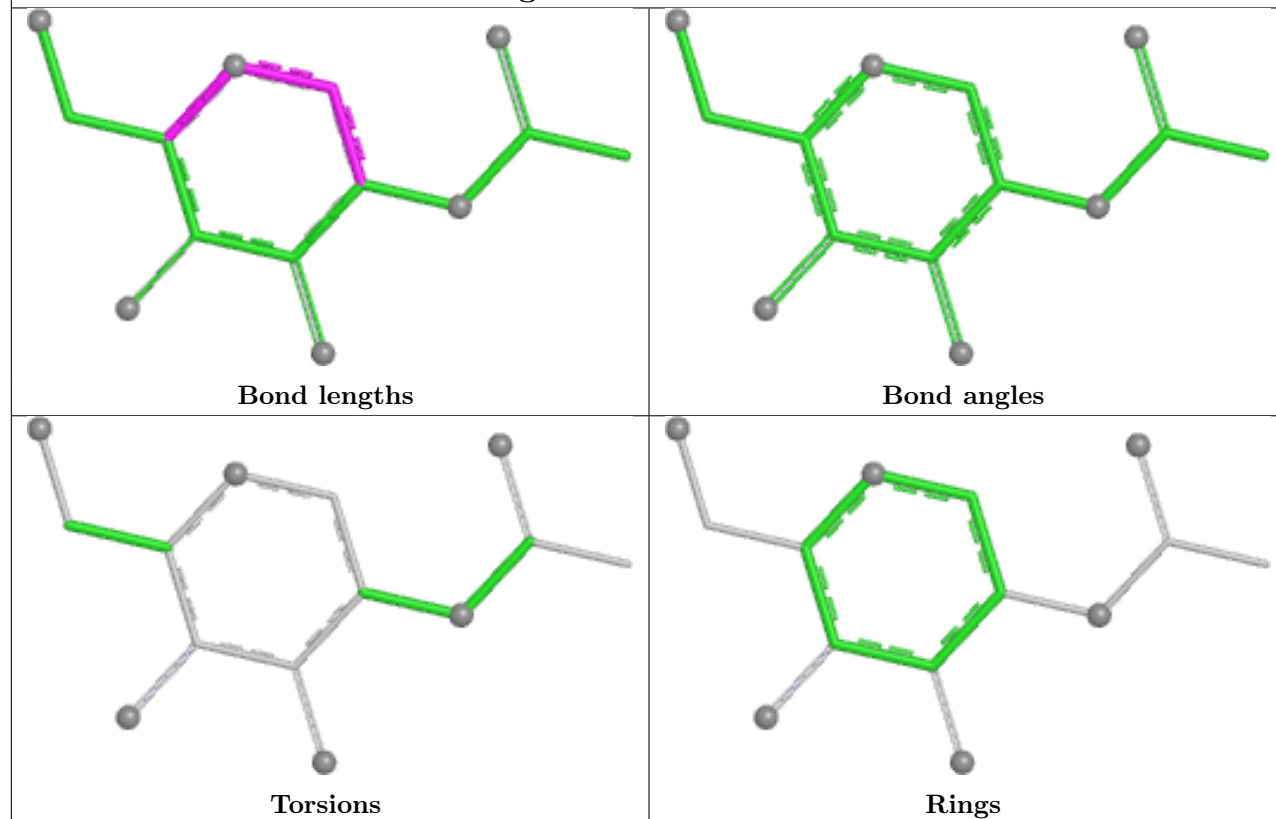


Ligand NAG A 1402

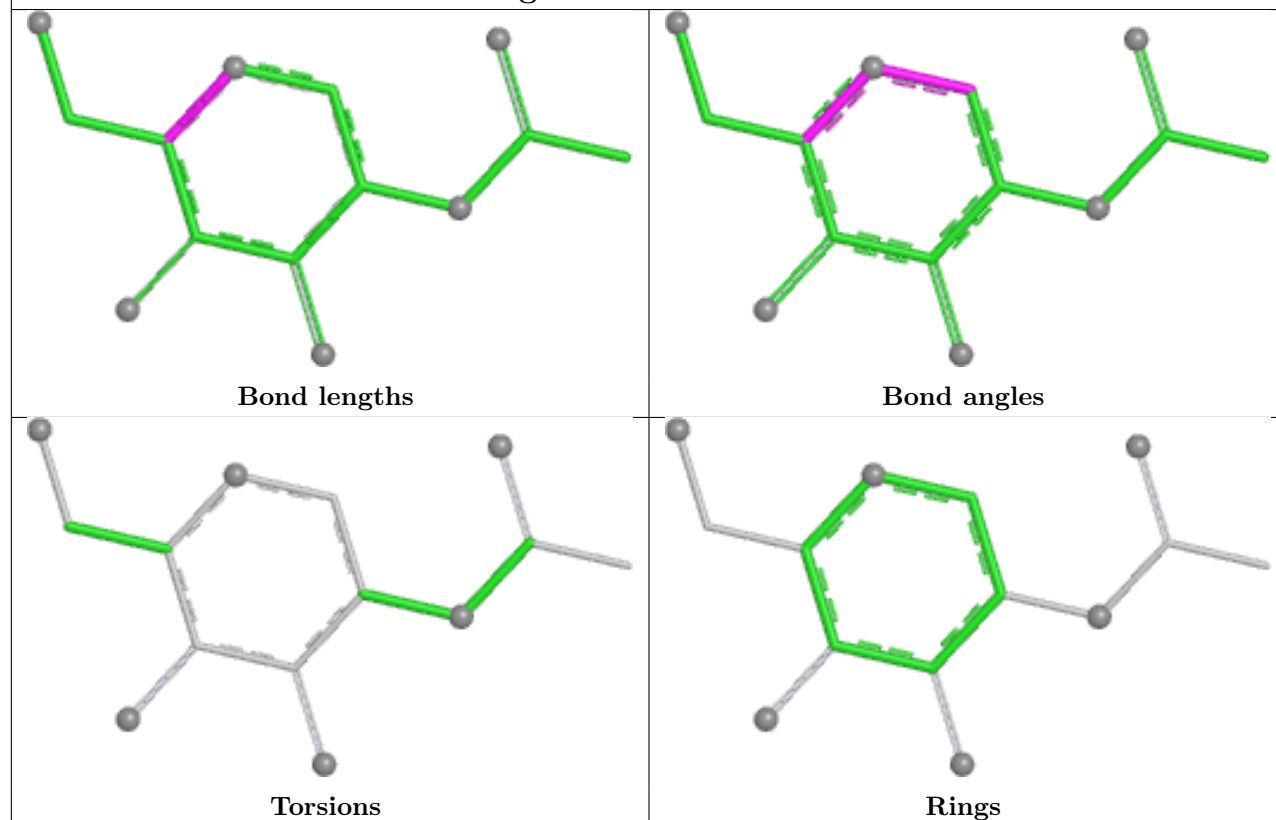


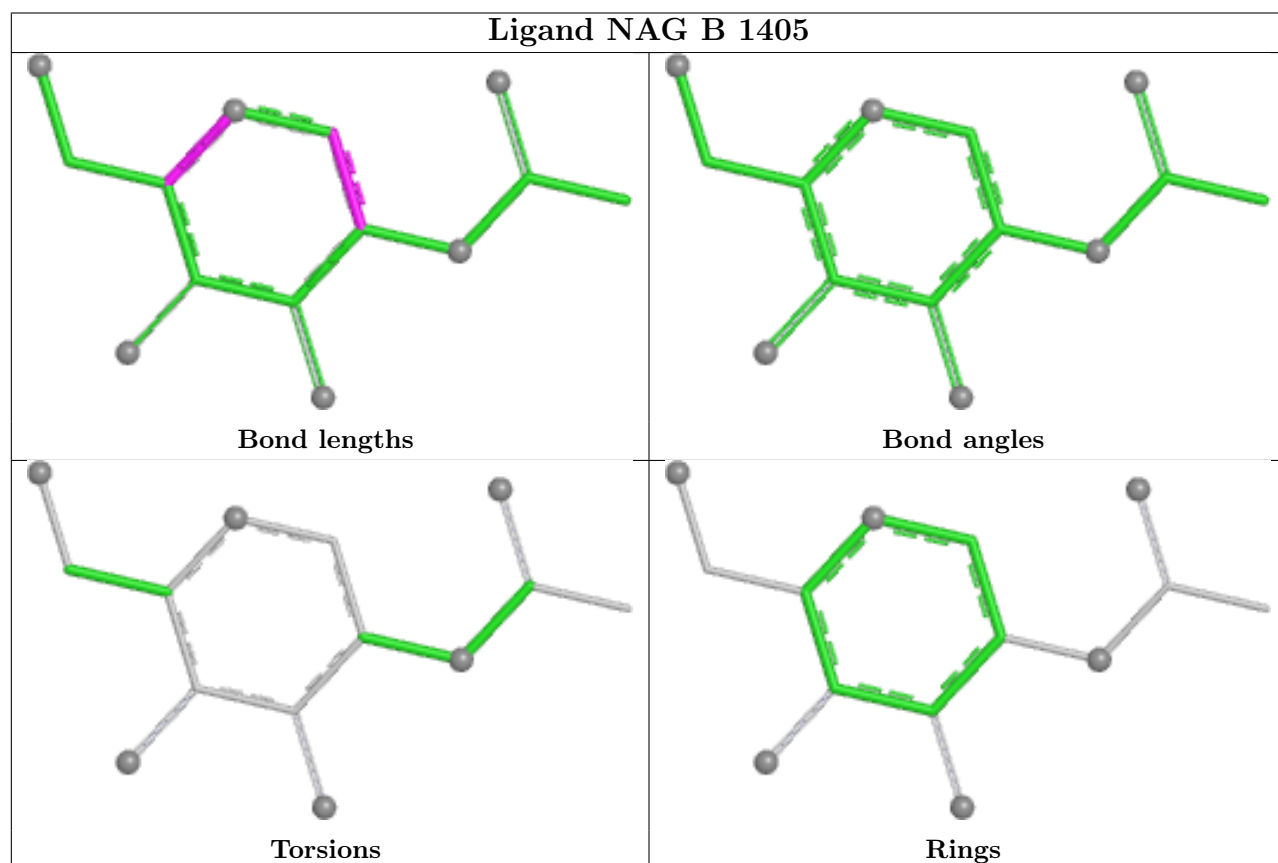
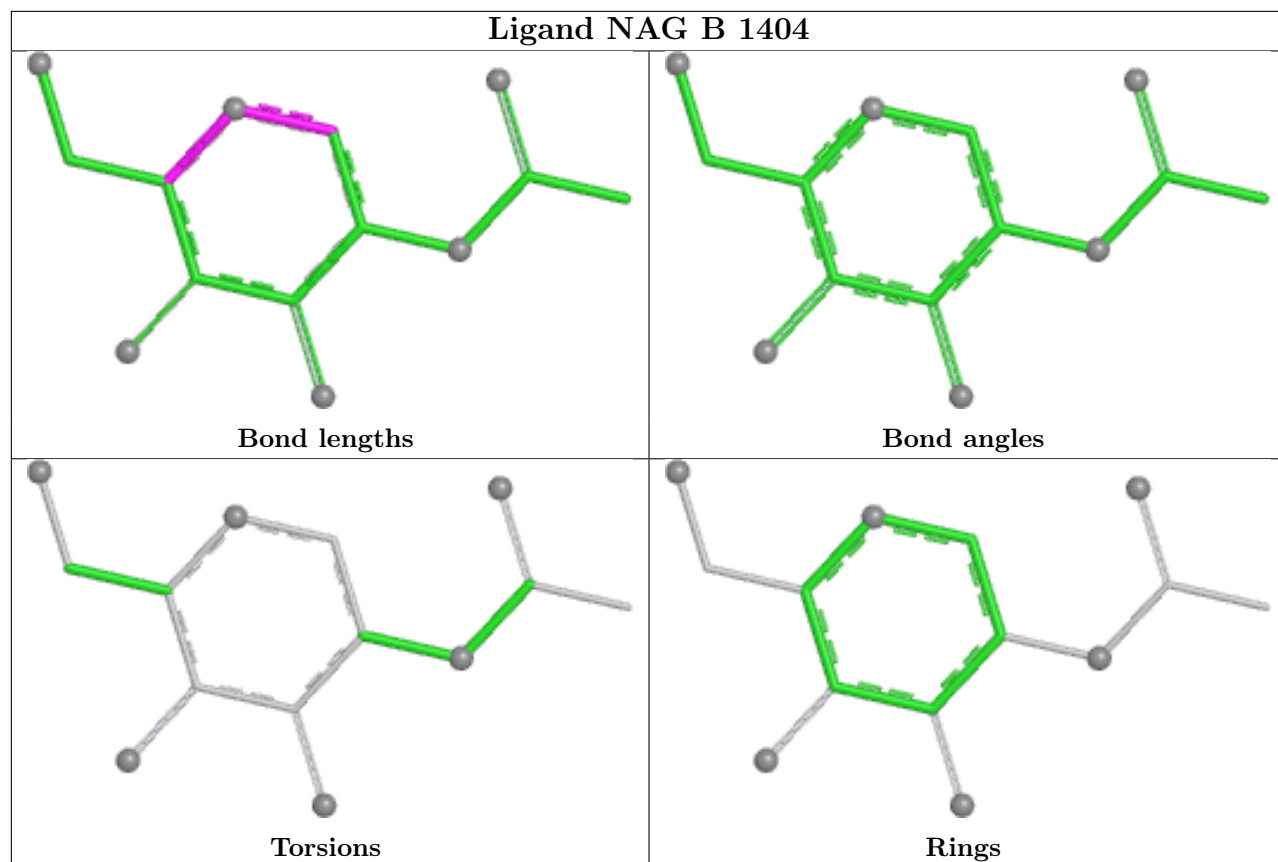


Ligand NAG A 1406

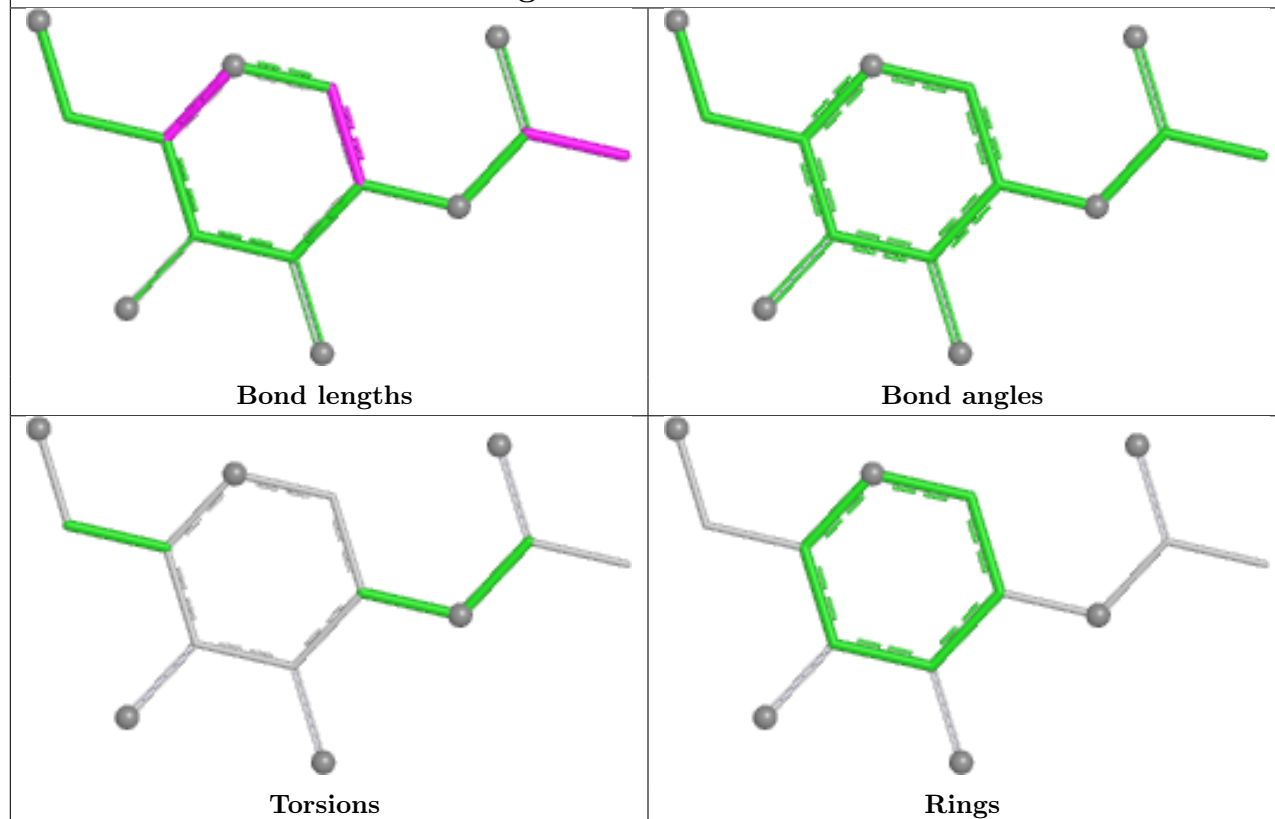


Ligand NAG C 1402

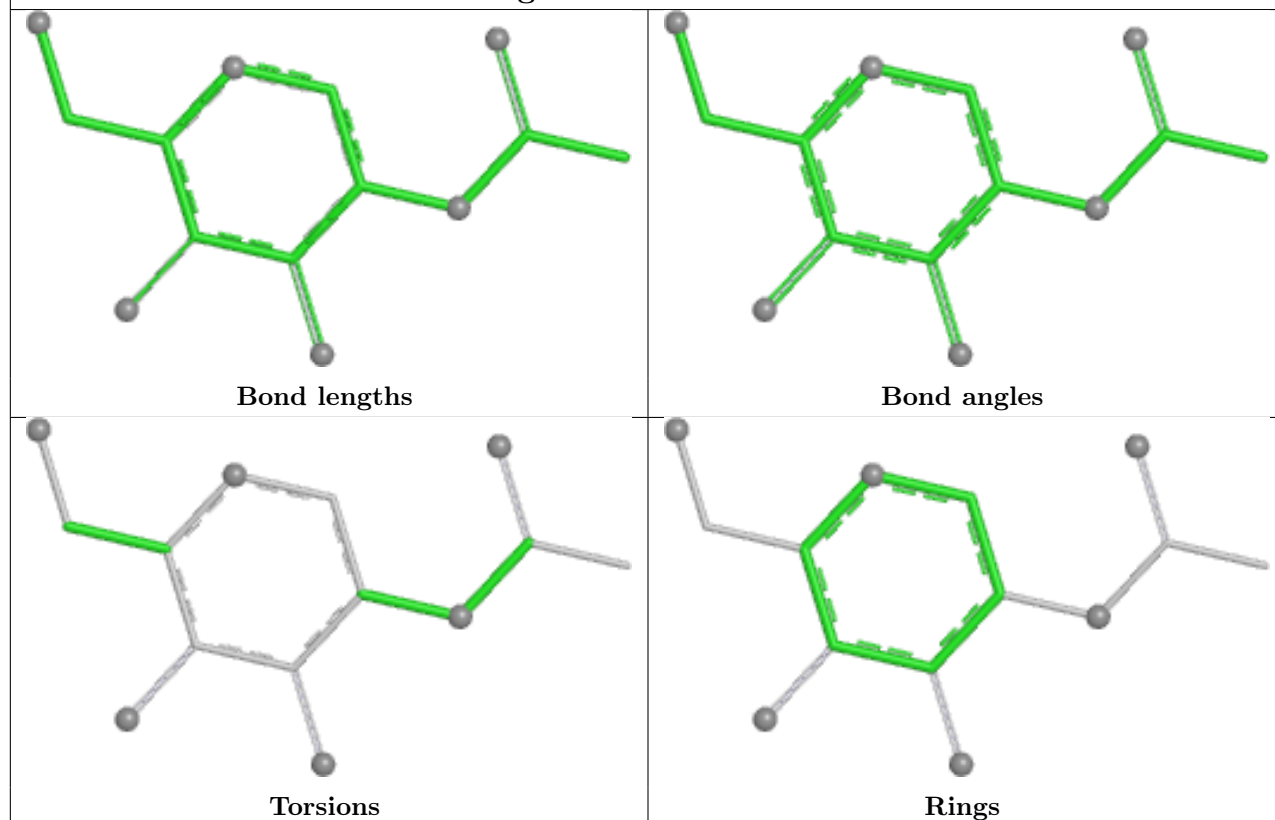




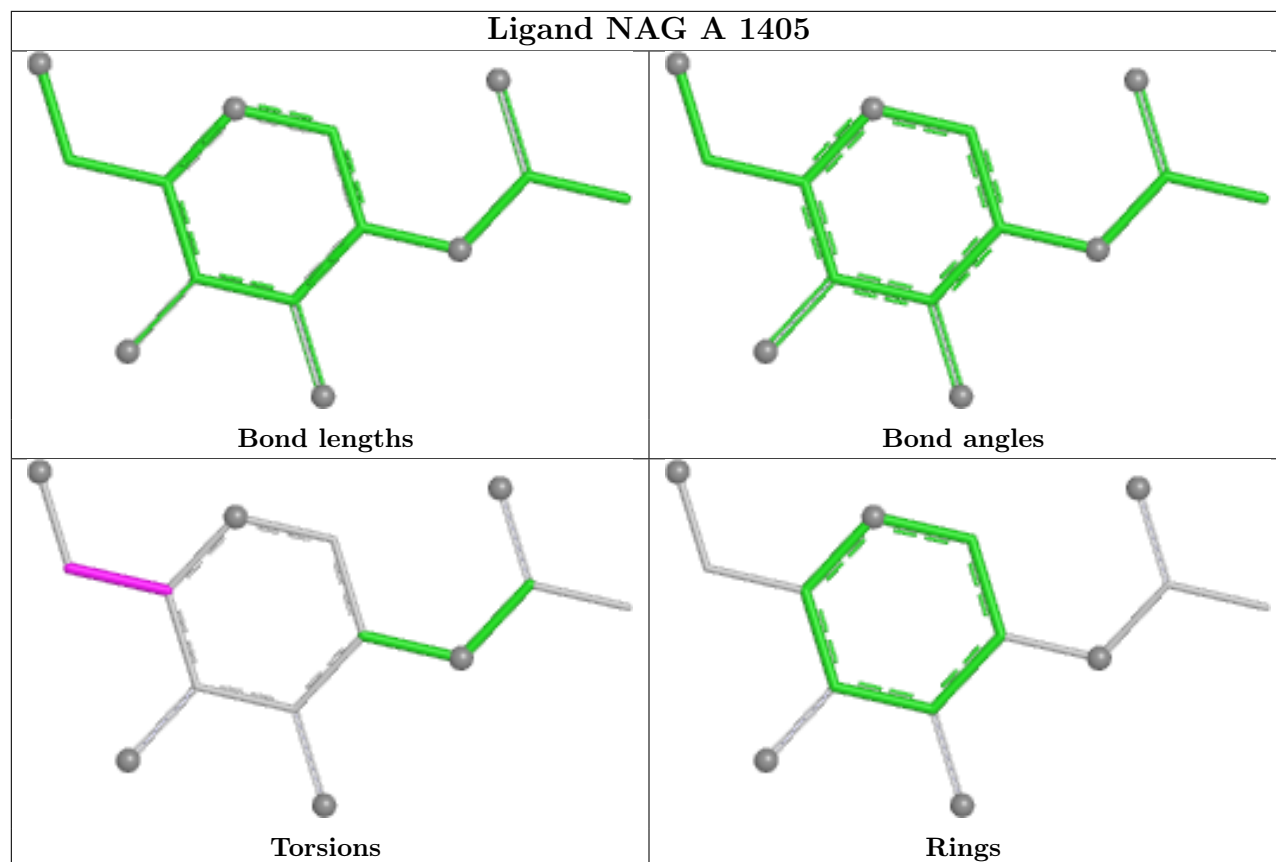
Ligand NAG C 1406



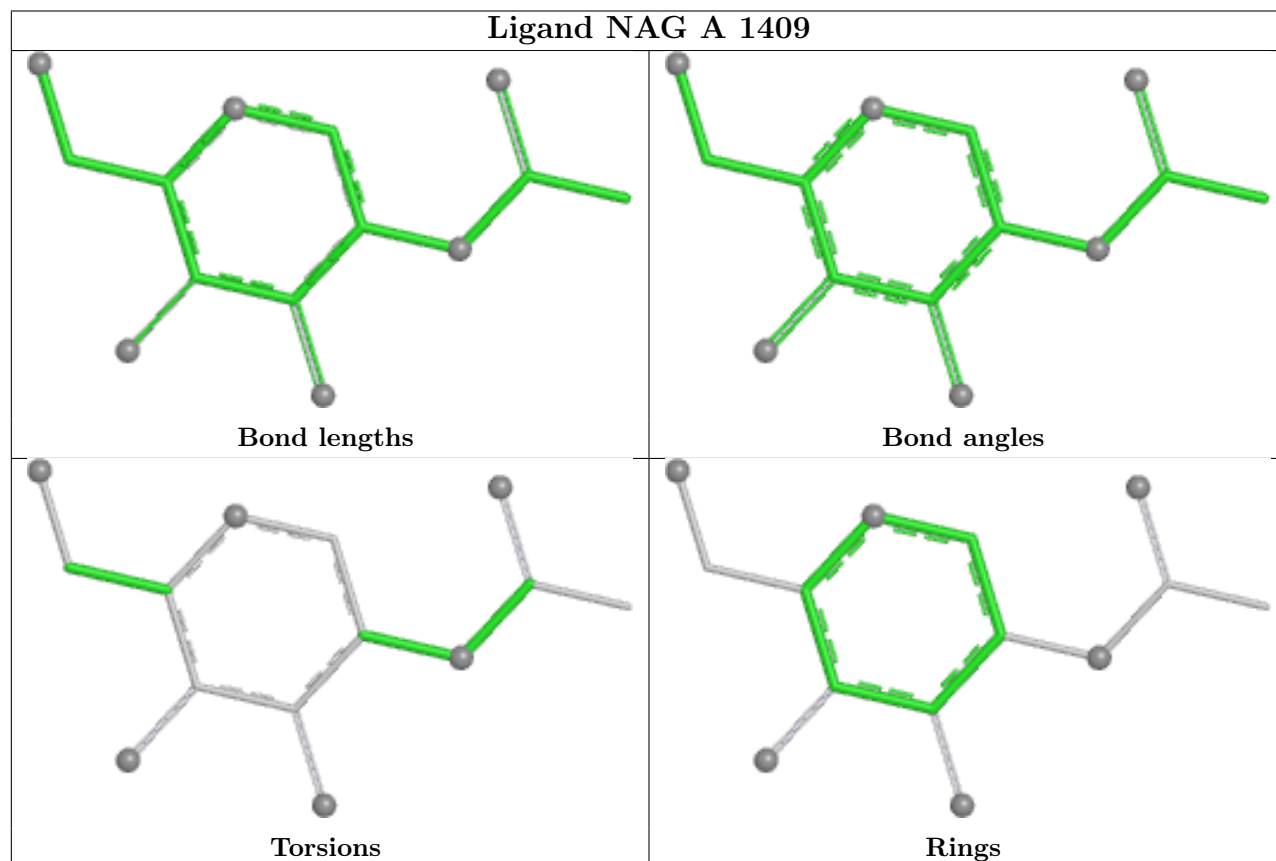
Ligand NAG A 1404

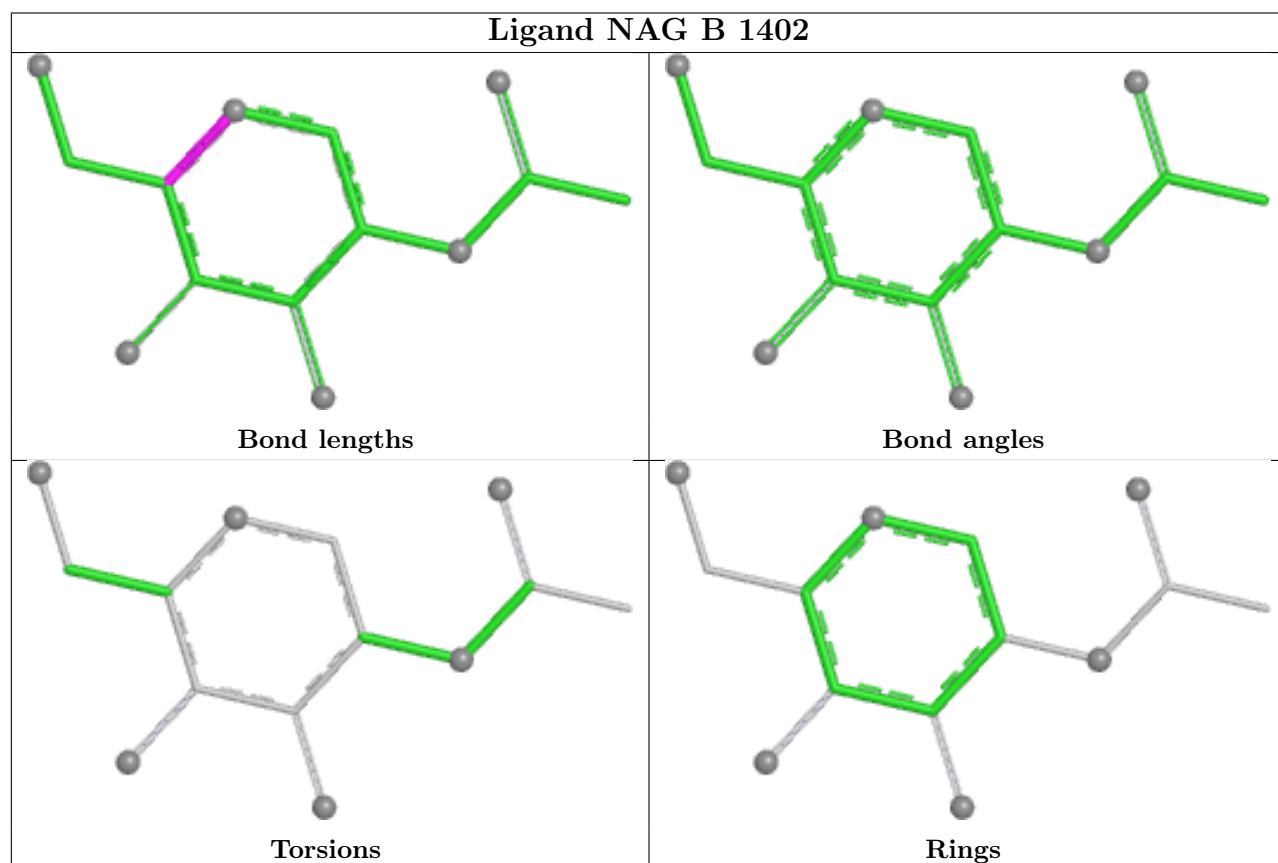
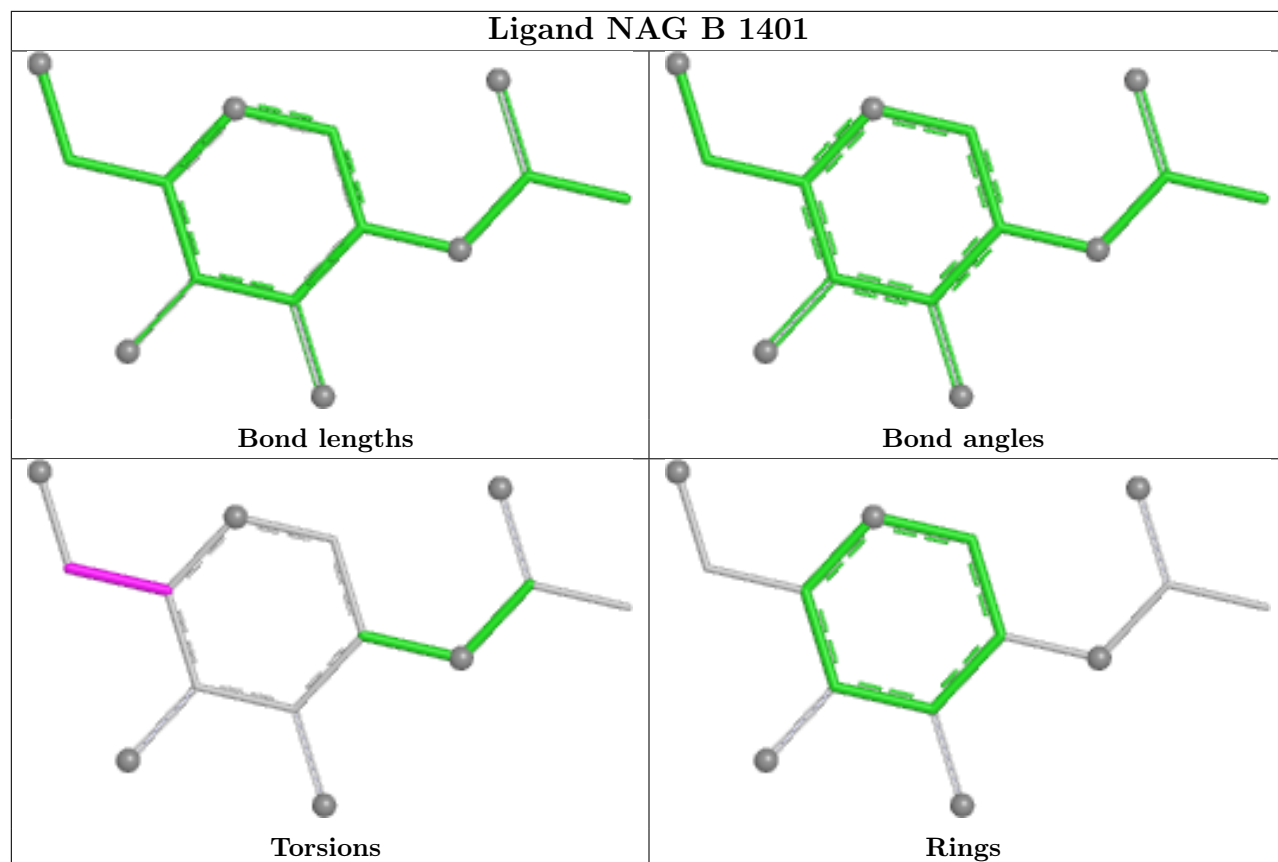


Ligand NAG A 1405

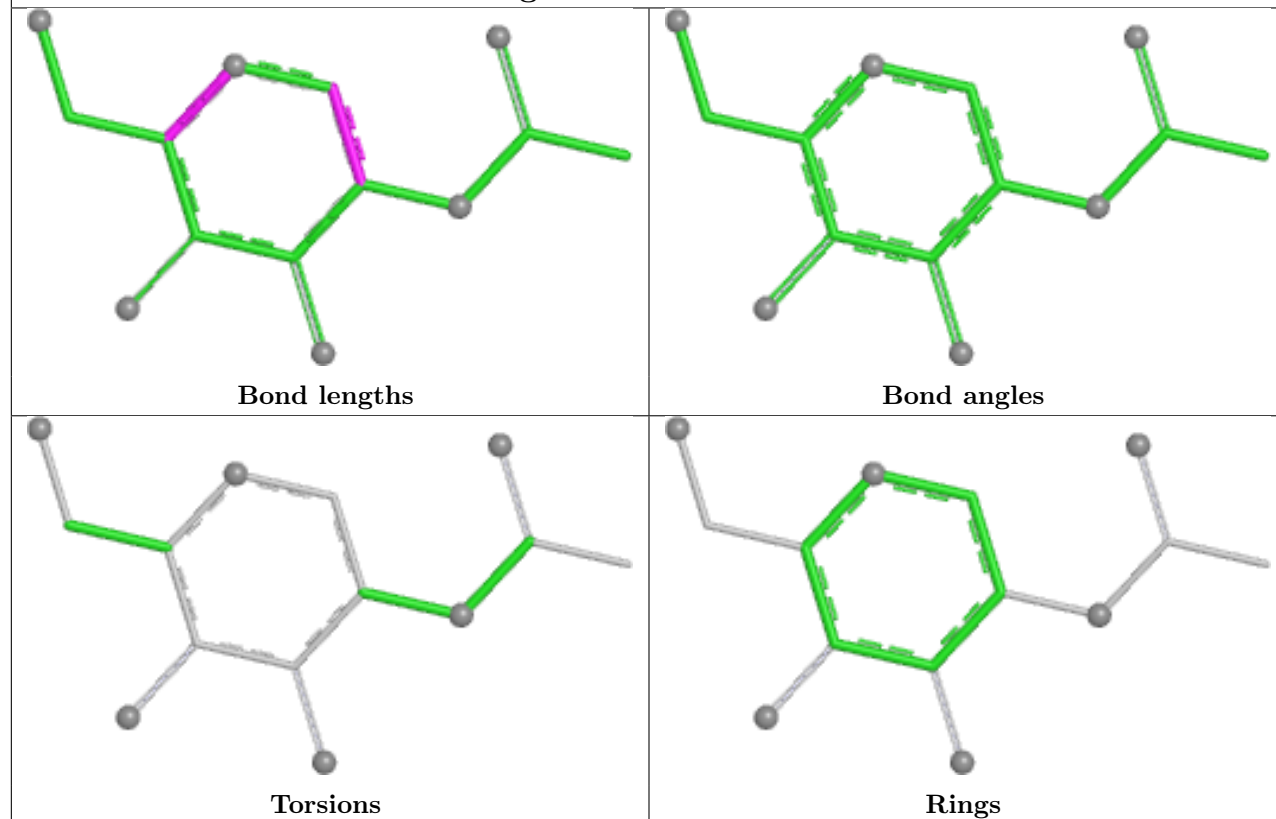


Ligand NAG A 1409

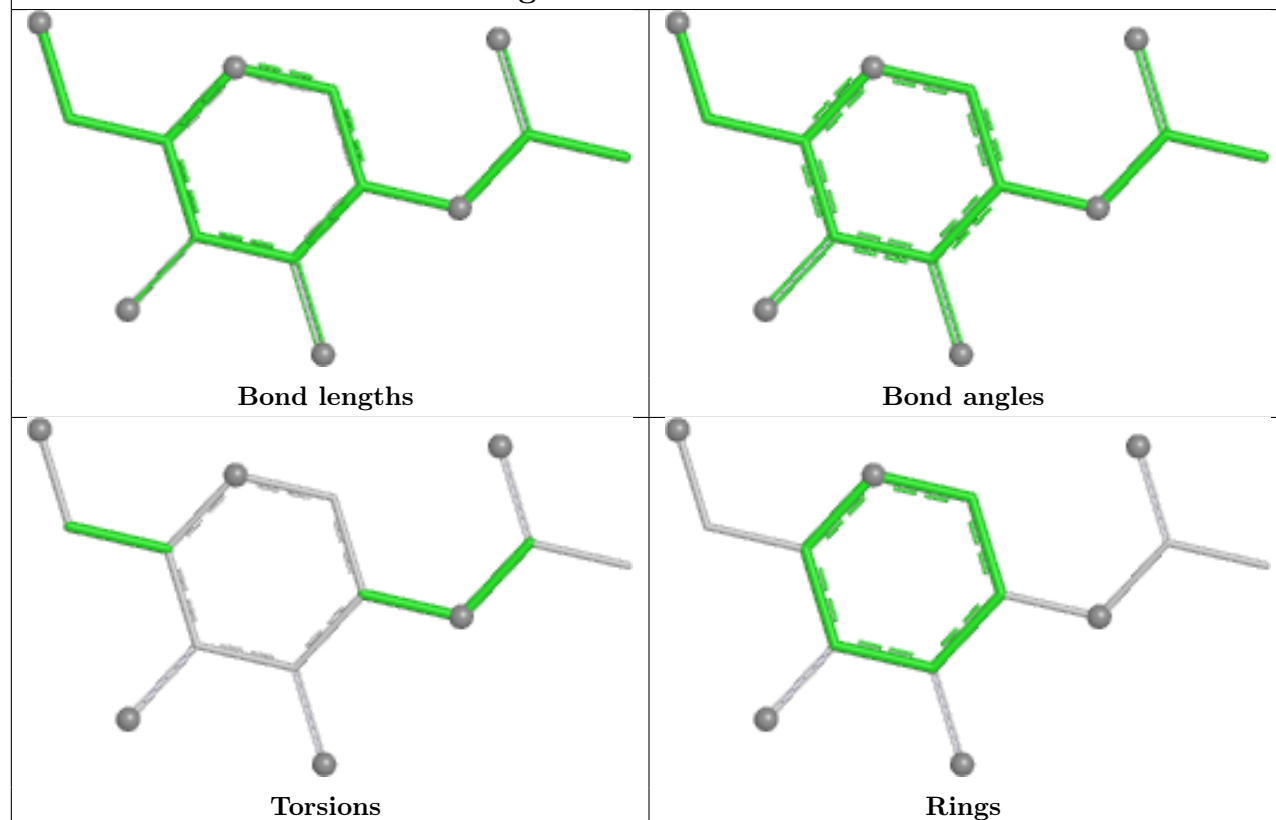


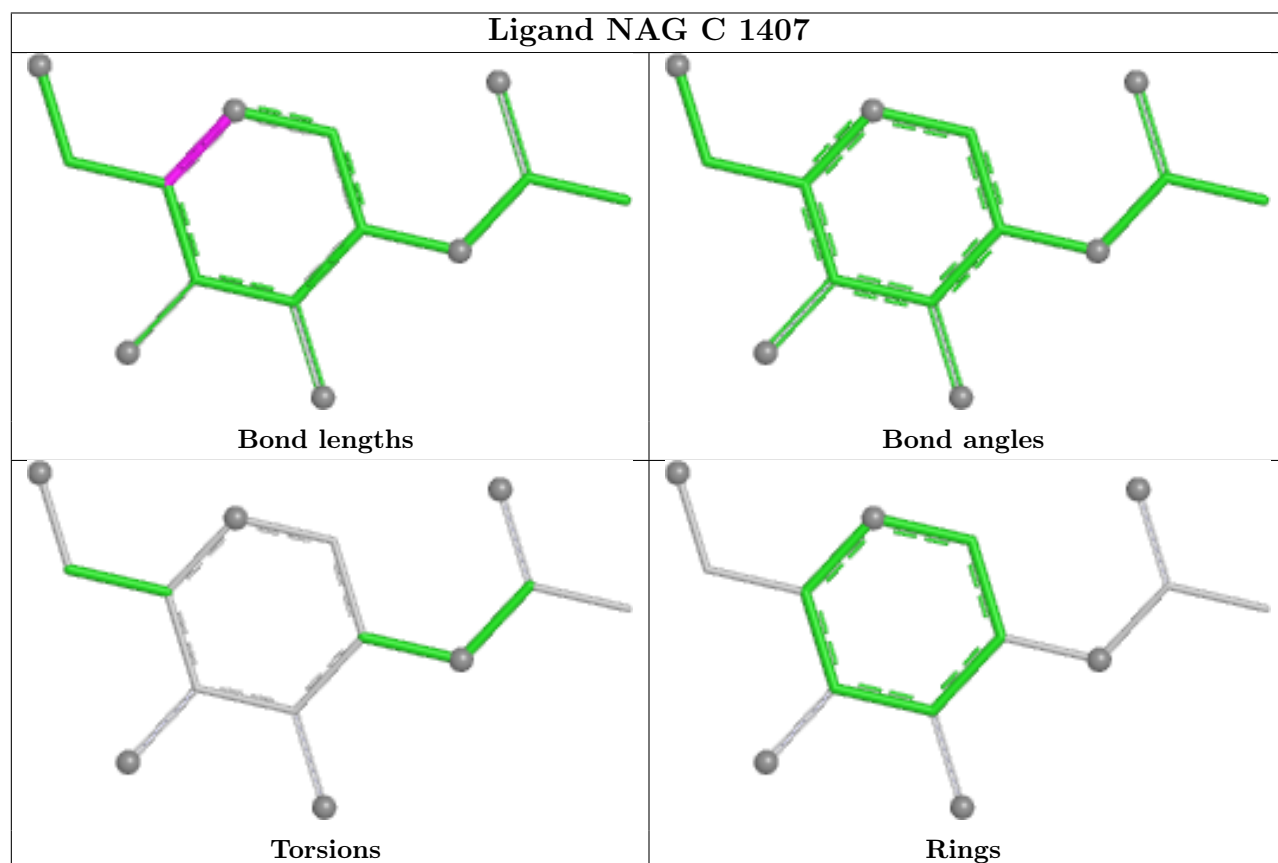
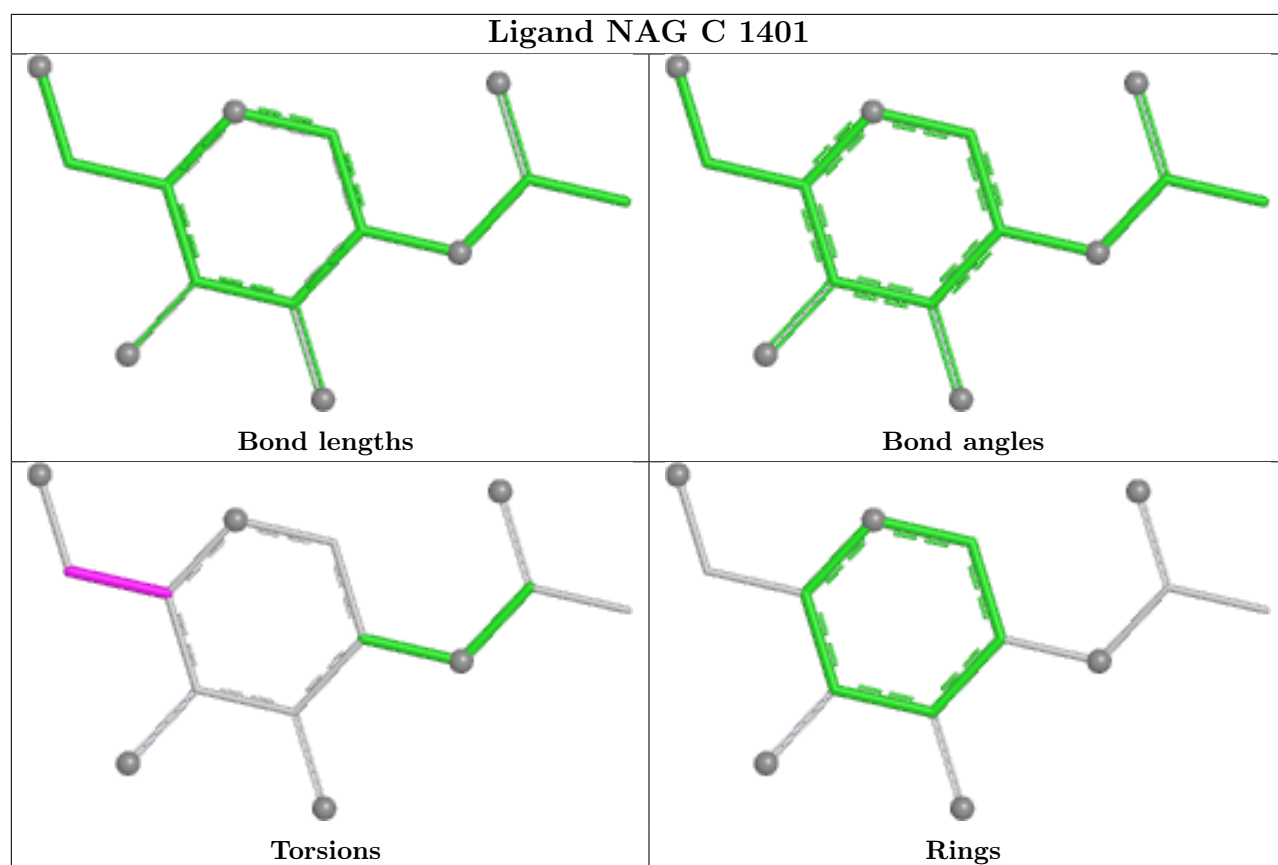


Ligand NAG B 1407



Ligand NAG A 1407





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.

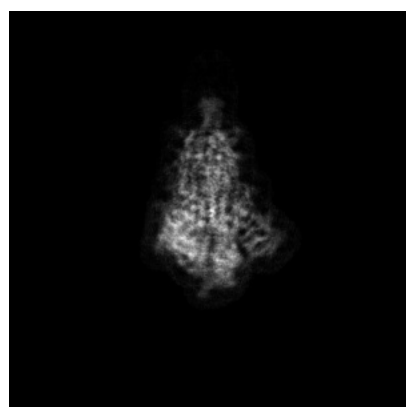
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24983. These allow visual inspection of the internal detail of the map and identification of artifacts.

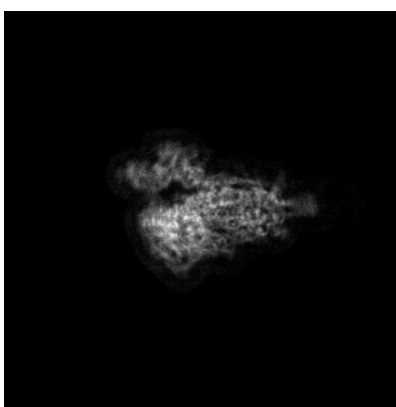
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

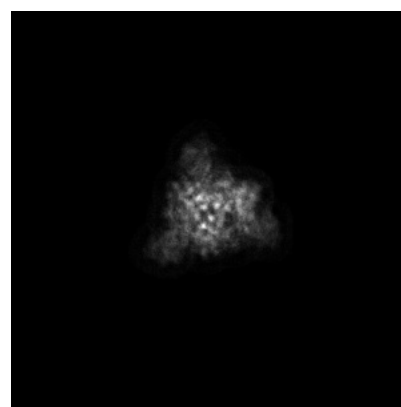
6.1.1 Primary map



X



Y



Z

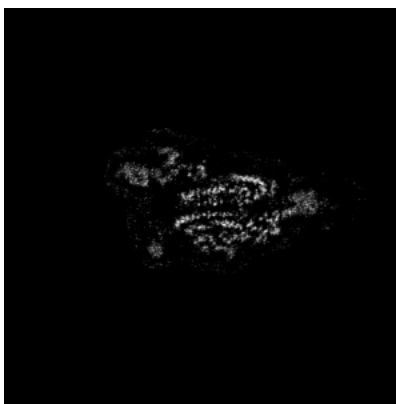
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

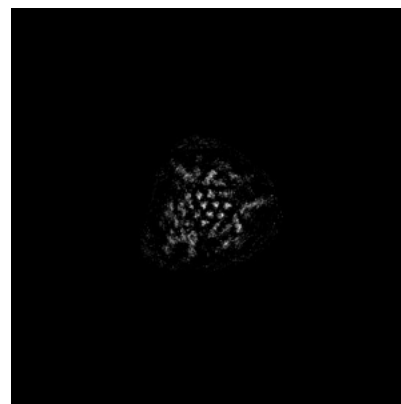
6.2.1 Primary map



X Index: 240



Y Index: 240

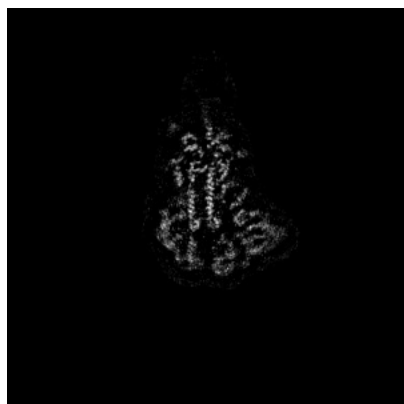


Z Index: 240

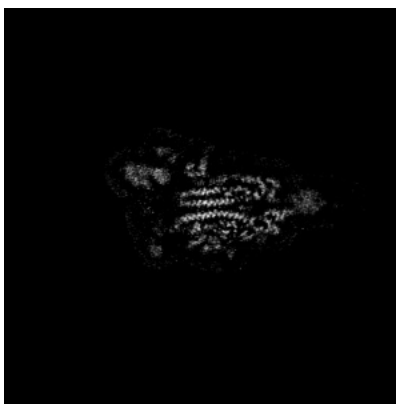
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

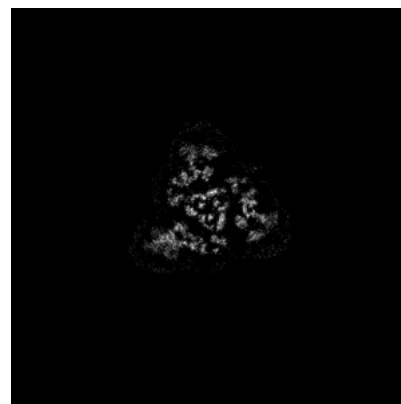
6.3.1 Primary map



X Index: 231



Y Index: 243

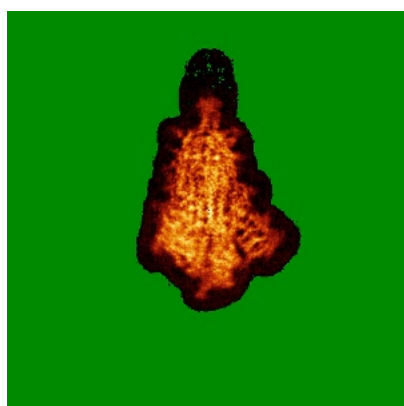


Z Index: 222

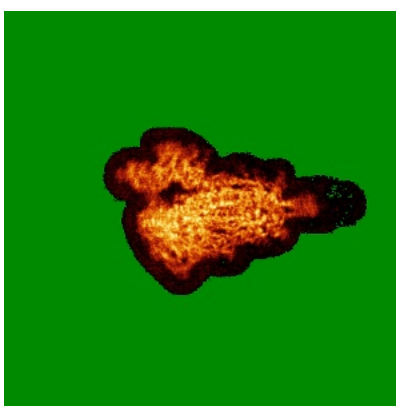
The images above show the largest variance slices of the map in three orthogonal directions.

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

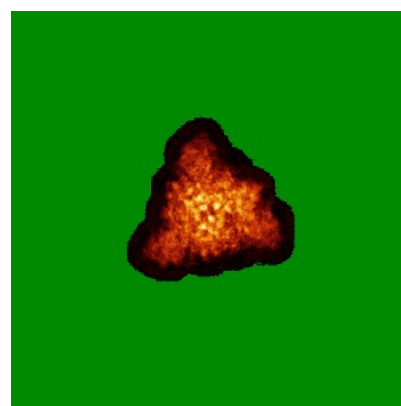
6.4.1 Primary map



X



Y

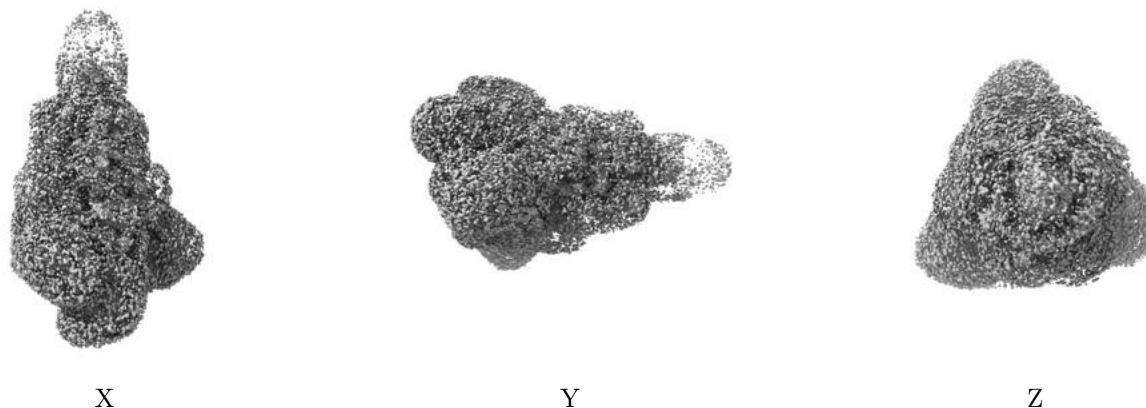


Z

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.

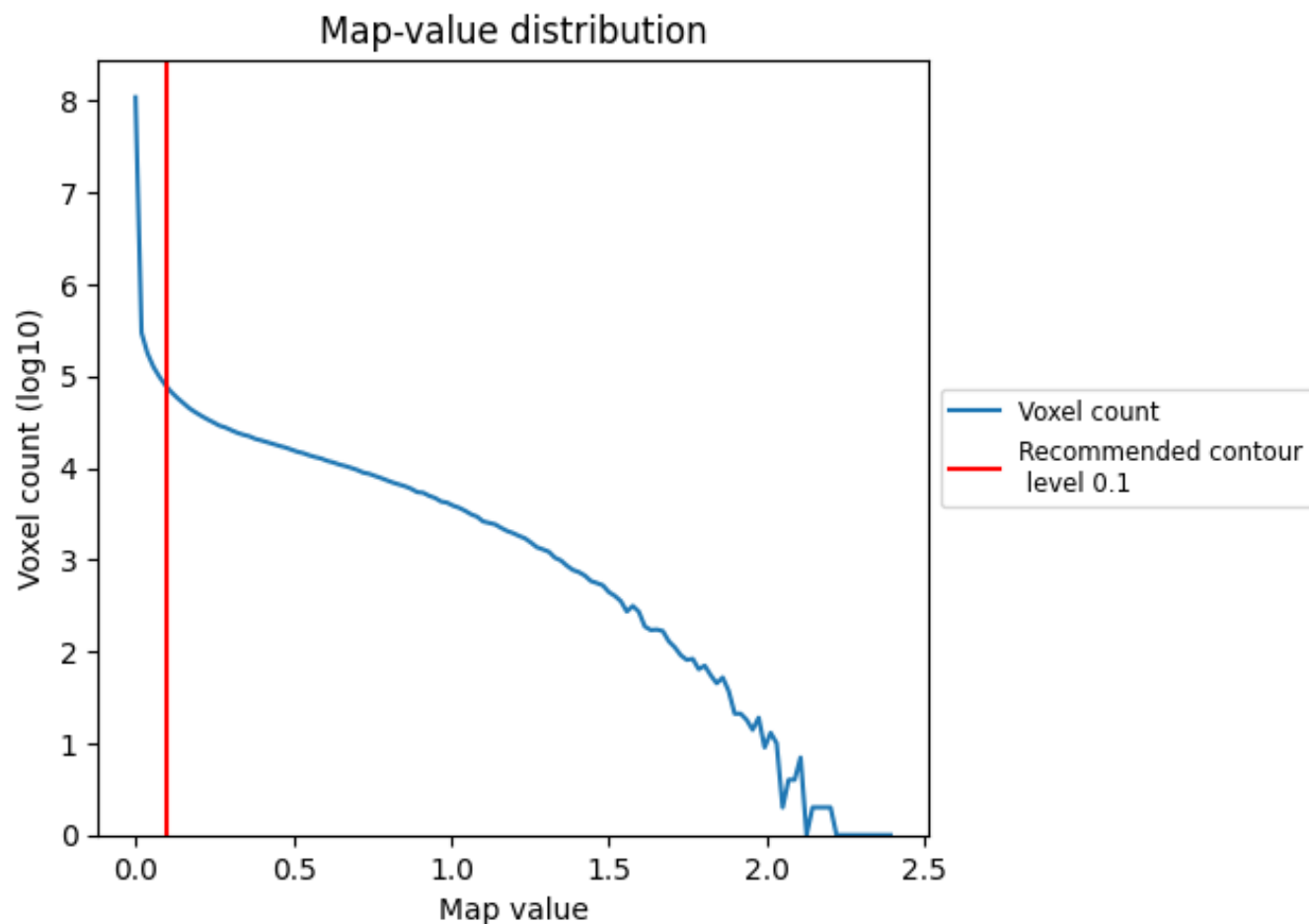
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

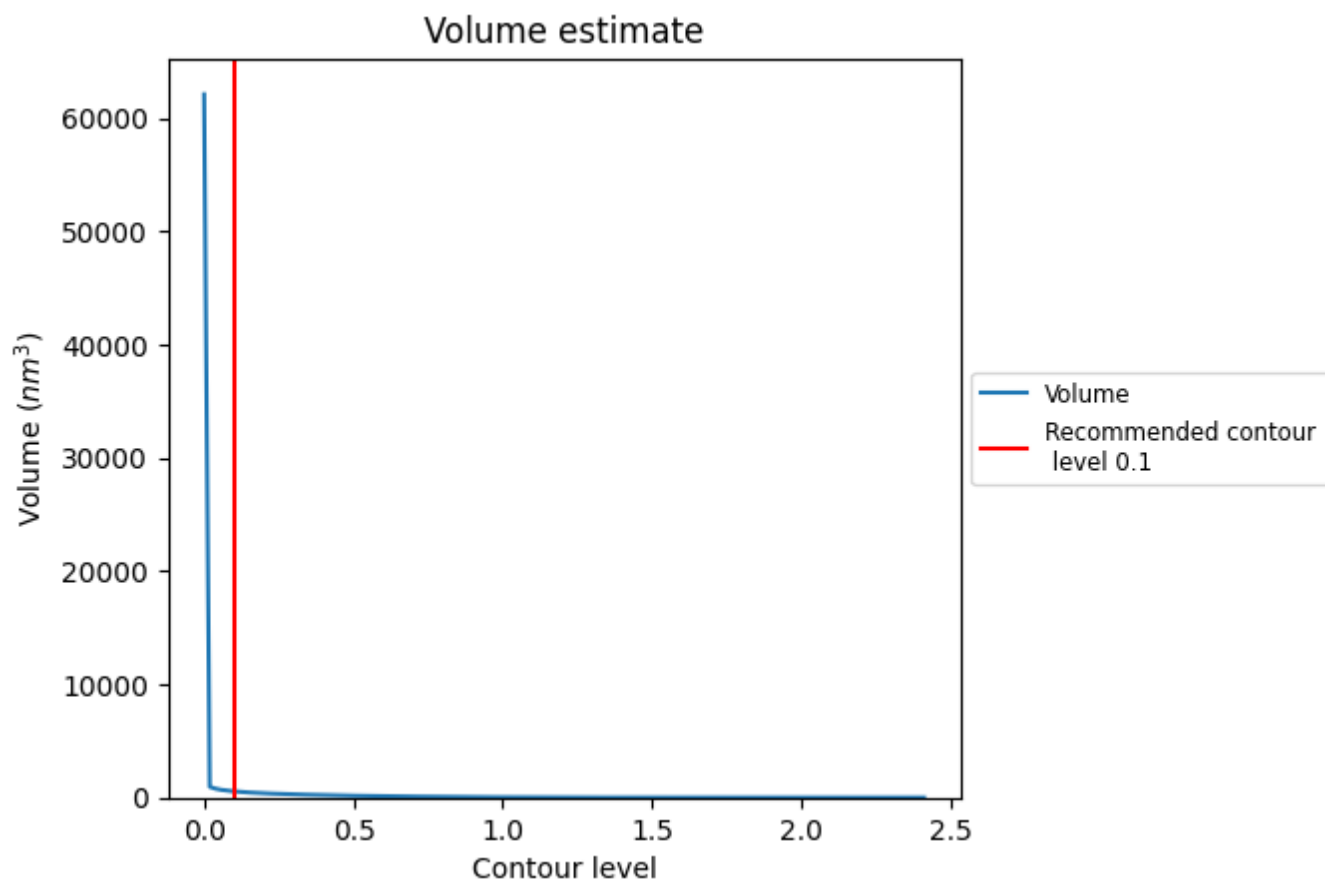
This section contains the results of statistical analysis of the map.

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.

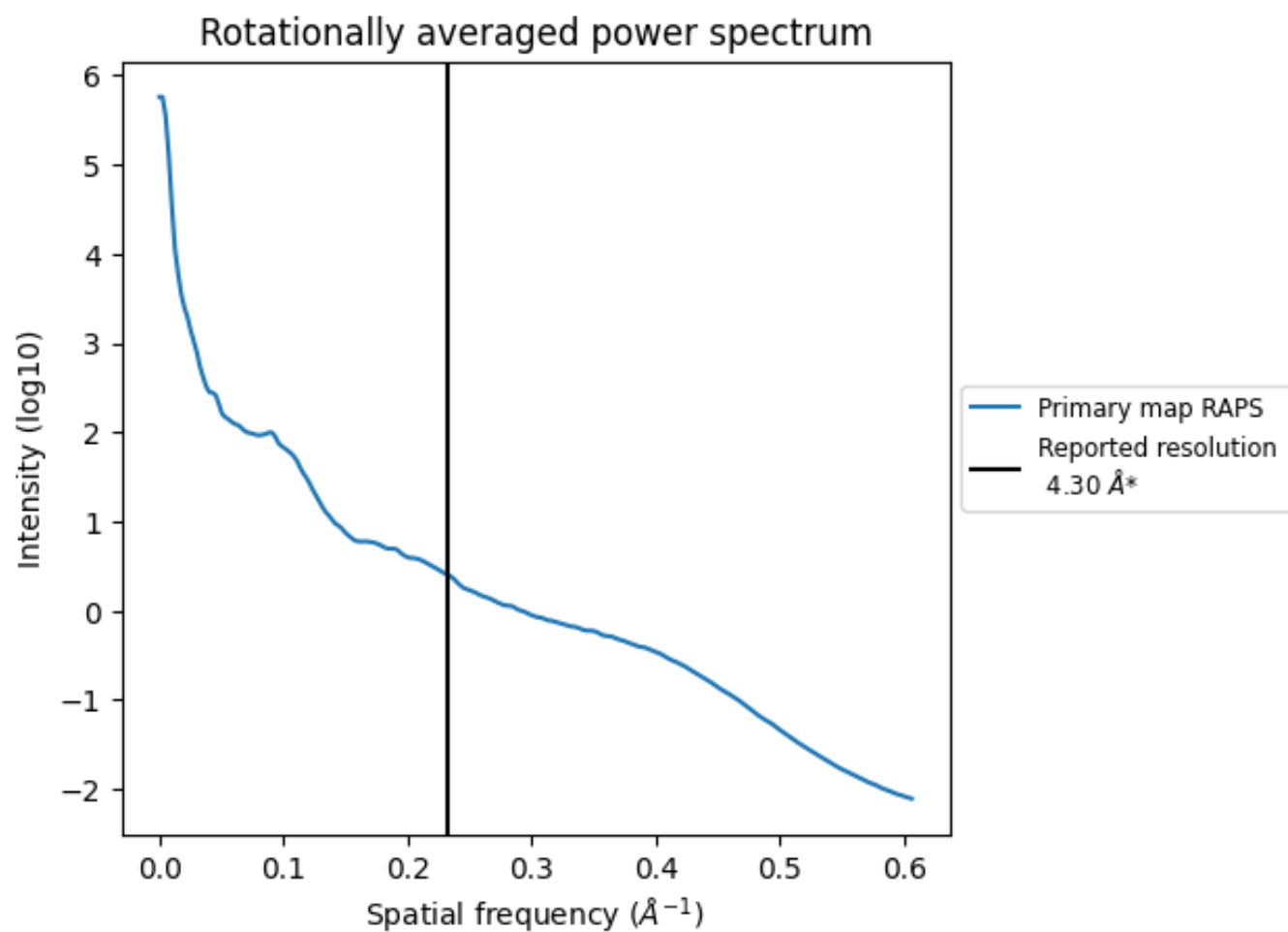
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm³; this corresponds to an approximate mass of 494 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 0.233 Å⁻¹

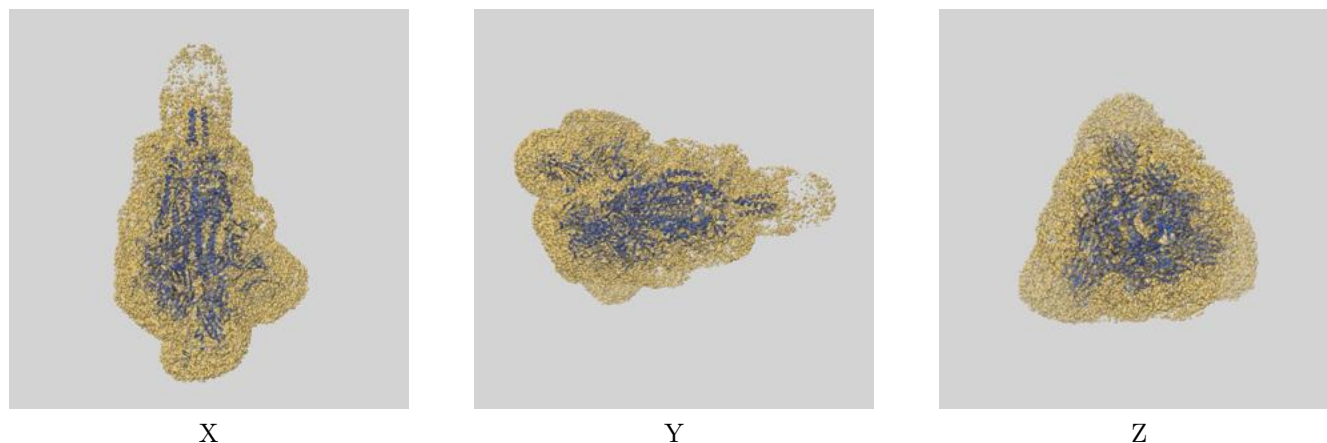
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

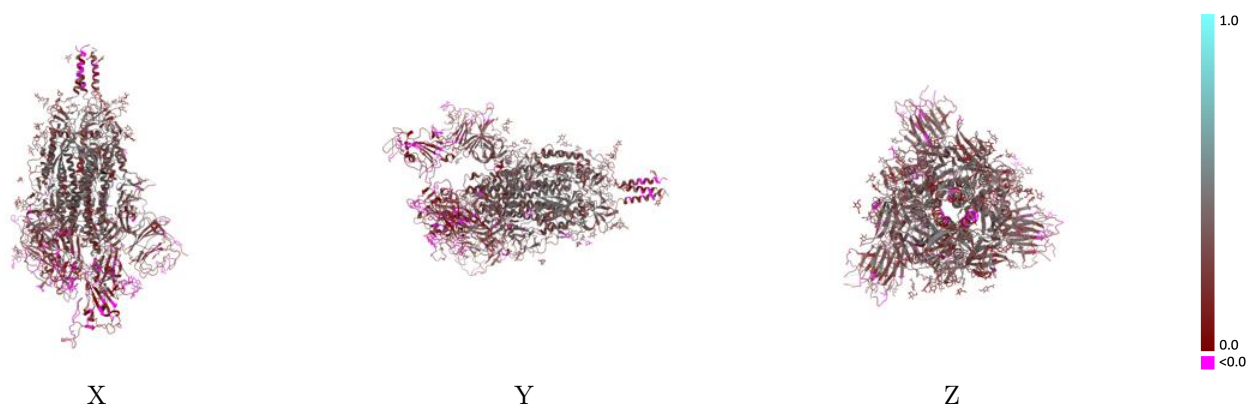
This section contains information regarding the fit between EMDB map EMD-24983 and PDB model 7SBO. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



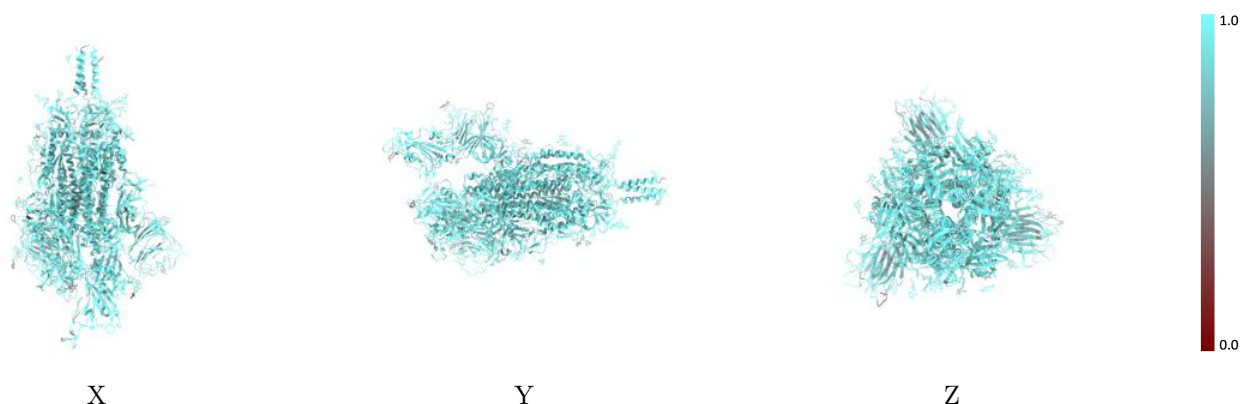
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



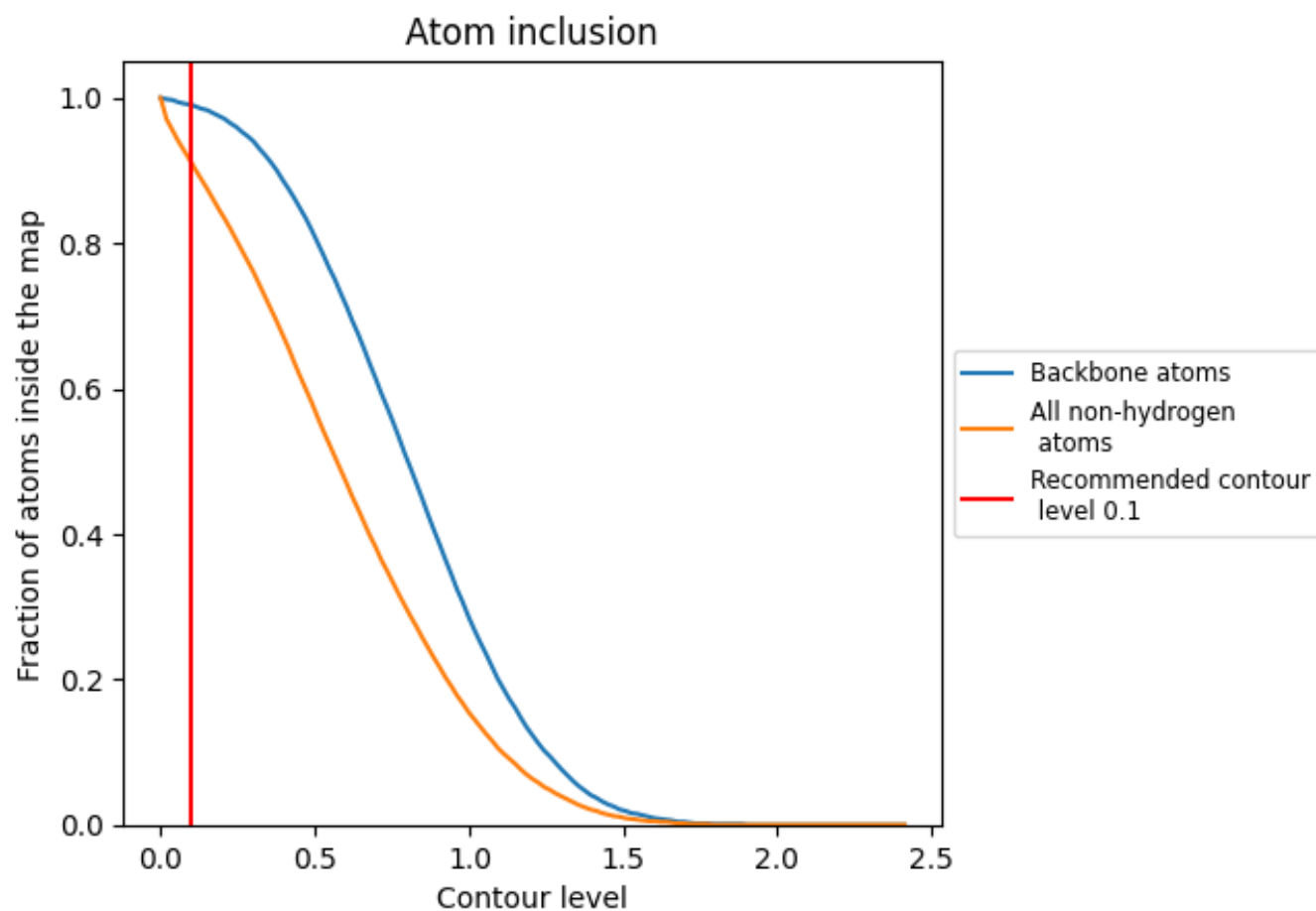
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.9100	 0.2660
A	 0.9100	 0.2660
B	 0.9150	 0.2760
C	 0.9090	 0.2680
D	 0.6670	 -0.0810
E	 0.9640	 0.2320
F	 0.9290	 0.2190
G	 0.9290	 0.2880
H	 0.9290	 0.1180
I	 0.8680	 0.1410
J	 0.9230	 0.1180
K	 0.9740	 0.1400
L	 0.8720	 0.0170
M	 0.5360	 -0.1580
N	 0.9290	 0.1900
O	 0.9640	 0.1200
P	 0.7500	 0.1720
Q	 0.9290	 0.2910
R	 0.8930	 0.2850
S	 0.7630	 0.1680
T	 0.8970	 0.1700
U	 0.9740	 0.2750
V	 0.7950	 0.1360
W	 0.7500	 0.0670
X	 1.0000	 0.2190
Y	 0.7140	 -0.0370
Z	 1.0000	 0.2440
a	 0.8210	 0.0890
b	 1.0000	 0.3280
c	 0.8570	 0.2450
d	 0.7630	 0.1730
e	 0.9740	 0.3270
f	 0.9740	 0.2570
g	 0.9740	 0.1210

