



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 07:17 AM UTC

PDB ID : 8ULS / pdb_00008uls
EMDB ID : EMD-42364
Title : Cryo-EM structure of the BG505 SOSIPv2 in complex with bNAb 01_D03 Fabs
Authors : DeLaitch, A.T.; Bjorkman, P.J.
Deposited on : 2023-10-16
Resolution : 3.20 Å (reported)
Based on initial models : 6UDJ, 8UKI

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

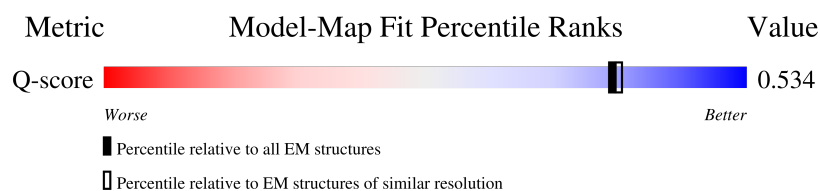
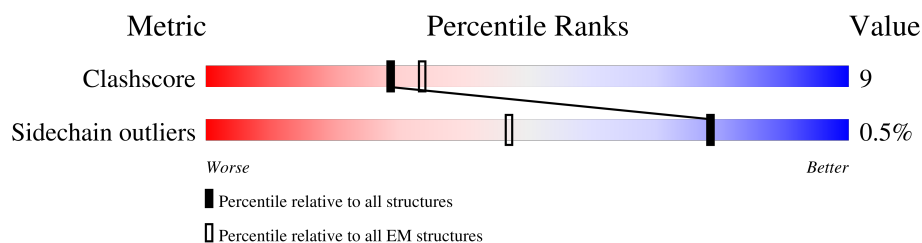
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	479	
1	C	479	
1	E	479	
2	B	153	
2	D	153	

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Mol	Chain	Length	Quality of chain
2	F	153	
3	H	249	
3	I	249	
3	J	249	
4	L	211	
4	M	211	
4	N	211	
5	G	2	
5	K	2	
5	O	2	
5	S	2	
5	T	2	
5	U	2	
5	X	2	
5	Y	2	
5	Z	2	
5	a	2	
5	b	2	
5	f	2	
5	g	2	
5	h	2	
5	k	2	
5	m	2	
5	n	2	
5	o	2	

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Mol	Chain	Length	Quality of chain
5	s	2	50%
5	t	2	50%
5	u	2	50%
5	v	2	50%
5	x	2	50%
5	y	2	100%
6	P	3	33%
6	Q	3	100%
6	c	3	33%
6	d	3	67%
6	l	3	33%
6	p	3	33%
6	q	3	100%
7	R	5	60%
7	e	5	40%
7	r	5	60%
8	V	4	25%
8	i	4	25%
9	W	4	25%
9	j	4	25%
9	w	4	25%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20959 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 gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	448	Total	C	N	O	S	0	0
			3523	2212	623	660	28		
1	C	448	Total	C	N	O	S	0	0
			3523	2212	623	660	28		
1	E	448	Total	C	N	O	S	0	0
			3523	2212	623	660	28		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	505	VAL	-	expression tag	UNP Q2N0S6
A	506	VAL	-	expression tag	UNP Q2N0S6
A	507	GLY	-	expression tag	UNP Q2N0S6
A	508	ARG	-	expression tag	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	505	VAL	-	expression tag	UNP Q2N0S6
C	506	VAL	-	expression tag	UNP Q2N0S6
C	507	GLY	-	expression tag	UNP Q2N0S6
C	508	ARG	-	expression tag	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	505	VAL	-	expression tag	UNP Q2N0S6
E	506	VAL	-	expression tag	UNP Q2N0S6
E	507	GLY	-	expression tag	UNP Q2N0S6
E	508	ARG	-	expression tag	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1049	668	181	194	6		
2	D	132	Total	C	N	O	S	0	0
			1049	668	181	194	6		
2	F	132	Total	C	N	O	S	0	0
			1049	668	181	194	6		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called 01_D03 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	137	Total	C	N	O	S	0	0
			1075	677	195	197	6		
3	I	137	Total	C	N	O	S	0	0
			1075	677	195	197	6		
3	J	137	Total	C	N	O	S	0	0
			1075	677	195	197	6		

- Molecule 4 is a protein called 01_D03 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	104	Total	C	N	O	S	0	0
			810	514	140	153	3		
4	M	104	Total	C	N	O	S	0	0
			810	514	140	153	3		
4	N	104	Total	C	N	O	S	0	0
			810	514	140	153	3		

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



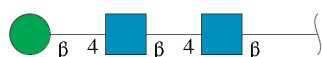
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		

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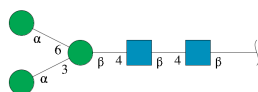
Mol	Chain	Residues	Atoms				AltConf	Trace
5	k	2	Total	C	N	O	0	0
			28	16	2	10		
5	m	2	Total	C	N	O	0	0
			28	16	2	10		
5	n	2	Total	C	N	O	0	0
			28	16	2	10		
5	o	2	Total	C	N	O	0	0
			28	16	2	10		
5	s	2	Total	C	N	O	0	0
			28	16	2	10		
5	t	2	Total	C	N	O	0	0
			28	16	2	10		
5	u	2	Total	C	N	O	0	0
			28	16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

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	3	Total	C	N	O	0	0
			39	22	2	15		
6	Q	3	Total	C	N	O	0	0
			39	22	2	15		
6	c	3	Total	C	N	O	0	0
			39	22	2	15		
6	d	3	Total	C	N	O	0	0
			39	22	2	15		
6	l	3	Total	C	N	O	0	0
			39	22	2	15		
6	p	3	Total	C	N	O	0	0
			39	22	2	15		
6	q	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 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
7	R	5	Total	C	N	O	0	0
			61	34	2	25		
7	e	5	Total	C	N	O	0	0
			61	34	2	25		
7	r	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 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
8	V	4	Total	C	N	O	0	0
			50	28	2	20		
8	i	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is an oligosaccharide called 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.



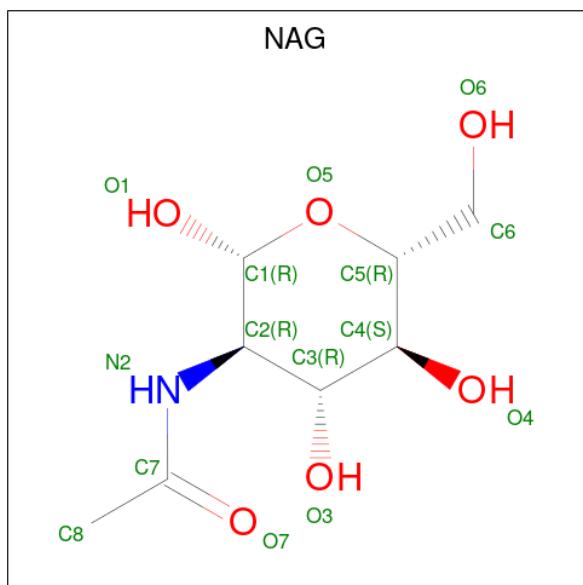
Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	4	Total	C	N	O	0	0
			50	28	2	20		
9	j	4	Total	C	N	O	0	0
			50	28	2	20		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	w	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: $C_8H_{15}NO_6$).



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	A	1	Total	C	N	O	0
			14	8	1	5	
10	A	1	Total	C	N	O	0
			14	8	1	5	
10	B	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	D	1	Total	C	N	O	0
			14	8	1	5	

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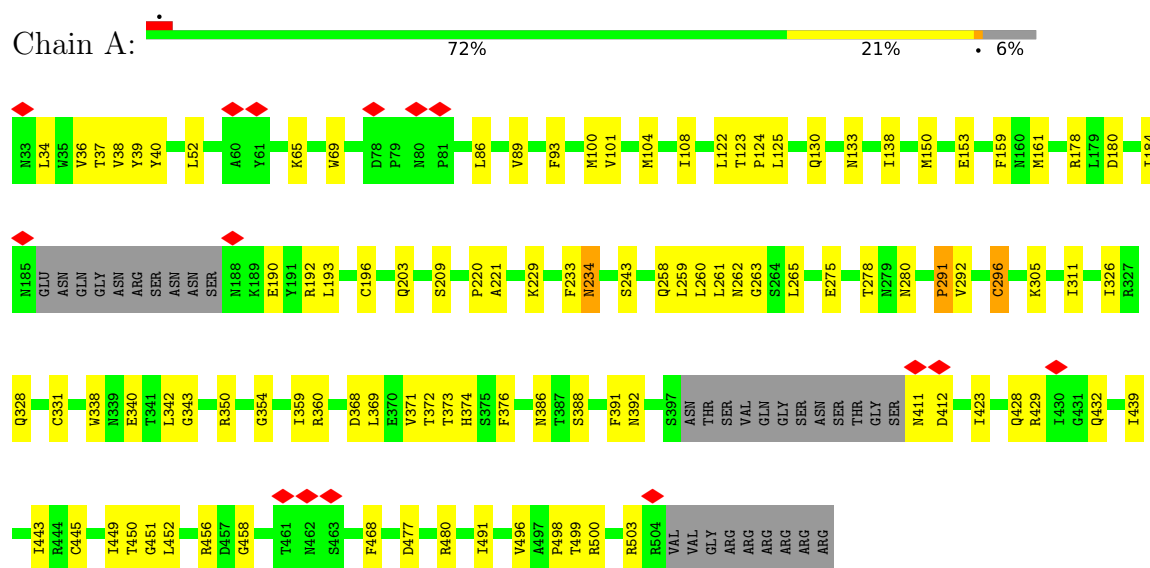
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Mol	Chain	Residues	Atoms				AltConf
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	E	1	Total	C	N	O	0
			14	8	1	5	
10	F	1	Total	C	N	O	0
			14	8	1	5	

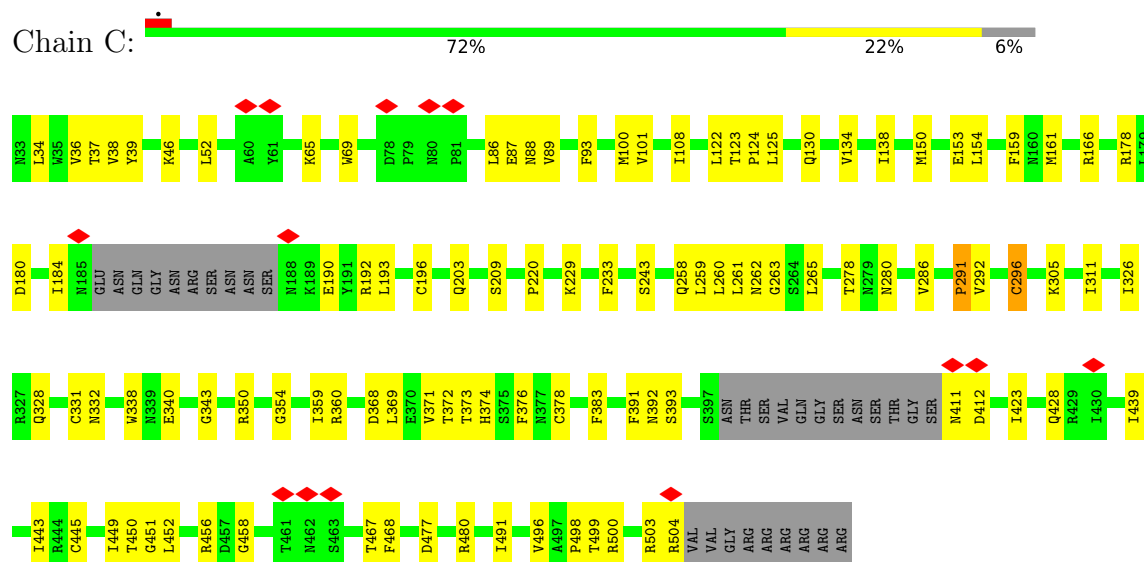
3 Residue-property plots

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 gp160

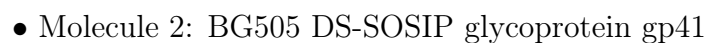


• Molecule 1: Envelope glycoprotein gp160

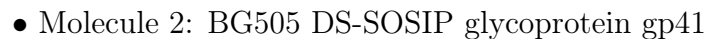


• Molecule 1: Envelope glycoprotein gp160

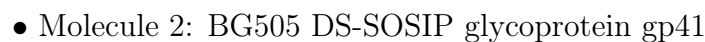
Frequency	Percentage
Daily	72%
Weekly	21%
Monthly	6%



Frequency	Percentage
Very often	9%
Often	63%
Sometimes	24%
Never	14%



Frequency	Percentage
Daily	9%
Often	64%
Sometimes	21%
Never	14%

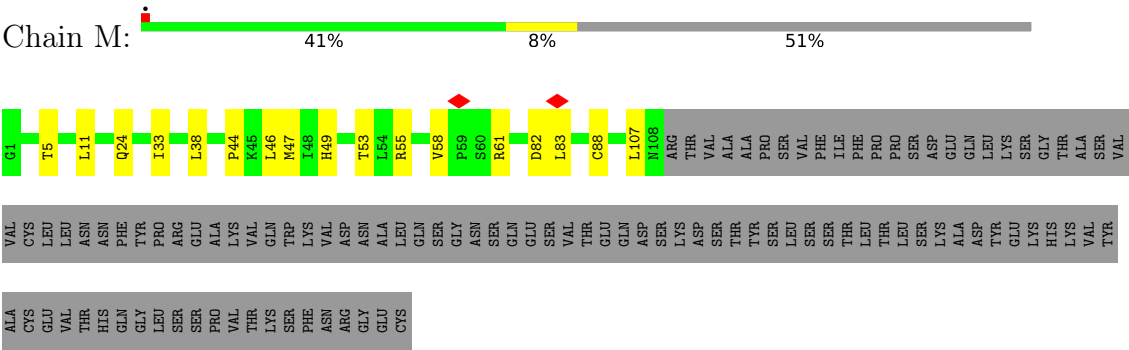


Frequency	Percentage
Daily	10%
Often	62%
Sometimes	23%
Never	14%

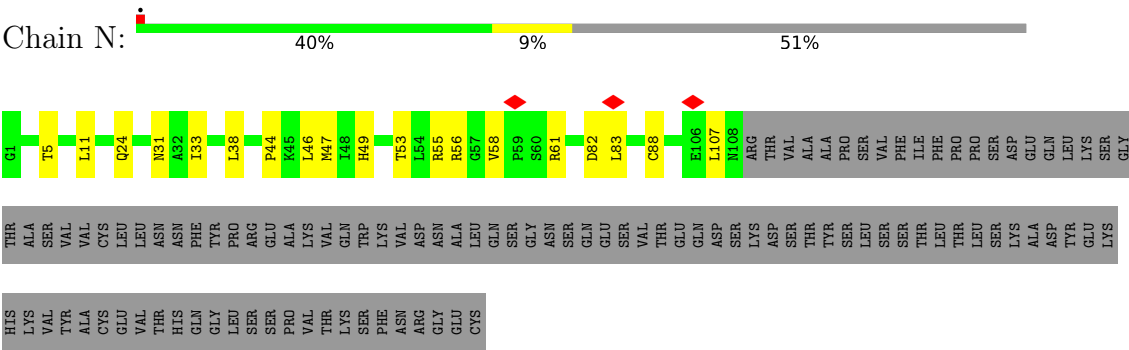


[illegible]

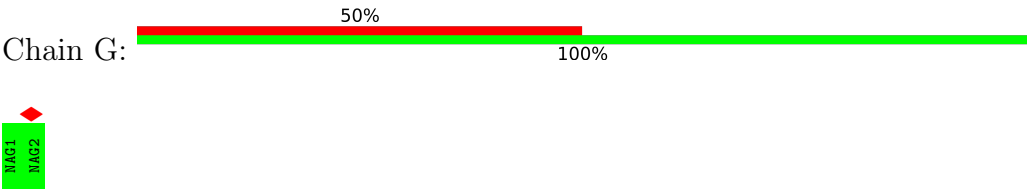
• Molecule 4: 01_D03 Fab Light Chain



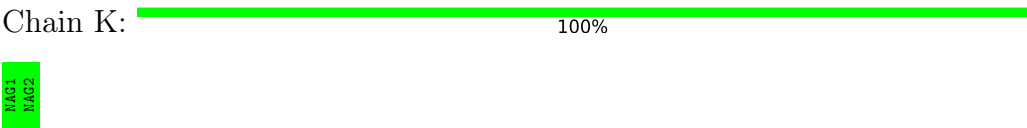
• Molecule 4: 01_D03 Fab Light Chain



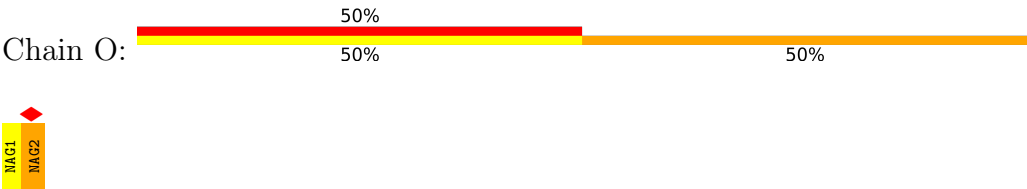
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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

Chain a: 



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

Chain b: 



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

Chain f: 



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

Chain g: 



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

Chain h: 



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

Chain k: 



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



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



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



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



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

Chain v:  50% 50%



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

Chain x:  50% 100%



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

Chain y:  50% 100%



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

Chain P:  33% 100%



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

Chain Q:  100%



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

Chain c:  33% 67% 33%



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

Chain d:  67% 33%



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

Chain l:  33% 67% 33%

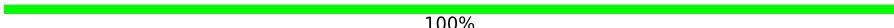


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  33% 67% 33%



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

Chain q:  100%

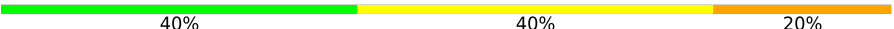


- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  60% 40%



- Molecule 7: 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

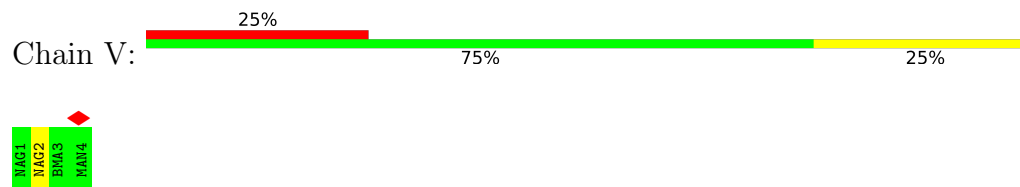
Chain e:  40% 40% 20%



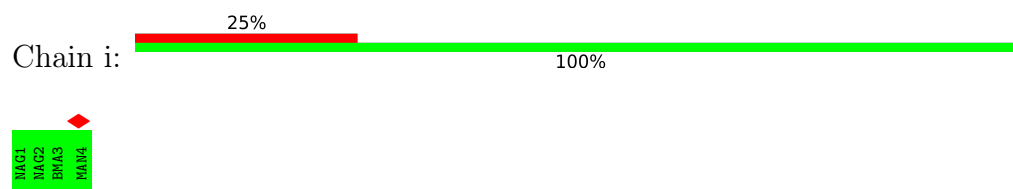
- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



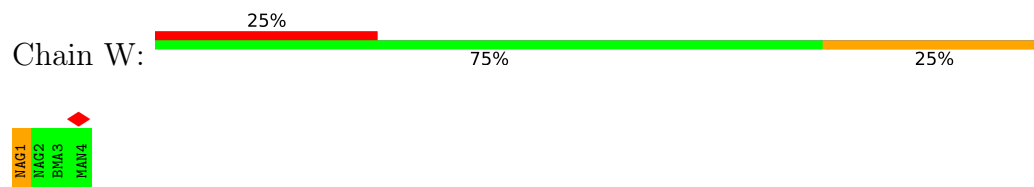
- Molecule 8: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 8: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



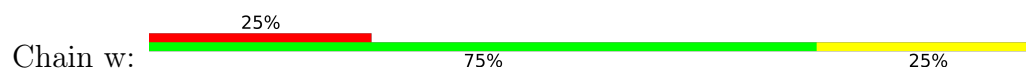
- Molecule 9: α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 9: α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 9: α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	149685	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.104	Depositor
Minimum map value	-0.730	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.18	Depositor
Map size ($\text{\AA}$)	326.144, 326.144, 326.144	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, 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	0.32	0/3597	0.57	2/4885 (0.0%)
1	C	0.32	0/3597	0.59	2/4885 (0.0%)
1	E	0.32	0/3597	0.59	3/4885 (0.1%)
2	B	0.17	0/1068	0.35	0/1448
2	D	0.21	0/1068	0.44	1/1448 (0.1%)
2	F	0.18	0/1068	0.42	1/1448 (0.1%)
3	H	0.12	0/1106	0.31	0/1500
3	I	0.12	0/1106	0.31	0/1500
3	J	0.12	0/1106	0.31	0/1500
4	L	0.08	0/832	0.28	0/1132
4	M	0.08	0/832	0.28	0/1132
4	N	0.08	0/832	0.28	0/1132
All	All	0.26	0/19809	0.49	9/26895 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	CYS	CB-CA-C	-15.59	82.85	109.51
1	E	296	CYS	CB-CA-C	-15.54	82.94	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	CYS	CB-CA-C	-14.14	83.45	109.46
1	E	354	GLY	CA-C-O	-6.61	117.92	122.22
1	A	291	PRO	CA-N-CD	-6.08	103.48	112.00
1	C	291	PRO	CA-N-CD	-6.08	103.48	112.00
1	E	291	PRO	CA-N-CD	-6.05	103.52	112.00
2	D	638	TYR	N-CA-CB	5.72	120.15	110.49
2	F	638	TYR	N-CA-CB	5.39	119.61	110.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	ARG	Sidechain
1	E	360	ARG	Sidechain

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	3523	0	3455	77	0
1	C	3523	0	3455	76	0
1	E	3523	0	3455	76	0
2	B	1049	0	1040	32	0
2	D	1049	0	1040	31	0
2	F	1049	0	1040	33	0
3	H	1075	0	1004	26	0
3	I	1075	0	1004	24	0
3	J	1075	0	1004	24	0
4	L	810	0	780	14	0
4	M	810	0	780	11	0
4	N	810	0	780	14	0
5	G	28	0	25	0	0
5	K	28	0	25	0	0
5	O	28	0	25	3	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	X	28	0	25	0	0
5	Y	28	0	25	1	0
5	Z	28	0	25	2	0
5	a	28	0	25	0	0
5	b	28	0	25	0	0
5	f	28	0	25	0	0
5	g	28	0	25	1	0
5	h	28	0	25	1	0
5	k	28	0	25	0	0
5	m	28	0	25	0	0
5	n	28	0	25	0	0
5	o	28	0	25	0	0
5	s	28	0	25	0	0
5	t	28	0	25	1	0
5	u	28	0	25	1	0
5	v	28	0	25	0	0
5	x	28	0	25	0	0
5	y	28	0	25	0	0
6	P	39	0	34	0	0
6	Q	39	0	34	0	0
6	c	39	0	34	0	0
6	d	39	0	34	1	0
6	l	39	0	34	1	0
6	p	39	0	34	1	0
6	q	39	0	34	0	0
7	R	61	0	52	2	0
7	e	61	0	52	2	0
7	r	61	0	52	2	0
8	V	50	0	43	0	0
8	i	50	0	43	0	0
9	W	50	0	43	2	0
9	j	50	0	43	1	0
9	w	50	0	43	0	0
10	A	56	0	52	1	0
10	B	14	0	13	0	0
10	C	56	0	52	0	0
10	D	14	0	13	0	0
10	E	56	0	52	0	0
10	F	14	0	13	0	0
All	All	20959	0	20241	387	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 9.

All (387) 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)
3:I:97:LEU:HD23	3:I:101:ASP:HB2	1.63	0.80
3:J:97:LEU:HD23	3:J:101:ASP:HB2	1.63	0.80
1:A:220:PRO:HB3	2:B:578:ALA:HB1	1.64	0.79
3:H:97:LEU:HD23	3:H:101:ASP:HB2	1.63	0.78
1:C:220:PRO:HB3	2:D:578:ALA:HB1	1.68	0.75
4:L:83:LEU:HD21	4:L:107:LEU:HB2	1.70	0.74
4:N:83:LEU:HD21	4:N:107:LEU:HB2	1.70	0.74
1:C:258:GLN:NE2	1:C:371:VAL:O	2.22	0.73
1:E:280:ASN:HD22	1:E:458:GLY:HA2	1.54	0.73
1:A:258:GLN:NE2	1:A:371:VAL:O	2.22	0.72
4:M:46:LEU:HD21	4:M:49:HIS:HB3	1.71	0.72
4:M:83:LEU:HD21	4:M:107:LEU:HB2	1.70	0.72
4:L:46:LEU:HD21	4:L:49:HIS:HB3	1.71	0.72
4:N:46:LEU:HD21	4:N:49:HIS:HB3	1.71	0.72
1:E:34:LEU:HD21	2:F:619:LEU:HD21	1.69	0.71
1:A:280:ASN:HD22	1:A:458:GLY:HA2	1.54	0.71
1:C:280:ASN:HD22	1:C:458:GLY:HA2	1.54	0.71
1:E:258:GLN:NE2	1:E:371:VAL:O	2.22	0.70
3:I:93:VAL:HG21	3:I:100(J):LEU:HD13	1.74	0.70
5:g:1:NAG:H61	5:g:2:NAG:HN2	1.57	0.70
1:C:296:CYS:HB2	1:C:445:CYS:HB2	1.74	0.69
3:J:93:VAL:HG21	3:J:100(J):LEU:HD13	1.74	0.69
1:A:296:CYS:HB2	1:A:445:CYS:HB2	1.74	0.69
3:H:93:VAL:HG21	3:H:100(J):LEU:HD13	1.74	0.69
1:E:296:CYS:HB2	1:E:445:CYS:HB2	1.76	0.68
1:A:161:MET:HG2	1:A:311:ILE:HG22	1.75	0.67
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.27	0.67
3:I:66:ARG:NH2	3:I:86:ASP:OD2	2.27	0.67
3:J:66:ARG:NH2	3:J:86:ASP:OD2	2.27	0.67
3:J:94:THR:HG22	3:J:95:HIS:H	1.60	0.67
3:I:94:THR:HG22	3:I:95:HIS:H	1.60	0.67
1:E:150:MET:HE3	1:E:328:GLN:HA	1.77	0.66
1:E:150:MET:HG3	1:E:153:GLU:HB3	1.77	0.66
1:A:150:MET:HG3	1:A:153:GLU:HB3	1.77	0.65
5:t:1:NAG:H61	5:t:2:NAG:HN2	1.60	0.65
3:H:94:THR:HG22	3:H:95:HIS:H	1.60	0.65
1:A:491:ILE:O	2:B:585:ARG:NH2	2.29	0.65
1:A:296:CYS:SG	1:A:445:CYS:HB2	2.37	0.65
1:C:150:MET:HE3	1:C:328:GLN:HA	1.77	0.65
1:C:296:CYS:SG	1:C:445:CYS:HB2	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:CYS:SG	1:E:445:CYS:HB2	2.37	0.65
1:C:150:MET:HG3	1:C:153:GLU:HB3	1.77	0.64
1:A:150:MET:HE3	1:A:328:GLN:HA	1.77	0.64
1:A:130:GLN:NE2	1:A:190:GLU:OE1	2.31	0.64
1:C:491:ILE:O	2:D:585:ARG:NH2	2.31	0.63
1:E:130:GLN:NE2	1:E:190:GLU:OE1	2.31	0.63
1:C:130:GLN:NE2	1:C:190:GLU:OE1	2.31	0.63
3:H:59:TYR:HE1	3:H:69:MET:HG3	1.65	0.62
1:E:37:THR:OG1	1:E:499:THR:OG1	2.17	0.61
3:I:59:TYR:HE1	3:I:69:MET:HG3	1.65	0.61
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.66	0.61
1:E:38:VAL:HG12	1:E:496:VAL:HG12	1.83	0.61
1:A:34:LEU:HD21	2:B:619:LEU:HD21	1.83	0.61
1:C:38:VAL:HG12	1:C:496:VAL:HG12	1.83	0.60
1:A:428:GLN:OE1	3:I:35(A):ARG:NH2	2.34	0.60
1:C:34:LEU:HD21	2:D:619:LEU:HD21	1.83	0.60
1:C:161:MET:HG2	1:C:311:ILE:HG22	1.84	0.60
3:J:59:TYR:HE1	3:J:69:MET:HG3	1.65	0.60
1:C:263:GLY:H	1:C:450:THR:HG21	1.67	0.60
1:E:161:MET:HG2	1:E:311:ILE:HG22	1.84	0.59
1:A:38:VAL:HG12	1:A:496:VAL:HG12	1.83	0.59
3:I:93:VAL:HG12	3:I:103:TRP:HA	1.84	0.59
1:A:411:ASN:OD1	1:A:412:ASP:N	2.36	0.59
1:E:411:ASN:OD1	1:E:412:ASP:N	2.36	0.59
1:A:500:ARG:HG3	2:F:662:ALA:HB1	1.84	0.59
1:E:111:LEU:HD11	2:F:571:TRP:CZ2	2.38	0.59
1:C:411:ASN:OD1	1:C:412:ASP:N	2.36	0.59
3:I:66:ARG:HH12	3:I:83:ARG:HE	1.51	0.59
1:E:93:PHE:HB2	1:E:233:PHE:HZ	1.69	0.58
3:J:93:VAL:HG12	3:J:103:TRP:HA	1.84	0.58
3:H:93:VAL:HG12	3:H:103:TRP:HA	1.84	0.58
3:H:66:ARG:HH12	3:H:83:ARG:HE	1.50	0.58
1:A:263:GLY:H	1:A:450:THR:HG21	1.68	0.58
1:C:93:PHE:HB2	1:C:233:PHE:HZ	1.68	0.58
1:A:138:ILE:HA	1:A:326:ILE:HB	1.86	0.57
1:E:138:ILE:HA	1:E:326:ILE:HB	1.86	0.57
1:A:36:VAL:O	2:B:606:THR:OG1	2.17	0.57
3:J:66:ARG:HH12	3:J:83:ARG:HE	1.51	0.57
3:I:24:ALA:HB1	3:I:27:PHE:HE1	1.70	0.57
1:C:138:ILE:HA	1:C:326:ILE:HB	1.86	0.56
1:A:372:THR:HG23	1:A:373:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:24:ALA:HB1	3:H:27:PHE:HE1	1.70	0.56
3:H:71(A):GLU:OE1	3:H:79:TYR:OH	2.24	0.56
3:H:97:LEU:HD12	3:H:100(I):ARG:HH21	1.71	0.56
3:J:97:LEU:HD12	3:J:100(I):ARG:HH21	1.71	0.56
3:J:24:ALA:HB1	3:J:27:PHE:HE1	1.70	0.56
3:J:71(A):GLU:OE1	3:J:79:TYR:OH	2.24	0.56
1:A:350:ARG:HG2	1:A:354:GLY:O	2.04	0.56
1:E:372:THR:HG23	1:E:373:THR:HG23	1.87	0.56
1:E:34:LEU:HD13	1:E:498:PRO:HB2	1.88	0.56
3:I:97:LEU:HD12	3:I:100(I):ARG:HH21	1.71	0.56
1:E:260:LEU:HD12	1:E:451:GLY:HA3	1.88	0.56
1:A:34:LEU:HD13	1:A:498:PRO:HB2	1.88	0.55
1:C:439:ILE:HB	1:C:443:ILE:HD11	1.88	0.55
1:E:439:ILE:HB	1:E:443:ILE:HD11	1.88	0.55
1:E:296:CYS:SG	1:E:376:PHE:CE2	3.00	0.55
1:C:296:CYS:CB	1:C:445:CYS:HB2	2.37	0.55
1:C:372:THR:HG23	1:C:373:THR:HG23	1.87	0.55
2:D:614:TRP:HE1	2:D:641:ILE:HD11	1.72	0.55
2:F:614:TRP:HE1	2:F:641:ILE:HD11	1.71	0.55
1:A:260:LEU:HD12	1:A:451:GLY:HA3	1.88	0.55
1:C:69:TRP:HE1	1:C:108:ILE:HG23	1.72	0.55
1:A:296:CYS:CB	1:A:445:CYS:HB2	2.37	0.55
1:A:439:ILE:HB	1:A:443:ILE:HD11	1.88	0.55
1:C:260:LEU:HD12	1:C:451:GLY:HA3	1.88	0.55
2:D:655:LYS:HE2	2:F:535:MET:HA	1.89	0.55
1:A:296:CYS:SG	1:A:376:PHE:CE2	3.00	0.55
1:A:391:PHE:O	1:A:392:ASN:C	2.49	0.54
1:C:34:LEU:HD13	1:C:498:PRO:HB2	1.88	0.54
1:A:69:TRP:HE1	1:A:108:ILE:HG23	1.72	0.54
1:C:350:ARG:HG2	1:C:354:GLY:O	2.08	0.54
1:C:296:CYS:SG	1:C:376:PHE:CE2	3.00	0.54
2:B:614:TRP:HE1	2:B:641:ILE:HD11	1.71	0.54
9:j:3:BMA:H4	9:j:4:MAN:H3	1.89	0.54
3:I:71(A):GLU:OE1	3:I:79:TYR:OH	2.24	0.54
2:B:546:SER:OG	2:F:588:ARG:NH1	2.41	0.54
2:D:587:LEU:HD22	2:F:586:TYR:HE2	1.72	0.54
1:A:292:VAL:HB	1:A:449:ILE:HB	1.89	0.53
1:E:193:LEU:HD22	1:E:423:ILE:HD11	1.89	0.53
2:B:545:LEU:HD21	2:F:587:LEU:HB3	1.91	0.53
1:E:69:TRP:HE1	1:E:108:ILE:HG23	1.72	0.53
2:F:637:ASN:N	2:F:637:ASN:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:CYS:CB	1:E:445:CYS:HB2	2.38	0.53
1:C:292:VAL:HB	1:C:449:ILE:HB	1.90	0.53
1:A:130:GLN:HG2	5:O:1:NAG:H81	1.91	0.53
1:C:37:THR:OG1	1:C:499:THR:OG1	2.17	0.53
1:E:46:LYS:NZ	2:F:632:ASP:OD2	2.42	0.53
1:A:37:THR:OG1	1:A:499:THR:OG1	2.17	0.53
1:C:428:GLN:OE1	3:J:35(A):ARG:NH2	2.42	0.53
1:C:193:LEU:HD22	1:C:423:ILE:HD11	1.89	0.52
1:A:193:LEU:HD22	1:A:423:ILE:HD11	1.89	0.52
1:C:369:LEU:O	1:C:373:THR:OG1	2.26	0.52
5:O:1:NAG:H61	5:O:2:NAG:H82	1.92	0.52
5:Z:1:NAG:H62	5:Z:2:NAG:O5	2.09	0.52
1:A:369:LEU:O	1:A:373:THR:OG1	2.26	0.52
3:H:97:LEU:HD21	4:L:46:LEU:HD22	1.91	0.52
2:D:651:ASN:ND2	2:F:535:MET:O	2.42	0.51
2:F:643:TYR:O	2:F:647:GLU:HG2	2.09	0.51
2:D:643:TYR:O	2:D:647:GLU:HG2	2.09	0.51
3:J:95:HIS:CG	3:J:100(G):THR:HA	2.45	0.51
1:A:292:VAL:HG11	1:A:338:TRP:HE3	1.75	0.51
1:A:340:GLU:O	1:A:343:GLY:N	2.44	0.51
1:E:259:LEU:HD12	1:E:374:HIS:CD2	2.46	0.51
1:A:291:PRO:HG3	5:Y:1:NAG:H62	1.93	0.51
3:I:95:HIS:CG	3:I:100(G):THR:HA	2.45	0.51
4:N:61:ARG:NH2	4:N:82:ASP:OD1	2.44	0.51
1:A:259:LEU:HD12	1:A:374:HIS:CD2	2.46	0.51
1:C:259:LEU:HD12	1:C:374:HIS:CD2	2.46	0.51
3:J:97:LEU:HD21	4:N:46:LEU:HD22	1.92	0.51
4:L:61:ARG:NH2	4:L:82:ASP:OD1	2.44	0.51
1:A:275:GLU:HG3	7:R:1:NAG:H83	1.92	0.51
1:E:369:LEU:O	1:E:373:THR:OG1	2.26	0.51
6:d:1:NAG:O6	6:l:1:NAG:H81	2.11	0.51
4:M:61:ARG:NH2	4:M:82:ASP:OD1	2.44	0.51
2:B:643:TYR:O	2:B:647:GLU:HG2	2.09	0.50
2:F:588:ARG:HH21	2:F:592:LEU:HD21	1.76	0.50
1:E:292:VAL:HG11	1:E:338:TRP:HE3	1.75	0.50
1:E:350:ARG:HG2	1:E:354:GLY:O	2.11	0.50
1:E:340:GLU:O	1:E:343:GLY:N	2.44	0.50
3:H:95:HIS:CG	3:H:100(G):THR:HA	2.45	0.50
1:E:263:GLY:H	1:E:450:THR:HG21	1.77	0.50
4:M:47:MET:HE3	4:M:47:MET:HA	1.94	0.50
2:D:588:ARG:HH21	2:D:592:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:LEU:HD21	2:F:596:TRP:CH2	2.46	0.50
4:L:47:MET:HA	4:L:47:MET:HE3	1.94	0.50
5:O:2:NAG:H83	5:O:2:NAG:H3	1.94	0.50
1:C:36:VAL:O	2:D:606:THR:OG1	2.24	0.49
2:B:580:VAL:O	2:B:584:GLU:HG2	2.12	0.49
1:C:340:GLU:O	1:C:343:GLY:N	2.45	0.49
2:D:580:VAL:O	2:D:584:GLU:HG2	2.12	0.49
1:E:220:PRO:HB3	2:F:578:ALA:HB1	1.94	0.49
1:A:101:VAL:HG11	1:A:480:ARG:HG3	1.95	0.49
1:A:292:VAL:HG11	1:A:338:TRP:CE3	2.48	0.49
2:B:588:ARG:HH21	2:B:592:LEU:HD21	1.76	0.49
1:C:265:LEU:HD21	1:C:291:PRO:HD3	1.95	0.49
2:F:620:SER:O	2:F:624:ASP:HB2	2.13	0.49
2:F:638:TYR:O	2:F:639:THR:C	2.52	0.49
1:C:338:TRP:HH2	1:C:452:LEU:HD21	1.77	0.49
1:E:338:TRP:HH2	1:E:452:LEU:HD21	1.77	0.49
1:A:386:ASN:HD22	9:W:1:NAG:H83	1.76	0.49
1:C:101:VAL:HG11	1:C:480:ARG:HG3	1.95	0.49
1:C:503:ARG:NH2	2:D:604:CYS:SG	2.86	0.49
1:E:153:GLU:O	1:E:178:ARG:N	2.45	0.49
1:C:39:TYR:HD2	2:D:537:LEU:HD11	1.78	0.48
3:I:94:THR:HG22	3:I:95:HIS:N	2.28	0.48
2:F:580:VAL:O	2:F:584:GLU:HG2	2.12	0.48
3:J:100(J):LEU:O	3:J:103:TRP:NE1	2.46	0.48
2:B:620:SER:O	2:B:624:ASP:HB2	2.13	0.48
2:D:620:SER:O	2:D:624:ASP:HB2	2.13	0.48
1:E:265:LEU:HD21	1:E:291:PRO:HD3	1.94	0.48
1:A:153:GLU:O	1:A:178:ARG:N	2.45	0.48
1:A:368:ASP:CG	3:I:71:ARG:HH22	2.21	0.48
3:H:98:TYR:CZ	4:L:56:ARG:HG3	2.48	0.48
1:A:265:LEU:HD21	1:A:291:PRO:HD3	1.95	0.48
1:E:101:VAL:HG11	1:E:480:ARG:HG3	1.95	0.48
3:J:94:THR:HG22	3:J:95:HIS:N	2.28	0.48
2:D:587:LEU:HD11	2:F:587:LEU:HG	1.96	0.48
2:D:637:ASN:OD1	2:D:637:ASN:N	2.46	0.48
3:H:100(J):LEU:O	3:H:103:TRP:NE1	2.46	0.48
4:N:47:MET:HA	4:N:47:MET:HE3	1.94	0.48
2:B:662:ALA:HB1	1:C:500:ARG:HG3	1.96	0.48
1:C:86:LEU:HB3	1:C:89:VAL:HG21	1.96	0.48
1:C:360:ARG:O	1:C:467:THR:HA	2.13	0.48
1:A:52:LEU:HD13	1:A:100:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HD13	1:C:100:MET:HE3	1.96	0.47
1:E:52:LEU:HD13	1:E:100:MET:HE3	1.96	0.47
3:H:35(A):ARG:O	3:H:53:ARG:HB2	2.15	0.47
2:D:587:LEU:HB3	2:F:545:LEU:HD21	1.96	0.47
1:C:93:PHE:HB2	1:C:233:PHE:CZ	2.48	0.47
1:C:196:CYS:O	1:C:196:CYS:SG	2.73	0.47
3:I:35(A):ARG:O	3:I:53:ARG:HB2	2.15	0.47
1:A:338:TRP:HH2	1:A:452:LEU:HD21	1.80	0.47
1:C:153:GLU:O	1:C:178:ARG:N	2.45	0.47
1:E:159:PHE:HE2	1:E:161:MET:HE2	1.78	0.47
1:E:292:VAL:HB	1:E:449:ILE:HB	1.96	0.47
3:J:38:ARG:O	3:J:46:GLN:N	2.47	0.47
1:A:180:ASP:HB3	1:A:423:ILE:HD12	1.97	0.47
1:C:123:THR:OG1	1:C:124:PRO:HD3	2.15	0.47
1:C:180:ASP:HB3	1:C:423:ILE:HD12	1.97	0.47
1:E:360:ARG:O	1:E:467:THR:HA	2.15	0.47
1:A:296:CYS:HA	1:A:331:CYS:SG	2.54	0.47
1:A:39:TYR:HD2	2:B:537:LEU:HD11	1.81	0.46
3:H:94:THR:HG22	3:H:95:HIS:N	2.28	0.46
2:B:587:LEU:HB3	2:D:545:LEU:HD21	1.97	0.46
1:A:93:PHE:HB2	1:A:233:PHE:CZ	2.47	0.46
1:C:292:VAL:HG11	1:C:338:TRP:HE3	1.80	0.46
3:I:38:ARG:O	3:I:46:GLN:N	2.47	0.46
3:I:100(J):LEU:O	3:I:103:TRP:NE1	2.46	0.46
1:A:124:PRO:HA	1:C:166:ARG:HD3	1.98	0.46
1:E:93:PHE:HB2	1:E:233:PHE:CZ	2.48	0.46
3:J:35(A):ARG:O	3:J:53:ARG:HB2	2.15	0.46
4:N:31:ASN:HD21	7:e:2:NAG:C3	2.28	0.46
1:A:123:THR:OG1	1:A:124:PRO:HD3	2.15	0.46
2:B:535:MET:HA	2:F:655:LYS:HE2	1.97	0.46
1:E:180:ASP:HB3	1:E:423:ILE:HD12	1.97	0.46
1:E:296:CYS:SG	1:E:376:PHE:CZ	3.09	0.46
1:C:46:LYS:NZ	2:D:632:ASP:OD2	2.49	0.46
1:E:44:VAL:HG23	2:F:628:TRP:HB3	1.98	0.46
4:N:53:THR:OG1	7:e:3:BMA:H4	2.16	0.46
1:A:234:ASN:HD22	10:A:602:NAG:C7	2.29	0.45
1:C:261:LEU:O	1:C:262:ASN:C	2.60	0.45
1:A:296:CYS:SG	1:A:376:PHE:CZ	3.09	0.45
2:B:655:LYS:HE2	2:D:535:MET:HA	1.99	0.45
1:E:391:PHE:O	1:E:392:ASN:C	2.59	0.45
3:J:63:PHE:O	3:J:67:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:587:LEU:HD11	2:D:587:LEU:HG	1.96	0.45
1:E:123:THR:OG1	1:E:124:PRO:HD3	2.15	0.45
1:A:86:LEU:HB3	1:A:89:VAL:HG21	1.97	0.45
1:C:296:CYS:SG	1:C:376:PHE:CZ	3.09	0.45
1:C:391:PHE:O	1:C:392:ASN:C	2.59	0.45
2:F:643:TYR:HA	2:F:646:LEU:HD12	1.99	0.45
2:B:643:TYR:HA	2:B:646:LEU:HD12	1.99	0.45
1:C:477:ASP:OD1	1:C:480:ARG:NH1	2.50	0.45
3:H:35(F):HIS:ND1	3:H:50:HIS:HB3	2.32	0.45
3:H:71:ARG:HG2	3:H:71:ARG:HH11	1.82	0.45
3:I:63:PHE:O	3:I:67:ILE:HG22	2.16	0.45
1:E:477:ASP:OD1	1:E:480:ARG:NH1	2.50	0.45
3:I:35(F):HIS:ND1	3:I:50:HIS:HB3	2.32	0.45
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.50	0.45
3:H:38:ARG:O	3:H:46:GLN:N	2.47	0.45
4:L:53:THR:OG1	7:r:3:BMA:H4	2.17	0.45
2:D:533:ALA:HA	2:D:536:THR:HG22	1.99	0.45
3:J:71:ARG:HG2	3:J:71:ARG:HH11	1.82	0.45
3:H:63:PHE:O	3:H:67:ILE:HG22	2.16	0.44
2:D:643:TYR:HA	2:D:646:LEU:HD12	1.99	0.44
1:E:428:GLN:OE1	3:H:35(A):ARG:NH2	2.49	0.44
1:E:503:ARG:NH2	2:F:604:CYS:SG	2.91	0.44
3:I:71:ARG:HG2	3:I:71:ARG:HH11	1.82	0.44
3:J:98:TYR:CZ	4:N:56:ARG:HG3	2.52	0.44
2:B:587:LEU:HD22	2:D:586:TYR:HE2	1.82	0.44
1:E:338:TRP:NE1	1:E:390:LEU:O	2.48	0.44
1:E:259:LEU:HD22	1:E:449:ILE:HG21	1.98	0.44
3:J:35(F):HIS:ND1	3:J:50:HIS:HB3	2.32	0.44
1:A:221:ALA:HB3	2:B:582:ALA:HB1	2.00	0.44
2:F:533:ALA:HA	2:F:536:THR:HG22	1.99	0.44
4:L:38:LEU:HD13	4:L:44:PRO:HG3	2.00	0.44
4:M:38:LEU:HD13	4:M:44:PRO:HG3	2.00	0.44
1:E:86:LEU:HB3	1:E:89:VAL:HG21	1.98	0.44
1:E:196:CYS:O	1:E:196:CYS:SG	2.75	0.44
2:B:533:ALA:HA	2:B:536:THR:HG22	1.99	0.44
1:E:296:CYS:SG	1:E:376:PHE:HE2	2.41	0.43
2:B:534:SER:HA	2:B:537:LEU:HG	2.01	0.43
1:A:498:PRO:HD3	2:B:631:TRP:CZ2	2.53	0.43
1:C:332:ASN:ND2	5:h:1:NAG:O7	2.52	0.43
4:N:33:ILE:HD11	4:N:88:CYS:HB2	2.00	0.43
1:A:65:LYS:HE2	1:A:209:SER:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:52:GLN:HA	3:H:52(A):PRO:HD3	1.87	0.43
1:A:122:LEU:HD11	1:A:203:GLN:HB2	2.01	0.43
4:N:38:LEU:HD13	4:N:44:PRO:HG3	2.00	0.43
1:A:159:PHE:HE2	1:A:161:MET:HE2	1.84	0.43
1:A:261:LEU:O	1:A:262:ASN:C	2.61	0.43
2:D:534:SER:HA	2:D:537:LEU:HG	2.01	0.43
2:D:638:TYR:O	2:D:639:THR:C	2.61	0.43
4:L:47:MET:HE1	4:L:58:VAL:HG11	2.01	0.43
2:B:661:LEU:HD11	1:C:504:ARG:HG3	2.01	0.42
1:A:359:ILE:HD12	1:A:468:PHE:HE1	1.84	0.42
1:C:87:GLU:HB2	5:Z:1:NAG:H83	2.01	0.42
1:C:259:LEU:HD22	1:C:449:ILE:HG21	2.01	0.42
4:N:11:LEU:HD12	4:N:11:LEU:HA	1.91	0.42
2:B:588:ARG:NH1	2:D:546:SER:OG	2.52	0.42
1:E:342:LEU:HD23	1:E:342:LEU:HA	1.90	0.42
4:M:53:THR:OG1	7:R:3:BMA:H4	2.18	0.42
1:A:296:CYS:SG	1:A:376:PHE:HE2	2.42	0.42
1:E:305:LYS:HB3	1:E:305:LYS:HE2	1.84	0.42
1:E:332:ASN:ND2	5:u:1:NAG:O7	2.53	0.42
2:F:534:SER:HA	2:F:537:LEU:HG	2.01	0.42
4:M:33:ILE:HD11	4:M:88:CYS:HB2	2.00	0.42
1:A:305:LYS:HB3	1:A:305:LYS:HE2	1.84	0.42
1:C:65:LYS:HE2	1:C:209:SER:HB2	2.00	0.42
1:C:134:VAL:CG1	1:C:154:LEU:HB2	2.49	0.42
1:E:229:LYS:HE2	1:E:243:SER:HB2	2.02	0.42
4:M:47:MET:HE1	4:M:58:VAL:HG11	2.01	0.42
2:F:651:ASN:O	2:F:655:LYS:HG3	2.20	0.42
1:A:229:LYS:HE2	1:A:243:SER:HB2	2.02	0.42
1:A:278:THR:O	1:A:456:ARG:NH2	2.53	0.42
1:C:229:LYS:HE2	1:C:243:SER:HB2	2.02	0.42
3:H:35(F):HIS:HB2	3:H:93:VAL:CG2	2.50	0.42
3:J:35(F):HIS:HB2	3:J:93:VAL:CG2	2.50	0.42
4:L:33:ILE:HD11	4:L:88:CYS:HB2	2.00	0.42
1:C:122:LEU:HD11	1:C:203:GLN:HB2	2.01	0.42
1:A:40:TYR:CG	2:B:593:LEU:HD11	2.54	0.42
1:A:386:ASN:ND2	9:W:1:NAG:H83	2.35	0.42
1:C:292:VAL:HG11	1:C:338:TRP:CE3	2.55	0.42
1:C:359:ILE:HD12	1:C:468:PHE:HE1	1.84	0.42
1:E:259:LEU:HD22	1:E:449:ILE:CG2	2.50	0.42
1:E:359:ILE:HD12	1:E:468:PHE:HE1	1.84	0.42
1:C:278:THR:O	1:C:456:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ASP:CG	3:J:71:ARG:HH22	2.28	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.90	0.41
1:C:296:CYS:SG	1:C:376:PHE:HE2	2.42	0.41
1:C:296:CYS:HA	1:C:331:CYS:SG	2.60	0.41
1:E:65:LYS:HE2	1:E:209:SER:HB2	2.00	0.41
1:E:360:ARG:HB3	1:E:467:THR:HG22	2.02	0.41
3:I:35(F):HIS:HB2	3:I:93:VAL:CG2	2.50	0.41
3:J:48:MET:HG2	3:J:63:PHE:CE2	2.55	0.41
2:B:583:VAL:HG13	2:F:587:LEU:CD1	2.50	0.41
1:C:159:PHE:HE2	1:C:161:MET:HE2	1.85	0.41
3:I:48:MET:HG2	3:I:63:PHE:CE2	2.55	0.41
4:L:55:ARG:HB3	4:L:58:VAL:HG22	2.02	0.41
4:M:11:LEU:HD12	4:M:11:LEU:HA	1.91	0.41
4:N:55:ARG:HB3	4:N:58:VAL:HG22	2.02	0.41
2:B:583:VAL:HG13	2:F:587:LEU:HD12	2.01	0.41
6:p:1:NAG:H83	6:p:1:NAG:H2	1.88	0.41
2:B:591:GLN:O	2:B:595:ILE:HG12	2.21	0.41
1:E:122:LEU:HD11	1:E:203:GLN:HB2	2.01	0.41
1:A:122:LEU:HD13	1:A:125:LEU:HD22	2.03	0.41
1:A:503:ARG:NH2	2:B:604:CYS:SG	2.93	0.41
2:B:605:CYS:SG	2:F:661:LEU:HD23	2.60	0.41
1:C:34:LEU:HD11	2:D:619:LEU:HD21	2.02	0.41
1:C:286:VAL:HB	1:C:452:LEU:HB2	2.03	0.41
1:E:43:PRO:HB2	2:F:526:ALA:HA	2.02	0.41
1:E:278:THR:O	1:E:456:ARG:NH2	2.53	0.41
4:M:5:THR:O	4:M:24:GLN:N	2.53	0.41
4:N:47:MET:HE1	4:N:58:VAL:HG11	2.01	0.41
1:A:196:CYS:SG	1:A:196:CYS:O	2.79	0.41
2:B:651:ASN:O	2:B:655:LYS:HG3	2.20	0.41
2:D:591:GLN:O	2:D:595:ILE:HG12	2.21	0.41
1:E:53:PHE:CE2	1:E:218:CYS:HB2	2.56	0.41
4:L:5:THR:O	4:L:24:GLN:N	2.53	0.41
4:L:31:ASN:HD21	7:r:2:NAG:C3	2.33	0.41
1:A:428:GLN:HB3	3:I:35(A):ARG:HH21	1.86	0.41
1:C:125:LEU:HA	1:C:161:MET:HE1	2.03	0.41
2:D:662:ALA:HA	1:E:501:CYS:HA	2.03	0.41
1:E:369:LEU:HA	1:E:372:THR:HG22	2.03	0.41
2:F:591:GLN:O	2:F:595:ILE:HG12	2.21	0.41
3:H:48:MET:HG2	3:H:63:PHE:CE2	2.55	0.41
1:C:134:VAL:O	1:C:138:ILE:HD13	2.20	0.40
1:A:104:MET:O	1:A:108:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ARG:HB2	1:A:432:GLN:HB3	2.04	0.40
1:C:184:ILE:HD11	1:C:192:ARG:HB3	2.03	0.40
1:E:184:ILE:HD11	1:E:192:ARG:HB3	2.03	0.40
3:H:101:ASP:HB3	3:H:102:PRO:HD3	2.02	0.40
4:M:55:ARG:HB3	4:M:58:VAL:HG22	2.02	0.40
1:C:305:LYS:HB3	1:C:305:LYS:HE2	1.84	0.40
1:C:378:CYS:HB3	1:C:383:PHE:CE1	2.57	0.40
1:E:104:MET:O	1:E:108:ILE:HG12	2.21	0.40
1:E:122:LEU:HD13	1:E:125:LEU:HD22	2.02	0.40
1:E:428:GLN:HB3	3:H:35(A):ARG:HH21	1.87	0.40
4:N:5:THR:O	4:N:24:GLN:N	2.53	0.40
1:A:184:ILE:HD11	1:A:192:ARG:HB3	2.03	0.40
2:D:662:ALA:HB1	1:E:500:ARG:HG3	2.04	0.40
1:E:36:VAL:O	2:F:606:THR:OG1	2.34	0.40
1:E:286:VAL:HB	1:E:452:LEU:HB2	2.03	0.40
3:I:101:ASP:HB3	3:I:102:PRO:HD3	2.02	0.40
4:L:48:ILE:HD13	4:L:54:LEU:HA	2.04	0.40
1:C:296:CYS:HG	1:C:376:PHE:HZ	1.68	0.40
1:E:378:CYS:HB3	1:E:383:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/427 (93%)	395 (99%)	3 (1%)	73	82
1	C	398/427 (93%)	396 (100%)	2 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	398/427 (93%)	395 (99%)	3 (1%)	73	82
2	B	113/129 (88%)	112 (99%)	1 (1%)	70	81
2	D	113/129 (88%)	112 (99%)	1 (1%)	70	81
2	F	113/129 (88%)	112 (99%)	1 (1%)	70	81
3	H	108/210 (51%)	108 (100%)	0	100	100
3	I	108/210 (51%)	108 (100%)	0	100	100
3	J	108/210 (51%)	108 (100%)	0	100	100
4	L	89/185 (48%)	89 (100%)	0	100	100
4	M	89/185 (48%)	89 (100%)	0	100	100
4	N	89/185 (48%)	89 (100%)	0	100	100
All	All	2124/2853 (74%)	2113 (100%)	11 (0%)	78	85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	234	ASN
1	A	388	SER
2	B	637	ASN
1	C	88	ASN
1	C	393	SER
2	D	637	ASN
1	E	388	SER
1	E	390	LEU
1	E	393	SER
2	F	637	ASN

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

Mol	Chain	Res	Type
1	A	99	ASN
1	A	425	ASN
2	B	590	GLN
1	C	66	HIS
1	C	99	ASN
1	C	425	ASN
2	D	590	GLN

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Mol	Chain	Res	Type
1	E	425	ASN
2	F	590	GLN
2	F	607	ASN
2	F	653	GLN
3	H	64	GLN
4	L	90	HIS
4	M	90	HIS
4	N	90	HIS

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](#)

104 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	G	1	1,5	14,14,15	0.38	0	17,19,21	0.52	0
5	NAG	G	2	5	14,14,15	0.38	0	17,19,21	0.47	0
5	NAG	K	1	1,5	14,14,15	0.38	0	17,19,21	0.48	0
5	NAG	K	2	5	14,14,15	0.37	0	17,19,21	0.48	0
5	NAG	O	1	1,5	14,14,15	0.38	0	17,19,21	0.78	0
5	NAG	O	2	5	14,14,15	0.36	0	17,19,21	1.69	1 (5%)
6	NAG	P	1	1,6	14,14,15	0.39	0	17,19,21	0.59	0
6	NAG	P	2	6	14,14,15	0.38	0	17,19,21	0.43	0
6	BMA	P	3	6	11,11,12	0.28	0	15,15,17	0.55	0
6	NAG	Q	1	1,6	14,14,15	0.39	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	Q	2	6	14,14,15	0.38	0	17,19,21	0.50	0
6	BMA	Q	3	6	11,11,12	0.41	0	15,15,17	0.47	0
7	NAG	R	1	1,7	14,14,15	0.36	0	17,19,21	0.76	0
7	NAG	R	2	7	14,14,15	0.36	0	17,19,21	0.59	0
7	BMA	R	3	7	11,11,12	0.45	0	15,15,17	0.54	0
7	MAN	R	4	7	11,11,12	0.32	0	15,15,17	0.49	0
7	MAN	R	5	7	11,11,12	0.32	0	15,15,17	0.53	0
5	NAG	S	1	1,5	14,14,15	0.37	0	17,19,21	0.83	0
5	NAG	S	2	5	14,14,15	0.39	0	17,19,21	0.86	2 (11%)
5	NAG	T	1	1,5	14,14,15	0.38	0	17,19,21	0.94	1 (5%)
5	NAG	T	2	5	14,14,15	0.37	0	17,19,21	0.50	0
5	NAG	U	1	1,5	14,14,15	0.38	0	17,19,21	0.89	1 (5%)
5	NAG	U	2	5	14,14,15	0.38	0	17,19,21	0.47	0
8	NAG	V	1	1,8	14,14,15	0.40	0	17,19,21	0.48	0
8	NAG	V	2	8	14,14,15	0.38	0	17,19,21	0.90	1 (5%)
8	BMA	V	3	8	11,11,12	0.46	0	15,15,17	0.48	0
8	MAN	V	4	8	11,11,12	0.28	0	15,15,17	0.56	0
9	NAG	W	1	1,9	14,14,15	0.39	0	17,19,21	1.37	3 (17%)
9	NAG	W	2	9	14,14,15	0.38	0	17,19,21	0.52	0
9	BMA	W	3	9	11,11,12	0.37	0	15,15,17	0.52	0
9	MAN	W	4	9	11,11,12	0.19	0	15,15,17	0.51	0
5	NAG	X	1	1,5	14,14,15	0.38	0	17,19,21	1.00	1 (5%)
5	NAG	X	2	5	14,14,15	0.40	0	17,19,21	0.34	0
5	NAG	Y	1	1,5	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
5	NAG	Y	2	5	14,14,15	0.38	0	17,19,21	0.55	0
5	NAG	Z	1	1,5	14,14,15	0.38	0	17,19,21	1.03	2 (11%)
5	NAG	Z	2	5	14,14,15	0.38	0	17,19,21	0.84	1 (5%)
5	NAG	a	1	1,5	14,14,15	0.38	0	17,19,21	0.52	0
5	NAG	a	2	5	14,14,15	0.39	0	17,19,21	0.89	2 (11%)
5	NAG	b	1	1,5	14,14,15	0.36	0	17,19,21	0.77	0
5	NAG	b	2	5	14,14,15	0.37	0	17,19,21	0.41	0
6	NAG	c	1	1,6	14,14,15	0.38	0	17,19,21	0.55	0
6	NAG	c	2	6	14,14,15	0.36	0	17,19,21	0.83	1 (5%)
6	BMA	c	3	6	11,11,12	0.29	0	15,15,17	0.53	0
6	NAG	d	1	1,6	14,14,15	0.39	0	17,19,21	0.59	0
6	NAG	d	2	6	14,14,15	0.38	0	17,19,21	0.56	0
6	BMA	d	3	6	11,11,12	0.41	0	15,15,17	0.54	0
7	NAG	e	1	1,7	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
7	NAG	e	2	7	14,14,15	0.38	0	17,19,21	0.63	0
7	BMA	e	3	7	11,11,12	0.89	1 (9%)	15,15,17	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	e	4	7	11,11,12	0.47	0	15,15,17	0.47	0
7	MAN	e	5	7	11,11,12	0.30	0	15,15,17	0.62	0
5	NAG	f	1	1,5	14,14,15	0.39	0	17,19,21	0.82	0
5	NAG	f	2	5	14,14,15	0.38	0	17,19,21	0.88	2 (11%)
5	NAG	g	1	1,5	14,14,15	0.39	0	17,19,21	0.96	1 (5%)
5	NAG	g	2	5	14,14,15	0.38	0	17,19,21	0.64	0
5	NAG	h	1	1,5	14,14,15	0.39	0	17,19,21	0.91	1 (5%)
5	NAG	h	2	5	14,14,15	0.39	0	17,19,21	0.49	0
8	NAG	i	1	1,8	14,14,15	0.39	0	17,19,21	0.53	0
8	NAG	i	2	8	14,14,15	0.37	0	17,19,21	0.68	0
8	BMA	i	3	8	11,11,12	0.34	0	15,15,17	0.46	0
8	MAN	i	4	8	11,11,12	0.31	0	15,15,17	0.52	0
9	NAG	j	1	1,9	14,14,15	0.41	0	17,19,21	0.64	1 (5%)
9	NAG	j	2	9	14,14,15	0.38	0	17,19,21	0.52	0
9	BMA	j	3	9	11,11,12	0.29	0	15,15,17	0.58	0
9	MAN	j	4	9	11,11,12	0.29	0	15,15,17	0.54	0
5	NAG	k	1	1,5	14,14,15	0.40	0	17,19,21	0.58	0
5	NAG	k	2	5	14,14,15	0.38	0	17,19,21	0.31	0
6	NAG	l	1	1,6	14,14,15	0.37	0	17,19,21	0.97	1 (5%)
6	NAG	l	2	6	14,14,15	0.37	0	17,19,21	0.49	0
6	BMA	l	3	6	11,11,12	0.28	0	15,15,17	0.53	0
5	NAG	m	1	1,5	14,14,15	0.37	0	17,19,21	0.50	0
5	NAG	m	2	5	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
5	NAG	n	1	1,5	14,14,15	0.37	0	17,19,21	0.56	0
5	NAG	n	2	5	14,14,15	0.40	0	17,19,21	0.91	2 (11%)
5	NAG	o	1	1,5	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
5	NAG	o	2	5	14,14,15	0.36	0	17,19,21	0.41	0
6	NAG	p	1	1,6	14,14,15	0.37	0	17,19,21	0.59	0
6	NAG	p	2	6	14,14,15	0.39	0	17,19,21	0.42	0
6	BMA	p	3	6	11,11,12	0.29	0	15,15,17	0.52	0
6	NAG	q	1	1,6	14,14,15	0.40	0	17,19,21	0.59	0
6	NAG	q	2	6	14,14,15	0.38	0	17,19,21	0.52	0
6	BMA	q	3	6	11,11,12	0.38	0	15,15,17	0.49	0
7	NAG	r	1	1,7	14,14,15	0.36	0	17,19,21	0.78	0
7	NAG	r	2	7	14,14,15	0.36	0	17,19,21	0.57	0
7	BMA	r	3	7	11,11,12	0.45	0	15,15,17	0.57	0
7	MAN	r	4	7	11,11,12	0.32	0	15,15,17	0.49	0
7	MAN	r	5	7	11,11,12	0.32	0	15,15,17	0.51	0
5	NAG	s	1	1,5	14,14,15	0.39	0	17,19,21	0.78	0
5	NAG	s	2	5	14,14,15	0.37	0	17,19,21	0.84	2 (11%)
5	NAG	t	1	1,5	14,14,15	0.38	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	t	2	5	14,14,15	0.36	0	17,19,21	0.62	0
5	NAG	u	1	1,5	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
5	NAG	u	2	5	14,14,15	0.39	0	17,19,21	0.47	0
5	NAG	v	1	1,5	14,14,15	0.38	0	17,19,21	0.56	0
5	NAG	v	2	5	14,14,15	0.39	0	17,19,21	1.02	1 (5%)
9	NAG	w	1	1,9	14,14,15	0.40	0	17,19,21	0.65	1 (5%)
9	NAG	w	2	9	14,14,15	0.39	0	17,19,21	0.48	0
9	BMA	w	3	9	11,11,12	0.36	0	15,15,17	0.52	0
9	MAN	w	4	9	11,11,12	0.22	0	15,15,17	0.49	0
5	NAG	x	1	1,5	14,14,15	0.41	0	17,19,21	0.57	0
5	NAG	x	2	5	14,14,15	0.39	0	17,19,21	0.31	0
5	NAG	y	1	1,5	14,14,15	0.38	0	17,19,21	0.80	0
5	NAG	y	2	5	14,14,15	0.39	0	17,19,21	0.46	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	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	5/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	1/2/19/22	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	0/2/19/22	0/1/1/1
7	NAG	R	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	R	2	7	-	2/6/23/26	0/1/1/1
7	BMA	R	3	7	-	0/2/19/22	0/1/1/1
7	MAN	R	4	7	-	0/2/19/22	0/1/1/1
7	MAN	R	5	7	-	1/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	S	2	5	-	3/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	3/6/23/26	0/1/1/1

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

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	e	3	BMA	C2-C3	-2.37	1.48	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	2	NAG	C2-N2-C7	6.65	131.81	122.90
9	W	1	NAG	C1-C2-N2	3.69	116.24	110.43
5	X	1	NAG	O5-C1-C2	-3.63	105.67	111.29
5	m	2	NAG	C2-N2-C7	3.45	127.52	122.90
5	t	1	NAG	C2-N2-C7	3.27	127.28	122.90
5	T	1	NAG	C2-N2-C7	3.25	127.25	122.90
5	v	2	NAG	C1-C2-N2	3.24	115.53	110.43
5	g	1	NAG	C2-N2-C7	3.21	127.20	122.90
9	W	1	NAG	C2-N2-C7	3.01	126.93	122.90
5	U	1	NAG	C1-C2-N2	2.66	114.63	110.43
5	u	1	NAG	C1-C2-N2	2.66	114.62	110.43
5	h	1	NAG	C1-C2-N2	2.64	114.59	110.43
6	c	2	NAG	C2-N2-C7	2.61	126.39	122.90
8	V	2	NAG	C1-C2-N2	2.50	114.37	110.43
7	e	1	NAG	C2-N2-C7	2.47	126.21	122.90
5	Z	2	NAG	C2-N2-C7	2.45	126.18	122.90
6	l	1	NAG	C2-N2-C7	2.41	126.13	122.90
5	Z	1	NAG	O4-C4-C3	-2.36	104.81	110.38
5	n	2	NAG	C2-N2-C7	2.29	125.96	122.90
5	f	2	NAG	C1-C2-N2	2.27	114.01	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2	NAG	C1-C2-N2	2.23	113.95	110.43
5	a	2	NAG	C2-N2-C7	2.19	125.83	122.90
5	f	2	NAG	C2-N2-C7	2.18	125.82	122.90
5	a	2	NAG	C1-C2-N2	2.14	113.81	110.43
5	S	2	NAG	C2-N2-C7	2.13	125.75	122.90
5	s	2	NAG	C1-C2-N2	2.10	113.74	110.43
9	w	1	NAG	C1-O5-C5	2.09	114.99	112.19
5	o	1	NAG	C2-N2-C7	2.09	125.70	122.90
5	Y	1	NAG	C1-O5-C5	2.08	114.98	112.19
9	j	1	NAG	C1-O5-C5	2.08	114.97	112.19
5	s	2	NAG	C2-N2-C7	2.05	125.65	122.90
5	n	2	NAG	C1-C2-N2	2.05	113.66	110.43
9	W	1	NAG	C1-O5-C5	2.04	114.92	112.19
5	Z	1	NAG	C2-N2-C7	2.02	125.60	122.90

There are no chirality outliers.

All (171) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	1	NAG	C8-C7-N2-C2
5	O	1	NAG	O7-C7-N2-C2
5	S	1	NAG	C1-C2-N2-C7
5	S	2	NAG	C1-C2-N2-C7
5	S	2	NAG	C8-C7-N2-C2
5	S	2	NAG	O7-C7-N2-C2
5	T	1	NAG	C3-C2-N2-C7
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	a	2	NAG	C8-C7-N2-C2
5	a	2	NAG	O7-C7-N2-C2
5	f	1	NAG	C1-C2-N2-C7
5	f	2	NAG	C1-C2-N2-C7
5	f	2	NAG	C8-C7-N2-C2
5	f	2	NAG	O7-C7-N2-C2
5	g	1	NAG	C3-C2-N2-C7
5	g	1	NAG	C8-C7-N2-C2
5	g	1	NAG	O7-C7-N2-C2
5	h	1	NAG	C3-C2-N2-C7
5	k	1	NAG	C8-C7-N2-C2
5	m	2	NAG	C3-C2-N2-C7
5	m	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	m	2	NAG	O7-C7-N2-C2
5	n	2	NAG	C8-C7-N2-C2
5	n	2	NAG	O7-C7-N2-C2
5	o	1	NAG	C8-C7-N2-C2
5	o	1	NAG	O7-C7-N2-C2
5	s	1	NAG	C1-C2-N2-C7
5	s	2	NAG	C1-C2-N2-C7
5	s	2	NAG	C8-C7-N2-C2
5	s	2	NAG	O7-C7-N2-C2
5	t	1	NAG	C3-C2-N2-C7
5	t	1	NAG	C8-C7-N2-C2
5	t	1	NAG	O7-C7-N2-C2
5	v	1	NAG	O7-C7-N2-C2
5	x	1	NAG	C8-C7-N2-C2
5	y	1	NAG	C8-C7-N2-C2
5	y	1	NAG	O7-C7-N2-C2
6	c	1	NAG	C8-C7-N2-C2
6	c	1	NAG	O7-C7-N2-C2
6	p	1	NAG	C8-C7-N2-C2
6	p	1	NAG	O7-C7-N2-C2
8	V	1	NAG	C8-C7-N2-C2
8	V	2	NAG	C8-C7-N2-C2
8	V	2	NAG	O7-C7-N2-C2
9	W	1	NAG	C8-C7-N2-C2
9	W	1	NAG	O7-C7-N2-C2
5	X	2	NAG	C8-C7-N2-C2
5	X	2	NAG	O7-C7-N2-C2
5	k	1	NAG	O7-C7-N2-C2
5	v	1	NAG	C8-C7-N2-C2
8	V	1	NAG	O7-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	x	1	NAG	O7-C7-N2-C2
8	i	1	NAG	C8-C7-N2-C2
8	i	1	NAG	O7-C7-N2-C2
9	j	3	BMA	C4-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
5	x	2	NAG	O5-C5-C6-O6
5	x	2	NAG	C4-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
7	R	2	NAG	C8-C7-N2-C2
7	R	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	X	1	NAG	C4-C5-C6-O6
6	d	3	BMA	O5-C5-C6-O6
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	S	1	NAG	C8-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	Y	1	NAG	C8-C7-N2-C2
5	Y	1	NAG	O7-C7-N2-C2
5	b	1	NAG	C8-C7-N2-C2
5	b	2	NAG	C8-C7-N2-C2
5	b	2	NAG	O7-C7-N2-C2
5	f	1	NAG	C8-C7-N2-C2
5	n	1	NAG	C8-C7-N2-C2
5	n	1	NAG	O7-C7-N2-C2
5	o	2	NAG	C8-C7-N2-C2
5	o	2	NAG	O7-C7-N2-C2
5	s	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
6	d	1	NAG	C8-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
6	p	2	NAG	C8-C7-N2-C2
6	p	2	NAG	O7-C7-N2-C2
6	q	1	NAG	C8-C7-N2-C2
6	q	1	NAG	O7-C7-N2-C2
7	e	1	NAG	C8-C7-N2-C2
7	e	1	NAG	O7-C7-N2-C2
7	e	2	NAG	C8-C7-N2-C2
7	e	2	NAG	O7-C7-N2-C2
7	r	2	NAG	C8-C7-N2-C2
7	r	2	NAG	O7-C7-N2-C2
9	j	1	NAG	C8-C7-N2-C2
9	j	1	NAG	O7-C7-N2-C2
9	w	1	NAG	C8-C7-N2-C2
9	w	1	NAG	O7-C7-N2-C2
9	j	3	BMA	O5-C5-C6-O6
6	d	3	BMA	C4-C5-C6-O6
5	o	1	NAG	O5-C5-C6-O6
5	b	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	s	1	NAG	O7-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
5	f	1	NAG	O7-C7-N2-C2
7	r	1	NAG	C8-C7-N2-C2
7	R	5	MAN	O5-C5-C6-O6
7	r	5	MAN	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
8	i	1	NAG	O5-C5-C6-O6
6	p	2	NAG	O5-C5-C6-O6
9	W	3	BMA	C4-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
7	e	3	BMA	O5-C5-C6-O6
6	c	3	BMA	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
6	p	3	BMA	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
6	P	1	NAG	C8-C7-N2-C2
5	S	1	NAG	C3-C2-N2-C7
5	U	1	NAG	C3-C2-N2-C7
5	a	2	NAG	C3-C2-N2-C7
5	f	1	NAG	C3-C2-N2-C7
5	n	2	NAG	C3-C2-N2-C7
5	u	1	NAG	C3-C2-N2-C7
8	V	2	NAG	C3-C2-N2-C7
9	W	1	NAG	C3-C2-N2-C7
9	w	3	BMA	C4-C5-C6-O6
5	x	2	NAG	C8-C7-N2-C2
7	r	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C1-C2-N2-C7
5	a	2	NAG	C1-C2-N2-C7
5	h	1	NAG	C1-C2-N2-C7
5	n	2	NAG	C1-C2-N2-C7
5	u	1	NAG	C1-C2-N2-C7
8	V	2	NAG	C1-C2-N2-C7
9	W	1	NAG	C1-C2-N2-C7
7	R	1	NAG	C8-C7-N2-C2
9	W	3	BMA	O5-C5-C6-O6
6	d	2	NAG	C8-C7-N2-C2
6	P	1	NAG	O7-C7-N2-C2
5	x	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C3-C2-N2-C7
5	O	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	Z	2	NAG	C3-C2-N2-C7
5	b	1	NAG	C3-C2-N2-C7
5	s	1	NAG	C3-C2-N2-C7
6	c	2	NAG	C3-C2-N2-C7
7	R	1	NAG	C3-C2-N2-C7
7	e	1	NAG	C3-C2-N2-C7
7	r	1	NAG	C3-C2-N2-C7
7	R	1	NAG	O7-C7-N2-C2
9	w	3	BMA	O5-C5-C6-O6
5	o	1	NAG	C4-C5-C6-O6
5	O	2	NAG	C1-C2-N2-C7
5	b	1	NAG	C1-C2-N2-C7
5	v	2	NAG	C1-C2-N2-C7
6	c	2	NAG	C1-C2-N2-C7
6	d	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C3-C2-N2-C7
5	Z	1	NAG	C3-C2-N2-C7
5	m	1	NAG	C3-C2-N2-C7
5	v	2	NAG	C3-C2-N2-C7
6	q	3	BMA	C4-C5-C6-O6
6	q	3	BMA	O5-C5-C6-O6
7	e	3	BMA	C4-C5-C6-O6

There are no ring outliers.

23 monomers are involved in 21 short contacts:

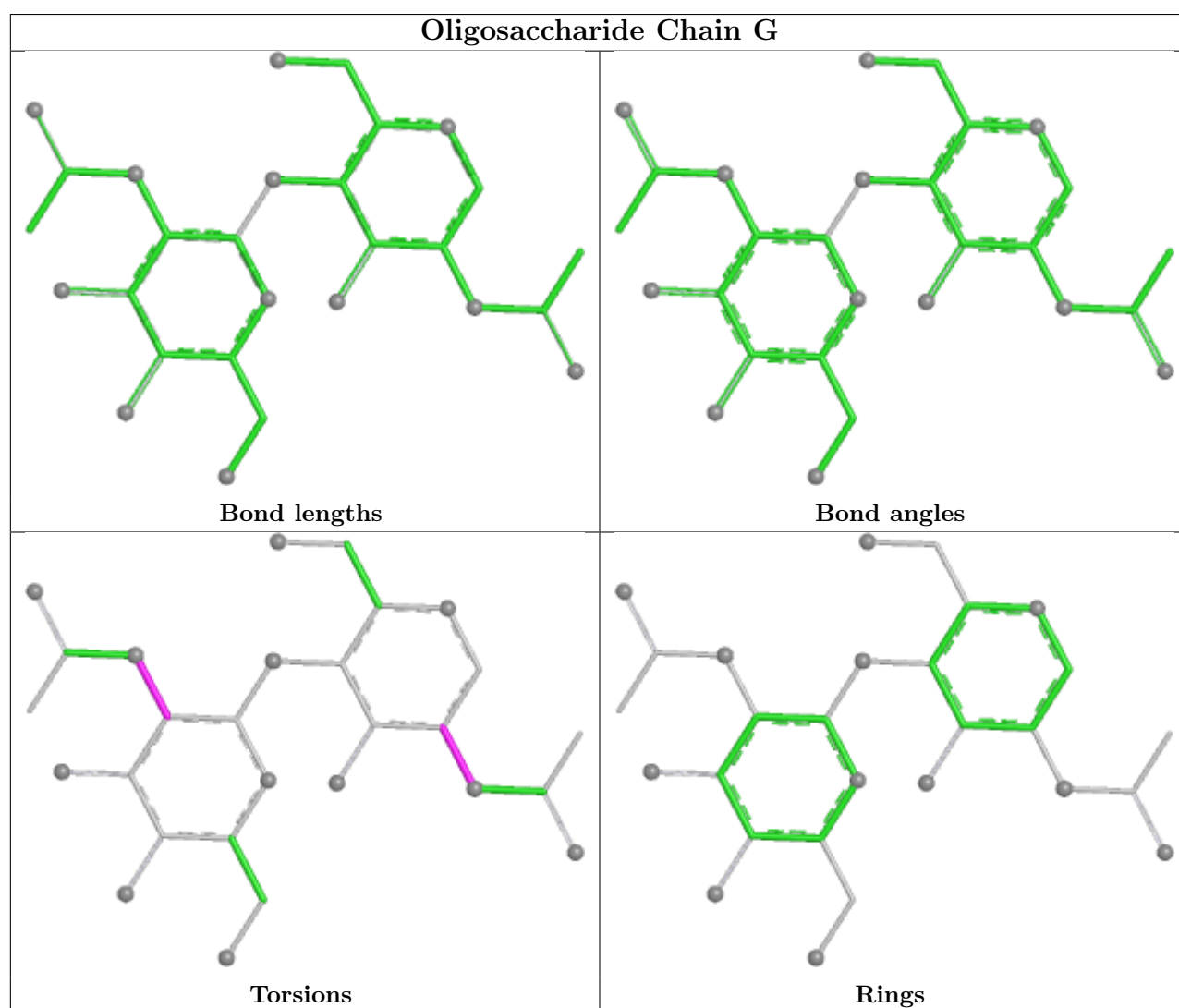
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	t	2	NAG	1	0
6	p	1	NAG	1	0
7	R	3	BMA	1	0
7	r	3	BMA	1	0
9	j	3	BMA	1	0
5	Y	1	NAG	1	0
5	u	1	NAG	1	0
5	O	2	NAG	2	0
9	j	4	MAN	1	0
7	R	1	NAG	1	0
5	t	1	NAG	1	0
5	O	1	NAG	2	0
7	r	2	NAG	1	0
5	Z	2	NAG	1	0
7	e	2	NAG	1	0

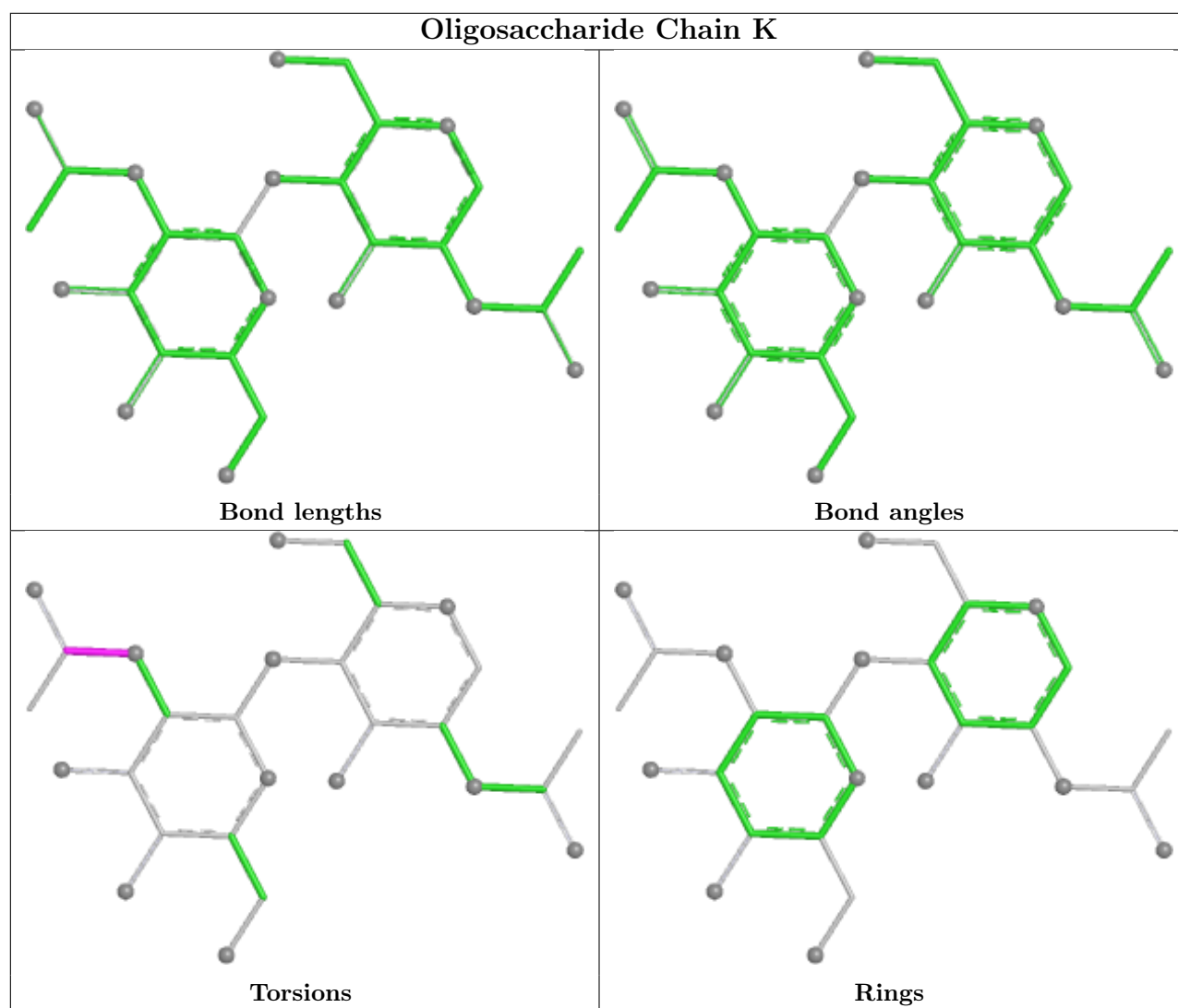
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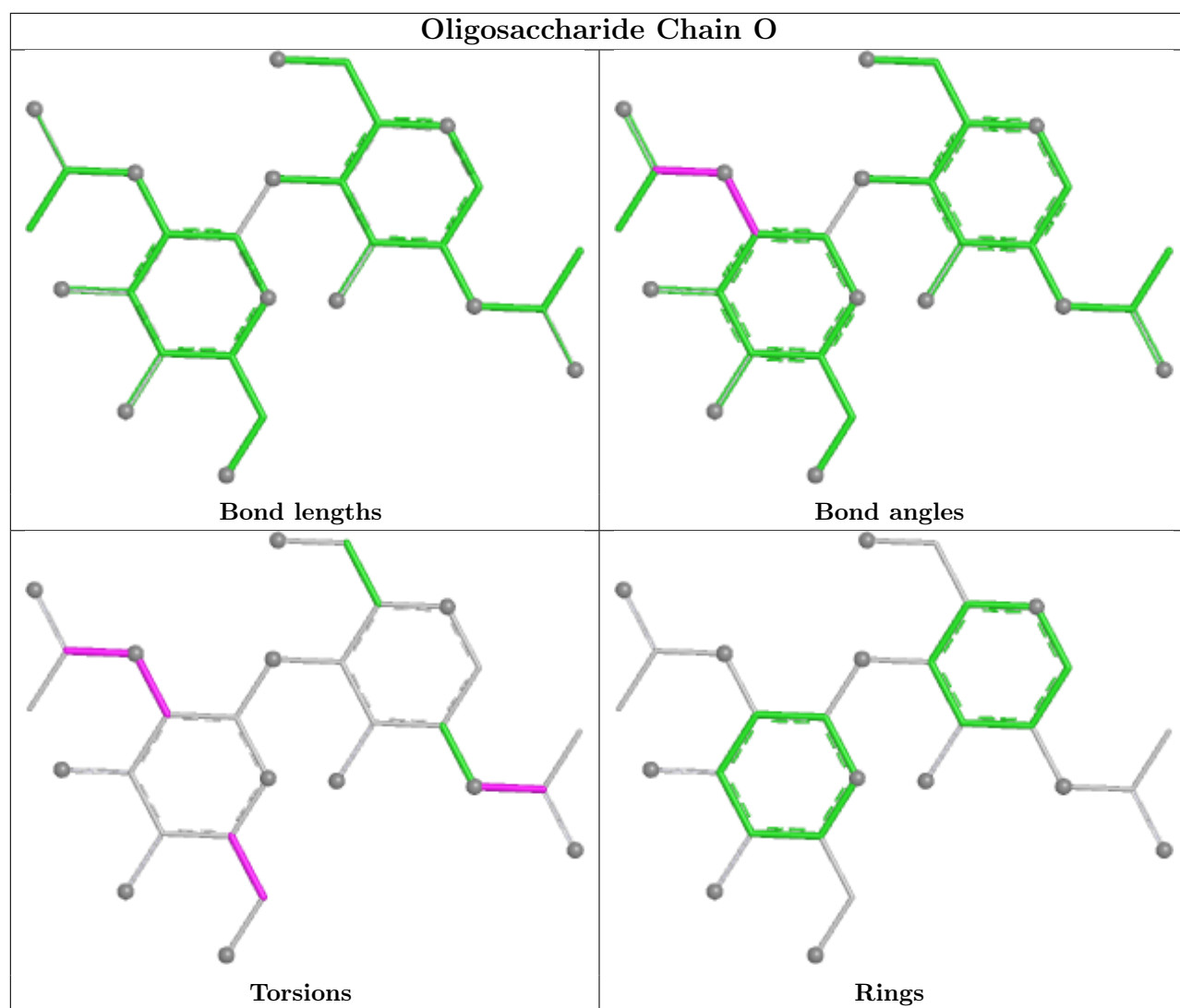
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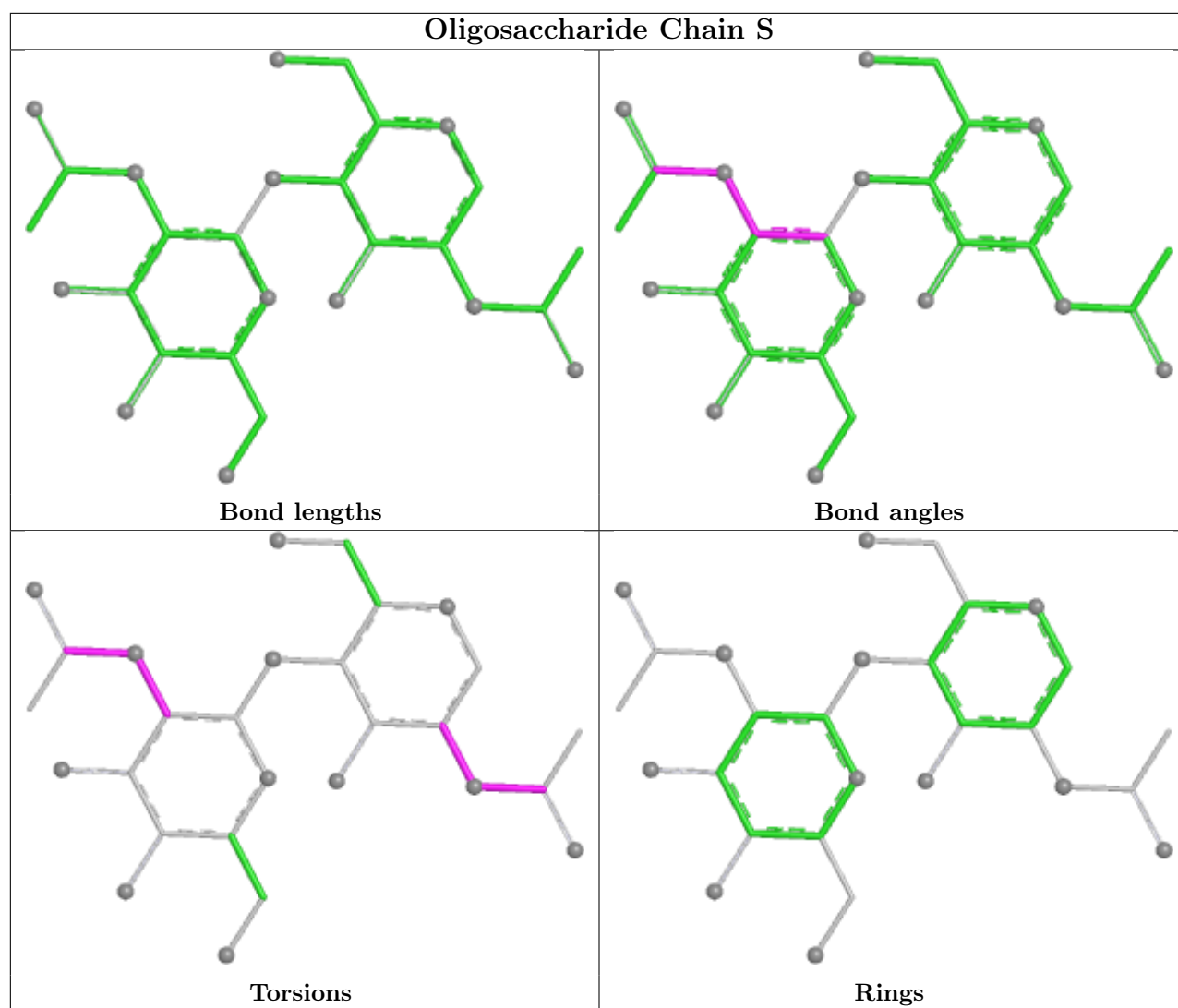
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	g	1	NAG	1	0
7	e	3	BMA	1	0
6	l	1	NAG	1	0
9	W	1	NAG	2	0
5	Z	1	NAG	2	0
5	g	2	NAG	1	0
5	h	1	NAG	1	0
6	d	1	NAG	1	0

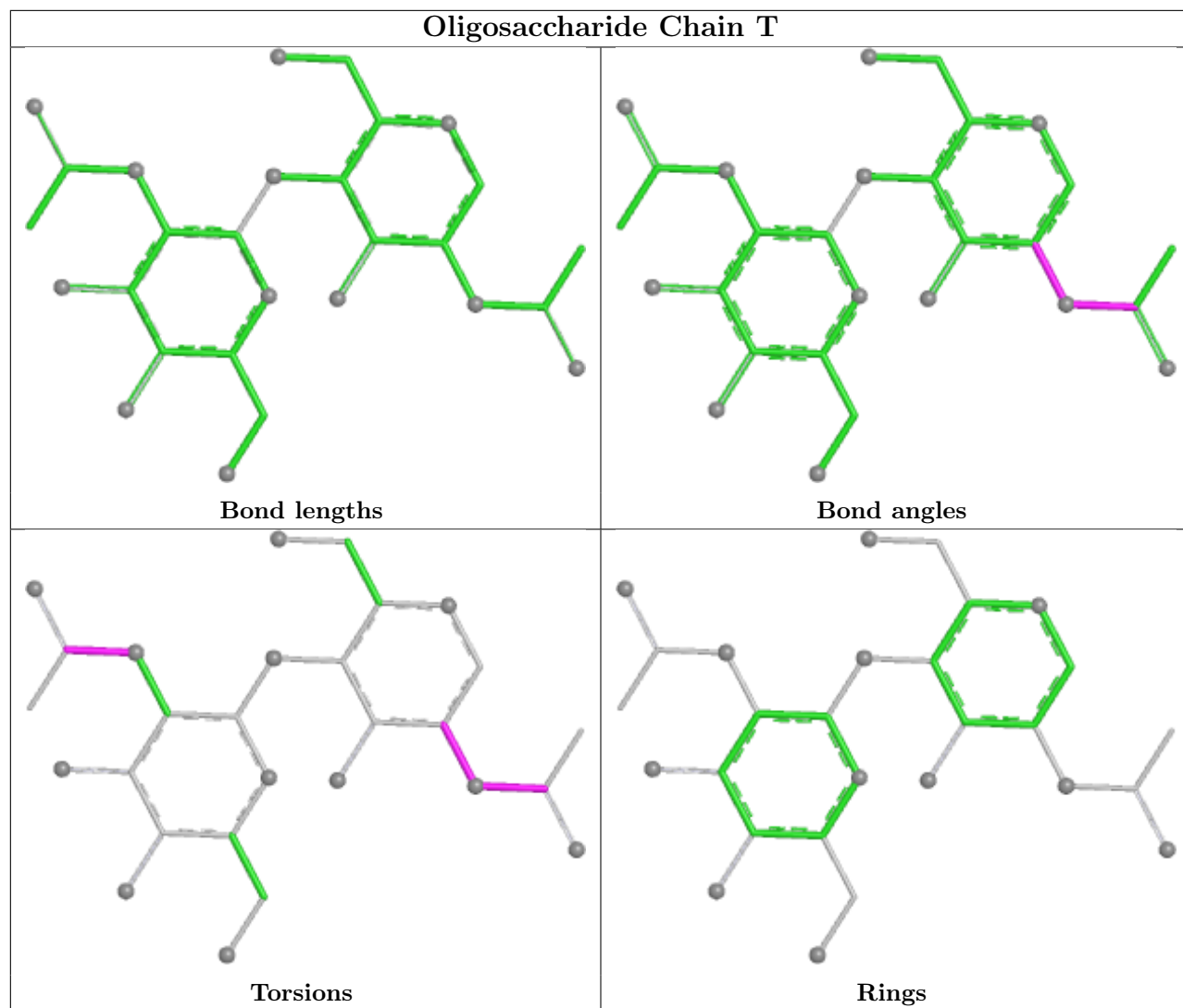
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

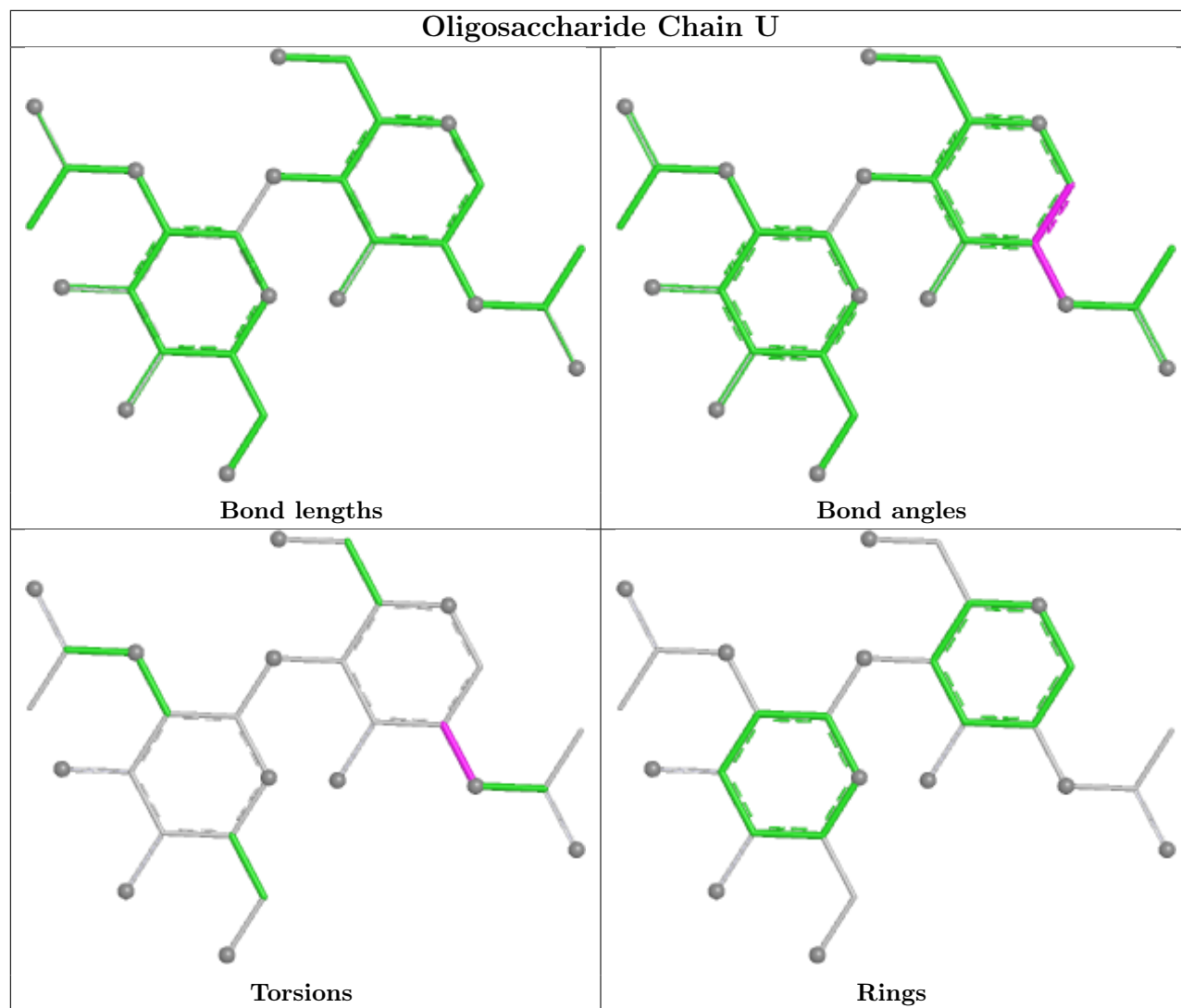


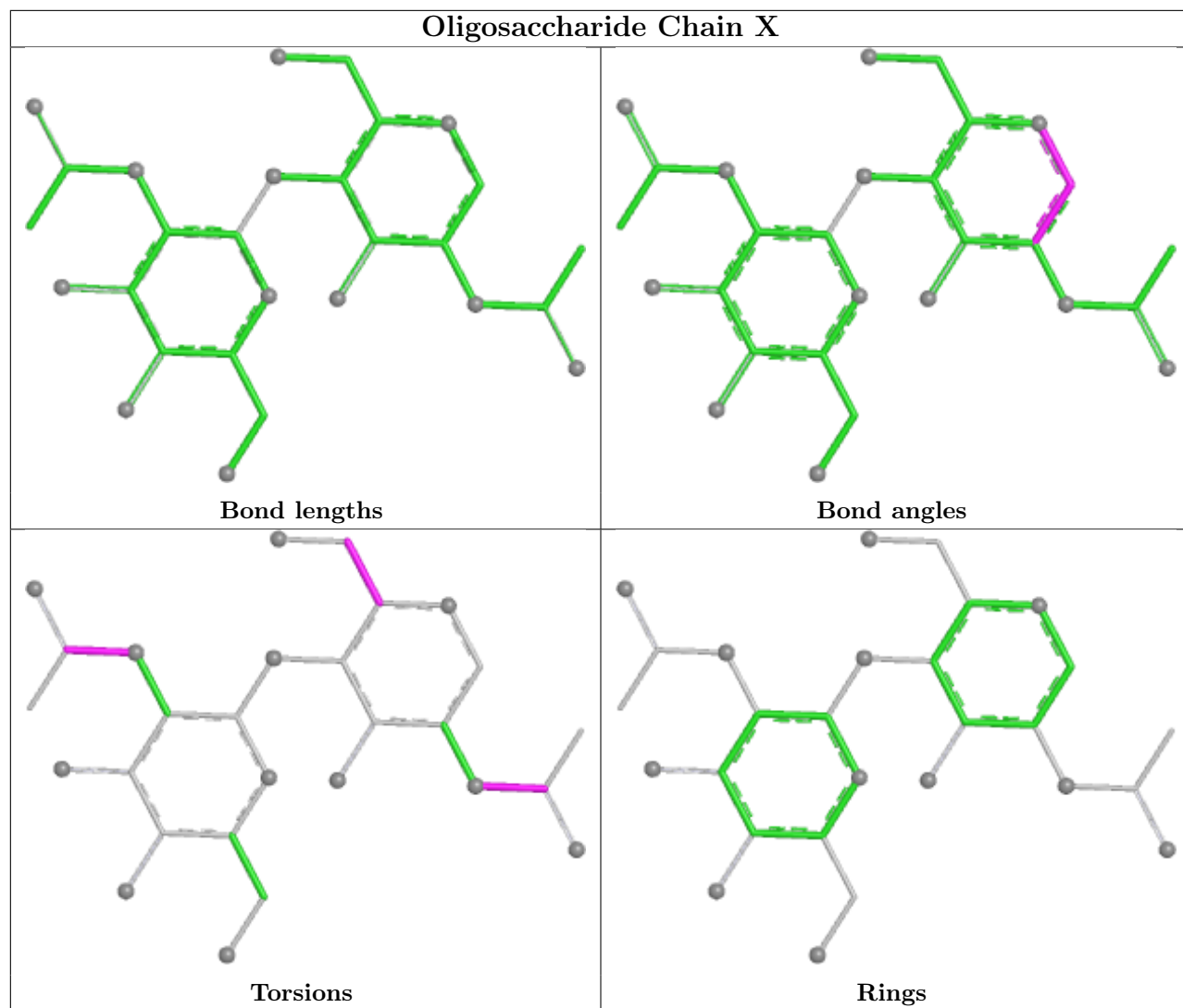


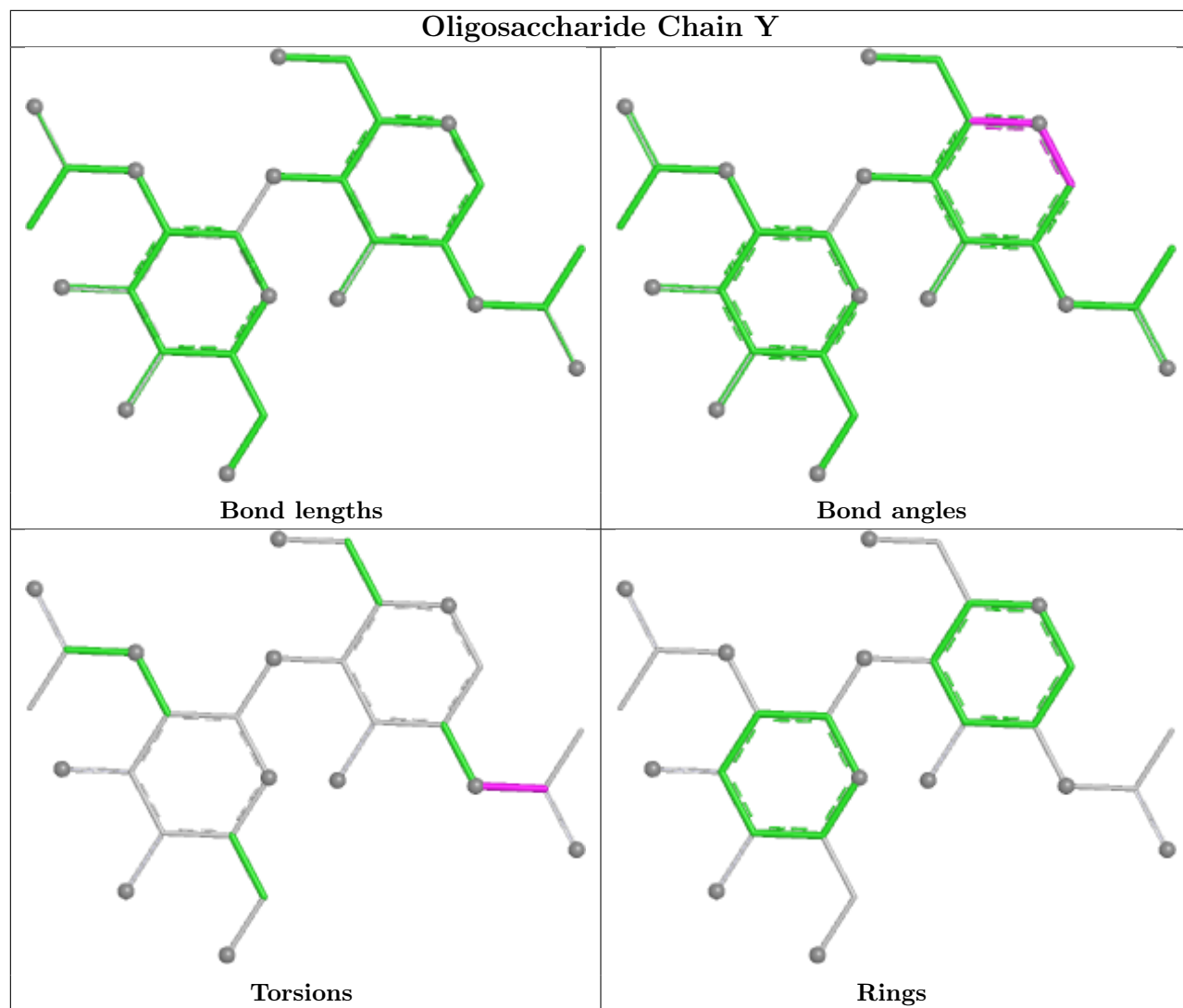


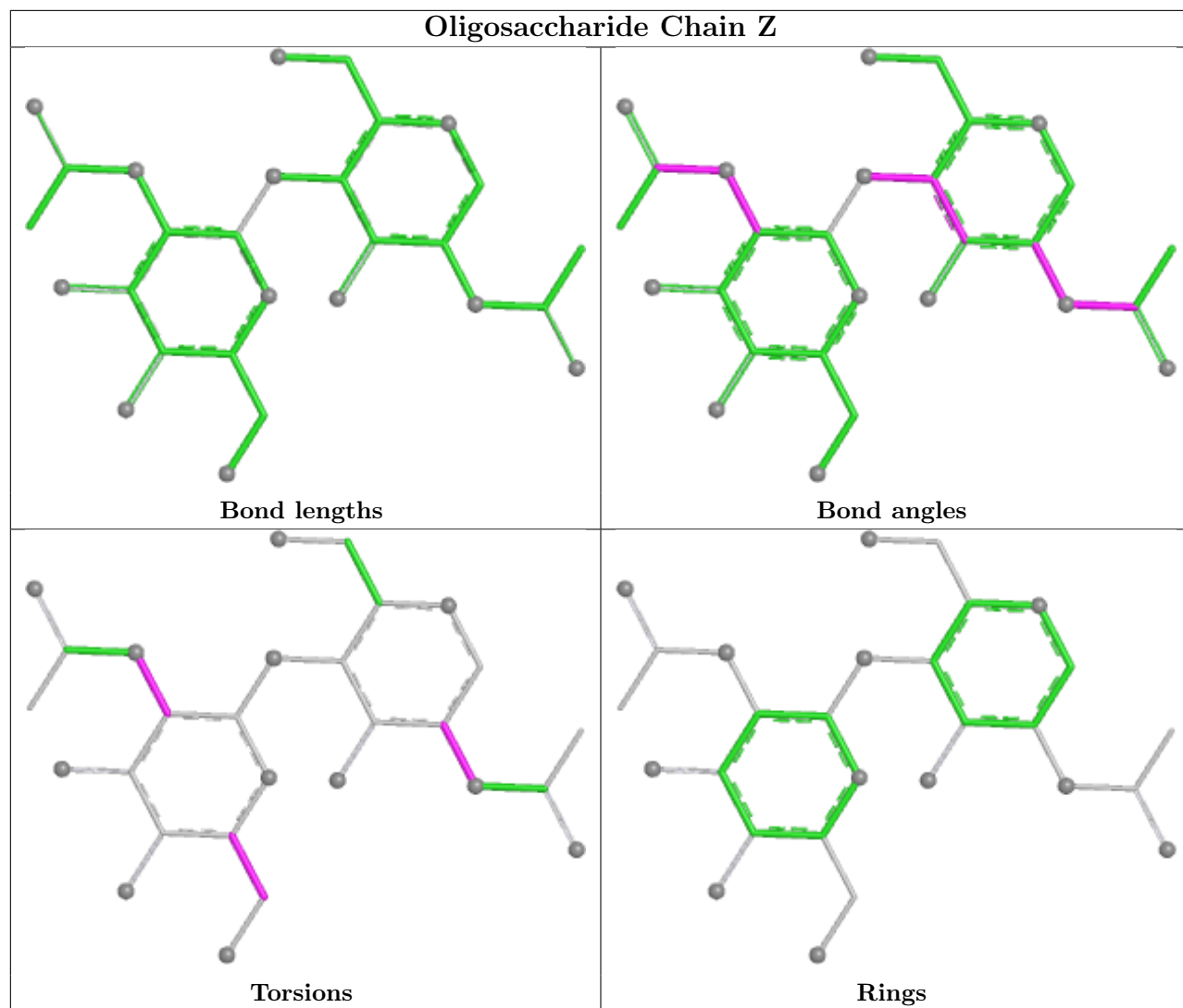


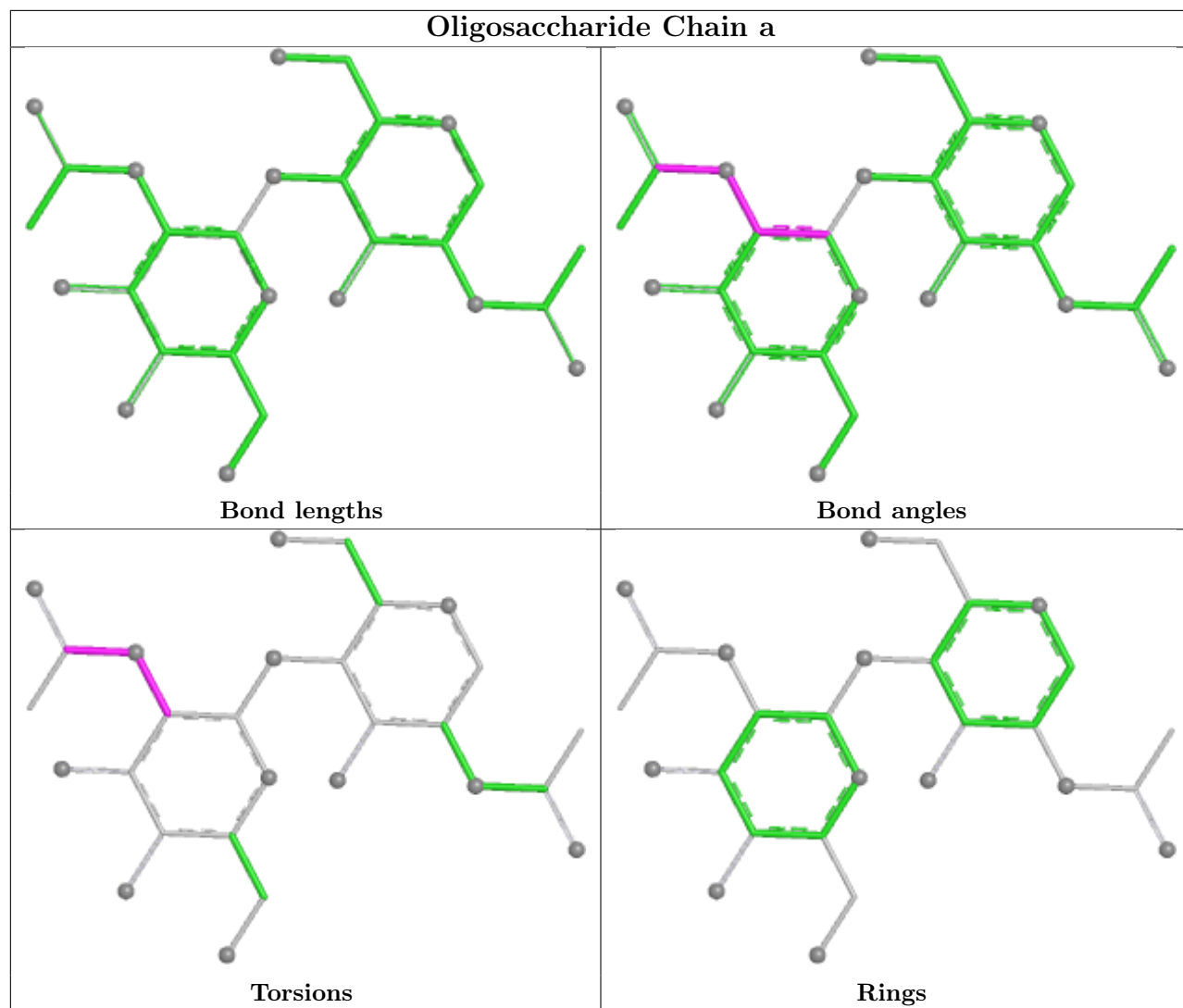


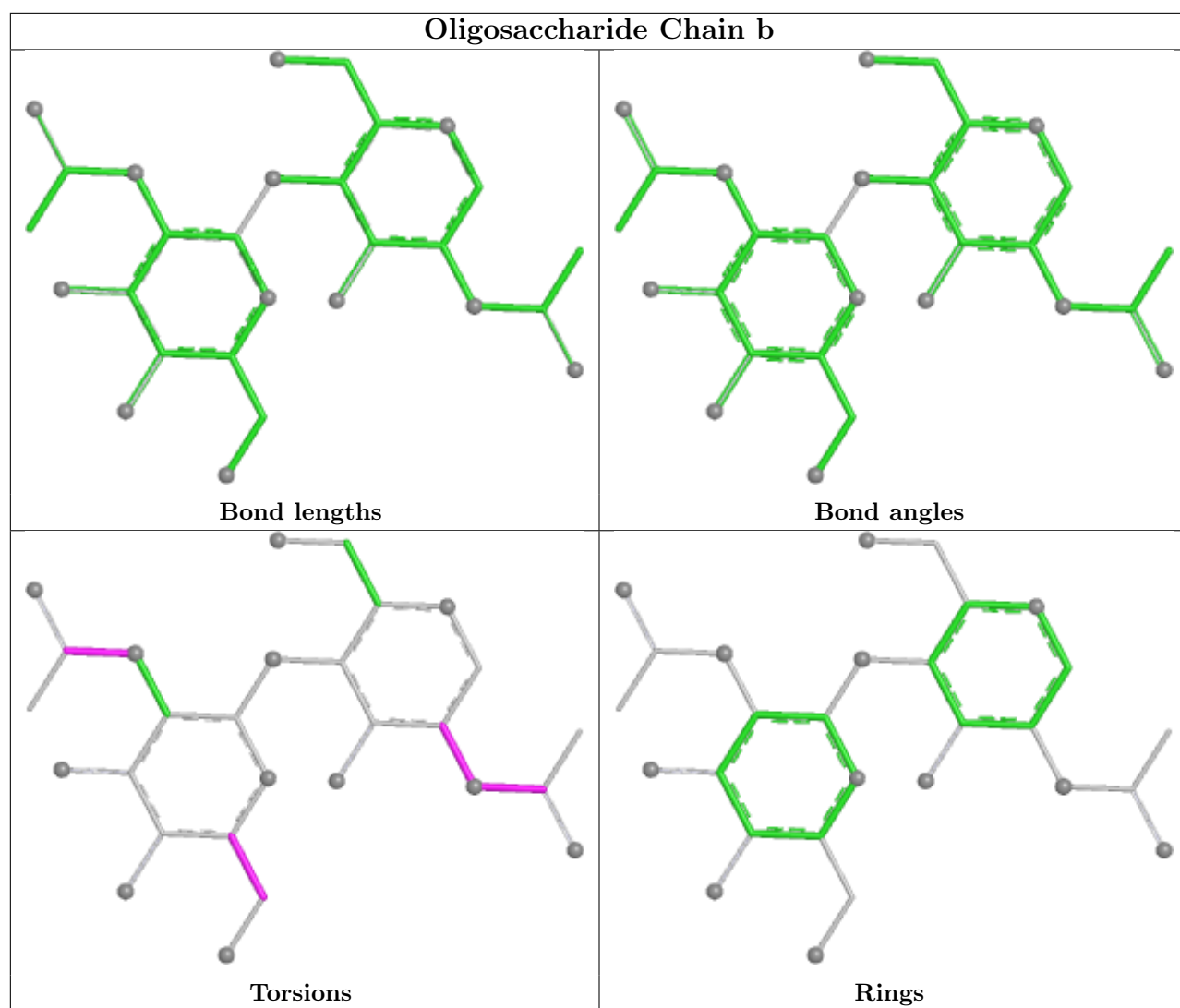


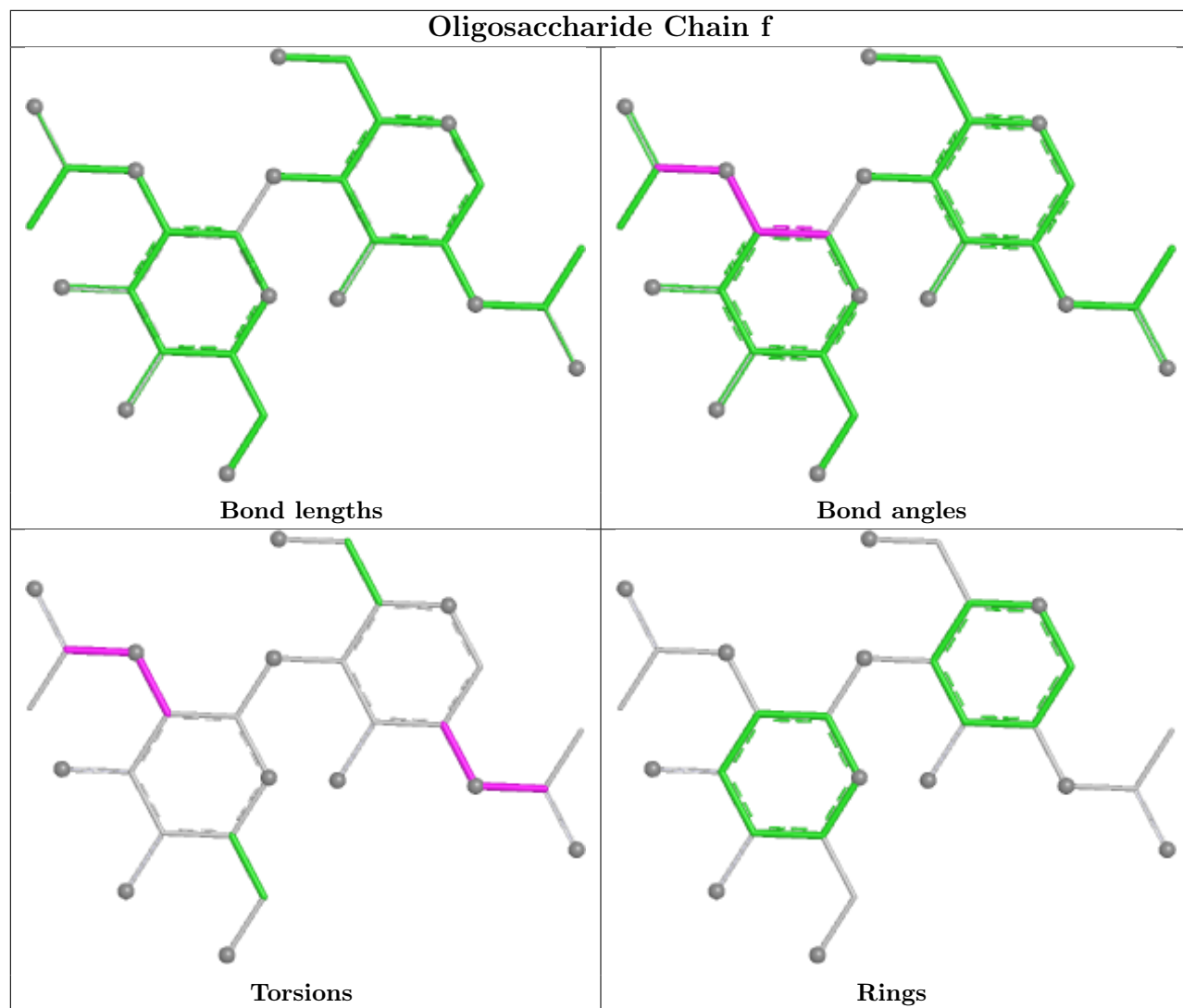


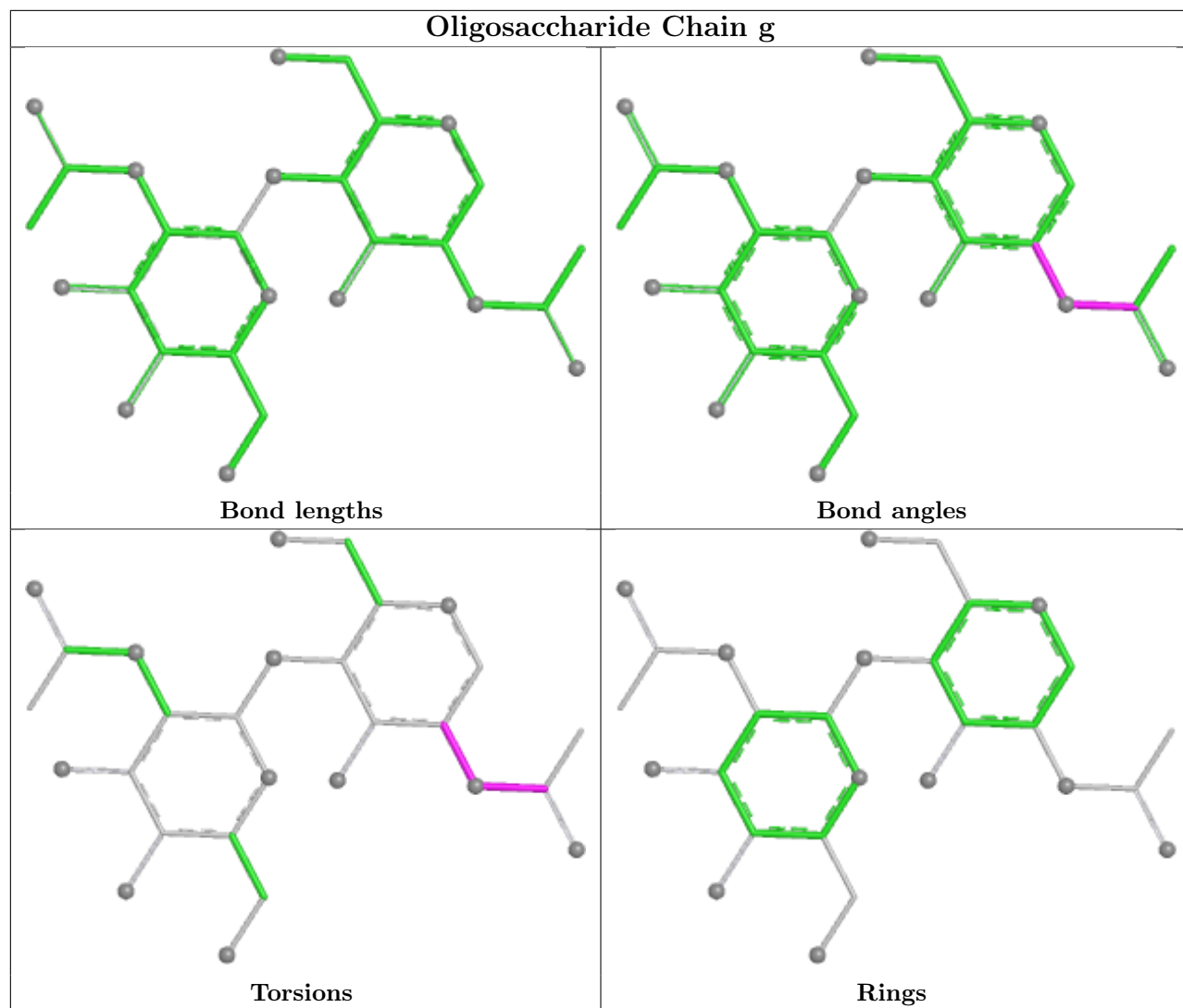


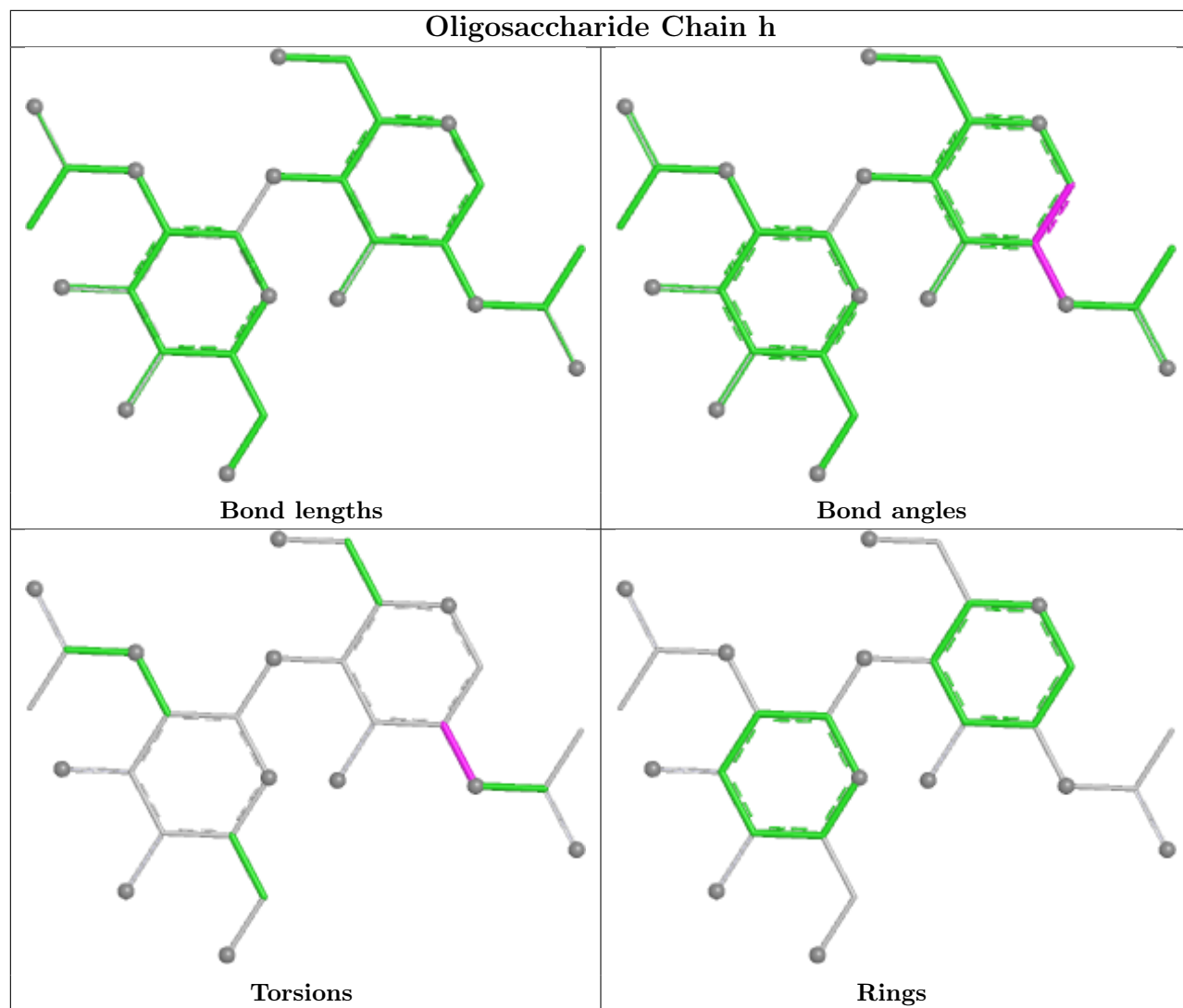


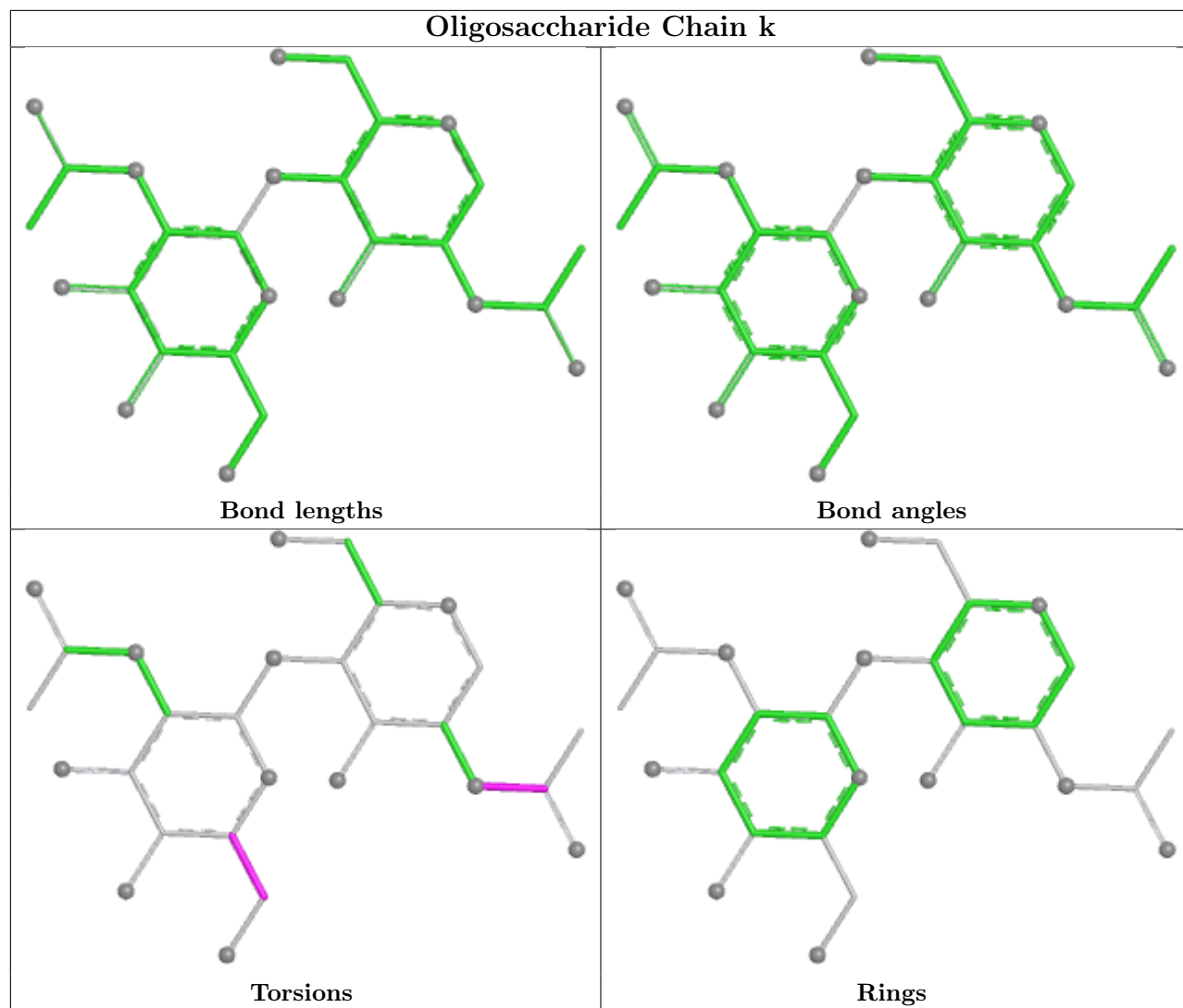


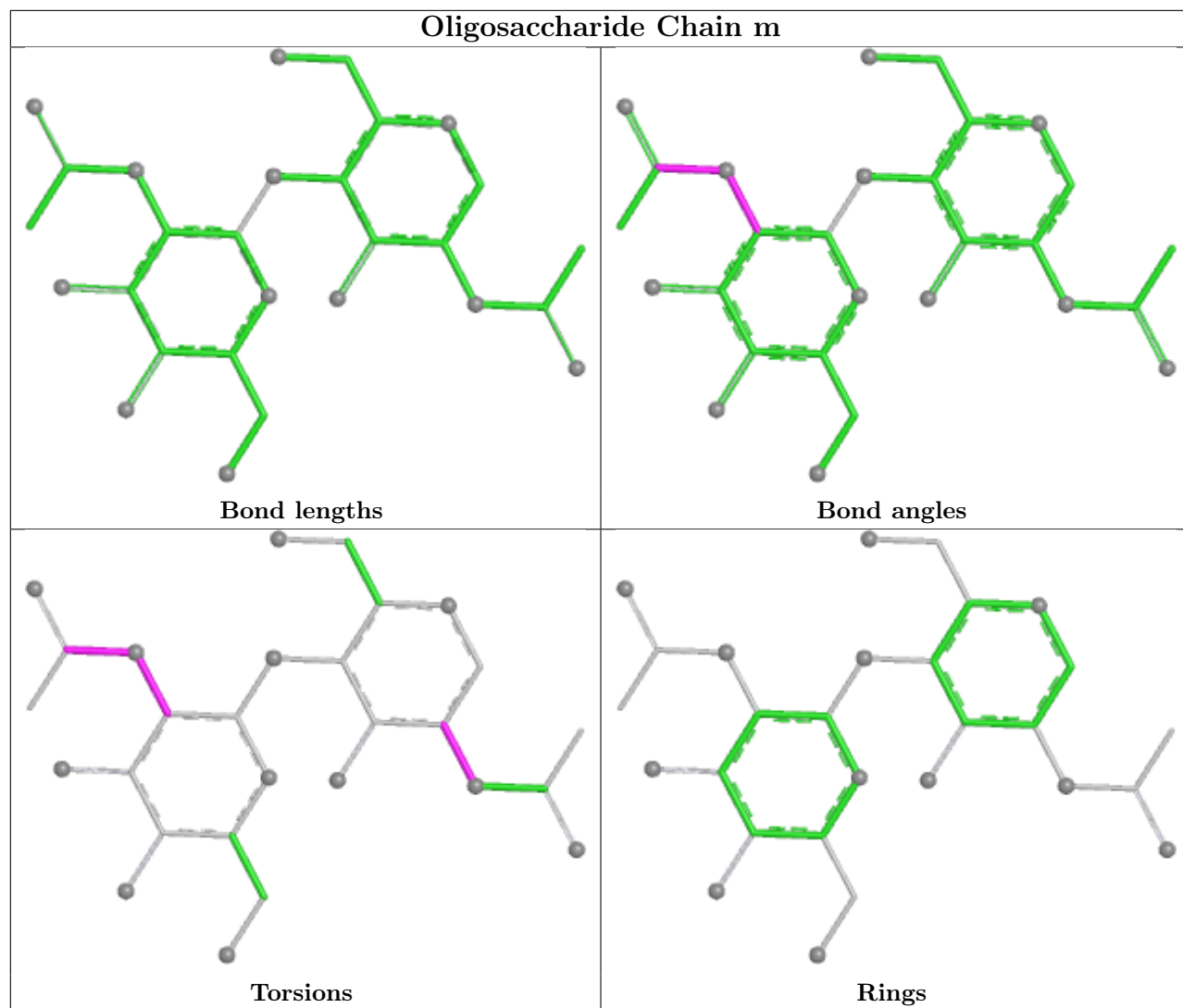


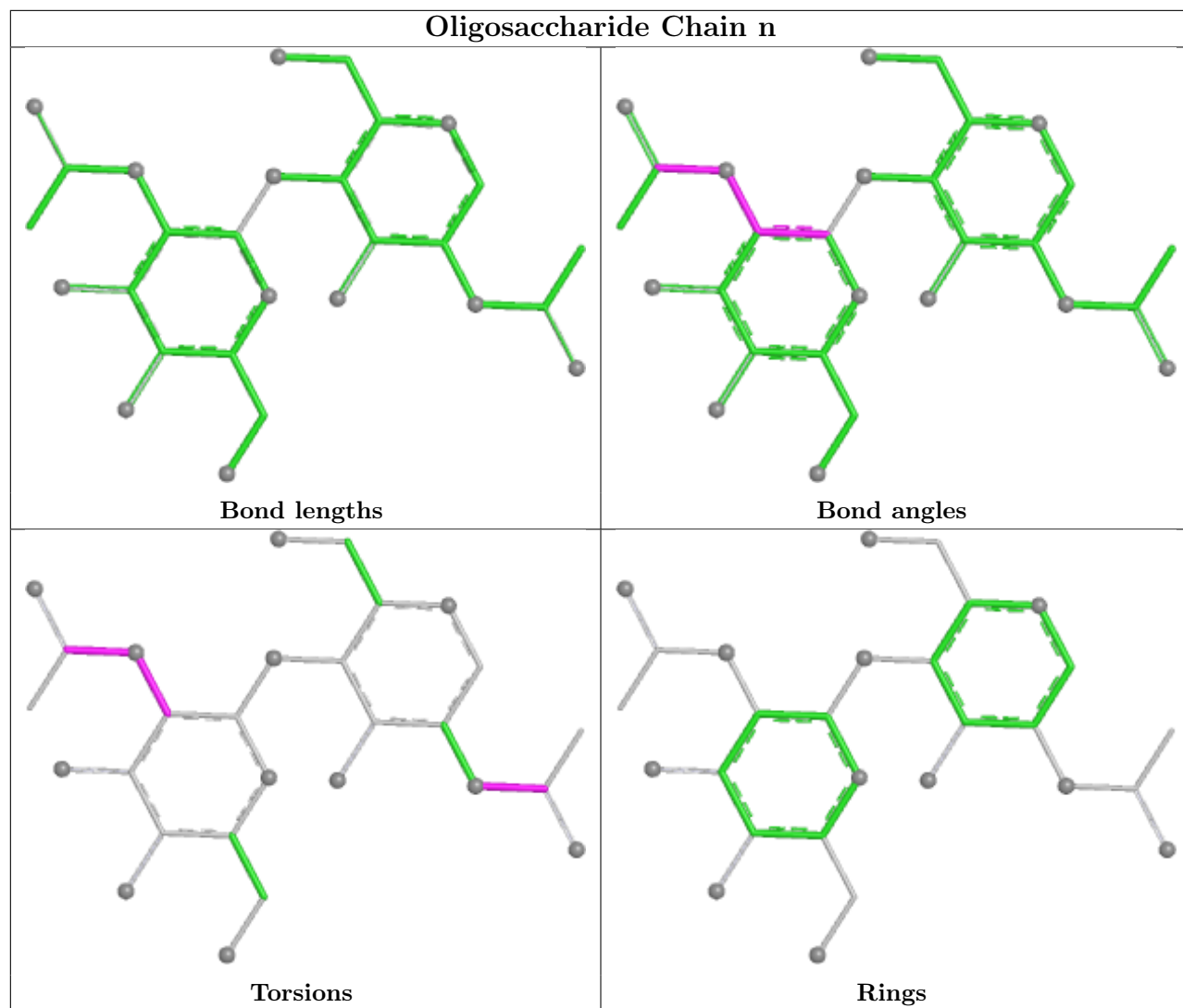


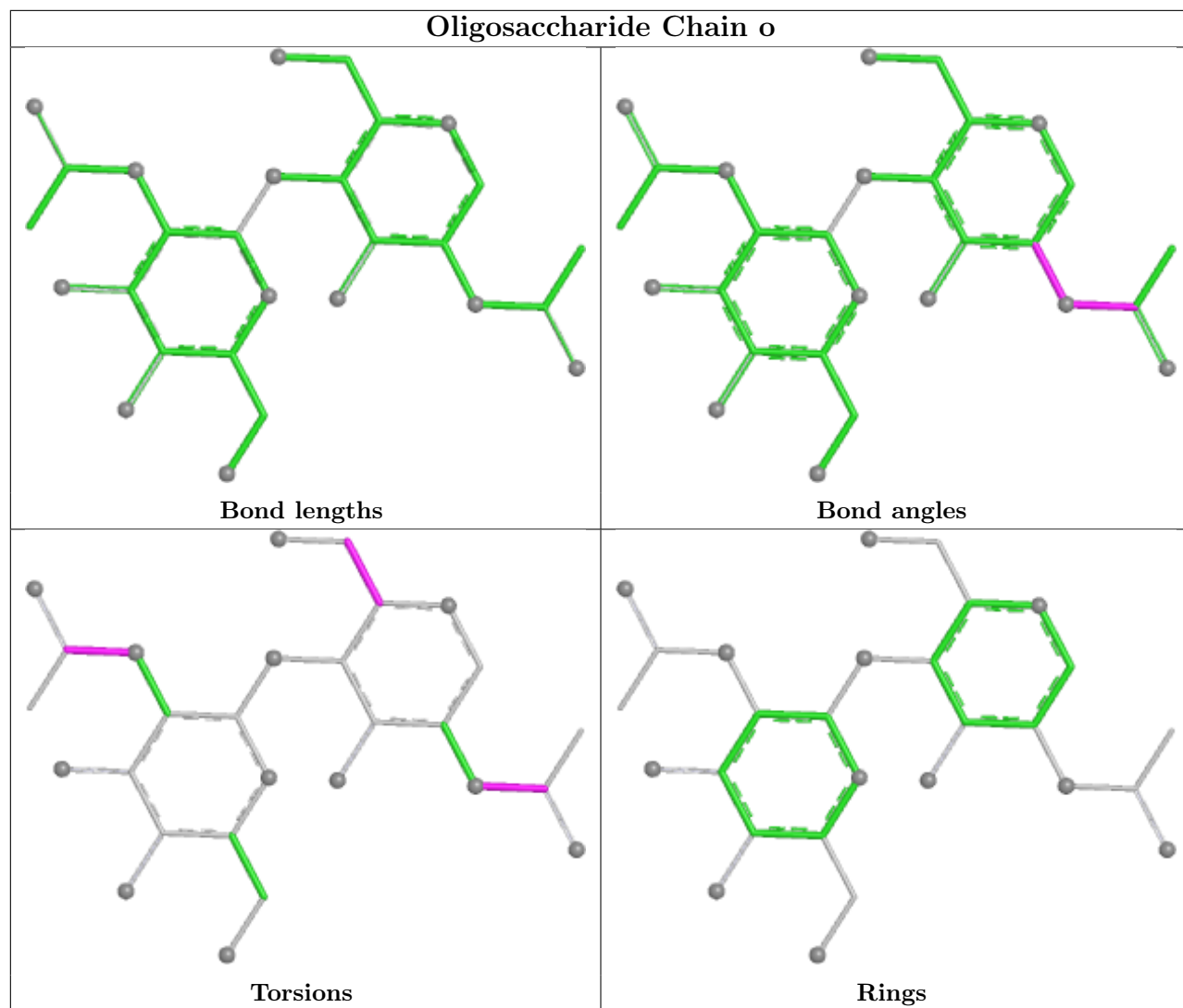


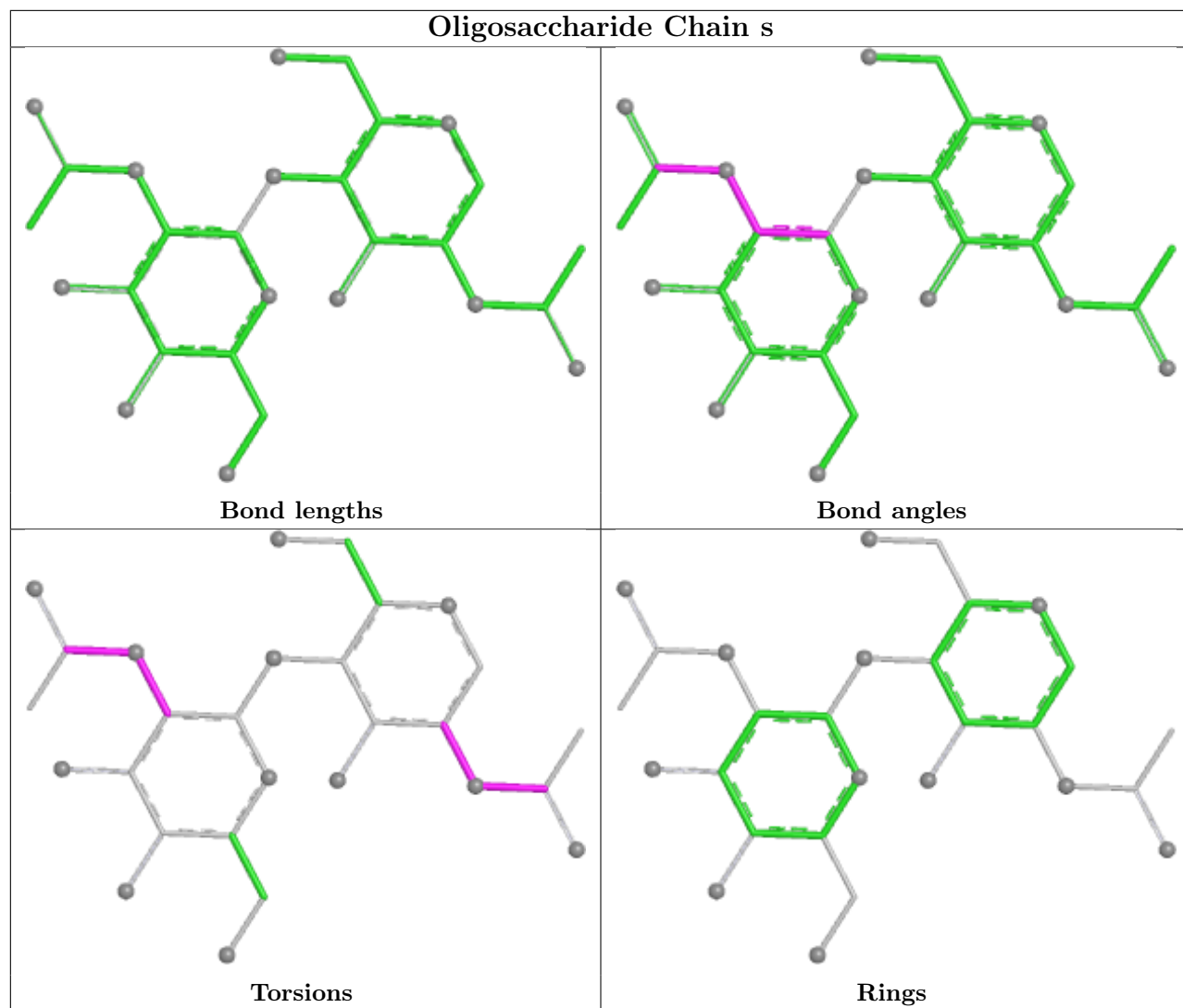


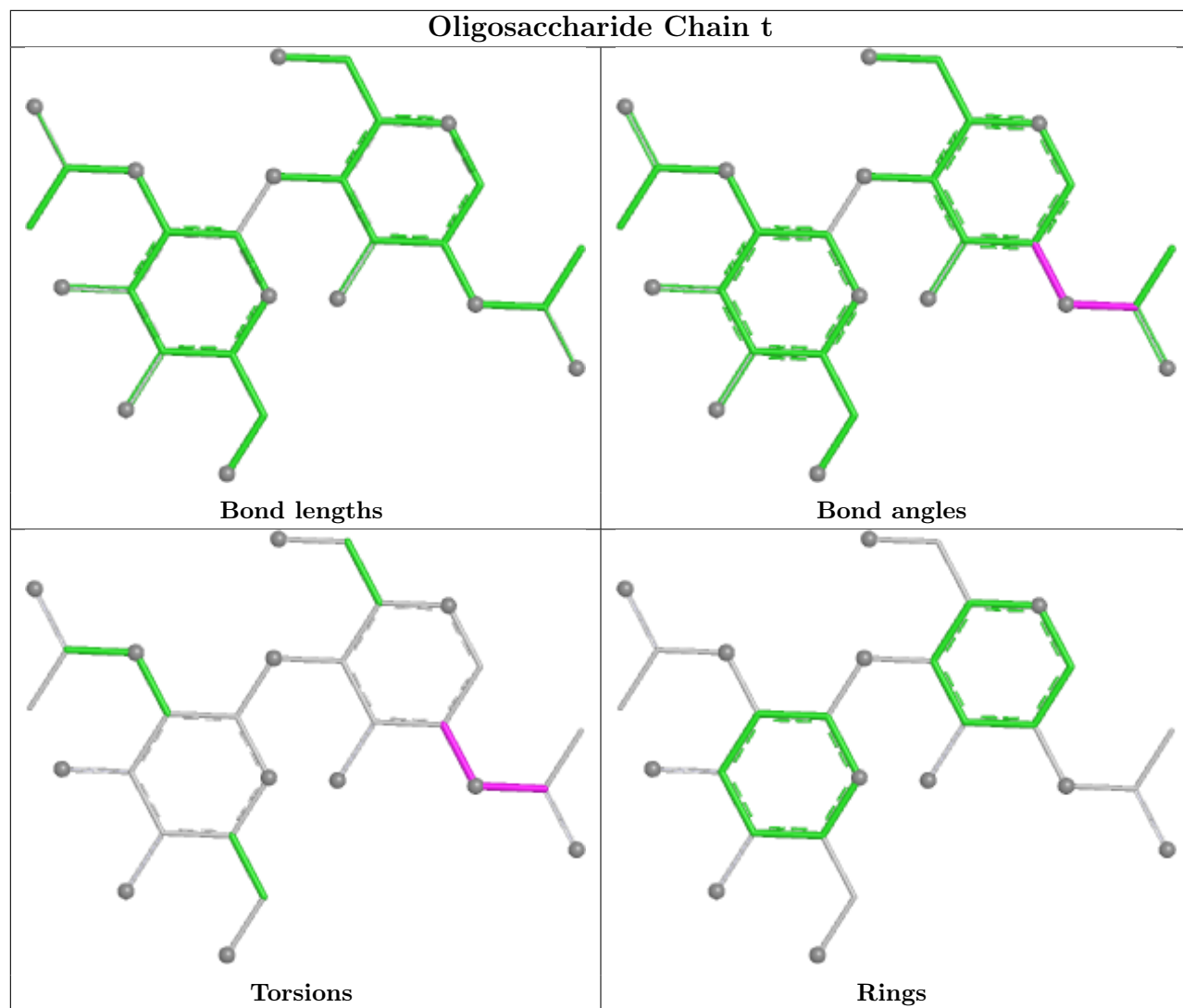


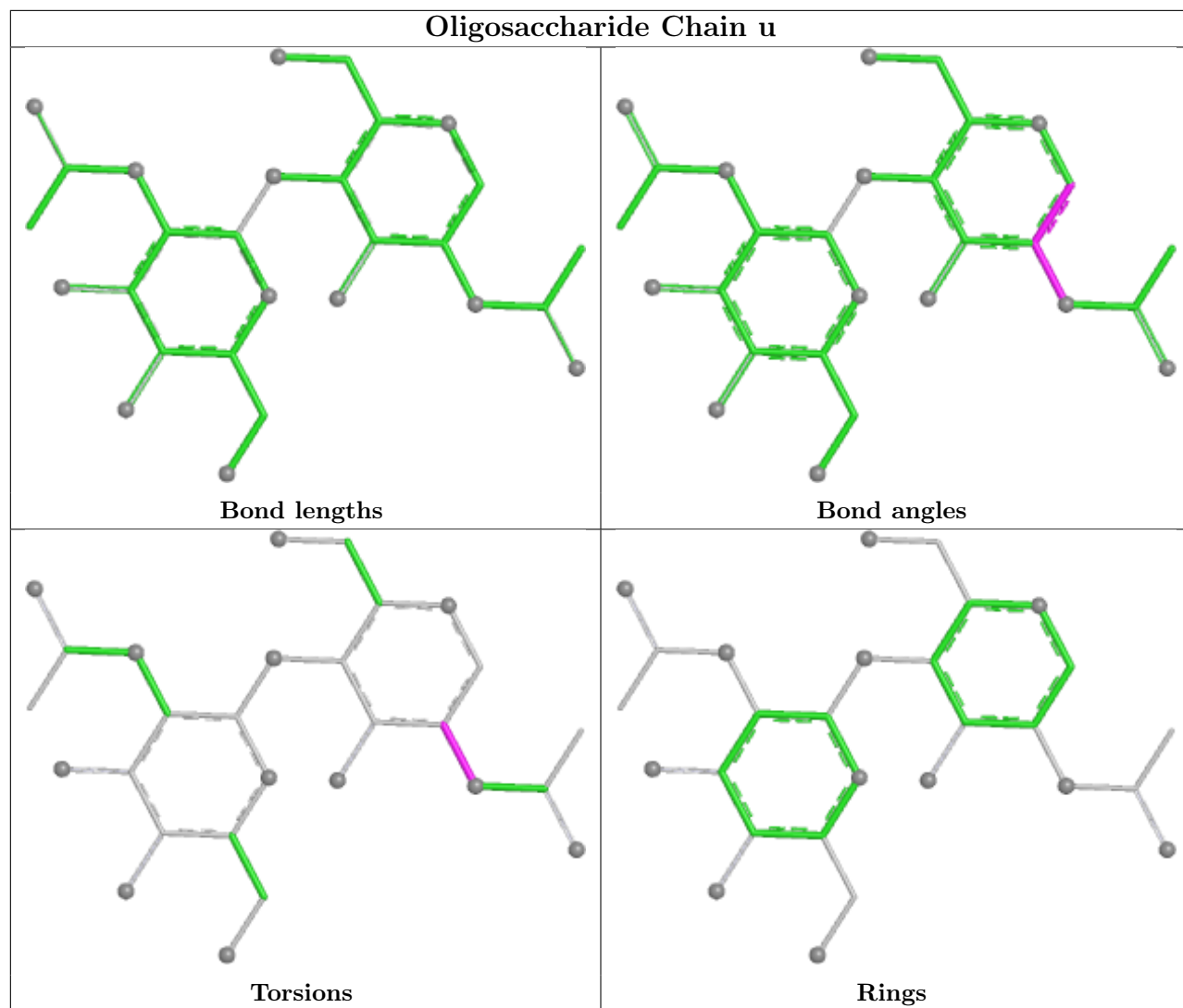


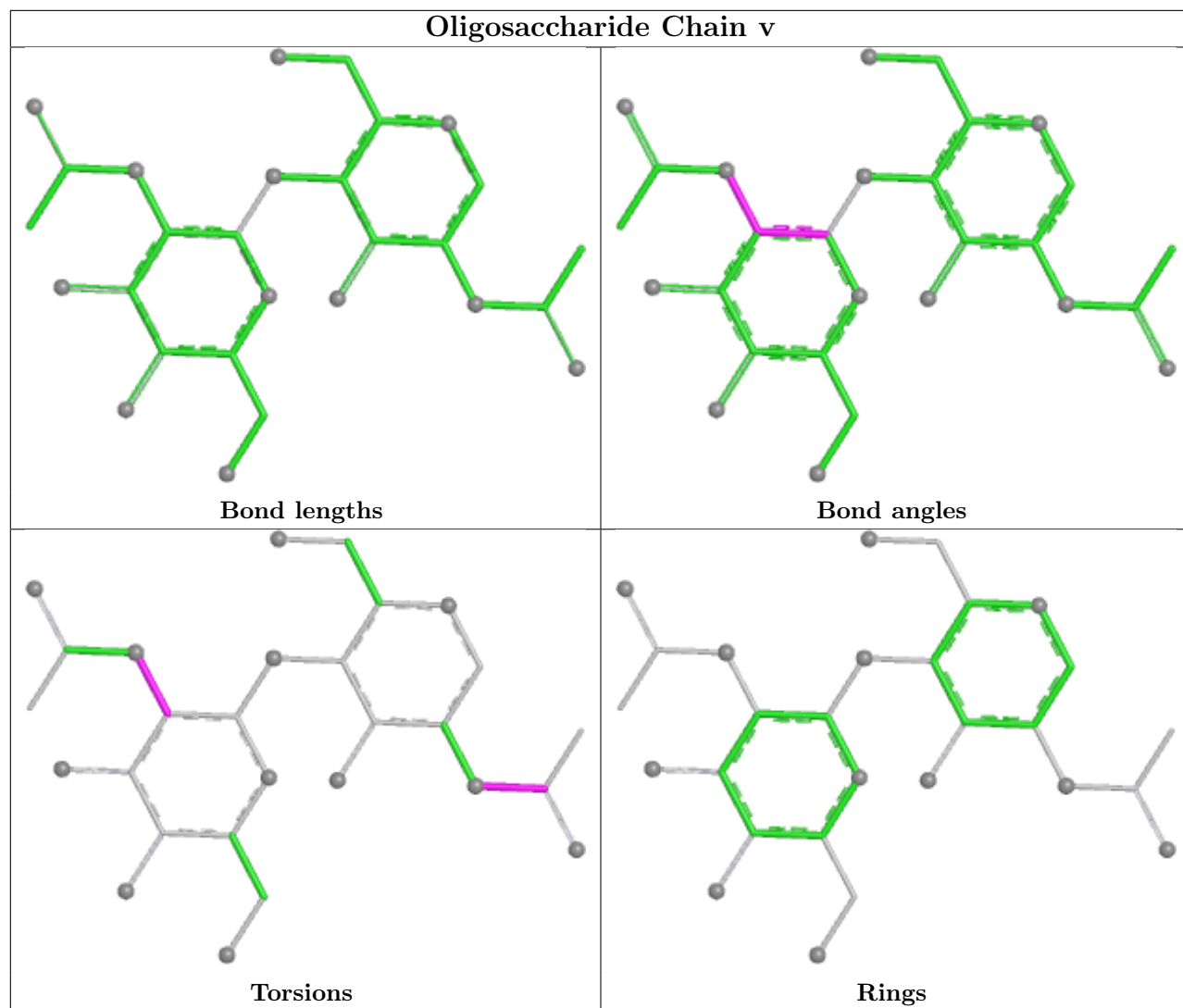


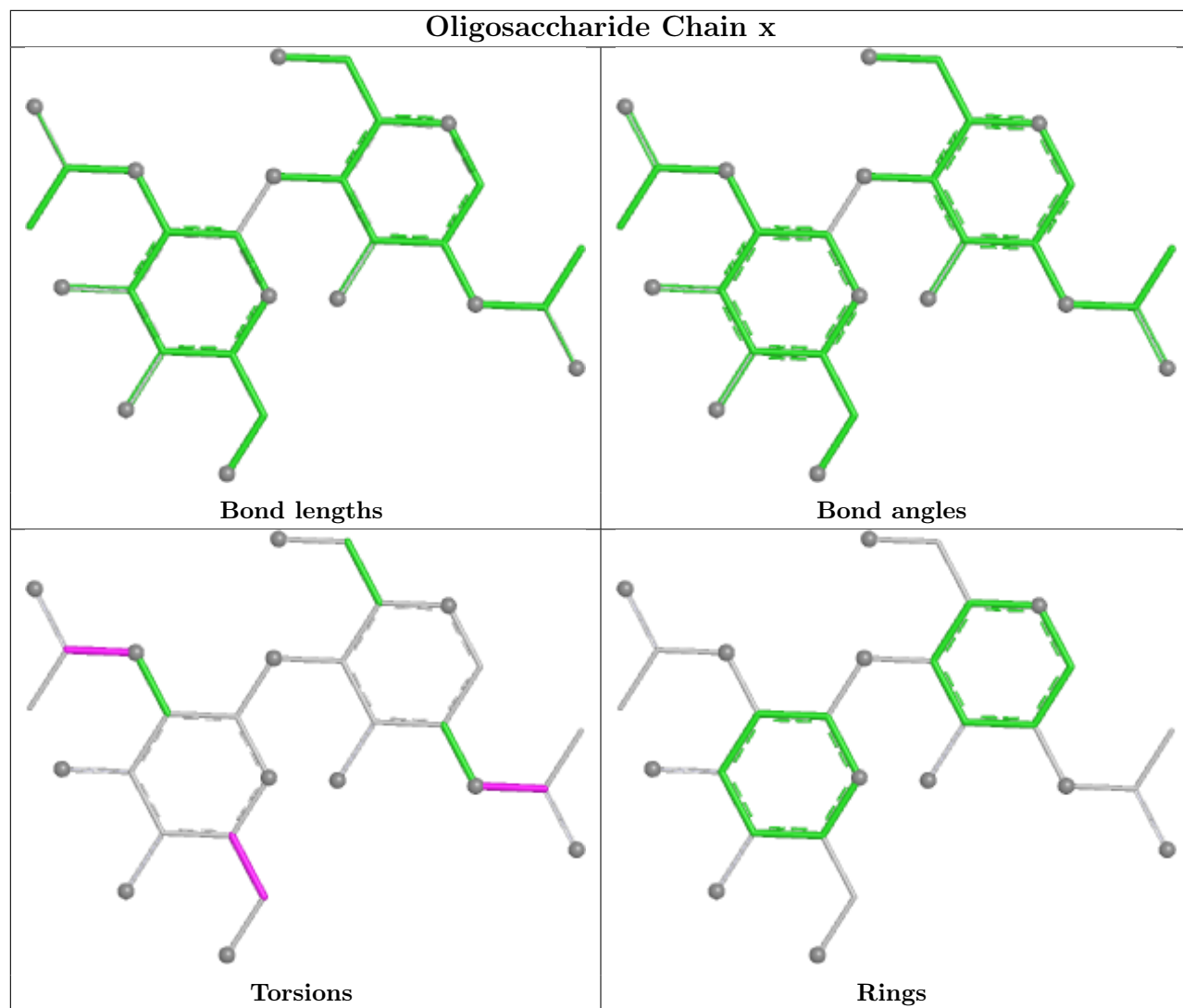


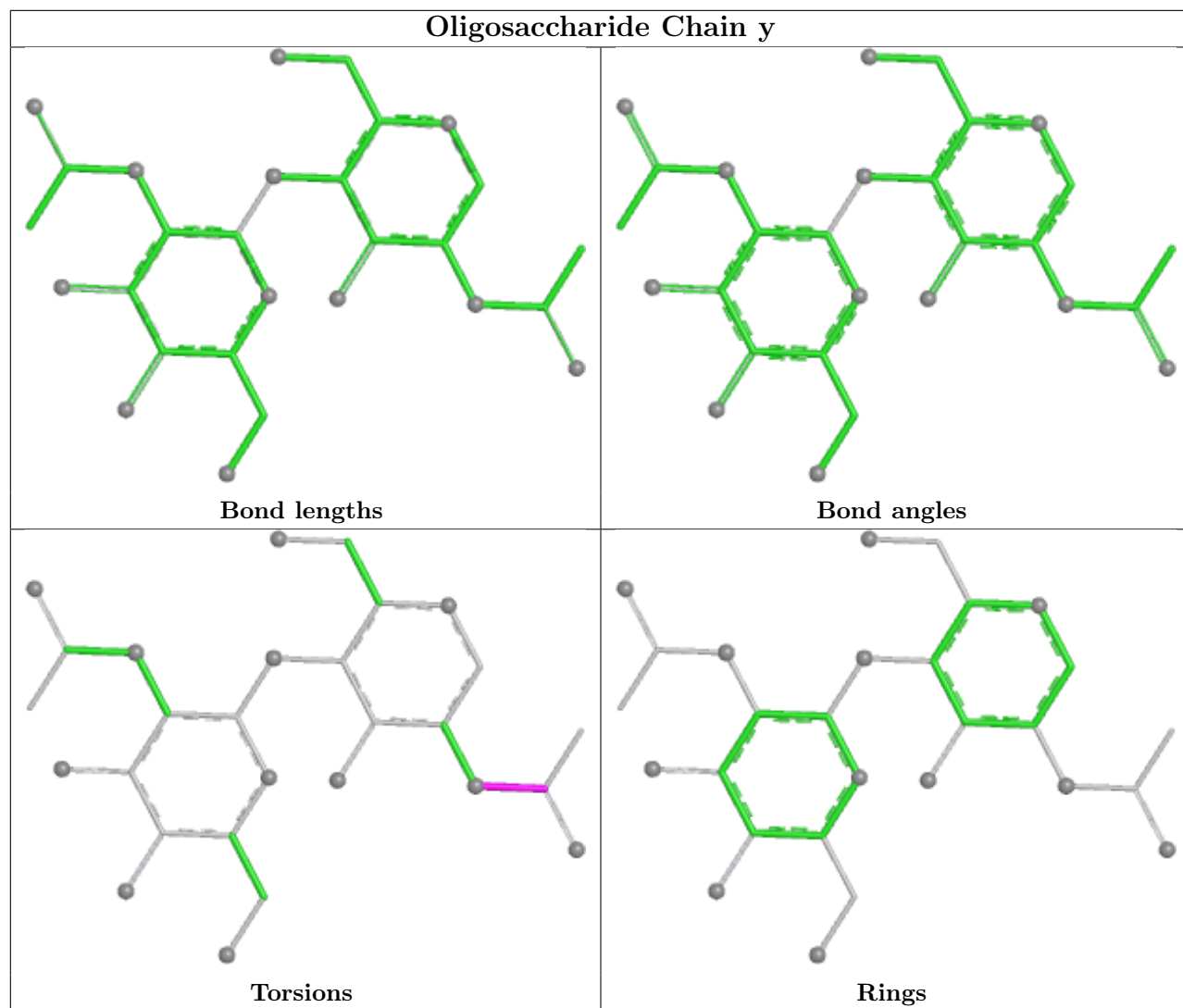


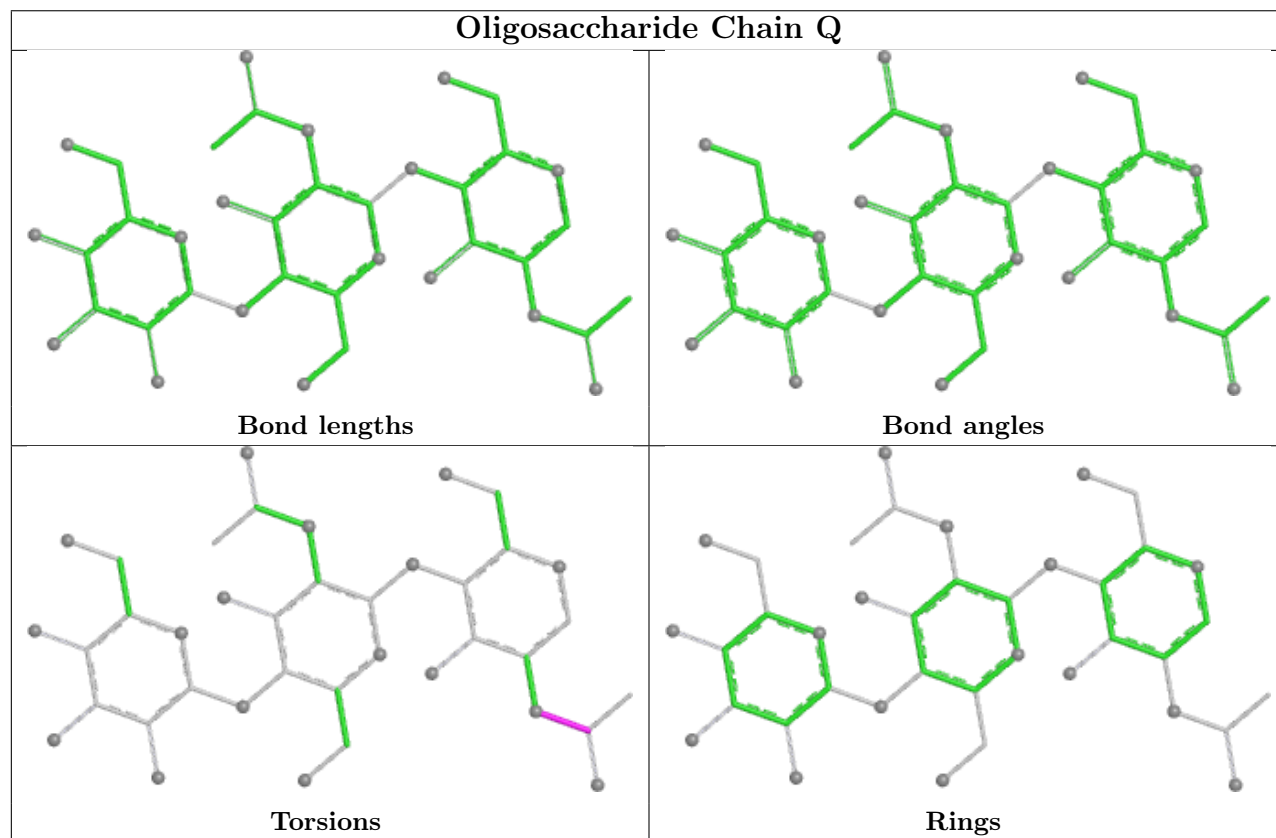
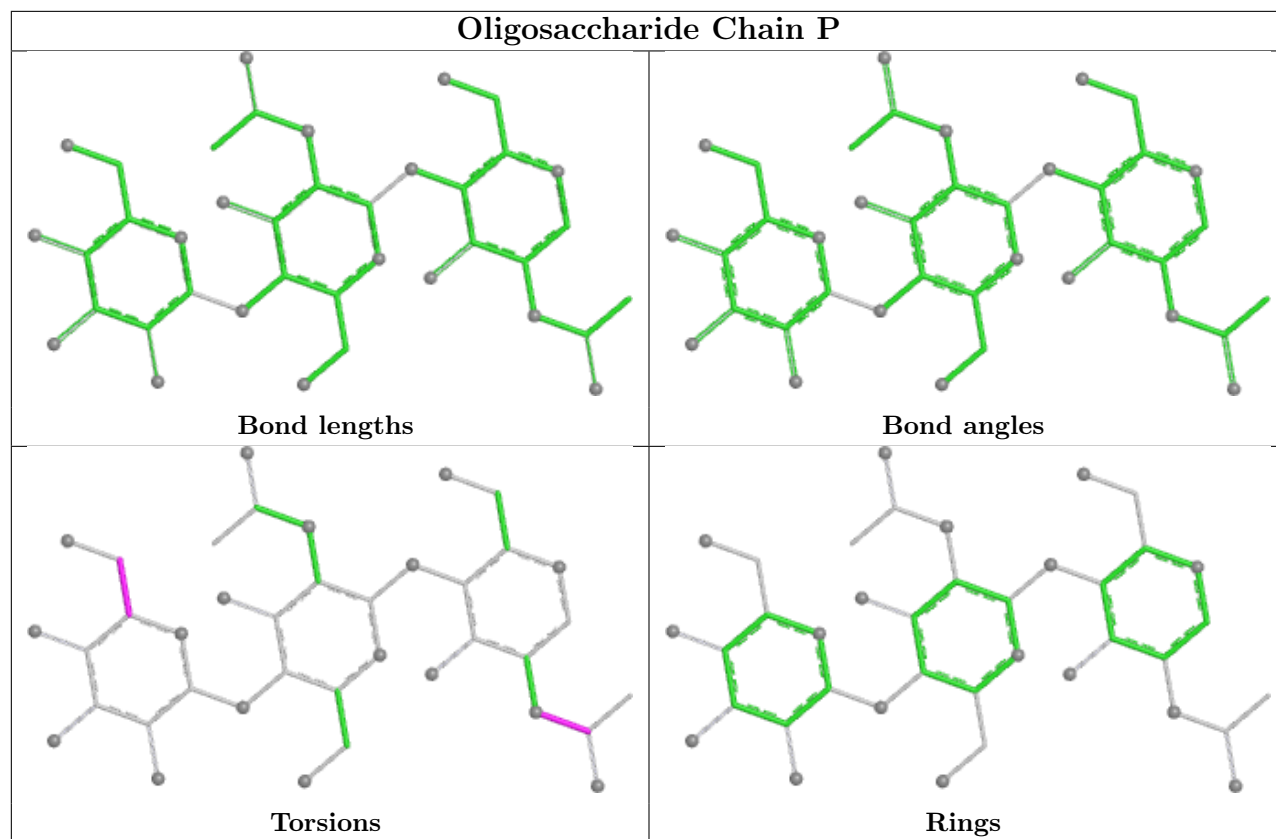


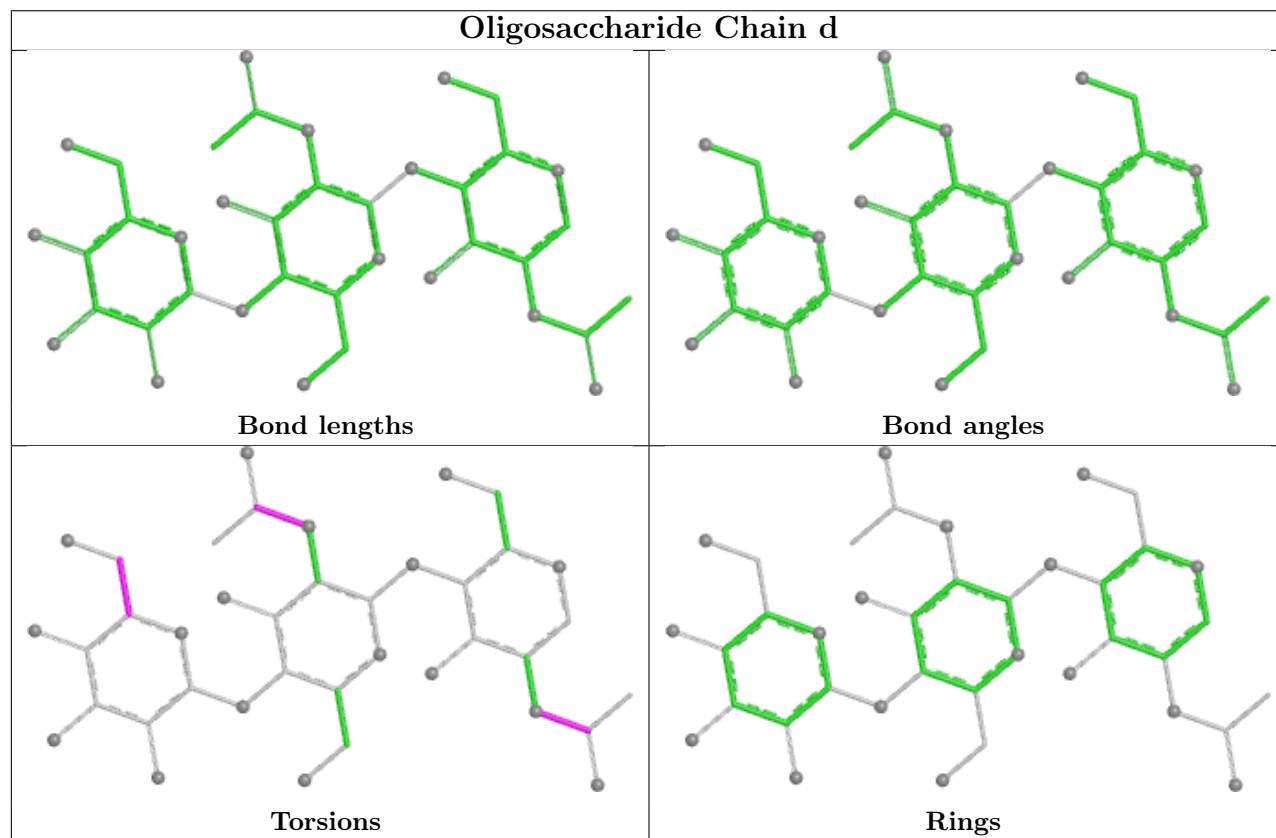
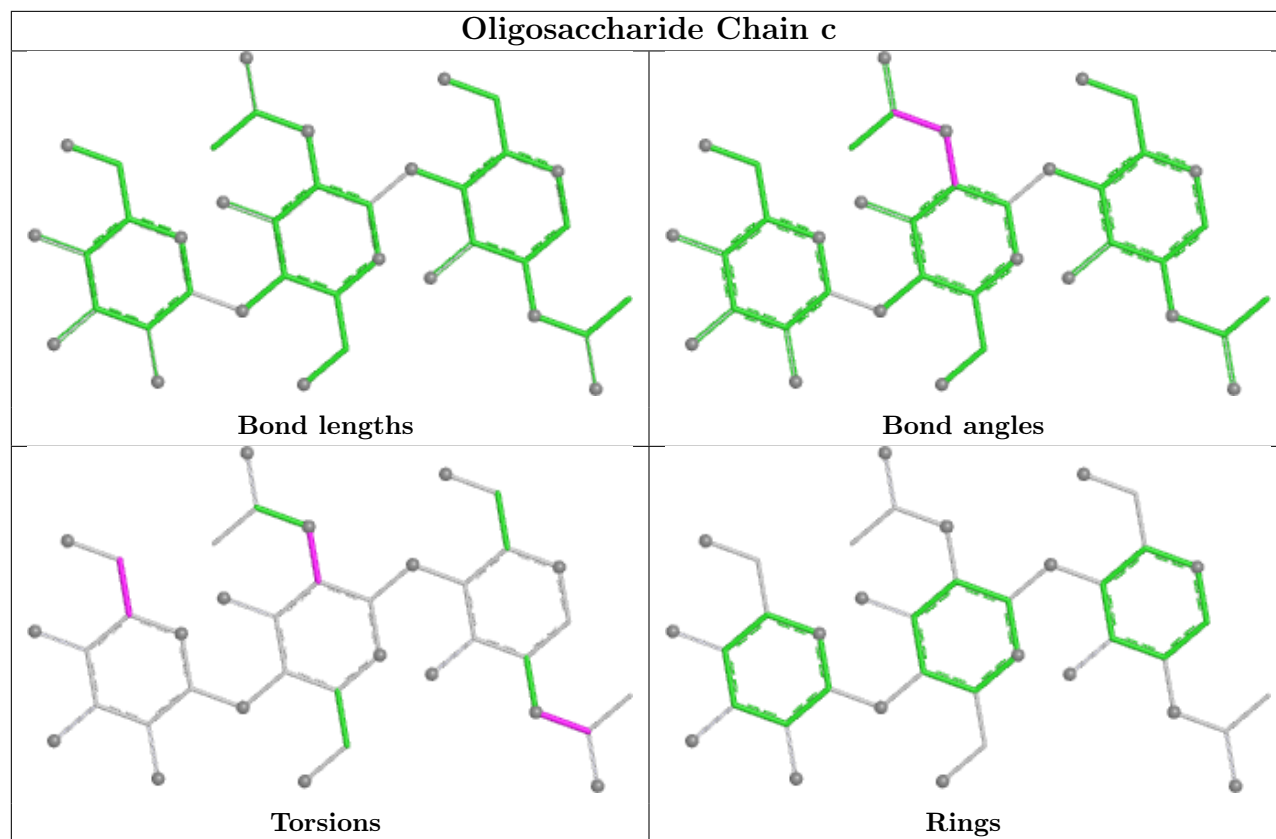


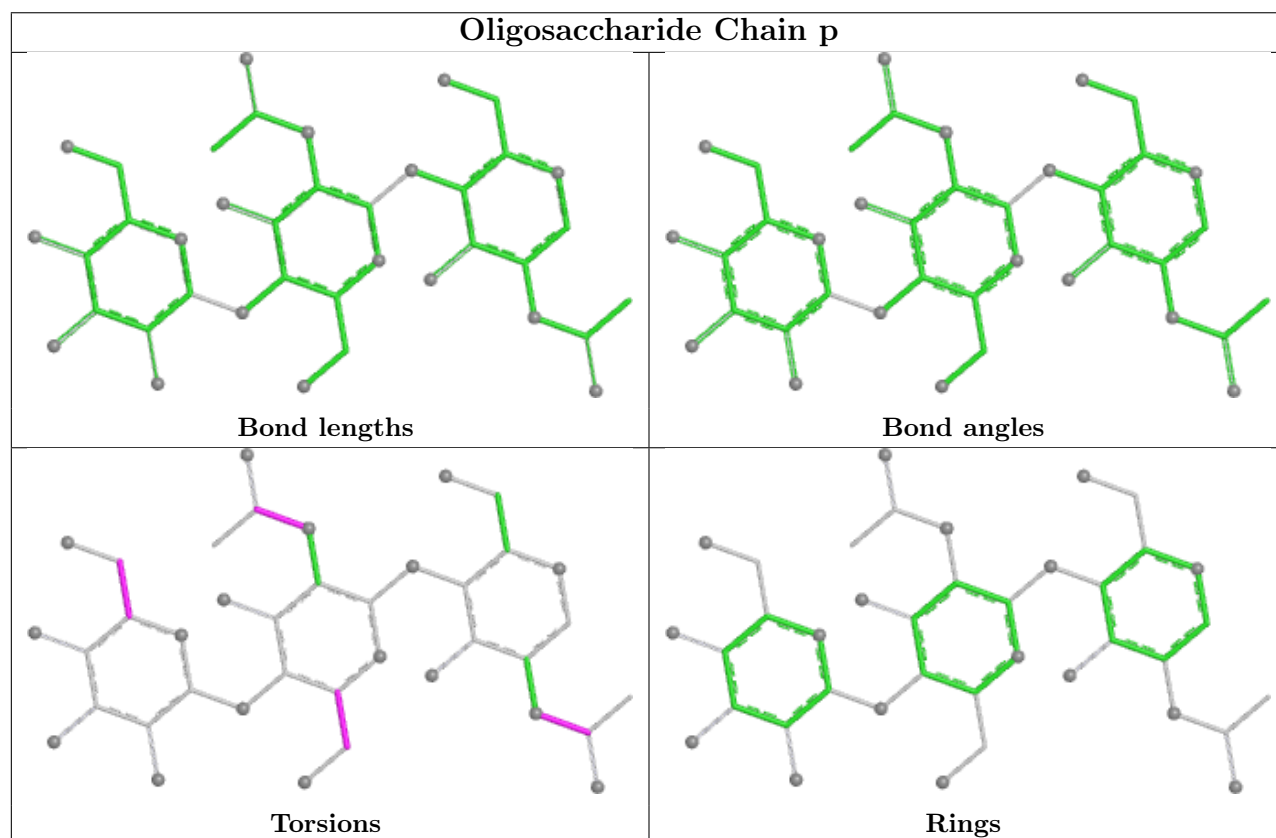
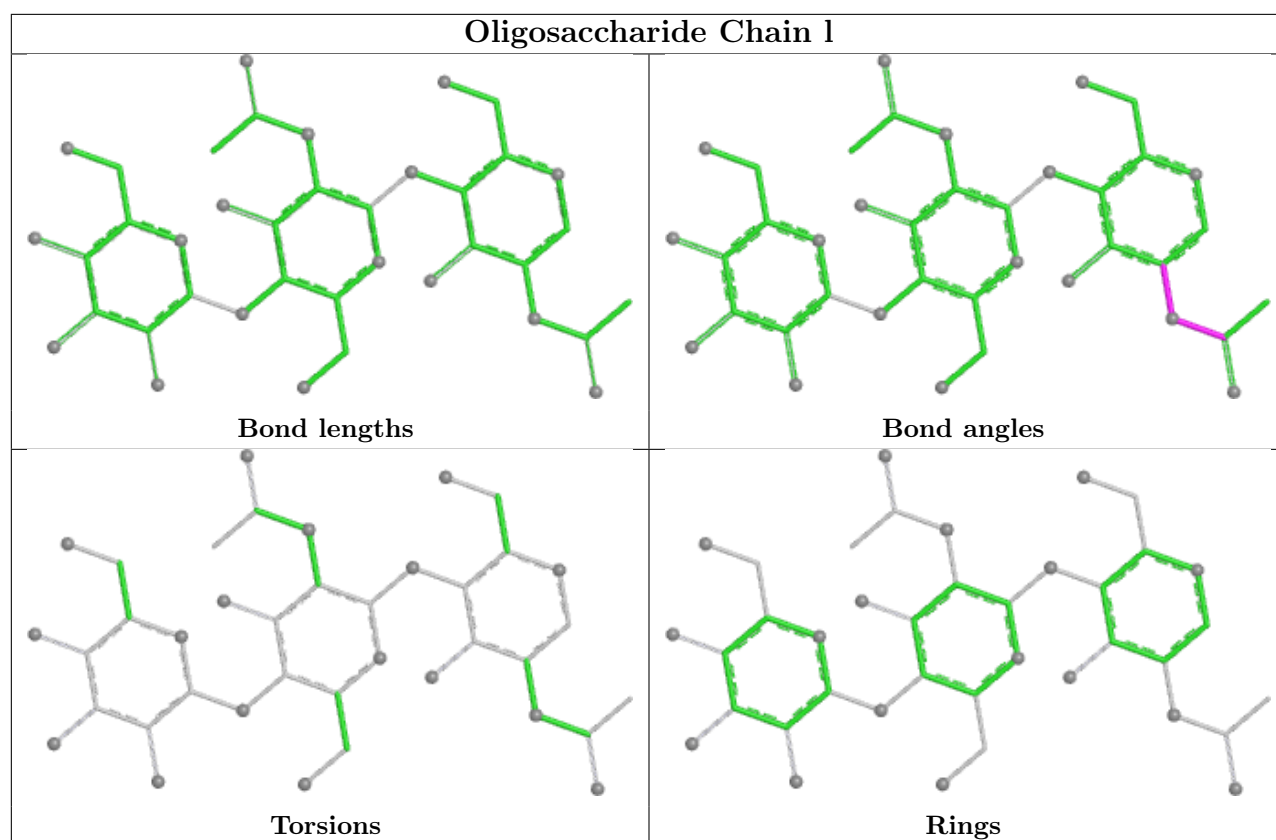


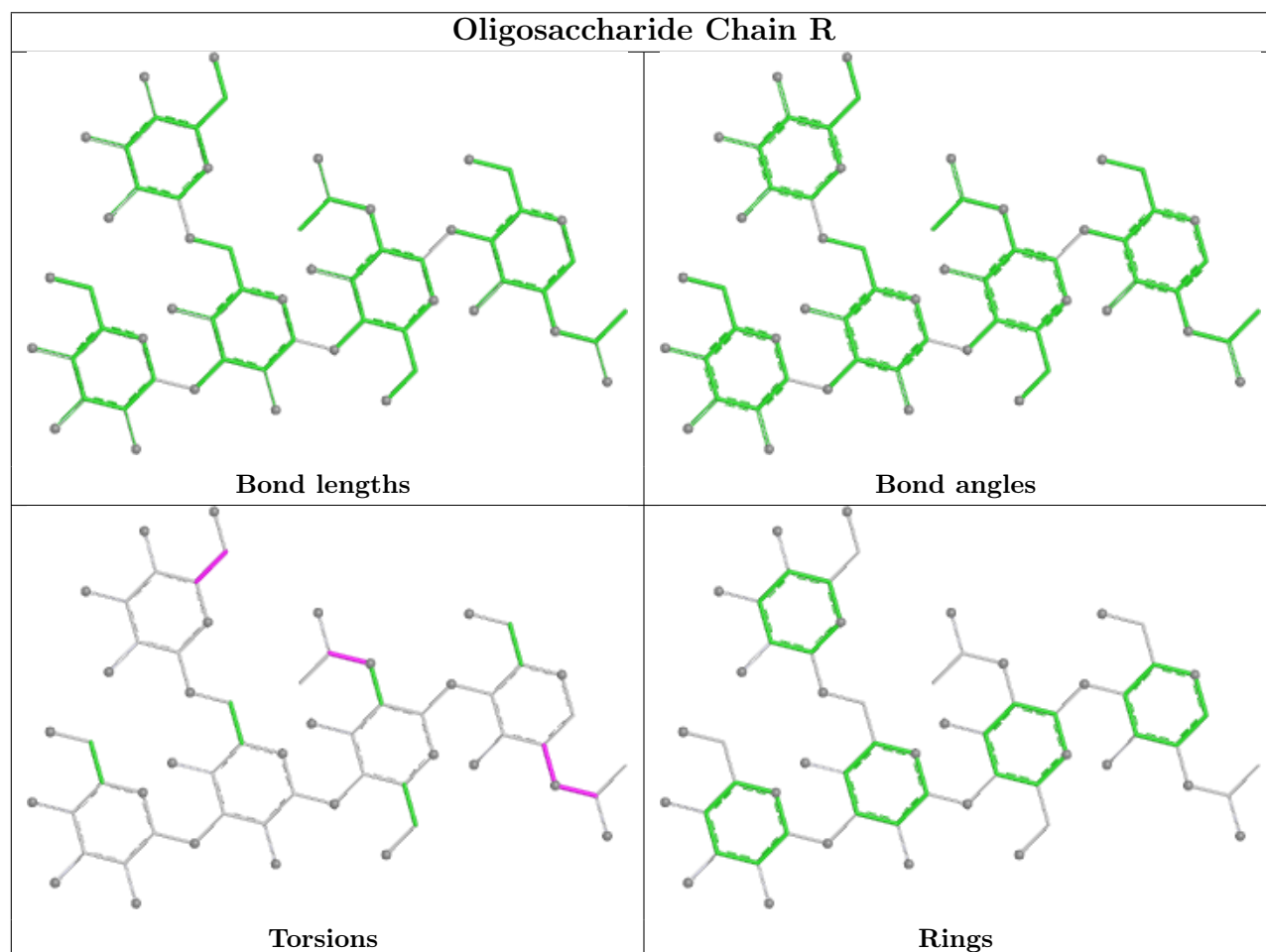
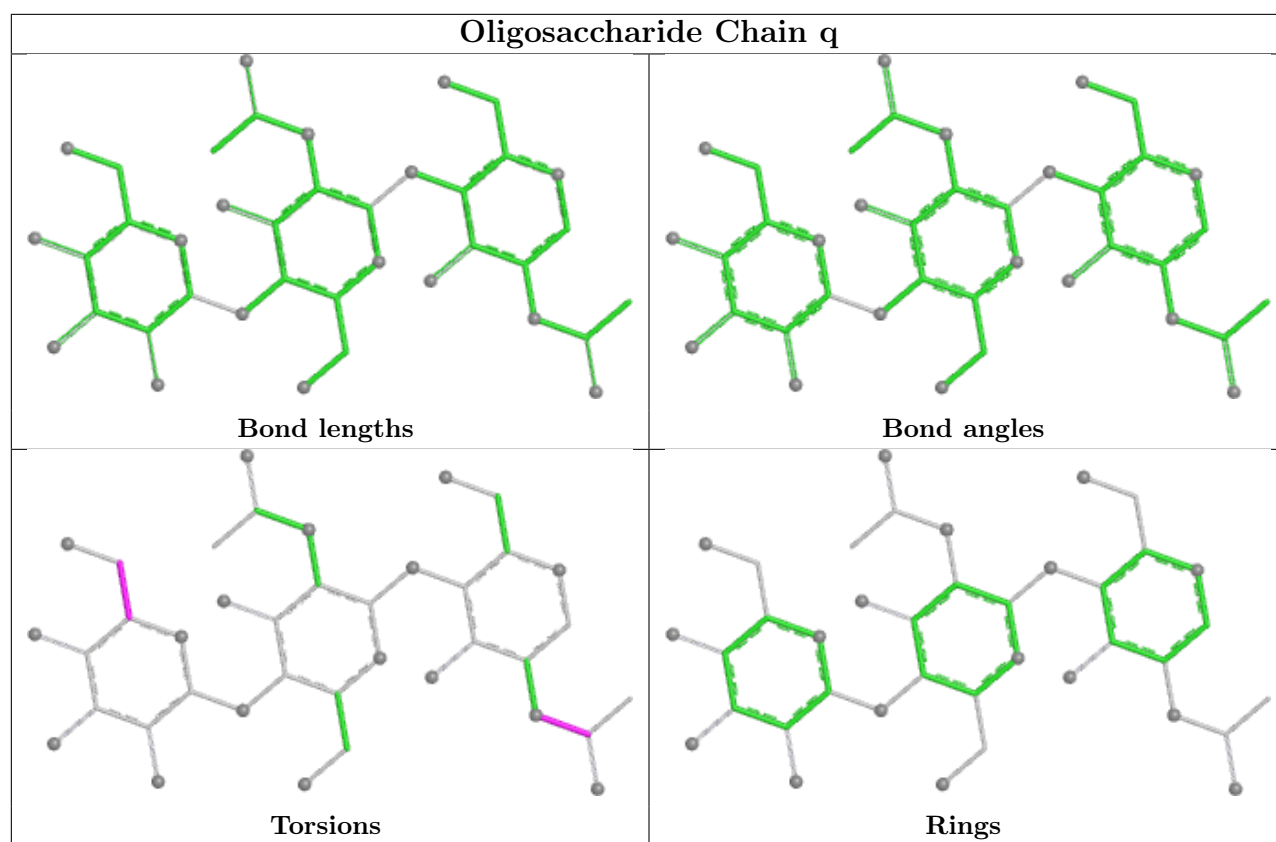


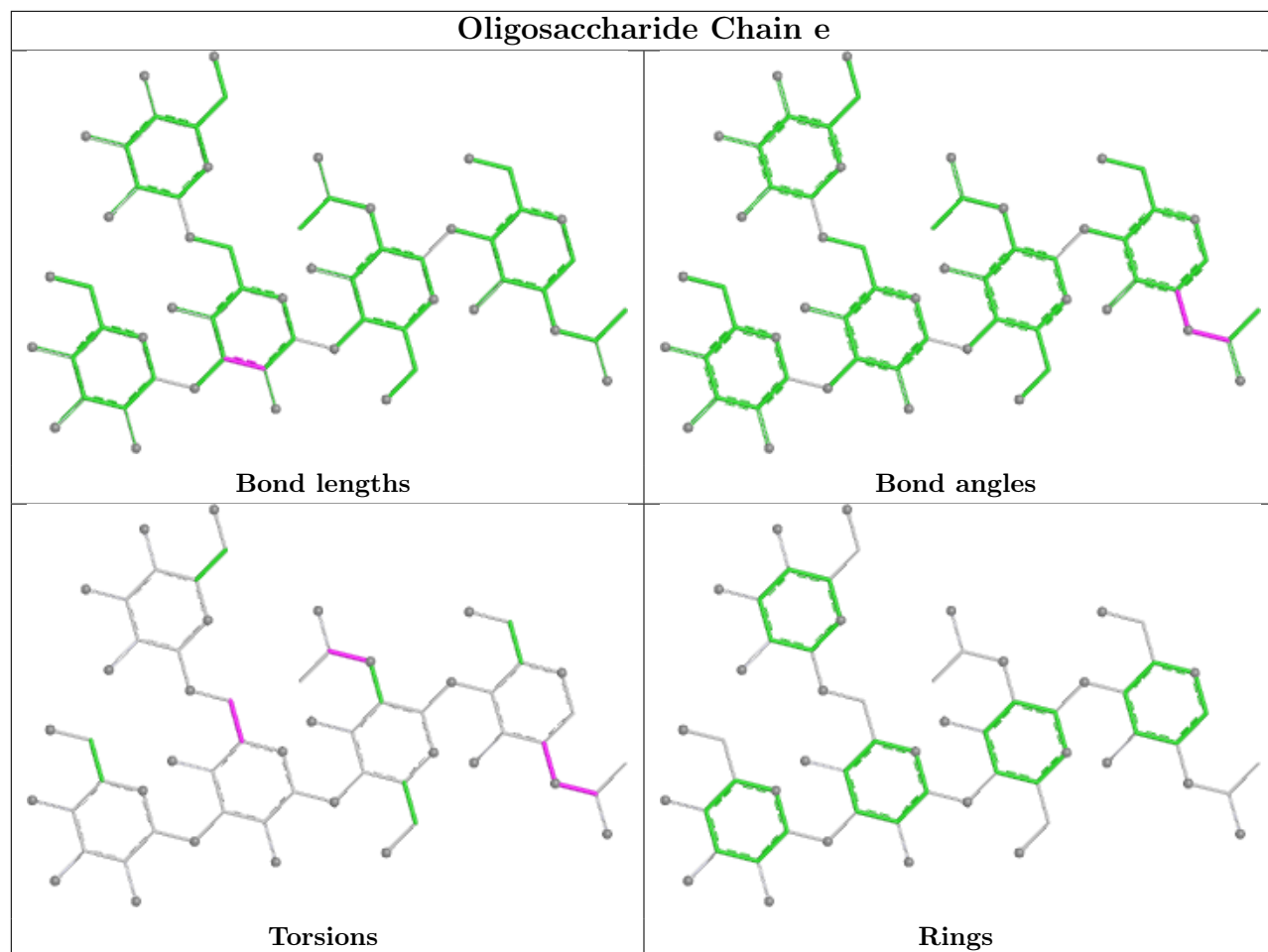


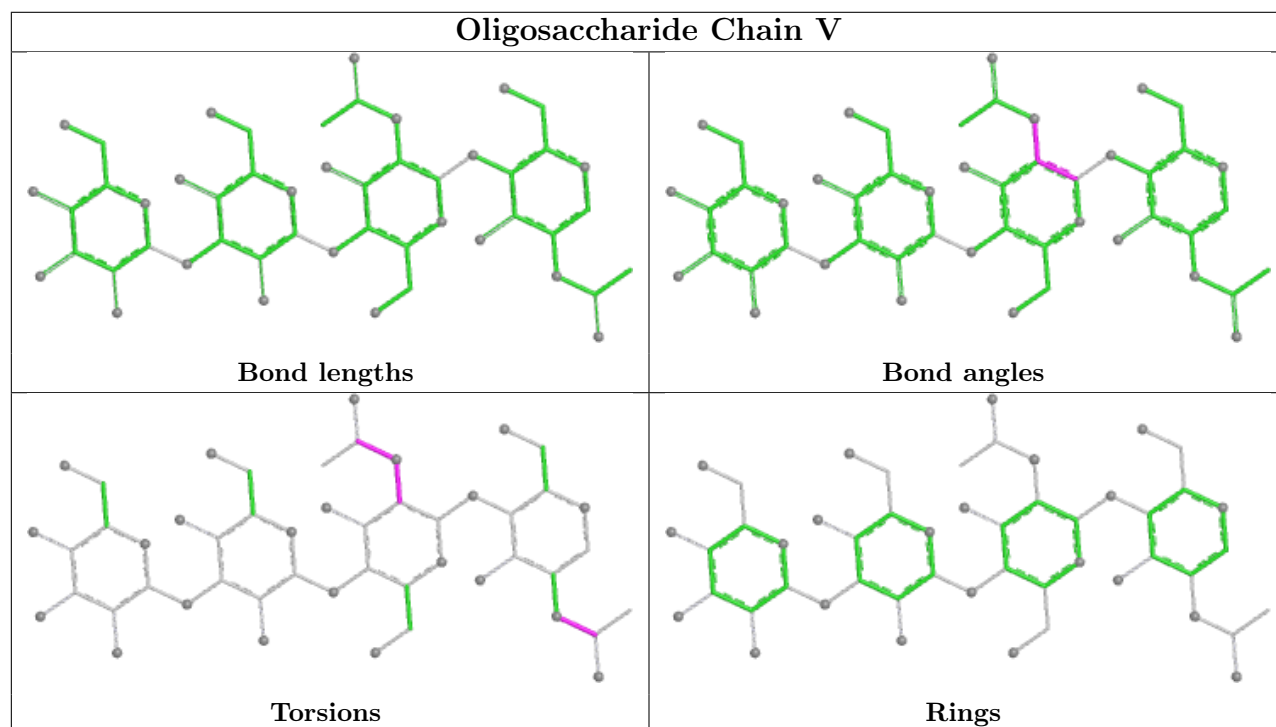
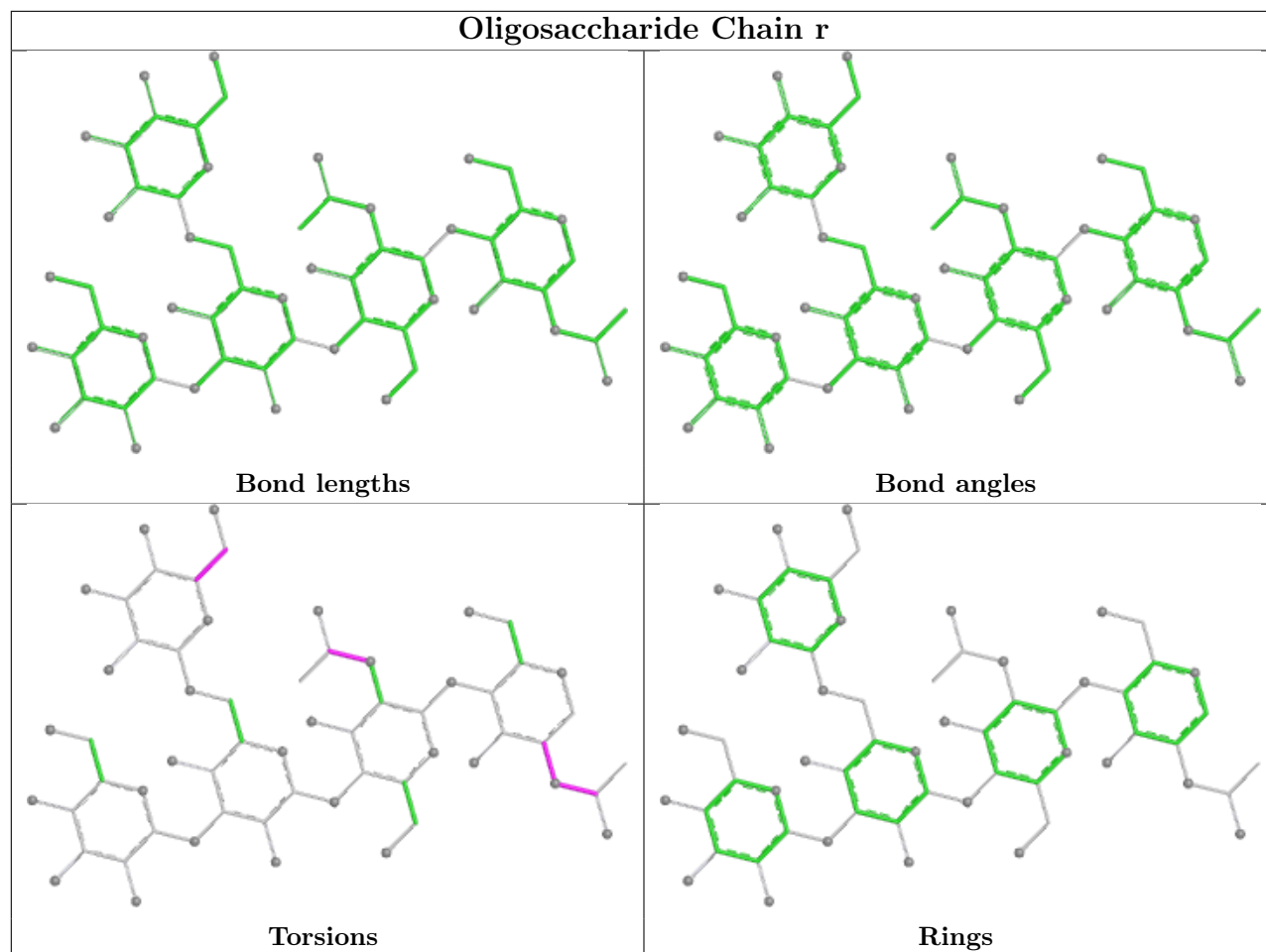


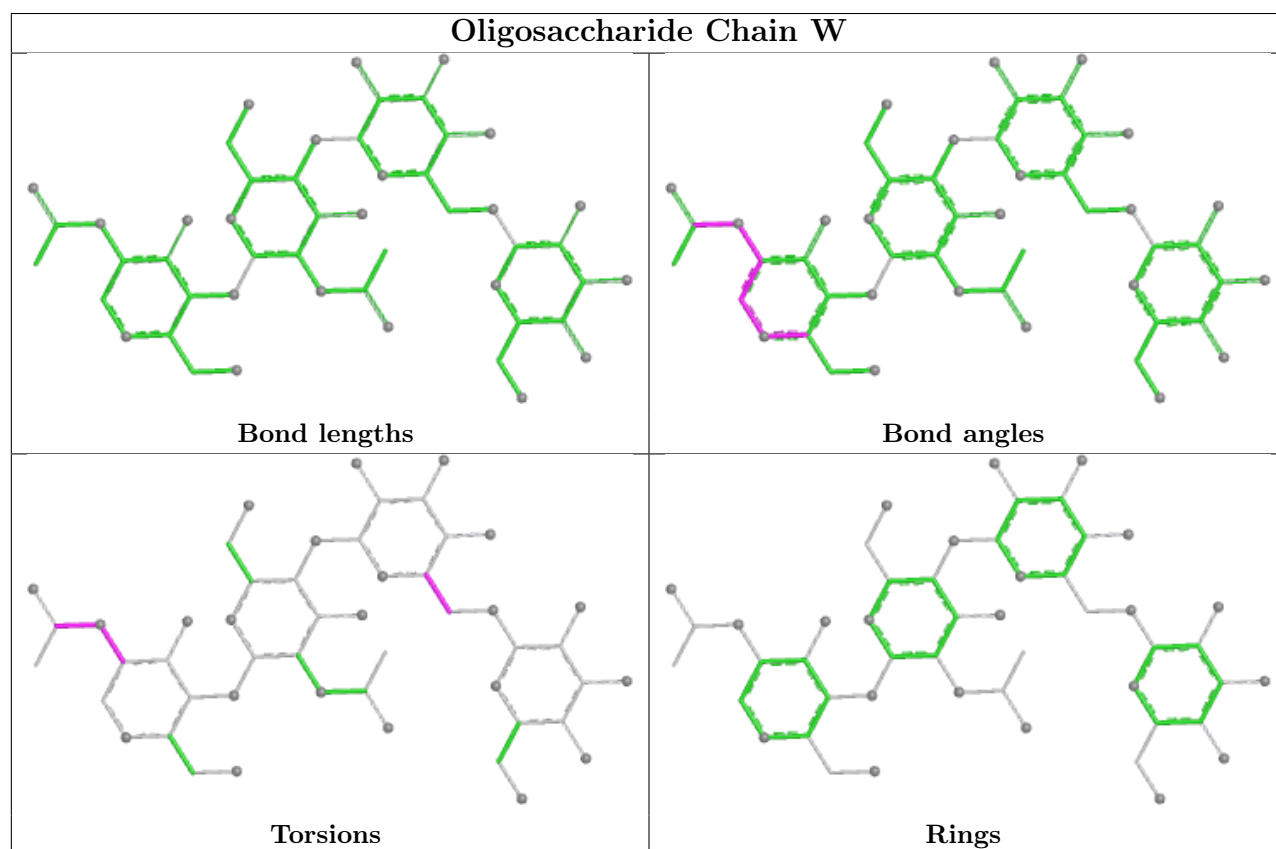
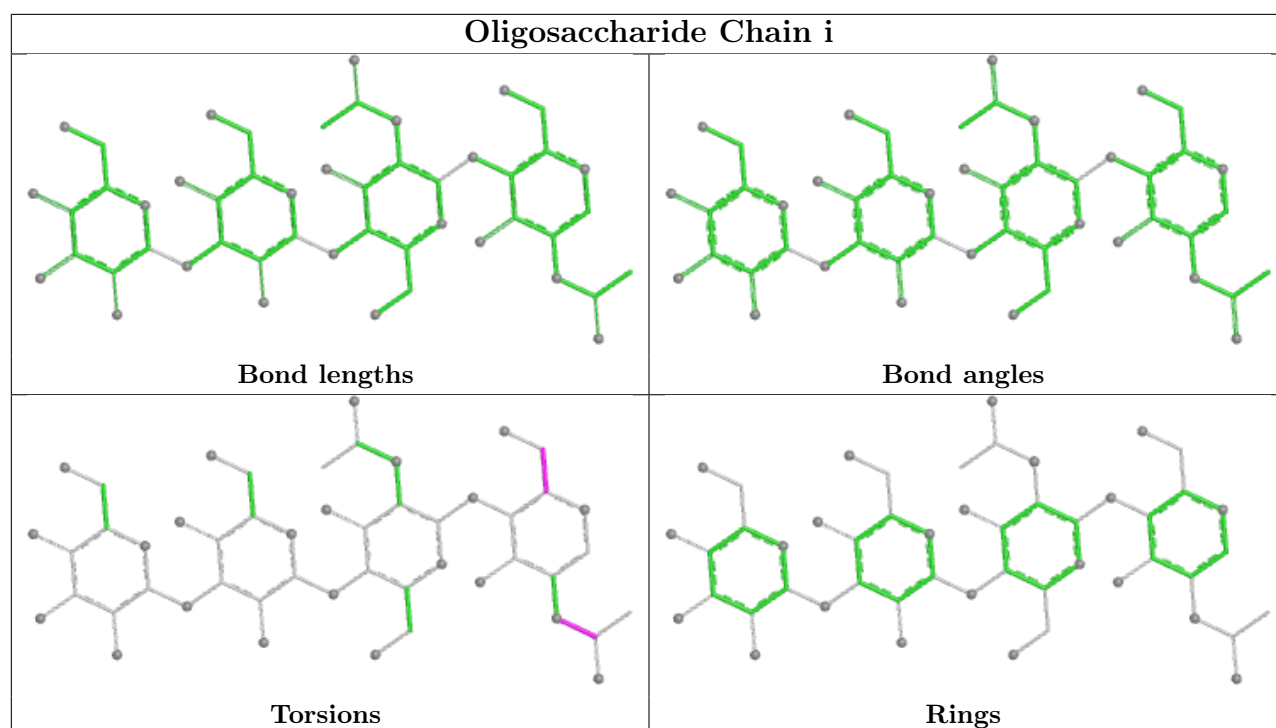


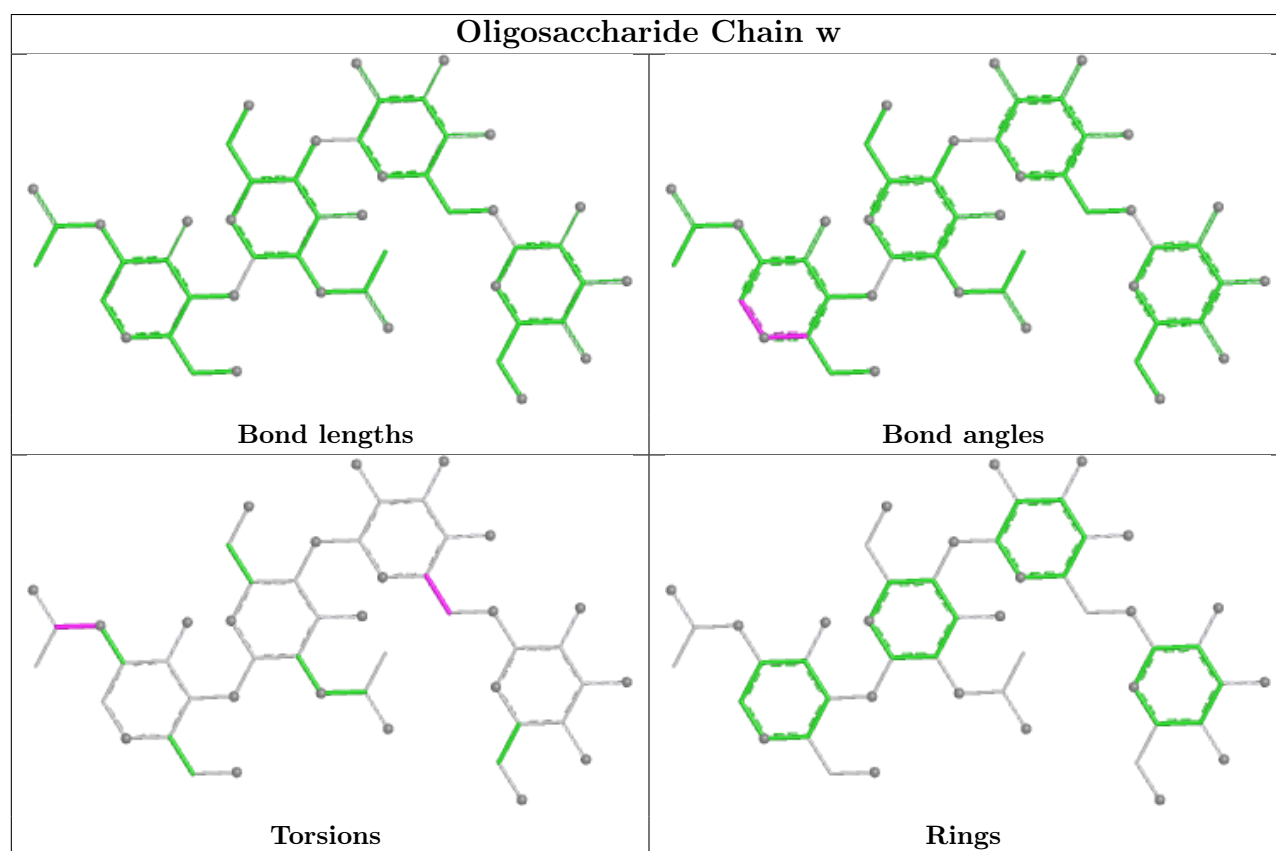
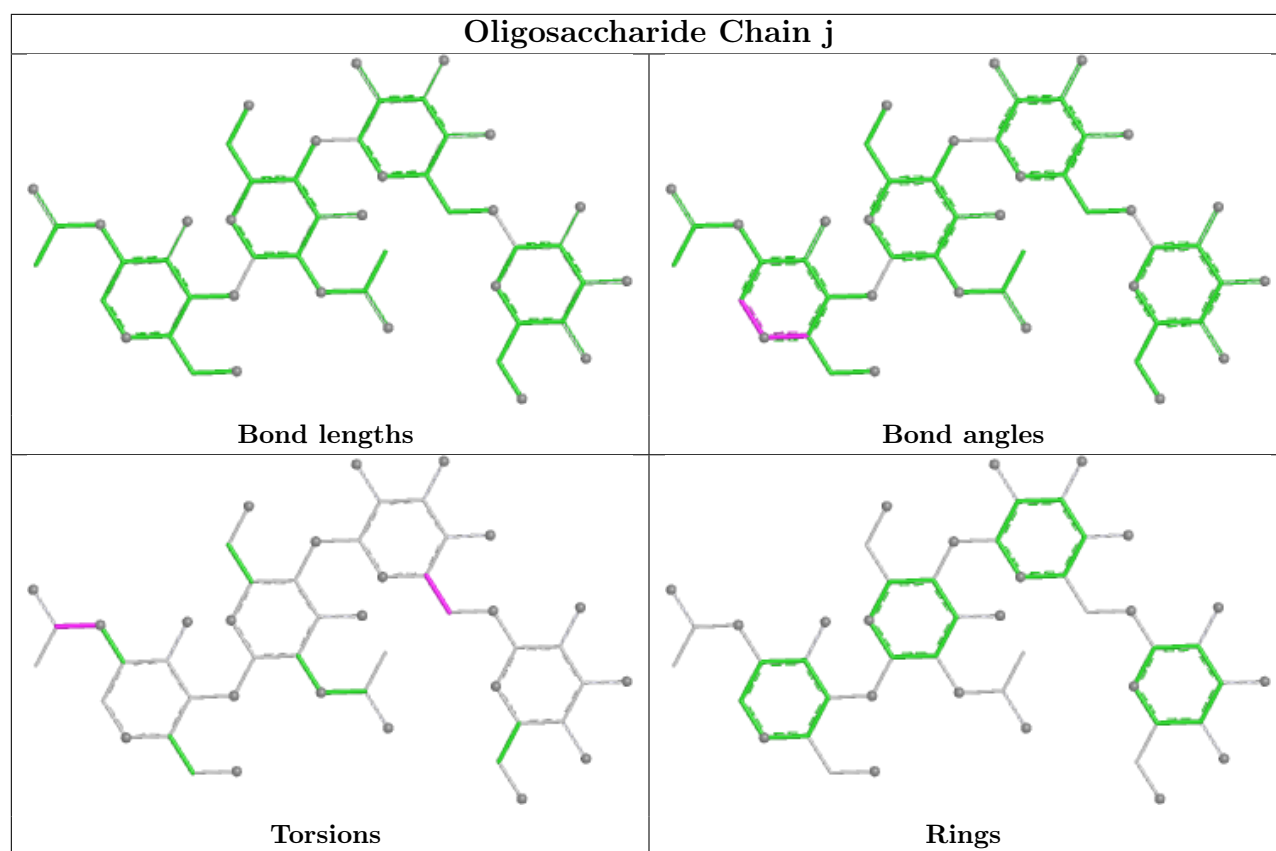












5.6 Ligand geometry

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	E	604	1	14,14,15	0.36	0	17,19,21	0.52	0
10	NAG	A	603	1	14,14,15	0.37	0	17,19,21	0.88	1 (5%)
10	NAG	E	602	1	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
10	NAG	B	701	2	14,14,15	0.39	0	17,19,21	1.15	2 (11%)
10	NAG	A	601	1	14,14,15	0.38	0	17,19,21	0.49	0
10	NAG	C	603	1	14,14,15	0.37	0	17,19,21	1.00	1 (5%)
10	NAG	E	603	1	14,14,15	0.37	0	17,19,21	1.03	1 (5%)
10	NAG	C	604	1	14,14,15	0.37	0	17,19,21	0.52	0
10	NAG	C	602	1	14,14,15	0.40	0	17,19,21	0.82	1 (5%)
10	NAG	F	701	2	14,14,15	0.39	0	17,19,21	1.31	2 (11%)
10	NAG	C	601	1	14,14,15	0.38	0	17,19,21	1.01	2 (11%)
10	NAG	E	601	1	14,14,15	0.36	0	17,19,21	0.55	0
10	NAG	D	701	2	14,14,15	0.40	0	17,19,21	0.63	0
10	NAG	A	602	1	14,14,15	0.39	0	17,19,21	0.92	1 (5%)
10	NAG	A	604	1	14,14,15	0.40	0	17,19,21	0.82	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	E	604	1	-	2/6/23/26	0/1/1/1
10	NAG	A	603	1	-	3/6/23/26	0/1/1/1
10	NAG	E	602	1	-	4/6/23/26	0/1/1/1
10	NAG	B	701	2	-	5/6/23/26	0/1/1/1
10	NAG	A	601	1	-	3/6/23/26	0/1/1/1
10	NAG	C	603	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	E	603	1	-	3/6/23/26	0/1/1/1
10	NAG	C	604	1	-	2/6/23/26	0/1/1/1
10	NAG	C	602	1	-	4/6/23/26	0/1/1/1
10	NAG	F	701	2	-	4/6/23/26	0/1/1/1
10	NAG	C	601	1	-	4/6/23/26	0/1/1/1
10	NAG	E	601	1	-	1/6/23/26	0/1/1/1
10	NAG	D	701	2	-	0/6/23/26	0/1/1/1
10	NAG	A	602	1	-	4/6/23/26	0/1/1/1
10	NAG	A	604	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	603	NAG	C2-N2-C7	3.84	128.04	122.90
10	C	603	NAG	C2-N2-C7	3.71	127.87	122.90
10	F	701	NAG	C2-N2-C7	3.68	127.84	122.90
10	F	701	NAG	C1-C2-N2	3.36	115.73	110.43
10	B	701	NAG	C2-N2-C7	3.25	127.26	122.90
10	A	603	NAG	C2-N2-C7	3.15	127.12	122.90
10	B	701	NAG	C1-C2-N2	2.87	114.96	110.43
10	C	601	NAG	C1-C2-N2	2.75	114.77	110.43
10	A	602	NAG	C1-C2-N2	2.74	114.76	110.43
10	C	601	NAG	C2-N2-C7	2.37	126.08	122.90
10	C	602	NAG	C1-C2-N2	2.24	113.96	110.43
10	E	602	NAG	C1-C2-N2	2.19	113.88	110.43
10	A	604	NAG	C1-C2-N2	2.16	113.83	110.43

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	603	NAG	C3-C2-N2-C7
10	A	603	NAG	C8-C7-N2-C2
10	A	603	NAG	O7-C7-N2-C2
10	A	604	NAG	C1-C2-N2-C7
10	A	604	NAG	C8-C7-N2-C2
10	A	604	NAG	O7-C7-N2-C2
10	B	701	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
10	C	602	NAG	C1-C2-N2-C7
10	C	603	NAG	C3-C2-N2-C7
10	C	603	NAG	O7-C7-N2-C2
10	E	602	NAG	C1-C2-N2-C7
10	E	603	NAG	C3-C2-N2-C7
10	E	603	NAG	O7-C7-N2-C2
10	F	701	NAG	C8-C7-N2-C2
10	F	701	NAG	O7-C7-N2-C2
10	C	603	NAG	C8-C7-N2-C2
10	E	603	NAG	C8-C7-N2-C2
10	C	604	NAG	C8-C7-N2-C2
10	C	604	NAG	O7-C7-N2-C2
10	E	604	NAG	C8-C7-N2-C2
10	E	604	NAG	O7-C7-N2-C2
10	C	602	NAG	C8-C7-N2-C2
10	E	602	NAG	C8-C7-N2-C2
10	C	602	NAG	O7-C7-N2-C2
10	A	602	NAG	C8-C7-N2-C2
10	B	701	NAG	O5-C5-C6-O6
10	A	601	NAG	O5-C5-C6-O6
10	E	601	NAG	O5-C5-C6-O6
10	E	602	NAG	O7-C7-N2-C2
10	A	604	NAG	O5-C5-C6-O6
10	A	602	NAG	C3-C2-N2-C7
10	B	701	NAG	C3-C2-N2-C7
10	C	601	NAG	C3-C2-N2-C7
10	C	602	NAG	C3-C2-N2-C7
10	E	602	NAG	C3-C2-N2-C7
10	F	701	NAG	C3-C2-N2-C7
10	A	602	NAG	O7-C7-N2-C2
10	A	602	NAG	C1-C2-N2-C7
10	C	601	NAG	C1-C2-N2-C7
10	F	701	NAG	C1-C2-N2-C7
10	C	601	NAG	C8-C7-N2-C2
10	B	701	NAG	C8-C7-N2-C2
10	C	601	NAG	O7-C7-N2-C2
10	B	701	NAG	O7-C7-N2-C2
10	A	601	NAG	C8-C7-N2-C2
10	A	604	NAG	C3-C2-N2-C7
10	A	601	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	602	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

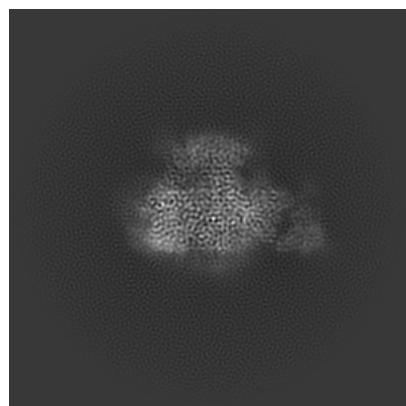
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42364. These allow visual inspection of the internal detail of the map and identification of artifacts.

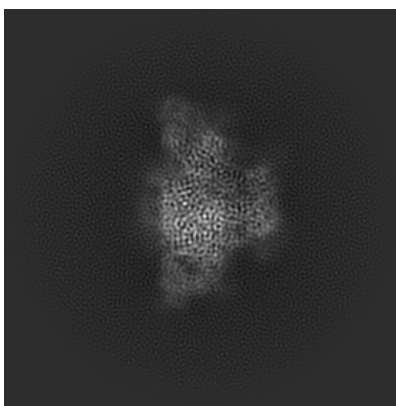
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

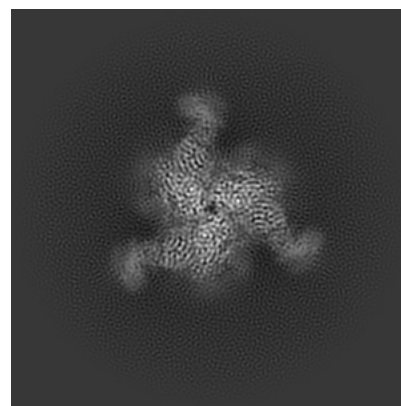
6.1.1 Primary map



X

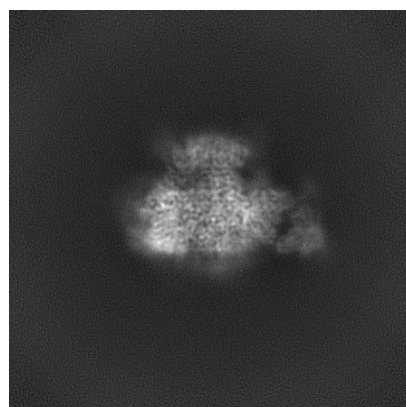


Y

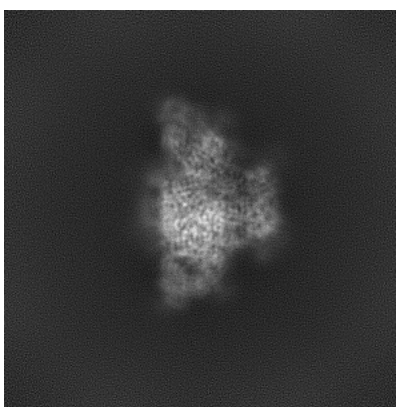


Z

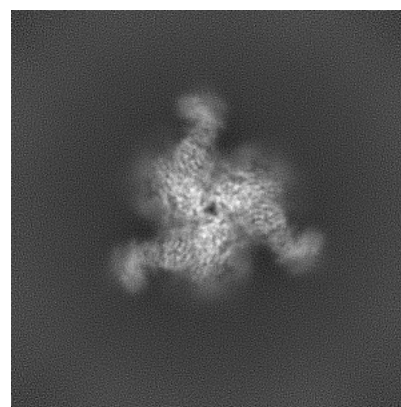
6.1.2 Raw map



X



Y

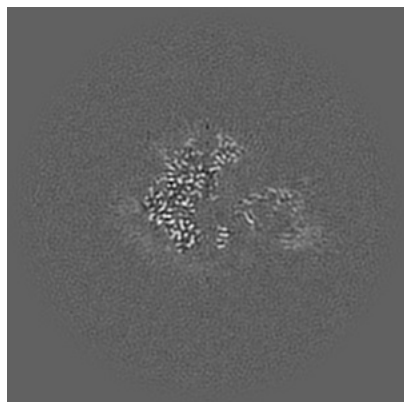


Z

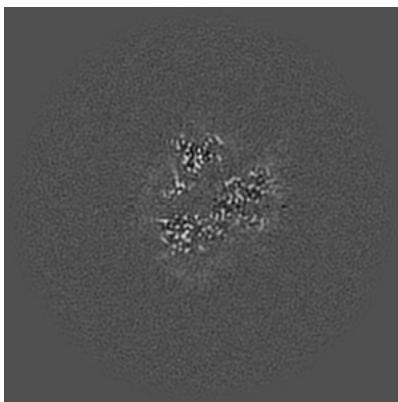
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

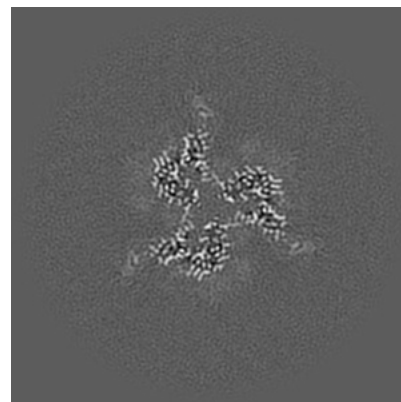
6.2.1 Primary map



X Index: 196

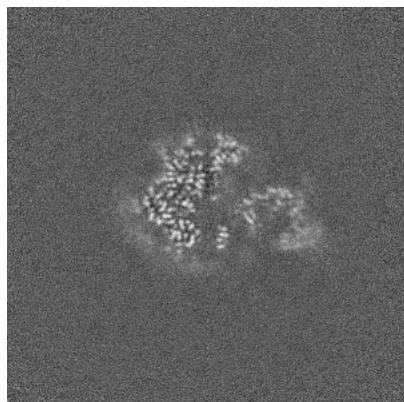


Y Index: 196

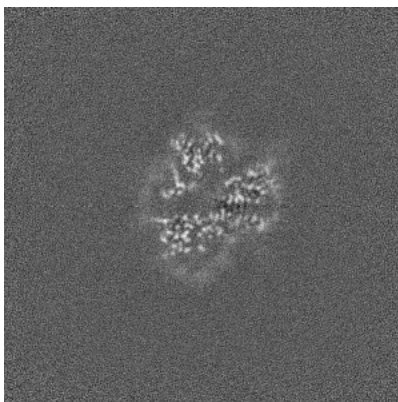


Z Index: 196

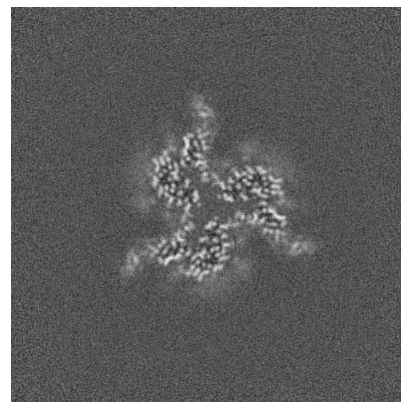
6.2.2 Raw map



X Index: 196



Y Index: 196

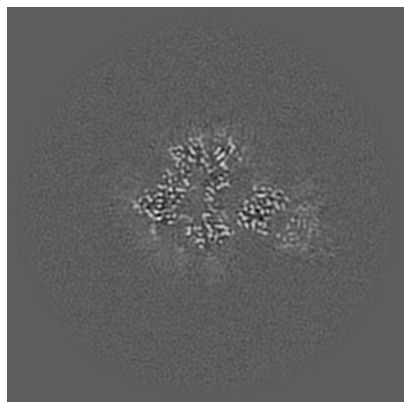


Z Index: 196

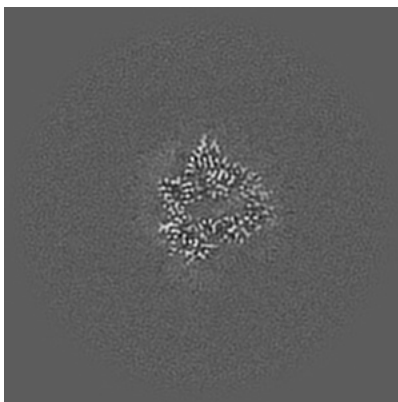
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

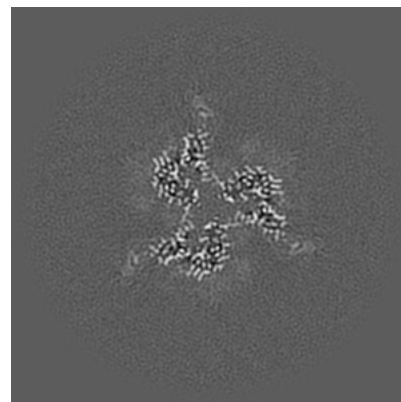
6.3.1 Primary map



X Index: 185

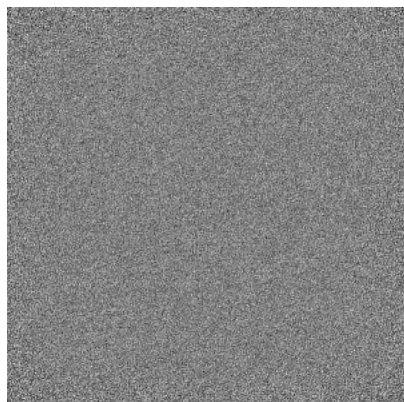


Y Index: 210

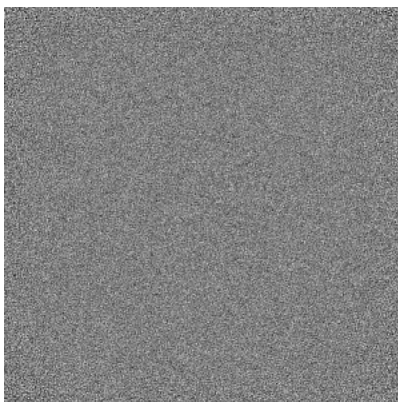


Z Index: 196

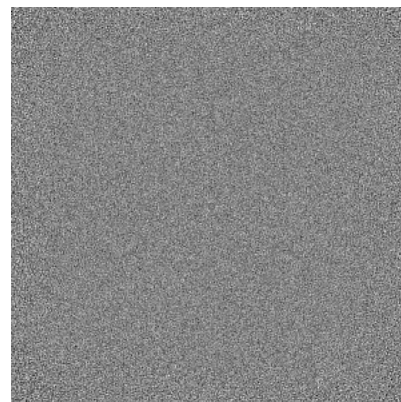
6.3.2 Raw map



X Index: 0



Y Index: 0

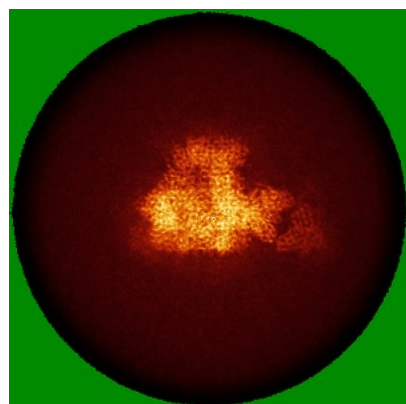


Z Index: 391

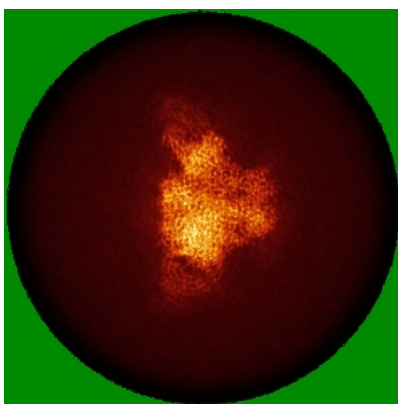
The images above show the largest variance slices of the map in three orthogonal directions.

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

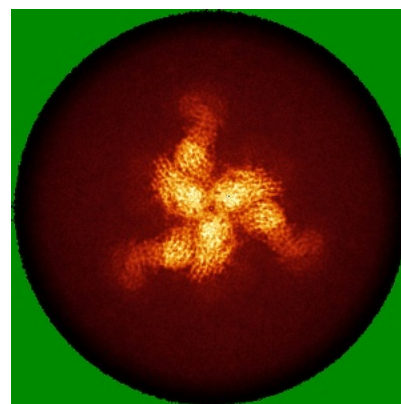
6.4.1 Primary map



X

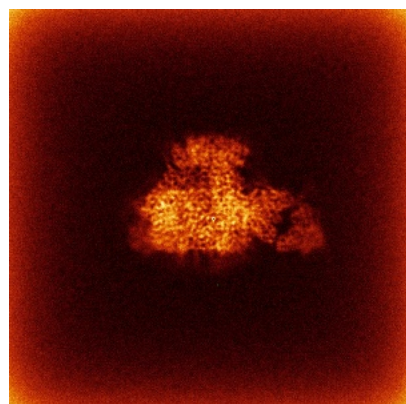


Y

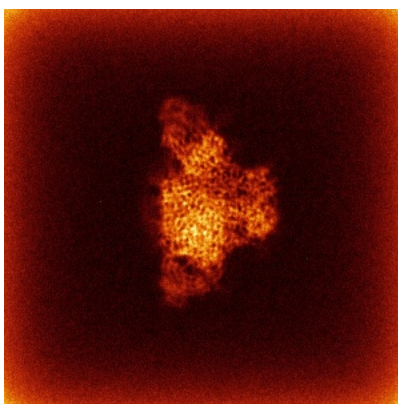


Z

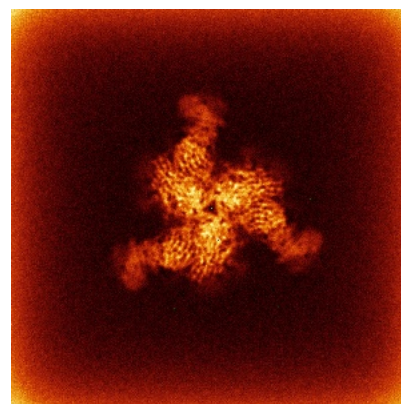
6.4.2 Raw map



X



Y

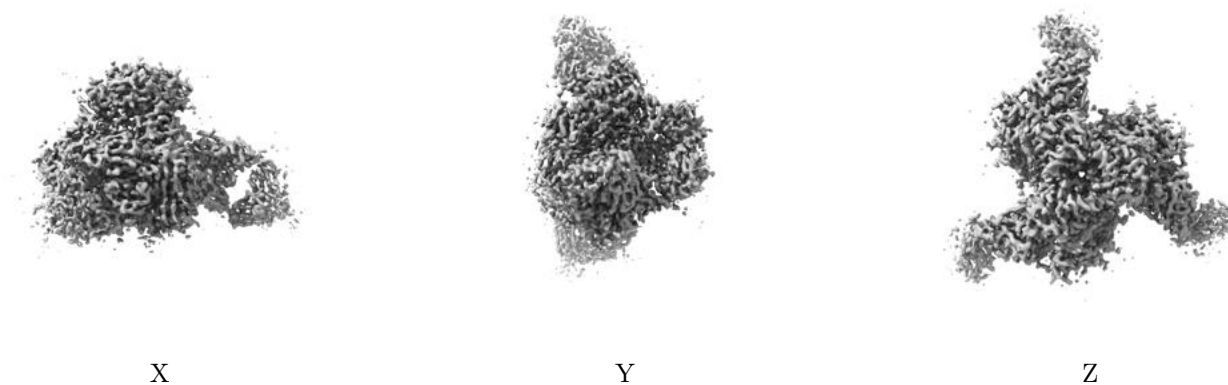


Z

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

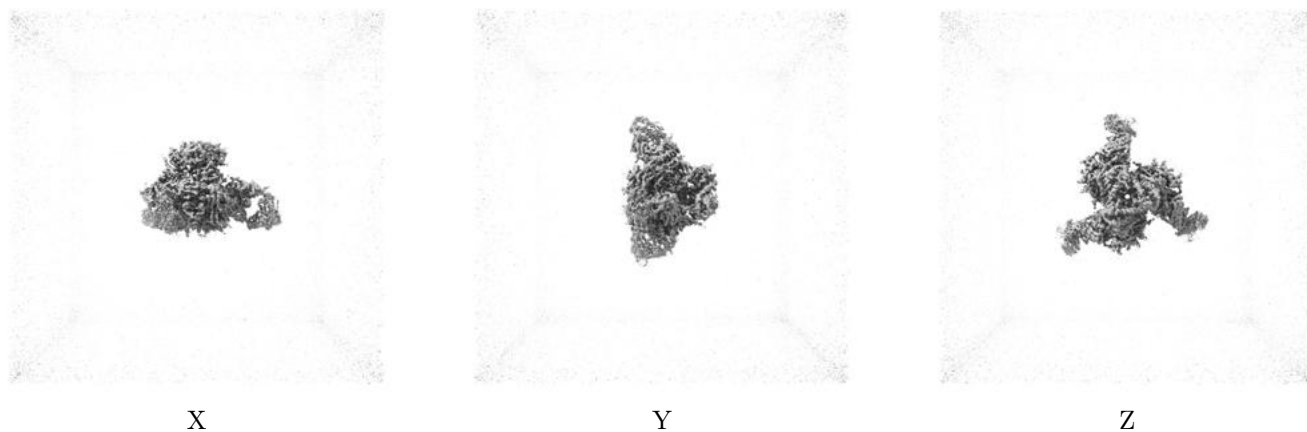
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

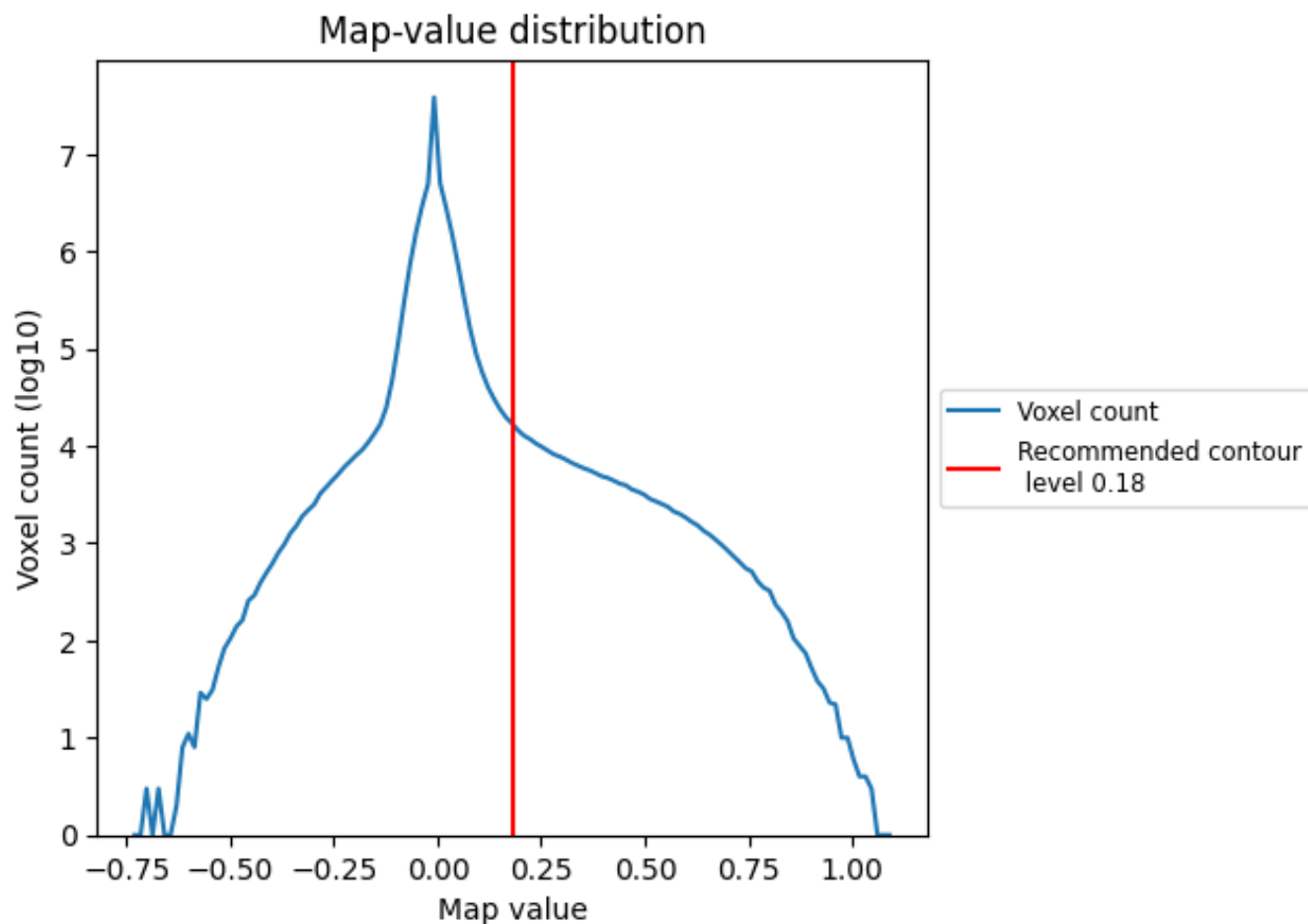
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

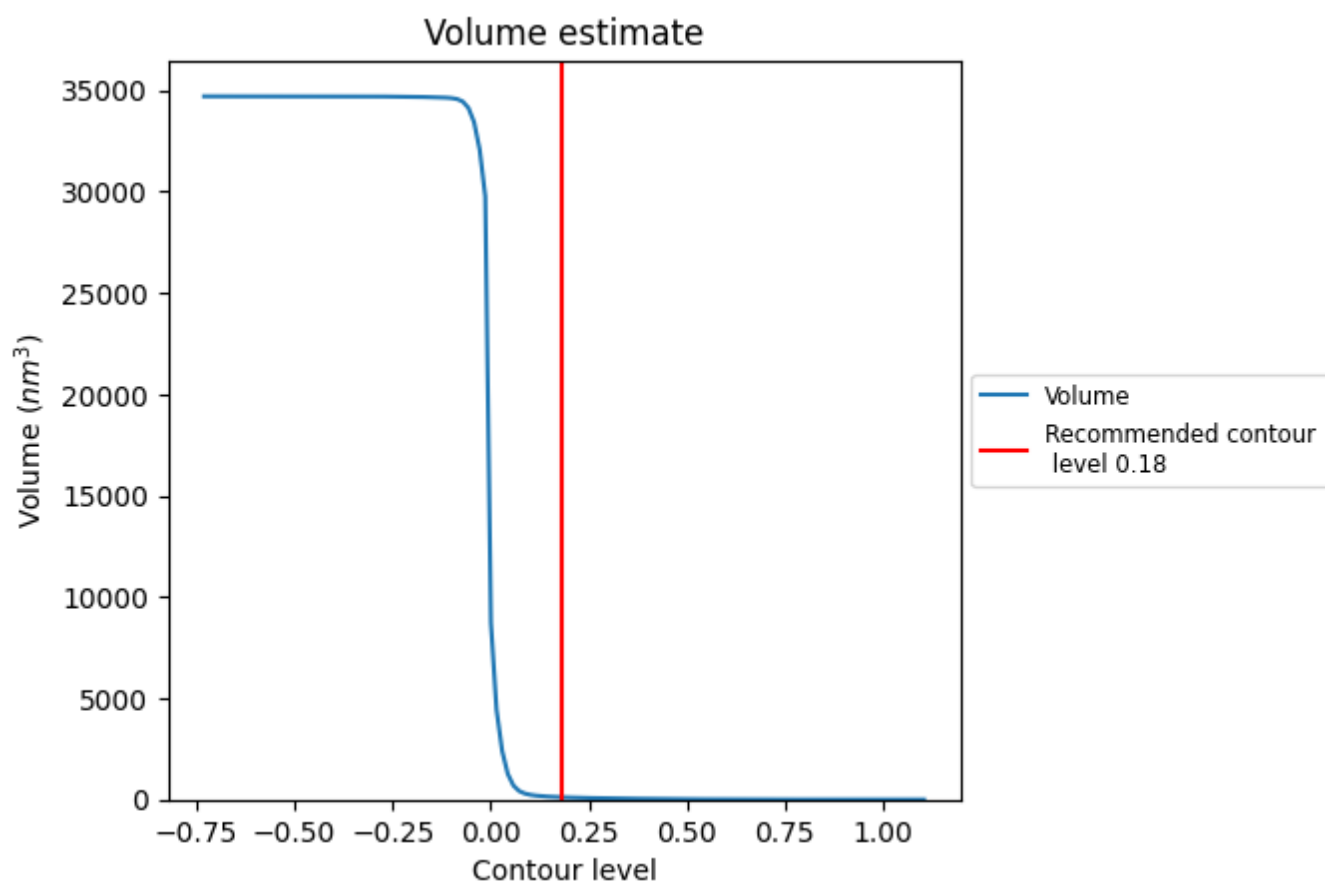
This section contains the results of statistical analysis of the map.

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.

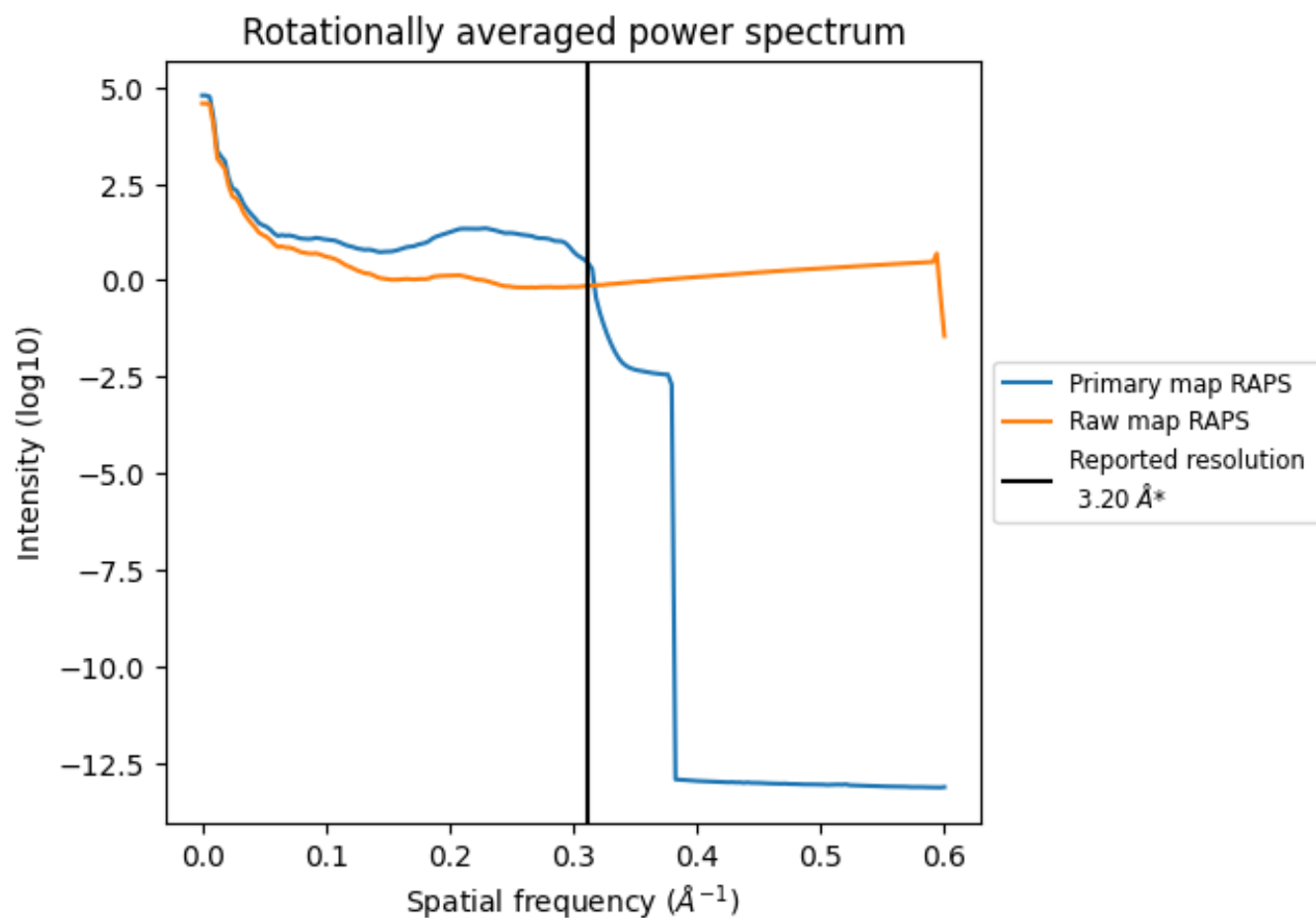
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

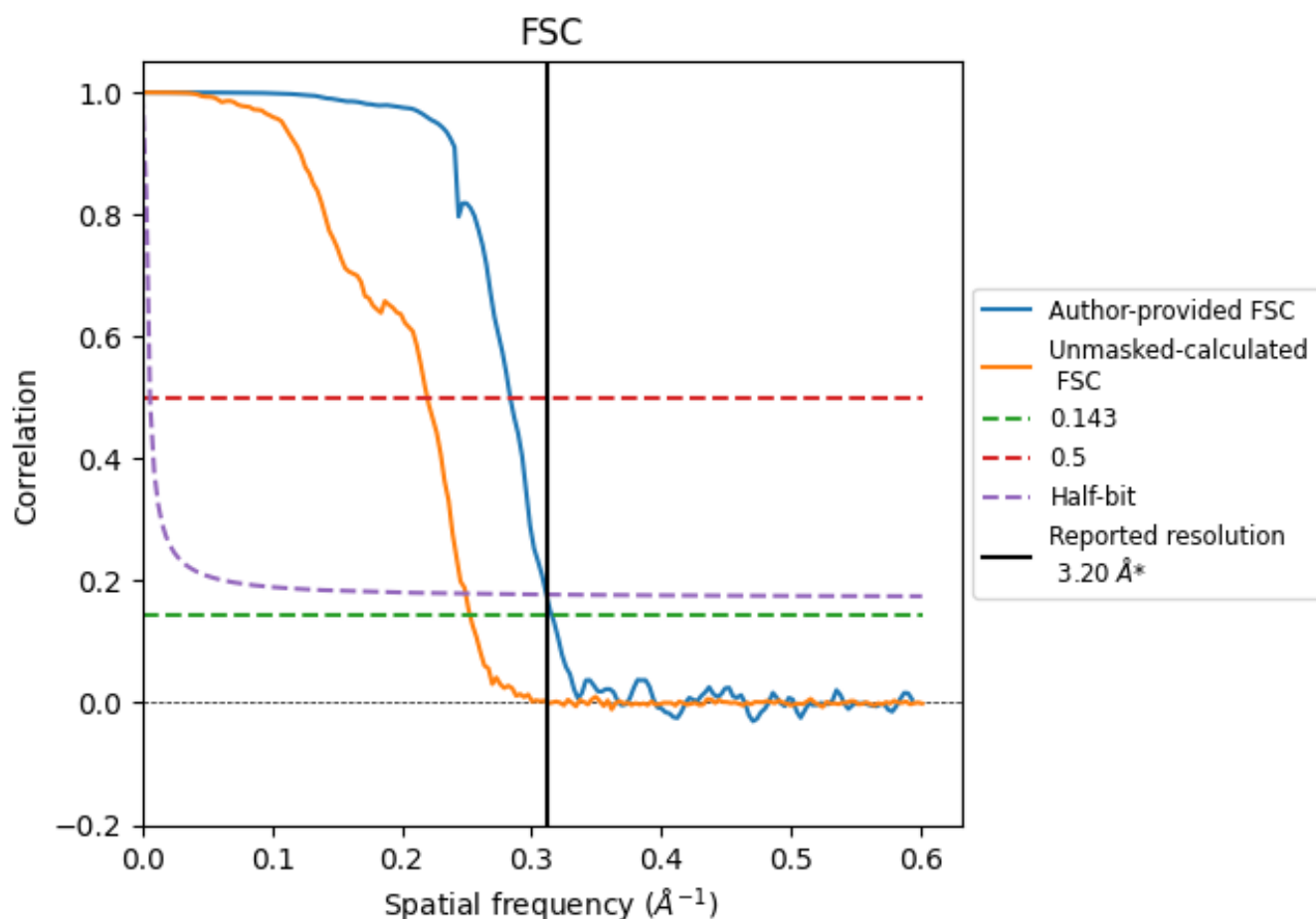


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

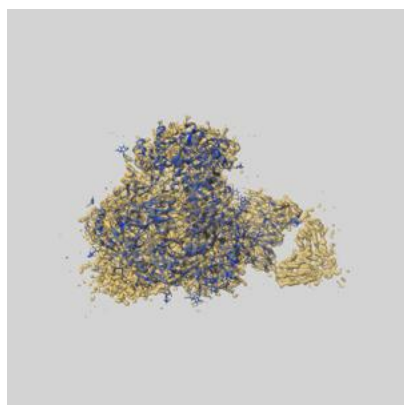
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.53	3.21
Unmasked-calculated*	3.96	4.55	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.2 by more than 10 %

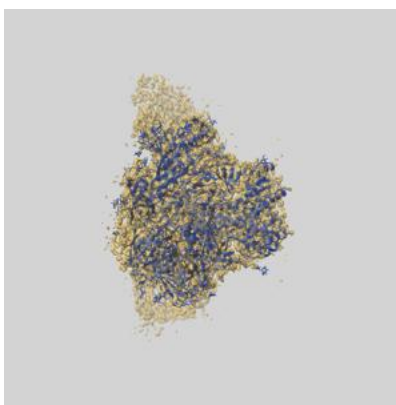
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42364 and PDB model 8ULS. Per-residue inclusion information can be found in section [3](#) on page [12](#).

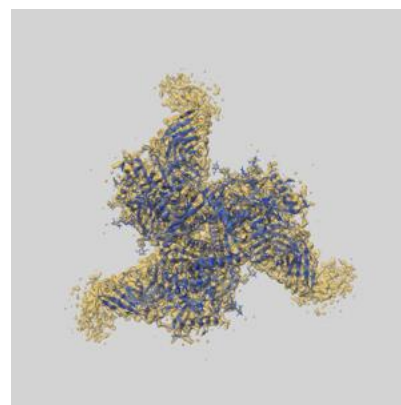
9.1 Map-model overlay [i](#)



X



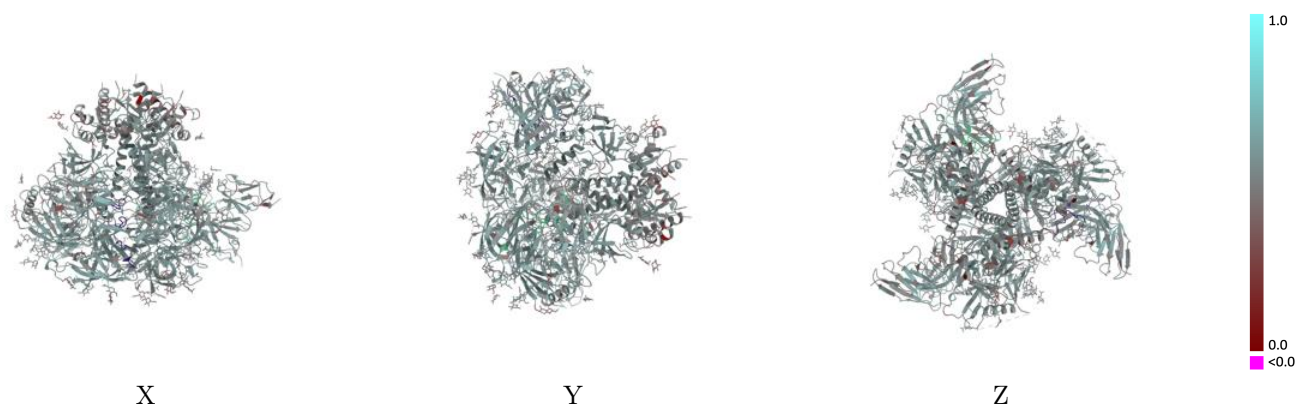
Y



Z

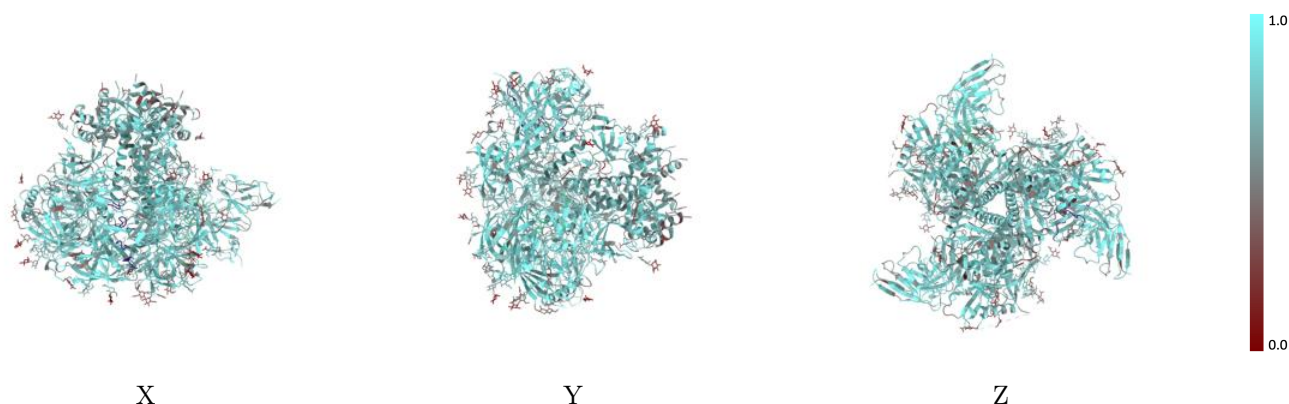
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



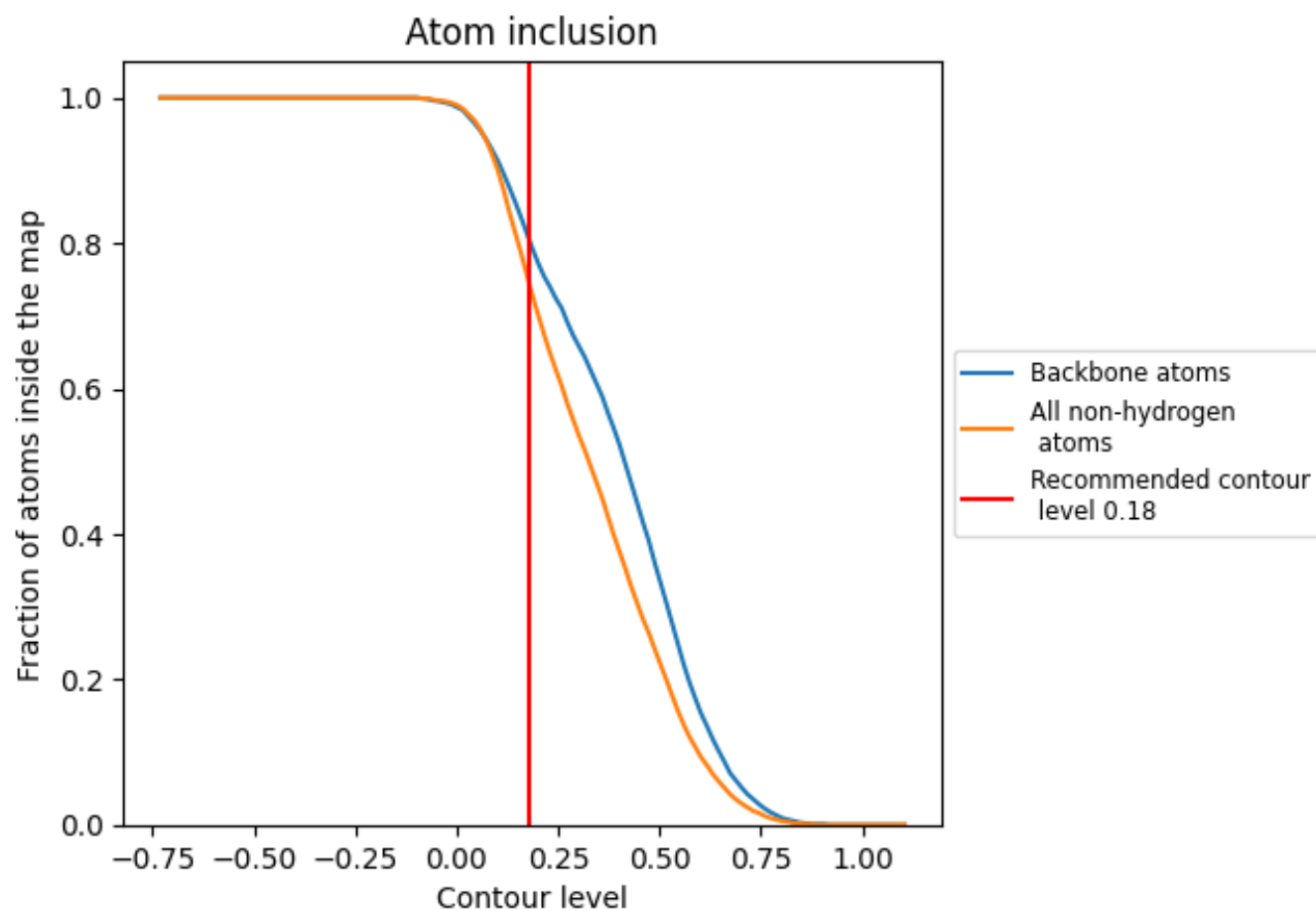
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.5340
A	 0.7600	 0.5450
B	 0.6790	 0.4980
C	 0.7600	 0.5470
D	 0.6790	 0.4960
E	 0.7590	 0.5450
F	 0.6740	 0.4920
G	 0.3930	 0.4090
H	 0.8060	 0.5500
I	 0.8030	 0.5530
J	 0.8060	 0.5510
K	 0.7140	 0.5480
L	 0.7540	 0.5270
M	 0.7570	 0.5240
N	 0.7550	 0.5290
O	 0.3930	 0.4620
P	 0.5380	 0.5040
Q	 0.7180	 0.5000
R	 0.8200	 0.5250
S	 0.5000	 0.4610
T	 0.4640	 0.4830
U	 0.6790	 0.5520
V	 0.6800	 0.4900
W	 0.5200	 0.4950
X	 0.2500	 0.4710
Y	 0.5000	 0.5130
Z	 0.3570	 0.3940
a	 0.7140	 0.5250
b	 0.4290	 0.4770
c	 0.5380	 0.5150
d	 0.6920	 0.4720
e	 0.8030	 0.5440
f	 0.5360	 0.4670
g	 0.5000	 0.4640
h	 0.6790	 0.5700



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Chain	Atom inclusion	Q-score
i	 0.6600	 0.5040
j	 0.5200	 0.5110
k	 0.2860	 0.4840
l	 0.3850	 0.5030
m	 0.3930	 0.3600
n	 0.7140	 0.5430
o	 0.3570	 0.4490
p	 0.5130	 0.5080
q	 0.7440	 0.5160
r	 0.8200	 0.5210
s	 0.5000	 0.4500
t	 0.5000	 0.4510
u	 0.7140	 0.5550
v	 0.7500	 0.5320
w	 0.5200	 0.5080
x	 0.2500	 0.4780
y	 0.5710	 0.5110