



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 10:30 PM UTC

PDB ID : 6V8Z / pdb_00006v8z
EMDB ID : EMD-21112
Title : VRC03 and 10-1074 Bound BG505 F14 HIV-1 SOSIP Envelope Trimer Structure
Authors : Henderson, R.; Acharya, P.
Deposited on : 2019-12-12
Resolution : 2.90 Å(reported)

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

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

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

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

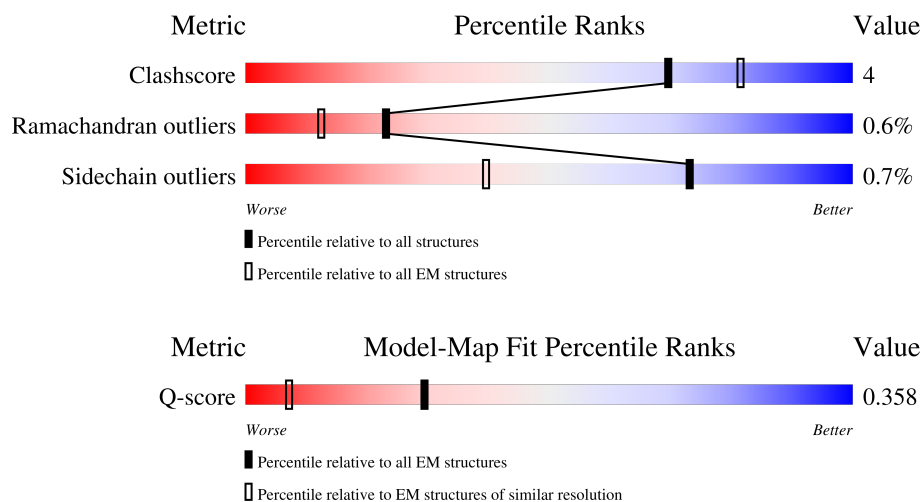
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.90 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	13054 (2.40 - 3.40)

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	472	25% 86% 8% • 5%
1	G	472	25% 86% 7% • 5%
1	M	472	26% 86% 7% • 5%
2	B	147	40% 89% 10% •

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Mol	Chain	Length	Quality of chain
2	H	147	39% 89% 10% ..
2	N	147	40% 89% 10% .
3	D	235	88% 87% 11% .
3	J	235	89% 86% 11% .
3	P	235	89% 87% 11% .
4	E	211	90% 85% 14%
4	K	211	90% 86% 14%
4	Q	211	90% 86% 14%
5	C	231	54% 90% 8% .
5	I	231	52% 89% 9% .
5	O	231	53% 90% 8% .
6	F	208	82% 95% 5%
6	L	208	82% 95% 5%
6	R	208	83% 95% 5%
7	0	2	100% 100%
7	1	2	100% 50% 50%
7	S	2	100% 100%
7	U	2	100% 50% 50%
7	V	2	50% 50% 50%
7	W	2	100% 100%
7	X	2	50% 100%
7	Y	2	100% 50% 50%
7	b	2	100% 100%
7	c	2	50% 100%
7	d	2	100% 50% 50%

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Mol	Chain	Length	Quality of chain
7	e	2	100%
7	g	2	100%
7	h	2	50%
7	i	2	100%
7	j	2	50%
7	k	2	100%
7	n	2	100%
7	o	2	50%
7	p	2	100%
7	q	2	50%
7	s	2	100%
7	t	2	50%
7	u	2	100%
7	v	2	50%
7	w	2	100%
7	z	2	100%
8	T	3	100%
8	f	3	100%
8	r	3	100%
9	Z	8	50%
9	l	8	25%
9	x	8	50%
10	a	4	75%
10	m	4	75%
10	y	4	75%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 35877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3534	2227	618	659	30		
1	G	449	Total	C	N	O	S	0	0
			3534	2227	618	659	30		
1	M	449	Total	C	N	O	S	0	0
			3534	2227	618	659	30		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ILE	VAL	conflict	UNP Q2N0S6
A	142	ALA	ASN	conflict	UNP Q2N0S6
A	203	MET	GLN	conflict	UNP Q2N0S6
A	204	VAL	ALA	conflict	UNP Q2N0S6
A	208	LEU	VAL	conflict	UNP Q2N0S6
A	255	LEU	VAL	conflict	UNP Q2N0S6
A	300	LEU	ASN	conflict	UNP Q2N0S6
A	302	LEU	ASN	conflict	UNP Q2N0S6
A	320	MET	THR	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	422	MET	GLN	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
G	68	ILE	VAL	conflict	UNP Q2N0S6
G	142	ALA	ASN	conflict	UNP Q2N0S6
G	203	MET	GLN	conflict	UNP Q2N0S6
G	204	VAL	ALA	conflict	UNP Q2N0S6
G	208	LEU	VAL	conflict	UNP Q2N0S6
G	255	LEU	VAL	conflict	UNP Q2N0S6
G	300	LEU	ASN	conflict	UNP Q2N0S6
G	302	LEU	ASN	conflict	UNP Q2N0S6
G	320	MET	THR	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	422	MET	GLN	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	68	ILE	VAL	conflict	UNP Q2N0S6
M	142	ALA	ASN	conflict	UNP Q2N0S6
M	203	MET	GLN	conflict	UNP Q2N0S6
M	204	VAL	ALA	conflict	UNP Q2N0S6
M	208	LEU	VAL	conflict	UNP Q2N0S6
M	255	LEU	VAL	conflict	UNP Q2N0S6
M	300	LEU	ASN	conflict	UNP Q2N0S6
M	302	LEU	ASN	conflict	UNP Q2N0S6
M	320	MET	THR	conflict	UNP Q2N0S6
M	332	ASN	THR	conflict	UNP Q2N0S6
M	422	MET	GLN	conflict	UNP Q2N0S6
M	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	147	Total	C	N	O	S	0	0
			1171	740	205	220	6		
2	H	147	Total	C	N	O	S	0	0
			1171	740	205	220	6		
2	N	147	Total	C	N	O	S	0	0
			1171	740	205	220	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S7
B	605	CYS	THR	conflict	UNP Q2N0S7
H	559	PRO	ILE	conflict	UNP Q2N0S7
H	605	CYS	THR	conflict	UNP Q2N0S7
N	559	PRO	ILE	conflict	UNP Q2N0S7
N	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called 10-1074 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	230	Total	C	N	O	S	0	0
			1753	1108	293	345	7		
3	J	230	Total	C	N	O	S	0	0
			1753	1108	293	345	7		
3	P	230	Total	C	N	O	S	0	0
			1753	1108	293	345	7		

- Molecule 4 is a protein called 10-1074 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	211	Total	C	N	O	S	0	0
			1607	1006	281	314	6		
4	K	211	Total	C	N	O	S	0	0
			1607	1006	281	314	6		
4	Q	211	Total	C	N	O	S	0	0
			1607	1006	281	314	6		

- Molecule 5 is a protein called VRC03 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	227	Total	C	N	O	S	0	0
			1739	1110	292	328	9		
5	I	227	Total	C	N	O	S	0	0
			1739	1110	292	328	9		
5	O	227	Total	C	N	O	S	0	0
			1739	1110	292	328	9		

- Molecule 6 is a protein called VRC03 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	208	Total	C	N	O	S	0	0
			1622	1020	276	321	5		
6	L	208	Total	C	N	O	S	0	0
			1622	1020	276	321	5		
6	R	208	Total	C	N	O	S	0	0
			1622	1020	276	321	5		

- 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	S	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	V	2	Total	C	N	O	0	0
			28	16	2	10		

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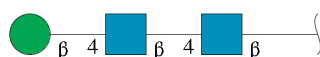
Mol	Chain	Residues	Atoms				AltConf	Trace
7	W	2	Total	C	N	O	0	0
			28	16	2	10		
7	X	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		
7	e	2	Total	C	N	O	0	0
			28	16	2	10		
7	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	i	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	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	o	2	Total	C	N	O	0	0
			28	16	2	10		
7	p	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	v	2	Total	C	N	O	0	0
			28	16	2	10		
7	w	2	Total	C	N	O	0	0
			28	16	2	10		

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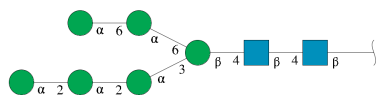
Mol	Chain	Residues	Atoms				AltConf	Trace
7	z	2	Total	C	N	O	0	0
			28	16	2	10		
7	0	2	Total	C	N	O	0	0
			28	16	2	10		
7	1	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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.



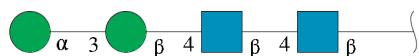
Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	3	Total	C	N	O	0	0
			39	22	2	15		
8	f	3	Total	C	N	O	0	0
			39	22	2	15		
8	r	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



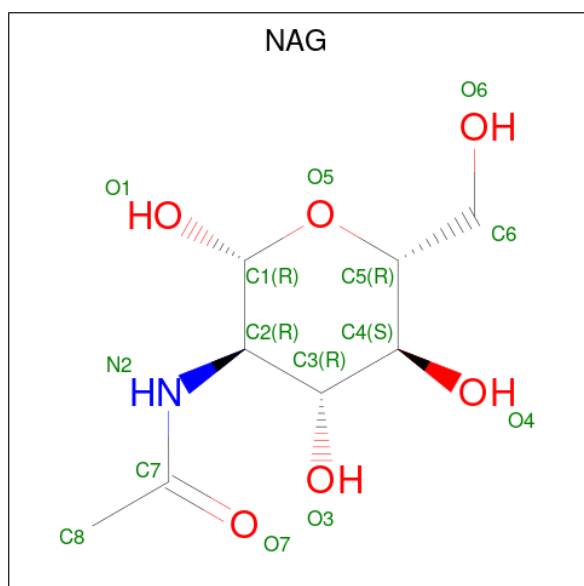
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	8	Total	C	N	O	0	0
			94	52	2	40		
9	l	8	Total	C	N	O	0	0
			94	52	2	40		
9	x	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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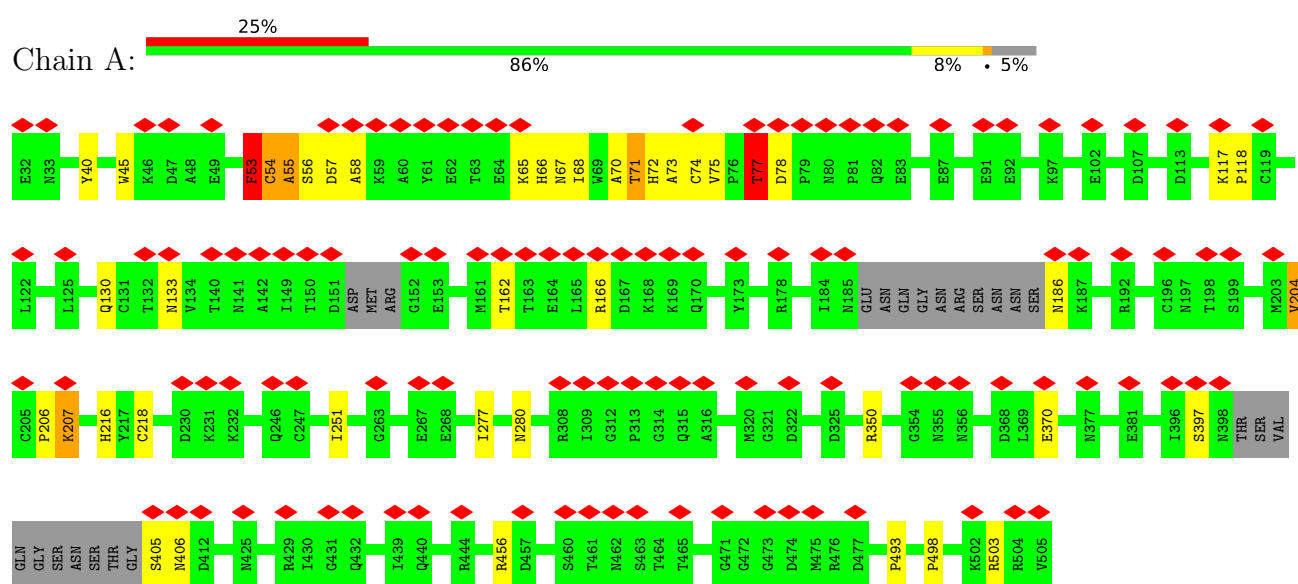
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Mol	Chain	Residues	Atoms				AltConf
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	H	1	Total	C	N	O	0
			14	8	1	5	
11	H	1	Total	C	N	O	0
			14	8	1	5	
11	H	1	Total	C	N	O	0
			14	8	1	5	
11	M	1	Total	C	N	O	0
			14	8	1	5	
11	M	1	Total	C	N	O	0
			14	8	1	5	
11	M	1	Total	C	N	O	0
			14	8	1	5	
11	M	1	Total	C	N	O	0
			14	8	1	5	
11	N	1	Total	C	N	O	0
			14	8	1	5	
11	N	1	Total	C	N	O	0
			14	8	1	5	
11	N	1	Total	C	N	O	0
			14	8	1	5	

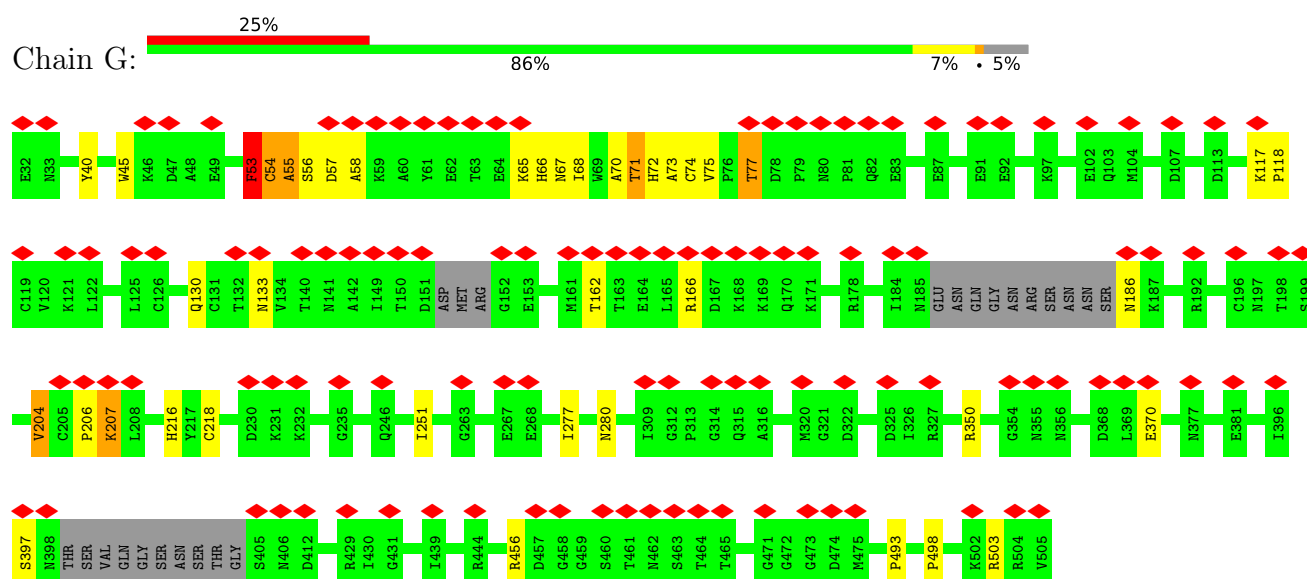
3 Residue-property plots [i](#)

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

• Molecule 1: Envelope glycoprotein gp120

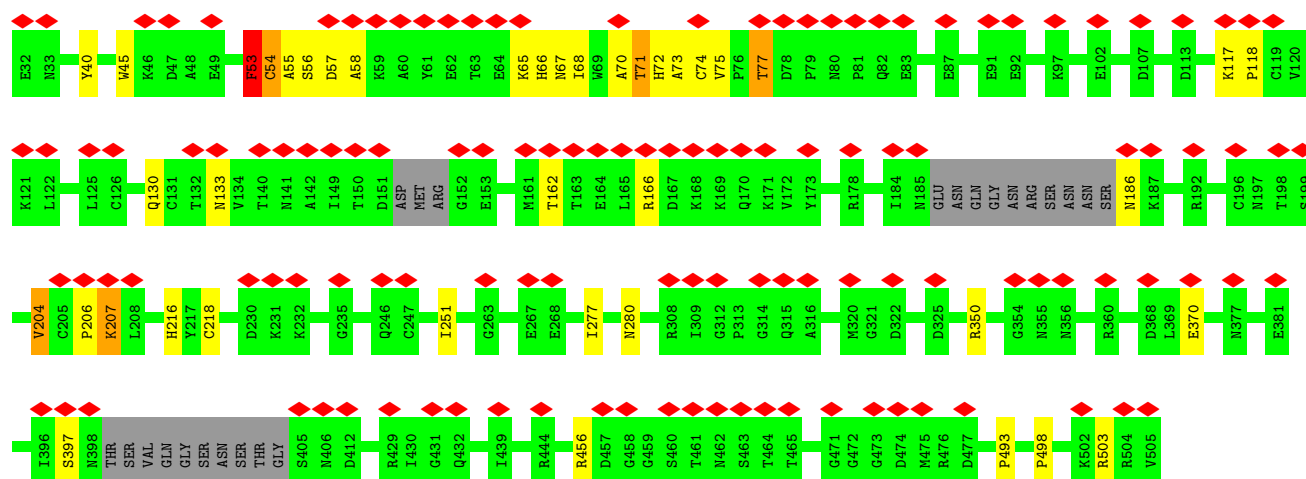


• Molecule 1: Envelope glycoprotein gp120



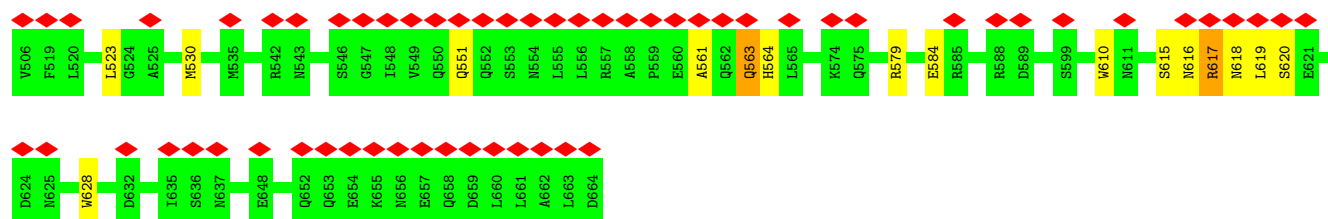
• Molecule 1: Envelope glycoprotein gp120

Chain M: 



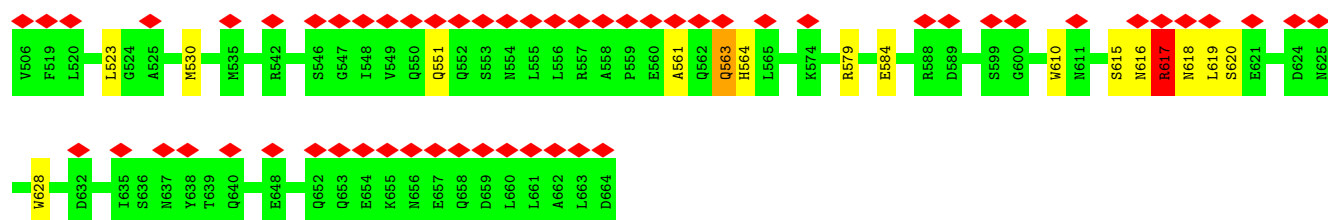
• Molecule 2: envelope glycoprotein gp41

Chain B: 



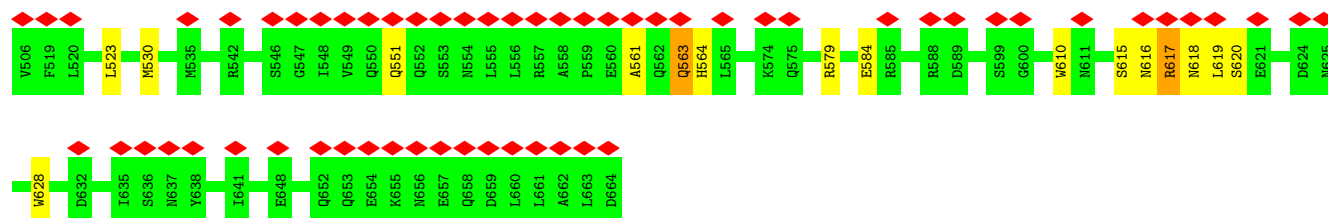
• Molecule 2: envelope glycoprotein gp41

Chain H: 

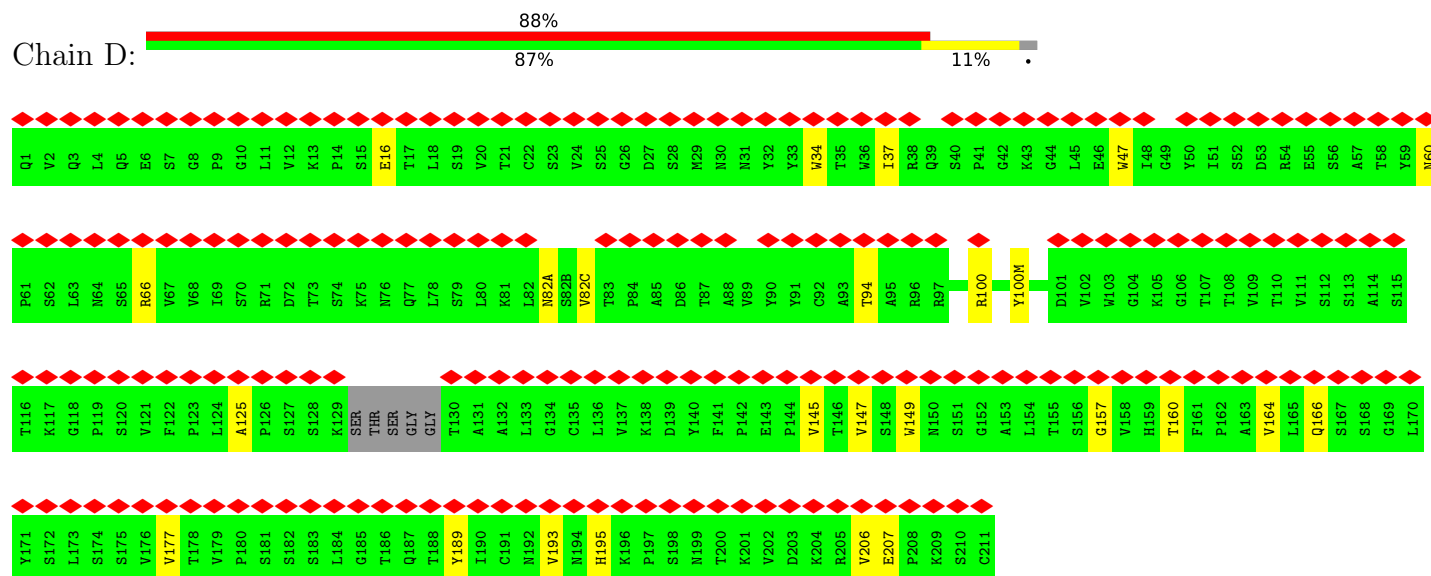


• Molecule 2: envelope glycoprotein gp41

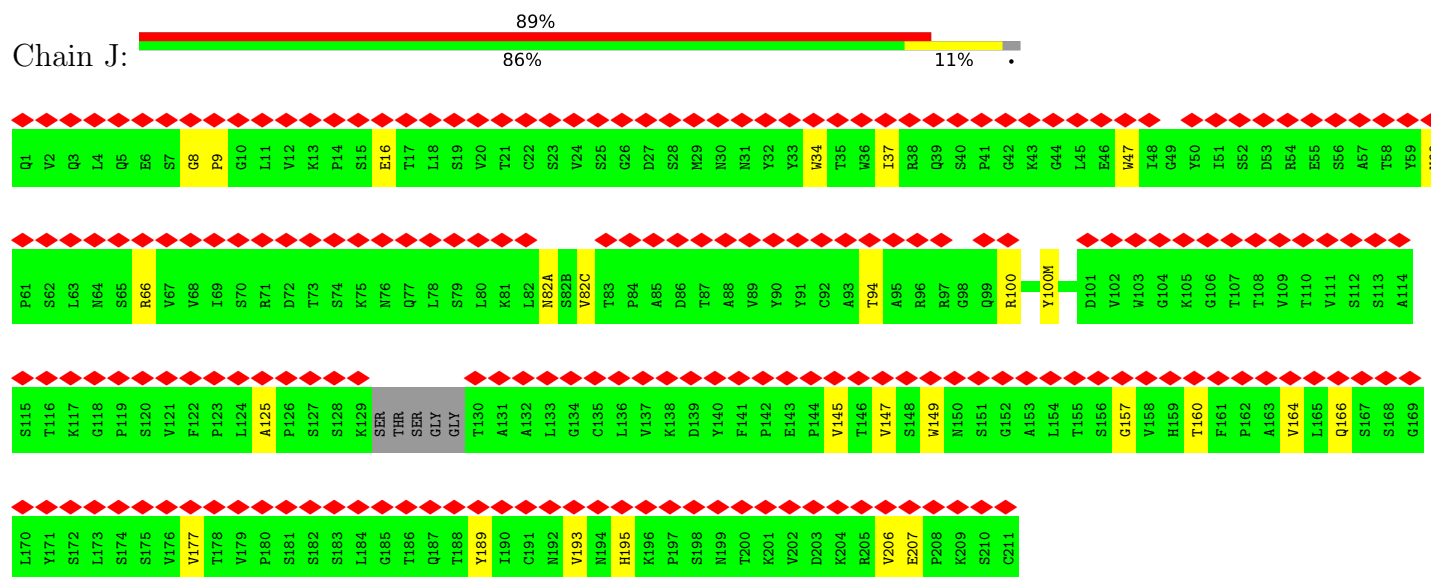
Chain N: 



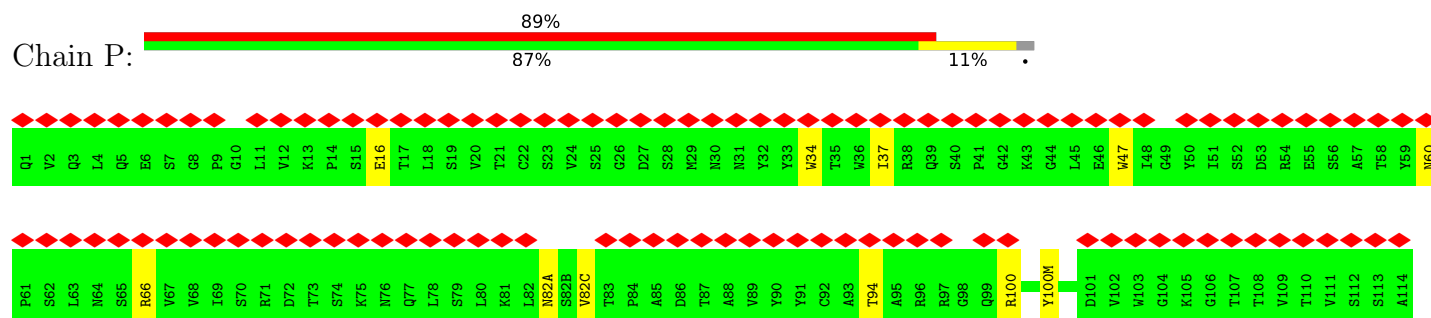
• Molecule 3: 10-1074 Fab Heavy Chain



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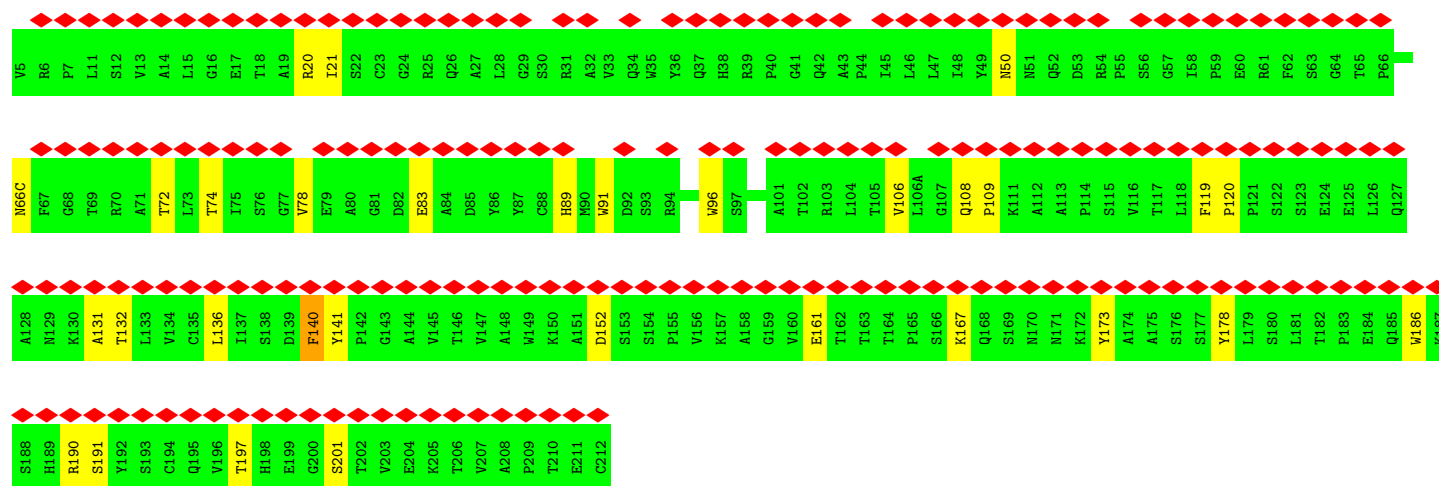
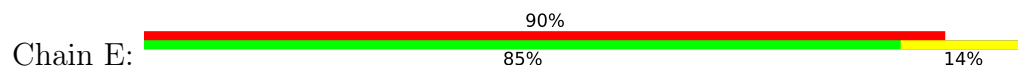


• Molecule 3: 10-1074 Fab Heavy Chain

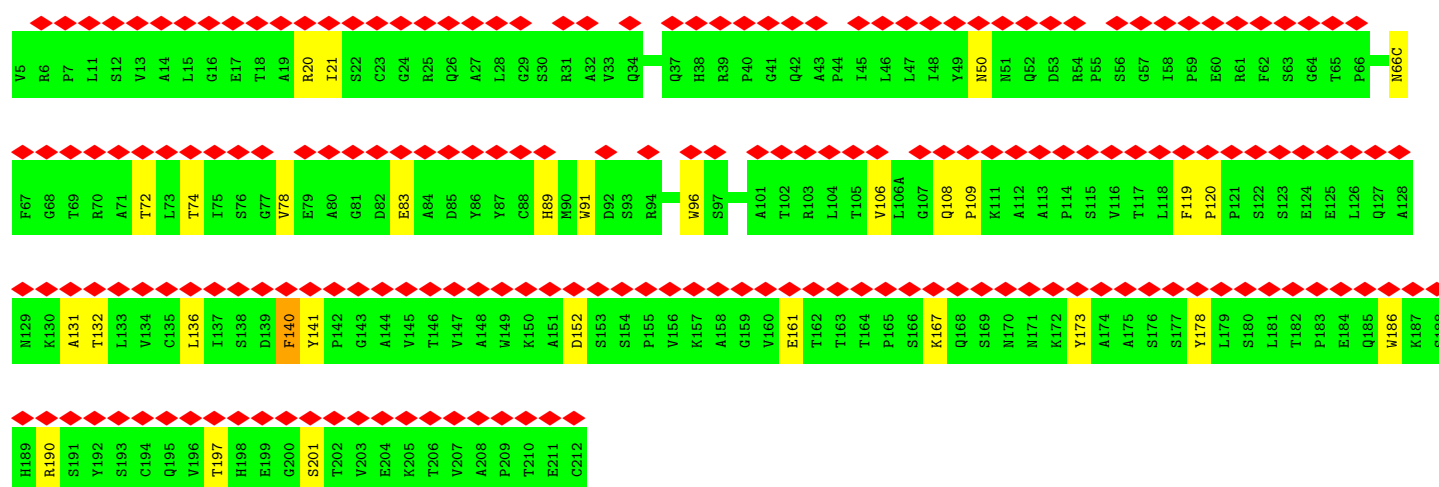
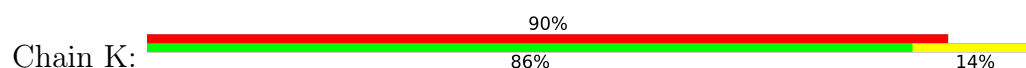




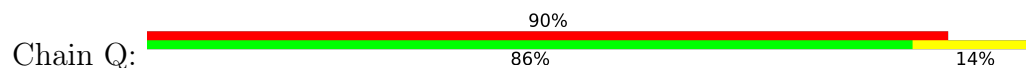
• Molecule 4: 10-1074 Fab Light Chain

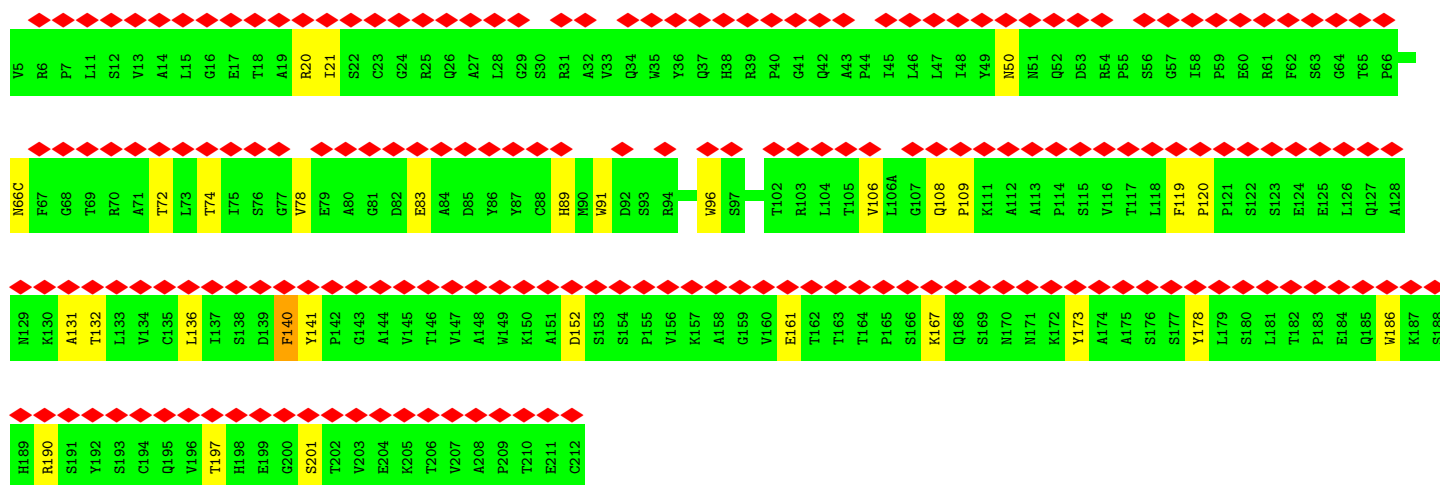


• Molecule 4: 10-1074 Fab Light Chain

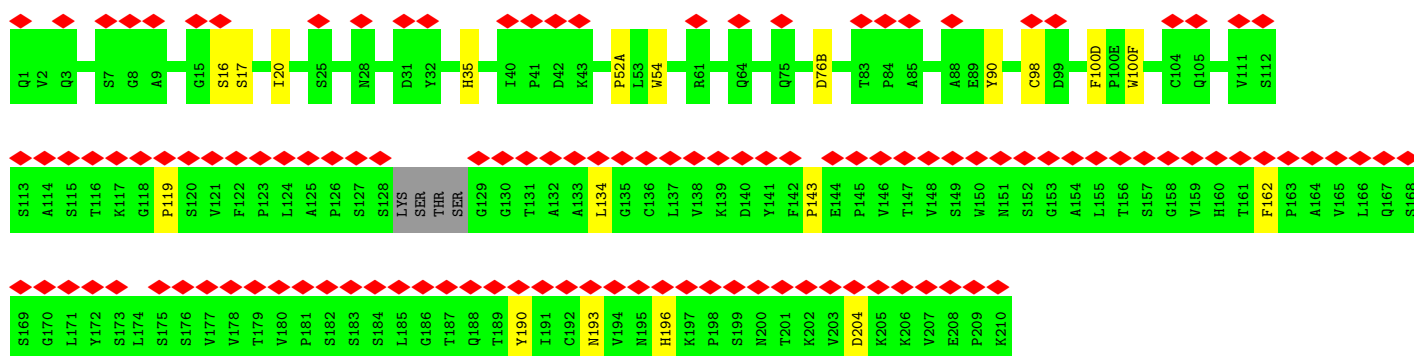
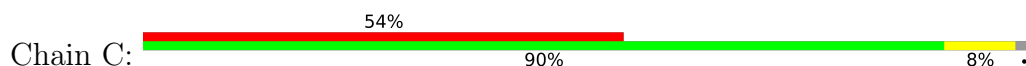


• Molecule 4: 10-1074 Fab Light Chain

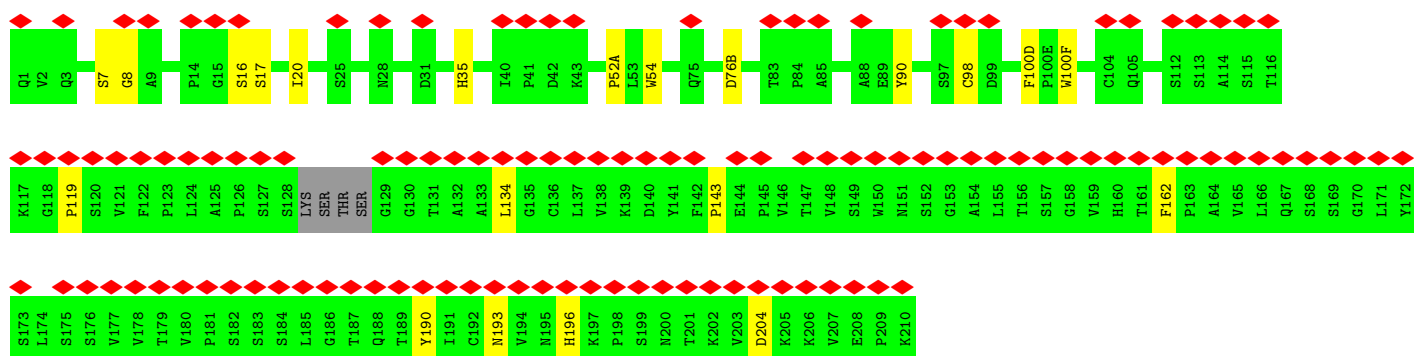
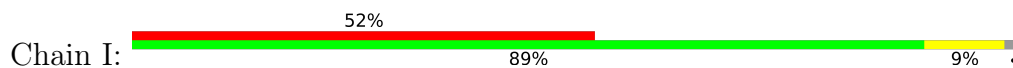




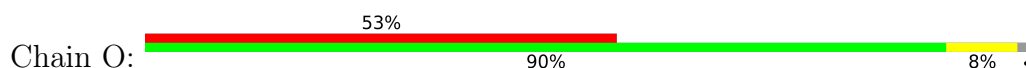
• Molecule 5: VRC03 Fab Heavy Chain

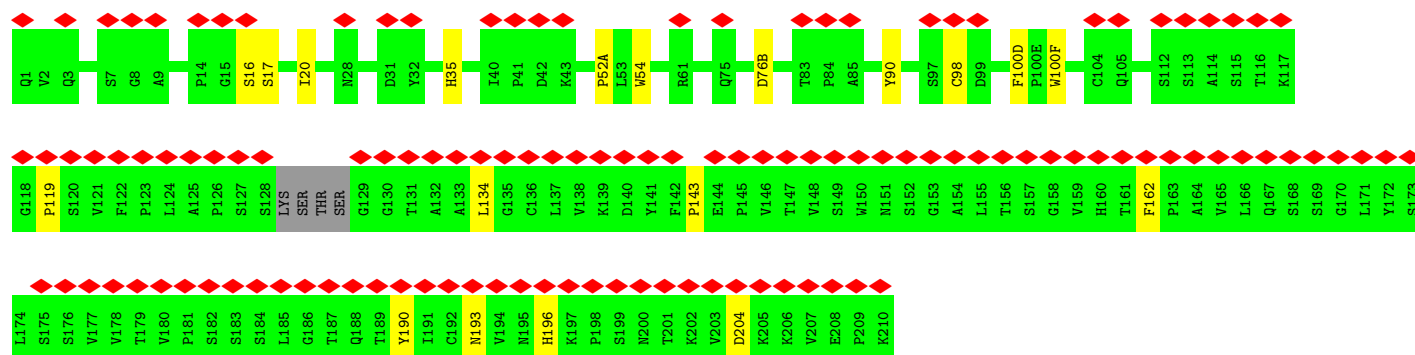


• Molecule 5: VRC03 Fab Heavy Chain

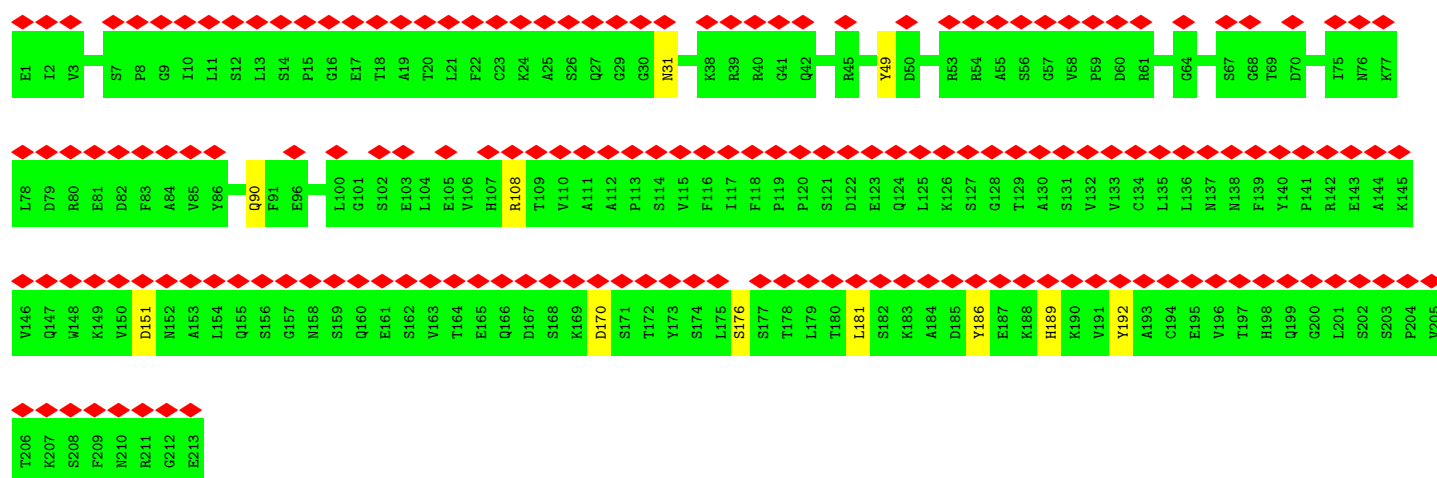
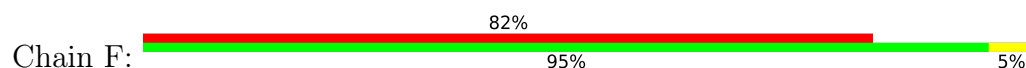


• Molecule 5: VRC03 Fab Heavy Chain

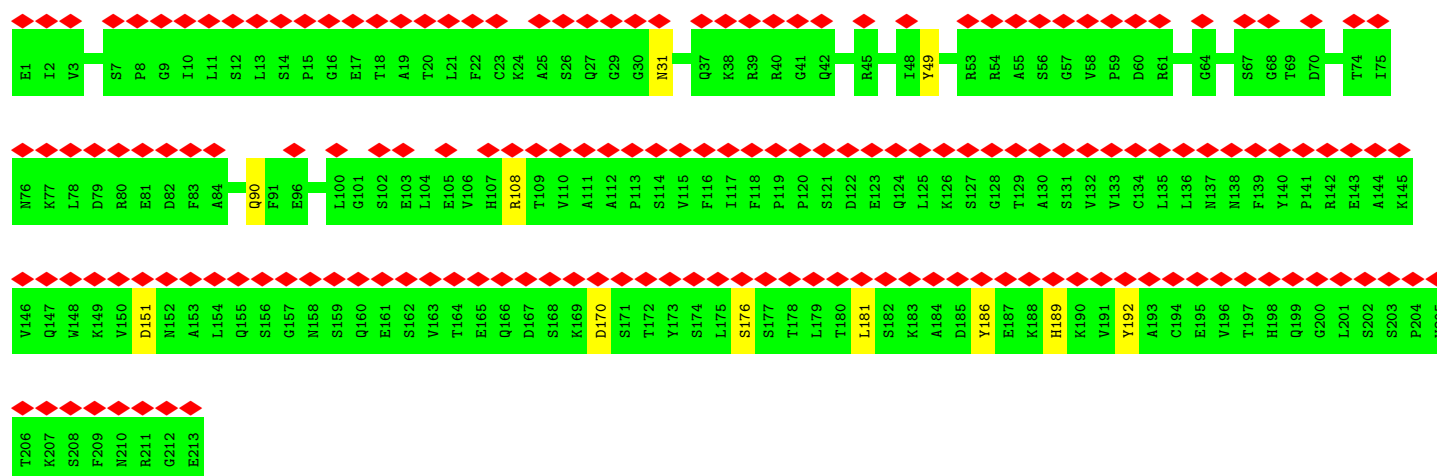
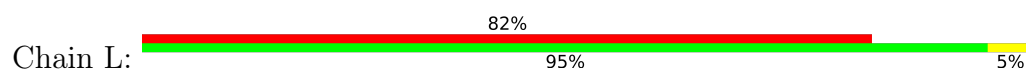




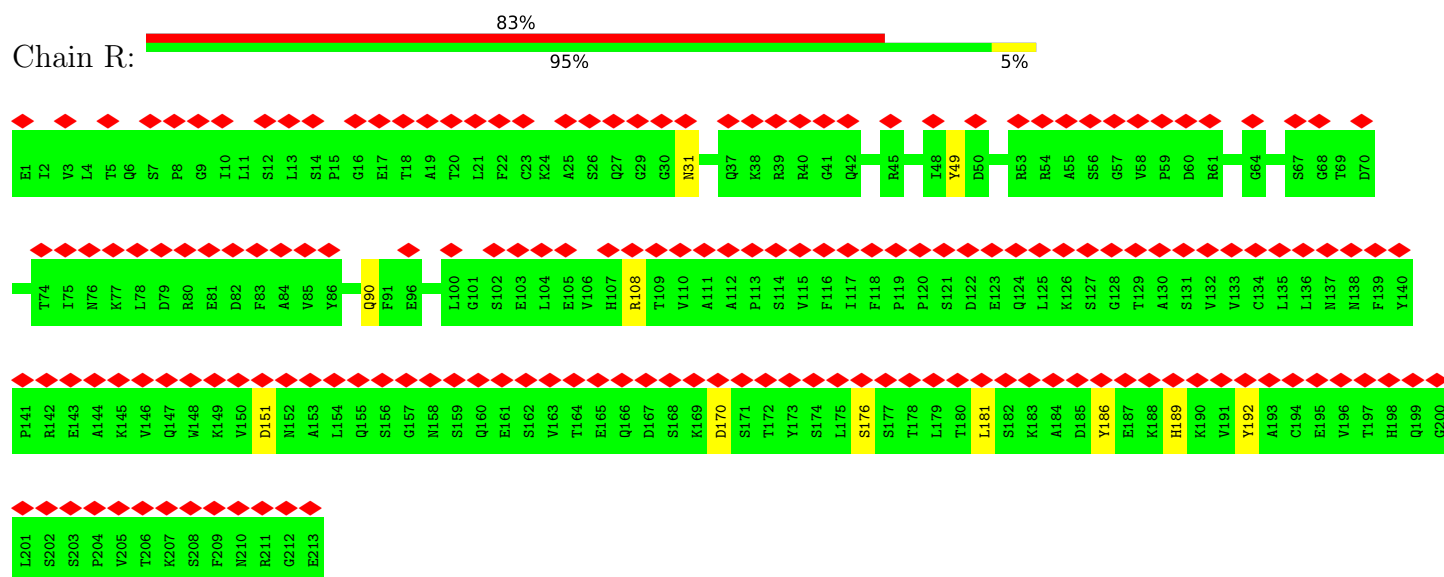
• Molecule 6: VRC03 Fab Light Chain



• Molecule 6: VRC03 Fab Light Chain



• Molecule 6: VRC03 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



- 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





- 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



- 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



- 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



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



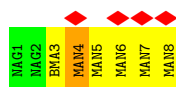
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



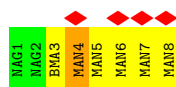
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



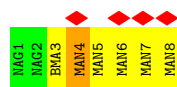
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



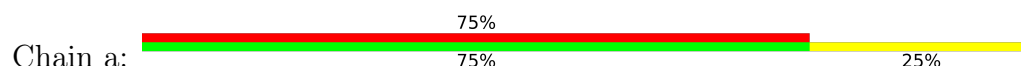
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



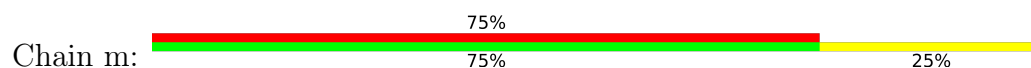
- Molecule 9: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 10: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 10: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



- Molecule 10: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	84378	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 ($e^-/\text{\AA}^2$)	54.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	37.497	Depositor
Minimum map value	-20.186	Depositor
Average map value	0.169	Depositor
Map value standard deviation	1.863	Depositor
Recommended contour level	10.5	Depositor
Map size (Å)	249.1176, 249.1176, 249.1176	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08312, 1.08312, 1.08312	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, 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	0.52	0/3607	0.85	8/4894 (0.2%)
1	G	0.52	0/3607	0.85	8/4894 (0.2%)
1	M	0.52	0/3607	0.85	7/4894 (0.1%)
2	B	0.43	0/1192	0.81	3/1618 (0.2%)
2	H	0.44	0/1192	0.81	3/1618 (0.2%)
2	N	0.43	0/1192	0.81	3/1618 (0.2%)
3	D	0.34	0/1796	0.76	2/2450 (0.1%)
3	J	0.34	0/1796	0.76	2/2450 (0.1%)
3	P	0.34	0/1796	0.76	2/2450 (0.1%)
4	E	0.38	0/1649	0.78	2/2250 (0.1%)
4	K	0.38	0/1649	0.78	2/2250 (0.1%)
4	Q	0.39	0/1649	0.78	2/2250 (0.1%)
5	C	0.39	0/1790	0.69	2/2444 (0.1%)
5	I	0.40	0/1790	0.69	2/2444 (0.1%)
5	O	0.40	0/1790	0.69	2/2444 (0.1%)
6	F	0.36	0/1657	0.71	0/2244
6	L	0.36	0/1657	0.71	0/2244
6	R	0.36	0/1657	0.71	0/2244
All	All	0.43	0/35073	0.78	50/47700 (0.1%)

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
2	B	0	2
2	H	0	2
2	N	0	2
4	E	0	1
4	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	Q	0	1
6	F	0	1
6	L	0	1
6	R	0	1
All	All	0	12

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	160	THR	CA-C-N	8.67	148.98	122.71
3	P	160	THR	C-N-CA	8.67	148.98	122.71
3	D	160	THR	CA-C-N	8.67	148.98	122.71
3	D	160	THR	C-N-CA	8.67	148.98	122.71
3	J	160	THR	CA-C-N	8.66	148.96	122.71
3	J	160	THR	C-N-CA	8.66	148.96	122.71
1	G	251	ILE	CA-C-N	8.37	142.23	121.80
1	G	251	ILE	C-N-CA	8.37	142.23	121.80
1	A	251	ILE	CA-C-N	8.37	142.22	121.80
1	A	251	ILE	C-N-CA	8.37	142.22	121.80
1	M	251	ILE	CA-C-N	8.37	142.21	121.80
1	M	251	ILE	C-N-CA	8.37	142.21	121.80
1	M	53	PHE	CB-CA-C	-7.83	96.61	109.53
1	A	53	PHE	CB-CA-C	-7.82	96.63	109.53
1	G	53	PHE	CB-CA-C	-7.80	96.65	109.53
2	H	617	ARG	N-CA-CB	-6.94	98.76	110.49
2	B	617	ARG	N-CA-CB	-6.93	98.77	110.49
2	N	617	ARG	N-CA-CB	-6.92	98.79	110.49
4	Q	109	PRO	CA-C-N	5.91	132.34	121.70
4	Q	109	PRO	C-N-CA	5.91	132.34	121.70
4	K	109	PRO	CA-C-N	5.91	132.34	121.70
4	K	109	PRO	C-N-CA	5.91	132.34	121.70
4	E	109	PRO	CA-C-N	5.90	132.32	121.70
4	E	109	PRO	C-N-CA	5.90	132.32	121.70
5	I	52(A)	PRO	CA-C-N	5.66	132.35	121.54
5	I	52(A)	PRO	C-N-CA	5.66	132.35	121.54
5	C	52(A)	PRO	CA-C-N	5.65	132.34	121.54
5	C	52(A)	PRO	C-N-CA	5.65	132.34	121.54
5	O	52(A)	PRO	CA-C-N	5.65	132.33	121.54
5	O	52(A)	PRO	C-N-CA	5.65	132.33	121.54
1	G	77	THR	N-CA-C	5.51	118.44	110.28
1	A	77	THR	N-CA-C	5.51	118.43	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	77	THR	N-CA-C	5.50	118.41	110.28
1	A	77	THR	CB-CA-C	-5.26	100.65	109.65
1	G	77	THR	CB-CA-C	-5.26	100.66	109.65
1	M	77	THR	CB-CA-C	-5.25	100.66	109.65
1	A	66	HIS	CB-CA-C	-5.16	101.85	109.90
1	M	66	HIS	CB-CA-C	-5.16	101.85	109.90
1	G	66	HIS	CB-CA-C	-5.16	101.86	109.90
1	G	207	LYS	N-CA-C	-5.15	106.97	113.20
1	A	207	LYS	N-CA-C	-5.12	107.00	113.20
2	H	563	GLN	CA-C-N	5.12	131.31	121.54
2	H	563	GLN	C-N-CA	5.12	131.31	121.54
2	N	563	GLN	CA-C-N	5.12	131.31	121.54
2	N	563	GLN	C-N-CA	5.12	131.31	121.54
2	B	563	GLN	CA-C-N	5.11	131.30	121.54
2	B	563	GLN	C-N-CA	5.11	131.30	121.54
1	M	207	LYS	N-CA-C	-5.10	107.03	113.20
1	G	55	ALA	N-CA-C	5.04	117.32	111.02
1	A	55	ALA	N-CA-C	5.02	117.29	111.02

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	615	SER	Peptide
2	B	616	ASN	Peptide
4	E	140	PHE	Peptide
6	F	90	GLN	Peptide
2	H	615	SER	Peptide
2	H	616	ASN	Peptide
4	K	140	PHE	Peptide
6	L	90	GLN	Peptide
2	N	615	SER	Peptide
2	N	616	ASN	Peptide
4	Q	140	PHE	Peptide
6	R	90	GLN	Peptide

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	3534	0	3488	29	0
1	G	3534	0	3488	27	0
1	M	3534	0	3488	27	0
2	B	1171	0	1158	11	0
2	H	1171	0	1158	12	0
2	N	1171	0	1158	11	0
3	D	1753	0	1721	17	0
3	J	1753	0	1721	18	0
3	P	1753	0	1721	17	0
4	E	1607	0	1552	21	0
4	K	1607	0	1552	20	0
4	Q	1607	0	1552	20	0
5	C	1739	0	1686	12	0
5	I	1739	0	1686	13	0
5	O	1739	0	1686	12	0
6	F	1622	0	1572	8	0
6	L	1622	0	1572	8	0
6	R	1622	0	1572	8	0
7	0	28	0	25	0	0
7	1	28	0	25	1	0
7	S	28	0	25	0	0
7	U	28	0	25	0	0
7	V	28	0	25	0	0
7	W	28	0	25	0	0
7	X	28	0	25	0	0
7	Y	28	0	25	0	0
7	b	28	0	25	1	0
7	c	28	0	25	0	0
7	d	28	0	25	1	0
7	e	28	0	25	0	0
7	g	28	0	25	0	0
7	h	28	0	25	0	0
7	i	28	0	25	0	0
7	j	28	0	25	0	0
7	k	28	0	25	0	0
7	n	28	0	25	1	0
7	o	28	0	25	0	0
7	p	28	0	25	1	0
7	q	28	0	25	0	0
7	s	28	0	25	0	0
7	t	28	0	25	0	0
7	u	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	v	28	0	25	0	0
7	w	28	0	25	0	0
7	z	28	0	25	0	0
8	T	39	0	34	0	0
8	f	39	0	34	0	0
8	r	39	0	34	0	0
9	Z	94	0	79	1	0
9	l	94	0	79	1	0
9	x	94	0	79	1	0
10	a	50	0	43	0	0
10	m	50	0	43	0	0
10	y	50	0	43	0	0
11	A	56	0	52	1	0
11	B	42	0	39	0	0
11	G	56	0	52	1	0
11	H	42	0	39	0	0
11	M	56	0	52	1	0
11	N	42	0	39	0	0
All	All	35877	0	34947	239	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 (239) 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:207:LYS:HZ1	2:B:563:GLN:HE21	1.34	0.76
5:I:76(B):ASP:OD2	1:M:206:PRO:HG2	1.89	0.73
1:A:206:PRO:HG2	5:O:76(B):ASP:OD2	1.89	0.73
5:C:76(B):ASP:OD2	1:G:206:PRO:HG2	1.89	0.72
1:G:57:ASP:OD1	1:G:58:ALA:N	2.23	0.72
1:M:57:ASP:OD1	1:M:58:ALA:N	2.23	0.72
1:A:57:ASP:OD1	1:A:58:ALA:N	2.23	0.70
1:G:207:LYS:HZ1	2:H:563:GLN:HE21	1.41	0.69
1:A:207:LYS:NZ	2:B:563:GLN:HE21	1.91	0.68
1:G:207:LYS:NZ	2:H:563:GLN:HE21	1.91	0.68
1:M:207:LYS:NZ	2:N:563:GLN:HE21	1.91	0.67
1:M:207:LYS:HZ1	2:N:563:GLN:HE21	1.46	0.63
4:K:120:PRO:O	4:K:132:THR:OG1	2.19	0.61
1:A:117:LYS:HB2	1:A:118:PRO:HD3	1.83	0.60
4:Q:108:GLN:O	4:Q:141:TYR:CD2	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:117:LYS:HB2	1:M:118:PRO:HD3	1.83	0.60
1:G:117:LYS:HB2	1:G:118:PRO:HD3	1.83	0.59
4:K:108:GLN:O	4:K:141:TYR:CD2	2.55	0.59
4:E:108:GLN:O	4:E:141:TYR:CD2	2.55	0.59
6:F:186:TYR:O	6:F:192:TYR:OH	2.21	0.58
6:L:186:TYR:O	6:L:192:TYR:OH	2.21	0.58
6:R:186:TYR:O	6:R:192:TYR:OH	2.21	0.57
6:R:108:ARG:NH1	6:R:170:ASP:O	2.37	0.57
2:B:584:GLU:OE2	2:H:579:ARG:NH2	2.38	0.57
6:L:108:ARG:NH1	6:L:170:ASP:O	2.37	0.57
2:H:584:GLU:OE2	2:N:579:ARG:NH2	2.38	0.56
2:B:579:ARG:NH2	2:N:584:GLU:OE2	2.38	0.56
6:F:108:ARG:NH1	6:F:170:ASP:O	2.37	0.56
4:Q:120:PRO:O	4:Q:132:THR:OG1	2.19	0.56
4:K:131:ALA:HB1	4:K:186:TRP:HE1	1.71	0.56
1:A:53:PHE:CZ	2:B:551:GLN:HG2	2.41	0.56
4:Q:131:ALA:HB1	4:Q:186:TRP:HE1	1.71	0.55
1:G:53:PHE:CZ	2:H:551:GLN:HG2	2.41	0.55
4:E:120:PRO:O	4:E:132:THR:OG1	2.18	0.55
4:E:131:ALA:HB1	4:E:186:TRP:HE1	1.71	0.55
1:A:56:SER:HB3	1:A:74:CYS:SG	2.47	0.54
1:G:56:SER:HB3	1:G:74:CYS:SG	2.48	0.54
4:Q:152:ASP:OD2	4:Q:190:ARG:HG2	2.08	0.54
4:K:152:ASP:OD2	4:K:190:ARG:HG2	2.08	0.54
1:M:53:PHE:CZ	2:N:551:GLN:HG2	2.41	0.54
4:E:152:ASP:OD2	4:E:190:ARG:HG2	2.08	0.54
1:M:55:ALA:HB3	1:M:216:HIS:O	2.08	0.53
1:G:55:ALA:HB3	1:G:216:HIS:O	2.08	0.53
1:A:55:ALA:HB3	1:A:216:HIS:O	2.08	0.53
1:G:498:PRO:HB3	2:H:610:TRP:CD2	2.44	0.53
2:N:618:ASN:O	2:N:620:SER:N	2.42	0.53
2:B:618:ASN:O	2:B:620:SER:N	2.42	0.53
1:M:56:SER:HB3	1:M:74:CYS:SG	2.47	0.53
1:M:130:GLN:OE1	1:M:186:ASN:N	2.42	0.52
3:D:100(M):TYR:OH	4:E:50:ASN:ND2	2.43	0.52
2:H:618:ASN:O	2:H:620:SER:N	2.42	0.52
3:P:100(M):TYR:OH	4:Q:50:ASN:ND2	2.43	0.52
1:A:498:PRO:HB3	2:B:610:TRP:CD2	2.44	0.52
1:M:498:PRO:HB3	2:N:610:TRP:CD2	2.44	0.52
1:A:130:GLN:OE1	1:A:186:ASN:N	2.42	0.52
3:D:66:ARG:NE	3:D:82(A):ASN:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ASN:OD1	1:A:456:ARG:HD3	2.10	0.52
1:G:280:ASN:OD1	1:G:456:ARG:HD3	2.10	0.52
3:J:100(M):TYR:OH	4:K:50:ASN:ND2	2.43	0.52
1:G:130:GLN:OE1	1:G:186:ASN:N	2.42	0.51
11:G:603:NAG:O7	6:L:31:ASN:ND2	2.44	0.51
4:Q:89:HIS:CE1	4:Q:91:TRP:HE1	2.29	0.51
3:J:66:ARG:NE	3:J:82(A):ASN:O	2.43	0.51
5:C:134:LEU:HD22	5:C:190:TYR:CD2	2.46	0.51
11:M:603:NAG:O7	6:R:31:ASN:ND2	2.44	0.51
11:A:603:NAG:O7	6:F:31:ASN:ND2	2.44	0.50
5:O:134:LEU:HD22	5:O:190:TYR:CD2	2.46	0.50
6:L:181:LEU:HB2	6:L:186:TYR:CZ	2.47	0.50
1:M:280:ASN:OD1	1:M:456:ARG:HD3	2.10	0.50
5:O:35:HIS:CD2	5:O:100(F):TRP:HE1	2.29	0.50
5:C:35:HIS:CD2	5:C:100(F):TRP:HE1	2.29	0.50
5:I:134:LEU:HD22	5:I:190:TYR:CD2	2.46	0.50
3:P:145:VAL:HG13	3:P:195:HIS:CE1	2.47	0.50
6:F:181:LEU:HB2	6:F:186:TYR:CZ	2.47	0.50
3:D:145:VAL:HG13	3:D:195:HIS:CE1	2.47	0.50
1:G:54:CYS:O	1:G:216:HIS:O	2.30	0.49
4:K:89:HIS:CE1	4:K:91:TRP:HE1	2.29	0.49
1:M:54:CYS:O	1:M:216:HIS:O	2.30	0.49
3:P:66:ARG:NE	3:P:82(A):ASN:O	2.43	0.49
6:R:181:LEU:HB2	6:R:186:TYR:CZ	2.47	0.49
3:J:145:VAL:HG13	3:J:195:HIS:CE1	2.47	0.49
5:I:35:HIS:CD2	5:I:100(F):TRP:HE1	2.29	0.49
3:D:60:ASN:HA	4:E:96:TRP:CZ3	2.48	0.49
1:A:54:CYS:O	1:A:216:HIS:O	2.30	0.49
4:E:89:HIS:CE1	4:E:91:TRP:HE1	2.29	0.49
5:I:98:CYS:SG	6:L:49:TYR:OH	2.71	0.49
6:L:181:LEU:N	6:L:186:TYR:OH	2.43	0.49
3:P:47:TRP:HE3	4:Q:96:TRP:CD1	2.31	0.49
1:M:53:PHE:HB2	1:M:218:CYS:O	2.13	0.49
3:P:60:ASN:HA	4:Q:96:TRP:CZ3	2.48	0.49
1:A:53:PHE:HB2	1:A:218:CYS:O	2.13	0.48
5:O:98:CYS:SG	6:R:49:TYR:OH	2.71	0.48
3:D:47:TRP:HE3	4:E:96:TRP:CD1	2.31	0.48
3:J:60:ASN:HA	4:K:96:TRP:CZ3	2.48	0.48
1:G:53:PHE:HB2	1:G:218:CYS:O	2.13	0.48
3:P:100:ARG:NH2	9:x:4:MAN:O6	2.44	0.48
5:C:98:CYS:SG	6:F:49:TYR:OH	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:47:TRP:HE3	4:K:96:TRP:CD1	2.31	0.48
1:M:40:TYR:CE1	1:M:493:PRO:HB2	2.49	0.48
1:M:67:ASN:H	1:M:71:THR:HG21	1.79	0.47
6:R:181:LEU:N	6:R:186:TYR:OH	2.43	0.47
5:O:143:PRO:O	5:O:196:HIS:NE2	2.44	0.47
1:A:40:TYR:CE1	1:A:493:PRO:HB2	2.49	0.47
1:G:40:TYR:CE1	1:G:493:PRO:HB2	2.49	0.47
1:G:67:ASN:H	1:G:71:THR:HG21	1.79	0.47
4:K:131:ALA:CB	4:K:186:TRP:HE1	2.28	0.47
5:O:193:ASN:ND2	5:O:204:ASP:OD1	2.48	0.47
1:A:133:ASN:OD1	7:d:1:NAG:N2	2.49	0.46
4:E:131:ALA:CB	4:E:186:TRP:HE1	2.28	0.46
4:K:78:VAL:HG11	4:K:106:VAL:HG11	1.97	0.46
1:G:204:VAL:O	1:G:204:VAL:HG12	2.15	0.46
1:M:133:ASN:OD1	7:l:1:NAG:N2	2.49	0.46
3:J:47:TRP:CE3	4:K:96:TRP:CD1	3.04	0.46
3:D:149:TRP:CD1	3:D:177:VAL:HG21	2.51	0.46
1:M:204:VAL:O	1:M:204:VAL:HG12	2.15	0.46
3:P:47:TRP:CE3	4:Q:96:TRP:CD1	3.04	0.46
1:A:67:ASN:H	1:A:71:THR:HG21	1.79	0.46
3:J:100:ARG:NH2	9:l:4:MAN:O6	2.44	0.46
1:G:133:ASN:OD1	7:p:1:NAG:N2	2.49	0.46
3:J:149:TRP:CD1	3:J:177:VAL:HG21	2.51	0.46
4:Q:131:ALA:CB	4:Q:186:TRP:HE1	2.28	0.46
3:D:47:TRP:CE3	4:E:96:TRP:CD1	3.04	0.46
1:A:204:VAL:O	1:A:204:VAL:HG12	2.15	0.46
1:G:56:SER:CB	1:G:74:CYS:SG	3.04	0.46
5:I:193:ASN:ND2	5:I:204:ASP:OD1	2.48	0.45
3:P:149:TRP:CD1	3:P:177:VAL:HG21	2.51	0.45
1:A:56:SER:CB	1:A:74:CYS:SG	3.04	0.45
1:A:162:THR:CG2	1:A:166:ARG:HA	2.47	0.45
6:F:181:LEU:N	6:F:186:TYR:OH	2.43	0.45
4:Q:78:VAL:HG11	4:Q:106:VAL:HG11	1.97	0.45
3:D:100:ARG:NH2	9:Z:4:MAN:O6	2.44	0.45
5:C:193:ASN:ND2	5:C:204:ASP:OD1	2.48	0.45
6:F:151:ASP:HB2	6:F:189:HIS:HB3	1.99	0.45
4:E:78:VAL:HG11	4:E:106:VAL:HG11	1.97	0.45
1:A:56:SER:HB3	1:A:74:CYS:CB	2.47	0.45
1:G:162:THR:CG2	1:G:166:ARG:HA	2.47	0.45
3:P:189:TYR:O	3:P:206:VAL:HG23	2.17	0.45
3:D:34:TRP:CD2	3:D:94:THR:HG22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:151:ASP:HB2	6:L:189:HIS:HB3	1.99	0.45
1:M:56:SER:CB	1:M:74:CYS:SG	3.04	0.45
3:P:34:TRP:CD2	3:P:94:THR:HG22	2.52	0.45
6:R:151:ASP:HB2	6:R:189:HIS:HB3	1.99	0.45
1:M:162:THR:CG2	1:M:166:ARG:HA	2.47	0.44
3:D:166:GLN:HA	4:E:161:GLU:CD	2.43	0.44
4:E:20:ARG:NH1	4:E:74:THR:OG1	2.50	0.44
5:I:143:PRO:O	5:I:196:HIS:NE2	2.44	0.44
1:M:118:PRO:HB3	2:N:563:GLN:NE2	2.33	0.44
1:M:350:ARG:NH1	1:M:397:SER:OG	2.50	0.44
1:A:118:PRO:HB3	2:B:563:GLN:NE2	2.32	0.44
1:G:56:SER:HB3	1:G:74:CYS:CB	2.47	0.44
1:G:118:PRO:HB3	2:H:563:GLN:NE2	2.32	0.44
3:J:34:TRP:CD2	3:J:94:THR:HG22	2.52	0.44
4:Q:20:ARG:NH1	4:Q:74:THR:OG1	2.51	0.44
1:A:405:SER:OG	1:A:406:ASN:N	2.50	0.44
3:D:189:TYR:O	3:D:206:VAL:HG23	2.17	0.44
5:C:35:HIS:CE1	5:C:100(D):PHE:CE1	3.06	0.44
3:J:125:ALA:CB	3:J:207:GLU:O	2.66	0.44
3:J:189:TYR:O	3:J:206:VAL:HG23	2.17	0.44
3:P:164:VAL:HG21	4:Q:178:TYR:CB	2.48	0.44
3:P:166:GLN:HA	4:Q:161:GLU:CD	2.43	0.44
5:O:119:PRO:HG3	5:O:196:HIS:HB2	2.00	0.44
5:O:35:HIS:CE1	5:O:100(D):PHE:CE1	3.06	0.44
4:K:20:ARG:NH1	4:K:74:THR:OG1	2.50	0.43
5:I:119:PRO:HG3	5:I:196:HIS:HB2	2.00	0.43
5:C:119:PRO:HG3	5:C:196:HIS:HB2	2.00	0.43
1:M:56:SER:HB3	1:M:74:CYS:CB	2.47	0.43
3:P:125:ALA:CB	3:P:207:GLU:O	2.66	0.43
5:C:143:PRO:O	5:C:196:HIS:NE2	2.44	0.43
5:C:162:PHE:CZ	6:F:176:SER:HB2	2.54	0.43
3:J:166:GLN:HA	4:K:161:GLU:CD	2.43	0.43
1:G:350:ARG:NH1	1:G:397:SER:OG	2.50	0.43
3:P:16:GLU:H	3:P:82(C):VAL:HG12	1.83	0.43
4:Q:21:ILE:C	4:Q:72:THR:HG23	2.44	0.43
4:Q:140:PHE:HB2	4:Q:173:TYR:HB2	2.01	0.43
3:D:157:GLY:O	3:D:177:VAL:HA	2.19	0.43
5:I:35:HIS:CE1	5:I:100(D):PHE:CE1	3.06	0.43
3:D:125:ALA:CB	3:D:207:GLU:O	2.66	0.43
4:K:21:ILE:C	4:K:72:THR:HG23	2.44	0.43
5:O:16:SER:OG	5:O:17:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:83:GLU:OE1	4:E:167:LYS:NZ	2.47	0.43
4:E:140:PHE:HB2	4:E:173:TYR:HB2	2.01	0.43
3:J:34:TRP:CZ3	3:J:94:THR:HG23	2.54	0.43
1:A:350:ARG:NH1	1:A:397:SER:OG	2.50	0.43
4:E:119:PHE:CE2	4:E:136:LEU:HD12	2.54	0.43
3:J:147:VAL:HG22	3:J:193:VAL:HG22	2.01	0.43
1:M:117:LYS:CB	1:M:118:PRO:HD3	2.49	0.43
4:E:152:ASP:OD1	4:E:191:SER:OG	2.35	0.43
1:G:117:LYS:CB	1:G:118:PRO:HD3	2.49	0.42
5:C:20:ILE:CD1	5:C:90:TYR:HD2	2.32	0.42
3:J:164:VAL:HG21	4:K:178:TYR:CB	2.48	0.42
4:K:140:PHE:HB2	4:K:173:TYR:HB2	2.01	0.42
3:J:8:GLY:HA2	3:J:9:PRO:HD3	1.92	0.42
4:K:119:PHE:CE2	4:K:136:LEU:HD12	2.54	0.42
1:A:117:LYS:CB	1:A:118:PRO:HD3	2.49	0.42
4:E:21:ILE:C	4:E:72:THR:HG23	2.44	0.42
3:P:147:VAL:HG22	3:P:193:VAL:HG22	2.01	0.42
4:Q:83:GLU:OE1	4:Q:167:LYS:NZ	2.47	0.42
3:J:16:GLU:H	3:J:82(C):VAL:HG12	1.83	0.42
3:D:164:VAL:HG21	4:E:178:TYR:CB	2.48	0.42
4:K:197:THR:HA	4:K:201:SER:O	2.20	0.42
4:Q:197:THR:HA	4:Q:201:SER:O	2.20	0.42
5:O:20:ILE:CD1	5:O:90:TYR:HD2	2.32	0.42
5:O:162:PHE:CZ	6:R:176:SER:HB2	2.54	0.42
4:E:197:THR:HA	4:E:201:SER:O	2.20	0.42
3:J:157:GLY:O	3:J:177:VAL:HA	2.19	0.42
5:I:162:PHE:CZ	6:L:176:SER:HB2	2.54	0.42
3:P:157:GLY:O	3:P:177:VAL:HA	2.19	0.42
4:Q:119:PHE:CE2	4:Q:136:LEU:HD12	2.54	0.42
1:A:45:TRP:HE1	2:B:523:LEU:HD22	1.85	0.42
1:M:45:TRP:HE1	2:N:523:LEU:HD22	1.85	0.42
2:N:530:MET:HE3	2:N:628:TRP:CZ3	2.55	0.42
2:H:530:MET:HE3	2:H:628:TRP:CZ3	2.55	0.42
3:P:34:TRP:CZ3	3:P:94:THR:HG23	2.54	0.42
3:D:34:TRP:CZ3	3:D:94:THR:HG23	2.54	0.41
1:A:370:GLU:HG3	5:C:54:TRP:CZ3	2.56	0.41
5:C:16:SER:OG	5:C:17:SER:N	2.52	0.41
5:I:20:ILE:CD1	5:I:90:TYR:HD2	2.32	0.41
3:D:16:GLU:H	3:D:82(C):VAL:HG12	1.83	0.41
3:D:147:VAL:HG22	3:D:193:VAL:HG22	2.01	0.41
1:G:70:ALA:O	1:G:71:THR:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:70:ALA:O	1:M:71:THR:O	2.39	0.41
5:I:16:SER:OG	5:I:17:SER:N	2.52	0.41
1:A:70:ALA:O	1:A:71:THR:O	2.39	0.41
2:B:530:MET:HE3	2:B:628:TRP:CZ3	2.55	0.41
7:b:1:NAG:H4	7:b:2:NAG:H2	1.92	0.41
1:G:45:TRP:HE1	2:H:523:LEU:HD22	1.85	0.41
1:G:370:GLU:HG3	5:I:54:TRP:CZ3	2.56	0.41
1:A:77:THR:O	1:A:78:ASP:C	2.64	0.41
1:G:45:TRP:HE1	2:H:523:LEU:CD2	2.34	0.41
5:I:7:SER:HA	5:I:8:GLY:HA2	1.88	0.41
1:M:45:TRP:HE1	2:N:523:LEU:CD2	2.34	0.41
4:E:108:GLN:HB3	4:E:141:TYR:CZ	2.56	0.41
4:K:108:GLN:HB3	4:K:141:TYR:CZ	2.56	0.40
4:K:83:GLU:OE1	4:K:167:LYS:NZ	2.47	0.40
7:n:1:NAG:H4	7:n:2:NAG:H2	1.92	0.40
1:A:45:TRP:HE1	2:B:523:LEU:CD2	2.34	0.40
2:H:617:ARG:HG3	2:H:618:ASN:H	1.86	0.40
4:Q:108:GLN:HB3	4:Q:141:TYR:CZ	2.56	0.40
1:M:370:GLU:HG3	5:O:54:TRP:CZ3	2.56	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	441/472 (93%)	399 (90%)	38 (9%)	4 (1%)	14	41
1	G	441/472 (93%)	399 (90%)	38 (9%)	4 (1%)	14	41
1	M	441/472 (93%)	399 (90%)	38 (9%)	4 (1%)	14	41
2	B	145/147 (99%)	131 (90%)	10 (7%)	4 (3%)	4	15
2	H	145/147 (99%)	131 (90%)	10 (7%)	4 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	145/147 (99%)	131 (90%)	10 (7%)	4 (3%)	4	15
3	D	226/235 (96%)	213 (94%)	13 (6%)	0	100	100
3	J	226/235 (96%)	214 (95%)	12 (5%)	0	100	100
3	P	226/235 (96%)	213 (94%)	13 (6%)	0	100	100
4	E	209/211 (99%)	190 (91%)	18 (9%)	1 (0%)	24	54
4	K	209/211 (99%)	190 (91%)	18 (9%)	1 (0%)	24	54
4	Q	209/211 (99%)	190 (91%)	18 (9%)	1 (0%)	24	54
5	C	223/231 (96%)	208 (93%)	15 (7%)	0	100	100
5	I	223/231 (96%)	208 (93%)	15 (7%)	0	100	100
5	O	223/231 (96%)	208 (93%)	15 (7%)	0	100	100
6	F	206/208 (99%)	191 (93%)	15 (7%)	0	100	100
6	L	206/208 (99%)	191 (93%)	15 (7%)	0	100	100
6	R	206/208 (99%)	191 (93%)	15 (7%)	0	100	100
All	All	4350/4512 (96%)	3997 (92%)	326 (8%)	27 (1%)	23	51

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	503	ARG
2	B	617	ARG
1	G	71	THR
1	G	503	ARG
2	H	617	ARG
1	M	71	THR
1	M	503	ARG
2	N	617	ARG
1	A	73	ALA
1	G	73	ALA
1	M	73	ALA
1	A	277	ILE
2	B	561	ALA
2	B	564	HIS
2	B	619	LEU
4	E	66(C)	ASN
1	G	277	ILE
2	H	561	ALA

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Mol	Chain	Res	Type
2	H	564	HIS
2	H	619	LEU
4	K	66(C)	ASN
1	M	277	ILE
2	N	561	ALA
2	N	564	HIS
2	N	619	LEU
4	Q	66(C)	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	401/421 (95%)	393 (98%)	8 (2%)	48	78
1	G	401/421 (95%)	393 (98%)	8 (2%)	48	78
1	M	401/421 (95%)	393 (98%)	8 (2%)	48	78
2	B	127/127 (100%)	127 (100%)	0	100	100
2	H	127/127 (100%)	127 (100%)	0	100	100
2	N	127/127 (100%)	127 (100%)	0	100	100
3	D	202/205 (98%)	201 (100%)	1 (0%)	81	93
3	J	202/205 (98%)	201 (100%)	1 (0%)	81	93
3	P	202/205 (98%)	201 (100%)	1 (0%)	81	93
4	E	175/175 (100%)	175 (100%)	0	100	100
4	K	175/175 (100%)	175 (100%)	0	100	100
4	Q	175/175 (100%)	175 (100%)	0	100	100
5	C	194/198 (98%)	194 (100%)	0	100	100
5	I	194/198 (98%)	194 (100%)	0	100	100
5	O	194/198 (98%)	194 (100%)	0	100	100
6	F	181/181 (100%)	181 (100%)	0	100	100
6	L	181/181 (100%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	R	181/181 (100%)	181 (100%)	0	100	100
All	All	3840/3921 (98%)	3813 (99%)	27 (1%)	73	92

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	54	CYS
1	A	65	LYS
1	A	68	ILE
1	A	72	HIS
1	A	75	VAL
1	A	77	THR
1	A	204	VAL
3	D	37	ILE
1	G	53	PHE
1	G	54	CYS
1	G	65	LYS
1	G	68	ILE
1	G	72	HIS
1	G	75	VAL
1	G	77	THR
1	G	204	VAL
3	J	37	ILE
1	M	53	PHE
1	M	54	CYS
1	M	65	LYS
1	M	68	ILE
1	M	72	HIS
1	M	75	VAL
1	M	77	THR
1	M	204	VAL
3	P	37	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	186	ASN
1	A	352	HIS
2	B	543	ASN

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Mol	Chain	Res	Type
2	B	550	GLN
2	B	554	ASN
2	B	563	GLN
2	B	590	GLN
4	E	50	ASN
4	E	89	HIS
4	E	189	HIS
5	C	35	HIS
6	F	198	HIS
1	G	66	HIS
1	G	186	ASN
1	G	352	HIS
2	H	550	GLN
2	H	554	ASN
2	H	563	GLN
2	H	590	GLN
4	K	50	ASN
4	K	89	HIS
4	K	189	HIS
5	I	35	HIS
6	L	198	HIS
1	M	66	HIS
1	M	186	ASN
1	M	352	HIS
2	N	543	ASN
2	N	550	GLN
2	N	554	ASN
2	N	563	GLN
2	N	590	GLN
4	Q	50	ASN
4	Q	89	HIS
4	Q	189	HIS
5	O	35	HIS
6	R	198	HIS

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 ⓘ

99 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	0	1	7,1	14,14,15	0.33	0	17,19,21	0.54	0
7	NAG	0	2	7	14,14,15	0.33	0	17,19,21	0.48	0
7	NAG	1	1	7,1	14,14,15	0.71	1 (7%)	17,19,21	0.88	1 (5%)
7	NAG	1	2	7	14,14,15	0.56	0	17,19,21	1.00	1 (5%)
7	NAG	S	1	7,1	14,14,15	0.55	0	17,19,21	1.01	1 (5%)
7	NAG	S	2	7	14,14,15	0.26	0	17,19,21	0.66	1 (5%)
8	NAG	T	1	1,8	14,14,15	0.21	0	17,19,21	0.48	0
8	NAG	T	2	8	14,14,15	0.34	0	17,19,21	0.51	0
8	BMA	T	3	8	11,11,12	0.84	0	15,15,17	0.70	0
7	NAG	U	1	7,1	14,14,15	0.70	1 (7%)	17,19,21	1.22	1 (5%)
7	NAG	U	2	7	14,14,15	0.28	0	17,19,21	0.57	0
7	NAG	V	1	7,1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
7	NAG	V	2	7	14,14,15	0.41	0	17,19,21	0.58	0
7	NAG	W	1	7,1	14,14,15	0.30	0	17,19,21	0.98	1 (5%)
7	NAG	W	2	7	14,14,15	0.84	1 (7%)	17,19,21	1.06	1 (5%)
7	NAG	X	1	7,1	14,14,15	0.22	0	17,19,21	0.56	0
7	NAG	X	2	7	14,14,15	0.31	0	17,19,21	0.50	0
7	NAG	Y	1	7,1	14,14,15	0.21	0	17,19,21	0.65	1 (5%)
7	NAG	Y	2	7	14,14,15	0.26	0	17,19,21	0.44	0
9	NAG	Z	1	9,1	14,14,15	0.58	0	17,19,21	0.57	0
9	NAG	Z	2	9	14,14,15	0.24	0	17,19,21	0.69	0
9	BMA	Z	3	9	11,11,12	0.96	0	15,15,17	1.76	4 (26%)
9	MAN	Z	4	9	11,11,12	0.98	0	15,15,17	1.61	2 (13%)
9	MAN	Z	5	9	11,11,12	0.60	0	15,15,17	1.03	1 (6%)
9	MAN	Z	6	9	11,11,12	1.07	1 (9%)	15,15,17	1.51	1 (6%)
9	MAN	Z	7	9	11,11,12	0.60	0	15,15,17	1.05	1 (6%)
9	MAN	Z	8	9	11,11,12	0.74	0	15,15,17	1.22	2 (13%)
10	NAG	a	1	1,10	14,14,15	0.45	0	17,19,21	0.53	0
10	NAG	a	2	10	14,14,15	0.38	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	a	3	10	11,11,12	0.59	0	15,15,17	0.74	0
10	MAN	a	4	10	11,11,12	0.88	0	15,15,17	1.09	2 (13%)
7	NAG	b	1	7,1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
7	NAG	b	2	7	14,14,15	0.63	1 (7%)	17,19,21	0.82	1 (5%)
7	NAG	c	1	7,1	14,14,15	0.32	0	17,19,21	0.55	0
7	NAG	c	2	7	14,14,15	0.32	0	17,19,21	0.48	0
7	NAG	d	1	7,1	14,14,15	0.70	1 (7%)	17,19,21	0.88	1 (5%)
7	NAG	d	2	7	14,14,15	0.56	0	17,19,21	1.00	1 (5%)
7	NAG	e	1	7,1	14,14,15	0.55	0	17,19,21	1.02	1 (5%)
7	NAG	e	2	7	14,14,15	0.25	0	17,19,21	0.65	1 (5%)
8	NAG	f	1	1,8	14,14,15	0.21	0	17,19,21	0.49	0
8	NAG	f	2	8	14,14,15	0.34	0	17,19,21	0.52	0
8	BMA	f	3	8	11,11,12	0.84	0	15,15,17	0.70	0
7	NAG	g	1	7,1	14,14,15	0.71	1 (7%)	17,19,21	1.22	1 (5%)
7	NAG	g	2	7	14,14,15	0.28	0	17,19,21	0.57	0
7	NAG	h	1	7,1	14,14,15	0.30	0	17,19,21	0.83	1 (5%)
7	NAG	h	2	7	14,14,15	0.40	0	17,19,21	0.58	0
7	NAG	i	1	7,1	14,14,15	0.30	0	17,19,21	0.97	1 (5%)
7	NAG	i	2	7	14,14,15	0.84	1 (7%)	17,19,21	1.06	1 (5%)
7	NAG	j	1	7,1	14,14,15	0.22	0	17,19,21	0.57	0
7	NAG	j	2	7	14,14,15	0.31	0	17,19,21	0.49	0
7	NAG	k	1	7,1	14,14,15	0.21	0	17,19,21	0.66	1 (5%)
7	NAG	k	2	7	14,14,15	0.26	0	17,19,21	0.44	0
9	NAG	l	1	9,1	14,14,15	0.58	0	17,19,21	0.56	0
9	NAG	l	2	9	14,14,15	0.25	0	17,19,21	0.69	0
9	BMA	l	3	9	11,11,12	0.96	0	15,15,17	1.76	4 (26%)
9	MAN	l	4	9	11,11,12	0.98	0	15,15,17	1.61	2 (13%)
9	MAN	l	5	9	11,11,12	0.61	0	15,15,17	1.03	1 (6%)
9	MAN	l	6	9	11,11,12	1.07	1 (9%)	15,15,17	1.51	2 (13%)
9	MAN	l	7	9	11,11,12	0.59	0	15,15,17	1.04	1 (6%)
9	MAN	l	8	9	11,11,12	0.74	0	15,15,17	1.22	2 (13%)
10	NAG	m	1	1,10	14,14,15	0.45	0	17,19,21	0.53	0
10	NAG	m	2	10	14,14,15	0.38	0	17,19,21	0.45	0
10	BMA	m	3	10	11,11,12	0.59	0	15,15,17	0.72	0
10	MAN	m	4	10	11,11,12	0.87	0	15,15,17	1.09	2 (13%)
7	NAG	n	1	7,1	14,14,15	0.38	0	17,19,21	0.75	1 (5%)
7	NAG	n	2	7	14,14,15	0.63	1 (7%)	17,19,21	0.82	1 (5%)
7	NAG	o	1	7,1	14,14,15	0.32	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	o	2	7	14,14,15	0.32	0	17,19,21	0.48	0
7	NAG	p	1	7,1	14,14,15	0.69	1 (7%)	17,19,21	0.88	1 (5%)
7	NAG	p	2	7	14,14,15	0.56	0	17,19,21	1.01	1 (5%)
7	NAG	q	1	7,1	14,14,15	0.54	0	17,19,21	1.01	1 (5%)
7	NAG	q	2	7	14,14,15	0.26	0	17,19,21	0.66	1 (5%)
8	NAG	r	1	1,8	14,14,15	0.23	0	17,19,21	0.48	0
8	NAG	r	2	8	14,14,15	0.33	0	17,19,21	0.51	0
8	BMA	r	3	8	11,11,12	0.83	0	15,15,17	0.71	0
7	NAG	s	1	7,1	14,14,15	0.71	1 (7%)	17,19,21	1.21	1 (5%)
7	NAG	s	2	7	14,14,15	0.29	0	17,19,21	0.57	0
7	NAG	t	1	7,1	14,14,15	0.30	0	17,19,21	0.83	1 (5%)
7	NAG	t	2	7	14,14,15	0.40	0	17,19,21	0.58	0
7	NAG	u	1	7,1	14,14,15	0.29	0	17,19,21	0.98	1 (5%)
7	NAG	u	2	7	14,14,15	0.84	1 (7%)	17,19,21	1.06	1 (5%)
7	NAG	v	1	7,1	14,14,15	0.22	0	17,19,21	0.56	0
7	NAG	v	2	7	14,14,15	0.31	0	17,19,21	0.50	0
7	NAG	w	1	7,1	14,14,15	0.22	0	17,19,21	0.66	1 (5%)
7	NAG	w	2	7	14,14,15	0.25	0	17,19,21	0.44	0
9	NAG	x	1	9,1	14,14,15	0.58	0	17,19,21	0.57	0
9	NAG	x	2	9	14,14,15	0.25	0	17,19,21	0.69	0
9	BMA	x	3	9	11,11,12	0.95	0	15,15,17	1.77	4 (26%)
9	MAN	x	4	9	11,11,12	0.99	0	15,15,17	1.61	2 (13%)
9	MAN	x	5	9	11,11,12	0.60	0	15,15,17	1.03	1 (6%)
9	MAN	x	6	9	11,11,12	1.07	1 (9%)	15,15,17	1.51	1 (6%)
9	MAN	x	7	9	11,11,12	0.59	0	15,15,17	1.05	1 (6%)
9	MAN	x	8	9	11,11,12	0.74	0	15,15,17	1.22	2 (13%)
10	NAG	y	1	1,10	14,14,15	0.45	0	17,19,21	0.53	0
10	NAG	y	2	10	14,14,15	0.38	0	17,19,21	0.45	0
10	BMA	y	3	10	11,11,12	0.59	0	15,15,17	0.74	0
10	MAN	y	4	10	11,11,12	0.88	0	15,15,17	1.09	2 (13%)
7	NAG	z	1	7,1	14,14,15	0.38	0	17,19,21	0.76	1 (5%)
7	NAG	z	2	7	14,14,15	0.63	1 (7%)	17,19,21	0.82	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	e	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	e	2	7	-	2/6/23/26	0/1/1/1
8	NAG	f	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	f	2	8	-	1/6/23/26	0/1/1/1
8	BMA	f	3	8	-	0/2/19/22	0/1/1/1
7	NAG	g	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	g	2	7	-	2/6/23/26	0/1/1/1
7	NAG	h	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	h	2	7	-	2/6/23/26	0/1/1/1
7	NAG	i	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	4/6/23/26	0/1/1/1
7	NAG	j	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	j	2	7	-	0/6/23/26	0/1/1/1
7	NAG	k	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	k	2	7	-	0/6/23/26	0/1/1/1
9	NAG	l	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	l	2	9	-	0/6/23/26	0/1/1/1
9	BMA	l	3	9	-	2/2/19/22	0/1/1/1
9	MAN	l	4	9	-	2/2/19/22	0/1/1/1
9	MAN	l	5	9	-	2/2/19/22	0/1/1/1
9	MAN	l	6	9	-	2/2/19/22	0/1/1/1
9	MAN	l	7	9	-	1/2/19/22	0/1/1/1
9	MAN	l	8	9	-	2/2/19/22	0/1/1/1
10	NAG	m	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	m	2	10	-	2/6/23/26	0/1/1/1
10	BMA	m	3	10	-	1/2/19/22	0/1/1/1
10	MAN	m	4	10	-	2/2/19/22	1/1/1/1
7	NAG	n	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	n	2	7	-	2/6/23/26	0/1/1/1
7	NAG	o	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	o	2	7	-	2/6/23/26	0/1/1/1
7	NAG	p	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	p	2	7	-	4/6/23/26	0/1/1/1
7	NAG	q	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	q	2	7	-	2/6/23/26	0/1/1/1
8	NAG	r	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	r	2	8	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	r	3	8	-	0/2/19/22	0/1/1/1
7	NAG	s	1	7,1	-	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	7,1	-	2/6/23/26	0/1/1/1
7	NAG	t	2	7	-	2/6/23/26	0/1/1/1
7	NAG	u	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	u	2	7	-	4/6/23/26	0/1/1/1
7	NAG	v	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	v	2	7	-	0/6/23/26	0/1/1/1
7	NAG	w	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	w	2	7	-	0/6/23/26	0/1/1/1
9	NAG	x	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	x	2	9	-	0/6/23/26	0/1/1/1
9	BMA	x	3	9	-	2/2/19/22	0/1/1/1
9	MAN	x	4	9	-	2/2/19/22	0/1/1/1
9	MAN	x	5	9	-	2/2/19/22	0/1/1/1
9	MAN	x	6	9	-	2/2/19/22	0/1/1/1
9	MAN	x	7	9	-	1/2/19/22	0/1/1/1
9	MAN	x	8	9	-	2/2/19/22	0/1/1/1
10	NAG	y	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	y	2	10	-	2/6/23/26	0/1/1/1
10	BMA	y	3	10	-	1/2/19/22	0/1/1/1
10	MAN	y	4	10	-	2/2/19/22	1/1/1/1
7	NAG	z	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	z	2	7	-	2/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	6	MAN	O5-C5	3.36	1.50	1.43
9	l	6	MAN	O5-C5	3.35	1.50	1.43
9	x	6	MAN	O5-C5	3.34	1.49	1.43
7	i	2	NAG	C1-C2	2.62	1.55	1.52
7	u	2	NAG	C1-C2	2.59	1.55	1.52
7	W	2	NAG	C1-C2	2.59	1.55	1.52
7	s	1	NAG	O5-C1	-2.46	1.39	1.43
7	g	1	NAG	O5-C1	-2.45	1.39	1.43
7	U	1	NAG	O5-C1	-2.44	1.39	1.43
7	1	1	NAG	C1-C2	2.13	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	n	2	NAG	C1-C2	2.07	1.55	1.52
7	d	1	NAG	C1-C2	2.07	1.55	1.52
7	p	1	NAG	C1-C2	2.05	1.55	1.52
7	z	2	NAG	C1-C2	2.05	1.55	1.52
7	b	2	NAG	C1-C2	2.05	1.55	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	l	4	MAN	C1-O5-C5	5.21	119.17	112.19
9	Z	4	MAN	C1-O5-C5	5.20	119.16	112.19
9	x	4	MAN	C1-O5-C5	5.18	119.12	112.19
9	Z	6	MAN	C1-O5-C5	4.93	118.79	112.19
9	l	6	MAN	C1-O5-C5	4.92	118.78	112.19
9	x	6	MAN	C1-O5-C5	4.90	118.75	112.19
9	x	3	BMA	C1-O5-C5	4.59	118.34	112.19
9	l	3	BMA	C1-O5-C5	4.58	118.33	112.19
9	Z	3	BMA	C1-O5-C5	4.56	118.30	112.19
9	Z	8	MAN	C1-O5-C5	3.81	117.29	112.19
9	x	8	MAN	C1-O5-C5	3.81	117.29	112.19
9	l	8	MAN	C1-O5-C5	3.79	117.27	112.19
7	g	1	NAG	C2-N2-C7	3.49	127.58	122.90
7	U	1	NAG	C2-N2-C7	3.49	127.57	122.90
7	s	1	NAG	C2-N2-C7	3.47	127.55	122.90
7	u	1	NAG	C1-O5-C5	3.24	116.52	112.19
7	W	1	NAG	C1-O5-C5	3.23	116.52	112.19
7	u	2	NAG	C2-N2-C7	3.21	127.20	122.90
7	i	1	NAG	C1-O5-C5	3.21	116.48	112.19
7	W	2	NAG	C2-N2-C7	3.19	127.18	122.90
7	i	2	NAG	C2-N2-C7	3.19	127.18	122.90
7	p	2	NAG	C2-N2-C7	3.16	127.13	122.90
7	l	2	NAG	C2-N2-C7	3.14	127.11	122.90
7	d	2	NAG	C2-N2-C7	3.13	127.09	122.90
7	n	2	NAG	C1-O5-C5	3.02	116.24	112.19
7	z	2	NAG	C1-O5-C5	3.00	116.20	112.19
7	b	2	NAG	C1-O5-C5	2.99	116.20	112.19
10	y	4	MAN	C1-O5-C5	2.95	116.15	112.19
10	m	4	MAN	C1-O5-C5	2.95	116.14	112.19
10	a	4	MAN	C1-O5-C5	2.94	116.13	112.19
9	l	5	MAN	C1-O5-C5	2.92	116.10	112.19
9	Z	5	MAN	C1-O5-C5	2.91	116.08	112.19
9	x	5	MAN	C1-O5-C5	2.88	116.05	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	t	1	NAG	C1-O5-C5	2.81	115.95	112.19
7	V	1	NAG	C1-O5-C5	2.80	115.94	112.19
7	h	1	NAG	C1-O5-C5	2.79	115.92	112.19
9	l	3	BMA	C1-C2-C3	2.57	113.38	109.64
10	a	4	MAN	O2-C2-C3	-2.56	104.84	110.15
9	Z	3	BMA	C1-C2-C3	2.56	113.37	109.64
9	x	3	BMA	C1-C2-C3	2.56	113.37	109.64
10	m	4	MAN	O2-C2-C3	-2.55	104.87	110.15
10	y	4	MAN	O2-C2-C3	-2.54	104.88	110.15
7	q	2	NAG	C1-O5-C5	2.30	115.27	112.19
7	S	2	NAG	C1-O5-C5	2.30	115.27	112.19
7	e	2	NAG	C1-O5-C5	2.25	115.20	112.19
9	l	3	BMA	C3-C4-C5	-2.23	106.19	110.23
7	w	1	NAG	C1-O5-C5	2.23	115.17	112.19
9	Z	3	BMA	C3-C4-C5	-2.23	106.19	110.23
9	Z	8	MAN	O2-C2-C3	-2.22	105.55	110.15
9	x	8	MAN	O2-C2-C3	-2.22	105.55	110.15
9	l	8	MAN	O2-C2-C3	-2.22	105.56	110.15
9	Z	7	MAN	O2-C2-C3	-2.21	105.58	110.15
7	k	1	NAG	C1-O5-C5	2.20	115.14	112.19
9	x	3	BMA	C3-C4-C5	-2.20	106.24	110.23
9	l	7	MAN	O2-C2-C3	-2.20	105.59	110.15
9	x	7	MAN	O2-C2-C3	-2.20	105.59	110.15
7	Y	1	NAG	C1-O5-C5	2.20	115.13	112.19
7	l	1	NAG	O4-C4-C5	-2.19	103.94	109.32
7	d	1	NAG	O4-C4-C5	-2.17	103.97	109.32
7	p	1	NAG	O4-C4-C5	-2.17	103.98	109.32
7	z	1	NAG	C1-O5-C5	2.08	114.97	112.19
7	b	1	NAG	C1-O5-C5	2.08	114.97	112.19
7	e	1	NAG	C1-O5-C5	2.07	114.96	112.19
7	n	1	NAG	C1-O5-C5	2.07	114.96	112.19
7	S	1	NAG	C1-O5-C5	2.05	114.94	112.19
9	l	4	MAN	O2-C2-C3	-2.05	105.91	110.15
9	Z	3	BMA	O5-C1-C2	2.05	115.67	110.79
9	x	4	MAN	O2-C2-C3	-2.05	105.91	110.15
9	x	3	BMA	O5-C1-C2	2.04	115.65	110.79
9	Z	4	MAN	O2-C2-C3	-2.03	105.94	110.15
9	l	3	BMA	O5-C1-C2	2.03	115.64	110.79
7	q	1	NAG	C1-O5-C5	2.03	114.91	112.19
9	l	6	MAN	C1-C2-C3	-2.00	106.73	109.64

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	V	2	NAG	C4-C5-C6-O6
7	h	2	NAG	C4-C5-C6-O6
7	t	2	NAG	C4-C5-C6-O6
9	Z	8	MAN	O5-C5-C6-O6
9	l	8	MAN	O5-C5-C6-O6
9	x	8	MAN	O5-C5-C6-O6
9	Z	1	NAG	O5-C5-C6-O6
9	l	1	NAG	O5-C5-C6-O6
9	x	1	NAG	O5-C5-C6-O6
7	d	2	NAG	C4-C5-C6-O6
7	p	2	NAG	C4-C5-C6-O6
7	l	2	NAG	C4-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
7	t	2	NAG	O5-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
7	s	1	NAG	O5-C5-C6-O6
8	T	1	NAG	O5-C5-C6-O6
8	f	1	NAG	O5-C5-C6-O6
8	r	1	NAG	O5-C5-C6-O6
10	a	4	MAN	O5-C5-C6-O6
10	m	4	MAN	O5-C5-C6-O6
10	y	4	MAN	O5-C5-C6-O6
9	Z	8	MAN	C4-C5-C6-O6
9	l	8	MAN	C4-C5-C6-O6
9	x	8	MAN	C4-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
7	u	2	NAG	O5-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
7	o	2	NAG	O5-C5-C6-O6
7	0	2	NAG	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
7	p	2	NAG	O5-C5-C6-O6
7	l	2	NAG	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	e	1	NAG	C4-C5-C6-O6
7	q	1	NAG	C4-C5-C6-O6
7	c	1	NAG	O5-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
7	0	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	T	1	NAG	C4-C5-C6-O6
8	f	1	NAG	C4-C5-C6-O6
8	r	1	NAG	C4-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
7	i	2	NAG	C4-C5-C6-O6
7	u	2	NAG	C4-C5-C6-O6
7	c	2	NAG	C4-C5-C6-O6
7	o	2	NAG	C4-C5-C6-O6
7	0	2	NAG	C4-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
7	e	1	NAG	O5-C5-C6-O6
7	q	1	NAG	O5-C5-C6-O6
9	Z	1	NAG	C4-C5-C6-O6
9	l	1	NAG	C4-C5-C6-O6
9	x	1	NAG	C4-C5-C6-O6
9	Z	3	BMA	C4-C5-C6-O6
9	Z	6	MAN	C4-C5-C6-O6
9	l	3	BMA	C4-C5-C6-O6
9	l	6	MAN	C4-C5-C6-O6
9	x	3	BMA	C4-C5-C6-O6
9	x	6	MAN	C4-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
10	m	2	NAG	O5-C5-C6-O6
10	y	2	NAG	O5-C5-C6-O6
7	U	1	NAG	C4-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
7	s	1	NAG	C4-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	n	2	NAG	O5-C5-C6-O6
7	z	2	NAG	O5-C5-C6-O6
10	m	4	MAN	C4-C5-C6-O6
7	b	2	NAG	C4-C5-C6-O6
7	n	2	NAG	C4-C5-C6-O6
7	o	1	NAG	C4-C5-C6-O6
7	z	2	NAG	C4-C5-C6-O6
10	a	4	MAN	C4-C5-C6-O6
10	y	4	MAN	C4-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	e	2	NAG	O5-C5-C6-O6
7	q	2	NAG	O5-C5-C6-O6
9	Z	6	MAN	O5-C5-C6-O6
9	l	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	x	6	MAN	O5-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
7	0	1	NAG	C4-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	e	2	NAG	C4-C5-C6-O6
7	q	2	NAG	C4-C5-C6-O6
9	x	4	MAN	O5-C5-C6-O6
9	Z	4	MAN	O5-C5-C6-O6
9	l	4	MAN	O5-C5-C6-O6
10	a	3	BMA	O5-C5-C6-O6
10	m	3	BMA	O5-C5-C6-O6
10	y	3	BMA	O5-C5-C6-O6
9	l	4	MAN	C4-C5-C6-O6
9	x	4	MAN	C4-C5-C6-O6
9	Z	4	MAN	C4-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
7	s	2	NAG	C4-C5-C6-O6
9	Z	7	MAN	O5-C5-C6-O6
9	l	7	MAN	O5-C5-C6-O6
9	x	7	MAN	O5-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
7	t	1	NAG	O5-C5-C6-O6
7	V	1	NAG	O5-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6
8	r	2	NAG	O5-C5-C6-O6
9	Z	3	BMA	O5-C5-C6-O6
9	l	3	BMA	O5-C5-C6-O6
9	x	3	BMA	O5-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	s	2	NAG	O5-C5-C6-O6
9	Z	5	MAN	C4-C5-C6-O6
9	l	5	MAN	C4-C5-C6-O6
9	x	5	MAN	C4-C5-C6-O6
10	y	2	NAG	C4-C5-C6-O6
10	a	2	NAG	C4-C5-C6-O6
10	m	2	NAG	C4-C5-C6-O6
7	U	1	NAG	C3-C2-N2-C7
7	W	2	NAG	C3-C2-N2-C7
7	g	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	i	2	NAG	C3-C2-N2-C7
7	s	1	NAG	C3-C2-N2-C7
7	u	2	NAG	C3-C2-N2-C7
10	a	1	NAG	C4-C5-C6-O6
10	m	1	NAG	C4-C5-C6-O6
10	y	1	NAG	C4-C5-C6-O6
7	d	1	NAG	C4-C5-C6-O6
7	p	1	NAG	C4-C5-C6-O6
7	l	1	NAG	C4-C5-C6-O6
7	U	1	NAG	C1-C2-N2-C7
7	W	2	NAG	C1-C2-N2-C7
7	d	2	NAG	C1-C2-N2-C7
7	g	1	NAG	C1-C2-N2-C7
7	i	2	NAG	C1-C2-N2-C7
7	p	2	NAG	C1-C2-N2-C7
7	s	1	NAG	C1-C2-N2-C7
7	u	2	NAG	C1-C2-N2-C7
7	l	2	NAG	C1-C2-N2-C7
7	d	2	NAG	C3-C2-N2-C7
7	p	2	NAG	C3-C2-N2-C7
7	l	2	NAG	C3-C2-N2-C7
7	V	1	NAG	C4-C5-C6-O6
7	h	1	NAG	C4-C5-C6-O6
7	t	1	NAG	C4-C5-C6-O6
7	d	1	NAG	O5-C5-C6-O6
7	p	1	NAG	O5-C5-C6-O6
7	l	1	NAG	O5-C5-C6-O6
9	x	5	MAN	O5-C5-C6-O6
9	Z	5	MAN	O5-C5-C6-O6
9	l	5	MAN	O5-C5-C6-O6

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	m	4	MAN	C1-C2-C3-C4-C5-O5
10	a	4	MAN	C1-C2-C3-C4-C5-O5
10	y	4	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 8 short contacts:

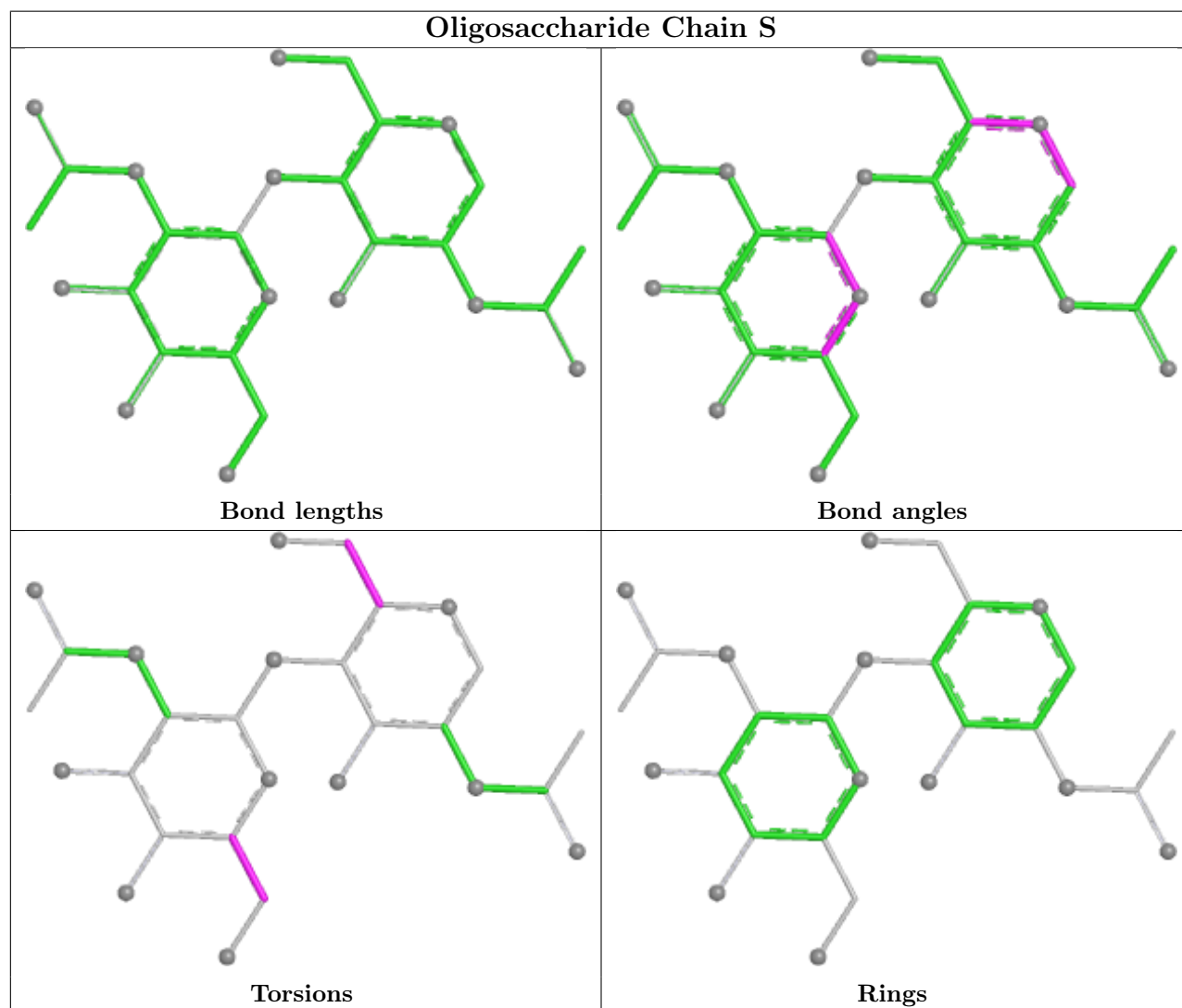
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	d	1	NAG	1	0

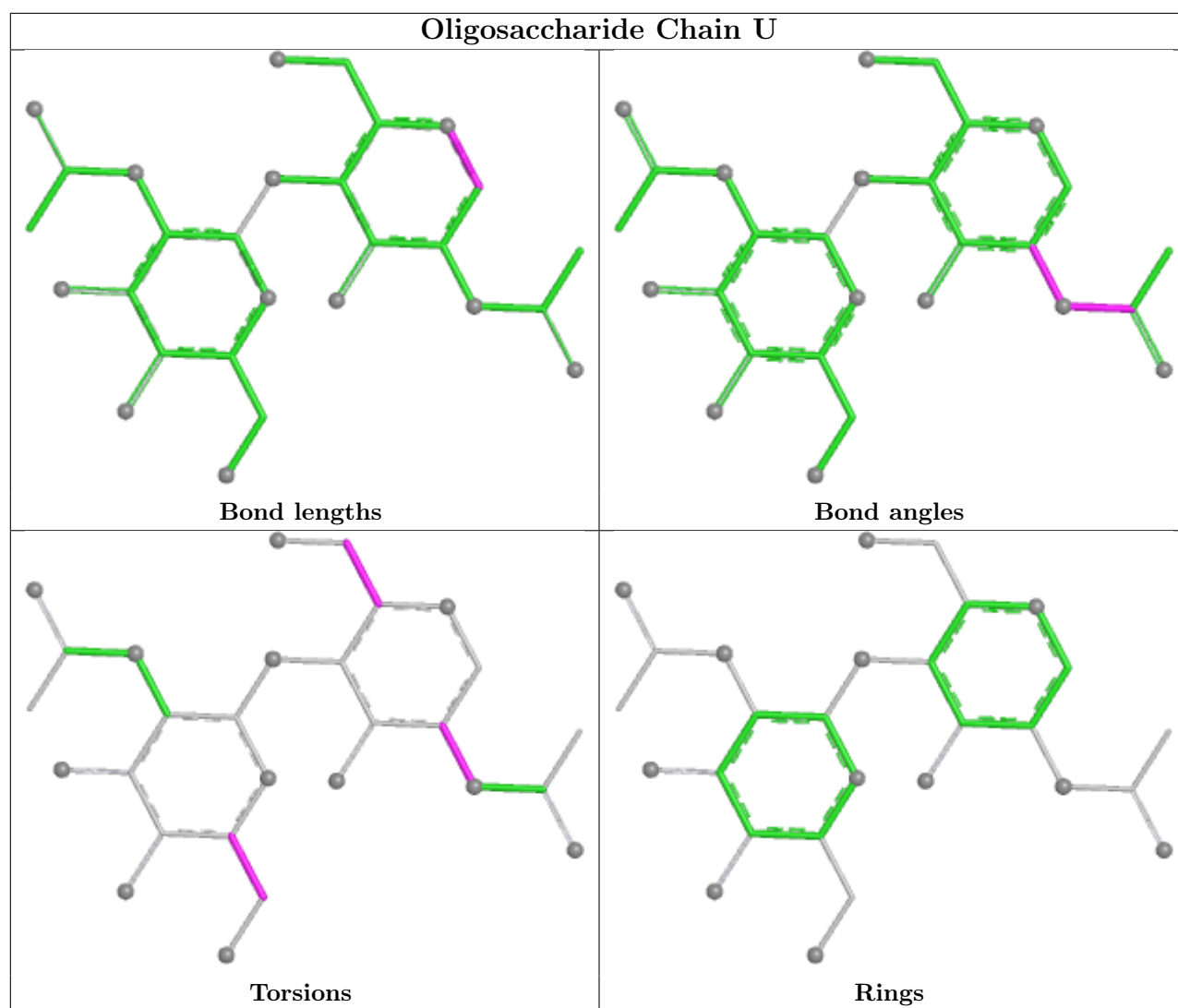
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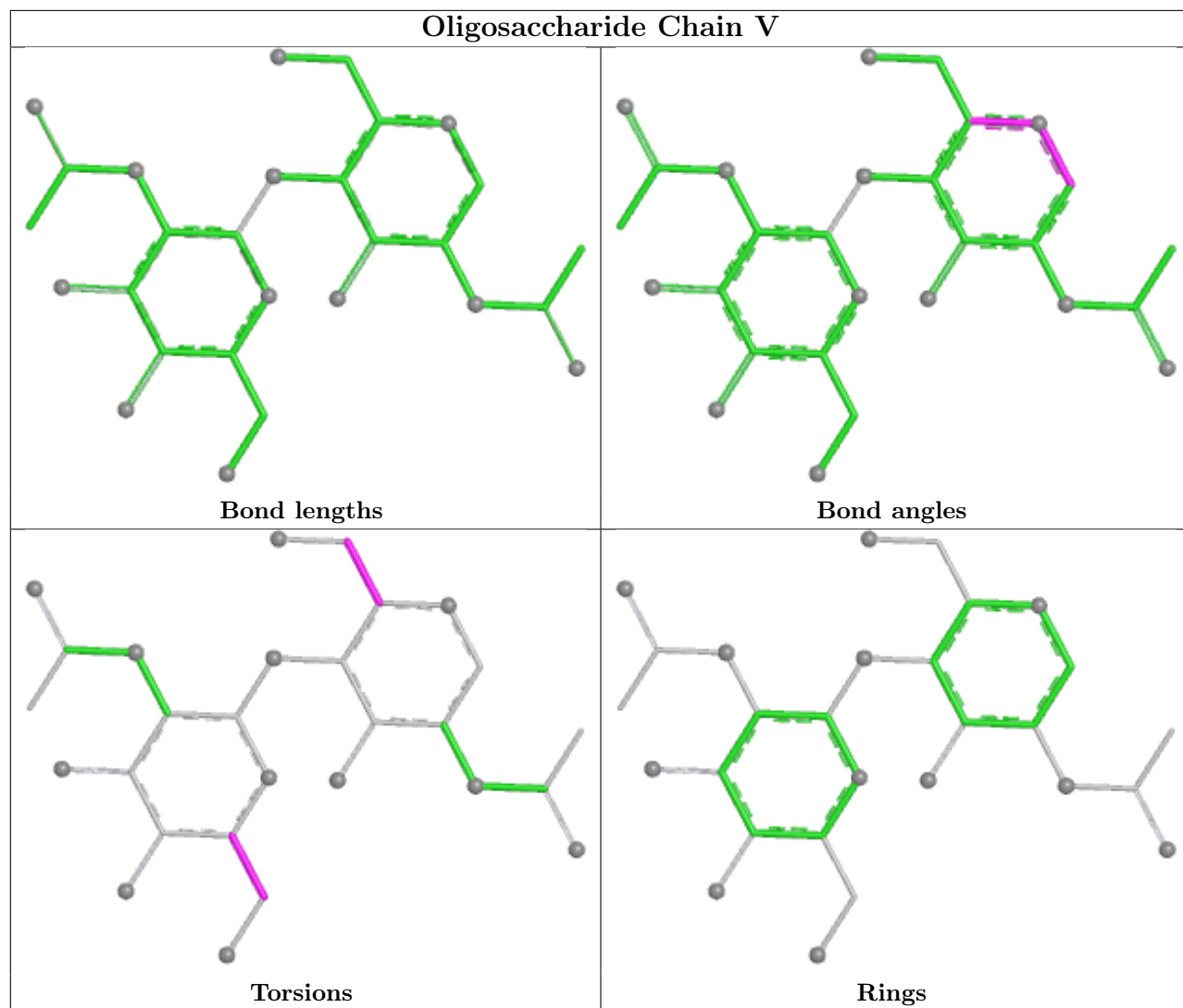
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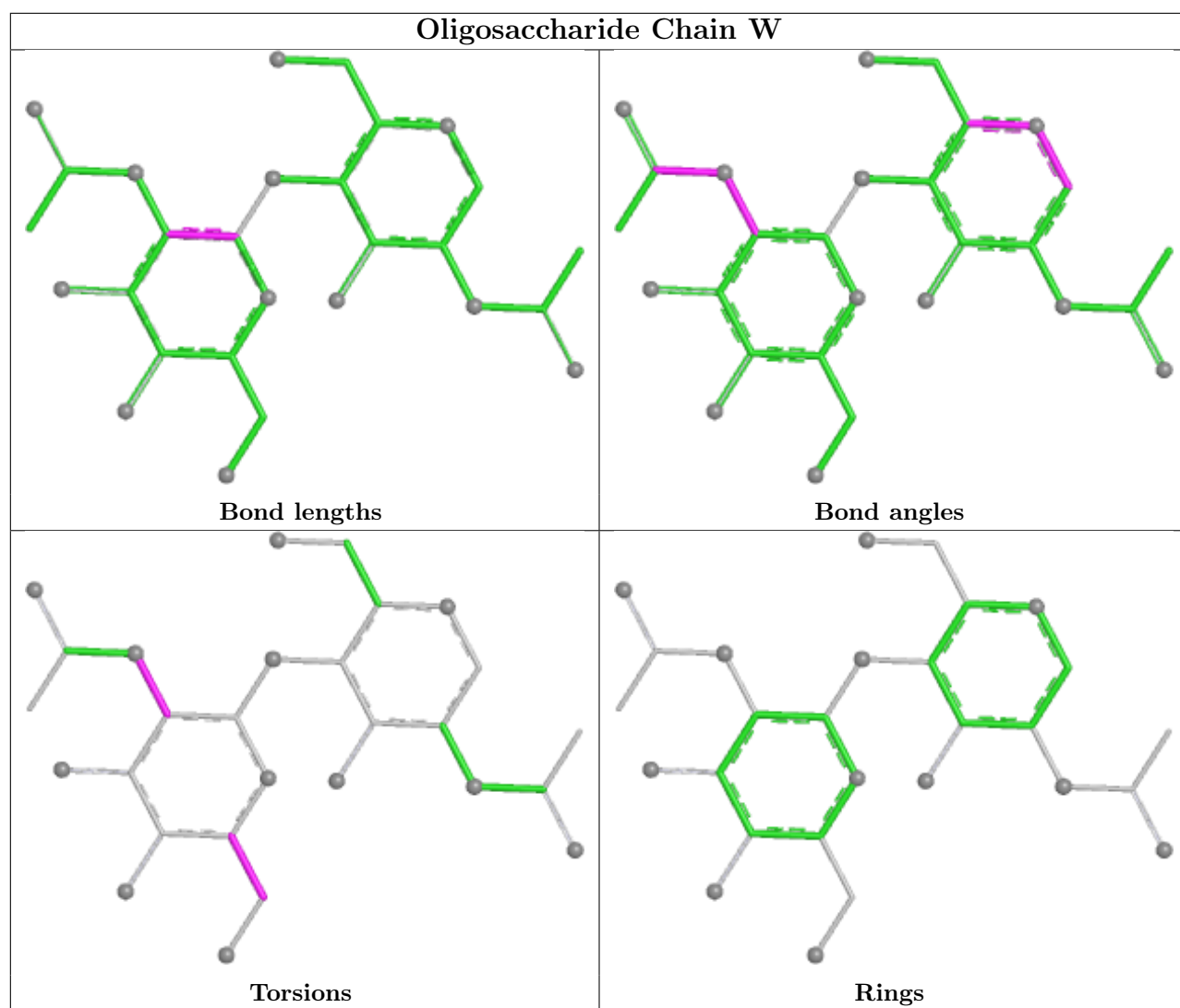
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	b	1	NAG	1	0
7	l	1	NAG	1	0
9	Z	4	MAN	1	0
7	n	1	NAG	1	0
9	l	4	MAN	1	0
7	b	2	NAG	1	0
7	n	2	NAG	1	0
7	p	1	NAG	1	0
9	x	4	MAN	1	0

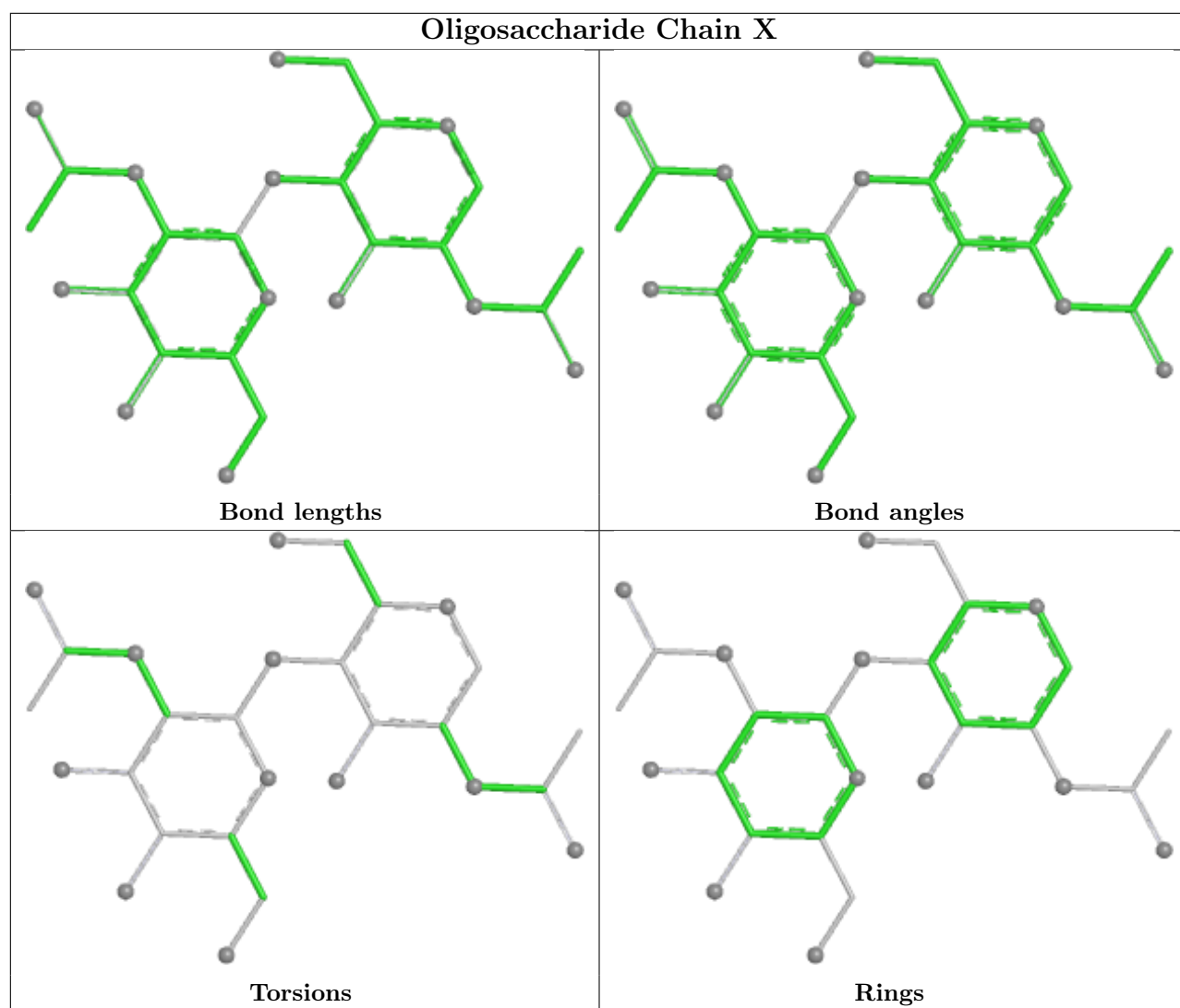
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

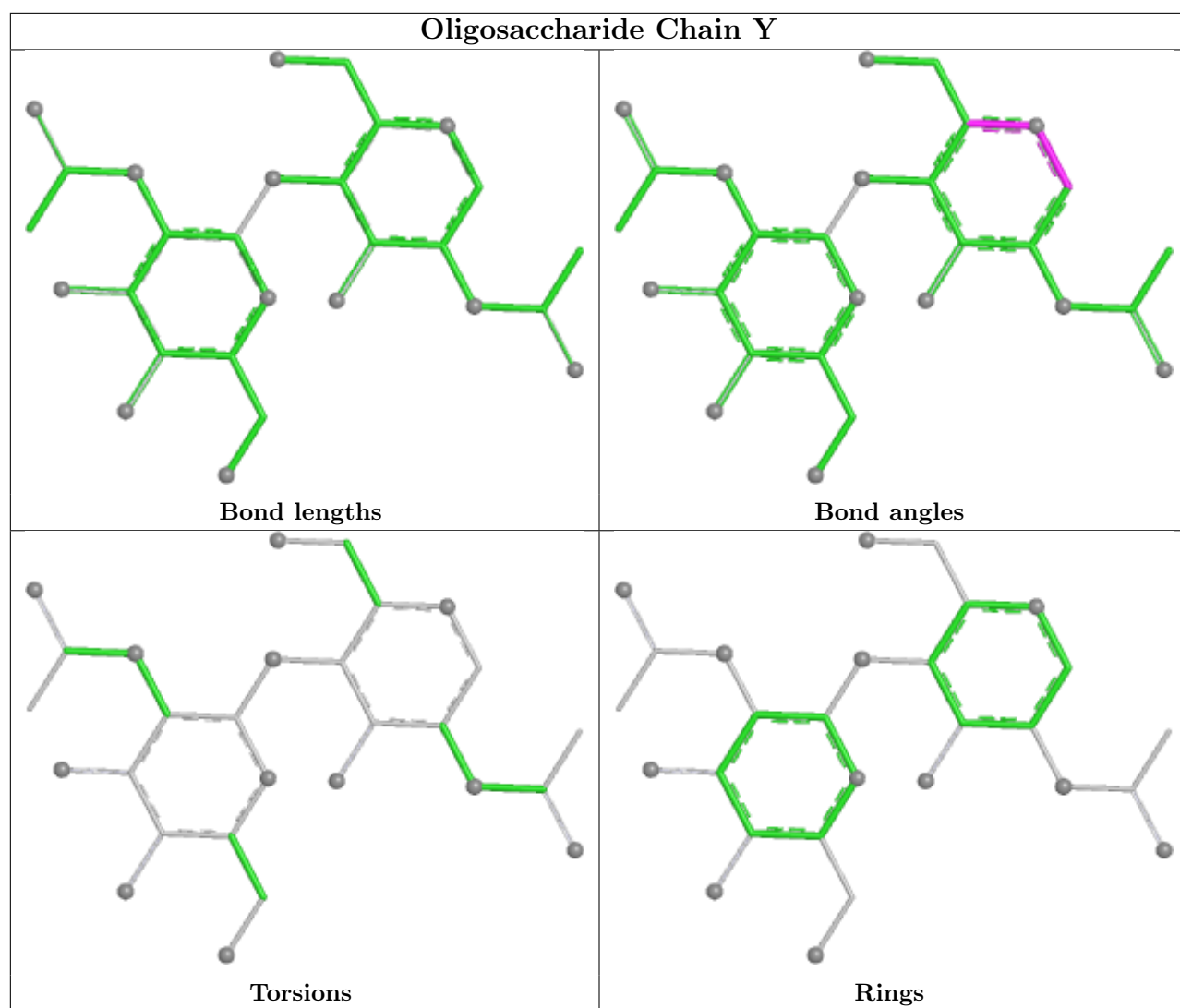


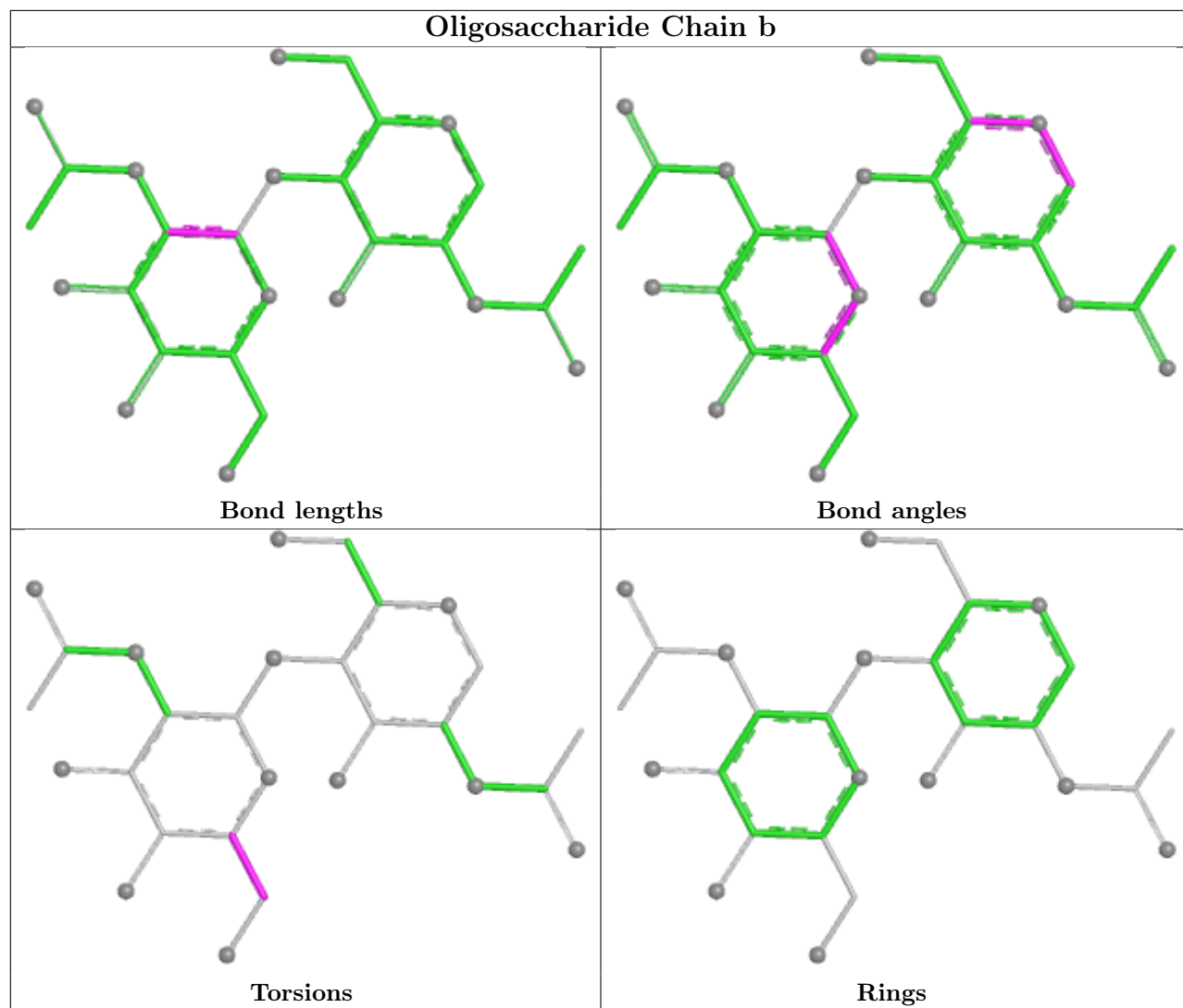


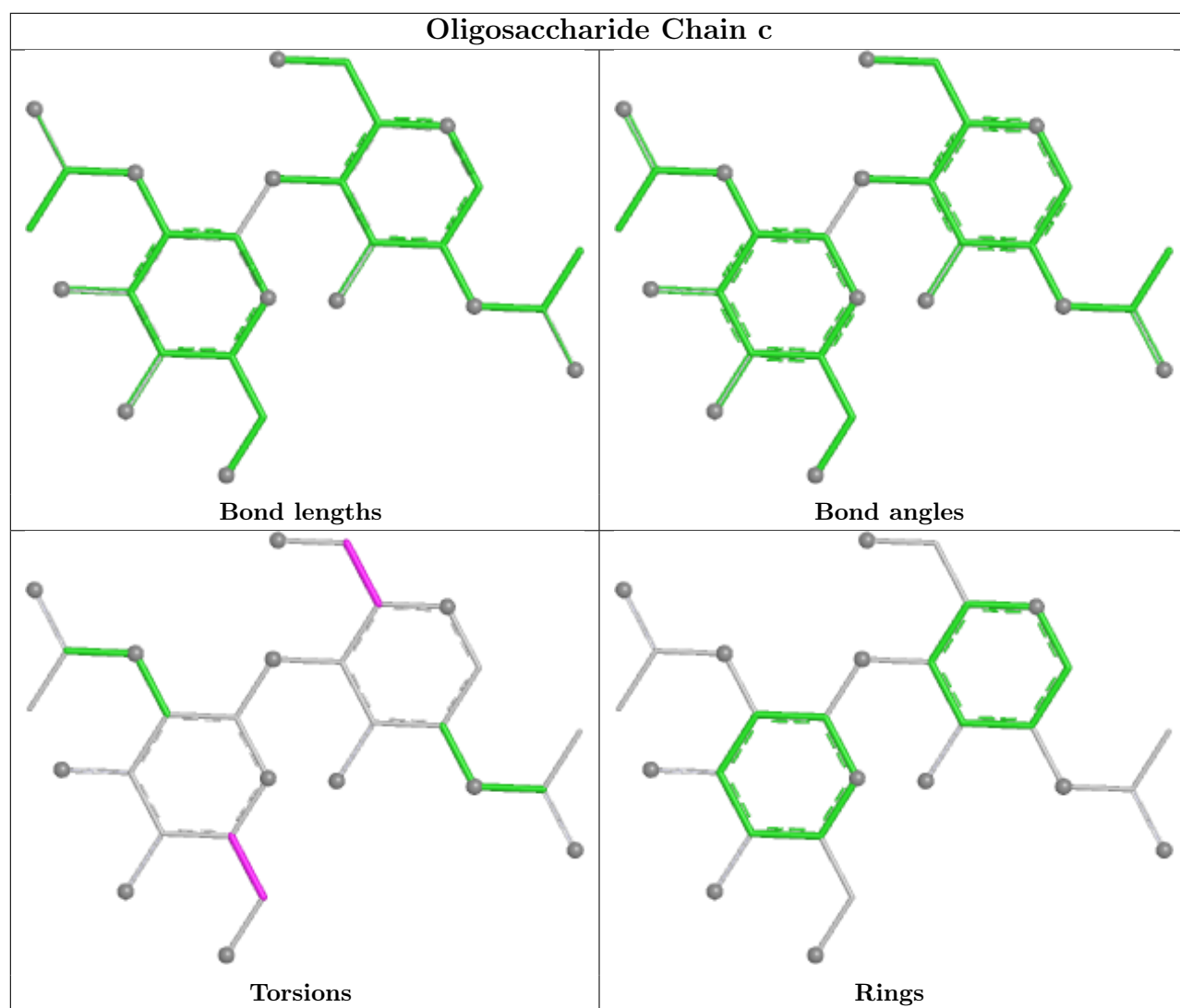


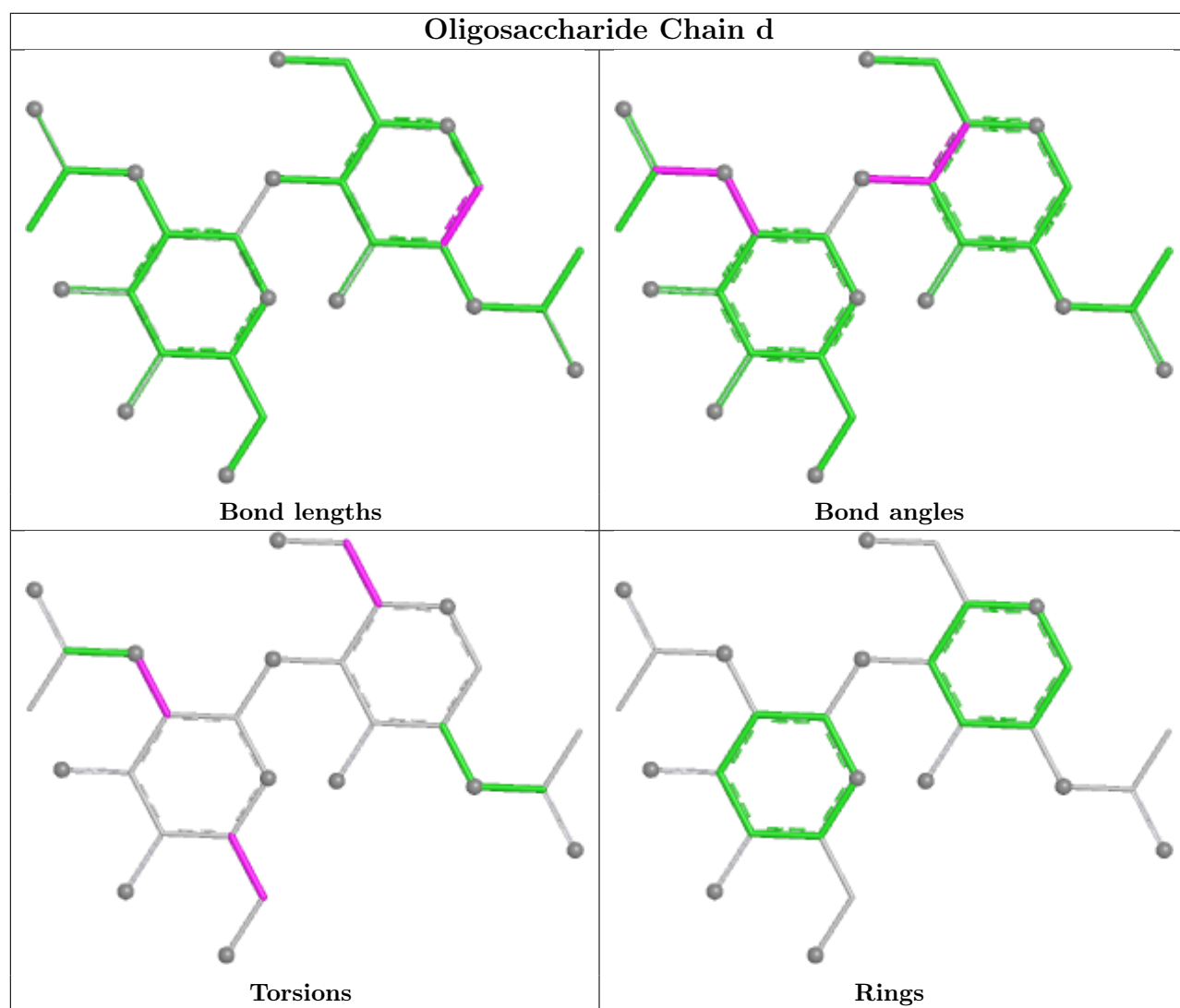


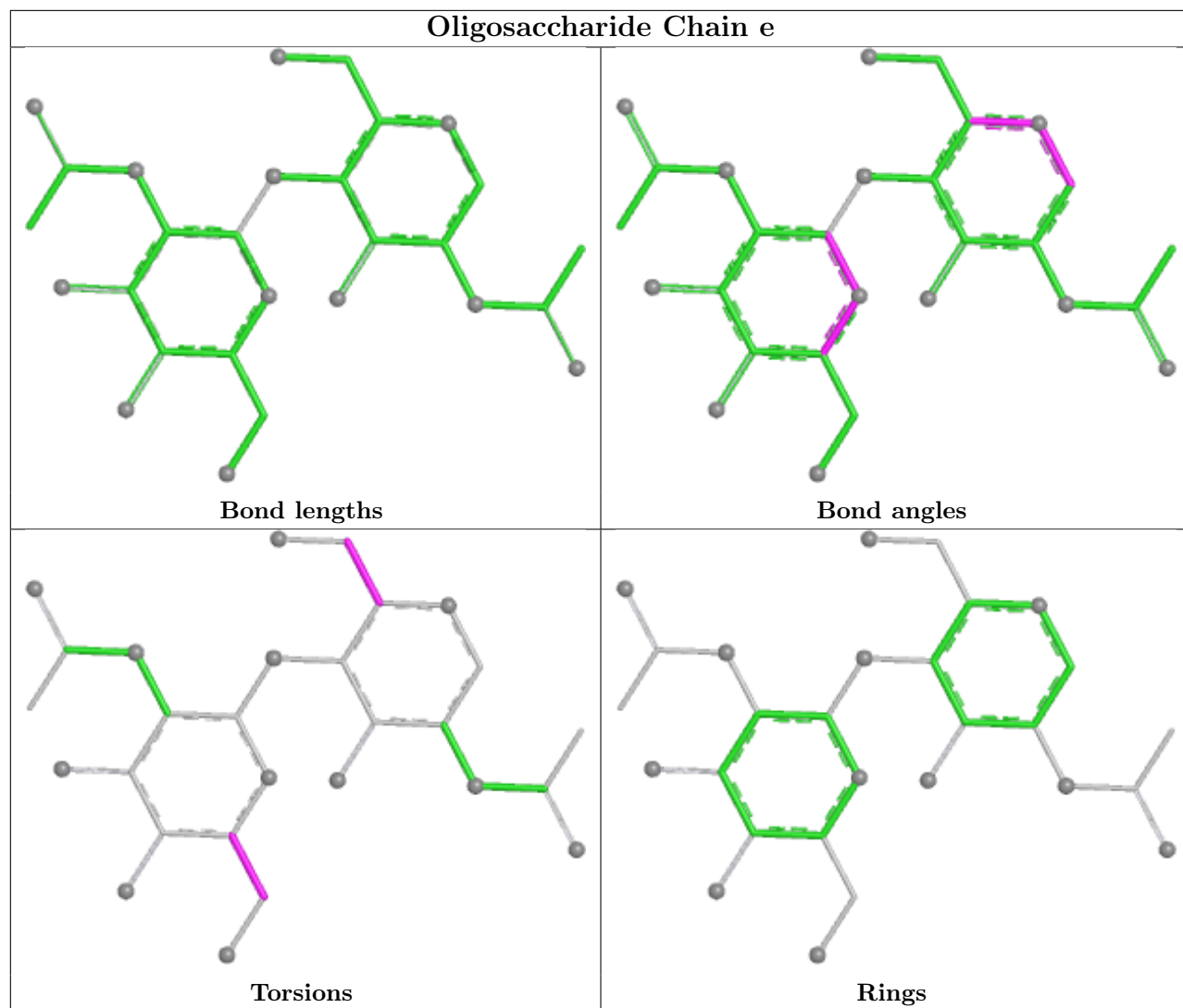


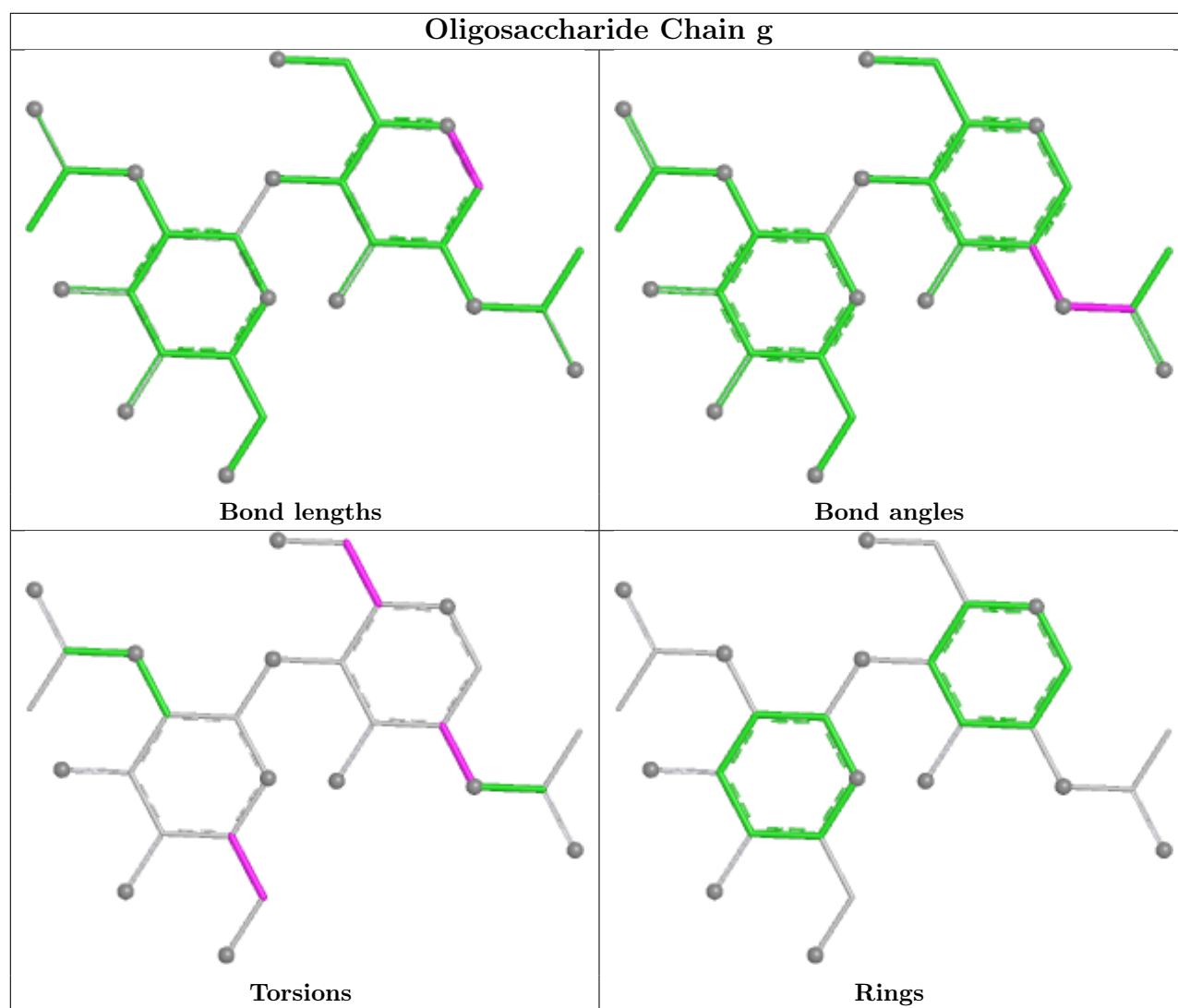


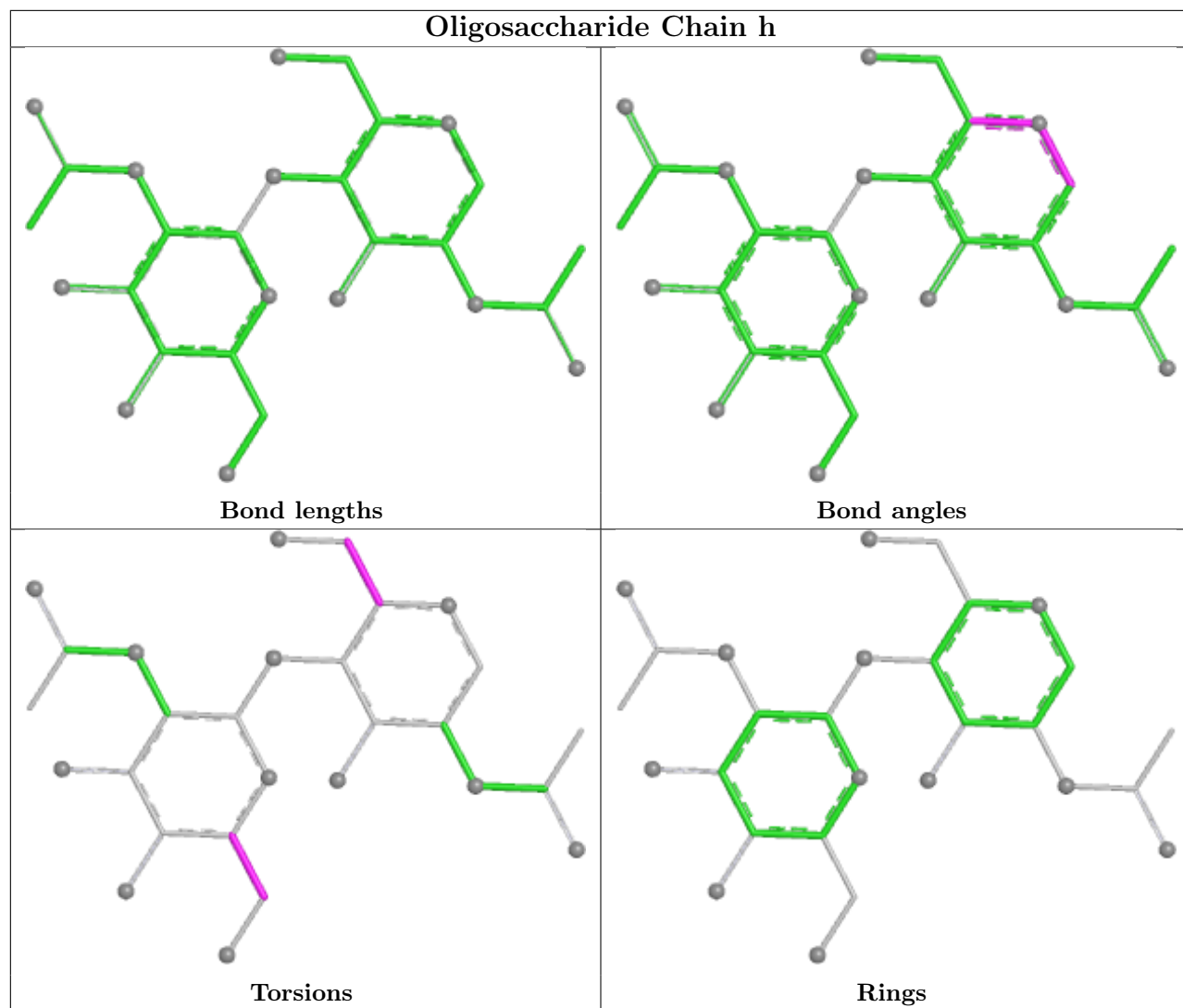


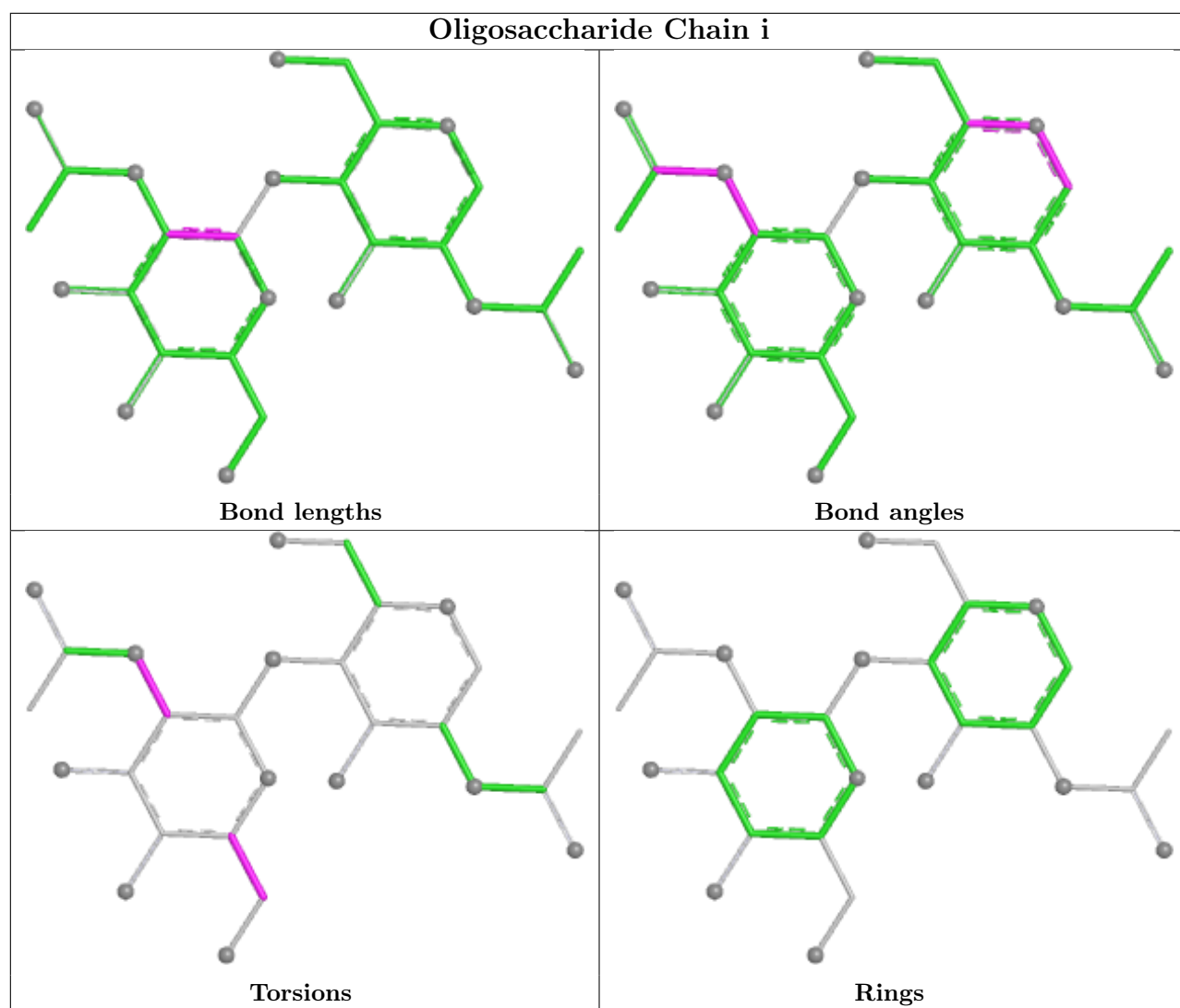


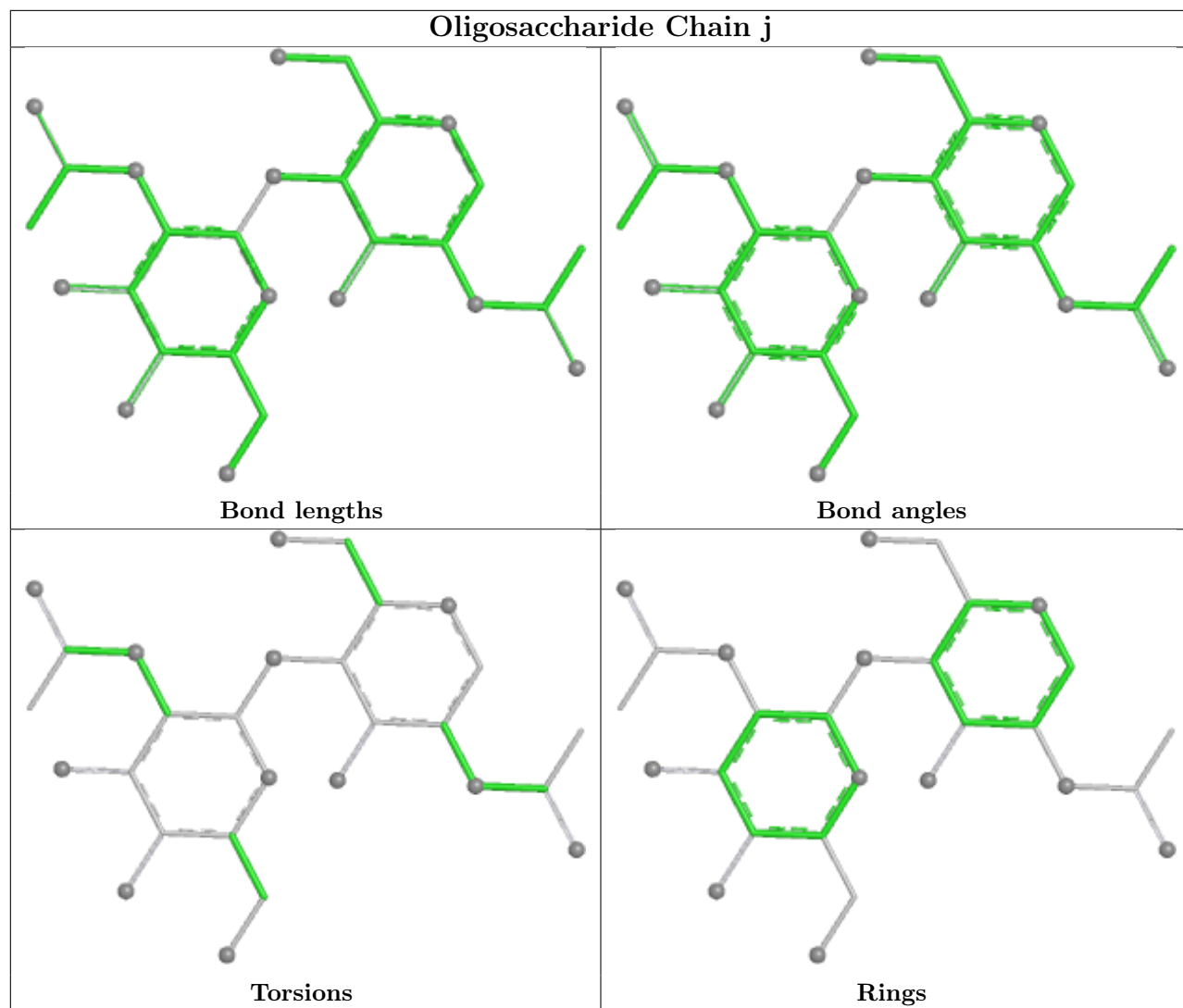


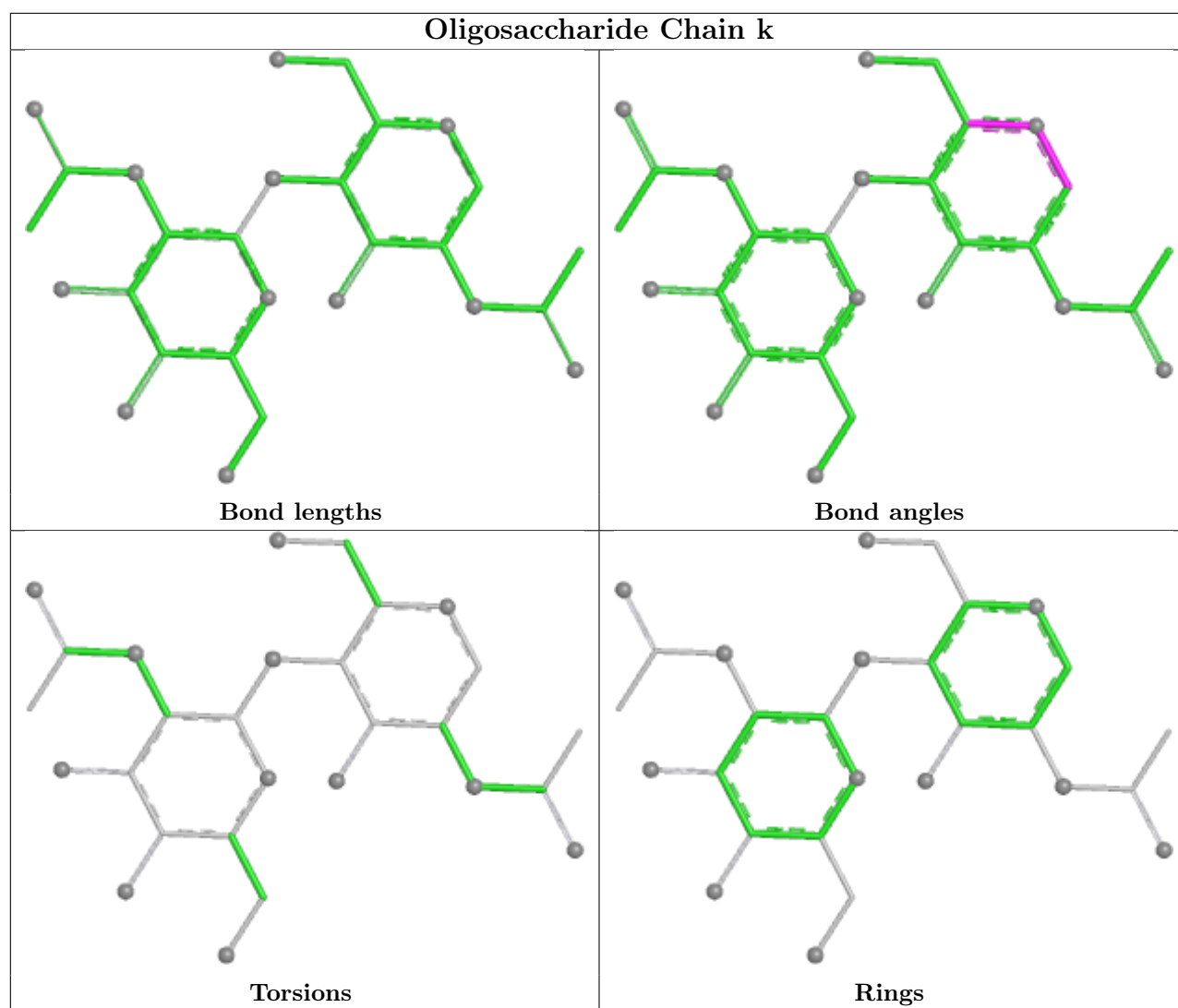


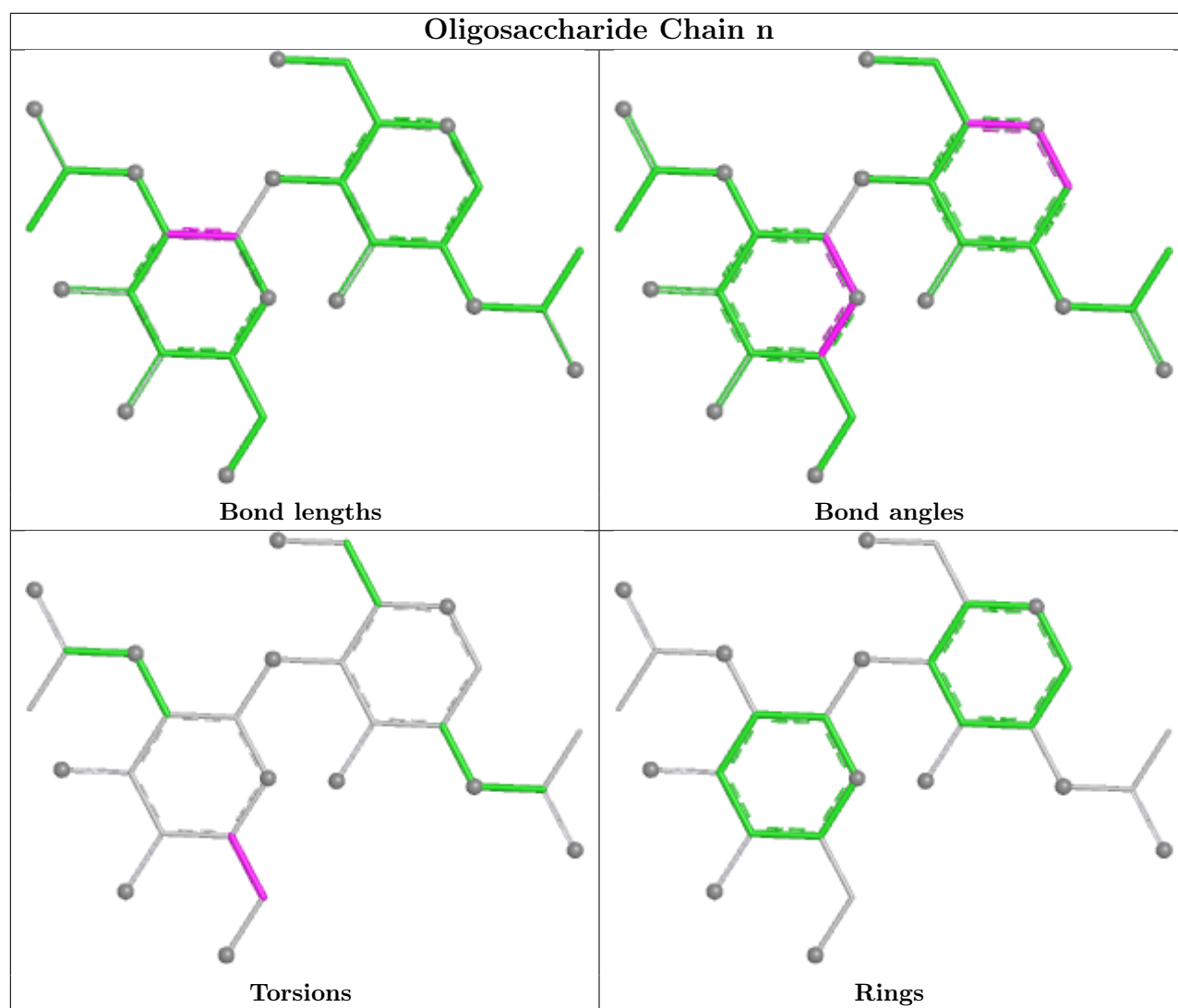


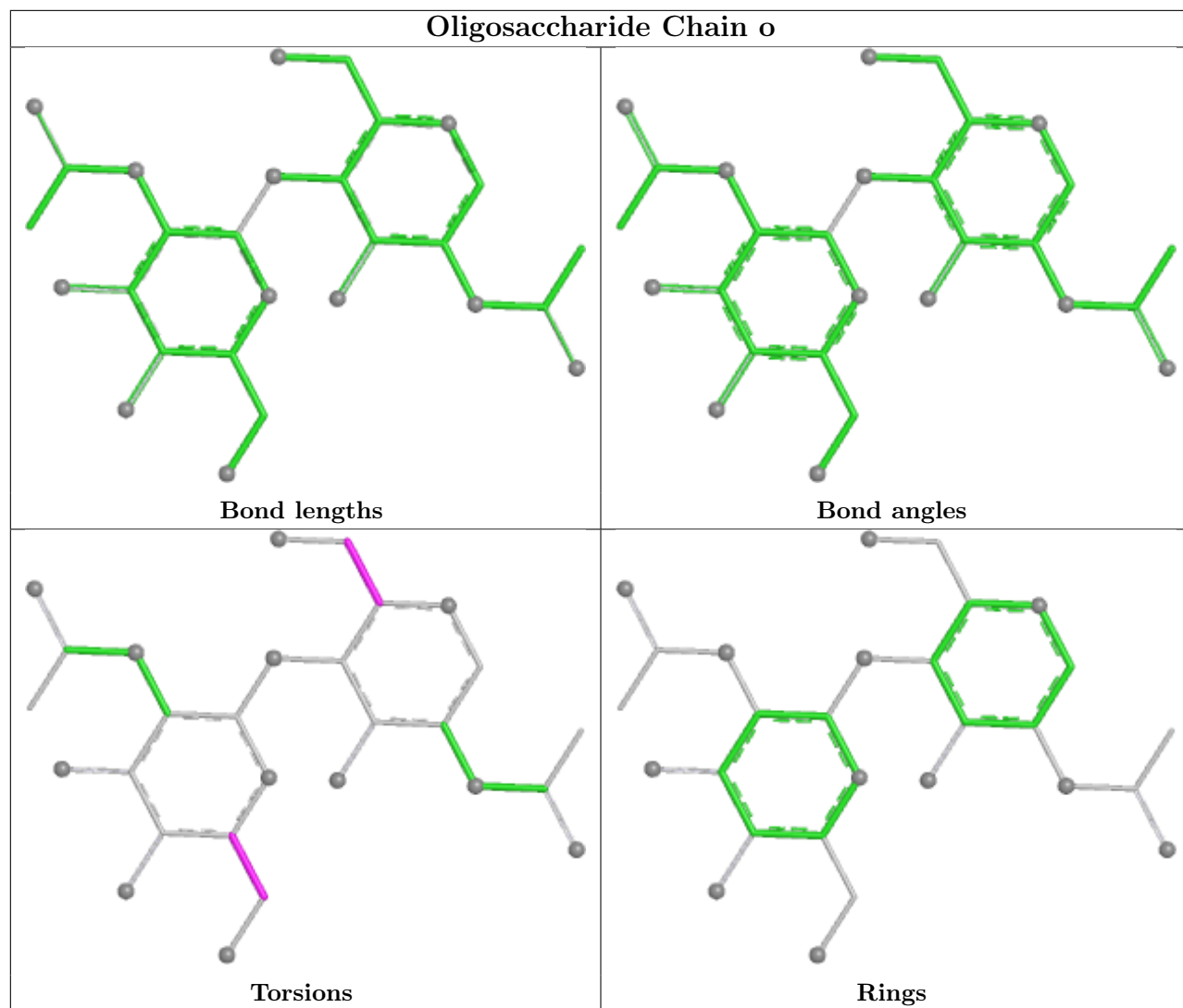


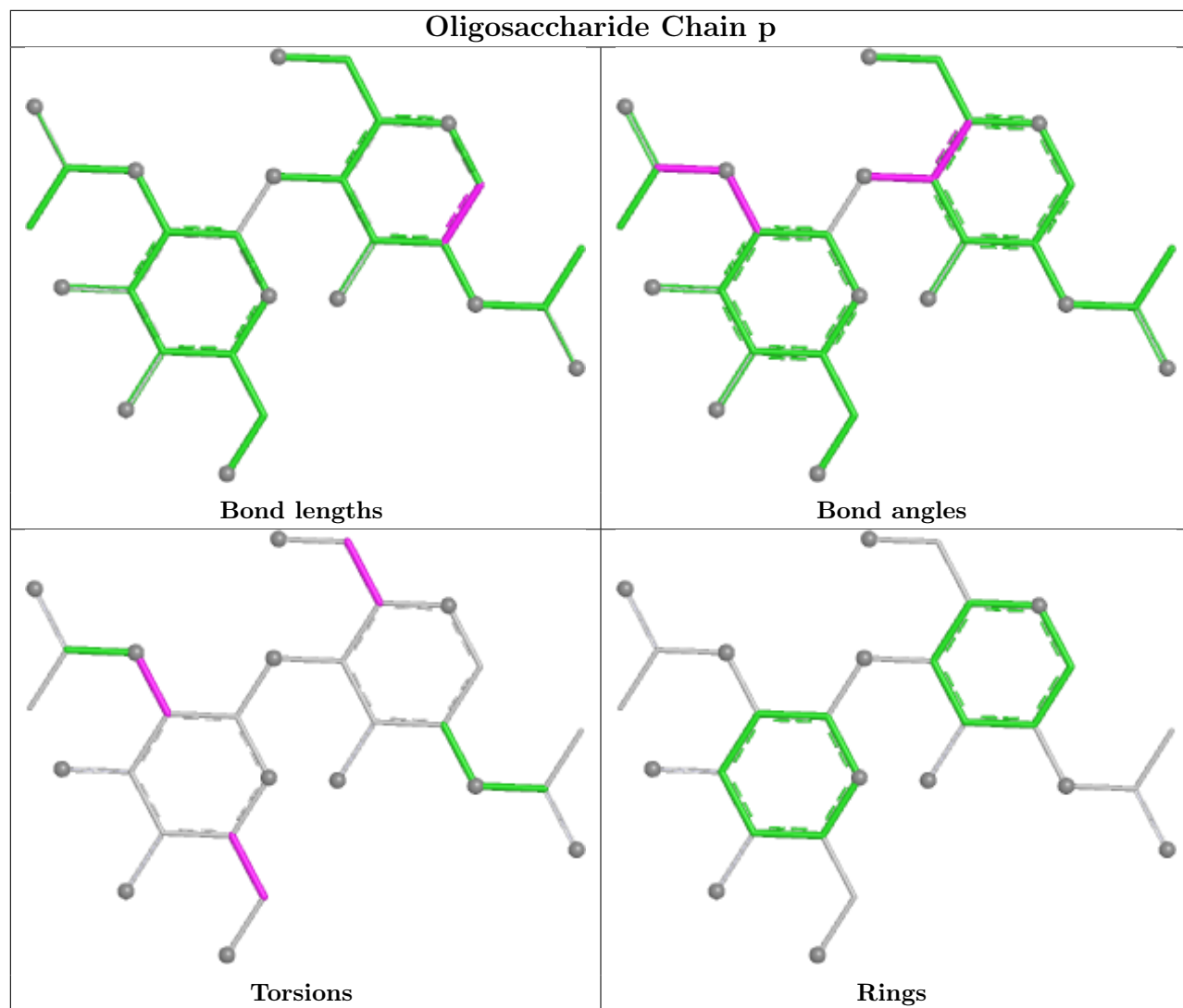


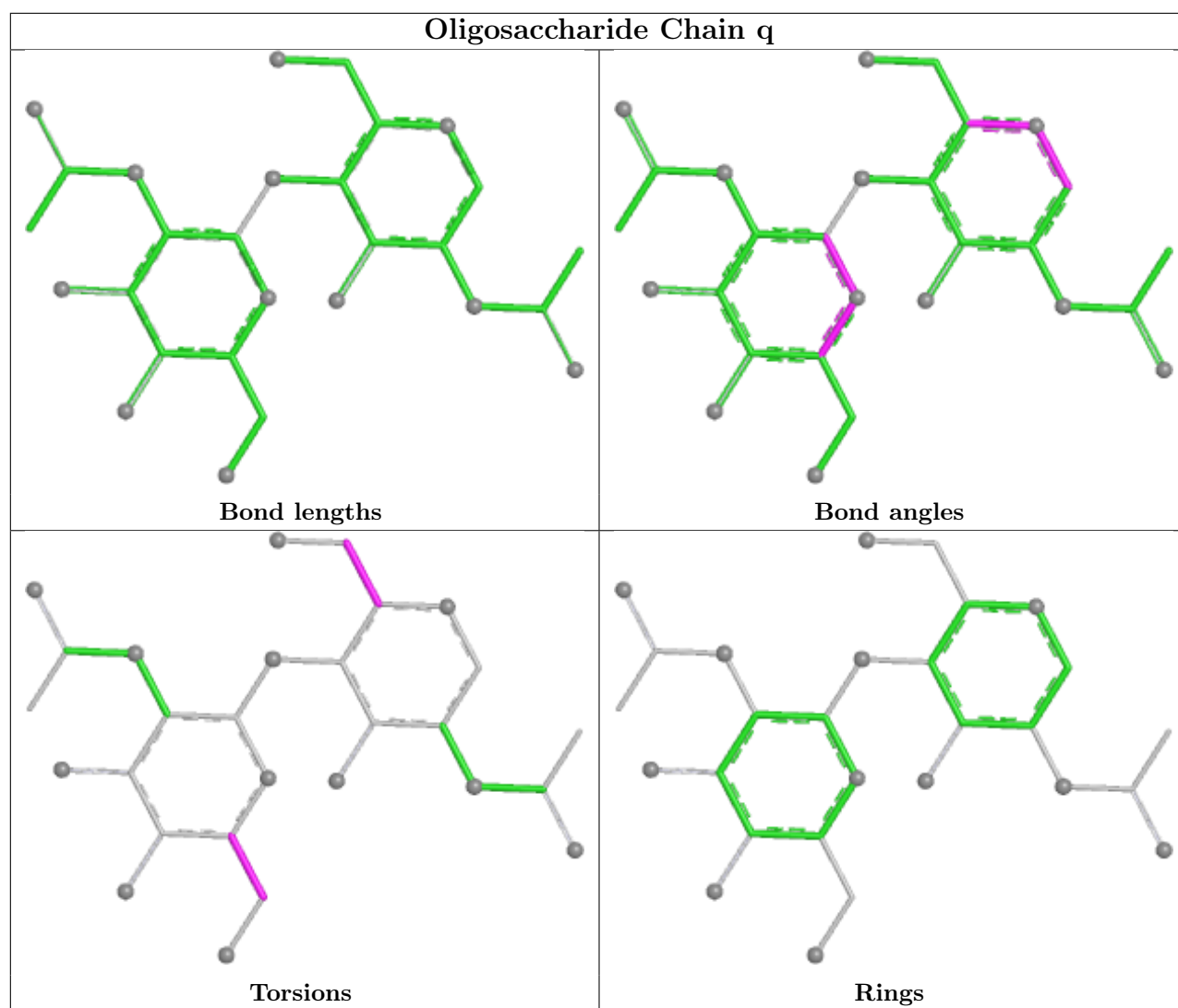


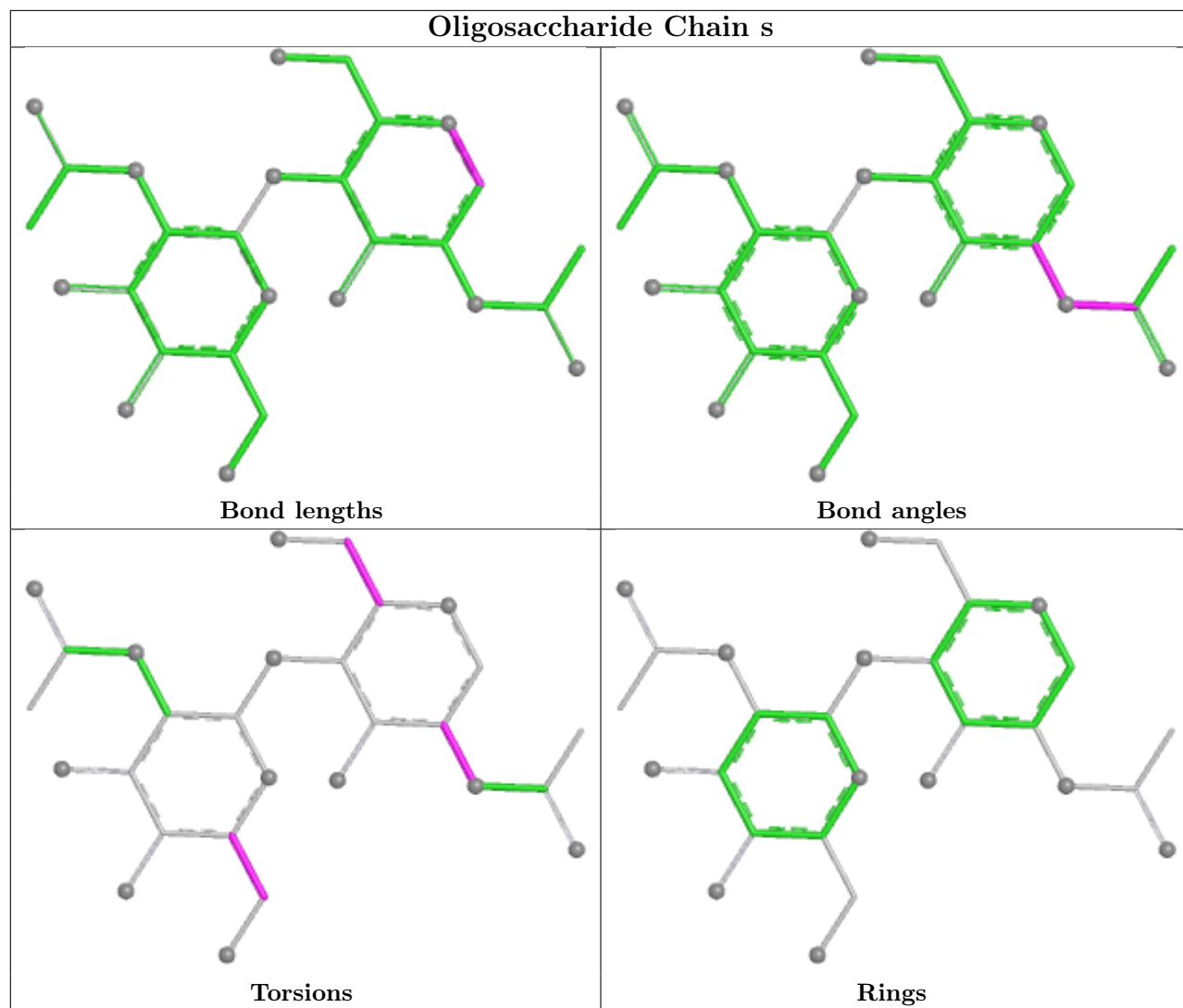


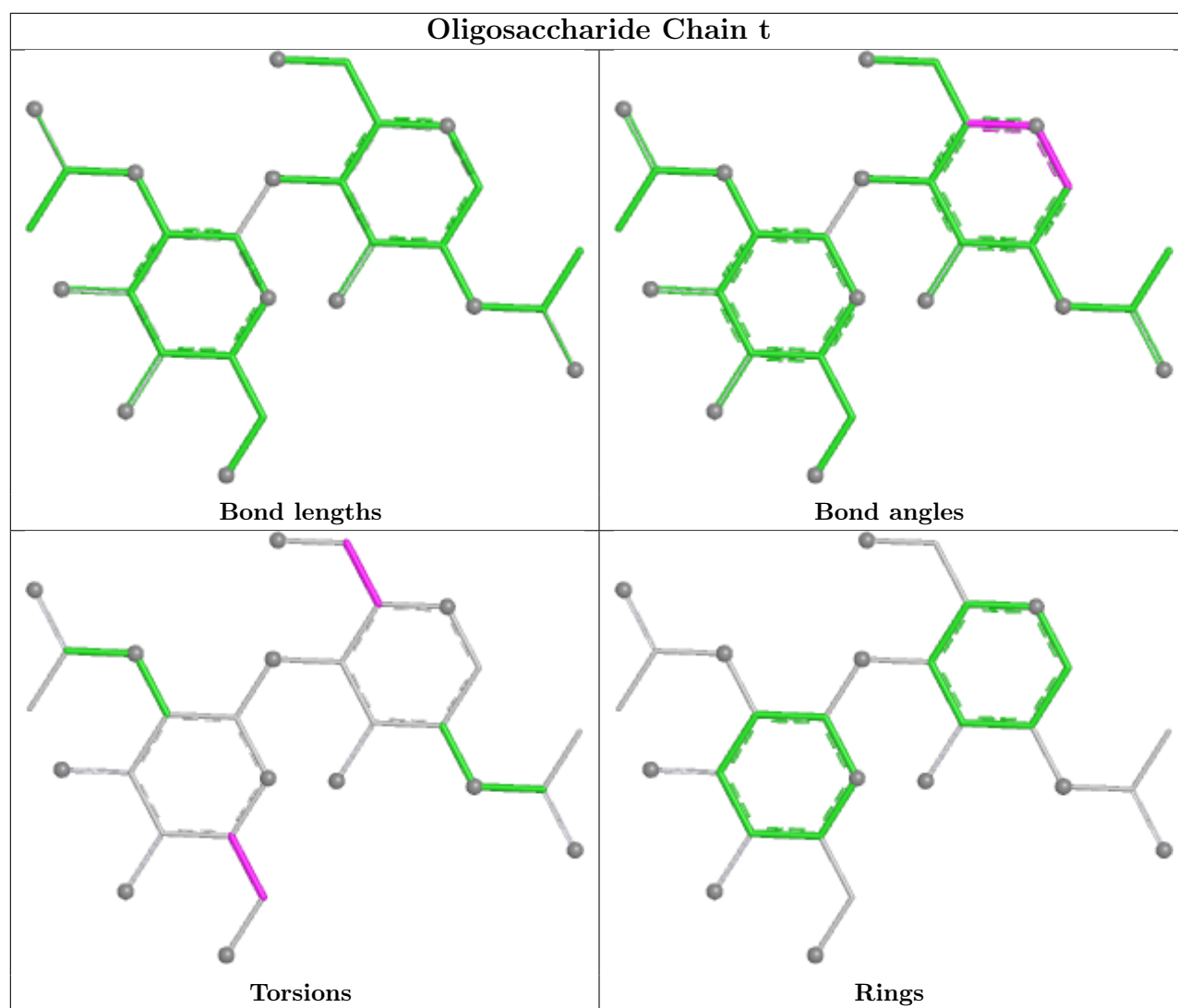


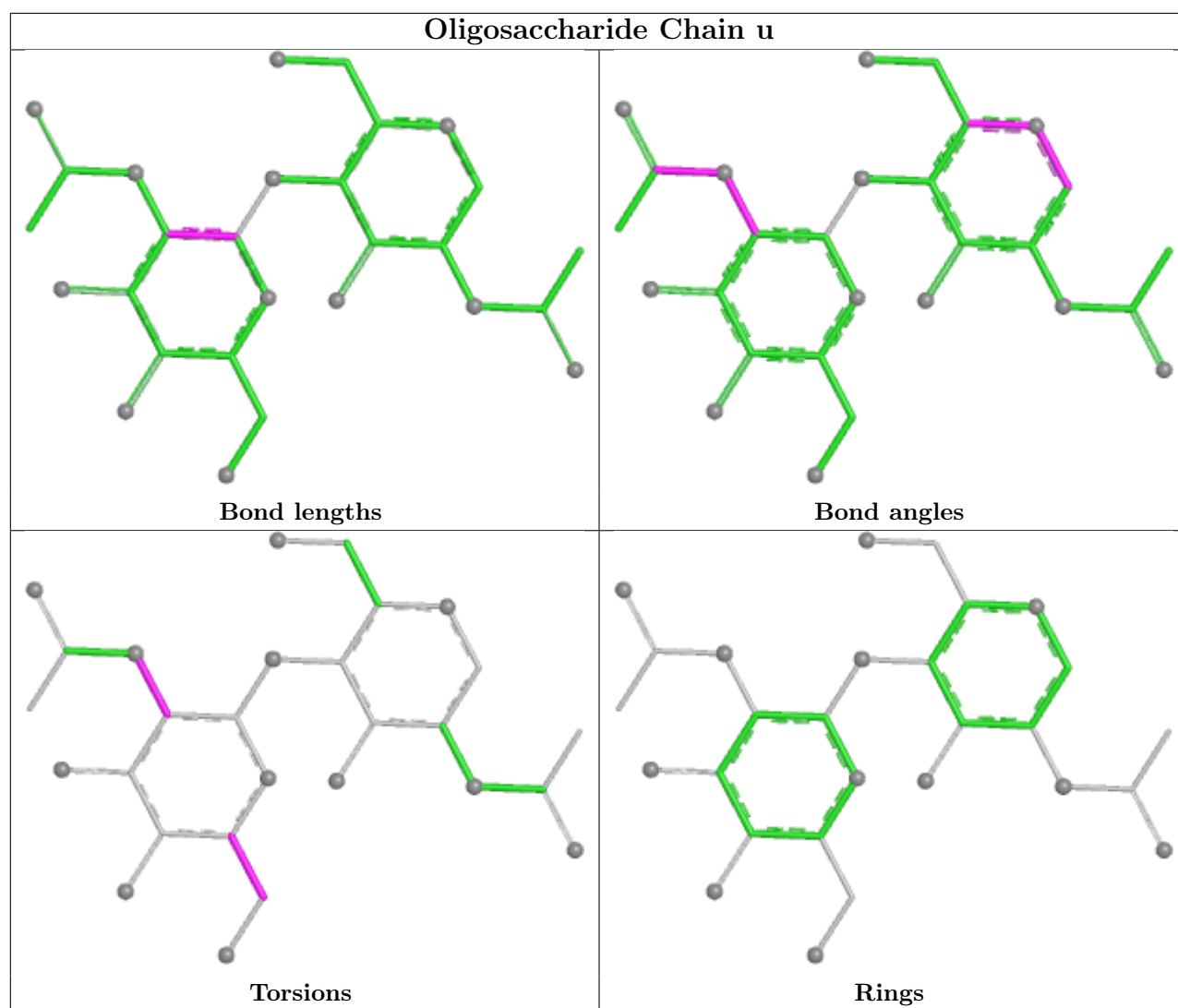


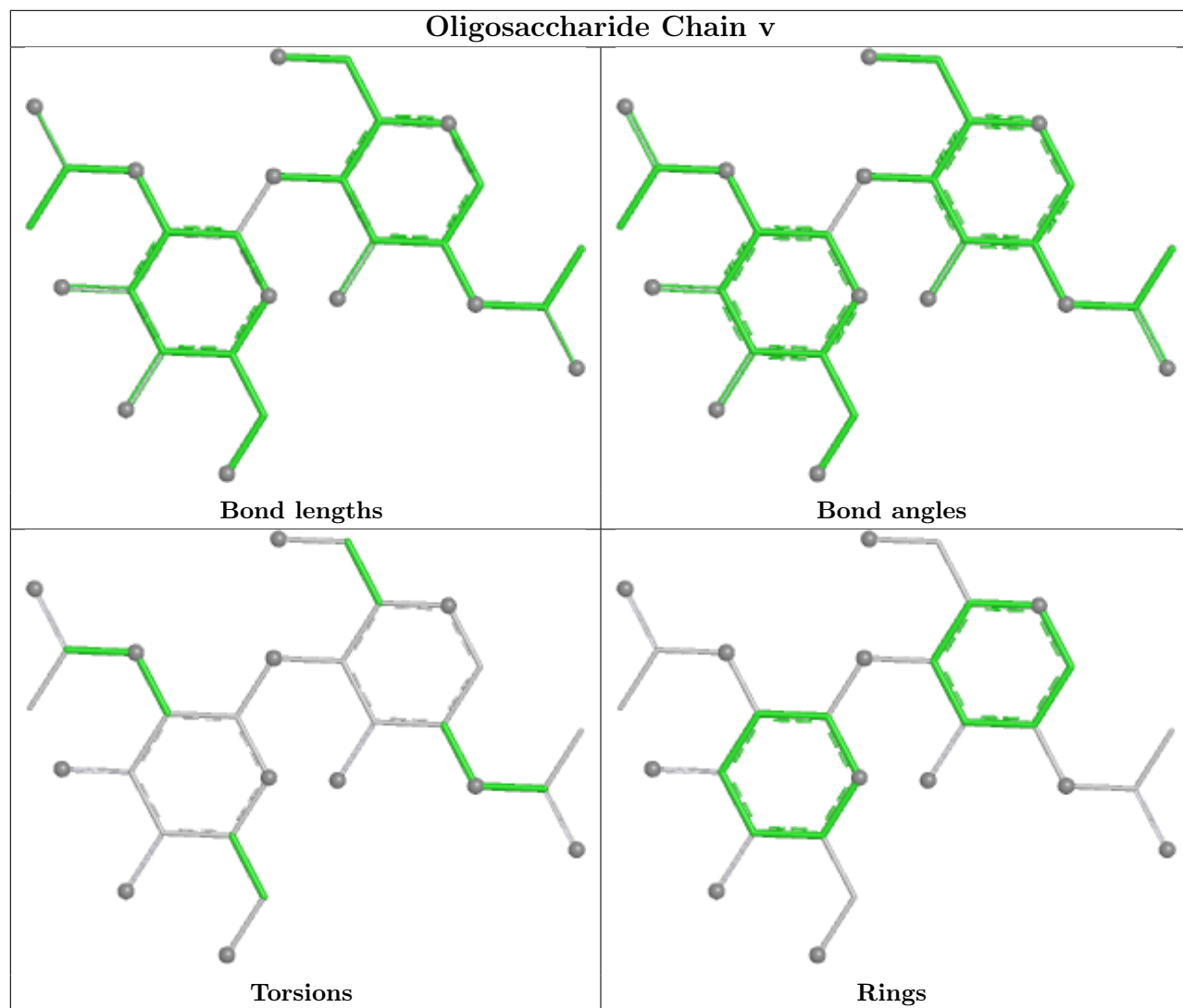


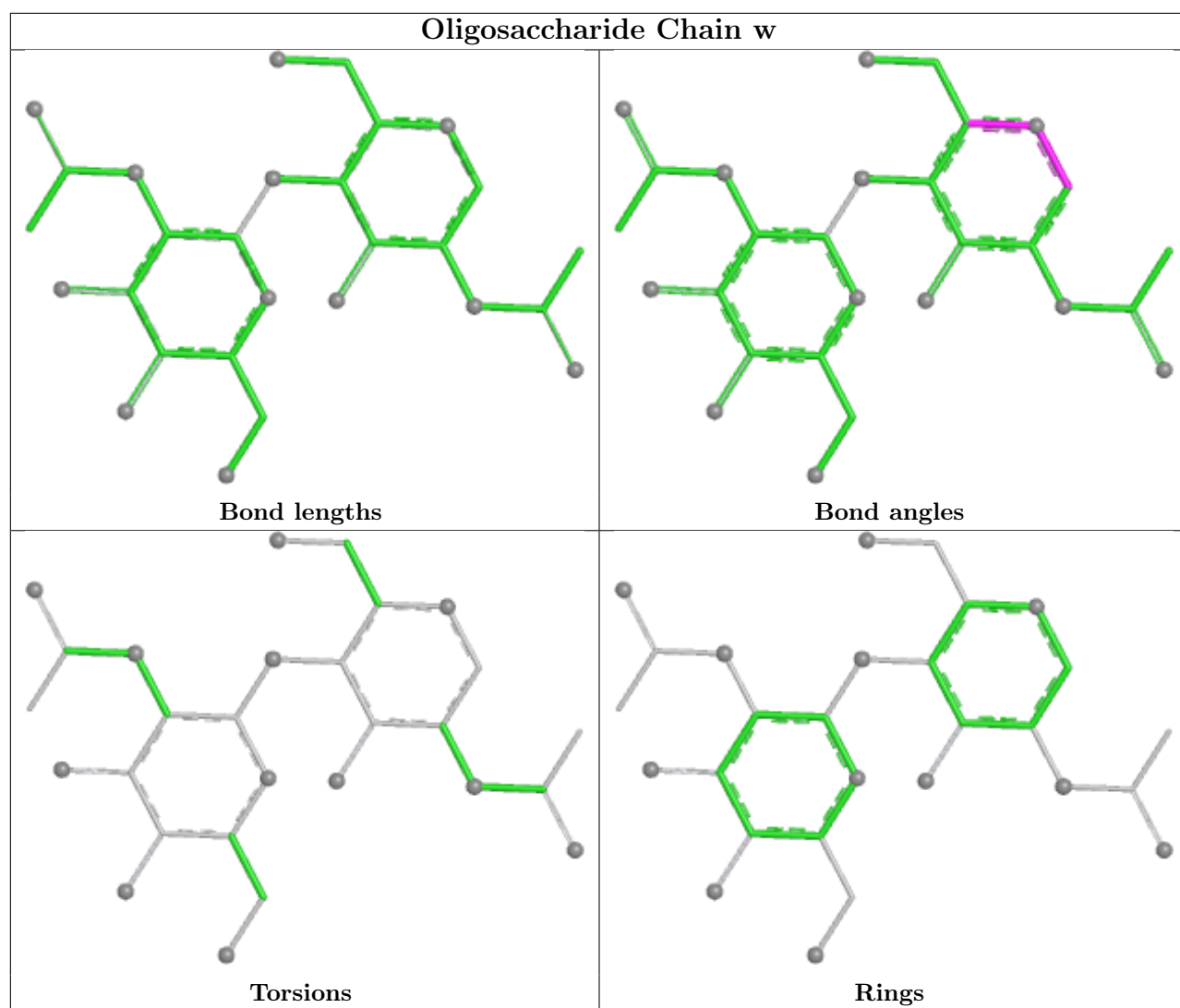


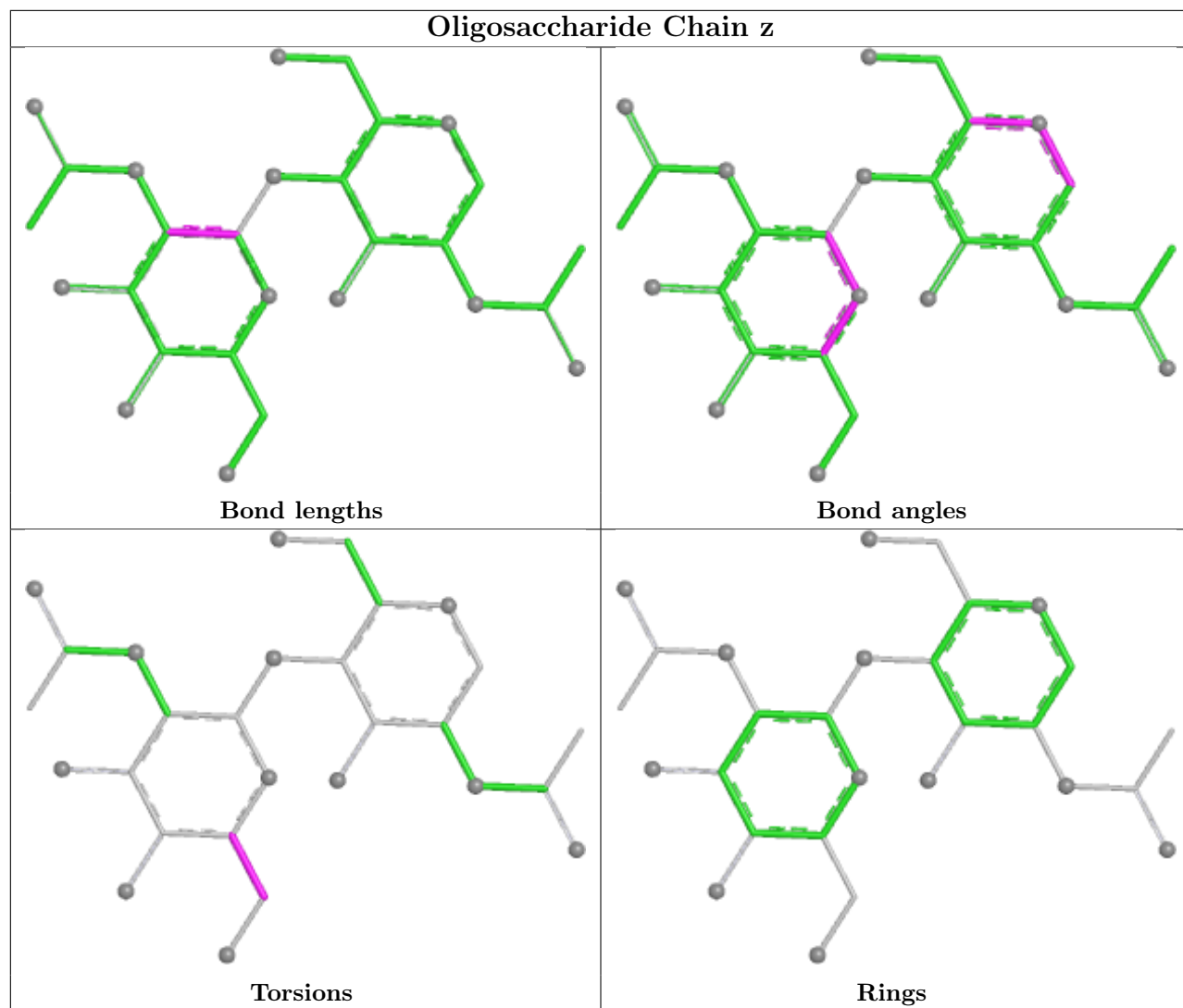


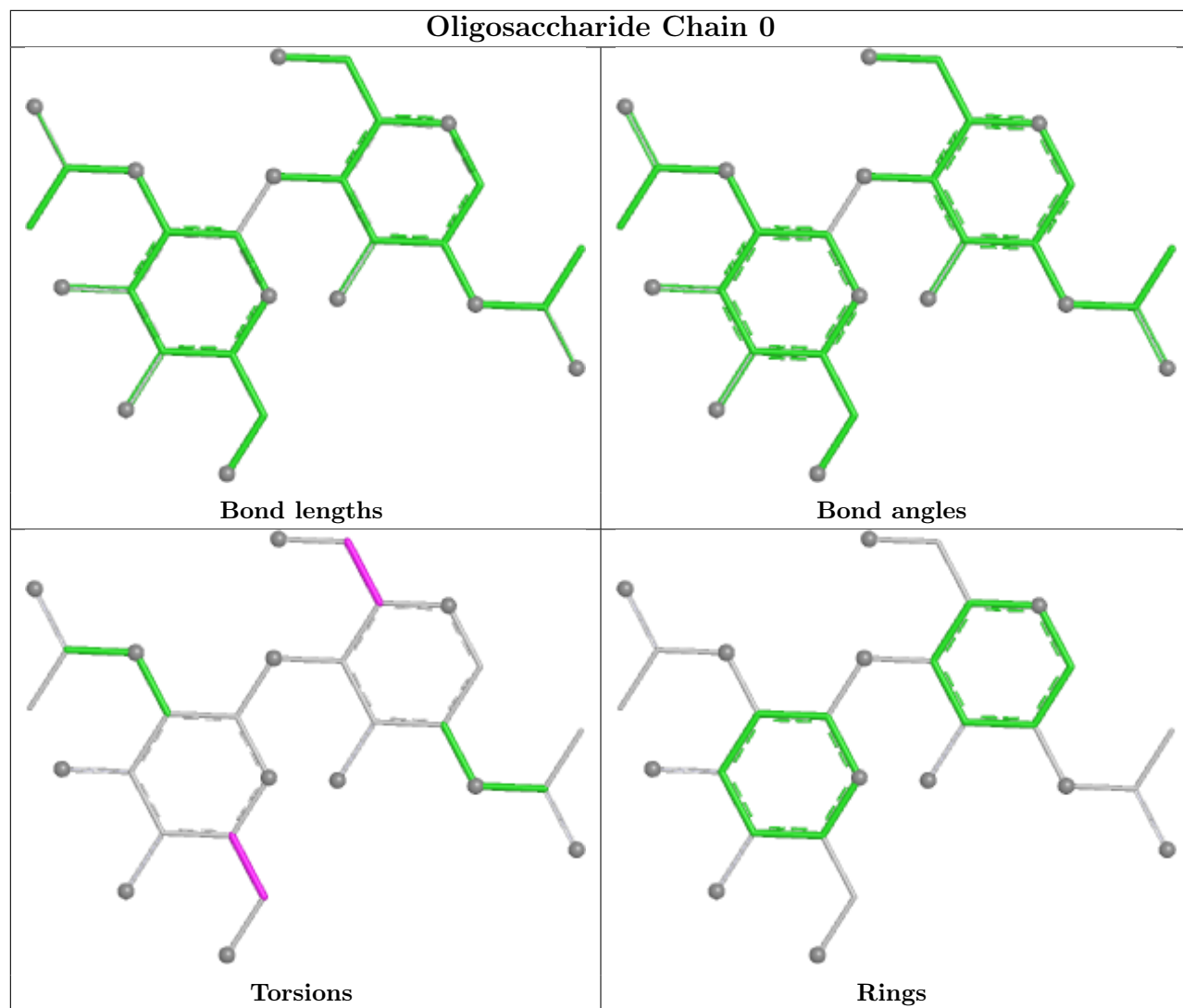


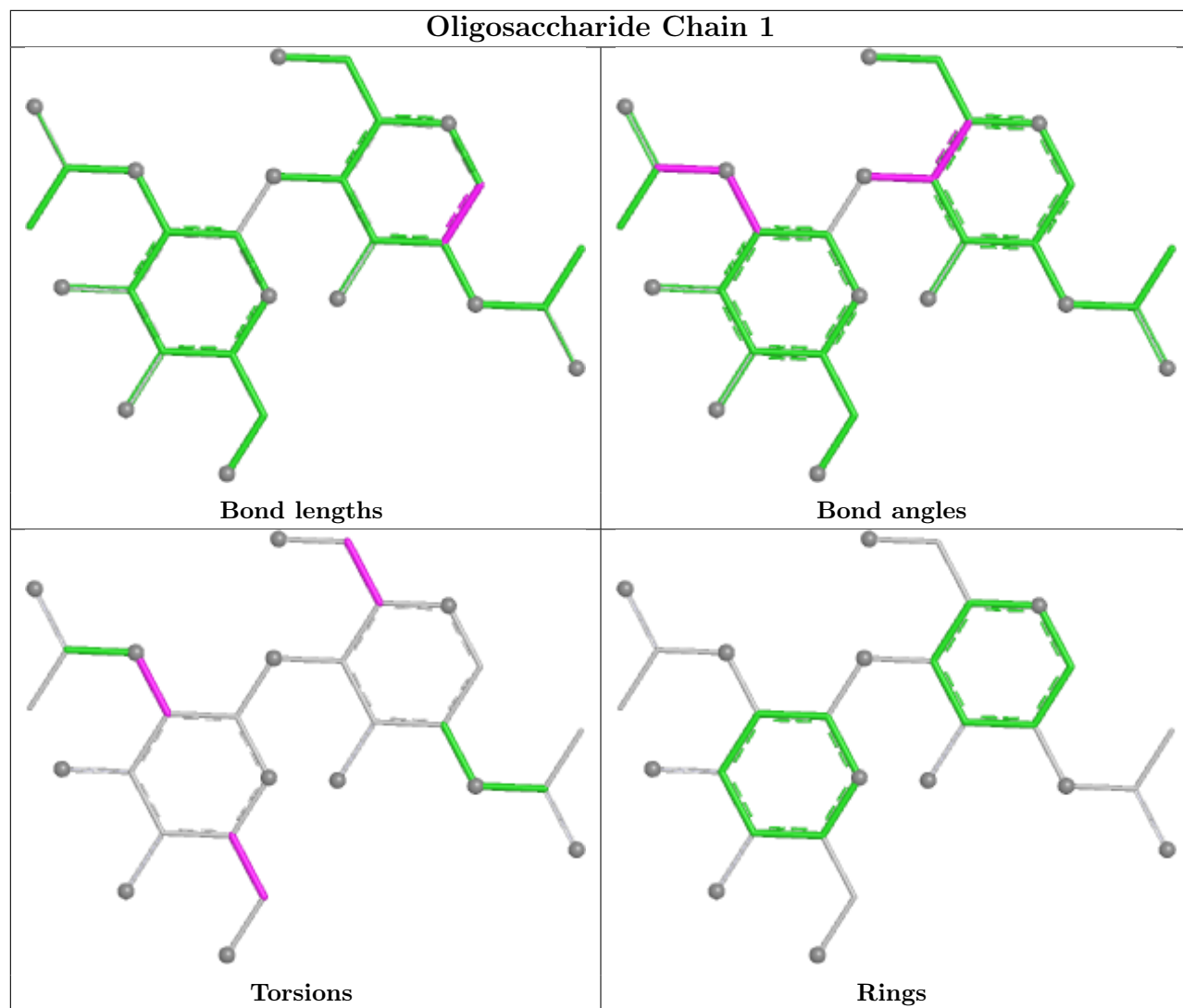


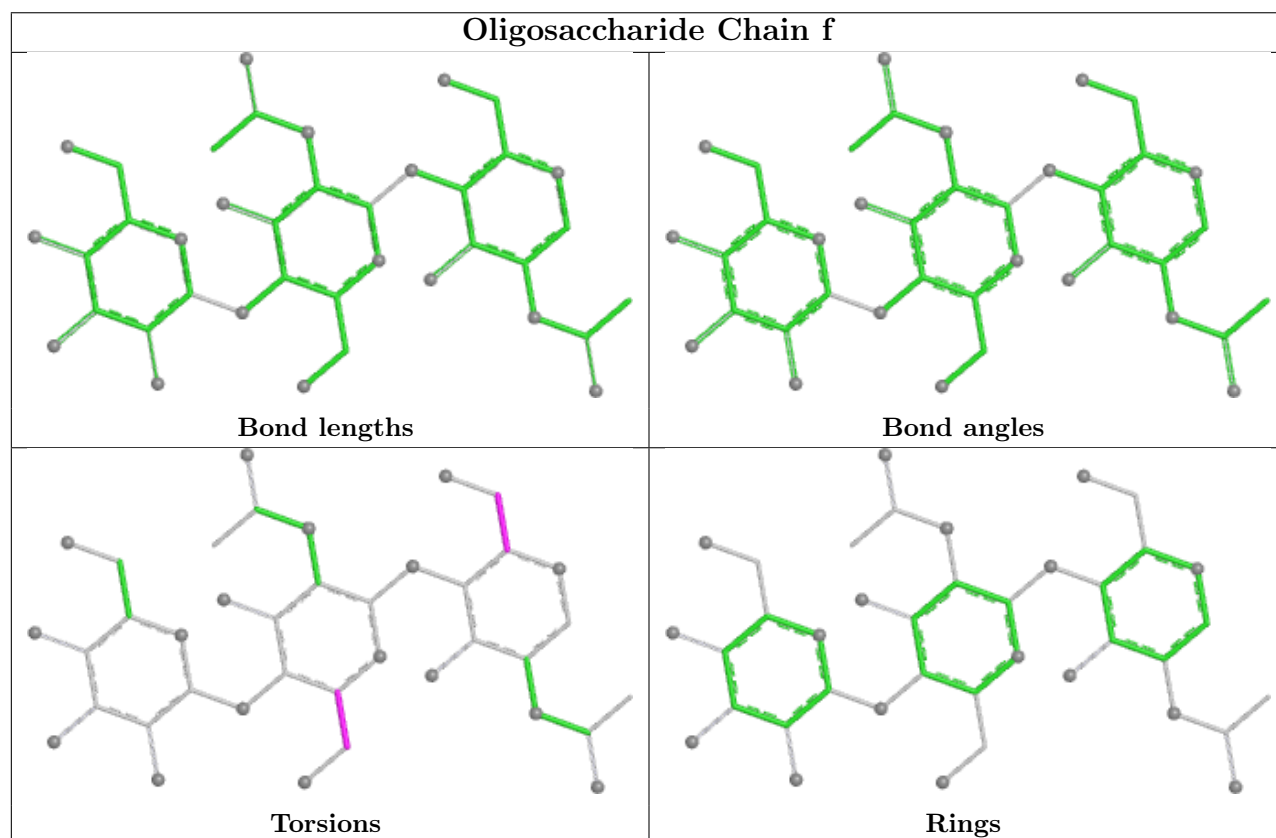
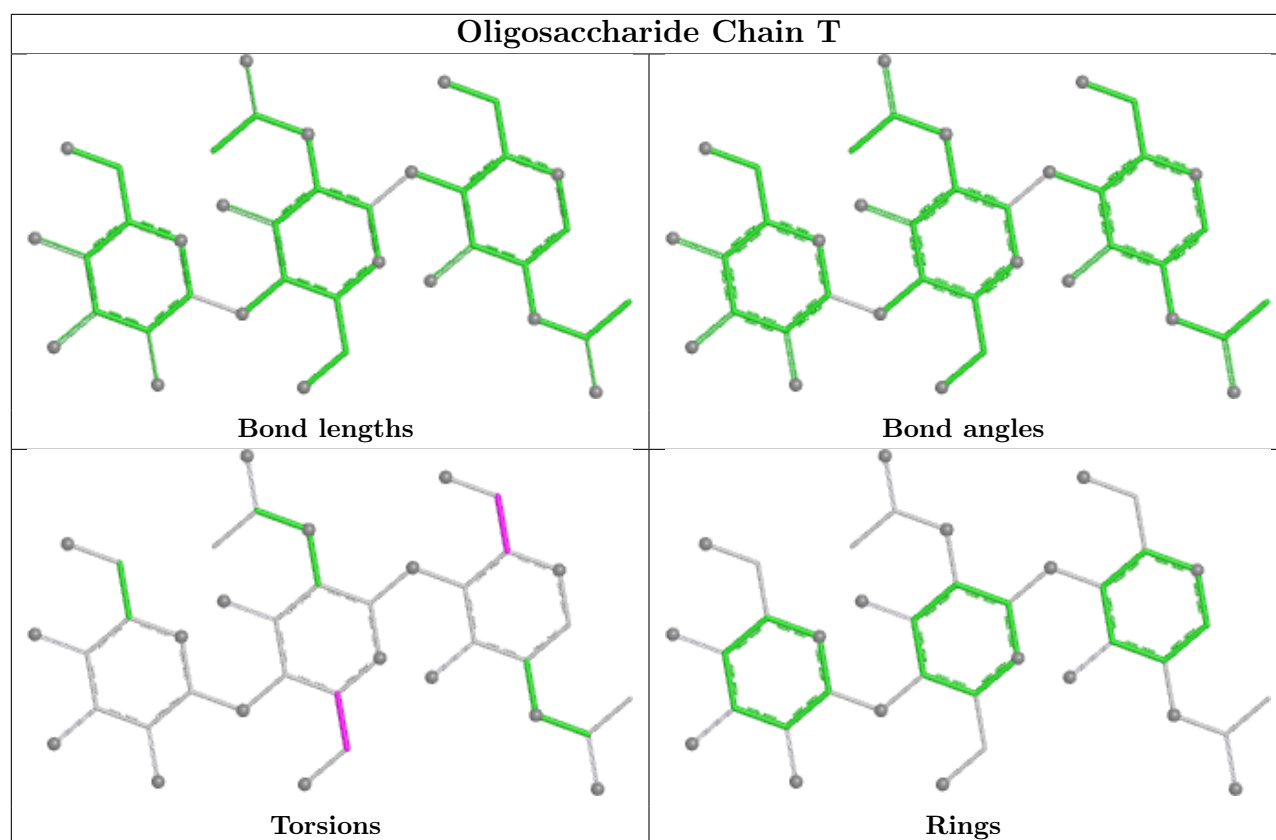


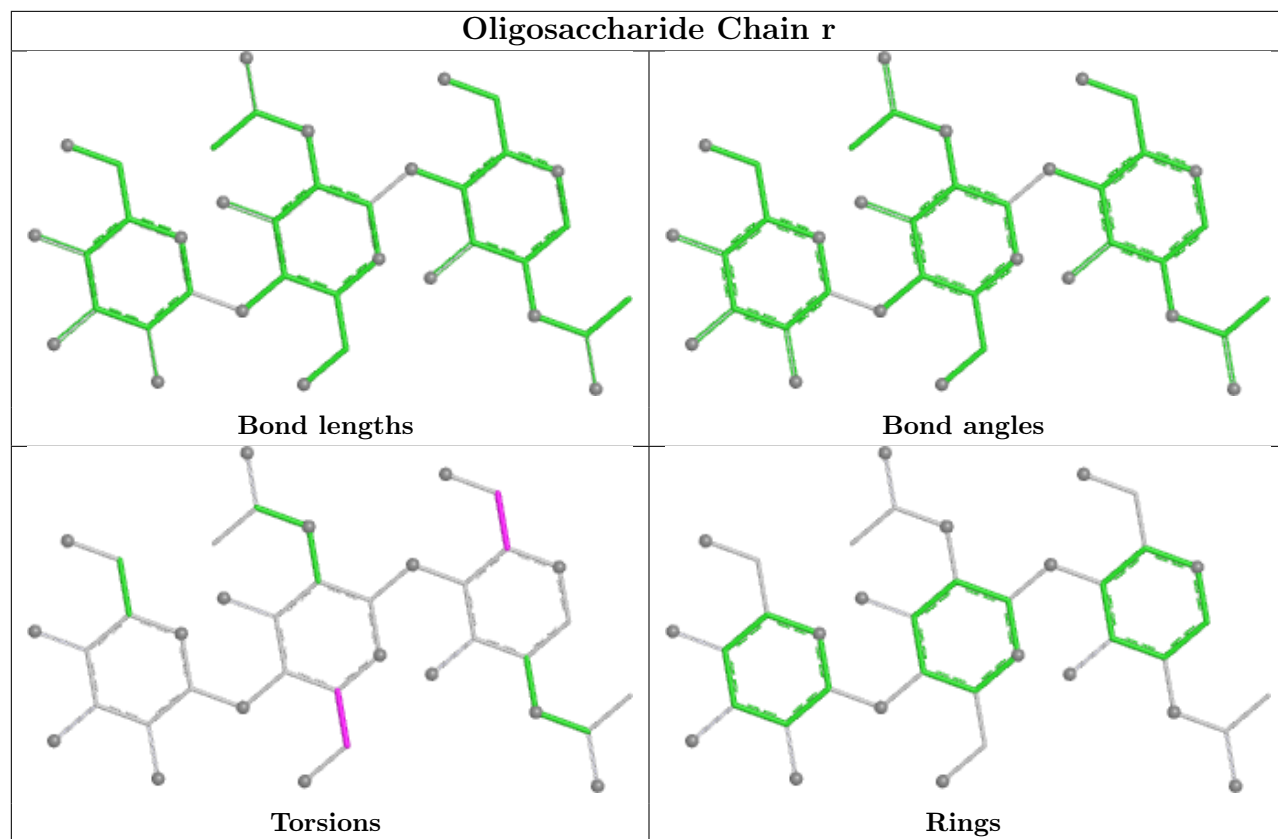


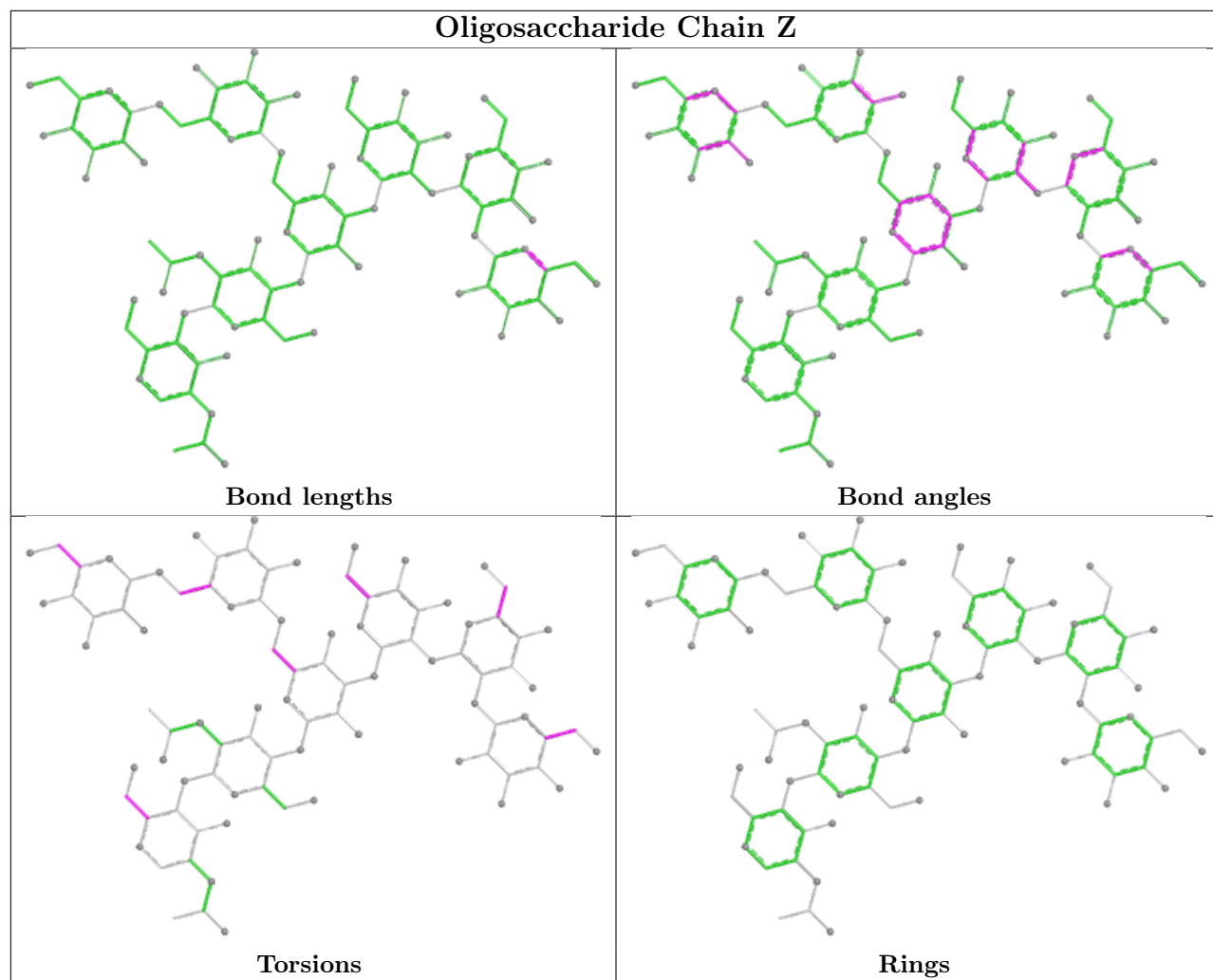


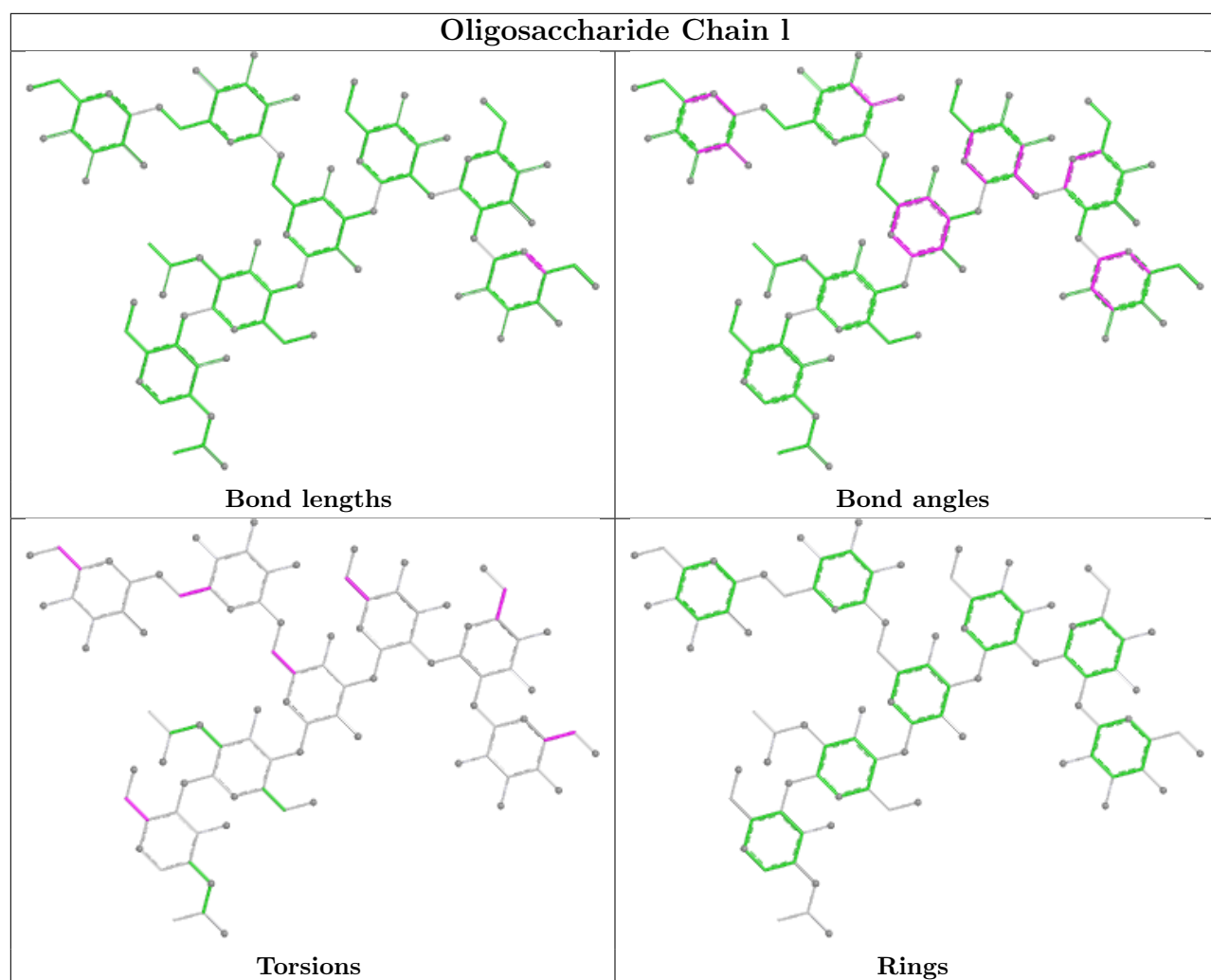


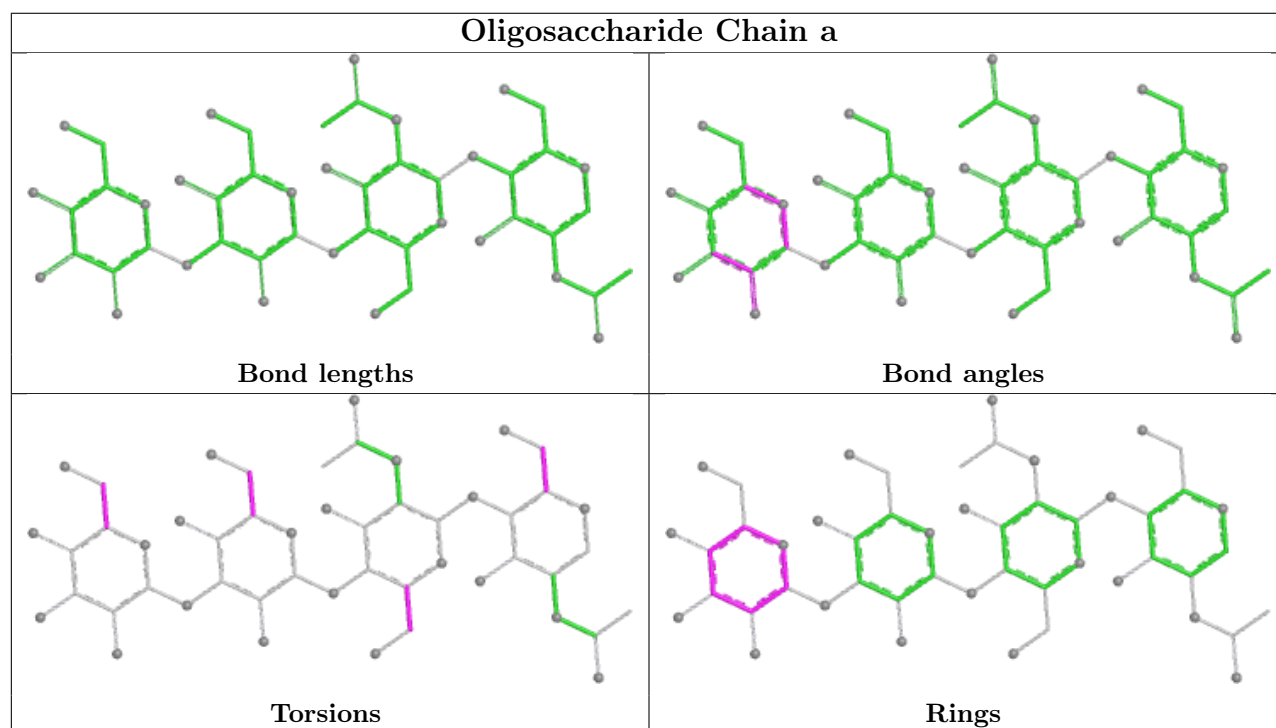
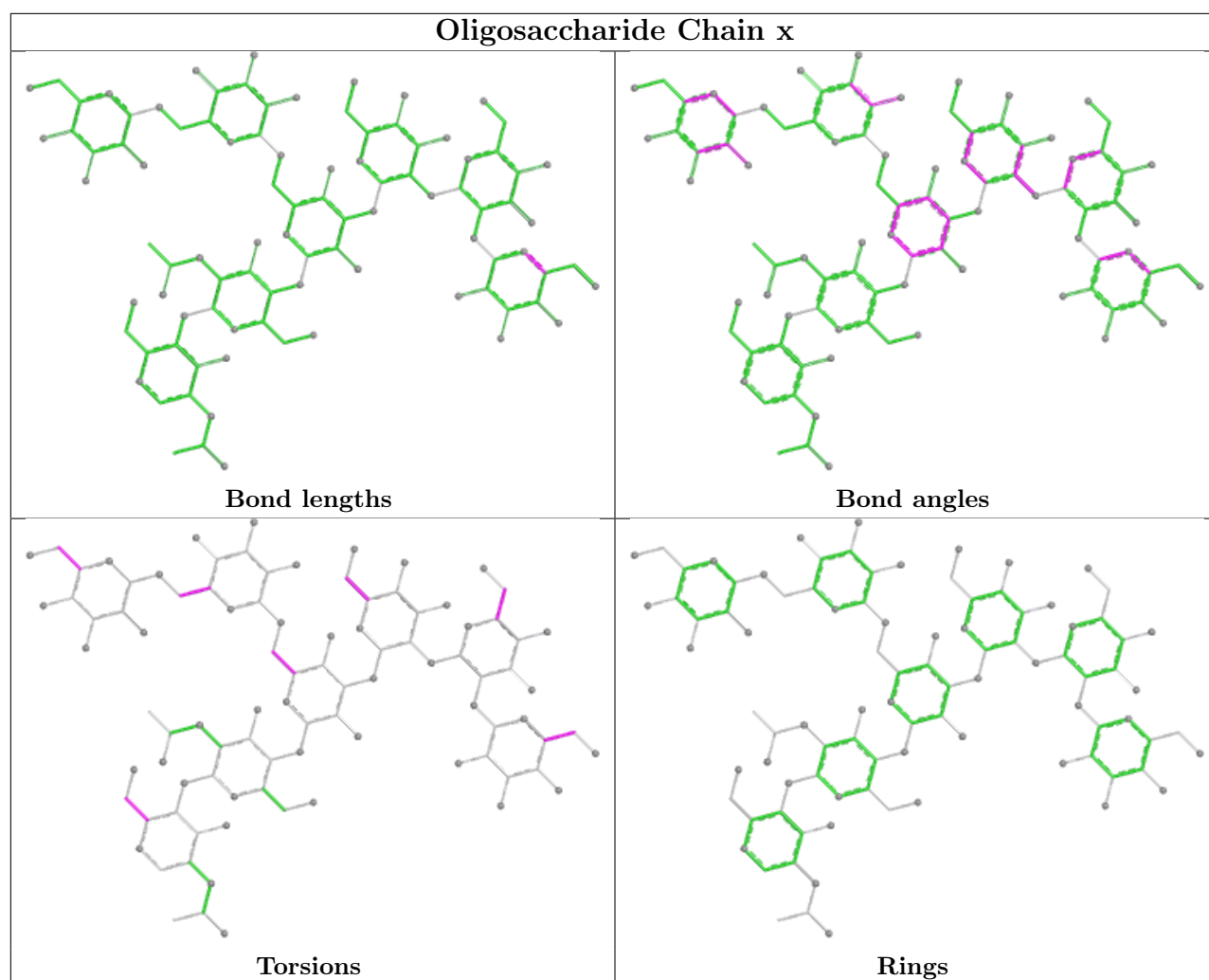


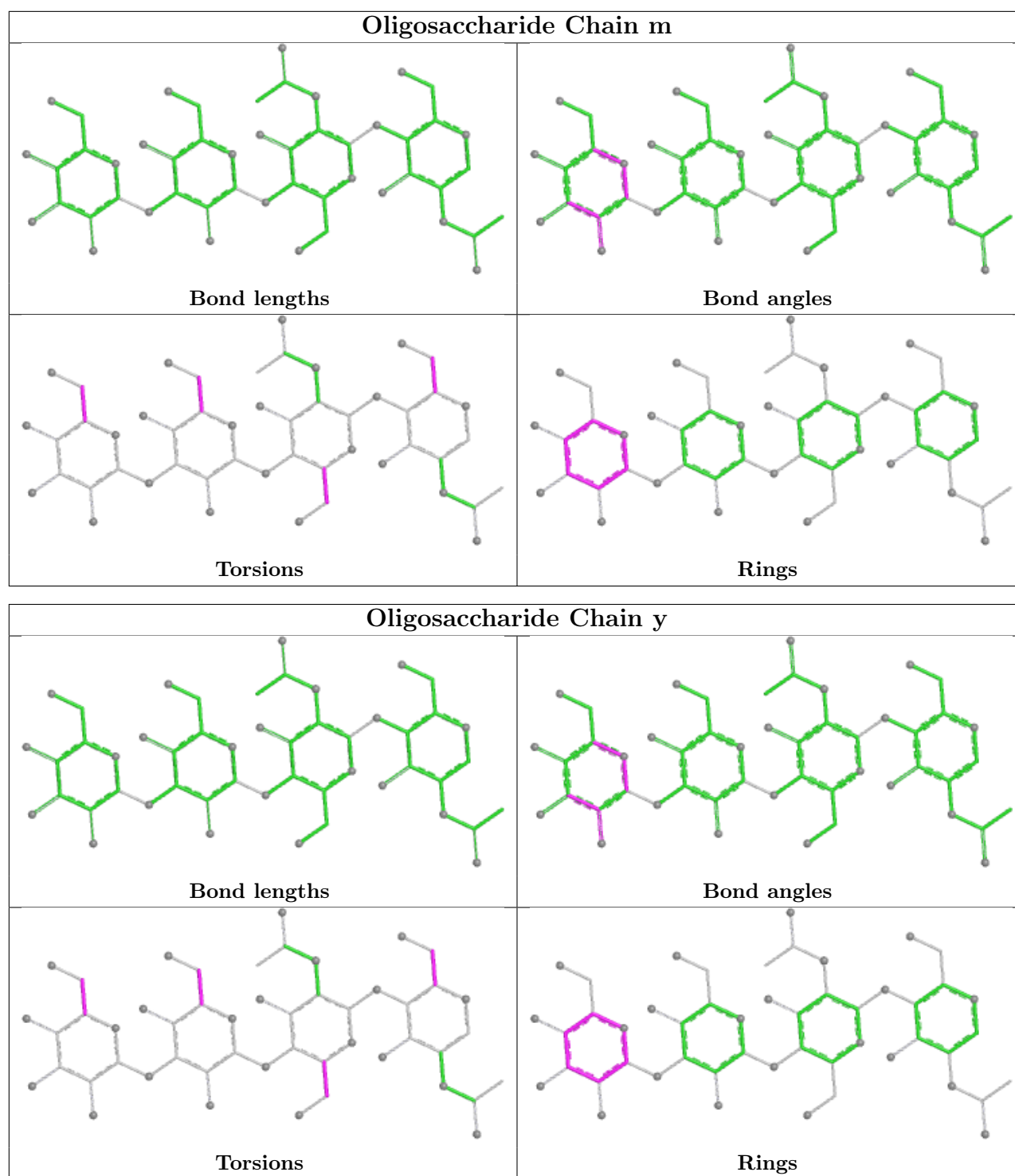












5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	G	609	1	14,14,15	0.32	0	17,19,21	0.66	1 (5%)
11	NAG	G	603	1	14,14,15	0.42	0	17,19,21	0.53	0
11	NAG	B	703	2	14,14,15	0.74	0	17,19,21	2.36	3 (17%)
11	NAG	A	603	1	14,14,15	0.43	0	17,19,21	0.54	0
11	NAG	M	603	1	14,14,15	0.44	0	17,19,21	0.54	0
11	NAG	B	701	2	14,14,15	0.29	0	17,19,21	0.58	0
11	NAG	N	702	2	14,14,15	0.72	0	17,19,21	2.41	4 (23%)
11	NAG	N	701	2	14,14,15	0.28	0	17,19,21	0.58	0
11	NAG	M	607	1	14,14,15	0.33	0	17,19,21	0.47	0
11	NAG	G	607	1	14,14,15	0.32	0	17,19,21	0.47	0
11	NAG	H	702	2	14,14,15	0.71	0	17,19,21	2.41	4 (23%)
11	NAG	M	609	1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
11	NAG	A	607	1	14,14,15	0.33	0	17,19,21	0.47	0
11	NAG	B	702	2	14,14,15	0.71	0	17,19,21	2.42	4 (23%)
11	NAG	A	609	1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
11	NAG	G	608	1	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
11	NAG	H	703	2	14,14,15	0.75	0	17,19,21	2.37	3 (17%)
11	NAG	A	608	1	14,14,15	0.49	0	17,19,21	1.02	1 (5%)
11	NAG	M	608	1	14,14,15	0.48	0	17,19,21	1.01	1 (5%)
11	NAG	H	701	2	14,14,15	0.30	0	17,19,21	0.59	0
11	NAG	N	703	2	14,14,15	0.74	0	17,19,21	2.36	3 (17%)

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
11	NAG	G	609	1	-	0/6/23/26	0/1/1/1
11	NAG	G	603	1	-	1/6/23/26	0/1/1/1
11	NAG	B	703	2	-	6/6/23/26	0/1/1/1
11	NAG	A	603	1	-	1/6/23/26	0/1/1/1
11	NAG	M	603	1	-	1/6/23/26	0/1/1/1
11	NAG	B	701	2	-	0/6/23/26	0/1/1/1
11	NAG	N	702	2	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	N	701	2	-	0/6/23/26	0/1/1/1
11	NAG	M	607	1	-	2/6/23/26	0/1/1/1
11	NAG	G	607	1	-	2/6/23/26	0/1/1/1
11	NAG	H	702	2	-	6/6/23/26	0/1/1/1
11	NAG	M	609	1	-	0/6/23/26	0/1/1/1
11	NAG	A	607	1	-	2/6/23/26	0/1/1/1
11	NAG	B	702	2	-	6/6/23/26	0/1/1/1
11	NAG	A	609	1	-	0/6/23/26	0/1/1/1
11	NAG	G	608	1	-	2/6/23/26	0/1/1/1
11	NAG	H	703	2	-	6/6/23/26	0/1/1/1
11	NAG	A	608	1	-	2/6/23/26	0/1/1/1
11	NAG	M	608	1	-	2/6/23/26	0/1/1/1
11	NAG	H	701	2	-	0/6/23/26	0/1/1/1
11	NAG	N	703	2	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	702	NAG	C2-N2-C7	8.32	134.06	122.90
11	H	702	NAG	C2-N2-C7	8.31	134.03	122.90
11	N	702	NAG	C2-N2-C7	8.29	134.01	122.90
11	H	703	NAG	C2-N2-C7	8.18	133.87	122.90
11	B	703	NAG	C2-N2-C7	8.18	133.86	122.90
11	N	703	NAG	C2-N2-C7	8.17	133.85	122.90
11	H	703	NAG	C1-C2-N2	4.19	117.03	110.43
11	B	703	NAG	C1-C2-N2	4.16	117.00	110.43
11	N	703	NAG	C1-C2-N2	4.16	116.99	110.43
11	B	702	NAG	C1-C2-N2	3.78	116.39	110.43
11	N	702	NAG	C1-C2-N2	3.76	116.36	110.43
11	H	702	NAG	C1-C2-N2	3.75	116.34	110.43
11	G	608	NAG	C2-N2-C7	3.15	127.13	122.90
11	A	608	NAG	C2-N2-C7	3.14	127.10	122.90
11	M	608	NAG	C2-N2-C7	3.13	127.09	122.90
11	N	702	NAG	C1-O5-C5	2.68	115.77	112.19
11	B	702	NAG	C1-O5-C5	2.66	115.76	112.19
11	H	702	NAG	C1-O5-C5	2.64	115.73	112.19
11	H	703	NAG	C8-C7-N2	2.35	120.02	116.12
11	B	703	NAG	C8-C7-N2	2.34	120.00	116.12
11	N	703	NAG	C8-C7-N2	2.34	119.99	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	609	NAG	C1-O5-C5	2.29	115.25	112.19
11	A	609	NAG	C1-O5-C5	2.27	115.23	112.19
11	G	609	NAG	C1-O5-C5	2.26	115.22	112.19
11	N	702	NAG	C8-C7-N2	2.19	119.75	116.12
11	H	702	NAG	C8-C7-N2	2.19	119.75	116.12
11	B	702	NAG	C8-C7-N2	2.19	119.74	116.12

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	703	NAG	O5-C5-C6-O6
11	H	703	NAG	O5-C5-C6-O6
11	N	703	NAG	O5-C5-C6-O6
11	A	607	NAG	O5-C5-C6-O6
11	B	702	NAG	O5-C5-C6-O6
11	G	607	NAG	O5-C5-C6-O6
11	H	702	NAG	O5-C5-C6-O6
11	M	607	NAG	O5-C5-C6-O6
11	N	702	NAG	O5-C5-C6-O6
11	B	703	NAG	C4-C5-C6-O6
11	H	703	NAG	C4-C5-C6-O6
11	N	703	NAG	C4-C5-C6-O6
11	A	607	NAG	C4-C5-C6-O6
11	B	702	NAG	C4-C5-C6-O6
11	G	607	NAG	C4-C5-C6-O6
11	H	702	NAG	C4-C5-C6-O6
11	M	607	NAG	C4-C5-C6-O6
11	N	702	NAG	C4-C5-C6-O6
11	B	702	NAG	C8-C7-N2-C2
11	B	702	NAG	O7-C7-N2-C2
11	B	703	NAG	C8-C7-N2-C2
11	B	703	NAG	O7-C7-N2-C2
11	H	702	NAG	C8-C7-N2-C2
11	H	702	NAG	O7-C7-N2-C2
11	H	703	NAG	C8-C7-N2-C2
11	H	703	NAG	O7-C7-N2-C2
11	N	702	NAG	C8-C7-N2-C2
11	N	702	NAG	O7-C7-N2-C2
11	N	703	NAG	C8-C7-N2-C2
11	N	703	NAG	O7-C7-N2-C2
11	G	603	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	A	603	NAG	O5-C5-C6-O6
11	M	603	NAG	O5-C5-C6-O6
11	A	608	NAG	C3-C2-N2-C7
11	B	702	NAG	C3-C2-N2-C7
11	G	608	NAG	C3-C2-N2-C7
11	H	702	NAG	C3-C2-N2-C7
11	M	608	NAG	C3-C2-N2-C7
11	N	702	NAG	C3-C2-N2-C7
11	A	608	NAG	C1-C2-N2-C7
11	B	702	NAG	C1-C2-N2-C7
11	B	703	NAG	C1-C2-N2-C7
11	G	608	NAG	C1-C2-N2-C7
11	H	702	NAG	C1-C2-N2-C7
11	H	703	NAG	C1-C2-N2-C7
11	M	608	NAG	C1-C2-N2-C7
11	N	702	NAG	C1-C2-N2-C7
11	N	703	NAG	C1-C2-N2-C7
11	B	703	NAG	C3-C2-N2-C7
11	H	703	NAG	C3-C2-N2-C7
11	N	703	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	603	NAG	1	0
11	A	603	NAG	1	0
11	M	603	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.

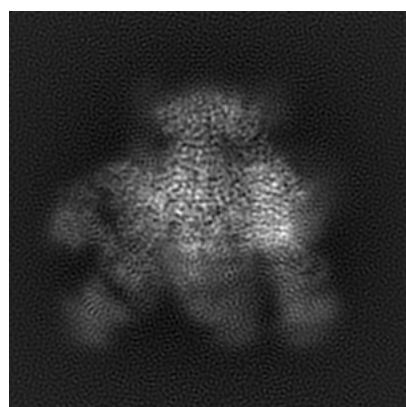
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21112. These allow visual inspection of the internal detail of the map and identification of artifacts.

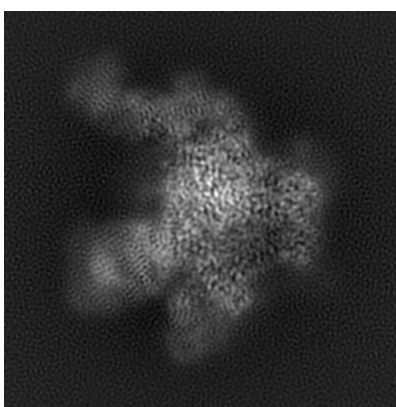
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

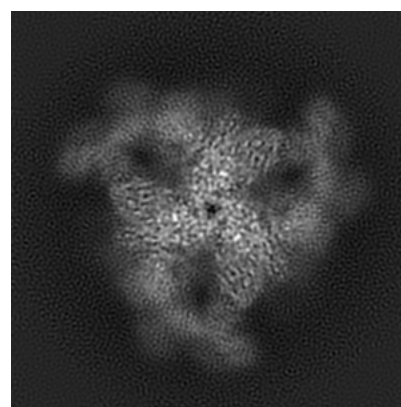
6.1.1 Primary map



X



Y

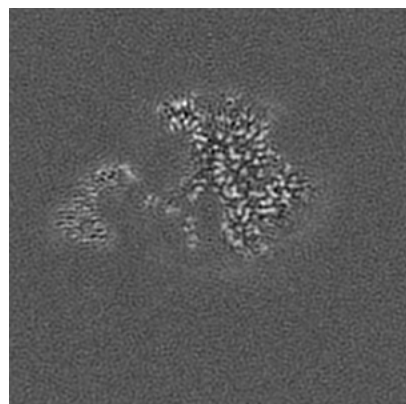


Z

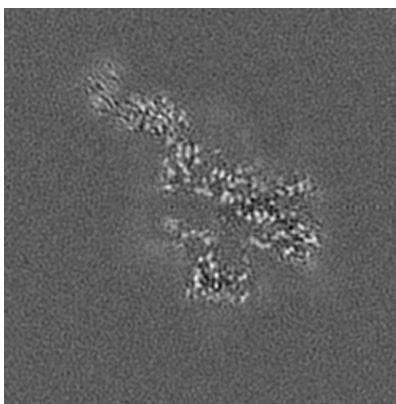
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

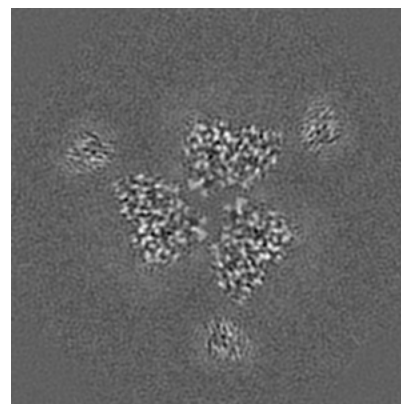
6.2.1 Primary map



X Index: 115



Y Index: 115

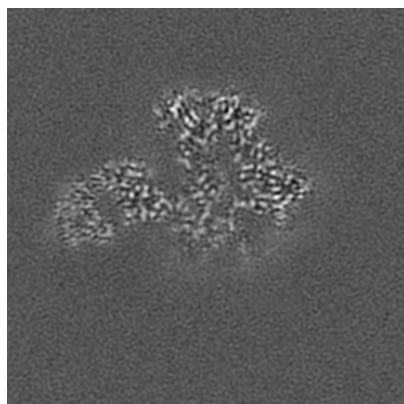


Z Index: 115

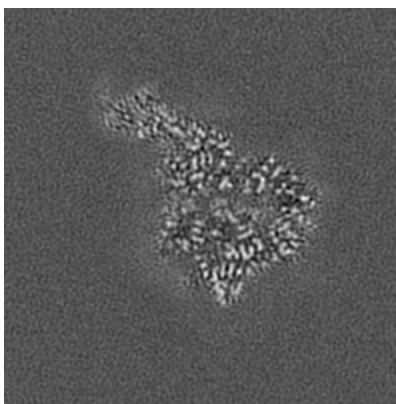
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

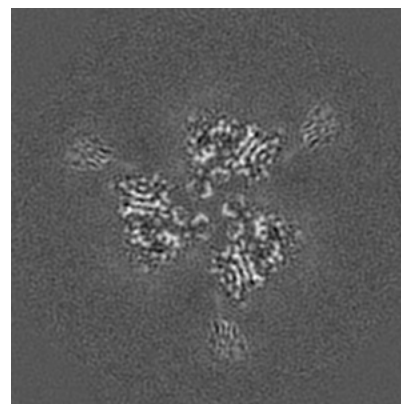
6.3.1 Primary map



X Index: 124



Y Index: 104

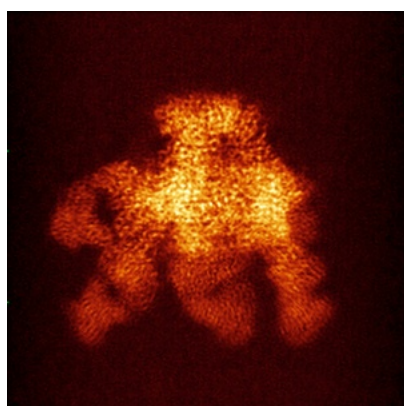


Z Index: 118

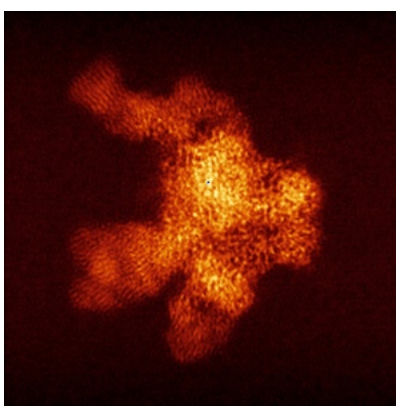
The images above show the largest variance slices of the map in three orthogonal directions.

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

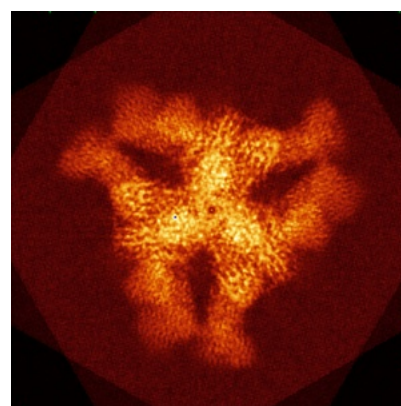
6.4.1 Primary map



X



Y

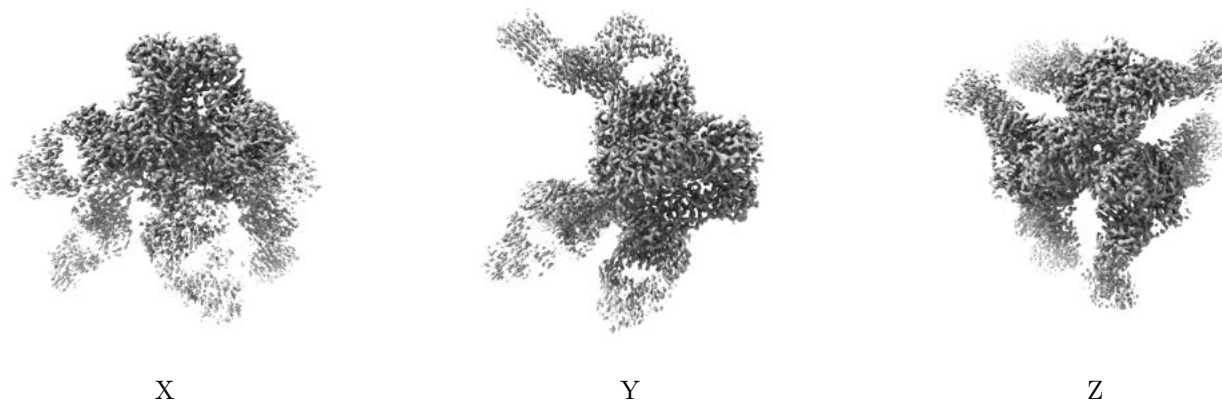


Z

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 10.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

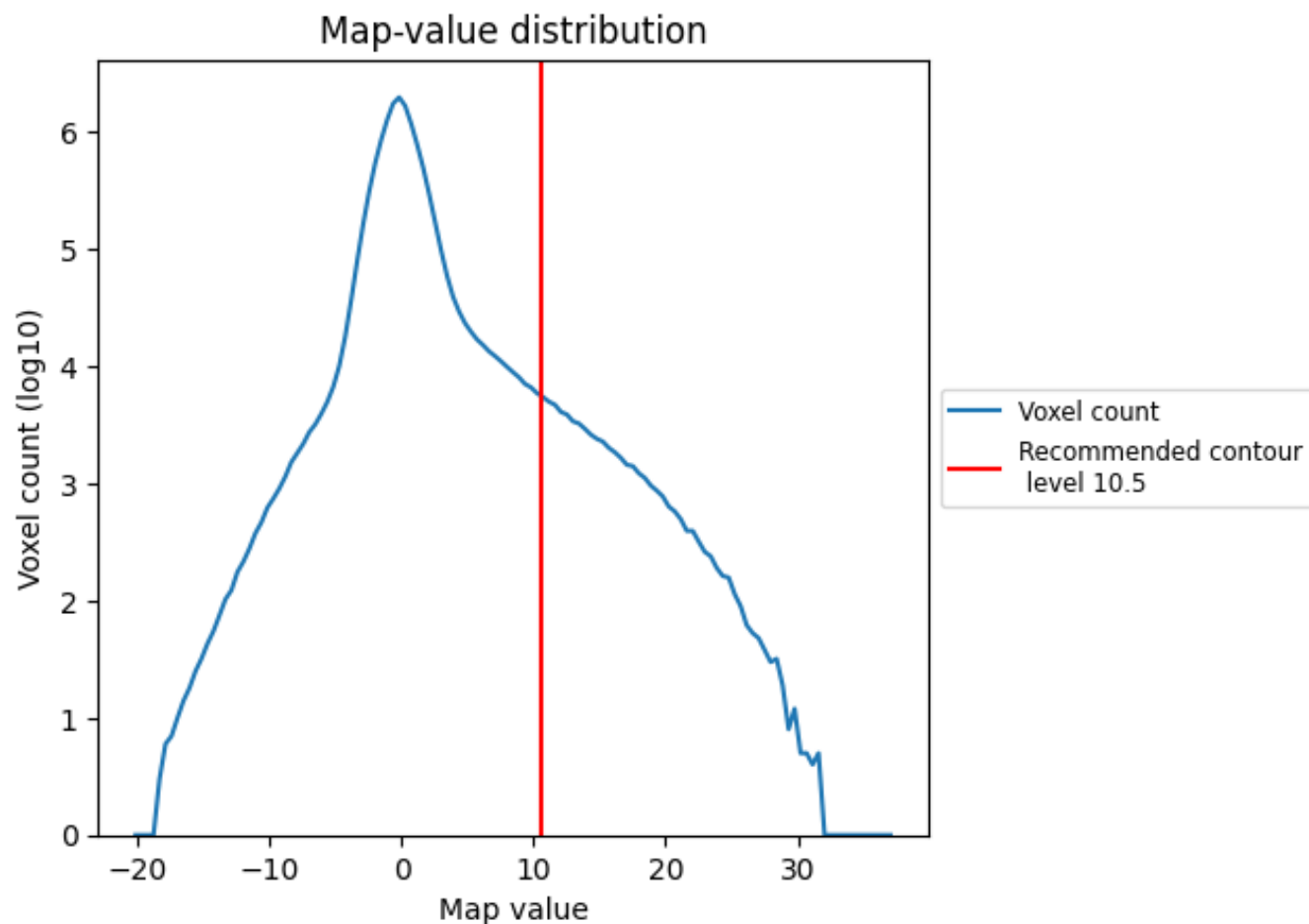
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

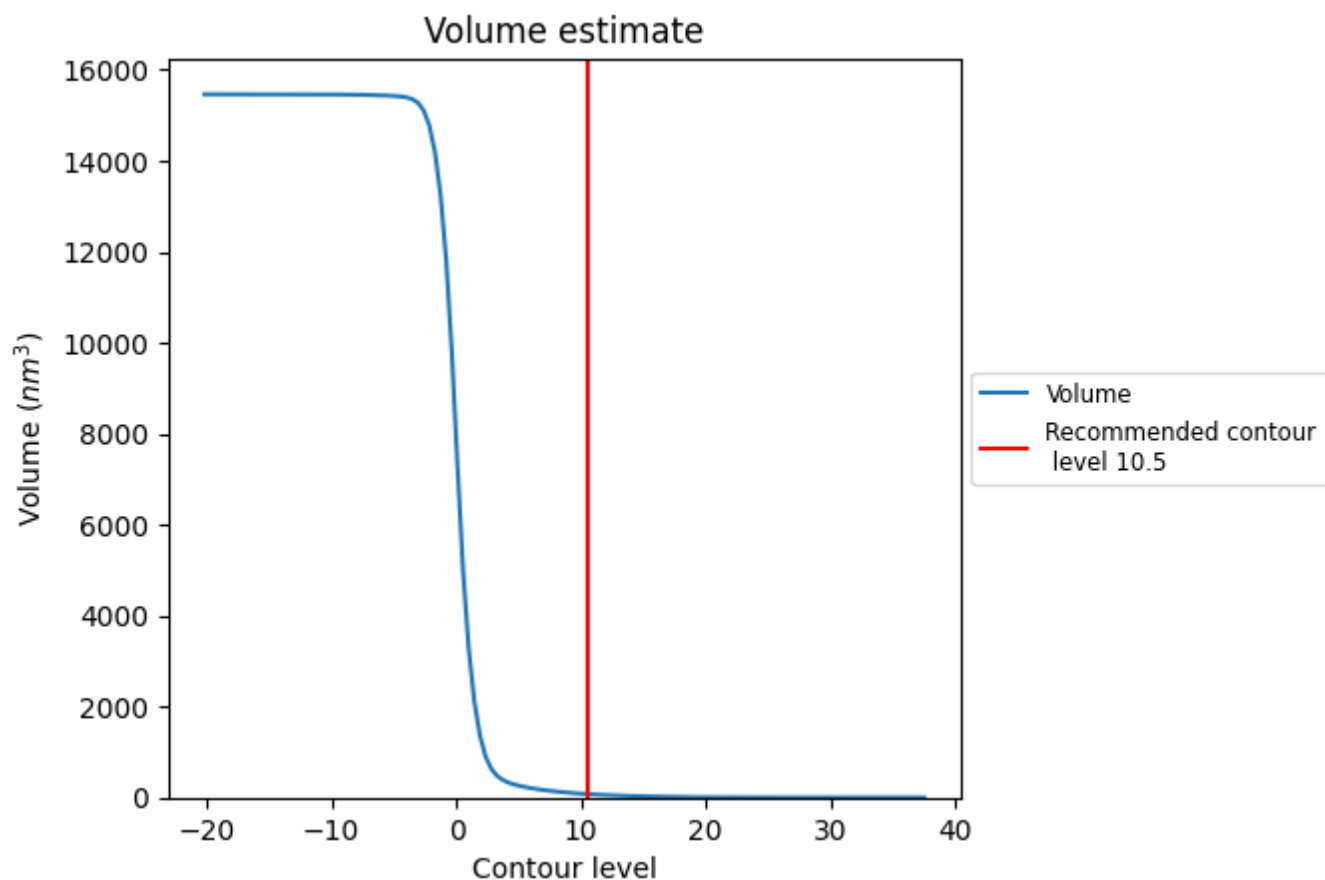
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

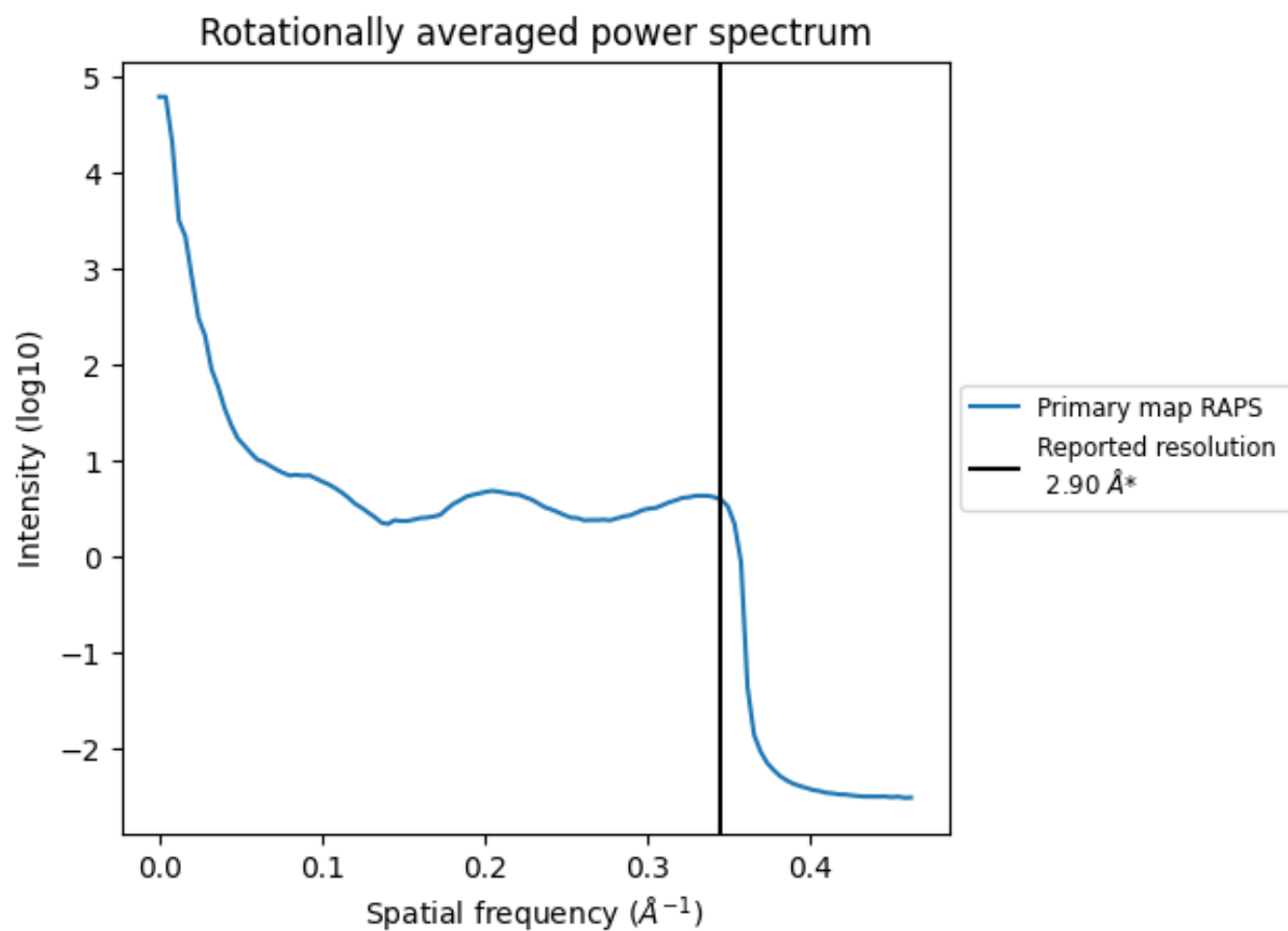
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm³; this corresponds to an approximate mass of 69 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 0.345 Å⁻¹

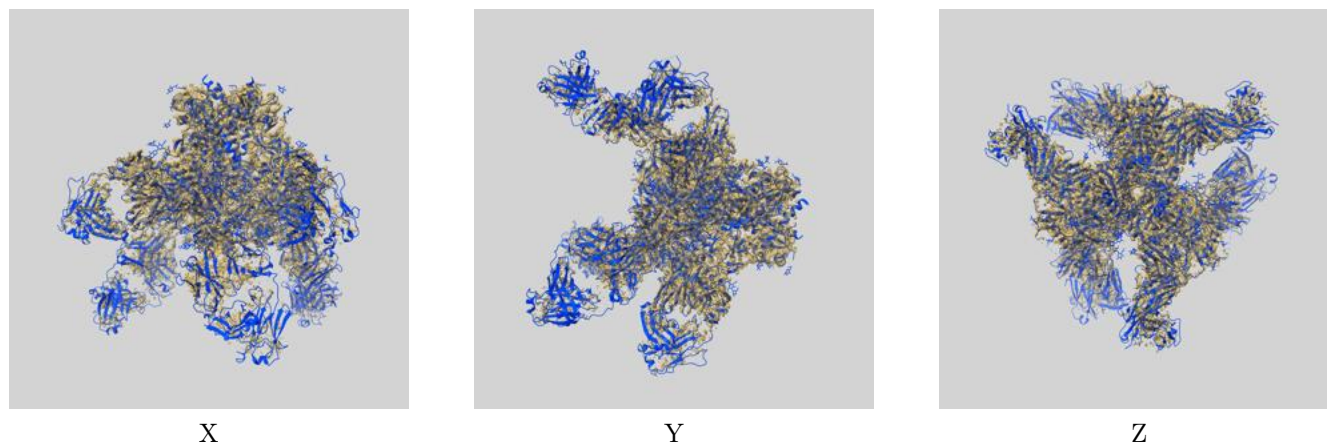
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

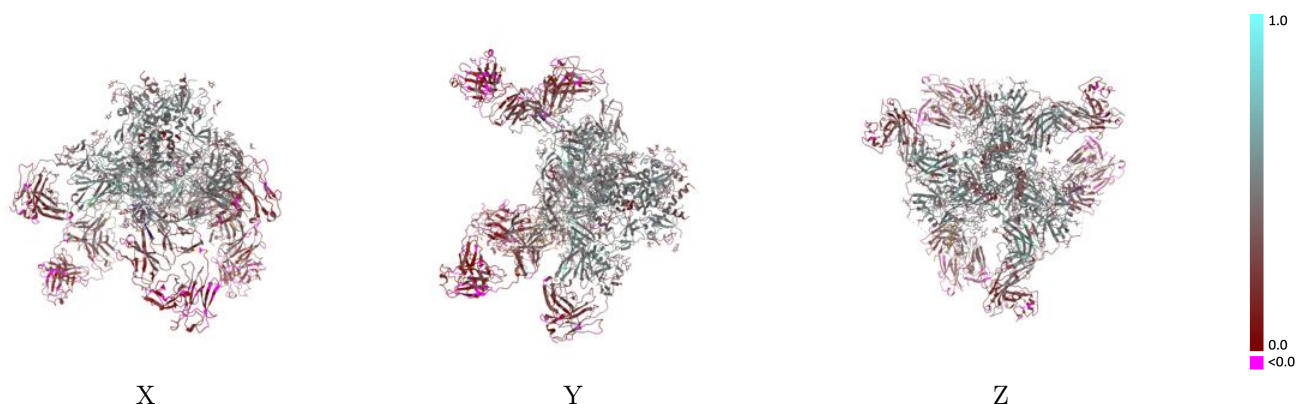
This section contains information regarding the fit between EMDB map EMD-21112 and PDB model 6V8Z. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



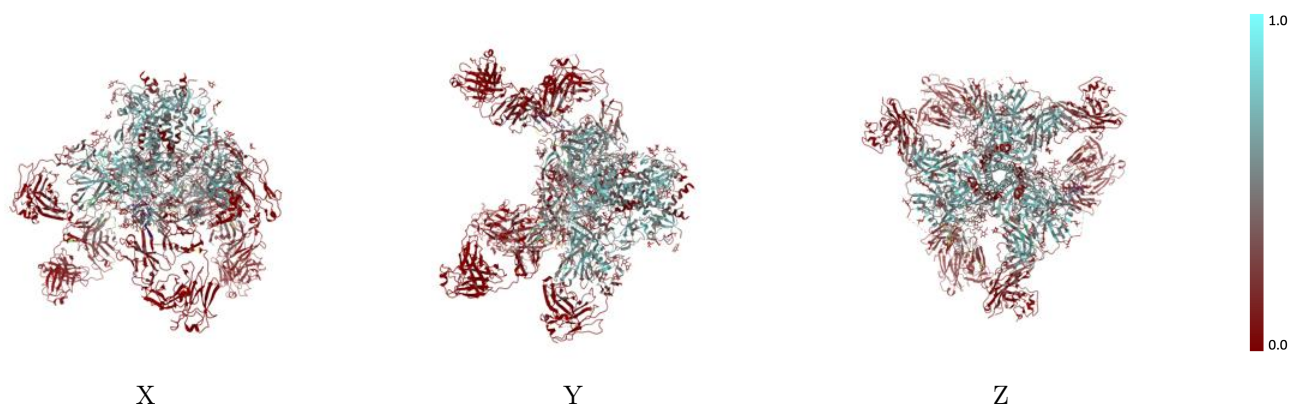
The images above show the 3D surface view of the map at the recommended contour level 10.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



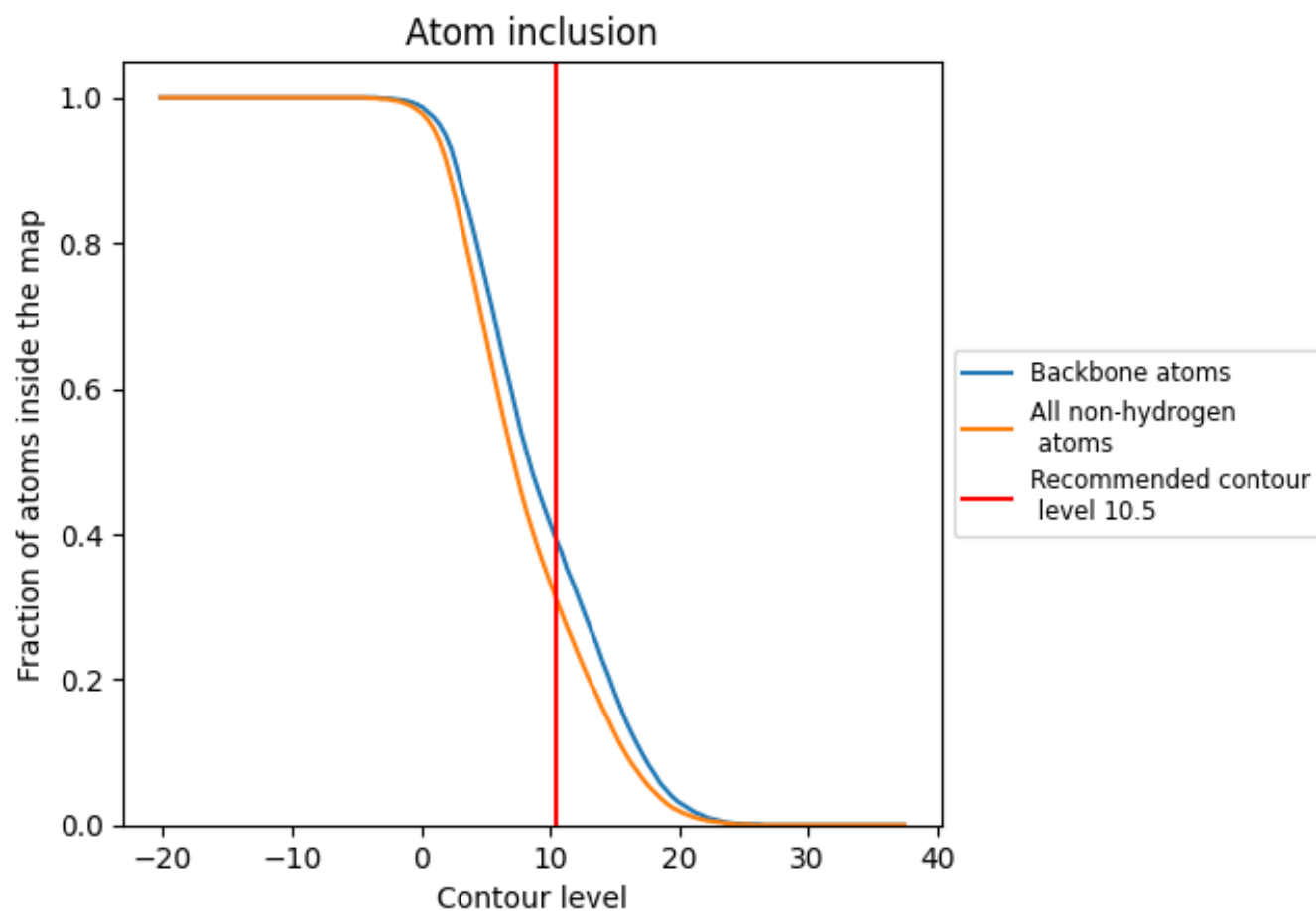
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 31% 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 (10.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3100	 0.3580
0	 0.1790	 0.5180
1	 0.0710	 0.3040
A	 0.5030	 0.4790
B	 0.4340	 0.4170
C	 0.3400	 0.3950
D	 0.1120	 0.2110
E	 0.1130	 0.2250
F	 0.2050	 0.3020
G	 0.5000	 0.4780
H	 0.4330	 0.4120
I	 0.3430	 0.3920
J	 0.1080	 0.2080
K	 0.1100	 0.2270
L	 0.2040	 0.3010
M	 0.5000	 0.4770
N	 0.4330	 0.4130
O	 0.3430	 0.3930
P	 0.1090	 0.2100
Q	 0.1150	 0.2260
R	 0.2030	 0.3030
S	 0.0710	 0.2560
T	 0.0510	 0.3000
U	 0.2140	 0.3980
V	 0.3570	 0.4660
W	 0.0360	 0.2730
X	 0.2500	 0.3310
Y	 0.0710	 0.3120
Z	 0.3400	 0.4280
a	 0.2200	 0.4150
b	 0.0000	 0.1160
c	 0.2140	 0.5100
d	 0.0710	 0.3070
e	 0.0710	 0.2460
f	 0.0770	 0.2760



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Chain	Atom inclusion	Q-score
g	 0.2140	 0.3970
h	 0.3210	 0.4600
i	 0.0360	 0.2620
j	 0.2140	 0.3080
k	 0.0710	 0.3300
l	 0.3620	 0.4330
m	 0.2400	 0.3960
n	 0.0000	 0.1090
o	 0.2140	 0.5130
p	 0.0710	 0.3110
q	 0.0710	 0.2470
r	 0.0770	 0.2990
s	 0.2500	 0.4000
t	 0.3210	 0.4610
u	 0.0710	 0.2480
v	 0.2500	 0.3420
w	 0.0710	 0.3360
x	 0.3620	 0.4340
y	 0.2400	 0.4060
z	 0.0000	 0.1070