



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 06:51 PM UTC

PDB ID : 8TL5 / pdb_00008tl5
EMDB ID : EMD-41362
Title : CRYO-EM STRUCTURE OF HIV-1 BG505DS-SOSIP.664 ENV TRIMER
BOUND TO HERH-c.01 FAB
Authors : Pletnev, S.; Hoyt, F.; Fischer, E.; Kwong, P.
Deposited on : 2023-07-26
Resolution : 3.30 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:

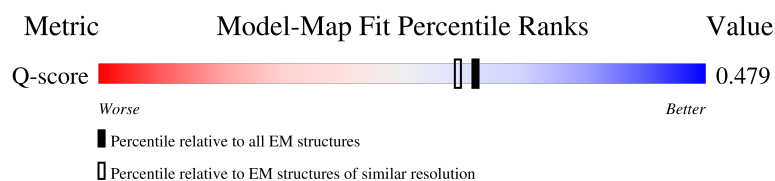
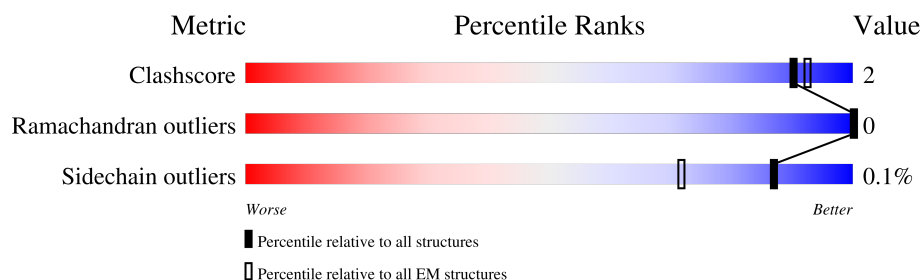
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.30 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.



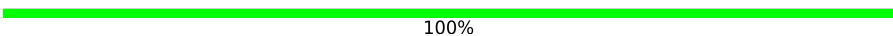
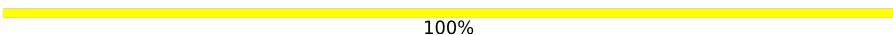
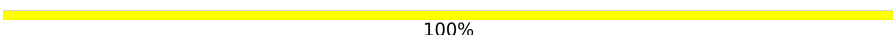
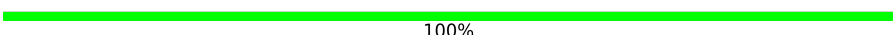
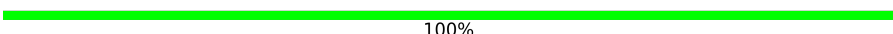
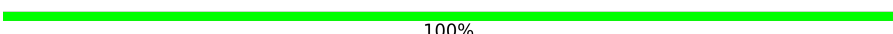
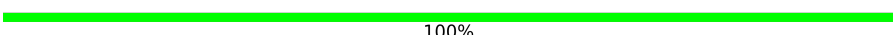
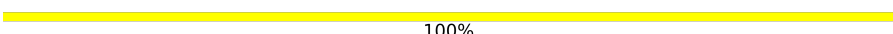
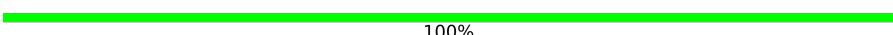
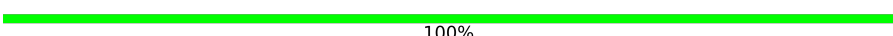
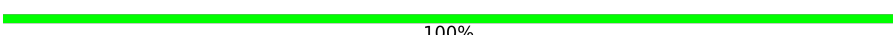
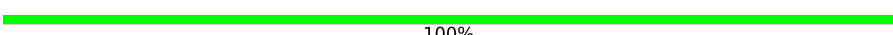
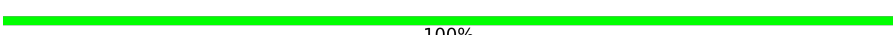
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	481	
1	C	481	
1	E	481	
2	B	153	

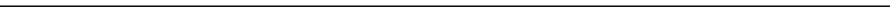
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Mol	Chain	Length	Quality of chain
2	D	153	
2	F	153	
3	G	237	
3	I	237	
3	K	237	
4	H	214	
4	J	214	
4	L	214	
5	M	2	
5	N	2	
5	P	2	
5	Q	2	
5	S	2	
5	T	2	
5	U	2	
5	V	2	
5	W	2	
5	Y	2	
5	Z	2	
5	a	2	
5	c	2	
5	d	2	
5	e	2	
5	f	2	
5	g	2	

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Mol	Chain	Length	Quality of chain
5	h	2	 100%
5	i	2	 50% 50%
5	k	2	 100%
5	l	2	 100%
5	n	2	 100%
5	o	2	 100%
5	p	2	 100%
6	O	3	 100%
6	X	3	 100%
6	j	3	 100%
7	R	5	 60% 40%
7	b	5	 60% 40%
7	m	5	 60% 40%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19830 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 BG505 DS-SOSIP Surface protein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3465	2173	611	651	30		
1	C	441	Total	C	N	O	S	0	0
			3465	2173	611	651	30		
1	E	441	Total	C	N	O	S	0	0
			3465	2173	611	651	30		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	CYS	ILE	engineered mutation	UNP Q2N0S5
A	332	ASN	THR	engineered mutation	UNP Q2N0S5
A	433	CYS	ALA	engineered mutation	UNP Q2N0S5
A	501	CYS	ALA	engineered mutation	UNP Q2N0S5
A	509	ARG	GLU	engineered mutation	UNP Q2N0S5
A	510	ARG	LYS	engineered mutation	UNP Q2N0S5
A	512	ARG	-	insertion	UNP Q2N0S5
A	513	ARG	-	insertion	UNP Q2N0S5
C	201	CYS	ILE	engineered mutation	UNP Q2N0S5
C	332	ASN	THR	engineered mutation	UNP Q2N0S5
C	433	CYS	ALA	engineered mutation	UNP Q2N0S5
C	501	CYS	ALA	engineered mutation	UNP Q2N0S5
C	509	ARG	GLU	engineered mutation	UNP Q2N0S5
C	510	ARG	LYS	engineered mutation	UNP Q2N0S5
C	512	ARG	-	insertion	UNP Q2N0S5
C	513	ARG	-	insertion	UNP Q2N0S5
E	201	CYS	ILE	engineered mutation	UNP Q2N0S5
E	332	ASN	THR	engineered mutation	UNP Q2N0S5
E	433	CYS	ALA	engineered mutation	UNP Q2N0S5
E	501	CYS	ALA	engineered mutation	UNP Q2N0S5
E	509	ARG	GLU	engineered mutation	UNP Q2N0S5
E	510	ARG	LYS	engineered mutation	UNP Q2N0S5
E	512	ARG	-	insertion	UNP Q2N0S5
E	513	ARG	-	insertion	UNP Q2N0S5

- Molecule 2 is a protein called BG505 DS-SOSIP Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	125	Total	C	N	O	S	0	0
			994	630	171	187	6		
2	D	125	Total	C	N	O	S	0	0
			994	630	171	187	6		
2	F	125	Total	C	N	O	S	0	0
			994	630	171	187	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S5
B	605	CYS	THR	engineered mutation	UNP Q2N0S5
D	559	PRO	ILE	engineered mutation	UNP Q2N0S5
D	605	CYS	THR	engineered mutation	UNP Q2N0S5
F	559	PRO	ILE	engineered mutation	UNP Q2N0S5
F	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 3 is a protein called HERH-c.01 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	126	Total	C	N	O	S	0	0
			934	574	173	182	5		
3	I	126	Total	C	N	O	S	0	0
			934	574	173	182	5		
3	K	126	Total	C	N	O	S	0	0
			934	574	173	182	5		

- Molecule 4 is a protein called HERH-c.01 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	107	Total	C	N	O	S	0	0
			823	523	139	158	3		
4	J	107	Total	C	N	O	S	0	0
			823	523	139	158	3		
4	L	107	Total	C	N	O	S	0	0
			823	523	139	158	3		

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



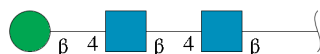
Mol	Chain	Residues	Atoms				AltConf	Trace
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	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	W	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	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	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		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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		
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		

- 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.



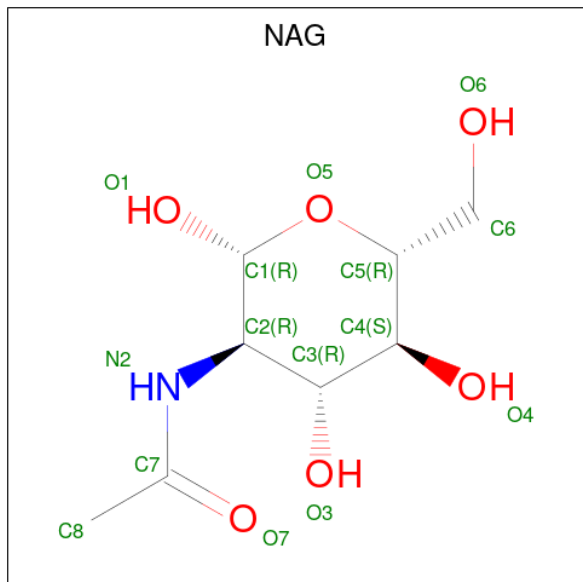
Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	3	Total	C	N	O	0	0
			39	22	2	15		
6	X	3	Total	C	N	O	0	0
			39	22	2	15		
6	j	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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	R	5	Total	C	N	O	0	0
			61	34	2	25		
7	b	5	Total	C	N	O	0	0
			61	34	2	25		
7	m	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	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	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	

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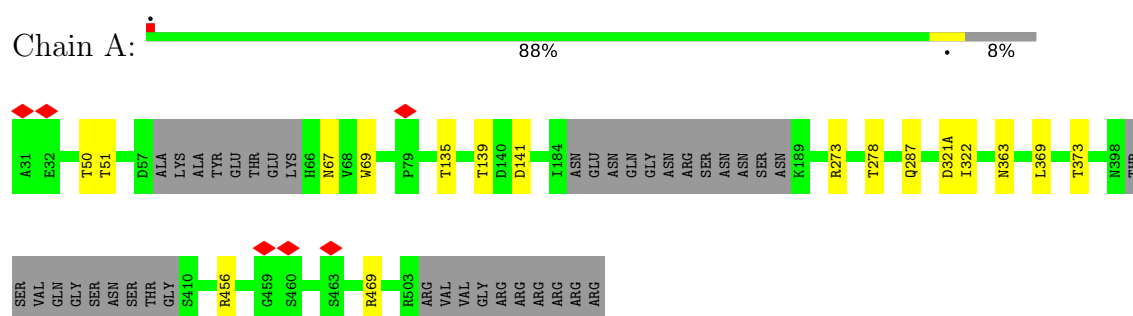
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Mol	Chain	Residues	Atoms				AltConf
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	

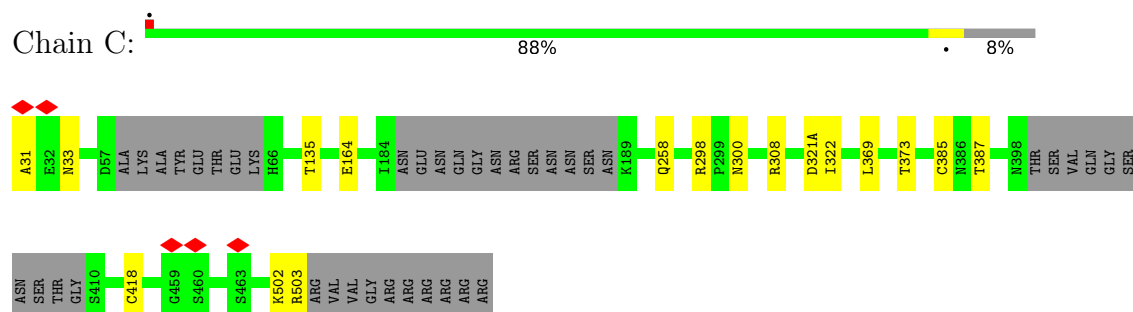
3 Residue-property plots [i](#)

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

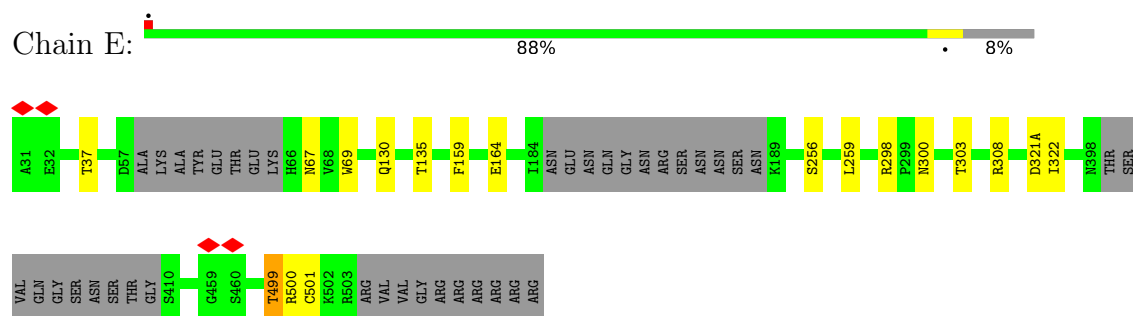
- Molecule 1: BG505 DS-SOSIP Surface protein gp120



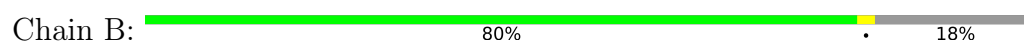
- Molecule 1: BG505 DS-SOSIP Surface protein gp120

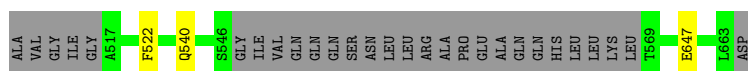


- Molecule 1: BG505 DS-SOSIP Surface protein gp120



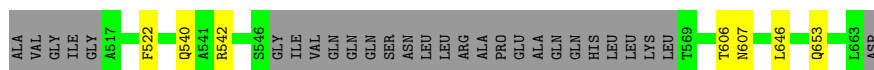
- Molecule 2: BG505 DS-SOSIP Transmembrane protein gp41





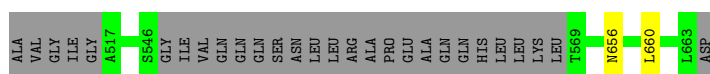
- Molecule 2: BG505 DS-SOSIP Transmembrane protein gp41

Chain D: 77% 5% 18%



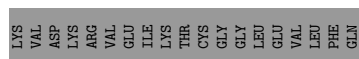
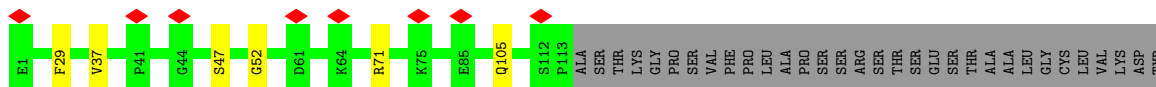
- Molecule 2: BG505 DS-SOSIP Transmembrane protein gp41

Chain F: 80% 18%



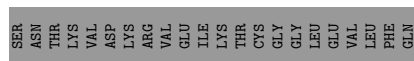
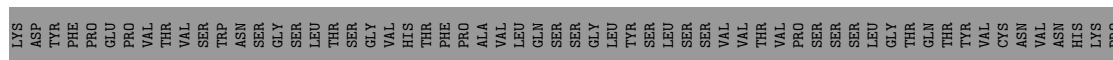
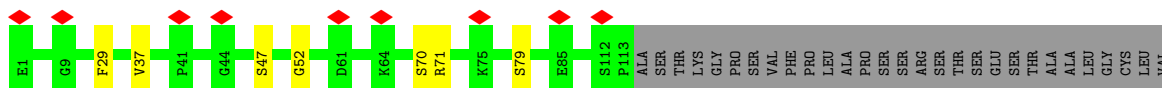
- Molecule 3: HERH-c.01 FAB HEAVY CHAIN

Chain G: 51% 47%



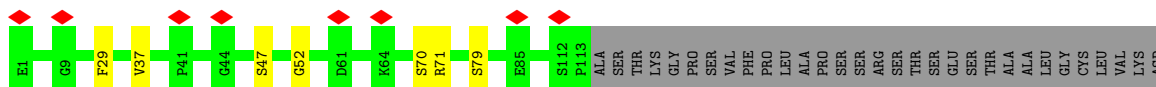
- Molecule 3: HERH-c.01 FAB HEAVY CHAIN

Chain I: 50% 47%



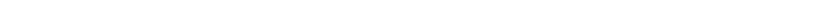
- Molecule 3: HERH-c.01 FAB HEAVY CHAIN

Chain K: 50% 47%



[illegible]

● Molecule 4: HERH-c.01 FAB LIGHT CHAIN

Chain H:  48% . 50%

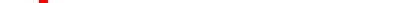
[illegible]

- Molecule 4: HERH-c.01 FAB LIGHT CHAIN

Chain J: 47% . 50%

ARG	ASP	D1
GLY	GLY	I2
GLU	ALA	Q3
CYS	LEU	Q37
	THR	L47
	GLY	
	ASN	T74
	SER	
	GLN	D82
	GLU	
	SER	Y86
	VAL	
	THR	D106
	GLU	V106
	GLN	K107
	ASP	ARG
	SER	THR
	LYS	VAL
	ASP	ALA
	ASN	ALA
	THR	PRO
	TYR	SER
	SER	VAL
	LEU	PHE
	SER	ILE
	THR	PHE
	LEU	PRO
	THR	PRO
	LEU	SER
	SER	GLU
	SER	GLY
	THR	THR
	GLY	VAL
	GLU	GLN
	TYR	LYS
	GLN	SER
	SER	GLY
	HIS	THR
	LYS	VAL
	VAL	SER
	TYR	VAL
	ALA	VAL
	CYS	CYS
	GLU	LEU
	VAL	LEU
	THR	ASN
	HIS	ASN
	GLN	PHE
	GLY	TYR
	LEU	PRO
	SER	ARG
	SER	GLU
	PRO	ALA
	VAL	SER
	THR	VAL
	LYS	THR
	SER	LYS
	PHE	TRP
	ASN	LYS

● Molecule 4: HERH-c.01 FAB LIGHT CHAIN

Chain L:  46% . 50%

[illegible]

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

Chain a: 100%

NAG1
NAG2

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

Chain M:  100%

NAG1
NAG2

- 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 P:  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:  100%

NAG1
NAG2

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

Chain U:  100%

NAG1
NAG2

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

Chain c:  100%



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

Chain V:  100%



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

Chain W:  100%



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

Chain Y:  100%



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

Chain Z:  100%



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

Chain d:  100%



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

Chain e:  100%

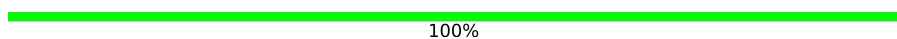
MAG1
MAG2

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

Chain f: 50%50%

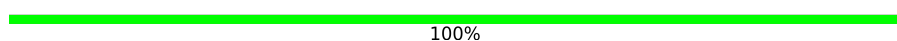
MAG1
MAG2

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

Chain g: 100%

MAG1
MAG2

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

Chain h: 100%

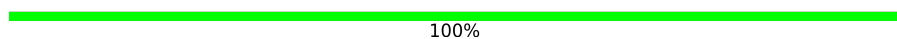
MAG1
MAG2

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

Chain i: 50%50%

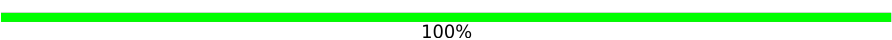
MAG1
MAG2

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

Chain k: 100%

MAG1
MAG2

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

Chain l: 100%

MAG1
MAG2

- 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:  100%

NAG1
NAG2

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

Chain p:  100%

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 O:  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 X:  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 j:  100%

NAG1
NAG2
BMA3

- Molecule 7: alpha-D-mannopyranose-(1-2)-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 R:  60% 40%

MAN1	MAN2	MAN3	MAN4	MAN5
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● Molecule 7: alpha-D-mannopyranose-(1-2)-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 b:  60% 40%

MAN1	MAN2	MAN3	MAN4	MAN5
------	------	------	------	------

● Molecule 7: alpha-D-mannopyranose-(1-2)-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 m:  60% 40%

MAN1	MAN2	MAN3	MAN4	MAN5
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	637576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.2	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.986	Depositor
Minimum map value	-1.322	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	397.302, 397.302, 397.302	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86370003, 0.86370003, 0.86370003	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.15	0/3537	0.32	0/4802
1	C	0.13	0/3537	0.30	0/4802
1	E	0.13	0/3537	0.30	0/4802
2	B	0.15	0/1012	0.31	0/1373
2	D	0.13	0/1012	0.29	0/1373
2	F	0.14	0/1012	0.31	0/1373
3	G	0.11	0/950	0.27	0/1280
3	I	0.12	0/950	0.28	0/1280
3	K	0.12	0/950	0.28	0/1280
4	H	0.15	0/846	0.33	0/1153
4	J	0.15	0/846	0.31	0/1153
4	L	0.14	0/846	0.31	0/1153
All	All	0.14	0/19035	0.30	0/25824

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3465	0	3391	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3465	0	3391	11	0
1	E	3465	0	3391	11	0
2	B	994	0	976	2	0
2	D	994	0	976	6	0
2	F	994	0	976	1	0
3	G	934	0	911	4	0
3	I	934	0	911	4	0
3	K	934	0	911	4	0
4	H	823	0	791	2	0
4	J	823	0	791	4	0
4	L	823	0	791	5	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	P	28	0	25	1	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	0	0
5	V	28	0	25	0	0
5	W	28	0	25	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	2	0
5	a	28	0	25	0	0
5	c	28	0	25	0	0
5	d	28	0	25	0	0
5	e	28	0	25	0	0
5	f	28	0	25	2	0
5	g	28	0	25	0	0
5	h	28	0	25	0	0
5	i	28	0	25	2	0
5	k	28	0	25	0	0
5	l	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
6	O	39	0	34	0	0
6	X	39	0	34	0	0
6	j	39	0	34	0	0
7	R	61	0	52	0	0
7	b	61	0	52	0	0
7	m	61	0	52	0	0
8	A	70	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	70	0	65	0	0
8	E	70	0	65	0	0
All	All	19830	0	19260	65	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 2.

All (65) 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:606:THR:HG21	2:D:646:LEU:CD2	2.27	0.65
1:A:278:THR:O	1:A:456:ARG:NH2	2.30	0.64
2:F:656:ASN:O	2:F:660:LEU:HD23	1.99	0.63
5:o:1:NAG:O3	5:o:2:NAG:O5	2.16	0.63
1:C:369:LEU:O	1:C:373:THR:OG1	2.16	0.63
3:I:70:SER:OG	3:I:79:SER:OG	2.17	0.63
1:C:258:GLN:OE1	1:C:387:THR:OG1	2.15	0.63
3:G:29:PHE:O	3:G:71:ARG:NH2	2.31	0.62
4:J:3:GLN:N	4:J:3:GLN:OE1	2.31	0.62
1:C:503:ARG:NH1	2:D:653:GLN:OE1	2.32	0.62
3:G:52:GLY:O	3:G:71:ARG:NH1	2.33	0.62
3:K:52:GLY:O	3:K:71:ARG:NH1	2.34	0.60
1:C:502:LYS:NZ	2:D:607:ASN:OD1	2.34	0.59
2:D:522:PHE:O	2:D:540:GLN:NE2	2.35	0.59
3:K:29:PHE:O	3:K:71:ARG:NH2	2.36	0.59
1:E:135:THR:HG22	1:E:135:THR:O	2.04	0.58
1:C:135:THR:O	1:C:135:THR:HG22	2.04	0.58
3:I:52:GLY:O	3:I:71:ARG:NH1	2.37	0.57
1:A:135:THR:HG22	1:A:135:THR:O	2.04	0.57
3:K:70:SER:OG	3:K:79:SER:OG	2.21	0.55
5:T:1:NAG:O3	5:T:2:NAG:O5	2.17	0.55
3:G:105:GLN:O	3:G:105:GLN:NE2	2.40	0.54
1:A:321(A):ASP:OD1	1:A:322:ILE:N	2.41	0.53
1:E:164:GLU:OE2	1:E:308:ARG:NH1	2.41	0.53
3:I:29:PHE:O	3:I:71:ARG:NH2	2.41	0.53
2:B:647:GLU:OE1	2:D:542:ARG:NH1	2.41	0.53
1:E:321(A):ASP:OD1	1:E:322:ILE:N	2.42	0.52
4:J:37:GLN:CB	4:J:47:LEU:HD11	2.39	0.52
3:G:37:VAL:HG22	3:G:47:SER:HA	1.91	0.51
3:K:37:VAL:HG22	3:K:47:SER:HA	1.92	0.51
1:C:385:CYS:HA	1:C:418:CYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:33:VAL:HG12	4:L:51:ALA:HB2	1.93	0.50
1:A:67:ASN:OD1	1:A:69:TRP:N	2.44	0.50
5:Z:1:NAG:N2	5:f:1:NAG:O7	2.45	0.49
3:I:37:VAL:HG22	3:I:47:SER:HA	1.92	0.49
1:C:321(A):ASP:OD1	1:C:322:ILE:N	2.47	0.48
2:D:606:THR:HG21	2:D:646:LEU:HD21	1.94	0.48
2:B:522:PHE:O	2:B:540:GLN:NE2	2.46	0.48
1:E:67:ASN:ND2	1:E:69:TRP:O	2.46	0.48
1:A:50:THR:OG1	1:A:51:THR:N	2.47	0.48
5:Z:2:NAG:O7	5:f:1:NAG:O6	2.32	0.48
1:E:303:THR:OG1	1:E:321(A):ASP:O	2.29	0.47
4:L:82:ASP:O	4:L:86:TYR:OH	2.27	0.47
1:E:256:SER:OG	1:E:259:LEU:O	2.30	0.47
1:A:139:THR:OG1	1:A:141:ASP:OD1	2.32	0.47
1:C:298:ARG:NH1	1:C:300:ASN:O	2.48	0.46
1:E:37:THR:HG1	1:E:499:THR:CB	2.26	0.46
1:E:298:ARG:NH1	1:E:300:ASN:O	2.48	0.45
1:E:159:PHE:HA	5:i:1:NAG:H82	1.97	0.45
4:J:82:ASP:O	4:J:86:TYR:OH	2.28	0.45
1:A:273:ARG:NH2	1:A:287:GLN:OE1	2.50	0.44
1:C:31:ALA:O	1:C:33:ASN:ND2	2.48	0.44
4:L:78:LEU:HD21	4:L:83:PHE:CZ	2.53	0.44
1:E:130:GLN:HG3	5:i:1:NAG:H81	2.00	0.44
4:J:37:GLN:HB3	4:J:47:LEU:HD11	1.99	0.43
4:H:37:GLN:HB3	4:H:47:LEU:HD11	2.01	0.43
1:A:369:LEU:O	1:A:373:THR:OG1	2.34	0.43
5:P:1:NAG:O6	5:P:2:NAG:N2	2.52	0.43
1:A:363:ASN:O	1:A:469:ARG:NH1	2.48	0.43
1:E:499:THR:HG22	1:E:500:ARG:H	1.84	0.42
4:L:25:THR:OG1	4:L:27:GLN:O	2.34	0.41
4:L:14:SER:O	4:L:78:LEU:HD23	2.20	0.41
1:C:385:CYS:HA	1:C:418:CYS:CB	2.51	0.41
4:H:35:TRP:CE3	4:H:73:LEU:HD22	2.56	0.41
1:C:164:GLU:OE2	1:C:308:ARG:NH1	2.55	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	433/481 (90%)	424 (98%)	9 (2%)	0	100	100
1	C	433/481 (90%)	427 (99%)	6 (1%)	0	100	100
1	E	433/481 (90%)	422 (98%)	11 (2%)	0	100	100
2	B	121/153 (79%)	117 (97%)	4 (3%)	0	100	100
2	D	121/153 (79%)	118 (98%)	3 (2%)	0	100	100
2	F	121/153 (79%)	118 (98%)	3 (2%)	0	100	100
3	G	124/237 (52%)	124 (100%)	0	0	100	100
3	I	124/237 (52%)	124 (100%)	0	0	100	100
3	K	124/237 (52%)	124 (100%)	0	0	100	100
4	H	105/214 (49%)	102 (97%)	3 (3%)	0	100	100
4	J	105/214 (49%)	101 (96%)	4 (4%)	0	100	100
4	L	105/214 (49%)	100 (95%)	5 (5%)	0	100	100
All	All	2349/3255 (72%)	2301 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	395/429 (92%)	395 (100%)	0	100	100
1	C	395/429 (92%)	395 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	395/429 (92%)	393 (100%)	2 (0%)	81	83
2	B	107/129 (83%)	107 (100%)	0	100	100
2	D	107/129 (83%)	107 (100%)	0	100	100
2	F	107/129 (83%)	107 (100%)	0	100	100
3	G	99/197 (50%)	99 (100%)	0	100	100
3	I	99/197 (50%)	99 (100%)	0	100	100
3	K	99/197 (50%)	99 (100%)	0	100	100
4	H	92/189 (49%)	92 (100%)	0	100	100
4	J	92/189 (49%)	91 (99%)	1 (1%)	65	76
4	L	92/189 (49%)	92 (100%)	0	100	100
All	All	2079/2832 (73%)	2076 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	499	THR
1	E	501	CYS
4	J	74	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	94	ASN
1	A	302	ASN
1	A	422	GLN
1	A	478	ASN
2	B	577	GLN
1	C	80	ASN
1	C	99	ASN
1	C	203	GLN
1	C	478	ASN
1	E	425	ASN
1	E	462	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

72 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	0.29	0	17,19,21	0.58	0
5	NAG	M	2	5	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	N	1	5,1	14,14,15	0.35	0	17,19,21	0.55	0
5	NAG	N	2	5	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	O	1	1,6	14,14,15	0.22	0	17,19,21	0.41	0
6	NAG	O	2	6	14,14,15	0.21	0	17,19,21	0.48	0
6	BMA	O	3	6	11,11,12	0.56	0	15,15,17	0.70	0
5	NAG	P	1	5,1	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	P	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	Q	1	5,1	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	Q	2	5	14,14,15	0.23	0	17,19,21	0.43	0
7	NAG	R	1	1,7	14,14,15	0.26	0	17,19,21	0.49	0
7	NAG	R	2	7	14,14,15	0.22	0	17,19,21	0.42	0
7	BMA	R	3	7	11,11,12	0.55	0	15,15,17	0.71	0
7	MAN	R	4	7	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
7	MAN	R	5	7	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
5	NAG	S	1	5,1	14,14,15	0.22	0	17,19,21	0.46	0
5	NAG	S	2	5	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	T	1	5,1	14,14,15	0.21	0	17,19,21	0.47	0
5	NAG	T	2	5	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	U	1	5,1	14,14,15	0.31	0	17,19,21	0.52	0
5	NAG	U	2	5	14,14,15	0.24	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	V	1	5,1	14,14,15	0.30	0	17,19,21	0.57	0
5	NAG	V	2	5	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	W	1	5,1	14,14,15	0.32	0	17,19,21	0.53	0
5	NAG	W	2	5	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	X	1	1,6	14,14,15	0.25	0	17,19,21	0.42	0
6	NAG	X	2	6	14,14,15	0.24	0	17,19,21	0.53	0
6	BMA	X	3	6	11,11,12	0.56	0	15,15,17	0.67	0
5	NAG	Y	1	5,1	14,14,15	0.26	0	17,19,21	0.47	0
5	NAG	Y	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	Z	1	5,1	14,14,15	0.21	0	17,19,21	0.53	0
5	NAG	Z	2	5	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	a	1	5,1	14,14,15	0.31	0	17,19,21	0.54	0
5	NAG	a	2	5	14,14,15	0.24	0	17,19,21	0.43	0
7	NAG	b	1	1,7	14,14,15	0.25	0	17,19,21	0.48	0
7	NAG	b	2	7	14,14,15	0.21	0	17,19,21	0.42	0
7	BMA	b	3	7	11,11,12	0.56	0	15,15,17	0.71	0
7	MAN	b	4	7	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
7	MAN	b	5	7	11,11,12	0.62	0	15,15,17	0.93	2 (13%)
5	NAG	c	1	5,1	14,14,15	0.31	0	17,19,21	0.57	0
5	NAG	c	2	5	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	d	1	5,1	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	d	2	5	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	e	1	5,1	14,14,15	0.25	0	17,19,21	0.49	0
5	NAG	e	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	f	1	5,1	14,14,15	0.30	0	17,19,21	0.49	0
5	NAG	f	2	5	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	g	1	5,1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	g	2	5	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	h	1	5,1	14,14,15	0.29	0	17,19,21	0.57	0
5	NAG	h	2	5	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	i	1	5,1	14,14,15	0.33	0	17,19,21	0.53	0
5	NAG	i	2	5	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	j	1	1,6	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	j	2	6	14,14,15	0.20	0	17,19,21	0.48	0
6	BMA	j	3	6	11,11,12	0.57	0	15,15,17	0.67	0
5	NAG	k	1	5,1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	k	2	5	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	l	1	5,1	14,14,15	0.27	0	17,19,21	0.51	0
5	NAG	l	2	5	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	m	1	1,7	14,14,15	0.23	0	17,19,21	0.49	0
7	NAG	m	2	7	14,14,15	0.20	0	17,19,21	0.43	0
7	BMA	m	3	7	11,11,12	0.56	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	m	4	7	11,11,12	0.60	0	15,15,17	0.96	2 (13%)
7	MAN	m	5	7	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
5	NAG	n	1	5,1	14,14,15	0.21	0	17,19,21	0.47	0
5	NAG	n	2	5	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	o	1	5,1	14,14,15	0.23	0	17,19,21	0.48	0
5	NAG	o	2	5	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	p	1	5,1	14,14,15	0.28	0	17,19,21	0.49	0
5	NAG	p	2	5	14,14,15	0.23	0	17,19,21	0.44	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	W	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	3/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	BMA	X	3	6	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Z	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	NAG	a	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
7	NAG	b	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
7	BMA	b	3	7	-	0/2/19/22	0/1/1/1
7	MAN	b	4	7	-	0/2/19/22	0/1/1/1
7	MAN	b	5	7	-	0/2/19/22	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	NAG	d	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1
5	NAG	e	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	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	-	0/6/23/26	0/1/1/1
5	NAG	i	2	5	-	2/6/23/26	0/1/1/1
6	NAG	j	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	j	2	6	-	2/6/23/26	0/1/1/1
6	BMA	j	3	6	-	1/2/19/22	0/1/1/1
5	NAG	k	1	5,1	-	0/6/23/26	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	-	2/6/23/26	0/1/1/1
7	NAG	m	1	1,7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	m	2	7	-	0/6/23/26	0/1/1/1
7	BMA	m	3	7	-	0/2/19/22	0/1/1/1
7	MAN	m	4	7	-	0/2/19/22	0/1/1/1
7	MAN	m	5	7	-	0/2/19/22	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	-	1/6/23/26	0/1/1/1
5	NAG	o	2	5	-	2/6/23/26	0/1/1/1
5	NAG	p	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	p	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	4	MAN	C1-O5-C5	2.36	115.35	112.19
7	b	4	MAN	C1-O5-C5	2.36	115.35	112.19
7	m	4	MAN	C1-O5-C5	2.35	115.34	112.19
7	R	4	MAN	O2-C2-C3	-2.25	105.50	110.15
7	m	4	MAN	O2-C2-C3	-2.23	105.53	110.15
7	b	4	MAN	O2-C2-C3	-2.23	105.54	110.15
7	m	5	MAN	C1-O5-C5	2.20	115.14	112.19
7	b	5	MAN	C1-O5-C5	2.20	115.13	112.19
7	R	5	MAN	C1-O5-C5	2.19	115.12	112.19
7	m	5	MAN	O2-C2-C3	-2.15	105.70	110.15
7	R	5	MAN	O2-C2-C3	-2.15	105.71	110.15
7	b	5	MAN	O2-C2-C3	-2.14	105.71	110.15

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	U	2	NAG	C4-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	n	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	p	1	NAG	O5-C5-C6-O6
6	j	1	NAG	O5-C5-C6-O6
6	X	1	NAG	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	p	1	NAG	C4-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
6	j	1	NAG	C4-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
5	n	2	NAG	C4-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
7	m	1	NAG	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
6	j	2	NAG	C4-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
5	l	2	NAG	C4-C5-C6-O6
5	o	2	NAG	O5-C5-C6-O6
7	m	1	NAG	C4-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	l	2	NAG	O5-C5-C6-O6

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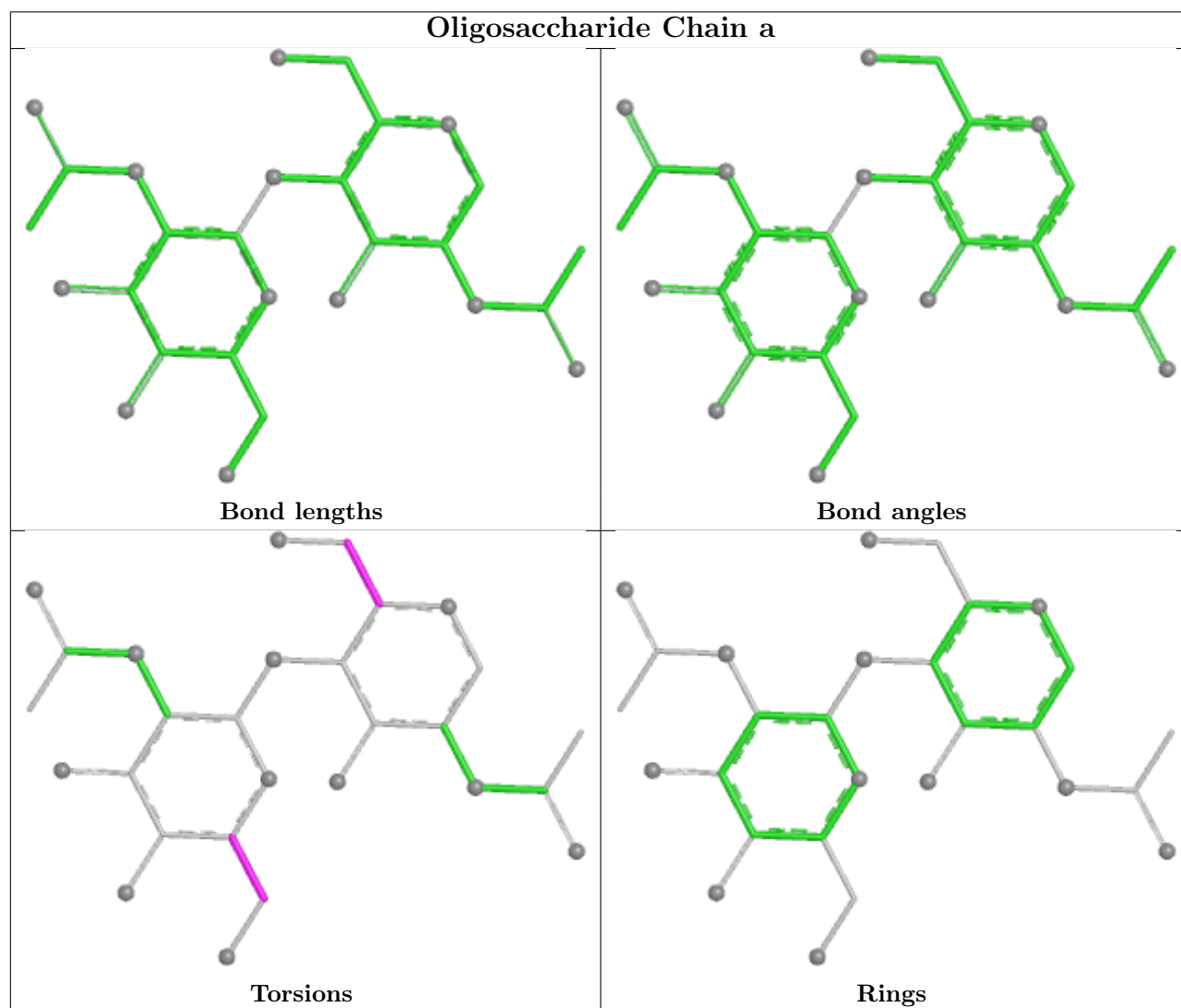
Mol	Chain	Res	Type	Atoms
5	e	2	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
6	X	2	NAG	C4-C5-C6-O6
6	j	3	BMA	O5-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
5	o	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
5	W	2	NAG	C1-C2-N2-C7
5	o	1	NAG	C1-C2-N2-C7
5	i	2	NAG	C4-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
6	O	3	BMA	O5-C5-C6-O6
6	O	3	BMA	C4-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6

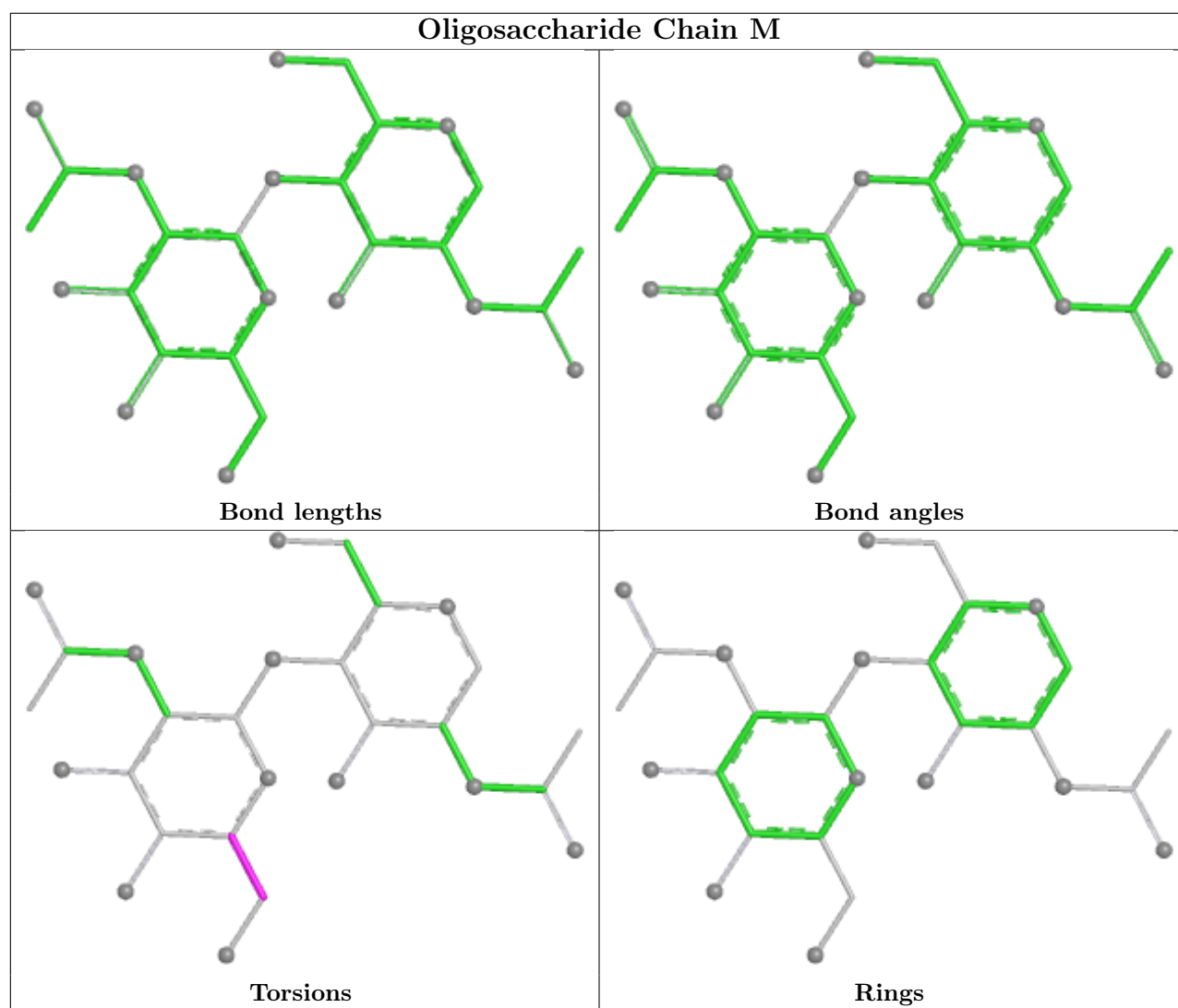
There are no ring outliers.

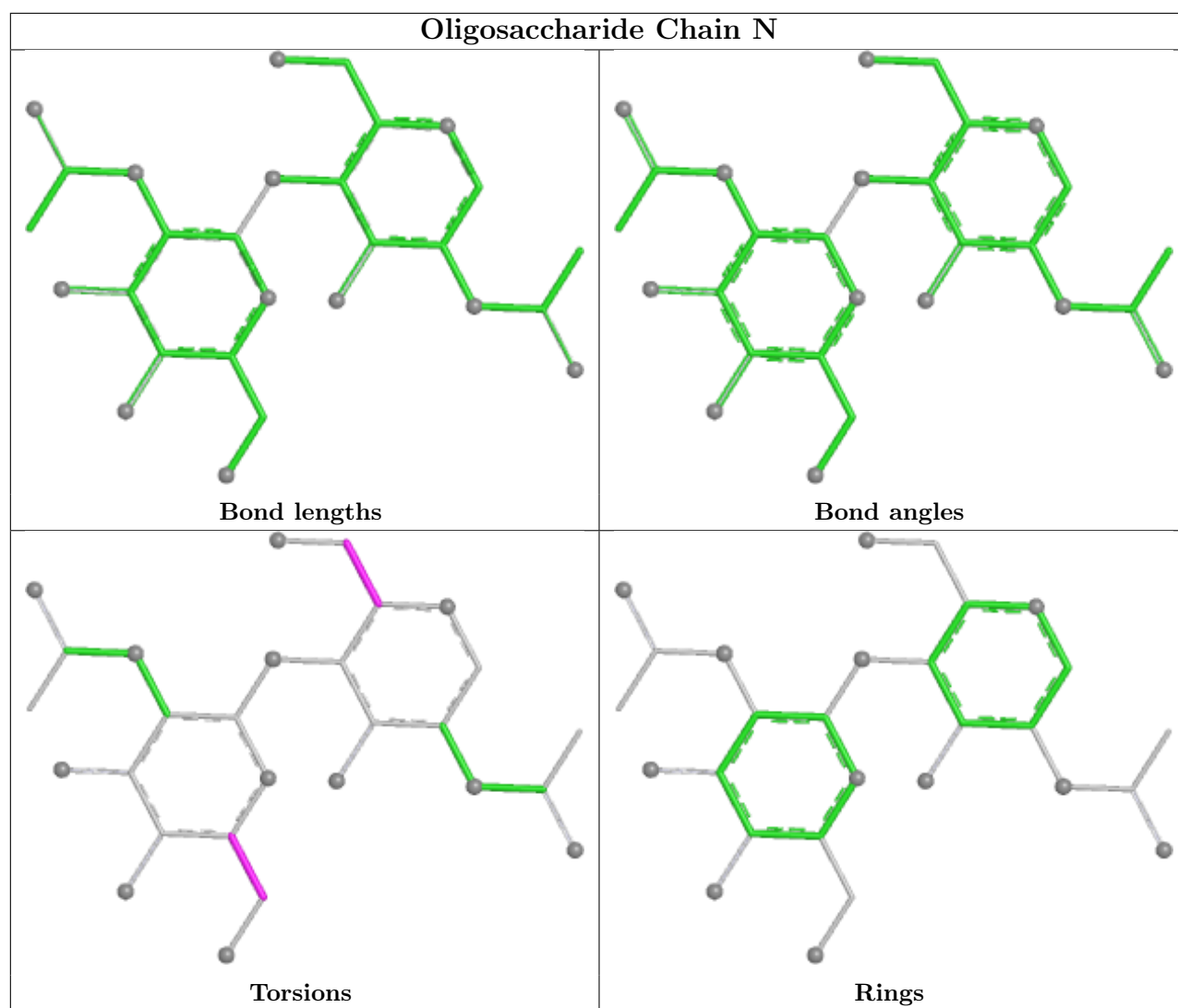
10 monomers are involved in 7 short contacts:

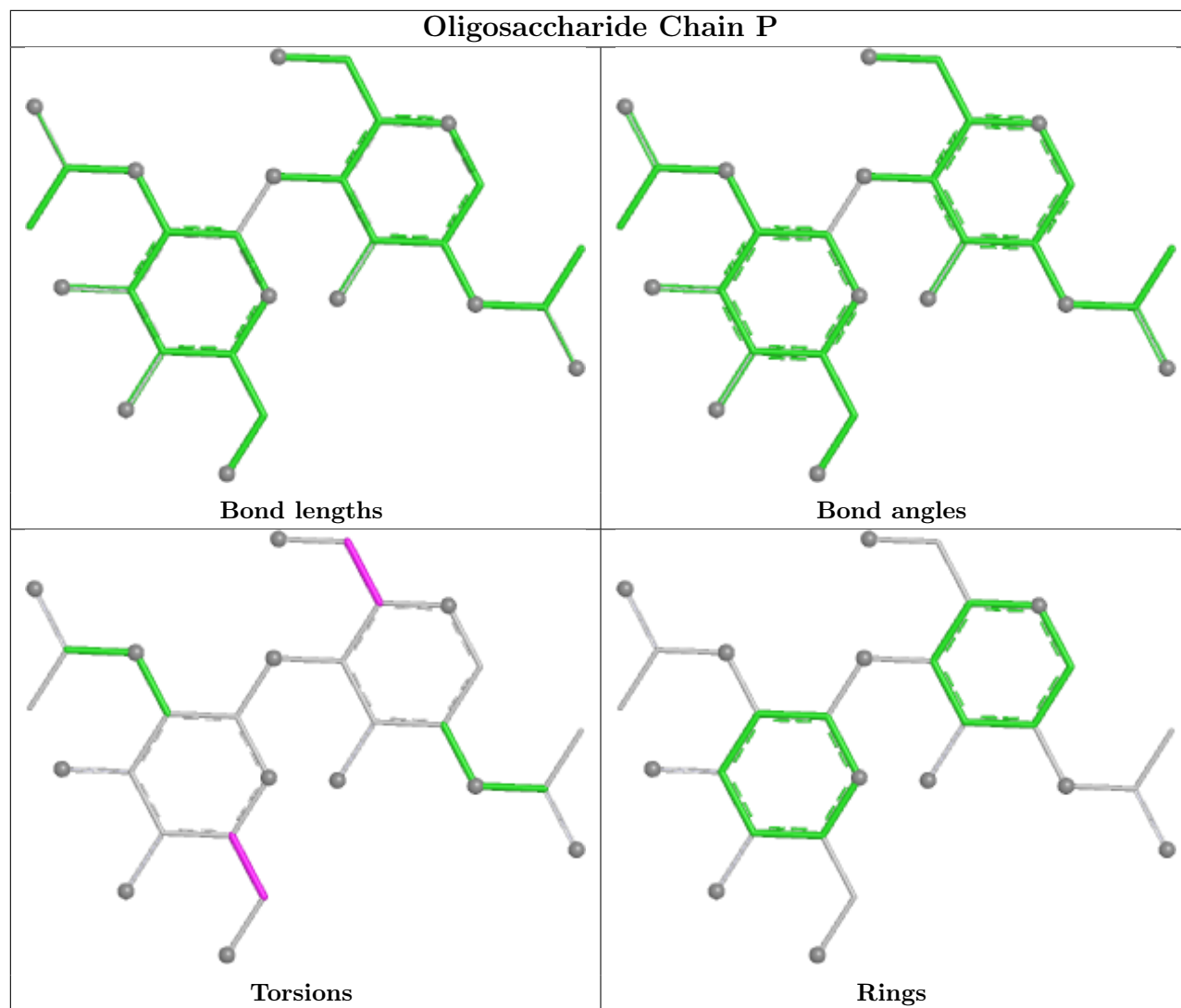
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	o	2	NAG	1	0
5	T	2	NAG	1	0
5	Z	2	NAG	1	0
5	i	1	NAG	2	0
5	T	1	NAG	1	0
5	Z	1	NAG	1	0
5	P	1	NAG	1	0
5	f	1	NAG	2	0
5	P	2	NAG	1	0
5	o	1	NAG	1	0

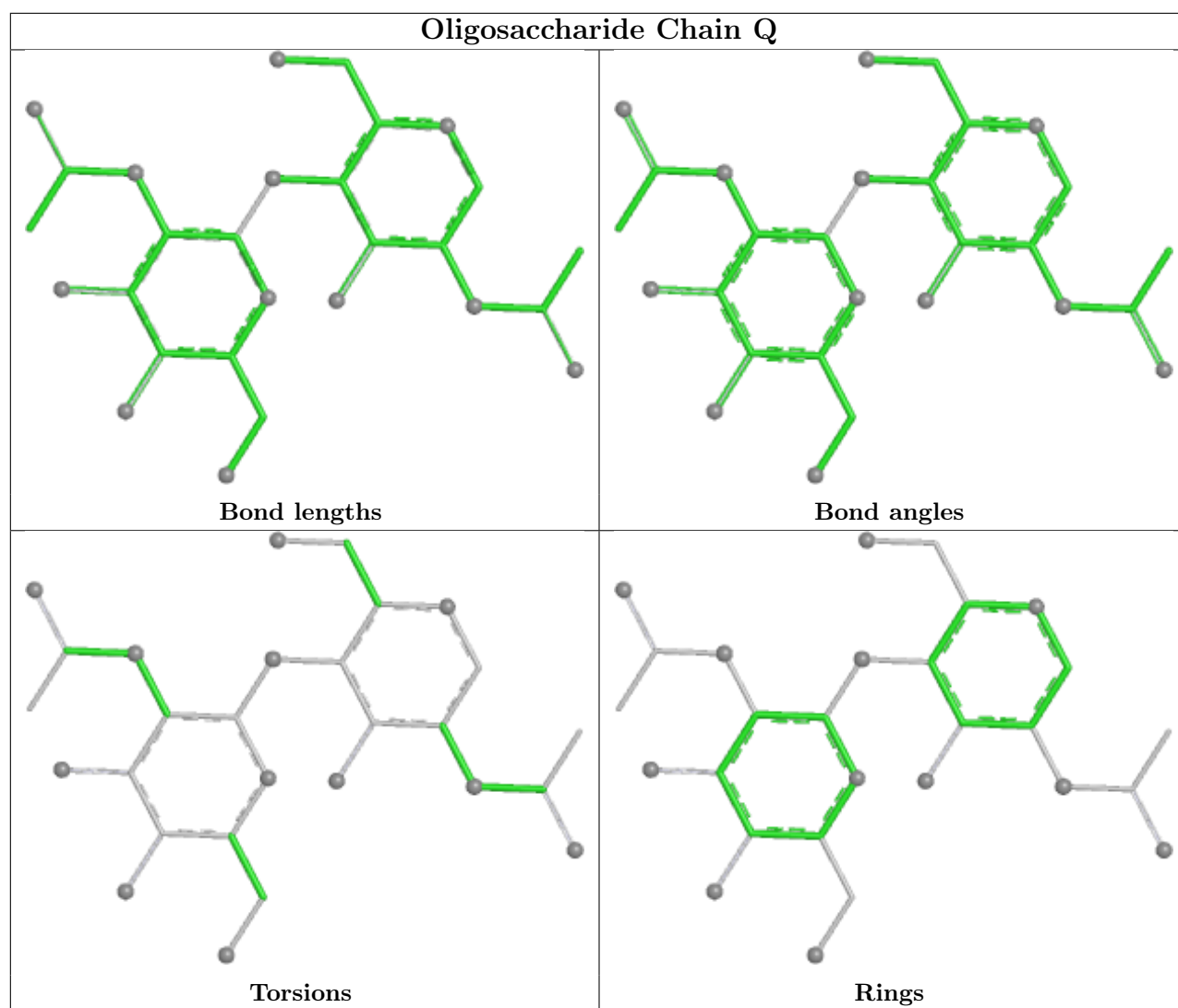
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

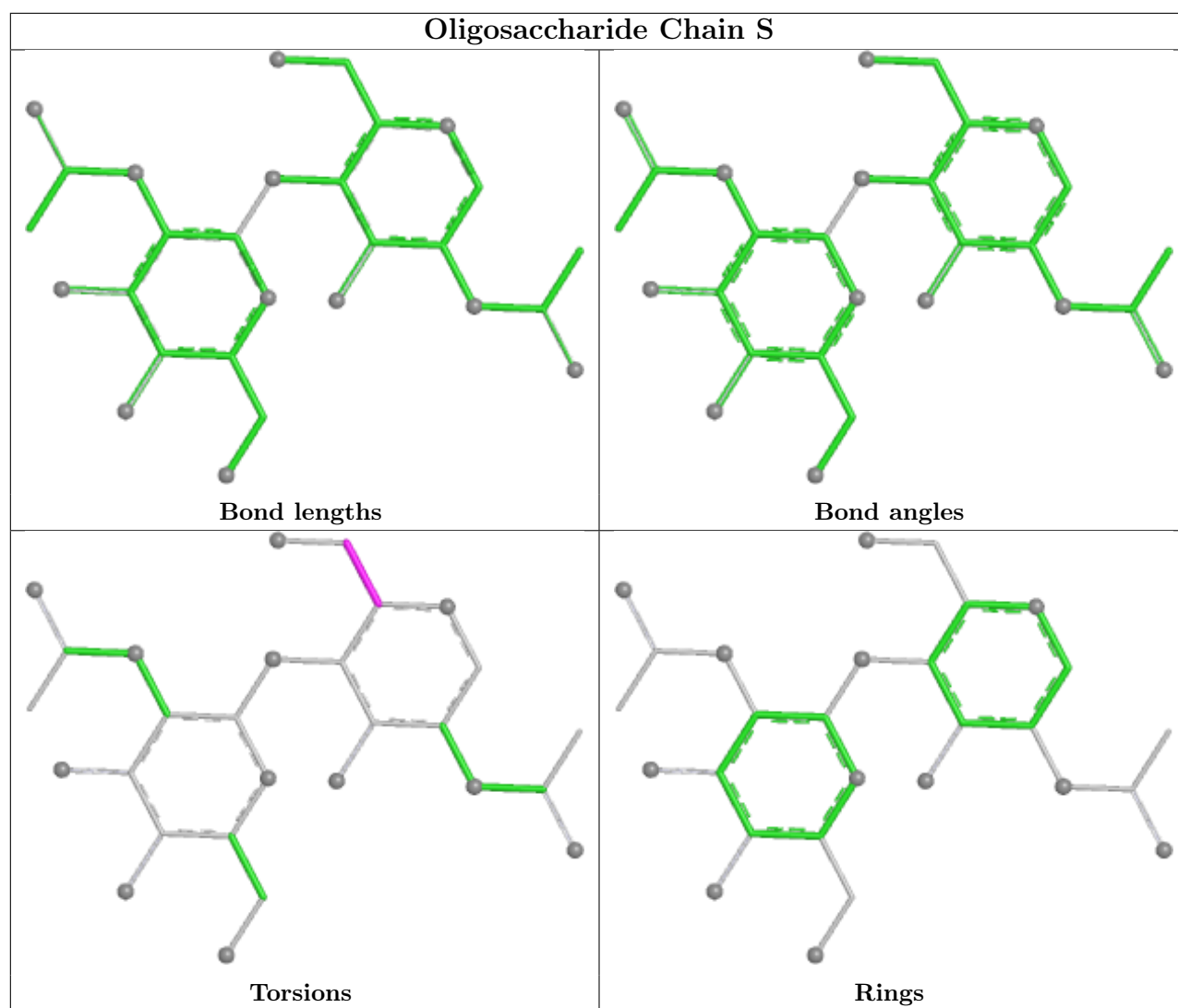


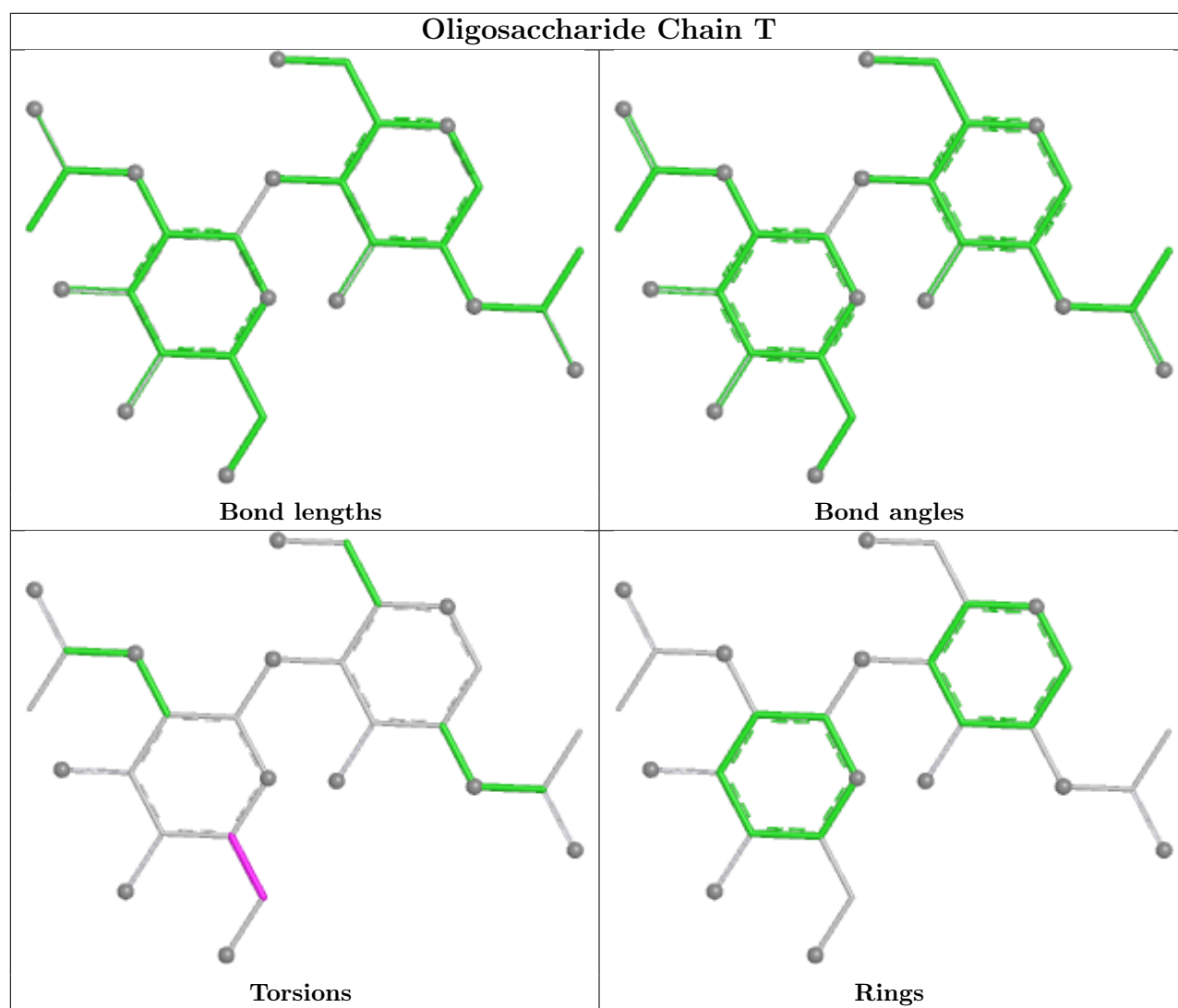


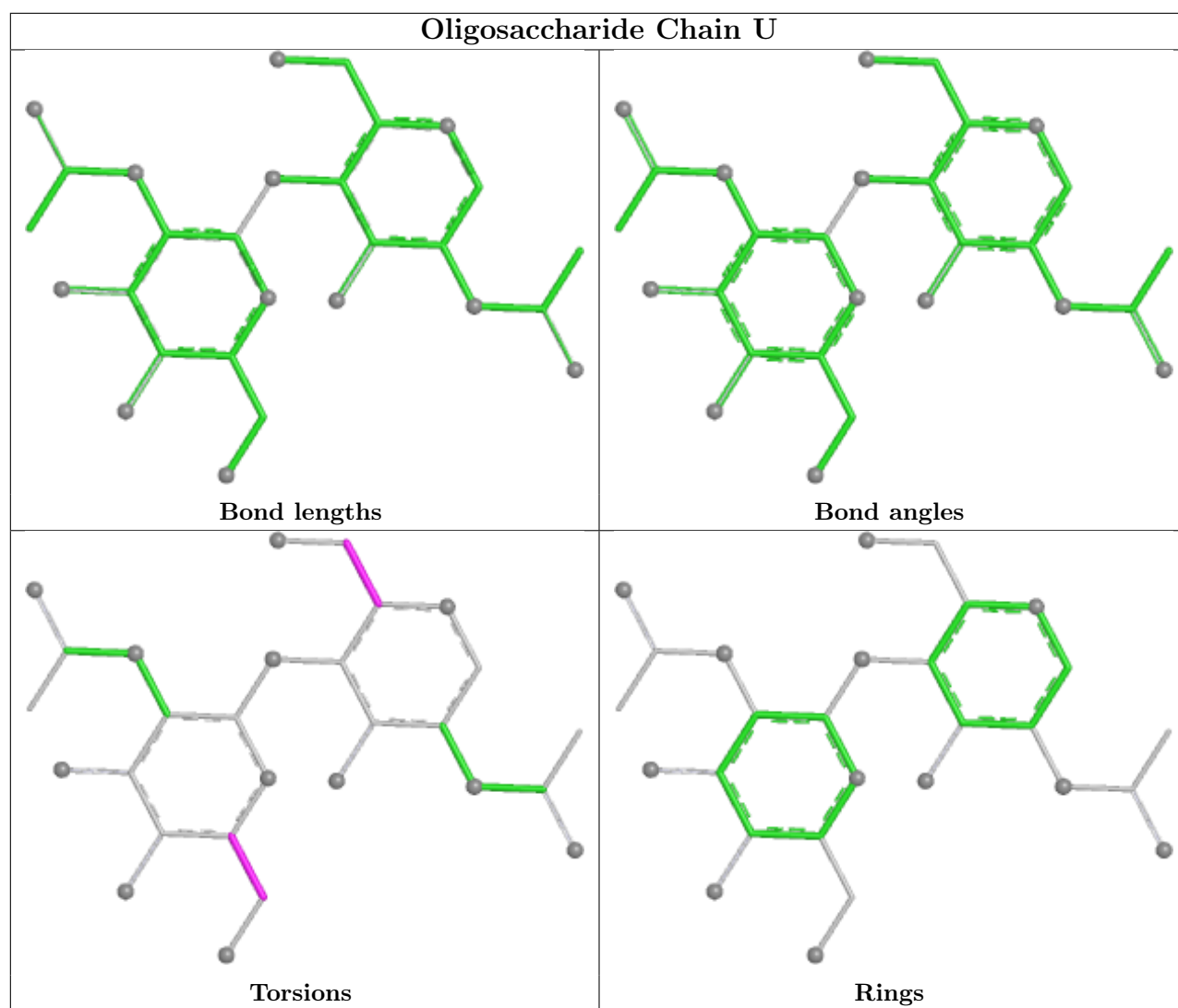


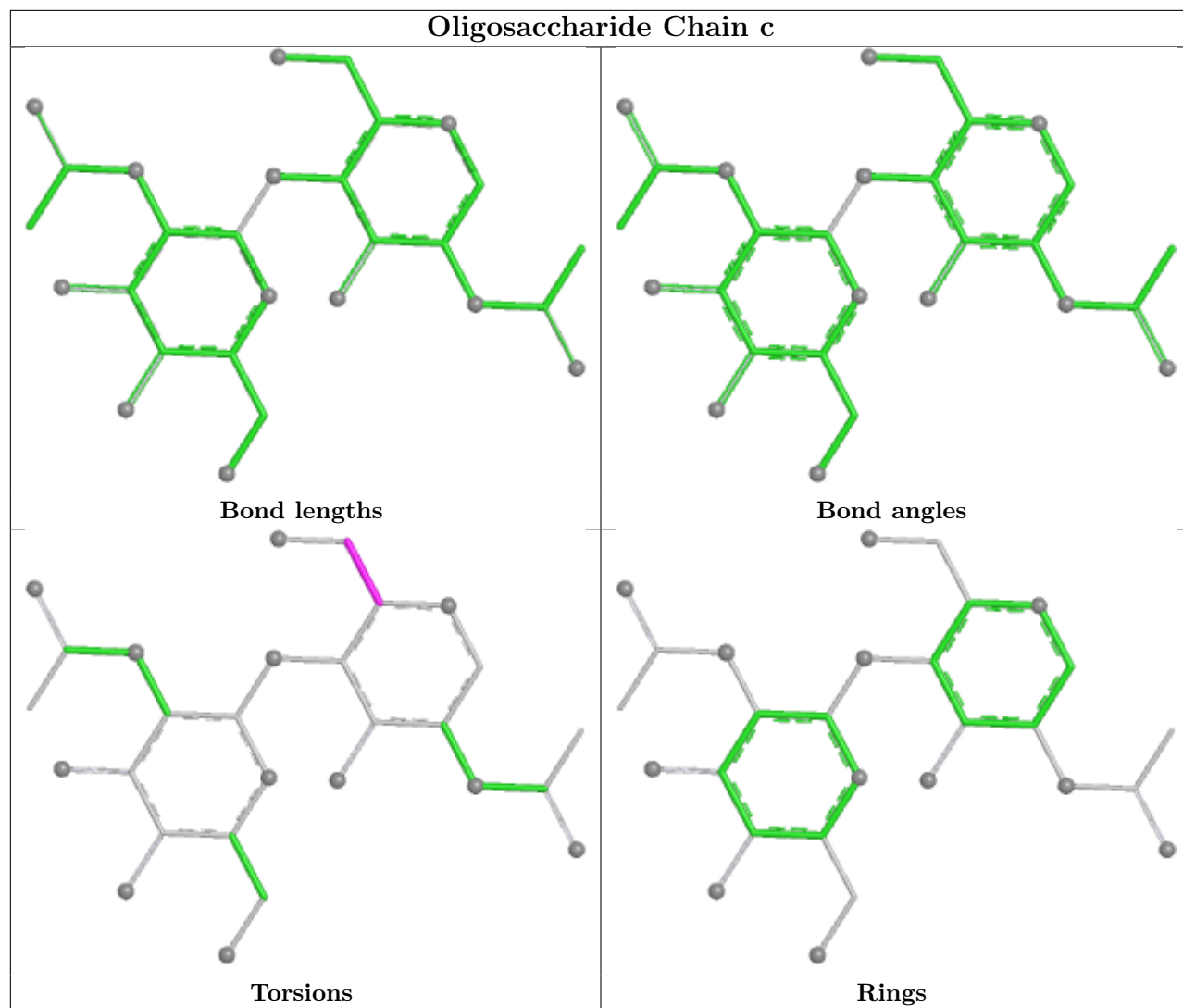


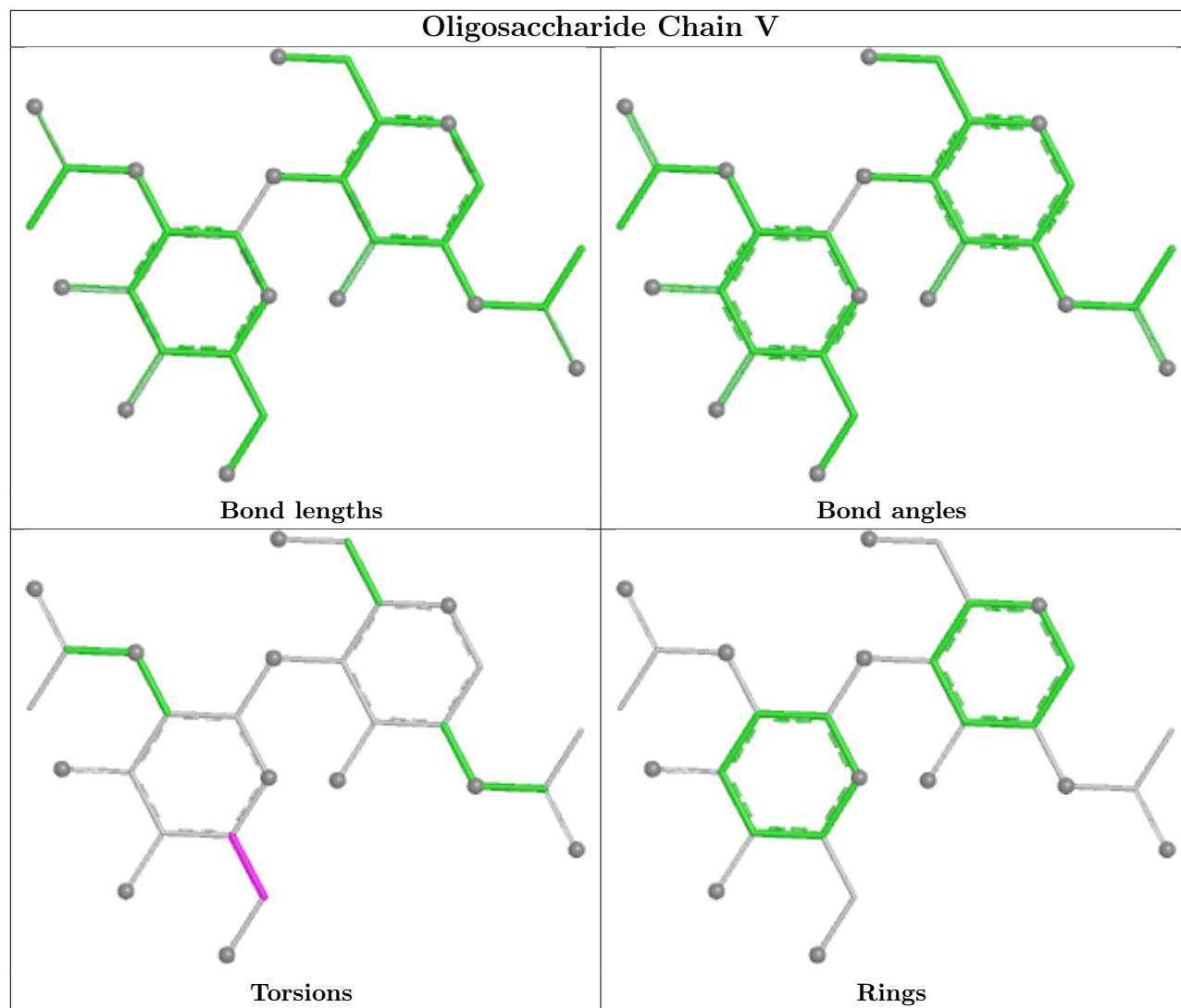


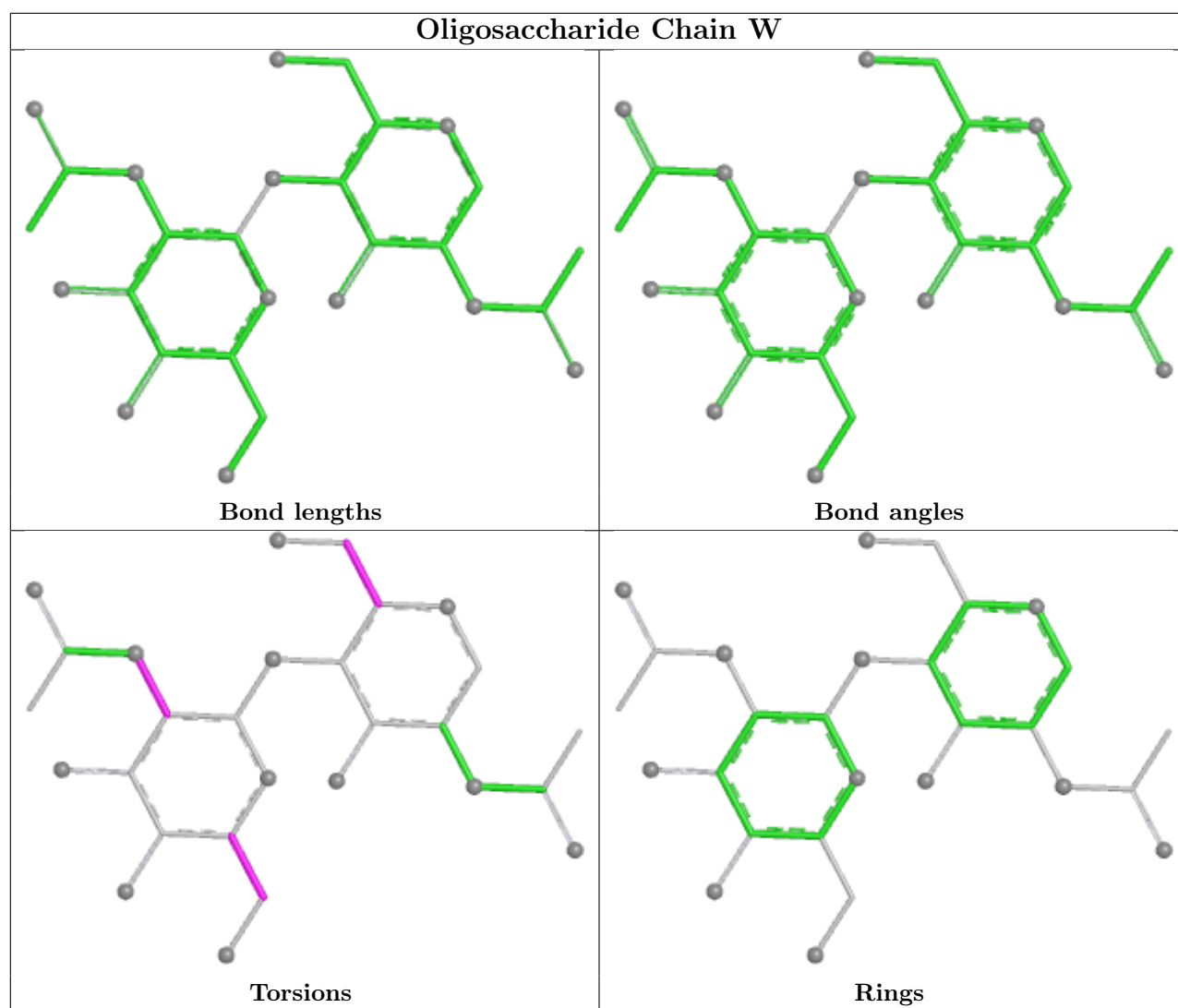


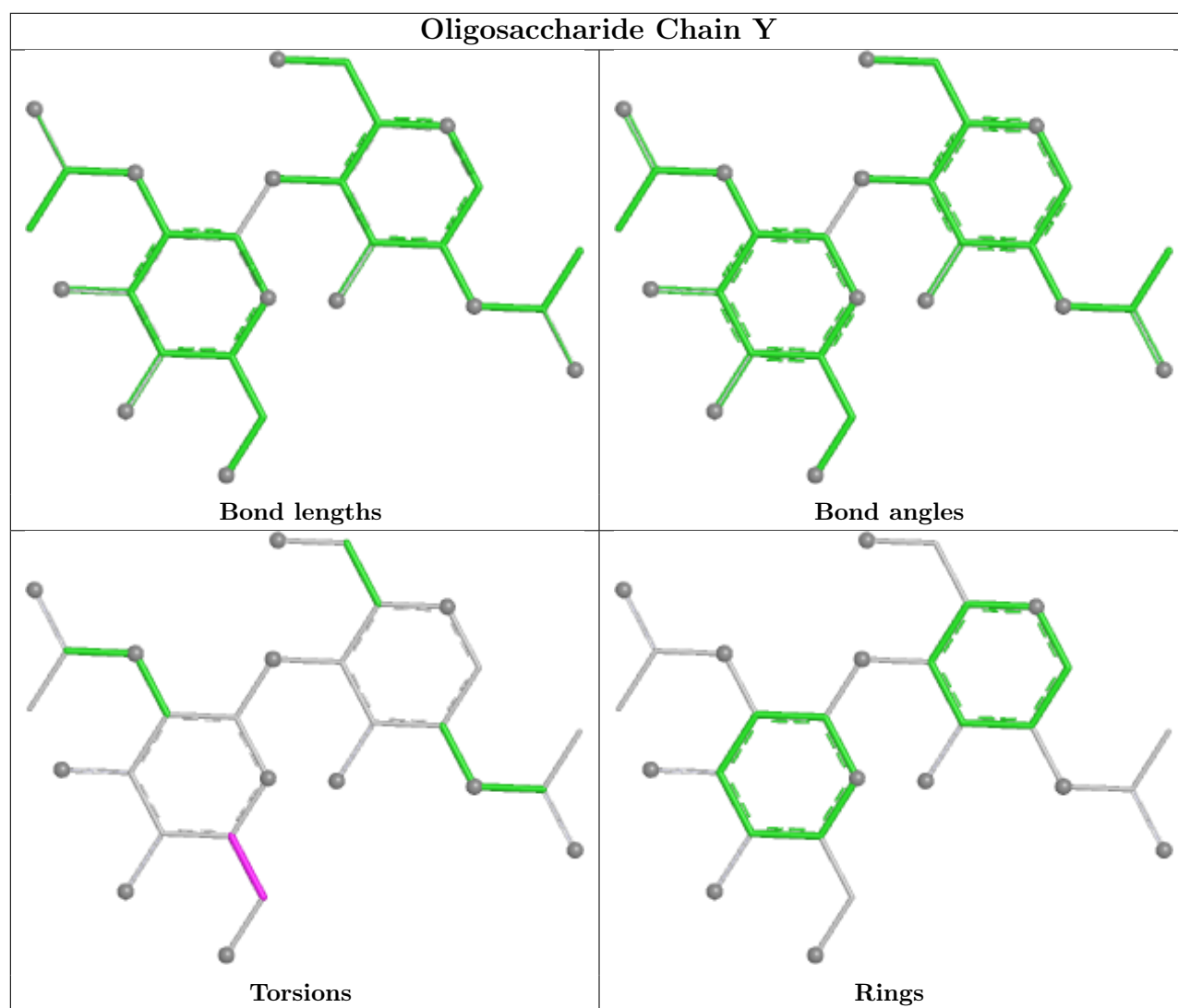


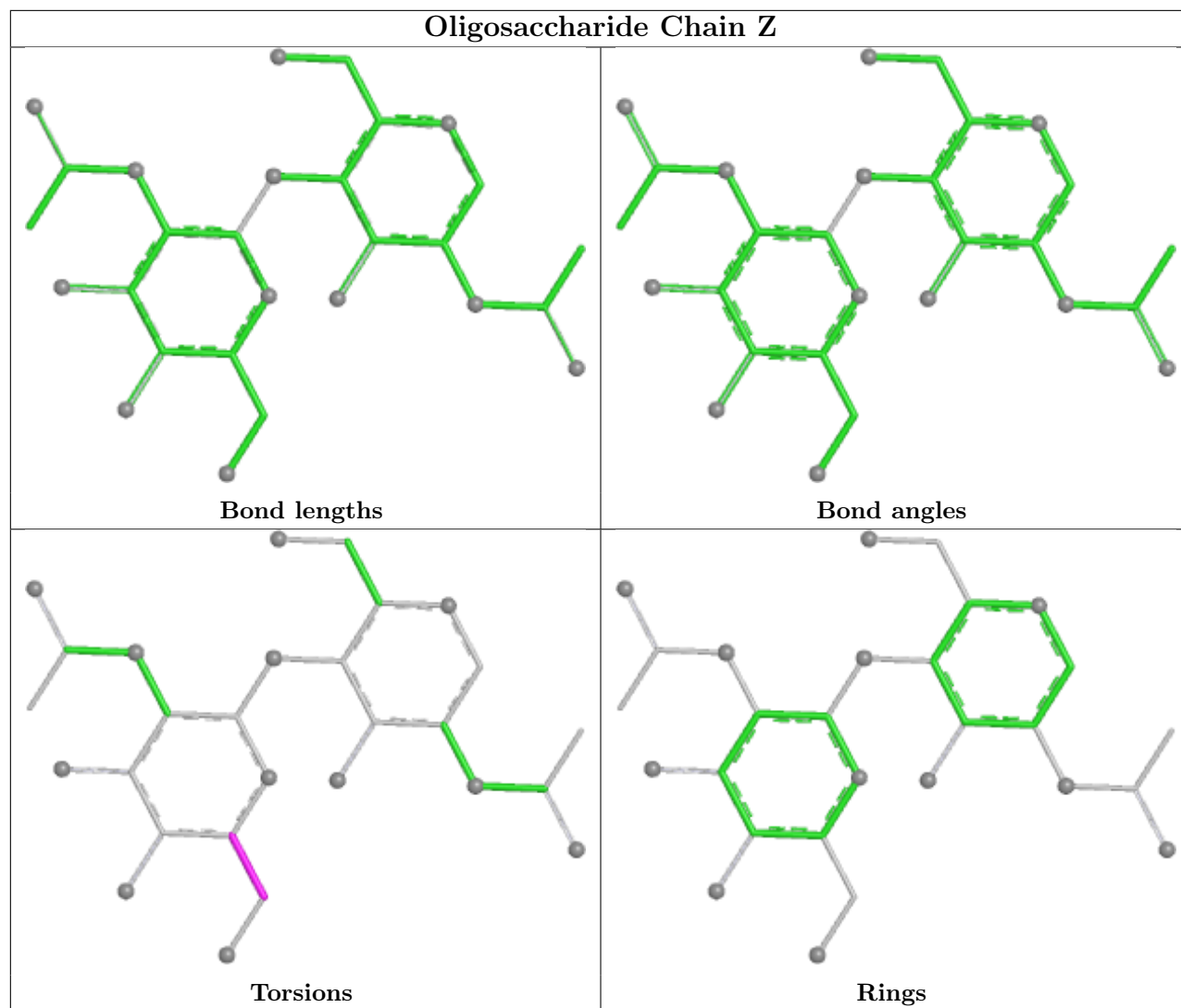


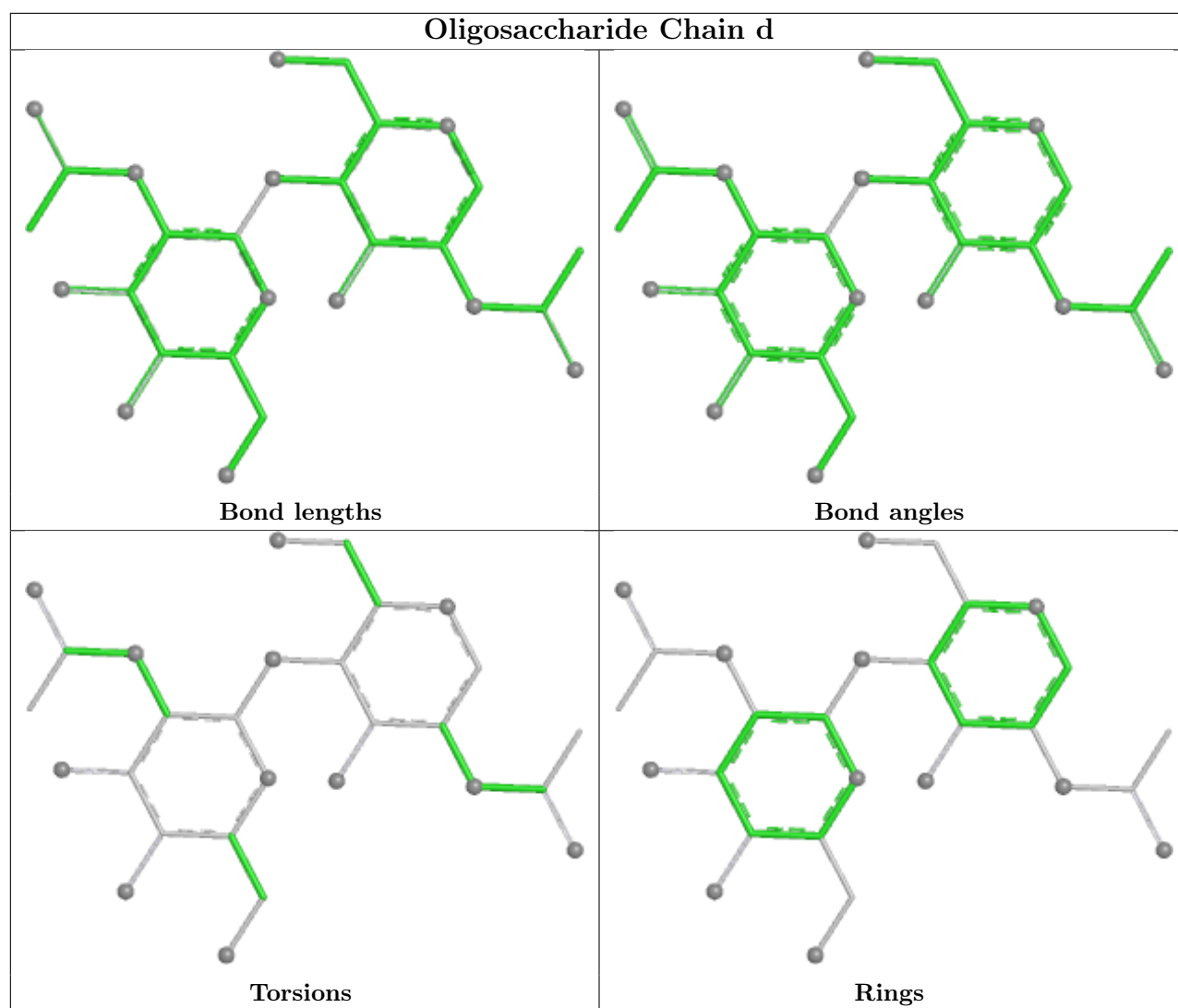


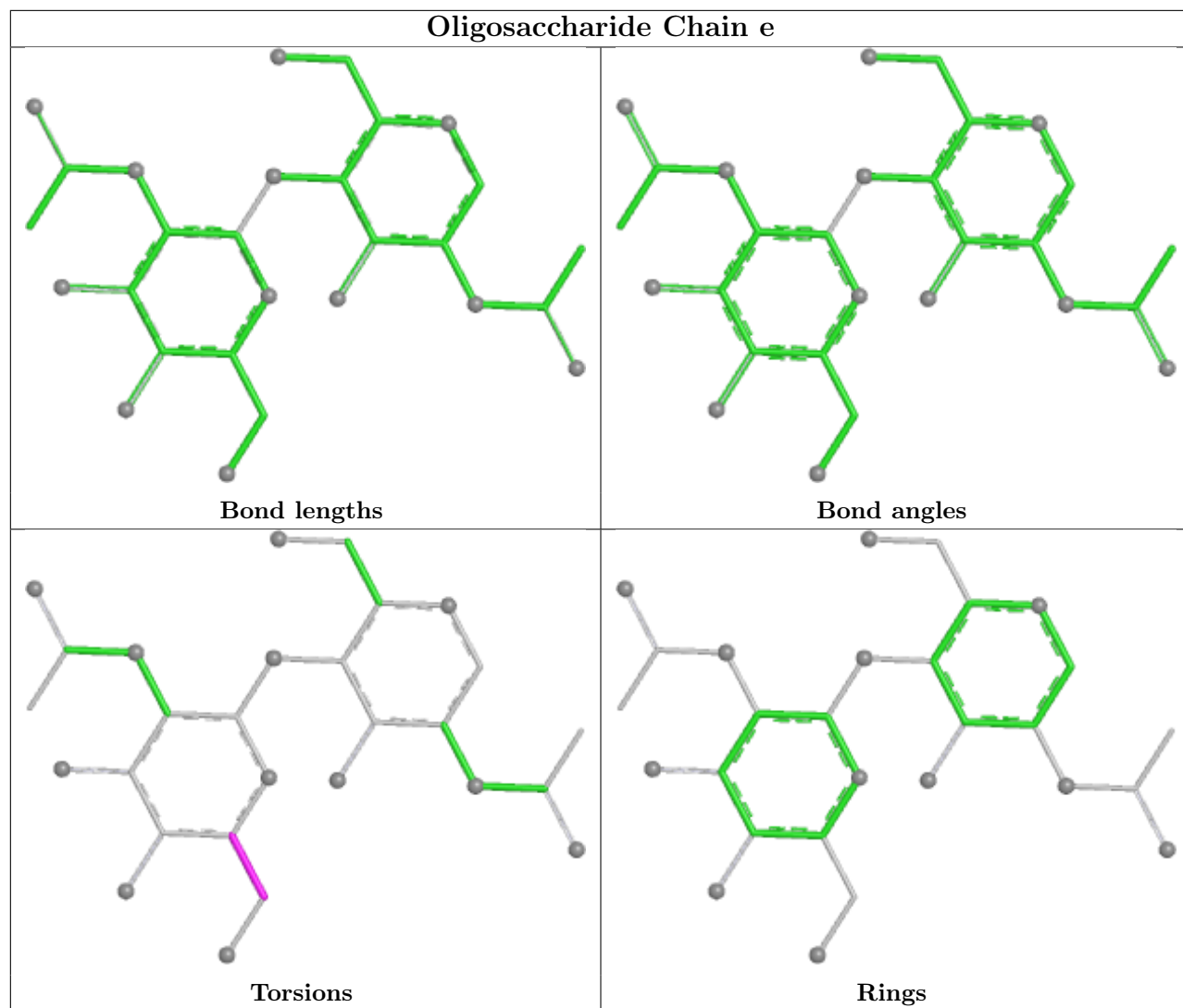


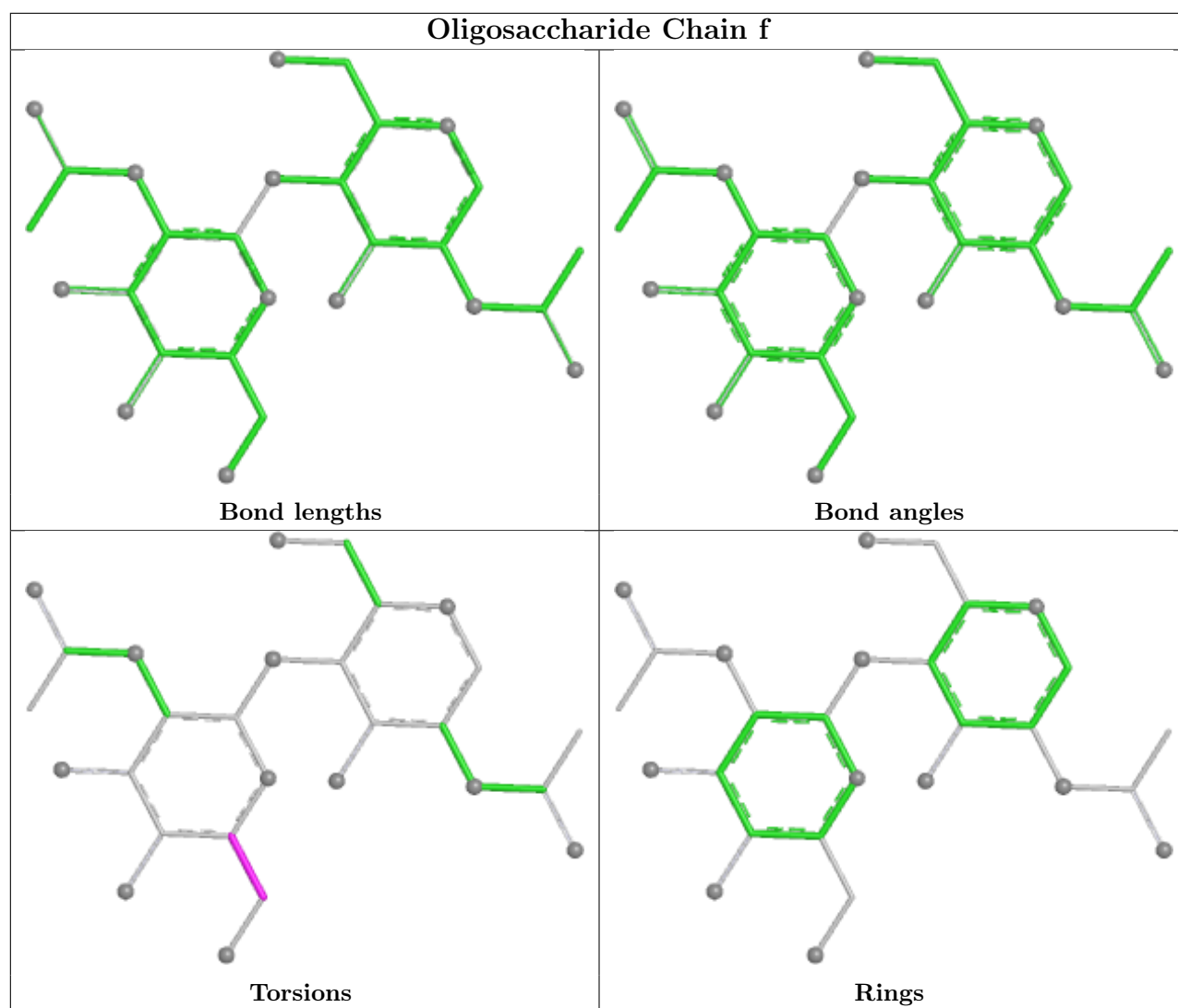


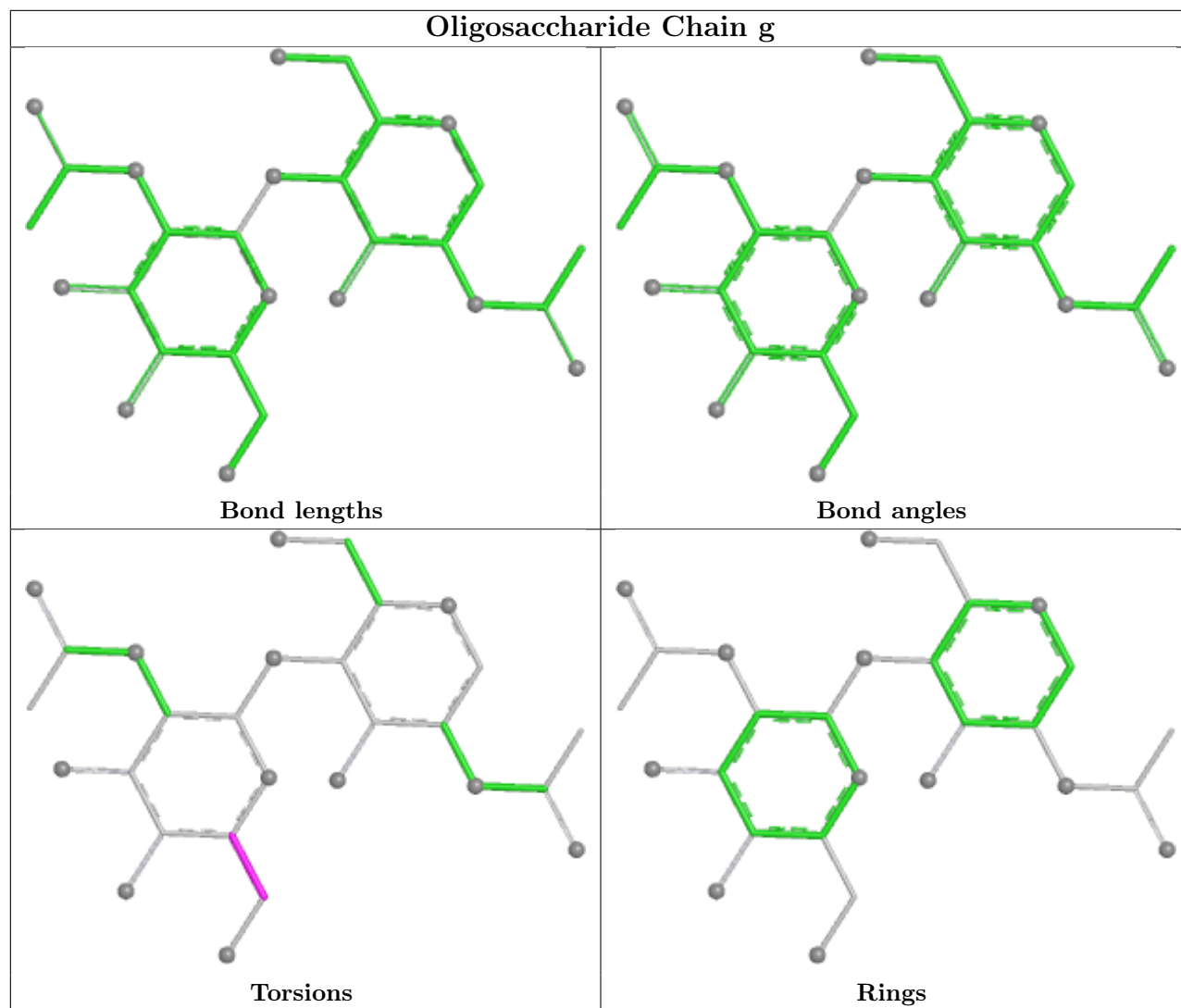


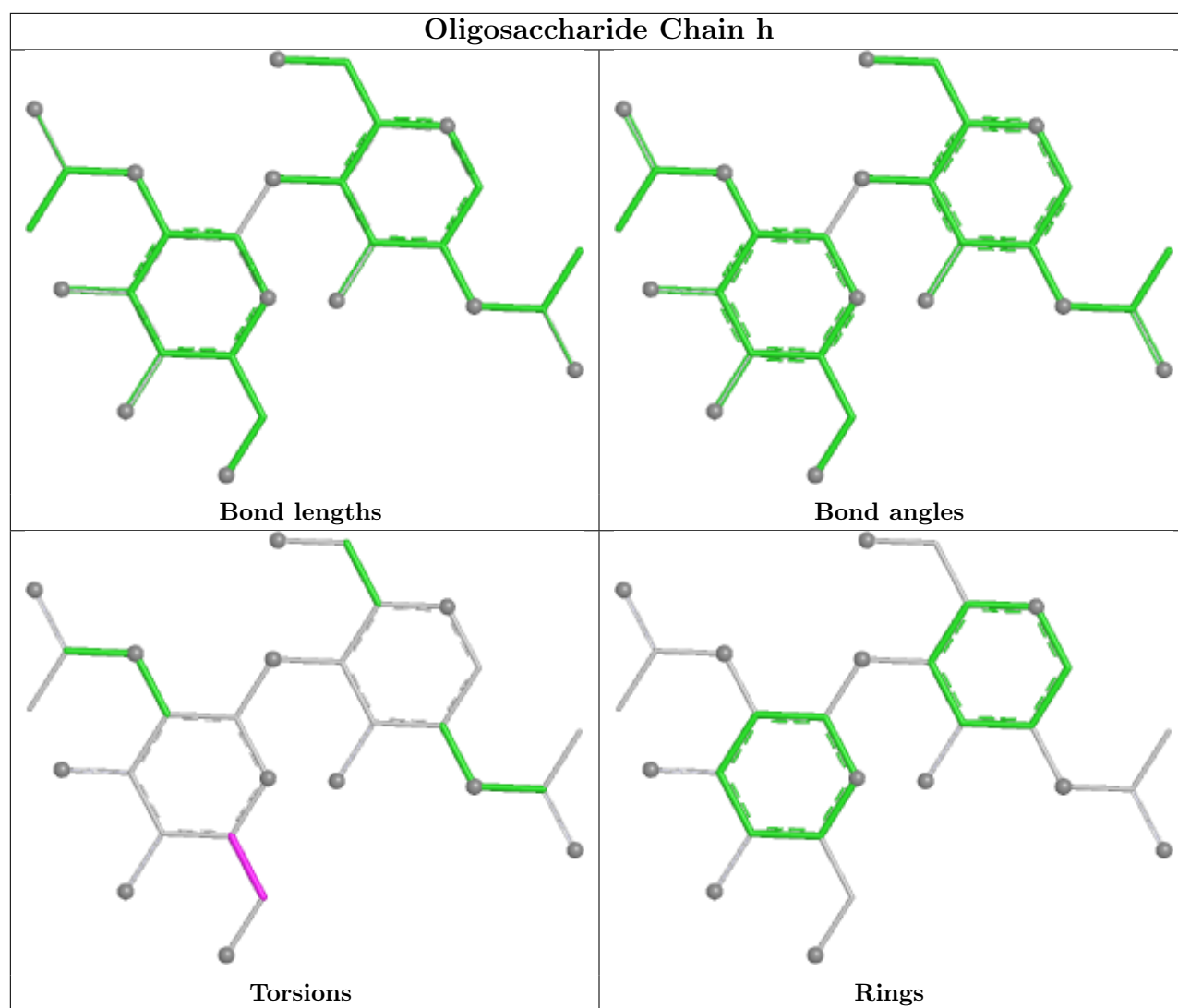


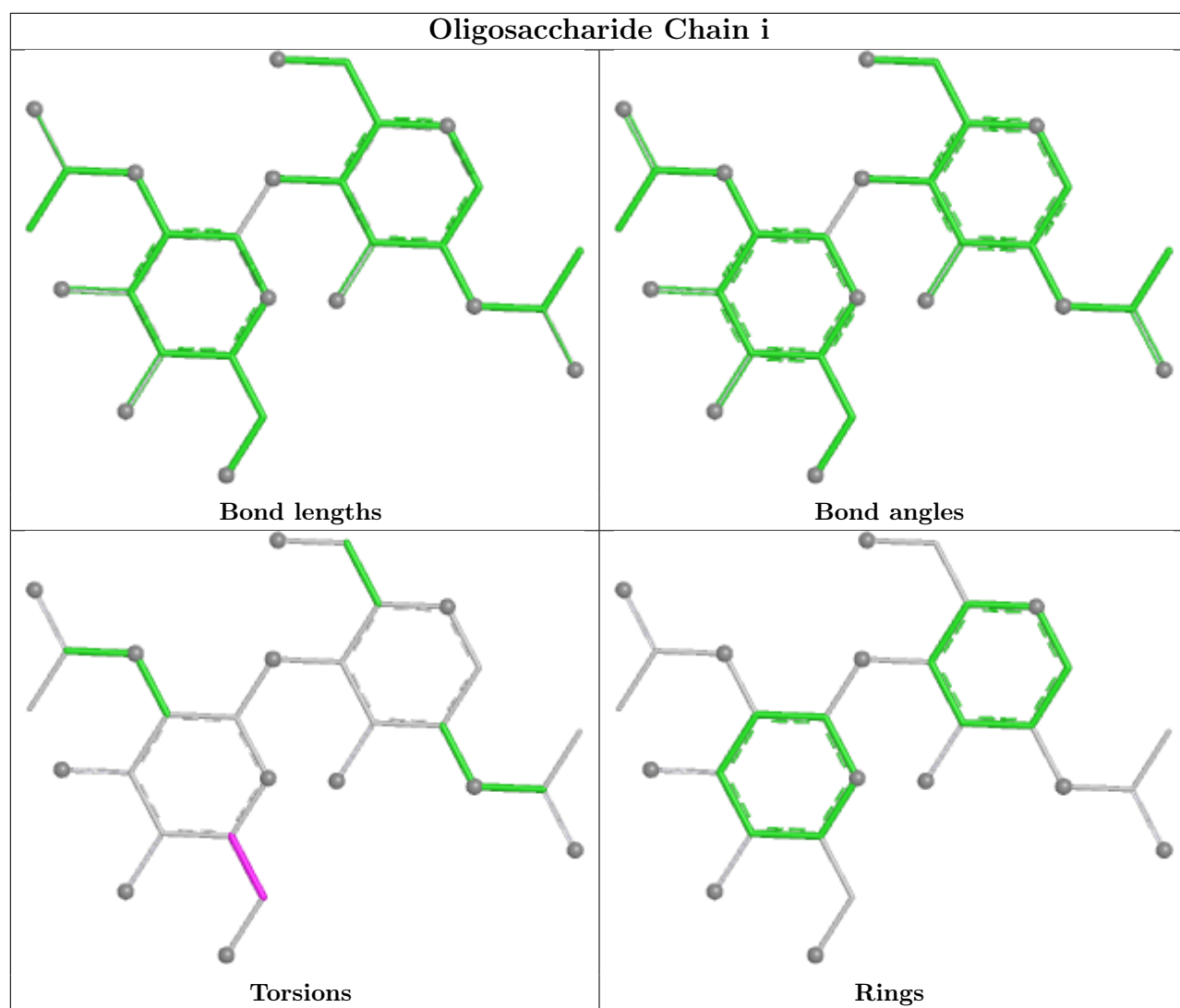


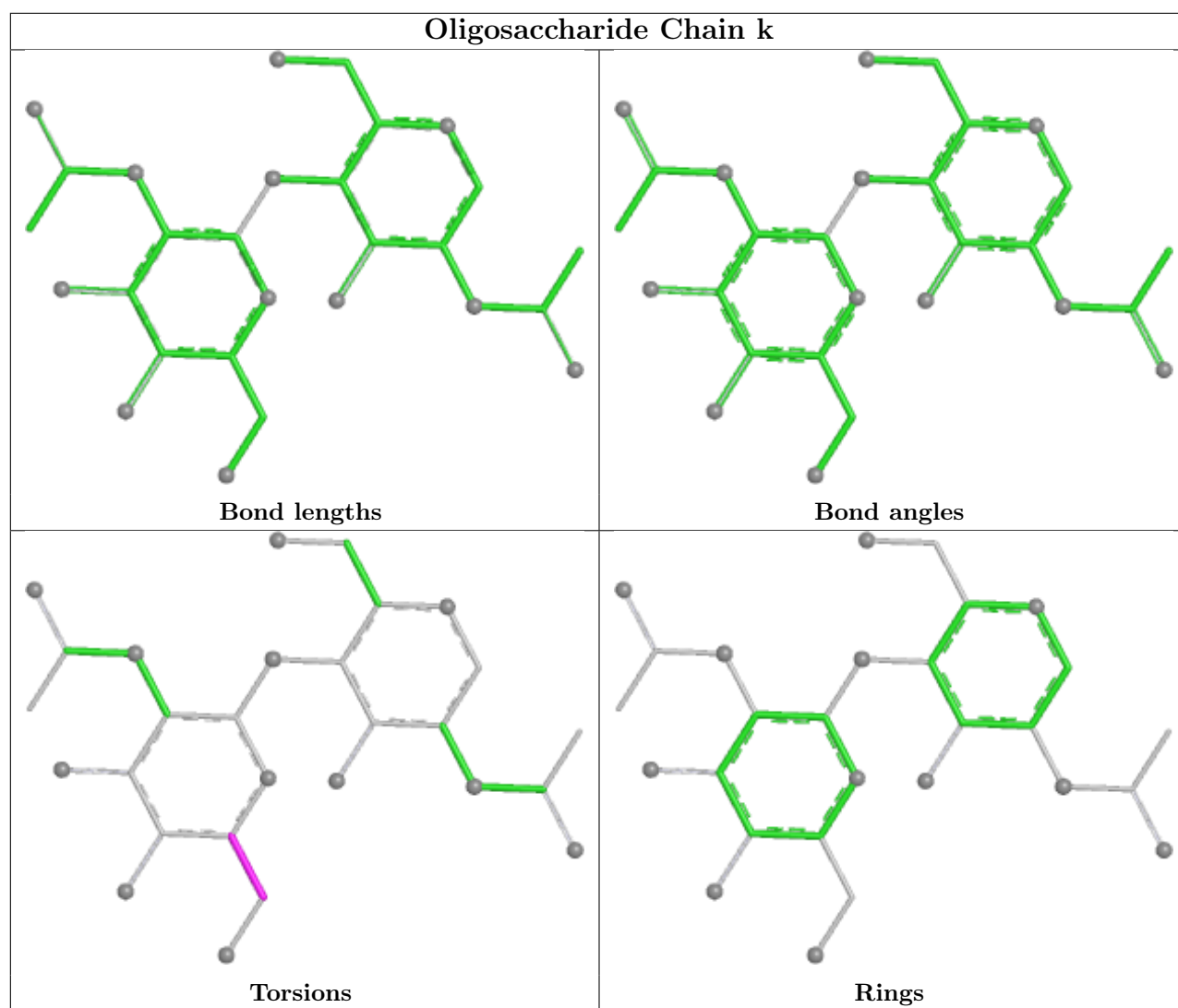


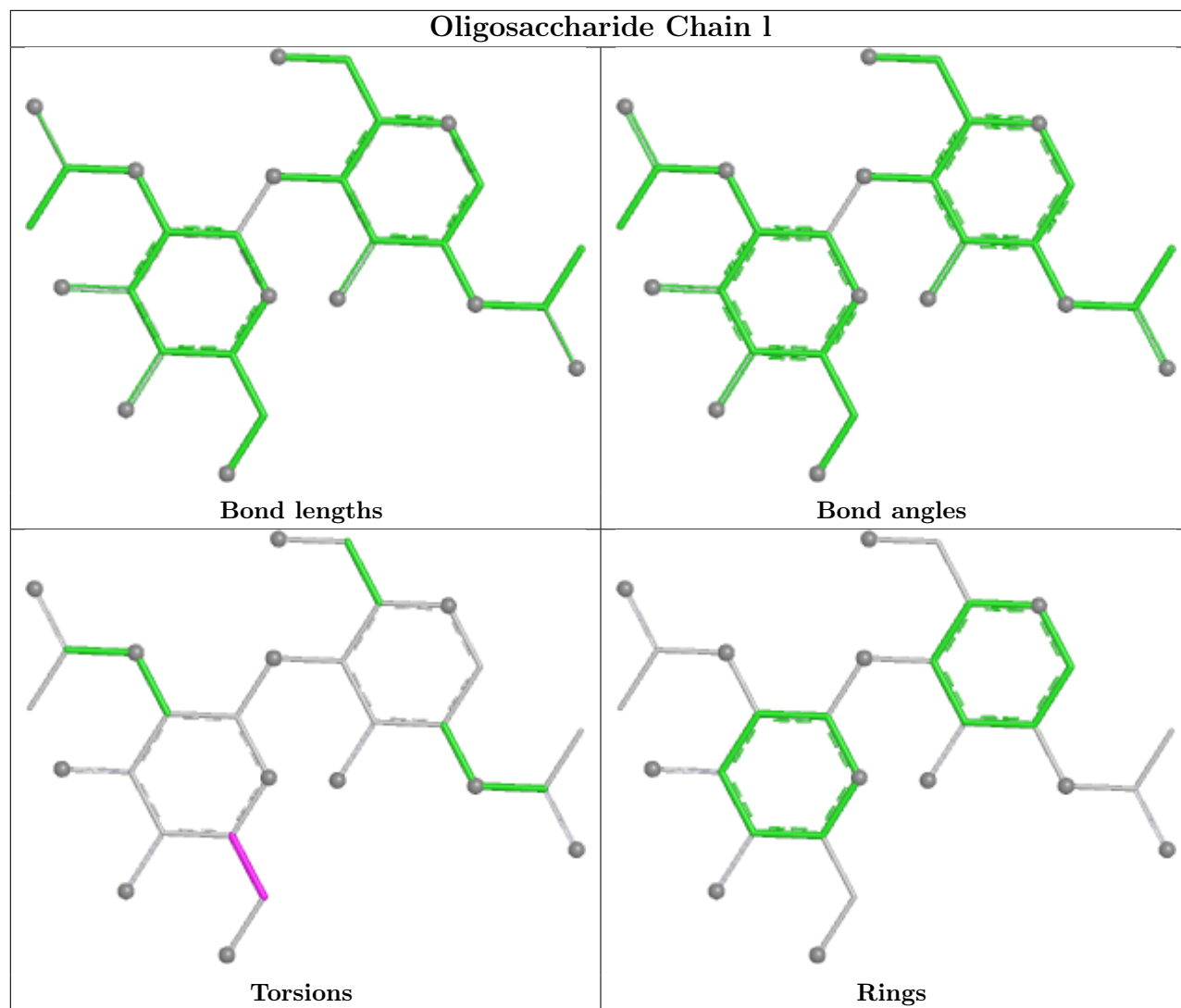


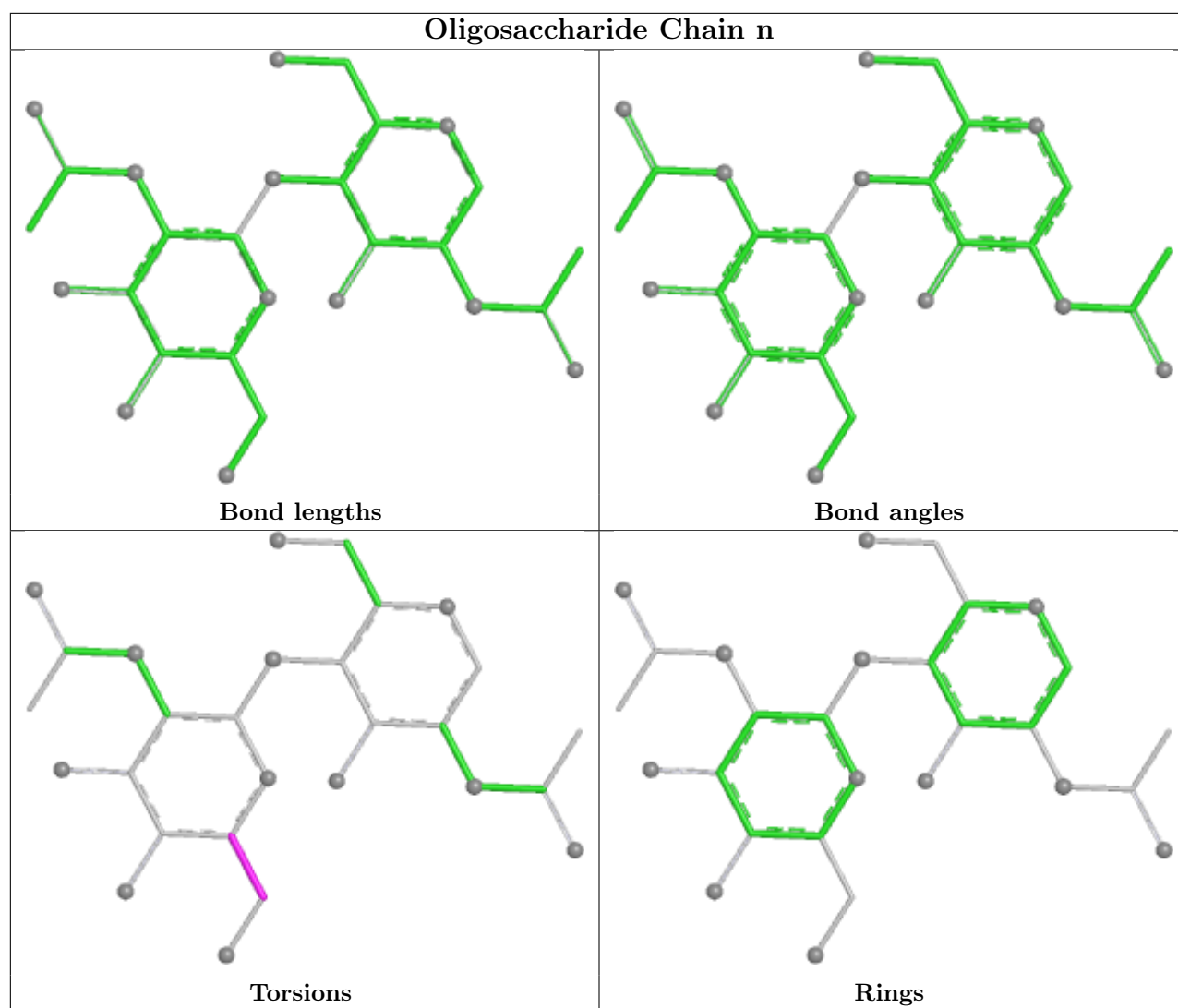


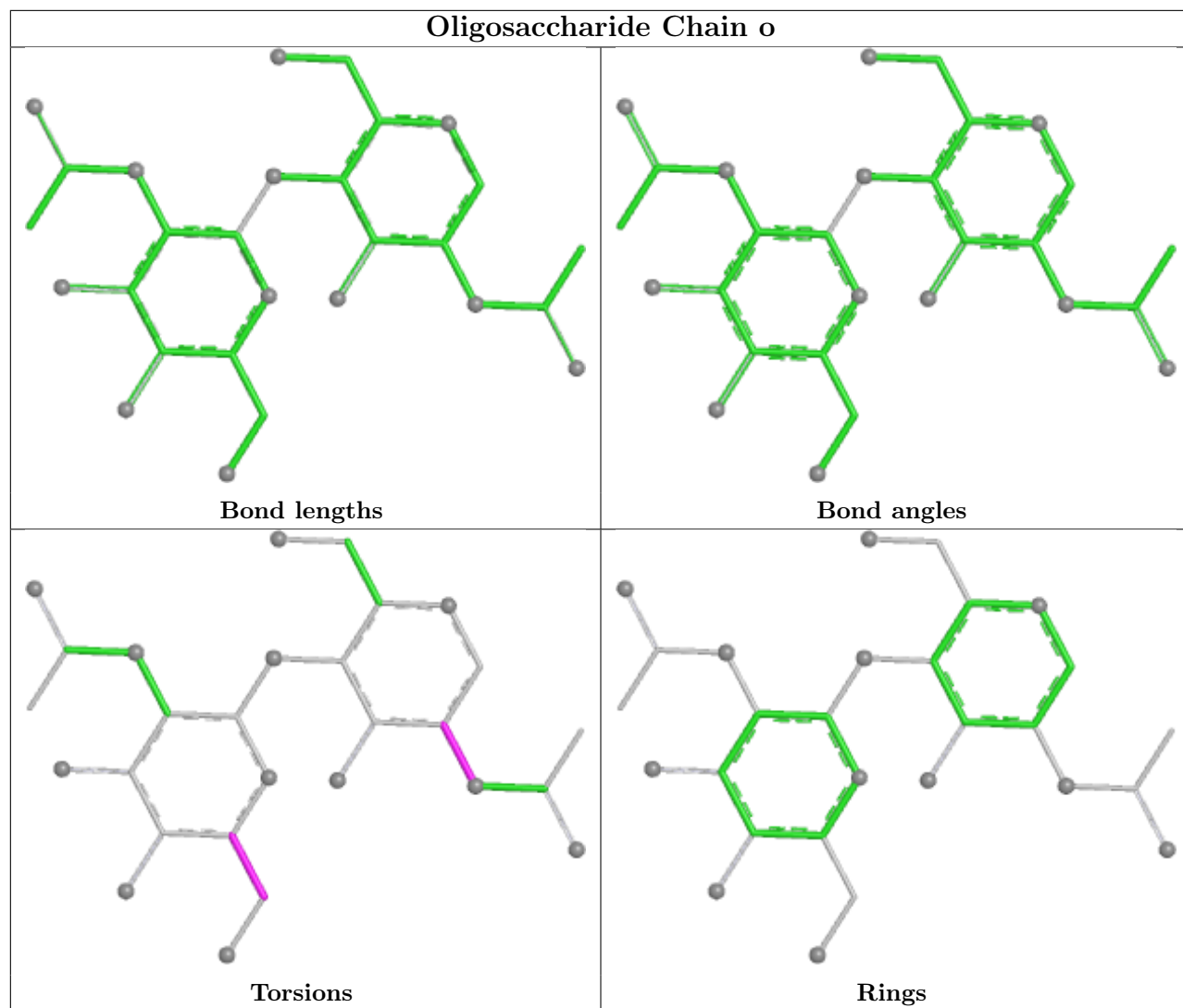


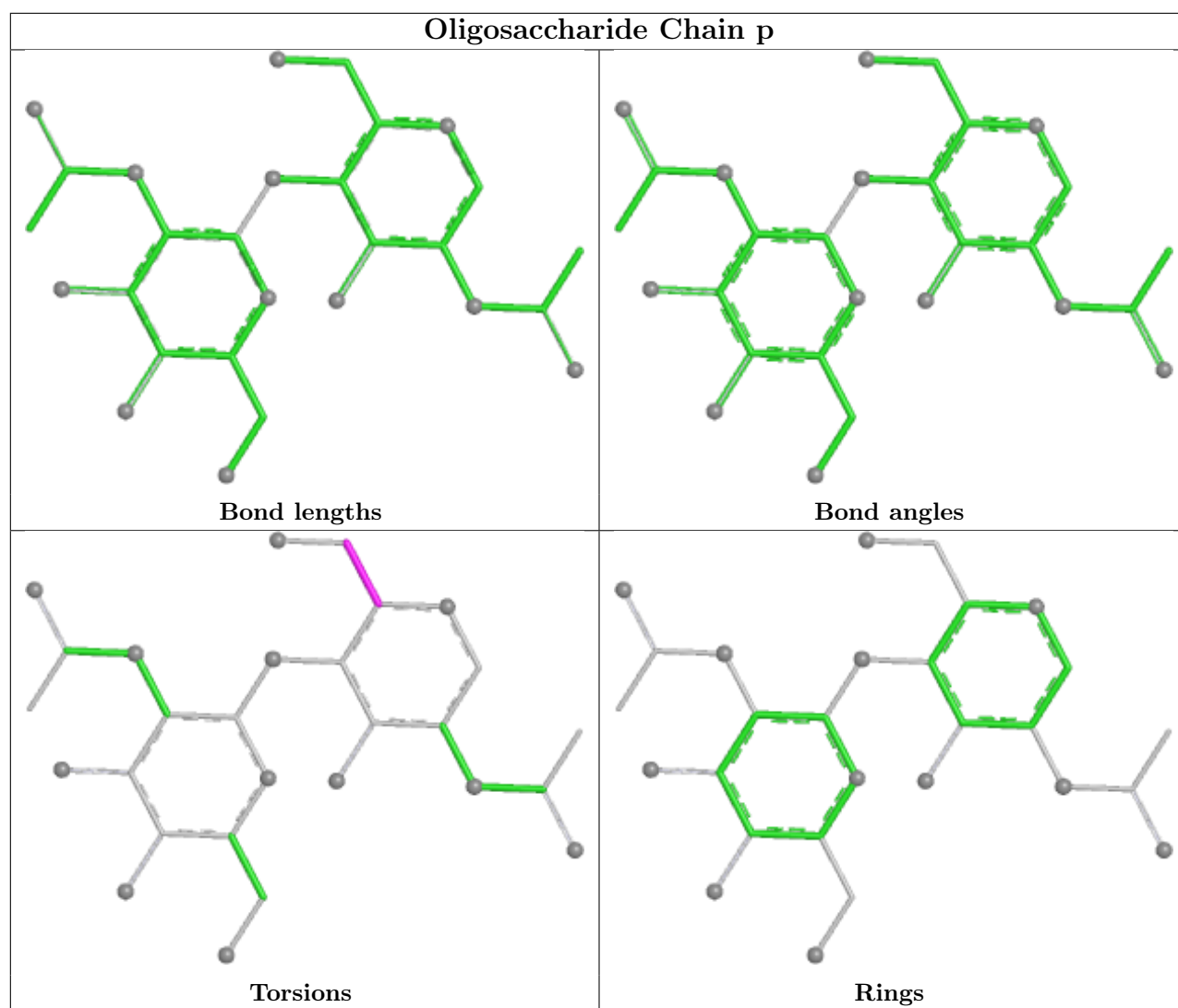


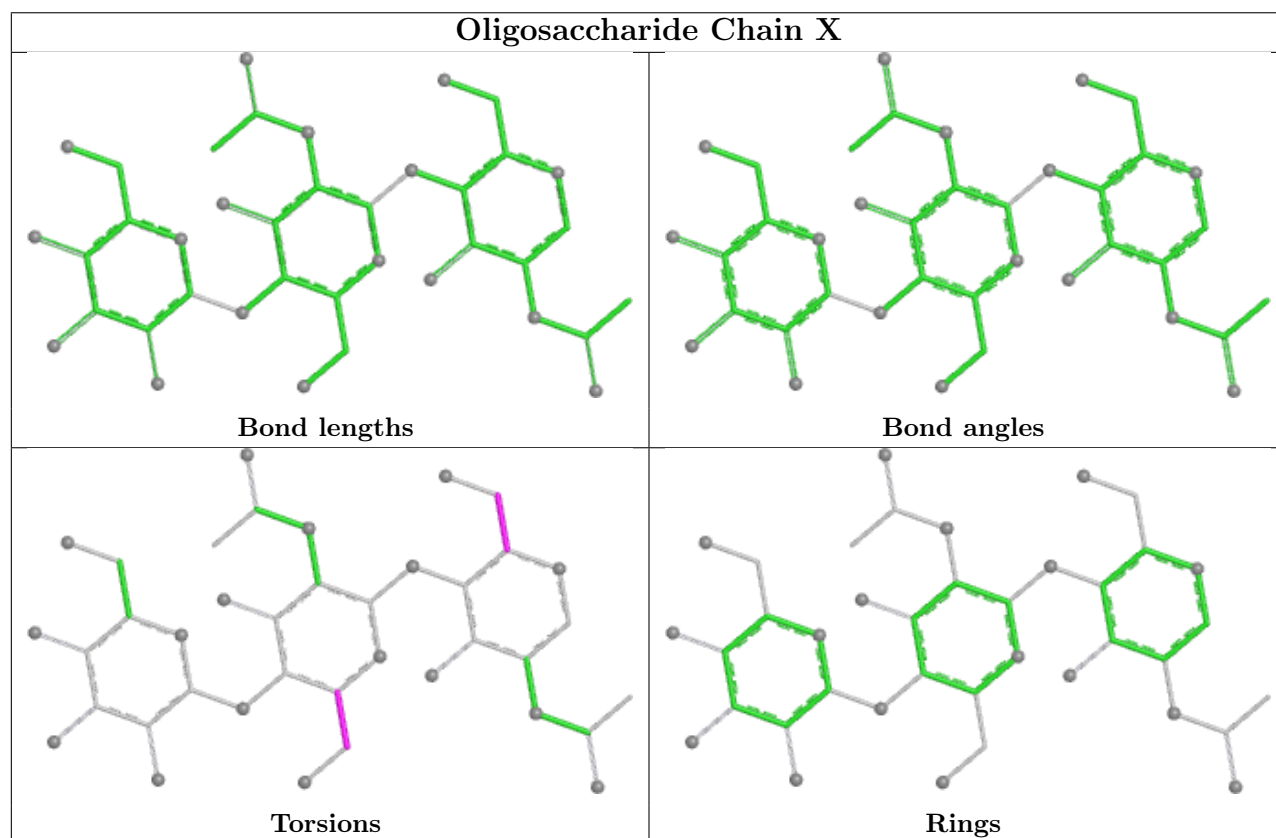
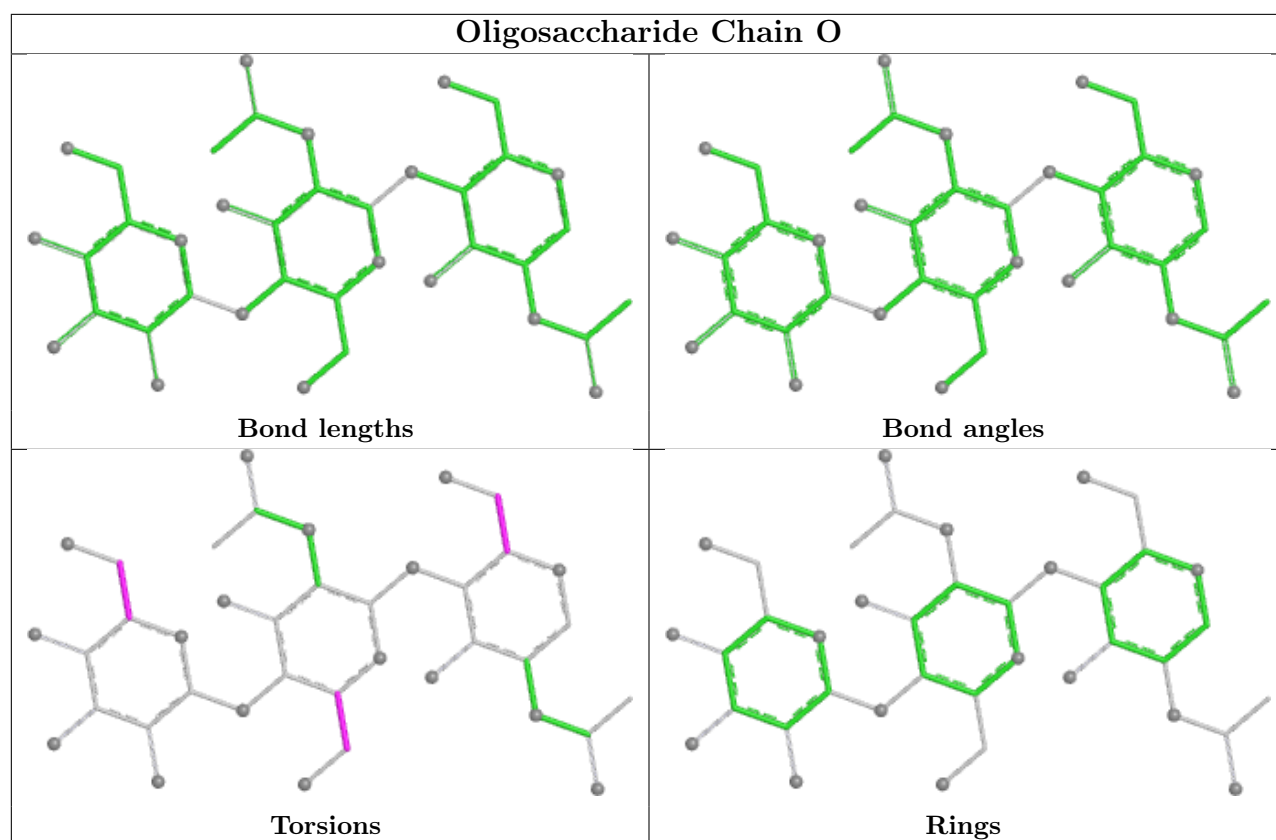


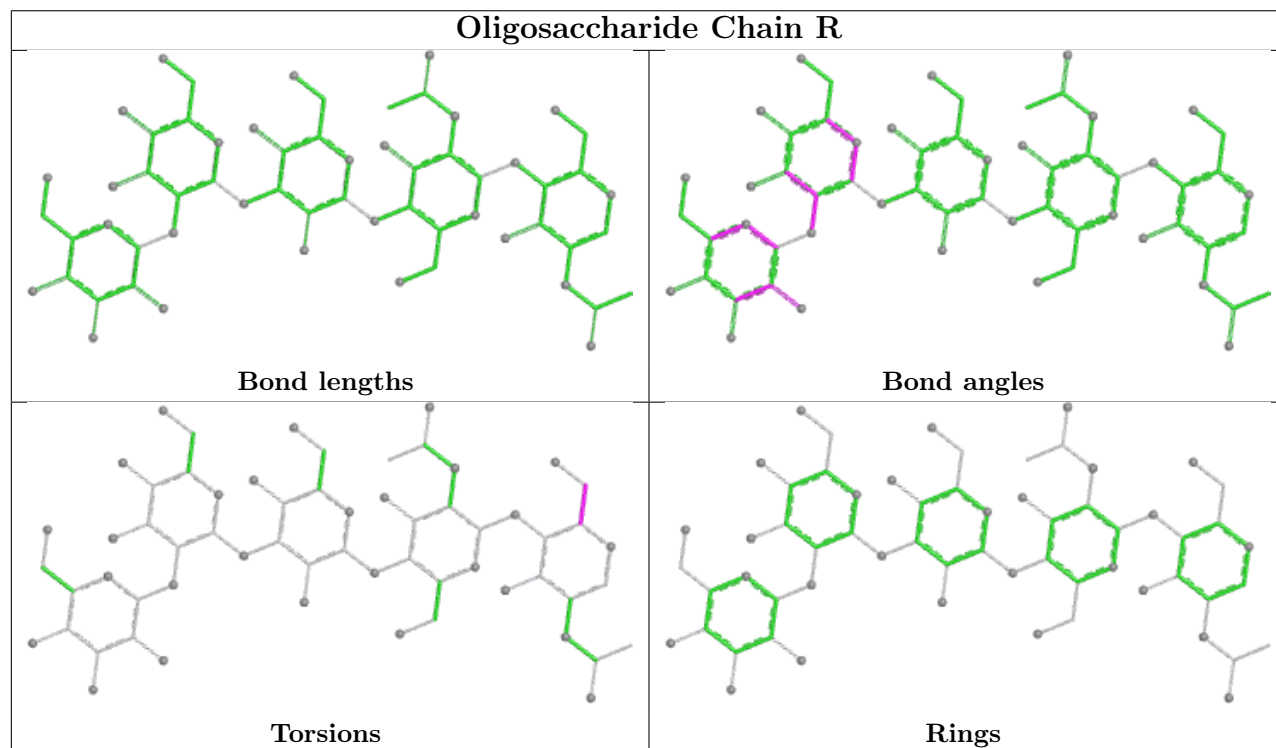
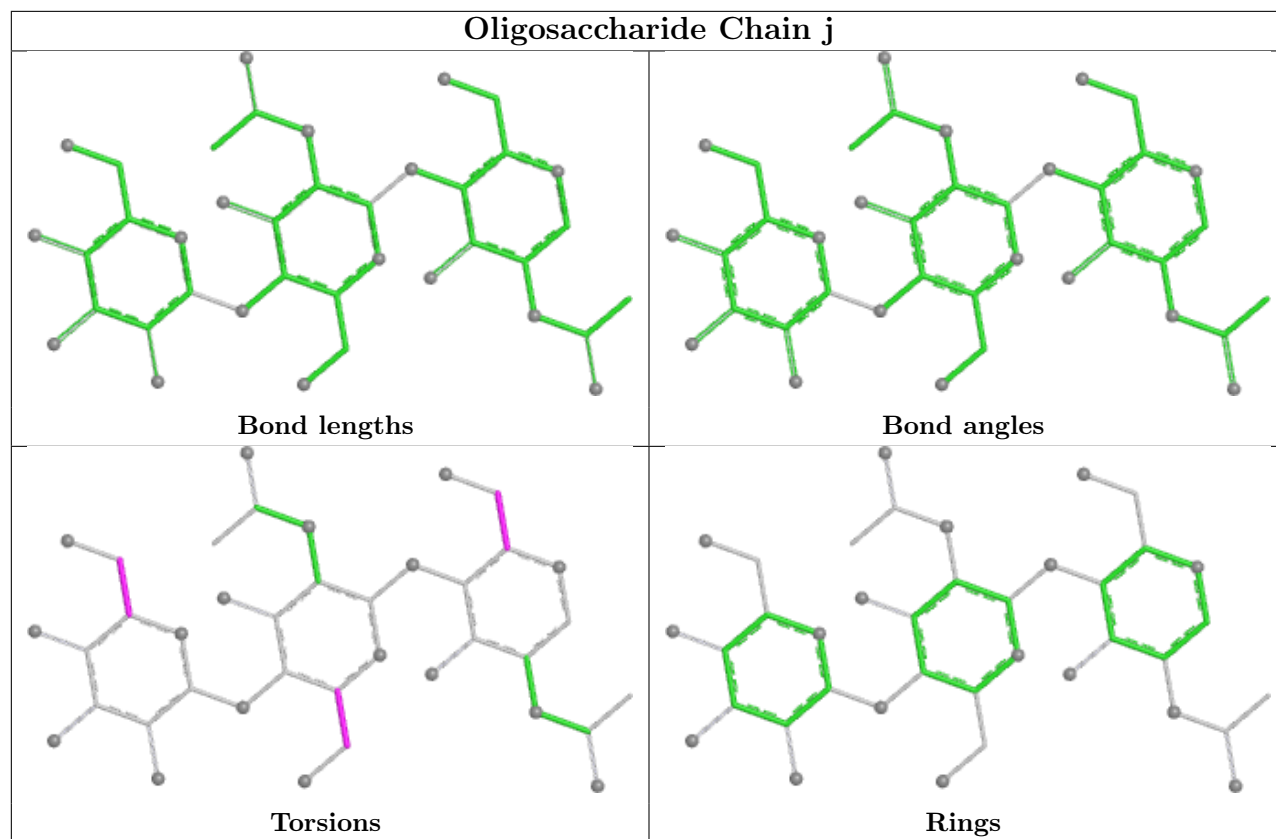


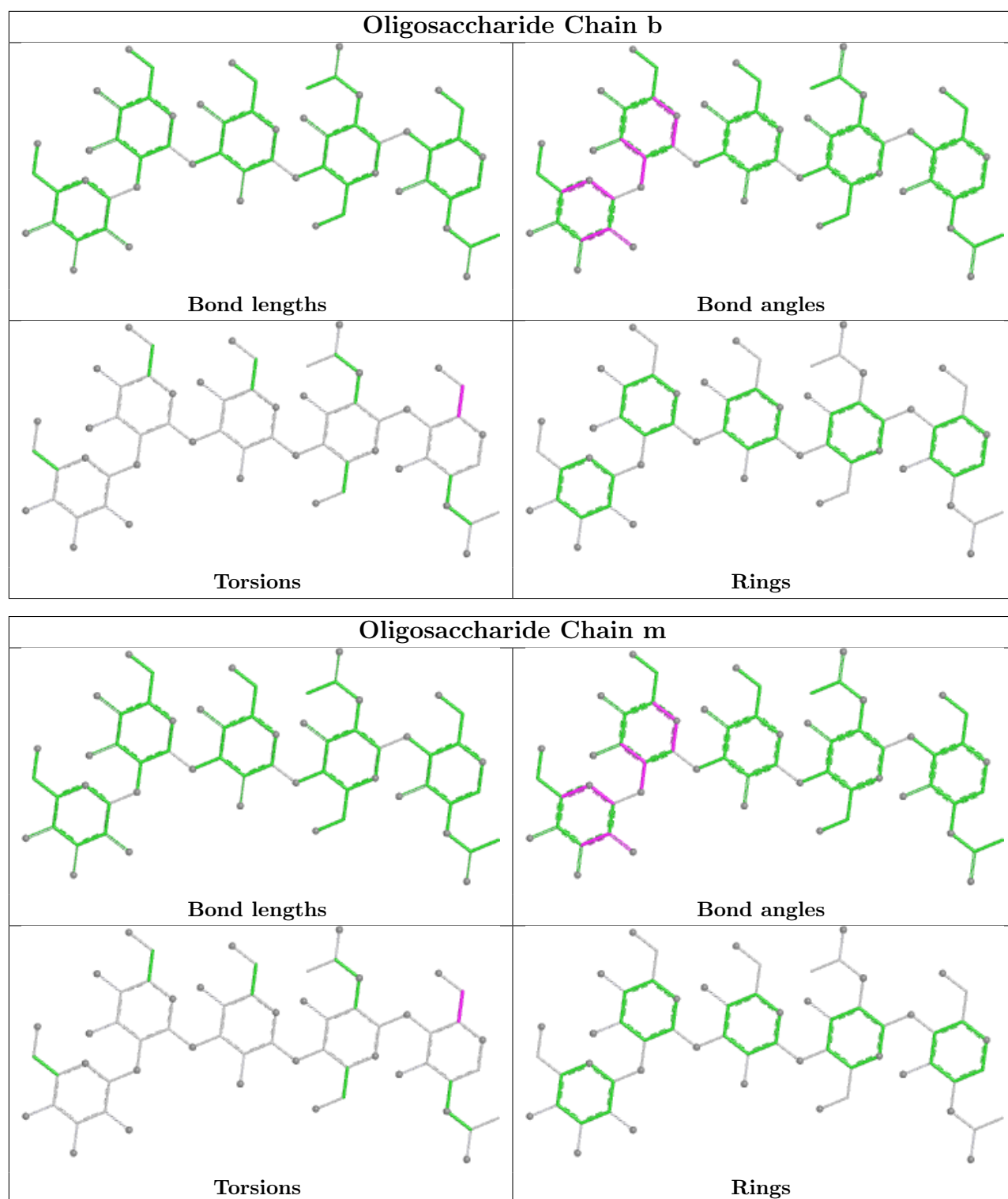












5.6 Ligand geometry [i](#)

15 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	A	603	1	14,14,15	0.19	0	17,19,21	0.44	0
8	NAG	E	605	1	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
8	NAG	E	603	1	14,14,15	0.22	0	17,19,21	0.46	0
8	NAG	C	604	1	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	C	605	1	14,14,15	0.25	0	17,19,21	0.72	1 (5%)
8	NAG	E	601	1	14,14,15	0.26	0	17,19,21	0.39	0
8	NAG	A	605	1	14,14,15	0.25	0	17,19,21	0.72	1 (5%)
8	NAG	C	603	1	14,14,15	0.22	0	17,19,21	0.45	0
8	NAG	E	602	1	14,14,15	0.19	0	17,19,21	0.45	0
8	NAG	A	604	1	14,14,15	0.23	0	17,19,21	0.47	0
8	NAG	C	601	1	14,14,15	0.24	0	17,19,21	0.39	0
8	NAG	A	602	1	14,14,15	0.21	0	17,19,21	0.45	0
8	NAG	A	601	1	14,14,15	0.25	0	17,19,21	0.39	0
8	NAG	E	604	1	14,14,15	0.23	0	17,19,21	0.47	0
8	NAG	C	602	1	14,14,15	0.19	0	17,19,21	0.44	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
8	NAG	A	603	1	-	0/6/23/26	0/1/1/1
8	NAG	E	605	1	-	2/6/23/26	0/1/1/1
8	NAG	E	603	1	-	0/6/23/26	0/1/1/1
8	NAG	C	604	1	-	2/6/23/26	0/1/1/1
8	NAG	C	605	1	-	2/6/23/26	0/1/1/1
8	NAG	E	601	1	-	1/6/23/26	0/1/1/1
8	NAG	A	605	1	-	4/6/23/26	0/1/1/1
8	NAG	C	603	1	-	0/6/23/26	0/1/1/1
8	NAG	E	602	1	-	0/6/23/26	0/1/1/1
8	NAG	A	604	1	-	2/6/23/26	0/1/1/1
8	NAG	C	601	1	-	1/6/23/26	0/1/1/1
8	NAG	A	602	1	-	0/6/23/26	0/1/1/1
8	NAG	A	601	1	-	1/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	E	604	1	-	2/6/23/26	0/1/1/1
8	NAG	C	602	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	605	NAG	C2-N2-C7	2.28	125.96	122.90
8	E	605	NAG	C2-N2-C7	2.28	125.95	122.90
8	A	605	NAG	C2-N2-C7	2.28	125.95	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	602	NAG	O5-C5-C6-O6
8	A	604	NAG	O5-C5-C6-O6
8	C	602	NAG	C4-C5-C6-O6
8	E	604	NAG	O5-C5-C6-O6
8	C	604	NAG	O5-C5-C6-O6
8	E	604	NAG	C4-C5-C6-O6
8	C	604	NAG	C4-C5-C6-O6
8	A	604	NAG	C4-C5-C6-O6
8	A	605	NAG	C8-C7-N2-C2
8	A	605	NAG	O7-C7-N2-C2
8	C	605	NAG	C8-C7-N2-C2
8	C	605	NAG	O7-C7-N2-C2
8	E	605	NAG	C8-C7-N2-C2
8	E	605	NAG	O7-C7-N2-C2
8	E	601	NAG	O5-C5-C6-O6
8	A	601	NAG	O5-C5-C6-O6
8	C	601	NAG	O5-C5-C6-O6
8	A	605	NAG	C4-C5-C6-O6
8	A	605	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

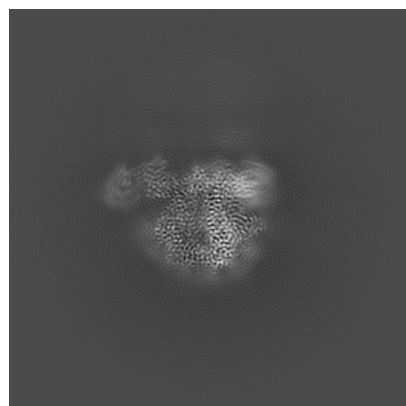
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41362. These allow visual inspection of the internal detail of the map and identification of artifacts.

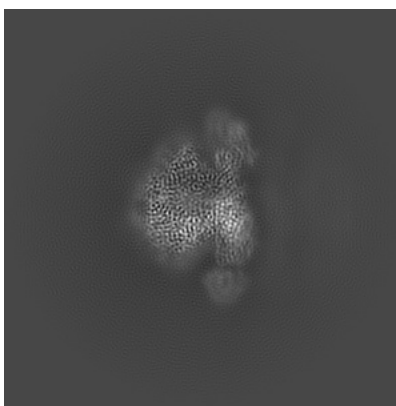
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

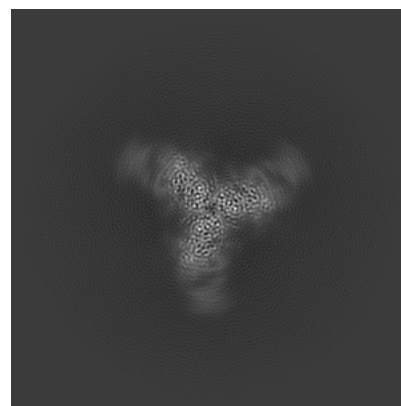
6.1.1 Primary map



X

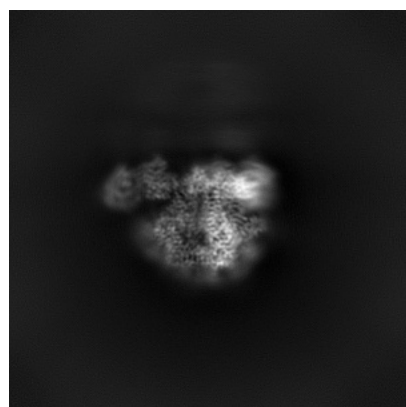


Y

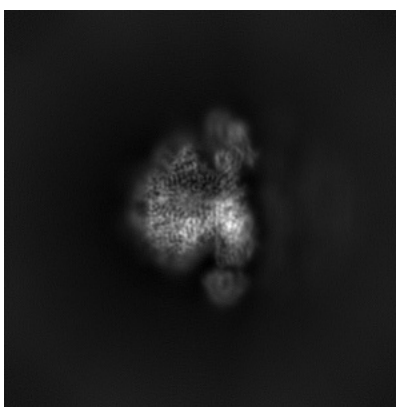


Z

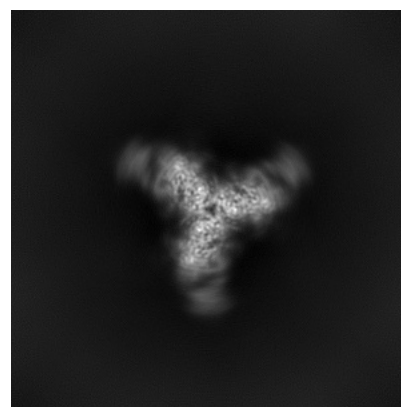
6.1.2 Raw map



X



Y

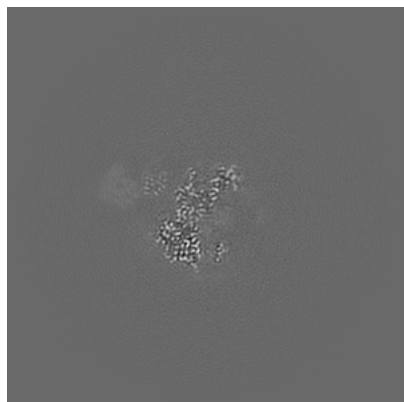


Z

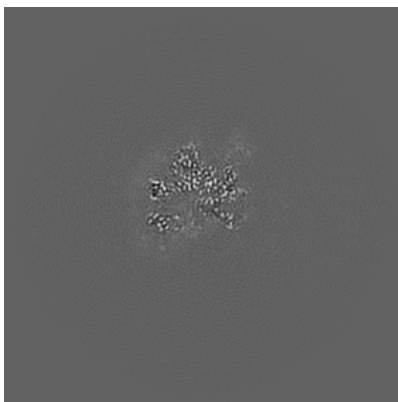
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

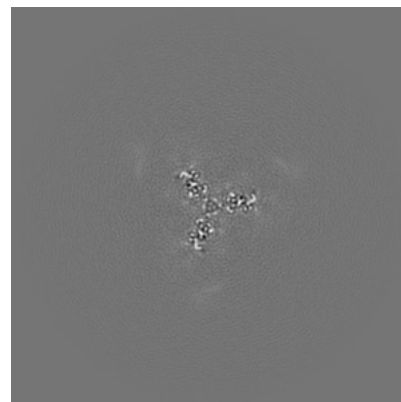
6.2.1 Primary map



X Index: 230

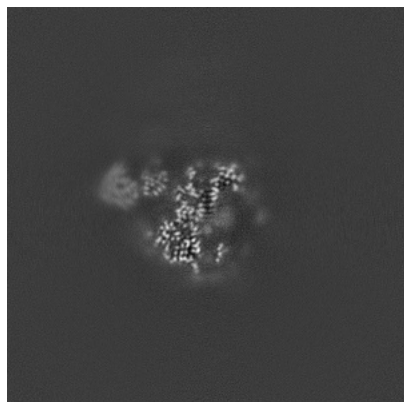


Y Index: 230

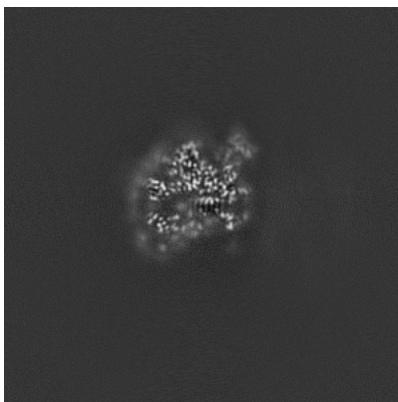


Z Index: 230

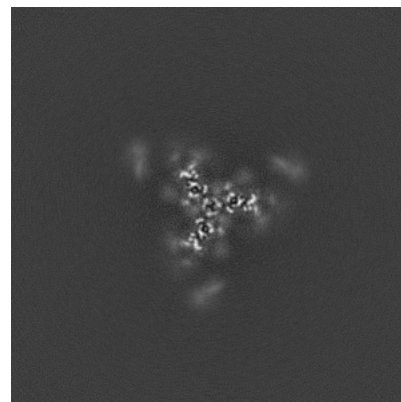
6.2.2 Raw map



X Index: 230



Y Index: 230

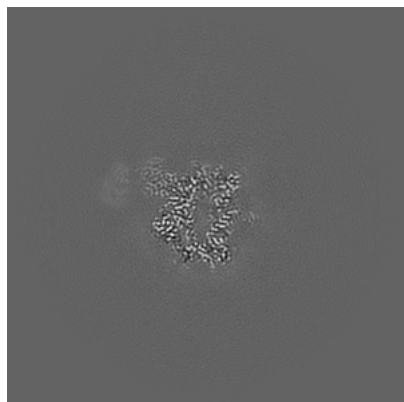


Z Index: 230

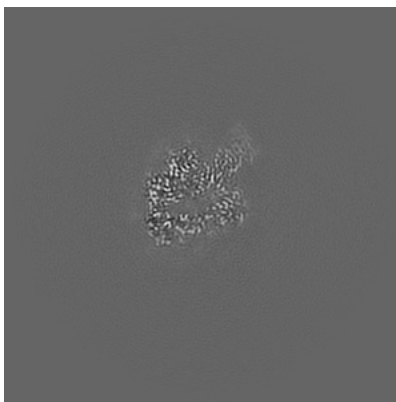
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

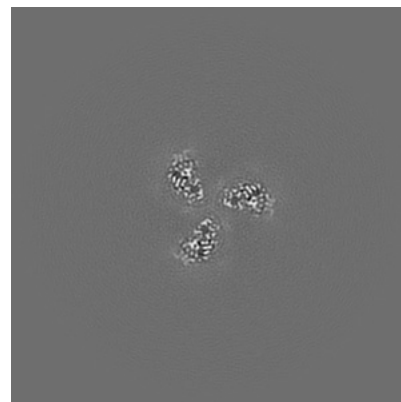
6.3.1 Primary map



X Index: 218

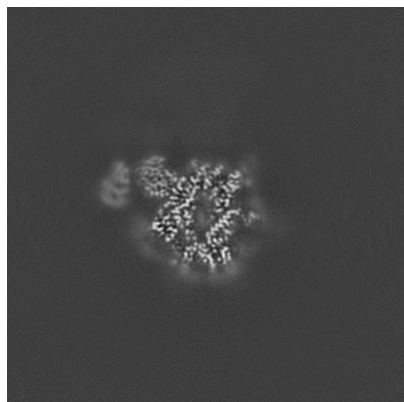


Y Index: 241

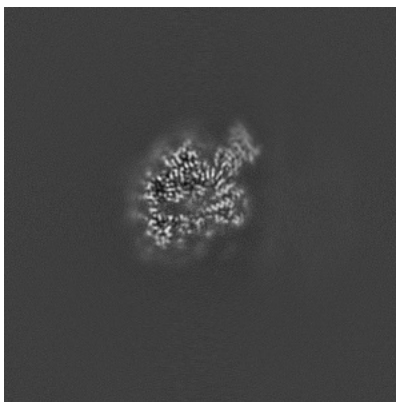


Z Index: 208

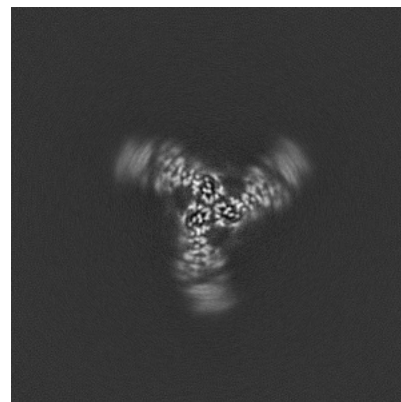
6.3.2 Raw map



X Index: 217



Y Index: 239



Z Index: 260

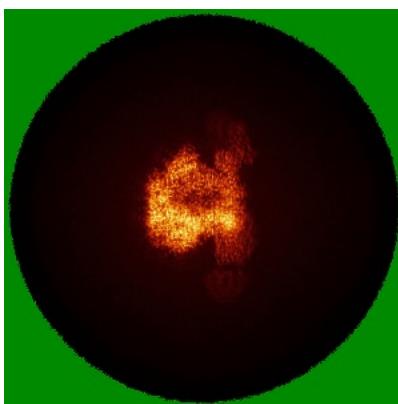
The images above show the largest variance slices of the map in three orthogonal directions.

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

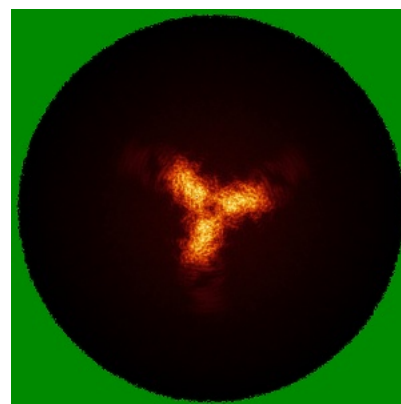
6.4.1 Primary map



X

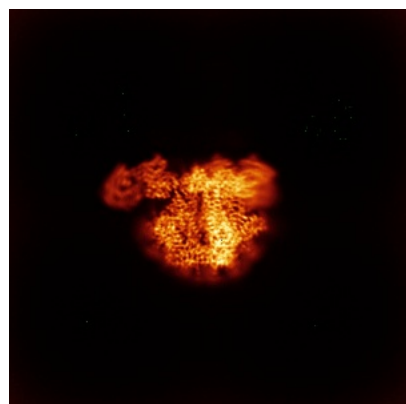


Y

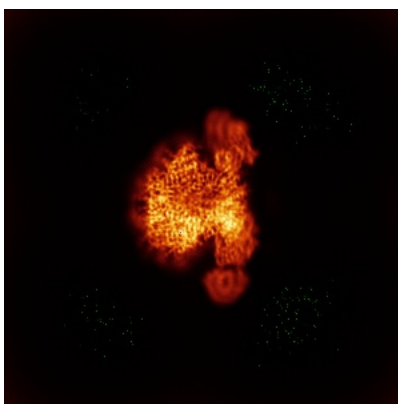


Z

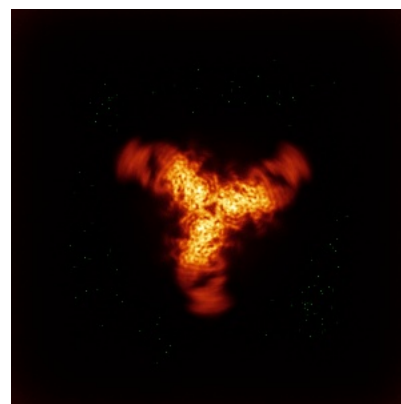
6.4.2 Raw map



X



Y

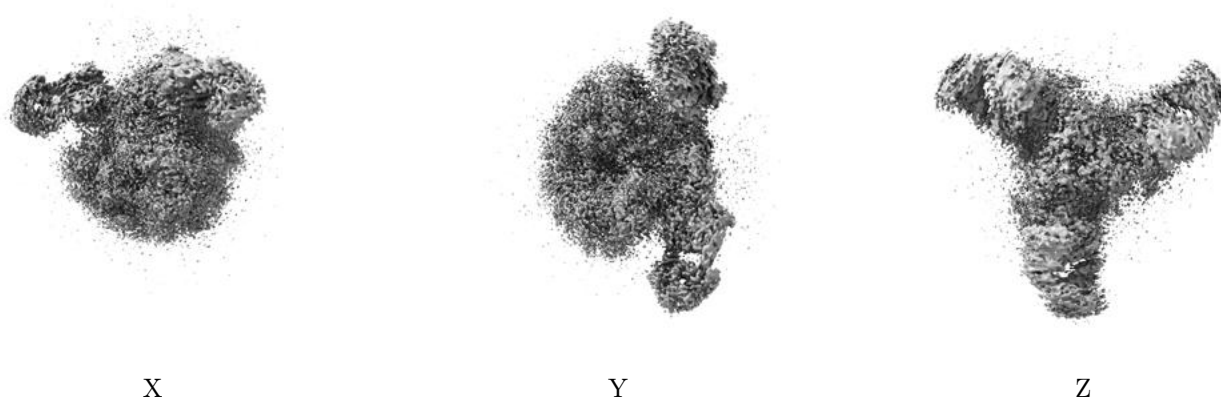


Z

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.

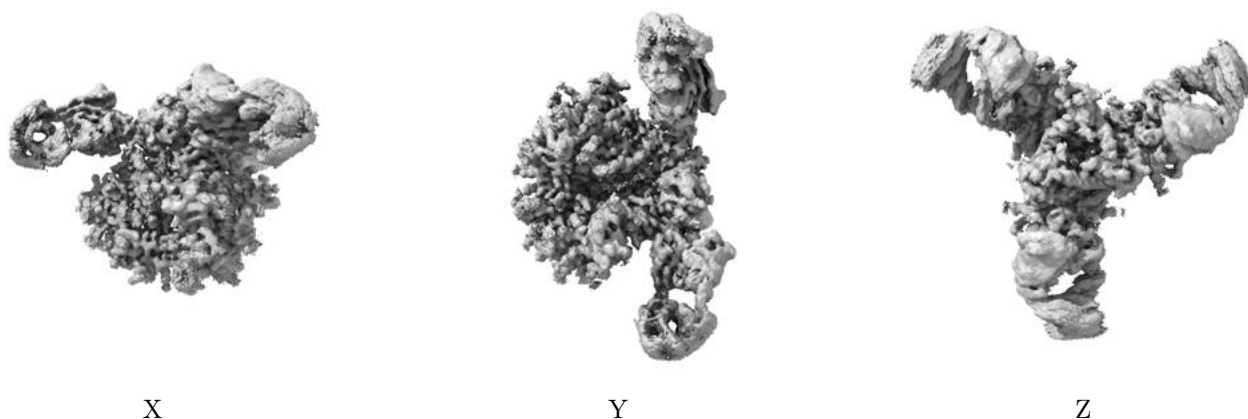
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

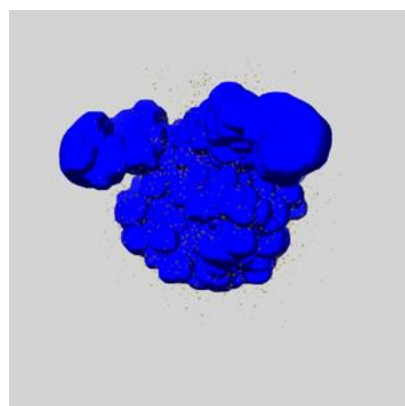
6.6 Mask visualisation [i](#)

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

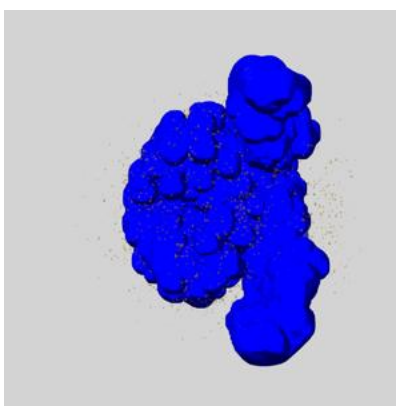
A mask typically either:

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

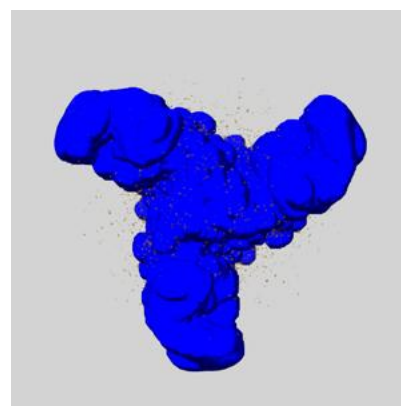
6.6.1 emd_41362_msk_1.map [i](#)



X



Y

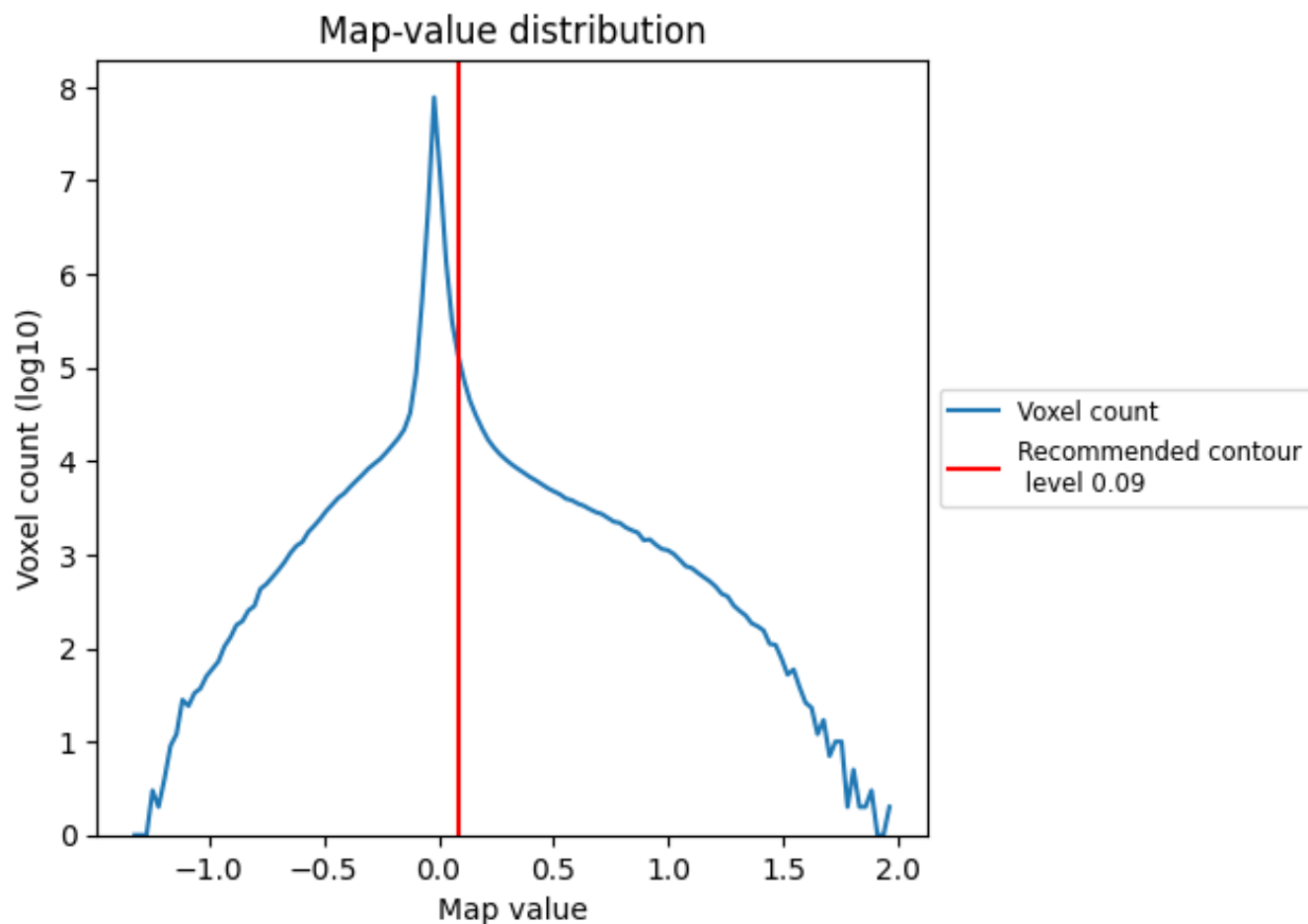


Z

7 Map analysis [i](#)

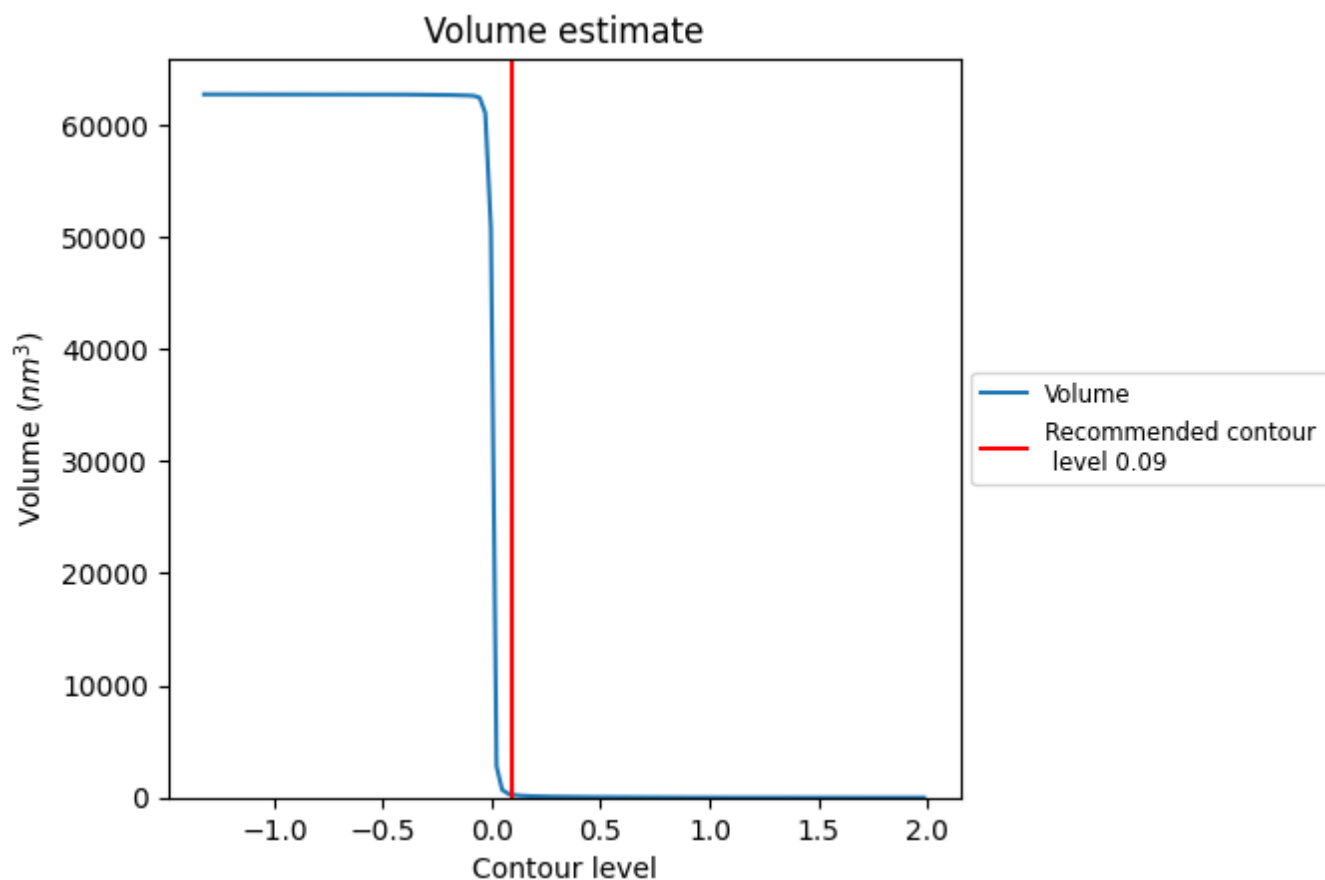
This section contains the results of statistical analysis of the map.

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.

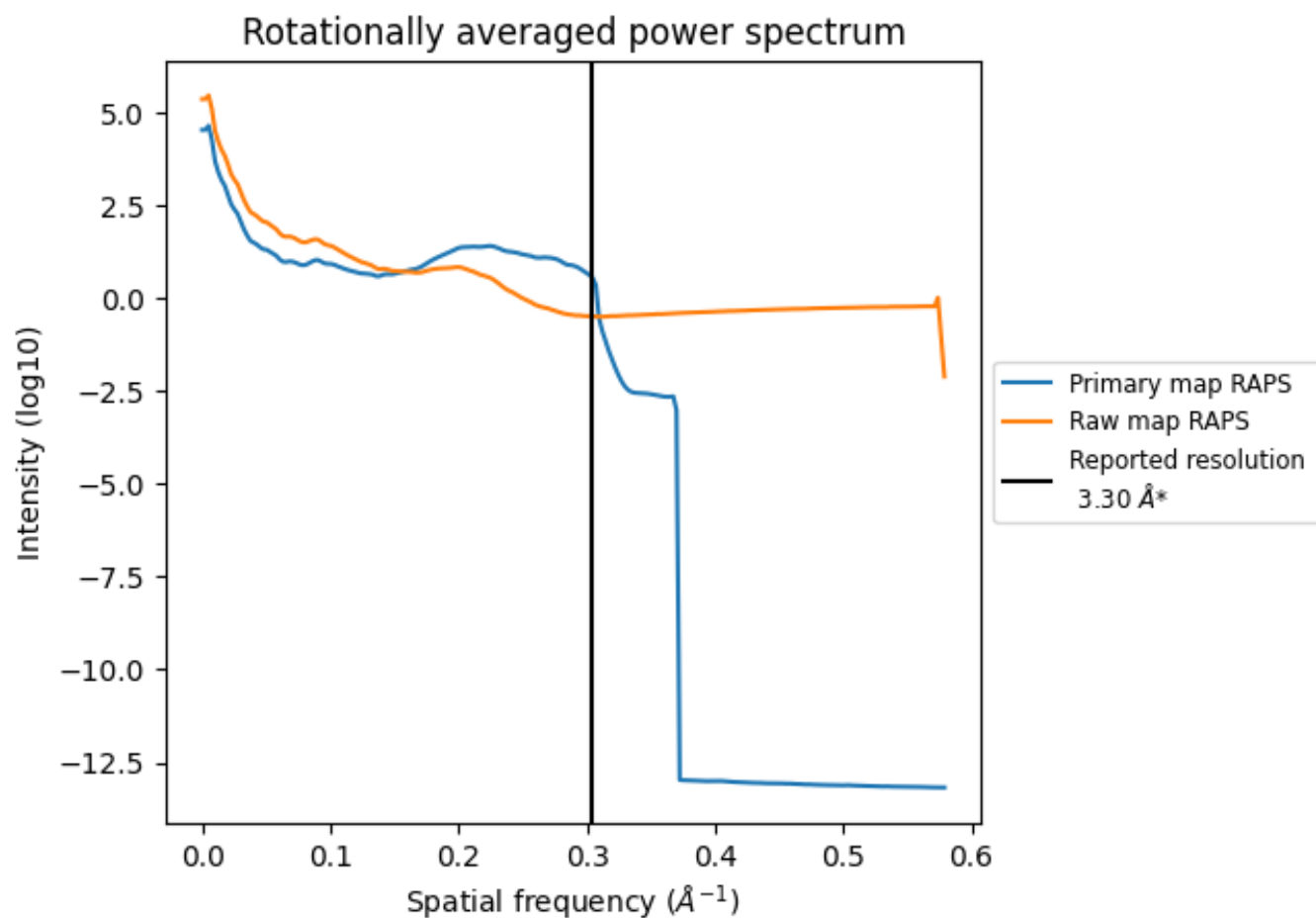
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm^3 ; this corresponds to an approximate mass of 259 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 ⓘ

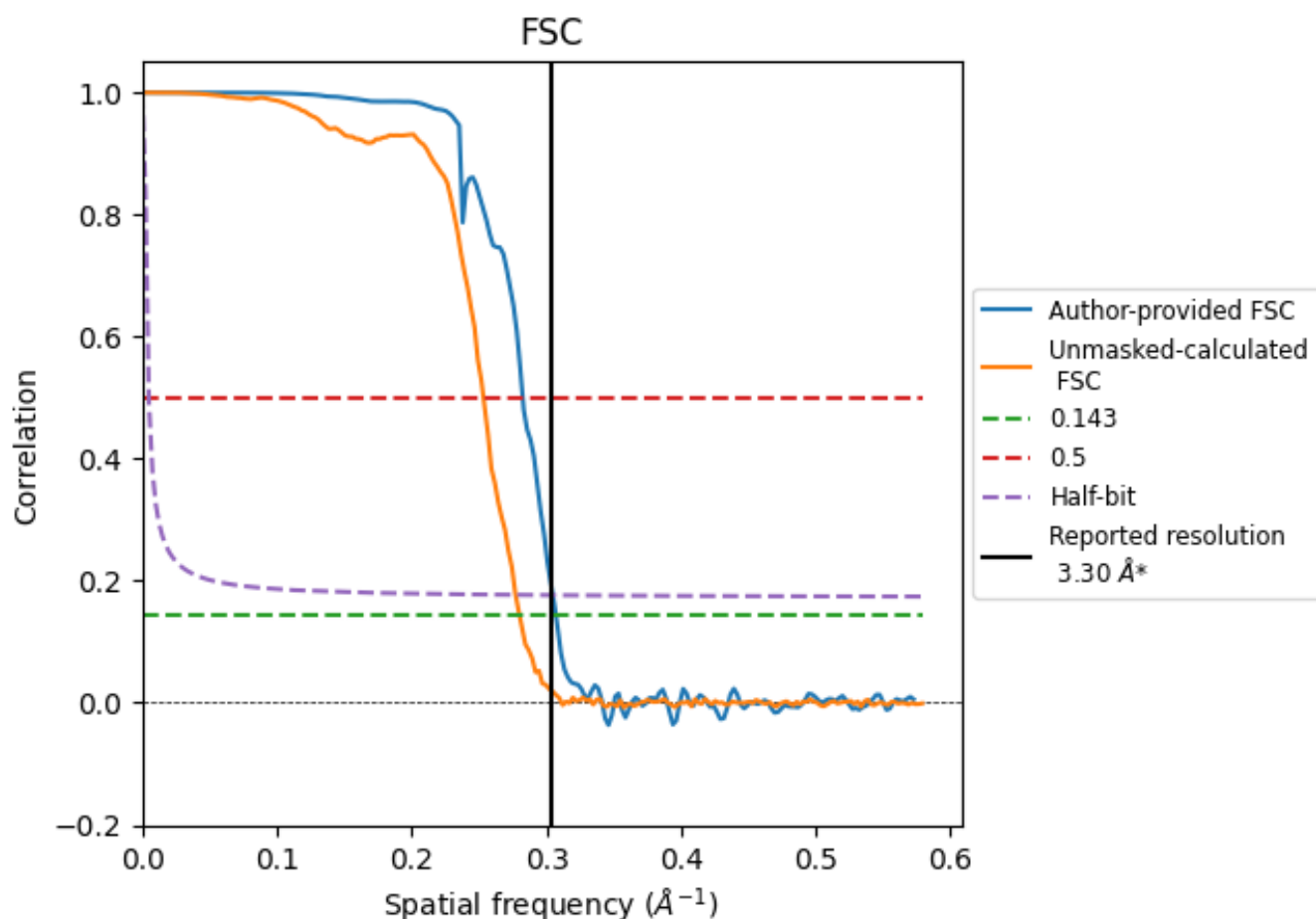


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

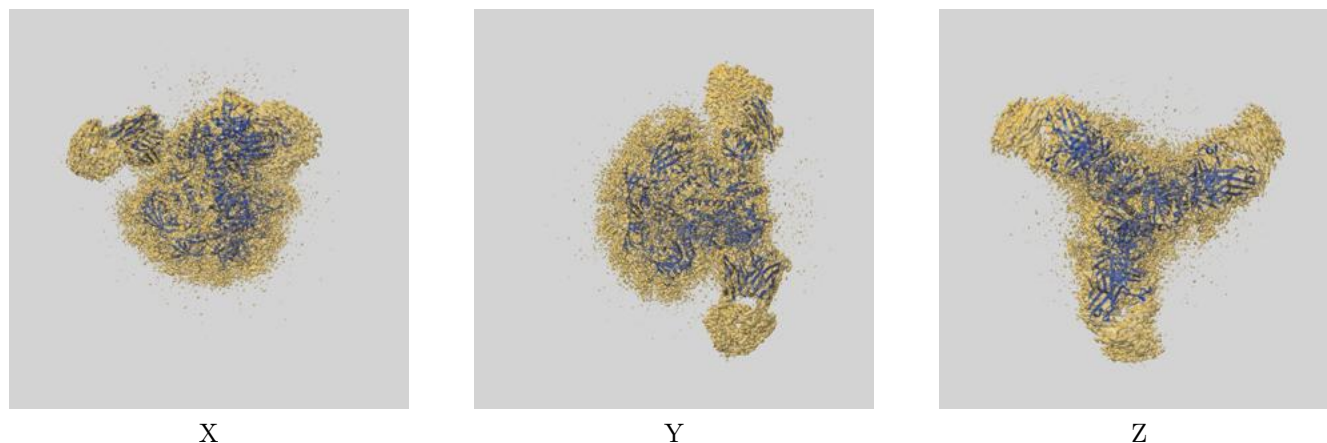
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.54	3.28
Unmasked-calculated*	3.57	3.95	3.61

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

9 Map-model fit [i](#)

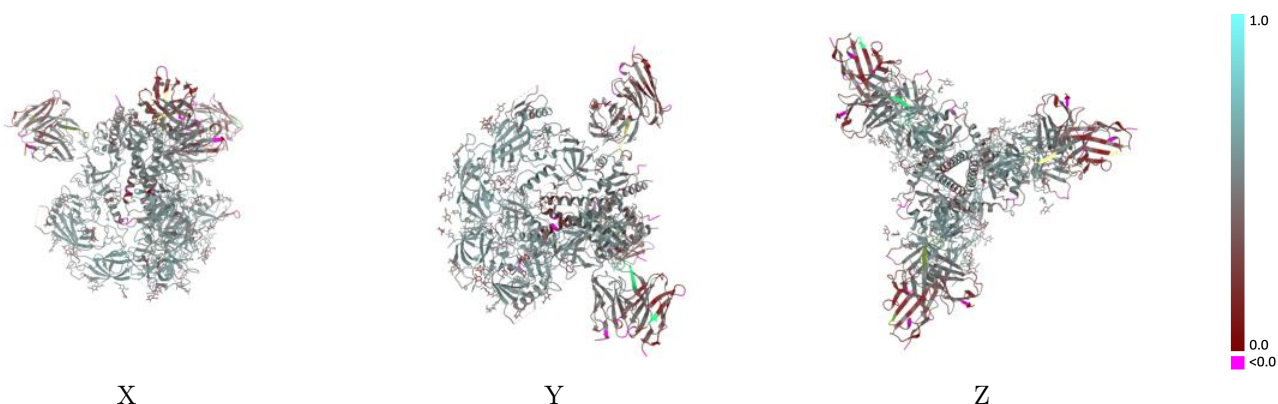
This section contains information regarding the fit between EMDB map EMD-41362 and PDB model 8TL5. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



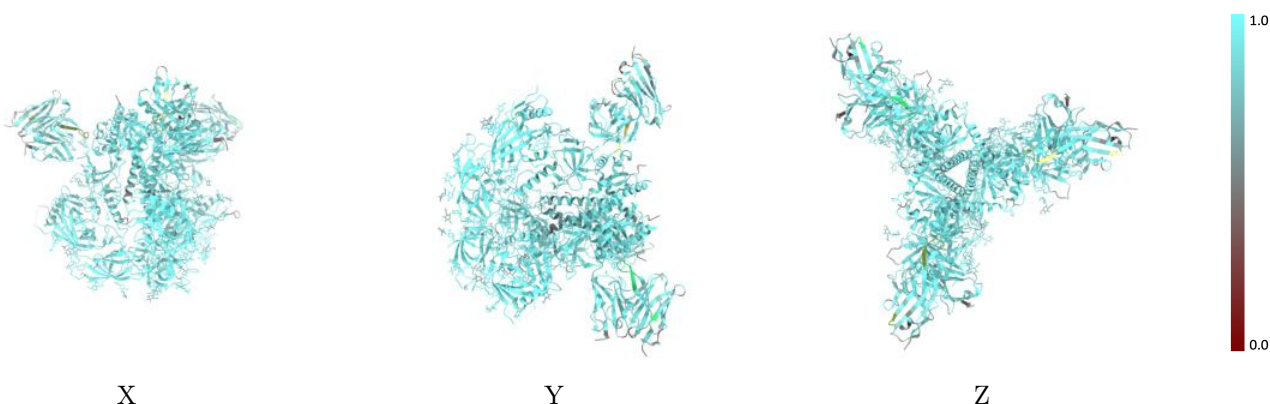
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



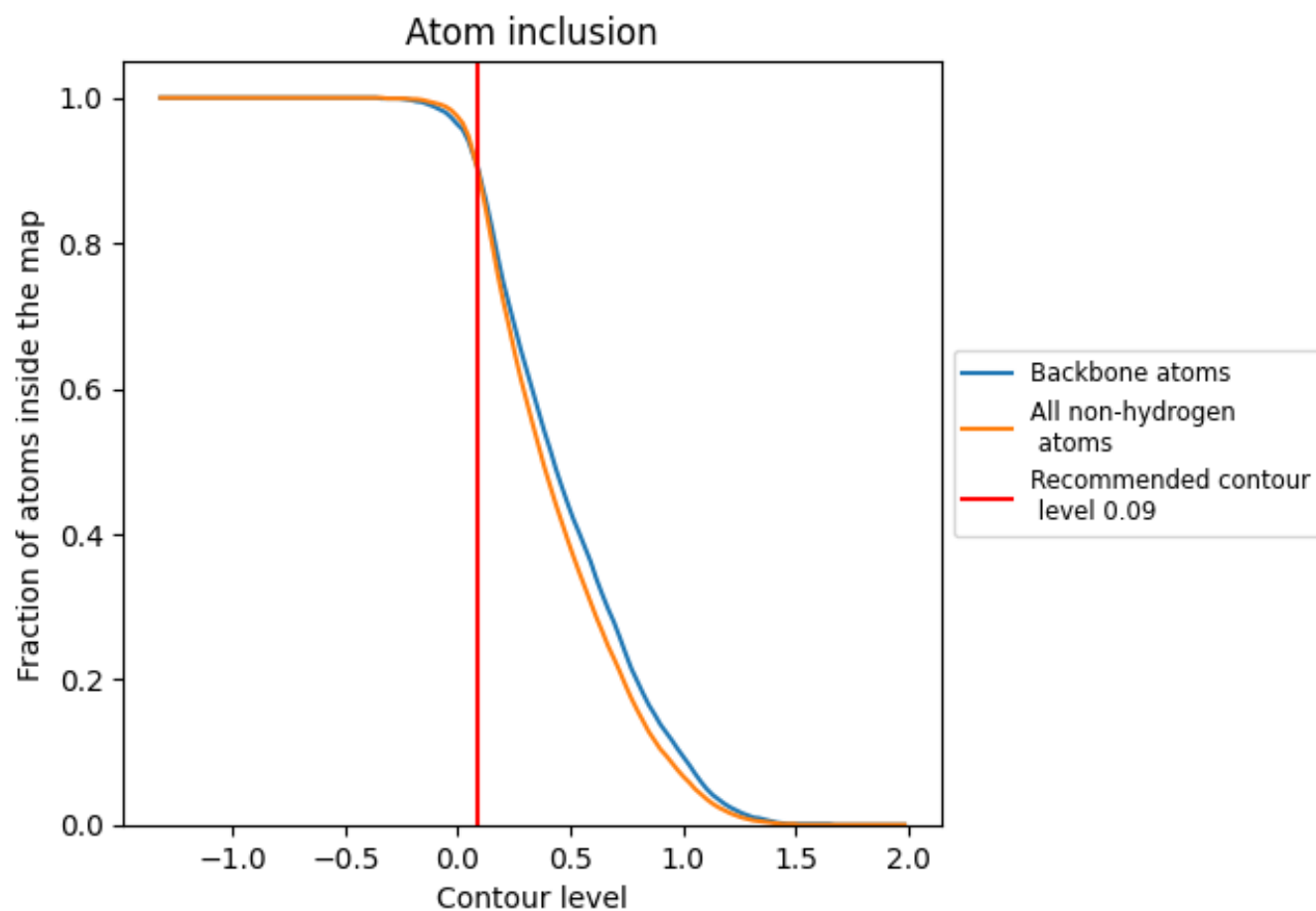
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8990	 0.4790
A	 0.9350	 0.5360
B	 0.9050	 0.4760
C	 0.9340	 0.5310
D	 0.9010	 0.4750
E	 0.9400	 0.5330
F	 0.9140	 0.4810
G	 0.7880	 0.3300
H	 0.8700	 0.4270
I	 0.7820	 0.3290
J	 0.8720	 0.4340
K	 0.7890	 0.3310
L	 0.8670	 0.4320
M	 0.8570	 0.4080
N	 0.8210	 0.3920
O	 0.9230	 0.5210
P	 0.7500	 0.3430
Q	 0.7860	 0.3730
R	 0.9180	 0.4600
S	 0.9290	 0.4730
T	 1.0000	 0.5100
U	 0.7860	 0.3460
V	 0.8570	 0.4070
W	 0.8210	 0.4030
X	 0.8970	 0.4840
Y	 0.7140	 0.3910
Z	 0.7860	 0.3730
a	 0.8210	 0.4870
b	 0.9340	 0.4590
c	 0.9290	 0.4710
d	 0.9290	 0.4720
e	 0.9290	 0.4960
f	 0.8570	 0.3640
g	 0.8210	 0.4740
h	 0.8570	 0.4040



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Chain	Atom inclusion	Q-score
i	 0.8210	 0.3990
j	 0.9490	 0.4830
k	 0.7140	 0.3980
l	 0.7860	 0.3670
m	 0.9020	 0.4600
n	 0.9290	 0.4720
o	 0.9640	 0.5210
p	 0.8210	 0.3170