



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 05:33 PM UTC

PDB ID : 7JJI / pdb_00007jji
EMDB ID : EMD-22352
Title : Structure of SARS-CoV-2 3Q-2P full-length prefusion spike trimer (C3 symmetry)
Authors : Bangaru, S.; Turner, H.L.; Ozorowski, G.; Antanasijevic, A.; Ward, A.B.
Deposited on : 2020-07-26
Resolution : 3.60 Å(reported)
Based on initial model : 6VXX

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

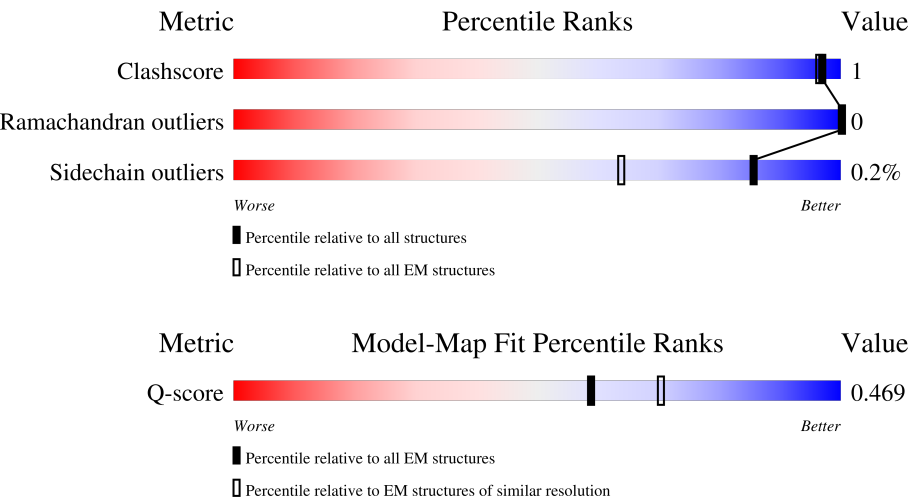
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	1273	82%5%13%
1	B	1273	82%5%13%
1	C	1273	82%5%13%
2	D	2	50% 100%

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

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Mol	Chain	Length	Quality of chain
2	d	2	50% 100%
2	e	2	100%
2	f	2	100%
2	g	2	100%
2	h	2	50% 100%
2	i	2	100%
2	j	2	100%
2	k	2	50% 100%
2	l	2	100%
2	m	2	50% 100%
2	n	2	100%
2	o	2	100%
2	p	2	50% 100%
2	q	2	50% 50%
2	r	2	100%
2	s	2	50% 100%
2	t	2	100%
2	u	2	100%
2	v	2	50% 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27459 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1109	Total	C	N	O	S	0	0
			8657	5516	1448	1653	40		
1	B	1109	Total	C	N	O	S	0	0
			8657	5516	1448	1653	40		
1	C	1109	Total	C	N	O	S	0	0
			8657	5516	1448	1653	40		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLN	ARG	engineered mutation	UNP P0DTC2
A	683	GLN	ARG	engineered mutation	UNP P0DTC2
A	685	GLN	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLN	ARG	engineered mutation	UNP P0DTC2
B	683	GLN	ARG	engineered mutation	UNP P0DTC2
B	685	GLN	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLN	ARG	engineered mutation	UNP P0DTC2
C	683	GLN	ARG	engineered mutation	UNP P0DTC2
C	685	GLN	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total 28	C 16	N 2	O 10	0	0
2	E	2	Total 28	C 16	N 2	O 10	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0
2	G	2	Total 28	C 16	N 2	O 10	0	0
2	H	2	Total 28	C 16	N 2	O 10	0	0
2	I	2	Total 28	C 16	N 2	O 10	0	0
2	J	2	Total 28	C 16	N 2	O 10	0	0
2	K	2	Total 28	C 16	N 2	O 10	0	0
2	L	2	Total 28	C 16	N 2	O 10	0	0
2	M	2	Total 28	C 16	N 2	O 10	0	0
2	N	2	Total 28	C 16	N 2	O 10	0	0
2	O	2	Total 28	C 16	N 2	O 10	0	0
2	P	2	Total 28	C 16	N 2	O 10	0	0
2	Q	2	Total 28	C 16	N 2	O 10	0	0
2	R	2	Total 28	C 16	N 2	O 10	0	0
2	S	2	Total 28	C 16	N 2	O 10	0	0
2	T	2	Total 28	C 16	N 2	O 10	0	0
2	U	2	Total 28	C 16	N 2	O 10	0	0
2	V	2	Total 28	C 16	N 2	O 10	0	0
2	W	2	Total 28	C 16	N 2	O 10	0	0
2	X	2	Total 28	C 16	N 2	O 10	0	0
2	Y	2	Total 28	C 16	N 2	O 10	0	0

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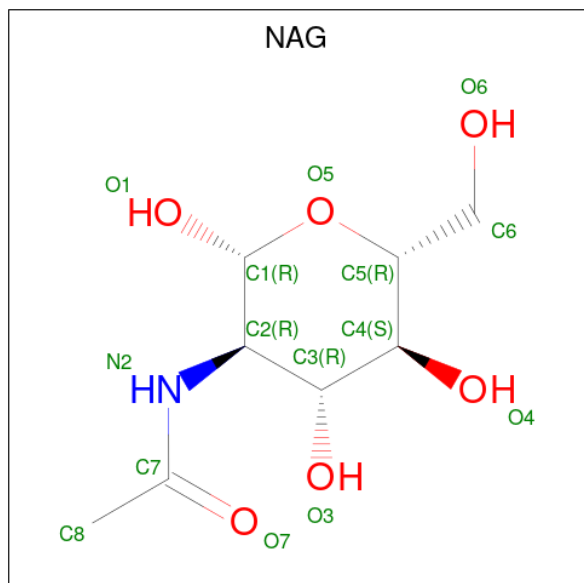
Mol	Chain	Residues	Atoms				AltConf	Trace
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	h	2	Total	C	N	O	0	0
			28	16	2	10		
2	i	2	Total	C	N	O	0	0
			28	16	2	10		
2	j	2	Total	C	N	O	0	0
			28	16	2	10		
2	k	2	Total	C	N	O	0	0
			28	16	2	10		
2	l	2	Total	C	N	O	0	0
			28	16	2	10		
2	m	2	Total	C	N	O	0	0
			28	16	2	10		
2	n	2	Total	C	N	O	0	0
			28	16	2	10		
2	o	2	Total	C	N	O	0	0
			28	16	2	10		
2	p	2	Total	C	N	O	0	0
			28	16	2	10		
2	q	2	Total	C	N	O	0	0
			28	16	2	10		
2	r	2	Total	C	N	O	0	0
			28	16	2	10		
2	s	2	Total	C	N	O	0	0
			28	16	2	10		
2	t	2	Total	C	N	O	0	0
			28	16	2	10		

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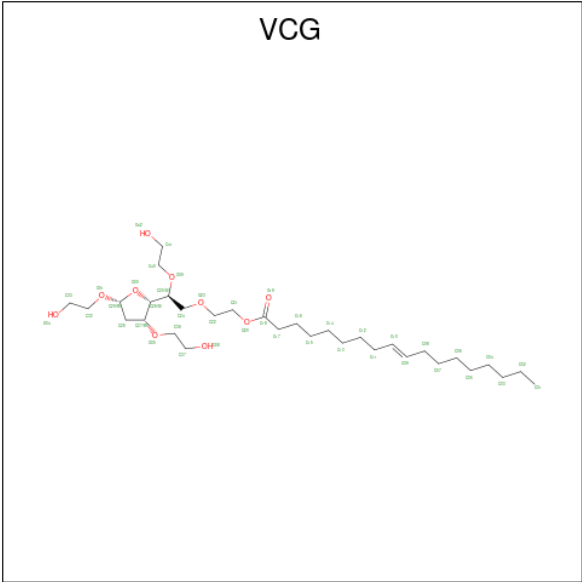
Mol	Chain	Residues	Atoms				AltConf	Trace
2	u	2	Total	C	N	O	0	0
			28	16	2	10		
2	v	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



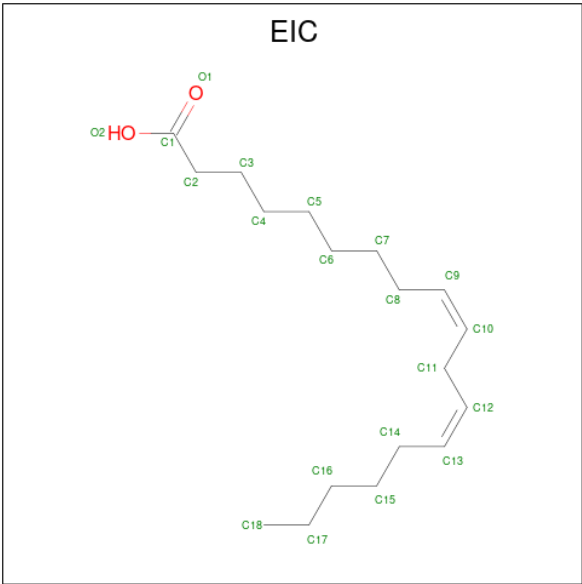
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is 2-hydroxyethyl 2-deoxy-3,5-bis-O-(2-hydroxyethyl)-6-O-(2-{[(9E)-octadec-9-enoyl]oxy}ethyl)-alpha-L-xylo-hexofuranoside (CCD ID: VCG) (formula: $C_{32}H_{60}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			42	32	10	
4	B	1	Total	C	O	0
			42	32	10	
4	C	1	Total	C	O	0
			42	32	10	

- Molecule 5 is LINOLEIC ACID (CCD ID: EIC) (formula: C₁₈H₃₂O₂) (labeled as "Ligand of Interest" by depositor).

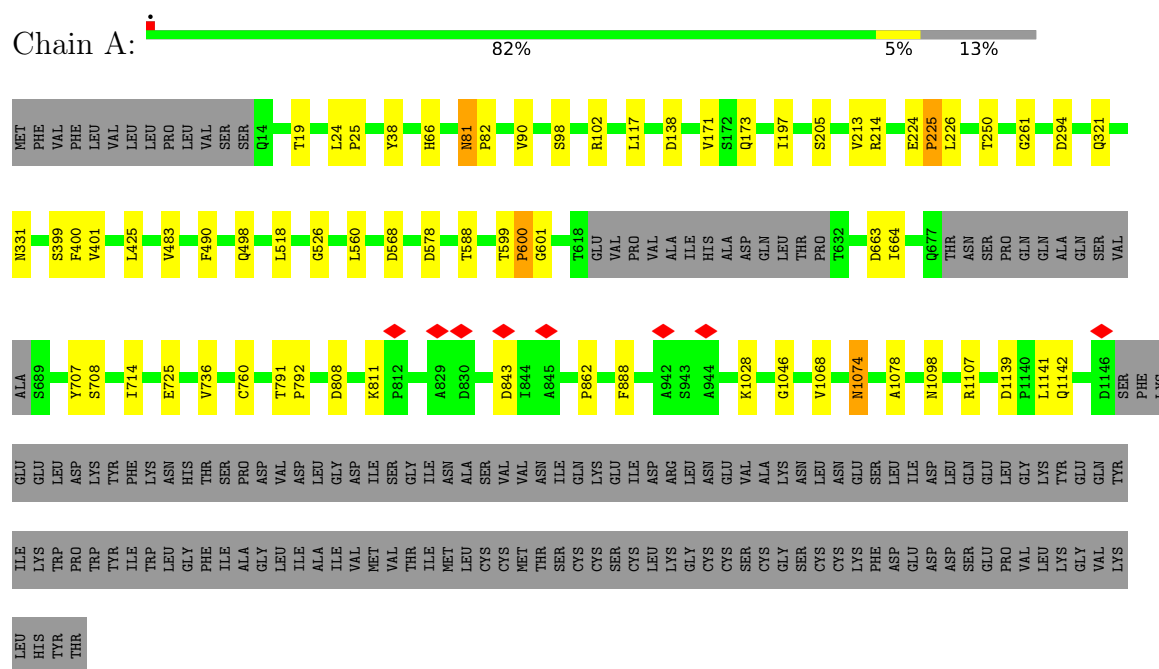


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 20	C 18	O 2	0
5	B	1	Total 20	C 18	O 2	0
5	C	1	Total 20	C 18	O 2	0

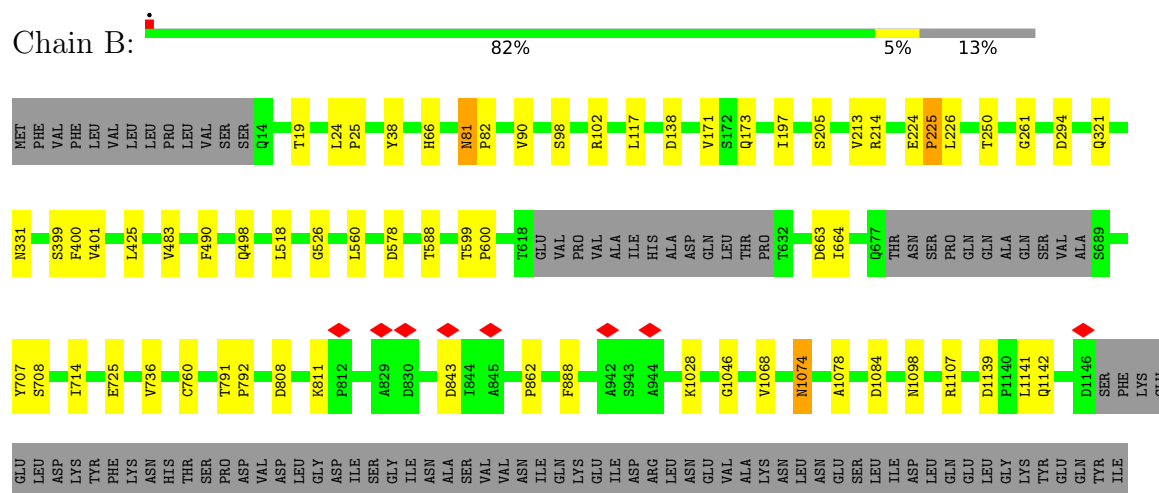
3 Residue-property plots [i](#)

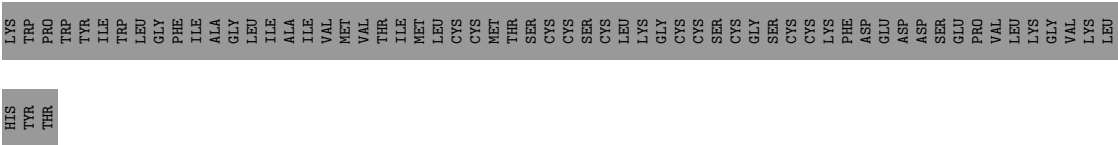
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

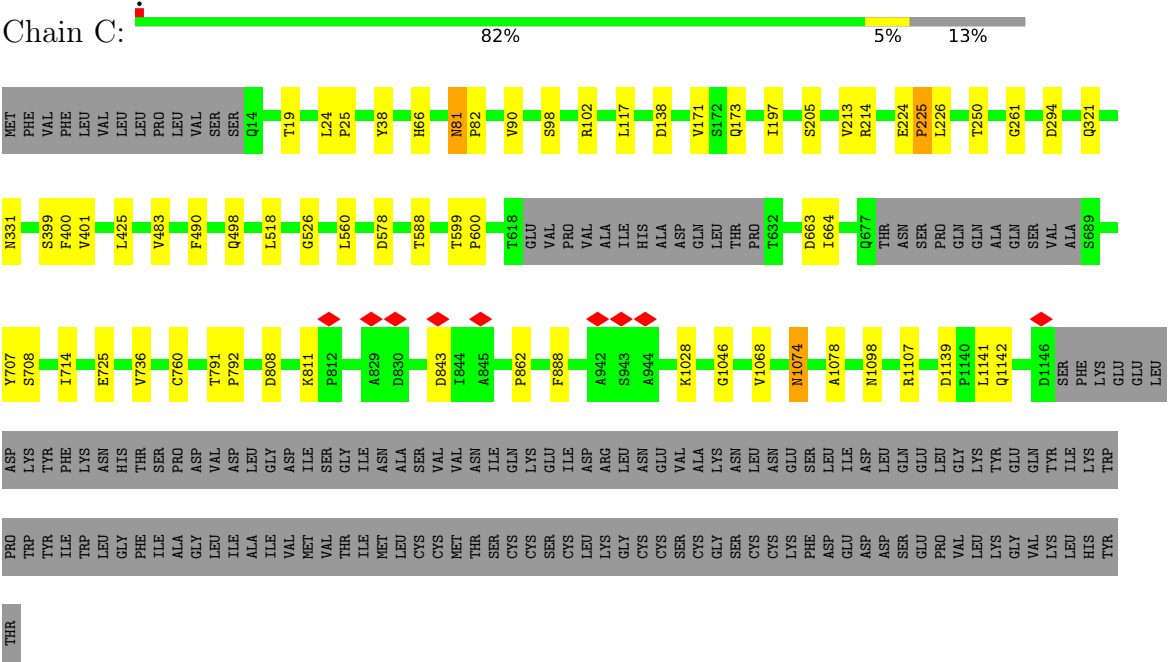


• Molecule 1: Spike glycoprotein

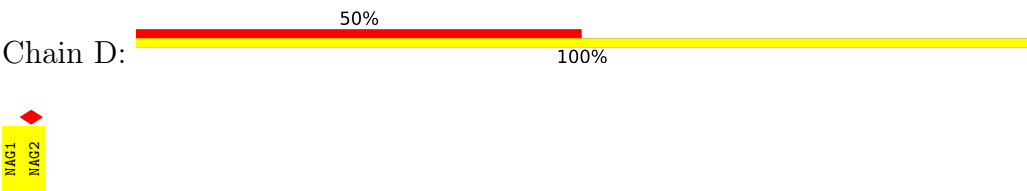




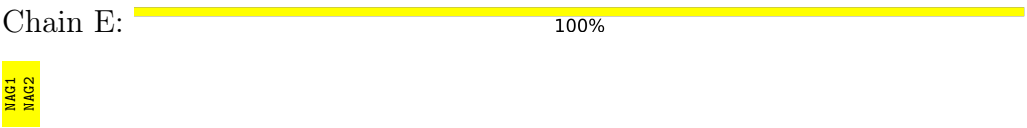
• Molecule 1: Spike glycoprotein



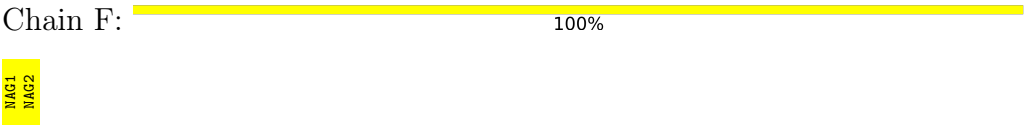
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• 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

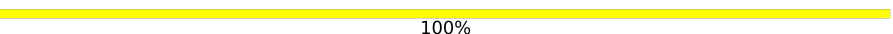


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

NAG1
NAG2

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

Chain N:  100%

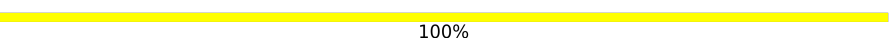
NAG1
NAG2

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

Chain O:  50% 100%

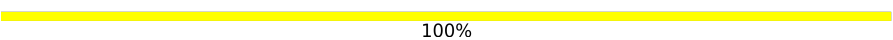
♦
NAG1
NAG2

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

Chain P:  100%

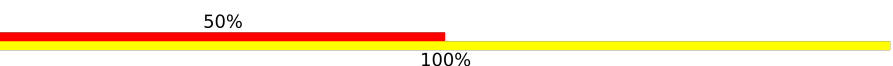
NAG1
NAG2

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

Chain Q:  100%

NAG1
NAG2

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

Chain R:  50% 100%

♦
NAG1
NAG2

- 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



NAG1
NAG2

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

Chain Z:  100%

NAG1
NAG2

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

Chain a:  50%
100%

NAG1
NAG2

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

Chain b:  50%
50%

NAG1
NAG2

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

Chain c:  100%

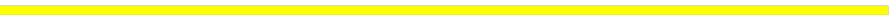
NAG1
NAG2

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

Chain d:  50%
100%

NAG1
NAG2

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

Chain e:  100%

NAG1
NAG2

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

Chain f:  100%

NAG1
NAG2

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

Chain g:  100%

NAG1
NAG2

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

Chain h:  50% 100%


NAG1
NAG2

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

Chain i:  100%

NAG1
NAG2

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

Chain j:  100%

NAG1
NAG2

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

Chain k:  50% 100%


NAG1
NAG2

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

Chain l:  100%

MAG1
MAG2

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

Chain m:  50%
100%

MAG1
MAG2

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

Chain n:  100%

MAG1
MAG2

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

Chain o:  100%

MAG1
MAG2

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

Chain p:  50%
100%

MAG1
MAG2

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

Chain q:  50%
50%

MAG1
MAG2

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

Chain r:  100%

NAG1
NAG2

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



NAG1
NAG2

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



NAG1
NAG2

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



NAG1
NAG2

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



NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	45374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.949	Depositor
Minimum map value	-1.152	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	437.0, 437.0, 437.0	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.02	0/8859	1.26	85/12059 (0.7%)
1	B	1.02	0/8859	1.26	85/12059 (0.7%)
1	C	1.02	0/8859	1.26	85/12059 (0.7%)
All	All	1.02	0/26577	1.26	255/36177 (0.7%)

There are no bond length outliers.

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	862	PRO	CA-C-N	8.03	127.98	120.03
1	B	862	PRO	C-N-CA	8.03	127.98	120.03
1	C	862	PRO	CA-C-N	8.02	127.97	120.03
1	C	862	PRO	C-N-CA	8.02	127.97	120.03
1	A	862	PRO	CA-C-N	8.00	127.95	120.03
1	A	862	PRO	C-N-CA	8.00	127.95	120.03
1	A	214	ARG	N-CA-C	7.83	121.32	111.69
1	B	214	ARG	N-CA-C	7.82	121.31	111.69
1	C	214	ARG	N-CA-C	7.80	121.28	111.69
1	A	1107	ARG	N-CA-C	7.52	119.56	111.36
1	C	1107	ARG	N-CA-C	7.49	119.53	111.36
1	B	1107	ARG	N-CA-C	7.47	119.50	111.36
1	C	792	PRO	CA-C-N	7.43	127.07	119.56
1	C	792	PRO	C-N-CA	7.43	127.07	119.56
1	A	792	PRO	CA-C-N	7.40	127.03	119.56
1	A	792	PRO	C-N-CA	7.40	127.03	119.56
1	B	792	PRO	CA-C-N	7.39	127.03	119.56
1	B	792	PRO	C-N-CA	7.39	127.03	119.56
1	B	90	VAL	N-CA-C	7.32	118.36	108.11
1	C	90	VAL	N-CA-C	7.32	118.36	108.11
1	A	90	VAL	N-CA-C	7.29	118.32	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	VAL	N-CA-C	7.25	117.79	111.56
1	B	213	VAL	N-CA-C	7.21	117.76	111.56
1	C	213	VAL	N-CA-C	7.16	117.72	111.56
1	C	400	PHE	N-CA-C	6.92	118.70	108.60
1	A	400	PHE	N-CA-C	6.92	118.70	108.60
1	B	400	PHE	N-CA-C	6.91	118.68	108.60
1	C	1074	ASN	CA-CB-CG	6.90	119.50	112.60
1	B	1074	ASN	CA-CB-CG	6.88	119.48	112.60
1	C	25	PRO	CA-C-N	6.88	126.80	119.85
1	C	25	PRO	C-N-CA	6.88	126.80	119.85
1	B	25	PRO	CA-C-N	6.87	126.79	119.85
1	B	25	PRO	C-N-CA	6.87	126.79	119.85
1	A	1074	ASN	CA-CB-CG	6.87	119.47	112.60
1	A	25	PRO	CA-C-N	6.86	126.78	119.85
1	A	25	PRO	C-N-CA	6.86	126.78	119.85
1	B	81	ASN	CA-C-N	6.78	126.75	120.03
1	B	81	ASN	C-N-CA	6.78	126.75	120.03
1	C	81	ASN	CA-C-N	6.78	126.74	120.03
1	C	81	ASN	C-N-CA	6.78	126.74	120.03
1	A	81	ASN	CA-C-N	6.76	126.73	120.03
1	A	81	ASN	C-N-CA	6.76	126.73	120.03
1	A	526	GLY	CA-C-N	6.75	127.71	120.83
1	A	526	GLY	C-N-CA	6.75	127.71	120.83
1	B	526	GLY	CA-C-N	6.72	127.69	120.83
1	B	526	GLY	C-N-CA	6.72	127.69	120.83
1	A	600	PRO	N-CA-C	-6.70	101.36	111.41
1	C	600	PRO	N-CA-C	-6.69	101.38	111.41
1	B	600	PRO	N-CA-C	-6.69	101.38	111.41
1	C	526	GLY	CA-C-N	6.68	127.64	120.83
1	C	526	GLY	C-N-CA	6.68	127.64	120.83
1	C	736	VAL	N-CA-C	6.55	117.28	108.11
1	A	736	VAL	N-CA-C	6.55	117.27	108.11
1	B	736	VAL	N-CA-C	6.53	117.26	108.11
1	B	19	THR	N-CA-C	6.51	121.28	112.88
1	A	19	THR	N-CA-C	6.50	121.27	112.88
1	C	19	THR	N-CA-C	6.50	121.27	112.88
1	C	498	GLN	CA-C-N	6.49	126.62	119.87
1	C	498	GLN	C-N-CA	6.49	126.62	119.87
1	A	498	GLN	CA-C-N	6.46	126.58	119.87
1	A	498	GLN	C-N-CA	6.46	126.58	119.87
1	B	498	GLN	CA-C-N	6.45	126.58	119.87
1	B	498	GLN	C-N-CA	6.45	126.58	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	N-CA-C	6.45	118.37	109.54
1	B	102	ARG	N-CA-C	6.44	118.36	109.54
1	C	102	ARG	N-CA-C	6.41	118.32	109.54
1	C	38	TYR	CA-C-N	6.35	125.97	119.56
1	C	38	TYR	C-N-CA	6.35	125.97	119.56
1	B	38	TYR	CA-C-N	6.34	125.96	119.56
1	B	38	TYR	C-N-CA	6.34	125.96	119.56
1	A	38	TYR	CA-C-N	6.33	125.96	119.56
1	A	38	TYR	C-N-CA	6.33	125.96	119.56
1	A	205	SER	N-CA-C	6.31	118.89	108.99
1	B	205	SER	N-CA-C	6.30	118.89	108.99
1	C	205	SER	N-CA-C	6.29	118.86	108.99
1	A	714	ILE	CA-C-N	6.20	126.17	119.78
1	A	714	ILE	C-N-CA	6.20	126.17	119.78
1	B	714	ILE	CA-C-N	6.20	126.16	119.78
1	B	714	ILE	C-N-CA	6.20	126.16	119.78
1	C	714	ILE	CA-C-N	6.19	126.16	119.78
1	C	714	ILE	C-N-CA	6.19	126.16	119.78
1	B	425	LEU	CA-C-N	6.14	126.11	120.03
1	B	425	LEU	C-N-CA	6.14	126.11	120.03
1	C	425	LEU	CA-C-N	6.13	126.10	120.03
1	C	425	LEU	C-N-CA	6.13	126.10	120.03
1	A	425	LEU	CA-C-N	6.12	126.09	120.03
1	A	425	LEU	C-N-CA	6.12	126.09	120.03
1	A	599	THR	CA-C-N	6.06	126.03	120.03
1	A	599	THR	C-N-CA	6.06	126.03	120.03
1	C	599	THR	CA-C-N	6.05	126.02	120.03
1	C	599	THR	C-N-CA	6.05	126.02	120.03
1	B	599	THR	CA-C-N	6.03	125.99	120.03
1	B	599	THR	C-N-CA	6.03	125.99	120.03
1	C	1078	ALA	CA-C-N	6.01	125.63	119.56
1	C	1078	ALA	C-N-CA	6.01	125.63	119.56
1	A	1078	ALA	CA-C-N	6.00	125.62	119.56
1	A	1078	ALA	C-N-CA	6.00	125.62	119.56
1	C	224	GLU	CA-C-N	5.99	125.67	119.56
1	C	224	GLU	C-N-CA	5.99	125.67	119.56
1	A	224	GLU	CA-C-N	5.98	125.66	119.56
1	A	224	GLU	C-N-CA	5.98	125.66	119.56
1	B	1078	ALA	CA-C-N	5.97	125.59	119.56
1	B	1078	ALA	C-N-CA	5.97	125.59	119.56
1	C	708	SER	N-CA-C	-5.97	102.08	110.50
1	B	224	GLU	CA-C-N	5.96	125.64	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	GLU	C-N-CA	5.96	125.64	119.56
1	B	708	SER	N-CA-C	-5.96	102.10	110.50
1	A	708	SER	N-CA-C	-5.95	102.11	110.50
1	B	808	ASP	CA-C-N	5.92	126.03	119.87
1	B	808	ASP	C-N-CA	5.92	126.03	119.87
1	A	808	ASP	CA-C-N	5.92	126.02	119.87
1	A	808	ASP	C-N-CA	5.92	126.02	119.87
1	C	808	ASP	CA-C-N	5.90	126.00	119.87
1	C	808	ASP	C-N-CA	5.90	126.00	119.87
1	B	518	LEU	N-CA-C	5.83	120.20	113.38
1	A	600	PRO	CA-C-N	-5.82	114.57	120.10
1	A	600	PRO	C-N-CA	-5.82	114.57	120.10
1	C	600	PRO	CA-C-N	-5.81	114.58	120.10
1	C	600	PRO	C-N-CA	-5.81	114.58	120.10
1	A	24	LEU	CA-C-N	5.81	126.36	120.38
1	A	24	LEU	C-N-CA	5.81	126.36	120.38
1	C	518	LEU	N-CA-C	5.81	120.17	113.38
1	C	24	LEU	CA-C-N	5.80	126.36	120.38
1	C	24	LEU	C-N-CA	5.80	126.36	120.38
1	B	600	PRO	CA-C-N	-5.80	114.59	120.10
1	B	600	PRO	C-N-CA	-5.80	114.59	120.10
1	A	518	LEU	N-CA-C	5.80	120.16	113.38
1	B	24	LEU	CA-C-N	5.76	126.32	120.38
1	B	24	LEU	C-N-CA	5.76	126.32	120.38
1	B	888	PHE	CA-CB-CG	5.69	119.49	113.80
1	C	225	PRO	N-CA-C	5.68	121.23	113.84
1	A	225	PRO	N-CA-C	5.68	121.22	113.84
1	C	888	PHE	CA-CB-CG	5.67	119.47	113.80
1	B	225	PRO	N-CA-C	5.67	121.21	113.84
1	B	1139	ASP	CA-C-N	5.62	125.71	119.87
1	B	1139	ASP	C-N-CA	5.62	125.71	119.87
1	A	888	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	1139	ASP	CA-C-N	5.60	125.70	119.87
1	A	1139	ASP	C-N-CA	5.60	125.70	119.87
1	C	1139	ASP	CA-C-N	5.60	125.70	119.87
1	C	1139	ASP	C-N-CA	5.60	125.70	119.87
1	A	250	THR	CA-C-N	5.49	125.47	120.03
1	A	250	THR	C-N-CA	5.49	125.47	120.03
1	C	250	THR	CA-C-N	5.48	125.45	120.03
1	C	250	THR	C-N-CA	5.48	125.45	120.03
1	B	250	THR	CA-C-N	5.45	125.42	120.03
1	B	250	THR	C-N-CA	5.45	125.42	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	760	CYS	N-CA-C	-5.45	105.26	111.14
1	A	760	CYS	N-CA-C	-5.44	105.26	111.14
1	B	197	ILE	N-CA-C	5.44	115.82	107.77
1	A	197	ILE	N-CA-C	5.44	115.82	107.77
1	B	760	CYS	N-CA-C	-5.43	105.28	111.14
1	C	197	ILE	N-CA-C	5.43	115.80	107.77
1	B	213	VAL	CB-CA-C	-5.42	106.29	111.44
1	B	490	PHE	CA-C-N	5.41	125.03	119.56
1	B	490	PHE	C-N-CA	5.41	125.03	119.56
1	A	490	PHE	CA-C-N	5.40	125.01	119.56
1	A	490	PHE	C-N-CA	5.40	125.01	119.56
1	C	490	PHE	CA-C-N	5.40	125.01	119.56
1	C	490	PHE	C-N-CA	5.40	125.01	119.56
1	A	213	VAL	CB-CA-C	-5.38	106.33	111.44
1	C	213	VAL	CB-CA-C	-5.34	106.37	111.44
1	C	490	PHE	N-CA-C	-5.30	101.71	109.50
1	A	490	PHE	N-CA-C	-5.29	101.73	109.50
1	A	888	PHE	N-CA-C	-5.28	106.10	112.54
1	C	888	PHE	N-CA-C	-5.27	106.11	112.54
1	B	888	PHE	N-CA-C	-5.26	106.12	112.54
1	B	490	PHE	N-CA-C	-5.26	101.77	109.50
1	A	173	GLN	CA-C-N	5.26	125.16	119.85
1	A	173	GLN	C-N-CA	5.26	125.16	119.85
1	B	173	GLN	CA-C-N	5.26	125.16	119.85
1	B	173	GLN	C-N-CA	5.26	125.16	119.85
1	C	173	GLN	CA-C-N	5.25	125.15	119.85
1	C	173	GLN	C-N-CA	5.25	125.15	119.85
1	A	483	VAL	N-CA-C	5.23	115.38	107.75
1	B	483	VAL	N-CA-C	5.23	115.38	107.75
1	C	483	VAL	N-CA-C	5.23	115.38	107.75
1	C	294	ASP	CA-C-N	5.22	125.53	119.47
1	C	294	ASP	C-N-CA	5.22	125.53	119.47
1	B	294	ASP	CA-C-N	5.21	125.52	119.47
1	B	294	ASP	C-N-CA	5.21	125.52	119.47
1	C	578	ASP	CA-C-N	5.21	124.82	119.56
1	C	578	ASP	C-N-CA	5.21	124.82	119.56
1	A	294	ASP	CA-C-N	5.20	125.50	119.47
1	A	294	ASP	C-N-CA	5.20	125.50	119.47
1	B	401	VAL	N-CA-C	5.20	115.45	108.17
1	C	401	VAL	N-CA-C	5.20	115.45	108.17
1	A	401	VAL	N-CA-C	5.19	115.43	108.17
1	B	578	ASP	CA-C-N	5.19	124.80	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	578	ASP	C-N-CA	5.19	124.80	119.56
1	A	588	THR	CA-C-N	5.17	125.10	119.78
1	A	588	THR	C-N-CA	5.17	125.10	119.78
1	A	98	SER	N-CA-C	5.16	118.69	111.56
1	C	138	ASP	CA-C-N	5.16	125.06	119.85
1	C	138	ASP	C-N-CA	5.16	125.06	119.85
1	C	588	THR	CA-C-N	5.16	125.09	119.78
1	C	588	THR	C-N-CA	5.16	125.09	119.78
1	A	811	LYS	CA-C-N	5.15	124.76	119.56
1	A	811	LYS	C-N-CA	5.15	124.76	119.56
1	A	138	ASP	CA-C-N	5.14	125.04	119.85
1	A	138	ASP	C-N-CA	5.14	125.04	119.85
1	B	98	SER	N-CA-C	5.14	118.65	111.56
1	A	261	GLY	N-CA-C	-5.13	104.72	112.41
1	A	578	ASP	CA-C-N	5.13	124.74	119.56
1	A	578	ASP	C-N-CA	5.13	124.74	119.56
1	C	98	SER	N-CA-C	5.12	118.63	111.56
1	B	138	ASP	CA-C-N	5.11	125.01	119.85
1	B	138	ASP	C-N-CA	5.11	125.01	119.85
1	B	811	LYS	CA-C-N	5.10	124.71	119.56
1	B	811	LYS	C-N-CA	5.10	124.71	119.56
1	A	1068	VAL	CA-C-N	5.10	125.00	119.85
1	A	1068	VAL	C-N-CA	5.10	125.00	119.85
1	B	261	GLY	N-CA-C	-5.10	104.76	112.41
1	B	588	THR	CA-C-N	5.10	125.03	119.78
1	B	588	THR	C-N-CA	5.10	125.03	119.78
1	B	1068	VAL	CA-C-N	5.10	125.00	119.85
1	B	1068	VAL	C-N-CA	5.10	125.00	119.85
1	C	261	GLY	N-CA-C	-5.10	104.77	112.41
1	C	1068	VAL	CA-C-N	5.09	125.00	119.85
1	C	1068	VAL	C-N-CA	5.09	125.00	119.85
1	C	811	LYS	CA-C-N	5.09	124.70	119.56
1	C	811	LYS	C-N-CA	5.09	124.70	119.56
1	B	321	GLN	CA-C-N	5.09	124.99	119.85
1	B	321	GLN	C-N-CA	5.09	124.99	119.85
1	B	1098	ASN	CA-CB-CG	5.09	117.69	112.60
1	C	1098	ASN	CA-CB-CG	5.08	117.67	112.60
1	B	560	LEU	CA-C-N	5.07	125.36	119.47
1	B	560	LEU	C-N-CA	5.07	125.36	119.47
1	A	1098	ASN	CA-CB-CG	5.07	117.67	112.60
1	C	791	THR	CA-C-N	5.06	123.36	119.66
1	C	791	THR	C-N-CA	5.06	123.36	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	791	THR	CA-C-N	5.06	123.35	119.66
1	B	791	THR	C-N-CA	5.06	123.35	119.66
1	A	66	HIS	N-CA-C	5.05	117.49	109.50
1	C	117	LEU	N-CA-C	5.05	116.97	108.73
1	A	560	LEU	CA-C-N	5.05	125.33	119.47
1	A	560	LEU	C-N-CA	5.05	125.33	119.47
1	C	66	HIS	N-CA-C	5.05	117.48	109.50
1	C	560	LEU	CA-C-N	5.05	125.33	119.47
1	C	560	LEU	C-N-CA	5.05	125.33	119.47
1	A	321	GLN	CA-C-N	5.05	124.95	119.85
1	A	321	GLN	C-N-CA	5.05	124.95	119.85
1	B	399	SER	N-CA-C	5.05	117.57	108.48
1	C	399	SER	N-CA-C	5.04	117.56	108.48
1	B	117	LEU	N-CA-C	5.04	116.95	108.73
1	C	321	GLN	CA-C-N	5.04	124.94	119.85
1	C	321	GLN	C-N-CA	5.04	124.94	119.85
1	B	66	HIS	N-CA-C	5.04	117.46	109.50
1	A	791	THR	CA-C-N	5.04	123.34	119.66
1	A	791	THR	C-N-CA	5.04	123.34	119.66
1	A	117	LEU	N-CA-C	5.04	116.94	108.73
1	A	399	SER	N-CA-C	5.03	117.54	108.48
1	C	1046	GLY	N-CA-C	-5.02	105.82	111.85
1	A	1046	GLY	N-CA-C	-5.02	105.83	111.85
1	B	1046	GLY	N-CA-C	-5.00	105.84	111.85

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	8657	0	8418	11	0
1	B	8657	0	8418	9	0
1	C	8657	0	8418	9	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	1	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	1	0
2	c	28	0	25	0	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
2	f	28	0	25	0	0
2	g	28	0	25	0	0
2	h	28	0	25	0	0
2	i	28	0	25	0	0
2	j	28	0	25	0	0
2	k	28	0	25	0	0
2	l	28	0	25	0	0
2	m	28	0	25	0	0
2	n	28	0	25	0	0
2	o	28	0	25	0	0
2	p	28	0	25	0	0
2	q	28	0	25	1	0
2	r	28	0	25	0	0
2	s	28	0	25	0	0
2	t	28	0	25	0	0
2	u	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	v	28	0	25	0	0
3	A	14	0	12	0	0
3	B	14	0	12	0	0
3	C	14	0	12	0	0
4	A	42	0	0	2	0
4	B	42	0	0	2	0
4	C	42	0	0	2	0
5	A	20	0	31	0	0
5	B	20	0	31	0	0
5	C	20	0	31	0	0
All	All	27459	0	26508	35	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 1.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.40	0.55
1:C:707:TYR:CG	1:C:707:TYR:O	2.59	0.54
1:A:707:TYR:O	1:A:707:TYR:CG	2.59	0.54
4:A:1302:VCG:O35	4:A:1302:VCG:C24	2.56	0.54
4:B:1503:VCG:O35	4:B:1503:VCG:C24	2.56	0.54
1:B:171:VAL:HG11	2:b:2:NAG:H82	1.90	0.53
4:C:1503:VCG:C24	4:C:1503:VCG:O35	2.56	0.53
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.40	0.53
1:C:663:ASP:O	1:C:664:ILE:C	2.52	0.53
1:A:663:ASP:O	1:A:664:ILE:C	2.52	0.53
1:A:171:VAL:HG11	2:M:2:NAG:H82	1.90	0.52
1:B:663:ASP:O	1:B:664:ILE:C	2.52	0.52
1:B:707:TYR:O	1:B:707:TYR:CG	2.59	0.52
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.40	0.52
1:C:171:VAL:HG11	2:q:2:NAG:H82	1.90	0.52
1:C:843:ASP:N	1:C:843:ASP:OD1	2.46	0.49
1:A:843:ASP:N	1:A:843:ASP:OD1	2.46	0.48
1:B:843:ASP:OD1	1:B:843:ASP:N	2.46	0.48
4:A:1302:VCG:C22	4:A:1302:VCG:C40	2.95	0.45
4:C:1503:VCG:C40	4:C:1503:VCG:C22	2.95	0.44
4:B:1503:VCG:C22	4:B:1503:VCG:C40	2.95	0.44
1:B:81:ASN:N	1:B:82:PRO:CD	2.82	0.43
1:B:225:PRO:O	1:B:226:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PRO:O	1:C:226:LEU:C	2.61	0.43
1:A:81:ASN:N	1:A:82:PRO:CD	2.82	0.43
1:A:1141:LEU:O	1:A:1142:GLN:C	2.62	0.43
1:C:81:ASN:N	1:C:82:PRO:CD	2.82	0.42
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.48	0.42
1:C:1141:LEU:O	1:C:1142:GLN:C	2.62	0.42
1:A:225:PRO:O	1:A:226:LEU:C	2.61	0.41
1:B:1141:LEU:O	1:B:1142:GLN:C	2.62	0.41
1:A:600:PRO:O	1:A:601:GLY:C	2.62	0.41
1:A:568:ASP:OD1	1:A:568:ASP:C	2.64	0.40
1:C:707:TYR:O	1:C:707:TYR:CD2	2.74	0.40
1:A:707:TYR:O	1:A:707:TYR:CD2	2.75	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	1103/1273 (87%)	1085 (98%)	18 (2%)	0	100	100
1	B	1103/1273 (87%)	1085 (98%)	18 (2%)	0	100	100
1	C	1103/1273 (87%)	1085 (98%)	18 (2%)	0	100	100
All	All	3309/3819 (87%)	3255 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	964/1112 (87%)	962 (100%)	2 (0%)	87	85
1	B	964/1112 (87%)	962 (100%)	2 (0%)	87	85
1	C	964/1112 (87%)	962 (100%)	2 (0%)	87	85
All	All	2892/3336 (87%)	2886 (100%)	6 (0%)	85	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	1074	ASN
1	B	331	ASN
1	B	1074	ASN
1	C	331	ASN
1	C	1074	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	125	ASN
1	A	641	ASN
1	A	836	GLN
1	A	901	GLN
1	A	955	ASN
1	A	1011	GLN
1	A	1058	HIS
1	B	52	GLN
1	B	66	HIS
1	B	125	ASN
1	B	836	GLN
1	B	856	ASN
1	B	901	GLN
1	B	955	ASN
1	B	1011	GLN
1	C	52	GLN
1	C	66	HIS
1	C	125	ASN
1	C	836	GLN

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Mol	Chain	Res	Type
1	C	856	ASN
1	C	901	GLN
1	C	955	ASN
1	C	1011	GLN
1	C	1058	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

90 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	2.25	6 (42%)	17,19,21	1.04	1 (5%)
2	NAG	D	2	2	14,14,15	2.11	5 (35%)	17,19,21	2.17	4 (23%)
2	NAG	E	1	2,1	14,14,15	2.06	6 (42%)	17,19,21	1.22	2 (11%)
2	NAG	E	2	2	14,14,15	2.04	5 (35%)	17,19,21	0.88	1 (5%)
2	NAG	F	1	2,1	14,14,15	2.10	6 (42%)	17,19,21	1.07	1 (5%)
2	NAG	F	2	2	14,14,15	2.03	6 (42%)	17,19,21	0.89	1 (5%)
2	NAG	G	1	2,1	14,14,15	2.13	6 (42%)	17,19,21	1.02	2 (11%)
2	NAG	G	2	2	14,14,15	2.06	7 (50%)	17,19,21	0.92	1 (5%)
2	NAG	H	1	2,1	14,14,15	2.06	6 (42%)	17,19,21	0.99	1 (5%)
2	NAG	H	2	2	14,14,15	2.04	6 (42%)	17,19,21	0.90	1 (5%)
2	NAG	I	1	2,1	14,14,15	2.09	6 (42%)	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	2	2	14,14,15	2.03	5 (35%)	17,19,21	0.85	1 (5%)
2	NAG	J	1	2,1	14,14,15	2.35	6 (42%)	17,19,21	1.11	2 (11%)
2	NAG	J	2	2	14,14,15	1.99	4 (28%)	17,19,21	0.91	1 (5%)
2	NAG	K	1	2,1	14,14,15	2.19	4 (28%)	17,19,21	1.10	1 (5%)
2	NAG	K	2	2	14,14,15	1.96	6 (42%)	17,19,21	0.96	1 (5%)
2	NAG	L	1	2,1	14,14,15	2.25	5 (35%)	17,19,21	0.97	0
2	NAG	L	2	2	14,14,15	2.07	6 (42%)	17,19,21	0.89	1 (5%)
2	NAG	M	1	2,1	14,14,15	2.13	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	M	2	2	14,14,15	2.01	5 (35%)	17,19,21	1.06	2 (11%)
2	NAG	N	1	2,1	14,14,15	1.99	6 (42%)	17,19,21	1.17	1 (5%)
2	NAG	N	2	2	14,14,15	1.98	6 (42%)	17,19,21	0.87	1 (5%)
2	NAG	O	1	2,1	14,14,15	2.18	5 (35%)	17,19,21	1.01	1 (5%)
2	NAG	O	2	2	14,14,15	2.02	6 (42%)	17,19,21	0.85	1 (5%)
2	NAG	P	1	2,1	14,14,15	2.18	7 (50%)	17,19,21	1.53	4 (23%)
2	NAG	P	2	2	14,14,15	2.12	5 (35%)	17,19,21	0.94	2 (11%)
2	NAG	Q	1	2,1	14,14,15	2.18	5 (35%)	17,19,21	0.94	0
2	NAG	Q	2	2	14,14,15	1.97	5 (35%)	17,19,21	0.89	1 (5%)
2	NAG	R	1	2,1	14,14,15	2.13	6 (42%)	17,19,21	1.21	3 (17%)
2	NAG	R	2	2	14,14,15	2.05	5 (35%)	17,19,21	0.92	1 (5%)
2	NAG	S	1	2,1	14,14,15	2.25	6 (42%)	17,19,21	1.04	1 (5%)
2	NAG	S	2	2	14,14,15	2.11	5 (35%)	17,19,21	2.17	4 (23%)
2	NAG	T	1	2,1	14,14,15	2.07	5 (35%)	17,19,21	1.22	2 (11%)
2	NAG	T	2	2	14,14,15	2.05	5 (35%)	17,19,21	0.88	1 (5%)
2	NAG	U	1	2,1	14,14,15	2.09	6 (42%)	17,19,21	1.08	1 (5%)
2	NAG	U	2	2	14,14,15	2.03	6 (42%)	17,19,21	0.89	1 (5%)
2	NAG	V	1	2,1	14,14,15	2.12	6 (42%)	17,19,21	1.03	2 (11%)
2	NAG	V	2	2	14,14,15	2.06	7 (50%)	17,19,21	0.92	1 (5%)
2	NAG	W	1	2,1	14,14,15	2.05	6 (42%)	17,19,21	0.99	1 (5%)
2	NAG	W	2	2	14,14,15	2.04	6 (42%)	17,19,21	0.91	1 (5%)
2	NAG	X	1	2,1	14,14,15	2.09	6 (42%)	17,19,21	0.98	1 (5%)
2	NAG	X	2	2	14,14,15	2.02	6 (42%)	17,19,21	0.86	1 (5%)
2	NAG	Y	1	2,1	14,14,15	2.33	6 (42%)	17,19,21	1.11	2 (11%)
2	NAG	Y	2	2	14,14,15	1.99	4 (28%)	17,19,21	0.91	1 (5%)
2	NAG	Z	1	2,1	14,14,15	2.19	4 (28%)	17,19,21	1.10	1 (5%)
2	NAG	Z	2	2	14,14,15	1.95	6 (42%)	17,19,21	0.96	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	a	1	2,1	14,14,15	2.25	5 (35%)	17,19,21	0.97	0
2	NAG	a	2	2	14,14,15	2.06	6 (42%)	17,19,21	0.89	1 (5%)
2	NAG	b	1	2,1	14,14,15	2.12	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	b	2	2	14,14,15	2.02	5 (35%)	17,19,21	1.05	2 (11%)
2	NAG	c	1	2,1	14,14,15	2.00	6 (42%)	17,19,21	1.18	1 (5%)
2	NAG	c	2	2	14,14,15	1.97	6 (42%)	17,19,21	0.87	1 (5%)
2	NAG	d	1	2,1	14,14,15	2.18	5 (35%)	17,19,21	1.01	1 (5%)
2	NAG	d	2	2	14,14,15	2.02	7 (50%)	17,19,21	0.86	1 (5%)
2	NAG	e	1	2,1	14,14,15	2.19	7 (50%)	17,19,21	1.53	4 (23%)
2	NAG	e	2	2	14,14,15	2.11	4 (28%)	17,19,21	0.93	2 (11%)
2	NAG	f	1	2,1	14,14,15	2.19	5 (35%)	17,19,21	0.94	0
2	NAG	f	2	2	14,14,15	1.98	5 (35%)	17,19,21	0.89	1 (5%)
2	NAG	g	1	2,1	14,14,15	2.13	6 (42%)	17,19,21	1.21	3 (17%)
2	NAG	g	2	2	14,14,15	2.04	5 (35%)	17,19,21	0.92	1 (5%)
2	NAG	h	1	2,1	14,14,15	2.25	6 (42%)	17,19,21	1.04	1 (5%)
2	NAG	h	2	2	14,14,15	2.11	5 (35%)	17,19,21	2.17	4 (23%)
2	NAG	i	1	2,1	14,14,15	2.07	6 (42%)	17,19,21	1.22	2 (11%)
2	NAG	i	2	2	14,14,15	2.04	5 (35%)	17,19,21	0.87	1 (5%)
2	NAG	j	1	2,1	14,14,15	2.09	6 (42%)	17,19,21	1.07	1 (5%)
2	NAG	j	2	2	14,14,15	2.04	6 (42%)	17,19,21	0.89	1 (5%)
2	NAG	k	1	2,1	14,14,15	2.12	6 (42%)	17,19,21	1.02	2 (11%)
2	NAG	k	2	2	14,14,15	2.06	7 (50%)	17,19,21	0.92	1 (5%)
2	NAG	l	1	2,1	14,14,15	2.05	6 (42%)	17,19,21	0.99	1 (5%)
2	NAG	l	2	2	14,14,15	2.02	6 (42%)	17,19,21	0.90	1 (5%)
2	NAG	m	1	2,1	14,14,15	2.09	6 (42%)	17,19,21	0.99	1 (5%)
2	NAG	m	2	2	14,14,15	2.02	5 (35%)	17,19,21	0.85	1 (5%)
2	NAG	n	1	2,1	14,14,15	2.34	6 (42%)	17,19,21	1.11	2 (11%)
2	NAG	n	2	2	14,14,15	2.00	5 (35%)	17,19,21	0.90	1 (5%)
2	NAG	o	1	2,1	14,14,15	2.20	4 (28%)	17,19,21	1.10	1 (5%)
2	NAG	o	2	2	14,14,15	1.96	6 (42%)	17,19,21	0.96	1 (5%)
2	NAG	p	1	2,1	14,14,15	2.24	5 (35%)	17,19,21	0.97	0
2	NAG	p	2	2	14,14,15	2.06	6 (42%)	17,19,21	0.88	1 (5%)
2	NAG	q	1	2,1	14,14,15	2.12	7 (50%)	17,19,21	1.10	2 (11%)
2	NAG	q	2	2	14,14,15	2.01	5 (35%)	17,19,21	1.05	2 (11%)
2	NAG	r	1	2,1	14,14,15	2.00	6 (42%)	17,19,21	1.18	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	r	2	2	14,14,15	1.98	6 (42%)	17,19,21	0.87	1 (5%)
2	NAG	s	1	2,1	14,14,15	2.18	5 (35%)	17,19,21	1.01	1 (5%)
2	NAG	s	2	2	14,14,15	2.02	7 (50%)	17,19,21	0.87	1 (5%)
2	NAG	t	1	2,1	14,14,15	2.19	7 (50%)	17,19,21	1.53	4 (23%)
2	NAG	t	2	2	14,14,15	2.12	4 (28%)	17,19,21	0.93	2 (11%)
2	NAG	u	1	2,1	14,14,15	2.18	5 (35%)	17,19,21	0.94	0
2	NAG	u	2	2	14,14,15	1.98	5 (35%)	17,19,21	0.89	1 (5%)
2	NAG	v	1	2,1	14,14,15	2.13	6 (42%)	17,19,21	1.21	3 (17%)
2	NAG	v	2	2	14,14,15	2.05	5 (35%)	17,19,21	0.92	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	P	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	NAG	W	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	NAG	a	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	NAG	b	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	NAG	c	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	NAG	d	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
2	NAG	e	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1
2	NAG	g	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
2	NAG	h	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	h	2	2	-	2/6/23/26	0/1/1/1
2	NAG	i	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	i	2	2	-	0/6/23/26	0/1/1/1
2	NAG	j	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	j	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	k	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	k	2	2	-	0/6/23/26	0/1/1/1
2	NAG	l	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	l	2	2	-	0/6/23/26	0/1/1/1
2	NAG	m	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	m	2	2	-	0/6/23/26	0/1/1/1
2	NAG	n	1	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	o	2	2	-	0/6/23/26	0/1/1/1
2	NAG	p	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	p	2	2	-	0/6/23/26	0/1/1/1
2	NAG	q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	r	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	r	2	2	-	0/6/23/26	0/1/1/1
2	NAG	s	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	s	2	2	-	0/6/23/26	0/1/1/1
2	NAG	t	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	t	2	2	-	0/6/23/26	0/1/1/1
2	NAG	u	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	u	2	2	-	0/6/23/26	0/1/1/1
2	NAG	v	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	v	2	2	-	0/6/23/26	0/1/1/1

All (508) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	NAG	C1-C2	6.12	1.60	1.52
2	D	1	NAG	C1-C2	6.11	1.60	1.52
2	h	1	NAG	C1-C2	6.10	1.60	1.52
2	a	1	NAG	C1-C2	6.03	1.60	1.52
2	L	1	NAG	C1-C2	6.02	1.60	1.52
2	p	1	NAG	C1-C2	5.99	1.60	1.52
2	o	1	NAG	C1-C2	5.87	1.60	1.52
2	Z	1	NAG	C1-C2	5.84	1.60	1.52
2	K	1	NAG	C1-C2	5.82	1.60	1.52
2	Q	1	NAG	C1-C2	5.77	1.60	1.52
2	u	1	NAG	C1-C2	5.77	1.60	1.52
2	f	1	NAG	C1-C2	5.76	1.60	1.52
2	d	1	NAG	C1-C2	5.61	1.60	1.52
2	P	2	NAG	C1-C2	5.60	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	t	2	NAG	C1-C2	5.59	1.60	1.52
2	e	2	NAG	C1-C2	5.59	1.60	1.52
2	s	1	NAG	C1-C2	5.58	1.59	1.52
2	O	1	NAG	C1-C2	5.56	1.59	1.52
2	J	1	NAG	C1-C2	5.43	1.59	1.52
2	n	1	NAG	C1-C2	5.37	1.59	1.52
2	Y	1	NAG	C1-C2	5.34	1.59	1.52
2	G	1	NAG	C1-C2	5.27	1.59	1.52
2	F	1	NAG	C1-C2	5.27	1.59	1.52
2	V	1	NAG	C1-C2	5.27	1.59	1.52
2	j	1	NAG	C1-C2	5.23	1.59	1.52
2	U	1	NAG	C1-C2	5.22	1.59	1.52
2	k	1	NAG	C1-C2	5.21	1.59	1.52
2	i	1	NAG	C1-C2	5.20	1.59	1.52
2	R	1	NAG	C1-C2	5.19	1.59	1.52
2	T	1	NAG	C1-C2	5.18	1.59	1.52
2	g	1	NAG	C1-C2	5.18	1.59	1.52
2	E	1	NAG	C1-C2	5.16	1.59	1.52
2	v	1	NAG	C1-C2	5.16	1.59	1.52
2	e	1	NAG	C1-C2	5.11	1.59	1.52
2	H	1	NAG	C1-C2	5.11	1.59	1.52
2	S	2	NAG	C1-C2	5.11	1.59	1.52
2	D	2	NAG	C1-C2	5.10	1.59	1.52
2	m	1	NAG	C1-C2	5.09	1.59	1.52
2	h	2	NAG	C1-C2	5.08	1.59	1.52
2	t	1	NAG	C1-C2	5.08	1.59	1.52
2	l	1	NAG	C1-C2	5.07	1.59	1.52
2	W	1	NAG	C1-C2	5.07	1.59	1.52
2	P	1	NAG	C1-C2	5.07	1.59	1.52
2	X	1	NAG	C1-C2	5.05	1.59	1.52
2	I	1	NAG	C1-C2	5.04	1.59	1.52
2	T	2	NAG	C1-C2	5.02	1.59	1.52
2	L	2	NAG	C1-C2	4.99	1.59	1.52
2	i	2	NAG	C1-C2	4.99	1.59	1.52
2	E	2	NAG	C1-C2	4.97	1.59	1.52
2	p	2	NAG	C1-C2	4.96	1.59	1.52
2	R	2	NAG	C1-C2	4.95	1.59	1.52
2	v	2	NAG	C1-C2	4.95	1.59	1.52
2	a	2	NAG	C1-C2	4.94	1.59	1.52
2	g	2	NAG	C1-C2	4.92	1.59	1.52
2	r	1	NAG	C1-C2	4.91	1.59	1.52
2	c	1	NAG	C1-C2	4.91	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	2	NAG	C1-C2	4.89	1.59	1.52
2	b	2	NAG	C1-C2	4.87	1.59	1.52
2	U	2	NAG	C1-C2	4.87	1.59	1.52
2	M	2	NAG	C1-C2	4.86	1.59	1.52
2	F	2	NAG	C1-C2	4.85	1.59	1.52
2	N	1	NAG	C1-C2	4.84	1.58	1.52
2	q	2	NAG	C1-C2	4.83	1.58	1.52
2	X	2	NAG	C1-C2	4.83	1.58	1.52
2	m	2	NAG	C1-C2	4.81	1.58	1.52
2	I	2	NAG	C1-C2	4.80	1.58	1.52
2	b	1	NAG	C1-C2	4.79	1.58	1.52
2	M	1	NAG	C1-C2	4.77	1.58	1.52
2	q	1	NAG	C1-C2	4.77	1.58	1.52
2	V	2	NAG	C1-C2	4.76	1.58	1.52
2	f	2	NAG	C1-C2	4.75	1.58	1.52
2	k	2	NAG	C1-C2	4.73	1.58	1.52
2	u	2	NAG	C1-C2	4.72	1.58	1.52
2	G	2	NAG	C1-C2	4.72	1.58	1.52
2	W	2	NAG	C1-C2	4.70	1.58	1.52
2	n	2	NAG	C1-C2	4.68	1.58	1.52
2	Q	2	NAG	C1-C2	4.67	1.58	1.52
2	J	2	NAG	C1-C2	4.66	1.58	1.52
2	Y	2	NAG	C1-C2	4.66	1.58	1.52
2	H	2	NAG	C1-C2	4.65	1.58	1.52
2	d	2	NAG	C1-C2	4.62	1.58	1.52
2	l	2	NAG	C1-C2	4.61	1.58	1.52
2	O	2	NAG	C1-C2	4.61	1.58	1.52
2	N	2	NAG	C1-C2	4.60	1.58	1.52
2	s	2	NAG	C1-C2	4.59	1.58	1.52
2	c	2	NAG	C1-C2	4.57	1.58	1.52
2	r	2	NAG	C1-C2	4.56	1.58	1.52
2	Z	2	NAG	C1-C2	4.29	1.58	1.52
2	o	2	NAG	C1-C2	4.29	1.58	1.52
2	K	2	NAG	C1-C2	4.28	1.58	1.52
2	J	1	NAG	O5-C5	3.49	1.50	1.43
2	n	1	NAG	O5-C5	3.44	1.50	1.43
2	Y	1	NAG	O5-C5	3.43	1.50	1.43
2	Z	1	NAG	O5-C5	3.38	1.50	1.43
2	K	1	NAG	O5-C5	3.38	1.50	1.43
2	o	1	NAG	O5-C5	3.37	1.50	1.43
2	o	2	NAG	O5-C5	3.29	1.49	1.43
2	O	2	NAG	O5-C5	3.29	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	NAG	O5-C5	3.28	1.49	1.43
2	Z	2	NAG	O5-C5	3.28	1.49	1.43
2	s	2	NAG	O5-C5	3.27	1.49	1.43
2	v	2	NAG	O5-C5	3.26	1.49	1.43
2	b	2	NAG	O5-C5	3.26	1.49	1.43
2	g	2	NAG	O5-C5	3.26	1.49	1.43
2	R	2	NAG	O5-C5	3.26	1.49	1.43
2	M	1	NAG	O5-C5	3.26	1.49	1.43
2	q	2	NAG	O5-C5	3.25	1.49	1.43
2	d	2	NAG	O5-C5	3.25	1.49	1.43
2	O	1	NAG	O5-C5	3.25	1.49	1.43
2	M	2	NAG	O5-C5	3.25	1.49	1.43
2	s	1	NAG	O5-C5	3.24	1.49	1.43
2	k	2	NAG	O5-C5	3.24	1.49	1.43
2	q	1	NAG	O5-C5	3.24	1.49	1.43
2	V	2	NAG	O5-C5	3.23	1.49	1.43
2	d	1	NAG	O5-C5	3.23	1.49	1.43
2	b	1	NAG	O5-C5	3.22	1.49	1.43
2	F	2	NAG	O5-C5	3.22	1.49	1.43
2	I	2	NAG	O5-C5	3.21	1.49	1.43
2	m	2	NAG	O5-C5	3.20	1.49	1.43
2	Y	2	NAG	O5-C5	3.20	1.49	1.43
2	G	2	NAG	O5-C5	3.20	1.49	1.43
2	j	2	NAG	O5-C5	3.20	1.49	1.43
2	J	2	NAG	O5-C5	3.19	1.49	1.43
2	n	2	NAG	O5-C5	3.18	1.49	1.43
2	U	2	NAG	O5-C5	3.18	1.49	1.43
2	E	2	NAG	O5-C5	3.18	1.49	1.43
2	L	2	NAG	O5-C5	3.18	1.49	1.43
2	X	2	NAG	O5-C5	3.18	1.49	1.43
2	T	2	NAG	O5-C5	3.17	1.49	1.43
2	h	2	NAG	O5-C5	3.17	1.49	1.43
2	i	2	NAG	O5-C5	3.16	1.49	1.43
2	D	2	NAG	O5-C5	3.16	1.49	1.43
2	a	2	NAG	O5-C5	3.16	1.49	1.43
2	H	2	NAG	O5-C5	3.15	1.49	1.43
2	N	2	NAG	O5-C5	3.15	1.49	1.43
2	c	2	NAG	O5-C5	3.14	1.49	1.43
2	S	2	NAG	O5-C5	3.14	1.49	1.43
2	W	2	NAG	O5-C5	3.14	1.49	1.43
2	p	2	NAG	O5-C5	3.14	1.49	1.43
2	l	2	NAG	O5-C5	3.11	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	r	2	NAG	O5-C5	3.10	1.49	1.43
2	u	2	NAG	O5-C5	3.10	1.49	1.43
2	f	2	NAG	O5-C5	3.10	1.49	1.43
2	Q	2	NAG	O5-C5	3.09	1.49	1.43
2	v	1	NAG	O5-C5	3.07	1.49	1.43
2	g	1	NAG	O5-C5	3.05	1.49	1.43
2	R	1	NAG	O5-C5	3.04	1.49	1.43
2	I	1	NAG	O5-C5	3.04	1.49	1.43
2	m	1	NAG	O5-C5	3.04	1.49	1.43
2	Q	1	NAG	O5-C5	3.03	1.49	1.43
2	u	1	NAG	O5-C5	3.02	1.49	1.43
2	f	1	NAG	O5-C5	3.02	1.49	1.43
2	X	1	NAG	O5-C5	2.98	1.49	1.43
2	G	1	NAG	O5-C5	2.97	1.49	1.43
2	a	1	NAG	O5-C5	2.97	1.49	1.43
2	V	1	NAG	O5-C5	2.97	1.49	1.43
2	L	1	NAG	O5-C5	2.95	1.49	1.43
2	k	1	NAG	O5-C5	2.95	1.49	1.43
2	p	1	NAG	O5-C5	2.95	1.49	1.43
2	H	1	NAG	O5-C5	2.87	1.49	1.43
2	l	1	NAG	O5-C5	2.85	1.49	1.43
2	t	2	NAG	O5-C5	2.84	1.49	1.43
2	W	1	NAG	O5-C5	2.84	1.49	1.43
2	e	2	NAG	O5-C5	2.82	1.48	1.43
2	N	1	NAG	O5-C5	2.80	1.48	1.43
2	e	2	NAG	C3-C2	2.80	1.58	1.52
2	P	2	NAG	C3-C2	2.80	1.58	1.52
2	P	2	NAG	O5-C5	2.79	1.48	1.43
2	t	2	NAG	C3-C2	2.79	1.58	1.52
2	c	1	NAG	O5-C5	2.78	1.48	1.43
2	r	1	NAG	O5-C5	2.77	1.48	1.43
2	D	1	NAG	O5-C5	2.75	1.48	1.43
2	j	1	NAG	O5-C5	2.74	1.48	1.43
2	S	1	NAG	O5-C5	2.73	1.48	1.43
2	h	1	NAG	O5-C5	2.72	1.48	1.43
2	F	1	NAG	O5-C5	2.71	1.48	1.43
2	U	1	NAG	O5-C5	2.70	1.48	1.43
2	t	1	NAG	C4-C3	2.69	1.59	1.52
2	e	1	NAG	O5-C5	2.69	1.48	1.43
2	o	1	NAG	O5-C1	2.69	1.48	1.43
2	J	1	NAG	C4-C3	2.68	1.59	1.52
2	t	1	NAG	O5-C5	2.68	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1	NAG	O5-C1	2.68	1.48	1.43
2	P	1	NAG	C4-C3	2.67	1.59	1.52
2	e	1	NAG	C4-C3	2.67	1.59	1.52
2	P	1	NAG	O5-C5	2.67	1.48	1.43
2	Z	1	NAG	O5-C1	2.67	1.48	1.43
2	n	1	NAG	C4-C3	2.66	1.59	1.52
2	Y	1	NAG	C4-C3	2.66	1.59	1.52
2	n	1	NAG	C4-C5	2.66	1.58	1.53
2	Y	1	NAG	C4-C5	2.65	1.58	1.53
2	T	1	NAG	O5-C5	2.64	1.48	1.43
2	J	1	NAG	C4-C5	2.64	1.58	1.53
2	E	1	NAG	O5-C5	2.63	1.48	1.43
2	i	1	NAG	O5-C5	2.62	1.48	1.43
2	G	2	NAG	C3-C2	2.61	1.58	1.52
2	n	1	NAG	O5-C1	2.58	1.48	1.43
2	J	1	NAG	O5-C1	2.58	1.48	1.43
2	k	2	NAG	C3-C2	2.58	1.57	1.52
2	Y	1	NAG	O5-C1	2.58	1.48	1.43
2	h	2	NAG	C3-C2	2.57	1.57	1.52
2	S	2	NAG	C3-C2	2.57	1.57	1.52
2	n	2	NAG	C3-C2	2.56	1.57	1.52
2	V	2	NAG	C3-C2	2.56	1.57	1.52
2	Y	2	NAG	C3-C2	2.56	1.57	1.52
2	J	2	NAG	C3-C2	2.55	1.57	1.52
2	D	2	NAG	C3-C2	2.54	1.57	1.52
2	t	1	NAG	C3-C2	2.52	1.57	1.52
2	e	1	NAG	C3-C2	2.52	1.57	1.52
2	J	1	NAG	C3-C2	2.51	1.57	1.52
2	R	1	NAG	C3-C2	2.50	1.57	1.52
2	H	2	NAG	C2-N2	2.50	1.50	1.46
2	n	1	NAG	C3-C2	2.50	1.57	1.52
2	L	2	NAG	C3-C2	2.50	1.57	1.52
2	P	1	NAG	C3-C2	2.49	1.57	1.52
2	W	2	NAG	C2-N2	2.49	1.50	1.46
2	g	1	NAG	C3-C2	2.49	1.57	1.52
2	H	2	NAG	C3-C2	2.49	1.57	1.52
2	v	1	NAG	C3-C2	2.49	1.57	1.52
2	l	2	NAG	C2-N2	2.49	1.50	1.46
2	Y	1	NAG	C3-C2	2.49	1.57	1.52
2	a	2	NAG	C3-C2	2.48	1.57	1.52
2	m	2	NAG	C3-C2	2.48	1.57	1.52
2	I	2	NAG	C3-C2	2.48	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	p	2	NAG	C3-C2	2.48	1.57	1.52
2	l	2	NAG	C3-C2	2.47	1.57	1.52
2	X	1	NAG	C4-C5	2.47	1.58	1.53
2	O	1	NAG	O5-C1	2.47	1.47	1.43
2	N	2	NAG	C3-C2	2.47	1.57	1.52
2	r	2	NAG	C3-C2	2.46	1.57	1.52
2	d	1	NAG	O5-C1	2.45	1.47	1.43
2	F	1	NAG	C4-C5	2.45	1.58	1.53
2	j	2	NAG	C3-C2	2.45	1.57	1.52
2	c	2	NAG	C3-C2	2.45	1.57	1.52
2	d	1	NAG	C4-C5	2.45	1.58	1.53
2	U	2	NAG	C3-C2	2.45	1.57	1.52
2	U	1	NAG	C4-C5	2.44	1.58	1.53
2	I	1	NAG	C4-C5	2.44	1.58	1.53
2	F	2	NAG	C3-C2	2.44	1.57	1.52
2	W	2	NAG	C3-C2	2.44	1.57	1.52
2	O	2	NAG	C3-C2	2.43	1.57	1.52
2	q	1	NAG	O5-C1	2.43	1.47	1.43
2	X	2	NAG	C3-C2	2.43	1.57	1.52
2	s	1	NAG	O5-C1	2.43	1.47	1.43
2	o	2	NAG	C4-C5	2.43	1.58	1.53
2	s	2	NAG	C3-C2	2.43	1.57	1.52
2	Z	2	NAG	C4-C5	2.43	1.58	1.53
2	b	1	NAG	C3-C2	2.43	1.57	1.52
2	m	1	NAG	C4-C5	2.42	1.58	1.53
2	K	2	NAG	C4-C5	2.42	1.58	1.53
2	b	1	NAG	O5-C1	2.42	1.47	1.43
2	O	1	NAG	C4-C5	2.42	1.58	1.53
2	M	1	NAG	O5-C1	2.42	1.47	1.43
2	j	1	NAG	C4-C5	2.42	1.58	1.53
2	s	1	NAG	C4-C5	2.42	1.58	1.53
2	d	2	NAG	C3-C2	2.41	1.57	1.52
2	M	1	NAG	C3-C2	2.40	1.57	1.52
2	S	1	NAG	C4-C5	2.40	1.58	1.53
2	q	1	NAG	C3-C2	2.39	1.57	1.52
2	h	1	NAG	C4-C5	2.39	1.58	1.53
2	g	2	NAG	C3-C2	2.39	1.57	1.52
2	t	1	NAG	C4-C5	2.38	1.58	1.53
2	f	2	NAG	C3-C2	2.38	1.57	1.52
2	P	1	NAG	C4-C5	2.38	1.58	1.53
2	R	2	NAG	C3-C2	2.38	1.57	1.52
2	v	2	NAG	C3-C2	2.38	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C4-C5	2.38	1.58	1.53
2	e	1	NAG	C4-C5	2.38	1.58	1.53
2	T	1	NAG	C3-C2	2.37	1.57	1.52
2	v	1	NAG	C4-C5	2.37	1.58	1.53
2	E	1	NAG	C3-C2	2.37	1.57	1.52
2	u	2	NAG	C3-C2	2.37	1.57	1.52
2	f	1	NAG	O5-C1	2.37	1.47	1.43
2	D	2	NAG	C2-N2	2.37	1.50	1.46
2	T	2	NAG	C3-C2	2.36	1.57	1.52
2	i	1	NAG	C3-C2	2.36	1.57	1.52
2	b	2	NAG	C3-C2	2.36	1.57	1.52
2	S	2	NAG	C2-N2	2.36	1.50	1.46
2	g	1	NAG	C4-C5	2.36	1.58	1.53
2	h	2	NAG	C2-N2	2.36	1.50	1.46
2	Q	2	NAG	C3-C2	2.35	1.57	1.52
2	q	2	NAG	C3-C2	2.35	1.57	1.52
2	R	1	NAG	C4-C5	2.35	1.58	1.53
2	M	2	NAG	C3-C2	2.34	1.57	1.52
2	k	1	NAG	O5-C1	2.34	1.47	1.43
2	W	1	NAG	C4-C5	2.34	1.58	1.53
2	K	2	NAG	C3-C2	2.33	1.57	1.52
2	X	1	NAG	O5-C1	2.33	1.47	1.43
2	i	2	NAG	C3-C2	2.33	1.57	1.52
2	G	2	NAG	C4-C5	2.33	1.58	1.53
2	d	2	NAG	C4-C5	2.33	1.58	1.53
2	o	2	NAG	C3-C2	2.33	1.57	1.52
2	m	1	NAG	O5-C1	2.33	1.47	1.43
2	a	1	NAG	O5-C1	2.33	1.47	1.43
2	v	1	NAG	O5-C1	2.33	1.47	1.43
2	H	1	NAG	C4-C5	2.33	1.58	1.53
2	G	1	NAG	O5-C1	2.32	1.47	1.43
2	L	1	NAG	O5-C1	2.32	1.47	1.43
2	b	1	NAG	C4-C5	2.32	1.58	1.53
2	M	1	NAG	C4-C5	2.32	1.58	1.53
2	E	2	NAG	C3-C2	2.32	1.57	1.52
2	q	1	NAG	C4-C3	2.32	1.58	1.52
2	l	1	NAG	C4-C5	2.32	1.58	1.53
2	V	1	NAG	O5-C1	2.32	1.47	1.43
2	Q	1	NAG	O5-C1	2.31	1.47	1.43
2	V	2	NAG	C4-C5	2.31	1.58	1.53
2	Z	2	NAG	C3-C2	2.31	1.57	1.52
2	p	1	NAG	O5-C1	2.31	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	1	NAG	C4-C5	2.31	1.58	1.53
2	u	1	NAG	C4-C5	2.31	1.58	1.53
2	u	1	NAG	O5-C1	2.31	1.47	1.43
2	k	2	NAG	C4-C5	2.31	1.57	1.53
2	s	2	NAG	C4-C5	2.31	1.57	1.53
2	Q	1	NAG	C4-C5	2.31	1.57	1.53
2	M	1	NAG	C4-C3	2.31	1.58	1.52
2	R	1	NAG	O5-C1	2.31	1.47	1.43
2	O	2	NAG	C4-C5	2.30	1.57	1.53
2	p	1	NAG	C4-C5	2.30	1.57	1.53
2	W	2	NAG	C4-C5	2.30	1.57	1.53
2	q	1	NAG	C4-C5	2.30	1.57	1.53
2	T	1	NAG	C4-C5	2.30	1.57	1.53
2	g	1	NAG	O5-C1	2.30	1.47	1.43
2	S	2	NAG	C4-C5	2.30	1.57	1.53
2	h	1	NAG	C3-C2	2.30	1.57	1.52
2	b	1	NAG	C4-C3	2.30	1.58	1.52
2	h	2	NAG	C4-C5	2.30	1.57	1.53
2	L	1	NAG	C4-C5	2.29	1.57	1.53
2	T	2	NAG	C4-C5	2.29	1.57	1.53
2	D	2	NAG	C4-C5	2.29	1.57	1.53
2	p	2	NAG	C4-C5	2.29	1.57	1.53
2	a	1	NAG	C4-C5	2.29	1.57	1.53
2	I	1	NAG	O5-C1	2.29	1.47	1.43
2	I	2	NAG	C4-C5	2.29	1.57	1.53
2	L	2	NAG	C4-C5	2.28	1.57	1.53
2	k	1	NAG	C4-C5	2.28	1.57	1.53
2	l	2	NAG	C4-C5	2.28	1.57	1.53
2	i	1	NAG	C4-C5	2.27	1.57	1.53
2	E	1	NAG	C4-C5	2.27	1.57	1.53
2	H	2	NAG	C4-C5	2.27	1.57	1.53
2	R	2	NAG	C4-C5	2.27	1.57	1.53
2	a	2	NAG	C4-C5	2.27	1.57	1.53
2	g	2	NAG	C4-C5	2.27	1.57	1.53
2	D	1	NAG	C3-C2	2.27	1.57	1.52
2	v	2	NAG	C4-C5	2.26	1.57	1.53
2	G	1	NAG	C4-C5	2.26	1.57	1.53
2	X	2	NAG	C4-C5	2.26	1.57	1.53
2	i	2	NAG	C4-C5	2.26	1.57	1.53
2	V	1	NAG	C4-C5	2.26	1.57	1.53
2	m	2	NAG	C4-C5	2.26	1.57	1.53
2	S	1	NAG	C3-C2	2.25	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C4-C5	2.25	1.57	1.53
2	Q	2	NAG	C4-C5	2.25	1.57	1.53
2	G	2	NAG	C2-N2	2.25	1.50	1.46
2	l	1	NAG	C3-C2	2.24	1.57	1.52
2	k	2	NAG	C2-N2	2.24	1.50	1.46
2	F	2	NAG	C4-C5	2.24	1.57	1.53
2	G	1	NAG	C4-C3	2.24	1.58	1.52
2	U	2	NAG	C4-C5	2.24	1.57	1.53
2	V	1	NAG	C4-C3	2.23	1.58	1.52
2	V	2	NAG	C2-N2	2.23	1.49	1.46
2	j	2	NAG	C4-C5	2.22	1.57	1.53
2	c	1	NAG	O5-C1	2.22	1.47	1.43
2	F	1	NAG	O5-C1	2.22	1.47	1.43
2	k	1	NAG	C4-C3	2.22	1.58	1.52
2	r	1	NAG	O5-C1	2.22	1.47	1.43
2	r	2	NAG	C4-C5	2.22	1.57	1.53
2	u	2	NAG	C4-C5	2.22	1.57	1.53
2	j	1	NAG	O5-C1	2.22	1.47	1.43
2	U	1	NAG	O5-C1	2.22	1.47	1.43
2	f	2	NAG	C4-C5	2.22	1.57	1.53
2	F	1	NAG	C2-N2	2.21	1.49	1.46
2	j	1	NAG	C2-N2	2.21	1.49	1.46
2	U	1	NAG	C2-N2	2.21	1.49	1.46
2	N	1	NAG	O5-C1	2.21	1.47	1.43
2	H	1	NAG	C3-C2	2.21	1.57	1.52
2	V	1	NAG	C3-C2	2.20	1.57	1.52
2	W	1	NAG	C3-C2	2.20	1.57	1.52
2	c	2	NAG	C4-C5	2.19	1.57	1.53
2	M	2	NAG	C4-C5	2.19	1.57	1.53
2	G	1	NAG	C3-C2	2.18	1.57	1.52
2	L	1	NAG	C3-C2	2.18	1.57	1.52
2	b	2	NAG	C4-C5	2.17	1.57	1.53
2	I	1	NAG	C4-C3	2.17	1.58	1.52
2	k	1	NAG	C3-C2	2.17	1.57	1.52
2	t	1	NAG	C2-N2	2.17	1.49	1.46
2	N	2	NAG	C4-C5	2.16	1.57	1.53
2	q	2	NAG	C4-C5	2.16	1.57	1.53
2	m	1	NAG	C4-C3	2.15	1.57	1.52
2	p	1	NAG	C3-C2	2.15	1.57	1.52
2	X	1	NAG	C4-C3	2.15	1.57	1.52
2	P	1	NAG	C2-N2	2.15	1.49	1.46
2	c	1	NAG	C4-C5	2.14	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	d	2	NAG	C2-N2	2.14	1.49	1.46
2	p	2	NAG	C2-N2	2.13	1.49	1.46
2	o	2	NAG	C4-C3	2.13	1.57	1.52
2	b	2	NAG	C2-N2	2.13	1.49	1.46
2	U	2	NAG	C2-N2	2.13	1.49	1.46
2	J	2	NAG	C4-C5	2.13	1.57	1.53
2	K	2	NAG	C4-C3	2.13	1.57	1.52
2	t	2	NAG	C4-C5	2.13	1.57	1.53
2	n	2	NAG	C4-C5	2.13	1.57	1.53
2	a	1	NAG	C3-C2	2.12	1.57	1.52
2	q	2	NAG	C2-N2	2.12	1.49	1.46
2	N	1	NAG	C3-C2	2.12	1.57	1.52
2	L	2	NAG	C2-N2	2.12	1.49	1.46
2	f	1	NAG	C3-C2	2.12	1.57	1.52
2	Y	2	NAG	C4-C5	2.12	1.57	1.53
2	S	1	NAG	C4-C3	2.12	1.57	1.52
2	N	1	NAG	C4-C5	2.12	1.57	1.53
2	h	1	NAG	O5-C1	2.11	1.47	1.43
2	D	1	NAG	C4-C3	2.11	1.57	1.52
2	c	1	NAG	C3-C2	2.11	1.56	1.52
2	a	2	NAG	C2-N2	2.11	1.49	1.46
2	r	1	NAG	C4-C5	2.11	1.57	1.53
2	F	2	NAG	C2-N2	2.11	1.49	1.46
2	Z	2	NAG	C4-C3	2.11	1.57	1.52
2	e	2	NAG	C4-C5	2.10	1.57	1.53
2	e	1	NAG	C2-N2	2.10	1.49	1.46
2	K	2	NAG	C2-N2	2.10	1.49	1.46
2	P	2	NAG	C4-C5	2.10	1.57	1.53
2	H	1	NAG	O5-C1	2.10	1.47	1.43
2	W	1	NAG	C4-C3	2.10	1.57	1.52
2	M	2	NAG	C2-N2	2.10	1.49	1.46
2	s	2	NAG	C2-N2	2.10	1.49	1.46
2	j	2	NAG	C2-N2	2.10	1.49	1.46
2	r	2	NAG	C2-N2	2.10	1.49	1.46
2	E	2	NAG	C2-N2	2.09	1.49	1.46
2	r	1	NAG	C3-C2	2.09	1.56	1.52
2	Q	1	NAG	C3-C2	2.09	1.56	1.52
2	l	1	NAG	C4-C3	2.09	1.57	1.52
2	D	1	NAG	O5-C1	2.09	1.47	1.43
2	h	1	NAG	C4-C3	2.09	1.57	1.52
2	W	1	NAG	O5-C1	2.09	1.47	1.43
2	o	2	NAG	C2-N2	2.09	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	1	NAG	O5-C1	2.09	1.47	1.43
2	I	1	NAG	C3-C2	2.09	1.56	1.52
2	u	1	NAG	C3-C2	2.08	1.56	1.52
2	i	2	NAG	C2-N2	2.08	1.49	1.46
2	O	2	NAG	C2-N2	2.08	1.49	1.46
2	P	1	NAG	O5-C1	2.08	1.47	1.43
2	e	1	NAG	O5-C1	2.08	1.47	1.43
2	X	1	NAG	C3-C2	2.08	1.56	1.52
2	Z	2	NAG	C2-N2	2.08	1.49	1.46
2	T	1	NAG	O5-C1	2.07	1.47	1.43
2	v	1	NAG	C4-C3	2.07	1.57	1.52
2	E	1	NAG	O5-C1	2.07	1.47	1.43
2	t	1	NAG	O5-C1	2.07	1.47	1.43
2	i	1	NAG	O5-C1	2.07	1.47	1.43
2	q	1	NAG	C2-N2	2.07	1.49	1.46
2	H	1	NAG	C4-C3	2.07	1.57	1.52
2	g	1	NAG	C4-C3	2.07	1.57	1.52
2	k	2	NAG	O5-C1	2.07	1.47	1.43
2	R	1	NAG	C4-C3	2.07	1.57	1.52
2	M	1	NAG	C2-N2	2.07	1.49	1.46
2	I	2	NAG	C4-C3	2.06	1.57	1.52
2	N	2	NAG	C2-N2	2.06	1.49	1.46
2	F	1	NAG	C4-C3	2.06	1.57	1.52
2	U	1	NAG	C4-C3	2.06	1.57	1.52
2	c	2	NAG	C2-N2	2.06	1.49	1.46
2	G	2	NAG	O5-C1	2.06	1.47	1.43
2	j	1	NAG	C4-C3	2.06	1.57	1.52
2	r	2	NAG	C4-C3	2.06	1.57	1.52
2	m	1	NAG	C3-C2	2.06	1.56	1.52
2	T	2	NAG	C2-N2	2.05	1.49	1.46
2	S	1	NAG	O5-C1	2.05	1.47	1.43
2	l	2	NAG	C4-C3	2.05	1.57	1.52
2	N	2	NAG	C4-C3	2.05	1.57	1.52
2	b	1	NAG	C2-N2	2.05	1.49	1.46
2	V	2	NAG	O5-C1	2.05	1.47	1.43
2	O	2	NAG	C4-C3	2.05	1.57	1.52
2	Z	1	NAG	C4-C5	2.05	1.57	1.53
2	c	2	NAG	C4-C3	2.05	1.57	1.52
2	W	2	NAG	C4-C3	2.05	1.57	1.52
2	s	2	NAG	C4-C3	2.05	1.57	1.52
2	H	2	NAG	C4-C3	2.04	1.57	1.52
2	s	1	NAG	C3-C2	2.04	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	2	NAG	C4-C3	2.04	1.57	1.52
2	f	2	NAG	C2-N2	2.04	1.49	1.46
2	i	1	NAG	C4-C3	2.03	1.57	1.52
2	u	2	NAG	C2-N2	2.03	1.49	1.46
2	d	2	NAG	O5-C1	2.03	1.47	1.43
2	m	2	NAG	C4-C3	2.03	1.57	1.52
2	d	1	NAG	C3-C2	2.03	1.56	1.52
2	p	2	NAG	C4-C3	2.03	1.57	1.52
2	Q	2	NAG	C2-N2	2.03	1.49	1.46
2	R	2	NAG	C2-N2	2.03	1.49	1.46
2	n	2	NAG	O5-C1	2.02	1.47	1.43
2	s	2	NAG	O5-C1	2.02	1.47	1.43
2	L	2	NAG	C4-C3	2.02	1.57	1.52
2	a	2	NAG	C4-C3	2.02	1.57	1.52
2	K	1	NAG	C4-C5	2.02	1.57	1.53
2	O	1	NAG	C3-C2	2.02	1.56	1.52
2	j	2	NAG	C4-C3	2.02	1.57	1.52
2	v	2	NAG	C2-N2	2.02	1.49	1.46
2	G	2	NAG	C4-C3	2.02	1.57	1.52
2	U	2	NAG	C4-C3	2.02	1.57	1.52
2	d	2	NAG	C4-C3	2.02	1.57	1.52
2	k	2	NAG	C4-C3	2.01	1.57	1.52
2	r	1	NAG	C4-C3	2.01	1.57	1.52
2	g	2	NAG	C2-N2	2.01	1.49	1.46
2	o	1	NAG	C4-C5	2.01	1.57	1.53
2	c	1	NAG	C4-C3	2.01	1.57	1.52
2	E	1	NAG	C4-C3	2.01	1.57	1.52
2	P	2	NAG	C4-C3	2.01	1.57	1.52
2	V	2	NAG	C4-C3	2.01	1.57	1.52
2	X	2	NAG	C2-N2	2.00	1.49	1.46
2	F	2	NAG	C4-C3	2.00	1.57	1.52
2	N	1	NAG	C4-C3	2.00	1.57	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C8-C7-N2	6.94	127.63	116.12
2	h	2	NAG	C8-C7-N2	6.93	127.62	116.12
2	S	2	NAG	C8-C7-N2	6.92	127.60	116.12
2	D	2	NAG	O7-C7-N2	-4.20	114.56	121.98
2	S	2	NAG	O7-C7-N2	-4.18	114.59	121.98
2	h	2	NAG	O7-C7-N2	-4.18	114.59	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	NAG	C8-C7-N2	2.92	120.96	116.12
2	t	1	NAG	C8-C7-N2	2.91	120.94	116.12
2	q	2	NAG	C8-C7-N2	2.90	120.93	116.12
2	P	1	NAG	O4-C4-C5	-2.90	102.19	109.32
2	b	2	NAG	C8-C7-N2	2.89	120.92	116.12
2	e	1	NAG	O4-C4-C5	-2.89	102.21	109.32
2	e	1	NAG	C8-C7-N2	2.89	120.91	116.12
2	t	1	NAG	O4-C4-C5	-2.88	102.22	109.32
2	P	1	NAG	C8-C7-N2	2.88	120.89	116.12
2	n	1	NAG	C8-C7-N2	2.62	120.47	116.12
2	J	1	NAG	C8-C7-N2	2.61	120.45	116.12
2	c	1	NAG	C8-C7-N2	2.61	120.45	116.12
2	r	1	NAG	C8-C7-N2	2.61	120.44	116.12
2	N	1	NAG	C8-C7-N2	2.60	120.43	116.12
2	Y	1	NAG	C8-C7-N2	2.60	120.43	116.12
2	K	1	NAG	O4-C4-C3	-2.60	104.25	110.38
2	o	1	NAG	O4-C4-C3	-2.59	104.26	110.38
2	Z	1	NAG	O4-C4-C3	-2.59	104.27	110.38
2	V	1	NAG	C8-C7-N2	2.57	120.37	116.12
2	G	1	NAG	C8-C7-N2	2.56	120.37	116.12
2	k	1	NAG	C8-C7-N2	2.56	120.36	116.12
2	E	1	NAG	C8-C7-N2	2.56	120.36	116.12
2	M	2	NAG	O7-C7-C8	-2.55	117.51	122.05
2	T	1	NAG	C8-C7-N2	2.55	120.35	116.12
2	b	2	NAG	O7-C7-C8	-2.54	117.53	122.05
2	i	1	NAG	C8-C7-N2	2.53	120.31	116.12
2	q	2	NAG	O7-C7-C8	-2.52	117.56	122.05
2	W	2	NAG	C8-C7-N2	2.49	120.25	116.12
2	l	2	NAG	C8-C7-N2	2.48	120.23	116.12
2	H	2	NAG	C8-C7-N2	2.48	120.22	116.12
2	g	1	NAG	C8-C7-N2	2.47	120.22	116.12
2	R	1	NAG	C8-C7-N2	2.46	120.19	116.12
2	v	1	NAG	C8-C7-N2	2.45	120.18	116.12
2	h	2	NAG	O7-C7-C8	-2.40	117.79	122.05
2	D	2	NAG	O7-C7-C8	-2.39	117.81	122.05
2	S	2	NAG	O7-C7-C8	-2.38	117.81	122.05
2	e	1	NAG	O7-C7-C8	-2.37	117.83	122.05
2	I	1	NAG	C8-C7-N2	2.36	120.03	116.12
2	t	1	NAG	O7-C7-C8	-2.36	117.86	122.05
2	P	1	NAG	O7-C7-C8	-2.35	117.87	122.05
2	m	1	NAG	C8-C7-N2	2.35	120.01	116.12
2	X	1	NAG	C8-C7-N2	2.34	120.01	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	t	1	NAG	O4-C4-C3	2.33	115.88	110.38
2	P	1	NAG	O4-C4-C3	2.32	115.85	110.38
2	e	1	NAG	O4-C4-C3	2.31	115.83	110.38
2	J	1	NAG	O7-C7-C8	-2.30	117.95	122.05
2	n	1	NAG	O7-C7-C8	-2.30	117.96	122.05
2	K	2	NAG	C8-C7-N2	2.30	119.93	116.12
2	Z	2	NAG	C8-C7-N2	2.30	119.93	116.12
2	Y	1	NAG	O7-C7-C8	-2.29	117.97	122.05
2	o	2	NAG	C8-C7-N2	2.28	119.91	116.12
2	q	1	NAG	C1-C2-N2	-2.25	106.89	110.43
2	M	1	NAG	C1-C2-N2	-2.25	106.89	110.43
2	b	1	NAG	C1-C2-N2	-2.25	106.89	110.43
2	H	1	NAG	C8-C7-N2	2.25	119.85	116.12
2	l	1	NAG	C8-C7-N2	2.25	119.85	116.12
2	W	1	NAG	C8-C7-N2	2.24	119.84	116.12
2	k	2	NAG	C8-C7-N2	2.23	119.82	116.12
2	g	2	NAG	C8-C7-N2	2.23	119.81	116.12
2	E	2	NAG	C8-C7-N2	2.22	119.79	116.12
2	G	2	NAG	C8-C7-N2	2.21	119.78	116.12
2	R	2	NAG	C8-C7-N2	2.21	119.78	116.12
2	V	2	NAG	C8-C7-N2	2.21	119.78	116.12
2	T	2	NAG	C8-C7-N2	2.20	119.77	116.12
2	v	2	NAG	C8-C7-N2	2.20	119.77	116.12
2	b	1	NAG	C8-C7-N2	2.19	119.74	116.12
2	j	1	NAG	C8-C7-N2	2.18	119.73	116.12
2	i	2	NAG	C8-C7-N2	2.17	119.72	116.12
2	q	1	NAG	C8-C7-N2	2.17	119.72	116.12
2	M	1	NAG	C8-C7-N2	2.17	119.72	116.12
2	U	1	NAG	C8-C7-N2	2.17	119.72	116.12
2	g	1	NAG	O7-C7-C8	-2.15	118.22	122.05
2	R	1	NAG	O7-C7-C8	-2.15	118.23	122.05
2	V	1	NAG	O7-C7-C8	-2.15	118.23	122.05
2	Q	2	NAG	C8-C7-N2	2.15	119.68	116.12
2	s	2	NAG	C8-C7-N2	2.14	119.67	116.12
2	c	2	NAG	C8-C7-N2	2.14	119.67	116.12
2	Y	2	NAG	C8-C7-N2	2.14	119.67	116.12
2	k	1	NAG	O7-C7-C8	-2.14	118.25	122.05
2	v	1	NAG	O7-C7-C8	-2.14	118.25	122.05
2	N	2	NAG	C8-C7-N2	2.14	119.66	116.12
2	L	2	NAG	C8-C7-N2	2.13	119.66	116.12
2	a	2	NAG	C8-C7-N2	2.13	119.66	116.12
2	F	1	NAG	C8-C7-N2	2.13	119.65	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	NAG	C8-C7-N2	2.13	119.65	116.12
2	r	2	NAG	C8-C7-N2	2.13	119.65	116.12
2	p	2	NAG	C8-C7-N2	2.13	119.65	116.12
2	d	2	NAG	C8-C7-N2	2.12	119.64	116.12
2	n	2	NAG	C8-C7-N2	2.12	119.63	116.12
2	f	2	NAG	C8-C7-N2	2.12	119.63	116.12
2	G	1	NAG	O7-C7-C8	-2.12	118.29	122.05
2	O	2	NAG	C8-C7-N2	2.11	119.62	116.12
2	u	2	NAG	C8-C7-N2	2.11	119.61	116.12
2	X	2	NAG	C8-C7-N2	2.09	119.59	116.12
2	I	2	NAG	C8-C7-N2	2.07	119.54	116.12
2	d	1	NAG	C8-C7-N2	2.07	119.54	116.12
2	m	2	NAG	C8-C7-N2	2.06	119.54	116.12
2	j	2	NAG	C8-C7-N2	2.06	119.53	116.12
2	g	1	NAG	O5-C1-C2	-2.06	108.11	111.29
2	E	1	NAG	O7-C7-C8	-2.05	118.39	122.05
2	U	2	NAG	C8-C7-N2	2.05	119.52	116.12
2	R	1	NAG	O5-C1-C2	-2.05	108.12	111.29
2	O	1	NAG	C8-C7-N2	2.05	119.52	116.12
2	s	1	NAG	C8-C7-N2	2.05	119.52	116.12
2	S	2	NAG	C2-N2-C7	2.05	125.65	122.90
2	i	1	NAG	O7-C7-C8	-2.05	118.40	122.05
2	v	1	NAG	O5-C1-C2	-2.05	108.12	111.29
2	P	2	NAG	C1-O5-C5	2.05	114.93	112.19
2	F	2	NAG	C8-C7-N2	2.05	119.51	116.12
2	h	2	NAG	C2-N2-C7	2.05	125.64	122.90
2	T	1	NAG	O7-C7-C8	-2.04	118.42	122.05
2	P	2	NAG	C8-C7-N2	2.04	119.50	116.12
2	t	2	NAG	C8-C7-N2	2.04	119.50	116.12
2	e	2	NAG	C1-O5-C5	2.03	114.91	112.19
2	D	2	NAG	C2-N2-C7	2.03	125.62	122.90
2	e	2	NAG	C8-C7-N2	2.03	119.48	116.12
2	D	1	NAG	C8-C7-N2	2.01	119.46	116.12
2	S	1	NAG	C8-C7-N2	2.01	119.45	116.12
2	h	1	NAG	C8-C7-N2	2.01	119.45	116.12
2	Z	2	NAG	O7-C7-C8	-2.01	118.48	122.05
2	t	2	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

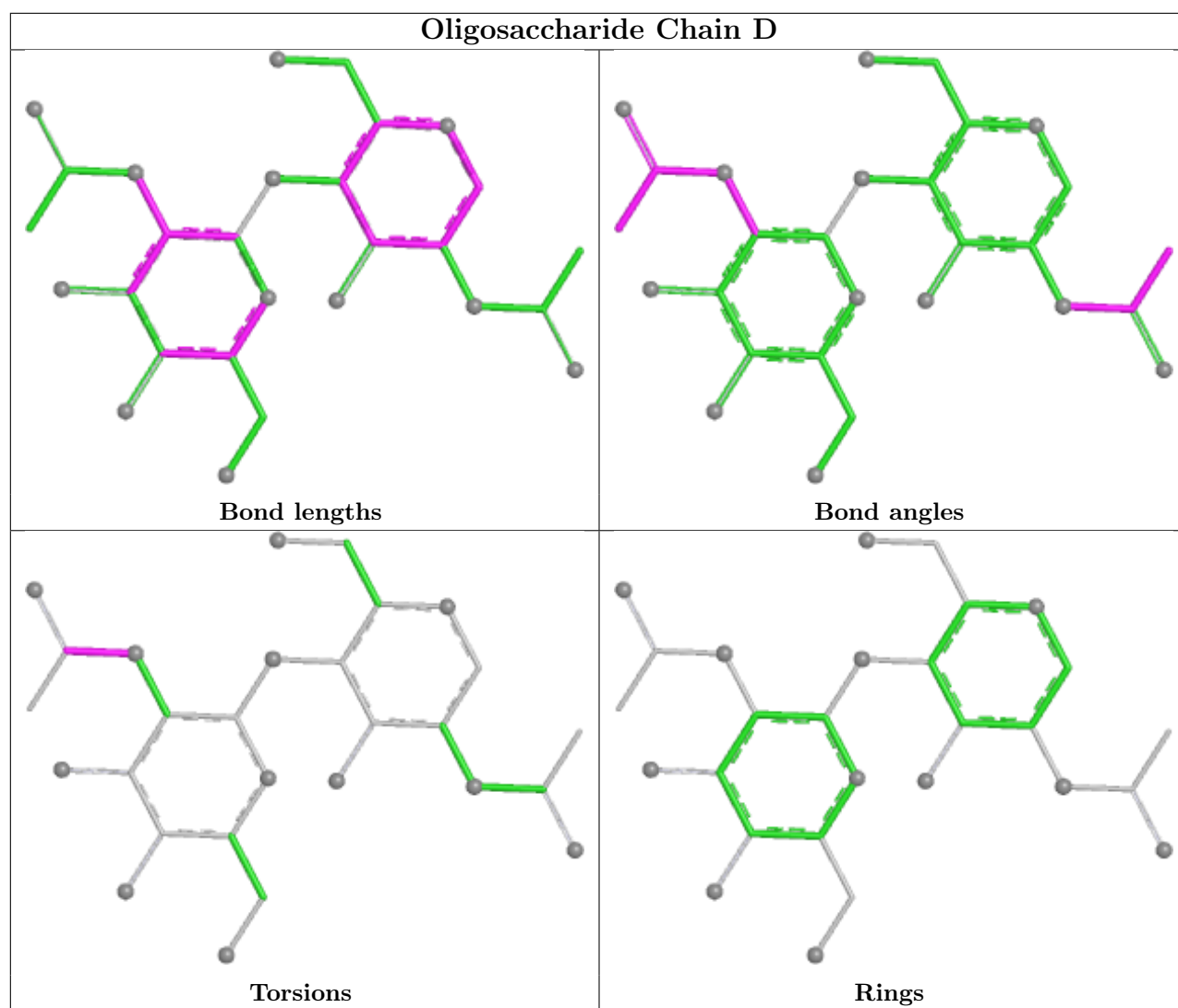
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	S	2	NAG	C8-C7-N2-C2
2	S	2	NAG	O7-C7-N2-C2
2	h	2	NAG	C8-C7-N2-C2
2	h	2	NAG	O7-C7-N2-C2
2	t	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6

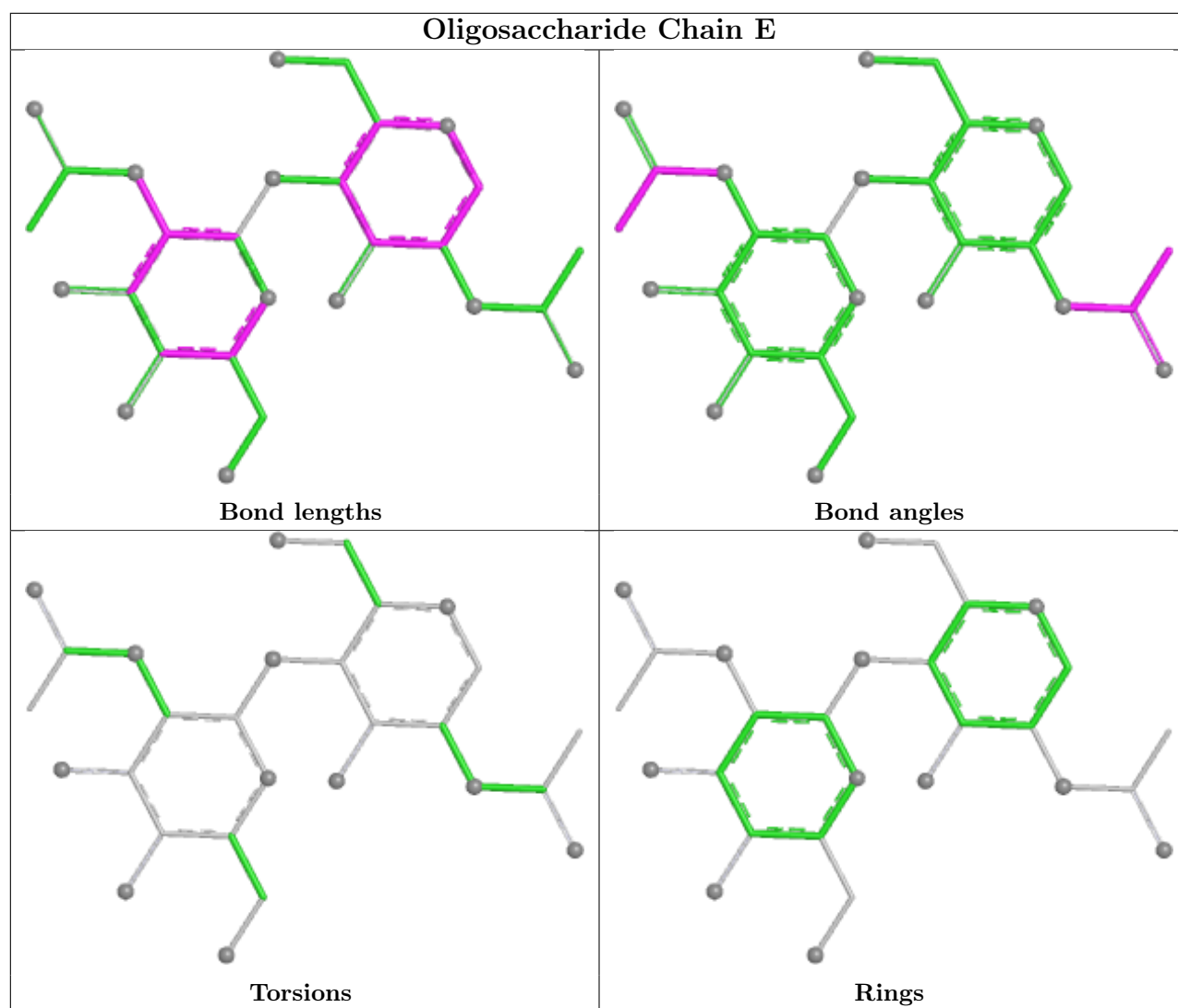
There are no ring outliers.

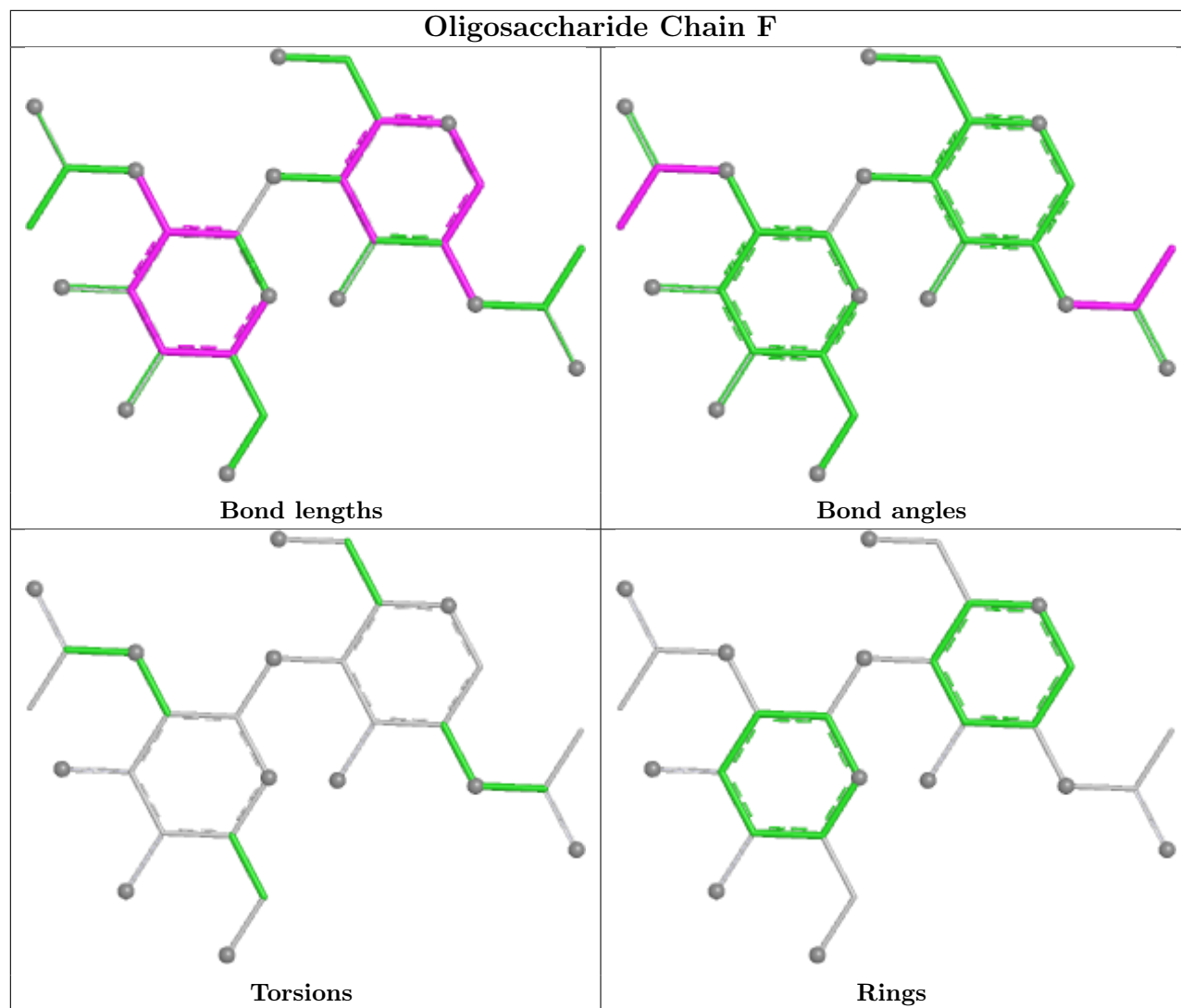
3 monomers are involved in 3 short contacts:

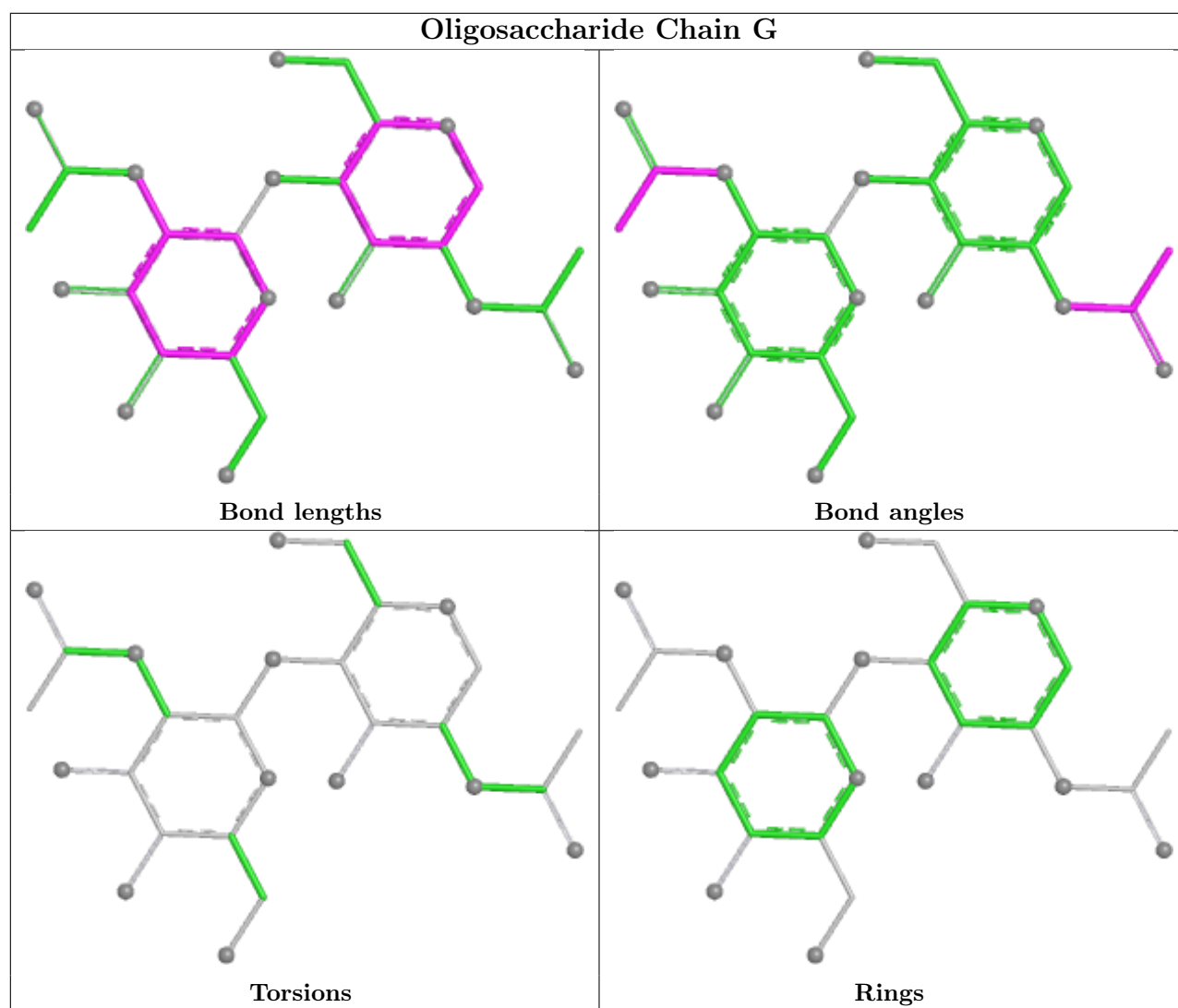
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	b	2	NAG	1	0
2	M	2	NAG	1	0
2	q	2	NAG	1	0

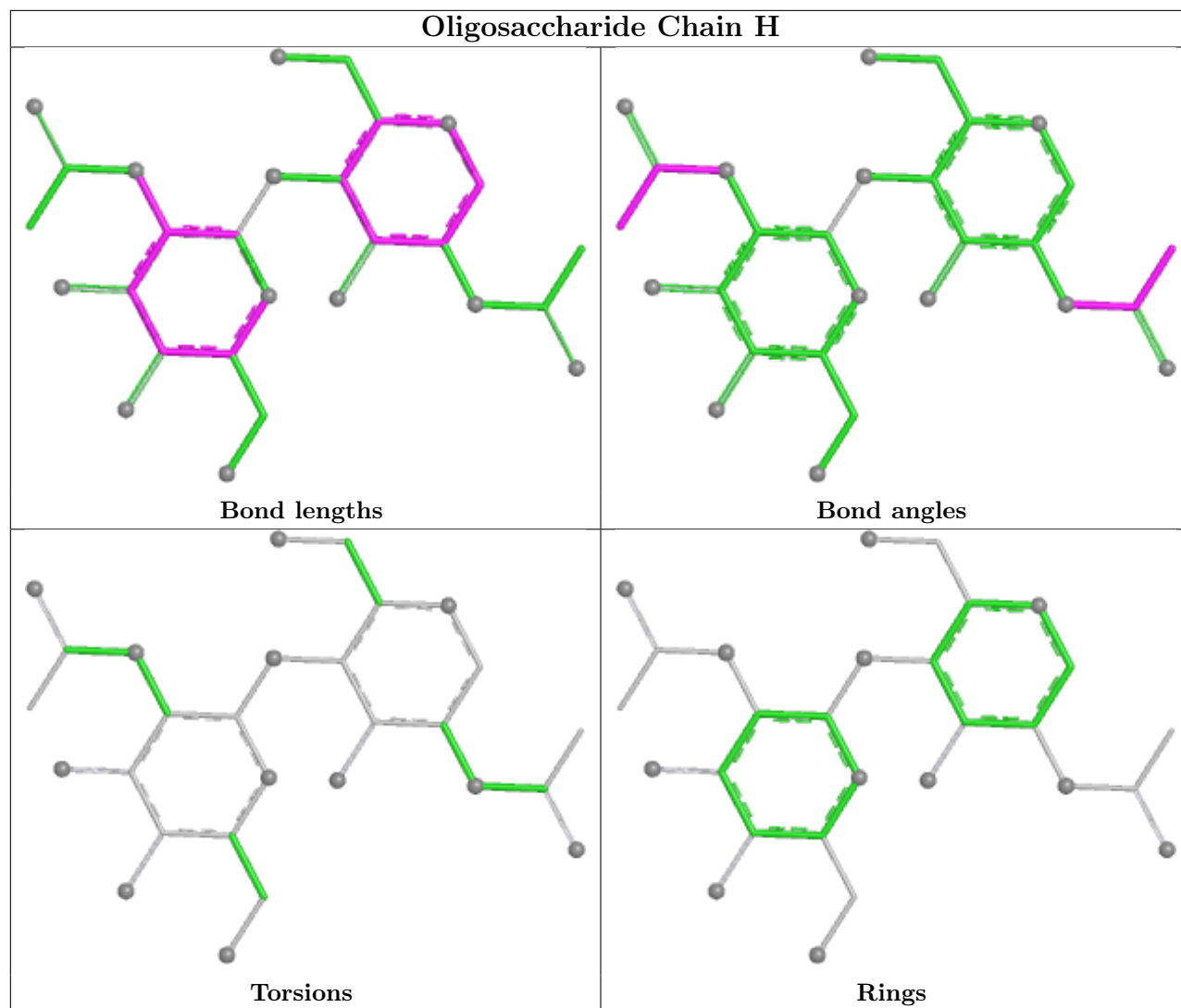
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

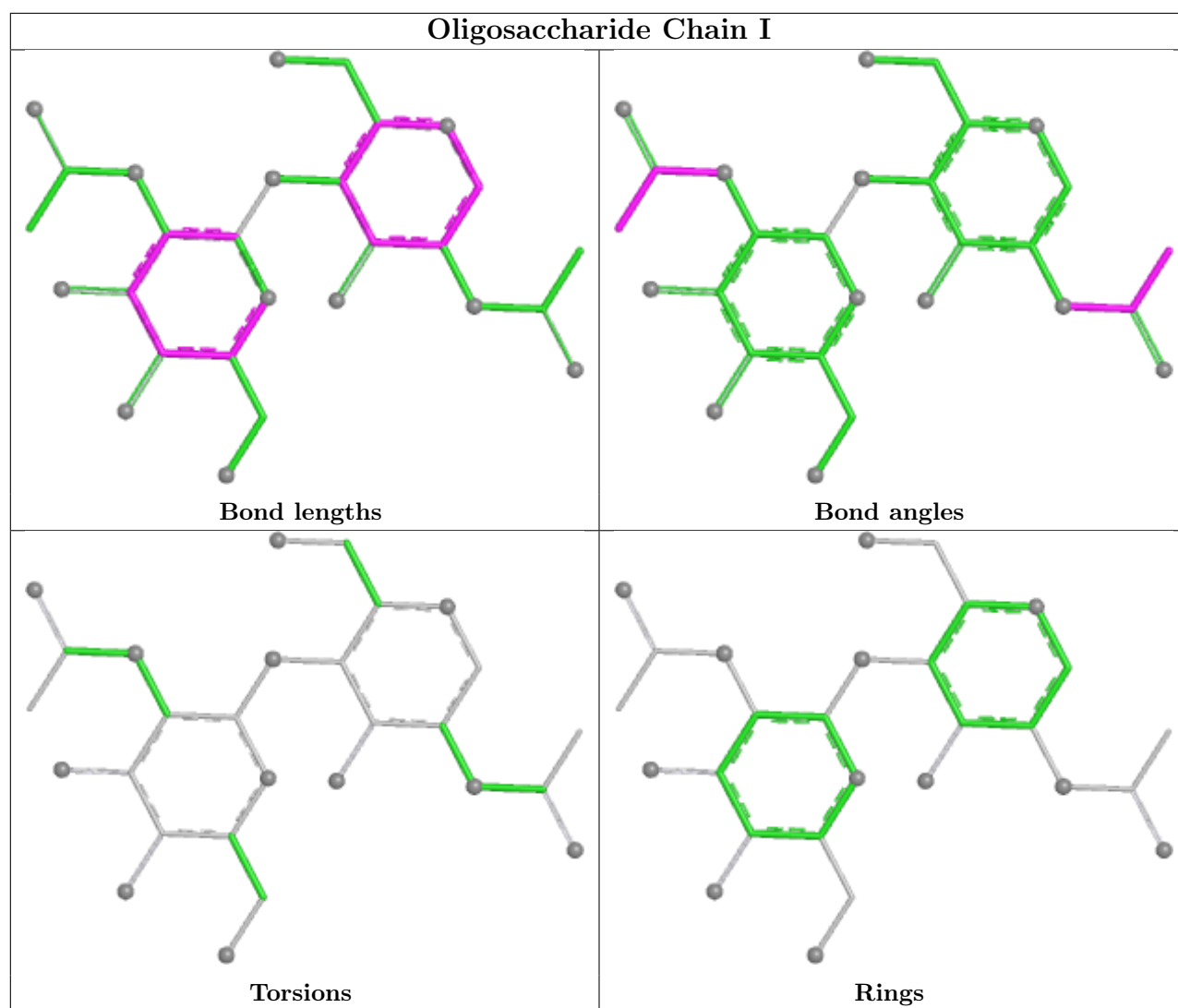


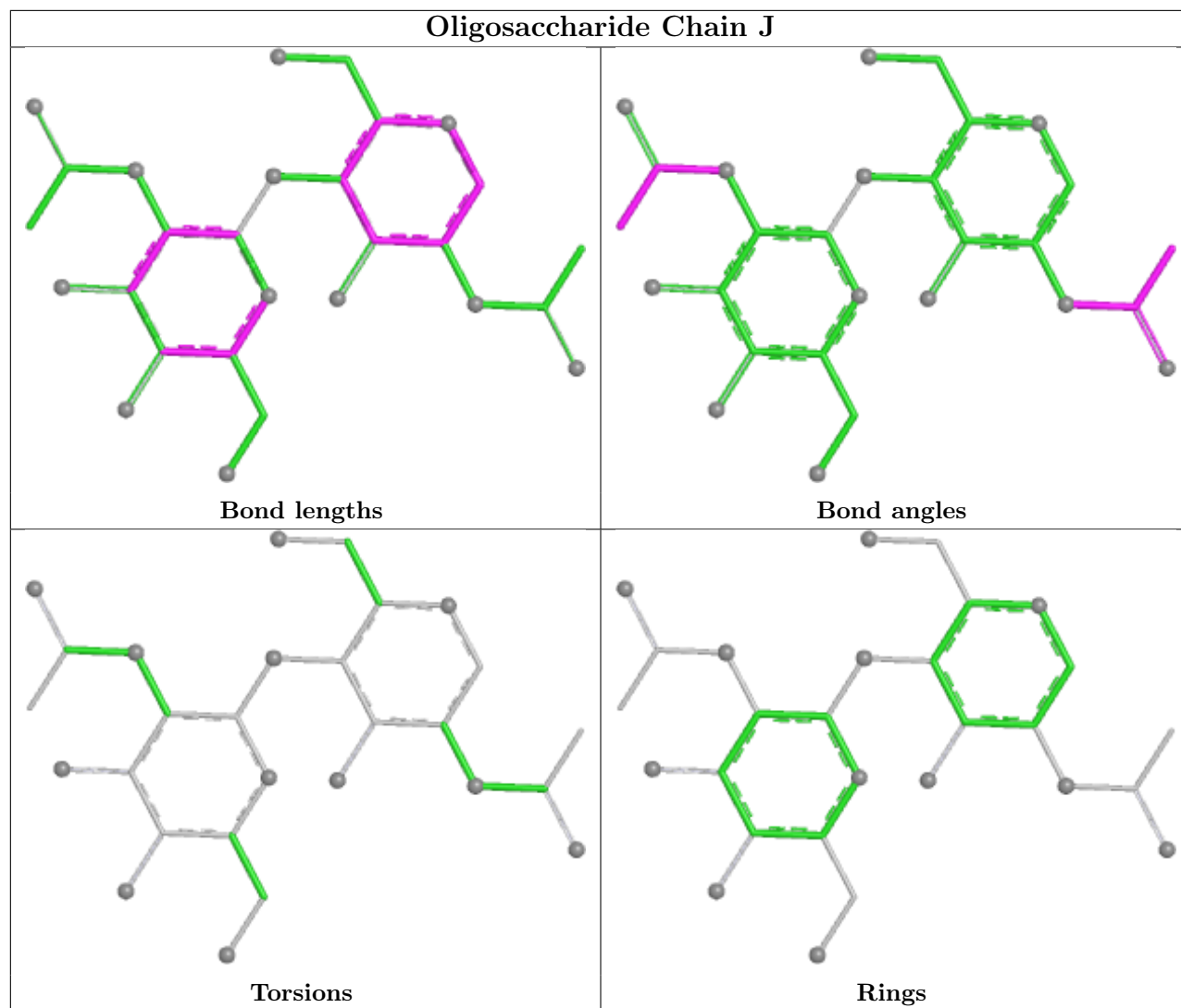


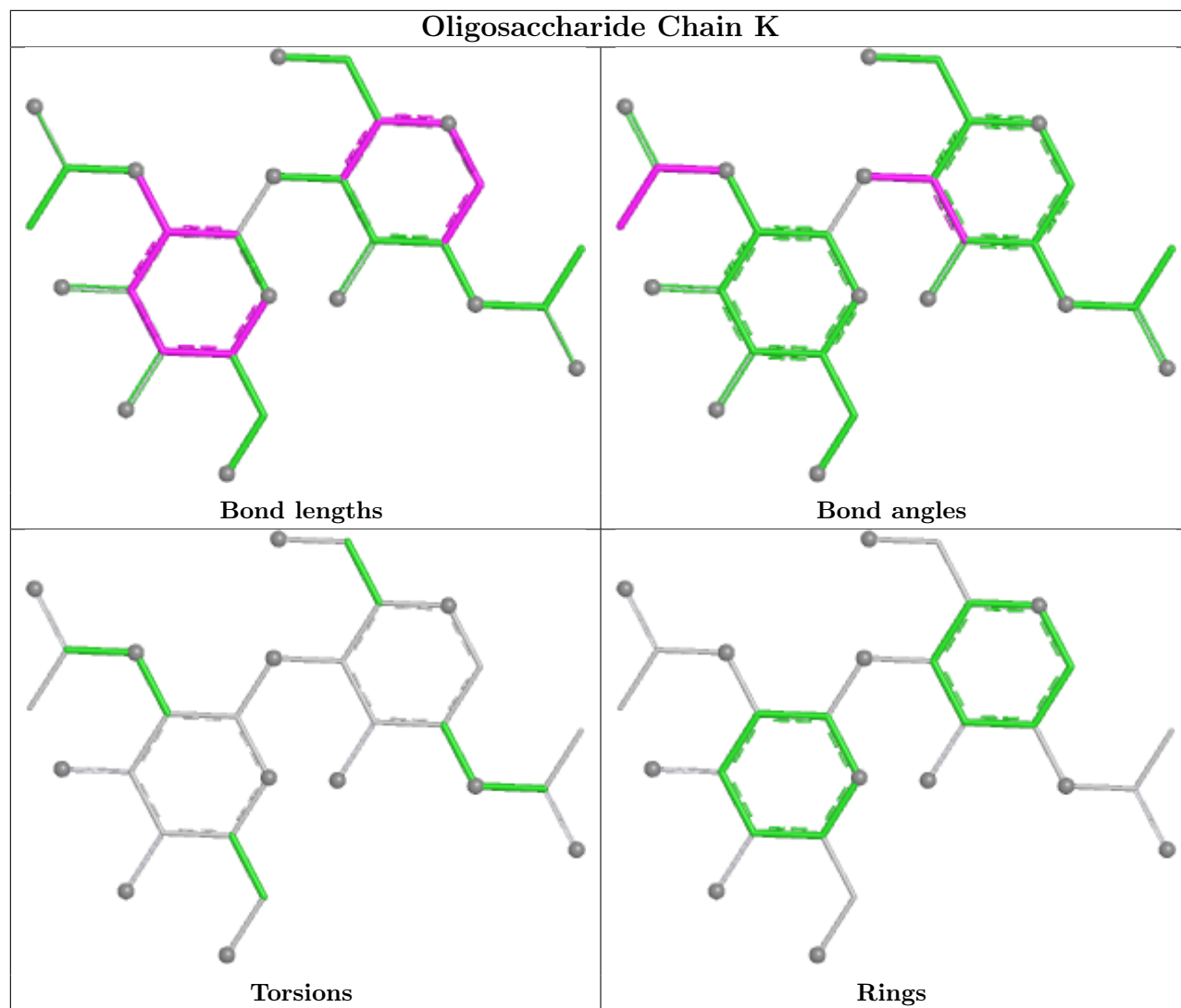


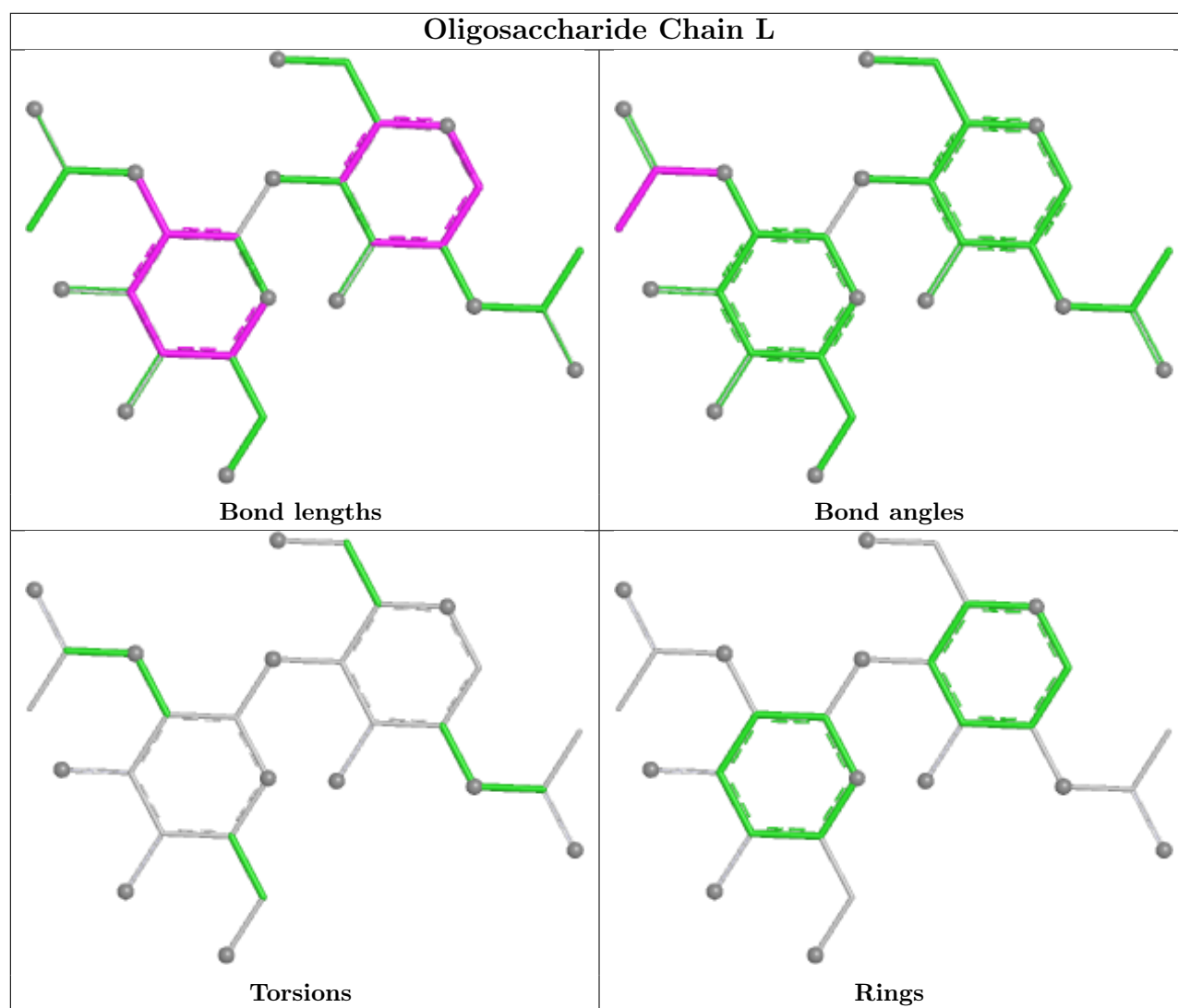


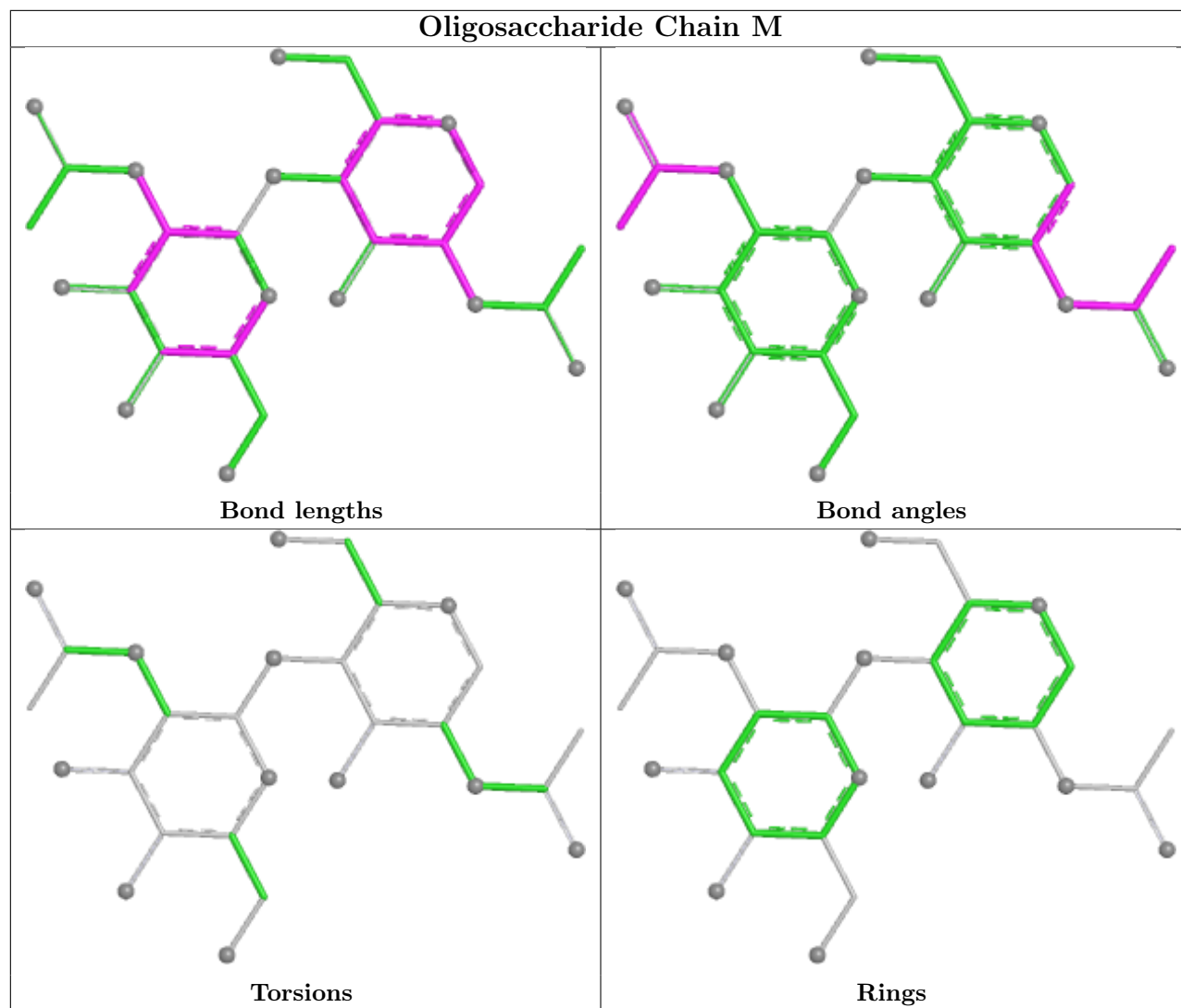


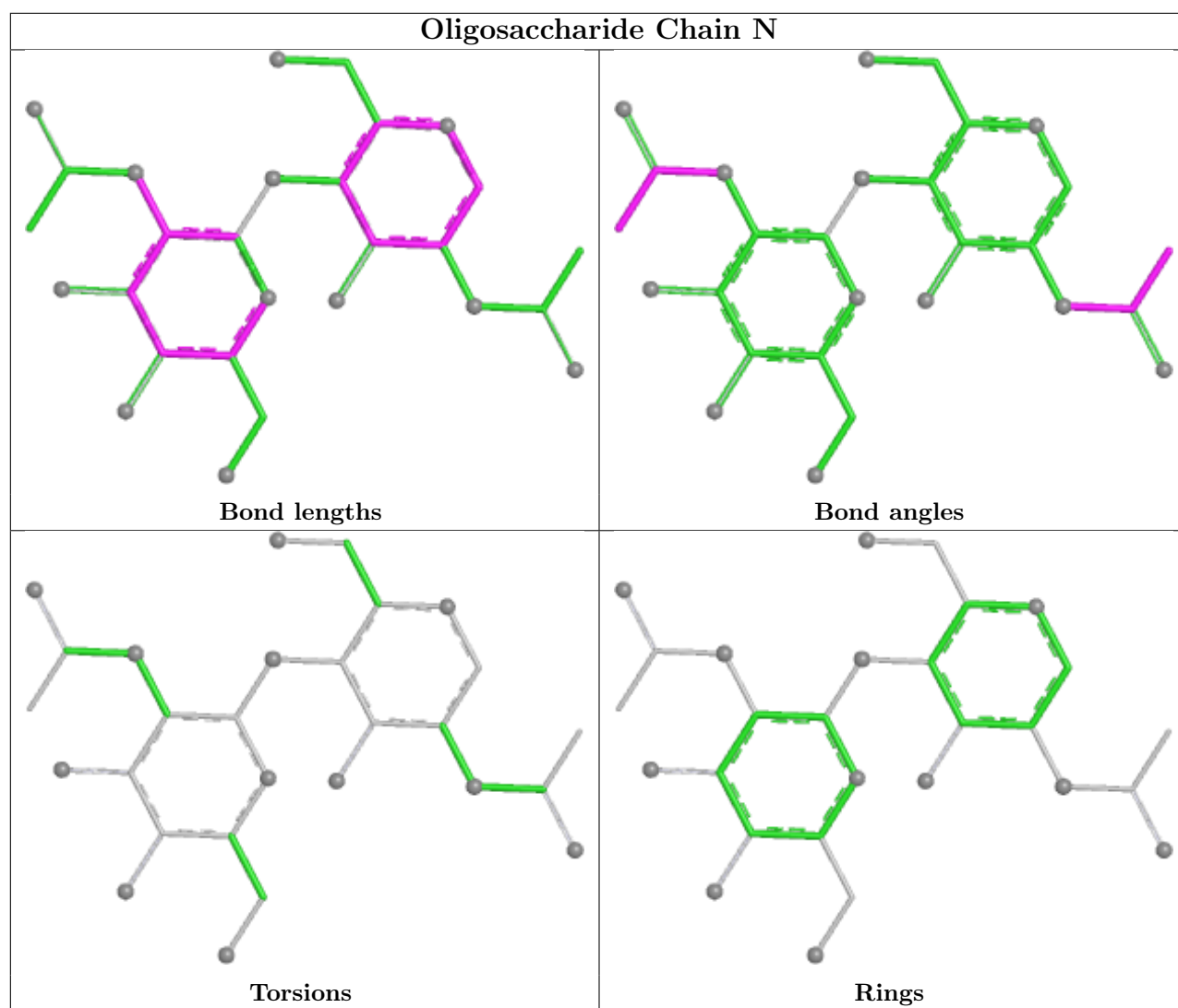


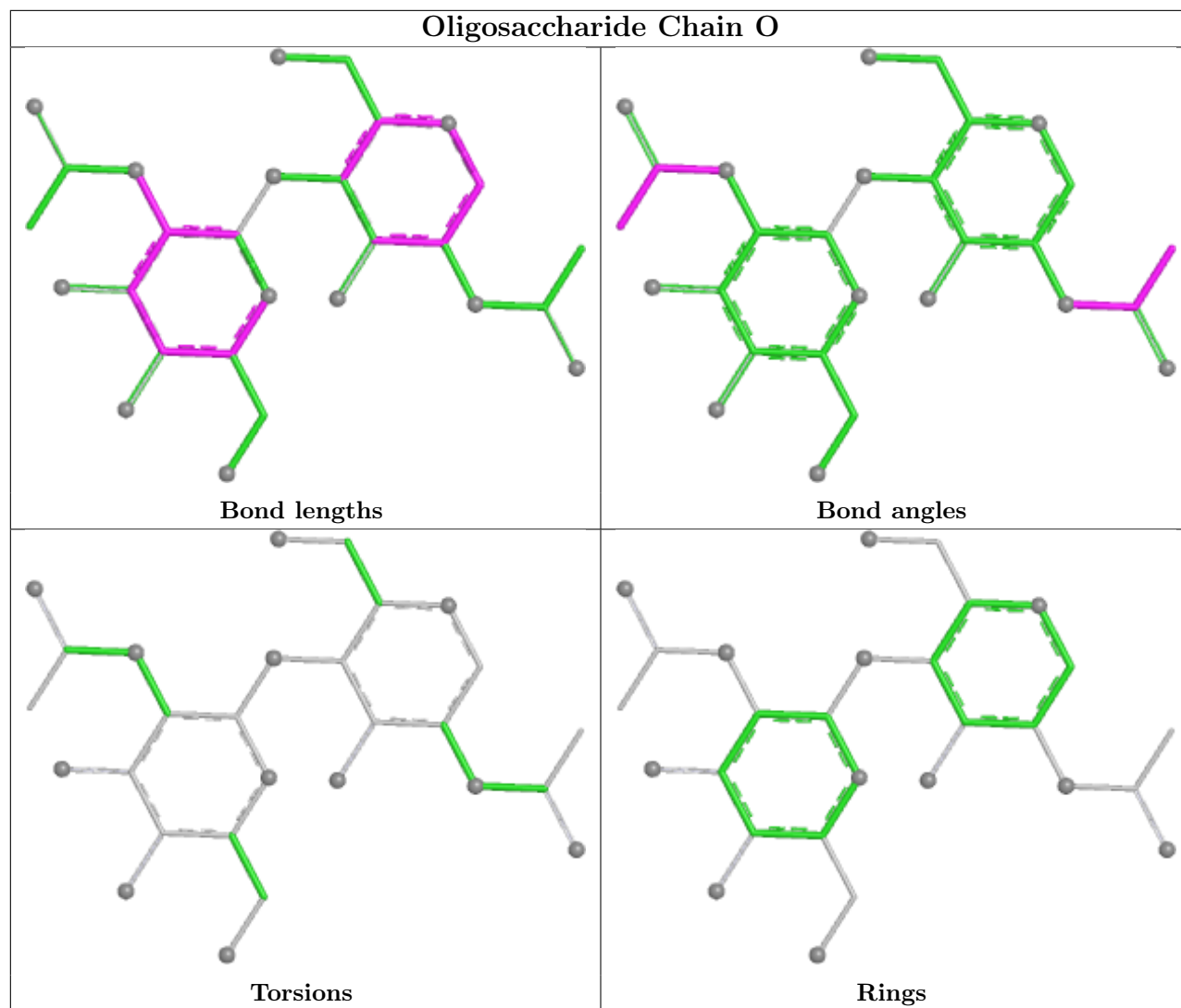


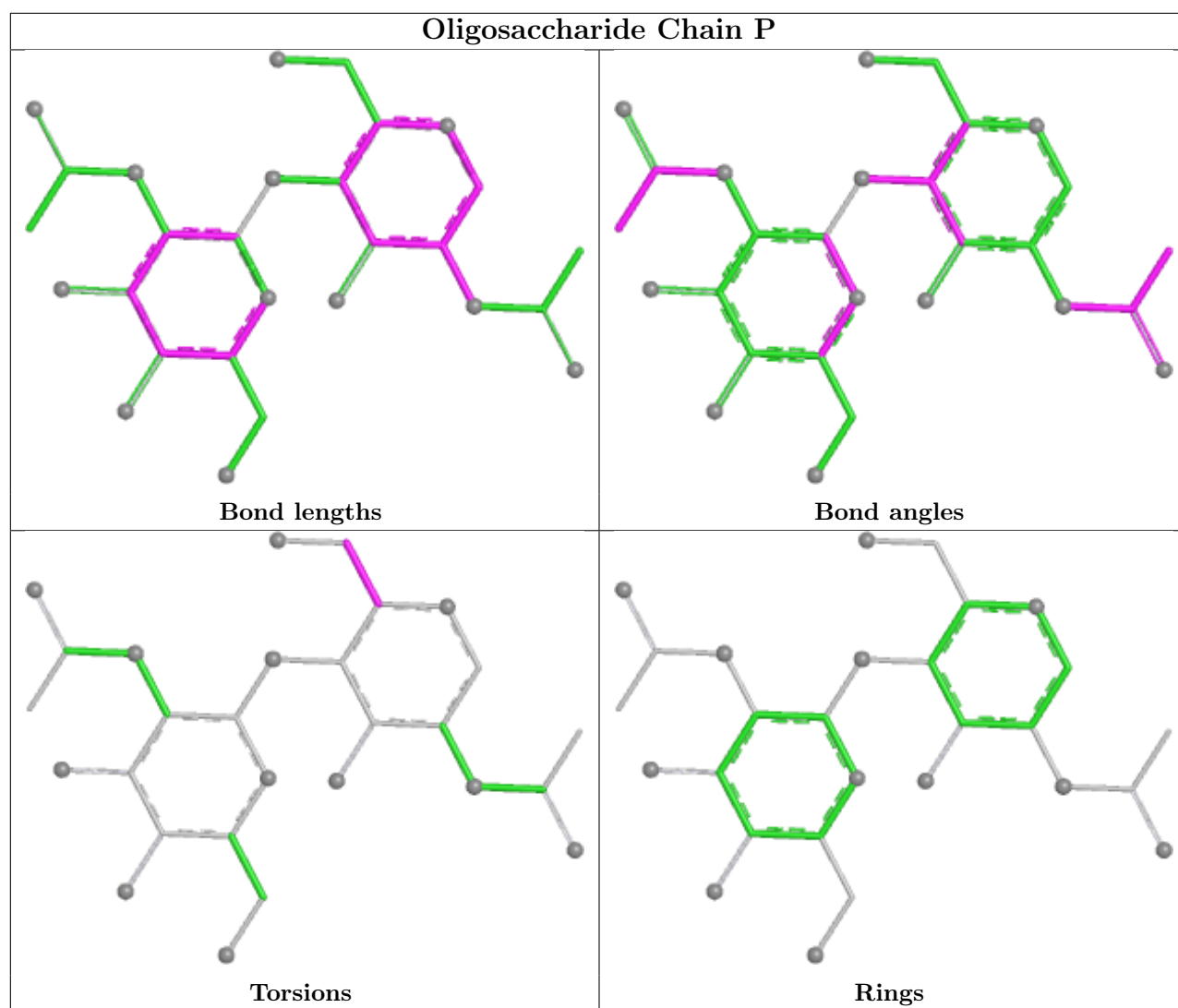


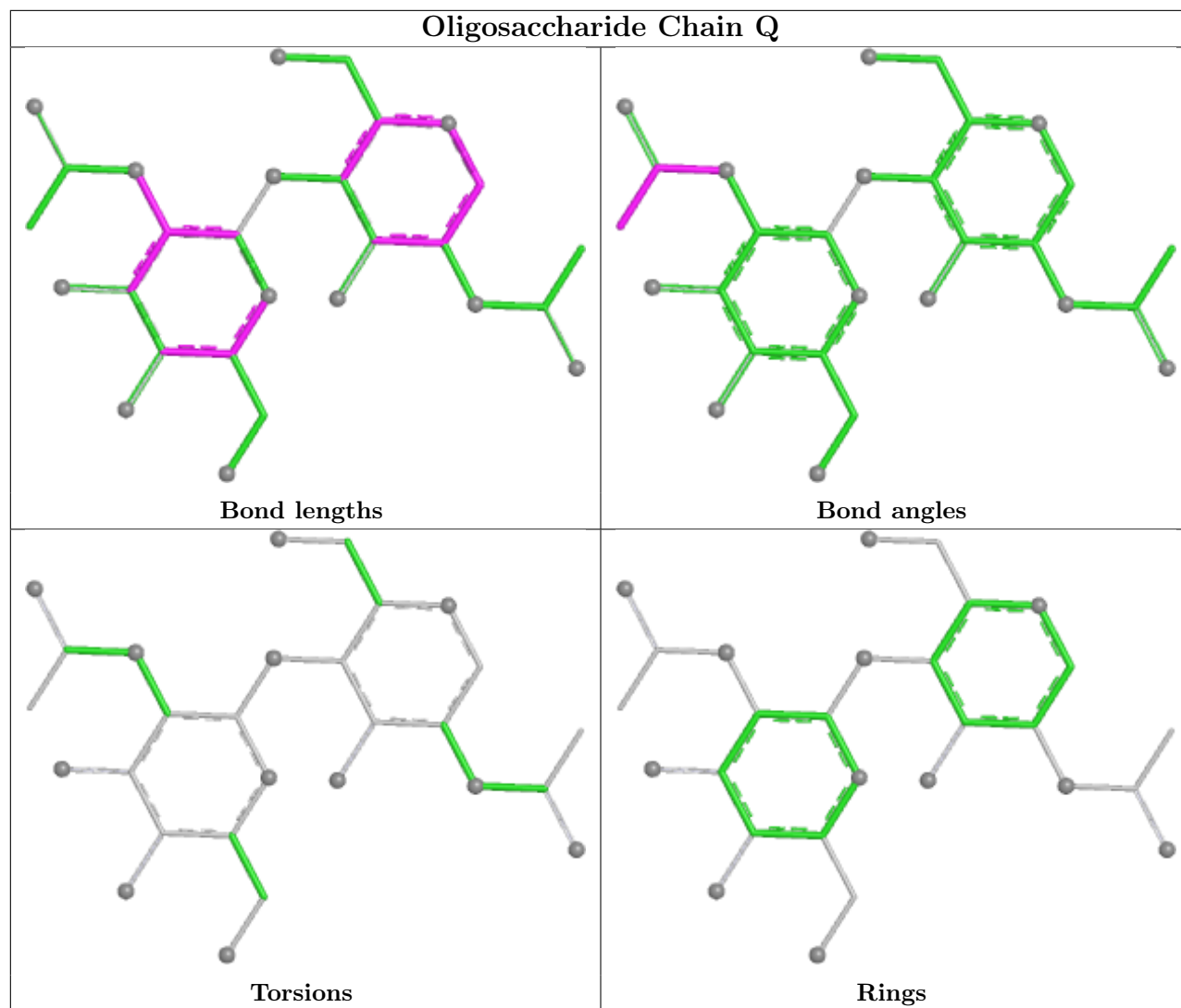


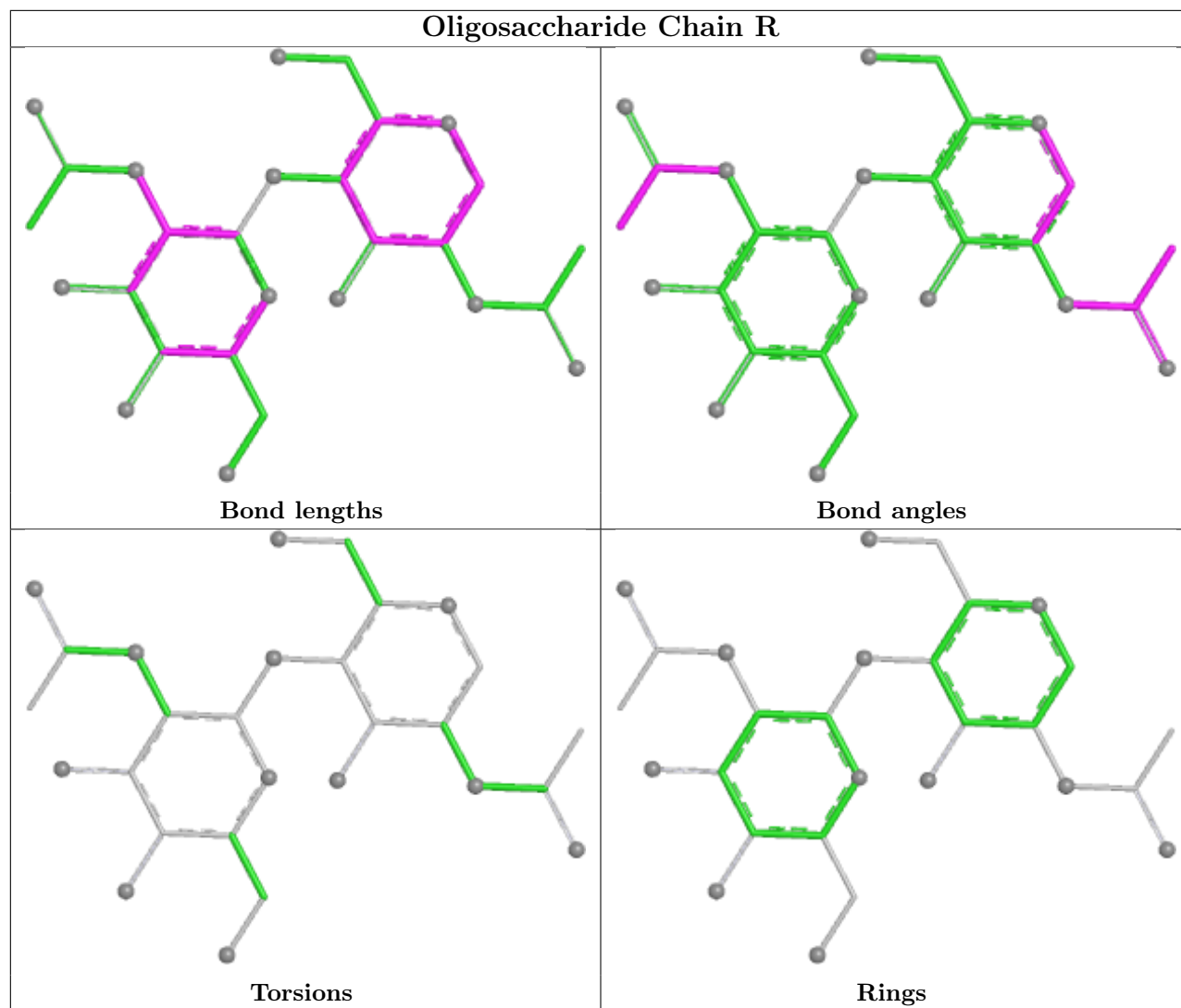


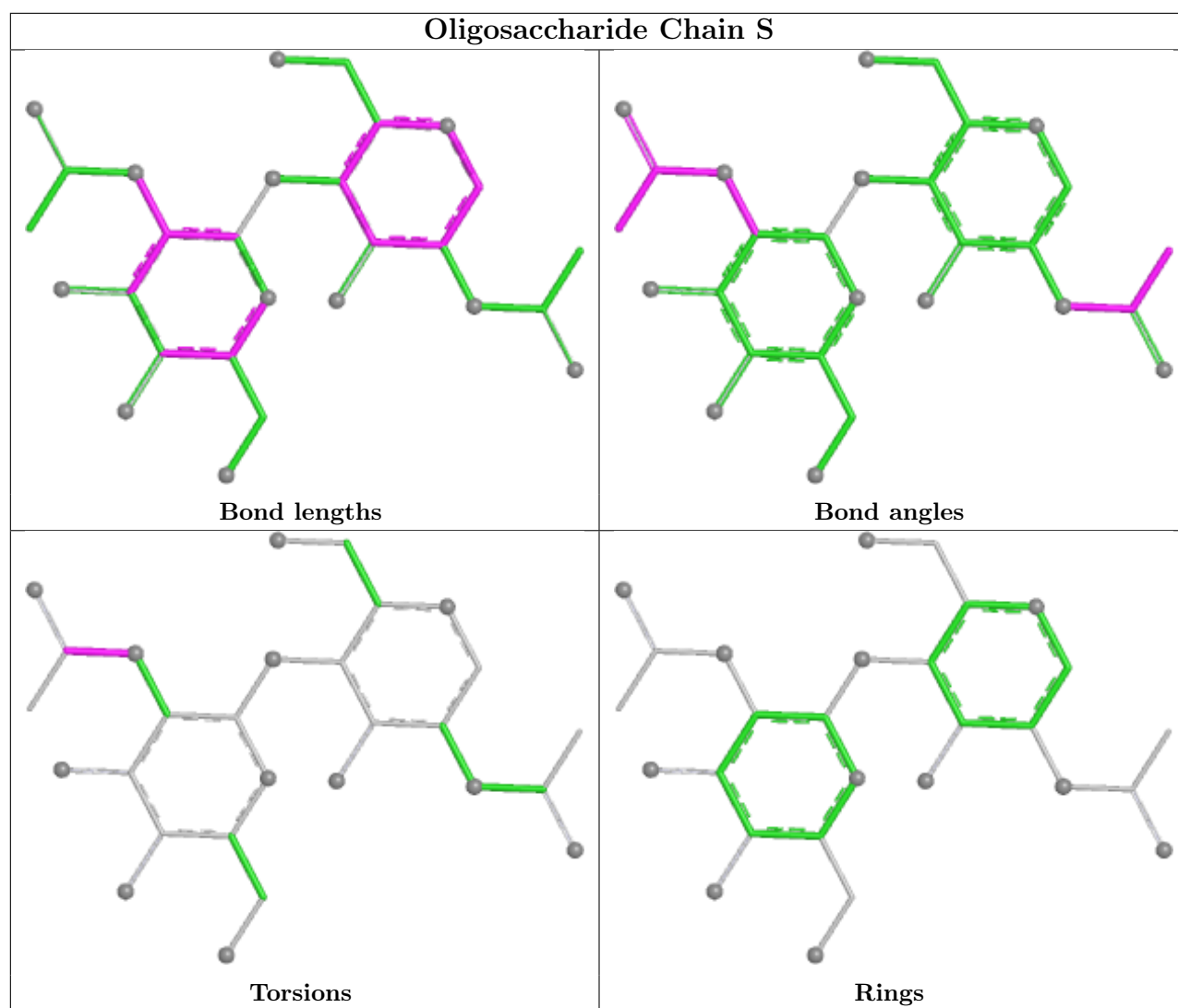


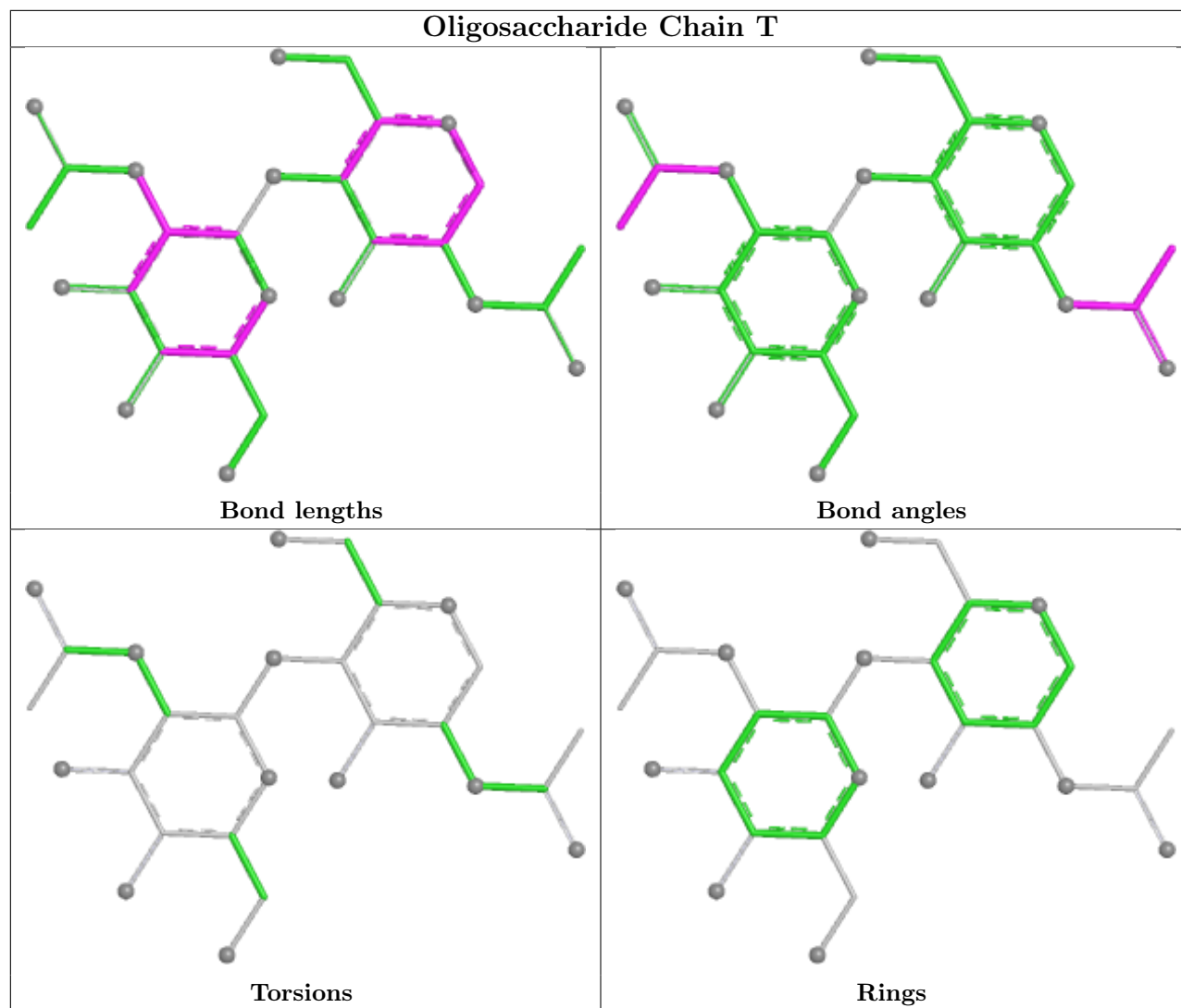


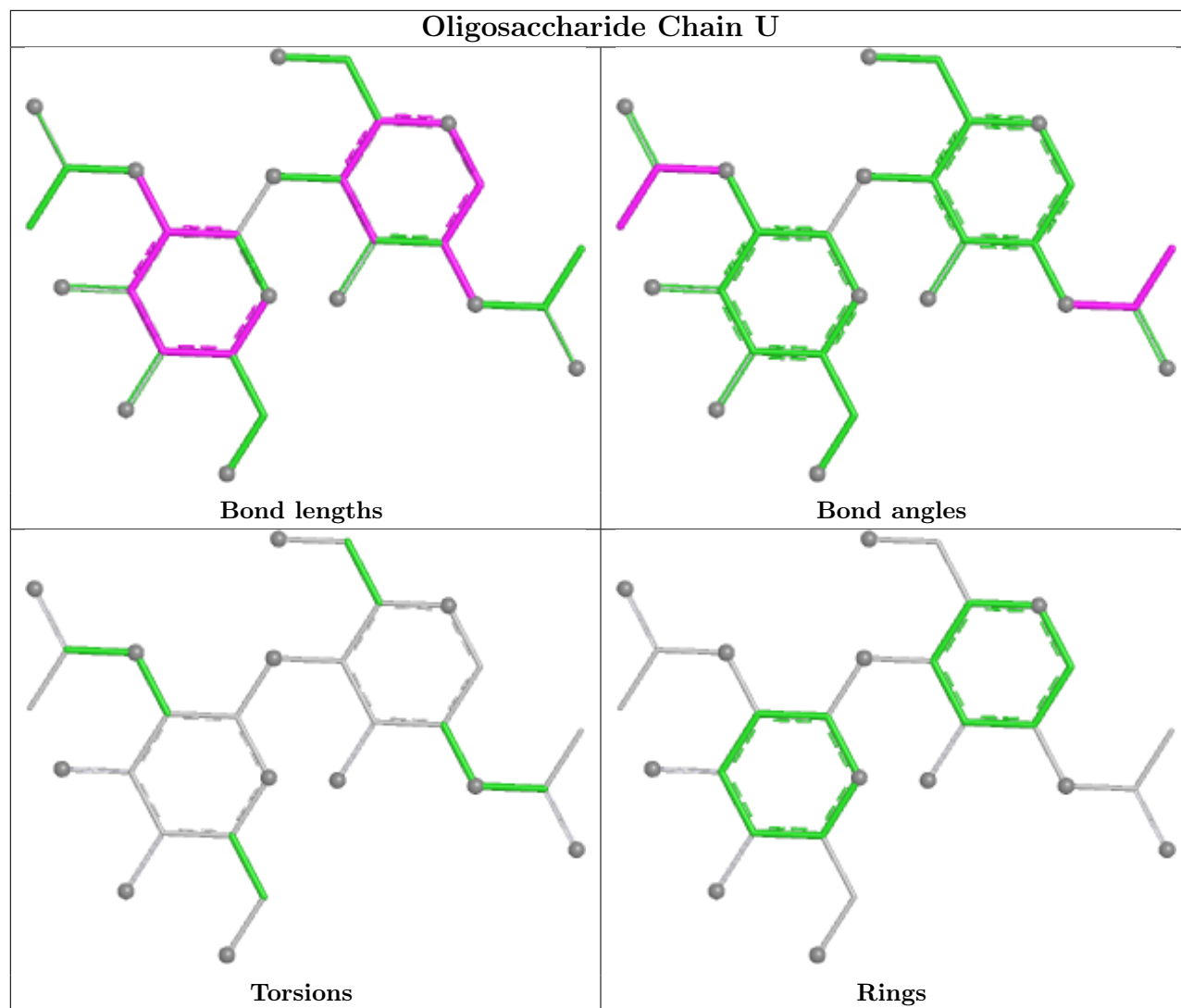


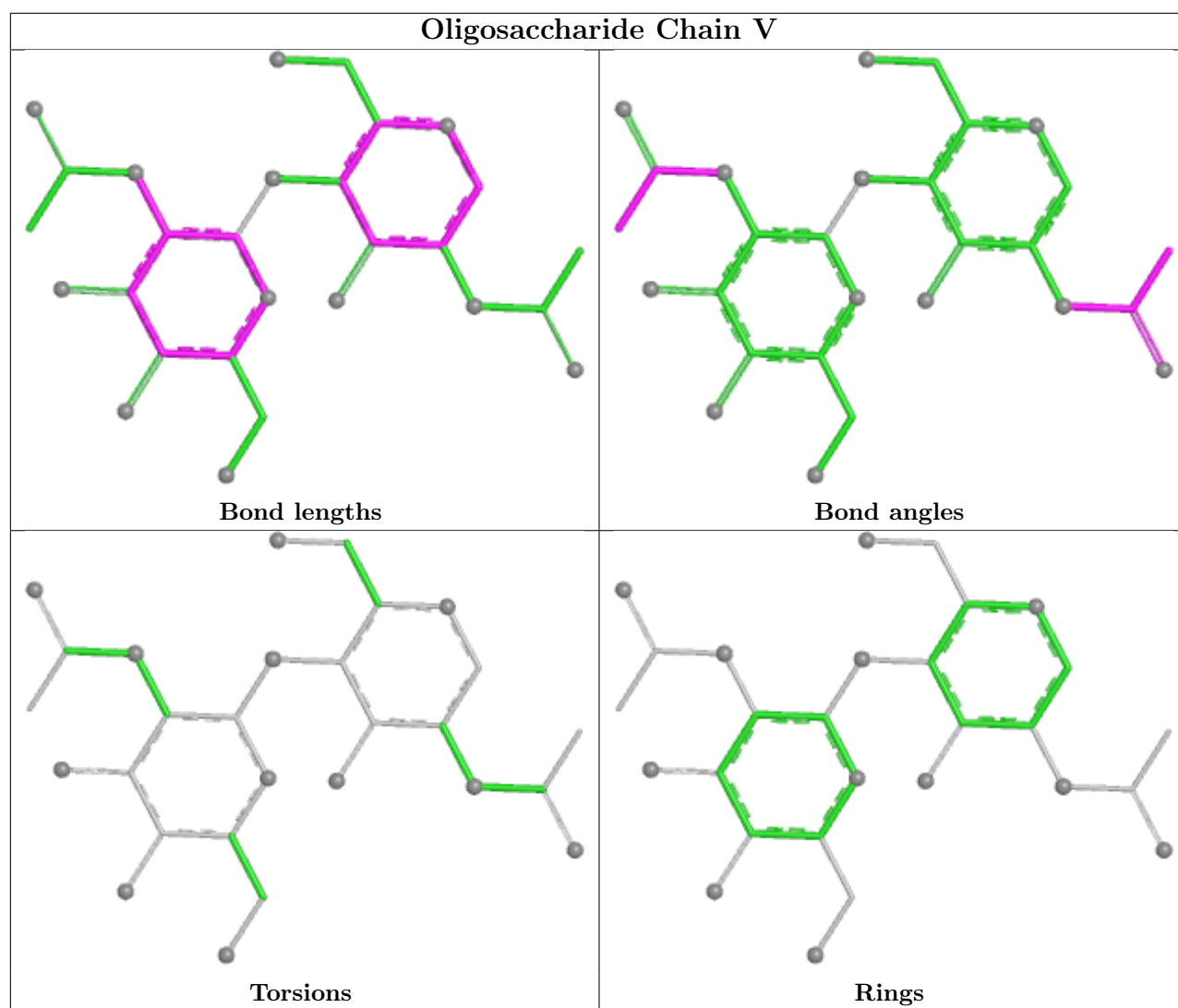


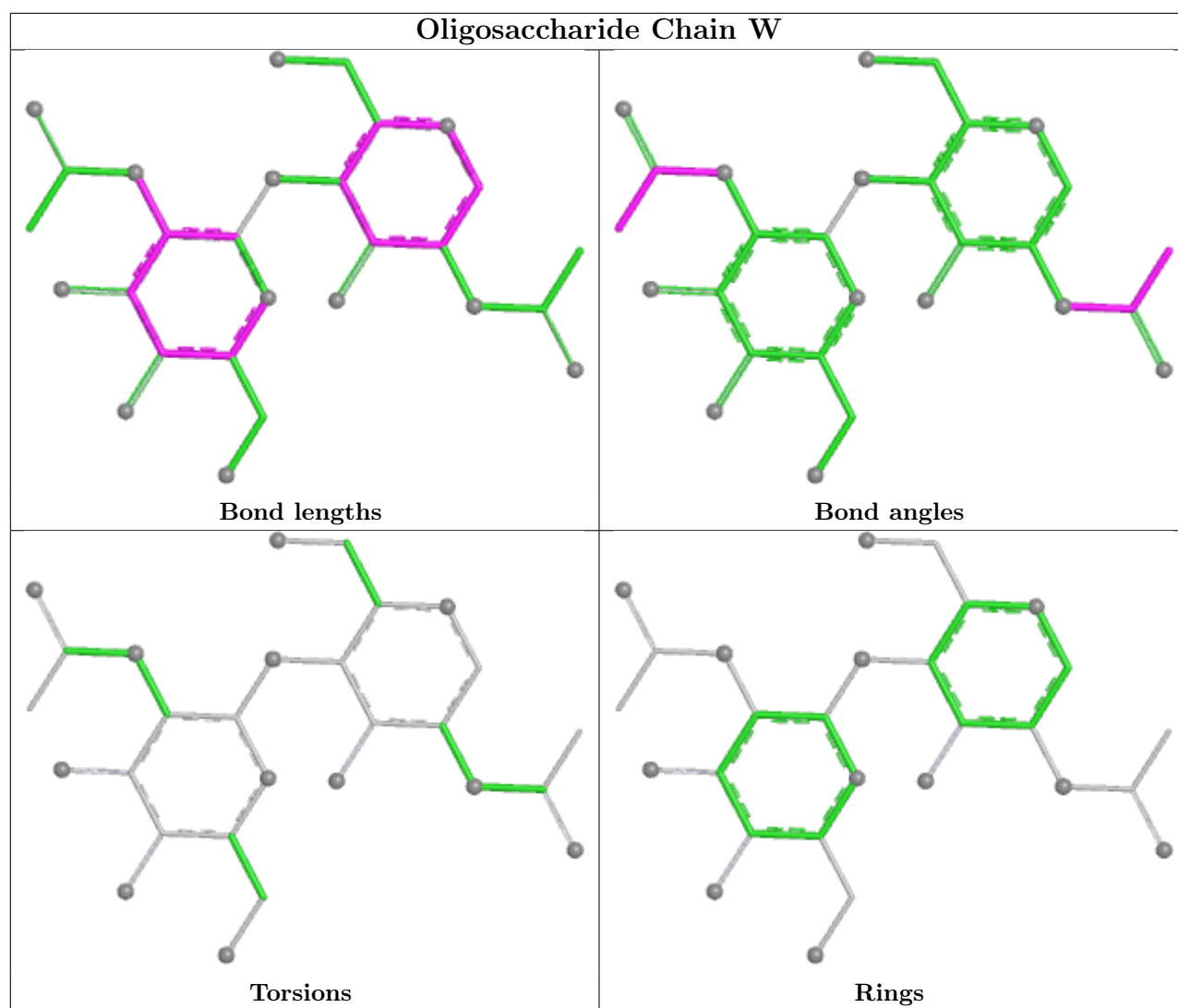


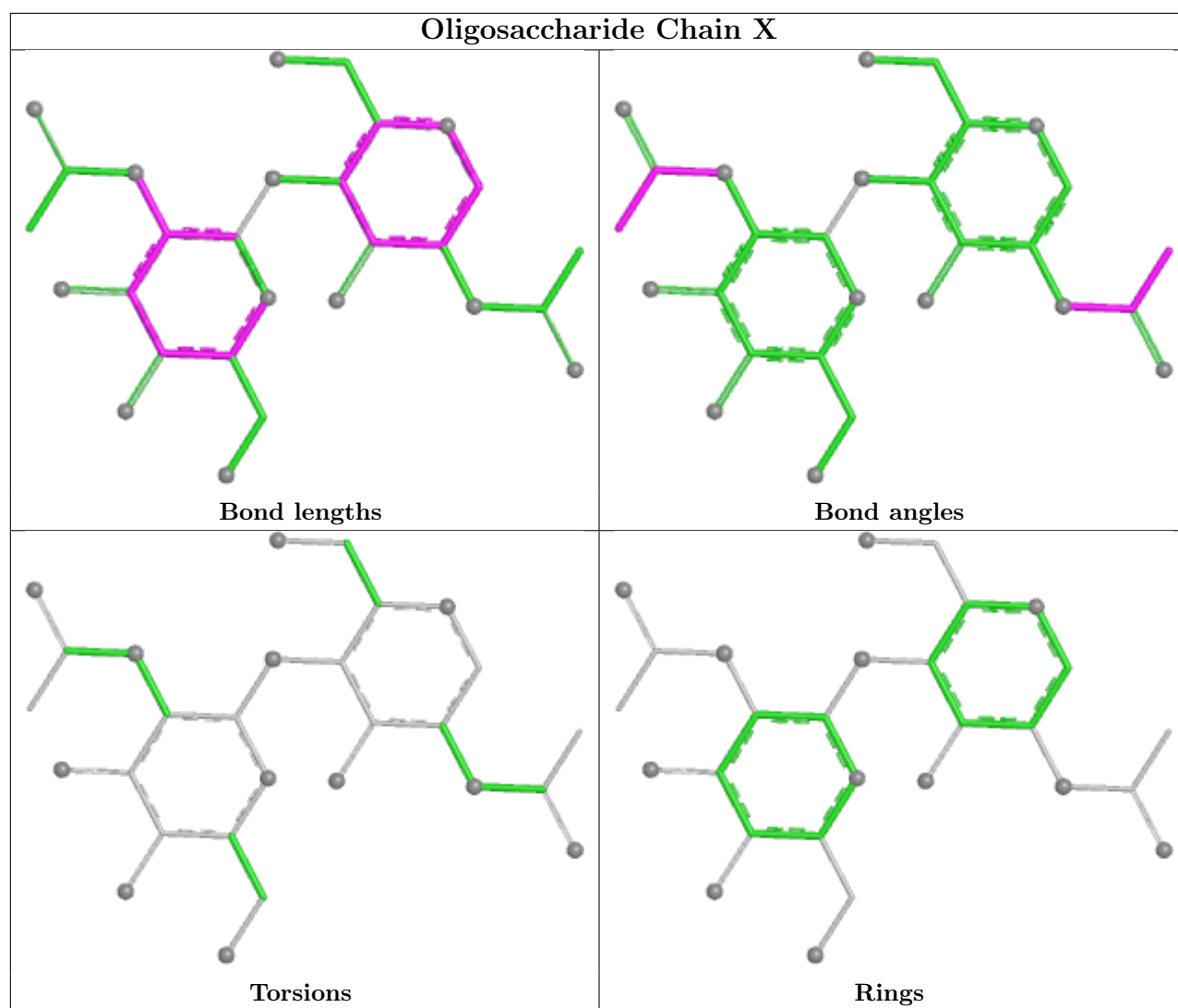


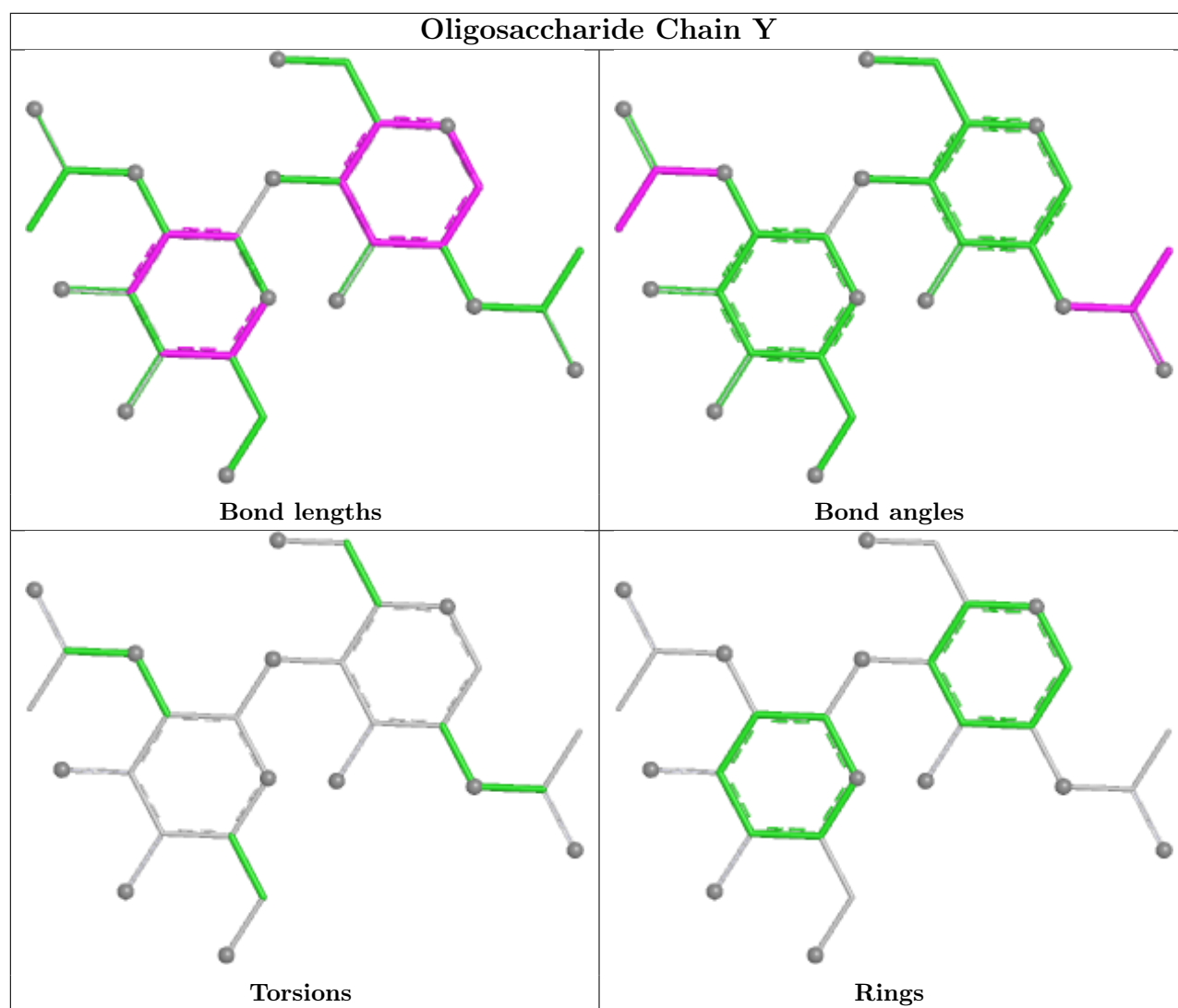


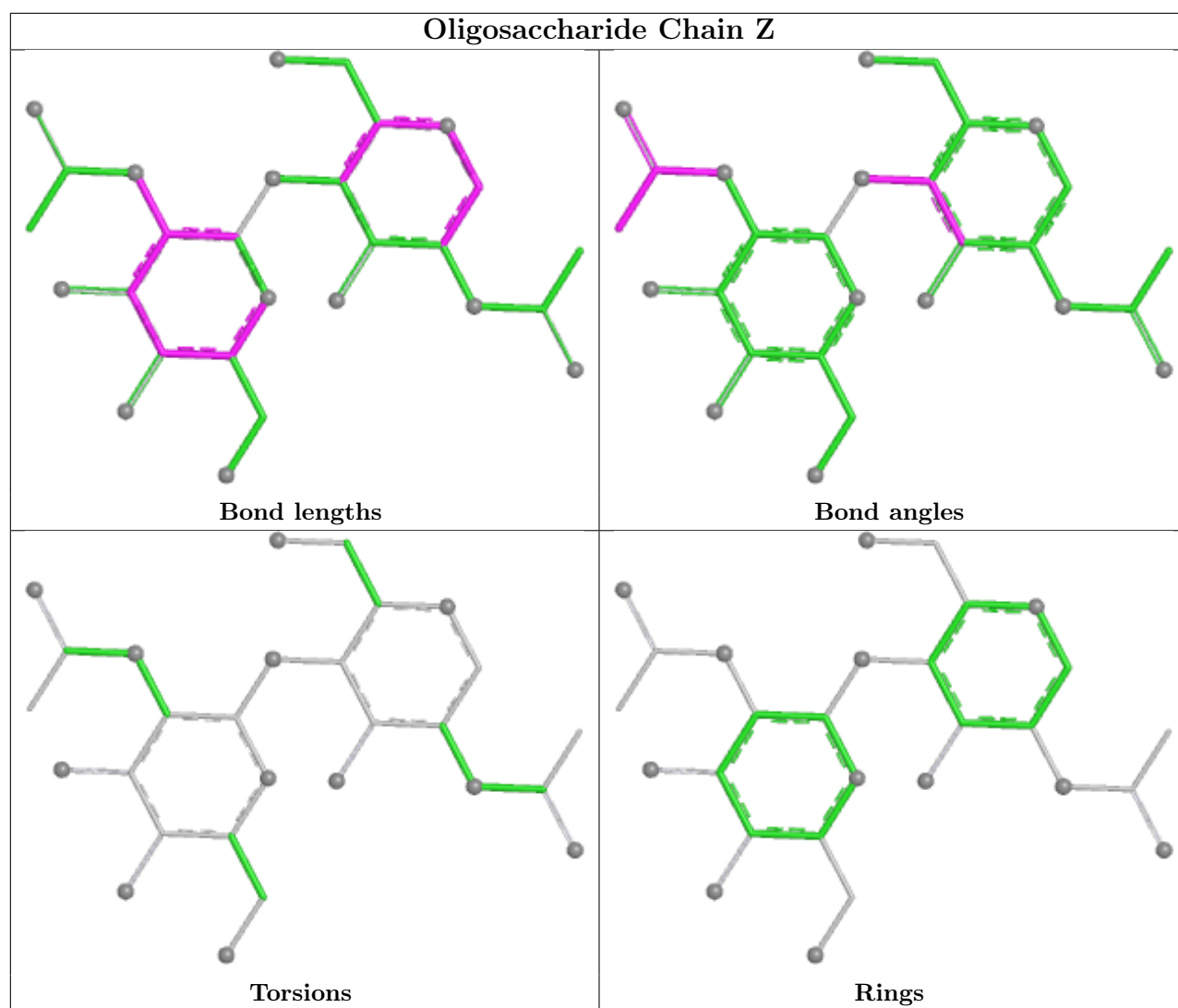


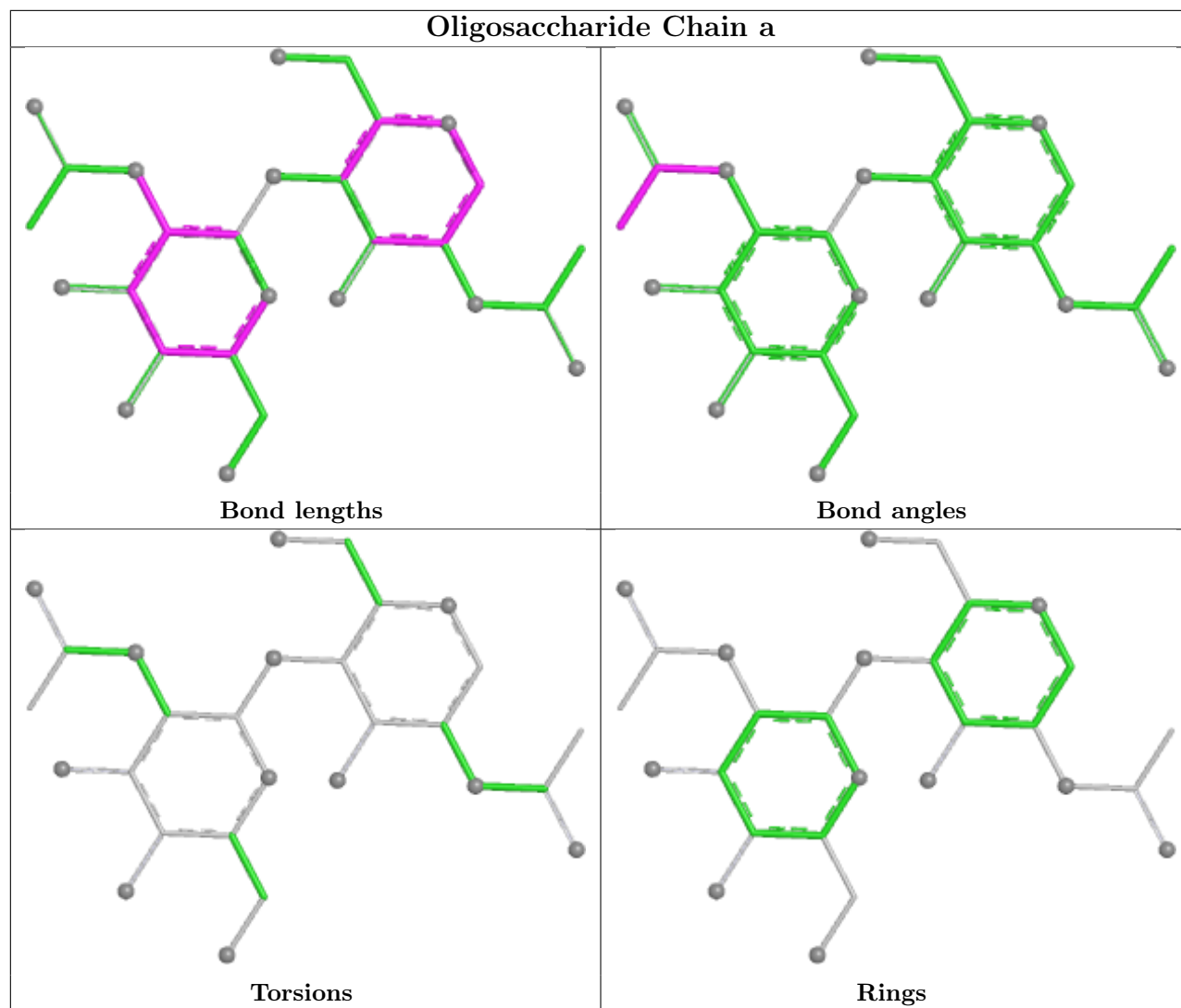


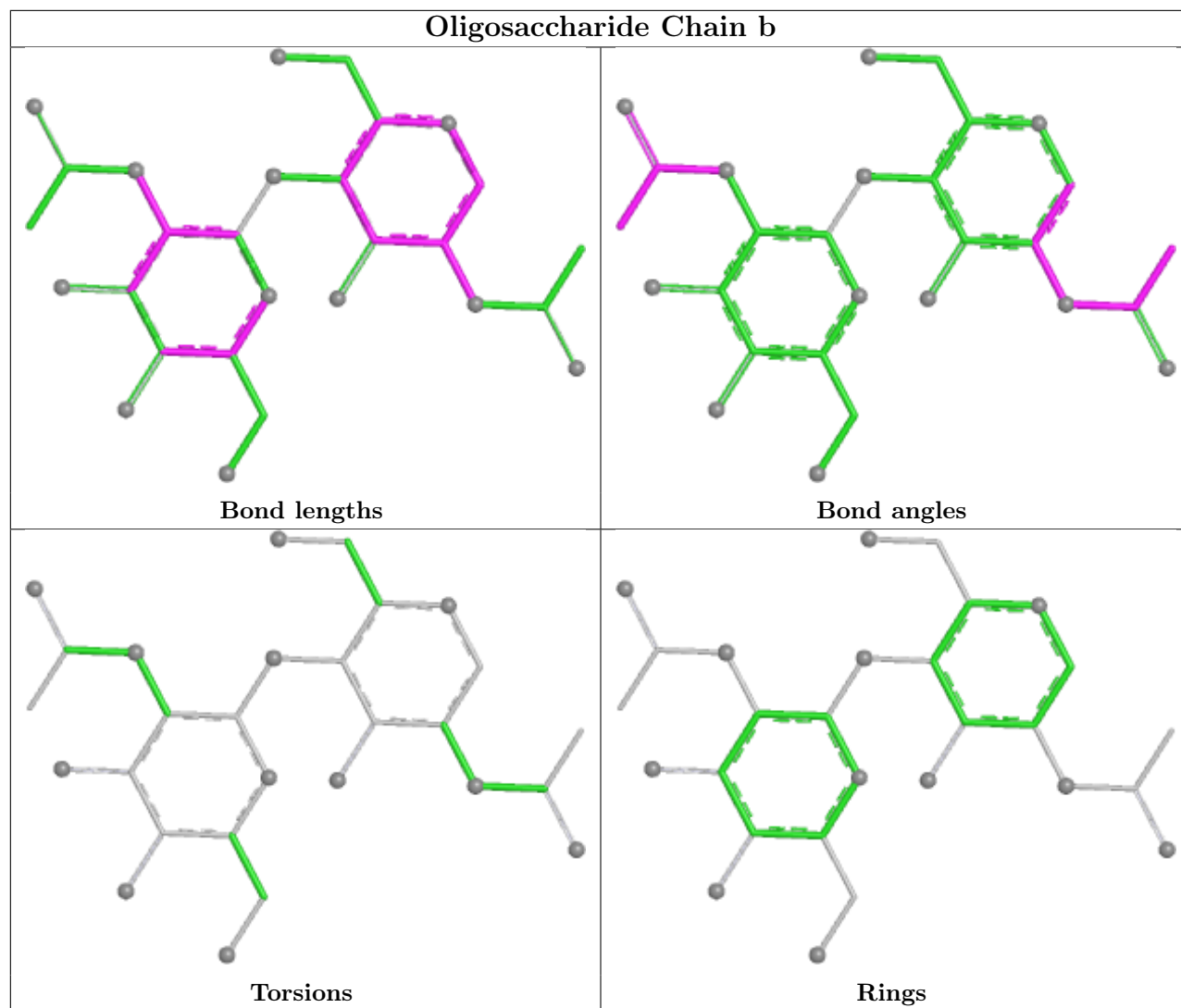


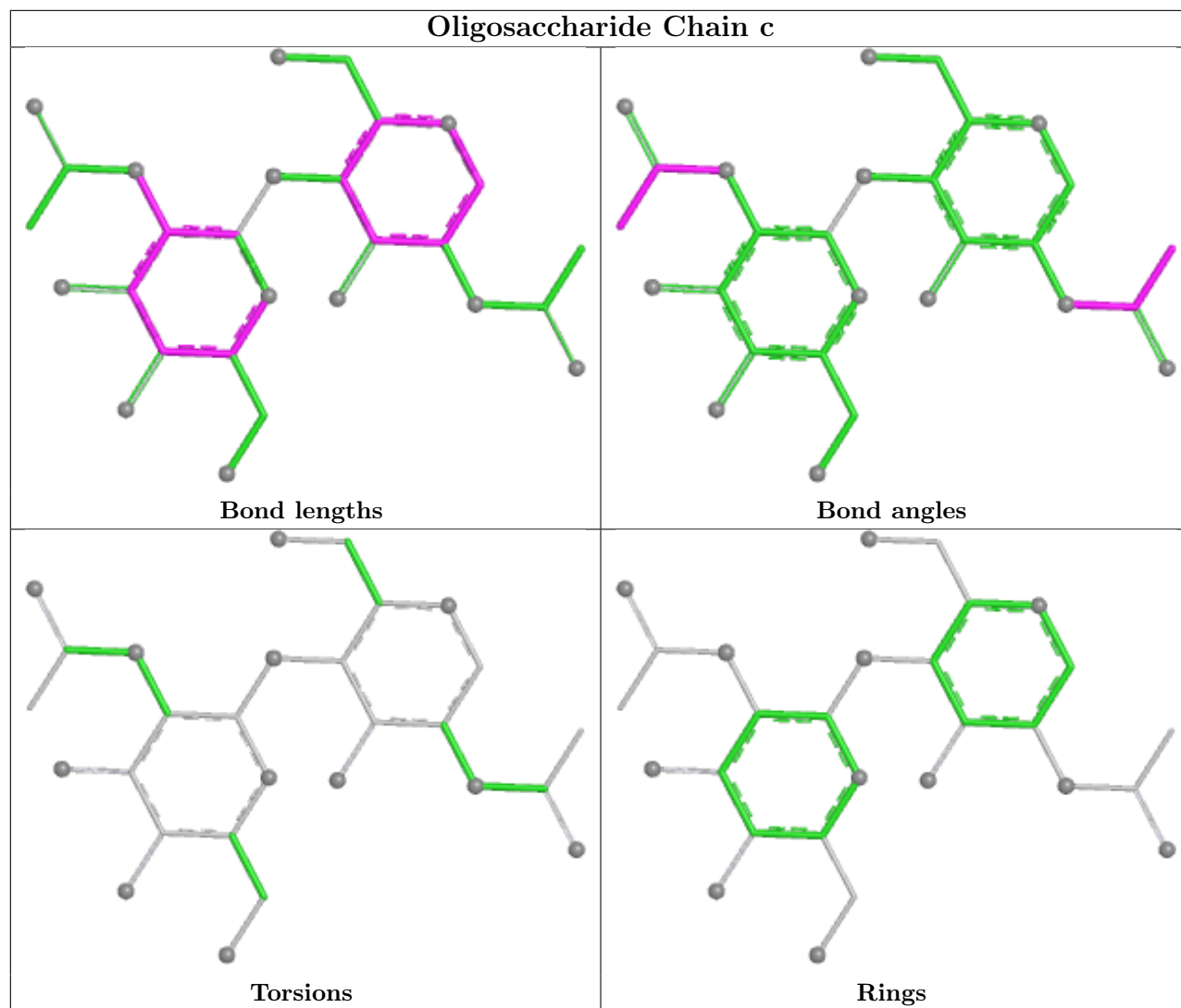


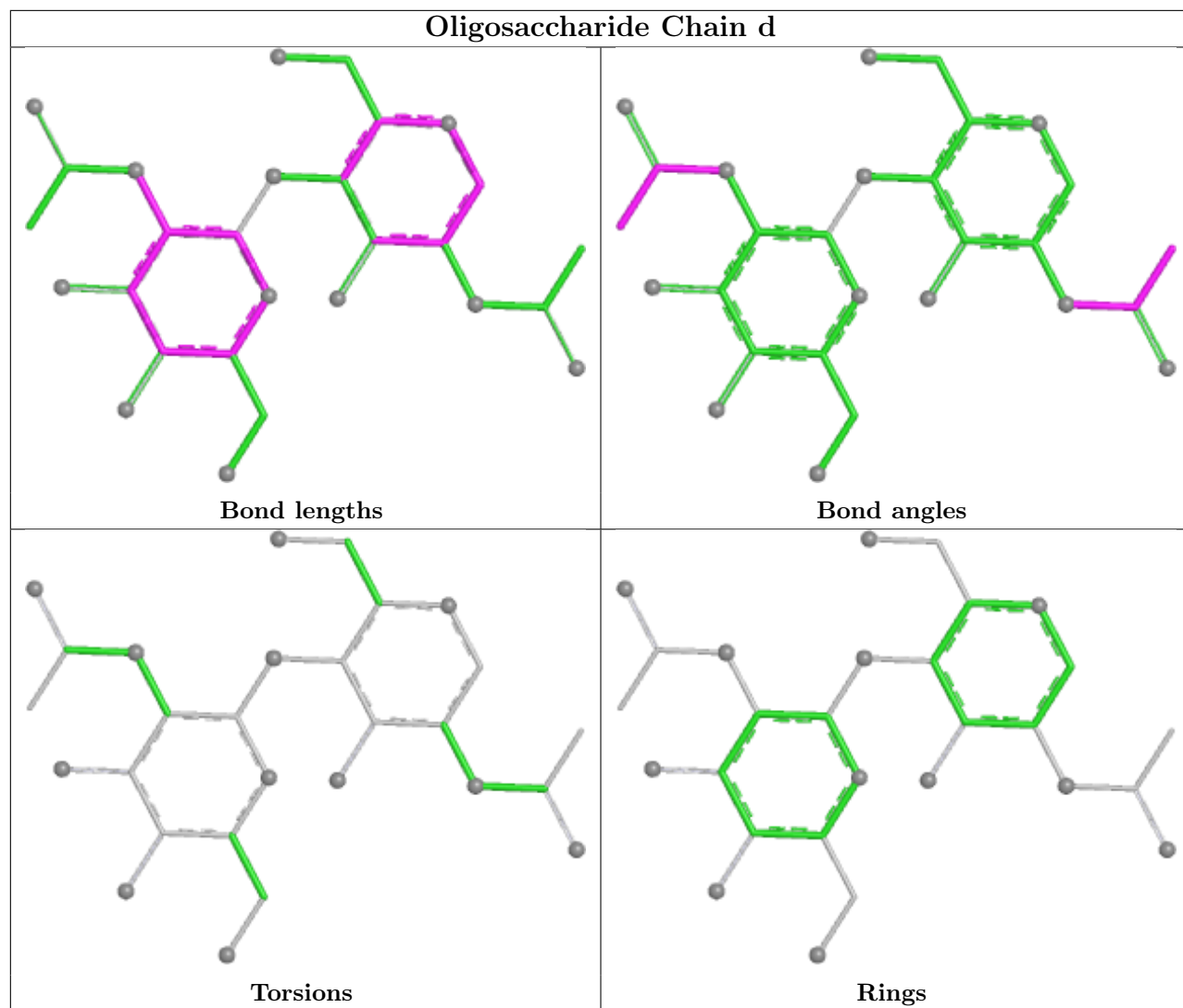


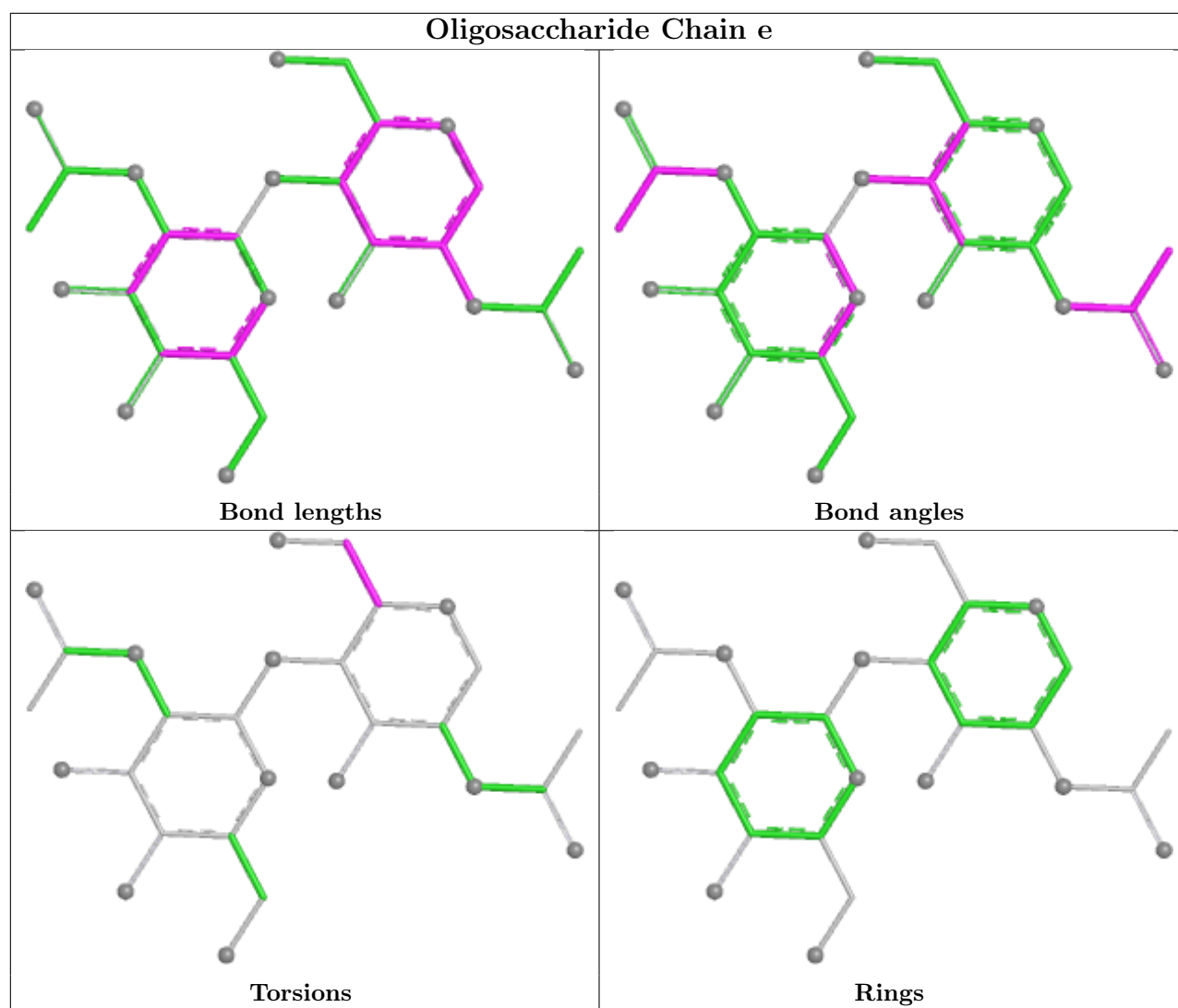


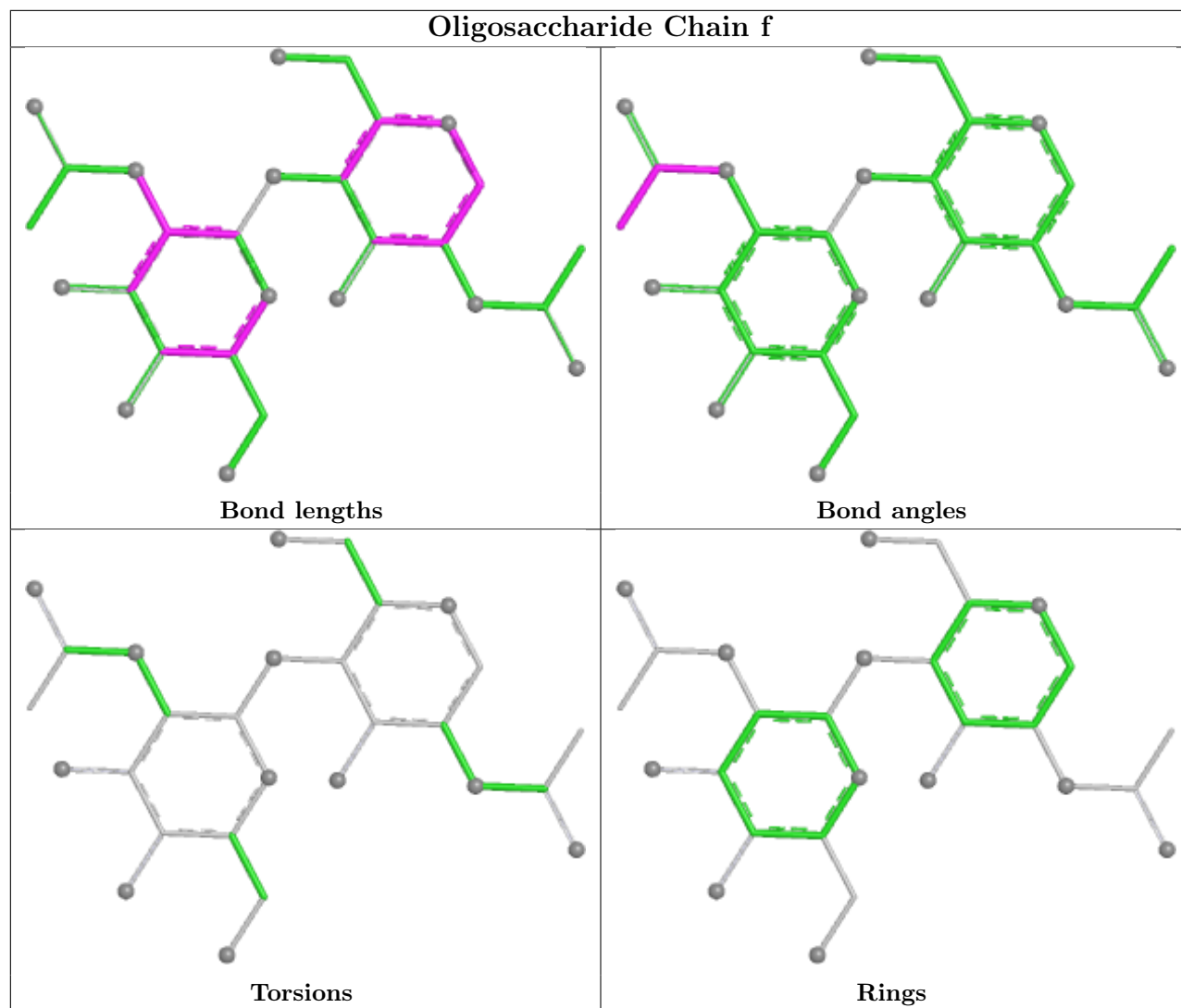


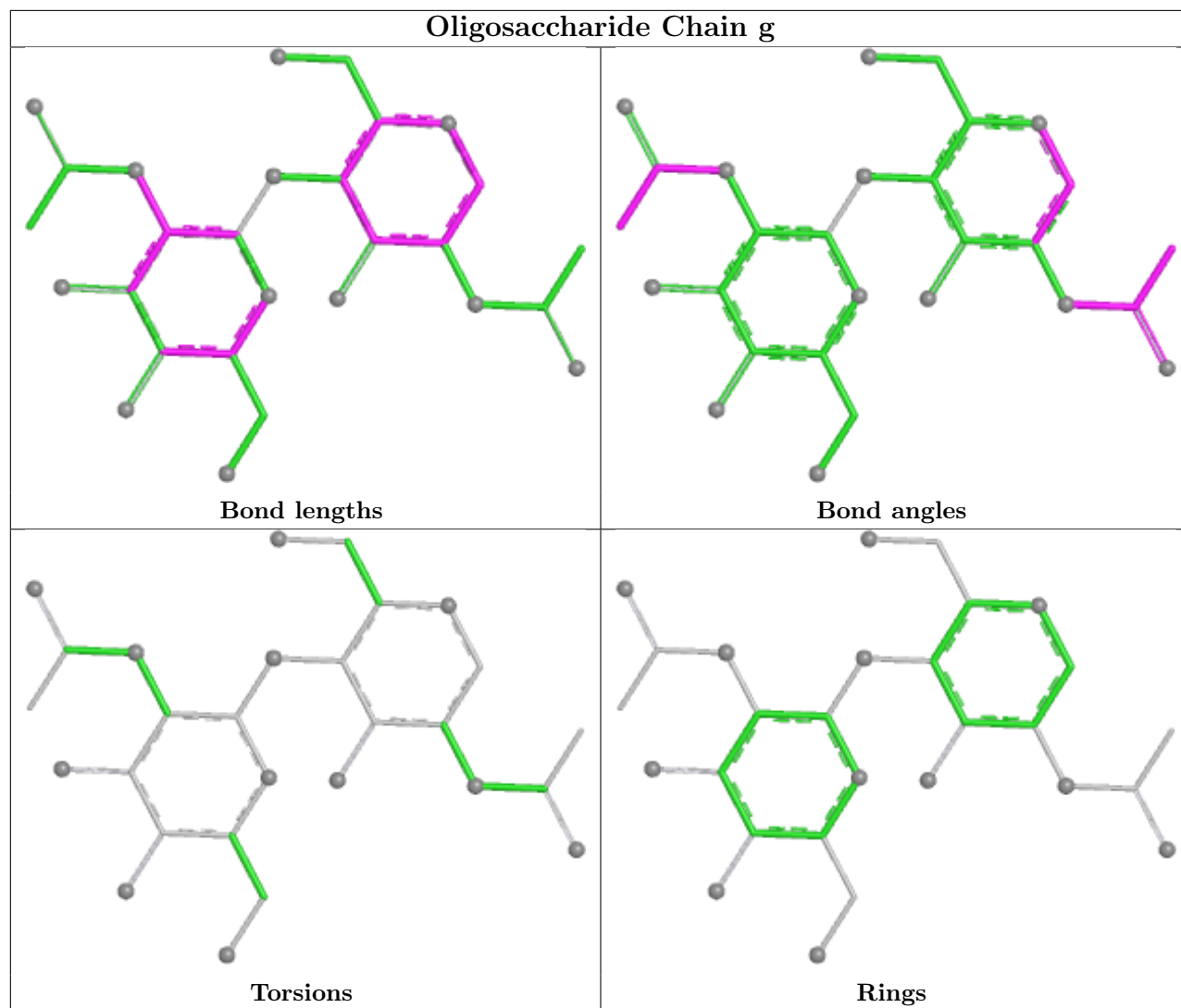


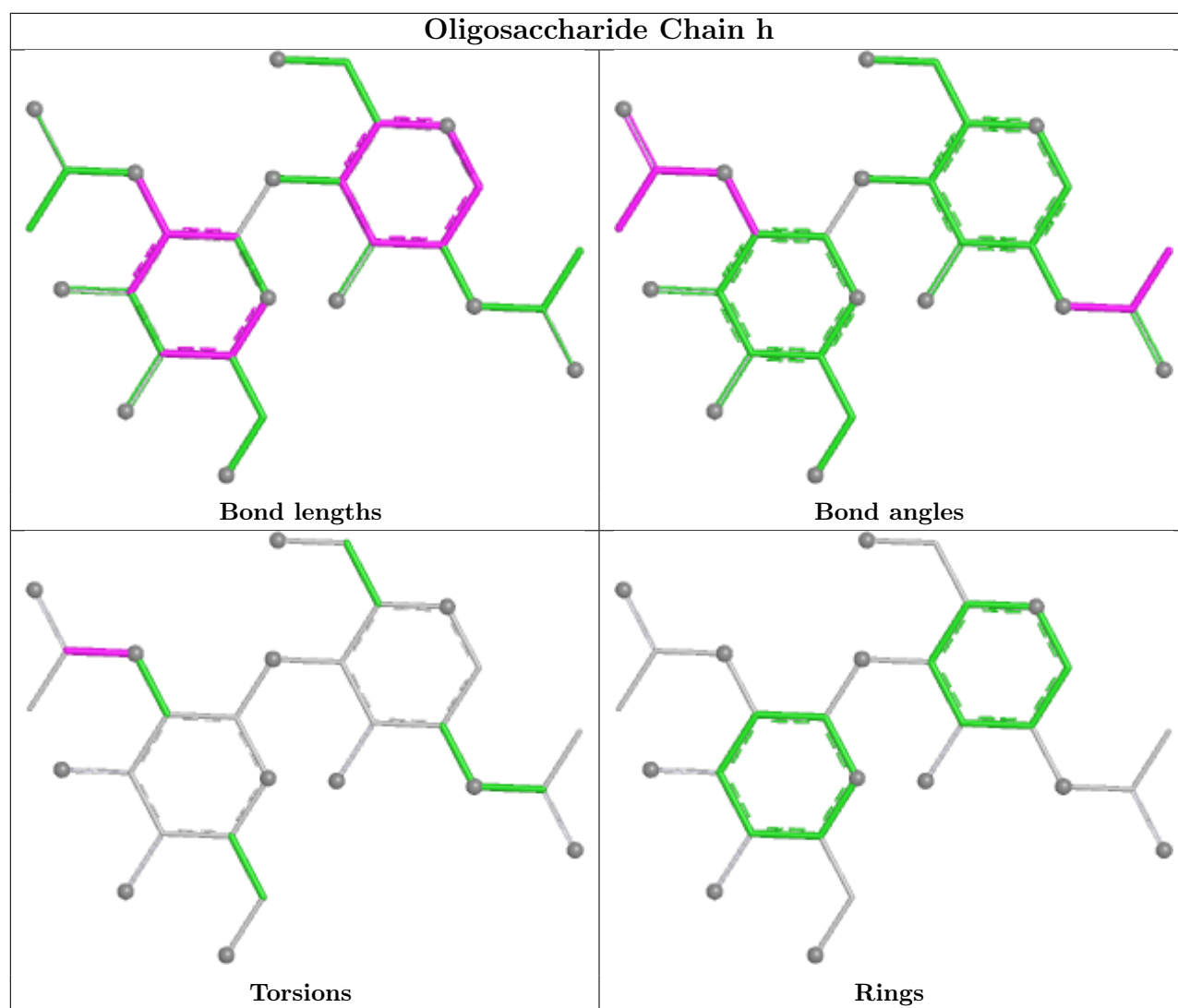


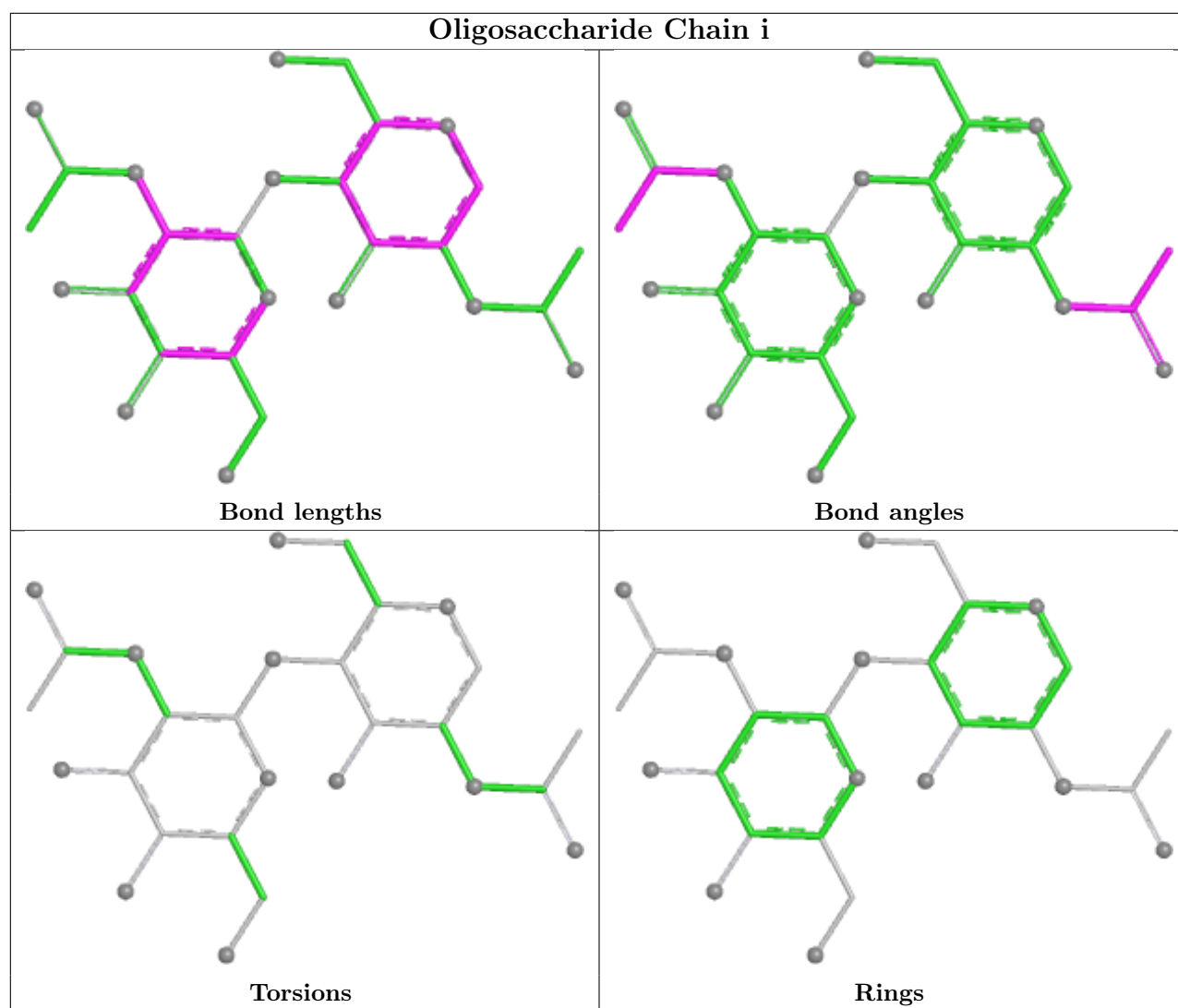


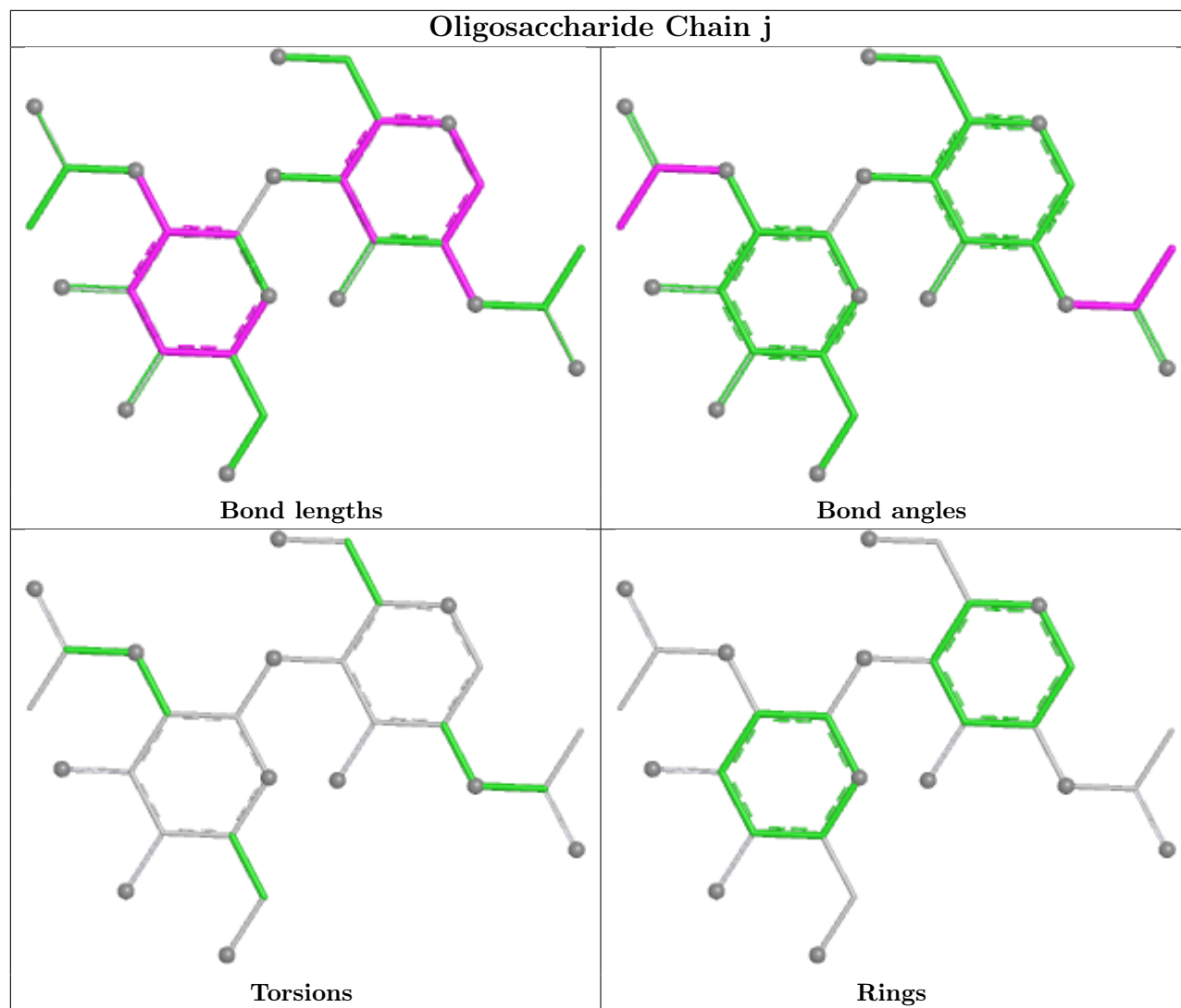


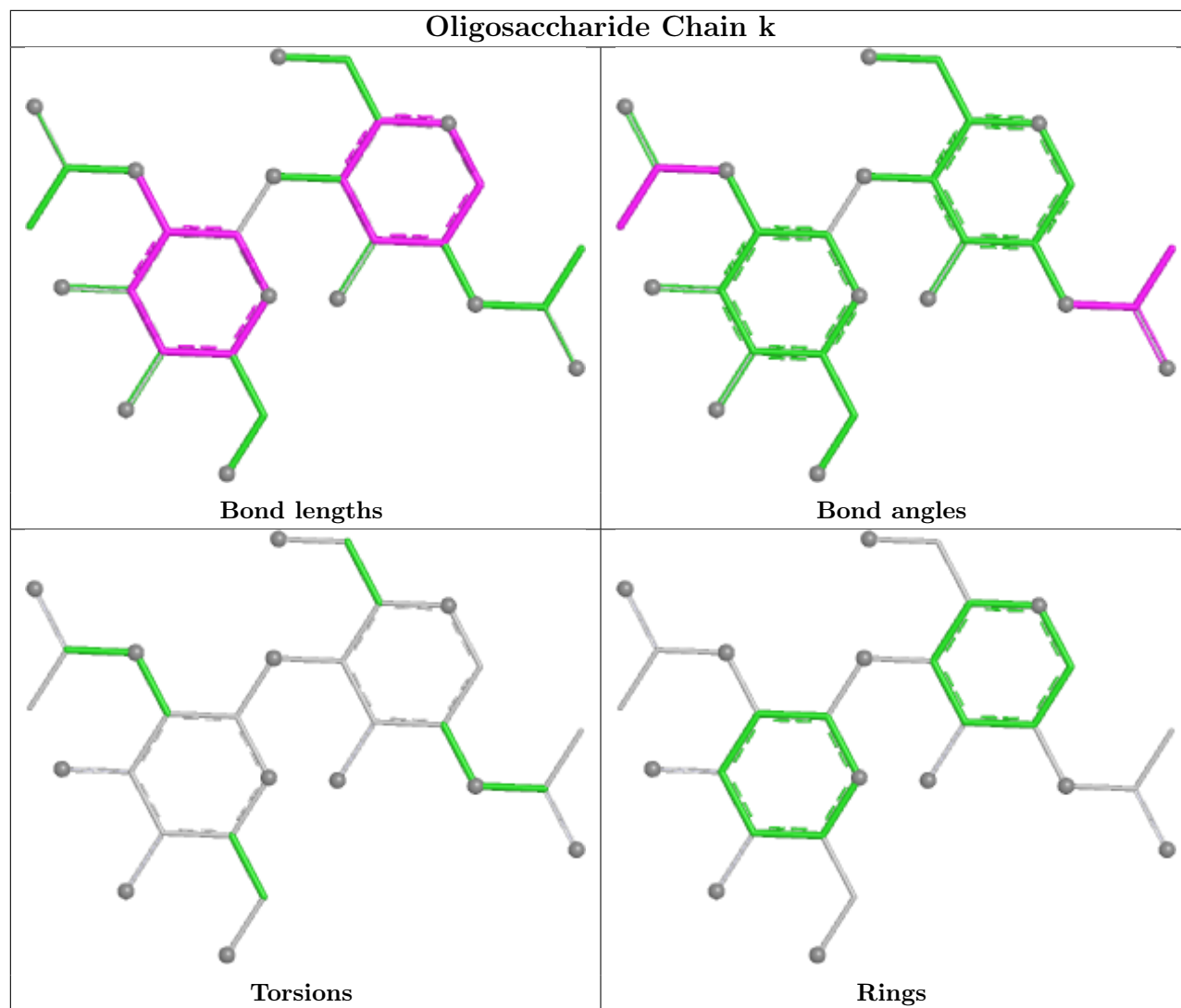


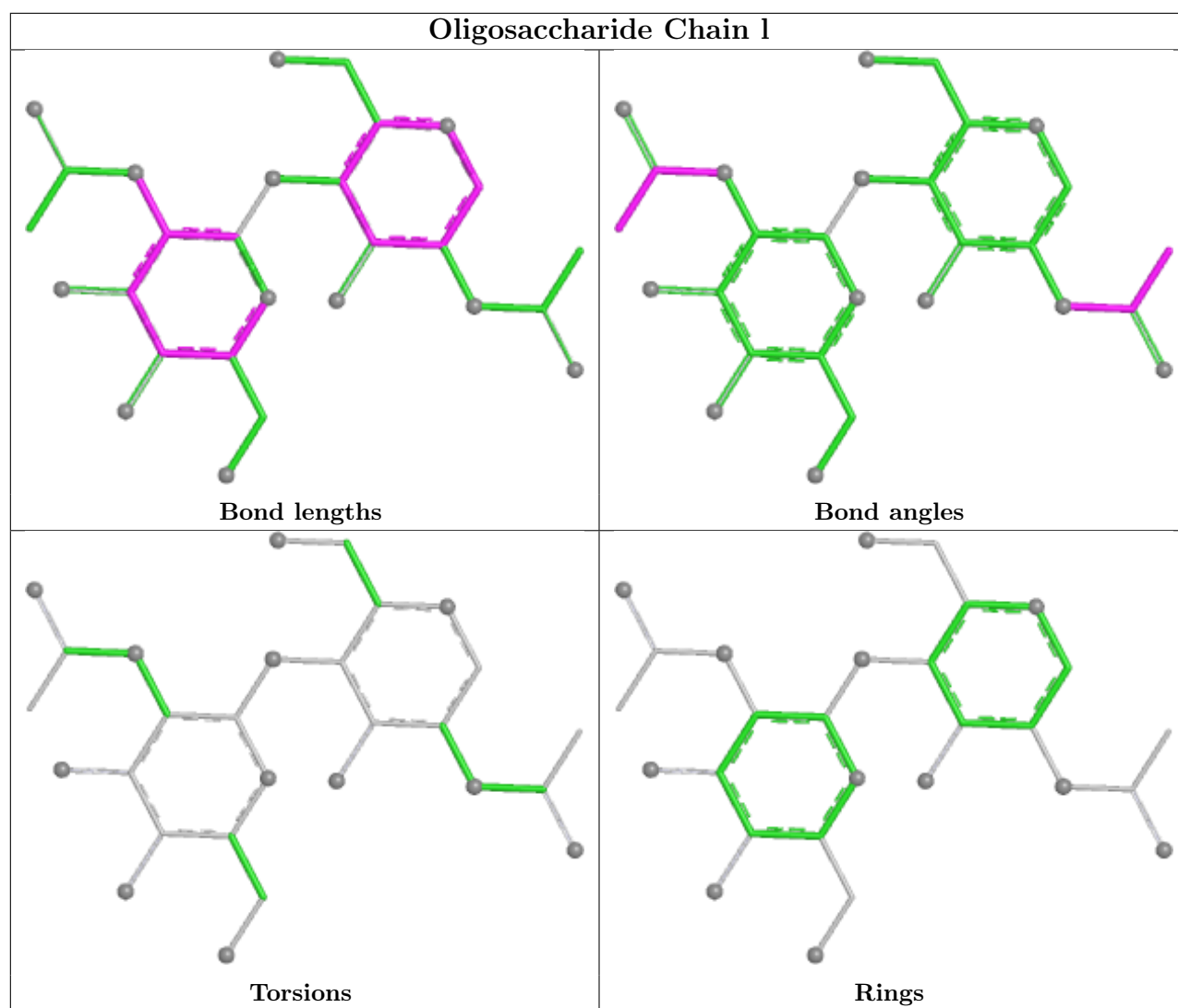


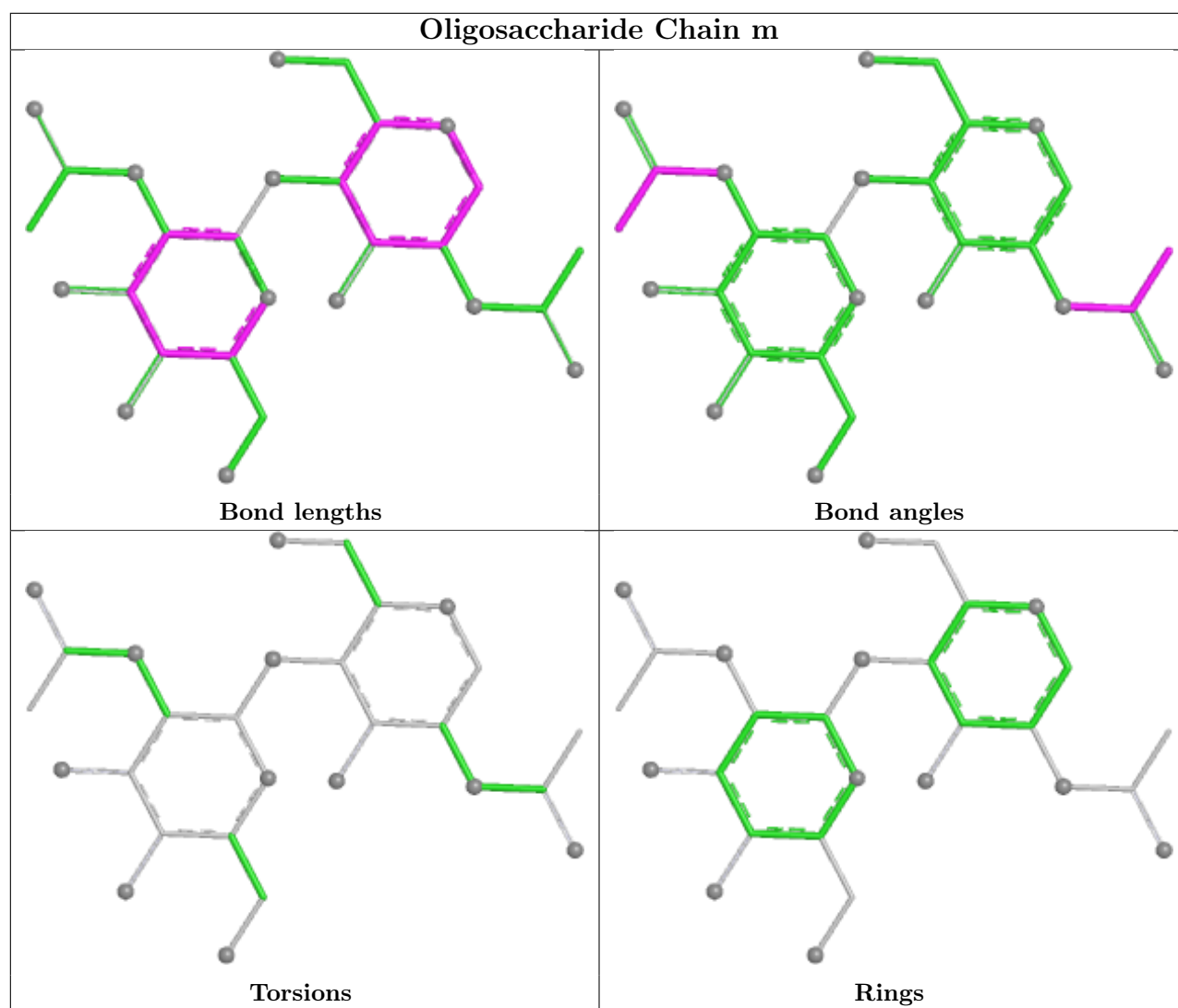


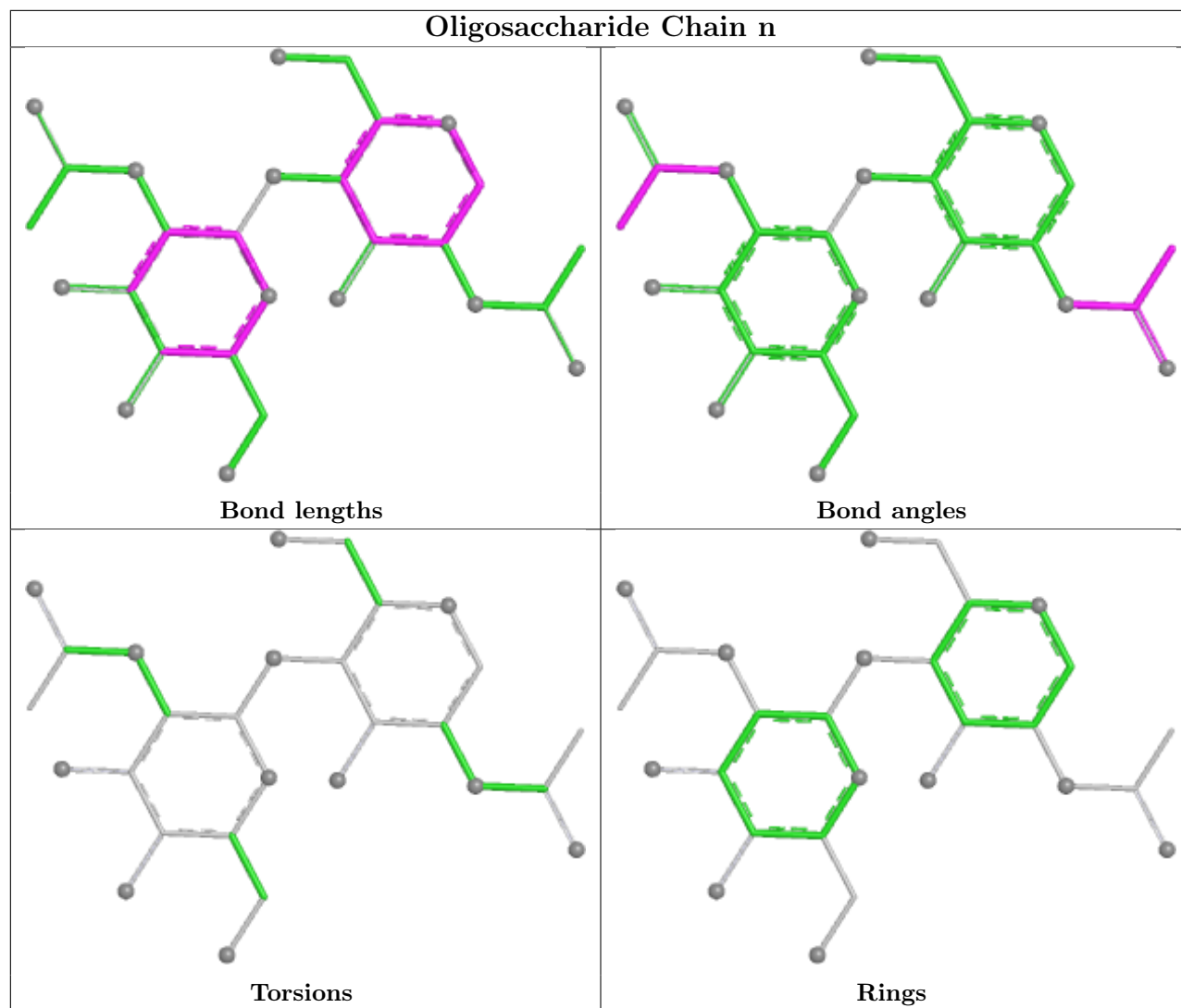


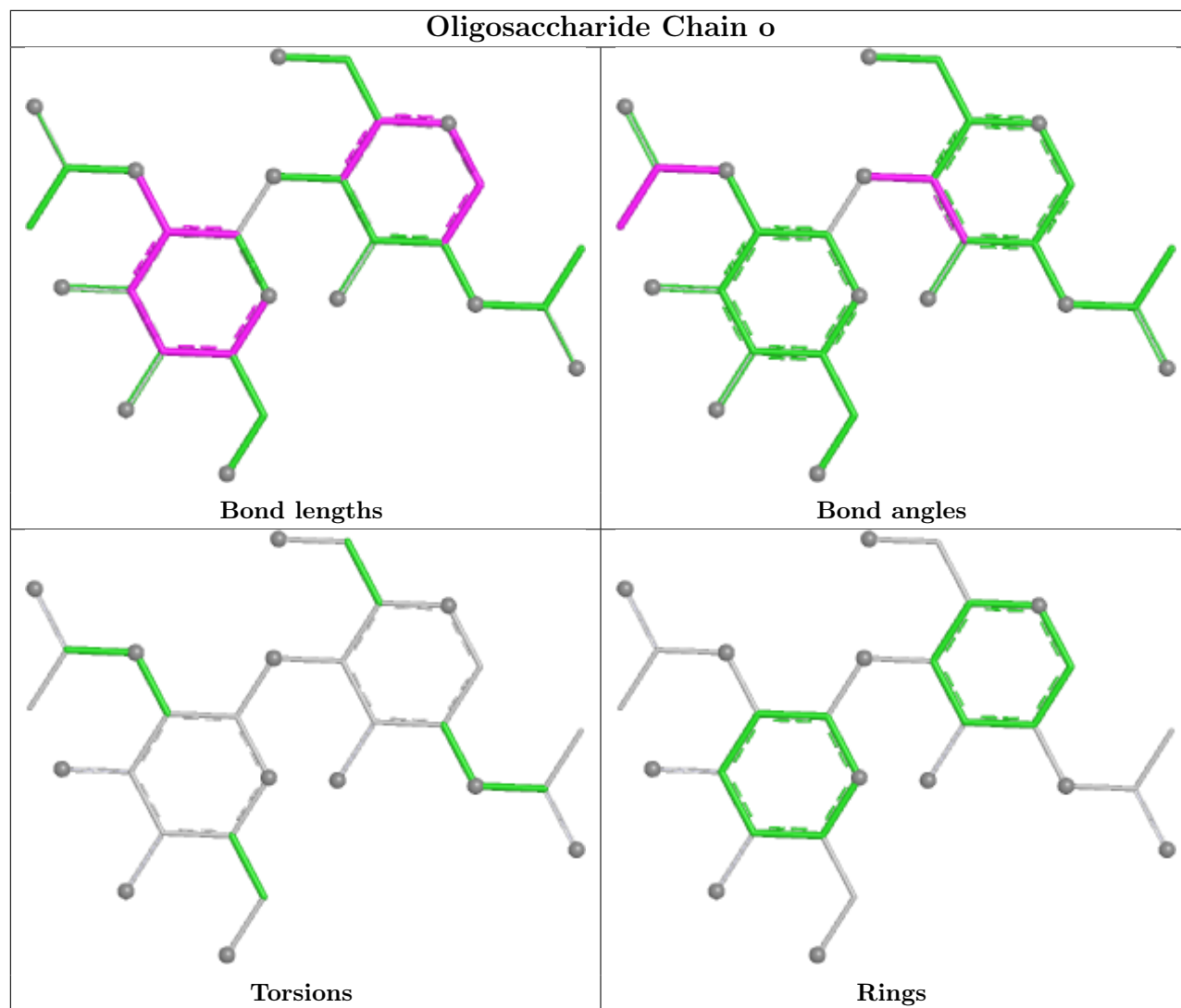


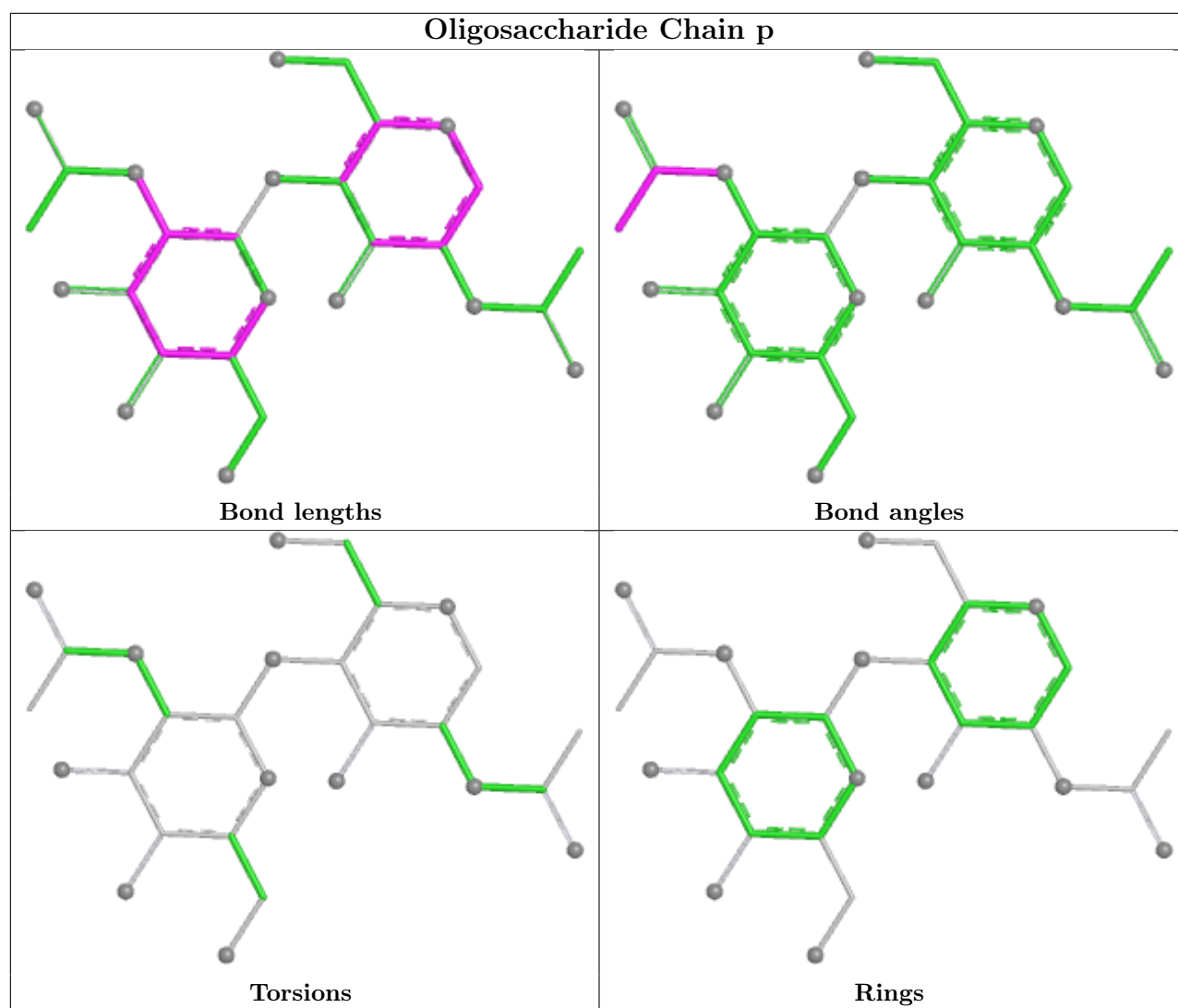


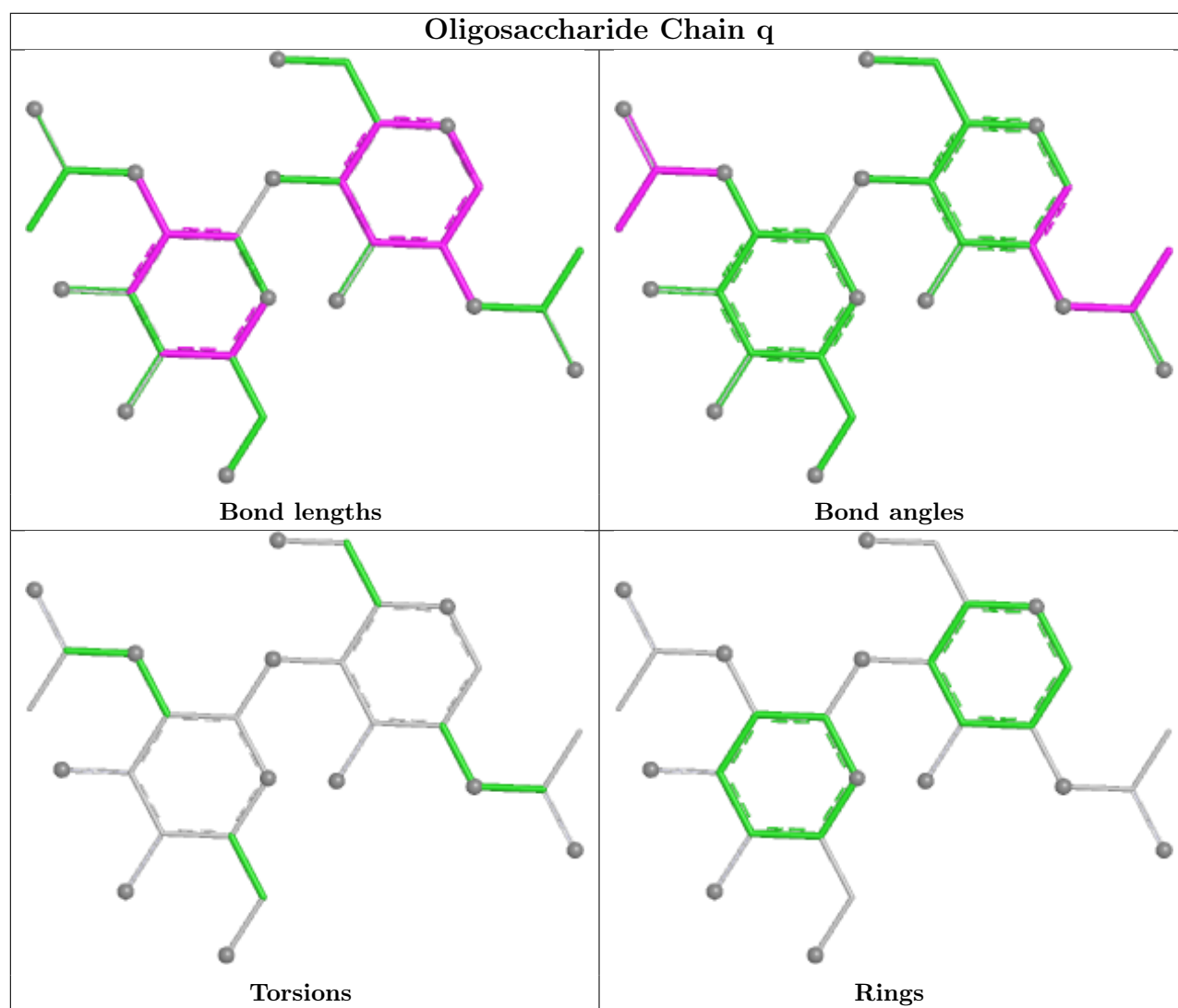


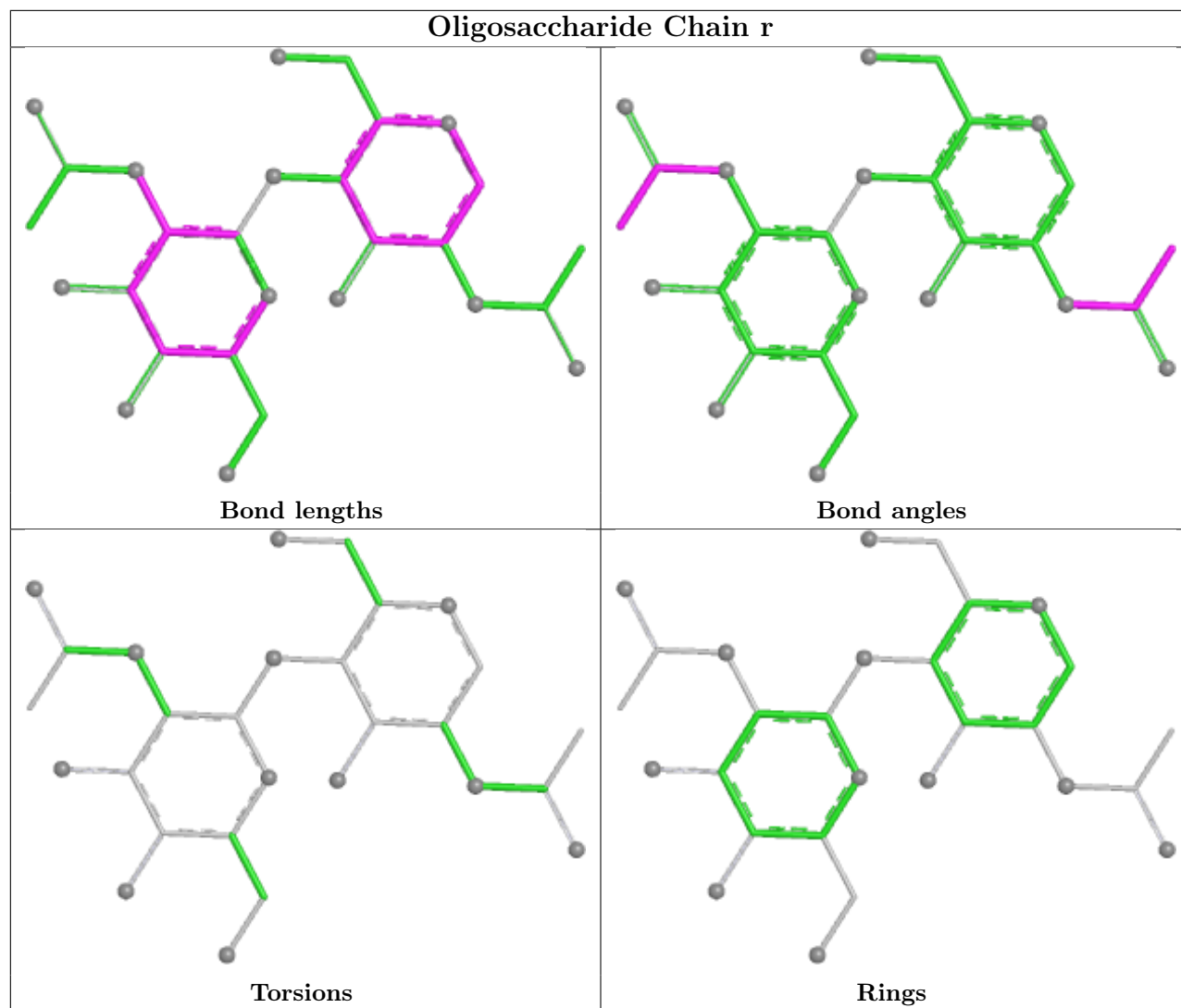


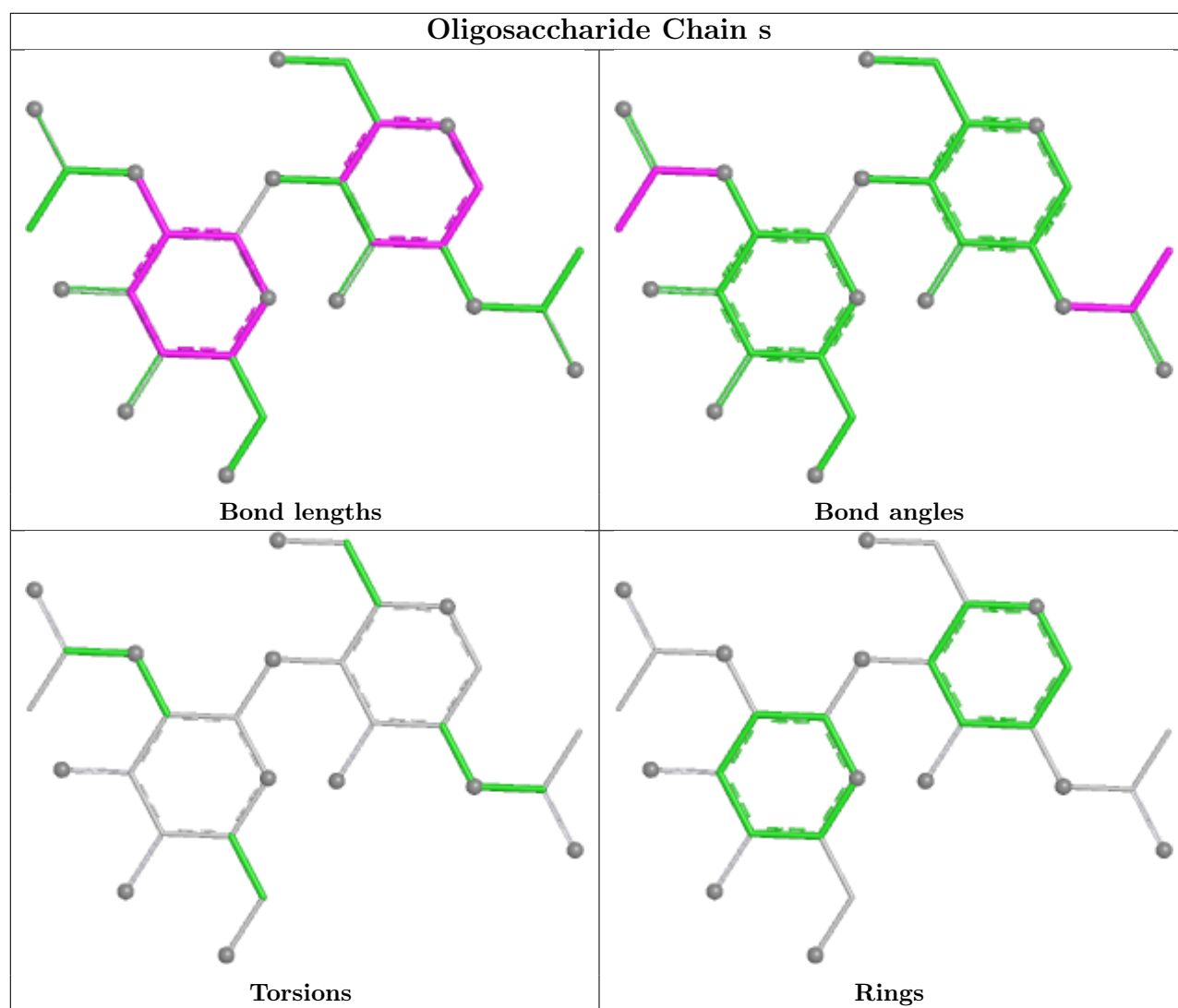


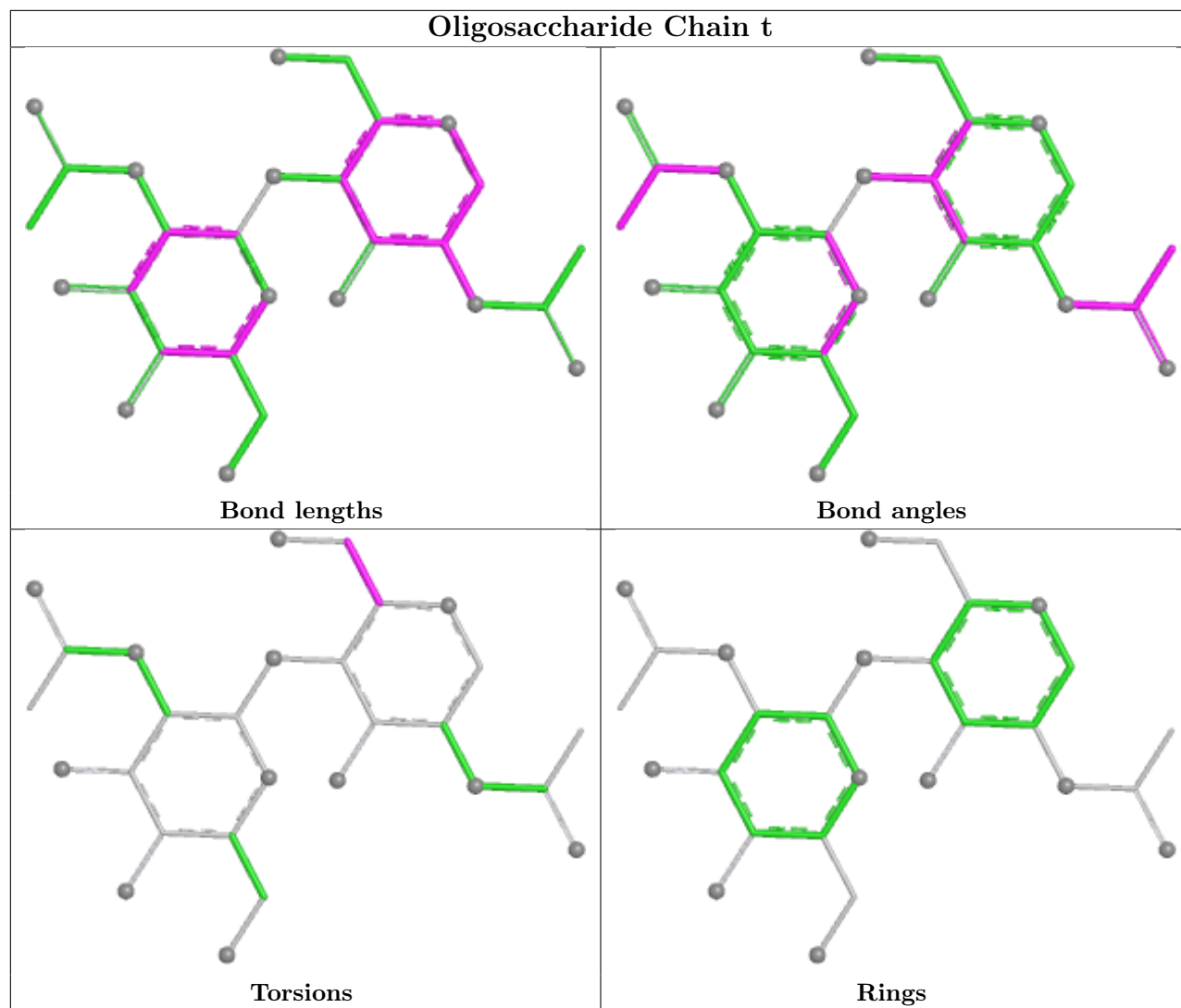


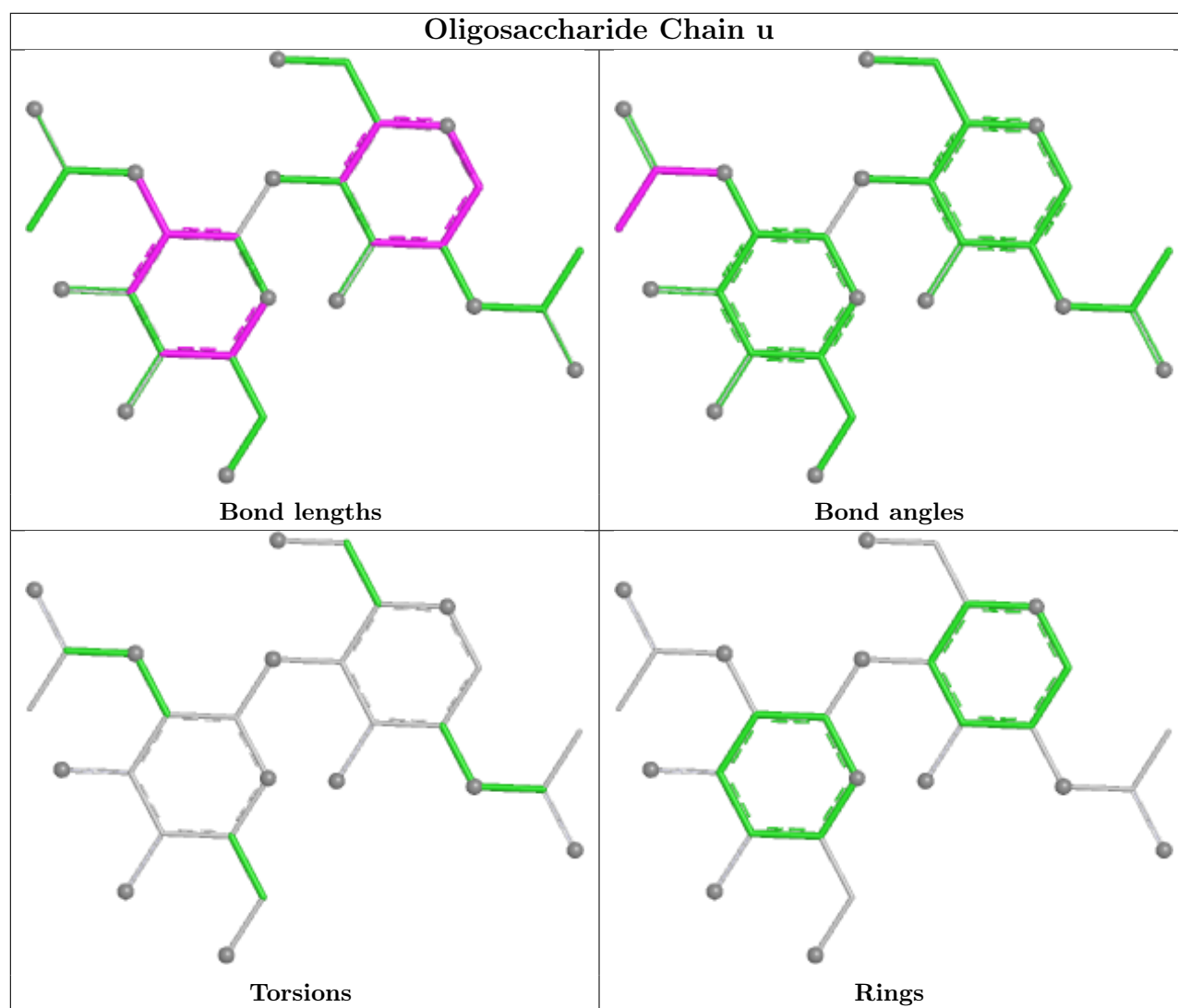


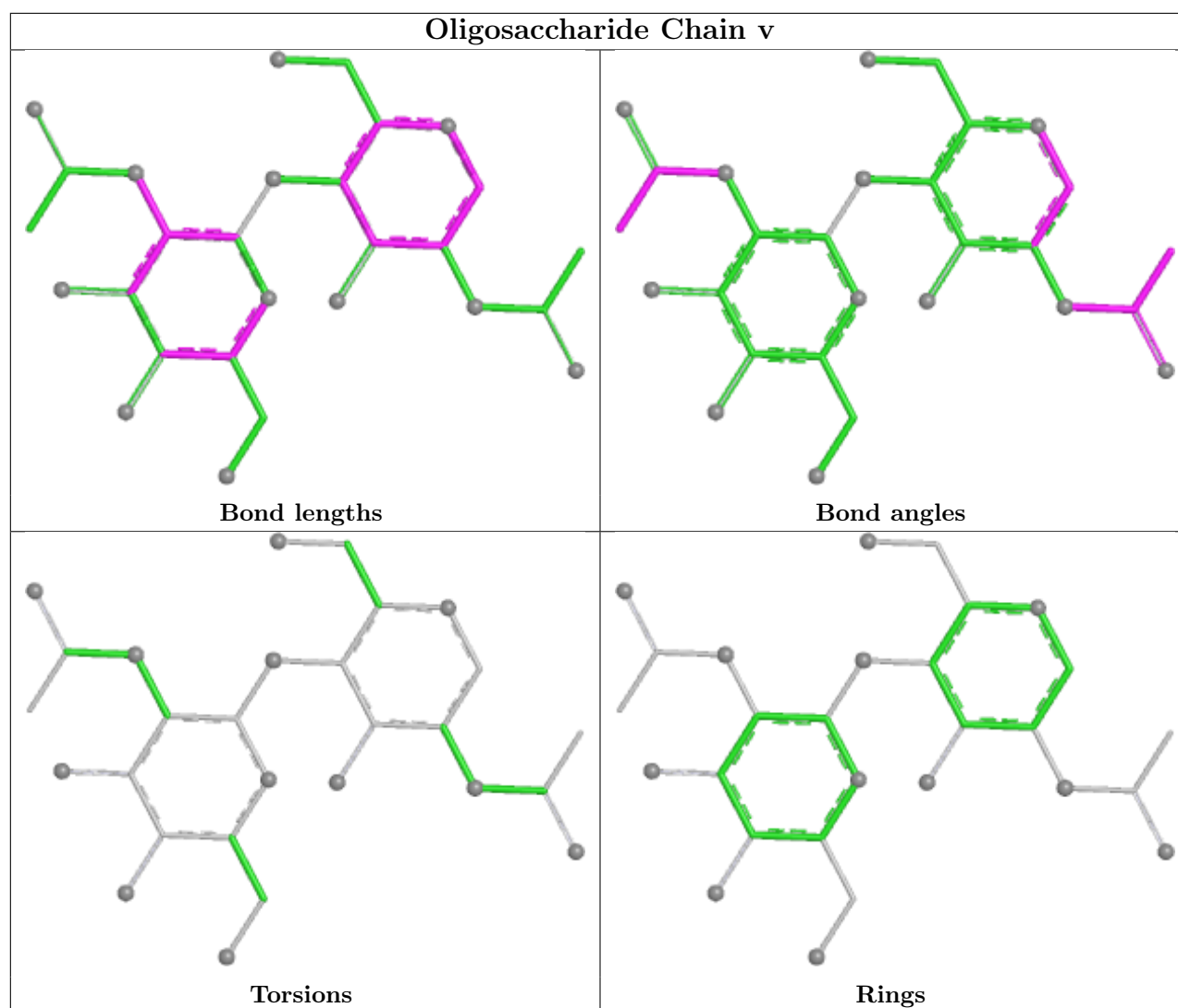












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	NAG	B	1502	1	14,14,15	2.10	5 (35%)	17,19,21	6.79	3 (17%)
4	VCG	C	1503	-	42,42,42	2.58	6 (14%)	46,47,47	0.99	3 (6%)
5	EIC	C	1501	-	19,19,19	0.95	0	19,19,19	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	VCG	B	1503	-	42,42,42	2.57	6 (14%)	46,47,47	0.99	3 (6%)
3	NAG	C	1502	1	14,14,15	2.10	5 (35%)	17,19,21	6.79	3 (17%)
5	EIC	B	1501	-	19,19,19	0.95	0	19,19,19	0.60	0
3	NAG	A	1301	1	14,14,15	2.09	5 (35%)	17,19,21	6.80	3 (17%)
4	VCG	A	1302	-	42,42,42	2.58	6 (14%)	46,47,47	0.99	3 (6%)
5	EIC	A	1303	-	19,19,19	0.96	0	19,19,19	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1502	1	-	2/6/23/26	0/1/1/1
4	VCG	C	1503	-	-	21/41/53/53	0/1/1/1
5	EIC	C	1501	-	-	5/17/17/17	-
4	VCG	B	1503	-	-	21/41/53/53	0/1/1/1
3	NAG	C	1502	1	-	2/6/23/26	0/1/1/1
5	EIC	B	1501	-	-	5/17/17/17	-
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	VCG	A	1302	-	-	21/41/53/53	0/1/1/1
5	EIC	A	1303	-	-	5/17/17/17	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1302	VCG	C28-C27	-11.03	1.29	1.52
4	C	1503	VCG	C28-C27	-11.01	1.29	1.52
4	B	1503	VCG	C28-C27	-11.01	1.29	1.52
4	C	1503	VCG	O30-C26	-9.50	1.30	1.44
4	A	1302	VCG	O30-C26	-9.49	1.30	1.44
4	B	1503	VCG	O30-C26	-9.49	1.30	1.44
3	B	1502	NAG	C1-C2	5.57	1.59	1.52
3	C	1502	NAG	C1-C2	5.54	1.59	1.52
3	A	1301	NAG	C1-C2	5.51	1.59	1.52
4	A	1302	VCG	C26-C27	4.15	1.63	1.52
4	B	1503	VCG	C26-C27	4.15	1.63	1.52
4	C	1503	VCG	C26-C27	4.13	1.63	1.52
4	A	1302	VCG	O30-C29	3.83	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1503	VCG	O30-C29	3.82	1.53	1.42
4	C	1503	VCG	O30-C29	3.82	1.53	1.42
3	A	1301	NAG	O5-C5	3.24	1.49	1.43
3	C	1502	NAG	O5-C5	3.23	1.49	1.43
3	B	1502	NAG	O5-C5	3.21	1.49	1.43
4	C	1503	VCG	C28-C29	3.13	1.56	1.52
4	A	1302	VCG	C28-C29	3.12	1.56	1.52
4	B	1503	VCG	C28-C29	3.11	1.56	1.52
3	B	1502	NAG	O5-C1	2.50	1.47	1.43
3	C	1502	NAG	O5-C1	2.50	1.47	1.43
3	A	1301	NAG	O5-C1	2.49	1.47	1.43
4	C	1503	VCG	O20-C18	2.27	1.40	1.33
4	B	1503	VCG	O20-C18	2.26	1.39	1.33
4	A	1302	VCG	O20-C18	2.24	1.39	1.33
3	C	1502	NAG	C4-C5	2.08	1.57	1.53
3	C	1502	NAG	C3-C2	2.07	1.56	1.52
3	B	1502	NAG	C3-C2	2.06	1.56	1.52
3	B	1502	NAG	C4-C5	2.06	1.57	1.53
3	A	1301	NAG	C4-C5	2.05	1.57	1.53
3	A	1301	NAG	C3-C2	2.04	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	NAG	C2-N2-C7	27.21	159.36	122.90
3	C	1502	NAG	C2-N2-C7	27.19	159.34	122.90
3	B	1502	NAG	C2-N2-C7	27.15	159.28	122.90
3	B	1502	NAG	C8-C7-N2	4.82	124.12	116.12
3	C	1502	NAG	C8-C7-N2	4.80	124.07	116.12
3	A	1301	NAG	C8-C7-N2	4.79	124.05	116.12
4	C	1503	VCG	C29-O30-C26	-3.69	100.94	107.67
4	B	1503	VCG	C29-O30-C26	-3.68	100.95	107.67
4	A	1302	VCG	C29-O30-C26	-3.68	100.96	107.67
3	B	1502	NAG	O7-C7-N2	-3.03	116.62	121.98
3	C	1502	NAG	O7-C7-N2	-3.00	116.68	121.98
3	A	1301	NAG	O7-C7-N2	-3.00	116.69	121.98
4	B	1503	VCG	O20-C18-C17	2.59	119.74	111.83
4	A	1302	VCG	O20-C18-C17	2.59	119.72	111.83
4	C	1503	VCG	O20-C18-C17	2.58	119.69	111.83
4	A	1302	VCG	O30-C26-C25	2.57	112.89	108.29
4	B	1503	VCG	O30-C26-C25	2.56	112.87	108.29
4	C	1503	VCG	O30-C26-C25	2.56	112.86	108.29

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	VCG	C24-C25-C26-C27
4	A	1302	VCG	C28-C29-O31-C32
4	A	1302	VCG	O30-C29-O31-C32
4	A	1302	VCG	C33-C32-O31-C29
4	B	1503	VCG	C24-C25-C26-C27
4	B	1503	VCG	C28-C29-O31-C32
4	B	1503	VCG	O30-C29-O31-C32
4	B	1503	VCG	C33-C32-O31-C29
4	C	1503	VCG	C24-C25-C26-C27
4	C	1503	VCG	C28-C29-O31-C32
4	C	1503	VCG	O30-C29-O31-C32
4	C	1503	VCG	C33-C32-O31-C29
4	A	1302	VCG	C37-C36-O35-C27
4	B	1503	VCG	C37-C36-O35-C27
4	C	1503	VCG	C37-C36-O35-C27
4	A	1302	VCG	C17-C18-O20-C21
4	B	1503	VCG	C17-C18-O20-C21
4	C	1503	VCG	C17-C18-O20-C21
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	B	1502	NAG	C8-C7-N2-C2
3	B	1502	NAG	O7-C7-N2-C2
3	C	1502	NAG	C8-C7-N2-C2
3	C	1502	NAG	O7-C7-N2-C2
4	A	1302	VCG	O19-C18-O20-C21
4	B	1503	VCG	O19-C18-O20-C21
4	C	1503	VCG	O19-C18-O20-C21
4	B	1503	VCG	C21-C22-O23-C24
4	A	1302	VCG	C21-C22-O23-C24
4	C	1503	VCG	C21-C22-O23-C24
4	A	1302	VCG	C13-C14-C15-C16
4	B	1503	VCG	C13-C14-C15-C16
4	C	1503	VCG	C13-C14-C15-C16
4	C	1503	VCG	C14-C15-C16-C17
4	A	1302	VCG	C14-C15-C16-C17
4	B	1503	VCG	C14-C15-C16-C17
5	A	1303	EIC	C13-C14-C15-C16
5	B	1501	EIC	C13-C14-C15-C16
5	C	1501	EIC	C13-C14-C15-C16
4	A	1302	VCG	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
4	B	1503	VCG	C02-C03-C04-C05
4	C	1503	VCG	C02-C03-C04-C05
5	B	1501	EIC	C14-C15-C16-C17
5	C	1501	EIC	C14-C15-C16-C17
5	A	1303	EIC	C14-C15-C16-C17
4	B	1503	VCG	C15-C16-C17-C18
4	A	1302	VCG	C15-C16-C17-C18
4	C	1503	VCG	C15-C16-C17-C18
5	A	1303	EIC	C3-C4-C5-C6
5	B	1501	EIC	C3-C4-C5-C6
5	C	1501	EIC	C3-C4-C5-C6
5	A	1303	EIC	C1-C2-C3-C4
5	B	1501	EIC	C1-C2-C3-C4
5	C	1501	EIC	C1-C2-C3-C4
4	C	1503	VCG	C05-C06-C07-C08
4	B	1503	VCG	C05-C06-C07-C08
4	A	1302	VCG	C05-C06-C07-C08
4	A	1302	VCG	O39-C40-C41-O42
4	B	1503	VCG	O39-C40-C41-O42
4	C	1503	VCG	O39-C40-C41-O42
4	A	1302	VCG	C11-C12-C13-C14
4	C	1503	VCG	C11-C12-C13-C14
4	B	1503	VCG	C11-C12-C13-C14
5	A	1303	EIC	C12-C13-C14-C15
5	B	1501	EIC	C12-C13-C14-C15
5	C	1501	EIC	C12-C13-C14-C15
4	C	1503	VCG	O20-C21-C22-O23
4	A	1302	VCG	O20-C21-C22-O23
4	B	1503	VCG	O20-C21-C22-O23
4	A	1302	VCG	C12-C13-C14-C15
4	B	1503	VCG	C12-C13-C14-C15
4	C	1503	VCG	C12-C13-C14-C15
4	A	1302	VCG	C16-C17-C18-O20
4	B	1503	VCG	C16-C17-C18-O20
4	C	1503	VCG	C16-C17-C18-O20
4	A	1302	VCG	C25-C24-O23-C22
4	B	1503	VCG	C25-C24-O23-C22
4	C	1503	VCG	C25-C24-O23-C22
4	A	1302	VCG	C10-C11-C12-C13
4	B	1503	VCG	C10-C11-C12-C13
4	C	1503	VCG	C10-C11-C12-C13
4	B	1503	VCG	C01-C02-C03-C04

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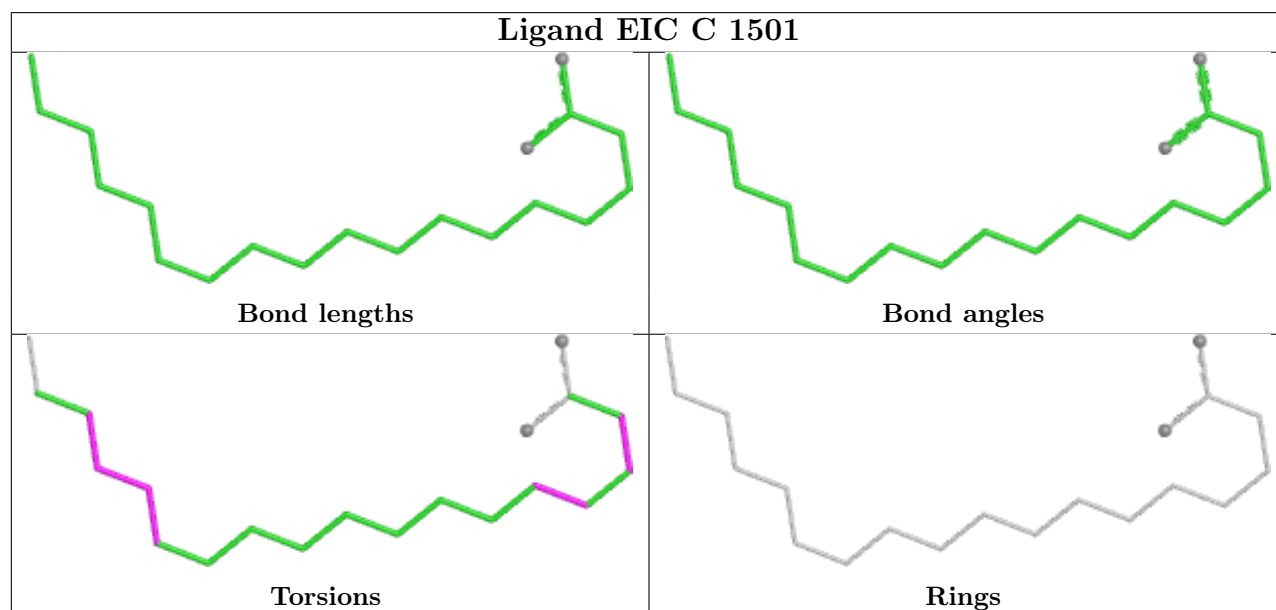
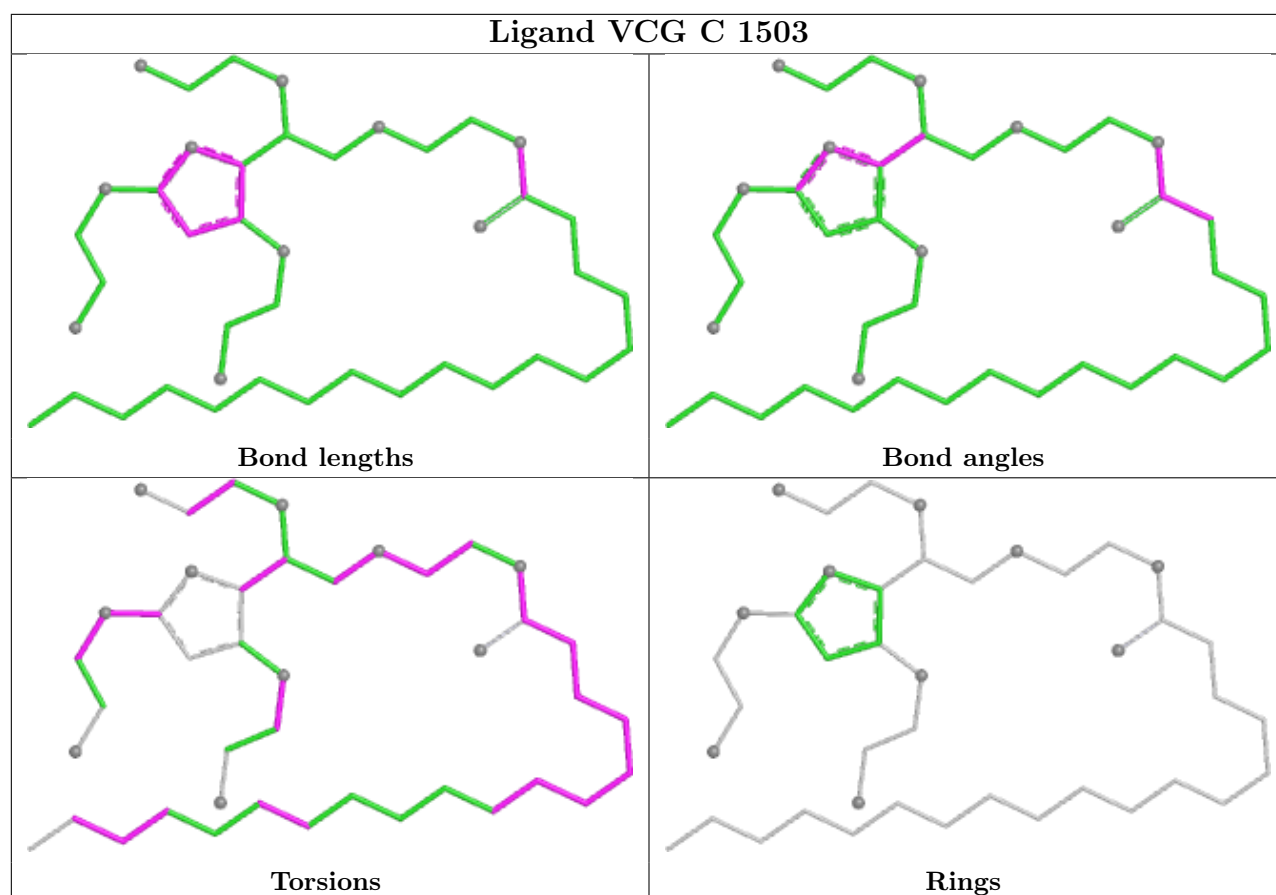
Mol	Chain	Res	Type	Atoms
4	C	1503	VCG	C01-C02-C03-C04
4	A	1302	VCG	C01-C02-C03-C04

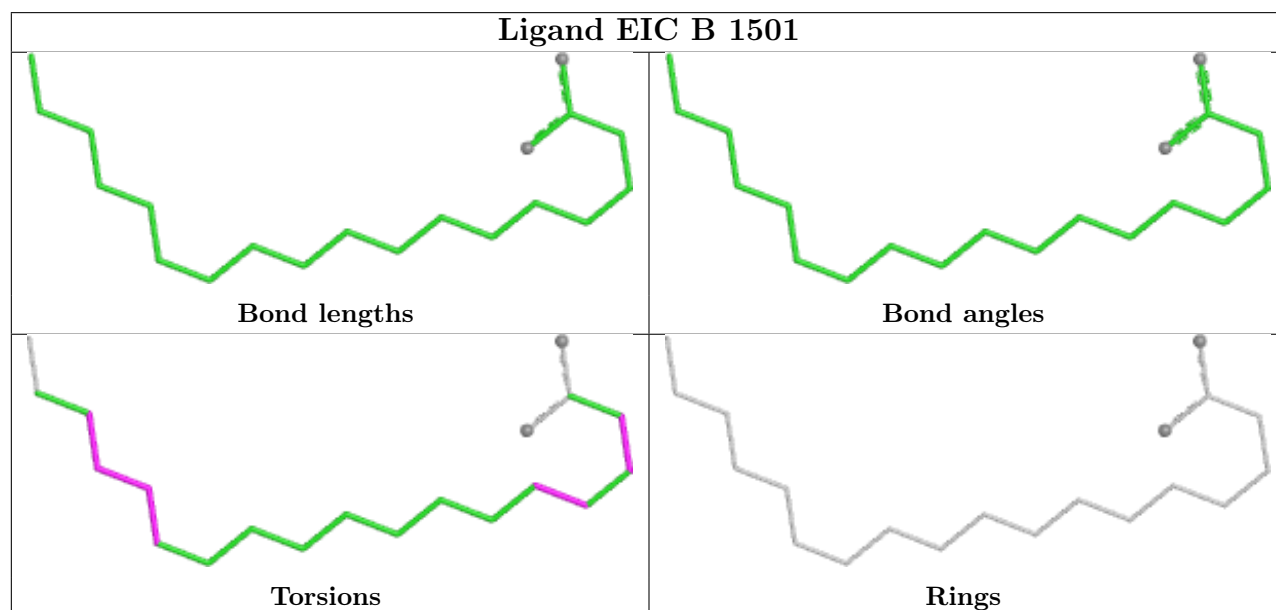
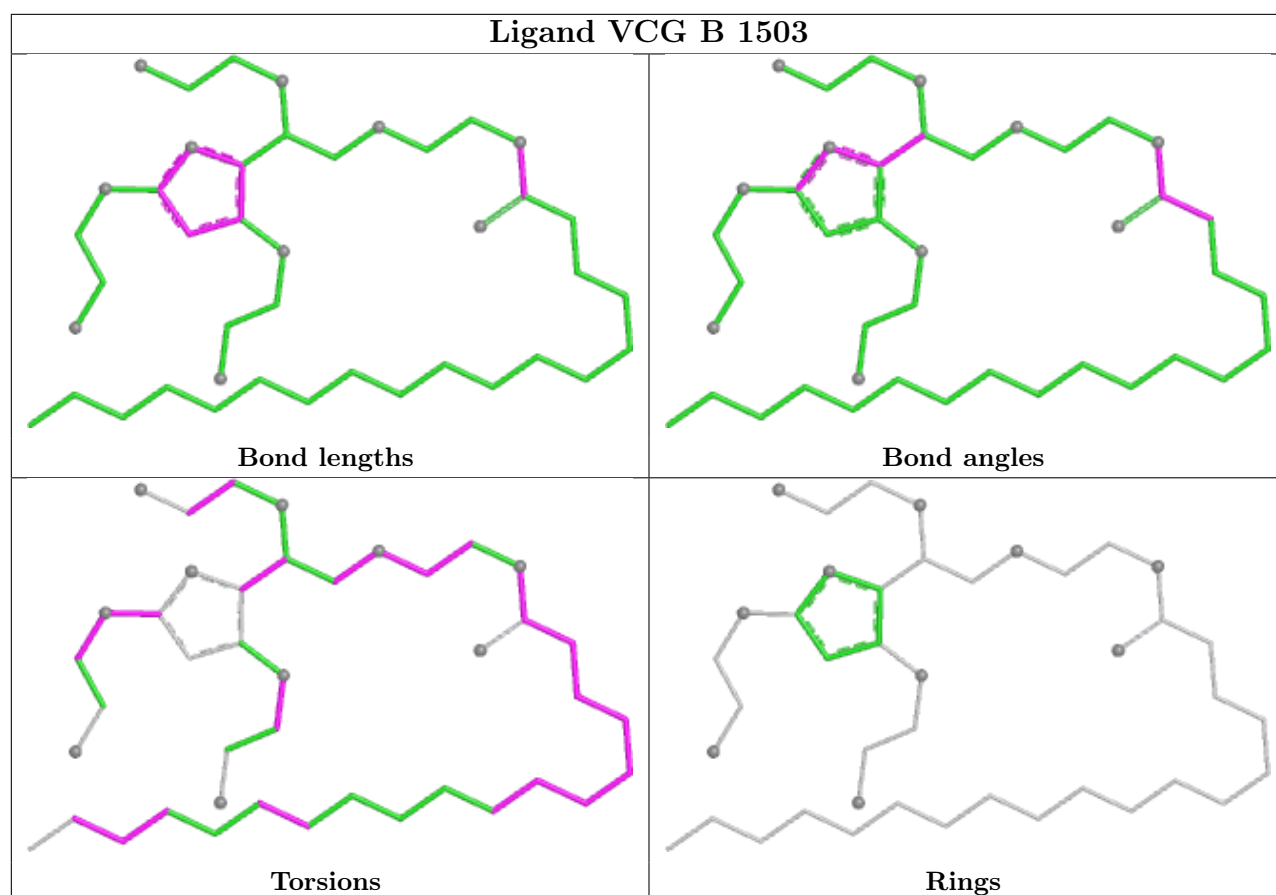
There are no ring outliers.

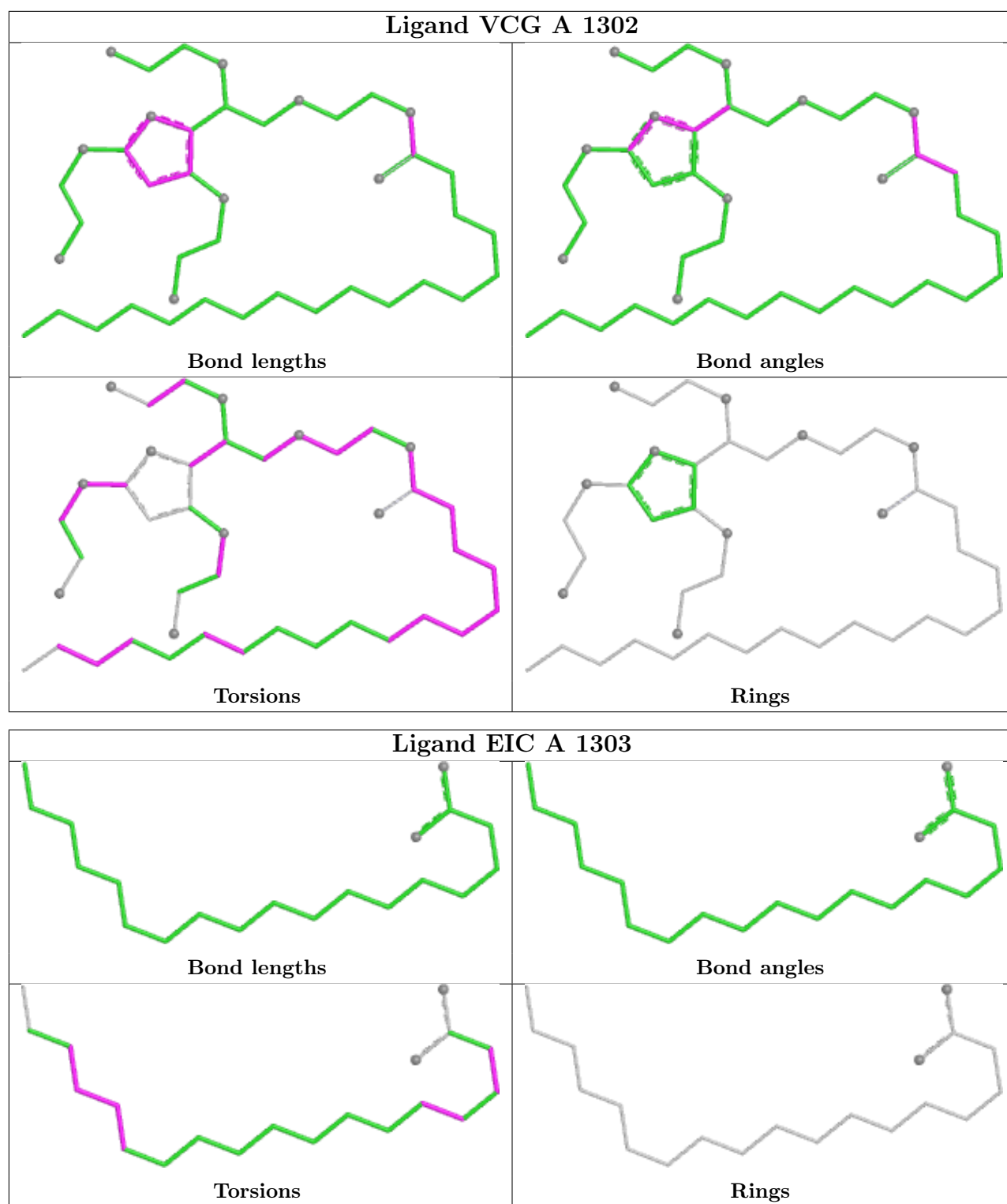
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1503	VCG	2	0
4	B	1503	VCG	2	0
4	A	1302	VCG	2	0

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

There are no chain breaks in this entry.

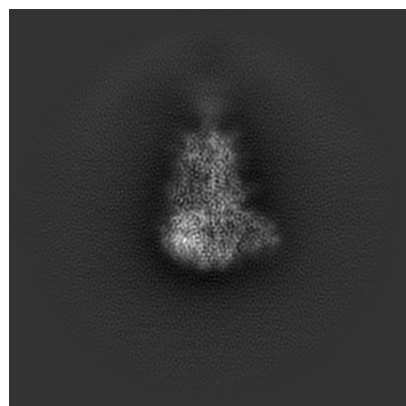
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22352. These allow visual inspection of the internal detail of the map and identification of artifacts.

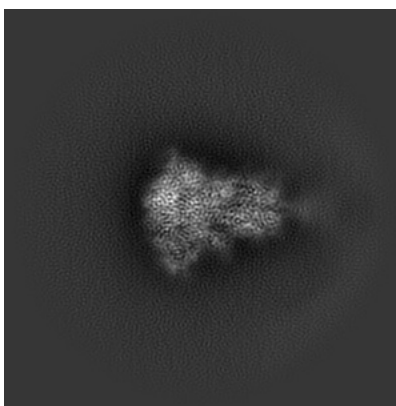
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

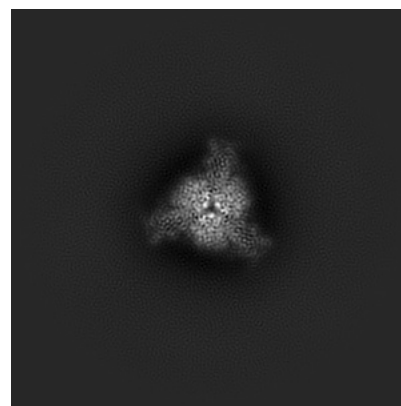
6.1.1 Primary map



X

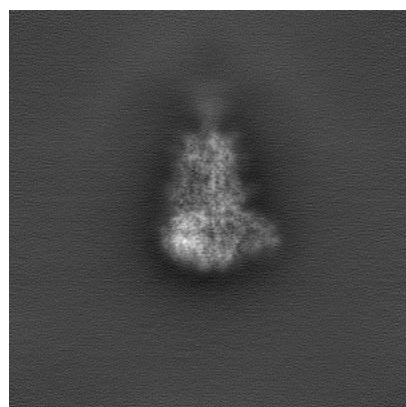


Y

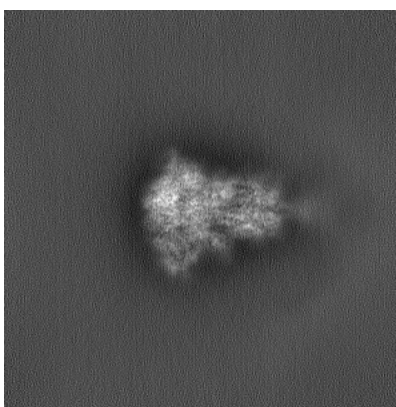


Z

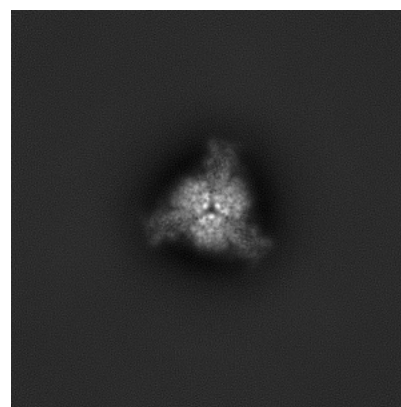
6.1.2 Raw map



X



Y

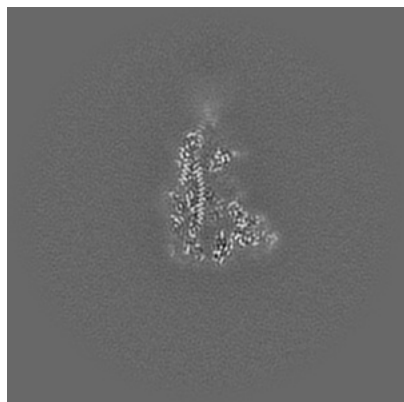


Z

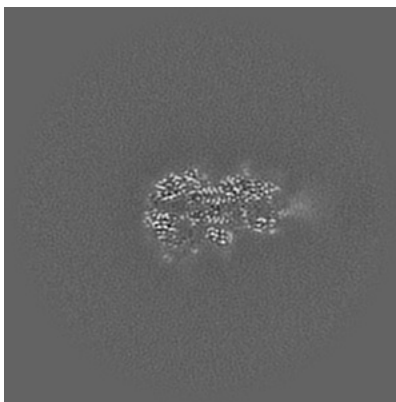
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

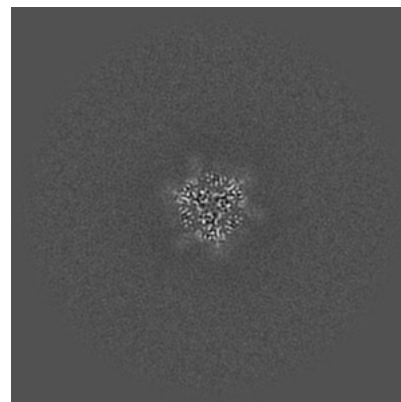
6.2.1 Primary map



X Index: 190

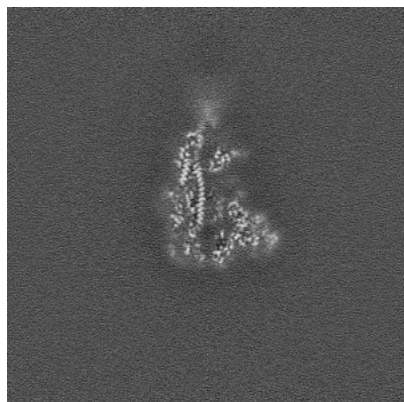


Y Index: 190

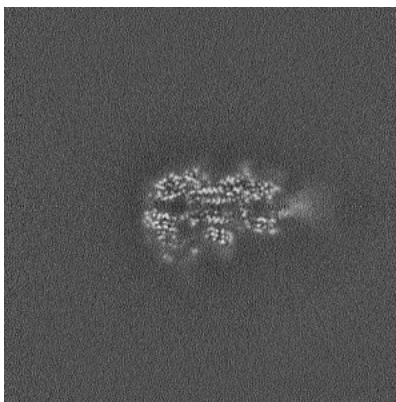


Z Index: 190

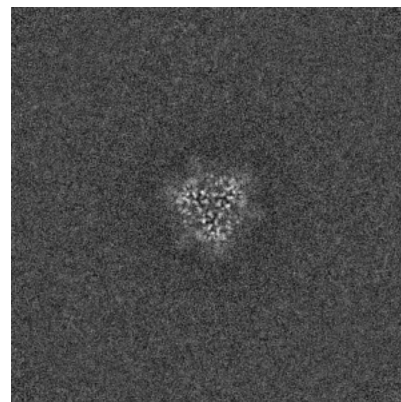
6.2.2 Raw map



X Index: 190



Y Index: 190

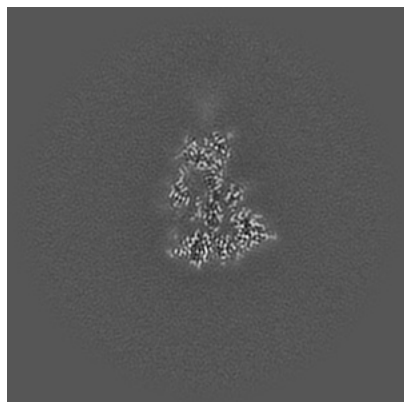


Z Index: 190

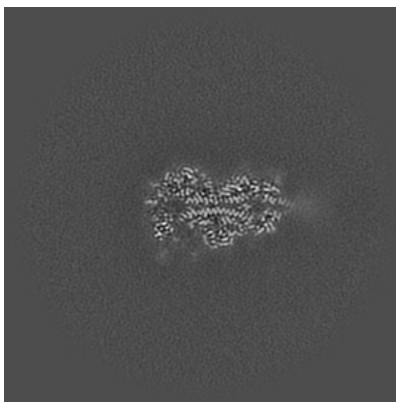
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

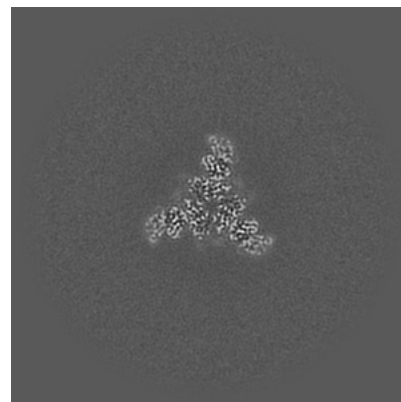
6.3.1 Primary map



X Index: 200

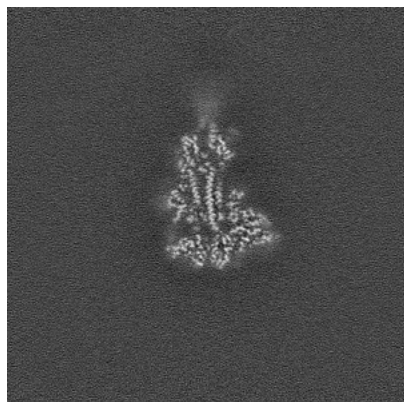


Y Index: 194

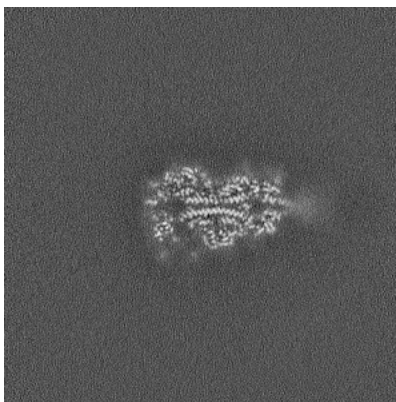


Z Index: 159

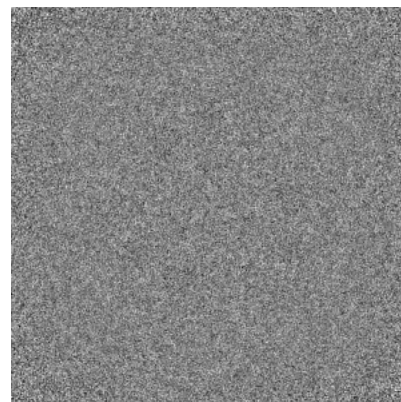
6.3.2 Raw map



X Index: 196



Y Index: 194

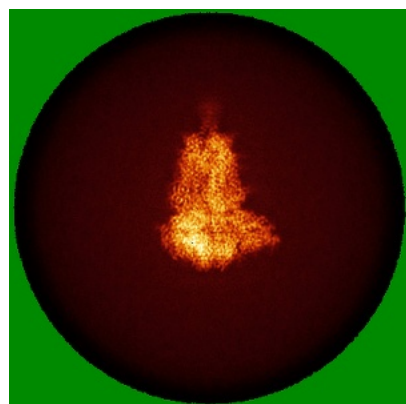


Z Index: 0

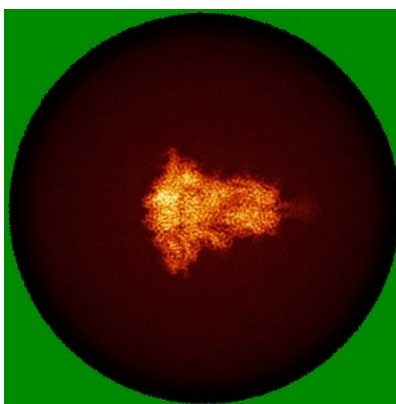
The images above show the largest variance slices of the map in three orthogonal directions.

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

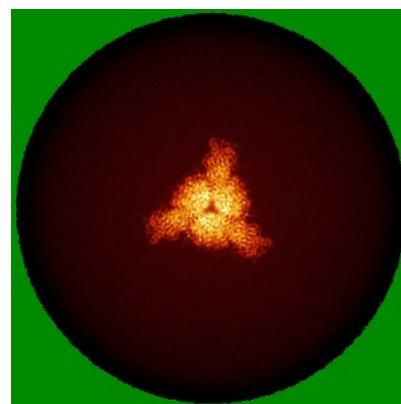
6.4.1 Primary map



X

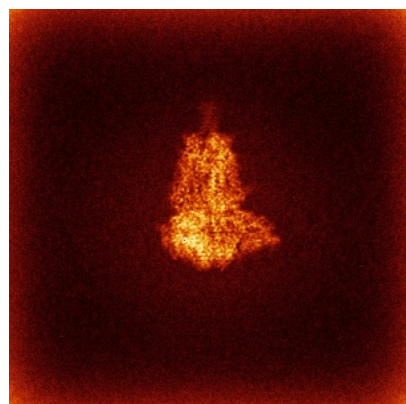


Y

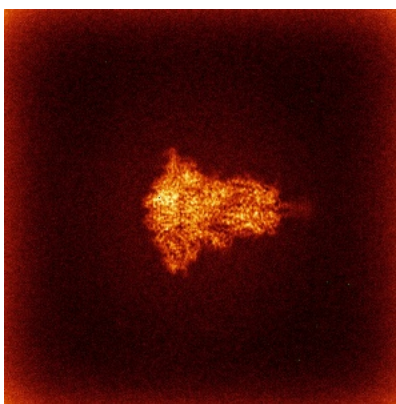


Z

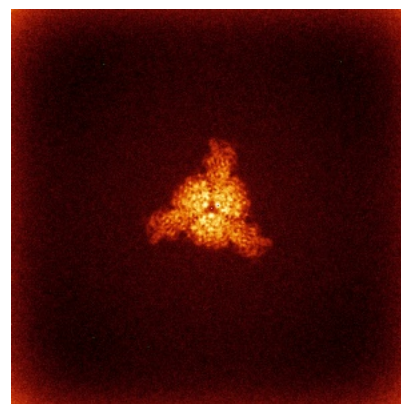
6.4.2 Raw map



X



Y

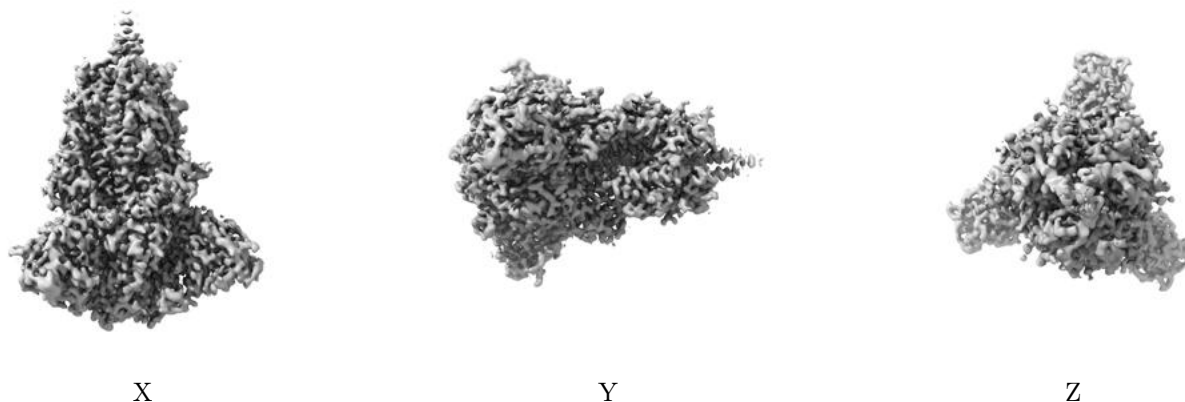


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

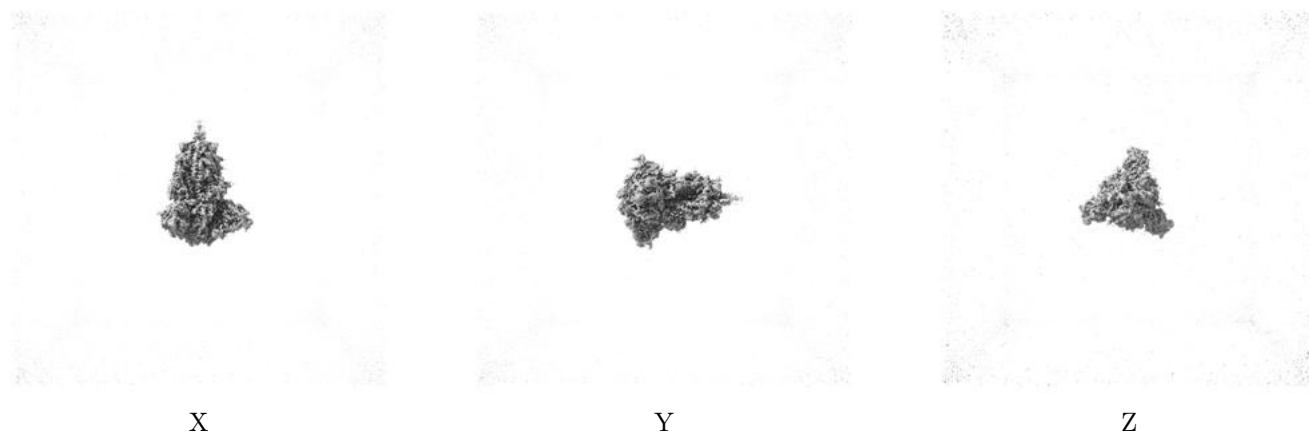
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

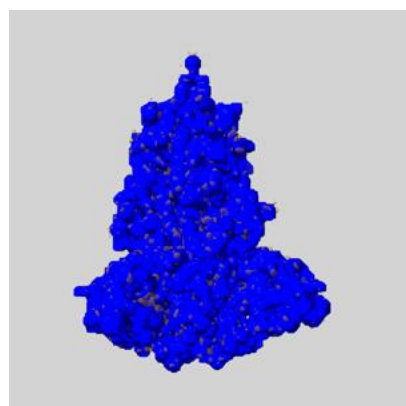
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

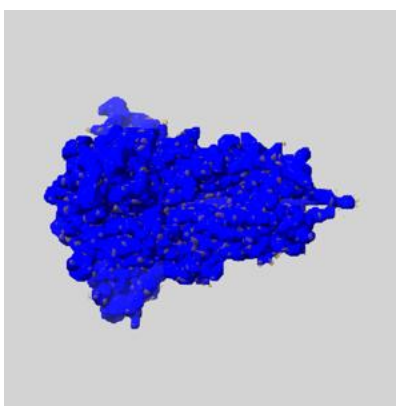
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

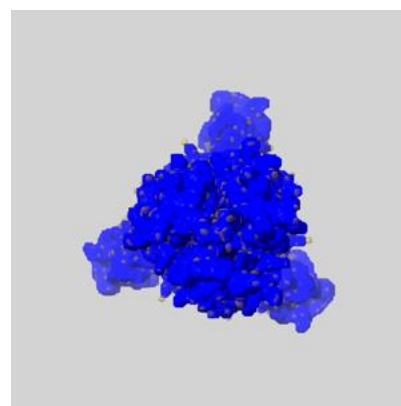
6.6.1 emd_22352_msk_1.map [i](#)



X



Y

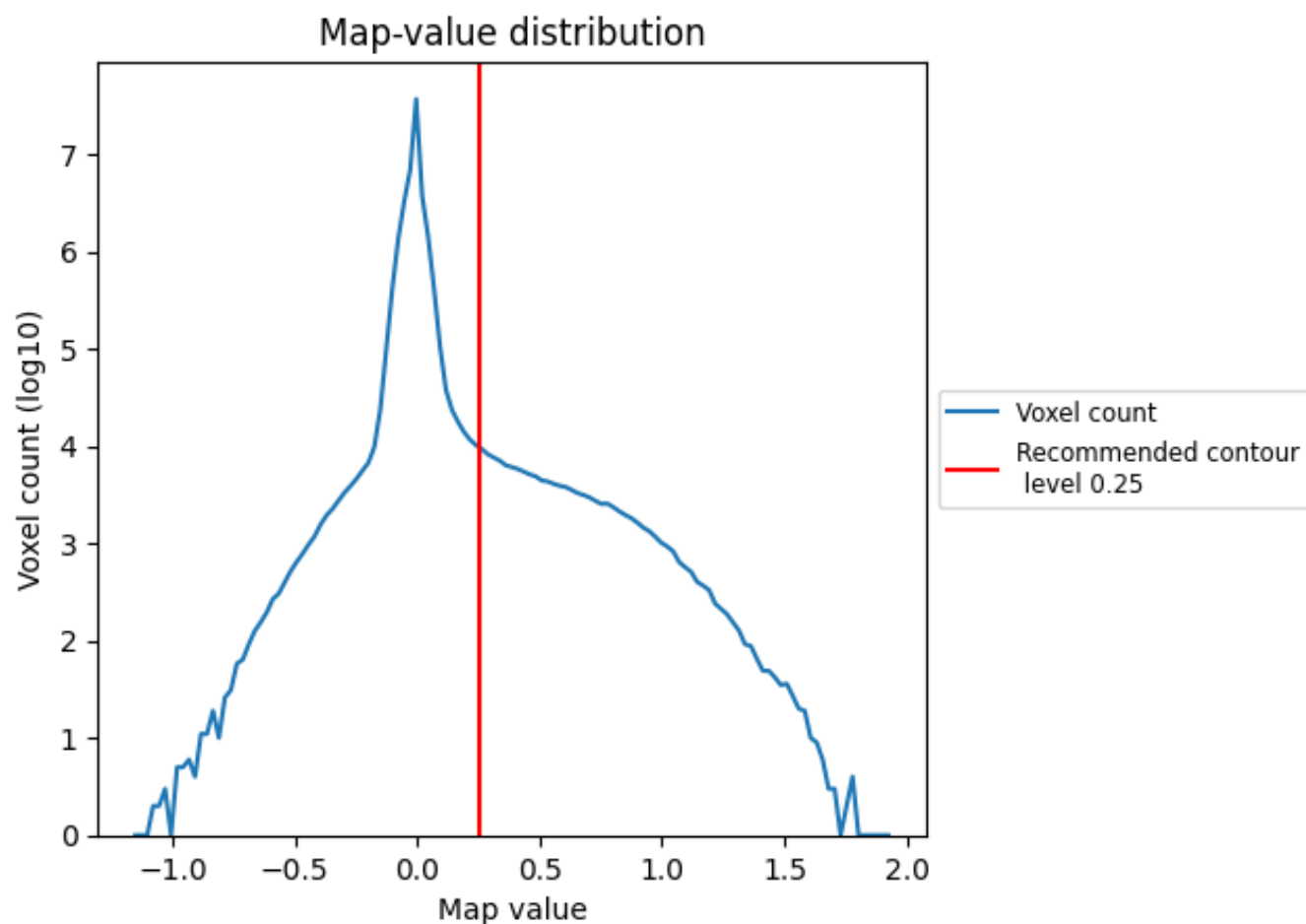


Z

7 Map analysis [i](#)

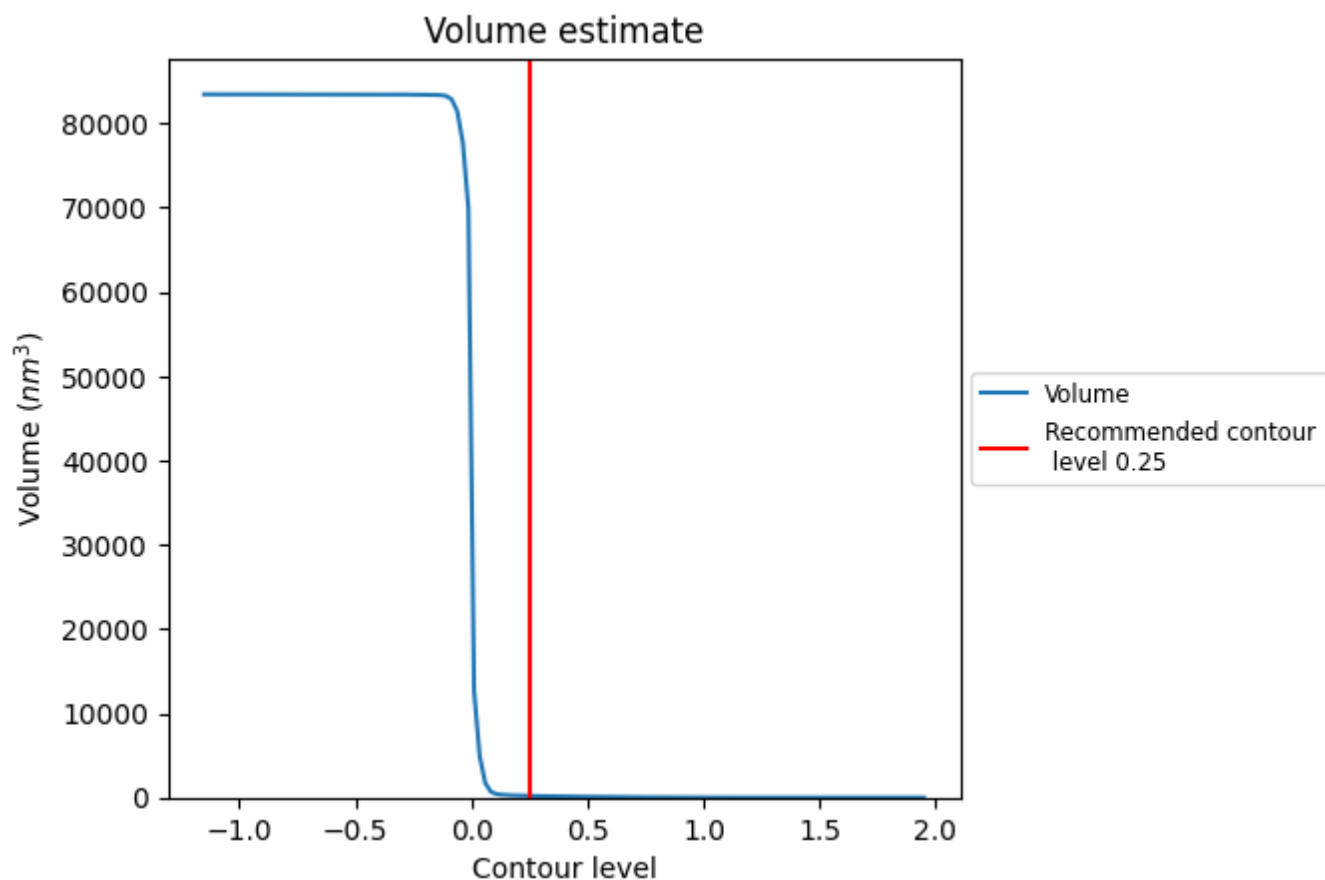
This section contains the results of statistical analysis of the map.

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.

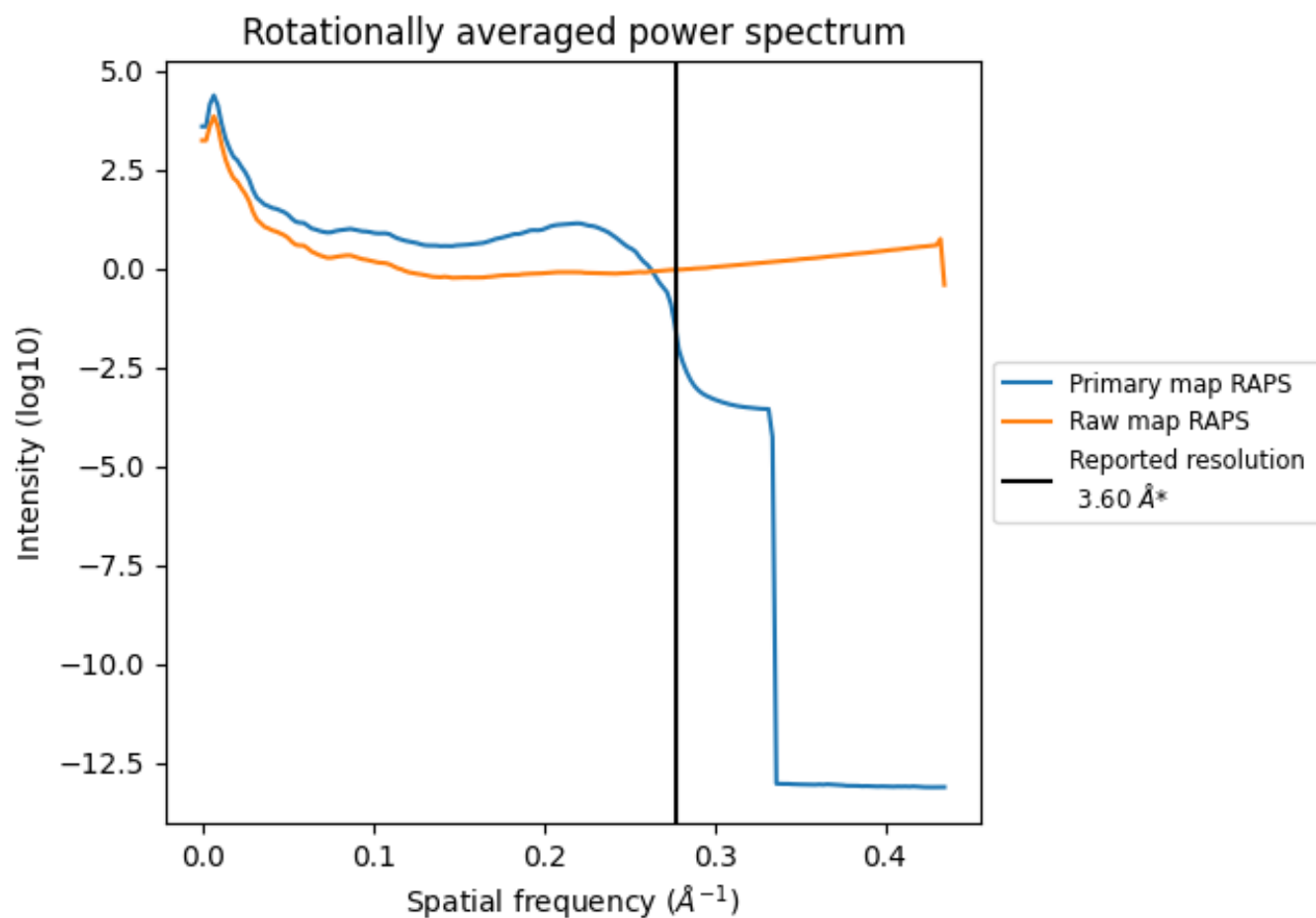
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm³; this corresponds to an approximate mass of 184 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 ⓘ

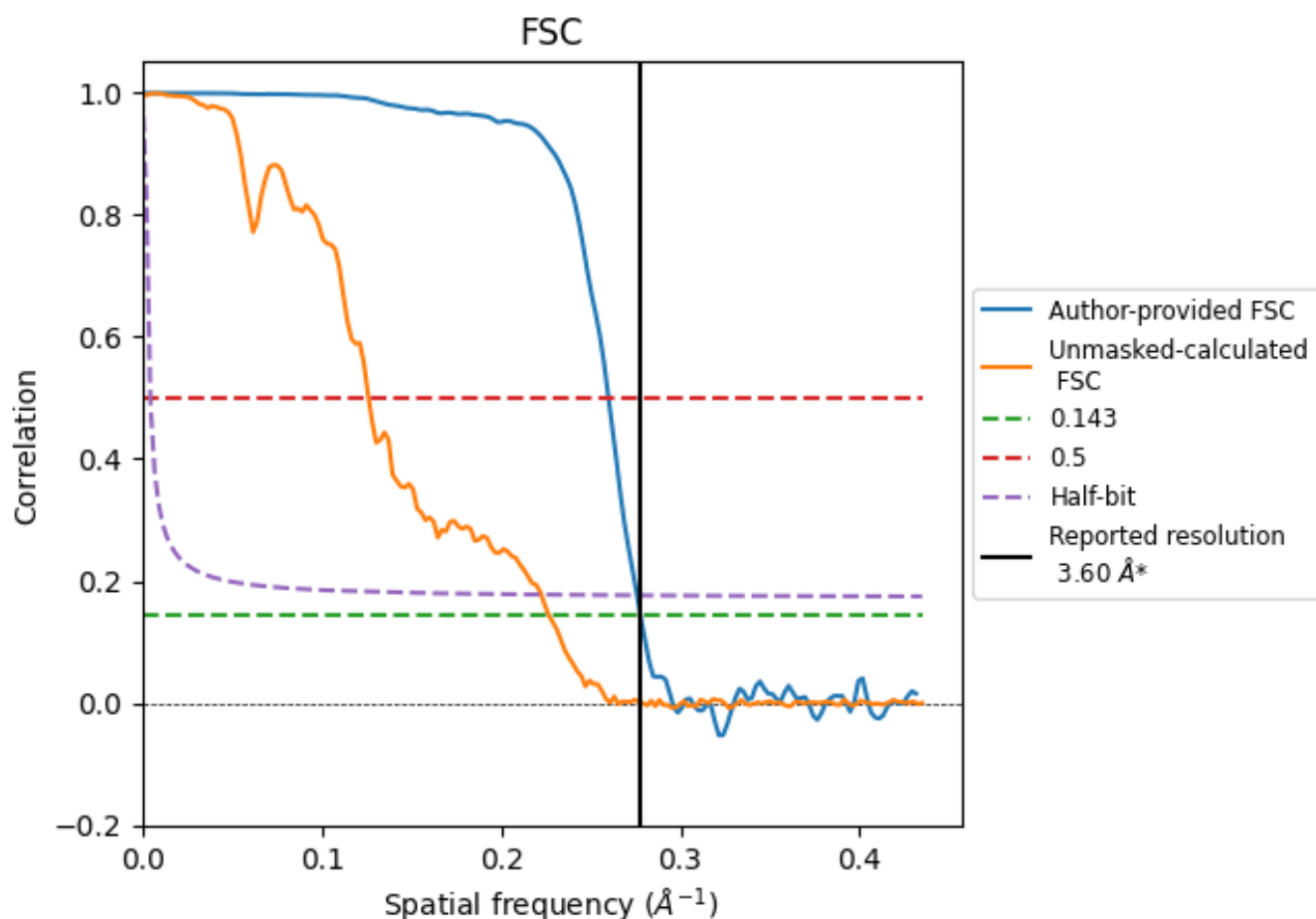


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

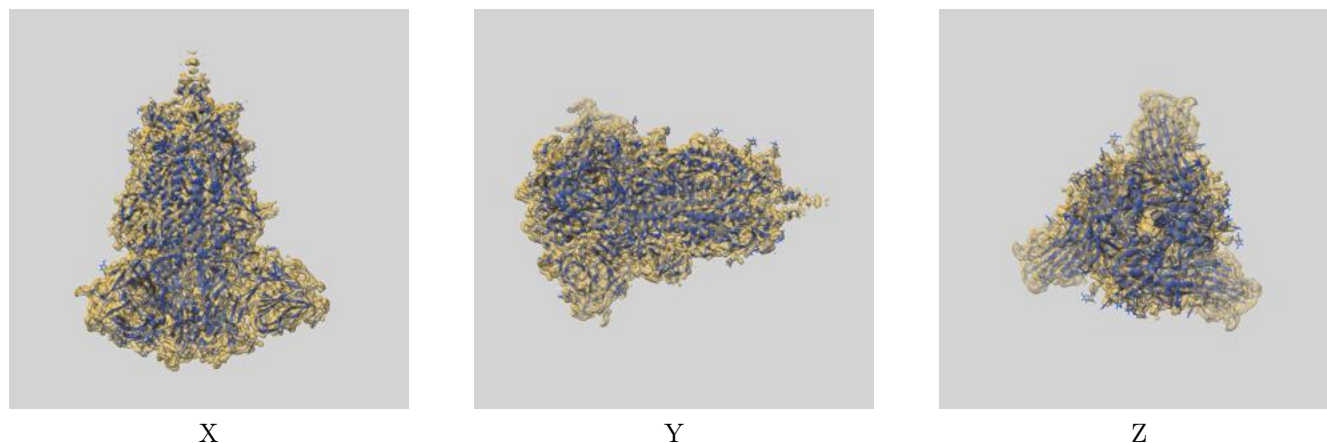
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	3.85	3.62
Unmasked-calculated*	4.41	7.92	4.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.41 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22352 and PDB model 7JJI. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



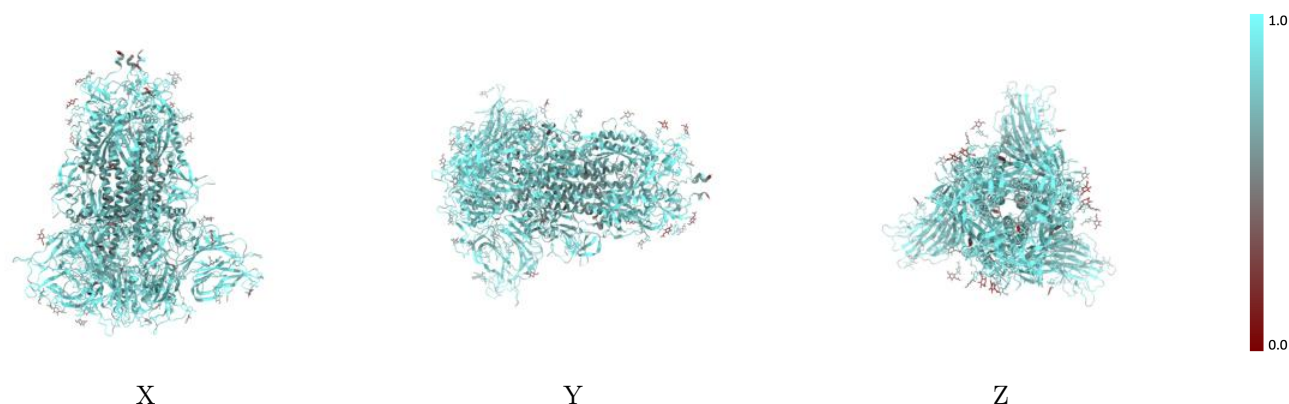
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



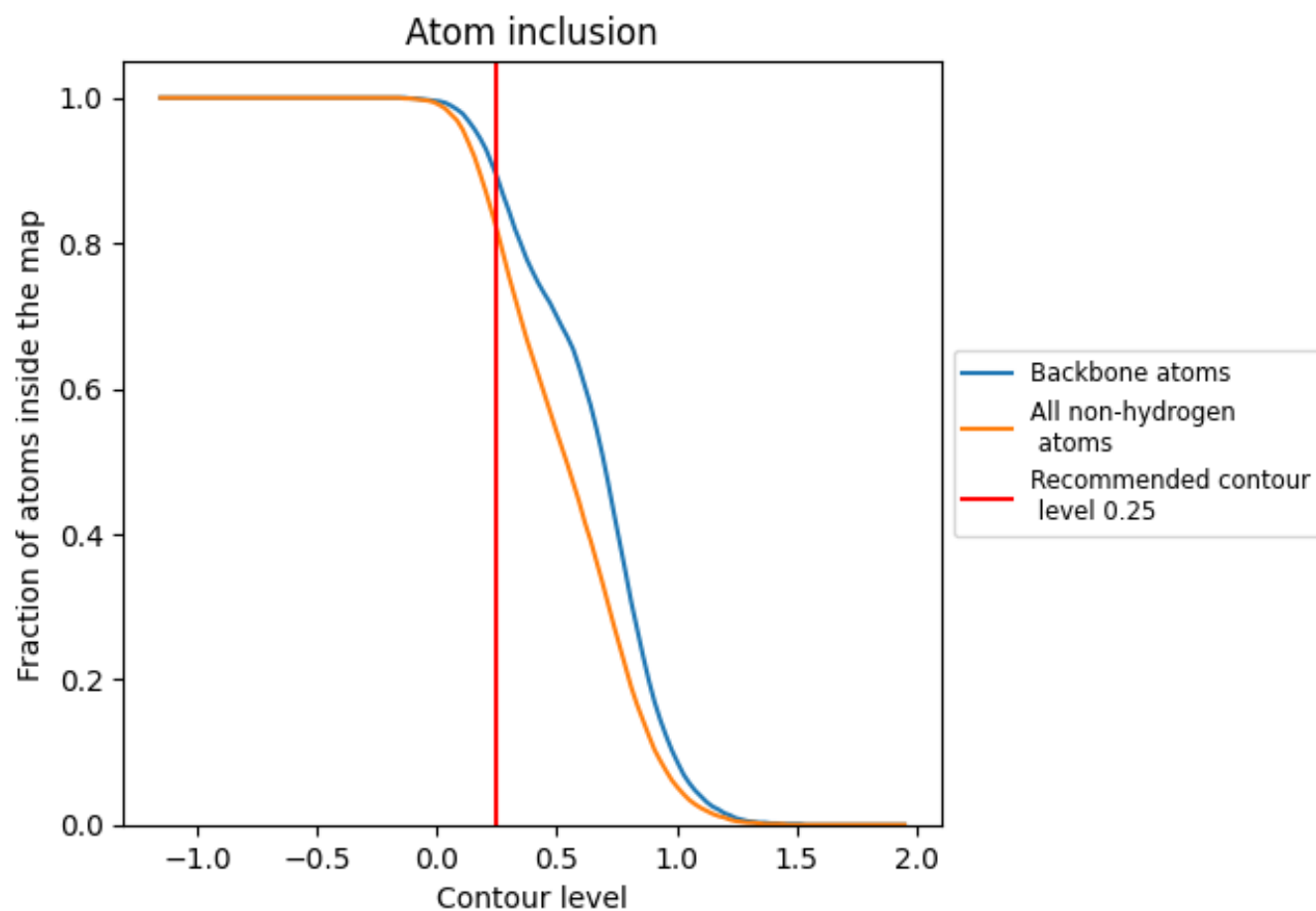
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.4690
A	 0.8270	 0.4730
B	 0.8280	 0.4720
C	 0.8290	 0.4720
D	 0.5710	 0.3300
E	 0.6790	 0.4360
F	 0.6430	 0.4760
G	 0.3930	 0.3550
H	 0.6790	 0.4420
I	 0.5710	 0.3240
J	 0.6430	 0.3790
K	 0.7140	 0.4270
L	 0.5360	 0.3890
M	 0.8210	 0.4760
N	 0.6790	 0.3880
O	 0.3930	 0.3130
P	 0.6790	 0.4360
Q	 0.7140	 0.4210
R	 0.5710	 0.4100
S	 0.5360	 0.3110
T	 0.6790	 0.4280
U	 0.6430	 0.4670
V	 0.3930	 0.3530
W	 0.6790	 0.4220
X	 0.5710	 0.3220
Y	 0.6430	 0.3840
Z	 0.7140	 0.4170
a	 0.5360	 0.3910
b	 0.8210	 0.4840
c	 0.6790	 0.3910
d	 0.4290	 0.3100
e	 0.6790	 0.4470
f	 0.7140	 0.4100
g	 0.6070	 0.4300
h	 0.5360	 0.3160



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Chain	Atom inclusion	Q-score
i	 0.6430	 0.4380
j	 0.6430	 0.4600
k	 0.3930	 0.3570
l	 0.6790	 0.4410
m	 0.5710	 0.3320
n	 0.6430	 0.3900
o	 0.7140	 0.4230
p	 0.5360	 0.3850
q	 0.8210	 0.4790
r	 0.6790	 0.3920
s	 0.4290	 0.3230
t	 0.6790	 0.4250
u	 0.7140	 0.4310
v	 0.5710	 0.4070