



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:09 PM UTC

PDB ID : 6MAR / pdb_00006mar
EMDB ID : EMD-9062
Title : HIV-1 Envelope Glycoprotein Clone BG505 delCT N332T in complex with broadly neutralizing antibody Fab PGT151
Authors : Berndsen, Z.T.; Ward, A.B.
Deposited on : 2018-08-28
Resolution : 4.50 Å(reported)
Based on initial model : 5FUU

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

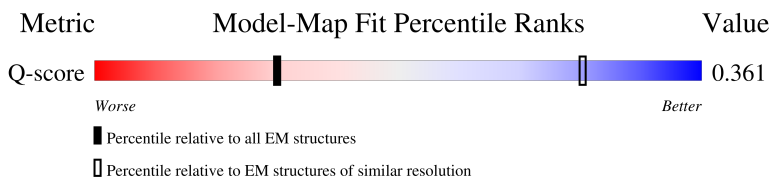
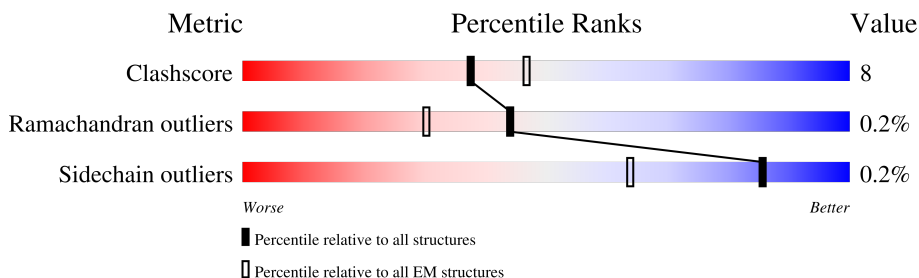
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



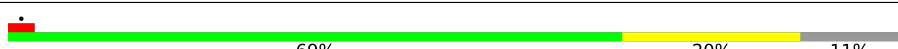
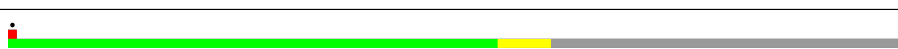
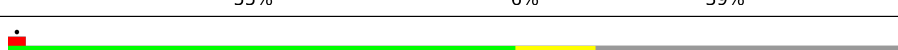
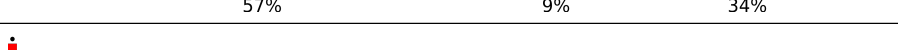
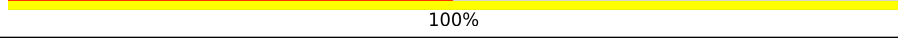
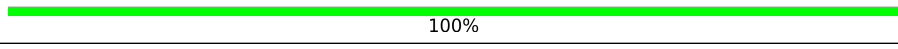
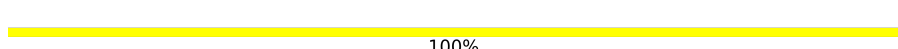
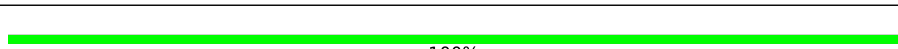
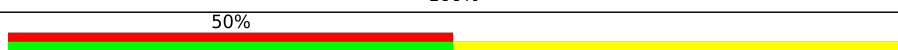
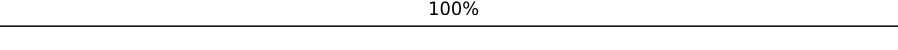
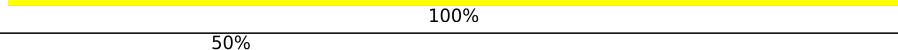
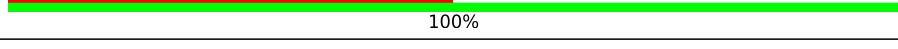
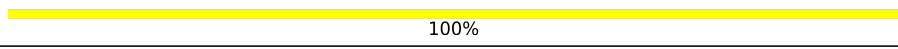
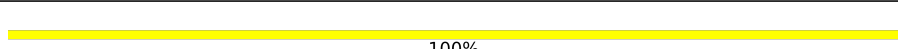
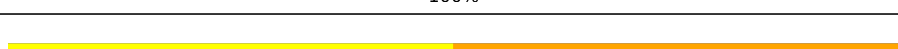
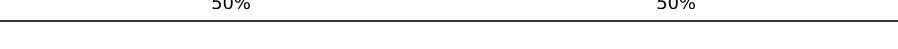
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	240	
1	M	240	
2	L	219	
2	N	219	

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Mol	Chain	Length	Quality of chain
3	A	494	
3	C	494	
3	E	494	
4	B	220	
4	D	220	
4	F	220	
5	G	2	
5	I	2	
5	J	2	
5	O	2	
5	P	2	
5	R	2	
5	S	2	
5	V	2	
5	W	2	
5	X	2	
5	Y	2	
5	Z	2	
5	a	2	
5	b	2	
5	c	2	
5	d	2	
5	f	2	
5	g	2	
5	i	2	

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Mol	Chain	Length	Quality of chain
5	k	2	
5	l	2	
5	m	2	
6	K	6	
7	Q	3	
7	j	3	
8	T	11	
9	U	10	
9	o	10	
10	e	4	
11	h	7	
12	n	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	BMA	T	3	-	-	X	-
8	NAG	T	5	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 19211 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 Immunoglobulin G PGT151 Fab, Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	135	Total	C	N	O	S	0	0
			1067	679	185	197	6		
1	H	135	Total	C	N	O	S	0	0
			1073	682	188	197	6		

- Molecule 2 is a protein called Immunoglobulin G PGT151, Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	112	Total	C	N	O	S	0	0
			866	545	149	168	4		
2	L	114	Total	C	N	O	S	0	0
			881	553	151	173	4		

- Molecule 3 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	440	Total	C	N	O	S	0	0
			3464	2177	612	648	27		
3	C	444	Total	C	N	O	S	0	0
			3493	2196	615	655	27		
3	E	438	Total	C	N	O	S	0	0
			3448	2168	608	645	27		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	expression tag	UNP Q2N0S6
A	11	GLU	-	expression tag	UNP Q2N0S6
A	12	THR	-	expression tag	UNP Q2N0S6
A	13	ASP	-	expression tag	UNP Q2N0S6
A	14	THR	-	expression tag	UNP Q2N0S6
A	15	LEU	-	expression tag	UNP Q2N0S6
A	16	LEU	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	17	LEU	-	expression tag	UNP Q2N0S6
A	18	TRP	-	expression tag	UNP Q2N0S6
A	19	VAL	-	expression tag	UNP Q2N0S6
A	20	LEU	-	expression tag	UNP Q2N0S6
A	21	LEU	-	expression tag	UNP Q2N0S6
A	22	LEU	-	expression tag	UNP Q2N0S6
A	23	TRP	-	expression tag	UNP Q2N0S6
A	24	VAL	-	expression tag	UNP Q2N0S6
A	25	PRO	-	expression tag	UNP Q2N0S6
A	26	GLY	-	expression tag	UNP Q2N0S6
A	27	SER	-	expression tag	UNP Q2N0S6
A	28	THR	-	expression tag	UNP Q2N0S6
A	29	GLY	-	expression tag	UNP Q2N0S6
A	30	ASP	-	expression tag	UNP Q2N0S6
C	10	MET	-	expression tag	UNP Q2N0S6
C	11	GLU	-	expression tag	UNP Q2N0S6
C	12	THR	-	expression tag	UNP Q2N0S6
C	13	ASP	-	expression tag	UNP Q2N0S6
C	14	THR	-	expression tag	UNP Q2N0S6
C	15	LEU	-	expression tag	UNP Q2N0S6
C	16	LEU	-	expression tag	UNP Q2N0S6
C	17	LEU	-	expression tag	UNP Q2N0S6
C	18	TRP	-	expression tag	UNP Q2N0S6
C	19	VAL	-	expression tag	UNP Q2N0S6
C	20	LEU	-	expression tag	UNP Q2N0S6
C	21	LEU	-	expression tag	UNP Q2N0S6
C	22	LEU	-	expression tag	UNP Q2N0S6
C	23	TRP	-	expression tag	UNP Q2N0S6
C	24	VAL	-	expression tag	UNP Q2N0S6
C	25	PRO	-	expression tag	UNP Q2N0S6
C	26	GLY	-	expression tag	UNP Q2N0S6
C	27	SER	-	expression tag	UNP Q2N0S6
C	28	THR	-	expression tag	UNP Q2N0S6
C	29	GLY	-	expression tag	UNP Q2N0S6
C	30	ASP	-	expression tag	UNP Q2N0S6
E	10	MET	-	expression tag	UNP Q2N0S6
E	11	GLU	-	expression tag	UNP Q2N0S6
E	12	THR	-	expression tag	UNP Q2N0S6
E	13	ASP	-	expression tag	UNP Q2N0S6
E	14	THR	-	expression tag	UNP Q2N0S6
E	15	LEU	-	expression tag	UNP Q2N0S6
E	16	LEU	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	17	LEU	-	expression tag	UNP Q2N0S6
E	18	TRP	-	expression tag	UNP Q2N0S6
E	19	VAL	-	expression tag	UNP Q2N0S6
E	20	LEU	-	expression tag	UNP Q2N0S6
E	21	LEU	-	expression tag	UNP Q2N0S6
E	22	LEU	-	expression tag	UNP Q2N0S6
E	23	TRP	-	expression tag	UNP Q2N0S6
E	24	VAL	-	expression tag	UNP Q2N0S6
E	25	PRO	-	expression tag	UNP Q2N0S6
E	26	GLY	-	expression tag	UNP Q2N0S6
E	27	SER	-	expression tag	UNP Q2N0S6
E	28	THR	-	expression tag	UNP Q2N0S6
E	29	GLY	-	expression tag	UNP Q2N0S6
E	30	ASP	-	expression tag	UNP Q2N0S6

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	134	Total	C	N	O	S	0	0
			1050	666	180	199	5		
4	D	146	Total	C	N	O	S	0	0
			1149	729	200	215	5		
4	F	127	Total	C	N	O	S	0	0
			1009	635	175	194	5		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	712	GLY	-	expression tag	UNP Q2N0S7
B	713	GLY	-	expression tag	UNP Q2N0S7
B	714	SER	-	expression tag	UNP Q2N0S7
B	715	GLY	-	expression tag	UNP Q2N0S7
B	716	GLY	-	expression tag	UNP Q2N0S7
B	717	GLY	-	expression tag	UNP Q2N0S7
B	718	TRP	-	expression tag	UNP Q2N0S7
B	719	SER	-	expression tag	UNP Q2N0S7
B	720	HIS	-	expression tag	UNP Q2N0S7
B	721	PRO	-	expression tag	UNP Q2N0S7
B	722	GLN	-	expression tag	UNP Q2N0S7
B	723	PHE	-	expression tag	UNP Q2N0S7
B	724	GLU	-	expression tag	UNP Q2N0S7
B	725	LYS	-	expression tag	UNP Q2N0S7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	712	GLY	-	expression tag	UNP Q2N0S7
D	713	GLY	-	expression tag	UNP Q2N0S7
D	714	SER	-	expression tag	UNP Q2N0S7
D	715	GLY	-	expression tag	UNP Q2N0S7
D	716	GLY	-	expression tag	UNP Q2N0S7
D	717	GLY	-	expression tag	UNP Q2N0S7
D	718	TRP	-	expression tag	UNP Q2N0S7
D	719	SER	-	expression tag	UNP Q2N0S7
D	720	HIS	-	expression tag	UNP Q2N0S7
D	721	PRO	-	expression tag	UNP Q2N0S7
D	722	GLN	-	expression tag	UNP Q2N0S7
D	723	PHE	-	expression tag	UNP Q2N0S7
D	724	GLU	-	expression tag	UNP Q2N0S7
D	725	LYS	-	expression tag	UNP Q2N0S7
F	712	GLY	-	expression tag	UNP Q2N0S7
F	713	GLY	-	expression tag	UNP Q2N0S7
F	714	SER	-	expression tag	UNP Q2N0S7
F	715	GLY	-	expression tag	UNP Q2N0S7
F	716	GLY	-	expression tag	UNP Q2N0S7
F	717	GLY	-	expression tag	UNP Q2N0S7
F	718	TRP	-	expression tag	UNP Q2N0S7
F	719	SER	-	expression tag	UNP Q2N0S7
F	720	HIS	-	expression tag	UNP Q2N0S7
F	721	PRO	-	expression tag	UNP Q2N0S7
F	722	GLN	-	expression tag	UNP Q2N0S7
F	723	PHE	-	expression tag	UNP Q2N0S7
F	724	GLU	-	expression tag	UNP Q2N0S7
F	725	LYS	-	expression tag	UNP Q2N0S7

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



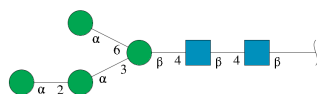
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		

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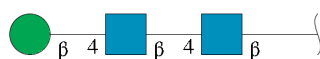
Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		
5	k	2	Total	C	N	O	0	0
			28	16	2	10		
5	l	2	Total	C	N	O	0	0
			28	16	2	10		
5	m	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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.



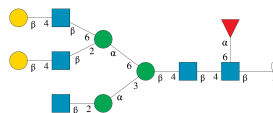
Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 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.



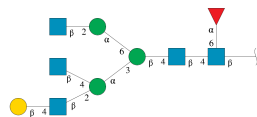
Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	3	Total	C	N	O	0	0
			39	22	2	15		
7	j	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	11	Total	C	N	O	0	0
			135	76	5	54		

- Molecule 9 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



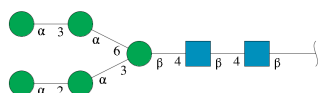
Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	10	Total	C	N	O	0	0
			124	70	5	49		
9	o	10	Total	C	N	O	0	0
			124	70	5	49		

- Molecule 10 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.



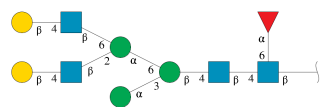
Mol	Chain	Residues	Atoms				AltConf	Trace
10	e	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



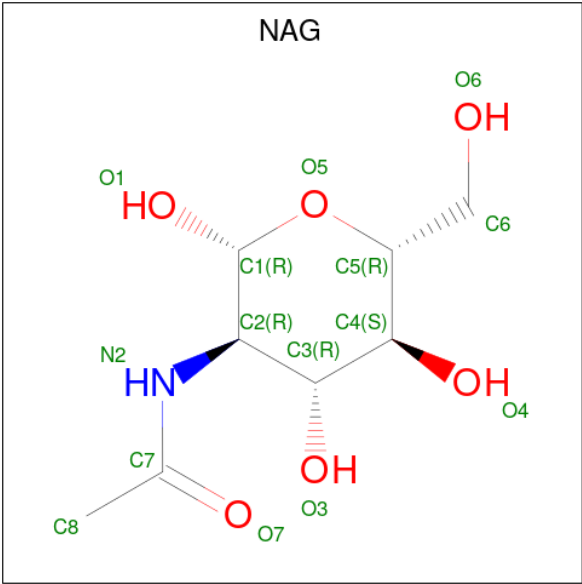
Mol	Chain	Residues	Atoms				AltConf	Trace
11	h	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 12 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	n	10	Total	C	N	O	0	0
			121	68	4	49		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



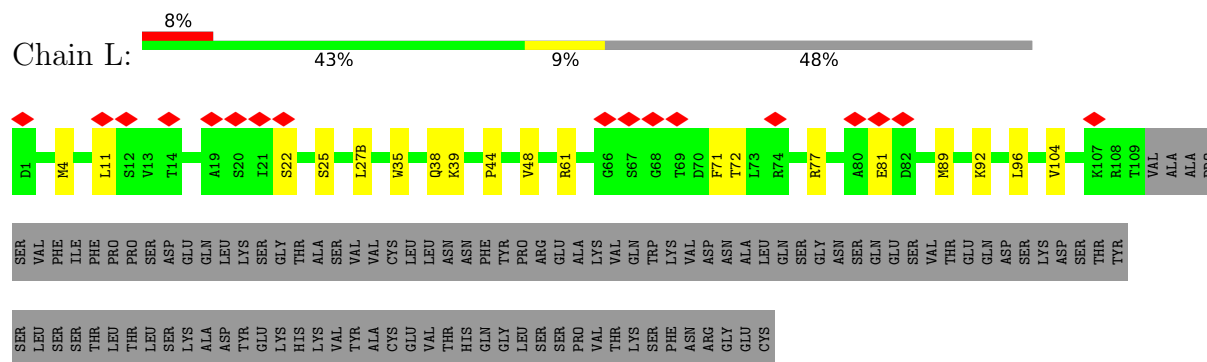
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	A	1	Total	C	N	O	0
			14	8	1	5	
13	B	1	Total	C	N	O	0
			14	8	1	5	
13	B	1	Total	C	N	O	0
			14	8	1	5	
13	D	1	Total	C	N	O	0
			14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

Continued on next page...

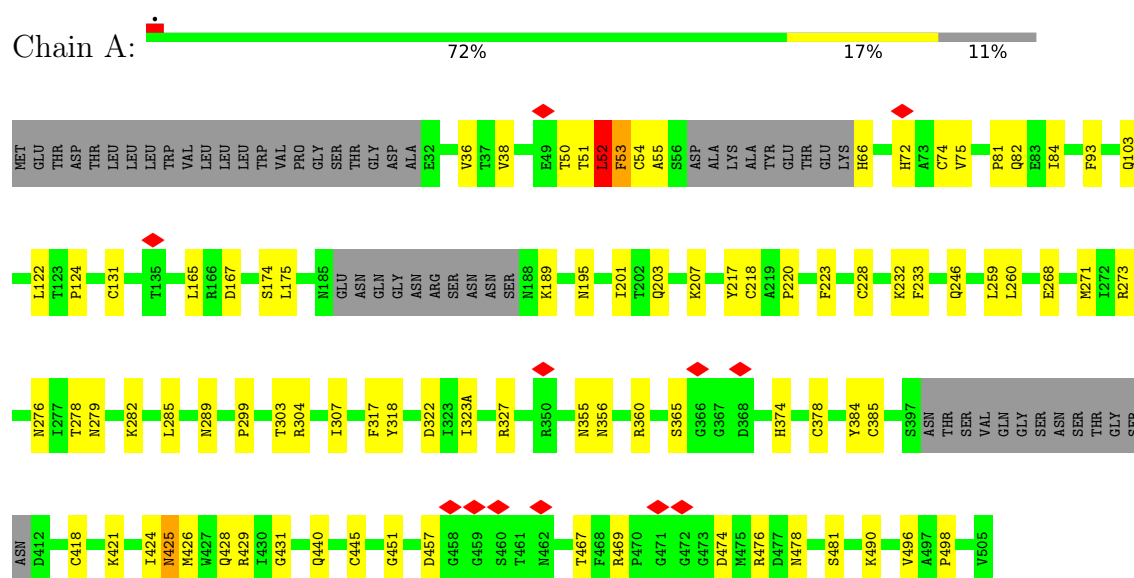
Continued from previous page...

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

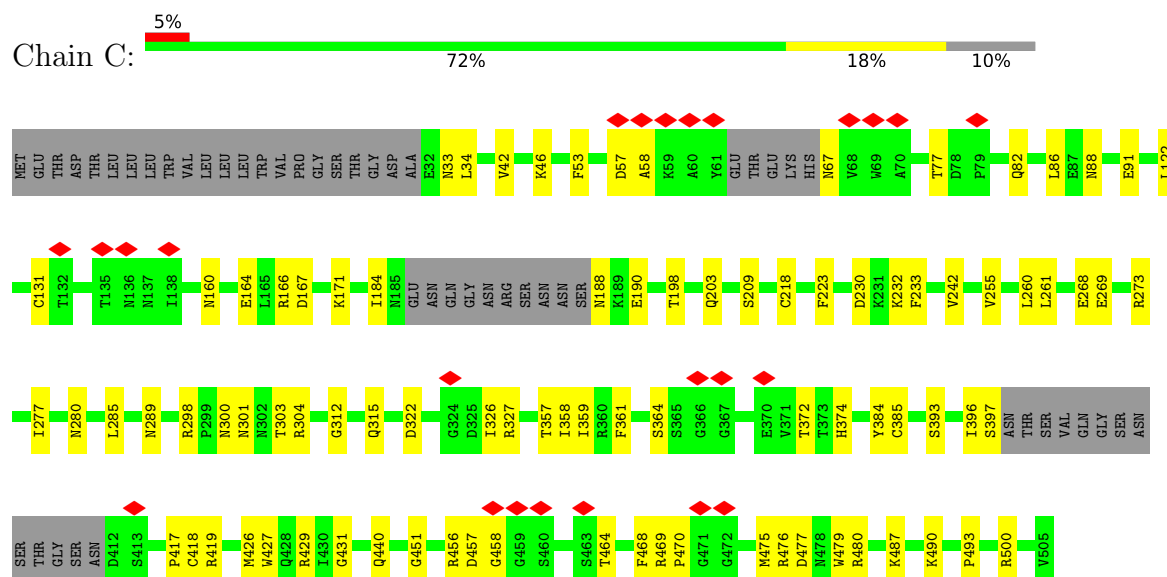
- Molecule 2: Immunoglobulin G PGT151, Light chain



- Molecule 3: Envelope glycoprotein gp160



- Molecule 3: Envelope glycoprotein gp160



- Molecule 3: Envelope glycoprotein gp160



PRO
GLN
PHE
GLU
LYS

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



MAG1
MAG2

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



MAG1
MAG2

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



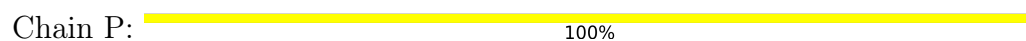
MAG1
MAG2

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



MAG1
MAG2

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



MAG1
MAG2

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



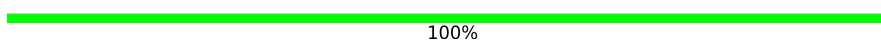
MAG1
MAG2

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

Chain S: 

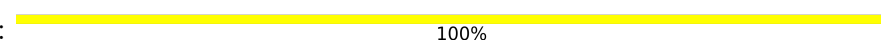


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 



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

Chain W: 

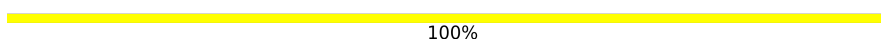


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 



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

Chain Y: 



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

Chain Z: 

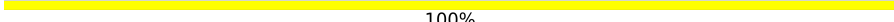


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%

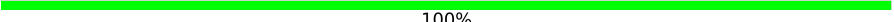
MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain d:  50% 50%

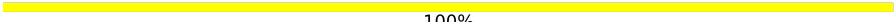
MAG1
MAG2

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

Chain f:  50% 50%

MAG1
MAG2

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

Chain g:  100%

MAG1
MAG2

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

Chain i:  50% 50%

MAG1
MAG2

- 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 6: 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



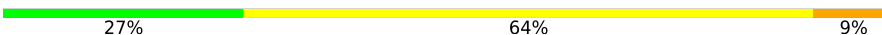
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



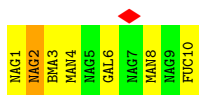
- Molecule 8: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyrano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

Chain T: 



- Molecule 9: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 



- Molecule 9: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 

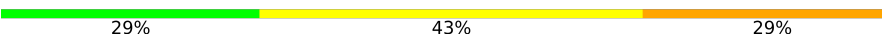


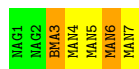
- Molecule 10: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 



- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 h: 



- Molecule 12: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  40% 60%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67010	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, GAL, MAN, FUC

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	H	0.27	0/1102	0.53	0/1496
1	M	0.27	0/1096	0.51	0/1489
2	L	0.22	0/899	0.49	0/1213
2	N	0.23	0/884	0.51	0/1192
3	A	0.27	0/3536	0.54	0/4800
3	C	0.27	0/3565	0.52	0/4839
3	E	0.29	1/3519 (0.0%)	0.50	0/4777
4	B	0.33	0/1068	0.60	0/1450
4	D	0.30	0/1168	0.54	0/1584
4	F	0.31	0/1026	0.53	0/1392
All	All	0.28	1/17863 (0.0%)	0.53	0/24232

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	117	LYS	C-N	5.40	1.38	1.33

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	H	1073	0	1040	45	0
1	M	1067	0	1029	22	0
2	L	881	0	868	13	0
2	N	866	0	854	12	0
3	A	3464	0	3410	62	0
3	C	3493	0	3439	55	0
3	E	3448	0	3398	59	0
4	B	1050	0	1033	10	0
4	D	1149	0	1142	14	0
4	F	1009	0	985	11	0
5	G	28	0	25	2	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	R	28	0	25	0	0
5	S	28	0	25	0	0
5	V	28	0	25	0	0
5	W	28	0	25	1	0
5	X	28	0	25	0	0
5	Y	28	0	25	1	0
5	Z	28	0	25	0	0
5	a	28	0	25	2	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
5	d	28	0	25	2	0
5	f	28	0	25	0	0
5	g	28	0	25	0	0
5	i	28	0	25	0	0
5	k	28	0	25	0	0
5	l	28	0	25	0	0
5	m	28	0	25	0	0
6	K	72	0	61	0	0
7	Q	39	0	34	0	0
7	j	39	0	34	0	0
8	T	135	0	115	22	0
9	U	124	0	106	1	0
9	o	124	0	106	2	0
10	e	50	0	43	1	0
11	h	83	0	70	1	0
12	n	121	0	103	0	0
13	A	70	0	65	0	0
13	B	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C	70	0	65	1	0
13	D	42	0	39	0	0
13	E	84	0	78	0	0
13	F	14	0	13	0	0
All	All	19211	0	18706	285	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 8.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:TRP:CZ3	8:T:3:BMA:H61	1.42	1.55
1:H:55:TRP:CD1	1:H:100(M):TYR:HH	1.48	1.30
1:H:55:TRP:CZ3	8:T:3:BMA:C6	2.21	1.22
1:H:55:TRP:CH2	8:T:3:BMA:C6	2.25	1.19
1:H:55:TRP:CH2	8:T:3:BMA:H62	1.82	1.14
1:H:55:TRP:CE2	8:T:5:NAG:O7	2.08	1.07
1:H:55:TRP:HD1	1:H:100(M):TYR:OH	1.46	0.98
3:A:52:LEU:CD1	3:A:217:TYR:CD2	2.50	0.95
1:H:55:TRP:HZ3	8:T:3:BMA:H61	1.17	0.94
1:H:55:TRP:HH2	8:T:3:BMA:H62	1.32	0.94
3:A:52:LEU:HD11	3:A:217:TYR:CD2	2.03	0.94
1:H:55:TRP:CH2	8:T:3:BMA:H61	1.95	0.93
2:N:50:GLU:OE1	2:N:53:ASN:ND2	2.03	0.92
1:H:55:TRP:CD1	1:H:100(M):TYR:OH	2.22	0.85
3:A:52:LEU:HD13	3:A:217:TYR:CG	2.14	0.83
1:H:55:TRP:NE1	8:T:5:NAG:H81	1.94	0.82
3:A:52:LEU:CD1	3:A:217:TYR:CE2	2.63	0.81
1:H:55:TRP:CD2	8:T:5:NAG:O7	2.34	0.80
1:H:55:TRP:HE1	8:T:5:NAG:H81	1.44	0.80
4:F:523:LEU:H	4:F:540:GLN:HE22	1.33	0.77
3:A:424:ILE:O	3:A:425:ASN:O	2.03	0.76
3:A:52:LEU:HD11	3:A:217:TYR:CE2	2.24	0.73
3:A:429:ARG:HG2	3:A:431:GLY:H	1.55	0.72
3:A:52:LEU:CD1	3:A:217:TYR:CG	2.74	0.70
3:E:273:ARG:HB2	3:E:285:LEU:HB3	1.74	0.69
1:H:39:GLN:HB2	1:H:89:VAL:HB	1.75	0.68
2:L:27(B):LEU:HA	2:L:92:LYS:HD2	1.74	0.68
1:M:100(J):ARG:CZ	3:A:82:GLN:HG2	2.24	0.68
3:A:52:LEU:O	3:A:53:PHE:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:323(A):ILE:HD12	5:G:1:NAG:HN2	1.59	0.66
3:A:52:LEU:HD12	3:A:217:TYR:CZ	2.31	0.66
1:H:55:TRP:NE1	8:T:5:NAG:O7	2.29	0.66
1:M:3:GLN:HB3	1:M:25:SER:HB3	1.78	0.65
2:N:50:GLU:O	2:N:52:SER:N	2.30	0.65
3:A:273:ARG:HB2	3:A:285:LEU:HB2	1.79	0.62
3:C:417:PRO:HG3	5:a:1:NAG:H82	1.81	0.62
1:M:97:GLN:NE2	9:o:2:NAG:O3	2.31	0.62
3:E:74:CYS:SG	3:E:75:VAL:N	2.69	0.62
3:A:74:CYS:SG	3:A:75:VAL:N	2.69	0.61
4:F:548:ILE:O	4:F:551:GLN:NE2	2.33	0.61
3:C:230:ASP:HB3	3:C:233:PHE:HB2	1.83	0.60
3:C:255:VAL:HG13	3:C:475:MET:HE1	1.83	0.60
3:C:304:ARG:HB3	3:C:440:GLN:HE21	1.65	0.60
3:E:230:ASP:HB3	3:E:233:PHE:HB2	1.83	0.59
1:M:100(C):ARG:NH1	9:o:10:FUC:O3	2.35	0.59
4:D:653:GLN:HA	4:D:657:GLU:H	1.67	0.59
3:A:304:ARG:HB3	3:A:440:GLN:HE21	1.68	0.58
4:F:652:GLN:HG3	4:F:653:GLN:HG2	1.85	0.58
1:M:38:ARG:NH1	1:M:46:GLU:OE1	2.36	0.58
3:A:93:PHE:HE2	3:A:228:CYS:HB2	1.68	0.57
3:A:52:LEU:HD12	3:A:217:TYR:CE2	2.38	0.57
3:A:36:VAL:HA	3:A:498:PRO:HA	1.87	0.57
4:B:538:THR:HG21	4:F:647:GLU:HB3	1.84	0.57
3:C:277:ILE:O	3:C:456:ARG:NH2	2.38	0.57
1:H:55:TRP:CZ3	8:T:3:BMA:C5	2.87	0.57
3:E:179:LEU:HB3	3:E:421:LYS:HE2	1.86	0.57
3:A:457:ASP:OD2	3:A:469:ARG:NH1	2.37	0.56
3:E:175:LEU:H	3:E:320:THR:HB	1.70	0.56
1:M:52(A):GLY:O	1:M:71:ARG:NH1	2.39	0.56
1:H:55:TRP:HZ3	8:T:3:BMA:C5	2.19	0.56
3:A:50:THR:O	3:A:103:GLN:NE2	2.34	0.56
1:H:55:TRP:NE1	8:T:5:NAG:C8	2.65	0.56
3:A:195:ASN:HD21	3:A:201:ILE:HD12	1.70	0.56
3:E:298:ARG:HD2	3:E:300:ASN:H	1.70	0.56
3:C:164:GLU:HA	3:C:312:GLY:HA2	1.87	0.55
2:N:36:TYR:HB3	2:N:46:LEU:HD12	1.88	0.55
3:A:474:ASP:OD2	3:A:476:ARG:NH1	2.39	0.55
3:A:232:LYS:HA	3:A:271:MET:HE1	1.88	0.55
3:C:385:CYS:HA	3:C:418:CYS:HA	1.89	0.55
2:N:22:SER:HA	2:N:72:THR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:TRP:HZ3	8:T:3:BMA:C6	1.88	0.55
1:M:100(G):TRP:NE1	3:A:84:ILE:HD11	2.20	0.55
1:H:93:ALA:O	1:H:94:ARG:NH1	2.39	0.55
3:C:232:LYS:NZ	3:C:269:GLU:OE2	2.40	0.54
3:E:258:GLN:NE2	3:E:372:THR:O	2.40	0.54
2:L:38:GLN:HB3	2:L:44:PRO:HA	1.88	0.54
1:M:33:PRO:HA	1:M:71:ARG:HH22	1.72	0.54
2:N:19:ALA:HB3	2:N:75:ILE:HB	1.89	0.54
2:L:27(B):LEU:HD12	2:L:71:PHE:HE2	1.73	0.53
3:E:457:ASP:OD2	3:E:469:ARG:NH1	2.41	0.53
3:C:233:PHE:O	3:C:273:ARG:NH2	2.40	0.53
2:L:39:LYS:NZ	2:L:81:GLU:OE1	2.40	0.53
3:E:304:ARG:HB3	3:E:440:GLN:HE21	1.74	0.53
3:A:52:LEU:HD13	3:A:217:TYR:CD1	2.43	0.53
3:C:131:CYS:O	3:C:188:ASN:ND2	2.39	0.53
3:C:268:GLU:O	3:C:289:ASN:ND2	2.42	0.52
3:C:359:ILE:HG12	3:C:397:SER:HB3	1.90	0.52
1:M:39:GLN:HB3	1:M:89:VAL:HB	1.92	0.52
3:E:272:ILE:HG12	3:E:286:VAL:HG22	1.91	0.52
3:A:233:PHE:O	3:A:273:ARG:NH2	2.42	0.52
5:a:2:NAG:HN2	5:d:2:NAG:H5	1.75	0.52
3:E:350:ARG:HB3	3:E:355:ASN:HA	1.92	0.52
1:H:55:TRP:CD1	8:T:5:NAG:O7	2.63	0.51
3:E:292:VAL:HB	3:E:449:ILE:HB	1.92	0.51
2:N:92:LYS:O	4:B:512:ALA:N	2.44	0.51
1:M:100(J):ARG:HA	4:B:517:ALA:HA	1.93	0.51
3:A:279:ASN:HD22	3:A:282:LYS:HE2	1.75	0.51
2:N:51:VAL:O	2:N:64:GLY:HA3	2.10	0.51
3:C:312:GLY:H	3:C:315:GLN:HB2	1.76	0.51
3:A:53:PHE:HD2	3:A:218:CYS:HB2	1.76	0.51
1:M:63:VAL:HG12	1:M:66:ARG:HD2	1.92	0.50
3:A:131:CYS:HB2	3:A:189:LYS:HB2	1.92	0.50
4:D:657:GLU:O	4:D:661:LEU:N	2.42	0.50
3:C:58:ALA:H	3:C:77:THR:H	1.59	0.50
3:E:98:ASN:ND2	3:E:100:MET:SD	2.85	0.50
1:H:53:ASP:OD1	1:H:53:ASP:N	2.43	0.50
3:C:122:LEU:HD11	3:C:203:GLN:HB2	1.94	0.50
3:E:54:CYS:SG	3:E:55:ALA:N	2.85	0.50
2:L:92:LYS:O	4:D:512:ALA:N	2.45	0.50
4:B:523:LEU:HD23	4:B:540:GLN:HE21	1.76	0.50
3:E:456:ARG:HG3	3:E:468:PHE:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:88:CYS:O	2:N:99:GLY:N	2.44	0.50
3:A:260:LEU:HD12	3:A:451:GLY:HA3	1.94	0.50
2:N:87:TYR:HE1	2:N:101:GLY:HA2	1.78	0.49
3:E:162:THR:HA	3:E:169:LYS:HA	1.94	0.49
4:F:597:GLY:N	4:F:650:GLN:OE1	2.45	0.49
3:A:54:CYS:SG	3:A:55:ALA:N	2.85	0.49
3:A:268:GLU:O	3:A:289:ASN:ND2	2.46	0.49
3:C:53:PHE:HD2	3:C:218:CYS:HB2	1.76	0.49
4:B:647:GLU:HB3	4:D:538:THR:HG21	1.95	0.49
3:E:69:TRP:HZ3	3:E:108:ILE:HG23	1.76	0.49
1:H:34:MET:HE3	1:H:71:ARG:HH11	1.78	0.49
4:B:594:GLY:HA2	4:B:599:SER:HB2	1.95	0.49
3:C:456:ARG:HD3	3:C:468:PHE:HE1	1.77	0.49
1:M:52:SER:HB3	1:M:56:HIS:HB3	1.95	0.48
1:H:100(H):SER:HB3	3:C:82:GLN:HG2	1.95	0.48
4:D:544:LEU:HD21	3:C:493:PRO:HG2	1.95	0.48
3:E:137:ASN:HB3	3:E:325:ASP:HA	1.95	0.48
3:A:52:LEU:CD1	3:A:217:TYR:CZ	2.95	0.48
3:E:298:ARG:NH2	3:E:441:GLY:O	2.46	0.48
2:L:61:ARG:HD2	2:L:77:ARG:HB2	1.94	0.48
3:C:384:TYR:O	3:C:419:ARG:N	2.44	0.48
4:B:596:TRP:HE1	4:B:647:GLU:HG3	1.78	0.48
3:C:298:ARG:HD2	3:C:300:ASN:H	1.78	0.48
1:H:20:LEU:HB2	1:H:80:LEU:HB3	1.94	0.48
1:H:55:TRP:CE2	8:T:5:NAG:C7	2.94	0.48
1:H:55:TRP:NE1	8:T:5:NAG:C7	2.77	0.48
3:C:67:ASN:HA	3:C:209:SER:H	1.79	0.48
3:C:91:GLU:OE2	3:C:487:LYS:NZ	2.38	0.48
3:E:304:ARG:HD2	3:E:318:TYR:HB3	1.94	0.48
1:H:97:GLN:OE1	9:U:2:NAG:O3	2.31	0.48
3:C:357:THR:HG23	3:C:464:THR:HA	1.96	0.48
2:L:11:LEU:HB3	2:L:104:VAL:HG22	1.96	0.47
3:A:323(A):ILE:H	5:G:1:NAG:H82	1.78	0.47
1:H:10:GLY:N	1:H:108:THR:O	2.43	0.47
3:C:384:TYR:HB2	3:C:419:ARG:HB2	1.96	0.47
3:E:271:MET:HB3	3:E:273:ARG:HH12	1.79	0.47
3:C:160:ASN:OD1	3:C:171:LYS:NZ	2.38	0.47
3:C:280:ASN:HD22	3:C:458:GLY:HA2	1.78	0.47
3:C:357:THR:O	3:C:397:SER:OG	2.31	0.47
3:C:303:THR:OG1	3:C:322:ASP:N	2.44	0.47
1:H:47:TRP:HH2	1:H:58:VAL:HG12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:22:SER:HA	2:L:72:THR:HA	1.95	0.47
3:A:38:VAL:HA	3:A:496:VAL:HG12	1.97	0.47
3:E:278:THR:O	3:E:456:ARG:NH2	2.47	0.47
3:C:476:ARG:HA	3:C:479:TRP:HD1	1.80	0.47
1:H:100(R):MET:HE3	2:L:89:MET:HE1	1.97	0.46
4:F:569:THR:HG23	4:F:572:GLY:H	1.80	0.46
1:M:12:VAL:HB	1:M:16:LYS:HG3	1.96	0.46
4:D:609:PRO:HB3	3:C:33:ASN:HD21	1.80	0.46
3:E:499:THR:HG23	3:E:501:ALA:H	1.79	0.46
1:H:4:LEU:HA	1:H:24:VAL:HG22	1.98	0.46
1:H:91:ARG:HD3	1:H:103:TRP:HB3	1.97	0.46
1:H:55:TRP:CG	8:T:5:NAG:O7	2.69	0.46
3:A:307:ILE:O	3:A:317:PHE:N	2.44	0.46
3:A:478:ASN:O	3:A:481:SER:OG	2.29	0.46
3:A:303:THR:OG1	3:A:322:ASP:O	2.29	0.46
3:A:378:CYS:HB3	3:A:445:CYS:HB2	1.89	0.46
3:E:138:ILE:HD11	3:E:143:ARG:HA	1.97	0.46
3:A:385:CYS:HA	3:A:418:CYS:HA	1.98	0.46
3:E:45:TRP:CD1	3:E:489:VAL:HG11	2.51	0.46
3:E:331:CYS:HB2	3:E:416:LEU:HB2	1.98	0.46
3:C:261:LEU:HD11	3:C:374:HIS:HE2	1.81	0.45
3:E:258:GLN:HB2	3:E:374:HIS:HD1	1.81	0.45
3:C:364:SER:HB3	3:C:470:PRO:HG2	1.98	0.45
3:E:206:PRO:HG3	3:E:318:TYR:HE2	1.82	0.45
3:A:66:HIS:N	3:A:207:LYS:O	2.49	0.45
1:M:38:ARG:N	1:M:46:GLU:O	2.50	0.45
3:C:260:LEU:HD12	3:C:451:GLY:HA3	1.98	0.45
3:E:209:SER:OG	3:E:210:PHE:N	2.49	0.45
3:A:81:PRO:HB3	3:A:246:GLN:HG2	1.99	0.45
3:A:165:LEU:HG	3:A:167:ASP:H	1.81	0.45
4:D:542:ARG:HH12	4:D:549:VAL:HG11	1.81	0.45
3:E:185:ASN:HD21	3:E:190:GLU:H	1.65	0.45
3:A:276:ASN:OD1	3:A:278:THR:OG1	2.31	0.45
4:D:617:ARG:HH11	4:D:621:GLU:HG2	1.82	0.45
4:D:655:LYS:HA	4:D:658:GLN:HB3	1.97	0.45
3:C:184:ILE:HD12	3:C:190:GLU:HB3	1.98	0.45
1:H:38:ARG:NH2	1:H:46:GLU:OE1	2.45	0.45
3:A:223:PHE:HE1	3:A:490:LYS:HG3	1.82	0.45
3:C:326:ILE:O	3:C:327:ARG:NH1	2.41	0.45
3:E:384:TYR:O	3:E:419:ARG:N	2.50	0.44
2:N:27(D):GLN:HG3	2:N:28:ASN:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:426:MET:HG3	3:C:427:TRP:CD1	2.53	0.44
3:E:228:CYS:SG	3:E:229:LYS:N	2.91	0.44
3:A:220:PRO:HB3	4:B:578:ALA:HB1	1.98	0.44
10:e:1:NAG:H61	10:e:2:NAG:H82	1.98	0.44
3:E:161:MET:HE2	3:E:172:VAL:HG21	2.00	0.44
1:M:41:PRO:HD3	1:M:88:ALA:HA	1.99	0.44
1:M:95:MET:HE2	1:M:100(P):SER:H	1.82	0.44
3:A:52:LEU:HB3	3:A:53:PHE:H	1.61	0.44
4:D:619:LEU:HB3	4:D:623:TRP:HD1	1.83	0.44
1:M:112:SER:OG	1:M:113:SER:N	2.51	0.44
2:L:35:TRP:HB2	2:L:48:VAL:HG22	2.00	0.44
4:D:530:MET:HG2	4:D:628:TRP:CD1	2.53	0.43
3:E:457:ASP:OD2	3:E:467:THR:OG1	2.33	0.43
3:C:273:ARG:HB2	3:C:285:LEU:HB3	2.00	0.43
3:E:224:ALA:HB2	3:E:491:ILE:HD11	2.00	0.43
3:A:384:TYR:HE2	3:A:421:LYS:HD3	1.83	0.43
3:C:223:PHE:HE1	3:C:490:LYS:HG3	1.83	0.43
3:C:361:PHE:HB2	3:C:393:SER:HB3	1.99	0.43
4:F:569:THR:OG1	4:F:570:VAL:N	2.52	0.43
3:E:155:LYS:HE2	3:E:178:ARG:HB3	2.00	0.43
3:E:185:ASN:HD21	3:E:189:LYS:HA	1.83	0.43
1:M:6:GLU:HG3	1:M:92:CYS:HB3	2.00	0.43
3:E:53:PHE:HE1	4:F:575:GLN:HG3	1.83	0.43
1:H:36:TRP:CE2	1:H:80:LEU:HD22	2.53	0.43
4:D:617:ARG:HD2	4:D:622:ILE:HG13	1.99	0.43
3:C:86:LEU:HD12	3:C:242:VAL:HG12	2.01	0.43
3:A:355:ASN:OD1	3:A:356:ASN:N	2.50	0.43
3:E:165:LEU:HB2	3:E:168:LYS:HB2	2.00	0.43
3:E:216:HIS:ND1	3:E:248:THR:O	2.44	0.43
4:D:570:VAL:HA	4:D:573:ILE:HD12	1.99	0.43
3:C:372:THR:HG23	5:d:1:NAG:H81	2.01	0.43
3:E:122:LEU:HB3	3:E:125:LEU:HD12	2.01	0.43
3:E:302:ASN:HB3	3:E:441:GLY:H	1.84	0.43
1:M:32:TYR:HD2	1:M:94:ARG:HD2	1.83	0.43
1:M:100(J):ARG:NH2	3:A:82:GLN:HB3	2.33	0.43
3:A:259:LEU:HB2	3:A:374:HIS:CE1	2.54	0.43
3:C:429:ARG:HG2	3:C:431:GLY:H	1.83	0.42
1:H:35:TYR:OH	1:H:100(P):SER:O	2.35	0.42
3:C:34:LEU:HG	3:C:500:ARG:HG2	2.00	0.42
3:E:45:TRP:HE3	4:F:629:LEU:HD21	1.84	0.42
3:E:350:ARG:HA	3:E:353:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:360:ARG:HB2	3:A:467:THR:HG22	2.02	0.42
3:A:174:SER:OG	3:A:175:LEU:N	2.50	0.42
3:C:167:ASP:OD1	3:C:167:ASP:N	2.52	0.42
3:E:53:PHE:HD2	3:E:218:CYS:HB2	1.84	0.42
2:L:4:MET:HA	2:L:25:SER:HA	2.00	0.42
3:A:304:ARG:HD2	3:A:318:TYR:HB3	2.01	0.42
1:H:55:TRP:CH2	8:T:3:BMA:O5	2.72	0.42
3:A:365:SER:HB3	3:A:469:ARG:HD3	2.02	0.42
4:B:652:GLN:HG3	4:B:653:GLN:HG2	2.01	0.42
3:C:57:ASP:HA	3:C:77:THR:HG22	2.01	0.42
3:E:90:THR:HG22	3:E:240:PRO:HA	2.01	0.42
3:C:46:LYS:HB2	3:C:490:LYS:HE2	2.00	0.42
3:E:122:LEU:HD11	3:E:203:GLN:HB2	2.02	0.42
3:A:50:THR:OG1	3:A:51:THR:N	2.52	0.42
3:A:299:PRO:O	3:A:327:ARG:NH2	2.52	0.42
3:E:180:ASP:OD2	3:E:422:GLN:N	2.52	0.42
3:E:107:ASP:OD2	4:F:574:LYS:NZ	2.51	0.41
11:h:3:BMA:H62	11:h:6:MAN:H2	1.89	0.41
4:D:658:GLN:HA	4:D:661:LEU:HB2	2.03	0.41
3:E:180:ASP:HB3	3:E:423:ILE:HD12	2.03	0.41
2:N:19:ALA:N	2:N:75:ILE:O	2.51	0.41
1:H:103:TRP:CD2	2:L:44:PRO:HB2	2.56	0.41
3:A:122:LEU:HD21	3:A:203:GLN:HB2	2.02	0.41
1:H:47:TRP:CD1	2:L:96:LEU:HD12	2.55	0.41
1:H:55:TRP:HH2	8:T:3:BMA:C6	1.96	0.41
3:A:52:LEU:CD1	3:A:217:TYR:CD1	3.03	0.41
4:B:541:ALA:O	4:F:591:GLN:NE2	2.53	0.41
3:A:124:PRO:HA	3:C:166:ARG:NE	2.35	0.41
3:C:88:ASN:OD1	13:C:611:NAG:N2	2.54	0.41
3:C:198:THR:HB	5:Y:1:NAG:H82	2.03	0.41
3:E:33:ASN:OD1	3:E:35:TRP:NE1	2.54	0.41
3:A:122:LEU:HB2	3:A:201:ILE:HG23	2.02	0.41
3:C:312:GLY:N	3:C:315:GLN:HB2	2.36	0.41
3:C:477:ASP:HA	3:C:480:ARG:HB2	2.03	0.41
1:M:104:GLY:O	2:N:43:SER:OG	2.37	0.40
1:H:55:TRP:HD1	1:H:100(M):TYR:HH	0.65	0.40
3:C:457:ASP:OD2	3:C:469:ARG:NH1	2.54	0.40
3:E:38:VAL:HG22	3:E:496:VAL:HG12	2.03	0.40
3:E:36:VAL:HA	3:E:498:PRO:HA	2.03	0.40
3:E:304:ARG:NH1	3:E:438:PRO:O	2.53	0.40
1:M:38:ARG:O	1:M:46:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100(H):SER:HB2	1:H:100(J):ARG:HD3	2.04	0.40
3:A:66:HIS:NE2	3:A:72:HIS:HB2	2.37	0.40
3:C:358:ILE:HG23	3:C:396:ILE:HA	2.02	0.40
3:E:233:PHE:O	3:E:273:ARG:NH2	2.54	0.40
3:E:302:ASN:ND2	3:E:439:ILE:O	2.54	0.40
3:E:338:TRP:CE2	3:E:390:LEU:HD22	2.56	0.40
3:E:426:MET:HB3	3:E:427:TRP:H	1.72	0.40
1:H:90:TYR:O	1:H:107:THR:N	2.47	0.40
3:C:301:ASN:OD1	5:W:1:NAG:N2	2.55	0.40
3:E:257:THR:OG1	3:E:375:SER:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	133/240 (55%)	120 (90%)	13 (10%)	0	100	100
1	M	133/240 (55%)	118 (89%)	14 (10%)	1 (1%)	16	53
2	L	112/219 (51%)	100 (89%)	12 (11%)	0	100	100
2	N	110/219 (50%)	94 (86%)	15 (14%)	1 (1%)	14	49
3	A	432/494 (87%)	385 (89%)	44 (10%)	3 (1%)	18	55
3	C	436/494 (88%)	397 (91%)	39 (9%)	0	100	100
3	E	430/494 (87%)	398 (93%)	32 (7%)	0	100	100
4	B	130/220 (59%)	118 (91%)	12 (9%)	0	100	100
4	D	142/220 (64%)	123 (87%)	19 (13%)	0	100	100
4	F	123/220 (56%)	109 (89%)	14 (11%)	0	100	100
All	All	2181/3060 (71%)	1962 (90%)	214 (10%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	52	LEU
3	A	425	ASN
2	N	51	VAL
3	A	53	PHE
1	M	100(I)	GLY

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	H	116/207 (56%)	116 (100%)	0	100	100
1	M	115/207 (56%)	115 (100%)	0	100	100
2	L	101/195 (52%)	101 (100%)	0	100	100
2	N	99/195 (51%)	99 (100%)	0	100	100
3	A	393/439 (90%)	390 (99%)	3 (1%)	73	77
3	C	395/439 (90%)	394 (100%)	1 (0%)	86	84
3	E	391/439 (89%)	391 (100%)	0	100	100
4	B	112/184 (61%)	112 (100%)	0	100	100
4	D	122/184 (66%)	122 (100%)	0	100	100
4	F	109/184 (59%)	109 (100%)	0	100	100
All	All	1953/2673 (73%)	1949 (100%)	4 (0%)	85	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	52	LEU
3	A	426	MET
3	A	428	GLN
3	C	42	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	76	ASN
1	M	97	GLN
1	H	76	ASN
1	H	100(K)	ASN
3	A	348	GLN
3	A	352	HIS
3	A	374	HIS
3	A	377	ASN
3	A	478	ASN
4	D	562	GLN
4	D	607	ASN
4	D	651	ASN
3	C	195	ASN
3	C	203	GLN
3	C	289	ASN
3	C	440	GLN
3	E	72	HIS
3	E	105	HIS
3	E	185	ASN
3	E	289	ASN
3	E	315	GLN
3	E	440	GLN
4	F	540	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

108 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	3,5	14,14,15	0.37	0	17,19,21	0.70	0
5	NAG	G	2	5	14,14,15	0.21	0	17,19,21	0.63	1 (5%)
5	NAG	I	1	3,5	14,14,15	0.20	0	17,19,21	0.57	0
5	NAG	I	2	5	14,14,15	0.39	0	17,19,21	0.49	0
5	NAG	J	1	3,5	14,14,15	0.51	0	17,19,21	0.78	0
5	NAG	J	2	5	14,14,15	0.71	1 (7%)	17,19,21	0.64	1 (5%)
6	NAG	K	1	6,3	14,14,15	0.22	0	17,19,21	0.56	0
6	NAG	K	2	6	14,14,15	0.34	0	17,19,21	0.67	0
6	BMA	K	3	6	11,11,12	0.84	0	15,15,17	0.86	0
6	MAN	K	4	6	11,11,12	0.70	0	15,15,17	1.52	3 (20%)
6	MAN	K	5	6	11,11,12	1.09	1 (9%)	15,15,17	1.18	1 (6%)
6	MAN	K	6	6	11,11,12	0.73	0	15,15,17	0.96	1 (6%)
5	NAG	O	1	3,5	14,14,15	0.44	0	17,19,21	0.58	0
5	NAG	O	2	5	14,14,15	0.24	0	17,19,21	0.61	1 (5%)
5	NAG	P	1	3,5	14,14,15	0.63	1 (7%)	17,19,21	0.67	0
5	NAG	P	2	5	14,14,15	0.53	0	17,19,21	0.73	1 (5%)
7	NAG	Q	1	7,3	14,14,15	0.27	0	17,19,21	0.59	0
7	NAG	Q	2	7	14,14,15	0.40	0	17,19,21	0.75	0
7	BMA	Q	3	7	11,11,12	0.95	0	15,15,17	0.84	0
5	NAG	R	1	3,5	14,14,15	0.37	0	17,19,21	0.56	0
5	NAG	R	2	5	14,14,15	0.33	0	17,19,21	0.46	0
5	NAG	S	1	3,5	14,14,15	0.32	0	17,19,21	0.66	0
5	NAG	S	2	5	14,14,15	0.46	0	17,19,21	0.69	1 (5%)
8	NAG	T	1	8,4	14,14,15	0.44	0	17,19,21	0.80	1 (5%)
8	NAG	T	10	8	14,14,15	0.25	0	17,19,21	0.52	0
8	FUC	T	11	8	10,10,11	0.75	0	14,14,16	0.90	0
8	NAG	T	2	8	14,14,15	0.34	0	17,19,21	0.68	0
8	BMA	T	3	8	11,11,12	1.08	1 (9%)	15,15,17	1.75	5 (33%)
8	MAN	T	4	8	11,11,12	1.13	2 (18%)	15,15,17	1.15	2 (13%)
8	NAG	T	5	8	14,14,15	0.51	0	17,19,21	0.55	0
8	GAL	T	6	8	11,11,12	0.74	0	15,15,17	0.97	1 (6%)
8	NAG	T	7	8	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
8	GAL	T	8	8	11,11,12	0.62	0	15,15,17	1.25	2 (13%)
8	MAN	T	9	8	11,11,12	0.97	0	15,15,17	1.84	4 (26%)
9	NAG	U	1	4,9	14,14,15	0.40	0	17,19,21	1.37	3 (17%)
9	FUC	U	10	9	10,10,11	0.86	1 (10%)	14,14,16	0.90	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	U	2	9	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
9	BMA	U	3	9	11,11,12	0.99	1 (9%)	15,15,17	1.25	2 (13%)
9	MAN	U	4	9	11,11,12	0.99	1 (9%)	15,15,17	1.60	3 (20%)
9	NAG	U	5	9	14,14,15	0.22	0	17,19,21	0.50	0
9	GAL	U	6	9	11,11,12	0.67	0	15,15,17	1.18	2 (13%)
9	NAG	U	7	9	14,14,15	0.36	0	17,19,21	0.44	0
9	MAN	U	8	9	11,11,12	0.88	0	15,15,17	1.47	2 (13%)
9	NAG	U	9	9	14,14,15	0.30	0	17,19,21	0.43	0
5	NAG	V	1	4,5	14,14,15	0.22	0	17,19,21	0.55	0
5	NAG	V	2	5	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	W	1	3,5	14,14,15	0.27	0	17,19,21	0.62	0
5	NAG	W	2	5	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
5	NAG	X	1	3,5	14,14,15	0.41	0	17,19,21	0.41	0
5	NAG	X	2	5	14,14,15	0.41	0	17,19,21	0.50	0
5	NAG	Y	1	3,5	14,14,15	0.25	0	17,19,21	0.64	0
5	NAG	Y	2	5	14,14,15	0.44	0	17,19,21	0.68	1 (5%)
5	NAG	Z	1	3,5	14,14,15	0.27	0	17,19,21	0.68	1 (5%)
5	NAG	Z	2	5	14,14,15	0.31	0	17,19,21	0.61	0
5	NAG	a	1	3,5	14,14,15	0.22	0	17,19,21	0.49	0
5	NAG	a	2	5	14,14,15	0.28	0	17,19,21	0.89	1 (5%)
5	NAG	b	1	3,5	14,14,15	0.78	0	17,19,21	2.42	3 (17%)
5	NAG	b	2	5	14,14,15	0.31	0	17,19,21	0.64	1 (5%)
5	NAG	c	1	3,5	14,14,15	0.34	0	17,19,21	0.57	0
5	NAG	c	2	5	14,14,15	0.28	0	17,19,21	0.59	0
5	NAG	d	1	3,5	14,14,15	0.28	0	17,19,21	0.54	0
5	NAG	d	2	5	14,14,15	0.33	0	17,19,21	0.62	1 (5%)
10	NAG	e	1	10,3	14,14,15	0.40	0	17,19,21	0.65	0
10	NAG	e	2	10	14,14,15	0.17	0	17,19,21	0.68	1 (5%)
10	BMA	e	3	10	11,11,12	0.80	0	15,15,17	1.16	1 (6%)
10	MAN	e	4	10	11,11,12	1.15	2 (18%)	15,15,17	1.18	1 (6%)
5	NAG	f	1	3,5	14,14,15	1.55	1 (7%)	17,19,21	1.41	2 (11%)
5	NAG	f	2	5	14,14,15	0.40	0	17,19,21	0.43	0
5	NAG	g	1	3,5	14,14,15	1.12	1 (7%)	17,19,21	1.81	1 (5%)
5	NAG	g	2	5	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
11	NAG	h	1	11,3	14,14,15	0.34	0	17,19,21	0.44	0
11	NAG	h	2	11	14,14,15	0.42	0	17,19,21	0.58	0
11	BMA	h	3	11	11,11,12	0.74	0	15,15,17	0.78	1 (6%)
11	MAN	h	4	11	11,11,12	0.75	0	15,15,17	1.21	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	h	5	11	11,11,12	0.79	0	15,15,17	1.04	2 (13%)
11	MAN	h	6	11	11,11,12	0.74	0	15,15,17	1.09	2 (13%)
11	MAN	h	7	11	11,11,12	0.81	0	15,15,17	0.96	2 (13%)
5	NAG	i	1	3,5	14,14,15	0.23	0	17,19,21	0.70	1 (5%)
5	NAG	i	2	5	14,14,15	0.27	0	17,19,21	0.50	0
7	NAG	j	1	7,3	14,14,15	1.20	2 (14%)	17,19,21	1.38	1 (5%)
7	NAG	j	2	7	14,14,15	0.18	0	17,19,21	0.63	1 (5%)
7	BMA	j	3	7	11,11,12	0.53	0	15,15,17	1.39	2 (13%)
5	NAG	k	1	3,5	14,14,15	0.83	1 (7%)	17,19,21	2.39	3 (17%)
5	NAG	k	2	5	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
5	NAG	l	1	3,5	14,14,15	0.22	0	17,19,21	0.59	0
5	NAG	l	2	5	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	m	1	3,5	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	m	2	5	14,14,15	0.27	0	17,19,21	0.61	1 (5%)
12	NAG	n	1	4,12	14,14,15	0.29	0	17,19,21	0.50	0
12	FUC	n	10	12	10,10,11	0.62	0	14,14,16	0.90	0
12	NAG	n	2	12	14,14,15	0.20	0	17,19,21	0.83	1 (5%)
12	BMA	n	3	12	11,11,12	1.00	1 (9%)	15,15,17	0.91	1 (6%)
12	MAN	n	4	12	11,11,12	1.04	2 (18%)	15,15,17	1.10	1 (6%)
12	NAG	n	5	12	14,14,15	0.58	0	17,19,21	0.79	1 (5%)
12	GAL	n	6	12	11,11,12	0.83	0	15,15,17	1.24	2 (13%)
12	NAG	n	7	12	14,14,15	0.21	0	17,19,21	0.50	0
12	GAL	n	8	12	11,11,12	0.74	0	15,15,17	0.98	0
12	MAN	n	9	12	11,11,12	0.67	0	15,15,17	1.17	2 (13%)
9	NAG	o	1	4,9	14,14,15	0.25	0	17,19,21	1.09	1 (5%)
9	FUC	o	10	9	10,10,11	0.90	0	14,14,16	1.13	1 (7%)
9	NAG	o	2	9	14,14,15	0.48	0	17,19,21	0.61	0
9	BMA	o	3	9	11,11,12	1.40	2 (18%)	15,15,17	1.42	1 (6%)
9	MAN	o	4	9	11,11,12	1.02	1 (9%)	15,15,17	1.75	2 (13%)
9	NAG	o	5	9	14,14,15	0.28	0	17,19,21	0.51	0
9	GAL	o	6	9	11,11,12	0.72	0	15,15,17	1.05	1 (6%)
9	NAG	o	7	9	14,14,15	0.23	0	17,19,21	0.40	0
9	MAN	o	8	9	11,11,12	0.64	0	15,15,17	1.36	2 (13%)
9	NAG	o	9	9	14,14,15	0.26	0	17,19,21	0.60	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
6	NAG	K	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	2/2/19/22	1/1/1/1
6	MAN	K	6	6	-	1/2/19/22	0/1/1/1
5	NAG	O	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	3/6/23/26	0/1/1/1
5	NAG	P	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
5	NAG	R	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	1/6/23/26	0/1/1/1
5	NAG	S	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	2/6/23/26	0/1/1/1
8	NAG	T	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	T	10	8	-	2/6/23/26	0/1/1/1
8	FUC	T	11	8	-	-	0/1/1/1
8	NAG	T	2	8	-	2/6/23/26	0/1/1/1
8	BMA	T	3	8	-	2/2/19/22	0/1/1/1
8	MAN	T	4	8	-	0/2/19/22	0/1/1/1
8	NAG	T	5	8	-	2/6/23/26	0/1/1/1
8	GAL	T	6	8	-	2/2/19/22	0/1/1/1
8	NAG	T	7	8	-	2/6/23/26	0/1/1/1
8	GAL	T	8	8	-	1/2/19/22	0/1/1/1
8	MAN	T	9	8	-	2/2/19/22	0/1/1/1
9	NAG	U	1	4,9	-	2/6/23/26	0/1/1/1
9	FUC	U	10	9	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	U	2	9	-	1/6/23/26	0/1/1/1
9	BMA	U	3	9	-	2/2/19/22	0/1/1/1
9	MAN	U	4	9	-	0/2/19/22	0/1/1/1
9	NAG	U	5	9	-	2/6/23/26	0/1/1/1
9	GAL	U	6	9	-	2/2/19/22	0/1/1/1
9	NAG	U	7	9	-	1/6/23/26	0/1/1/1
9	MAN	U	8	9	-	0/2/19/22	0/1/1/1
9	NAG	U	9	9	-	1/6/23/26	0/1/1/1
5	NAG	V	1	4,5	-	1/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	NAG	W	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	NAG	X	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Y	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	NAG	Z	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	NAG	a	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	NAG	b	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	NAG	c	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	NAG	d	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	0/6/23/26	0/1/1/1
10	NAG	e	1	10,3	-	2/6/23/26	0/1/1/1
10	NAG	e	2	10	-	0/6/23/26	0/1/1/1
10	BMA	e	3	10	-	1/2/19/22	0/1/1/1
10	MAN	e	4	10	-	0/2/19/22	0/1/1/1
5	NAG	f	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	1/6/23/26	0/1/1/1
5	NAG	g	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
11	NAG	h	1	11,3	-	2/6/23/26	0/1/1/1
11	NAG	h	2	11	-	0/6/23/26	0/1/1/1
11	BMA	h	3	11	-	2/2/19/22	0/1/1/1
11	MAN	h	4	11	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	h	5	11	-	1/2/19/22	0/1/1/1
11	MAN	h	6	11	-	0/2/19/22	0/1/1/1
11	MAN	h	7	11	-	2/2/19/22	0/1/1/1
5	NAG	i	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	i	2	5	-	2/6/23/26	0/1/1/1
7	NAG	j	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
7	BMA	j	3	7	-	2/2/19/22	0/1/1/1
5	NAG	k	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	k	2	5	-	2/6/23/26	0/1/1/1
5	NAG	l	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	l	2	5	-	3/6/23/26	0/1/1/1
5	NAG	m	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	m	2	5	-	2/6/23/26	0/1/1/1
12	NAG	n	1	4,12	-	0/6/23/26	0/1/1/1
12	FUC	n	10	12	-	-	0/1/1/1
12	NAG	n	2	12	-	2/6/23/26	0/1/1/1
12	BMA	n	3	12	-	1/2/19/22	0/1/1/1
12	MAN	n	4	12	-	0/2/19/22	0/1/1/1
12	NAG	n	5	12	-	0/6/23/26	0/1/1/1
12	GAL	n	6	12	-	2/2/19/22	0/1/1/1
12	NAG	n	7	12	-	1/6/23/26	0/1/1/1
12	GAL	n	8	12	-	2/2/19/22	0/1/1/1
12	MAN	n	9	12	-	1/2/19/22	0/1/1/1
9	NAG	o	1	4,9	-	4/6/23/26	0/1/1/1
9	FUC	o	10	9	-	-	0/1/1/1
9	NAG	o	2	9	-	2/6/23/26	0/1/1/1
9	BMA	o	3	9	-	0/2/19/22	0/1/1/1
9	MAN	o	4	9	-	0/2/19/22	0/1/1/1
9	NAG	o	5	9	-	1/6/23/26	0/1/1/1
9	GAL	o	6	9	-	2/2/19/22	0/1/1/1
9	NAG	o	7	9	-	1/6/23/26	0/1/1/1
9	MAN	o	8	9	-	2/2/19/22	0/1/1/1
9	NAG	o	9	9	-	2/6/23/26	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	f	1	NAG	O5-C1	-5.48	1.34	1.43
5	g	1	NAG	O5-C1	4.07	1.50	1.43
7	j	1	NAG	O5-C1	3.87	1.50	1.43
9	o	3	BMA	C1-C2	3.25	1.60	1.52
9	U	4	MAN	C1-C2	2.99	1.59	1.52
10	e	4	MAN	C2-C3	2.68	1.56	1.52
9	o	3	BMA	C2-C3	2.62	1.56	1.52
5	J	2	NAG	C1-C2	2.53	1.55	1.52
6	K	5	MAN	O5-C5	2.40	1.48	1.43
8	T	4	MAN	O5-C1	-2.32	1.39	1.43
8	T	3	BMA	C2-C3	2.31	1.56	1.52
8	T	4	MAN	C1-C2	2.28	1.57	1.52
10	e	4	MAN	C1-C2	2.27	1.57	1.52
12	n	3	BMA	C1-C2	2.27	1.57	1.52
9	o	4	MAN	C1-C2	2.25	1.57	1.52
9	U	10	FUC	C1-C2	2.20	1.57	1.52
9	U	3	BMA	C1-C2	2.18	1.57	1.52
5	P	1	NAG	O5-C1	-2.15	1.40	1.43
7	j	1	NAG	C1-C2	2.14	1.55	1.52
12	n	4	MAN	O5-C1	-2.06	1.40	1.43
5	k	1	NAG	C1-C2	2.05	1.55	1.52
12	n	4	MAN	O2-C2	-2.02	1.39	1.43

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	b	1	NAG	C2-N2-C7	8.34	134.08	122.90
5	k	1	NAG	C2-N2-C7	8.29	134.01	122.90
5	g	1	NAG	C1-O5-C5	7.10	121.71	112.19
7	j	1	NAG	C1-O5-C5	5.25	119.22	112.19
7	j	3	BMA	C1-O5-C5	4.46	118.17	112.19
9	U	8	MAN	C1-O5-C5	4.37	118.04	112.19
5	f	1	NAG	C4-C3-C2	4.33	117.36	111.02
9	U	4	MAN	C1-O5-C5	4.31	117.97	112.19
8	T	9	MAN	C1-O5-C5	4.12	117.70	112.19
5	b	1	NAG	C1-C2-N2	4.08	116.87	110.43
9	o	8	MAN	C1-O5-C5	4.08	117.66	112.19
8	T	9	MAN	O2-C2-C3	-4.07	101.72	110.15
6	K	4	MAN	C1-O5-C5	4.01	117.56	112.19
5	k	1	NAG	C1-C2-N2	3.95	116.67	110.43
9	o	4	MAN	C1-O5-C5	3.89	117.41	112.19
9	o	4	MAN	O2-C2-C3	-3.84	102.21	110.15
12	n	4	MAN	O2-C2-C3	-3.65	102.59	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	3	BMA	C1-O5-C5	3.55	116.95	112.19
6	K	5	MAN	C1-O5-C5	3.46	116.83	112.19
9	o	3	BMA	C1-C2-C3	3.39	114.59	109.64
8	T	4	MAN	O2-C2-C3	-3.37	103.17	110.15
5	a	2	NAG	C1-O5-C5	3.25	116.54	112.19
11	h	4	MAN	C1-O5-C5	3.21	116.49	112.19
9	U	1	NAG	C2-N2-C7	3.19	127.17	122.90
12	n	6	GAL	O2-C2-C3	-3.16	103.60	110.15
9	o	1	NAG	C2-N2-C7	3.12	127.08	122.90
9	U	1	NAG	C1-O5-C5	3.08	116.32	112.19
9	U	4	MAN	O2-C2-C3	-3.08	103.76	110.15
8	T	3	BMA	C1-C2-C3	3.07	114.12	109.64
12	n	9	MAN	C1-O5-C5	3.07	116.30	112.19
9	U	3	BMA	O2-C2-C3	-3.05	103.83	110.15
8	T	9	MAN	O2-C2-C1	2.97	116.02	109.22
8	T	8	GAL	C1-O5-C5	2.94	116.12	112.19
9	U	6	GAL	C1-O5-C5	2.91	116.09	112.19
12	n	2	NAG	C1-O5-C5	2.88	116.05	112.19
8	T	3	BMA	C2-C3-C4	2.85	115.88	110.86
9	U	3	BMA	C1-C2-C3	2.80	113.72	109.64
11	h	5	MAN	C1-O5-C5	2.74	115.86	112.19
10	e	3	BMA	C1-O5-C5	2.73	115.85	112.19
9	U	8	MAN	O2-C2-C3	-2.71	104.53	110.15
5	P	2	NAG	C1-O5-C5	2.69	115.80	112.19
11	h	6	MAN	C1-O5-C5	2.63	115.71	112.19
12	n	6	GAL	C1-O5-C5	2.63	115.71	112.19
5	W	2	NAG	C1-O5-C5	2.60	115.67	112.19
9	o	8	MAN	O2-C2-C3	-2.59	104.78	110.15
5	f	1	NAG	C3-C4-C5	2.56	114.88	110.23
11	h	6	MAN	O2-C2-C3	-2.56	104.84	110.15
9	o	6	GAL	C1-O5-C5	2.54	115.59	112.19
6	K	4	MAN	O3-C3-C2	2.50	115.17	110.05
12	n	9	MAN	O2-C2-C3	-2.45	105.08	110.15
8	T	1	NAG	C1-O5-C5	2.42	115.43	112.19
9	U	1	NAG	C1-C2-N2	2.41	114.23	110.43
11	h	5	MAN	O2-C2-C3	-2.40	105.18	110.15
5	k	2	NAG	C1-O5-C5	2.40	115.40	112.19
8	T	3	BMA	O2-C2-C3	-2.39	105.19	110.15
5	S	2	NAG	C1-O5-C5	2.39	115.38	112.19
5	i	1	NAG	C1-O5-C5	2.38	115.37	112.19
8	T	9	MAN	C1-C2-C3	-2.37	106.20	109.64
5	Y	2	NAG	C1-O5-C5	2.35	115.34	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	h	4	MAN	O2-C2-C3	-2.27	105.45	110.15
6	K	6	MAN	O2-C2-C3	-2.27	105.45	110.15
10	e	2	NAG	C1-O5-C5	2.25	115.20	112.19
5	g	2	NAG	C1-O5-C5	2.24	115.19	112.19
8	T	8	GAL	C1-C2-C3	2.23	112.90	109.64
10	e	4	MAN	C1-O5-C5	2.22	115.16	112.19
5	k	1	NAG	C8-C7-N2	2.22	119.79	116.12
8	T	7	NAG	C1-O5-C5	2.21	115.15	112.19
11	h	7	MAN	C1-O5-C5	2.19	115.12	112.19
9	o	10	FUC	O5-C5-C4	2.19	113.49	109.55
5	b	1	NAG	C8-C7-N2	2.18	119.74	116.12
9	U	4	MAN	C3-C4-C5	-2.17	106.30	110.23
5	b	2	NAG	C1-O5-C5	2.17	115.09	112.19
11	h	7	MAN	O2-C2-C3	-2.17	105.67	110.15
5	G	2	NAG	C1-O5-C5	2.16	115.09	112.19
9	U	2	NAG	C1-O5-C5	2.15	115.07	112.19
5	m	2	NAG	C1-O5-C5	2.14	115.06	112.19
12	n	5	NAG	C1-O5-C5	2.13	115.04	112.19
8	T	4	MAN	C2-C3-C4	2.12	114.60	110.86
11	h	3	BMA	O2-C2-C3	-2.11	105.79	110.15
5	d	2	NAG	C1-O5-C5	2.10	115.01	112.19
12	n	3	BMA	O2-C2-C3	-2.10	105.81	110.15
7	j	2	NAG	C1-O5-C5	2.09	114.98	112.19
5	O	2	NAG	C1-O5-C5	2.08	114.98	112.19
8	T	3	BMA	C3-C4-C5	2.08	114.01	110.23
9	U	10	FUC	O2-C2-C1	2.07	113.97	109.22
5	J	2	NAG	C1-O5-C5	2.07	114.96	112.19
5	Z	1	NAG	C1-O5-C5	2.07	114.96	112.19
7	j	3	BMA	O2-C2-C3	-2.06	105.88	110.15
6	K	4	MAN	O2-C2-C3	-2.03	105.94	110.15
9	U	6	GAL	O2-C2-C3	-2.02	105.96	110.15
9	o	9	NAG	C1-O5-C5	2.02	114.89	112.19
8	T	6	GAL	O3-C3-C4	-2.01	105.65	110.38

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
9	o	9	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
8	T	5	NAG	C4-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
9	o	9	NAG	O5-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
5	l	2	NAG	O5-C5-C6-O6
5	m	1	NAG	O5-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
9	o	6	GAL	O5-C5-C6-O6
12	n	8	GAL	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
11	h	3	BMA	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	m	1	NAG	C4-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
12	n	2	NAG	O5-C5-C6-O6
9	o	2	NAG	C4-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
8	T	3	BMA	O5-C5-C6-O6
8	T	5	NAG	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
6	K	3	BMA	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
8	T	1	NAG	C4-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	k	2	NAG	C4-C5-C6-O6
9	o	6	GAL	C4-C5-C6-O6
12	n	8	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	j	3	BMA	O5-C5-C6-O6
9	o	2	NAG	O5-C5-C6-O6
7	Q	2	NAG	C4-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
9	U	6	GAL	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
5	l	2	NAG	C4-C5-C6-O6
7	Q	3	BMA	C4-C5-C6-O6
5	b	1	NAG	C8-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
5	k	1	NAG	C8-C7-N2-C2
5	k	1	NAG	O7-C7-N2-C2
8	T	8	GAL	O5-C5-C6-O6
9	U	9	NAG	O5-C5-C6-O6
9	o	8	MAN	O5-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
12	n	2	NAG	C4-C5-C6-O6
11	h	4	MAN	O5-C5-C6-O6
9	U	6	GAL	C4-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
9	o	1	NAG	O5-C5-C6-O6
7	j	3	BMA	C4-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
8	T	10	NAG	O5-C5-C6-O6
9	U	5	NAG	C4-C5-C6-O6
8	T	10	NAG	C4-C5-C6-O6
9	o	8	MAN	C4-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
12	n	6	GAL	C4-C5-C6-O6
8	T	6	GAL	C4-C5-C6-O6
5	m	2	NAG	C4-C5-C6-O6
8	T	2	NAG	C4-C5-C6-O6
9	o	7	NAG	O5-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
8	T	9	MAN	C4-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
10	e	1	NAG	C4-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
11	h	3	BMA	C4-C5-C6-O6
8	T	9	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	T	6	GAL	O5-C5-C6-O6
5	f	1	NAG	C4-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
9	U	3	BMA	O5-C5-C6-O6
8	T	7	NAG	C4-C5-C6-O6
9	U	5	NAG	O5-C5-C6-O6
7	j	2	NAG	C4-C5-C6-O6
12	n	6	GAL	O5-C5-C6-O6
9	U	2	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
7	j	1	NAG	C4-C5-C6-O6
12	n	9	MAN	O5-C5-C6-O6
6	K	6	MAN	O5-C5-C6-O6
11	h	7	MAN	O5-C5-C6-O6
9	o	5	NAG	O5-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
12	n	3	BMA	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
9	U	7	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
10	e	1	NAG	O5-C5-C6-O6
11	h	7	MAN	C4-C5-C6-O6
8	T	7	NAG	O5-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	i	2	NAG	C4-C5-C6-O6
6	K	5	MAN	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
9	o	1	NAG	C4-C5-C6-O6
11	h	1	NAG	C4-C5-C6-O6
6	K	5	MAN	C4-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
8	T	3	BMA	C4-C5-C6-O6
11	h	5	MAN	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	i	1	NAG	C4-C5-C6-O6
10	e	3	BMA	C4-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
12	n	7	NAG	C4-C5-C6-O6
5	O	2	NAG	C1-C2-N2-C7
5	R	2	NAG	C1-C2-N2-C7
5	b	1	NAG	C1-C2-N2-C7
5	k	1	NAG	C1-C2-N2-C7
5	l	2	NAG	C1-C2-N2-C7
9	U	1	NAG	C1-C2-N2-C7
9	o	1	NAG	C1-C2-N2-C7
5	b	1	NAG	C3-C2-N2-C7
5	k	1	NAG	C3-C2-N2-C7
9	U	1	NAG	C3-C2-N2-C7
9	o	1	NAG	C3-C2-N2-C7
9	U	3	BMA	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
11	h	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	5	MAN	C1-C2-C3-C4-C5-O5

16 monomers are involved in 34 short contacts:

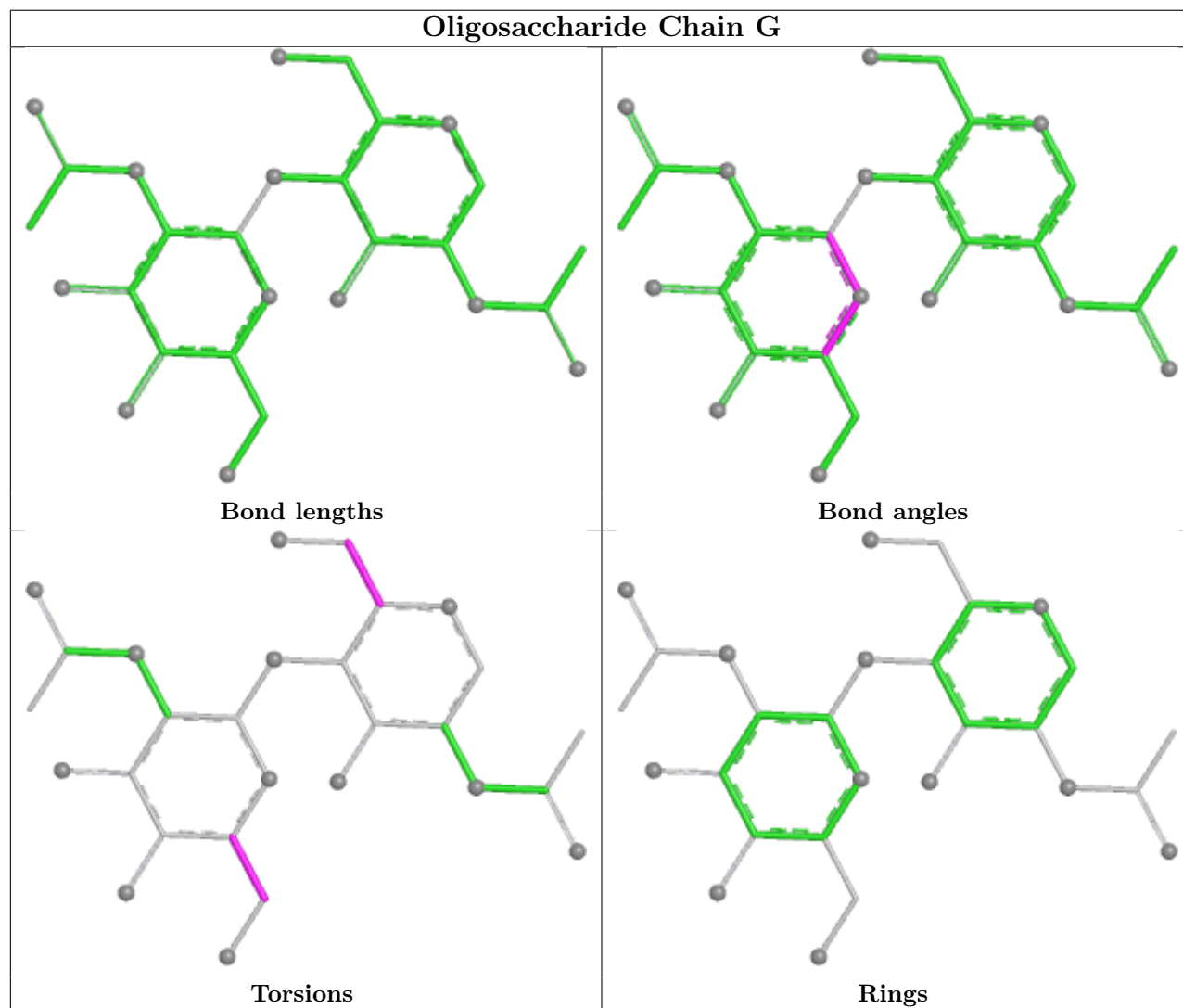
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	e	2	NAG	1	0
9	o	2	NAG	1	0
5	Y	1	NAG	1	0
11	h	6	MAN	1	0
5	d	1	NAG	1	0
8	T	5	NAG	10	0
10	e	1	NAG	1	0
5	a	2	NAG	1	0
9	o	10	FUC	1	0
8	T	3	BMA	12	0
5	G	1	NAG	2	0
5	d	2	NAG	1	0

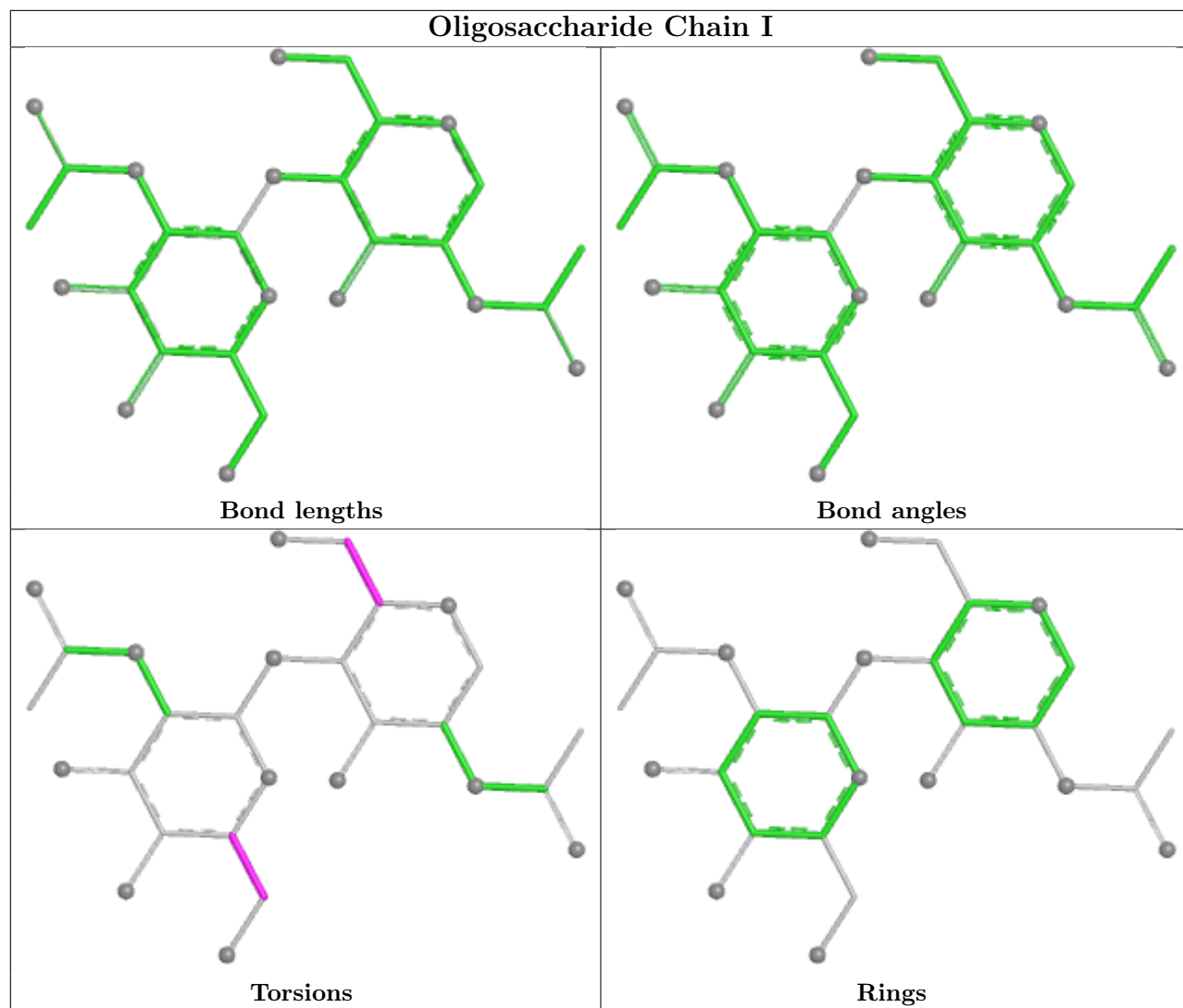
Continued on next page...

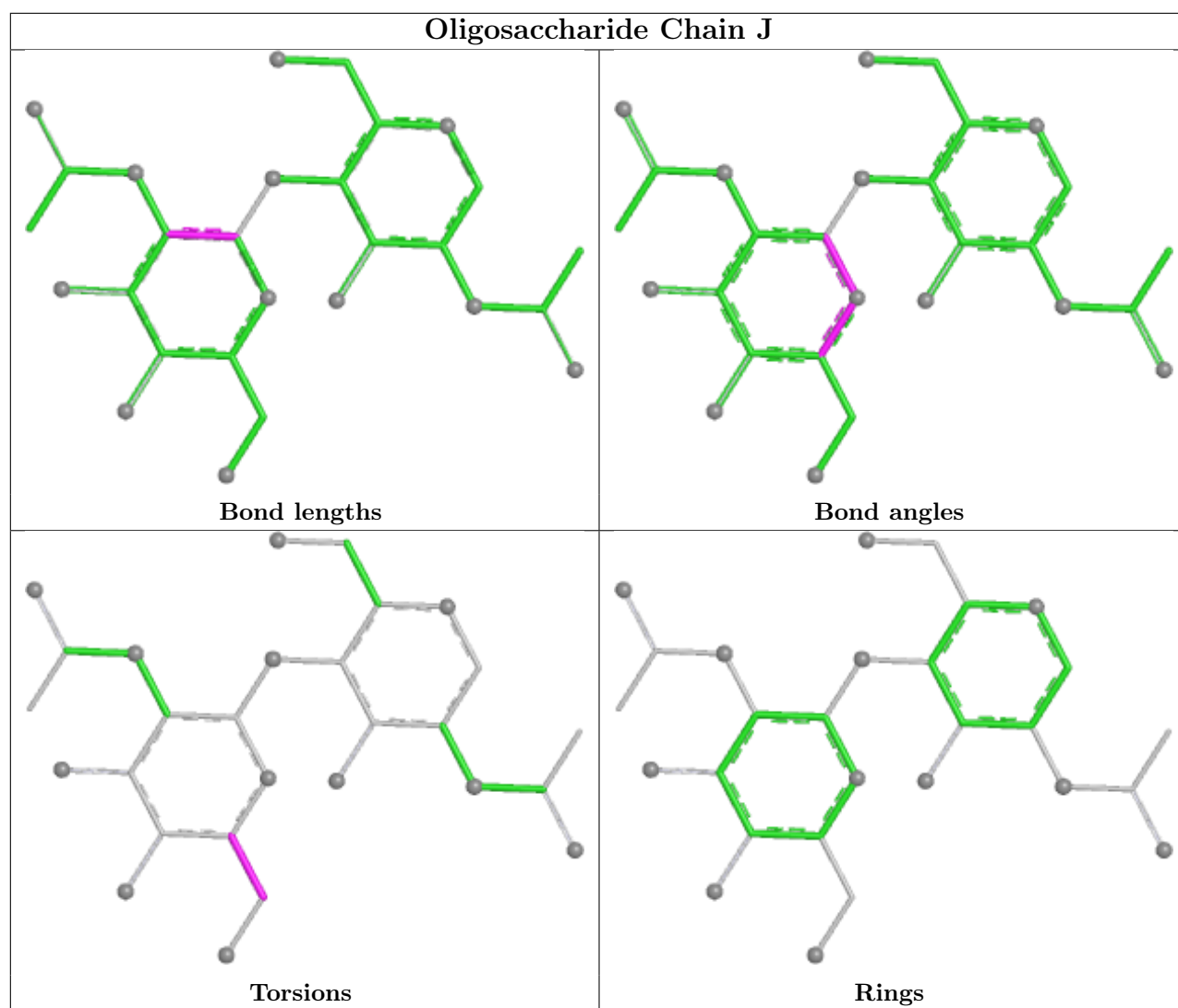
Continued from previous page...

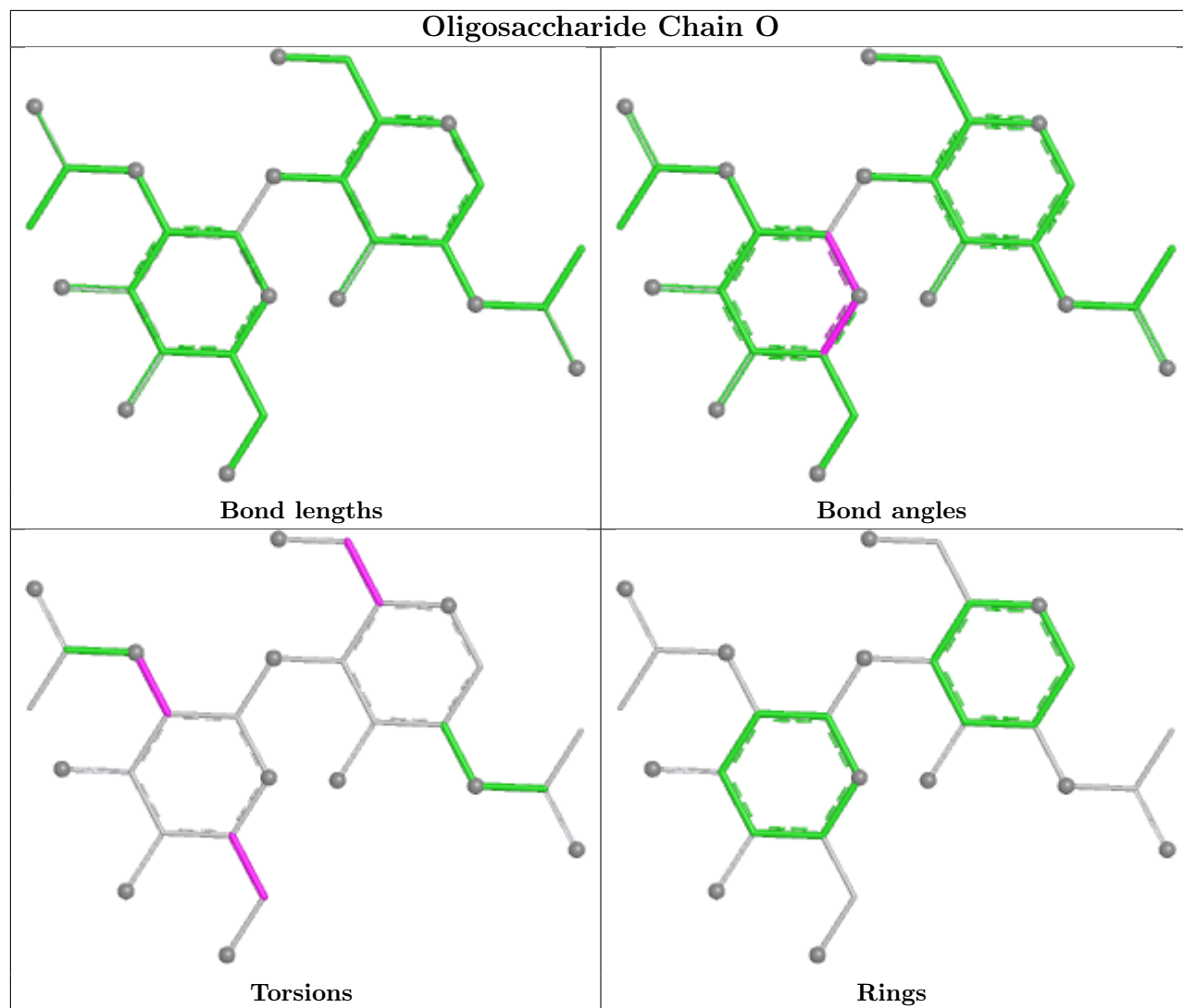
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	W	1	NAG	1	0
5	a	1	NAG	1	0
9	U	2	NAG	1	0
11	h	3	BMA	1	0

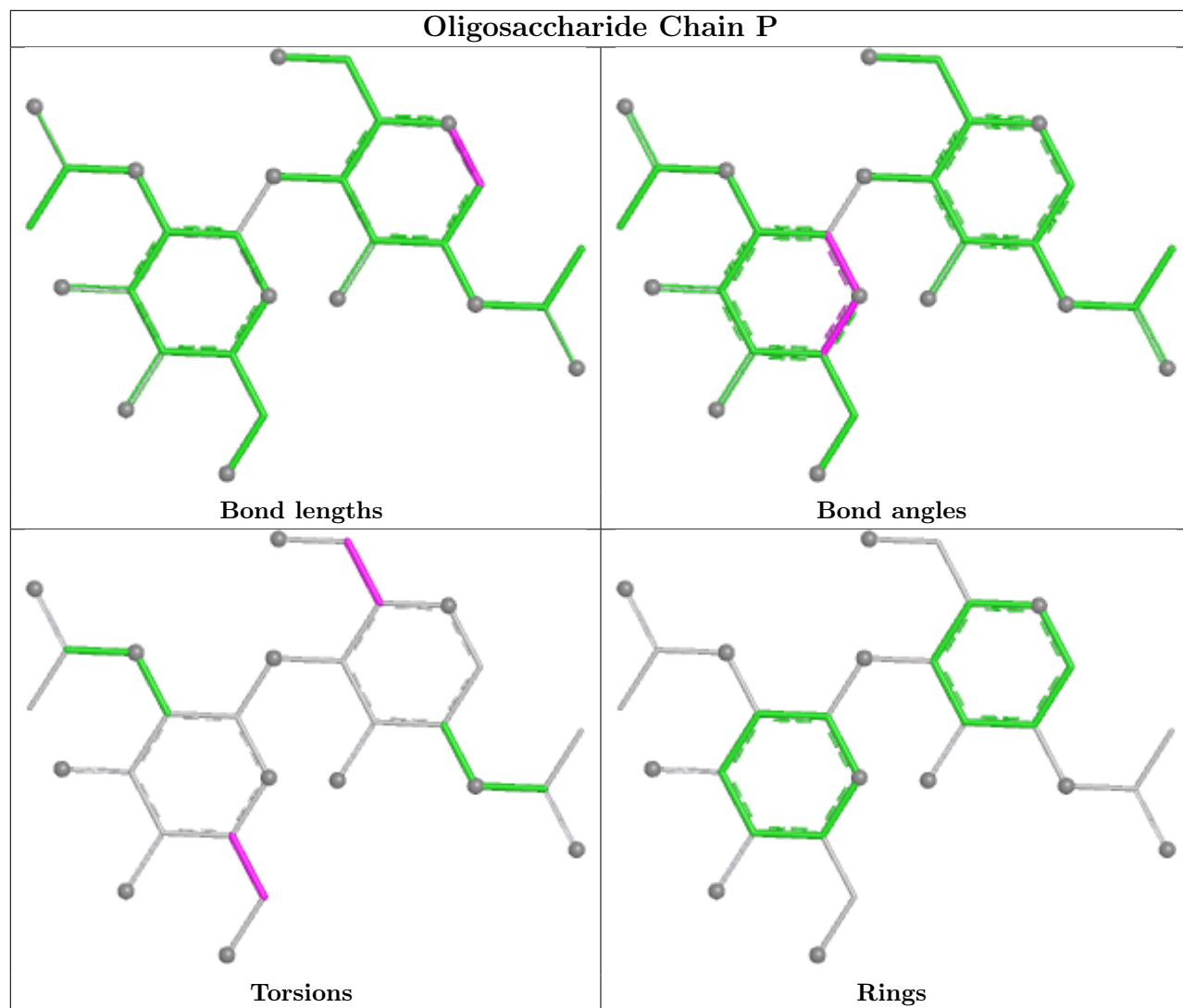
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

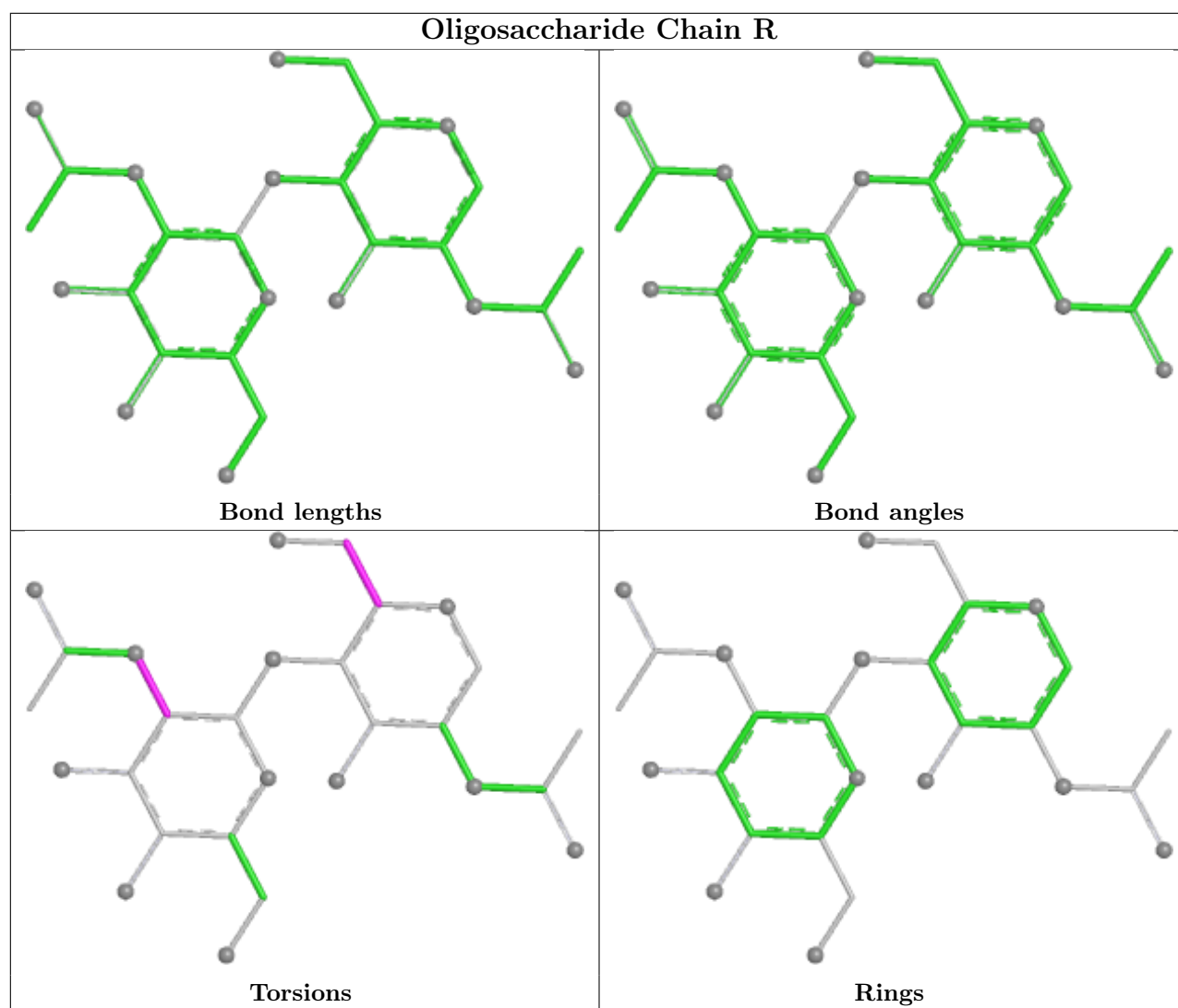


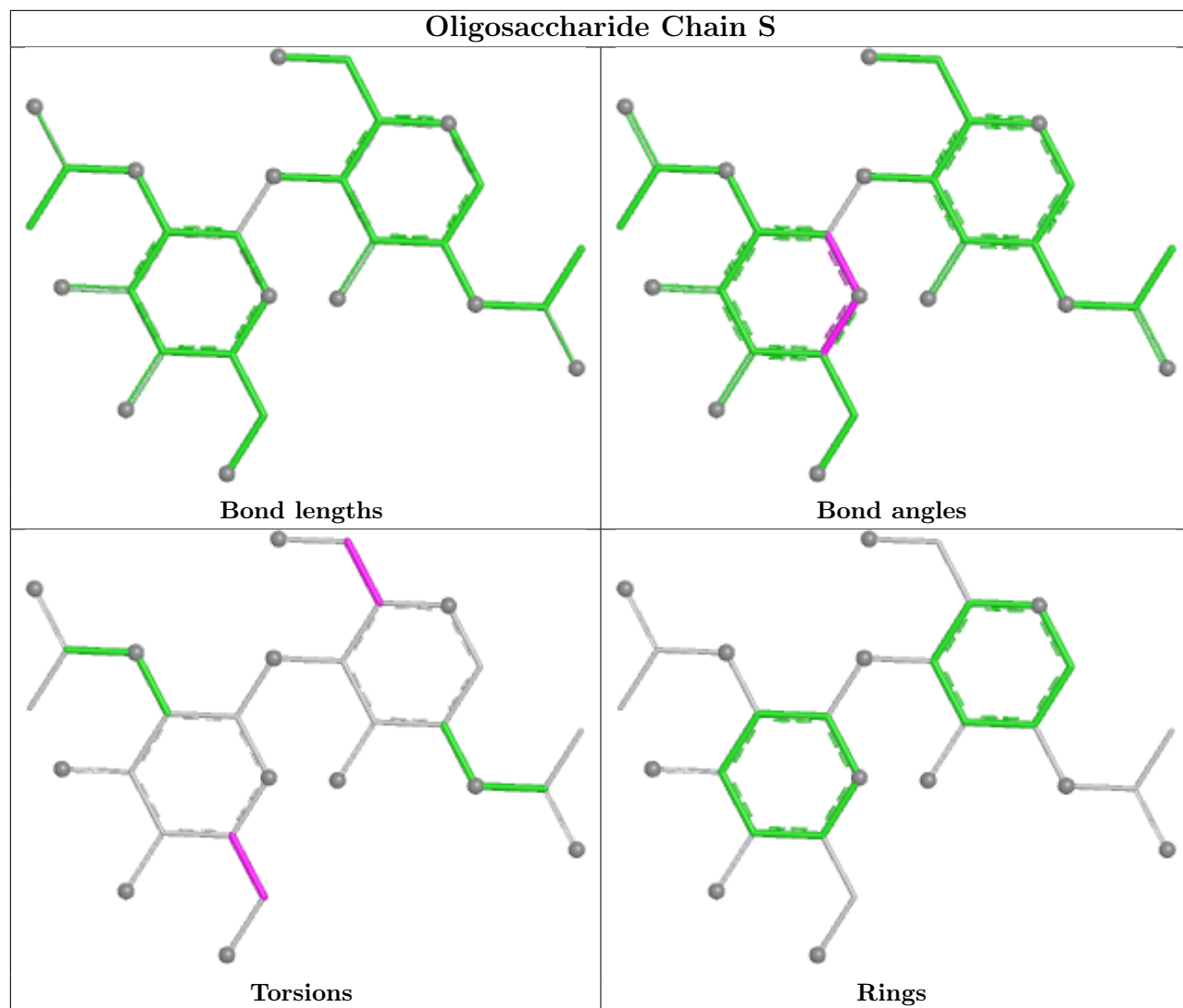


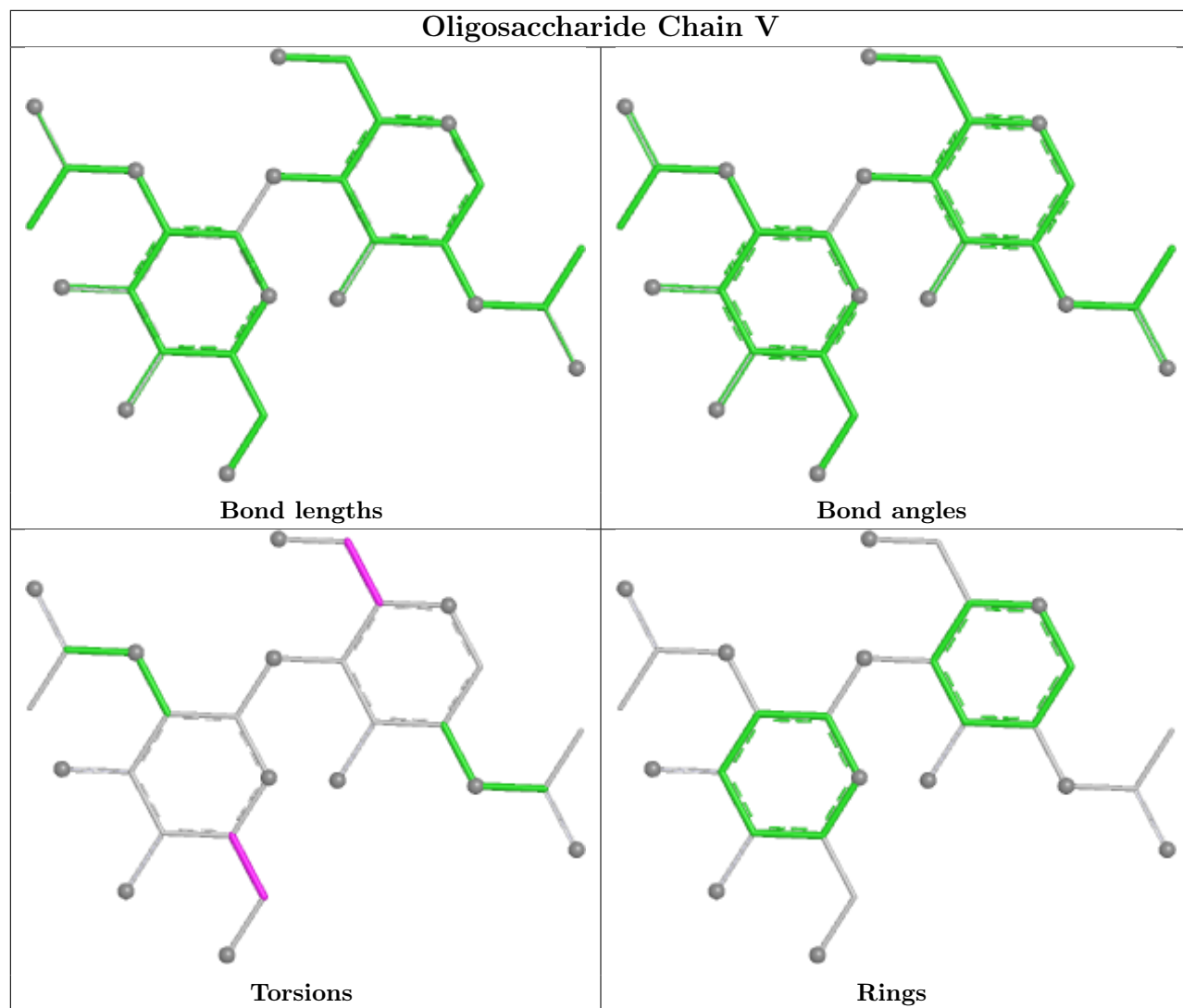


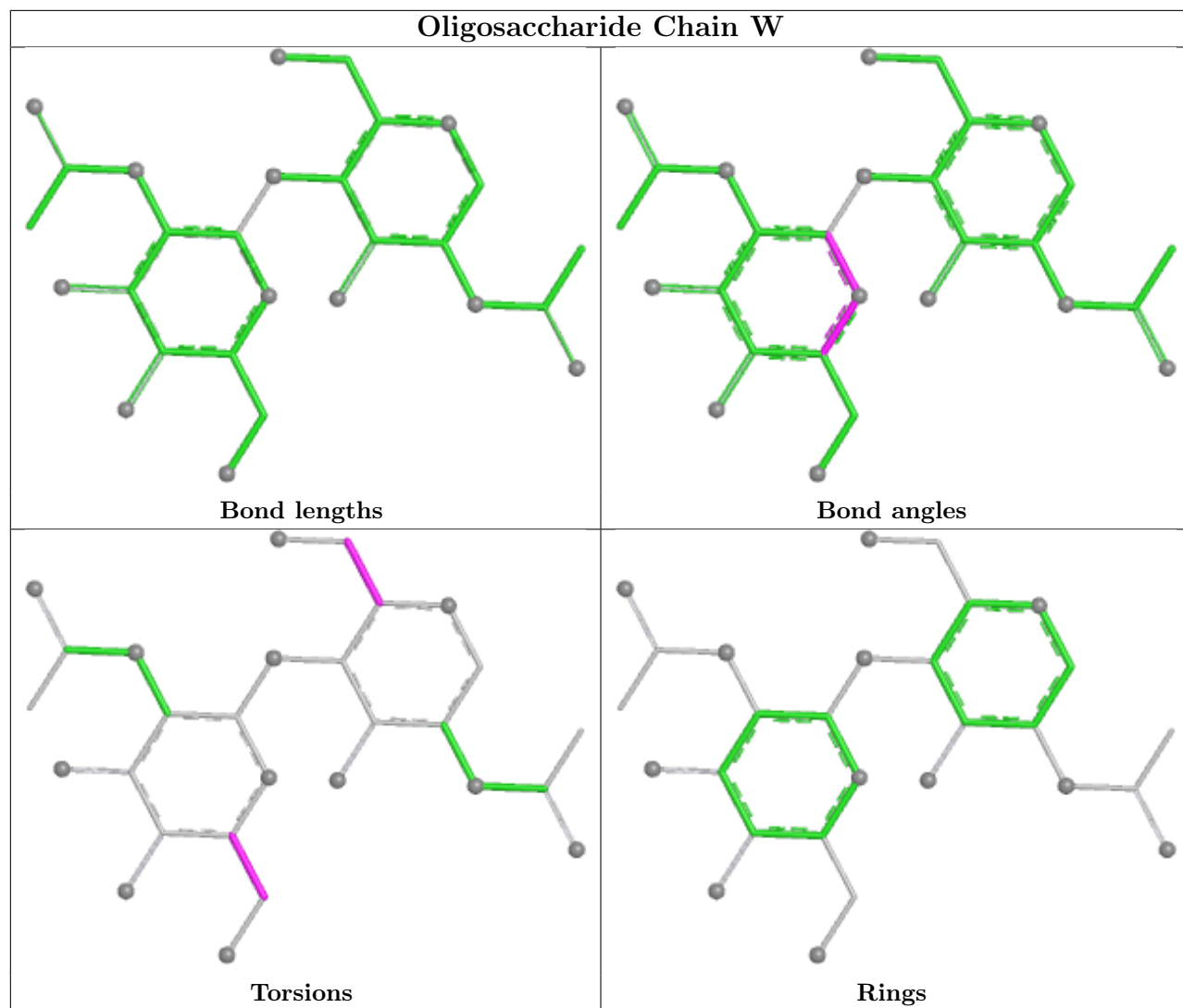


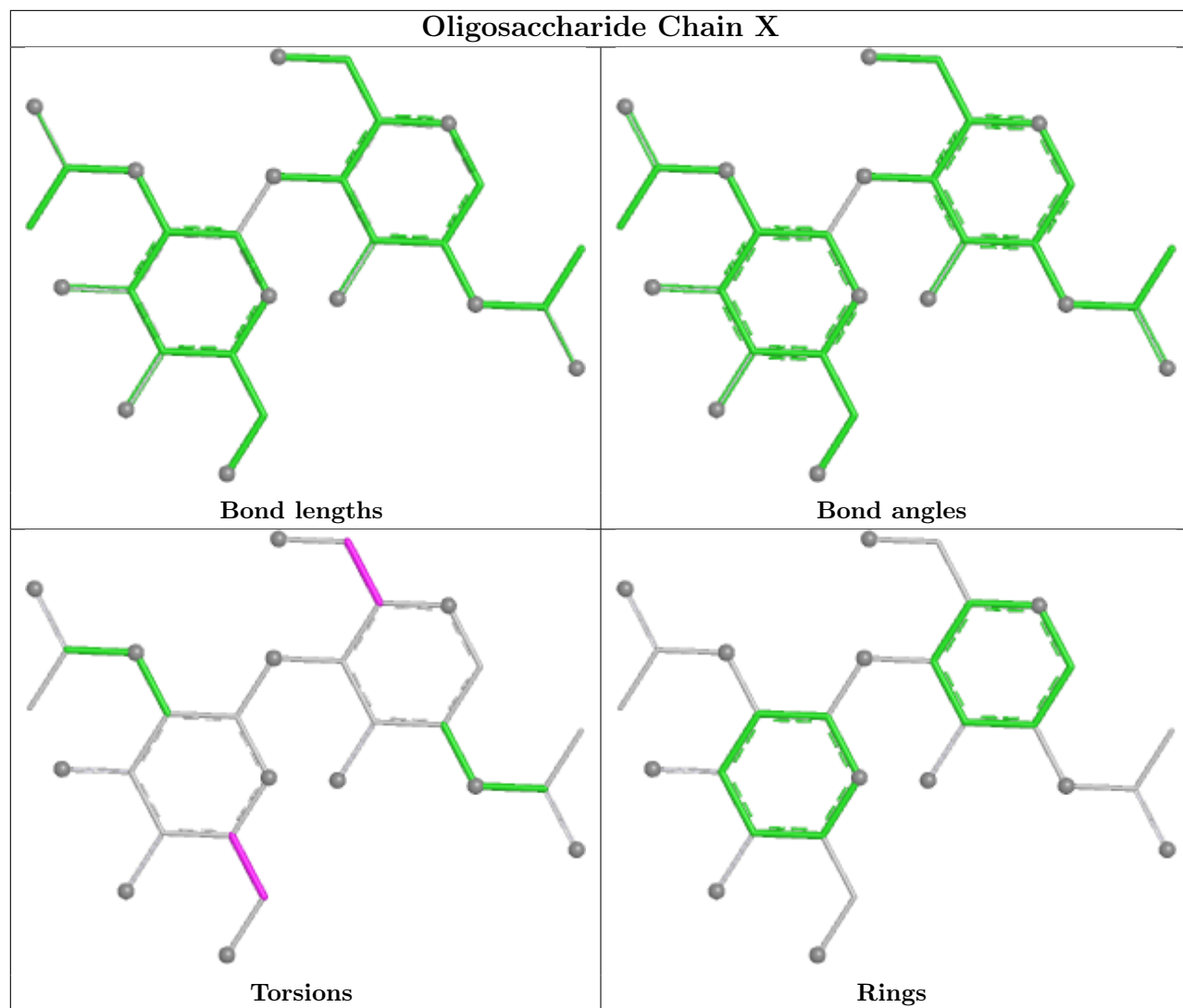


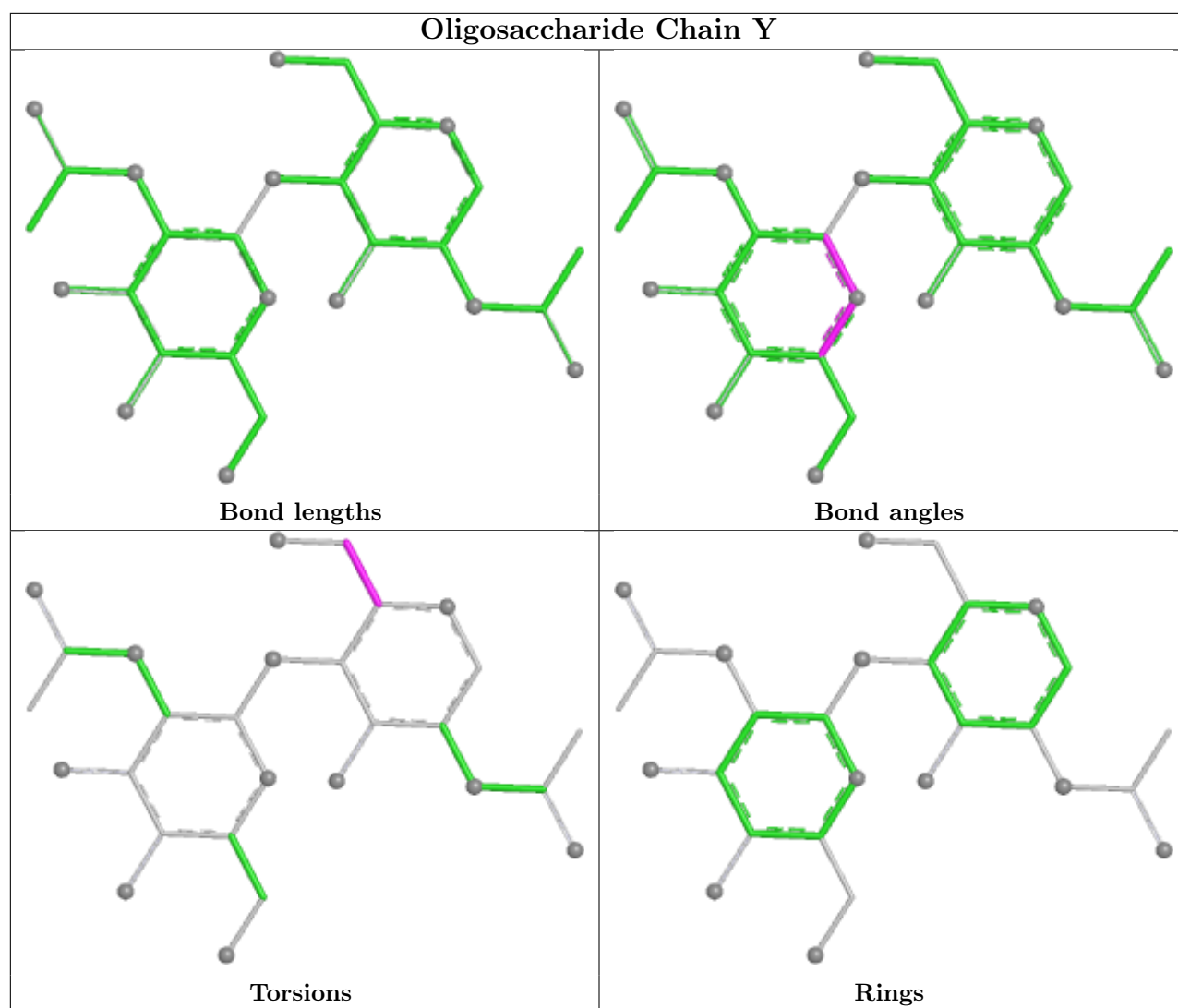


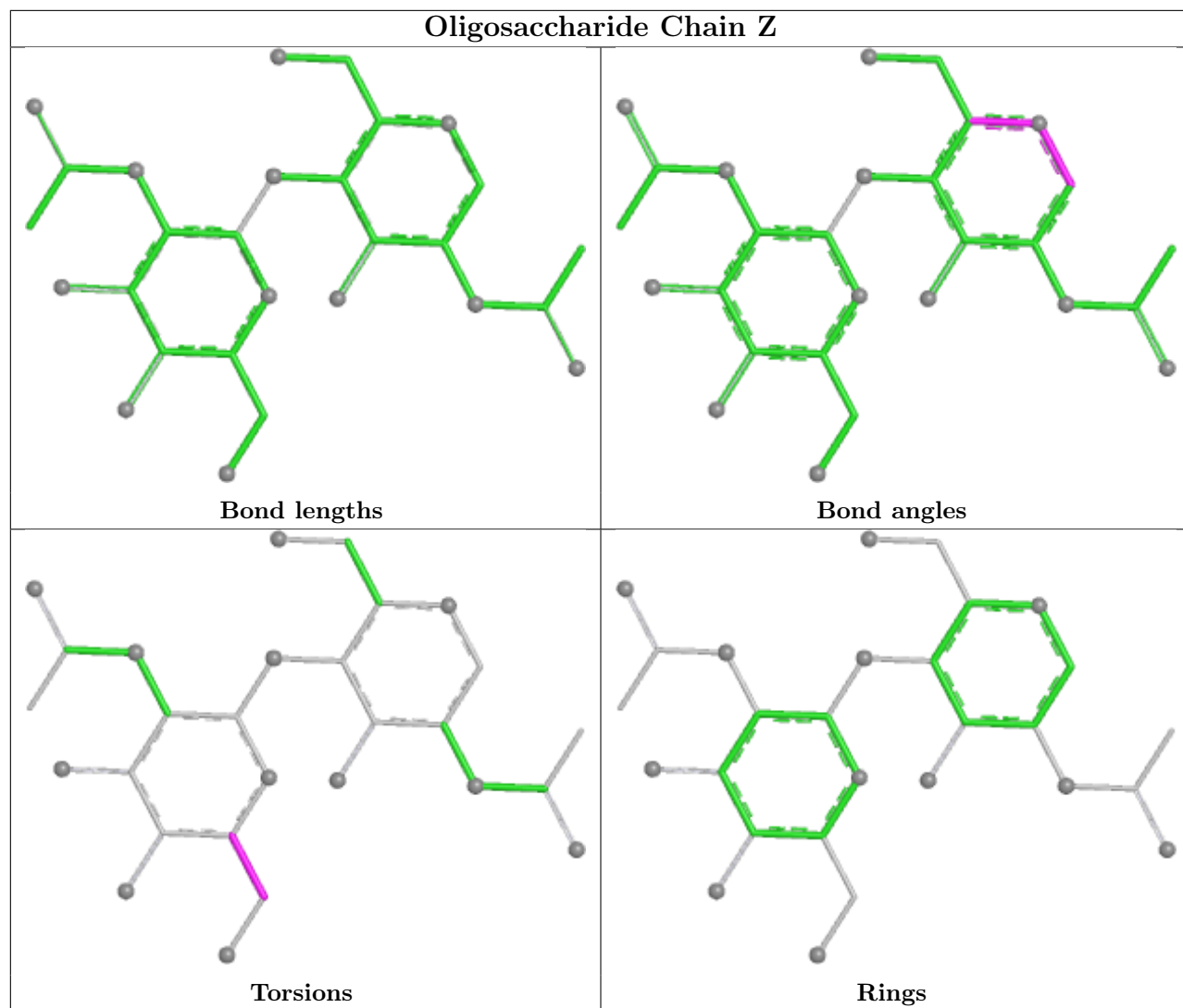


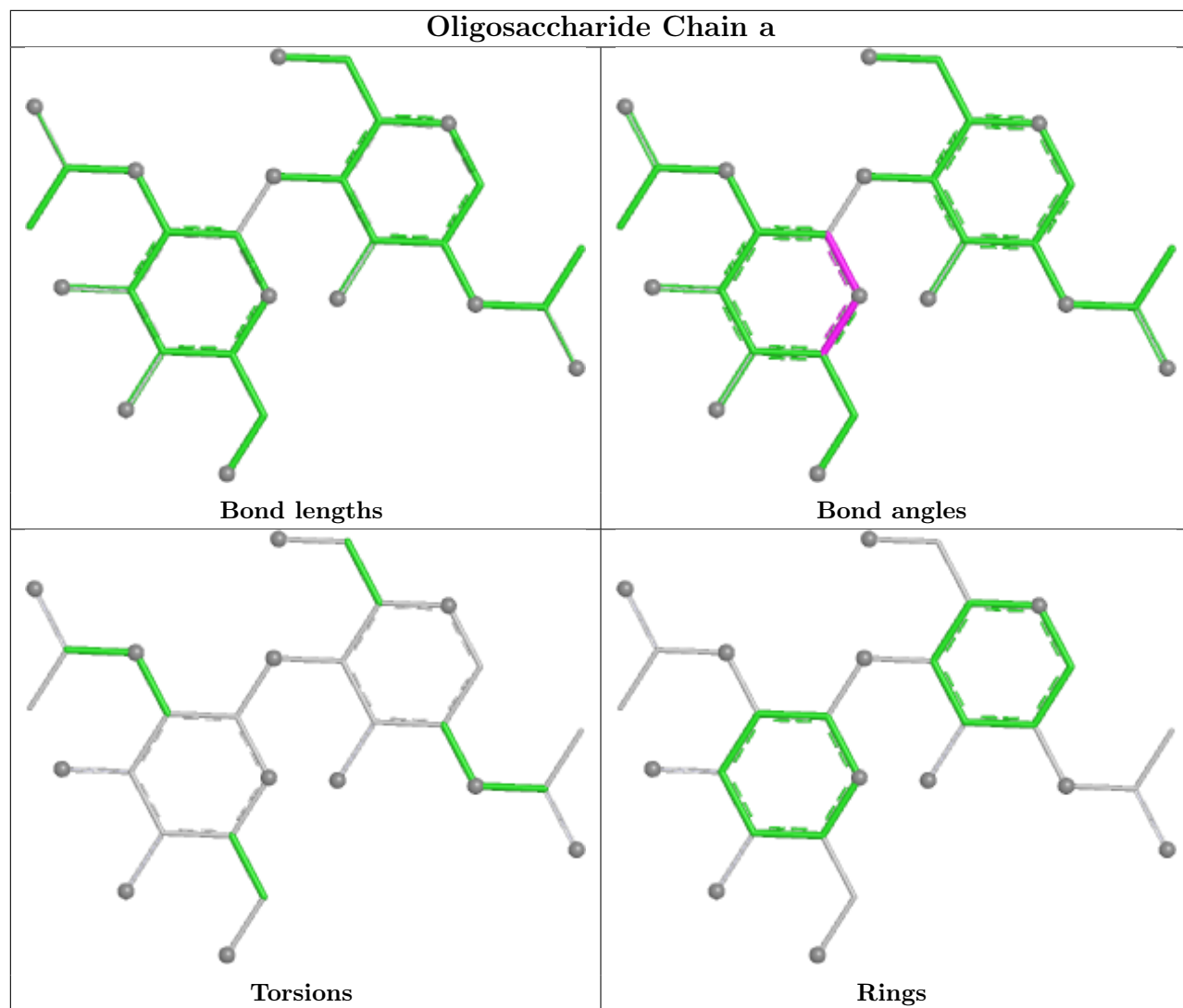


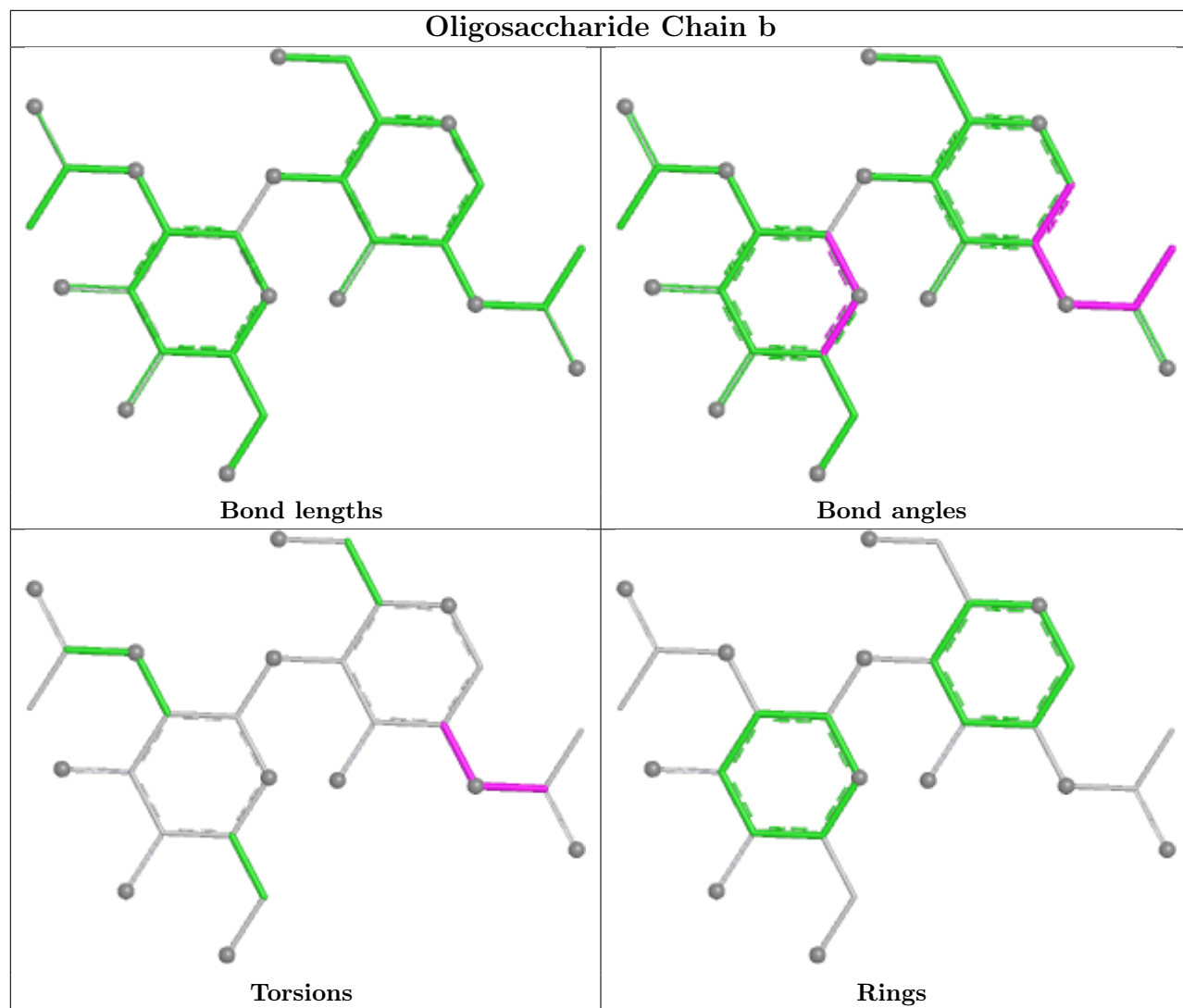


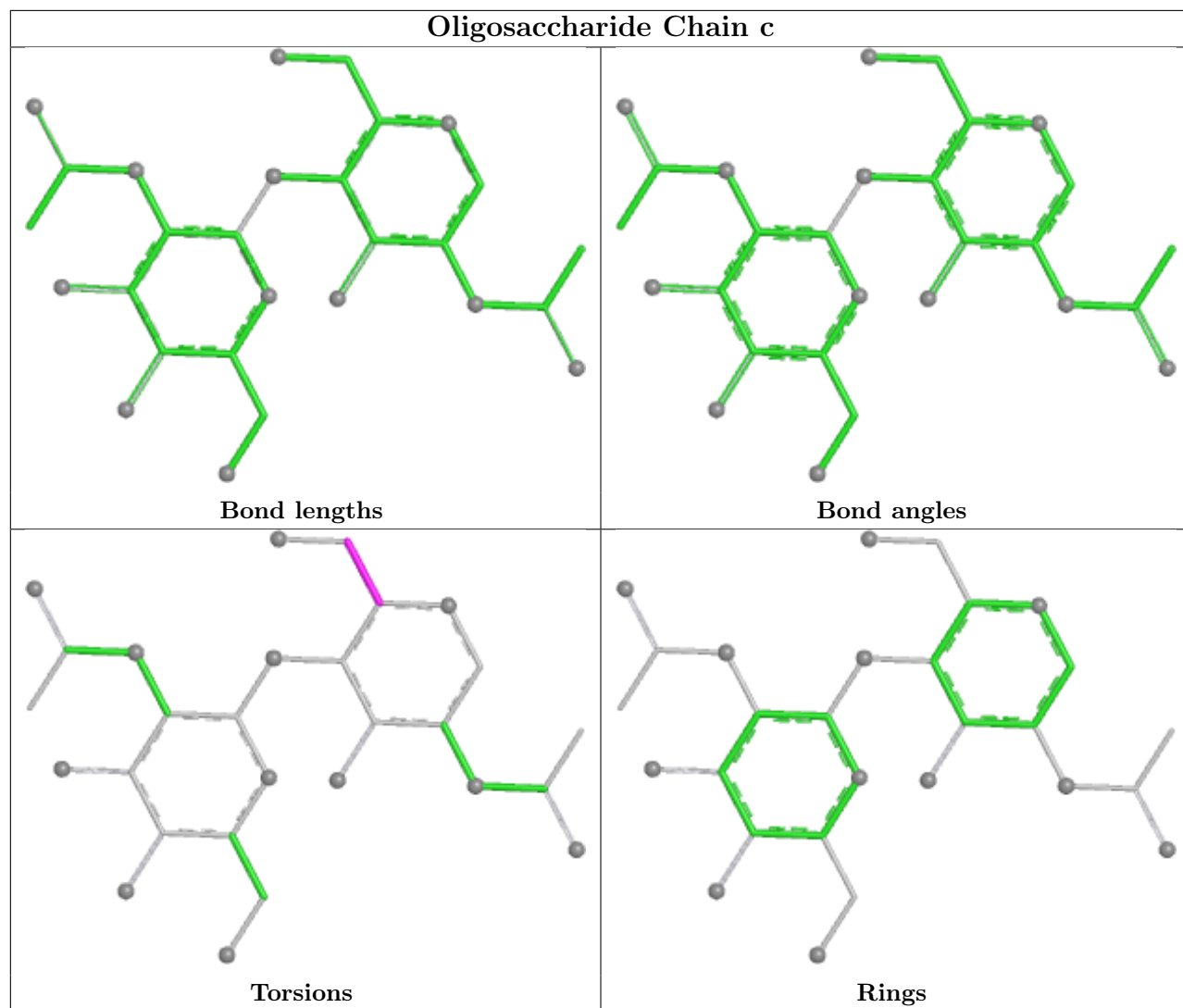


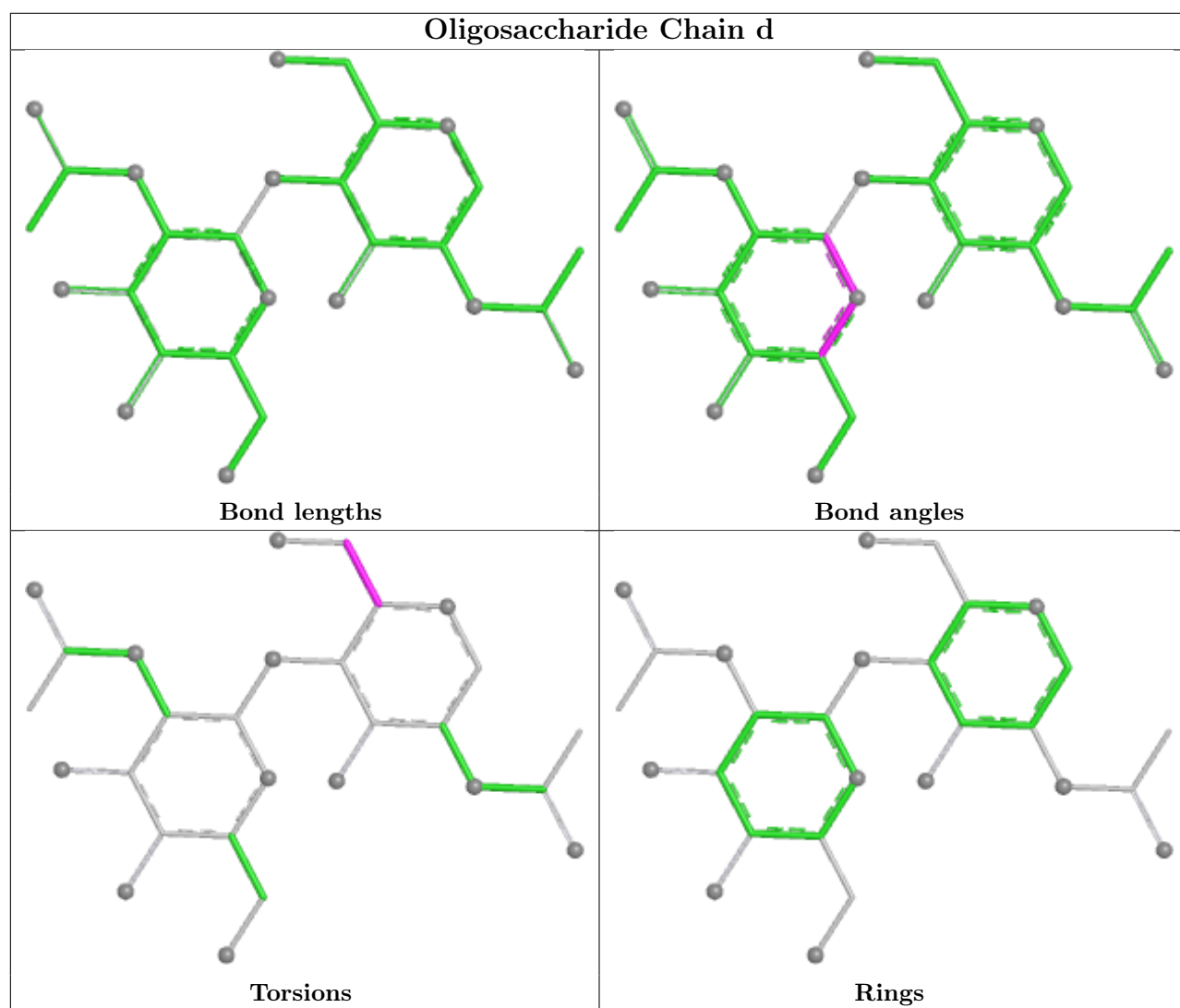


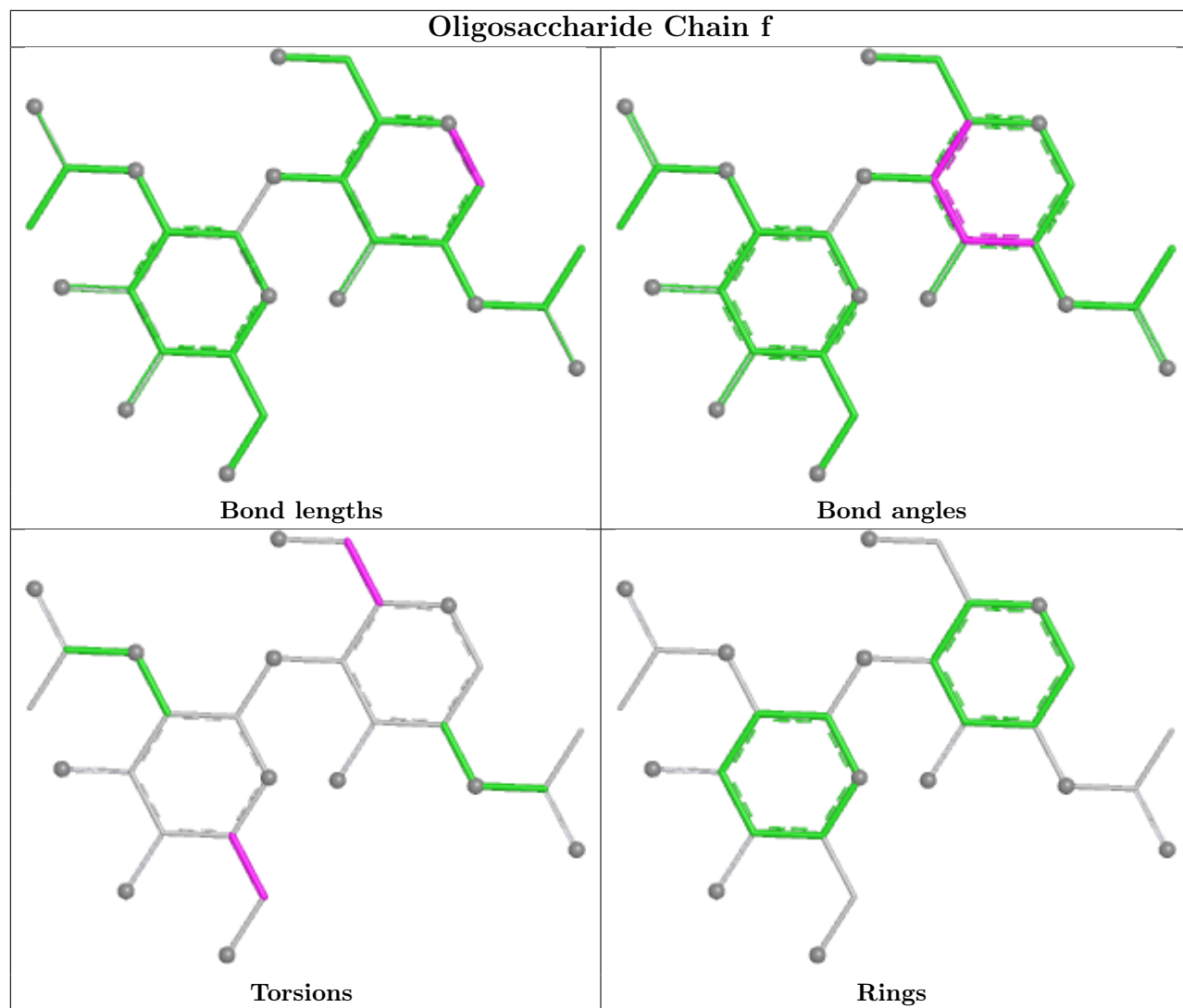


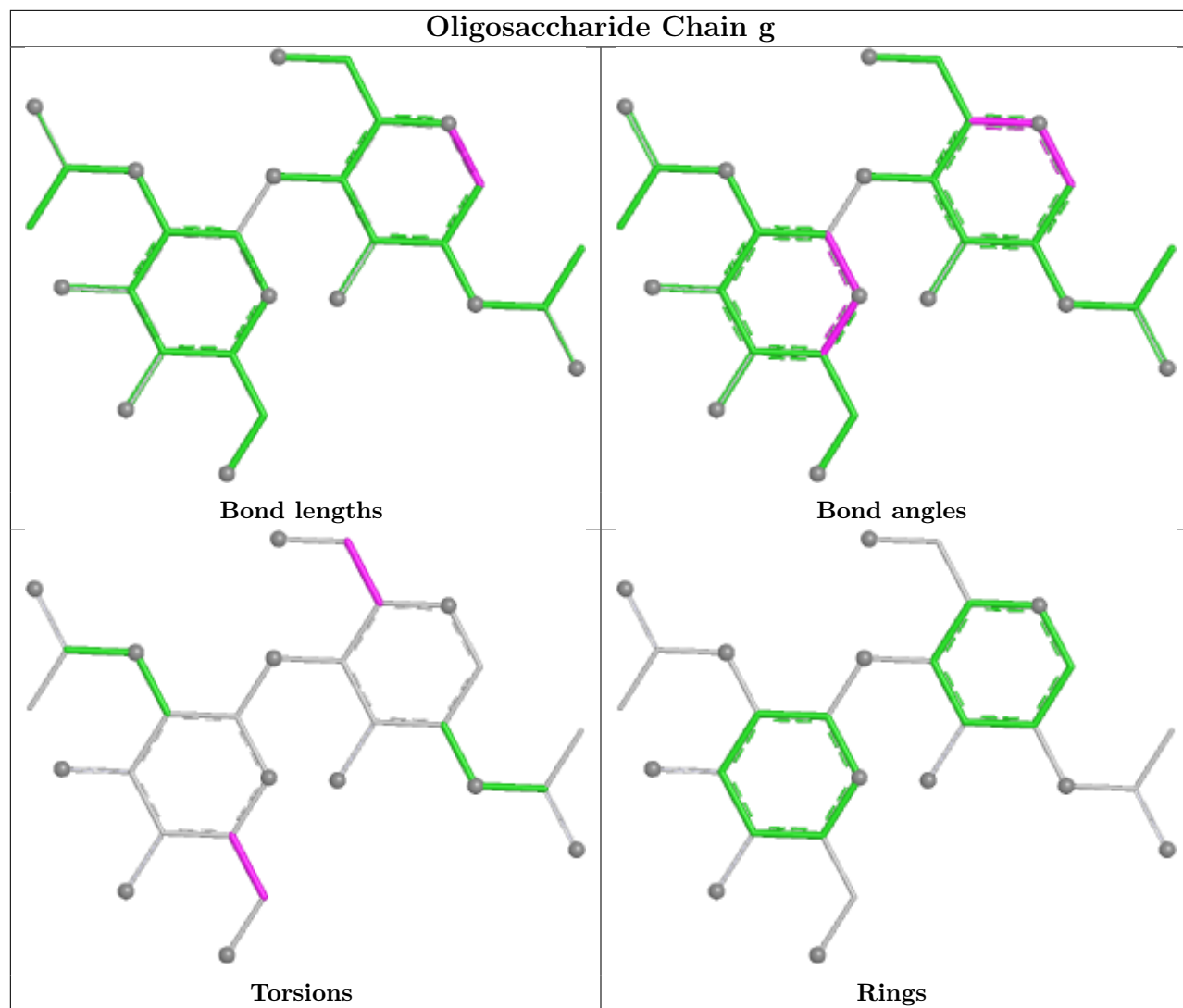


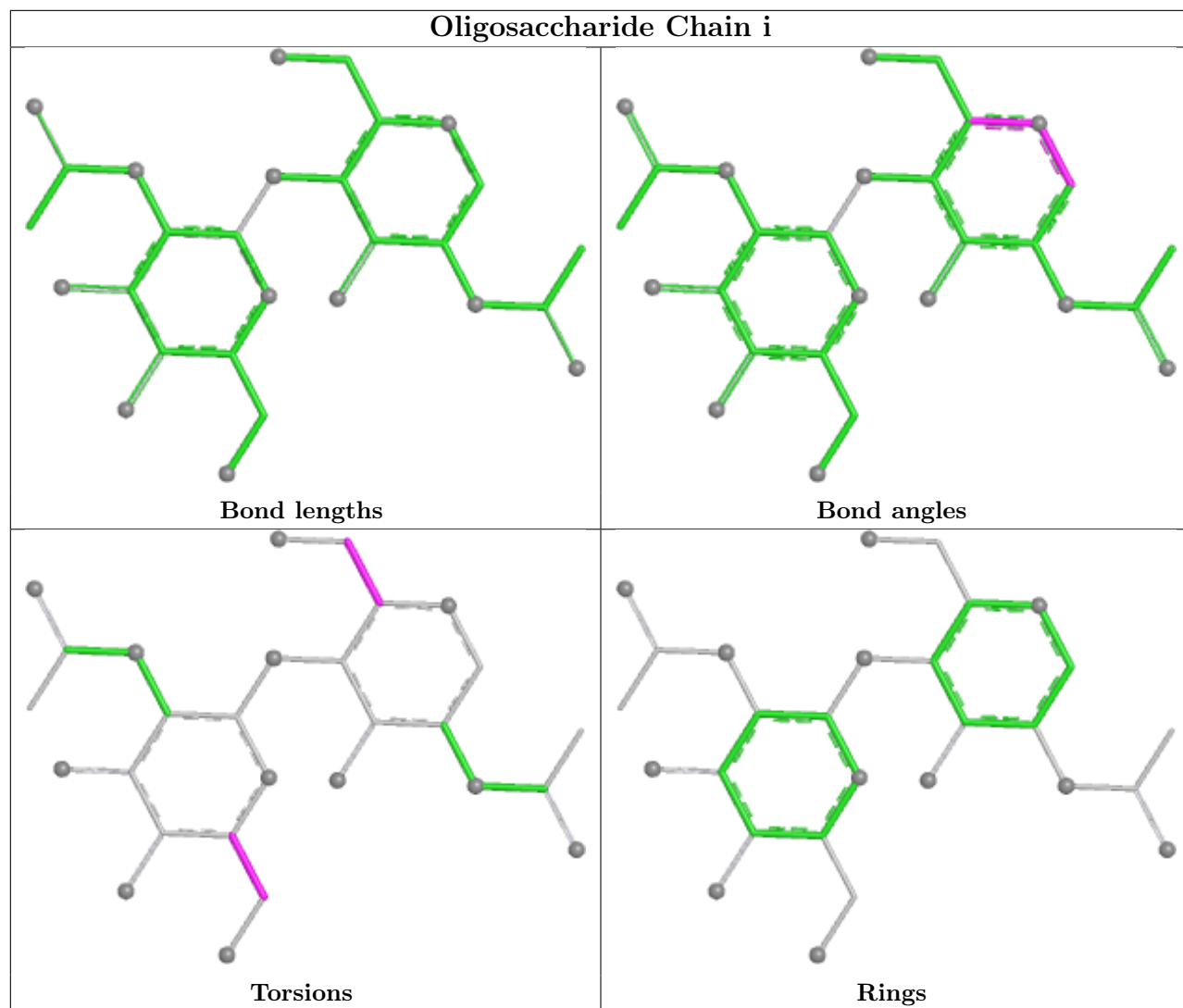


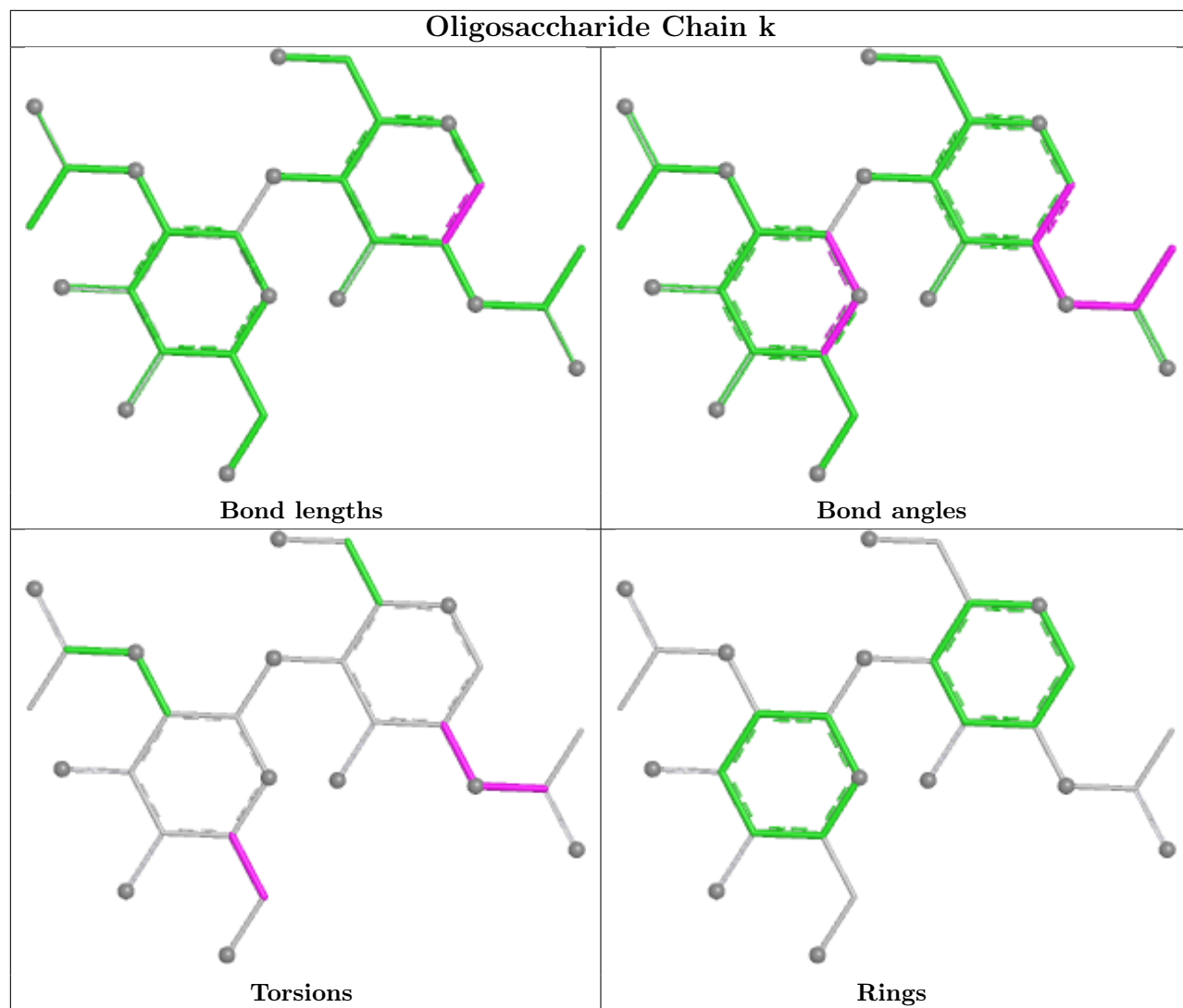


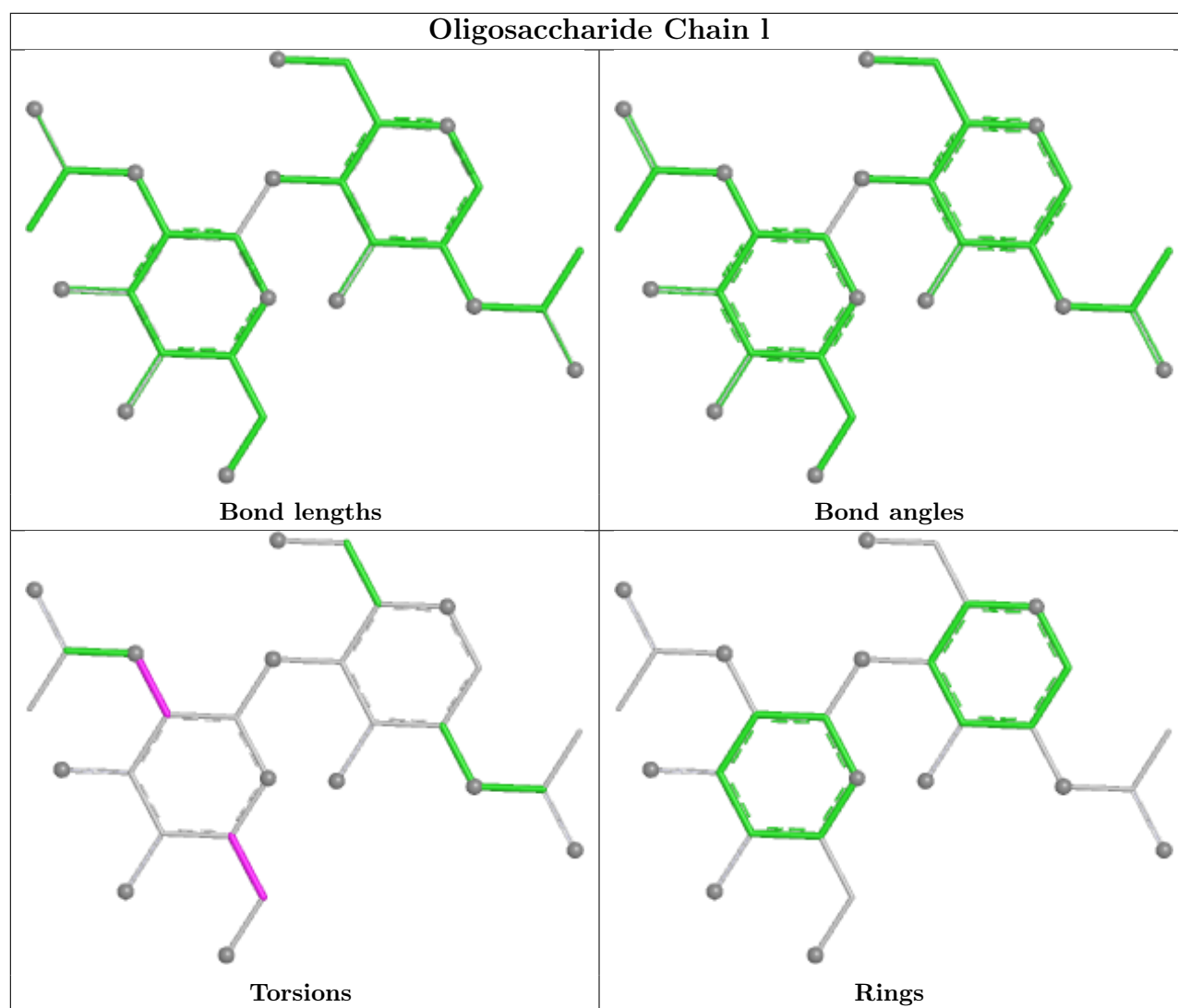


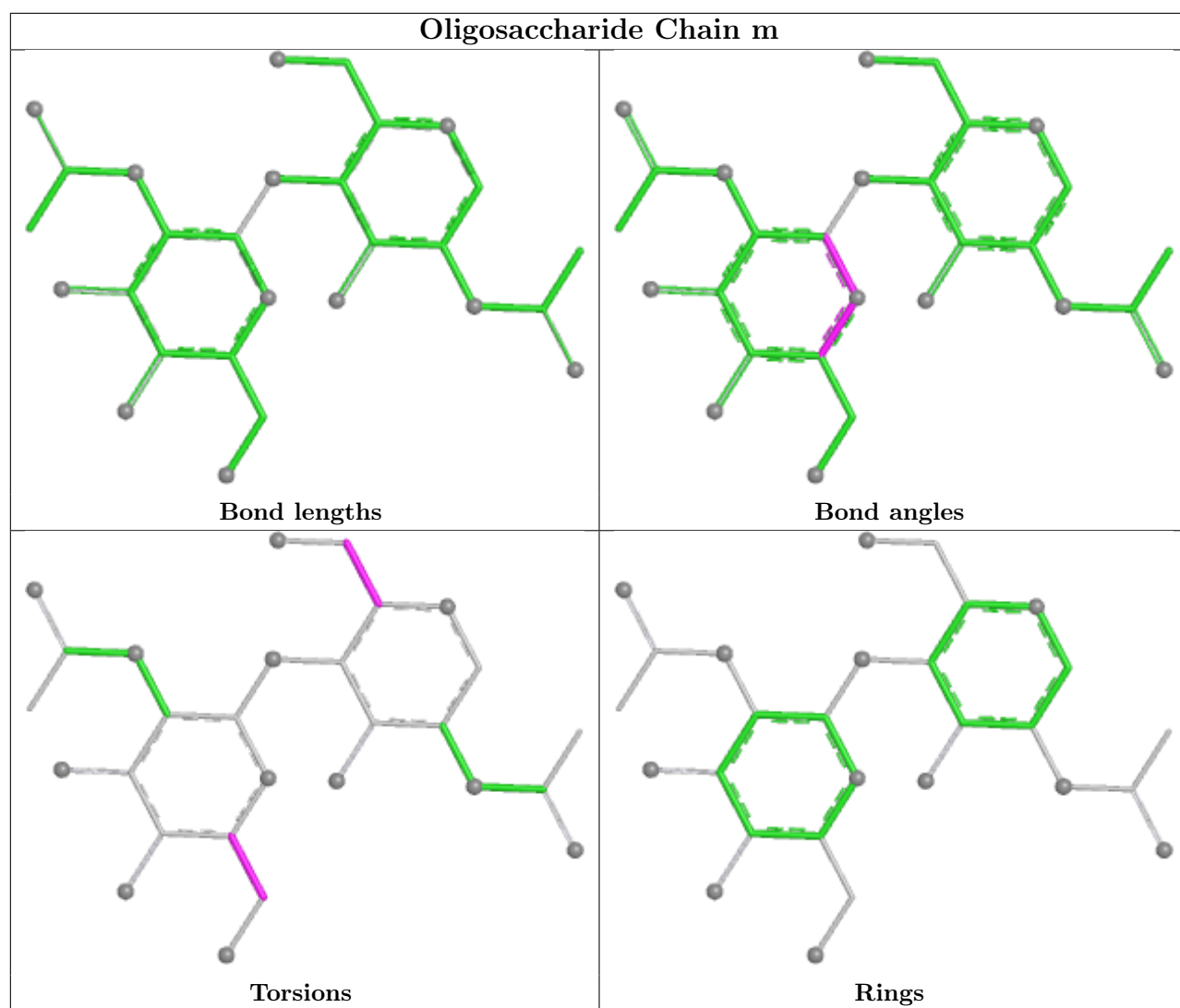


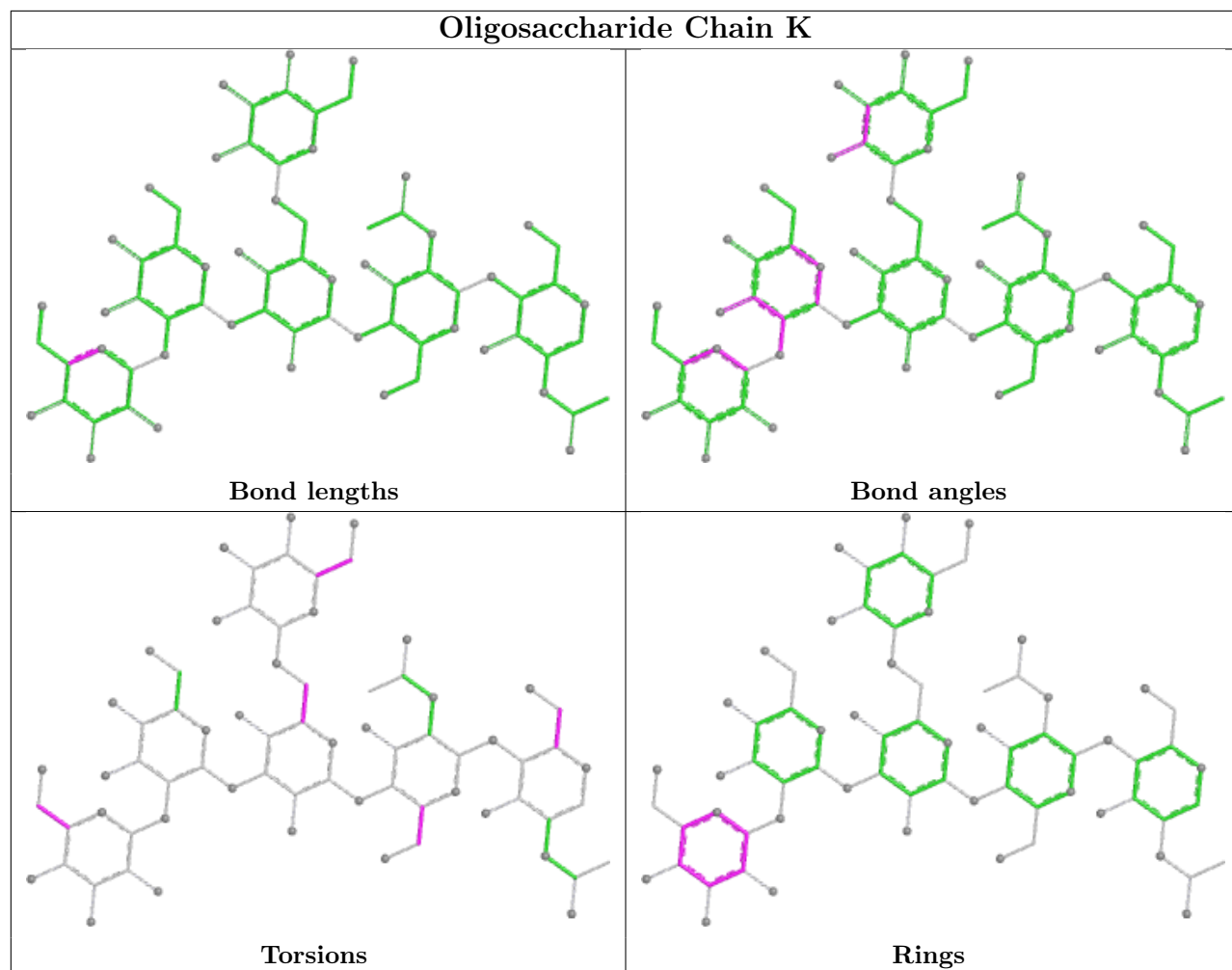


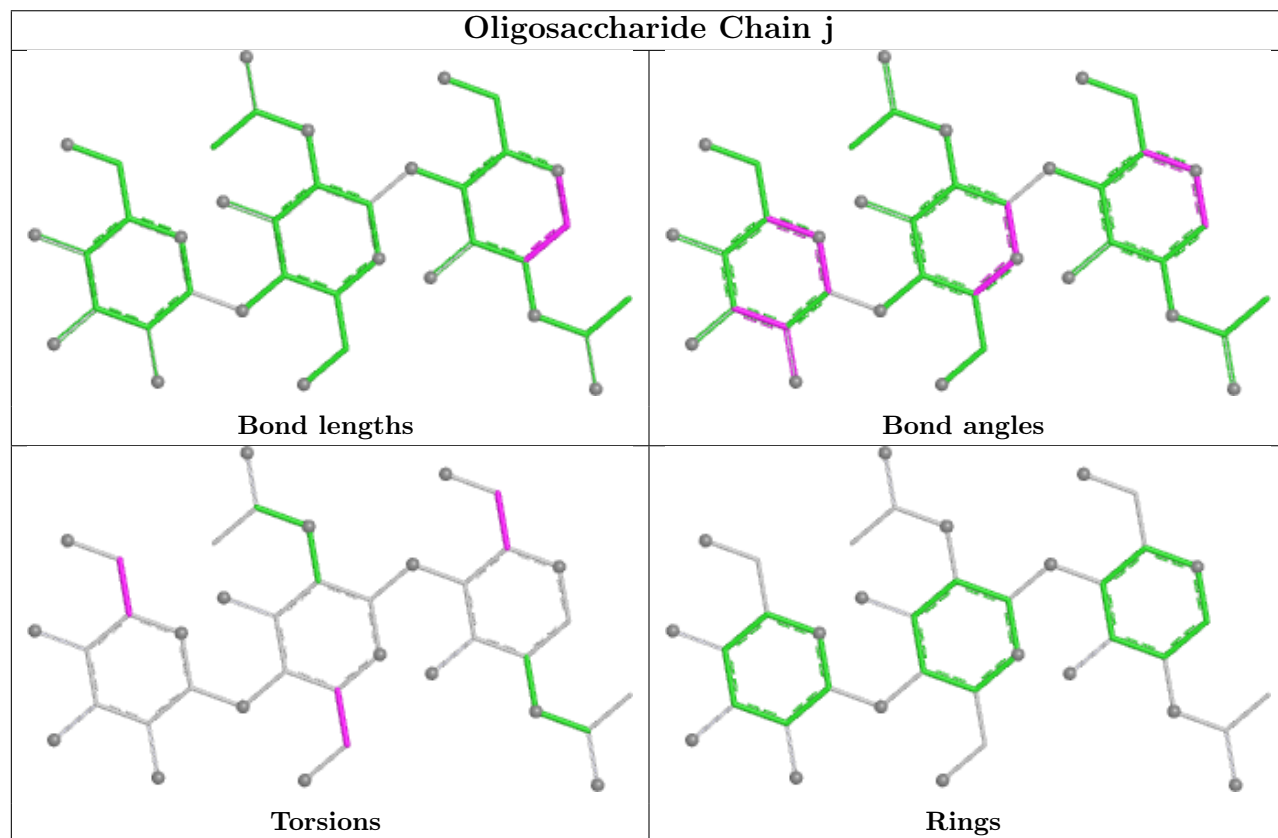
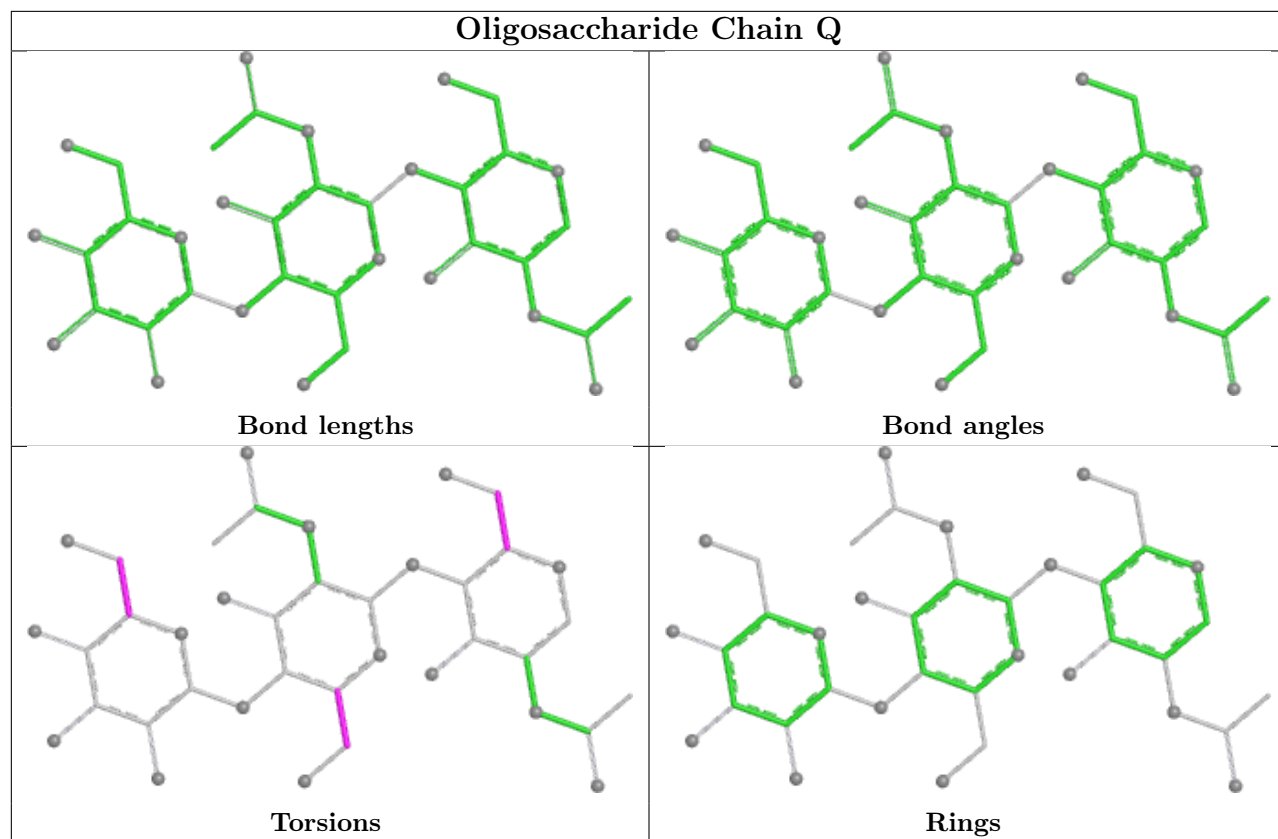


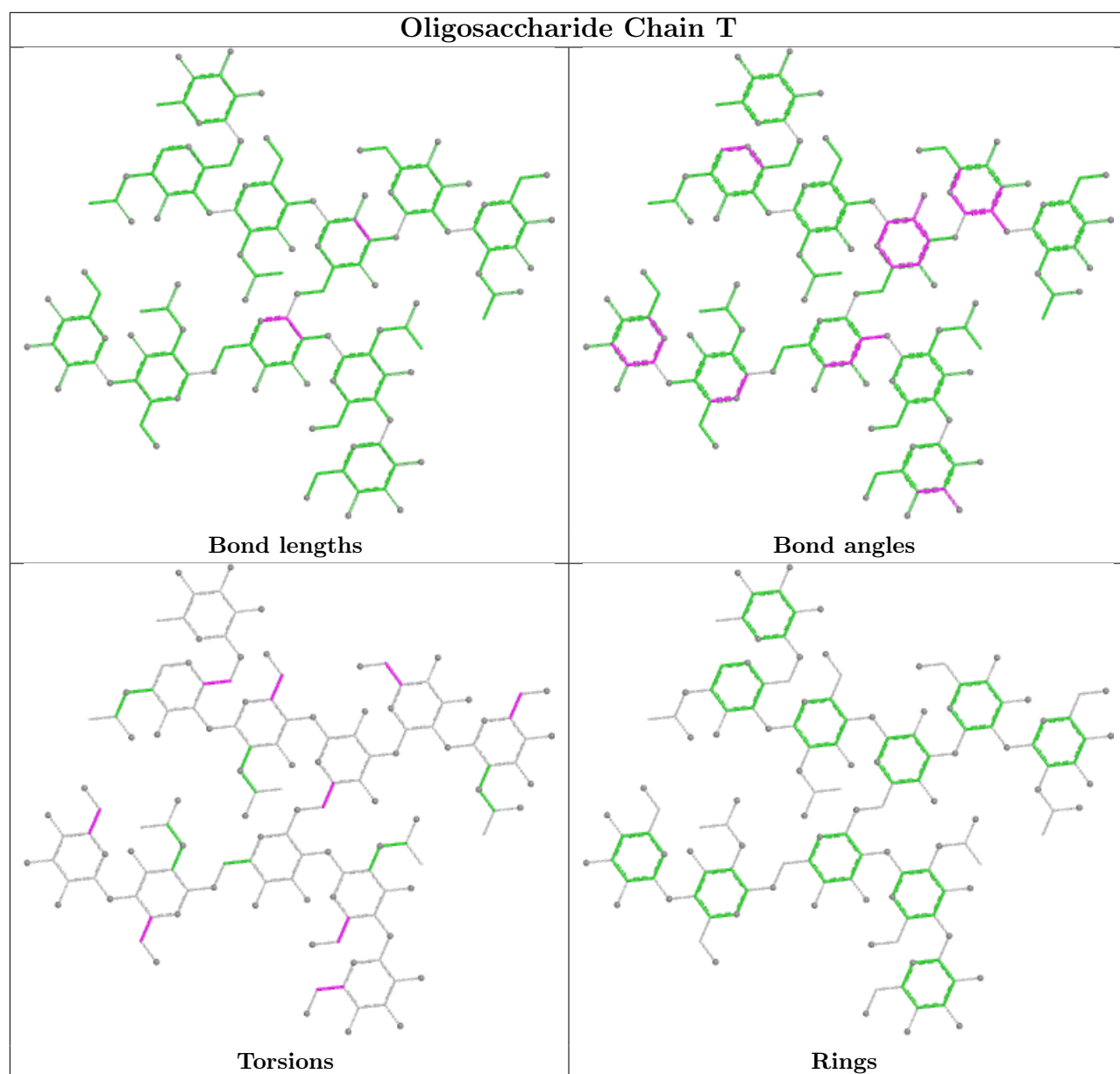


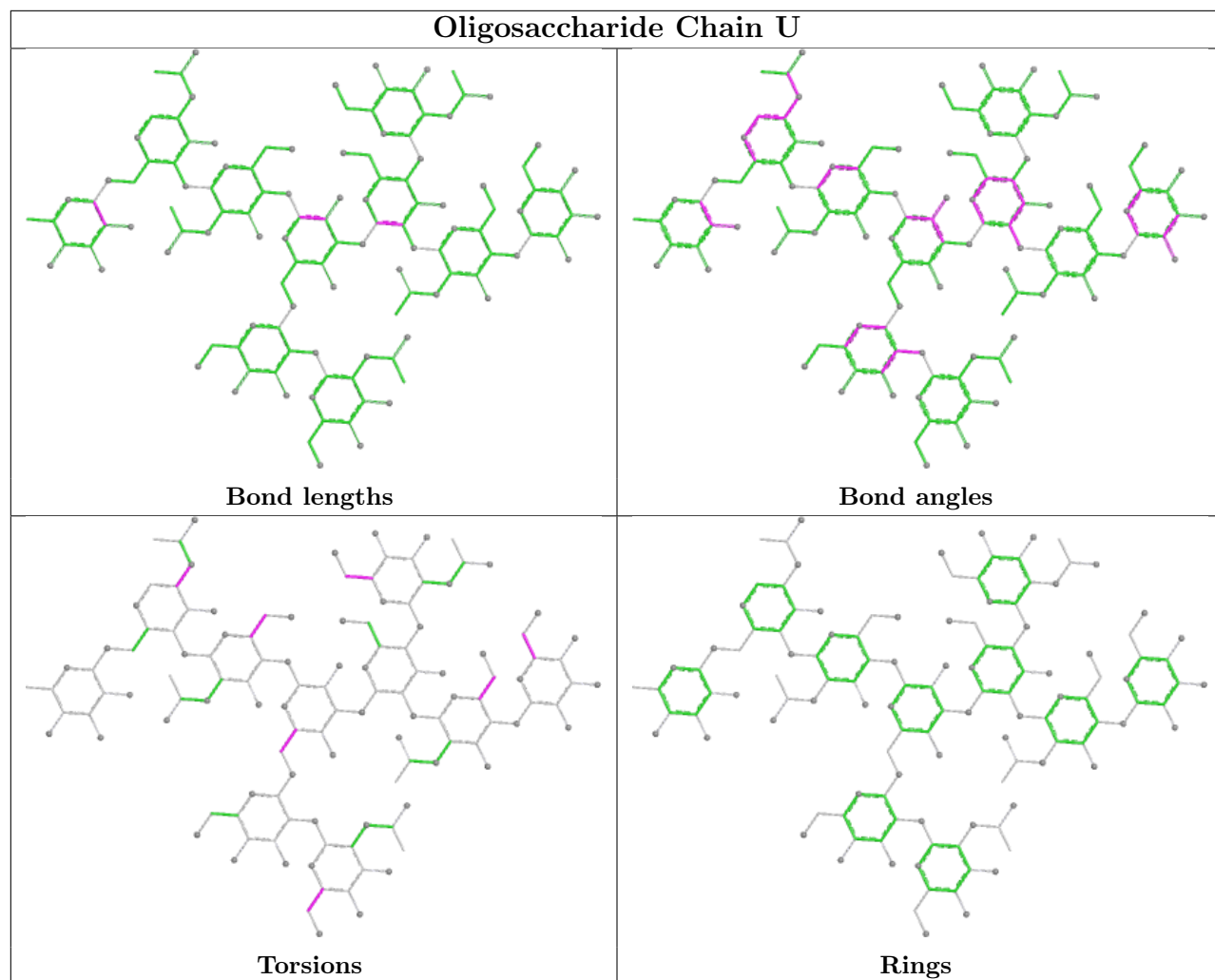


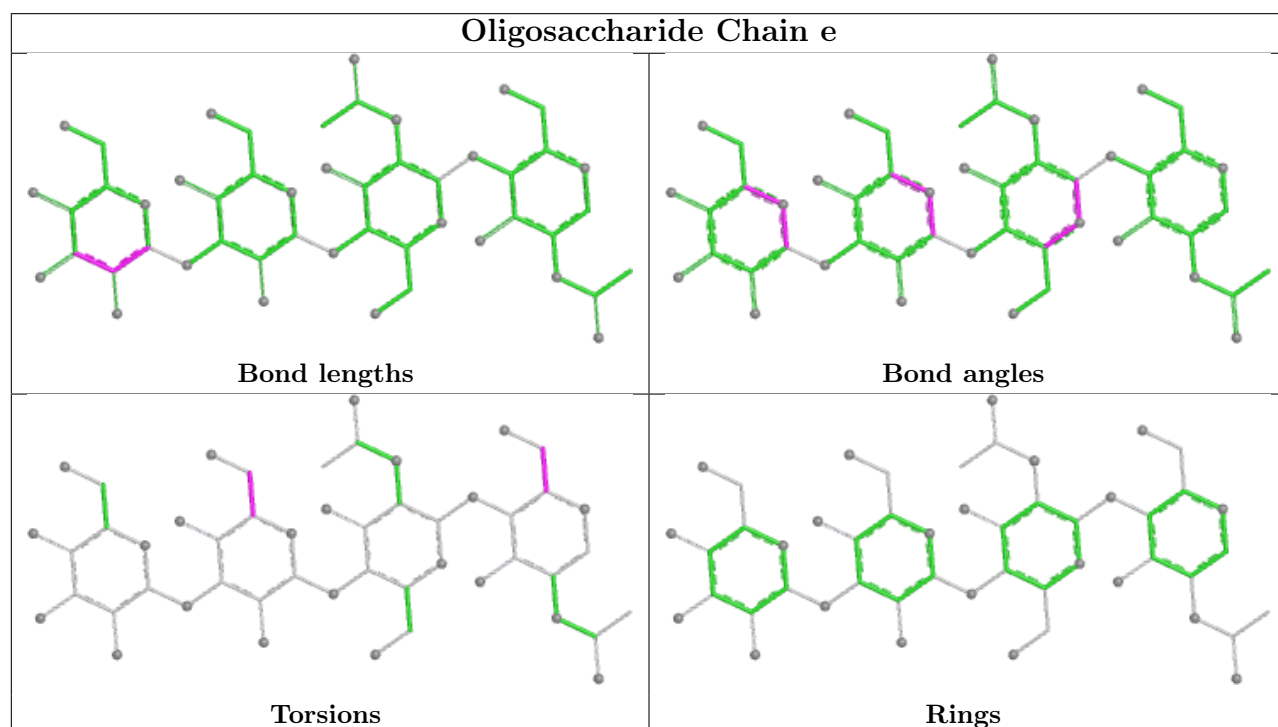
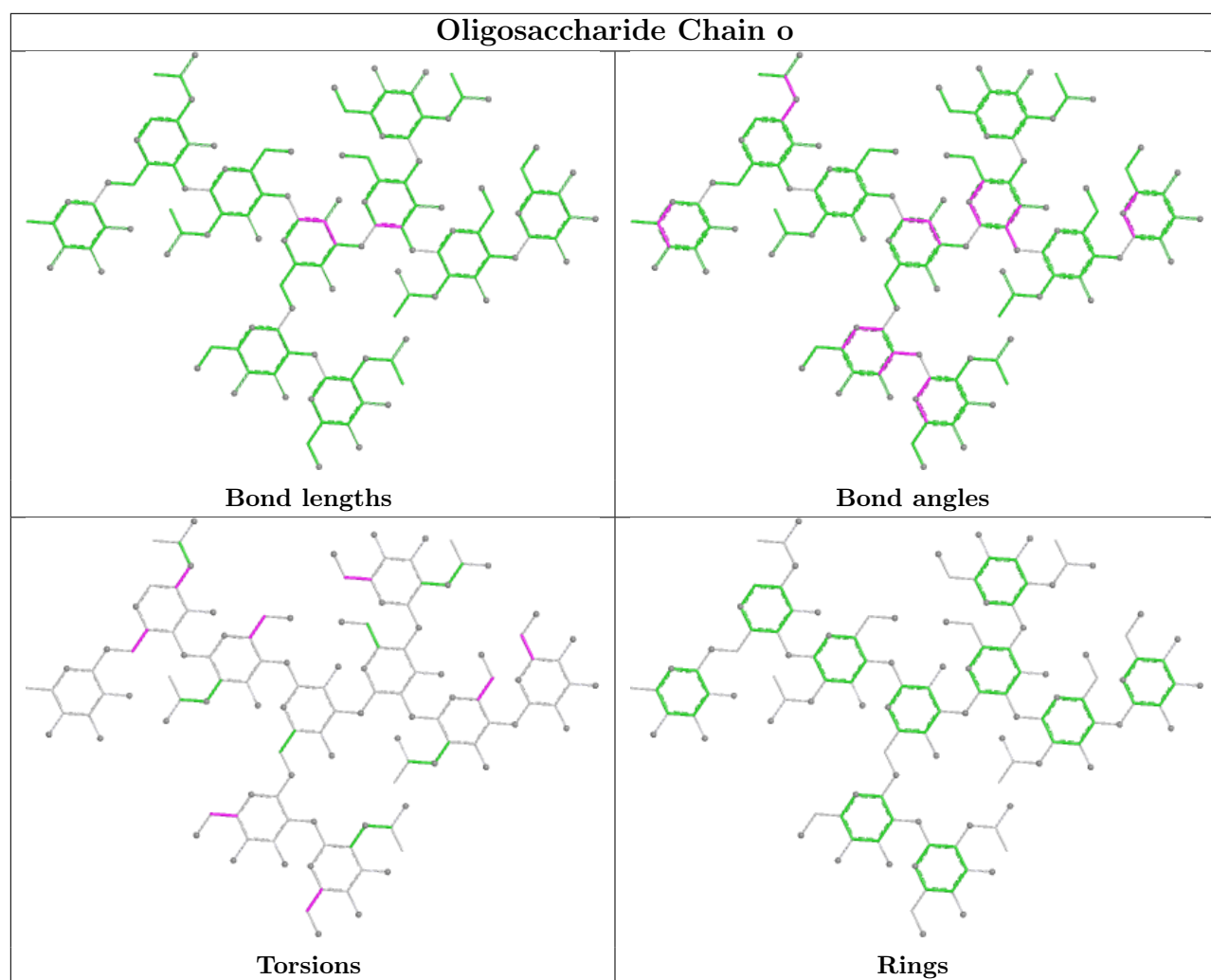


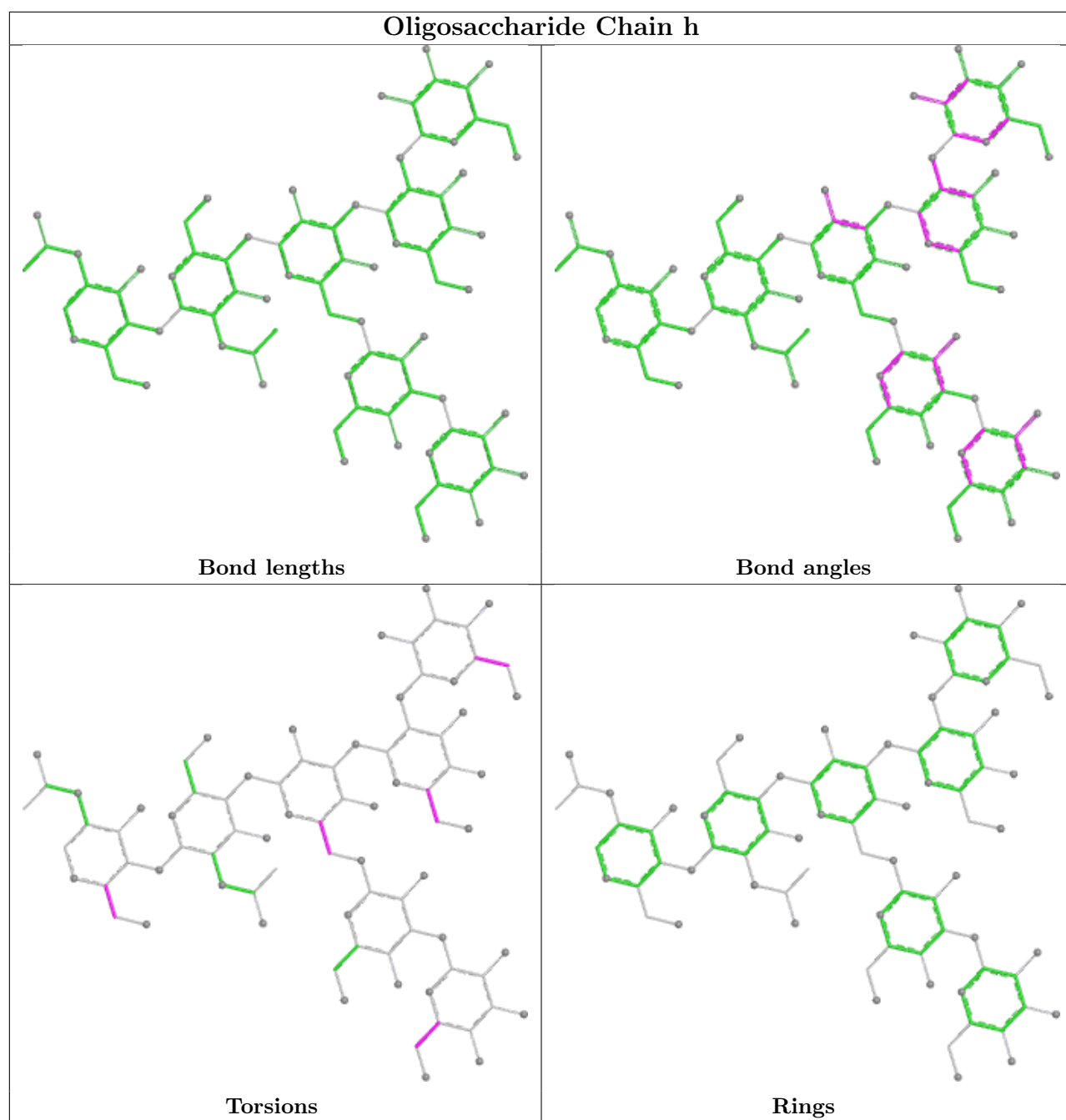


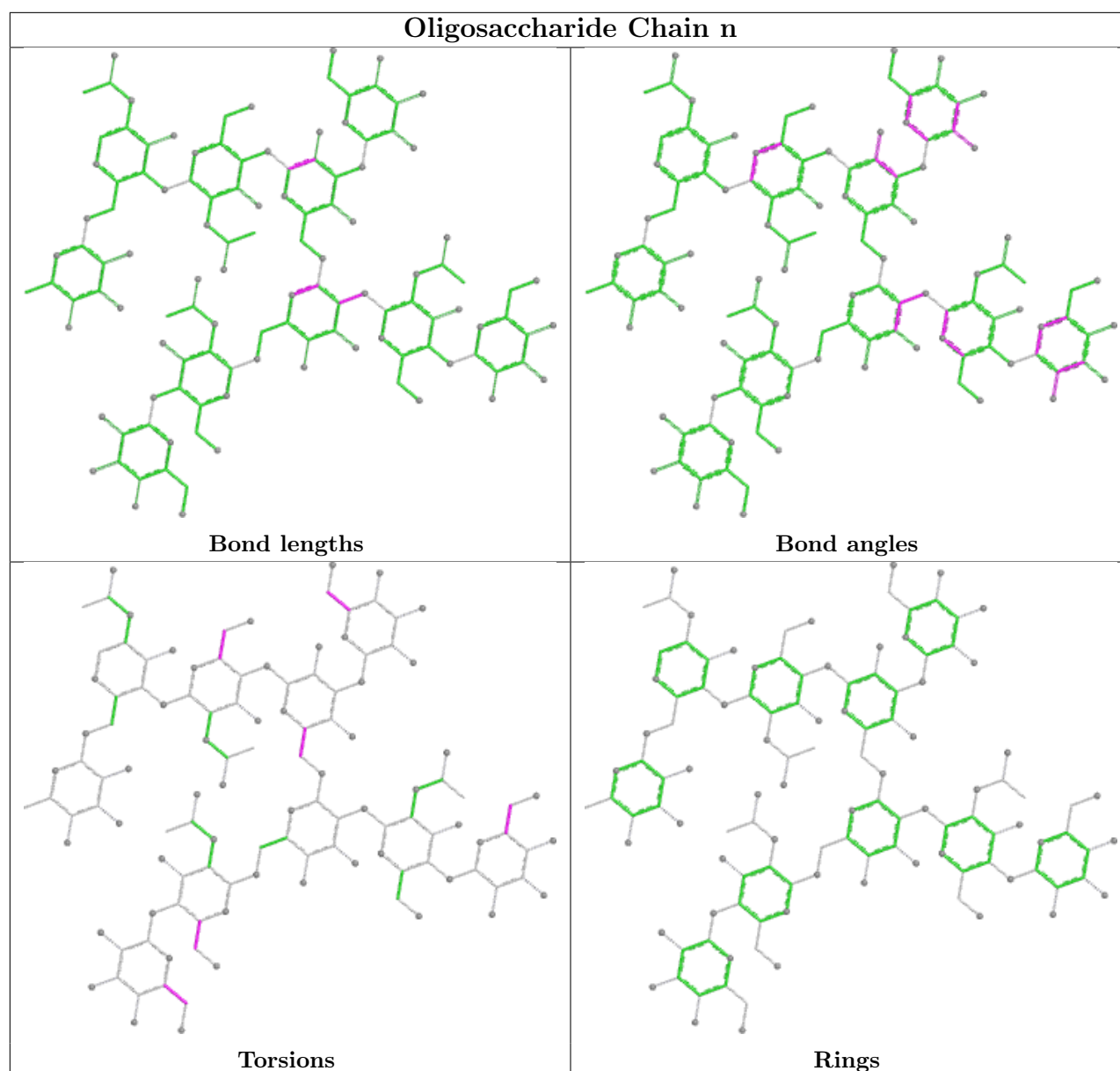












5.6 Ligand geometry [i](#)

22 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
13	NAG	C	611	3	14,14,15	0.28	0	17,19,21	0.53	0
13	NAG	B	802	4	14,14,15	0.55	0	17,19,21	0.83	1 (5%)
13	NAG	E	1001	3	14,14,15	0.45	0	17,19,21	0.60	0
13	NAG	A	1015	3	14,14,15	0.43	0	17,19,21	0.61	0
13	NAG	A	1000	3	14,14,15	0.27	0	17,19,21	0.71	1 (5%)
13	NAG	E	1017	3	14,14,15	0.34	0	17,19,21	0.55	0
13	NAG	C	601	3	14,14,15	0.45	0	17,19,21	0.55	0
13	NAG	E	1016	3	14,14,15	0.26	0	17,19,21	0.47	0
13	NAG	E	1000	3	14,14,15	0.20	0	17,19,21	0.57	0
13	NAG	D	1000	4	14,14,15	0.27	0	17,19,21	0.63	1 (5%)
13	NAG	D	1004	4	14,14,15	0.55	0	17,19,21	1.05	1 (5%)
13	NAG	C	610	3	14,14,15	0.35	0	17,19,21	0.59	0
13	NAG	F	1000	4	14,14,15	0.44	0	17,19,21	0.37	0
13	NAG	E	1015	3	14,14,15	0.46	0	17,19,21	0.41	0
13	NAG	C	612	3	14,14,15	0.19	0	17,19,21	0.51	0
13	NAG	B	801	4	14,14,15	0.32	0	17,19,21	0.43	0
13	NAG	A	1023	3	14,14,15	0.88	1 (7%)	17,19,21	2.41	3 (17%)
13	NAG	C	615	3	14,14,15	0.54	0	17,19,21	0.75	1 (5%)
13	NAG	A	1022	3	14,14,15	0.53	0	17,19,21	0.75	1 (5%)
13	NAG	D	1001	4	14,14,15	0.26	0	17,19,21	0.50	0
13	NAG	E	1021	3	14,14,15	0.51	0	17,19,21	0.60	0
13	NAG	A	1018	3	14,14,15	0.21	0	17,19,21	0.60	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
13	NAG	C	611	3	-	2/6/23/26	0/1/1/1
13	NAG	B	802	4	-	2/6/23/26	0/1/1/1
13	NAG	E	1001	3	-	2/6/23/26	0/1/1/1
13	NAG	A	1015	3	-	2/6/23/26	0/1/1/1
13	NAG	A	1000	3	-	0/6/23/26	0/1/1/1
13	NAG	E	1017	3	-	2/6/23/26	0/1/1/1
13	NAG	C	601	3	-	0/6/23/26	0/1/1/1
13	NAG	E	1016	3	-	2/6/23/26	0/1/1/1
13	NAG	E	1000	3	-	2/6/23/26	0/1/1/1
13	NAG	D	1000	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	D	1004	4	-	3/6/23/26	0/1/1/1
13	NAG	C	610	3	-	2/6/23/26	0/1/1/1
13	NAG	F	1000	4	-	3/6/23/26	0/1/1/1
13	NAG	E	1015	3	-	0/6/23/26	0/1/1/1
13	NAG	C	612	3	-	2/6/23/26	0/1/1/1
13	NAG	B	801	4	-	2/6/23/26	0/1/1/1
13	NAG	A	1023	3	-	4/6/23/26	0/1/1/1
13	NAG	C	615	3	-	0/6/23/26	0/1/1/1
13	NAG	A	1022	3	-	0/6/23/26	0/1/1/1
13	NAG	D	1001	4	-	0/6/23/26	0/1/1/1
13	NAG	E	1021	3	-	0/6/23/26	0/1/1/1
13	NAG	A	1018	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1023	NAG	C1-C2	2.74	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1023	NAG	C2-N2-C7	8.25	133.95	122.90
13	A	1023	NAG	C1-C2-N2	4.40	117.37	110.43
13	D	1004	NAG	C2-N2-C7	3.12	127.08	122.90
13	B	802	NAG	C1-O5-C5	2.98	116.18	112.19
13	C	615	NAG	C1-O5-C5	2.61	115.69	112.19
13	A	1022	NAG	C1-O5-C5	2.33	115.31	112.19
13	D	1000	NAG	C1-O5-C5	2.12	115.03	112.19
13	A	1023	NAG	C8-C7-N2	2.11	119.61	116.12
13	A	1000	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1018	NAG	O5-C5-C6-O6
13	C	610	NAG	O5-C5-C6-O6
13	C	611	NAG	O5-C5-C6-O6
13	A	1015	NAG	O5-C5-C6-O6
13	B	802	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	E	1017	NAG	O5-C5-C6-O6
13	C	610	NAG	C4-C5-C6-O6
13	B	801	NAG	O5-C5-C6-O6
13	A	1018	NAG	C4-C5-C6-O6
13	B	802	NAG	C4-C5-C6-O6
13	C	611	NAG	C4-C5-C6-O6
13	E	1016	NAG	C4-C5-C6-O6
13	E	1001	NAG	O5-C5-C6-O6
13	E	1016	NAG	O5-C5-C6-O6
13	E	1017	NAG	C4-C5-C6-O6
13	A	1015	NAG	C4-C5-C6-O6
13	A	1023	NAG	C8-C7-N2-C2
13	A	1023	NAG	O7-C7-N2-C2
13	B	801	NAG	C4-C5-C6-O6
13	F	1000	NAG	O5-C5-C6-O6
13	C	612	NAG	C4-C5-C6-O6
13	C	612	NAG	O5-C5-C6-O6
13	D	1004	NAG	O5-C5-C6-O6
13	E	1000	NAG	C4-C5-C6-O6
13	E	1000	NAG	O5-C5-C6-O6
13	E	1001	NAG	C4-C5-C6-O6
13	D	1004	NAG	C3-C2-N2-C7
13	F	1000	NAG	C4-C5-C6-O6
13	D	1000	NAG	C4-C5-C6-O6
13	A	1023	NAG	C1-C2-N2-C7
13	D	1004	NAG	C1-C2-N2-C7
13	F	1000	NAG	C1-C2-N2-C7
13	D	1000	NAG	O5-C5-C6-O6
13	A	1023	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	611	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.

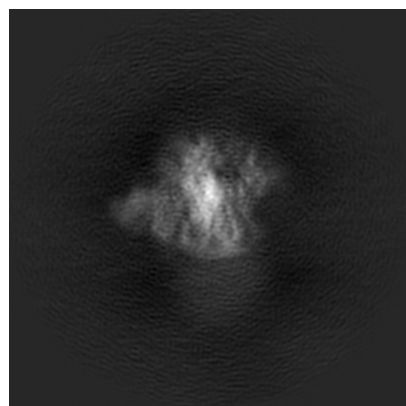
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9062. These allow visual inspection of the internal detail of the map and identification of artifacts.

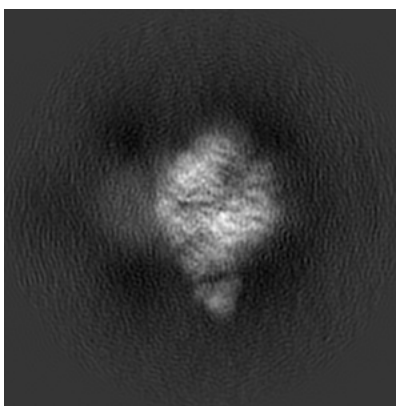
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

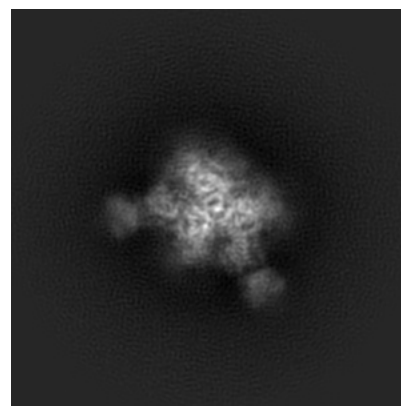
6.1.1 Primary map



X

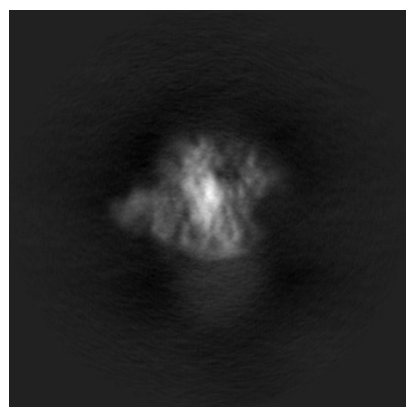


Y

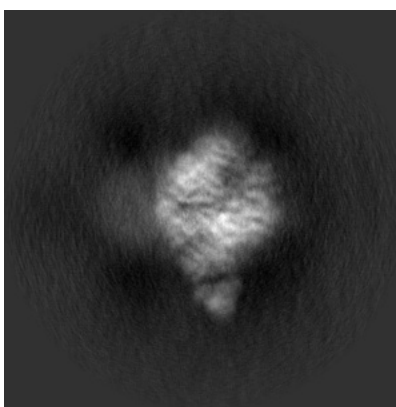


Z

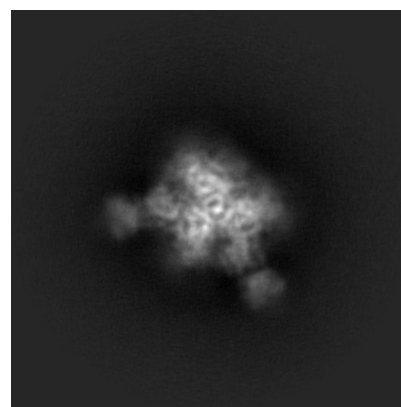
6.1.2 Raw map



X



Y

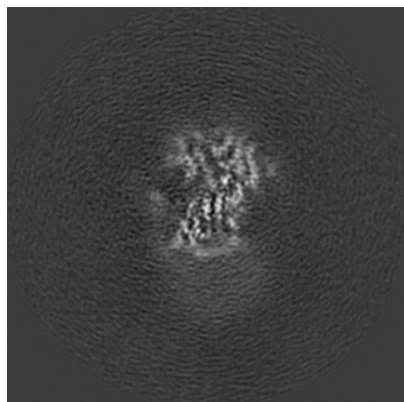


Z

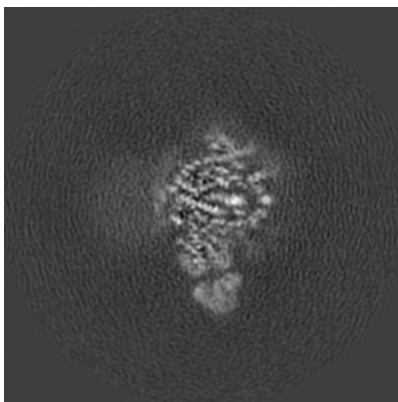
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

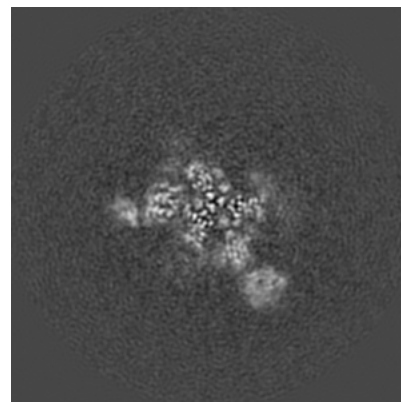
6.2.1 Primary map



X Index: 160

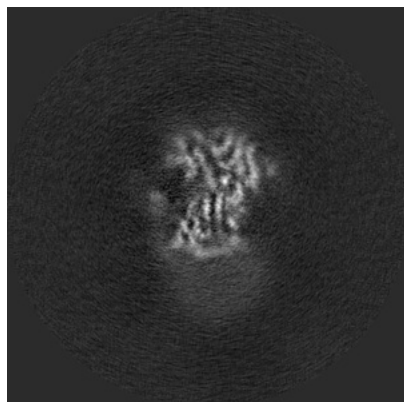


Y Index: 160

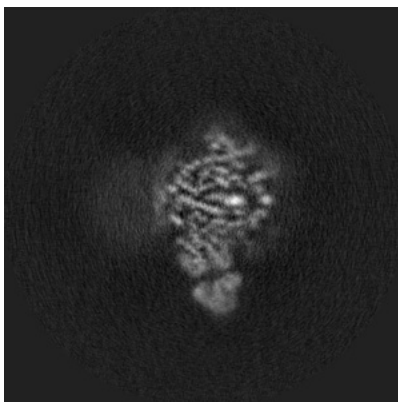


Z Index: 160

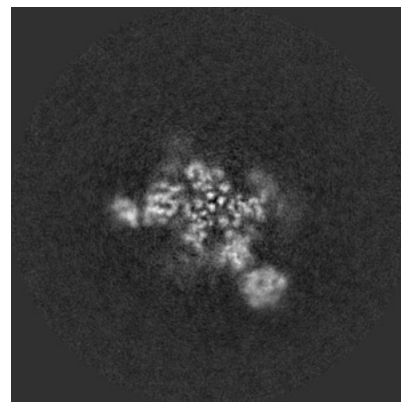
6.2.2 Raw map



X Index: 160



Y Index: 160

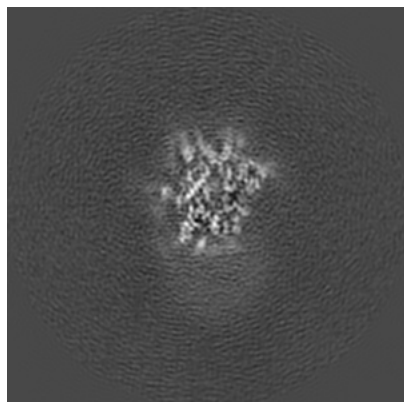


Z Index: 160

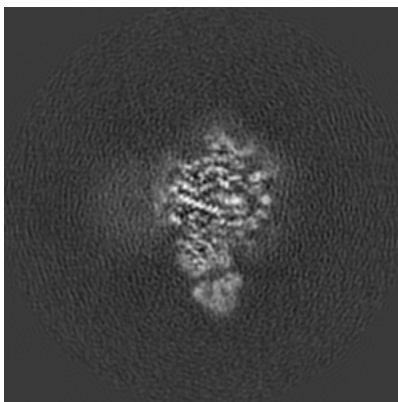
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

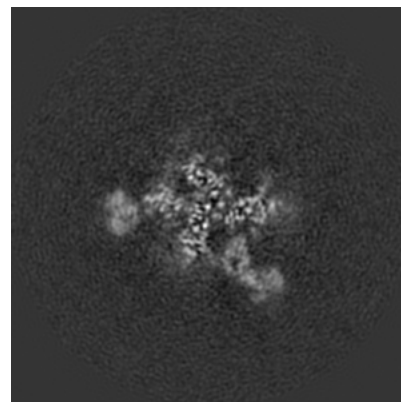
6.3.1 Primary map



X Index: 155

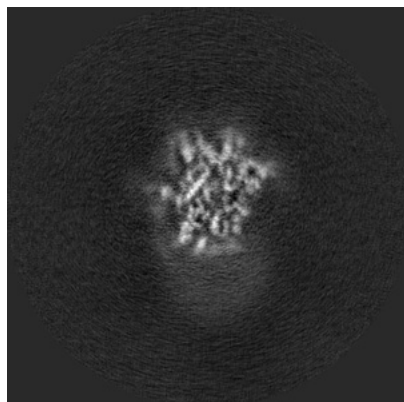


Y Index: 159

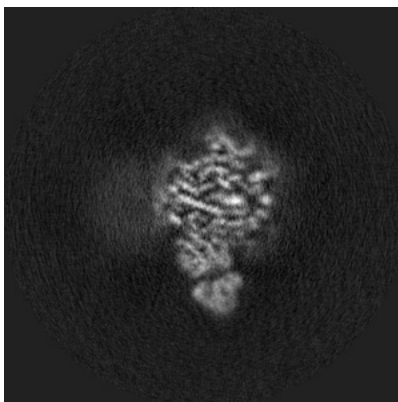


Z Index: 168

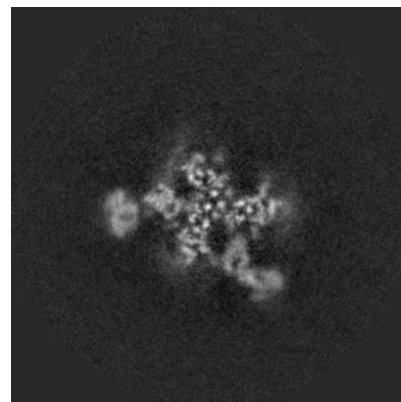
6.3.2 Raw map



X Index: 155



Y Index: 159

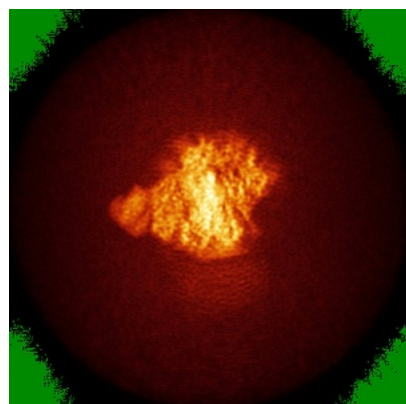


Z Index: 169

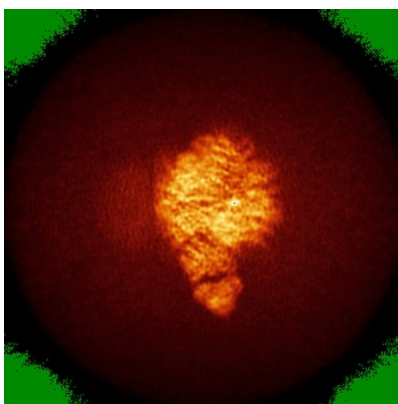
The images above show the largest variance slices of the map in three orthogonal directions.

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

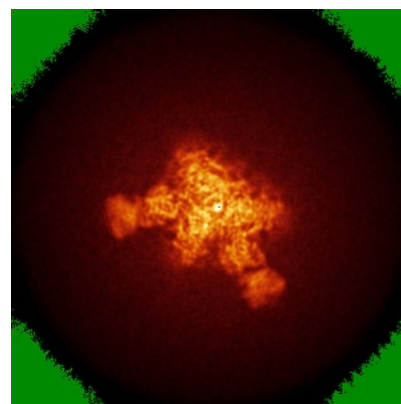
6.4.1 Primary map



X

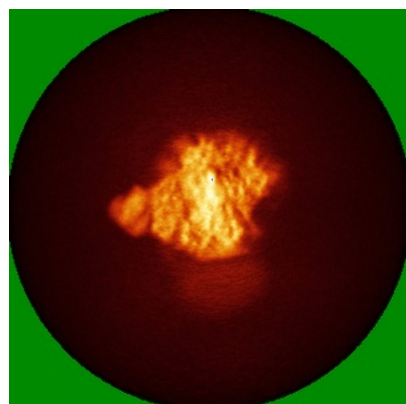


Y

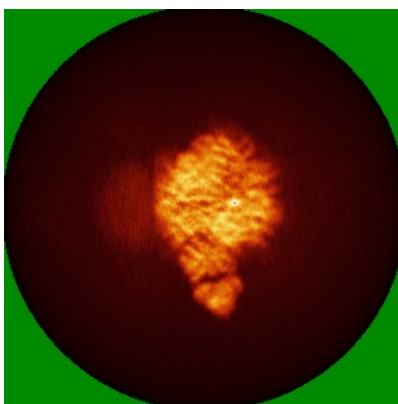


Z

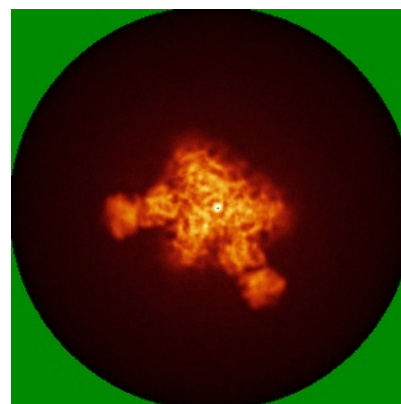
6.4.2 Raw map



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.

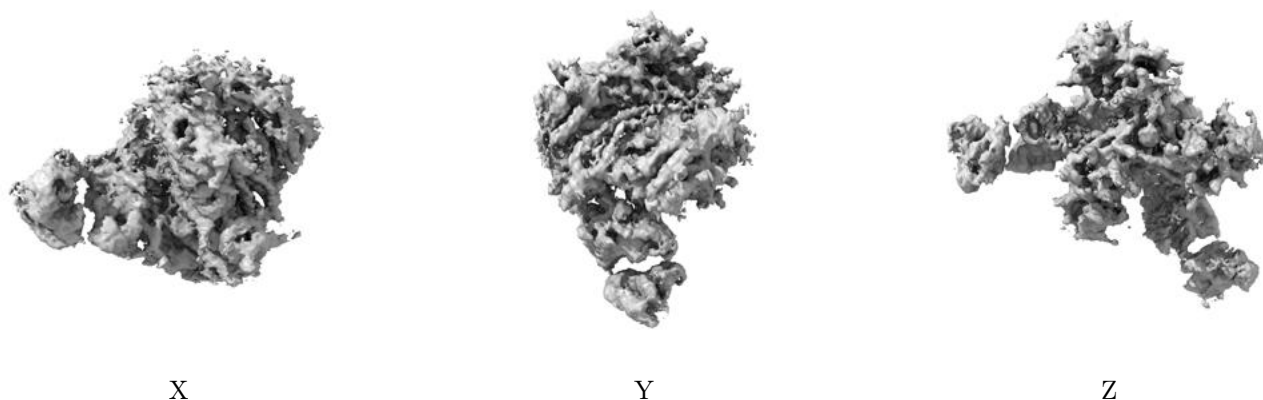
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

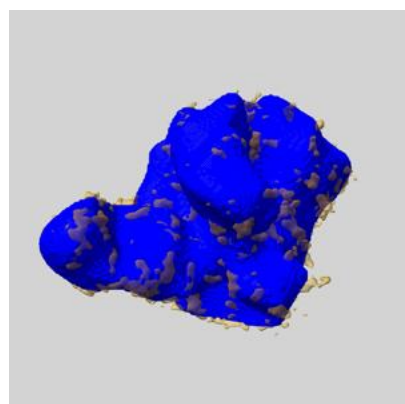
6.6 Mask visualisation [i](#)

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

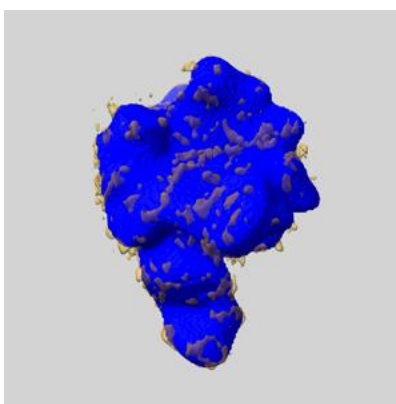
A mask typically either:

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

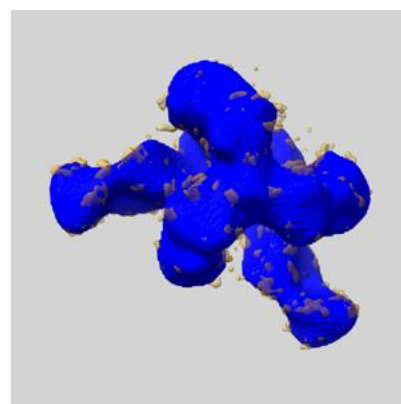
6.6.1 emd_9062_msk_1.map [i](#)



X



Y

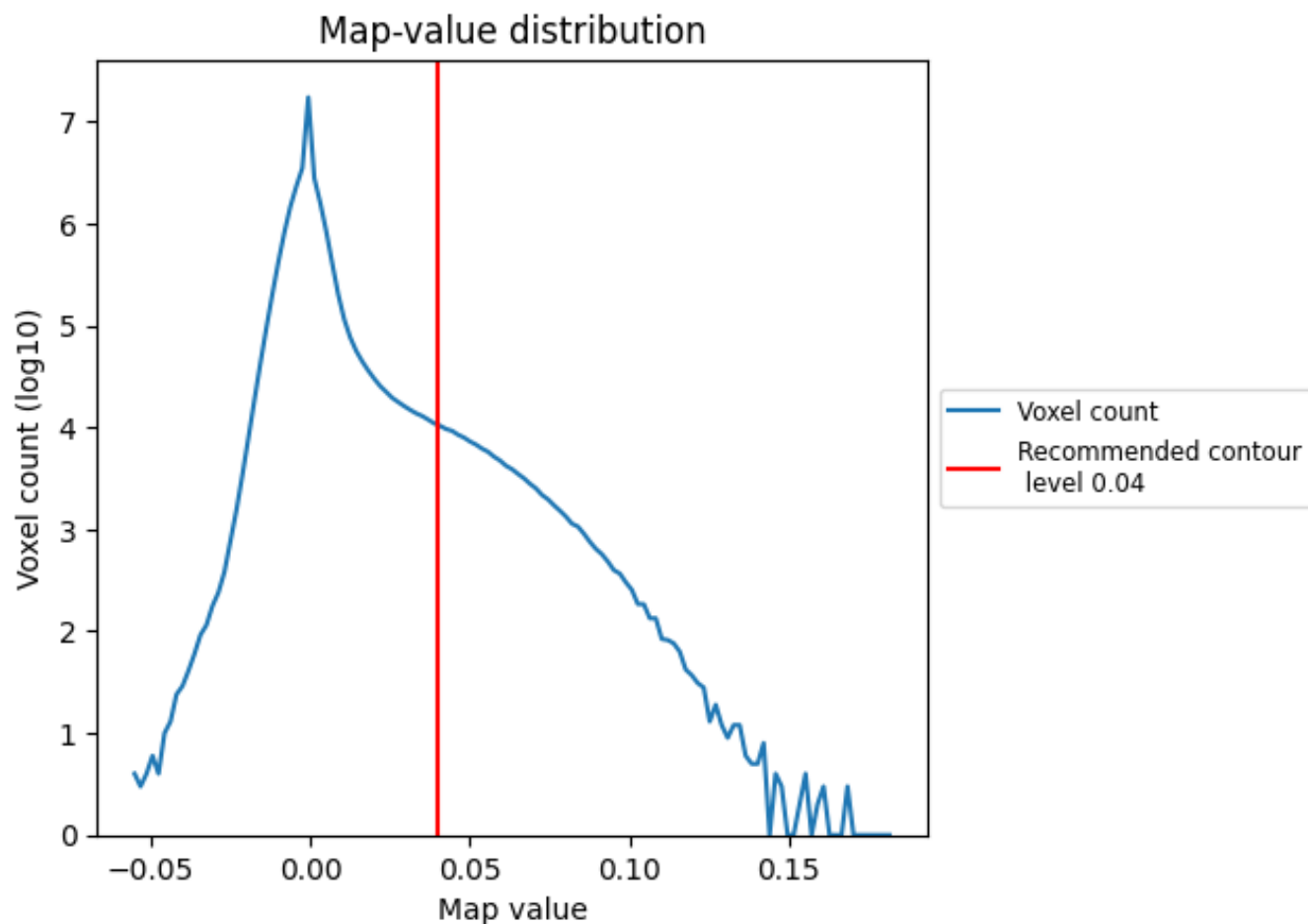


Z

7 Map analysis [i](#)

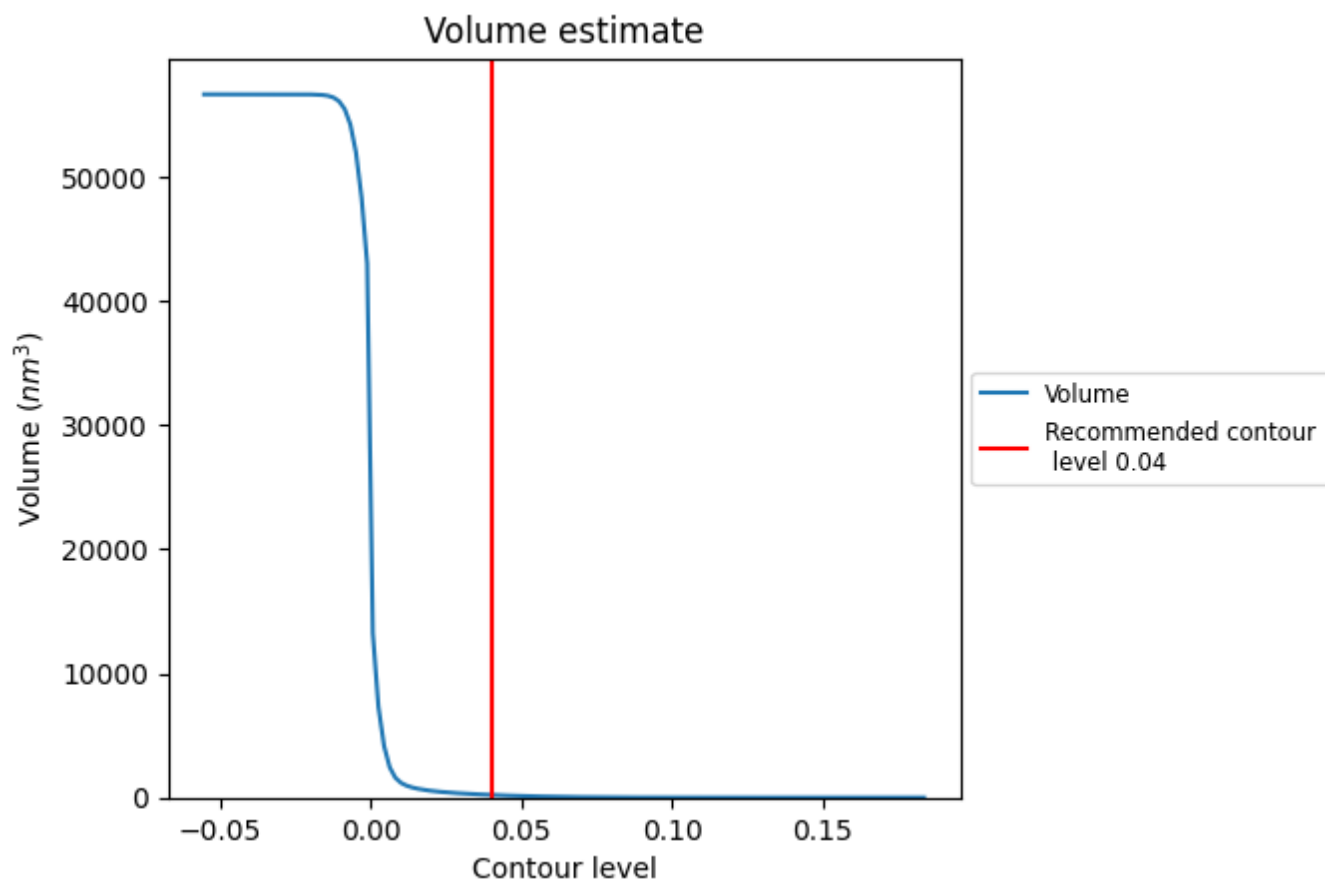
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

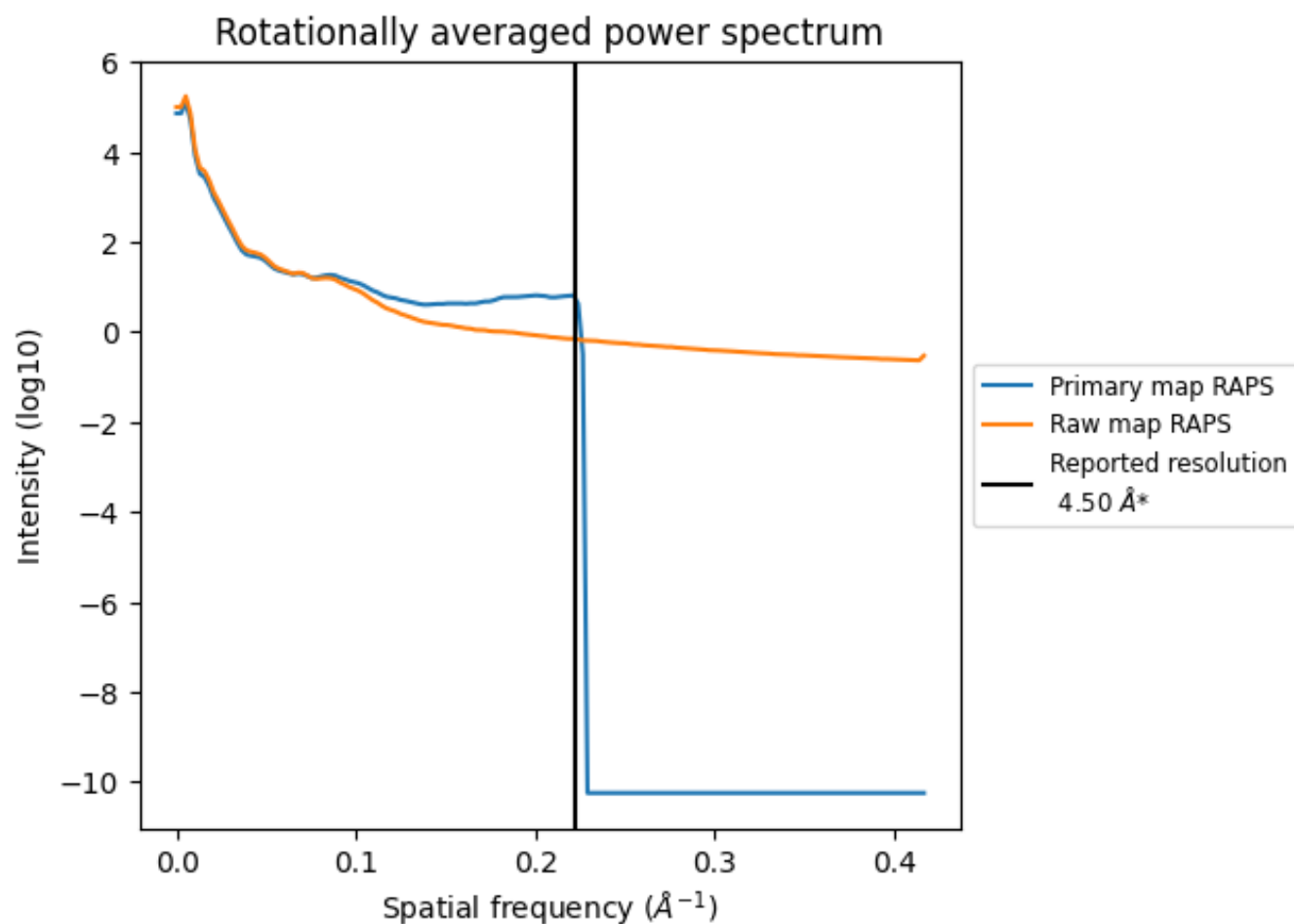
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 191 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 ⓘ

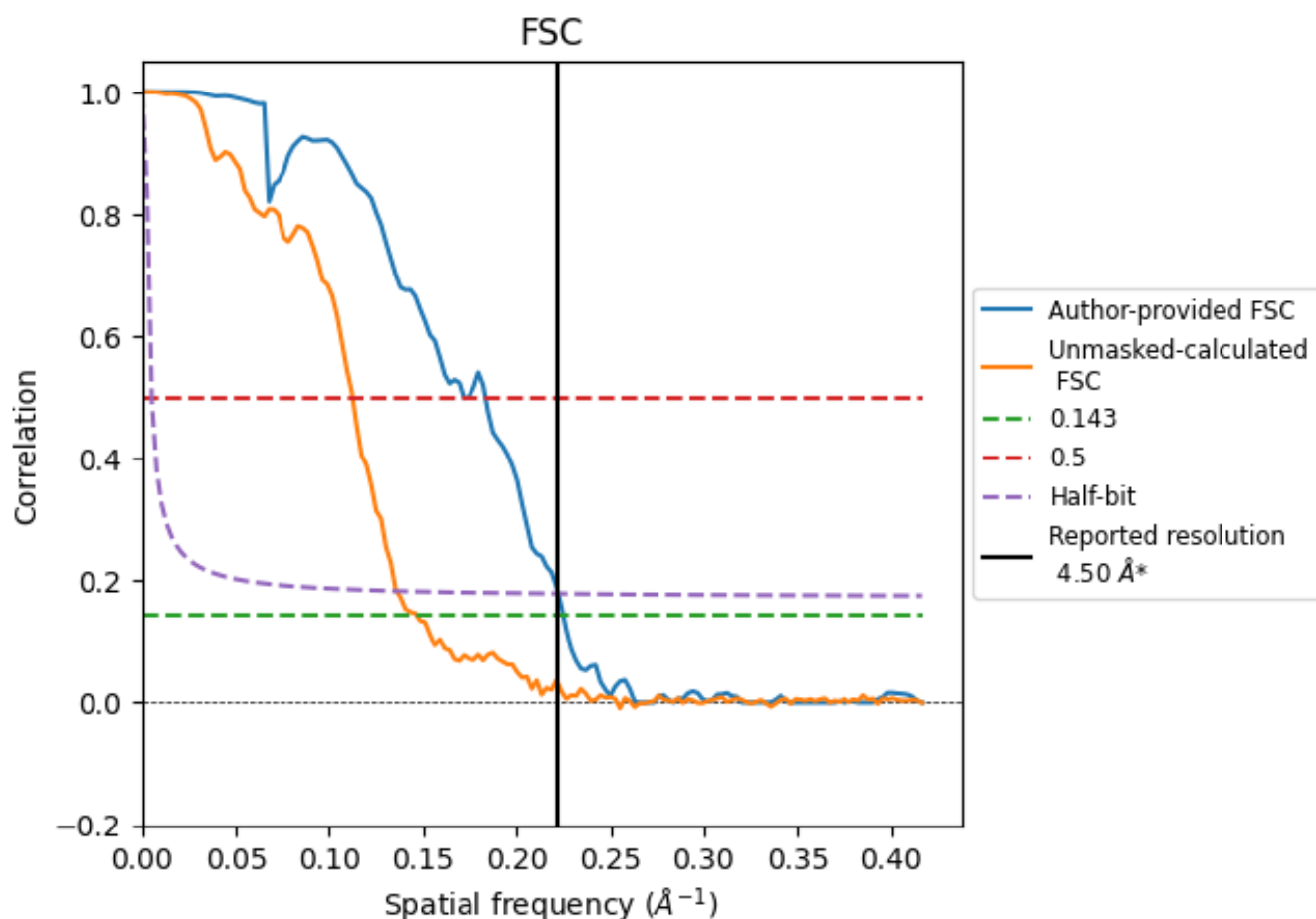


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

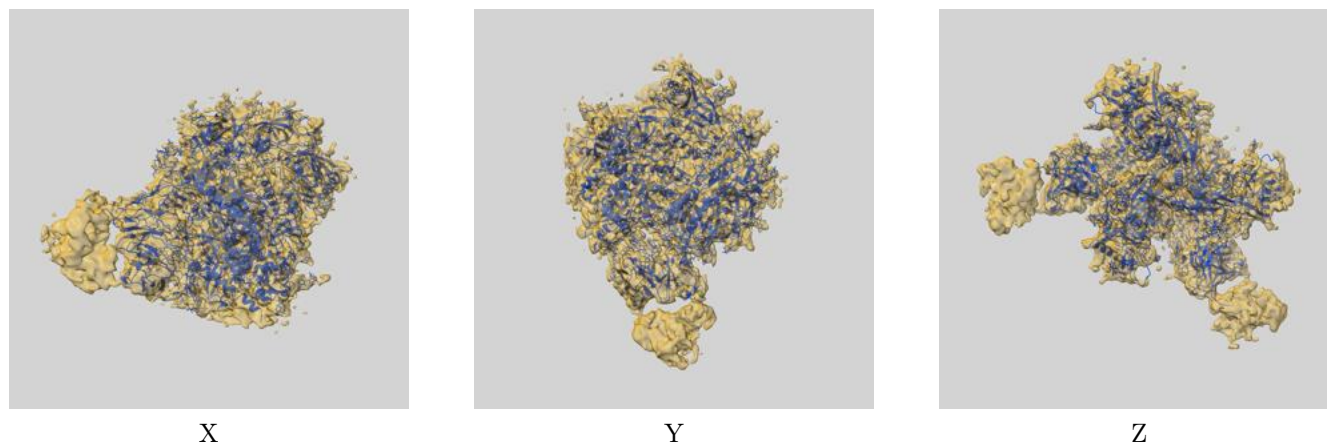
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.45	5.82	4.50
Unmasked-calculated*	6.82	8.90	7.36

*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 6.82 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9062 and PDB model 6MAR. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



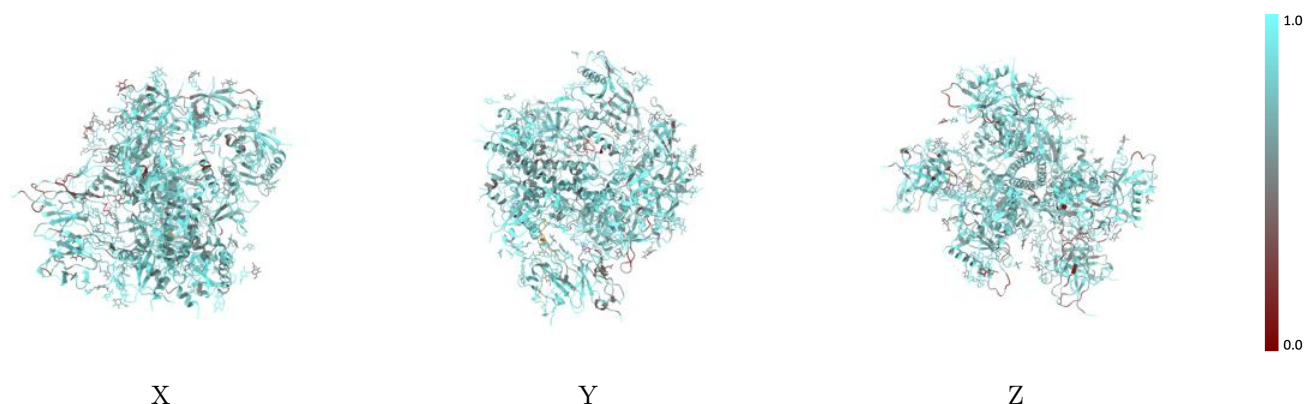
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



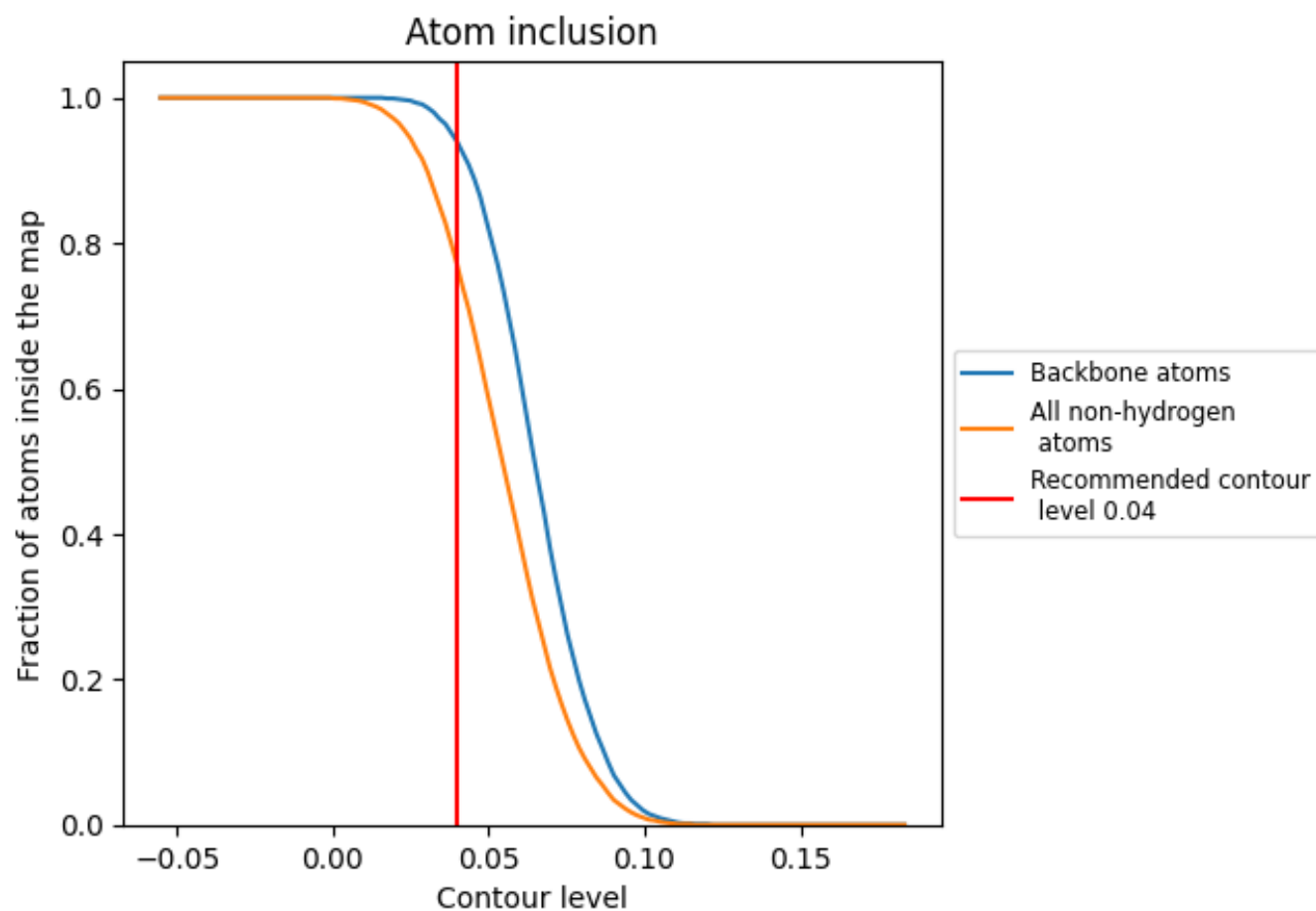
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 77% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.3610
A	 0.7690	 0.3710
B	 0.8130	 0.3670
C	 0.7570	 0.3550
D	 0.7490	 0.3360
E	 0.7770	 0.3600
F	 0.8050	 0.3560
G	 0.5360	 0.3550
H	 0.8170	 0.3680
I	 0.7500	 0.4130
J	 0.5710	 0.4030
K	 0.7360	 0.4490
L	 0.6740	 0.3310
M	 0.8440	 0.3640
N	 0.7520	 0.3490
O	 0.5360	 0.4080
P	 0.7140	 0.4240
Q	 0.6150	 0.2260
R	 0.8570	 0.4140
S	 0.5710	 0.2700
T	 0.7930	 0.4160
U	 0.7420	 0.4240
V	 0.6790	 0.4360
W	 0.5000	 0.3630
X	 0.5360	 0.3790
Y	 0.7500	 0.4070
Z	 0.5360	 0.4160
a	 0.8210	 0.3780
b	 0.6430	 0.3940
c	 0.7860	 0.4060
d	 0.7500	 0.3010
e	 0.6000	 0.2820
f	 0.6790	 0.3980
g	 0.6430	 0.4150
h	 0.7590	 0.4450



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Chain	Atom inclusion	Q-score
i	 0.6070	 0.4110
j	 0.8720	 0.3140
k	 0.5360	 0.4230
l	 0.6790	 0.3620
m	 0.7500	 0.2570
n	 0.8680	 0.4370
o	 0.7500	 0.4280