



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:27 AM UTC

PDB ID : 7TNW / pdb_00007tnw
EMDB ID : EMD-26021
Title : Structural and functional impact by SARS-CoV-2 Omicron spike mutations
Authors : Zhang, J.; Xiao, T.S.; Cai, Y.F.; Peng, H.Q.; Volloch, S.R.; Chen, B.
Deposited on : 2022-01-21
Resolution : 3.10 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:

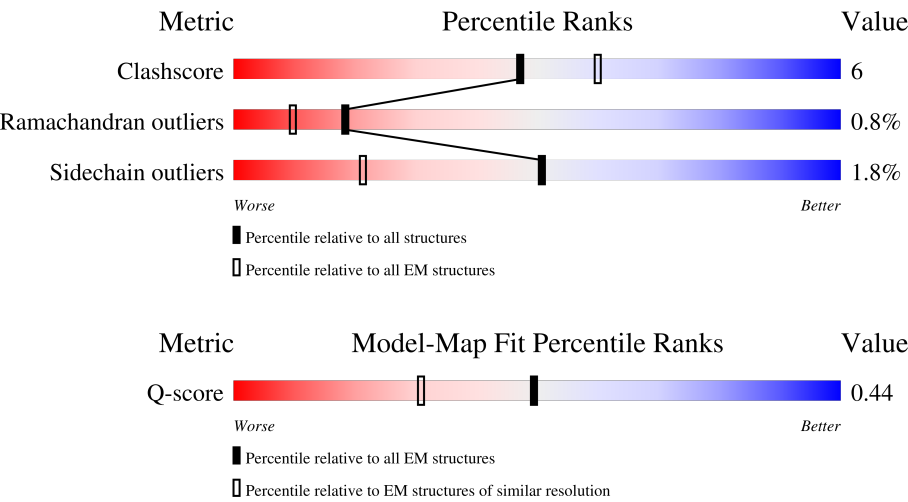
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 Å.

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



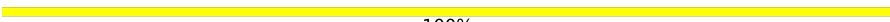
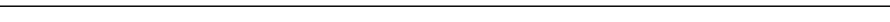
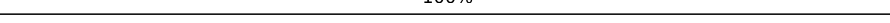
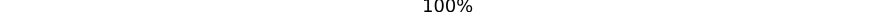
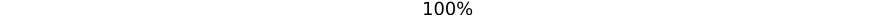
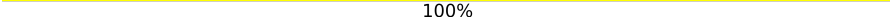
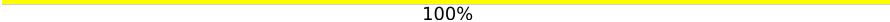
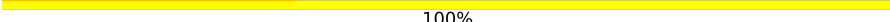
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1270	
1	B	1270	
1	C	1270	
2	D	2	

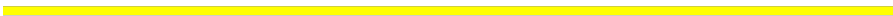
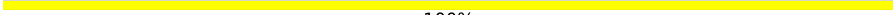
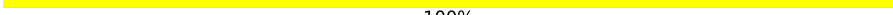
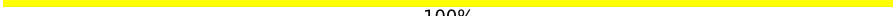
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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	I	2	 100%
2	O	2	 50% 100%
2	Q	2	 100%
2	T	2	 100%
2	Z	2	 50% 100%
2	b	2	 100%
2	e	2	 50% 50%
3	E	3	 67% 33%
3	G	3	 67% 33%
3	H	3	 100%
3	J	3	 100%
3	K	3	 100%
3	M	3	 100%
3	N	3	 100%
3	P	3	 67% 33%
3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

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Mol	Chain	Length	Quality of chain
3	f	3	 100%
3	g	3	 100%
3	i	3	 100%
3	j	3	 100%
4	L	3	 100%
4	W	3	 100%
4	h	3	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27846 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	C	1119	Total	C	N	O	S	0	0
			8789	5624	1466	1659	40		
1	A	1119	Total	C	N	O	S	0	0
			8789	5624	1466	1659	40		
1	B	1119	Total	C	N	O	S	0	0
			8789	5624	1466	1659	40		

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	144	PHE	TYR	variant	UNP P0DTC2
C	145	ASP	TYR	variant	UNP P0DTC2
C	212	ILE	-	insertion	UNP P0DTC2
C	213	VAL	-	insertion	UNP P0DTC2
C	214	ARG	ASN	variant	UNP P0DTC2
C	214A	GLU	LEU	variant	UNP P0DTC2
C	214B	PRO	VAL	variant	UNP P0DTC2
C	214C	GLU	ARG	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	144	PHE	TYR	variant	UNP P0DTC2
A	145	ASP	TYR	variant	UNP P0DTC2
A	212	ILE	-	insertion	UNP P0DTC2
A	213	VAL	-	insertion	UNP P0DTC2
A	214	ARG	ASN	variant	UNP P0DTC2
A	214A	GLU	LEU	variant	UNP P0DTC2
A	214B	PRO	VAL	variant	UNP P0DTC2
A	214C	GLU	ARG	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	144	PHE	TYR	variant	UNP P0DTC2
B	145	ASP	TYR	variant	UNP P0DTC2
B	212	ILE	-	insertion	UNP P0DTC2
B	213	VAL	-	insertion	UNP P0DTC2
B	214	ARG	ASN	variant	UNP P0DTC2
B	214A	GLU	LEU	variant	UNP P0DTC2
B	214B	PRO	VAL	variant	UNP P0DTC2
B	214C	GLU	ARG	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	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	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	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	b	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 alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



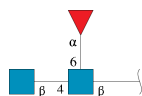
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	N	3	Total	C	N	O	0	0
			39	22	2	15		
3	P	3	Total	C	N	O	0	0
			39	22	2	15		
3	R	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	Y	3	Total	C	N	O	0	0
			39	22	2	15		
3	a	3	Total	C	N	O	0	0
			39	22	2	15		
3	c	3	Total	C	N	O	0	0
			39	22	2	15		
3	d	3	Total	C	N	O	0	0
			39	22	2	15		
3	f	3	Total	C	N	O	0	0
			39	22	2	15		

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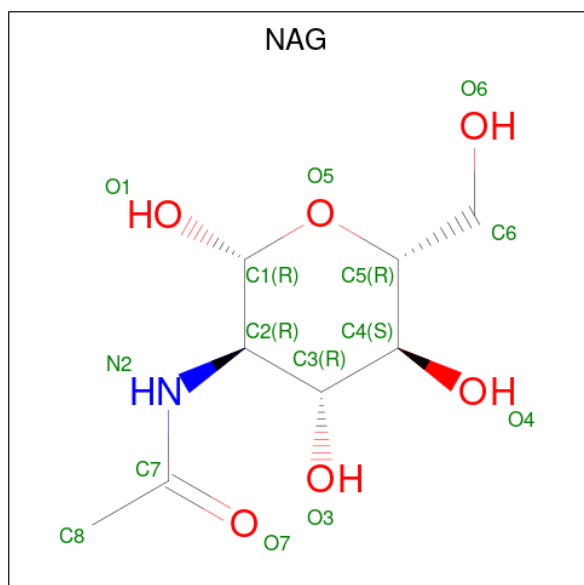
Mol	Chain	Residues	Atoms				AltConf	Trace
3	g	3	Total	C	N	O	0	0
			39	22	2	15		
3	i	3	Total	C	N	O	0	0
			39	22	2	15		
3	j	3	Total	C	N	O	0	0
			39	22	2	15		

- 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.

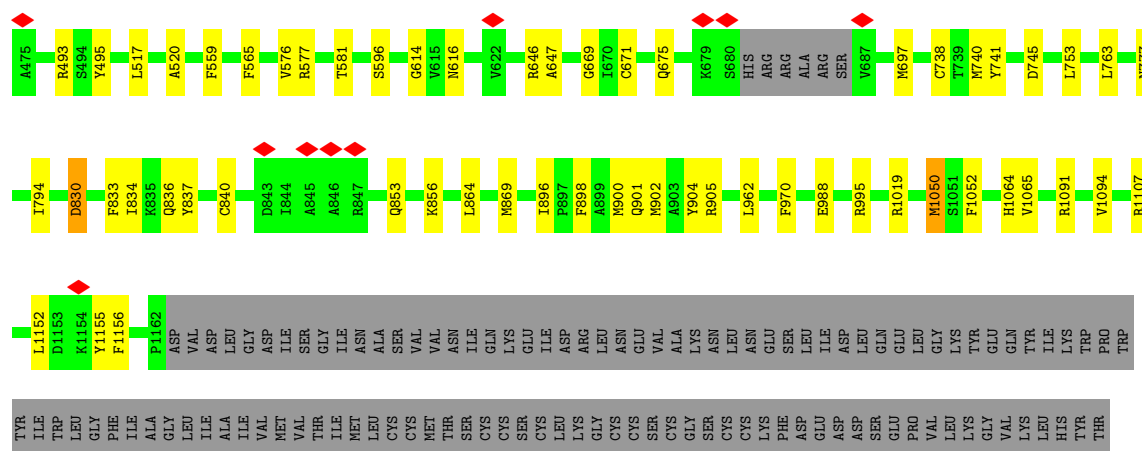


Mol	Chain	Residues	Atoms				AltConf	Trace
4	L	3	Total	C	N	O	0	0
			38	22	2	14		
4	W	3	Total	C	N	O	0	0
			38	22	2	14		
4	h	3	Total	C	N	O	0	0
			38	22	2	14		

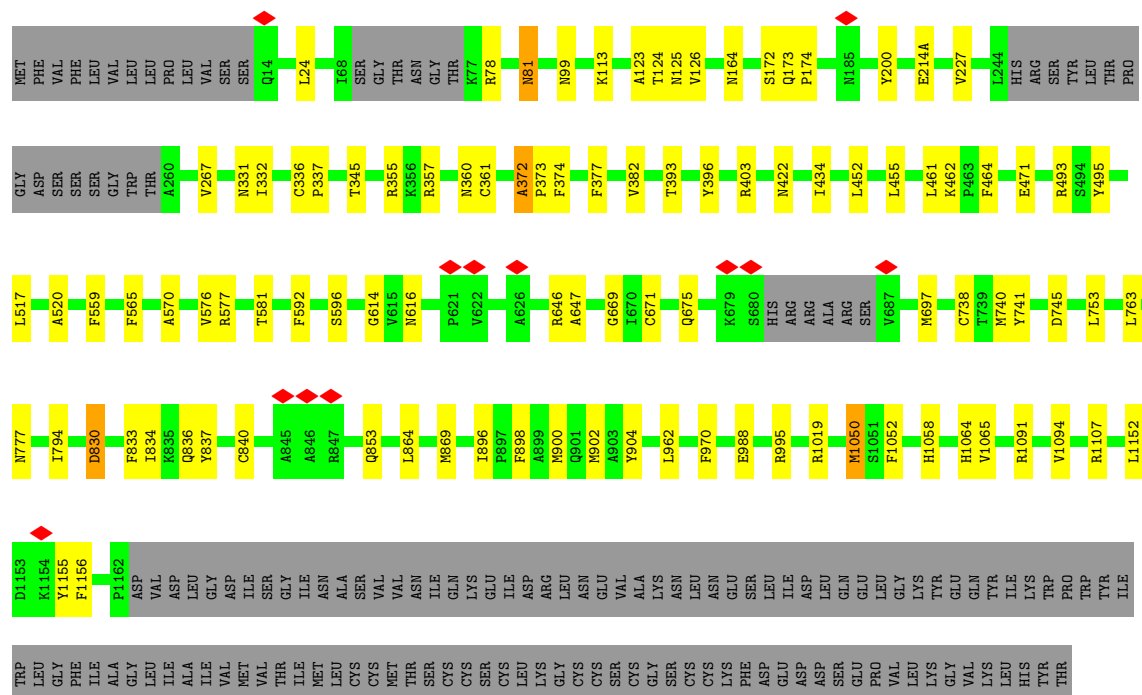
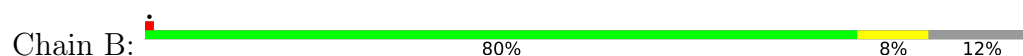
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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



• Molecule 1: Spike glycoprotein



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



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

Chain F:  100%



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

Chain I:  100%



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

Chain O:  50%
100%



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

Chain Q:  100%



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

Chain T:  100%



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

Chain Z:  50%
100%



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

Chain b:  100%



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

Chain e:  50% 50%



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

Chain E:  67% 33%



- Molecule 3: 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%



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

Chain H:  100%

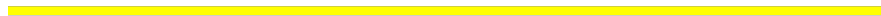


- Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



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

Chain K:  100%



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

Chain M:  100%

NAG1
NAG2
MAN3

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

Chain N:  100%

NAG1
NAG2
MAN3

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

Chain P:  67% 33%

NAG1
NAG2
MAN3

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

Chain R:  33% 67% 33%

NAG1
NAG2
MAN3

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

Chain S:  100%

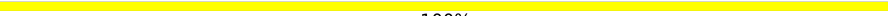
NAG1
NAG2
MAN3

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

Chain U:  100%

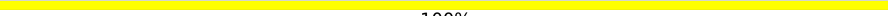
NAG1
NAG2
MAN3

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

Chain V:  100%

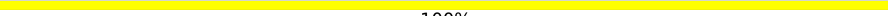
MAG1
MAG2
MAN3

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

Chain X:  100%

MAG1
MAG2
MAN3

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

Chain Y:  100%

MAG1
MAG2
MAN3

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

Chain a:  67% 33%

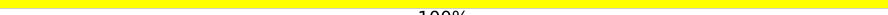
MAG1
MAG2
MAN3

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

Chain c:  33% 100%

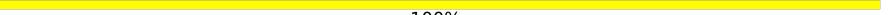

MAG1
MAG2
MAN3

- Molecule 3: 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
MAN3

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

Chain f:  100%

MAG1
MAG2
MAN3

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

Chain g:  100%

MAG1
MAG2
MAN3

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

Chain i:  100%

MAG1
MAG2
MAN3

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

Chain j:  100%

MAG1
MAG2
MAN3

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

Chain L:  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 W:  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 h:  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	69374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.592	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.037	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/8996	1.26	15/12233 (0.1%)
1	B	0.71	0/8996	1.26	18/12233 (0.1%)
1	C	0.70	0/8996	1.26	18/12233 (0.1%)
All	All	0.71	0/26988	1.26	51/36699 (0.1%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1091	ARG	N-CA-C	-7.17	103.07	111.03
1	C	1091	ARG	N-CA-C	-7.16	103.08	111.03
1	B	1091	ARG	N-CA-C	-7.13	103.12	111.03
1	A	422	ASN	CA-CB-CG	6.97	119.57	112.60
1	B	422	ASN	CA-CB-CG	6.97	119.57	112.60
1	C	422	ASN	CA-CB-CG	6.96	119.56	112.60
1	A	1050	MET	CA-C-N	-6.20	113.08	122.81
1	A	1050	MET	C-N-CA	-6.20	113.08	122.81
1	C	1050	MET	CA-C-N	-6.19	113.08	122.81
1	C	1050	MET	C-N-CA	-6.19	113.08	122.81
1	B	1050	MET	CA-C-N	-6.17	113.12	122.81
1	B	1050	MET	C-N-CA	-6.17	113.12	122.81
1	B	81	ASN	CA-CB-CG	6.06	118.66	112.60
1	C	81	ASN	CA-CB-CG	6.02	118.62	112.60
1	A	81	ASN	CA-CB-CG	6.01	118.61	112.60
1	A	336	CYS	CA-C-N	5.66	126.91	119.84
1	A	336	CYS	C-N-CA	5.66	126.91	119.84
1	A	559	PHE	CA-CB-CG	5.65	119.45	113.80
1	C	336	CYS	CA-C-N	5.64	126.89	119.84
1	C	336	CYS	C-N-CA	5.64	126.89	119.84
1	B	559	PHE	CA-CB-CG	5.64	119.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	CYS	CA-C-N	5.64	126.89	119.84
1	B	336	CYS	C-N-CA	5.64	126.89	119.84
1	C	559	PHE	CA-CB-CG	5.63	119.43	113.80
1	A	331	ASN	N-CA-C	5.45	118.06	109.39
1	C	331	ASN	N-CA-C	5.45	118.05	109.39
1	B	331	ASN	N-CA-C	5.45	118.05	109.39
1	A	464	PHE	CA-CB-CG	5.35	119.15	113.80
1	C	464	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	464	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	745	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	745	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	745	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	372	ALA	CA-C-N	5.26	126.42	119.84
1	A	372	ALA	C-N-CA	5.26	126.42	119.84
1	C	372	ALA	CA-C-N	5.25	126.40	119.84
1	C	372	ALA	C-N-CA	5.25	126.40	119.84
1	B	372	ALA	CA-C-N	5.24	126.39	119.84
1	B	372	ALA	C-N-CA	5.24	126.39	119.84
1	C	1064	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	B	1064	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	A	1064	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	B	267	VAL	CA-C-N	5.05	125.92	121.58
1	B	267	VAL	C-N-CA	5.05	125.92	121.58
1	C	853	GLN	OE1-CD-NE2	-5.03	117.58	122.60
1	A	853	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	853	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	B	1058	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	C	267	VAL	CA-C-N	5.02	125.89	121.58
1	C	267	VAL	C-N-CA	5.02	125.89	121.58
1	C	1058	HIS	CB-CG-CD2	-5.01	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	8789	0	8593	139	0
1	B	8789	0	8593	134	0
1	C	8789	0	8593	141	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	I	28	0	25	4	0
2	O	28	0	25	0	0
2	Q	28	0	25	0	0
2	T	28	0	25	3	0
2	Z	28	0	25	0	0
2	b	28	0	25	0	0
2	e	28	0	25	2	0
3	E	39	0	34	0	0
3	G	39	0	34	4	0
3	H	39	0	34	0	0
3	J	39	0	34	0	0
3	K	39	0	34	0	0
3	M	39	0	34	0	0
3	N	39	0	34	0	0
3	P	39	0	34	0	0
3	R	39	0	34	4	0
3	S	39	0	34	0	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
3	X	39	0	34	0	0
3	Y	39	0	34	0	0
3	a	39	0	34	0	0
3	c	39	0	34	3	0
3	d	39	0	34	0	0
3	f	39	0	34	0	0
3	g	39	0	34	0	0
3	i	39	0	34	0	0
3	j	39	0	34	0	0
4	L	38	0	34	0	0
4	W	38	0	34	0	0
4	h	38	0	34	0	0
5	A	98	0	91	2	0
5	B	98	0	91	2	0
5	C	98	0	91	4	0
All	All	27846	0	27093	331	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 6.

All (331) 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:C:740:MET:HE1	1:B:592:PHE:CZ	1.48	1.46
1:C:592:PHE:CZ	1:A:740:MET:HE1	1.47	1.46
1:C:173:GLN:HB3	1:C:174:PRO:CD	1.62	1.29
1:B:173:GLN:HB3	1:B:174:PRO:CD	1.62	1.29
1:A:173:GLN:HB3	1:A:174:PRO:CD	1.62	1.27
1:C:592:PHE:CZ	1:A:740:MET:CE	2.20	1.25
1:C:740:MET:CE	1:B:592:PHE:CZ	2.21	1.23
1:C:904:TYR:CE2	1:B:1107:ARG:HD3	1.78	1.18
1:C:1107:ARG:HD3	1:A:904:TYR:CE2	1.79	1.18
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	1.78	1.17
1:C:740:MET:HE1	1:B:592:PHE:CE1	1.81	1.16
1:B:173:GLN:HB3	1:B:174:PRO:HD2	1.24	1.14
1:C:592:PHE:CE1	1:A:740:MET:HE1	1.81	1.14
1:B:24:LEU:HD22	1:B:78:ARG:NH1	1.64	1.13
1:C:24:LEU:HD22	1:C:78:ARG:NH1	1.64	1.11
1:A:24:LEU:HD22	1:A:78:ARG:NH1	1.64	1.10
1:C:173:GLN:HB3	1:C:174:PRO:HD2	1.24	1.09
1:A:173:GLN:HB3	1:A:174:PRO:HD2	1.24	1.07
1:B:24:LEU:HD22	1:B:78:ARG:HH12	1.21	1.03
1:A:173:GLN:CB	1:A:174:PRO:HD2	1.89	1.02
1:C:173:GLN:CB	1:C:174:PRO:HD2	1.89	1.01
1:B:173:GLN:CB	1:B:174:PRO:HD2	1.90	1.01
1:A:1107:ARG:HD3	1:B:904:TYR:CD2	1.97	0.99
1:C:24:LEU:HD22	1:C:78:ARG:HH12	1.22	0.99
1:C:904:TYR:CD2	1:B:1107:ARG:HD3	1.96	0.99
1:A:24:LEU:HD22	1:A:78:ARG:HH12	1.22	0.99
1:C:1107:ARG:HD3	1:A:904:TYR:CD2	1.97	0.98
1:A:173:GLN:CB	1:A:174:PRO:CD	2.39	0.98
1:B:173:GLN:HB3	1:B:174:PRO:HD3	1.46	0.97
1:A:462:LYS:HG2	3:c:1:NAG:C8	1.97	0.95
1:C:462:LYS:HG2	3:R:1:NAG:C8	1.97	0.95
1:A:173:GLN:HB3	1:A:174:PRO:HD3	1.45	0.94
1:C:173:GLN:HB3	1:C:174:PRO:HD3	1.45	0.94
1:B:462:LYS:HG2	3:G:1:NAG:C8	1.98	0.93
1:C:904:TYR:HE2	1:B:1107:ARG:HD3	1.35	0.90
1:C:455:LEU:HD22	1:C:493:ARG:HD2	1.54	0.88
1:B:455:LEU:HD22	1:B:493:ARG:HD2	1.54	0.88
1:A:1107:ARG:HD3	1:B:904:TYR:HE2	1.35	0.87
1:A:493:ARG:HG3	1:A:493:ARG:HH11	1.39	0.87
1:A:455:LEU:HD22	1:A:493:ARG:HD2	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HG21	1:B:361:CYS:CA	2.05	0.87
1:C:1107:ARG:HD3	1:A:904:TYR:HE2	1.36	0.87
1:C:332:ILE:HG21	1:C:361:CYS:CA	2.05	0.86
1:A:332:ILE:HG21	1:A:361:CYS:CA	2.05	0.86
1:B:493:ARG:HG3	1:B:493:ARG:HH11	1.39	0.86
1:C:493:ARG:HG3	1:C:493:ARG:HH11	1.39	0.86
1:C:1019:ARG:HG3	1:C:1019:ARG:HH11	1.41	0.86
1:B:332:ILE:HG21	1:B:361:CYS:N	1.90	0.86
1:C:332:ILE:HG21	1:C:361:CYS:N	1.90	0.86
1:A:1019:ARG:HH11	1:A:1019:ARG:HG3	1.41	0.85
1:B:1019:ARG:HG3	1:B:1019:ARG:HH11	1.41	0.85
1:A:332:ILE:HG21	1:A:361:CYS:N	1.90	0.85
1:A:403:ARG:CZ	1:A:495:TYR:CE1	2.62	0.83
1:B:403:ARG:CZ	1:B:495:TYR:CE1	2.62	0.83
1:C:900:MET:O	1:C:904:TYR:HD1	1.63	0.82
1:C:403:ARG:CZ	1:C:495:TYR:CE1	2.62	0.82
1:C:403:ARG:CZ	1:C:495:TYR:CD1	2.63	0.81
1:A:403:ARG:CZ	1:A:495:TYR:CD1	2.63	0.81
1:B:403:ARG:CZ	1:B:495:TYR:CD1	2.63	0.81
1:A:900:MET:O	1:A:904:TYR:HD1	1.63	0.81
1:B:900:MET:O	1:B:904:TYR:HD1	1.63	0.81
1:B:403:ARG:NH1	1:B:495:TYR:HE1	1.80	0.80
1:B:836:GLN:HE21	2:T:1:NAG:H2	1.47	0.80
1:A:403:ARG:NH1	1:A:495:TYR:HE1	1.80	0.80
1:C:403:ARG:NH1	1:C:495:TYR:HE1	1.80	0.79
1:A:836:GLN:NE2	2:I:1:NAG:H2	1.97	0.79
1:A:836:GLN:HE21	2:I:1:NAG:H2	1.48	0.79
1:B:830:ASP:HA	1:B:833:PHE:HE1	1.48	0.77
1:A:830:ASP:HA	1:A:833:PHE:HE1	1.49	0.77
1:C:900:MET:O	1:C:904:TYR:CD1	2.38	0.77
1:C:830:ASP:HA	1:C:833:PHE:HE1	1.49	0.76
1:A:900:MET:O	1:A:904:TYR:CD1	2.38	0.76
1:B:332:ILE:CG2	1:B:361:CYS:HA	2.16	0.76
1:C:592:PHE:CE2	1:A:740:MET:CE	2.69	0.75
1:A:1019:ARG:HG3	1:A:1019:ARG:NH1	1.99	0.75
1:C:332:ILE:CG2	1:C:361:CYS:HA	2.17	0.75
1:B:836:GLN:NE2	2:T:1:NAG:H2	2.02	0.75
1:B:900:MET:O	1:B:904:TYR:CD1	2.38	0.75
1:A:332:ILE:CG2	1:A:361:CYS:HA	2.16	0.75
1:C:740:MET:CE	1:B:592:PHE:CE2	2.70	0.75
1:C:740:MET:HE2	1:B:592:PHE:CZ	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:PHE:CZ	1:A:740:MET:HE2	2.21	0.74
1:A:1107:ARG:CD	1:B:904:TYR:CE2	2.67	0.73
1:C:904:TYR:HE2	1:B:1107:ARG:CD	2.02	0.73
1:B:1019:ARG:HG3	1:B:1019:ARG:NH1	1.99	0.72
1:A:1107:ARG:CD	1:B:904:TYR:HE2	2.02	0.72
1:B:830:ASP:HA	1:B:833:PHE:CE1	2.25	0.72
1:C:1107:ARG:CD	1:A:904:TYR:HE2	2.03	0.71
1:A:697:MET:HE1	1:B:864:LEU:HG	1.72	0.71
1:C:1019:ARG:HG3	1:C:1019:ARG:NH1	1.99	0.71
1:C:697:MET:HE1	1:A:864:LEU:HG	1.72	0.71
1:C:864:LEU:HG	1:B:697:MET:HE1	1.73	0.71
1:A:830:ASP:HA	1:A:833:PHE:CE1	2.25	0.71
1:C:830:ASP:HA	1:C:833:PHE:CE1	2.25	0.71
1:C:741:TYR:OH	1:C:962:LEU:HD12	1.91	0.70
1:A:741:TYR:OH	1:A:962:LEU:HD12	1.91	0.70
1:A:896:ILE:HD11	1:A:904:TYR:CE1	2.27	0.70
1:C:896:ILE:HD11	1:C:904:TYR:CE1	2.27	0.70
5:C:1306:NAG:H83	1:A:794:ILE:HD13	1.72	0.70
1:B:896:ILE:HD11	1:B:904:TYR:CE1	2.27	0.70
1:A:462:LYS:HG2	3:c:1:NAG:H82	1.74	0.69
1:C:836:GLN:HE21	2:e:1:NAG:H2	1.58	0.69
1:B:741:TYR:OH	1:B:962:LEU:HD12	1.91	0.69
1:C:836:GLN:NE2	2:e:1:NAG:H2	2.08	0.69
1:C:904:TYR:CE2	1:B:1107:ARG:CD	2.66	0.69
1:C:332:ILE:CG2	1:C:361:CYS:CA	2.72	0.68
1:B:403:ARG:NH1	1:B:495:TYR:CE1	2.62	0.68
1:C:403:ARG:NH1	1:C:495:TYR:CE1	2.62	0.68
1:C:455:LEU:HD23	1:C:493:ARG:CZ	2.24	0.68
1:A:455:LEU:HD23	1:A:493:ARG:CZ	2.24	0.68
1:B:332:ILE:CG2	1:B:361:CYS:CA	2.71	0.68
1:C:462:LYS:HG2	3:R:1:NAG:H82	1.74	0.68
1:C:565:PHE:CD2	1:C:576:VAL:HG23	2.29	0.67
1:B:462:LYS:HG2	3:G:1:NAG:H82	1.76	0.67
1:B:898:PHE:HZ	1:B:1050:MET:HE1	1.59	0.67
1:B:565:PHE:CD2	1:B:576:VAL:HG23	2.29	0.67
1:A:565:PHE:CD2	1:A:576:VAL:HG23	2.29	0.67
1:B:455:LEU:HD23	1:B:493:ARG:CZ	2.24	0.67
1:A:24:LEU:CD2	1:A:78:ARG:HH12	2.04	0.67
1:C:898:PHE:HZ	1:C:1050:MET:HE1	1.59	0.66
1:C:455:LEU:HD22	1:C:493:ARG:CD	2.26	0.66
1:C:1050:MET:SD	1:C:1052:PHE:CZ	2.89	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1107:ARG:CD	1:A:904:TYR:CE2	2.68	0.66
1:C:740:MET:HE1	1:B:592:PHE:CE2	2.25	0.66
1:A:1050:MET:SD	1:A:1052:PHE:CZ	2.89	0.66
1:B:462:LYS:HG2	3:G:1:NAG:H81	1.79	0.65
1:C:794:ILE:HD13	5:B:1306:NAG:H83	1.77	0.65
1:A:898:PHE:HZ	1:A:1050:MET:HE1	1.59	0.65
1:C:898:PHE:CZ	1:C:1050:MET:HE1	2.32	0.65
1:A:455:LEU:HD22	1:A:493:ARG:CD	2.26	0.65
1:B:1050:MET:SD	1:B:1052:PHE:CZ	2.89	0.65
1:A:902:MET:SD	1:A:1050:MET:HE3	2.38	0.64
1:C:24:LEU:CD2	1:C:78:ARG:HH12	2.04	0.64
1:A:493:ARG:HH11	1:A:493:ARG:CG	2.11	0.64
1:A:898:PHE:CZ	1:A:1050:MET:HE1	2.32	0.64
1:B:902:MET:SD	1:B:1050:MET:HE3	2.38	0.64
1:A:332:ILE:CG2	1:A:361:CYS:CA	2.71	0.63
1:B:455:LEU:HD22	1:B:493:ARG:CD	2.26	0.63
1:B:898:PHE:CZ	1:B:1050:MET:HE1	2.32	0.63
1:B:493:ARG:HH11	1:B:493:ARG:CG	2.11	0.63
1:C:493:ARG:HH11	1:C:493:ARG:CG	2.11	0.63
1:C:592:PHE:CE2	1:A:740:MET:HE1	2.25	0.63
1:B:24:LEU:CD2	1:B:78:ARG:HH12	2.04	0.63
1:C:902:MET:SD	1:C:1050:MET:HE3	2.38	0.63
1:A:741:TYR:OH	1:A:962:LEU:CD1	2.47	0.62
1:C:462:LYS:HG2	3:R:1:NAG:H81	1.78	0.62
1:B:741:TYR:OH	1:B:962:LEU:CD1	2.47	0.62
1:C:741:TYR:OH	1:C:962:LEU:CD1	2.47	0.61
1:C:592:PHE:CE2	1:A:740:MET:HE2	2.34	0.61
1:A:403:ARG:NH1	1:A:495:TYR:CE1	2.62	0.61
1:C:697:MET:HE1	1:A:864:LEU:CG	2.30	0.61
1:C:740:MET:HE2	1:B:592:PHE:CE2	2.35	0.61
1:A:697:MET:HE1	1:B:864:LEU:CG	2.31	0.61
1:C:864:LEU:CG	1:B:697:MET:HE1	2.31	0.60
1:B:455:LEU:CD2	1:B:493:ARG:HD2	2.31	0.59
5:C:1306:NAG:C8	1:A:794:ILE:HD13	2.33	0.59
5:A:1306:NAG:H83	1:B:794:ILE:HD13	1.84	0.59
1:A:462:LYS:HG2	3:c:1:NAG:H81	1.78	0.58
1:C:646:ARG:O	1:A:834:ILE:HD11	2.03	0.58
1:A:646:ARG:O	1:B:834:ILE:HD11	2.03	0.58
1:C:125:ASN:HB2	1:C:172:SER:O	2.04	0.58
1:C:455:LEU:CD2	1:C:493:ARG:HD2	2.31	0.58
1:C:403:ARG:CZ	1:C:495:TYR:HD1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:ILE:HD11	1:C:904:TYR:HE1	1.68	0.58
1:A:896:ILE:HD11	1:A:904:TYR:HE1	1.68	0.57
1:C:357:ARG:HB2	1:C:396:TYR:CE1	2.39	0.57
1:A:357:ARG:HB2	1:A:396:TYR:CE1	2.39	0.57
1:A:125:ASN:HB2	1:A:172:SER:O	2.04	0.57
1:B:125:ASN:HB2	1:B:172:SER:O	2.04	0.57
1:B:357:ARG:HB2	1:B:396:TYR:CE1	2.39	0.57
1:A:403:ARG:NH2	1:A:495:TYR:CD1	2.74	0.56
1:C:834:ILE:HD11	1:B:646:ARG:O	2.04	0.56
1:B:124:THR:O	1:B:124:THR:HG22	2.05	0.56
1:B:403:ARG:NH2	1:B:495:TYR:CD1	2.74	0.56
1:C:834:ILE:HG23	1:B:614:GLY:C	2.30	0.56
1:A:614:GLY:C	1:B:834:ILE:HG23	2.32	0.56
1:A:403:ARG:CZ	1:A:495:TYR:HD1	2.17	0.55
1:C:403:ARG:NH2	1:C:495:TYR:CD1	2.74	0.55
1:C:124:THR:HG22	1:C:124:THR:O	2.05	0.55
1:A:124:THR:HG22	1:A:124:THR:O	2.05	0.55
1:A:455:LEU:CD2	1:A:493:ARG:HD2	2.31	0.55
1:C:614:GLY:C	1:A:834:ILE:HG23	2.32	0.55
1:C:647:ALA:C	1:A:834:ILE:HD11	2.32	0.55
1:C:834:ILE:HD11	1:B:647:ALA:C	2.31	0.55
1:A:403:ARG:NE	1:A:495:TYR:HD1	2.05	0.55
1:C:471:GLU:OE2	1:A:113:LYS:HE2	2.07	0.55
1:B:403:ARG:NE	1:B:495:TYR:HD1	2.05	0.55
1:B:896:ILE:HD11	1:B:904:TYR:HE1	1.68	0.54
1:C:455:LEU:HD23	1:C:493:ARG:NE	2.23	0.54
1:A:647:ALA:C	1:B:834:ILE:HD11	2.32	0.54
1:C:403:ARG:NE	1:C:495:TYR:HD1	2.05	0.54
1:C:671:CYS:SG	1:C:697:MET:HE2	2.48	0.54
1:A:455:LEU:HD23	1:A:493:ARG:NE	2.23	0.54
1:A:671:CYS:SG	1:A:697:MET:HE2	2.48	0.54
1:B:671:CYS:SG	1:B:697:MET:HE2	2.48	0.54
1:C:777:ASN:OD1	1:C:1019:ARG:NH1	2.41	0.54
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.41	0.54
1:A:455:LEU:CD2	1:A:493:ARG:NE	2.72	0.53
1:A:125:ASN:HA	1:A:173:GLN:C	2.33	0.53
1:B:455:LEU:HD23	1:B:493:ARG:NE	2.23	0.53
1:A:1050:MET:SD	1:A:1052:PHE:HZ	2.31	0.53
1:B:403:ARG:CZ	1:B:495:TYR:HD1	2.17	0.53
1:C:125:ASN:HA	1:C:173:GLN:C	2.33	0.53
1:C:1050:MET:SD	1:C:1052:PHE:HZ	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LEU:CD2	1:B:493:ARG:NE	2.72	0.53
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.41	0.53
1:B:125:ASN:HA	1:B:173:GLN:C	2.33	0.53
1:B:1050:MET:SD	1:B:1052:PHE:HZ	2.31	0.53
1:C:455:LEU:CD2	1:C:493:ARG:NE	2.72	0.52
1:C:493:ARG:CG	1:C:493:ARG:NH1	2.72	0.52
1:C:794:ILE:HD13	5:B:1306:NAG:C8	2.40	0.52
1:A:471:GLU:OE2	1:B:113:LYS:HE2	2.11	0.51
1:C:493:ARG:HG3	1:C:493:ARG:NH1	2.18	0.50
1:C:355:ARG:NH2	1:A:200:TYR:OH	2.44	0.50
1:A:355:ARG:NH2	1:B:200:TYR:OH	2.44	0.50
1:C:834:ILE:HG23	1:B:614:GLY:O	2.11	0.50
1:C:200:TYR:OH	1:B:355:ARG:NH2	2.44	0.49
1:C:646:ARG:O	1:A:834:ILE:CD1	2.61	0.49
1:A:902:MET:SD	1:A:1050:MET:CE	3.01	0.49
1:B:902:MET:SD	1:B:1050:MET:CE	3.00	0.49
1:C:113:LYS:HE2	1:B:471:GLU:OE2	2.11	0.49
1:B:332:ILE:HG22	1:B:361:CYS:HA	1.94	0.49
1:B:493:ARG:CG	1:B:493:ARG:NH1	2.72	0.48
1:A:614:GLY:O	1:B:834:ILE:HG23	2.12	0.48
1:A:646:ARG:O	1:B:834:ILE:CD1	2.61	0.48
1:C:614:GLY:O	1:A:834:ILE:HG23	2.12	0.48
1:C:902:MET:SD	1:C:1050:MET:CE	3.01	0.48
1:C:970:PHE:O	1:C:995:ARG:HD3	2.14	0.48
5:C:1306:NAG:H83	1:A:794:ILE:CD1	2.41	0.48
1:A:1156:PHE:CZ	1:B:1155:TYR:HB3	2.48	0.48
1:A:970:PHE:O	1:A:995:ARG:HD3	2.14	0.48
1:C:332:ILE:HG22	1:C:361:CYS:HA	1.94	0.48
1:C:834:ILE:CD1	1:B:646:ARG:O	2.62	0.48
1:A:646:ARG:O	1:B:834:ILE:HG12	2.14	0.48
1:C:834:ILE:HG12	1:B:646:ARG:O	2.14	0.47
1:A:332:ILE:HG22	1:A:361:CYS:HA	1.94	0.47
1:B:970:PHE:O	1:B:995:ARG:HD3	2.14	0.47
1:C:403:ARG:NE	1:C:495:TYR:CD1	2.82	0.47
1:C:126:VAL:HG23	1:C:173:GLN:O	2.14	0.47
1:A:493:ARG:CG	1:A:493:ARG:NH1	2.72	0.47
1:B:126:VAL:HG23	1:B:173:GLN:O	2.15	0.47
1:C:646:ARG:O	1:A:834:ILE:HG12	2.14	0.47
1:A:493:ARG:HG3	1:A:493:ARG:NH1	2.17	0.47
1:A:1107:ARG:NH1	1:B:904:TYR:CE2	2.68	0.47
1:A:173:GLN:HB2	1:A:174:PRO:HD2	1.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1155:TYR:HB3	1:B:1156:PHE:CZ	2.49	0.47
1:B:403:ARG:NE	1:B:495:TYR:CD1	2.82	0.47
1:C:403:ARG:CZ	1:C:495:TYR:HE1	2.14	0.47
1:A:126:VAL:HG23	1:A:173:GLN:O	2.14	0.46
1:B:173:GLN:HB2	1:B:174:PRO:HD2	1.91	0.46
1:C:173:GLN:CB	1:C:174:PRO:CD	2.39	0.46
1:A:455:LEU:CD2	1:A:493:ARG:CD	2.93	0.46
1:A:1107:ARG:HD3	1:B:904:TYR:HD2	1.73	0.46
1:C:1094:VAL:HB	1:A:904:TYR:OH	2.16	0.46
1:A:403:ARG:NE	1:A:495:TYR:CD1	2.82	0.46
1:A:836:GLN:NE2	2:I:1:NAG:O7	2.49	0.46
1:A:1019:ARG:NH1	1:A:1019:ARG:CG	2.72	0.46
1:C:1156:PHE:CZ	1:A:1155:TYR:HB3	2.51	0.45
1:B:372:ALA:HB1	1:B:374:PHE:CD2	2.52	0.45
1:C:372:ALA:HB1	1:C:374:PHE:CD2	2.52	0.45
1:C:869:MET:HE1	1:B:669:GLY:HA2	1.98	0.45
5:A:1306:NAG:C8	1:B:794:ILE:HD13	2.46	0.45
1:C:904:TYR:OH	1:B:1094:VAL:HB	2.16	0.45
1:A:1094:VAL:HB	1:B:904:TYR:OH	2.16	0.45
1:C:669:GLY:HA2	1:A:869:MET:HE1	1.99	0.44
1:A:616:ASN:HD22	1:B:836:GLN:HB2	1.82	0.44
1:C:1155:TYR:HB3	1:B:1156:PHE:CE2	2.53	0.44
1:A:457:ARG:NE	1:A:459:SER:O	2.48	0.44
5:C:1306:NAG:C8	1:A:794:ILE:CD1	2.95	0.44
1:A:669:GLY:HA2	1:B:869:MET:HE1	1.98	0.44
1:C:616:ASN:HD22	1:A:836:GLN:HB2	1.83	0.44
1:A:372:ALA:HB1	1:A:374:PHE:CD2	2.52	0.44
1:A:393:THR:HG21	1:A:520:ALA:HB3	2.00	0.44
1:B:493:ARG:HG3	1:B:493:ARG:NH1	2.18	0.44
1:C:836:GLN:HB2	1:B:616:ASN:HD22	1.82	0.44
1:C:332:ILE:HG21	1:C:360:ASN:C	2.43	0.43
1:B:357:ARG:HB2	1:B:396:TYR:HE1	1.84	0.43
1:B:393:THR:HG21	1:B:520:ALA:HB3	2.00	0.43
1:B:332:ILE:CG2	1:B:361:CYS:N	2.74	0.43
1:C:357:ARG:HB2	1:C:396:TYR:HE1	1.84	0.43
1:C:565:PHE:CD2	1:C:576:VAL:CG2	2.98	0.43
1:C:393:THR:HG21	1:C:520:ALA:HB3	2.00	0.43
1:C:452:LEU:HD13	1:C:493:ARG:O	2.19	0.43
1:C:1107:ARG:NH1	1:A:904:TYR:CD2	2.87	0.43
1:C:646:ARG:O	1:A:834:ILE:CG1	2.67	0.42
1:A:741:TYR:CE1	1:A:962:LEU:HG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:MET:HG3	1:A:1065:VAL:CG2	2.50	0.42
1:A:1156:PHE:CE2	1:B:1155:TYR:HB3	2.54	0.42
1:B:565:PHE:CD2	1:B:576:VAL:CG2	2.98	0.42
1:B:1050:MET:HG3	1:B:1065:VAL:CG2	2.50	0.42
1:A:1107:ARG:CG	1:B:904:TYR:HE2	2.32	0.42
1:B:455:LEU:CD2	1:B:493:ARG:CD	2.93	0.42
1:B:741:TYR:CE1	1:B:962:LEU:HG	2.54	0.42
1:C:834:ILE:CG1	1:B:646:ARG:O	2.68	0.42
1:A:646:ARG:O	1:B:834:ILE:CG1	2.68	0.42
1:C:173:GLN:HB2	1:C:174:PRO:HD2	1.91	0.42
1:C:904:TYR:HE2	1:B:1107:ARG:CG	2.32	0.42
1:C:1107:ARG:CG	1:A:904:TYR:HE2	2.33	0.42
1:A:332:ILE:HD13	1:A:360:ASN:HA	2.01	0.42
1:B:452:LEU:HD13	1:B:493:ARG:O	2.19	0.42
1:C:741:TYR:CE1	1:C:962:LEU:HG	2.54	0.42
1:C:1050:MET:HG3	1:C:1065:VAL:CG2	2.50	0.42
1:C:1050:MET:HG2	1:C:1065:VAL:HB	2.02	0.42
1:A:452:LEU:HD13	1:A:493:ARG:O	2.19	0.42
1:A:565:PHE:CD2	1:A:576:VAL:CG2	2.98	0.42
1:A:741:TYR:CZ	1:A:962:LEU:HD11	2.55	0.42
1:B:1050:MET:HG2	1:B:1065:VAL:HB	2.02	0.42
1:C:904:TYR:CD2	1:B:1107:ARG:NH1	2.88	0.42
1:C:741:TYR:CZ	1:C:962:LEU:HD11	2.55	0.41
1:C:856:LYS:HE2	1:B:570:ALA:CB	2.51	0.41
1:B:332:ILE:HG21	1:B:360:ASN:C	2.43	0.41
1:B:332:ILE:HG21	1:B:361:CYS:C	2.45	0.41
1:B:332:ILE:HD13	1:B:360:ASN:HA	2.01	0.41
1:C:457:ARG:NE	1:C:459:SER:O	2.48	0.41
1:A:332:ILE:CG2	1:A:361:CYS:N	2.74	0.41
1:A:1050:MET:HG2	1:A:1065:VAL:HB	2.02	0.41
1:C:332:ILE:HD13	1:C:360:ASN:HA	2.01	0.41
1:C:1156:PHE:CE2	1:A:1155:TYR:HB3	2.56	0.41
1:A:357:ARG:HB2	1:A:396:TYR:HE1	1.84	0.41
1:A:332:ILE:HG21	1:A:360:ASN:C	2.43	0.41
1:A:901:GLN:O	1:A:905:ARG:HG2	2.21	0.41
1:A:1107:ARG:NH1	1:B:904:TYR:CD2	2.87	0.41
3:R:1:NAG:H61	3:R:2:NAG:N2	2.36	0.41
1:C:901:GLN:O	1:C:905:ARG:HG2	2.21	0.40
1:B:741:TYR:CZ	1:B:962:LEU:HD11	2.55	0.40
1:C:570:ALA:CB	1:A:856:LYS:HE2	2.51	0.40
1:C:408:ARG:C	1:C:408:ARG:HD2	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:NAG:H61	3:G:2:NAG:N2	2.36	0.40
2:T:1:NAG:H62	2:T:2:NAG:C7	2.51	0.40
1:B:740:MET:O	1:B:740:MET:HG3	2.20	0.40
2:I:1:NAG:H62	2:I:2:NAG:C7	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1111/1270 (88%)	1017 (92%)	85 (8%)	9 (1%)	16	47
1	B	1111/1270 (88%)	1017 (92%)	85 (8%)	9 (1%)	16	47
1	C	1111/1270 (88%)	1017 (92%)	85 (8%)	9 (1%)	16	47
All	All	3333/3810 (88%)	3051 (92%)	255 (8%)	27 (1%)	18	47

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	ASN
1	C	830	ASP
1	A	164	ASN
1	A	830	ASP
1	B	164	ASN
1	B	830	ASP
1	C	123	ALA
1	C	345	THR
1	A	123	ALA
1	A	345	THR
1	B	123	ALA
1	B	345	THR
1	C	99	ASN

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Mol	Chain	Res	Type
1	C	214(A)	GLU
1	A	99	ASN
1	A	214(A)	GLU
1	B	99	ASN
1	B	214(A)	GLU
1	C	81	ASN
1	A	81	ASN
1	B	81	ASN
1	C	337	PRO
1	C	373	PRO
1	A	337	PRO
1	A	373	PRO
1	B	337	PRO
1	B	373	PRO

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	978/1112 (88%)	960 (98%)	18 (2%)	51	73
1	B	978/1112 (88%)	961 (98%)	17 (2%)	53	74
1	C	978/1112 (88%)	960 (98%)	18 (2%)	51	73
All	All	2934/3336 (88%)	2881 (98%)	53 (2%)	51	73

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	87	ASN
1	C	227	VAL
1	C	377	PHE
1	C	382	VAL
1	C	434	ILE
1	C	461	LEU
1	C	517	LEU
1	C	577	ARG

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Mol	Chain	Res	Type
1	C	581	THR
1	C	596	SER
1	C	675	GLN
1	C	738	CYS
1	C	753	LEU
1	C	763	LEU
1	C	837	TYR
1	C	840	CYS
1	C	988	GLU
1	C	1152	LEU
1	A	87	ASN
1	A	227	VAL
1	A	377	PHE
1	A	382	VAL
1	A	434	ILE
1	A	461	LEU
1	A	517	LEU
1	A	577	ARG
1	A	581	THR
1	A	596	SER
1	A	675	GLN
1	A	738	CYS
1	A	753	LEU
1	A	763	LEU
1	A	837	TYR
1	A	840	CYS
1	A	988	GLU
1	A	1152	LEU
1	B	227	VAL
1	B	377	PHE
1	B	382	VAL
1	B	434	ILE
1	B	461	LEU
1	B	517	LEU
1	B	577	ARG
1	B	581	THR
1	B	596	SER
1	B	675	GLN
1	B	738	CYS
1	B	753	LEU
1	B	763	LEU
1	B	837	TYR

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Mol	Chain	Res	Type
1	B	840	CYS
1	B	988	GLU
1	B	1152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	183	GLN
1	C	218	GLN
1	C	334	ASN
1	C	544	ASN
1	C	613	GLN
1	C	677	GLN
1	C	751	ASN
1	C	779	GLN
1	C	836	GLN
1	C	907	ASN
1	C	914	ASN
1	C	1011	GLN
1	C	1058	HIS
1	A	183	GLN
1	A	218	GLN
1	A	334	ASN
1	A	544	ASN
1	A	613	GLN
1	A	751	ASN
1	A	755	GLN
1	A	779	GLN
1	A	836	GLN
1	A	914	ASN
1	A	1011	GLN
1	B	149	ASN
1	B	183	GLN
1	B	218	GLN
1	B	334	ASN
1	B	544	ASN
1	B	751	ASN
1	B	779	GLN
1	B	836	GLN
1	B	907	ASN
1	B	914	ASN
1	B	1011	GLN

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Mol	Chain	Res	Type
1	B	1023	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 ⓘ

90 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	1,2	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	D	2	2	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	E	1	1,3	14,14,15	0.17	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.36	0	17,19,21	0.78	0
3	MAN	E	3	3	11,11,12	1.52	2 (18%)	15,15,17	0.94	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.33	0	17,19,21	0.40	0
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	G	1	1,3	14,14,15	0.42	0	17,19,21	0.44	0
3	NAG	G	2	3	14,14,15	1.16	2 (14%)	17,19,21	1.11	1 (5%)
3	MAN	G	3	3	11,11,12	1.46	2 (18%)	15,15,17	0.56	0
3	NAG	H	1	1,3	14,14,15	1.21	2 (14%)	17,19,21	0.60	0
3	NAG	H	2	3	14,14,15	1.41	3 (21%)	17,19,21	0.80	1 (5%)
3	MAN	H	3	3	11,11,12	1.54	2 (18%)	15,15,17	0.97	0
2	NAG	I	1	1,2	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	I	2	2	14,14,15	0.30	0	17,19,21	0.54	0
3	NAG	J	1	1,3	14,14,15	1.12	1 (7%)	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	2	3	14,14,15	1.23	2 (14%)	17,19,21	0.66	0
3	MAN	J	3	3	11,11,12	1.49	2 (18%)	15,15,17	1.00	0
3	NAG	K	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	0.69	0
3	NAG	K	2	3	14,14,15	1.37	3 (21%)	17,19,21	0.68	0
3	MAN	K	3	3	11,11,12	1.49	2 (18%)	15,15,17	0.74	0
4	NAG	L	1	1,4	14,14,15	1.33	1 (7%)	17,19,21	0.97	2 (11%)
4	NAG	L	2	4	14,14,15	1.26	1 (7%)	17,19,21	0.82	1 (5%)
4	FUC	L	3	4	10,10,11	1.65	2 (20%)	14,14,16	1.08	1 (7%)
3	NAG	M	1	1,3	14,14,15	1.17	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	M	2	3	14,14,15	1.40	2 (14%)	17,19,21	1.05	2 (11%)
3	MAN	M	3	3	11,11,12	1.47	2 (18%)	15,15,17	0.73	0
3	NAG	N	1	1,3	14,14,15	1.21	2 (14%)	17,19,21	0.72	0
3	NAG	N	2	3	14,14,15	1.25	2 (14%)	17,19,21	1.00	1 (5%)
3	MAN	N	3	3	11,11,12	1.54	2 (18%)	15,15,17	0.78	1 (6%)
2	NAG	O	1	1,2	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	O	2	2	14,14,15	0.27	0	17,19,21	0.53	0
3	NAG	P	1	1,3	14,14,15	0.18	0	17,19,21	0.51	0
3	NAG	P	2	3	14,14,15	0.36	0	17,19,21	0.78	0
3	MAN	P	3	3	11,11,12	1.51	2 (18%)	15,15,17	0.94	1 (6%)
2	NAG	Q	1	1,2	14,14,15	0.33	0	17,19,21	0.40	0
2	NAG	Q	2	2	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	R	1	1,3	14,14,15	0.42	0	17,19,21	0.44	0
3	NAG	R	2	3	14,14,15	1.17	2 (14%)	17,19,21	1.11	1 (5%)
3	MAN	R	3	3	11,11,12	1.46	2 (18%)	15,15,17	0.56	0
3	NAG	S	1	1,3	14,14,15	1.20	2 (14%)	17,19,21	0.59	0
3	NAG	S	2	3	14,14,15	1.41	3 (21%)	17,19,21	0.80	1 (5%)
3	MAN	S	3	3	11,11,12	1.54	2 (18%)	15,15,17	0.97	0
2	NAG	T	1	1,2	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	T	2	2	14,14,15	0.29	0	17,19,21	0.55	0
3	NAG	U	1	1,3	14,14,15	1.11	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	U	2	3	14,14,15	1.23	2 (14%)	17,19,21	0.67	0
3	MAN	U	3	3	11,11,12	1.50	2 (18%)	15,15,17	1.00	0
3	NAG	V	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	0.69	0
3	NAG	V	2	3	14,14,15	1.38	3 (21%)	17,19,21	0.68	0
3	MAN	V	3	3	11,11,12	1.48	2 (18%)	15,15,17	0.74	0
4	NAG	W	1	1,4	14,14,15	1.32	1 (7%)	17,19,21	0.97	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	W	2	4	14,14,15	1.27	1 (7%)	17,19,21	0.82	1 (5%)
4	FUC	W	3	4	10,10,11	1.65	2 (20%)	14,14,16	1.08	1 (7%)
3	NAG	X	1	1,3	14,14,15	1.17	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	X	2	3	14,14,15	1.40	2 (14%)	17,19,21	1.05	2 (11%)
3	MAN	X	3	3	11,11,12	1.47	2 (18%)	15,15,17	0.73	0
3	NAG	Y	1	1,3	14,14,15	1.22	2 (14%)	17,19,21	0.71	0
3	NAG	Y	2	3	14,14,15	1.25	2 (14%)	17,19,21	1.00	1 (5%)
3	MAN	Y	3	3	11,11,12	1.55	2 (18%)	15,15,17	0.78	1 (6%)
2	NAG	Z	1	1,2	14,14,15	0.22	0	17,19,21	0.47	0
2	NAG	Z	2	2	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	a	1	1,3	14,14,15	0.17	0	17,19,21	0.51	0
3	NAG	a	2	3	14,14,15	0.37	0	17,19,21	0.78	0
3	MAN	a	3	3	11,11,12	1.51	2 (18%)	15,15,17	0.94	1 (6%)
2	NAG	b	1	1,2	14,14,15	0.33	0	17,19,21	0.40	0
2	NAG	b	2	2	14,14,15	0.28	0	17,19,21	0.52	0
3	NAG	c	1	1,3	14,14,15	0.42	0	17,19,21	0.44	0
3	NAG	c	2	3	14,14,15	1.16	2 (14%)	17,19,21	1.11	1 (5%)
3	MAN	c	3	3	11,11,12	1.46	2 (18%)	15,15,17	0.56	0
3	NAG	d	1	1,3	14,14,15	1.21	2 (14%)	17,19,21	0.59	0
3	NAG	d	2	3	14,14,15	1.42	3 (21%)	17,19,21	0.80	1 (5%)
3	MAN	d	3	3	11,11,12	1.54	2 (18%)	15,15,17	0.97	0
2	NAG	e	1	1,2	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	e	2	2	14,14,15	0.29	0	17,19,21	0.55	0
3	NAG	f	1	1,3	14,14,15	1.12	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	f	2	3	14,14,15	1.24	2 (14%)	17,19,21	0.66	0
3	MAN	f	3	3	11,11,12	1.49	2 (18%)	15,15,17	1.00	0
3	NAG	g	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	0.69	0
3	NAG	g	2	3	14,14,15	1.37	3 (21%)	17,19,21	0.68	0
3	MAN	g	3	3	11,11,12	1.49	2 (18%)	15,15,17	0.74	0
4	NAG	h	1	1,4	14,14,15	1.33	1 (7%)	17,19,21	0.97	2 (11%)
4	NAG	h	2	4	14,14,15	1.26	1 (7%)	17,19,21	0.83	1 (5%)
4	FUC	h	3	4	10,10,11	1.65	2 (20%)	14,14,16	1.08	1 (7%)
3	NAG	i	1	1,3	14,14,15	1.17	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	i	2	3	14,14,15	1.39	2 (14%)	17,19,21	1.04	2 (11%)
3	MAN	i	3	3	11,11,12	1.47	2 (18%)	15,15,17	0.73	0
3	NAG	j	1	1,3	14,14,15	1.21	2 (14%)	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	j	2	3	14,14,15	1.25	2 (14%)	17,19,21	1.01	1 (5%)
3	MAN	j	3	3	11,11,12	1.55	2 (18%)	15,15,17	0.78	1 (6%)

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
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	MAN	E	3	3	-	1/2/19/22	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
3	NAG	G	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	MAN	G	3	3	-	1/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	MAN	H	3	3	-	0/2/19/22	1/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	MAN	J	3	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	MAN	K	3	3	-	1/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	FUC	L	3	4	-	-	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	MAN	M	3	3	-	1/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	MAN	N	3	3	-	0/2/19/22	1/1/1/1
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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	NAG	f	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	f	2	3	-	0/6/23/26	0/1/1/1
3	MAN	f	3	3	-	0/2/19/22	0/1/1/1
3	NAG	g	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	g	2	3	-	0/6/23/26	0/1/1/1
3	MAN	g	3	3	-	1/2/19/22	0/1/1/1
4	NAG	h	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	h	2	4	-	0/6/23/26	0/1/1/1
4	FUC	h	3	4	-	-	0/1/1/1
3	NAG	i	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	0/6/23/26	0/1/1/1
3	MAN	i	3	3	-	1/2/19/22	0/1/1/1
3	NAG	j	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	j	2	3	-	0/6/23/26	0/1/1/1
3	MAN	j	3	3	-	0/2/19/22	1/1/1/1

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	3	MAN	O5-C5	3.35	1.50	1.43
3	N	3	MAN	O5-C5	3.31	1.49	1.43
3	d	3	MAN	O5-C5	3.31	1.49	1.43
3	j	3	MAN	O5-C5	3.31	1.49	1.43
3	H	3	MAN	O5-C5	3.30	1.49	1.43
3	S	3	MAN	O5-C5	3.28	1.49	1.43
3	i	3	MAN	O5-C5	3.21	1.49	1.43
3	M	3	MAN	O5-C5	3.19	1.49	1.43
3	g	3	MAN	O5-C5	3.19	1.49	1.43
3	X	3	MAN	O5-C5	3.19	1.49	1.43
3	K	3	MAN	O5-C5	3.16	1.49	1.43
3	V	3	MAN	O5-C5	3.13	1.49	1.43
3	X	2	NAG	O5-C5	3.09	1.49	1.43
3	M	2	NAG	O5-C5	3.08	1.49	1.43
3	i	2	NAG	O5-C5	3.06	1.49	1.43
4	W	3	FUC	O5-C5	2.97	1.49	1.43
4	L	3	FUC	O5-C5	2.96	1.49	1.43
4	h	3	FUC	O5-C5	2.93	1.49	1.43
3	J	3	MAN	O5-C5	2.91	1.49	1.43
3	f	3	MAN	O5-C5	2.90	1.49	1.43
3	U	3	MAN	O5-C5	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	NAG	O5-C5	2.88	1.49	1.43
3	g	2	NAG	O5-C5	2.88	1.49	1.43
3	V	2	NAG	O5-C5	2.88	1.49	1.43
3	E	3	MAN	O5-C5	2.85	1.49	1.43
3	a	3	MAN	O5-C5	2.85	1.49	1.43
3	P	3	MAN	O5-C5	2.84	1.49	1.43
4	W	2	NAG	O5-C5	2.84	1.49	1.43
3	d	2	NAG	O5-C5	2.83	1.48	1.43
4	L	2	NAG	O5-C5	2.83	1.48	1.43
4	h	1	NAG	O5-C5	2.81	1.48	1.43
4	h	2	NAG	O5-C5	2.81	1.48	1.43
3	H	2	NAG	O5-C5	2.81	1.48	1.43
3	S	2	NAG	O5-C5	2.80	1.48	1.43
3	E	3	MAN	O5-C1	2.79	1.48	1.43
3	a	3	MAN	O5-C1	2.78	1.48	1.43
3	G	3	MAN	O5-C5	2.76	1.48	1.43
4	W	1	NAG	O5-C5	2.76	1.48	1.43
3	c	3	MAN	O5-C5	2.76	1.48	1.43
4	L	1	NAG	O5-C5	2.76	1.48	1.43
3	P	3	MAN	O5-C1	2.76	1.48	1.43
3	R	3	MAN	O5-C5	2.73	1.48	1.43
3	N	2	NAG	O5-C5	2.60	1.48	1.43
3	Y	2	NAG	O5-C5	2.60	1.48	1.43
3	j	2	NAG	O5-C5	2.58	1.48	1.43
3	i	1	NAG	O5-C5	2.55	1.48	1.43
3	M	1	NAG	O5-C5	2.55	1.48	1.43
3	X	1	NAG	O5-C5	2.54	1.48	1.43
3	f	2	NAG	O5-C5	2.52	1.48	1.43
3	d	3	MAN	O5-C1	2.51	1.47	1.43
3	J	2	NAG	O5-C5	2.51	1.48	1.43
4	h	3	FUC	O5-C1	2.51	1.47	1.43
3	H	3	MAN	O5-C1	2.50	1.47	1.43
3	U	2	NAG	O5-C5	2.50	1.48	1.43
3	S	3	MAN	O5-C1	2.49	1.47	1.43
4	L	3	FUC	O5-C1	2.49	1.47	1.43
3	G	2	NAG	O5-C5	2.49	1.48	1.43
3	c	2	NAG	O5-C5	2.49	1.48	1.43
3	R	2	NAG	O5-C5	2.48	1.48	1.43
4	W	3	FUC	O5-C1	2.48	1.47	1.43
3	U	3	MAN	O5-C1	2.45	1.47	1.43
3	J	3	MAN	O5-C1	2.44	1.47	1.43
3	X	2	NAG	O4-C4	2.44	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	f	3	MAN	O5-C1	2.44	1.47	1.43
3	M	2	NAG	O4-C4	2.43	1.49	1.43
3	i	2	NAG	O4-C4	2.42	1.49	1.43
3	d	2	NAG	O4-C4	2.39	1.48	1.43
3	H	2	NAG	O4-C4	2.39	1.48	1.43
3	S	2	NAG	O4-C4	2.35	1.48	1.43
3	d	1	NAG	O5-C5	2.33	1.48	1.43
3	H	1	NAG	O5-C5	2.33	1.48	1.43
3	S	1	NAG	O5-C5	2.31	1.47	1.43
3	j	3	MAN	O5-C1	2.26	1.47	1.43
3	f	1	NAG	O5-C5	2.26	1.47	1.43
3	K	2	NAG	O4-C4	2.25	1.48	1.43
3	V	2	NAG	O4-C4	2.25	1.48	1.43
3	N	3	MAN	O5-C1	2.24	1.47	1.43
3	c	3	MAN	O5-C1	2.24	1.47	1.43
3	g	2	NAG	O4-C4	2.23	1.48	1.43
3	j	2	NAG	O4-C4	2.23	1.48	1.43
3	G	3	MAN	O5-C1	2.23	1.47	1.43
3	Y	3	MAN	O5-C1	2.23	1.47	1.43
3	Y	2	NAG	O4-C4	2.22	1.48	1.43
3	N	2	NAG	O4-C4	2.22	1.48	1.43
3	J	1	NAG	O5-C5	2.22	1.47	1.43
3	R	3	MAN	O5-C1	2.22	1.47	1.43
3	g	1	NAG	O5-C5	2.21	1.47	1.43
3	K	1	NAG	O5-C5	2.21	1.47	1.43
3	X	3	MAN	O5-C1	2.20	1.47	1.43
3	V	1	NAG	O5-C5	2.19	1.47	1.43
3	f	2	NAG	O4-C4	2.19	1.48	1.43
3	U	1	NAG	O5-C5	2.19	1.47	1.43
3	i	3	MAN	O5-C1	2.19	1.47	1.43
3	M	3	MAN	O5-C1	2.18	1.47	1.43
3	J	2	NAG	O4-C4	2.18	1.48	1.43
3	U	2	NAG	O4-C4	2.18	1.48	1.43
3	R	2	NAG	O4-C4	2.16	1.48	1.43
3	G	2	NAG	O4-C4	2.15	1.48	1.43
3	c	2	NAG	O4-C4	2.15	1.48	1.43
3	Y	1	NAG	C1-C2	2.15	1.55	1.52
3	S	2	NAG	O5-C1	2.13	1.47	1.43
3	g	2	NAG	O5-C1	2.13	1.47	1.43
3	N	1	NAG	C1-C2	2.13	1.55	1.52
3	H	2	NAG	O5-C1	2.12	1.47	1.43
3	K	2	NAG	O5-C1	2.11	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	2	NAG	O5-C1	2.11	1.47	1.43
3	j	1	NAG	C1-C2	2.11	1.55	1.52
3	d	2	NAG	O5-C1	2.10	1.47	1.43
3	Y	1	NAG	O5-C5	2.08	1.47	1.43
3	K	3	MAN	O5-C1	2.07	1.47	1.43
3	j	1	NAG	O5-C5	2.06	1.47	1.43
3	N	1	NAG	O5-C5	2.06	1.47	1.43
3	V	3	MAN	O5-C1	2.05	1.47	1.43
3	g	3	MAN	O5-C1	2.04	1.47	1.43
3	H	1	NAG	O4-C4	2.03	1.48	1.43
3	S	1	NAG	O4-C4	2.03	1.48	1.43
3	d	1	NAG	O4-C4	2.00	1.47	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C1-O5-C5	3.51	116.89	112.19
3	R	2	NAG	C1-O5-C5	3.49	116.86	112.19
3	c	2	NAG	C1-O5-C5	3.49	116.86	112.19
3	j	2	NAG	C1-O5-C5	3.38	116.71	112.19
3	Y	2	NAG	C1-O5-C5	3.36	116.69	112.19
3	N	2	NAG	C1-O5-C5	3.36	116.69	112.19
3	X	2	NAG	C4-C3-C2	-2.93	106.73	111.02
3	M	2	NAG	C4-C3-C2	-2.92	106.73	111.02
3	i	2	NAG	C4-C3-C2	-2.91	106.75	111.02
3	H	2	NAG	C1-O5-C5	2.71	115.81	112.19
3	d	2	NAG	C1-O5-C5	2.70	115.81	112.19
3	S	2	NAG	C1-O5-C5	2.69	115.79	112.19
4	W	1	NAG	O5-C5-C6	2.57	112.66	107.66
4	L	1	NAG	O5-C5-C6	2.56	112.65	107.66
4	h	1	NAG	O5-C5-C6	2.56	112.64	107.66
3	P	3	MAN	C1-O5-C5	2.32	115.30	112.19
3	E	3	MAN	C1-O5-C5	2.31	115.28	112.19
3	a	3	MAN	C1-O5-C5	2.31	115.28	112.19
3	X	1	NAG	O4-C4-C3	-2.31	104.94	110.38
3	i	1	NAG	O4-C4-C3	-2.30	104.96	110.38
3	M	1	NAG	O4-C4-C3	-2.30	104.96	110.38
4	W	1	NAG	C1-O5-C5	2.23	115.17	112.19
4	L	1	NAG	C1-O5-C5	2.19	115.13	112.19
4	h	1	NAG	C1-O5-C5	2.18	115.11	112.19
3	Y	3	MAN	C1-O5-C5	2.16	115.08	112.19
3	N	3	MAN	C1-O5-C5	2.16	115.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	j	3	MAN	C1-O5-C5	2.13	115.04	112.19
4	L	3	FUC	C1-C2-C3	2.12	112.73	109.64
4	W	3	FUC	C1-C2-C3	2.12	112.73	109.64
4	h	3	FUC	C1-C2-C3	2.11	112.72	109.64
4	h	2	NAG	C1-O5-C5	2.09	114.99	112.19
3	M	2	NAG	C1-O5-C5	2.06	114.95	112.19
4	L	2	NAG	C1-O5-C5	2.06	114.95	112.19
3	X	2	NAG	C1-O5-C5	2.06	114.94	112.19
4	W	2	NAG	C1-O5-C5	2.05	114.94	112.19
3	i	2	NAG	C1-O5-C5	2.05	114.93	112.19
3	f	1	NAG	C1-O5-C5	2.04	114.92	112.19
3	J	1	NAG	C1-O5-C5	2.04	114.91	112.19
3	U	1	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	c	1	NAG	C4-C5-C6-O6
3	M	3	MAN	O5-C5-C6-O6
3	X	3	MAN	O5-C5-C6-O6
3	i	3	MAN	O5-C5-C6-O6
3	K	3	MAN	O5-C5-C6-O6
3	V	3	MAN	O5-C5-C6-O6
3	g	3	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	3	MAN	O5-C5-C6-O6
3	P	3	MAN	O5-C5-C6-O6
3	a	3	MAN	O5-C5-C6-O6
3	c	3	MAN	O5-C5-C6-O6
3	G	3	MAN	O5-C5-C6-O6
3	R	3	MAN	O5-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	a	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	a	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C1-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
3	U	1	NAG	C1-C2-N2-C7
3	c	1	NAG	C1-C2-N2-C7
3	f	1	NAG	C1-C2-N2-C7

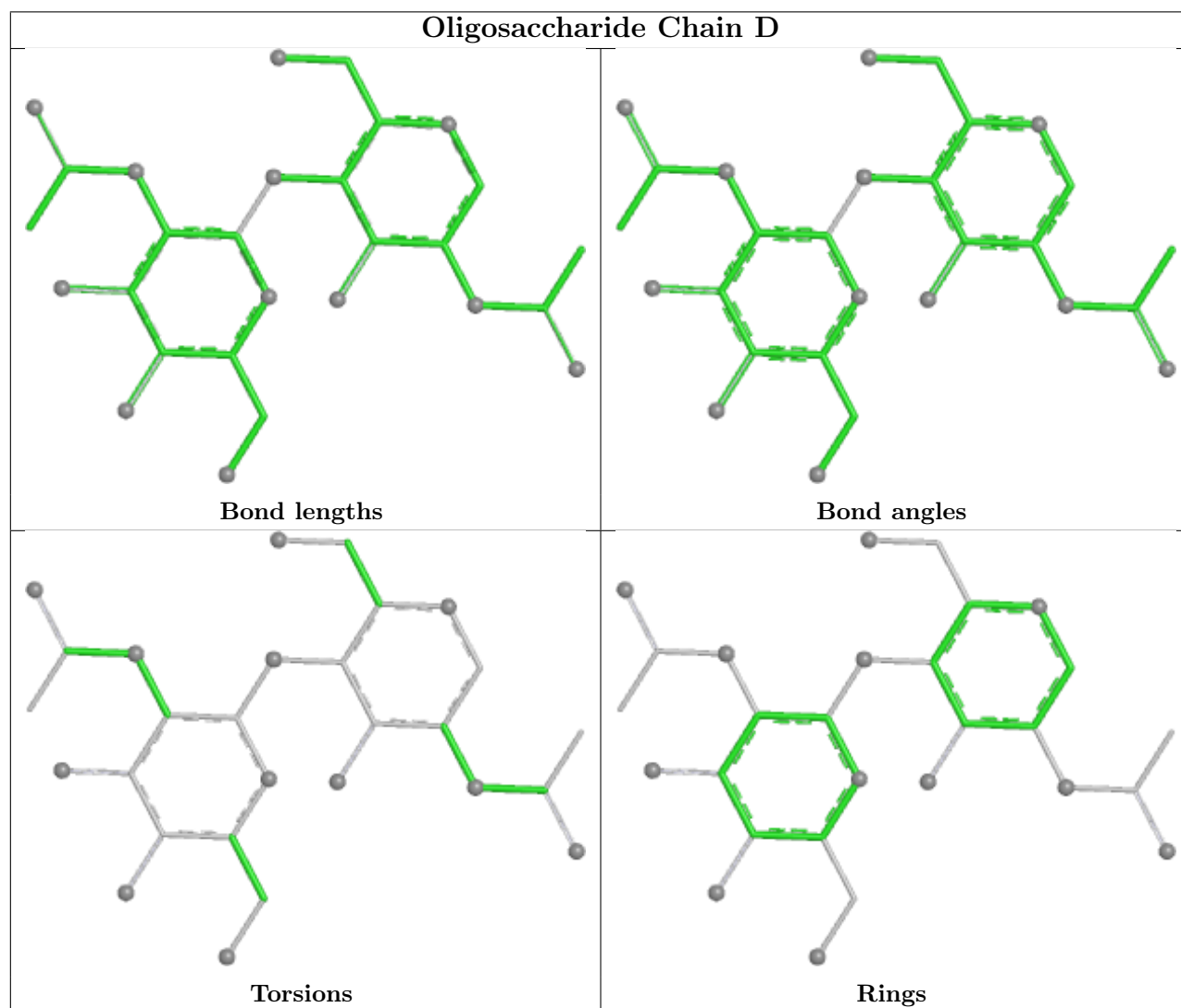
All (6) ring outliers are listed below:

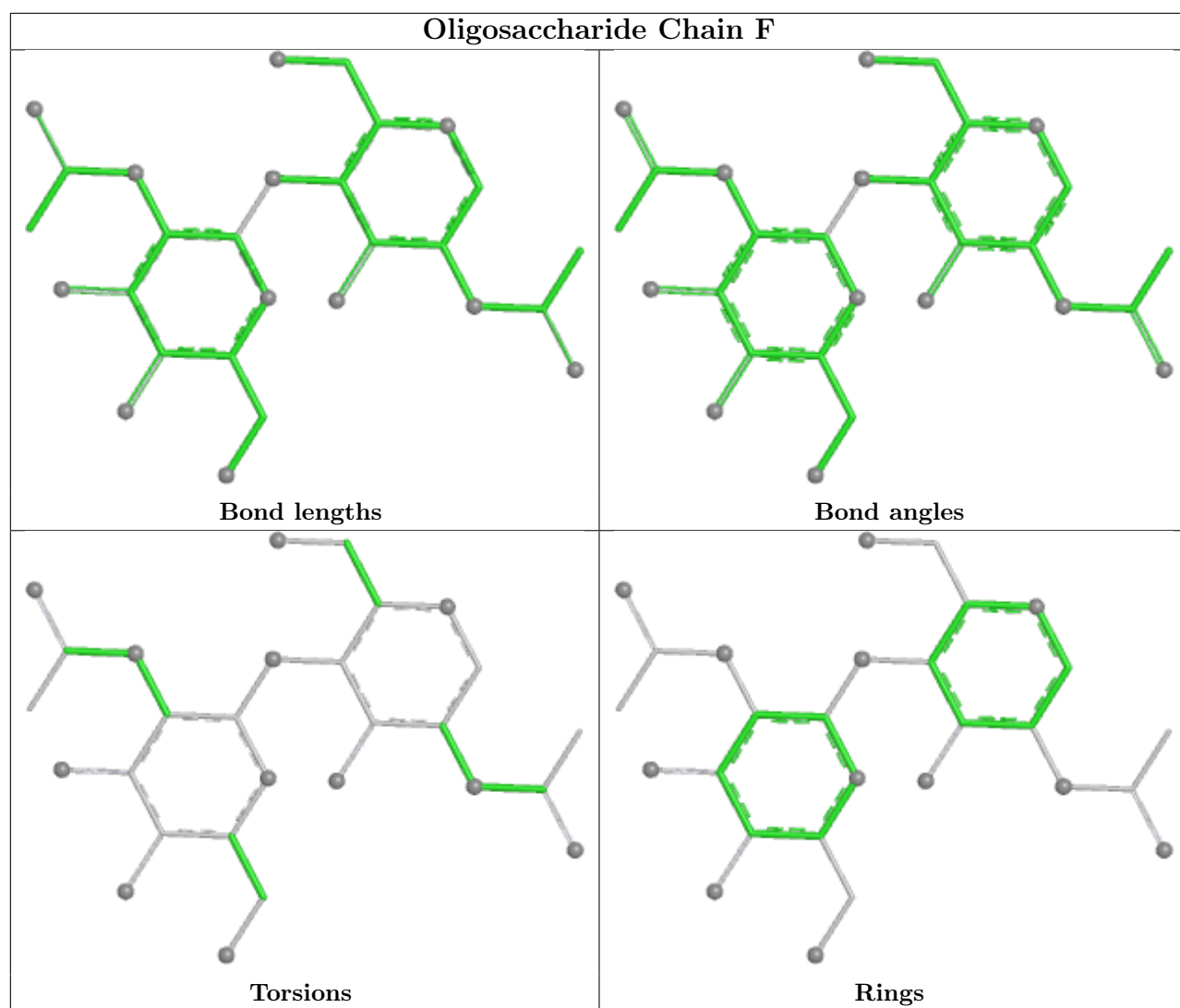
Mol	Chain	Res	Type	Atoms
3	d	3	MAN	C1-C2-C3-C4-C5-O5
3	S	3	MAN	C1-C2-C3-C4-C5-O5
3	H	3	MAN	C1-C2-C3-C4-C5-O5
3	Y	3	MAN	C1-C2-C3-C4-C5-O5
3	N	3	MAN	C1-C2-C3-C4-C5-O5
3	j	3	MAN	C1-C2-C3-C4-C5-O5

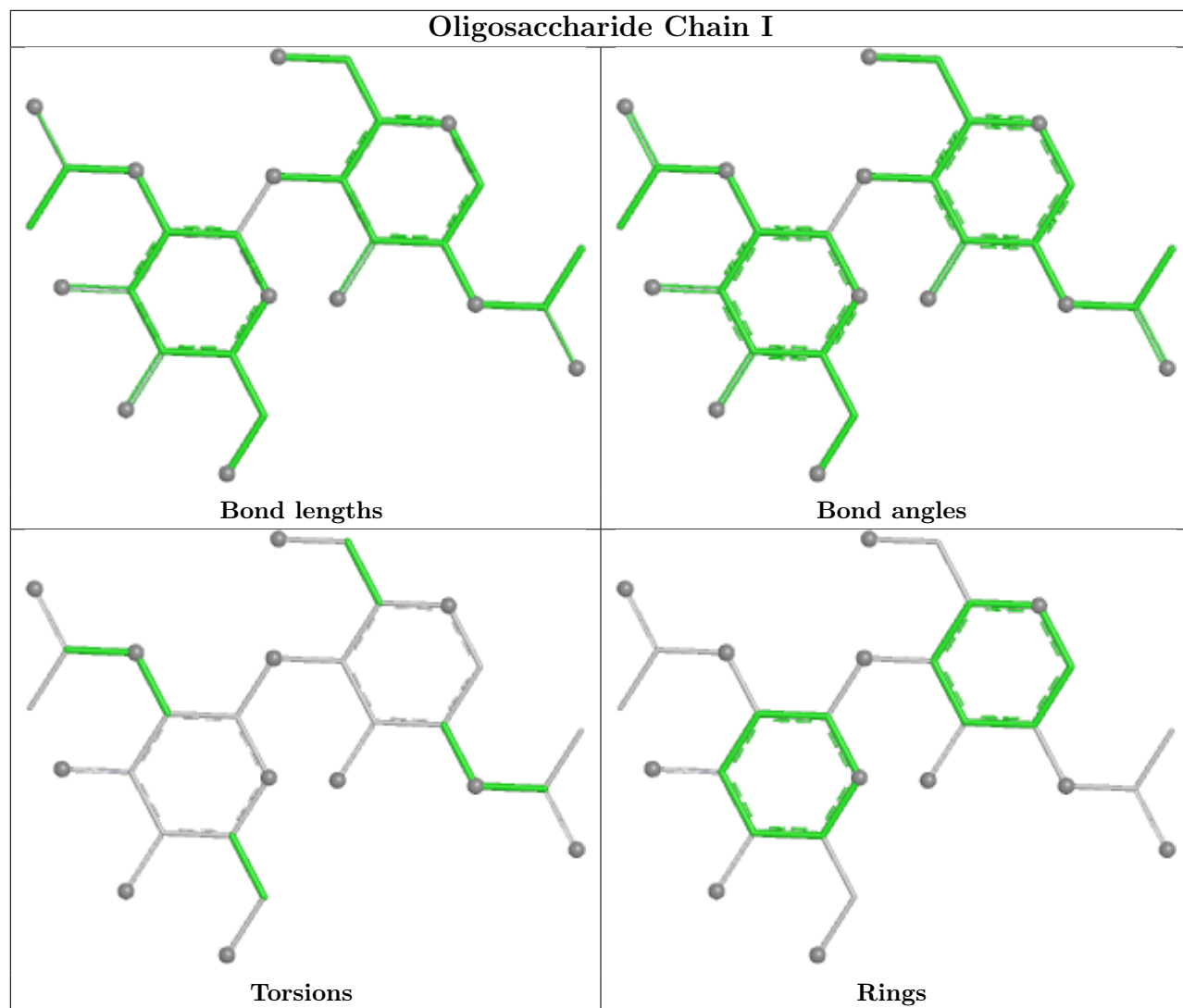
10 monomers are involved in 20 short contacts:

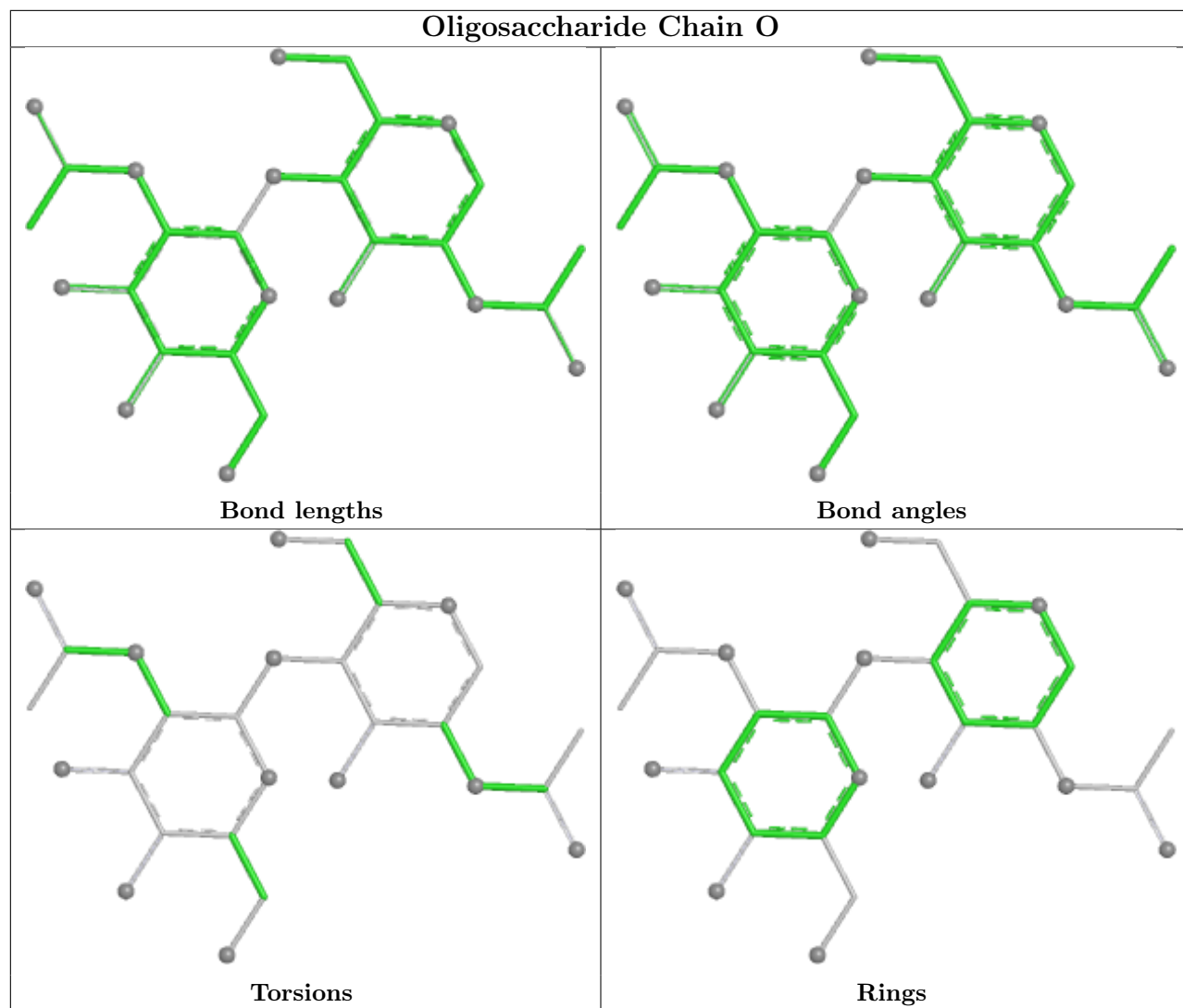
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1	NAG	4	0
3	c	1	NAG	3	0
2	I	2	NAG	1	0
3	R	2	NAG	1	0
2	I	1	NAG	4	0
3	G	2	NAG	1	0
3	G	1	NAG	4	0
2	T	1	NAG	3	0
2	T	2	NAG	1	0
2	e	1	NAG	2	0

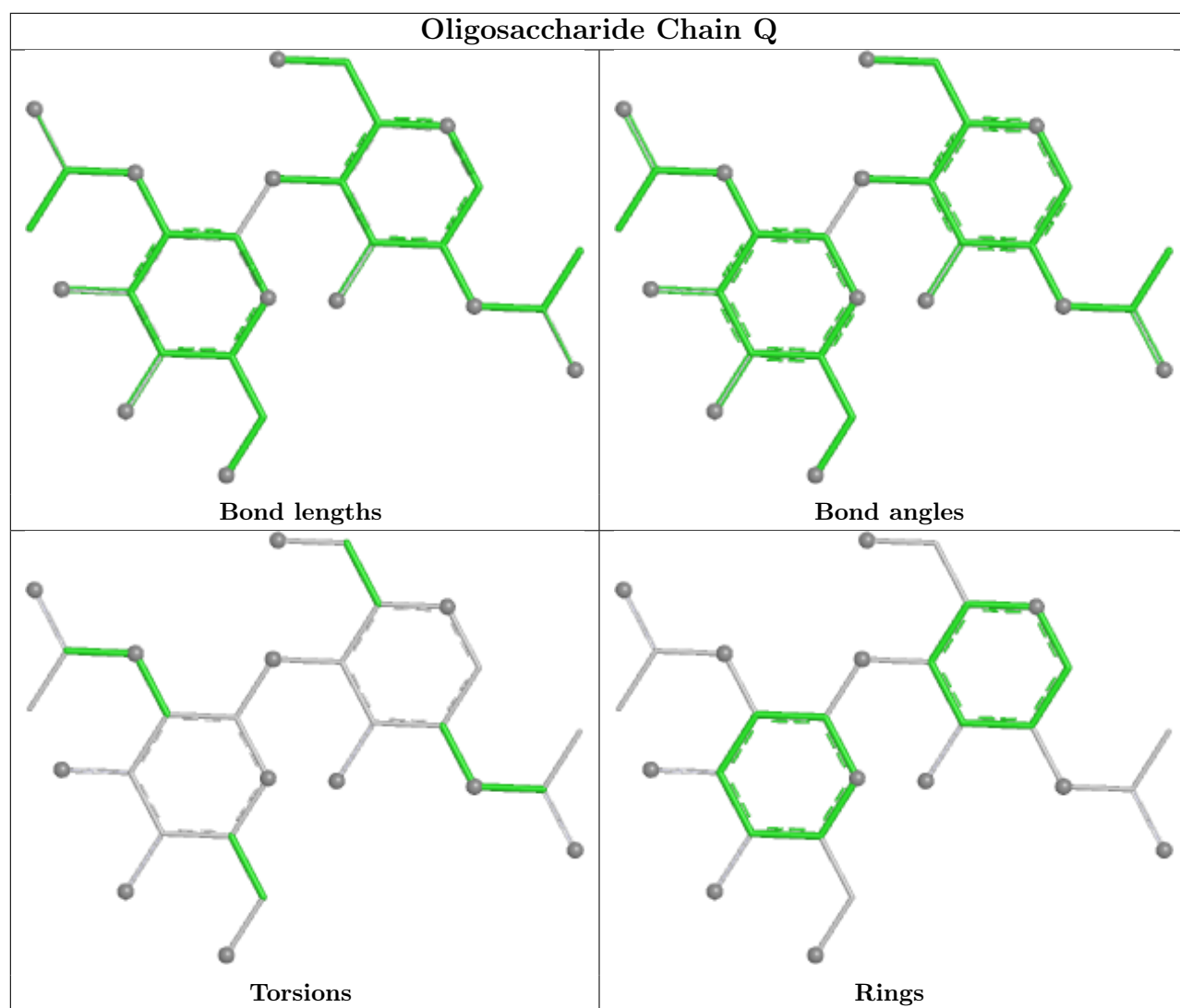
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

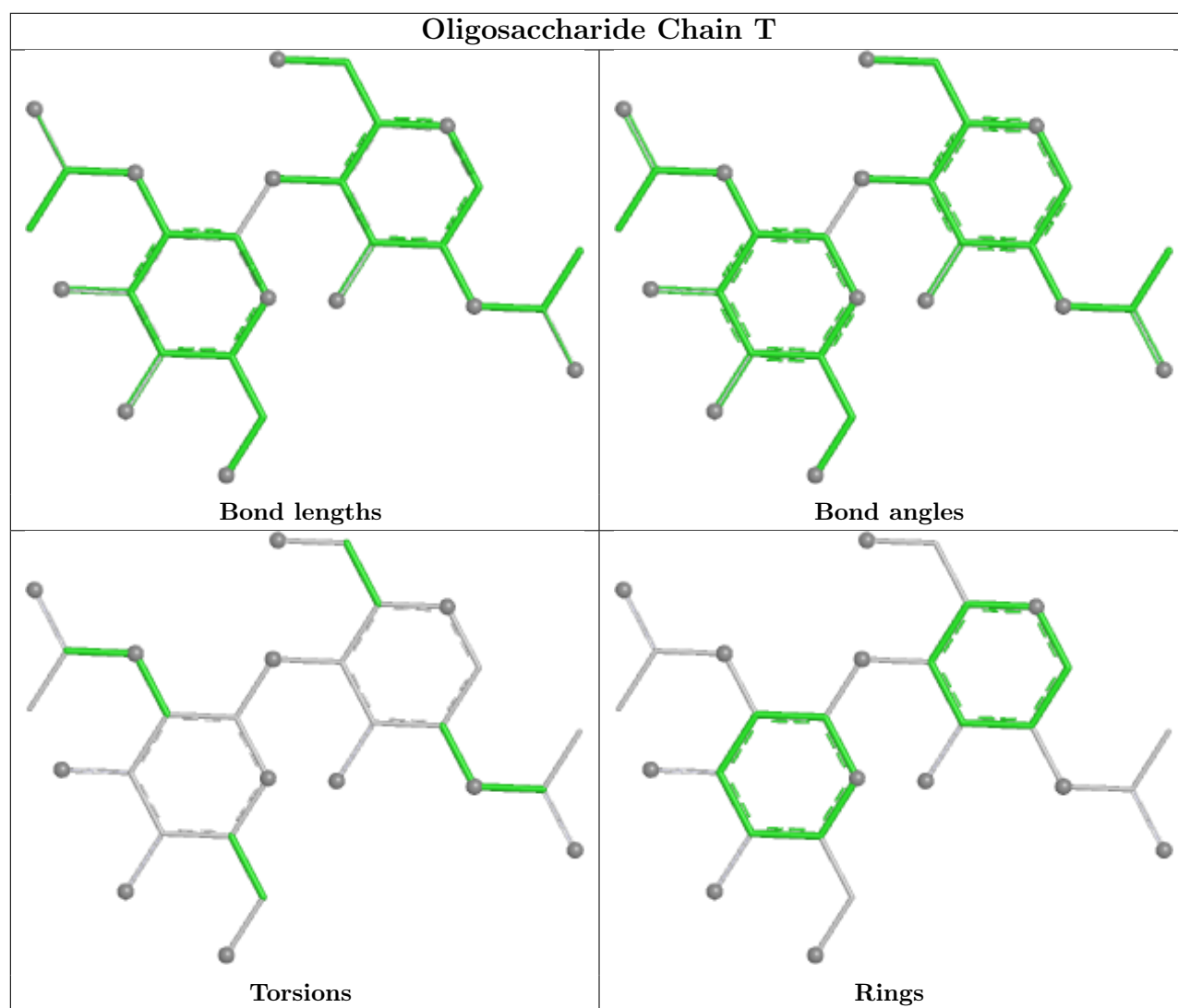


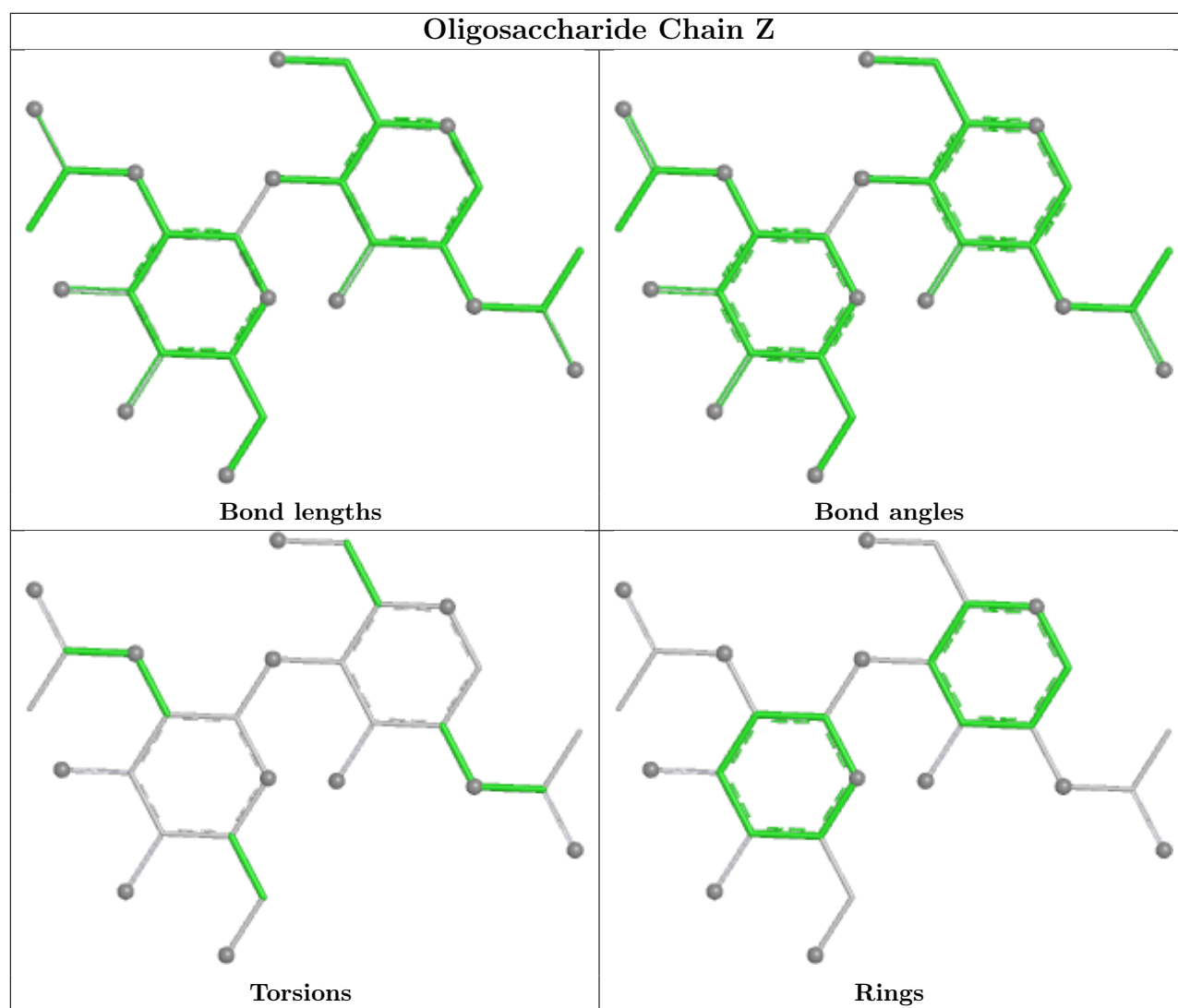


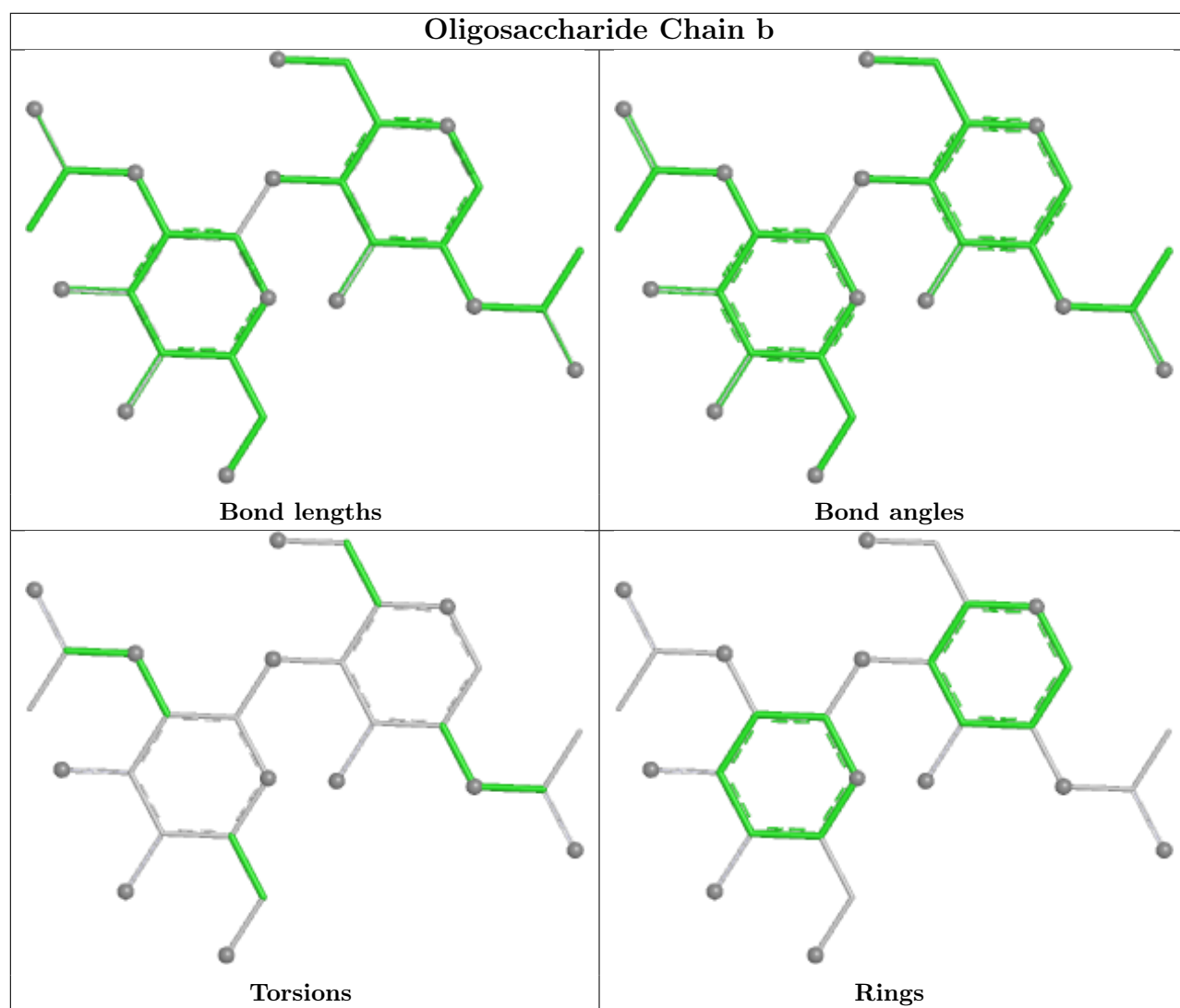


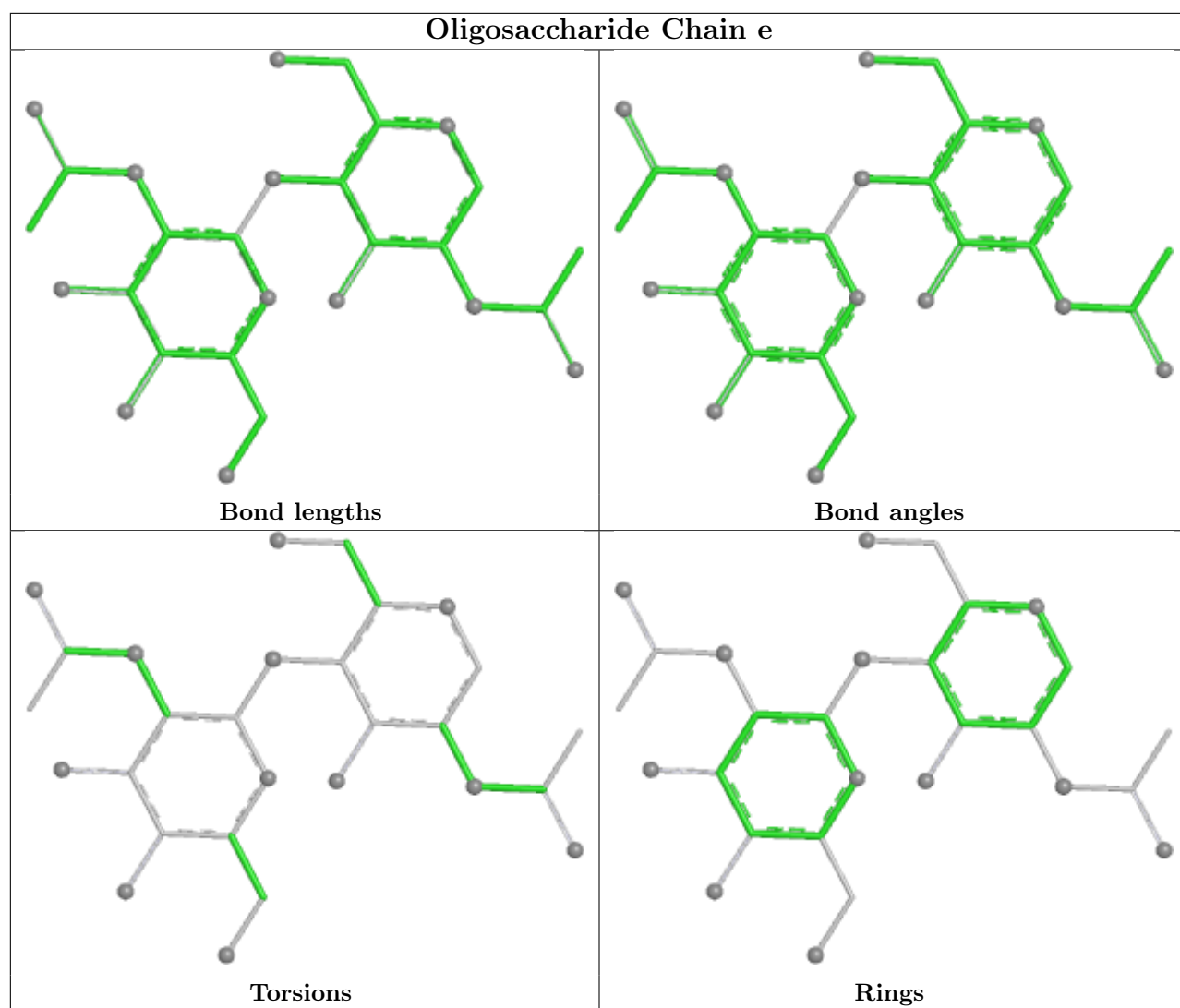


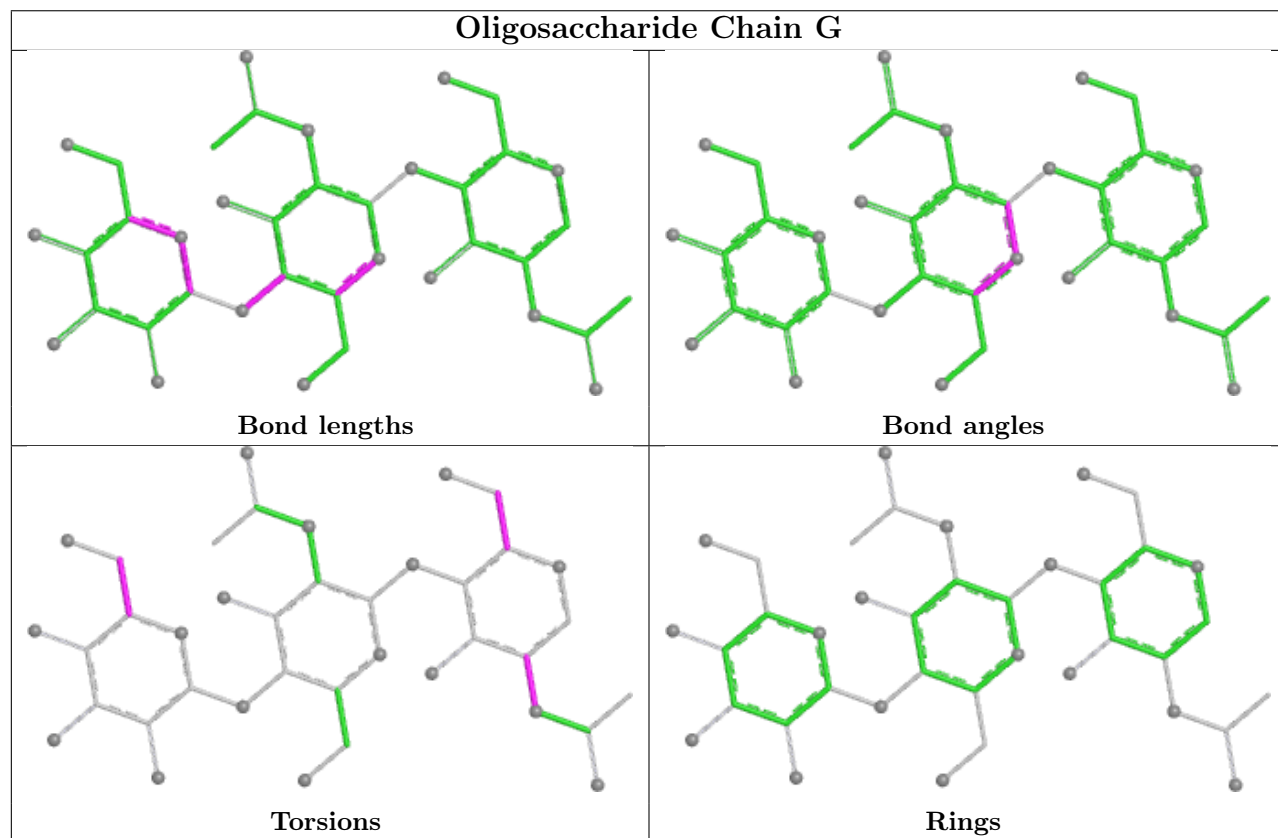
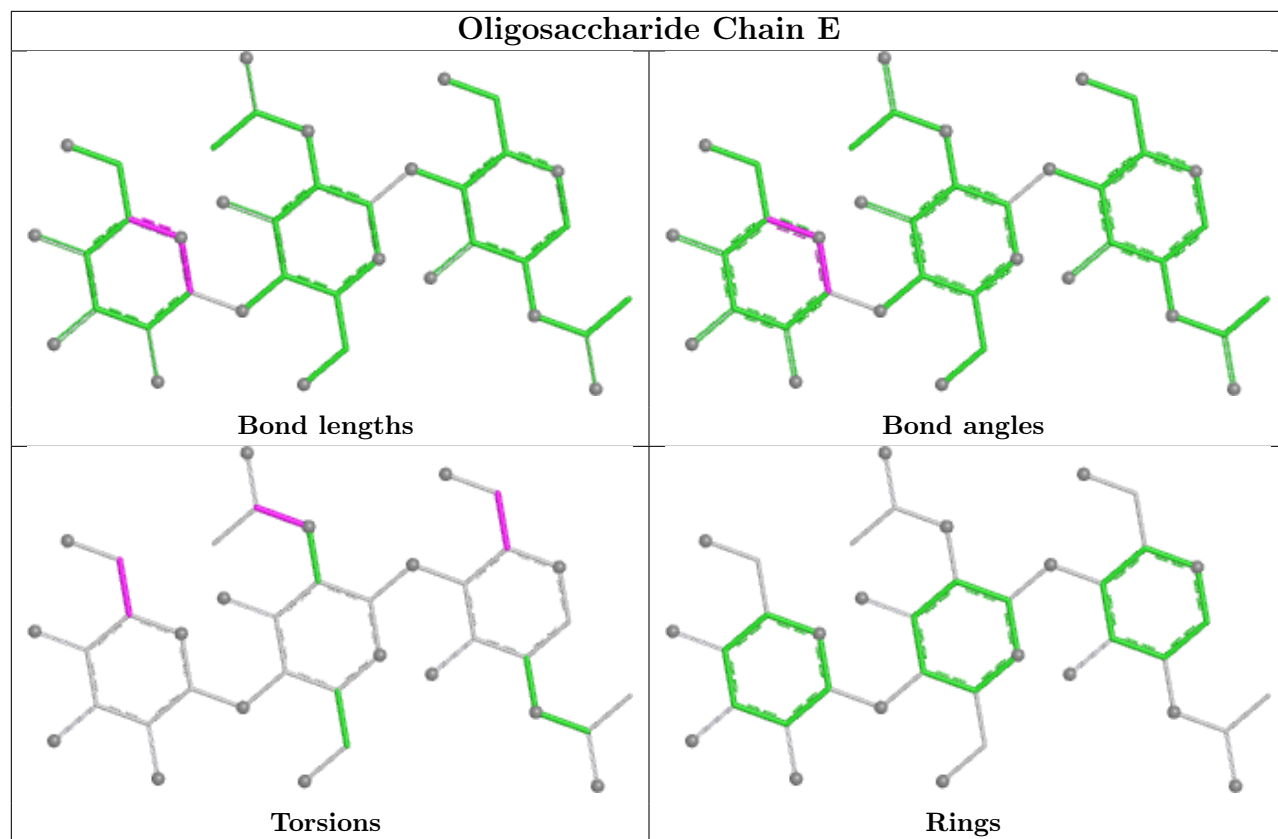


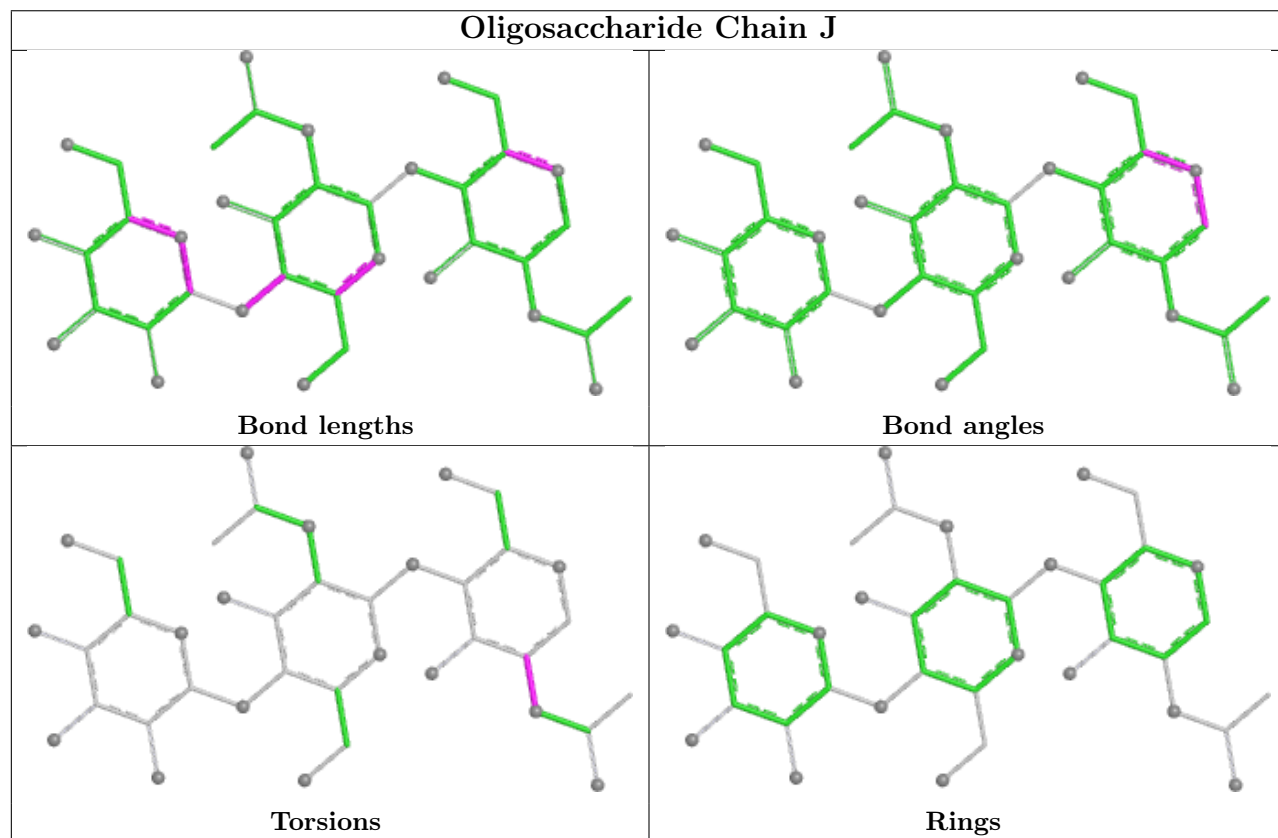
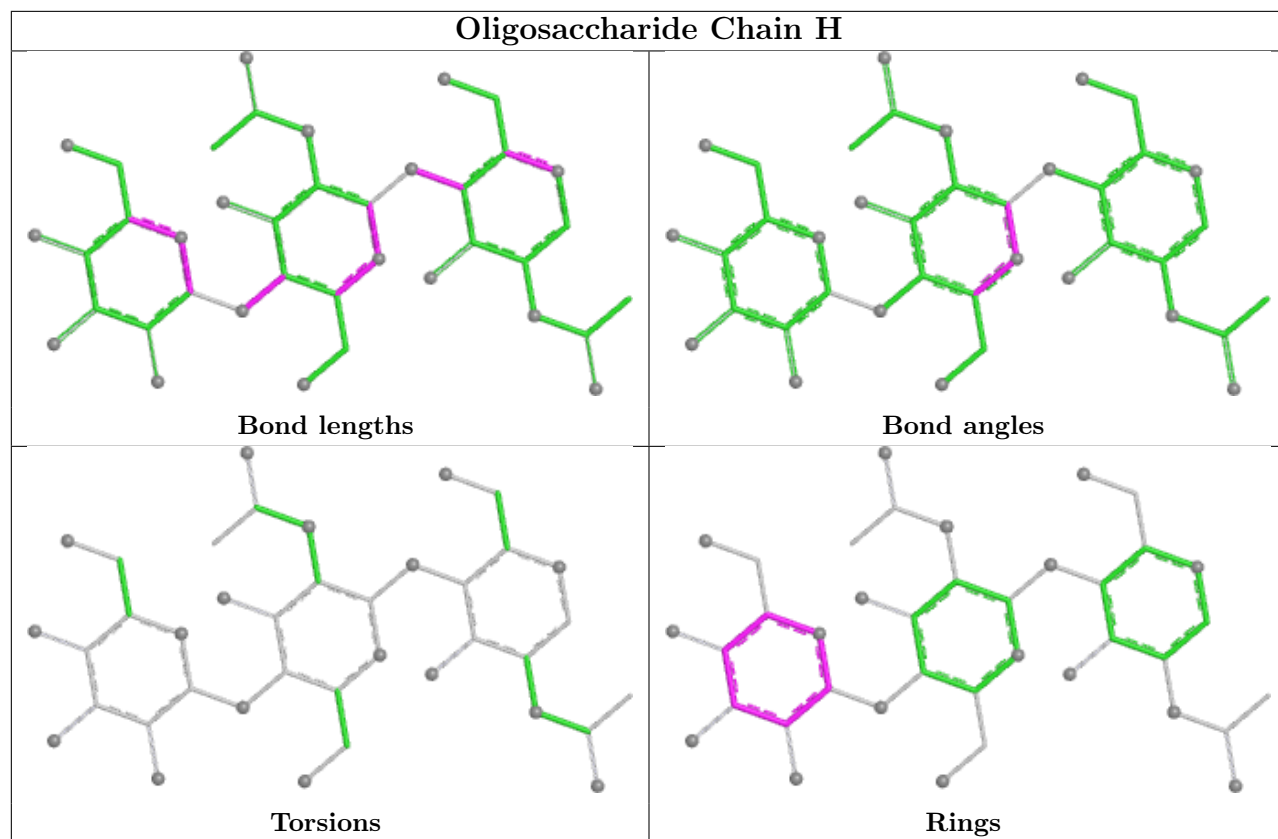


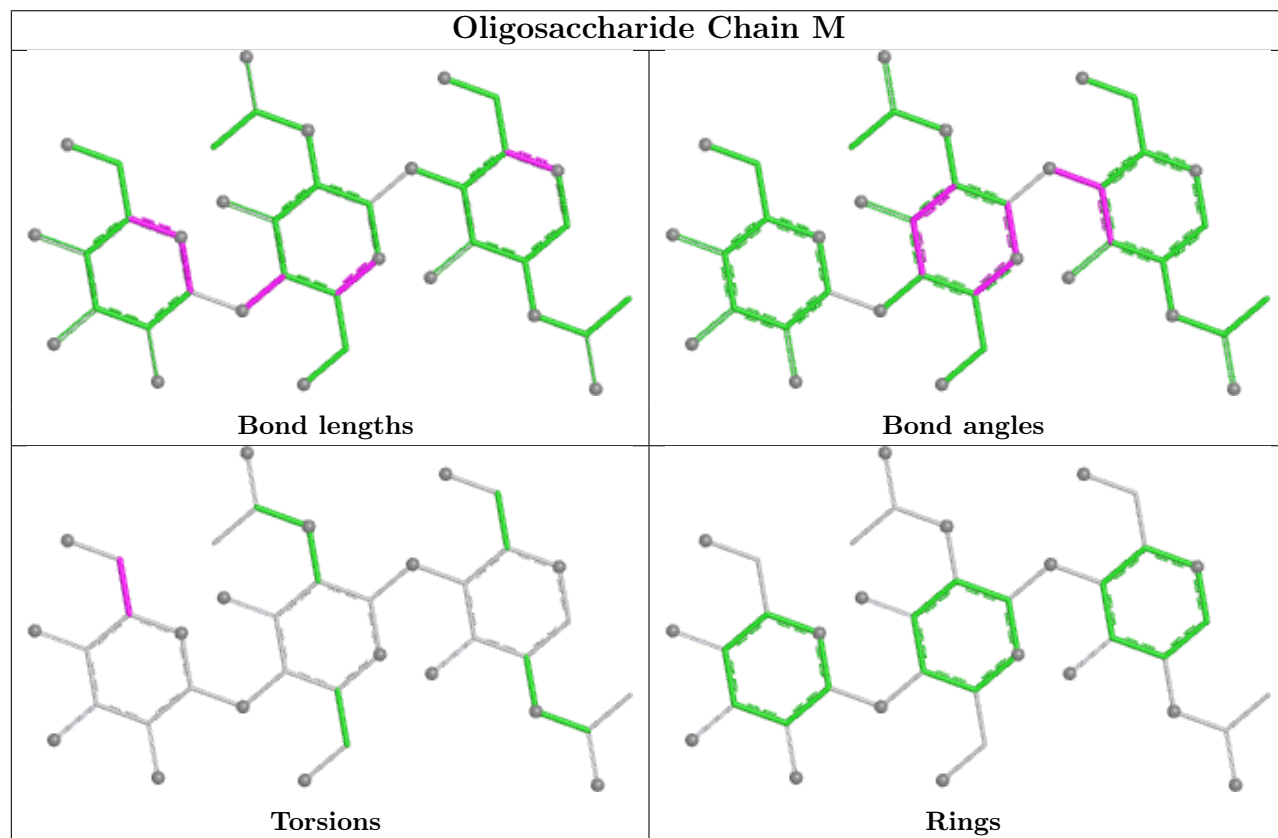
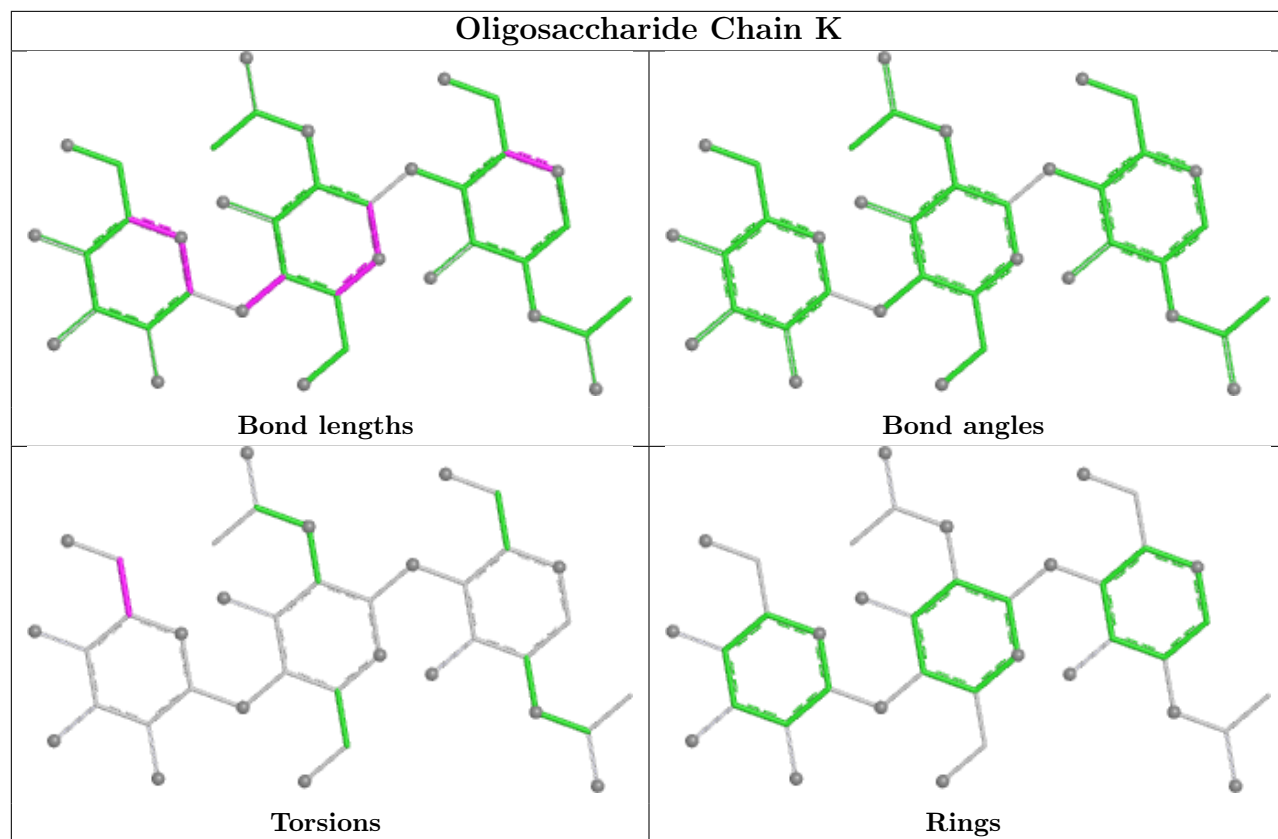


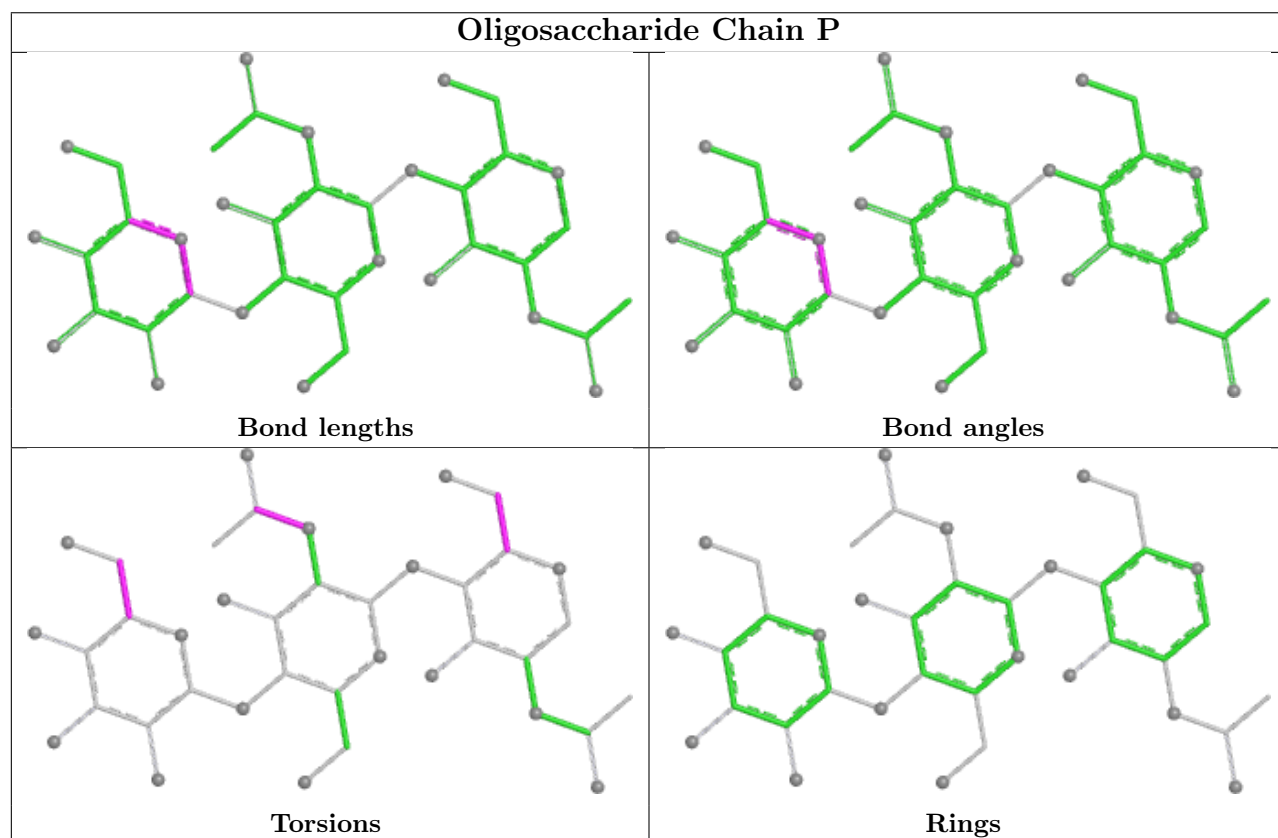
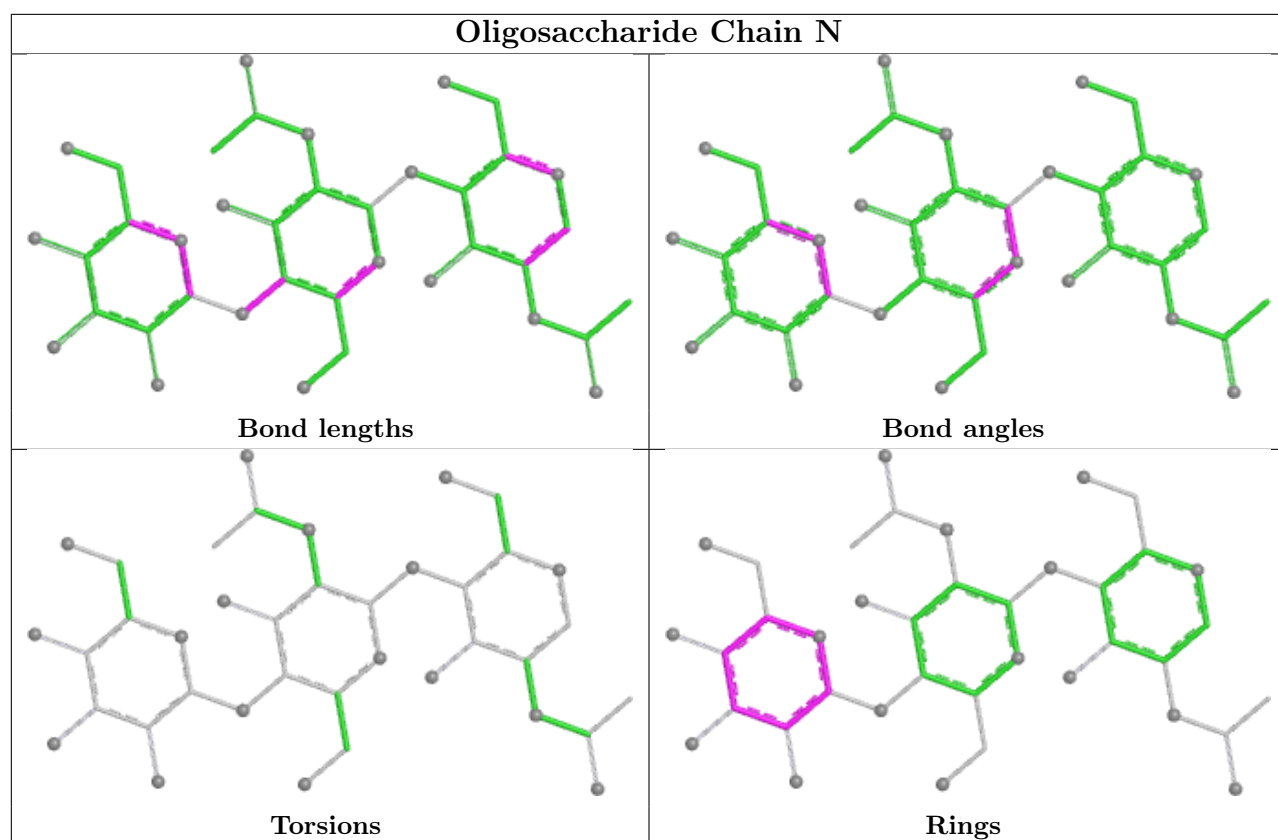


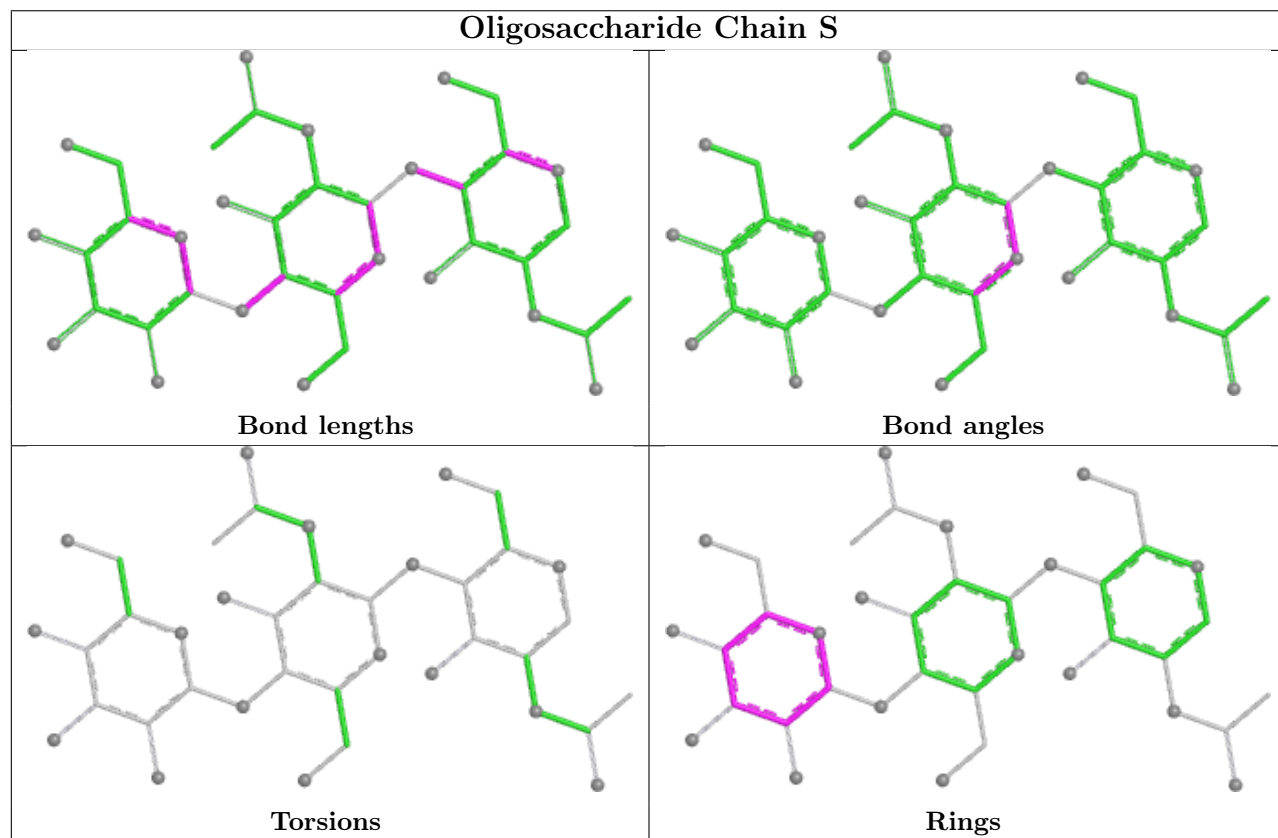
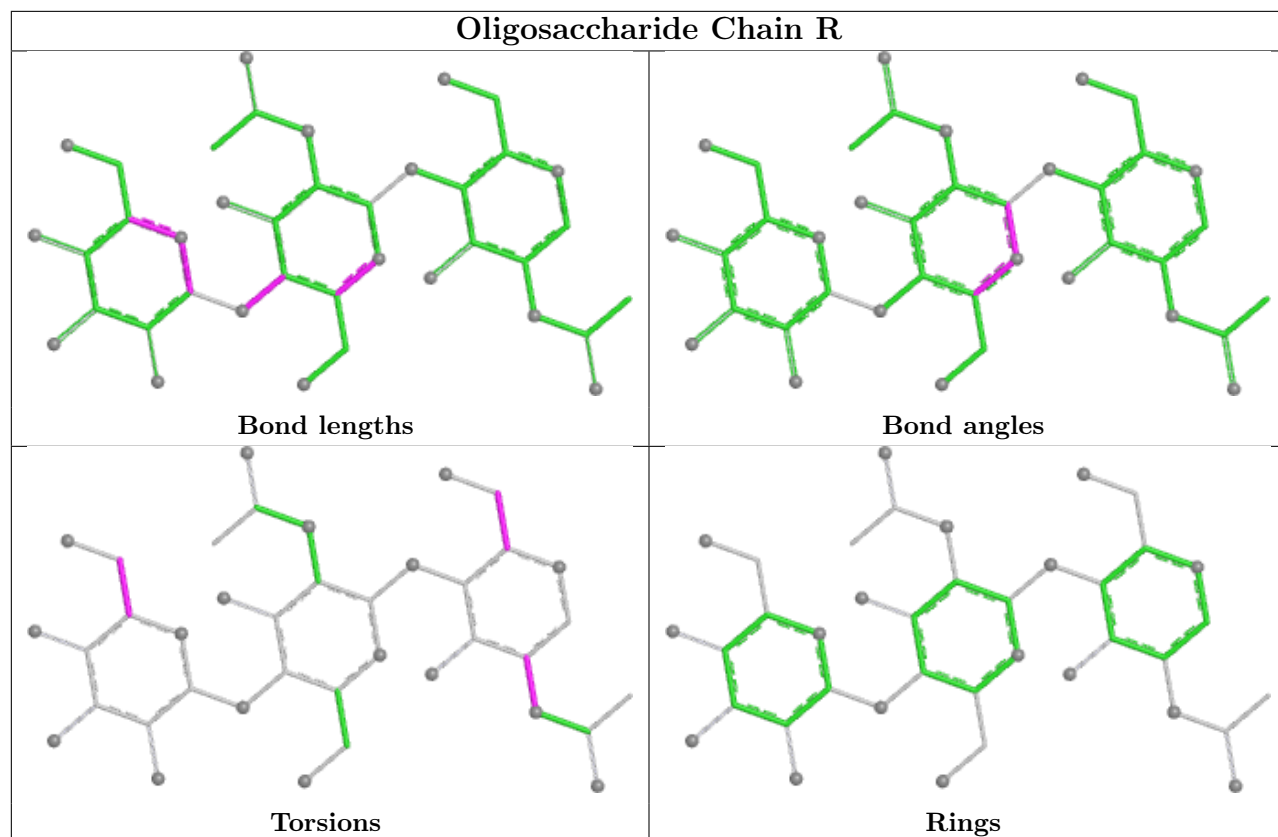


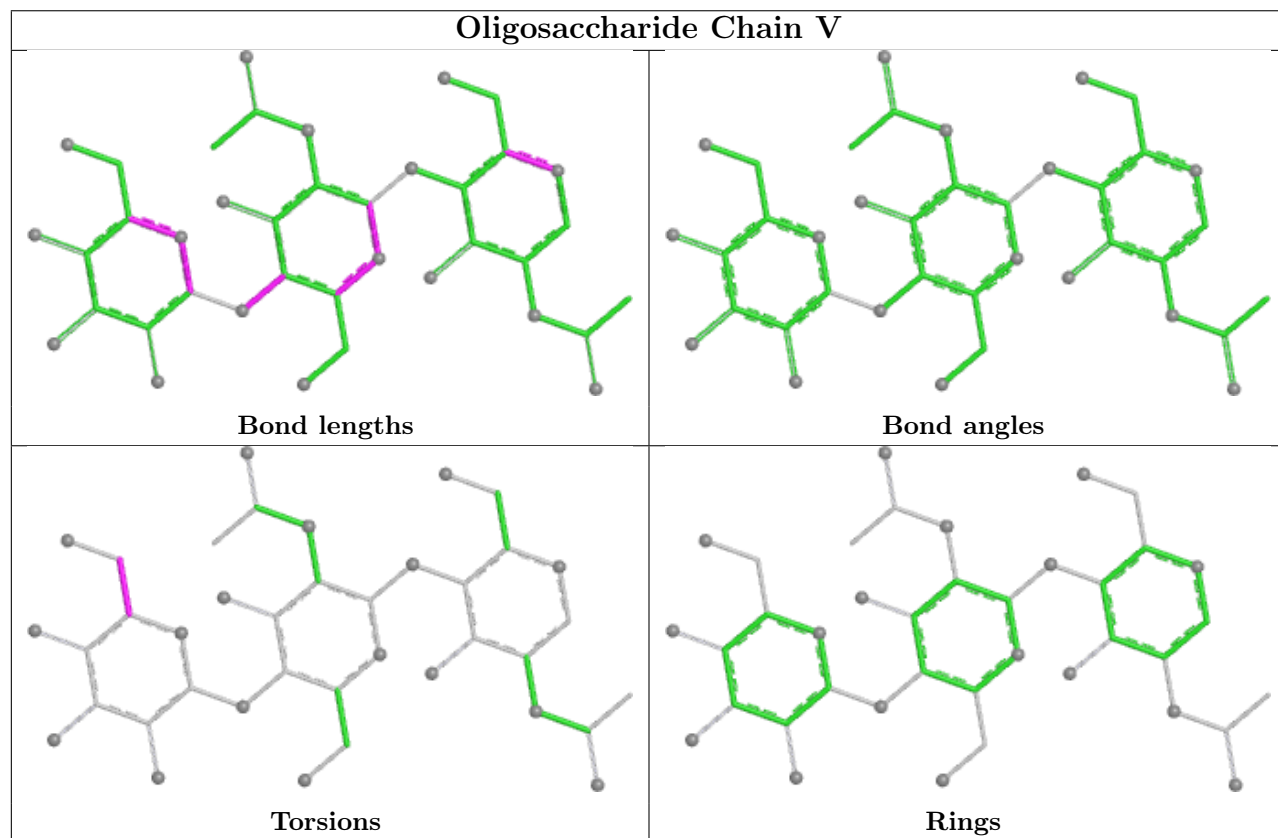
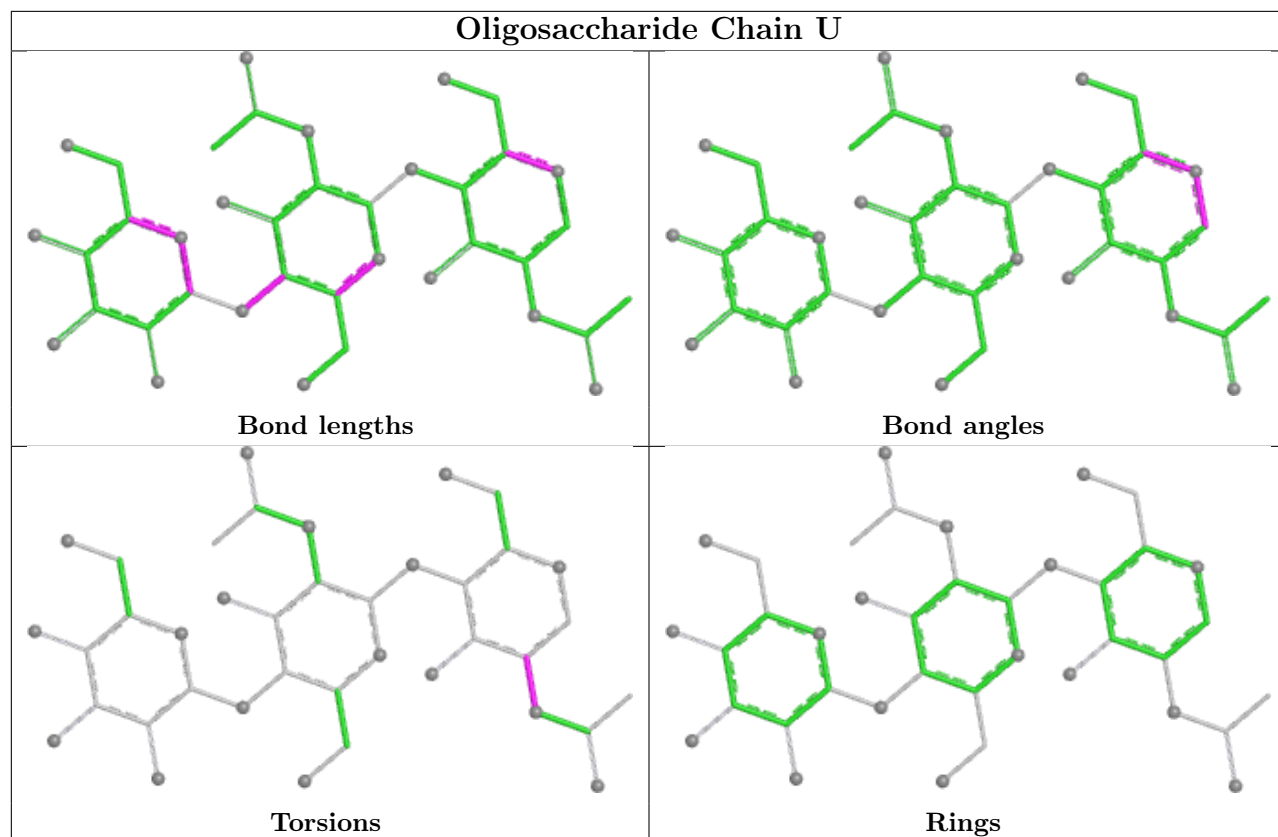


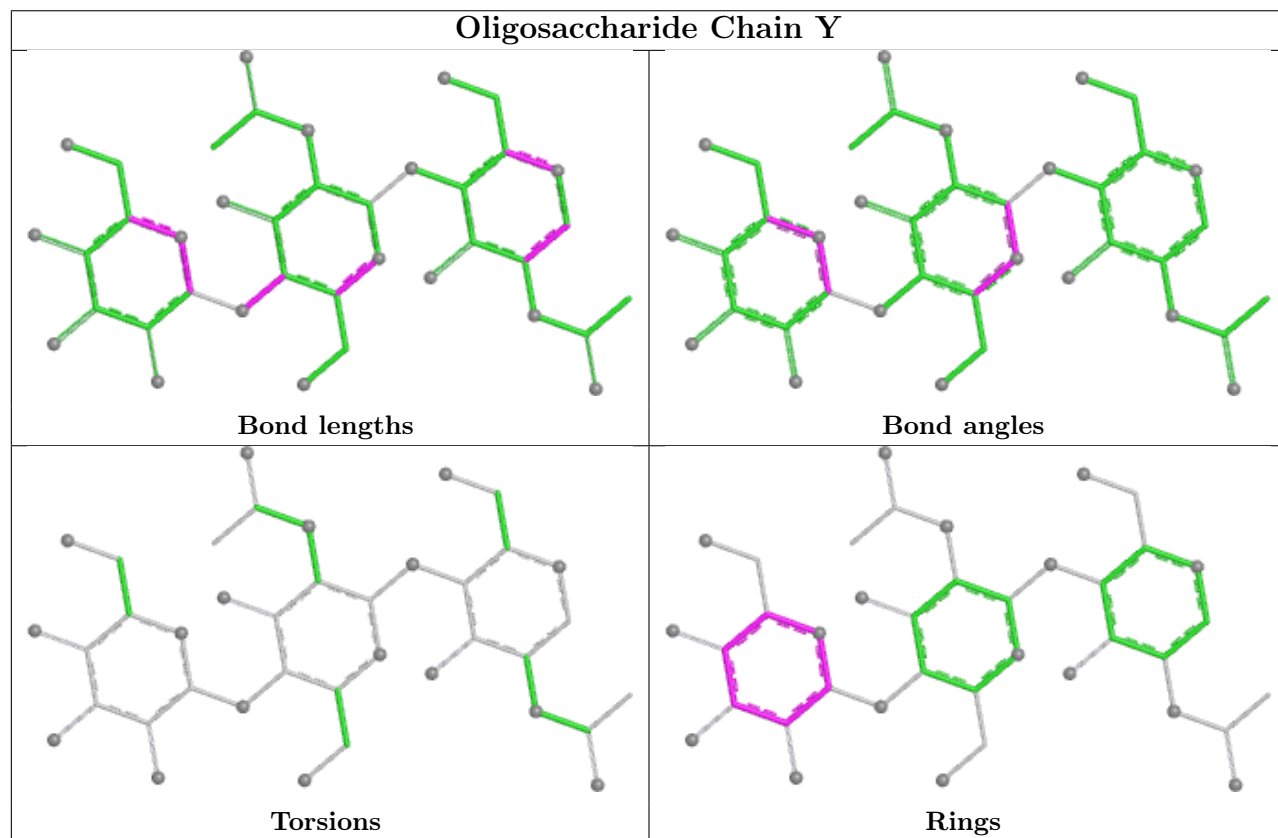
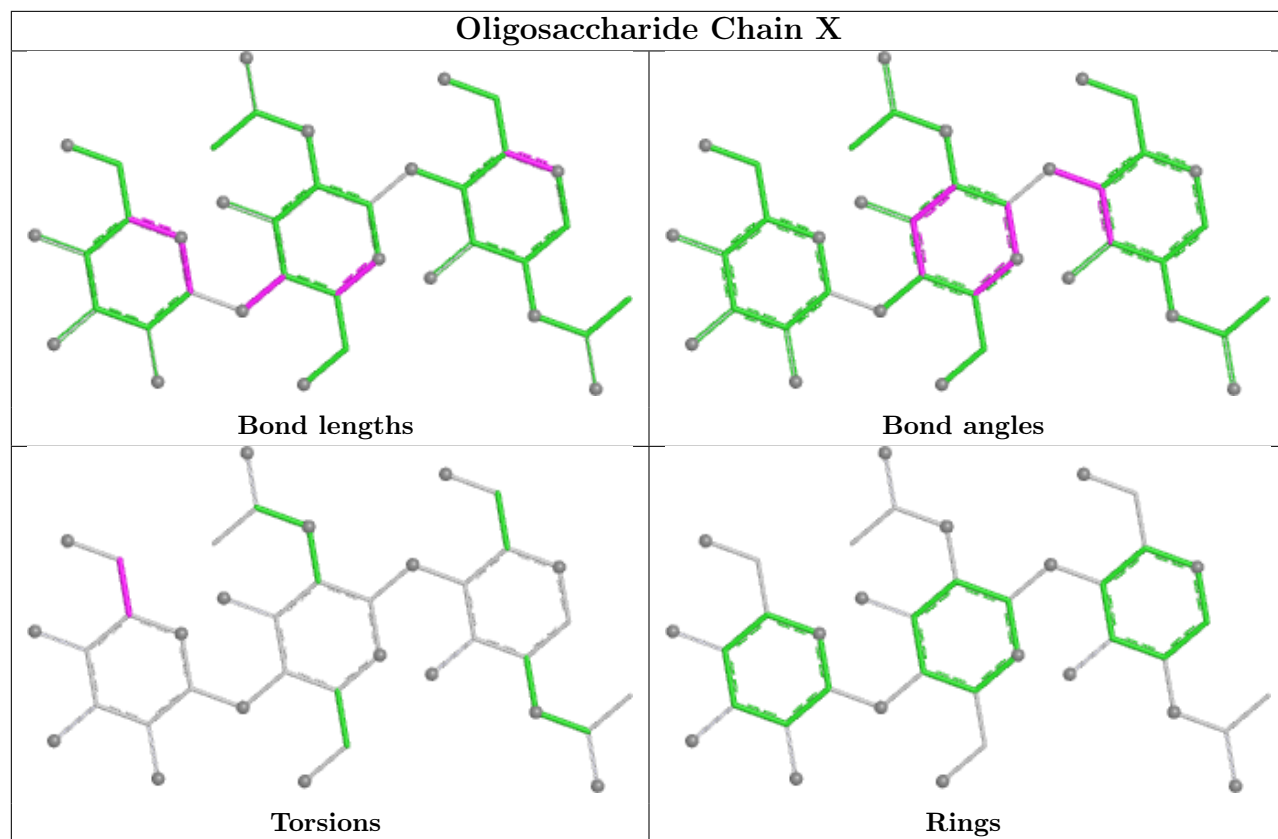


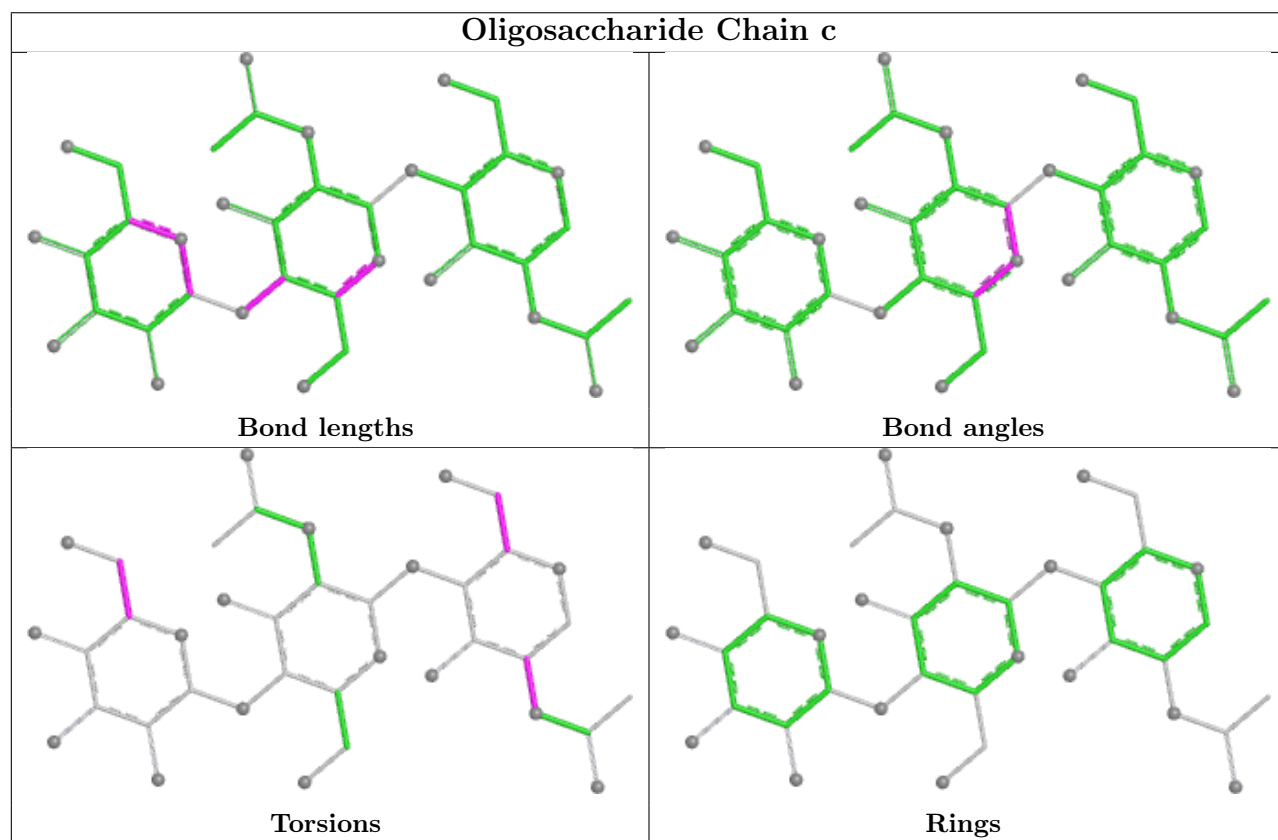
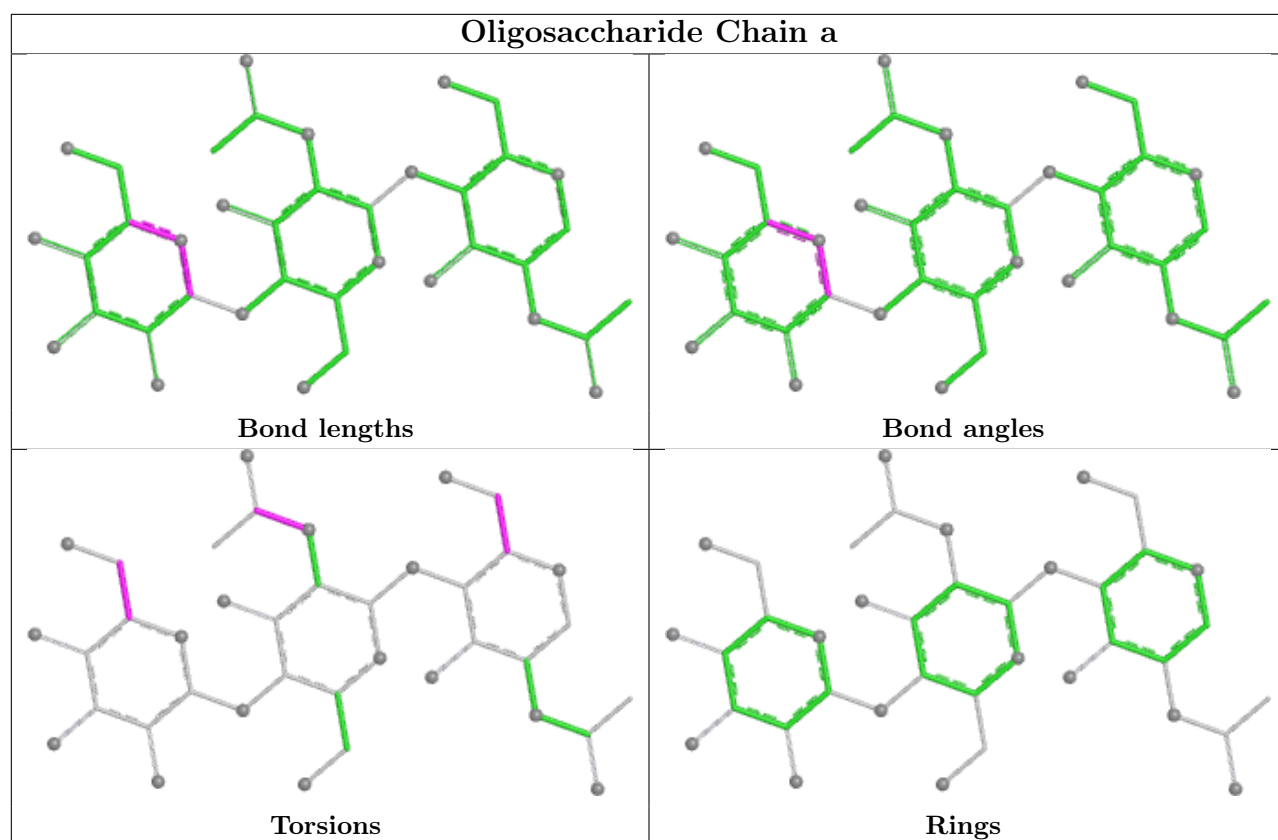


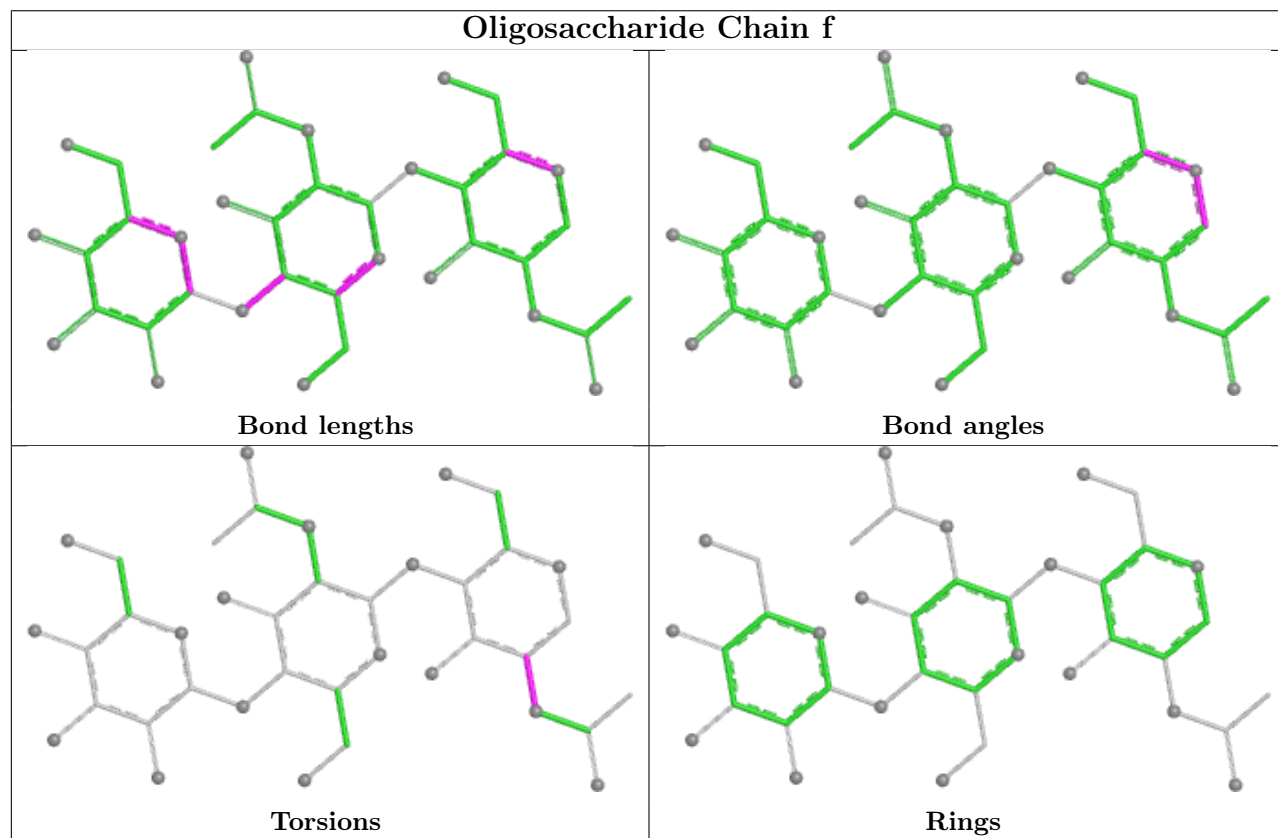
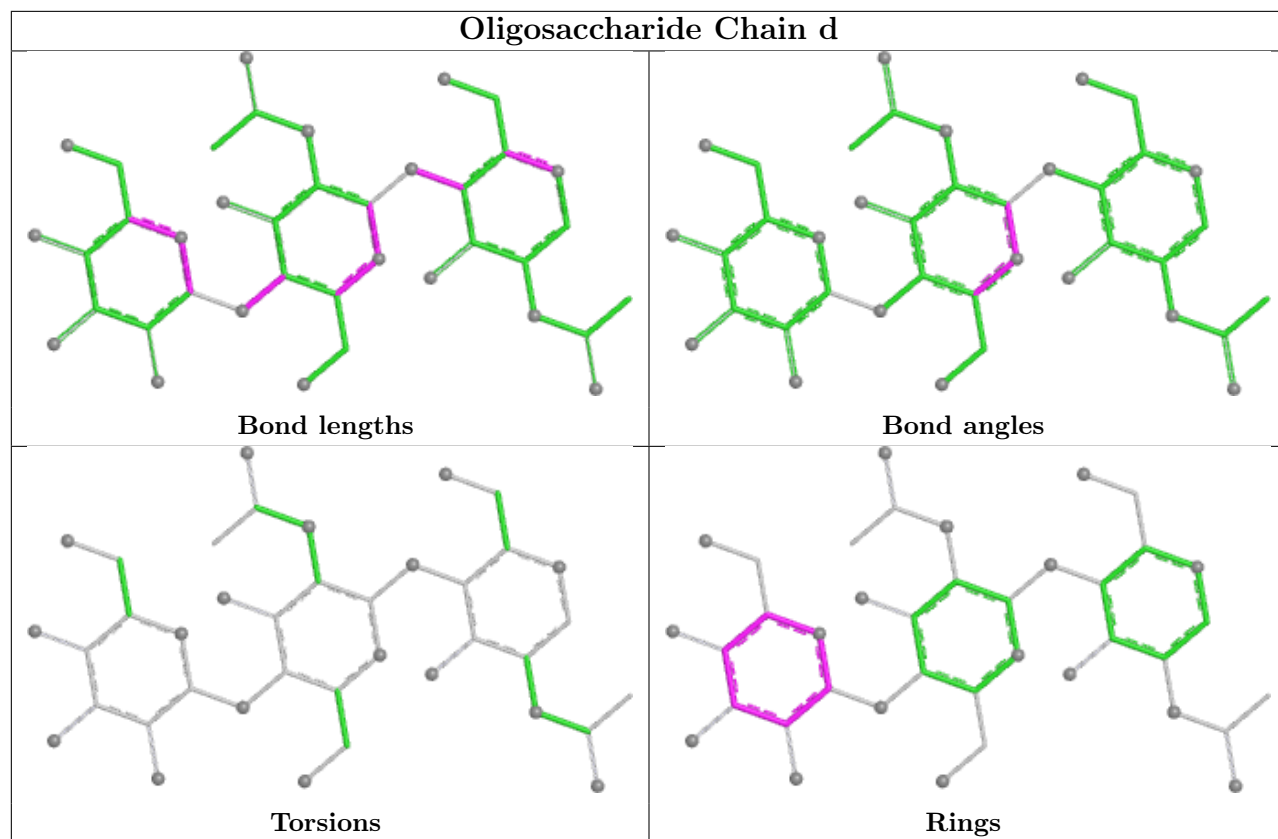


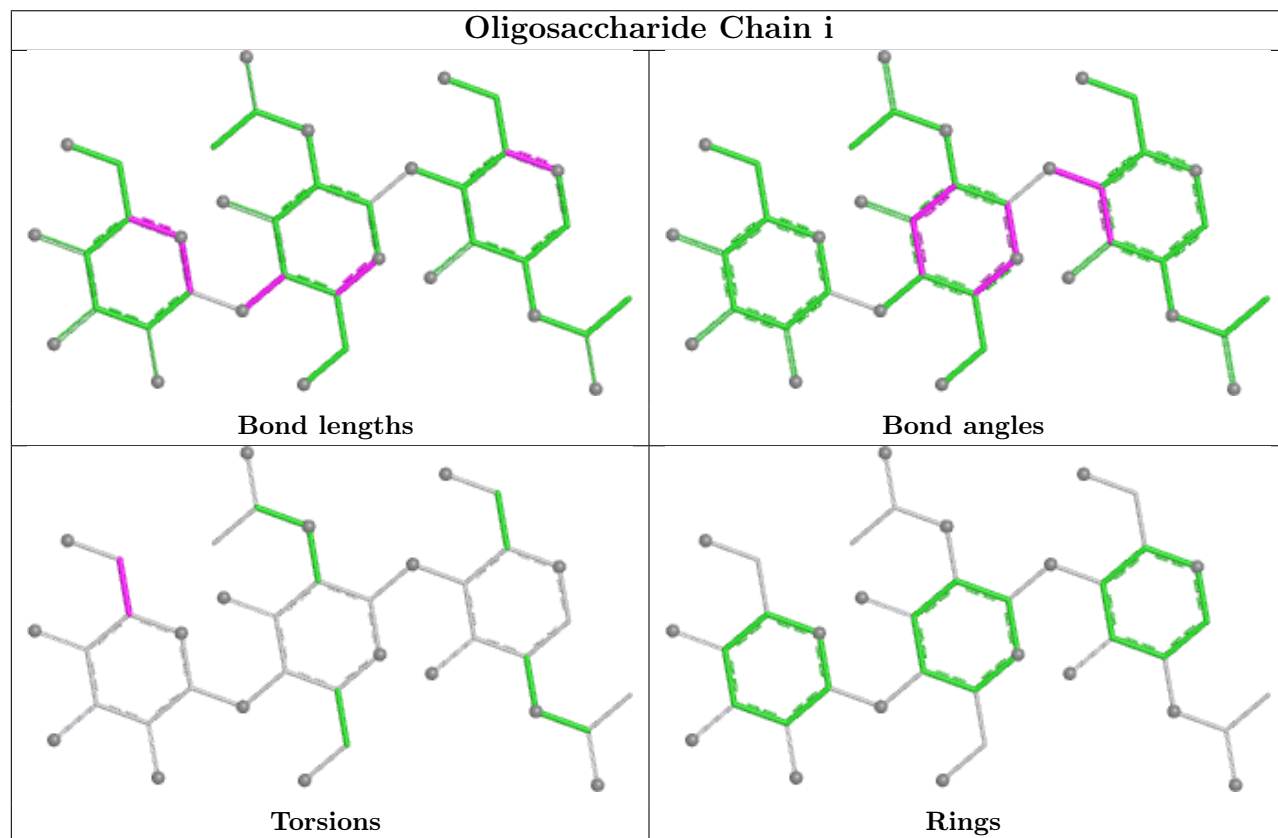
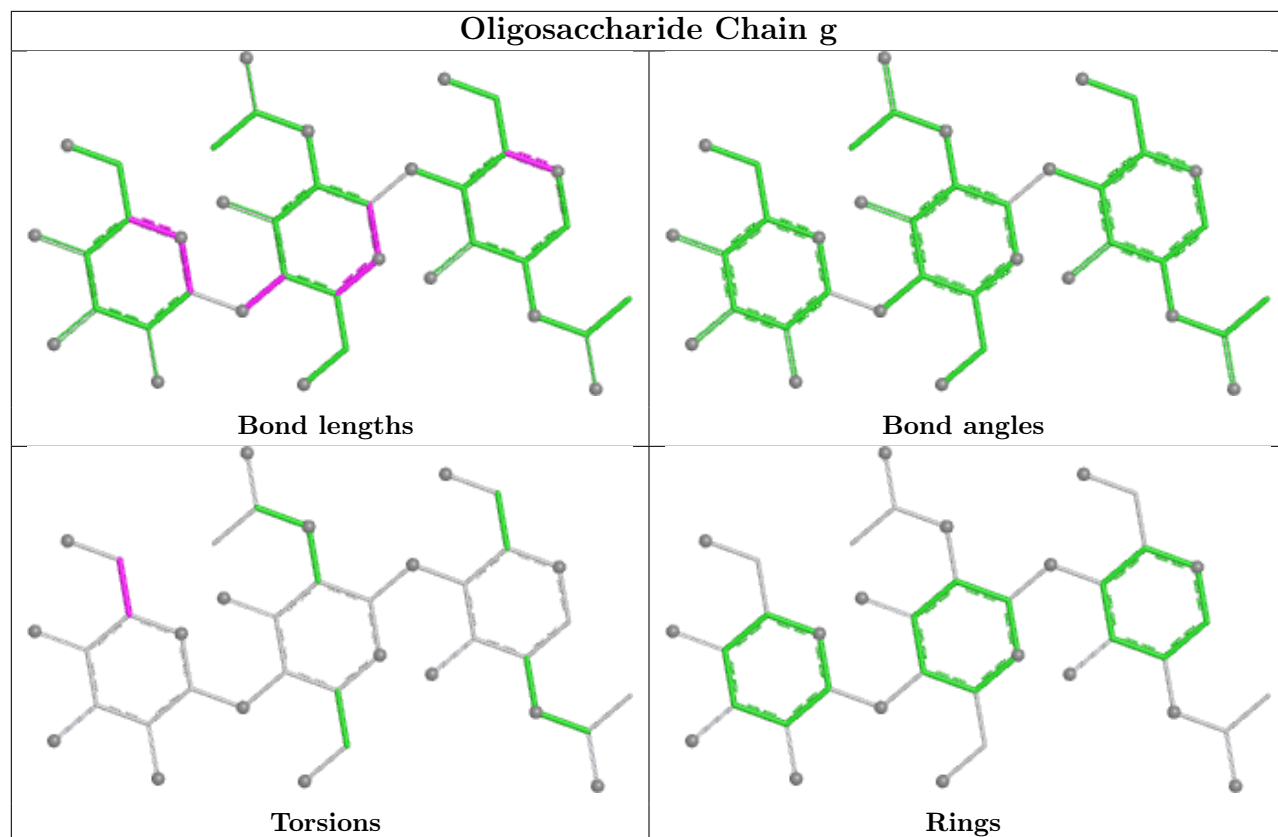


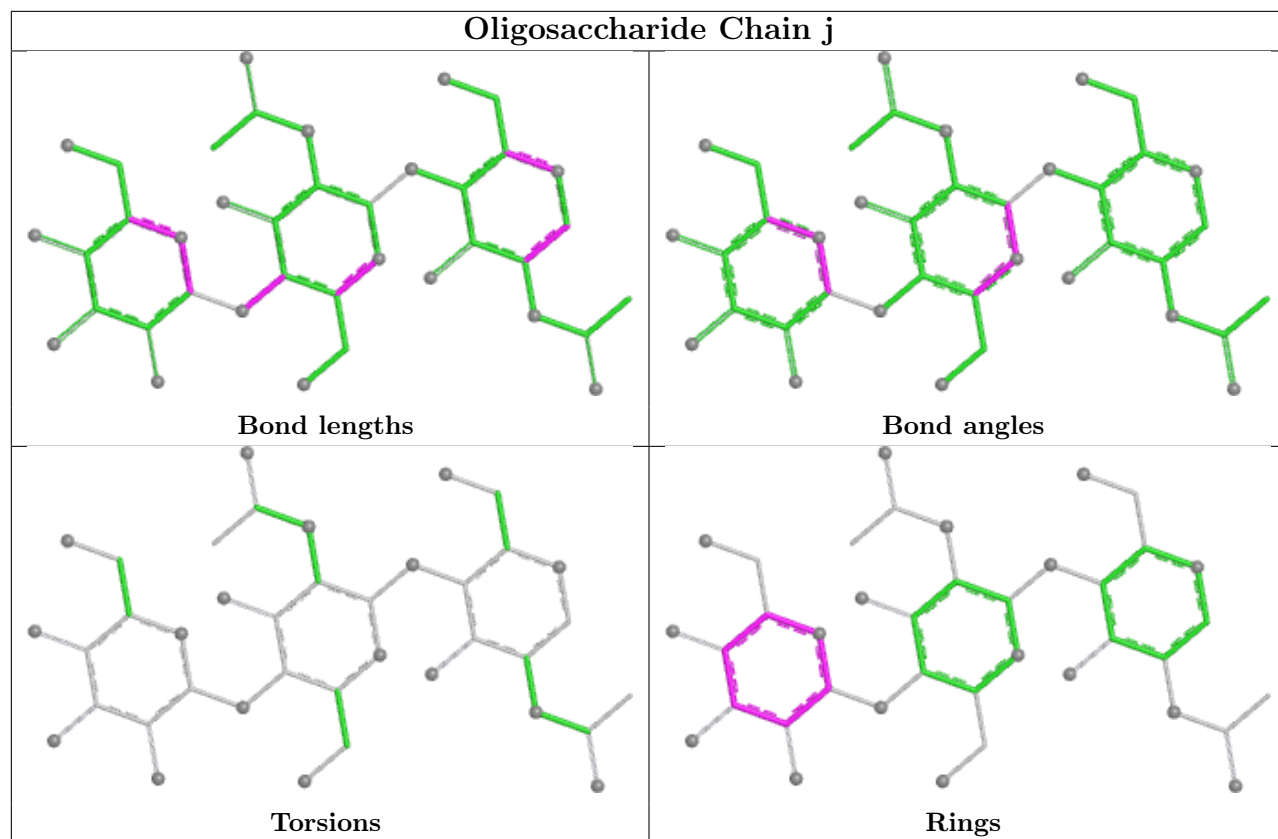


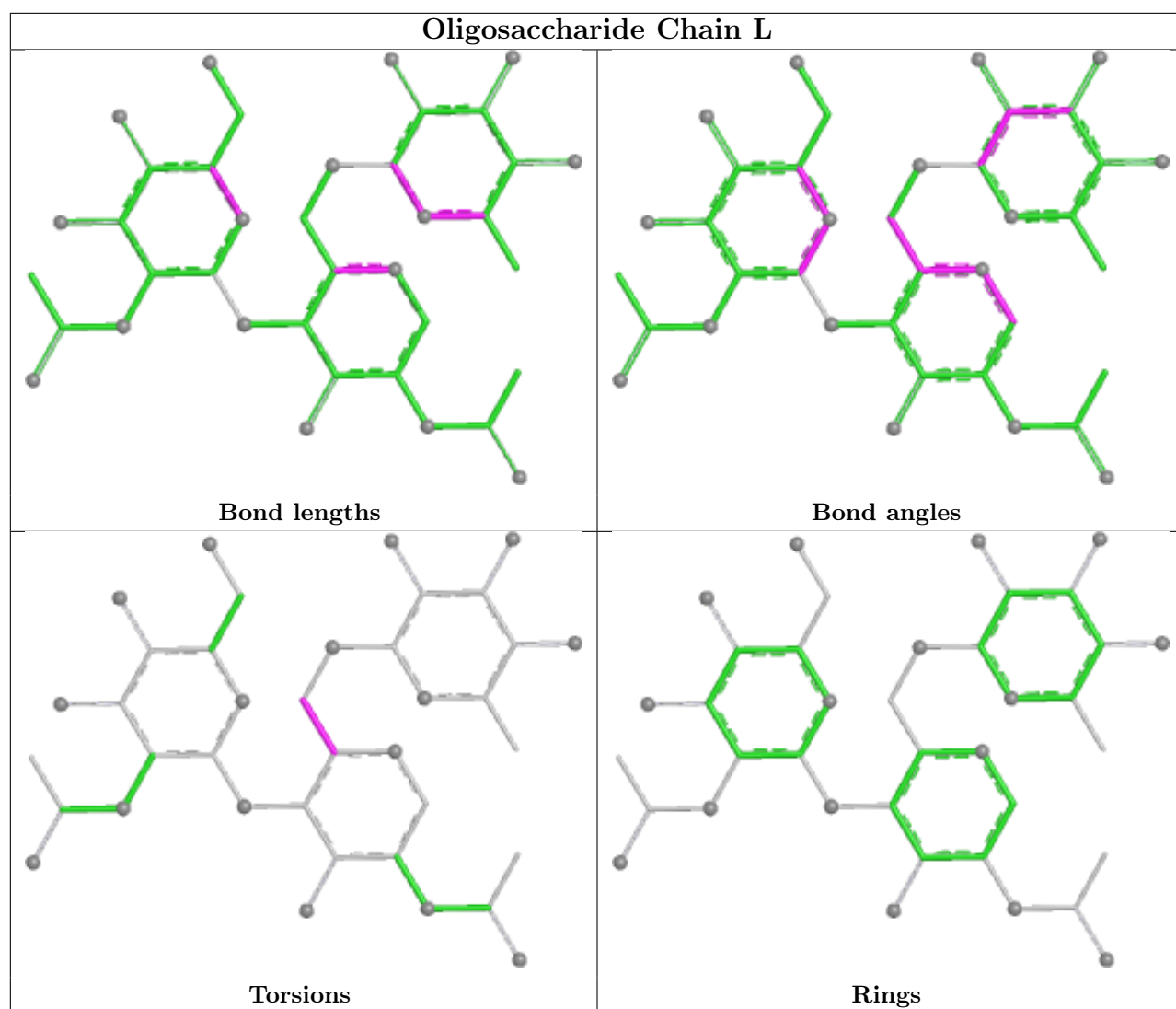


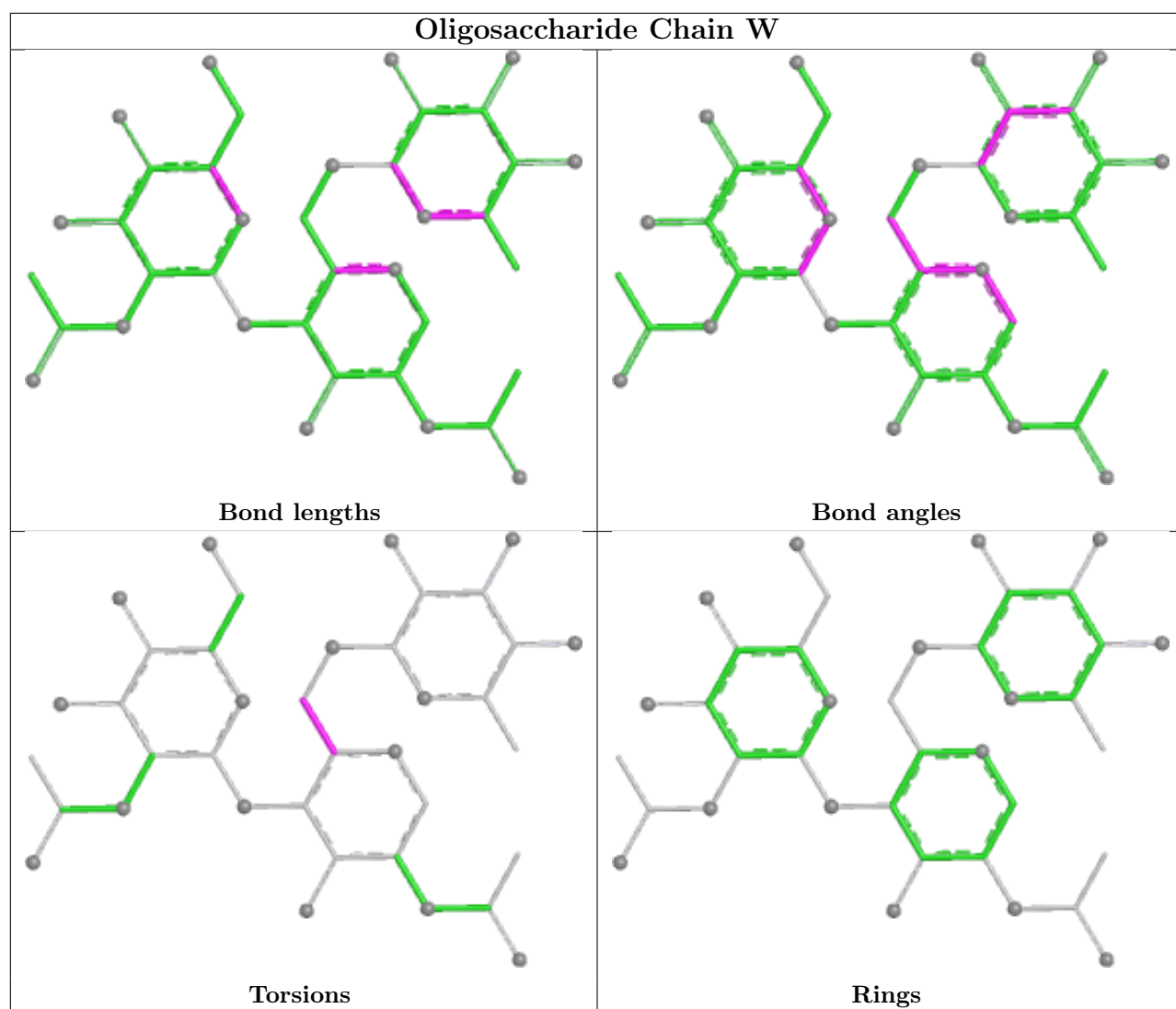


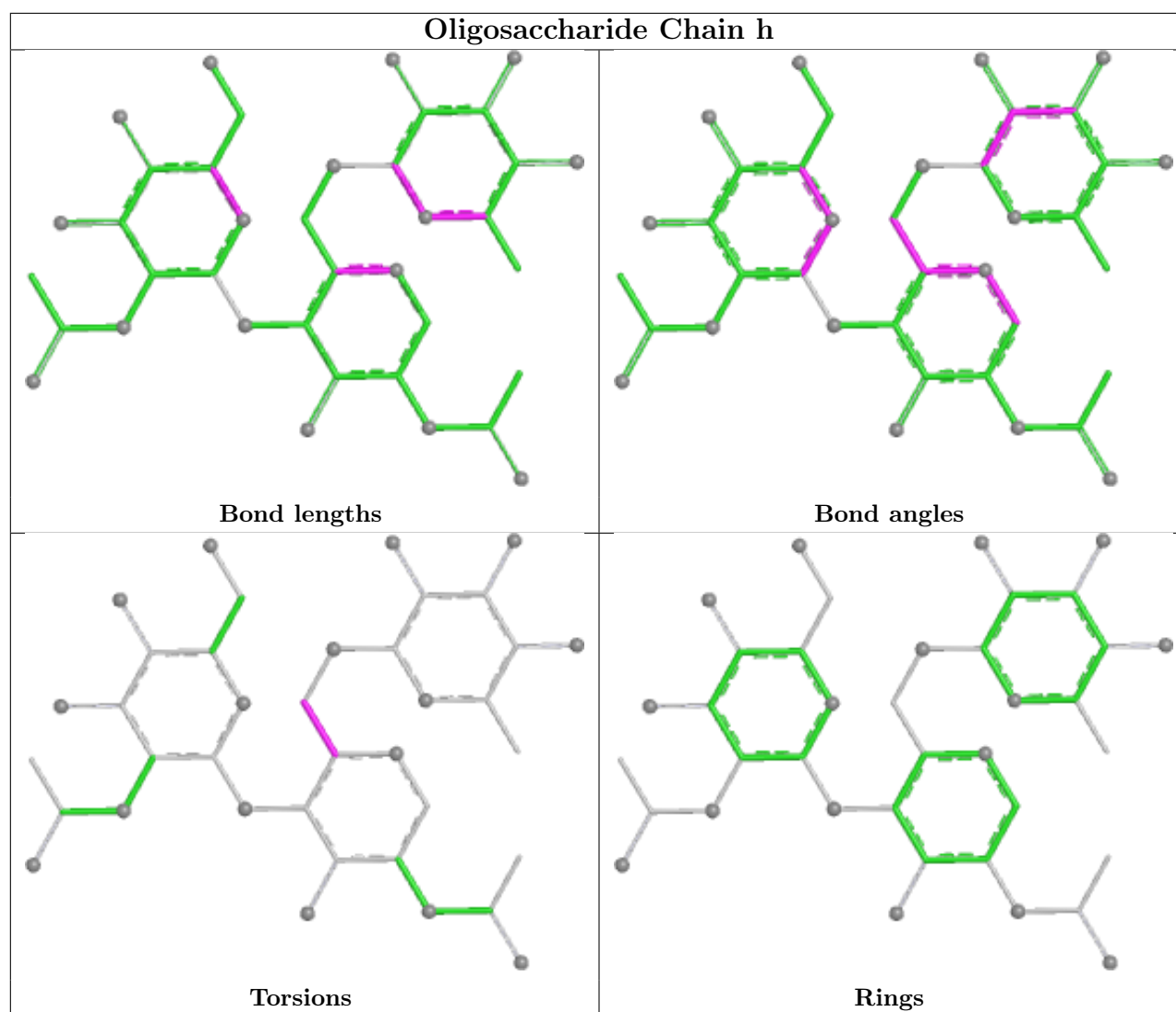












5.6 Ligand geometry [i](#)

21 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	C	1307	1	14,14,15	1.38	3 (21%)	17,19,21	0.70	0
5	NAG	C	1301	1	14,14,15	1.34	2 (14%)	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1303	1	14,14,15	1.26	2 (14%)	17,19,21	0.82	1 (5%)
5	NAG	B	1304	1	14,14,15	1.28	2 (14%)	17,19,21	0.82	0
5	NAG	B	1303	1	14,14,15	1.26	2 (14%)	17,19,21	0.81	1 (5%)
5	NAG	B	1301	1	14,14,15	1.35	2 (14%)	17,19,21	0.93	1 (5%)
5	NAG	C	1303	1	14,14,15	1.26	2 (14%)	17,19,21	0.82	1 (5%)
5	NAG	A	1306	1	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	B	1305	1	14,14,15	1.26	2 (14%)	17,19,21	0.90	0
5	NAG	A	1305	1	14,14,15	1.27	2 (14%)	17,19,21	0.90	0
5	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	B	1307	1	14,14,15	1.38	3 (21%)	17,19,21	0.70	0
5	NAG	A	1307	1	14,14,15	1.37	3 (21%)	17,19,21	0.71	0
5	NAG	B	1306	1	14,14,15	0.26	0	17,19,21	0.39	0
5	NAG	A	1304	1	14,14,15	1.29	2 (14%)	17,19,21	0.82	0
5	NAG	C	1304	1	14,14,15	1.29	2 (14%)	17,19,21	0.82	0
5	NAG	C	1306	1	14,14,15	0.25	0	17,19,21	0.39	0
5	NAG	C	1302	1	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	A	1301	1	14,14,15	1.34	2 (14%)	17,19,21	0.93	1 (5%)
5	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	C	1305	1	14,14,15	1.26	2 (14%)	17,19,21	0.90	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	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	0/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1307	NAG	O5-C5	2.93	1.49	1.43
5	C	1307	NAG	O5-C5	2.92	1.49	1.43
5	A	1307	NAG	O5-C5	2.90	1.49	1.43
5	B	1301	NAG	O5-C5	2.81	1.48	1.43
5	A	1301	NAG	O5-C5	2.77	1.48	1.43
5	C	1301	NAG	O5-C5	2.77	1.48	1.43
5	C	1304	NAG	O5-C5	2.77	1.48	1.43
5	B	1304	NAG	O5-C5	2.76	1.48	1.43
5	A	1304	NAG	O5-C5	2.75	1.48	1.43
5	B	1303	NAG	O5-C5	2.59	1.48	1.43
5	B	1307	NAG	C1-C2	2.58	1.55	1.52
5	C	1307	NAG	C1-C2	2.57	1.55	1.52
5	A	1305	NAG	O5-C5	2.57	1.48	1.43
5	C	1305	NAG	O5-C5	2.55	1.48	1.43
5	A	1307	NAG	C1-C2	2.55	1.55	1.52
5	A	1303	NAG	O5-C5	2.54	1.48	1.43
5	C	1303	NAG	O5-C5	2.54	1.48	1.43
5	B	1305	NAG	O5-C5	2.54	1.48	1.43
5	B	1301	NAG	C1-C2	2.48	1.55	1.52
5	A	1301	NAG	C1-C2	2.47	1.55	1.52
5	C	1301	NAG	C1-C2	2.43	1.55	1.52
5	A	1303	NAG	C1-C2	2.31	1.55	1.52
5	C	1303	NAG	C1-C2	2.31	1.55	1.52
5	B	1303	NAG	C1-C2	2.29	1.55	1.52
5	C	1305	NAG	C1-C2	2.22	1.55	1.52
5	A	1305	NAG	C1-C2	2.21	1.55	1.52
5	B	1305	NAG	C1-C2	2.21	1.55	1.52
5	B	1307	NAG	O5-C1	2.16	1.47	1.43
5	C	1307	NAG	O5-C1	2.14	1.47	1.43
5	A	1307	NAG	O5-C1	2.12	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1304	NAG	C1-C2	2.05	1.55	1.52
5	B	1304	NAG	C1-C2	2.04	1.55	1.52
5	A	1304	NAG	C1-C2	2.04	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1301	NAG	C1-O5-C5	2.71	115.82	112.19
5	C	1301	NAG	C1-O5-C5	2.71	115.82	112.19
5	A	1301	NAG	C1-O5-C5	2.71	115.82	112.19
5	A	1303	NAG	C1-O5-C5	2.32	115.30	112.19
5	C	1303	NAG	C1-O5-C5	2.31	115.29	112.19
5	B	1303	NAG	C1-O5-C5	2.29	115.26	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1302	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6

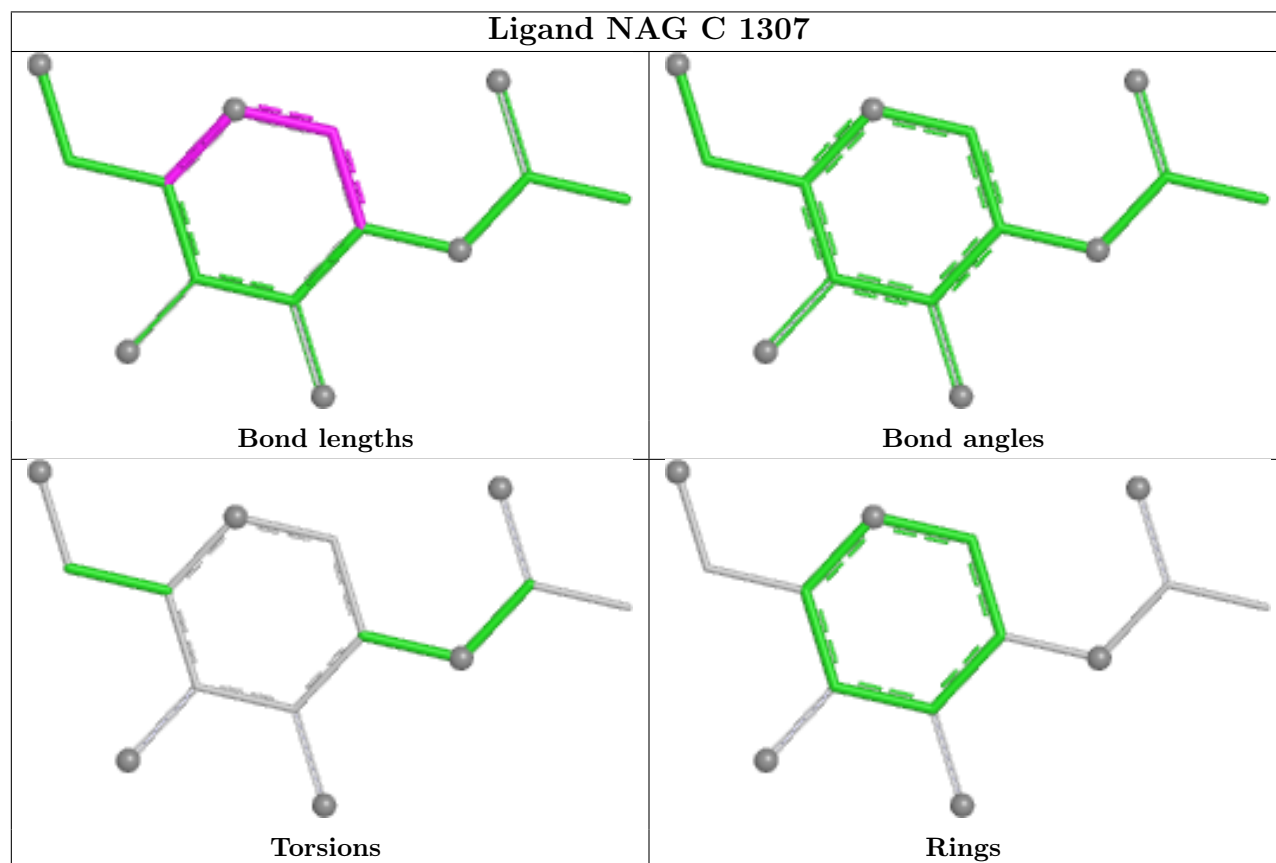
There are no ring outliers.

3 monomers are involved in 8 short contacts:

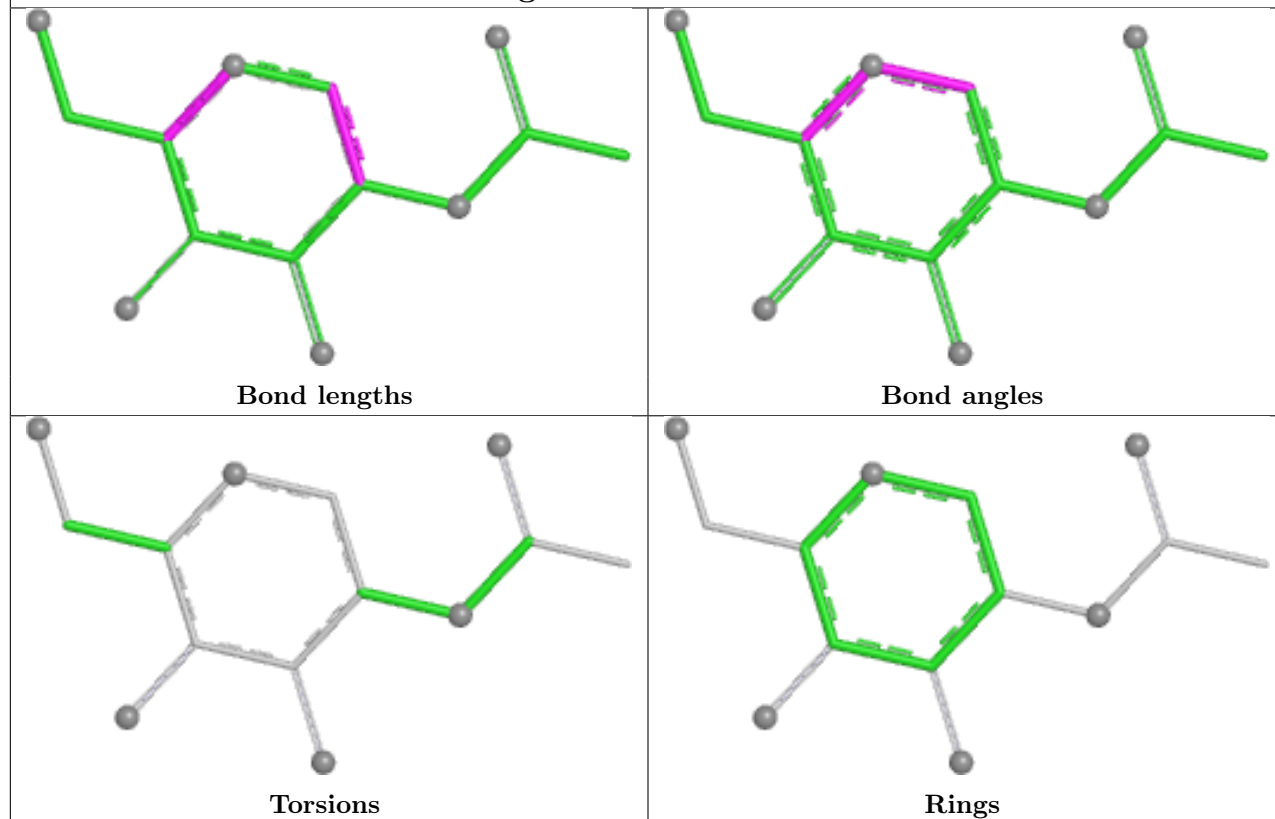
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1306	NAG	2	0
5	B	1306	NAG	2	0
5	C	1306	NAG	4	0

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

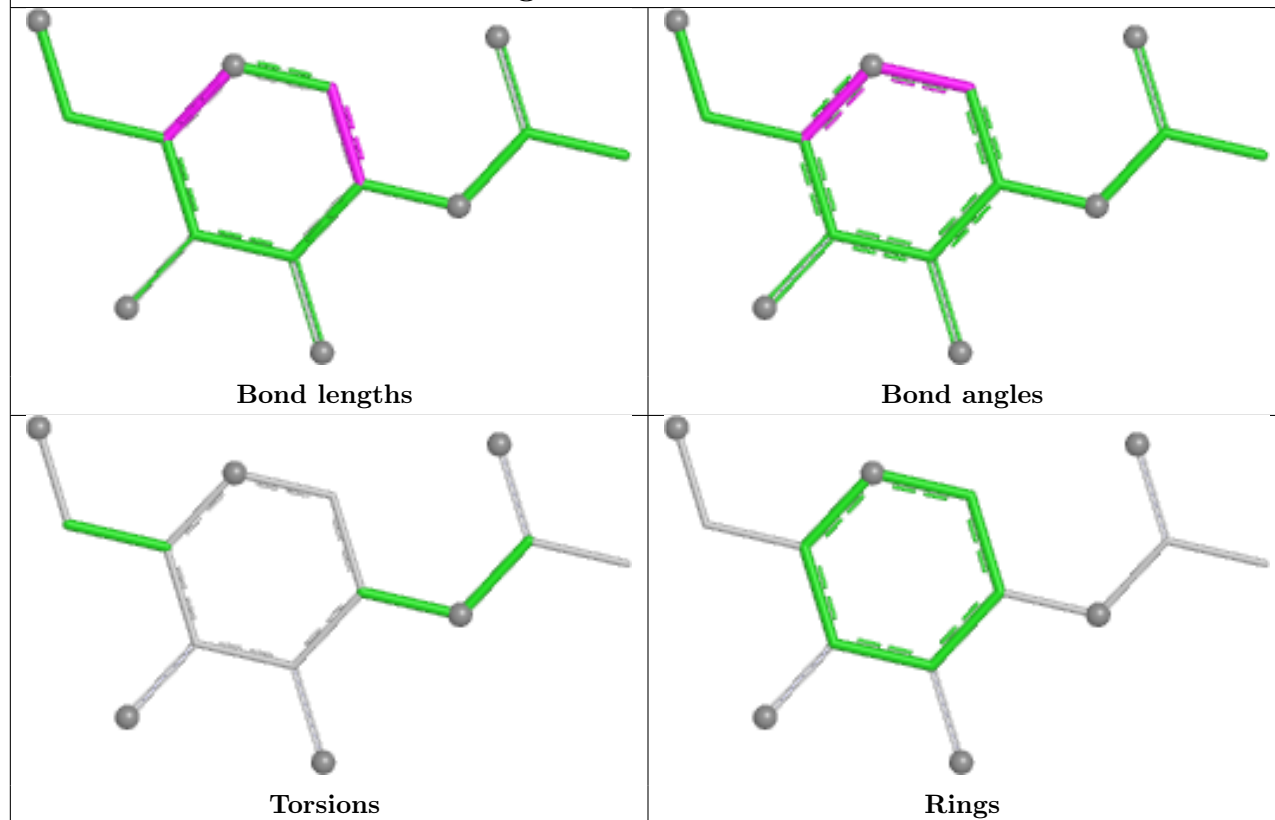
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

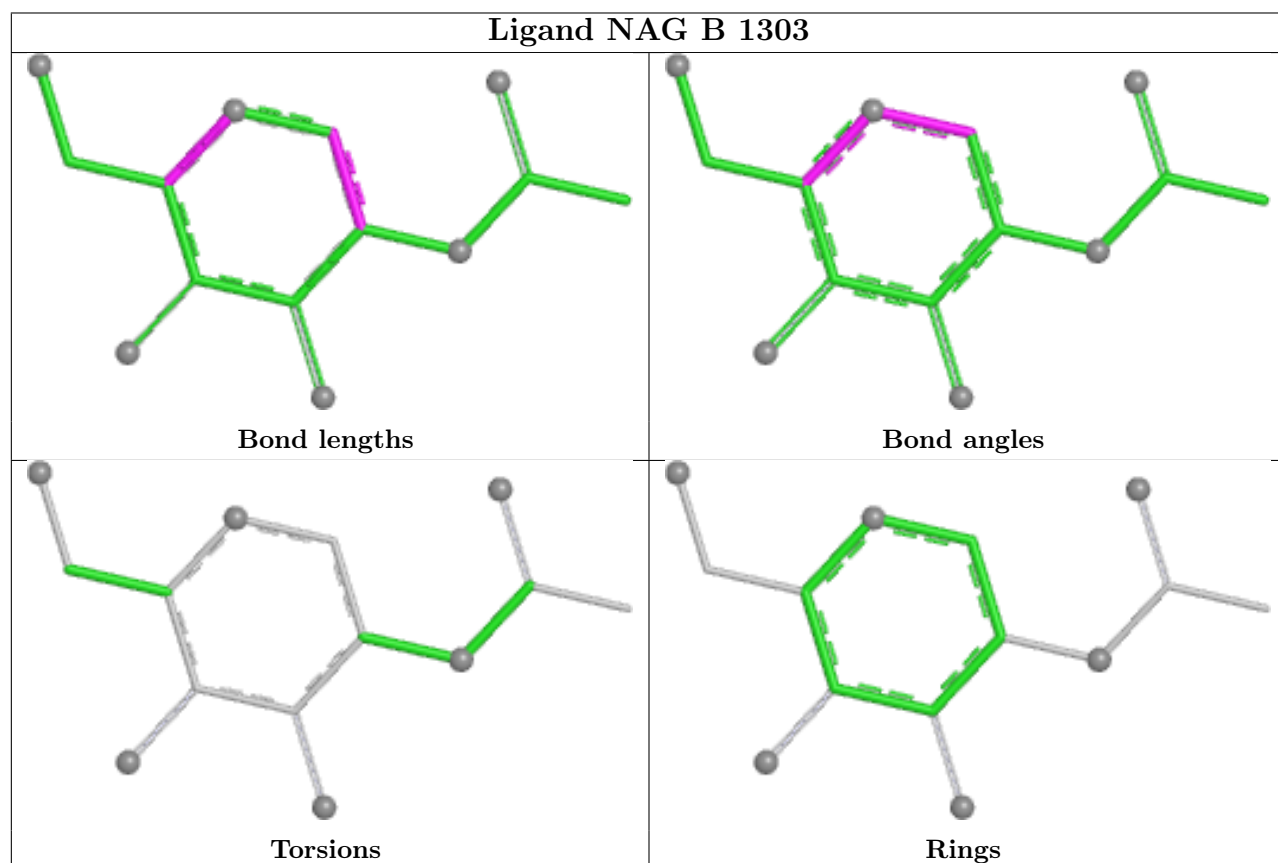
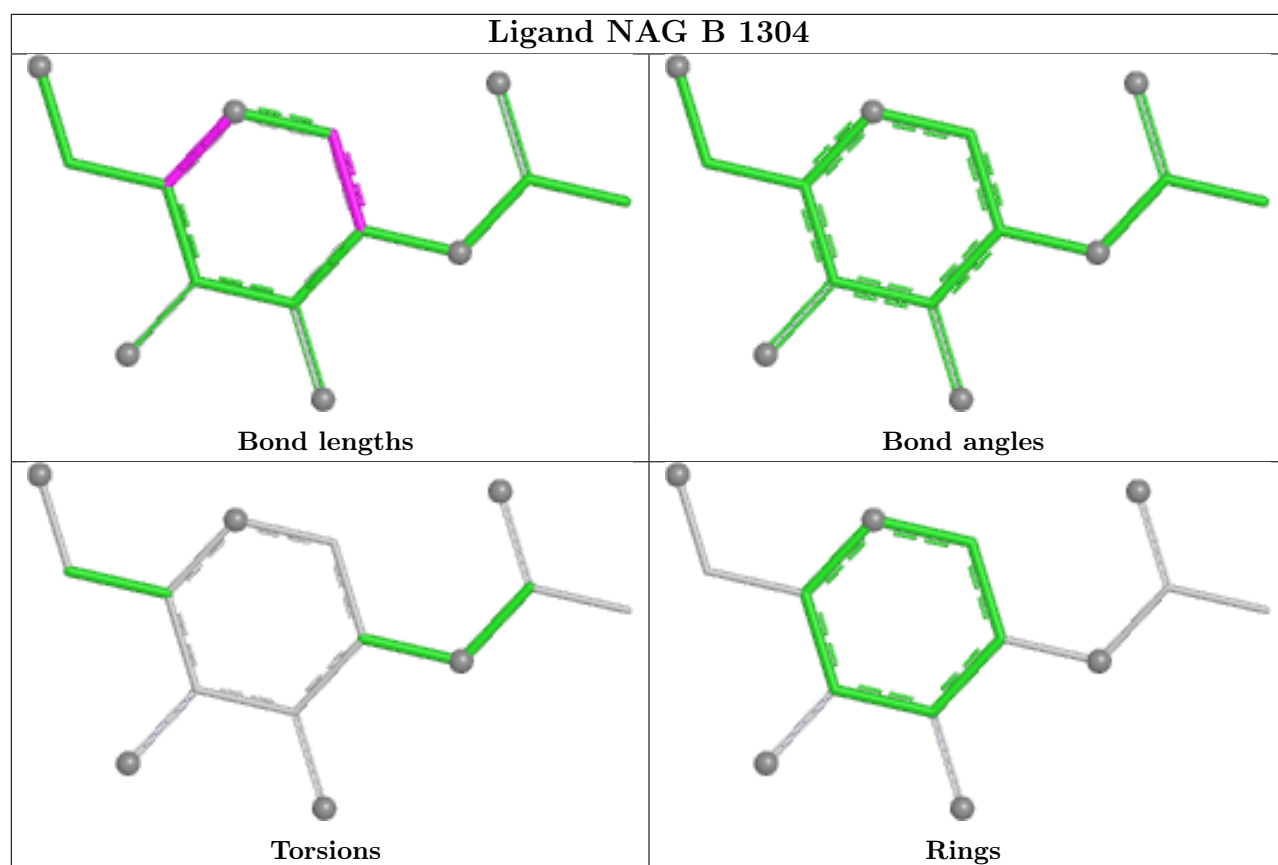


Ligand NAG C 1301

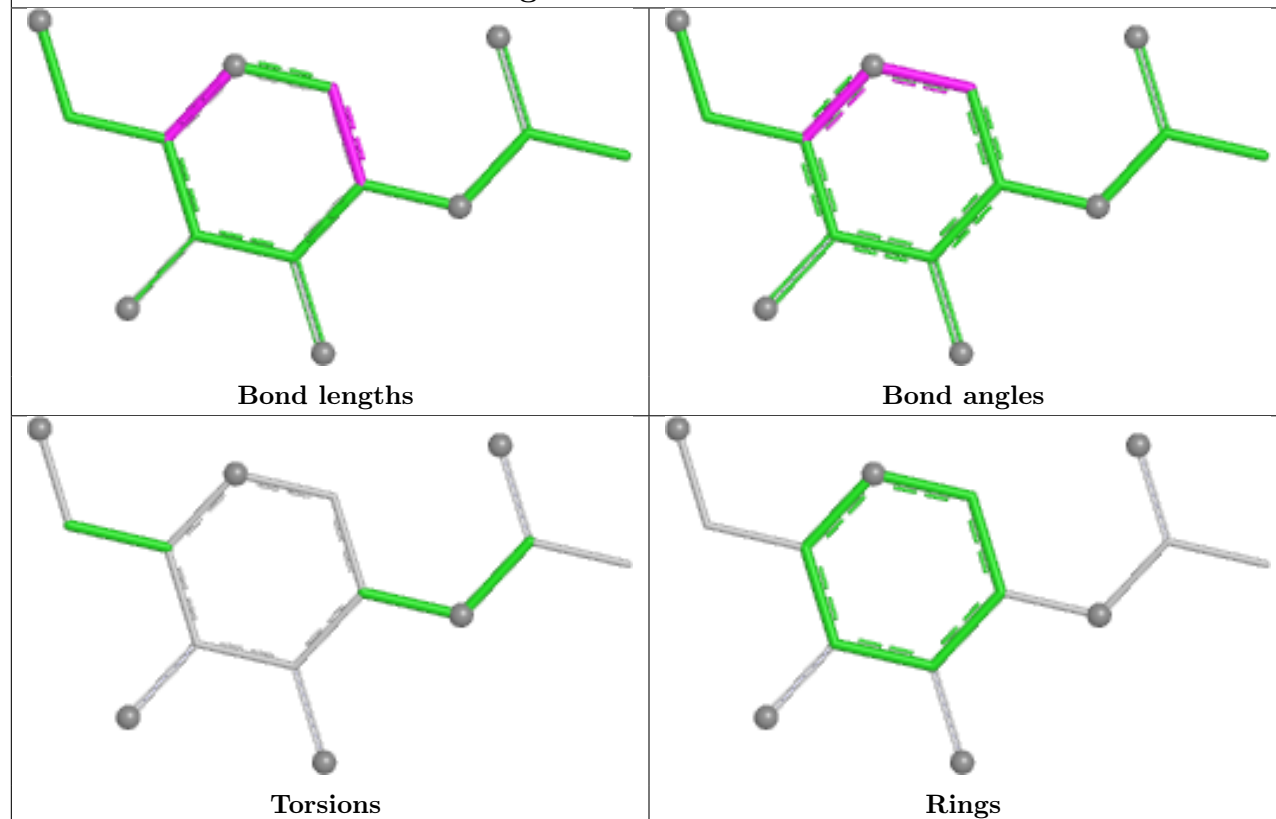


Ligand NAG A 1303

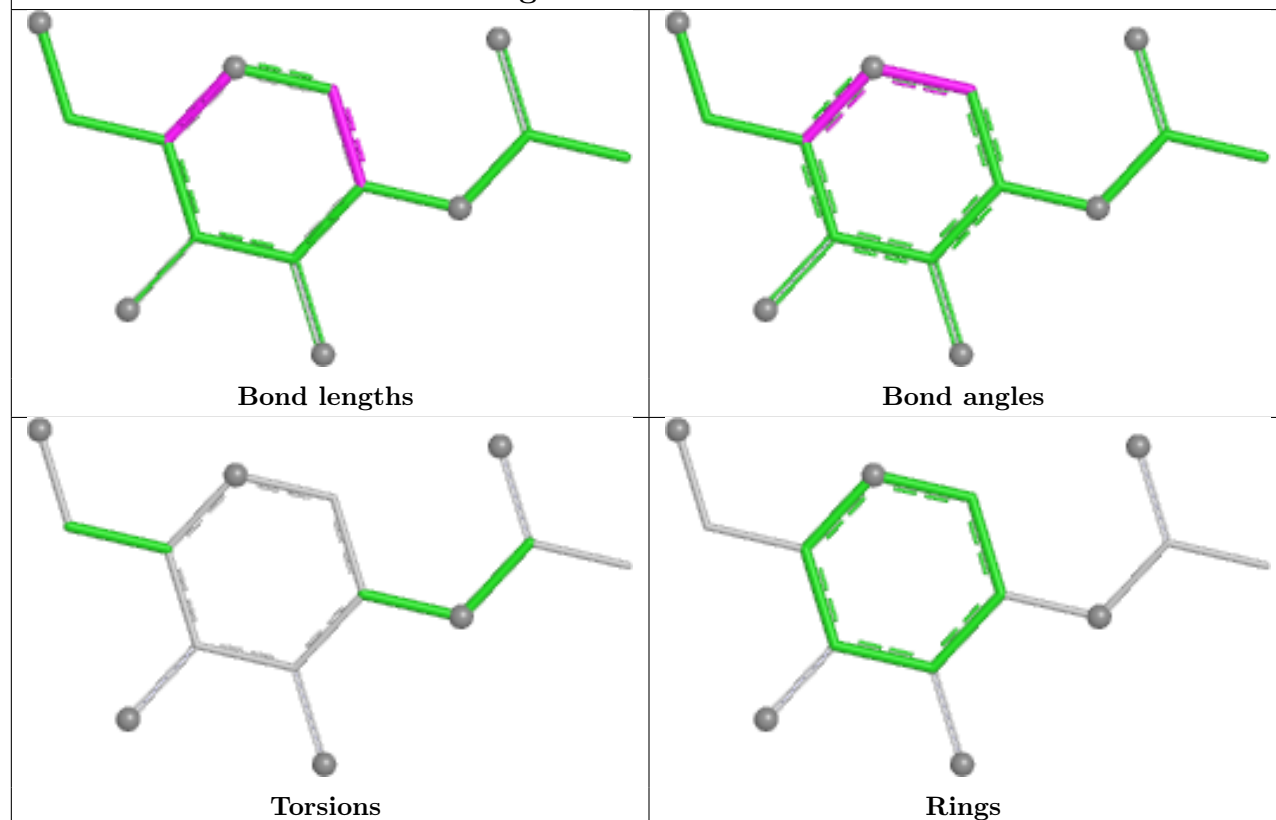




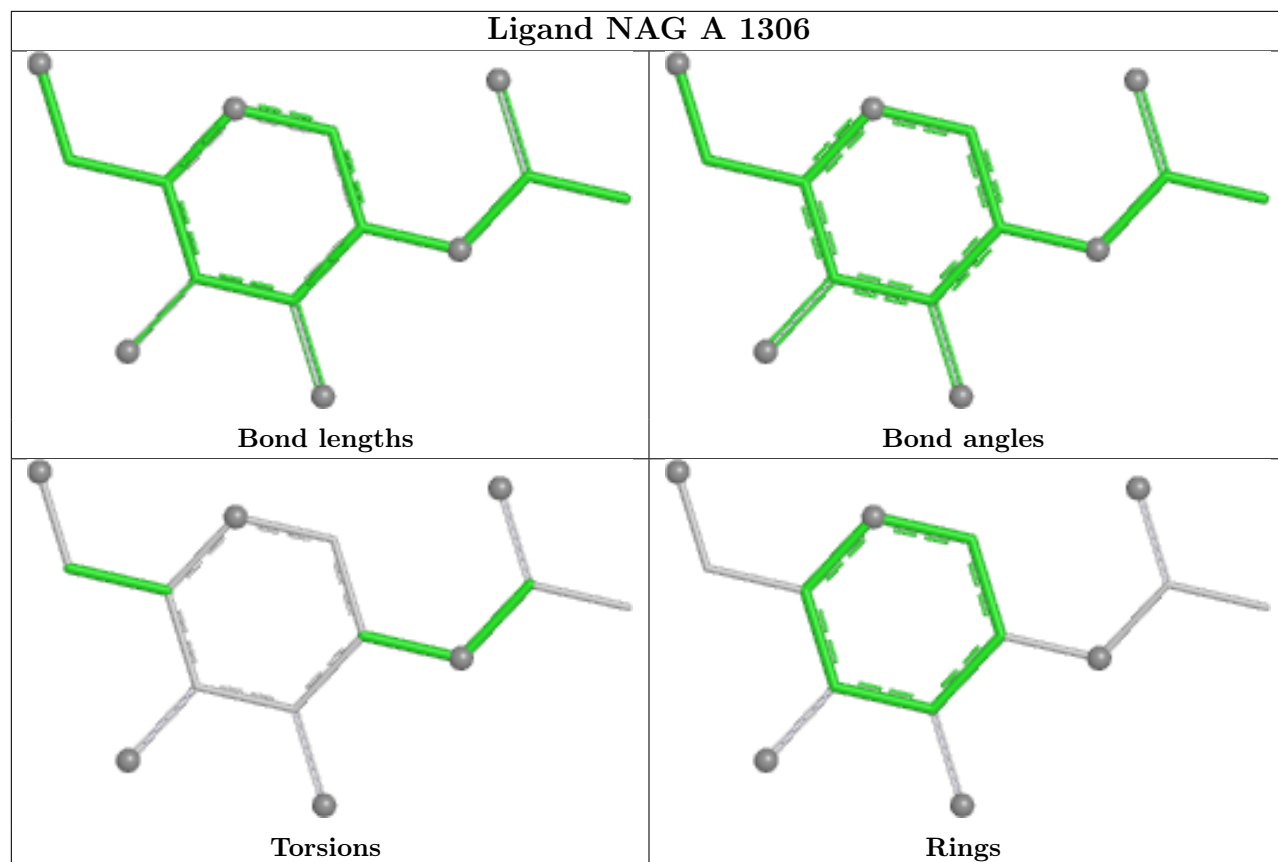
Ligand NAG B 1301



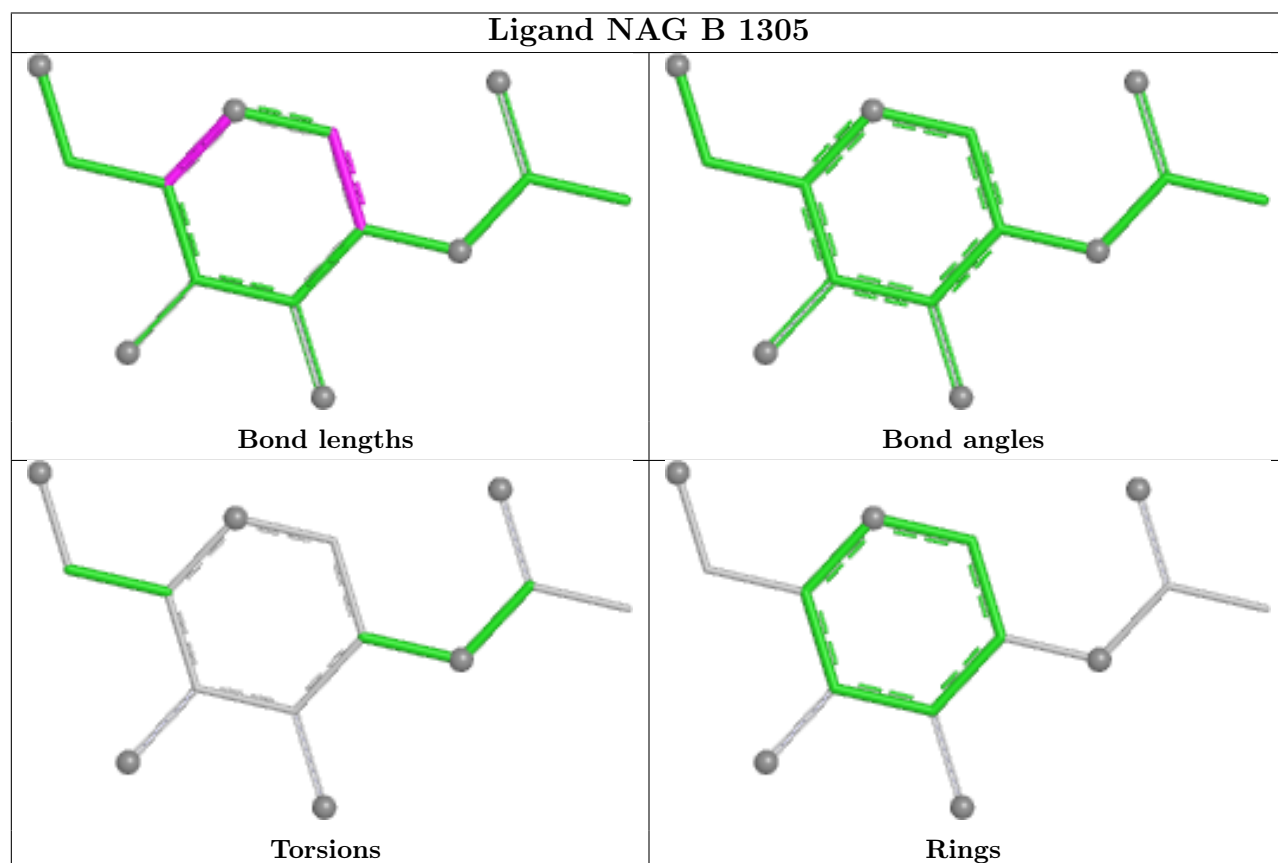
Ligand NAG C 1303



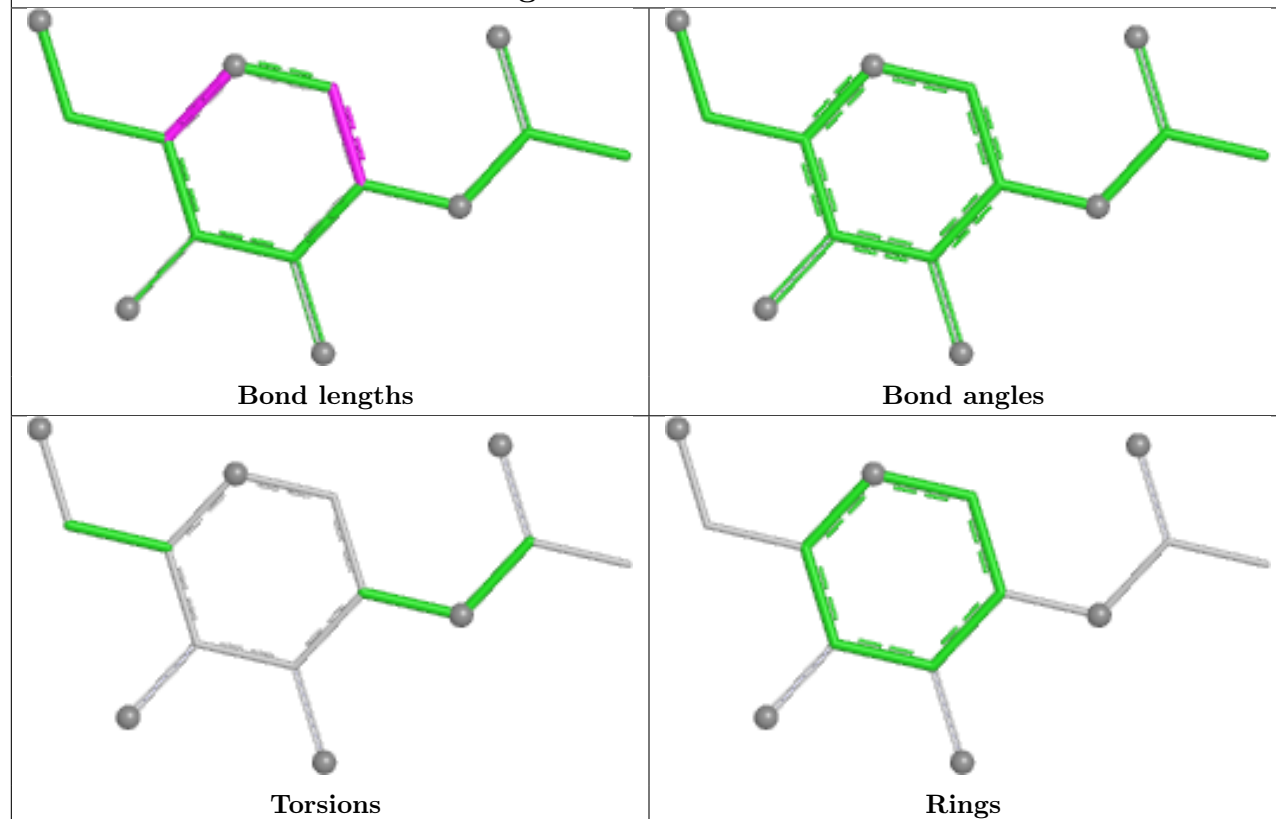
Ligand NAG A 1306



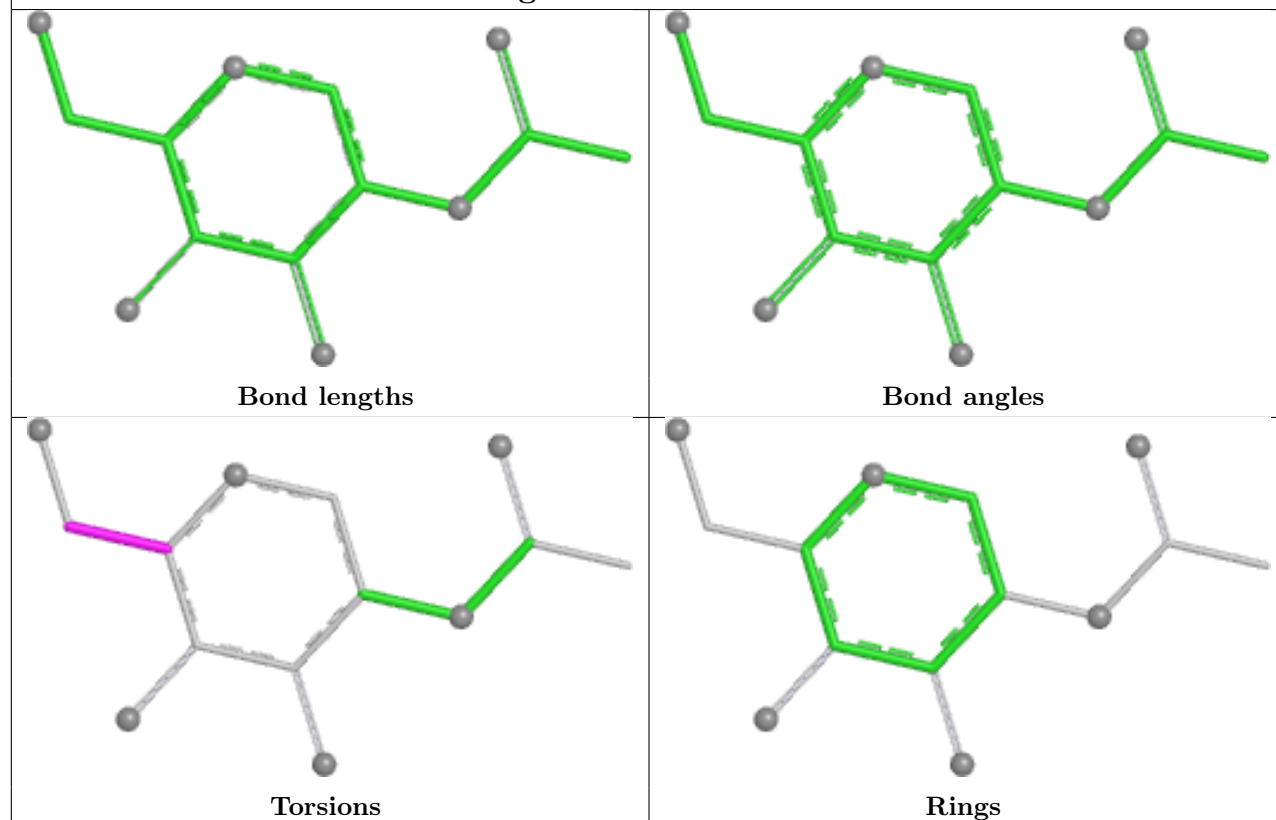
Ligand NAG B 1305

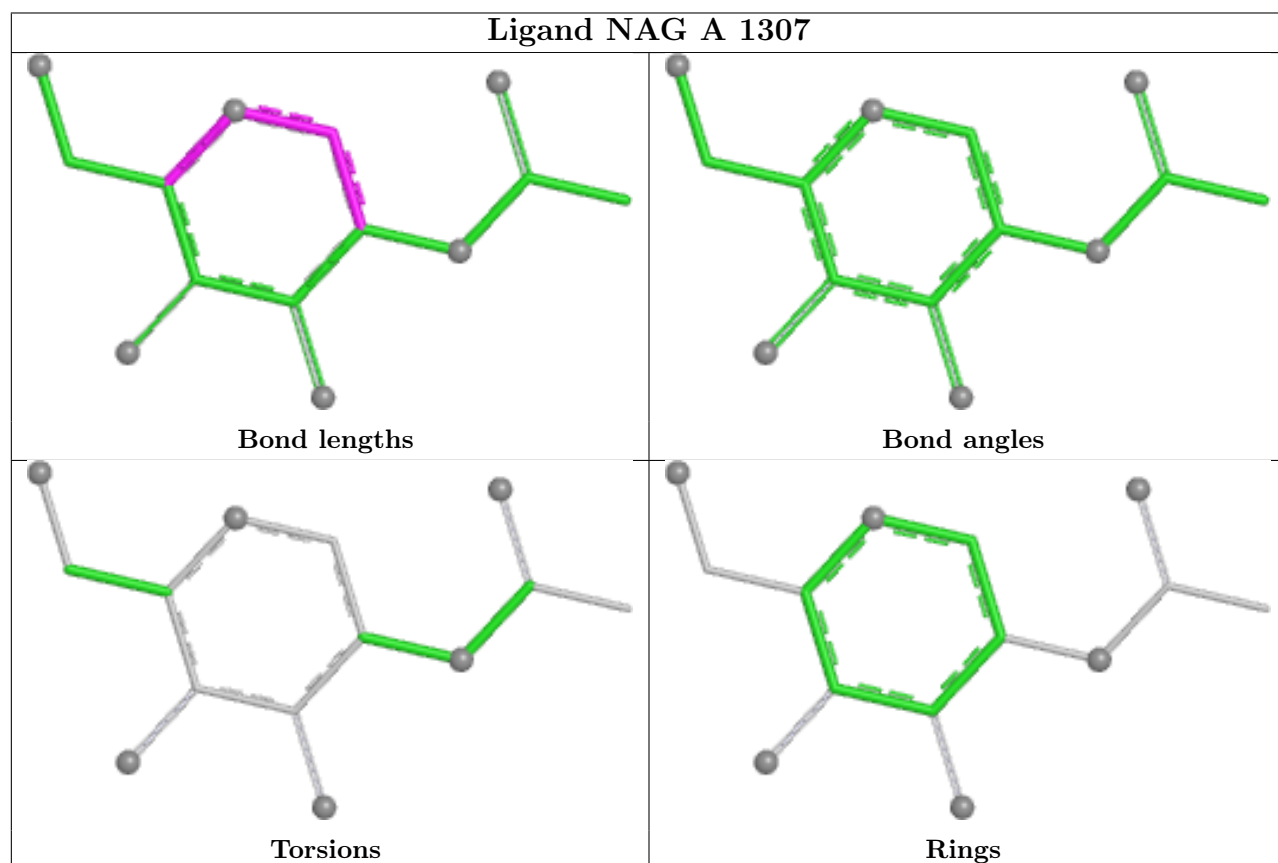
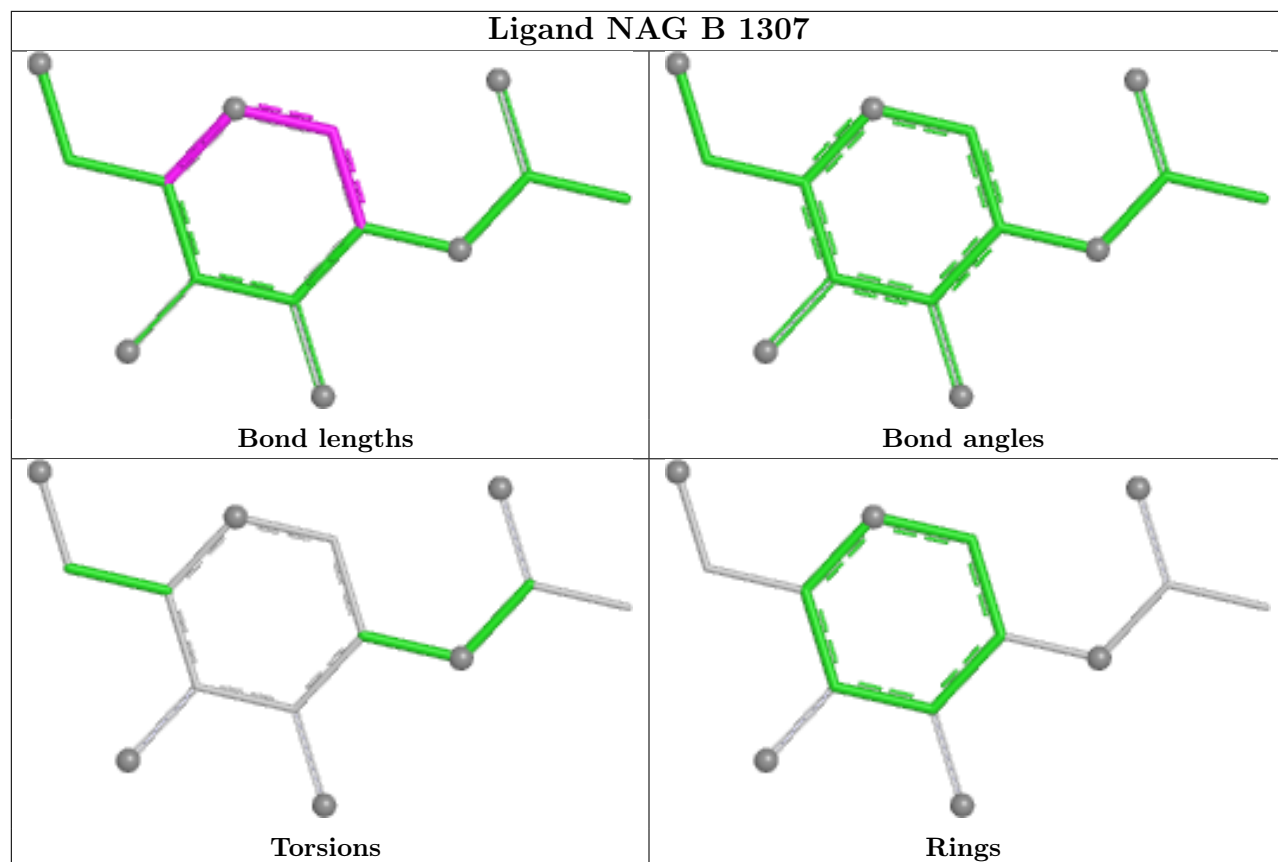


Ligand NAG A 1305

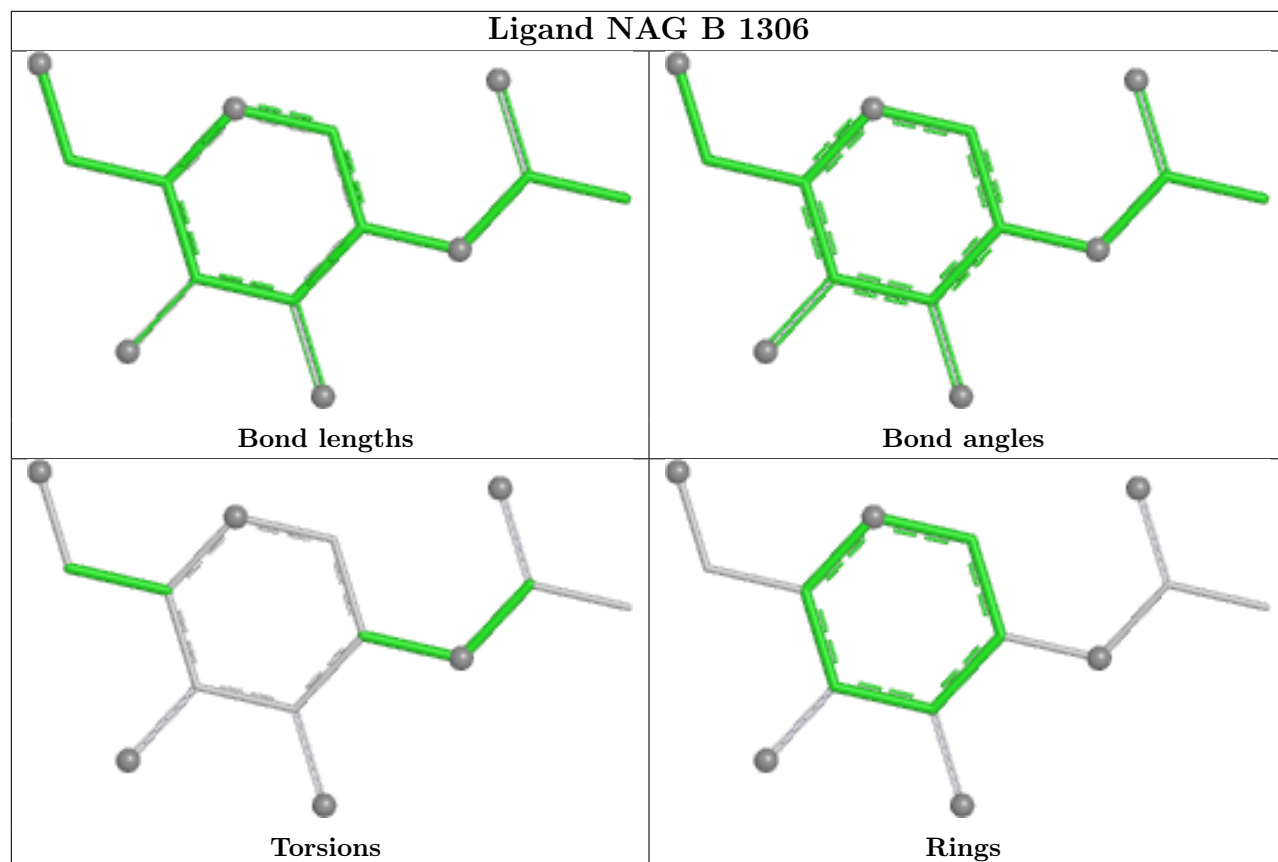


Ligand NAG A 1302

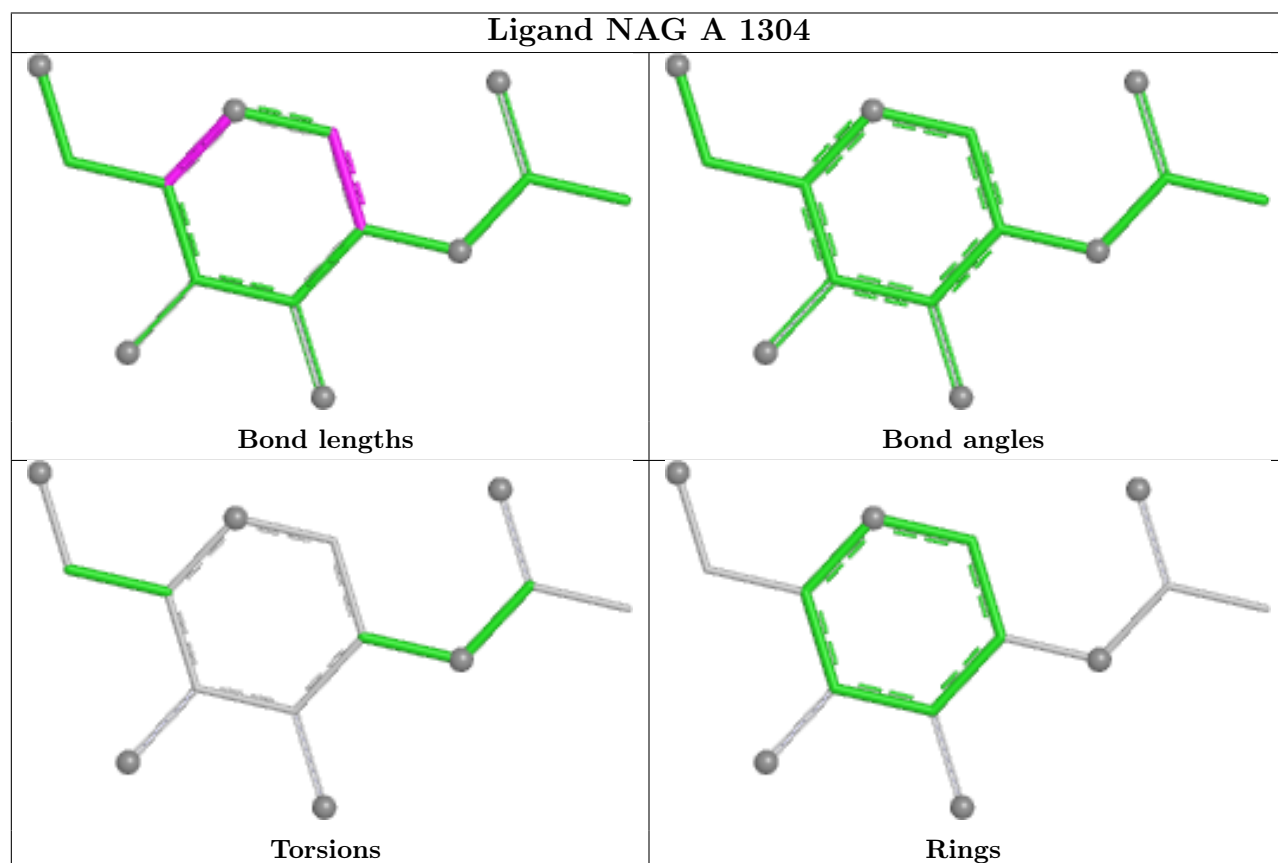




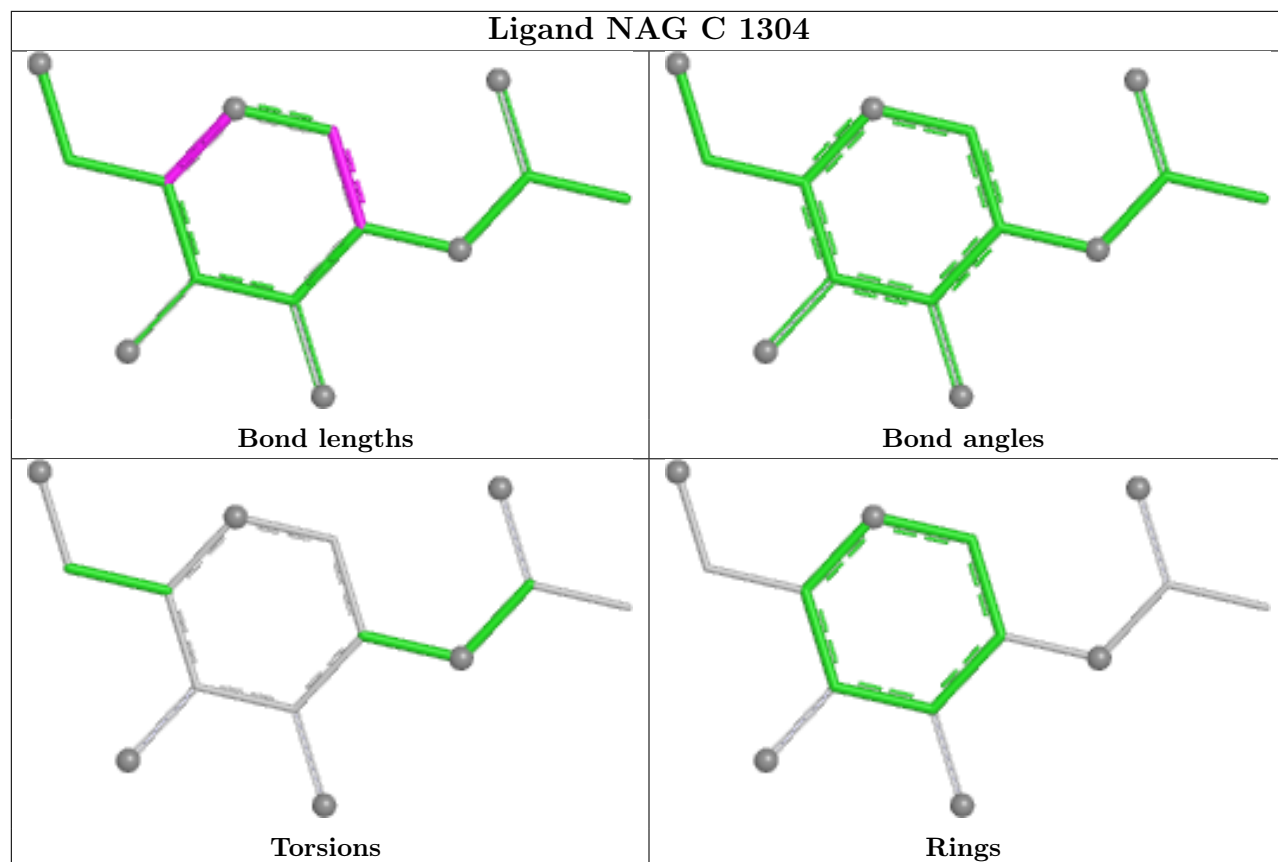
Ligand NAG B 1306



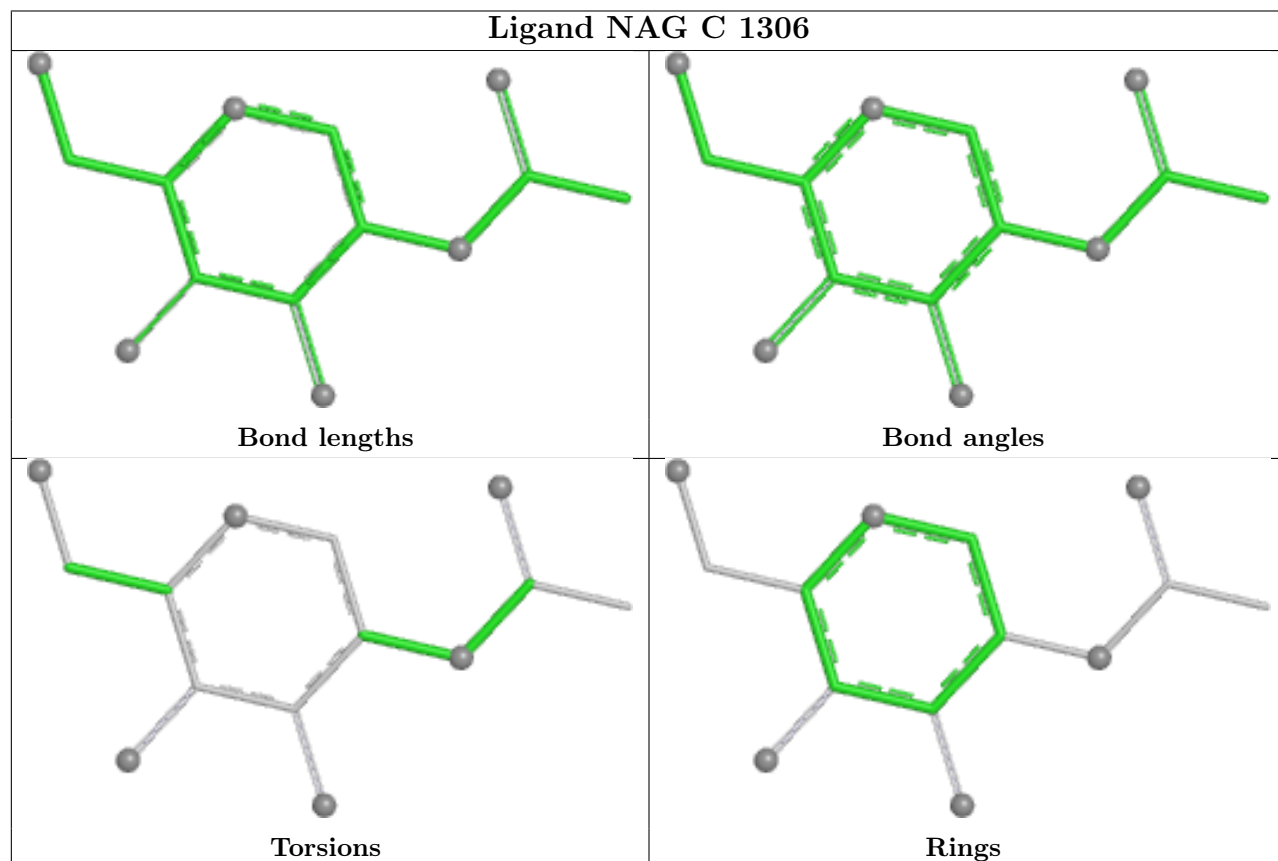
Ligand NAG A 1304



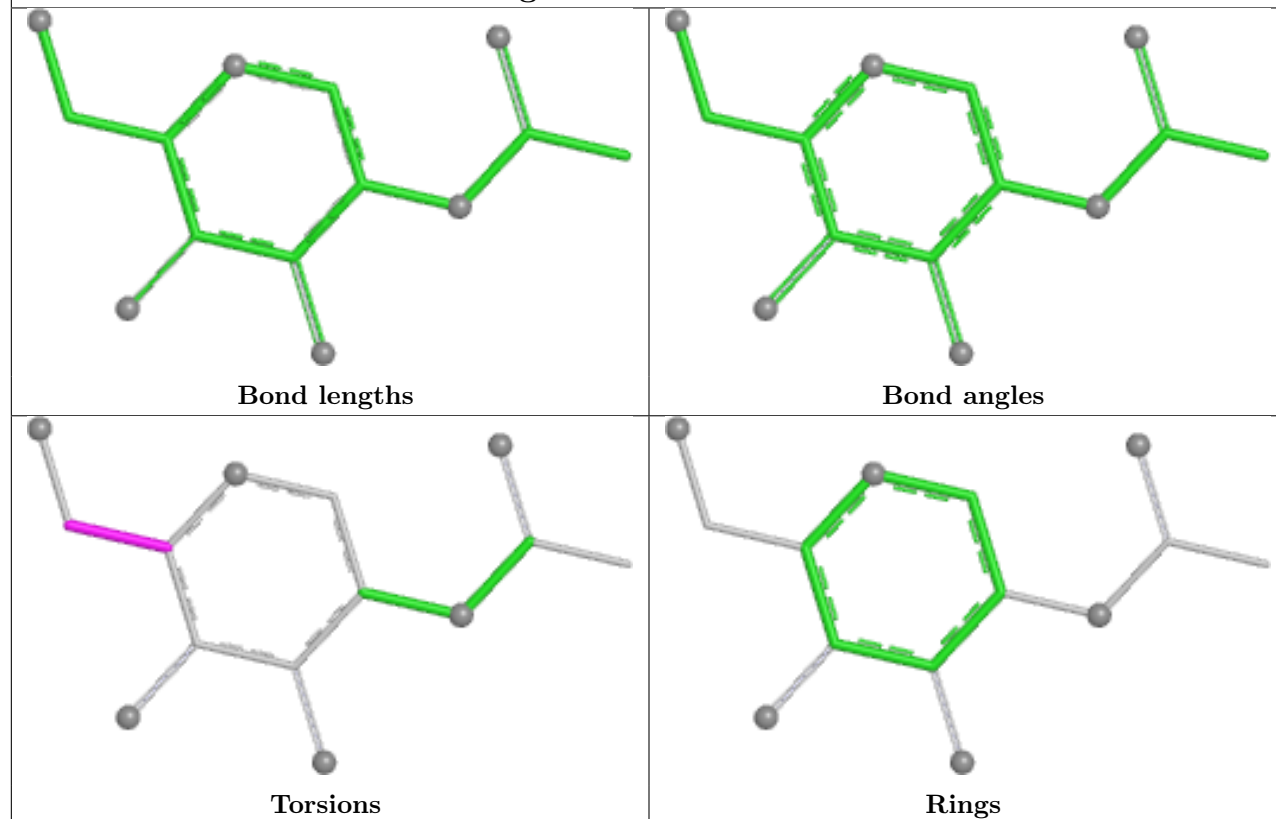
Ligand NAG C 1304



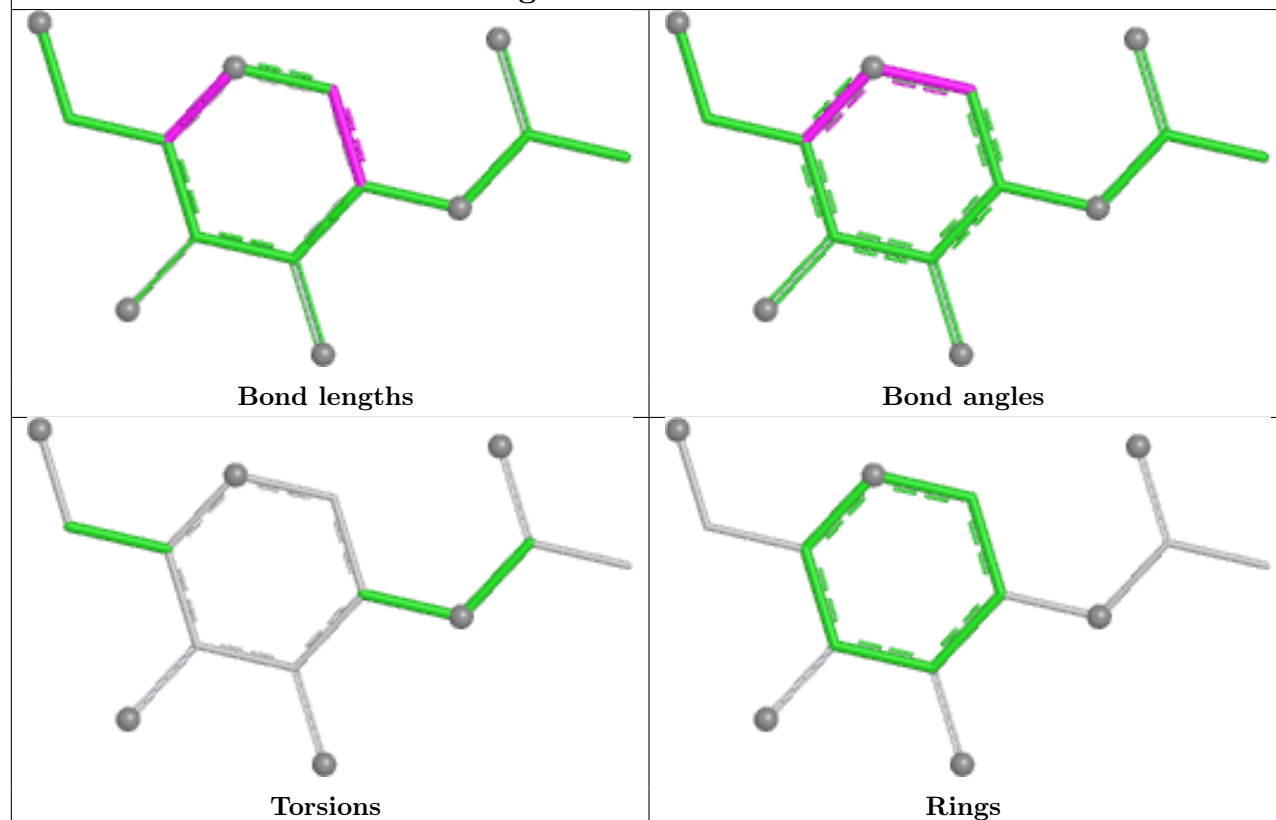
Ligand NAG C 1306



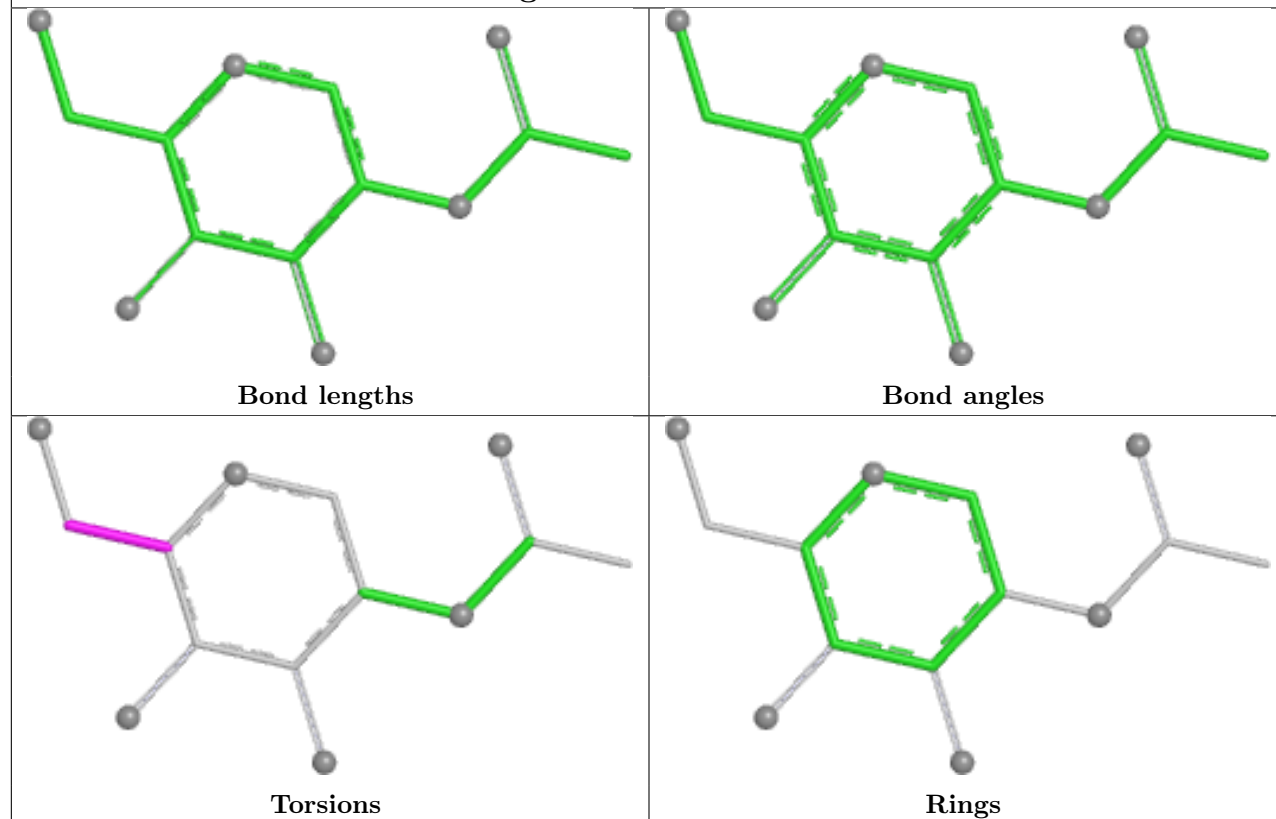
Ligand NAG C 1302



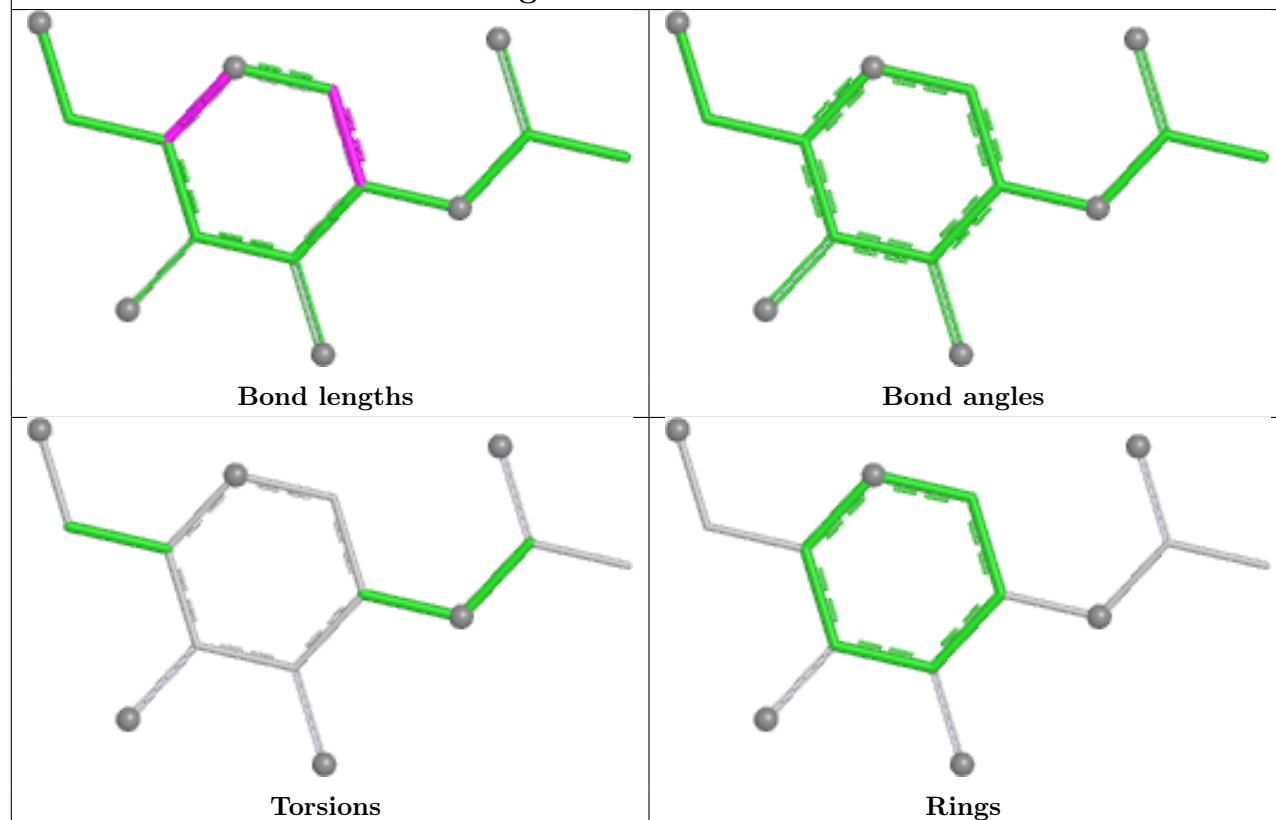
Ligand NAG A 1301



Ligand NAG B 1302



Ligand NAG C 1305



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.

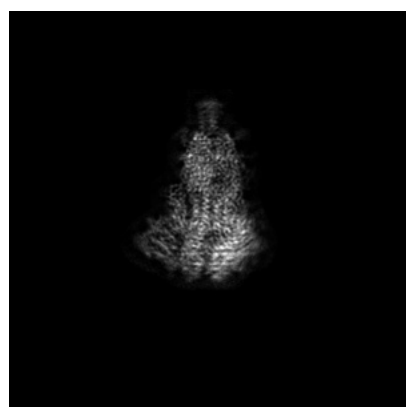
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26021. These allow visual inspection of the internal detail of the map and identification of artifacts.

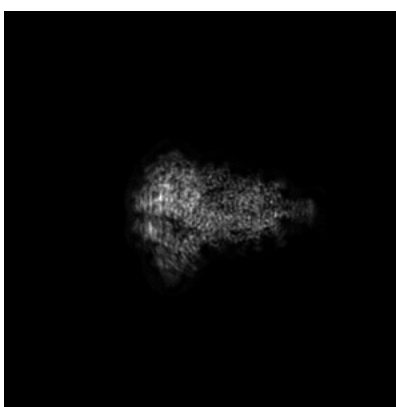
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

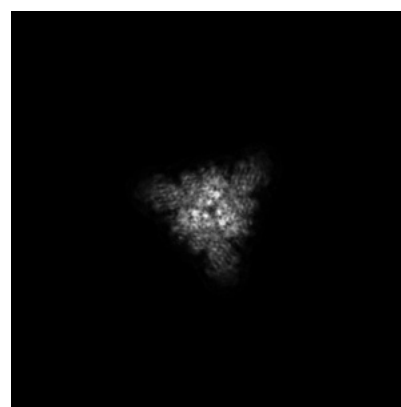
6.1.1 Primary map



X



Y



Z

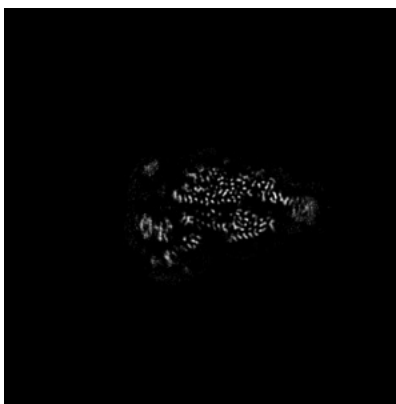
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 240



Y Index: 240

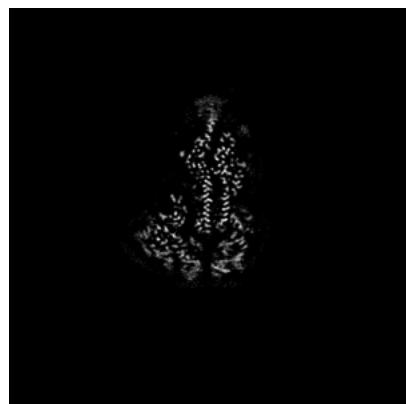


Z Index: 240

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

6.3 Largest variance slices [i](#)

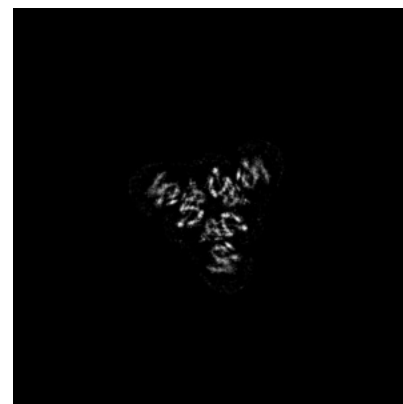
6.3.1 Primary map



X Index: 248



Y Index: 228

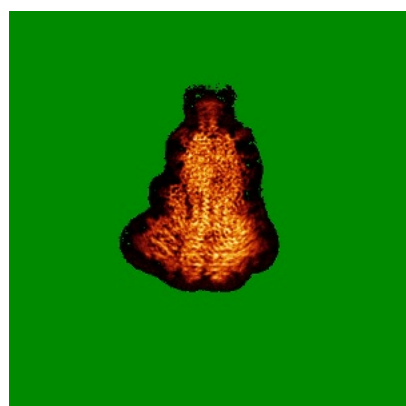


Z Index: 188

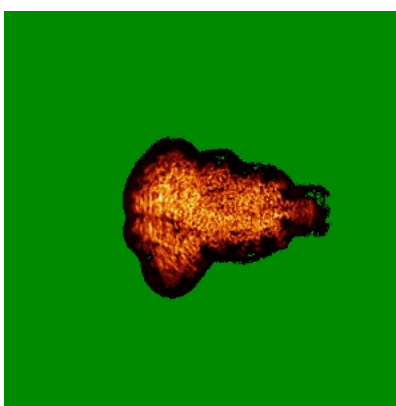
The images above show the largest variance slices of the map in three orthogonal directions.

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

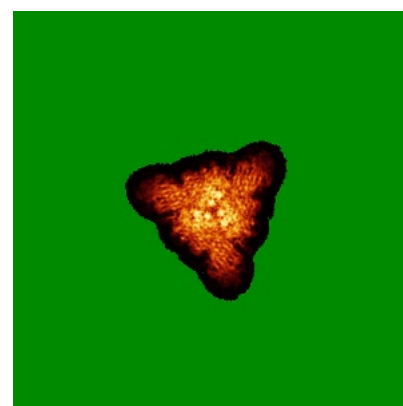
6.4.1 Primary map



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

This section was not generated.

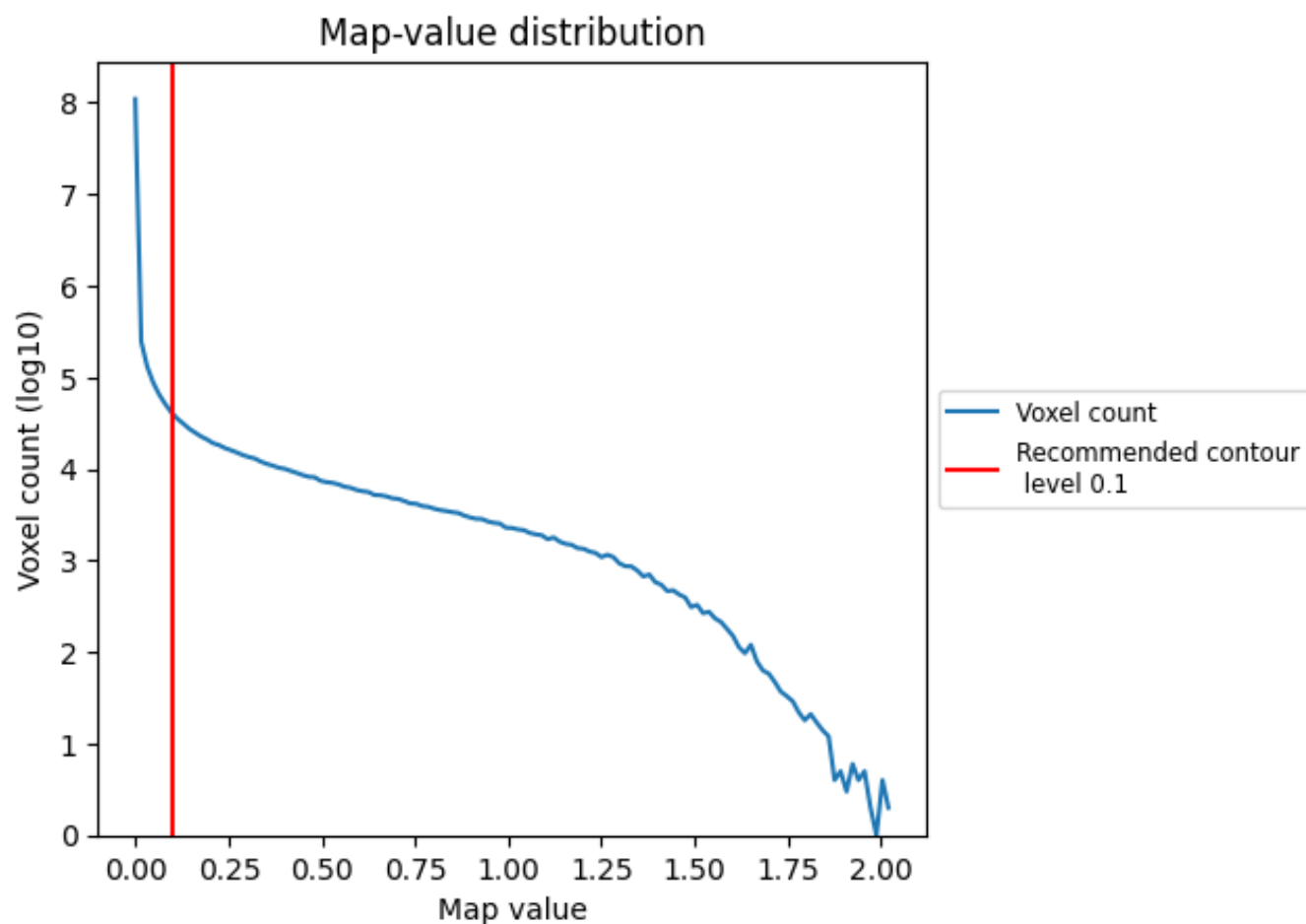
6.6 Mask visualisation

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

7 Map analysis [i](#)

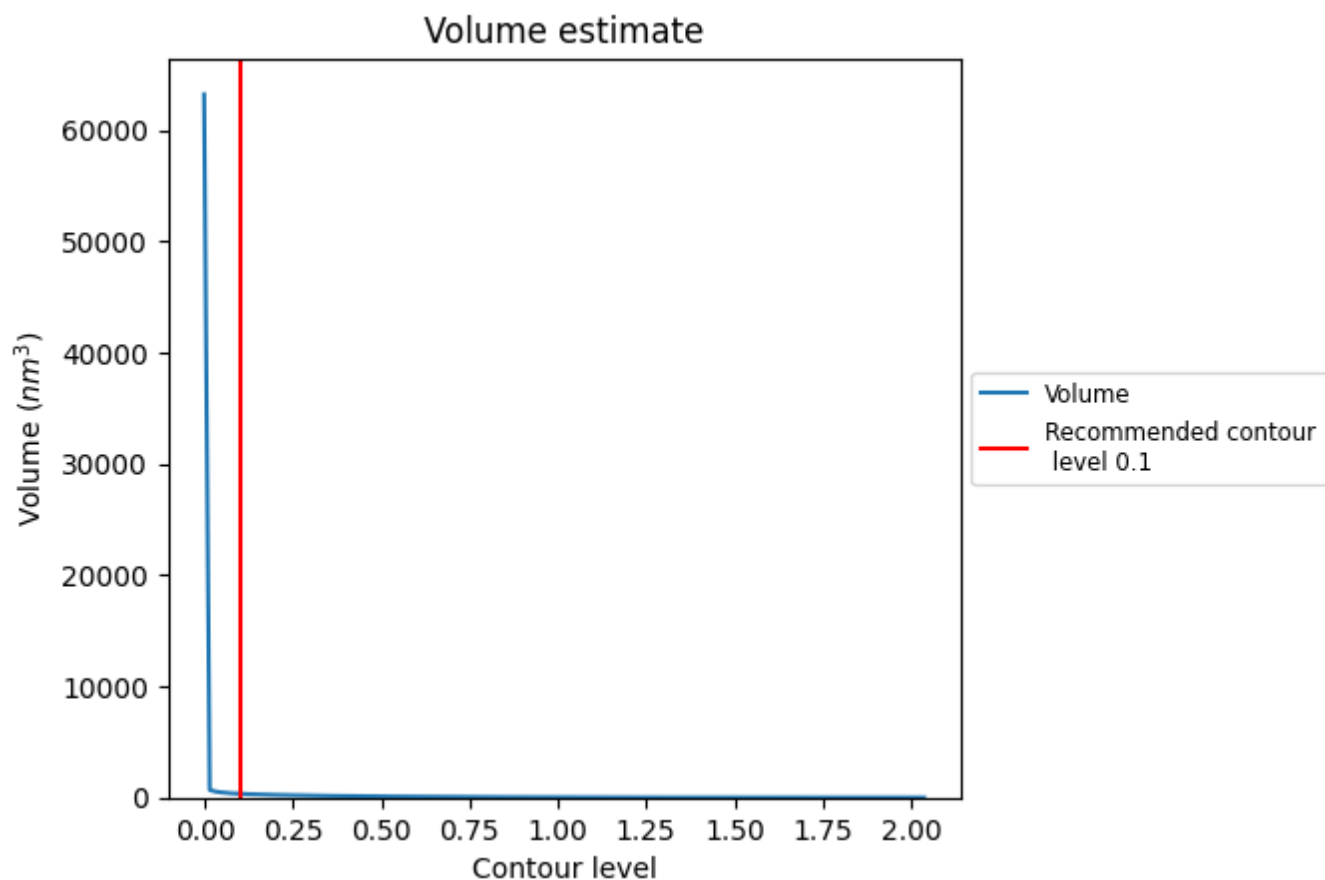
This section contains the results of statistical analysis of the map.

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.

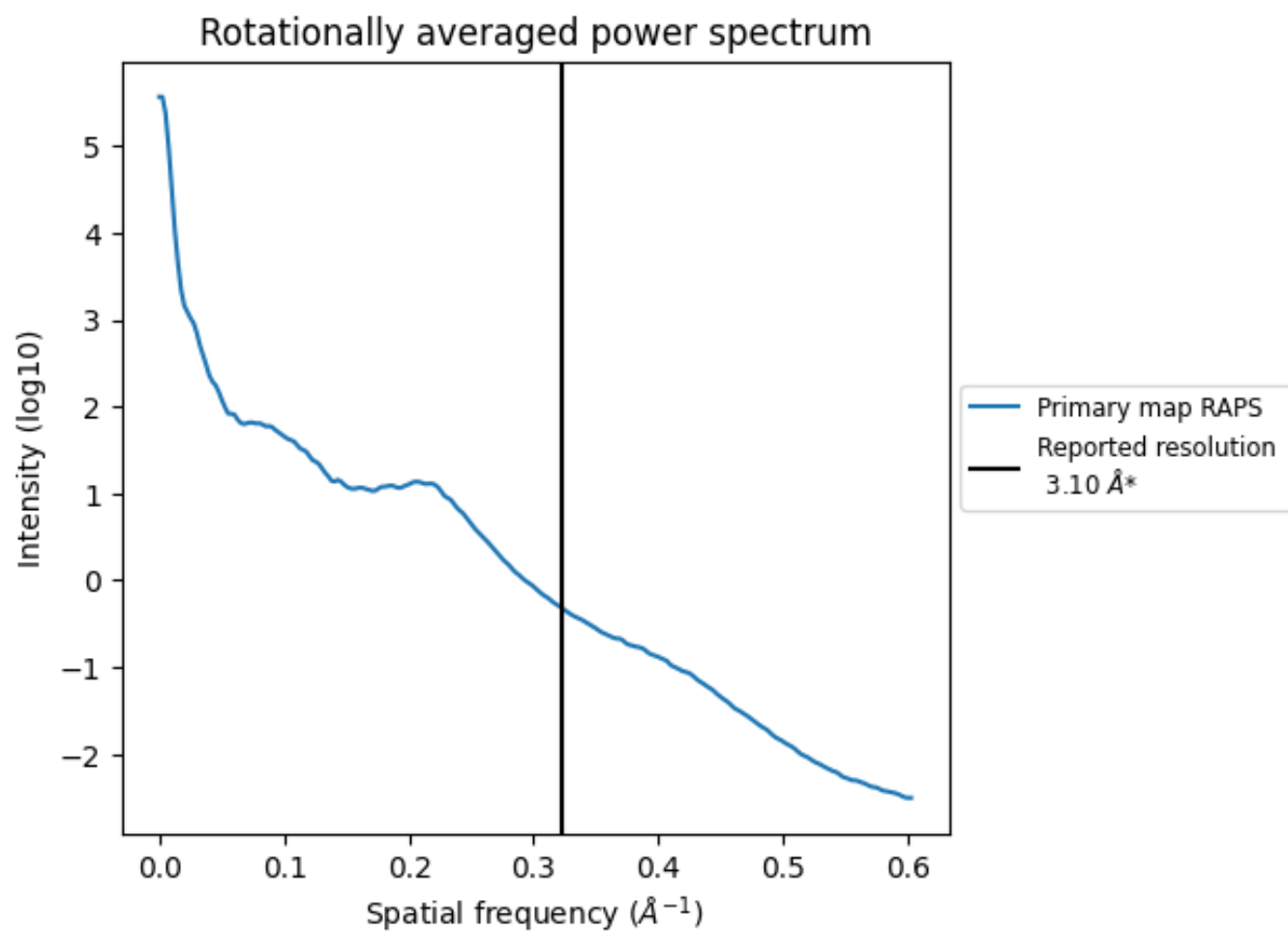
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm^3 ; this corresponds to an approximate mass of 309 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

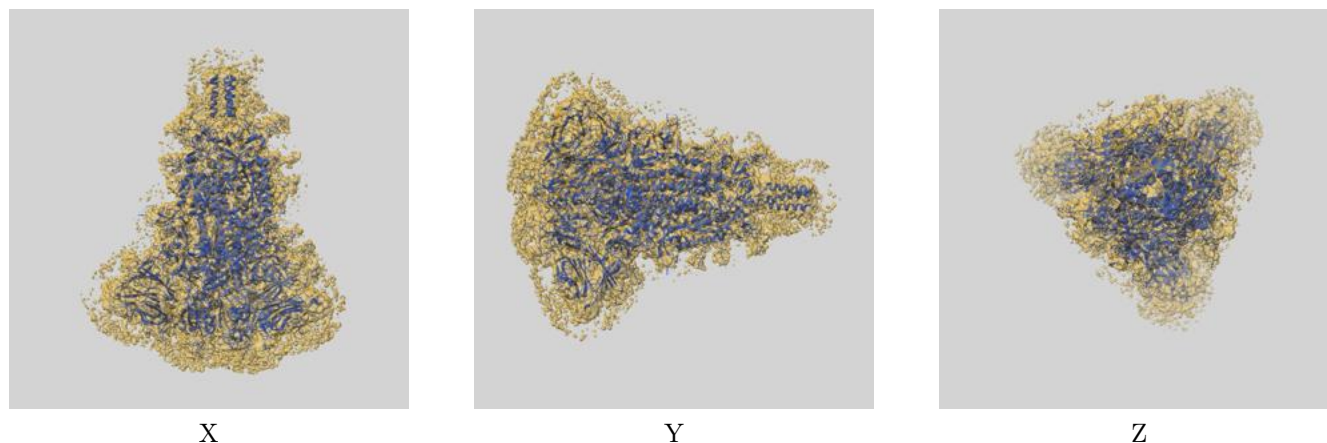
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

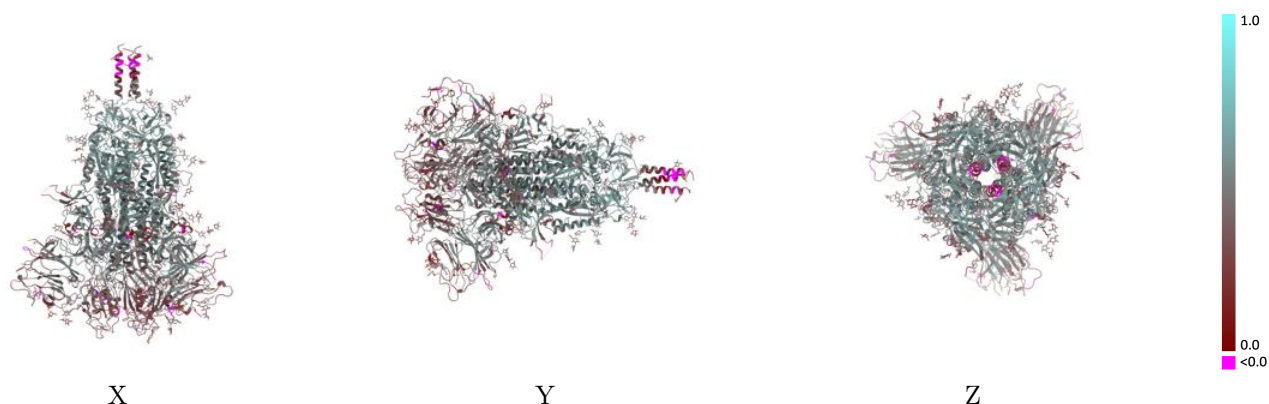
This section contains information regarding the fit between EMDB map EMD-26021 and PDB model 7TNW. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



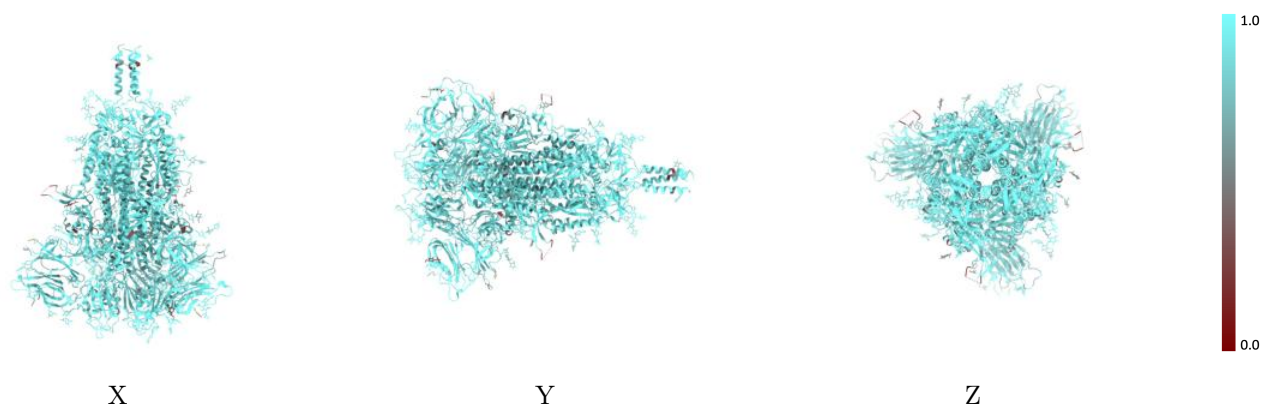
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



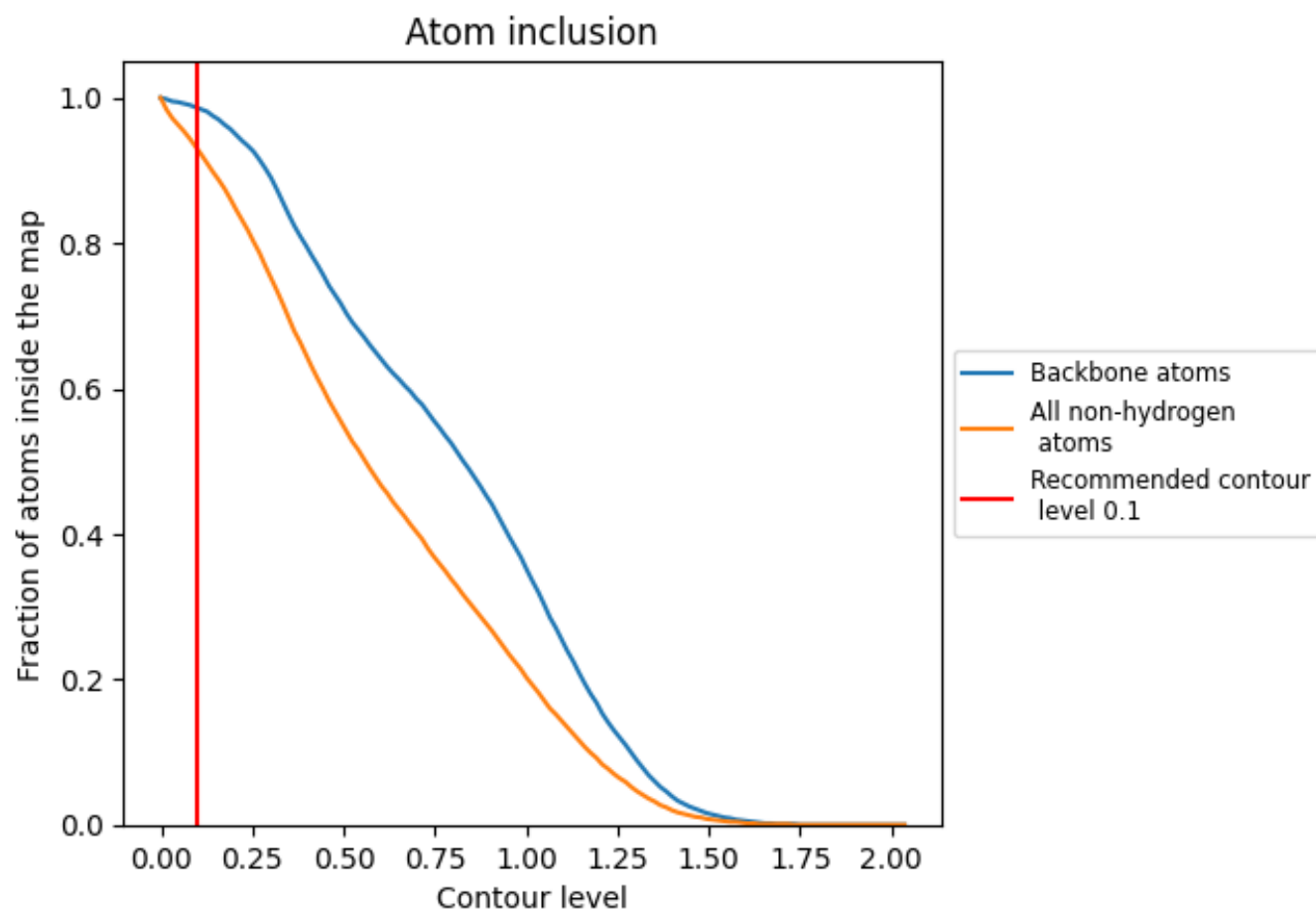
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% 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	 0.9290	 0.4400
A	 0.9330	 0.4450
B	 0.9330	 0.4480
C	 0.9310	 0.4440
D	 0.5710	 0.0090
E	 0.8970	 0.2520
F	 0.9640	 0.1910
G	 0.7690	 0.2930
H	 0.8720	 0.3180
I	 0.8930	 0.2650
J	 0.9490	 0.4690
K	 0.8720	 0.3470
L	 0.8420	 0.3880
M	 0.9490	 0.3990
N	 0.8970	 0.3670
O	 0.5000	 0.1210
P	 0.9740	 0.2700
Q	 0.9640	 0.1930
R	 0.7690	 0.2730
S	 0.8460	 0.3190
T	 0.7860	 0.2640
U	 0.9490	 0.4540
V	 0.8720	 0.3720
W	 0.8420	 0.4040
X	 0.9740	 0.4000
Y	 0.9230	 0.3850
Z	 0.5000	 0.0070
a	 0.9740	 0.2860
b	 0.9640	 0.2180
c	 0.7180	 0.2650
d	 0.8970	 0.3030
e	 0.7860	 0.2750
f	 0.9490	 0.4540
g	 0.8460	 0.3890
h	 0.8680	 0.4190



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Chain	Atom inclusion	Q-score
i	 0.9740	 0.4250
j	 0.9230	 0.4060