



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:32 PM UTC

PDB ID : 7CN8 / pdb_00007cn8
EMDB ID : EMD-30418
Title : Cryo-EM structure of PCoV_GX spike glycoprotein
Authors : Wang, X.; Yu, J.; Zhang, S.; Qiao, S.; Zeng, J.; Tian, L.
Deposited on : 2020-07-30
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

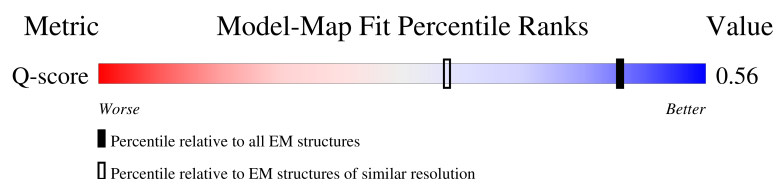
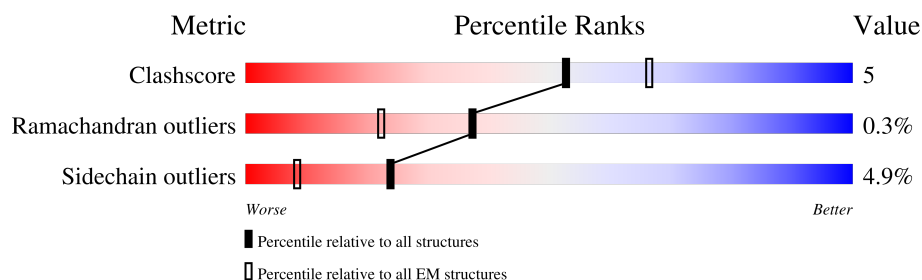
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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.



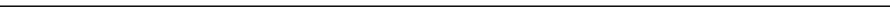
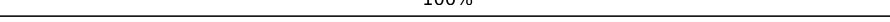
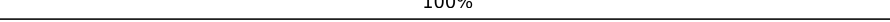
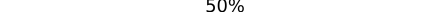
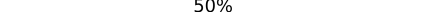
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	1295	
1	B	1295	
1	C	1295	
2	D	2	

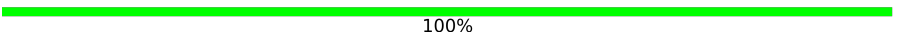
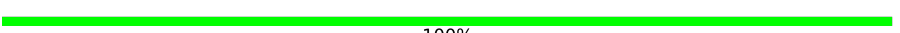
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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%
2	I	2	 50%  50%
2	J	2	 50%  50%
2	K	2	 50%  50%
2	L	2	 50%  50%
2	M	2	 50%  50%
2	N	2	 50%  50%
2	O	2	 100%
2	P	2	 100%
2	Q	2	 100%
2	R	2	 100%
2	S	2	 50%  50%
2	T	2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

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Mol	Chain	Length	Quality of chain
2	f	2	 50%50%
2	g	2	 100%
2	h	2	 50%50%
2	i	2	 50%50%
2	k	2	 50%50%
2	l	2	 100%
2	m	2	 50%50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EIC	A	1310	-	-	X	-
4	EIC	B	1310	-	-	X	-
4	EIC	C	1310	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27675 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 Glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1125	Total	C	N	O	S	0	0
			8771	5596	1466	1668	41		
1	B	1125	Total	C	N	O	S	0	0
			8771	5596	1466	1668	41		
1	C	1125	Total	C	N	O	S	0	0
			8771	5596	1466	1668	41		

- 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	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	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	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	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	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	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	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	k	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	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	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	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	m	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	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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



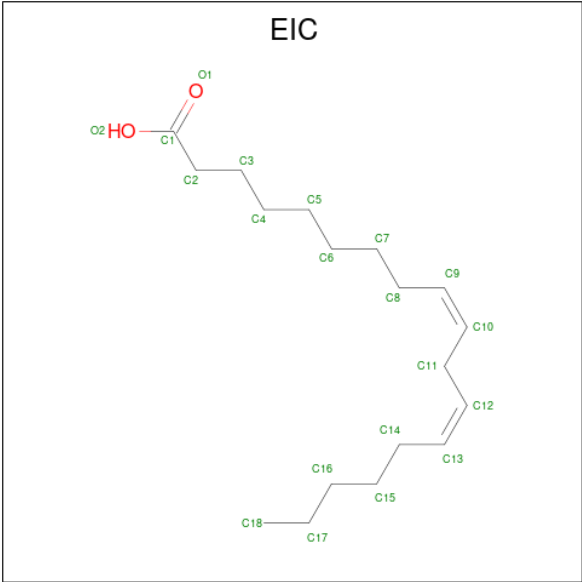
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	

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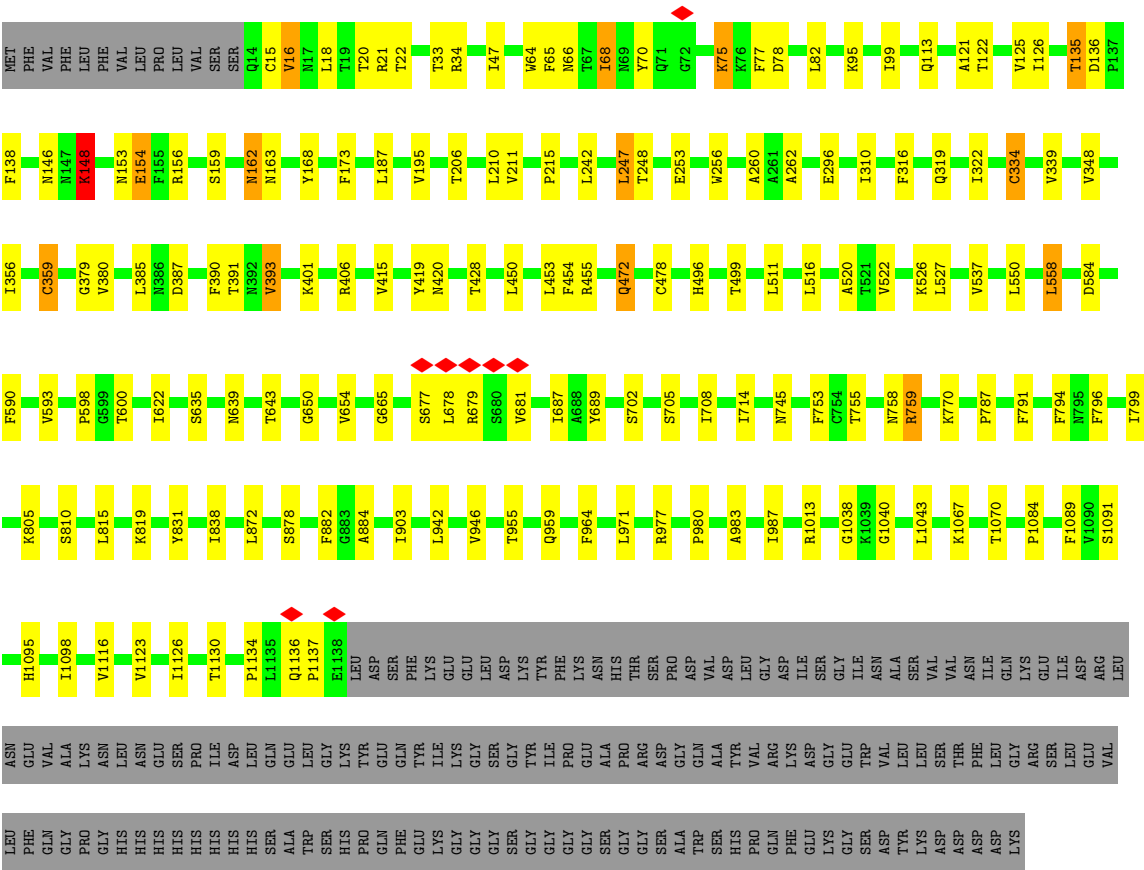
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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C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

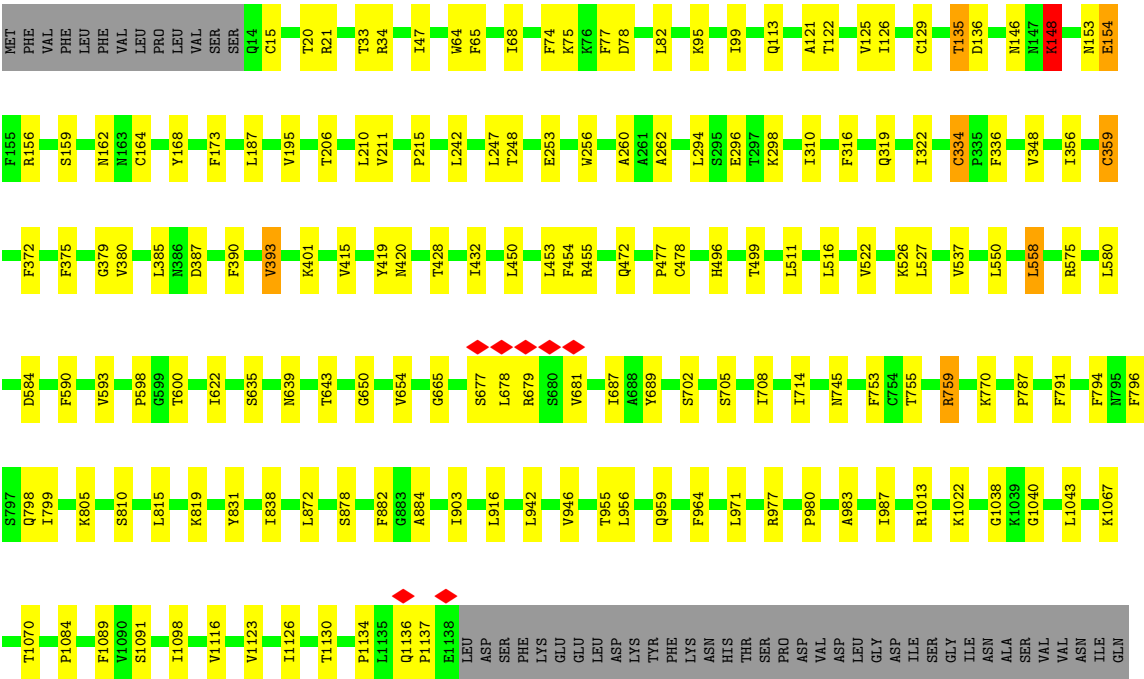
- Molecule 4 is LINOLEIC ACID (CCD ID: EIC) (formula: C₁₈H₃₂O₂).



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



● Molecule 1: Glycoprotein



LYS
GLU
ILE
SER
ASP
ARG
LEU
ASN
GLU
VAL
ALA
LYS
ASN
LEU
ASN
GLU
SER
PRO
ILE
ASP
LEU
GLN
GLU
LEU
GLY
LYS
TYR
GLU
GLN
TYR
ILE
LYS
GLY
SER
GLY
TYR
ILE
PRO
GLU
ALA
PRO
GLY
ARG
ASP
GLY
GLN
ALA
TYR
VAL
ARG
LYS
ASP
GLY
GLU
TRP
VAL
LEU
SER
THR
PHE
LEU

GLY
ARG
SER
LEU
GLU
VAL
LEU
PHE
GLN
GLY
PRO
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS
SER
ALA
TRP
SER
HIS
PRO
PHE
GLN
GLU
LYS
GLY
GLY
SER
GLY
GLY
GLY
GLY
SER
GLY
GLY
GLY
ALA
SER
ALA
TRP
SER
HIS
PRO
VAL
GLN
PHE
GLY
LYS
GLY
SER
ASP
VAL
TYR
LYS
ASP
ASP
PHE
LEU

LYS

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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain J:  50%  50%

MAG1
MAG2

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

Chain L:  50%  50%

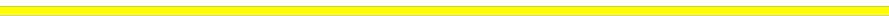
MAG1
MAG2

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

Chain M:  50%  50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2

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

Chain S:  50% 50%

MAG1
MAG2

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

Chain T:  100%

MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2

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

Chain W:  50% 50%

MAG1
MAG2

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

Chain X:  50% 50%

MAG1
MAG2

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

Chain a:  100%

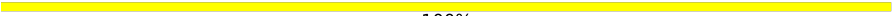
MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain e:  100%

MAG1
MAG2

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

Chain f:  50%  50%

MAG1
MAG2

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

Chain g:  100%

MAG1
MAG2

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

Chain h:  50%  50%

MAG1
MAG2

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

Chain i:  50%  50%



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

Chain k:  50% 50%



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

Chain D:  50% 50%



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

Chain G:  100%



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

Chain H:  100%



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

Chain I:  50% 50%



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

Chain K:  50% 50%



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

Chain I:  100%

MAG1
MAG2

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

Chain N:  50%  50%

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 R:  100%

MAG1
MAG2

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

Chain m:  50%  50%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain Z: 

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	263901	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0077	Depositor
Map size ($\text{\AA}$)	320.41998, 320.41998, 320.41998	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.98	1/8975 (0.0%)	1.18	7/12223 (0.1%)
1	B	0.99	1/8975 (0.0%)	1.18	7/12223 (0.1%)
1	C	0.99	1/8975 (0.0%)	1.19	9/12223 (0.1%)
All	All	0.99	3/26925 (0.0%)	1.18	23/36669 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	THR	N-CA	5.28	1.50	1.46
1	A	248	THR	N-CA	5.18	1.50	1.46
1	C	248	THR	N-CA	5.16	1.50	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	THR	CB-CA-C	8.76	117.42	111.20
1	A	248	THR	CB-CA-C	8.76	117.42	111.20
1	C	248	THR	CB-CA-C	8.73	117.40	111.20
1	C	980	PRO	N-CA-C	7.26	119.56	110.70
1	A	980	PRO	N-CA-C	7.23	119.53	110.70
1	B	980	PRO	N-CA-C	7.23	119.53	110.70
1	B	665	GLY	CA-C-O	-7.07	117.63	122.22
1	A	665	GLY	CA-C-O	-7.01	117.66	122.22
1	C	665	GLY	CA-C-O	-6.96	117.69	122.22
1	A	787	PRO	N-CA-C	-6.62	100.81	111.14
1	C	787	PRO	N-CA-C	-6.61	100.83	111.14
1	B	787	PRO	N-CA-C	-6.60	100.85	111.14
1	C	1038	GLY	CA-C-O	-6.12	118.24	122.22
1	A	1038	GLY	CA-C-O	-6.06	118.28	122.22
1	B	1038	GLY	CA-C-O	-6.05	118.28	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	745	ASN	N-CA-C	-5.89	104.94	111.36
1	A	745	ASN	N-CA-C	-5.89	104.94	111.36
1	C	745	ASN	N-CA-C	-5.86	104.97	111.36
1	C	478	CYS	CA-CB-SG	-5.72	101.23	114.40
1	B	598	PRO	N-CA-C	-5.42	103.64	111.22
1	A	598	PRO	N-CA-C	-5.41	103.64	111.22
1	C	598	PRO	N-CA-C	-5.41	103.64	111.22
1	C	477	PRO	N-CA-CB	5.09	107.73	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8771	0	8571	99	0
1	B	8771	0	8571	96	0
1	C	8771	0	8571	93	0
2	D	28	0	25	2	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	2	0
2	H	28	0	25	2	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	1	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	5	0
2	O	28	0	25	1	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	7	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
2	Z	28	0	25	1	0
2	a	28	0	25	0	0
2	b	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	k	28	0	25	1	0
2	l	28	0	25	0	0
2	m	28	0	25	3	0
3	A	126	0	117	1	0
3	B	126	0	117	1	0
3	C	126	0	117	1	0
4	A	20	0	31	27	0
4	B	20	0	31	18	0
4	C	20	0	31	24	0
All	All	27675	0	26982	289	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 5.

All (289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:PHE:CE2	4:A:1310:EIC:H121	1.29	1.64
1:C:375:PHE:CE1	4:C:1310:EIC:H52	1.62	1.34
1:A:390:PHE:CE2	4:A:1310:EIC:C12	2.12	1.33
1:B:393:VAL:HG21	4:B:1310:EIC:H142	1.24	1.18
1:A:838:ILE:HG21	1:C:584:ASP:OD2	1.41	1.18
1:A:584:ASP:OD2	1:B:838:ILE:HG21	1.41	1.17
1:C:393:VAL:CG2	4:C:1310:EIC:H142	1.77	1.15
1:B:584:ASP:OD2	1:C:838:ILE:HG21	1.42	1.14
1:C:393:VAL:HG21	4:C:1310:EIC:C14	1.79	1.11
1:A:385:LEU:HD13	4:A:1310:EIC:H81	1.32	1.08
1:A:390:PHE:CZ	4:A:1310:EIC:H121	1.92	1.05
1:C:511:LEU:HD13	4:C:1310:EIC:H1O1	1.36	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:VAL:HG21	4:A:1310:EIC:H142	1.35	1.05
1:A:356:ILE:CD1	4:A:1310:EIC:H183	1.89	1.03
1:A:356:ILE:HD13	4:A:1310:EIC:H183	1.42	1.01
1:B:406:ARG:NH2	4:C:1310:EIC:O2	1.97	0.98
1:B:385:LEU:HD13	4:B:1310:EIC:H81	1.47	0.97
1:A:390:PHE:CD2	4:A:1310:EIC:C12	2.49	0.95
1:C:375:PHE:CE1	4:C:1310:EIC:C5	2.52	0.93
1:A:390:PHE:CD2	4:A:1310:EIC:H121	2.01	0.93
1:A:334:CYS:SG	4:A:1310:EIC:H171	2.08	0.92
1:A:584:ASP:CG	1:B:838:ILE:HG21	1.95	0.92
1:C:375:PHE:CZ	4:C:1310:EIC:H52	2.05	0.92
1:A:838:ILE:HG21	1:C:584:ASP:CG	1.95	0.91
1:B:584:ASP:CG	1:C:838:ILE:HG21	1.95	0.90
1:C:393:VAL:HG21	4:C:1310:EIC:H142	0.91	0.89
1:B:1095:HIS:ND1	2:R:1:NAG:H5	1.88	0.89
1:B:393:VAL:HG21	4:B:1310:EIC:C14	2.02	0.89
1:A:15:CYS:HB3	1:A:156:ARG:HB2	1.53	0.88
1:C:375:PHE:HE1	4:C:1310:EIC:H52	1.38	0.88
1:C:15:CYS:HB3	1:C:156:ARG:HB2	1.56	0.87
1:B:15:CYS:HB3	1:B:156:ARG:HB2	1.55	0.86
1:C:432:ILE:HD13	4:C:1310:EIC:H51	1.58	0.85
1:C:511:LEU:CD1	4:C:1310:EIC:H1O1	2.07	0.85
1:A:390:PHE:CD2	4:A:1310:EIC:C13	2.58	0.85
1:C:135:THR:HG21	2:U:1:NAG:H5	1.56	0.85
1:B:390:PHE:CD2	4:B:1310:EIC:H121	2.12	0.84
1:C:372:PHE:HD2	4:C:1310:EIC:H22	1.43	0.82
1:A:361:ALA:HB1	4:A:1310:EIC:C11	2.12	0.78
1:C:372:PHE:CD2	4:C:1310:EIC:H22	2.19	0.78
1:A:361:ALA:HB1	4:A:1310:EIC:H111	1.64	0.78
1:B:393:VAL:CG2	4:B:1310:EIC:H142	2.09	0.77
1:A:584:ASP:OD2	1:B:838:ILE:CG2	2.29	0.76
1:A:356:ILE:HD13	4:A:1310:EIC:C18	2.14	0.76
1:B:522:VAL:HG11	4:B:1310:EIC:H131	1.67	0.76
1:B:584:ASP:OD2	1:C:838:ILE:CG2	2.29	0.75
1:A:838:ILE:CG2	1:C:584:ASP:OD2	2.28	0.74
1:A:522:VAL:HG11	4:A:1310:EIC:H131	1.68	0.74
1:B:339:VAL:HG21	4:B:1310:EIC:H183	1.71	0.73
2:Y:2:NAG:O7	2:Y:2:NAG:O3	2.06	0.73
1:B:511:LEU:HD13	4:B:1310:EIC:H1O1	1.70	0.72
2:K:2:NAG:O7	2:K:2:NAG:O3	2.07	0.71
1:B:472:GLN:HB3	1:B:478:CYS:SG	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:CYS:HA	1:C:359:CYS:HB2	1.73	0.70
1:B:334:CYS:HA	1:B:359:CYS:HB2	1.73	0.70
1:B:16:VAL:HA	2:N:1:NAG:H81	1.72	0.69
1:A:334:CYS:SG	4:A:1310:EIC:C17	2.80	0.69
1:A:472:GLN:HB3	1:A:478:CYS:SG	2.33	0.68
1:A:334:CYS:HA	1:A:359:CYS:HB2	1.73	0.68
1:A:390:PHE:CD2	4:A:1310:EIC:H131	2.26	0.68
1:C:432:ILE:CD1	4:C:1310:EIC:H51	2.23	0.67
1:B:1136:GLN:HG3	1:B:1137:PRO:HD3	1.77	0.66
1:C:1136:GLN:HG3	1:C:1137:PRO:HD3	1.77	0.66
1:A:522:VAL:CG1	4:A:1310:EIC:H131	2.26	0.66
1:A:1136:GLN:HG3	1:A:1137:PRO:HD3	1.78	0.65
1:B:390:PHE:CE2	4:B:1310:EIC:H121	2.31	0.65
1:C:916:LEU:CD1	2:m:2:NAG:H83	2.28	0.63
1:C:379:GLY:HA3	1:C:428:THR:HG23	1.80	0.63
1:A:379:GLY:HA3	1:A:428:THR:HG23	1.80	0.63
1:B:334:CYS:SG	4:B:1310:EIC:H171	2.39	0.62
1:A:125:VAL:HG21	3:A:1306:NAG:H61	1.82	0.62
1:B:379:GLY:HA3	1:B:428:THR:HG23	1.80	0.62
1:B:125:VAL:HG21	3:B:1306:NAG:H61	1.82	0.61
1:B:16:VAL:HA	2:N:1:NAG:C8	2.30	0.61
2:R:1:NAG:H61	2:R:2:NAG:H83	1.82	0.60
1:C:125:VAL:HG21	3:C:1306:NAG:H61	1.82	0.60
1:C:375:PHE:CD1	4:C:1310:EIC:H31	2.36	0.59
4:C:1310:EIC:H112	4:C:1310:EIC:H161	1.83	0.59
1:C:916:LEU:HD12	2:m:2:NAG:H83	1.85	0.59
1:B:21:ARG:HH21	1:B:77:PHE:HB3	1.68	0.59
1:A:393:VAL:HG21	4:A:1310:EIC:C14	2.24	0.59
1:A:21:ARG:HH21	1:A:77:PHE:HB3	1.68	0.58
1:A:126:ILE:HB	1:A:168:TYR:HB3	1.86	0.58
1:B:126:ILE:HB	1:B:168:TYR:HB3	1.86	0.58
1:C:21:ARG:HH21	1:C:77:PHE:HB3	1.68	0.58
1:B:390:PHE:CD2	4:B:1310:EIC:C12	2.84	0.58
1:A:390:PHE:HE2	4:A:1310:EIC:C12	2.03	0.58
1:A:702:SER:HB3	1:A:705:SER:HB3	1.86	0.57
1:A:393:VAL:CG2	4:A:1310:EIC:H142	2.23	0.57
1:C:702:SER:HB3	1:C:705:SER:HB3	1.86	0.57
1:C:126:ILE:HB	1:C:168:TYR:HB3	1.86	0.57
1:C:322:ILE:HB	1:C:537:VAL:HG12	1.87	0.57
1:B:702:SER:HB3	1:B:705:SER:HB3	1.86	0.56
1:B:1070:THR:HB	1:B:1091:SER:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ILE:HB	1:B:537:VAL:HG12	1.87	0.56
1:B:356:ILE:HG21	4:B:1310:EIC:H151	1.87	0.56
1:A:135:THR:HG21	2:D:1:NAG:H5	1.88	0.56
1:C:187:LEU:HD22	1:C:215:PRO:HG2	1.89	0.55
1:B:187:LEU:HD22	1:B:215:PRO:HG2	1.89	0.55
1:A:322:ILE:HB	1:A:537:VAL:HG12	1.87	0.55
1:A:187:LEU:HD22	1:A:215:PRO:HG2	1.89	0.55
2:R:2:NAG:O7	2:R:2:NAG:H3	2.05	0.55
1:B:955:THR:O	1:B:959:GLN:HG2	2.07	0.55
1:A:955:THR:O	1:A:959:GLN:HG2	2.07	0.54
1:C:955:THR:O	1:C:959:GLN:HG2	2.07	0.54
1:C:20:THR:HG22	1:C:20:THR:O	2.08	0.54
1:A:390:PHE:HD2	4:A:1310:EIC:H131	1.72	0.54
1:A:639:ASN:HB3	1:A:650:GLY:H	1.73	0.54
1:C:639:ASN:HB3	1:C:650:GLY:H	1.73	0.54
1:A:20:THR:O	1:A:20:THR:HG22	2.08	0.53
2:H:2:NAG:O7	2:H:2:NAG:H3	2.07	0.53
1:C:654:VAL:HG21	1:C:687:ILE:HD12	1.91	0.53
1:C:390:PHE:CE2	4:C:1310:EIC:H121	2.43	0.53
1:B:20:THR:HG22	1:B:20:THR:O	2.08	0.53
1:B:639:ASN:HB3	1:B:650:GLY:H	1.73	0.53
1:B:654:VAL:HG21	1:B:687:ILE:HD12	1.91	0.53
1:C:453:LEU:HD23	1:C:454:PHE:CE2	2.44	0.53
1:C:296:GLU:HG3	1:C:316:PHE:HD2	1.74	0.52
1:B:64:TRP:HE1	1:B:262:ALA:HB1	1.75	0.52
1:B:296:GLU:HG3	1:B:316:PHE:HD2	1.74	0.52
1:A:64:TRP:HE1	1:A:262:ALA:HB1	1.75	0.52
1:B:390:PHE:CE2	4:B:1310:EIC:C12	2.92	0.52
1:B:453:LEU:HD23	1:B:454:PHE:CE2	2.44	0.52
1:C:64:TRP:HE1	1:C:262:ALA:HB1	1.75	0.52
1:A:296:GLU:HG3	1:A:316:PHE:HD2	1.74	0.52
1:A:453:LEU:HD23	1:A:454:PHE:CE2	2.44	0.52
1:C:522:VAL:HG11	4:C:1310:EIC:H131	1.91	0.51
1:A:654:VAL:HG21	1:A:687:ILE:HD12	1.90	0.51
1:B:654:VAL:HG23	1:B:689:TYR:HB3	1.93	0.51
1:C:356:ILE:HD12	4:C:1310:EIC:H151	1.93	0.51
1:A:361:ALA:CB	4:A:1310:EIC:C11	2.86	0.51
1:B:393:VAL:HG21	4:B:1310:EIC:C13	2.40	0.50
1:A:1123:VAL:HB	1:A:1126:ILE:HB	1.94	0.50
1:B:622:ILE:HD11	1:B:635:SER:HB3	1.94	0.50
1:A:654:VAL:HG23	1:A:689:TYR:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:CYS:SG	1:A:164:CYS:N	2.85	0.50
1:C:1123:VAL:HB	1:C:1126:ILE:HB	1.94	0.50
1:A:711:ASN:HB3	1:A:1064:ALA:HB3	1.93	0.49
1:C:654:VAL:HG23	1:C:689:TYR:HB3	1.93	0.49
1:C:622:ILE:HD11	1:C:635:SER:HB3	1.94	0.49
1:A:622:ILE:HD11	1:A:635:SER:HB3	1.94	0.49
1:B:1134:PRO:O	1:B:1137:PRO:HD2	2.13	0.49
4:B:1310:EIC:H141	4:B:1310:EIC:C10	2.42	0.49
1:C:1134:PRO:O	1:C:1137:PRO:HD2	2.13	0.49
1:B:1040:GLY:HA2	1:C:884:ALA:HB1	1.94	0.49
1:C:148:LYS:HB3	1:C:148:LYS:HE2	1.55	0.49
1:B:1123:VAL:HB	1:B:1126:ILE:HB	1.94	0.48
1:A:884:ALA:HB1	1:C:1040:GLY:HA2	1.95	0.48
1:B:380:VAL:HG12	1:C:977:ARG:HB3	1.95	0.48
1:A:1134:PRO:O	1:A:1137:PRO:HD2	2.13	0.48
1:B:135:THR:CG2	2:N:1:NAG:H3	2.44	0.48
1:B:356:ILE:CD1	4:B:1310:EIC:H162	2.44	0.48
1:B:1095:HIS:CE1	2:R:1:NAG:H5	2.47	0.48
1:A:1040:GLY:HA2	1:B:884:ALA:HB1	1.95	0.47
2:G:1:NAG:H61	2:G:2:NAG:HN2	1.79	0.47
1:A:903:ILE:HD13	1:A:1043:LEU:HD21	1.96	0.47
1:B:1095:HIS:CG	2:R:1:NAG:H5	2.49	0.47
1:A:361:ALA:HB1	4:A:1310:EIC:H112	1.92	0.47
1:B:135:THR:HG21	2:N:1:NAG:H3	1.96	0.47
1:B:791:PHE:O	1:B:794:PHE:HD1	1.97	0.47
1:B:903:ILE:HD13	1:B:1043:LEU:HD21	1.97	0.47
2:O:1:NAG:H61	2:O:2:NAG:N2	2.30	0.47
4:C:1310:EIC:H112	4:C:1310:EIC:C16	2.45	0.47
2:G:1:NAG:H61	2:G:2:NAG:N2	2.30	0.47
1:A:977:ARG:HB3	1:C:380:VAL:HG12	1.96	0.47
1:C:796:PHE:HD1	1:C:799:ILE:HD11	1.79	0.46
1:A:122:THR:HB	1:A:173:PHE:O	2.15	0.46
2:R:1:NAG:O7	2:R:1:NAG:H3	2.16	0.46
1:A:1075:ILE:HD13	1:A:1127:VAL:HG22	1.97	0.46
1:A:380:VAL:HG12	1:B:977:ARG:HB3	1.96	0.46
4:A:1310:EIC:H141	4:A:1310:EIC:C10	2.45	0.46
1:A:815:LEU:O	1:A:819:LYS:HG2	2.16	0.46
1:B:815:LEU:O	1:B:819:LYS:HG2	2.16	0.46
1:A:253:GLU:HA	1:A:256:TRP:HE1	1.81	0.46
1:C:122:THR:HB	1:C:173:PHE:O	2.15	0.46
1:C:187:LEU:HB3	1:C:206:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ILE:HD12	1:B:70:TYR:HE1	1.81	0.46
1:B:253:GLU:HA	1:B:256:TRP:HE1	1.81	0.46
1:C:903:ILE:HD13	1:C:1043:LEU:HD21	1.97	0.46
1:C:385:LEU:HD13	4:C:1310:EIC:H81	1.98	0.46
1:B:122:THR:HB	1:B:173:PHE:O	2.15	0.45
1:B:187:LEU:HB3	1:B:206:THR:O	2.16	0.45
1:A:148:LYS:HB3	1:A:148:LYS:HE2	1.53	0.45
1:A:522:VAL:HG11	4:A:1310:EIC:C13	2.41	0.45
1:C:74:PHE:HD1	1:C:74:PHE:O	1.98	0.45
1:A:187:LEU:HB3	1:A:206:THR:O	2.16	0.45
1:C:348:VAL:HG22	1:C:420:ASN:HB3	1.99	0.45
1:B:348:VAL:HG22	1:B:420:ASN:HB3	1.99	0.45
1:C:336:PHE:CE1	4:C:1310:EIC:H172	2.52	0.45
1:B:796:PHE:HD1	1:B:799:ILE:HD11	1.81	0.45
1:C:1067:LYS:HE2	1:C:1067:LYS:HB3	1.68	0.45
1:B:334:CYS:SG	4:B:1310:EIC:C17	3.05	0.45
1:A:356:ILE:HD11	4:A:1310:EIC:H183	1.89	0.45
1:B:872:LEU:HD12	1:B:872:LEU:HA	1.85	0.45
1:C:815:LEU:O	1:C:819:LYS:HG2	2.16	0.45
1:C:253:GLU:HA	1:C:256:TRP:HE1	1.81	0.44
1:C:74:PHE:O	1:C:74:PHE:CD1	2.70	0.44
1:A:419:TYR:CD1	1:A:455:ARG:HB3	2.53	0.44
1:C:419:TYR:CD1	1:C:455:ARG:HB3	2.53	0.44
1:C:1070:THR:HB	1:C:1091:SER:HB3	2.00	0.44
1:A:348:VAL:HG22	1:A:420:ASN:HB3	1.99	0.44
4:B:1310:EIC:H1O1	4:B:1310:EIC:H141	2.00	0.44
1:A:983:ALA:O	1:A:987:ILE:HG12	2.18	0.44
2:k:1:NAG:O7	2:k:1:NAG:H3	2.17	0.44
1:A:791:PHE:O	1:A:794:PHE:HD1	2.01	0.44
1:C:798:GLN:NE2	2:Y:1:NAG:O6	2.51	0.44
1:C:872:LEU:HD12	1:C:872:LEU:HA	1.85	0.44
1:C:95:LYS:NZ	1:C:260:ALA:HB3	2.33	0.43
1:B:135:THR:HG21	2:N:1:NAG:H5	2.00	0.43
1:B:22:THR:OG1	1:B:75:LYS:O	2.25	0.43
1:B:419:TYR:CD1	1:B:455:ARG:HB3	2.53	0.43
1:C:983:ALA:O	1:C:987:ILE:HG12	2.18	0.43
1:A:95:LYS:NZ	1:A:260:ALA:HB3	2.33	0.43
1:A:1070:THR:HB	1:A:1091:SER:HB3	2.00	0.43
1:C:1084:PRO:HD3	1:C:1089:PHE:CE2	2.54	0.43
1:A:474:GLY:H	1:A:485:ASN:HB3	1.82	0.43
1:B:983:ALA:O	1:B:987:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:HH21	1:C:215:PRO:HB2	1.83	0.43
1:C:558:LEU:HD13	1:C:558:LEU:HA	1.90	0.43
1:A:789:LYS:HE2	1:A:789:LYS:HB3	1.94	0.43
2:Z:2:NAG:O7	2:Z:2:NAG:H3	2.19	0.43
1:A:34:ARG:HH21	1:A:215:PRO:HB2	1.83	0.43
1:C:375:PHE:CE1	4:C:1310:EIC:H31	2.54	0.43
1:C:387:ASP:HA	1:C:526:LYS:HD2	2.01	0.43
1:A:387:ASP:HA	1:A:526:LYS:HD2	2.01	0.43
1:B:95:LYS:NZ	1:B:260:ALA:HB3	2.33	0.43
1:C:956:LEU:HD12	1:C:956:LEU:HA	1.90	0.43
1:B:34:ARG:HH21	1:B:215:PRO:HB2	1.83	0.42
1:B:1084:PRO:HD3	1:B:1089:PHE:CE2	2.54	0.42
1:A:755:THR:HG22	1:A:759:ARG:HD3	2.00	0.42
1:C:755:THR:HG22	1:C:759:ARG:HD3	2.00	0.42
1:B:677:SER:O	1:B:678:LEU:HB2	2.20	0.42
2:U:1:NAG:H62	2:U:2:NAG:C7	2.50	0.42
1:A:677:SER:O	1:A:678:LEU:HB2	2.20	0.42
1:B:148:LYS:HB3	1:B:148:LYS:HE2	1.70	0.42
1:B:247:LEU:HD13	1:B:247:LEU:HA	1.89	0.42
2:D:1:NAG:H62	2:D:2:NAG:N2	2.34	0.42
1:A:964:PHE:HE1	1:B:753:PHE:HZ	1.67	0.42
1:B:65:PHE:HB3	1:B:78:ASP:HB3	2.01	0.42
1:C:677:SER:O	1:C:678:LEU:HB2	2.20	0.42
1:C:679:ARG:HA	1:C:679:ARG:HD3	1.86	0.42
2:m:2:NAG:O7	2:m:2:NAG:H3	2.19	0.42
1:A:1084:PRO:HD3	1:A:1089:PHE:CE2	2.54	0.42
1:B:1067:LYS:HE2	1:B:1067:LYS:HB3	1.79	0.42
1:A:496:HIS:HB2	1:A:499:THR:HB	2.02	0.42
1:B:755:THR:HG22	1:B:759:ARG:HD3	2.00	0.42
1:B:758:ASN:HD22	1:B:758:ASN:HA	1.70	0.42
1:A:516:LEU:H	1:A:516:LEU:HG	1.70	0.42
1:A:780:LYS:HD3	1:A:780:LYS:HA	1.83	0.42
1:B:387:ASP:HA	1:B:526:LYS:HD2	2.01	0.42
1:B:496:HIS:HB2	1:B:499:THR:HB	2.02	0.42
1:B:590:PHE:CD1	1:C:831:TYR:HD1	2.38	0.42
1:C:153:ASN:HB2	1:C:154:GLU:H	1.68	0.42
1:A:590:PHE:CD1	1:B:831:TYR:HD1	2.38	0.41
1:A:65:PHE:HB3	1:A:78:ASP:HB3	2.01	0.41
1:A:878:SER:OG	1:A:882:PHE:HB3	2.20	0.41
1:B:878:SER:OG	1:B:882:PHE:HB3	2.20	0.41
1:B:964:PHE:HE1	1:C:753:PHE:HZ	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD21	1:B:138:PHE:CE2	2.56	0.41
1:B:679:ARG:HA	1:B:679:ARG:HD3	1.86	0.41
1:C:65:PHE:HB3	1:C:78:ASP:HB3	2.01	0.41
1:A:74:PHE:O	1:A:74:PHE:CD1	2.73	0.41
1:C:575:ARG:HD3	1:C:580:LEU:HG	2.02	0.41
1:C:770:LYS:HD2	1:C:1013:ARG:HH12	1.86	0.41
1:A:74:PHE:O	1:A:74:PHE:HD1	2.03	0.41
1:A:391:THR:HA	1:A:520:ALA:HA	2.03	0.41
1:B:153:ASN:HB2	1:B:154:GLU:H	1.69	0.41
1:C:496:HIS:HB2	1:C:499:THR:HB	2.02	0.41
1:A:770:LYS:HD2	1:A:1013:ARG:HH12	1.86	0.41
1:A:894:MET:HE2	1:A:894:MET:HB3	1.92	0.41
1:B:391:THR:HA	1:B:520:ALA:HA	2.03	0.41
1:B:558:LEU:HD13	1:B:558:LEU:HA	1.89	0.41
1:B:770:LYS:HD2	1:B:1013:ARG:HH12	1.86	0.41
1:A:483:GLY:H	1:A:486:CYS:HB2	1.86	0.41
1:A:831:TYR:HD1	1:C:590:PHE:CD1	2.39	0.41
1:B:162:ASN:HB3	1:B:163:ASN:H	1.54	0.41
1:B:64:TRP:NE1	1:B:66:ASN:HB3	2.36	0.40
1:C:294:LEU:HG	1:C:298:LYS:HE3	2.03	0.40
1:C:878:SER:OG	1:C:882:PHE:HB3	2.20	0.40
1:A:208:ILE:HD12	1:A:208:ILE:HA	1.95	0.40
1:A:575:ARG:HD3	1:A:580:LEU:HG	2.03	0.40
1:C:393:VAL:HG21	4:C:1310:EIC:C15	2.45	0.40
2:R:1:NAG:H61	2:R:2:NAG:C8	2.51	0.40
2:Y:2:NAG:HO3	2:Y:2:NAG:C7	2.26	0.40
1:C:791:PHE:O	1:C:794:PHE:HD1	2.04	0.40
1:A:753:PHE:HZ	1:C:964:PHE:HE1	1.68	0.40
2:H:1:NAG:H61	2:H:2:NAG:N2	2.36	0.40
1:A:214:LEU:HA	1:A:215:PRO:HD3	1.95	0.40
1:C:1022:LYS:HE3	1:C:1022:LYS:HB2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	937/1295 (72%)	909 (97%)	26 (3%)	2 (0%)	43	63
1	B	1123/1295 (87%)	1080 (96%)	39 (4%)	4 (0%)	30	49
1	C	1123/1295 (87%)	1079 (96%)	40 (4%)	4 (0%)	30	49
All	All	3183/3885 (82%)	3068 (96%)	105 (3%)	10 (0%)	37	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	LYS
1	C	148	LYS
1	A	481	GLN
1	B	162	ASN
1	C	162	ASN
1	B	121	ALA
1	C	121	ALA
1	A	319	GLN
1	B	319	GLN
1	C	319	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	976/1120 (87%)	926 (95%)	50 (5%)	21	43
1	B	976/1120 (87%)	930 (95%)	46 (5%)	23	47
1	C	976/1120 (87%)	929 (95%)	47 (5%)	23	46
All	All	2928/3360 (87%)	2785 (95%)	143 (5%)	24	45

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL

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Mol	Chain	Res	Type
1	A	18	LEU
1	A	33	THR
1	A	47	ILE
1	A	68	ILE
1	A	75	LYS
1	A	82	LEU
1	A	99	ILE
1	A	113	GLN
1	A	129	CYS
1	A	135	THR
1	A	136	ASP
1	A	146	ASN
1	A	148	LYS
1	A	154	GLU
1	A	159	SER
1	A	160	SER
1	A	195	VAL
1	A	210	LEU
1	A	211	VAL
1	A	242	LEU
1	A	247	LEU
1	A	310	ILE
1	A	334	CYS
1	A	359	CYS
1	A	393	VAL
1	A	401	LYS
1	A	415	VAL
1	A	450	LEU
1	A	472	GLN
1	A	481	GLN
1	A	516	LEU
1	A	527	LEU
1	A	550	LEU
1	A	558	LEU
1	A	593	VAL
1	A	600	THR
1	A	643	THR
1	A	681	VAL
1	A	708	ILE
1	A	714	ILE
1	A	759	ARG
1	A	805	LYS

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Mol	Chain	Res	Type
1	A	810	SER
1	A	942	LEU
1	A	946	VAL
1	A	971	LEU
1	A	1098	ILE
1	A	1116	VAL
1	A	1130	THR
1	B	16	VAL
1	B	33	THR
1	B	47	ILE
1	B	68	ILE
1	B	75	LYS
1	B	82	LEU
1	B	99	ILE
1	B	113	GLN
1	B	135	THR
1	B	136	ASP
1	B	146	ASN
1	B	148	LYS
1	B	154	GLU
1	B	159	SER
1	B	195	VAL
1	B	210	LEU
1	B	211	VAL
1	B	242	LEU
1	B	247	LEU
1	B	310	ILE
1	B	334	CYS
1	B	359	CYS
1	B	393	VAL
1	B	401	LYS
1	B	415	VAL
1	B	450	LEU
1	B	472	GLN
1	B	516	LEU
1	B	527	LEU
1	B	550	LEU
1	B	558	LEU
1	B	593	VAL
1	B	600	THR
1	B	643	THR
1	B	681	VAL

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Mol	Chain	Res	Type
1	B	708	ILE
1	B	714	ILE
1	B	759	ARG
1	B	805	LYS
1	B	810	SER
1	B	942	LEU
1	B	946	VAL
1	B	971	LEU
1	B	1098	ILE
1	B	1116	VAL
1	B	1130	THR
1	C	33	THR
1	C	47	ILE
1	C	68	ILE
1	C	75	LYS
1	C	82	LEU
1	C	99	ILE
1	C	113	GLN
1	C	129	CYS
1	C	135	THR
1	C	136	ASP
1	C	146	ASN
1	C	148	LYS
1	C	154	GLU
1	C	159	SER
1	C	164	CYS
1	C	195	VAL
1	C	210	LEU
1	C	211	VAL
1	C	242	LEU
1	C	247	LEU
1	C	310	ILE
1	C	334	CYS
1	C	359	CYS
1	C	393	VAL
1	C	401	LYS
1	C	415	VAL
1	C	450	LEU
1	C	472	GLN
1	C	516	LEU
1	C	527	LEU
1	C	550	LEU

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Mol	Chain	Res	Type
1	C	558	LEU
1	C	593	VAL
1	C	600	THR
1	C	643	THR
1	C	681	VAL
1	C	708	ILE
1	C	714	ILE
1	C	759	ARG
1	C	805	LYS
1	C	810	SER
1	C	942	LEU
1	C	946	VAL
1	C	971	LEU
1	C	1098	ILE
1	C	1116	VAL
1	C	1130	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	119	ASN
1	A	132	GLN
1	A	251	ASN
1	A	623	HIS
1	A	626	GLN
1	A	653	HIS
1	A	673	HIS
1	A	697	ASN
1	A	758	ASN
1	A	895	GLN
1	A	1005	GLN
1	A	1129	ASN
1	B	71	GLN
1	B	119	ASN
1	B	251	ASN
1	B	623	HIS
1	B	626	GLN
1	B	653	HIS
1	B	673	HIS
1	B	697	ASN
1	B	758	ASN

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Mol	Chain	Res	Type
1	B	895	GLN
1	B	1005	GLN
1	B	1129	ASN
1	C	71	GLN
1	C	113	GLN
1	C	119	ASN
1	C	132	GLN
1	C	623	HIS
1	C	626	GLN
1	C	653	HIS
1	C	673	HIS
1	C	697	ASN
1	C	758	ASN
1	C	798	GLN
1	C	895	GLN
1	C	1005	GLN
1	C	1129	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

66 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	-	14,14,15	0.31	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	2	-	14,14,15	0.31	0	17,19,21	0.84	1 (5%)
2	NAG	E	1	-	14,14,15	0.36	0	17,19,21	1.03	2 (11%)
2	NAG	E	2	-	14,14,15	0.36	0	17,19,21	1.25	2 (11%)
2	NAG	F	1	-	14,14,15	0.33	0	17,19,21	0.69	0
2	NAG	F	2	-	14,14,15	0.30	0	17,19,21	0.69	0
2	NAG	G	1	-	14,14,15	0.30	0	17,19,21	0.56	0
2	NAG	G	2	-	14,14,15	0.30	0	17,19,21	0.63	0
2	NAG	H	1	-	14,14,15	0.30	0	17,19,21	0.73	0
2	NAG	H	2	-	14,14,15	0.29	0	17,19,21	0.89	0
2	NAG	I	1	-	14,14,15	0.31	0	17,19,21	0.75	1 (5%)
2	NAG	I	2	-	14,14,15	0.28	0	17,19,21	0.62	0
2	NAG	J	1	-	14,14,15	0.36	0	17,19,21	1.28	3 (17%)
2	NAG	J	2	-	14,14,15	0.31	0	17,19,21	0.61	0
2	NAG	K	1	-	14,14,15	0.29	0	17,19,21	0.98	2 (11%)
2	NAG	K	2	-	14,14,15	0.33	0	17,19,21	0.87	1 (5%)
2	NAG	L	1	-	14,14,15	0.34	0	17,19,21	0.96	1 (5%)
2	NAG	L	2	-	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	M	1	-	14,14,15	0.46	0	17,19,21	1.33	3 (17%)
2	NAG	M	2	-	14,14,15	0.31	0	17,19,21	0.54	0
2	NAG	N	1	-	14,14,15	0.27	0	17,19,21	0.63	0
2	NAG	N	2	-	14,14,15	0.26	0	17,19,21	0.65	0
2	NAG	O	1	-	14,14,15	0.30	0	17,19,21	0.69	0
2	NAG	O	2	-	14,14,15	0.29	0	17,19,21	0.64	0
2	NAG	P	1	-	14,14,15	0.36	0	17,19,21	1.03	2 (11%)
2	NAG	P	2	-	14,14,15	0.37	0	17,19,21	1.25	2 (11%)
2	NAG	Q	1	-	14,14,15	0.32	0	17,19,21	0.70	0
2	NAG	Q	2	-	14,14,15	0.31	0	17,19,21	0.68	0
2	NAG	R	1	-	14,14,15	0.26	0	17,19,21	0.65	0
2	NAG	R	2	-	14,14,15	0.27	0	17,19,21	0.62	0
2	NAG	S	1	-	14,14,15	0.38	0	17,19,21	0.74	1 (5%)
2	NAG	S	2	-	14,14,15	0.31	0	17,19,21	0.71	0
2	NAG	T	1	-	14,14,15	0.36	0	17,19,21	1.22	1 (5%)
2	NAG	T	2	-	14,14,15	0.36	0	17,19,21	1.31	3 (17%)
2	NAG	U	1	-	14,14,15	0.29	0	17,19,21	0.62	0
2	NAG	U	2	-	14,14,15	0.27	0	17,19,21	0.69	0
2	NAG	V	1	-	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	V	2	-	14,14,15	0.30	0	17,19,21	0.66	0
2	NAG	W	1	-	14,14,15	0.34	0	17,19,21	0.96	1 (5%)
2	NAG	W	2	-	14,14,15	0.29	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	X	1	-	14,14,15	0.45	0	17,19,21	1.33	3 (17%)
2	NAG	X	2	-	14,14,15	0.31	0	17,19,21	0.53	0
2	NAG	Y	1	-	14,14,15	0.33	0	17,19,21	0.85	0
2	NAG	Y	2	-	14,14,15	0.32	0	17,19,21	0.72	0
2	NAG	Z	1	-	14,14,15	0.28	0	17,19,21	0.65	0
2	NAG	Z	2	-	14,14,15	0.27	0	17,19,21	0.61	0
2	NAG	a	1	-	14,14,15	0.37	0	17,19,21	1.02	2 (11%)
2	NAG	a	2	-	14,14,15	0.37	0	17,19,21	1.25	1 (5%)
2	NAG	b	1	-	14,14,15	0.33	0	17,19,21	0.70	0
2	NAG	b	2	-	14,14,15	0.31	0	17,19,21	0.69	0
2	NAG	e	1	-	14,14,15	0.37	0	17,19,21	1.22	1 (5%)
2	NAG	e	2	-	14,14,15	0.35	0	17,19,21	1.31	3 (17%)
2	NAG	f	1	-	14,14,15	0.35	0	17,19,21	1.28	3 (17%)
2	NAG	f	2	-	14,14,15	0.31	0	17,19,21	0.61	0
2	NAG	g	1	-	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	g	2	-	14,14,15	0.30	0	17,19,21	0.67	0
2	NAG	h	1	-	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
2	NAG	h	2	-	14,14,15	0.31	0	17,19,21	0.53	0
2	NAG	i	1	-	14,14,15	0.46	0	17,19,21	1.33	3 (17%)
2	NAG	i	2	-	14,14,15	0.30	0	17,19,21	0.54	0
2	NAG	k	1	-	14,14,15	0.28	0	17,19,21	0.66	0
2	NAG	k	2	-	14,14,15	0.26	0	17,19,21	0.63	0
2	NAG	l	1	-	14,14,15	0.28	0	17,19,21	0.77	0
2	NAG	l	2	-	14,14,15	0.28	0	17,19,21	0.64	0
2	NAG	m	1	-	14,14,15	0.29	0	17,19,21	0.67	0
2	NAG	m	2	-	14,14,15	0.28	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	-	-	2/6/23/26	0/1/1/1
2	NAG	D	2	-	-	2/6/23/26	0/1/1/1
2	NAG	E	1	-	-	2/6/23/26	0/1/1/1
2	NAG	E	2	-	-	2/6/23/26	0/1/1/1
2	NAG	F	1	-	-	1/6/23/26	0/1/1/1
2	NAG	F	2	-	-	0/6/23/26	0/1/1/1
2	NAG	G	1	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	-	-	0/6/23/26	0/1/1/1
2	NAG	H	1	-	-	2/6/23/26	0/1/1/1
2	NAG	H	2	-	-	1/6/23/26	0/1/1/1
2	NAG	I	1	-	-	2/6/23/26	0/1/1/1
2	NAG	I	2	-	-	3/6/23/26	0/1/1/1
2	NAG	J	1	-	-	4/6/23/26	0/1/1/1
2	NAG	J	2	-	-	4/6/23/26	0/1/1/1
2	NAG	K	1	-	-	2/6/23/26	0/1/1/1
2	NAG	K	2	-	-	1/6/23/26	0/1/1/1
2	NAG	L	1	-	-	3/6/23/26	0/1/1/1
2	NAG	L	2	-	-	0/6/23/26	0/1/1/1
2	NAG	M	1	-	-	4/6/23/26	0/1/1/1
2	NAG	M	2	-	-	0/6/23/26	0/1/1/1
2	NAG	N	1	-	-	1/6/23/26	0/1/1/1
2	NAG	N	2	-	-	0/6/23/26	0/1/1/1
2	NAG	O	1	-	-	3/6/23/26	0/1/1/1
2	NAG	O	2	-	-	0/6/23/26	0/1/1/1
2	NAG	P	1	-	-	2/6/23/26	0/1/1/1
2	NAG	P	2	-	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	-	-	1/6/23/26	0/1/1/1
2	NAG	Q	2	-	-	0/6/23/26	0/1/1/1
2	NAG	R	1	-	-	2/6/23/26	0/1/1/1
2	NAG	R	2	-	-	6/6/23/26	0/1/1/1
2	NAG	S	1	-	-	2/6/23/26	0/1/1/1
2	NAG	S	2	-	-	0/6/23/26	0/1/1/1
2	NAG	T	1	-	-	2/6/23/26	0/1/1/1
2	NAG	T	2	-	-	2/6/23/26	0/1/1/1
2	NAG	U	1	-	-	0/6/23/26	0/1/1/1
2	NAG	U	2	-	-	1/6/23/26	0/1/1/1
2	NAG	V	1	-	-	2/6/23/26	0/1/1/1
2	NAG	V	2	-	-	2/6/23/26	0/1/1/1
2	NAG	W	1	-	-	3/6/23/26	0/1/1/1
2	NAG	W	2	-	-	0/6/23/26	0/1/1/1
2	NAG	X	1	-	-	4/6/23/26	0/1/1/1
2	NAG	X	2	-	-	0/6/23/26	0/1/1/1
2	NAG	Y	1	-	-	2/6/23/26	0/1/1/1
2	NAG	Y	2	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Z	1	-	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	-	-	5/6/23/26	0/1/1/1
2	NAG	a	1	-	-	2/6/23/26	0/1/1/1
2	NAG	a	2	-	-	2/6/23/26	0/1/1/1
2	NAG	b	1	-	-	1/6/23/26	0/1/1/1
2	NAG	b	2	-	-	0/6/23/26	0/1/1/1
2	NAG	e	1	-	-	2/6/23/26	0/1/1/1
2	NAG	e	2	-	-	2/6/23/26	0/1/1/1
2	NAG	f	1	-	-	4/6/23/26	0/1/1/1
2	NAG	f	2	-	-	4/6/23/26	0/1/1/1
2	NAG	g	1	-	-	2/6/23/26	0/1/1/1
2	NAG	g	2	-	-	2/6/23/26	0/1/1/1
2	NAG	h	1	-	-	3/6/23/26	0/1/1/1
2	NAG	h	2	-	-	0/6/23/26	0/1/1/1
2	NAG	i	1	-	-	4/6/23/26	0/1/1/1
2	NAG	i	2	-	-	0/6/23/26	0/1/1/1
2	NAG	k	1	-	-	3/6/23/26	0/1/1/1
2	NAG	k	2	-	-	1/6/23/26	0/1/1/1
2	NAG	l	1	-	-	2/6/23/26	0/1/1/1
2	NAG	l	2	-	-	0/6/23/26	0/1/1/1
2	NAG	m	1	-	-	2/6/23/26	0/1/1/1
2	NAG	m	2	-	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	2	NAG	C2-N2-C7	3.68	127.83	122.90
2	e	2	NAG	C2-N2-C7	3.67	127.81	122.90
2	T	1	NAG	C2-N2-C7	3.45	127.52	122.90
2	f	1	NAG	C2-N2-C7	3.44	127.51	122.90
2	a	2	NAG	C2-N2-C7	3.44	127.51	122.90
2	E	2	NAG	C2-N2-C7	3.43	127.50	122.90
2	P	2	NAG	C2-N2-C7	3.43	127.50	122.90
2	J	1	NAG	C2-N2-C7	3.43	127.49	122.90
2	e	1	NAG	C2-N2-C7	3.39	127.44	122.90
2	M	1	NAG	C3-C4-C5	2.88	115.45	110.23
2	X	1	NAG	C3-C4-C5	2.88	115.45	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	i	1	NAG	C3-C4-C5	2.88	115.45	110.23
2	i	1	NAG	C2-N2-C7	2.63	126.42	122.90
2	X	1	NAG	C2-N2-C7	2.62	126.41	122.90
2	M	1	NAG	C2-N2-C7	2.61	126.40	122.90
2	E	1	NAG	O5-C1-C2	-2.61	107.26	111.29
2	P	1	NAG	O5-C1-C2	-2.60	107.27	111.29
2	a	1	NAG	O5-C1-C2	-2.59	107.29	111.29
2	K	1	NAG	C1-O5-C5	2.58	115.65	112.19
2	f	1	NAG	O5-C1-C2	-2.52	107.40	111.29
2	J	1	NAG	O5-C1-C2	-2.51	107.40	111.29
2	X	1	NAG	C1-C2-N2	2.50	114.37	110.43
2	i	1	NAG	C1-C2-N2	2.50	114.36	110.43
2	M	1	NAG	C1-C2-N2	2.48	114.34	110.43
2	h	1	NAG	C2-N2-C7	2.42	126.14	122.90
2	W	1	NAG	C2-N2-C7	2.42	126.14	122.90
2	L	1	NAG	C2-N2-C7	2.41	126.13	122.90
2	P	1	NAG	C2-N2-C7	-2.31	119.80	122.90
2	E	1	NAG	C2-N2-C7	-2.31	119.80	122.90
2	a	1	NAG	C2-N2-C7	-2.30	119.81	122.90
2	D	2	NAG	O5-C1-C2	-2.20	107.88	111.29
2	K	1	NAG	O4-C4-C3	-2.20	105.19	110.38
2	e	2	NAG	C1-C2-N2	2.12	113.78	110.43
2	I	1	NAG	C1-O5-C5	2.10	115.00	112.19
2	T	2	NAG	C1-C2-N2	2.09	113.72	110.43
2	J	1	NAG	C1-C2-N2	2.07	113.69	110.43
2	f	1	NAG	C1-C2-N2	2.06	113.69	110.43
2	T	2	NAG	O5-C1-C2	-2.03	108.14	111.29
2	e	2	NAG	O5-C1-C2	-2.03	108.15	111.29
2	S	1	NAG	O5-C1-C2	-2.03	108.15	111.29
2	K	2	NAG	C2-N2-C7	-2.02	120.19	122.90
2	P	2	NAG	C1-C2-N2	2.01	113.59	110.43
2	E	2	NAG	C1-C2-N2	2.01	113.59	110.43

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	NAG	C1-C2-N2-C7
2	L	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C1-C2-N2-C7
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	V	2	NAG	C8-C7-N2-C2
2	V	2	NAG	O7-C7-N2-C2
2	W	1	NAG	C1-C2-N2-C7
2	W	1	NAG	O7-C7-N2-C2
2	X	1	NAG	C1-C2-N2-C7
2	X	1	NAG	C8-C7-N2-C2
2	X	1	NAG	O7-C7-N2-C2
2	g	2	NAG	C8-C7-N2-C2
2	g	2	NAG	O7-C7-N2-C2
2	h	1	NAG	C1-C2-N2-C7
2	h	1	NAG	O7-C7-N2-C2
2	i	1	NAG	C1-C2-N2-C7
2	i	1	NAG	C8-C7-N2-C2
2	i	1	NAG	O7-C7-N2-C2
2	k	1	NAG	C3-C2-N2-C7
2	k	2	NAG	C1-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	U	2	NAG	C1-C2-N2-C7
2	Y	2	NAG	C3-C2-N2-C7
2	Z	2	NAG	C3-C2-N2-C7
2	L	1	NAG	C8-C7-N2-C2
2	W	1	NAG	C8-C7-N2-C2
2	h	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O5-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	f	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	C8-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6
2	m	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	V	1	NAG	C4-C5-C6-O6
2	g	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	S	1	NAG	C8-C7-N2-C2
2	S	1	NAG	O7-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	Y	1	NAG	C8-C7-N2-C2
2	Y	2	NAG	O7-C7-N2-C2
2	R	2	NAG	C4-C5-C6-O6
2	l	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O7-C7-N2-C2
2	Z	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
2	m	1	NAG	C8-C7-N2-C2
2	Y	1	NAG	O7-C7-N2-C2
2	m	2	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	g	1	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
2	m	1	NAG	O7-C7-N2-C2
2	Z	2	NAG	C8-C7-N2-C2
2	N	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	R	2	NAG	C8-C7-N2-C2
2	k	1	NAG	C8-C7-N2-C2
2	J	1	NAG	C1-C2-N2-C7
2	T	2	NAG	C1-C2-N2-C7
2	e	2	NAG	C1-C2-N2-C7
2	f	1	NAG	C1-C2-N2-C7
2	m	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	l	1	NAG	C4-C5-C6-O6
2	Z	2	NAG	O7-C7-N2-C2
2	M	1	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	i	1	NAG	C4-C5-C6-O6
2	R	2	NAG	O7-C7-N2-C2
2	T	1	NAG	C3-C2-N2-C7
2	e	1	NAG	C3-C2-N2-C7
2	R	1	NAG	C3-C2-N2-C7
2	R	2	NAG	C3-C2-N2-C7
2	m	2	NAG	C3-C2-N2-C7
2	k	1	NAG	O7-C7-N2-C2
2	K	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C1-C2-N2-C7
2	P	2	NAG	C1-C2-N2-C7
2	T	1	NAG	C1-C2-N2-C7
2	a	2	NAG	C1-C2-N2-C7
2	e	1	NAG	C1-C2-N2-C7
2	R	1	NAG	C1-C2-N2-C7
2	R	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7
2	T	2	NAG	C3-C2-N2-C7
2	a	2	NAG	C3-C2-N2-C7
2	e	2	NAG	C3-C2-N2-C7
2	f	1	NAG	C3-C2-N2-C7
2	K	2	NAG	C3-C2-N2-C7
2	I	1	NAG	O5-C5-C6-O6

There are no ring outliers.

19 monomers are involved in 30 short contacts:

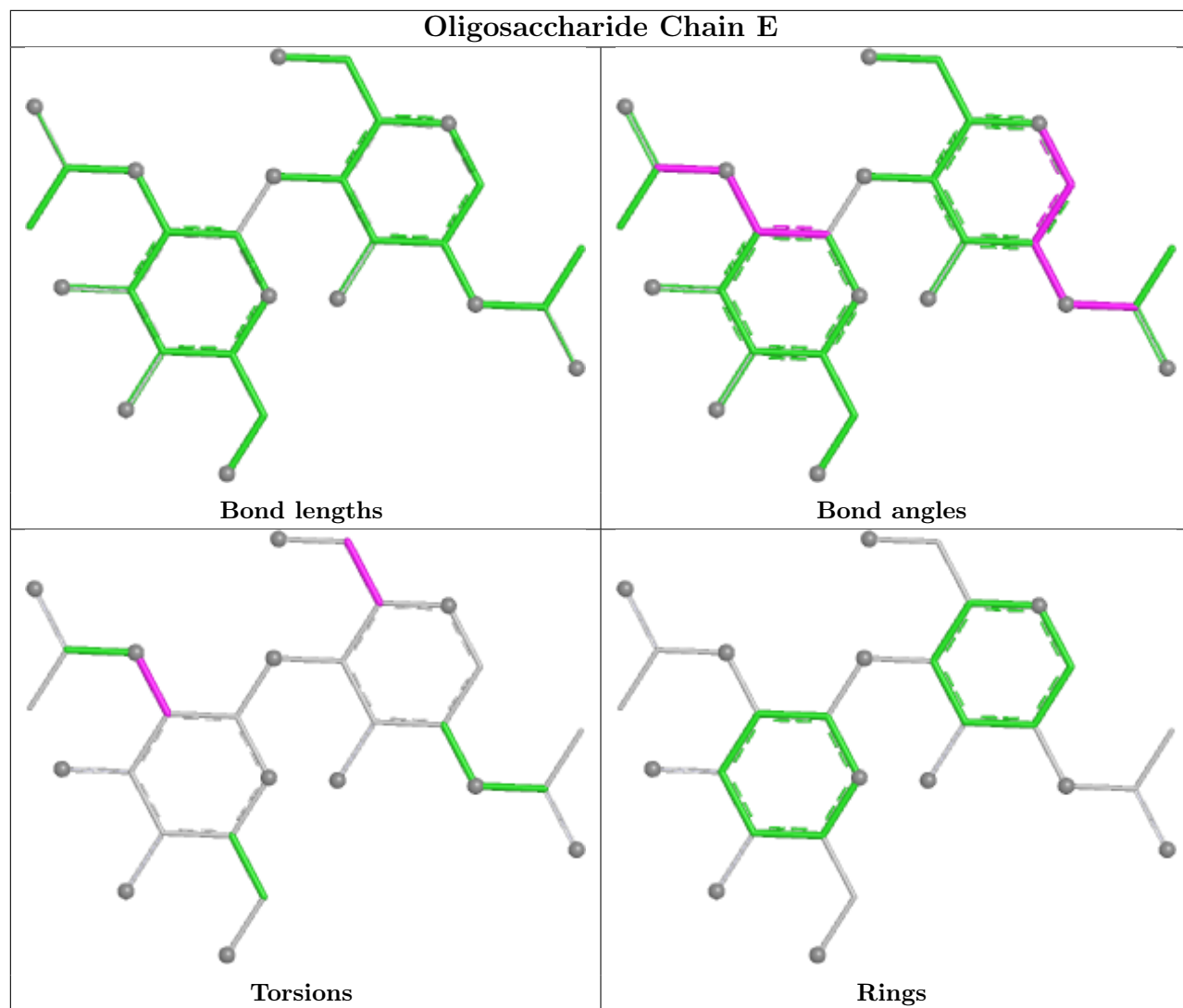
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	2	NAG	2	0
2	D	1	NAG	2	0
2	O	2	NAG	1	0
2	U	2	NAG	1	0
2	G	1	NAG	2	0
2	H	2	NAG	2	0

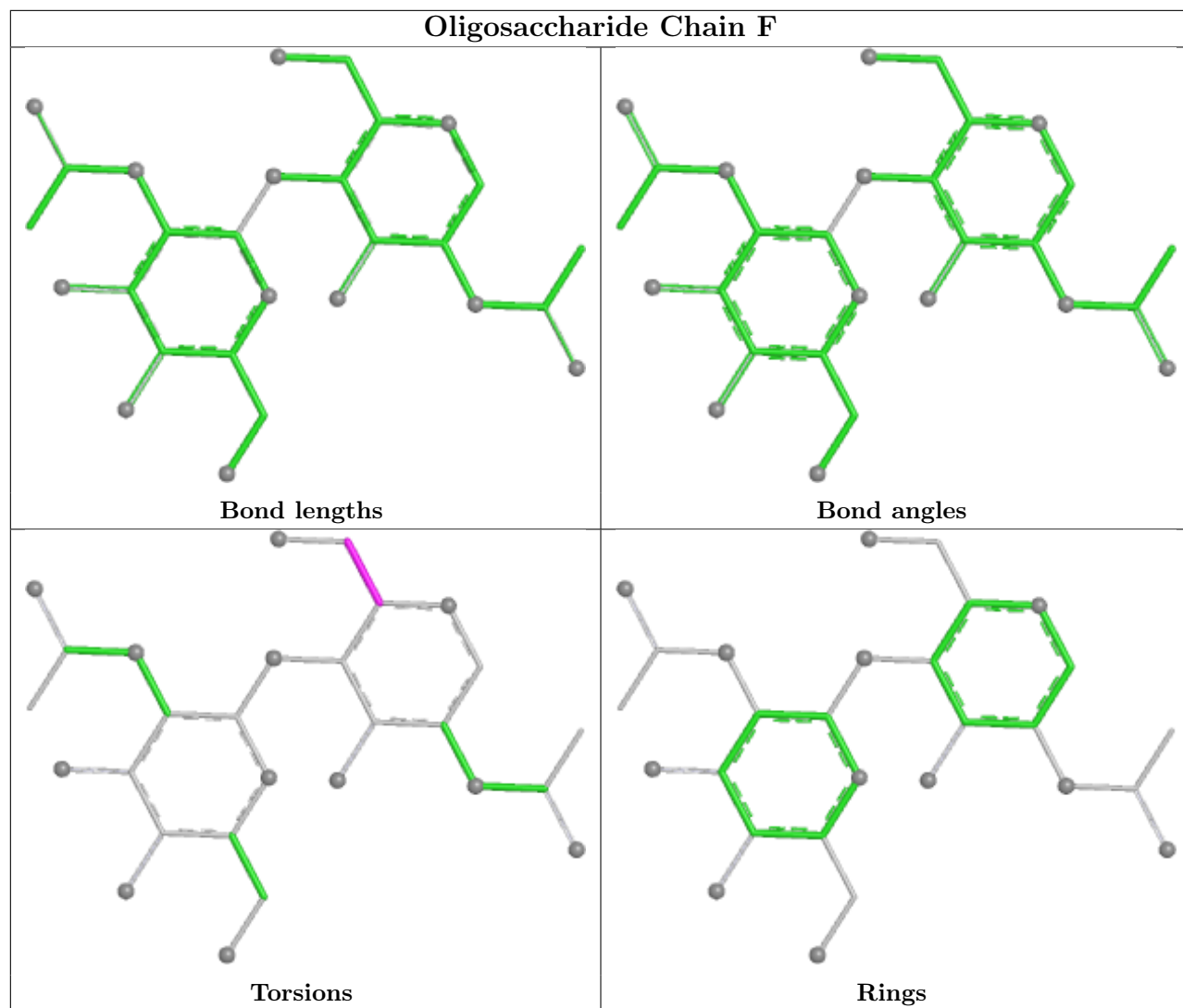
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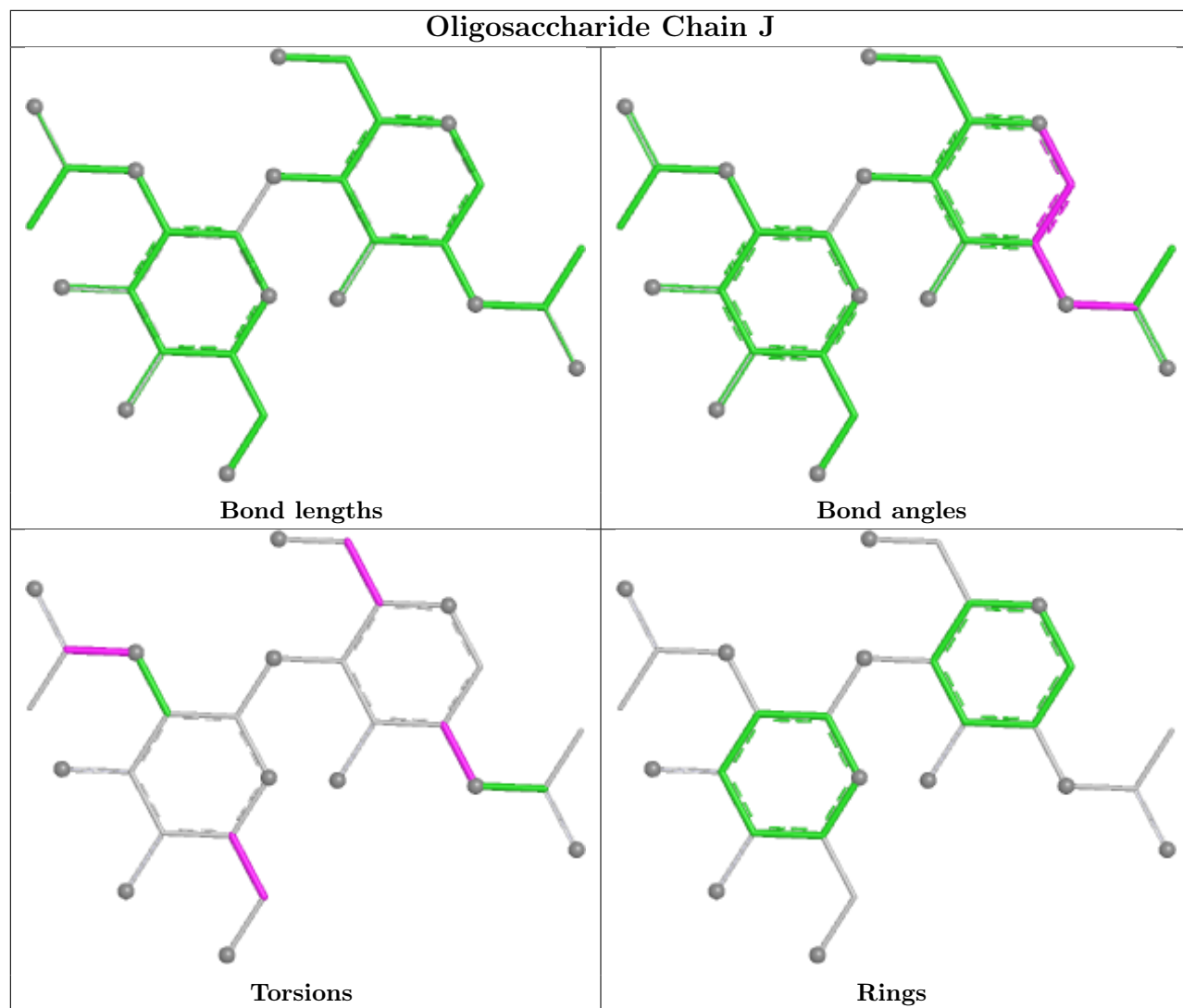
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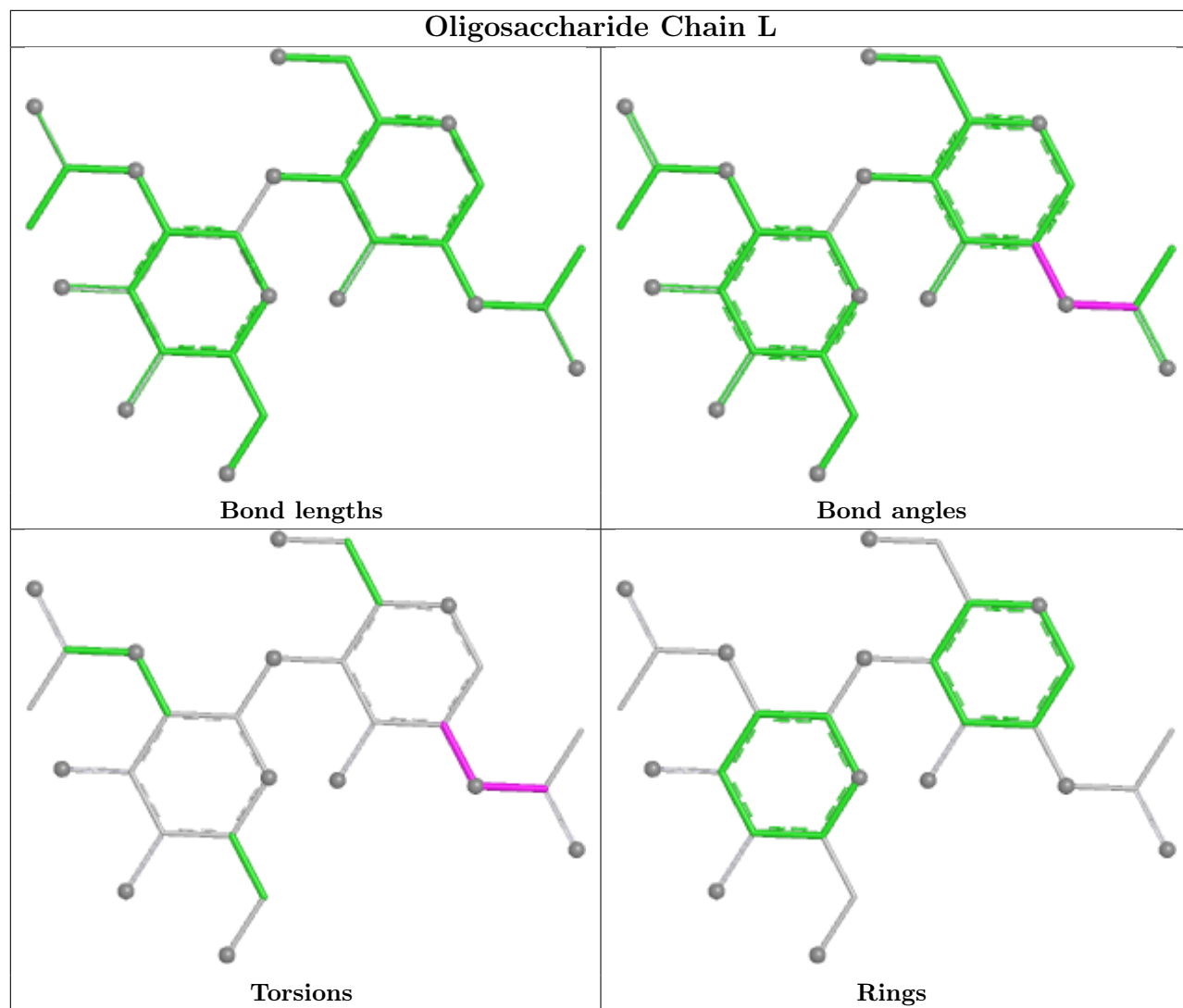
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	N	1	NAG	5	0
2	U	1	NAG	2	0
2	O	1	NAG	1	0
2	K	2	NAG	1	0
2	m	2	NAG	3	0
2	k	1	NAG	1	0
2	Z	2	NAG	1	0
2	R	2	NAG	3	0
2	Y	1	NAG	1	0
2	D	2	NAG	1	0
2	G	2	NAG	2	0
2	R	1	NAG	6	0

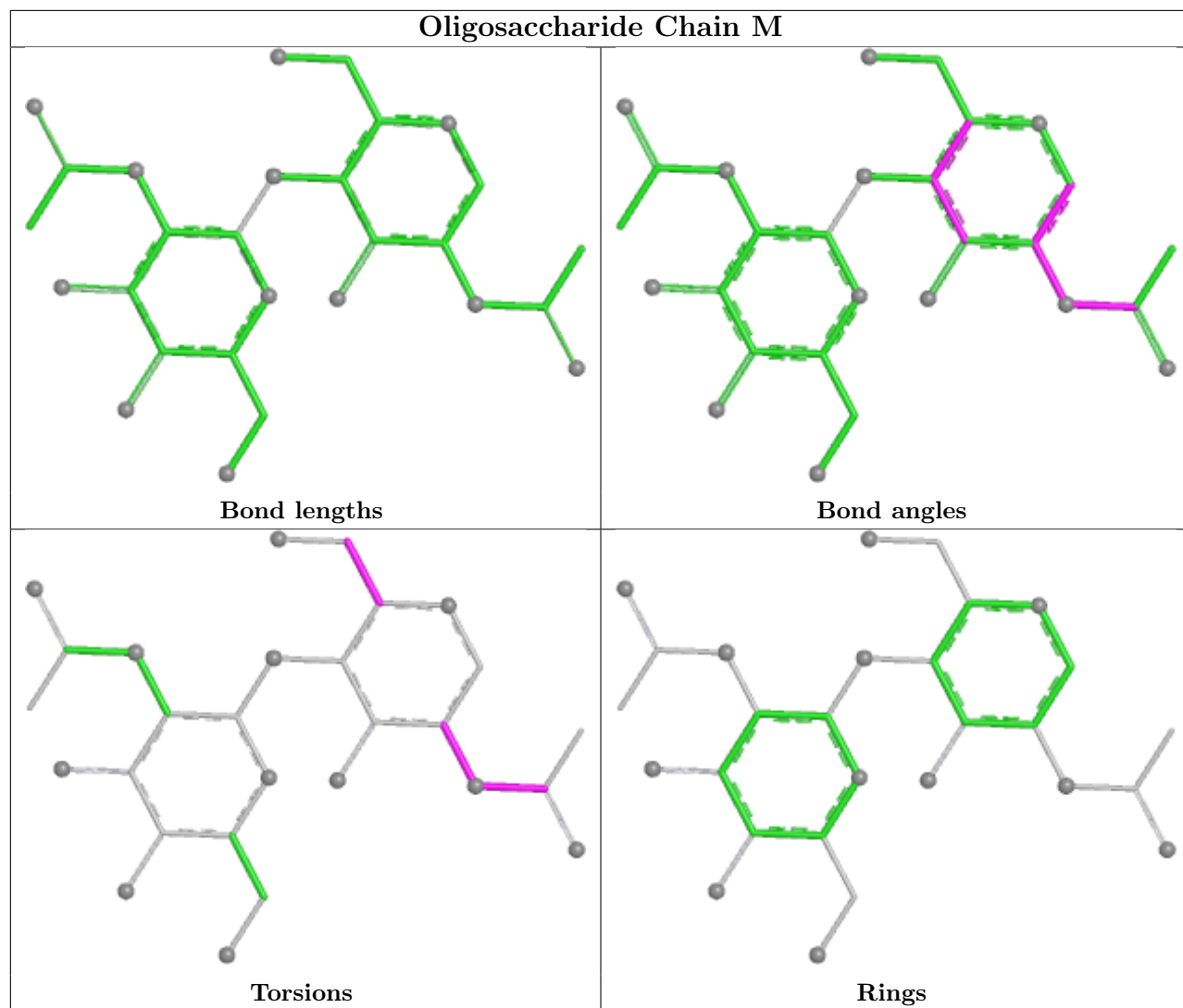
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

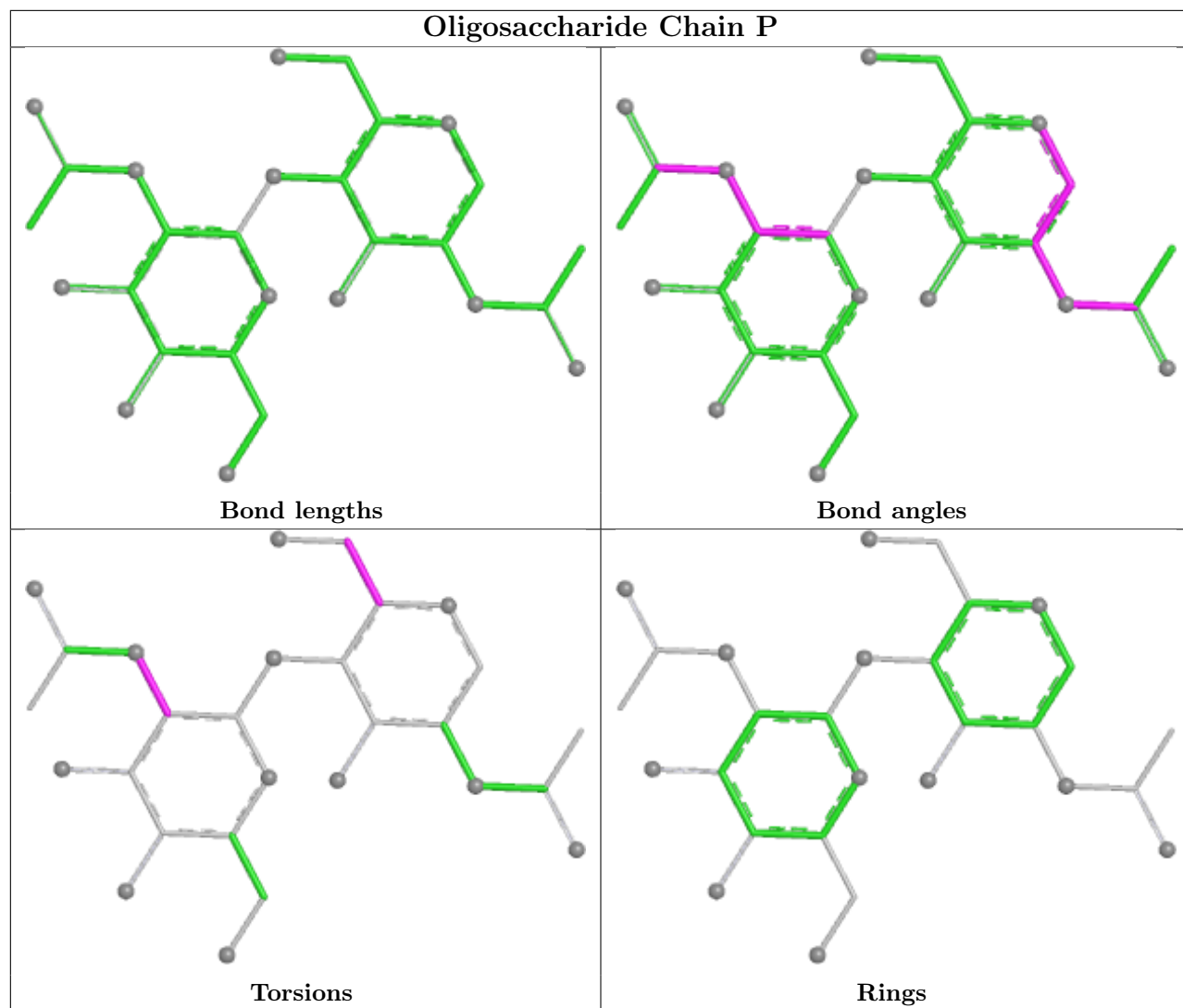


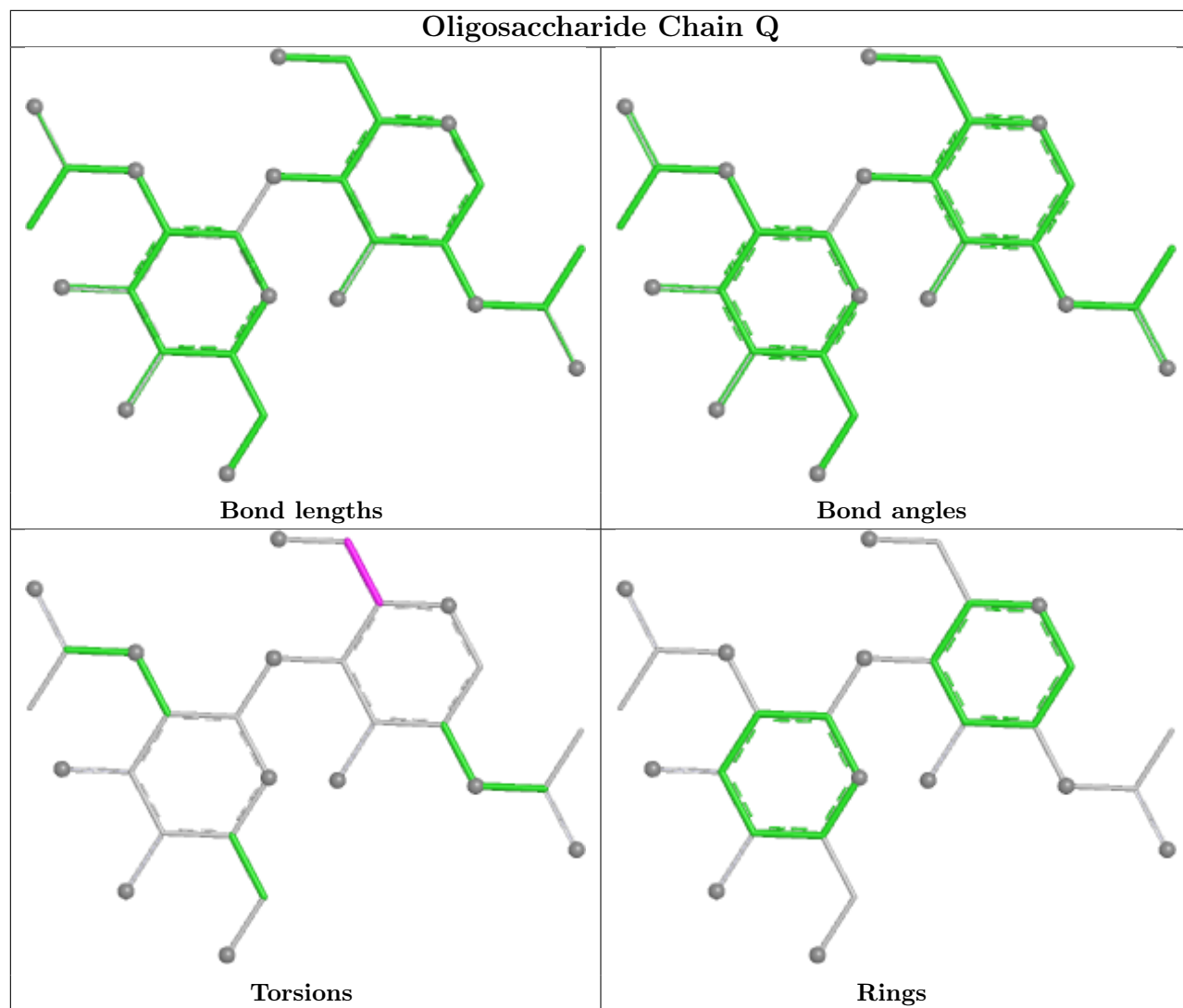


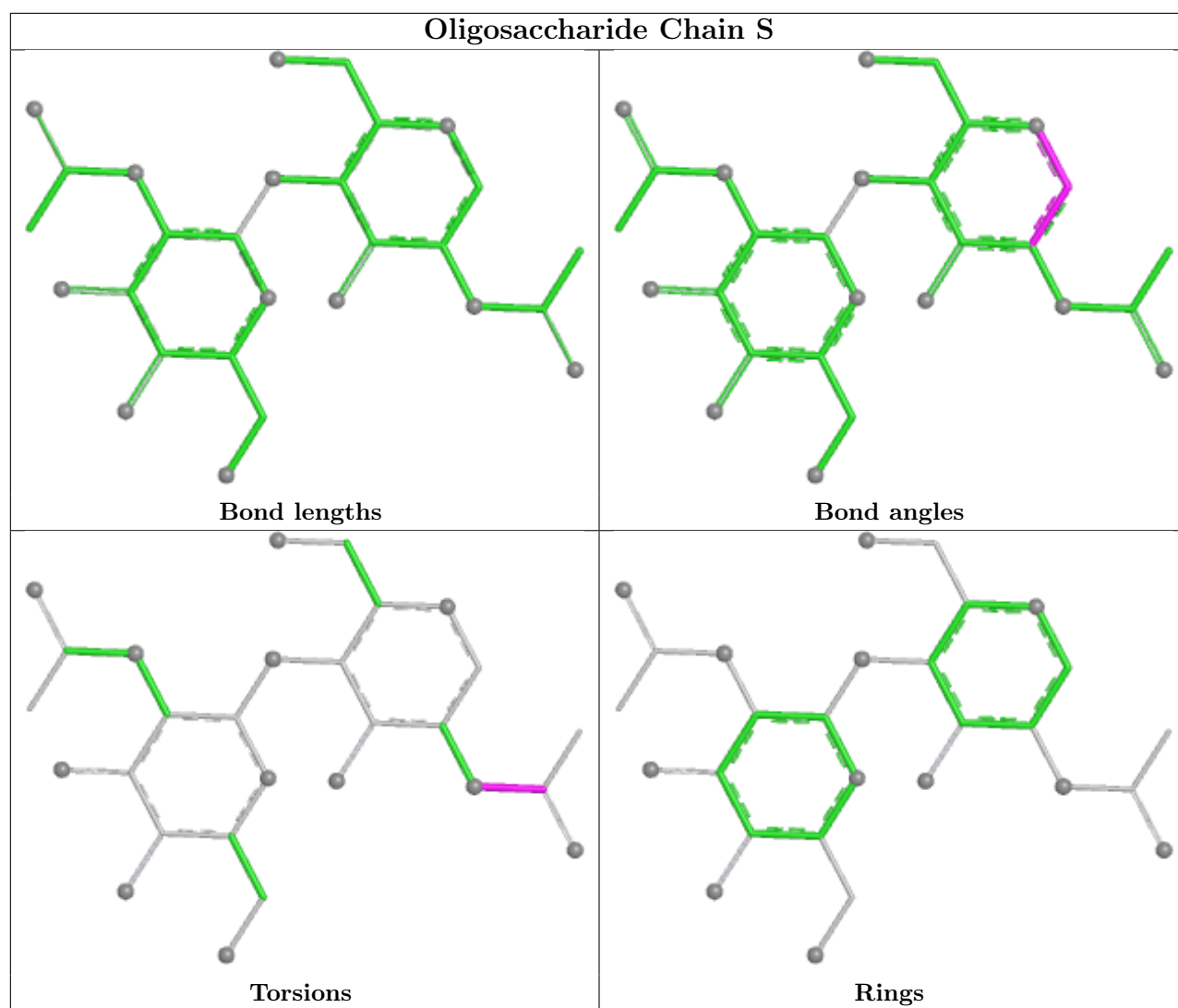


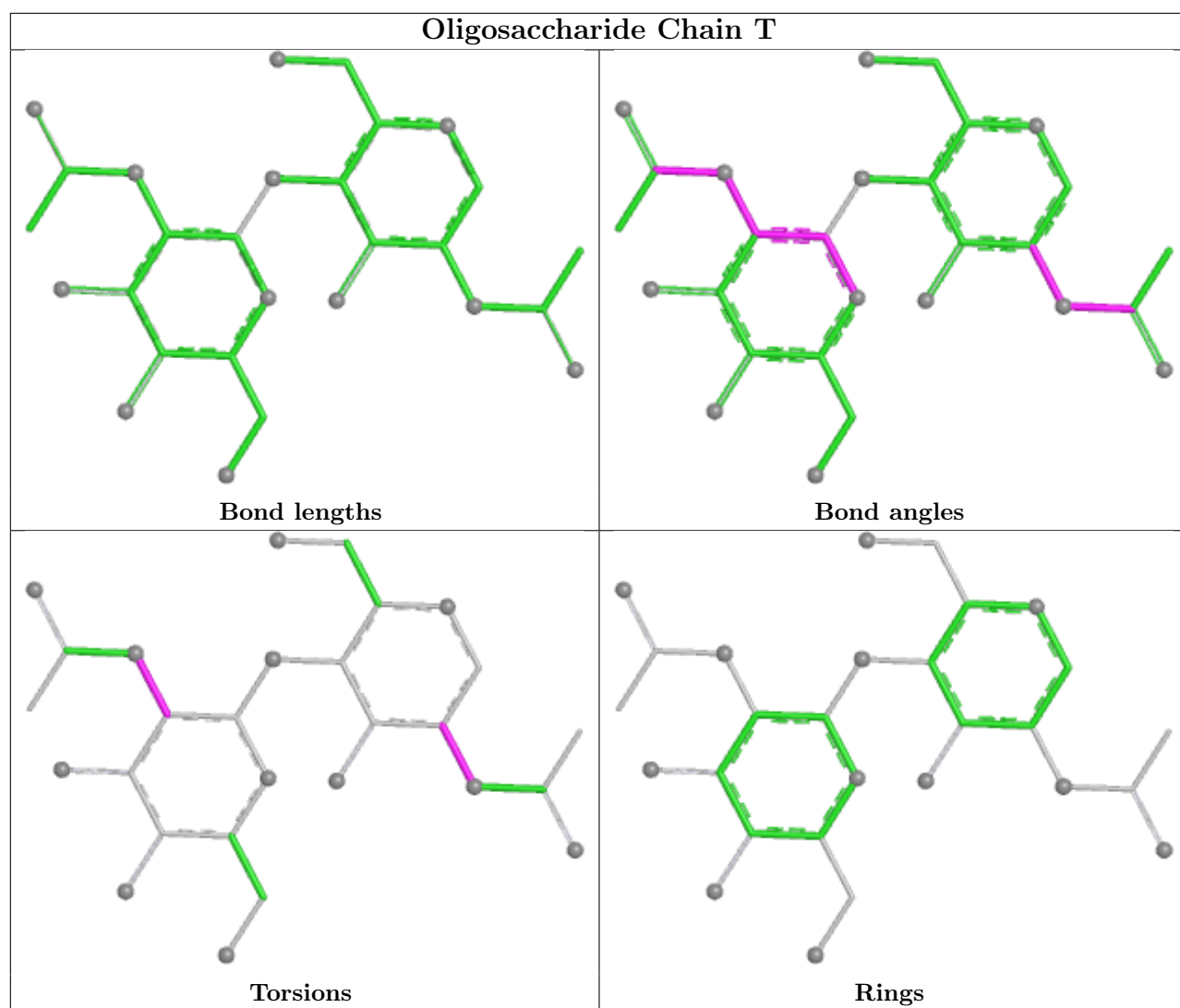


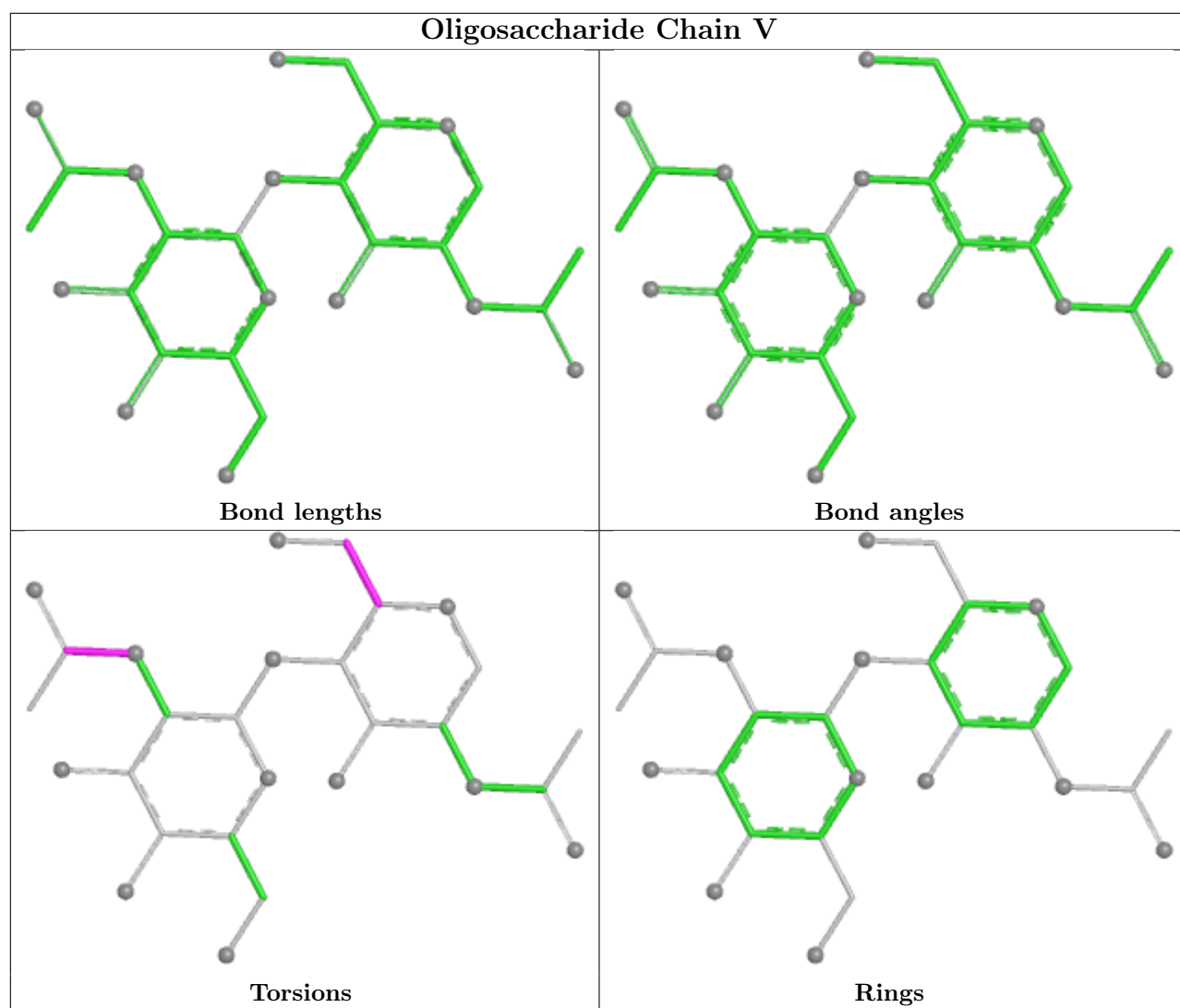


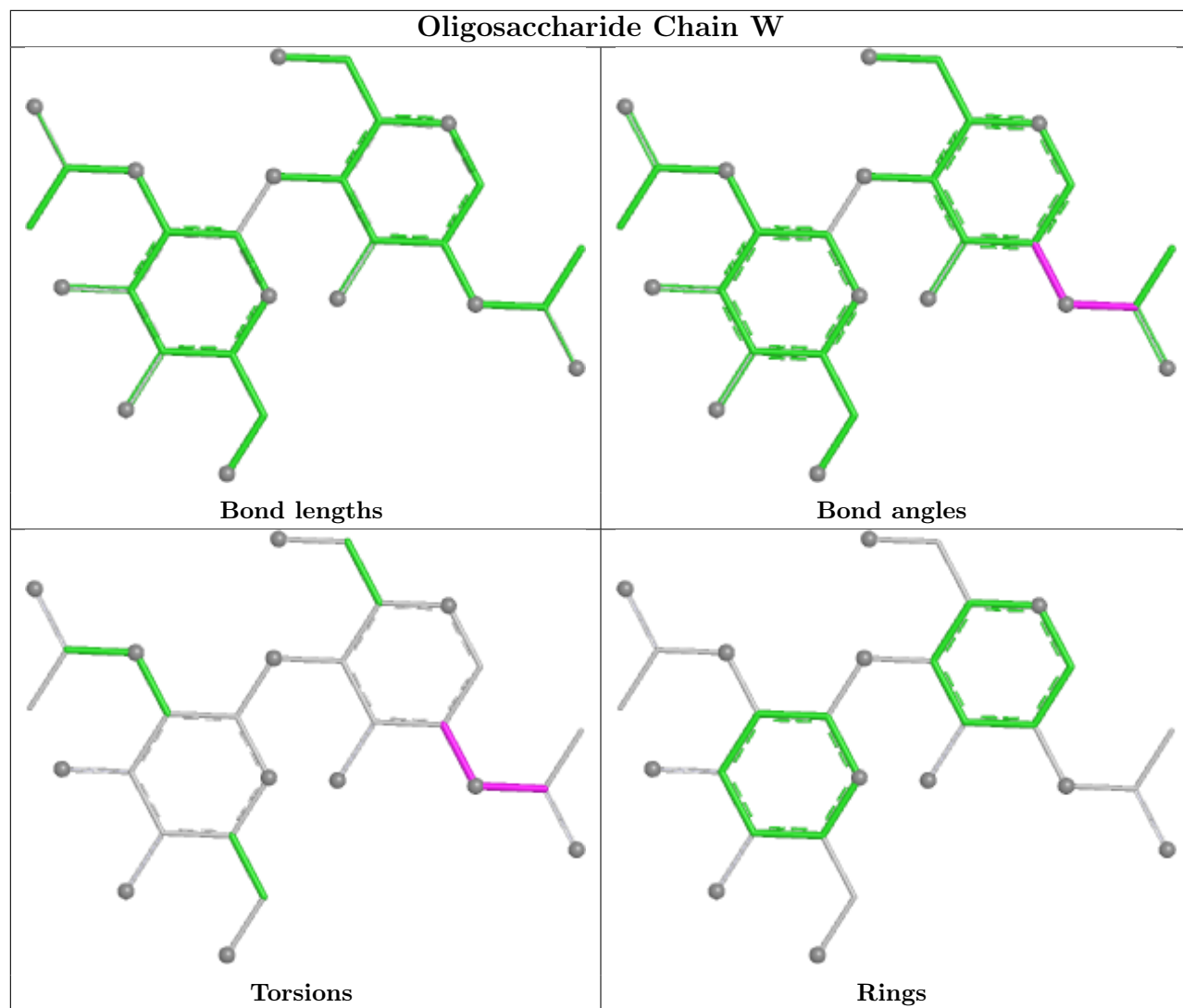


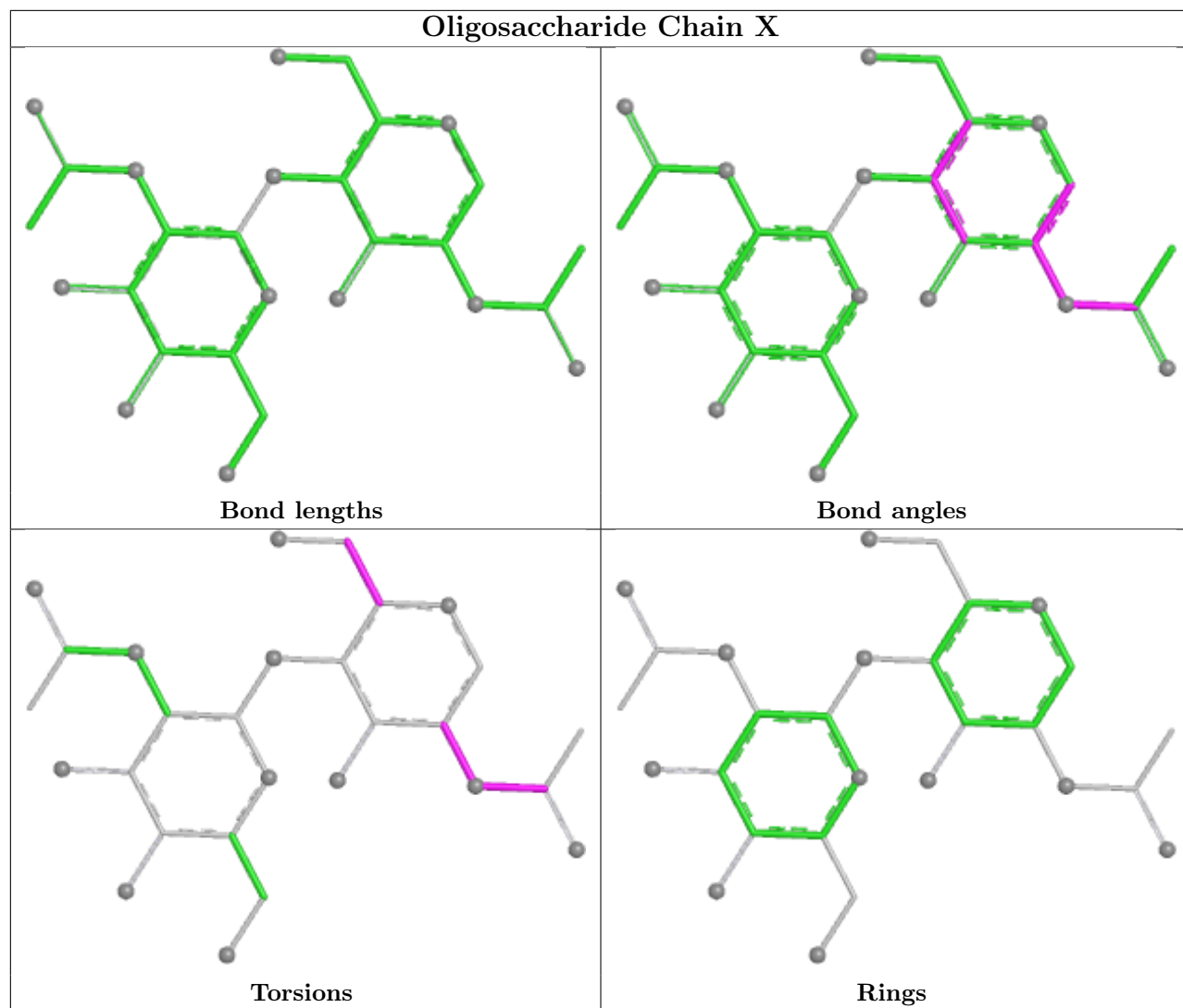


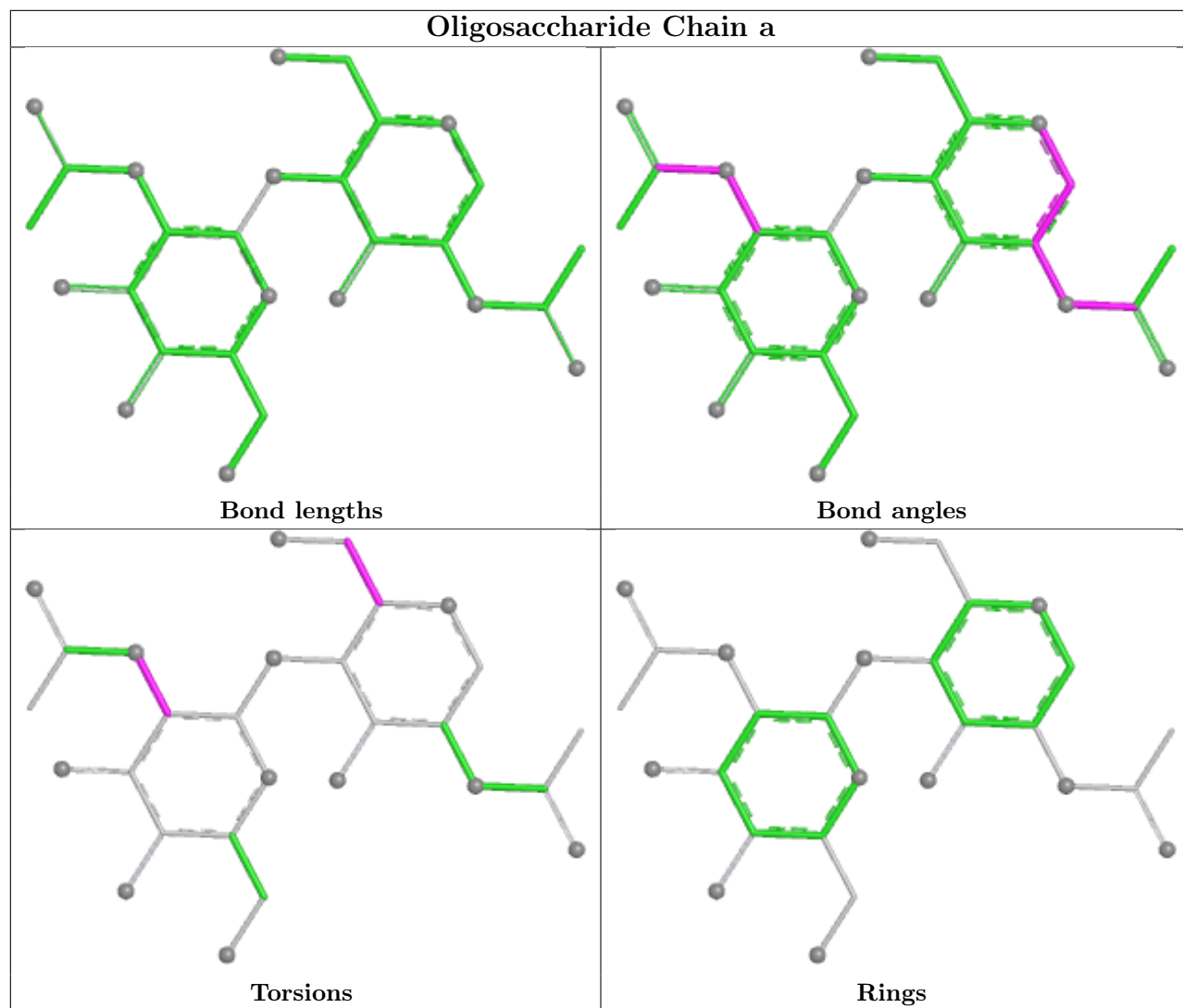


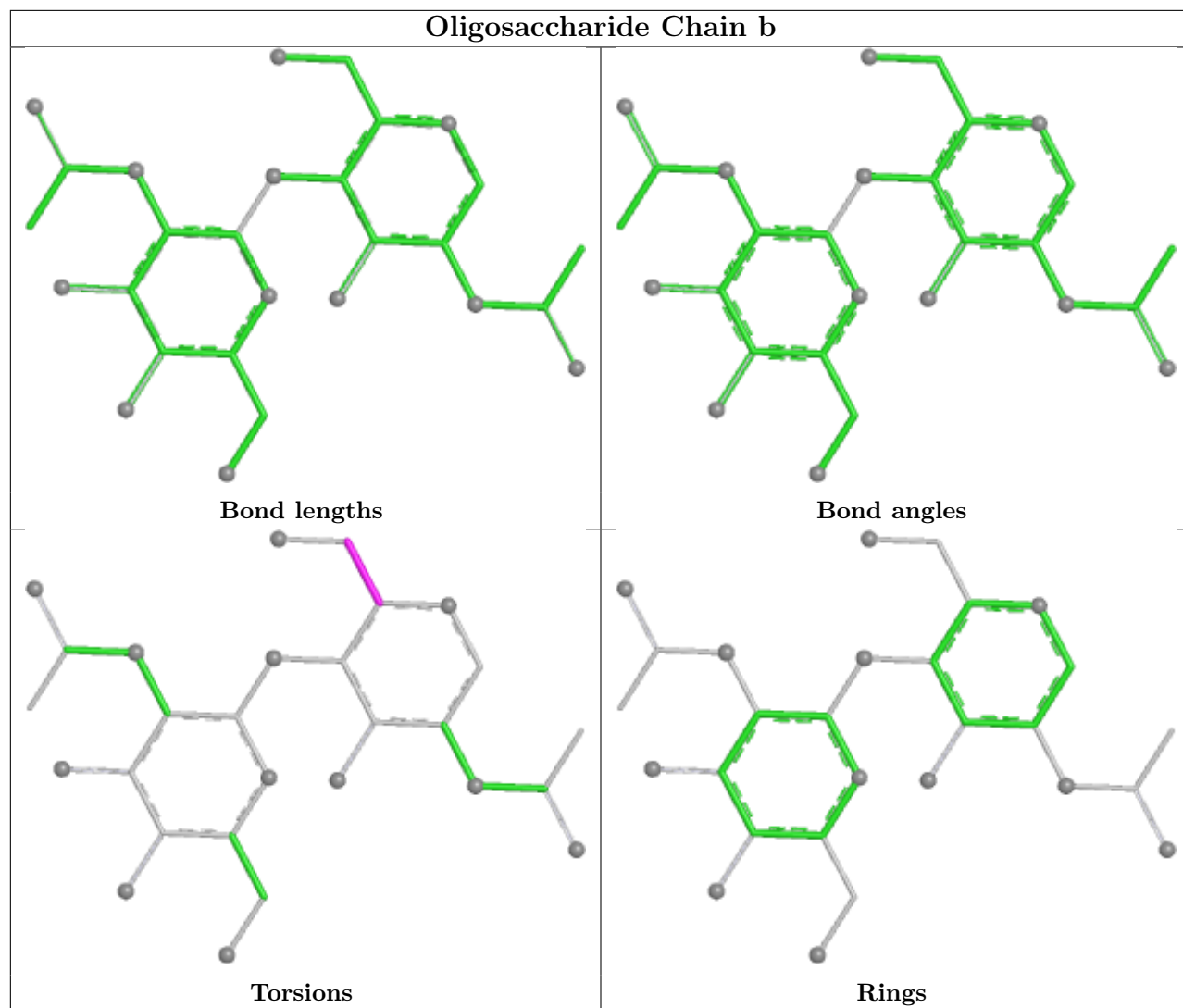


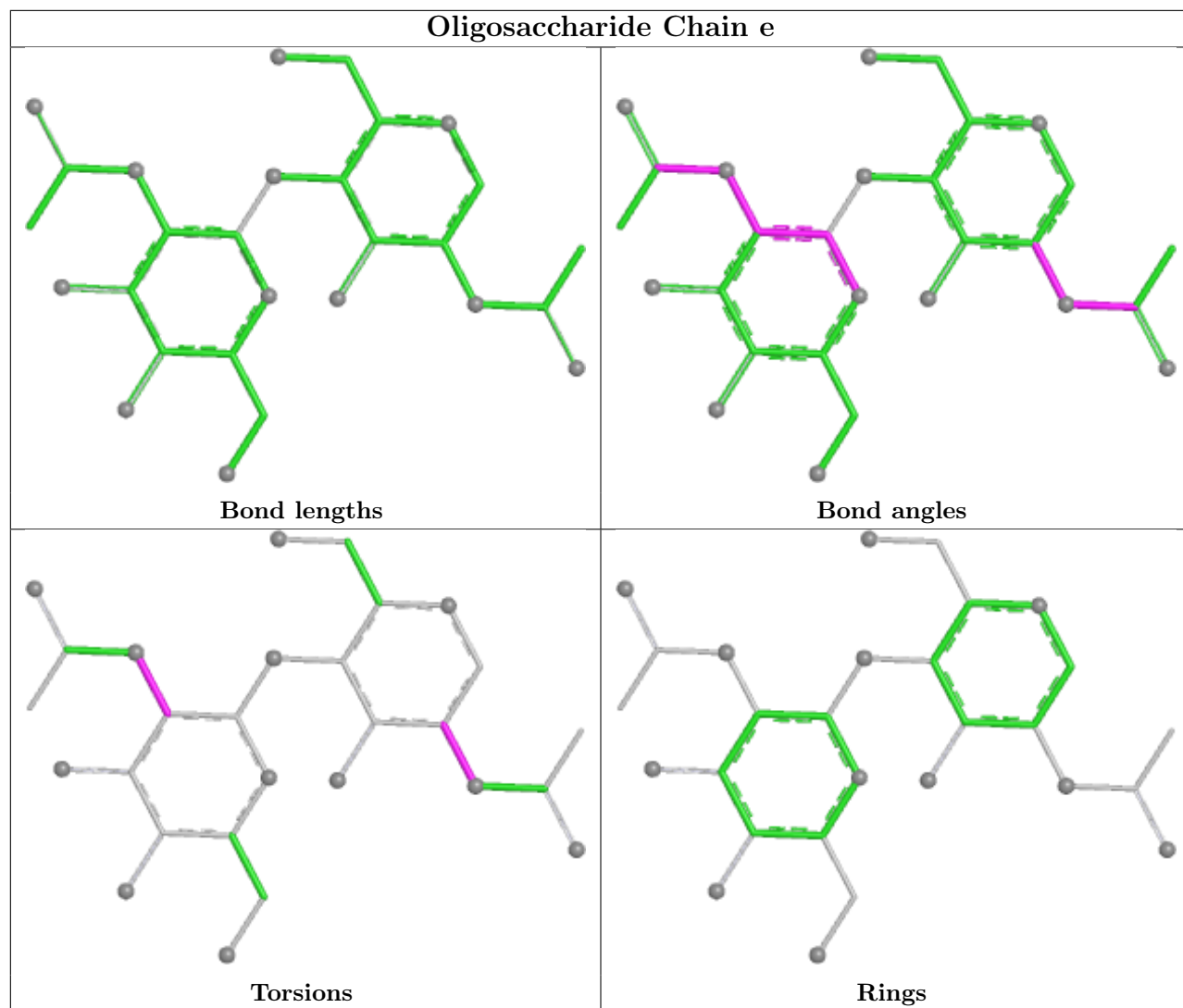


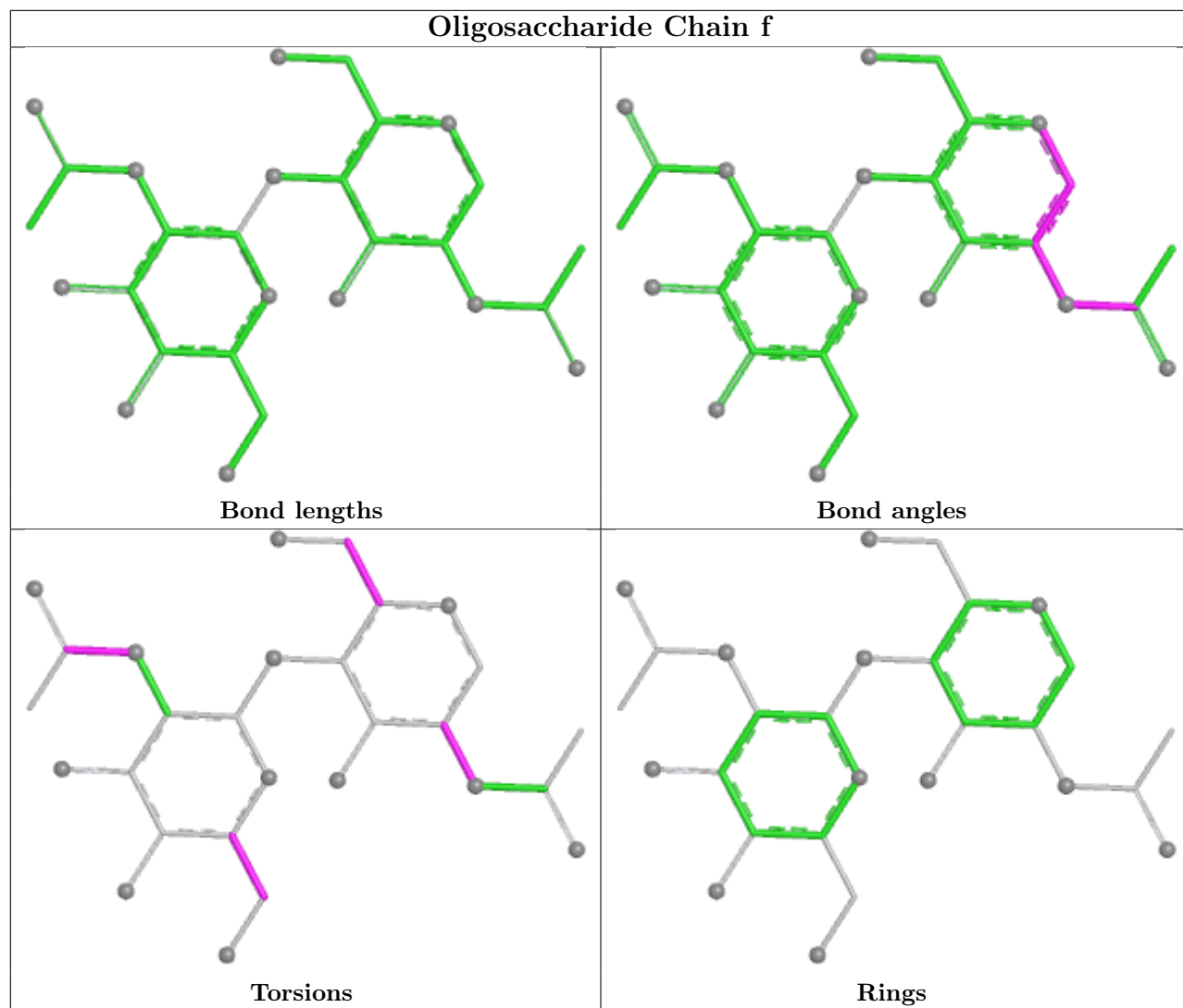


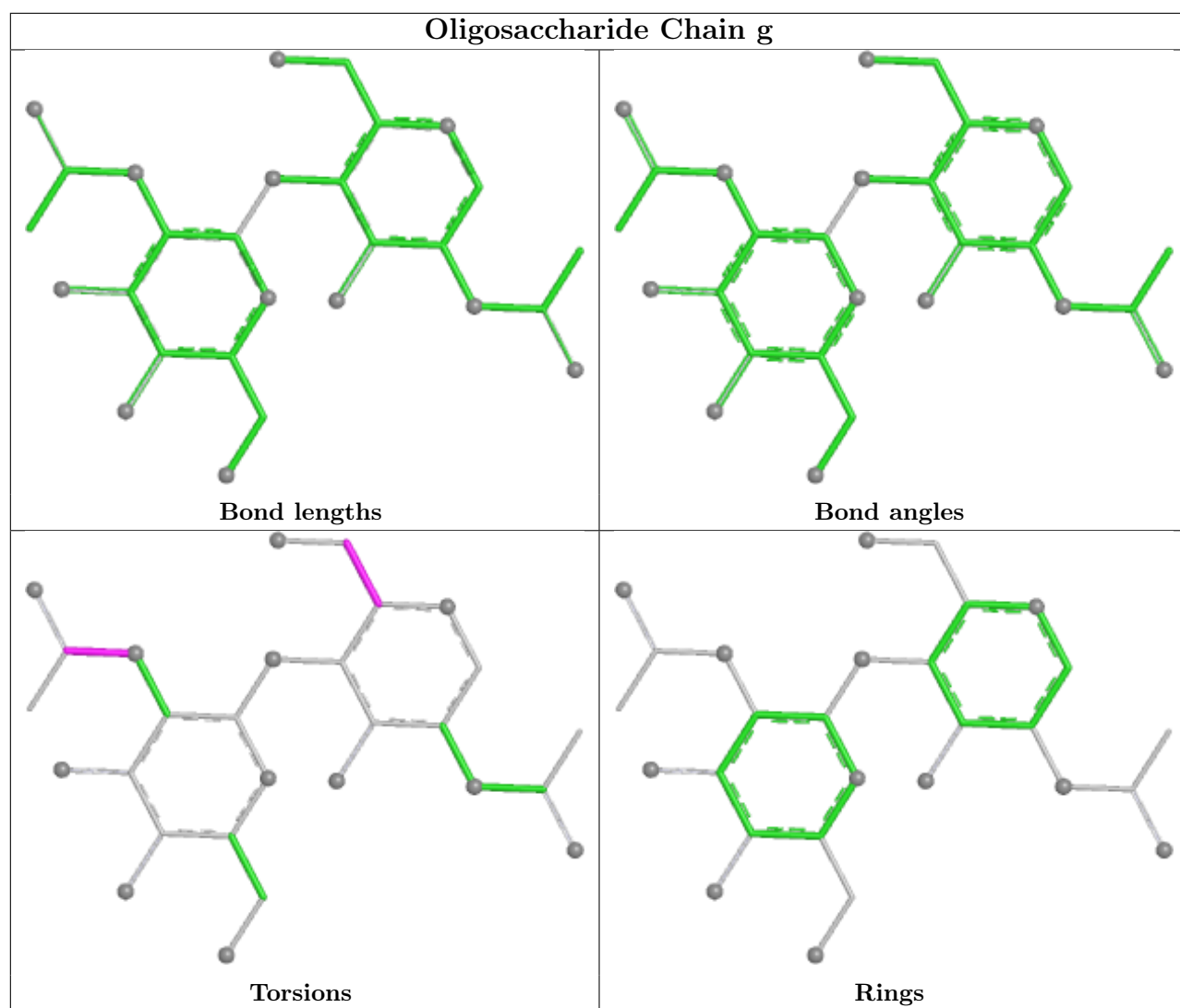


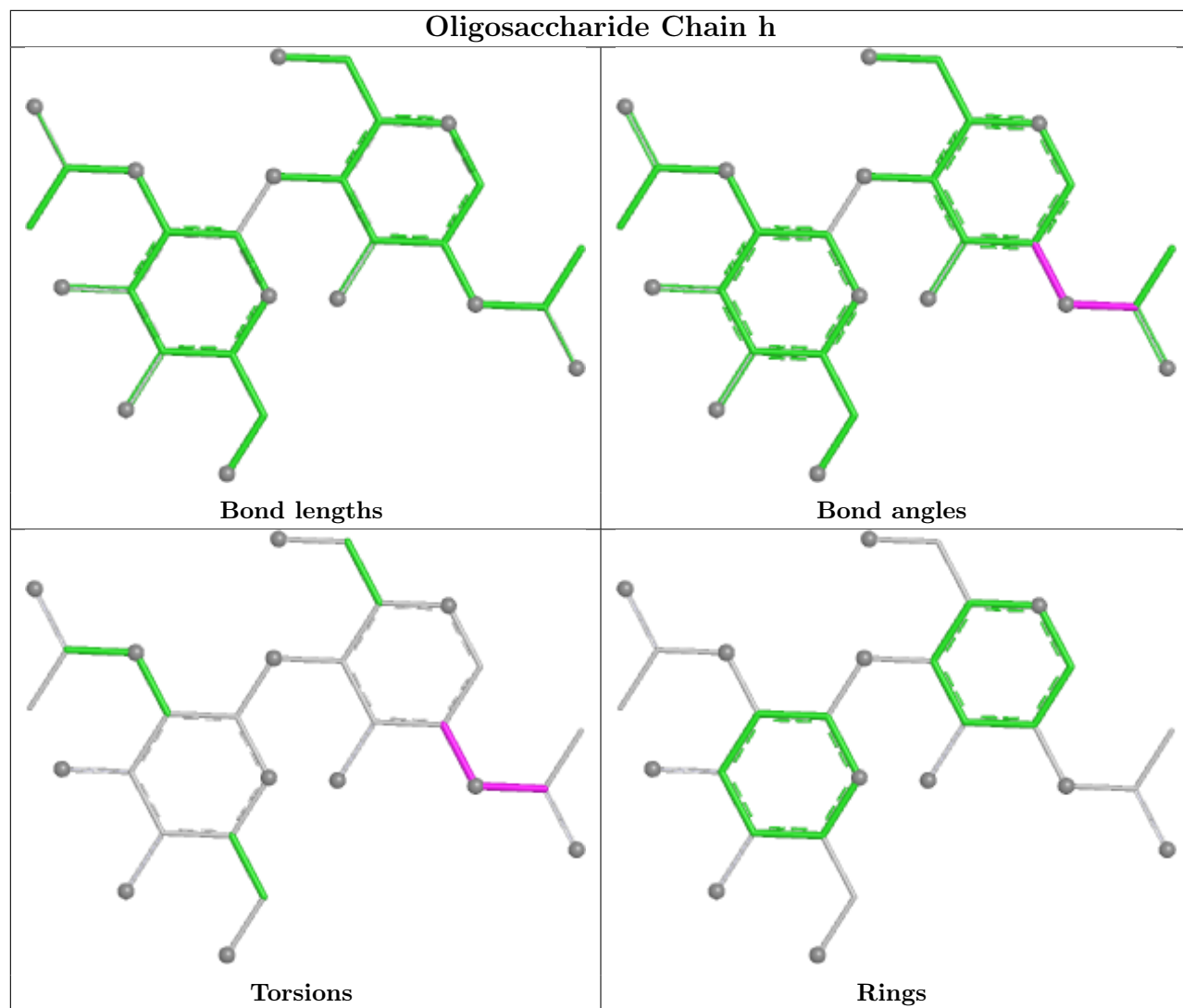


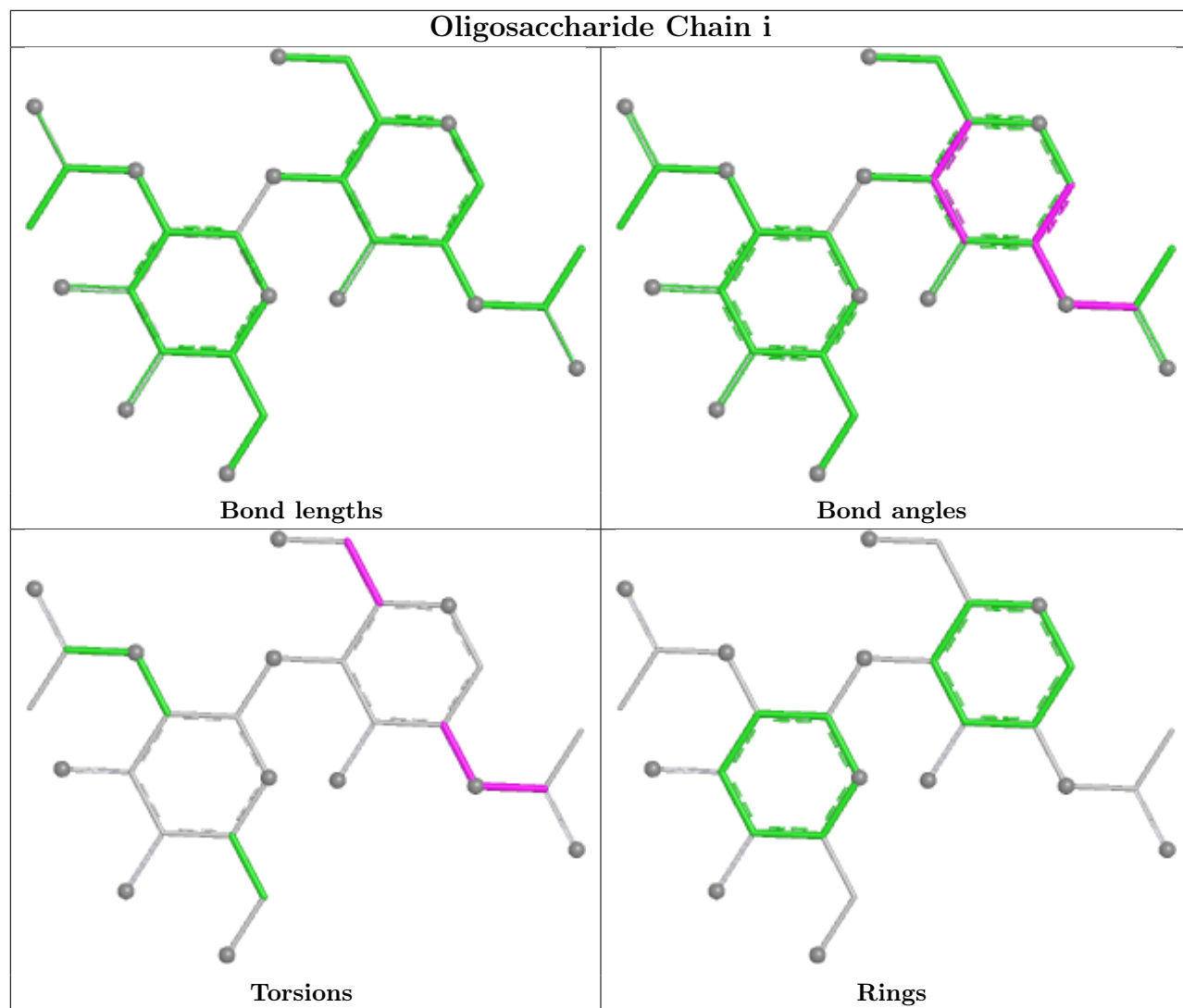


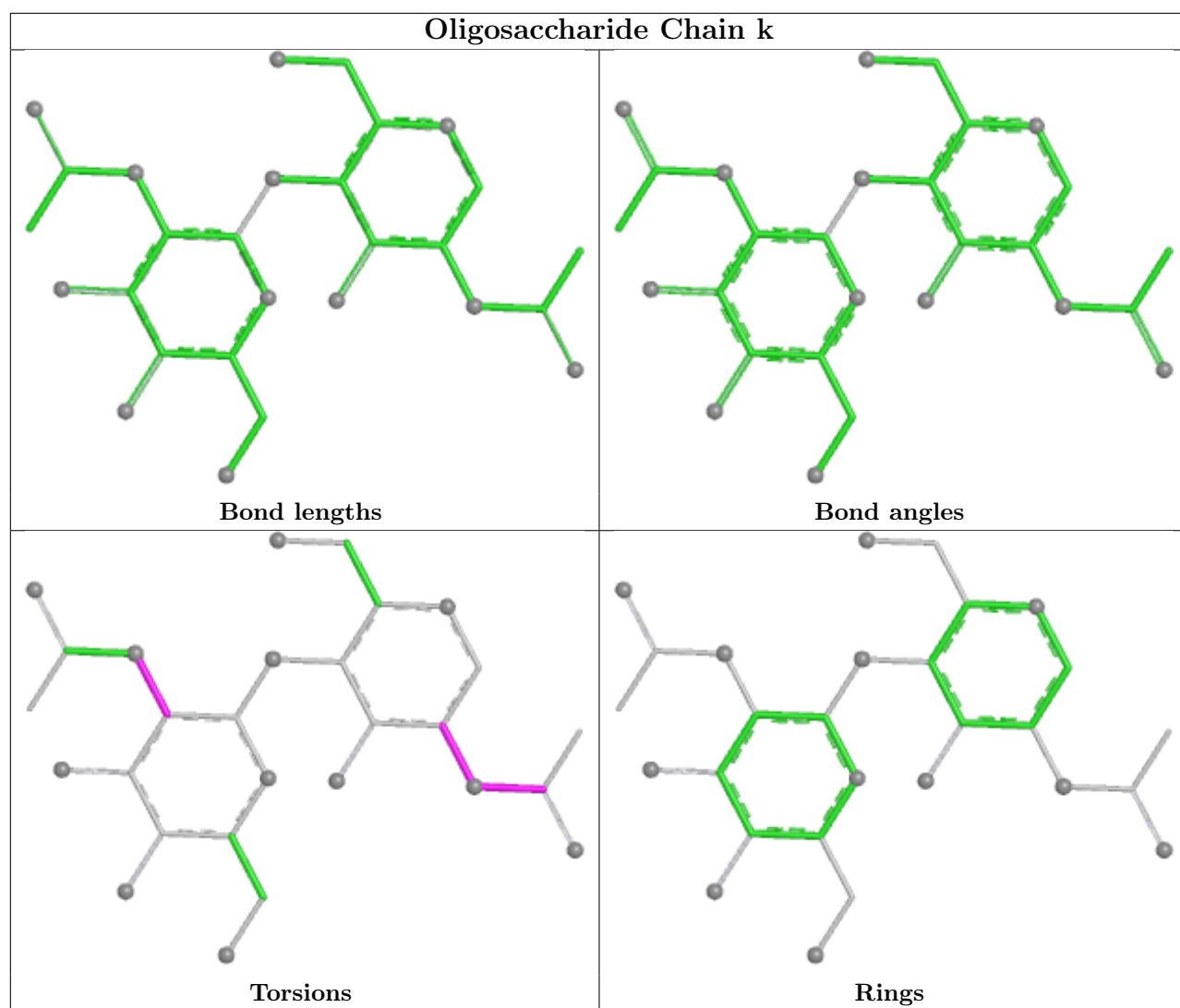


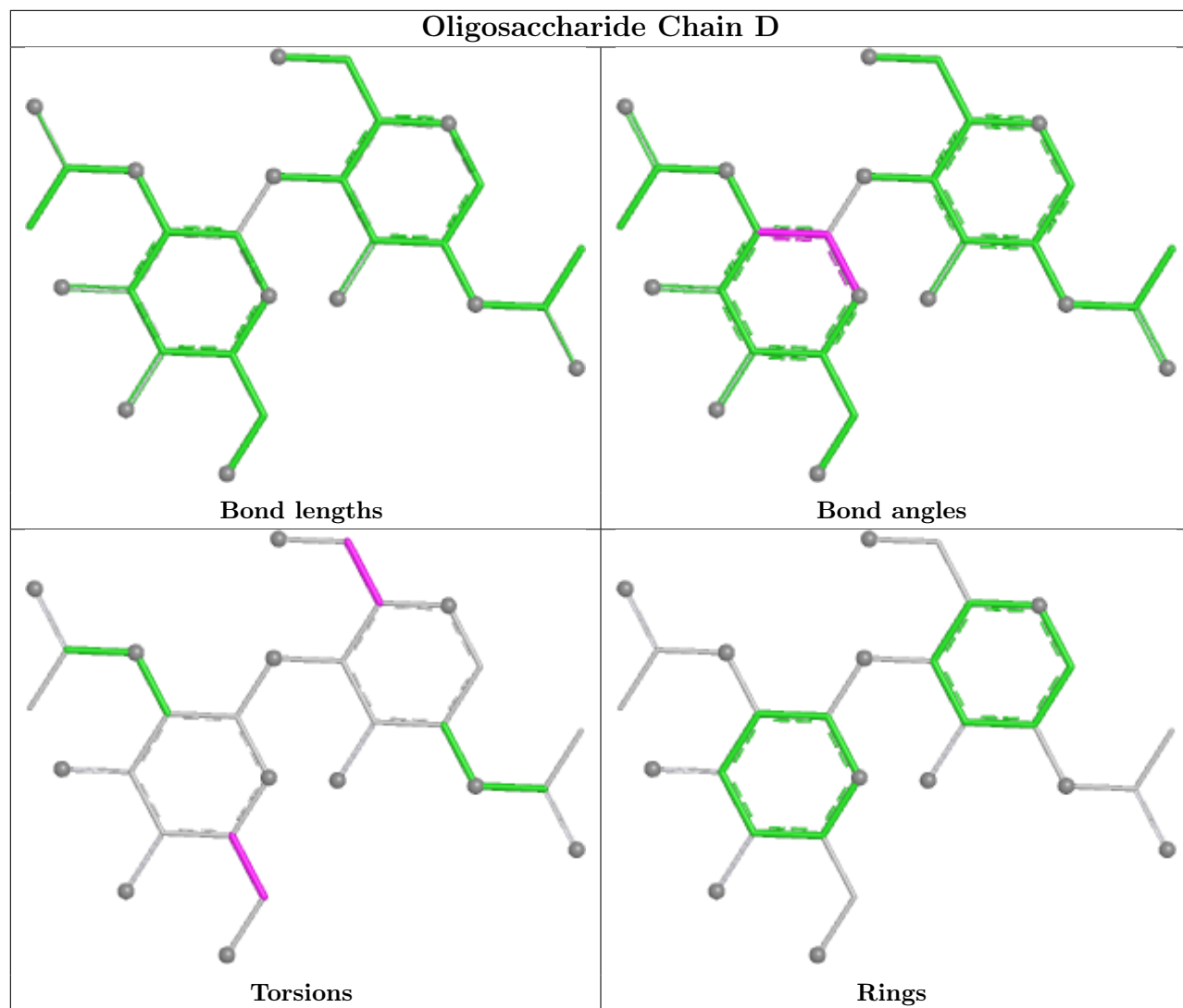


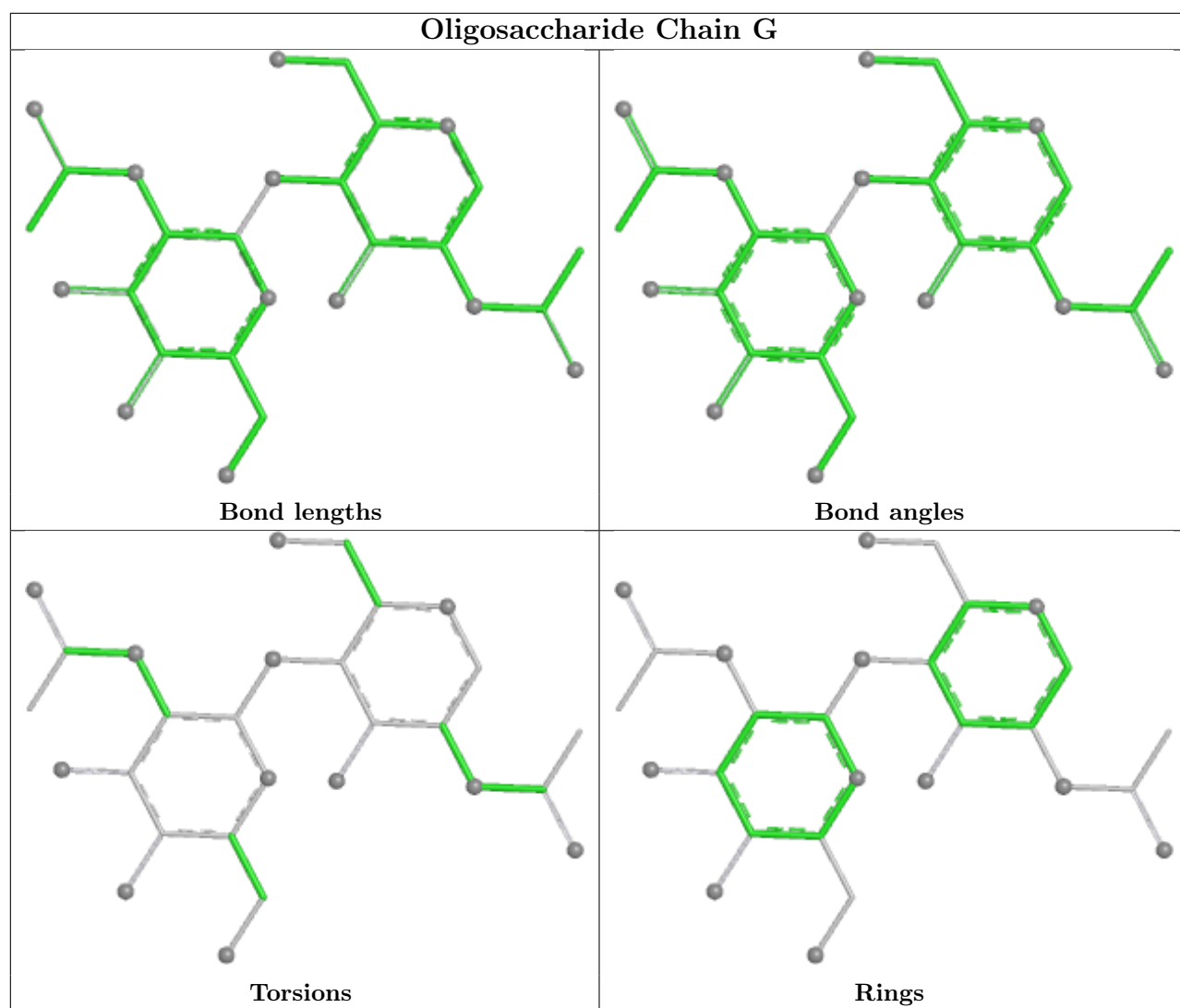


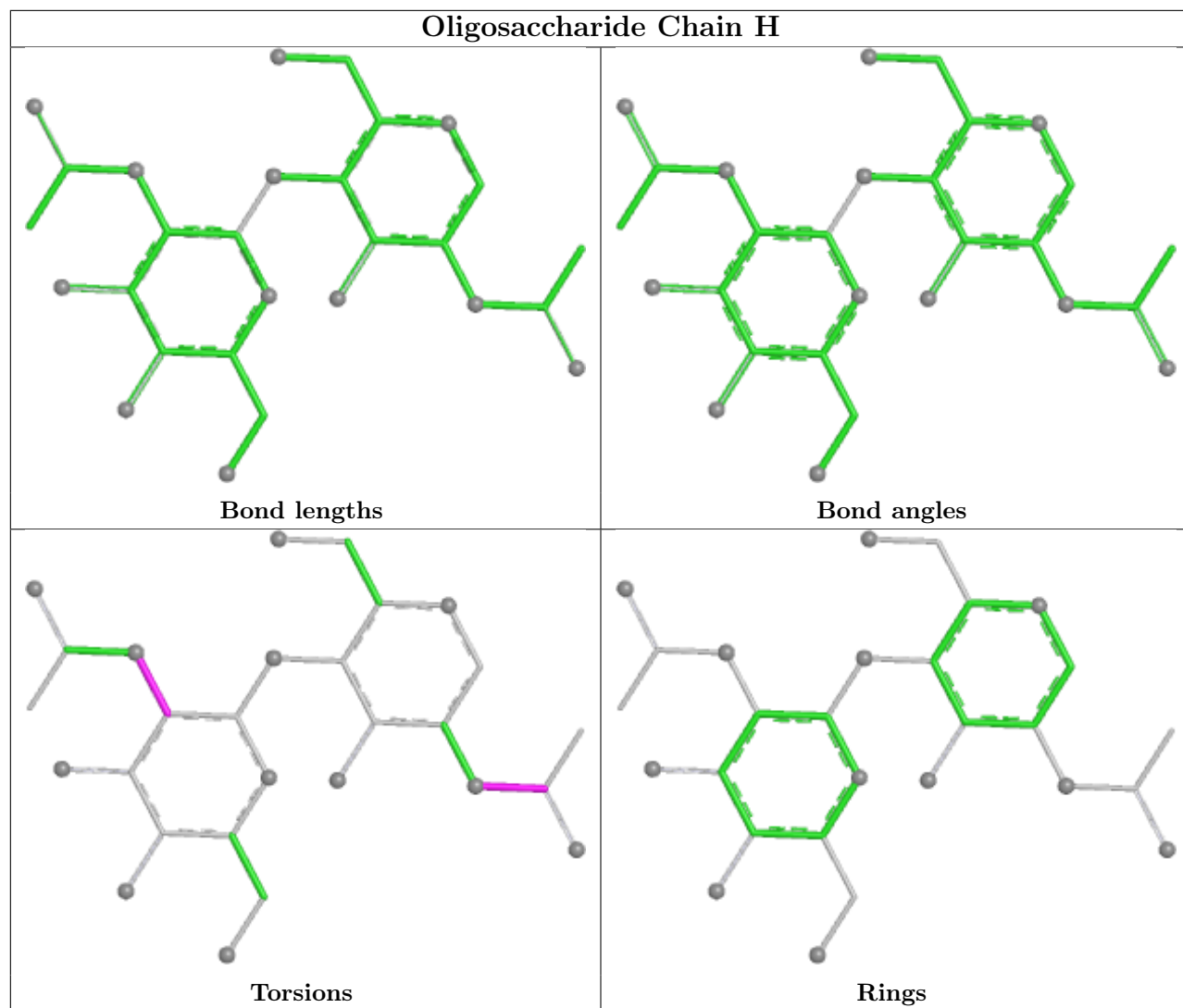


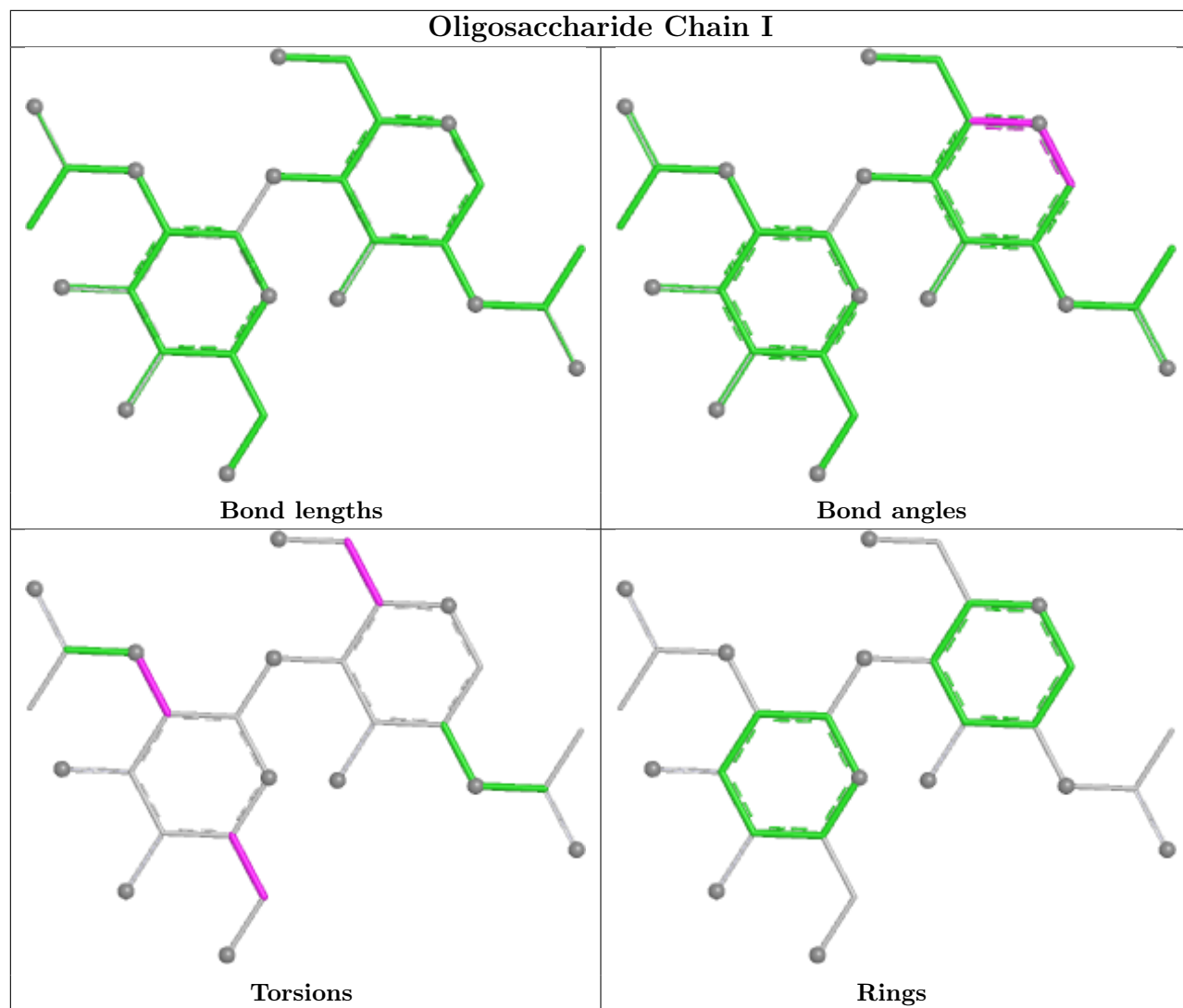


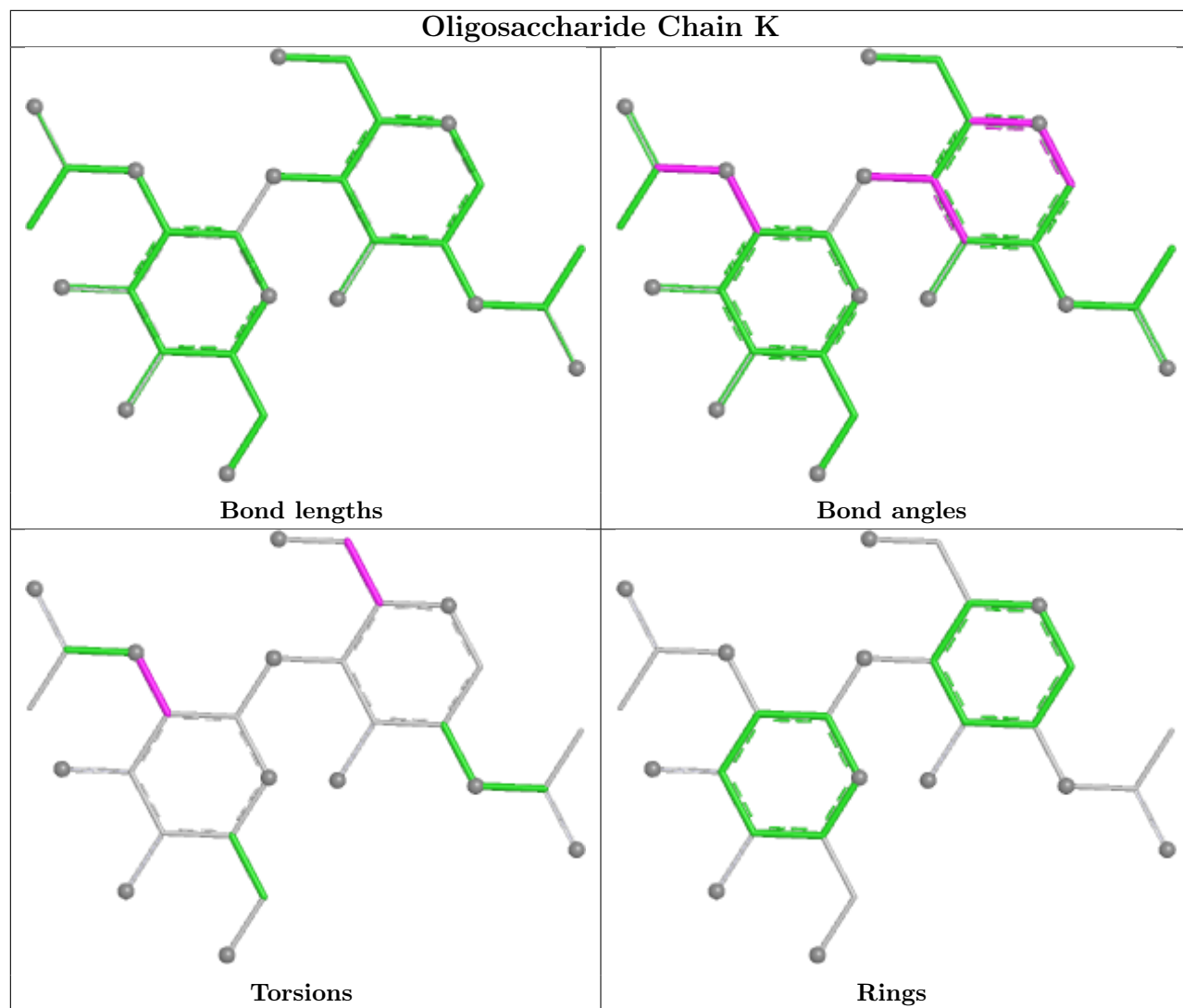


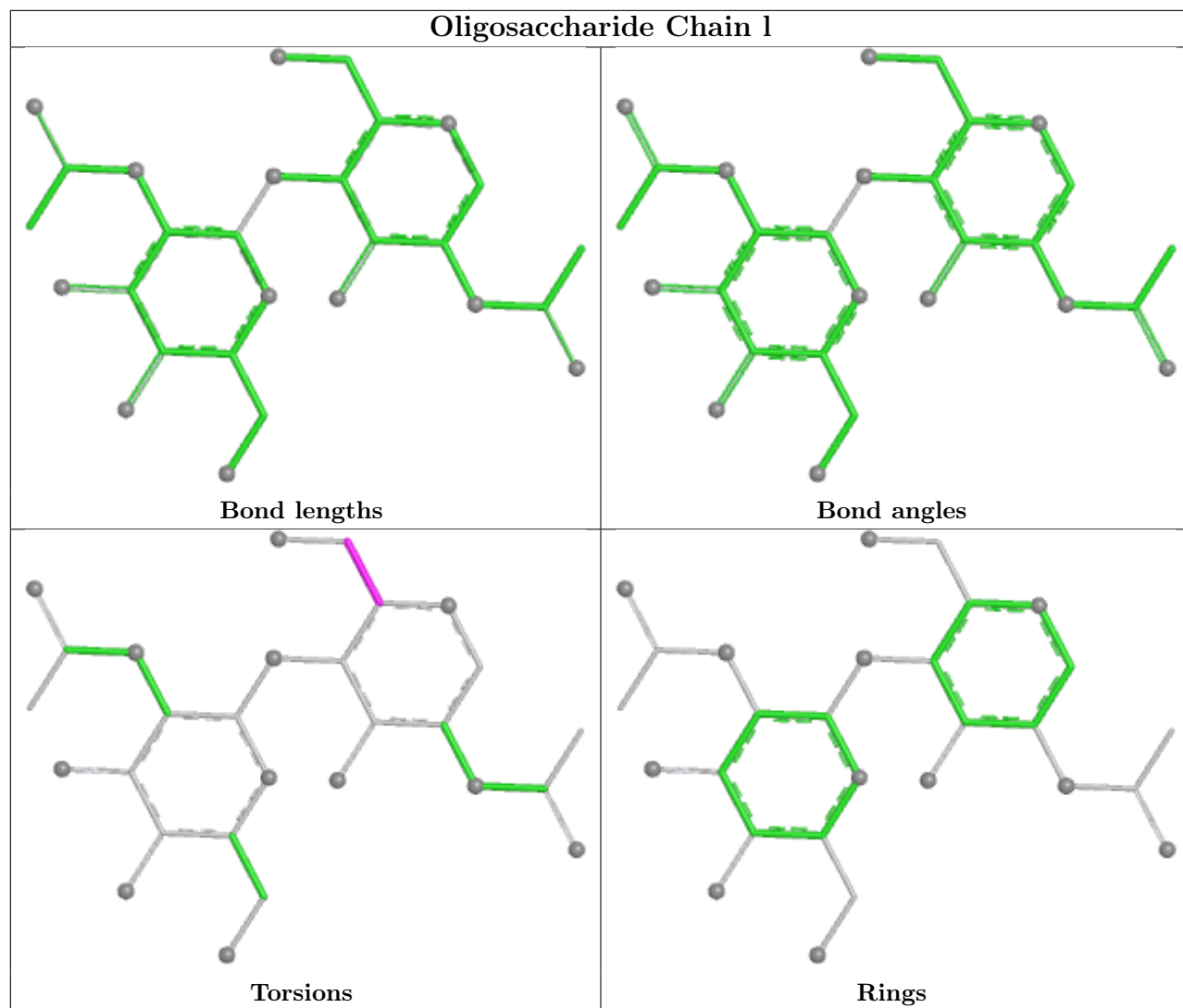


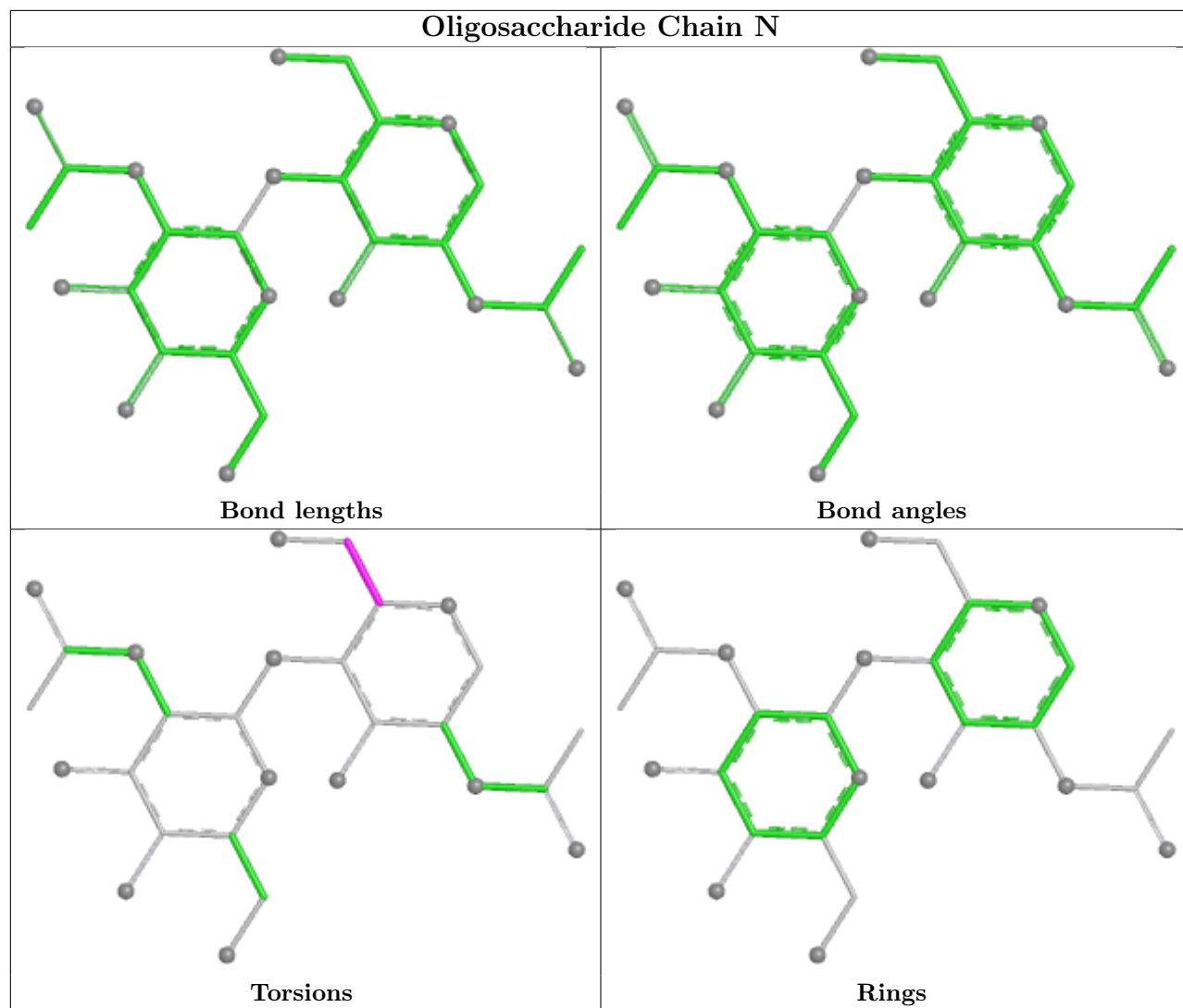


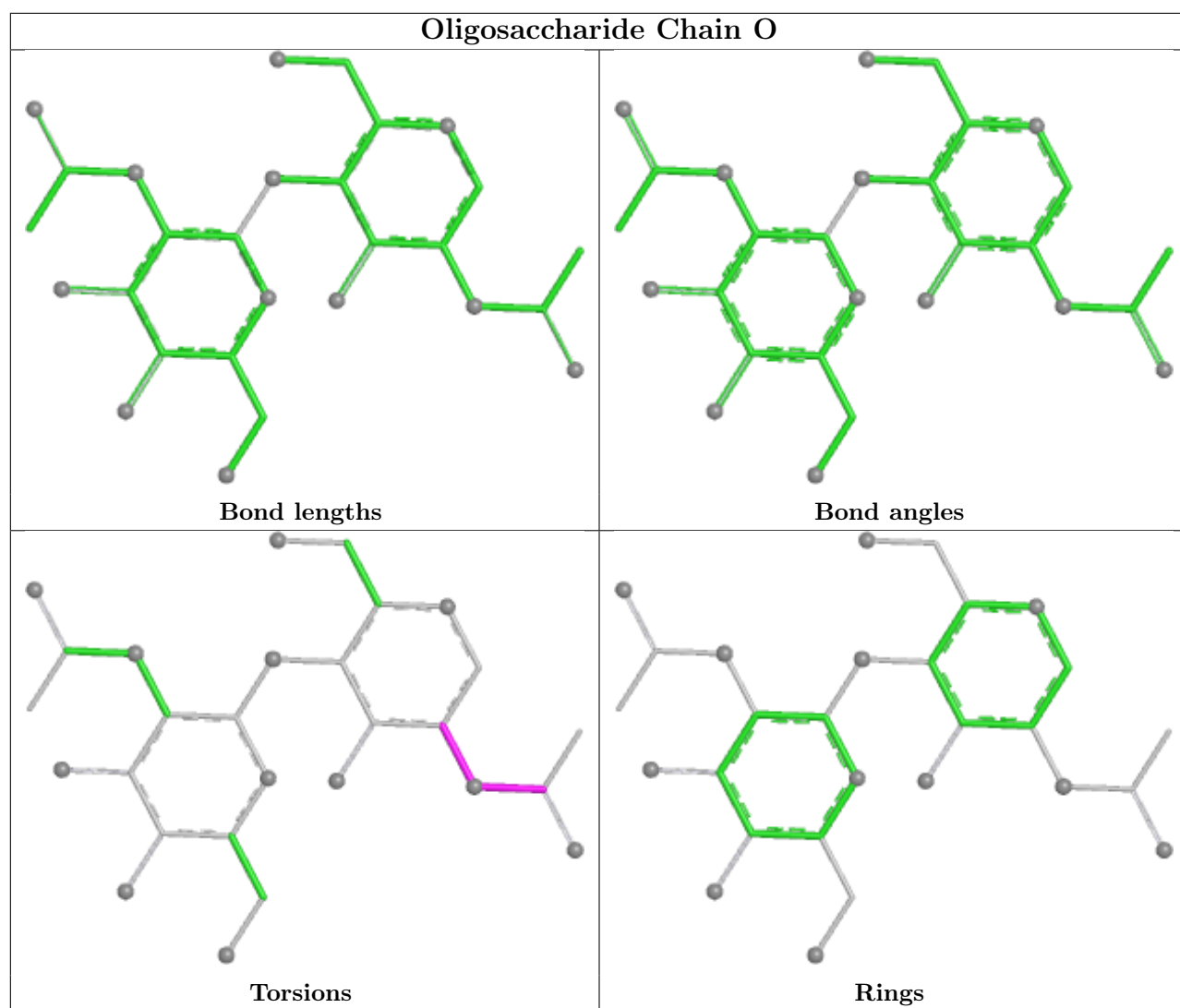


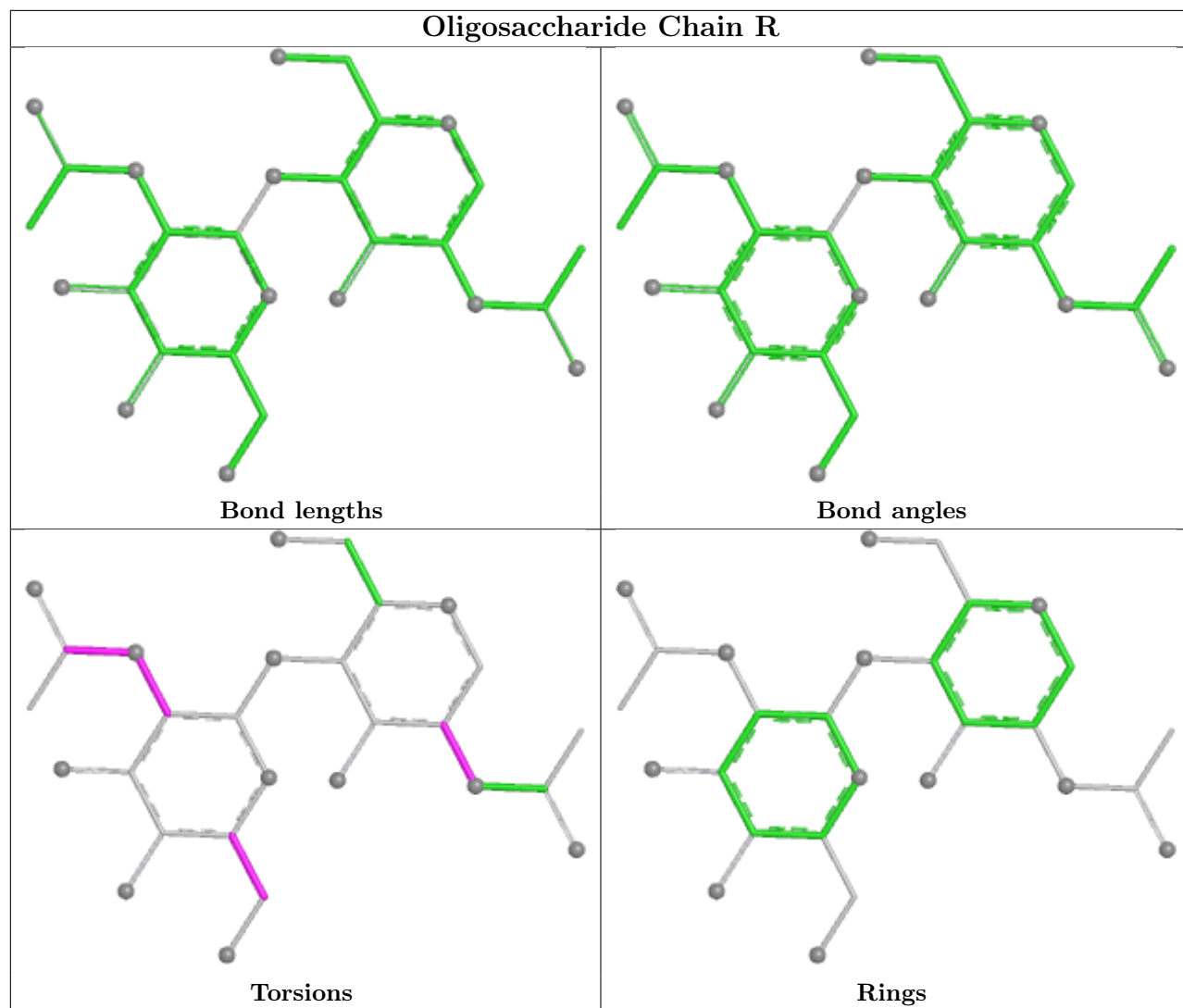


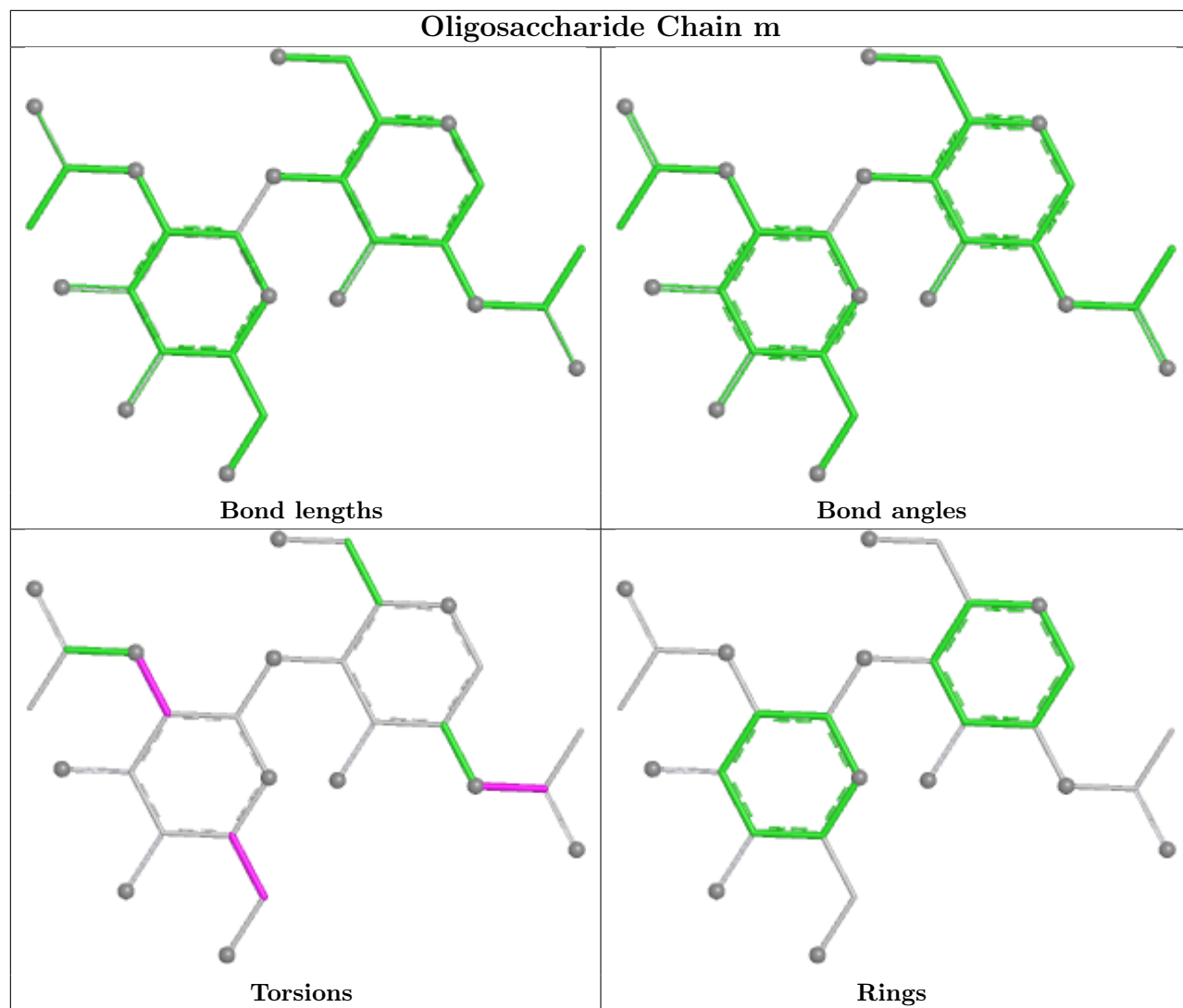


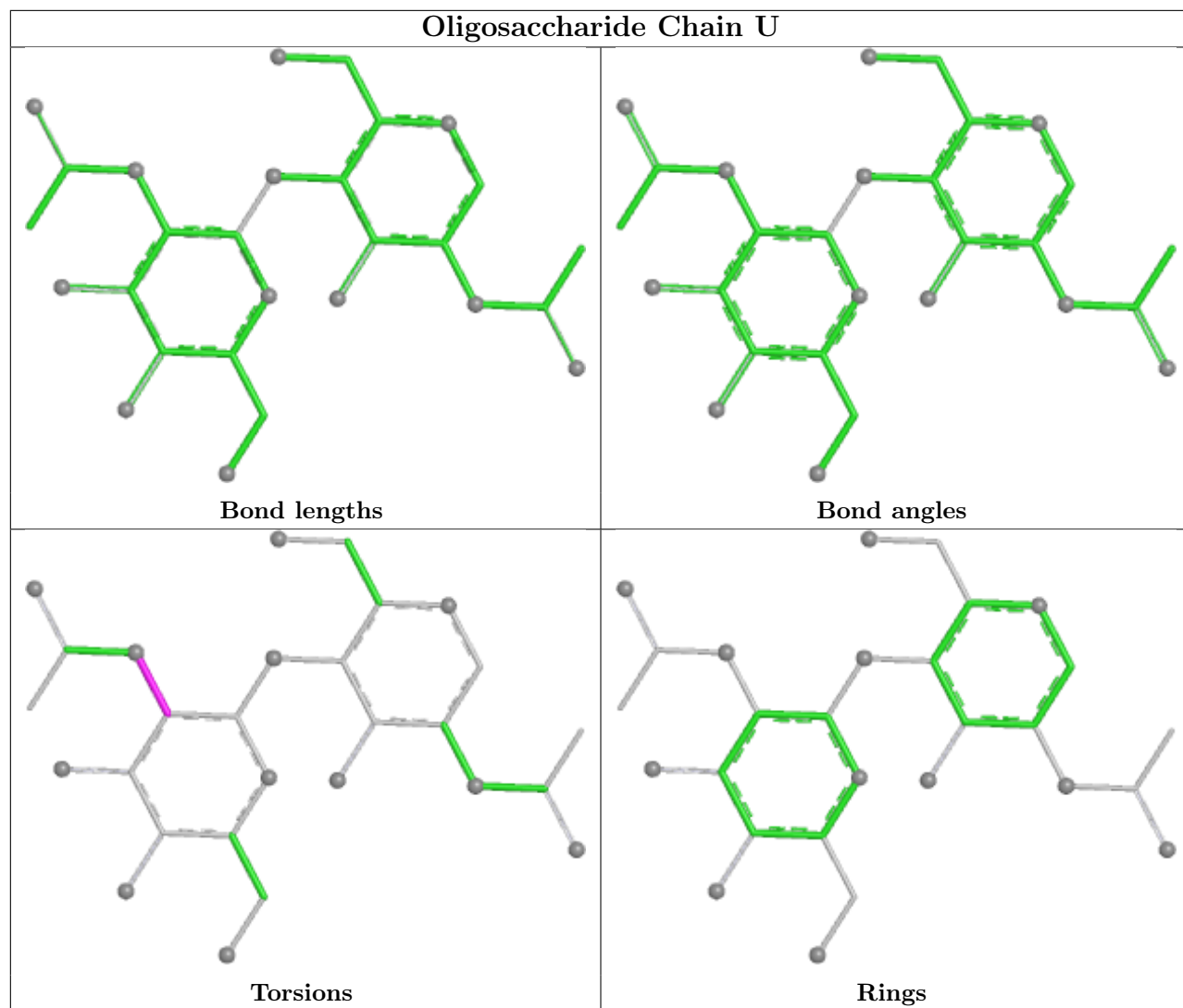


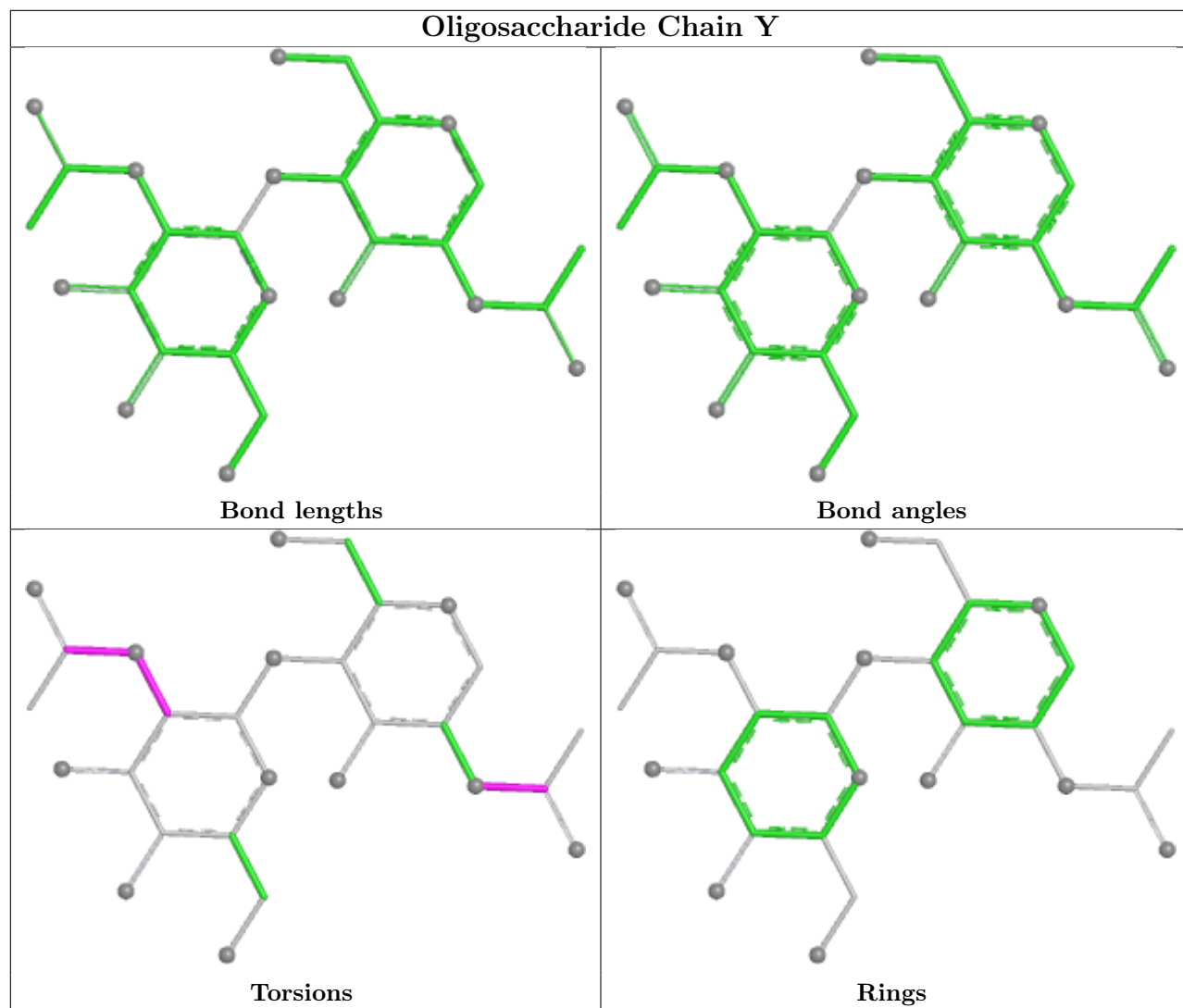


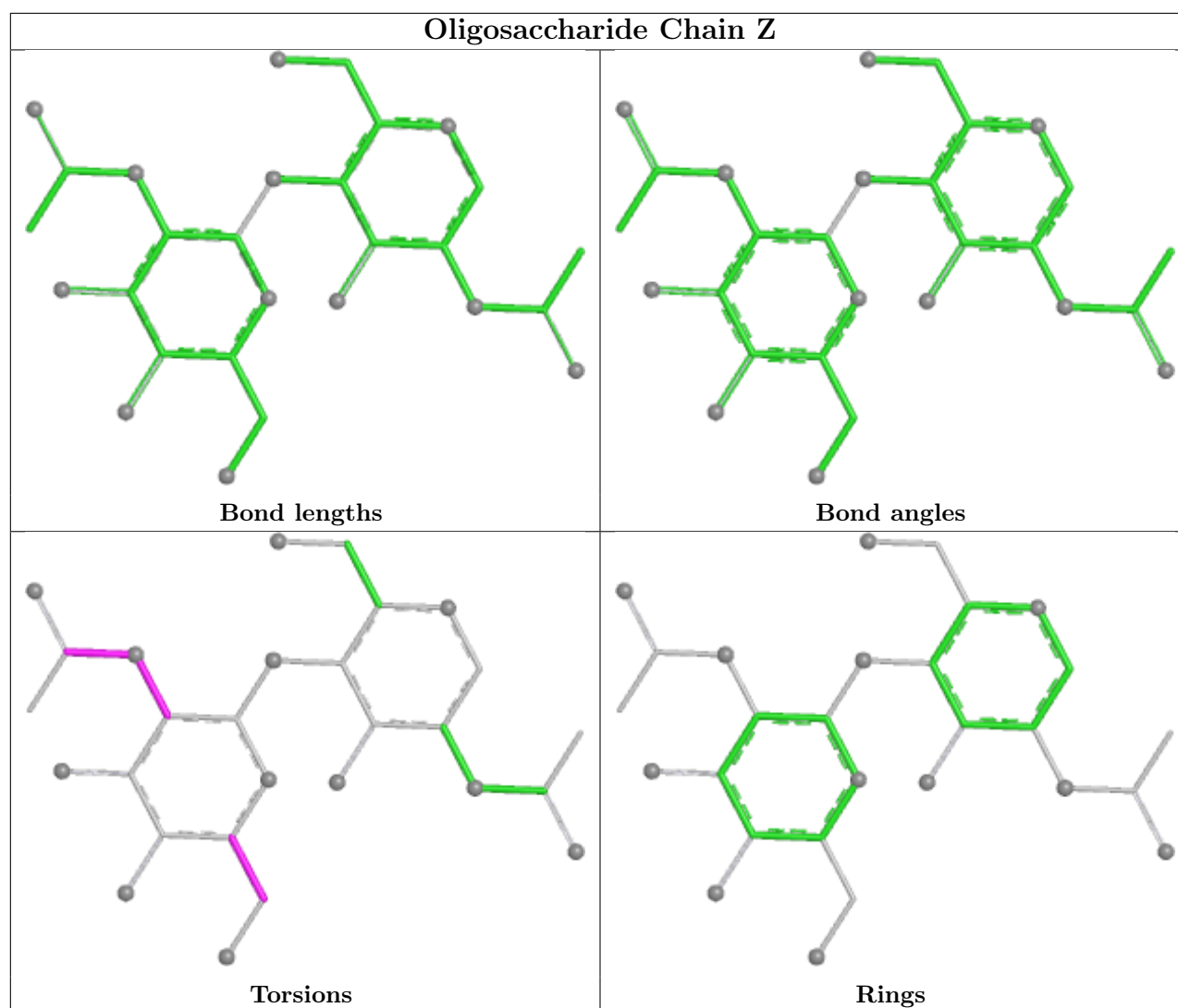












5.6 Ligand geometry [i](#)

30 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	1302	-	14,14,15	0.30	0	17,19,21	1.03	1 (5%)
3	NAG	A	1309	-	14,14,15	0.32	0	17,19,21	0.61	0
3	NAG	C	1307	-	14,14,15	0.30	0	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1305	-	14,14,15	0.33	0	17,19,21	0.63	0
3	NAG	C	1306	-	14,14,15	0.29	0	17,19,21	1.05	1 (5%)
4	EIC	C	1310	-	19,19,19	1.35	2 (10%)	19,19,19	1.15	0
3	NAG	C	1305	-	14,14,15	0.33	0	17,19,21	0.63	0
4	EIC	A	1310	-	19,19,19	1.36	2 (10%)	19,19,19	1.15	0
3	NAG	A	1308	-	14,14,15	0.29	0	17,19,21	1.08	1 (5%)
3	NAG	C	1304	-	14,14,15	0.28	0	17,19,21	0.60	0
3	NAG	C	1303	-	14,14,15	0.28	0	17,19,21	0.92	1 (5%)
3	NAG	A	1307	-	14,14,15	0.30	0	17,19,21	1.08	1 (5%)
3	NAG	B	1309	-	14,14,15	0.32	0	17,19,21	0.61	0
3	NAG	C	1302	-	14,14,15	0.29	0	17,19,21	1.03	1 (5%)
3	NAG	C	1308	-	14,14,15	0.29	0	17,19,21	1.08	1 (5%)
3	NAG	A	1304	-	14,14,15	0.28	0	17,19,21	0.60	0
3	NAG	A	1303	-	14,14,15	0.27	0	17,19,21	0.92	1 (5%)
3	NAG	B	1307	-	14,14,15	0.29	0	17,19,21	1.08	1 (5%)
3	NAG	A	1306	-	14,14,15	0.29	0	17,19,21	1.04	1 (5%)
3	NAG	B	1304	-	14,14,15	0.28	0	17,19,21	0.60	0
3	NAG	A	1301	-	14,14,15	0.32	0	17,19,21	0.92	1 (5%)
3	NAG	B	1306	-	14,14,15	0.29	0	17,19,21	1.04	1 (5%)
3	NAG	C	1301	-	14,14,15	0.32	0	17,19,21	0.92	1 (5%)
3	NAG	B	1303	-	14,14,15	0.28	0	17,19,21	0.92	1 (5%)
3	NAG	B	1301	-	14,14,15	0.32	0	17,19,21	0.92	1 (5%)
3	NAG	C	1309	-	14,14,15	0.32	0	17,19,21	0.61	0
4	EIC	B	1310	-	19,19,19	1.36	2 (10%)	19,19,19	1.16	0
3	NAG	B	1308	-	14,14,15	0.30	0	17,19,21	1.07	1 (5%)
3	NAG	A	1302	-	14,14,15	0.29	0	17,19,21	1.03	1 (5%)
3	NAG	B	1305	-	14,14,15	0.33	0	17,19,21	0.63	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	1302	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1309	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1305	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
4	EIC	C	1310	-	-	11/17/17/17	-
3	NAG	C	1305	-	-	0/6/23/26	0/1/1/1
4	EIC	A	1310	-	-	8/17/17/17	-
3	NAG	A	1308	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1307	-	-	3/6/23/26	0/1/1/1
3	NAG	B	1309	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1308	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1304	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	-	-	3/6/23/26	0/1/1/1
3	NAG	B	1307	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1306	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	-	-	3/6/23/26	0/1/1/1
3	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	-	-	3/6/23/26	0/1/1/1
3	NAG	B	1303	-	-	3/6/23/26	0/1/1/1
3	NAG	B	1301	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1309	-	-	2/6/23/26	0/1/1/1
4	EIC	B	1310	-	-	8/17/17/17	-
3	NAG	B	1308	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1302	-	-	3/6/23/26	0/1/1/1
3	NAG	B	1305	-	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1310	EIC	C13-C12	3.79	1.53	1.31
4	A	1310	EIC	C13-C12	3.79	1.53	1.31
4	A	1310	EIC	C10-C9	3.78	1.53	1.31
4	C	1310	EIC	C13-C12	3.78	1.53	1.31
4	C	1310	EIC	C10-C9	3.78	1.53	1.31
4	B	1310	EIC	C10-C9	3.77	1.53	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1306	NAG	C1-O5-C5	3.56	116.95	112.19
3	A	1306	NAG	C1-O5-C5	3.56	116.95	112.19
3	B	1306	NAG	C1-O5-C5	3.55	116.95	112.19
3	C	1308	NAG	C2-N2-C7	2.98	126.89	122.90
3	A	1308	NAG	C2-N2-C7	2.98	126.89	122.90
3	B	1308	NAG	C2-N2-C7	2.96	126.87	122.90
3	C	1302	NAG	C2-N2-C7	2.92	126.81	122.90
3	B	1302	NAG	C2-N2-C7	2.91	126.80	122.90
3	A	1302	NAG	C2-N2-C7	2.90	126.79	122.90
3	C	1301	NAG	C2-N2-C7	2.71	126.53	122.90
3	C	1307	NAG	C1-O5-C5	2.69	115.80	112.19
3	B	1301	NAG	C2-N2-C7	2.69	126.50	122.90
3	A	1301	NAG	C2-N2-C7	2.69	126.50	122.90
3	A	1307	NAG	C1-O5-C5	2.69	115.79	112.19
3	B	1307	NAG	C1-O5-C5	2.67	115.77	112.19
3	C	1303	NAG	C2-N2-C7	2.16	125.80	122.90
3	A	1303	NAG	C2-N2-C7	2.16	125.80	122.90
3	B	1303	NAG	C2-N2-C7	2.15	125.78	122.90

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	NAG	C1-C2-N2-C7
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	A	1302	NAG	C1-C2-N2-C7
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	A	1303	NAG	C1-C2-N2-C7
3	A	1303	NAG	O7-C7-N2-C2
3	A	1307	NAG	C8-C7-N2-C2
3	A	1307	NAG	O7-C7-N2-C2
3	A	1308	NAG	C1-C2-N2-C7
3	A	1308	NAG	C8-C7-N2-C2
3	A	1308	NAG	O7-C7-N2-C2
3	B	1301	NAG	C1-C2-N2-C7
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	B	1302	NAG	C1-C2-N2-C7
3	B	1302	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	B	1302	NAG	O7-C7-N2-C2
3	B	1303	NAG	C1-C2-N2-C7
3	B	1303	NAG	O7-C7-N2-C2
3	B	1307	NAG	C8-C7-N2-C2
3	B	1307	NAG	O7-C7-N2-C2
3	B	1308	NAG	C1-C2-N2-C7
3	B	1308	NAG	C8-C7-N2-C2
3	B	1308	NAG	O7-C7-N2-C2
3	C	1301	NAG	C1-C2-N2-C7
3	C	1301	NAG	C8-C7-N2-C2
3	C	1301	NAG	O7-C7-N2-C2
3	C	1302	NAG	C1-C2-N2-C7
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	C	1303	NAG	C1-C2-N2-C7
3	C	1303	NAG	O7-C7-N2-C2
3	C	1307	NAG	C8-C7-N2-C2
3	C	1307	NAG	O7-C7-N2-C2
3	C	1308	NAG	C1-C2-N2-C7
3	C	1308	NAG	C8-C7-N2-C2
3	C	1308	NAG	O7-C7-N2-C2
3	A	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	C8-C7-N2-C2
3	C	1303	NAG	C8-C7-N2-C2
4	B	1310	EIC	C11-C10-C9-C8
4	A	1310	EIC	C11-C10-C9-C8
4	C	1310	EIC	C11-C10-C9-C8
3	A	1309	NAG	C8-C7-N2-C2
3	B	1309	NAG	C8-C7-N2-C2
3	C	1309	NAG	C8-C7-N2-C2
3	A	1309	NAG	O7-C7-N2-C2
3	B	1309	NAG	O7-C7-N2-C2
3	C	1309	NAG	O7-C7-N2-C2
4	B	1310	EIC	C1-C2-C3-C4
4	A	1310	EIC	C1-C2-C3-C4
3	A	1304	NAG	C8-C7-N2-C2
3	B	1304	NAG	C8-C7-N2-C2
3	C	1304	NAG	C8-C7-N2-C2
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
4	A	1310	EIC	C4-C5-C6-C7

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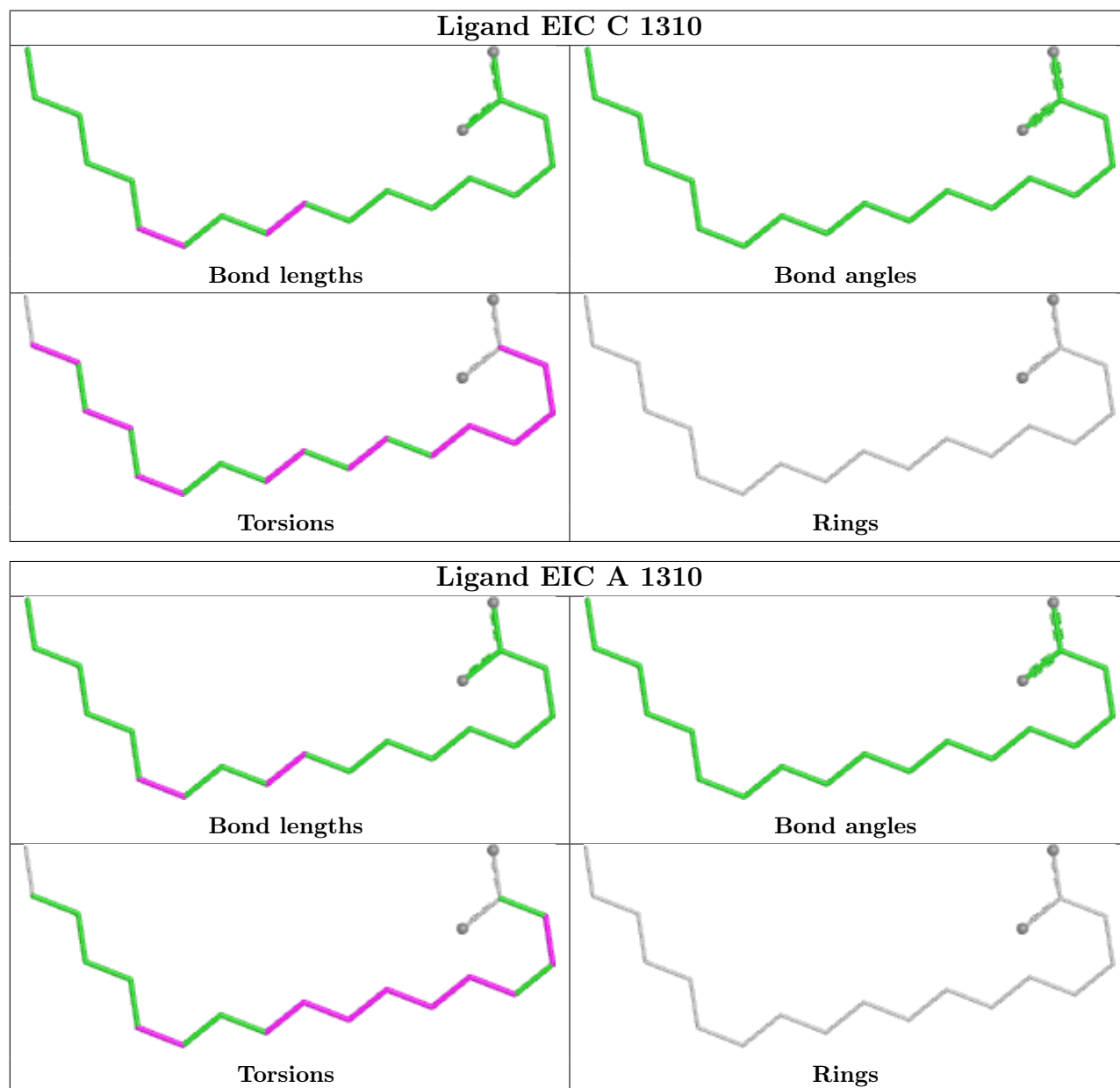
Mol	Chain	Res	Type	Atoms
4	B	1310	EIC	C4-C5-C6-C7
4	C	1310	EIC	C4-C5-C6-C7
4	C	1310	EIC	C13-C14-C15-C16
4	A	1310	EIC	C6-C7-C8-C9
4	C	1310	EIC	C6-C7-C8-C9
4	C	1310	EIC	C11-C12-C13-C14
4	B	1310	EIC	C6-C7-C8-C9
4	B	1310	EIC	C11-C12-C13-C14
3	A	1307	NAG	C3-C2-N2-C7
3	B	1307	NAG	C3-C2-N2-C7
3	C	1307	NAG	C3-C2-N2-C7
3	A	1304	NAG	O7-C7-N2-C2
3	B	1304	NAG	O7-C7-N2-C2
3	C	1304	NAG	O7-C7-N2-C2
4	A	1310	EIC	C11-C12-C13-C14
4	B	1310	EIC	C7-C8-C9-C10
4	A	1310	EIC	C7-C8-C9-C10
4	A	1310	EIC	C3-C4-C5-C6
3	A	1306	NAG	C1-C2-N2-C7
3	B	1306	NAG	C1-C2-N2-C7
3	C	1306	NAG	C1-C2-N2-C7
4	C	1310	EIC	O1-C1-C2-C3
4	C	1310	EIC	O2-C1-C2-C3
4	C	1310	EIC	C3-C4-C5-C6
4	B	1310	EIC	C3-C4-C5-C6
4	B	1310	EIC	C5-C6-C7-C8
4	C	1310	EIC	C2-C3-C4-C5
4	C	1310	EIC	C1-C2-C3-C4
4	C	1310	EIC	C15-C16-C17-C18
4	A	1310	EIC	C5-C6-C7-C8

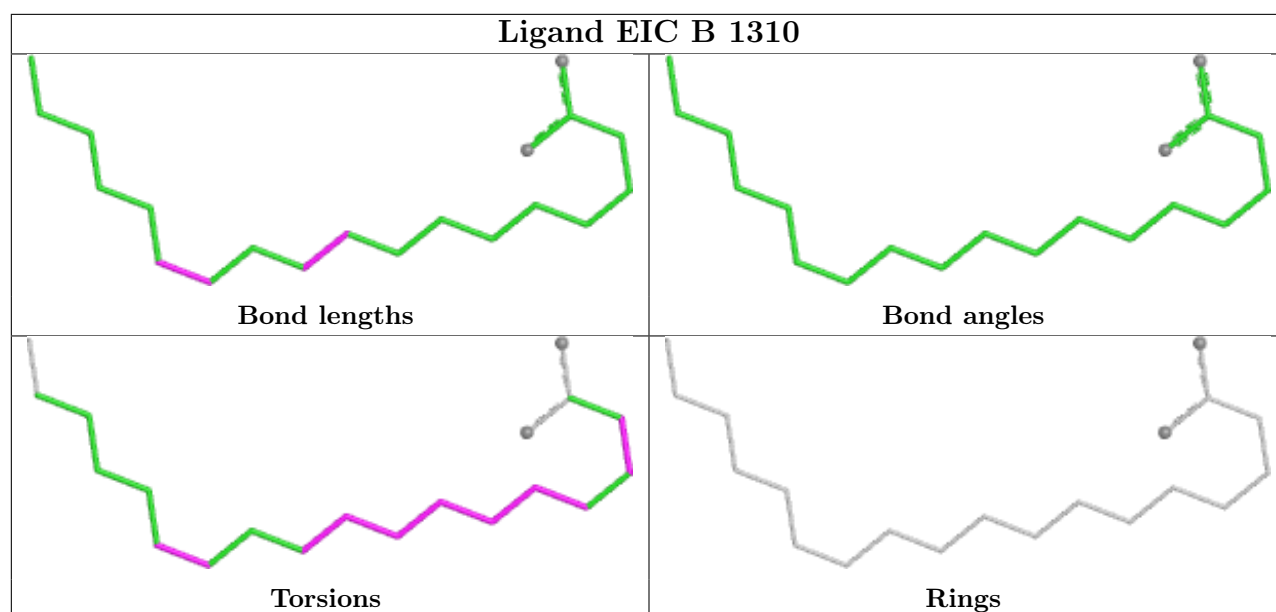
There are no ring outliers.

6 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1306	NAG	1	0
4	C	1310	EIC	24	0
4	A	1310	EIC	27	0
3	A	1306	NAG	1	0
3	B	1306	NAG	1	0
4	B	1310	EIC	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

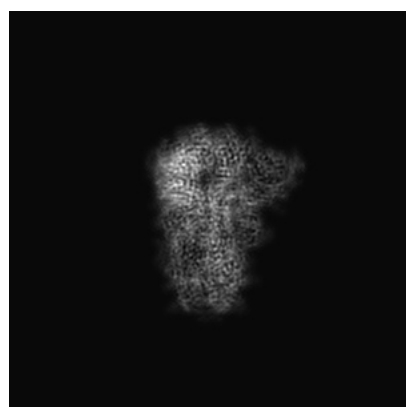
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30418. These allow visual inspection of the internal detail of the map and identification of artifacts.

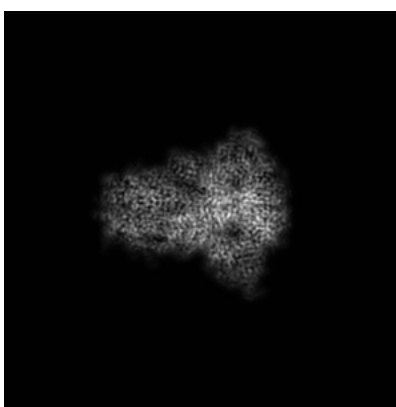
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

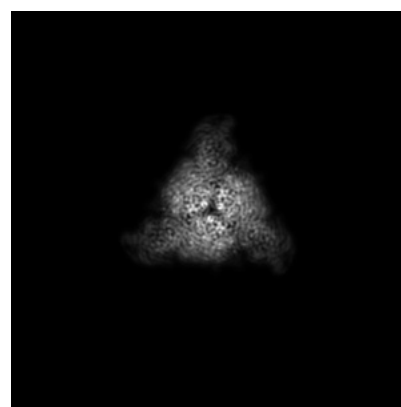
6.1.1 Primary map



X



Y



Z

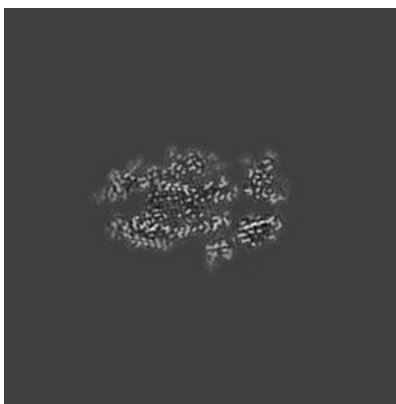
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

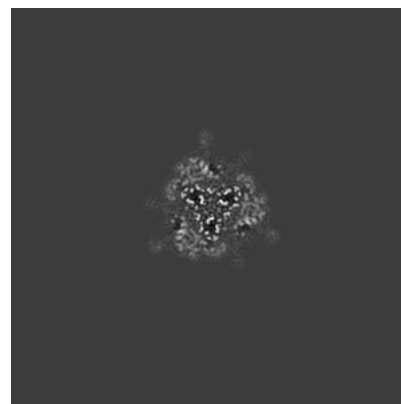
6.2.1 Primary map



X Index: 148



Y Index: 148

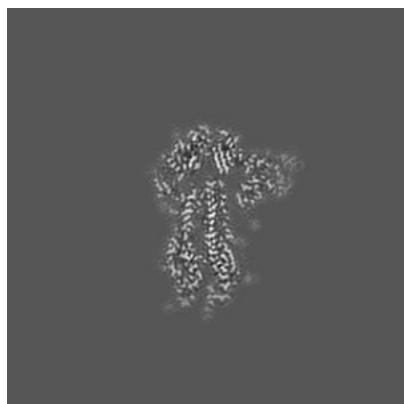


Z Index: 148

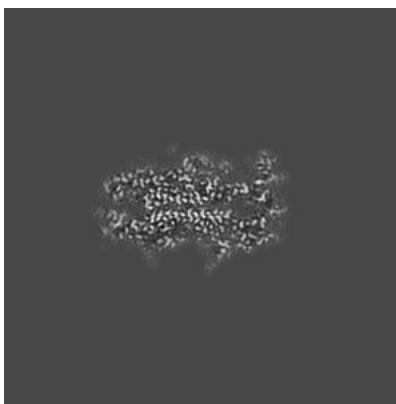
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

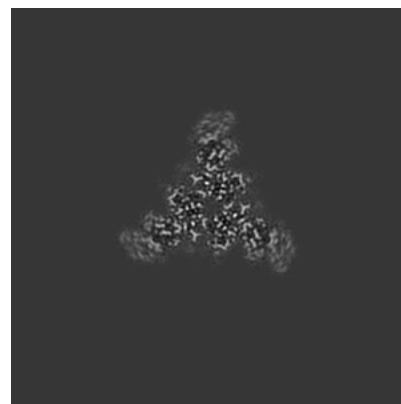
6.3.1 Primary map



X Index: 155



Y Index: 153

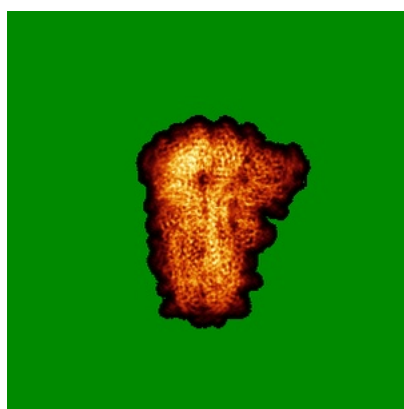


Z Index: 182

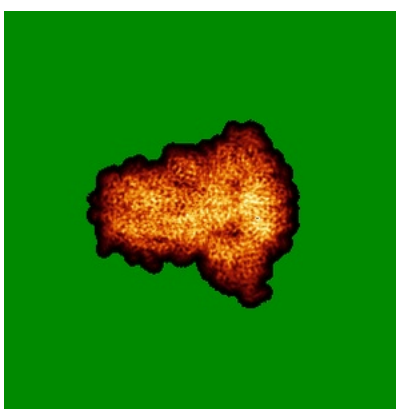
The images above show the largest variance slices of the map in three orthogonal directions.

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

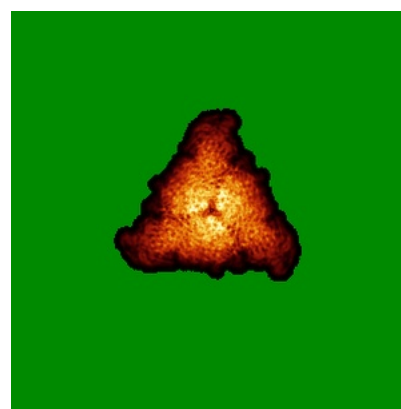
6.4.1 Primary map



X



Y

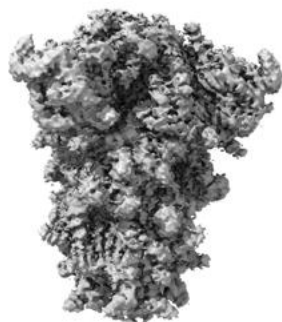


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

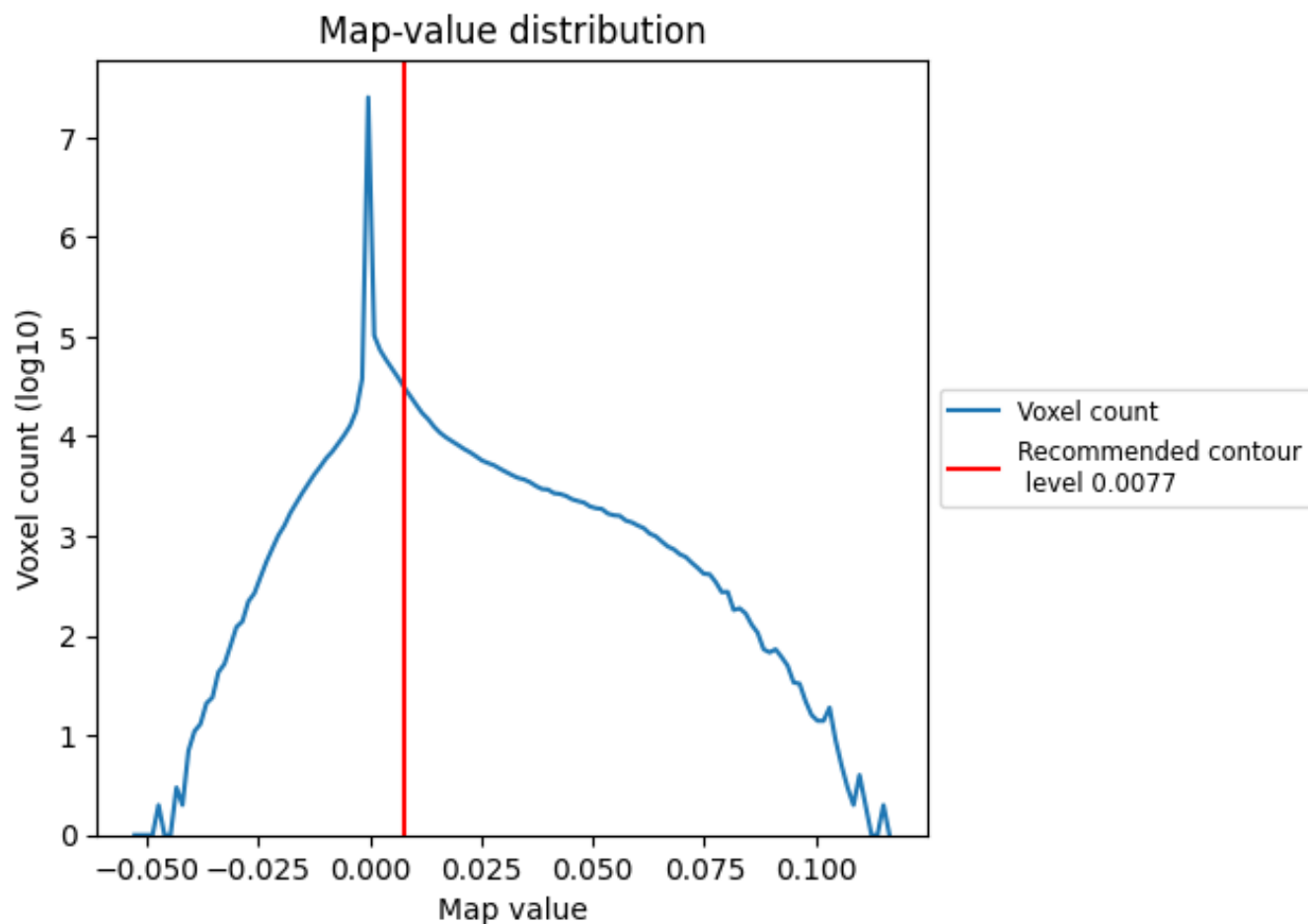
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

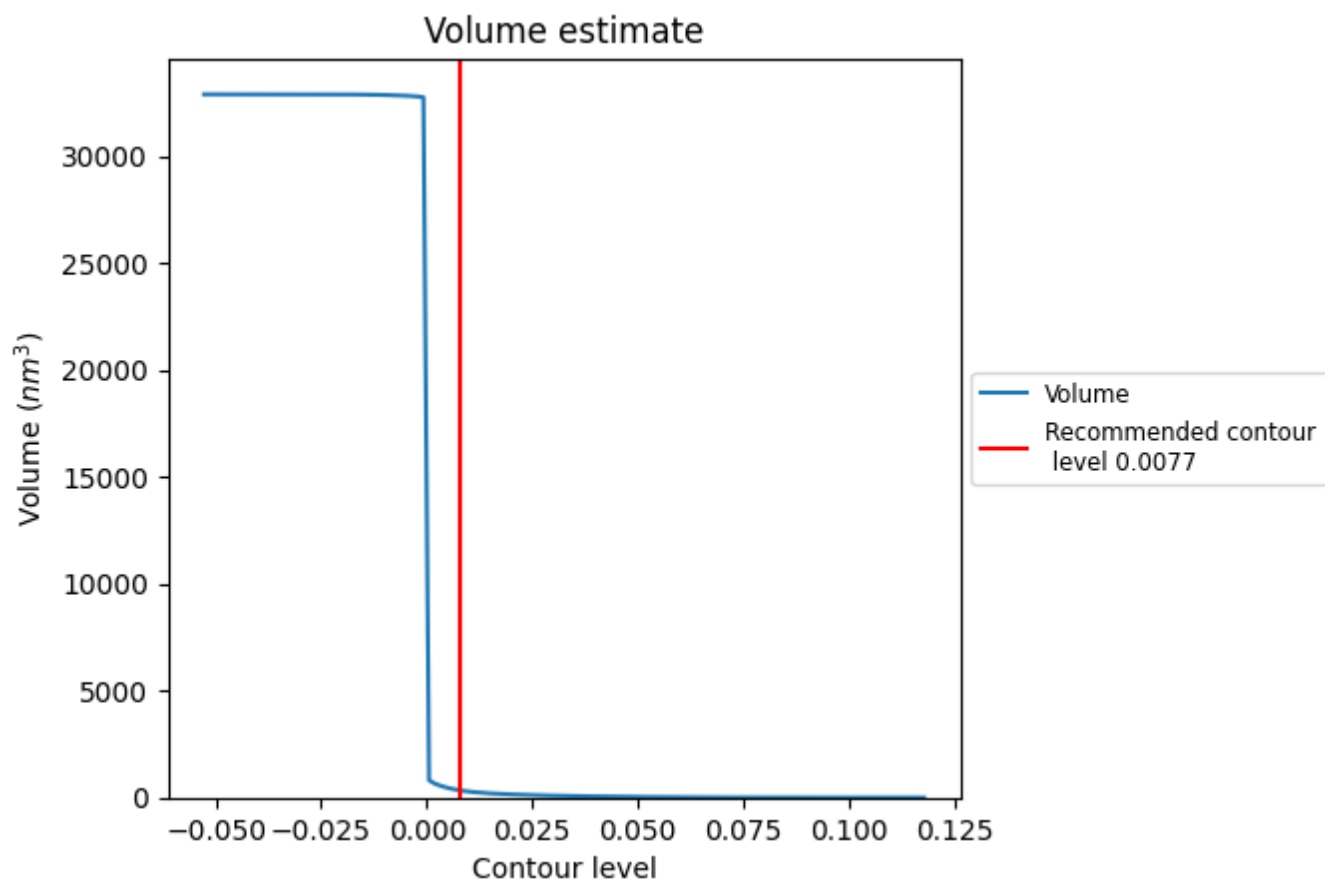
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

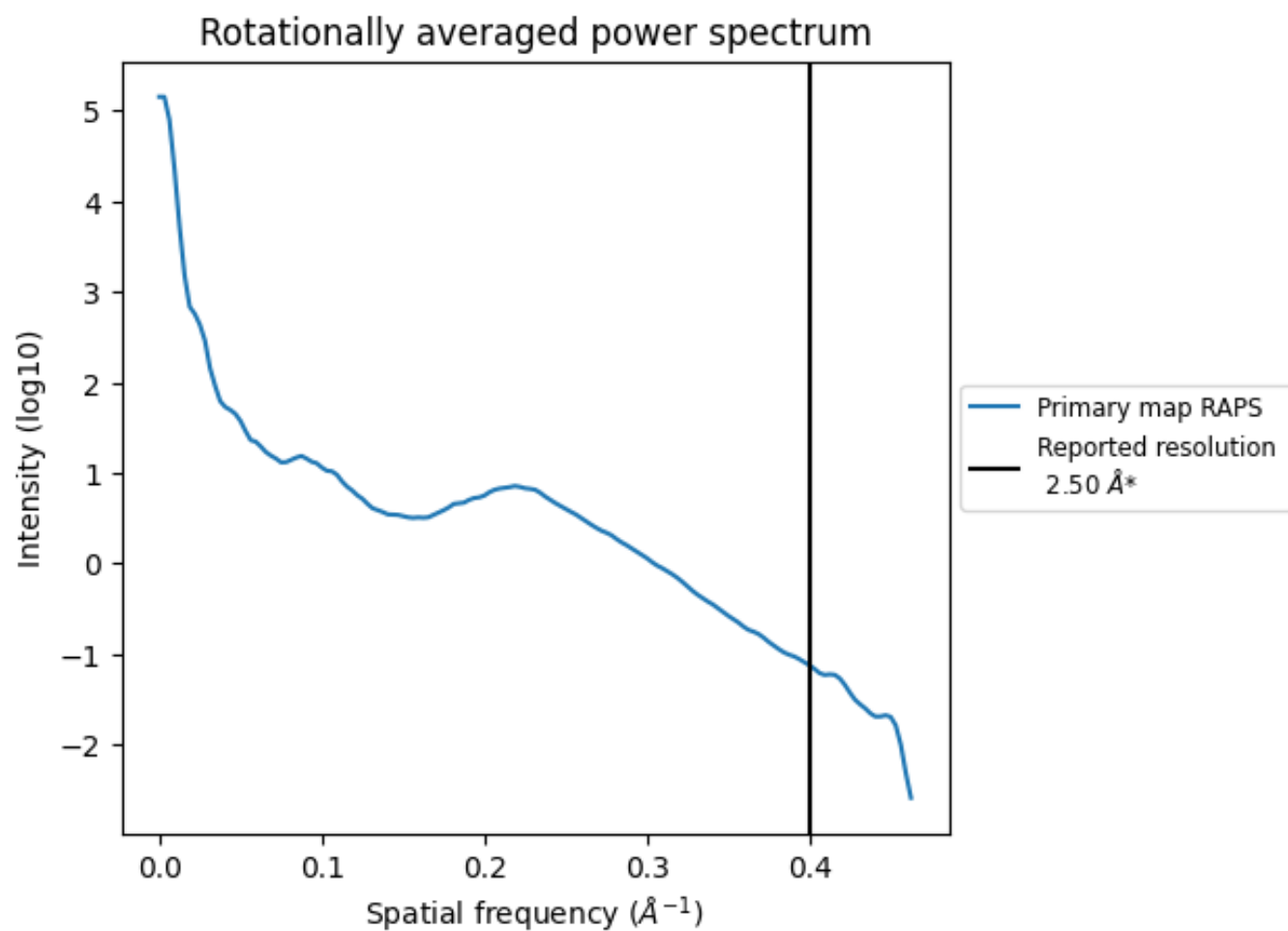
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 343 nm³; this corresponds to an approximate mass of 310 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 ⓘ

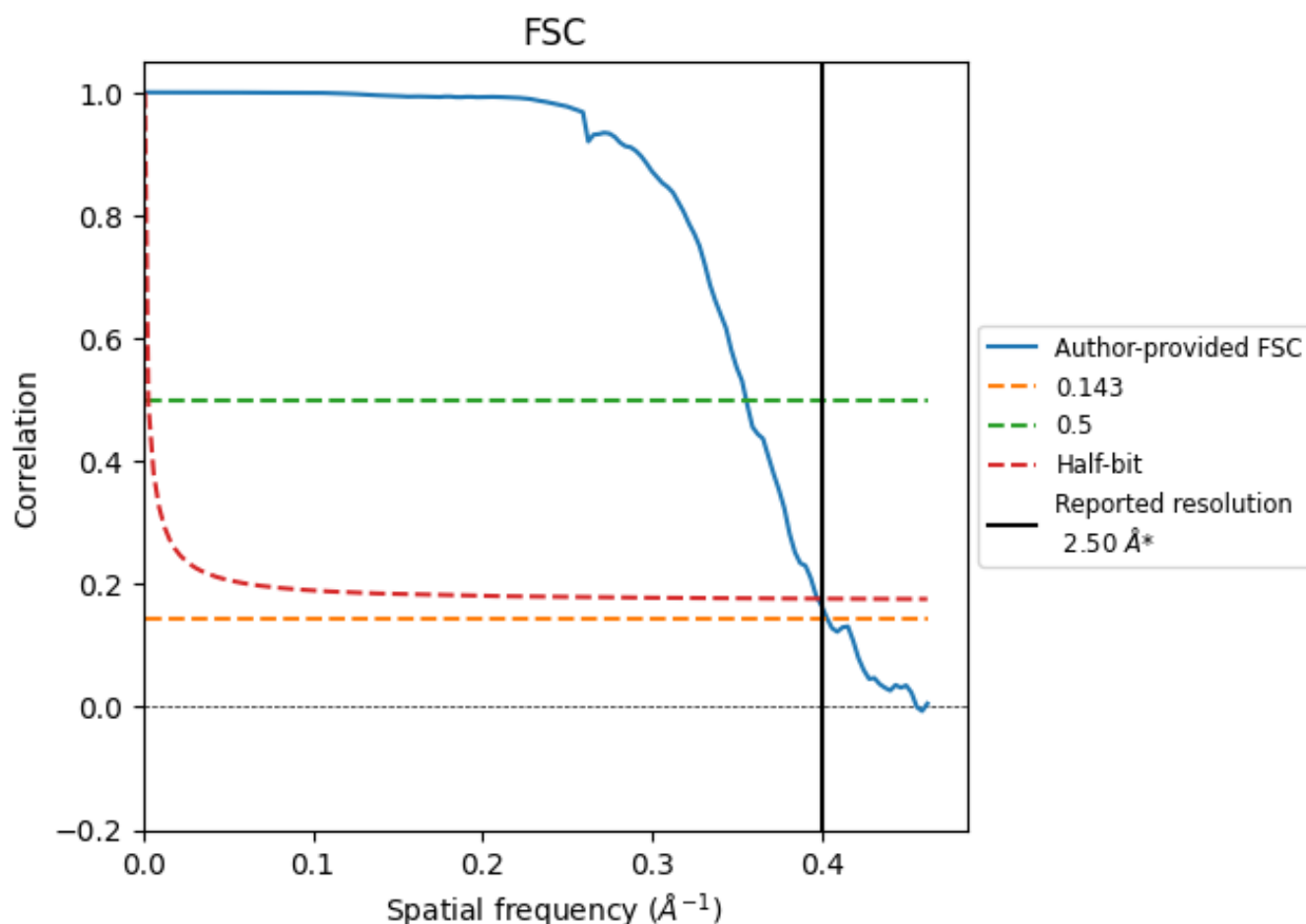


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

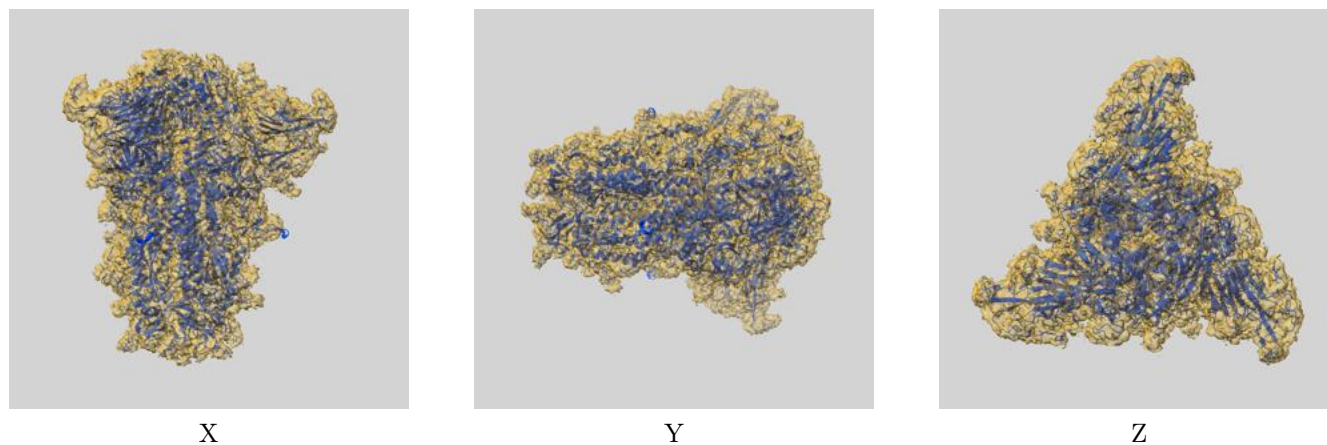
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.48	2.82	2.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

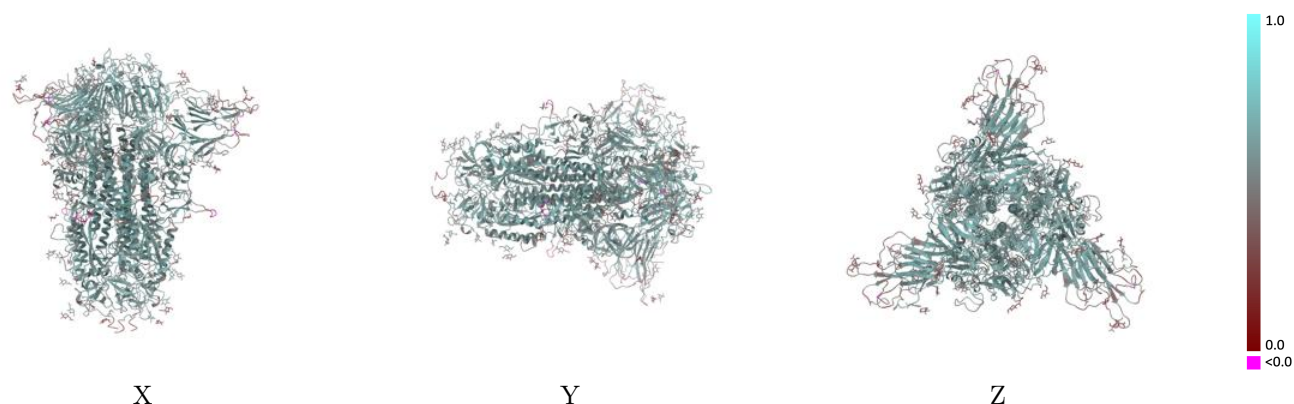
This section contains information regarding the fit between EMDB map EMD-30418 and PDB model 7CN8. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



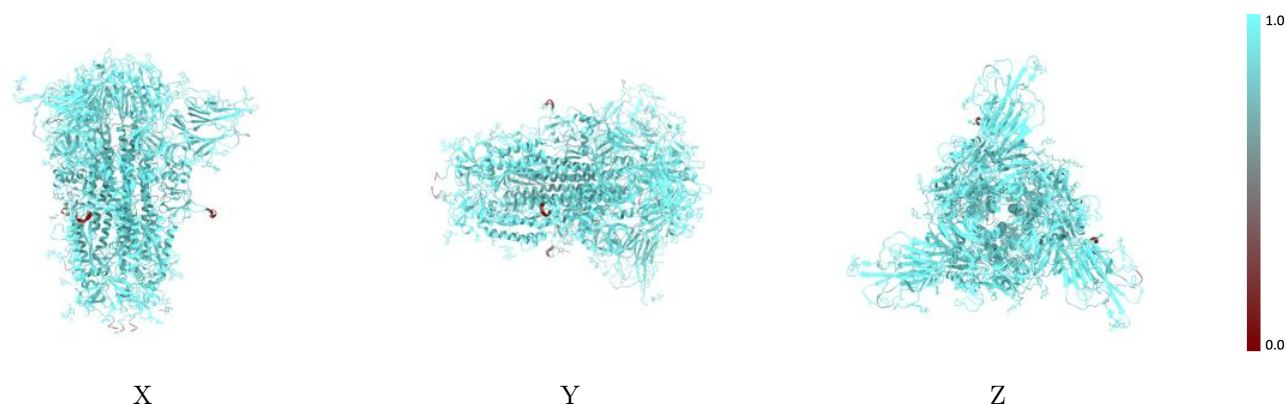
The images above show the 3D surface view of the map at the recommended contour level 0.0077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



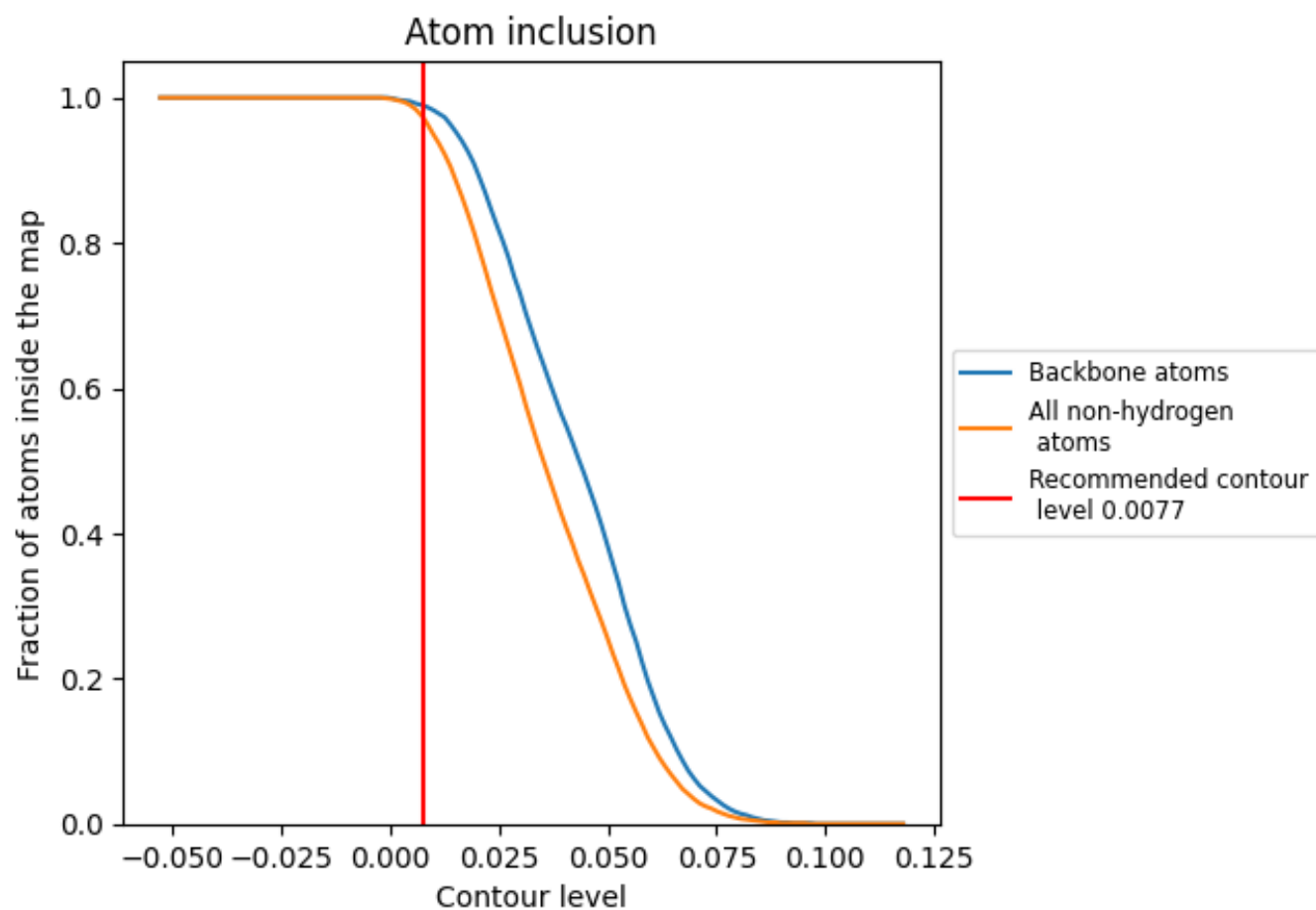
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0077).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.0077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9720	 0.5600
A	 0.9720	 0.5640
B	 0.9740	 0.5640
C	 0.9730	 0.5630
D	 0.9290	 0.3920
E	 0.9640	 0.5450
F	 1.0000	 0.5390
G	 1.0000	 0.5350
H	 0.9640	 0.4740
I	 1.0000	 0.5240
J	 0.9290	 0.4110
K	 0.9640	 0.4100
L	 0.9290	 0.3480
M	 0.8570	 0.3380
N	 0.8930	 0.2610
O	 1.0000	 0.5130
P	 0.9640	 0.5400
Q	 1.0000	 0.5500
R	 0.8570	 0.3940
S	 0.9640	 0.5230
T	 0.9290	 0.4390
U	 0.9640	 0.4790
V	 0.9290	 0.3080
W	 0.9290	 0.3370
X	 0.8210	 0.3160
Y	 0.9640	 0.4350
Z	 1.0000	 0.4750
a	 0.9640	 0.5430
b	 1.0000	 0.5440
e	 0.9290	 0.4470
f	 0.9290	 0.4170
g	 0.9290	 0.3140
h	 0.9290	 0.3390
i	 0.8570	 0.3160
k	 0.9640	 0.4580



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Chain	Atom inclusion	Q-score
l	 1.0000	 0.5400
m	 1.0000	 0.5360