



## Full wwPDB EM Validation Report ⓘ

Oct 2, 2025 – 06:49 PM EDT

PDB ID : 9OGU / pdb\_00009ogu  
EMDB ID : EMD-70476  
Title : HIV-1 Env BG505 SOSIP.664-dPG-His in complex with PGT122 and 3BNC117 Fabs  
Authors : Andrade, T.G.; Ozorowski, G.; Ward, A.B.  
Deposited on : 2025-05-01  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

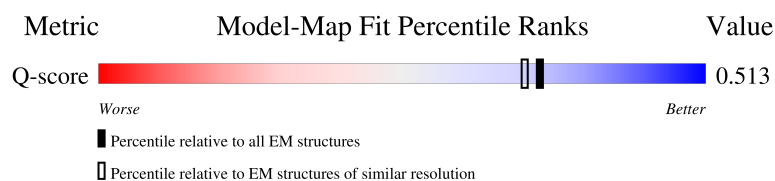
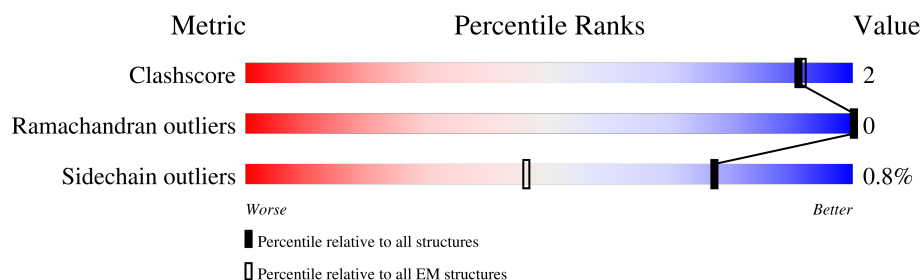


# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	516	
1	C	516	
1	E	516	
2	B	168	

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Mol	Chain	Length	Quality of chain
2	D	168	
2	F	168	
3	H	226	
3	M	226	
3	P	226	
4	I	206	
4	L	206	
4	Q	206	
5	J	235	
5	N	235	
5	R	235	
6	K	211	
6	O	211	
6	S	211	
7	G	2	
7	T	2	
7	W	2	
7	X	2	
7	a	2	
7	b	2	
7	g	2	
7	h	2	
7	j	2	
7	n	2	
7	q	2	

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Mol	Chain	Length	Quality of chain
8	U	4	 25% 100%
9	V	6	 100%
10	Y	4	 100%
10	k	4	 100%
11	Z	5	 20% 40% 60% 20%
11	f	5	 40% 40% 60%
11	i	5	 20% 100%
11	r	5	 40% 100%
12	c	3	 33% 67%
12	d	3	 100%
12	l	3	 33% 100%
12	p	3	 33% 33% 33% 33%
13	e	7	 100%
13	o	7	 100%
14	m	2	 50% 50% 50%



## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 25622 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 HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	435	Total	C	N	O	S	0	0
			3423	2153	605	637	28		
1	E	440	Total	C	N	O	S	0	0
			3463	2174	611	650	28		
1	C	437	Total	C	N	O	S	0	0
			3440	2162	608	642	28		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP Q2N0S6
A	-3	ASP	-	expression tag	UNP Q2N0S6
A	-2	ALA	-	expression tag	UNP Q2N0S6
A	-1	MET	-	expression tag	UNP Q2N0S6
A	0	LYS	-	expression tag	UNP Q2N0S6
A	1	ARG	-	expression tag	UNP Q2N0S6
A	2	GLY	-	expression tag	UNP Q2N0S6
A	3	LEU	-	expression tag	UNP Q2N0S6
A	4	CYS	-	expression tag	UNP Q2N0S6
A	5	CYS	-	expression tag	UNP Q2N0S6
A	6	VAL	-	expression tag	UNP Q2N0S6
A	7	LEU	-	expression tag	UNP Q2N0S6
A	8	LEU	-	expression tag	UNP Q2N0S6
A	9	LEU	-	expression tag	UNP Q2N0S6
A	10	CYS	-	expression tag	UNP Q2N0S6
A	11	GLY	-	expression tag	UNP Q2N0S6
A	12	ALA	-	expression tag	UNP Q2N0S6
A	13	VAL	-	expression tag	UNP Q2N0S6
A	14	PHE	-	expression tag	UNP Q2N0S6
A	15	VAL	-	expression tag	UNP Q2N0S6
A	16	SER	-	expression tag	UNP Q2N0S6
A	17	PRO	-	expression tag	UNP Q2N0S6
A	18	SER	-	expression tag	UNP Q2N0S6
A	19	GLN	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLU	-	expression tag	UNP Q2N0S6
A	21	ILE	-	expression tag	UNP Q2N0S6
A	22	HIS	-	expression tag	UNP Q2N0S6
A	23	ALA	-	expression tag	UNP Q2N0S6
A	24	ARG	-	expression tag	UNP Q2N0S6
A	25	PHE	-	expression tag	UNP Q2N0S6
A	26	ARG	-	expression tag	UNP Q2N0S6
A	27	ARG	-	expression tag	UNP Q2N0S6
A	28	GLY	-	expression tag	UNP Q2N0S6
A	29	ALA	-	expression tag	UNP Q2N0S6
A	30	ARG	-	expression tag	UNP Q2N0S6
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
E	-4	MET	-	expression tag	UNP Q2N0S6
E	-3	ASP	-	expression tag	UNP Q2N0S6
E	-2	ALA	-	expression tag	UNP Q2N0S6
E	-1	MET	-	expression tag	UNP Q2N0S6
E	0	LYS	-	expression tag	UNP Q2N0S6
E	1	ARG	-	expression tag	UNP Q2N0S6
E	2	GLY	-	expression tag	UNP Q2N0S6
E	3	LEU	-	expression tag	UNP Q2N0S6
E	4	CYS	-	expression tag	UNP Q2N0S6
E	5	CYS	-	expression tag	UNP Q2N0S6
E	6	VAL	-	expression tag	UNP Q2N0S6
E	7	LEU	-	expression tag	UNP Q2N0S6
E	8	LEU	-	expression tag	UNP Q2N0S6
E	9	LEU	-	expression tag	UNP Q2N0S6
E	10	CYS	-	expression tag	UNP Q2N0S6
E	11	GLY	-	expression tag	UNP Q2N0S6
E	12	ALA	-	expression tag	UNP Q2N0S6
E	13	VAL	-	expression tag	UNP Q2N0S6
E	14	PHE	-	expression tag	UNP Q2N0S6
E	15	VAL	-	expression tag	UNP Q2N0S6
E	16	SER	-	expression tag	UNP Q2N0S6
E	17	PRO	-	expression tag	UNP Q2N0S6
E	18	SER	-	expression tag	UNP Q2N0S6
E	19	GLN	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	20	GLU	-	expression tag	UNP Q2N0S6
E	21	ILE	-	expression tag	UNP Q2N0S6
E	22	HIS	-	expression tag	UNP Q2N0S6
E	23	ALA	-	expression tag	UNP Q2N0S6
E	24	ARG	-	expression tag	UNP Q2N0S6
E	25	PHE	-	expression tag	UNP Q2N0S6
E	26	ARG	-	expression tag	UNP Q2N0S6
E	27	ARG	-	expression tag	UNP Q2N0S6
E	28	GLY	-	expression tag	UNP Q2N0S6
E	29	ALA	-	expression tag	UNP Q2N0S6
E	30	ARG	-	expression tag	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6
C	-4	MET	-	expression tag	UNP Q2N0S6
C	-3	ASP	-	expression tag	UNP Q2N0S6
C	-2	ALA	-	expression tag	UNP Q2N0S6
C	-1	MET	-	expression tag	UNP Q2N0S6
C	0	LYS	-	expression tag	UNP Q2N0S6
C	1	ARG	-	expression tag	UNP Q2N0S6
C	2	GLY	-	expression tag	UNP Q2N0S6
C	3	LEU	-	expression tag	UNP Q2N0S6
C	4	CYS	-	expression tag	UNP Q2N0S6
C	5	CYS	-	expression tag	UNP Q2N0S6
C	6	VAL	-	expression tag	UNP Q2N0S6
C	7	LEU	-	expression tag	UNP Q2N0S6
C	8	LEU	-	expression tag	UNP Q2N0S6
C	9	LEU	-	expression tag	UNP Q2N0S6
C	10	CYS	-	expression tag	UNP Q2N0S6
C	11	GLY	-	expression tag	UNP Q2N0S6
C	12	ALA	-	expression tag	UNP Q2N0S6
C	13	VAL	-	expression tag	UNP Q2N0S6
C	14	PHE	-	expression tag	UNP Q2N0S6
C	15	VAL	-	expression tag	UNP Q2N0S6
C	16	SER	-	expression tag	UNP Q2N0S6
C	17	PRO	-	expression tag	UNP Q2N0S6
C	18	SER	-	expression tag	UNP Q2N0S6
C	19	GLN	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLU	-	expression tag	UNP Q2N0S6
C	21	ILE	-	expression tag	UNP Q2N0S6
C	22	HIS	-	expression tag	UNP Q2N0S6
C	23	ALA	-	expression tag	UNP Q2N0S6
C	24	ARG	-	expression tag	UNP Q2N0S6
C	25	PHE	-	expression tag	UNP Q2N0S6
C	26	ARG	-	expression tag	UNP Q2N0S6
C	27	ARG	-	expression tag	UNP Q2N0S6
C	28	GLY	-	expression tag	UNP Q2N0S6
C	29	ALA	-	expression tag	UNP Q2N0S6
C	30	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	125	Total	C	N	O	S	0	0
			986	622	171	187	6		
2	D	124	Total	C	N	O	S	0	0
			982	620	170	186	6		
2	B	121	Total	C	N	O	S	0	0
			958	604	166	182	6		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	560	PRO	ILE	conflict	UNP A0A6H1VYE9
F	?	-	LEU	deletion	UNP A0A6H1VYE9
F	567	PRO	LYS	engineered mutation	UNP A0A6H1VYE9
F	568	GLY	LEU	engineered mutation	UNP A0A6H1VYE9
F	605	CYS	THR	conflict	UNP A0A6H1VYE9
F	665	GLY	-	expression tag	UNP A0A6H1VYE9
F	666	SER	-	expression tag	UNP A0A6H1VYE9
F	667	GLY	-	expression tag	UNP A0A6H1VYE9
F	668	SER	-	expression tag	UNP A0A6H1VYE9
F	669	GLY	-	expression tag	UNP A0A6H1VYE9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	670	GLY	-	expression tag	UNP A0A6H1VYE9
F	671	SER	-	expression tag	UNP A0A6H1VYE9
F	672	GLY	-	expression tag	UNP A0A6H1VYE9
F	673	HIS	-	expression tag	UNP A0A6H1VYE9
F	674	HIS	-	expression tag	UNP A0A6H1VYE9
F	675	HIS	-	expression tag	UNP A0A6H1VYE9
F	676	HIS	-	expression tag	UNP A0A6H1VYE9
F	677	HIS	-	expression tag	UNP A0A6H1VYE9
F	678	HIS	-	expression tag	UNP A0A6H1VYE9
F	679	HIS	-	expression tag	UNP A0A6H1VYE9
F	680	HIS	-	expression tag	UNP A0A6H1VYE9
D	560	PRO	ILE	conflict	UNP A0A6H1VYE9
D	?	-	LEU	deletion	UNP A0A6H1VYE9
D	567	PRO	LYS	engineered mutation	UNP A0A6H1VYE9
D	568	GLY	LEU	engineered mutation	UNP A0A6H1VYE9
D	605	CYS	THR	conflict	UNP A0A6H1VYE9
D	665	GLY	-	expression tag	UNP A0A6H1VYE9
D	666	SER	-	expression tag	UNP A0A6H1VYE9
D	667	GLY	-	expression tag	UNP A0A6H1VYE9
D	668	SER	-	expression tag	UNP A0A6H1VYE9
D	669	GLY	-	expression tag	UNP A0A6H1VYE9
D	670	GLY	-	expression tag	UNP A0A6H1VYE9
D	671	SER	-	expression tag	UNP A0A6H1VYE9
D	672	GLY	-	expression tag	UNP A0A6H1VYE9
D	673	HIS	-	expression tag	UNP A0A6H1VYE9
D	674	HIS	-	expression tag	UNP A0A6H1VYE9
D	675	HIS	-	expression tag	UNP A0A6H1VYE9
D	676	HIS	-	expression tag	UNP A0A6H1VYE9
D	677	HIS	-	expression tag	UNP A0A6H1VYE9
D	678	HIS	-	expression tag	UNP A0A6H1VYE9
D	679	HIS	-	expression tag	UNP A0A6H1VYE9
D	680	HIS	-	expression tag	UNP A0A6H1VYE9
B	560	PRO	ILE	conflict	UNP A0A6H1VYE9
B	?	-	LEU	deletion	UNP A0A6H1VYE9
B	567	PRO	LYS	engineered mutation	UNP A0A6H1VYE9
B	568	GLY	LEU	engineered mutation	UNP A0A6H1VYE9
B	605	CYS	THR	conflict	UNP A0A6H1VYE9
B	665	GLY	-	expression tag	UNP A0A6H1VYE9
B	666	SER	-	expression tag	UNP A0A6H1VYE9
B	667	GLY	-	expression tag	UNP A0A6H1VYE9
B	668	SER	-	expression tag	UNP A0A6H1VYE9
B	669	GLY	-	expression tag	UNP A0A6H1VYE9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	670	GLY	-	expression tag	UNP A0A6H1VYE9
B	671	SER	-	expression tag	UNP A0A6H1VYE9
B	672	GLY	-	expression tag	UNP A0A6H1VYE9
B	673	HIS	-	expression tag	UNP A0A6H1VYE9
B	674	HIS	-	expression tag	UNP A0A6H1VYE9
B	675	HIS	-	expression tag	UNP A0A6H1VYE9
B	676	HIS	-	expression tag	UNP A0A6H1VYE9
B	677	HIS	-	expression tag	UNP A0A6H1VYE9
B	678	HIS	-	expression tag	UNP A0A6H1VYE9
B	679	HIS	-	expression tag	UNP A0A6H1VYE9
B	680	HIS	-	expression tag	UNP A0A6H1VYE9

- Molecule 3 is a protein called 3BNC117 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	M	121	Total	C	N	O	S	0	0
			985	626	177	179	3		
3	P	121	Total	C	N	O	S	0	0
			985	626	177	179	3		

- Molecule 4 is a protein called 3BNC117 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
4	L	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
4	Q	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

- Molecule 5 is a protein called PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
5	N	131	Total	C	N	O	S	0	0
			1041	666	179	193	3		
5	R	131	Total	C	N	O	S	0	0
			1038	664	178	193	3		



- Molecule 6 is a protein called PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	106	Total	C	N	O	S	0	0
			811	507	140	162	2		
6	O	106	Total	C	N	O	S	0	0
			811	507	140	162	2		
6	S	105	Total	C	N	O	S	0	0
			805	504	139	160	2		

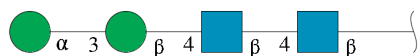
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	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	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	h	2	Total	C	N	O	0	0
			28	16	2	10		
7	j	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		

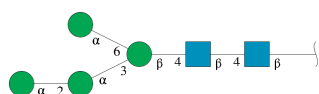
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	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.



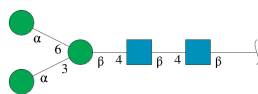
Mol	Chain	Residues	Atoms				AltConf	Trace
9	V	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

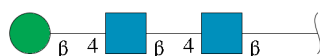
- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





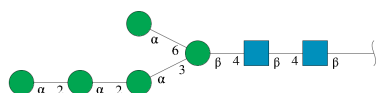
Mol	Chain	Residues	Atoms				AltConf	Trace
11	Z	5	Total	C	N	O	0	0
			61	34	2	25		
11	f	5	Total	C	N	O	0	0
			61	34	2	25		
11	i	5	Total	C	N	O	0	0
			61	34	2	25		
11	r	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 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
12	c	3	Total	C	N	O	0	0
			39	22	2	15		
12	d	3	Total	C	N	O	0	0
			39	22	2	15		
12	l	3	Total	C	N	O	0	0
			39	22	2	15		
12	p	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
13	e	7	Total	C	N	O	0	0
			83	46	2	35		
13	o	7	Total	C	N	O	0	0
			83	46	2	35		

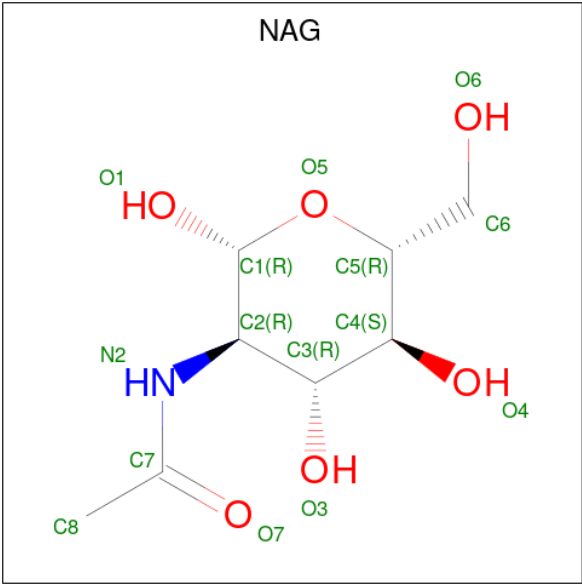
- Molecule 14 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	m	2	25	14	1	10	0	0

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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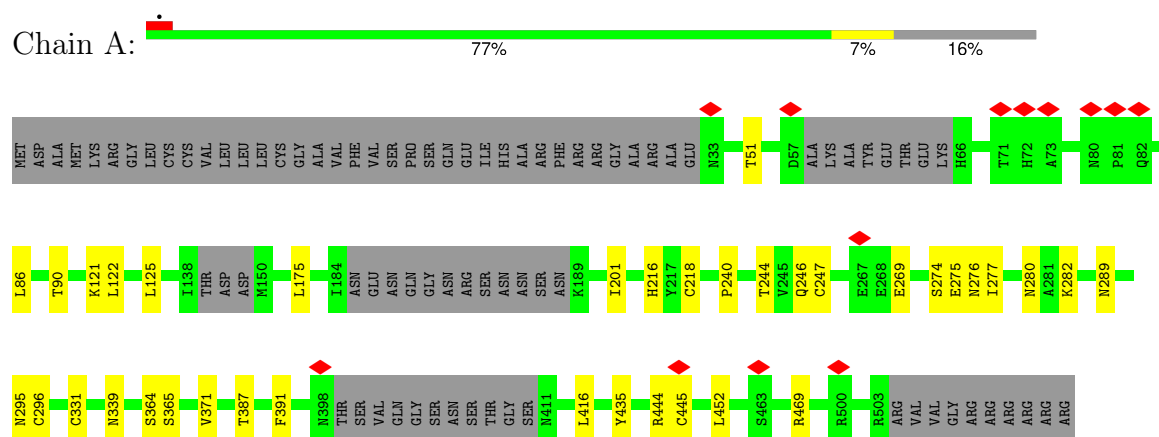
Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total 14	C 8	N 1	O 5	0
15	F	1	Total 14	C 8	N 1	O 5	0
15	D	1	Total 14	C 8	N 1	O 5	0
15	B	1	Total 14	C 8	N 1	O 5	0
15	E	1	Total 14	C 8	N 1	O 5	0
15	E	1	Total 14	C 8	N 1	O 5	0
15	E	1	Total 14	C 8	N 1	O 5	0
15	E	1	Total 14	C 8	N 1	O 5	0
15	E	1	Total 14	C 8	N 1	O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



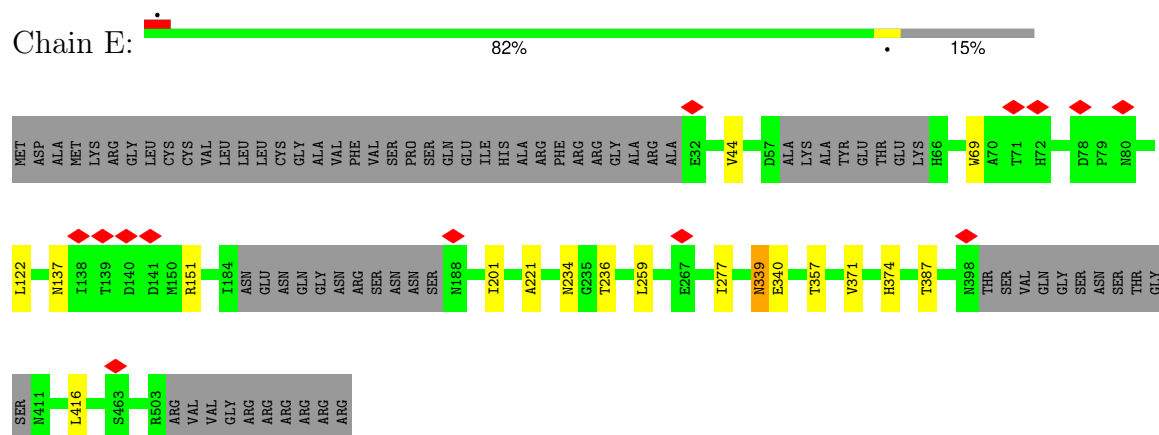
### 3 Residue-property plots

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

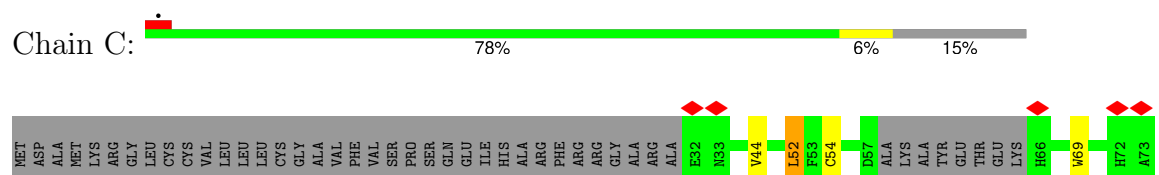
#### • Molecule 1: HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp120



#### • Molecule 1: HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp120



#### • Molecule 1: HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp120







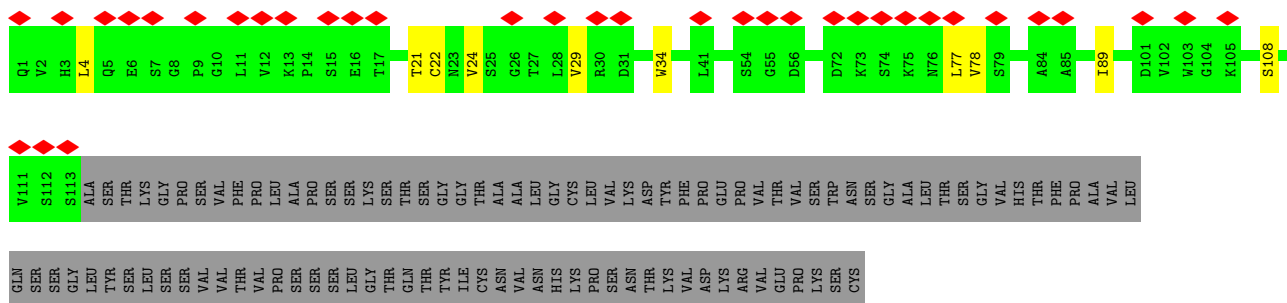




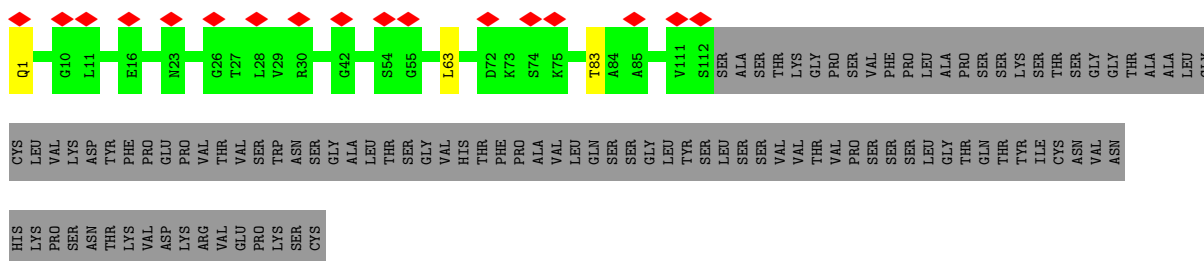


VAL  
THR  
LYS  
SER  
PHE  
ASN  
ARG  
GLY  
GLU  
CYS

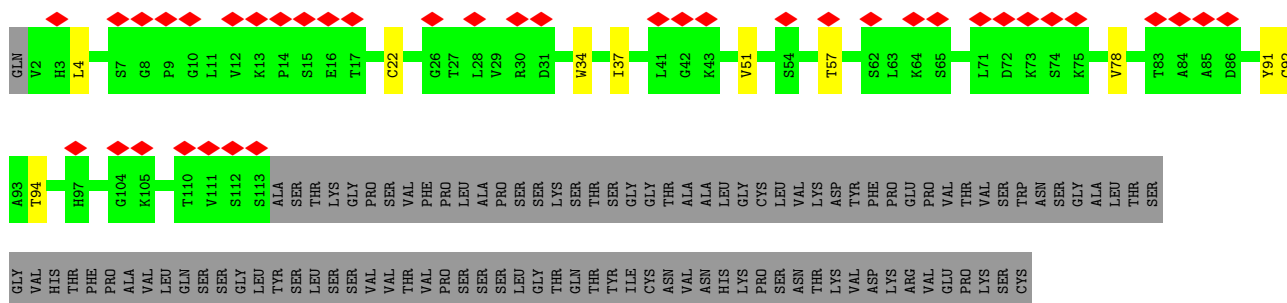
Chain J: 



Chain N:  7% 54% 44%

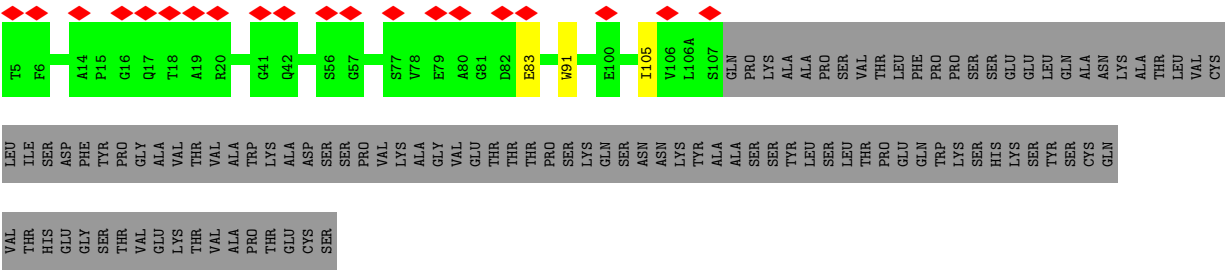


Chain B:  17% 51% 44%

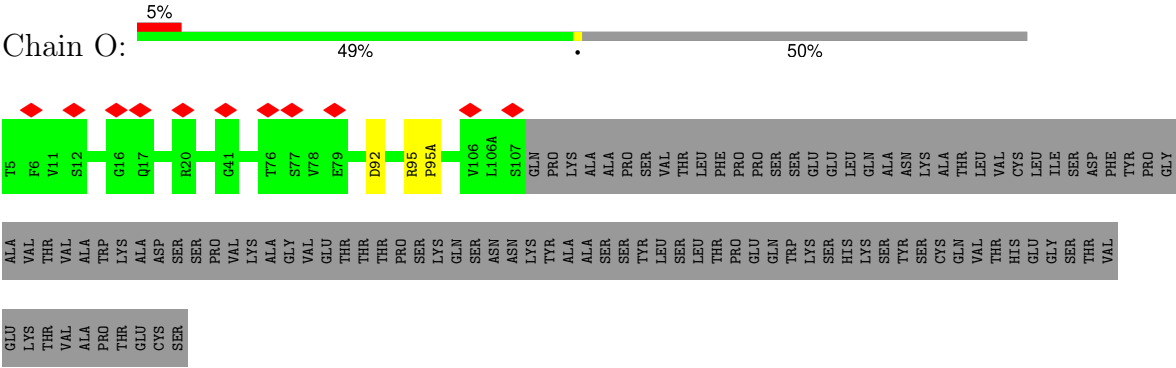


Chain K:  9% 49% 50%

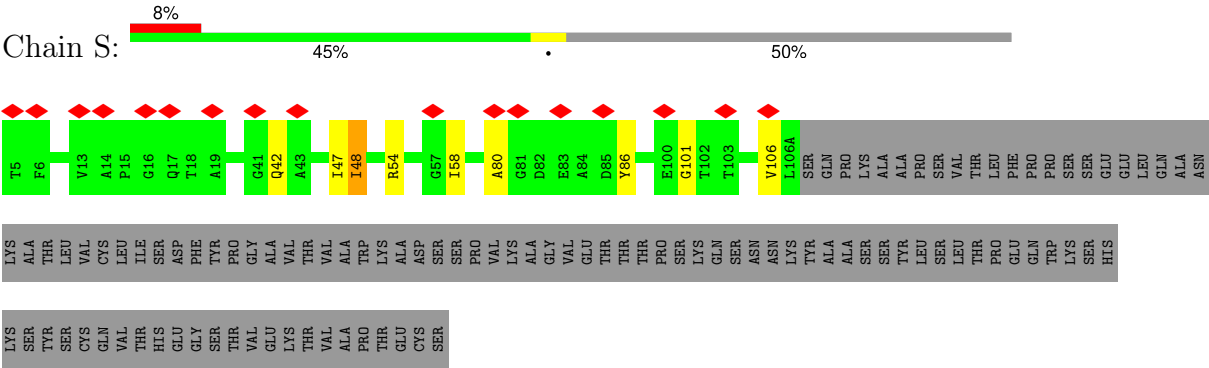




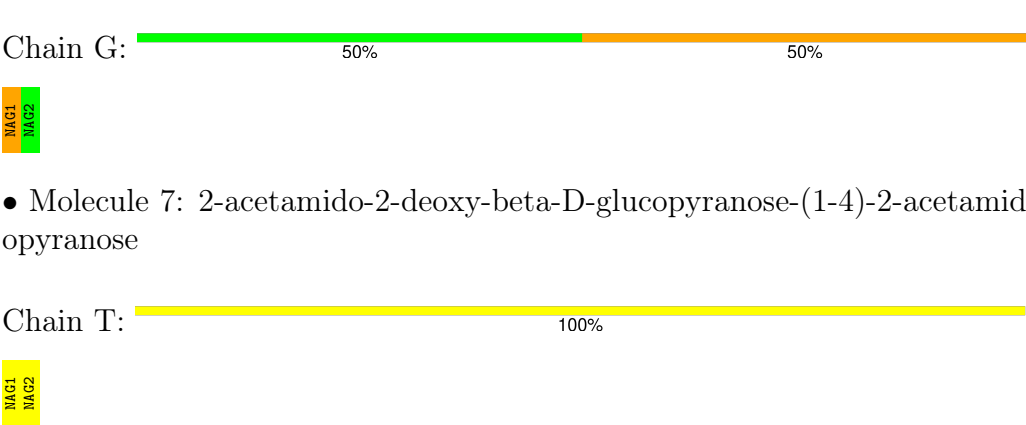
• Molecule 6: PGT122 Fab light chain



• 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

Chain W:  50% 50%

NAG1  
NAG2

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

Chain X:  100%

NAG1  
NAG2

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

Chain a:  100%

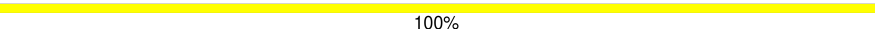
NAG1  
NAG2

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

Chain b:  50% 100%

◆  
NAG1  
NAG2

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

Chain g:  100%

NAG1  
NAG2

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

Chain h:  50% 100%

◆  
NAG1  
NAG2

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



Chain j:  100%

NAG1  
NAG2

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

Chain n:  100%

NAG1  
NAG2

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

Chain q:  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 U:  25% 100%


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 V:  100%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 10: 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:  100%

NAG1  
NAG2  
BMA3  
MAN4

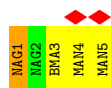
- Molecule 10: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%

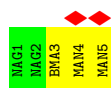




- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



- 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



- 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



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain d:  100%

MAG1  
MAG2  
BMA3

- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%

MAG1  
MAG2  
BMA3

- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  33% 33% 33%

MAG1  
MAG2  
BMA3

- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 13: alpha-D-mannopyranose-(1-2)-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 o:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 14: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  50% 50%

MAG1  
BMA2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	210222	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.796	Depositor
Minimum map value	-0.445	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	406.0, 406.0, 406.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	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, MAN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/3494	0.62	2/4742 (0.0%)
1	C	0.26	0/3511	0.61	1/4765 (0.0%)
1	E	0.25	0/3535	0.58	2/4800 (0.0%)
2	B	0.21	0/974	0.45	0/1318
2	D	0.23	0/1000	0.51	0/1356
2	F	0.19	0/1004	0.43	0/1361
3	H	0.21	0/1017	0.47	0/1386
3	M	0.23	0/1017	0.53	0/1386
3	P	0.23	0/1017	0.51	0/1386
4	I	0.22	0/800	0.53	0/1086
4	L	0.25	0/800	0.62	0/1086
4	Q	0.27	0/800	0.69	0/1086
5	J	0.23	0/1076	0.52	0/1465
5	N	0.22	0/1070	0.58	1/1457 (0.1%)
5	R	0.23	0/1067	0.58	0/1453
6	K	0.22	0/832	0.48	0/1138
6	O	0.21	0/832	0.50	0/1138
6	S	0.22	0/826	0.52	0/1130
All	All	0.24	0/24672	0.56	6/33539 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	339	ASN	CA-C-N	7.90	136.62	121.54
1	E	339	ASN	C-N-CA	7.90	136.62	121.54
1	C	501	CYS	CA-CB-SG	6.45	129.24	114.40
1	A	339	ASN	CA-C-N	5.15	131.37	121.54
1	A	339	ASN	C-N-CA	5.15	131.37	121.54
5	N	63	LEU	CA-CB-CG	5.03	133.90	116.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	304	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3423	0	3365	19	0
1	C	3440	0	3377	16	0
1	E	3463	0	3392	9	0
2	B	958	0	938	1	0
2	D	982	0	963	3	0
2	F	986	0	966	2	0
3	H	985	0	919	1	0
3	M	985	0	919	2	0
3	P	985	0	919	4	0
4	I	783	0	764	6	0
4	L	783	0	764	2	0
4	Q	783	0	764	0	0
5	J	1047	0	1026	5	0
5	N	1041	0	1021	0	0
5	R	1038	0	1015	5	0
6	K	811	0	766	2	0
6	O	811	0	766	3	0
6	S	805	0	761	4	0
7	G	28	0	25	1	0
7	T	28	0	25	0	0
7	W	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	g	28	0	25	0	0
7	h	28	0	25	0	0
7	j	28	0	25	1	0
7	n	28	0	25	0	0
7	q	28	0	25	0	0
8	U	50	0	43	0	0
9	V	72	0	61	0	0
10	Y	50	0	43	0	0
10	k	50	0	43	0	0
11	Z	61	0	52	1	0
11	f	61	0	52	0	0
11	i	61	0	52	0	0
11	r	61	0	52	0	0
12	c	39	0	34	0	0
12	d	39	0	34	0	0
12	l	39	0	34	0	0
12	p	39	0	34	1	0
13	e	83	0	70	0	0
13	o	83	0	70	0	0
14	m	25	0	22	0	0
15	A	126	0	117	0	0
15	B	14	0	13	0	0
15	C	112	0	104	0	0
15	D	14	0	13	0	0
15	E	112	0	104	1	0
15	F	14	0	13	0	0
All	All	25622	0	24740	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (76) 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:A:387:THR:HG22	1:A:416:LEU:HD13	1.78	0.66
1:E:387:THR:HG22	1:E:416:LEU:HD13	1.78	0.65
1:C:371:VAL:HG21	3:P:55:THR:HB	1.78	0.63
1:C:255:VAL:HG21	1:C:426:MET:HE1	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG22	1:A:240:PRO:HA	1.86	0.57
5:J:21:THR:HG22	5:J:77:LEU:HD12	1.85	0.57
1:A:274:SER:HB3	1:A:277:ILE:HD13	1.86	0.56
1:E:371:VAL:HG21	3:M:55:THR:HB	1.86	0.56
5:R:51:VAL:HG12	5:R:57:THR:HB	1.88	0.55
1:C:204:ALA:HB3	1:C:437:PRO:HD3	1.88	0.54
1:A:122:LEU:HB3	1:A:125:LEU:HD13	1.90	0.54
1:A:201:ILE:HD11	1:A:435:TYR:HB2	1.89	0.54
6:S:47:ILE:HG22	6:S:48:ILE:HG13	1.89	0.53
1:C:364:SER:HB2	1:C:470:PRO:HG2	1.90	0.53
2:F:629:LEU:HD23	1:E:44:VAL:HG23	1.91	0.52
1:C:156:ASN:HA	1:C:175:LEU:HD23	1.92	0.52
1:A:275:GLU:HB3	1:A:282:LYS:HD3	1.91	0.51
1:A:296:CYS:O	1:A:444:ARG:HA	2.10	0.51
5:R:34:TRP:HZ3	5:R:94:THR:HG22	1.75	0.51
1:A:371:VAL:HG21	3:H:55:THR:HB	1.92	0.51
2:F:547:GLY:H	1:E:221:ALA:HB2	1.76	0.51
2:D:617:ARG:HG2	2:D:622:ILE:HD11	1.93	0.51
4:I:65:ARG:HH12	4:I:67:TRP:HB2	1.74	0.51
1:C:121:LYS:HB3	1:C:202:THR:HG22	1.93	0.51
1:A:364:SER:HB3	7:W:1:NAG:H82	1.94	0.50
6:O:95:ARG:HD3	6:O:95(A):PRO:HD2	1.93	0.50
3:P:95:THR:HG22	3:P:120:THR:HA	1.92	0.49
1:A:175:LEU:HD11	7:G:1:NAG:H82	1.95	0.49
1:C:201:ILE:HD11	1:C:435:TYR:HB2	1.95	0.49
4:I:37:GLN:HB2	4:I:47:LEU:HD11	1.95	0.48
5:J:4:LEU:HD23	5:J:24:VAL:HG22	1.95	0.47
1:C:69:TRP:HA	1:C:111:LEU:HD13	1.96	0.47
1:A:269:GLU:HA	1:A:289:ASN:HD21	1.78	0.47
3:P:10:ALA:HB3	3:P:119:VAL:HG12	1.96	0.47
1:A:365:SER:HB3	1:A:469:ARG:HD3	1.98	0.46
3:M:37:TRP:HB3	3:M:45:LEU:HD22	1.97	0.46
5:R:37:ILE:HB	5:R:91:TYR:HB2	1.97	0.46
4:I:4:MET:HE3	4:I:99:VAL:HB	1.98	0.46
6:O:92:ASP:HB3	6:O:95:ARG:HB2	1.96	0.46
1:C:363:ASN:HD22	12:p:1:NAG:H83	1.80	0.45
5:J:29:VAL:HA	5:J:34:TRP:HZ2	1.82	0.45
5:R:4:LEU:HD23	5:R:92:CYS:HB3	1.99	0.45
1:E:122:LEU:HB2	1:E:201:ILE:HG13	1.97	0.45
1:A:218:CYS:HA	1:A:247:CYS:HB3	1.99	0.45
4:I:33:LEU:HA	4:I:90:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:89:ILE:HA	5:J:108:SER:HA	1.99	0.44
4:L:38:GLN:HB2	4:L:87:PHE:HE2	1.83	0.44
6:K:83:GLU:HG3	6:K:105:ILE:HA	1.98	0.44
6:K:91:TRP:HE3	11:Z:1:NAG:H83	1.82	0.44
1:C:120:VAL:HG13	1:C:203:GLN:HB3	2.00	0.43
2:D:546:SER:HB2	1:C:221:ALA:HB2	2.01	0.43
6:S:47:ILE:HD13	6:S:58:ILE:HD12	2.00	0.43
1:A:296:CYS:HA	1:A:331:CYS:HA	1.99	0.43
2:D:629:LEU:HA	1:C:44:VAL:HG23	2.01	0.43
1:E:151:ARG:HG2	15:E:602:NAG:H83	2.01	0.43
1:C:251:ILE:HG23	1:C:482:GLU:HG3	2.01	0.43
4:L:37:GLN:HB2	4:L:47:LEU:HD11	2.01	0.43
1:C:204:ALA:HB1	1:C:210:PHE:HZ	1.83	0.43
5:R:22:CYS:HB3	5:R:78:VAL:HG13	2.01	0.42
4:I:16:GLY:H	4:I:78:LEU:HB3	1.84	0.42
1:A:295:ASN:HA	1:A:445:CYS:O	2.20	0.41
1:A:391:PHE:HZ	1:A:452:LEU:HD22	1.85	0.41
5:J:22:CYS:HB3	5:J:78:VAL:HG13	2.01	0.41
1:A:86:LEU:HD21	1:A:244:THR:HG22	2.01	0.41
1:A:121:LYS:HB3	1:A:121:LYS:HE3	1.85	0.41
3:P:67:ARG:HD2	3:P:89:ALA:HB3	2.03	0.41
1:C:52:LEU:HD11	1:C:488:VAL:HG21	2.02	0.41
1:C:323(A):ILE:HD13	1:C:323(A):ILE:HA	1.96	0.41
6:S:86:TYR:O	6:S:101:GLY:HA3	2.20	0.41
1:E:259:LEU:HD12	1:E:374:HIS:CD2	2.56	0.41
1:E:137:ASN:HD22	6:O:95(A):PRO:HA	1.85	0.41
1:A:51:THR:HG21	2:B:574:LYS:HB3	2.02	0.41
4:I:33:LEU:HD13	4:I:71:TYR:CD1	2.55	0.40
7:j:1:NAG:H62	7:j:2:NAG:H82	2.02	0.40
6:S:80:ALA:HA	6:S:106:VAL:HG11	2.02	0.40
1:E:339:ASN:O	1:E:340:GLU:HG2	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	425/516 (82%)	394 (93%)	31 (7%)	0	100	100
1	C	427/516 (83%)	402 (94%)	25 (6%)	0	100	100
1	E	432/516 (84%)	411 (95%)	21 (5%)	0	100	100
2	B	117/168 (70%)	116 (99%)	1 (1%)	0	100	100
2	D	120/168 (71%)	119 (99%)	1 (1%)	0	100	100
2	F	121/168 (72%)	118 (98%)	3 (2%)	0	100	100
3	H	119/226 (53%)	115 (97%)	4 (3%)	0	100	100
3	M	119/226 (53%)	116 (98%)	3 (2%)	0	100	100
3	P	119/226 (53%)	114 (96%)	5 (4%)	0	100	100
4	I	96/206 (47%)	88 (92%)	8 (8%)	0	100	100
4	L	96/206 (47%)	88 (92%)	8 (8%)	0	100	100
4	Q	96/206 (47%)	90 (94%)	6 (6%)	0	100	100
5	J	130/235 (55%)	127 (98%)	3 (2%)	0	100	100
5	N	129/235 (55%)	127 (98%)	2 (2%)	0	100	100
5	R	129/235 (55%)	119 (92%)	10 (8%)	0	100	100
6	K	104/211 (49%)	99 (95%)	5 (5%)	0	100	100
6	O	104/211 (49%)	99 (95%)	5 (5%)	0	100	100
6	S	103/211 (49%)	97 (94%)	6 (6%)	0	100	100
All	All	2986/4686 (64%)	2839 (95%)	147 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/456 (85%)	385 (99%)	4 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	391/456 (86%)	384 (98%)	7 (2%)	54	77
1	E	394/456 (86%)	389 (99%)	5 (1%)	65	83
2	B	103/138 (75%)	103 (100%)	0	100	100
2	D	106/138 (77%)	106 (100%)	0	100	100
2	F	106/138 (77%)	106 (100%)	0	100	100
3	H	102/193 (53%)	102 (100%)	0	100	100
3	M	102/193 (53%)	102 (100%)	0	100	100
3	P	102/193 (53%)	102 (100%)	0	100	100
4	I	86/183 (47%)	86 (100%)	0	100	100
4	L	86/183 (47%)	85 (99%)	1 (1%)	67	85
4	Q	86/183 (47%)	86 (100%)	0	100	100
5	J	116/205 (57%)	116 (100%)	0	100	100
5	N	115/205 (56%)	113 (98%)	2 (2%)	56	78
5	R	115/205 (56%)	115 (100%)	0	100	100
6	K	89/180 (49%)	89 (100%)	0	100	100
6	O	89/180 (49%)	89 (100%)	0	100	100
6	S	88/180 (49%)	85 (97%)	3 (3%)	32	63
All	All	2665/4065 (66%)	2643 (99%)	22 (1%)	77	90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	HIS
1	A	246	GLN
1	A	276	ASN
1	A	280	ASN
1	E	69	TRP
1	E	234	ASN
1	E	236	THR
1	E	277	ILE
1	E	357	THR
1	C	52	LEU
1	C	54	CYS
1	C	88	ASN
1	C	158	SER
1	C	161	MET

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Mol	Chain	Res	Type
1	C	299	PRO
1	C	365	SER
4	L	39	ARG
5	N	1	GLN
5	N	83	THR
6	S	42	GLN
6	S	48	ILE
6	S	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	82	GLN
1	A	280	ASN
1	A	315	GLN
1	A	377	ASN
1	A	432	GLN
1	A	462	ASN
2	F	652	GLN
2	F	656	ASN
2	D	543	ASN
2	D	653	GLN
2	D	658	GLN
2	B	591	GLN
1	E	99	ASN
1	E	302	ASN
1	E	478	ASN
1	C	99	ASN
1	C	315	GLN
1	C	348	GLN
1	C	425	ASN
3	H	35	HIS
3	H	60	ASN
3	H	65	GLN
3	H	103	GLN
4	I	77	ASN
4	I	89	GLN
6	K	50	ASN
3	M	28	ASN
3	M	60	ASN
3	M	63	GLN

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Mol	Chain	Res	Type
3	M	103	GLN
3	M	118	GLN
4	L	3	GLN
4	L	37	GLN
5	N	23	ASN
6	O	50	ASN
3	P	65	GLN
4	Q	37	GLN
4	Q	69	GLN
4	Q	79	GLN
4	Q	89	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 ⓘ

88 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	G	1	1,7	14,14,15	0.71	0	17,19,21	1.07	2 (11%)
7	NAG	G	2	7	14,14,15	0.71	0	17,19,21	0.91	0
7	NAG	T	1	1,7	14,14,15	0.67	0	17,19,21	1.41	3 (17%)
7	NAG	T	2	7	14,14,15	0.74	0	17,19,21	2.80	6 (35%)
8	NAG	U	1	8,1	14,14,15	0.78	0	17,19,21	1.09	1 (5%)
8	NAG	U	2	8	14,14,15	0.83	0	17,19,21	3.45	6 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BMA	U	3	8	11,11,12	0.77	0	15,15,17	2.65	6 (40%)
8	MAN	U	4	8	11,11,12	0.59	0	15,15,17	1.77	1 (6%)
9	NAG	V	1	9,1	14,14,15	0.78	0	17,19,21	1.08	2 (11%)
9	NAG	V	2	9	14,14,15	0.80	0	17,19,21	1.39	3 (17%)
9	BMA	V	3	9	11,11,12	0.98	0	15,15,17	2.39	5 (33%)
9	MAN	V	4	9	11,11,12	0.58	0	15,15,17	1.94	1 (6%)
9	MAN	V	5	9	11,11,12	0.65	0	15,15,17	1.64	1 (6%)
9	MAN	V	6	9	11,11,12	0.64	0	15,15,17	1.50	1 (6%)
7	NAG	W	1	1,7	14,14,15	0.97	0	17,19,21	2.11	6 (35%)
7	NAG	W	2	7	14,14,15	0.70	0	17,19,21	0.83	0
7	NAG	X	1	1,7	14,14,15	0.78	0	17,19,21	1.18	1 (5%)
7	NAG	X	2	7	14,14,15	0.81	0	17,19,21	3.44	4 (23%)
10	NAG	Y	1	1,10	14,14,15	0.83	0	17,19,21	1.25	2 (11%)
10	NAG	Y	2	10	14,14,15	0.72	0	17,19,21	1.31	2 (11%)
10	BMA	Y	3	10	11,11,12	0.85	0	15,15,17	3.50	5 (33%)
10	MAN	Y	4	10	11,11,12	0.73	0	15,15,17	1.30	1 (6%)
11	NAG	Z	1	11,1	14,14,15	0.78	0	17,19,21	1.14	1 (5%)
11	NAG	Z	2	11	14,14,15	0.71	0	17,19,21	0.87	0
11	BMA	Z	3	11	11,11,12	0.68	0	15,15,17	2.83	4 (26%)
11	MAN	Z	4	11	11,11,12	0.59	0	15,15,17	1.95	1 (6%)
11	MAN	Z	5	11	11,11,12	0.70	0	15,15,17	1.27	1 (6%)
7	NAG	a	1	1,7	14,14,15	0.73	0	17,19,21	1.11	1 (5%)
7	NAG	a	2	7	14,14,15	0.77	0	17,19,21	1.48	1 (5%)
7	NAG	b	1	1,7	14,14,15	0.75	0	17,19,21	1.59	2 (11%)
7	NAG	b	2	7	14,14,15	0.68	0	17,19,21	1.14	1 (5%)
12	NAG	c	1	1,12	14,14,15	0.72	0	17,19,21	1.37	2 (11%)
12	NAG	c	2	12	14,14,15	0.70	0	17,19,21	0.85	0
12	BMA	c	3	12	11,11,12	0.85	0	15,15,17	2.76	6 (40%)
12	NAG	d	1	1,12	14,14,15	0.80	0	17,19,21	1.50	4 (23%)
12	NAG	d	2	12	14,14,15	0.76	0	17,19,21	1.30	2 (11%)
12	BMA	d	3	12	11,11,12	0.98	1 (9%)	15,15,17	2.24	4 (26%)
13	NAG	e	1	1,13	14,14,15	0.77	0	17,19,21	0.86	1 (5%)
13	NAG	e	2	13	14,14,15	0.75	0	17,19,21	3.48	5 (29%)
13	BMA	e	3	13	11,11,12	1.02	0	15,15,17	2.22	4 (26%)
13	MAN	e	4	13	11,11,12	0.59	0	15,15,17	1.81	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	MAN	e	5	13	11,11,12	0.62	0	15,15,17	1.89	1 (6%)
13	MAN	e	6	13	11,11,12	0.74	0	15,15,17	1.30	1 (6%)
13	MAN	e	7	13	11,11,12	0.72	0	15,15,17	1.51	1 (6%)
11	NAG	f	1	11,1	14,14,15	0.73	0	17,19,21	0.96	0
11	NAG	f	2	11	14,14,15	0.73	0	17,19,21	0.97	0
11	BMA	f	3	11	11,11,12	0.82	0	15,15,17	2.50	6 (40%)
11	MAN	f	4	11	11,11,12	0.59	0	15,15,17	1.92	1 (6%)
11	MAN	f	5	11	11,11,12	0.69	0	15,15,17	1.42	1 (6%)
7	NAG	g	1	1,7	14,14,15	0.80	0	17,19,21	2.00	7 (41%)
7	NAG	g	2	7	14,14,15	0.85	1 (7%)	17,19,21	1.05	1 (5%)
7	NAG	h	1	1,7	14,14,15	0.96	0	17,19,21	2.28	5 (29%)
7	NAG	h	2	7	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
11	NAG	i	1	11,1	14,14,15	0.84	0	17,19,21	1.61	3 (17%)
11	NAG	i	2	11	14,14,15	0.77	0	17,19,21	1.32	1 (5%)
11	BMA	i	3	11	11,11,12	0.86	0	15,15,17	2.76	7 (46%)
11	MAN	i	4	11	11,11,12	0.58	0	15,15,17	1.99	1 (6%)
11	MAN	i	5	11	11,11,12	0.69	0	15,15,17	1.52	1 (6%)
7	NAG	j	1	1,7	14,14,15	0.74	0	17,19,21	1.62	1 (5%)
7	NAG	j	2	7	14,14,15	0.76	0	17,19,21	3.35	3 (17%)
10	NAG	k	1	1,10	14,14,15	0.75	0	17,19,21	1.14	1 (5%)
10	NAG	k	2	10	14,14,15	0.68	0	17,19,21	2.81	6 (35%)
10	BMA	k	3	10	11,11,12	1.04	1 (9%)	15,15,17	1.89	6 (40%)
10	MAN	k	4	10	11,11,12	0.63	0	15,15,17	1.65	1 (6%)
12	NAG	l	1	1,12	14,14,15	0.78	0	17,19,21	2.06	3 (17%)
12	NAG	l	2	12	14,14,15	0.75	0	17,19,21	2.04	3 (17%)
12	BMA	l	3	12	11,11,12	0.88	0	15,15,17	3.60	5 (33%)
14	NAG	m	1	1,14	14,14,15	0.72	0	17,19,21	0.96	0
14	BMA	m	2	14	11,11,12	0.85	0	15,15,17	2.78	5 (33%)
7	NAG	n	1	1,7	14,14,15	0.70	0	17,19,21	0.81	0
7	NAG	n	2	7	14,14,15	0.71	0	17,19,21	0.84	0
13	NAG	o	1	1,13	14,14,15	0.78	0	17,19,21	1.52	2 (11%)
13	NAG	o	2	13	14,14,15	0.78	0	17,19,21	3.44	5 (29%)
13	BMA	o	3	13	11,11,12	1.01	0	15,15,17	2.78	6 (40%)
13	MAN	o	4	13	11,11,12	0.58	0	15,15,17	1.99	1 (6%)
13	MAN	o	5	13	11,11,12	0.61	0	15,15,17	1.84	1 (6%)
13	MAN	o	6	13	11,11,12	0.75	0	15,15,17	1.19	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	MAN	o	7	13	11,11,12	0.60	0	15,15,17	2.05	1 (6%)
12	NAG	p	1	1,12	14,14,15	0.76	0	17,19,21	1.48	1 (5%)
12	NAG	p	2	12	14,14,15	0.75	0	17,19,21	0.97	0
12	BMA	p	3	12	11,11,12	0.82	0	15,15,17	2.99	6 (40%)
7	NAG	q	1	1,7	14,14,15	0.68	0	17,19,21	1.35	2 (11%)
7	NAG	q	2	7	14,14,15	0.72	0	17,19,21	1.13	1 (5%)
11	NAG	r	1	11,1	14,14,15	0.75	0	17,19,21	0.96	1 (5%)
11	NAG	r	2	11	14,14,15	0.73	0	17,19,21	1.56	2 (11%)
11	BMA	r	3	11	11,11,12	0.84	0	15,15,17	3.00	7 (46%)
11	MAN	r	4	11	11,11,12	0.68	0	15,15,17	1.34	1 (6%)
11	MAN	r	5	11	11,11,12	0.59	0	15,15,17	1.77	1 (6%)

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	G	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	1/6/23/26	0/1/1/1
7	NAG	T	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
8	NAG	U	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	U	2	8	-	4/6/23/26	0/1/1/1
8	BMA	U	3	8	-	0/2/19/22	0/1/1/1
8	MAN	U	4	8	-	0/2/19/22	0/1/1/1
9	NAG	V	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	0/6/23/26	0/1/1/1
9	BMA	V	3	9	-	0/2/19/22	0/1/1/1
9	MAN	V	4	9	-	0/2/19/22	0/1/1/1
9	MAN	V	5	9	-	2/2/19/22	0/1/1/1
9	MAN	V	6	9	-	0/2/19/22	0/1/1/1
7	NAG	W	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	0/6/23/26	0/1/1/1
7	NAG	X	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	X	2	7	-	4/6/23/26	0/1/1/1
10	NAG	Y	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	2/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	j	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	j	2	7	-	4/6/23/26	0/1/1/1
10	NAG	k	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	k	2	10	-	3/6/23/26	0/1/1/1
10	BMA	k	3	10	-	2/2/19/22	0/1/1/1
10	MAN	k	4	10	-	2/2/19/22	0/1/1/1
12	NAG	l	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	l	2	12	-	2/6/23/26	0/1/1/1
12	BMA	l	3	12	-	0/2/19/22	0/1/1/1
14	NAG	m	1	1,14	-	0/6/23/26	0/1/1/1
14	BMA	m	2	14	-	0/2/19/22	0/1/1/1
7	NAG	n	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	n	2	7	-	0/6/23/26	0/1/1/1
13	NAG	o	1	1,13	-	2/6/23/26	0/1/1/1
13	NAG	o	2	13	-	4/6/23/26	0/1/1/1
13	BMA	o	3	13	-	0/2/19/22	0/1/1/1
13	MAN	o	4	13	-	2/2/19/22	0/1/1/1
13	MAN	o	5	13	-	2/2/19/22	0/1/1/1
13	MAN	o	6	13	-	0/2/19/22	0/1/1/1
13	MAN	o	7	13	-	2/2/19/22	1/1/1/1
12	NAG	p	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	p	2	12	-	0/6/23/26	0/1/1/1
12	BMA	p	3	12	-	0/2/19/22	0/1/1/1
7	NAG	q	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	q	2	7	-	2/6/23/26	0/1/1/1
11	NAG	r	1	11,1	-	0/6/23/26	0/1/1/1
11	NAG	r	2	11	-	0/6/23/26	0/1/1/1
11	BMA	r	3	11	-	1/2/19/22	0/1/1/1
11	MAN	r	4	11	-	0/2/19/22	0/1/1/1
11	MAN	r	5	11	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	2	NAG	C1-C2	2.31	1.55	1.52
12	d	3	BMA	C2-C3	2.27	1.56	1.52
10	k	3	BMA	C2-C3	2.26	1.55	1.52



All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	j	2	NAG	C2-N2-C7	12.37	139.48	122.90
7	X	2	NAG	C2-N2-C7	12.37	139.47	122.90
13	e	2	NAG	C2-N2-C7	12.29	139.37	122.90
13	o	2	NAG	C2-N2-C7	12.14	139.18	122.90
8	U	2	NAG	C2-N2-C7	11.93	138.89	122.90
12	l	3	BMA	C1-O5-C5	11.22	127.22	112.19
10	Y	3	BMA	C1-O5-C5	10.82	126.68	112.19
7	T	2	NAG	C2-N2-C7	9.58	135.73	122.90
11	Z	3	BMA	C1-O5-C5	9.35	124.72	112.19
12	p	3	BMA	C1-O5-C5	9.12	124.41	112.19
14	m	2	BMA	C1-O5-C5	8.87	124.08	112.19
11	r	3	BMA	C1-O5-C5	8.80	123.97	112.19
13	o	3	BMA	C1-O5-C5	8.27	123.27	112.19
12	c	3	BMA	C1-O5-C5	8.02	122.93	112.19
8	U	3	BMA	C1-O5-C5	7.76	122.59	112.19
11	i	3	BMA	C1-O5-C5	7.65	122.43	112.19
13	o	7	MAN	C1-O5-C5	7.33	122.02	112.19
11	f	3	BMA	C1-O5-C5	7.13	121.75	112.19
10	k	2	NAG	C1-O5-C5	7.13	121.74	112.19
11	i	4	MAN	C1-O5-C5	7.13	121.74	112.19
11	Z	4	MAN	C1-O5-C5	7.02	121.60	112.19
13	o	4	MAN	C1-O5-C5	6.96	121.52	112.19
9	V	4	MAN	C1-O5-C5	6.88	121.41	112.19
11	f	4	MAN	C1-O5-C5	6.80	121.30	112.19
9	V	3	BMA	C1-O5-C5	6.73	121.20	112.19
13	e	5	MAN	C1-O5-C5	6.63	121.07	112.19
12	l	1	NAG	C2-N2-C7	6.55	131.67	122.90
13	o	5	MAN	C1-O5-C5	6.31	120.64	112.19
8	U	4	MAN	C1-O5-C5	6.26	120.58	112.19
12	d	3	BMA	C1-O5-C5	6.23	120.53	112.19
11	r	5	MAN	C1-O5-C5	6.20	120.50	112.19
13	e	4	MAN	C1-O5-C5	6.14	120.42	112.19
13	e	3	BMA	C1-O5-C5	5.97	120.19	112.19
12	l	2	NAG	C2-N2-C7	5.65	130.47	122.90
10	k	4	MAN	C1-O5-C5	5.43	119.47	112.19
12	l	3	BMA	C1-C2-C3	5.41	117.52	109.64
9	V	5	MAN	C1-O5-C5	5.38	119.39	112.19
7	b	1	NAG	C2-N2-C7	5.23	129.91	122.90
7	j	1	NAG	C2-N2-C7	5.17	129.83	122.90
9	V	6	MAN	C1-O5-C5	5.02	118.91	112.19
7	h	1	NAG	C2-N2-C7	4.98	129.57	122.90
13	o	1	NAG	C2-N2-C7	4.96	129.55	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	k	2	NAG	C4-C3-C2	4.91	118.22	111.02
11	i	5	MAN	C1-O5-C5	4.88	118.72	112.19
7	W	1	NAG	C1-O5-C5	-4.84	105.70	112.19
7	a	2	NAG	C2-N2-C7	4.82	129.36	122.90
11	i	1	NAG	C2-N2-C7	4.82	129.36	122.90
10	Y	3	BMA	C1-C2-C3	4.81	116.66	109.64
8	U	2	NAG	C8-C7-N2	4.72	123.95	116.12
7	W	1	NAG	O5-C1-C2	-4.64	104.12	111.29
7	h	1	NAG	O5-C1-C2	-4.57	104.23	111.29
11	r	3	BMA	C1-C2-C3	-4.49	103.11	109.64
12	p	1	NAG	C2-N2-C7	4.48	128.91	122.90
13	e	7	MAN	C1-O5-C5	4.44	118.14	112.19
7	X	2	NAG	C8-C7-N2	4.43	123.46	116.12
11	f	5	MAN	C1-O5-C5	4.36	118.03	112.19
13	o	2	NAG	C8-C7-N2	4.26	123.19	116.12
7	j	2	NAG	C8-C7-N2	4.26	123.19	116.12
11	r	4	MAN	C1-O5-C5	4.23	117.86	112.19
10	k	2	NAG	O4-C4-C3	-4.11	100.68	110.38
13	e	2	NAG	C8-C7-N2	4.06	122.86	116.12
7	h	1	NAG	C1-O5-C5	-4.05	106.76	112.19
13	e	6	MAN	C1-O5-C5	4.02	117.58	112.19
10	k	3	BMA	C2-C3-C4	4.02	117.93	110.86
11	Z	5	MAN	C1-O5-C5	4.01	117.56	112.19
7	g	1	NAG	C2-N2-C7	3.98	128.23	122.90
10	k	1	NAG	C2-N2-C7	3.93	128.17	122.90
13	o	2	NAG	O5-C1-C2	-3.84	105.34	111.29
12	c	1	NAG	C2-N2-C7	3.83	128.03	122.90
12	c	3	BMA	C3-C4-C5	3.81	117.13	110.23
12	p	3	BMA	C3-C4-C5	3.79	117.11	110.23
11	i	2	NAG	C2-N2-C7	3.77	127.96	122.90
10	Y	3	BMA	C2-C3-C4	3.75	117.45	110.86
12	d	1	NAG	C2-N2-C7	3.72	127.88	122.90
12	c	3	BMA	C2-C3-C4	3.66	117.31	110.86
13	e	2	NAG	O5-C1-C2	-3.64	105.66	111.29
12	l	3	BMA	C2-C3-C4	3.60	117.19	110.86
7	g	1	NAG	O4-C4-C3	-3.59	101.91	110.38
7	q	1	NAG	C2-N2-C7	3.59	127.71	122.90
7	g	1	NAG	C1-O5-C5	3.58	116.98	112.19
13	o	3	BMA	C2-C3-C4	3.53	117.07	110.86
8	U	3	BMA	C3-C4-C5	3.53	116.63	110.23
11	r	2	NAG	O5-C1-C2	-3.52	105.84	111.29
10	k	2	NAG	C2-N2-C7	3.51	127.60	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	1	NAG	C2-N2-C7	3.50	127.59	122.90
10	Y	4	MAN	C1-O5-C5	3.48	116.85	112.19
12	p	3	BMA	C2-C3-C4	3.48	116.98	110.86
9	V	3	BMA	C2-C3-C4	3.48	116.98	110.86
7	T	2	NAG	O7-C7-N2	3.47	128.10	121.98
11	i	3	BMA	C2-C3-C4	3.44	116.91	110.86
11	i	3	BMA	C3-C4-C5	3.43	116.44	110.23
13	o	6	MAN	C1-O5-C5	3.40	116.74	112.19
12	d	3	BMA	C2-C3-C4	3.40	116.83	110.86
10	k	2	NAG	O5-C5-C6	-3.38	101.09	107.66
13	e	3	BMA	C2-C3-C4	3.34	116.73	110.86
7	q	2	NAG	C2-N2-C7	3.32	127.34	122.90
11	f	3	BMA	C3-C4-C5	3.32	116.24	110.23
7	b	2	NAG	C2-N2-C7	3.27	127.29	122.90
11	i	3	BMA	O3-C3-C2	-3.23	103.46	110.05
13	o	3	BMA	C3-C4-C5	3.23	116.08	110.23
9	V	2	NAG	C4-C3-C2	3.19	115.69	111.02
14	m	2	BMA	C2-C3-C4	3.17	116.44	110.86
14	m	2	BMA	C3-C4-C5	3.11	115.88	110.23
10	Y	3	BMA	C3-C4-C5	3.11	115.87	110.23
10	Y	1	NAG	O5-C1-C2	-3.06	106.56	111.29
10	k	2	NAG	C3-C4-C5	3.03	115.72	110.23
7	X	1	NAG	C1-O5-C5	2.99	116.19	112.19
13	e	2	NAG	C1-C2-N2	2.98	115.12	110.43
8	U	1	NAG	C1-O5-C5	2.98	116.17	112.19
10	k	3	BMA	C3-C4-C5	2.96	115.60	110.23
7	a	1	NAG	C2-N2-C7	2.95	126.86	122.90
7	W	1	NAG	C4-C3-C2	2.95	115.33	111.02
9	V	2	NAG	C2-N2-C7	2.94	126.84	122.90
7	g	2	NAG	O5-C1-C2	-2.92	106.77	111.29
8	U	2	NAG	O7-C7-C8	-2.90	116.89	122.05
13	e	3	BMA	O3-C3-C2	-2.88	104.17	110.05
11	f	3	BMA	C2-C3-C4	2.86	115.89	110.86
12	l	2	NAG	O7-C7-N2	2.80	126.92	121.98
7	g	1	NAG	C4-C3-C2	2.79	115.11	111.02
11	r	3	BMA	C3-C4-C5	2.78	115.27	110.23
7	q	1	NAG	C1-O5-C5	2.77	115.91	112.19
12	d	1	NAG	O3-C3-C2	-2.77	103.65	109.40
12	l	3	BMA	C3-C4-C5	2.76	115.24	110.23
9	V	3	BMA	O3-C3-C2	-2.75	104.44	110.05
7	X	2	NAG	C1-C2-N2	2.73	114.74	110.43
12	l	1	NAG	O7-C7-N2	2.73	126.81	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	2	NAG	O7-C7-C8	-2.69	117.26	122.05
12	l	2	NAG	O4-C4-C3	-2.69	104.04	110.38
8	U	3	BMA	O5-C5-C4	2.66	117.31	110.83
12	p	3	BMA	O5-C5-C4	2.64	117.25	110.83
13	o	3	BMA	O3-C3-C2	-2.64	104.67	110.05
11	i	3	BMA	O4-C4-C3	-2.63	104.18	110.38
8	U	2	NAG	O4-C4-C3	-2.59	104.28	110.38
11	r	2	NAG	O3-C3-C4	2.58	116.46	110.38
12	c	3	BMA	O5-C5-C4	2.57	117.08	110.83
8	U	2	NAG	C1-C2-N2	2.56	114.47	110.43
7	j	2	NAG	O7-C7-C8	-2.56	117.50	122.05
12	c	1	NAG	C1-O5-C5	2.54	115.59	112.19
8	U	3	BMA	O4-C4-C3	-2.54	104.39	110.38
11	i	1	NAG	C4-C3-C2	2.54	114.74	111.02
11	i	3	BMA	C1-C2-C3	2.54	113.34	109.64
10	k	3	BMA	O5-C5-C6	2.51	112.55	107.66
8	U	3	BMA	O3-C3-C2	-2.51	104.94	110.05
11	f	3	BMA	O3-C3-C2	-2.50	104.96	110.05
11	f	3	BMA	O4-C4-C3	-2.49	104.50	110.38
12	d	3	BMA	C3-C4-C5	2.49	114.75	110.23
11	r	3	BMA	C2-C3-C4	2.48	115.23	110.86
13	o	2	NAG	O7-C7-C8	-2.48	117.63	122.05
11	Z	3	BMA	O5-C5-C4	2.48	116.85	110.83
9	V	1	NAG	O5-C1-C2	-2.48	107.46	111.29
11	Z	1	NAG	C2-N2-C7	2.47	126.22	122.90
12	l	1	NAG	O5-C1-C2	-2.47	107.47	111.29
11	Z	3	BMA	O3-C3-C4	2.46	116.17	110.38
13	o	3	BMA	O4-C4-C3	-2.46	104.59	110.38
7	W	1	NAG	C1-C2-N2	2.45	114.29	110.43
10	Y	3	BMA	O4-C4-C3	-2.43	104.65	110.38
9	V	3	BMA	C3-C4-C5	2.41	114.60	110.23
10	k	3	BMA	O3-C3-C2	-2.40	105.16	110.05
8	U	3	BMA	C2-C3-C4	2.39	115.06	110.86
12	c	3	BMA	O4-C4-C3	-2.37	104.79	110.38
12	l	3	BMA	O4-C4-C3	-2.35	104.84	110.38
12	p	3	BMA	O4-C4-C3	-2.35	104.85	110.38
9	V	2	NAG	O3-C3-C2	-2.34	104.55	109.40
13	o	1	NAG	O3-C3-C2	-2.34	104.55	109.40
10	Y	1	NAG	O3-C3-C2	-2.33	104.56	109.40
13	e	2	NAG	O7-C7-C8	-2.31	117.93	122.05
11	f	3	BMA	O5-C5-C4	2.31	116.45	110.83
9	V	3	BMA	O4-C4-C3	-2.29	104.97	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Y	2	NAG	C1-O5-C5	2.28	115.25	112.19
11	r	3	BMA	O2-C2-C3	2.28	114.87	110.15
12	d	2	NAG	C1-O5-C5	2.27	115.23	112.19
10	k	3	BMA	O4-C4-C3	-2.25	105.07	110.38
13	o	2	NAG	C1-C2-N2	2.24	113.97	110.43
12	d	1	NAG	C1-O5-C5	-2.22	109.22	112.19
12	p	3	BMA	O3-C3-C2	-2.21	105.55	110.05
7	T	2	NAG	O5-C1-C2	-2.19	107.90	111.29
12	d	1	NAG	O3-C3-C4	2.19	115.54	110.38
12	c	3	BMA	O3-C3-C2	-2.19	105.59	110.05
11	r	3	BMA	O4-C4-C3	-2.18	105.23	110.38
7	h	1	NAG	C3-C4-C5	2.17	114.17	110.23
7	T	1	NAG	C1-O5-C5	2.17	115.10	112.19
7	g	1	NAG	O5-C5-C6	-2.17	103.44	107.66
7	W	1	NAG	C3-C4-C5	2.16	114.15	110.23
7	W	1	NAG	O4-C4-C3	-2.16	105.29	110.38
7	b	1	NAG	C1-O5-C5	2.16	115.08	112.19
11	r	3	BMA	O5-C5-C4	2.16	116.07	110.83
12	d	2	NAG	C3-C4-C5	-2.15	106.33	110.23
14	m	2	BMA	O3-C3-C2	-2.15	105.67	110.05
10	Y	2	NAG	C2-N2-C7	2.15	125.78	122.90
7	T	2	NAG	C4-C3-C2	2.15	114.16	111.02
7	g	1	NAG	O5-C1-C2	-2.14	107.98	111.29
7	h	2	NAG	C1-O5-C5	2.14	115.05	112.19
9	V	1	NAG	C1-O5-C5	2.14	115.05	112.19
8	U	2	NAG	C1-O5-C5	2.13	115.04	112.19
11	Z	3	BMA	O4-C4-C3	-2.12	105.37	110.38
14	m	2	BMA	O4-C4-C3	-2.12	105.38	110.38
13	e	3	BMA	O4-C4-C3	-2.11	105.39	110.38
7	T	2	NAG	C1-C2-N2	-2.10	107.12	110.43
7	T	1	NAG	C3-C4-C5	-2.07	106.47	110.23
13	e	1	NAG	O3-C3-C2	-2.07	105.09	109.40
11	r	1	NAG	O5-C1-C2	-2.07	108.08	111.29
12	d	3	BMA	O4-C4-C3	-2.04	105.56	110.38
7	G	1	NAG	C1-O5-C5	2.03	114.91	112.19
10	k	3	BMA	O2-C2-C1	2.03	113.87	109.22
7	T	2	NAG	C8-C7-N2	-2.02	112.76	116.12
7	G	1	NAG	O5-C1-C2	-2.02	108.17	111.29
11	i	3	BMA	O5-C5-C4	2.02	115.74	110.83
7	g	1	NAG	O4-C4-C5	2.02	114.29	109.32
11	i	1	NAG	O5-C1-C2	-2.01	108.18	111.29
13	o	3	BMA	O5-C5-C4	2.01	115.71	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	h	1	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	T	2	NAG	C3-C2-N2-C7
12	l	1	NAG	C1-C2-N2-C7
12	l	2	NAG	C1-C2-N2-C7
10	Y	4	MAN	C4-C5-C6-O6
13	e	6	MAN	O5-C5-C6-O6
13	o	5	MAN	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
11	Z	4	MAN	O5-C5-C6-O6
10	Y	4	MAN	O5-C5-C6-O6
10	k	4	MAN	O5-C5-C6-O6
10	Y	3	BMA	O5-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
13	e	6	MAN	C4-C5-C6-O6
13	o	7	MAN	C4-C5-C6-O6
12	d	3	BMA	O5-C5-C6-O6
11	Z	4	MAN	C4-C5-C6-O6
9	V	5	MAN	O5-C5-C6-O6
13	e	5	MAN	O5-C5-C6-O6
11	r	5	MAN	C4-C5-C6-O6
13	o	5	MAN	C4-C5-C6-O6
11	i	3	BMA	O5-C5-C6-O6
11	f	5	MAN	O5-C5-C6-O6
10	k	3	BMA	C4-C5-C6-O6
10	k	4	MAN	C4-C5-C6-O6
11	f	5	MAN	C4-C5-C6-O6
11	r	5	MAN	O5-C5-C6-O6
13	o	7	MAN	O5-C5-C6-O6
11	f	4	MAN	O5-C5-C6-O6
13	o	4	MAN	O5-C5-C6-O6
11	i	3	BMA	C4-C5-C6-O6
7	T	1	NAG	C8-C7-N2-C2
7	T	1	NAG	O7-C7-N2-C2
7	X	2	NAG	C8-C7-N2-C2
7	X	2	NAG	O7-C7-N2-C2
7	a	1	NAG	C8-C7-N2-C2
7	a	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	a	2	NAG	C8-C7-N2-C2
7	a	2	NAG	O7-C7-N2-C2
7	b	1	NAG	C8-C7-N2-C2
7	b	1	NAG	O7-C7-N2-C2
7	b	2	NAG	C8-C7-N2-C2
7	b	2	NAG	O7-C7-N2-C2
7	g	1	NAG	C8-C7-N2-C2
7	g	1	NAG	O7-C7-N2-C2
7	h	1	NAG	C8-C7-N2-C2
7	h	1	NAG	O7-C7-N2-C2
7	j	1	NAG	C8-C7-N2-C2
7	j	1	NAG	O7-C7-N2-C2
7	j	2	NAG	C8-C7-N2-C2
7	j	2	NAG	O7-C7-N2-C2
7	q	1	NAG	C8-C7-N2-C2
7	q	1	NAG	O7-C7-N2-C2
7	q	2	NAG	C8-C7-N2-C2
7	q	2	NAG	O7-C7-N2-C2
8	U	2	NAG	C8-C7-N2-C2
8	U	2	NAG	O7-C7-N2-C2
10	Y	1	NAG	C8-C7-N2-C2
10	Y	1	NAG	O7-C7-N2-C2
10	k	1	NAG	C8-C7-N2-C2
10	k	1	NAG	O7-C7-N2-C2
10	k	2	NAG	C8-C7-N2-C2
10	k	2	NAG	O7-C7-N2-C2
11	i	1	NAG	C8-C7-N2-C2
11	i	1	NAG	O7-C7-N2-C2
11	i	2	NAG	C8-C7-N2-C2
11	i	2	NAG	O7-C7-N2-C2
12	c	1	NAG	C8-C7-N2-C2
12	c	1	NAG	O7-C7-N2-C2
12	d	1	NAG	C8-C7-N2-C2
12	d	1	NAG	O7-C7-N2-C2
12	p	1	NAG	C8-C7-N2-C2
12	p	1	NAG	O7-C7-N2-C2
13	e	2	NAG	C8-C7-N2-C2
13	e	2	NAG	O7-C7-N2-C2
13	o	1	NAG	C8-C7-N2-C2
13	o	1	NAG	O7-C7-N2-C2
13	o	2	NAG	C8-C7-N2-C2
13	o	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
11	r	3	BMA	O5-C5-C6-O6
11	f	4	MAN	C4-C5-C6-O6
13	e	3	BMA	C4-C5-C6-O6
11	i	4	MAN	C4-C5-C6-O6
13	e	5	MAN	C4-C5-C6-O6
11	i	4	MAN	O5-C5-C6-O6
9	V	5	MAN	C4-C5-C6-O6
10	k	3	BMA	O5-C5-C6-O6
11	i	2	NAG	O5-C5-C6-O6
13	e	3	BMA	O5-C5-C6-O6
10	Y	3	BMA	C4-C5-C6-O6
12	d	1	NAG	O5-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
11	f	2	NAG	O5-C5-C6-O6
13	o	4	MAN	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
10	k	2	NAG	O5-C5-C6-O6
7	X	2	NAG	C1-C2-N2-C7
7	X	2	NAG	C3-C2-N2-C7
7	j	2	NAG	C3-C2-N2-C7
8	U	2	NAG	C3-C2-N2-C7
13	e	2	NAG	C3-C2-N2-C7
13	o	2	NAG	C3-C2-N2-C7
11	Z	5	MAN	O5-C5-C6-O6
7	G	1	NAG	C1-C2-N2-C7
7	j	2	NAG	C1-C2-N2-C7
8	U	2	NAG	C1-C2-N2-C7
13	e	2	NAG	C1-C2-N2-C7
13	o	2	NAG	C1-C2-N2-C7
12	l	1	NAG	C3-C2-N2-C7
12	l	2	NAG	C3-C2-N2-C7
12	d	3	BMA	C4-C5-C6-O6

All (2) ring outliers are listed below:

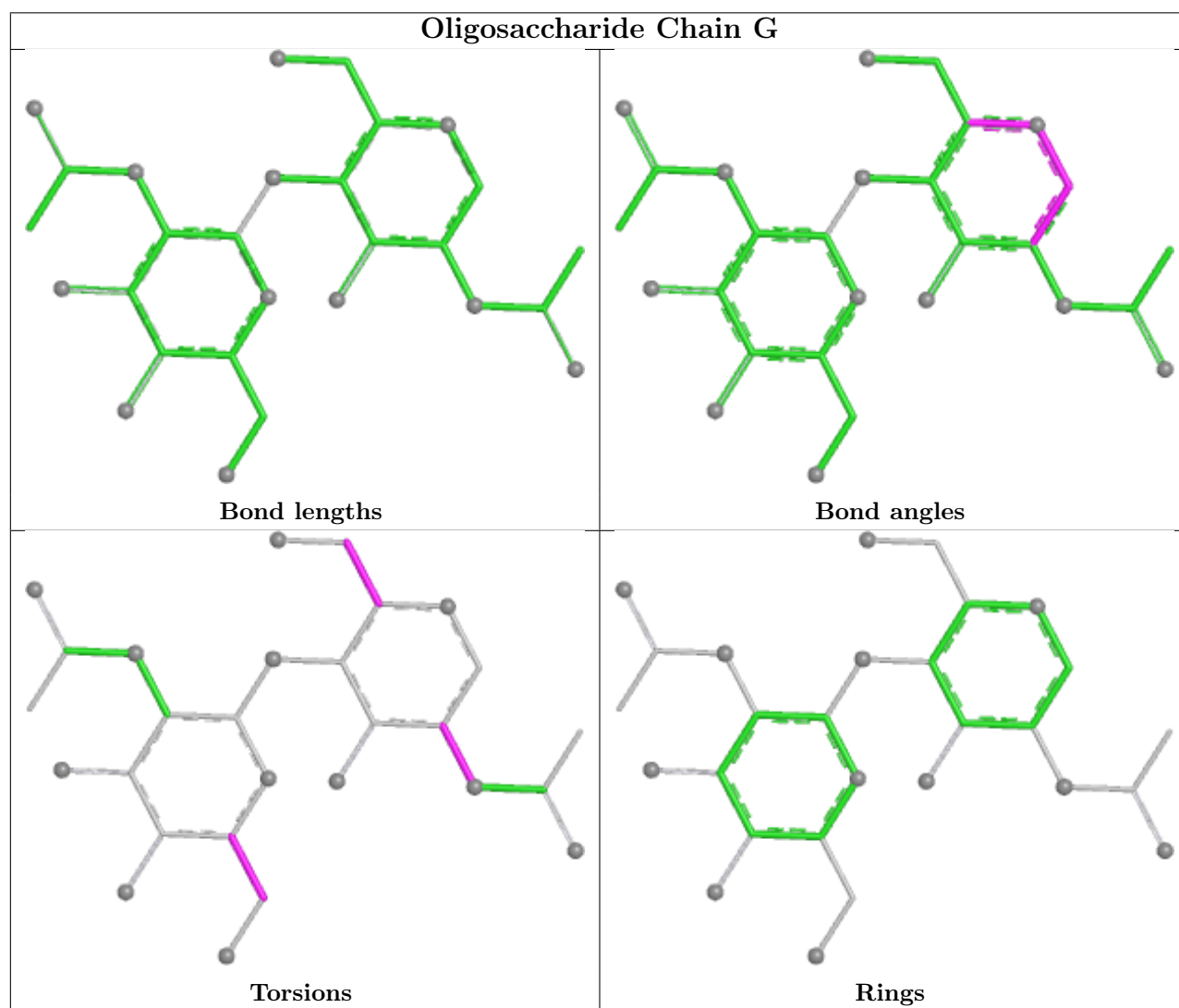
Mol	Chain	Res	Type	Atoms
11	i	5	MAN	C1-C2-C3-C4-C5-O5
13	o	7	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 5 short contacts:

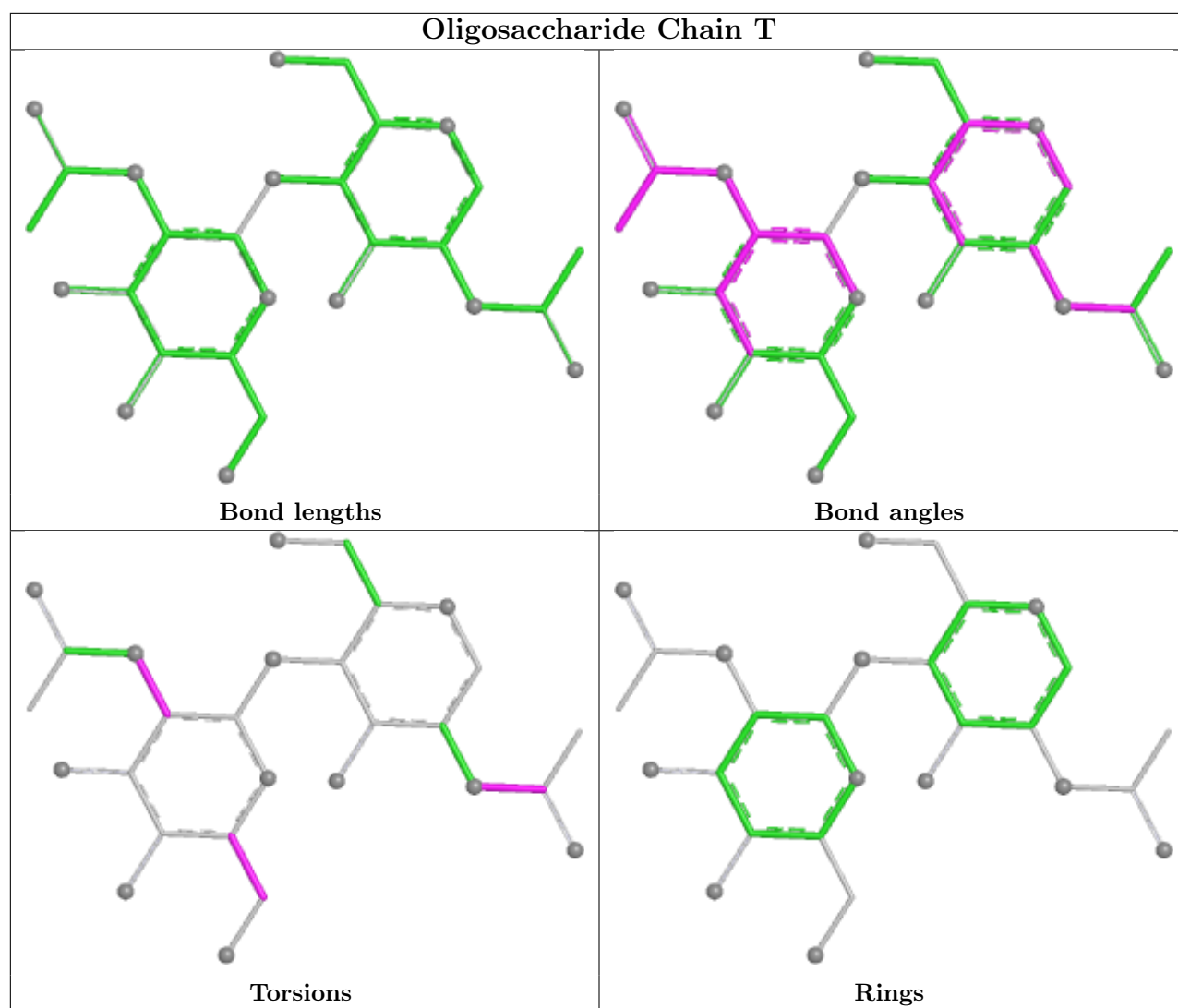


Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	j	1	NAG	1	0
11	Z	1	NAG	1	0
7	W	1	NAG	1	0
7	j	2	NAG	1	0
12	p	1	NAG	1	0
7	G	1	NAG	1	0

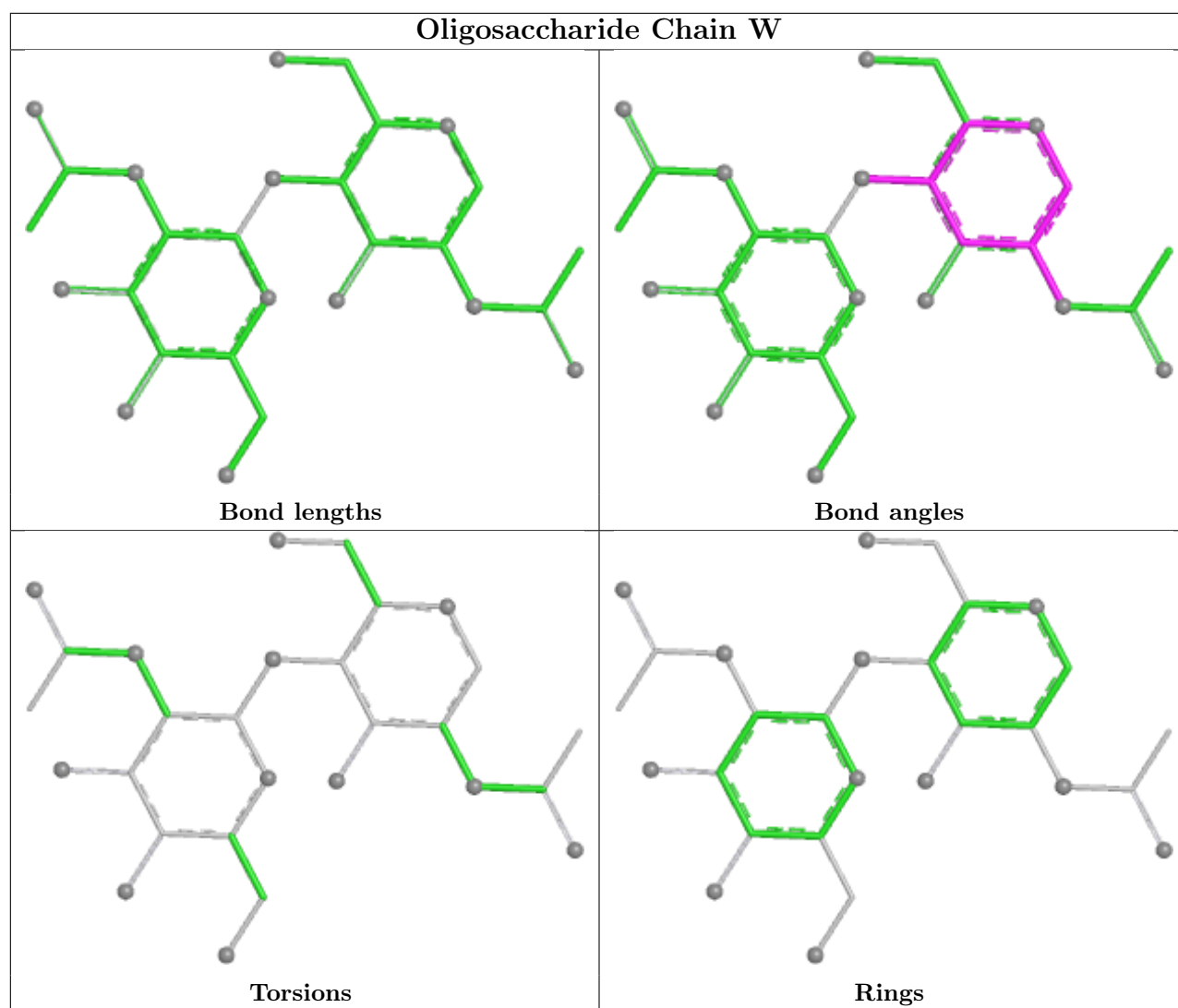
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



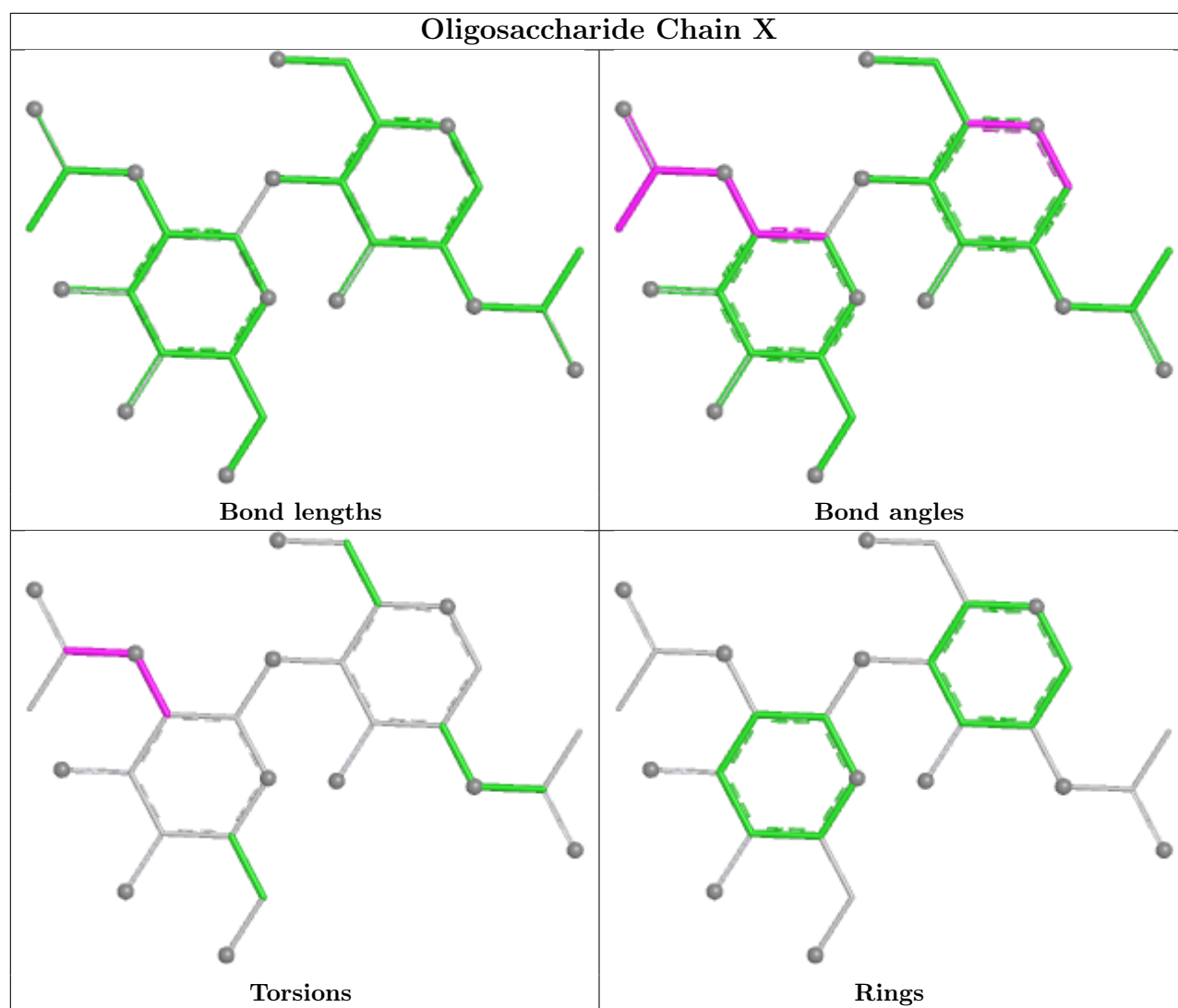




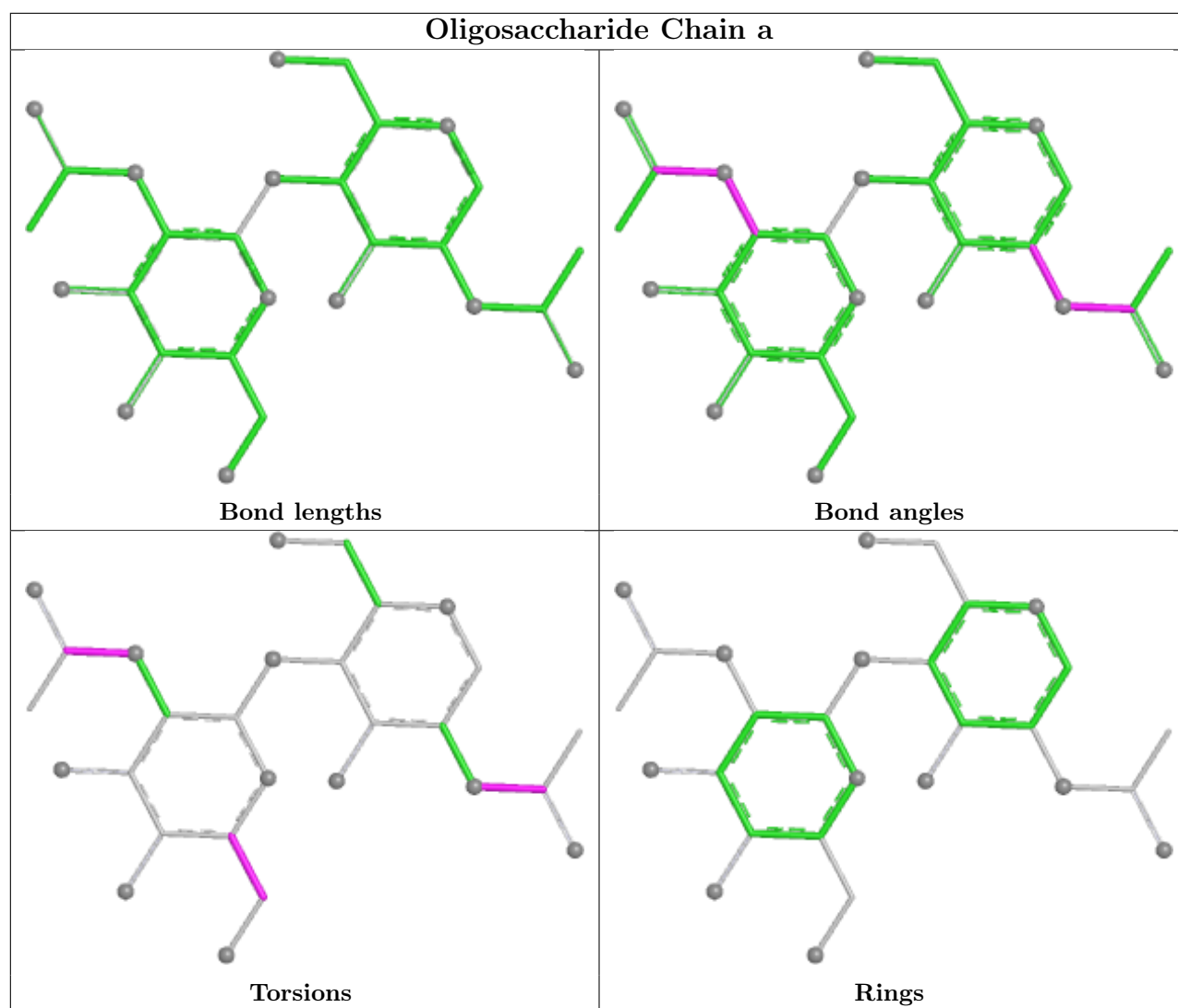




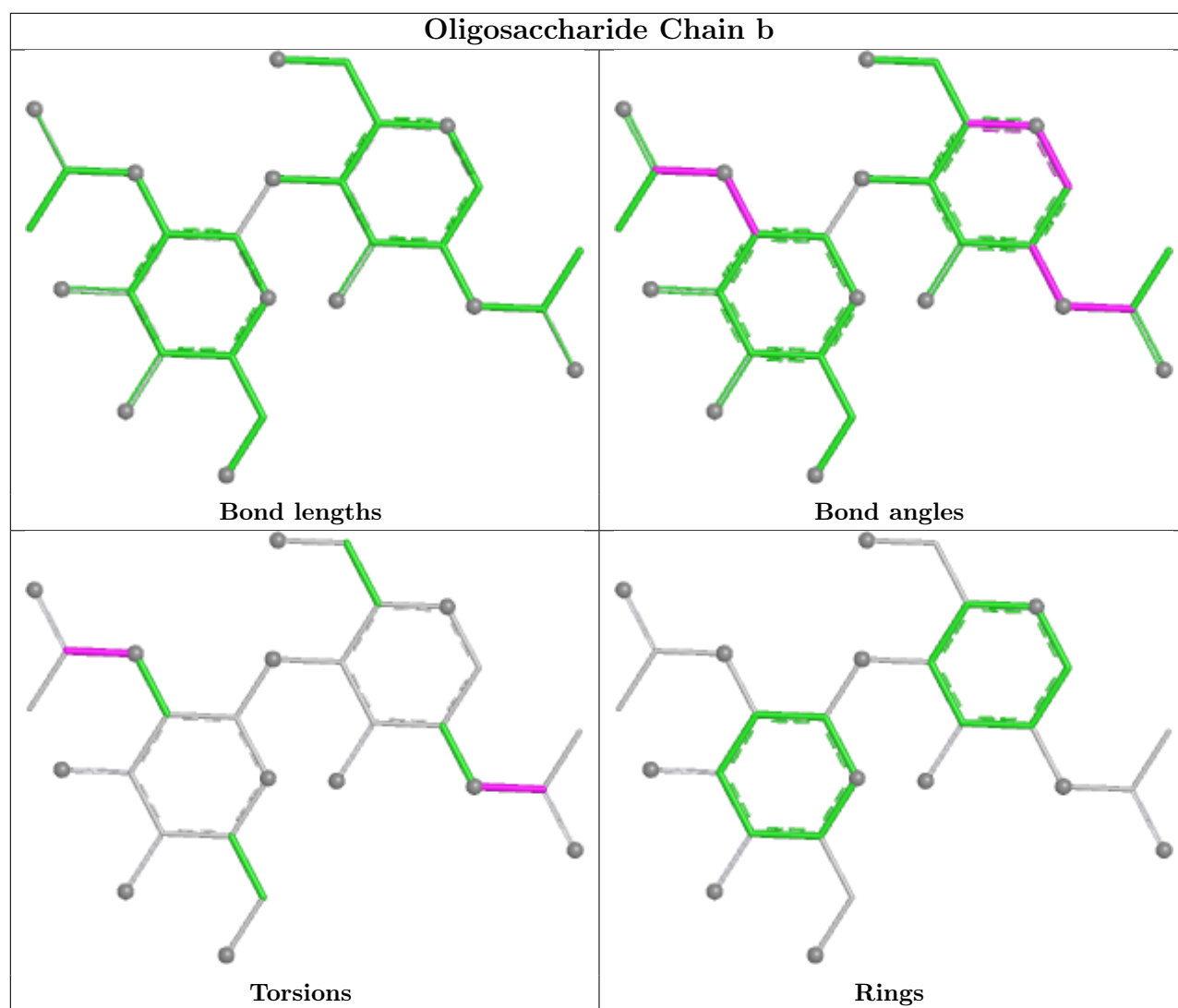




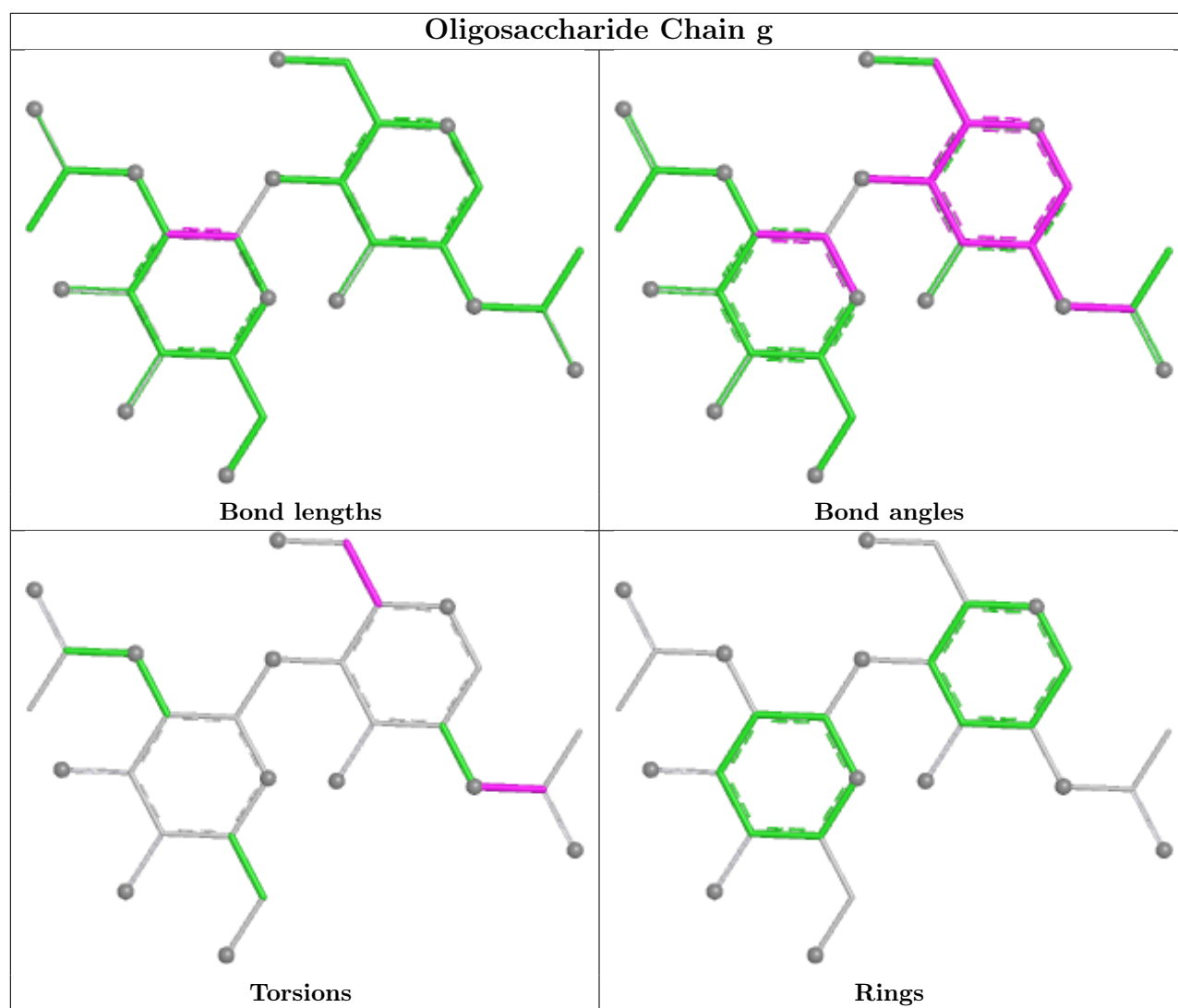




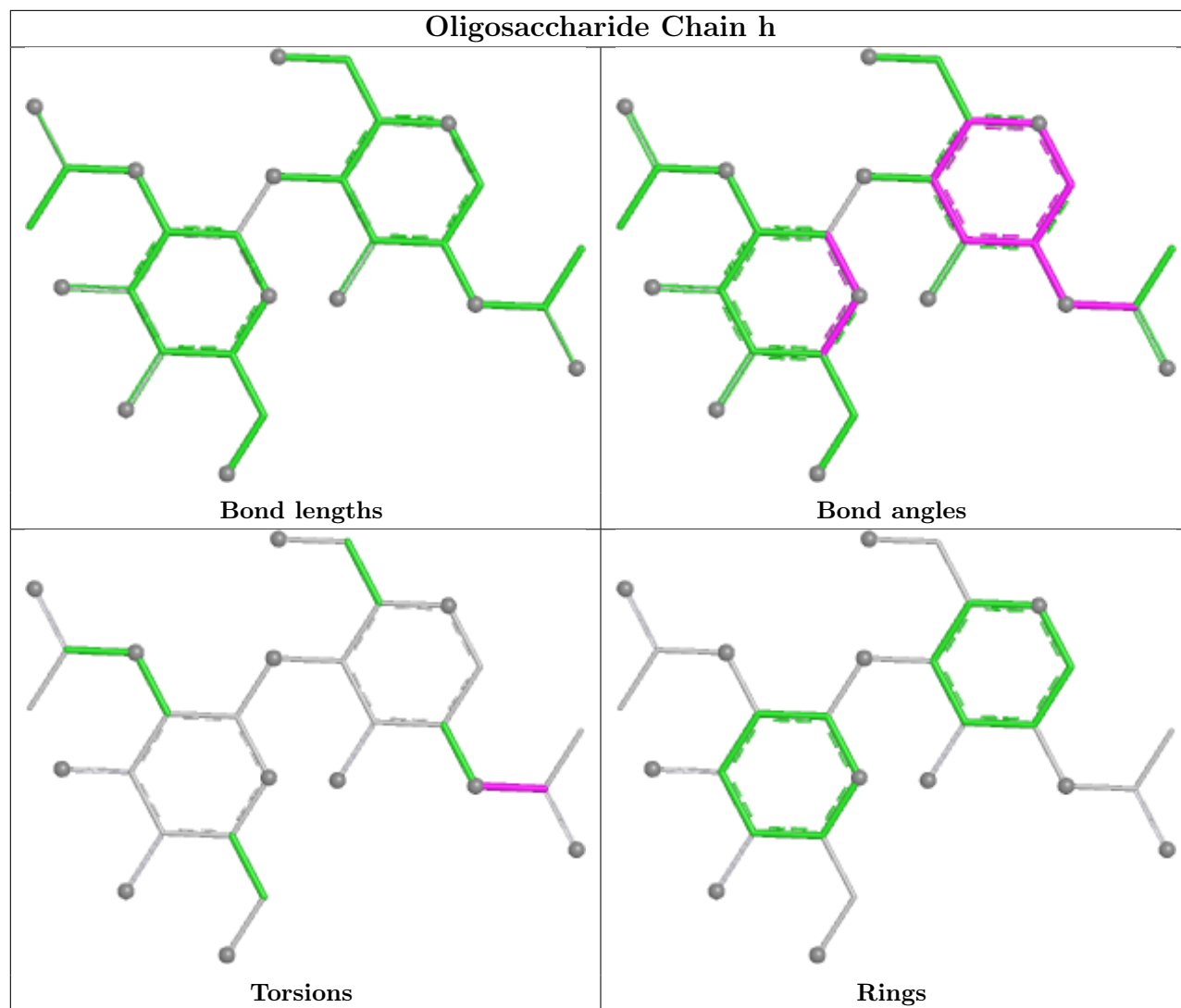




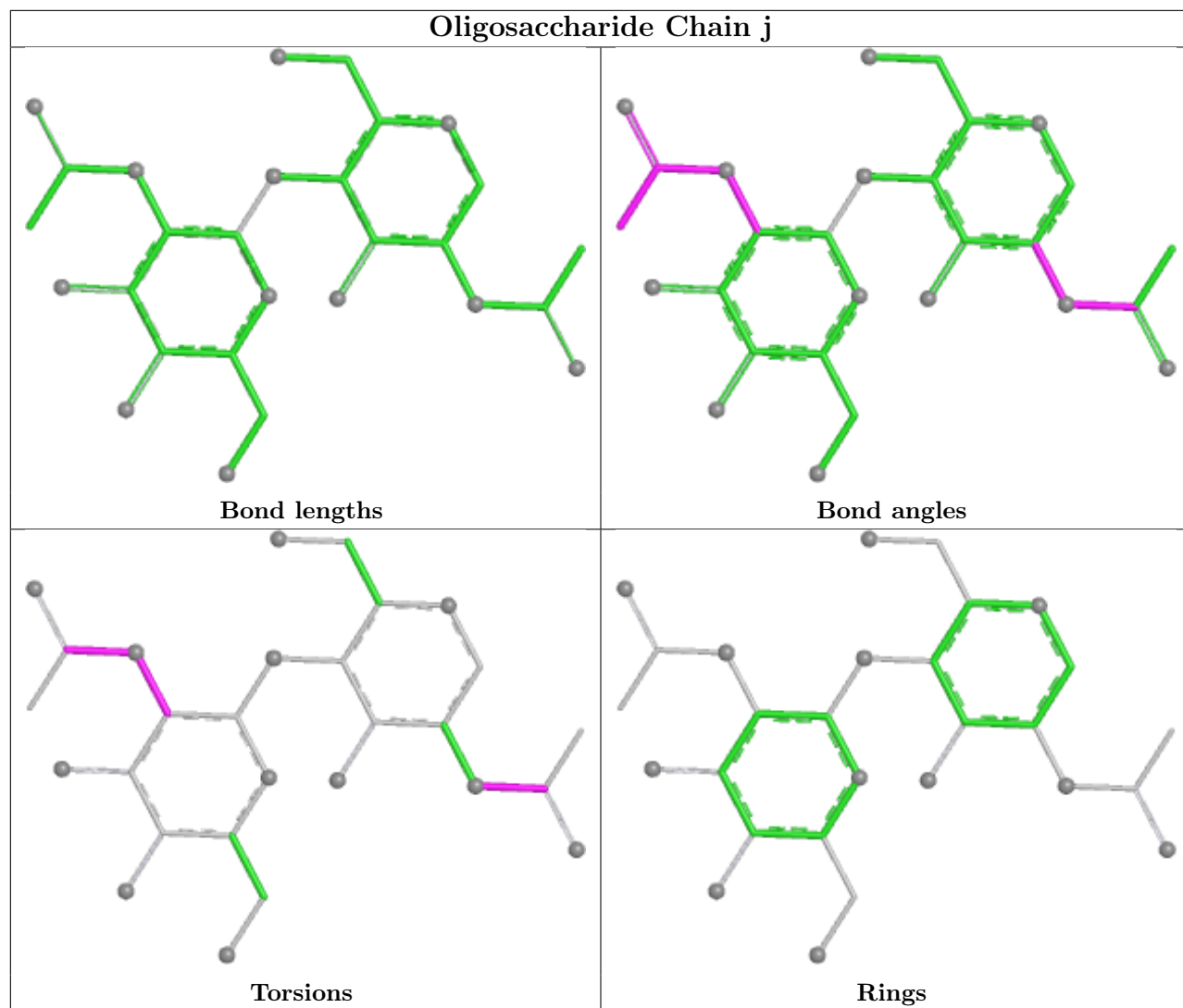




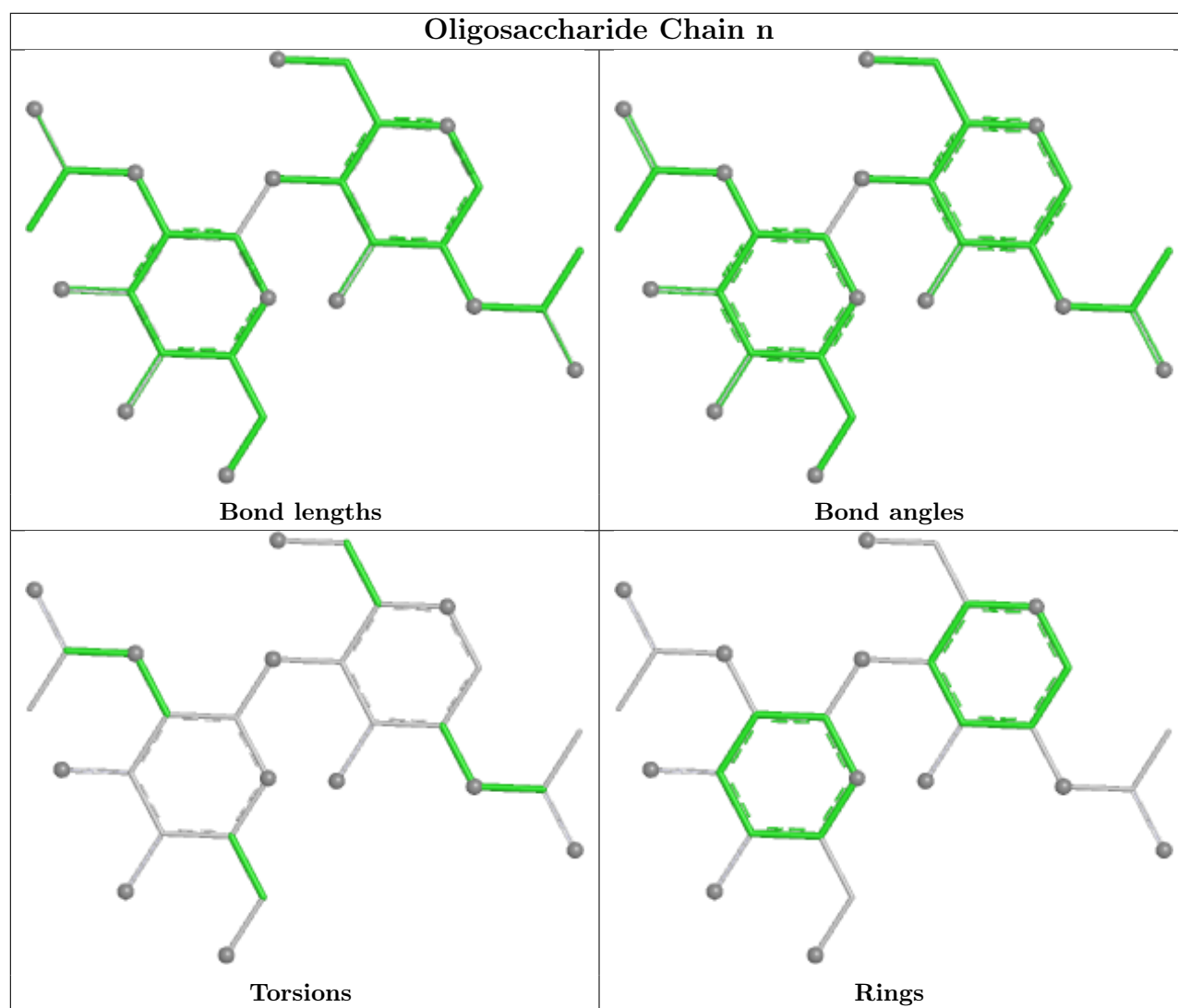




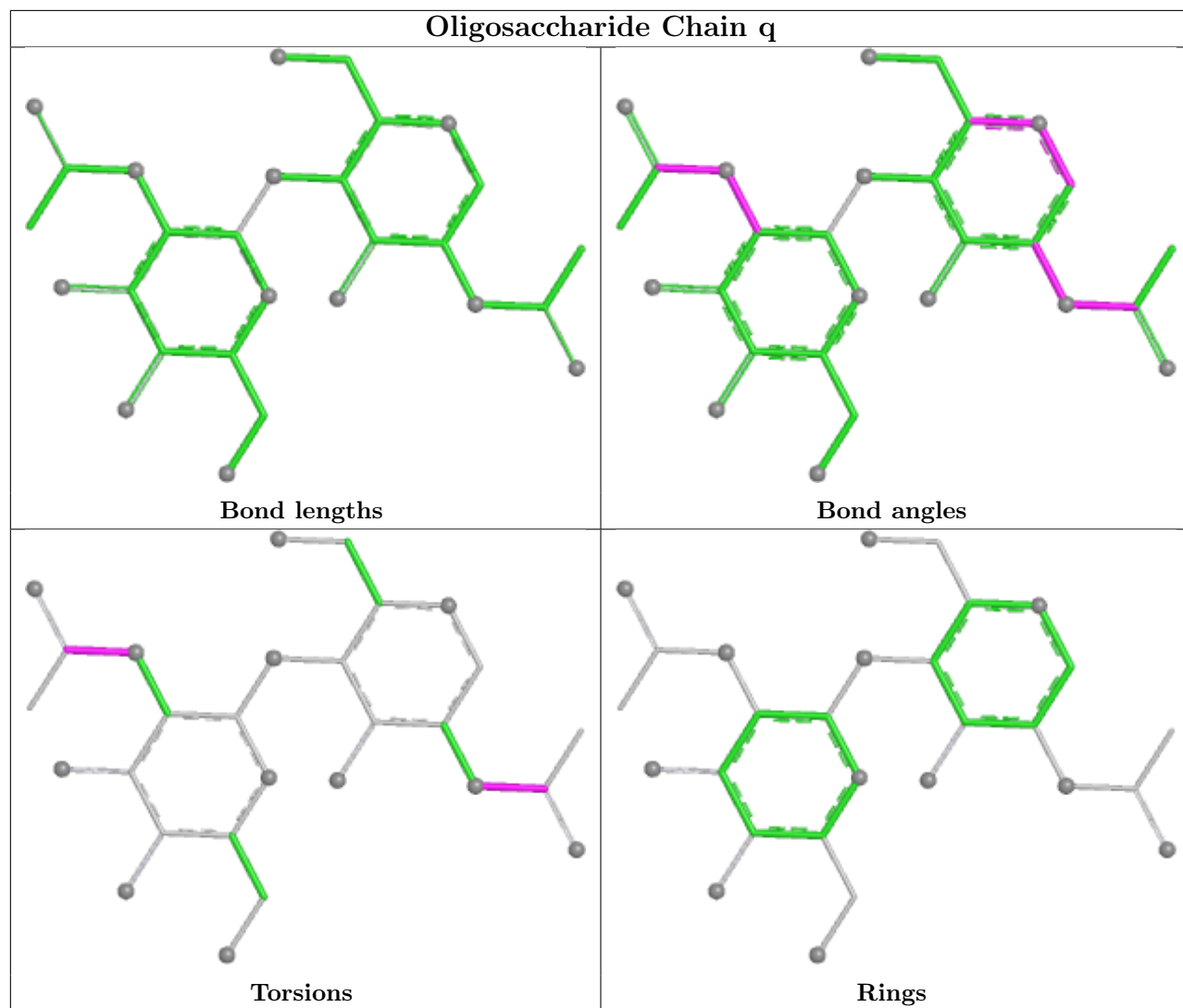




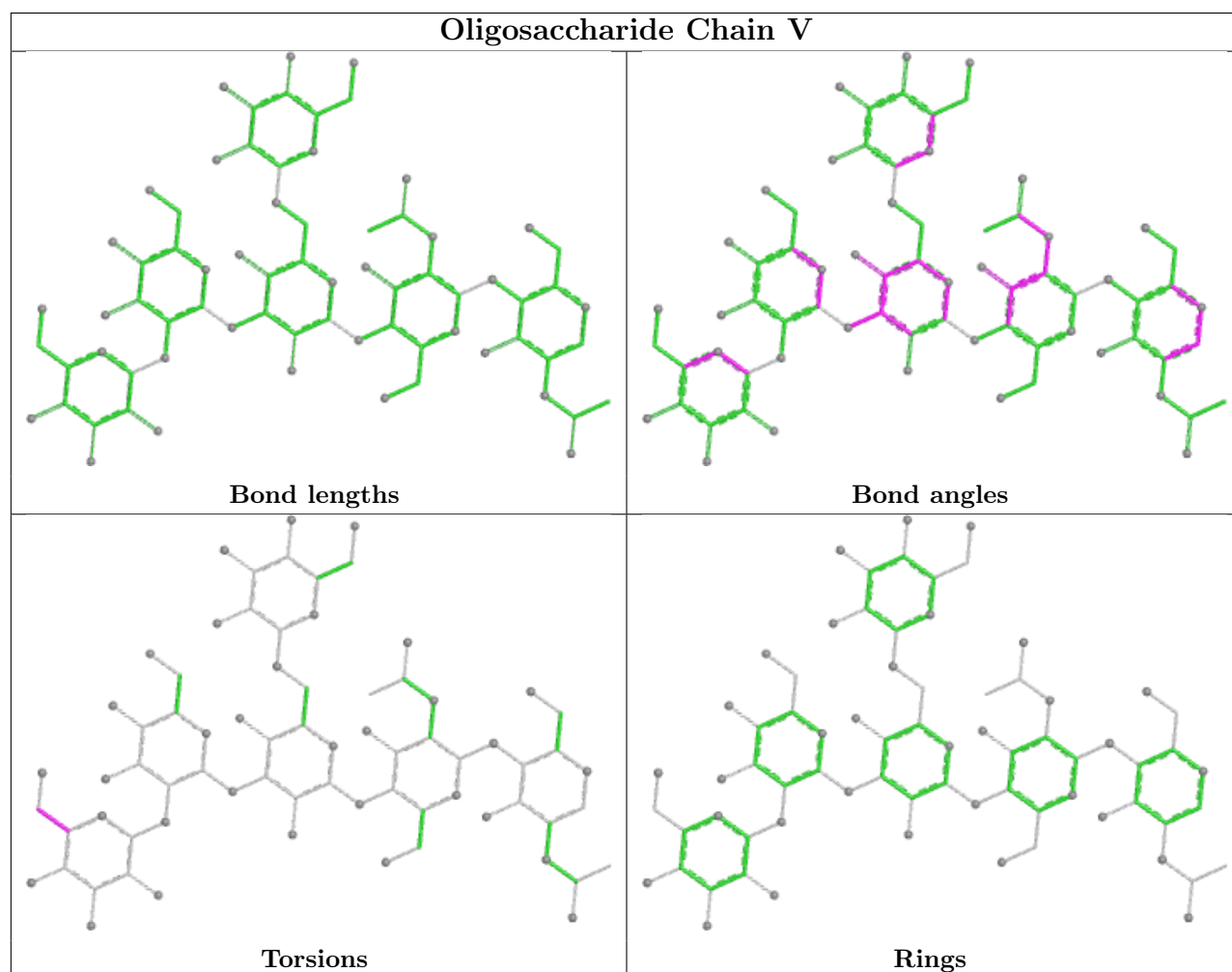
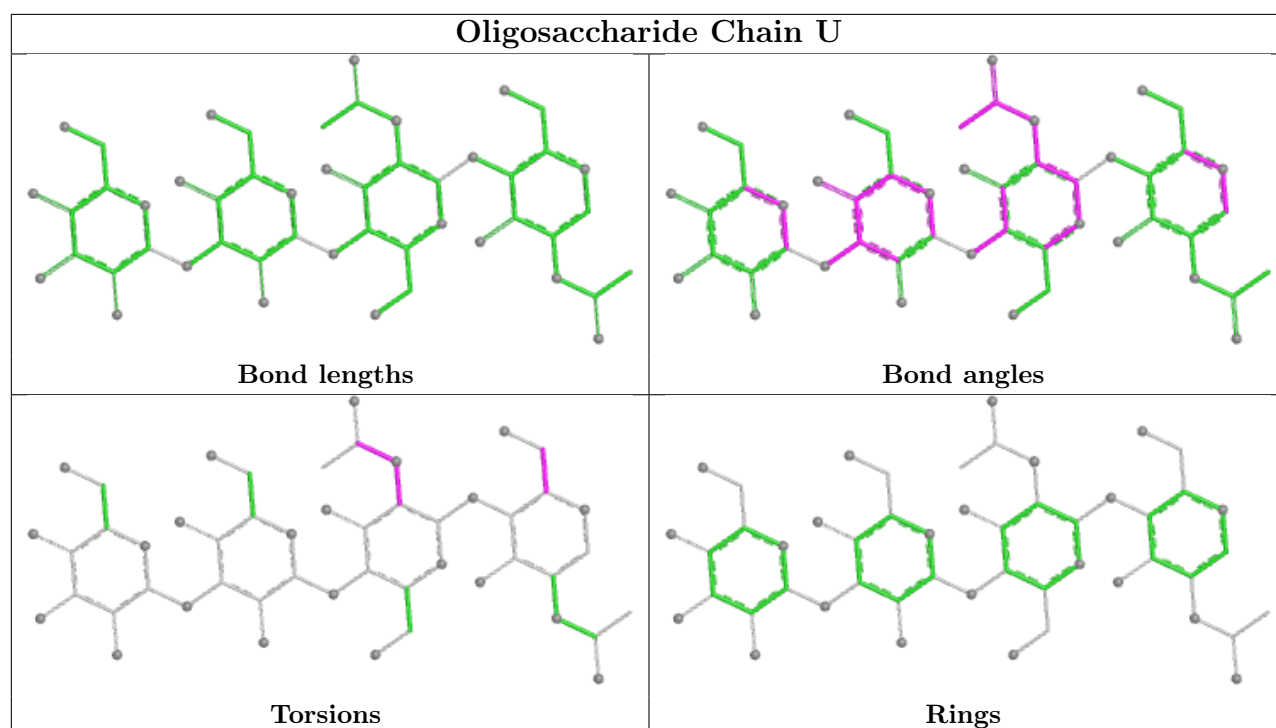




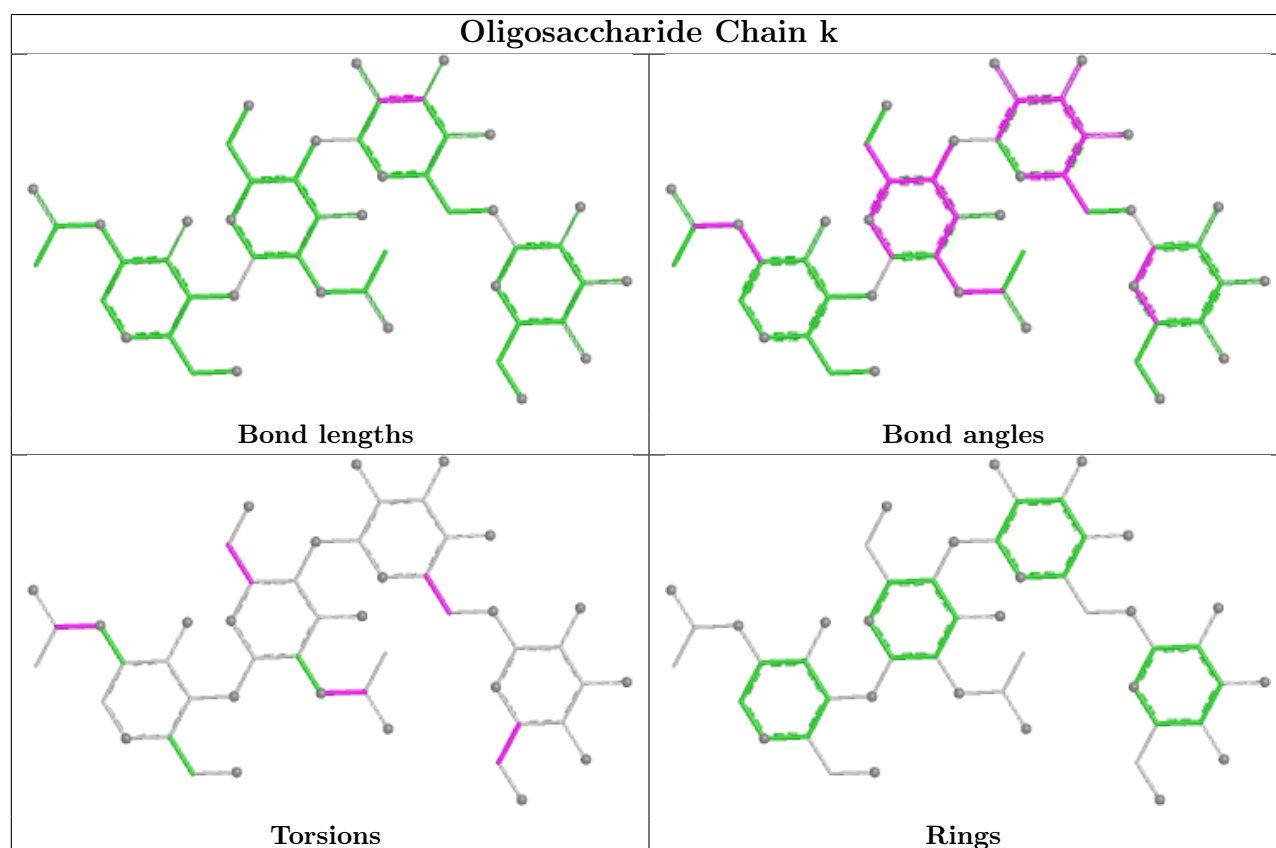
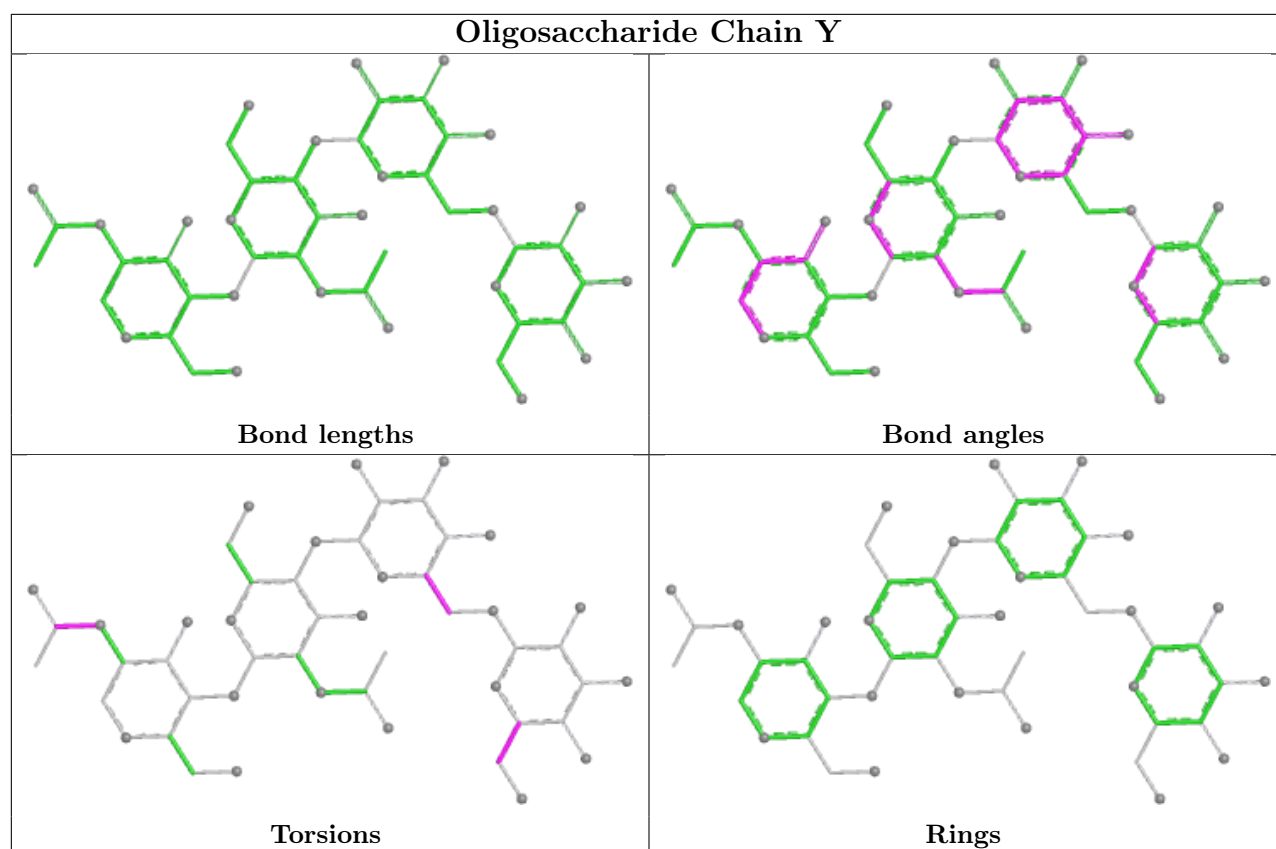




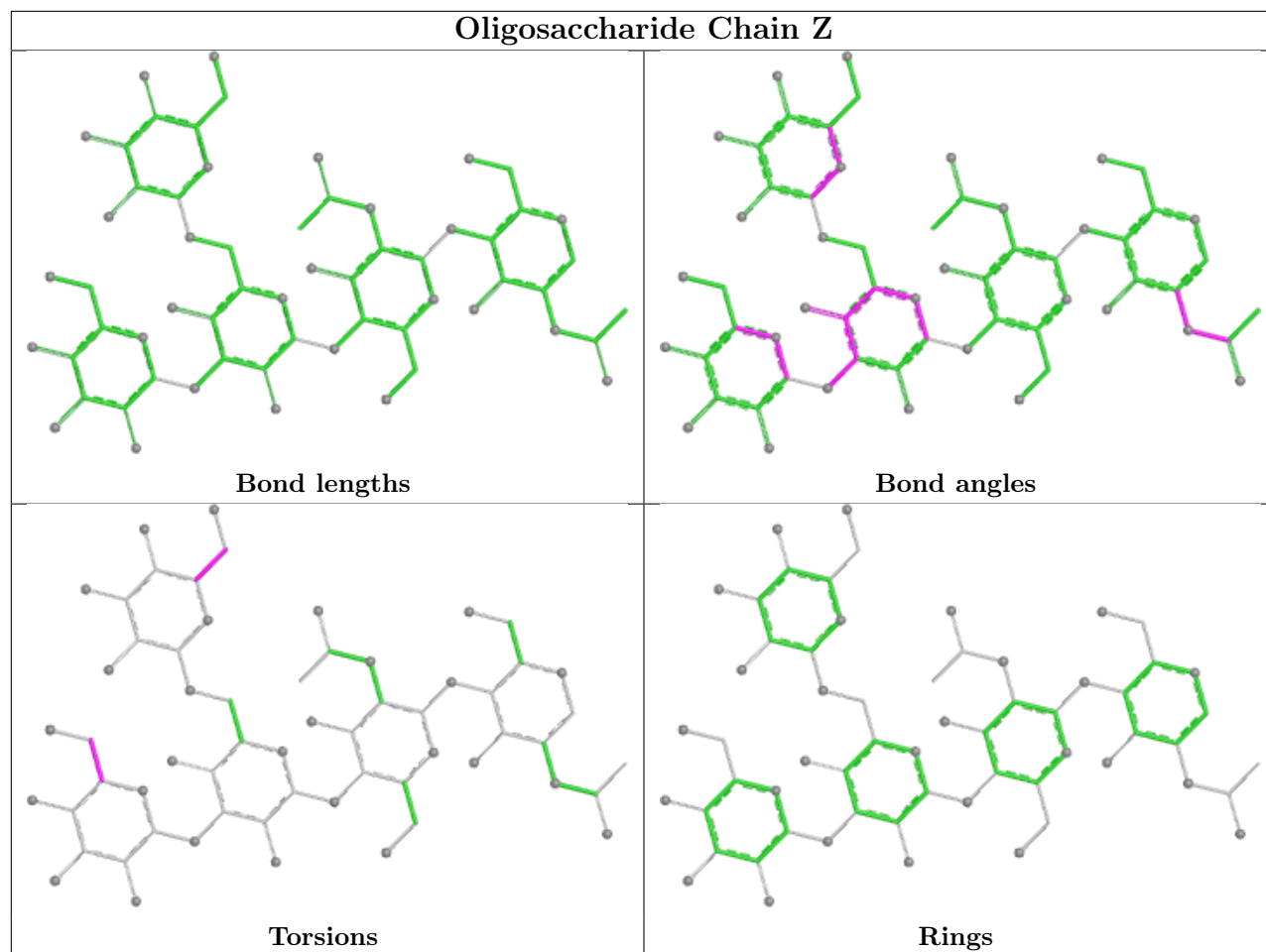




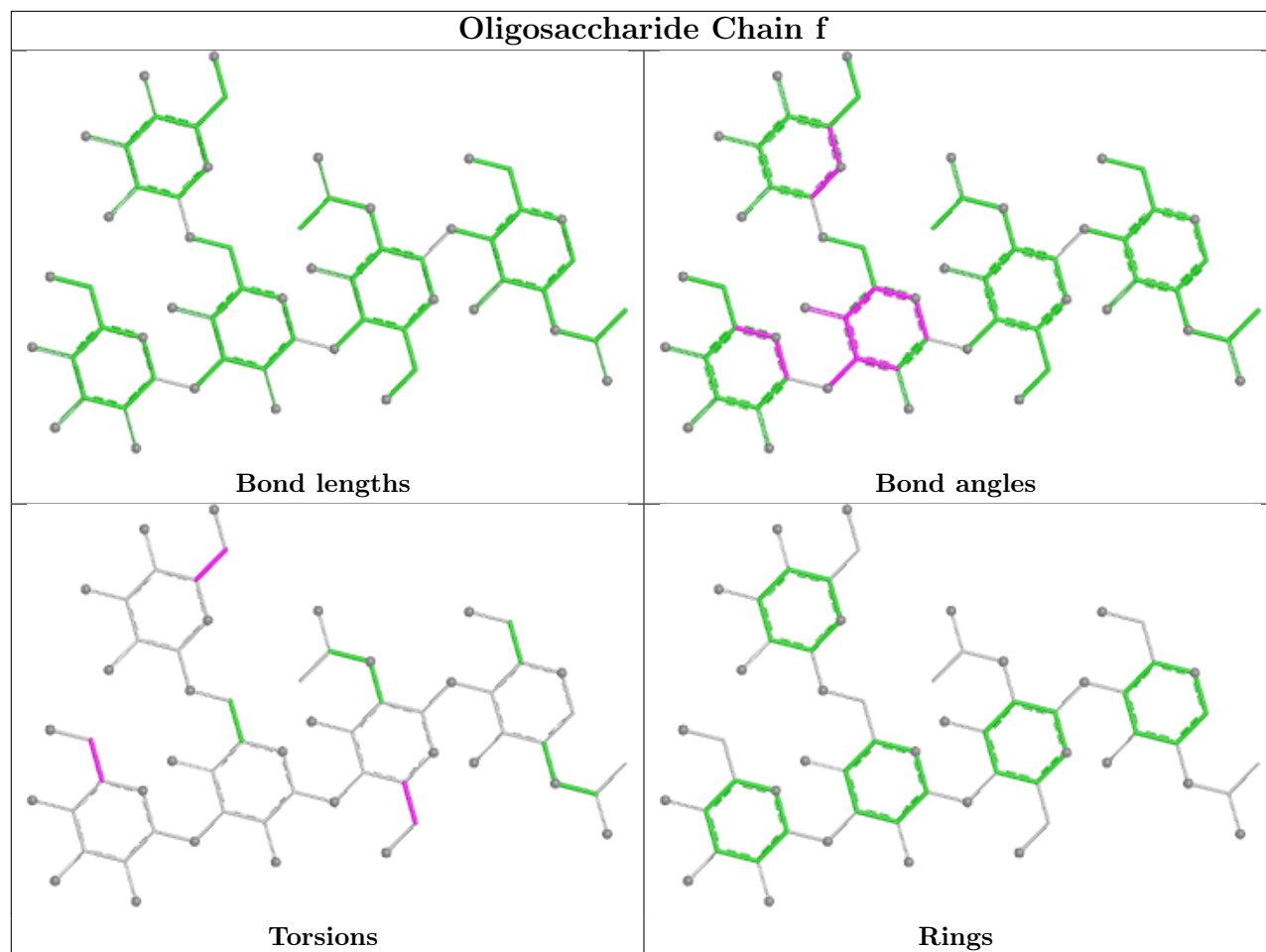




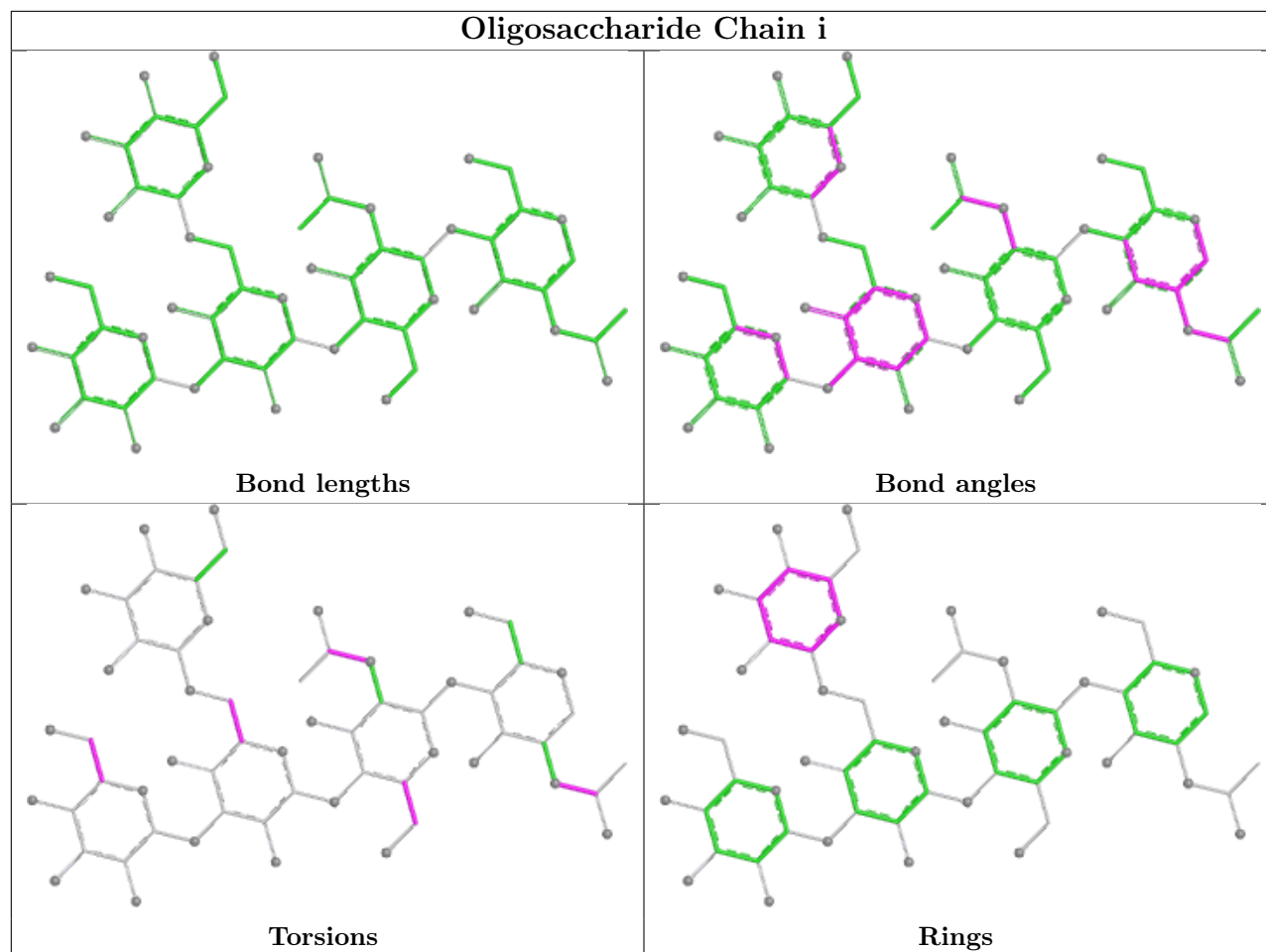




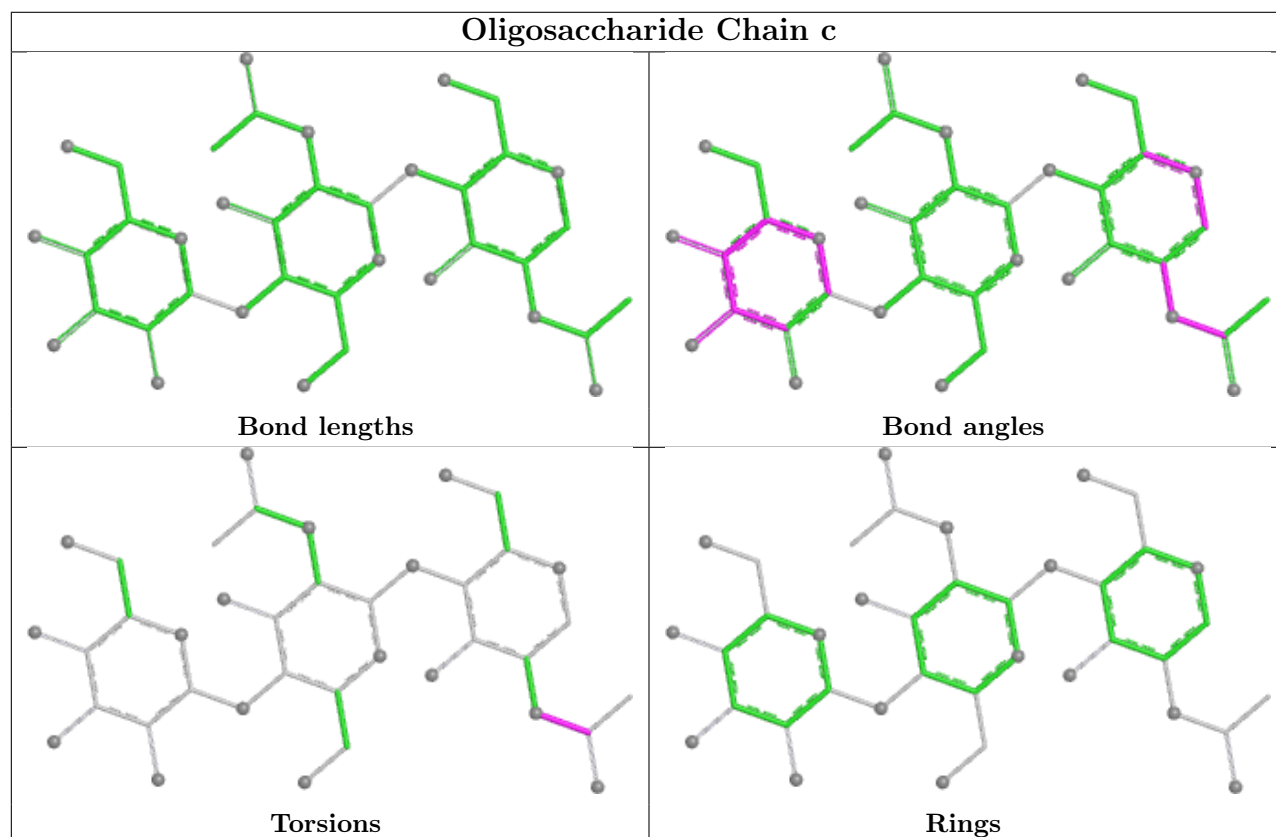
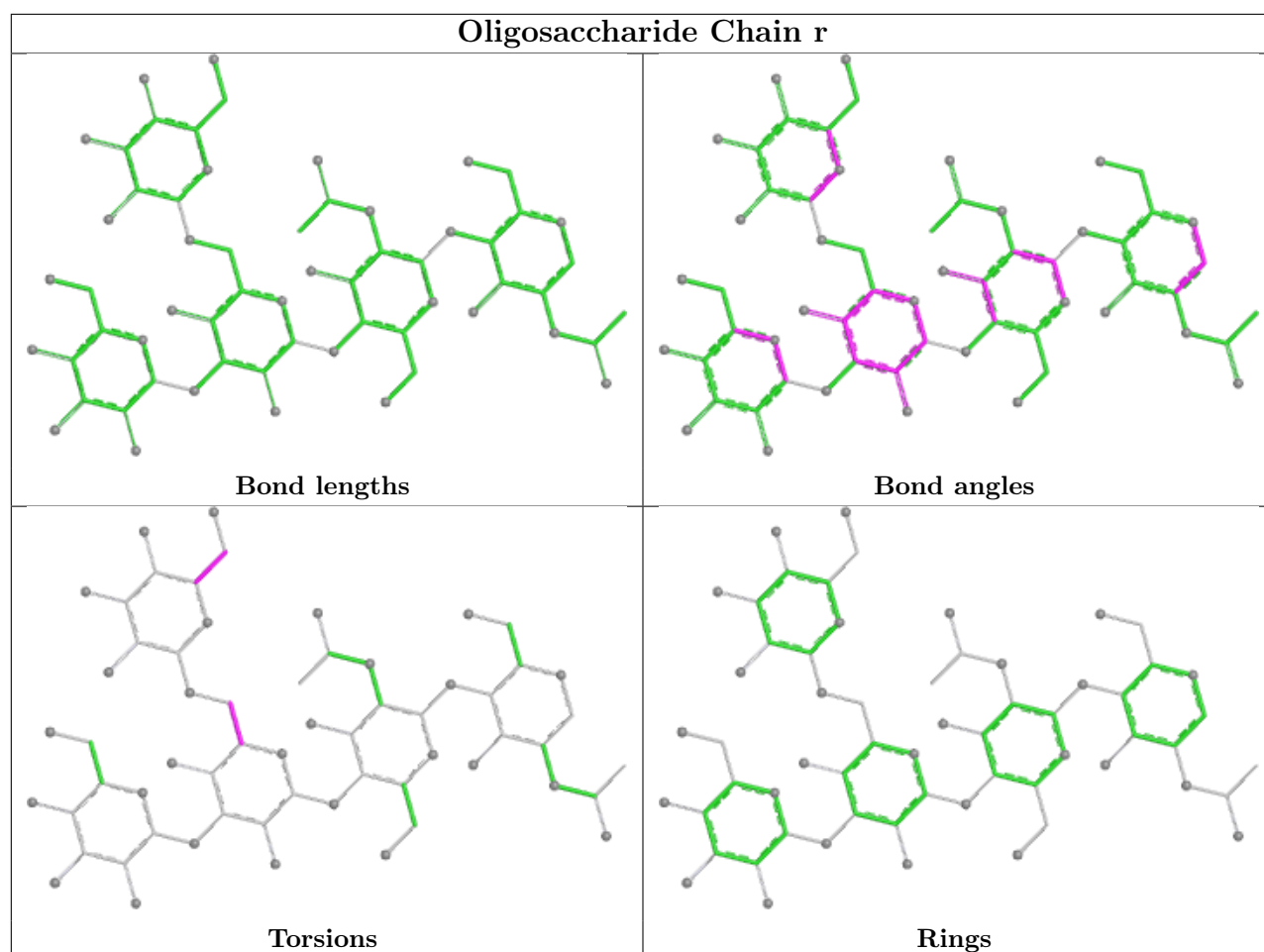




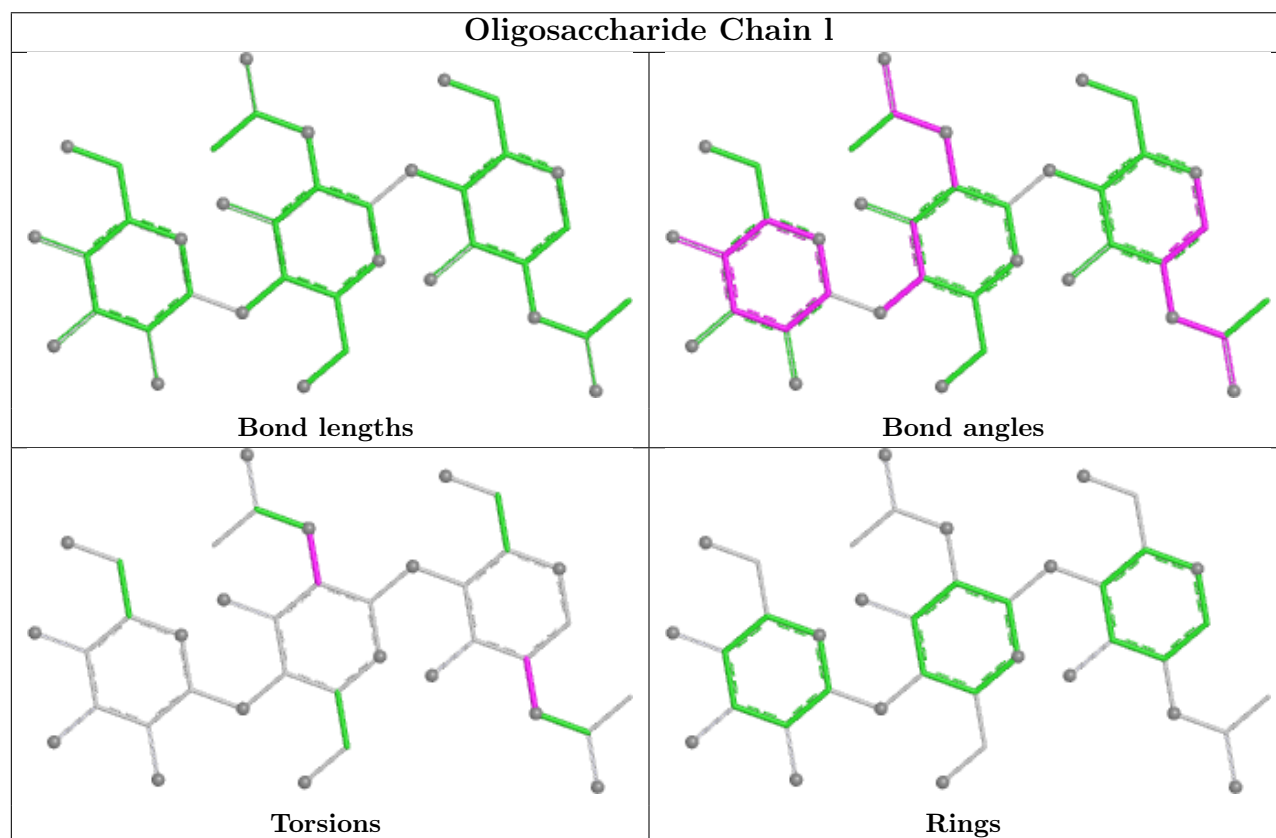
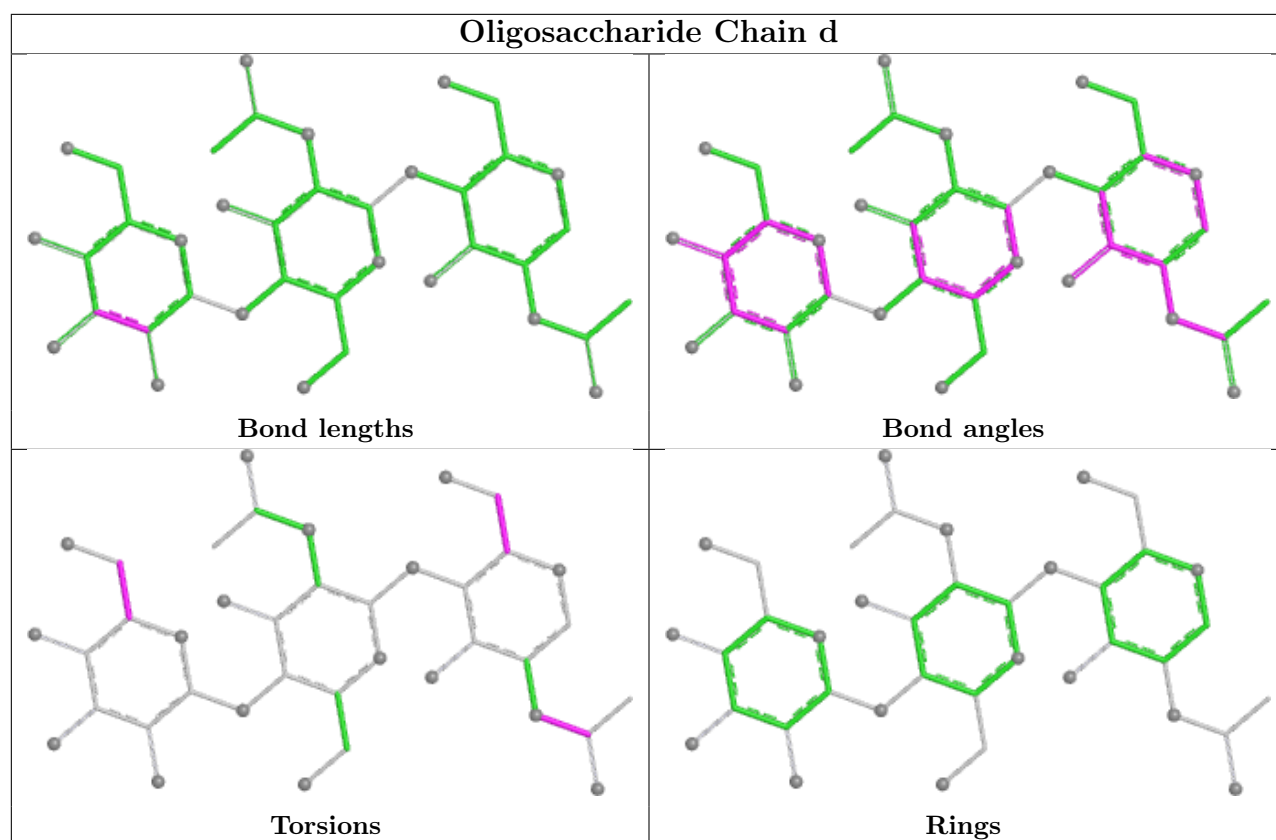




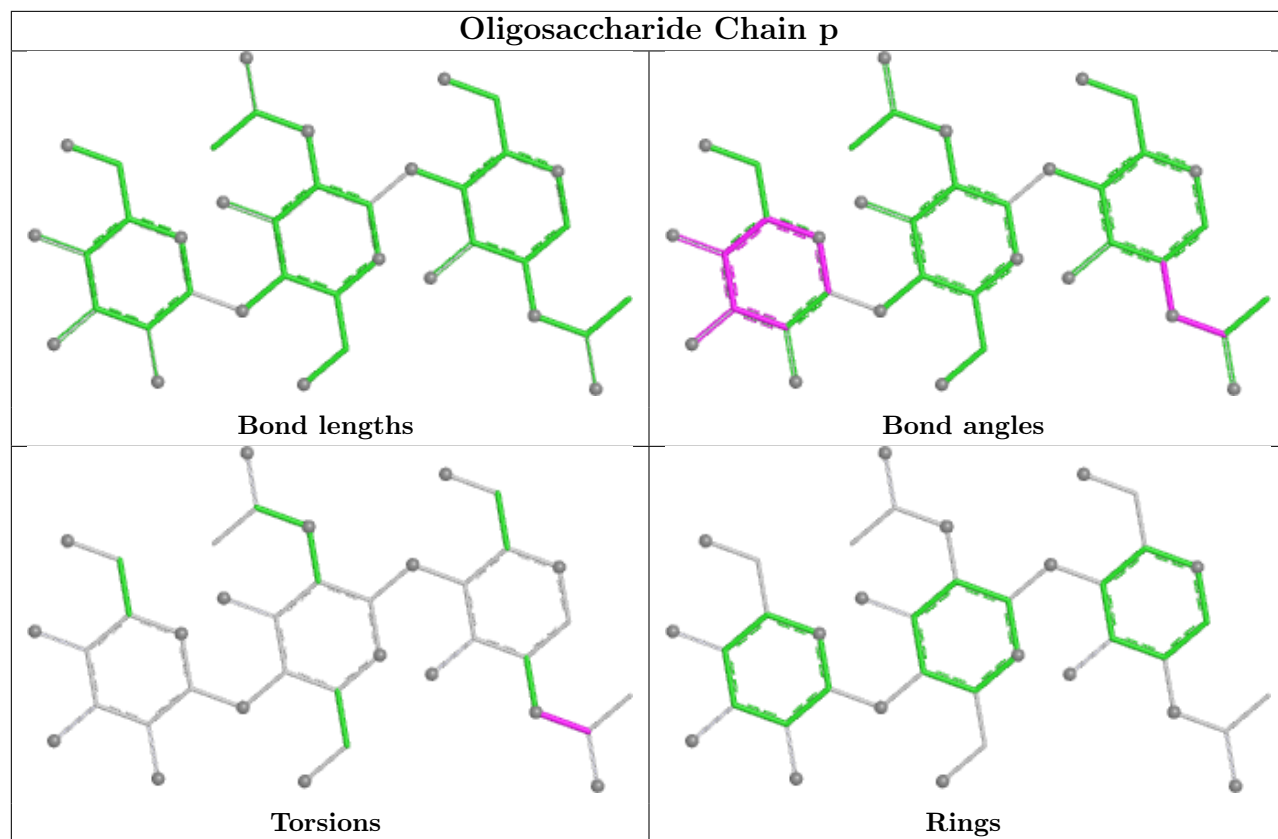




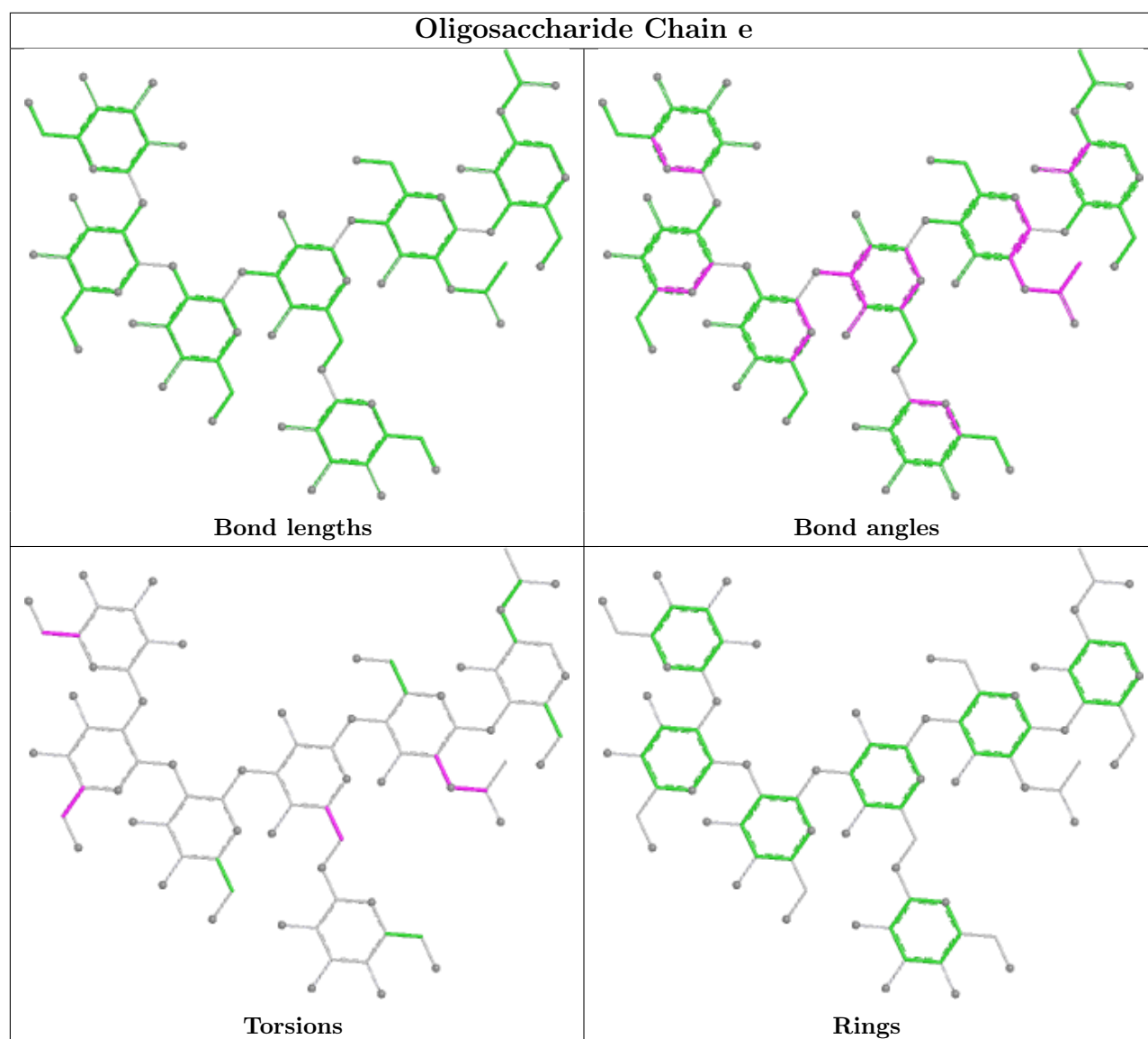




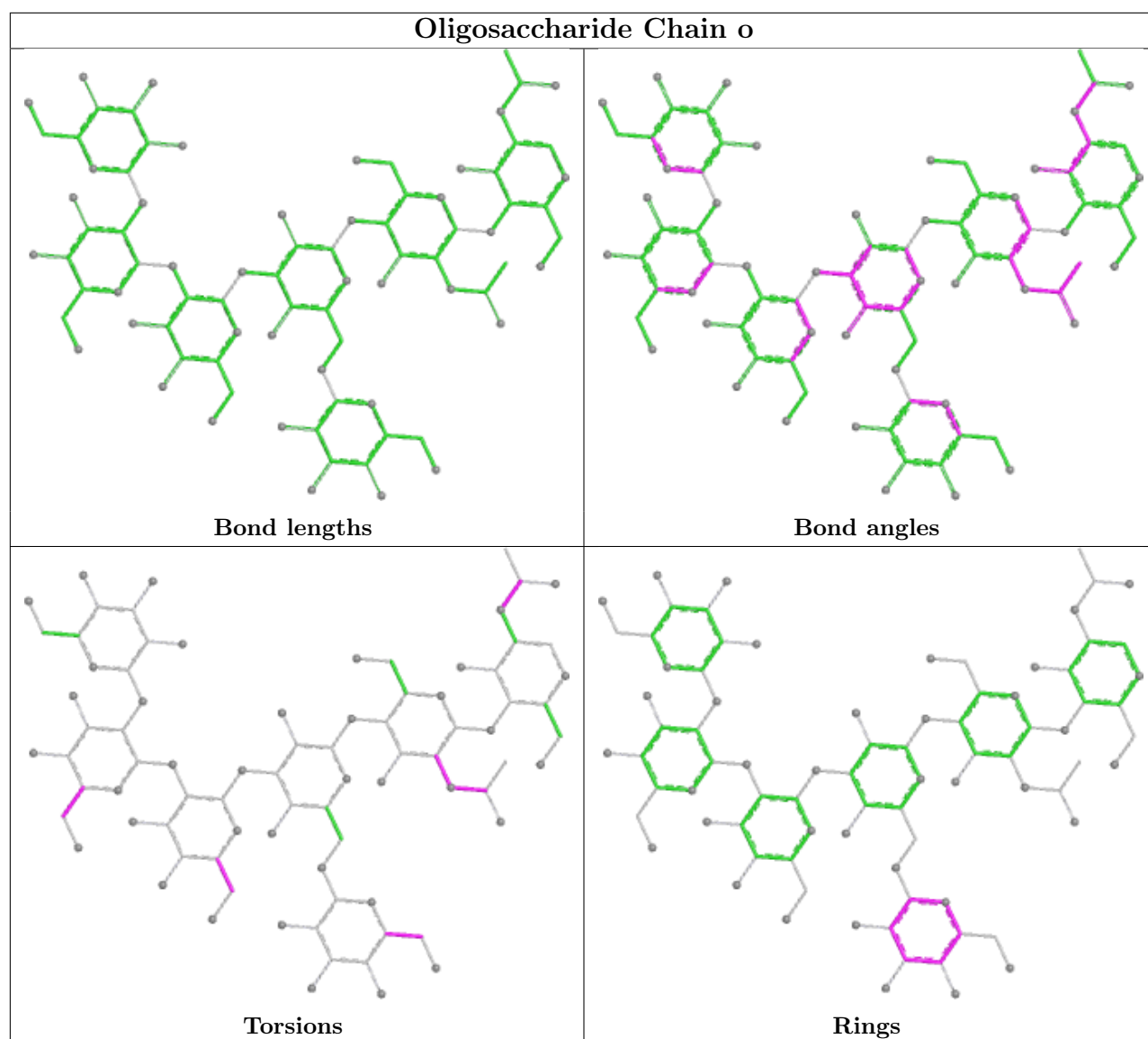




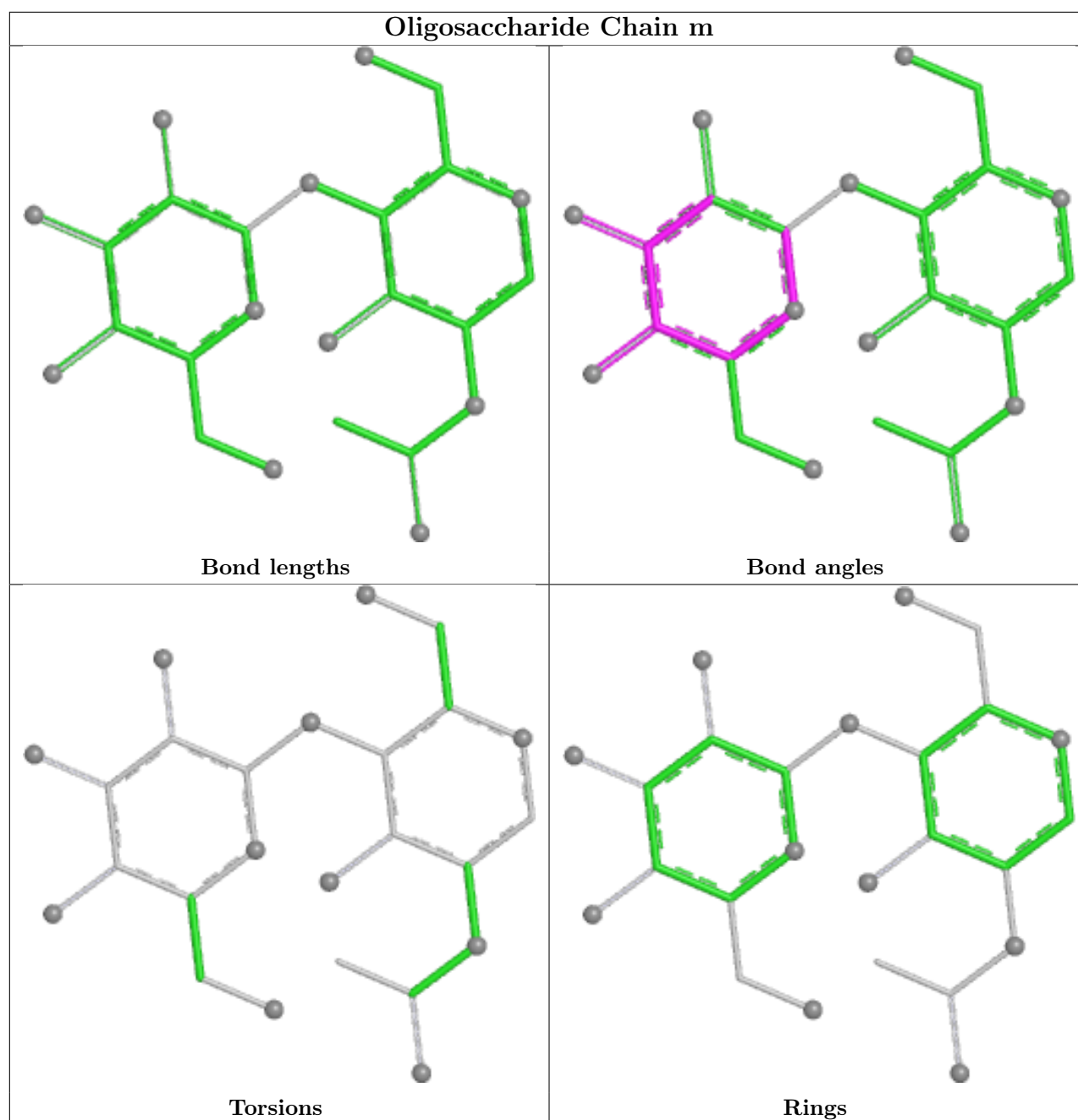












## 5.6 Ligand geometry [i](#)

28 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
15	NAG	D	701	2	14,14,15	0.85	1 (7%)	17,19,21	1.94	3 (17%)
15	NAG	A	606	1	14,14,15	0.74	0	17,19,21	1.16	1 (5%)
15	NAG	C	607	1	14,14,15	0.81	1 (7%)	17,19,21	3.57	5 (29%)
15	NAG	C	608	1	14,14,15	0.75	0	17,19,21	1.15	2 (11%)
15	NAG	E	603	1	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
15	NAG	E	608	1	14,14,15	0.72	0	17,19,21	0.98	1 (5%)
15	NAG	E	607	1	14,14,15	0.75	0	17,19,21	1.09	1 (5%)
15	NAG	B	701	2	14,14,15	0.67	0	17,19,21	1.22	2 (11%)
15	NAG	A	608	1	14,14,15	0.70	0	17,19,21	0.89	0
15	NAG	C	601	1	14,14,15	0.68	0	17,19,21	2.16	2 (11%)
15	NAG	A	604	1	14,14,15	0.72	0	17,19,21	1.11	1 (5%)
15	NAG	A	605	1	14,14,15	0.77	0	17,19,21	1.49	1 (5%)
15	NAG	E	605	1	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
15	NAG	E	602	1	14,14,15	0.80	0	17,19,21	1.94	2 (11%)
15	NAG	C	603	1	14,14,15	0.72	0	17,19,21	1.32	2 (11%)
15	NAG	C	606	1	14,14,15	0.73	0	17,19,21	1.28	2 (11%)
15	NAG	A	601	1	14,14,15	0.65	0	17,19,21	2.02	3 (17%)
15	NAG	E	606	1	14,14,15	0.71	0	17,19,21	1.20	2 (11%)
15	NAG	E	601	1	14,14,15	0.71	0	17,19,21	1.19	2 (11%)
15	NAG	C	604	1	14,14,15	0.81	0	17,19,21	2.11	2 (11%)
15	NAG	C	602	1	14,14,15	0.72	0	17,19,21	1.63	2 (11%)
15	NAG	A	607	1	14,14,15	0.76	0	17,19,21	1.35	1 (5%)
15	NAG	A	603	1	14,14,15	0.69	0	17,19,21	1.39	2 (11%)
15	NAG	A	609	1	14,14,15	0.72	0	17,19,21	1.33	2 (11%)
15	NAG	A	602	1	14,14,15	0.72	0	17,19,21	0.85	0
15	NAG	E	604	1	14,14,15	0.72	0	17,19,21	1.22	1 (5%)
15	NAG	F	701	2	14,14,15	0.82	0	17,19,21	1.61	3 (17%)
15	NAG	C	605	1	14,14,15	0.81	0	17,19,21	1.52	2 (11%)

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
15	NAG	D	701	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	A	606	1	-	1/6/23/26	0/1/1/1
15	NAG	C	607	1	-	3/6/23/26	0/1/1/1
15	NAG	C	608	1	-	0/6/23/26	0/1/1/1
15	NAG	E	603	1	-	1/6/23/26	0/1/1/1
15	NAG	E	608	1	-	1/6/23/26	0/1/1/1
15	NAG	E	607	1	-	2/6/23/26	0/1/1/1
15	NAG	B	701	2	-	2/6/23/26	0/1/1/1
15	NAG	A	608	1	-	0/6/23/26	0/1/1/1
15	NAG	C	601	1	-	3/6/23/26	0/1/1/1
15	NAG	A	604	1	-	0/6/23/26	0/1/1/1
15	NAG	A	605	1	-	2/6/23/26	0/1/1/1
15	NAG	E	605	1	-	2/6/23/26	0/1/1/1
15	NAG	E	602	1	-	2/6/23/26	0/1/1/1
15	NAG	C	603	1	-	3/6/23/26	0/1/1/1
15	NAG	C	606	1	-	2/6/23/26	0/1/1/1
15	NAG	A	601	1	-	2/6/23/26	0/1/1/1
15	NAG	E	606	1	-	2/6/23/26	0/1/1/1
15	NAG	E	601	1	-	2/6/23/26	0/1/1/1
15	NAG	C	604	1	-	3/6/23/26	0/1/1/1
15	NAG	C	602	1	-	2/6/23/26	0/1/1/1
15	NAG	A	607	1	-	2/6/23/26	0/1/1/1
15	NAG	A	603	1	-	3/6/23/26	0/1/1/1
15	NAG	A	609	1	-	2/6/23/26	0/1/1/1
15	NAG	A	602	1	-	0/6/23/26	0/1/1/1
15	NAG	E	604	1	-	1/6/23/26	0/1/1/1
15	NAG	F	701	2	-	0/6/23/26	0/1/1/1
15	NAG	C	605	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	701	NAG	C1-C2	2.53	1.55	1.52
15	C	607	NAG	C1-C2	2.01	1.55	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	607	NAG	C2-N2-C7	12.62	139.81	122.90

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	601	NAG	C1-O5-C5	7.61	122.38	112.19
15	C	604	NAG	C2-N2-C7	6.84	132.07	122.90
15	E	602	NAG	C2-N2-C7	6.19	131.19	122.90
15	A	601	NAG	C2-N2-C7	5.84	130.72	122.90
15	D	701	NAG	C2-N2-C7	5.68	130.51	122.90
15	C	602	NAG	C2-N2-C7	5.22	129.90	122.90
15	A	605	NAG	C2-N2-C7	4.97	129.55	122.90
15	C	607	NAG	C8-C7-N2	4.64	123.81	116.12
15	F	701	NAG	C2-N2-C7	4.44	128.85	122.90
15	A	607	NAG	C2-N2-C7	4.42	128.82	122.90
15	C	605	NAG	O5-C1-C2	-4.17	104.83	111.29
15	A	601	NAG	C1-O5-C5	4.05	117.61	112.19
15	C	604	NAG	O5-C1-C2	-4.05	105.03	111.29
15	C	607	NAG	C1-C2-N2	3.58	116.08	110.43
15	C	603	NAG	C2-N2-C7	3.51	127.60	122.90
15	A	603	NAG	C2-N2-C7	3.44	127.51	122.90
15	A	609	NAG	C2-N2-C7	3.40	127.46	122.90
15	A	603	NAG	C1-O5-C5	3.38	116.72	112.19
15	E	605	NAG	C2-N2-C7	3.35	127.39	122.90
15	D	701	NAG	C1-O5-C5	3.34	116.67	112.19
15	C	606	NAG	C2-N2-C7	3.34	127.38	122.90
15	C	605	NAG	C1-O5-C5	-3.33	107.72	112.19
15	E	604	NAG	C1-O5-C5	3.27	116.58	112.19
15	E	603	NAG	C1-O5-C5	3.26	116.56	112.19
15	A	604	NAG	C1-O5-C5	3.19	116.47	112.19
15	E	607	NAG	C2-N2-C7	3.19	127.18	122.90
15	E	601	NAG	C2-N2-C7	3.17	127.15	122.90
15	C	608	NAG	O5-C1-C2	-3.13	106.45	111.29
15	C	606	NAG	C1-O5-C5	3.12	116.37	112.19
15	E	606	NAG	C2-N2-C7	3.10	127.06	122.90
15	A	606	NAG	C1-O5-C5	3.10	116.34	112.19
15	C	601	NAG	C2-N2-C7	3.08	127.03	122.90
15	B	701	NAG	C2-N2-C7	2.97	126.88	122.90
15	A	609	NAG	C1-O5-C5	2.87	116.03	112.19
15	C	607	NAG	O7-C7-C8	-2.82	117.03	122.05
15	F	701	NAG	O5-C1-C2	-2.76	107.02	111.29
15	E	602	NAG	O7-C7-N2	2.71	126.76	121.98
15	B	701	NAG	C1-O5-C5	2.56	115.61	112.19
15	C	607	NAG	C1-O5-C5	2.49	115.52	112.19
15	A	601	NAG	O7-C7-N2	2.45	126.31	121.98
15	E	606	NAG	C1-O5-C5	2.40	115.40	112.19
15	C	602	NAG	O7-C7-N2	2.36	126.16	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	608	NAG	C2-N2-C7	2.36	126.07	122.90
15	F	701	NAG	C1-O5-C5	2.36	115.35	112.19
15	D	701	NAG	O7-C7-N2	2.35	126.14	121.98
15	E	608	NAG	C1-O5-C5	2.33	115.31	112.19
15	E	601	NAG	C1-O5-C5	2.23	115.18	112.19
15	C	603	NAG	O5-C1-C2	-2.12	108.01	111.29

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	602	NAG	C1-C2-N2-C7
15	C	607	NAG	C1-C2-N2-C7
15	A	603	NAG	C8-C7-N2-C2
15	A	603	NAG	O7-C7-N2-C2
15	A	605	NAG	C8-C7-N2-C2
15	A	605	NAG	O7-C7-N2-C2
15	A	607	NAG	C8-C7-N2-C2
15	A	607	NAG	O7-C7-N2-C2
15	A	609	NAG	C8-C7-N2-C2
15	A	609	NAG	O7-C7-N2-C2
15	B	701	NAG	C8-C7-N2-C2
15	B	701	NAG	O7-C7-N2-C2
15	E	601	NAG	C8-C7-N2-C2
15	E	601	NAG	O7-C7-N2-C2
15	E	605	NAG	C8-C7-N2-C2
15	E	605	NAG	O7-C7-N2-C2
15	E	606	NAG	C8-C7-N2-C2
15	E	606	NAG	O7-C7-N2-C2
15	E	607	NAG	C8-C7-N2-C2
15	E	607	NAG	O7-C7-N2-C2
15	C	601	NAG	C8-C7-N2-C2
15	C	601	NAG	O7-C7-N2-C2
15	C	603	NAG	C8-C7-N2-C2
15	C	603	NAG	O7-C7-N2-C2
15	C	604	NAG	C8-C7-N2-C2
15	C	604	NAG	O7-C7-N2-C2
15	C	606	NAG	C8-C7-N2-C2
15	C	606	NAG	O7-C7-N2-C2
15	C	607	NAG	C8-C7-N2-C2
15	C	607	NAG	O7-C7-N2-C2
15	C	603	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	A	601	NAG	O5-C5-C6-O6
15	A	603	NAG	O5-C5-C6-O6
15	E	608	NAG	O5-C5-C6-O6
15	A	606	NAG	O5-C5-C6-O6
15	E	603	NAG	O5-C5-C6-O6
15	E	604	NAG	O5-C5-C6-O6
15	C	601	NAG	O5-C5-C6-O6
15	D	701	NAG	C1-C2-N2-C7
15	C	602	NAG	C1-C2-N2-C7
15	A	601	NAG	C3-C2-N2-C7
15	C	602	NAG	C3-C2-N2-C7
15	C	604	NAG	O5-C5-C6-O6
15	D	701	NAG	C3-C2-N2-C7
15	E	602	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
15	E	602	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



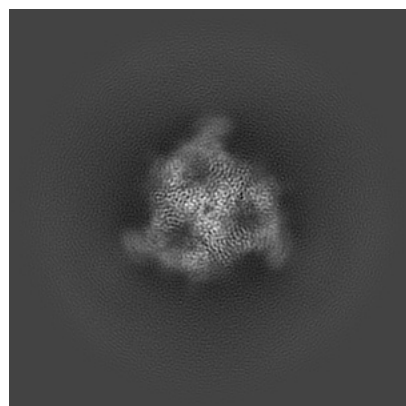
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70476. These allow visual inspection of the internal detail of the map and identification of artifacts.

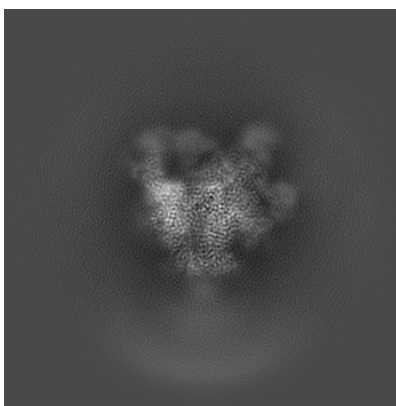
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

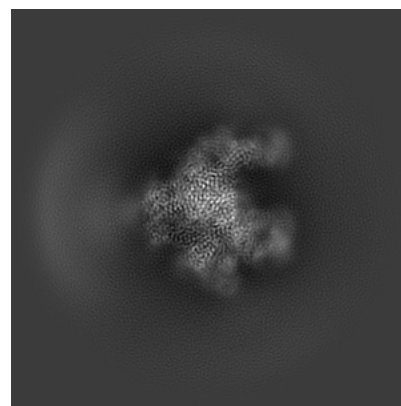
#### 6.1.1 Primary map



X

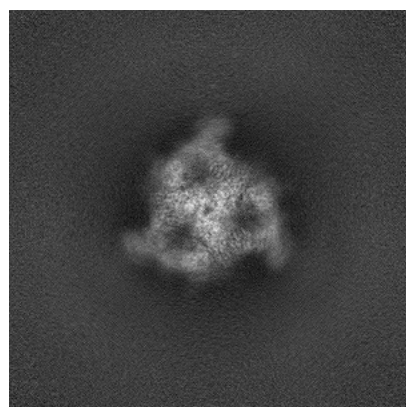


Y

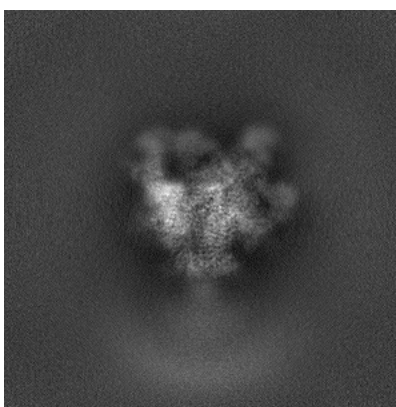


Z

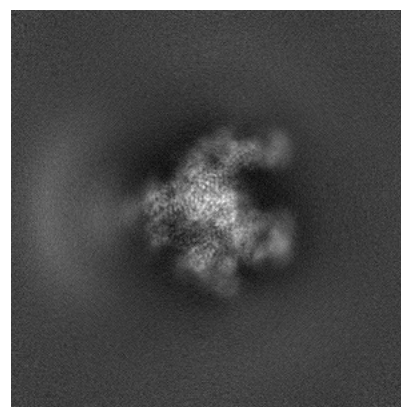
#### 6.1.2 Raw map



X



Y



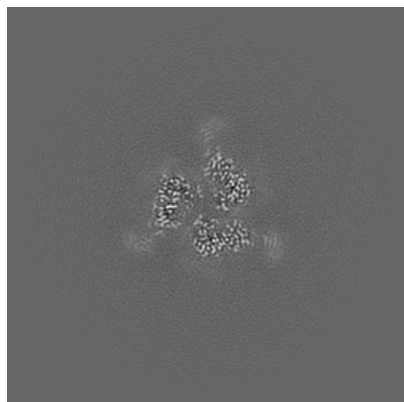
Z

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

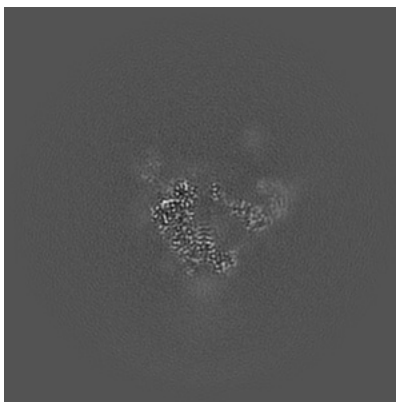


## 6.2 Central slices [i](#)

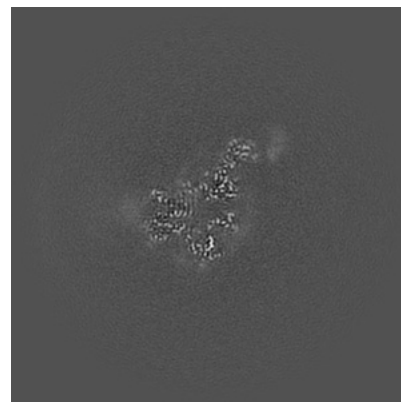
### 6.2.1 Primary map



X Index: 280

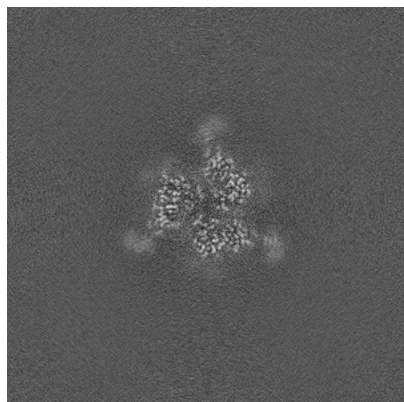


Y Index: 280

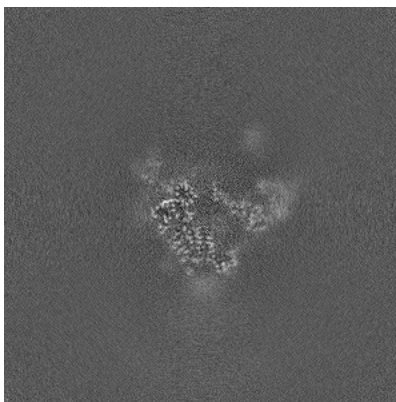


Z Index: 280

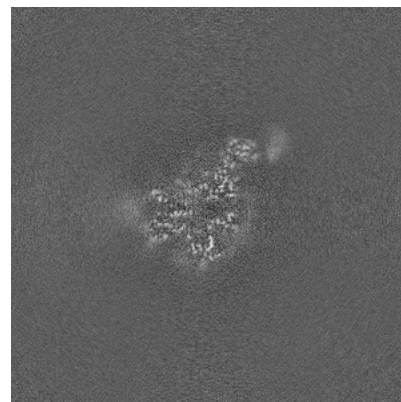
### 6.2.2 Raw map



X Index: 280



Y Index: 280



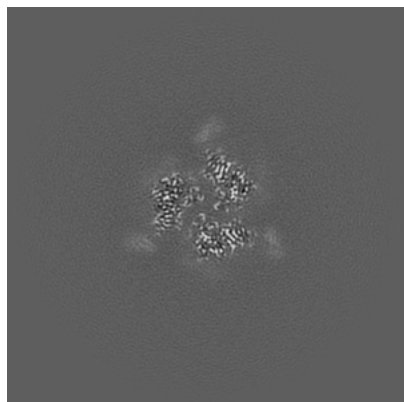
Z Index: 280

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

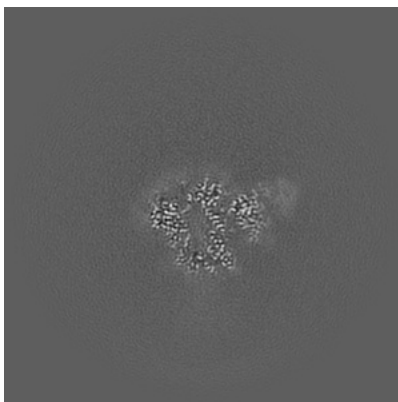


## 6.3 Largest variance slices [i](#)

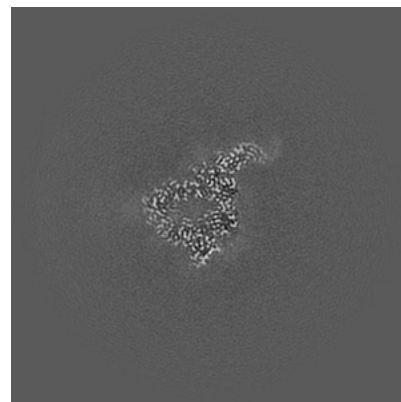
### 6.3.1 Primary map



X Index: 275

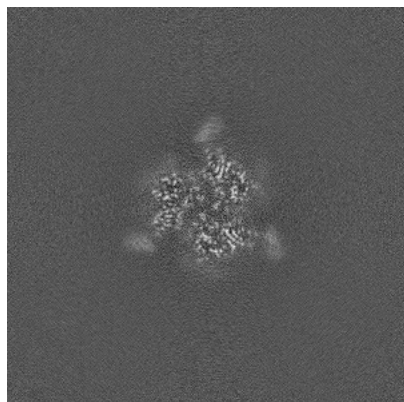


Y Index: 295

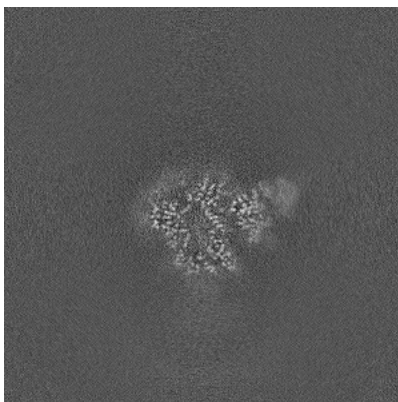


Z Index: 295

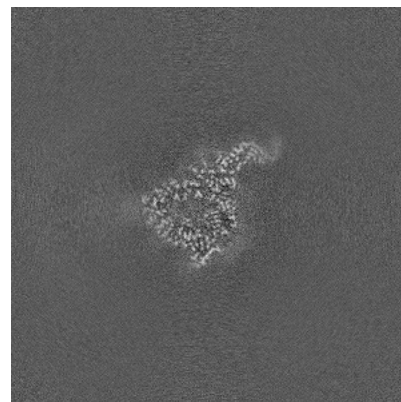
### 6.3.2 Raw map



X Index: 275



Y Index: 295



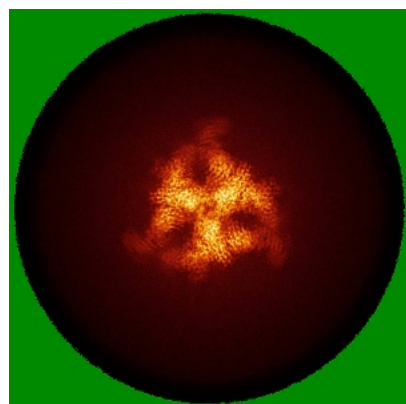
Z Index: 295

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

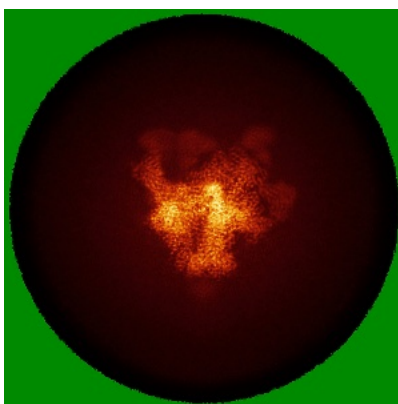


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

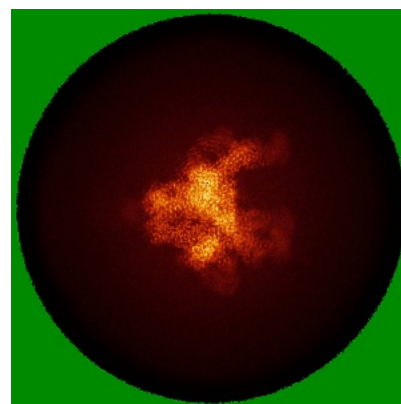
### 6.4.1 Primary map



X

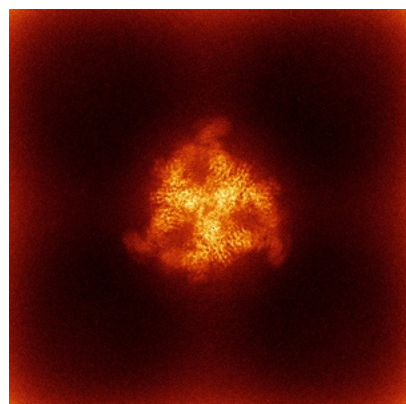


Y

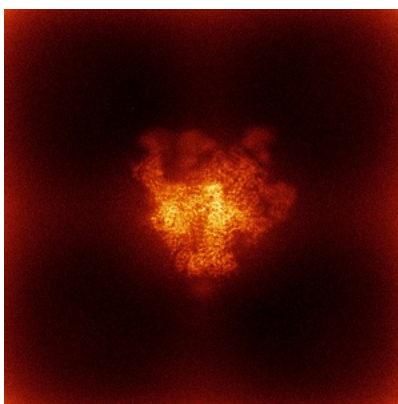


Z

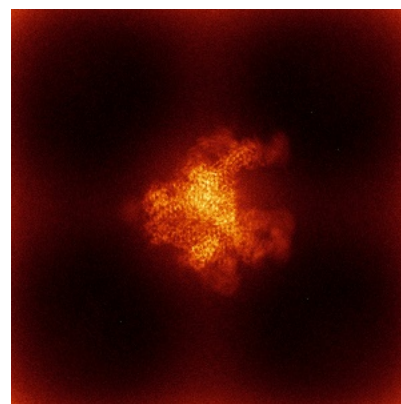
### 6.4.2 Raw map



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



X



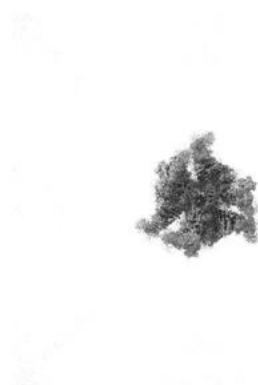
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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



X



Y



Z

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.



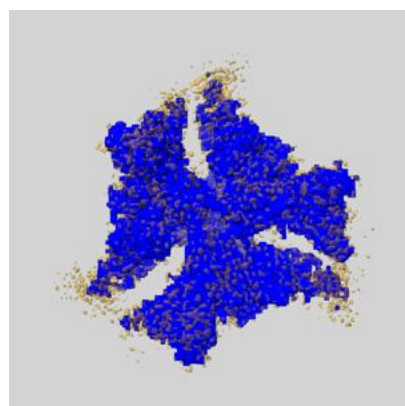
## 6.6 Mask visualisation [i](#)

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

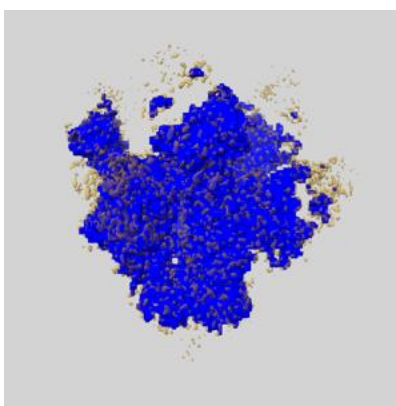
A mask typically either:

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

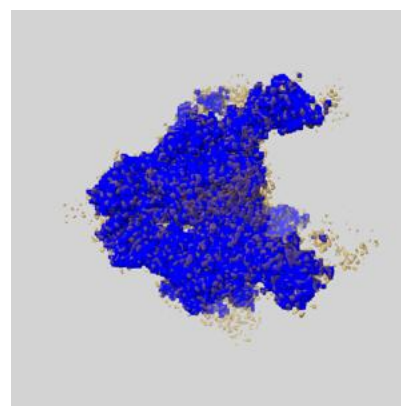
### 6.6.1 emd\_70476\_msk\_1.map [i](#)



X



Y



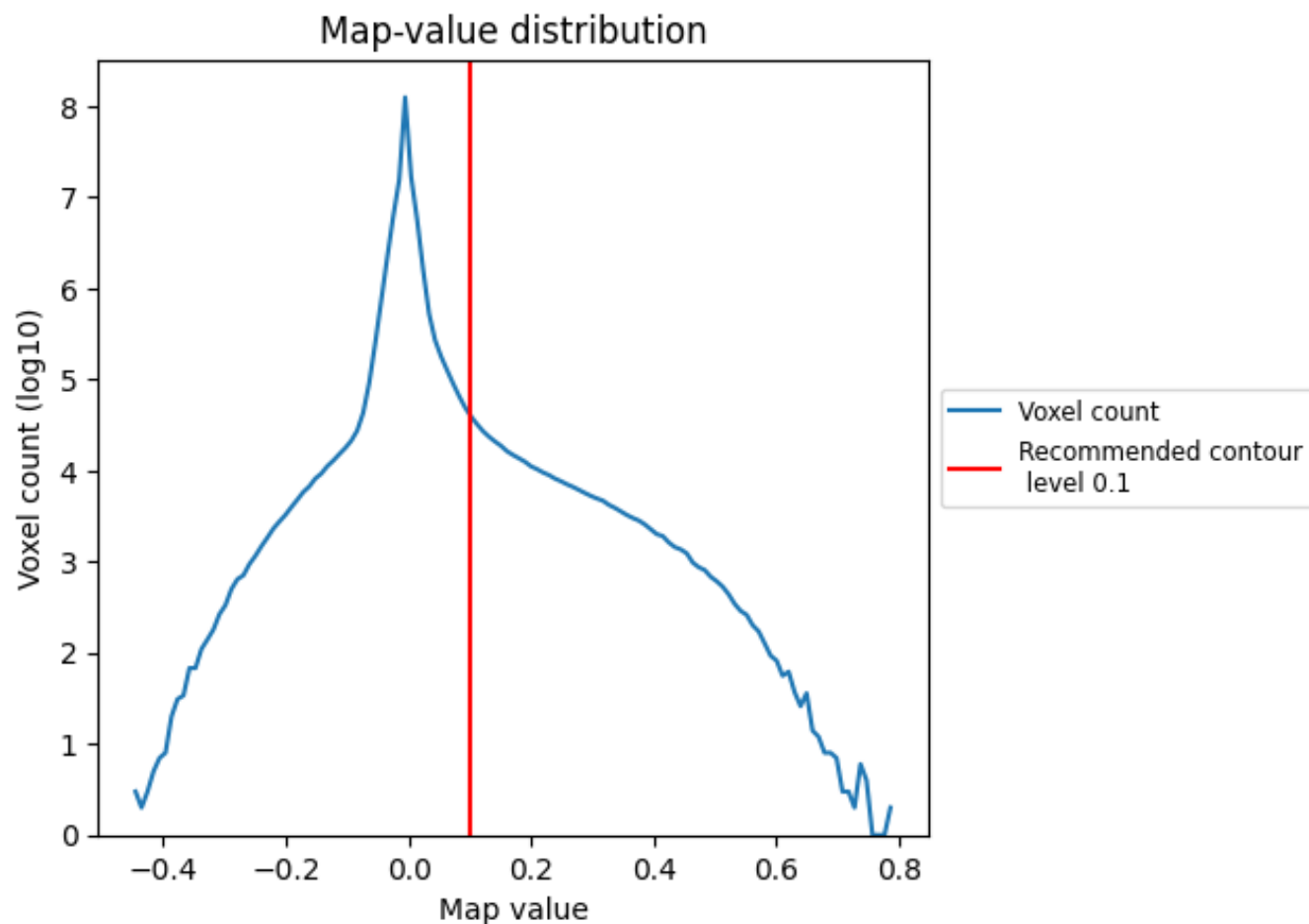
Z



## 7 Map analysis [i](#)

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

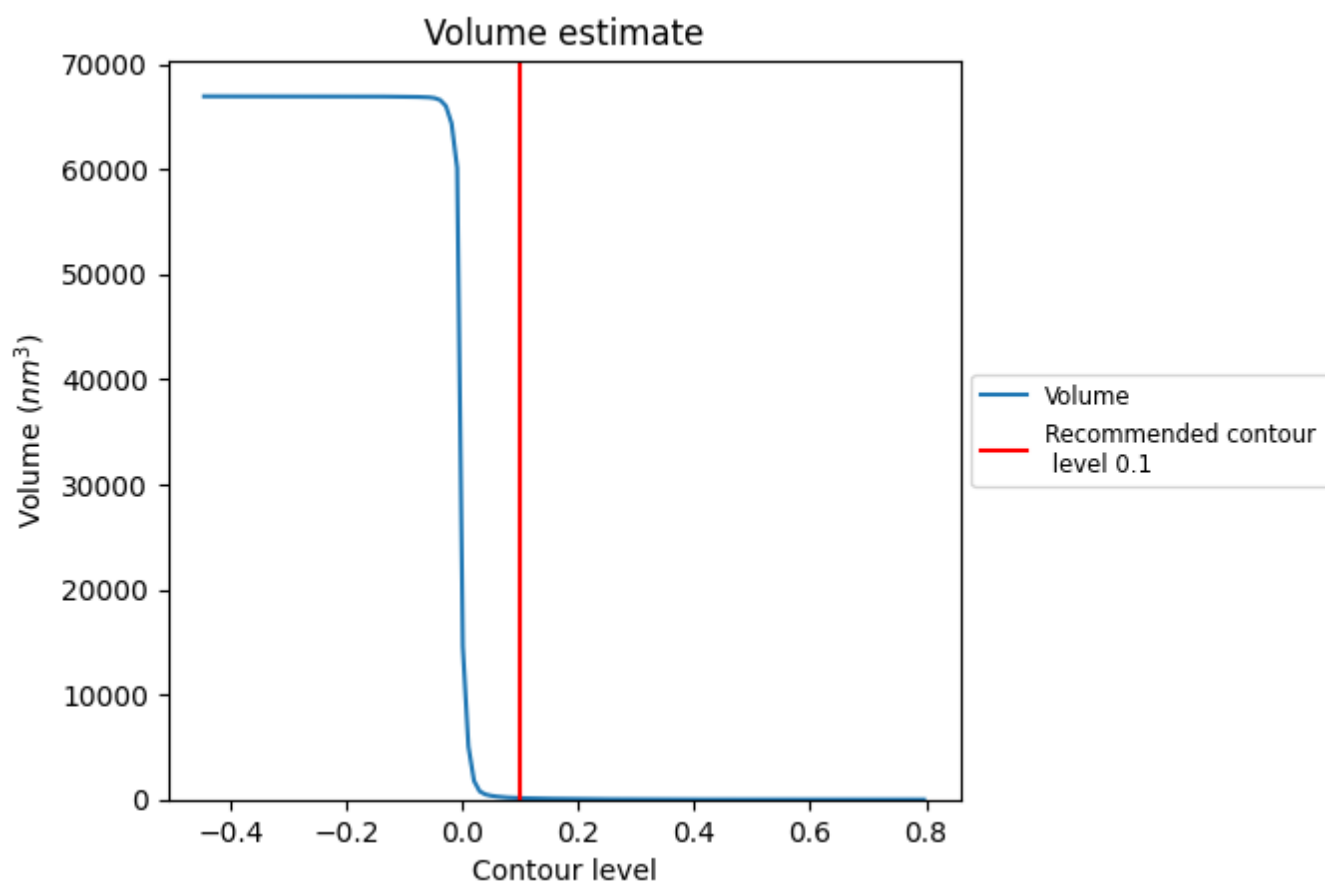
### 7.1 Map-value distribution [i](#)



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](#)

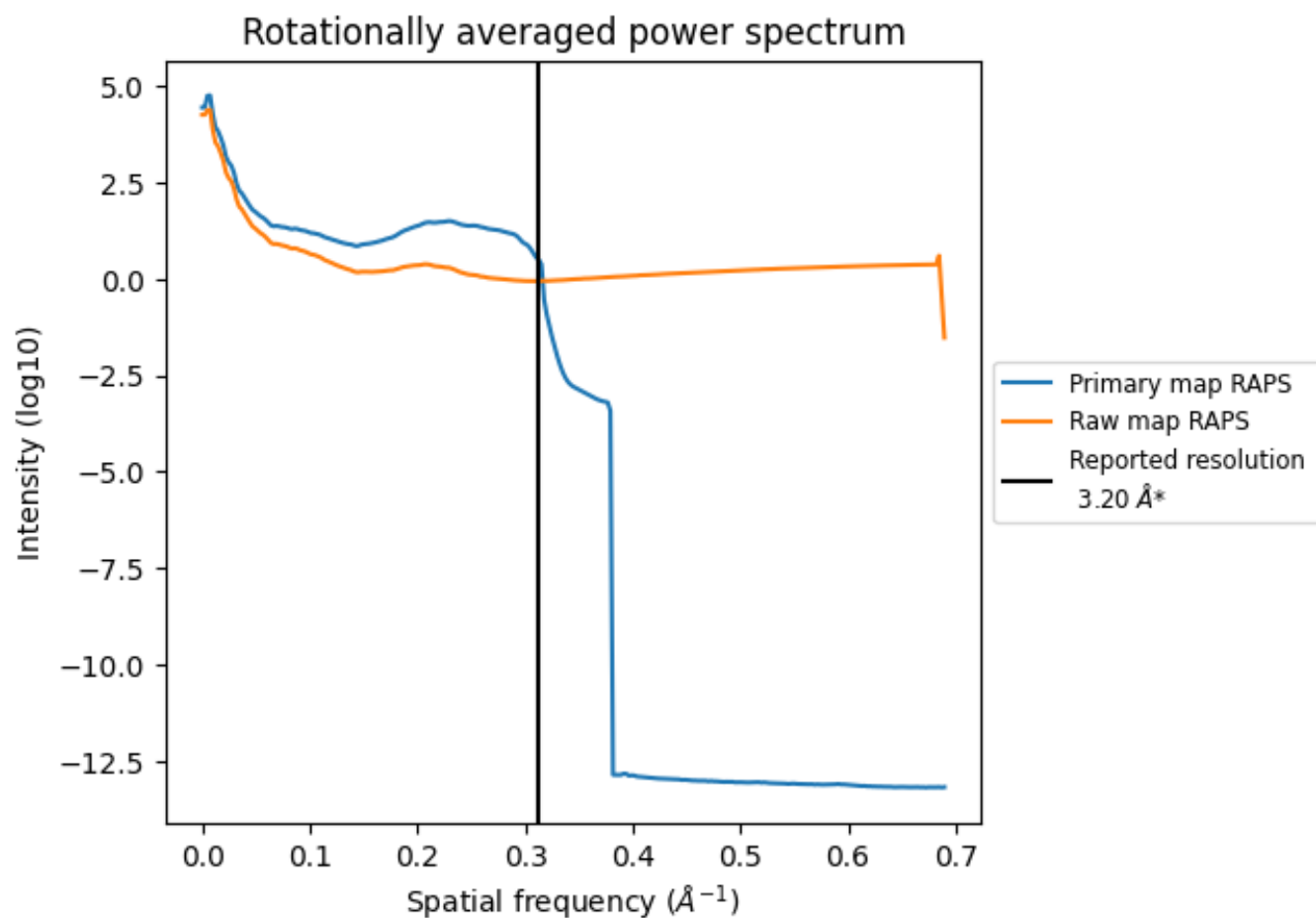


The volume at the recommended contour level is 140 nm<sup>3</sup>; this corresponds to an approximate mass of 127 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ



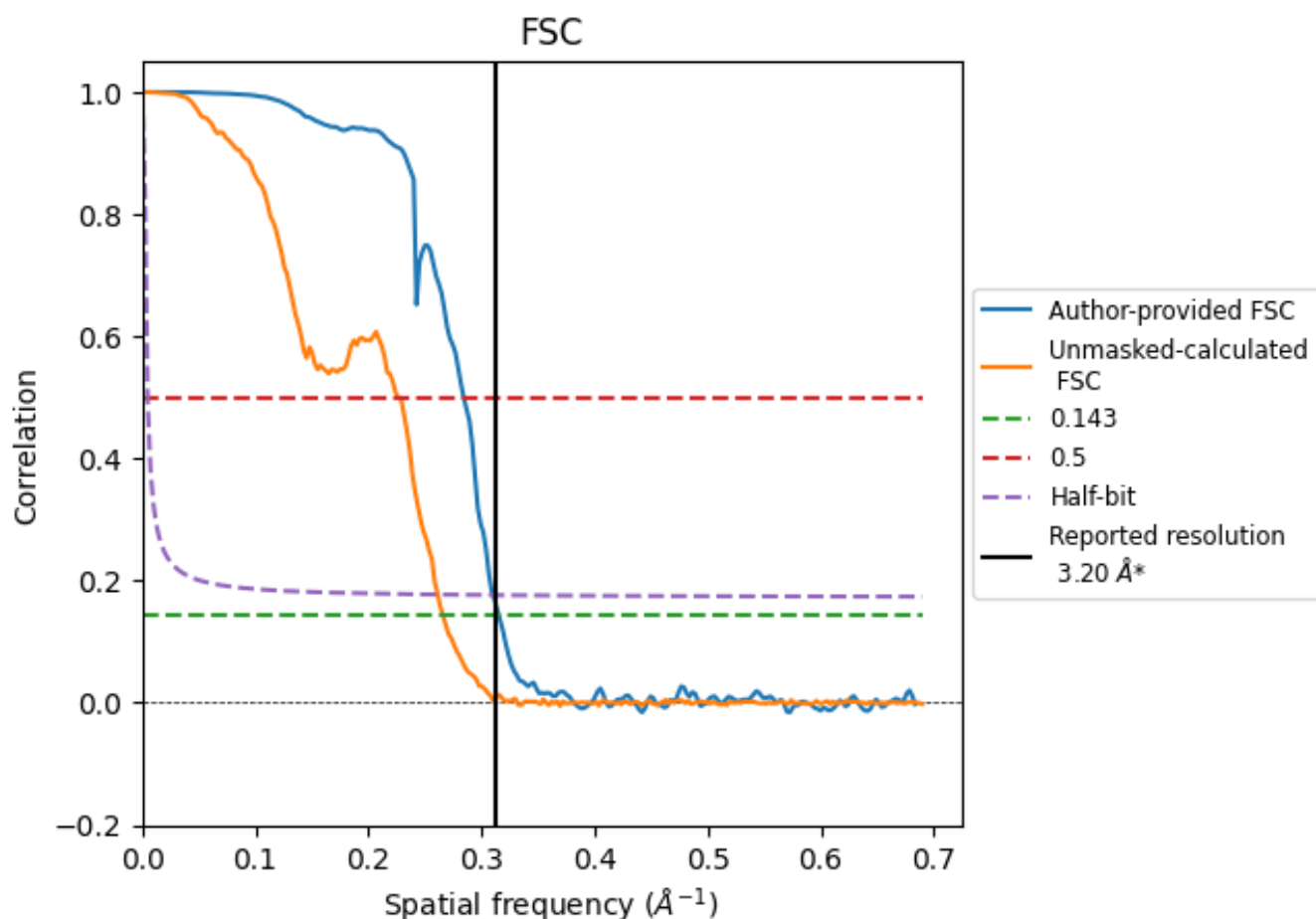
\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



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



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.52	3.22
Unmasked-calculated*	3.76	4.42	3.83

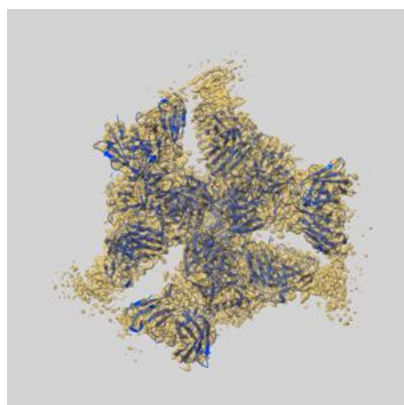
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.2 by more than 10 %



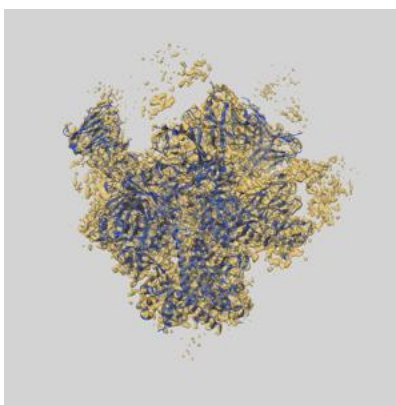
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70476 and PDB model 9OGU. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

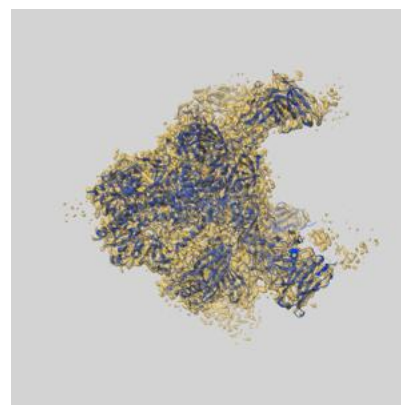
### 9.1 Map-model overlay [i](#)



X



Y

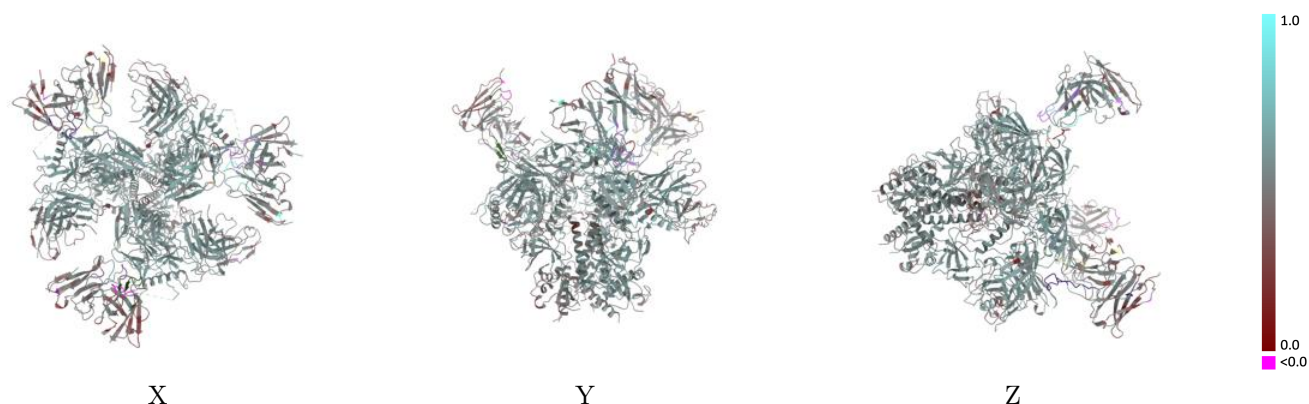


Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

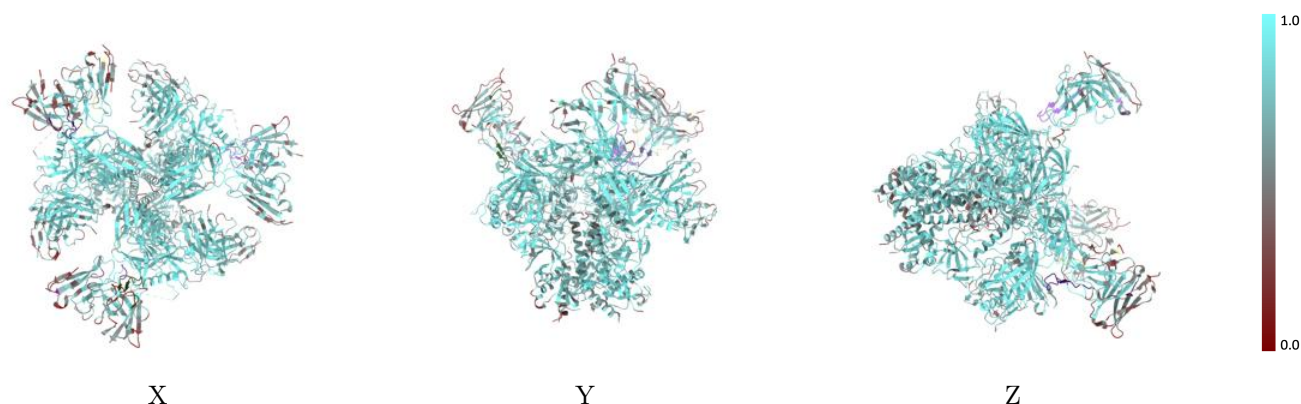


## 9.2 Q-score mapped to coordinate model [i](#)



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.

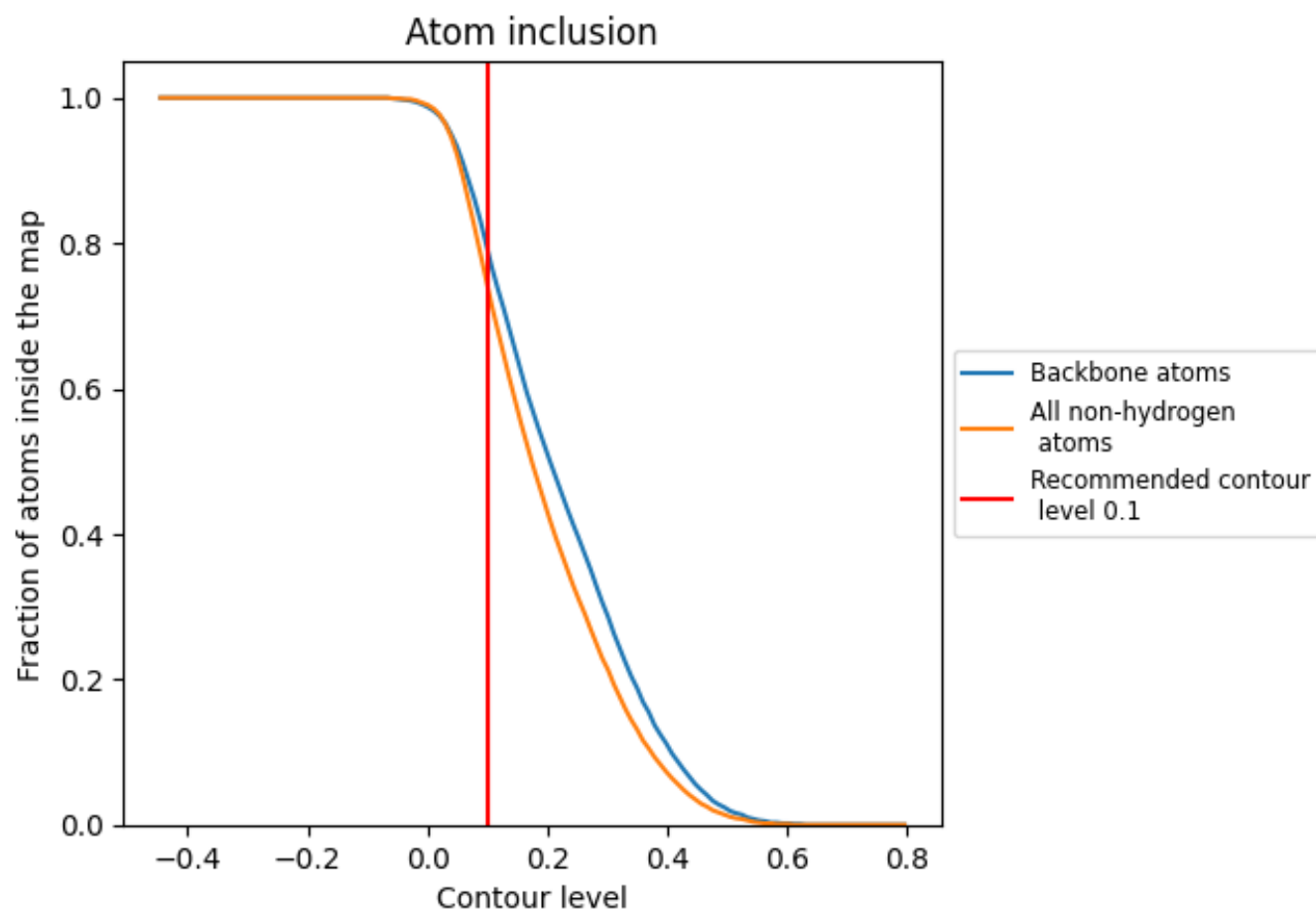
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.1).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 79% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.





















Chain	Atom inclusion	Q-score
All	 0.7420	 0.5130
A	 0.8090	 0.5450
B	 0.7000	 0.5120
C	 0.8010	 0.5420
D	 0.6790	 0.4730
E	 0.8160	 0.5490
F	 0.7340	 0.5170
G	 0.7140	 0.4960
H	 0.7760	 0.5420
I	 0.6780	 0.4800
J	 0.6020	 0.4590
K	 0.6650	 0.4730
L	 0.6660	 0.4660
M	 0.7770	 0.5250
N	 0.6930	 0.5000
O	 0.7290	 0.5090
P	 0.7960	 0.5460
Q	 0.6890	 0.4780
R	 0.5760	 0.4130
S	 0.6730	 0.4800
T	 0.5360	 0.4350
U	 0.6000	 0.4390
V	 0.9170	 0.5540
W	 0.7140	 0.5000
X	 0.7500	 0.5310
Y	 0.7400	 0.4410
Z	 0.5570	 0.4690
a	 0.7140	 0.5450
b	 0.5710	 0.5190
c	 0.7950	 0.5000
d	 0.7180	 0.4000
e	 0.8190	 0.5140
f	 0.4920	 0.4200
g	 0.7500	 0.4950
h	 0.4640	 0.3800



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Chain	Atom inclusion	Q-score
i	 0.6560	 0.4570
j	 0.7140	 0.4730
k	 0.6600	 0.4470
l	 0.6410	 0.4310
m	 0.4800	 0.3830
n	 0.5360	 0.4770
o	 0.7590	 0.4900
p	 0.6670	 0.5090
q	 0.7500	 0.5510
r	 0.5740	 0.3810