



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:20 PM UTC

PDB ID : 6U59 / pdb_00006u59
EMDB ID : EMD-20642
Title : HIV-1 B41 SOSIP.664 in complex with rabbit antibody 13B
Authors : Yang, Y.R.; Ward, A.B.
Deposited on : 2019-08-27
Resolution : 3.86 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:

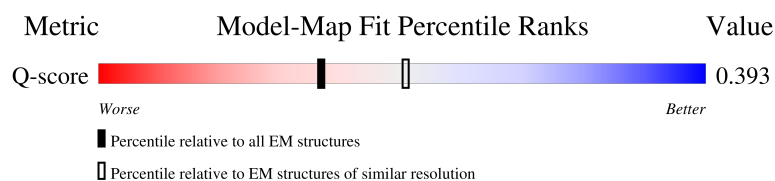
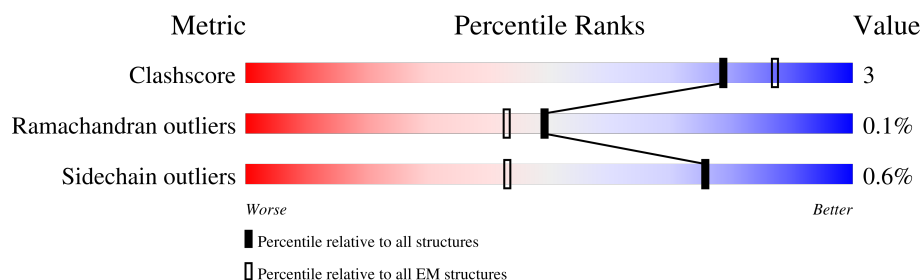
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.86 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	8889 (3.36 - 4.35)

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	524	
1	C	524	
1	G	524	
2	B	153	

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Mol	Chain	Length	Quality of chain
2	D	153	
2	I	153	
3	E	112	
3	J	112	
3	L	112	
4	F	119	
4	H	119	
4	K	119	
5	M	2	
5	N	2	
5	O	2	
5	P	2	
5	Q	2	
5	S	2	
5	T	2	
5	U	2	
5	V	2	
5	X	2	
5	Y	2	
5	Z	2	
5	a	2	
5	b	2	
5	c	2	
5	d	2	
5	f	2	

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Mol	Chain	Length	Quality of chain
5	g	2	
5	h	2	
5	i	2	
5	k	2	
5	l	2	
5	m	2	
5	n	2	
5	o	2	
5	p	2	
5	q	2	
5	s	2	
5	t	2	
5	u	2	
5	v	2	
5	x	2	
5	y	2	
6	R	3	
6	e	3	
6	r	3	
7	W	4	
7	j	4	
7	w	4	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20439 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 SOSIP.664 gp120,SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	454	Total	C	N	O	S	0	0
			3562	2234	629	672	27		
1	C	454	Total	C	N	O	S	0	0
			3562	2234	629	672	27		
1	G	454	Total	C	N	O	S	0	0
			3562	2234	629	672	27		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	CYS	ALA	engineered mutation	UNP B3UES2
A	509	ARG	GLU	engineered mutation	UNP B3UES2
A	510	ARG	LYS	engineered mutation	UNP B3UES2
A	512	ARG	ALA	engineered mutation	UNP B3UES2
A	513	ARG	VAL	engineered mutation	UNP B3UES2
C	501	CYS	ALA	engineered mutation	UNP B3UES2
C	509	ARG	GLU	engineered mutation	UNP B3UES2
C	510	ARG	LYS	engineered mutation	UNP B3UES2
C	512	ARG	ALA	engineered mutation	UNP B3UES2
C	513	ARG	VAL	engineered mutation	UNP B3UES2
G	501	CYS	ALA	engineered mutation	UNP B3UES2
G	509	ARG	GLU	engineered mutation	UNP B3UES2
G	510	ARG	LYS	engineered mutation	UNP B3UES2
G	512	ARG	ALA	engineered mutation	UNP B3UES2
G	513	ARG	VAL	engineered mutation	UNP B3UES2

- Molecule 2 is a protein called SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			975	616	167	184	8		
2	D	120	Total	C	N	O	S	0	0
			975	616	167	184	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	120	Total	C	N	O	S	0	0
			975	616	167	184	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6
D	559	PRO	ILE	engineered mutation	UNP B3UEZ6
D	605	CYS	THR	engineered mutation	UNP B3UEZ6
I	559	PRO	ILE	engineered mutation	UNP B3UEZ6
I	605	CYS	THR	engineered mutation	UNP B3UEZ6

- Molecule 3 is a protein called rabbit antibody 13B Fragment antigen binding light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	112	Total	C	N	O	S	0	0
			842	527	139	172	4		
3	E	112	Total	C	N	O	S	0	0
			842	527	139	172	4		
3	J	112	Total	C	N	O	S	0	0
			842	527	139	172	4		

- Molecule 4 is a protein called rabbit antibody 13B Fragment antigen binding heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	118	Total	C	N	O	S	0	0
			897	577	143	174	3		
4	F	118	Total	C	N	O	S	0	0
			897	577	143	174	3		
4	K	118	Total	C	N	O	S	0	0
			897	577	143	174	3		

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



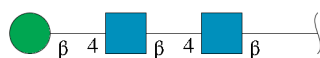
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
5	k	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			28	16	2	10		

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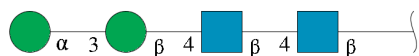
Mol	Chain	Residues	Atoms				AltConf	Trace
5	m	2	Total	C	N	O	0	0
			28	16	2	10		
5	n	2	Total	C	N	O	0	0
			28	16	2	10		
5	o	2	Total	C	N	O	0	0
			28	16	2	10		
5	p	2	Total	C	N	O	0	0
			28	16	2	10		
5	q	2	Total	C	N	O	0	0
			28	16	2	10		
5	s	2	Total	C	N	O	0	0
			28	16	2	10		
5	t	2	Total	C	N	O	0	0
			28	16	2	10		
5	u	2	Total	C	N	O	0	0
			28	16	2	10		
5	v	2	Total	C	N	O	0	0
			28	16	2	10		
5	x	2	Total	C	N	O	0	0
			28	16	2	10		
5	y	2	Total	C	N	O	0	0
			28	16	2	10		

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



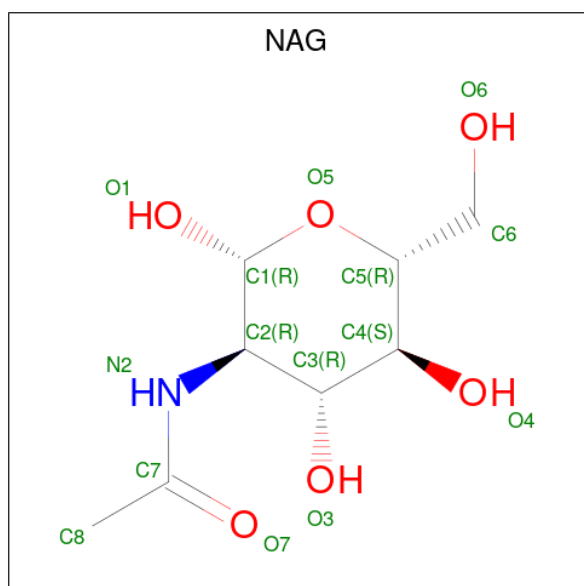
Mol	Chain	Residues	Atoms				AltConf	Trace
6	R	3	Total	C	N	O	0	0
			39	22	2	15		
6	e	3	Total	C	N	O	0	0
			39	22	2	15		
6	r	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	W	4	Total	C	N	O	0	0
			50	28	2	20		
7	j	4	Total	C	N	O	0	0
			50	28	2	20		
7	w	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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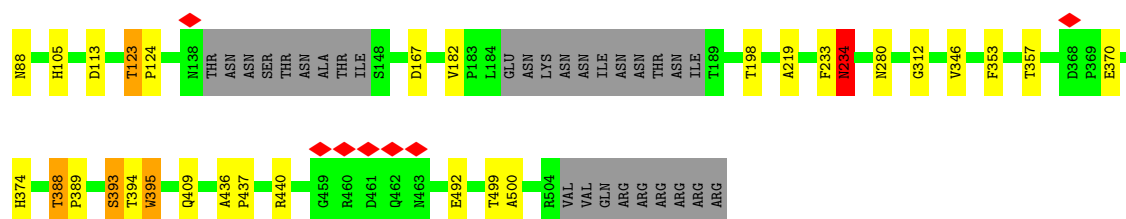
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Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C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

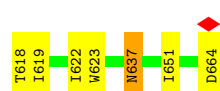
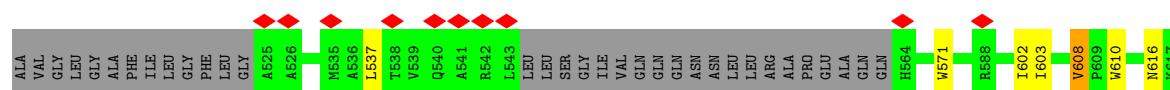
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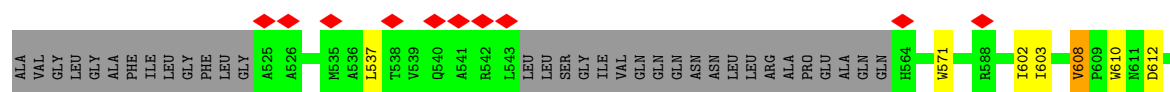
Mol	Chain	Residues	Atoms				AltConf
8	I	1	Total	C	N	O	0
			14	8	1	5	
8	I	1	Total	C	N	O	0
			14	8	1	5	
8	I	1	Total	C	N	O	0
			14	8	1	5	



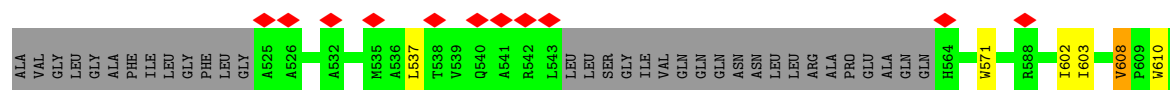
• Molecule 2: SOSIP.664 gp41



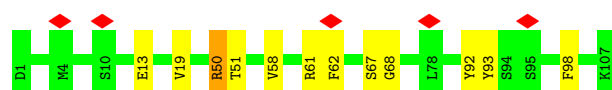
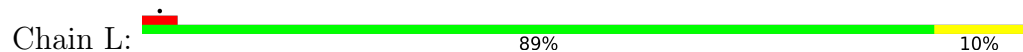
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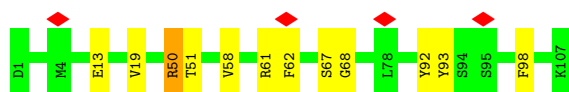


• Molecule 3: rabbit antibody 13B Fragment antigen binding light chain



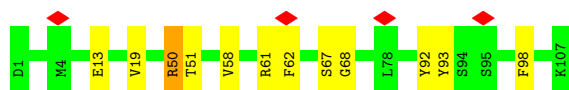
• Molecule 3: rabbit antibody 13B Fragment antigen binding light chain

Chain E:  89% 10% .



- Molecule 3: rabbit antibody 13B Fragment antigen binding light chain

Chain J:  89% 10% .



- Molecule 4: rabbit antibody 13B Fragment antigen binding heavy chain

Chain H:  90% 8% ..



- Molecule 4: rabbit antibody 13B Fragment antigen binding heavy chain

Chain F:  90% 8% ..

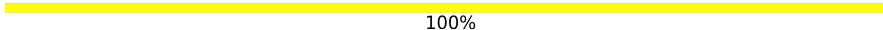


- Molecule 4: rabbit antibody 13B Fragment antigen binding heavy chain

Chain K:  90% 8% ..

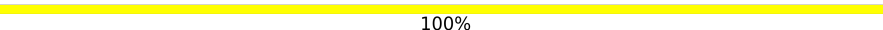


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



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

Chain N:  100%

NAG1
NAG2

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

Chain O:  50% 50%

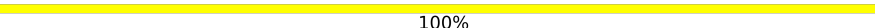
NAG1
NAG2

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

Chain P:  50% 100%

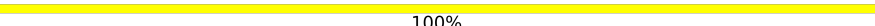
NAG1
NAG2

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

Chain Q:  100%

NAG1
NAG2

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

Chain S:  100%

NAG1
NAG2

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

Chain T:  50% 50% 50%

NAG1
NAG2

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

Chain U:  50% 50%

NAG1
NAG2

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



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



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

Chain l:  50% 50%



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

Chain m:  50% 50%

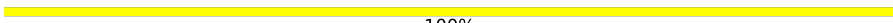


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  50% 100%



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

Chain o:  100%



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

Chain p:  50% 100%



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

Chain q:  50% 50%



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

Chain s:  100%

NAG1
NAG2

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

Chain t:  50% 100%

♦
NAG1
NAG2

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

Chain u:  50% 50%

NAG1
NAG2

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

Chain v:  50% 50%

♦
NAG1
NAG2

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

Chain x:  50% 50%

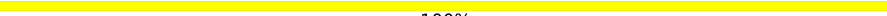
NAG1
NAG2

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

Chain y:  50% 50%

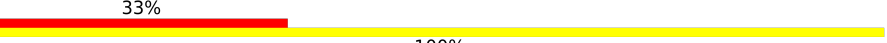
NAG1
NAG2

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

NAG1
NAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

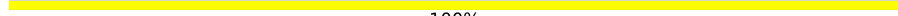
NAG1
NAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  67%

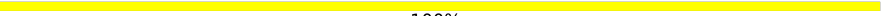
NAG1
NAG2
BMA3

- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

NAG1
NAG2
BMA3
MAN4

- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%

NAG1
NAG2
BMA3
MAN4

- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  100%

NAG1
NAG2
BMA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	147520	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.700	Depositor
Minimum map value	-1.588	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.53	Depositor
Map size (Å)	294.4, 294.4, 294.4	wwPDB
Map dimensions	256, 256, 256	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: MAN, BMA, 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	1.04	2/3638 (0.1%)	1.25	31/4945 (0.6%)
1	C	1.04	2/3638 (0.1%)	1.25	29/4945 (0.6%)
1	G	1.04	2/3638 (0.1%)	1.25	29/4945 (0.6%)
2	B	1.03	0/993	1.18	9/1347 (0.7%)
2	D	1.03	0/993	1.18	9/1347 (0.7%)
2	I	1.03	0/993	1.18	9/1347 (0.7%)
3	E	1.04	0/861	1.38	7/1171 (0.6%)
3	J	1.04	0/861	1.38	7/1171 (0.6%)
3	L	1.04	0/861	1.38	7/1171 (0.6%)
4	F	1.05	1/922 (0.1%)	1.25	3/1257 (0.2%)
4	H	1.04	1/922 (0.1%)	1.25	3/1257 (0.2%)
4	K	1.04	1/922 (0.1%)	1.25	3/1257 (0.2%)
All	All	1.04	9/19242 (0.0%)	1.26	146/26160 (0.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	374	HIS	CE1-NE2	-5.33	1.27	1.32
1	G	374	HIS	CE1-NE2	-5.29	1.27	1.32
1	A	374	HIS	CE1-NE2	-5.25	1.27	1.32
1	G	105	HIS	CB-CG	-5.11	1.43	1.50
1	C	105	HIS	CB-CG	-5.11	1.43	1.50
4	K	100(G)	PHE	CB-CG	-5.05	1.39	1.50
4	H	100(G)	PHE	CB-CG	-5.05	1.39	1.50
1	A	105	HIS	CB-CG	-5.04	1.43	1.50
4	F	100(G)	PHE	CB-CG	-5.00	1.39	1.50

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	GLU	N-CA-C	-10.50	102.65	114.62
1	G	370	GLU	N-CA-C	-10.46	102.69	114.62
1	C	370	GLU	N-CA-C	-10.46	102.70	114.62
2	I	602	ILE	N-CA-C	-8.20	103.88	111.67
2	B	602	ILE	N-CA-C	-8.19	103.89	111.67
2	D	602	ILE	N-CA-C	-8.16	103.92	111.67
1	G	393	SER	N-CA-C	8.10	118.93	108.24
1	A	393	SER	N-CA-C	8.09	118.91	108.24
1	C	393	SER	N-CA-C	8.06	118.89	108.24
3	J	58	VAL	CA-C-N	7.21	127.13	120.21
3	J	58	VAL	C-N-CA	7.21	127.13	120.21
3	E	58	VAL	CA-C-N	7.20	127.12	120.21
3	E	58	VAL	C-N-CA	7.20	127.12	120.21
3	L	58	VAL	CA-C-N	7.19	127.12	120.21
3	L	58	VAL	C-N-CA	7.19	127.12	120.21
1	A	395	TRP	N-CA-C	7.18	119.77	108.79
1	C	395	TRP	N-CA-C	7.18	119.77	108.79
1	G	395	TRP	N-CA-C	7.18	119.77	108.79
3	E	98	PHE	CA-CB-CG	7.15	120.95	113.80
3	J	98	PHE	CA-CB-CG	7.13	120.93	113.80
3	L	98	PHE	CA-CB-CG	7.04	120.84	113.80
1	G	280	ASN	CA-CB-CG	-6.85	105.75	112.60
1	A	280	ASN	CA-CB-CG	-6.84	105.75	112.60
1	A	492	GLU	CA-C-N	6.83	126.97	119.87
1	A	492	GLU	C-N-CA	6.83	126.97	119.87
1	C	492	GLU	CA-C-N	6.82	126.96	119.87
1	C	492	GLU	C-N-CA	6.82	126.96	119.87
1	G	492	GLU	CA-C-N	6.80	126.94	119.87
1	G	492	GLU	C-N-CA	6.80	126.94	119.87
1	A	233	PHE	N-CA-C	6.79	118.34	111.07
1	C	280	ASN	CA-CB-CG	-6.79	105.81	112.60
1	G	233	PHE	N-CA-C	6.75	118.30	111.07
1	C	233	PHE	N-CA-C	6.74	118.28	111.07
4	H	104	GLY	CA-C-N	6.22	125.84	119.56
4	H	104	GLY	C-N-CA	6.22	125.84	119.56
4	K	104	GLY	CA-C-N	6.21	125.84	119.56
4	K	104	GLY	C-N-CA	6.21	125.84	119.56
4	F	104	GLY	CA-C-N	6.21	125.83	119.56
4	F	104	GLY	C-N-CA	6.21	125.83	119.56
1	C	312	GLY	CA-C-N	6.13	127.51	119.84
1	C	312	GLY	C-N-CA	6.13	127.51	119.84
1	G	312	GLY	CA-C-N	6.11	127.48	119.84
1	G	312	GLY	C-N-CA	6.11	127.48	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	123	THR	CA-C-N	6.11	125.81	119.82
1	G	123	THR	C-N-CA	6.11	125.81	119.82
1	A	312	GLY	CA-C-N	6.09	127.45	119.84
1	A	312	GLY	C-N-CA	6.09	127.45	119.84
2	B	608	VAL	CA-C-N	6.09	126.06	120.03
2	B	608	VAL	C-N-CA	6.09	126.06	120.03
2	I	608	VAL	CA-C-N	6.08	126.05	120.03
2	I	608	VAL	C-N-CA	6.08	126.05	120.03
1	A	123	THR	CA-C-N	6.07	125.77	119.82
1	A	123	THR	C-N-CA	6.07	125.77	119.82
2	D	608	VAL	CA-C-N	6.07	126.04	120.03
2	D	608	VAL	C-N-CA	6.07	126.04	120.03
3	L	50	ARG	N-CA-C	-6.05	100.15	109.52
1	A	113	ASP	N-CA-C	-6.04	102.01	110.35
1	C	123	THR	CA-C-N	6.04	125.74	119.82
1	C	123	THR	C-N-CA	6.04	125.74	119.82
1	C	113	ASP	N-CA-C	-6.04	102.02	110.35
1	C	437	PRO	CA-C-N	6.03	125.94	119.85
1	C	437	PRO	C-N-CA	6.03	125.94	119.85
2	D	537	LEU	CB-CA-C	-6.02	109.62	116.54
3	E	50	ARG	N-CA-C	-6.02	100.19	109.52
3	J	50	ARG	N-CA-C	-6.01	100.20	109.52
1	G	113	ASP	N-CA-C	-6.00	102.07	110.35
1	G	437	PRO	CA-C-N	5.99	125.90	119.85
1	G	437	PRO	C-N-CA	5.99	125.90	119.85
1	A	437	PRO	CA-C-N	5.98	125.89	119.85
1	A	437	PRO	C-N-CA	5.98	125.89	119.85
2	B	537	LEU	CB-CA-C	-5.98	109.66	116.54
2	I	537	LEU	CB-CA-C	-5.94	109.71	116.54
1	G	72	HIS	CA-CB-CG	-5.92	107.88	113.80
1	G	353	PHE	CA-C-N	5.92	125.83	119.85
1	G	353	PHE	C-N-CA	5.92	125.83	119.85
1	A	72	HIS	CA-CB-CG	-5.91	107.89	113.80
1	C	72	HIS	CA-CB-CG	-5.89	107.91	113.80
1	C	353	PHE	CA-C-N	5.88	125.79	119.85
1	C	353	PHE	C-N-CA	5.88	125.79	119.85
1	A	353	PHE	CA-C-N	5.86	125.77	119.85
1	A	353	PHE	C-N-CA	5.86	125.77	119.85
1	C	182	VAL	CA-C-N	5.76	125.73	120.03
1	C	182	VAL	C-N-CA	5.76	125.73	120.03
2	B	622	ILE	CB-CA-C	-5.76	105.01	111.80
1	A	182	VAL	CA-C-N	5.75	125.73	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	VAL	C-N-CA	5.75	125.73	120.03
1	G	182	VAL	CA-C-N	5.75	125.72	120.03
1	G	182	VAL	C-N-CA	5.75	125.72	120.03
2	D	622	ILE	CB-CA-C	-5.74	105.03	111.80
2	I	622	ILE	CB-CA-C	-5.73	105.04	111.80
4	H	100	SER	N-CA-C	5.72	115.66	108.45
4	K	100	SER	N-CA-C	5.70	115.64	108.45
4	F	100	SER	N-CA-C	5.70	115.63	108.45
1	A	219	ALA	CA-C-N	5.65	125.56	119.85
1	A	219	ALA	C-N-CA	5.65	125.56	119.85
1	C	219	ALA	CA-C-N	5.65	125.55	119.85
1	C	219	ALA	C-N-CA	5.65	125.55	119.85
1	G	219	ALA	CA-C-N	5.62	125.53	119.85
1	G	219	ALA	C-N-CA	5.62	125.53	119.85
2	B	623	TRP	N-CA-C	-5.62	105.07	111.14
3	E	19	VAL	N-CA-C	5.59	116.80	108.46
2	D	623	TRP	N-CA-C	-5.58	105.12	111.14
2	I	623	TRP	N-CA-C	-5.57	105.12	111.14
3	L	19	VAL	N-CA-C	5.57	116.75	108.46
3	J	19	VAL	N-CA-C	5.57	116.75	108.46
1	C	388	THR	CA-C-N	5.49	125.16	119.56
1	C	388	THR	C-N-CA	5.49	125.16	119.56
1	A	388	THR	CA-C-N	5.48	125.15	119.56
1	A	388	THR	C-N-CA	5.48	125.15	119.56
1	G	388	THR	CA-C-N	5.46	125.13	119.56
1	G	388	THR	C-N-CA	5.46	125.13	119.56
1	G	78	ASP	CA-C-N	5.37	125.03	119.56
1	G	78	ASP	C-N-CA	5.37	125.03	119.56
2	I	651	ILE	N-CA-C	-5.36	107.20	111.81
2	B	651	ILE	N-CA-C	-5.36	107.20	111.81
2	D	651	ILE	N-CA-C	-5.33	107.23	111.81
3	L	13	GLU	CA-C-N	5.30	125.20	119.85
3	L	13	GLU	C-N-CA	5.30	125.20	119.85
1	A	78	ASP	CA-C-N	5.30	124.96	119.56
1	A	78	ASP	C-N-CA	5.30	124.96	119.56
1	C	78	ASP	CA-C-N	5.28	124.94	119.56
1	C	78	ASP	C-N-CA	5.28	124.94	119.56
1	A	436	ALA	CA-C-N	5.28	123.46	119.66
1	A	436	ALA	C-N-CA	5.28	123.46	119.66
1	G	436	ALA	CA-C-N	5.27	123.45	119.66
1	G	436	ALA	C-N-CA	5.27	123.45	119.66
3	E	13	GLU	CA-C-N	5.26	125.16	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	13	GLU	C-N-CA	5.26	125.16	119.85
1	C	436	ALA	CA-C-N	5.25	123.44	119.66
1	C	436	ALA	C-N-CA	5.25	123.44	119.66
3	J	13	GLU	CA-C-N	5.23	125.14	119.85
3	J	13	GLU	C-N-CA	5.23	125.14	119.85
1	C	440	ARG	N-CA-C	5.21	120.81	113.56
1	G	440	ARG	N-CA-C	5.19	120.77	113.56
1	A	440	ARG	N-CA-C	5.14	120.70	113.56
2	D	603	ILE	CA-C-N	-5.12	115.50	122.93
2	D	603	ILE	C-N-CA	-5.12	115.50	122.93
2	I	603	ILE	CA-C-N	-5.12	115.51	122.93
2	I	603	ILE	C-N-CA	-5.12	115.51	122.93
2	B	603	ILE	CA-C-N	-5.10	115.54	122.93
2	B	603	ILE	C-N-CA	-5.10	115.54	122.93
1	G	234	ASN	CA-CB-CG	5.02	117.62	112.60
1	A	234	ASN	CA-CB-CG	5.02	117.62	112.60
1	C	234	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	357	THR	CA-C-N	-5.01	115.91	122.37
1	A	357	THR	C-N-CA	-5.01	115.91	122.37

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	3562	0	3475	14	0
1	C	3562	0	3475	15	0
1	G	3562	0	3475	15	0
2	B	975	0	949	6	0
2	D	975	0	949	6	0
2	I	975	0	949	7	0
3	E	842	0	807	5	0
3	J	842	0	807	5	0
3	L	842	0	807	5	0
4	F	897	0	854	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	897	0	854	7	0
4	K	897	0	854	7	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	1	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	1	0
5	U	28	0	25	1	0
5	V	28	0	25	1	0
5	X	28	0	25	0	0
5	Y	28	0	25	1	0
5	Z	28	0	25	0	0
5	a	28	0	25	1	0
5	b	28	0	25	1	0
5	c	28	0	25	0	0
5	d	28	0	25	1	0
5	f	28	0	25	0	0
5	g	28	0	25	0	0
5	h	28	0	25	1	0
5	i	28	0	25	0	0
5	k	28	0	25	1	0
5	l	28	0	25	1	0
5	m	28	0	25	1	0
5	n	28	0	25	0	0
5	o	28	0	25	0	0
5	p	28	0	25	0	0
5	q	28	0	25	1	0
5	s	28	0	25	0	0
5	t	28	0	25	0	0
5	u	28	0	25	1	0
5	v	28	0	25	1	0
5	x	28	0	25	1	0
5	y	28	0	25	1	0
6	R	39	0	34	0	0
6	e	39	0	34	0	0
6	r	39	0	34	1	0
7	W	50	0	43	0	0
7	j	50	0	43	0	0
7	w	50	0	43	0	0
8	A	84	0	78	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	56	0	52	1	0
8	C	84	0	78	5	0
8	D	56	0	52	2	0
8	G	84	0	78	6	0
8	I	56	0	52	1	0
All	All	20439	0	19701	114	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 3.

All (114) 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)
2:D:637:ASN:N	2:D:637:ASN:OD1	2.33	0.62
2:I:637:ASN:OD1	2:I:637:ASN:N	2.33	0.61
1:A:54:CYS:HG	2:B:571:TRP:CG	2.20	0.60
1:G:54:CYS:HG	2:I:571:TRP:CG	2.20	0.59
1:C:54:CYS:HG	2:D:571:TRP:CG	2.21	0.59
2:B:637:ASN:OD1	2:B:637:ASN:N	2.33	0.58
4:K:31:ASP:OD1	4:K:31:ASP:N	2.35	0.58
4:F:31:ASP:N	4:F:31:ASP:OD1	2.35	0.54
8:C:614:NAG:O6	8:C:614:NAG:O4	2.26	0.53
1:A:198:THR:HG21	8:A:606:NAG:H82	1.91	0.52
8:B:701:NAG:O6	8:B:701:NAG:O4	2.26	0.52
4:H:31:ASP:N	4:H:31:ASP:OD1	2.35	0.52
8:A:618:NAG:O6	8:A:618:NAG:O4	2.26	0.52
1:C:198:THR:HG21	8:C:606:NAG:H82	1.91	0.52
1:G:198:THR:HG21	8:G:606:NAG:H82	1.91	0.51
1:G:499:THR:OG1	1:G:500:ALA:N	2.43	0.51
1:C:499:THR:OG1	1:C:500:ALA:N	2.43	0.51
1:A:389:PRO:O	5:U:1:NAG:H82	2.11	0.50
1:G:389:PRO:O	5:u:1:NAG:H82	2.11	0.50
1:C:389:PRO:O	5:h:1:NAG:H82	2.11	0.50
5:a:2:NAG:O6	5:a:2:NAG:O4	2.26	0.50
1:A:499:THR:OG1	1:A:500:ALA:N	2.43	0.50
2:B:664:ASP:OD1	2:B:664:ASP:C	2.54	0.50
2:D:664:ASP:OD1	2:D:664:ASP:C	2.54	0.50
2:I:610:TRP:O	2:I:610:TRP:CG	2.65	0.49
2:D:610:TRP:CG	2:D:610:TRP:O	2.65	0.49
2:B:610:TRP:O	2:B:610:TRP:CG	2.65	0.49
5:q:2:NAG:O6	5:q:2:NAG:O4	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:r:3:BMA:O6	6:r:3:BMA:O4	2.29	0.48
5:x:2:NAG:O6	5:x:2:NAG:O4	2.23	0.48
2:I:616:ASN:OD1	2:I:616:ASN:N	2.43	0.48
4:H:100:SER:OG	4:H:100(A):ALA:N	2.46	0.48
4:K:100:SER:OG	4:K:100(A):ALA:N	2.46	0.48
2:I:664:ASP:OD1	2:I:664:ASP:C	2.54	0.48
4:K:100(A):ALA:HB3	4:K:100(B):PRO:CD	2.44	0.47
4:F:100(A):ALA:HB3	4:F:100(B):PRO:CD	2.44	0.47
4:F:82:THR:OG1	4:F:82(A):THR:N	2.48	0.47
4:F:100:SER:OG	4:F:100(A):ALA:N	2.46	0.47
1:A:393:SER:OG	1:A:394:THR:N	2.47	0.47
5:m:2:NAG:O6	5:m:2:NAG:O4	2.27	0.47
4:H:100(A):ALA:HB3	4:H:100(B):PRO:CD	2.45	0.46
5:v:2:NAG:O6	5:v:2:NAG:O4	2.28	0.46
1:C:234:ASN:OD1	1:C:234:ASN:C	2.59	0.46
1:A:234:ASN:OD1	1:A:234:ASN:C	2.59	0.46
4:K:82:THR:OG1	4:K:82(A):THR:N	2.48	0.46
1:G:234:ASN:OD1	1:G:234:ASN:C	2.59	0.46
8:I:701:NAG:O6	8:I:701:NAG:O4	2.26	0.46
8:G:614:NAG:O6	8:G:614:NAG:O4	2.26	0.46
5:T:2:NAG:O6	5:T:2:NAG:O4	2.25	0.46
4:H:82:THR:OG1	4:H:82(A):THR:N	2.48	0.45
3:L:50:ARG:O	3:L:51:THR:C	2.58	0.45
8:C:618:NAG:O6	8:C:618:NAG:O4	2.26	0.45
2:B:616:ASN:OD1	2:B:616:ASN:N	2.43	0.45
3:E:93:TYR:HB3	4:F:100(C):TYR:HB2	1.99	0.45
8:G:618:NAG:O6	8:G:618:NAG:O4	2.26	0.45
1:C:34:LYS:NZ	2:D:612:ASP:OD1	2.49	0.45
1:G:123:THR:N	1:G:124:PRO:CD	2.80	0.45
1:G:346:VAL:HG11	1:G:395:TRP:HE1	1.82	0.45
5:b:2:NAG:O6	5:b:2:NAG:O4	2.27	0.45
8:D:701:NAG:O6	8:D:701:NAG:O4	2.26	0.45
1:C:88:ASN:OD1	1:C:88:ASN:N	2.50	0.44
2:B:618:THR:OG1	2:B:619:ILE:N	2.51	0.44
1:C:393:SER:OG	1:C:394:THR:N	2.47	0.44
3:E:67:SER:O	3:E:68:GLY:C	2.60	0.44
5:d:2:NAG:O6	5:d:2:NAG:O4	2.25	0.44
1:A:346:VAL:HG11	1:A:395:TRP:HE1	1.82	0.44
3:E:50:ARG:O	3:E:51:THR:C	2.58	0.44
5:k:2:NAG:O6	5:k:2:NAG:O4	2.23	0.44
1:C:346:VAL:HG11	1:C:395:TRP:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:93:TYR:HB3	4:K:100(C):TYR:HB2	1.99	0.44
1:A:123:THR:N	1:A:124:PRO:CD	2.80	0.44
1:C:123:THR:N	1:C:124:PRO:CD	2.80	0.43
3:J:50:ARG:O	3:J:51:THR:C	2.58	0.43
4:H:100(A):ALA:HB3	4:H:100(B):PRO:HD3	2.00	0.43
4:F:100(A):ALA:HB3	4:F:100(B):PRO:HD3	2.00	0.43
3:J:67:SER:O	3:J:68:GLY:C	2.60	0.43
2:D:618:THR:OG1	2:D:619:ILE:N	2.51	0.43
1:A:357:THR:OG1	8:A:635:NAG:H81	2.19	0.43
3:L:93:TYR:HB3	4:H:100(C):TYR:HB2	1.99	0.43
1:G:357:THR:OG1	8:G:635:NAG:H81	2.19	0.43
1:C:357:THR:OG1	8:C:635:NAG:H81	2.19	0.43
4:K:100(A):ALA:HB3	4:K:100(B):PRO:HD3	2.00	0.43
1:G:34:LYS:NZ	2:I:612:ASP:OD1	2.49	0.43
3:L:67:SER:O	3:L:68:GLY:C	2.60	0.42
1:C:87:GLY:HA2	8:C:601:NAG:H82	2.00	0.42
3:J:92:TYR:O	3:J:93:TYR:C	2.60	0.42
1:A:87:GLY:HA2	8:A:601:NAG:H82	2.00	0.42
1:C:409:GLN:HG2	5:I:1:NAG:H82	2.01	0.42
3:E:92:TYR:O	3:E:93:TYR:C	2.60	0.42
4:K:83:THR:OG1	4:K:84:ALA:N	2.52	0.42
8:A:614:NAG:O6	8:A:614:NAG:O4	2.26	0.42
8:D:703:NAG:O6	8:D:703:NAG:O4	2.30	0.42
1:G:388:THR:N	1:G:389:PRO:CD	2.82	0.42
1:C:388:THR:N	1:C:389:PRO:CD	2.82	0.42
3:J:61:ARG:HG3	3:J:62:PHE:CD1	2.55	0.42
1:A:409:GLN:HG2	5:Y:1:NAG:H82	2.01	0.42
1:A:388:THR:N	1:A:389:PRO:CD	2.82	0.42
3:E:61:ARG:HG3	3:E:62:PHE:CD1	2.55	0.42
1:G:87:GLY:HA2	8:G:601:NAG:H82	2.00	0.42
3:L:61:ARG:HG3	3:L:62:PHE:CD1	2.55	0.42
3:L:92:TYR:O	3:L:93:TYR:C	2.60	0.41
4:H:83:THR:OG1	4:H:84:ALA:N	2.53	0.41
1:G:409:GLN:HG2	5:y:1:NAG:H82	2.01	0.41
5:V:2:NAG:O6	5:V:2:NAG:O4	2.28	0.41
1:G:393:SER:OG	1:G:394:THR:N	2.47	0.41
1:G:167:ASP:OD1	1:G:167:ASP:N	2.50	0.41
2:I:618:THR:OG1	2:I:619:ILE:N	2.51	0.41
4:F:83:THR:OG1	4:F:84:ALA:N	2.53	0.41
8:G:606:NAG:O6	8:G:606:NAG:O4	2.34	0.41
5:O:2:NAG:O6	5:O:2:NAG:O4	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASN:OD1	1:A:289:ASN:N	2.46	0.40
1:A:50:THR:OG1	1:A:51:THR:N	2.55	0.40
1:C:358:ILE:O	1:C:358:ILE:HG23	2.21	0.40
1:G:50:THR:OG1	1:G:51:THR:N	2.54	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	446/524 (85%)	435 (98%)	11 (2%)	0	100	100
1	C	446/524 (85%)	435 (98%)	11 (2%)	0	100	100
1	G	446/524 (85%)	435 (98%)	11 (2%)	0	100	100
2	B	116/153 (76%)	113 (97%)	3 (3%)	0	100	100
2	D	116/153 (76%)	113 (97%)	3 (3%)	0	100	100
2	I	116/153 (76%)	113 (97%)	3 (3%)	0	100	100
3	E	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
3	J	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
3	L	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
4	F	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	14	47
4	H	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	14	47
4	K	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	14	47
All	All	2364/2724 (87%)	2301 (97%)	60 (2%)	3 (0%)	49	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	100(A)	ALA
4	F	100(A)	ALA
4	K	100(A)	ALA

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	401/461 (87%)	399 (100%)	2 (0%)	81	82
1	C	401/461 (87%)	399 (100%)	2 (0%)	81	82
1	G	401/461 (87%)	399 (100%)	2 (0%)	81	82
2	B	106/130 (82%)	104 (98%)	2 (2%)	50	66
2	D	106/130 (82%)	104 (98%)	2 (2%)	50	66
2	I	106/130 (82%)	104 (98%)	2 (2%)	50	66
3	E	93/93 (100%)	93 (100%)	0	100	100
3	J	93/93 (100%)	93 (100%)	0	100	100
3	L	93/93 (100%)	93 (100%)	0	100	100
4	F	92/93 (99%)	92 (100%)	0	100	100
4	H	92/93 (99%)	92 (100%)	0	100	100
4	K	92/93 (99%)	92 (100%)	0	100	100
All	All	2076/2331 (89%)	2064 (99%)	12 (1%)	76	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	234	ASN
2	B	608	VAL
2	B	637	ASN
1	C	88	ASN
1	C	234	ASN
2	D	608	VAL
2	D	637	ASN

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Mol	Chain	Res	Type
1	G	88	ASN
1	G	234	ASN
2	I	608	VAL
2	I	637	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	105	HIS
2	B	575	GLN
3	L	30	ASN
4	H	56	ASN
1	C	92	ASN
1	C	105	HIS
2	D	575	GLN
3	E	30	ASN
4	F	56	ASN
1	G	92	ASN
1	G	105	HIS
2	I	575	GLN
3	J	30	ASN
4	K	56	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](#)

87 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
5	NAG	M	1	5,1	14,14,15	0.71	0	17,19,21	1.19	3 (17%)
5	NAG	M	2	5	14,14,15	0.83	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	N	1	5,1	14,14,15	0.77	1 (7%)	17,19,21	0.86	1 (5%)
5	NAG	N	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	O	1	5,1	14,14,15	0.67	0	17,19,21	1.11	2 (11%)
5	NAG	O	2	5	14,14,15	0.78	1 (7%)	17,19,21	0.83	1 (5%)
5	NAG	P	1	5,1	14,14,15	0.72	0	17,19,21	0.91	1 (5%)
5	NAG	P	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.76	1 (5%)
5	NAG	Q	1	5,1	14,14,15	0.82	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	Q	2	5	14,14,15	0.70	1 (7%)	17,19,21	0.93	1 (5%)
6	NAG	R	1	6,1	14,14,15	0.93	1 (7%)	17,19,21	1.90	4 (23%)
6	NAG	R	2	6	14,14,15	0.73	0	17,19,21	1.16	1 (5%)
6	BMA	R	3	6	11,11,12	0.69	0	15,15,17	0.89	1 (6%)
5	NAG	S	1	5,1	14,14,15	0.69	0	17,19,21	0.82	1 (5%)
5	NAG	S	2	5	14,14,15	0.81	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	T	1	5,1	14,14,15	0.68	0	17,19,21	1.19	2 (11%)
5	NAG	T	2	5	14,14,15	0.83	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	U	1	5,1	14,14,15	0.82	0	17,19,21	1.46	3 (17%)
5	NAG	U	2	5	14,14,15	0.73	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	V	1	5,1	14,14,15	0.84	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	V	2	5	14,14,15	0.71	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	W	1	1,7	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
7	NAG	W	2	7	14,14,15	0.76	1 (7%)	17,19,21	0.79	0
7	BMA	W	3	7	11,11,12	0.59	0	15,15,17	0.90	1 (6%)
7	MAN	W	4	7	11,11,12	0.57	0	15,15,17	0.86	1 (6%)
5	NAG	X	1	5,1	14,14,15	0.80	0	17,19,21	1.47	4 (23%)
5	NAG	X	2	5	14,14,15	0.80	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	Y	1	5,1	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
5	NAG	Y	2	5	14,14,15	0.82	1 (7%)	17,19,21	0.86	1 (5%)
5	NAG	Z	1	5,1	14,14,15	0.71	0	17,19,21	1.19	3 (17%)
5	NAG	Z	2	5	14,14,15	0.84	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	a	1	5,1	14,14,15	0.77	1 (7%)	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	a	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	b	1	5,1	14,14,15	0.68	0	17,19,21	1.10	2 (11%)
5	NAG	b	2	5	14,14,15	0.80	1 (7%)	17,19,21	0.83	1 (5%)
5	NAG	c	1	5,1	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
5	NAG	c	2	5	14,14,15	0.78	1 (7%)	17,19,21	0.76	1 (5%)
5	NAG	d	1	5,1	14,14,15	0.81	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	d	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.93	1 (5%)
6	NAG	e	1	6,1	14,14,15	0.93	1 (7%)	17,19,21	1.90	4 (23%)
6	NAG	e	2	6	14,14,15	0.73	0	17,19,21	1.16	1 (5%)
6	BMA	e	3	6	11,11,12	0.68	0	15,15,17	0.89	1 (6%)
5	NAG	f	1	5,1	14,14,15	0.69	0	17,19,21	0.82	1 (5%)
5	NAG	f	2	5	14,14,15	0.80	1 (7%)	17,19,21	0.95	1 (5%)
5	NAG	g	1	5,1	14,14,15	0.67	0	17,19,21	1.20	2 (11%)
5	NAG	g	2	5	14,14,15	0.84	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	h	1	5,1	14,14,15	0.82	0	17,19,21	1.46	4 (23%)
5	NAG	h	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	i	1	5,1	14,14,15	0.83	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	i	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	j	1	1,7	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
7	NAG	j	2	7	14,14,15	0.75	1 (7%)	17,19,21	0.80	0
7	BMA	j	3	7	11,11,12	0.58	0	15,15,17	0.91	1 (6%)
7	MAN	j	4	7	11,11,12	0.58	0	15,15,17	0.86	1 (6%)
5	NAG	k	1	5,1	14,14,15	0.79	0	17,19,21	1.47	4 (23%)
5	NAG	k	2	5	14,14,15	0.80	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	l	1	5,1	14,14,15	0.68	0	17,19,21	0.98	1 (5%)
5	NAG	l	2	5	14,14,15	0.85	1 (7%)	17,19,21	0.87	1 (5%)
5	NAG	m	1	5,1	14,14,15	0.70	0	17,19,21	1.20	3 (17%)
5	NAG	m	2	5	14,14,15	0.84	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	n	1	5,1	14,14,15	0.77	1 (7%)	17,19,21	0.86	1 (5%)
5	NAG	n	2	5	14,14,15	0.73	1 (7%)	17,19,21	0.98	1 (5%)
5	NAG	o	1	5,1	14,14,15	0.67	0	17,19,21	1.11	2 (11%)
5	NAG	o	2	5	14,14,15	0.78	1 (7%)	17,19,21	0.83	1 (5%)
5	NAG	p	1	5,1	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
5	NAG	p	2	5	14,14,15	0.77	1 (7%)	17,19,21	0.76	1 (5%)
5	NAG	q	1	5,1	14,14,15	0.80	1 (7%)	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	q	2	5	14,14,15	0.69	1 (7%)	17,19,21	0.93	1 (5%)
6	NAG	r	1	6,1	14,14,15	0.92	1 (7%)	17,19,21	1.90	4 (23%)
6	NAG	r	2	6	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
6	BMA	r	3	6	11,11,12	0.71	0	15,15,17	0.90	1 (6%)
5	NAG	s	1	5,1	14,14,15	0.70	0	17,19,21	0.82	1 (5%)
5	NAG	s	2	5	14,14,15	0.81	1 (7%)	17,19,21	0.94	1 (5%)
5	NAG	t	1	5,1	14,14,15	0.67	0	17,19,21	1.19	2 (11%)
5	NAG	t	2	5	14,14,15	0.85	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	u	1	5,1	14,14,15	0.82	0	17,19,21	1.46	3 (17%)
5	NAG	u	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.97	1 (5%)
5	NAG	v	1	5,1	14,14,15	0.83	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	v	2	5	14,14,15	0.72	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	w	1	1,7	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
7	NAG	w	2	7	14,14,15	0.74	1 (7%)	17,19,21	0.80	0
7	BMA	w	3	7	11,11,12	0.58	0	15,15,17	0.91	1 (6%)
7	MAN	w	4	7	11,11,12	0.59	0	15,15,17	0.86	1 (6%)
5	NAG	x	1	5,1	14,14,15	0.79	0	17,19,21	1.47	4 (23%)
5	NAG	x	2	5	14,14,15	0.80	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	y	1	5,1	14,14,15	0.67	0	17,19,21	0.98	1 (5%)
5	NAG	y	2	5	14,14,15	0.83	1 (7%)	17,19,21	0.87	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
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	NAG	Q	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	R	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	1/2/19/22	0/1/1/1
5	NAG	S	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
5	NAG	T	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	NAG	V	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
7	NAG	W	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	W	2	7	-	1/6/23/26	0/1/1/1
7	BMA	W	3	7	-	1/2/19/22	0/1/1/1
7	MAN	W	4	7	-	1/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
5	NAG	Z	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	1/6/23/26	0/1/1/1
5	NAG	a	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	NAG	c	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	c	2	5	-	1/6/23/26	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1
6	NAG	e	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	BMA	e	3	6	-	1/2/19/22	0/1/1/1
5	NAG	f	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
5	NAG	g	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
5	NAG	h	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	h	2	5	-	2/6/23/26	0/1/1/1
5	NAG	i	1	5,1	-	1/6/23/26	0/1/1/1

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

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	1	NAG	C1-C2	3.08	1.56	1.52
6	e	1	NAG	C1-C2	3.07	1.56	1.52
6	r	1	NAG	C1-C2	3.02	1.56	1.52
5	Z	2	NAG	C1-C2	2.74	1.56	1.52
5	V	1	NAG	C1-C2	2.70	1.56	1.52
5	t	2	NAG	C1-C2	2.70	1.56	1.52
5	m	2	NAG	C1-C2	2.69	1.56	1.52
5	g	2	NAG	C1-C2	2.68	1.56	1.52
5	v	1	NAG	C1-C2	2.67	1.56	1.52
5	M	2	NAG	C1-C2	2.66	1.56	1.52
5	l	2	NAG	C1-C2	2.65	1.56	1.52
5	T	2	NAG	C1-C2	2.65	1.55	1.52
5	i	1	NAG	C1-C2	2.65	1.55	1.52
5	k	2	NAG	C1-C2	2.62	1.55	1.52
5	X	2	NAG	C1-C2	2.60	1.55	1.52
5	x	2	NAG	C1-C2	2.60	1.55	1.52
5	y	2	NAG	C1-C2	2.59	1.55	1.52
5	b	2	NAG	C1-C2	2.59	1.55	1.52
5	Y	2	NAG	C1-C2	2.53	1.55	1.52
5	S	2	NAG	C1-C2	2.52	1.55	1.52
5	O	2	NAG	C1-C2	2.51	1.55	1.52
5	s	2	NAG	C1-C2	2.50	1.55	1.52
5	f	2	NAG	C1-C2	2.50	1.55	1.52
5	o	2	NAG	C1-C2	2.50	1.55	1.52
5	c	2	NAG	C1-C2	2.42	1.55	1.52
5	P	2	NAG	C1-C2	2.39	1.55	1.52
5	p	2	NAG	C1-C2	2.38	1.55	1.52
5	n	1	NAG	C1-C2	2.37	1.55	1.52
5	N	1	NAG	C1-C2	2.37	1.55	1.52
5	a	1	NAG	C1-C2	2.34	1.55	1.52
5	Q	1	NAG	C1-C2	2.31	1.55	1.52
5	q	1	NAG	C1-C2	2.26	1.55	1.52
5	d	1	NAG	C1-C2	2.25	1.55	1.52
5	U	2	NAG	C1-C2	2.25	1.55	1.52
5	h	2	NAG	C1-C2	2.17	1.55	1.52
5	n	2	NAG	C1-C2	2.16	1.55	1.52
5	u	2	NAG	C1-C2	2.16	1.55	1.52
5	a	2	NAG	C1-C2	2.16	1.55	1.52
5	N	2	NAG	C1-C2	2.14	1.55	1.52
5	i	2	NAG	C1-C2	2.10	1.55	1.52
5	v	2	NAG	C1-C2	2.09	1.55	1.52
7	W	2	NAG	C1-C2	2.09	1.55	1.52
7	j	2	NAG	C1-C2	2.08	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	2	NAG	C1-C2	2.06	1.55	1.52
7	w	2	NAG	C1-C2	2.06	1.55	1.52
5	V	2	NAG	C1-C2	2.03	1.55	1.52
5	q	2	NAG	C1-C2	2.02	1.55	1.52
5	d	2	NAG	C1-C2	2.02	1.55	1.52

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	e	1	NAG	C2-N2-C7	4.68	129.17	122.90
6	r	1	NAG	C2-N2-C7	4.67	129.15	122.90
6	R	1	NAG	C2-N2-C7	4.64	129.12	122.90
6	R	1	NAG	C1-C2-N2	4.40	117.37	110.43
6	e	1	NAG	C1-C2-N2	4.39	117.36	110.43
6	r	1	NAG	C1-C2-N2	4.39	117.35	110.43
5	h	1	NAG	C4-C3-C2	-3.50	105.89	111.02
5	U	1	NAG	C4-C3-C2	-3.48	105.92	111.02
5	u	1	NAG	C4-C3-C2	-3.46	105.95	111.02
5	Y	1	NAG	C3-C4-C5	-3.45	103.98	110.23
5	l	1	NAG	C3-C4-C5	-3.45	103.98	110.23
5	y	1	NAG	C3-C4-C5	-3.43	104.01	110.23
6	R	2	NAG	C3-C4-C5	-3.19	104.45	110.23
6	e	2	NAG	C3-C4-C5	-3.19	104.45	110.23
6	r	2	NAG	C3-C4-C5	-3.18	104.47	110.23
5	g	1	NAG	C3-C4-C5	-3.05	104.71	110.23
5	t	1	NAG	C3-C4-C5	-3.04	104.72	110.23
5	T	1	NAG	C3-C4-C5	-3.04	104.72	110.23
5	k	1	NAG	O5-C5-C6	-3.04	101.75	107.66
5	X	1	NAG	O5-C5-C6	-3.03	101.76	107.66
5	x	1	NAG	O5-C5-C6	-3.02	101.79	107.66
5	V	1	NAG	C4-C3-C2	-2.96	106.68	111.02
5	v	1	NAG	C4-C3-C2	-2.95	106.69	111.02
5	i	1	NAG	C4-C3-C2	-2.94	106.71	111.02
5	g	2	NAG	C4-C3-C2	-2.92	106.73	111.02
5	a	2	NAG	C4-C3-C2	-2.91	106.75	111.02
5	n	2	NAG	C4-C3-C2	-2.91	106.75	111.02
5	t	2	NAG	C4-C3-C2	-2.91	106.76	111.02
5	T	2	NAG	C4-C3-C2	-2.90	106.76	111.02
5	N	2	NAG	C4-C3-C2	-2.90	106.76	111.02
7	j	3	BMA	C2-C3-C4	-2.83	105.89	110.86
7	w	3	BMA	C2-C3-C4	-2.83	105.89	110.86
7	W	3	BMA	C2-C3-C4	-2.80	105.94	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	w	1	NAG	C3-C4-C5	-2.77	105.21	110.23
7	j	1	NAG	C3-C4-C5	-2.76	105.22	110.23
7	W	1	NAG	C3-C4-C5	-2.75	105.24	110.23
5	P	1	NAG	C3-C4-C5	-2.68	105.37	110.23
5	f	2	NAG	C4-C3-C2	-2.68	107.09	111.02
5	V	2	NAG	C4-C3-C2	-2.68	107.10	111.02
5	i	2	NAG	C4-C3-C2	-2.67	107.10	111.02
5	p	1	NAG	C3-C4-C5	-2.67	105.39	110.23
5	v	2	NAG	C4-C3-C2	-2.67	107.11	111.02
5	c	1	NAG	C3-C4-C5	-2.66	105.40	110.23
5	S	2	NAG	C4-C3-C2	-2.66	107.12	111.02
5	u	2	NAG	C4-C3-C2	-2.64	107.15	111.02
5	U	2	NAG	C4-C3-C2	-2.64	107.15	111.02
5	s	2	NAG	C4-C3-C2	-2.64	107.15	111.02
5	N	1	NAG	C3-C4-C5	-2.63	105.46	110.23
5	a	1	NAG	C3-C4-C5	-2.63	105.47	110.23
5	h	2	NAG	C4-C3-C2	-2.63	107.17	111.02
7	w	4	MAN	C2-C3-C4	-2.63	106.24	110.86
5	Q	2	NAG	C4-C3-C2	-2.62	107.18	111.02
7	W	4	MAN	C2-C3-C4	-2.62	106.26	110.86
5	d	2	NAG	C4-C3-C2	-2.61	107.19	111.02
5	n	1	NAG	C3-C4-C5	-2.61	105.50	110.23
5	q	2	NAG	C4-C3-C2	-2.61	107.19	111.02
7	j	4	MAN	C2-C3-C4	-2.60	106.28	110.86
5	O	1	NAG	C4-C3-C2	-2.60	107.21	111.02
5	o	1	NAG	C4-C3-C2	-2.60	107.21	111.02
5	b	1	NAG	C4-C3-C2	-2.59	107.22	111.02
5	k	2	NAG	C4-C3-C2	-2.56	107.26	111.02
5	x	2	NAG	C4-C3-C2	-2.56	107.27	111.02
5	m	1	NAG	C4-C3-C2	-2.55	107.27	111.02
5	X	2	NAG	C4-C3-C2	-2.54	107.29	111.02
5	Z	1	NAG	C4-C3-C2	-2.54	107.29	111.02
5	d	1	NAG	C3-C4-C5	-2.53	105.65	110.23
5	M	1	NAG	C4-C3-C2	-2.53	107.31	111.02
5	Q	1	NAG	C3-C4-C5	-2.52	105.67	110.23
5	X	1	NAG	C4-C3-C2	-2.51	107.34	111.02
5	x	1	NAG	C4-C3-C2	-2.50	107.35	111.02
5	q	1	NAG	C3-C4-C5	-2.50	105.70	110.23
5	k	1	NAG	C4-C3-C2	-2.50	107.35	111.02
5	f	1	NAG	C3-C4-C5	-2.49	105.72	110.23
5	s	1	NAG	C3-C4-C5	-2.49	105.72	110.23
5	S	1	NAG	C3-C4-C5	-2.49	105.72	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	u	1	NAG	C2-N2-C7	-2.45	119.62	122.90
5	U	1	NAG	C2-N2-C7	-2.45	119.62	122.90
5	M	2	NAG	C4-C3-C2	-2.43	107.45	111.02
5	h	1	NAG	C2-N2-C7	-2.43	119.65	122.90
5	Z	2	NAG	C4-C3-C2	-2.42	107.47	111.02
5	m	2	NAG	C4-C3-C2	-2.41	107.48	111.02
6	R	1	NAG	C3-C4-C5	-2.34	105.99	110.23
5	Z	1	NAG	O5-C5-C6	-2.33	103.13	107.66
5	m	1	NAG	O5-C5-C6	-2.33	103.13	107.66
6	R	1	NAG	O5-C1-C2	-2.33	107.69	111.29
5	c	2	NAG	C4-C3-C2	-2.33	107.61	111.02
6	e	1	NAG	O5-C1-C2	-2.33	107.69	111.29
5	M	1	NAG	O5-C5-C6	-2.32	103.14	107.66
6	r	1	NAG	C3-C4-C5	-2.32	106.02	110.23
5	P	2	NAG	C4-C3-C2	-2.32	107.62	111.02
6	r	1	NAG	O5-C1-C2	-2.31	107.71	111.29
5	p	2	NAG	C4-C3-C2	-2.31	107.63	111.02
6	e	1	NAG	C3-C4-C5	-2.31	106.04	110.23
5	O	2	NAG	C4-C3-C2	-2.26	107.70	111.02
5	o	2	NAG	C4-C3-C2	-2.26	107.71	111.02
5	b	2	NAG	C4-C3-C2	-2.24	107.73	111.02
5	y	2	NAG	C4-C3-C2	-2.24	107.74	111.02
5	Y	2	NAG	C4-C3-C2	-2.23	107.75	111.02
5	l	2	NAG	C4-C3-C2	-2.22	107.76	111.02
5	k	1	NAG	C3-C4-C5	-2.22	106.20	110.23
5	t	1	NAG	O4-C4-C3	-2.22	105.14	110.38
5	X	1	NAG	C3-C4-C5	-2.21	106.22	110.23
5	x	1	NAG	C3-C4-C5	-2.21	106.23	110.23
5	T	1	NAG	O4-C4-C3	-2.21	105.18	110.38
5	g	1	NAG	O4-C4-C3	-2.20	105.18	110.38
5	Z	1	NAG	C3-C4-C5	-2.19	106.26	110.23
5	m	1	NAG	C3-C4-C5	-2.19	106.27	110.23
5	x	1	NAG	C1-O5-C5	2.18	115.11	112.19
5	M	1	NAG	C3-C4-C5	-2.17	106.30	110.23
5	k	1	NAG	C1-O5-C5	2.16	115.08	112.19
5	X	1	NAG	C1-O5-C5	2.15	115.07	112.19
6	r	3	BMA	C2-C3-C4	-2.12	107.13	110.86
6	e	3	BMA	C2-C3-C4	-2.09	107.19	110.86
6	R	3	BMA	C2-C3-C4	-2.09	107.19	110.86
5	U	1	NAG	C3-C4-C5	-2.08	106.47	110.23
5	u	1	NAG	C3-C4-C5	-2.06	106.50	110.23
5	O	1	NAG	C2-N2-C7	-2.06	120.14	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	h	1	NAG	C3-C4-C5	-2.05	106.51	110.23
5	o	1	NAG	C2-N2-C7	-2.05	120.15	122.90
5	b	1	NAG	C2-N2-C7	-2.04	120.16	122.90
5	h	1	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	1	NAG	C1-C2-N2-C7
6	e	1	NAG	C1-C2-N2-C7
6	r	1	NAG	C1-C2-N2-C7
5	M	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
5	m	1	NAG	O5-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
5	u	2	NAG	C4-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
5	q	1	NAG	O5-C5-C6-O6
5	x	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
5	u	2	NAG	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
5	m	1	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	n	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
5	q	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	s	2	NAG	O5-C5-C6-O6
5	t	2	NAG	O5-C5-C6-O6
5	v	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	o	2	NAG	O5-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
5	q	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
7	j	3	BMA	O5-C5-C6-O6
7	w	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
6	e	3	BMA	O5-C5-C6-O6
6	r	3	BMA	O5-C5-C6-O6
7	W	4	MAN	O5-C5-C6-O6
7	j	4	MAN	O5-C5-C6-O6
7	w	4	MAN	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	l	2	NAG	O5-C5-C6-O6
5	y	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	p	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
7	w	2	NAG	O5-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
5	x	2	NAG	C4-C5-C6-O6
5	v	1	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
5	x	1	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	k	1	NAG	O5-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	k	1	NAG	C4-C5-C6-O6
5	x	1	NAG	C4-C5-C6-O6

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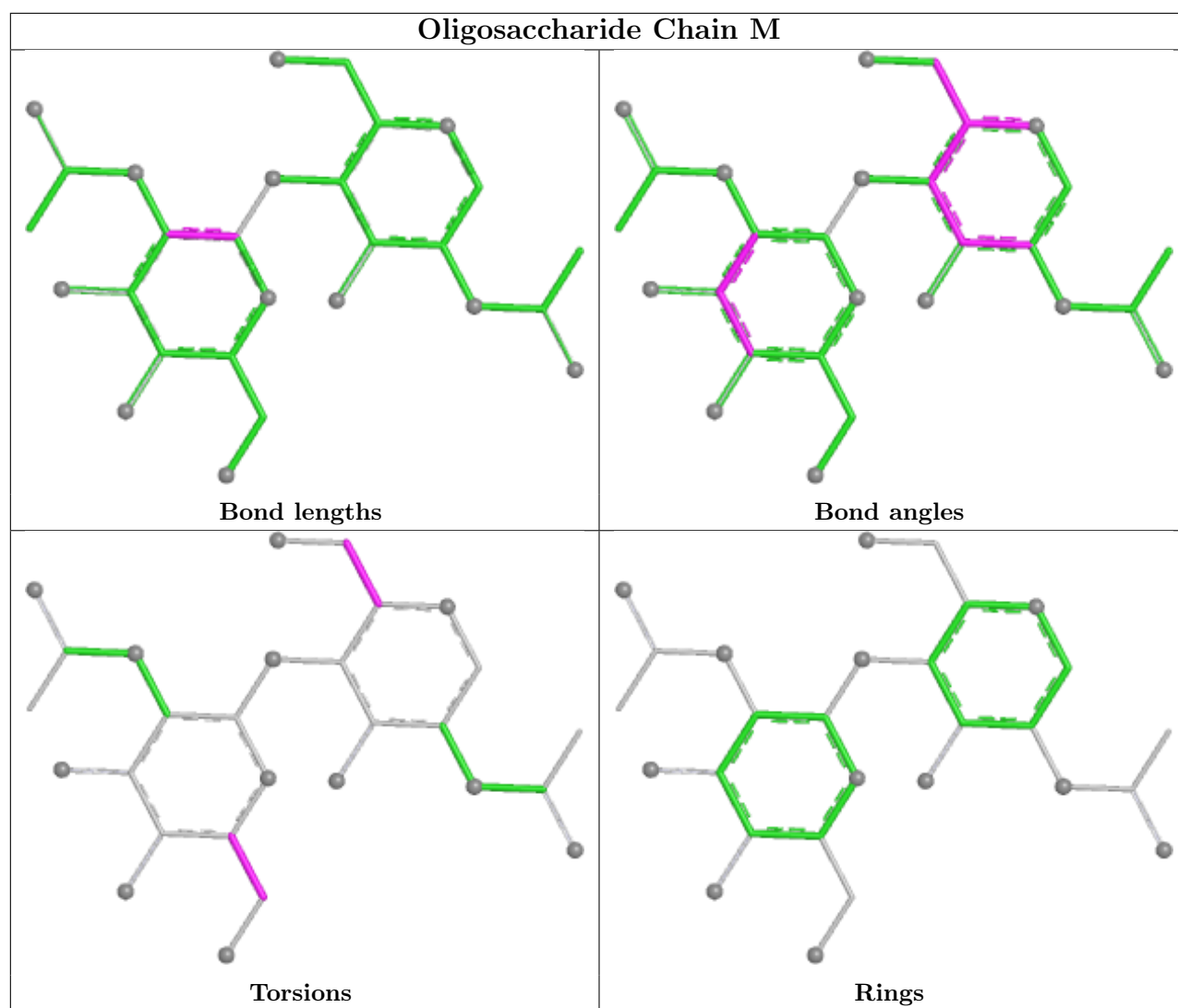
Mol	Chain	Res	Type	Atoms
7	w	1	NAG	O5-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	t	2	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
5	s	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	n	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
5	q	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6

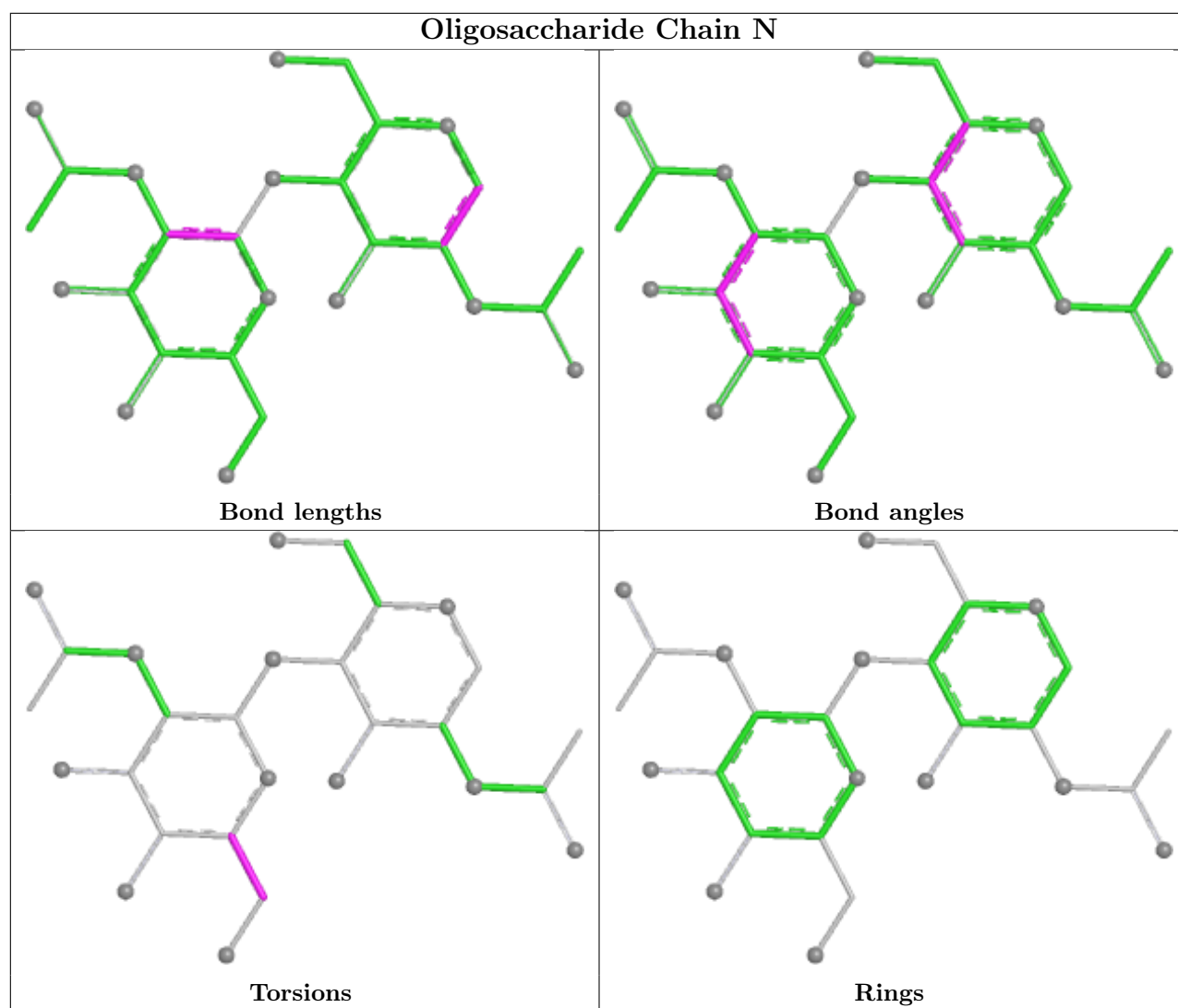
There are no ring outliers.

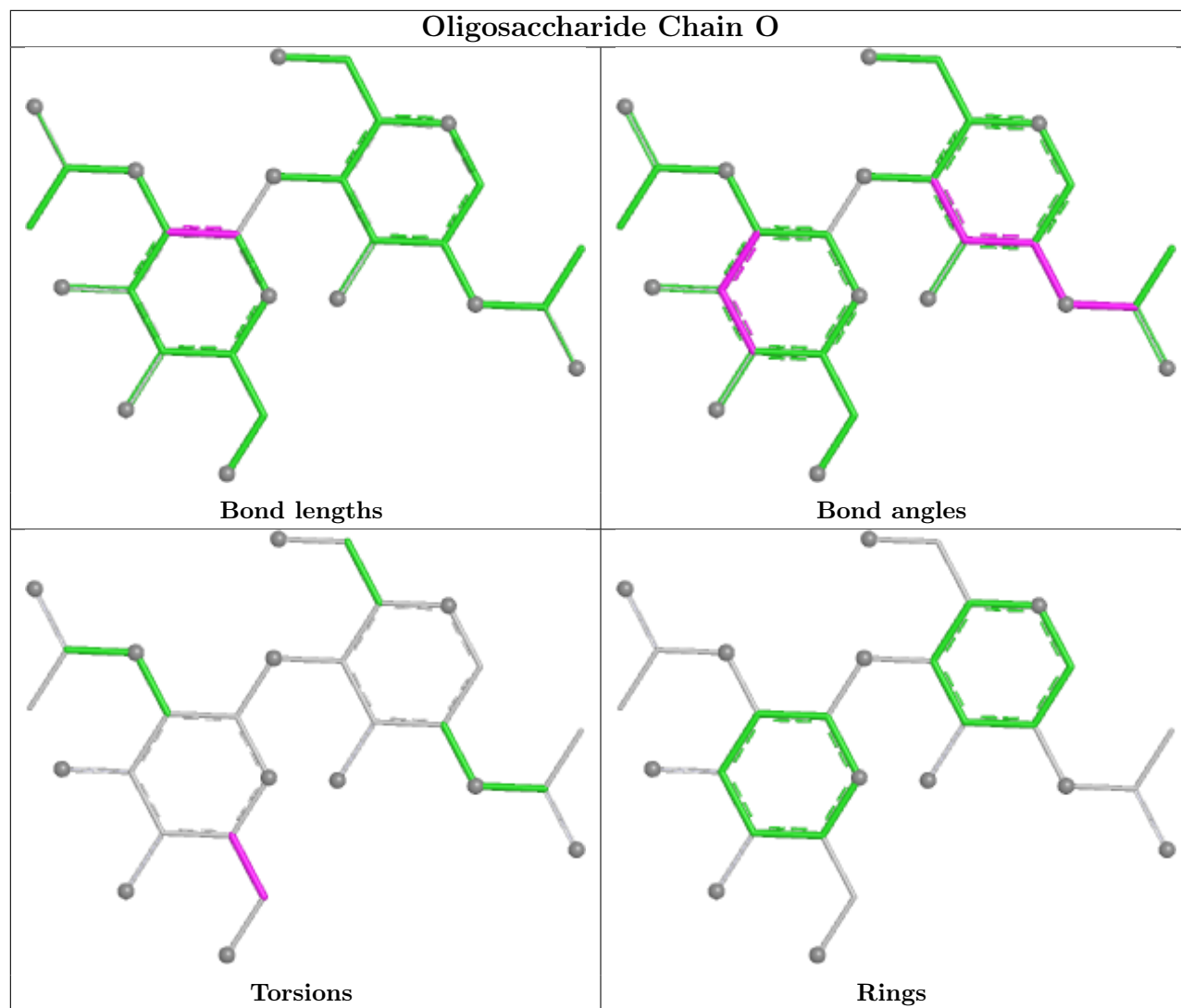
18 monomers are involved in 18 short contacts:

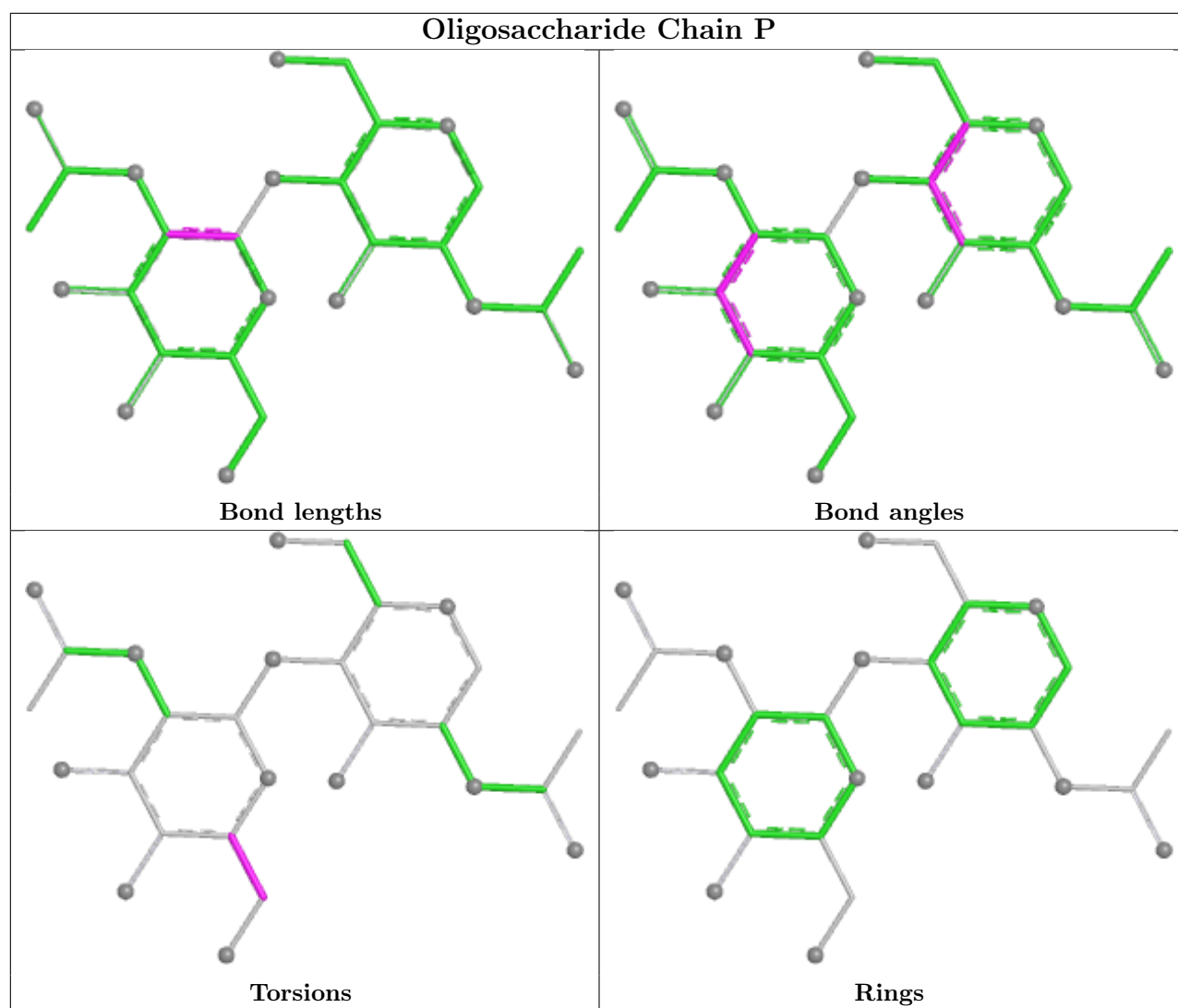
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	v	2	NAG	1	0
5	V	2	NAG	1	0
5	T	2	NAG	1	0
5	q	2	NAG	1	0
5	k	2	NAG	1	0
5	O	2	NAG	1	0
5	Y	1	NAG	1	0
5	d	2	NAG	1	0
5	a	2	NAG	1	0
5	m	2	NAG	1	0
5	u	1	NAG	1	0
5	y	1	NAG	1	0
5	h	1	NAG	1	0
6	r	3	BMA	1	0
5	x	2	NAG	1	0
5	l	1	NAG	1	0
5	U	1	NAG	1	0
5	b	2	NAG	1	0

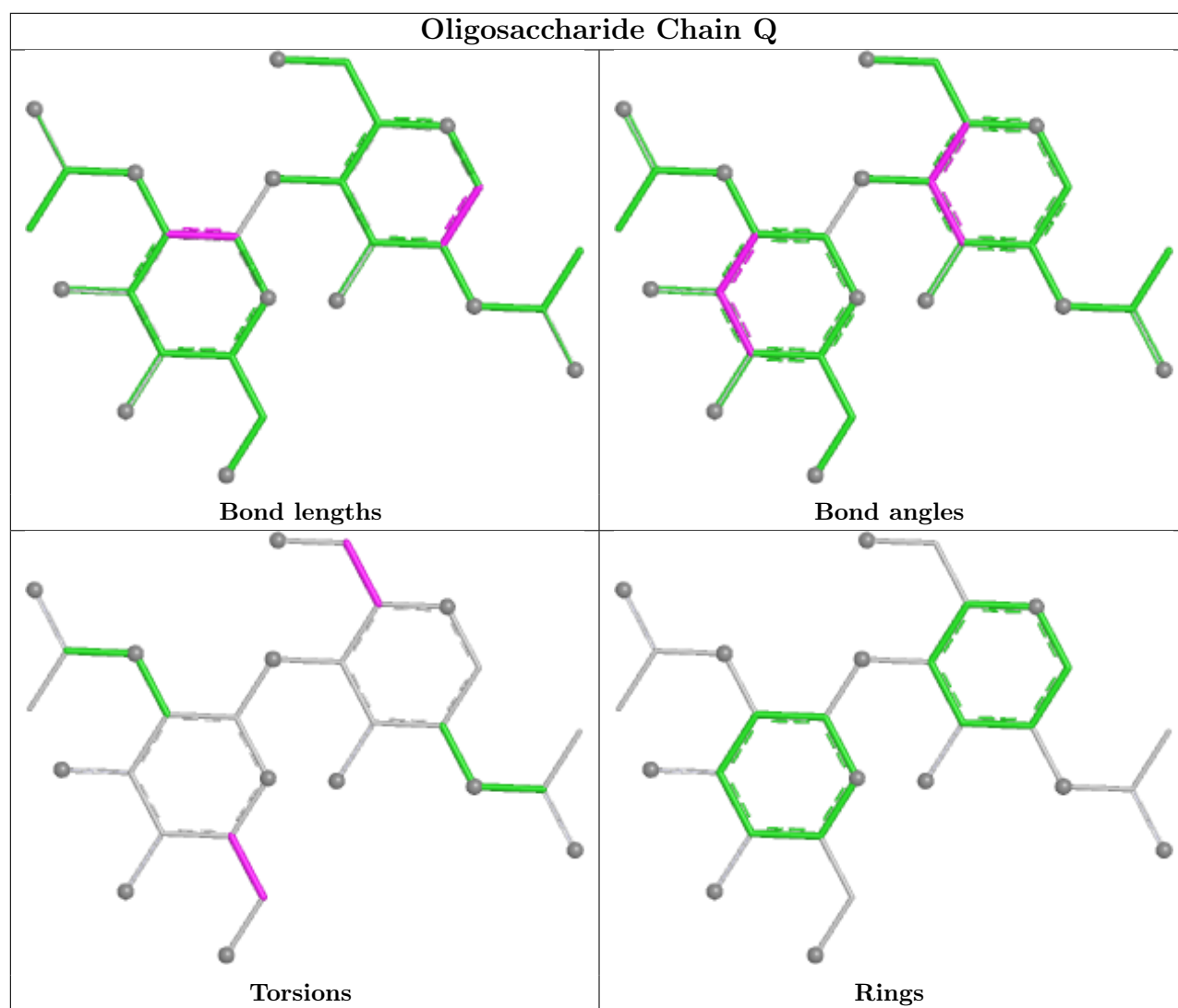
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

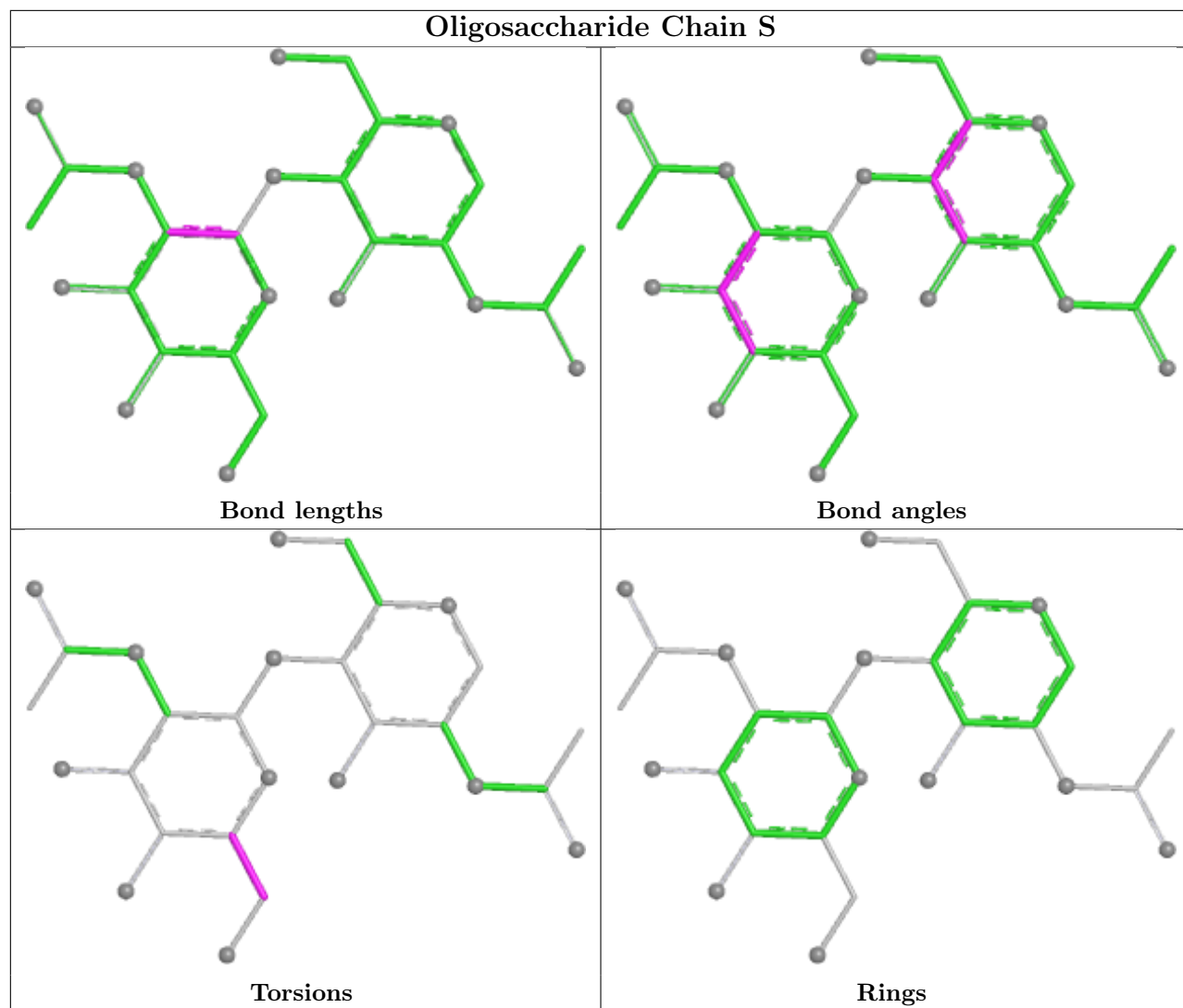


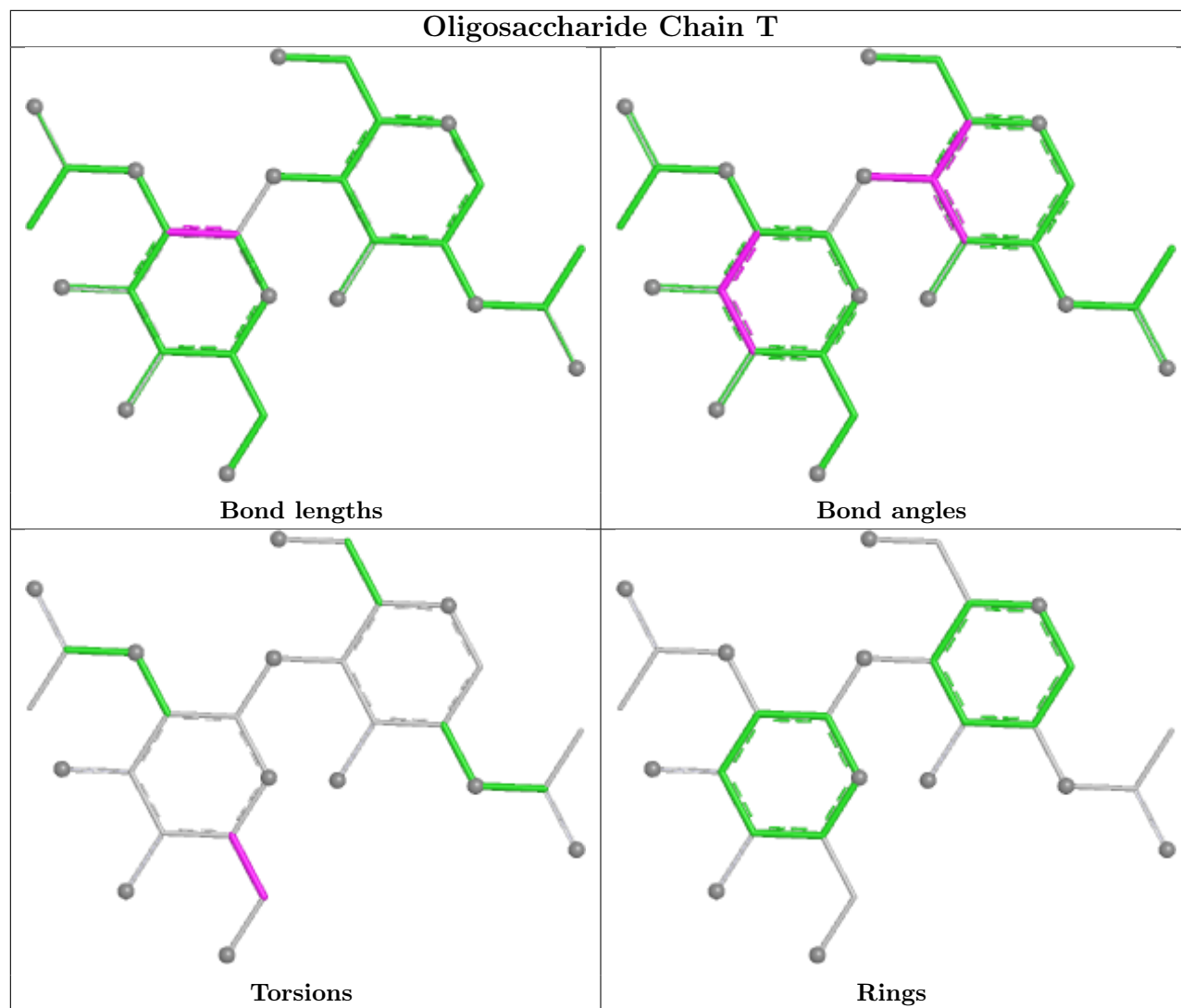


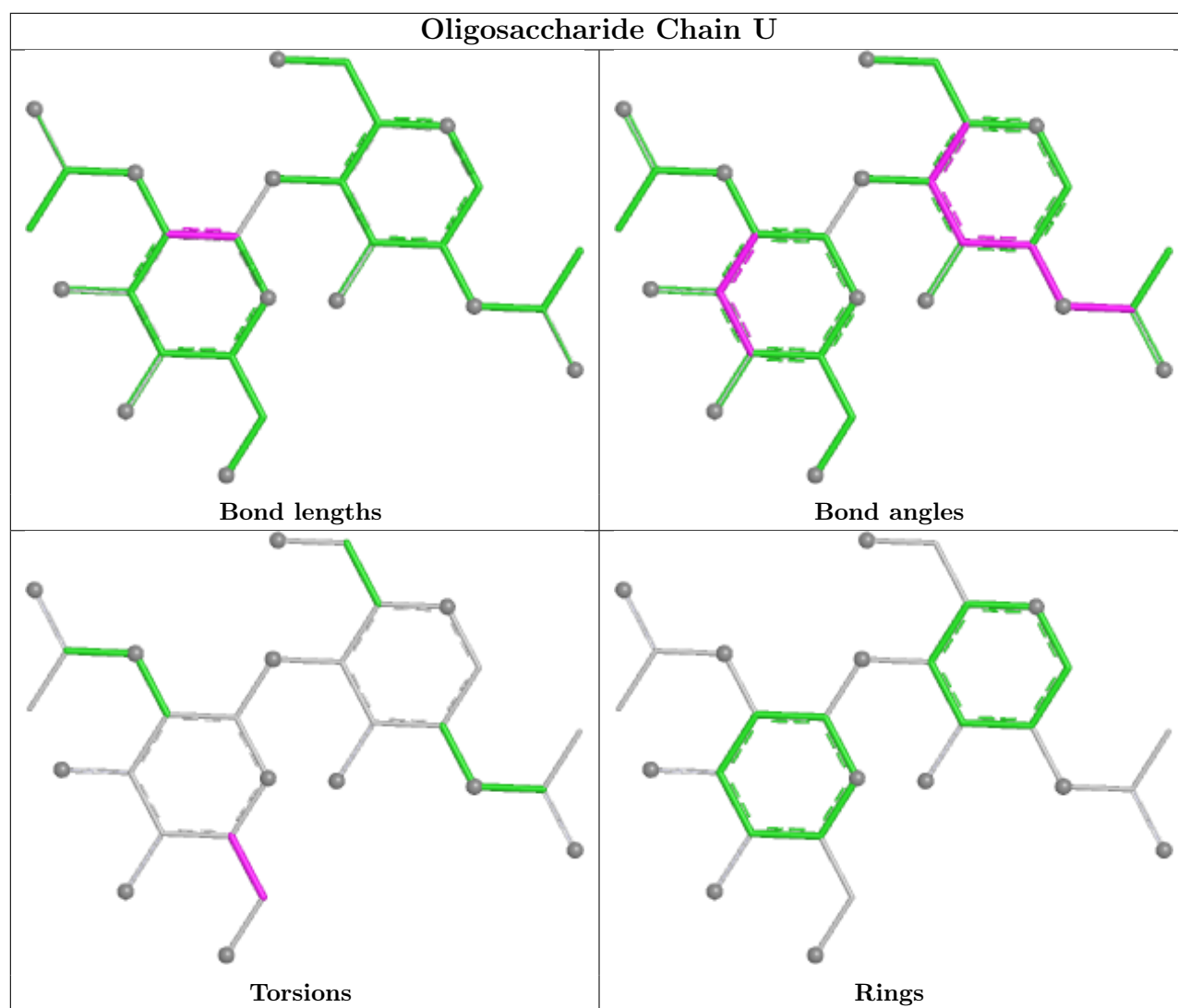


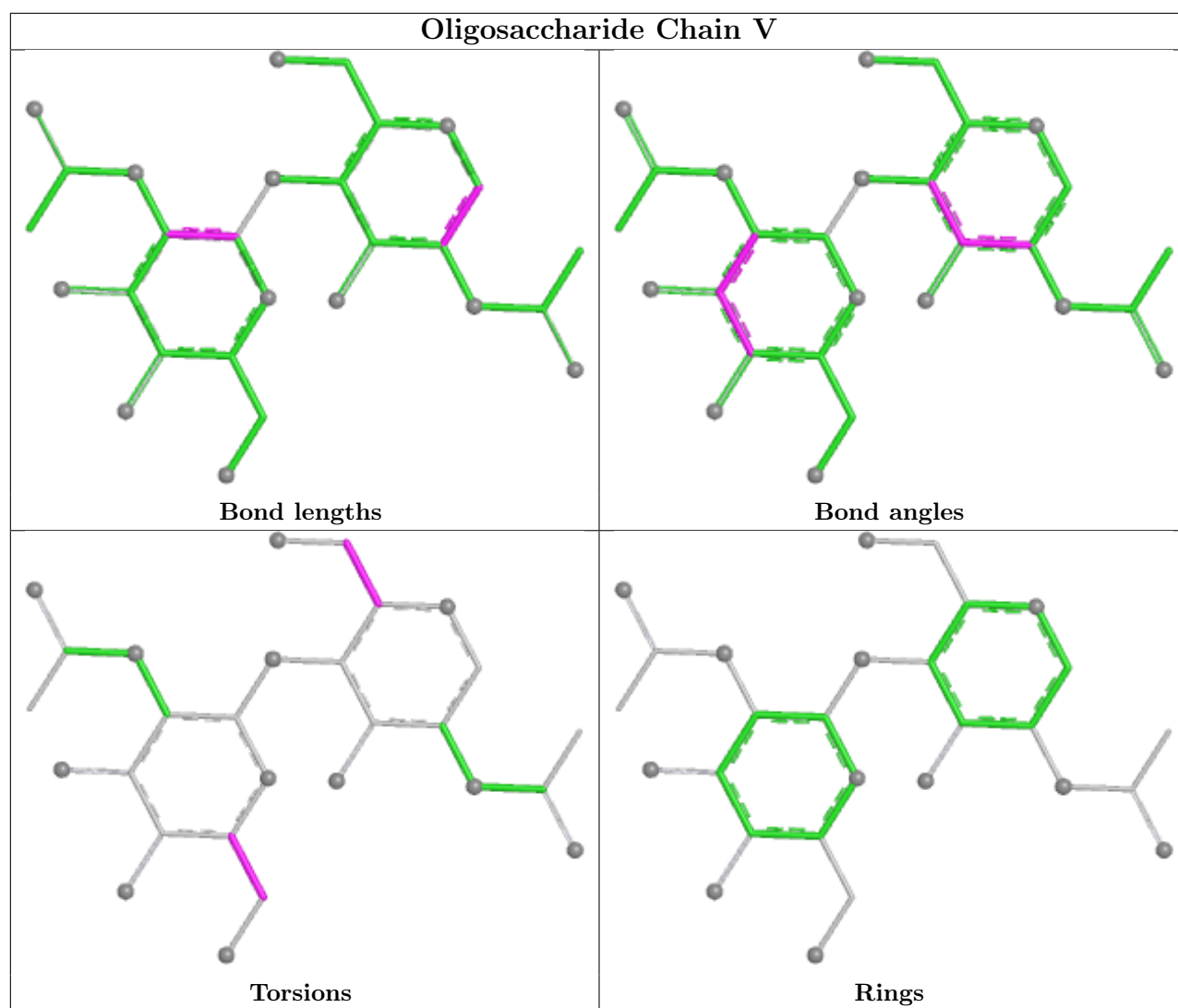


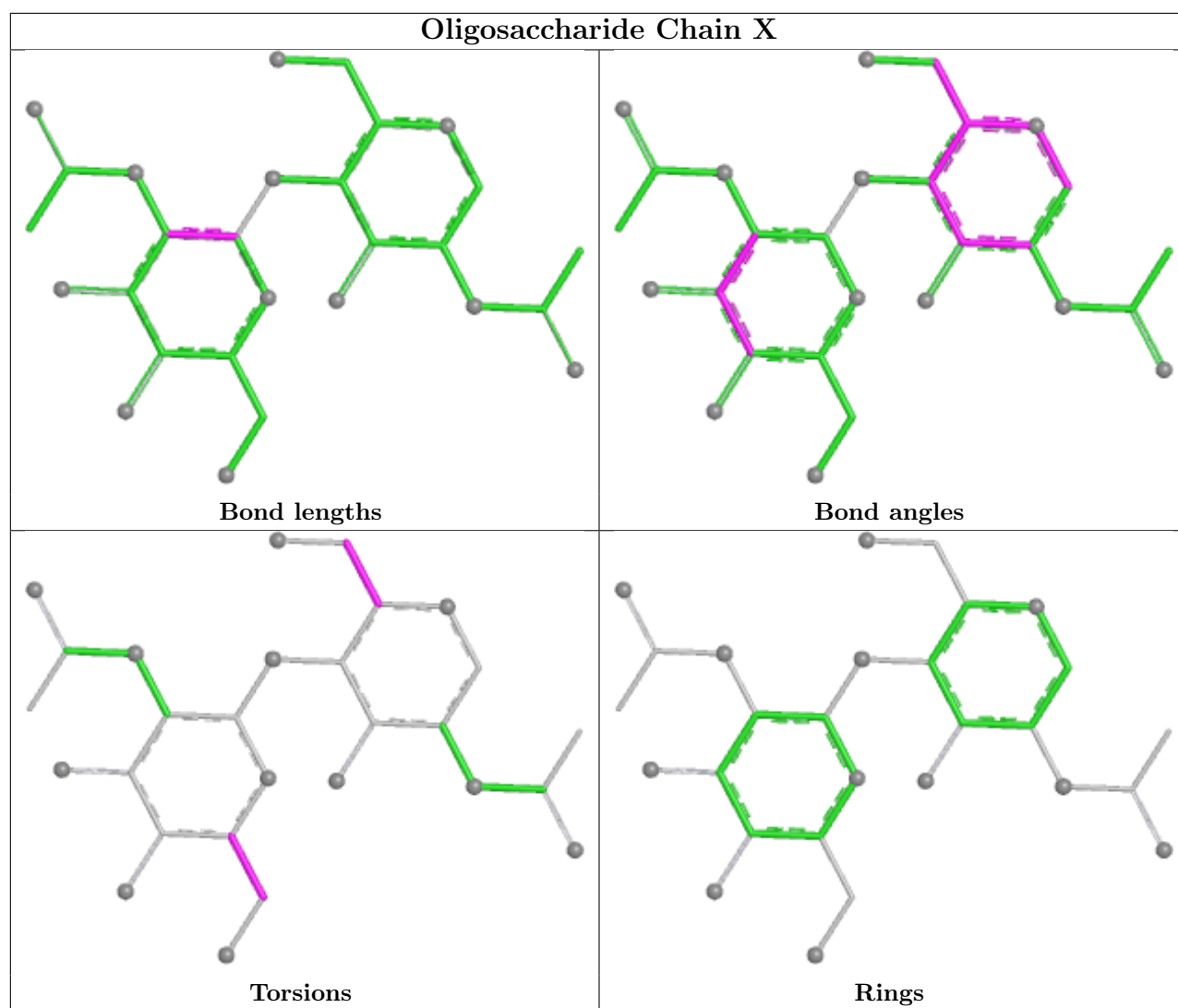


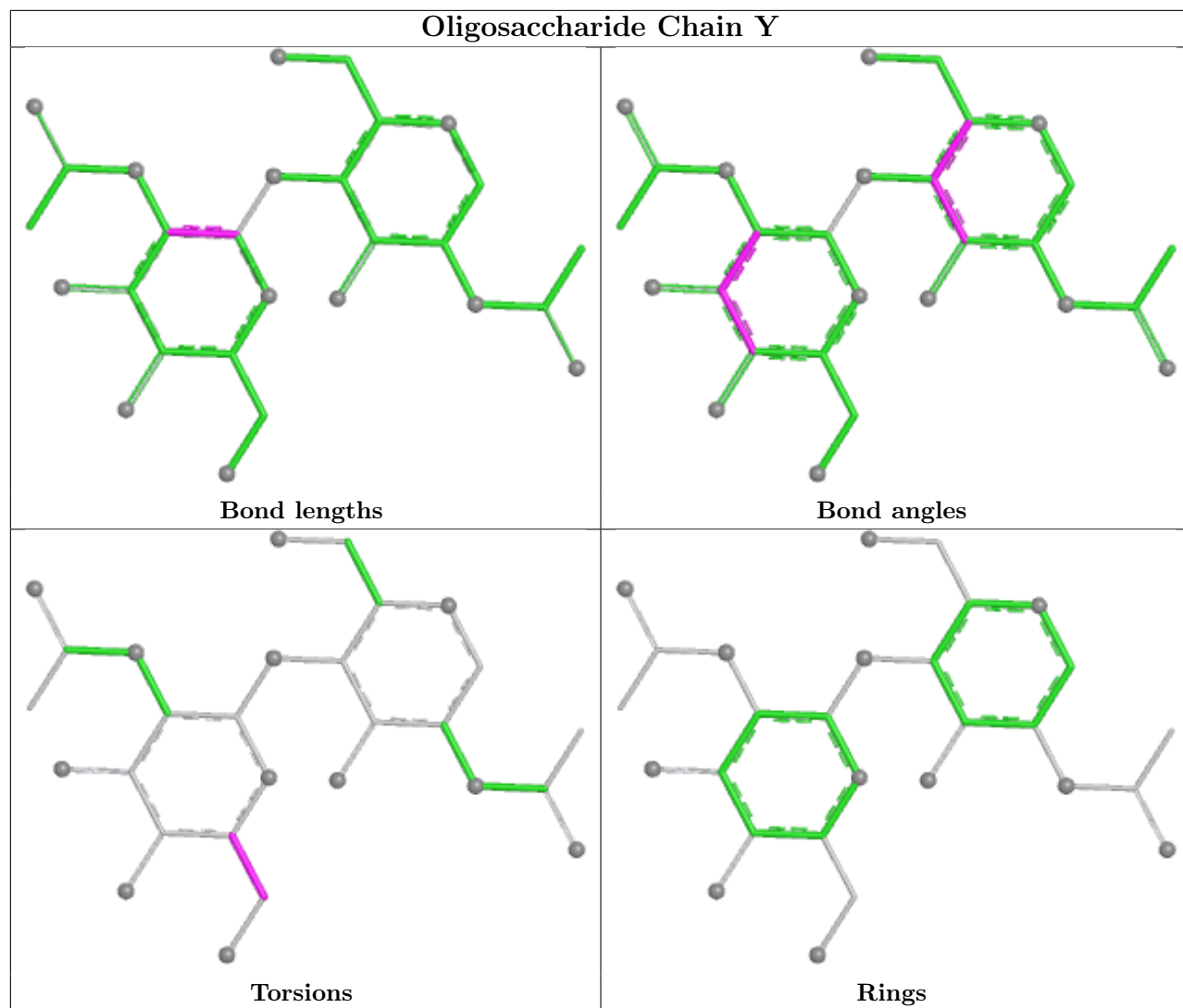


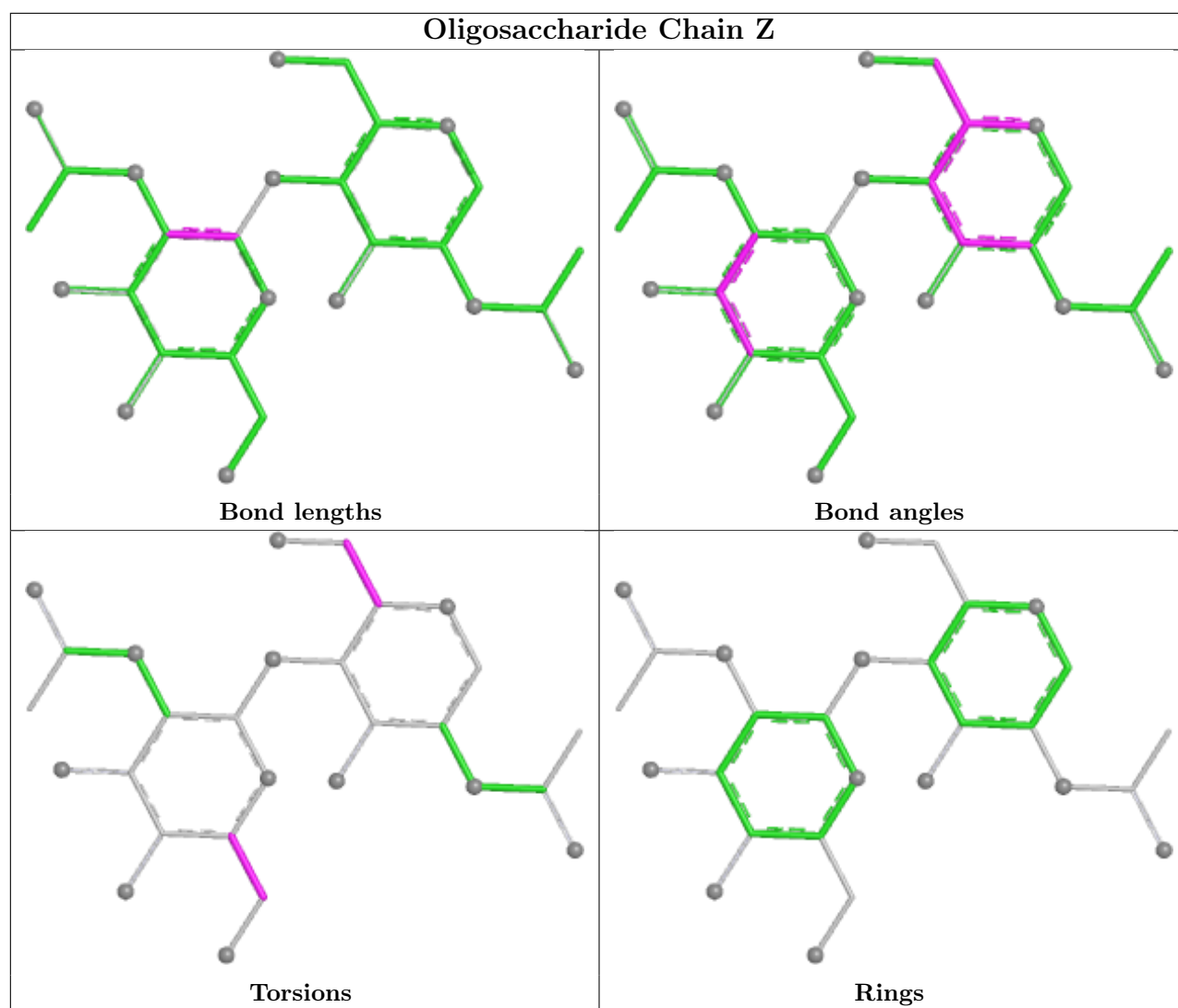


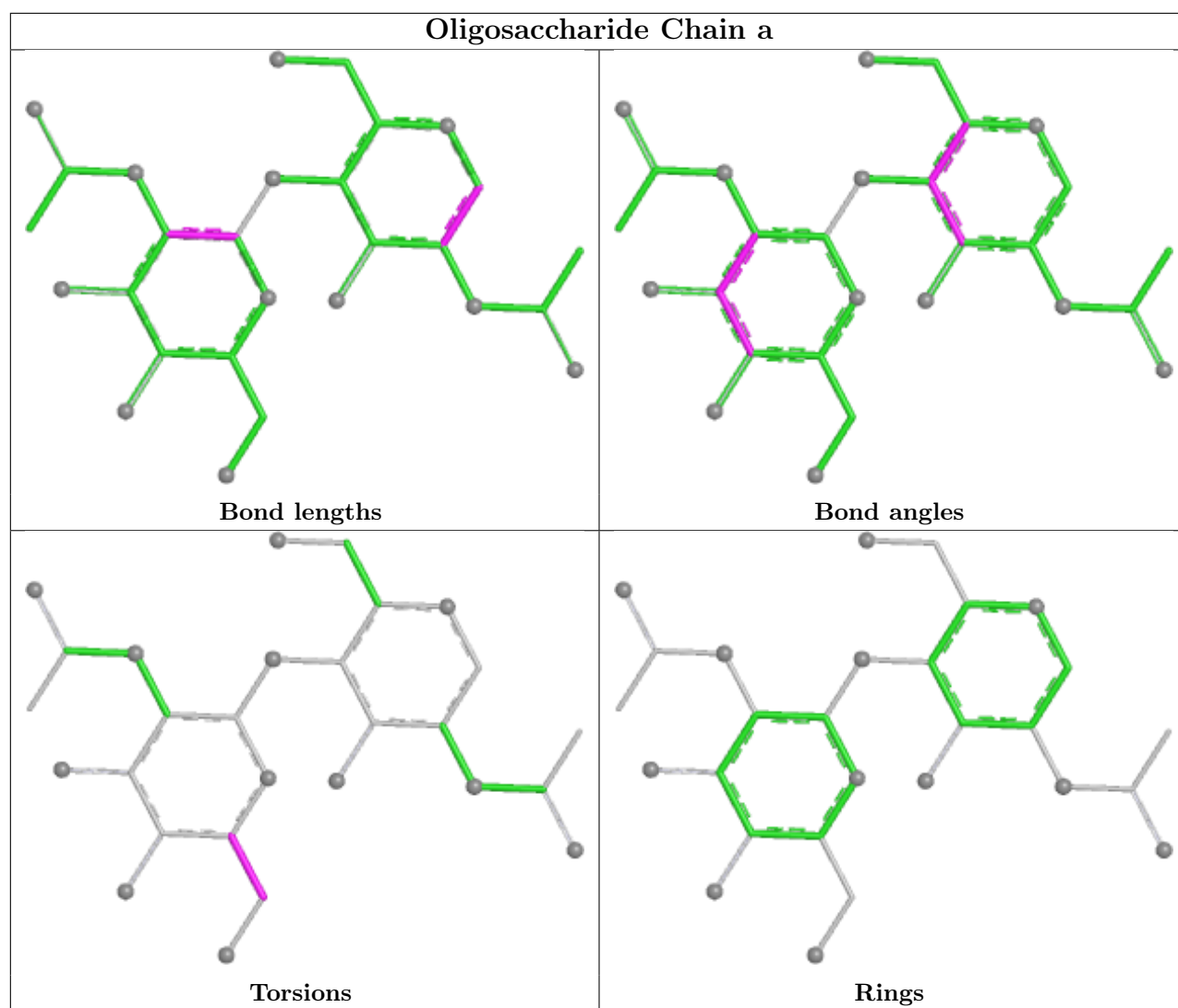


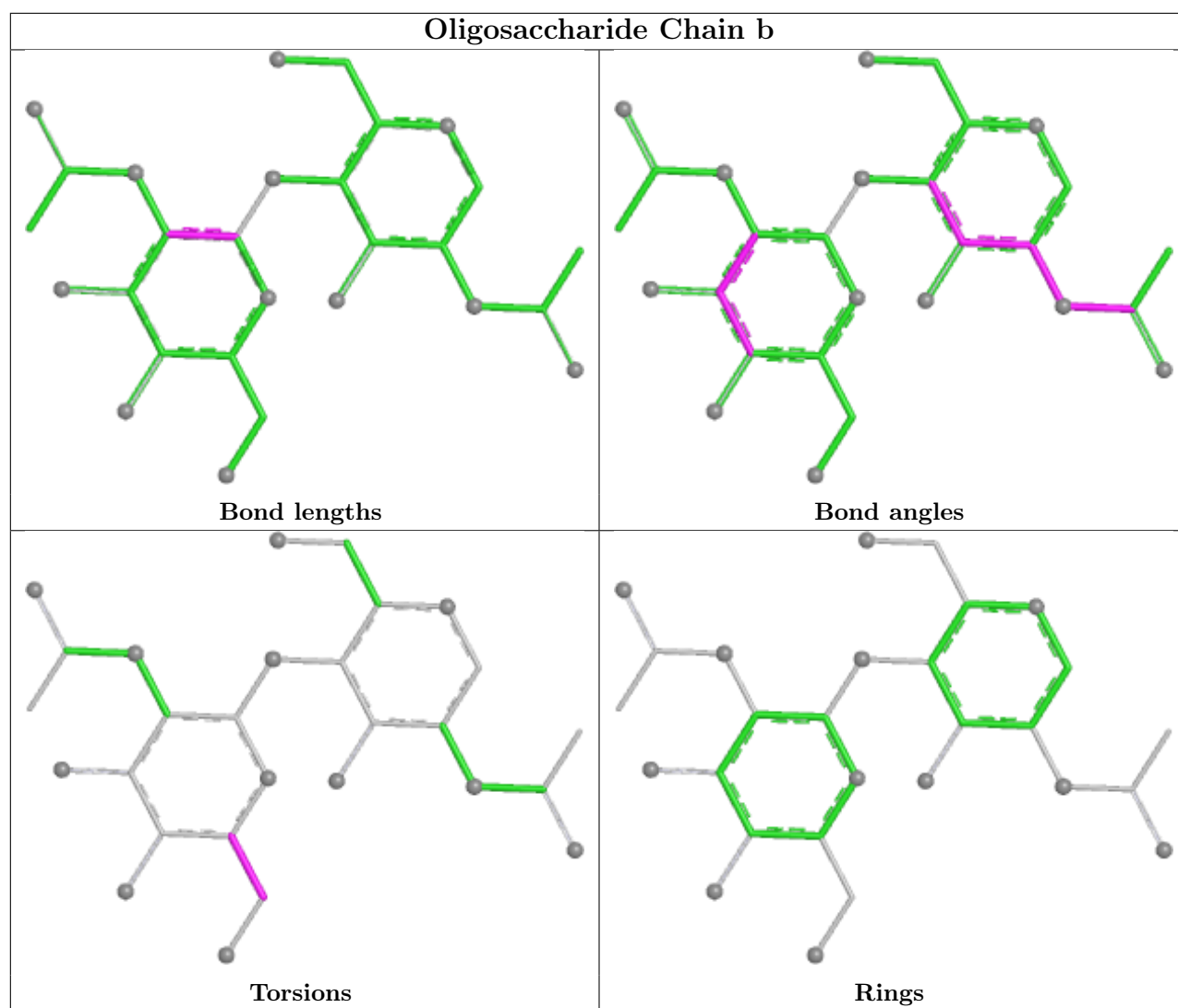


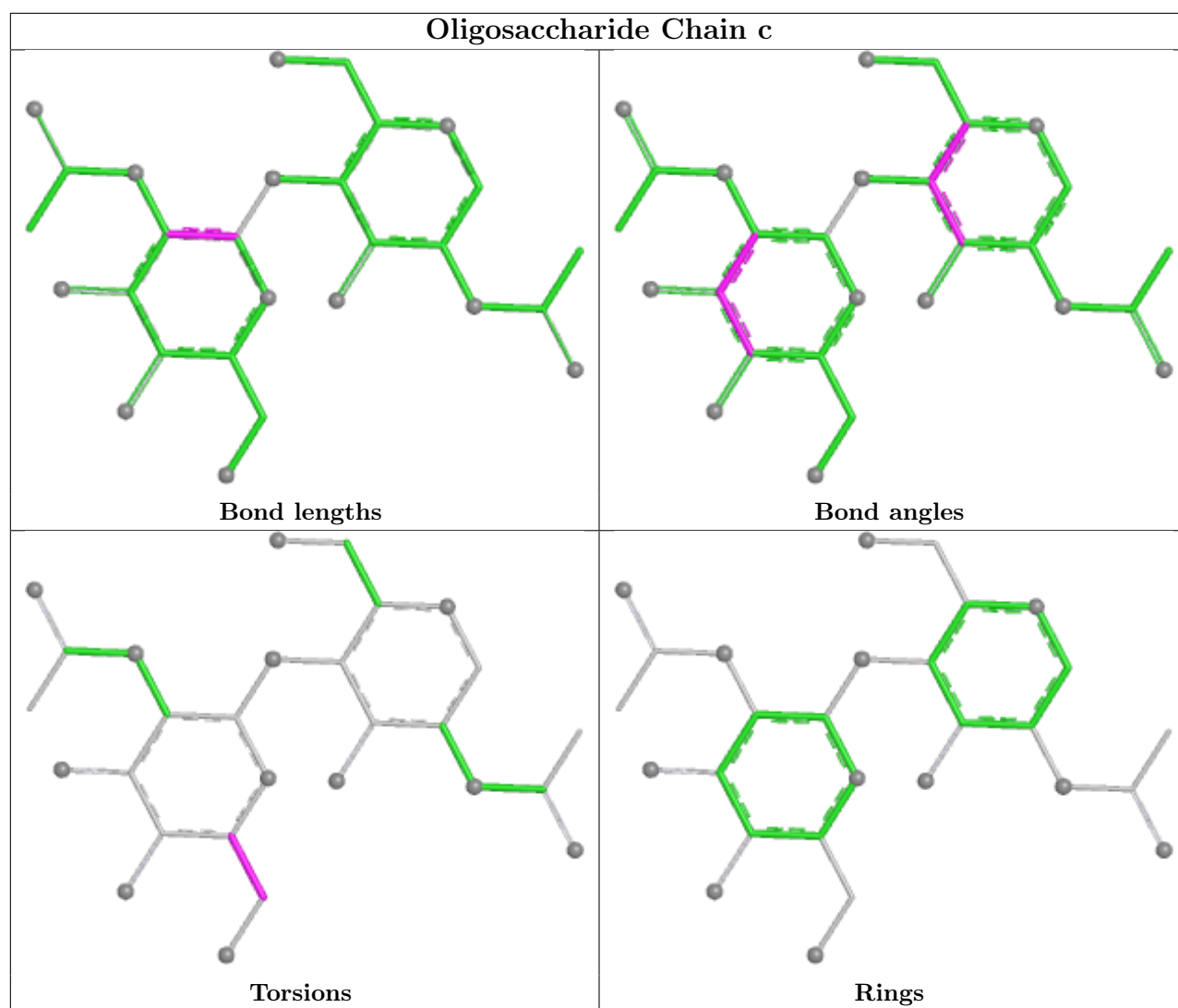


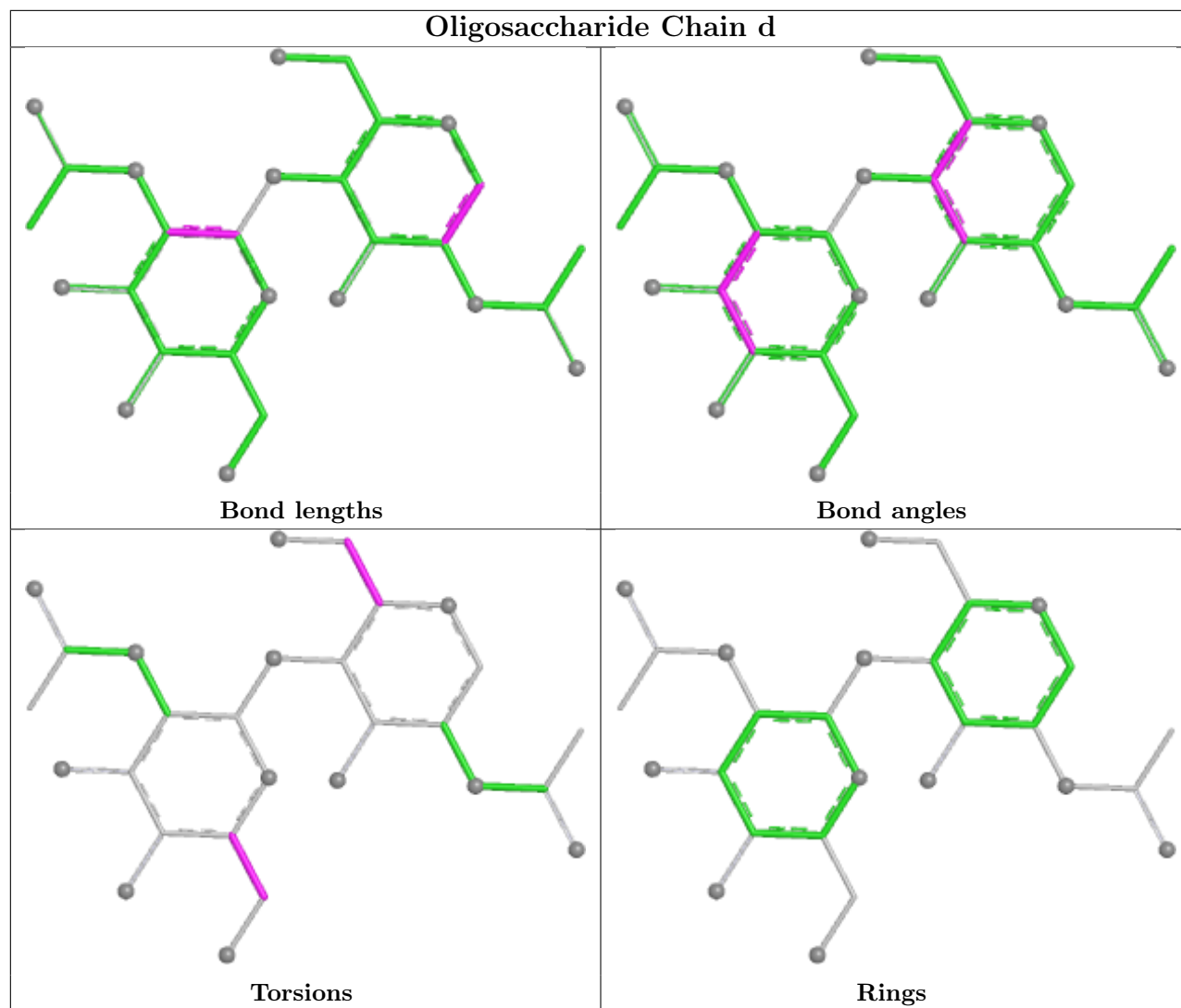


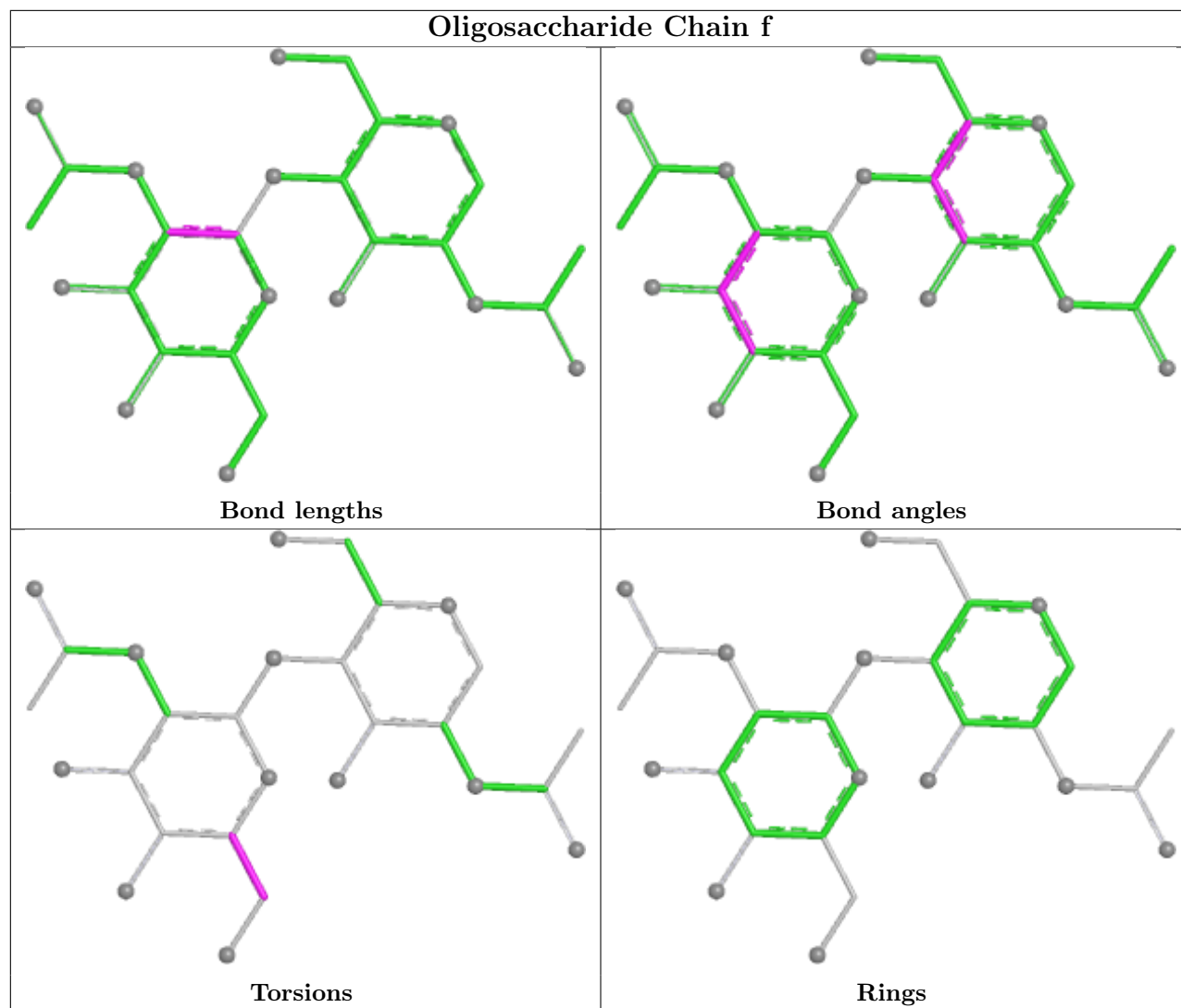


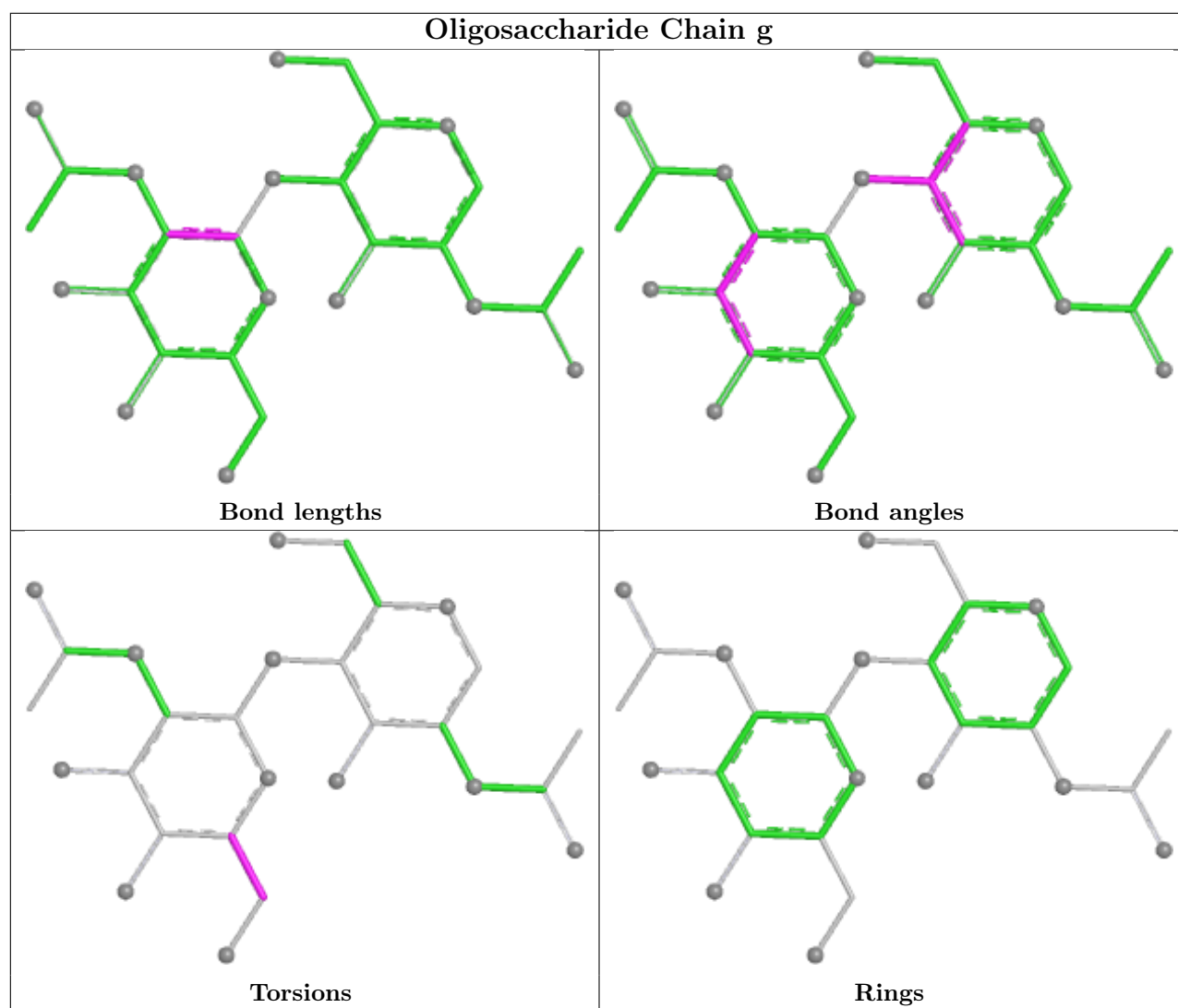


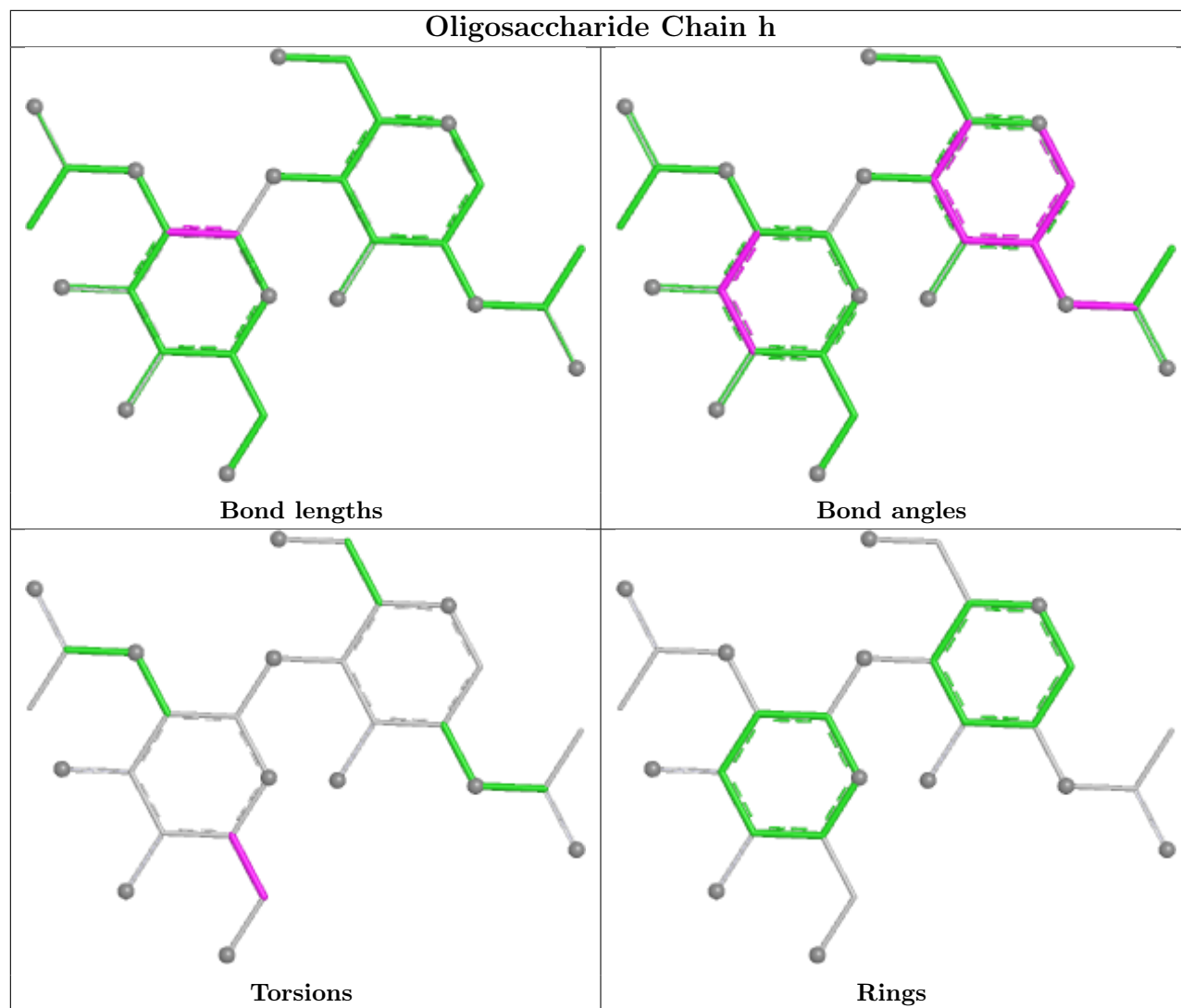


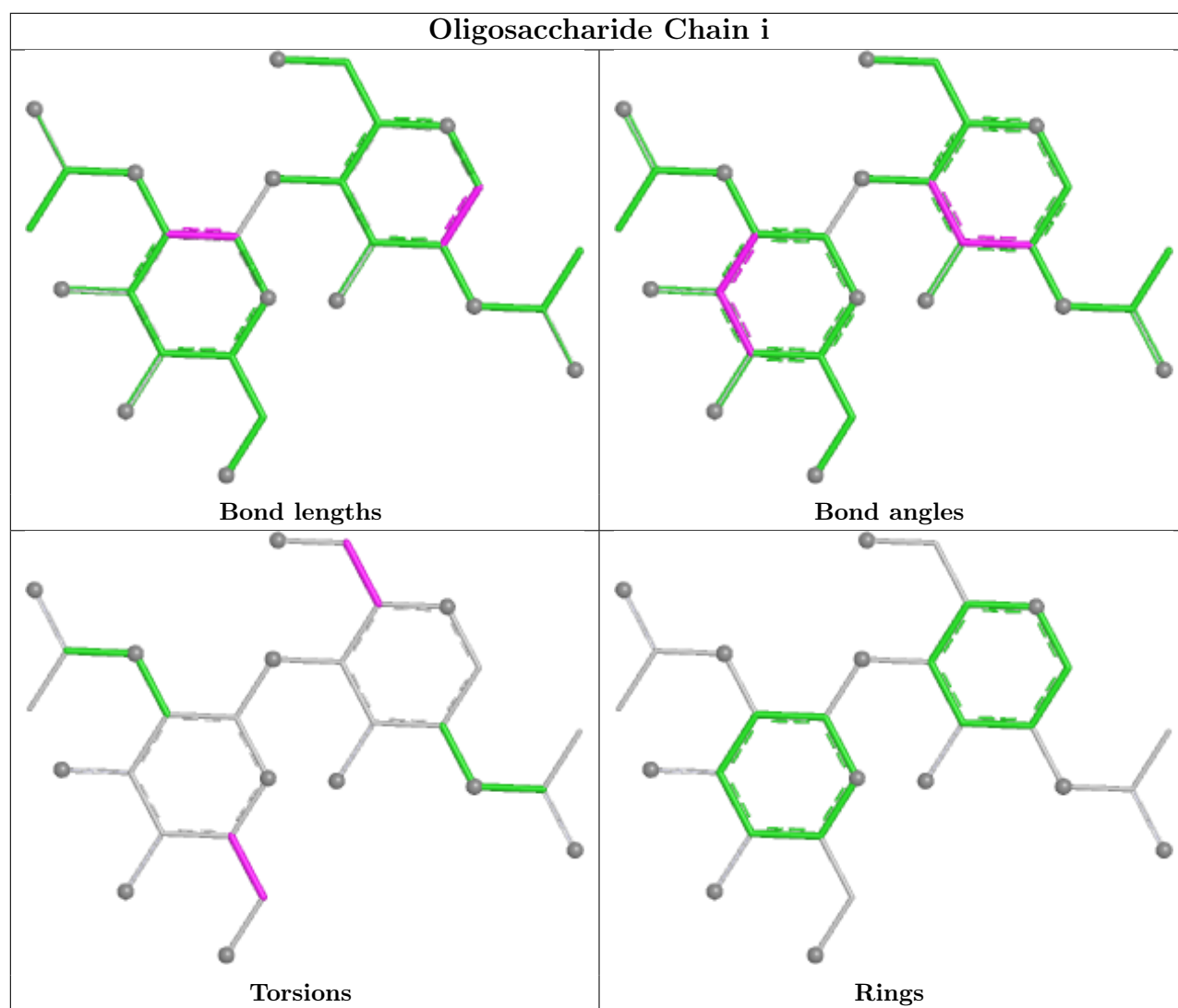


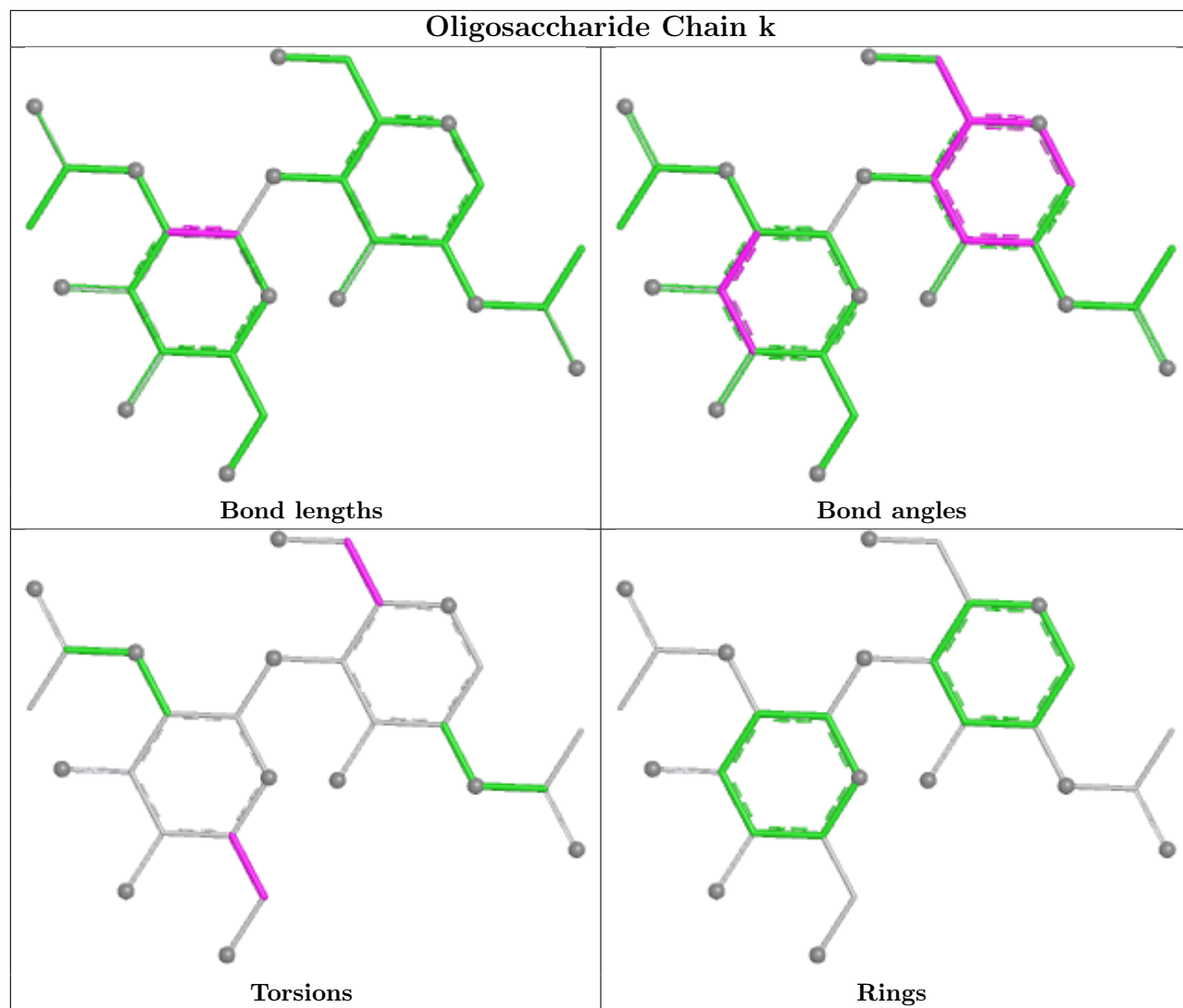


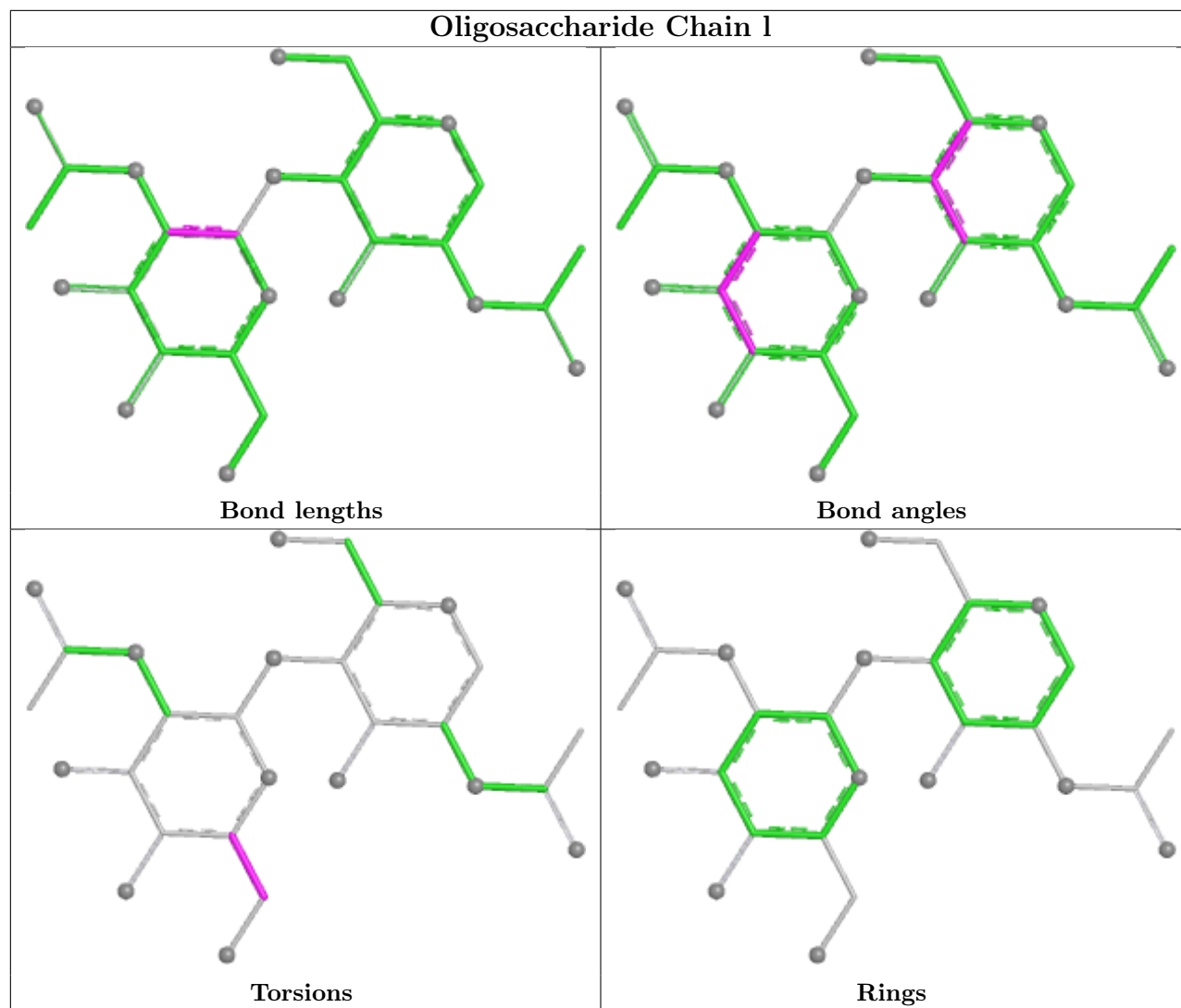


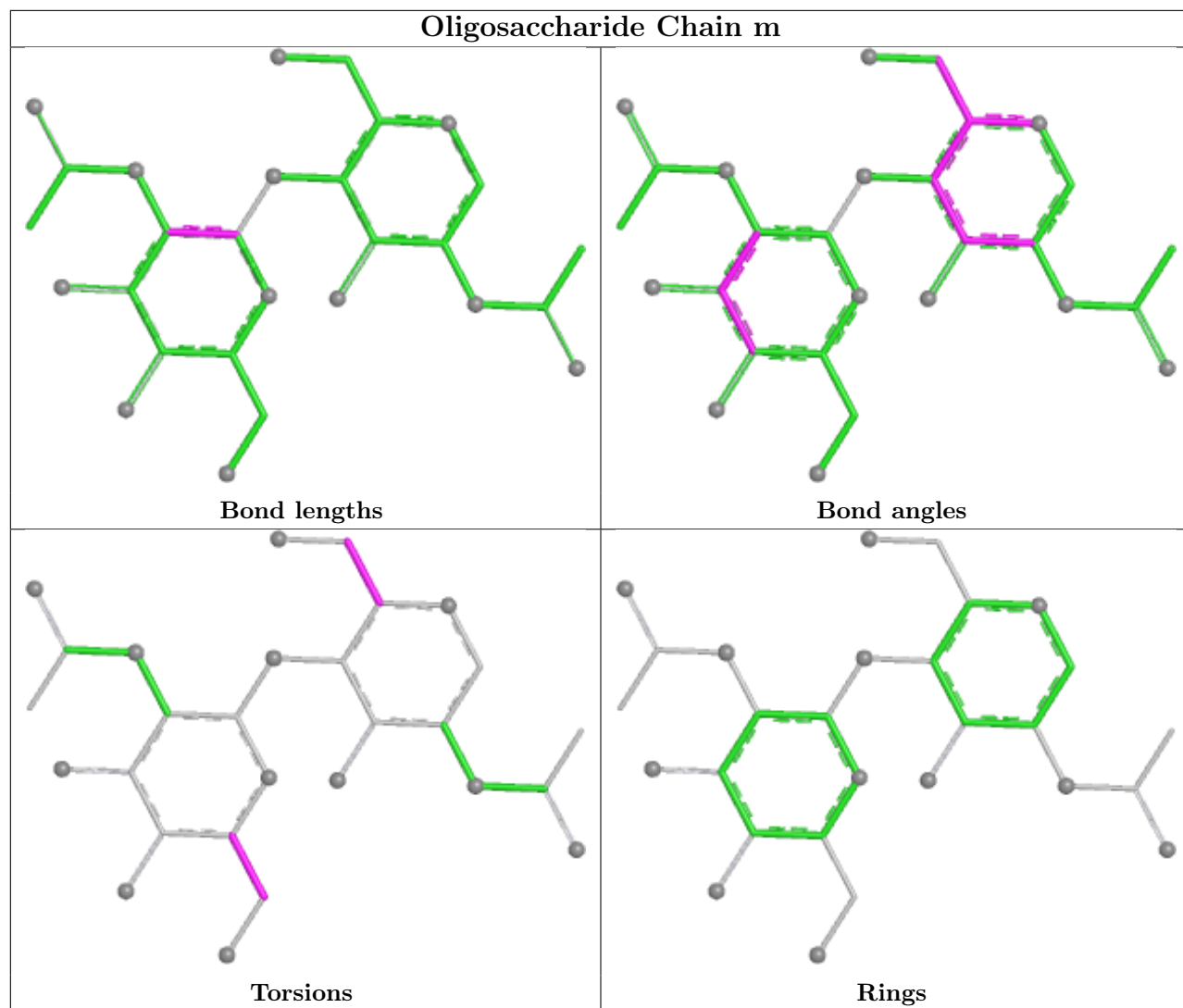


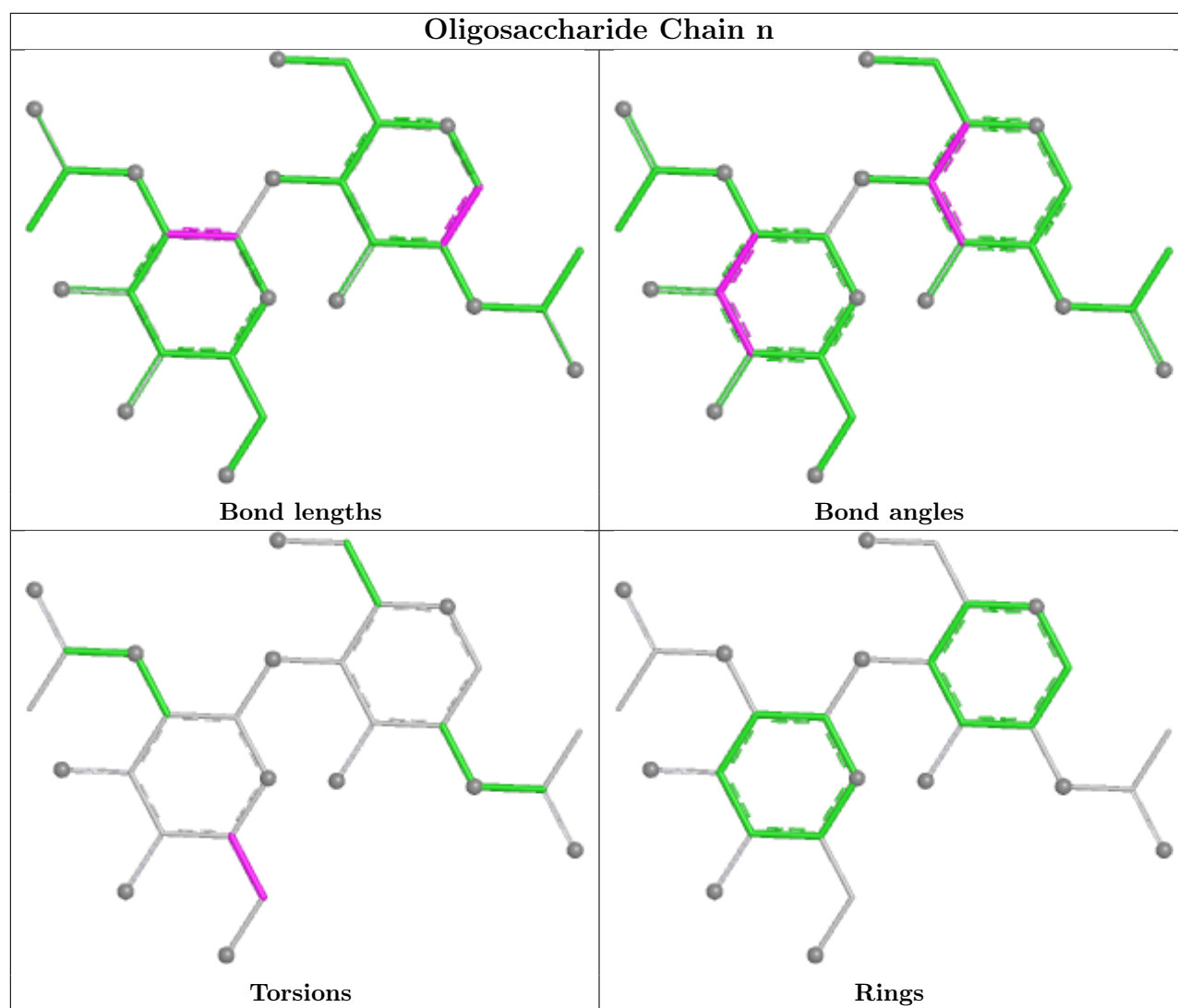


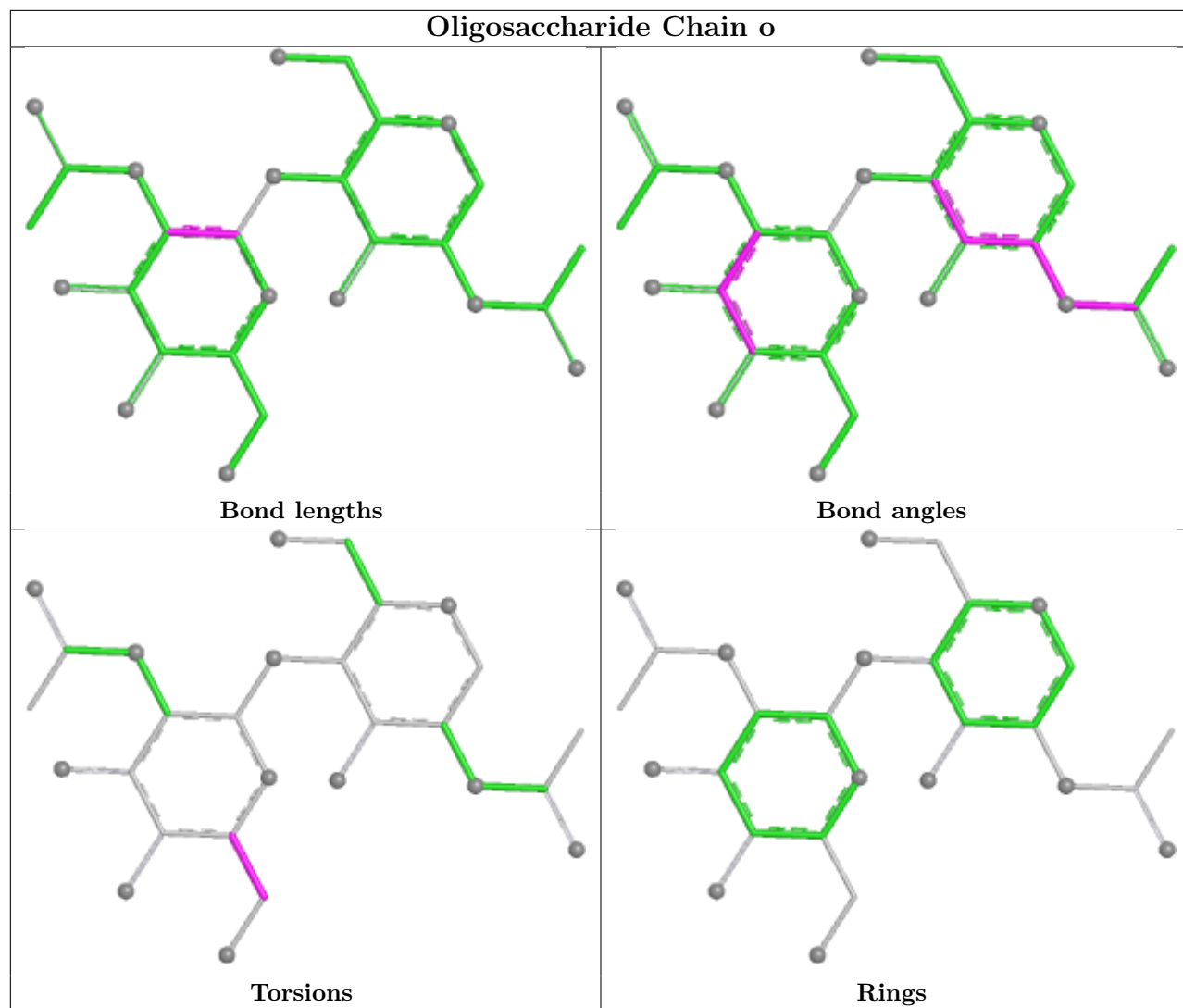


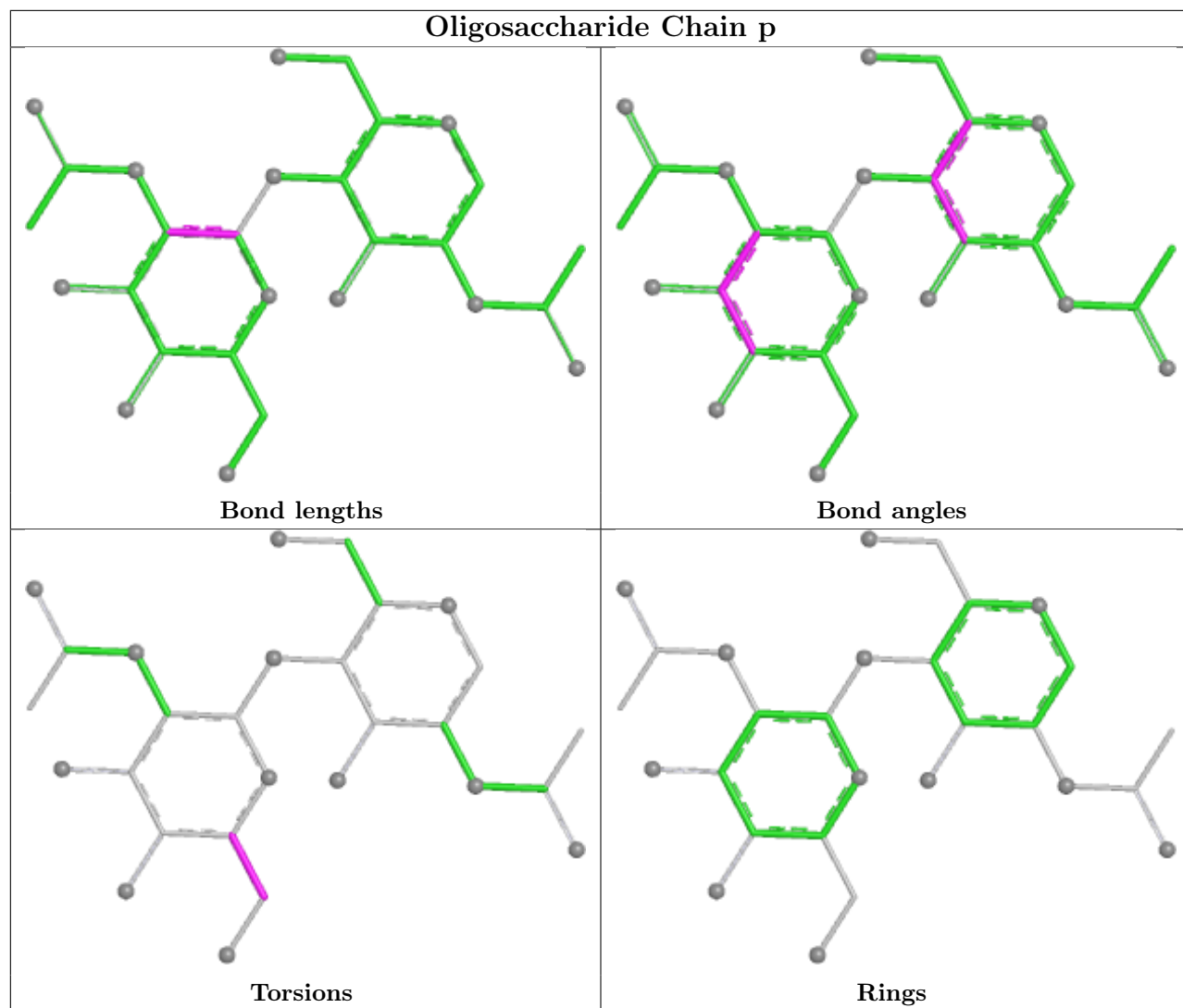


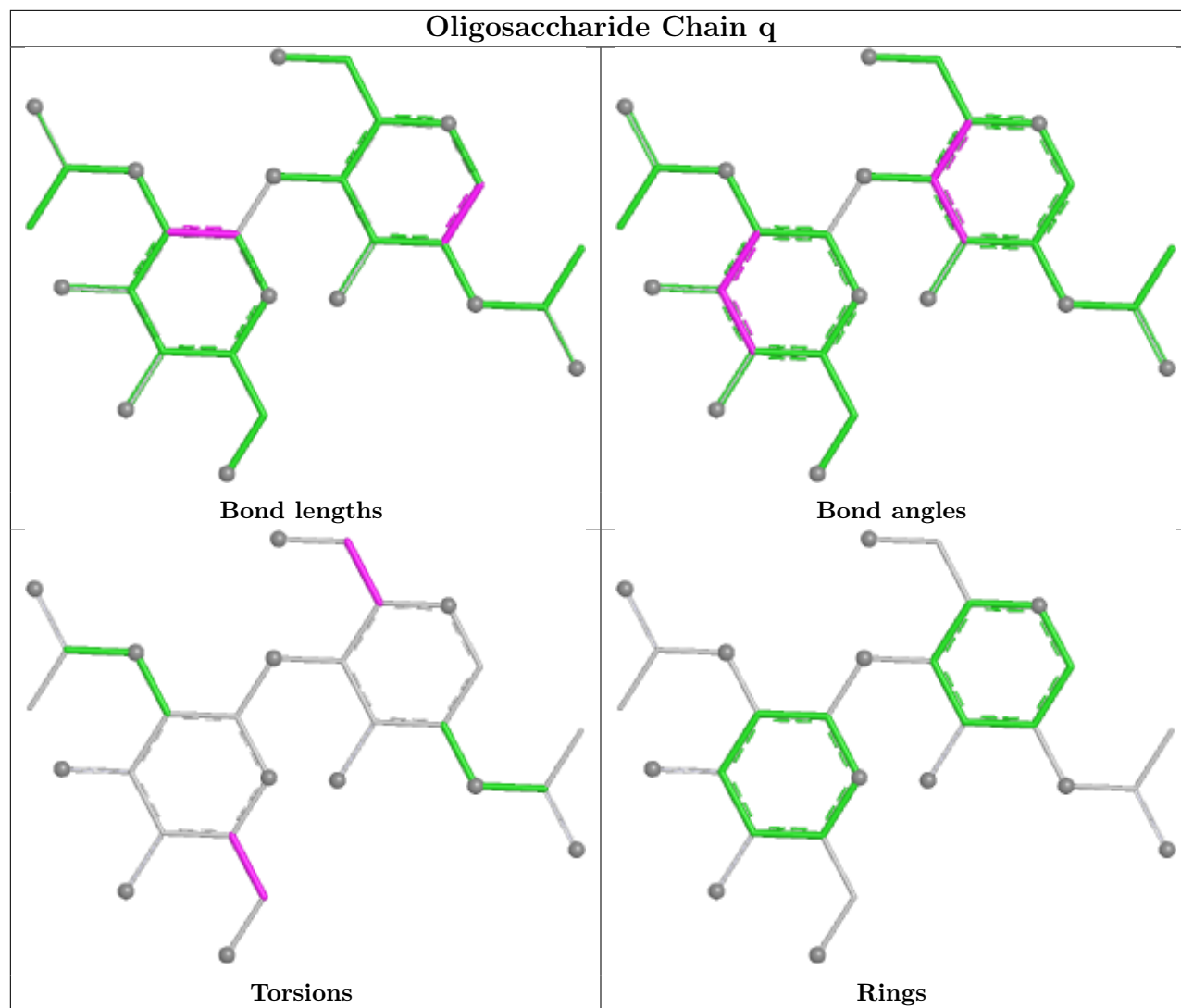


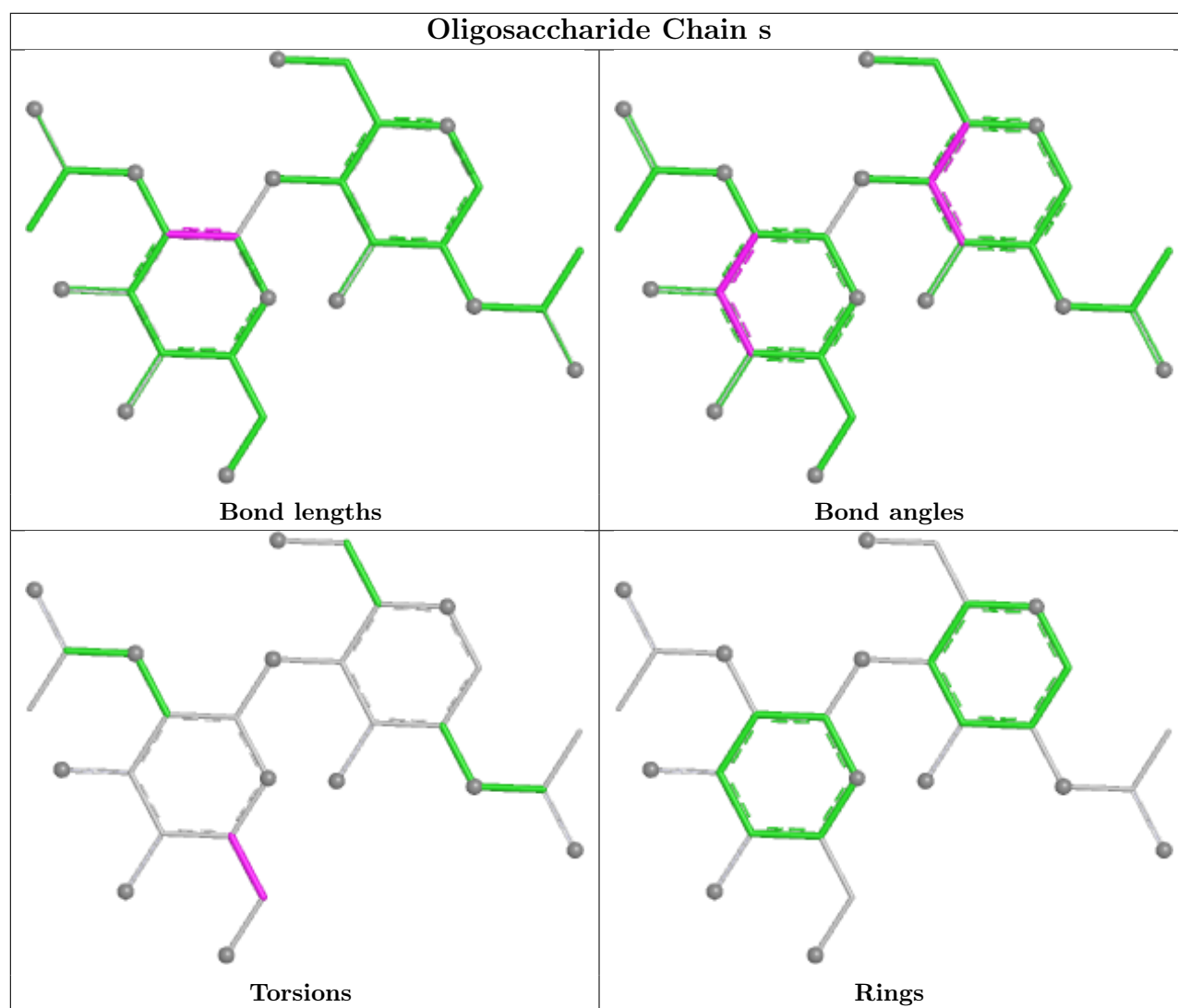


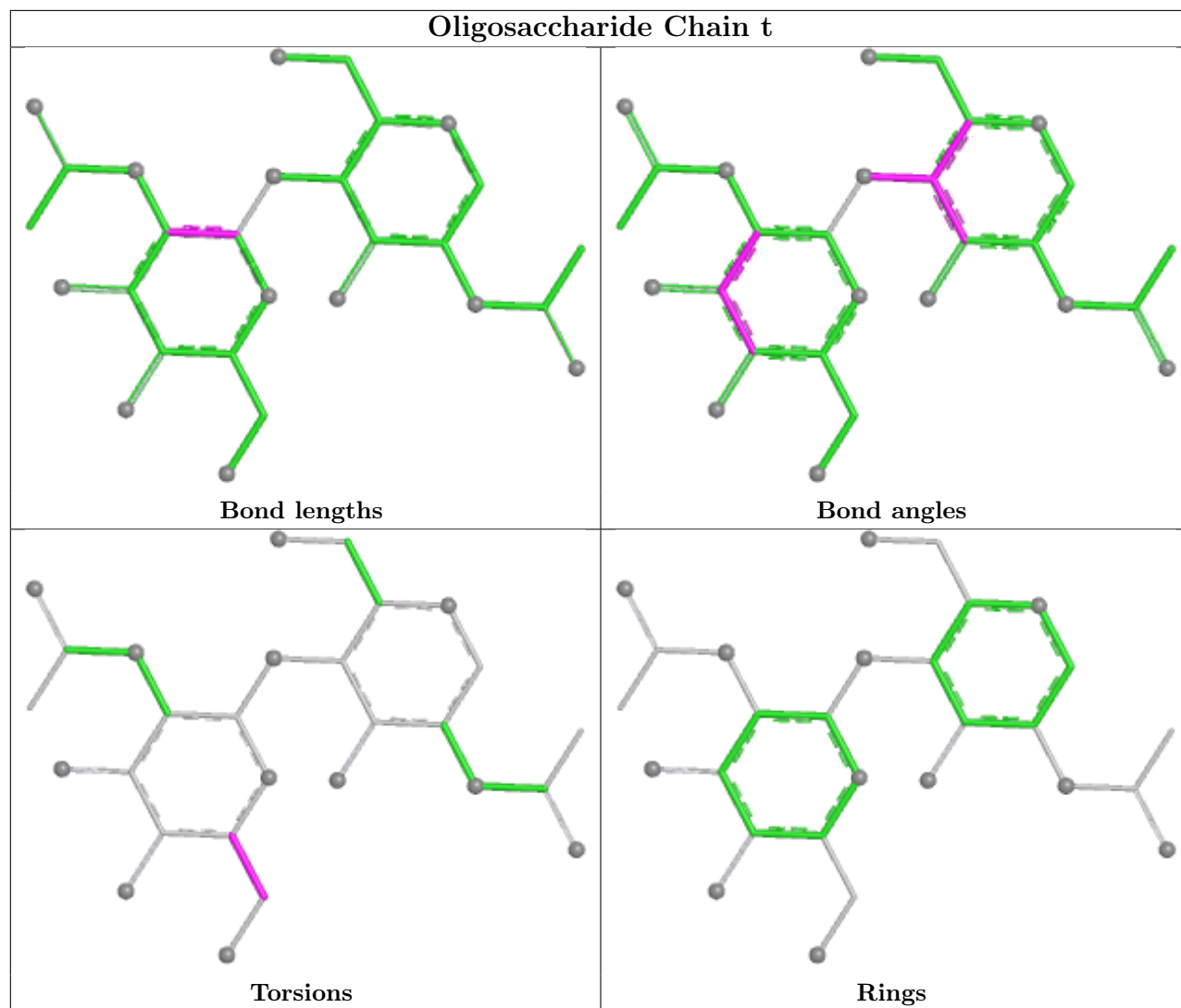


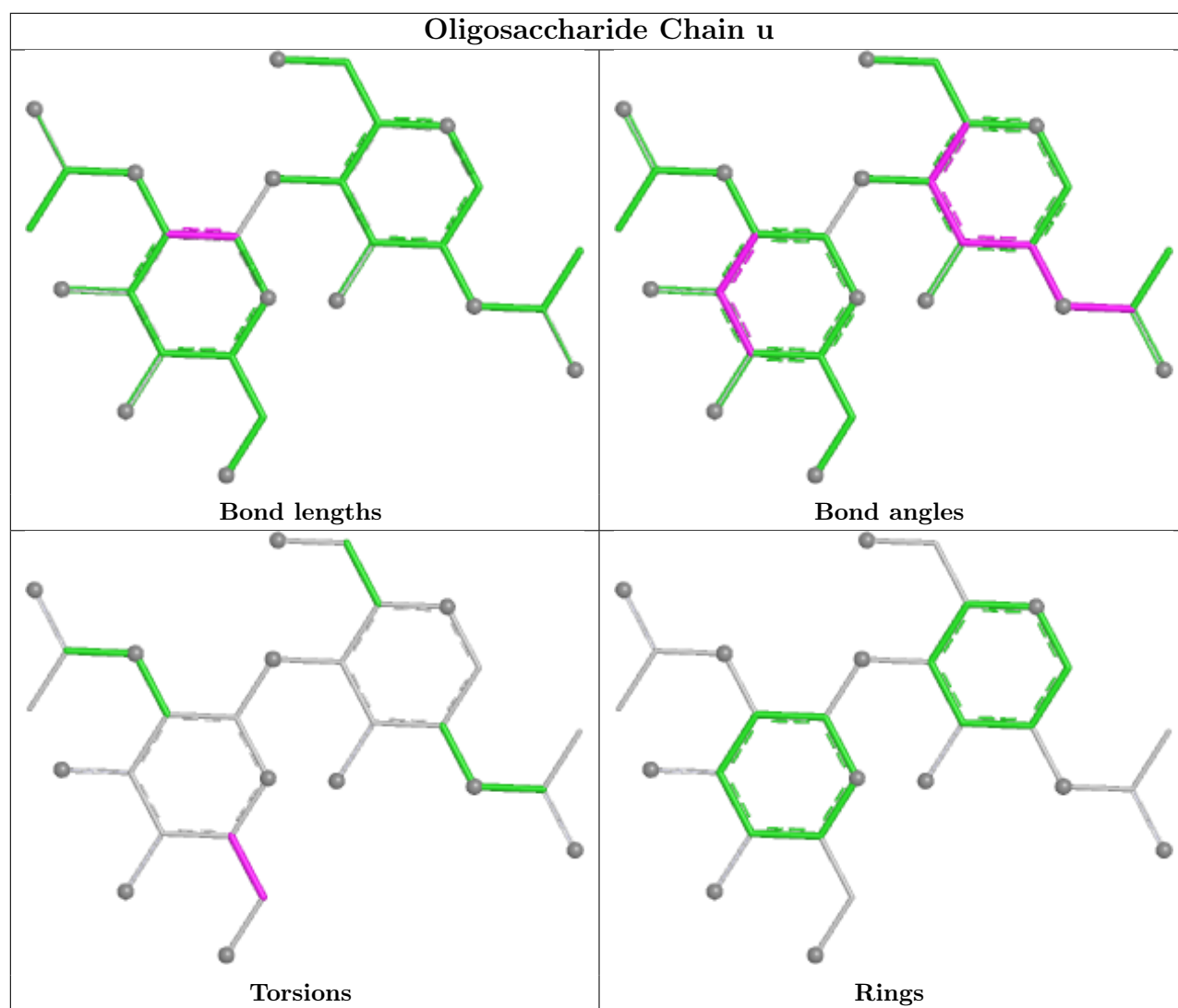


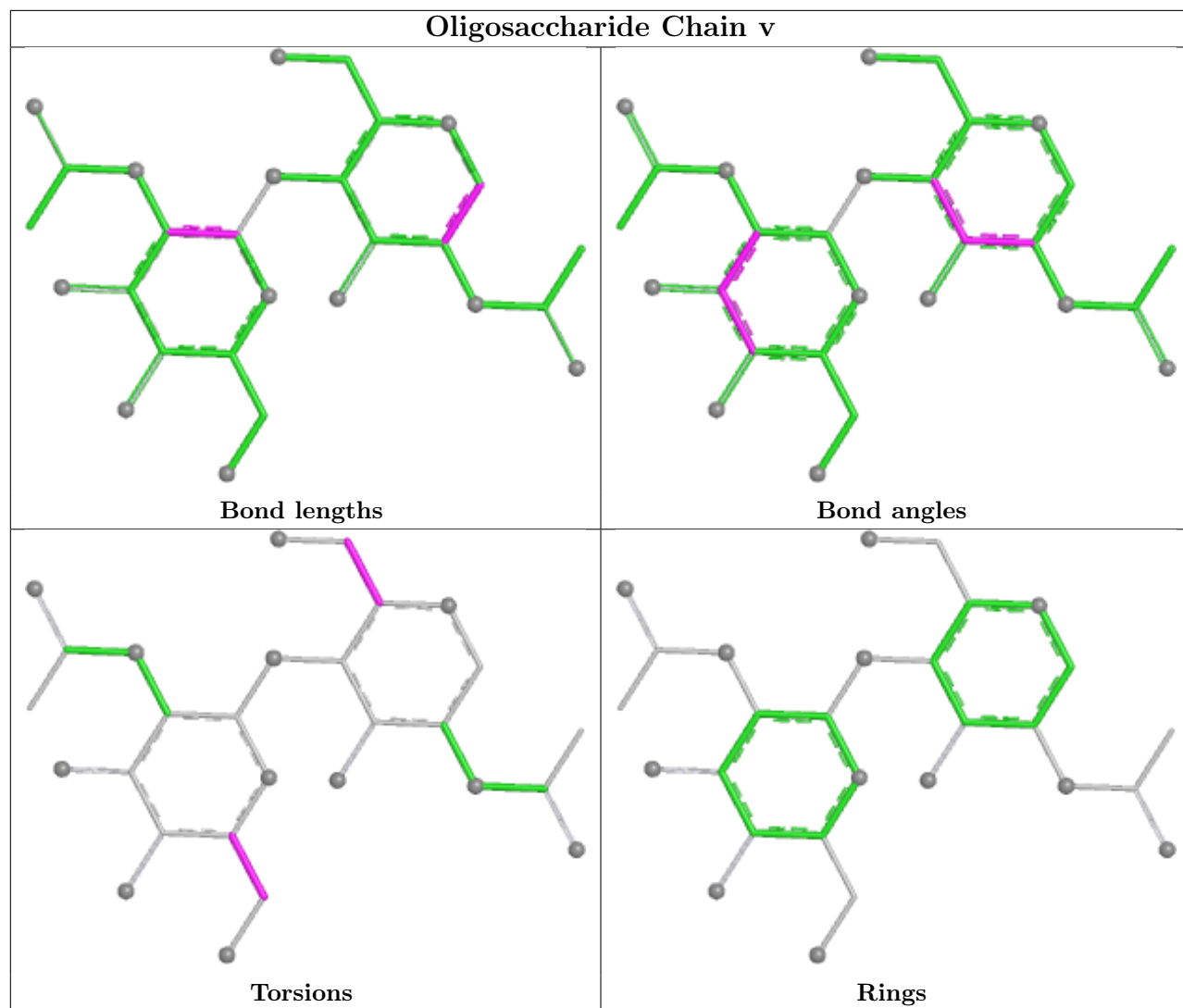


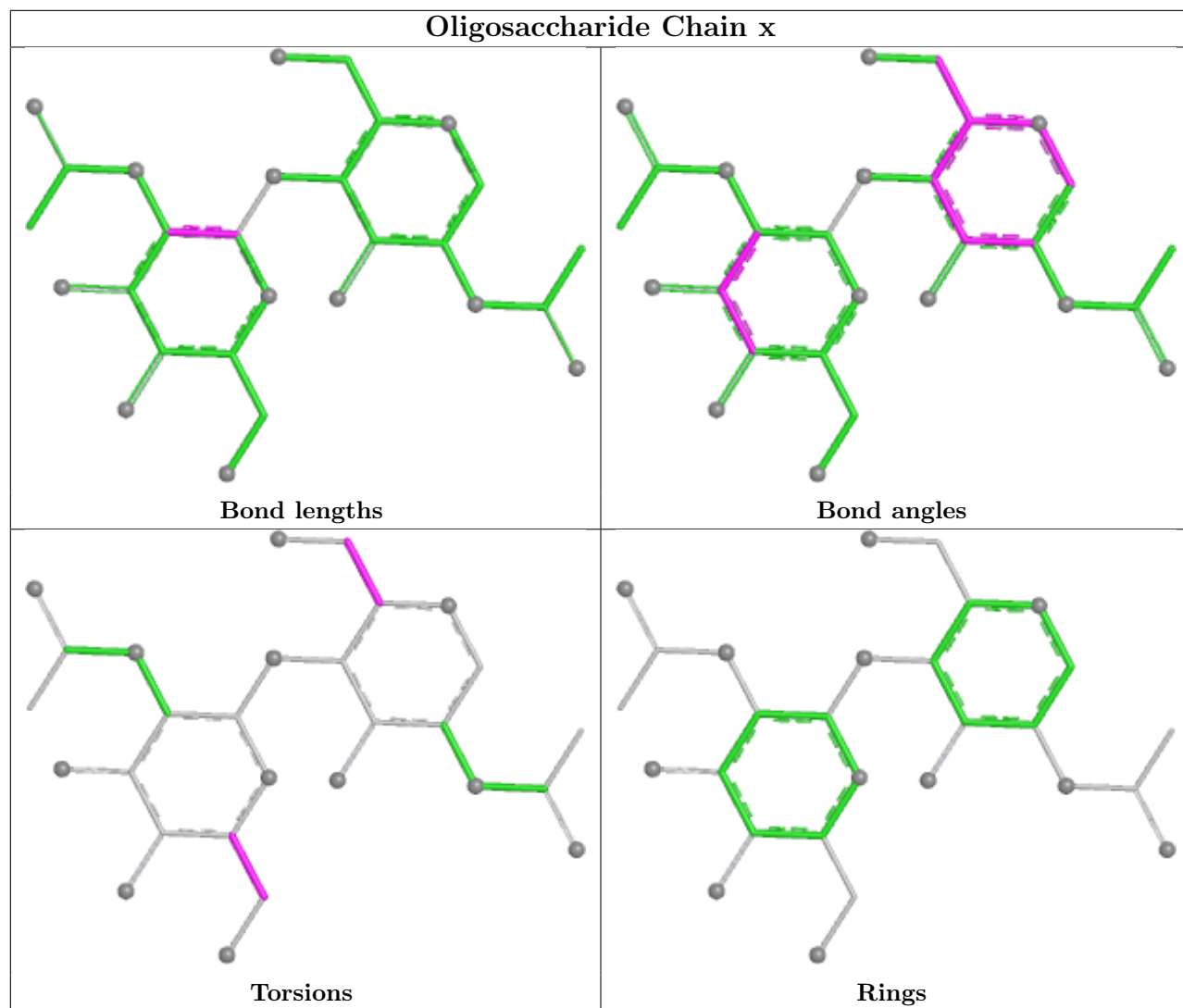


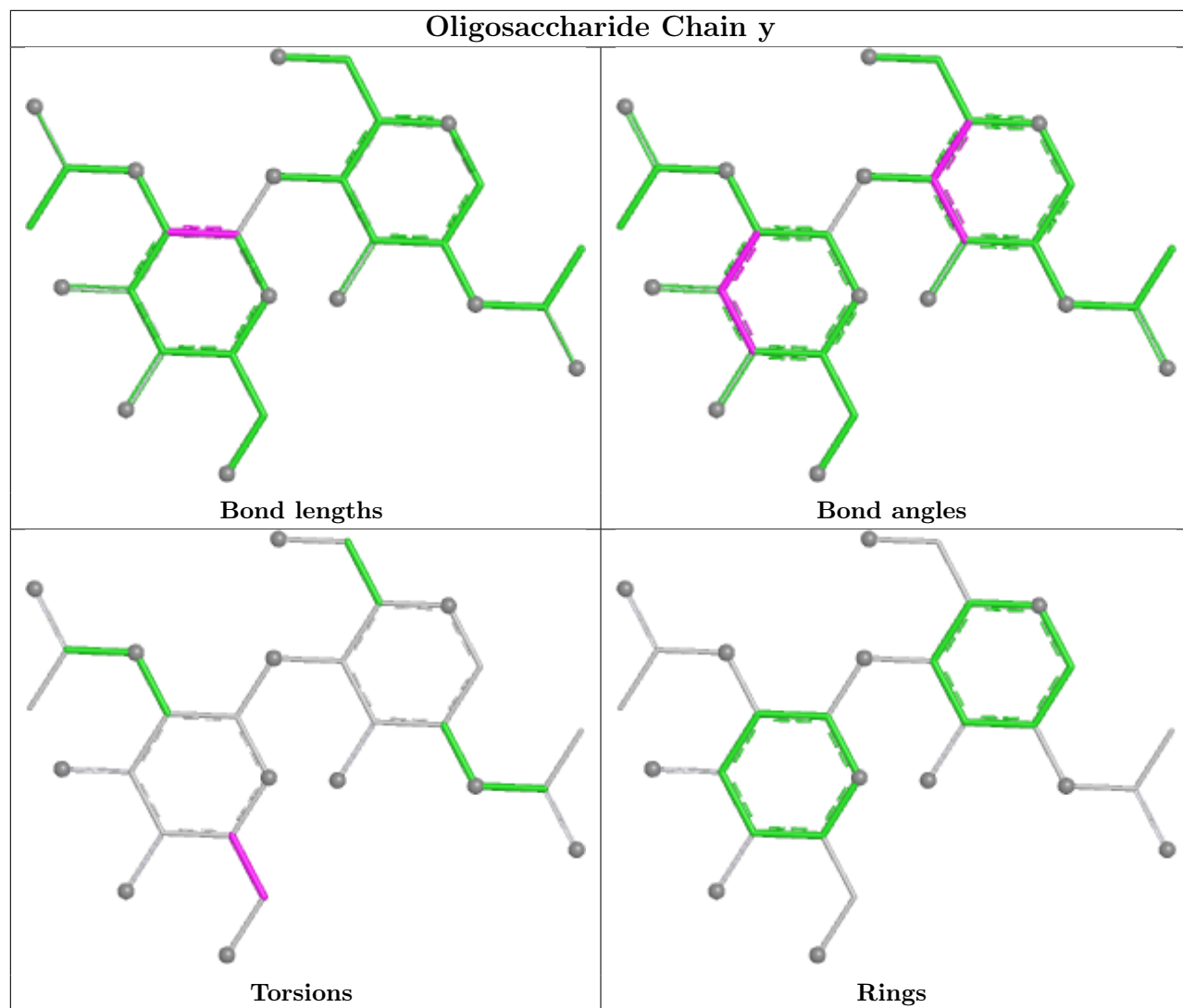


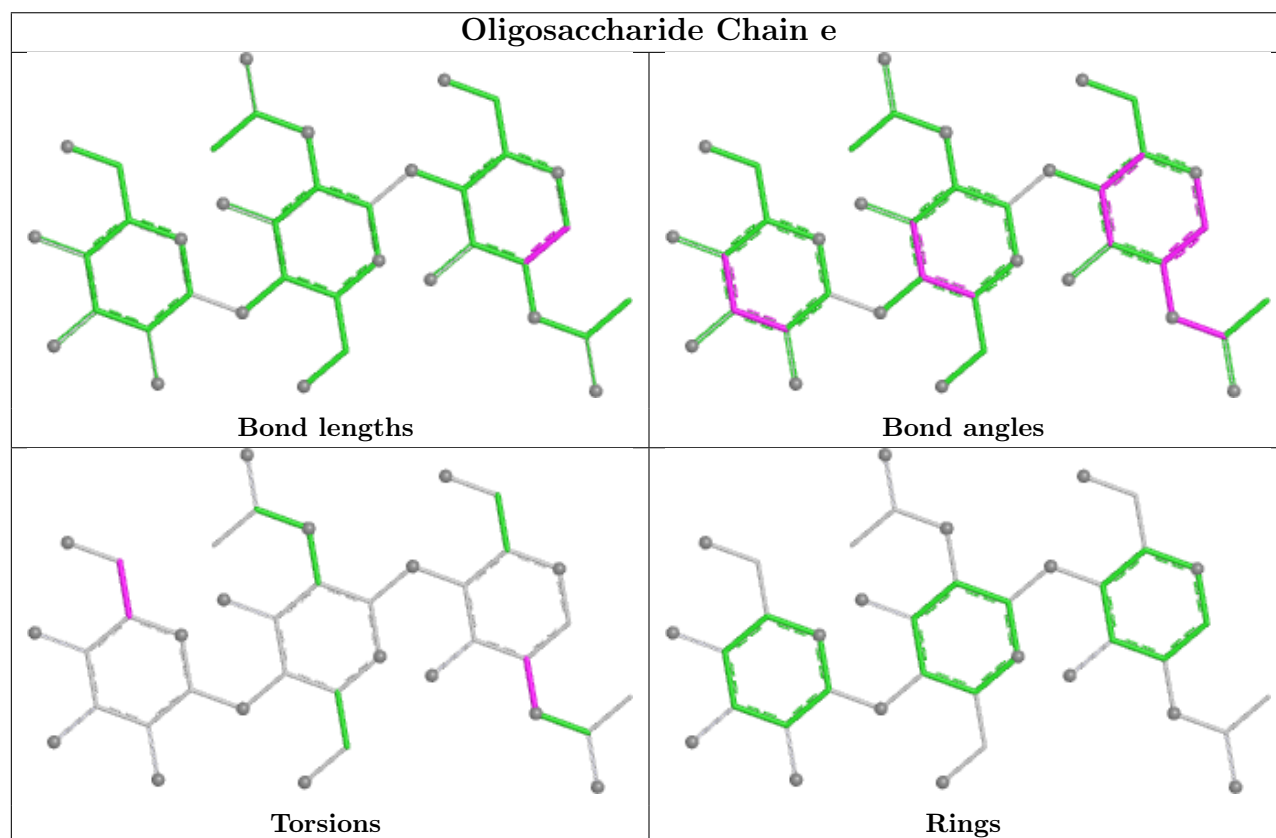
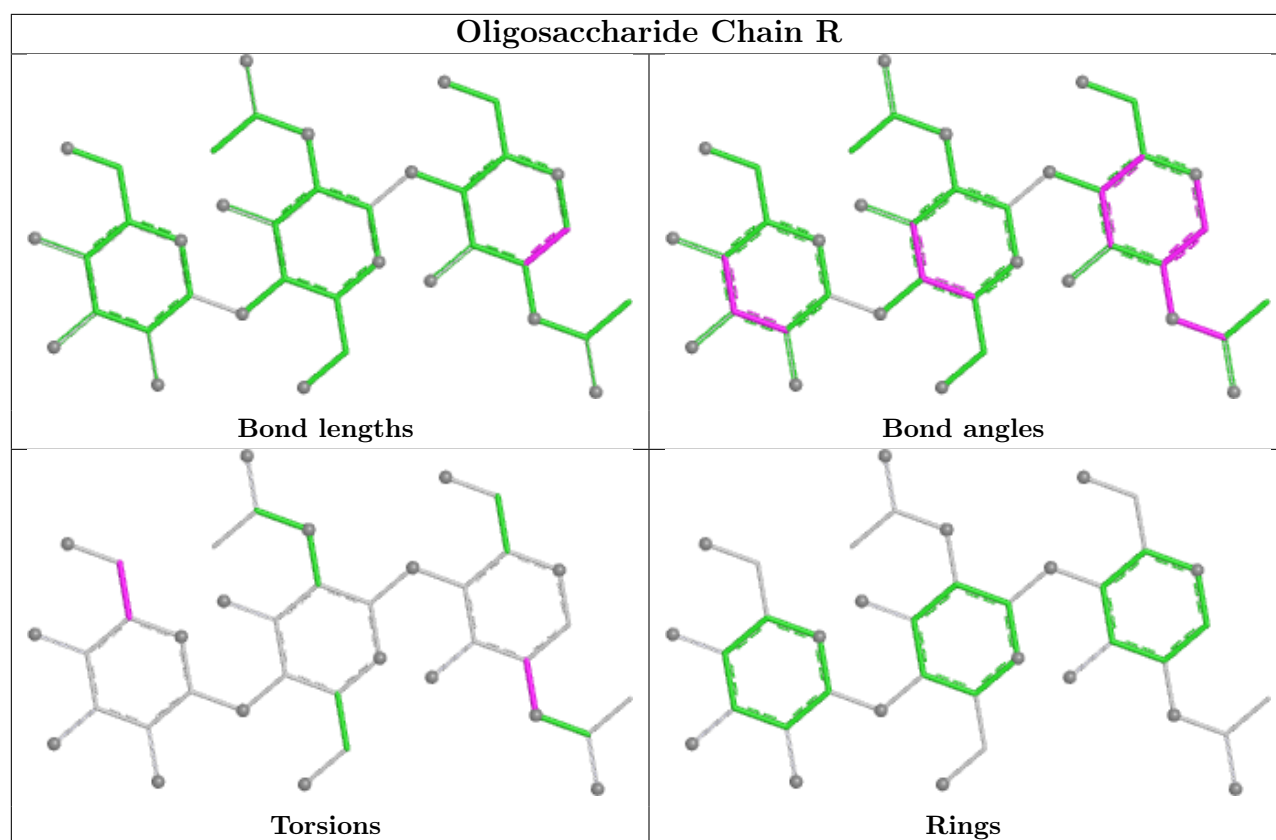


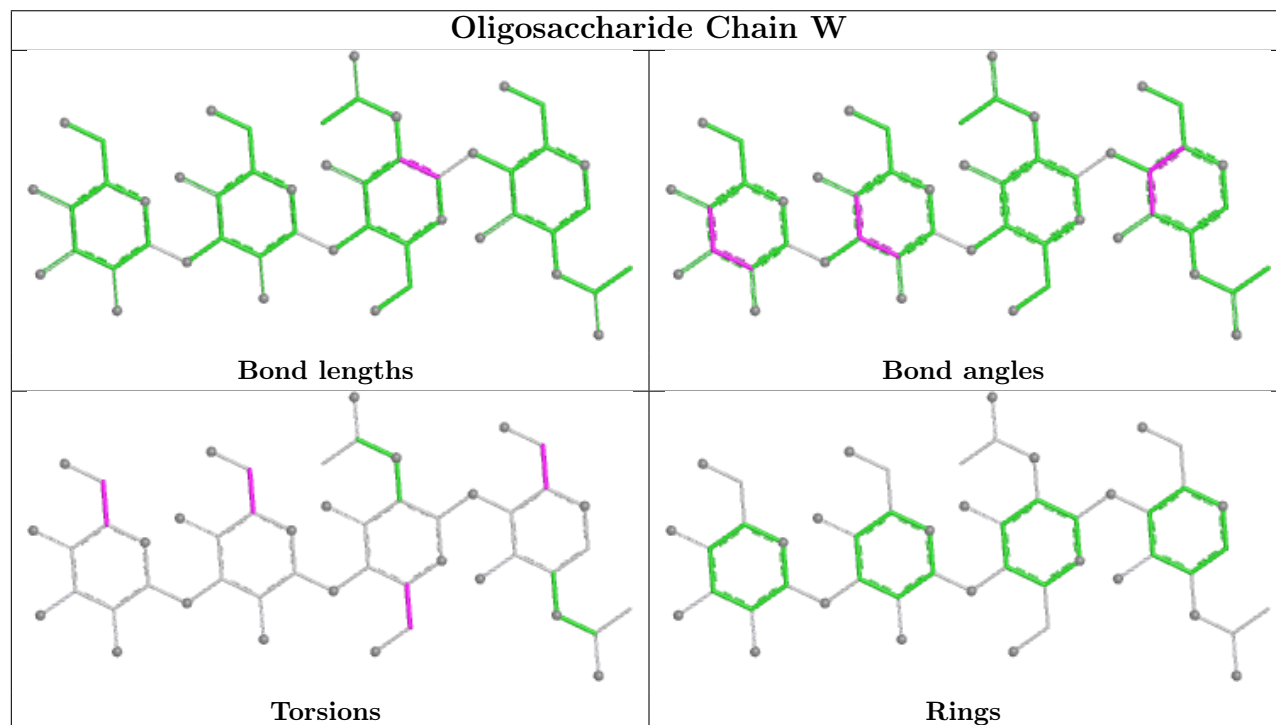
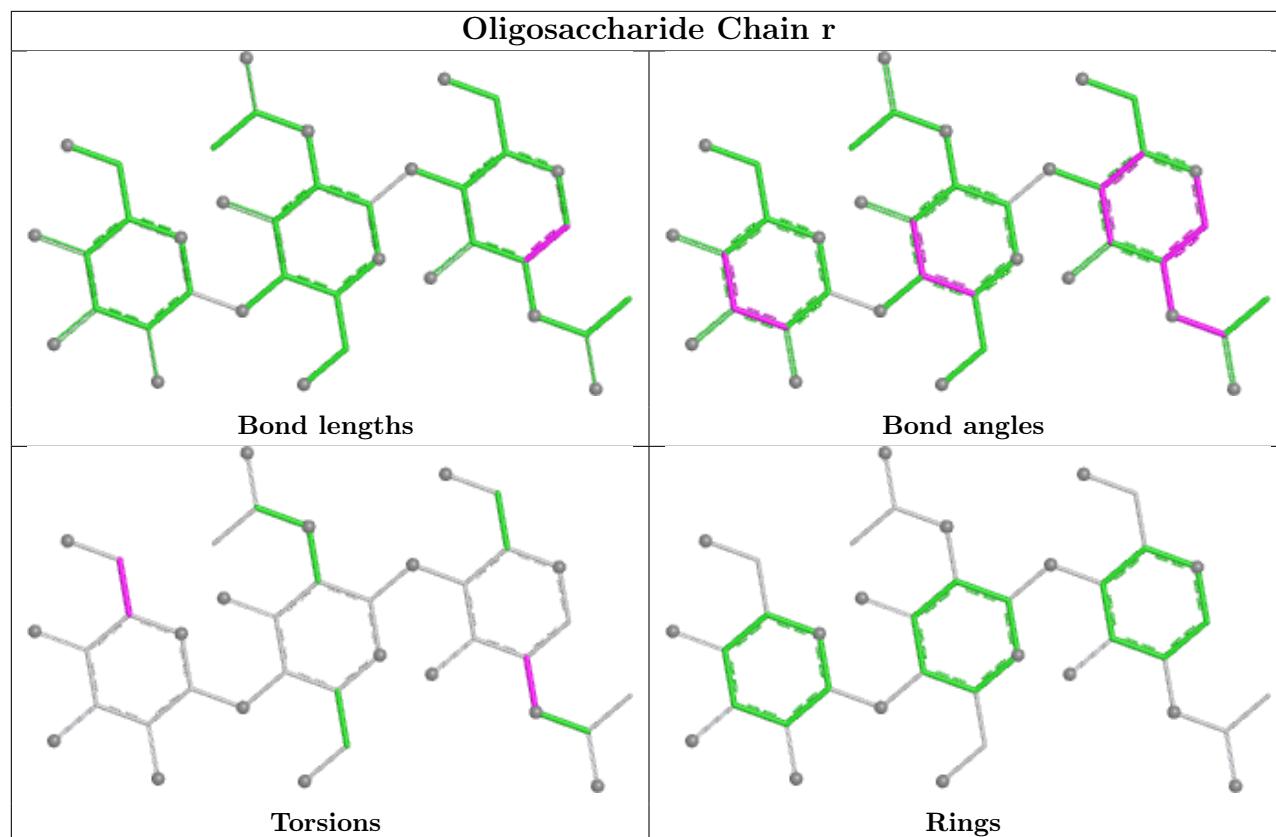


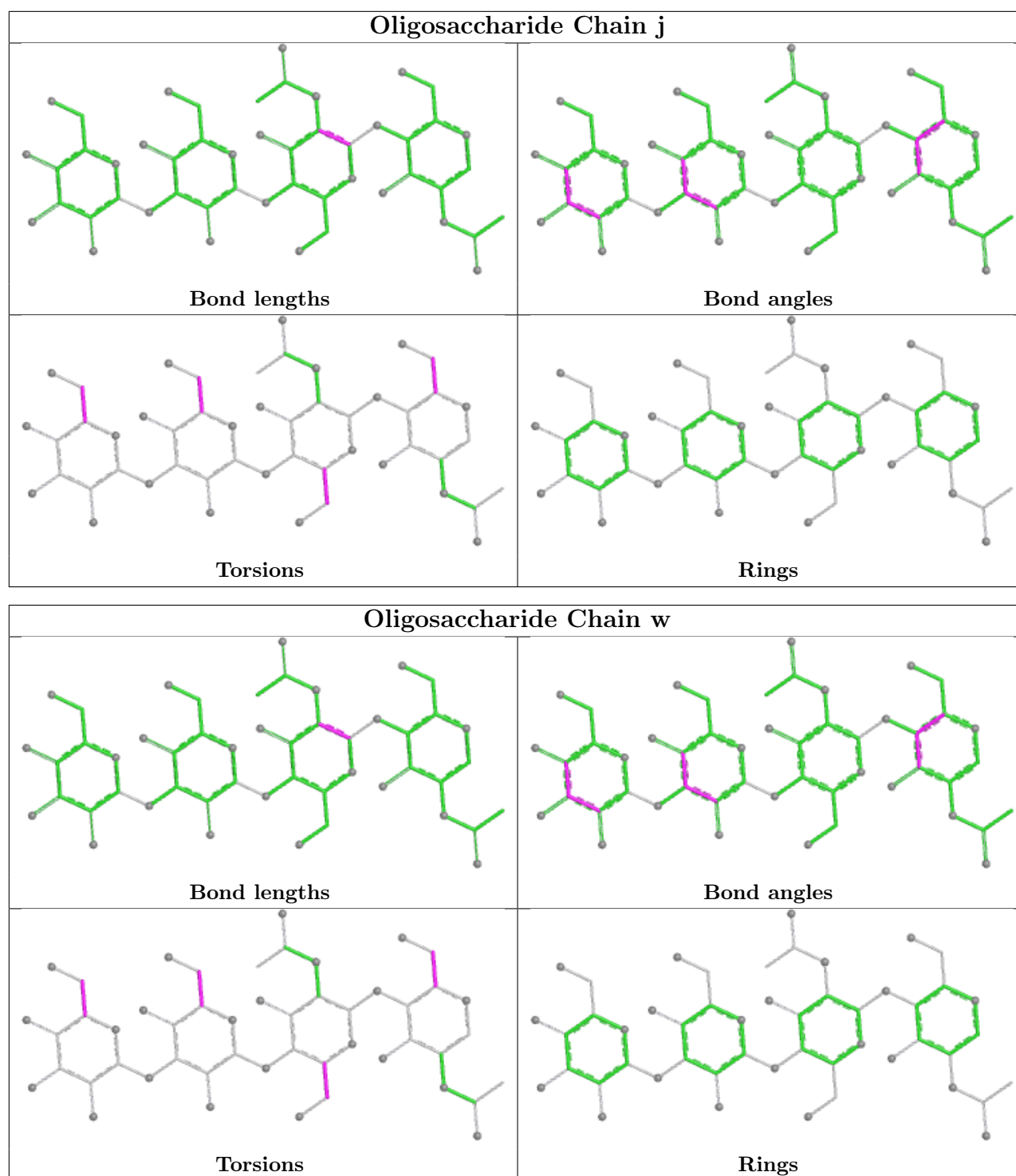












5.6 Ligand geometry [i](#)

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
8	NAG	B	703	2	14,14,15	0.76	1 (7%)	17,19,21	0.93	1 (5%)
8	NAG	C	601	1	14,14,15	0.95	1 (7%)	17,19,21	0.73	0
8	NAG	A	618	1	14,14,15	0.95	1 (7%)	17,19,21	1.07	1 (5%)
8	NAG	I	701	2	14,14,15	0.90	1 (7%)	17,19,21	0.94	1 (5%)
8	NAG	G	635	1	14,14,15	0.96	1 (7%)	17,19,21	0.71	0
8	NAG	B	704	2	14,14,15	0.92	1 (7%)	17,19,21	0.76	0
8	NAG	G	614	1	14,14,15	0.97	1 (7%)	17,19,21	1.15	1 (5%)
8	NAG	C	635	1	14,14,15	0.96	1 (7%)	17,19,21	0.71	1 (5%)
8	NAG	G	606	1	14,14,15	0.80	1 (7%)	17,19,21	1.05	1 (5%)
8	NAG	C	618	1	14,14,15	0.95	1 (7%)	17,19,21	1.07	1 (5%)
8	NAG	B	702	2	14,14,15	0.90	1 (7%)	17,19,21	0.77	1 (5%)
8	NAG	A	635	1	14,14,15	0.96	1 (7%)	17,19,21	0.71	0
8	NAG	G	613	1	14,14,15	0.77	1 (7%)	17,19,21	0.97	1 (5%)
8	NAG	D	704	2	14,14,15	0.91	1 (7%)	17,19,21	0.76	0
8	NAG	G	601	1	14,14,15	0.94	1 (7%)	17,19,21	0.73	0
8	NAG	A	601	1	14,14,15	0.95	1 (7%)	17,19,21	0.73	0
8	NAG	A	614	1	14,14,15	0.98	1 (7%)	17,19,21	1.14	1 (5%)
8	NAG	I	703	2	14,14,15	0.76	1 (7%)	17,19,21	0.93	1 (5%)
8	NAG	D	702	2	14,14,15	0.90	1 (7%)	17,19,21	0.77	1 (5%)
8	NAG	D	703	2	14,14,15	0.74	1 (7%)	17,19,21	0.93	1 (5%)
8	NAG	I	704	2	14,14,15	0.91	1 (7%)	17,19,21	0.76	0
8	NAG	D	701	2	14,14,15	0.90	1 (7%)	17,19,21	0.94	1 (5%)
8	NAG	C	614	1	14,14,15	0.97	1 (7%)	17,19,21	1.15	1 (5%)
8	NAG	G	618	1	14,14,15	0.94	1 (7%)	17,19,21	1.08	1 (5%)
8	NAG	A	606	1	14,14,15	0.81	1 (7%)	17,19,21	1.06	1 (5%)
8	NAG	B	701	2	14,14,15	0.89	1 (7%)	17,19,21	0.95	1 (5%)
8	NAG	C	613	1	14,14,15	0.80	1 (7%)	17,19,21	0.96	1 (5%)
8	NAG	I	702	2	14,14,15	0.90	1 (7%)	17,19,21	0.77	1 (5%)
8	NAG	A	613	1	14,14,15	0.78	1 (7%)	17,19,21	0.97	1 (5%)
8	NAG	C	606	1	14,14,15	0.80	1 (7%)	17,19,21	1.05	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
8	NAG	B	703	2	-	1/6/23/26	0/1/1/1
8	NAG	C	601	1	-	1/6/23/26	0/1/1/1
8	NAG	A	618	1	-	2/6/23/26	0/1/1/1
8	NAG	I	701	2	-	1/6/23/26	0/1/1/1
8	NAG	G	635	1	-	1/6/23/26	0/1/1/1
8	NAG	B	704	2	-	1/6/23/26	0/1/1/1
8	NAG	G	614	1	-	1/6/23/26	0/1/1/1
8	NAG	C	635	1	-	1/6/23/26	0/1/1/1
8	NAG	G	606	1	-	2/6/23/26	0/1/1/1
8	NAG	C	618	1	-	2/6/23/26	0/1/1/1
8	NAG	B	702	2	-	1/6/23/26	0/1/1/1
8	NAG	A	635	1	-	1/6/23/26	0/1/1/1
8	NAG	G	613	1	-	1/6/23/26	0/1/1/1
8	NAG	D	704	2	-	1/6/23/26	0/1/1/1
8	NAG	G	601	1	-	1/6/23/26	0/1/1/1
8	NAG	A	601	1	-	1/6/23/26	0/1/1/1
8	NAG	A	614	1	-	1/6/23/26	0/1/1/1
8	NAG	I	703	2	-	1/6/23/26	0/1/1/1
8	NAG	D	702	2	-	1/6/23/26	0/1/1/1
8	NAG	D	703	2	-	1/6/23/26	0/1/1/1
8	NAG	I	704	2	-	1/6/23/26	0/1/1/1
8	NAG	D	701	2	-	1/6/23/26	0/1/1/1
8	NAG	C	614	1	-	1/6/23/26	0/1/1/1
8	NAG	G	618	1	-	2/6/23/26	0/1/1/1
8	NAG	A	606	1	-	2/6/23/26	0/1/1/1
8	NAG	B	701	2	-	1/6/23/26	0/1/1/1
8	NAG	C	613	1	-	1/6/23/26	0/1/1/1
8	NAG	I	702	2	-	1/6/23/26	0/1/1/1
8	NAG	A	613	1	-	1/6/23/26	0/1/1/1
8	NAG	C	606	1	-	2/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	635	NAG	C1-C2	3.26	1.56	1.52
8	G	635	NAG	C1-C2	3.26	1.56	1.52
8	A	635	NAG	C1-C2	3.22	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	618	NAG	C1-C2	3.13	1.56	1.52
8	A	618	NAG	C1-C2	3.12	1.56	1.52
8	G	618	NAG	C1-C2	3.08	1.56	1.52
8	C	601	NAG	C1-C2	3.08	1.56	1.52
8	A	601	NAG	C1-C2	3.01	1.56	1.52
8	D	702	NAG	C1-C2	2.99	1.56	1.52
8	G	601	NAG	C1-C2	2.98	1.56	1.52
8	I	702	NAG	C1-C2	2.98	1.56	1.52
8	B	702	NAG	C1-C2	2.96	1.56	1.52
8	I	701	NAG	C1-C2	2.94	1.56	1.52
8	D	701	NAG	C1-C2	2.94	1.56	1.52
8	B	704	NAG	C1-C2	2.92	1.56	1.52
8	D	704	NAG	C1-C2	2.89	1.56	1.52
8	B	701	NAG	C1-C2	2.89	1.56	1.52
8	I	704	NAG	C1-C2	2.89	1.56	1.52
8	A	614	NAG	C1-C2	2.55	1.55	1.52
8	A	606	NAG	C1-C2	2.54	1.55	1.52
8	C	614	NAG	C1-C2	2.51	1.55	1.52
8	G	614	NAG	C1-C2	2.51	1.55	1.52
8	C	606	NAG	C1-C2	2.49	1.55	1.52
8	B	703	NAG	C1-C2	2.48	1.55	1.52
8	G	606	NAG	C1-C2	2.48	1.55	1.52
8	I	703	NAG	C1-C2	2.47	1.55	1.52
8	C	613	NAG	C1-C2	2.47	1.55	1.52
8	D	703	NAG	C1-C2	2.40	1.55	1.52
8	A	613	NAG	C1-C2	2.40	1.55	1.52
8	G	613	NAG	C1-C2	2.37	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	618	NAG	C4-C3-C2	-3.37	106.07	111.02
8	A	618	NAG	C4-C3-C2	-3.33	106.14	111.02
8	C	618	NAG	C4-C3-C2	-3.33	106.14	111.02
8	C	614	NAG	C4-C3-C2	-3.27	106.22	111.02
8	G	614	NAG	C4-C3-C2	-3.26	106.25	111.02
8	A	614	NAG	C4-C3-C2	-3.24	106.26	111.02
8	D	703	NAG	C4-C3-C2	-2.96	106.67	111.02
8	I	703	NAG	C4-C3-C2	-2.96	106.68	111.02
8	B	703	NAG	C4-C3-C2	-2.95	106.69	111.02
8	A	613	NAG	C4-C3-C2	-2.83	106.86	111.02
8	G	613	NAG	C4-C3-C2	-2.81	106.90	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	613	NAG	C4-C3-C2	-2.78	106.94	111.02
8	A	606	NAG	C4-C3-C2	-2.68	107.10	111.02
8	B	701	NAG	C4-C3-C2	-2.64	107.15	111.02
8	C	606	NAG	C4-C3-C2	-2.62	107.17	111.02
8	I	701	NAG	C4-C3-C2	-2.62	107.18	111.02
8	G	606	NAG	C4-C3-C2	-2.62	107.19	111.02
8	D	701	NAG	C4-C3-C2	-2.61	107.20	111.02
8	I	702	NAG	C4-C3-C2	-2.30	107.64	111.02
8	B	702	NAG	C4-C3-C2	-2.30	107.65	111.02
8	D	702	NAG	C4-C3-C2	-2.28	107.67	111.02
8	C	635	NAG	C4-C3-C2	-2.00	108.09	111.02

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	606	NAG	O5-C5-C6-O6
8	C	606	NAG	O5-C5-C6-O6
8	G	606	NAG	O5-C5-C6-O6
8	A	618	NAG	O5-C5-C6-O6
8	C	618	NAG	O5-C5-C6-O6
8	G	618	NAG	O5-C5-C6-O6
8	A	614	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	C	614	NAG	O5-C5-C6-O6
8	D	701	NAG	O5-C5-C6-O6
8	G	614	NAG	O5-C5-C6-O6
8	I	701	NAG	O5-C5-C6-O6
8	D	703	NAG	O5-C5-C6-O6
8	I	703	NAG	O5-C5-C6-O6
8	B	703	NAG	O5-C5-C6-O6
8	B	704	NAG	O5-C5-C6-O6
8	D	704	NAG	O5-C5-C6-O6
8	I	704	NAG	O5-C5-C6-O6
8	A	613	NAG	O5-C5-C6-O6
8	C	613	NAG	O5-C5-C6-O6
8	G	613	NAG	O5-C5-C6-O6
8	B	702	NAG	O5-C5-C6-O6
8	D	702	NAG	O5-C5-C6-O6
8	I	702	NAG	O5-C5-C6-O6
8	A	606	NAG	C4-C5-C6-O6
8	C	606	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	G	606	NAG	C4-C5-C6-O6
8	A	635	NAG	O5-C5-C6-O6
8	C	635	NAG	O5-C5-C6-O6
8	G	635	NAG	O5-C5-C6-O6
8	A	601	NAG	O5-C5-C6-O6
8	C	601	NAG	O5-C5-C6-O6
8	G	601	NAG	O5-C5-C6-O6
8	C	618	NAG	C4-C5-C6-O6
8	A	618	NAG	C4-C5-C6-O6
8	G	618	NAG	C4-C5-C6-O6

There are no ring outliers.

19 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	601	NAG	1	0
8	A	618	NAG	1	0
8	I	701	NAG	1	0
8	G	635	NAG	1	0
8	G	614	NAG	1	0
8	C	635	NAG	1	0
8	G	606	NAG	2	0
8	C	618	NAG	1	0
8	A	635	NAG	1	0
8	G	601	NAG	1	0
8	A	601	NAG	1	0
8	A	614	NAG	1	0
8	D	703	NAG	1	0
8	D	701	NAG	1	0
8	C	614	NAG	1	0
8	G	618	NAG	1	0
8	A	606	NAG	1	0
8	B	701	NAG	1	0
8	C	606	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

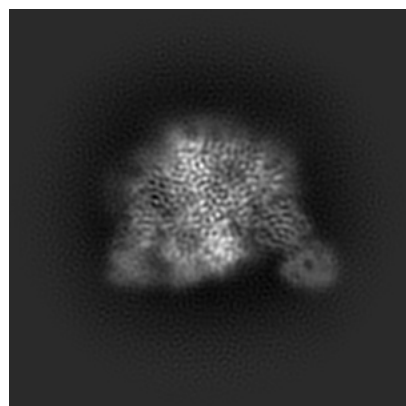
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20642. These allow visual inspection of the internal detail of the map and identification of artifacts.

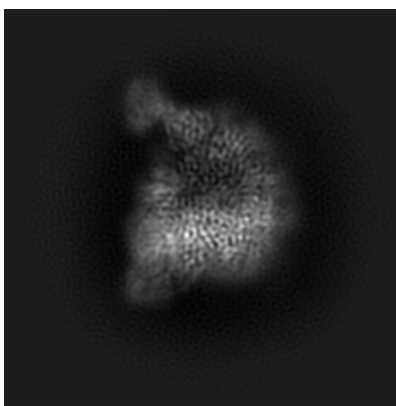
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

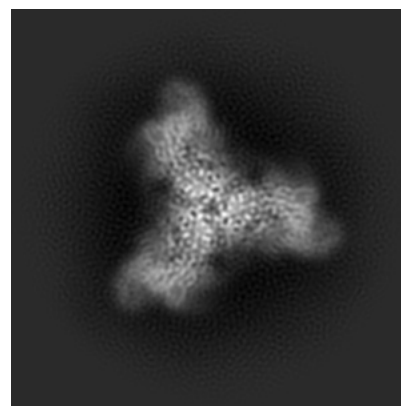
6.1.1 Primary map



X

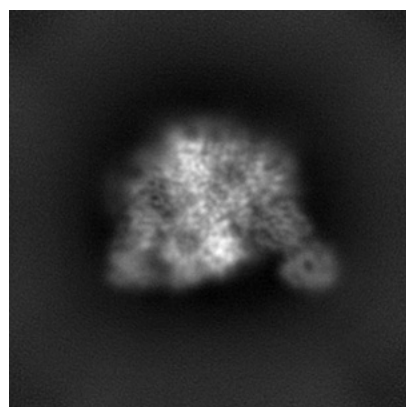


Y

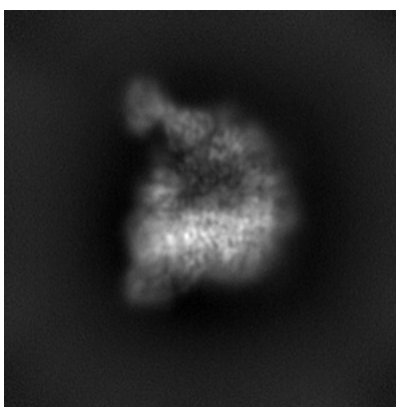


Z

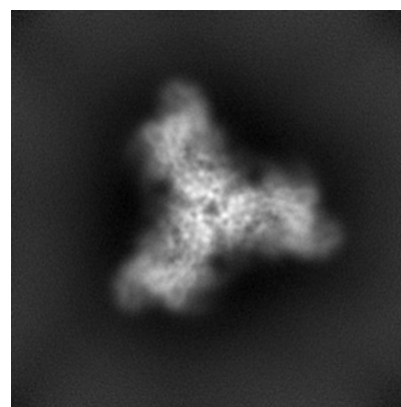
6.1.2 Raw map



X



Y

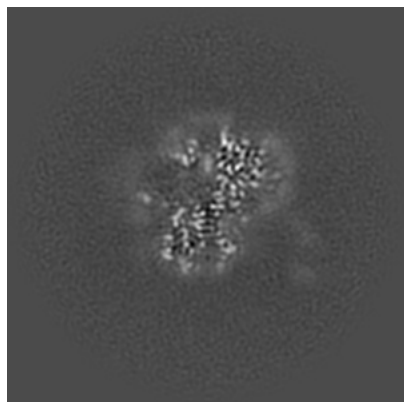


Z

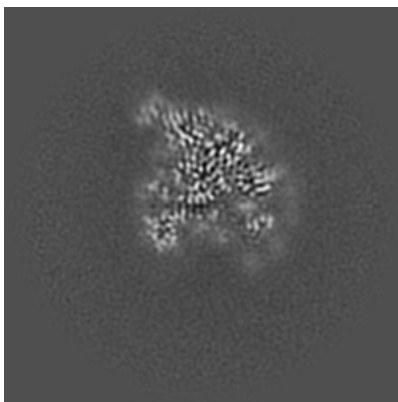
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

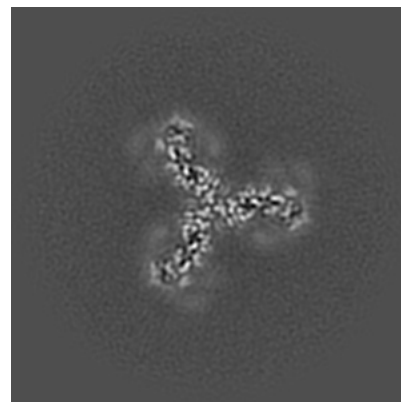
6.2.1 Primary map



X Index: 128

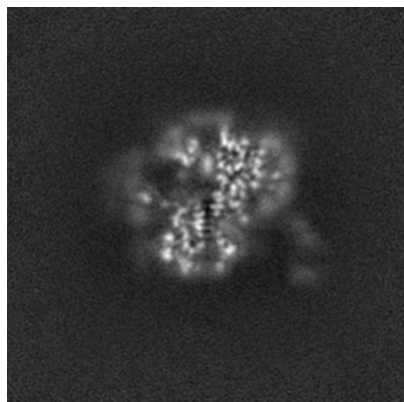


Y Index: 128

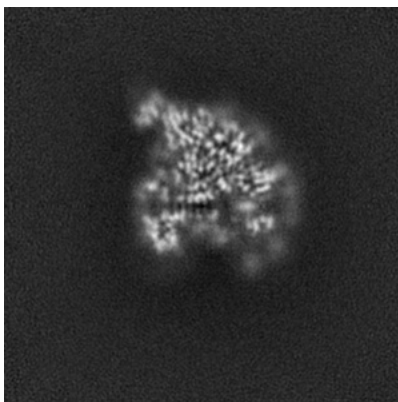


Z Index: 128

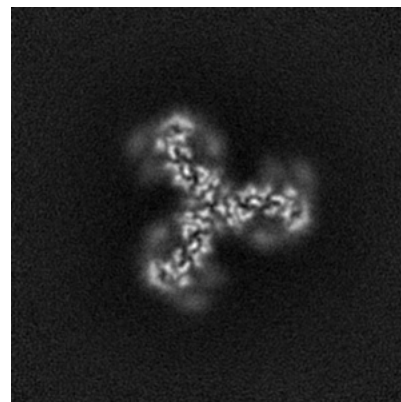
6.2.2 Raw map



X Index: 128



Y Index: 128

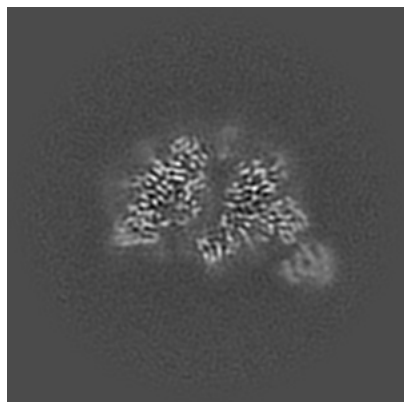


Z Index: 128

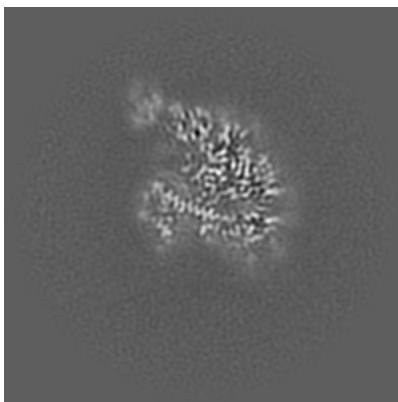
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

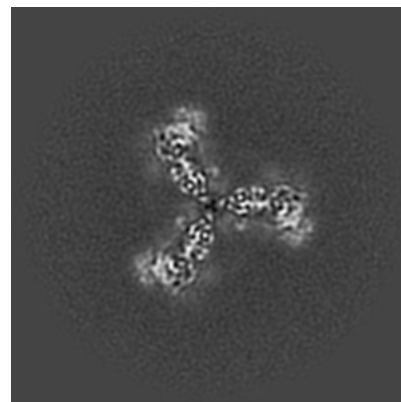
6.3.1 Primary map



X Index: 110

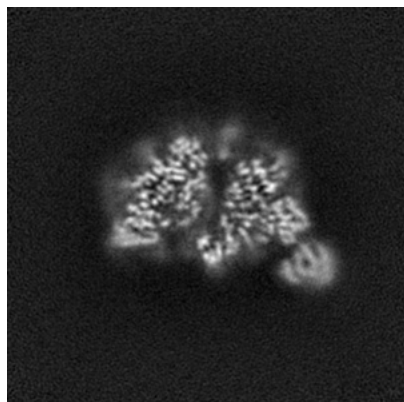


Y Index: 123

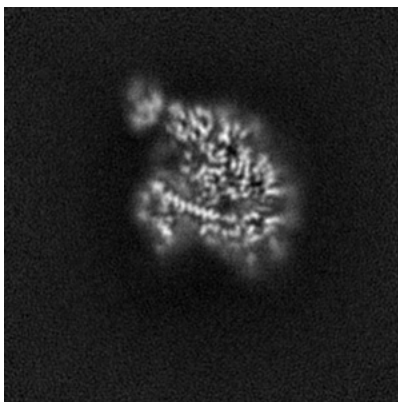


Z Index: 121

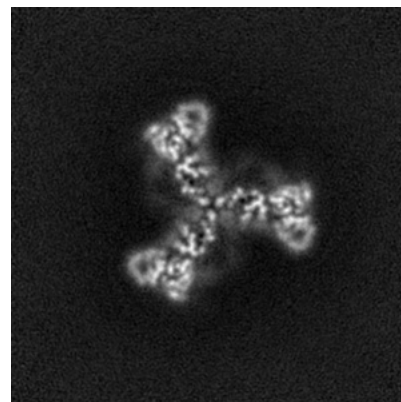
6.3.2 Raw map



X Index: 110



Y Index: 123

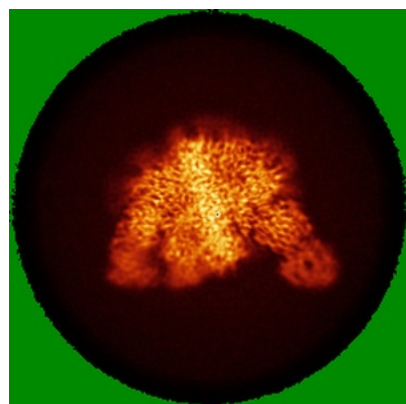


Z Index: 117

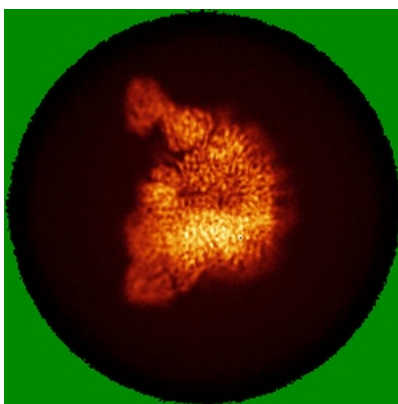
The images above show the largest variance slices of the map in three orthogonal directions.

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

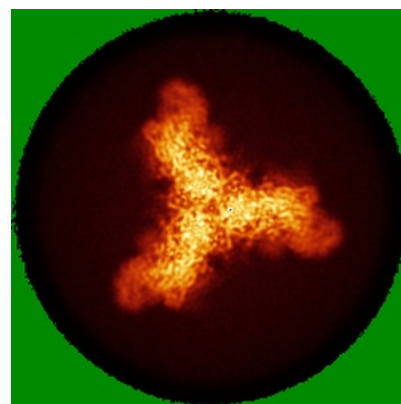
6.4.1 Primary map



X

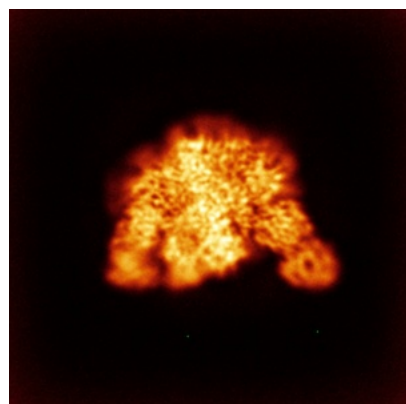


Y

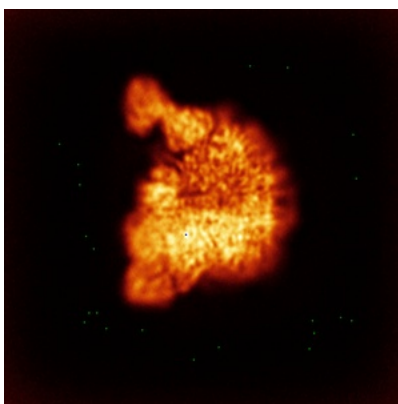


Z

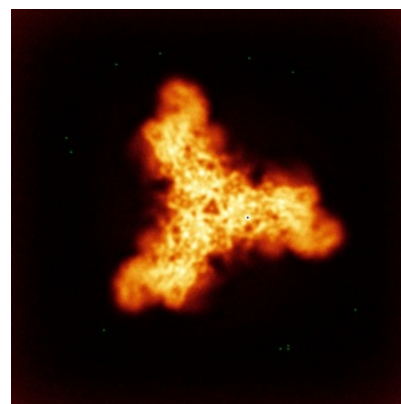
6.4.2 Raw map



X



Y

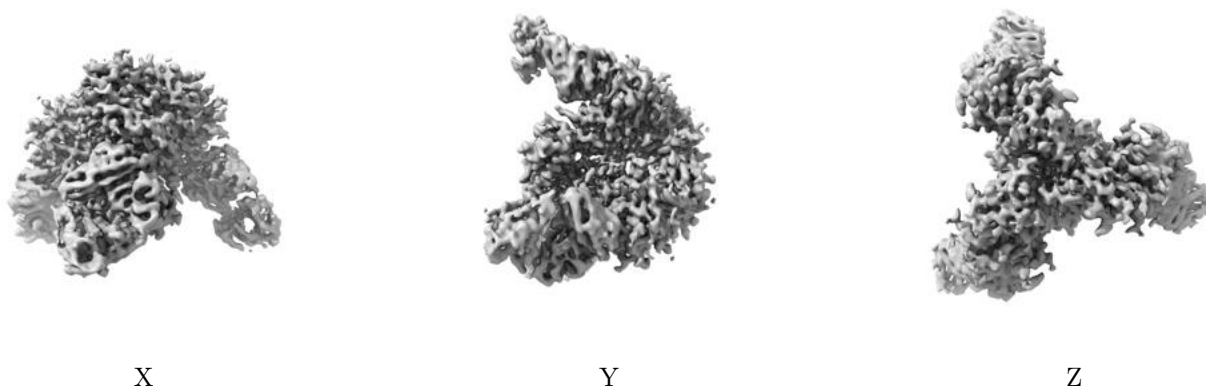


Z

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 0.53. 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.

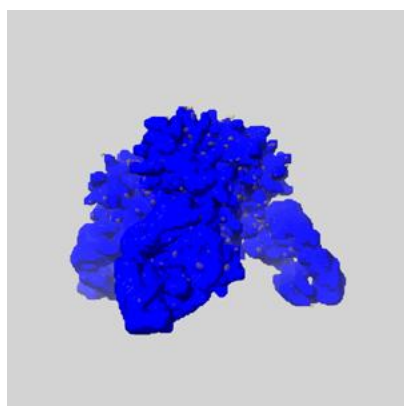
6.6 Mask visualisation [i](#)

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

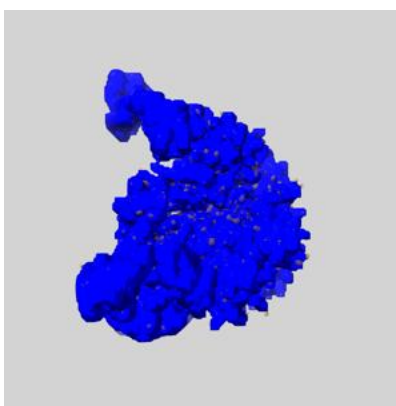
A mask typically either:

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

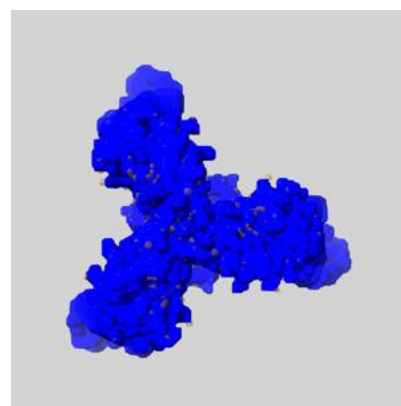
6.6.1 emd_20642_msk_1.map [i](#)



X



Y

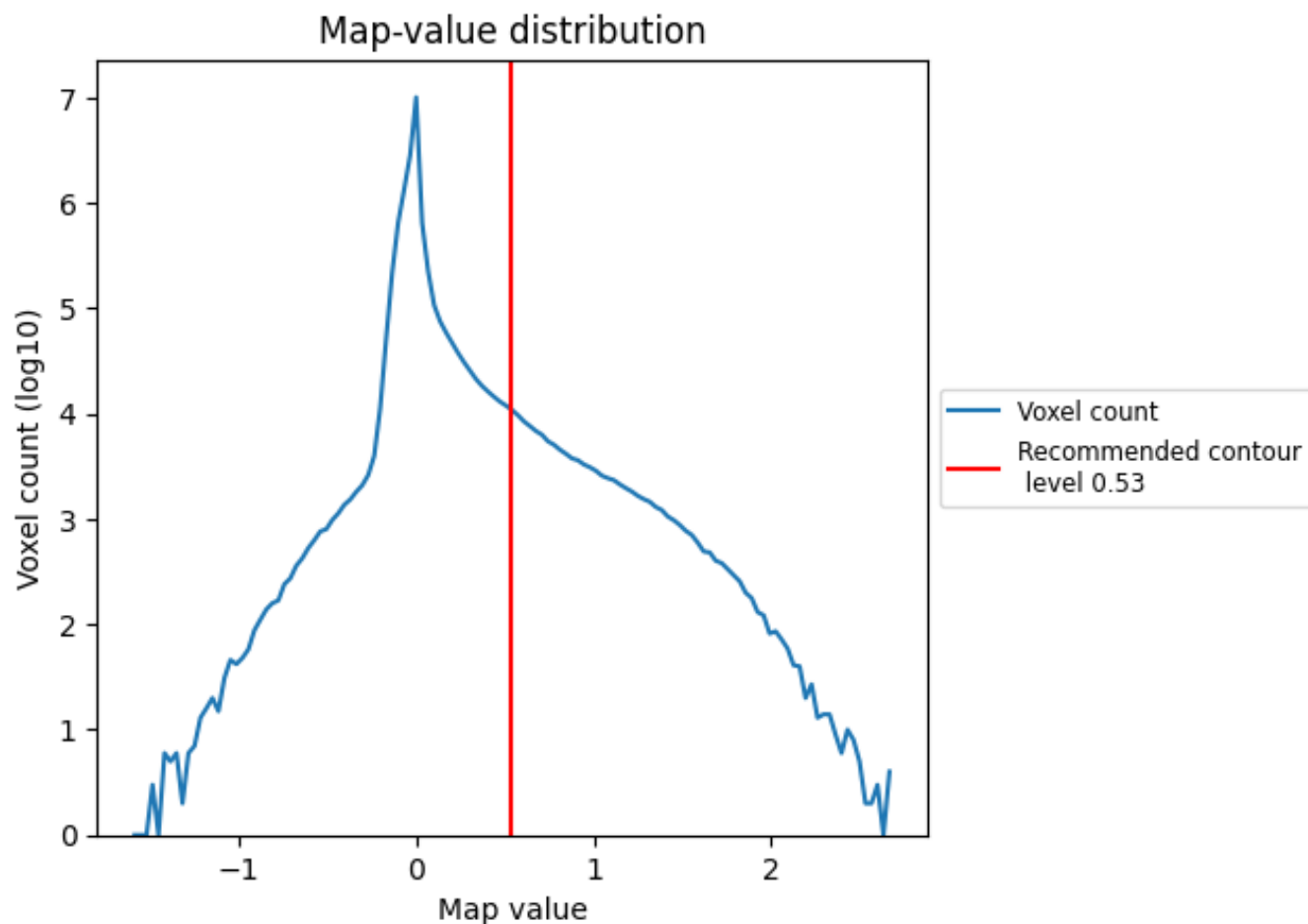


Z

7 Map analysis [i](#)

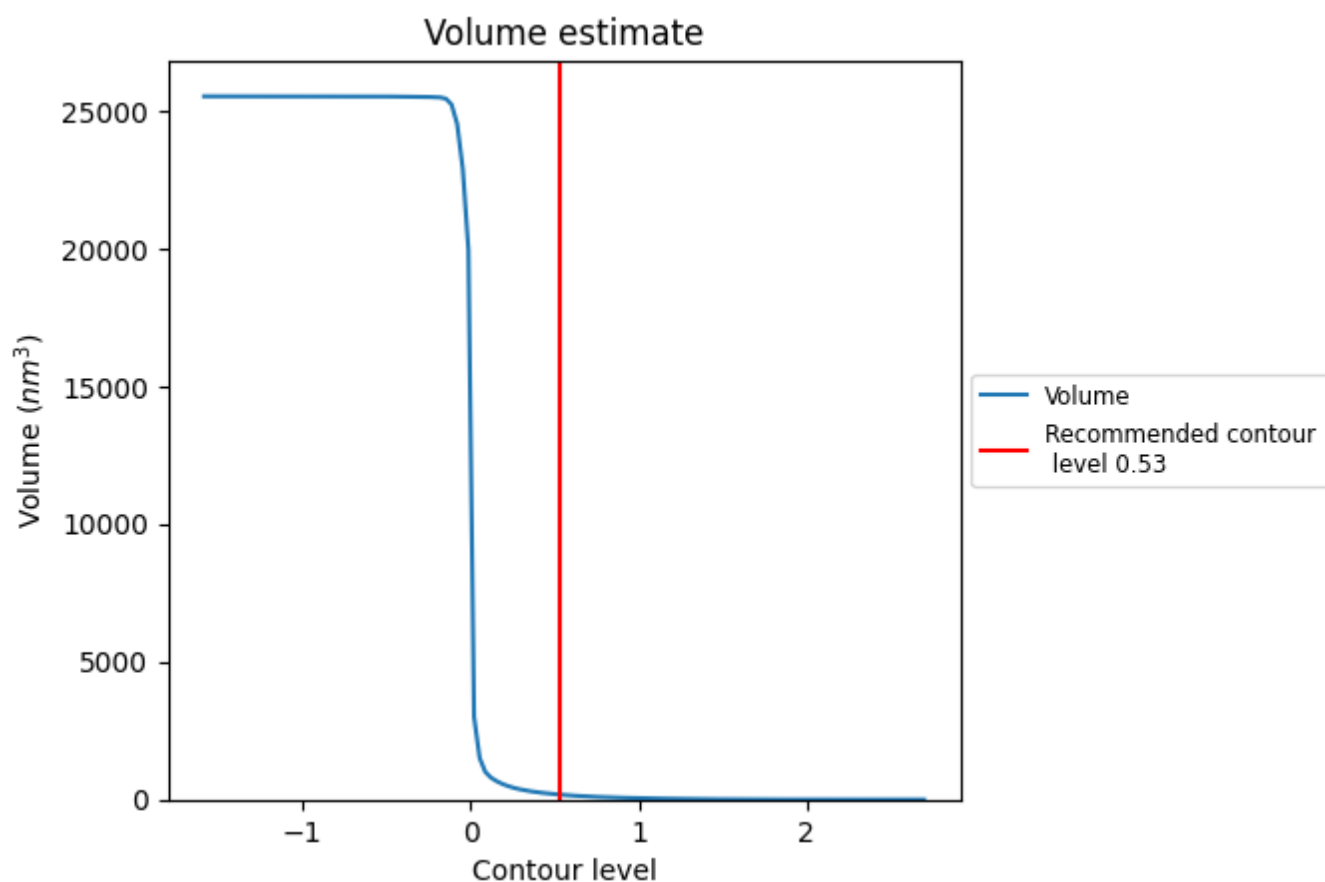
This section contains the results of statistical analysis of the map.

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.

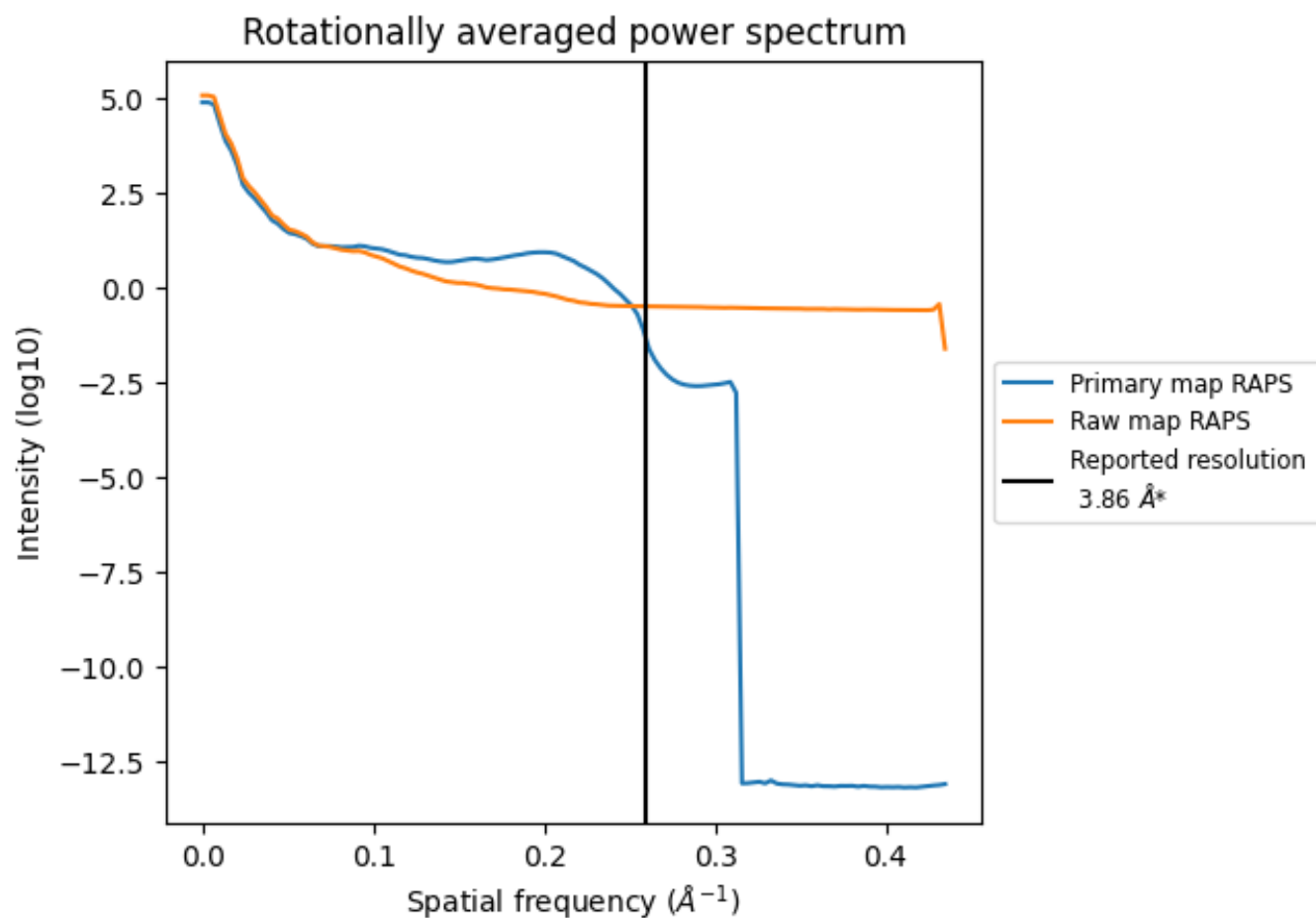
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 162 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 ⓘ

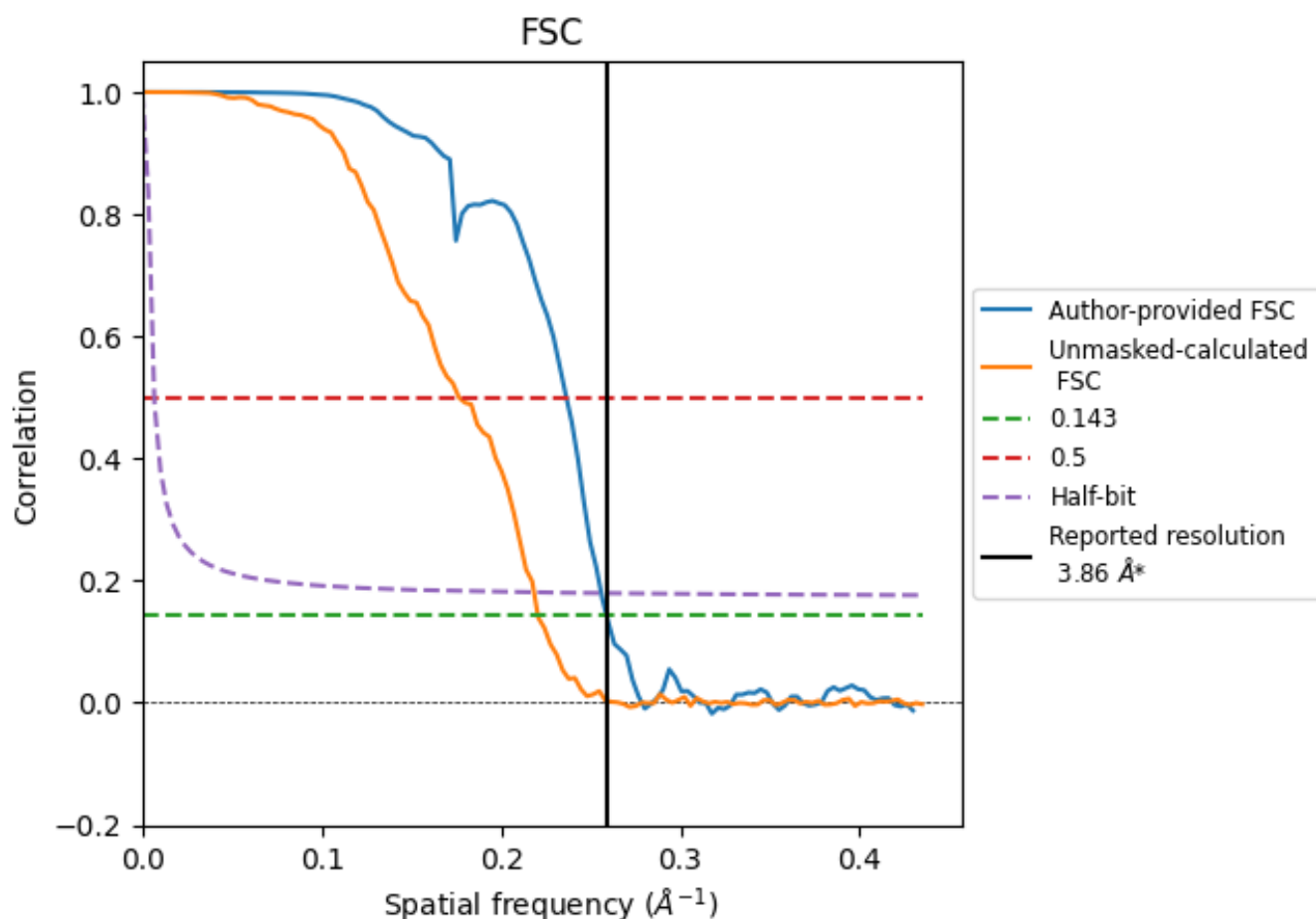


*Reported resolution corresponds to spatial frequency of 0.259 Å⁻¹

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 0.259 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

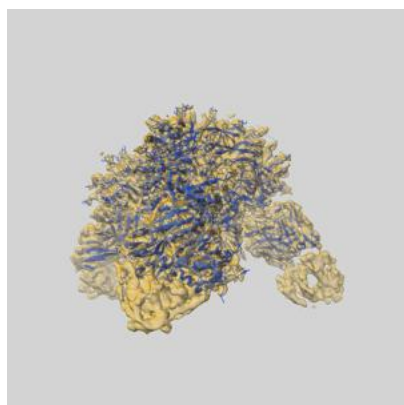
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.86	-	-
Author-provided FSC curve	3.86	4.23	3.91
Unmasked-calculated*	4.53	5.66	4.58

*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 4.53 differs from the reported value 3.86 by more than 10 %

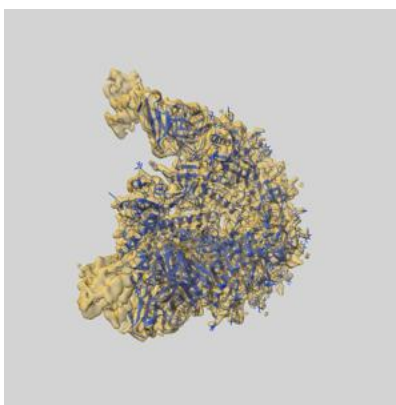
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20642 and PDB model 6U59. Per-residue inclusion information can be found in section 3 on page 12.

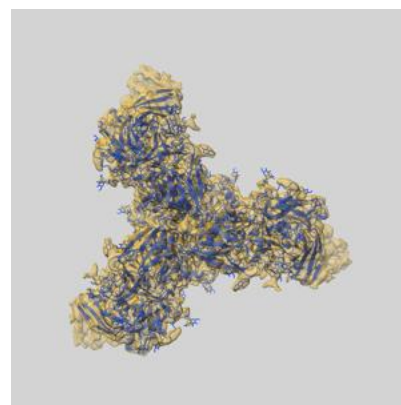
9.1 Map-model overlay [i](#)



X



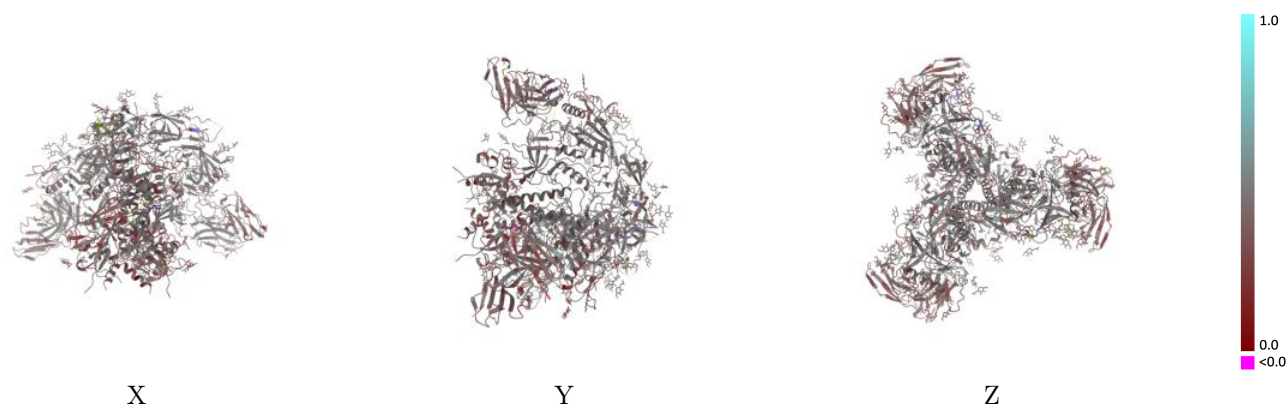
Y



Z

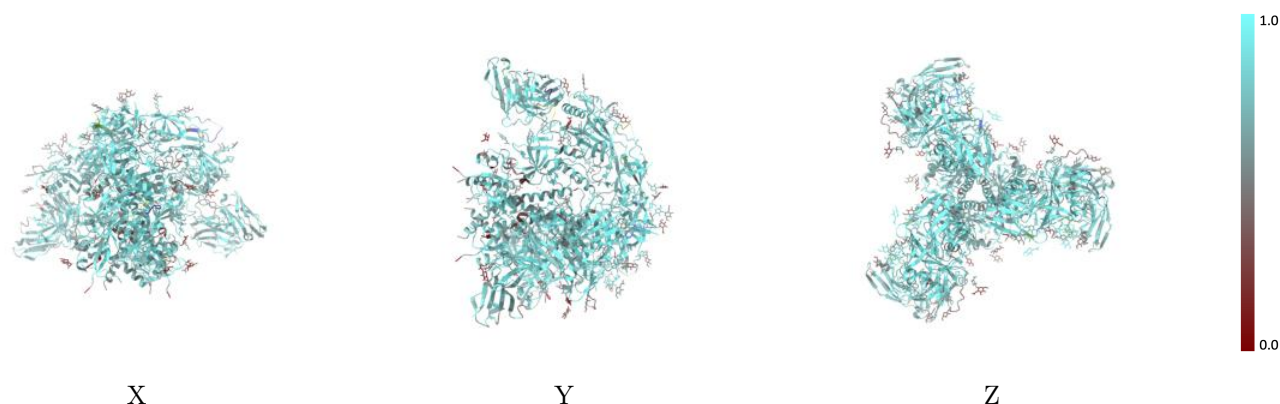
The images above show the 3D surface view of the map at the recommended contour level 0.53 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



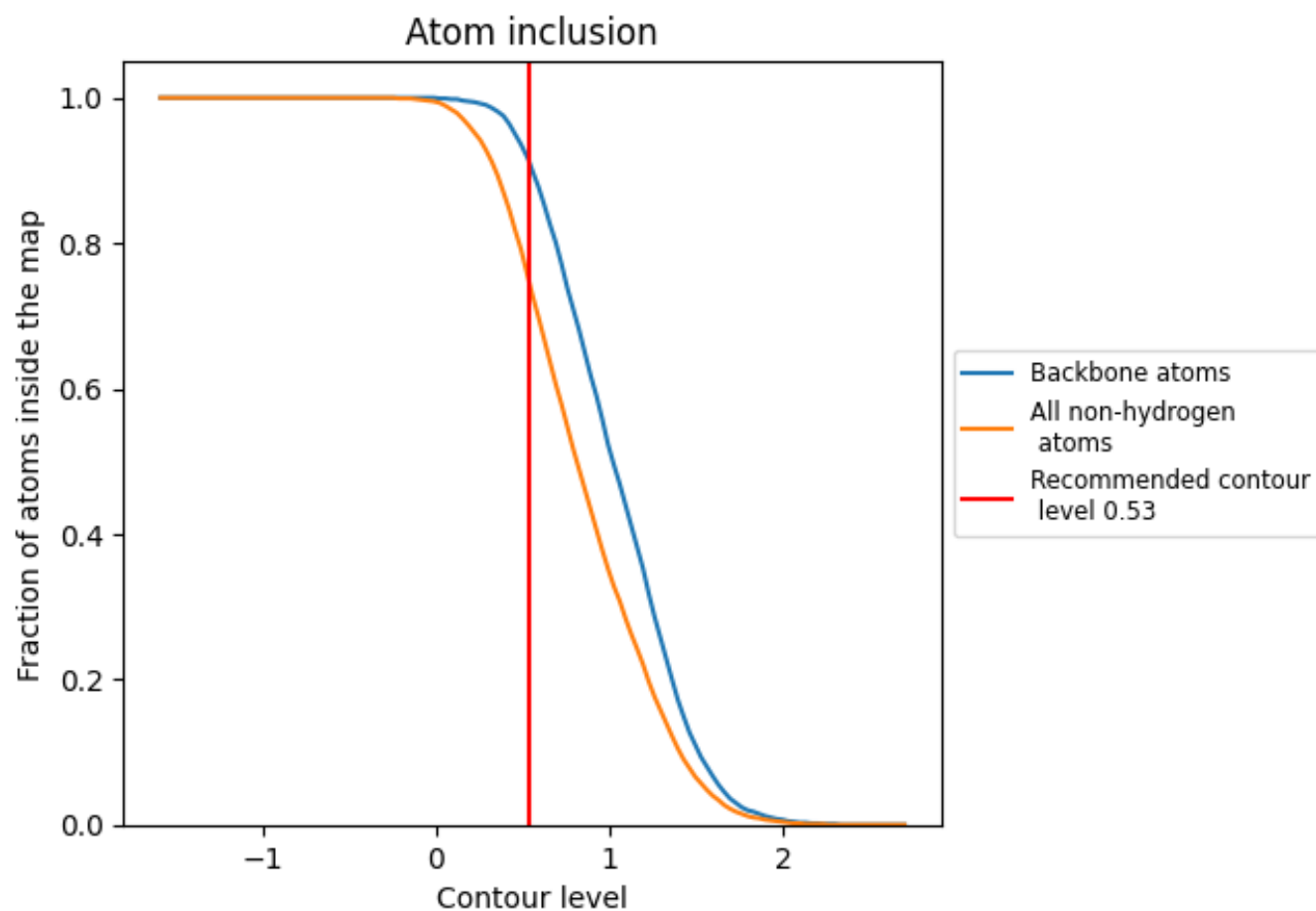
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.53).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 75% 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 (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7530	 0.3930
A	 0.7840	 0.4130
B	 0.6990	 0.3630
C	 0.7860	 0.4130
D	 0.6950	 0.3640
E	 0.7390	 0.3550
F	 0.7550	 0.3760
G	 0.7810	 0.4130
H	 0.7550	 0.3760
I	 0.7020	 0.3620
J	 0.7420	 0.3570
K	 0.7580	 0.3760
L	 0.7390	 0.3560
M	 0.6070	 0.3840
N	 0.6070	 0.4090
O	 0.7140	 0.4690
P	 0.3570	 0.3960
Q	 0.6790	 0.4110
R	 0.7690	 0.4110
S	 0.6430	 0.3670
T	 0.5710	 0.4200
U	 0.5360	 0.3160
V	 0.4640	 0.4120
W	 0.8200	 0.4560
X	 0.6430	 0.3900
Y	 0.8210	 0.4110
Z	 0.6070	 0.3950
a	 0.5000	 0.4000
b	 0.7140	 0.4660
c	 0.3570	 0.3870
d	 0.6790	 0.3950
e	 0.7440	 0.4220
f	 0.6430	 0.3630
g	 0.5710	 0.4030
h	 0.5360	 0.3200



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Chain	Atom inclusion	Q-score
i	 0.4290	 0.4040
j	 0.8200	 0.4550
k	 0.6430	 0.3810
l	 0.8210	 0.4280
m	 0.6070	 0.3790
n	 0.5360	 0.4220
o	 0.7140	 0.4680
p	 0.3570	 0.3840
q	 0.6790	 0.4080
r	 0.7440	 0.4220
s	 0.6430	 0.3790
t	 0.5710	 0.4050
u	 0.5710	 0.2980
v	 0.4290	 0.3970
w	 0.8000	 0.4570
x	 0.6430	 0.3750
y	 0.8210	 0.4020