



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:57 PM UTC

PDB ID : 7N6U / pdb_00007n6u
EMDB ID : EMD-23860
Title : Structure of uncleaved HIV-1 JR-FL Env glycoprotein trimer in state U1
bound to small Molecule HIV-1 Entry Inhibitor BMS-378806
Authors : Zhang, S.; Wang, K.; Mao, Y.
Deposited on : 2021-06-09
Resolution : 4.10 Å(reported)

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

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

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

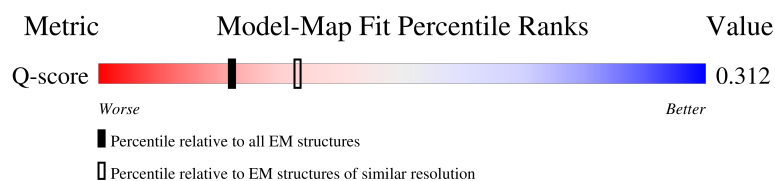
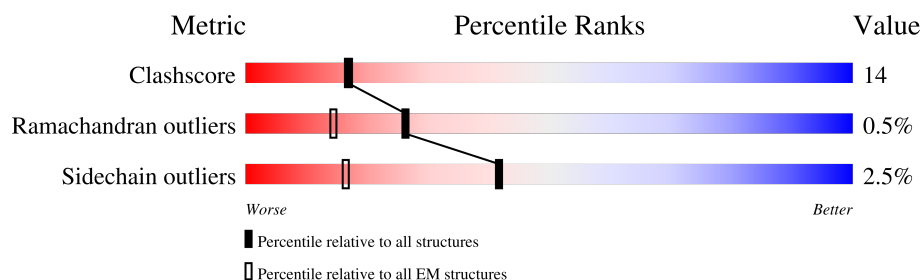
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	848	8% 48% 21% • 30%
1	B	848	9% 46% 23% • 30%
1	C	848	7% 46% 22% • 30%
2	D	2	50% 100%

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Mol	Chain	Length	Quality of chain
2	I	2	50% 100%
2	J	2	50% 100%
2	L	2	50% 50%
2	R	2	50% 100%
2	S	2	50% 100%
2	V	2	50% 50%
2	W	2	50% 100%
2	Z	2	50% 100%
2	a	2	50% 50%
2	d	2	50% 100%
2	g	2	50% 50%
2	h	2	50% 50%
2	j	2	50% 100%
2	m	2	50% 100%
2	n	2	50% 50%
2	o	2	50% 50%
2	q	2	50% 100%
2	r	2	100%
2	s	2	50% 50%
2	x	2	50% 50%
3	E	3	67% 33% 67%
3	F	3	33% 100%
3	H	3	33% 67% 33%
3	K	3	33% 67% 33%
3	M	3	67% 33% 67%

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Mol	Chain	Length	Quality of chain
3	N	3	
3	O	3	
3	Q	3	
3	X	3	
3	Y	3	
3	b	3	
3	c	3	
3	i	3	
3	k	3	
3	p	3	
3	t	3	
3	u	3	
3	y	3	
4	G	7	
4	U	7	
4	l	7	
4	v	7	
5	P	4	
5	T	4	
5	e	4	
6	f	3	
6	w	3	

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	N	2	-	-	X	-
3	NAG	O	1	-	-	X	-
3	NAG	Q	1	-	-	X	-
6	FUC	f	3	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16092 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	591	Total	C	N	O	S	0	0
			4686	2953	816	885	32		
1	B	595	Total	C	N	O	S	0	0
			4711	2967	820	892	32		
1	C	590	Total	C	N	O	S	0	0
			4673	2940	815	886	32		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q75760
A	?	-	ILE	deletion	UNP Q75760
A	?	-	ARG	deletion	UNP Q75760
A	5	GLU	LYS	conflict	UNP Q75760
A	6	LYS	SER	conflict	UNP Q75760
A	9	HIS	TYR	conflict	UNP Q75760
A	12	ARG	LYS	conflict	UNP Q75760
A	13	TRP	GLY	conflict	UNP Q75760
A	15	TRP	-	insertion	UNP Q75760
A	16	ARG	-	insertion	UNP Q75760
A	17	TRP	-	insertion	UNP Q75760
A	18	GLY	-	insertion	UNP Q75760
A	20	MET	LEU	conflict	UNP Q75760
A	24	MET	ILE	conflict	UNP Q75760
A	31	THR	VAL	conflict	UNP Q75760
A	508	SER	ARG	conflict	UNP Q75760
A	511	SER	ARG	conflict	UNP Q75760
A	752	SER	PHE	conflict	UNP Q75760
A	758	ASP	VAL	conflict	UNP Q75760
A	777	ILE	THR	conflict	UNP Q75760
A	792	ALA	VAL	conflict	UNP Q75760
A	829	VAL	ILE	conflict	UNP Q75760
A	832	VAL	ALA	conflict	UNP Q75760
A	833	VAL	LEU	conflict	UNP Q75760

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Chain	Residue	Modelled	Actual	Comment	Reference
A	835	GLY	ARG	conflict	UNP Q75760
A	836	ALA	THR	conflict	UNP Q75760
A	837	CYS	TYR	conflict	UNP Q75760
A	841	ARG	LEU	conflict	UNP Q75760
A	845	ARG	THR	conflict	UNP Q75760
A	854	ILE	ALA	conflict	UNP Q75760
B	?	-	GLY	deletion	UNP Q75760
B	?	-	ILE	deletion	UNP Q75760
B	?	-	ARG	deletion	UNP Q75760
B	5	GLU	LYS	conflict	UNP Q75760
B	6	LYS	SER	conflict	UNP Q75760
B	9	HIS	TYR	conflict	UNP Q75760
B	12	ARG	LYS	conflict	UNP Q75760
B	13	TRP	GLY	conflict	UNP Q75760
B	15	TRP	-	insertion	UNP Q75760
B	16	ARG	-	insertion	UNP Q75760
B	17	TRP	-	insertion	UNP Q75760
B	18	GLY	-	insertion	UNP Q75760
B	20	MET	LEU	conflict	UNP Q75760
B	24	MET	ILE	conflict	UNP Q75760
B	31	THR	VAL	conflict	UNP Q75760
B	508	SER	ARG	conflict	UNP Q75760
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B	835	GLY	ARG	conflict	UNP Q75760
B	836	ALA	THR	conflict	UNP Q75760
B	837	CYS	TYR	conflict	UNP Q75760
B	841	ARG	LEU	conflict	UNP Q75760
B	845	ARG	THR	conflict	UNP Q75760
B	854	ILE	ALA	conflict	UNP Q75760
C	?	-	GLY	deletion	UNP Q75760
C	?	-	ILE	deletion	UNP Q75760
C	?	-	ARG	deletion	UNP Q75760
C	5	GLU	LYS	conflict	UNP Q75760
C	6	LYS	SER	conflict	UNP Q75760
C	9	HIS	TYR	conflict	UNP Q75760

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Chain	Residue	Modelled	Actual	Comment	Reference
C	12	ARG	LYS	conflict	UNP Q75760
C	13	TRP	GLY	conflict	UNP Q75760
C	15	TRP	-	insertion	UNP Q75760
C	16	ARG	-	insertion	UNP Q75760
C	17	TRP	-	insertion	UNP Q75760
C	18	GLY	-	insertion	UNP Q75760
C	20	MET	LEU	conflict	UNP Q75760
C	24	MET	ILE	conflict	UNP Q75760
C	31	THR	VAL	conflict	UNP Q75760
C	508	SER	ARG	conflict	UNP Q75760
C	511	SER	ARG	conflict	UNP Q75760
C	752	SER	PHE	conflict	UNP Q75760
C	758	ASP	VAL	conflict	UNP Q75760
C	777	ILE	THR	conflict	UNP Q75760
C	792	ALA	VAL	conflict	UNP Q75760
C	829	VAL	ILE	conflict	UNP Q75760
C	832	VAL	ALA	conflict	UNP Q75760
C	833	VAL	LEU	conflict	UNP Q75760
C	835	GLY	ARG	conflict	UNP Q75760
C	836	ALA	THR	conflict	UNP Q75760
C	837	CYS	TYR	conflict	UNP Q75760
C	841	ARG	LEU	conflict	UNP Q75760
C	845	ARG	THR	conflict	UNP Q75760
C	854	ILE	ALA	conflict	UNP Q75760

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



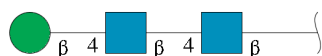
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		

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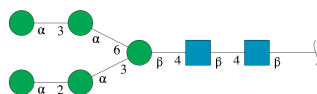
Mol	Chain	Residues	Atoms				AltConf	Trace
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	h	2	Total	C	N	O	0	0
			28	16	2	10		
2	j	2	Total	C	N	O	0	0
			28	16	2	10		
2	m	2	Total	C	N	O	0	0
			28	16	2	10		
2	n	2	Total	C	N	O	0	0
			28	16	2	10		
2	o	2	Total	C	N	O	0	0
			28	16	2	10		
2	q	2	Total	C	N	O	0	0
			28	16	2	10		
2	r	2	Total	C	N	O	0	0
			28	16	2	10		
2	s	2	Total	C	N	O	0	0
			28	16	2	10		
2	x	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called beta-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	F	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	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	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	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	b	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	i	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	p	3	Total	C	N	O	0	0
			39	22	2	15		
3	t	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	y	3	Total	C	N	O	0	0
			39	22	2	15		

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



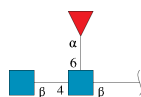
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	7	Total	C	N	O	0	0
			83	46	2	35		
4	U	7	Total	C	N	O	0	0
			83	46	2	35		
4	l	7	Total	C	N	O	0	0
			83	46	2	35		
4	v	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



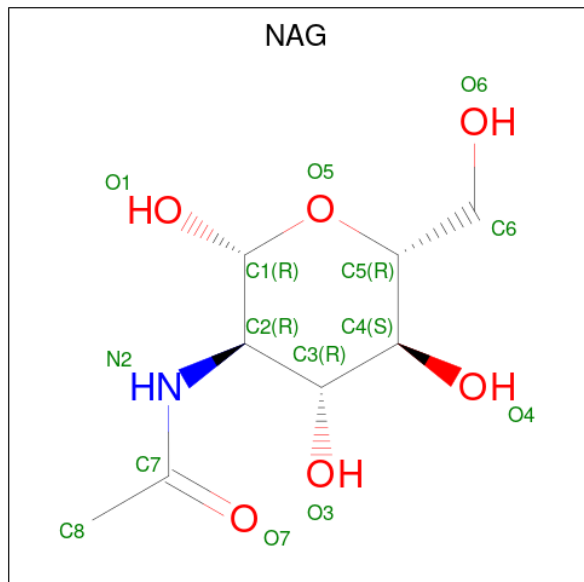
Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	4	Total	C	N	O	0	0
			50	28	2	20		
5	T	4	Total	C	N	O	0	0
			50	28	2	20		
5	e	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 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.



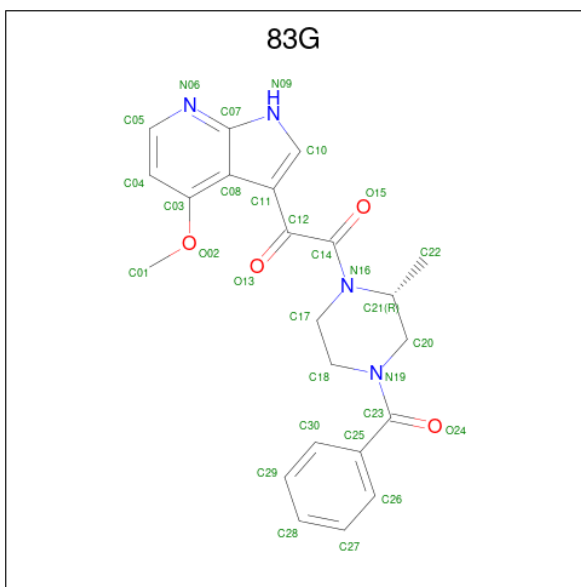
Mol	Chain	Residues	Atoms				AltConf	Trace
6	f	3	Total	C	N	O	0	0
			38	22	2	14		
6	w	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is 1-[(2R)-4-(benzenecarbonyl)-2-methylpiperazin-1-yl]-2-(4-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)ethane-1,2-dione (CCD ID: 83G) (formula: $C_{22}H_{22}N_4O_4$) (labeled as "Ligand of Interest" by depositor).

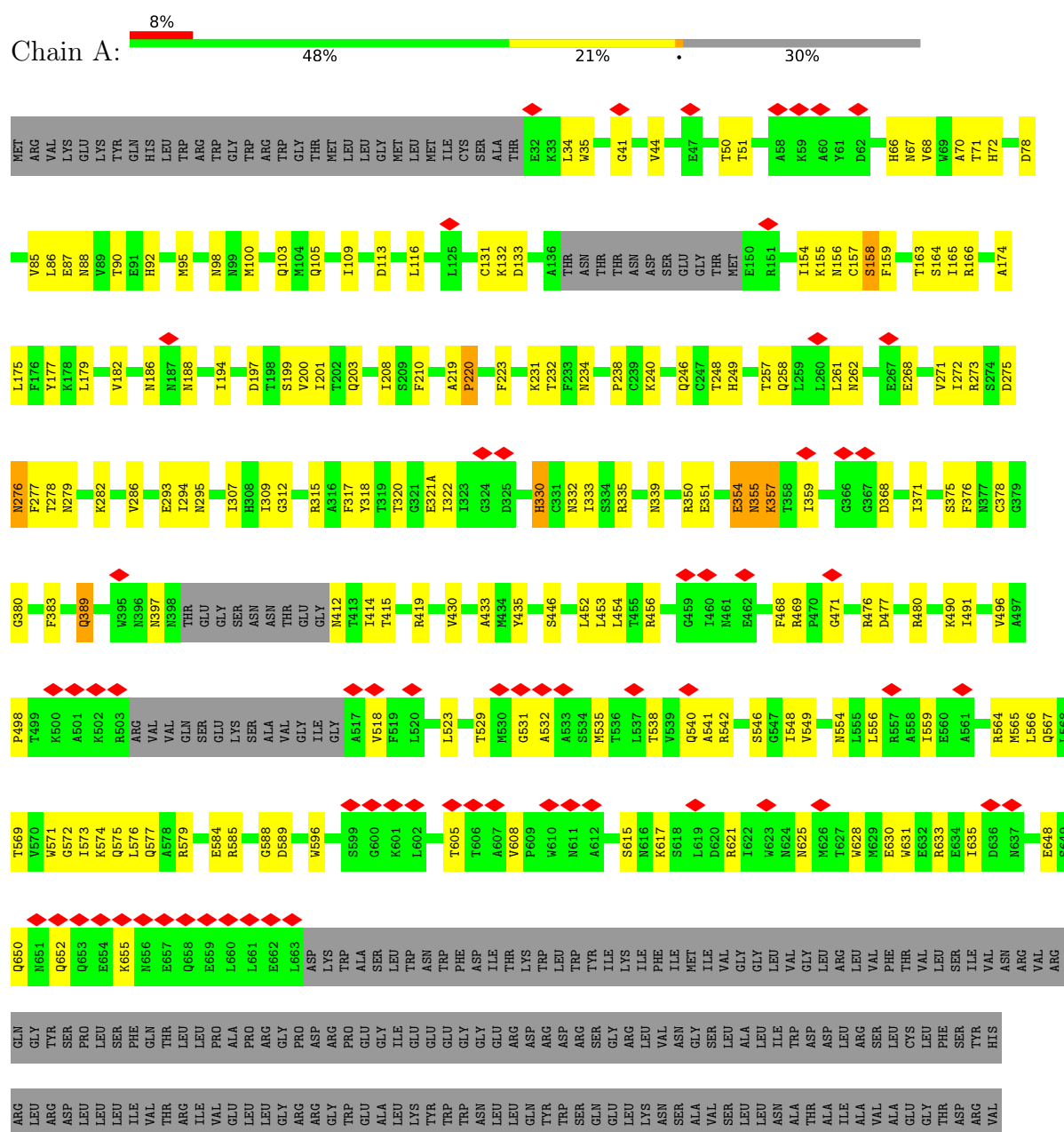


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			30	22	4	4	
8	B	1	Total	C	N	O	0
			30	22	4	4	
8	C	1	Total	C	N	O	0
			30	22	4	4	

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.

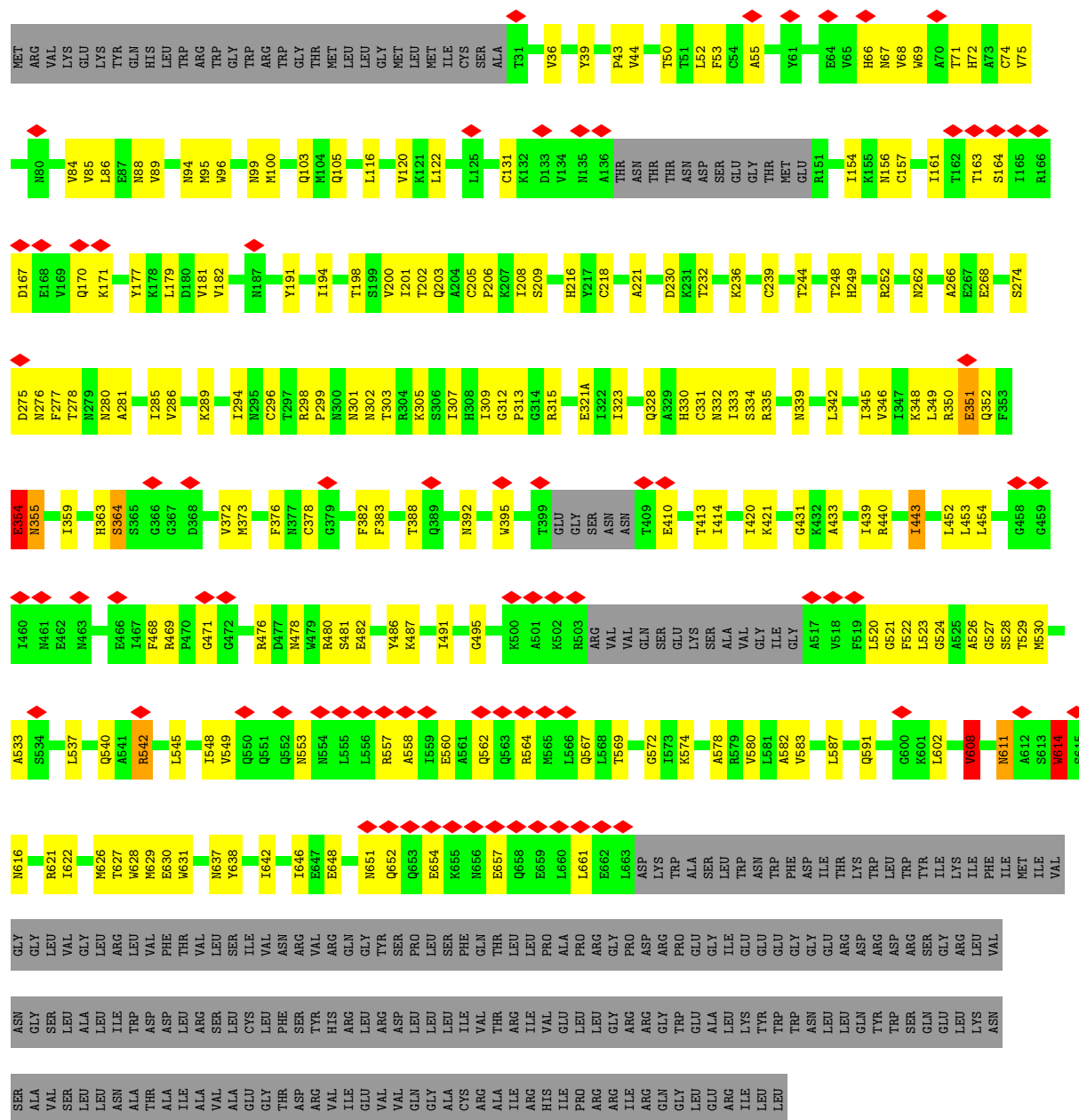
• Molecule 1: Envelope glycoprotein gp160



ILE
GLU
VAL
VAL
GLN
GLY
ALA
CYS
ARG
ALA
ILE
ARG
HIS
ILE
PRO
ARG
ARG
ILE
GLN
GLY
GLU
ARG
ILE
LEU

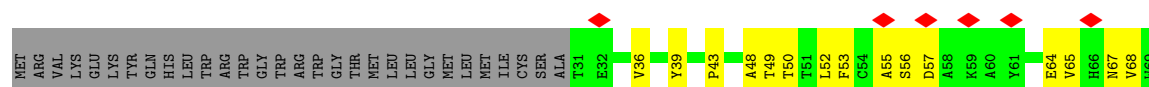
• Molecule 1: Envelope glycoprotein gp160

Chain B: 9% 46% 23% 30%



• Molecule 1: Envelope glycoprotein gp160

Chain C: 7% 46% 22% 30%



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



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



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



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



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



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



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



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



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



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



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



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





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



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

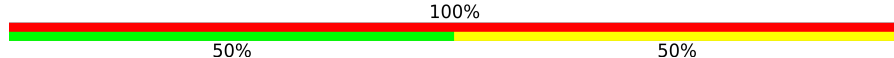


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s: 



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

Chain x: 



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

Chain E: 

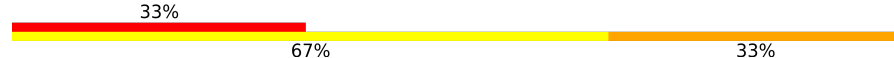


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 



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

Chain H: 



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

Chain K: 



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



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



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



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



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



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



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

Chain b: 



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

Chain c: 



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

Chain i: 



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

Chain k: 

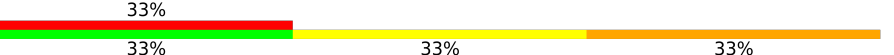


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p: 



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

Chain t: 



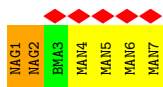
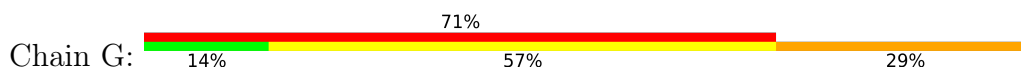
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



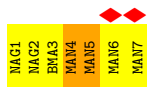
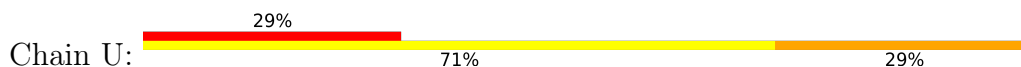
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



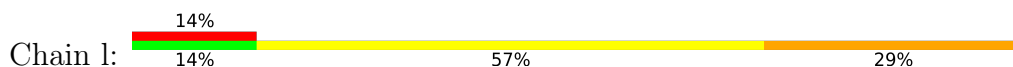
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



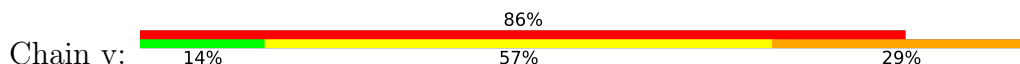
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



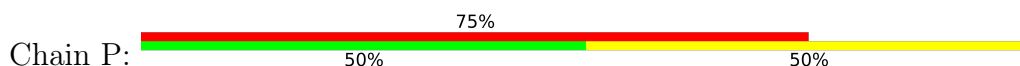
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



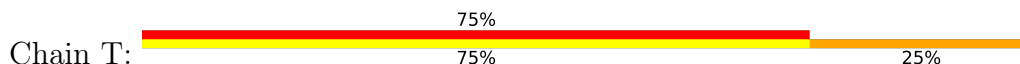
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



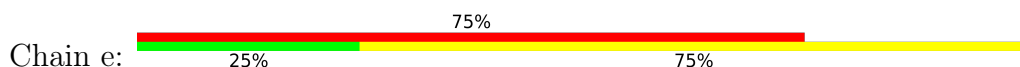
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123372	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	230.16, 230.16, 230.16	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN, 83G, 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	0.42	0/4779	0.79	7/6487 (0.1%)
1	B	0.48	2/4804 (0.0%)	0.82	10/6522 (0.2%)
1	C	0.44	0/4765	0.85	14/6468 (0.2%)
All	All	0.45	2/14348 (0.0%)	0.82	31/19477 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	GLU	C-O	-5.62	1.17	1.24
1	B	608	VAL	N-CA	5.57	1.50	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	GLU	CA-C-N	9.86	135.92	119.35
1	B	354	GLU	C-N-CA	9.86	135.92	119.35
1	B	392	ASN	N-CA-C	-9.41	98.65	111.55
1	A	165	ILE	N-CA-C	-8.12	104.79	112.83
1	C	301	ASN	CA-CB-CG	8.02	120.62	112.60
1	C	53	PHE	CB-CA-C	-7.73	96.60	110.36
1	C	637	ASN	N-CA-CB	-7.02	105.06	111.59
1	A	430	VAL	N-CA-C	-6.93	106.55	113.20
1	C	637	ASN	CB-CA-C	-6.88	106.50	116.54
1	C	53	PHE	CA-CB-CG	6.58	120.39	113.80
1	B	614	TRP	N-CA-CB	6.46	119.34	109.98
1	C	543	LEU	CA-C-N	6.42	130.45	120.82
1	C	543	LEU	C-N-CA	6.42	130.45	120.82
1	B	637	ASN	CA-CB-CG	-6.40	106.20	112.60
1	B	392	ASN	CB-CA-C	6.17	119.35	111.40
1	A	275	ASP	N-CA-C	-6.05	104.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	637	ASN	CA-CB-CG	-6.00	106.60	112.60
1	A	276	ASN	CA-CB-CG	-5.96	106.64	112.60
1	B	364	SER	N-CA-C	5.55	117.79	111.02
1	A	354	GLU	CA-C-O	-5.49	115.34	122.14
1	B	392	ASN	CA-CB-CG	5.39	118.00	112.60
1	C	173	TYR	N-CA-C	-5.38	101.11	109.72
1	B	611	ASN	CA-CB-CG	5.29	117.89	112.60
1	C	230	ASP	N-CA-C	-5.28	102.10	109.96
1	C	553	ASN	CA-C-N	5.26	131.59	121.54
1	C	553	ASN	C-N-CA	5.26	131.59	121.54
1	B	354	GLU	CA-C-O	-5.15	113.15	120.51
1	A	116	LEU	CA-C-N	5.05	129.55	121.62
1	A	116	LEU	C-N-CA	5.05	129.55	121.62
1	C	474	ASP	CA-C-N	5.03	131.15	121.54
1	C	474	ASP	C-N-CA	5.03	131.15	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4686	0	4604	126	0
1	B	4711	0	4622	158	0
1	C	4673	0	4579	120	0
2	D	28	0	25	4	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	L	28	0	25	1	0
2	R	28	0	25	2	0
2	S	28	0	25	2	0
2	V	28	0	25	4	0
2	W	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	1	0
2	d	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	g	28	0	25	2	0
2	h	28	0	25	1	0
2	j	28	0	25	2	0
2	m	28	0	25	3	0
2	n	28	0	25	0	0
2	o	28	0	25	2	0
2	q	28	0	25	0	0
2	r	28	0	25	1	0
2	s	28	0	25	2	0
2	x	28	0	25	0	0
3	E	39	0	34	1	0
3	F	39	0	34	2	0
3	H	39	0	34	7	0
3	K	39	0	34	0	0
3	M	39	0	34	2	0
3	N	39	0	34	8	0
3	O	39	0	34	12	0
3	Q	39	0	34	9	0
3	X	39	0	34	6	0
3	Y	39	0	34	2	0
3	b	39	0	34	2	0
3	c	39	0	34	1	0
3	i	39	0	34	1	0
3	k	39	0	34	1	0
3	p	39	0	34	1	0
3	t	39	0	34	2	0
3	u	39	0	34	0	0
3	y	39	0	34	2	0
4	G	83	0	70	5	0
4	U	83	0	70	6	0
4	l	83	0	70	3	0
4	v	83	0	70	2	0
5	P	50	0	43	2	0
5	T	50	0	43	2	0
5	e	50	0	43	2	0
6	f	38	0	34	6	0
6	w	38	0	34	0	0
7	A	56	0	52	6	0
7	B	14	0	13	2	0
7	C	14	0	13	1	0
8	A	30	0	0	0	0
8	B	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	30	0	0	1	0
All	All	16092	0	15497	439	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 14.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:TRP:CE3	6:f:3:FUC:H62	1.94	1.01
1:B:388:THR:HG21	3:c:1:NAG:H5	1.45	0.96
1:A:446:SER:O	4:G:2:NAG:O7	1.87	0.92
1:B:528:SER:CB	3:Q:1:NAG:O5	2.23	0.86
1:C:323:ILE:HG21	2:o:1:NAG:O6	1.76	0.85
3:N:2:NAG:H82	3:O:1:NAG:C8	2.06	0.85
1:B:614:TRP:CE3	6:f:3:FUC:C6	2.63	0.82
1:C:227:LYS:HE2	1:C:229:ASN:HD21	1.45	0.82
1:A:378:CYS:SG	4:G:1:NAG:O3	2.39	0.81
3:N:2:NAG:C8	3:O:1:NAG:H83	2.12	0.80
1:B:528:SER:HB3	3:Q:1:NAG:O5	1.84	0.78
1:B:528:SER:OG	3:Q:1:NAG:H2	1.84	0.77
1:A:293:GLU:OE1	5:P:1:NAG:O6	2.03	0.76
1:B:439:ILE:HG23	4:U:5:MAN:O6	1.87	0.74
3:N:2:NAG:H82	3:O:1:NAG:H83	1.70	0.73
1:B:84:VAL:HG21	1:B:521:GLY:HA3	1.69	0.73
3:N:2:NAG:C8	3:O:1:NAG:C8	2.68	0.71
1:A:85:VAL:HG11	3:F:1:NAG:O3	1.90	0.71
1:B:55:ALA:HB3	1:B:216:HIS:HB2	1.74	0.70
1:C:86:LEU:H	1:C:243:SER:HA	1.58	0.69
3:O:2:NAG:H3	3:O:3:BMA:O5	1.92	0.69
1:A:51:THR:HA	1:A:103:GLN:HE22	1.58	0.69
1:B:621:ARG:HH22	2:g:1:NAG:C7	2.06	0.68
1:B:302:ASN:HB2	1:B:440:ARG:HA	1.76	0.68
1:C:323:ILE:HG21	2:o:1:NAG:HO6	1.57	0.68
6:f:2:NAG:N2	6:f:3:FUC:O2	2.27	0.68
1:A:86:LEU:HB3	1:A:523:LEU:HD12	1.76	0.67
1:A:279:ASN:HB2	3:H:1:NAG:O5	1.93	0.67
1:C:294:ILE:HD11	1:C:331:CYS:HB3	1.76	0.67
1:B:346:VAL:HG13	1:B:359:ILE:HD13	1.74	0.67
1:C:429:GLU:HG3	1:C:431:GLY:H	1.59	0.67
1:B:262:ASN:OD1	5:e:1:NAG:H83	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ILE:HG12	3:X:1:NAG:H83	1.76	0.66
3:O:2:NAG:C3	3:O:3:BMA:O5	2.44	0.66
1:B:182:VAL:HG23	1:B:194:ILE:HG12	1.78	0.65
1:C:65:VAL:O	1:C:72:HIS:ND1	2.29	0.65
1:B:85:VAL:HG11	5:T:1:NAG:H61	1.77	0.65
1:C:227:LYS:HE2	1:C:229:ASN:ND2	2.11	0.64
4:v:3:BMA:H4	4:v:6:MAN:H5	1.80	0.63
1:A:596:TRP:O	1:A:650:GLN:NE2	2.32	0.63
3:H:1:NAG:H5	3:H:2:NAG:HN2	1.64	0.63
1:B:621:ARG:HH12	2:g:1:NAG:H2	1.63	0.63
3:F:1:NAG:H83	3:F:2:NAG:H2	1.80	0.62
1:B:105:GLN:HG3	1:B:476:ARG:HG2	1.81	0.62
1:B:383:PHE:HA	1:B:420:ILE:HG22	1.80	0.62
1:A:154:ILE:HD13	1:A:177:TYR:HB3	1.80	0.62
1:B:67:ASN:HB3	1:B:208:ILE:HA	1.82	0.62
1:B:614:TRP:CD2	6:f:3:FUC:H62	2.34	0.62
1:C:156:ASN:HB2	3:i:1:NAG:O7	1.98	0.62
1:A:158:SER:HB3	2:D:1:NAG:H81	1.81	0.62
1:C:305:LYS:HG3	1:C:321:GLY:HA2	1.81	0.62
1:A:564:ARG:HH22	1:B:52:LEU:HD23	1.64	0.62
1:A:354:GLU:HA	7:A:903:NAG:H81	1.82	0.61
1:B:528:SER:OG	3:Q:1:NAG:O5	2.18	0.61
1:A:454:LEU:HD11	1:A:468:PHE:HB3	1.81	0.61
1:A:258:GLN:NE2	1:A:371:ILE:O	2.34	0.61
1:B:350:ARG:HG2	1:B:355:ASN:HA	1.82	0.61
7:B:901:NAG:C1	7:B:901:NAG:O7	2.48	0.61
3:N:2:NAG:H82	3:O:1:NAG:H82	1.82	0.61
3:O:2:NAG:O3	3:O:3:BMA:C1	2.47	0.61
2:j:1:NAG:O3	2:j:2:NAG:O5	2.19	0.60
1:A:286:VAL:HB	1:A:452:LEU:H	1.67	0.60
1:C:426:MET:HB2	1:C:432:LYS:HB2	1.82	0.60
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.83	0.60
1:C:639:THR:C	1:C:641:GLU:H	2.09	0.60
1:A:577:GLN:HE22	1:C:566:LEU:HD13	1.66	0.60
1:B:614:TRP:CZ3	6:f:3:FUC:H62	2.35	0.60
1:A:272:ILE:HG13	1:A:286:VAL:HA	1.84	0.59
1:B:528:SER:OG	3:Q:1:NAG:C1	2.50	0.59
1:B:528:SER:OG	3:Q:1:NAG:C2	2.49	0.59
1:C:299:PRO:O	1:C:442:GLN:NE2	2.36	0.59
1:A:67:ASN:O	1:A:70:ALA:N	2.36	0.59
1:B:616:ASN:ND2	7:B:901:NAG:O7	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:MET:O	1:A:480:ARG:NH1	2.36	0.59
1:B:99:ASN:OD1	1:B:103:GLN:NE2	2.34	0.59
1:B:266:ALA:HB3	1:B:289:LYS:HA	1.85	0.58
4:v:1:NAG:H3	4:v:1:NAG:H83	1.85	0.58
1:B:564:ARG:HG3	1:B:567:GLN:HA	1.85	0.58
1:C:265:LEU:HD11	1:C:291:SER:HB3	1.84	0.58
1:B:627:THR:HG22	1:B:629:MET:H	1.68	0.58
1:B:530:MET:HG3	1:B:627:THR:HA	1.85	0.58
1:A:163:THR:HB	1:A:309:ILE:HA	1.85	0.58
1:A:330:HIS:HB2	1:A:415:THR:HG23	1.85	0.58
1:B:372:VAL:HG13	1:B:373:MET:HG3	1.86	0.58
1:C:98:ASN:ND2	1:C:486:TYR:O	2.37	0.58
2:S:1:NAG:O3	2:S:2:NAG:O5	2.20	0.58
1:C:256:SER:OG	1:C:478:ASN:ND2	2.37	0.57
1:A:279:ASN:CG	3:H:2:NAG:H82	2.28	0.57
1:A:576:LEU:HA	1:A:579:ARG:HE	1.69	0.57
1:C:652:GLN:O	1:C:656:ASN:ND2	2.38	0.57
1:B:209:SER:HB2	4:U:4:MAN:O6	2.04	0.57
2:r:1:NAG:H62	2:r:2:NAG:HN2	1.70	0.57
1:C:359:ILE:HA	1:C:466:GLU:HB2	1.86	0.57
1:B:286:VAL:HB	1:B:452:LEU:H	1.70	0.57
1:B:52:LEU:H	1:B:574:LYS:HZ1	1.53	0.57
1:B:549:VAL:HG12	1:B:553:ASN:HD22	1.70	0.56
1:A:628:TRP:HD1	1:A:630:GLU:HB2	1.69	0.56
1:C:49:THR:HG22	1:C:99:ASN:HD22	1.69	0.56
1:C:334:SER:HA	1:C:413:THR:HA	1.87	0.56
4:U:1:NAG:C6	5:e:1:NAG:H81	2.35	0.56
1:C:229:ASN:HB2	3:k:1:NAG:O5	2.05	0.56
1:B:335:ARG:NH2	1:B:410:GLU:O	2.38	0.56
1:B:351:GLU:HA	2:a:1:NAG:H81	1.88	0.56
1:A:276:ASN:HB3	1:A:282:LYS:HG3	1.86	0.56
1:C:426:MET:HG2	1:C:429:GLU:HB3	1.87	0.56
1:C:371:ILE:HG23	1:C:472:GLY:HA3	1.87	0.56
1:A:354:GLU:HA	7:A:903:NAG:C8	2.36	0.56
1:B:294:ILE:HG22	1:B:333:ILE:HB	1.88	0.56
1:B:548:ILE:HD12	1:B:582:ALA:HB1	1.88	0.56
1:B:627:THR:HB	1:B:630:GLU:HG3	1.88	0.56
1:A:312:GLY:H	1:A:315:ARG:HB2	1.70	0.55
1:C:235:GLY:HA2	1:C:273:ARG:HH11	1.71	0.55
1:C:577:GLN:HA	1:C:580:VAL:HG12	1.88	0.55
1:A:210:PHE:HB2	1:A:380:GLY:HA2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:VAL:HB	1:C:449:ILE:HB	1.89	0.55
1:B:88:ASN:ND2	3:Q:1:NAG:O7	2.40	0.55
1:B:96:TRP:O	1:B:480:ARG:NH2	2.40	0.55
1:A:278:THR:OG1	3:H:1:NAG:N2	2.33	0.54
1:A:469:ARG:NH2	3:M:1:NAG:O5	2.40	0.54
1:A:66:HIS:HB2	1:A:208:ILE:HD12	1.89	0.54
1:B:346:VAL:HG13	1:B:359:ILE:CD1	2.37	0.54
1:C:113:ASP:OD1	8:C:902:83G:N09	2.41	0.54
1:A:565:MET:HE3	1:A:566:LEU:HG	1.90	0.54
1:C:70:ALA:HB1	1:C:111:LEU:HB3	1.89	0.54
1:B:528:SER:HB2	3:Q:1:NAG:O6	2.07	0.54
1:B:334:SER:HA	1:B:413:THR:HA	1.89	0.54
1:C:374:HIS:HB3	1:C:385:CYS:HB2	1.88	0.54
1:C:64:GLU:HG2	1:C:67:ASN:HB2	1.90	0.54
1:B:249:HIS:ND1	1:B:486:TYR:OH	2.41	0.53
1:B:354:GLU:O	1:B:355:ASN:ND2	2.40	0.53
1:B:280:ASN:OD1	2:V:1:NAG:H82	2.08	0.53
1:C:159:PHE:HB2	1:C:172:GLU:HB2	1.90	0.53
1:C:230:ASP:HB2	1:C:241:ASN:HB2	1.91	0.53
1:A:585:ARG:NH1	1:A:589:ASP:OD2	2.41	0.53
1:C:597:GLY:HA3	1:C:650:GLN:HE22	1.74	0.53
1:B:68:VAL:O	1:B:72:HIS:N	2.40	0.53
1:C:43:PRO:HB3	1:C:523:LEU:HD12	1.91	0.53
1:C:312:GLY:H	1:C:315:ARG:HB2	1.73	0.53
1:B:156:ASN:ND2	2:R:1:NAG:O7	2.42	0.53
1:B:181:VAL:HB	1:B:191:TYR:HB3	1.90	0.53
1:C:131:CYS:HA	1:C:157:CYS:HA	1.90	0.53
3:y:1:NAG:C1	3:y:1:NAG:O7	2.57	0.53
1:B:244:THR:HG21	1:B:522:PHE:HB2	1.91	0.53
2:D:1:NAG:O3	2:D:2:NAG:O5	2.26	0.53
2:R:1:NAG:H61	2:R:2:NAG:HN2	1.72	0.53
1:B:648:GLU:O	1:B:652:GLN:N	2.41	0.53
1:A:71:THR:OG1	1:A:571:TRP:NE1	2.40	0.52
1:A:538:THR:O	1:A:542:ARG:N	2.42	0.52
1:C:39:TYR:N	1:C:495:GLY:O	2.41	0.52
1:C:387:SER:HA	1:C:416:LEU:HD11	1.90	0.52
1:A:279:ASN:H	3:H:1:NAG:C1	2.22	0.52
1:C:565:MET:HG3	1:C:568:LEU:HD23	1.91	0.52
1:B:276:ASN:OD1	2:V:1:NAG:C2	2.55	0.52
1:A:92:HIS:HA	1:A:238:PRO:HA	1.91	0.52
1:A:309:ILE:HB	1:A:315:ARG:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ARG:C	1:B:352:GLN:N	2.67	0.52
1:B:587:LEU:O	1:B:591:GLN:N	2.42	0.52
1:C:114:GLN:HG2	1:C:570:VAL:HG11	1.91	0.52
1:C:285:ILE:HG12	1:C:453:LEU:HG	1.91	0.52
1:A:182:VAL:HB	1:A:194:ILE:HG22	1.92	0.52
1:C:184:ILE:H	1:C:190:SER:HB3	1.75	0.52
1:A:376:PHE:O	1:A:383:PHE:N	2.39	0.52
1:A:573:ILE:HG21	1:C:567:GLN:HG3	1.92	0.51
1:A:596:TRP:HA	1:A:650:GLN:HG2	1.92	0.51
1:B:528:SER:CB	3:Q:1:NAG:O6	2.58	0.51
1:B:94:ASN:OD1	1:B:236:LYS:NZ	2.44	0.51
1:B:323:ILE:CG1	3:X:1:NAG:H83	2.41	0.51
1:B:342:LEU:HA	1:B:345:ILE:HD12	1.93	0.51
1:A:548:ILE:HG22	1:A:549:VAL:HG23	1.93	0.51
1:B:36:VAL:HG11	1:B:646:ILE:HD13	1.93	0.51
1:A:234:ASN:HA	1:A:273:ARG:HG2	1.91	0.51
1:C:65:VAL:HG12	1:C:73:ALA:HB3	1.91	0.51
1:A:133:ASP:HA	1:A:155:LYS:HA	1.93	0.51
1:A:454:LEU:HA	1:A:471:GLY:H	1.76	0.51
1:C:522:PHE:O	1:C:540:GLN:NE2	2.39	0.51
3:M:1:NAG:H61	3:M:2:NAG:C7	2.40	0.51
1:B:520:LEU:HB3	1:B:524:GLY:HA3	1.92	0.51
1:C:555:LEU:HA	1:C:558:ALA:HB3	1.93	0.51
1:A:652:GLN:HA	1:A:655:LYS:HE3	1.92	0.51
1:C:130:ASN:HA	1:C:189:THR:HB	1.94	0.50
1:A:538:THR:HA	1:A:541:ALA:HB3	1.92	0.50
1:B:350:ARG:C	1:B:352:GLN:H	2.19	0.50
1:B:85:VAL:HG11	5:T:1:NAG:C6	2.41	0.50
1:A:159:PHE:HE1	1:A:174:ALA:HB2	1.77	0.50
1:B:350:ARG:CG	1:B:355:ASN:HA	2.41	0.50
1:B:558:ALA:O	1:B:562:GLN:N	2.44	0.50
1:B:221:ALA:HB1	1:B:545:LEU:HA	1.93	0.50
1:B:309:ILE:HB	1:B:315:ARG:HG3	1.94	0.50
1:B:478:ASN:O	1:B:481:SER:OG	2.29	0.50
1:C:184:ILE:HG13	1:C:188:ASN:HD22	1.77	0.50
1:C:181:VAL:HB	1:C:191:TYR:HB3	1.93	0.50
1:C:286:VAL:HG21	1:C:345:ILE:HD11	1.94	0.50
1:A:571:TRP:O	1:A:575:GLN:N	2.42	0.49
1:B:622:ILE:HA	1:B:626:MET:HG2	1.93	0.49
1:C:50:THR:O	1:C:103:GLN:NE2	2.39	0.49
1:B:163:THR:OG1	1:B:164:SER:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:LEU:HA	1:B:471:GLY:H	1.77	0.49
3:y:1:NAG:O3	3:y:2:NAG:O5	2.25	0.49
1:B:651:ASN:HA	1:B:654:GLU:HB2	1.94	0.49
1:B:574:LYS:O	1:B:578:ALA:N	2.46	0.49
1:C:386:ASN:CG	3:t:1:NAG:C7	2.85	0.49
1:A:279:ASN:HB2	3:H:1:NAG:C1	2.42	0.49
1:C:198:THR:OG1	1:C:199:SER:N	2.46	0.49
1:A:87:GLU:OE2	7:A:901:NAG:O5	2.31	0.49
1:A:615:SER:O	1:A:617:LYS:NZ	2.35	0.49
1:B:120:VAL:HG22	1:B:203:GLN:HE21	1.76	0.49
1:C:52:LEU:HD22	1:C:217:TYR:HB3	1.95	0.48
1:C:55:ALA:HB1	1:C:78:ASP:HB2	1.94	0.48
1:B:43:PRO:HB3	1:B:540:GLN:HG2	1.94	0.48
1:B:301:ASN:HB2	1:B:323:ILE:HB	1.94	0.48
1:B:537:LEU:HB2	1:B:602:LEU:HD21	1.96	0.48
1:B:608:VAL:HG11	1:B:646:ILE:HG12	1.93	0.48
1:B:39:TYR:O	1:B:495:GLY:N	2.40	0.48
1:C:175:LEU:HB2	1:C:320:THR:HB	1.95	0.48
1:C:288:LEU:HD23	1:C:451:GLY:HA2	1.94	0.48
3:N:1:NAG:H61	3:N:2:NAG:H82	1.96	0.48
1:C:574:LYS:O	1:C:578:ALA:N	2.41	0.48
1:C:637:ASN:HB3	1:C:638:TYR:H	1.37	0.48
1:B:100:MET:SD	1:B:100:MET:N	2.87	0.48
1:B:116:LEU:HD11	1:B:202:THR:HB	1.95	0.48
1:C:386:ASN:OD1	3:t:1:NAG:C7	2.62	0.48
1:B:280:ASN:HD21	2:V:1:NAG:H83	1.79	0.48
1:C:303:THR:OG1	1:C:321(A):GLU:N	2.47	0.48
1:A:223:PHE:HB3	1:A:490:LYS:HD2	1.96	0.47
1:A:376:PHE:N	1:A:383:PHE:O	2.43	0.47
1:B:179:LEU:HB3	1:B:421:LYS:HE2	1.95	0.47
1:C:227:LYS:O	1:C:243:SER:OG	2.28	0.47
1:B:285:ILE:HG22	1:B:453:LEU:HG	1.97	0.47
1:B:342:LEU:HB3	1:B:395:TRP:HZ2	1.78	0.47
1:B:364:SER:HA	1:B:469:ARG:HB3	1.95	0.47
1:B:378:CYS:HB2	4:U:2:NAG:H62	1.96	0.47
1:C:559:ILE:O	1:C:562:GLN:NE2	2.46	0.47
1:B:530:MET:HE3	1:B:627:THR:HG23	1.96	0.47
1:C:182:VAL:HG23	1:C:194:ILE:HG12	1.97	0.47
1:A:567:GLN:HA	1:A:572:GLY:HA3	1.96	0.47
1:C:568:LEU:HD12	1:C:570:VAL:H	1.80	0.47
1:C:295:ASN:HA	1:C:446:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ALA:O	1:C:99:ASN:ND2	2.48	0.47
1:C:192:ARG:NH2	1:C:197:ASP:OD2	2.48	0.47
1:C:299:PRO:HD3	1:C:329:ALA:HA	1.96	0.47
3:X:1:NAG:O7	3:X:1:NAG:O3	2.24	0.47
1:A:86:LEU:HD22	1:A:523:LEU:HB3	1.97	0.47
1:A:531:GLY:HA2	1:A:535:MET:HG2	1.96	0.47
1:C:129:LEU:HD12	1:C:192:ARG:HA	1.97	0.47
1:C:155:LYS:O	1:C:176:PHE:N	2.45	0.47
1:A:199:SER:OG	1:A:200:VAL:N	2.48	0.46
1:C:210:PHE:HB2	1:C:380:GLY:HA2	1.97	0.46
1:C:564:ARG:O	1:C:567:GLN:NE2	2.38	0.46
1:A:397:ASN:OD1	7:A:904:NAG:N2	2.48	0.46
1:B:209:SER:CB	4:U:4:MAN:O6	2.63	0.46
1:B:313:PRO:HB3	1:C:125:LEU:HD12	1.98	0.46
1:B:346:VAL:O	1:B:350:ARG:HG3	2.15	0.46
1:C:478:ASN:O	1:C:481:SER:OG	2.24	0.46
1:A:564:ARG:NH1	1:B:50:THR:O	2.48	0.46
1:A:584:GLU:O	1:A:588:GLY:N	2.45	0.46
1:B:74:CYS:N	1:B:560:GLU:OE2	2.48	0.46
1:B:202:THR:OG1	1:B:433:ALA:O	2.33	0.46
1:B:481:SER:OG	1:B:482:GLU:N	2.49	0.46
1:C:300:ASN:OD1	1:C:300:ASN:N	2.47	0.46
1:A:232:THR:HA	1:A:271:VAL:HG21	1.97	0.46
1:B:301:ASN:CG	3:X:1:NAG:N2	2.72	0.46
1:B:303:THR:HB	1:B:321(A):GLU:H	1.81	0.46
1:A:223:PHE:HA	1:A:491:ILE:HG12	1.96	0.46
1:B:75:VAL:HG12	1:B:560:GLU:HG3	1.97	0.46
1:A:105:GLN:OE1	1:A:476:ARG:NE	2.49	0.46
1:A:179:LEU:HD11	1:A:419:ARG:HD3	1.98	0.46
1:C:258:GLN:HB2	1:C:374:HIS:HD2	1.80	0.46
1:A:131:CYS:HA	1:A:157:CYS:HA	1.96	0.46
1:A:339:ASN:OD1	2:L:1:NAG:C7	2.63	0.46
1:B:74:CYS:SG	1:B:75:VAL:N	2.88	0.45
1:B:529:THR:O	1:B:533:ALA:N	2.49	0.45
1:C:209:SER:OG	1:C:210:PHE:N	2.49	0.45
1:C:350:ARG:HB3	1:C:355:ASN:HA	1.97	0.45
1:A:279:ASN:CB	3:H:2:NAG:H82	2.46	0.45
1:A:518:VAL:HG23	1:A:540:GLN:HE22	1.81	0.45
4:G:1:NAG:H62	5:P:1:NAG:O7	2.16	0.45
1:A:354:GLU:O	1:A:355:ASN:C	2.59	0.45
1:B:86:LEU:HD13	1:B:86:LEU:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ASN:OD1	1:C:234:ASN:N	2.49	0.45
1:C:616:ASN:OD1	7:C:901:NAG:O5	2.28	0.45
1:B:275:ASP:O	1:B:278:THR:OG1	2.34	0.45
1:B:354:GLU:C	1:B:355:ASN:ND2	2.74	0.45
1:C:163:THR:OG1	1:C:309:ILE:O	2.26	0.45
1:A:87:GLU:OE2	7:A:901:NAG:C6	2.65	0.45
1:A:158:SER:HB3	2:D:1:NAG:C8	2.45	0.45
1:A:605:THR:HA	1:A:608:VAL:HG22	1.97	0.45
1:B:95:MET:HG3	1:B:96:TRP:CD1	2.51	0.45
1:A:332:ASN:HA	1:A:414:ILE:HG22	1.97	0.45
1:C:383:PHE:HB3	1:C:420:ILE:HG12	1.99	0.45
1:A:109:ILE:O	1:A:113:ASP:N	2.49	0.45
1:A:132:LYS:O	1:A:156:ASN:N	2.50	0.45
4:l:5:MAN:O6	4:l:5:MAN:O4	2.26	0.45
1:A:90:THR:HG22	1:A:240:LYS:HG3	1.99	0.44
1:A:257:THR:HG22	1:A:375:SER:HB3	1.98	0.44
1:A:219:ALA:O	1:A:246:GLN:NE2	2.50	0.44
1:A:648:GLU:O	1:A:652:GLN:N	2.47	0.44
1:B:305:LYS:HE3	1:B:307:ILE:HD11	1.98	0.44
1:B:323:ILE:HG13	3:X:1:NAG:N2	2.32	0.44
1:C:36:VAL:HG12	1:C:608:VAL:HB	1.99	0.44
3:N:2:NAG:H83	3:O:1:NAG:H83	1.96	0.44
2:h:1:NAG:H62	2:h:2:NAG:N2	2.32	0.44
2:m:1:NAG:O6	2:m:2:NAG:N2	2.49	0.44
1:B:200:VAL:HA	1:B:433:ALA:HB3	1.99	0.44
1:C:632:GLU:HA	1:C:636:ASP:HB2	1.99	0.44
1:A:571:TRP:HA	1:A:574:LYS:HE2	1.99	0.44
1:B:230:ASP:HB3	1:B:239:CYS:HB2	2.00	0.44
1:B:277:PHE:O	1:B:281:ALA:N	2.49	0.44
1:B:580:VAL:HA	1:B:583:VAL:HG22	2.00	0.44
1:C:360:VAL:HG11	2:s:1:NAG:C8	2.47	0.44
3:E:2:NAG:O3	3:E:3:BMA:C1	2.65	0.44
2:j:1:NAG:C3	2:j:2:NAG:O5	2.66	0.44
1:A:175:LEU:HB2	1:A:320:THR:HB	2.00	0.44
1:A:621:ARG:O	1:A:625:ASN:N	2.51	0.44
1:B:89:VAL:HG23	1:B:527:GLY:HA2	1.99	0.44
1:B:100:MET:HE1	1:B:487:LYS:HA	1.99	0.44
1:B:205:CYS:HA	1:B:206:PRO:HD3	1.83	0.44
1:A:44:VAL:HG13	1:A:633:ARG:HH11	1.82	0.44
1:A:231:LYS:HE3	1:A:268:GLU:HG2	2.00	0.44
1:B:328:GLN:HB2	1:B:330:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LEU:HB3	1:A:559:ILE:HG12	1.99	0.44
1:B:164:SER:HB3	1:B:312:GLY:HA2	1.99	0.44
1:B:332:ASN:OD1	3:Y:1:NAG:O5	2.30	0.44
1:C:276:ASN:HB3	1:C:282:LYS:HG3	2.00	0.44
1:B:298:ARG:HB2	1:B:443:ILE:HD12	1.99	0.43
1:C:258:GLN:NE2	1:C:373:MET:O	2.51	0.43
1:C:278:THR:OG1	2:m:1:NAG:H5	2.18	0.43
1:A:157:CYS:N	1:A:174:ALA:O	2.39	0.43
1:A:569:THR:HG23	1:A:571:TRP:HB2	2.00	0.43
1:B:198:THR:OG1	1:B:431:GLY:O	2.33	0.43
1:B:248:THR:OG1	1:B:249:HIS:N	2.50	0.43
1:A:546:SER:HB3	1:B:591:GLN:HB3	2.00	0.43
1:B:86:LEU:HD21	1:B:524:GLY:HA2	2.00	0.43
1:B:522:PHE:HB3	1:B:523:LEU:HD22	2.00	0.43
1:C:533:ALA:O	1:C:536:THR:OG1	2.35	0.43
1:C:639:THR:C	1:C:641:GLU:N	2.75	0.43
1:A:556:LEU:HD22	1:A:559:ILE:HG23	1.99	0.43
1:B:569:THR:HG23	1:B:572:GLY:H	1.83	0.43
3:O:1:NAG:H61	3:O:2:NAG:H82	2.00	0.43
1:B:296:CYS:HA	1:B:331:CYS:HA	2.01	0.43
1:B:611:ASN:O	1:B:614:TRP:CD1	2.72	0.43
1:A:276:ASN:ND2	1:A:279:ASN:H	2.17	0.43
1:B:66:HIS:HA	1:B:69:TRP:HB3	2.00	0.43
1:C:105:GLN:HE22	1:C:475:MET:HE3	1.83	0.43
1:A:197:ASP:OD1	1:A:197:ASP:N	2.52	0.43
1:A:200:VAL:O	1:A:433:ALA:N	2.50	0.43
1:A:201:ILE:HD11	1:A:435:TYR:HB2	2.00	0.43
1:A:389:GLN:H	1:A:389:GLN:HG2	1.58	0.43
1:B:363:HIS:CD2	3:b:1:NAG:H82	2.52	0.43
1:C:298:ARG:NH1	1:C:300:ASN:O	2.52	0.43
2:D:1:NAG:C3	2:D:2:NAG:O5	2.67	0.43
2:S:1:NAG:C3	2:S:2:NAG:O5	2.66	0.43
1:A:617:LYS:HE2	1:A:635:ILE:HG23	2.01	0.43
1:A:66:HIS:ND1	1:A:72:HIS:HB2	2.33	0.42
1:A:529:THR:HG21	1:A:532:ALA:HB3	2.01	0.42
1:B:55:ALA:O	1:B:216:HIS:N	2.52	0.42
1:C:100:MET:HE2	1:C:100:MET:HB2	1.95	0.42
1:C:279:ASN:HB2	2:m:1:NAG:O5	2.19	0.42
1:C:361:PHE:HB3	1:C:391:PHE:HB3	2.01	0.42
3:O:1:NAG:C6	3:O:2:NAG:H82	2.48	0.42
1:B:100:MET:HE2	1:B:100:MET:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:HA	1:A:498:PRO:HB3	2.02	0.42
1:A:477:ASP:HA	1:A:480:ARG:HG3	2.01	0.42
1:C:259:LEU:HB2	1:C:374:HIS:NE2	2.34	0.42
1:A:78:ASP:OD1	1:A:78:ASP:N	2.51	0.42
1:B:553:ASN:O	1:B:557:ARG:NE	2.46	0.42
1:C:360:VAL:HG22	1:C:394:THR:HG23	2.01	0.42
1:C:543:LEU:HG	1:C:552:GLN:HB2	2.02	0.42
3:X:1:NAG:HO3	3:X:1:NAG:C7	2.27	0.42
1:A:307:ILE:O	1:A:317:PHE:N	2.47	0.42
1:A:335:ARG:NH2	1:A:412:ASN:OD1	2.53	0.42
1:B:43:PRO:HB2	1:B:526:ALA:HB2	2.01	0.42
1:B:232:THR:OG1	1:B:268:GLU:OE1	2.36	0.42
4:l:6:MAN:O6	4:l:6:MAN:O4	2.38	0.42
1:B:44:VAL:HA	1:B:629:MET:HE2	2.00	0.42
1:B:205:CYS:HB2	1:B:208:ILE:HD12	2.02	0.42
1:A:277:PHE:O	1:A:456:ARG:NH2	2.53	0.42
1:A:453:LEU:HA	1:A:453:LEU:HD12	1.83	0.42
1:B:335:ARG:HD3	1:B:414:ILE:HB	2.02	0.42
1:C:198:THR:HB	1:C:430:VAL:HG22	2.02	0.42
1:A:41:GLY:HA2	1:A:538:THR:HB	2.01	0.41
1:A:88:ASN:OD1	7:A:901:NAG:O5	2.35	0.41
1:A:98:ASN:HD21	1:A:100:MET:HE2	1.85	0.41
1:A:203:GLN:HE22	1:A:318:TYR:H	1.66	0.41
1:B:363:HIS:HD2	3:b:1:NAG:H82	1.85	0.41
1:A:95:MET:HE1	1:A:480:ARG:HB3	2.02	0.41
1:A:335:ARG:O	1:A:339:ASN:N	2.42	0.41
1:B:131:CYS:HA	1:B:157:CYS:HA	2.01	0.41
1:C:56:SER:OG	1:C:57:ASP:N	2.53	0.41
3:N:2:NAG:C8	3:O:1:NAG:H82	2.44	0.41
1:A:262:ASN:HD22	4:G:1:NAG:C7	2.32	0.41
1:A:368:ASP:HB2	1:A:371:ILE:HD12	2.02	0.41
1:A:584:GLU:HB2	1:C:545:LEU:HD21	2.02	0.41
1:B:614:TRP:CE3	6:f:3:FUC:H63	2.53	0.41
1:B:96:TRP:NE1	1:B:274:SER:O	2.53	0.41
1:C:125:LEU:HD23	1:C:125:LEU:HA	1.92	0.41
1:C:244:THR:HG21	1:C:523:LEU:HD23	2.03	0.41
1:C:328:GLN:HE22	1:C:330:HIS:HB3	1.86	0.41
1:A:262:ASN:ND2	4:G:1:NAG:O7	2.42	0.41
1:A:321(A):GLU:HB3	1:A:322:ILE:H	1.75	0.41
3:Y:1:NAG:O7	3:Y:1:NAG:O3	2.27	0.41
1:B:163:THR:HG21	1:B:167:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:PHE:O	1:B:382:PHE:HA	2.21	0.41
1:B:657:GLU:O	1:B:661:LEU:N	2.50	0.41
1:C:104:MET:SD	1:C:217:TYR:OH	2.72	0.41
1:A:220:PRO:HD2	1:A:223:PHE:CE2	2.55	0.41
1:C:345:ILE:HD12	1:C:345:ILE:HA	1.93	0.41
1:C:635:ILE:HD12	1:C:635:ILE:HA	1.98	0.41
1:A:186:ASN:ND2	1:A:188:ASN:OD1	2.54	0.41
1:B:71:THR:OG1	1:B:72:HIS:ND1	2.52	0.41
1:B:154:ILE:HG22	1:B:177:TYR:CD1	2.56	0.41
1:B:468:PHE:HD1	1:B:468:PHE:HA	1.71	0.41
1:C:587:LEU:HA	1:C:590:GLN:HB2	2.02	0.41
1:A:554:ASN:OD1	1:A:575:GLN:NE2	2.54	0.41
1:B:86:LEU:HD11	1:B:524:GLY:HA2	2.03	0.41
1:B:122:LEU:N	1:B:201:ILE:O	2.33	0.41
1:B:628:TRP:HA	1:B:631:TRP:HB3	2.03	0.41
1:C:203:GLN:HE22	1:C:318:TYR:H	1.68	0.41
1:C:469:ARG:HH22	2:s:1:NAG:H61	1.85	0.41
4:l:1:NAG:O4	4:l:2:NAG:O7	2.38	0.41
1:A:295:ASN:HA	1:A:446:SER:HA	2.02	0.41
1:C:190:SER:O	1:C:190:SER:OG	2.37	0.41
1:C:568:LEU:HD13	1:C:570:VAL:HG12	2.03	0.41
1:B:53:PHE:HD2	1:B:218:CYS:HB2	1.86	0.40
1:B:376:PHE:HB2	1:B:383:PHE:CD2	2.57	0.40
1:C:346:VAL:HA	1:C:349:LEU:HD12	2.04	0.40
1:A:294:ILE:HD12	1:A:333:ILE:HA	2.02	0.40
1:C:332:ASN:HA	1:C:415:THR:HA	2.02	0.40
1:C:368:ASP:HB2	1:C:371:ILE:HB	2.04	0.40
1:C:535:MET:O	1:C:538:THR:OG1	2.29	0.40
1:A:164:SER:HB2	1:A:166:ARG:CZ	2.51	0.40
1:A:248:THR:OG1	1:A:249:HIS:N	2.47	0.40
1:A:357:LYS:HD3	1:A:357:LYS:HA	1.37	0.40
1:B:376:PHE:HD2	1:B:383:PHE:HB2	1.86	0.40
1:C:523:LEU:HD13	1:C:523:LEU:HA	1.93	0.40
3:p:1:NAG:H61	3:p:2:NAG:N2	2.36	0.40
1:A:631:TRP:O	1:A:635:ILE:HG13	2.21	0.40
1:B:252:ARG:NH2	4:U:1:NAG:O6	2.55	0.40
1:B:276:ASN:OD1	2:V:1:NAG:H2	2.20	0.40
1:B:335:ARG:O	1:B:339:ASN:N	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	583/848 (69%)	508 (87%)	72 (12%)	3 (0%)	24	61
1	B	587/848 (69%)	502 (86%)	83 (14%)	2 (0%)	36	70
1	C	582/848 (69%)	481 (83%)	98 (17%)	3 (0%)	24	61
All	All	1752/2544 (69%)	1491 (85%)	253 (14%)	8 (0%)	26	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	542	ARG
1	C	354	GLU
1	A	355	ASN
1	C	231	LYS
1	B	299	PRO
1	C	640	SER
1	A	68	VAL
1	A	220	PRO

5.3.2 Protein sidechains [i](#)

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	523/744 (70%)	512 (98%)	11 (2%)	47	65
1	B	526/744 (71%)	511 (97%)	15 (3%)	37	58
1	C	522/744 (70%)	509 (98%)	13 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1571/2232 (70%)	1532 (98%)	39 (2%)	42 62

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	50	THR
1	A	158	SER
1	A	261	LEU
1	A	330	HIS
1	A	350	ARG
1	A	351	GLU
1	A	357	LYS
1	A	359	ILE
1	A	389	GLN
1	A	496	VAL
1	B	161	ILE
1	B	170	GLN
1	B	171	LYS
1	B	348	LYS
1	B	349	LEU
1	B	351	GLU
1	B	354	GLU
1	B	355	ASN
1	B	443	ILE
1	B	491	ILE
1	B	542	ARG
1	B	608	VAL
1	B	614	TRP
1	B	638	TYR
1	B	642	ILE
1	C	68	VAL
1	C	101	VAL
1	C	116	LEU
1	C	213	ILE
1	C	301	ASN
1	C	354	GLU
1	C	355	ASN
1	C	357	LYS
1	C	358	THR
1	C	389	GLN
1	C	390	LEU

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Mol	Chain	Res	Type
1	C	613	SER
1	C	637	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	302	ASN
1	A	396	ASN
1	A	428	GLN
1	A	540	GLN
1	A	551	GLN
1	A	563	GLN
1	A	577	GLN
1	A	652	GLN
1	A	656	ASN
1	A	658	GLN
1	B	82	GLN
1	B	203	GLN
1	B	302	ASN
1	B	352	GLN
1	B	363	HIS
1	B	374	HIS
1	B	553	ASN
1	B	590	GLN
1	B	653	GLN
1	B	656	ASN
1	C	92	HIS
1	C	105	GLN
1	C	188	ASN
1	C	203	GLN
1	C	229	ASN
1	C	328	GLN
1	C	330	HIS
1	C	389	GLN
1	C	425	ASN
1	C	478	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 ⓘ

142 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	0.51	0	17,19,21	2.26	3 (17%)
2	NAG	D	2	2	14,14,15	0.49	0	17,19,21	1.33	3 (17%)
3	NAG	E	1	1,3	14,14,15	0.52	0	17,19,21	0.47	0
3	NAG	E	2	3	14,14,15	0.15	0	17,19,21	0.57	0
3	BMA	E	3	3	11,11,12	0.65	0	15,15,17	0.70	0
3	NAG	F	1	1,3	14,14,15	0.14	0	17,19,21	0.60	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.55	0
3	BMA	F	3	3	11,11,12	0.52	0	15,15,17	0.97	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	0.62	0
4	NAG	G	2	4	14,14,15	0.65	1 (7%)	17,19,21	0.44	0
4	BMA	G	3	4	11,11,12	0.69	0	15,15,17	0.77	0
4	MAN	G	4	4	11,11,12	0.62	0	15,15,17	0.96	1 (6%)
4	MAN	G	5	4	11,11,12	0.50	0	15,15,17	0.93	2 (13%)
4	MAN	G	6	4	11,11,12	0.59	0	15,15,17	0.95	2 (13%)
4	MAN	G	7	4	11,11,12	0.49	0	15,15,17	0.99	2 (13%)
3	NAG	H	1	1,3	14,14,15	0.61	1 (7%)	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.35	0	17,19,21	0.57	0
3	BMA	H	3	3	11,11,12	0.49	0	15,15,17	0.88	1 (6%)
2	NAG	I	1	1,2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	I	2	2	14,14,15	0.26	0	17,19,21	0.42	0
2	NAG	J	1	1,2	14,14,15	0.35	0	17,19,21	0.49	0
2	NAG	J	2	2	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	K	1	1,3	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	K	2	3	14,14,15	0.29	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	K	3	3	11,11,12	0.54	0	15,15,17	0.78	1 (6%)
2	NAG	L	1	1,2	14,14,15	0.51	0	17,19,21	2.29	3 (17%)
2	NAG	L	2	2	14,14,15	0.51	0	17,19,21	1.32	3 (17%)
3	NAG	M	1	1,3	14,14,15	0.56	0	17,19,21	0.44	0
3	NAG	M	2	3	14,14,15	0.31	0	17,19,21	0.56	0
3	BMA	M	3	3	11,11,12	0.52	0	15,15,17	0.71	0
3	NAG	N	1	1,3	14,14,15	0.67	1 (7%)	17,19,21	0.48	0
3	NAG	N	2	3	14,14,15	0.17	0	17,19,21	0.51	0
3	BMA	N	3	3	11,11,12	0.60	0	15,15,17	0.69	0
3	NAG	O	1	1,3	14,14,15	0.52	0	17,19,21	2.28	3 (17%)
3	NAG	O	2	3	14,14,15	0.49	0	17,19,21	1.34	3 (17%)
3	BMA	O	3	3	11,11,12	0.65	0	15,15,17	1.44	3 (20%)
5	NAG	P	1	1,5	14,14,15	0.48	0	17,19,21	0.53	0
5	NAG	P	2	5	14,14,15	0.17	0	17,19,21	0.62	0
5	BMA	P	3	5	11,11,12	0.53	0	15,15,17	0.83	0
5	MAN	P	4	5	11,11,12	0.90	1 (9%)	15,15,17	0.79	1 (6%)
3	NAG	Q	1	1,3	14,14,15	0.65	1 (7%)	17,19,21	0.69	0
3	NAG	Q	2	3	14,14,15	0.34	0	17,19,21	0.62	0
3	BMA	Q	3	3	11,11,12	0.59	0	15,15,17	0.73	0
2	NAG	R	1	1,2	14,14,15	0.49	0	17,19,21	0.44	0
2	NAG	R	2	2	14,14,15	0.30	0	17,19,21	0.52	0
2	NAG	S	1	1,2	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
2	NAG	S	2	2	14,14,15	0.52	0	17,19,21	1.32	3 (17%)
5	NAG	T	1	1,5	14,14,15	0.50	0	17,19,21	2.29	3 (17%)
5	NAG	T	2	5	14,14,15	0.49	0	17,19,21	1.36	3 (17%)
5	BMA	T	3	5	11,11,12	0.64	0	15,15,17	1.44	3 (20%)
5	MAN	T	4	5	11,11,12	0.55	0	15,15,17	1.48	2 (13%)
4	NAG	U	1	1,4	14,14,15	0.54	0	17,19,21	0.45	0
4	NAG	U	2	4	14,14,15	0.46	0	17,19,21	0.82	0
4	BMA	U	3	4	11,11,12	0.72	0	15,15,17	0.80	1 (6%)
4	MAN	U	4	4	11,11,12	0.65	0	15,15,17	1.28	2 (13%)
4	MAN	U	5	4	11,11,12	0.60	0	15,15,17	0.93	2 (13%)
4	MAN	U	6	4	11,11,12	0.60	0	15,15,17	0.88	1 (6%)
4	MAN	U	7	4	11,11,12	0.62	0	15,15,17	1.05	2 (13%)
2	NAG	V	1	1,2	14,14,15	0.18	0	17,19,21	0.40	0
2	NAG	V	2	2	14,14,15	0.16	0	17,19,21	0.58	0
2	NAG	W	1	1,2	14,14,15	0.36	0	17,19,21	0.43	0
2	NAG	W	2	2	14,14,15	0.18	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	X	1	1,3	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
3	NAG	X	2	3	14,14,15	0.49	0	17,19,21	1.31	3 (17%)
3	BMA	X	3	3	11,11,12	0.65	0	15,15,17	1.43	3 (20%)
3	NAG	Y	1	1,3	14,14,15	0.58	0	17,19,21	0.69	1 (5%)
3	NAG	Y	2	3	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
3	BMA	Y	3	3	11,11,12	0.74	0	15,15,17	0.80	0
2	NAG	Z	1	1,2	14,14,15	0.43	0	17,19,21	0.44	0
2	NAG	Z	2	2	14,14,15	0.34	0	17,19,21	0.52	0
2	NAG	a	1	1,2	14,14,15	0.48	0	17,19,21	2.29	3 (17%)
2	NAG	a	2	2	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
3	NAG	b	1	1,3	14,14,15	0.73	1 (7%)	17,19,21	0.54	0
3	NAG	b	2	3	14,14,15	0.18	0	17,19,21	0.48	0
3	BMA	b	3	3	11,11,12	0.50	0	15,15,17	0.91	0
3	NAG	c	1	1,3	14,14,15	0.47	0	17,19,21	0.49	0
3	NAG	c	2	3	14,14,15	0.29	0	17,19,21	0.47	0
3	BMA	c	3	3	11,11,12	0.66	0	15,15,17	0.85	0
2	NAG	d	1	1,2	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
2	NAG	d	2	2	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
5	NAG	e	1	1,5	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	e	2	5	14,14,15	0.19	0	17,19,21	0.47	0
5	BMA	e	3	5	11,11,12	0.55	0	15,15,17	0.95	1 (6%)
5	MAN	e	4	5	11,11,12	0.84	1 (9%)	15,15,17	1.39	2 (13%)
6	NAG	f	1	1,6	14,14,15	1.52	4 (28%)	17,19,21	1.10	1 (5%)
6	NAG	f	2	6	14,14,15	1.36	2 (14%)	17,19,21	1.29	1 (5%)
6	FUC	f	3	6	10,10,11	1.49	2 (20%)	14,14,16	0.87	0
2	NAG	g	1	1,2	14,14,15	0.21	0	17,19,21	0.54	0
2	NAG	g	2	2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	h	1	1,2	14,14,15	1.18	1 (7%)	17,19,21	0.97	2 (11%)
2	NAG	h	2	2	14,14,15	0.24	0	17,19,21	0.59	0
3	NAG	i	1	1,3	14,14,15	0.92	1 (7%)	17,19,21	0.84	0
3	NAG	i	2	3	14,14,15	0.15	0	17,19,21	0.65	0
3	BMA	i	3	3	11,11,12	0.57	0	15,15,17	0.77	0
2	NAG	j	1	1,2	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
2	NAG	j	2	2	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
3	NAG	k	1	1,3	14,14,15	0.22	0	17,19,21	0.63	0
3	NAG	k	2	3	14,14,15	0.17	0	17,19,21	0.52	0
3	BMA	k	3	3	11,11,12	0.52	0	15,15,17	0.90	0
4	NAG	l	1	1,4	14,14,15	0.32	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	l	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	BMA	l	3	4	11,11,12	0.66	0	15,15,17	0.94	0
4	MAN	l	4	4	11,11,12	0.90	0	15,15,17	1.20	1 (6%)
4	MAN	l	5	4	11,11,12	0.77	1 (9%)	15,15,17	1.26	2 (13%)
4	MAN	l	6	4	11,11,12	0.70	0	15,15,17	0.88	1 (6%)
4	MAN	l	7	4	11,11,12	0.70	0	15,15,17	0.93	1 (6%)
2	NAG	m	1	1,2	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	m	2	2	14,14,15	0.35	0	17,19,21	0.40	0
2	NAG	n	1	1,2	14,14,15	0.78	1 (7%)	17,19,21	0.56	0
2	NAG	n	2	2	14,14,15	0.19	0	17,19,21	0.54	0
2	NAG	o	1	1,2	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
2	NAG	o	2	2	14,14,15	0.49	0	17,19,21	1.32	3 (17%)
3	NAG	p	1	1,3	14,14,15	0.45	0	17,19,21	0.43	0
3	NAG	p	2	3	14,14,15	0.17	0	17,19,21	0.58	0
3	BMA	p	3	3	11,11,12	0.66	0	15,15,17	0.94	0
2	NAG	q	1	1,2	14,14,15	0.60	0	17,19,21	0.57	0
2	NAG	q	2	2	14,14,15	0.18	0	17,19,21	0.51	0
2	NAG	r	1	1,2	14,14,15	0.45	0	17,19,21	0.45	0
2	NAG	r	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	s	1	1,2	14,14,15	0.49	0	17,19,21	2.28	3 (17%)
2	NAG	s	2	2	14,14,15	0.50	0	17,19,21	1.34	3 (17%)
3	NAG	t	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.44	0
3	NAG	t	2	3	14,14,15	0.19	0	17,19,21	0.54	0
3	BMA	t	3	3	11,11,12	0.65	0	15,15,17	0.91	1 (6%)
3	NAG	u	1	1,3	14,14,15	0.73	1 (7%)	17,19,21	0.76	0
3	NAG	u	2	3	14,14,15	0.27	0	17,19,21	0.52	0
3	BMA	u	3	3	11,11,12	0.75	0	15,15,17	0.89	0
4	NAG	v	1	1,4	14,14,15	0.74	1 (7%)	17,19,21	1.30	1 (5%)
4	NAG	v	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	BMA	v	3	4	11,11,12	0.53	0	15,15,17	0.72	0
4	MAN	v	4	4	11,11,12	1.28	2 (18%)	15,15,17	1.93	2 (13%)
4	MAN	v	5	4	11,11,12	0.72	0	15,15,17	1.31	1 (6%)
4	MAN	v	6	4	11,11,12	0.77	0	15,15,17	1.06	1 (6%)
4	MAN	v	7	4	11,11,12	0.67	0	15,15,17	0.93	1 (6%)
6	NAG	w	1	1,6	14,14,15	1.53	4 (28%)	17,19,21	1.10	1 (5%)
6	NAG	w	2	6	14,14,15	1.33	2 (14%)	17,19,21	1.30	1 (5%)
6	FUC	w	3	6	10,10,11	1.52	2 (20%)	14,14,16	0.87	0
2	NAG	x	1	1,2	14,14,15	0.46	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	x	2	2	14,14,15	0.31	0	17,19,21	0.62	1 (5%)
3	NAG	y	1	1,3	14,14,15	1.52	3 (21%)	17,19,21	1.08	1 (5%)
3	NAG	y	2	3	14,14,15	1.35	2 (14%)	17,19,21	1.30	1 (5%)
3	BMA	y	3	3	11,11,12	1.36	2 (18%)	15,15,17	1.22	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	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	MAN	G	5	4	-	1/2/19/22	0/1/1/1
4	MAN	G	6	4	-	2/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	2/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
5	BMA	P	3	5	-	0/2/19/22	0/1/1/1
5	MAN	P	4	5	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	BMA	T	3	5	-	0/2/19/22	0/1/1/1
5	MAN	T	4	5	-	0/2/19/22	0/1/1/1
4	NAG	U	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	BMA	U	3	4	-	0/2/19/22	0/1/1/1
4	MAN	U	4	4	-	0/2/19/22	0/1/1/1
4	MAN	U	5	4	-	2/2/19/22	0/1/1/1
4	MAN	U	6	4	-	0/2/19/22	0/1/1/1
4	MAN	U	7	4	-	0/2/19/22	0/1/1/1
2	NAG	V	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	BMA	X	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Y	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	3/6/23/26	0/1/1/1
3	BMA	Y	3	3	-	0/2/19/22	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
2	NAG	a	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	0/6/23/26	0/1/1/1
3	BMA	b	3	3	-	0/2/19/22	0/1/1/1
3	NAG	c	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	BMA	c	3	3	-	0/2/19/22	0/1/1/1
2	NAG	d	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
5	NAG	e	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
5	BMA	e	3	5	-	2/2/19/22	0/1/1/1
5	MAN	e	4	5	-	0/2/19/22	0/1/1/1
6	NAG	f	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	0/6/23/26	0/1/1/1
6	FUC	f	3	6	-	-	0/1/1/1
2	NAG	g	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	g	2	2	-	1/6/23/26	0/1/1/1
2	NAG	h	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	0/6/23/26	0/1/1/1
3	NAG	i	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	BMA	i	3	3	-	2/2/19/22	0/1/1/1
2	NAG	j	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	j	2	2	-	0/6/23/26	0/1/1/1
3	NAG	k	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	k	2	3	-	0/6/23/26	0/1/1/1
3	BMA	k	3	3	-	0/2/19/22	0/1/1/1
4	NAG	l	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	l	2	4	-	2/6/23/26	0/1/1/1
4	BMA	l	3	4	-	0/2/19/22	0/1/1/1
4	MAN	l	4	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	l	5	4	-	1/2/19/22	0/1/1/1
4	MAN	l	6	4	-	1/2/19/22	0/1/1/1
4	MAN	l	7	4	-	0/2/19/22	0/1/1/1
2	NAG	m	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	m	2	2	-	2/6/23/26	0/1/1/1
2	NAG	n	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	n	2	2	-	0/6/23/26	0/1/1/1
2	NAG	o	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	o	2	2	-	0/6/23/26	0/1/1/1
3	NAG	p	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	p	2	3	-	0/6/23/26	0/1/1/1
3	BMA	p	3	3	-	0/2/19/22	0/1/1/1
2	NAG	q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	q	2	2	-	1/6/23/26	0/1/1/1
2	NAG	r	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	r	2	2	-	2/6/23/26	0/1/1/1
2	NAG	s	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	s	2	2	-	0/6/23/26	0/1/1/1
3	NAG	t	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	t	2	3	-	2/6/23/26	0/1/1/1
3	BMA	t	3	3	-	0/2/19/22	0/1/1/1
3	NAG	u	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	u	2	3	-	2/6/23/26	0/1/1/1
3	BMA	u	3	3	-	2/2/19/22	0/1/1/1
4	NAG	v	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	v	2	4	-	2/6/23/26	0/1/1/1
4	BMA	v	3	4	-	2/2/19/22	0/1/1/1
4	MAN	v	4	4	-	2/2/19/22	0/1/1/1
4	MAN	v	5	4	-	0/2/19/22	0/1/1/1
4	MAN	v	6	4	-	2/2/19/22	0/1/1/1
4	MAN	v	7	4	-	0/2/19/22	0/1/1/1
6	NAG	w	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	w	2	6	-	0/6/23/26	0/1/1/1
6	FUC	w	3	6	-	-	0/1/1/1
2	NAG	x	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	x	2	2	-	1/6/23/26	0/1/1/1
3	NAG	y	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	y	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	y	3	3	-	0/2/19/22	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	1	NAG	O5-C1	-4.02	1.36	1.43
3	i	1	NAG	O5-C1	-3.37	1.38	1.43
3	y	1	NAG	O5-C1	3.06	1.48	1.43
6	w	1	NAG	O5-C1	3.05	1.48	1.43
4	G	1	NAG	O5-C1	-3.01	1.38	1.43
6	f	1	NAG	O5-C1	2.99	1.48	1.43
6	w	3	FUC	O5-C1	2.91	1.48	1.43
6	f	2	NAG	O5-C1	2.90	1.48	1.43
6	f	3	FUC	O5-C1	2.80	1.48	1.43
3	y	2	NAG	O5-C1	2.75	1.48	1.43
6	w	2	NAG	O5-C1	2.74	1.48	1.43
2	n	1	NAG	O5-C1	-2.71	1.39	1.43
6	w	3	FUC	O5-C5	2.68	1.48	1.43
4	v	4	MAN	O5-C5	2.68	1.48	1.43
3	y	1	NAG	O5-C5	2.67	1.48	1.43
6	f	1	NAG	O5-C5	2.64	1.48	1.43
4	v	1	NAG	O5-C1	-2.62	1.39	1.43
6	f	3	FUC	O5-C5	2.60	1.48	1.43
3	y	3	BMA	O5-C1	2.56	1.48	1.43
6	w	1	NAG	O5-C5	2.56	1.48	1.43
3	b	1	NAG	O5-C1	-2.56	1.39	1.43
3	y	3	BMA	O5-C5	2.53	1.48	1.43
5	P	4	MAN	O5-C1	-2.53	1.39	1.43
3	u	1	NAG	O5-C1	-2.40	1.39	1.43
4	G	2	NAG	O5-C1	-2.34	1.39	1.43
3	Q	1	NAG	O5-C1	-2.30	1.39	1.43
4	v	4	MAN	O5-C1	2.29	1.47	1.43
3	N	1	NAG	O5-C1	-2.28	1.39	1.43
6	w	2	NAG	O5-C5	2.27	1.47	1.43
6	f	2	NAG	O5-C5	2.26	1.47	1.43
4	l	5	MAN	C1-C2	2.25	1.57	1.52
3	y	2	NAG	O5-C5	2.24	1.47	1.43
3	t	1	NAG	O5-C1	-2.24	1.39	1.43
5	e	4	MAN	C1-C2	2.17	1.57	1.52
3	H	1	NAG	O5-C1	-2.11	1.40	1.43
6	f	1	NAG	C8-C7	2.08	1.54	1.50
6	f	1	NAG	O4-C4	2.08	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	y	1	NAG	O4-C4	2.07	1.48	1.43
6	w	1	NAG	C8-C7	2.04	1.54	1.50
6	w	1	NAG	O4-C4	2.03	1.48	1.43

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	1	NAG	O5-C1-C2	-7.57	99.58	111.29
2	L	1	NAG	O5-C1-C2	-7.57	99.58	111.29
5	T	1	NAG	O5-C1-C2	-7.55	99.61	111.29
2	s	1	NAG	O5-C1-C2	-7.54	99.62	111.29
3	X	1	NAG	O5-C1-C2	-7.54	99.62	111.29
2	d	1	NAG	O5-C1-C2	-7.52	99.65	111.29
3	O	1	NAG	O5-C1-C2	-7.52	99.66	111.29
2	j	1	NAG	O5-C1-C2	-7.51	99.66	111.29
2	S	1	NAG	O5-C1-C2	-7.51	99.67	111.29
2	o	1	NAG	O5-C1-C2	-7.48	99.71	111.29
2	D	1	NAG	O5-C1-C2	-7.45	99.76	111.29
4	v	4	MAN	C1-O5-C5	6.57	120.99	112.19
4	v	1	NAG	C2-N2-C7	4.47	128.89	122.90
5	e	4	MAN	C1-O5-C5	4.37	118.04	112.19
4	v	5	MAN	C1-O5-C5	4.21	117.83	112.19
6	w	2	NAG	C1-O5-C5	4.11	117.69	112.19
3	y	2	NAG	C1-O5-C5	4.09	117.67	112.19
6	f	2	NAG	C1-O5-C5	4.02	117.58	112.19
3	y	3	BMA	C1-O5-C5	3.87	117.38	112.19
6	f	1	NAG	C1-O5-C5	3.41	116.75	112.19
6	w	1	NAG	C1-O5-C5	3.38	116.71	112.19
3	y	1	NAG	C1-O5-C5	3.33	116.65	112.19
4	U	4	MAN	C1-O5-C5	3.20	116.48	112.19
2	s	2	NAG	O5-C5-C6	-3.13	101.57	107.66
4	U	4	MAN	O2-C2-C3	-3.10	103.74	110.15
2	o	2	NAG	O5-C5-C6	-3.09	101.64	107.66
3	O	2	NAG	O5-C5-C6	-3.09	101.65	107.66
3	X	2	NAG	O5-C5-C6	-3.06	101.71	107.66
2	D	2	NAG	O5-C5-C6	-3.05	101.72	107.66
2	S	2	NAG	O5-C5-C6	-3.05	101.72	107.66
2	a	2	NAG	O5-C5-C6	-3.05	101.73	107.66
2	L	2	NAG	O5-C5-C6	-3.05	101.73	107.66
5	T	2	NAG	O5-C5-C6	-3.04	101.74	107.66
2	d	2	NAG	O5-C5-C6	-3.04	101.75	107.66
2	j	2	NAG	O5-C5-C6	-3.02	101.79	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1	NAG	O7-C7-C8	-2.96	116.78	122.05
2	j	1	NAG	O7-C7-C8	-2.95	116.81	122.05
2	d	1	NAG	O7-C7-C8	-2.94	116.83	122.05
5	T	1	NAG	O7-C7-C8	-2.92	116.85	122.05
2	S	1	NAG	O7-C7-C8	-2.91	116.86	122.05
2	L	1	NAG	O7-C7-C8	-2.91	116.87	122.05
2	a	1	NAG	O7-C7-C8	-2.88	116.92	122.05
2	o	1	NAG	O7-C7-C8	-2.88	116.92	122.05
2	D	1	NAG	O7-C7-C8	-2.87	116.94	122.05
3	X	1	NAG	O7-C7-C8	-2.86	116.95	122.05
3	O	3	BMA	O2-C2-C3	2.86	116.07	110.15
3	X	3	BMA	O2-C2-C3	2.86	116.06	110.15
2	s	1	NAG	O7-C7-C8	-2.84	116.99	122.05
5	T	3	BMA	O2-C2-C3	2.84	116.03	110.15
2	s	1	NAG	C4-C3-C2	-2.72	107.03	111.02
2	D	1	NAG	C4-C3-C2	-2.71	107.05	111.02
2	d	1	NAG	C4-C3-C2	-2.71	107.05	111.02
3	O	1	NAG	C4-C3-C2	-2.68	107.08	111.02
5	T	1	NAG	C4-C3-C2	-2.68	107.09	111.02
3	O	3	BMA	O4-C4-C5	-2.67	102.74	109.32
2	a	1	NAG	C4-C3-C2	-2.67	107.11	111.02
2	o	1	NAG	C4-C3-C2	-2.67	107.11	111.02
4	v	4	MAN	O2-C2-C3	-2.67	104.63	110.15
4	l	5	MAN	C1-O5-C5	2.66	115.76	112.19
3	X	3	BMA	O4-C4-C5	-2.66	102.78	109.32
2	L	1	NAG	C4-C3-C2	-2.65	107.13	111.02
3	X	1	NAG	C4-C3-C2	-2.64	107.15	111.02
2	j	1	NAG	C4-C3-C2	-2.63	107.16	111.02
2	S	1	NAG	C4-C3-C2	-2.61	107.19	111.02
5	T	3	BMA	O4-C4-C5	-2.59	102.94	109.32
4	U	7	MAN	C1-O5-C5	2.53	115.57	112.19
4	G	7	MAN	C1-O5-C5	2.49	115.52	112.19
5	T	4	MAN	O5-C5-C6	2.42	112.37	107.66
4	l	6	MAN	O2-C2-C3	-2.42	105.15	110.15
5	T	2	NAG	O5-C1-C2	-2.41	107.56	111.29
4	U	7	MAN	O2-C2-C3	-2.38	105.21	110.15
5	T	3	BMA	C6-C5-C4	-2.36	107.22	113.02
4	l	4	MAN	C1-C2-C3	2.35	113.07	109.64
2	j	2	NAG	O5-C1-C2	-2.35	107.66	111.29
3	O	2	NAG	O5-C1-C2	-2.35	107.66	111.29
2	s	2	NAG	O5-C1-C2	-2.34	107.67	111.29
5	T	2	NAG	C4-C3-C2	-2.34	107.59	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	O5-C1-C2	-2.33	107.69	111.29
2	L	2	NAG	O5-C1-C2	-2.31	107.71	111.29
3	O	3	BMA	C6-C5-C4	-2.31	107.36	113.02
3	X	3	BMA	C6-C5-C4	-2.30	107.37	113.02
2	d	2	NAG	O5-C1-C2	-2.30	107.73	111.29
2	S	2	NAG	O5-C1-C2	-2.30	107.74	111.29
4	l	7	MAN	O2-C2-C3	-2.30	105.40	110.15
2	a	2	NAG	O5-C1-C2	-2.29	107.74	111.29
4	G	5	MAN	C1-O5-C5	2.28	115.25	112.19
5	e	4	MAN	O2-C2-C3	-2.28	105.44	110.15
4	v	7	MAN	O2-C2-C3	-2.27	105.44	110.15
2	o	2	NAG	O5-C1-C2	-2.26	107.79	111.29
3	X	2	NAG	O5-C1-C2	-2.26	107.80	111.29
4	U	6	MAN	O2-C2-C3	-2.26	105.48	110.15
2	d	2	NAG	C4-C3-C2	-2.25	107.73	111.02
3	O	2	NAG	C4-C3-C2	-2.23	107.75	111.02
2	a	2	NAG	C4-C3-C2	-2.23	107.75	111.02
3	H	3	BMA	C1-O5-C5	2.22	115.17	112.19
2	D	2	NAG	C4-C3-C2	-2.22	107.76	111.02
2	s	2	NAG	C4-C3-C2	-2.22	107.77	111.02
4	l	5	MAN	O2-C2-C3	-2.21	105.58	110.15
3	Y	2	NAG	C1-O5-C5	2.20	115.14	112.19
2	S	2	NAG	C4-C3-C2	-2.19	107.81	111.02
4	v	6	MAN	C1-O5-C5	2.19	115.12	112.19
2	L	2	NAG	C4-C3-C2	-2.19	107.81	111.02
4	G	7	MAN	O2-C2-C3	-2.18	105.63	110.15
2	j	2	NAG	C4-C3-C2	-2.18	107.82	111.02
4	G	6	MAN	O2-C2-C3	-2.17	105.65	110.15
4	U	5	MAN	C1-O5-C5	2.17	115.09	112.19
4	U	5	MAN	O2-C2-C3	-2.16	105.69	110.15
3	K	3	BMA	O2-C2-C3	-2.15	105.69	110.15
2	h	1	NAG	C1-O5-C5	-2.14	109.32	112.19
4	G	4	MAN	C1-O5-C5	2.13	115.04	112.19
2	o	2	NAG	C4-C3-C2	-2.12	107.91	111.02
4	G	5	MAN	O2-C2-C3	-2.12	105.75	110.15
3	X	2	NAG	C4-C3-C2	-2.12	107.91	111.02
2	x	2	NAG	C1-O5-C5	2.10	115.00	112.19
2	h	1	NAG	C3-C4-C5	2.10	114.04	110.23
5	P	4	MAN	O2-C2-C3	-2.10	105.81	110.15
3	Y	1	NAG	C1-O5-C5	2.09	114.98	112.19
5	T	4	MAN	O3-C3-C4	2.07	115.26	110.38
5	e	3	BMA	C1-C2-C3	2.05	112.63	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	6	MAN	C1-O5-C5	2.03	114.91	112.19
3	t	3	BMA	C1-O5-C5	2.02	114.90	112.19
4	U	3	BMA	O2-C2-C3	-2.01	105.98	110.15
3	F	3	BMA	C1-O5-C5	2.01	114.87	112.19

There are no chirality outliers.

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	h	1	NAG	C1-C2-N2-C7
3	Q	1	NAG	C1-C2-N2-C7
3	i	1	NAG	C1-C2-N2-C7
3	y	1	NAG	C1-C2-N2-C7
3	Q	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
3	i	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	p	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	U	5	MAN	O5-C5-C6-O6
4	v	4	MAN	O5-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
2	r	2	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	m	2	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
3	t	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	P	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	v	4	MAN	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
3	u	1	NAG	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
3	N	3	BMA	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
4	l	2	NAG	C4-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
2	r	1	NAG	C4-C5-C6-O6
3	i	1	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	p	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
4	U	5	MAN	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	i	3	BMA	C4-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
2	r	2	NAG	C4-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
4	l	2	NAG	O5-C5-C6-O6
4	l	1	NAG	C4-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
4	l	5	MAN	O5-C5-C6-O6
4	v	1	NAG	C8-C7-N2-C2
4	v	1	NAG	O7-C7-N2-C2
2	Z	1	NAG	O5-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
2	r	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	t	1	NAG	C4-C5-C6-O6
3	u	2	NAG	O5-C5-C6-O6
3	u	3	BMA	C4-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
4	v	6	MAN	C4-C5-C6-O6
2	q	1	NAG	O5-C5-C6-O6
5	e	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	Y	1	NAG	C4-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	u	1	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
4	l	1	NAG	O5-C5-C6-O6
4	v	3	BMA	O5-C5-C6-O6
4	v	3	BMA	C4-C5-C6-O6
2	g	1	NAG	C4-C5-C6-O6
4	l	4	MAN	O5-C5-C6-O6
5	e	2	NAG	C4-C5-C6-O6
3	i	3	BMA	O5-C5-C6-O6
4	l	6	MAN	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	u	3	BMA	O5-C5-C6-O6
2	V	2	NAG	C4-C5-C6-O6
2	m	1	NAG	O5-C5-C6-O6
2	q	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
3	i	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	v	2	NAG	C4-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
3	u	2	NAG	C4-C5-C6-O6
4	v	6	MAN	O5-C5-C6-O6
4	l	4	MAN	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
2	g	1	NAG	O5-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
2	x	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
4	G	6	MAN	O5-C5-C6-O6
3	X	3	BMA	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
2	m	1	NAG	C1-C2-N2-C7
4	G	1	NAG	C1-C2-N2-C7
5	P	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	G	6	MAN	C4-C5-C6-O6
2	V	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
4	v	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	X	3	BMA	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
2	q	1	NAG	C4-C5-C6-O6
3	t	2	NAG	C4-C5-C6-O6
2	h	1	NAG	C3-C2-N2-C7
2	m	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	X	1	NAG	C3-C2-N2-C7
3	Y	1	NAG	C3-C2-N2-C7
5	e	1	NAG	C3-C2-N2-C7
2	x	1	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	V	1	NAG	C4-C5-C6-O6
4	v	1	NAG	C1-C2-N2-C7
5	e	1	NAG	C1-C2-N2-C7
3	Q	1	NAG	C3-C2-N2-C7
3	Y	2	NAG	C3-C2-N2-C7
4	v	1	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
3	K	1	NAG	O5-C5-C6-O6
3	t	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O7-C7-N2-C2
2	a	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	S	1	NAG	O7-C7-N2-C2
2	d	1	NAG	O7-C7-N2-C2
2	j	1	NAG	O7-C7-N2-C2
2	o	1	NAG	O7-C7-N2-C2
2	s	1	NAG	O7-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	X	1	NAG	O7-C7-N2-C2

There are no ring outliers.

63 monomers are involved in 105 short contacts:

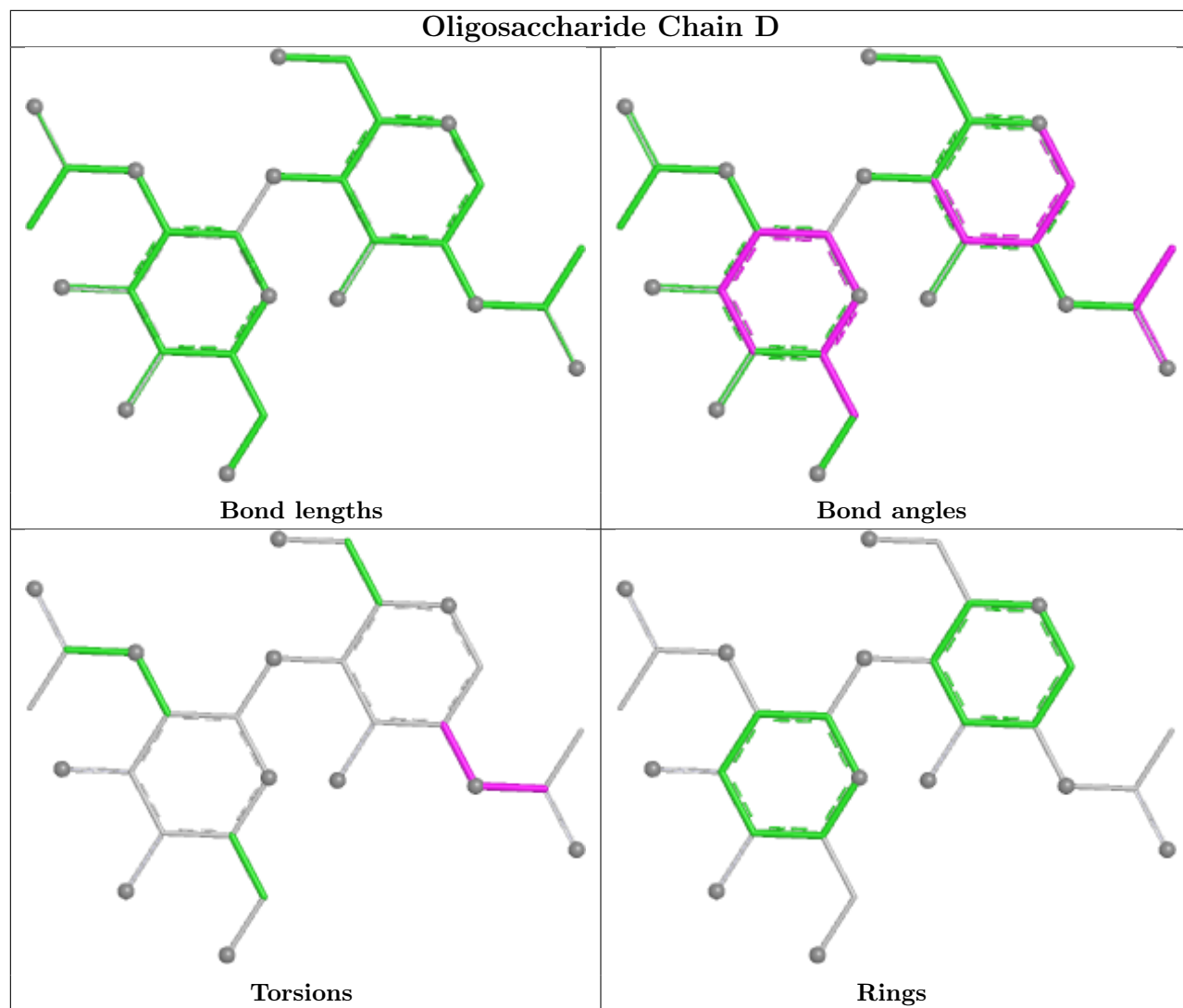
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0
3	H	1	NAG	5	0
5	e	1	NAG	2	0
6	f	2	NAG	1	0
4	U	5	MAN	1	0
3	E	2	NAG	1	0
2	S	2	NAG	2	0
3	k	1	NAG	1	0
2	h	2	NAG	1	0
2	m	2	NAG	1	0
3	M	2	NAG	1	0
3	N	1	NAG	1	0
6	f	3	FUC	6	0
2	D	1	NAG	4	0
3	H	2	NAG	3	0
2	R	1	NAG	2	0
2	s	1	NAG	2	0
4	G	1	NAG	4	0
5	T	1	NAG	2	0
4	U	4	MAN	2	0
3	t	1	NAG	2	0
5	P	1	NAG	2	0
3	E	3	BMA	1	0
2	S	1	NAG	2	0
3	p	1	NAG	1	0
2	o	1	NAG	2	0
2	r	2	NAG	1	0
3	N	2	NAG	8	0
2	h	1	NAG	1	0
3	y	2	NAG	1	0
2	g	1	NAG	2	0
2	r	1	NAG	1	0
3	F	1	NAG	2	0
4	U	1	NAG	2	0
3	O	2	NAG	5	0
3	y	1	NAG	2	0
3	b	1	NAG	2	0
4	v	1	NAG	1	0
2	L	1	NAG	1	0
3	Q	1	NAG	9	0
3	X	1	NAG	6	0
2	D	2	NAG	2	0

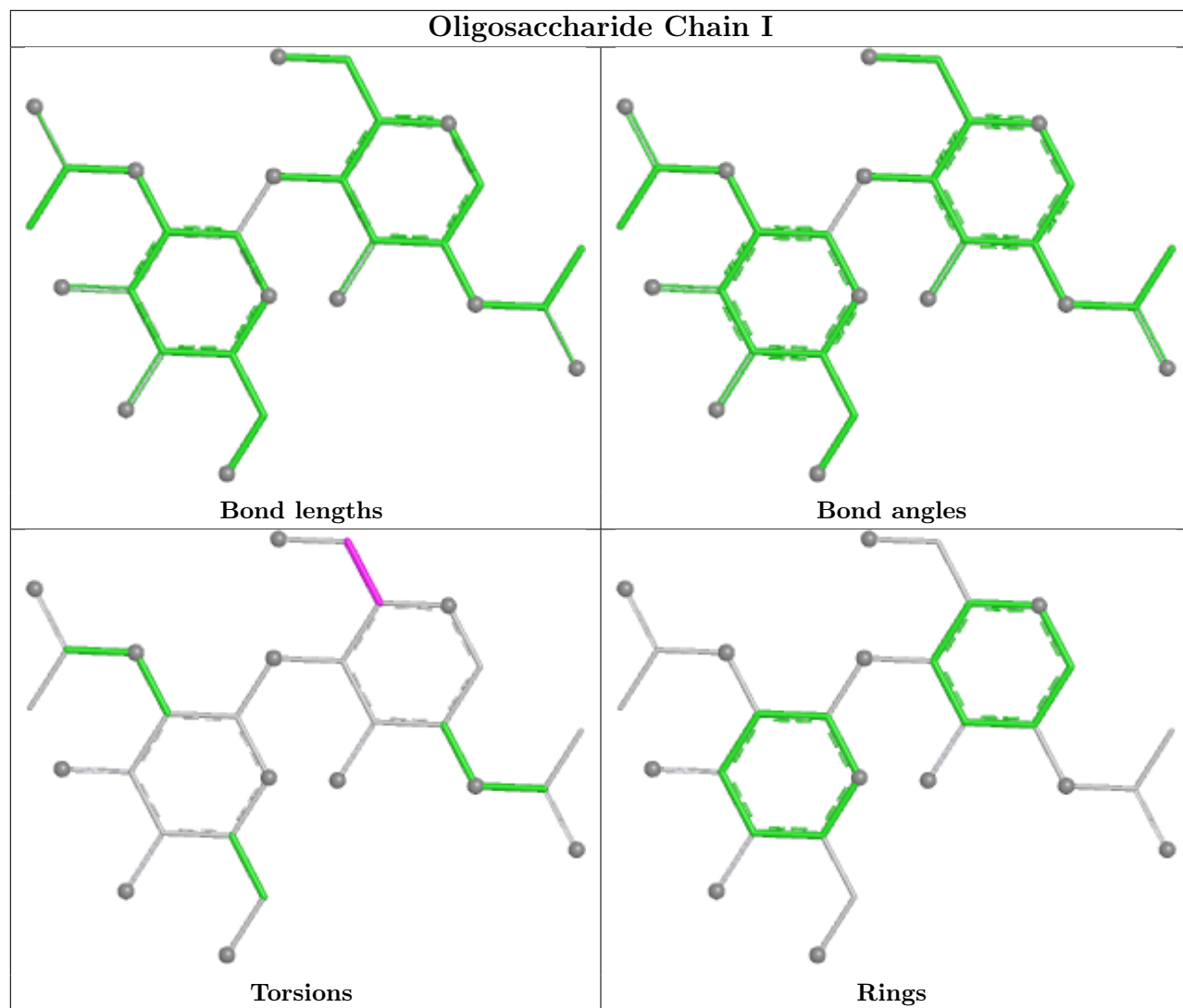
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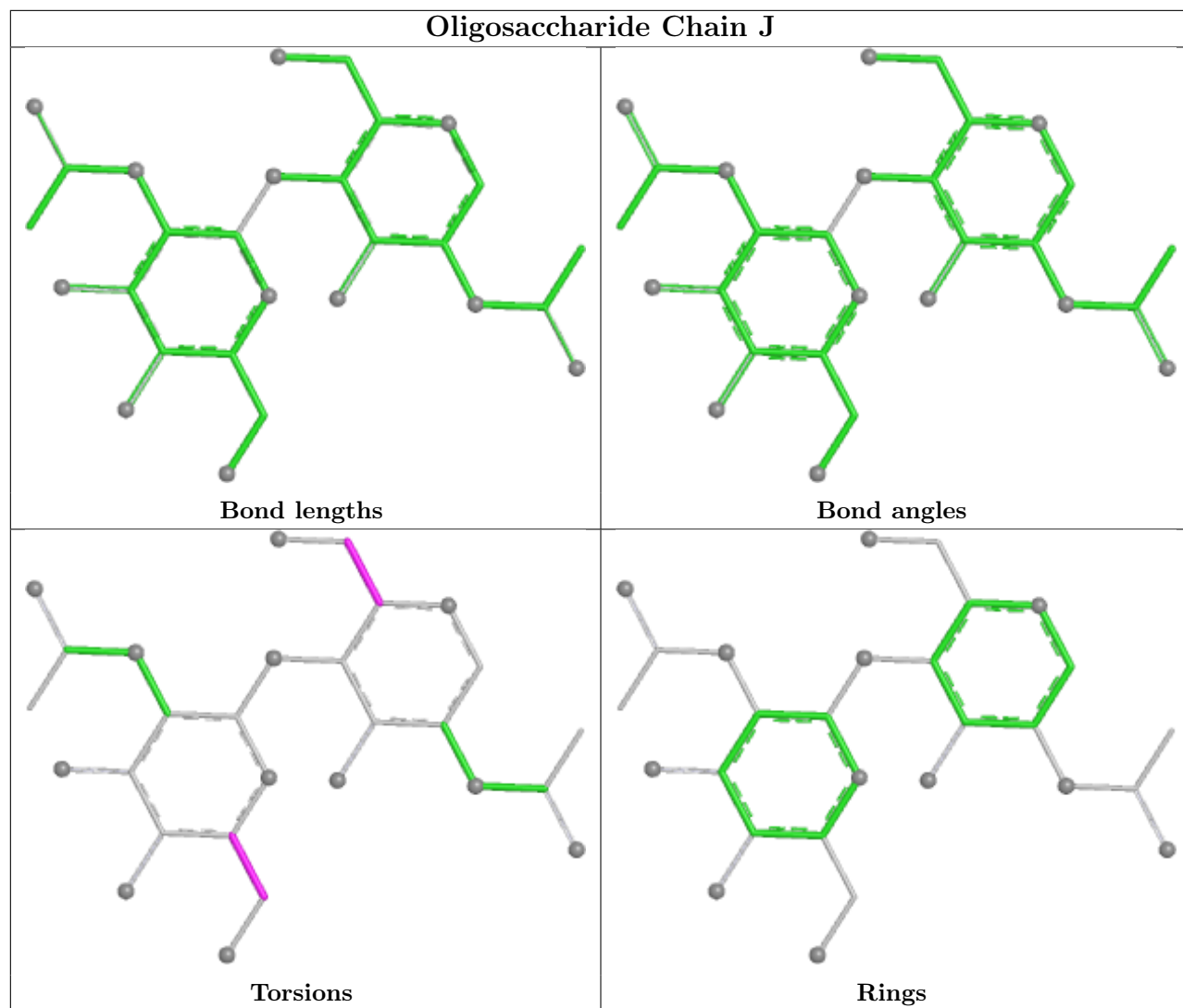
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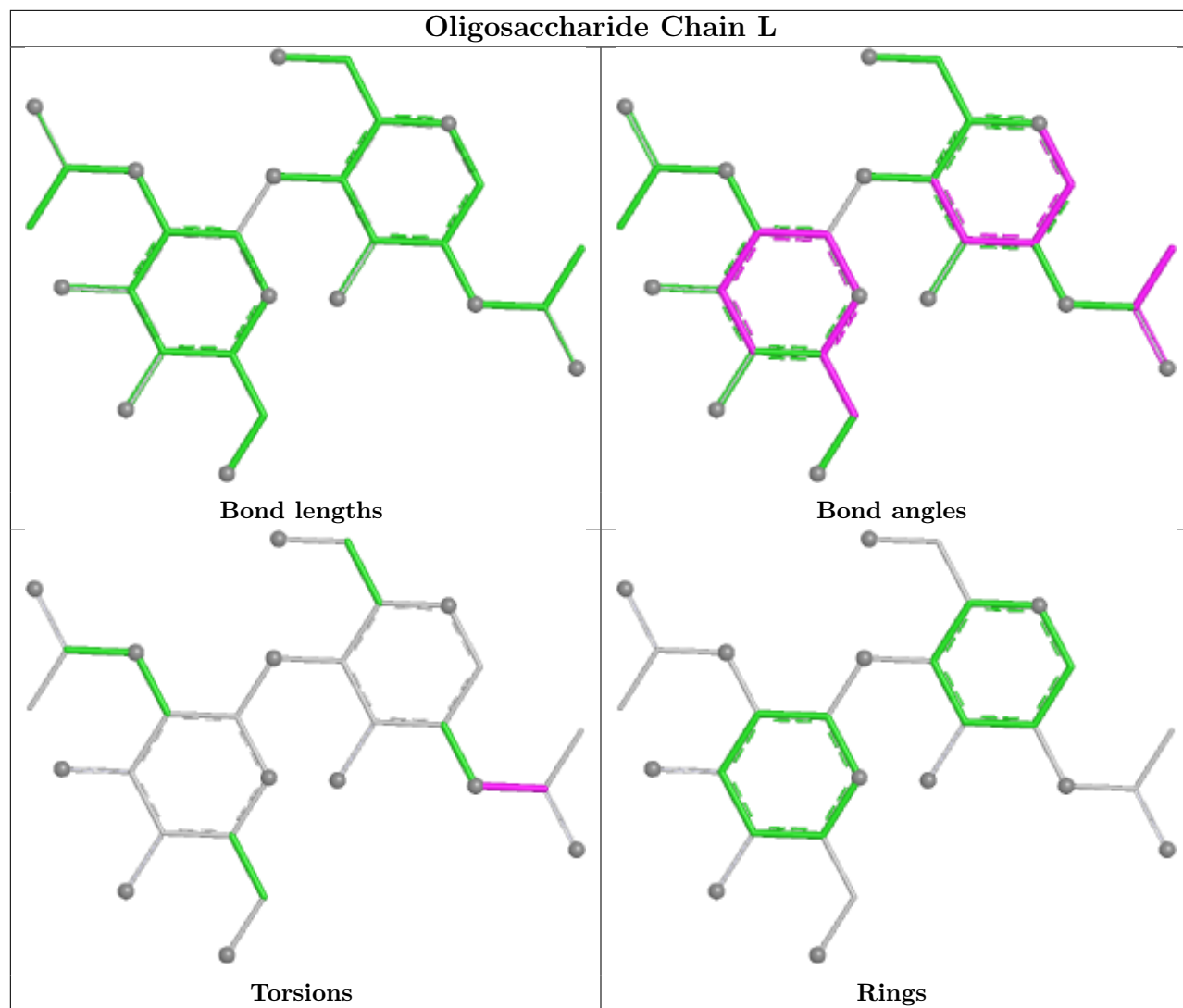
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	1	NAG	4	0
4	l	1	NAG	1	0
3	i	1	NAG	1	0
4	v	6	MAN	1	0
3	O	3	BMA	3	0
3	M	1	NAG	2	0
3	Y	1	NAG	2	0
3	F	2	NAG	1	0
2	j	1	NAG	2	0
3	p	2	NAG	1	0
2	m	1	NAG	3	0
2	R	2	NAG	1	0
4	v	3	BMA	1	0
2	a	1	NAG	1	0
3	O	1	NAG	9	0
4	l	6	MAN	1	0
4	U	2	NAG	1	0
2	j	2	NAG	2	0
3	c	1	NAG	1	0
4	l	5	MAN	1	0
4	l	2	NAG	1	0

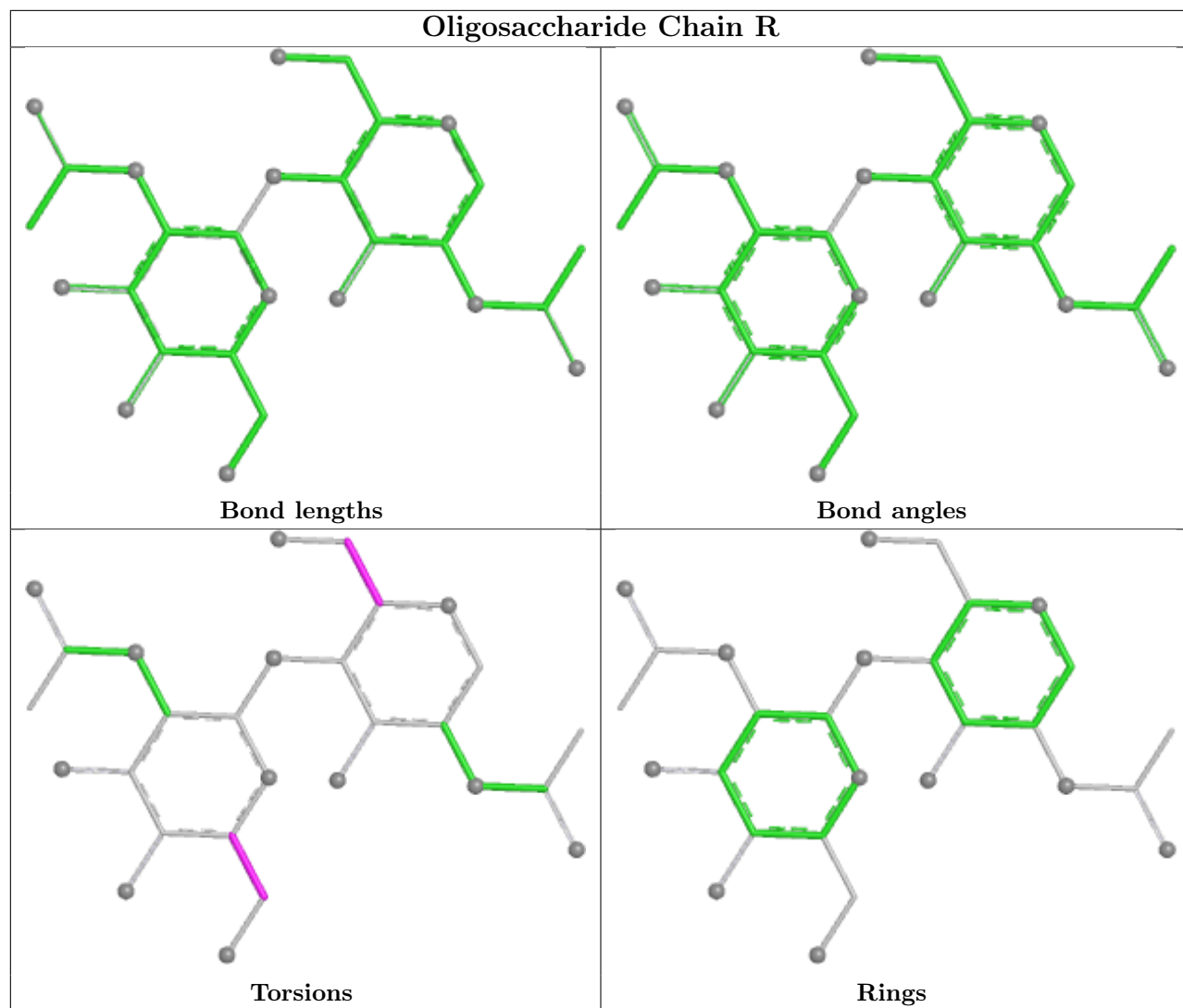
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

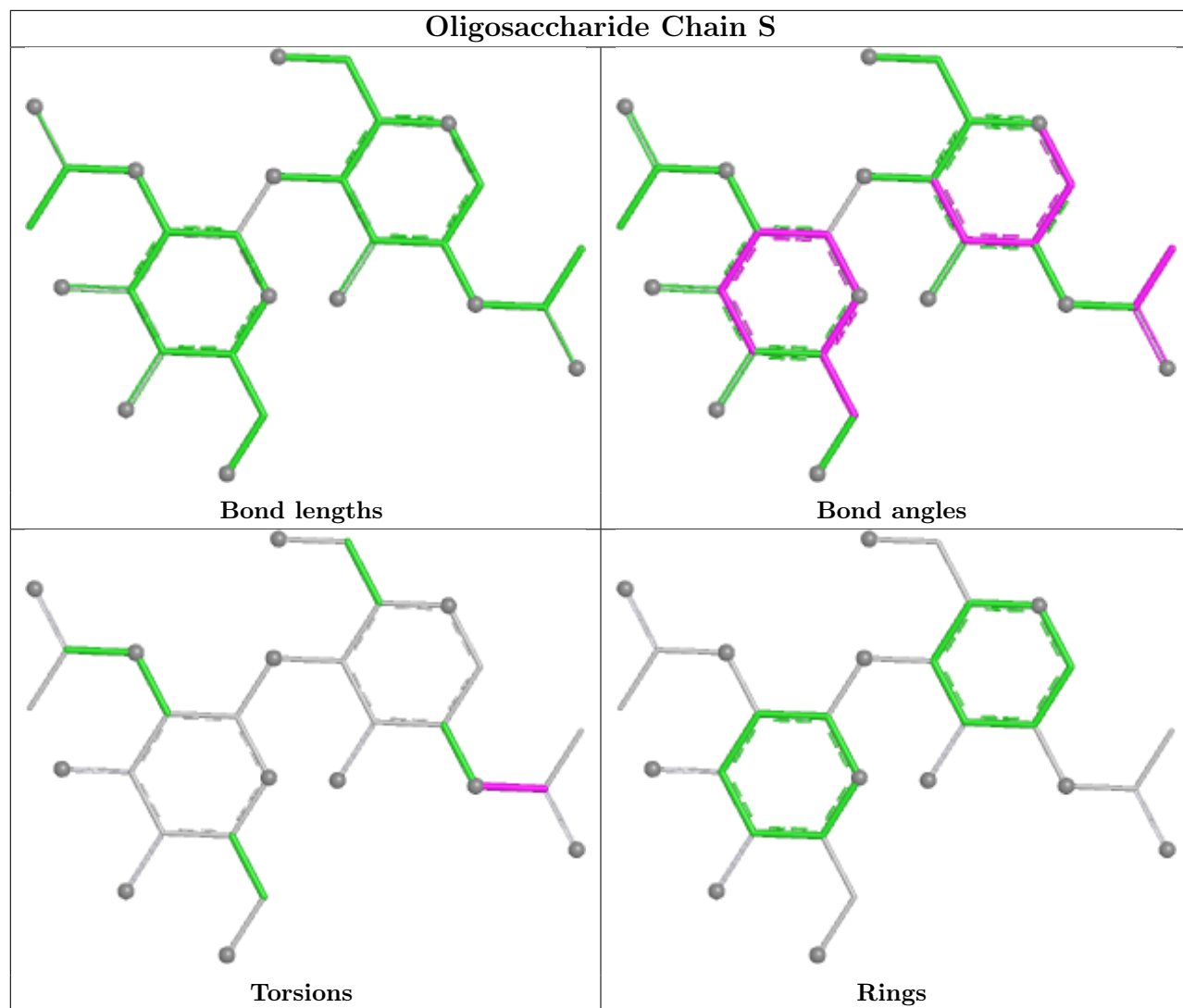


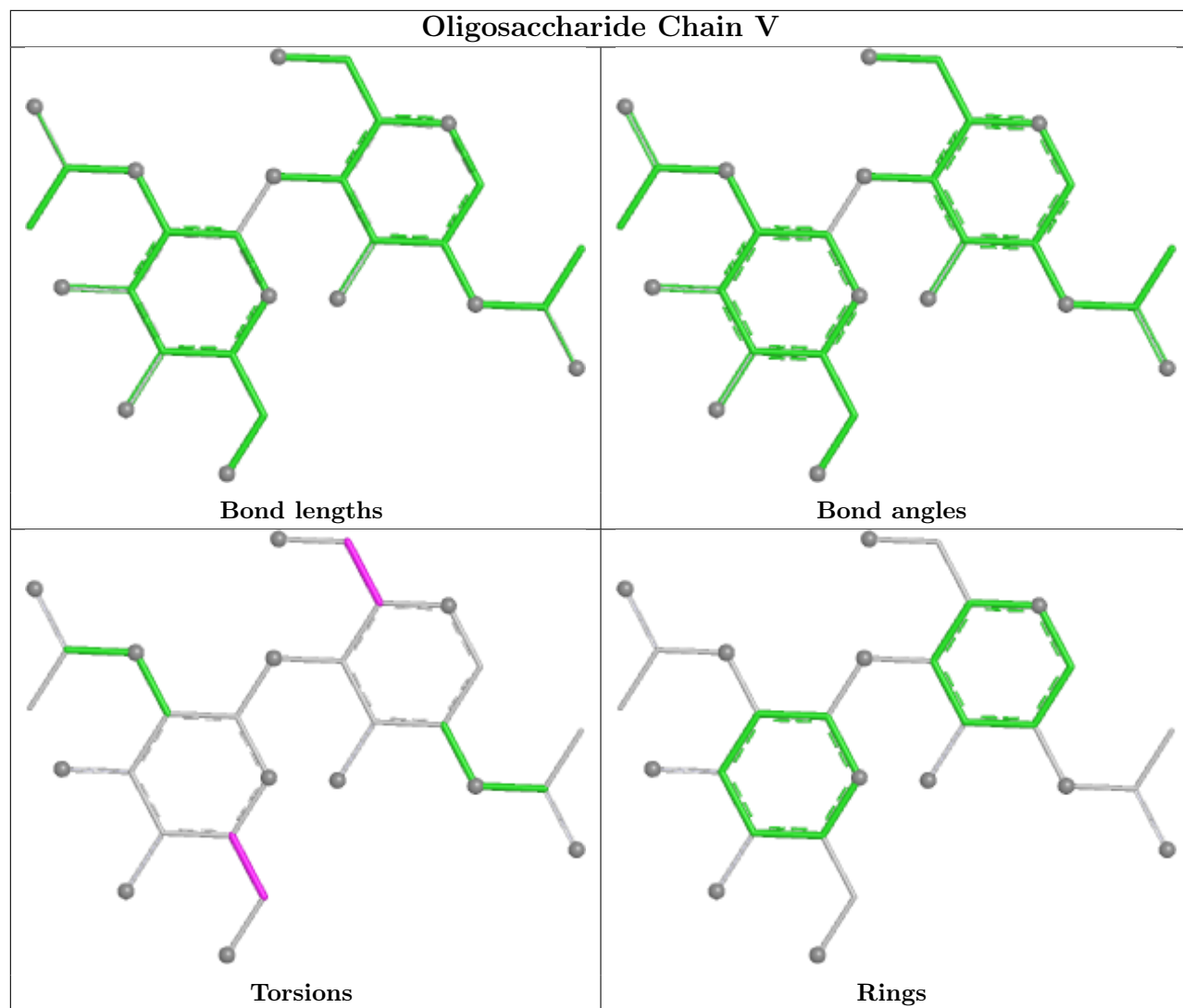


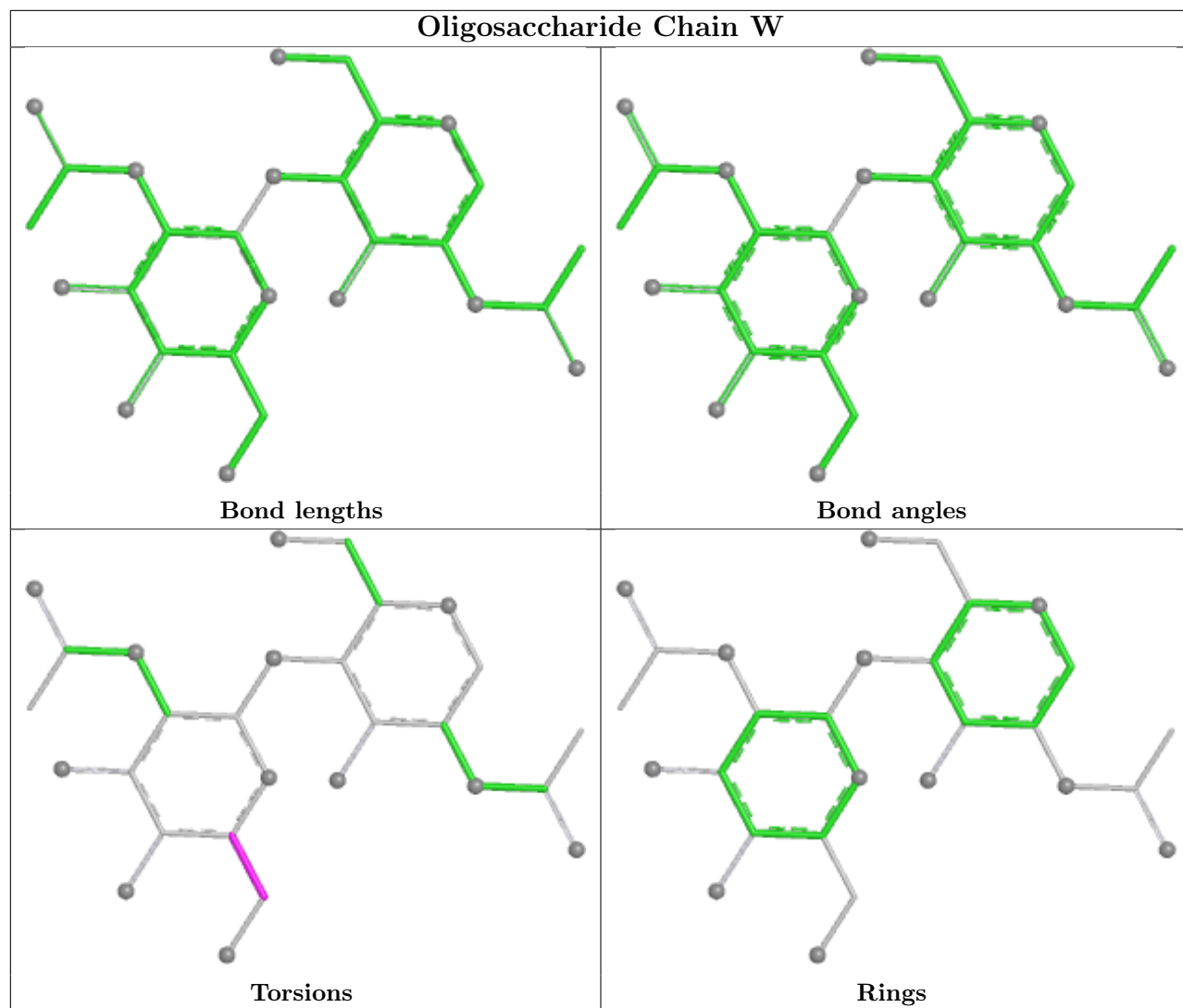


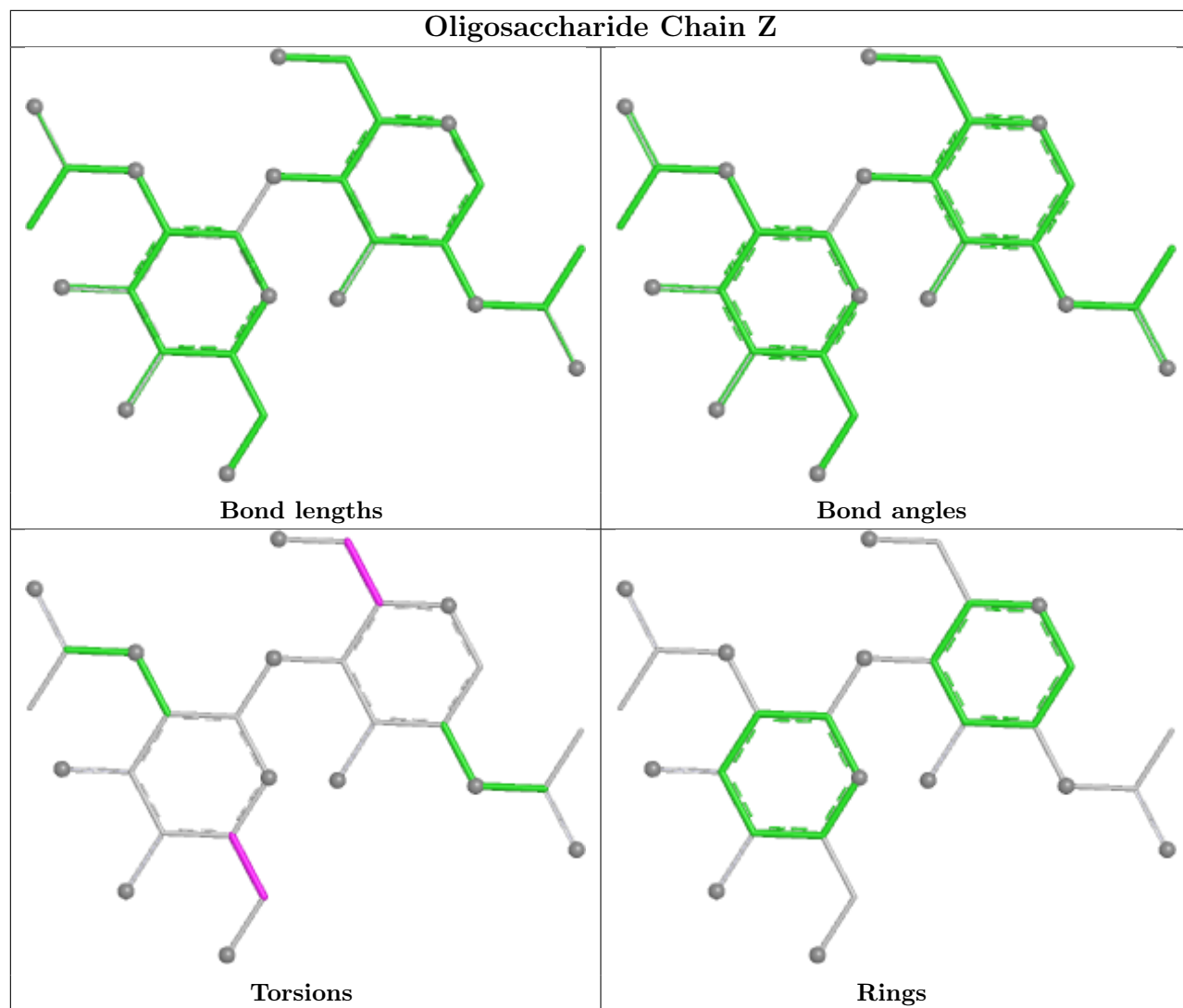


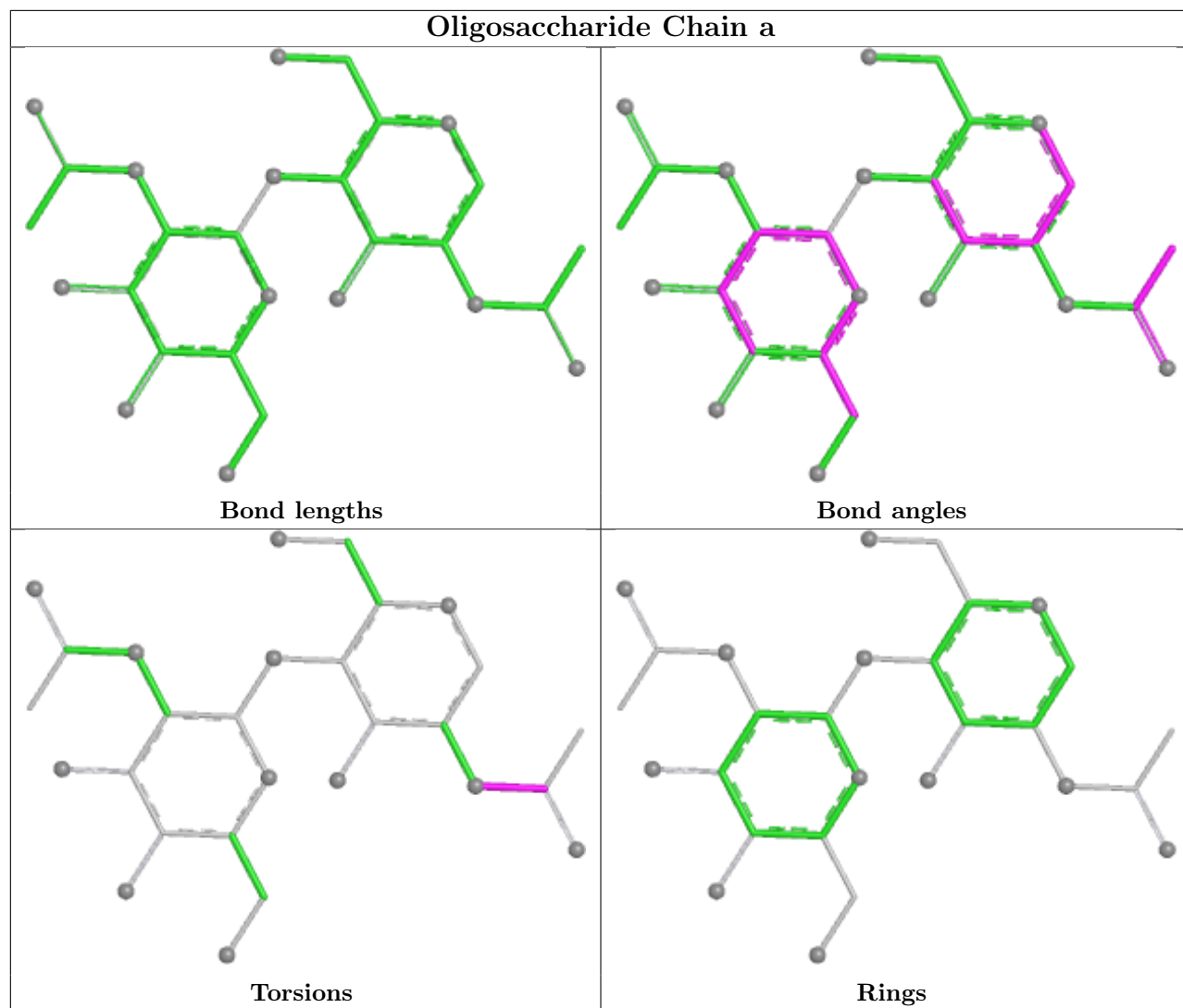


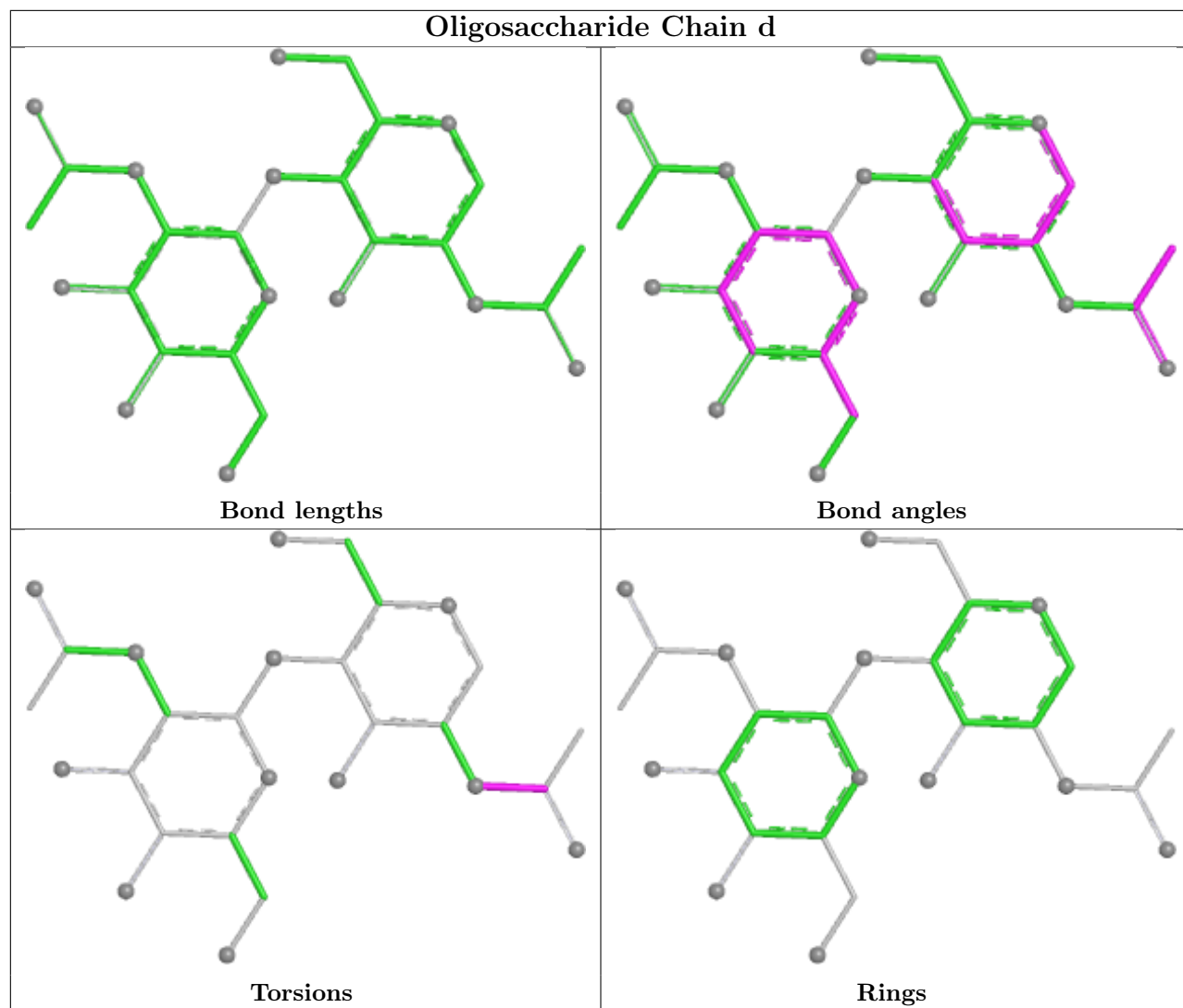


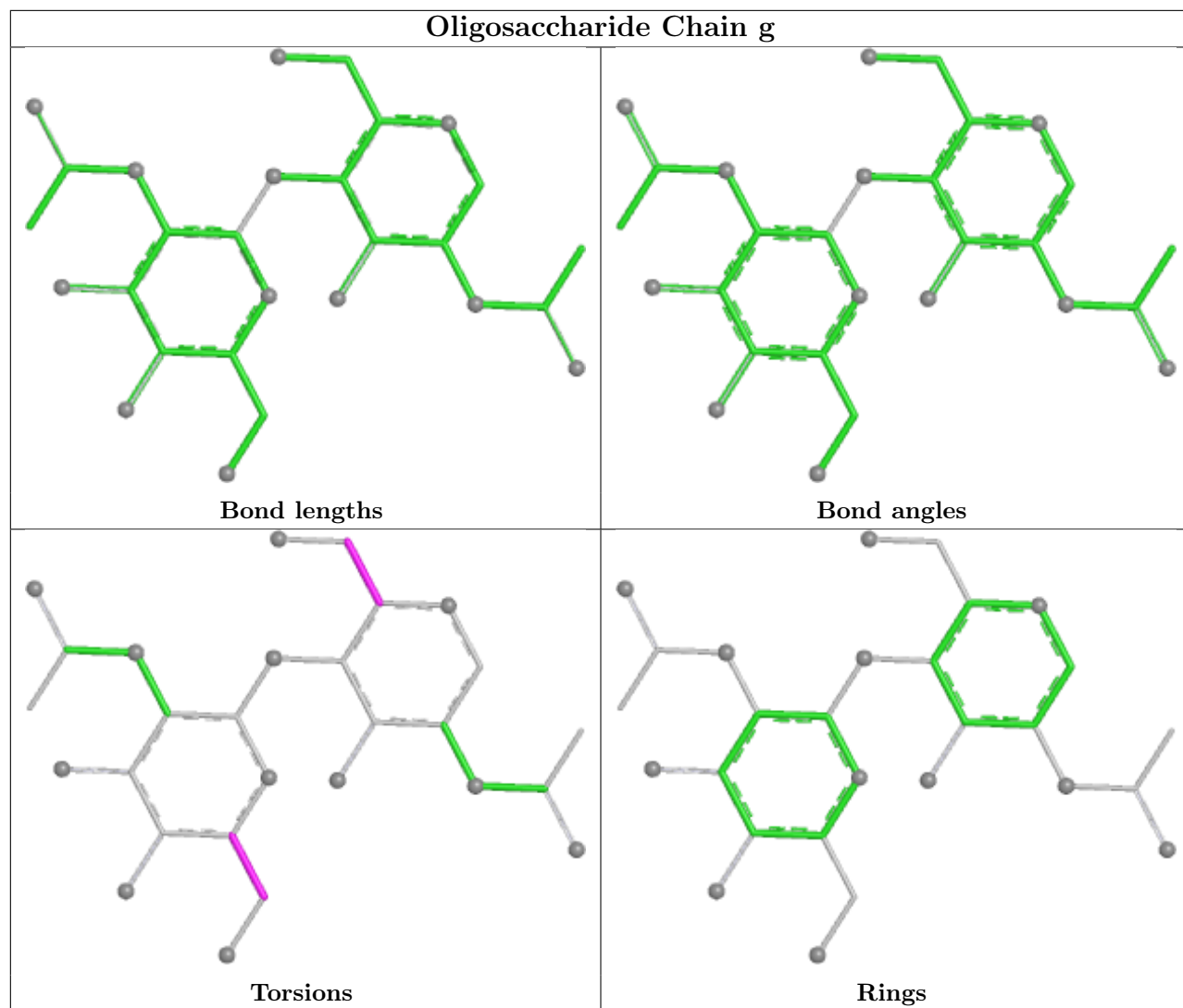


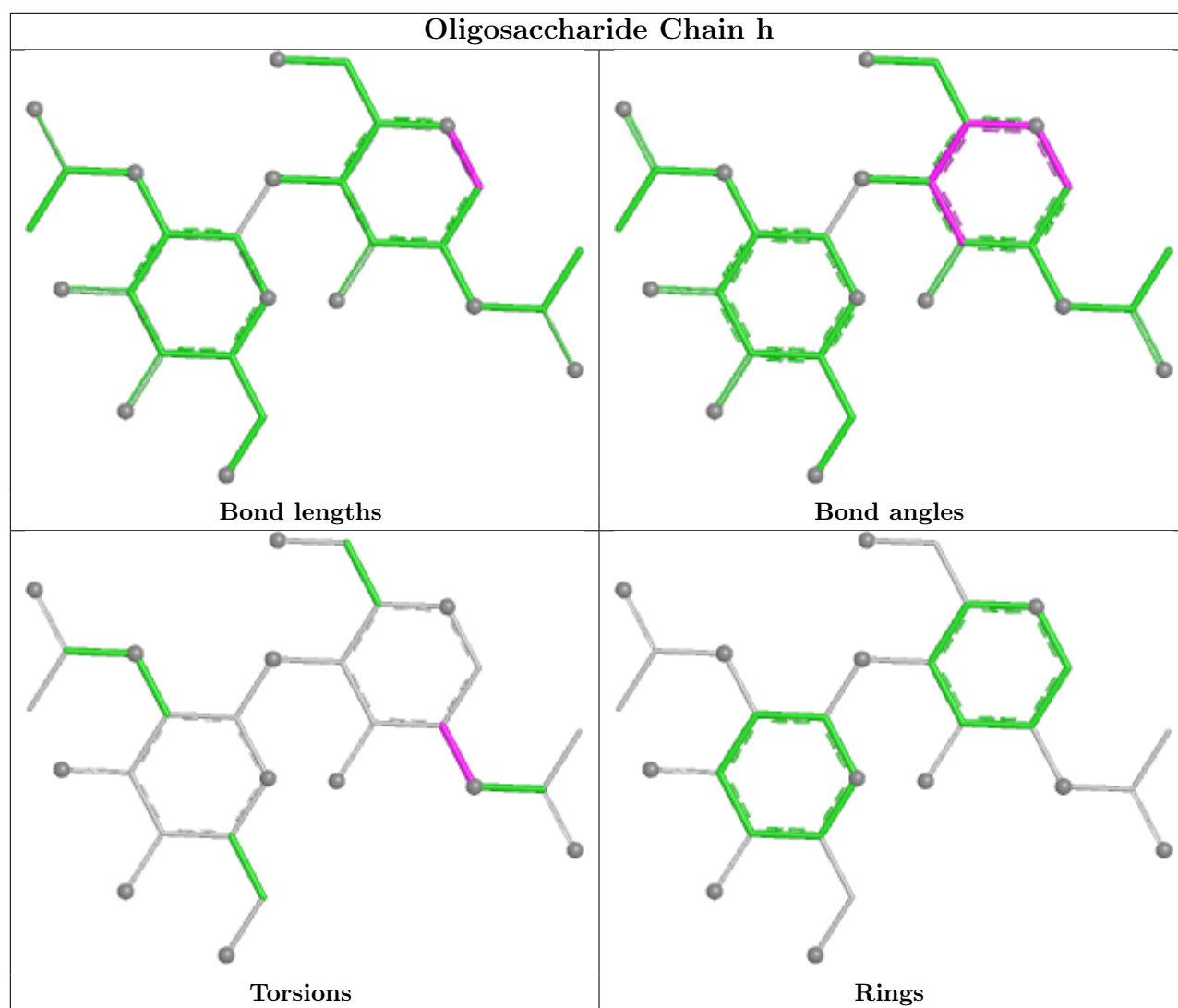


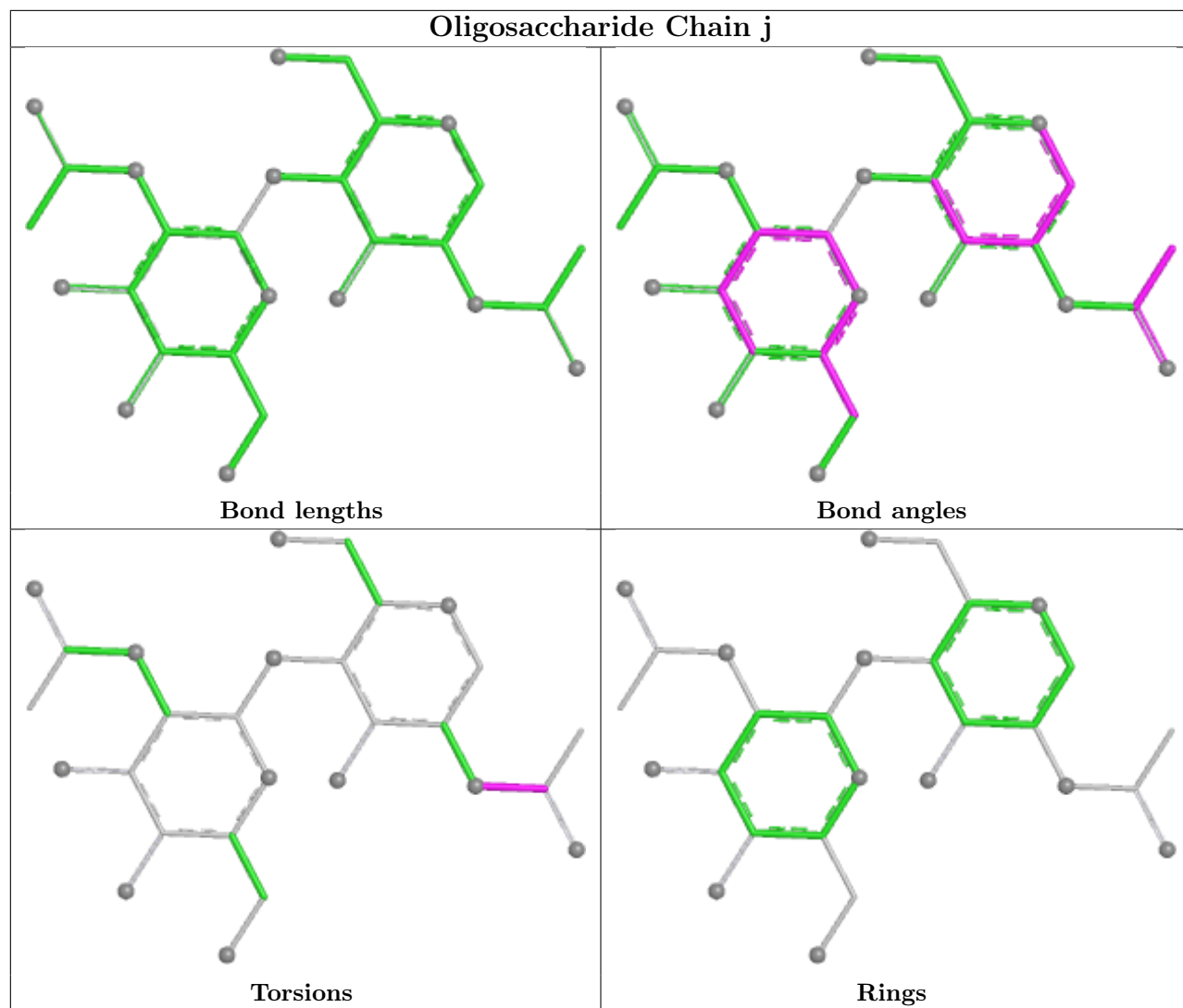


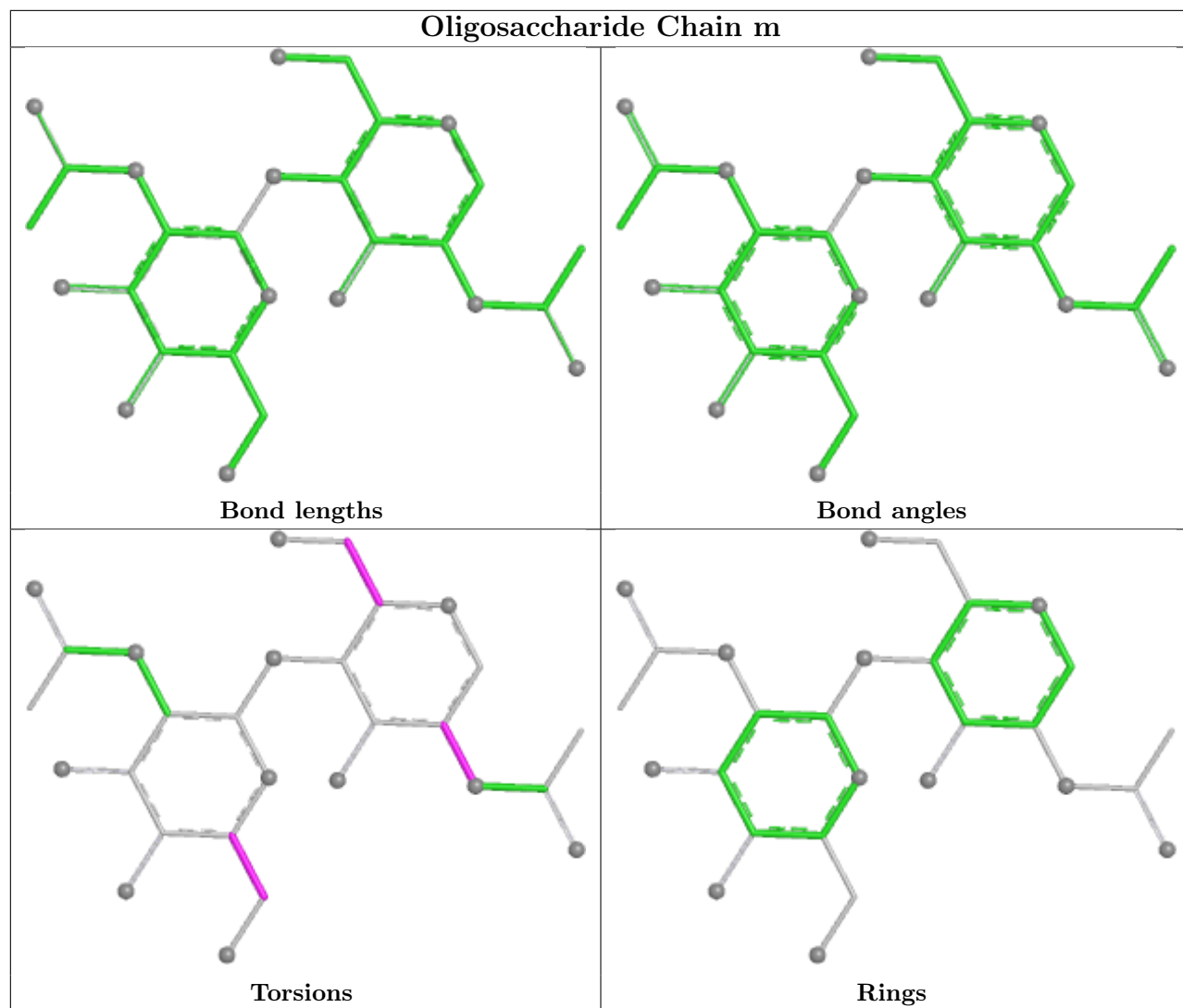


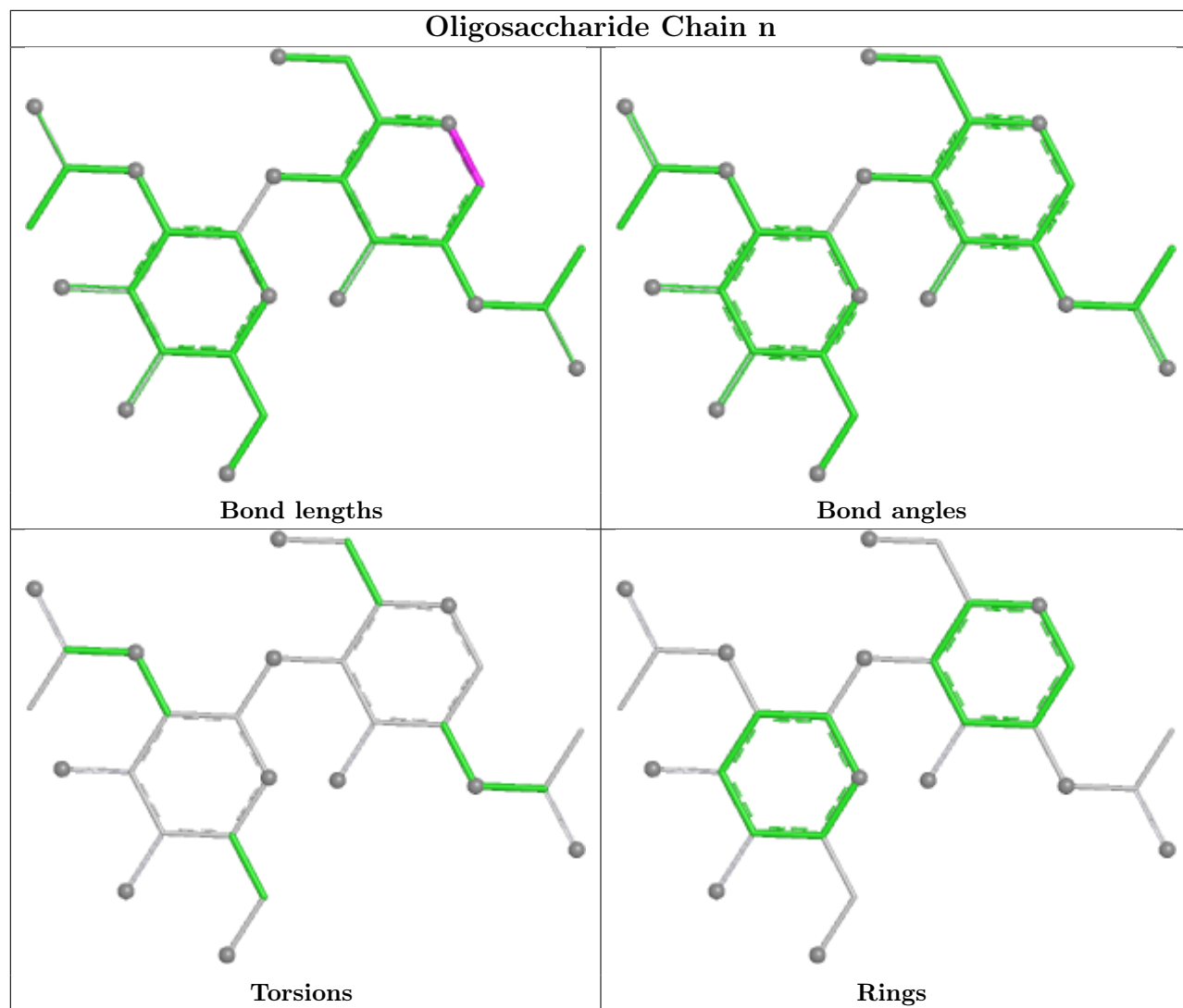


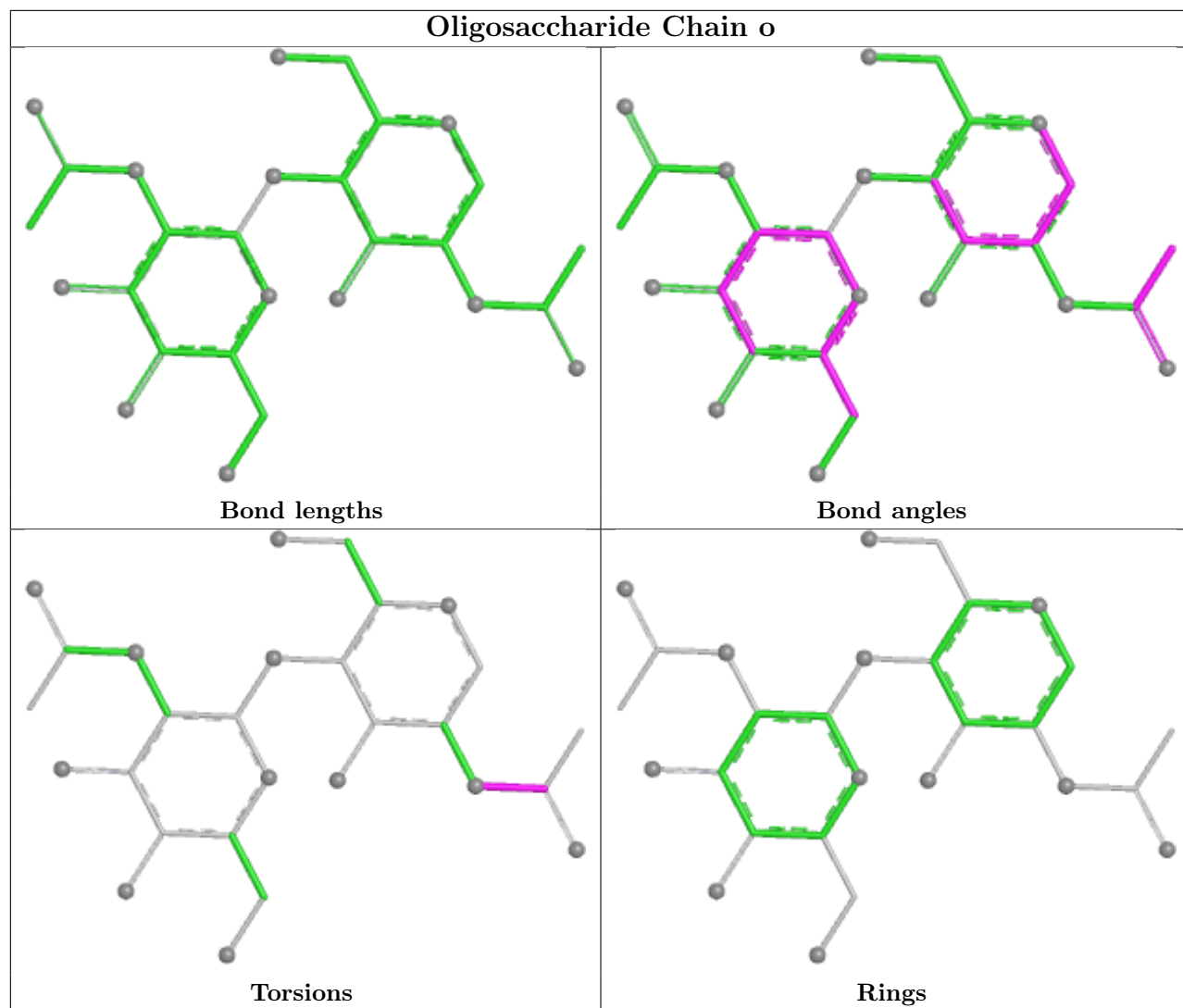


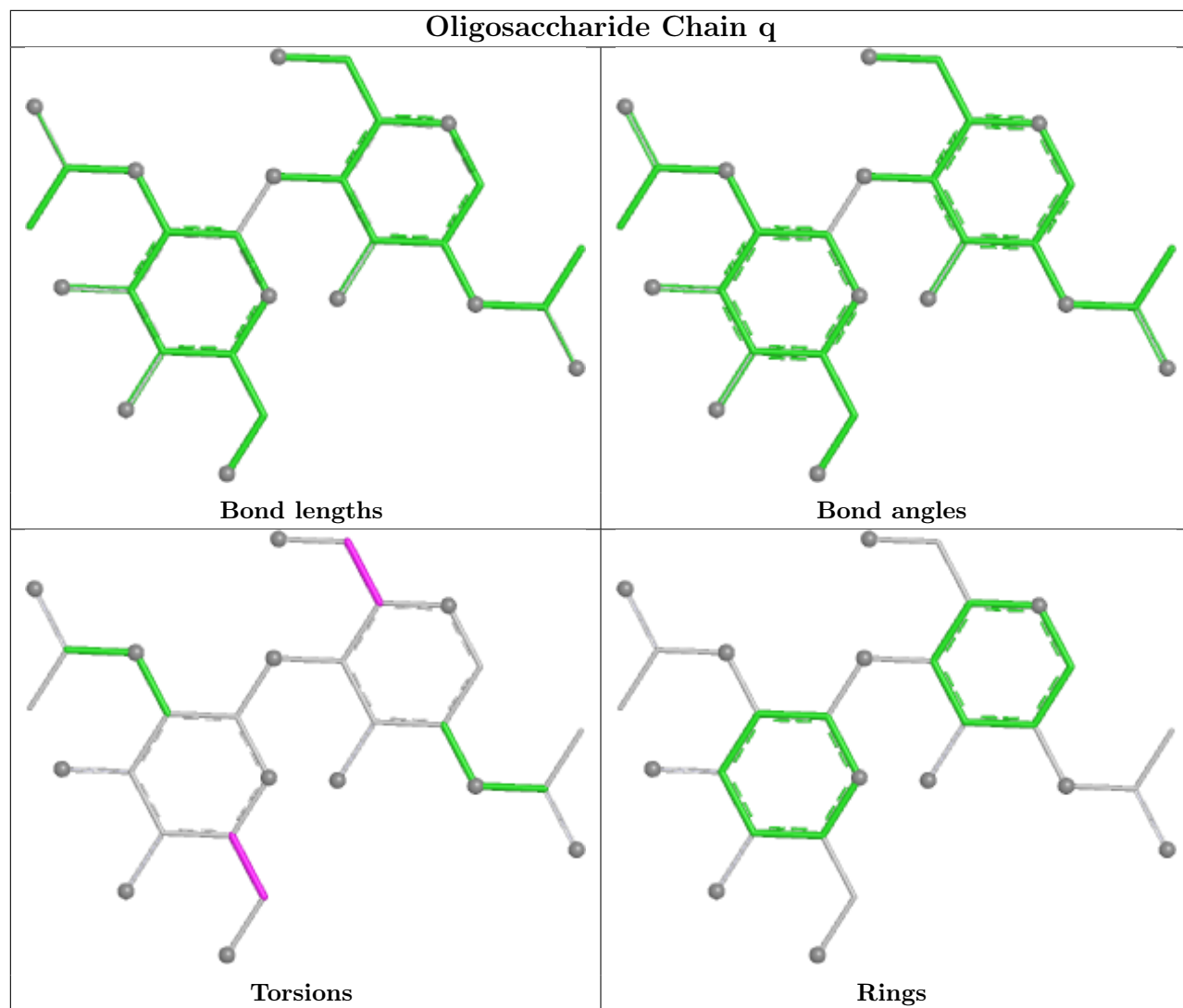


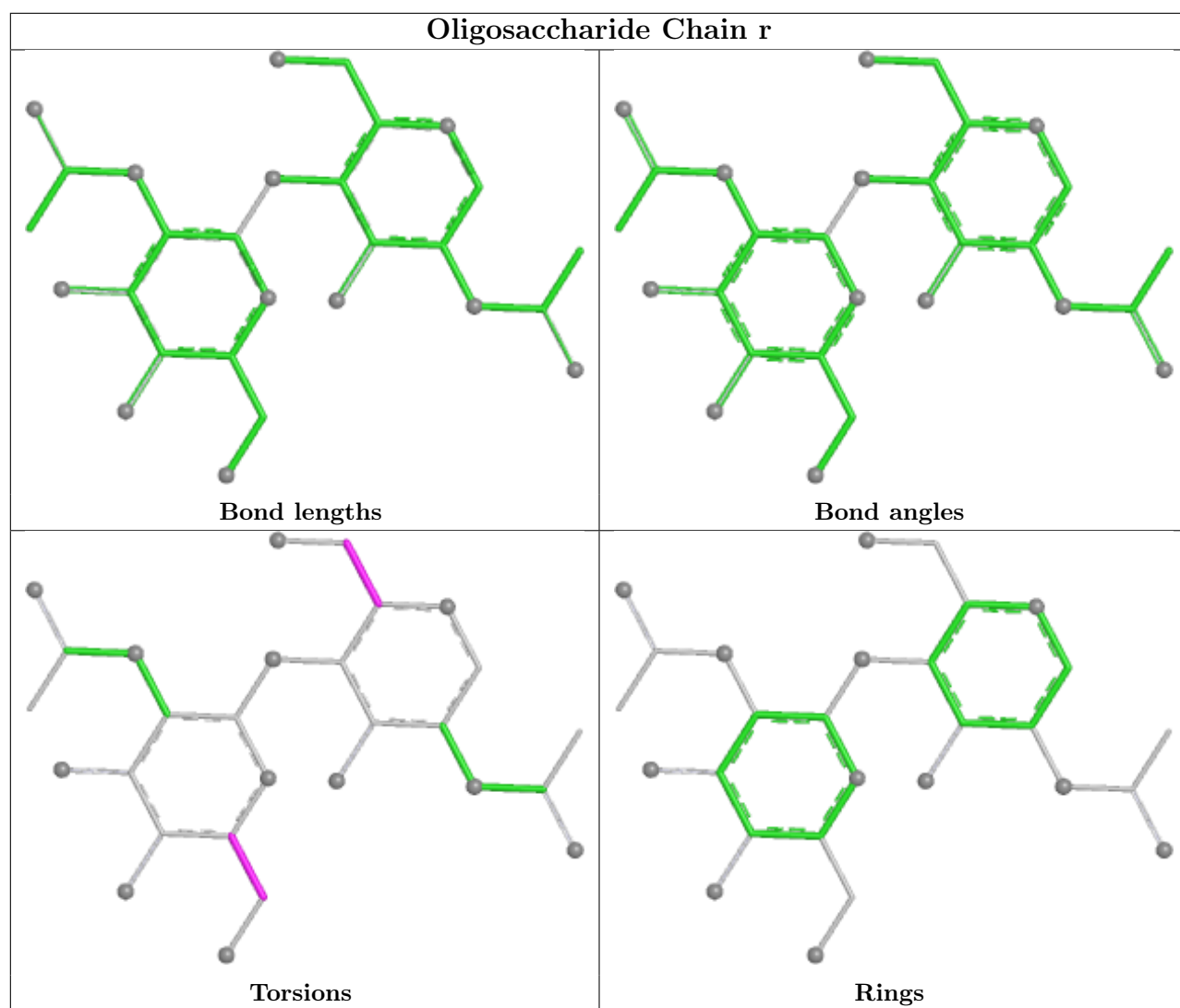


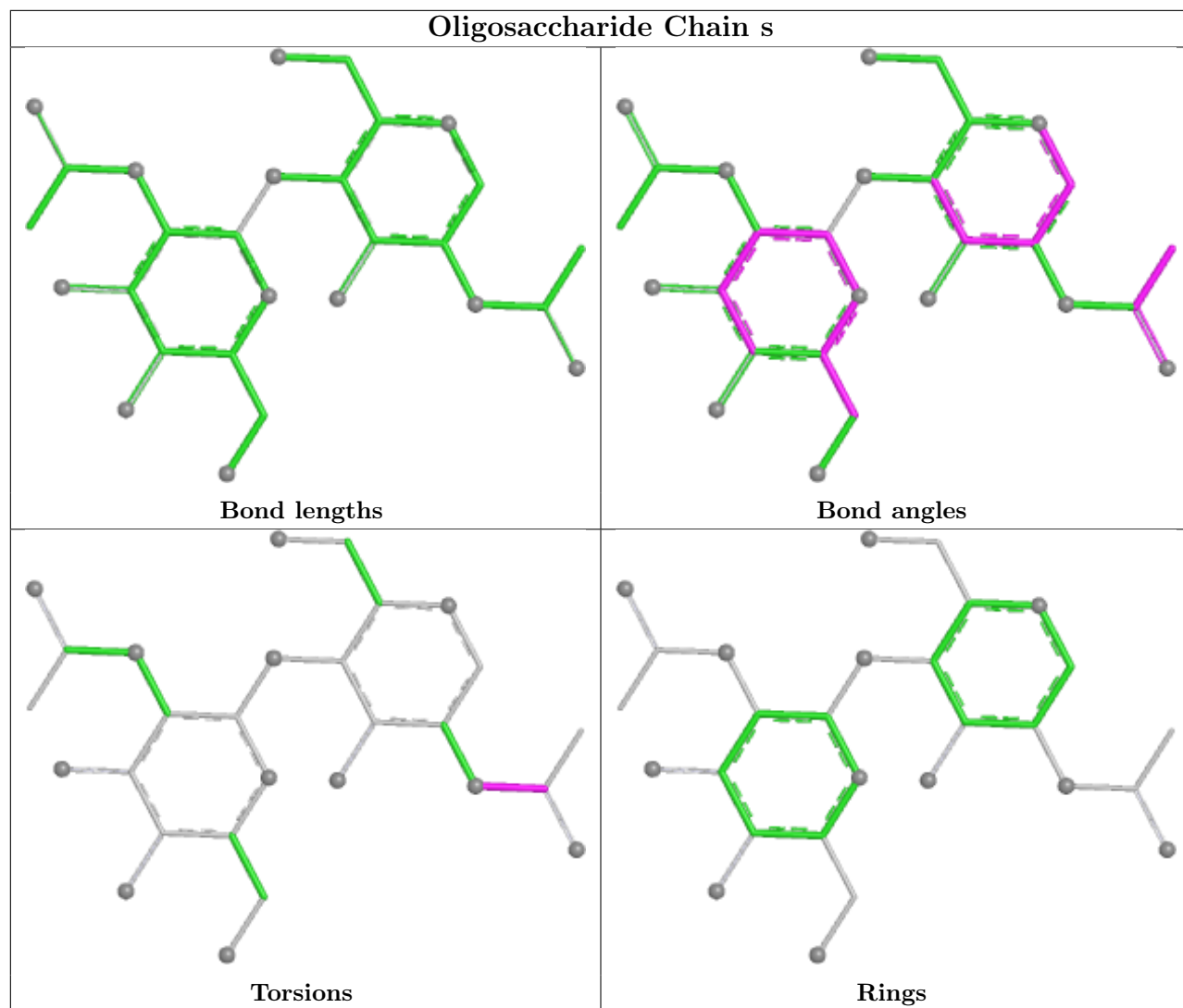


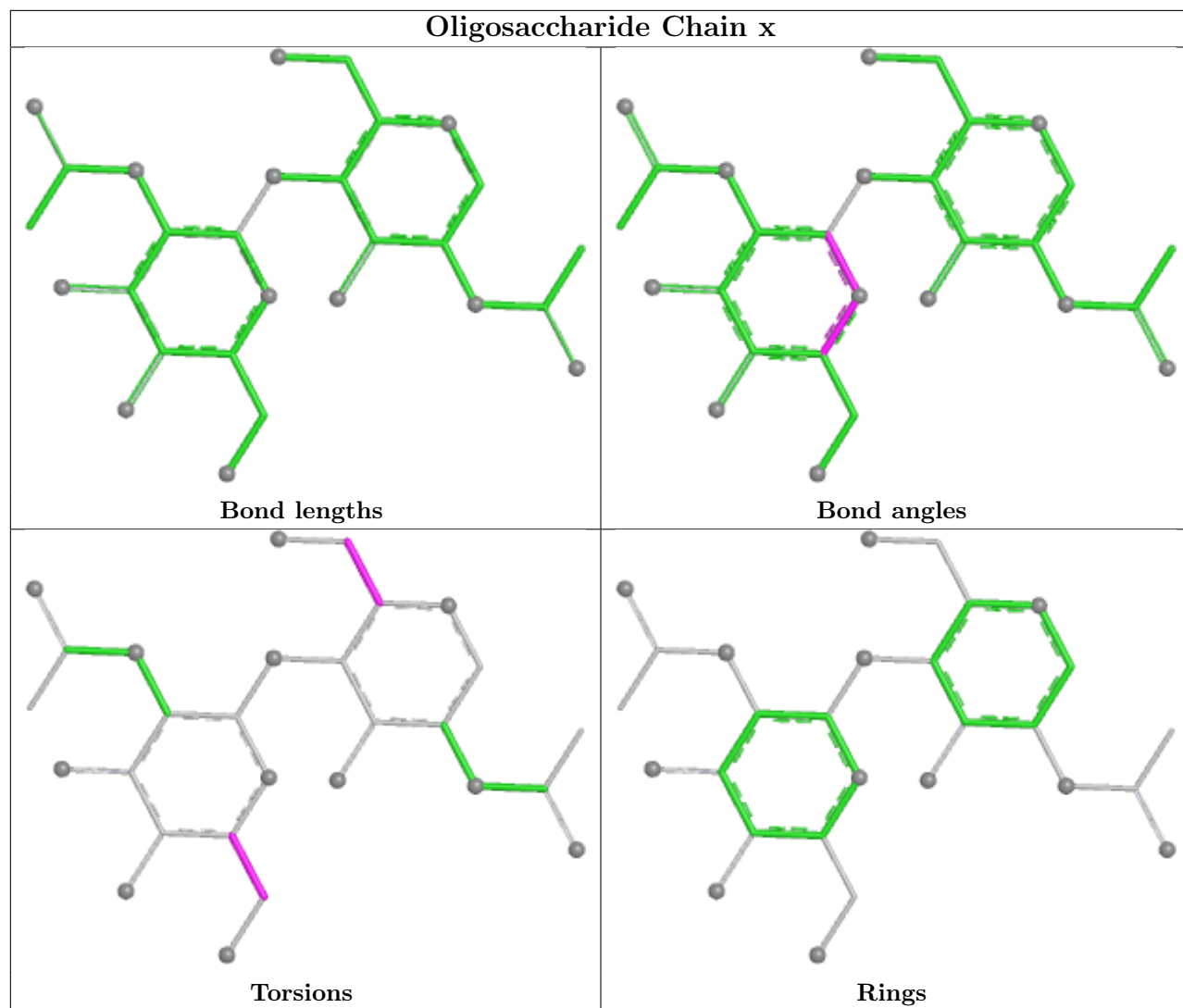


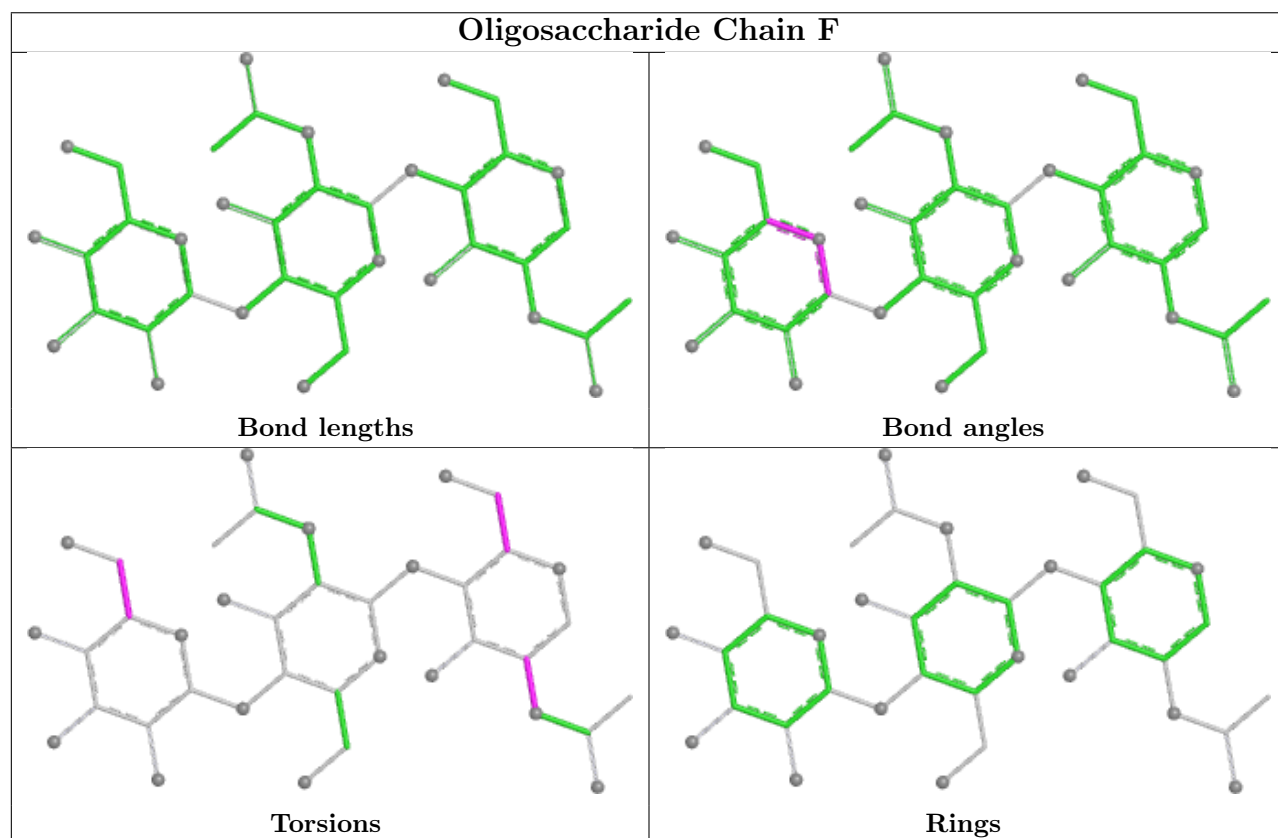
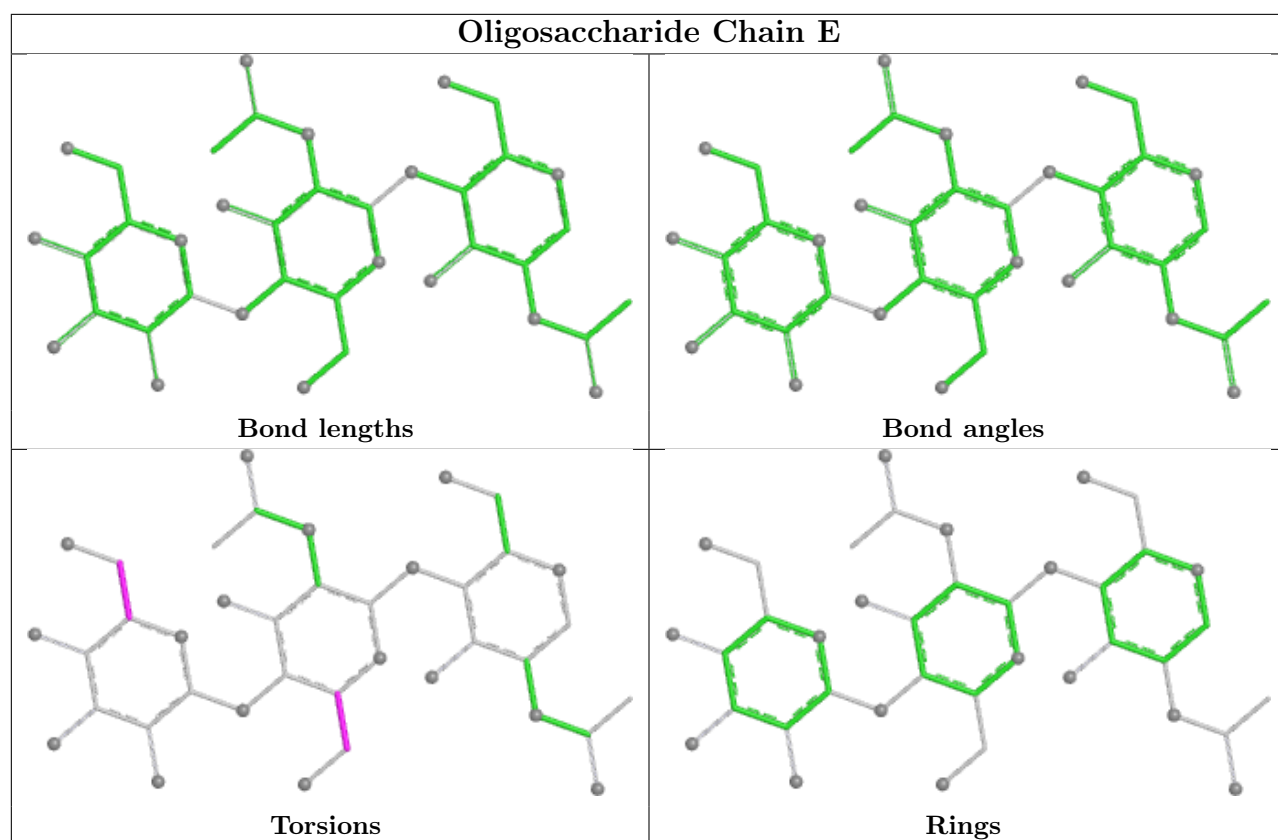


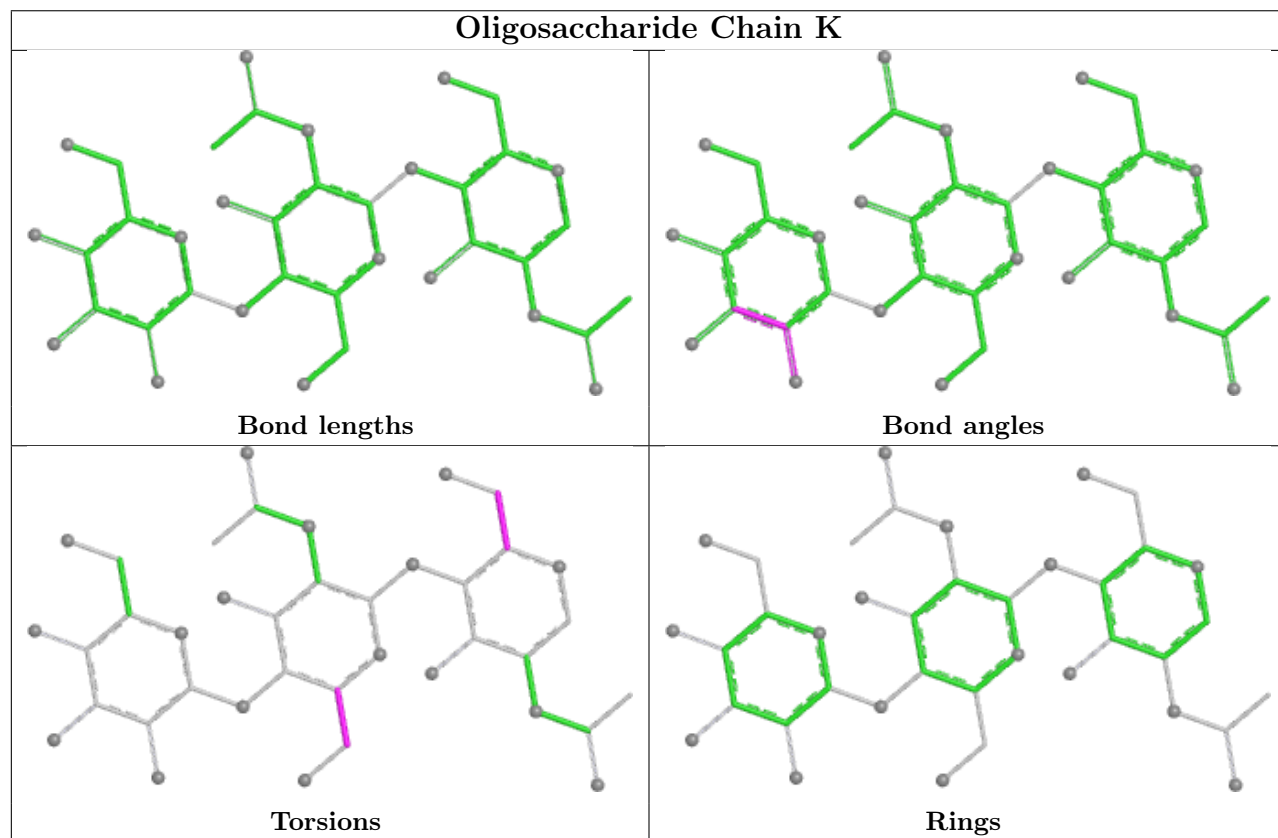
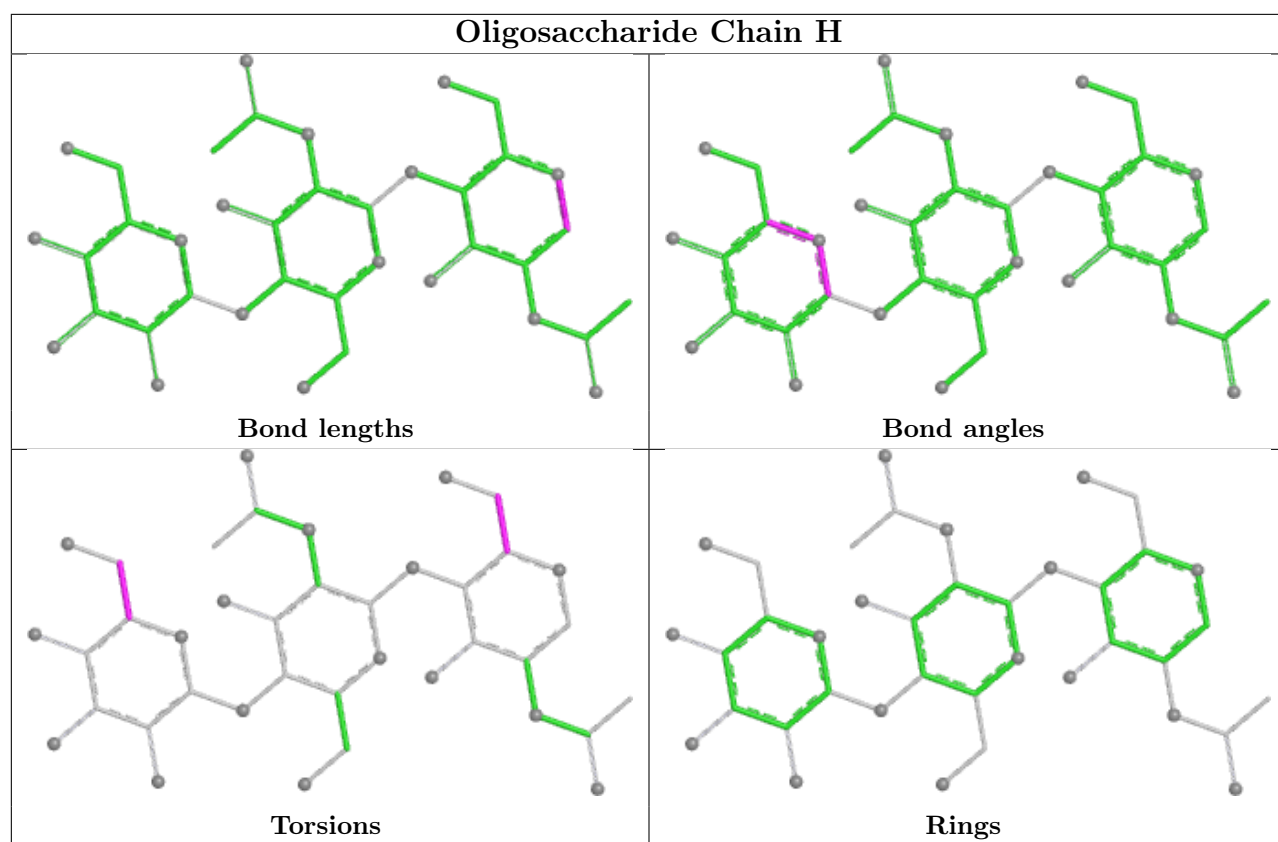


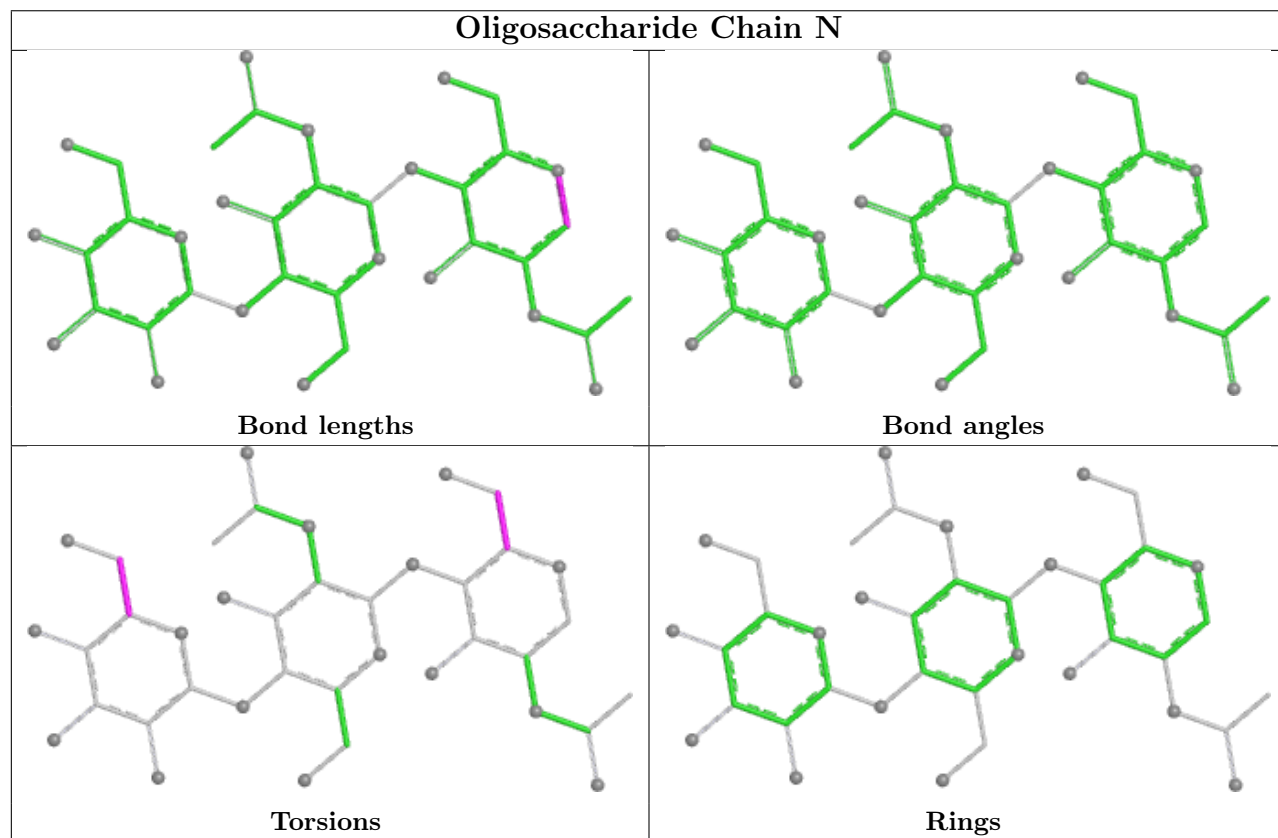
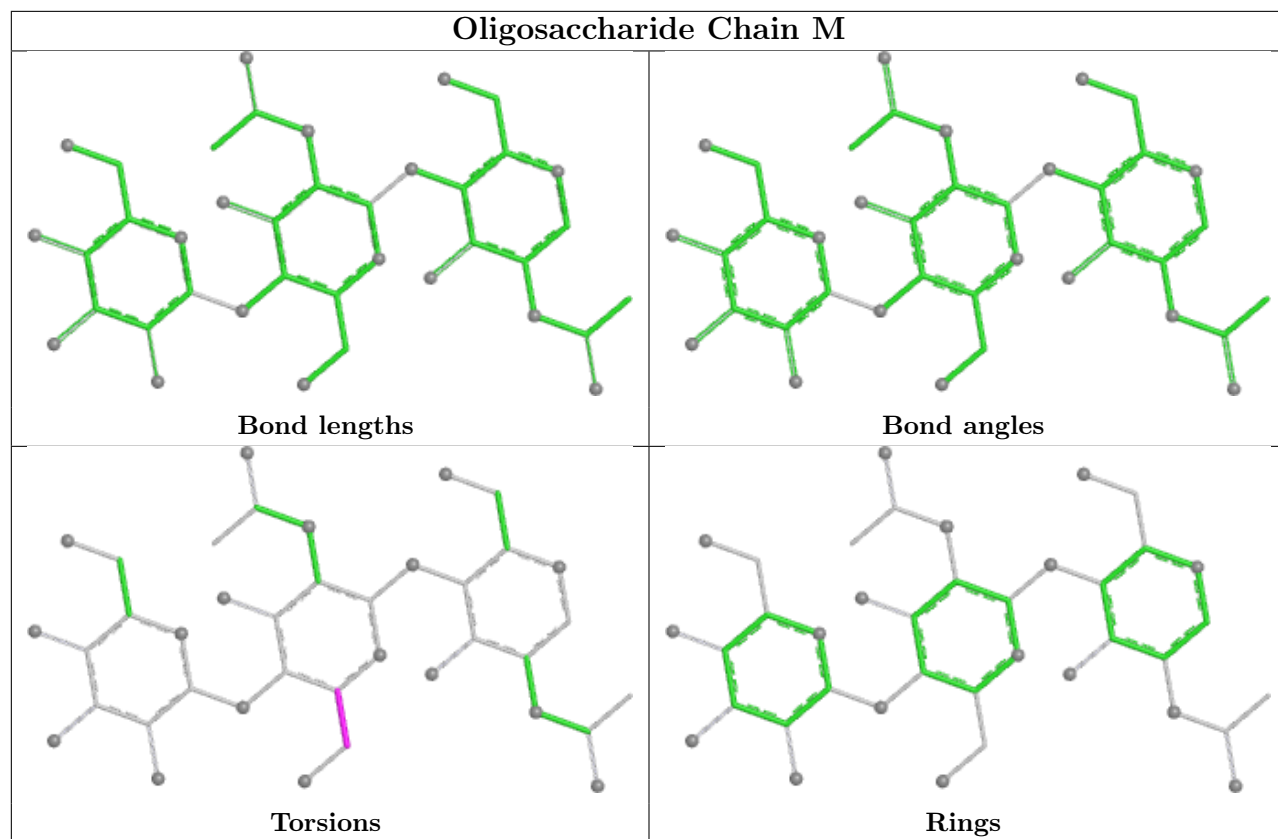


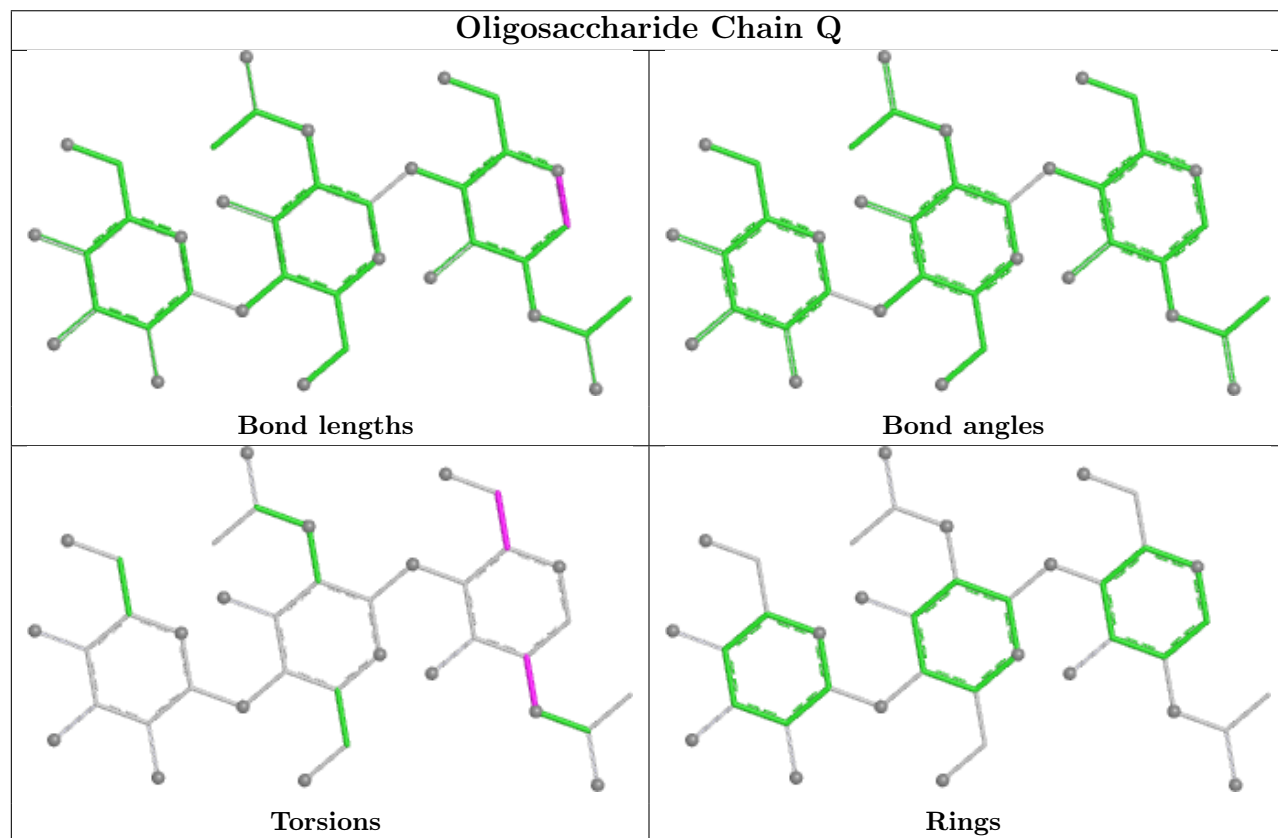
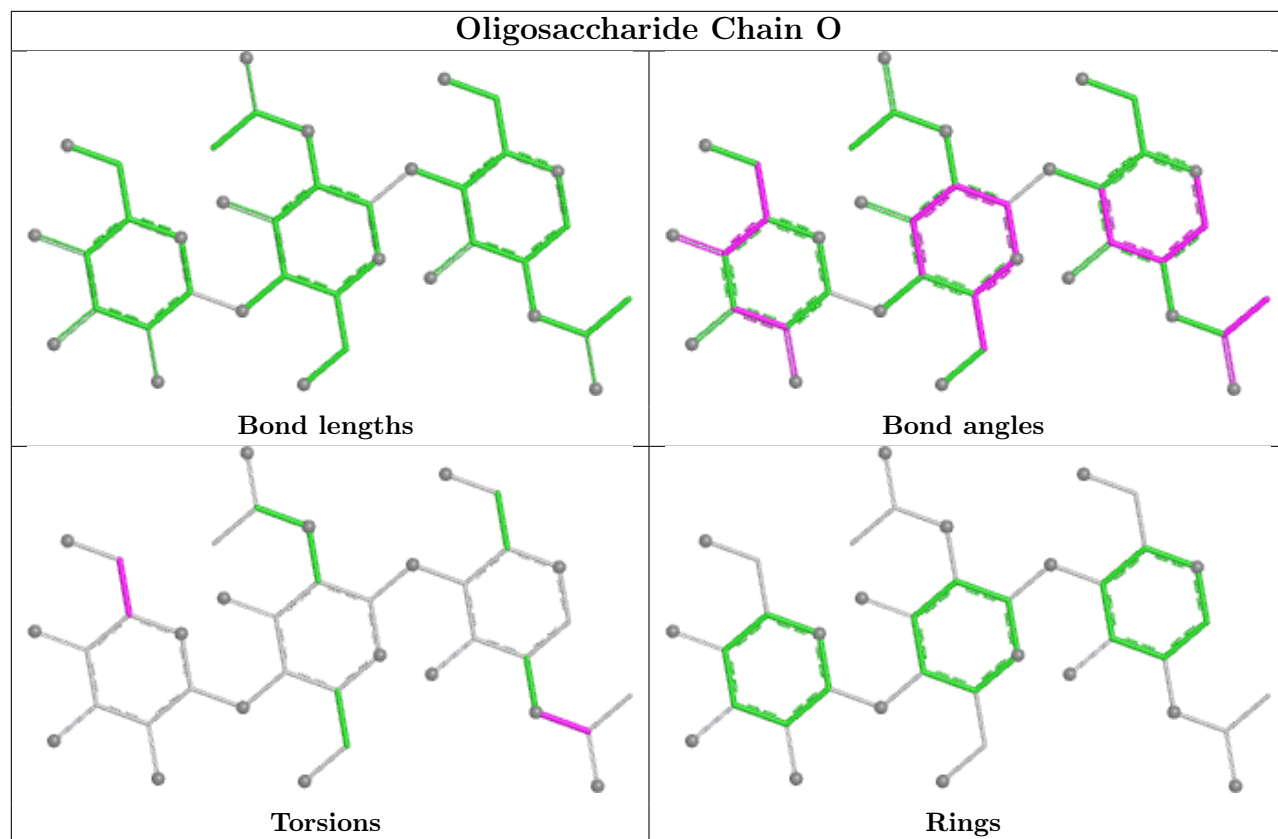


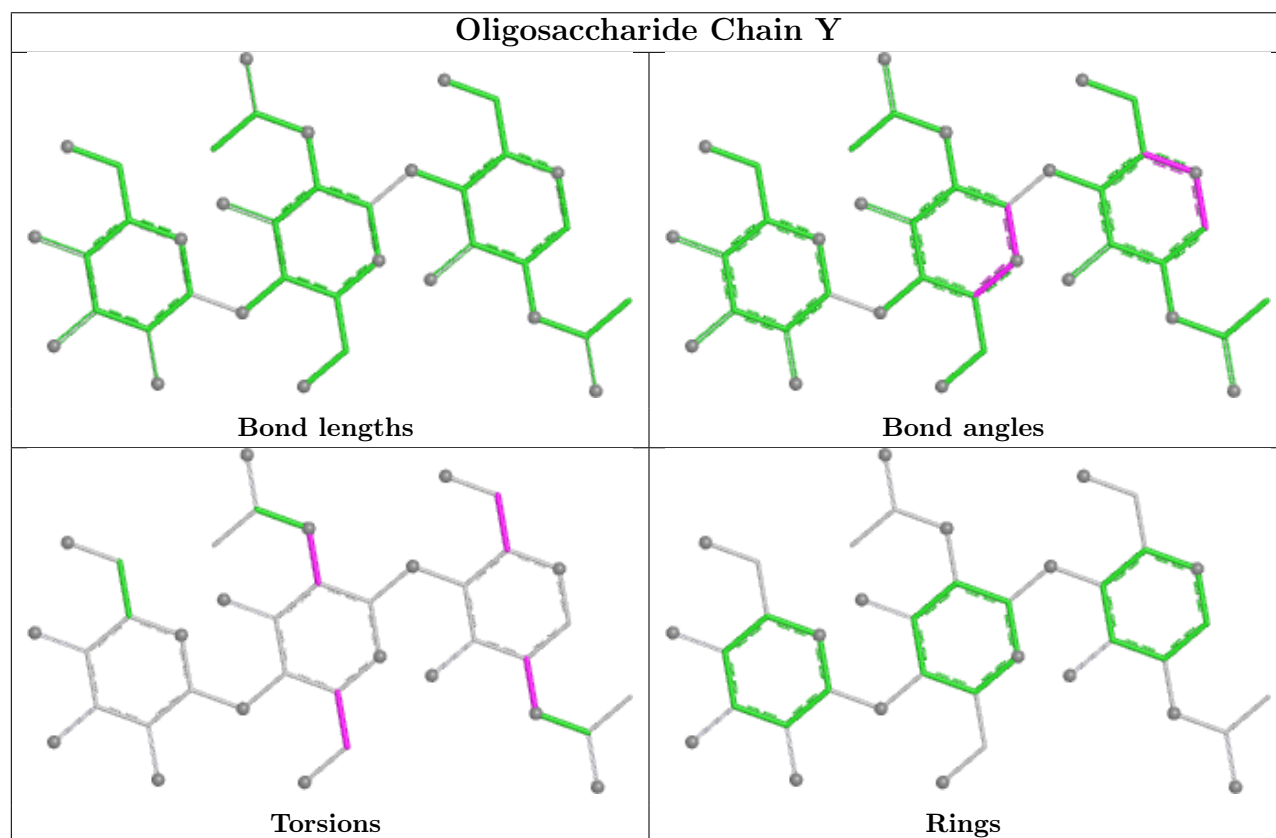
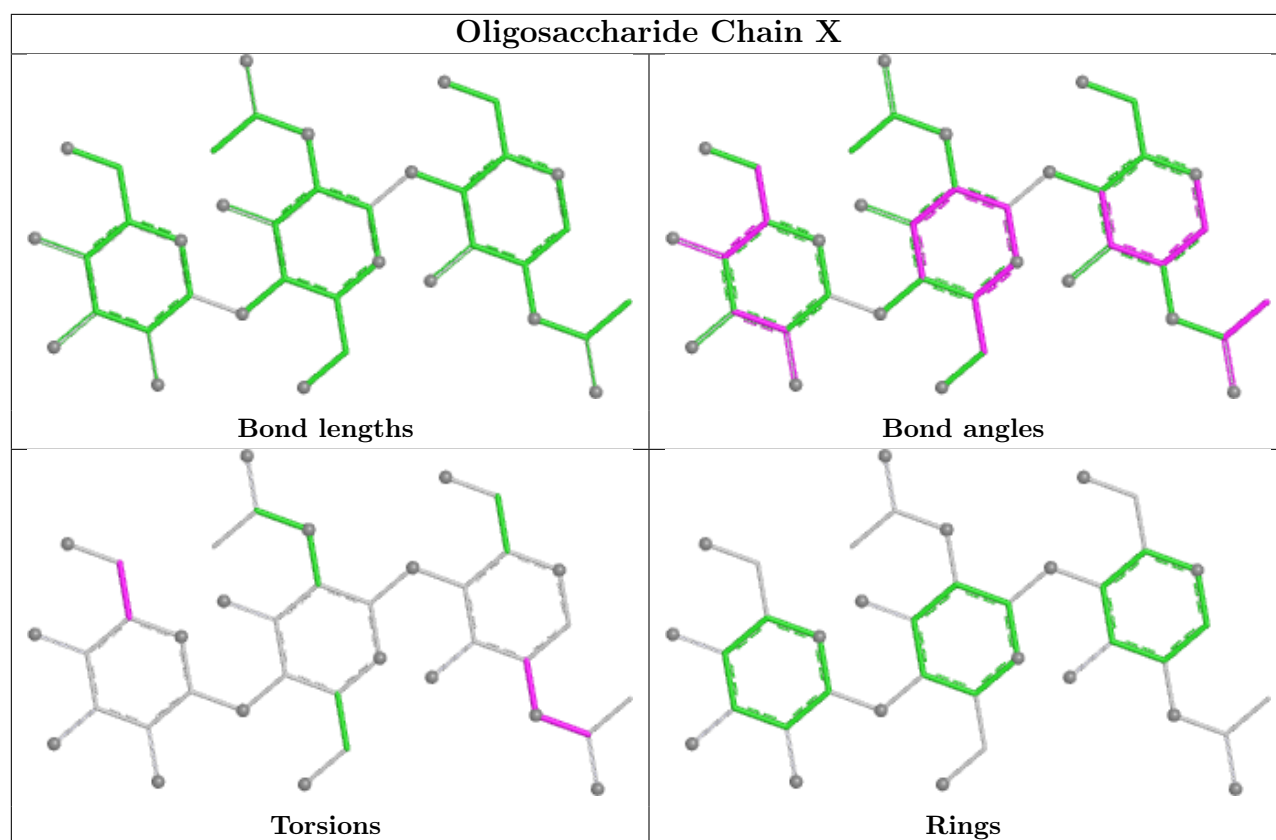


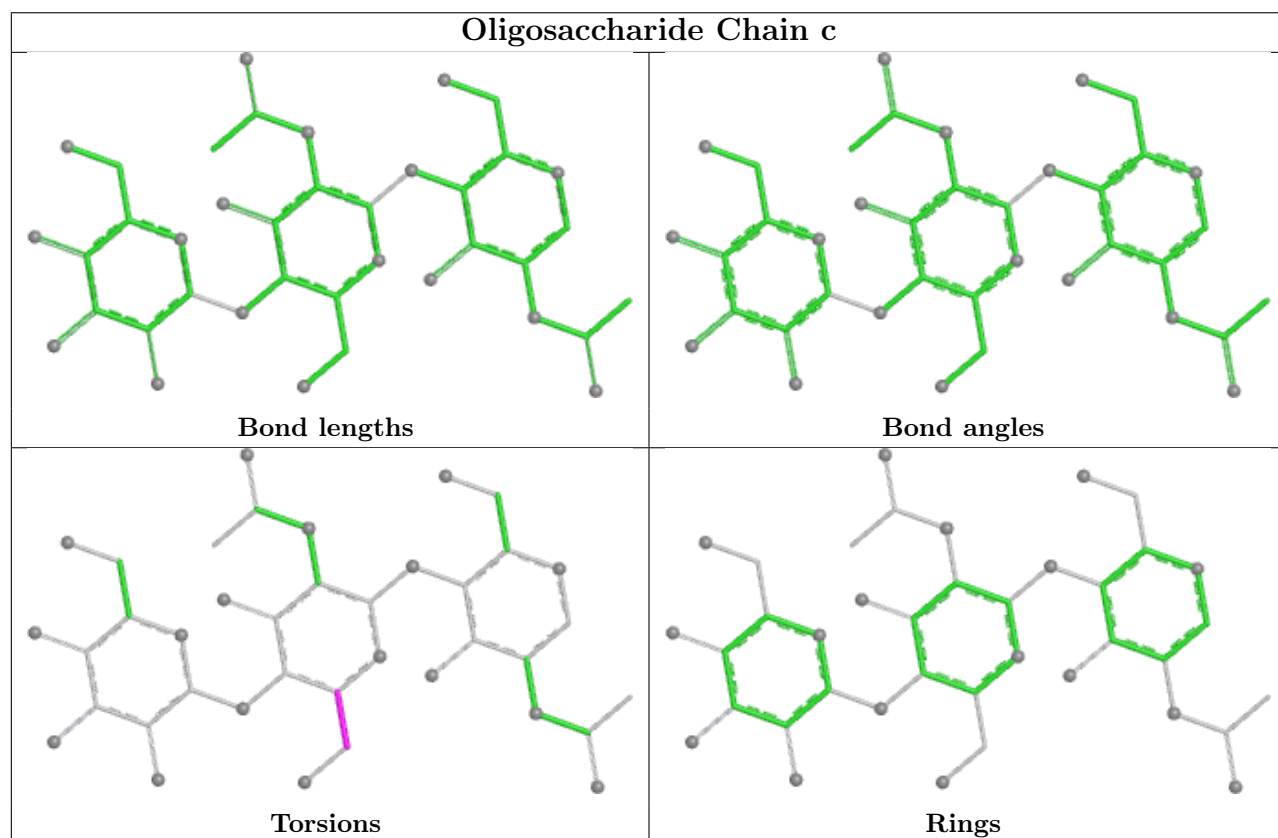
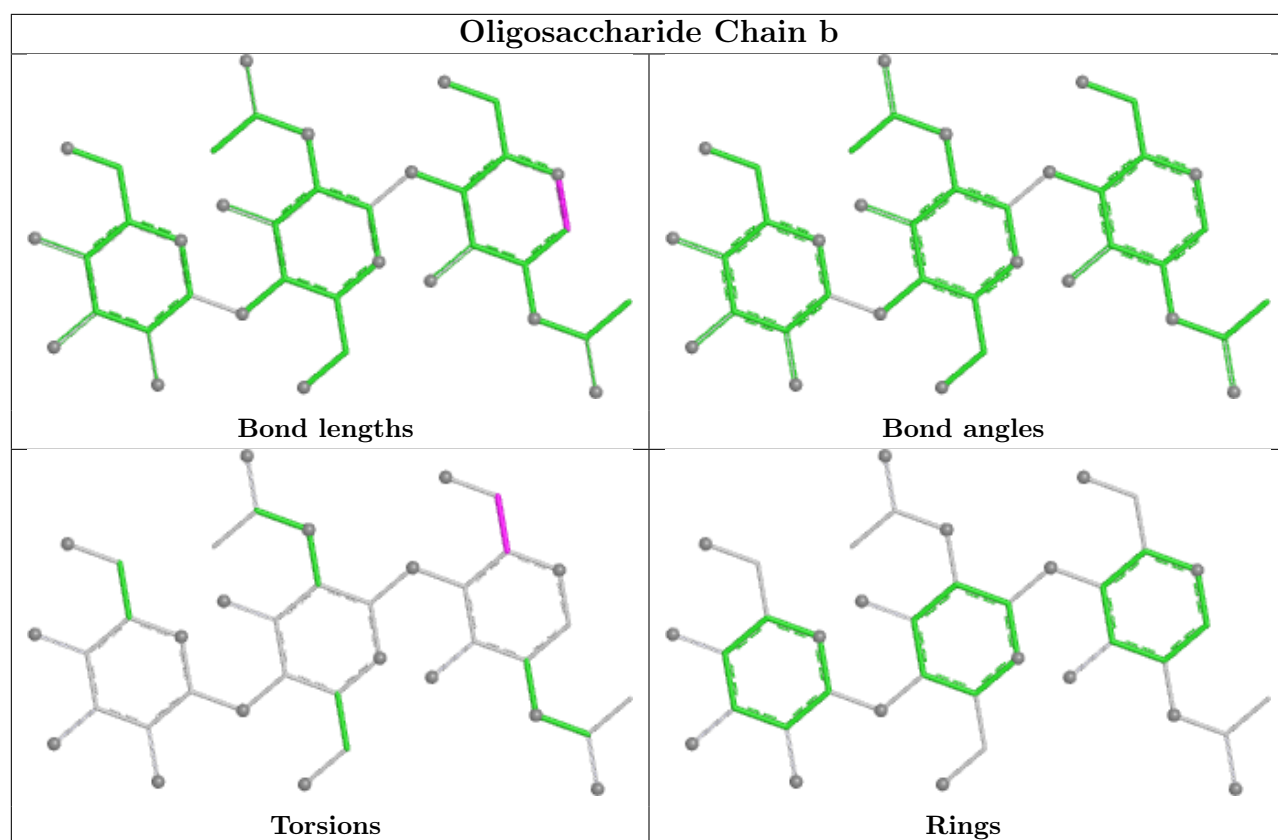


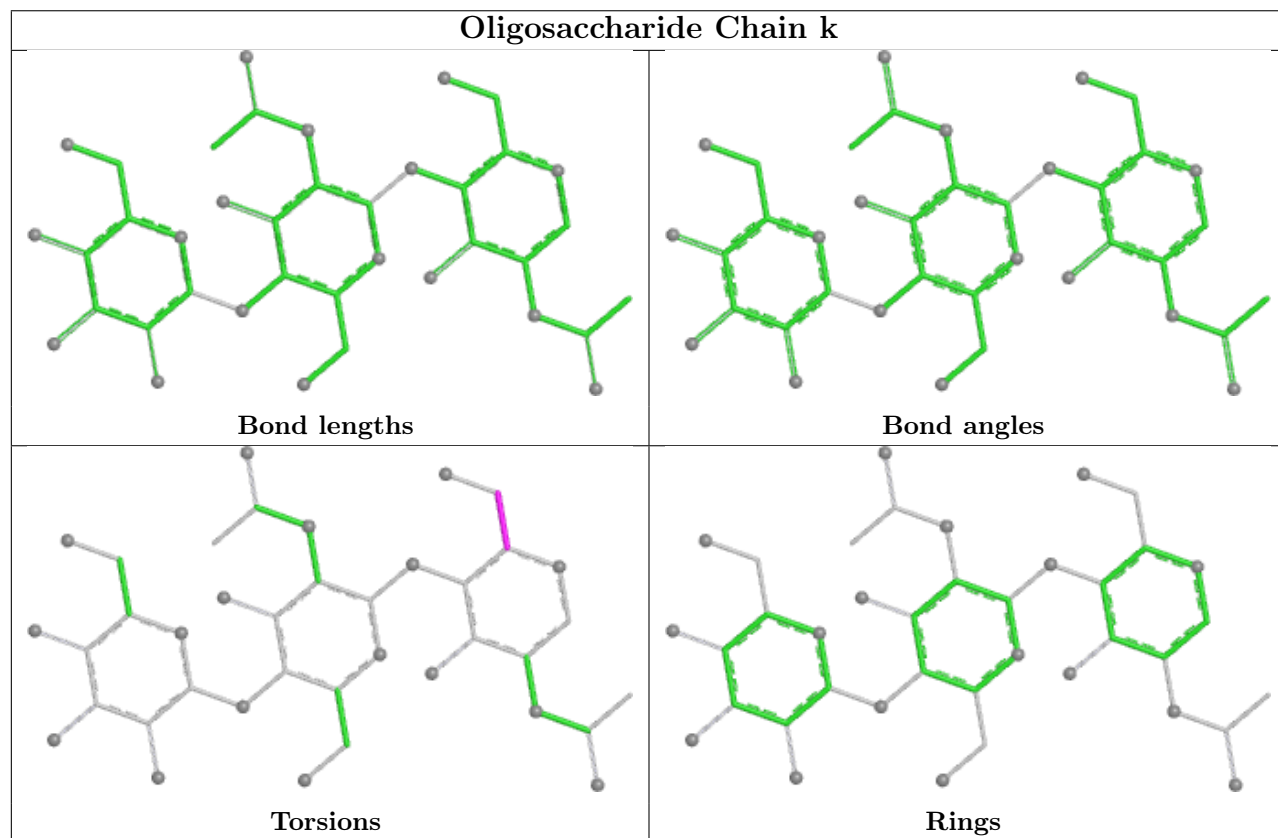
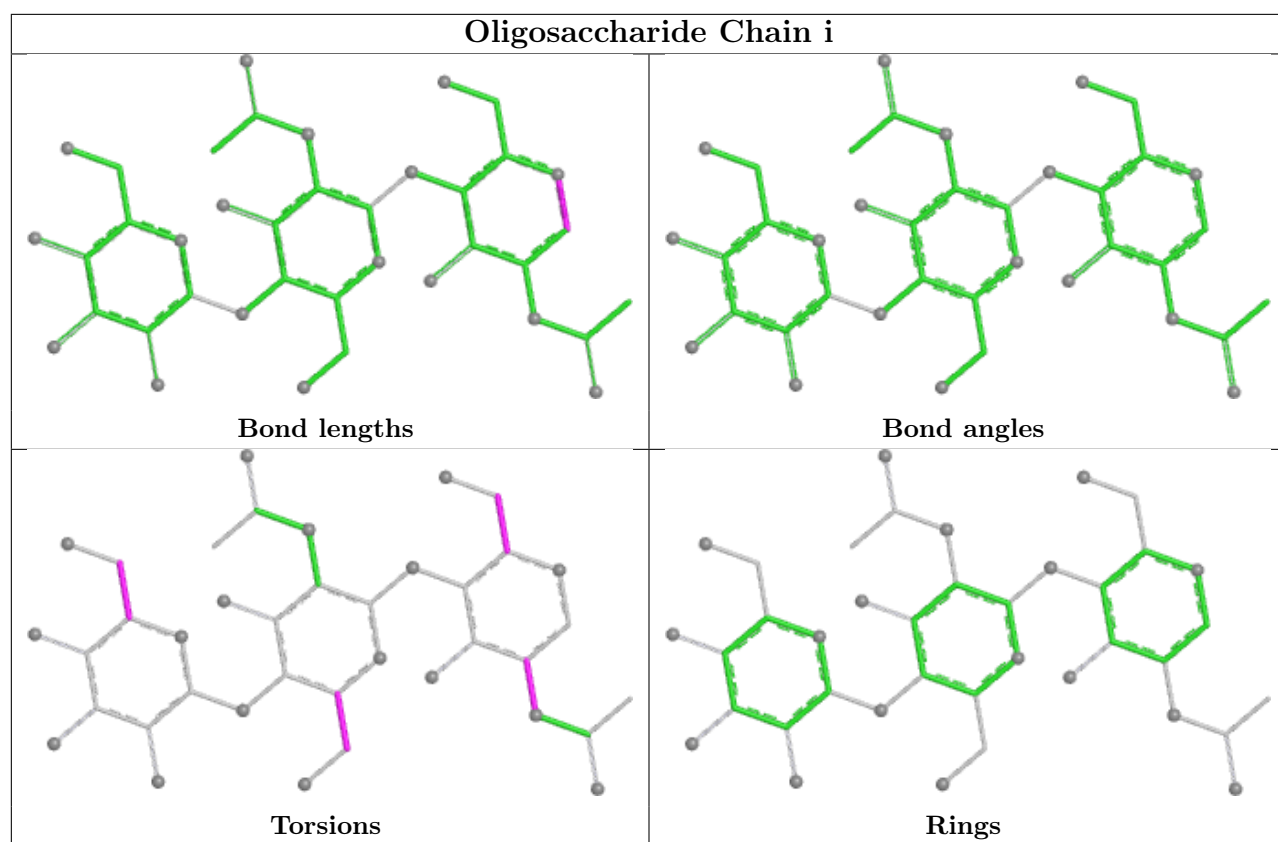


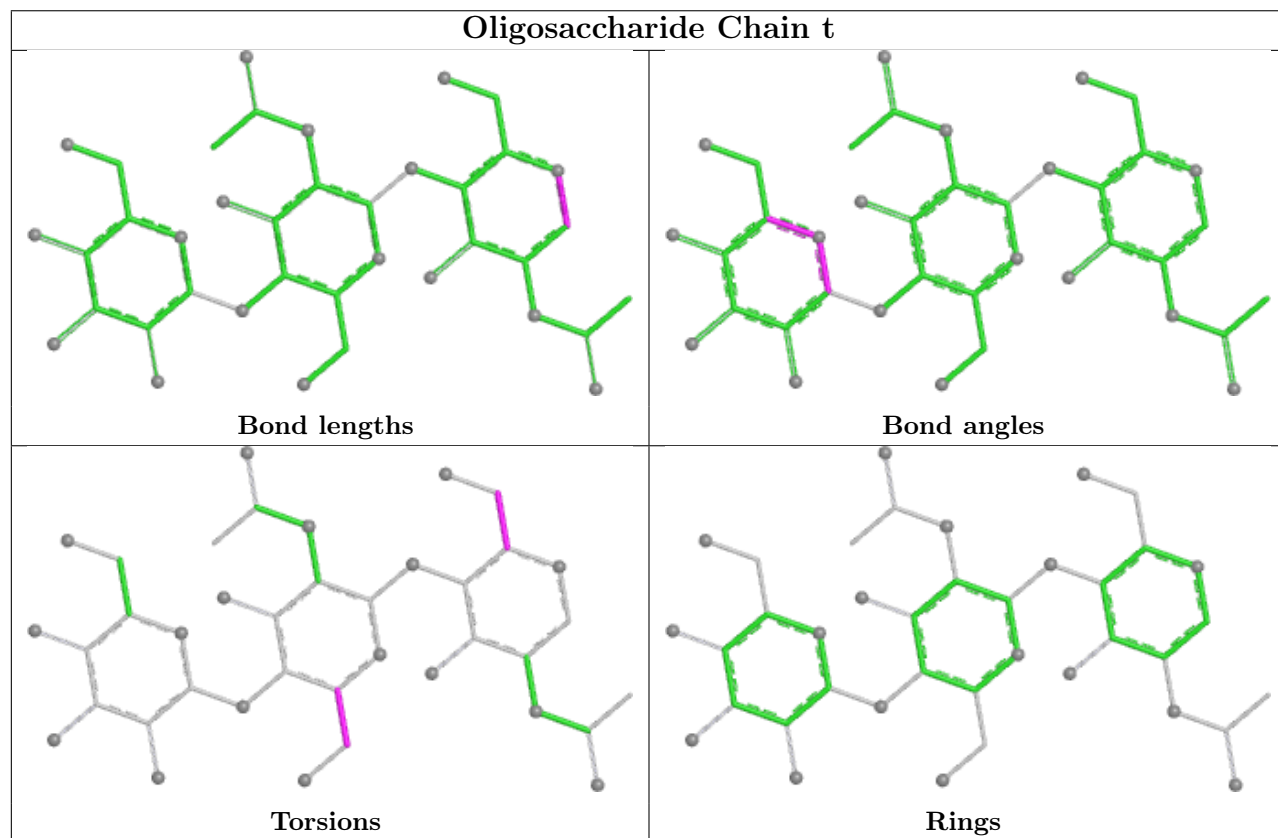
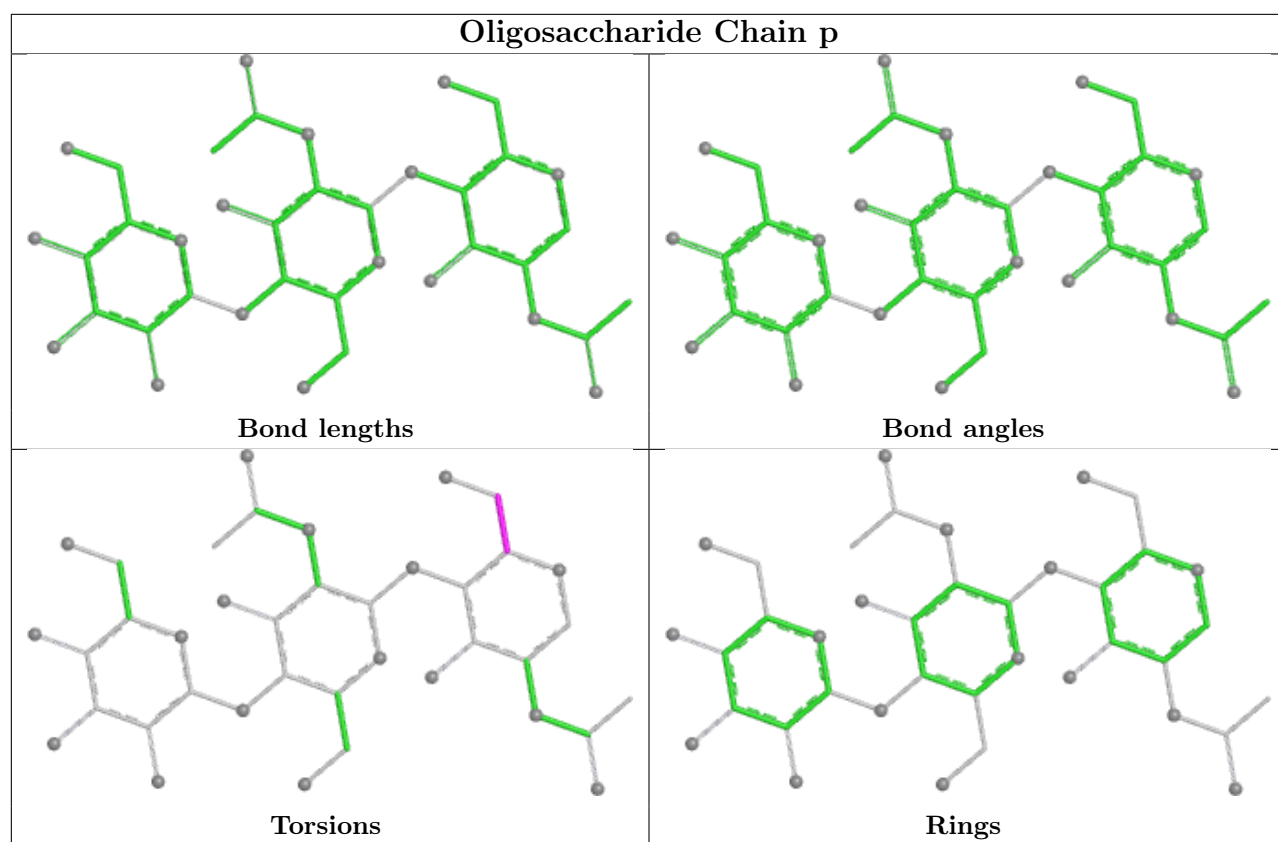


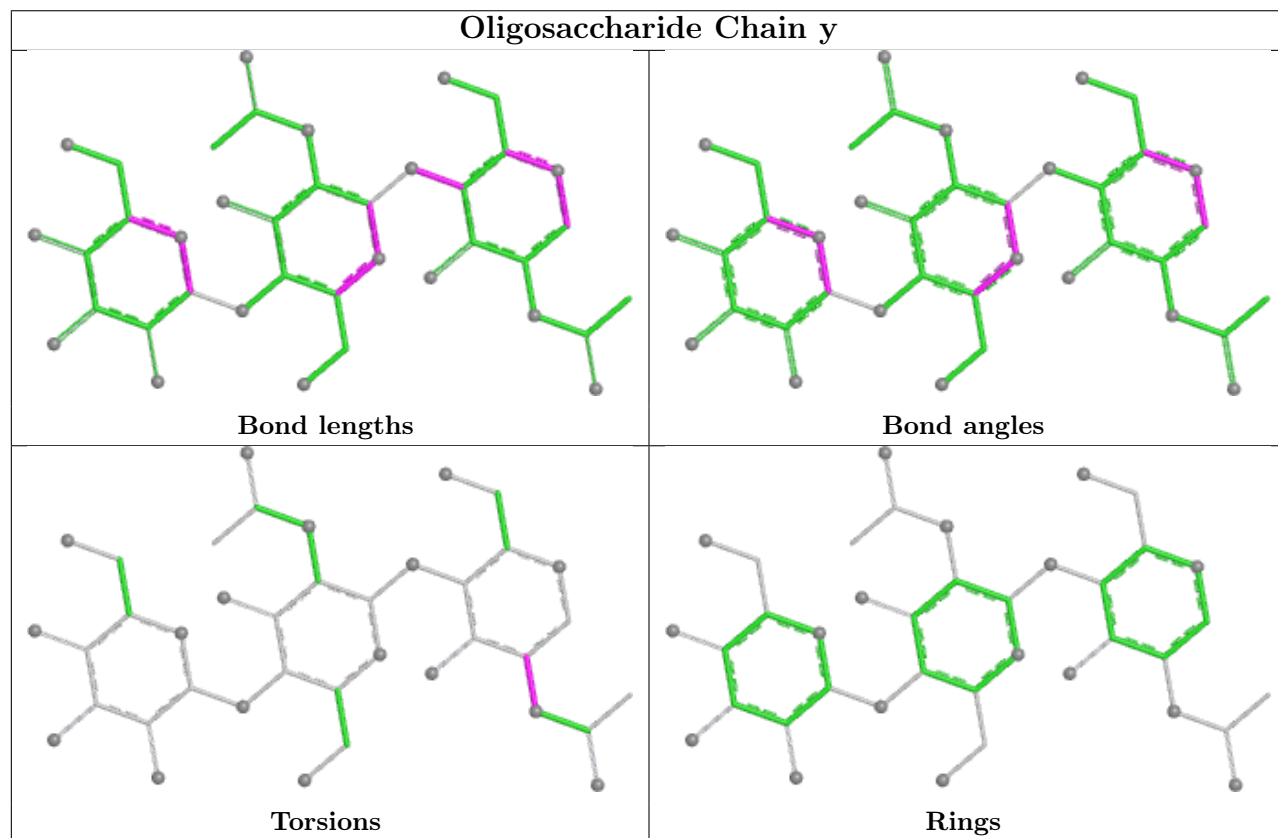
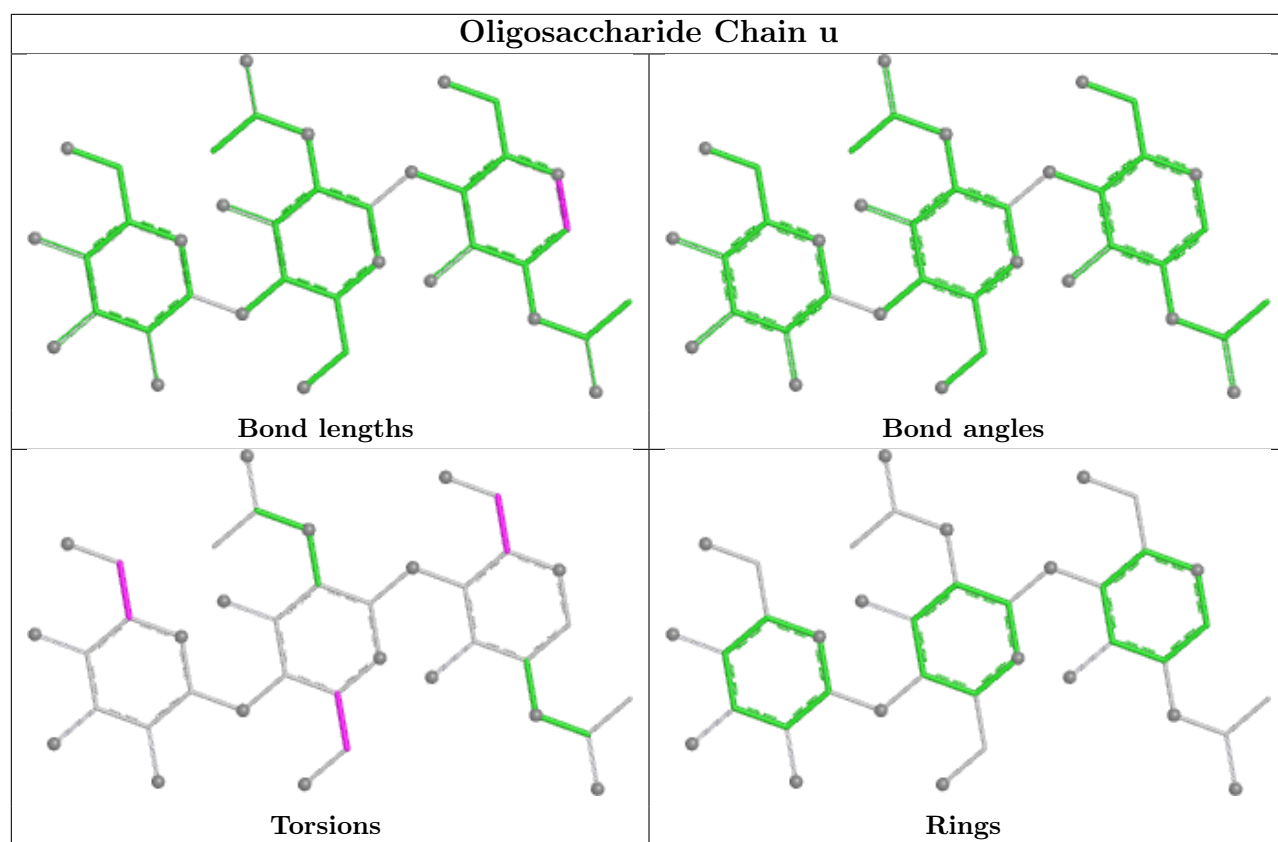


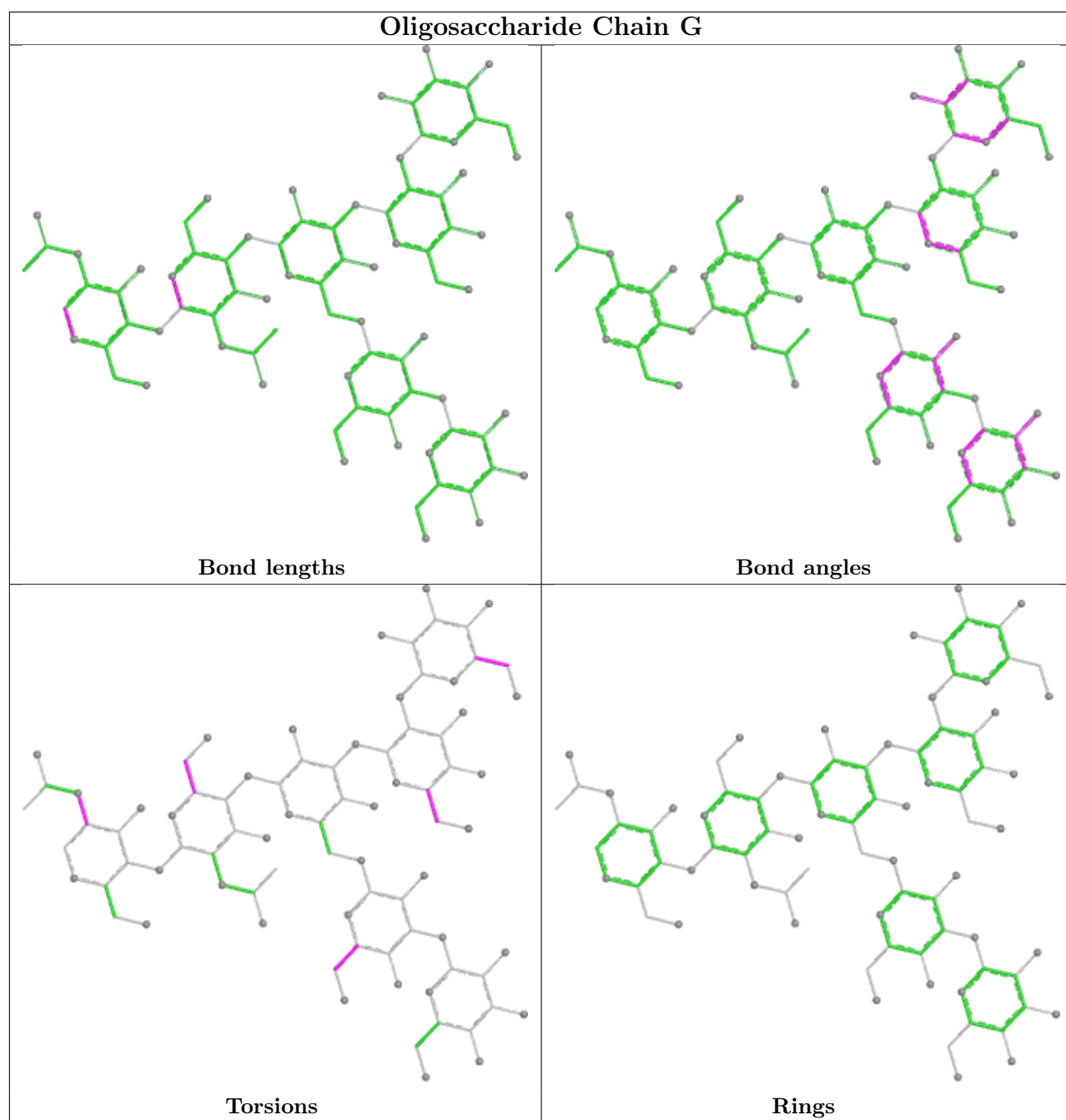


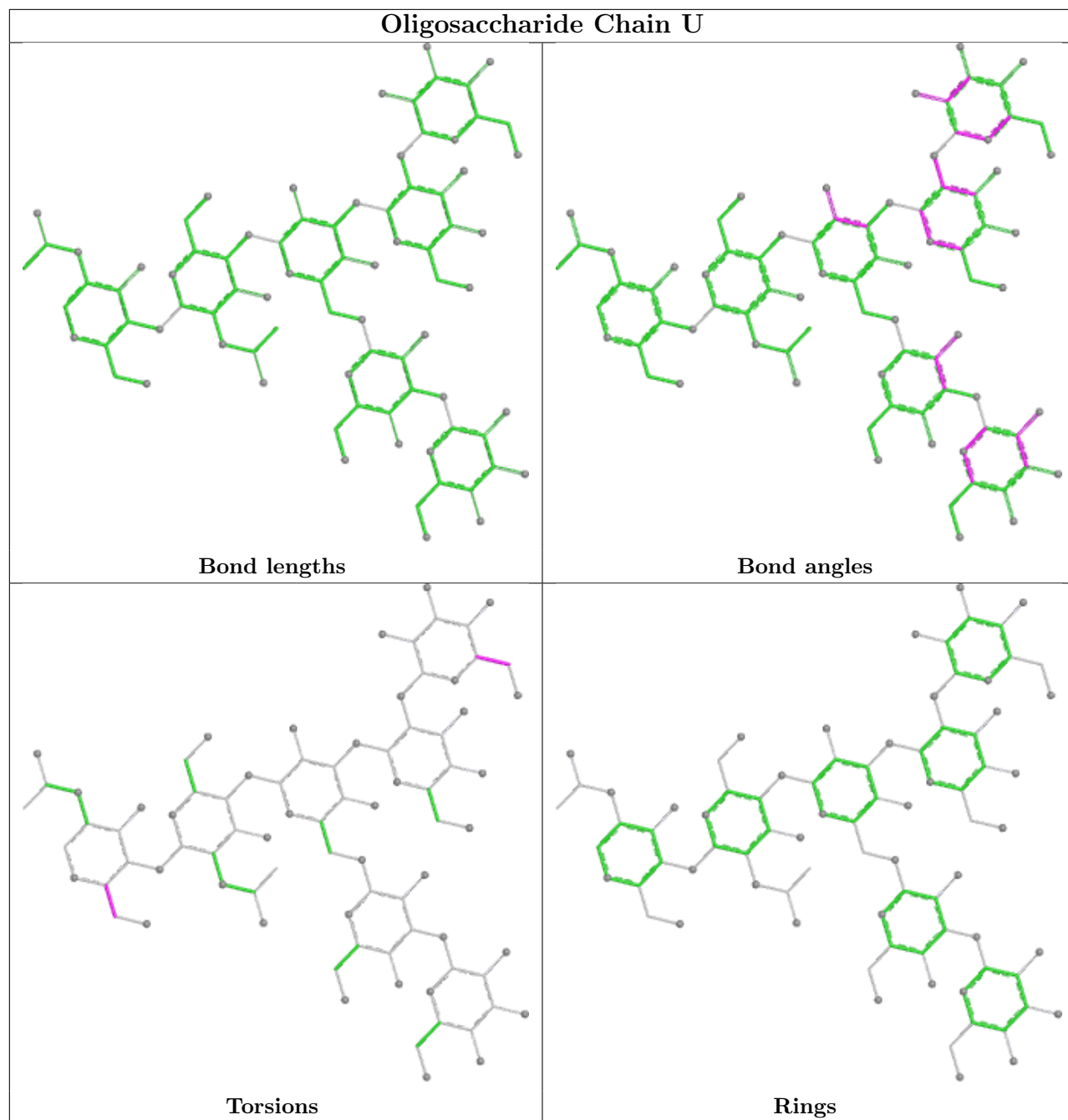


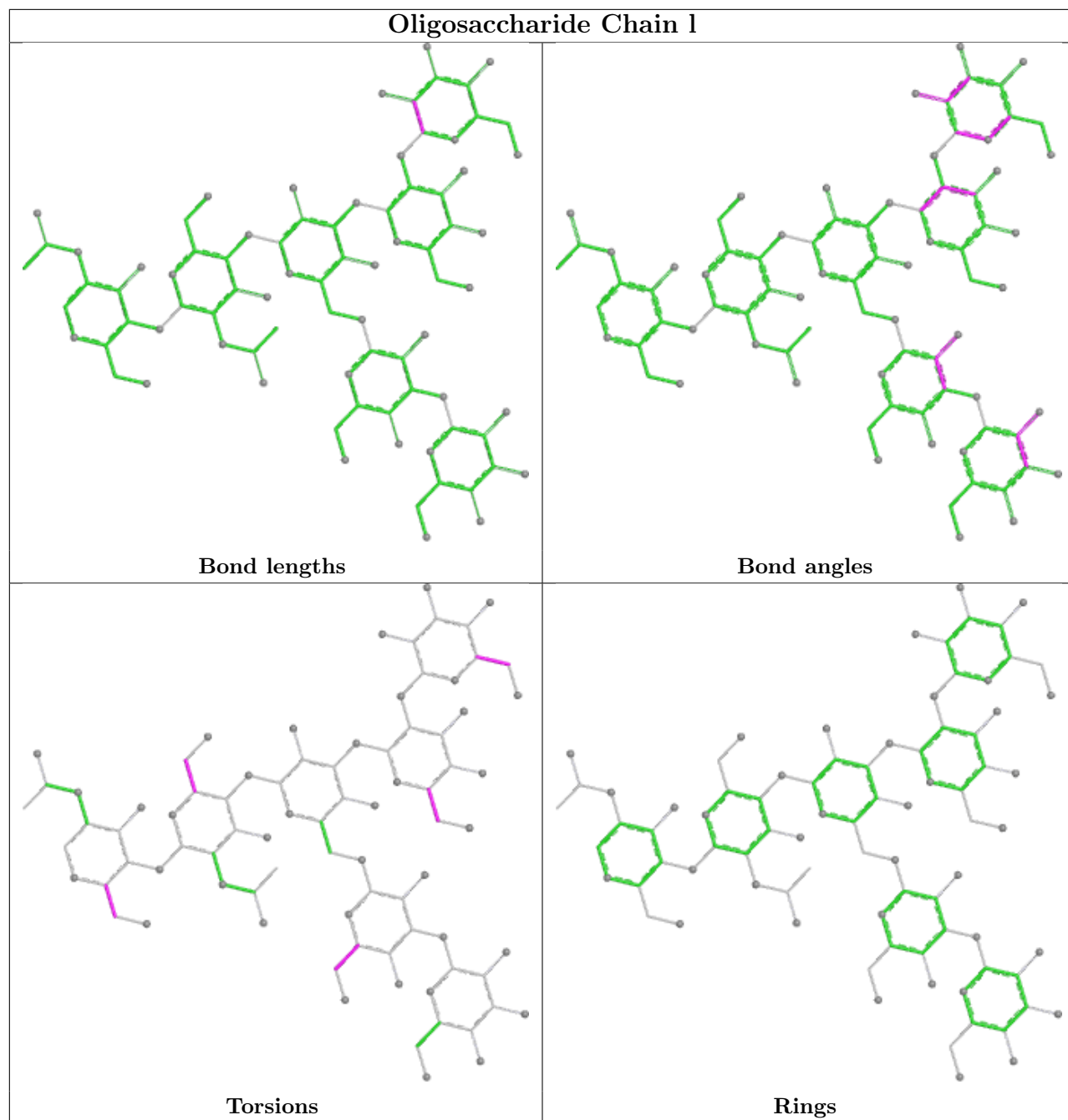


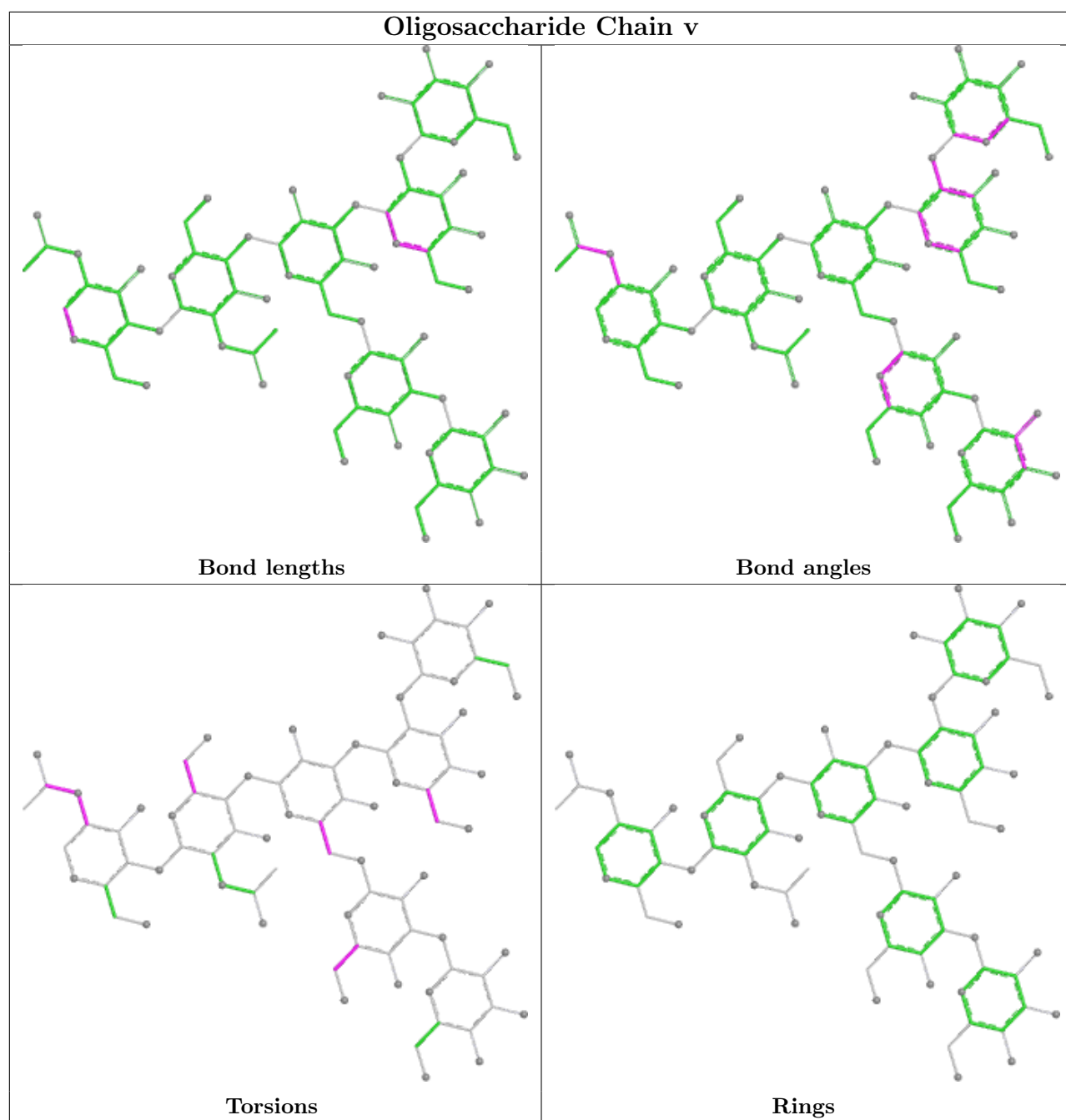


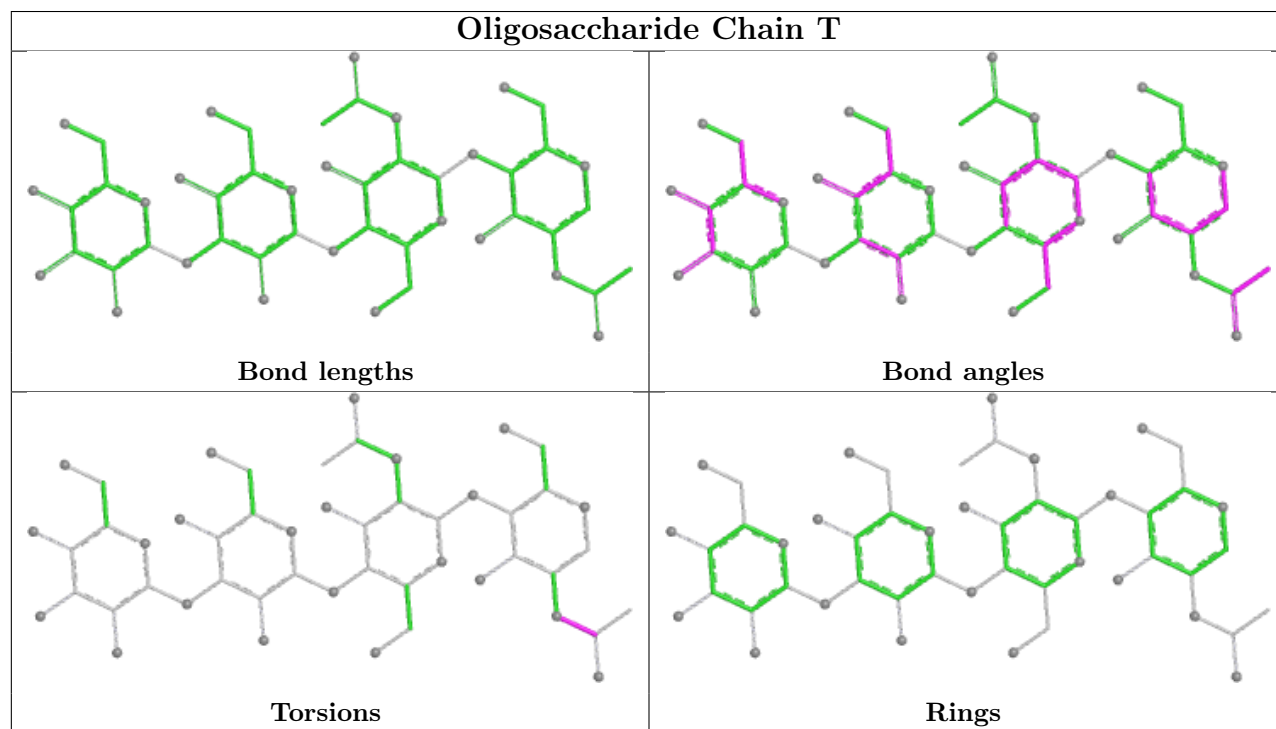
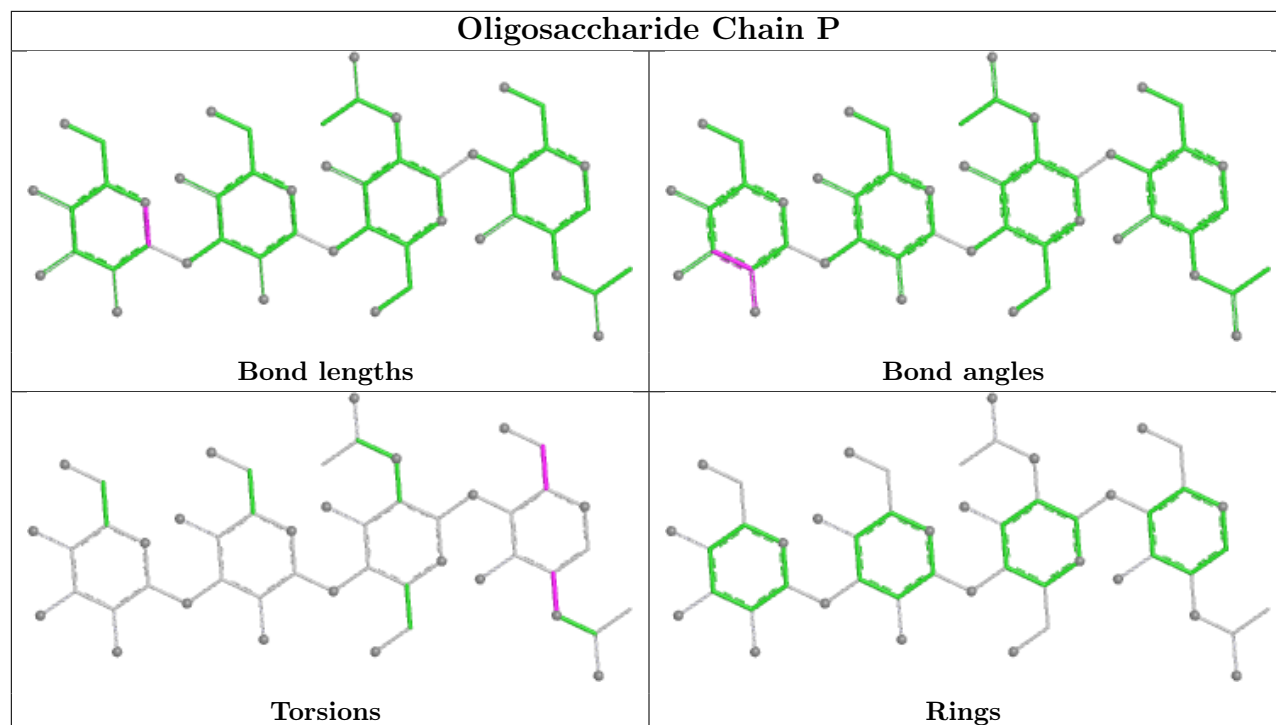


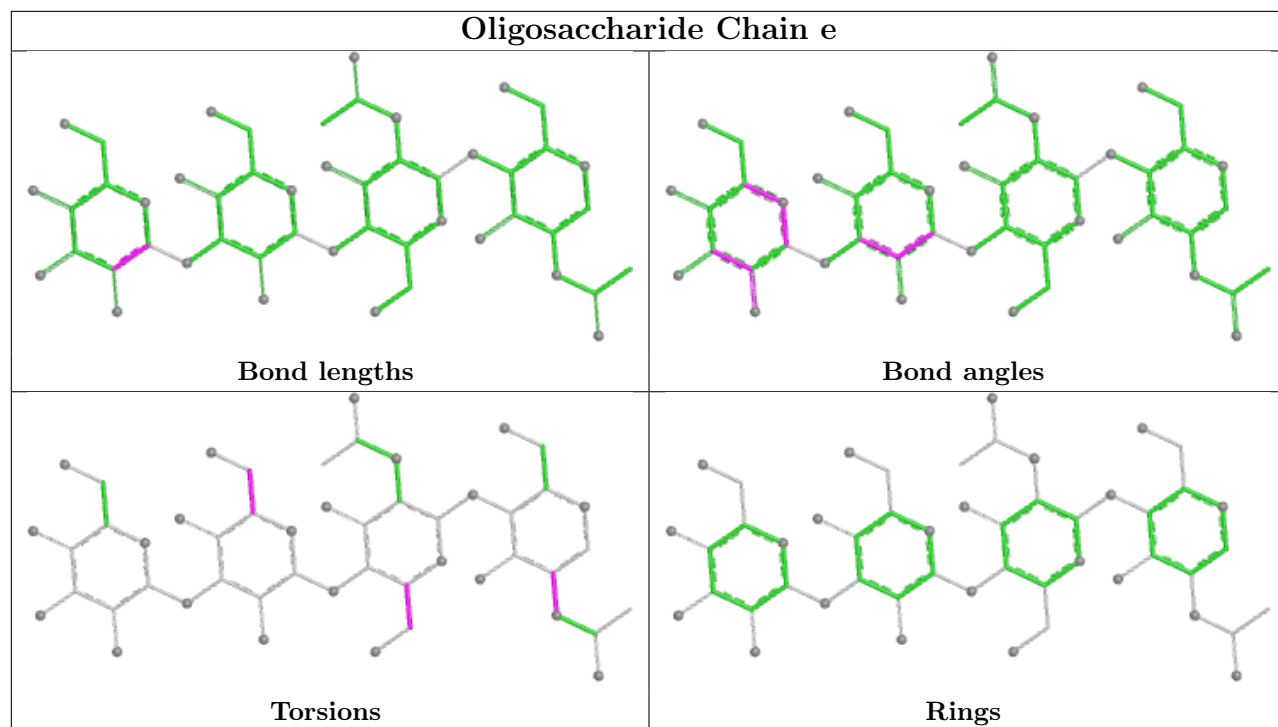


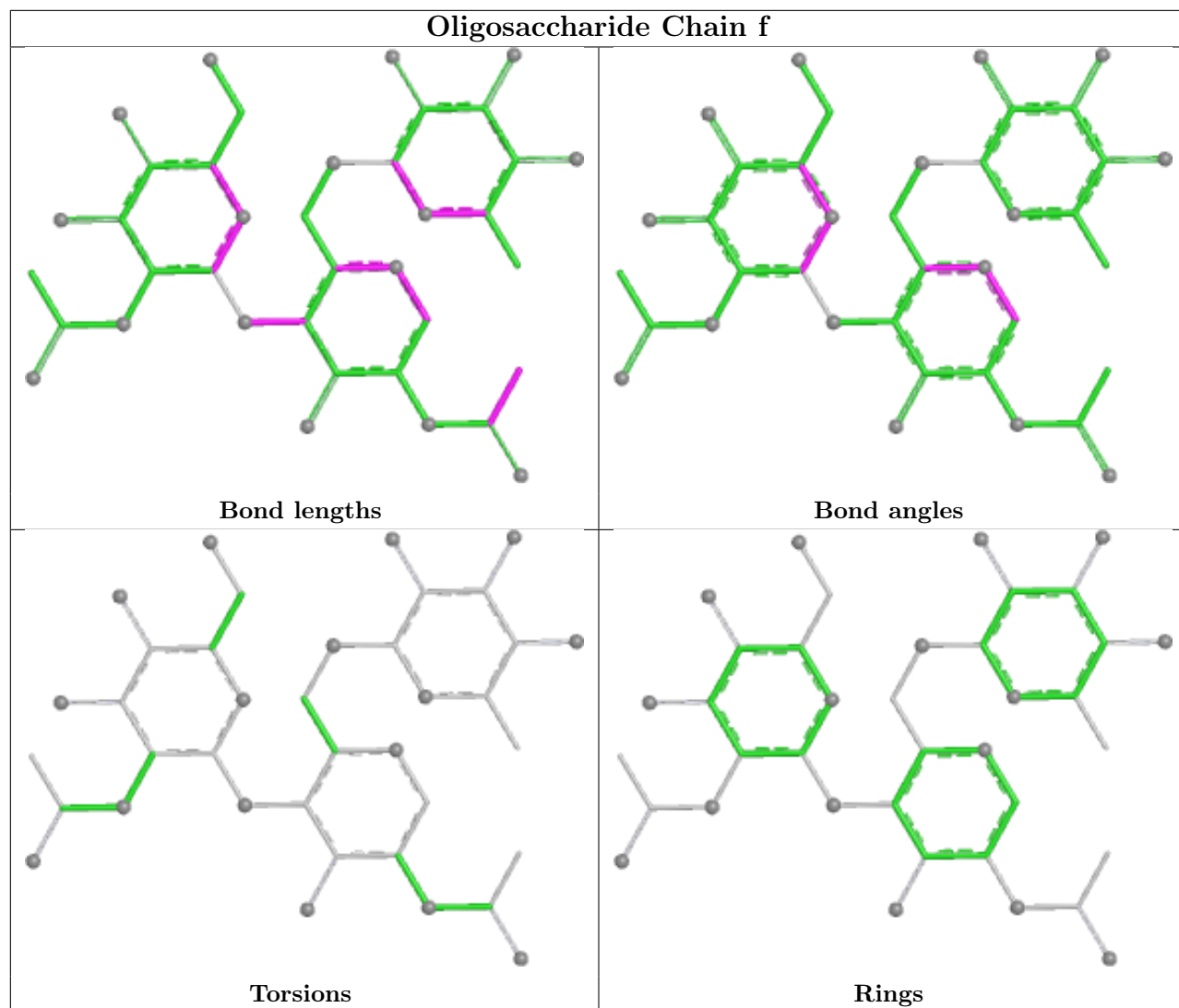


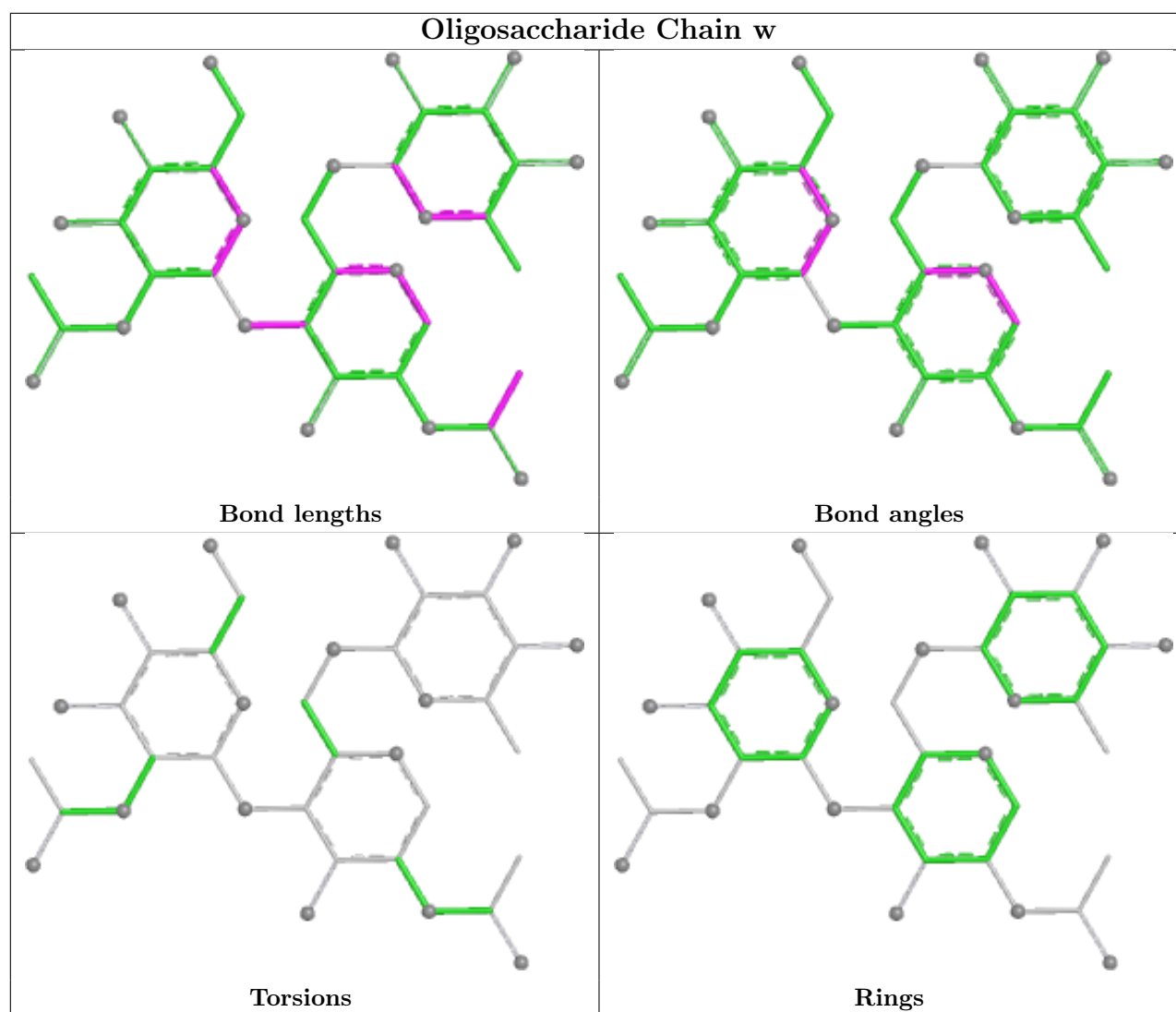












5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
7	NAG	A	901	1	14,14,15	0.34	0	17,19,21	1.06	2 (11%)
8	83G	A	905	-	33,33,33	2.28	11 (33%)	44,47,47	3.12	13 (29%)
7	NAG	B	901	1	14,14,15	0.41	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	902	1	14,14,15	0.40	0	17,19,21	0.76	0
8	83G	B	902	-	33,33,33	2.36	12 (36%)	44,47,47	3.29	16 (36%)
7	NAG	A	903	1	14,14,15	0.49	0	17,19,21	2.28	3 (17%)
7	NAG	C	901	1	14,14,15	0.24	0	17,19,21	0.46	0
7	NAG	A	904	1	14,14,15	0.49	0	17,19,21	2.26	3 (17%)
8	83G	C	902	-	33,33,33	2.40	11 (33%)	44,47,47	3.18	15 (34%)

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
7	NAG	A	901	1	-	2/6/23/26	0/1/1/1
8	83G	A	905	-	-	6/22/35/35	0/4/4/4
7	NAG	B	901	1	-	3/6/23/26	0/1/1/1
7	NAG	A	902	1	-	1/6/23/26	0/1/1/1
8	83G	B	902	-	-	2/22/35/35	0/4/4/4
7	NAG	A	903	1	-	1/6/23/26	0/1/1/1
7	NAG	C	901	1	-	2/6/23/26	0/1/1/1
7	NAG	A	904	1	-	1/6/23/26	0/1/1/1
8	83G	C	902	-	-	5/22/35/35	0/4/4/4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	902	83G	C14-N16	6.54	1.44	1.34
8	C	902	83G	C14-N16	6.49	1.44	1.34
8	A	905	83G	C14-N16	6.36	1.44	1.34
8	B	902	83G	C23-N19	5.76	1.46	1.34
8	C	902	83G	C23-N19	5.65	1.46	1.34
8	C	902	83G	C08-C11	-5.56	1.33	1.45
8	A	905	83G	C23-N19	5.29	1.45	1.34
8	B	902	83G	C08-C11	-4.80	1.34	1.45
8	A	905	83G	C08-C11	-4.41	1.35	1.45
8	C	902	83G	C08-C07	-4.05	1.35	1.41
8	A	905	83G	C08-C07	-3.90	1.35	1.41
8	B	902	83G	C08-C07	-3.82	1.35	1.41
8	A	905	83G	C11-C12	3.55	1.52	1.45
8	B	902	83G	C11-C12	3.34	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	905	83G	C18-N19	-3.22	1.41	1.47
8	B	902	83G	C18-N19	-3.16	1.41	1.47
8	C	902	83G	C08-C03	-3.11	1.35	1.40
8	C	902	83G	O15-C14	-2.97	1.17	1.23
8	C	902	83G	C11-C12	2.77	1.51	1.45
8	C	902	83G	C18-N19	-2.57	1.42	1.47
8	B	902	83G	O15-C14	-2.55	1.17	1.23
8	C	902	83G	O13-C12	-2.54	1.17	1.23
8	B	902	83G	O13-C12	-2.50	1.17	1.23
8	A	905	83G	O24-C23	-2.46	1.17	1.22
8	C	902	83G	C04-C03	-2.40	1.34	1.39
8	A	905	83G	O15-C14	-2.38	1.18	1.23
8	B	902	83G	C08-C03	-2.32	1.36	1.40
8	C	902	83G	O24-C23	-2.31	1.17	1.22
8	A	905	83G	O13-C12	-2.30	1.18	1.23
8	B	902	83G	O24-C23	-2.26	1.17	1.22
8	B	902	83G	C04-C03	-2.22	1.35	1.39
8	A	905	83G	C04-C03	-2.22	1.35	1.39
8	A	905	83G	C08-C03	-2.19	1.36	1.40
8	B	902	83G	C25-C23	2.07	1.53	1.50

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	905	83G	C10-C11-C12	-11.13	100.84	126.74
8	C	902	83G	C10-C11-C12	-10.86	101.46	126.74
8	B	902	83G	C10-C11-C12	-10.74	101.76	126.74
8	B	902	83G	C11-C10-N09	-10.25	103.28	110.22
8	A	905	83G	C11-C10-N09	-9.54	103.76	110.22
8	C	902	83G	C11-C10-N09	-8.94	104.16	110.22
7	A	903	NAG	O5-C1-C2	-7.54	99.62	111.29
7	A	904	NAG	O5-C1-C2	-7.46	99.75	111.29
8	C	902	83G	C08-C07-N06	-7.26	118.90	126.64
8	B	902	83G	C08-C11-C10	7.14	114.11	106.10
8	B	902	83G	C08-C07-N06	-6.92	119.27	126.64
8	A	905	83G	C08-C07-N06	-6.85	119.33	126.64
8	A	905	83G	C08-C11-C10	6.57	113.47	106.10
8	C	902	83G	C08-C11-C10	6.53	113.43	106.10
8	B	902	83G	C25-C23-N19	5.90	126.03	118.66
8	A	905	83G	C01-O02-C03	-4.68	110.65	117.51
8	C	902	83G	C12-C14-N16	4.61	123.53	118.81
8	C	902	83G	C01-O02-C03	-4.61	110.75	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	905	83G	C04-C05-N06	-3.73	119.41	123.97
8	A	905	83G	O02-C03-C08	3.57	120.90	115.84
8	B	902	83G	O02-C03-C08	3.54	120.85	115.84
8	C	902	83G	N09-C07-N06	3.53	132.40	126.69
8	C	902	83G	C25-C23-N19	3.52	123.06	118.66
8	C	902	83G	C04-C05-N06	-3.48	119.70	123.97
8	B	902	83G	C12-C14-N16	3.46	122.35	118.81
8	A	905	83G	O02-C03-C04	-3.43	118.52	124.30
7	A	901	NAG	C1-O5-C5	3.20	116.47	112.19
8	B	902	83G	C04-C05-N06	-3.15	120.11	123.97
8	B	902	83G	O24-C23-N19	-3.15	117.39	122.35
8	B	902	83G	N09-C07-N06	3.12	131.75	126.69
8	A	905	83G	N09-C07-N06	3.08	131.67	126.69
7	A	904	NAG	O7-C7-C8	-2.89	116.90	122.05
7	A	903	NAG	O7-C7-C8	-2.88	116.93	122.05
8	C	902	83G	O15-C14-N16	-2.86	116.58	122.17
8	B	902	83G	O02-C03-C04	-2.83	119.53	124.30
8	C	902	83G	O02-C03-C08	2.74	119.72	115.84
7	A	903	NAG	C4-C3-C2	-2.69	107.07	111.02
7	A	904	NAG	C4-C3-C2	-2.59	107.22	111.02
8	A	905	83G	C21-C20-N19	-2.52	108.11	110.99
8	A	905	83G	C22-C21-N16	-2.51	107.54	111.55
8	A	905	83G	C17-C18-N19	-2.50	105.45	110.42
8	B	902	83G	C18-C17-N16	2.50	114.84	110.33
8	C	902	83G	C21-C20-N19	-2.47	108.16	110.99
8	B	902	83G	C21-C20-N19	-2.45	108.19	110.99
8	C	902	83G	O13-C12-C11	-2.44	117.26	122.48
8	B	902	83G	C18-N19-C20	-2.36	108.52	113.07
8	A	905	83G	C05-N06-C07	2.17	120.97	116.74
8	C	902	83G	O24-C23-N19	-2.17	118.93	122.35
8	C	902	83G	O02-C03-C04	-2.13	120.71	124.30
8	B	902	83G	C07-N09-C10	2.09	109.47	108.48
8	B	902	83G	C22-C21-N16	-2.07	108.24	111.55
7	A	901	NAG	C2-N2-C7	2.04	125.64	122.90

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	901	NAG	C1-C2-N2-C7
8	C	902	83G	C08-C11-C12-O13
7	B	901	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	B	901	NAG	O5-C5-C6-O6
8	C	902	83G	C04-C03-O02-C01
8	A	905	83G	C04-C03-O02-C01
7	C	901	NAG	O5-C5-C6-O6
7	C	901	NAG	C4-C5-C6-O6
8	A	905	83G	C08-C03-O02-C01
8	B	902	83G	C04-C03-O02-C01
8	C	902	83G	C08-C03-O02-C01
8	B	902	83G	C08-C03-O02-C01
7	A	901	NAG	C8-C7-N2-C2
7	A	901	NAG	O7-C7-N2-C2
7	A	902	NAG	C1-C2-N2-C7
8	A	905	83G	C08-C11-C12-O13
8	A	905	83G	C10-C11-C12-O13
8	C	902	83G	C10-C11-C12-O13
8	A	905	83G	C10-C11-C12-C14
8	A	905	83G	C08-C11-C12-C14
8	C	902	83G	C10-C11-C12-C14
7	A	903	NAG	O7-C7-N2-C2
7	A	904	NAG	O7-C7-N2-C2

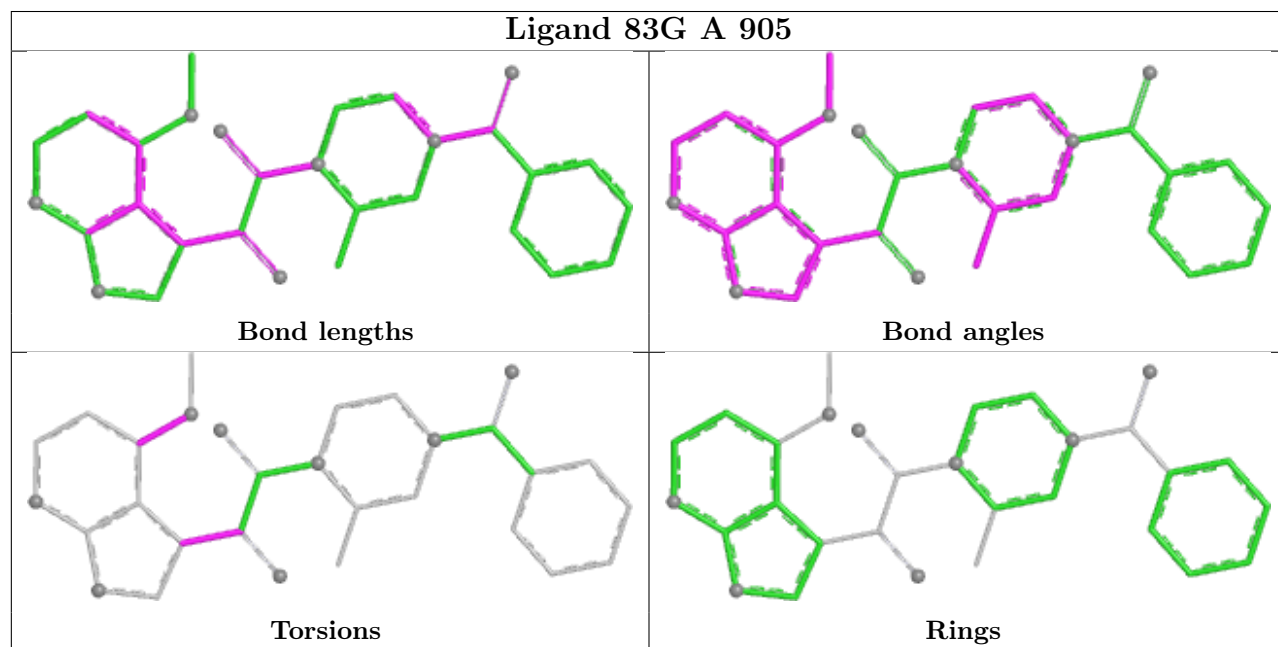
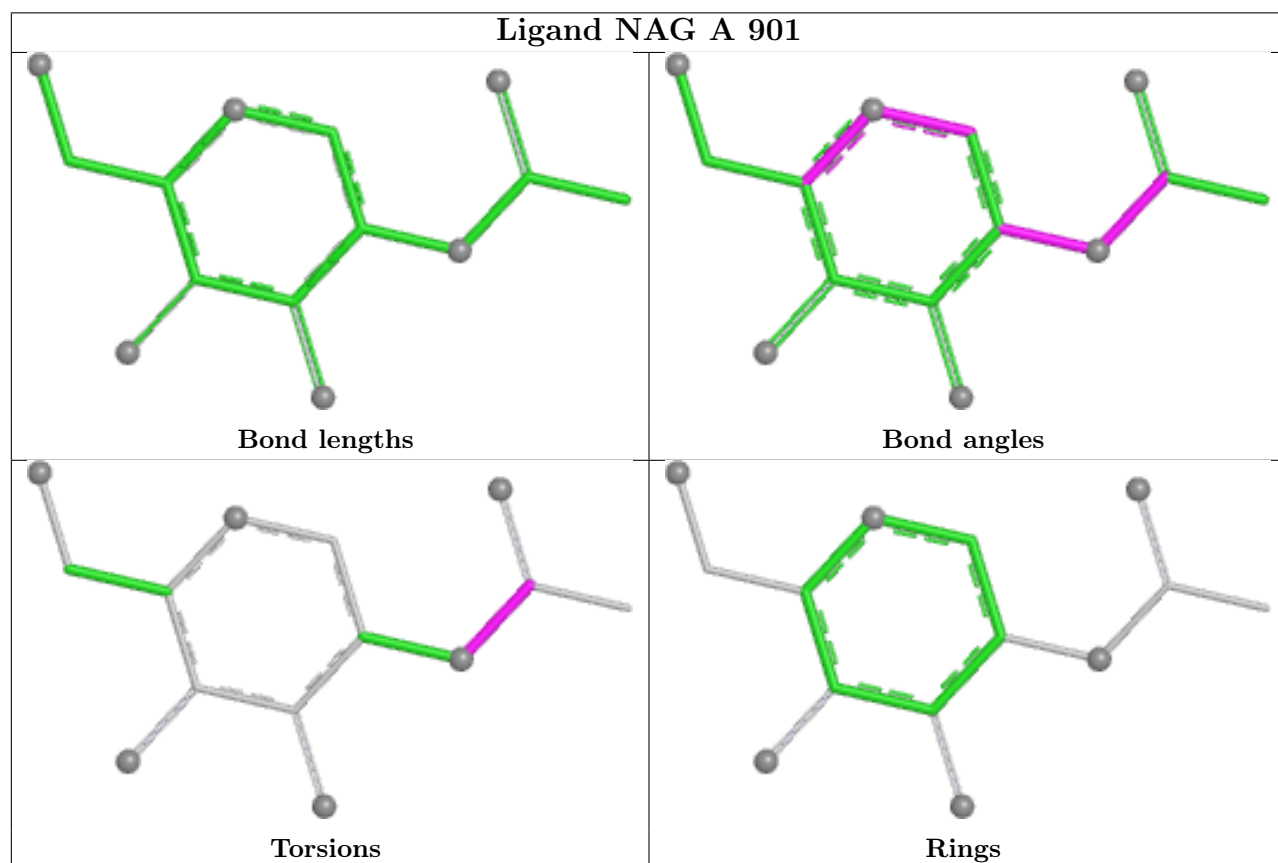
There are no ring outliers.

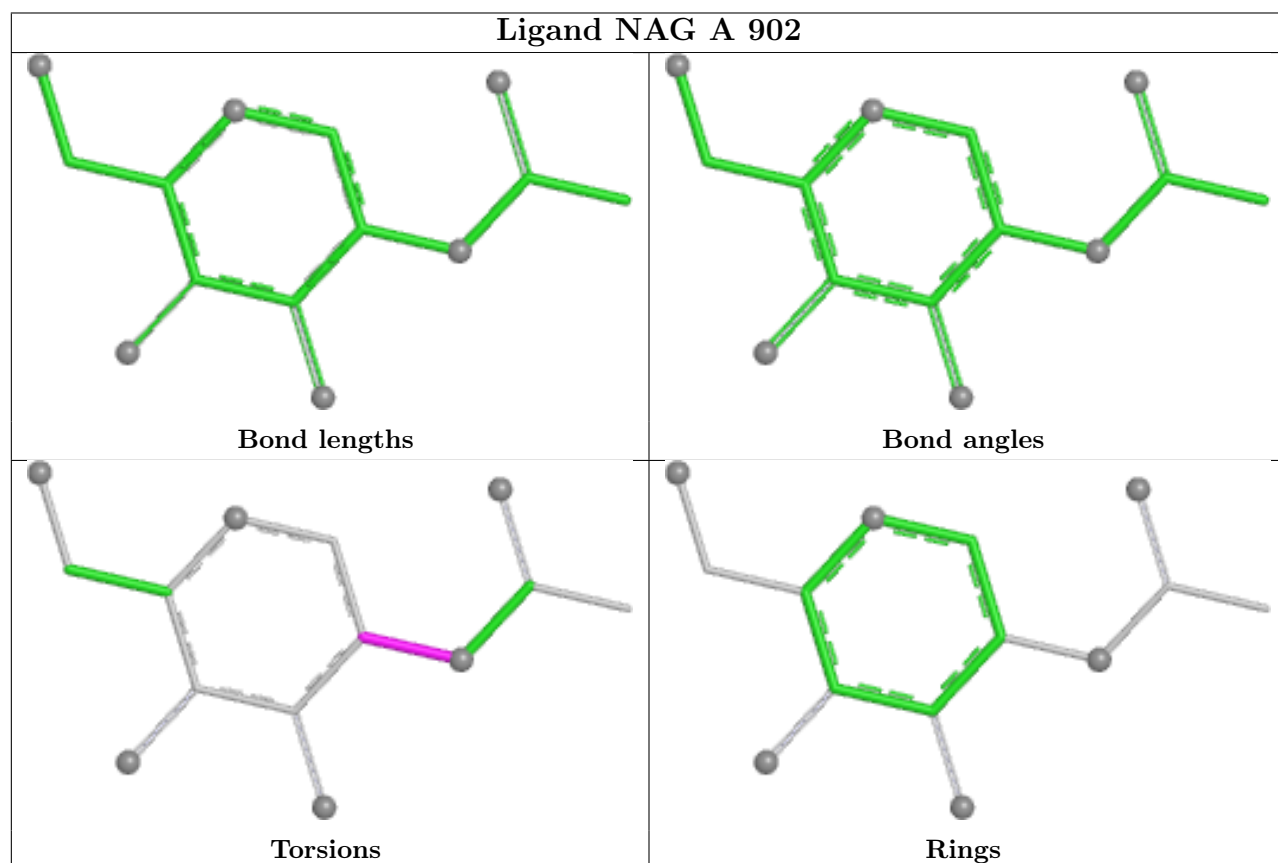
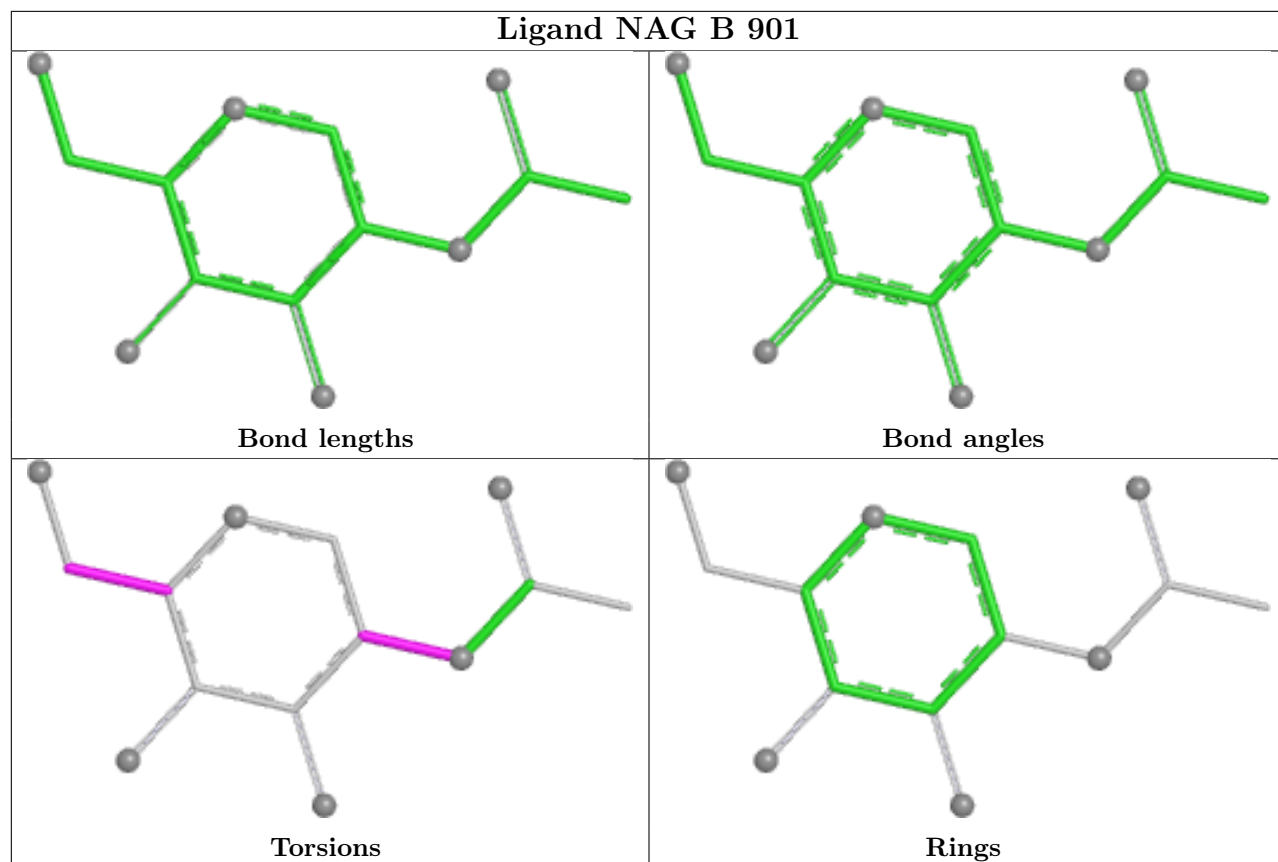
6 monomers are involved in 10 short contacts:

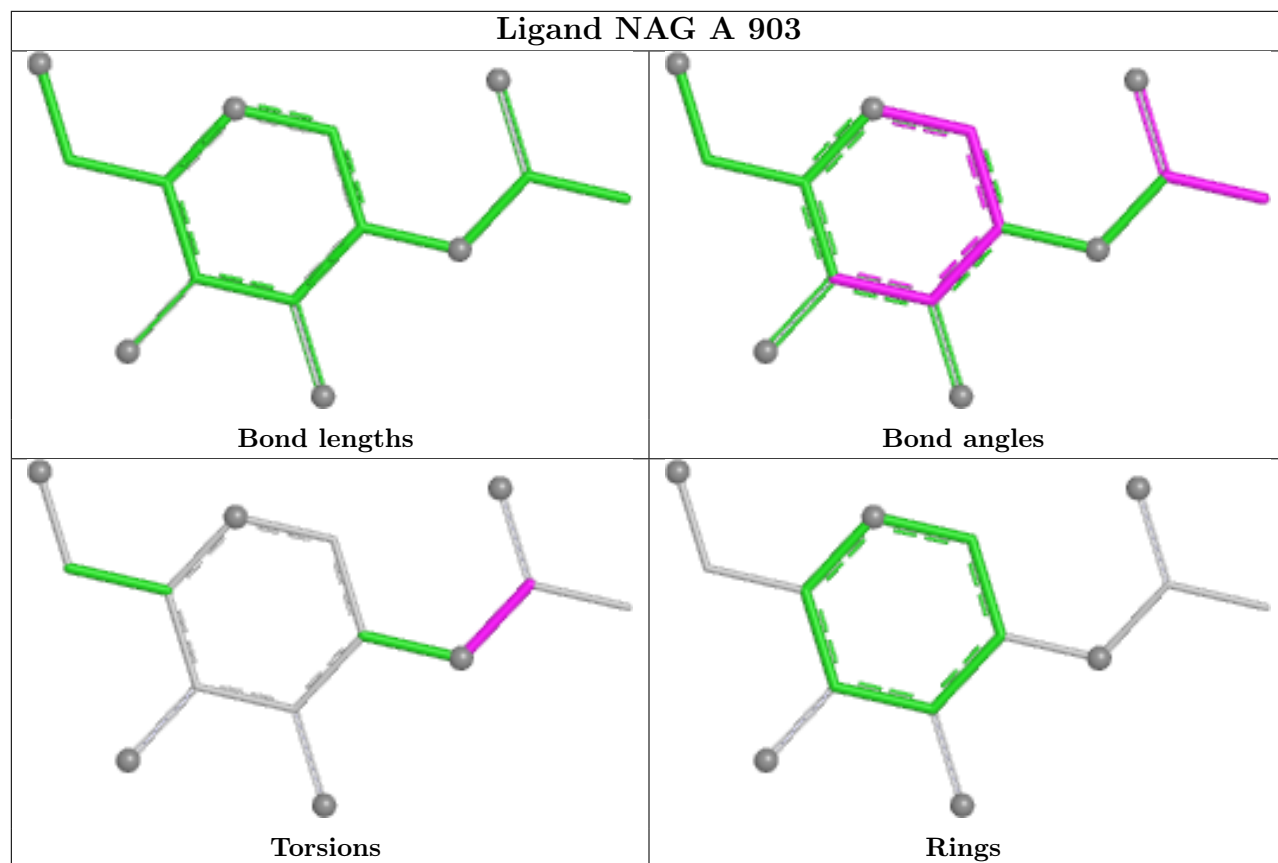
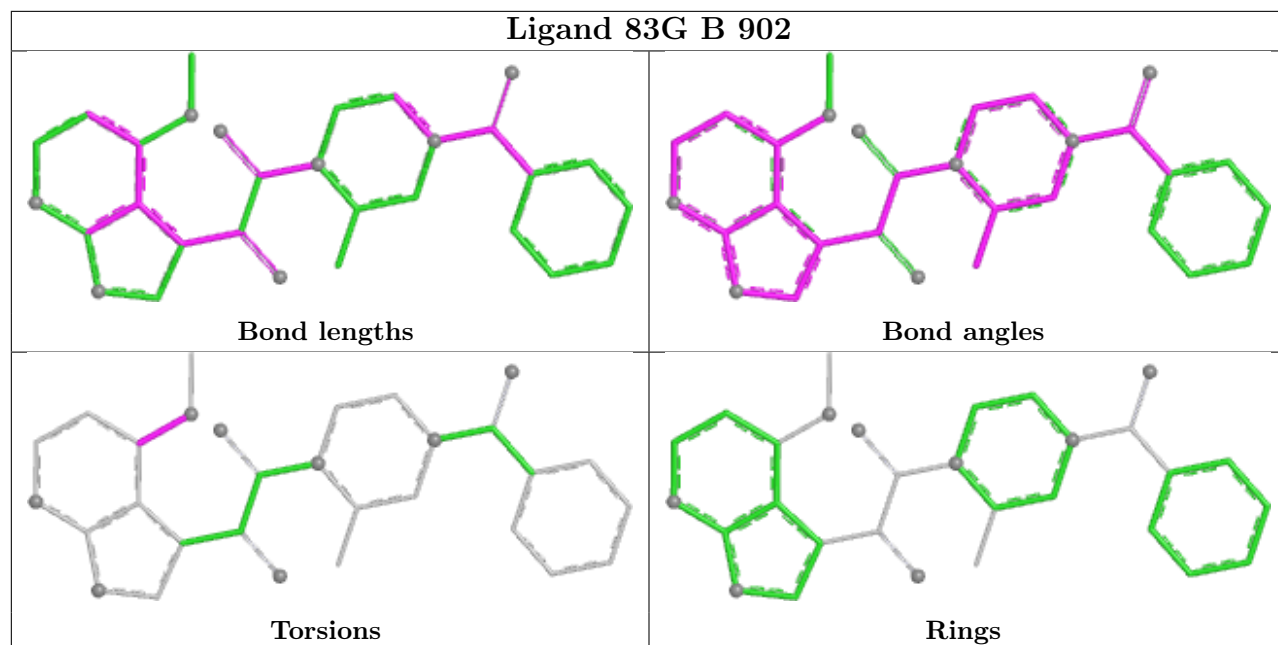
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	901	NAG	3	0
7	B	901	NAG	2	0
7	A	903	NAG	2	0
7	C	901	NAG	1	0
7	A	904	NAG	1	0
8	C	902	83G	1	0

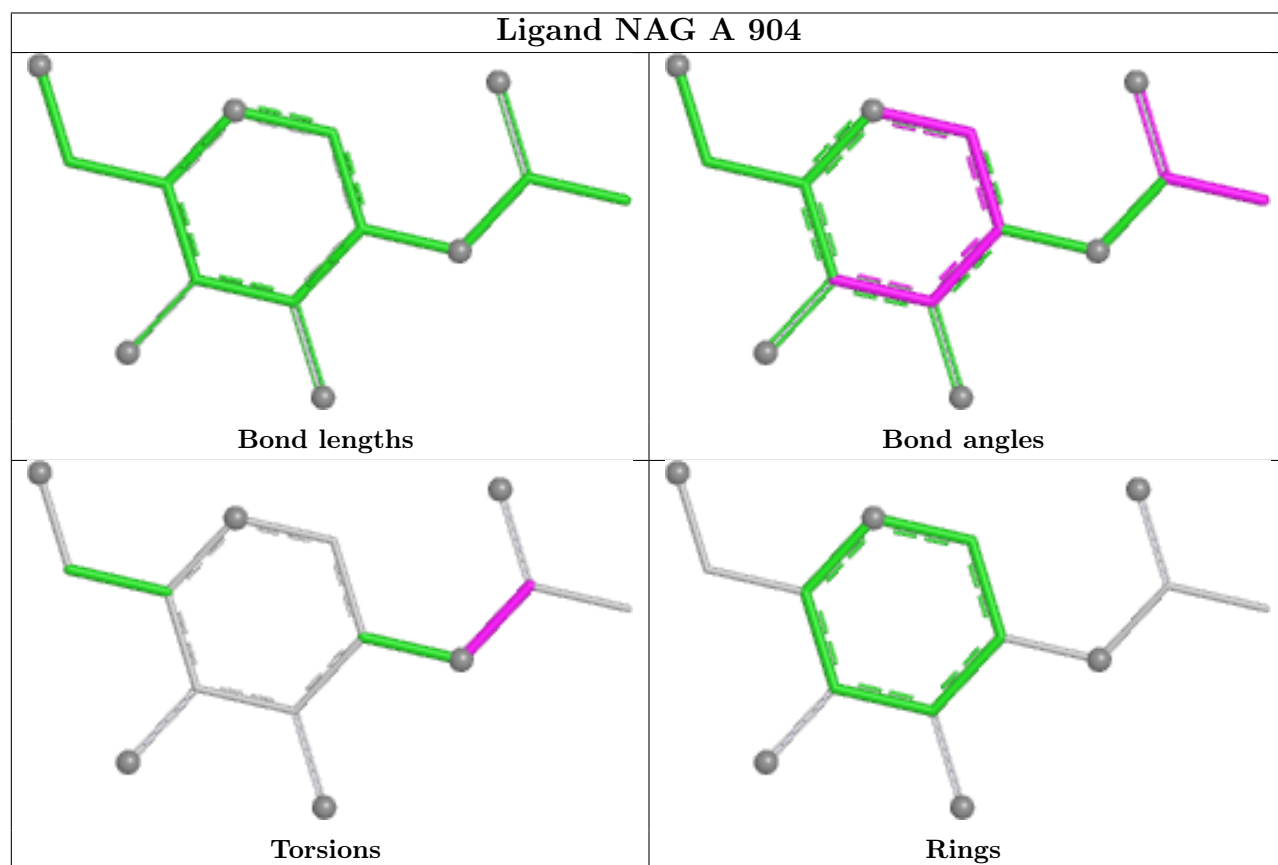
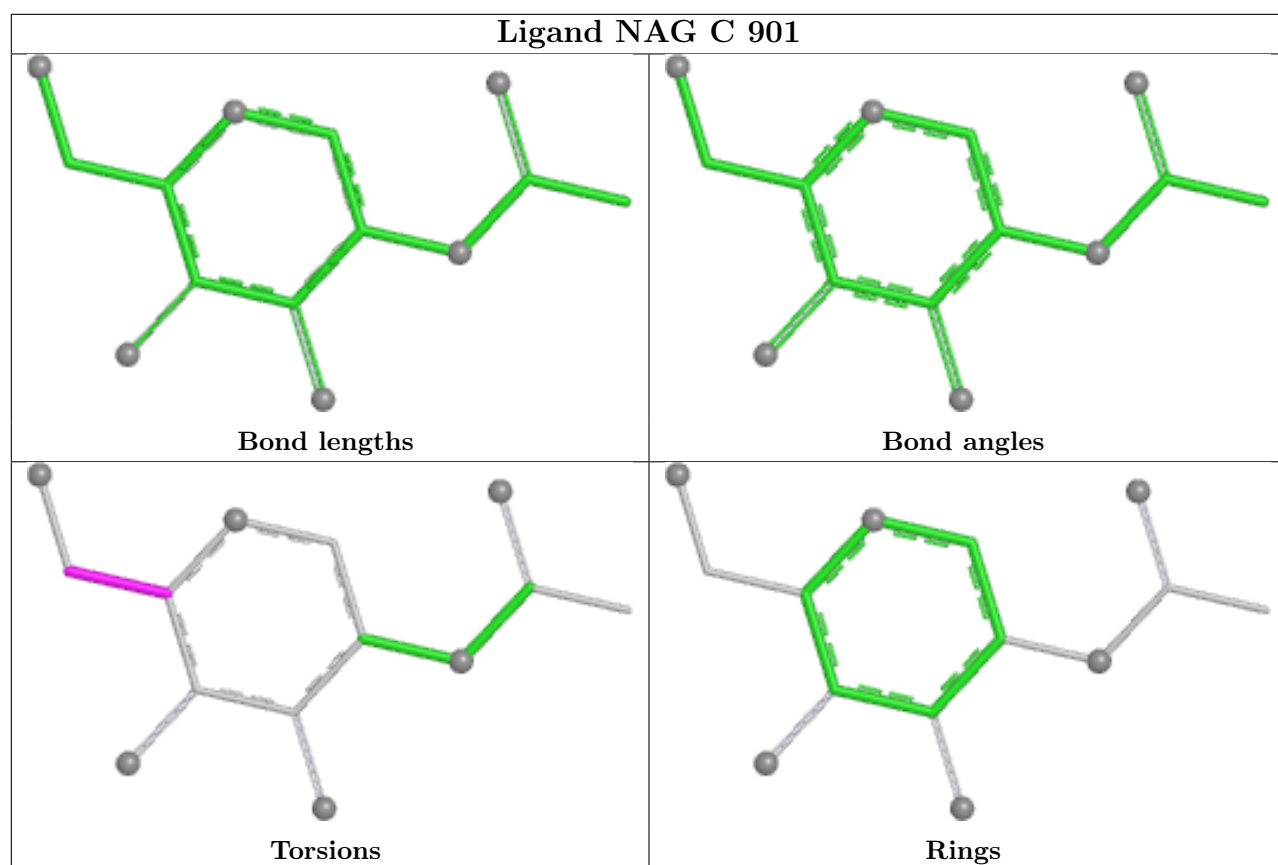
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

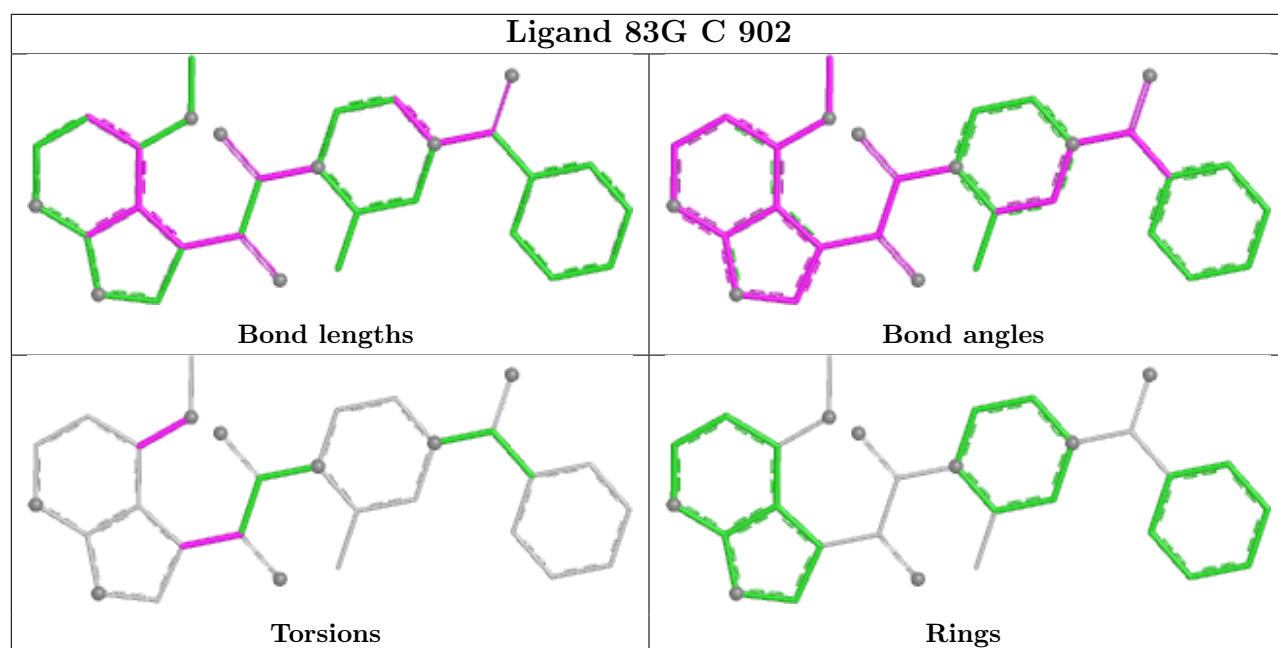
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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.

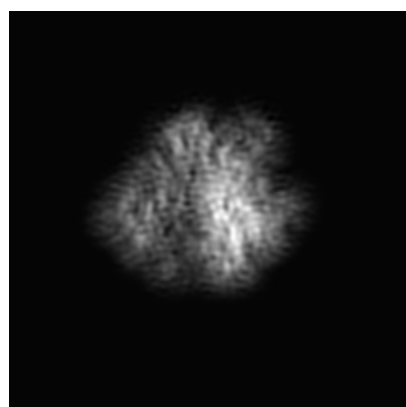
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23860. These allow visual inspection of the internal detail of the map and identification of artifacts.

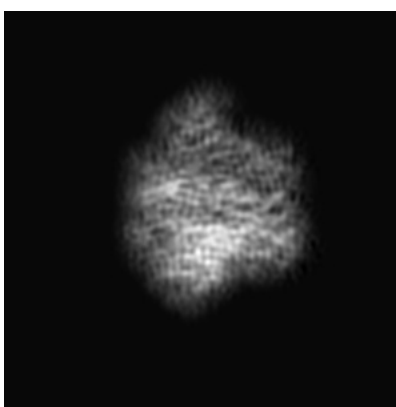
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

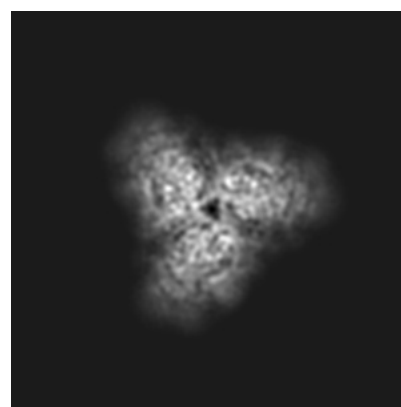
6.1.1 Primary map



X



Y

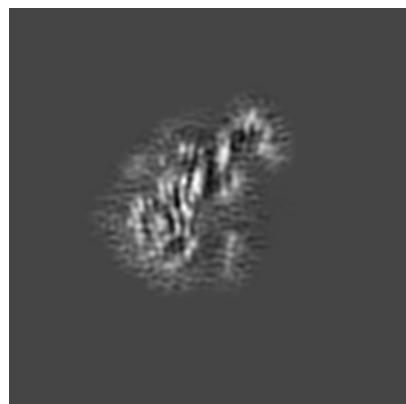


Z

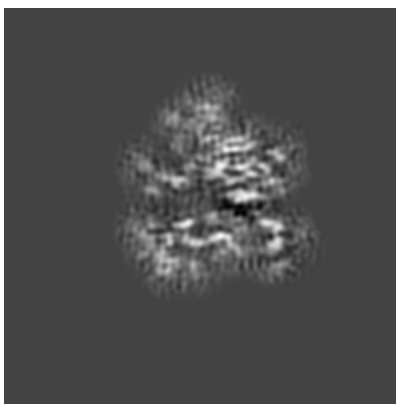
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

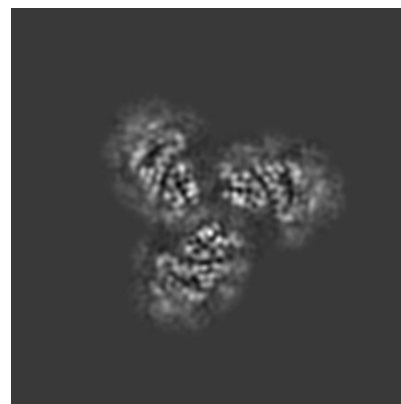
6.2.1 Primary map



X Index: 168



Y Index: 168

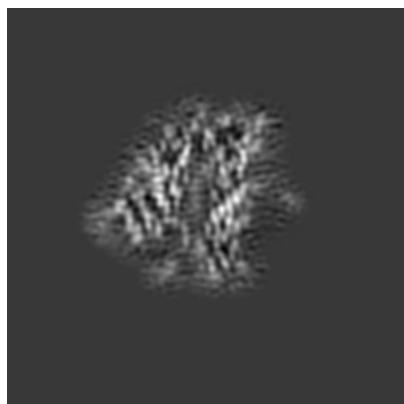


Z Index: 168

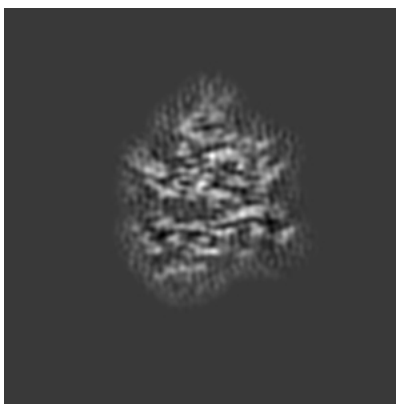
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

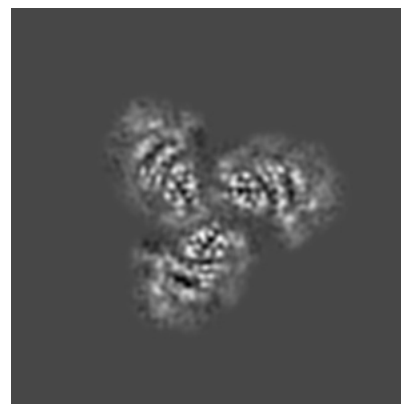
6.3.1 Primary map



X Index: 151



Y Index: 177

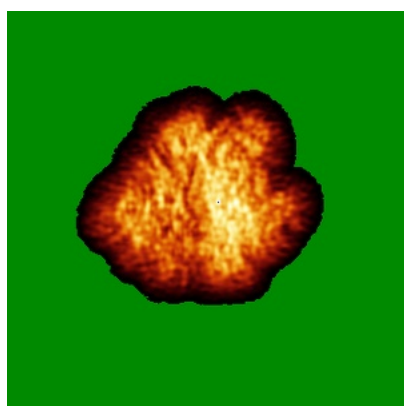


Z Index: 171

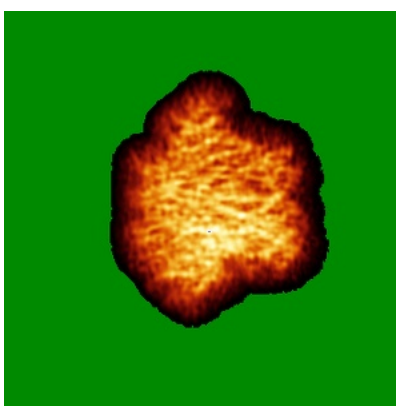
The images above show the largest variance slices of the map in three orthogonal directions.

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

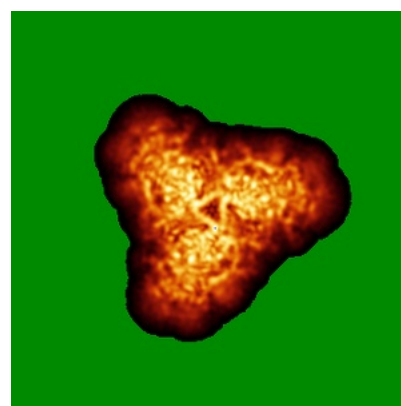
6.4.1 Primary map



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.

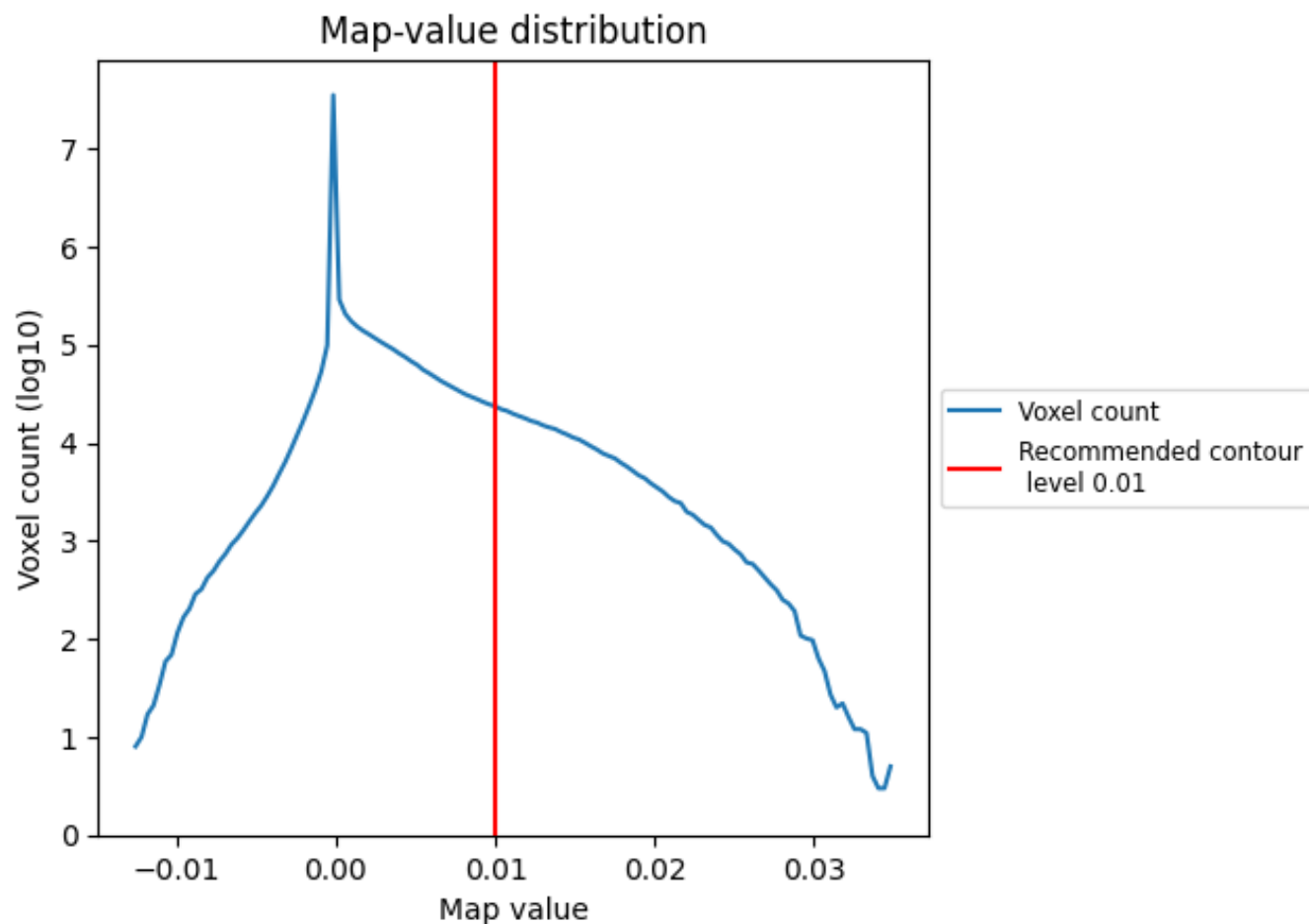
6.6 Mask visualisation

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

7 Map analysis [i](#)

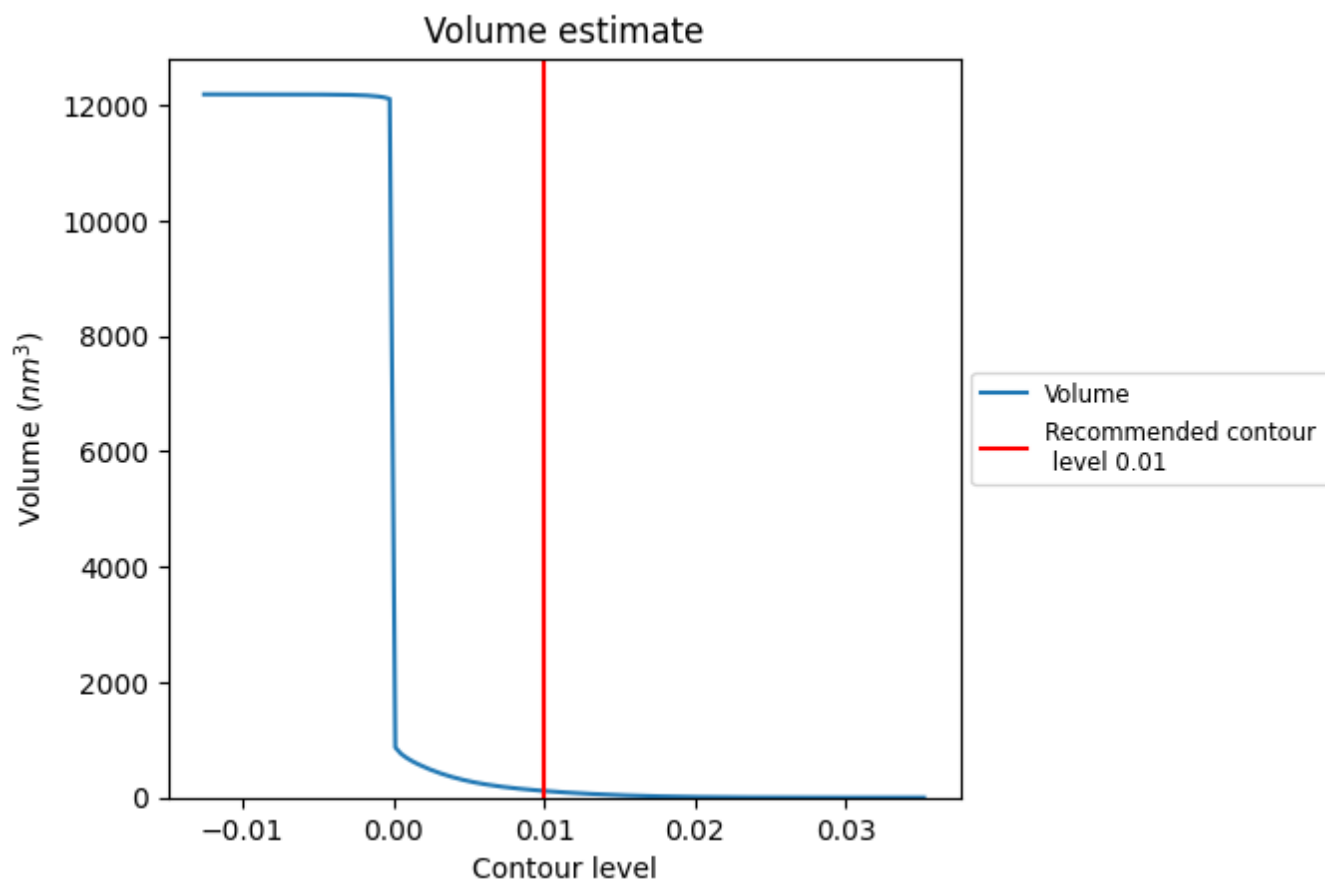
This section contains the results of statistical analysis of the map.

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.

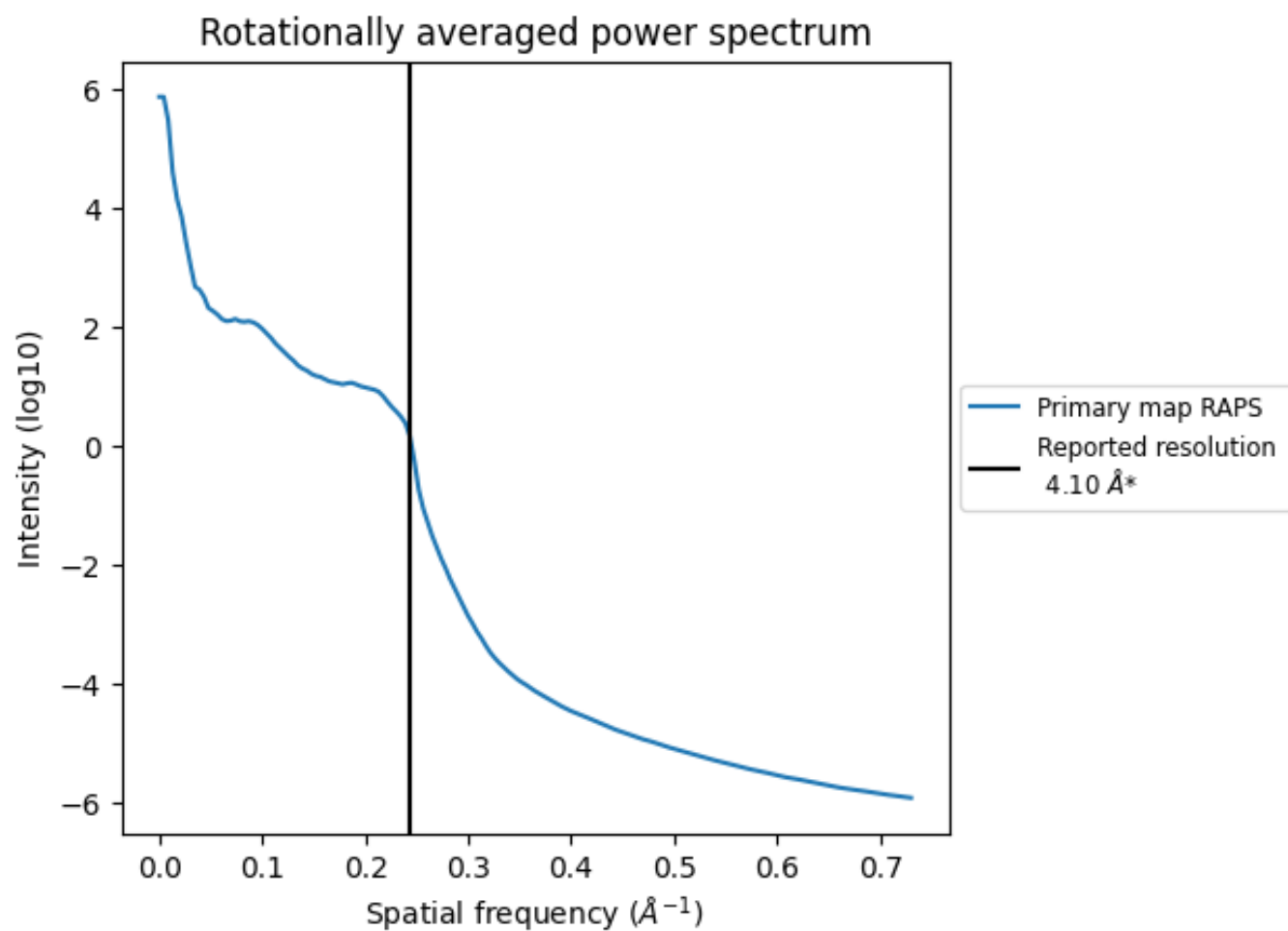
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 0.244 Å⁻¹

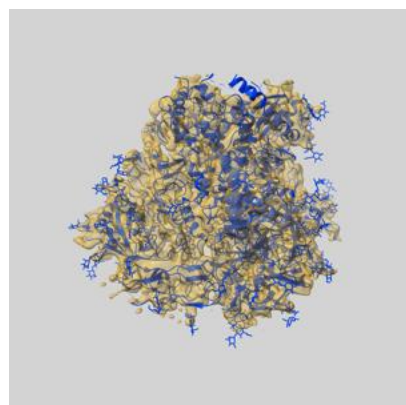
8 Fourier-Shell correlation ⓘ

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

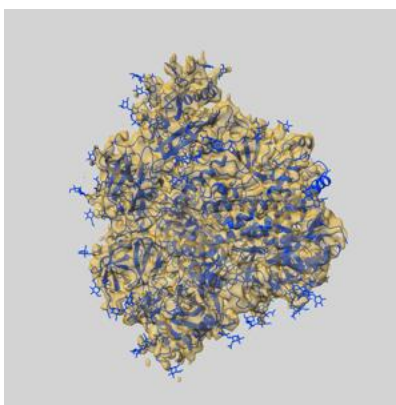
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23860 and PDB model 7N6U. Per-residue inclusion information can be found in section [3](#) on page [14](#).

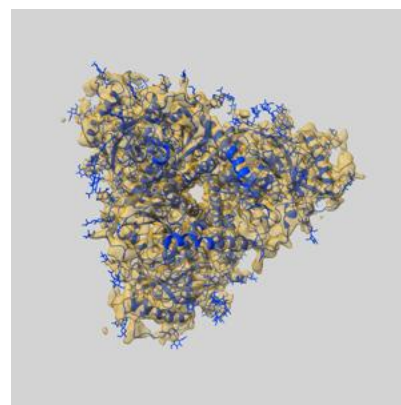
9.1 Map-model overlay [i](#)



X



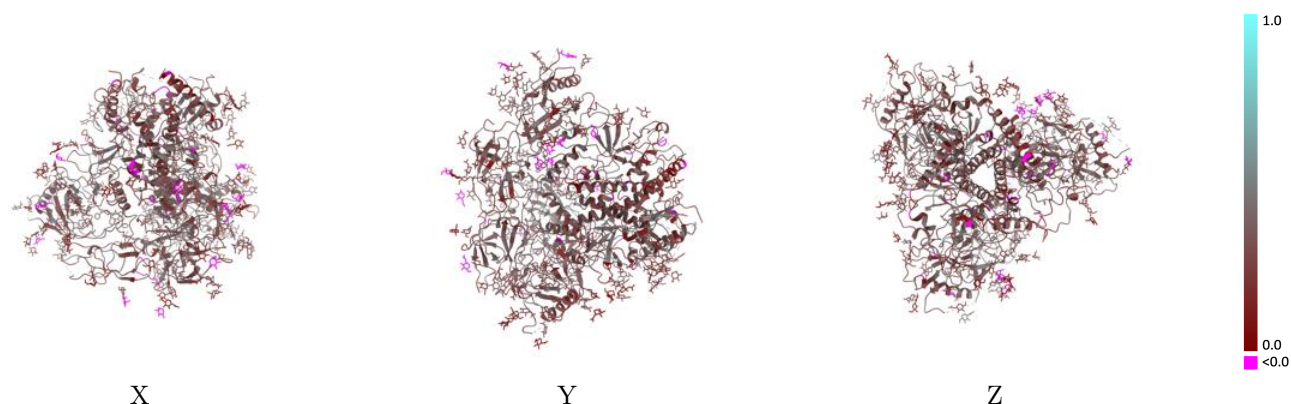
Y



Z

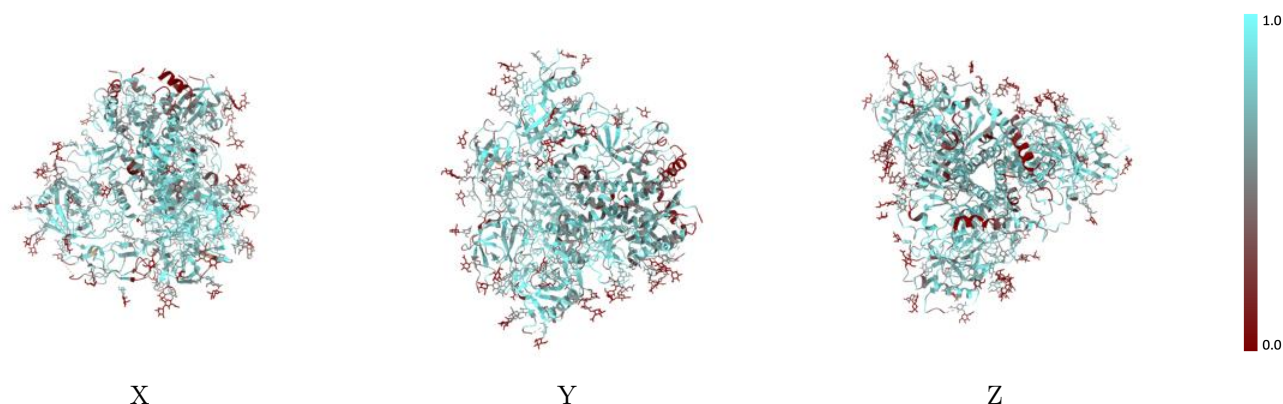
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



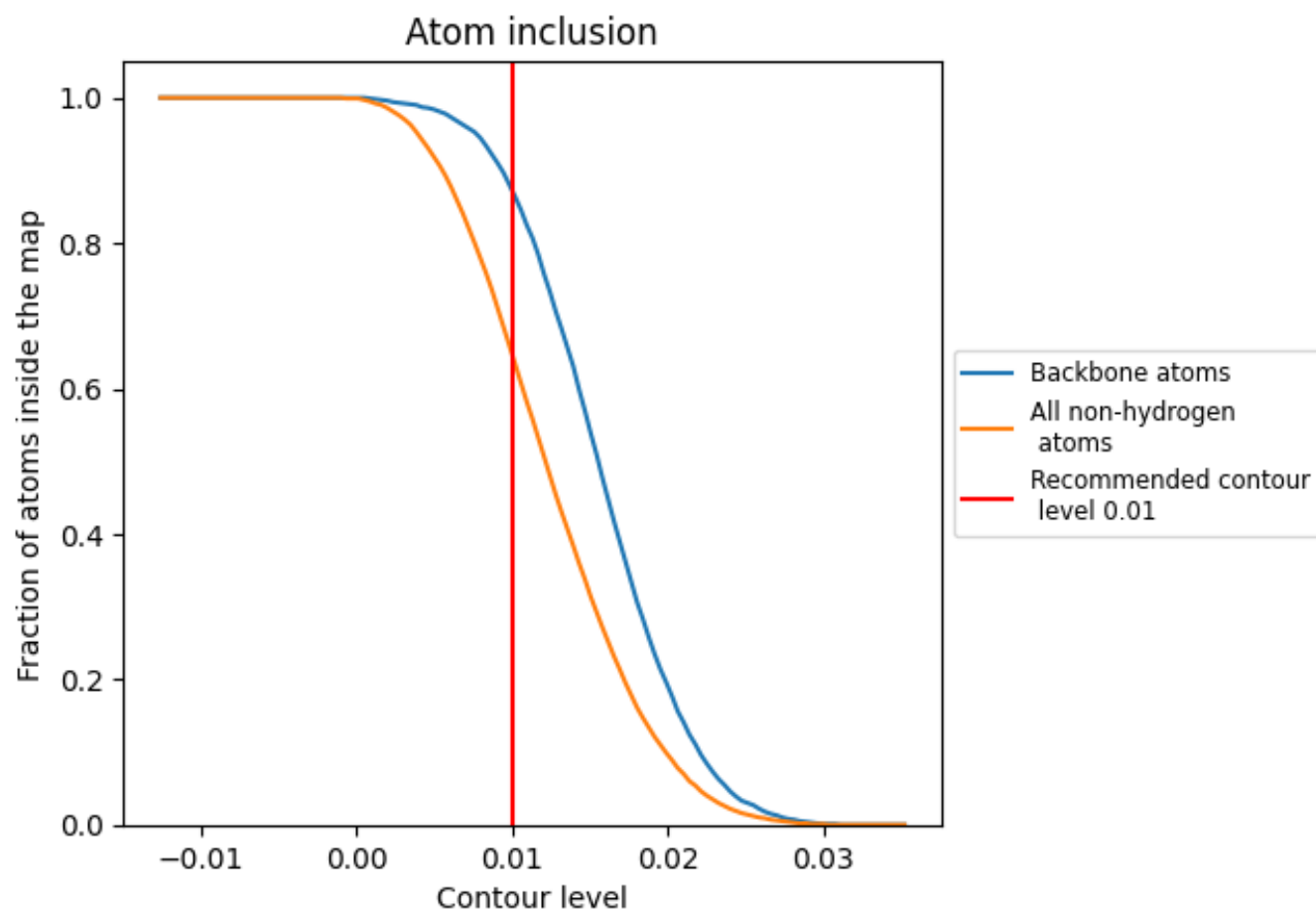
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 65% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6470	 0.3120
A	 0.6860	 0.3230
B	 0.6800	 0.3230
C	 0.7020	 0.3280
D	 0.4640	 0.2690
E	 0.1540	 0.1050
F	 0.3850	 0.2330
G	 0.2530	 0.0430
H	 0.3590	 0.1660
I	 0.3570	 0.1940
J	 0.3930	 0.2910
K	 0.6410	 0.3500
L	 0.6430	 0.3300
M	 0.4360	 0.2630
N	 0.4100	 0.3620
O	 0.2560	 0.1160
P	 0.2000	 0.2230
Q	 0.1790	 0.2040
R	 0.2140	 0.0870
S	 0.2500	 0.1180
T	 0.3400	 0.1870
U	 0.4940	 0.3120
V	 0.3930	 0.3110
W	 0.2500	 0.3250
X	 0.1790	 0.1490
Y	 0.4100	 0.2360
Z	 0.3210	 0.2040
a	 0.1070	 0.1740
b	 0.4100	 0.2940
c	 0.3850	 0.2810
d	 0.2860	 0.1460
e	 0.2200	 0.2090
f	 0.1840	 0.1720
g	 0.1790	 0.2460
h	 0.1790	 0.1850



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Chain	Atom inclusion	Q-score
i	 0.3080	 0.1860
j	 0.3210	 0.0670
k	 0.4100	 0.1930
l	 0.5180	 0.3080
m	 0.3930	 0.2540
n	 0.3570	 0.1430
o	 0.2500	 0.1570
p	 0.3850	 0.2900
q	 0.3570	 0.3000
r	 0.1430	 0.2350
s	 0.5360	 0.2550
t	 0.4870	 0.3290
u	 0.2310	 0.1360
v	 0.2170	 0.1500
w	 0.2100	 0.2070
x	 0.1430	 0.2600
y	 0.2310	 0.1940