



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 7MXE / pdb_00007mx
EMDB ID : EMD-24072
Title : Ab1245 Fab in complex with BG505 SOSIP.664 and 8ANC195 Fab
Authors : Abernathy, M.E.; Bjorkman, P.J.
Deposited on : 2021-05-19
Resolution : 3.70 Å (reported)
Based on initial models : 5CJX, 6NC3

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:

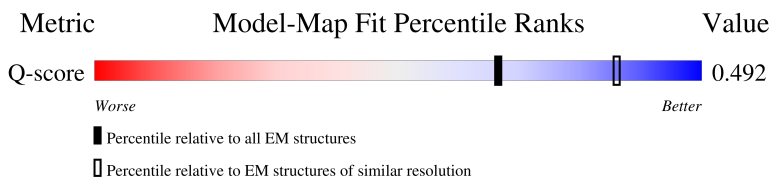
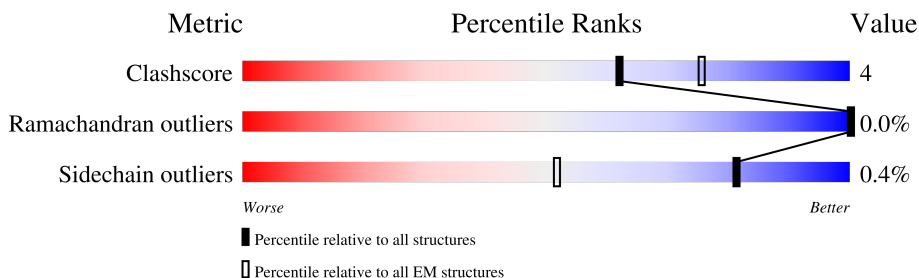
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.70 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.



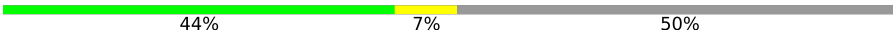
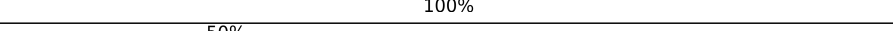
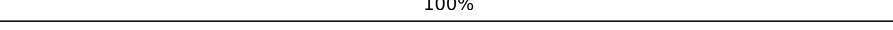
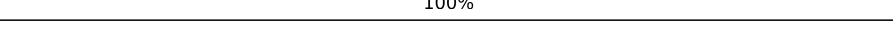
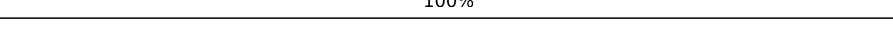
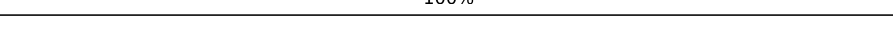
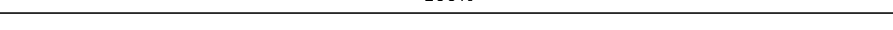
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	244	
1	H	244	
1	M	244	
2	B	215	

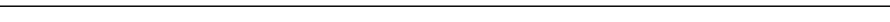
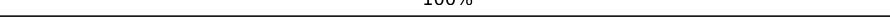
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Mol	Chain	Length	Quality of chain
2	L	215	
2	O	215	
3	C	153	
3	D	153	
3	F	153	
4	G	479	
4	J	479	
4	P	479	
5	R	263	
6	W	241	
7	E	2	
7	I	2	
7	K	2	
7	N	2	
7	Q	2	
7	S	2	
7	T	2	
7	U	2	
7	Z	2	
7	a	2	
7	b	2	
7	c	2	
7	d	2	
7	e	2	
7	f	2	

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Mol	Chain	Length	Quality of chain
7	g	2	 100%
7	l	2	 100%
7	m	2	 100%
7	n	2	 50% 50%
7	o	2	 50% 100%
7	t	2	 100%
8	V	4	 75% 25%
9	X	6	 17% 50% 50%
10	Y	11	 18% 82%
11	h	5	 40% 60%
11	s	5	 60% 40%
12	i	10	 20% 80%
12	r	10	 20% 80%
13	j	3	 33% 67%
13	k	3	 33% 67% 33%
13	p	3	 100%
13	q	3	 100%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22149 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 8ANC195 G52K5 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1014	642	176	193	3		
1	H	132	Total	C	N	O	S	0	0
			1014	642	176	193	3		
1	M	132	Total	C	N	O	S	0	0
			1014	642	176	193	3		

- Molecule 2 is a protein called 8ANC195 G52K5 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	108	Total	C	N	O	S	0	0
			795	499	135	158	3		
2	L	108	Total	C	N	O	S	0	0
			823	516	145	159	3		
2	O	108	Total	C	N	O	S	0	0
			799	502	136	158	3		

- Molecule 3 is a protein called HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	124	Total	C	N	O	S	0	0
			988	625	171	186	6		
3	D	122	Total	C	N	O	S	0	0
			975	616	169	184	6		
3	F	99	Total	C	N	O	S	0	0
			822	524	141	153	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	559	PRO	ILE	engineered mutation	UNP Q2N0S6
C	605	CYS	THR	engineered mutation	UNP Q2N0S6
D	559	PRO	ILE	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	605	CYS	THR	engineered mutation	UNP Q2N0S6
F	559	PRO	ILE	engineered mutation	UNP Q2N0S6
F	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 4 is a protein called Envelope glycoprotein BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	442	Total	C	N	O	S	0	0
			3479	2184	617	650	28		
4	J	442	Total	C	N	O	S	0	0
			3479	2184	617	650	28		
4	P	438	Total	C	N	O	S	0	0
			3449	2166	612	643	28		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	GLU	engineered mutation	UNP Q2N0S6
G	510	ARG	LYS	engineered mutation	UNP Q2N0S6
G	511	ARG	-	insertion	UNP Q2N0S6
G	512	ARG	-	insertion	UNP Q2N0S6
J	332	ASN	THR	engineered mutation	UNP Q2N0S6
J	501	CYS	ALA	engineered mutation	UNP Q2N0S6
J	509	ARG	GLU	engineered mutation	UNP Q2N0S6
J	510	ARG	LYS	engineered mutation	UNP Q2N0S6
J	511	ARG	-	insertion	UNP Q2N0S6
J	512	ARG	-	insertion	UNP Q2N0S6
P	332	ASN	THR	engineered mutation	UNP Q2N0S6
P	501	CYS	ALA	engineered mutation	UNP Q2N0S6
P	509	ARG	GLU	engineered mutation	UNP Q2N0S6
P	510	ARG	LYS	engineered mutation	UNP Q2N0S6
P	511	ARG	-	insertion	UNP Q2N0S6
P	512	ARG	-	insertion	UNP Q2N0S6

- Molecule 5 is a protein called Ab1245 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	129	Total	C	N	O	S	0	0
			989	631	166	189	3		

- Molecule 6 is a protein called Ab1245 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	W	116	Total	C	N	O	S	0	0
			840	518	148	171	3		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	2	Total	C	N	O		0	0
			28	16	2	10			
7	I	2	Total	C	N	O		0	0
			28	16	2	10			
7	K	2	Total	C	N	O		0	0
			28	16	2	10			
7	N	2	Total	C	N	O		0	0
			28	16	2	10			
7	Q	2	Total	C	N	O		0	0
			28	16	2	10			
7	S	2	Total	C	N	O		0	0
			28	16	2	10			
7	T	2	Total	C	N	O		0	0
			28	16	2	10			
7	U	2	Total	C	N	O		0	0
			28	16	2	10			
7	Z	2	Total	C	N	O		0	0
			28	16	2	10			
7	a	2	Total	C	N	O		0	0
			28	16	2	10			
7	b	2	Total	C	N	O		0	0
			28	16	2	10			
7	c	2	Total	C	N	O		0	0
			28	16	2	10			
7	d	2	Total	C	N	O		0	0
			28	16	2	10			
7	e	2	Total	C	N	O		0	0
			28	16	2	10			
7	f	2	Total	C	N	O		0	0
			28	16	2	10			

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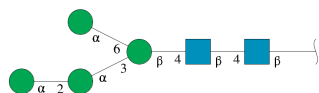
Mol	Chain	Residues	Atoms				AltConf	Trace
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	l	2	Total	C	N	O	0	0
			28	16	2	10		
7	m	2	Total	C	N	O	0	0
			28	16	2	10		
7	n	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	2	Total	C	N	O	0	0
			28	16	2	10		
7	t	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.



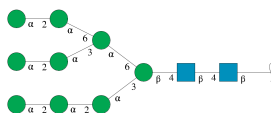
Mol	Chain	Residues	Atoms				AltConf	Trace
8	V	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 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.



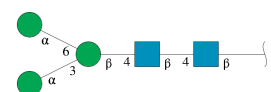
Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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.



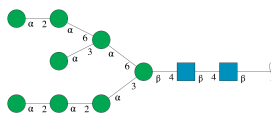
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Y	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 11 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.



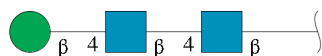
Mol	Chain	Residues	Atoms				AltConf	Trace
11	h	5	Total	C	N	O	0	0
			61	34	2	25		
11	s	5	Total	C	N	O	0	0
			61	34	2	25		

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



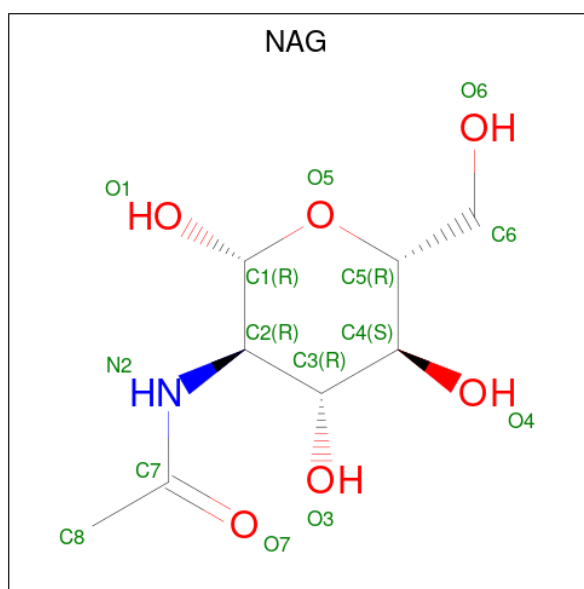
Mol	Chain	Residues	Atoms				AltConf	Trace
12	i	10	Total	C	N	O	0	0
			116	64	2	50		
12	r	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 13 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
13	j	3	Total	C	N	O	0	0
			39	22	2	15		
13	k	3	Total	C	N	O	0	0
			39	22	2	15		
13	p	3	Total	C	N	O	0	0
			39	22	2	15		
13	q	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				AltConf
14	G	1	Total 14	C 8	N 1	O 5	0
14	G	1	Total 14	C 8	N 1	O 5	0
14	G	1	Total 14	C 8	N 1	O 5	0
14	G	1	Total 14	C 8	N 1	O 5	0
14	G	1	Total 14	C 8	N 1	O 5	0
14	G	1	Total 14	C 8	N 1	O 5	0
14	J	1	Total 14	C 8	N 1	O 5	0
14	J	1	Total 14	C 8	N 1	O 5	0
14	J	1	Total 14	C 8	N 1	O 5	0
14	J	1	Total 14	C 8	N 1	O 5	0
14	J	1	Total 14	C 8	N 1	O 5	0
14	P	1	Total 14	C 8	N 1	O 5	0
14	P	1	Total 14	C 8	N 1	O 5	0
14	P	1	Total 14	C 8	N 1	O 5	0
14	P	1	Total 14	C 8	N 1	O 5	0
14	P	1	Total 14	C 8	N 1	O 5	0
14	P	1	Total 14	C 8	N 1	O 5	0

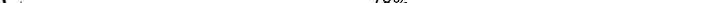
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D1	C23	Q37	R45	F71	K107	ARG	THR	VAL	ALA	ALA	ALA	ALA	PRO	PRO	SER	ASP	GLU	GLN	LEU	LYS	THR	GLY	SER	LYS	THR	ALA	ALA	SER	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	THR	THR	PRO	ARG	GLU	ALA	LYS	VAL	GLN	THR	TRP	LYS	VAL	ASN	GLY	ASP	ALA	LEU	GLN	CYS										

- Chain L: 46% . 50%

[illegible]

- Chain O:

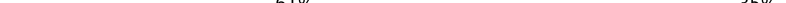
[illegible]

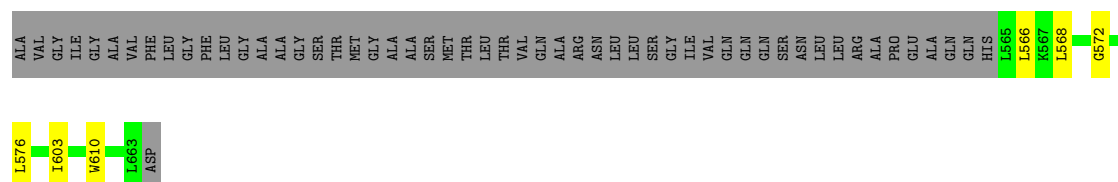
- Chain C:  78% • 19%

ALA	VAL	GLY	ILE	GLY	ALA	VAL	PHE	LS20	SS46	GLY	ILE	VAL	GLN	GLN	GLN	SER	ASN	LEU	LEU	ARG	ALA	ALA	PRO	GLU	ALA	ALA	GLN	GLN	HIS	LEU	LEU	K567	C605	N637	Q652	K655	Q658	L663	ASP
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- Chain D: 69% 8% • 20%

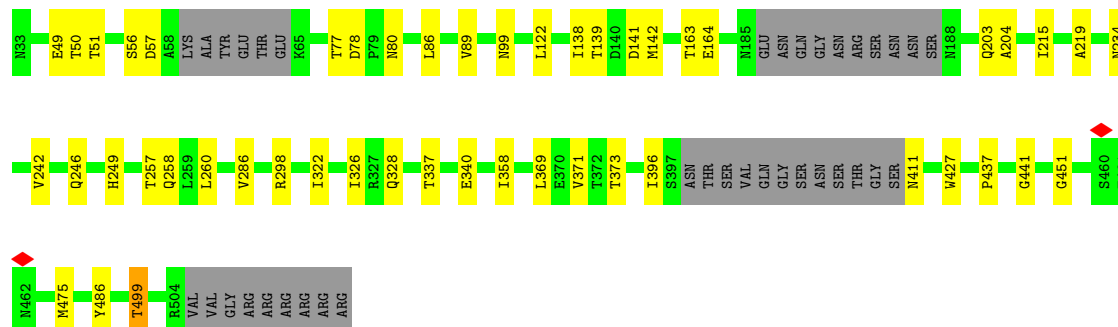
ALA	VAL	GLY	ILE	GLY	ALA	VAL	PHE	L520	G546	GLY	ILE	VAL	GLN	GLN	GLN	ASN	LEU	ARG	ALA	ALA	PRO	GLU	GLN	GLN	HIS	LEU	L566	Q577	V580	G597	M616	E648	S649	Q650	M651	Q652	E653	E654	K655	N656	E657	Q658	D659	L660	LEU	ALA	LEU	ASP
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- Chain F:  61% 0 35%



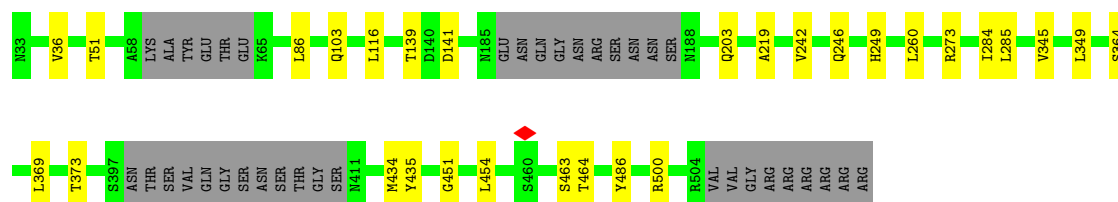
- Molecule 4: Envelope glycoprotein BG505 SOSIP.664 gp120

Chain G: 82% 10% 8%



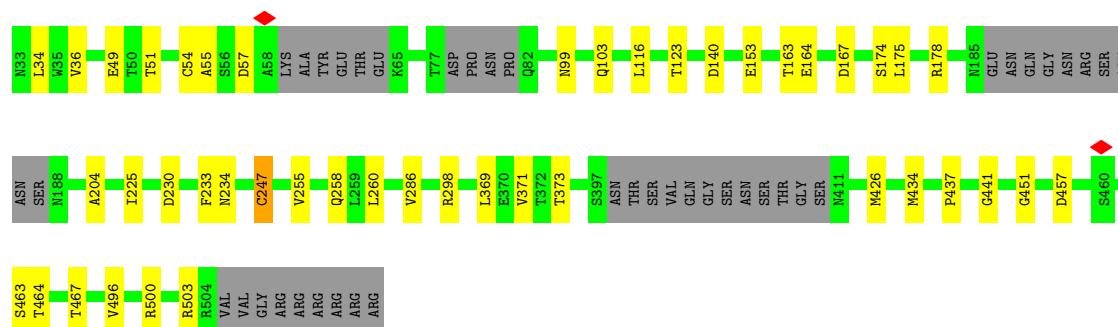
- Molecule 4: Envelope glycoprotein BG505 SOSIP.664 gp120

Chain J: 86% 6% 8%



- Molecule 4: Envelope glycoprotein BG505 SOSIP.664 gp120

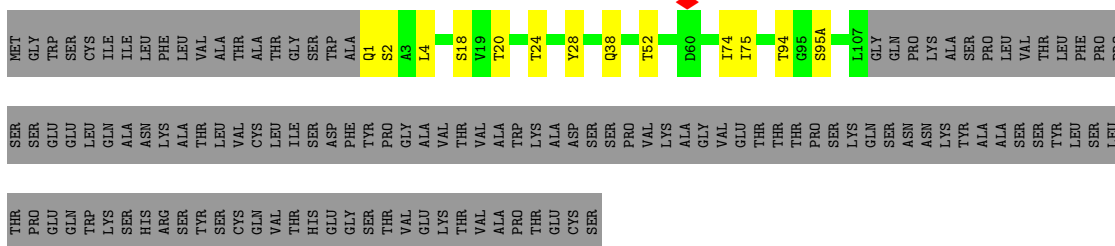
Chain P: 82% 9% 9%



- Molecule 5: Ab1245 Fab heavy chain

Chain R: 42% 7% 51%

- Molecule 6: Ab1245 Fab light chain



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



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



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

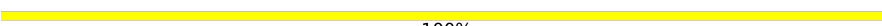


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain Q:  100%



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

Chain S:  100%



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

Chain T:  50%  50%

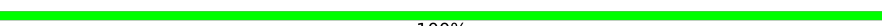


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

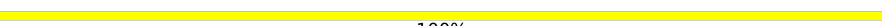


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



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

Chain a:  100%



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

Chain b:  50% 50%



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

Chain c:  50% 50%



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

Chain d:  50% 50%



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

Chain e:  50% 50%



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

Chain f:  50% 50% 50%



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

Chain g:  100%

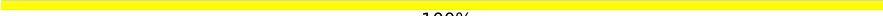


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%

NAG1
NAG2

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

Chain m:  100%

NAG1
NAG2

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

Chain n:  50% 50%

NAG1
NAG2

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

Chain o:  50% 100%

NAG1
NAG2

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

Chain t:  100%

NAG1
NAG2

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

Chain V:  75% 25%

NAG1
NAG2
BMA3
MAN4

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

Chain X:  17% 50% 50%



- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 Y: 18% 82%



- Molecule 11: 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: 40% 60%



- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s: 60% 40%



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

Chain i: 20% 80%



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

Chain r: 20% 80%



- Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	172731	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0154	Depositor
Map size (Å)	290.7744, 290.7744, 290.7744	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8654, 0.8654, 0.8654	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/1041	0.49	2/1418 (0.1%)
1	H	0.14	0/1041	0.38	0/1418
1	M	0.14	0/1041	0.35	0/1418
2	B	0.12	0/813	0.34	0/1110
2	L	0.12	0/841	0.32	0/1141
2	O	0.12	0/817	0.34	0/1114
3	C	0.11	0/1005	0.28	0/1362
3	D	0.24	0/992	0.42	0/1344
3	F	0.11	0/839	0.28	0/1140
4	G	0.14	0/3551	0.35	0/4820
4	J	0.15	0/3551	0.36	0/4820
4	P	0.20	1/3518 (0.0%)	0.39	2/4771 (0.0%)
5	R	0.13	0/1014	0.34	0/1381
6	W	0.13	0/856	0.36	0/1157
All	All	0.16	1/20920 (0.0%)	0.36	4/28414 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	123	THR	C-N	8.02	1.40	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	PRO	CA-C-N	-5.68	113.91	119.76
1	A	75	PRO	C-N-CA	-5.68	113.91	119.76
4	P	140	ASP	CA-C-N	5.31	130.89	122.61
4	P	140	ASP	C-N-CA	5.31	130.89	122.61

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1014	0	984	19	0
1	H	1014	0	984	10	0
1	M	1014	0	984	22	0
2	B	795	0	739	2	0
2	L	823	0	800	5	0
2	O	799	0	750	10	0
3	C	988	0	976	4	0
3	D	975	0	959	35	0
3	F	822	0	807	5	0
4	G	3479	0	3418	29	0
4	J	3479	0	3418	16	0
4	P	3449	0	3395	24	0
5	R	989	0	975	11	0
6	W	840	0	805	9	0
7	E	28	0	25	0	0
7	I	28	0	25	0	0
7	K	28	0	25	0	0
7	N	28	0	25	0	0
7	Q	28	0	24	0	0
7	S	28	0	25	0	0
7	T	28	0	25	0	0
7	U	28	0	25	0	0
7	Z	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	d	28	0	25	0	0
7	e	28	0	25	0	0
7	f	28	0	25	1	0
7	g	28	0	25	0	0
7	l	28	0	25	0	0
7	m	28	0	25	0	0
7	n	28	0	25	0	0
7	o	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	t	28	0	25	0	0
8	V	50	0	43	0	0
9	X	72	0	61	0	0
10	Y	127	0	106	1	0
11	h	61	0	52	0	0
11	s	61	0	52	1	0
12	i	116	0	97	1	0
12	r	116	0	97	2	0
13	j	39	0	34	0	0
13	k	39	0	34	0	0
13	p	39	0	34	0	0
13	q	39	0	34	0	0
14	C	14	0	13	0	0
14	F	14	0	13	0	0
14	G	126	0	117	0	0
14	J	70	0	65	0	0
14	P	98	0	91	0	0
All	All	22149	0	21461	188	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 4.

All (188) 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:D:655:LYS:CE	3:D:658:GLN:NE2	1.70	1.53
3:D:655:LYS:HE3	3:D:658:GLN:NE2	0.85	1.18
3:D:655:LYS:CG	3:D:658:GLN:HE21	1.61	1.14
3:D:655:LYS:HG3	3:D:658:GLN:HE21	0.94	1.10
3:D:597:GLY:HA3	3:D:650:GLN:OE1	1.49	1.09
3:D:657:GLU:O	3:D:660:LEU:N	1.97	0.97
3:D:655:LYS:CD	3:D:658:GLN:NE2	2.28	0.95
3:D:655:LYS:HG3	3:D:658:GLN:NE2	1.79	0.94
3:D:656:ASN:HD21	6:W:52:THR:HG21	1.33	0.92
3:D:655:LYS:HE3	3:D:658:GLN:CD	1.93	0.92
1:A:81:GLU:OE2	1:A:82(A):LYS:HG3	1.71	0.91
3:D:597:GLY:CA	3:D:650:GLN:OE1	2.21	0.88
3:D:657:GLU:O	3:D:659:ASP:N	2.12	0.82
1:M:90:TYR:O	1:M:106:GLY:HA2	1.80	0.82
1:M:87:THR:HA	1:M:109:ILE:O	1.83	0.79
1:A:3:HIS:C	1:A:4:LEU:HD22	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:OE2	1:A:82(A):LYS:CG	2.33	0.76
5:R:90:TYR:O	5:R:106:GLY:HA2	1.87	0.75
1:H:2:ILE:HA	1:H:25:TYR:O	1.90	0.71
3:D:655:LYS:HB2	3:F:603:ILE:HB	1.73	0.71
3:D:657:GLU:C	3:D:659:ASP:N	2.49	0.70
3:D:650:GLN:O	3:D:650:GLN:HG3	1.91	0.70
3:D:655:LYS:CG	3:D:658:GLN:NE2	2.39	0.69
1:A:2:ILE:O	1:A:3:HIS:ND1	2.29	0.66
1:H:87:THR:HA	1:H:109:ILE:O	1.94	0.66
3:D:656:ASN:ND2	6:W:52:THR:HG21	2.09	0.65
3:D:654:GLU:HA	3:D:654:GLU:OE1	1.95	0.65
1:A:4:LEU:HD22	1:A:4:LEU:N	2.16	0.61
3:D:651:ASN:C	3:D:653:GLN:H	2.09	0.61
3:D:657:GLU:C	3:D:659:ASP:H	2.08	0.61
3:D:655:LYS:CD	3:D:658:GLN:HE21	1.94	0.61
1:A:29:THR:HG22	1:A:31:GLY:H	1.65	0.60
1:M:61:HIS:HA	1:M:64:ARG:NE	2.17	0.60
3:D:653:GLN:HG2	3:D:653:GLN:O	2.01	0.60
2:L:65:SER:HG	2:L:72:THR:HG1	1.52	0.58
3:D:648:GLU:OE1	3:D:652:GLN:NE2	2.37	0.58
6:W:18:SER:HA	6:W:75:ILE:O	2.04	0.58
3:D:649:SER:C	3:D:651:ASN:H	2.11	0.57
4:J:273:ARG:HG3	4:J:285:LEU:HB2	1.87	0.57
1:M:55:TRP:CD1	12:r:2:NAG:H83	2.40	0.57
1:M:87:THR:HG22	1:M:111:VAL:H	1.68	0.57
1:A:51:ILE:O	1:A:51:ILE:HG23	2.05	0.56
4:P:230:ASP:HB3	4:P:233:PHE:HB2	1.86	0.56
1:H:37:VAL:HG12	1:H:47:TYR:HA	1.89	0.55
2:L:37:GLN:HE21	2:L:45:ARG:HD3	1.72	0.55
1:M:60:SER:O	1:M:64:ARG:HG3	2.07	0.54
4:G:49:GLU:OE1	4:G:99:ASN:ND2	2.41	0.54
1:H:99:ASP:HB3	1:H:100(B):SER:HB2	1.89	0.54
3:D:657:GLU:O	3:D:658:GLN:C	2.52	0.53
1:H:90:TYR:O	1:H:106:GLY:HA2	2.09	0.53
5:R:2:VAL:N	5:R:25:SER:O	2.43	0.52
5:R:35(A):LYS:HG2	5:R:50:ARG:HG3	1.91	0.51
1:M:67:VAL:HG12	1:M:82:ILE:HG12	1.92	0.51
5:R:40:PRO:HG2	5:R:43:LYS:HB2	1.92	0.51
1:H:72:ASP:HB2	10:Y:2:NAG:H61	1.93	0.51
4:J:203:GLN:HG3	4:J:435:TYR:HD2	1.75	0.50
4:J:249:HIS:HD1	4:J:486:TYR:HH	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:258:GLN:NE2	4:G:371:VAL:O	2.44	0.50
5:R:39:GLN:HE22	6:W:38:GLN:HE22	1.58	0.50
5:R:66:ARG:NH2	5:R:82(B):SER:O	2.44	0.50
1:M:99:ASP:HB3	1:M:100(B):SER:HB3	1.94	0.50
1:A:81:GLU:CD	1:A:82(A):LYS:HG3	2.36	0.50
4:G:257:THR:HG22	4:G:258:GLN:HG3	1.93	0.50
1:A:4:LEU:N	1:A:4:LEU:CD2	2.75	0.49
4:J:219:ALA:O	4:J:246:GLN:NE2	2.46	0.49
3:D:580:VAL:HG21	3:F:576:LEU:HD11	1.93	0.49
4:G:298:ARG:NH2	4:G:441:GLY:O	2.44	0.49
5:R:101:ASP:OD1	5:R:101:ASP:N	2.45	0.49
1:M:51:ILE:O	1:M:51:ILE:HG23	2.11	0.49
4:P:49:GLU:OE1	4:P:99:ASN:ND2	2.46	0.49
1:A:36:TRP:CZ3	1:A:92:CYS:HB2	2.48	0.49
4:J:51:THR:HA	4:J:103:GLN:HE22	1.76	0.49
1:A:40:ALA:HB3	1:A:43:GLN:HB2	1.94	0.49
4:P:298:ARG:NH2	4:P:441:GLY:O	2.45	0.49
4:G:57:ASP:OD1	4:G:57:ASP:N	2.45	0.48
4:P:463:SER:OG	4:P:464:THR:N	2.46	0.48
4:G:358:ILE:HG22	4:G:396:ILE:HA	1.95	0.48
3:C:652:GLN:HA	3:C:655:LYS:HG2	1.95	0.48
4:G:286:VAL:O	4:G:451:GLY:HA2	2.13	0.48
4:P:258:GLN:NE2	4:P:371:VAL:O	2.46	0.48
5:R:12:VAL:HB	5:R:111:VAL:HG22	1.94	0.48
5:R:83:THR:HG22	5:R:85:ALA:H	1.78	0.48
4:J:345:VAL:O	4:J:349:LEU:HB2	2.12	0.48
3:F:568:LEU:HA	3:F:572:GLY:HA3	1.94	0.48
1:M:7:SER:OG	1:M:8:GLY:N	2.46	0.48
3:D:656:ASN:O	3:D:659:ASP:OD2	2.31	0.48
1:M:34:ALA:HB2	1:M:53:TRP:HD1	1.79	0.47
2:O:61:ARG:NH1	2:O:82:ASP:OD2	2.42	0.47
1:M:40:ALA:HB3	1:M:43:GLN:HB2	1.96	0.47
4:P:255:VAL:HG11	4:P:426:MET:HE1	1.95	0.47
4:G:80:ASN:OD1	4:G:80:ASN:N	2.48	0.47
1:A:99:ASP:HB3	1:A:100(B):SER:HB3	1.96	0.47
3:D:649:SER:C	3:D:651:ASN:N	2.73	0.47
4:G:337:THR:HA	4:G:340:GLU:HG2	1.97	0.47
1:M:72:ASP:HB2	12:r:2:NAG:H61	1.97	0.47
5:R:52(A):GLY:O	5:R:71:LYS:NZ	2.48	0.47
6:W:4:LEU:O	6:W:24:THR:OG1	2.27	0.47
3:C:637:ASN:OD1	2:O:50:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:30:PHE:HB2	1:M:55:TRP:CH2	2.50	0.47
4:G:86:LEU:HD23	4:G:89:VAL:HG21	1.97	0.47
1:M:39:GLN:HE22	2:O:38:GLN:HE22	1.61	0.47
2:L:18:THR:HA	2:L:75:ILE:O	2.14	0.46
2:O:39:ARG:NH2	2:O:81:GLU:O	2.47	0.46
1:A:60:SER:OG	1:A:61:HIS:N	2.48	0.46
4:P:286:VAL:O	4:P:451:GLY:HA2	2.15	0.46
6:W:94:THR:HG23	6:W:95(A):SER:H	1.81	0.46
4:G:219:ALA:O	4:G:246:GLN:NE2	2.47	0.46
1:M:37:VAL:HG12	1:M:47:TYR:HA	1.98	0.46
4:G:138:ILE:HG22	4:G:326:ILE:HB	1.96	0.46
4:P:260:LEU:HD12	4:P:451:GLY:HA3	1.97	0.46
1:M:34:ALA:HB2	1:M:53:TRP:CD1	2.51	0.46
4:P:174:SER:OG	4:P:175:LEU:N	2.48	0.46
4:P:204:ALA:HB3	4:P:437:PRO:HD3	1.99	0.45
4:G:204:ALA:HB3	4:G:437:PRO:HD3	1.99	0.45
6:W:20:THR:HG22	6:W:74:ILE:HG12	1.98	0.45
3:C:605:CYS:O	4:P:503:ARG:NE	2.46	0.45
4:G:322:ILE:HG21	4:G:326:ILE:HG12	1.96	0.45
4:P:57:ASP:OD1	4:P:57:ASP:N	2.43	0.45
3:D:616:ASN:ND2	2:L:27(A):SER:OG	2.44	0.45
4:G:249:HIS:ND1	4:G:486:TYR:OH	2.49	0.45
1:H:12:LYS:HG3	1:H:18:VAL:HG22	1.98	0.44
1:H:38:ARG:HD3	1:H:48:ILE:HD11	1.99	0.44
1:A:35:VAL:HB	1:A:51:ILE:HG22	1.99	0.44
4:G:369:LEU:O	4:G:373:THR:OG1	2.35	0.44
4:G:427:TRP:HZ3	4:G:475:MET:HG2	1.83	0.44
4:J:364:SER:HB3	7:f:1:NAG:H82	1.98	0.44
4:P:163:THR:OG1	4:P:164:GLU:N	2.51	0.44
1:A:37:VAL:O	1:A:91:PHE:HB2	2.17	0.44
4:J:139:THR:OG1	4:J:141:ASP:OD2	2.35	0.44
1:A:72:ASP:HB2	12:i:2:NAG:H61	2.00	0.44
4:G:56:SER:HB2	4:G:215:ILE:HG22	1.99	0.44
4:J:116:LEU:HD21	4:J:434:MET:HG3	2.00	0.44
4:J:369:LEU:O	4:J:373:THR:OG1	2.34	0.44
2:O:11:LEU:HD11	2:O:19:VAL:HG13	1.99	0.44
4:P:369:LEU:O	4:P:373:THR:OG1	2.33	0.44
1:A:35:VAL:HB	1:A:51:ILE:CG2	2.48	0.44
11:s:2:NAG:H4	11:s:3:BMA:H2	1.82	0.44
1:A:83:THR:OG1	1:A:84:SER:N	2.50	0.43
3:C:658:GLN:HE21	4:G:499:THR:HG21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:153:GLU:HA	4:P:178:ARG:HB2	2.00	0.43
4:P:457:ASP:OD2	4:P:467:THR:OG1	2.36	0.43
3:F:610:TRP:HE3	4:J:36:VAL:HG22	1.83	0.43
2:L:39:ARG:NH2	2:L:81:GLU:O	2.47	0.43
1:M:66:ARG:HH11	1:M:82(C):LEU:HA	1.83	0.43
4:G:260:LEU:HD12	4:G:451:GLY:HA3	2.00	0.43
4:J:86:LEU:HB3	4:J:242:VAL:HG23	2.01	0.43
4:J:260:LEU:HD12	4:J:451:GLY:HA3	2.01	0.43
3:D:652:GLN:HG2	6:W:28:TYR:O	2.19	0.42
4:G:139:THR:OG1	4:G:141:ASP:OD1	2.34	0.42
4:G:411:ASN:N	4:G:411:ASN:OD1	2.52	0.42
3:D:577:GLN:HB2	3:F:566:LEU:HD13	2.01	0.42
1:M:72(B):THR:HB	1:M:74:SER:HB3	2.00	0.42
2:O:106:VAL:HG13	2:O:106:VAL:O	2.20	0.42
3:D:660:LEU:HB3	4:J:500:ARG:HH21	1.85	0.42
6:W:1:GLN:HB3	6:W:2:SER:H	1.69	0.42
1:M:12:LYS:HE2	1:M:12:LYS:HB2	1.86	0.42
4:P:54:CYS:SG	4:P:55:ALA:N	2.92	0.42
2:B:23:CYS:HB3	2:B:71:PHE:HB2	2.00	0.42
4:G:77:THR:OG1	4:G:78:ASP:N	2.51	0.42
4:P:36:VAL:HG13	4:P:496:VAL:HG13	2.01	0.42
4:P:167:ASP:OD1	4:P:167:ASP:N	2.47	0.42
1:A:2:ILE:C	1:A:3:HIS:ND1	2.77	0.42
4:G:50:THR:OG1	4:G:51:THR:N	2.53	0.42
4:G:234:ASN:OD1	4:G:234:ASN:N	2.52	0.42
4:G:163:THR:OG1	4:G:164:GLU:N	2.52	0.42
2:O:106:VAL:O	2:O:107:LYS:HG3	2.19	0.42
4:P:225:ILE:HD12	4:P:247:CYS:HA	2.02	0.42
1:H:84:SER:O	1:H:84:SER:OG	2.33	0.41
4:P:51:THR:HA	4:P:103:GLN:HE22	1.85	0.41
3:D:651:ASN:C	3:D:653:GLN:N	2.73	0.41
1:M:61:HIS:HA	1:M:64:ARG:HE	1.84	0.41
2:O:14:SER:OG	2:O:17:ASP:OD2	2.37	0.41
4:P:234:ASN:OD1	4:P:234:ASN:N	2.54	0.41
4:P:34:LEU:HD23	4:P:500:ARG:HG2	2.03	0.41
5:R:2:VAL:HG13	5:R:3:GLN:HG3	2.02	0.41
4:J:463:SER:OG	4:J:464:THR:N	2.54	0.41
1:M:44:SER:OG	1:M:45:LEU:N	2.54	0.41
2:O:18:THR:HA	2:O:75:ILE:O	2.21	0.41
2:B:37:GLN:HE21	2:B:45:ARG:HD3	1.86	0.40
3:D:648:GLU:HA	3:D:651:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:122:LEU:HG	4:G:203:GLN:HB2	2.02	0.40
2:O:39:ARG:NH2	2:O:81:GLU:OE1	2.53	0.40
3:D:657:GLU:OE1	3:D:657:GLU:HA	2.11	0.40
4:G:249:HIS:HD1	4:G:486:TYR:HH	1.67	0.40
1:H:12:LYS:HD3	1:H:12:LYS:HA	1.96	0.40
4:P:116:LEU:HD21	4:P:434:MET:HG3	2.04	0.40
4:G:142:MET:HE3	4:G:328:GLN:HG2	2.04	0.40
4:J:284:ILE:HB	4:J:454:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/244 (53%)	127 (98%)	3 (2%)	0	100	100
1	H	130/244 (53%)	127 (98%)	3 (2%)	0	100	100
1	M	130/244 (53%)	125 (96%)	5 (4%)	0	100	100
2	B	106/215 (49%)	102 (96%)	4 (4%)	0	100	100
2	L	106/215 (49%)	104 (98%)	2 (2%)	0	100	100
2	O	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
3	C	120/153 (78%)	118 (98%)	2 (2%)	0	100	100
3	D	118/153 (77%)	112 (95%)	5 (4%)	1 (1%)	16	48
3	F	97/153 (63%)	93 (96%)	4 (4%)	0	100	100
4	G	434/479 (91%)	419 (96%)	15 (4%)	0	100	100
4	J	434/479 (91%)	419 (96%)	15 (4%)	0	100	100
4	P	428/479 (89%)	414 (97%)	14 (3%)	0	100	100
5	R	127/263 (48%)	122 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	W	114/241 (47%)	107 (94%)	7 (6%)	0	100	100
All	All	2580/3777 (68%)	2492 (97%)	87 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	658	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/210 (53%)	111 (99%)	1 (1%)	70	75
1	H	112/210 (53%)	112 (100%)	0	100	100
1	M	112/210 (53%)	112 (100%)	0	100	100
2	B	80/182 (44%)	80 (100%)	0	100	100
2	L	86/182 (47%)	86 (100%)	0	100	100
2	O	81/182 (44%)	81 (100%)	0	100	100
3	C	107/129 (83%)	107 (100%)	0	100	100
3	D	106/129 (82%)	102 (96%)	4 (4%)	29	53
3	F	91/129 (70%)	91 (100%)	0	100	100
4	G	395/427 (92%)	393 (100%)	2 (0%)	81	80
4	J	395/427 (92%)	395 (100%)	0	100	100
4	P	391/427 (92%)	390 (100%)	1 (0%)	86	83
5	R	109/225 (48%)	109 (100%)	0	100	100
6	W	90/196 (46%)	90 (100%)	0	100	100
All	All	2267/3265 (69%)	2259 (100%)	8 (0%)	81	81

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
3	D	652	GLN
3	D	655	LYS
3	D	656	ASN
3	D	657	GLU
4	G	242	VAL
4	G	499	THR
4	P	247	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	100(F)	HIS
2	B	37	GLN
2	B	38	GLN
3	C	543	ASN
3	C	575	GLN
3	C	577	GLN
3	C	590	GLN
3	C	650	GLN
3	C	652	GLN
3	C	658	GLN
3	D	543	ASN
3	D	590	GLN
3	D	616	ASN
3	D	656	ASN
3	F	575	GLN
3	F	625	ASN
3	F	650	GLN
4	G	82	GLN
4	G	103	GLN
4	G	411	ASN
1	H	6	GLN
1	H	100(F)	HIS
4	J	80	ASN
4	J	103	GLN
4	J	136	ASN
4	J	188	ASN
4	J	203	GLN
4	J	258	GLN
2	L	31	ASN
2	L	37	GLN

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Mol	Chain	Res	Type
1	M	6	GLN
1	M	35(A)	ASN
1	M	43	GLN
1	M	50	GLN
1	M	100(F)	HIS
1	M	105	GLN
2	O	3	GLN
2	O	38	GLN
4	P	33	ASN
4	P	103	GLN
4	P	137	ASN
4	P	280	ASN
4	P	422	GLN
4	P	428	GLN
4	P	478	ASN
5	R	39	GLN
5	R	77	HIS
5	R	100(L)	ASN
6	W	1	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

105 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
7	NAG	E	1	3,7	14,14,15	0.33	0	17,19,21	0.61	0
7	NAG	E	2	7	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
7	NAG	I	1	3,7	14,14,15	0.36	0	17,19,21	0.57	0
7	NAG	I	2	7	14,14,15	0.89	1 (7%)	17,19,21	2.37	3 (17%)
7	NAG	K	1	3,7	14,14,15	0.35	0	17,19,21	0.55	0
7	NAG	K	2	7	14,14,15	0.36	0	17,19,21	0.51	0
7	NAG	N	1	7,4	14,14,15	0.33	0	17,19,21	0.53	0
7	NAG	N	2	7	14,14,15	0.45	0	17,19,21	0.51	0
7	NAG	Q	1	7,4	14,14,15	0.56	0	17,19,21	1.02	1 (5%)
7	NAG	Q	2	7	14,14,15	0.58	0	17,19,21	1.07	1 (5%)
7	NAG	S	1	7,4	14,14,15	0.50	0	17,19,21	1.06	1 (5%)
7	NAG	S	2	7	14,14,15	0.52	0	17,19,21	1.05	1 (5%)
7	NAG	T	1	7,4	14,14,15	0.37	0	17,19,21	0.54	0
7	NAG	T	2	7	14,14,15	0.56	0	17,19,21	1.03	1 (5%)
7	NAG	U	1	7,4	14,14,15	0.29	0	17,19,21	0.52	0
7	NAG	U	2	7	14,14,15	0.37	0	17,19,21	0.53	0
8	NAG	V	1	8,4	14,14,15	0.38	0	17,19,21	0.57	0
8	NAG	V	2	8	14,14,15	0.33	0	17,19,21	0.47	0
8	BMA	V	3	8	11,11,12	0.77	0	15,15,17	0.83	0
8	MAN	V	4	8	11,11,12	0.81	0	15,15,17	1.08	2 (13%)
9	NAG	X	1	9,4	14,14,15	0.25	0	17,19,21	0.44	0
9	NAG	X	2	9	14,14,15	0.30	0	17,19,21	0.53	0
9	BMA	X	3	9	11,11,12	0.80	0	15,15,17	0.77	0
9	MAN	X	4	9	11,11,12	0.84	0	15,15,17	1.14	1 (6%)
9	MAN	X	5	9	11,11,12	0.82	0	15,15,17	1.16	2 (13%)
9	MAN	X	6	9	11,11,12	0.82	0	15,15,17	1.07	2 (13%)
10	NAG	Y	1	10,4	14,14,15	0.30	0	17,19,21	0.52	0
10	MAN	Y	10	10	11,11,12	0.81	0	15,15,17	1.12	2 (13%)
10	MAN	Y	11	10	11,11,12	0.79	0	15,15,17	1.06	2 (13%)
10	NAG	Y	2	10	14,14,15	0.33	0	17,19,21	0.53	0
10	BMA	Y	3	10	11,11,12	0.83	0	15,15,17	0.75	0
10	MAN	Y	4	10	11,11,12	0.78	0	15,15,17	1.04	2 (13%)
10	MAN	Y	5	10	11,11,12	0.80	0	15,15,17	1.09	2 (13%)
10	MAN	Y	6	10	11,11,12	0.82	0	15,15,17	0.99	2 (13%)
10	MAN	Y	7	10	11,11,12	0.81	0	15,15,17	1.12	2 (13%)
10	MAN	Y	8	10	11,11,12	0.79	0	15,15,17	1.05	2 (13%)
10	MAN	Y	9	10	11,11,12	0.81	0	15,15,17	1.06	2 (13%)
7	NAG	Z	1	7,4	14,14,15	0.32	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	Z	2	7	14,14,15	0.38	0	17,19,21	0.50	0
7	NAG	a	1	7,4	14,14,15	0.48	0	17,19,21	1.04	1 (5%)
7	NAG	a	2	7	14,14,15	0.52	0	17,19,21	1.04	1 (5%)
7	NAG	b	1	7,4	14,14,15	0.37	0	17,19,21	0.52	0
7	NAG	b	2	7	14,14,15	0.61	0	17,19,21	1.03	1 (5%)
7	NAG	c	1	7,4	14,14,15	0.37	0	17,19,21	0.58	0
7	NAG	c	2	7	14,14,15	0.52	0	17,19,21	1.03	1 (5%)
7	NAG	d	1	7,4	14,14,15	0.40	0	17,19,21	0.62	1 (5%)
7	NAG	d	2	7	14,14,15	0.40	0	17,19,21	0.49	0
7	NAG	e	1	7,4	14,14,15	0.34	0	17,19,21	0.55	0
7	NAG	e	2	7	14,14,15	0.55	0	17,19,21	1.04	1 (5%)
7	NAG	f	1	7,4	14,14,15	0.28	0	17,19,21	0.50	0
7	NAG	f	2	7	14,14,15	0.36	0	17,19,21	0.51	0
7	NAG	g	1	7,4	14,14,15	0.31	0	17,19,21	0.53	0
7	NAG	g	2	7	14,14,15	0.36	0	17,19,21	0.52	0
11	NAG	h	1	11,4	14,14,15	0.28	0	17,19,21	0.50	0
11	NAG	h	2	11	14,14,15	0.34	0	17,19,21	0.57	0
11	BMA	h	3	11	11,11,12	0.81	0	15,15,17	0.88	1 (6%)
11	MAN	h	4	11	11,11,12	0.83	0	15,15,17	1.06	2 (13%)
11	MAN	h	5	11	11,11,12	0.87	1 (9%)	15,15,17	1.23	2 (13%)
12	NAG	i	1	12,4	14,14,15	0.37	0	17,19,21	0.56	0
12	MAN	i	10	12	11,11,12	0.81	0	15,15,17	1.06	2 (13%)
12	NAG	i	2	12	14,14,15	0.36	0	17,19,21	0.51	0
12	BMA	i	3	12	11,11,12	0.86	0	15,15,17	0.75	0
12	MAN	i	4	12	11,11,12	0.79	0	15,15,17	1.03	2 (13%)
12	MAN	i	5	12	11,11,12	0.79	0	15,15,17	1.12	2 (13%)
12	MAN	i	6	12	11,11,12	0.78	0	15,15,17	1.04	2 (13%)
12	MAN	i	7	12	11,11,12	0.80	0	15,15,17	1.13	2 (13%)
12	MAN	i	8	12	11,11,12	0.81	0	15,15,17	1.13	2 (13%)
12	MAN	i	9	12	11,11,12	0.80	0	15,15,17	1.06	2 (13%)
13	NAG	j	1	13,4	14,14,15	0.36	0	17,19,21	0.61	1 (5%)
13	NAG	j	2	13	14,14,15	0.50	0	17,19,21	1.06	1 (5%)
13	BMA	j	3	13	11,11,12	0.79	0	15,15,17	0.83	0
13	NAG	k	1	13,4	14,14,15	0.48	0	17,19,21	1.03	1 (5%)
13	NAG	k	2	13	14,14,15	0.30	0	17,19,21	0.63	0
13	BMA	k	3	13	11,11,12	0.81	0	15,15,17	0.81	0
7	NAG	l	1	7,4	14,14,15	0.33	0	17,19,21	0.54	0
7	NAG	l	2	7	14,14,15	0.39	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	m	1	7,4	14,14,15	0.50	0	17,19,21	1.05	1 (5%)
7	NAG	m	2	7	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
7	NAG	n	1	7,4	14,14,15	0.37	0	17,19,21	0.60	0
7	NAG	n	2	7	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
7	NAG	o	1	7,4	14,14,15	0.45	0	17,19,21	0.61	1 (5%)
7	NAG	o	2	7	14,14,15	0.54	0	17,19,21	1.03	1 (5%)
13	NAG	p	1	13,4	14,14,15	0.29	0	17,19,21	0.49	0
13	NAG	p	2	13	14,14,15	0.32	0	17,19,21	0.54	0
13	BMA	p	3	13	11,11,12	0.79	0	15,15,17	0.80	0
13	NAG	q	1	13,4	14,14,15	0.36	0	17,19,21	0.55	0
13	NAG	q	2	13	14,14,15	0.32	0	17,19,21	0.48	0
13	BMA	q	3	13	11,11,12	0.79	0	15,15,17	0.81	0
12	NAG	r	1	12,4	14,14,15	0.33	0	17,19,21	0.55	0
12	MAN	r	10	12	11,11,12	0.80	0	15,15,17	1.06	2 (13%)
12	NAG	r	2	12	14,14,15	0.34	0	17,19,21	0.62	0
12	BMA	r	3	12	11,11,12	0.85	0	15,15,17	0.73	0
12	MAN	r	4	12	11,11,12	0.79	0	15,15,17	1.05	2 (13%)
12	MAN	r	5	12	11,11,12	0.80	0	15,15,17	1.08	2 (13%)
12	MAN	r	6	12	11,11,12	0.79	0	15,15,17	1.06	2 (13%)
12	MAN	r	7	12	11,11,12	0.80	0	15,15,17	1.11	2 (13%)
12	MAN	r	8	12	11,11,12	0.81	0	15,15,17	1.11	2 (13%)
12	MAN	r	9	12	11,11,12	0.80	0	15,15,17	1.07	2 (13%)
11	NAG	s	1	11,4	14,14,15	0.62	0	17,19,21	0.88	1 (5%)
11	NAG	s	2	11	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
11	BMA	s	3	11	11,11,12	1.03	1 (9%)	15,15,17	0.90	0
11	MAN	s	4	11	11,11,12	1.08	1 (9%)	15,15,17	1.30	2 (13%)
11	MAN	s	5	11	11,11,12	0.82	0	15,15,17	1.10	2 (13%)
7	NAG	t	1	7,4	14,14,15	0.36	0	17,19,21	0.56	0
7	NAG	t	2	7	14,14,15	0.57	0	17,19,21	0.57	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
7	NAG	E	1	3,7	-	4/6/23/26	0/1/1/1
7	NAG	E	2	7	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	6/6/23/26	0/1/1/1
7	NAG	K	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
7	NAG	N	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	7,4	-	4/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	NAG	S	1	7,4	-	4/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	NAG	T	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	3/6/23/26	0/1/1/1
7	NAG	U	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	U	2	7	-	2/6/23/26	0/1/1/1
8	NAG	V	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	V	2	8	-	0/6/23/26	0/1/1/1
8	BMA	V	3	8	-	0/2/19/22	0/1/1/1
8	MAN	V	4	8	-	1/2/19/22	0/1/1/1
9	NAG	X	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	1/6/23/26	0/1/1/1
9	BMA	X	3	9	-	0/2/19/22	0/1/1/1
9	MAN	X	4	9	-	1/2/19/22	0/1/1/1
9	MAN	X	5	9	-	0/2/19/22	0/1/1/1
9	MAN	X	6	9	-	1/2/19/22	0/1/1/1
10	NAG	Y	1	10,4	-	2/6/23/26	0/1/1/1
10	MAN	Y	10	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	11	10	-	0/2/19/22	0/1/1/1
10	NAG	Y	2	10	-	2/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	2/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	5	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	6	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	7	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	8	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	9	10	-	0/2/19/22	0/1/1/1
7	NAG	Z	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	NAG	a	1	7,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	a	2	7	-	4/6/23/26	0/1/1/1
7	NAG	b	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	4/6/23/26	0/1/1/1
7	NAG	c	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	3/6/23/26	0/1/1/1
7	NAG	d	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
7	NAG	e	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	e	2	7	-	4/6/23/26	0/1/1/1
7	NAG	f	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	f	2	7	-	2/6/23/26	0/1/1/1
7	NAG	g	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	0/6/23/26	0/1/1/1
11	NAG	h	1	11,4	-	0/6/23/26	0/1/1/1
11	NAG	h	2	11	-	1/6/23/26	0/1/1/1
11	BMA	h	3	11	-	1/2/19/22	0/1/1/1
11	MAN	h	4	11	-	0/2/19/22	0/1/1/1
11	MAN	h	5	11	-	0/2/19/22	0/1/1/1
12	NAG	i	1	12,4	-	2/6/23/26	0/1/1/1
12	MAN	i	10	12	-	0/2/19/22	0/1/1/1
12	NAG	i	2	12	-	2/6/23/26	0/1/1/1
12	BMA	i	3	12	-	2/2/19/22	0/1/1/1
12	MAN	i	4	12	-	1/2/19/22	0/1/1/1
12	MAN	i	5	12	-	2/2/19/22	0/1/1/1
12	MAN	i	6	12	-	0/2/19/22	0/1/1/1
12	MAN	i	7	12	-	0/2/19/22	0/1/1/1
12	MAN	i	8	12	-	0/2/19/22	0/1/1/1
12	MAN	i	9	12	-	0/2/19/22	0/1/1/1
13	NAG	j	1	13,4	-	2/6/23/26	0/1/1/1
13	NAG	j	2	13	-	4/6/23/26	0/1/1/1
13	BMA	j	3	13	-	0/2/19/22	0/1/1/1
13	NAG	k	1	13,4	-	2/6/23/26	0/1/1/1
13	NAG	k	2	13	-	3/6/23/26	0/1/1/1
13	BMA	k	3	13	-	1/2/19/22	0/1/1/1
7	NAG	l	1	7,4	-	1/6/23/26	0/1/1/1
7	NAG	l	2	7	-	2/6/23/26	0/1/1/1
7	NAG	m	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	m	2	7	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	n	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	n	2	7	-	2/6/23/26	0/1/1/1
7	NAG	o	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	o	2	7	-	2/6/23/26	0/1/1/1
13	NAG	p	1	13,4	-	2/6/23/26	0/1/1/1
13	NAG	p	2	13	-	1/6/23/26	0/1/1/1
13	BMA	p	3	13	-	0/2/19/22	0/1/1/1
13	NAG	q	1	13,4	-	0/6/23/26	0/1/1/1
13	NAG	q	2	13	-	0/6/23/26	0/1/1/1
13	BMA	q	3	13	-	1/2/19/22	0/1/1/1
12	NAG	r	1	12,4	-	2/6/23/26	0/1/1/1
12	MAN	r	10	12	-	1/2/19/22	0/1/1/1
12	NAG	r	2	12	-	4/6/23/26	0/1/1/1
12	BMA	r	3	12	-	2/2/19/22	0/1/1/1
12	MAN	r	4	12	-	0/2/19/22	0/1/1/1
12	MAN	r	5	12	-	0/2/19/22	0/1/1/1
12	MAN	r	6	12	-	0/2/19/22	0/1/1/1
12	MAN	r	7	12	-	0/2/19/22	0/1/1/1
12	MAN	r	8	12	-	0/2/19/22	0/1/1/1
12	MAN	r	9	12	-	0/2/19/22	0/1/1/1
11	NAG	s	1	11,4	-	2/6/23/26	0/1/1/1
11	NAG	s	2	11	-	1/6/23/26	0/1/1/1
11	BMA	s	3	11	-	0/2/19/22	0/1/1/1
11	MAN	s	4	11	-	0/2/19/22	1/1/1/1
11	MAN	s	5	11	-	0/2/19/22	0/1/1/1
7	NAG	t	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	t	2	7	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	2	NAG	C1-C2	2.68	1.56	1.52
11	s	3	BMA	C1-C2	2.38	1.57	1.52
11	s	4	MAN	O5-C5	2.27	1.47	1.43
11	h	5	MAN	C1-C2	2.10	1.57	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	2	NAG	C2-N2-C7	8.30	134.02	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	s	4	MAN	C1-O5-C5	4.06	117.63	112.19
7	I	2	NAG	C1-C2-N2	4.01	116.76	110.43
11	h	5	MAN	C1-O5-C5	3.62	117.04	112.19
9	X	4	MAN	C1-O5-C5	3.41	116.76	112.19
9	X	5	MAN	C1-O5-C5	3.40	116.74	112.19
7	n	2	NAG	C2-N2-C7	3.30	127.33	122.90
12	i	7	MAN	C1-O5-C5	3.28	116.58	112.19
7	e	2	NAG	C2-N2-C7	3.28	127.30	122.90
7	S	1	NAG	C2-N2-C7	3.26	127.27	122.90
7	c	2	NAG	C2-N2-C7	3.26	127.26	122.90
7	S	2	NAG	C2-N2-C7	3.26	127.26	122.90
7	T	2	NAG	C2-N2-C7	3.25	127.26	122.90
7	m	1	NAG	C2-N2-C7	3.25	127.25	122.90
7	E	2	NAG	C2-N2-C7	3.24	127.25	122.90
7	o	2	NAG	C2-N2-C7	3.24	127.25	122.90
7	a	1	NAG	C2-N2-C7	3.24	127.24	122.90
7	a	2	NAG	C2-N2-C7	3.24	127.24	122.90
10	Y	10	MAN	C1-O5-C5	3.24	116.53	112.19
12	i	8	MAN	C1-O5-C5	3.24	116.52	112.19
7	Q	1	NAG	C2-N2-C7	3.23	127.23	122.90
7	b	2	NAG	C2-N2-C7	3.23	127.23	122.90
13	k	1	NAG	C2-N2-C7	3.23	127.22	122.90
13	j	2	NAG	C2-N2-C7	3.23	127.22	122.90
10	Y	7	MAN	C1-O5-C5	3.23	116.51	112.19
12	i	5	MAN	C1-O5-C5	3.22	116.51	112.19
12	r	7	MAN	C1-O5-C5	3.21	116.49	112.19
7	m	2	NAG	C2-N2-C7	3.20	127.19	122.90
7	Q	2	NAG	C2-N2-C7	3.19	127.17	122.90
12	r	8	MAN	C1-O5-C5	3.18	116.44	112.19
11	s	5	MAN	C1-O5-C5	3.12	116.37	112.19
12	r	5	MAN	C1-O5-C5	3.10	116.34	112.19
10	Y	5	MAN	C1-O5-C5	2.95	116.14	112.19
10	Y	11	MAN	C1-O5-C5	2.94	116.12	112.19
9	X	6	MAN	C1-O5-C5	2.93	116.11	112.19
12	r	9	MAN	C1-O5-C5	2.92	116.10	112.19
12	r	6	MAN	C1-O5-C5	2.92	116.10	112.19
8	V	4	MAN	C1-O5-C5	2.91	116.09	112.19
10	Y	9	MAN	C1-O5-C5	2.90	116.07	112.19
12	i	9	MAN	C1-O5-C5	2.88	116.05	112.19
12	r	10	MAN	C1-O5-C5	2.88	116.04	112.19
11	s	1	NAG	C1-O5-C5	2.87	116.04	112.19
12	i	10	MAN	C1-O5-C5	2.86	116.02	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Y	8	MAN	C1-O5-C5	2.85	116.01	112.19
12	i	6	MAN	C1-O5-C5	2.84	115.99	112.19
11	h	4	MAN	C1-O5-C5	2.81	115.95	112.19
10	Y	4	MAN	C1-O5-C5	2.72	115.83	112.19
12	r	4	MAN	C1-O5-C5	2.67	115.77	112.19
12	i	4	MAN	C1-O5-C5	2.65	115.73	112.19
10	Y	6	MAN	C1-O5-C5	2.55	115.60	112.19
10	Y	4	MAN	O2-C2-C3	-2.36	105.27	110.15
11	h	3	BMA	C1-O5-C5	2.28	115.24	112.19
10	Y	5	MAN	O2-C2-C3	-2.25	105.50	110.15
12	r	4	MAN	O2-C2-C3	-2.24	105.51	110.15
12	i	4	MAN	O2-C2-C3	-2.24	105.51	110.15
12	i	5	MAN	O2-C2-C3	-2.21	105.56	110.15
11	s	2	NAG	C1-O5-C5	2.21	115.15	112.19
10	Y	8	MAN	O2-C2-C3	-2.20	105.60	110.15
11	h	5	MAN	O2-C2-C3	-2.16	105.68	110.15
7	I	2	NAG	C8-C7-N2	2.16	119.69	116.12
11	s	4	MAN	O2-C2-C3	-2.15	105.70	110.15
12	r	8	MAN	O2-C2-C3	-2.14	105.71	110.15
12	r	7	MAN	O2-C2-C3	-2.14	105.72	110.15
11	s	5	MAN	O2-C2-C3	-2.14	105.73	110.15
10	Y	10	MAN	O2-C2-C3	-2.14	105.73	110.15
8	V	4	MAN	O2-C2-C3	-2.13	105.73	110.15
12	i	8	MAN	O2-C2-C3	-2.13	105.73	110.15
12	i	10	MAN	O2-C2-C3	-2.13	105.73	110.15
10	Y	7	MAN	O2-C2-C3	-2.13	105.73	110.15
11	h	4	MAN	O2-C2-C3	-2.13	105.74	110.15
12	i	9	MAN	O2-C2-C3	-2.12	105.75	110.15
12	i	7	MAN	O2-C2-C3	-2.12	105.76	110.15
10	Y	6	MAN	O2-C2-C3	-2.12	105.77	110.15
12	r	9	MAN	O2-C2-C3	-2.12	105.77	110.15
12	i	6	MAN	O2-C2-C3	-2.11	105.78	110.15
10	Y	9	MAN	O2-C2-C3	-2.11	105.78	110.15
12	r	6	MAN	O2-C2-C3	-2.11	105.78	110.15
9	X	5	MAN	O2-C2-C3	-2.11	105.79	110.15
9	X	6	MAN	O2-C2-C3	-2.11	105.79	110.15
10	Y	11	MAN	O2-C2-C3	-2.10	105.81	110.15
12	r	10	MAN	O2-C2-C3	-2.09	105.81	110.15
7	d	1	NAG	C1-O5-C5	2.09	114.99	112.19
7	o	1	NAG	C1-O5-C5	2.09	114.98	112.19
13	j	1	NAG	C1-O5-C5	2.07	114.95	112.19
12	r	5	MAN	O2-C2-C3	-2.05	105.90	110.15

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	d	1	NAG	O5-C5-C6-O6
8	V	1	NAG	O5-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6
7	E	1	NAG	O5-C5-C6-O6
12	r	2	NAG	O5-C5-C6-O6
13	j	2	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
12	i	2	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
10	Y	3	BMA	O5-C5-C6-O6
12	i	1	NAG	O5-C5-C6-O6
12	i	5	MAN	O5-C5-C6-O6
12	r	3	BMA	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
12	i	3	BMA	O5-C5-C6-O6
7	E	1	NAG	C4-C5-C6-O6
10	Y	2	NAG	O5-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
7	n	1	NAG	O5-C5-C6-O6
12	i	2	NAG	C4-C5-C6-O6
10	Y	1	NAG	O5-C5-C6-O6
7	d	1	NAG	C4-C5-C6-O6
8	V	1	NAG	C4-C5-C6-O6
12	r	1	NAG	O5-C5-C6-O6
13	j	1	NAG	O5-C5-C6-O6
12	i	1	NAG	C4-C5-C6-O6
12	r	2	NAG	C4-C5-C6-O6
7	E	2	NAG	O5-C5-C6-O6
7	t	2	NAG	O5-C5-C6-O6
13	j	2	NAG	C4-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
10	Y	2	NAG	C4-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
7	U	1	NAG	C4-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
7	t	2	NAG	C4-C5-C6-O6
12	r	1	NAG	C4-C5-C6-O6
7	f	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	g	1	NAG	C4-C5-C6-O6
12	i	5	MAN	C4-C5-C6-O6
13	j	1	NAG	C4-C5-C6-O6
13	p	1	NAG	O5-C5-C6-O6
10	Y	1	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
7	K	1	NAG	O5-C5-C6-O6
7	m	2	NAG	C4-C5-C6-O6
10	Y	3	BMA	C4-C5-C6-O6
7	E	1	NAG	C8-C7-N2-C2
7	E	1	NAG	O7-C7-N2-C2
7	I	2	NAG	C8-C7-N2-C2
7	I	2	NAG	O7-C7-N2-C2
7	t	2	NAG	C8-C7-N2-C2
7	t	2	NAG	O7-C7-N2-C2
12	r	2	NAG	C8-C7-N2-C2
12	r	2	NAG	O7-C7-N2-C2
13	k	2	NAG	C8-C7-N2-C2
13	k	2	NAG	O7-C7-N2-C2
7	U	1	NAG	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
7	n	1	NAG	C4-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
7	l	2	NAG	C4-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
12	r	3	BMA	C4-C5-C6-O6
7	f	2	NAG	O5-C5-C6-O6
7	f	2	NAG	C4-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
7	m	2	NAG	O5-C5-C6-O6
12	i	3	BMA	C4-C5-C6-O6
13	k	2	NAG	O5-C5-C6-O6
13	p	1	NAG	C4-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
11	h	2	NAG	O5-C5-C6-O6
13	k	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	Z	2	NAG	C4-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
11	s	2	NAG	O5-C5-C6-O6
11	h	3	BMA	O5-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6
9	X	6	MAN	O5-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
8	V	4	MAN	O5-C5-C6-O6
9	X	4	MAN	O5-C5-C6-O6
12	i	4	MAN	O5-C5-C6-O6
13	q	3	BMA	O5-C5-C6-O6
12	r	10	MAN	O5-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
11	s	1	NAG	C4-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
7	c	1	NAG	O5-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
11	s	1	NAG	O5-C5-C6-O6
7	E	2	NAG	C1-C2-N2-C7
7	I	2	NAG	C1-C2-N2-C7
7	Q	1	NAG	C1-C2-N2-C7
7	Q	2	NAG	C1-C2-N2-C7
7	S	1	NAG	C1-C2-N2-C7
7	S	2	NAG	C1-C2-N2-C7
7	T	2	NAG	C1-C2-N2-C7
7	a	1	NAG	C1-C2-N2-C7
7	a	2	NAG	C1-C2-N2-C7
7	b	2	NAG	C1-C2-N2-C7
7	c	2	NAG	C1-C2-N2-C7
7	e	2	NAG	C1-C2-N2-C7
7	m	1	NAG	C1-C2-N2-C7
7	m	2	NAG	C1-C2-N2-C7
7	n	2	NAG	C1-C2-N2-C7
7	o	2	NAG	C1-C2-N2-C7
13	j	2	NAG	C1-C2-N2-C7
13	k	1	NAG	C1-C2-N2-C7
7	E	2	NAG	C3-C2-N2-C7
7	I	2	NAG	C3-C2-N2-C7
7	Q	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	Q	2	NAG	C3-C2-N2-C7
7	S	1	NAG	C3-C2-N2-C7
7	S	2	NAG	C3-C2-N2-C7
7	T	2	NAG	C3-C2-N2-C7
7	a	1	NAG	C3-C2-N2-C7
7	a	2	NAG	C3-C2-N2-C7
7	b	2	NAG	C3-C2-N2-C7
7	c	2	NAG	C3-C2-N2-C7
7	e	2	NAG	C3-C2-N2-C7
7	m	1	NAG	C3-C2-N2-C7
7	m	2	NAG	C3-C2-N2-C7
7	n	2	NAG	C3-C2-N2-C7
7	o	2	NAG	C3-C2-N2-C7
13	j	2	NAG	C3-C2-N2-C7
13	k	1	NAG	C3-C2-N2-C7
7	l	1	NAG	O5-C5-C6-O6
13	p	2	NAG	C4-C5-C6-O6

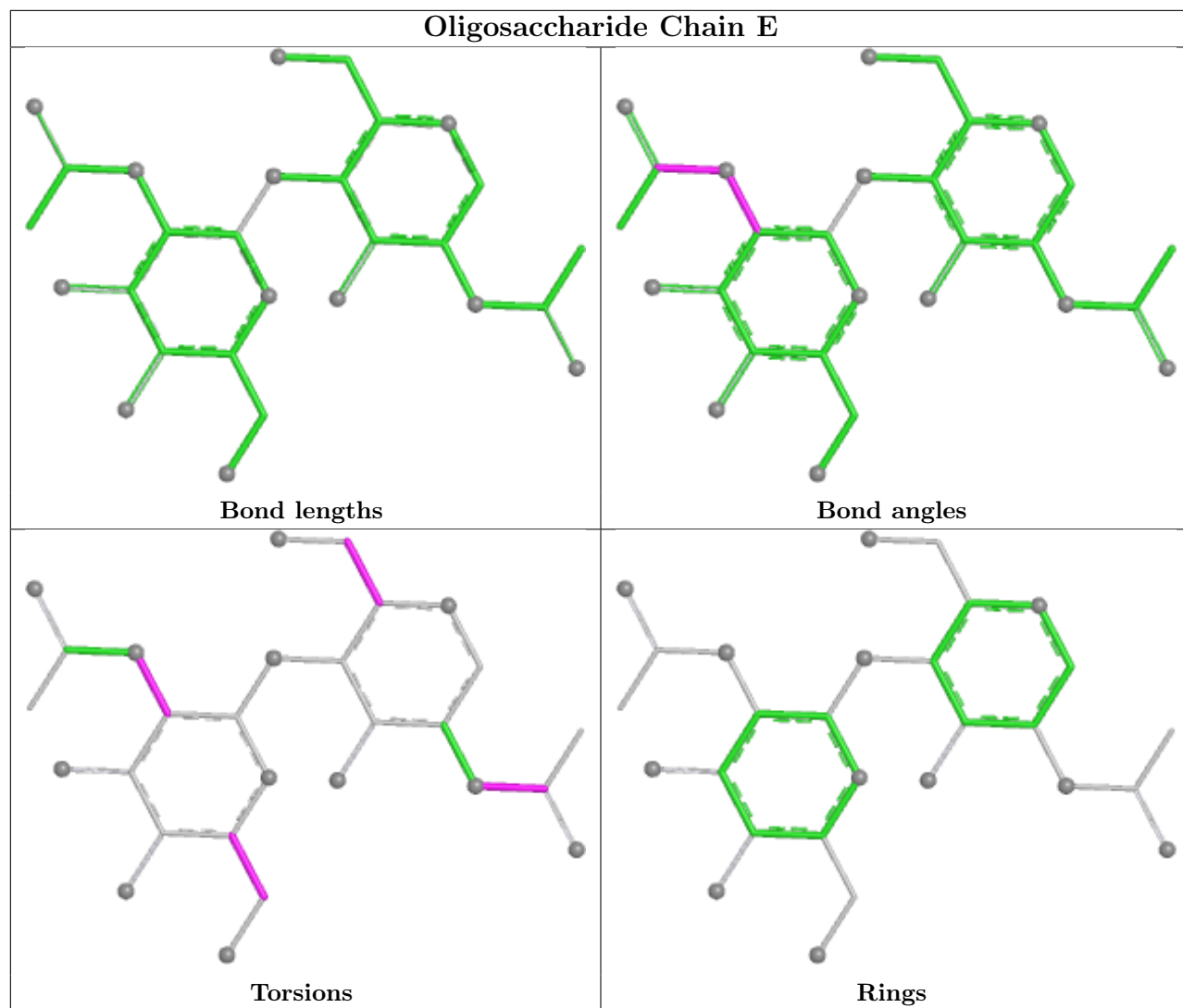
All (1) ring outliers are listed below:

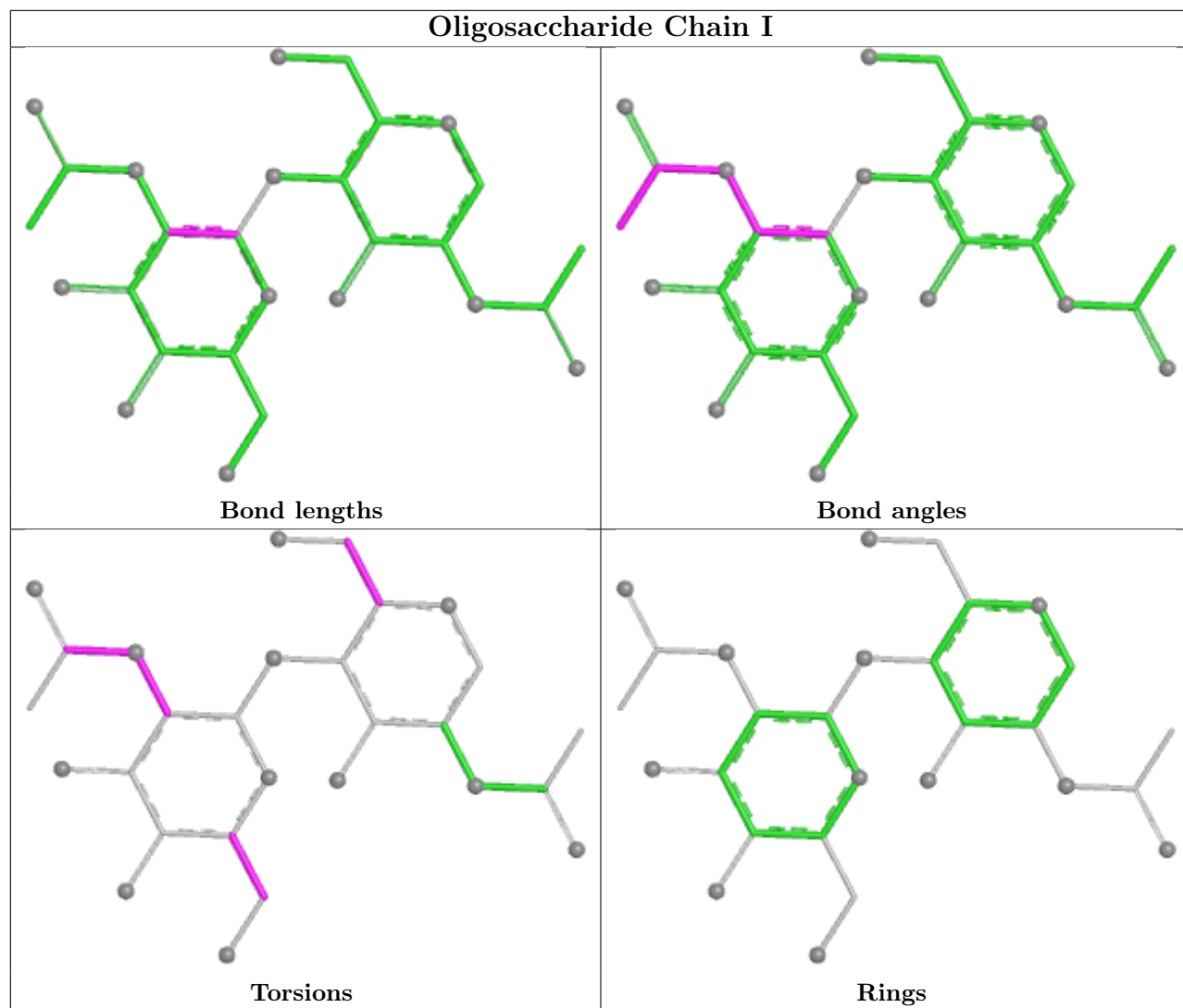
Mol	Chain	Res	Type	Atoms
11	s	4	MAN	C1-C2-C3-C4-C5-O5

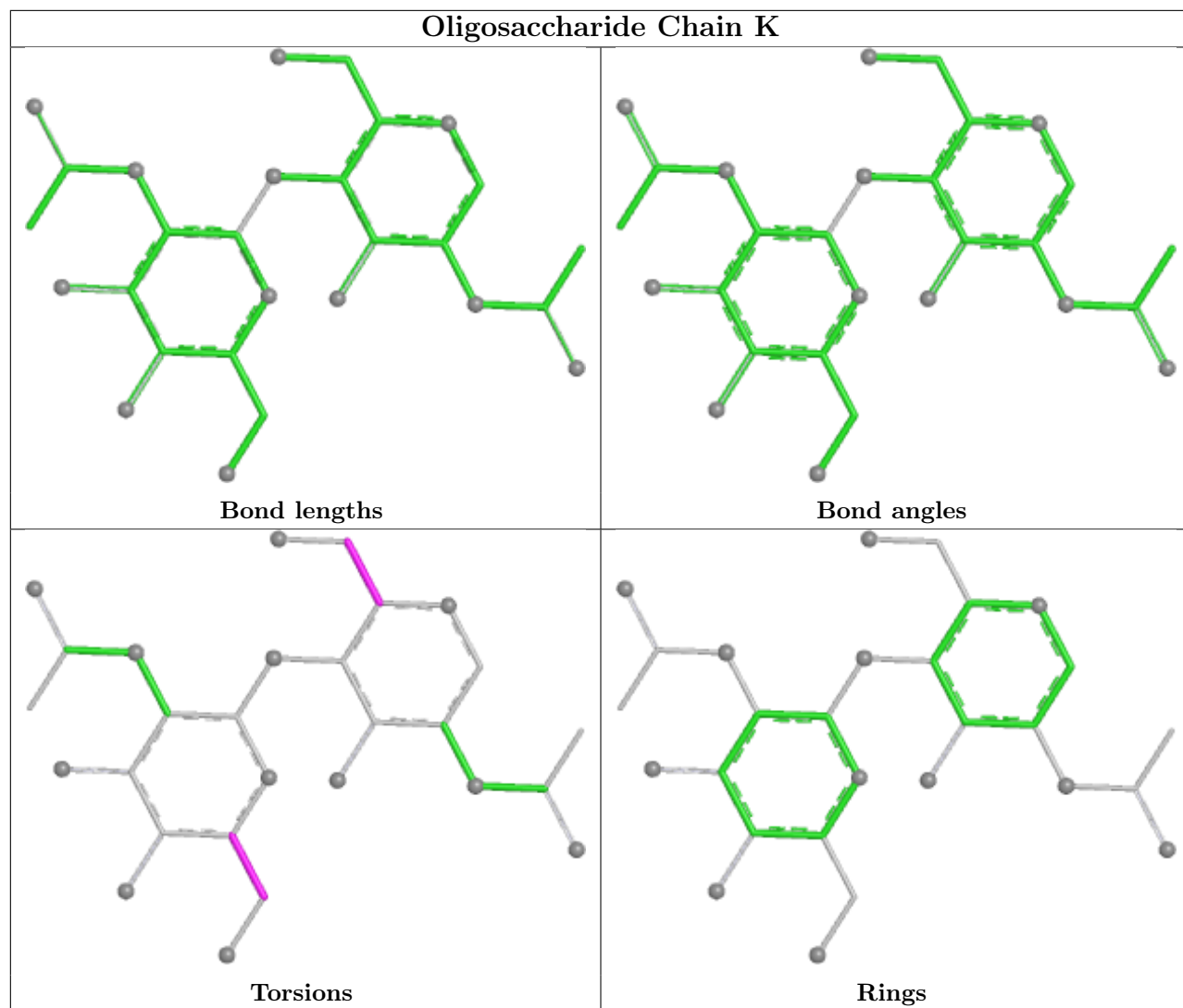
6 monomers are involved in 6 short contacts:

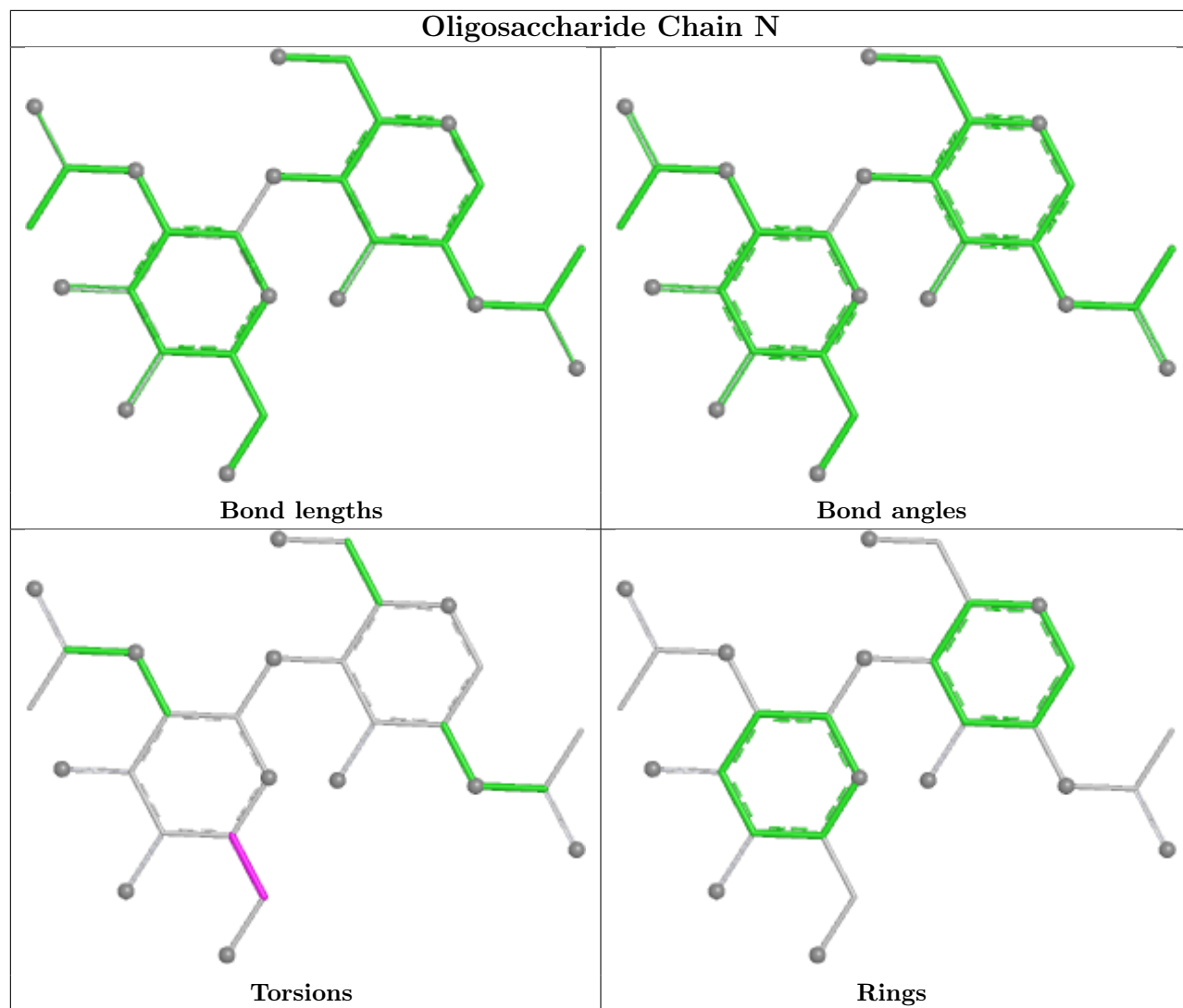
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	f	1	NAG	1	0
11	s	3	BMA	1	0
11	s	2	NAG	1	0
10	Y	2	NAG	1	0
12	i	2	NAG	1	0
12	r	2	NAG	2	0

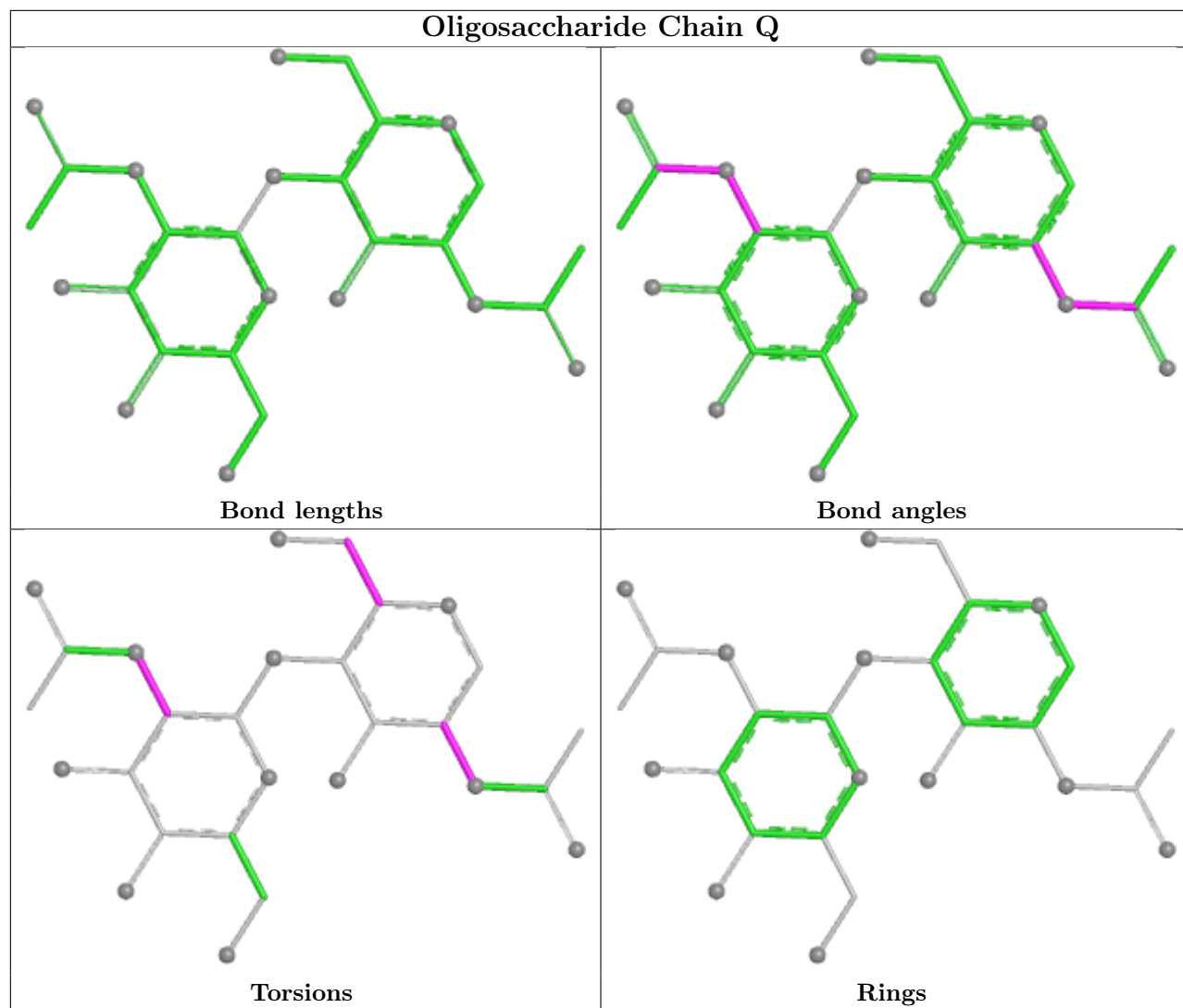
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

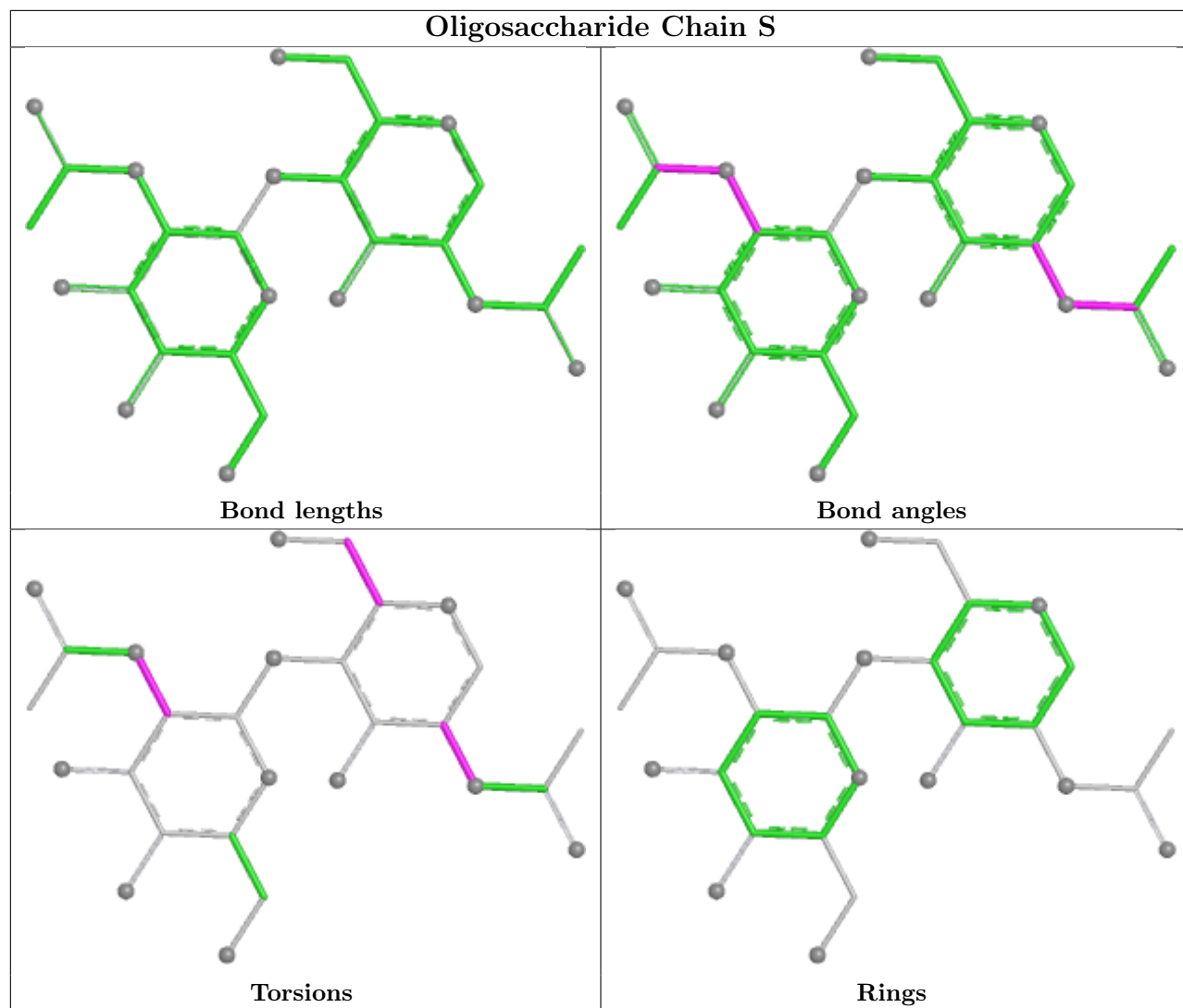


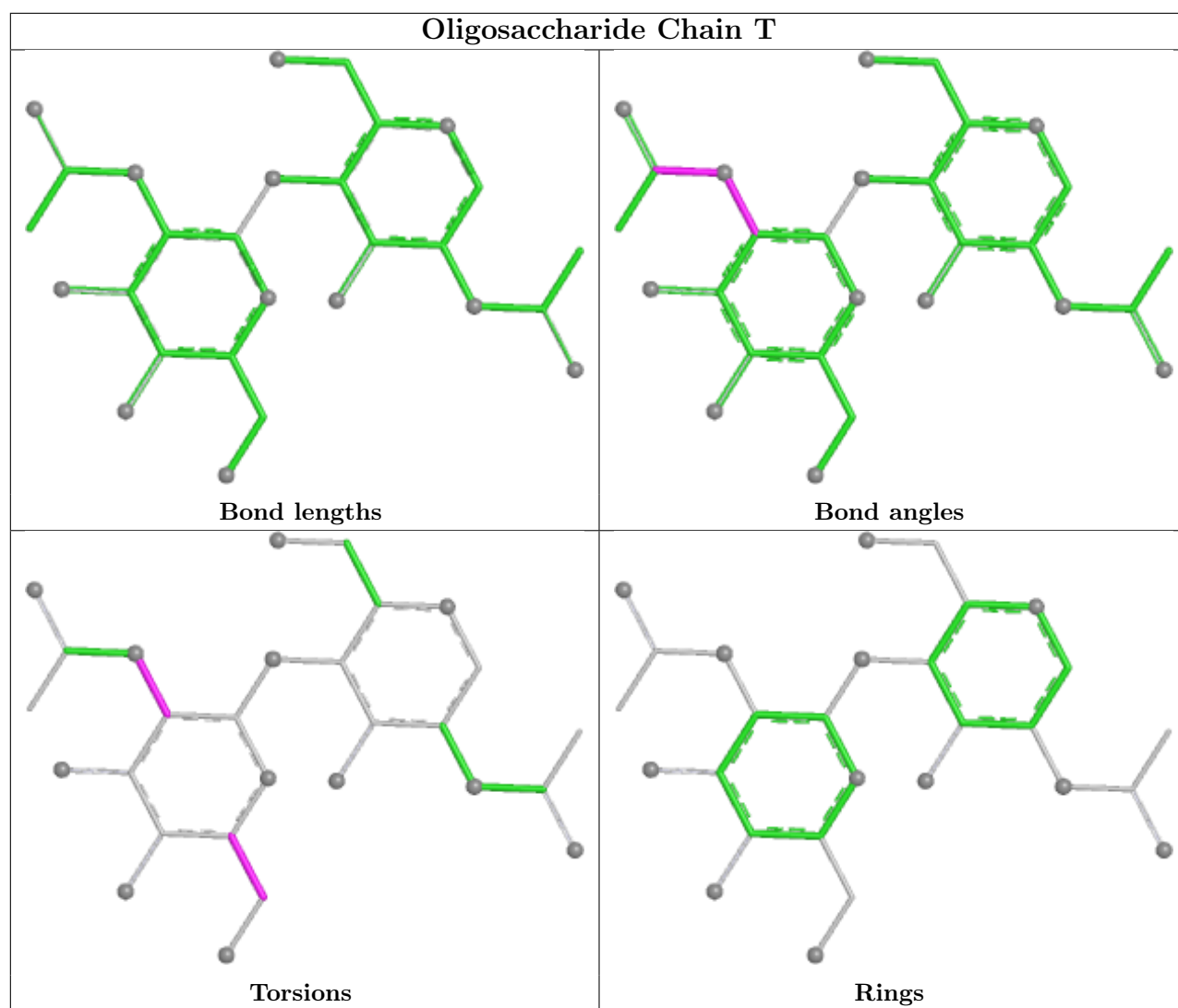


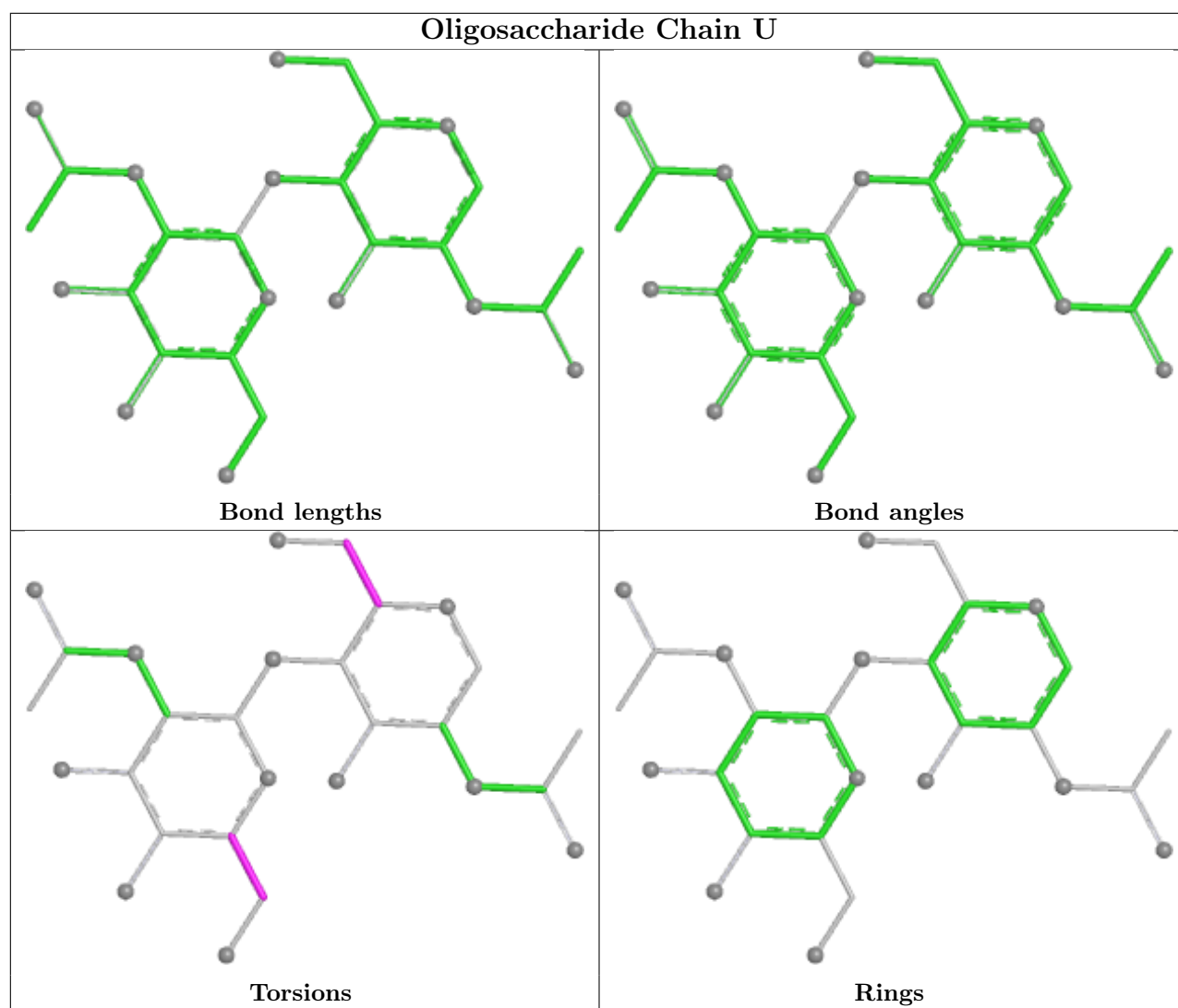


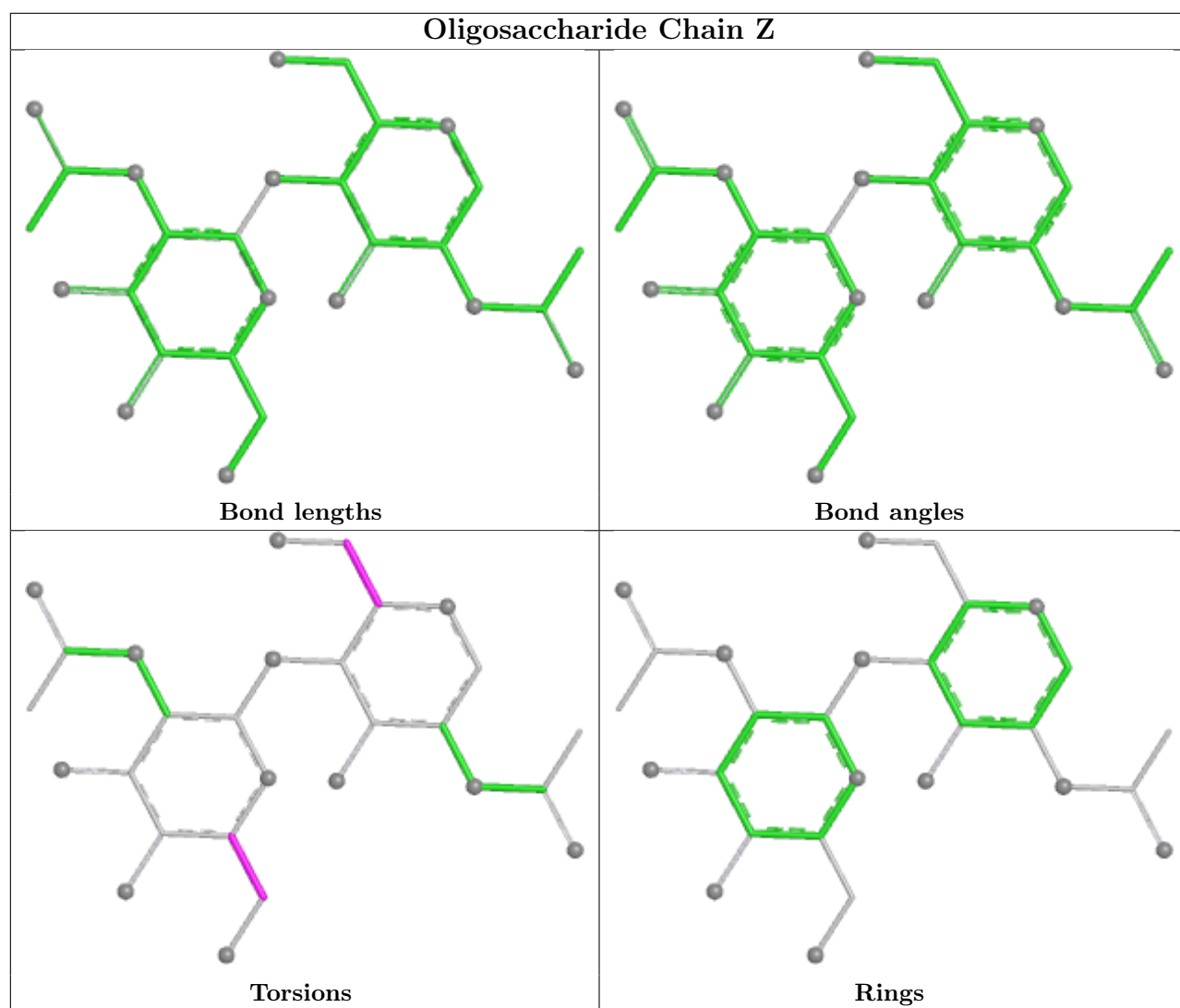


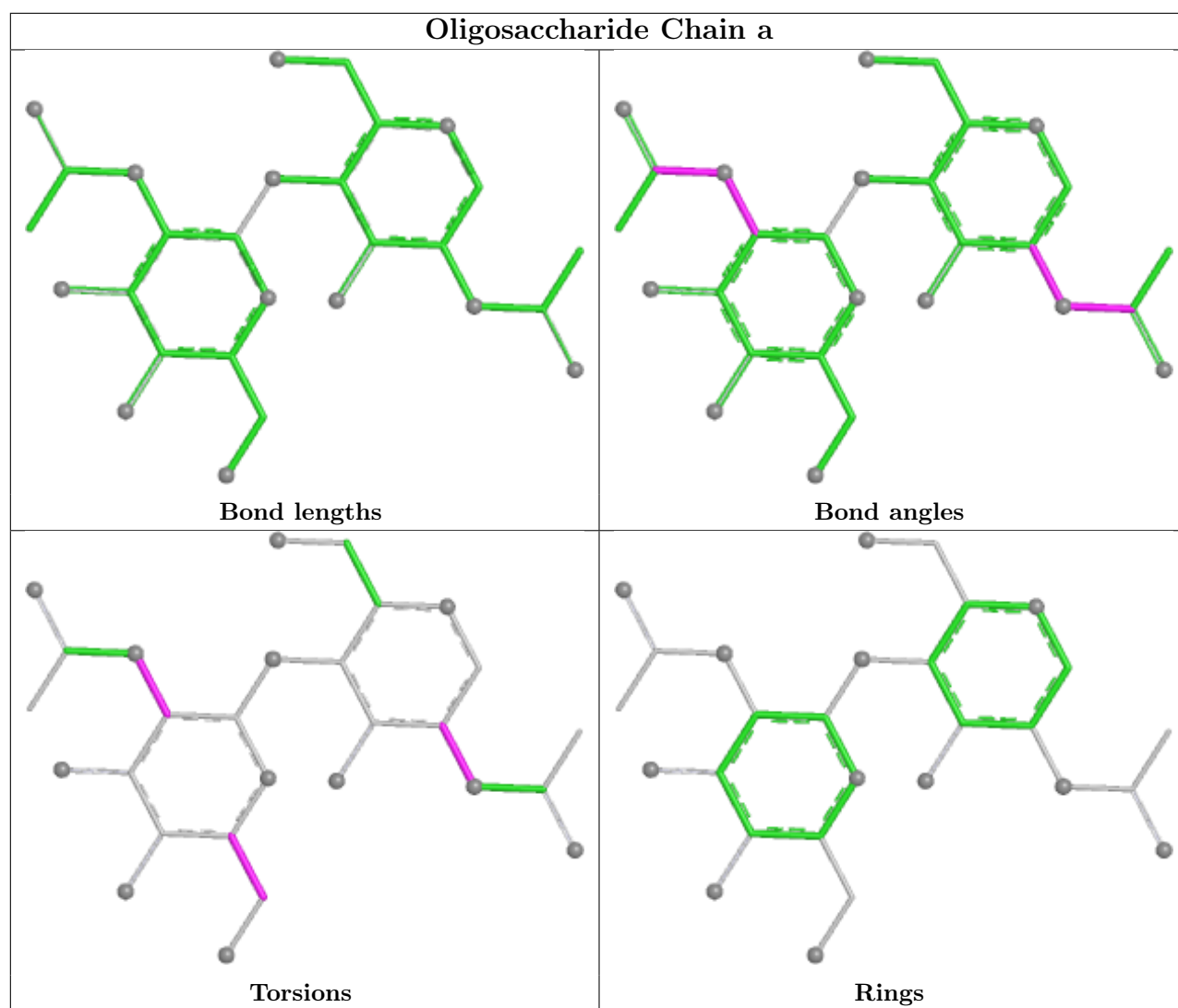


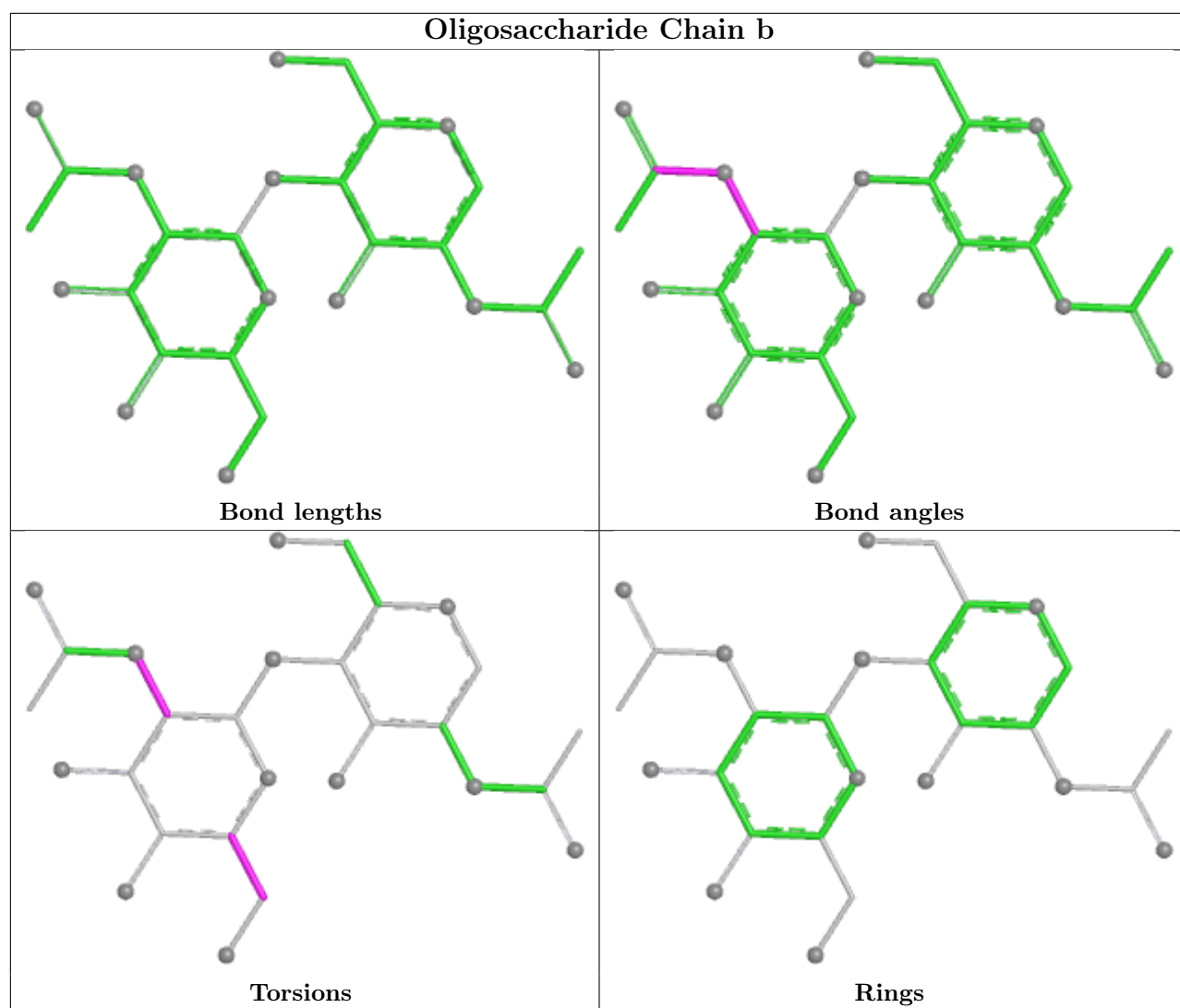


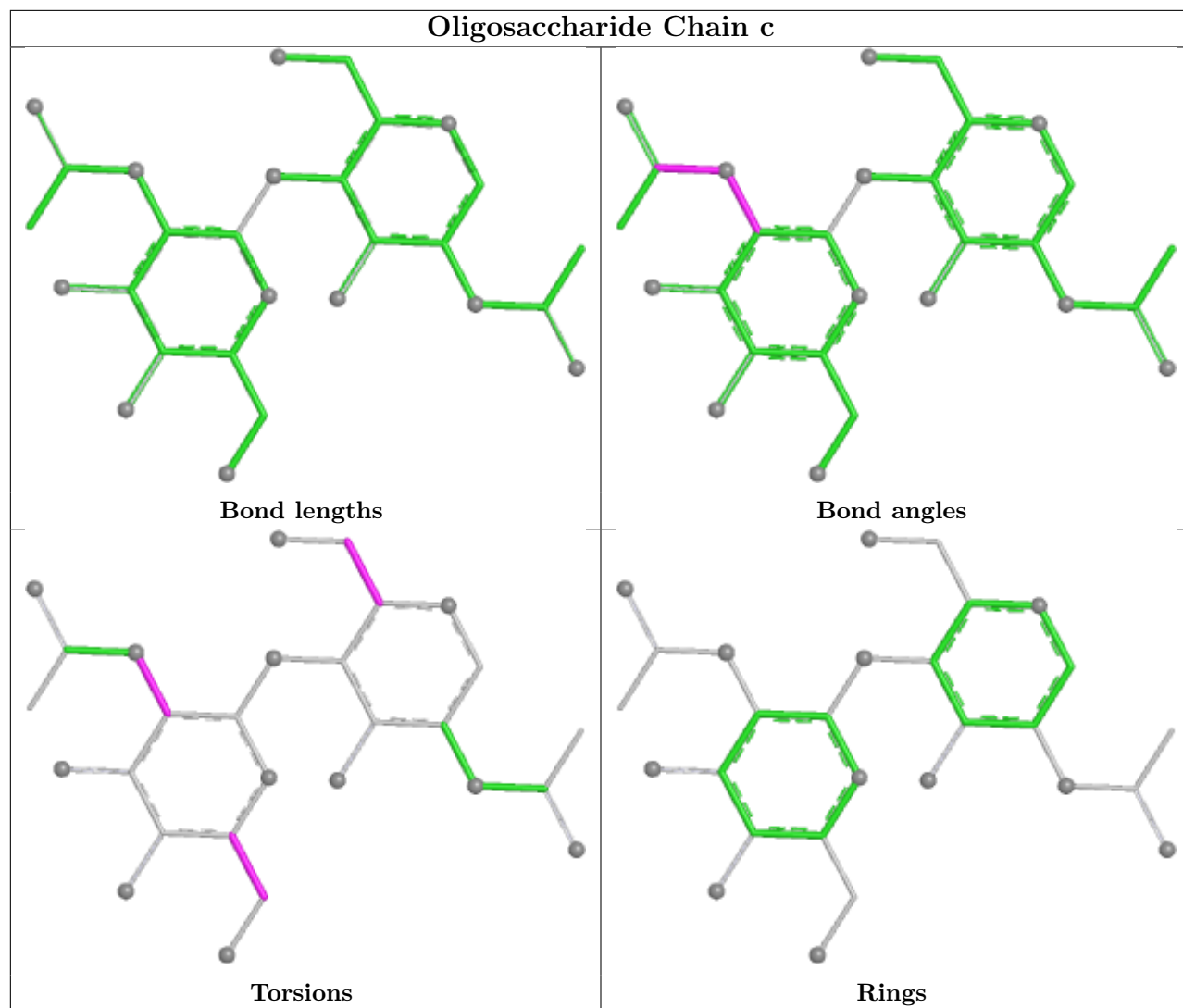


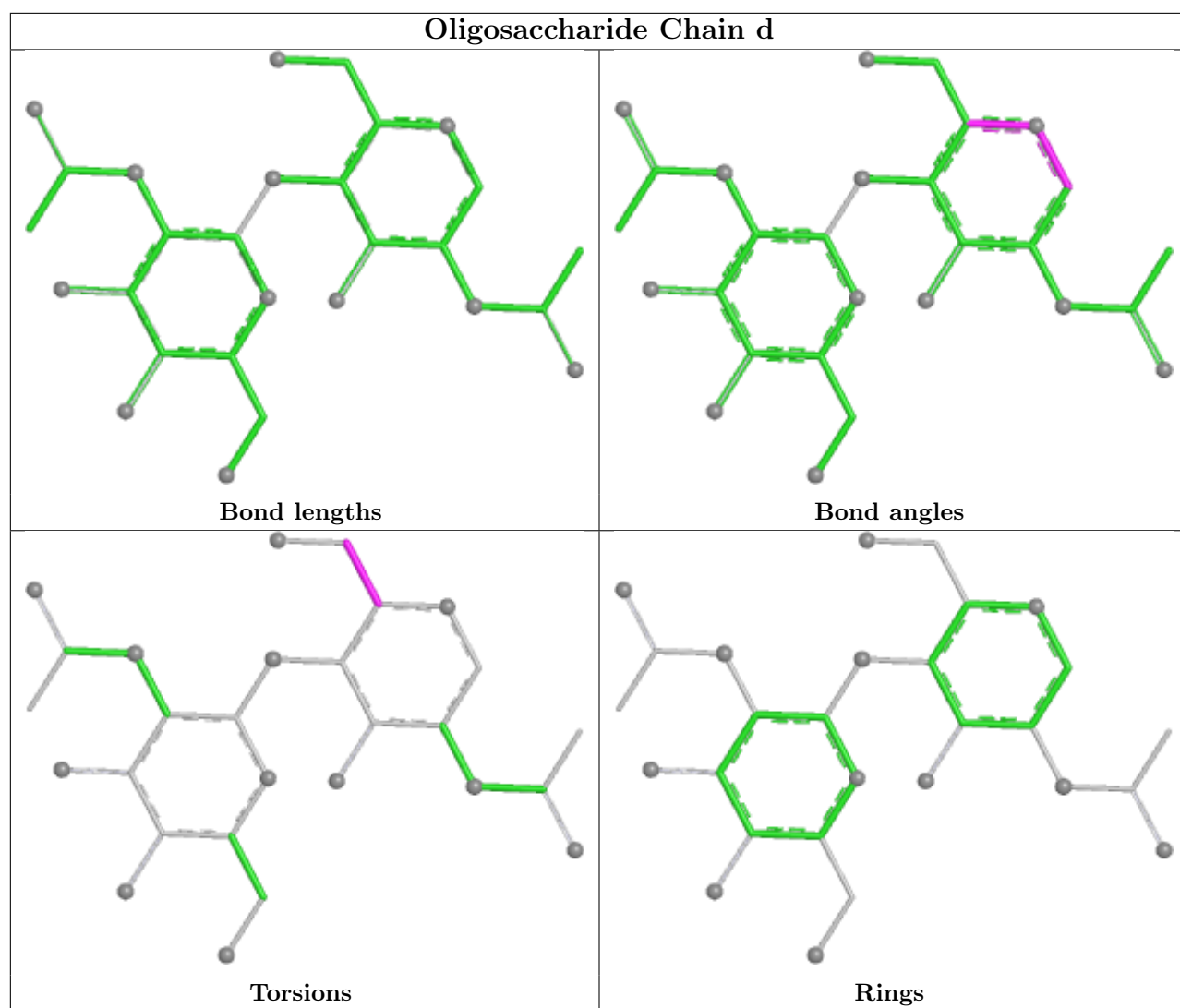


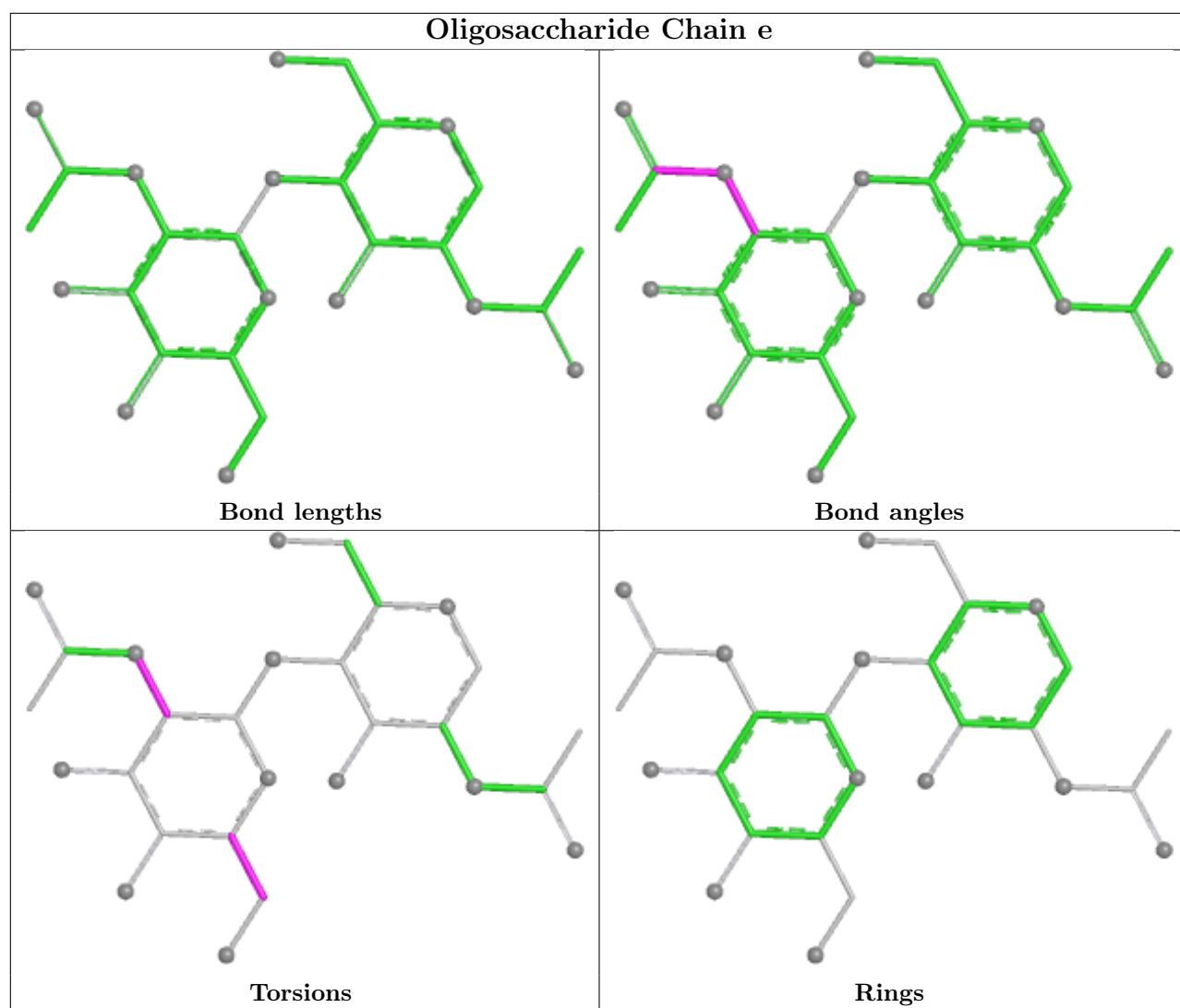


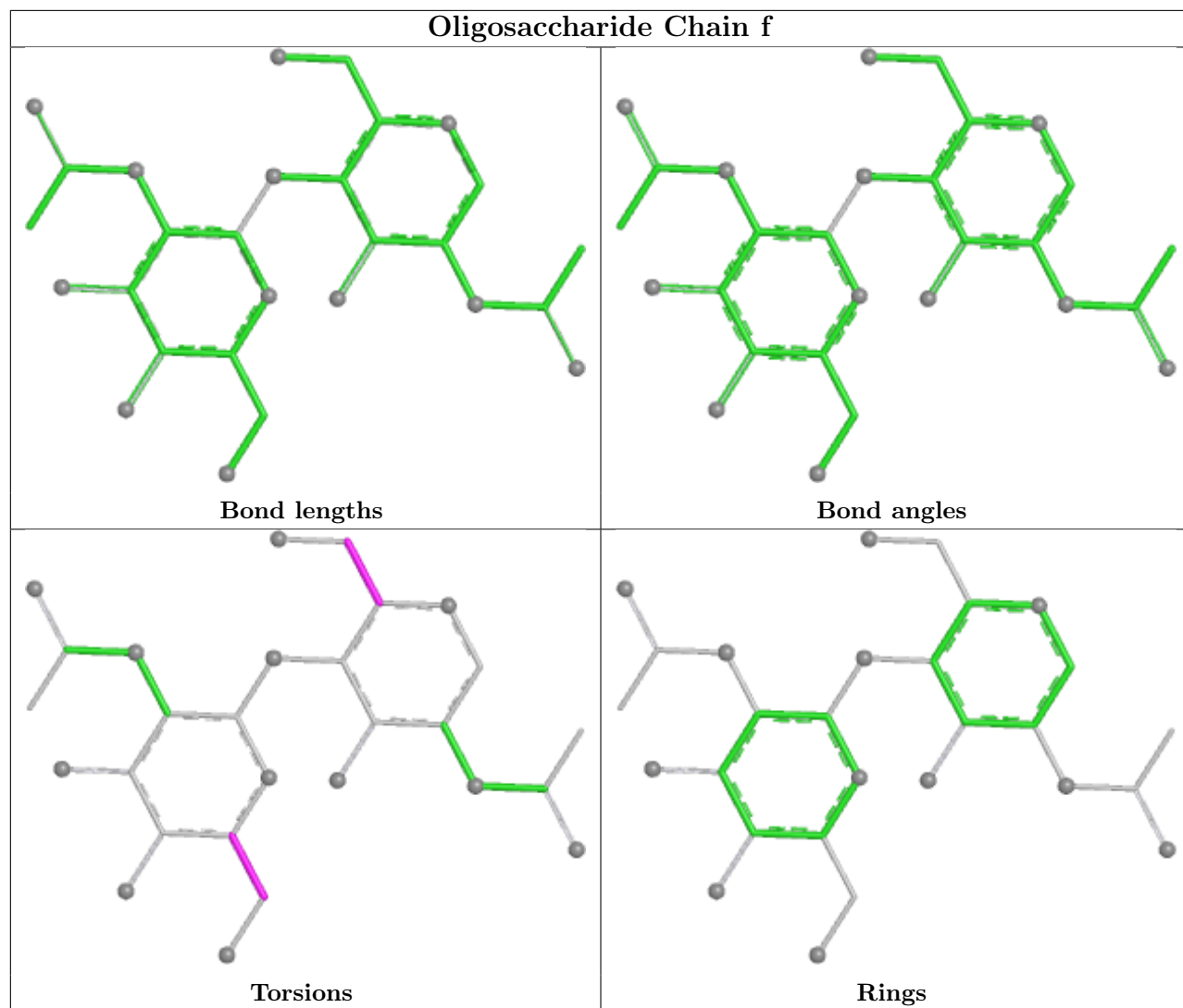


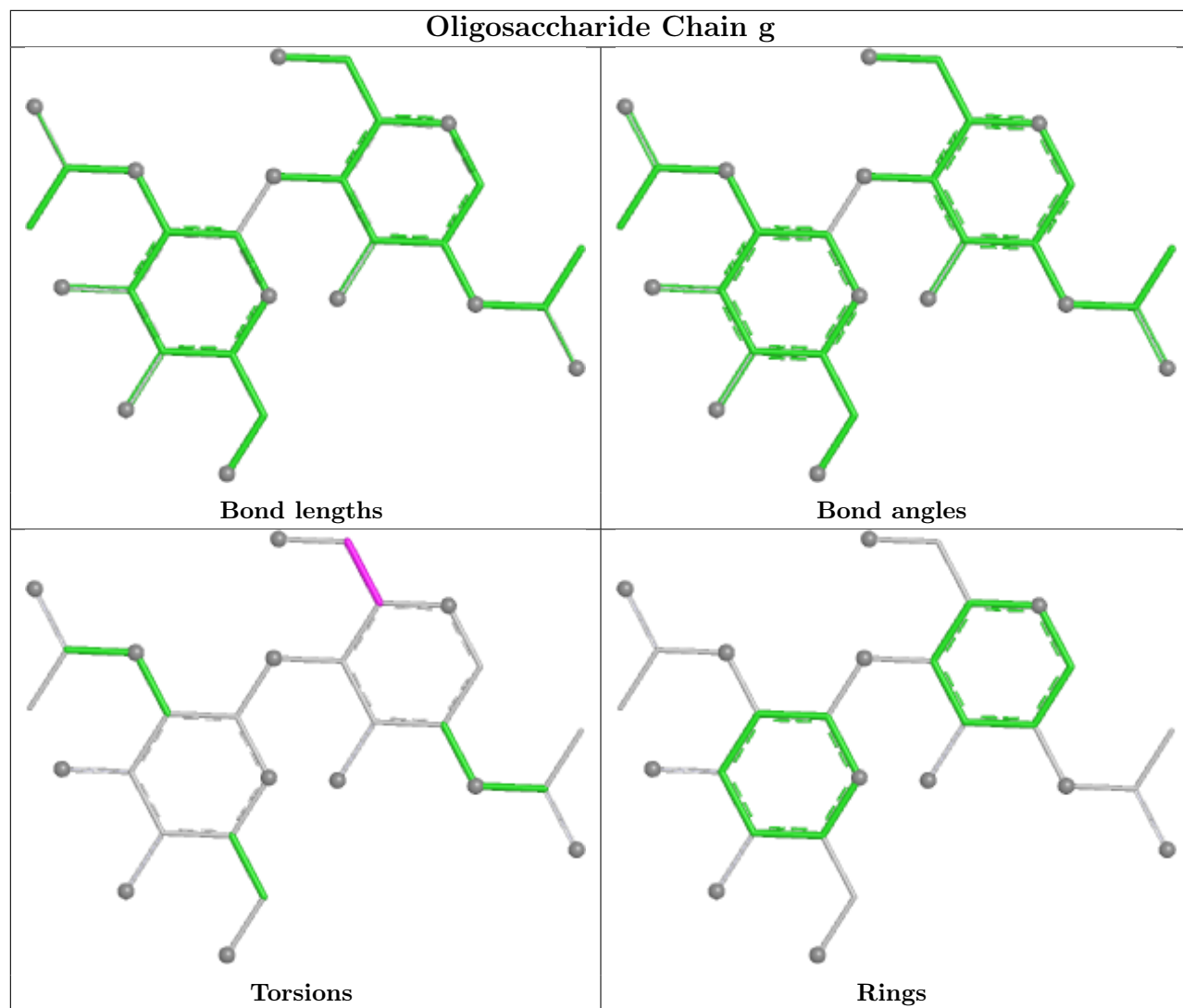


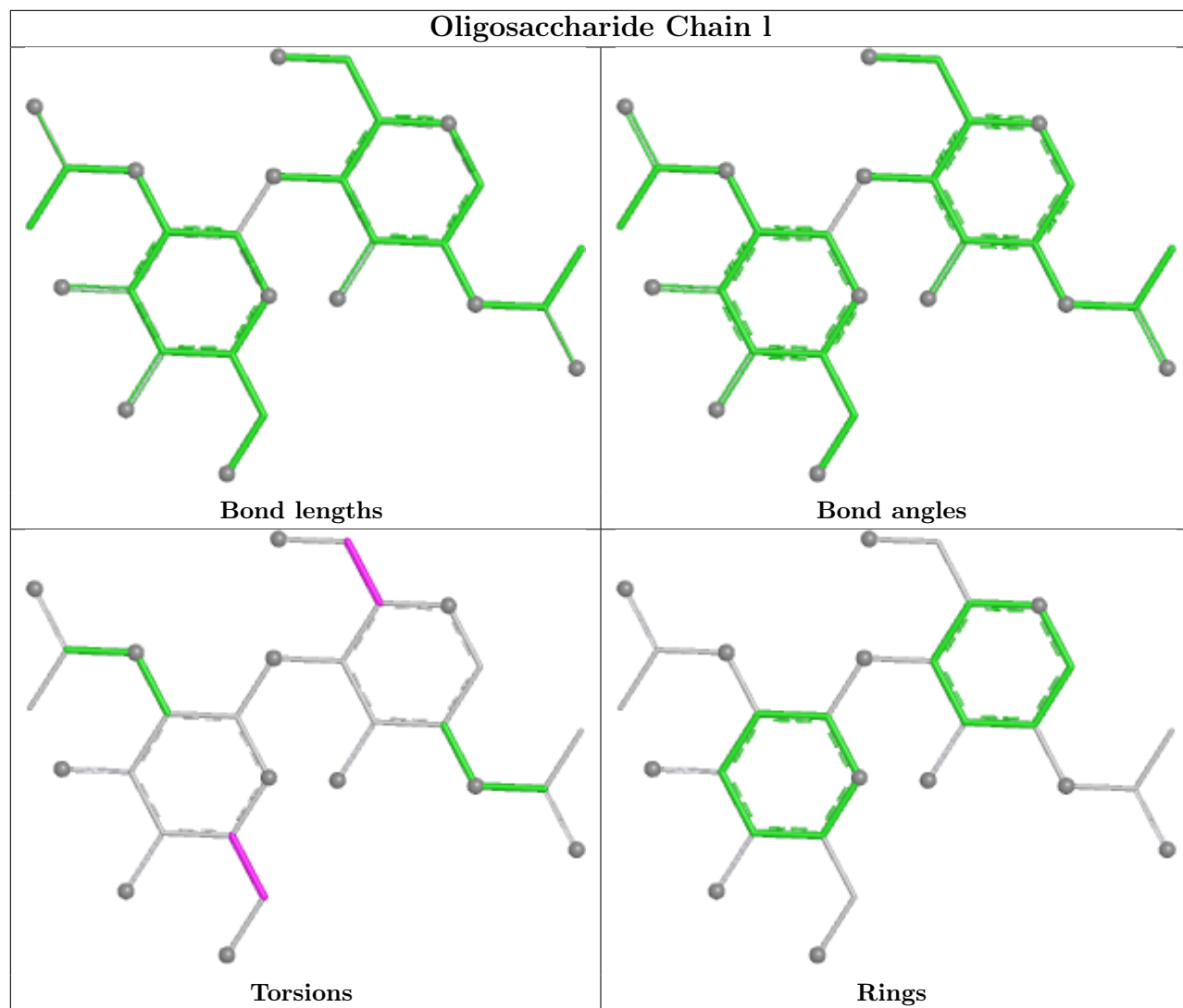


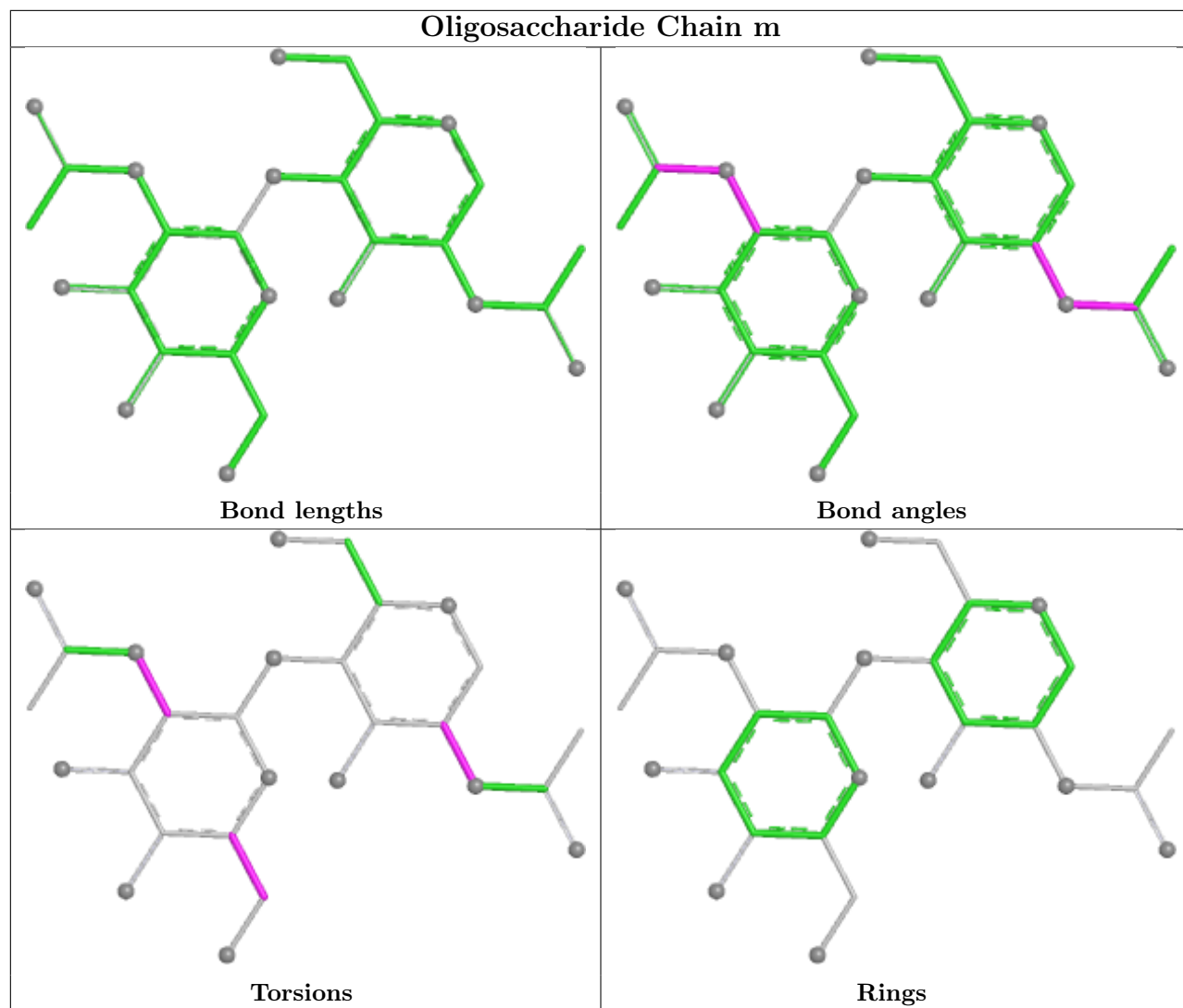


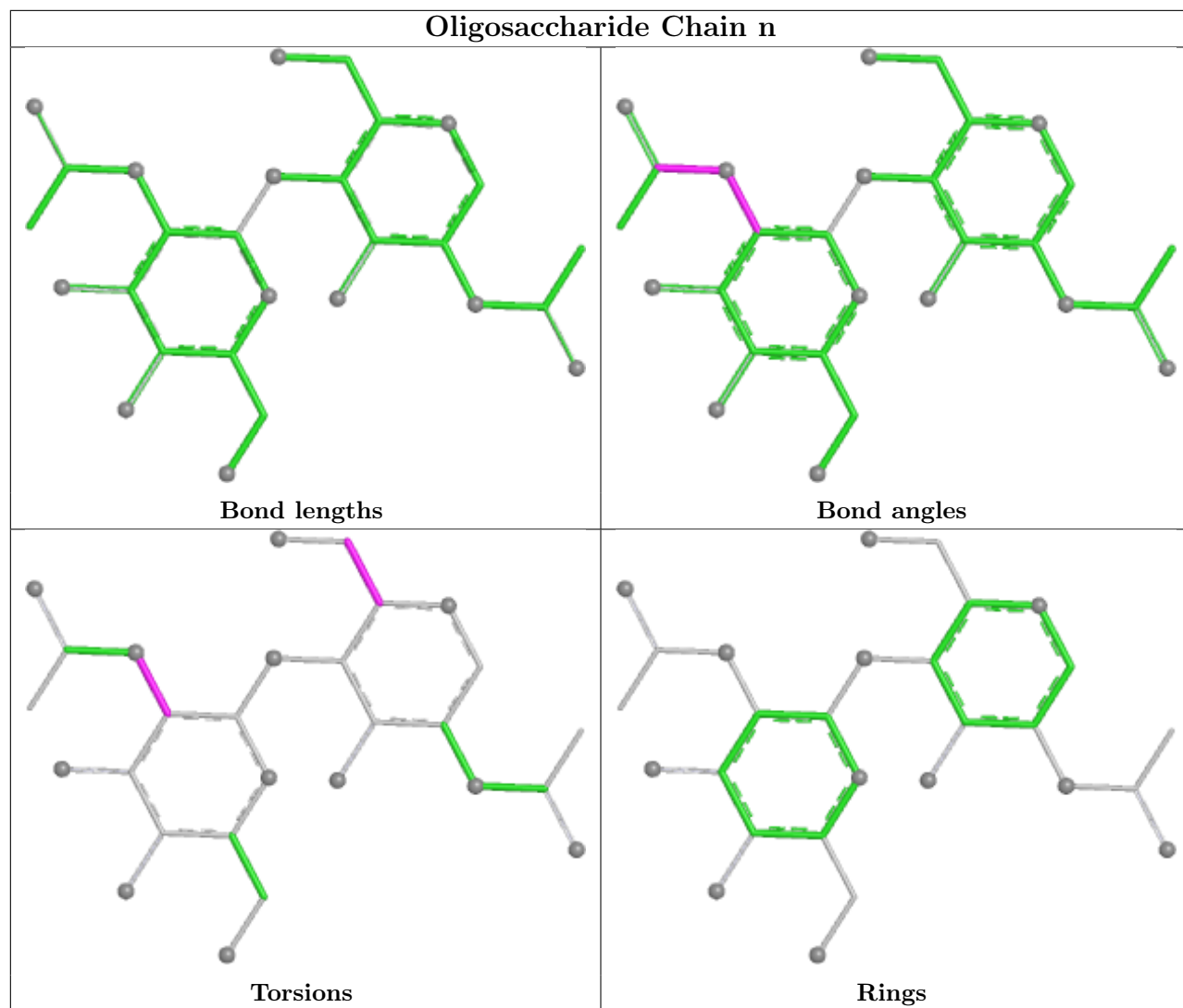


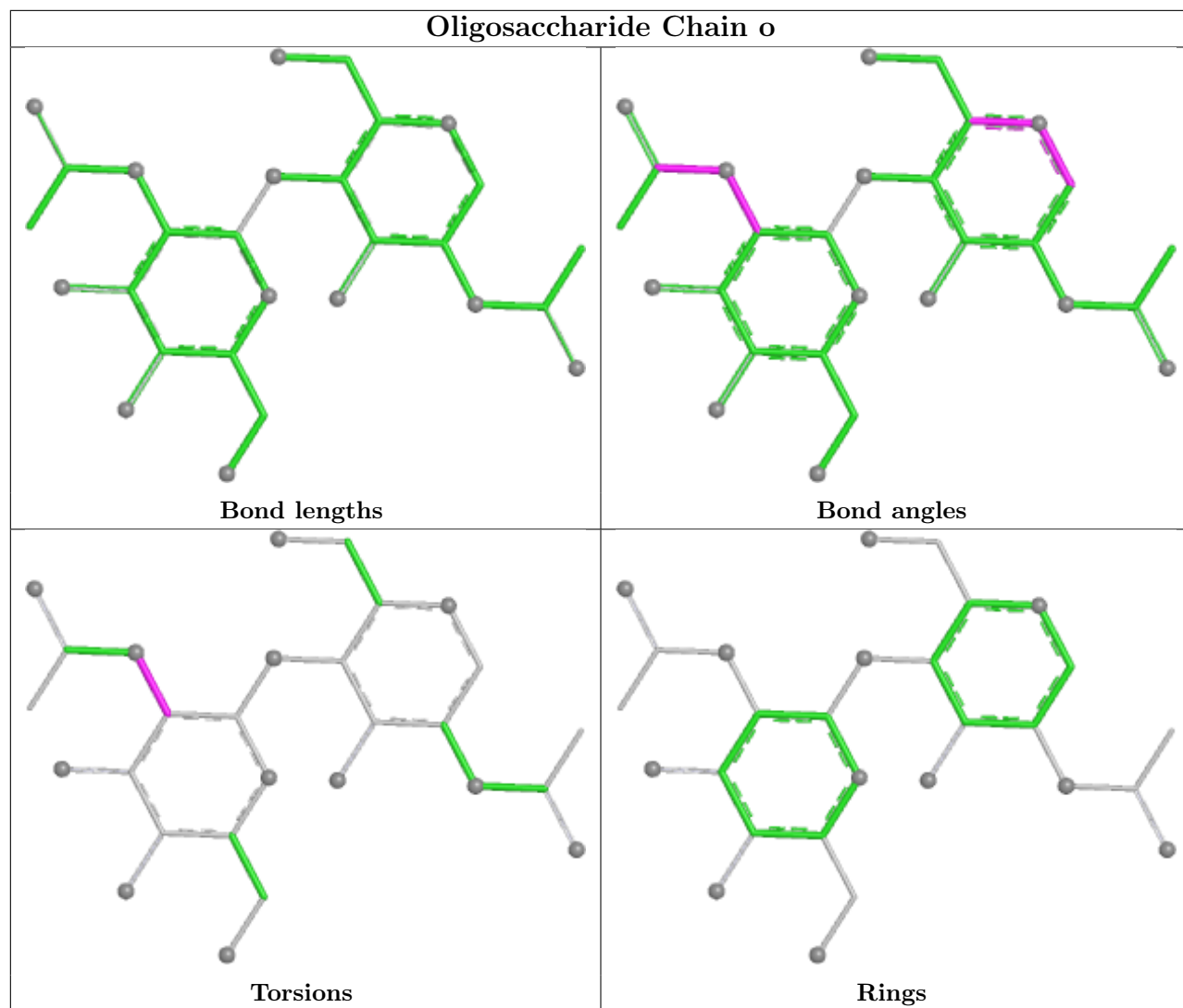


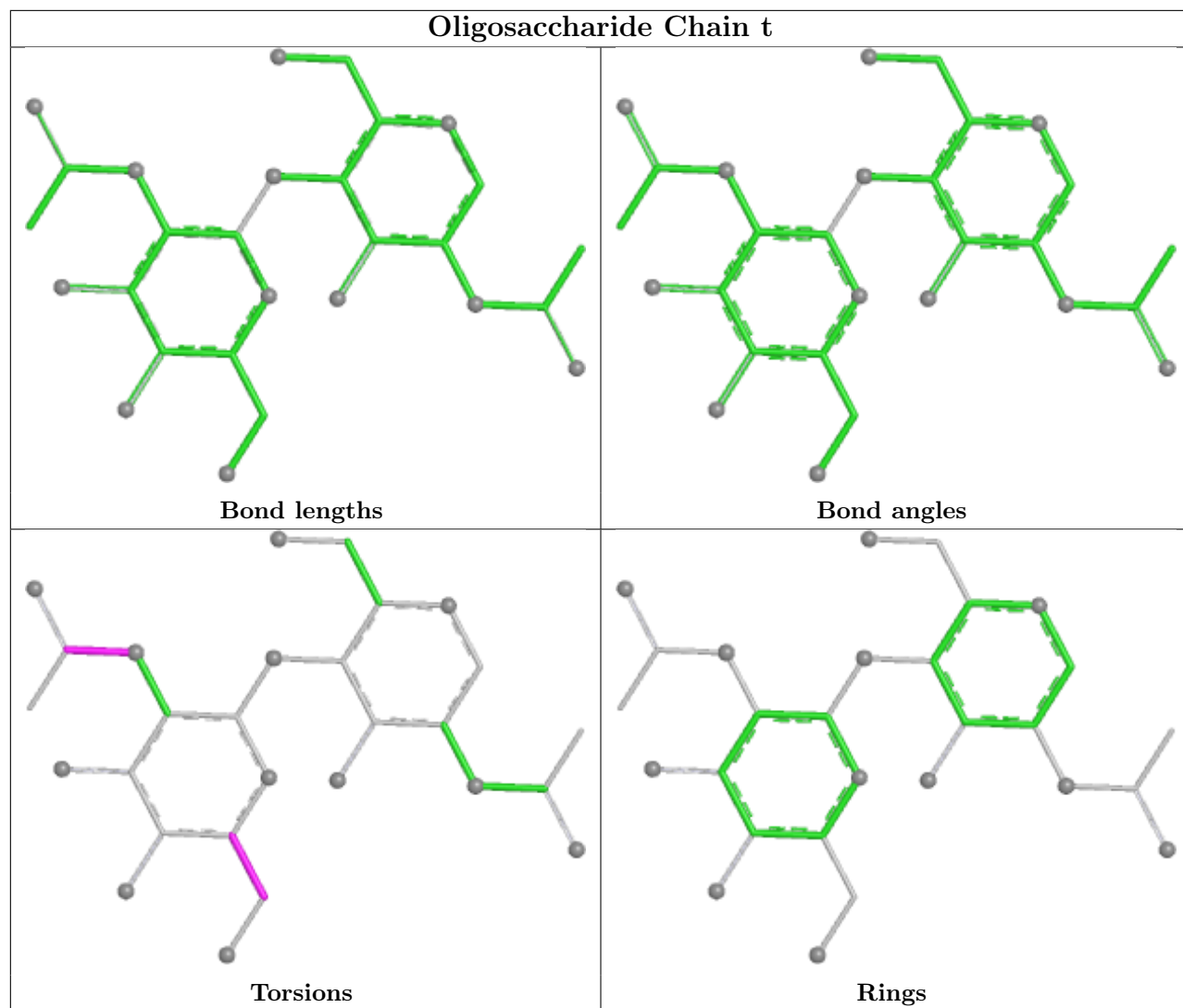


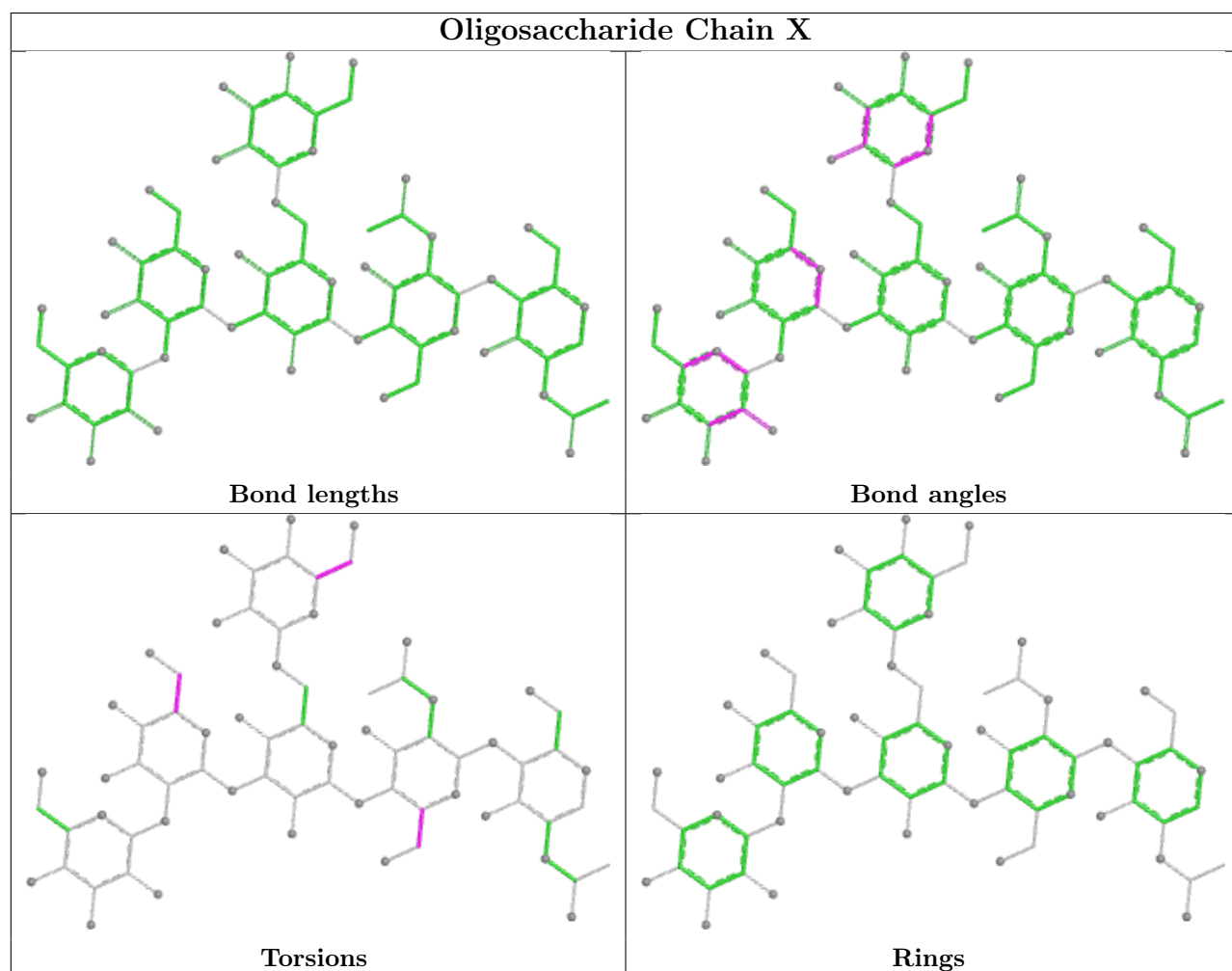
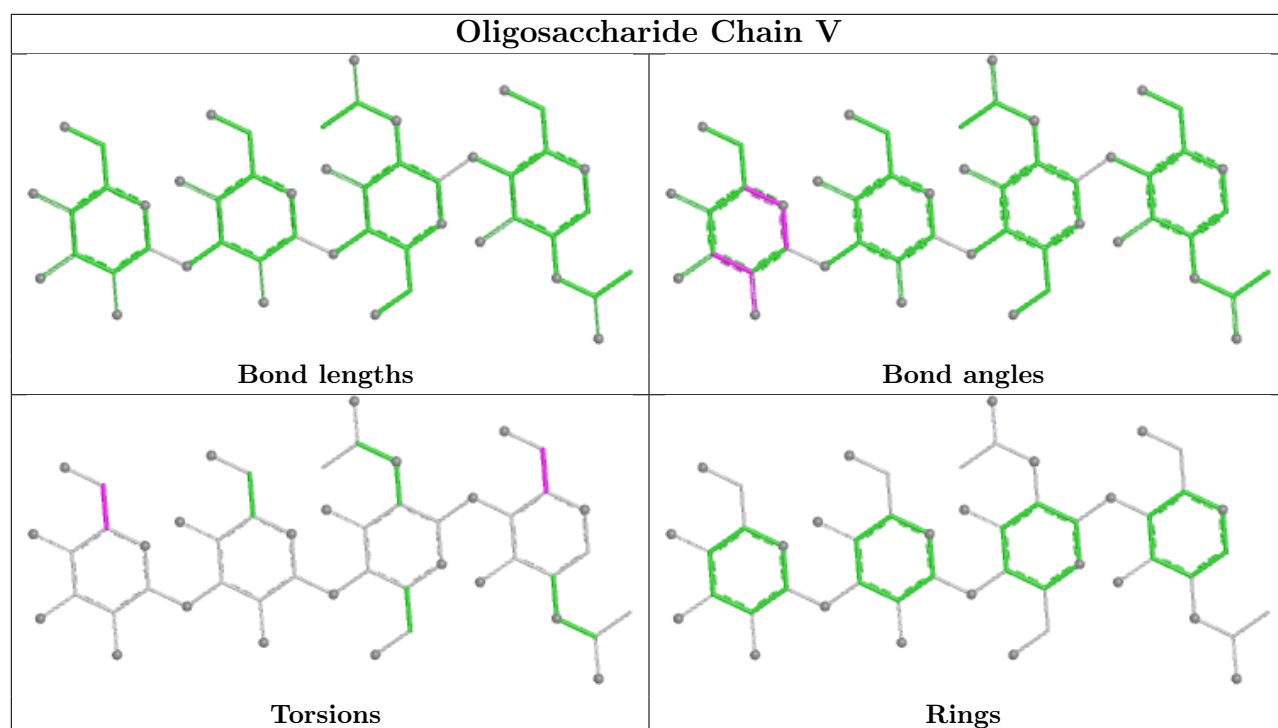


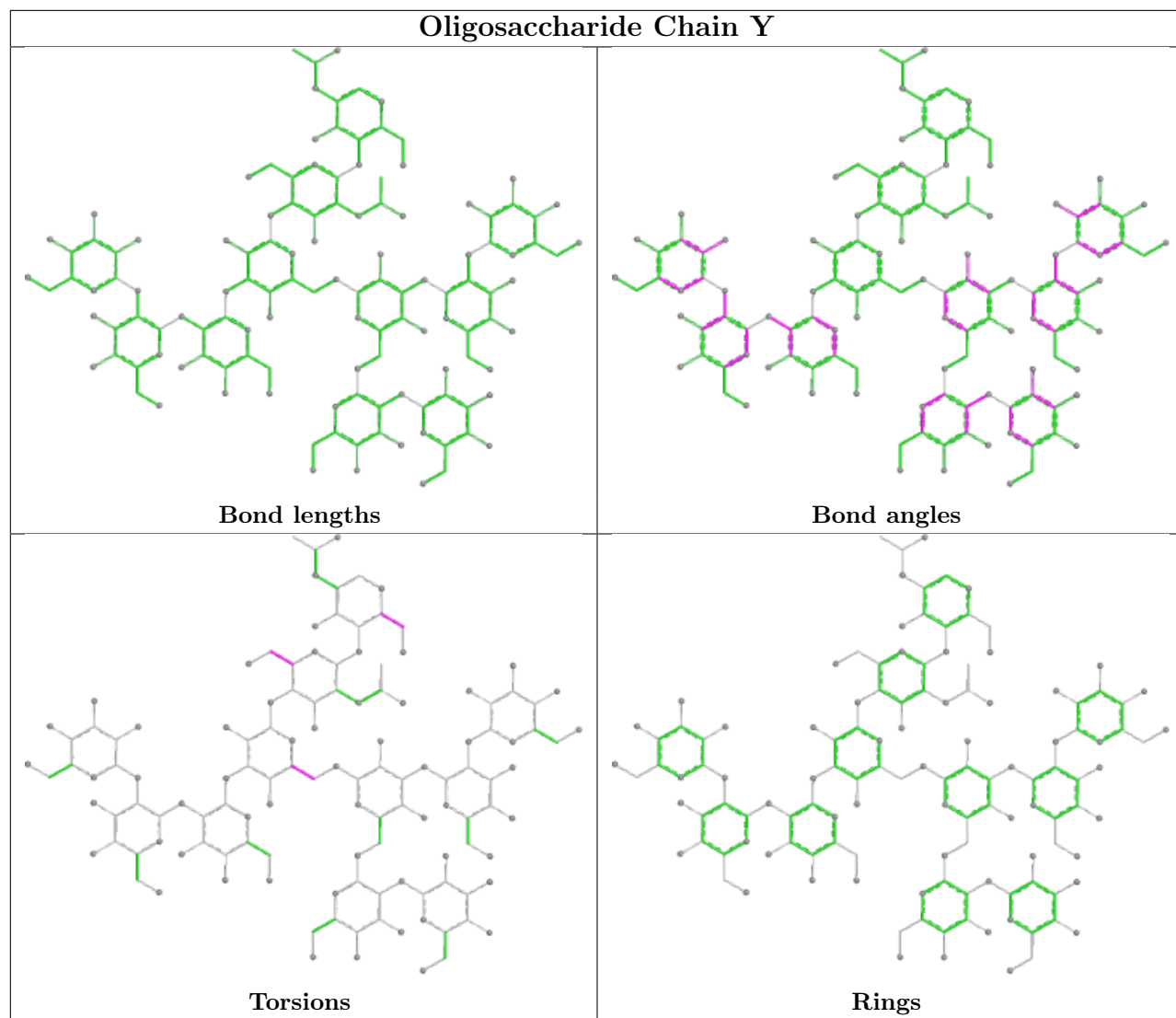


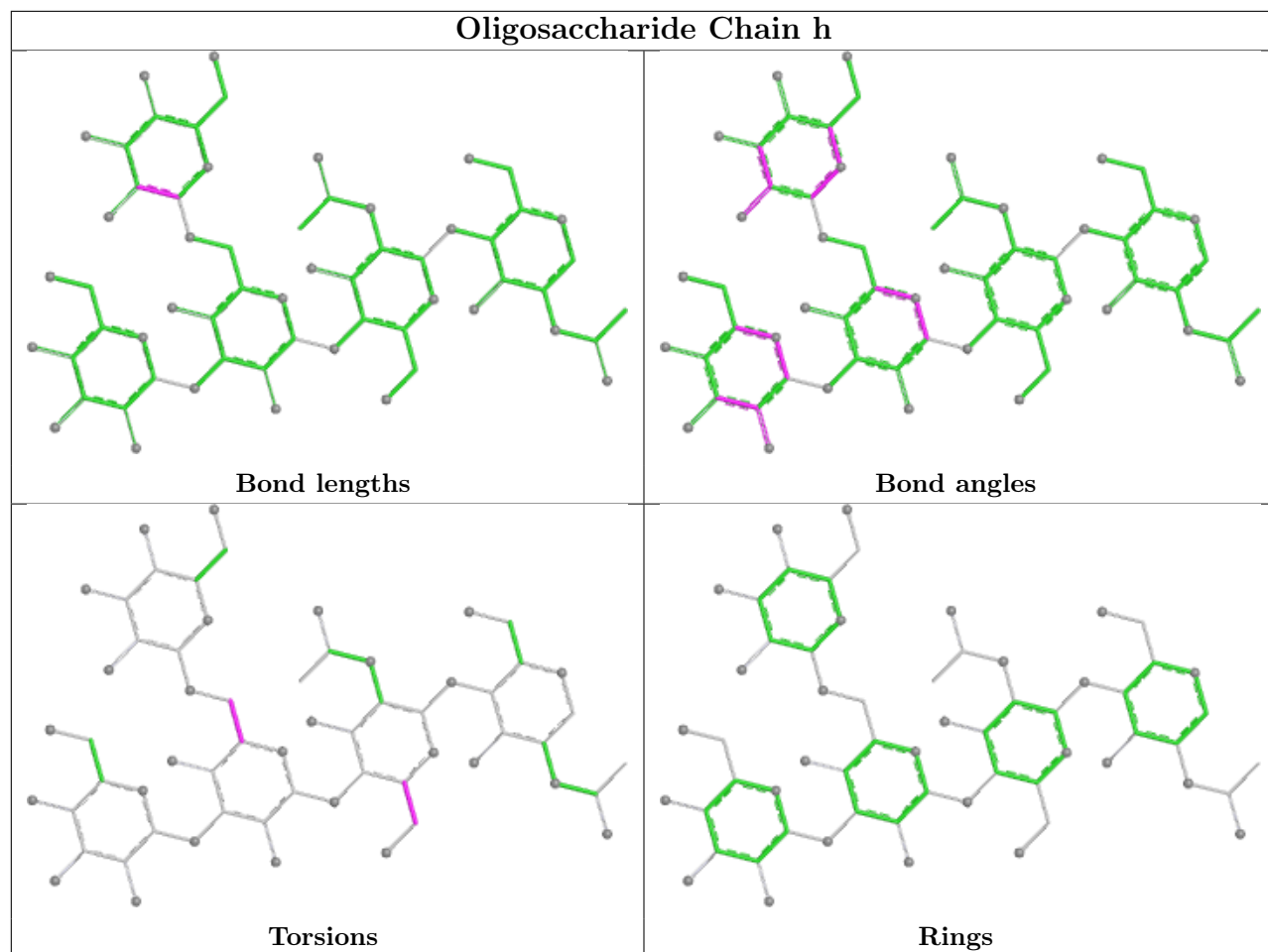


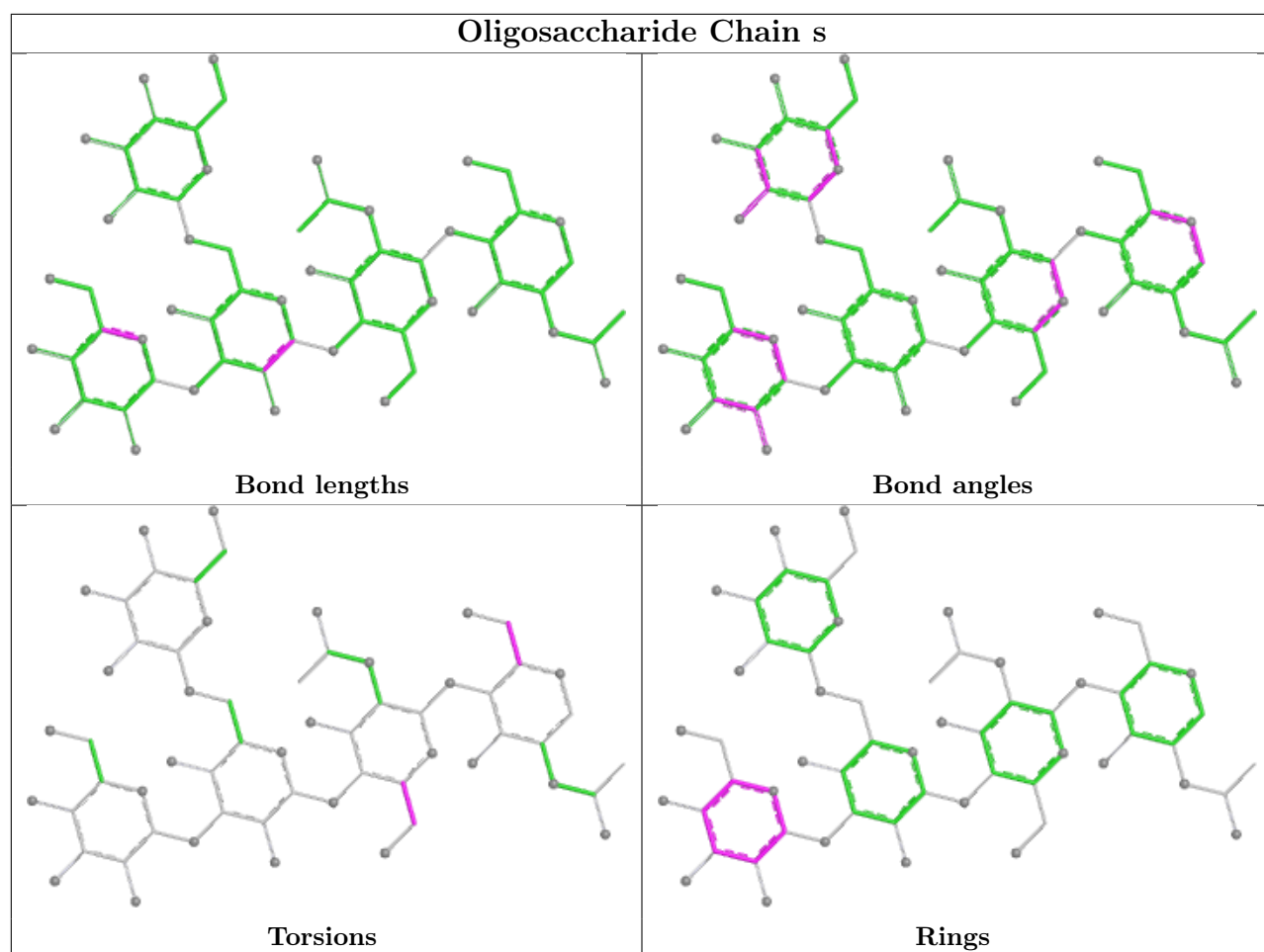


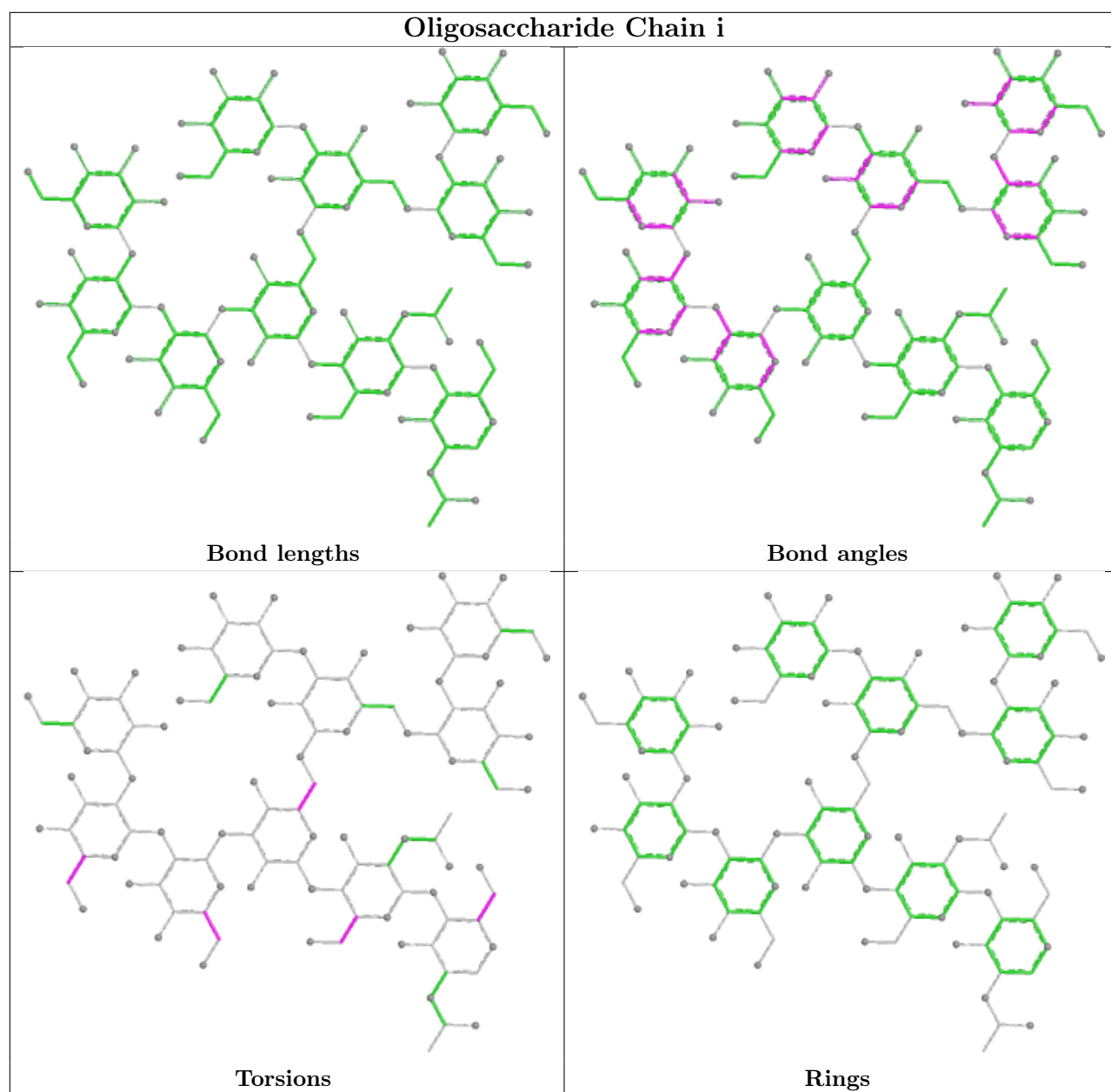


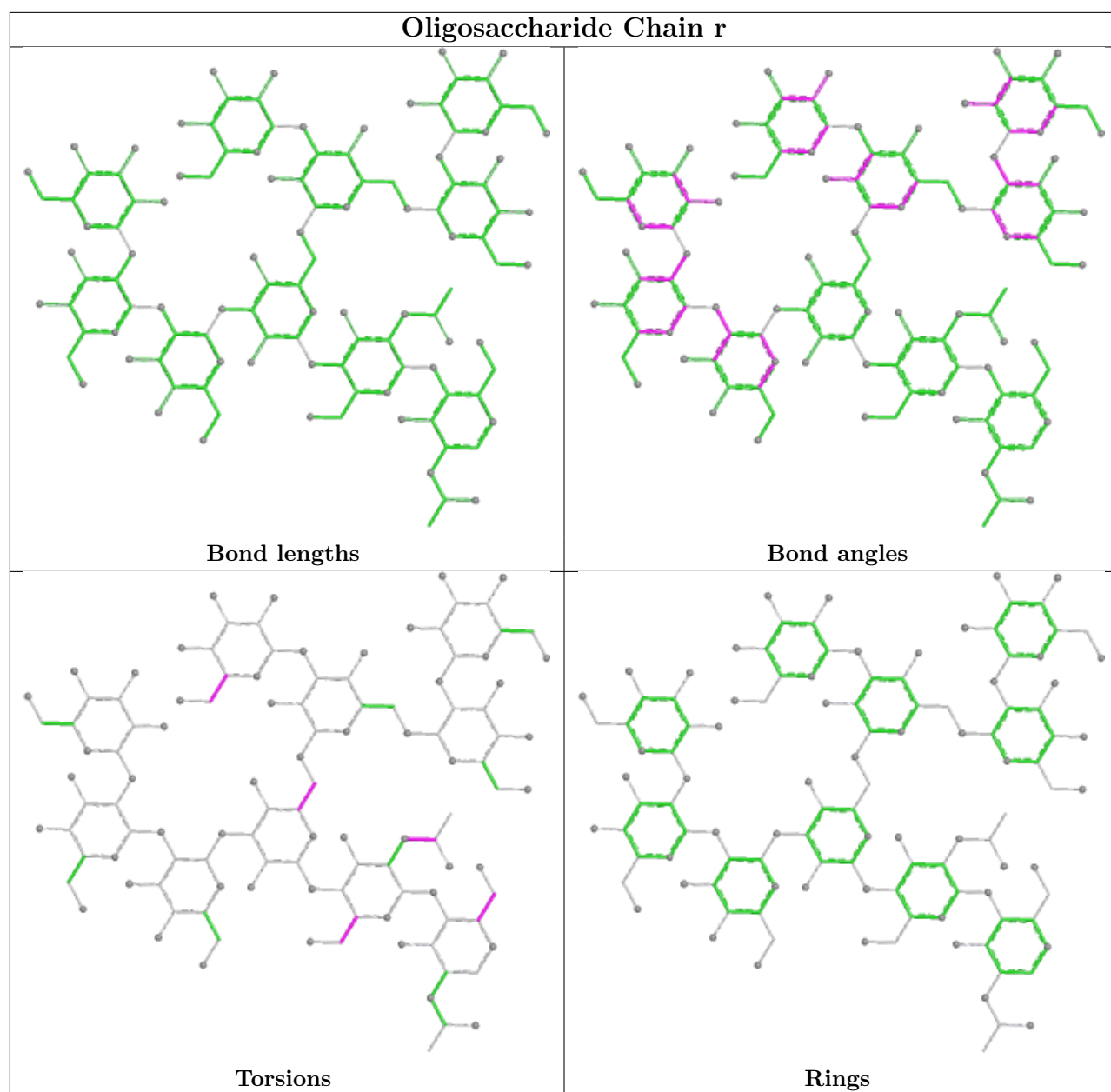


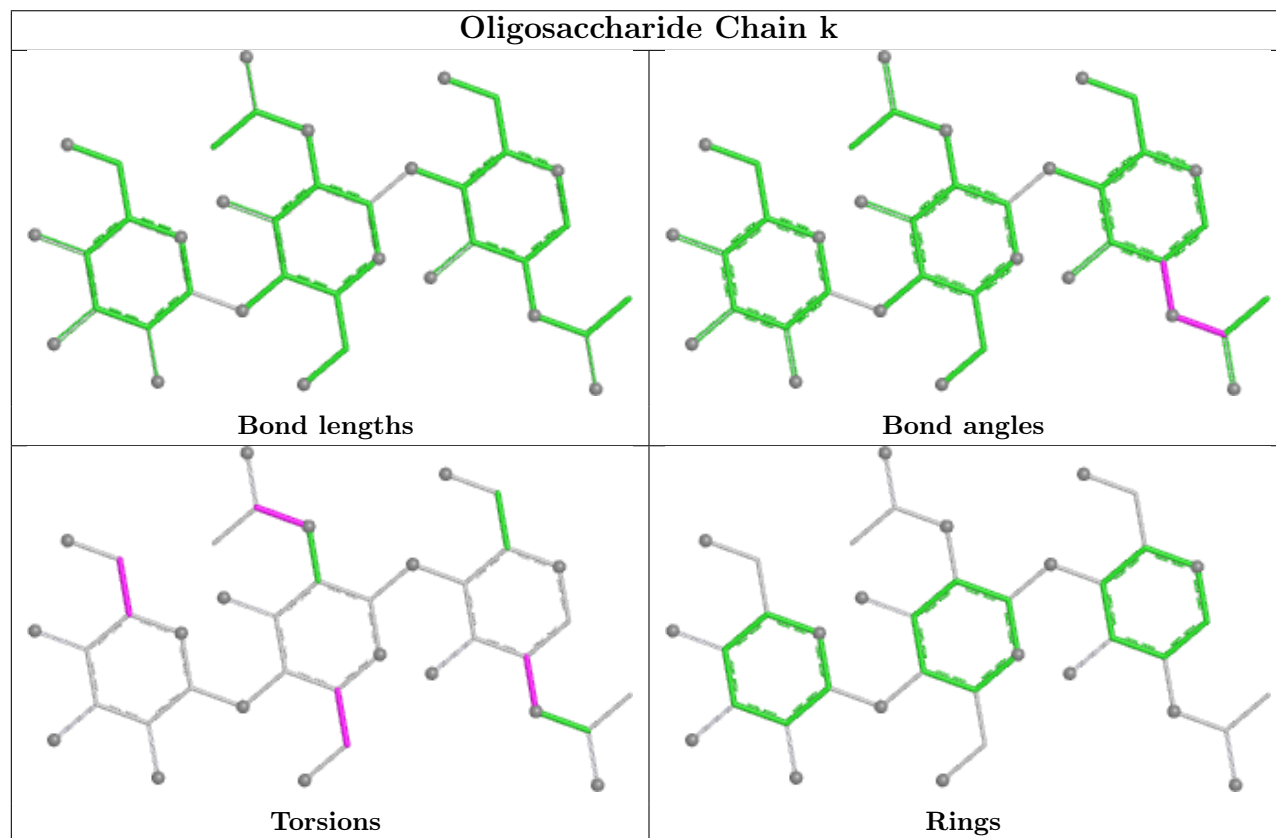
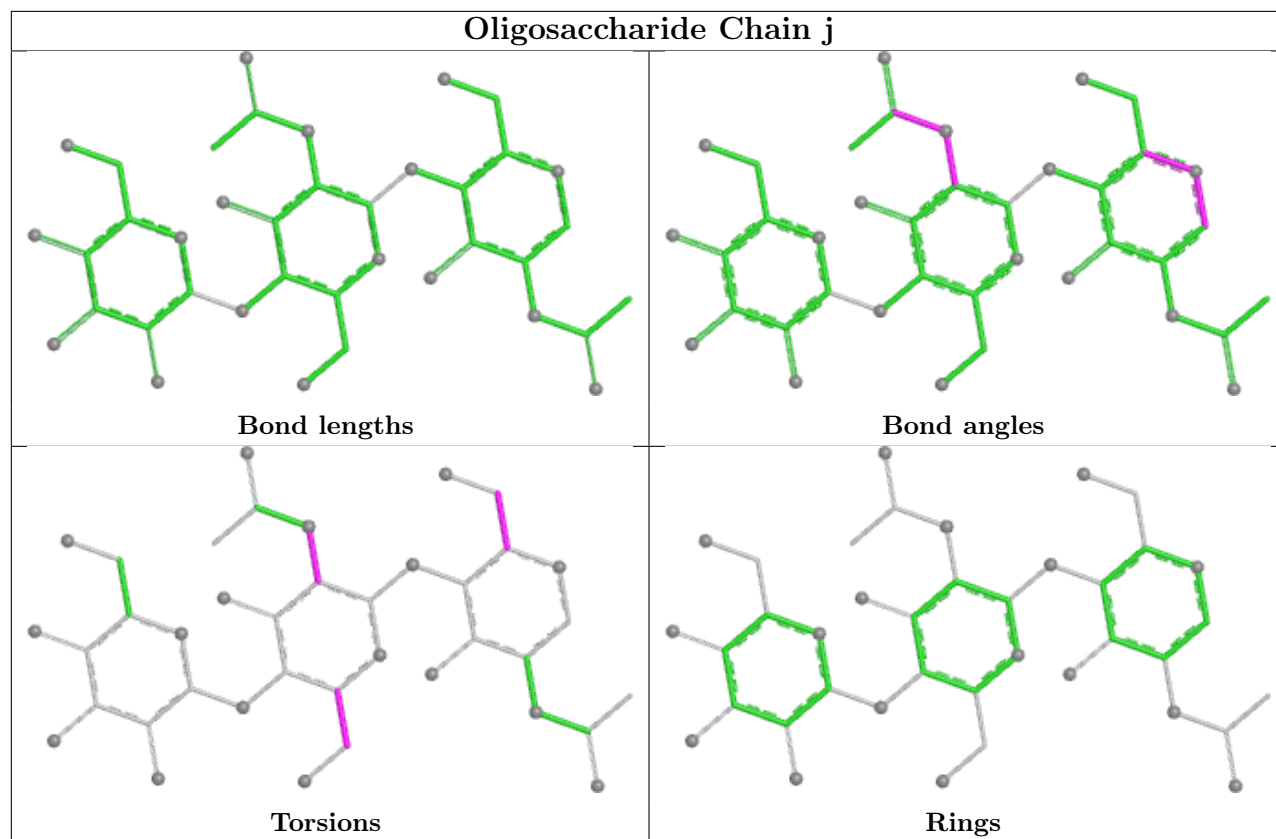


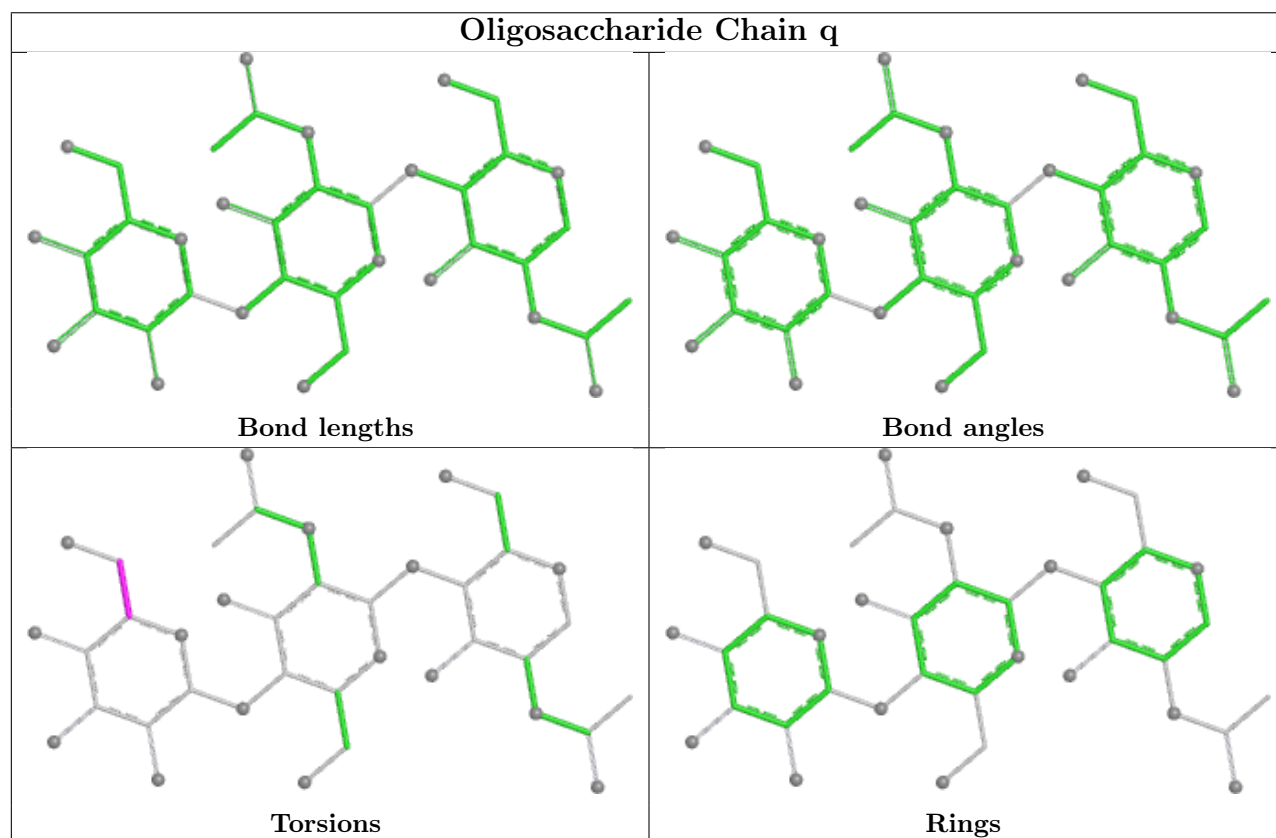
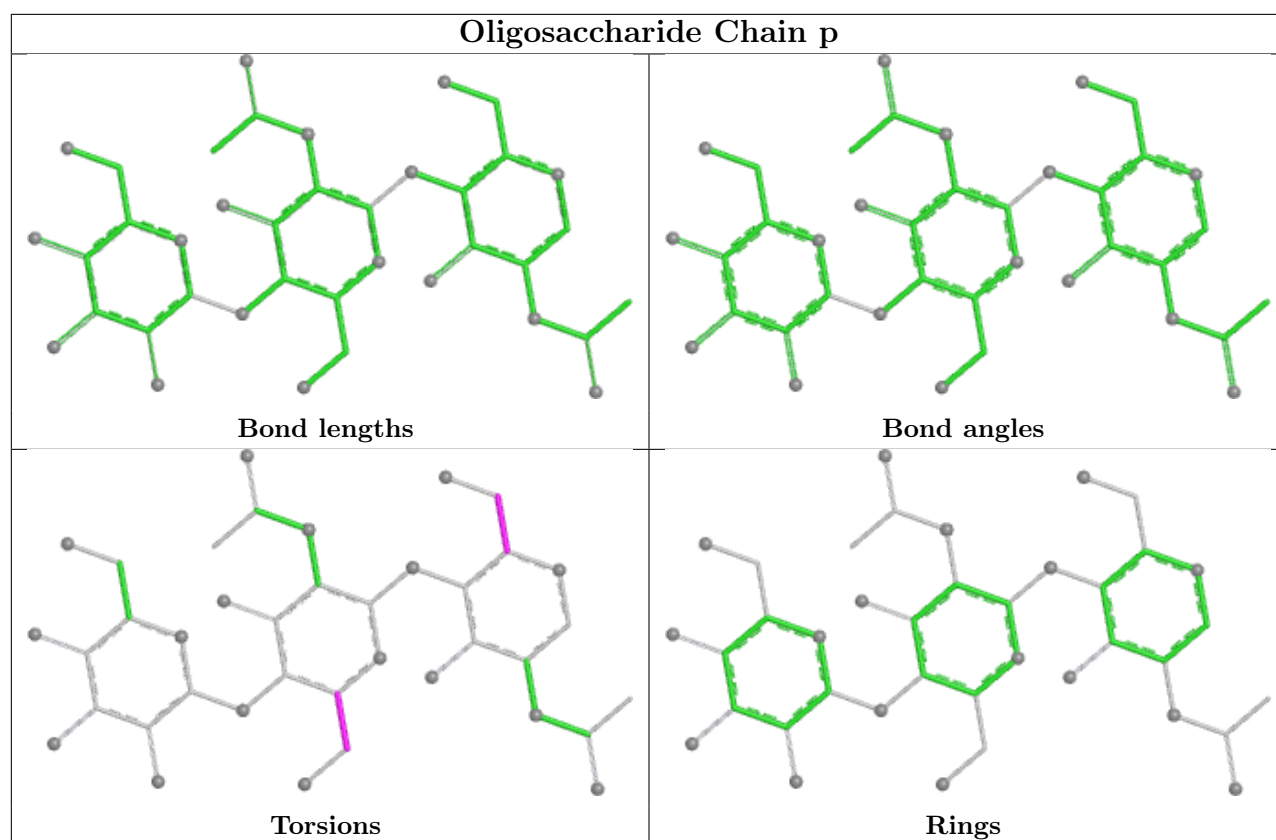












5.6 Ligand geometry

23 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	$\# Z > 2$
14	NAG	G	602	4	14,14,15	0.37	0	17,19,21	0.53	0
14	NAG	G	604	4	14,14,15	0.41	0	17,19,21	0.55	0
14	NAG	J	603	4	14,14,15	0.37	0	17,19,21	0.51	0
14	NAG	P	602	4	14,14,15	0.40	0	17,19,21	0.51	0
14	NAG	P	605	4	14,14,15	0.37	0	17,19,21	0.51	0
14	NAG	J	604	4	14,14,15	0.37	0	17,19,21	0.51	0
14	NAG	F	701	3	14,14,15	0.27	0	17,19,21	0.55	0
14	NAG	G	608	4	14,14,15	0.41	0	17,19,21	0.55	0
14	NAG	J	602	4	14,14,15	0.39	0	17,19,21	0.51	0
14	NAG	G	607	4	14,14,15	0.37	0	17,19,21	0.51	0
14	NAG	P	601	4	14,14,15	0.38	0	17,19,21	0.52	0
14	NAG	P	603	4	14,14,15	0.37	0	17,19,21	0.51	0
14	NAG	G	603	4	14,14,15	0.37	0	17,19,21	0.50	0
14	NAG	P	607	4	14,14,15	0.39	0	17,19,21	0.60	0
14	NAG	J	605	4	14,14,15	0.37	0	17,19,21	0.50	0
14	NAG	C	701	3	14,14,15	0.40	0	17,19,21	0.75	0
14	NAG	P	604	4	14,14,15	0.37	0	17,19,21	0.51	0
14	NAG	G	601	4	14,14,15	0.38	0	17,19,21	0.53	0
14	NAG	G	606	4	14,14,15	0.36	0	17,19,21	0.51	0
14	NAG	P	606	4	14,14,15	0.35	0	17,19,21	0.51	0
14	NAG	J	601	4	14,14,15	0.37	0	17,19,21	0.51	0
14	NAG	G	605	4	14,14,15	0.38	0	17,19,21	0.54	0
14	NAG	G	609	4	14,14,15	0.37	0	17,19,21	0.48	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
14	NAG	G	602	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	G	604	4	-	2/6/23/26	0/1/1/1
14	NAG	J	603	4	-	1/6/23/26	0/1/1/1
14	NAG	P	602	4	-	0/6/23/26	0/1/1/1
14	NAG	P	605	4	-	0/6/23/26	0/1/1/1
14	NAG	J	604	4	-	1/6/23/26	0/1/1/1
14	NAG	F	701	3	-	1/6/23/26	0/1/1/1
14	NAG	G	608	4	-	0/6/23/26	0/1/1/1
14	NAG	J	602	4	-	2/6/23/26	0/1/1/1
14	NAG	G	607	4	-	2/6/23/26	0/1/1/1
14	NAG	P	601	4	-	2/6/23/26	0/1/1/1
14	NAG	P	603	4	-	0/6/23/26	0/1/1/1
14	NAG	G	603	4	-	1/6/23/26	0/1/1/1
14	NAG	P	607	4	-	2/6/23/26	0/1/1/1
14	NAG	J	605	4	-	0/6/23/26	0/1/1/1
14	NAG	C	701	3	-	1/6/23/26	0/1/1/1
14	NAG	P	604	4	-	1/6/23/26	0/1/1/1
14	NAG	G	601	4	-	2/6/23/26	0/1/1/1
14	NAG	G	606	4	-	2/6/23/26	0/1/1/1
14	NAG	P	606	4	-	0/6/23/26	0/1/1/1
14	NAG	J	601	4	-	0/6/23/26	0/1/1/1
14	NAG	G	605	4	-	2/6/23/26	0/1/1/1
14	NAG	G	609	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	P	601	NAG	O5-C5-C6-O6
14	P	601	NAG	C4-C5-C6-O6
14	J	602	NAG	C4-C5-C6-O6
14	G	605	NAG	O5-C5-C6-O6
14	J	602	NAG	O5-C5-C6-O6
14	P	607	NAG	C8-C7-N2-C2
14	P	607	NAG	O7-C7-N2-C2
14	G	605	NAG	C4-C5-C6-O6
14	G	601	NAG	C4-C5-C6-O6
14	G	606	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	G	609	NAG	C4-C5-C6-O6
14	G	601	NAG	O5-C5-C6-O6
14	J	604	NAG	O5-C5-C6-O6
14	G	604	NAG	C4-C5-C6-O6
14	G	607	NAG	C4-C5-C6-O6
14	G	604	NAG	O5-C5-C6-O6
14	P	604	NAG	O5-C5-C6-O6
14	G	609	NAG	O5-C5-C6-O6
14	G	607	NAG	O5-C5-C6-O6
14	G	606	NAG	O5-C5-C6-O6
14	G	603	NAG	O5-C5-C6-O6
14	C	701	NAG	C1-C2-N2-C7
14	F	701	NAG	C1-C2-N2-C7
14	J	603	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

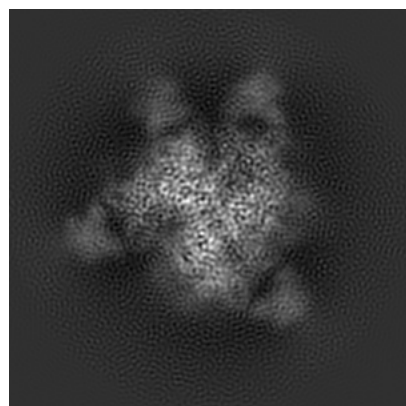
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24072. These allow visual inspection of the internal detail of the map and identification of artifacts.

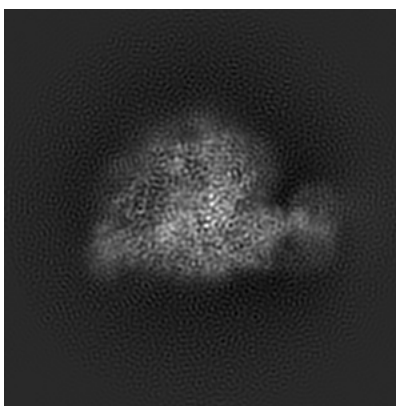
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

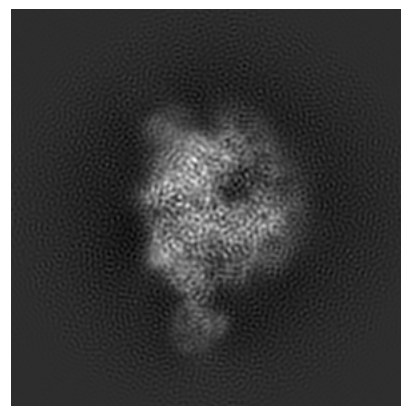
6.1.1 Primary map



X

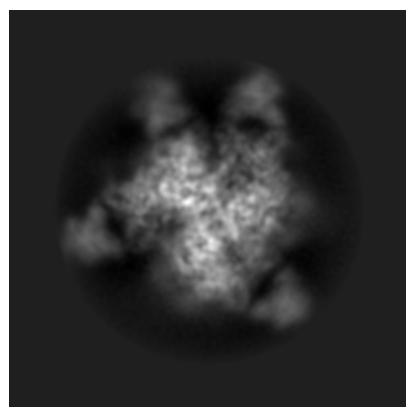


Y

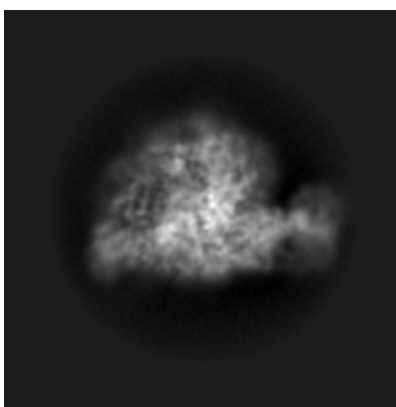


Z

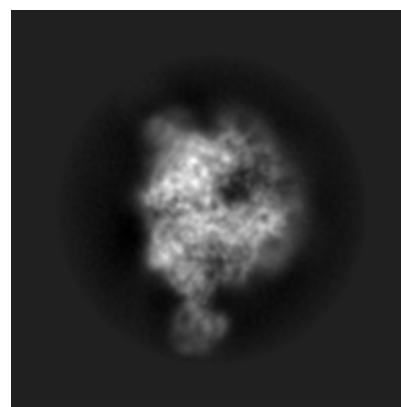
6.1.2 Raw map



X



Y

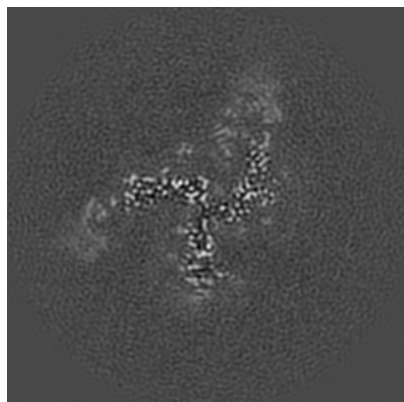


Z

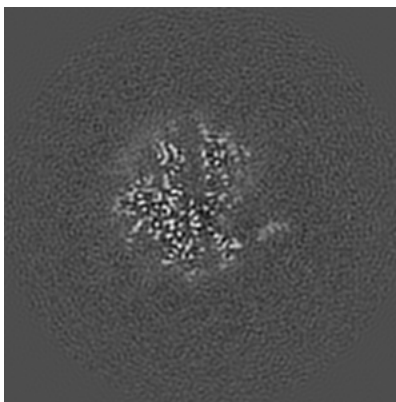
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

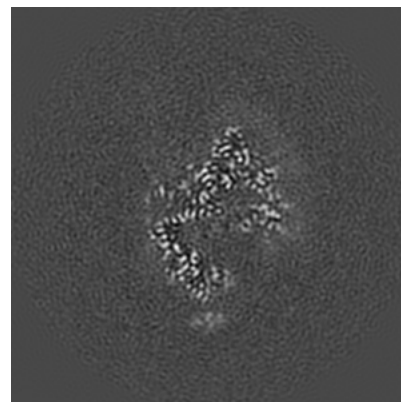
6.2.1 Primary map



X Index: 168

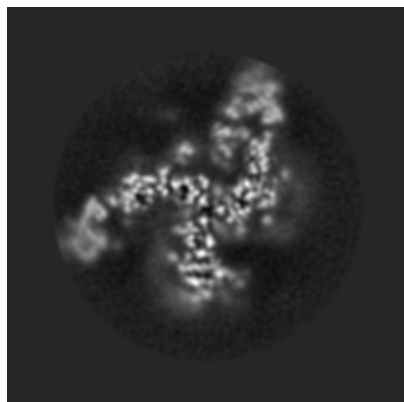


Y Index: 168

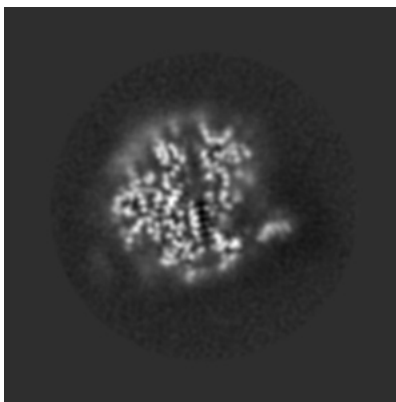


Z Index: 168

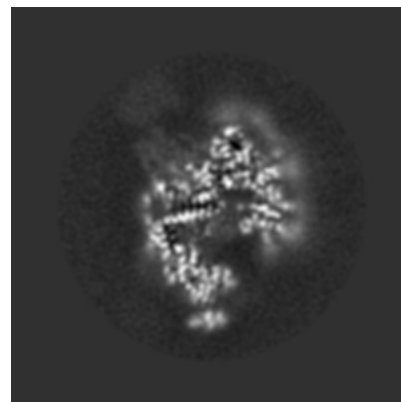
6.2.2 Raw map



X Index: 168



Y Index: 168

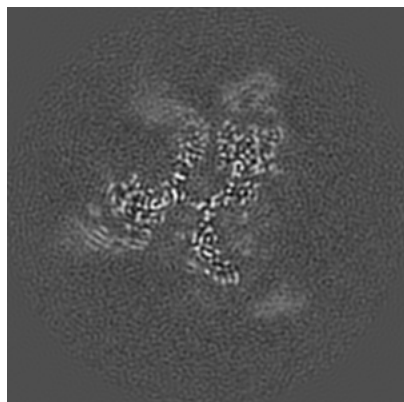


Z Index: 168

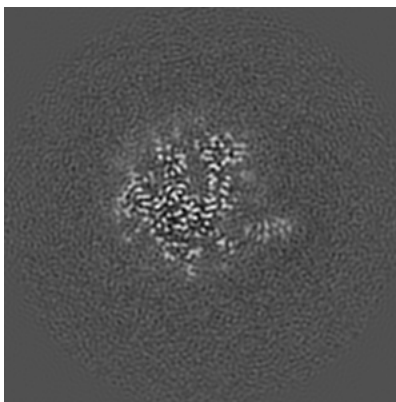
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

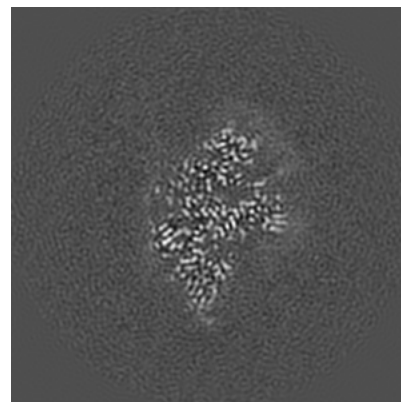
6.3.1 Primary map



X Index: 153

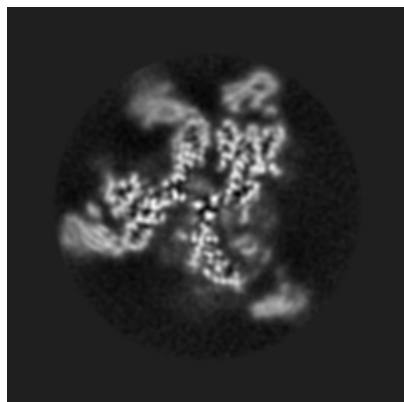


Y Index: 165

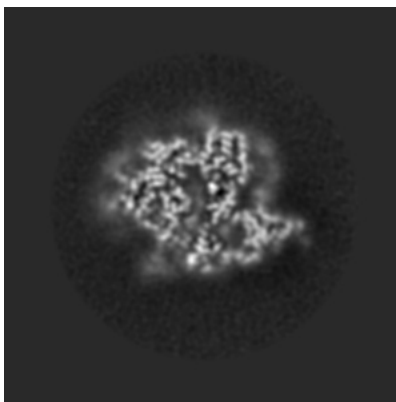


Z Index: 173

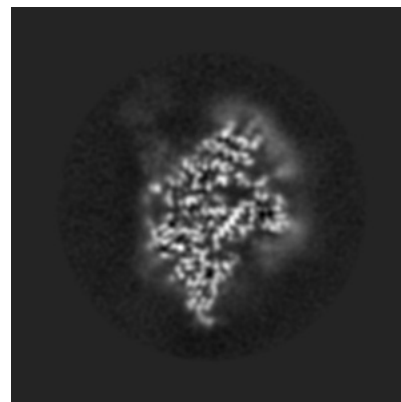
6.3.2 Raw map



X Index: 152



Y Index: 155

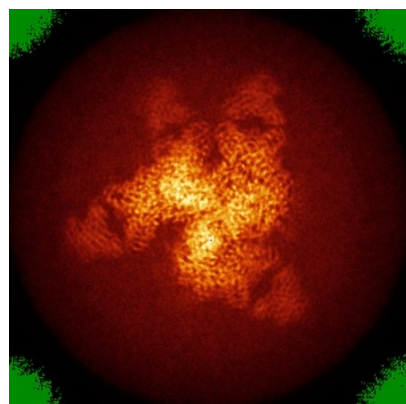


Z Index: 174

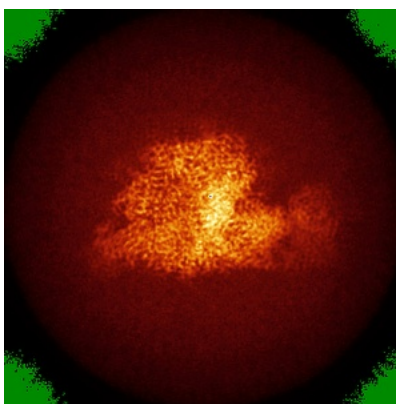
The images above show the largest variance slices of the map in three orthogonal directions.

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

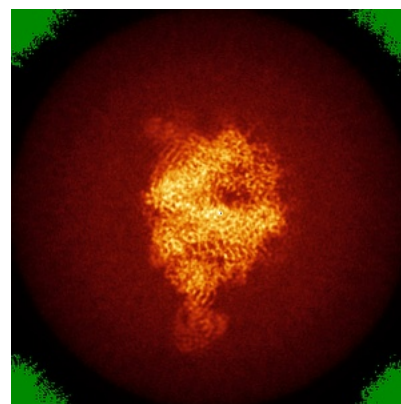
6.4.1 Primary map



X

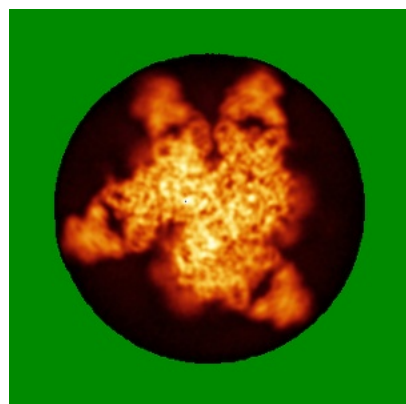


Y

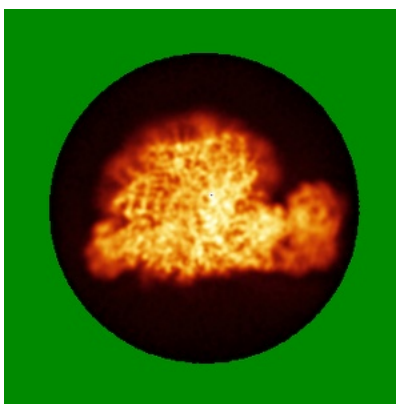


Z

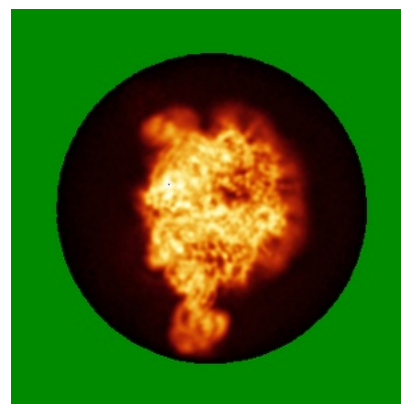
6.4.2 Raw map



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 0.0154. 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.

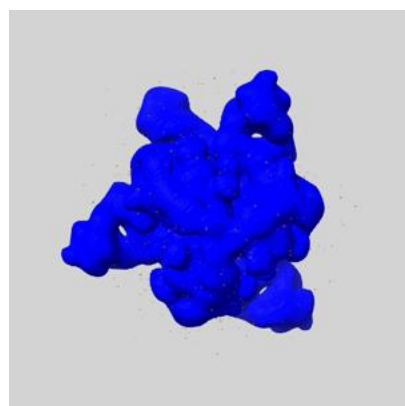
6.6 Mask visualisation [i](#)

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

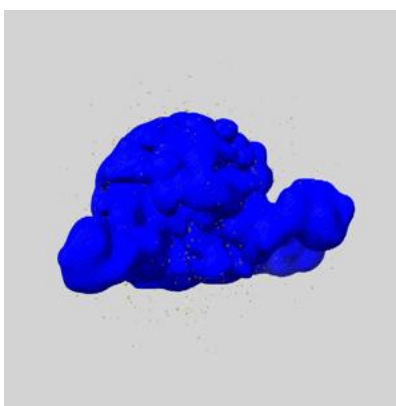
A mask typically either:

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

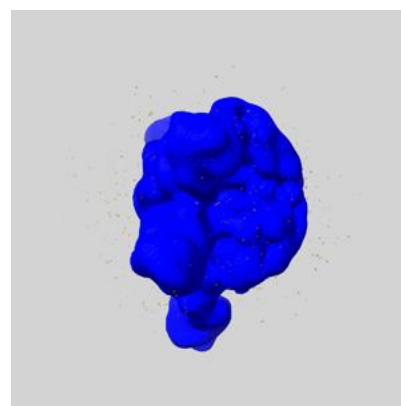
6.6.1 emd_24072_msk_1.map [i](#)



X



Y

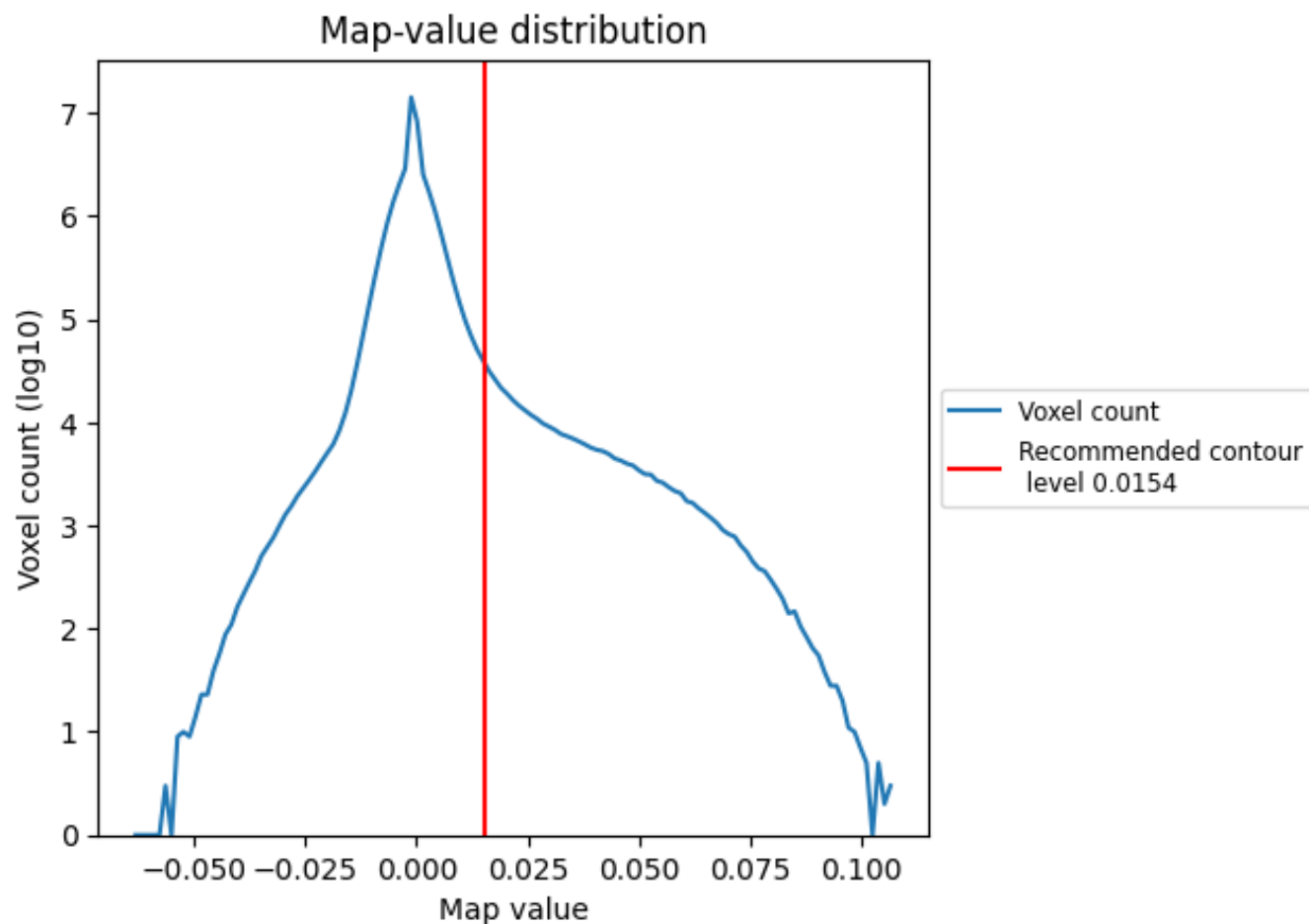


Z

7 Map analysis [i](#)

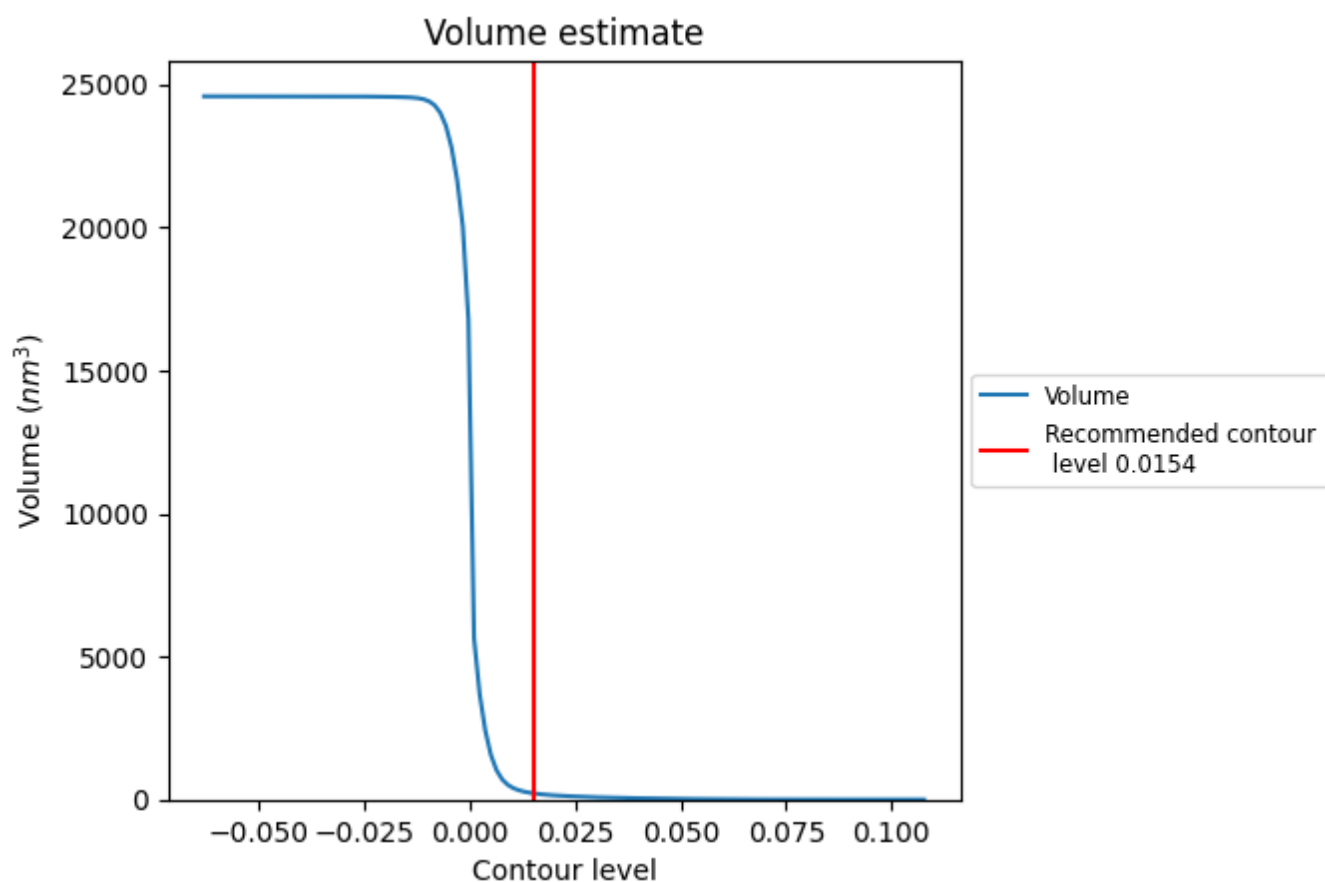
This section contains the results of statistical analysis of the map.

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.

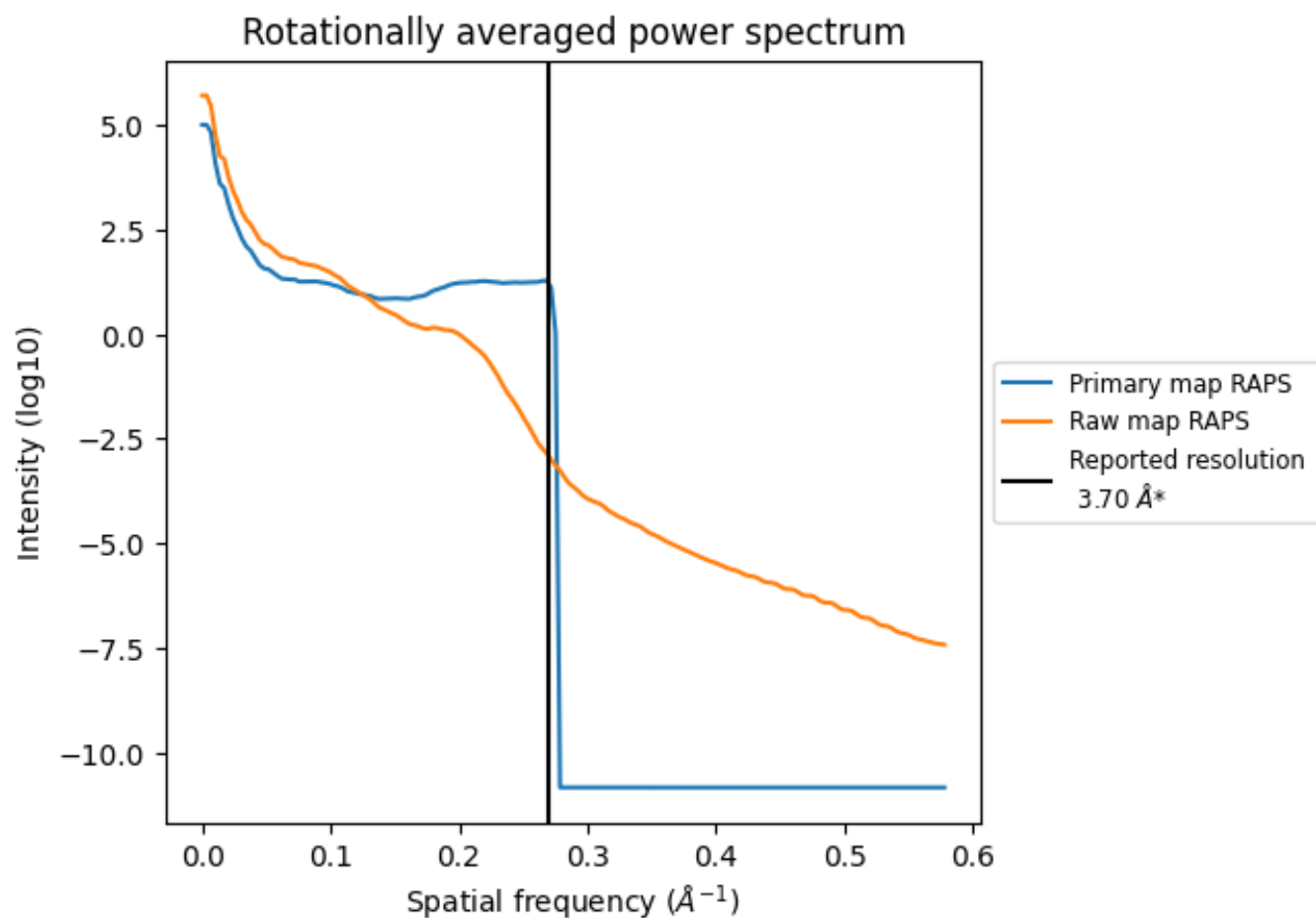
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 192 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 ⓘ

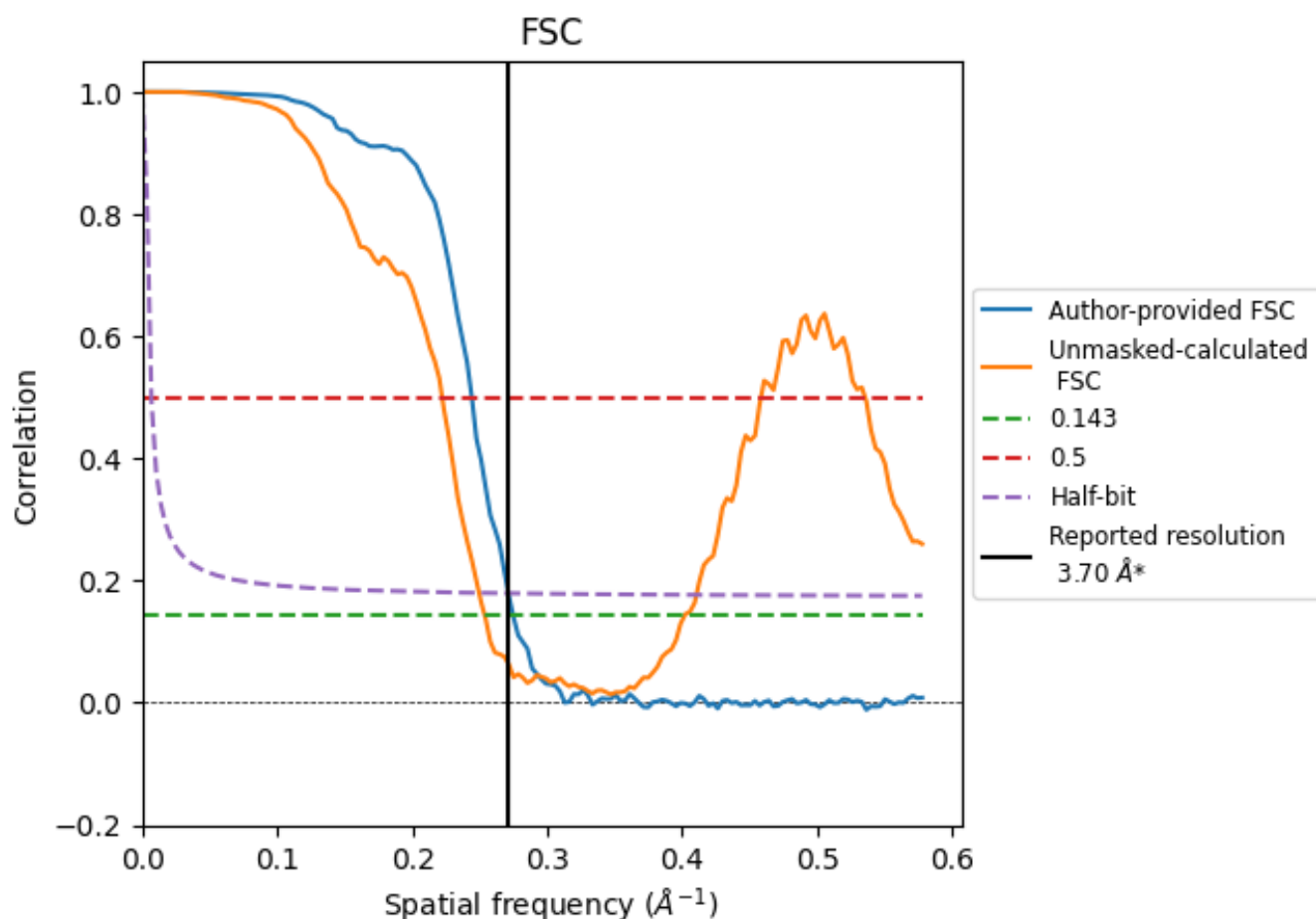


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.64	4.10	3.69
Unmasked-calculated*	3.94	4.50	4.01

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

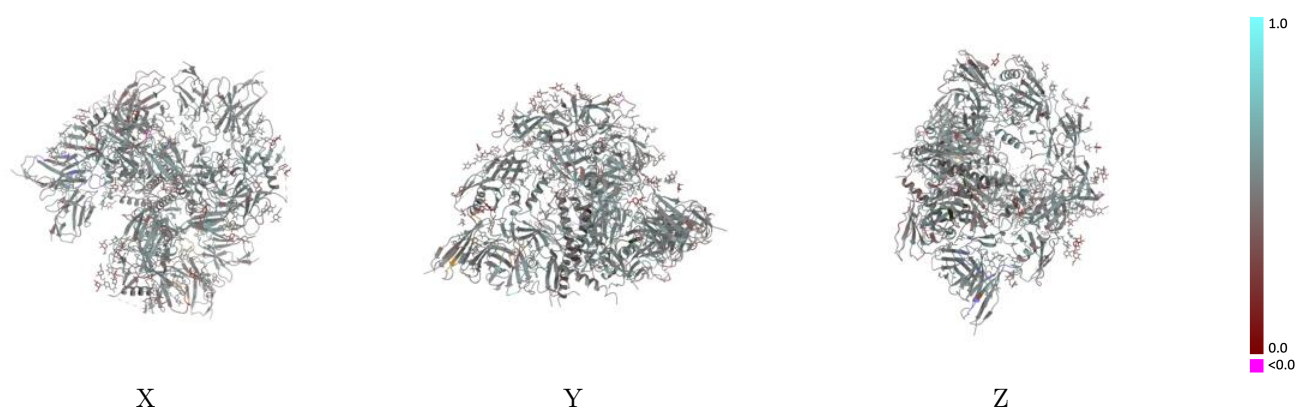
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24072 and PDB model 7MXE. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

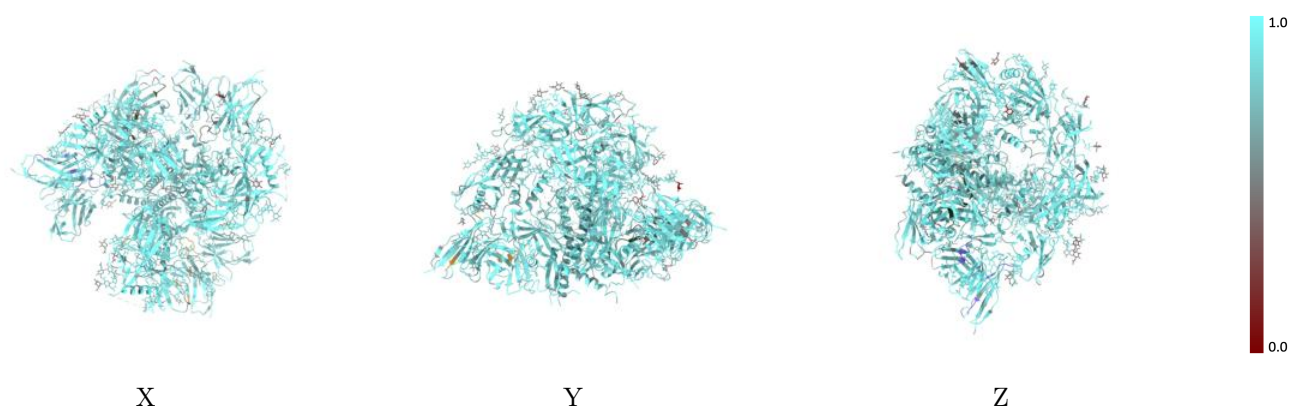
This section was not generated.

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



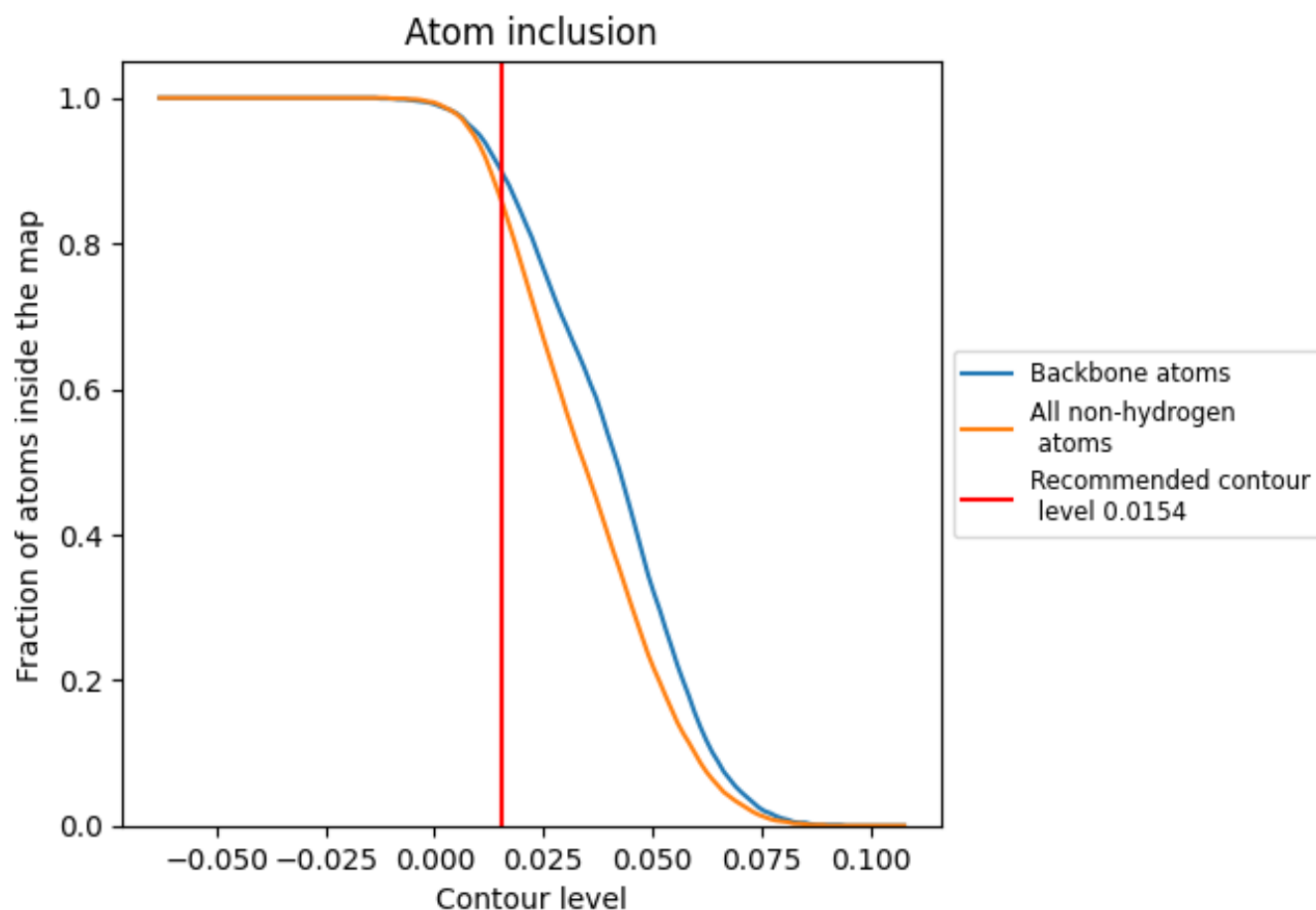
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0154).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.0154) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.4920
A	 0.8870	 0.5090
B	 0.8840	 0.5030
C	 0.8600	 0.5030
D	 0.8890	 0.5140
E	 0.9640	 0.5140
F	 0.8420	 0.4770
G	 0.8720	 0.5020
H	 0.8770	 0.5010
I	 0.8930	 0.5060
J	 0.8720	 0.5090
K	 0.8930	 0.5330
L	 0.8540	 0.4970
M	 0.8550	 0.4860
N	 0.5360	 0.3710
O	 0.8540	 0.4830
P	 0.8660	 0.4950
Q	 0.7500	 0.3380
R	 0.8180	 0.4560
S	 0.6790	 0.3350
T	 0.6790	 0.4280
U	 0.7860	 0.4570
V	 0.8400	 0.4810
W	 0.8130	 0.4620
X	 0.6810	 0.4360
Y	 0.8660	 0.4900
Z	 0.7140	 0.4150
a	 0.6430	 0.3850
b	 0.6070	 0.3220
c	 0.7500	 0.4680
d	 0.7500	 0.3920
e	 0.5360	 0.3870
f	 0.6070	 0.2870
g	 0.8570	 0.4900
h	 0.8360	 0.4640



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.9050	 0.5010
j	 0.7690	 0.4110
k	 0.5130	 0.2400
l	 0.7500	 0.4720
m	 0.6790	 0.3890
n	 0.6790	 0.4040
o	 0.5710	 0.3320
p	 0.6920	 0.4020
q	 0.8970	 0.5020
r	 0.8020	 0.4650
s	 0.6070	 0.2720
t	 0.8210	 0.3500