



Full wwPDB EM Validation Report ⓘ

Dec 10, 2025 – 04:49 PM EST

PDB ID : 9PNI / pdb_00009pni
EMDB ID : EMD-71766
Title : Cryo-EM structure of J601-1B2 Fab in complex with HIV-1 BG505 DS-SOSIP Env trimer
Authors : Wang, S.; Zhou, T.; Kwong, P.D.
Deposited on : 2025-07-21
Resolution : 3.83 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:

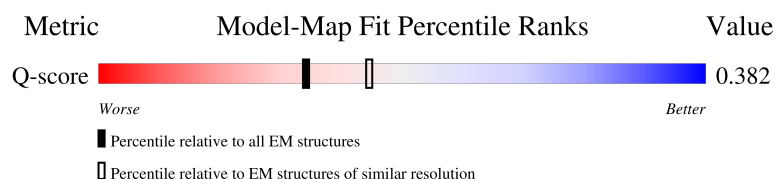
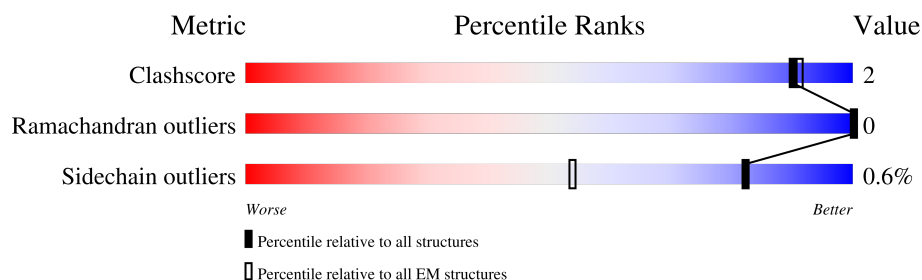
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

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 3.83 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.



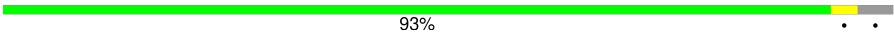

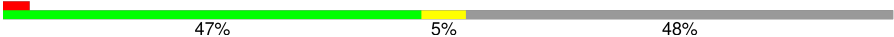





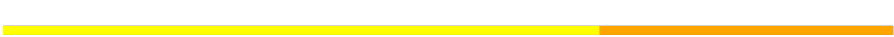

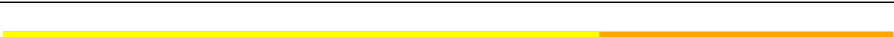
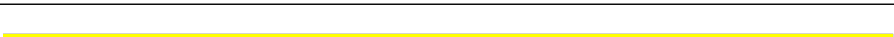

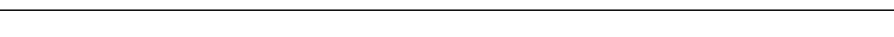
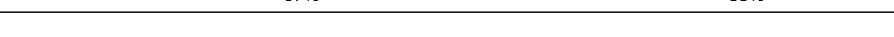
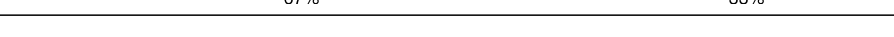

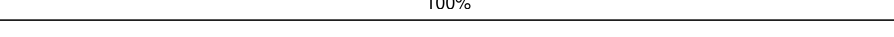
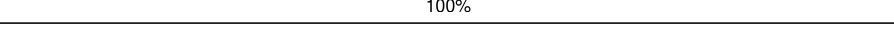
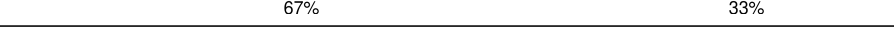


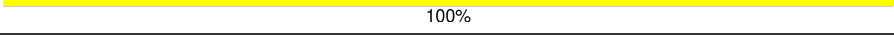

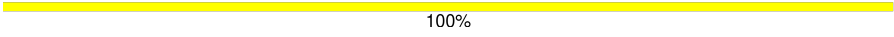
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	9087 (3.33 - 4.33)

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	153	
1	B	153	
1	F	153	
2	C	473	




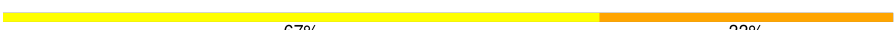
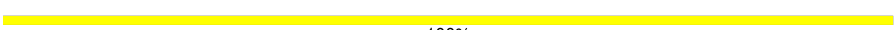





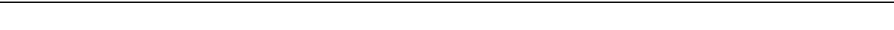

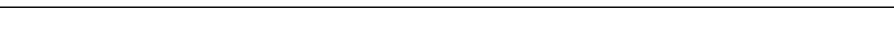
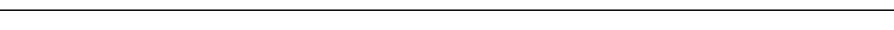
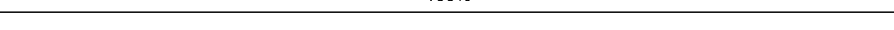
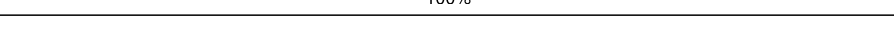


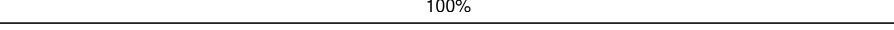
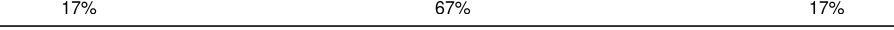




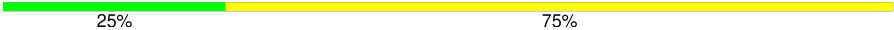
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Mol	Chain	Length	Quality of chain
2	G	473	
2	I	473	
3	D	234	
3	H	234	
3	J	234	
4	E	214	
4	K	214	
4	L	214	
5	0	3	
5	1	3	
5	M	3	
5	Q	3	
5	R	3	
5	U	3	
5	Y	3	
5	Z	3	
5	f	3	
5	g	3	
5	i	3	
5	j	3	
5	k	3	
5	m	3	
5	n	3	
5	t	3	
5	u	3	

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Mol	Chain	Length	Quality of chain
5	v	3	 67% 33%
5	w	3	 67% 33%
5	x	3	 67% 33%
5	y	3	 67% 33%
6	N	5	 100%
6	b	5	 100%
6	p	5	 80% 20%
7	O	2	 50% 50%
7	S	2	 100%
7	X	2	 50% 50%
7	a	2	 50% 50%
7	c	2	 50% 50%
7	d	2	 50% 50%
7	h	2	 100%
7	o	2	 100%
7	q	2	 50% 50%
7	r	2	 50% 50%
8	P	6	 100%
8	e	6	 17% 67% 17%
8	s	6	 17% 83%
9	T	4	 25% 75%
9	V	4	 50% 50%
9	W	4	 75% 25%
9	l	4	 25% 75%
9	z	4	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein BG505 DS-SOSIP gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
1	B	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
1	F	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	605	CYS	THR	engineered mutation	UNP Q2N0S7
B	605	CYS	THR	engineered mutation	UNP Q2N0S7
F	605	CYS	THR	engineered mutation	UNP Q2N0S7

- Molecule 2 is a protein called Envelope glycoprotein BG505 DS-SOSIP gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	453	Total	C	N	O	S	0	0
			3564	2233	630	671	30		
2	G	453	Total	C	N	O	S	0	0
			3564	2233	630	671	30		
2	I	453	Total	C	N	O	S	0	0
			3564	2233	630	671	30		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	201	CYS	ILE	engineered mutation	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	433	CYS	ALA	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
I	201	CYS	ILE	engineered mutation	UNP Q2N0S6
I	332	ASN	THR	engineered mutation	UNP Q2N0S6
I	433	CYS	ALA	engineered mutation	UNP Q2N0S6
I	501	CYS	ALA	engineered mutation	UNP Q2N0S6

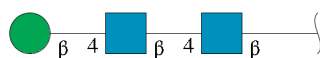
- Molecule 3 is a protein called J601-1B2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	122	Total	C	N	O	S	0	0
			953	605	162	184	2		
3	J	122	Total	C	N	O	S	0	0
			953	605	162	184	2		
3	D	122	Total	C	N	O	S	0	0
			953	605	162	184	2		

- Molecule 4 is a protein called J601-1B2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	107	Total	C	N	O	S	0	0
			824	518	137	167	2		
4	K	107	Total	C	N	O	S	0	0
			824	518	137	167	2		
4	E	107	Total	C	N	O	S	0	0
			824	518	137	167	2		

- Molecule 5 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.



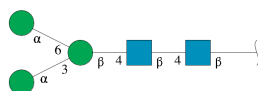
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	Q	3	Total	C	N	O	0	0
			39	22	2	15		
5	R	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	U	3	Total	C	N	O	0	0
			39	22	2	15		
5	Y	3	Total	C	N	O	0	0
			39	22	2	15		
5	Z	3	Total	C	N	O	0	0
			39	22	2	15		
5	f	3	Total	C	N	O	0	0
			39	22	2	15		
5	g	3	Total	C	N	O	0	0
			39	22	2	15		
5	i	3	Total	C	N	O	0	0
			39	22	2	15		
5	j	3	Total	C	N	O	0	0
			39	22	2	15		
5	k	3	Total	C	N	O	0	0
			39	22	2	15		
5	m	3	Total	C	N	O	0	0
			39	22	2	15		
5	n	3	Total	C	N	O	0	0
			39	22	2	15		
5	t	3	Total	C	N	O	0	0
			39	22	2	15		
5	u	3	Total	C	N	O	0	0
			39	22	2	15		
5	v	3	Total	C	N	O	0	0
			39	22	2	15		
5	w	3	Total	C	N	O	0	0
			39	22	2	15		
5	x	3	Total	C	N	O	0	0
			39	22	2	15		
5	y	3	Total	C	N	O	0	0
			39	22	2	15		
5	0	3	Total	C	N	O	0	0
			39	22	2	15		
5	1	3	Total	C	N	O	0	0
			39	22	2	15		

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



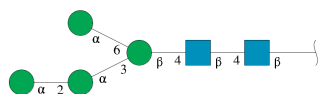
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	5	Total	C	N	O	0	0
			61	34	2	25		
6	b	5	Total	C	N	O	0	0
			61	34	2	25		
6	p	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 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
7	O	2	Total	C	N	O	0	0
			28	16	2	10		
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	h	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	2	Total	C	N	O	0	0
			28	16	2	10		
7	q	2	Total	C	N	O	0	0
			28	16	2	10		
7	r	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	6	Total	C	N	O	0	0
			72	40	2	30		
8	e	6	Total	C	N	O	0	0
			72	40	2	30		
8	s	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 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
9	T	4	Total	C	N	O	0	0
			50	28	2	20		
9	V	4	Total	C	N	O	0	0
			50	28	2	20		
9	W	4	Total	C	N	O	0	0
			50	28	2	20		
9	l	4	Total	C	N	O	0	0
			50	28	2	20		
9	z	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



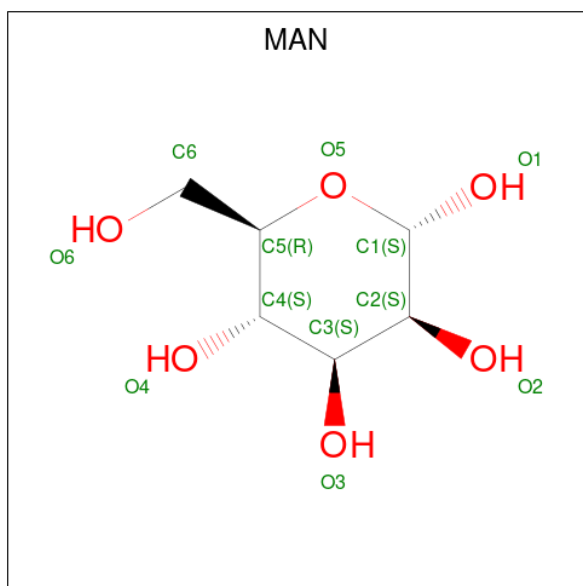
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	B	1	Total	C	N	O	0
			14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

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

- Molecule 11 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).




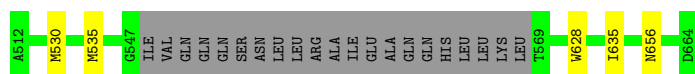
Mol	Chain	Residues	Atoms			AltConf
11	G	1	Total	C	O	0
			11	6	5	
11	I	1	Total	C	O	0
			11	6	5	

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.

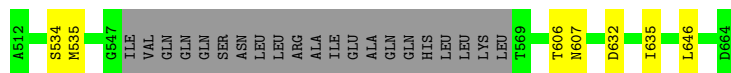
- Molecule 1: Envelope glycoprotein BG505 DS-SOSIP gp41

Chain A: 




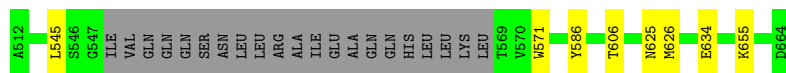
- Molecule 1: Envelope glycoprotein BG505 DS-SOSIP gp41

Chain B: 



- Molecule 1: Envelope glycoprotein BG505 DS-SOSIP gp41

Chain F: 



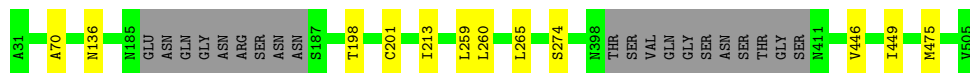
- Molecule 2: Envelope glycoprotein BG505 DS-SOSIP gp120

Chain C: 

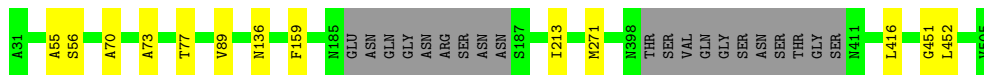


- Molecule 2: Envelope glycoprotein BG505 DS-SOSIP gp120

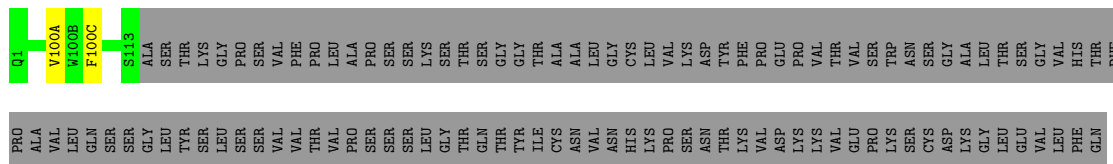
Chain G: 



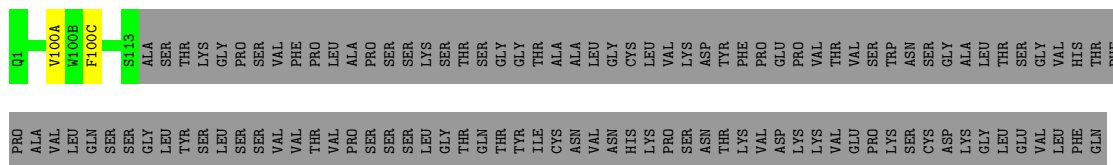
- Molecule 2: Envelope glycoprotein BG505 DS-SOSIP gp120



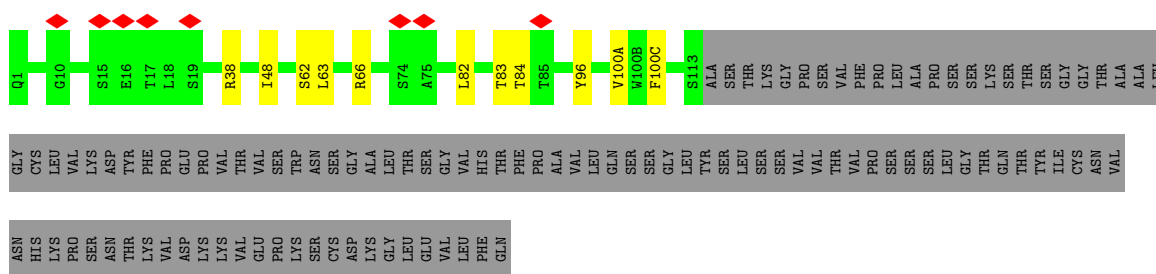
- Molecule 3: J601-1B2 heavy chain



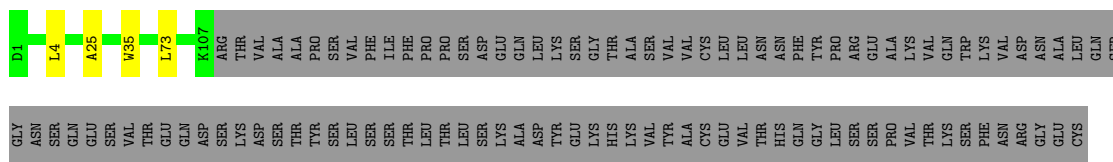
- Molecule 3: J601-1B2 heavy chain



- Molecule 3: J601-1B2 heavy chain

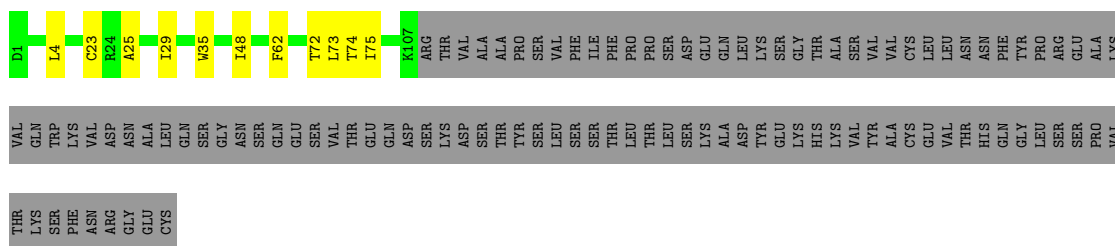


- Molecule 4: J601-1B2 light chain

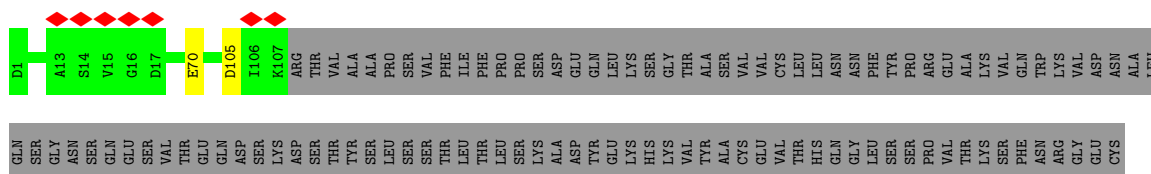


- Molecule 4: J601-1B2 light chain





- Molecule 4: J601-1B2 light chain



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



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



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



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



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

Chain Y:  67% 33%

MAG1
MAG2
BMA3

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

Chain Z:  67% 33%

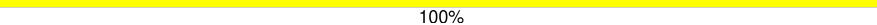
MAG1
MAG2
BMA3

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

Chain f:  100%

MAG1
MAG2
BMA3

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

Chain g:  100%

MAG1
MAG2
BMA3

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

Chain i:  67% 33%

MAG1
MAG2
BMA3

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

Chain j:  67% 33%

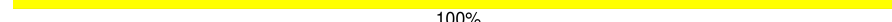
MAG1
MAG2
BMA3

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

Chain k:  33% 67%


NAG1
NAG2
BMA3

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

Chain m:  100%

NAG1
NAG2
BMA3

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

Chain n:  33% 67%

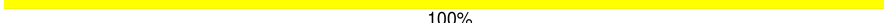
NAG1
NAG2
BMA3

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

Chain t:  100%

NAG1
NAG2
BMA3

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

Chain u:  100%

NAG1
NAG2
BMA3

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

Chain v:  67% 33%

NAG1
NAG2
BMA3

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

Chain w:  67% 33%


NAG1
NAG2
BMA3

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

Chain x:  67% 33%

MAG1
MAG2
BMA3

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

Chain y:  67% 33%

MAG1
MAG2
BMA3

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

Chain 0:  67% 33%

MAG1
MAG2
BMA3

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

Chain 1:  67% 33%

MAG1
MAG2
BMA3

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

Chain N:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

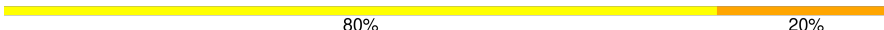
- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

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

nose

Chain p:  80% 20%



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

Chain O:  50% 50%



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

Chain S:  100%



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

Chain X:  50% 50%



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

Chain a:  50% 50%



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

Chain c:  50% 50%




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

Chain d:  50% 50%



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

Chain h:  100%



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

Chain o:  100%



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

Chain q:  50% 50%



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

Chain r:  50% 50%




- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

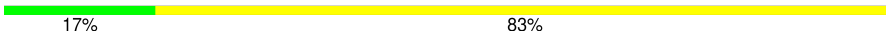


- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  17% 67% 17%



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  17% 83%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 9: 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 T:  25% 75%

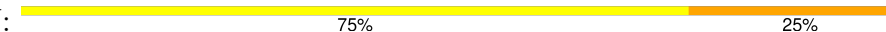
MAG1
MAG2
BMA3
MAN4

- Molecule 9: 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 V:  50% 50%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: 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:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: 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 l:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: 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 z:  100%

MAG1
MAG2
BMA3
MAN4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	806645	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON APOLLO (4k x 4k)	Depositor
Maximum map value	0.699	Depositor
Minimum map value	-0.268	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.0823	Depositor
Map size (\AA)	387.84, 387.84, 387.84	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.01, 1.01, 1.01	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, NAG, BMA

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	0.21	0/1052	0.47	0/1427
1	B	0.20	0/1052	0.42	0/1427
1	F	0.19	0/1052	0.42	0/1427
2	C	0.19	0/3638	0.36	0/4939
2	G	0.20	0/3638	0.36	0/4939
2	I	0.20	0/3638	0.36	0/4939
3	D	0.16	0/982	0.39	0/1341
3	H	0.17	0/982	0.34	0/1341
3	J	0.17	0/982	0.35	0/1341
4	E	0.15	0/841	0.34	0/1141
4	K	0.16	0/841	0.30	0/1141
4	L	0.16	0/841	0.32	0/1141
All	All	0.19	0/19539	0.37	0/26544

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

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	1034	0	1012	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1034	0	1011	6	0
1	F	1034	0	1013	5	0
2	C	3564	0	3487	4	0
2	G	3564	0	3487	8	0
2	I	3564	0	3488	11	0
3	D	953	0	895	5	0
3	H	953	0	895	1	0
3	J	953	0	895	1	0
4	E	824	0	801	0	0
4	K	824	0	801	9	0
4	L	824	0	801	3	0
5	0	39	0	34	1	0
5	1	39	0	34	1	0
5	M	39	0	34	1	0
5	Q	39	0	34	0	0
5	R	39	0	34	0	0
5	U	39	0	34	1	0
5	Y	39	0	34	2	0
5	Z	39	0	34	1	0
5	f	39	0	34	0	0
5	g	39	0	34	0	0
5	i	39	0	34	0	0
5	j	39	0	34	0	0
5	k	39	0	34	0	0
5	m	39	0	34	0	0
5	n	39	0	34	0	0
5	t	39	0	34	0	0
5	u	39	0	34	0	0
5	v	39	0	34	0	0
5	w	39	0	34	0	0
5	x	39	0	34	1	0
5	y	39	0	34	1	0
6	N	61	0	52	0	0
6	b	61	0	52	0	0
6	p	61	0	52	1	0
7	O	28	0	25	0	0
7	S	28	0	25	0	0
7	X	28	0	25	1	0
7	a	28	0	25	0	0
7	c	28	0	25	1	0
7	d	28	0	25	0	0
7	h	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	o	28	0	25	0	0
7	q	28	0	25	0	0
7	r	28	0	25	0	0
8	P	72	0	61	1	0
8	e	72	0	61	1	0
8	s	72	0	61	0	0
9	T	50	0	43	0	0
9	V	50	0	43	3	0
9	W	50	0	43	1	0
9	l	50	0	43	0	0
9	z	50	0	43	0	0
10	A	28	0	26	0	0
10	B	42	0	39	0	0
10	C	70	0	65	1	0
10	F	28	0	26	1	0
10	G	42	0	39	1	0
10	I	56	0	52	3	0
11	G	11	0	10	0	0
11	I	11	0	10	0	0
All	All	21161	0	20371	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)
9:V:2:NAG:H82	5:Y:1:NAG:H83	1.54	0.89
2:C:70:ALA:HB2	2:C:213:ILE:HD11	1.67	0.77
1:A:535:MET:HE2	1:A:535:MET:N	2.10	0.66
2:G:475:MET:N	2:G:475:MET:HE2	2.13	0.62
3:H:100(A):VAL:HG11	3:H:100(C):PHE:CZ	2.34	0.62
3:J:100(A):VAL:HG11	3:J:100(C):PHE:CZ	2.38	0.58
2:G:70:ALA:HB2	2:G:213:ILE:HD11	1.85	0.58
1:B:535:MET:N	1:B:535:MET:HE2	2.19	0.57
2:I:271:MET:HE3	2:I:271:MET:HA	1.85	0.57
4:L:35:TRP:CE3	4:L:73:LEU:HD22	2.40	0.56
5:x:1:NAG:O6	5:x:2:NAG:H82	2.06	0.56
2:C:309:ILE:HD12	2:C:315:GLN:O	2.07	0.55
1:F:571:TRP:HD1	2:I:73:ALA:HB3	1.72	0.55
2:I:70:ALA:HB2	2:I:213:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:136:ASN:OD1	10:G:601:NAG:H82	2.08	0.53
8:P:1:NAG:H62	9:W:1:NAG:H83	1.90	0.53
1:B:606:THR:HG21	1:B:646:LEU:CD2	2.39	0.53
2:G:446:VAL:HB	8:e:2:NAG:H81	1.90	0.53
4:K:62:PHE:CD2	4:K:75:ILE:HD12	2.44	0.53
1:A:530:MET:HE1	1:A:628:TRP:CZ2	2.43	0.53
5:y:2:NAG:H82	5:1:1:NAG:H83	1.92	0.52
2:G:259:LEU:HB3	2:G:449:ILE:HD11	1.92	0.52
2:I:451:GLY:C	2:I:452:LEU:HD12	2.35	0.51
4:K:62:PHE:HD2	4:K:75:ILE:HD12	1.74	0.51
3:D:100(A):VAL:HG11	3:D:100(C):PHE:CZ	2.45	0.51
1:F:545:LEU:HD21	1:F:586:TYR:CG	2.46	0.51
1:A:635:ILE:O	1:A:635:ILE:HG22	2.11	0.50
4:K:35:TRP:CE2	4:K:73:LEU:HD13	2.47	0.49
4:K:35:TRP:HB2	4:K:48:ILE:HG22	1.95	0.49
3:D:62:SER:C	3:D:63:LEU:HD22	2.38	0.49
1:F:625:ASN:O	1:F:626:MET:HE2	2.12	0.49
1:F:571:TRP:CD1	2:I:73:ALA:HB3	2.49	0.48
2:I:159:PHE:HA	5:0:1:NAG:H81	1.97	0.47
9:V:2:NAG:H82	5:Y:1:NAG:C8	2.35	0.47
3:D:38:ARG:HG2	3:D:48:ILE:HD11	1.97	0.46
2:C:122:LEU:HD12	2:C:125:LEU:HD22	1.97	0.46
1:B:635:ILE:O	1:B:635:ILE:HG22	2.15	0.46
2:I:136:ASN:CG	10:I:602:NAG:H82	2.40	0.46
1:F:634:GLU:O	10:F:702:NAG:H81	2.16	0.46
2:I:136:ASN:ND2	10:I:602:NAG:H82	2.31	0.46
7:X:1:NAG:H83	7:X:1:NAG:H3	1.99	0.45
4:K:4:LEU:HD12	4:K:23:CYS:SG	2.57	0.44
1:B:534:SER:C	1:B:535:MET:HE2	2.42	0.44
1:B:535:MET:HE2	1:B:535:MET:CA	2.48	0.44
2:G:198:THR:OG1	7:c:1:NAG:H82	2.17	0.44
5:Z:1:NAG:H3	5:Z:1:NAG:H83	2.00	0.44
2:G:260:LEU:O	2:G:449:ILE:HD12	2.18	0.44
2:I:56:SER:O	2:I:77:THR:HG23	2.18	0.44
2:I:55:ALA:HB1	2:I:77:THR:HG22	1.99	0.44
4:K:29:ILE:HG22	4:K:29:ILE:O	2.18	0.43
3:D:66:ARG:NH2	3:D:82:LEU:HD11	2.33	0.43
2:G:265:LEU:H	2:G:265:LEU:HD23	1.83	0.42
2:I:70:ALA:CB	2:I:213:ILE:HD11	2.49	0.42
4:K:74:THR:C	4:K:75:ILE:HD13	2.45	0.42
1:B:606:THR:HG22	1:B:607:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:601:NAG:H3	10:I:601:NAG:H83	2.00	0.42
6:p:1:NAG:H83	6:p:1:NAG:H3	2.01	0.42
4:L:4:LEU:HD13	4:L:25:ALA:HA	2.00	0.42
5:M:1:NAG:H83	5:M:1:NAG:H3	2.00	0.42
2:C:136:ASN:OD1	10:C:602:NAG:H82	2.20	0.41
4:K:4:LEU:HD13	4:K:25:ALA:HA	2.03	0.41
5:U:3:BMA:H61	9:V:4:MAN:H2	2.03	0.41
4:K:72:THR:O	4:K:73:LEU:HD12	2.21	0.41
4:L:35:TRP:CE2	4:L:73:LEU:HD13	2.56	0.40
3:D:83:THR:HG22	3:D:84:THR:N	2.37	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	128/153 (84%)	117 (91%)	11 (9%)	0	100	100
1	B	128/153 (84%)	118 (92%)	10 (8%)	0	100	100
1	F	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
2	C	447/473 (94%)	421 (94%)	26 (6%)	0	100	100
2	G	447/473 (94%)	419 (94%)	28 (6%)	0	100	100
2	I	447/473 (94%)	417 (93%)	30 (7%)	0	100	100
3	D	120/234 (51%)	109 (91%)	11 (9%)	0	100	100
3	H	120/234 (51%)	108 (90%)	12 (10%)	0	100	100
3	J	120/234 (51%)	108 (90%)	12 (10%)	0	100	100
4	E	105/214 (49%)	99 (94%)	6 (6%)	0	100	100
4	K	105/214 (49%)	101 (96%)	4 (4%)	0	100	100
4	L	105/214 (49%)	98 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2400/3222 (74%)	2235 (93%)	165 (7%)	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	110/129 (85%)	109 (99%)	1 (1%)	75	83
1	B	110/129 (85%)	109 (99%)	1 (1%)	75	83
1	F	110/129 (85%)	108 (98%)	2 (2%)	54	71
2	C	405/422 (96%)	403 (100%)	2 (0%)	86	90
2	G	405/422 (96%)	403 (100%)	2 (0%)	86	90
2	I	405/422 (96%)	403 (100%)	2 (0%)	86	90
3	D	103/200 (52%)	102 (99%)	1 (1%)	73	80
3	H	103/200 (52%)	103 (100%)	0	100	100
3	J	103/200 (52%)	103 (100%)	0	100	100
4	E	92/188 (49%)	90 (98%)	2 (2%)	47	65
4	K	92/188 (49%)	92 (100%)	0	100	100
4	L	92/188 (49%)	92 (100%)	0	100	100
All	All	2130/2817 (76%)	2117 (99%)	13 (1%)	82	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	656	ASN
2	C	236	THR
2	C	342	LEU
1	B	632	ASP
2	G	201	CYS
2	G	274	SER

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Mol	Chain	Res	Type
1	F	606	THR
1	F	655	LYS
2	I	89	VAL
2	I	416	LEU
3	D	96	TYR
4	E	70	GLU
4	E	105	ASP

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	625	ASN
1	B	640	GLN
2	G	72	HIS
2	G	203	GLN
2	I	105	HIS
2	I	283	ASN
2	I	411	ASN
3	J	3	GLN
4	K	30	ASN
3	D	33	HIS
3	D	99	ASN
4	E	6	GLN

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](#)

136 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	0	1	5,2	14,14,15	0.81	0	17,19,21	1.08	2 (11%)
5	NAG	0	2	5	14,14,15	0.74	0	17,19,21	0.96	1 (5%)
5	BMA	0	3	5	11,11,12	0.87	0	15,15,17	1.87	4 (26%)
5	NAG	1	1	5,2	14,14,15	0.76	0	17,19,21	1.00	1 (5%)
5	NAG	1	2	5	14,14,15	0.69	0	17,19,21	1.57	2 (11%)
5	BMA	1	3	5	11,11,12	0.82	0	15,15,17	1.80	2 (13%)
5	NAG	M	1	5,2	14,14,15	0.71	0	17,19,21	1.94	4 (23%)
5	NAG	M	2	5	14,14,15	0.71	0	17,19,21	1.34	1 (5%)
5	BMA	M	3	5	11,11,12	0.83	0	15,15,17	1.94	3 (20%)
6	NAG	N	1	6,2	14,14,15	0.77	0	17,19,21	1.92	4 (23%)
6	NAG	N	2	6	14,14,15	0.76	0	17,19,21	1.27	2 (11%)
6	BMA	N	3	6	11,11,12	0.84	0	15,15,17	1.90	3 (20%)
6	MAN	N	4	6	11,11,12	0.78	0	15,15,17	1.00	1 (6%)
6	MAN	N	5	6	11,11,12	0.71	0	15,15,17	1.20	1 (6%)
7	NAG	O	1	7,2	14,14,15	0.75	0	17,19,21	1.05	2 (11%)
7	NAG	O	2	7	14,14,15	0.74	0	17,19,21	0.74	0
8	NAG	P	1	8,2	14,14,15	0.80	0	17,19,21	0.82	0
8	NAG	P	2	8	14,14,15	0.81	0	17,19,21	1.16	1 (5%)
8	BMA	P	3	8	11,11,12	0.81	0	15,15,17	1.60	3 (20%)
8	MAN	P	4	8	11,11,12	0.80	0	15,15,17	1.03	1 (6%)
8	MAN	P	5	8	11,11,12	0.78	0	15,15,17	0.93	1 (6%)
8	MAN	P	6	8	11,11,12	0.75	0	15,15,17	1.08	1 (6%)
5	NAG	Q	1	5,2	14,14,15	0.62	0	17,19,21	1.56	4 (23%)
5	NAG	Q	2	5	14,14,15	0.79	0	17,19,21	1.13	1 (5%)
5	BMA	Q	3	5	11,11,12	0.91	0	15,15,17	1.92	4 (26%)
5	NAG	R	1	5,2	14,14,15	0.76	0	17,19,21	0.80	0
5	NAG	R	2	5	14,14,15	0.73	0	17,19,21	0.86	0
5	BMA	R	3	5	11,11,12	0.80	0	15,15,17	1.77	2 (13%)
7	NAG	S	1	7,2	14,14,15	0.74	0	17,19,21	1.86	3 (17%)
7	NAG	S	2	7	14,14,15	0.72	0	17,19,21	1.36	1 (5%)
9	NAG	T	1	9,2	14,14,15	0.81	0	17,19,21	0.89	1 (5%)
9	NAG	T	2	9	14,14,15	0.72	0	17,19,21	1.00	0
9	BMA	T	3	9	11,11,12	0.83	0	15,15,17	2.11	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	T	4	9	11,11,12	0.59	0	15,15,17	2.83	3 (20%)
5	NAG	U	1	5,2	14,14,15	0.76	0	17,19,21	0.87	0
5	NAG	U	2	5	14,14,15	0.73	0	17,19,21	0.90	0
5	BMA	U	3	5	11,11,12	0.85	0	15,15,17	2.10	4 (26%)
9	NAG	V	1	9,2	14,14,15	0.79	0	17,19,21	0.88	1 (5%)
9	NAG	V	2	9	14,14,15	0.73	0	17,19,21	1.25	2 (11%)
9	BMA	V	3	9	11,11,12	0.84	0	15,15,17	2.23	3 (20%)
9	MAN	V	4	9	11,11,12	0.58	0	15,15,17	2.75	2 (13%)
9	NAG	W	1	9,2	14,14,15	0.78	0	17,19,21	1.02	1 (5%)
9	NAG	W	2	9	14,14,15	0.72	0	17,19,21	1.01	1 (5%)
9	BMA	W	3	9	11,11,12	1.16	1 (9%)	15,15,17	2.10	6 (40%)
9	MAN	W	4	9	11,11,12	0.65	0	15,15,17	1.90	1 (6%)
7	NAG	X	1	7,2	14,14,15	0.74	0	17,19,21	1.82	2 (11%)
7	NAG	X	2	7	14,14,15	0.71	0	17,19,21	0.88	0
5	NAG	Y	1	5,2	14,14,15	0.76	0	17,19,21	1.02	2 (11%)
5	NAG	Y	2	5	14,14,15	0.70	0	17,19,21	1.03	1 (5%)
5	BMA	Y	3	5	11,11,12	0.82	0	15,15,17	1.83	2 (13%)
5	NAG	Z	1	5,2	14,14,15	0.73	0	17,19,21	1.87	3 (17%)
5	NAG	Z	2	5	14,14,15	0.71	0	17,19,21	1.35	1 (5%)
5	BMA	Z	3	5	11,11,12	0.98	1 (9%)	15,15,17	2.95	7 (46%)
7	NAG	a	1	7,2	14,14,15	0.70	0	17,19,21	0.92	0
7	NAG	a	2	7	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
6	NAG	b	1	6,2	14,14,15	0.79	0	17,19,21	1.94	4 (23%)
6	NAG	b	2	6	14,14,15	0.80	0	17,19,21	1.12	1 (5%)
6	BMA	b	3	6	11,11,12	0.81	0	15,15,17	1.81	3 (20%)
6	MAN	b	4	6	11,11,12	0.85	1 (9%)	15,15,17	0.92	0
6	MAN	b	5	6	11,11,12	0.69	0	15,15,17	1.20	1 (6%)
7	NAG	c	1	7,2	14,14,15	0.76	0	17,19,21	0.73	0
7	NAG	c	2	7	14,14,15	0.73	0	17,19,21	0.87	0
7	NAG	d	1	7,2	14,14,15	0.80	0	17,19,21	1.05	2 (11%)
7	NAG	d	2	7	14,14,15	0.71	0	17,19,21	0.85	0
8	NAG	e	1	8,2	14,14,15	0.83	0	17,19,21	0.81	0
8	NAG	e	2	8	14,14,15	0.80	0	17,19,21	1.10	1 (5%)
8	BMA	e	3	8	11,11,12	0.81	0	15,15,17	1.71	3 (20%)
8	MAN	e	4	8	11,11,12	0.79	1 (9%)	15,15,17	0.98	0
8	MAN	e	5	8	11,11,12	0.76	0	15,15,17	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	e	6	8	11,11,12	0.74	0	15,15,17	1.01	1 (6%)
5	NAG	f	1	5,2	14,14,15	0.65	0	17,19,21	1.38	1 (5%)
5	NAG	f	2	5	14,14,15	0.78	0	17,19,21	1.10	2 (11%)
5	BMA	f	3	5	11,11,12	0.91	0	15,15,17	1.96	4 (26%)
5	NAG	g	1	5,2	14,14,15	0.75	0	17,19,21	1.98	5 (29%)
5	NAG	g	2	5	14,14,15	0.71	0	17,19,21	1.02	2 (11%)
5	BMA	g	3	5	11,11,12	0.81	0	15,15,17	1.68	2 (13%)
7	NAG	h	1	7,2	14,14,15	0.73	0	17,19,21	1.05	1 (5%)
7	NAG	h	2	7	14,14,15	0.72	0	17,19,21	1.42	1 (5%)
5	NAG	i	1	5,2	14,14,15	0.81	0	17,19,21	0.81	0
5	NAG	i	2	5	14,14,15	0.75	0	17,19,21	0.97	0
5	BMA	i	3	5	11,11,12	0.83	0	15,15,17	2.03	5 (33%)
5	NAG	j	1	5,2	14,14,15	0.77	0	17,19,21	0.86	0
5	NAG	j	2	5	14,14,15	0.71	0	17,19,21	0.90	0
5	BMA	j	3	5	11,11,12	0.80	0	15,15,17	1.82	2 (13%)
5	NAG	k	1	5,2	14,14,15	0.76	0	17,19,21	1.01	2 (11%)
5	NAG	k	2	5	14,14,15	0.73	0	17,19,21	1.04	0
5	BMA	k	3	5	11,11,12	0.81	0	15,15,17	1.75	3 (20%)
9	NAG	l	1	9,2	14,14,15	0.73	0	17,19,21	1.21	1 (5%)
9	NAG	l	2	9	14,14,15	0.73	0	17,19,21	0.92	0
9	BMA	l	3	9	11,11,12	0.81	0	15,15,17	1.91	3 (20%)
9	MAN	l	4	9	11,11,12	0.78	1 (9%)	15,15,17	0.88	0
5	NAG	m	1	5,2	14,14,15	0.76	0	17,19,21	1.90	3 (17%)
5	NAG	m	2	5	14,14,15	0.69	0	17,19,21	1.09	2 (11%)
5	BMA	m	3	5	11,11,12	0.80	0	15,15,17	1.87	1 (6%)
5	NAG	n	1	5,2	14,14,15	0.76	0	17,19,21	0.94	1 (5%)
5	NAG	n	2	5	14,14,15	0.70	0	17,19,21	0.93	0
5	BMA	n	3	5	11,11,12	0.83	0	15,15,17	1.80	2 (13%)
7	NAG	o	1	7,2	14,14,15	0.71	0	17,19,21	1.00	0
7	NAG	o	2	7	14,14,15	0.74	0	17,19,21	0.96	0
6	NAG	p	1	6,2	14,14,15	0.77	0	17,19,21	1.95	4 (23%)
6	NAG	p	2	6	14,14,15	0.78	0	17,19,21	1.30	2 (11%)
6	BMA	p	3	6	11,11,12	0.86	0	15,15,17	1.96	3 (20%)
6	MAN	p	4	6	11,11,12	0.76	0	15,15,17	0.92	1 (6%)
6	MAN	p	5	6	11,11,12	0.74	0	15,15,17	1.05	1 (6%)
7	NAG	q	1	7,2	14,14,15	0.75	0	17,19,21	0.77	0
7	NAG	q	2	7	14,14,15	0.72	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	r	1	7,2	14,14,15	0.77	0	17,19,21	1.21	2 (11%)
7	NAG	r	2	7	14,14,15	0.69	0	17,19,21	0.80	0
8	NAG	s	1	8,2	14,14,15	0.87	0	17,19,21	0.70	0
8	NAG	s	2	8	14,14,15	0.80	0	17,19,21	1.02	1 (5%)
8	BMA	s	3	8	11,11,12	0.82	0	15,15,17	1.54	2 (13%)
8	MAN	s	4	8	11,11,12	0.78	0	15,15,17	1.06	1 (6%)
8	MAN	s	5	8	11,11,12	0.72	0	15,15,17	1.04	1 (6%)
8	MAN	s	6	8	11,11,12	0.72	0	15,15,17	1.13	1 (6%)
5	NAG	t	1	5,2	14,14,15	0.60	0	17,19,21	1.59	3 (17%)
5	NAG	t	2	5	14,14,15	0.79	0	17,19,21	1.14	2 (11%)
5	BMA	t	3	5	11,11,12	0.90	0	15,15,17	2.01	4 (26%)
5	NAG	u	1	5,2	14,14,15	0.80	0	17,19,21	0.81	1 (5%)
5	NAG	u	2	5	14,14,15	0.65	0	17,19,21	1.44	2 (11%)
5	BMA	u	3	5	11,11,12	0.91	1 (9%)	15,15,17	3.27	6 (40%)
5	NAG	v	1	5,2	14,14,15	0.77	0	17,19,21	0.94	0
5	NAG	v	2	5	14,14,15	0.72	0	17,19,21	0.87	0
5	BMA	v	3	5	11,11,12	0.83	0	15,15,17	2.05	4 (26%)
5	NAG	w	1	5,2	14,14,15	0.80	0	17,19,21	0.85	0
5	NAG	w	2	5	14,14,15	0.74	0	17,19,21	0.96	0
5	BMA	w	3	5	11,11,12	0.80	0	15,15,17	1.83	2 (13%)
5	NAG	x	1	5,2	14,14,15	0.77	0	17,19,21	0.94	0
5	NAG	x	2	5	14,14,15	0.71	0	17,19,21	1.12	1 (5%)
5	BMA	x	3	5	11,11,12	0.80	0	15,15,17	1.75	1 (6%)
5	NAG	y	1	5,2	14,14,15	0.85	0	17,19,21	0.97	1 (5%)
5	NAG	y	2	5	14,14,15	0.71	0	17,19,21	1.30	3 (17%)
5	BMA	y	3	5	11,11,12	0.90	1 (9%)	15,15,17	3.42	7 (46%)
9	NAG	z	1	9,2	14,14,15	0.73	0	17,19,21	1.02	1 (5%)
9	NAG	z	2	9	14,14,15	0.71	0	17,19,21	1.54	2 (11%)
9	BMA	z	3	9	11,11,12	0.80	0	15,15,17	1.91	2 (13%)
9	MAN	z	4	9	11,11,12	0.79	1 (9%)	15,15,17	0.88	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	0	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	0	2	5	-	0/6/23/26	0/1/1/1
5	BMA	0	3	5	-	1/2/19/22	0/1/1/1
5	NAG	1	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	1	2	5	-	2/6/23/26	0/1/1/1
5	BMA	1	3	5	-	0/2/19/22	0/1/1/1
5	NAG	M	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	1/2/19/22	0/1/1/1
6	NAG	N	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
7	NAG	O	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
8	NAG	P	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
8	BMA	P	3	8	-	2/2/19/22	0/1/1/1
8	MAN	P	4	8	-	1/2/19/22	0/1/1/1
8	MAN	P	5	8	-	0/2/19/22	0/1/1/1
8	MAN	P	6	8	-	0/2/19/22	0/1/1/1
5	NAG	Q	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
5	BMA	R	3	5	-	0/2/19/22	0/1/1/1
7	NAG	S	1	7,2	-	4/6/23/26	0/1/1/1
7	NAG	S	2	7	-	4/6/23/26	0/1/1/1
9	NAG	T	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
9	BMA	T	3	9	-	0/2/19/22	0/1/1/1
9	MAN	T	4	9	-	2/2/19/22	0/1/1/1
5	NAG	U	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1
5	BMA	U	3	5	-	1/2/19/22	0/1/1/1
9	NAG	V	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	0/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	V	4	9	-	2/2/19/22	0/1/1/1
9	NAG	W	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	W	2	9	-	0/6/23/26	0/1/1/1
9	BMA	W	3	9	-	2/2/19/22	0/1/1/1
9	MAN	W	4	9	-	1/2/19/22	0/1/1/1
7	NAG	X	1	7,2	-	4/6/23/26	0/1/1/1
7	NAG	X	2	7	-	0/6/23/26	0/1/1/1
5	NAG	Y	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	1/2/19/22	0/1/1/1
7	NAG	a	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
6	NAG	b	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1
6	BMA	b	3	6	-	1/2/19/22	0/1/1/1
6	MAN	b	4	6	-	0/2/19/22	0/1/1/1
6	MAN	b	5	6	-	1/2/19/22	0/1/1/1
7	NAG	c	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	1/6/23/26	0/1/1/1
7	NAG	d	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
8	NAG	e	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	0/6/23/26	0/1/1/1
8	BMA	e	3	8	-	2/2/19/22	0/1/1/1
8	MAN	e	4	8	-	1/2/19/22	0/1/1/1
8	MAN	e	5	8	-	0/2/19/22	0/1/1/1
8	MAN	e	6	8	-	0/2/19/22	0/1/1/1
5	NAG	f	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
5	BMA	f	3	5	-	0/2/19/22	0/1/1/1
5	NAG	g	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	g	2	5	-	0/6/23/26	0/1/1/1
5	BMA	g	3	5	-	0/2/19/22	0/1/1/1
7	NAG	h	1	7,2	-	3/6/23/26	0/1/1/1
7	NAG	h	2	7	-	3/6/23/26	0/1/1/1
5	NAG	i	1	5,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	i	2	5	-	2/6/23/26	0/1/1/1
5	BMA	i	3	5	-	0/2/19/22	0/1/1/1
5	NAG	j	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	j	2	5	-	0/6/23/26	0/1/1/1
5	BMA	j	3	5	-	1/2/19/22	0/1/1/1
5	NAG	k	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	k	2	5	-	0/6/23/26	0/1/1/1
5	BMA	k	3	5	-	2/2/19/22	0/1/1/1
9	NAG	l	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	l	2	9	-	0/6/23/26	0/1/1/1
9	BMA	l	3	9	-	1/2/19/22	0/1/1/1
9	MAN	l	4	9	-	0/2/19/22	0/1/1/1
5	NAG	m	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	m	2	5	-	0/6/23/26	0/1/1/1
5	BMA	m	3	5	-	1/2/19/22	0/1/1/1
5	NAG	n	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	n	2	5	-	0/6/23/26	0/1/1/1
5	BMA	n	3	5	-	0/2/19/22	0/1/1/1
7	NAG	o	1	7,2	-	1/6/23/26	0/1/1/1
7	NAG	o	2	7	-	2/6/23/26	0/1/1/1
6	NAG	p	1	6,2	-	5/6/23/26	0/1/1/1
6	NAG	p	2	6	-	0/6/23/26	0/1/1/1
6	BMA	p	3	6	-	2/2/19/22	0/1/1/1
6	MAN	p	4	6	-	0/2/19/22	0/1/1/1
6	MAN	p	5	6	-	0/2/19/22	0/1/1/1
7	NAG	q	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	q	2	7	-	1/6/23/26	0/1/1/1
7	NAG	r	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	r	2	7	-	1/6/23/26	0/1/1/1
8	NAG	s	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	s	2	8	-	0/6/23/26	0/1/1/1
8	BMA	s	3	8	-	1/2/19/22	0/1/1/1
8	MAN	s	4	8	-	1/2/19/22	0/1/1/1
8	MAN	s	5	8	-	0/2/19/22	0/1/1/1
8	MAN	s	6	8	-	0/2/19/22	0/1/1/1
5	NAG	t	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	t	2	5	-	2/6/23/26	0/1/1/1
5	BMA	t	3	5	-	0/2/19/22	0/1/1/1
5	NAG	u	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	u	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	u	3	5	-	0/2/19/22	0/1/1/1
5	NAG	v	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	v	2	5	-	1/6/23/26	0/1/1/1
5	BMA	v	3	5	-	0/2/19/22	0/1/1/1
5	NAG	w	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	w	2	5	-	1/6/23/26	0/1/1/1
5	BMA	w	3	5	-	0/2/19/22	0/1/1/1
5	NAG	x	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	x	2	5	-	0/6/23/26	0/1/1/1
5	BMA	x	3	5	-	1/2/19/22	0/1/1/1
5	NAG	y	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	y	3	5	-	1/2/19/22	0/1/1/1
9	NAG	z	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	z	3	9	-	1/2/19/22	1/1/1/1
9	MAN	z	4	9	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	3	BMA	C2-C3	3.21	1.57	1.52
5	Z	3	BMA	C2-C3	2.36	1.56	1.52
6	b	4	MAN	O5-C1	-2.26	1.39	1.43
9	z	4	MAN	O5-C1	-2.08	1.40	1.43
5	y	3	BMA	C2-C3	2.05	1.55	1.52
9	l	4	MAN	O5-C1	-2.05	1.40	1.43
8	e	4	MAN	O5-C1	-2.05	1.40	1.43
5	u	3	BMA	C2-C3	2.02	1.55	1.52

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	u	3	BMA	C1-O5-C5	10.34	126.04	112.19
5	y	3	BMA	C1-O5-C5	9.70	125.18	112.19
9	T	4	MAN	C1-O5-C5	9.53	124.96	112.19
9	V	4	MAN	C1-O5-C5	9.37	124.75	112.19
5	Z	3	BMA	C1-O5-C5	7.72	122.53	112.19
9	V	3	BMA	C1-O5-C5	6.74	121.22	112.19
9	W	4	MAN	C1-O5-C5	6.60	121.04	112.19
9	T	3	BMA	C1-O5-C5	6.47	120.86	112.19
9	z	3	BMA	C1-O5-C5	6.23	120.53	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	3	BMA	C1-O5-C5	6.23	120.53	112.19
5	v	3	BMA	C1-O5-C5	6.09	120.34	112.19
6	p	3	BMA	C1-O5-C5	5.98	120.19	112.19
9	l	3	BMA	C1-O5-C5	5.91	120.11	112.19
6	N	1	NAG	C2-N2-C7	5.84	130.72	122.90
7	X	1	NAG	C2-N2-C7	5.82	130.69	122.90
7	S	1	NAG	C2-N2-C7	5.80	130.67	122.90
6	b	1	NAG	C2-N2-C7	5.77	130.64	122.90
5	g	1	NAG	C2-N2-C7	5.76	130.62	122.90
5	m	3	BMA	C1-O5-C5	5.76	119.90	112.19
5	i	3	BMA	C1-O5-C5	5.76	119.90	112.19
6	p	1	NAG	C2-N2-C7	5.76	130.61	122.90
5	m	1	NAG	C2-N2-C7	5.72	130.56	122.90
6	N	3	BMA	C1-O5-C5	5.71	119.84	112.19
5	M	3	BMA	C1-O5-C5	5.69	119.81	112.19
5	Z	1	NAG	C2-N2-C7	5.62	130.43	122.90
5	M	1	NAG	C2-N2-C7	5.57	130.37	122.90
5	w	3	BMA	C1-O5-C5	5.37	119.38	112.19
5	0	3	BMA	C1-O5-C5	5.31	119.30	112.19
5	t	3	BMA	C1-O5-C5	5.28	119.26	112.19
5	j	3	BMA	C1-O5-C5	5.24	119.21	112.19
5	Y	3	BMA	C1-O5-C5	5.21	119.17	112.19
5	f	3	BMA	C1-O5-C5	5.19	119.14	112.19
5	R	3	BMA	C1-O5-C5	5.18	119.12	112.19
5	n	3	BMA	C1-O5-C5	5.16	119.10	112.19
5	l	3	BMA	C1-O5-C5	5.11	119.04	112.19
5	Q	3	BMA	C1-O5-C5	5.03	118.92	112.19
6	b	3	BMA	C1-O5-C5	4.94	118.81	112.19
5	x	3	BMA	C1-O5-C5	4.94	118.81	112.19
5	k	3	BMA	C1-O5-C5	4.85	118.69	112.19
5	Z	3	BMA	C1-C2-C3	4.83	116.67	109.64
5	y	3	BMA	C1-C2-C3	4.82	116.67	109.64
8	e	3	BMA	C1-O5-C5	4.71	118.50	112.19
9	W	3	BMA	O2-C2-C3	4.61	119.70	110.15
5	l	2	NAG	C2-N2-C7	4.58	129.04	122.90
9	z	2	NAG	C2-N2-C7	4.54	128.99	122.90
7	h	2	NAG	C2-N2-C7	4.43	128.83	122.90
5	y	3	BMA	C2-C3-C4	4.40	118.60	110.86
5	Z	3	BMA	C2-C3-C4	4.40	118.60	110.86
8	P	3	BMA	C1-O5-C5	4.35	118.02	112.19
5	t	1	NAG	C2-N2-C7	4.34	128.71	122.90
7	S	2	NAG	C2-N2-C7	4.33	128.70	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	u	2	NAG	C2-N2-C7	4.30	128.66	122.90
8	s	3	BMA	C1-O5-C5	4.23	117.86	112.19
5	Z	2	NAG	C2-N2-C7	4.17	128.49	122.90
5	g	3	BMA	C1-O5-C5	4.17	117.77	112.19
5	M	2	NAG	C2-N2-C7	4.16	128.47	122.90
9	W	3	BMA	C1-O5-C5	4.07	117.65	112.19
5	u	3	BMA	C1-C2-C3	4.02	115.50	109.64
5	Q	1	NAG	C2-N2-C7	3.72	127.88	122.90
5	y	3	BMA	C3-C4-C5	3.56	116.69	110.23
6	b	5	MAN	C1-O5-C5	3.56	116.95	112.19
5	u	3	BMA	C2-C3-C4	3.40	116.85	110.86
5	f	1	NAG	C2-N2-C7	3.23	127.23	122.90
6	N	5	MAN	C1-O5-C5	3.20	116.47	112.19
5	y	2	NAG	C1-O5-C5	3.17	116.43	112.19
5	t	3	BMA	C3-C4-C5	3.14	115.93	110.23
8	s	6	MAN	C1-O5-C5	3.12	116.36	112.19
7	r	1	NAG	O4-C4-C3	-3.01	103.29	110.38
5	f	3	BMA	C3-C4-C5	2.97	115.62	110.23
9	T	4	MAN	C1-C2-C3	2.96	113.96	109.64
8	e	3	BMA	O3-C3-C2	-2.96	104.02	110.05
5	y	3	BMA	O5-C1-C2	2.94	117.80	110.79
5	Q	3	BMA	C3-C4-C5	2.92	115.52	110.23
5	g	1	NAG	C8-C7-N2	2.90	120.93	116.12
8	e	2	NAG	C4-C3-C2	-2.89	106.78	111.02
6	b	1	NAG	C8-C7-N2	2.89	120.90	116.12
5	Q	2	NAG	O4-C4-C3	2.89	117.18	110.38
6	p	2	NAG	C1-O5-C5	2.88	116.05	112.19
5	Z	3	BMA	C3-C4-C5	2.88	115.45	110.23
5	m	1	NAG	C8-C7-N2	2.86	120.86	116.12
9	V	3	BMA	O3-C3-C2	-2.85	104.23	110.05
6	N	2	NAG	C1-O5-C5	2.84	115.99	112.19
8	P	6	MAN	C1-O5-C5	2.81	115.95	112.19
5	y	1	NAG	O5-C1-C2	-2.81	106.94	111.29
6	p	2	NAG	C4-C3-C2	-2.81	106.90	111.02
6	b	3	BMA	O3-C3-C2	-2.78	104.38	110.05
6	p	1	NAG	O5-C1-C2	-2.78	106.99	111.29
9	V	2	NAG	C4-C3-C2	-2.77	106.96	111.02
7	X	1	NAG	C8-C7-N2	2.77	120.70	116.12
8	s	5	MAN	C1-O5-C5	2.76	115.89	112.19
9	W	3	BMA	O3-C3-C2	2.75	115.67	110.05
9	l	1	NAG	C4-C3-C2	-2.75	106.99	111.02
6	b	2	NAG	C4-C3-C2	-2.72	107.03	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	2	NAG	O4-C4-C3	2.72	116.79	110.38
6	p	5	MAN	C1-O5-C5	2.71	115.82	112.19
6	N	2	NAG	C4-C3-C2	-2.71	107.05	111.02
7	S	1	NAG	C8-C7-N2	2.69	120.58	116.12
6	p	1	NAG	C8-C7-N2	2.66	120.53	116.12
5	t	2	NAG	O4-C4-C3	2.66	116.64	110.38
6	N	1	NAG	C8-C7-N2	2.66	120.52	116.12
5	g	1	NAG	O5-C1-C2	-2.65	107.19	111.29
5	i	3	BMA	C3-C4-C5	2.64	115.03	110.23
5	t	2	NAG	O5-C1-C2	-2.64	107.21	111.29
9	l	3	BMA	O3-C3-C2	-2.63	104.69	110.05
5	t	3	BMA	C2-C3-C4	2.63	115.48	110.86
6	b	1	NAG	C1-C2-N2	2.63	114.57	110.43
5	k	1	NAG	O5-C1-C2	-2.61	107.25	111.29
9	W	3	BMA	C3-C4-C5	2.60	114.95	110.23
5	g	1	NAG	C1-C2-N2	2.60	114.53	110.43
5	f	3	BMA	C2-C3-C4	2.59	115.42	110.86
6	N	4	MAN	C1-O5-C5	2.58	115.65	112.19
5	x	2	NAG	C1-O5-C5	2.58	115.64	112.19
5	Z	1	NAG	C8-C7-N2	2.58	120.39	116.12
5	U	3	BMA	C3-C4-C5	2.57	114.90	110.23
9	W	1	NAG	C4-C3-C2	-2.56	107.27	111.02
5	Y	1	NAG	O5-C1-C2	-2.56	107.33	111.29
5	Q	1	NAG	O5-C1-C2	-2.56	107.33	111.29
5	m	1	NAG	C1-C2-N2	2.55	114.46	110.43
5	Q	3	BMA	C2-C3-C4	2.54	115.33	110.86
9	V	4	MAN	C1-C2-C3	2.52	113.31	109.64
5	l	1	NAG	O5-C1-C2	-2.51	107.41	111.29
9	z	2	NAG	O5-C1-C2	-2.50	107.42	111.29
8	s	2	NAG	C4-C3-C2	-2.50	107.35	111.02
8	P	3	BMA	O3-C3-C2	-2.49	104.97	110.05
5	u	3	BMA	C3-C4-C5	2.48	114.73	110.23
9	T	3	BMA	O3-C3-C2	-2.48	104.99	110.05
7	O	1	NAG	O5-C1-C2	-2.48	107.45	111.29
5	y	3	BMA	O4-C4-C3	-2.46	104.58	110.38
9	W	3	BMA	O4-C4-C3	-2.43	104.64	110.38
5	y	2	NAG	C4-C3-C2	-2.43	107.46	111.02
6	N	1	NAG	C1-C2-N2	2.42	114.25	110.43
5	g	2	NAG	O5-C1-C2	-2.42	107.55	111.29
5	M	1	NAG	C1-C2-N2	2.42	114.24	110.43
9	T	4	MAN	O5-C1-C2	2.42	116.55	110.79
5	g	3	BMA	C3-C4-C5	2.41	114.61	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	3	BMA	C2-C3-C4	2.40	115.09	110.86
5	M	1	NAG	C8-C7-N2	2.40	120.10	116.12
7	O	1	NAG	O4-C4-C3	-2.39	104.75	110.38
5	v	3	BMA	C3-C4-C5	2.38	114.56	110.23
5	i	3	BMA	C2-C3-C4	2.38	115.05	110.86
5	Z	3	BMA	O5-C1-C2	2.38	116.46	110.79
5	k	3	BMA	C3-C4-C5	2.37	114.53	110.23
7	S	1	NAG	C1-C2-N2	2.36	114.14	110.43
6	b	3	BMA	C2-C3-C4	2.35	115.00	110.86
8	P	2	NAG	C4-C3-C2	-2.35	107.58	111.02
8	e	6	MAN	C1-O5-C5	2.35	115.33	112.19
6	p	3	BMA	C2-C3-C4	2.34	114.98	110.86
9	z	3	BMA	O3-C3-C2	-2.34	105.28	110.05
5	y	3	BMA	O3-C3-C2	-2.34	105.28	110.05
8	s	4	MAN	C1-O5-C5	2.33	115.31	112.19
5	0	3	BMA	C3-C4-C5	2.33	114.45	110.23
6	b	1	NAG	O5-C1-C2	-2.31	107.72	111.29
5	t	1	NAG	O7-C7-N2	2.31	126.06	121.98
5	n	3	BMA	C3-C4-C5	2.30	114.40	110.23
5	Z	3	BMA	O4-C4-C3	-2.30	104.96	110.38
5	0	3	BMA	C2-C3-C4	2.30	114.90	110.86
5	m	2	NAG	O5-C1-C2	-2.30	107.74	111.29
5	Q	1	NAG	C4-C3-C2	-2.28	107.67	111.02
5	Y	3	BMA	C3-C4-C5	2.26	114.34	110.23
9	T	3	BMA	C2-C3-C4	2.25	114.82	110.86
5	M	3	BMA	C3-C4-C5	2.25	114.32	110.23
9	z	1	NAG	C4-C3-C2	-2.25	107.72	111.02
5	t	3	BMA	O4-C4-C3	-2.24	105.09	110.38
8	P	4	MAN	C1-O5-C5	2.24	115.18	112.19
5	g	2	NAG	O4-C4-C3	-2.23	105.12	110.38
5	f	2	NAG	O5-C1-C2	-2.23	107.85	111.29
6	N	1	NAG	O5-C1-C2	-2.22	107.86	111.29
9	T	1	NAG	O5-C1-C2	-2.21	107.88	111.29
7	d	1	NAG	O4-C4-C3	-2.20	105.19	110.38
5	t	1	NAG	O5-C1-C2	-2.20	107.89	111.29
6	p	4	MAN	C1-O5-C5	2.20	115.14	112.19
5	0	1	NAG	O5-C1-C2	-2.20	107.89	111.29
9	V	3	BMA	C1-C2-C3	2.20	112.84	109.64
5	Y	2	NAG	C4-C3-C2	-2.20	107.80	111.02
5	l	3	BMA	C3-C4-C5	2.19	114.21	110.23
7	a	2	NAG	O5-C1-C2	-2.18	107.91	111.29
7	r	1	NAG	O5-C1-C2	-2.18	107.91	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	k	1	NAG	O4-C4-C3	-2.18	105.24	110.38
7	d	1	NAG	O5-C1-C2	-2.17	107.93	111.29
5	Y	1	NAG	O4-C4-C3	-2.17	105.25	110.38
5	v	3	BMA	C2-C3-C4	2.17	114.68	110.86
9	W	3	BMA	C6-C5-C4	2.17	118.35	113.02
8	s	3	BMA	O3-C3-C2	-2.17	105.64	110.05
9	V	1	NAG	O5-C1-C2	-2.16	107.95	111.29
5	Q	3	BMA	O4-C4-C3	-2.15	105.30	110.38
5	f	3	BMA	O4-C4-C3	-2.15	105.30	110.38
6	N	3	BMA	C2-C3-C4	2.15	114.64	110.86
5	0	3	BMA	O4-C4-C3	-2.14	105.32	110.38
5	u	3	BMA	O4-C4-C3	-2.14	105.33	110.38
5	w	3	BMA	C3-C4-C5	2.13	114.09	110.23
5	j	3	BMA	C3-C4-C5	2.13	114.09	110.23
9	l	3	BMA	C2-C3-C4	2.12	114.59	110.86
6	p	1	NAG	C1-C2-N2	2.12	113.77	110.43
5	Z	1	NAG	C1-C2-N2	2.09	113.73	110.43
8	e	3	BMA	C2-C3-C4	2.09	114.54	110.86
5	u	2	NAG	O3-C3-C2	-2.08	105.08	109.40
5	u	1	NAG	O4-C4-C3	-2.07	105.50	110.38
8	P	3	BMA	C2-C3-C4	2.07	114.50	110.86
5	0	2	NAG	O5-C1-C2	-2.06	108.10	111.29
5	M	1	NAG	C4-C3-C2	-2.05	108.01	111.02
5	v	3	BMA	O4-C4-C3	-2.05	105.54	110.38
5	Z	3	BMA	O3-C3-C2	-2.05	105.87	110.05
6	p	3	BMA	O3-C3-C2	-2.05	105.87	110.05
5	k	3	BMA	O4-C4-C3	-2.05	105.55	110.38
5	M	3	BMA	C2-C3-C4	2.05	114.46	110.86
9	W	2	NAG	C4-C3-C2	-2.04	108.02	111.02
5	i	3	BMA	O4-C4-C3	-2.04	105.57	110.38
7	q	2	NAG	O5-C1-C2	-2.04	108.14	111.29
7	h	1	NAG	C1-O5-C5	2.04	114.91	112.19
8	e	5	MAN	C1-O5-C5	2.04	114.91	112.19
5	l	2	NAG	C4-C3-C2	-2.04	108.03	111.02
5	U	3	BMA	O4-C4-C3	-2.03	105.58	110.38
8	P	5	MAN	C1-O5-C5	2.03	114.91	112.19
5	g	1	NAG	O4-C4-C3	-2.03	105.59	110.38
5	i	3	BMA	O3-C3-C2	-2.03	105.92	110.05
6	N	3	BMA	O3-C3-C2	-2.02	105.92	110.05
5	u	3	BMA	O5-C1-C2	2.02	115.61	110.79
5	m	2	NAG	C4-C3-C2	-2.02	108.06	111.02
9	V	2	NAG	C3-C4-C5	-2.02	106.58	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	y	2	NAG	O4-C4-C5	2.01	114.28	109.32
5	Q	1	NAG	O7-C7-N2	2.01	125.53	121.98
5	n	1	NAG	C4-C3-C2	-2.01	108.07	111.02
5	R	3	BMA	O4-C4-C3	-2.01	105.64	110.38
5	0	1	NAG	O4-C4-C3	-2.00	105.65	110.38

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	1	NAG	C3-C2-N2-C7
5	Q	2	NAG	C1-C2-N2-C7
5	f	1	NAG	C3-C2-N2-C7
5	f	2	NAG	C1-C2-N2-C7
5	g	1	NAG	C1-C2-N2-C7
5	m	1	NAG	C1-C2-N2-C7
5	t	1	NAG	C3-C2-N2-C7
5	t	2	NAG	C1-C2-N2-C7
5	w	2	NAG	C1-C2-N2-C7
6	N	1	NAG	C1-C2-N2-C7
6	b	1	NAG	C1-C2-N2-C7
7	S	1	NAG	C1-C2-N2-C7
7	a	1	NAG	C1-C2-N2-C7
7	a	2	NAG	C1-C2-N2-C7
7	o	1	NAG	C1-C2-N2-C7
7	o	2	NAG	C1-C2-N2-C7
9	T	1	NAG	C1-C2-N2-C7
9	W	3	BMA	C4-C5-C6-O6
9	T	4	MAN	O5-C5-C6-O6
9	W	3	BMA	O5-C5-C6-O6
9	V	3	BMA	C4-C5-C6-O6
9	V	3	BMA	O5-C5-C6-O6
5	M	1	NAG	C8-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
5	g	1	NAG	C8-C7-N2-C2
5	g	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	m	1	NAG	C8-C7-N2-C2
5	m	1	NAG	O7-C7-N2-C2
5	u	2	NAG	C8-C7-N2-C2
5	u	2	NAG	O7-C7-N2-C2
5	l	2	NAG	C8-C7-N2-C2
5	l	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	b	1	NAG	C8-C7-N2-C2
6	b	1	NAG	O7-C7-N2-C2
6	p	1	NAG	C8-C7-N2-C2
6	p	1	NAG	O7-C7-N2-C2
7	S	1	NAG	C8-C7-N2-C2
7	S	1	NAG	O7-C7-N2-C2
7	S	2	NAG	C8-C7-N2-C2
7	S	2	NAG	O7-C7-N2-C2
7	X	1	NAG	C8-C7-N2-C2
7	X	1	NAG	O7-C7-N2-C2
7	h	2	NAG	C8-C7-N2-C2
7	h	2	NAG	O7-C7-N2-C2
9	z	2	NAG	C8-C7-N2-C2
9	z	2	NAG	O7-C7-N2-C2
8	e	3	BMA	C4-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
9	V	4	MAN	O5-C5-C6-O6
9	z	4	MAN	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	j	3	BMA	O5-C5-C6-O6
5	m	3	BMA	O5-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
6	p	3	BMA	C4-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
5	k	3	BMA	C4-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6
8	P	4	MAN	O5-C5-C6-O6
8	s	4	MAN	O5-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
5	y	1	NAG	O5-C5-C6-O6
7	q	2	NAG	O5-C5-C6-O6
9	z	3	BMA	O5-C5-C6-O6
6	b	5	MAN	O5-C5-C6-O6
9	W	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	b	1	NAG	O5-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
5	v	2	NAG	O5-C5-C6-O6
5	x	3	BMA	O5-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
9	l	3	BMA	O5-C5-C6-O6
5	y	3	BMA	C4-C5-C6-O6
5	0	3	BMA	O5-C5-C6-O6
8	e	4	MAN	O5-C5-C6-O6
6	p	1	NAG	O5-C5-C6-O6
8	P	3	BMA	C4-C5-C6-O6
9	T	4	MAN	C4-C5-C6-O6
6	b	3	BMA	C4-C5-C6-O6
5	i	2	NAG	C1-C2-N2-C7
9	T	2	NAG	C1-C2-N2-C7
5	M	1	NAG	C3-C2-N2-C7
5	Z	1	NAG	C3-C2-N2-C7
5	i	2	NAG	C3-C2-N2-C7
6	p	1	NAG	C3-C2-N2-C7
7	X	1	NAG	C3-C2-N2-C7
7	h	1	NAG	C3-C2-N2-C7
9	T	1	NAG	C3-C2-N2-C7
8	s	3	BMA	C4-C5-C6-O6
6	p	3	BMA	O5-C5-C6-O6
9	V	4	MAN	C4-C5-C6-O6
5	M	1	NAG	C1-C2-N2-C7
5	Q	1	NAG	C1-C2-N2-C7
5	Z	1	NAG	C1-C2-N2-C7
6	p	1	NAG	C1-C2-N2-C7
7	S	2	NAG	C1-C2-N2-C7
7	X	1	NAG	C1-C2-N2-C7
7	h	1	NAG	C1-C2-N2-C7
7	r	2	NAG	C1-C2-N2-C7
5	Q	2	NAG	C3-C2-N2-C7
5	f	2	NAG	C3-C2-N2-C7
5	t	2	NAG	C3-C2-N2-C7
7	a	1	NAG	C3-C2-N2-C7
7	a	2	NAG	C3-C2-N2-C7
7	o	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	T	2	NAG	C3-C2-N2-C7
9	z	4	MAN	C4-C5-C6-O6
8	P	3	BMA	O5-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
5	k	3	BMA	O5-C5-C6-O6

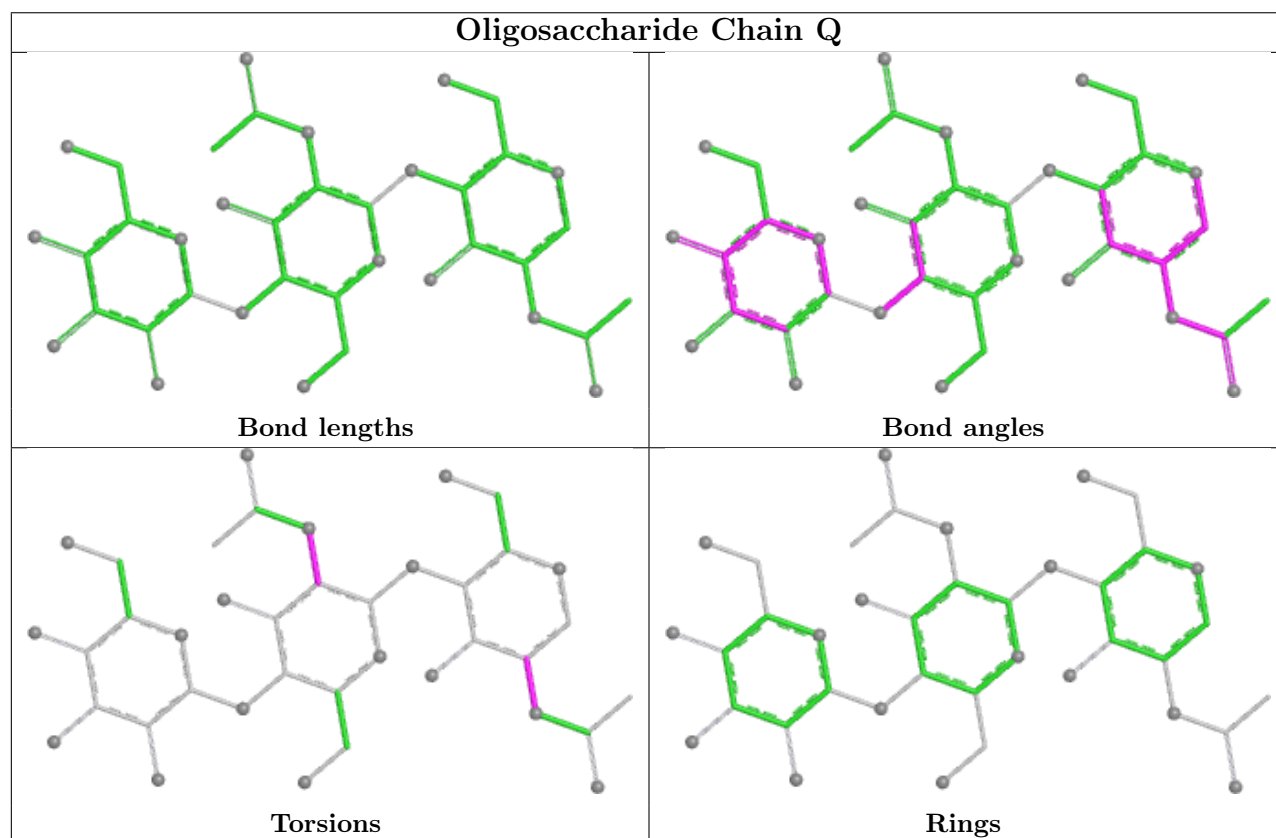
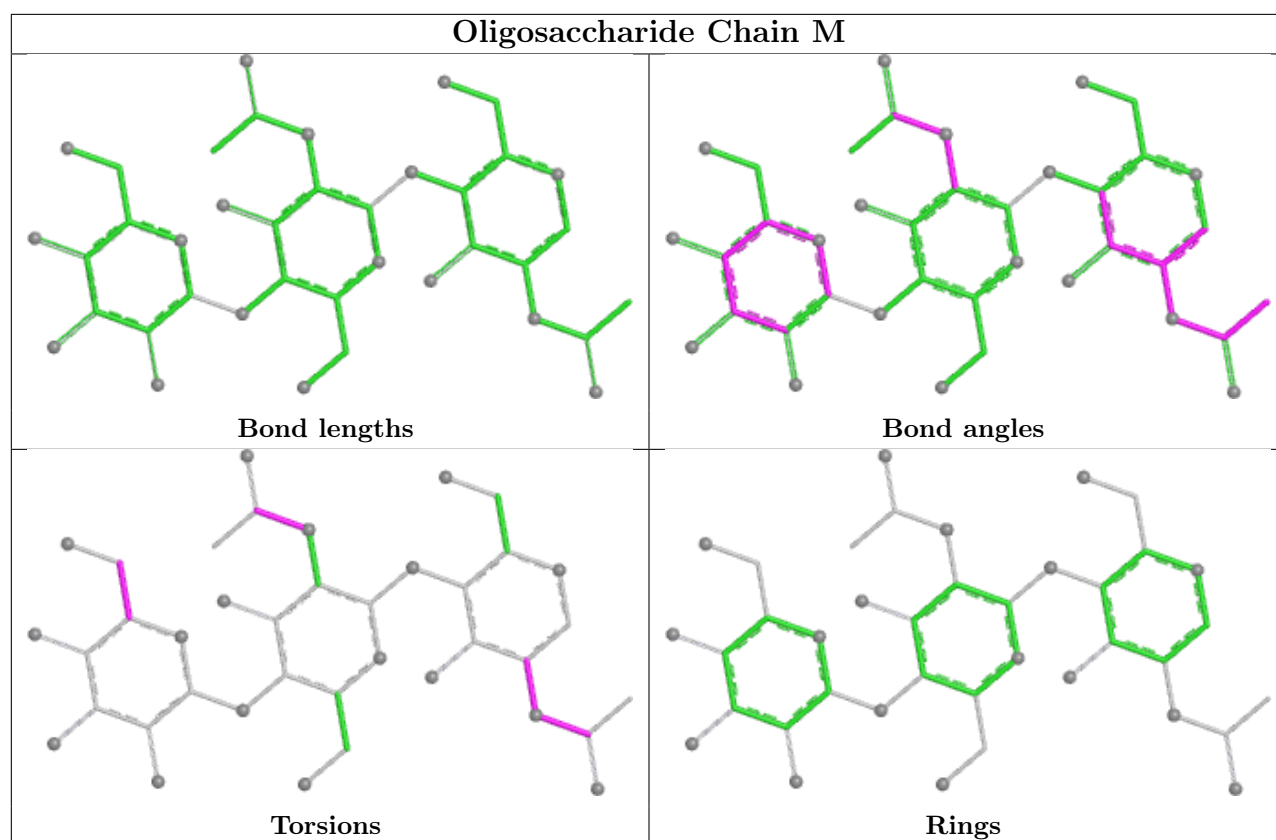
All (1) ring outliers are listed below:

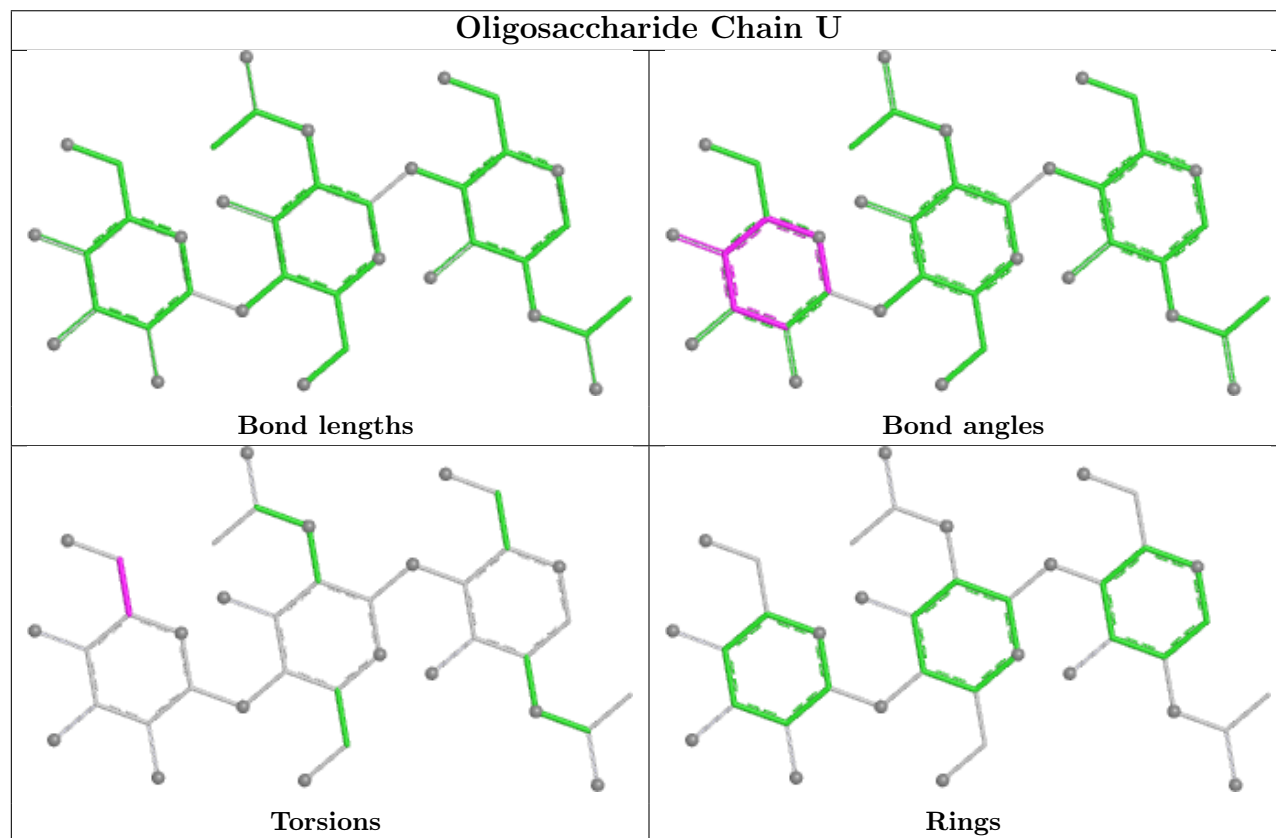
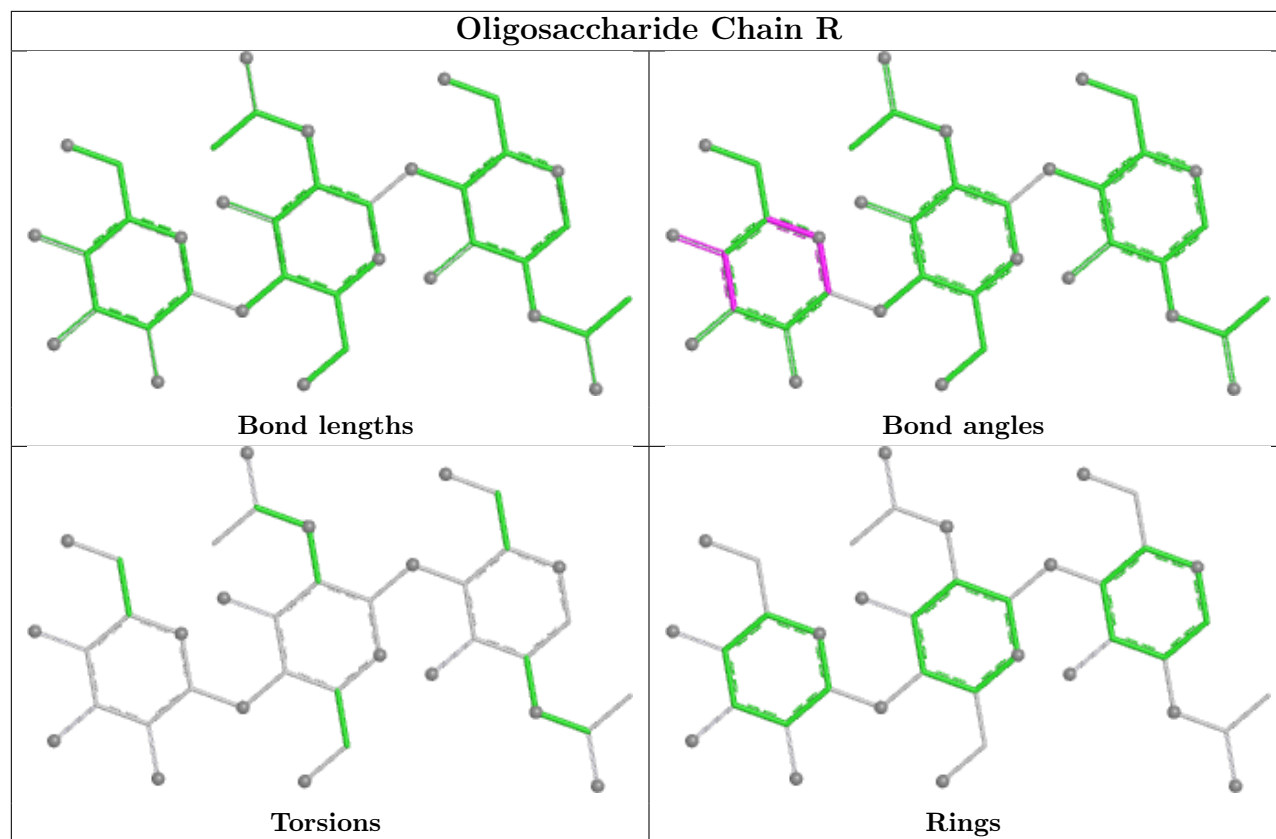
Mol	Chain	Res	Type	Atoms
9	z	3	BMA	C1-C2-C3-C4-C5-O5

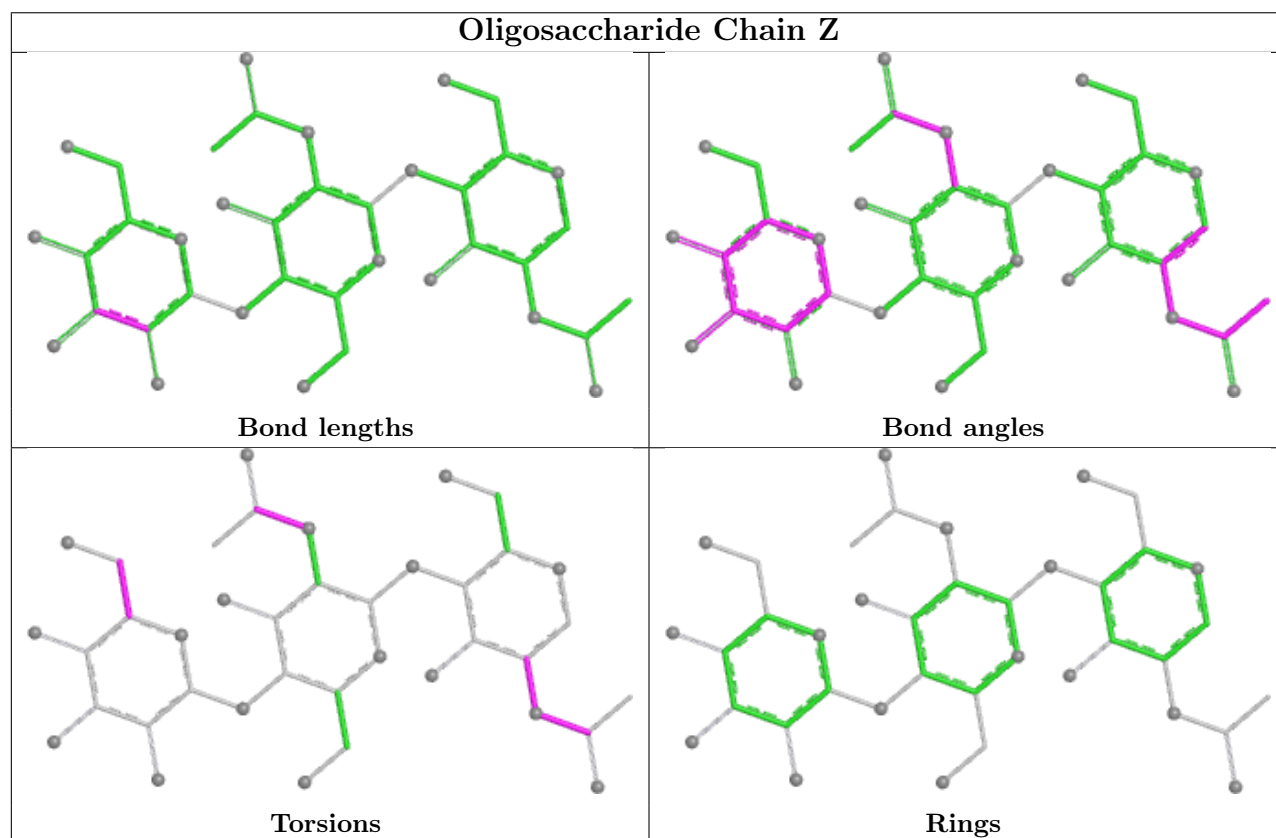
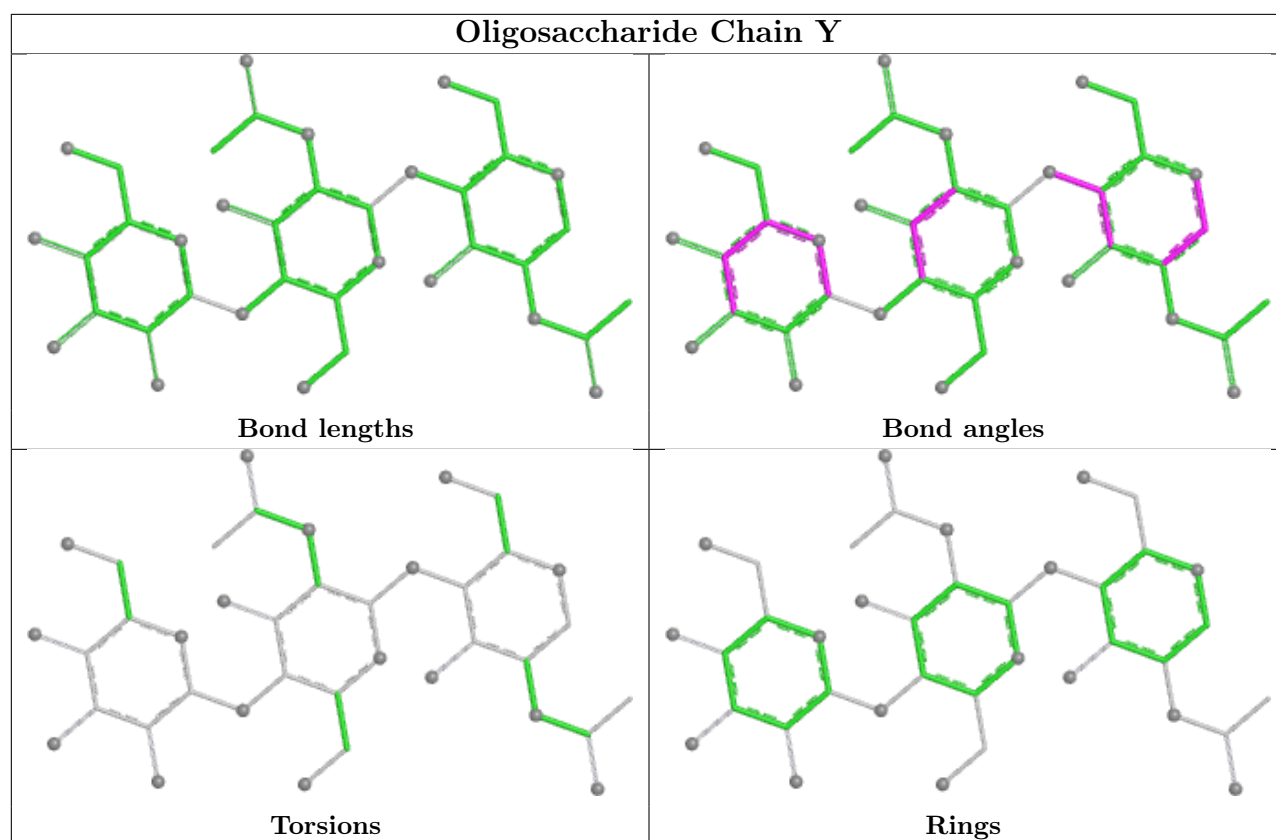
17 monomers are involved in 13 short contacts:

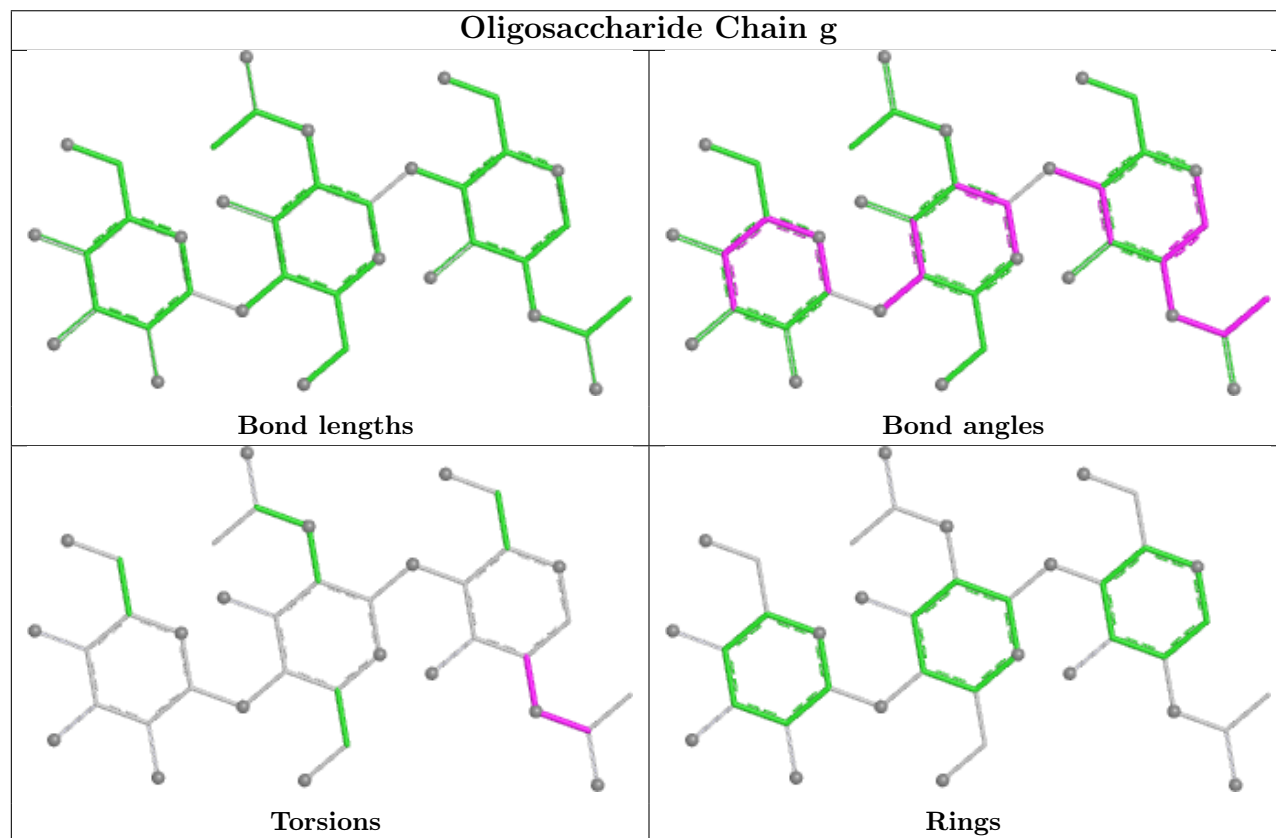
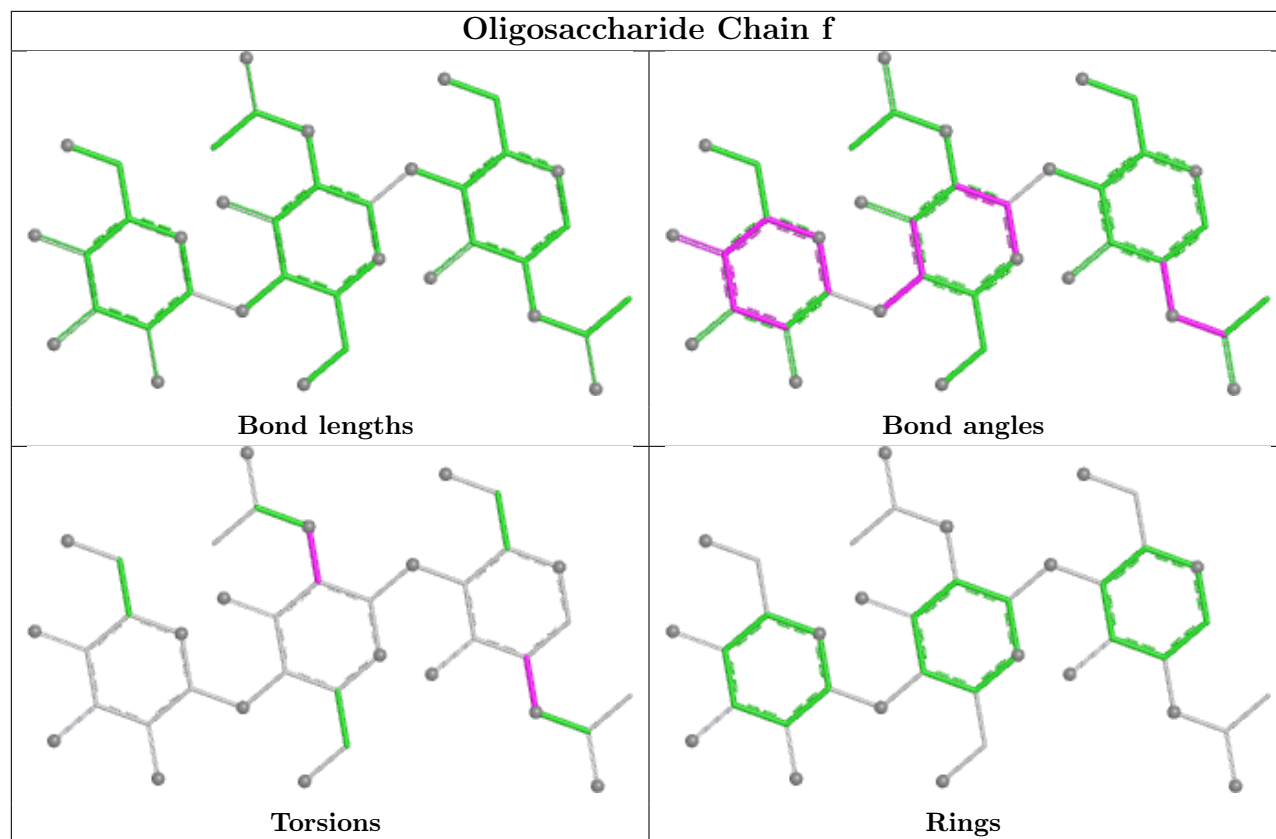
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	x	2	NAG	1	0
5	U	3	BMA	1	0
5	Y	1	NAG	2	0
5	1	1	NAG	1	0
9	V	4	MAN	1	0
6	p	1	NAG	1	0
9	V	2	NAG	2	0
5	0	1	NAG	1	0
9	W	1	NAG	1	0
8	P	1	NAG	1	0
8	e	2	NAG	1	0
5	x	1	NAG	1	0
5	M	1	NAG	1	0
7	X	1	NAG	1	0
5	Z	1	NAG	1	0
5	y	2	NAG	1	0
7	c	1	NAG	1	0

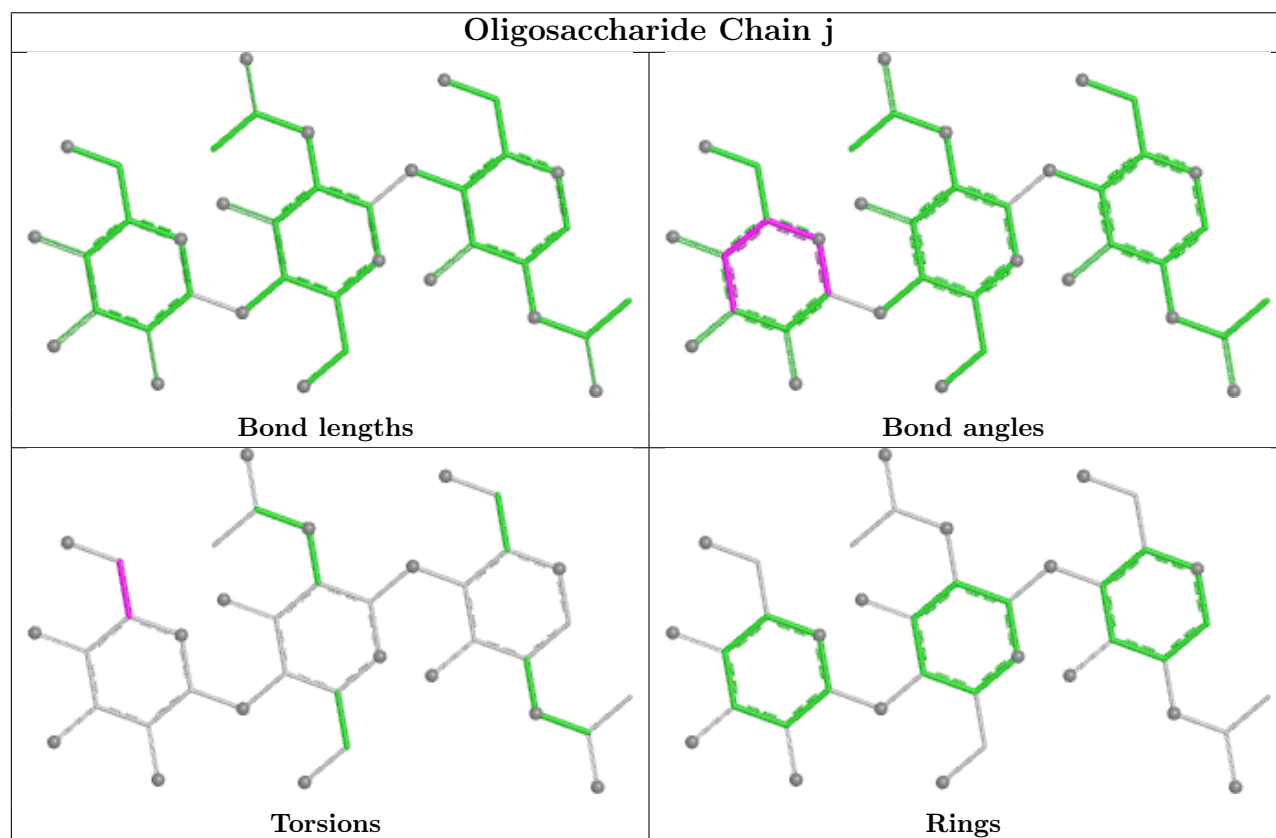
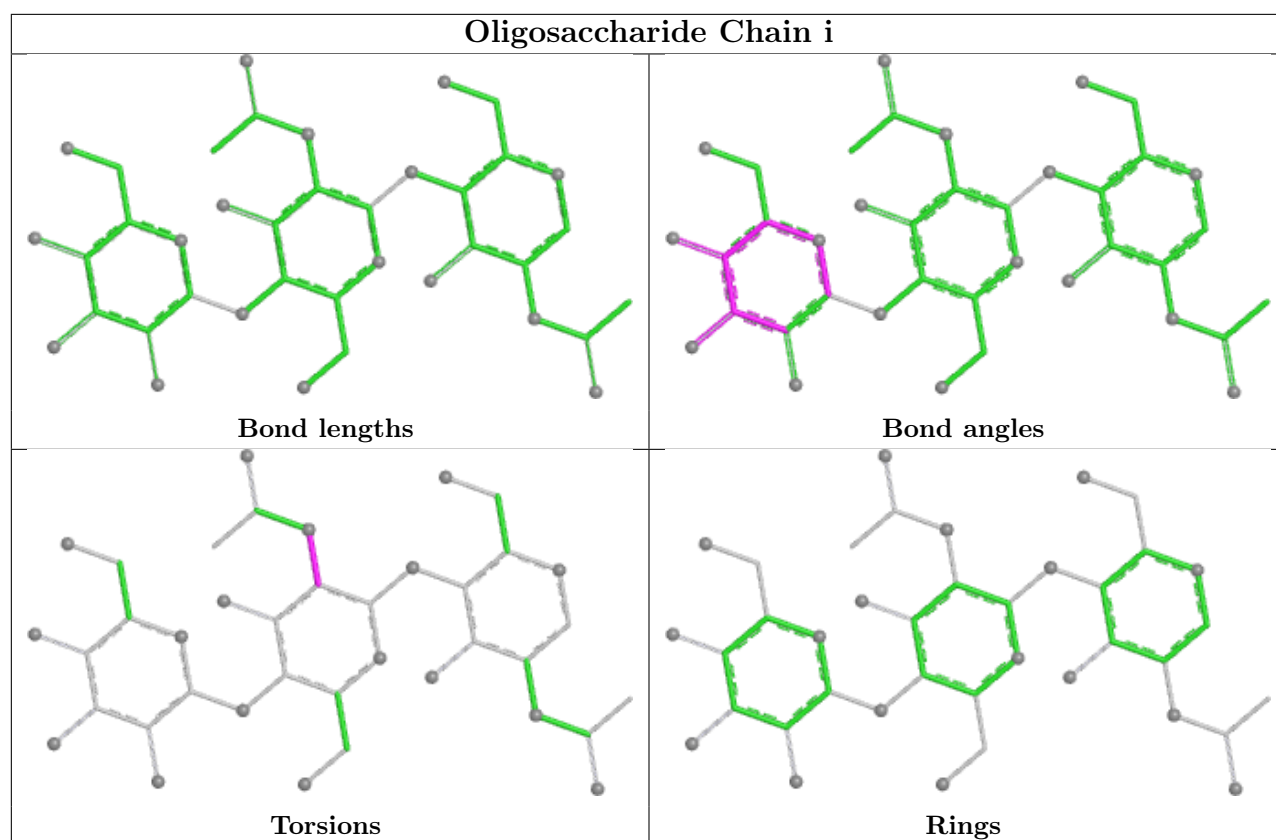
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

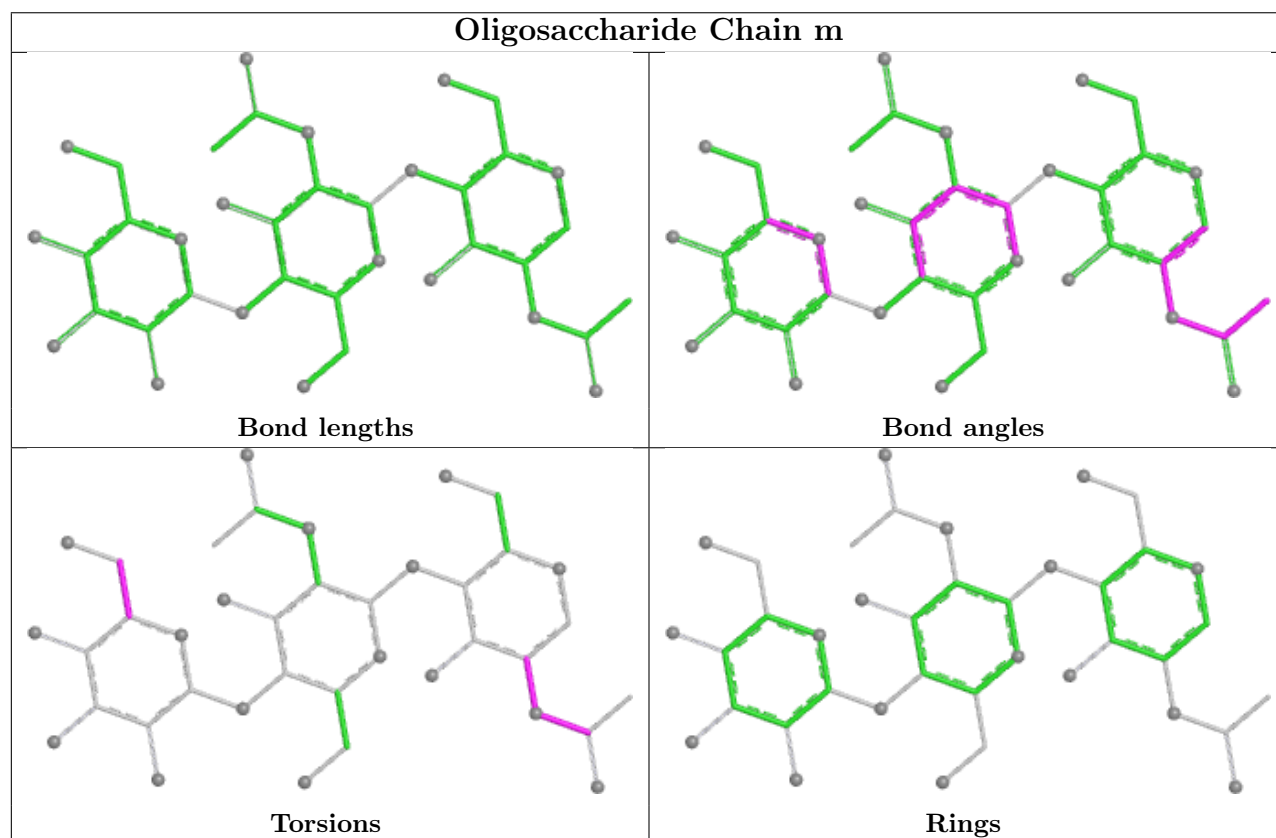
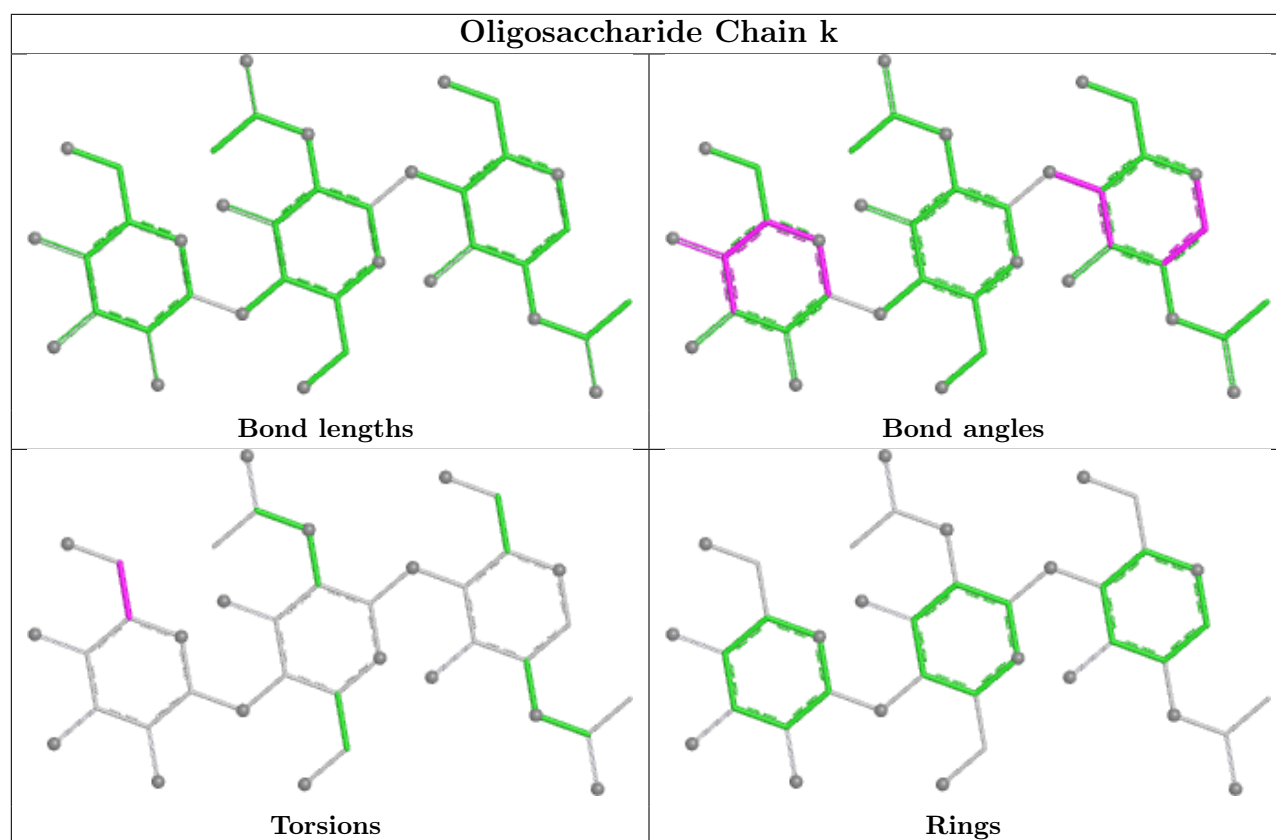


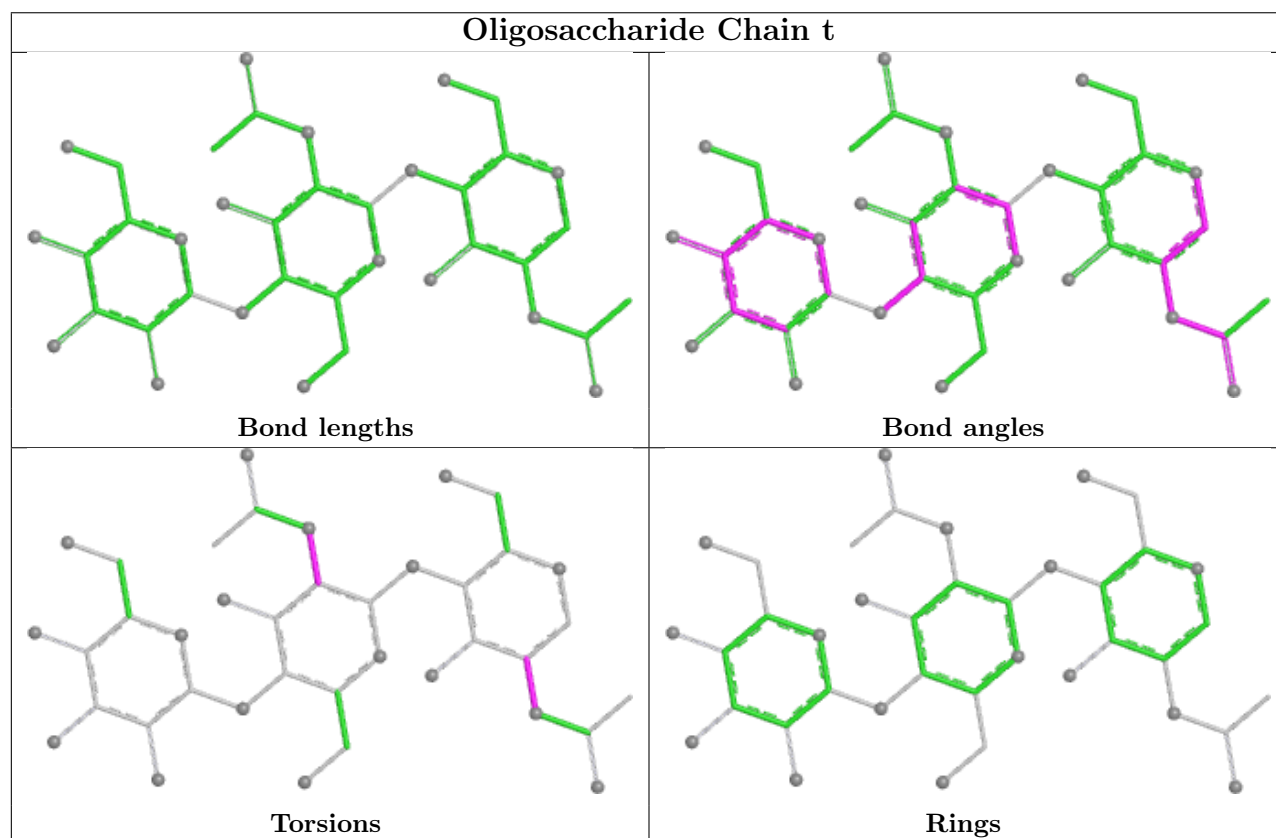
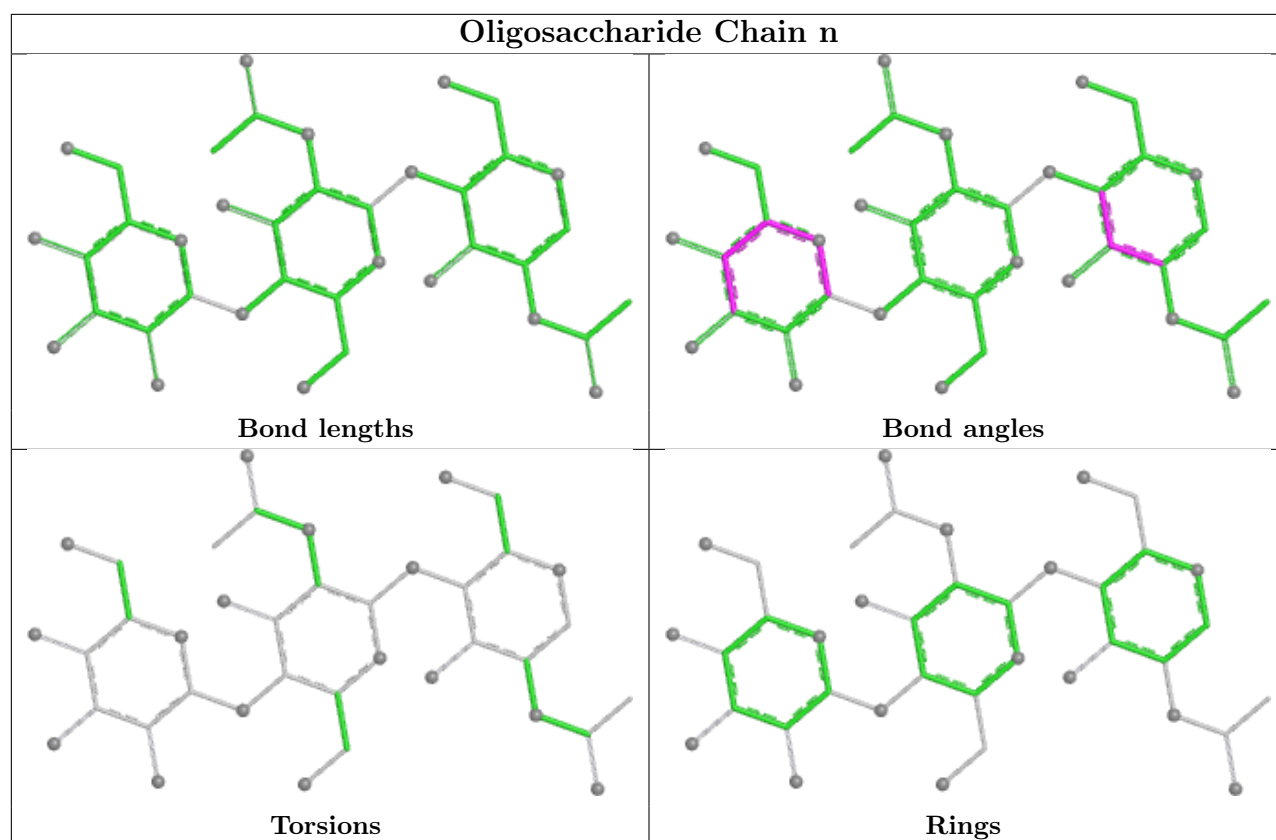


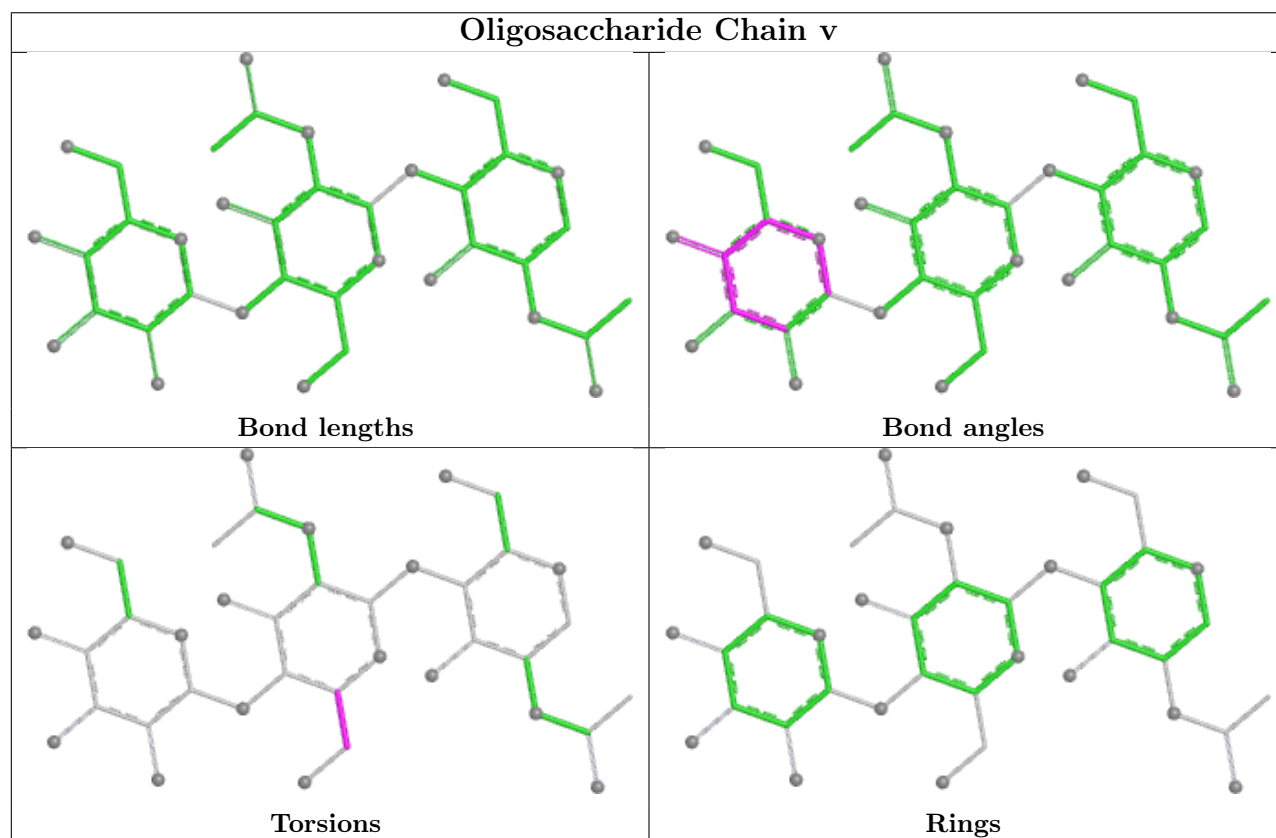
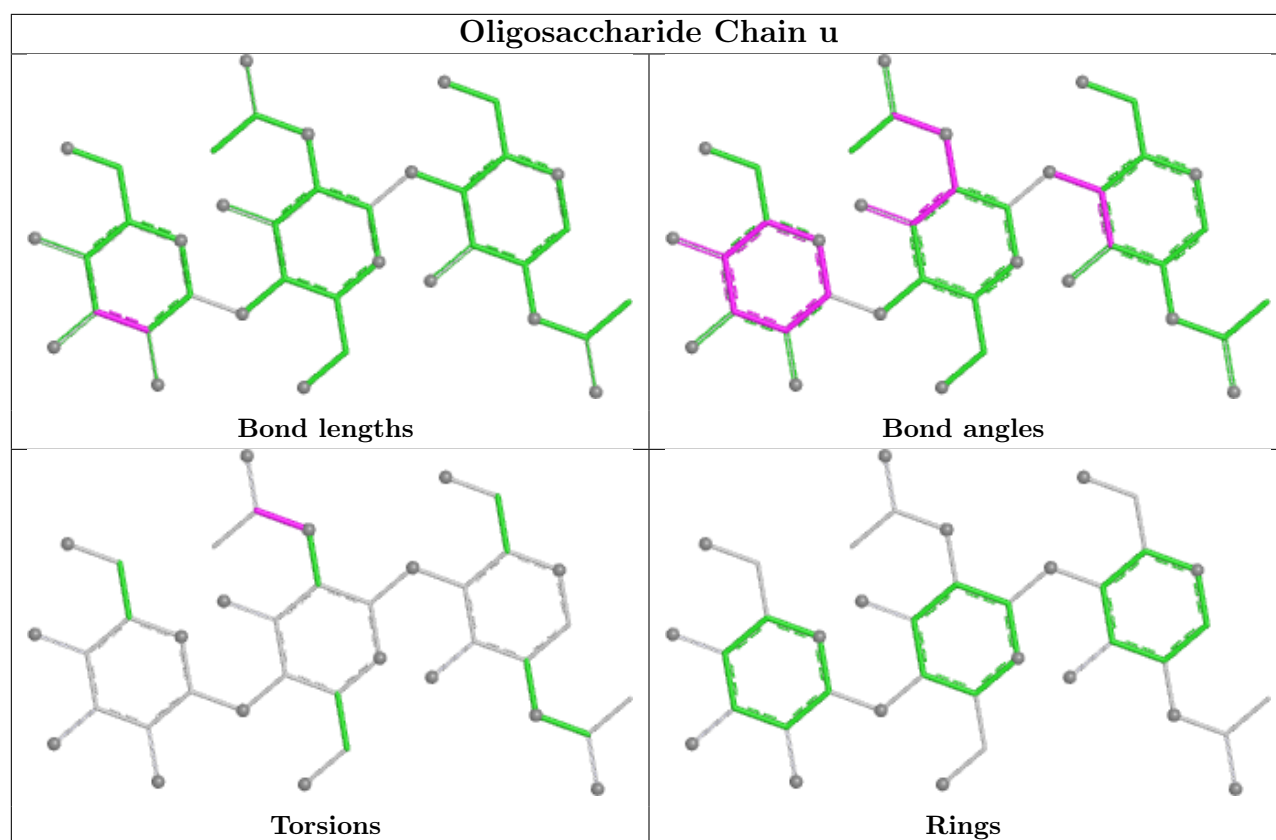


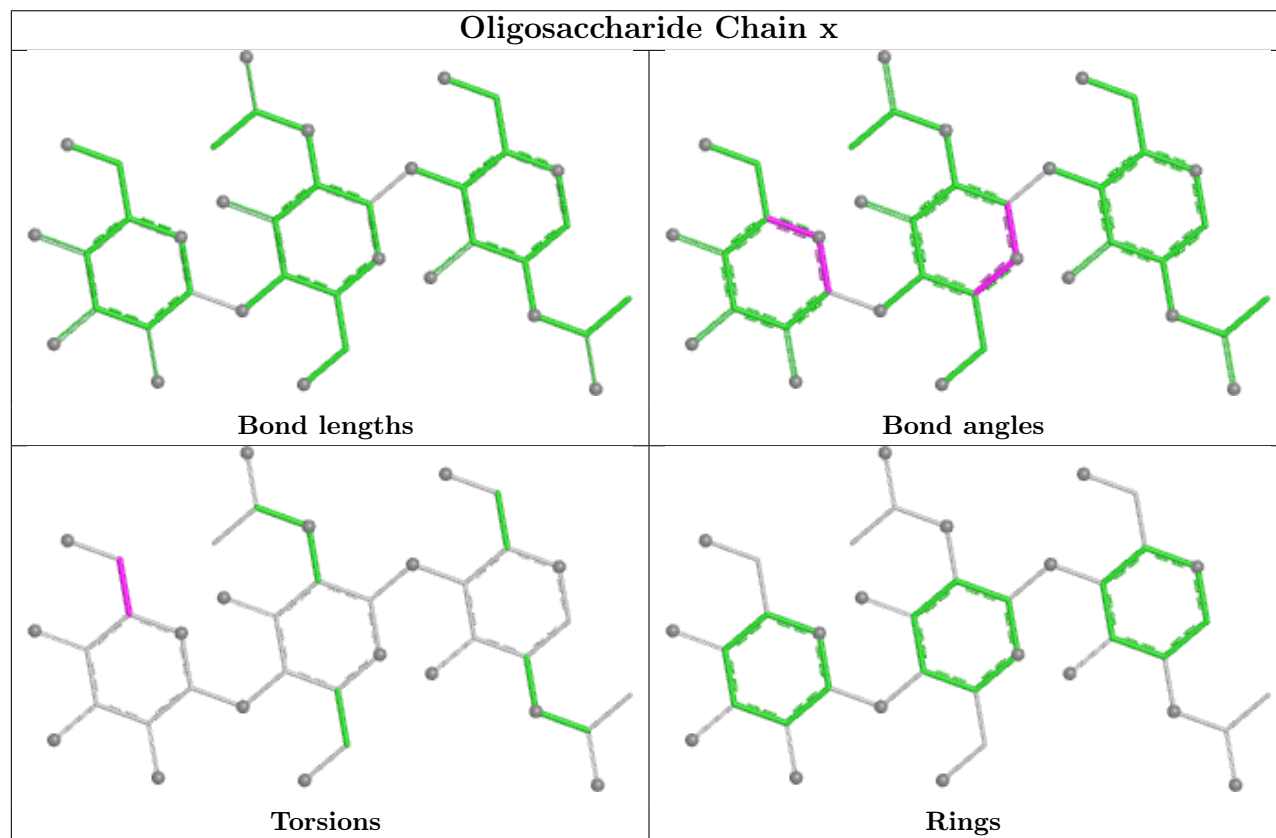
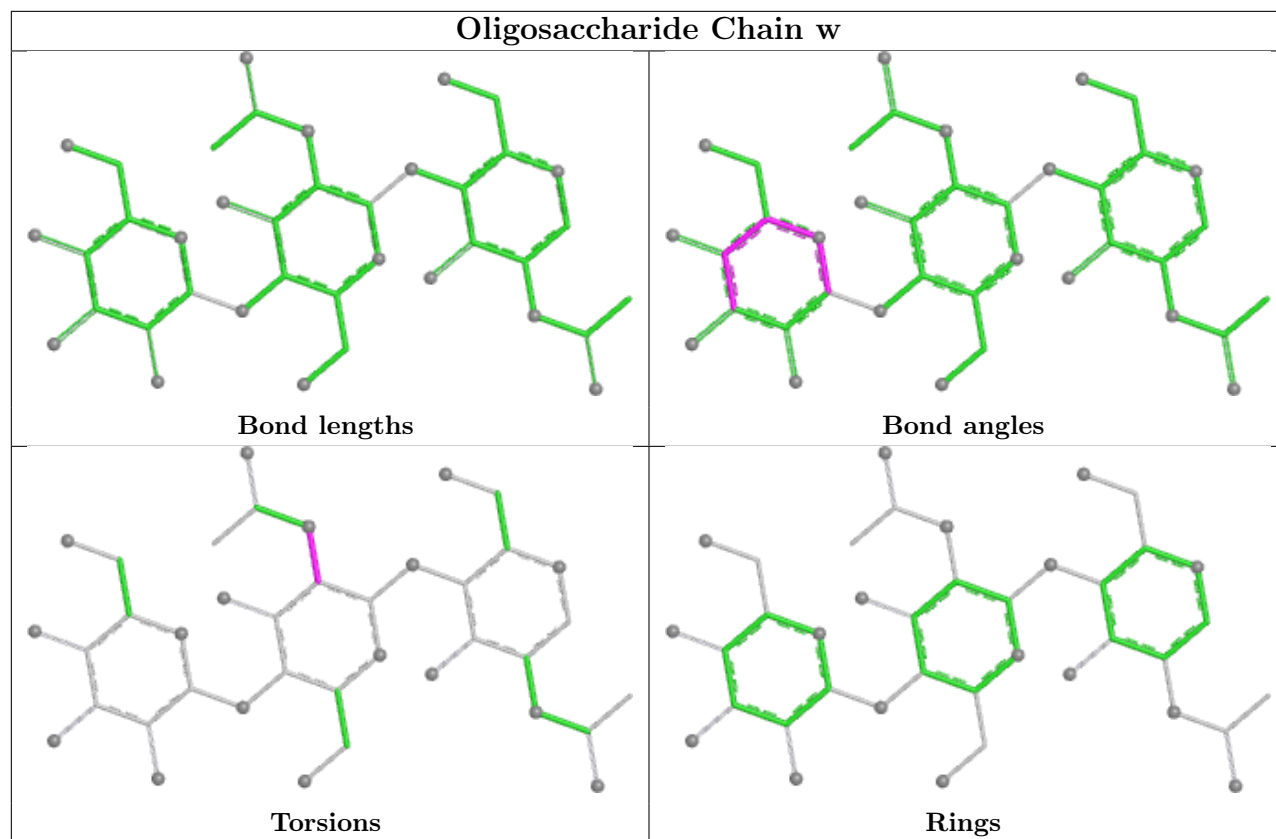


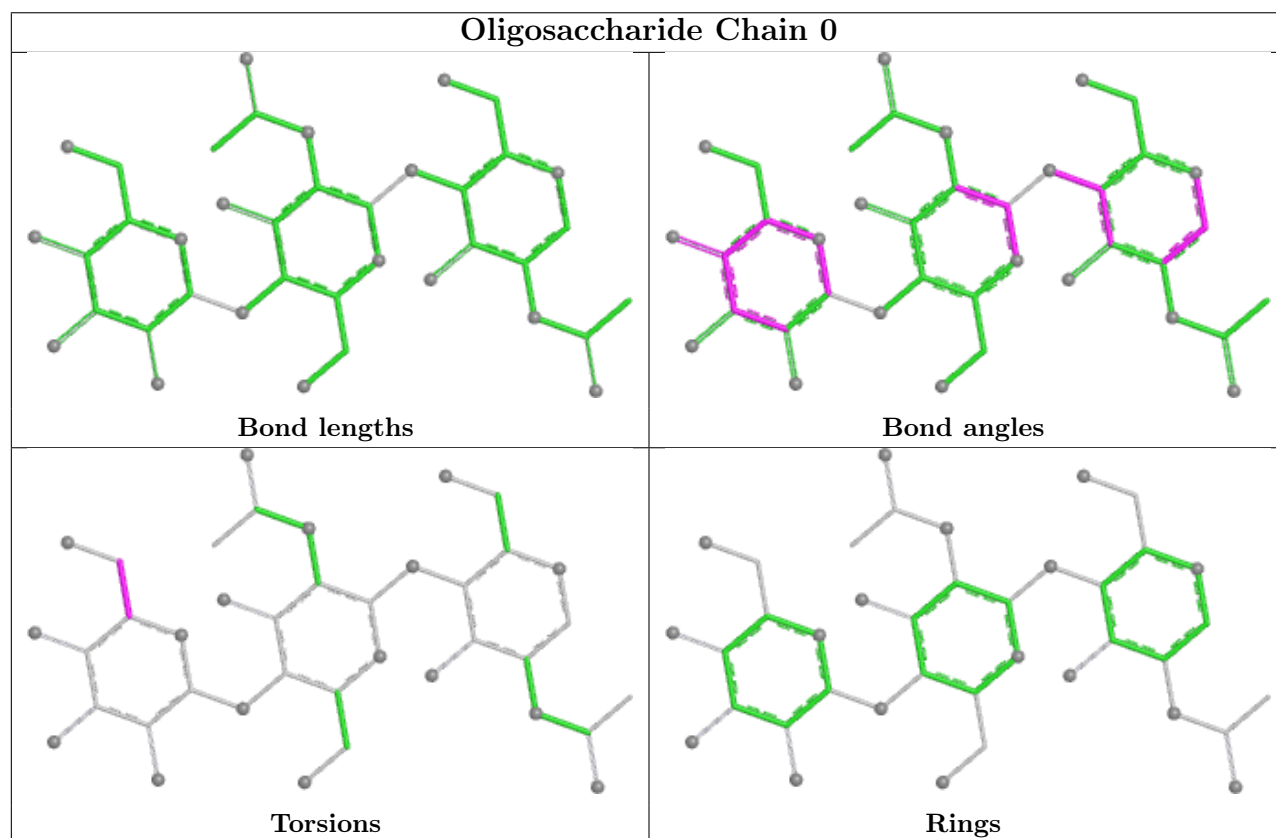
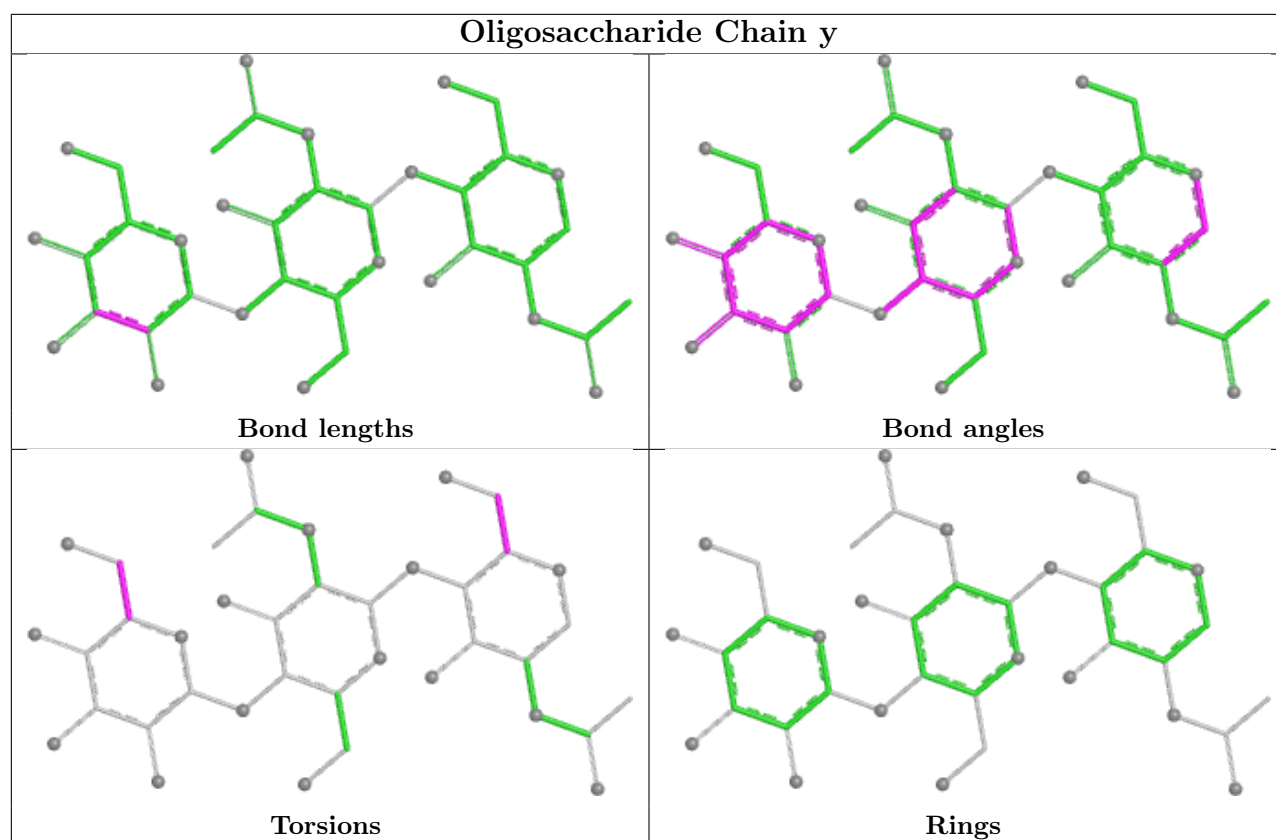


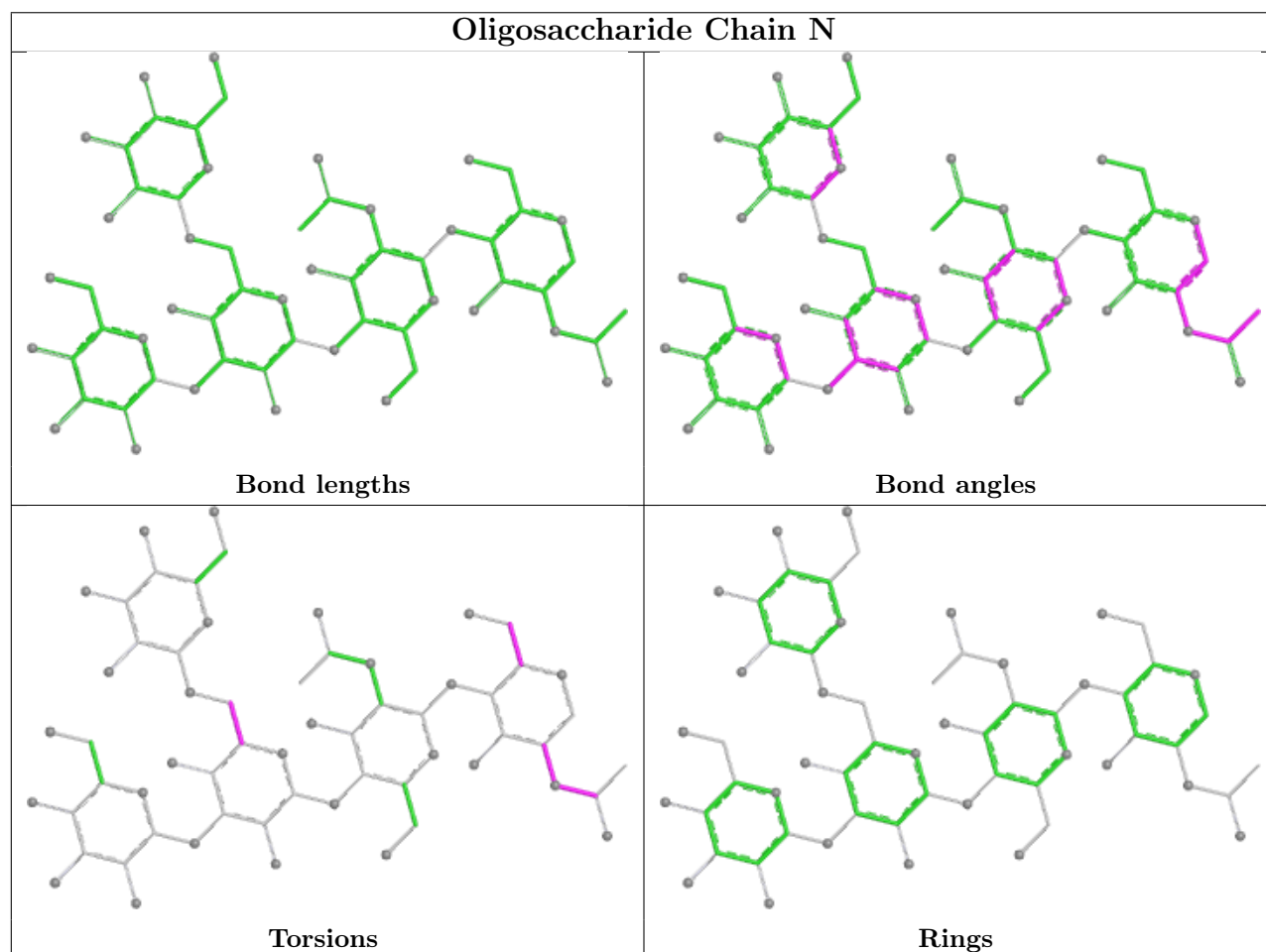
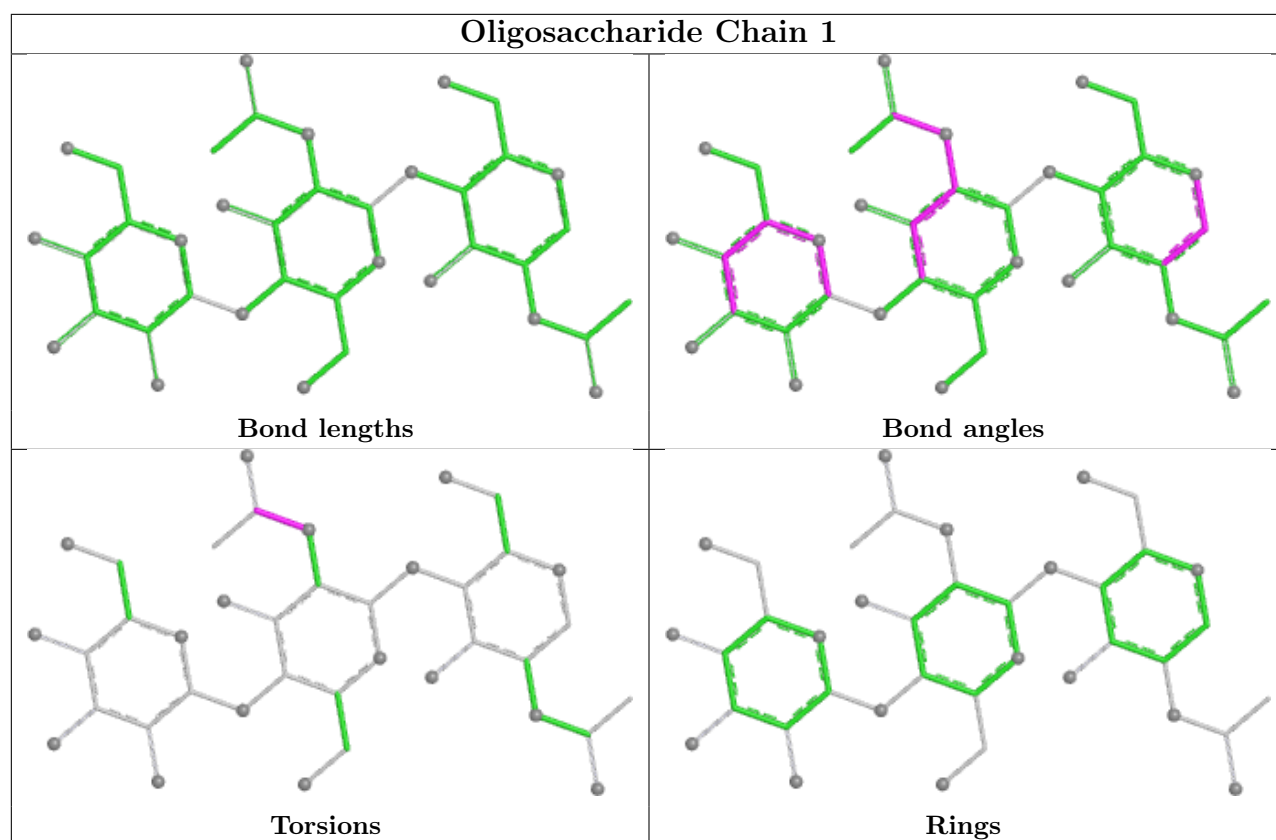


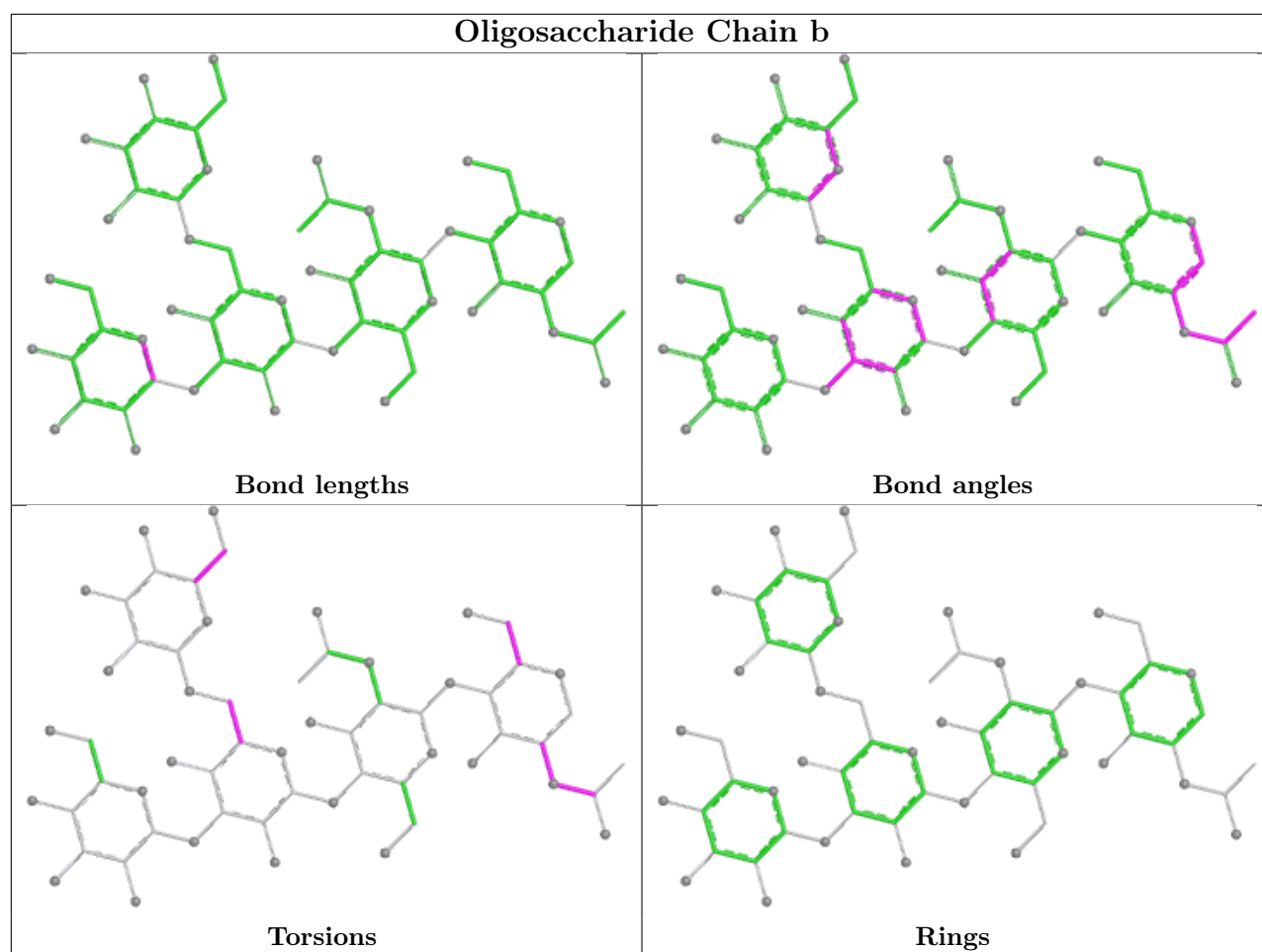


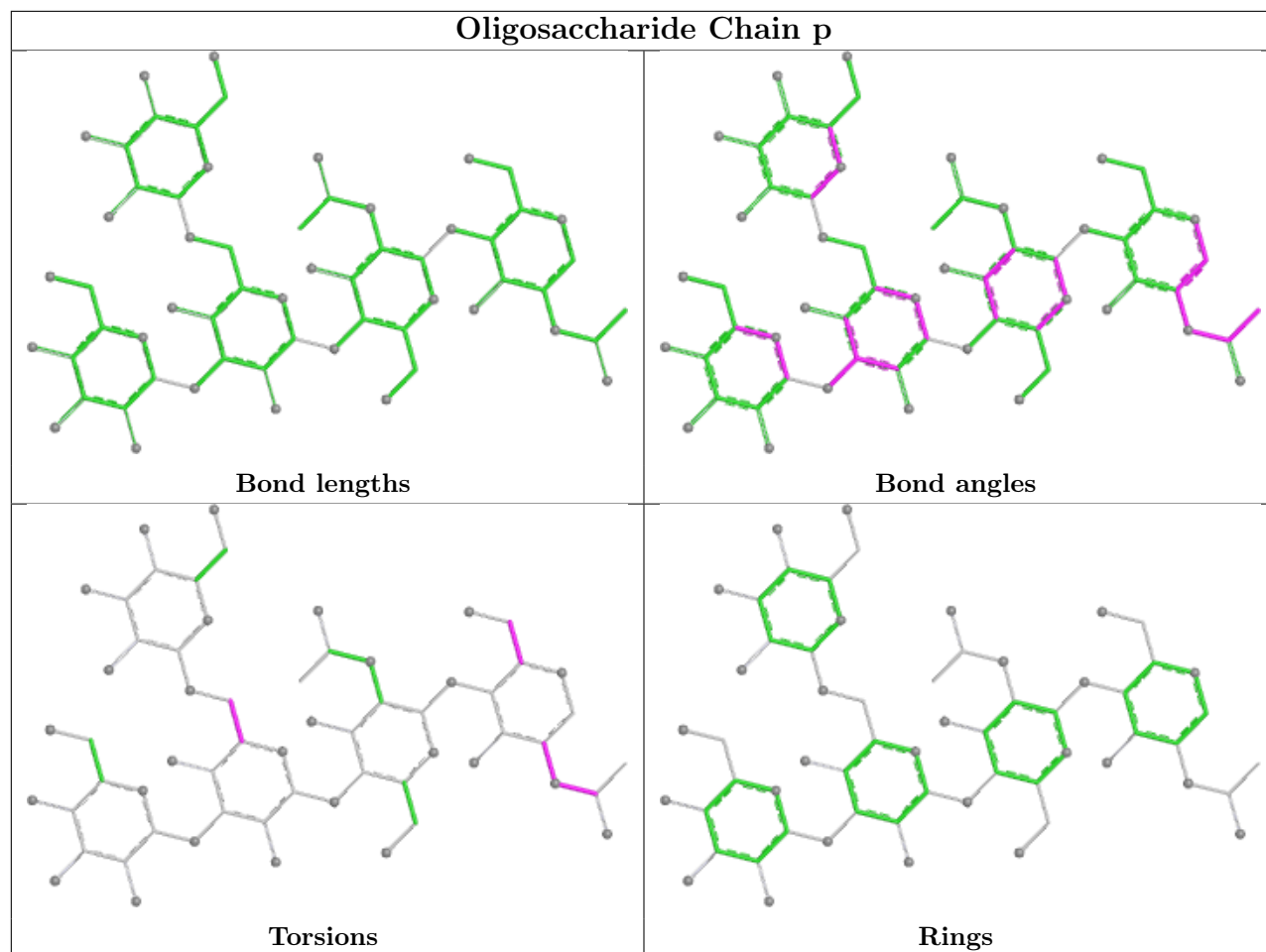


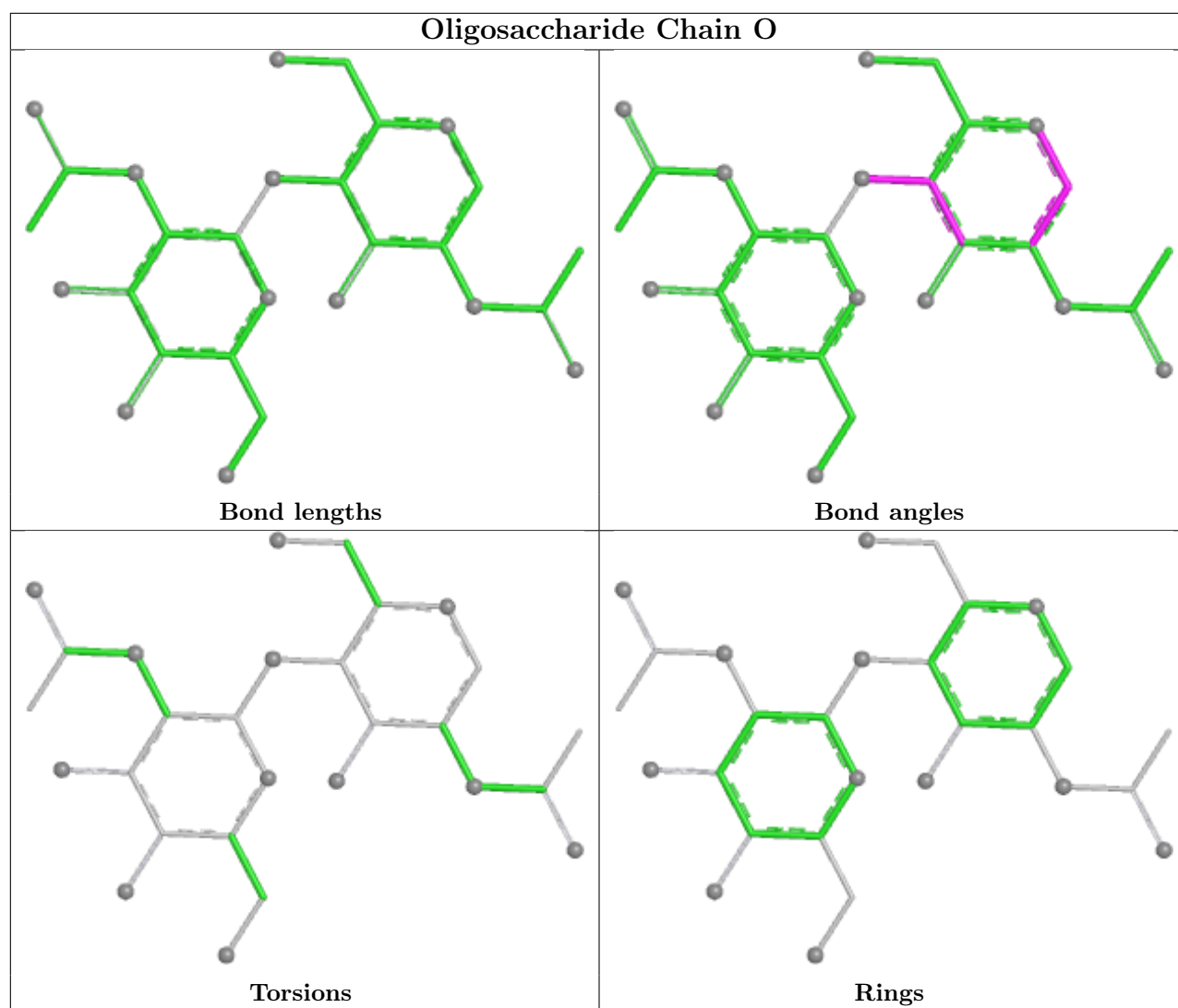


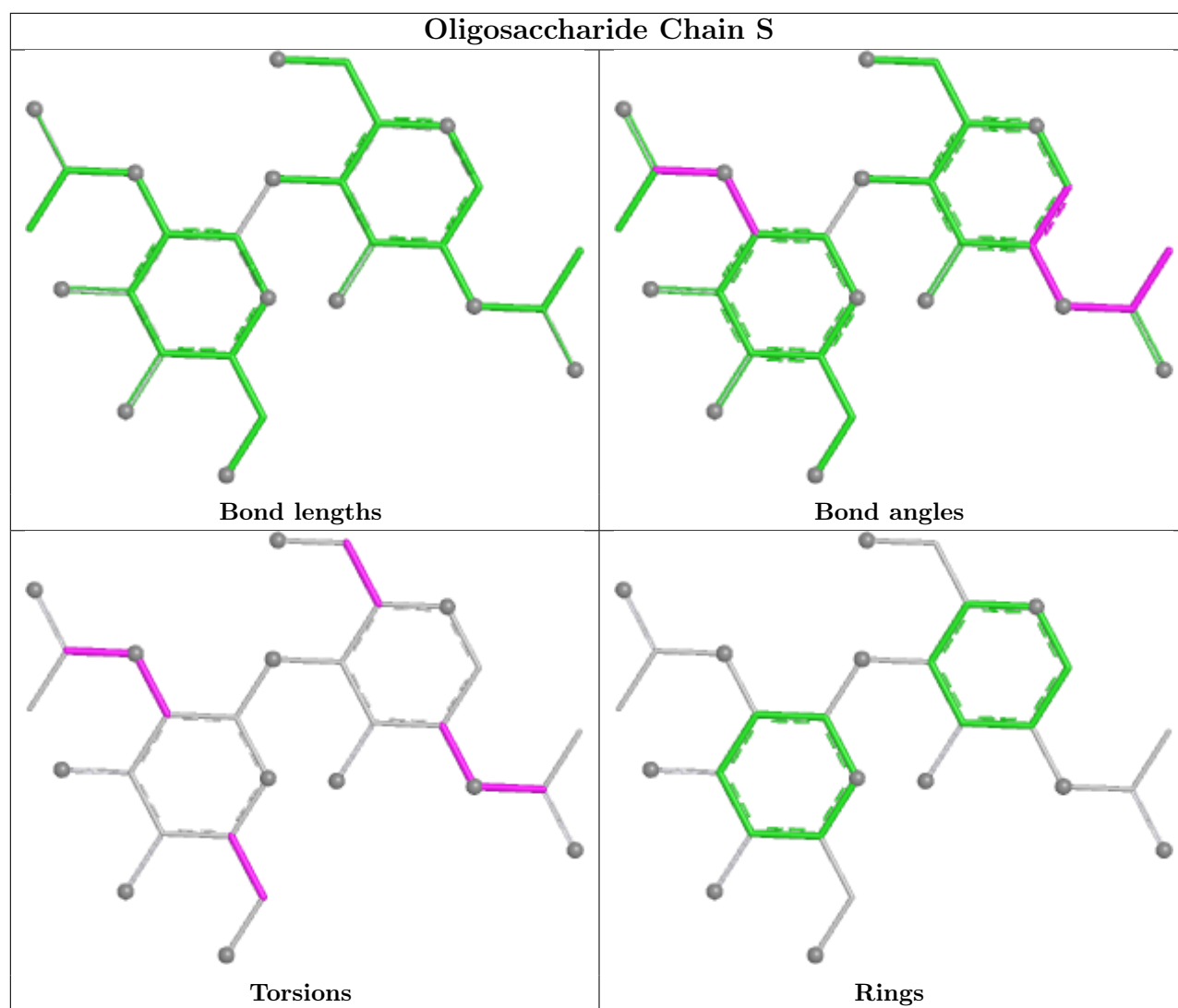


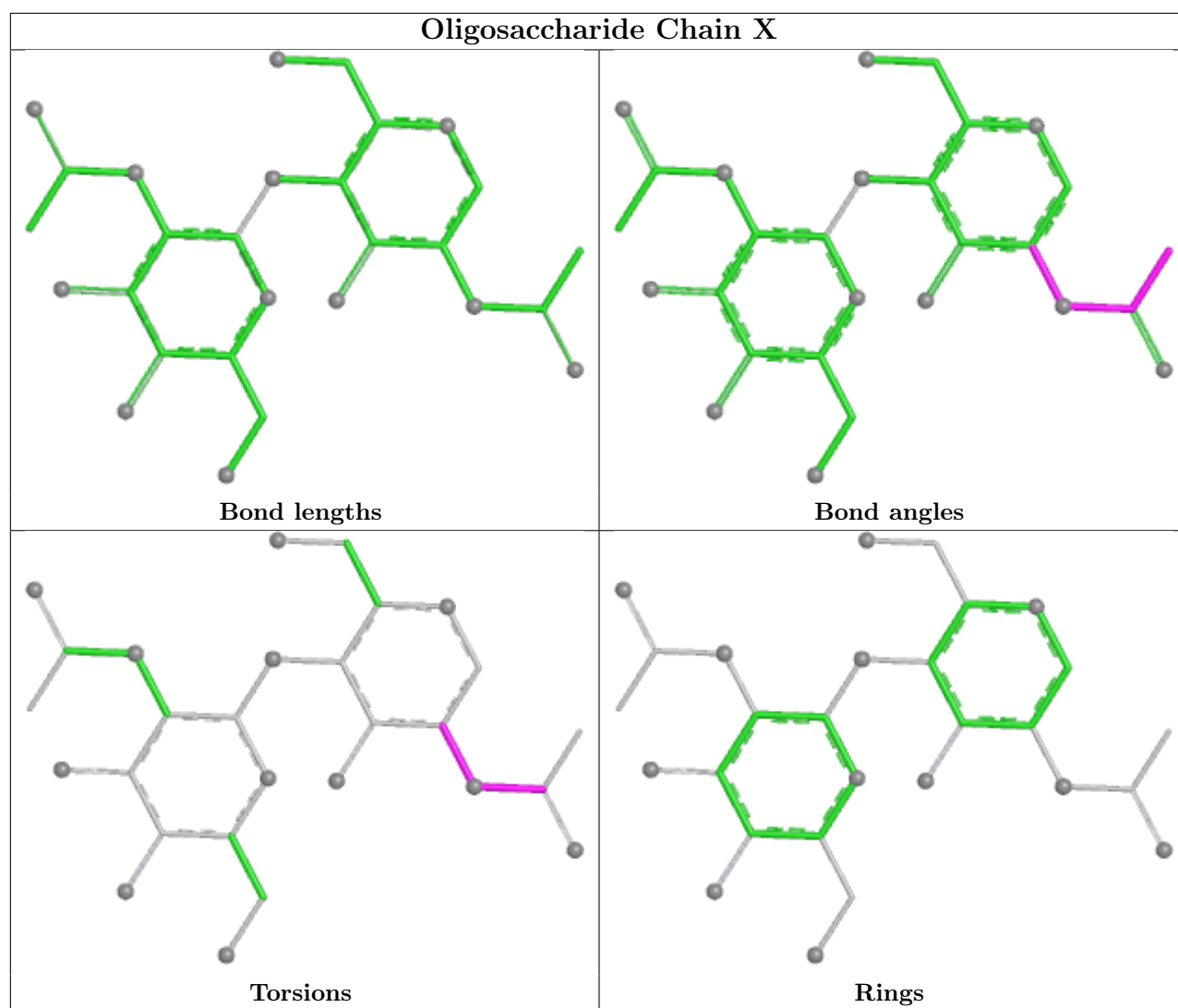


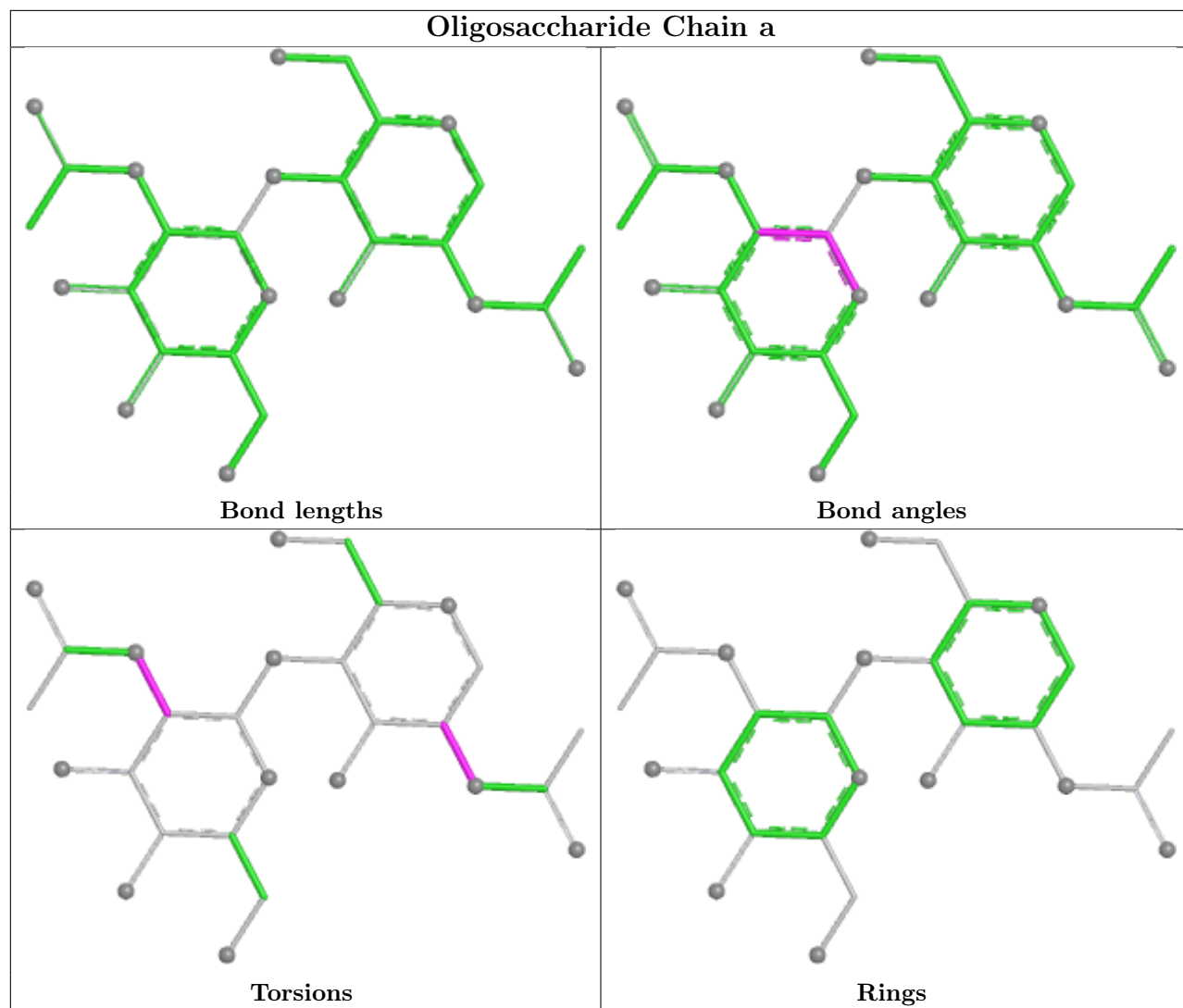


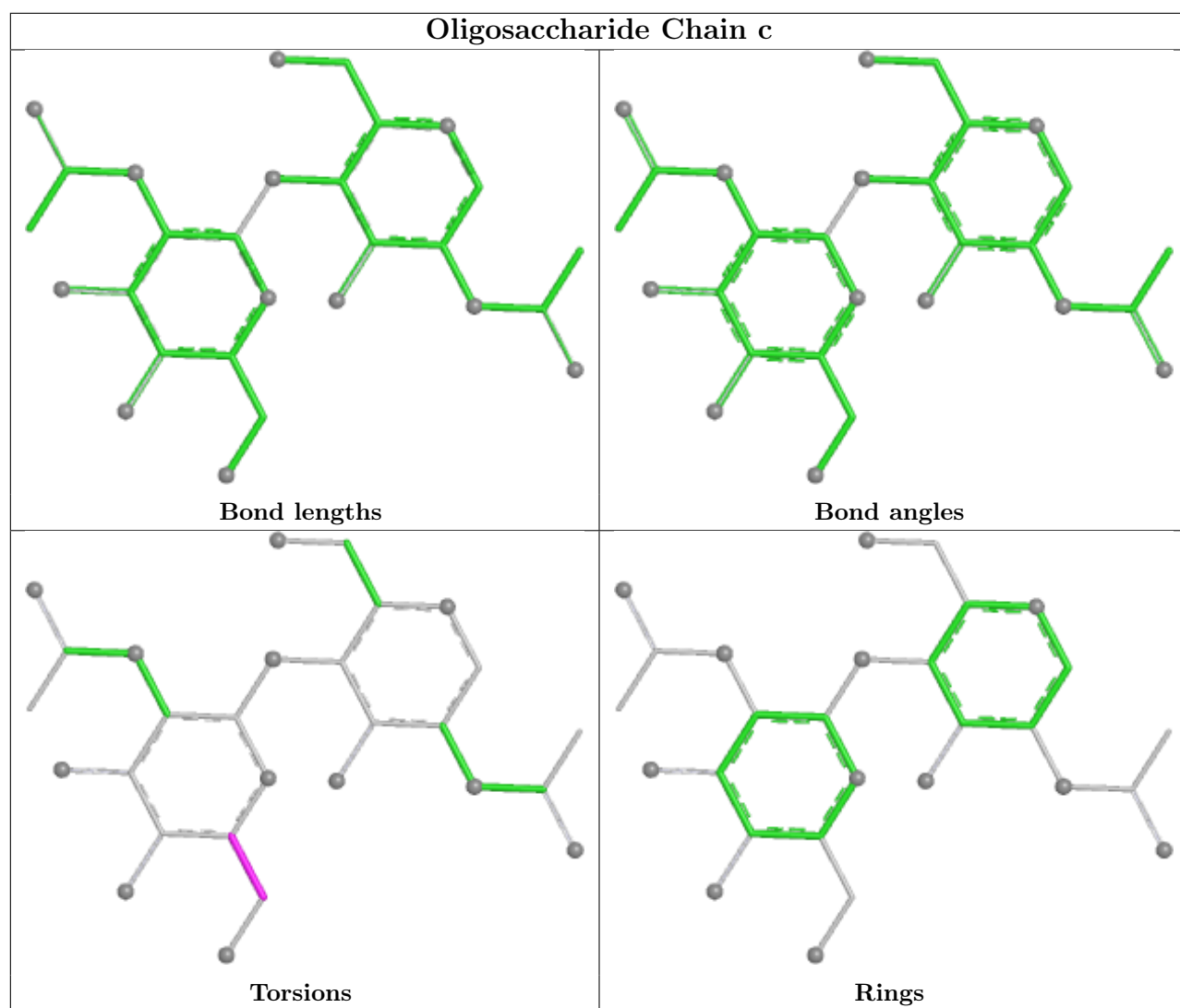


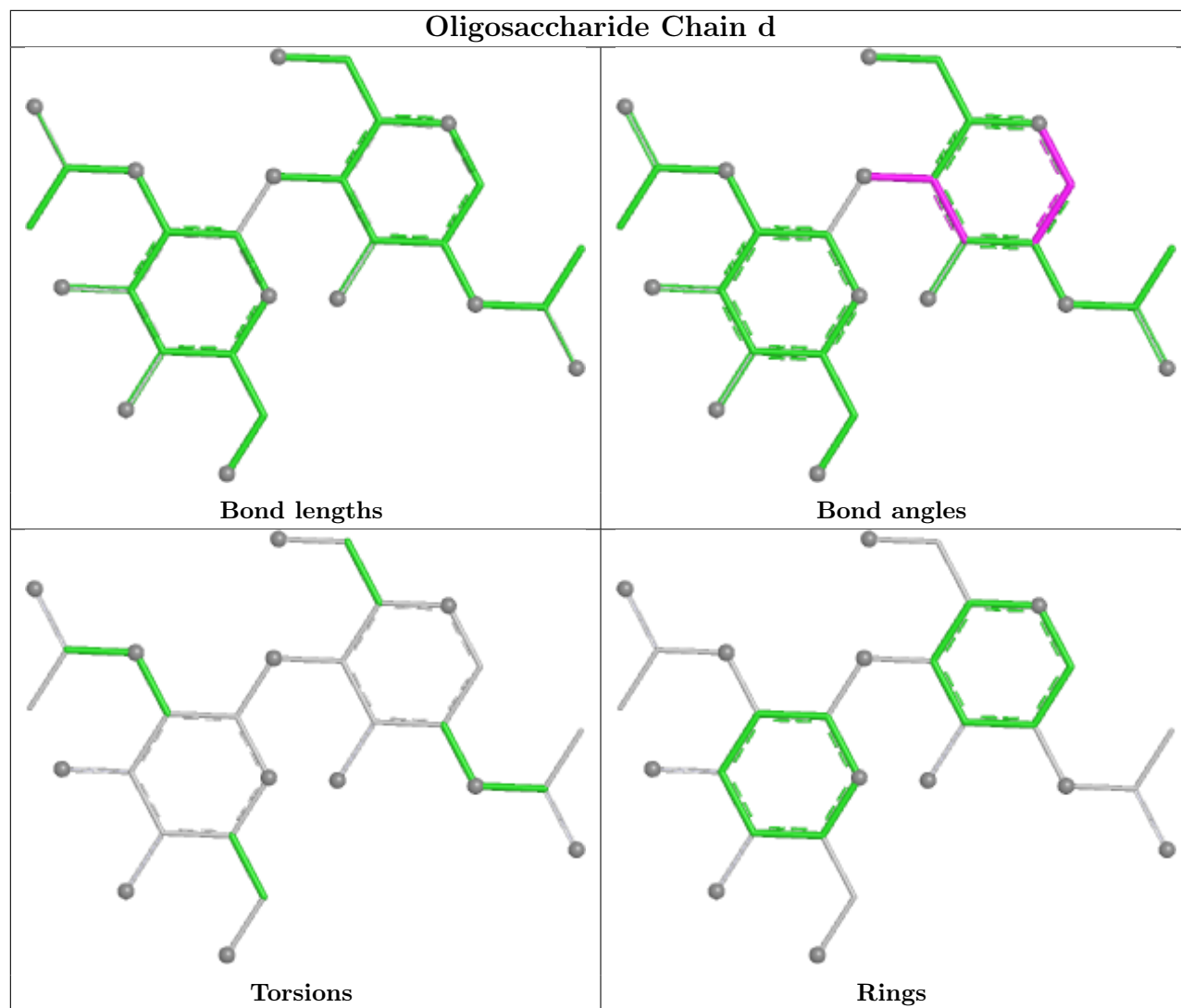


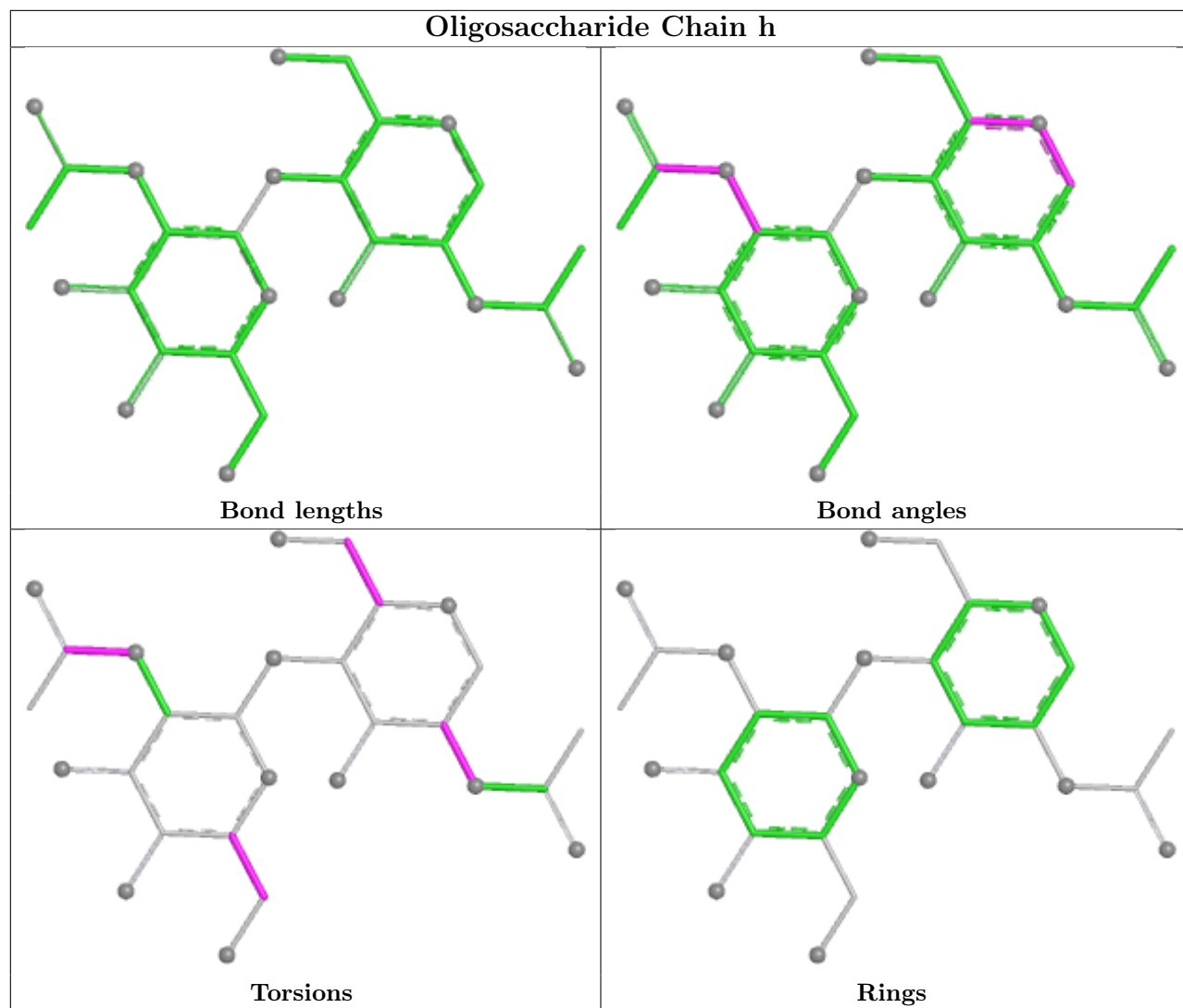


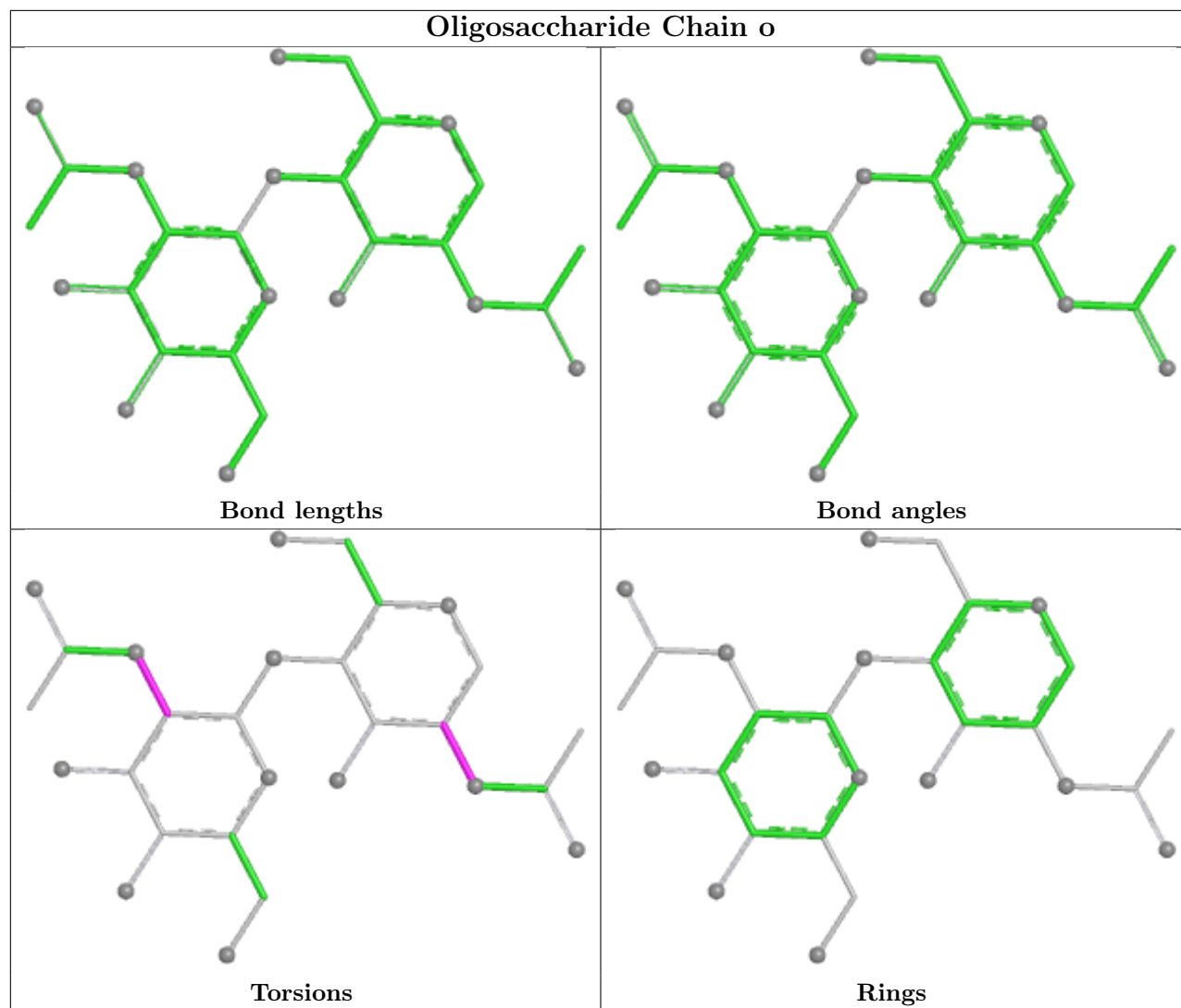


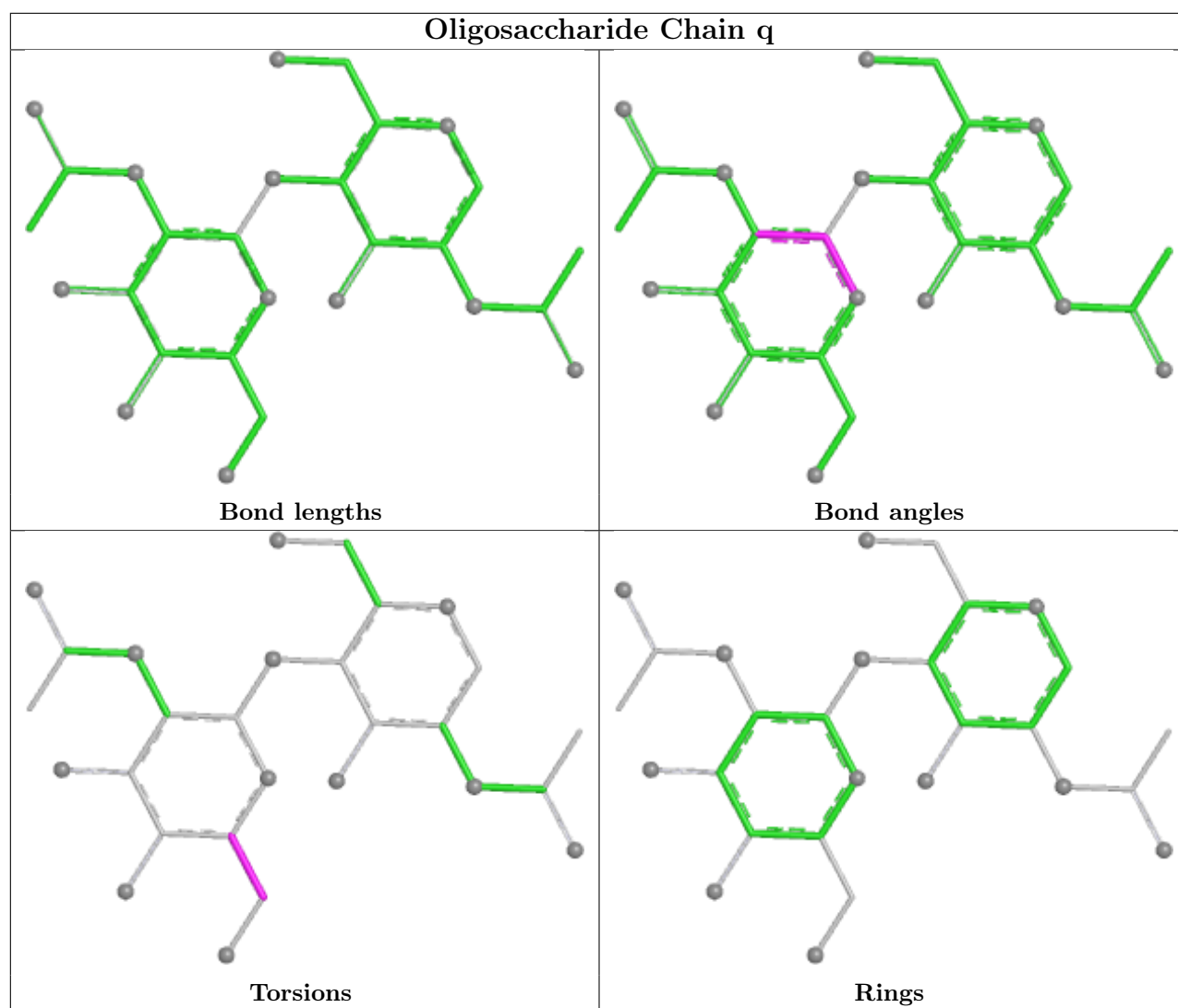


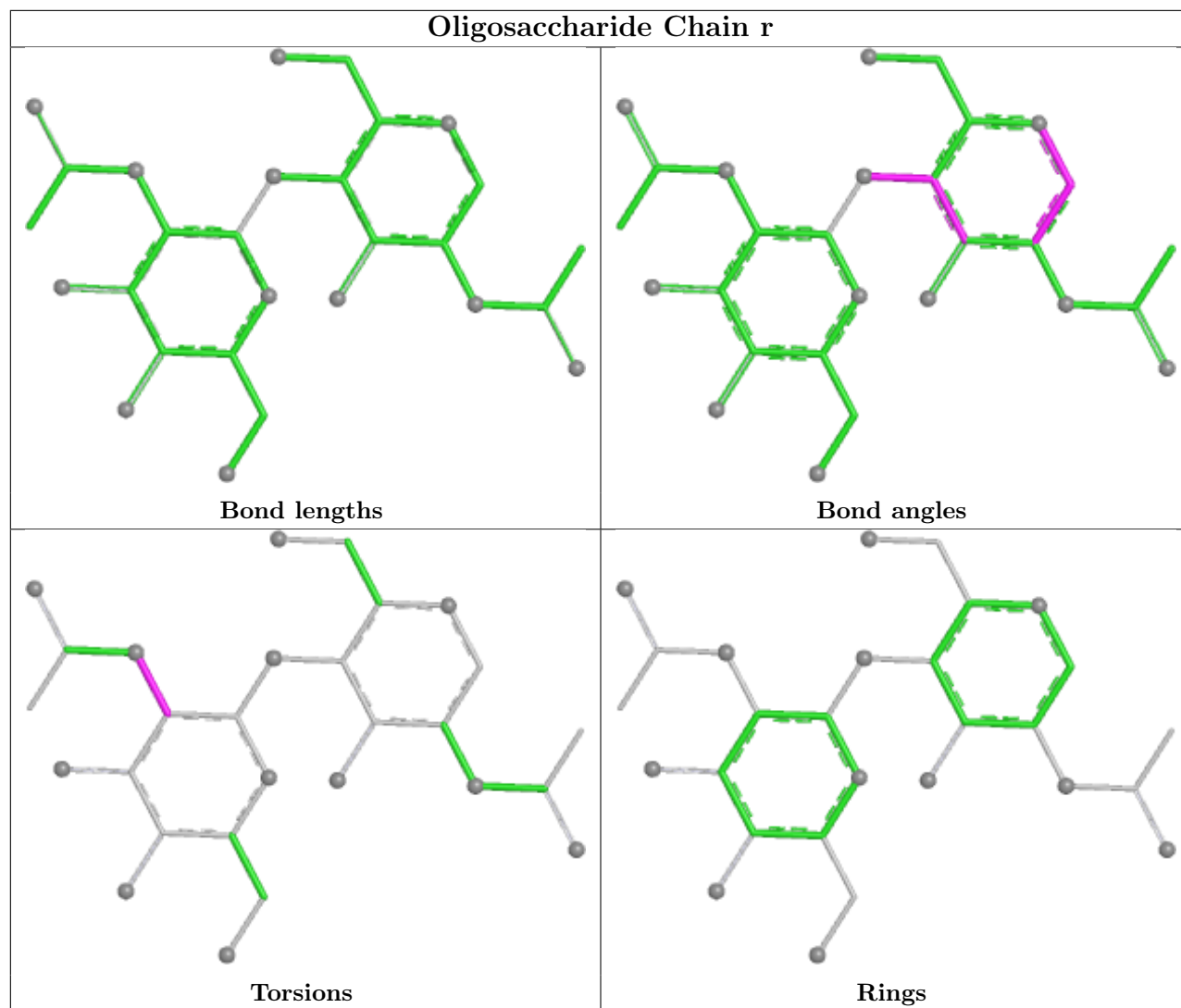


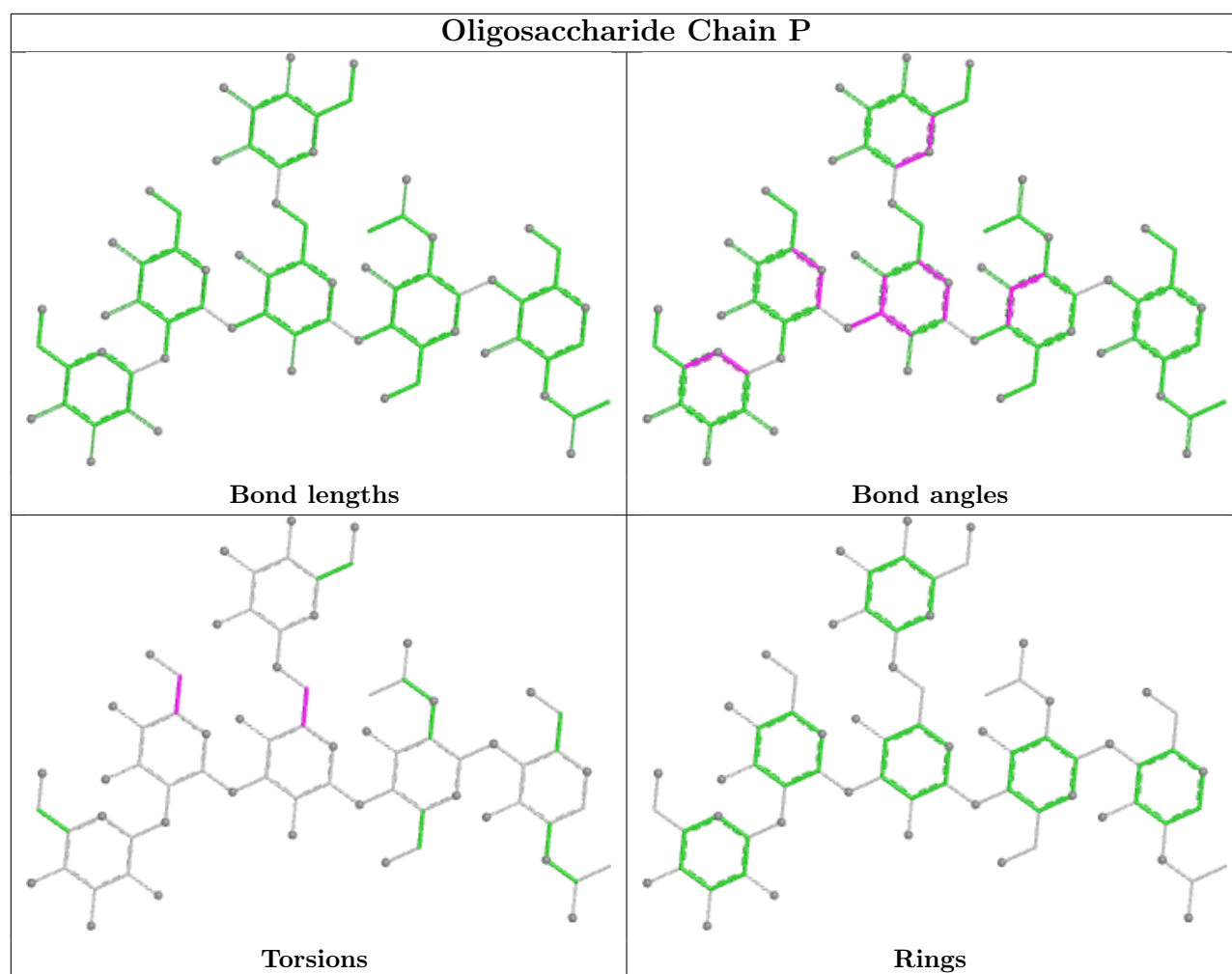


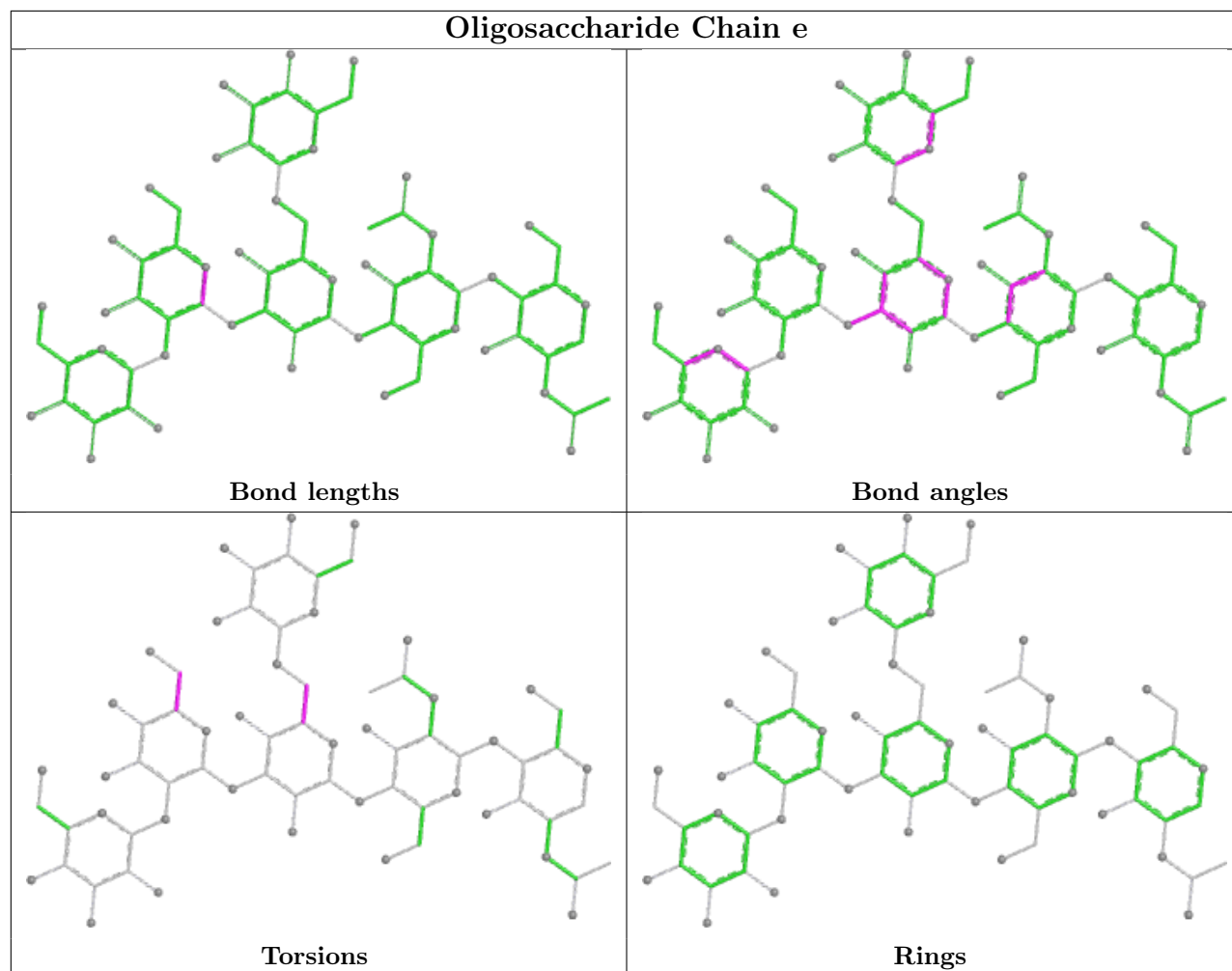


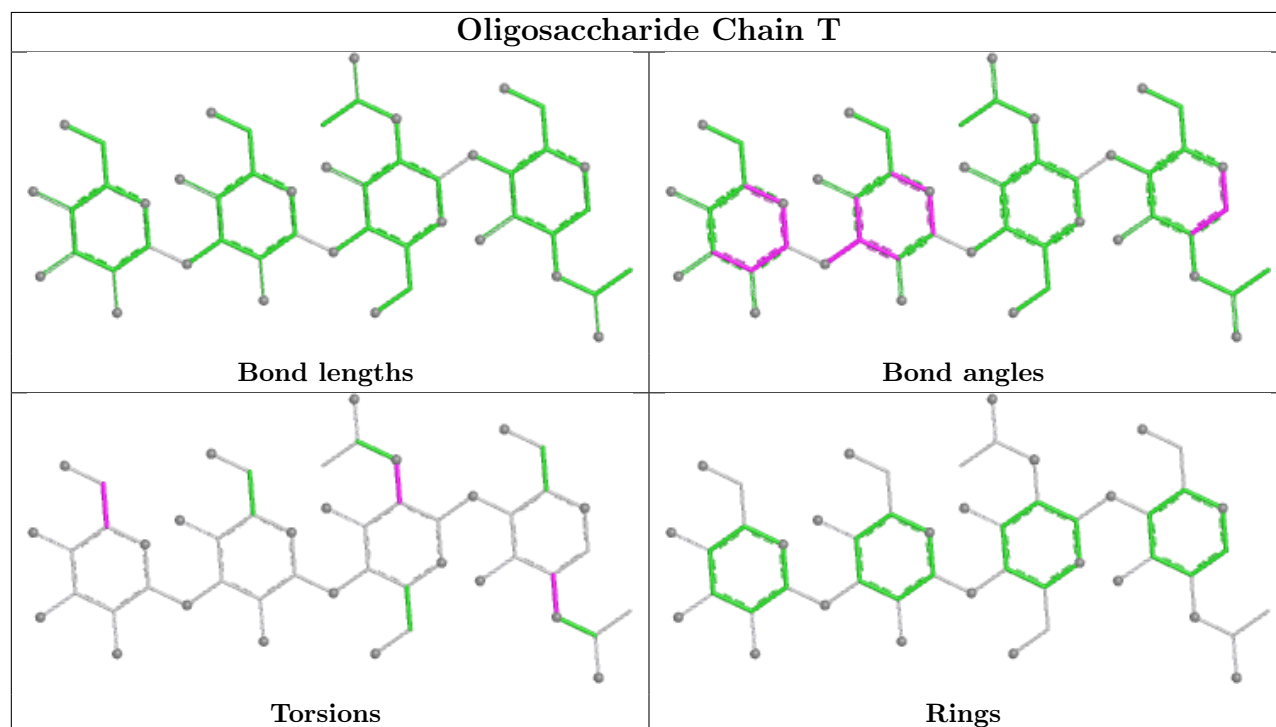
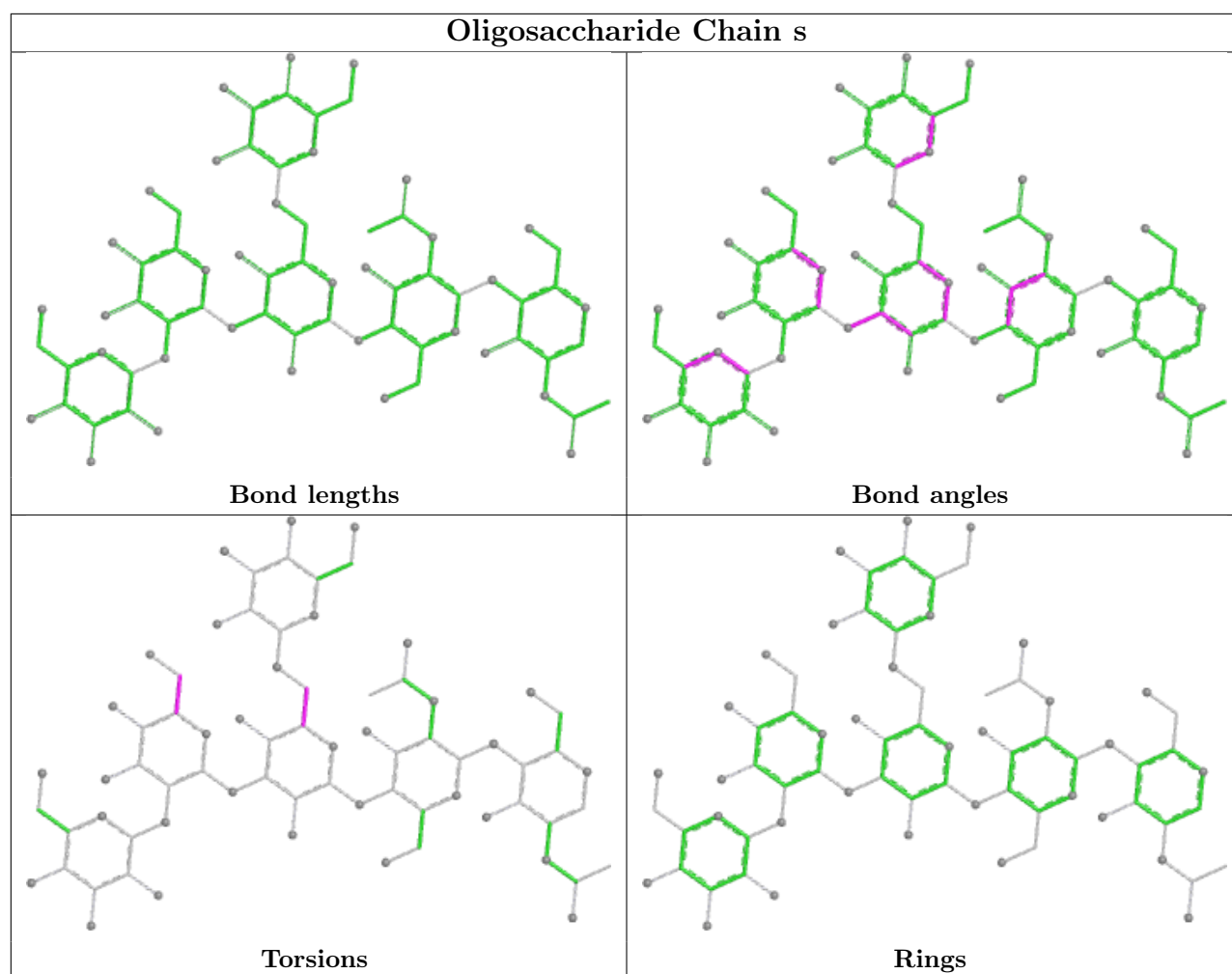


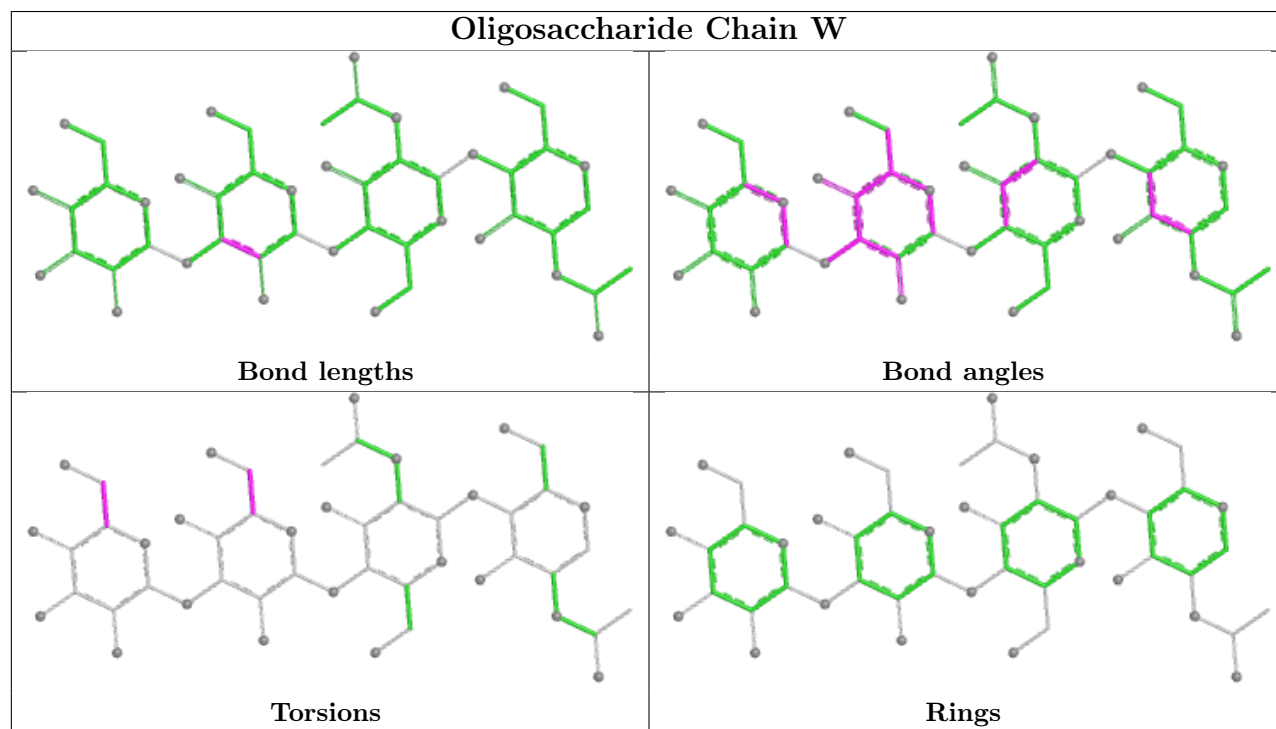
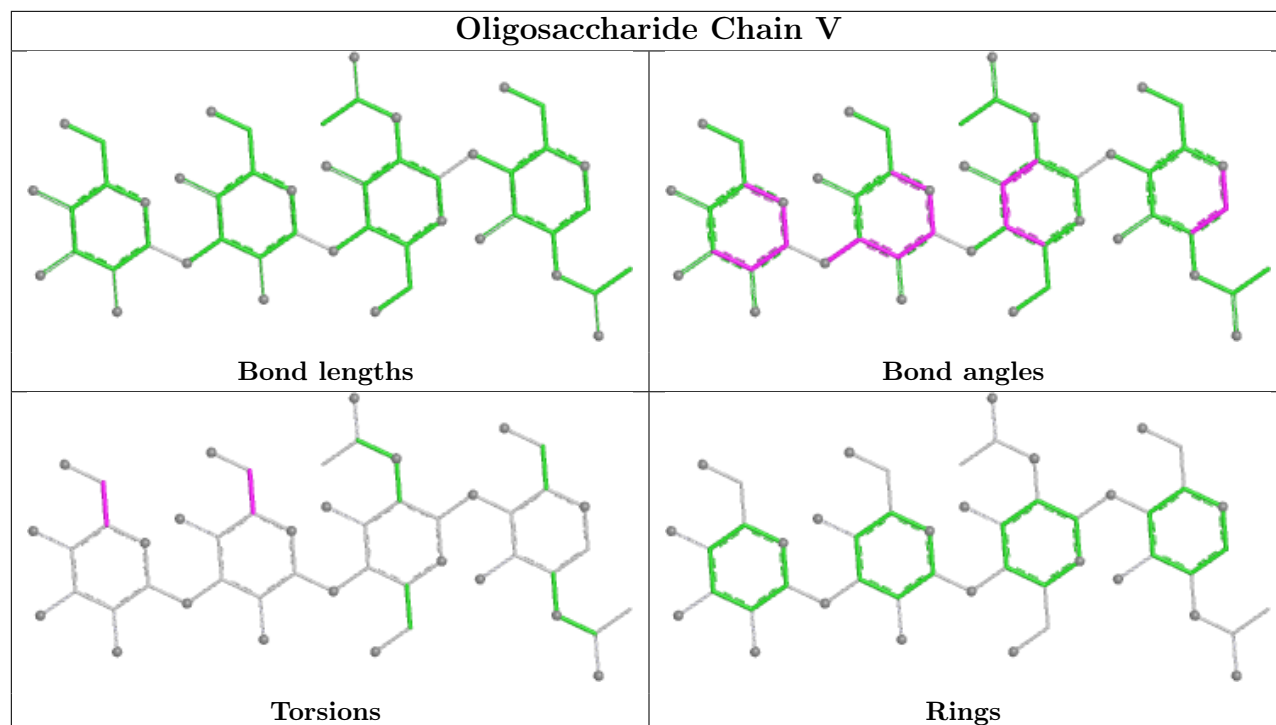


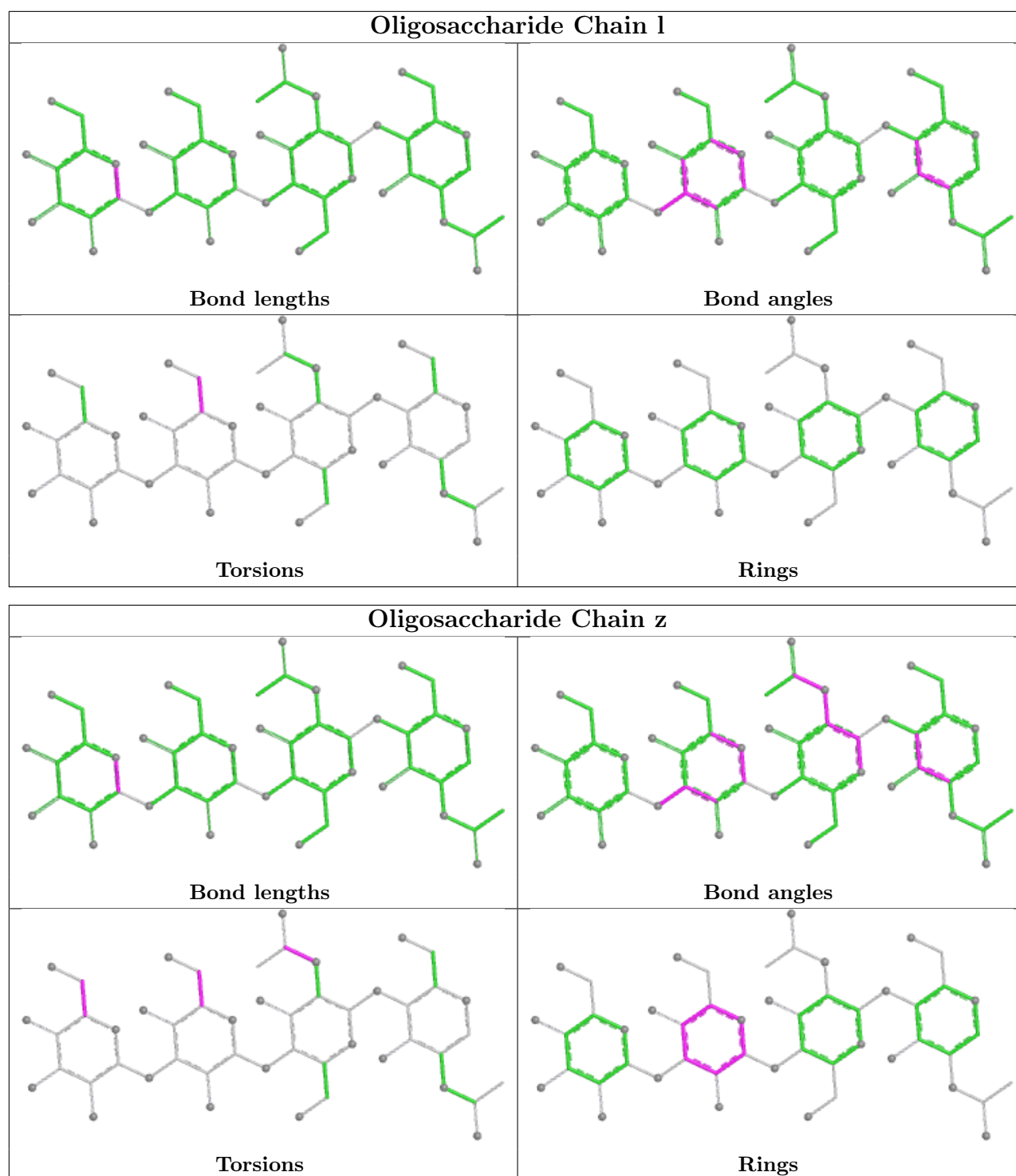












5.6 Ligand geometry [i](#)

21 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
10	NAG	F	701	1	14,14,15	0.70	0	17,19,21	1.38	1 (5%)
10	NAG	I	602	2	14,14,15	0.72	0	17,19,21	0.95	0
10	NAG	A	702	1	14,14,15	0.72	0	17,19,21	0.84	0
10	NAG	B	703	1	14,14,15	0.73	0	17,19,21	0.82	0
10	NAG	C	605	2	14,14,15	0.70	0	17,19,21	1.37	1 (5%)
10	NAG	C	602	2	14,14,15	0.72	0	17,19,21	0.90	0
11	MAN	I	603	-	11,11,12	0.78	1 (9%)	15,15,17	1.07	1 (6%)
10	NAG	C	601	2	14,14,15	0.75	0	17,19,21	0.86	0
10	NAG	A	701	1	14,14,15	0.70	0	17,19,21	1.43	1 (5%)
10	NAG	G	601	2	14,14,15	0.75	0	17,19,21	0.94	1 (5%)
10	NAG	F	702	1	14,14,15	0.75	0	17,19,21	0.83	0
10	NAG	G	604	2	14,14,15	0.71	0	17,19,21	1.35	1 (5%)
11	MAN	G	602	-	11,11,12	0.78	1 (9%)	15,15,17	1.07	1 (6%)
10	NAG	G	603	2	14,14,15	0.72	0	17,19,21	0.97	0
10	NAG	C	604	2	14,14,15	0.74	0	17,19,21	0.77	0
10	NAG	B	702	1	14,14,15	0.70	0	17,19,21	1.42	1 (5%)
10	NAG	C	603	2	14,14,15	0.72	0	17,19,21	0.89	0
10	NAG	I	601	2	14,14,15	0.72	0	17,19,21	1.85	3 (17%)
10	NAG	B	701	1	14,14,15	0.75	0	17,19,21	0.82	0
10	NAG	I	604	2	14,14,15	0.74	0	17,19,21	0.85	0
10	NAG	I	605	2	14,14,15	0.70	0	17,19,21	1.39	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
10	NAG	F	701	1	-	2/6/23/26	0/1/1/1
10	NAG	I	602	2	-	0/6/23/26	0/1/1/1
10	NAG	A	702	1	-	0/6/23/26	0/1/1/1
10	NAG	B	703	1	-	0/6/23/26	0/1/1/1
10	NAG	C	605	2	-	3/6/23/26	0/1/1/1
10	NAG	C	602	2	-	0/6/23/26	0/1/1/1
11	MAN	I	603	-	-	0/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	C	601	2	-	2/6/23/26	0/1/1/1
10	NAG	A	701	1	-	2/6/23/26	0/1/1/1
10	NAG	G	601	2	-	0/6/23/26	0/1/1/1
10	NAG	F	702	1	-	0/6/23/26	0/1/1/1
10	NAG	G	604	2	-	3/6/23/26	0/1/1/1
11	MAN	G	602	-	-	0/2/19/22	1/1/1/1
10	NAG	G	603	2	-	1/6/23/26	0/1/1/1
10	NAG	C	604	2	-	0/6/23/26	0/1/1/1
10	NAG	B	702	1	-	2/6/23/26	0/1/1/1
10	NAG	C	603	2	-	0/6/23/26	0/1/1/1
10	NAG	I	601	2	-	4/6/23/26	0/1/1/1
10	NAG	B	701	1	-	0/6/23/26	0/1/1/1
10	NAG	I	604	2	-	2/6/23/26	0/1/1/1
10	NAG	I	605	2	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	602	MAN	O5-C1	-2.01	1.40	1.43
11	I	603	MAN	O5-C1	-2.00	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	601	NAG	C2-N2-C7	5.61	130.42	122.90
10	A	701	NAG	C2-N2-C7	4.54	128.99	122.90
10	I	605	NAG	C2-N2-C7	4.50	128.93	122.90
10	G	604	NAG	C2-N2-C7	4.41	128.82	122.90
10	C	605	NAG	C2-N2-C7	4.34	128.71	122.90
10	F	701	NAG	C2-N2-C7	4.32	128.69	122.90
10	B	702	NAG	C2-N2-C7	4.20	128.53	122.90
11	G	602	MAN	C1-O5-C5	3.03	116.25	112.19
11	I	603	MAN	C1-O5-C5	3.03	116.25	112.19
10	I	601	NAG	C8-C7-N2	2.39	120.08	116.12
10	I	601	NAG	C1-O5-C5	2.31	115.28	112.19
10	G	601	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	601	NAG	C1-C2-N2-C7
10	G	603	NAG	C1-C2-N2-C7
10	A	701	NAG	C8-C7-N2-C2
10	A	701	NAG	O7-C7-N2-C2
10	C	605	NAG	C8-C7-N2-C2
10	C	605	NAG	O7-C7-N2-C2
10	B	702	NAG	C8-C7-N2-C2
10	B	702	NAG	O7-C7-N2-C2
10	G	604	NAG	C8-C7-N2-C2
10	G	604	NAG	O7-C7-N2-C2
10	F	701	NAG	C8-C7-N2-C2
10	F	701	NAG	O7-C7-N2-C2
10	I	601	NAG	C8-C7-N2-C2
10	I	601	NAG	O7-C7-N2-C2
10	I	605	NAG	C8-C7-N2-C2
10	I	605	NAG	O7-C7-N2-C2
10	G	604	NAG	O5-C5-C6-O6
10	C	605	NAG	O5-C5-C6-O6
10	I	605	NAG	O5-C5-C6-O6
10	I	604	NAG	C1-C2-N2-C7
10	C	601	NAG	C3-C2-N2-C7
10	I	601	NAG	C3-C2-N2-C7
10	I	601	NAG	C1-C2-N2-C7
10	I	604	NAG	C3-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	G	602	MAN	C1-C2-C3-C4-C5-O5
11	I	603	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	602	NAG	2	0
10	C	602	NAG	1	0
10	G	601	NAG	1	0
10	F	702	NAG	1	0
10	I	601	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.

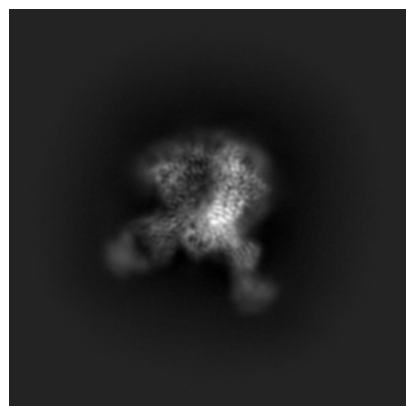
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71766. These allow visual inspection of the internal detail of the map and identification of artifacts.

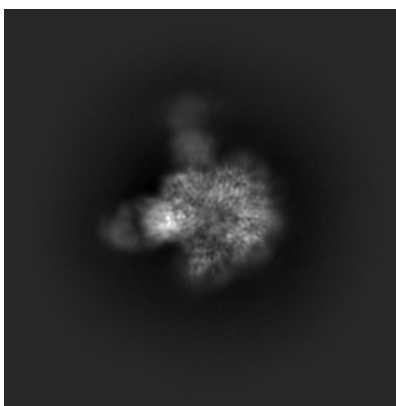
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

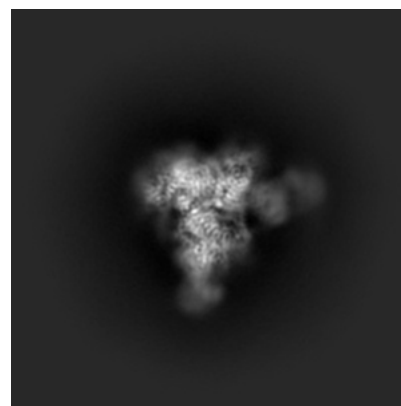
6.1.1 Primary map



X

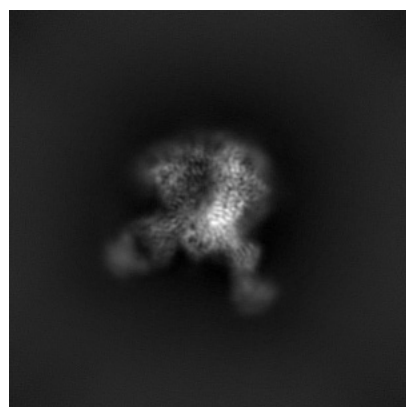


Y

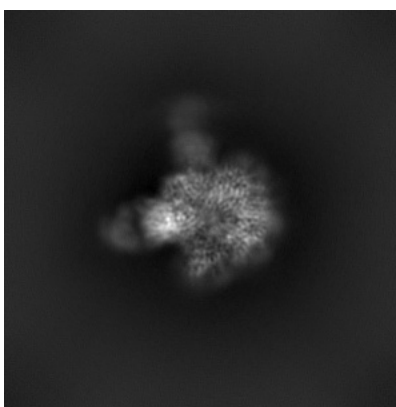


Z

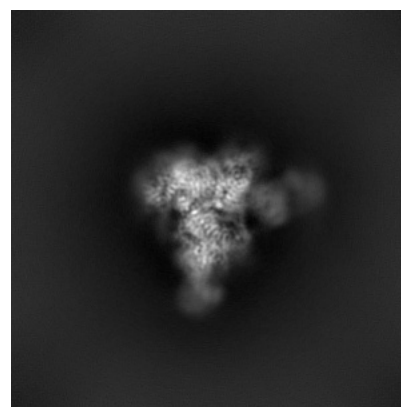
6.1.2 Raw map



X



Y

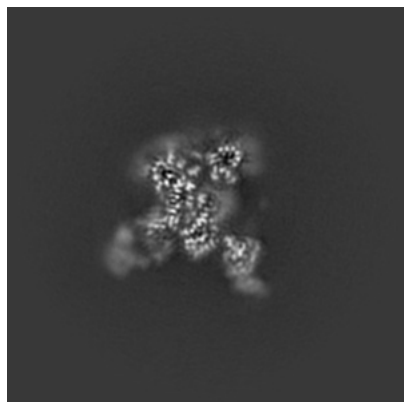


Z

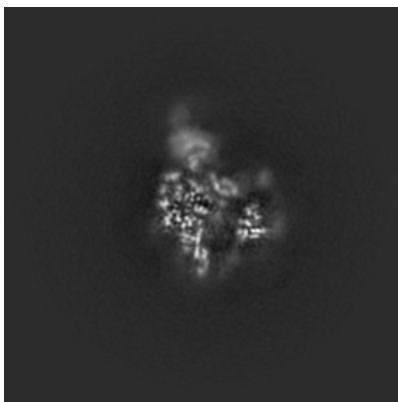
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

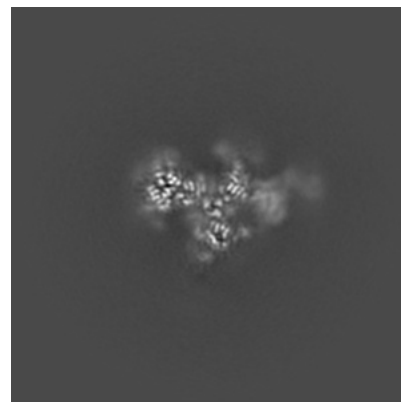
6.2.1 Primary map



X Index: 192

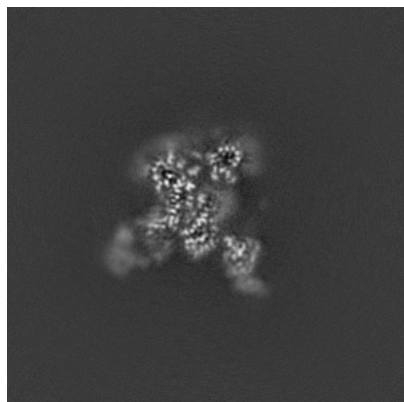


Y Index: 192

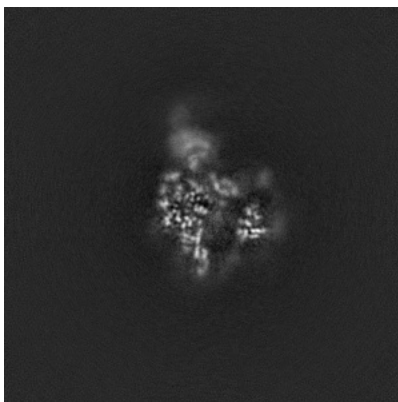


Z Index: 192

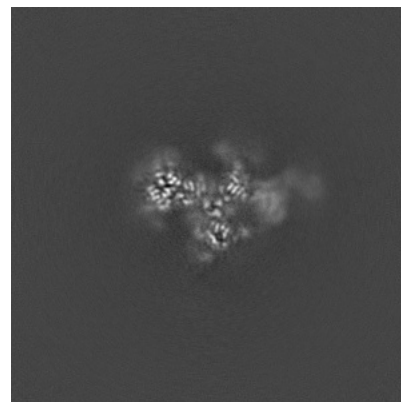
6.2.2 Raw map



X Index: 192



Y Index: 192

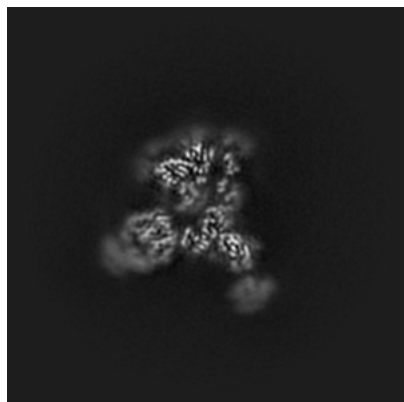


Z Index: 192

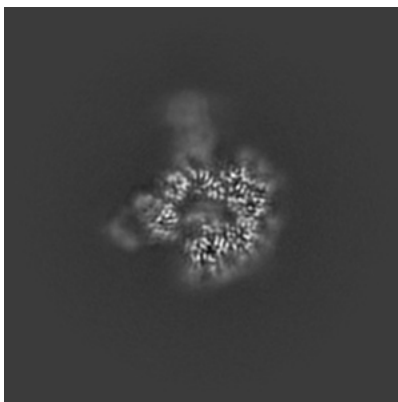
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

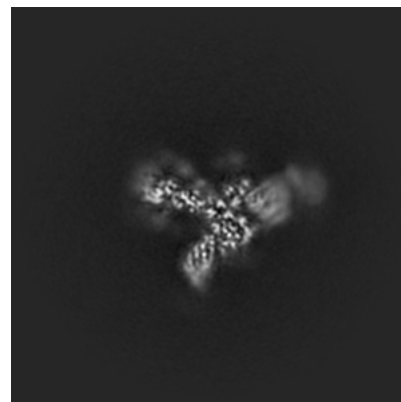
6.3.1 Primary map



X Index: 178

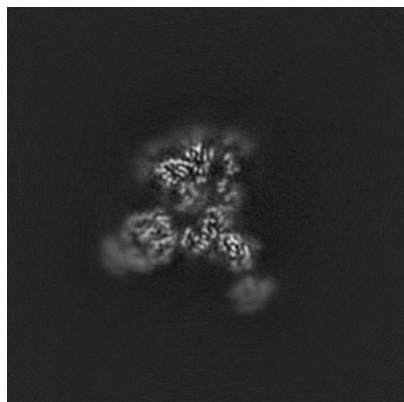


Y Index: 214

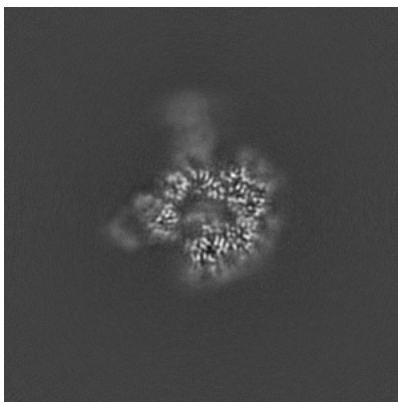


Z Index: 180

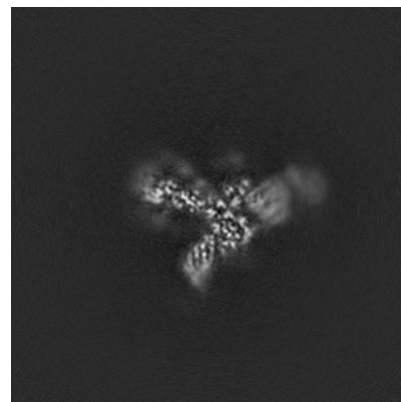
6.3.2 Raw map



X Index: 178



Y Index: 214

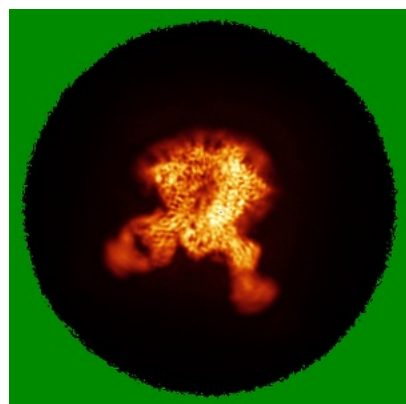


Z Index: 180

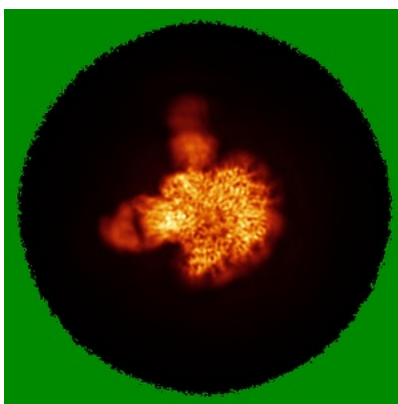
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

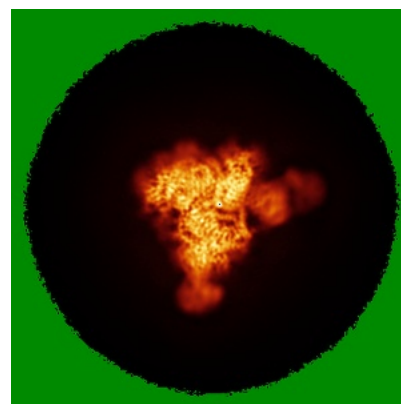
6.4.1 Primary map



X

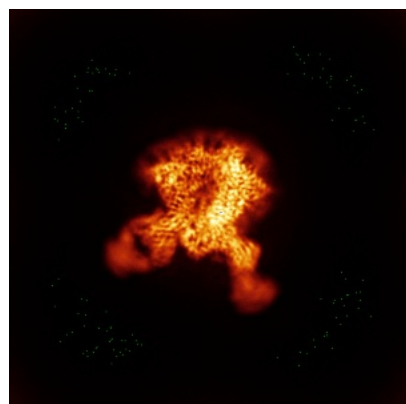


Y

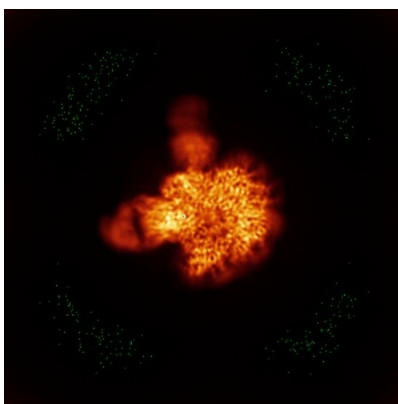


Z

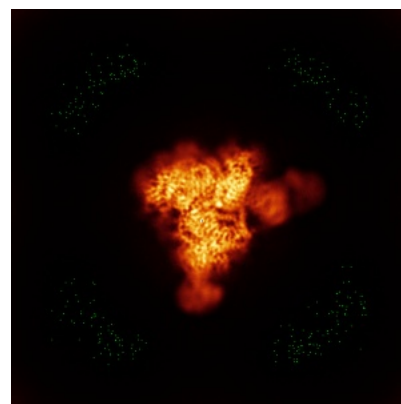
6.4.2 Raw map



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.

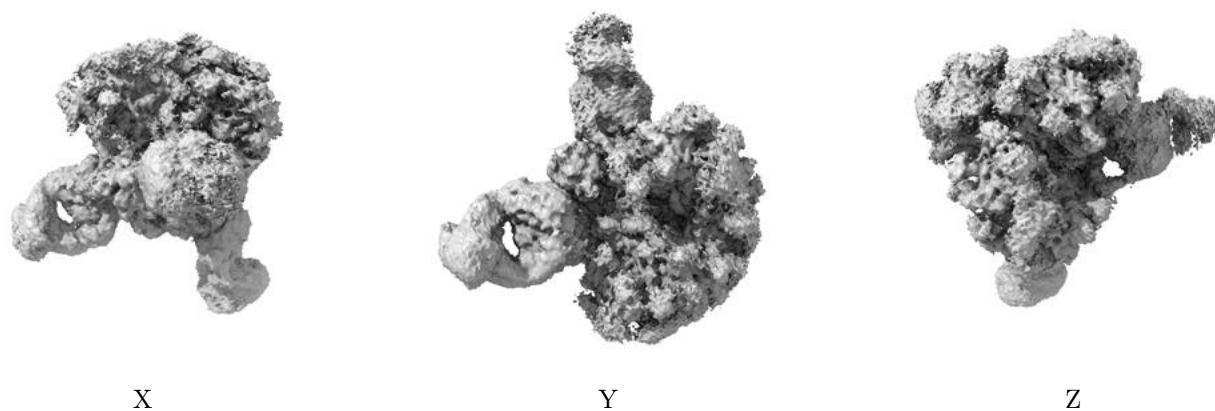
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0823. 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.

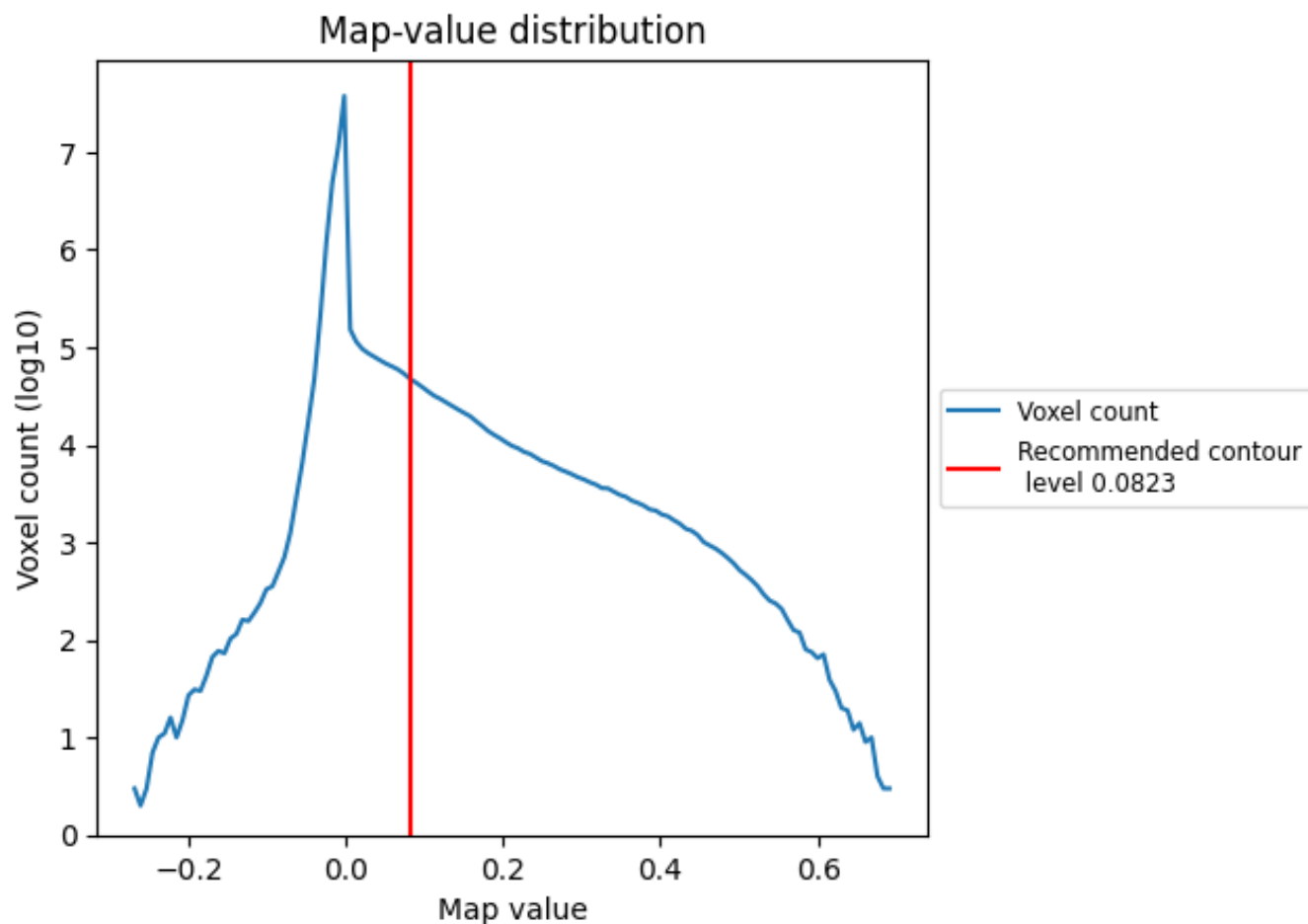
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

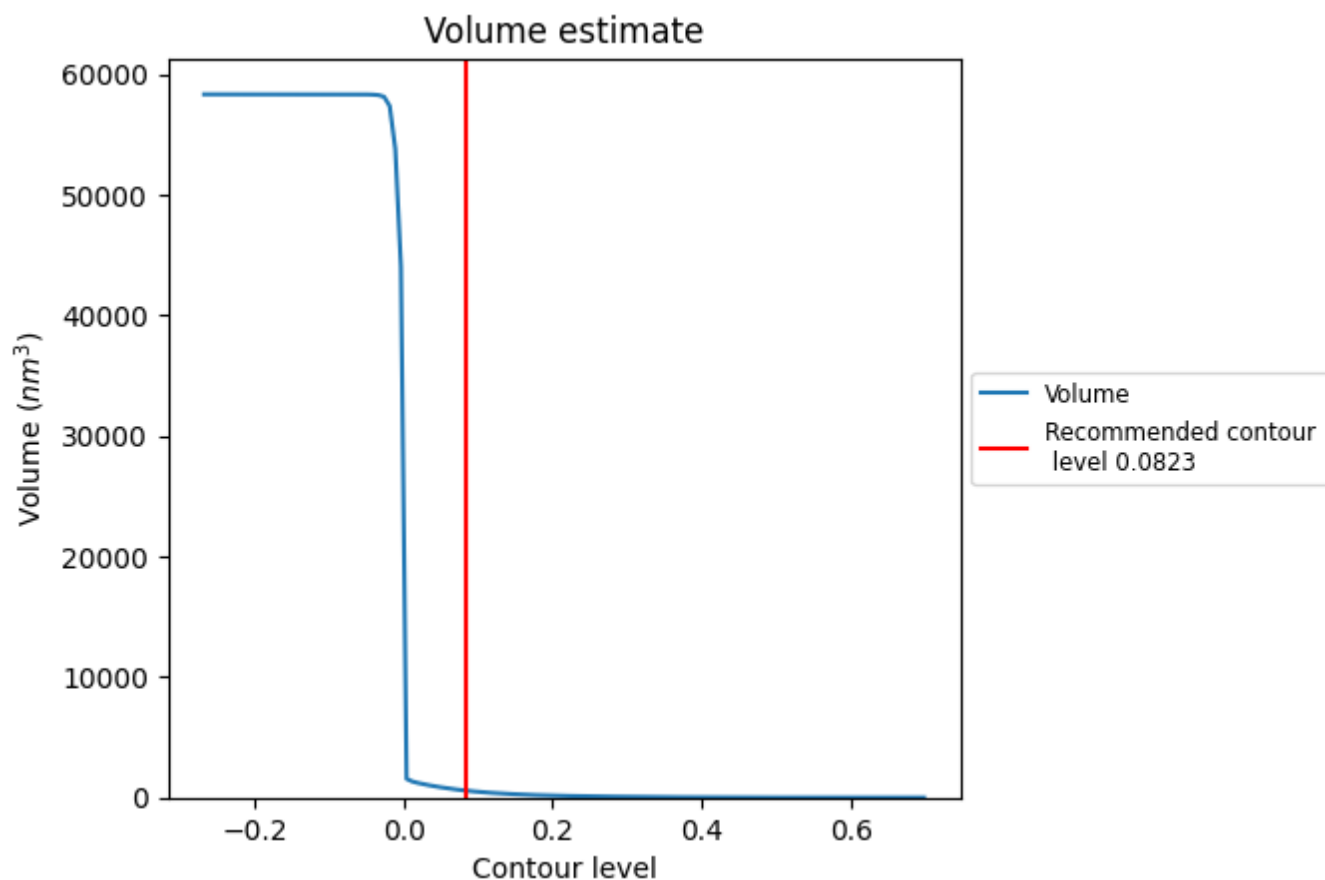
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

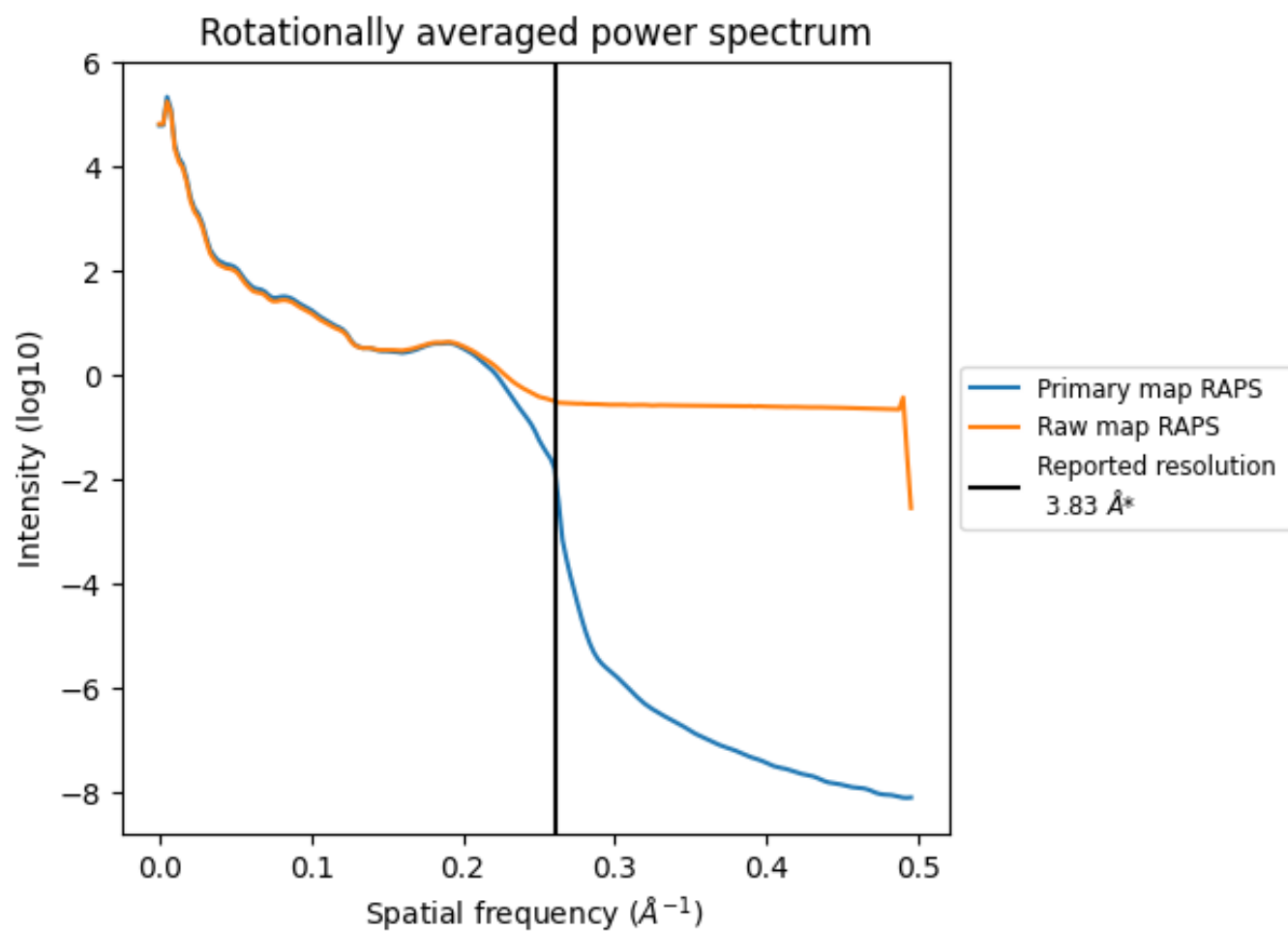
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 583 nm^3 ; this corresponds to an approximate mass of 526 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 ⓘ

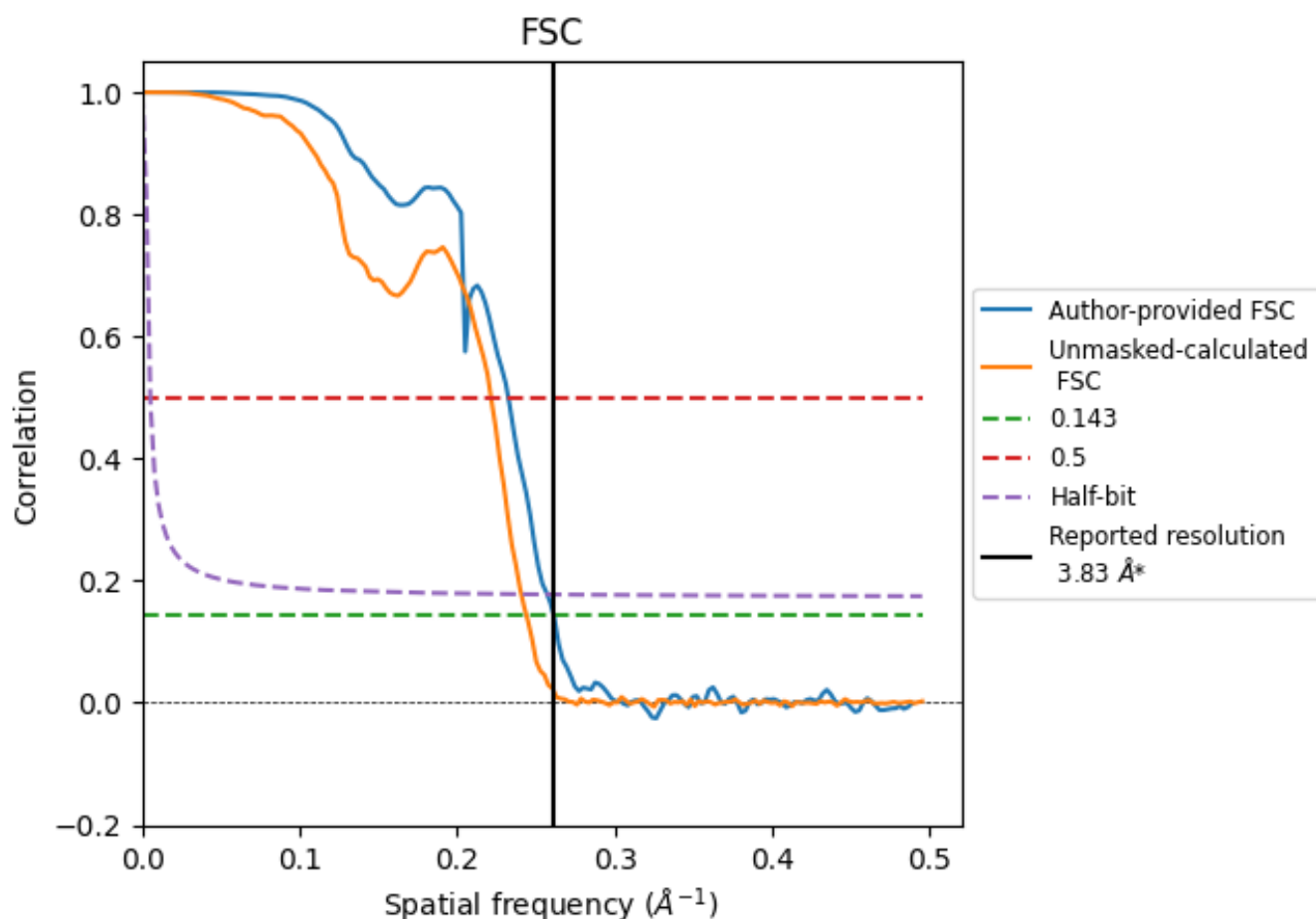


*Reported resolution corresponds to spatial frequency of 0.261 \AA^{-1}

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 0.261 \AA^{-1}

8.2 Resolution estimates [i](#)

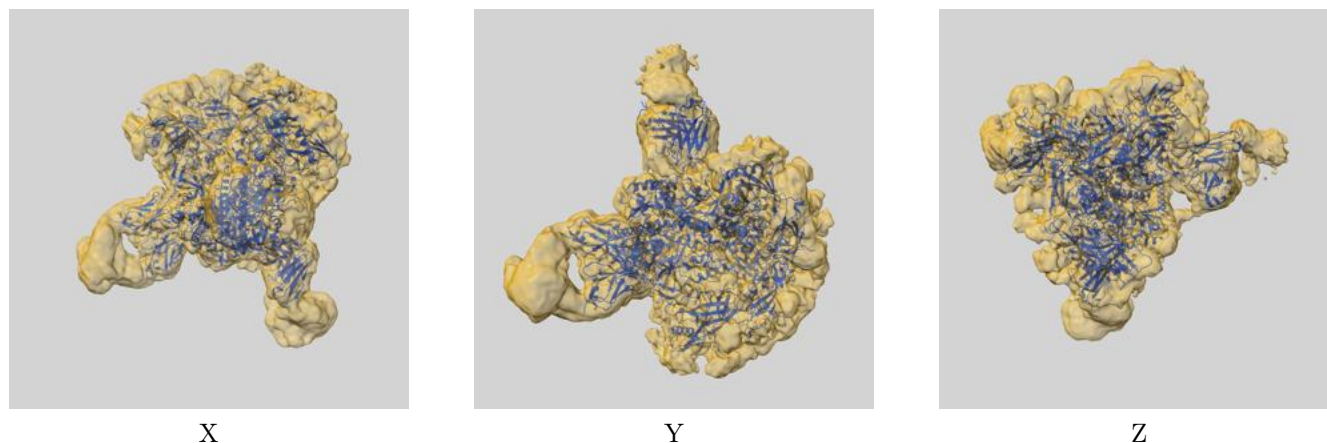
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	3.83	4.30	3.89
Unmasked-calculated*	4.10	4.52	4.16

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

9 Map-model fit [i](#)

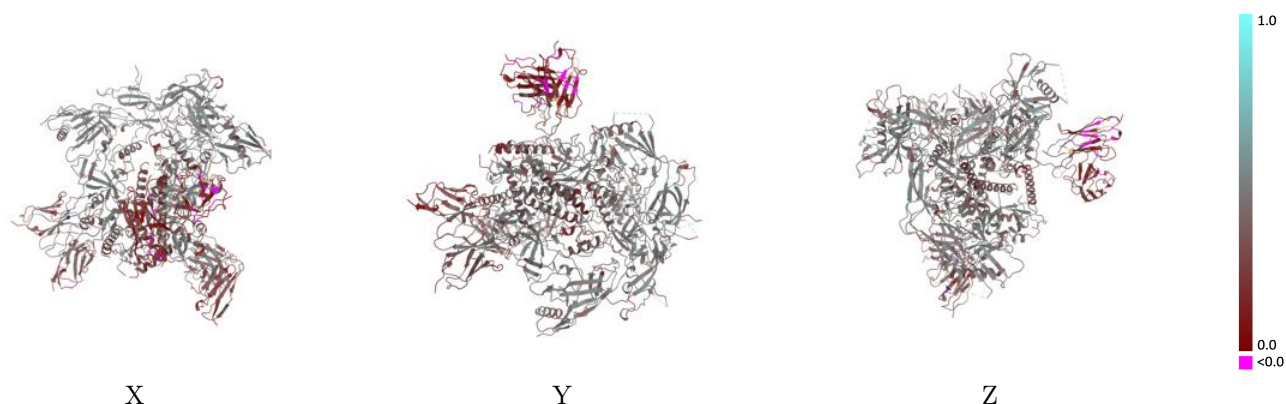
This section contains information regarding the fit between EMDB map EMD-71766 and PDB model 9PNI. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0823 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](#)



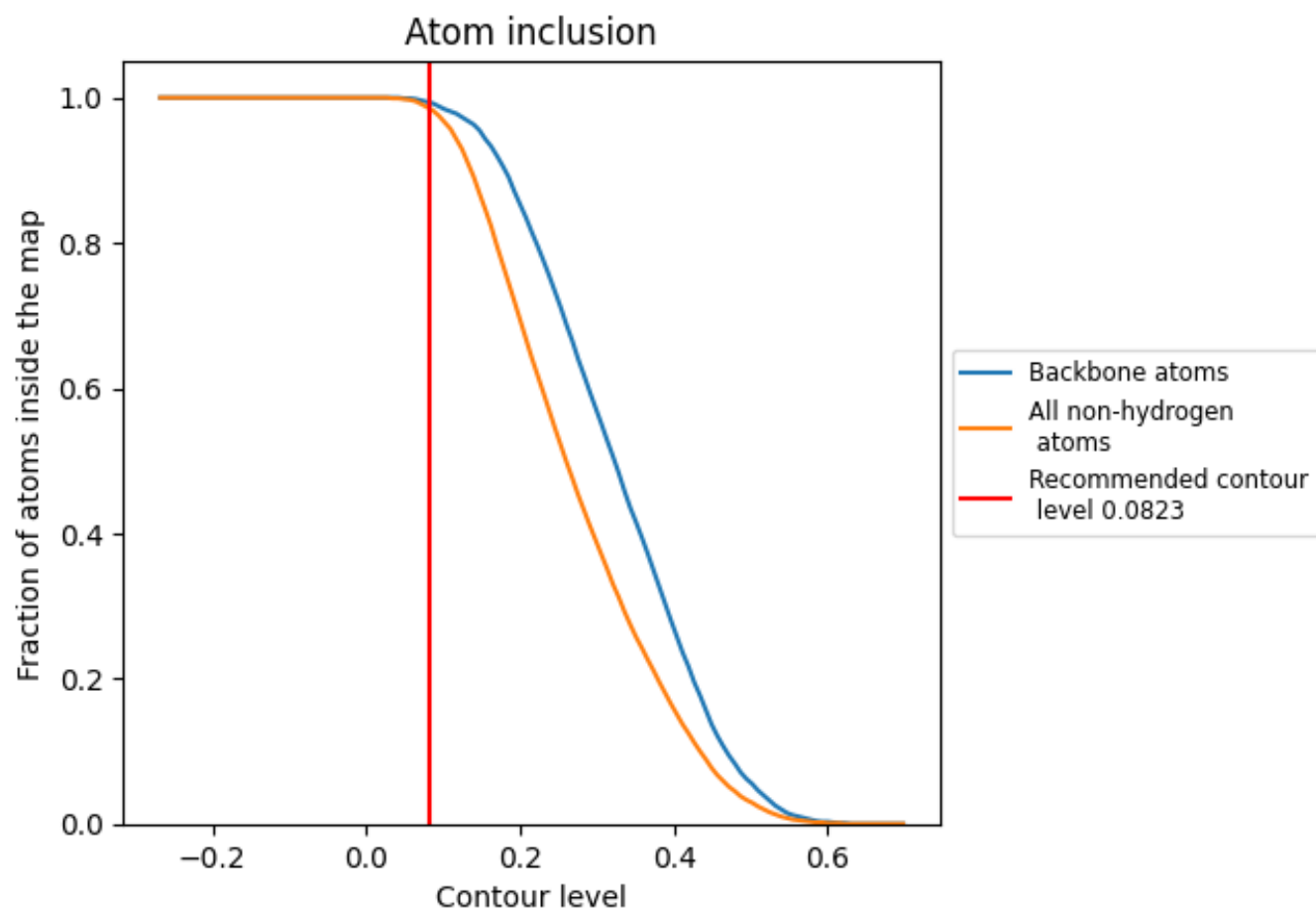
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0823).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.0823) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9850	 0.3820
0	 1.0000	 0.3900
1	 0.9490	 0.3590
A	 0.9940	 0.3950
B	 0.9910	 0.3820
C	 0.9910	 0.4370
D	 0.9050	 0.1760
E	 0.9340	 0.1450
F	 0.9930	 0.3800
G	 0.9910	 0.4360
H	 1.0000	 0.3610
I	 0.9910	 0.4370
J	 0.9990	 0.3530
K	 0.9900	 0.2990
L	 0.9960	 0.3070
M	 1.0000	 0.4000
N	 0.9510	 0.2960
O	 0.8570	 0.3210
P	 1.0000	 0.3350
Q	 1.0000	 0.3810
R	 1.0000	 0.4000
S	 0.9640	 0.3250
T	 1.0000	 0.4070
U	 1.0000	 0.3910
V	 0.9800	 0.3630
W	 0.9800	 0.3570
X	 1.0000	 0.3830
Y	 0.9740	 0.3980
Z	 0.9740	 0.4120
a	 0.9640	 0.3600
b	 0.9840	 0.3560
c	 0.8930	 0.3510
d	 0.9640	 0.3080
e	 0.9860	 0.3510
f	 1.0000	 0.3450



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Chain	Atom inclusion	Q-score
g	 1.0000	 0.4030
h	 0.9290	 0.3440
i	 1.0000	 0.3780
j	 1.0000	 0.3990
k	 1.0000	 0.3840
l	 1.0000	 0.3470
m	 0.9740	 0.3780
n	 0.9740	 0.2650
o	 1.0000	 0.2930
p	 0.9840	 0.2800
q	 0.8930	 0.3940
r	 1.0000	 0.3240
s	 0.9860	 0.3550
t	 1.0000	 0.3280
u	 1.0000	 0.4080
v	 0.9230	 0.3280
w	 1.0000	 0.3980
x	 0.9740	 0.3810
y	 1.0000	 0.3410
z	 0.9800	 0.3470