



Full wwPDB EM Validation Report ⓘ

May 21, 2026 – 02:49 PM EDT

PDB ID : 9Q3X / pdb_00009q3x
EMDB ID : EMD-72216
Title : The CryoEM structure of Rhesus macaque 1G3 and PGT121 Fabs in complex with BG505 SOSIP.664
Authors : Nguyen, D.N.; Tolbert, W.D.; Pazgier, M.
Deposited on : 2025-08-19
Resolution : 3.64 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:

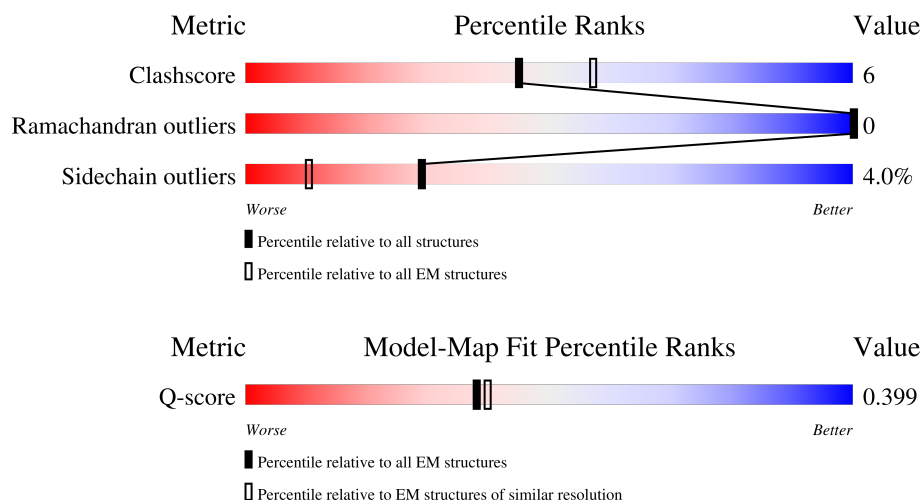
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.64 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	11633 (3.14 - 4.14)

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	481	
1	G	481	
1	I	481	
2	B	153	

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Mol	Chain	Length	Quality of chain
2	C	153	
2	J	153	
3	D	115	
3	H	115	
3	K	115	
4	E	106	
4	L	106	
4	M	106	
5	d	235	
5	h	235	
5	k	235	
6	e	213	
6	l	213	
6	m	213	
7	1	2	
7	2	2	
7	N	2	
7	P	2	
7	Q	2	
7	R	2	
7	S	2	
7	T	2	
7	V	2	
7	W	2	
7	Z	2	

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Mol	Chain	Length	Quality of chain
7	a	2	100%
7	b	2	50% 50%
7	c	2	100%
7	g	2	50% 50%
7	i	2	100%
7	o	2	100%
7	q	2	50% 50%
7	r	2	50% 50%
7	s	2	100%
7	t	2	50% 50%
7	u	2	100%
7	w	2	50% 50%
7	x	2	100%
8	U	4	100%
8	f	4	75% 25%
8	v	4	100%
9	X	3	33% 67%
9	j	3	33% 100%
9	y	3	33% 67%
10	Y	5	60% 80% 20%
10	n	5	40% 60%
10	z	5	40% 60%
11	0	9	11% 100%
11	O	9	11% 78% 11%
11	p	9	11% 100%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 25890 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 BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	452	Total	C	N	O	S	0	0
			3559	2233	629	669	28		
1	A	452	Total	C	N	O	S	0	0
			3559	2233	629	669	28		
1	I	452	Total	C	N	O	S	0	0
			3559	2233	629	669	28		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S5
G	501	CYS	ALA	engineered mutation	UNP Q2N0S5
G	509	ARG	GLU	engineered mutation	UNP Q2N0S5
G	510	ARG	LYS	engineered mutation	UNP Q2N0S5
G	512	ARG	-	insertion	UNP Q2N0S5
G	513	ARG	-	insertion	UNP Q2N0S5
A	332	ASN	THR	engineered mutation	UNP Q2N0S5
A	501	CYS	ALA	engineered mutation	UNP Q2N0S5
A	509	ARG	GLU	engineered mutation	UNP Q2N0S5
A	510	ARG	LYS	engineered mutation	UNP Q2N0S5
A	512	ARG	-	insertion	UNP Q2N0S5
A	513	ARG	-	insertion	UNP Q2N0S5
I	332	ASN	THR	engineered mutation	UNP Q2N0S5
I	501	CYS	ALA	engineered mutation	UNP Q2N0S5
I	509	ARG	GLU	engineered mutation	UNP Q2N0S5
I	510	ARG	LYS	engineered mutation	UNP Q2N0S5
I	512	ARG	-	insertion	UNP Q2N0S5
I	513	ARG	-	insertion	UNP Q2N0S5

- Molecule 2 is a protein called BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	129	Total	C	N	O	S	0	0
			1018	644	175	193	6		
2	C	129	Total	C	N	O	S	0	0
			1018	644	175	193	6		
2	J	129	Total	C	N	O	S	0	0
			1018	644	175	193	6		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called 1G3 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	109	Total	C	N	O	S	0	0
			828	524	139	163	2		
3	D	109	Total	C	N	O	S	0	0
			828	524	139	163	2		
3	K	109	Total	C	N	O	S	0	0
			828	524	139	163	2		

- Molecule 4 is a protein called 1G3 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	102	Total	C	N	O	S	0	0
			793	503	130	157	3		
4	E	102	Total	C	N	O	S	0	0
			793	503	130	157	3		
4	M	102	Total	C	N	O	S	0	0
			793	503	130	157	3		

- Molecule 5 is a protein called PGT121 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	131	Total	C	N	O	S	0	0
			1017	644	173	196	4		

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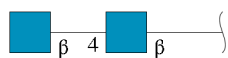
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	131	Total	C	N	O	S	0	0
			1017	644	173	196	4		
5	k	131	Total	C	N	O	S	0	0
			1017	644	173	196	4		

- Molecule 6 is a protein called PGT121 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	l	108	Total	C	N	O	S	0	0
			824	516	143	163	2		
6	e	108	Total	C	N	O	S	0	0
			824	516	143	163	2		
6	m	108	Total	C	N	O	S	0	0
			824	516	143	163	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	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	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	o	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	r	2	Total	C	N	O	0	0
			28	16	2	10		
7	s	2	Total	C	N	O	0	0
			28	16	2	10		

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



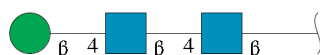
Mol	Chain	Residues	Atoms				AltConf	Trace
8	f	4	Total	C	N	O	0	0
			50	28	2	20		

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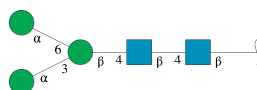
Mol	Chain	Residues	Atoms				AltConf	Trace
8	v	4	Total	C	N	O	0	0
			50	28	2	20		
8	U	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 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.



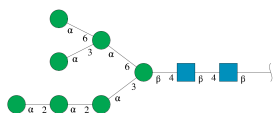
Mol	Chain	Residues	Atoms				AltConf	Trace
9	j	3	Total	C	N	O	0	0
			39	22	2	15		
9	y	3	Total	C	N	O	0	0
			39	22	2	15		
9	X	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 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.



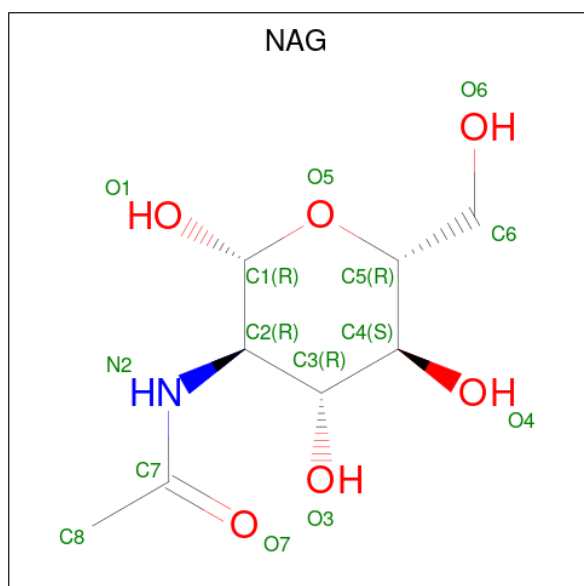
Mol	Chain	Residues	Atoms				AltConf	Trace
10	n	5	Total	C	N	O	0	0
			61	34	2	25		
10	z	5	Total	C	N	O	0	0
			61	34	2	25		
10	Y	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
11	p	9	Total	C	N	O	0	0
			105	58	2	45		
11	O	9	Total	C	N	O	0	0
			105	58	2	45		
11	0	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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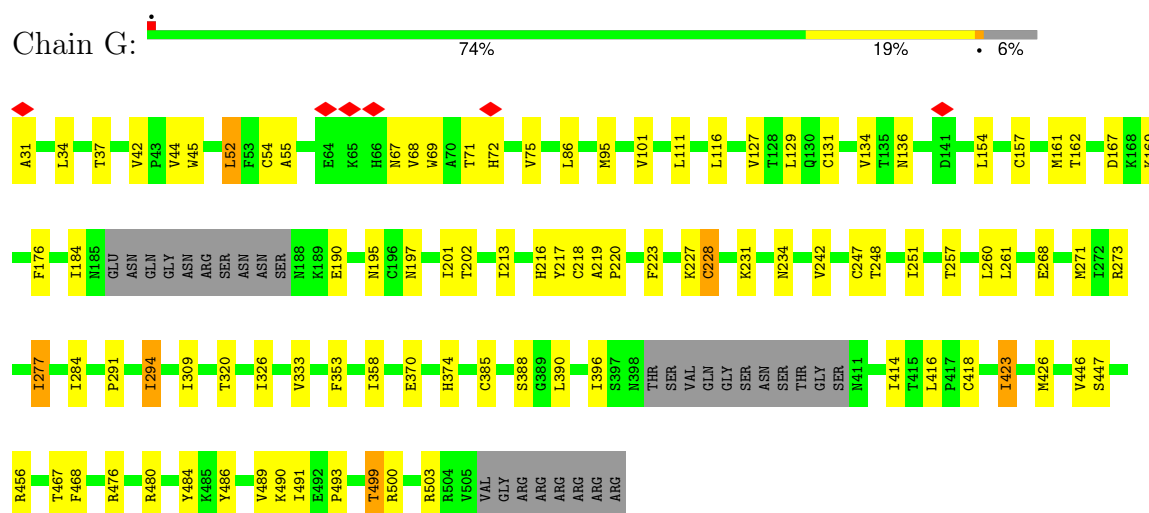
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Mol	Chain	Residues	Atoms				AltConf
12	G	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	C	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	J	1	Total	C	N	O	0
			14	8	1	5	

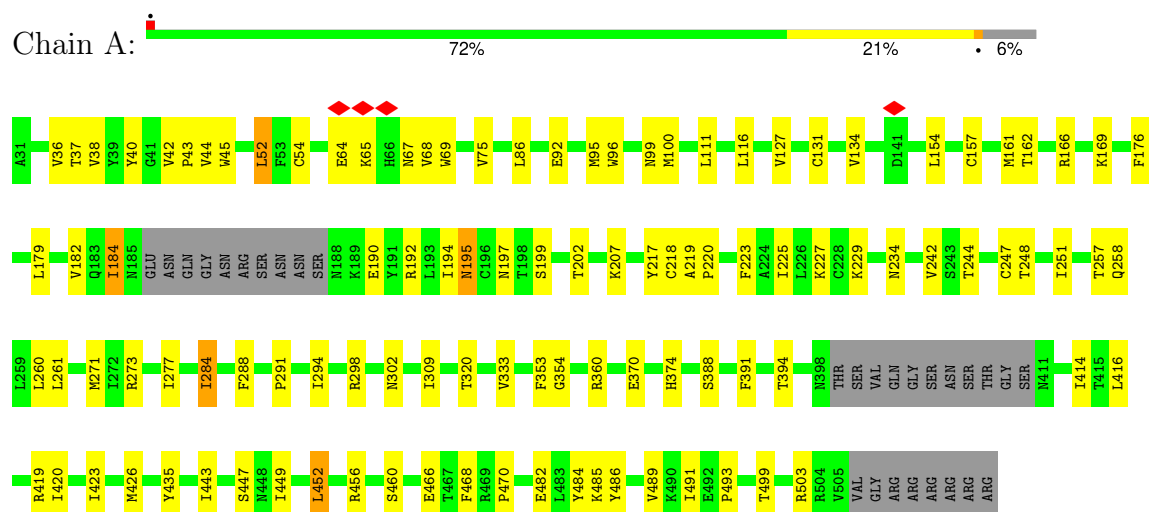
3 Residue-property plots

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

• Molecule 1: BG505 SOSIP.664 gp120

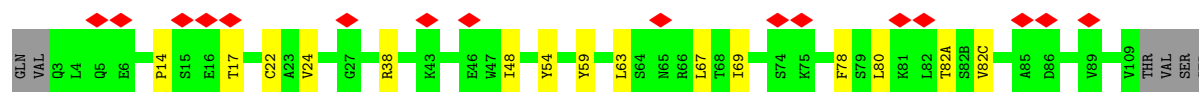


• Molecule 1: BG505 SOSIP.664 gp120

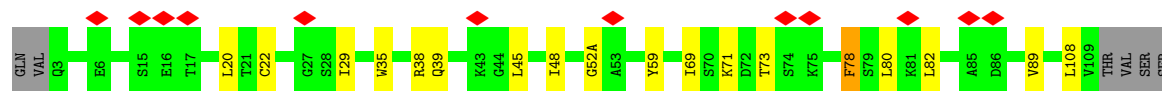
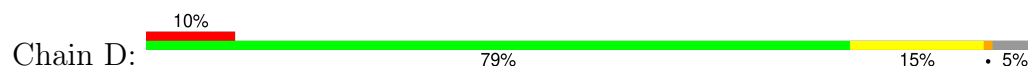


• Molecule 1: BG505 SOSIP.664 gp120

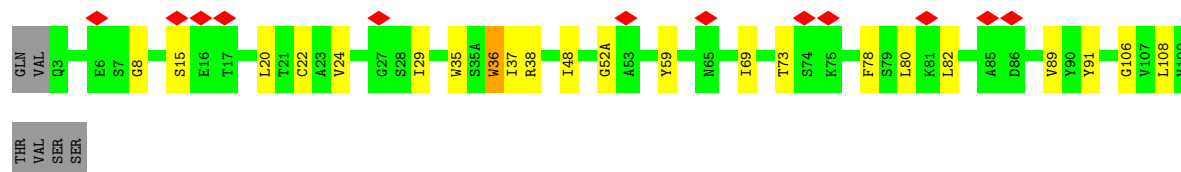
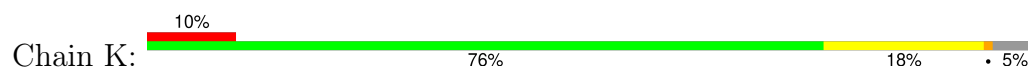




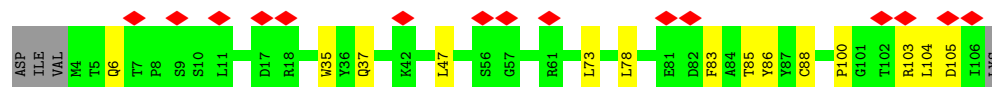
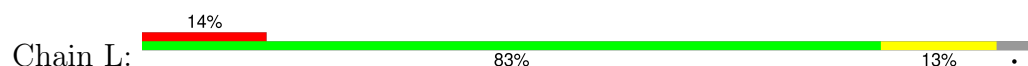
- Molecule 3: 1G3 Fab heavy chain



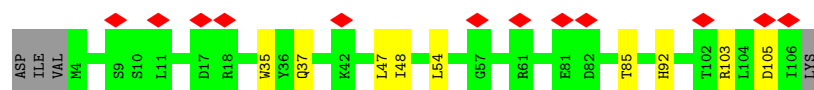
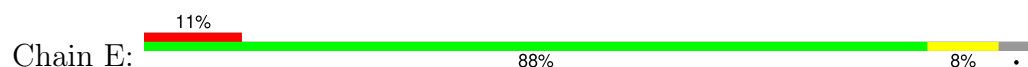
- Molecule 3: 1G3 Fab heavy chain



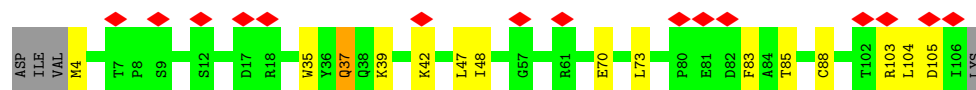
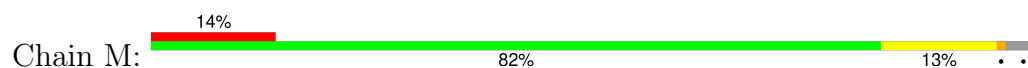
- Molecule 4: 1G3 Fab light chain



- Molecule 4: 1G3 Fab light chain

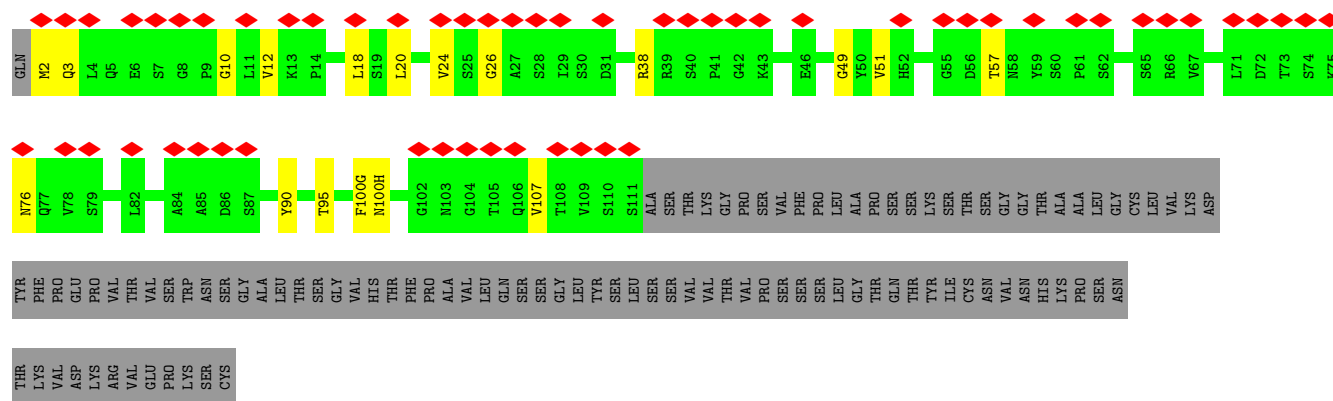


- Molecule 4: 1G3 Fab light chain

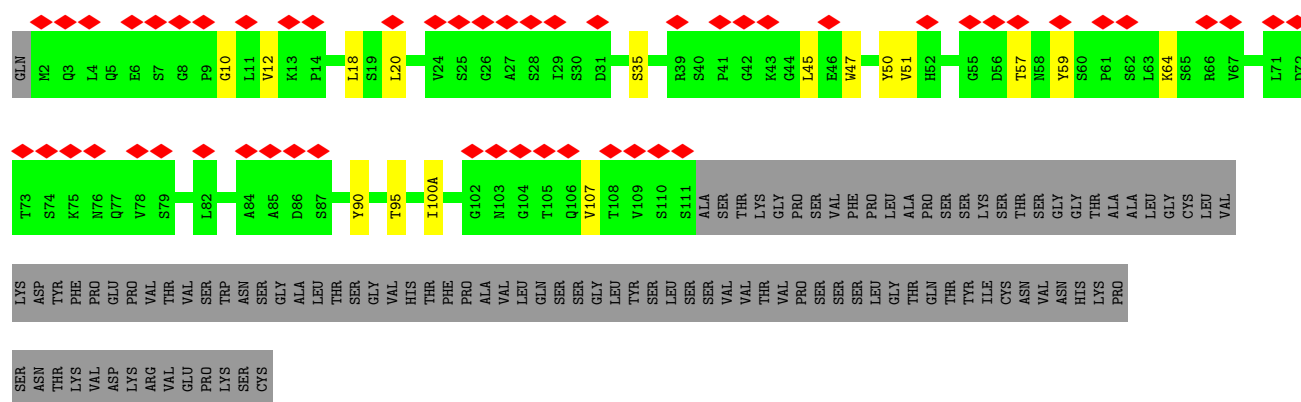


- Molecule 5: PGT121 Fab heavy chain

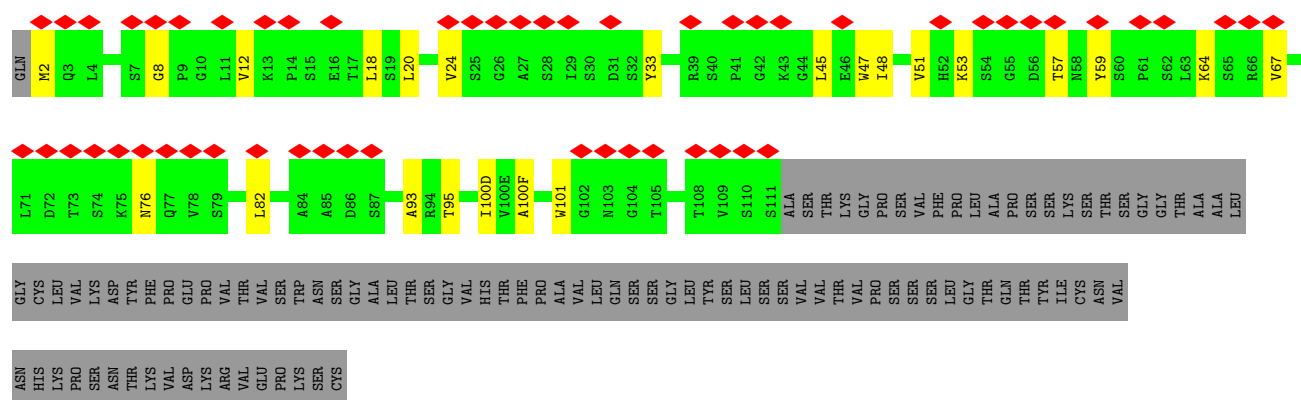




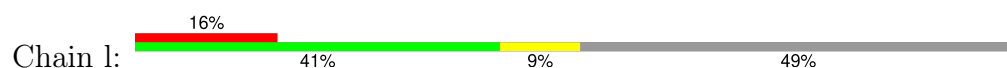
• Molecule 5: PGT121 Fab heavy chain

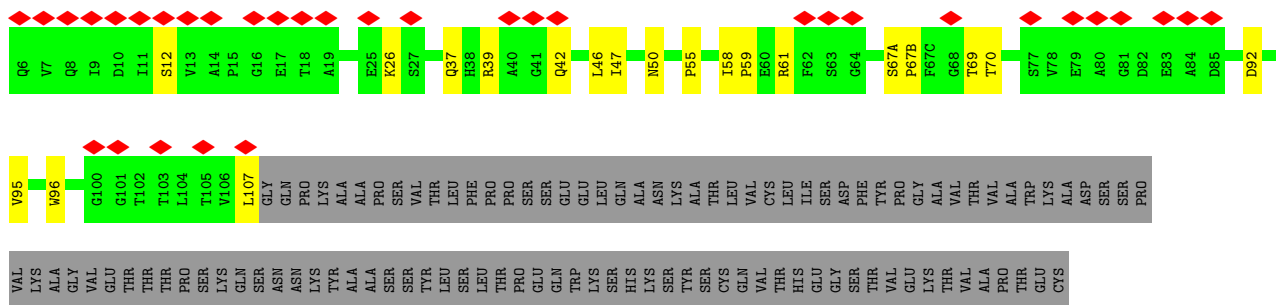


• Molecule 5: PGT121 Fab heavy chain

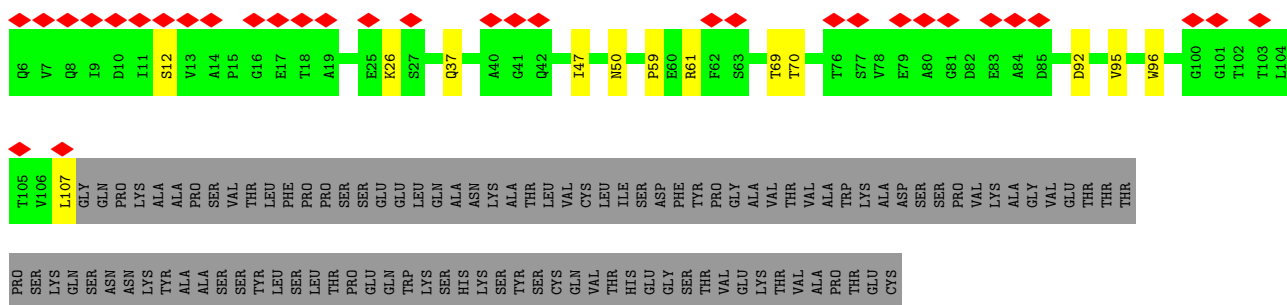
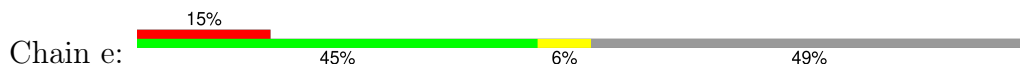


• Molecule 6: PGT121 Fab light chain

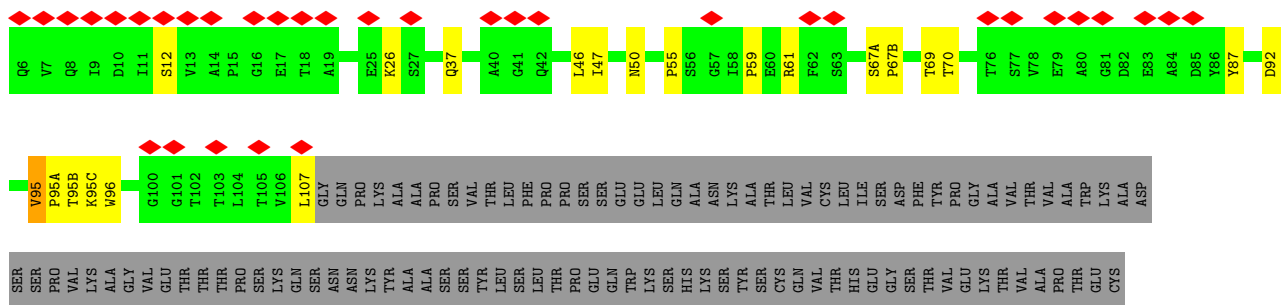




- Molecule 6: PGT121 Fab light chain



- Molecule 6: PGT121 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 c:  100%



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

Chain g:  50% 50%




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

Chain i:  100%



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

Chain o:  100%



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

Chain q:  50% 50%



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

Chain r:  50% 50% 50%



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

Chain s:  100%

MAG1
MAG2

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

Chain t:  50% 50%

MAG1
MAG2

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

Chain u:  100%

MAG1
MAG2

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

Chain w:  50% 50%

MAG1
MAG2

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

Chain x:  100%

MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain P:  50% 50%



- 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

Chain Z:  100%

MAG1
MAG2

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

Chain 1:  50% 50%

MAG1
MAG2

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

Chain 2:  50% 50% 50%

MAG1
MAG2

- 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 f:  75% 25%

MAG1
MAG2
BMA3
MAN4

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

Chain v:  100%

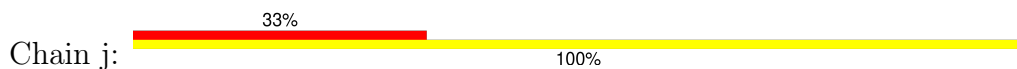
MAG1
MAG2
BMA3
MAN4

- 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

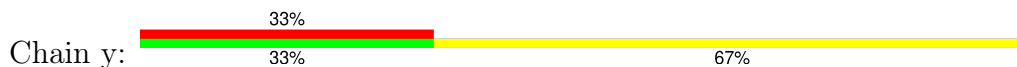
Chain U:  100%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



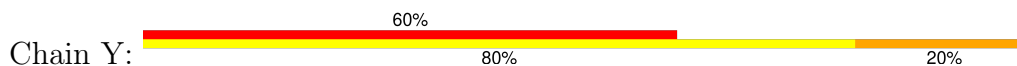
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 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 10: 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-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	425978	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.643	Depositor
Minimum map value	-1.211	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.094	Depositor
Map size (\AA)	355.72, 355.72, 355.72	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8893, 0.8893, 0.8893	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/3633	0.34	0/4933
1	G	0.14	0/3633	0.35	0/4933
1	I	0.14	0/3633	0.35	0/4933
2	B	0.14	0/1036	0.38	0/1405
2	C	0.12	0/1036	0.32	0/1405
2	J	0.12	0/1036	0.34	0/1405
3	D	0.08	0/850	0.29	0/1160
3	H	0.09	0/850	0.29	0/1160
3	K	0.10	0/850	0.29	0/1160
4	E	0.06	0/813	0.21	0/1104
4	L	0.09	0/813	0.24	0/1104
4	M	0.08	0/813	0.24	0/1104
5	d	0.07	0/1043	0.25	0/1417
5	h	0.08	0/1043	0.25	0/1417
5	k	0.09	0/1043	0.28	0/1417
6	e	0.09	0/845	0.25	0/1154
6	l	0.08	0/845	0.25	0/1154
6	m	0.08	0/845	0.27	0/1154
All	All	0.12	0/24660	0.31	0/33519

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3559	0	3489	64	0
1	G	3559	0	3489	60	0
1	I	3559	0	3489	47	0
2	B	1018	0	996	26	0
2	C	1018	0	996	18	0
2	J	1018	0	996	19	0
3	D	828	0	797	11	0
3	H	828	0	797	8	0
3	K	828	0	797	12	0
4	E	793	0	766	7	0
4	L	793	0	766	9	0
4	M	793	0	766	7	0
5	d	1017	0	983	10	0
5	h	1017	0	983	14	0
5	k	1017	0	983	13	0
6	e	824	0	785	9	0
6	l	824	0	785	10	0
6	m	824	0	785	9	0
7	1	28	0	25	1	0
7	2	28	0	25	0	0
7	N	28	0	25	0	0
7	P	28	0	25	1	0
7	Q	28	0	25	0	0
7	R	28	0	25	0	0
7	S	28	0	25	0	0
7	T	28	0	25	0	0
7	V	28	0	25	0	0
7	W	28	0	25	0	0
7	Z	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	g	28	0	25	0	0
7	i	28	0	25	0	0
7	o	28	0	25	0	0
7	q	28	0	25	1	0
7	r	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
7	w	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	x	28	0	25	0	0
8	U	50	0	43	0	0
8	f	50	0	43	1	0
8	v	50	0	43	0	0
9	X	39	0	34	0	0
9	j	39	0	34	0	0
9	y	39	0	34	0	0
10	Y	61	0	52	1	0
10	n	61	0	52	2	0
10	z	61	0	52	2	0
11	0	105	0	88	0	0
11	O	105	0	88	1	0
11	p	105	0	88	0	0
12	A	98	0	91	1	0
12	B	14	0	13	0	0
12	C	14	0	13	0	0
12	G	98	0	91	1	0
12	I	98	0	91	1	0
12	J	14	0	13	0	0
All	All	25890	0	25011	320	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 6.

All (320) 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:I:67:ASN:HB2	1:I:71:THR:HG21	1.56	0.88
1:G:95:MET:HE1	1:G:273:ARG:HD3	1.60	0.82
1:A:95:MET:HE1	1:A:273:ARG:HD3	1.64	0.78
1:I:218:CYS:HA	1:I:247:CYS:HB2	1.69	0.75
4:E:48:ILE:HG22	4:E:54:LEU:HA	1.68	0.73
1:A:218:CYS:HA	1:A:247:CYS:HB2	1.71	0.73
1:I:37:THR:HG22	2:J:605:CYS:HA	1.71	0.72
1:G:52:LEU:HD12	1:G:219:ALA:HA	1.73	0.71
1:G:218:CYS:HA	1:G:247:CYS:HB2	1.72	0.71
1:A:37:THR:HG22	2:C:605:CYS:HA	1.74	0.70
4:M:37:GLN:HG2	4:M:47:LEU:HD21	1.74	0.70
1:I:52:LEU:HD12	1:I:219:ALA:HA	1.73	0.69
1:A:52:LEU:HD12	1:A:219:ALA:HA	1.75	0.68
2:B:606:THR:HG21	2:B:646:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:MET:HE1	1:G:309:ILE:HG12	1.76	0.67
2:J:606:THR:HG21	2:J:646:LEU:HD21	1.77	0.67
2:C:606:THR:HG21	2:C:646:LEU:HD21	1.77	0.66
4:L:6:GLN:HB3	4:L:100:PRO:HD2	1.78	0.66
5:d:51:VAL:HA	5:d:57:THR:HG22	1.78	0.66
5:k:2:MET:HE2	5:k:2:MET:HA	1.78	0.66
3:H:63:LEU:HD12	3:H:67:LEU:HD13	1.78	0.65
1:A:353:PHE:HE1	1:A:456:ARG:HH21	1.45	0.65
2:B:576:LEU:O	2:B:580:VAL:HG23	1.97	0.64
2:C:523:LEU:H	2:C:540:GLN:HE21	1.45	0.63
4:E:85:THR:HA	4:E:103:ARG:HA	1.79	0.63
5:h:51:VAL:HA	5:h:57:THR:HG22	1.80	0.63
1:I:182:VAL:HG13	1:I:194:ILE:HG22	1.80	0.63
1:A:491:ILE:HG22	1:A:493:PRO:HD3	1.81	0.62
5:k:18:LEU:HB3	5:k:82:LEU:HD23	1.79	0.62
1:G:195:ASN:HB2	1:G:423:ILE:HD11	1.79	0.62
1:G:491:ILE:HG22	1:G:493:PRO:HD3	1.81	0.62
3:H:22:CYS:HB3	3:H:78:PHE:HB2	1.80	0.62
6:l:37:GLN:HB2	6:l:47:ILE:HD11	1.80	0.62
1:A:184:ILE:HD11	1:A:192:ARG:HE	1.65	0.62
1:A:261:LEU:HD11	1:A:374:HIS:NE2	2.14	0.62
1:I:360:ARG:HB2	1:I:394:THR:HG22	1.80	0.62
1:A:503:ARG:HH21	2:C:606:THR:HG22	1.65	0.62
4:M:85:THR:HA	4:M:103:ARG:HA	1.81	0.61
1:G:353:PHE:HE1	1:G:456:ARG:HH21	1.47	0.61
5:k:51:VAL:HA	5:k:57:THR:HG22	1.80	0.61
1:G:503:ARG:HH21	2:B:606:THR:HG22	1.65	0.61
4:L:85:THR:HA	4:L:103:ARG:HA	1.81	0.61
1:I:261:LEU:HD11	1:I:374:HIS:NE2	2.16	0.61
3:K:8:GLY:HA3	3:K:20:LEU:HD23	1.83	0.61
1:G:68:VAL:HG11	1:G:213:ILE:HD12	1.83	0.61
1:I:55:ALA:HB3	1:I:216:HIS:HB2	1.83	0.60
1:I:353:PHE:HE1	1:I:456:ARG:HH21	1.49	0.60
1:A:277:ILE:HD11	1:A:284:ILE:HD12	1.83	0.60
6:e:92:ASP:HB3	6:e:95:VAL:HG22	1.83	0.60
5:h:2:MET:HE1	5:h:26:GLY:H	1.66	0.60
5:h:12:VAL:HG21	5:h:18:LEU:HA	1.84	0.60
1:I:271:MET:HE3	1:I:273:ARG:HH12	1.67	0.60
1:G:294:ILE:HG23	1:G:447:SER:HB2	1.85	0.59
2:J:576:LEU:O	2:J:580:VAL:HG22	2.01	0.59
1:A:503:ARG:HH22	2:C:597:GLY:HA3	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:37:GLN:HB2	6:e:47:ILE:HD11	1.83	0.59
1:G:42:VAL:HG12	1:G:493:PRO:HA	1.84	0.59
1:A:234:ASN:HB3	12:A:606:NAG:O5	2.01	0.59
1:I:64:GLU:O	1:I:65:LYS:HG3	2.02	0.59
2:B:523:LEU:H	2:B:540:GLN:HE21	1.50	0.59
1:I:491:ILE:HG22	1:I:493:PRO:HD3	1.84	0.58
1:I:503:ARG:HH22	2:J:597:GLY:HA3	1.68	0.58
1:G:86:LEU:HD13	1:G:242:VAL:HG23	1.85	0.58
1:A:182:VAL:HG13	1:A:194:ILE:HG22	1.85	0.58
1:G:261:LEU:HD11	1:G:374:HIS:NE2	2.18	0.58
1:A:391:PHE:HD2	1:A:470:PRO:HG3	1.68	0.58
3:H:59:TYR:HE1	3:H:69:ILE:HG22	1.68	0.58
4:L:37:GLN:HB3	4:L:47:LEU:HD21	1.86	0.58
1:I:86:LEU:HD13	1:I:242:VAL:HG23	1.84	0.58
1:A:161:MET:HE1	1:A:309:ILE:HG12	1.86	0.58
1:I:234:ASN:HB3	12:I:606:NAG:O5	2.03	0.58
1:I:184:ILE:HD11	1:I:192:ARG:HE	1.67	0.58
4:E:37:GLN:HB3	4:E:47:LEU:HD21	1.85	0.57
1:G:277:ILE:HG22	1:G:456:ARG:HD2	1.86	0.57
1:A:42:VAL:HG12	1:A:493:PRO:HA	1.86	0.57
5:k:12:VAL:HG21	5:k:18:LEU:HA	1.86	0.57
1:I:294:ILE:HG23	1:I:447:SER:HB2	1.86	0.57
3:D:29:ILE:HD11	3:D:73:THR:HA	1.85	0.57
1:G:503:ARG:HH22	2:B:597:GLY:HA3	1.70	0.57
2:B:639:THR:HG22	2:B:640:GLN:H	1.69	0.57
1:A:391:PHE:CD2	1:A:470:PRO:HG3	2.39	0.57
3:H:17:THR:HA	3:H:82(A):THR:HA	1.86	0.56
2:B:538:THR:HG21	2:C:647:GLU:OE2	2.05	0.56
3:K:38:ARG:HB3	3:K:48:ILE:HD11	1.87	0.56
6:l:92:ASP:HB3	6:l:95:VAL:HG22	1.87	0.56
6:m:92:ASP:HB3	6:m:95:VAL:HG22	1.86	0.56
1:G:234:ASN:HB3	12:G:606:NAG:O5	2.05	0.56
2:J:523:LEU:H	2:J:540:GLN:HE21	1.52	0.56
1:A:294:ILE:HG23	1:A:447:SER:HB2	1.87	0.56
3:D:22:CYS:HB3	3:D:78:PHE:HB3	1.87	0.56
1:I:68:VAL:HG12	1:I:69:TRP:CD1	2.40	0.56
1:A:134:VAL:HG21	1:A:154:LEU:HB3	1.88	0.56
1:I:353:PHE:HZ	1:I:456:ARG:HE	1.54	0.56
2:C:639:THR:HG23	2:C:640:GLN:OE1	2.06	0.55
5:d:12:VAL:HG21	5:d:18:LEU:HA	1.85	0.55
3:K:36:TRP:CZ3	3:K:80:LEU:HB2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:67:LEU:H	3:H:67:LEU:HD23	1.72	0.55
6:l:46:LEU:HD11	6:l:55:PRO:HG3	1.87	0.55
1:A:360:ARG:HB2	1:A:394:THR:HG22	1.89	0.55
1:I:68:VAL:HG11	1:I:211:GLU:O	2.06	0.55
1:I:503:ARG:HH21	2:J:606:THR:HG22	1.72	0.54
1:A:86:LEU:HD13	1:A:242:VAL:HG23	1.88	0.54
1:A:353:PHE:HZ	1:A:456:ARG:HE	1.56	0.54
2:B:639:THR:CG2	2:B:640:GLN:H	2.21	0.54
1:G:261:LEU:HD23	1:G:447:SER:HB3	1.89	0.54
1:A:45:TRP:HB2	1:A:489:VAL:HB	1.91	0.53
3:K:22:CYS:HB3	3:K:78:PHE:HB2	1.90	0.53
1:G:388:SER:HB3	10:n:1:NAG:H5	1.91	0.53
1:G:68:VAL:HG13	1:G:69:TRP:H	1.73	0.53
1:G:111:LEU:HG	2:B:571:TRP:HZ2	1.73	0.53
3:D:20:LEU:HD12	3:D:80:LEU:HB3	1.91	0.53
1:I:95:MET:HE1	1:I:273:ARG:HB3	1.90	0.52
6:m:46:LEU:HD11	6:m:55:PRO:HG3	1.92	0.52
2:B:639:THR:HG22	2:B:640:GLN:N	2.25	0.52
1:G:31:ALA:HB3	1:G:500:ARG:HH22	1.74	0.52
1:G:271:MET:HE3	1:G:273:ARG:HH12	1.75	0.52
3:K:29:ILE:HD11	3:K:73:THR:HA	1.93	0.51
1:G:162:THR:HG22	1:G:169:LYS:HE2	1.92	0.51
1:G:333:VAL:HG11	1:G:390:LEU:HD21	1.92	0.51
1:A:251:ILE:HG23	1:A:482:GLU:HG2	1.92	0.51
1:G:71:THR:HG23	1:G:72:HIS:H	1.76	0.51
2:B:647:GLU:OE2	2:J:538:THR:HG21	2.11	0.50
5:k:8:GLY:HA3	5:k:20:LEU:HG	1.92	0.50
1:G:68:VAL:HG22	1:G:69:TRP:HB2	1.92	0.50
2:B:614:TRP:HZ3	2:B:637:ASN:HD21	1.57	0.50
1:A:388:SER:HB3	10:z:1:NAG:H5	1.93	0.50
1:G:291:PRO:HG2	7:q:1:NAG:H61	1.93	0.50
1:I:217:TYR:O	1:I:248:THR:HG22	2.11	0.50
1:A:456:ARG:HG2	1:A:468:PHE:HE1	1.75	0.50
2:B:538:THR:HA	2:B:541:ALA:HB3	1.93	0.50
1:I:45:TRP:HB2	1:I:489:VAL:HB	1.94	0.50
1:I:220:PRO:HG2	1:I:223:PHE:HD2	1.77	0.50
2:B:652:GLN:O	2:B:655:LYS:HG2	2.12	0.49
1:A:68:VAL:HG22	1:A:69:TRP:H	1.77	0.49
1:A:162:THR:HG22	1:A:169:LYS:HE2	1.94	0.49
1:A:333:VAL:HG13	1:A:414:ILE:HB	1.94	0.49
2:C:538:THR:HG21	2:J:647:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:291:PRO:HG2	7:1:1:NAG:H61	1.94	0.49
4:M:39:LYS:HB2	4:M:42:LYS:HB2	1.94	0.49
6:m:26:LYS:HE3	6:m:69:THR:N	2.27	0.49
1:A:40:TYR:HB3	2:C:602:LEU:HD23	1.94	0.49
1:A:68:VAL:HG22	1:A:69:TRP:N	2.28	0.49
6:e:26:LYS:HE3	6:e:69:THR:N	2.28	0.49
5:d:12:VAL:HB	5:d:18:LEU:HD12	1.94	0.48
1:I:55:ALA:HB1	1:I:77:THR:HA	1.94	0.48
1:I:162:THR:HG22	1:I:169:LYS:HE2	1.93	0.48
5:k:45:LEU:H	6:m:87:TYR:HE2	1.60	0.48
1:A:99:ASN:O	1:A:100:MET:HG2	2.13	0.48
1:G:257:THR:HG21	1:G:370:GLU:O	2.14	0.48
3:D:29:ILE:HD12	3:D:71:LYS:HG3	1.95	0.48
3:D:35:TRP:HE1	3:D:52(A):GLY:HA2	1.78	0.48
2:J:614:TRP:HZ3	2:J:637:ASN:HD21	1.61	0.48
2:J:655:LYS:O	2:J:658:GLN:HG2	2.13	0.48
3:K:35:TRP:HE1	3:K:52(A):GLY:HA2	1.79	0.48
1:I:257:THR:HG21	1:I:370:GLU:O	2.14	0.48
2:J:645:LEU:O	2:J:648:GLU:HG3	2.14	0.48
5:h:18:LEU:HD11	5:h:107:VAL:HG21	1.96	0.48
6:l:39:ARG:HG2	6:l:42:GLN:HB2	1.96	0.48
1:G:136:ASN:ND2	1:G:326:ILE:HD12	2.29	0.48
6:e:96:TRP:HD1	6:e:96:TRP:O	1.96	0.48
1:A:64:GLU:O	1:A:65:LYS:HG3	2.14	0.47
1:A:220:PRO:HG2	1:A:223:PHE:HD2	1.78	0.47
6:m:37:GLN:HB2	6:m:47:ILE:HD11	1.95	0.47
1:A:257:THR:HG21	1:A:370:GLU:O	2.14	0.47
3:K:59:TYR:HE1	3:K:69:ILE:HG22	1.80	0.47
1:G:37:THR:HG21	1:G:499:THR:HG22	1.95	0.47
1:A:218:CYS:HA	1:A:247:CYS:CB	2.43	0.47
6:e:12:SER:HB3	6:e:107:LEU:HG	1.94	0.47
1:G:456:ARG:HG2	1:G:468:PHE:HE1	1.80	0.47
3:H:14:PRO:HA	3:H:82(C):VAL:HG23	1.95	0.47
6:l:12:SER:HB3	6:l:107:LEU:HG	1.95	0.47
1:A:197:ASN:C	1:A:197:ASN:OD1	2.58	0.47
1:A:423:ILE:HG22	1:A:435:TYR:HD2	1.80	0.47
6:m:12:SER:HB3	6:m:107:LEU:HG	1.96	0.46
1:I:388:SER:HB3	10:Y:1:NAG:H5	1.96	0.46
2:B:655:LYS:O	2:B:658:GLN:HG2	2.16	0.46
2:B:655:LYS:HA	2:B:658:GLN:CD	2.41	0.46
1:G:134:VAL:HG21	1:G:154:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:LYS:HG3	1:G:486:TYR:HE1	1.80	0.46
5:h:24:VAL:HG13	5:h:76:ASN:HB3	1.97	0.46
1:A:38:VAL:HG22	2:C:604:CYS:HB3	1.96	0.46
5:d:100(A):ILE:HB	11:O:3:BMA:H5	1.97	0.46
1:G:248:THR:HB	1:G:486:TYR:CE2	2.51	0.46
1:I:111:LEU:HG	2:J:571:TRP:HZ2	1.81	0.46
3:K:36:TRP:HZ3	3:K:80:LEU:HB2	1.81	0.46
3:D:39:GLN:HB3	3:D:45:LEU:HD23	1.98	0.45
1:G:333:VAL:HG13	1:G:414:ILE:HB	1.98	0.45
1:A:503:ARG:HE	2:C:606:THR:HA	1.80	0.45
3:D:69:ILE:HD11	3:D:78:PHE:CE1	2.51	0.45
1:I:423:ILE:HG22	1:I:435:TYR:HD2	1.81	0.45
1:I:100:MET:HG2	1:I:483:LEU:HD13	1.97	0.45
1:G:34:LEU:HD11	2:B:619:LEU:HD11	1.98	0.45
1:A:227:LYS:HD3	1:A:486:TYR:HE1	1.81	0.45
1:G:358:ILE:HD12	3:H:54:TYR:HD2	1.81	0.45
5:d:10:GLY:HA2	5:d:107:VAL:HG23	1.99	0.45
1:G:167:ASP:OD1	1:A:127:VAL:HG13	2.17	0.45
1:G:248:THR:HB	1:G:486:TYR:HE2	1.81	0.45
6:l:67(A):SER:HB3	6:l:67(B):PRO:HD3	1.99	0.45
4:M:103:ARG:HH12	4:M:105:ASP:HB2	1.80	0.45
5:h:20:LEU:HD23	5:h:90:TYR:HD2	1.82	0.45
1:A:271:MET:HE3	1:A:273:ARG:HH12	1.82	0.45
1:G:157:CYS:HB2	1:G:176:PHE:HD2	1.82	0.44
2:B:575:GLN:O	2:B:579:ARG:HD3	2.16	0.44
5:d:59:TYR:HB2	5:d:64:LYS:HD2	1.98	0.44
5:h:10:GLY:HA2	5:h:107:VAL:HG23	1.98	0.44
2:C:614:TRP:CH2	2:C:638:TYR:HB2	2.52	0.44
1:I:503:ARG:HE	2:J:606:THR:HA	1.82	0.44
1:G:95:MET:HE3	1:G:484:TYR:HB2	1.99	0.44
5:h:12:VAL:HB	5:h:18:LEU:HD12	2.00	0.44
5:h:38:ARG:HG3	5:h:90:TYR:CE1	2.52	0.44
1:G:503:ARG:HH12	2:B:597:GLY:HA3	1.82	0.44
6:l:59:PRO:HB2	6:l:61:ARG:HG2	1.99	0.44
4:M:35:TRP:CE2	4:M:73:LEU:HB2	2.53	0.44
4:L:37:GLN:HB2	4:L:86:TYR:CE1	2.53	0.44
4:L:83:PHE:HA	4:L:104:LEU:HD23	2.00	0.44
1:I:43:PRO:HB3	2:J:523:LEU:HD23	2.00	0.44
1:A:248:THR:HB	1:A:486:TYR:HE2	1.83	0.44
1:A:485:LYS:HG3	1:A:486:TYR:CD1	2.52	0.44
5:k:59:TYR:HB2	5:k:64:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:PHE:CD2	1:G:490:LYS:HA	2.53	0.44
4:L:103:ARG:HH12	4:L:105:ASP:HB2	1.82	0.43
1:A:298:ARG:HH12	1:A:302:ASN:HB2	1.83	0.43
3:D:59:TYR:HE1	3:D:69:ILE:HG22	1.82	0.43
3:D:82:LEU:HD12	3:D:82:LEU:HA	1.88	0.43
1:I:503:ARG:HH12	2:J:597:GLY:HA3	1.82	0.43
3:K:91:TYR:CE1	3:K:106:GLY:HA3	2.53	0.43
5:k:33:TYR:HE1	5:k:53:LYS:HG2	1.83	0.43
2:J:588:ARG:HD2	2:J:588:ARG:O	2.18	0.43
1:G:45:TRP:HB2	1:G:489:VAL:HB	2.00	0.43
6:m:59:PRO:HB2	6:m:61:ARG:HG2	1.99	0.43
1:G:127:VAL:HG13	1:I:167:ASP:OD1	2.17	0.43
1:A:95:MET:HE3	1:A:484:TYR:HB2	1.99	0.43
1:A:195:ASN:HD21	1:A:199:SER:HB3	1.83	0.43
3:D:38:ARG:HB3	3:D:48:ILE:HD11	1.99	0.43
5:k:93:ALA:HB2	5:k:101:TRP:HA	2.01	0.43
1:A:166:ARG:HA	1:A:166:ARG:HD2	1.82	0.43
1:A:217:TYR:O	1:A:248:THR:HG23	2.18	0.43
2:C:538:THR:HA	2:C:541:ALA:HB3	2.00	0.43
5:d:47:TRP:HB3	6:e:96:TRP:CD1	2.52	0.43
2:J:614:TRP:CH2	2:J:638:TYR:HB2	2.53	0.43
1:G:31:ALA:N	1:G:500:ARG:HH12	2.16	0.43
2:B:614:TRP:CH2	2:B:638:TYR:HB2	2.53	0.43
1:A:179:LEU:HD21	1:A:419:ARG:HH12	1.83	0.43
2:C:575:GLN:O	2:C:579:ARG:HD3	2.18	0.43
3:K:82:LEU:HD12	3:K:82:LEU:HA	1.84	0.43
1:A:111:LEU:HD21	2:C:571:TRP:HE1	1.83	0.43
3:D:89:VAL:HG22	3:D:108:LEU:HB2	2.00	0.43
4:E:103:ARG:HH12	4:E:105:ASP:HB2	1.82	0.43
1:I:32:GLU:N	1:I:500:ARG:HH22	2.17	0.43
1:G:500:ARG:HD3	2:B:619:LEU:HD13	2.01	0.43
4:E:35:TRP:CD1	4:E:48:ILE:HD11	2.53	0.43
1:I:485:LYS:C	1:I:486:TYR:HD1	2.27	0.43
2:B:639:THR:CG2	2:B:640:GLN:N	2.82	0.43
6:m:67(A):SER:HB3	6:m:67(B):PRO:HD3	2.00	0.43
2:B:588:ARG:HD2	2:B:588:ARG:O	2.19	0.43
1:A:95:MET:HG2	1:A:96:TRP:CD1	2.54	0.42
5:d:20:LEU:HD23	5:d:90:TYR:HD2	1.84	0.42
4:L:35:TRP:CZ3	4:L:88:CYS:HB3	2.54	0.42
6:l:26:LYS:HE3	6:l:69:THR:N	2.34	0.42
5:k:48:ILE:HG12	5:k:67:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ALA:O	1:G:216:HIS:HB2	2.19	0.42
4:E:35:TRP:HD1	4:E:48:ILE:HD11	1.85	0.42
1:I:317:PHE:CE2	1:I:319:ALA:HB2	2.53	0.42
1:G:385:CYS:HA	1:G:418:CYS:HA	2.02	0.42
1:A:291:PRO:HG2	7:P:1:NAG:H61	2.00	0.42
1:I:54:CYS:HB2	1:I:74:CYS:HB3	1.33	0.42
1:G:220:PRO:HG2	1:G:223:PHE:HD1	1.84	0.42
6:e:59:PRO:HB2	6:e:61:ARG:HG2	2.02	0.42
5:h:20:LEU:HD23	5:h:90:TYR:CD2	2.54	0.42
1:I:166:ARG:HA	1:I:166:ARG:HD2	1.87	0.42
3:K:89:VAL:HG22	3:K:108:LEU:HB2	2.02	0.42
4:M:83:PHE:HA	4:M:104:LEU:HD23	2.02	0.42
1:G:476:ARG:HE	1:G:476:ARG:HB2	1.64	0.42
6:l:58:ILE:HD13	6:l:58:ILE:HA	1.89	0.42
1:A:485:LYS:HG3	1:A:486:TYR:CE1	2.55	0.42
1:G:231:LYS:HE2	1:G:268:GLU:HG2	2.01	0.42
5:h:2:MET:HE3	5:h:3:GLN:N	2.35	0.42
2:B:587:LEU:HD22	2:J:586:TYR:HE2	1.84	0.42
2:B:658:GLN:HA	2:B:661:LEU:HG	2.02	0.42
5:h:38:ARG:HE	5:h:38:ARG:HB3	1.67	0.42
1:A:298:ARG:HE	1:A:443:ILE:HD11	1.85	0.42
6:e:61:ARG:HG2	6:e:61:ARG:H	1.70	0.42
1:G:353:PHE:HZ	1:G:456:ARG:HE	1.67	0.41
5:d:47:TRP:HB3	6:e:96:TRP:HD1	1.85	0.41
1:I:207:LYS:HA	1:I:207:LYS:HD3	1.79	0.41
3:K:36:TRP:HD1	3:K:91:TYR:O	2.03	0.41
1:G:101:VAL:HG21	1:G:480:ARG:HA	2.02	0.41
1:G:227:LYS:HG2	1:G:228:CYS:N	2.34	0.41
1:A:288:PHE:HE2	1:A:452:LEU:HD13	1.85	0.41
5:h:49:GLY:HA2	6:l:96:TRP:HZ2	1.85	0.41
1:G:217:TYR:O	1:G:248:THR:HG23	2.21	0.41
1:G:446:VAL:O	8:f:1:NAG:H5	2.21	0.41
1:A:229:LYS:HE3	1:A:229:LYS:HB3	1.88	0.41
2:C:586:TYR:HE2	2:J:587:LEU:HD22	1.84	0.41
5:d:35:SER:HA	5:d:50:TYR:HA	2.02	0.41
4:M:4:MET:HE1	4:M:88:CYS:SG	2.60	0.41
1:G:184:ILE:HD13	1:G:184:ILE:HA	1.84	0.41
2:B:633:LYS:HA	2:B:633:LYS:HD3	1.84	0.41
1:G:358:ILE:HD11	1:G:396:ILE:HG23	2.01	0.41
1:A:460:SER:HB3	1:A:466:GLU:HG3	2.03	0.41
4:L:78:LEU:HD23	4:L:78:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:z:2:NAG:H4	10:z:3:BMA:O2	2.20	0.41
3:H:38:ARG:HB3	3:H:48:ILE:HD11	2.03	0.41
5:h:100(G):PHE:O	5:h:100(H):ASN:HB2	2.20	0.41
1:A:43:PRO:HB3	2:C:523:LEU:HD23	2.02	0.41
1:I:136:ASN:ND2	1:I:326:ILE:HD12	2.36	0.41
10:n:2:NAG:H4	10:n:3:BMA:O2	2.20	0.41
1:G:197:ASN:OD1	1:G:197:ASN:C	2.64	0.41
1:A:157:CYS:HB2	1:A:176:PHE:HD2	1.86	0.41
5:k:47:TRP:CG	6:m:96:TRP:HE1	2.39	0.41
1:A:294:ILE:HG21	1:A:449:ILE:HG13	2.03	0.40
1:A:354:GLY:HA2	4:E:92:HIS:CE1	2.56	0.40
2:C:618:ASN:HB3	2:C:621:GLU:OE1	2.21	0.40
1:I:368:ASP:HB2	1:I:371:VAL:HG12	2.03	0.40
4:L:35:TRP:CE2	4:L:73:LEU:HB2	2.56	0.40
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.88	0.40
1:I:95:MET:SD	1:I:484:TYR:HB2	2.61	0.40
5:k:24:VAL:HG12	5:k:76:ASN:HB3	2.03	0.40
1:I:157:CYS:HB2	1:I:176:PHE:HD2	1.86	0.40
5:k:100(D):ILE:HG22	5:k:100(F):ALA:H	1.85	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	446/481 (93%)	420 (94%)	26 (6%)	0	100	100
1	G	446/481 (93%)	416 (93%)	30 (7%)	0	100	100
1	I	446/481 (93%)	417 (94%)	29 (6%)	0	100	100
2	B	125/153 (82%)	121 (97%)	4 (3%)	0	100	100
2	C	125/153 (82%)	122 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	125/153 (82%)	121 (97%)	4 (3%)	0	100	100
3	D	107/115 (93%)	99 (92%)	8 (8%)	0	100	100
3	H	107/115 (93%)	99 (92%)	8 (8%)	0	100	100
3	K	107/115 (93%)	99 (92%)	8 (8%)	0	100	100
4	E	100/106 (94%)	94 (94%)	6 (6%)	0	100	100
4	L	100/106 (94%)	94 (94%)	6 (6%)	0	100	100
4	M	100/106 (94%)	93 (93%)	7 (7%)	0	100	100
5	d	129/235 (55%)	124 (96%)	5 (4%)	0	100	100
5	h	129/235 (55%)	125 (97%)	4 (3%)	0	100	100
5	k	129/235 (55%)	124 (96%)	5 (4%)	0	100	100
6	e	106/213 (50%)	103 (97%)	3 (3%)	0	100	100
6	l	106/213 (50%)	101 (95%)	5 (5%)	0	100	100
6	m	106/213 (50%)	102 (96%)	4 (4%)	0	100	100
All	All	3039/3909 (78%)	2874 (95%)	165 (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	403/428 (94%)	379 (94%)	24 (6%)	17	42
1	G	403/428 (94%)	380 (94%)	23 (6%)	18	43
1	I	403/428 (94%)	384 (95%)	19 (5%)	23	47
2	B	109/129 (84%)	103 (94%)	6 (6%)	19	44
2	C	109/129 (84%)	104 (95%)	5 (5%)	24	47
2	J	109/129 (84%)	102 (94%)	7 (6%)	16	40
3	D	90/96 (94%)	89 (99%)	1 (1%)	65	71
3	H	90/96 (94%)	88 (98%)	2 (2%)	45	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	90/96 (94%)	86 (96%)	4 (4%)	25	48
4	E	90/94 (96%)	90 (100%)	0	100	100
4	L	90/94 (96%)	90 (100%)	0	100	100
4	M	90/94 (96%)	87 (97%)	3 (3%)	33	54
5	d	112/202 (55%)	110 (98%)	2 (2%)	51	64
5	h	112/202 (55%)	111 (99%)	1 (1%)	70	73
5	k	112/202 (55%)	111 (99%)	1 (1%)	70	73
6	e	89/179 (50%)	87 (98%)	2 (2%)	45	61
6	l	89/179 (50%)	87 (98%)	2 (2%)	45	61
6	m	89/179 (50%)	83 (93%)	6 (7%)	15	40
All	All	2679/3384 (79%)	2571 (96%)	108 (4%)	29	50

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	44	VAL
1	G	52	LEU
1	G	54	CYS
1	G	67	ASN
1	G	75	VAL
1	G	116	LEU
1	G	129	LEU
1	G	131	CYS
1	G	190	GLU
1	G	201	ILE
1	G	202	THR
1	G	228	CYS
1	G	251	ILE
1	G	260	LEU
1	G	277	ILE
1	G	284	ILE
1	G	294	ILE
1	G	320	THR
1	G	416	LEU
1	G	423	ILE
1	G	426	MET
1	G	467	THR
1	G	499	THR

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Mol	Chain	Res	Type
2	B	544	LEU
2	B	583	VAL
2	B	593	LEU
2	B	627	THR
2	B	641	ILE
2	B	645	LEU
3	H	24	VAL
3	H	80	LEU
5	h	95	THR
6	l	50	ASN
6	l	70	THR
1	A	36	VAL
1	A	44	VAL
1	A	52	LEU
1	A	54	CYS
1	A	67	ASN
1	A	75	VAL
1	A	92	GLU
1	A	116	LEU
1	A	131	CYS
1	A	184	ILE
1	A	190	GLU
1	A	195	ASN
1	A	202	THR
1	A	225	ILE
1	A	244	THR
1	A	258	GLN
1	A	260	LEU
1	A	284	ILE
1	A	320	THR
1	A	416	LEU
1	A	420	ILE
1	A	426	MET
1	A	452	LEU
1	A	499	THR
2	C	544	LEU
2	C	593	LEU
2	C	625	ASN
2	C	627	THR
2	C	645	LEU
3	D	78	PHE
5	d	45	LEU

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Mol	Chain	Res	Type
5	d	95	THR
6	e	50	ASN
6	e	70	THR
1	I	44	VAL
1	I	52	LEU
1	I	75	VAL
1	I	92	GLU
1	I	95	MET
1	I	101	VAL
1	I	116	LEU
1	I	131	CYS
1	I	175	LEU
1	I	201	ILE
1	I	202	THR
1	I	260	LEU
1	I	284	ILE
1	I	357	THR
1	I	370	GLU
1	I	416	LEU
1	I	426	MET
1	I	443	ILE
1	I	499	THR
2	J	544	LEU
2	J	584	GLU
2	J	593	LEU
2	J	603	ILE
2	J	627	THR
2	J	641	ILE
2	J	646	LEU
3	K	15	SER
3	K	24	VAL
3	K	36	TRP
3	K	37	ILE
4	M	37	GLN
4	M	48	ILE
4	M	70	GLU
5	k	95	THR
6	m	50	ASN
6	m	70	THR
6	m	95	VAL
6	m	95(A)	PRO
6	m	95(B)	THR

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Mol	Chain	Res	Type
6	m	95(C)	LYS

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

Mol	Chain	Res	Type
1	G	67	ASN
1	G	283	ASN
1	G	432	GLN
2	B	540	GLN
2	B	640	GLN
5	h	5	GLN
5	h	76	ASN
6	l	51	ASN
1	A	66	HIS
2	C	540	GLN
2	C	630	GLN
5	d	5	GLN
6	e	51	ASN
1	I	195	ASN
1	I	328	GLN
2	J	540	GLN
2	J	616	ASN
3	K	39	GLN
4	M	38	GLN
5	k	5	GLN
5	k	77	GLN
6	m	37	GLN
6	m	52	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 ⓘ

111 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	$\# Z > 2$
11	NAG	0	1	1,11	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
11	NAG	0	2	11	14,14,15	0.71	0	17,19,21	1.46	3 (17%)
11	BMA	0	3	11	11,11,12	0.98	0	15,15,17	2.11	4 (26%)
11	MAN	0	4	11	11,11,12	0.61	0	15,15,17	1.55	1 (6%)
11	MAN	0	5	11	11,11,12	0.70	0	15,15,17	1.20	1 (6%)
11	MAN	0	6	11	11,11,12	0.71	0	15,15,17	1.14	1 (6%)
11	MAN	0	7	11	11,11,12	0.69	0	15,15,17	1.33	1 (6%)
11	MAN	0	8	11	11,11,12	0.68	0	15,15,17	1.15	1 (6%)
11	MAN	0	9	11	11,11,12	0.67	0	15,15,17	1.25	1 (6%)
7	NAG	1	1	1,7	14,14,15	0.70	0	17,19,21	1.25	1 (5%)
7	NAG	1	2	7	14,14,15	0.72	0	17,19,21	0.80	0
7	NAG	2	1	1,7	14,14,15	0.74	0	17,19,21	1.01	1 (5%)
7	NAG	2	2	7	14,14,15	0.72	0	17,19,21	0.79	0
7	NAG	N	1	1,7	14,14,15	0.74	0	17,19,21	1.05	1 (5%)
7	NAG	N	2	7	14,14,15	0.70	0	17,19,21	1.20	1 (5%)
11	NAG	O	1	1,11	14,14,15	0.74	0	17,19,21	1.00	0
11	NAG	O	2	11	14,14,15	0.71	0	17,19,21	1.44	3 (17%)
11	BMA	O	3	11	11,11,12	0.98	0	15,15,17	2.18	4 (26%)
11	MAN	O	4	11	11,11,12	0.60	0	15,15,17	1.58	1 (6%)
11	MAN	O	5	11	11,11,12	0.69	0	15,15,17	1.14	1 (6%)
11	MAN	O	6	11	11,11,12	0.72	0	15,15,17	1.16	1 (6%)
11	MAN	O	7	11	11,11,12	0.69	0	15,15,17	1.32	1 (6%)
11	MAN	O	8	11	11,11,12	0.67	0	15,15,17	1.13	1 (6%)
11	MAN	O	9	11	11,11,12	0.67	0	15,15,17	1.24	1 (6%)
7	NAG	P	1	1,7	14,14,15	0.69	0	17,19,21	1.25	1 (5%)
7	NAG	P	2	7	14,14,15	0.72	0	17,19,21	0.81	0
7	NAG	Q	1	1,7	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
7	NAG	Q	2	7	14,14,15	0.71	0	17,19,21	0.80	0
7	NAG	R	1	1,7	14,14,15	0.75	0	17,19,21	0.88	0
7	NAG	R	2	7	14,14,15	0.72	0	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	S	1	1,7	14,14,15	0.70	0	17,19,21	1.15	1 (5%)
7	NAG	S	2	7	14,14,15	0.73	0	17,19,21	0.80	0
7	NAG	T	1	1,7	14,14,15	0.70	0	17,19,21	1.11	2 (11%)
7	NAG	T	2	7	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
8	NAG	U	1	1,8	14,14,15	0.85	0	17,19,21	1.68	2 (11%)
8	NAG	U	2	8	14,14,15	0.73	0	17,19,21	1.05	1 (5%)
8	BMA	U	3	8	11,11,12	0.85	0	15,15,17	2.32	4 (26%)
8	MAN	U	4	8	11,11,12	0.66	0	15,15,17	1.42	1 (6%)
7	NAG	V	1	1,7	14,14,15	0.69	0	17,19,21	1.14	1 (5%)
7	NAG	V	2	7	14,14,15	0.72	0	17,19,21	0.87	0
7	NAG	W	1	1,7	14,14,15	0.74	0	17,19,21	0.89	0
7	NAG	W	2	7	14,14,15	0.71	0	17,19,21	0.81	0
9	NAG	X	1	1,9	14,14,15	0.69	0	17,19,21	0.95	1 (5%)
9	NAG	X	2	9	14,14,15	0.72	0	17,19,21	0.86	0
9	BMA	X	3	9	11,11,12	0.84	0	15,15,17	2.09	4 (26%)
10	NAG	Y	1	1,10	14,14,15	0.68	0	17,19,21	1.06	1 (5%)
10	NAG	Y	2	10	14,14,15	0.77	0	17,19,21	1.39	4 (23%)
10	BMA	Y	3	10	11,11,12	0.89	0	15,15,17	1.95	6 (40%)
10	MAN	Y	4	10	11,11,12	0.72	0	15,15,17	1.10	1 (6%)
10	MAN	Y	5	10	11,11,12	0.74	0	15,15,17	0.94	1 (6%)
7	NAG	Z	1	1,7	14,14,15	0.74	0	17,19,21	1.07	1 (5%)
7	NAG	Z	2	7	14,14,15	0.68	0	17,19,21	1.20	2 (11%)
7	NAG	a	1	1,7	14,14,15	0.75	0	17,19,21	0.89	0
7	NAG	a	2	7	14,14,15	0.72	0	17,19,21	0.81	0
7	NAG	b	1	1,7	14,14,15	0.71	0	17,19,21	1.15	1 (5%)
7	NAG	b	2	7	14,14,15	0.72	0	17,19,21	0.81	0
7	NAG	c	1	1,7	14,14,15	0.69	0	17,19,21	1.11	2 (11%)
7	NAG	c	2	7	14,14,15	0.74	0	17,19,21	0.95	1 (5%)
8	NAG	f	1	1,8	14,14,15	0.82	0	17,19,21	1.66	2 (11%)
8	NAG	f	2	8	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
8	BMA	f	3	8	11,11,12	0.86	0	15,15,17	2.30	4 (26%)
8	MAN	f	4	8	11,11,12	0.65	0	15,15,17	1.44	1 (6%)
7	NAG	g	1	1,7	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
7	NAG	g	2	7	14,14,15	0.73	0	17,19,21	0.87	0
7	NAG	i	1	1,7	14,14,15	0.71	0	17,19,21	0.86	0
7	NAG	i	2	7	14,14,15	0.69	0	17,19,21	0.80	0
9	NAG	j	1	1,9	14,14,15	0.70	0	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	j	2	9	14,14,15	0.72	0	17,19,21	0.88	1 (5%)
9	BMA	j	3	9	11,11,12	0.86	0	15,15,17	2.08	4 (26%)
10	NAG	n	1	1,10	14,14,15	0.70	0	17,19,21	1.02	1 (5%)
10	NAG	n	2	10	14,14,15	0.78	0	17,19,21	1.36	3 (17%)
10	BMA	n	3	10	11,11,12	0.91	0	15,15,17	1.96	6 (40%)
10	MAN	n	4	10	11,11,12	0.73	0	15,15,17	1.09	1 (6%)
10	MAN	n	5	10	11,11,12	0.75	0	15,15,17	0.96	1 (6%)
7	NAG	o	1	1,7	14,14,15	0.78	0	17,19,21	1.04	1 (5%)
7	NAG	o	2	7	14,14,15	0.69	0	17,19,21	1.20	1 (5%)
11	NAG	p	1	1,11	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
11	NAG	p	2	11	14,14,15	0.71	0	17,19,21	1.46	3 (17%)
11	BMA	p	3	11	11,11,12	0.96	0	15,15,17	2.13	4 (26%)
11	MAN	p	4	11	11,11,12	0.61	0	15,15,17	1.58	1 (6%)
11	MAN	p	5	11	11,11,12	0.71	0	15,15,17	1.17	1 (6%)
11	MAN	p	6	11	11,11,12	0.71	0	15,15,17	1.14	1 (6%)
11	MAN	p	7	11	11,11,12	0.69	0	15,15,17	1.35	1 (6%)
11	MAN	p	8	11	11,11,12	0.69	0	15,15,17	1.15	1 (6%)
11	MAN	p	9	11	11,11,12	0.67	0	15,15,17	1.26	1 (6%)
7	NAG	q	1	1,7	14,14,15	0.69	0	17,19,21	1.25	1 (5%)
7	NAG	q	2	7	14,14,15	0.72	0	17,19,21	0.80	0
7	NAG	r	1	1,7	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
7	NAG	r	2	7	14,14,15	0.72	0	17,19,21	0.80	0
7	NAG	s	1	1,7	14,14,15	0.77	0	17,19,21	0.90	0
7	NAG	s	2	7	14,14,15	0.71	0	17,19,21	0.81	0
7	NAG	t	1	1,7	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
7	NAG	t	2	7	14,14,15	0.73	0	17,19,21	0.80	0
7	NAG	u	1	1,7	14,14,15	0.70	0	17,19,21	1.12	2 (11%)
7	NAG	u	2	7	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
8	NAG	v	1	1,8	14,14,15	0.83	0	17,19,21	1.69	2 (11%)
8	NAG	v	2	8	14,14,15	0.73	0	17,19,21	1.05	1 (5%)
8	BMA	v	3	8	11,11,12	0.85	0	15,15,17	2.30	4 (26%)
8	MAN	v	4	8	11,11,12	0.67	0	15,15,17	1.43	1 (6%)
7	NAG	w	1	1,7	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
7	NAG	w	2	7	14,14,15	0.73	0	17,19,21	0.87	0
7	NAG	x	1	1,7	14,14,15	0.75	0	17,19,21	0.87	0
7	NAG	x	2	7	14,14,15	0.69	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	y	1	1,9	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
9	NAG	y	2	9	14,14,15	0.74	0	17,19,21	0.85	0
9	BMA	y	3	9	11,11,12	0.85	0	15,15,17	2.08	4 (26%)
10	NAG	z	1	1,10	14,14,15	0.69	0	17,19,21	1.06	1 (5%)
10	NAG	z	2	10	14,14,15	0.76	0	17,19,21	1.31	3 (17%)
10	BMA	z	3	10	11,11,12	0.89	0	15,15,17	1.95	6 (40%)
10	MAN	z	4	10	11,11,12	0.72	0	15,15,17	1.09	1 (6%)
10	MAN	z	5	10	11,11,12	0.77	0	15,15,17	0.95	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
11	NAG	0	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	0	2	11	-	3/6/23/26	0/1/1/1
11	BMA	0	3	11	-	0/2/19/22	0/1/1/1
11	MAN	0	4	11	-	1/2/19/22	0/1/1/1
11	MAN	0	5	11	-	2/2/19/22	0/1/1/1
11	MAN	0	6	11	-	2/2/19/22	1/1/1/1
11	MAN	0	7	11	-	2/2/19/22	0/1/1/1
11	MAN	0	8	11	-	2/2/19/22	0/1/1/1
11	MAN	0	9	11	-	2/2/19/22	1/1/1/1
7	NAG	1	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	1	2	7	-	0/6/23/26	0/1/1/1
7	NAG	2	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	2	2	7	-	0/6/23/26	0/1/1/1
7	NAG	N	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
11	NAG	O	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	O	2	11	-	3/6/23/26	0/1/1/1
11	BMA	O	3	11	-	0/2/19/22	0/1/1/1
11	MAN	O	4	11	-	1/2/19/22	0/1/1/1
11	MAN	O	5	11	-	2/2/19/22	0/1/1/1
11	MAN	O	6	11	-	2/2/19/22	1/1/1/1
11	MAN	O	7	11	-	2/2/19/22	0/1/1/1
11	MAN	O	8	11	-	2/2/19/22	0/1/1/1

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

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

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

There are no bond length outliers.

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	3	BMA	C1-O5-C5	7.03	121.61	112.19
8	f	3	BMA	C1-O5-C5	6.97	121.52	112.19
8	v	3	BMA	C1-O5-C5	6.96	121.52	112.19
9	X	3	BMA	C1-O5-C5	6.17	120.46	112.19
9	y	3	BMA	C1-O5-C5	6.11	120.38	112.19
9	j	3	BMA	C1-O5-C5	6.07	120.32	112.19
8	v	1	NAG	C1-O5-C5	5.77	119.92	112.19
8	U	1	NAG	C1-O5-C5	5.67	119.78	112.19
8	f	1	NAG	C1-O5-C5	5.59	119.68	112.19
11	O	3	BMA	C1-O5-C5	5.56	119.64	112.19
11	p	4	MAN	C1-O5-C5	5.33	119.33	112.19
11	O	4	MAN	C1-O5-C5	5.32	119.31	112.19
11	0	4	MAN	C1-O5-C5	5.23	119.19	112.19
11	0	3	BMA	C1-O5-C5	4.97	118.84	112.19
11	p	3	BMA	C1-O5-C5	4.92	118.79	112.19
8	f	4	MAN	C1-O5-C5	4.30	117.95	112.19
8	v	4	MAN	C1-O5-C5	4.26	117.89	112.19
8	U	4	MAN	C1-O5-C5	4.21	117.83	112.19
11	p	7	MAN	C1-O5-C5	4.11	117.69	112.19
11	0	7	MAN	C1-O5-C5	4.00	117.54	112.19
11	p	9	MAN	C1-O5-C5	3.99	117.54	112.19
11	0	9	MAN	C1-O5-C5	3.98	117.53	112.19
11	O	7	MAN	C1-O5-C5	3.94	117.47	112.19
11	O	9	MAN	C1-O5-C5	3.91	117.43	112.19
11	p	3	BMA	C3-C4-C5	3.70	116.94	110.23
10	n	3	BMA	C1-C2-C3	-3.61	104.38	109.64
11	0	5	MAN	C1-O5-C5	3.58	116.99	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	0	3	BMA	C3-C4-C5	3.57	116.70	110.23
10	Y	3	BMA	C1-C2-C3	-3.57	104.45	109.64
10	z	3	BMA	C1-C2-C3	-3.56	104.46	109.64
10	Y	3	BMA	C1-O5-C5	3.56	116.96	112.19
10	z	3	BMA	C1-O5-C5	3.55	116.95	112.19
11	0	2	NAG	C2-N2-C7	3.51	127.60	122.90
10	n	3	BMA	C1-O5-C5	3.49	116.87	112.19
11	O	3	BMA	C3-C4-C5	3.47	116.53	110.23
11	O	6	MAN	C1-O5-C5	3.47	116.84	112.19
11	p	2	NAG	C2-N2-C7	3.46	127.54	122.90
11	O	2	NAG	C2-N2-C7	3.45	127.53	122.90
11	p	5	MAN	C1-O5-C5	3.44	116.80	112.19
11	p	6	MAN	C1-O5-C5	3.42	116.77	112.19
11	0	6	MAN	C1-O5-C5	3.42	116.76	112.19
11	0	8	MAN	C1-O5-C5	3.33	116.65	112.19
11	O	5	MAN	C1-O5-C5	3.33	116.65	112.19
11	p	8	MAN	C1-O5-C5	3.33	116.64	112.19
10	z	1	NAG	O5-C1-C2	-3.31	106.17	111.29
10	Y	1	NAG	O5-C1-C2	-3.28	106.21	111.29
11	O	8	MAN	C1-O5-C5	3.26	116.56	112.19
7	N	2	NAG	C2-N2-C7	3.24	127.24	122.90
7	o	2	NAG	C2-N2-C7	3.23	127.23	122.90
7	Z	2	NAG	C2-N2-C7	3.22	127.21	122.90
7	t	1	NAG	C2-N2-C7	3.14	127.11	122.90
7	b	1	NAG	C2-N2-C7	3.13	127.10	122.90
11	0	2	NAG	O5-C1-C2	-3.11	106.48	111.29
7	S	1	NAG	C2-N2-C7	3.11	127.06	122.90
10	n	3	BMA	C3-C4-C5	3.10	115.85	110.23
10	Y	4	MAN	C1-O5-C5	3.09	116.33	112.19
10	n	1	NAG	O5-C1-C2	-3.09	106.51	111.29
11	p	2	NAG	O5-C1-C2	-3.08	106.53	111.29
10	z	3	BMA	C3-C4-C5	3.08	115.81	110.23
10	Y	3	BMA	C3-C4-C5	3.07	115.80	110.23
11	p	3	BMA	C2-C3-C4	3.07	116.26	110.86
10	n	4	MAN	C1-O5-C5	3.05	116.28	112.19
10	z	4	MAN	C1-O5-C5	3.05	116.27	112.19
11	0	3	BMA	C2-C3-C4	3.05	116.22	110.86
7	q	1	NAG	C2-N2-C7	3.05	126.98	122.90
7	l	1	NAG	C2-N2-C7	3.04	126.98	122.90
7	P	1	NAG	C2-N2-C7	3.03	126.97	122.90
11	O	2	NAG	O5-C1-C2	-2.97	106.70	111.29
8	f	3	BMA	C3-C4-C5	2.95	115.57	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	3	BMA	C3-C4-C5	2.94	115.57	110.23
10	z	2	NAG	O5-C1-C2	-2.94	106.74	111.29
11	O	3	BMA	C2-C3-C4	2.94	116.03	110.86
10	Y	2	NAG	C4-C3-C2	2.93	115.32	111.02
8	v	3	BMA	C3-C4-C5	2.93	115.55	110.23
10	n	2	NAG	O4-C4-C3	-2.86	103.63	110.38
10	n	2	NAG	O5-C1-C2	-2.84	106.89	111.29
10	Y	2	NAG	O4-C4-C3	-2.82	103.72	110.38
7	V	1	NAG	C1-O5-C5	2.79	115.93	112.19
10	n	2	NAG	C4-C3-C2	2.78	115.09	111.02
10	z	2	NAG	O4-C4-C3	-2.77	103.84	110.38
7	g	1	NAG	C1-O5-C5	2.77	115.90	112.19
7	w	1	NAG	C1-O5-C5	2.77	115.89	112.19
10	Y	2	NAG	O5-C1-C2	-2.72	107.08	111.29
9	j	3	BMA	C3-C4-C5	2.68	115.10	110.23
7	u	1	NAG	O4-C4-C5	2.65	115.86	109.32
9	X	3	BMA	C3-C4-C5	2.65	115.03	110.23
9	y	3	BMA	C3-C4-C5	2.63	115.01	110.23
7	c	1	NAG	O4-C4-C5	2.61	115.75	109.32
10	z	2	NAG	C4-C3-C2	2.58	114.80	111.02
7	Q	1	NAG	O5-C1-C2	-2.57	107.32	111.29
7	T	1	NAG	O4-C4-C5	2.57	115.64	109.32
7	2	1	NAG	O5-C1-C2	-2.52	107.39	111.29
7	r	1	NAG	O5-C1-C2	-2.49	107.44	111.29
8	U	1	NAG	C3-C4-C5	-2.46	105.77	110.23
8	f	1	NAG	C3-C4-C5	-2.44	105.81	110.23
7	Z	1	NAG	O4-C4-C3	-2.44	104.63	110.38
7	o	1	NAG	O4-C4-C3	-2.43	104.65	110.38
11	p	3	BMA	O4-C4-C3	-2.42	104.66	110.38
7	N	1	NAG	O4-C4-C3	-2.41	104.69	110.38
9	j	1	NAG	O5-C1-C2	-2.39	107.60	111.29
11	0	3	BMA	O4-C4-C3	-2.39	104.75	110.38
8	v	1	NAG	C3-C4-C5	-2.38	105.92	110.23
9	y	1	NAG	O5-C1-C2	-2.34	107.67	111.29
9	y	3	BMA	C2-C3-C4	2.33	114.96	110.86
9	X	3	BMA	C2-C3-C4	2.33	114.96	110.86
8	U	3	BMA	C2-C3-C4	2.33	114.95	110.86
8	v	3	BMA	C2-C3-C4	2.32	114.94	110.86
8	v	2	NAG	O5-C1-C2	-2.32	107.71	111.29
8	f	2	NAG	O5-C1-C2	-2.31	107.72	111.29
9	X	1	NAG	O5-C1-C2	-2.31	107.72	111.29
9	j	3	BMA	C2-C3-C4	2.30	114.91	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	3	BMA	C2-C3-C4	2.30	114.90	110.86
7	c	2	NAG	C1-O5-C5	2.29	115.26	112.19
9	j	2	NAG	O5-C1-C2	-2.28	107.76	111.29
8	U	2	NAG	O5-C1-C2	-2.27	107.77	111.29
7	u	1	NAG	C1-O5-C5	2.27	115.23	112.19
10	n	3	BMA	O5-C1-C2	-2.26	105.40	110.79
7	u	2	NAG	C1-O5-C5	2.26	115.21	112.19
11	O	3	BMA	O4-C4-C3	-2.24	105.10	110.38
10	z	3	BMA	O5-C1-C2	-2.23	105.47	110.79
7	T	1	NAG	C1-O5-C5	2.23	115.17	112.19
10	Y	3	BMA	O5-C1-C2	-2.22	105.50	110.79
7	T	2	NAG	C1-O5-C5	2.21	115.14	112.19
10	n	5	MAN	C1-O5-C5	2.18	115.11	112.19
11	p	2	NAG	C1-C2-N2	2.16	113.84	110.43
11	0	2	NAG	C1-C2-N2	2.15	113.82	110.43
7	c	1	NAG	C1-O5-C5	2.13	115.04	112.19
11	0	1	NAG	O5-C1-C2	-2.11	108.02	111.29
10	Y	5	MAN	C1-O5-C5	2.11	115.02	112.19
11	O	2	NAG	C1-C2-N2	2.11	113.76	110.43
10	z	5	MAN	C1-O5-C5	2.11	115.01	112.19
8	U	3	BMA	O4-C4-C3	-2.11	105.41	110.38
8	f	3	BMA	O4-C4-C3	-2.10	105.42	110.38
10	Y	2	NAG	C2-N2-C7	2.10	125.72	122.90
8	v	3	BMA	O4-C4-C3	-2.09	105.45	110.38
10	n	3	BMA	O4-C4-C3	-2.08	105.48	110.38
10	z	3	BMA	O4-C4-C3	-2.06	105.51	110.38
10	Y	3	BMA	O4-C4-C3	-2.06	105.53	110.38
9	j	3	BMA	O4-C4-C3	-2.03	105.58	110.38
7	Z	2	NAG	O5-C1-C2	-2.02	108.16	111.29
9	X	3	BMA	O4-C4-C3	-2.02	105.61	110.38
10	n	3	BMA	C2-C3-C4	2.02	114.41	110.86
10	z	3	BMA	C2-C3-C4	2.02	114.41	110.86
10	Y	3	BMA	C2-C3-C4	2.00	114.39	110.86
9	y	3	BMA	O4-C4-C3	-2.00	105.65	110.38
11	p	1	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	p	7	MAN	C4-C5-C6-O6
11	O	7	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	0	7	MAN	C4-C5-C6-O6
11	p	5	MAN	C4-C5-C6-O6
11	p	1	NAG	O5-C5-C6-O6
11	0	1	NAG	O5-C5-C6-O6
11	O	6	MAN	C4-C5-C6-O6
11	O	1	NAG	O5-C5-C6-O6
11	p	6	MAN	C4-C5-C6-O6
11	0	6	MAN	C4-C5-C6-O6
11	0	8	MAN	C4-C5-C6-O6
11	0	7	MAN	O5-C5-C6-O6
11	p	8	MAN	C4-C5-C6-O6
11	O	8	MAN	C4-C5-C6-O6
11	0	5	MAN	C4-C5-C6-O6
10	n	3	BMA	O5-C5-C6-O6
10	z	3	BMA	O5-C5-C6-O6
11	p	7	MAN	O5-C5-C6-O6
11	O	6	MAN	O5-C5-C6-O6
10	Y	3	BMA	O5-C5-C6-O6
11	O	7	MAN	O5-C5-C6-O6
10	Y	3	BMA	C4-C5-C6-O6
10	n	2	NAG	O5-C5-C6-O6
11	0	8	MAN	O5-C5-C6-O6
10	n	3	BMA	C4-C5-C6-O6
10	z	3	BMA	C4-C5-C6-O6
10	Y	2	NAG	O5-C5-C6-O6
11	p	6	MAN	O5-C5-C6-O6
11	p	8	MAN	O5-C5-C6-O6
11	O	8	MAN	O5-C5-C6-O6
11	0	6	MAN	O5-C5-C6-O6
10	z	2	NAG	O5-C5-C6-O6
11	p	5	MAN	O5-C5-C6-O6
11	O	9	MAN	C4-C5-C6-O6
11	0	5	MAN	O5-C5-C6-O6
11	O	5	MAN	C4-C5-C6-O6
11	0	9	MAN	C4-C5-C6-O6
11	p	9	MAN	C4-C5-C6-O6
10	n	4	MAN	C4-C5-C6-O6
10	z	4	MAN	C4-C5-C6-O6
11	O	9	MAN	O5-C5-C6-O6
8	U	4	MAN	C4-C5-C6-O6
10	Y	4	MAN	C4-C5-C6-O6
8	v	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	i	2	NAG	O5-C5-C6-O6
11	O	1	NAG	C4-C5-C6-O6
11	0	9	MAN	O5-C5-C6-O6
7	x	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	q	1	NAG	O5-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
11	p	4	MAN	O5-C5-C6-O6
11	p	9	MAN	O5-C5-C6-O6
11	O	4	MAN	O5-C5-C6-O6
7	w	2	NAG	O5-C5-C6-O6
7	l	1	NAG	O5-C5-C6-O6
11	0	4	MAN	O5-C5-C6-O6
11	p	1	NAG	C4-C5-C6-O6
11	0	1	NAG	C4-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
7	u	2	NAG	O5-C5-C6-O6
11	O	5	MAN	O5-C5-C6-O6
10	n	4	MAN	O5-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
10	z	4	MAN	O5-C5-C6-O6
7	V	1	NAG	O5-C5-C6-O6
8	f	4	MAN	C4-C5-C6-O6
7	w	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
10	Y	4	MAN	O5-C5-C6-O6
10	n	2	NAG	C4-C5-C6-O6
7	o	2	NAG	C1-C2-N2-C7
7	q	1	NAG	C1-C2-N2-C7
7	N	2	NAG	C1-C2-N2-C7
7	P	1	NAG	C1-C2-N2-C7
7	Z	2	NAG	C1-C2-N2-C7
7	l	1	NAG	C1-C2-N2-C7
8	U	4	MAN	O5-C5-C6-O6
10	z	1	NAG	O5-C5-C6-O6
10	Y	2	NAG	C4-C5-C6-O6
8	v	4	MAN	O5-C5-C6-O6
10	z	1	NAG	C4-C5-C6-O6
10	z	2	NAG	C4-C5-C6-O6
7	b	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	q	1	NAG	C3-C2-N2-C7
7	t	1	NAG	C3-C2-N2-C7
7	P	1	NAG	C3-C2-N2-C7
7	S	1	NAG	C3-C2-N2-C7
7	l	1	NAG	C3-C2-N2-C7
11	p	2	NAG	C3-C2-N2-C7
11	O	2	NAG	C3-C2-N2-C7
11	0	2	NAG	C3-C2-N2-C7
8	f	4	MAN	O5-C5-C6-O6
10	Y	1	NAG	O5-C5-C6-O6
11	p	2	NAG	O5-C5-C6-O6
11	O	2	NAG	O5-C5-C6-O6
10	n	1	NAG	O5-C5-C6-O6
7	b	1	NAG	C1-C2-N2-C7
7	t	1	NAG	C1-C2-N2-C7
7	S	1	NAG	C1-C2-N2-C7
11	p	2	NAG	C1-C2-N2-C7
11	O	2	NAG	C1-C2-N2-C7
11	0	2	NAG	C1-C2-N2-C7
11	0	2	NAG	O5-C5-C6-O6
10	Y	1	NAG	C4-C5-C6-O6
7	o	2	NAG	C3-C2-N2-C7
7	N	2	NAG	C3-C2-N2-C7
7	Z	2	NAG	C3-C2-N2-C7
10	n	1	NAG	C4-C5-C6-O6

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	0	9	MAN	C1-C2-C3-C4-C5-O5
11	0	6	MAN	C1-C2-C3-C4-C5-O5
11	p	6	MAN	C1-C2-C3-C4-C5-O5
11	O	6	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 10 short contacts:

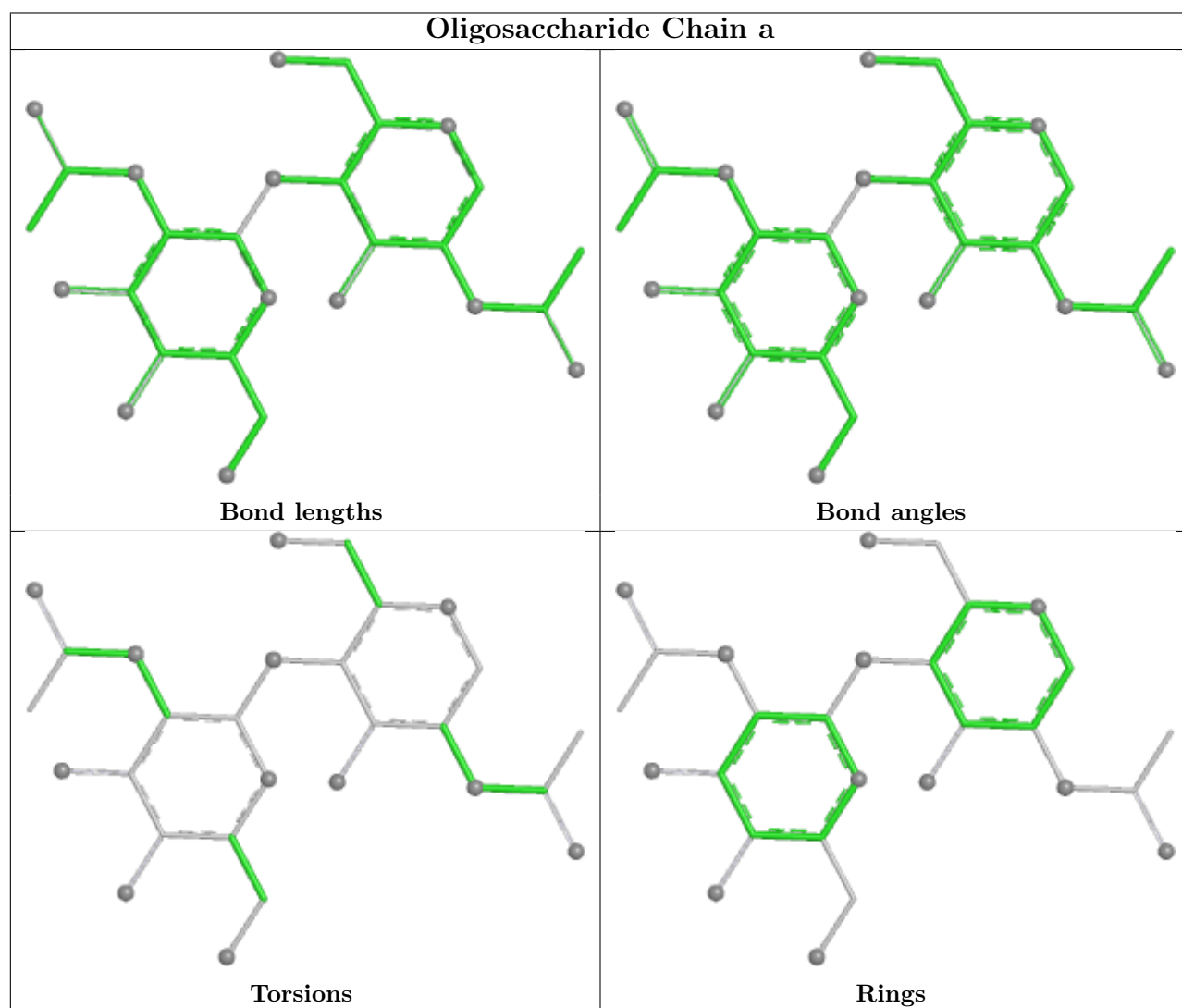
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	q	1	NAG	1	0
7	P	1	NAG	1	0
10	z	1	NAG	1	0
10	n	1	NAG	1	0
10	Y	1	NAG	1	0

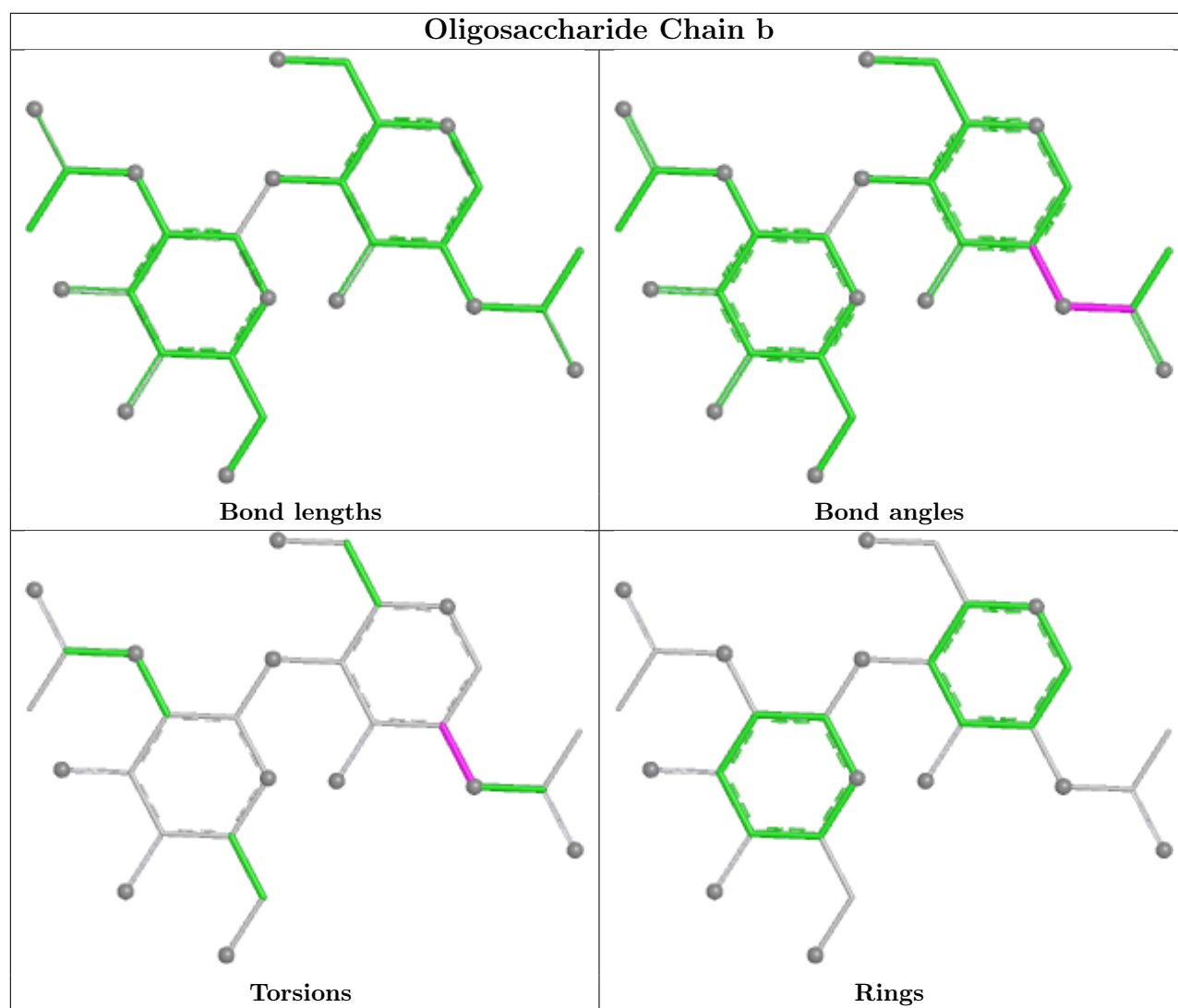
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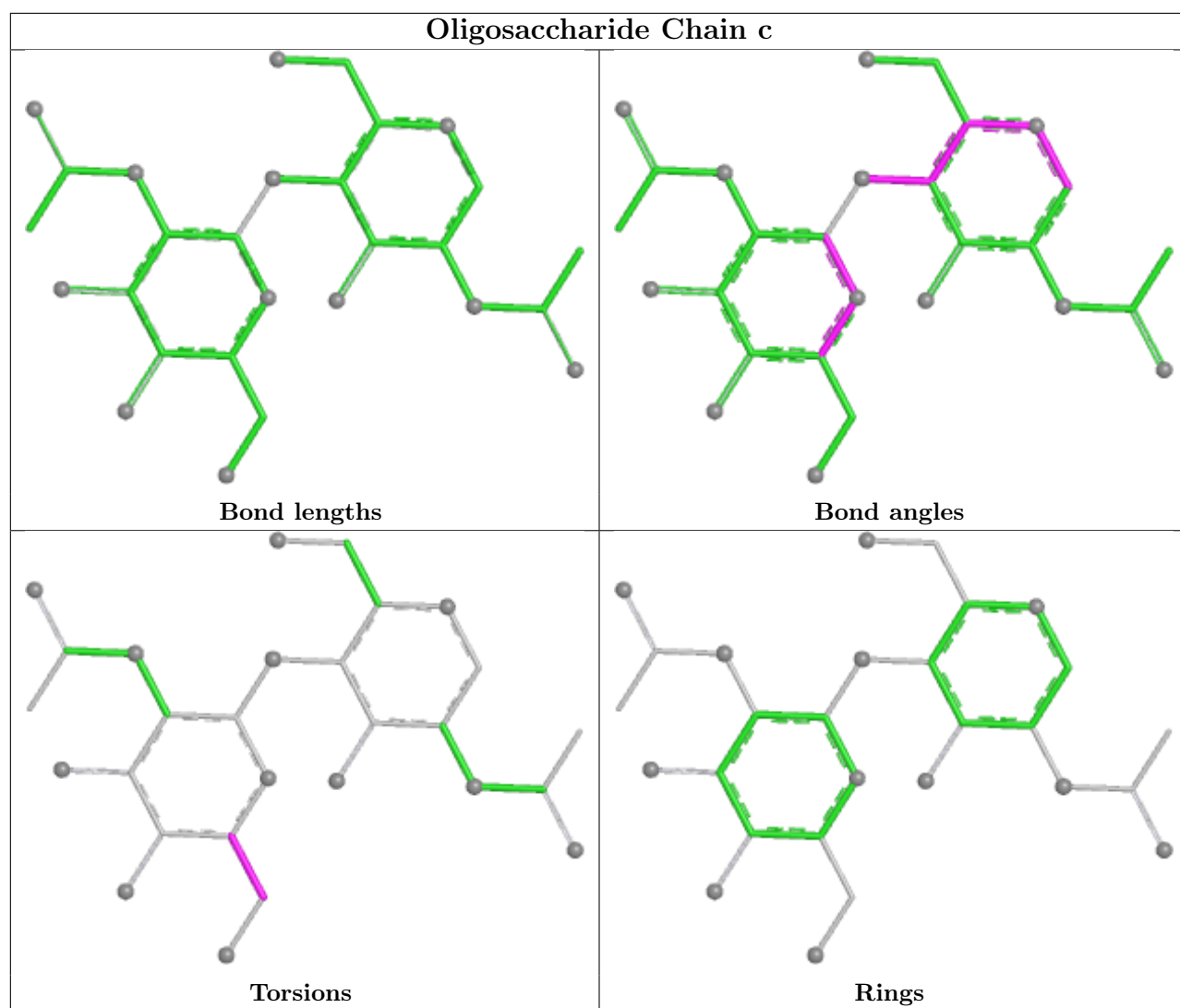
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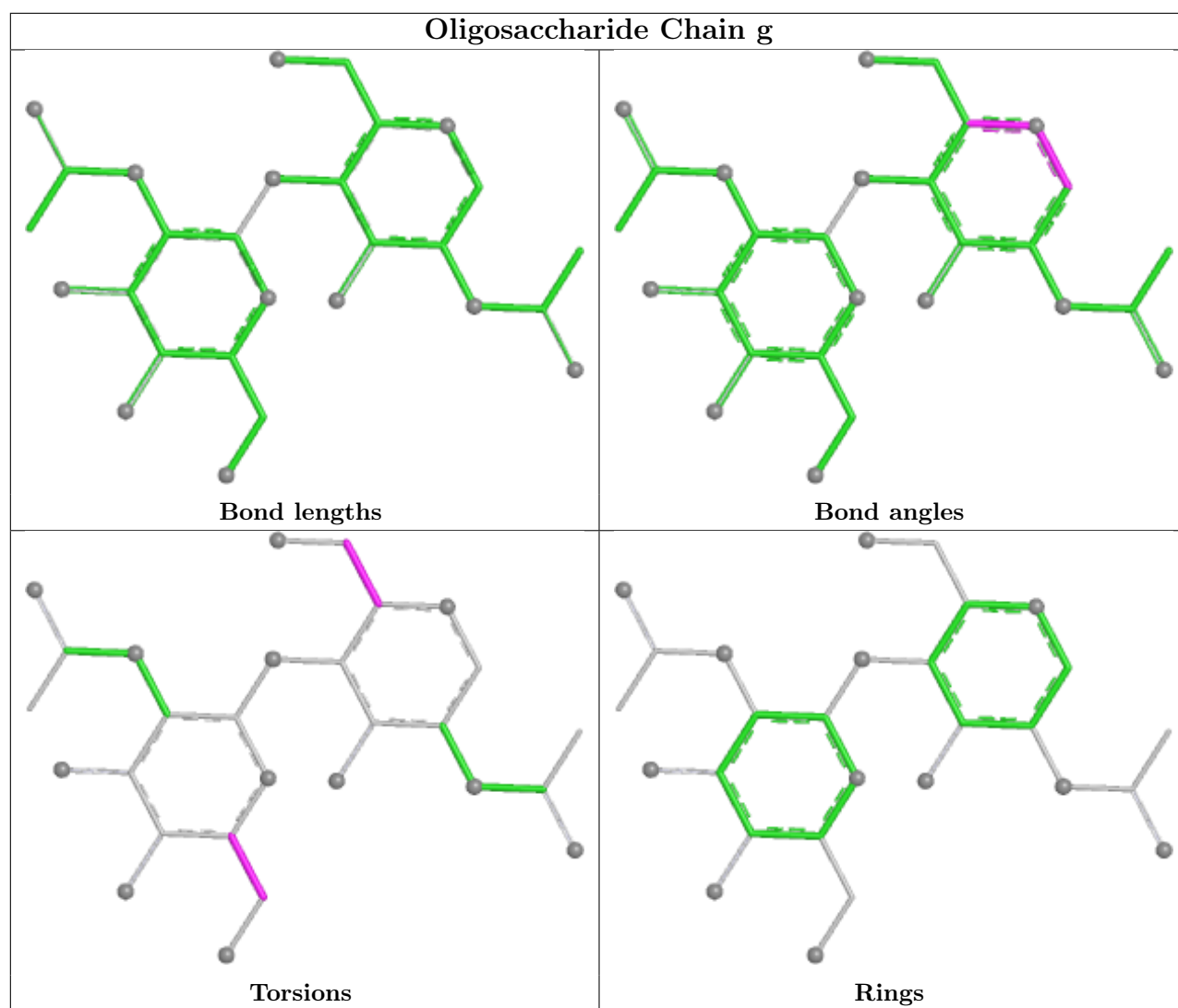
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	n	3	BMA	1	0
7	1	1	NAG	1	0
10	z	2	NAG	1	0
11	O	3	BMA	1	0
10	z	3	BMA	1	0
10	n	2	NAG	1	0
8	f	1	NAG	1	0

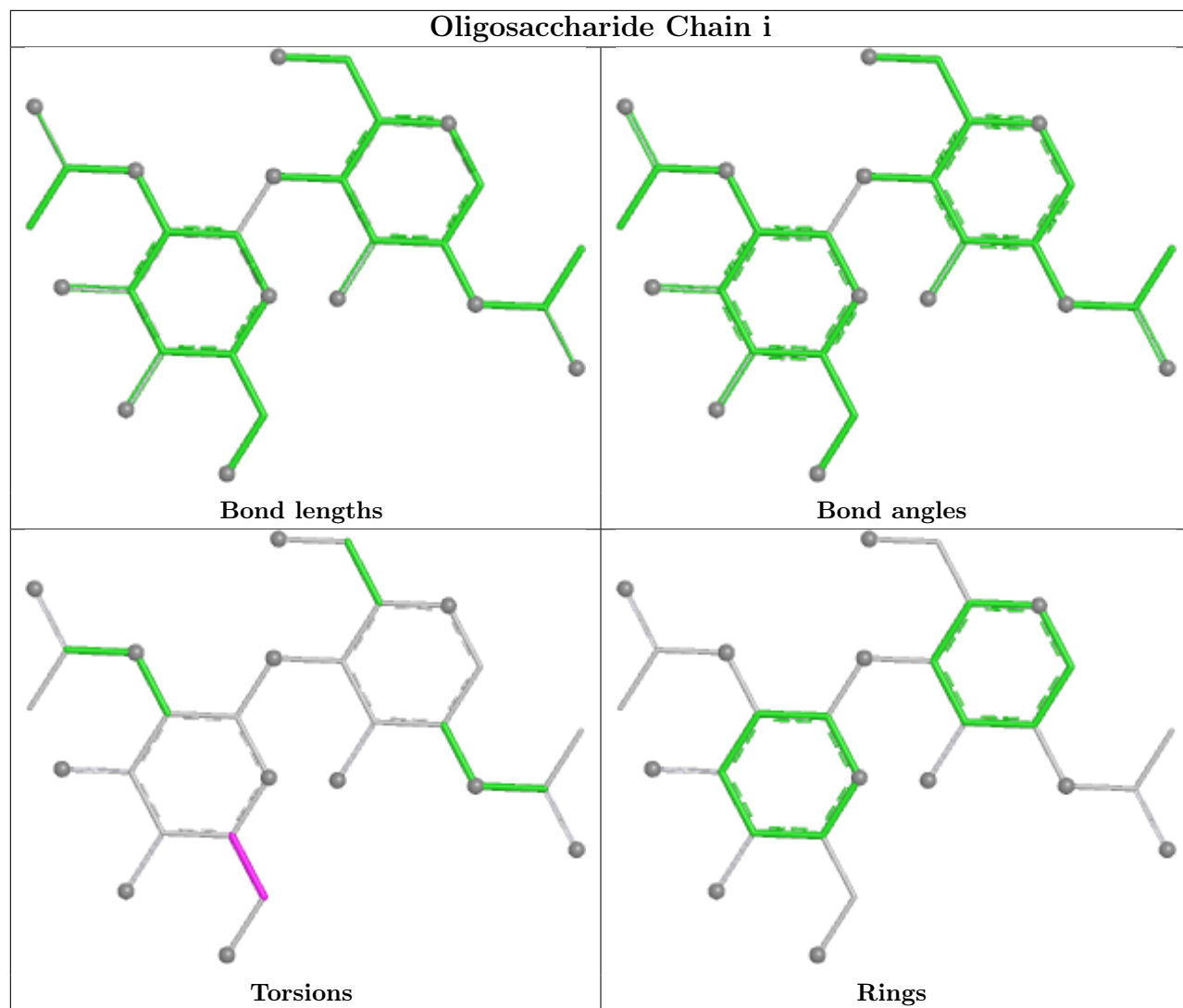
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

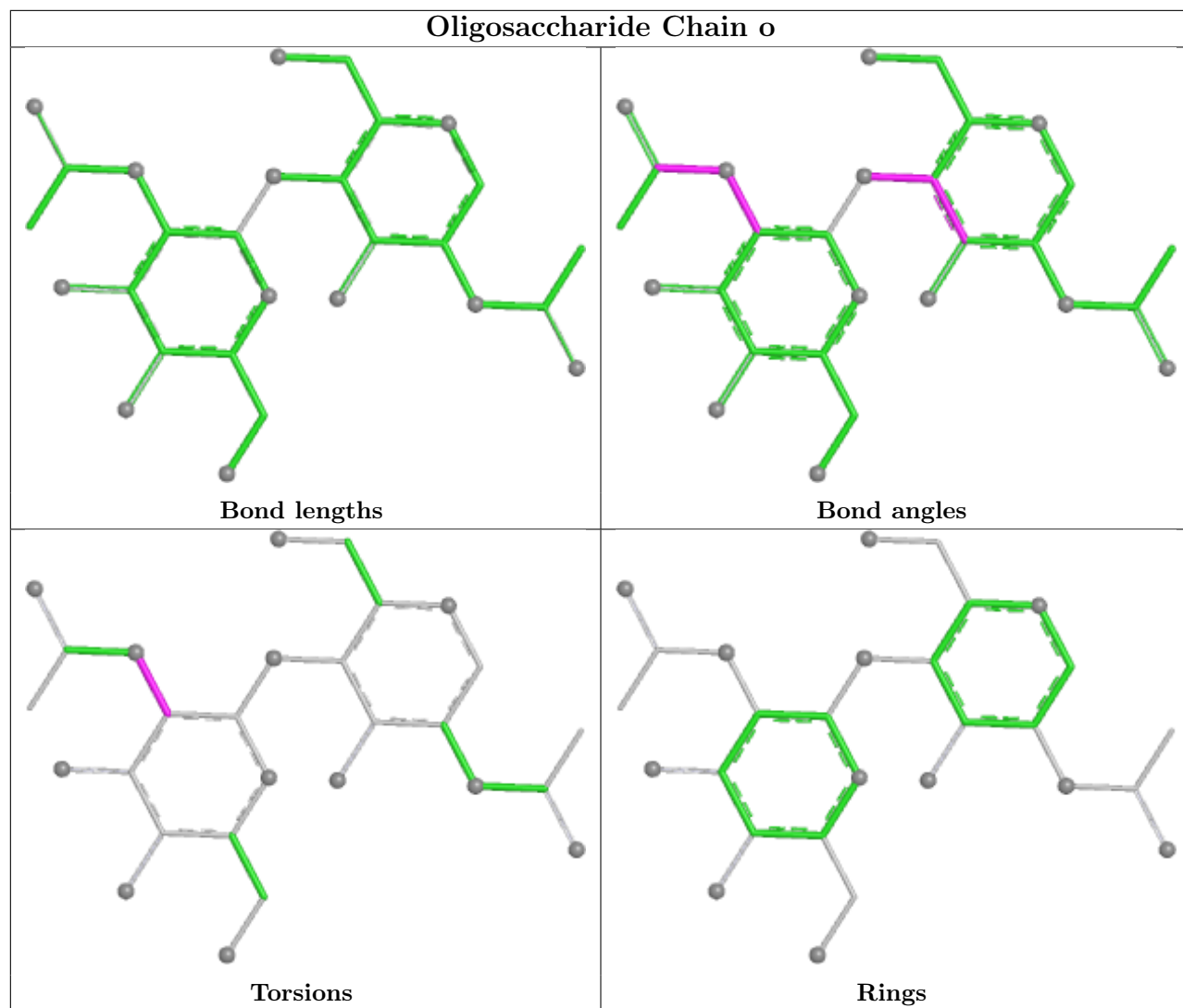


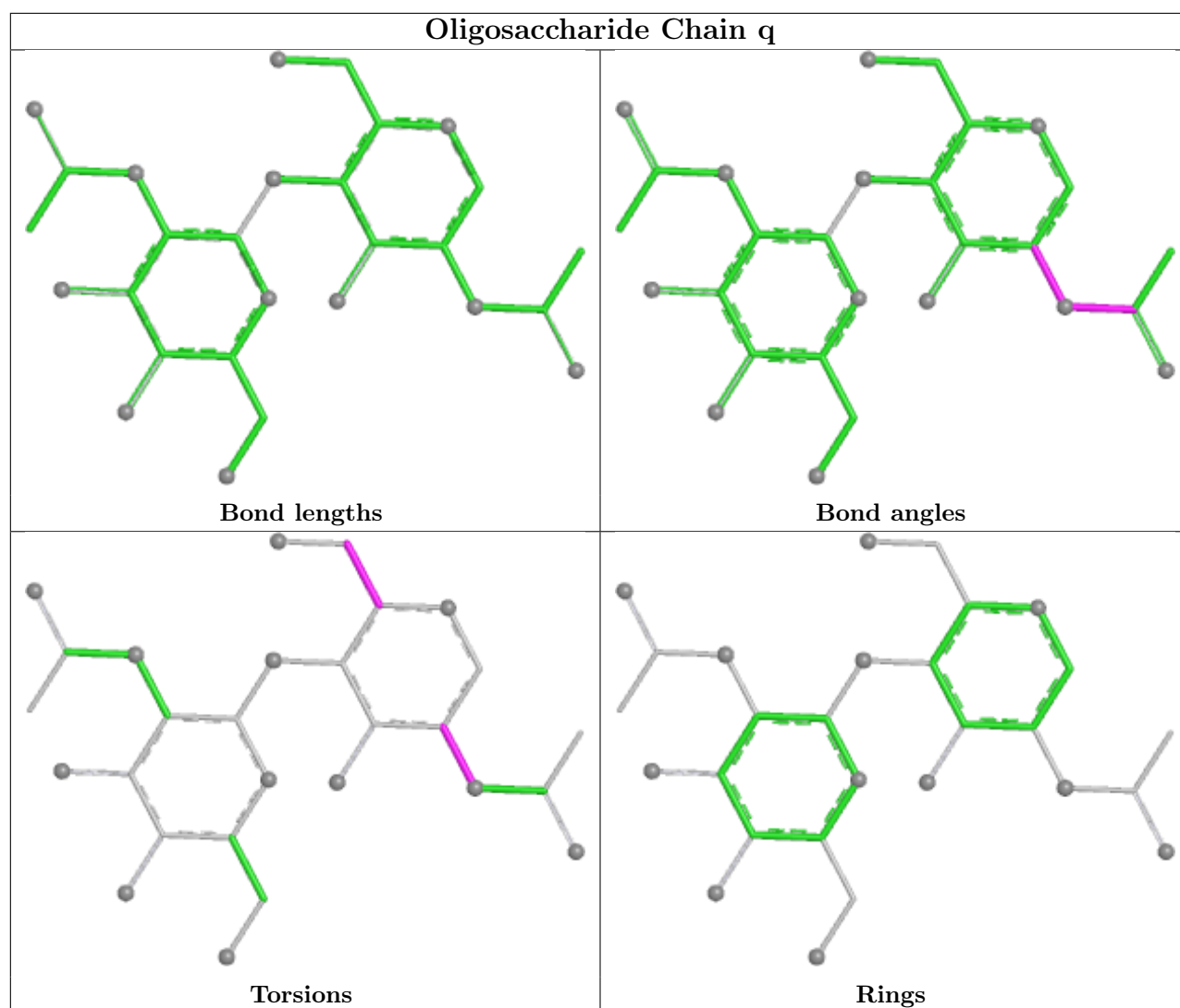


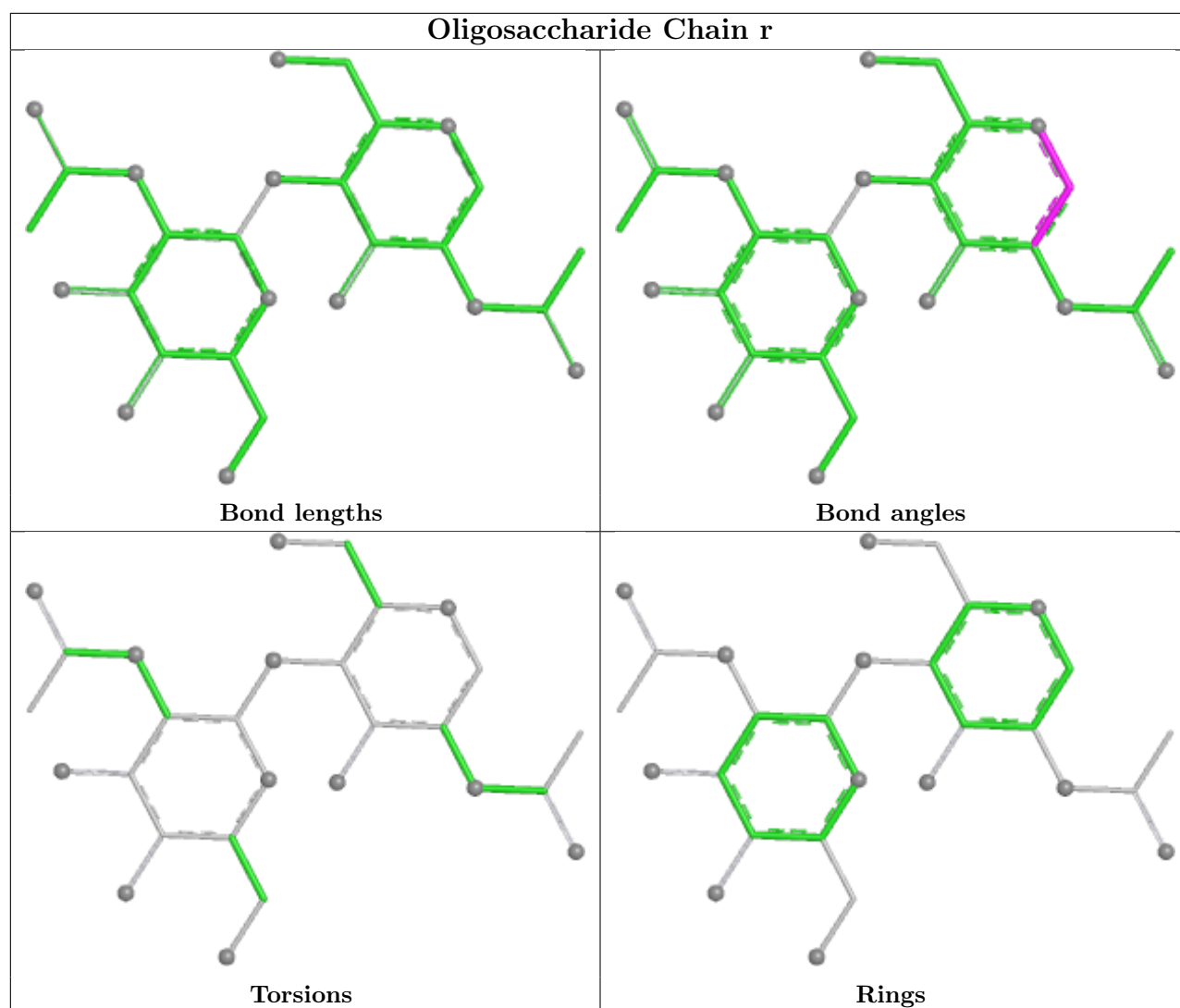


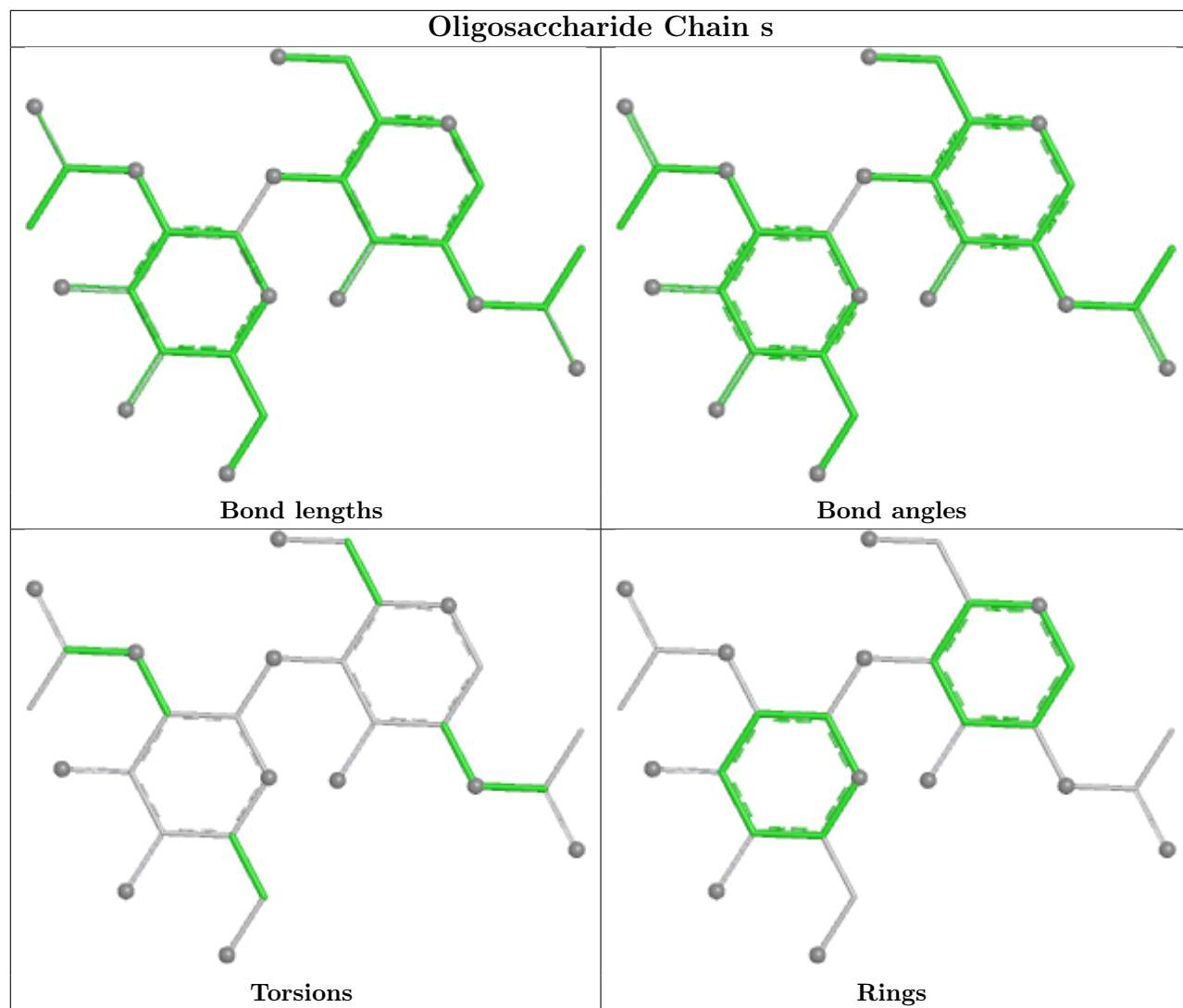


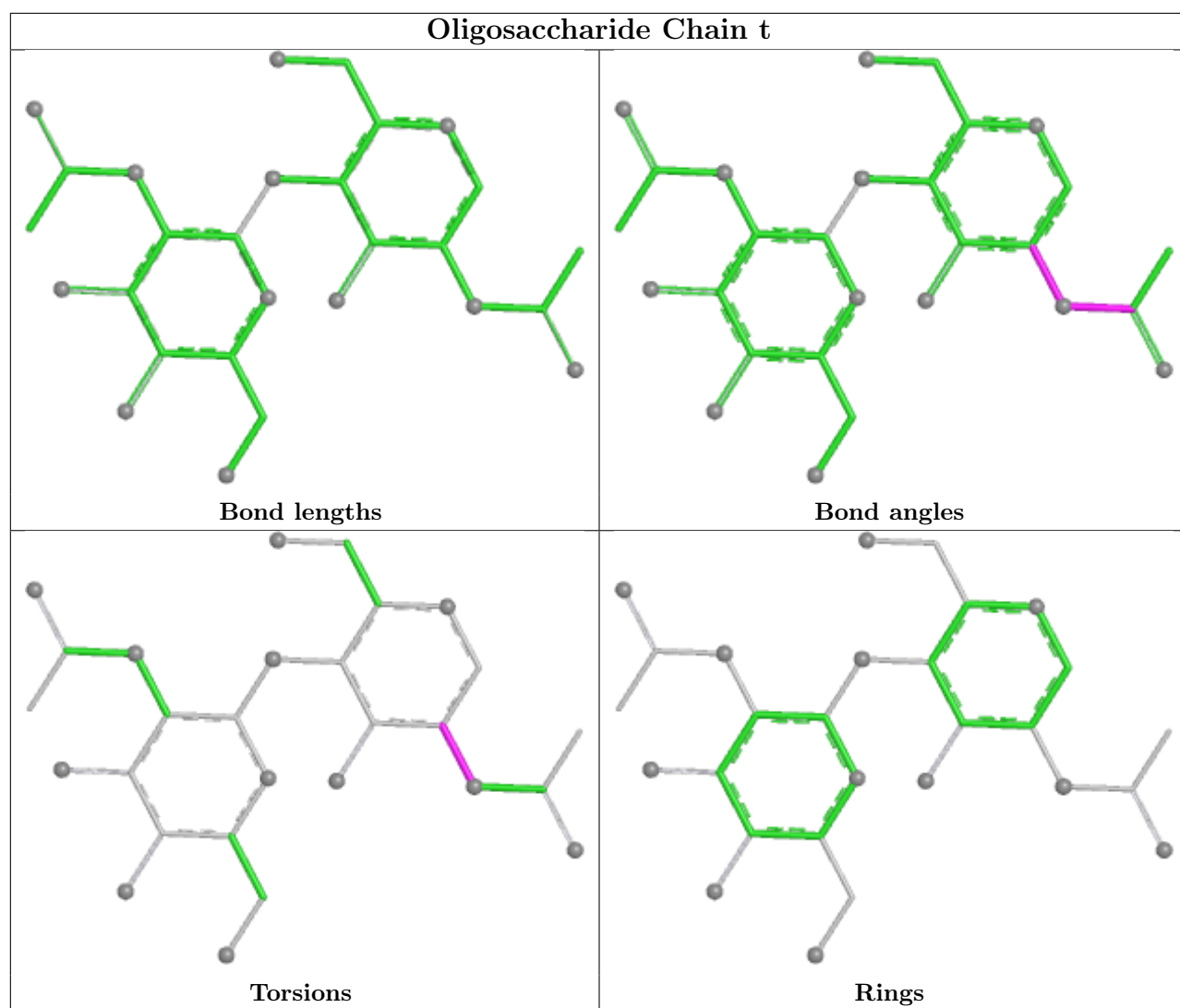


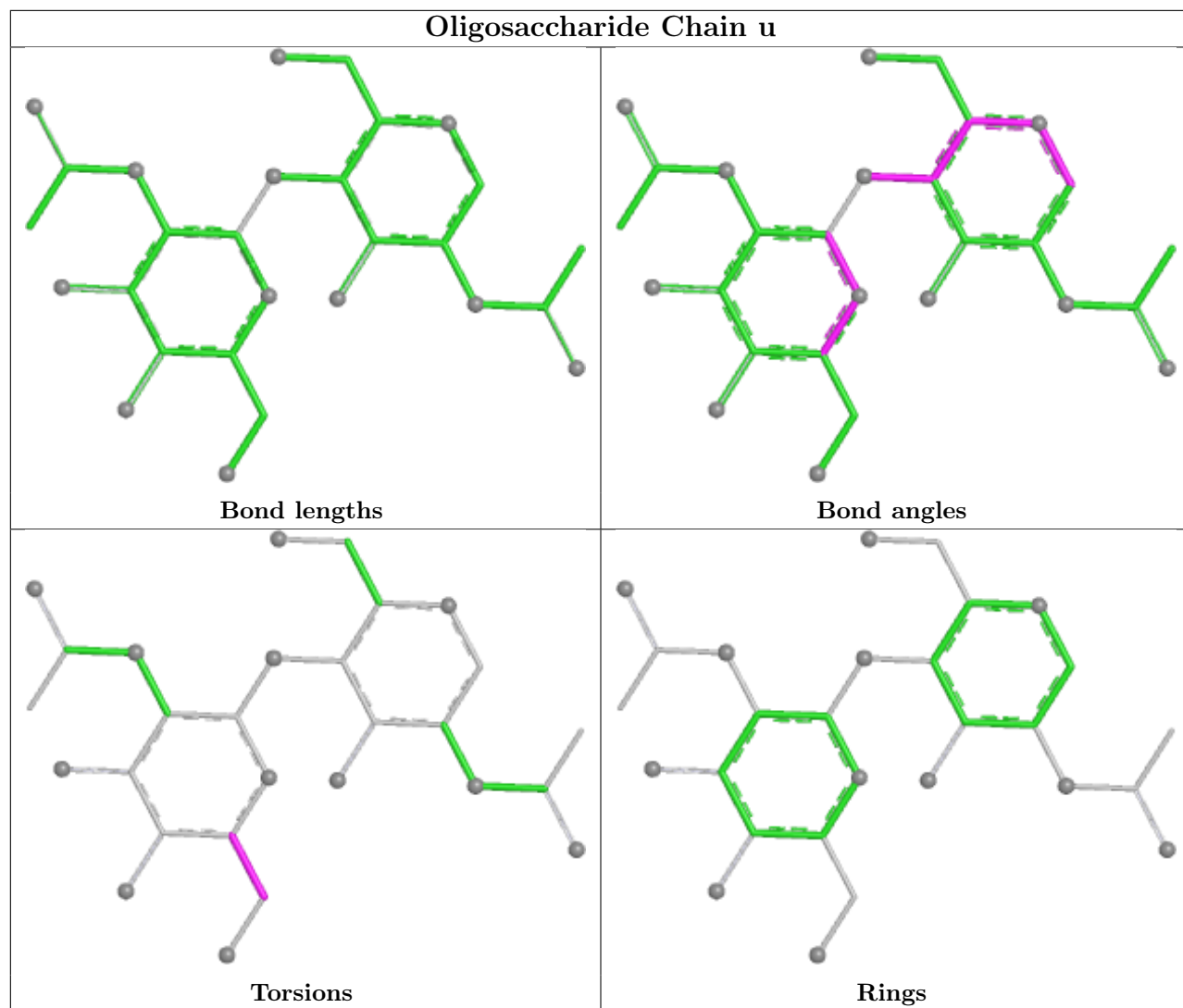


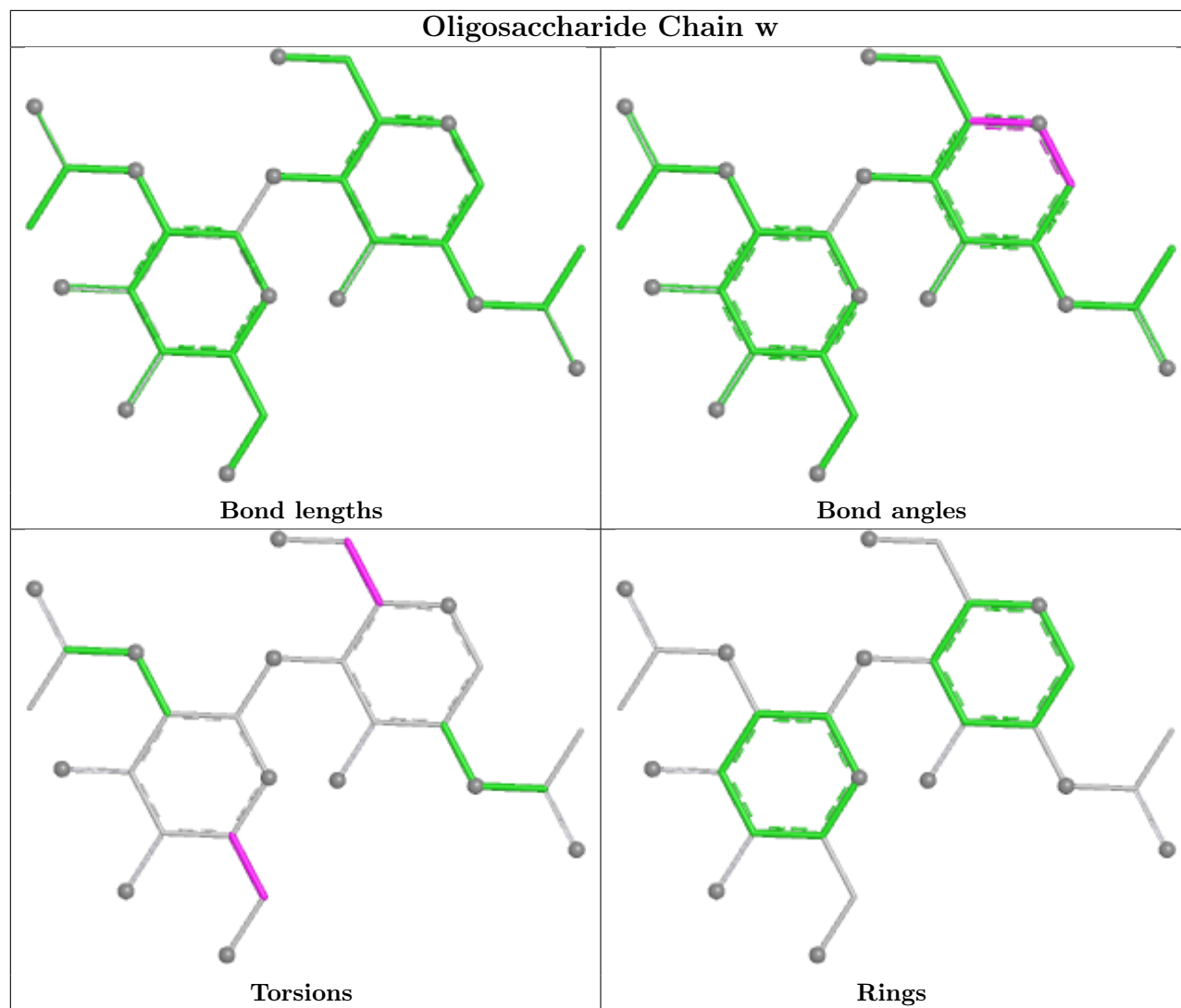


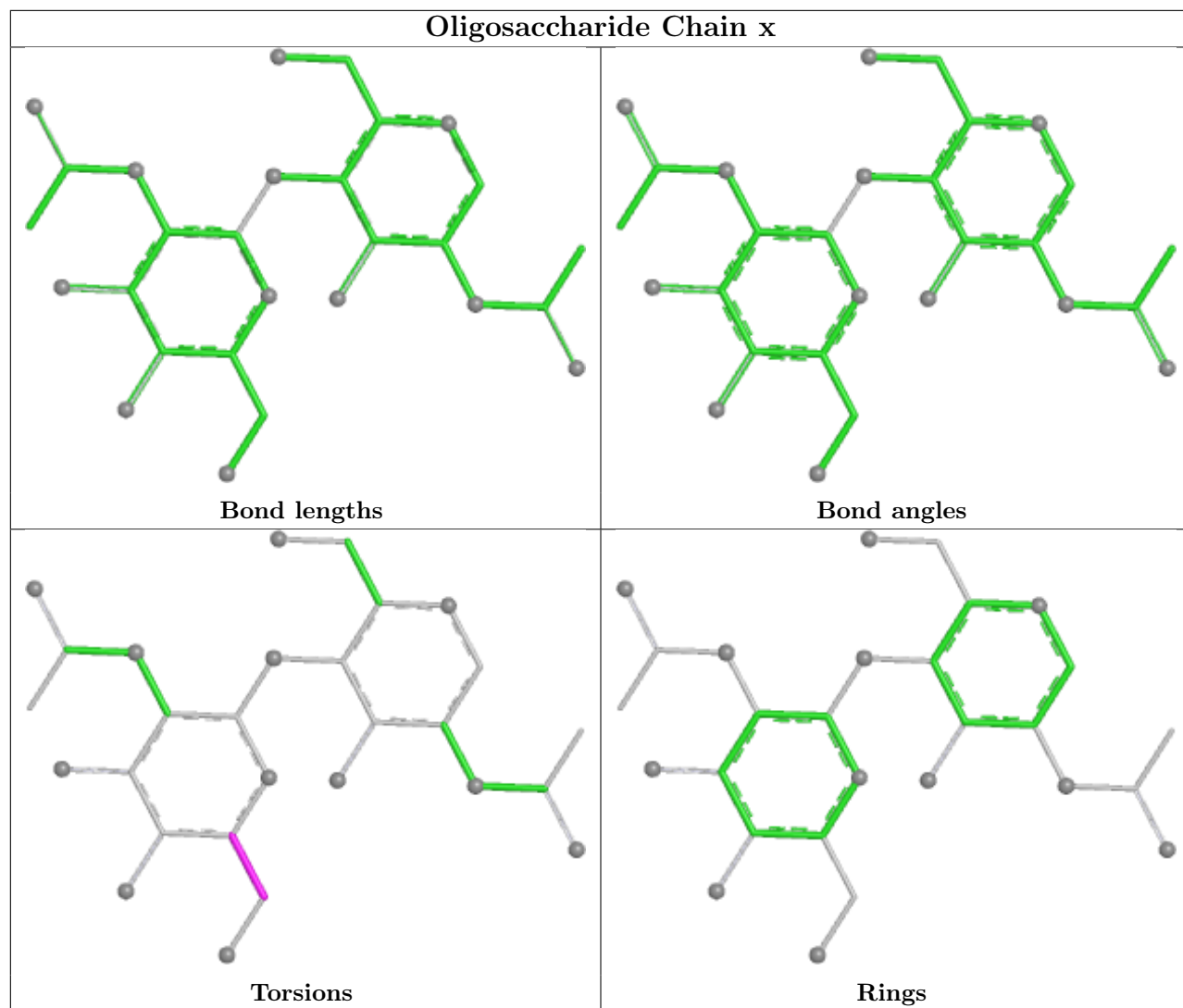


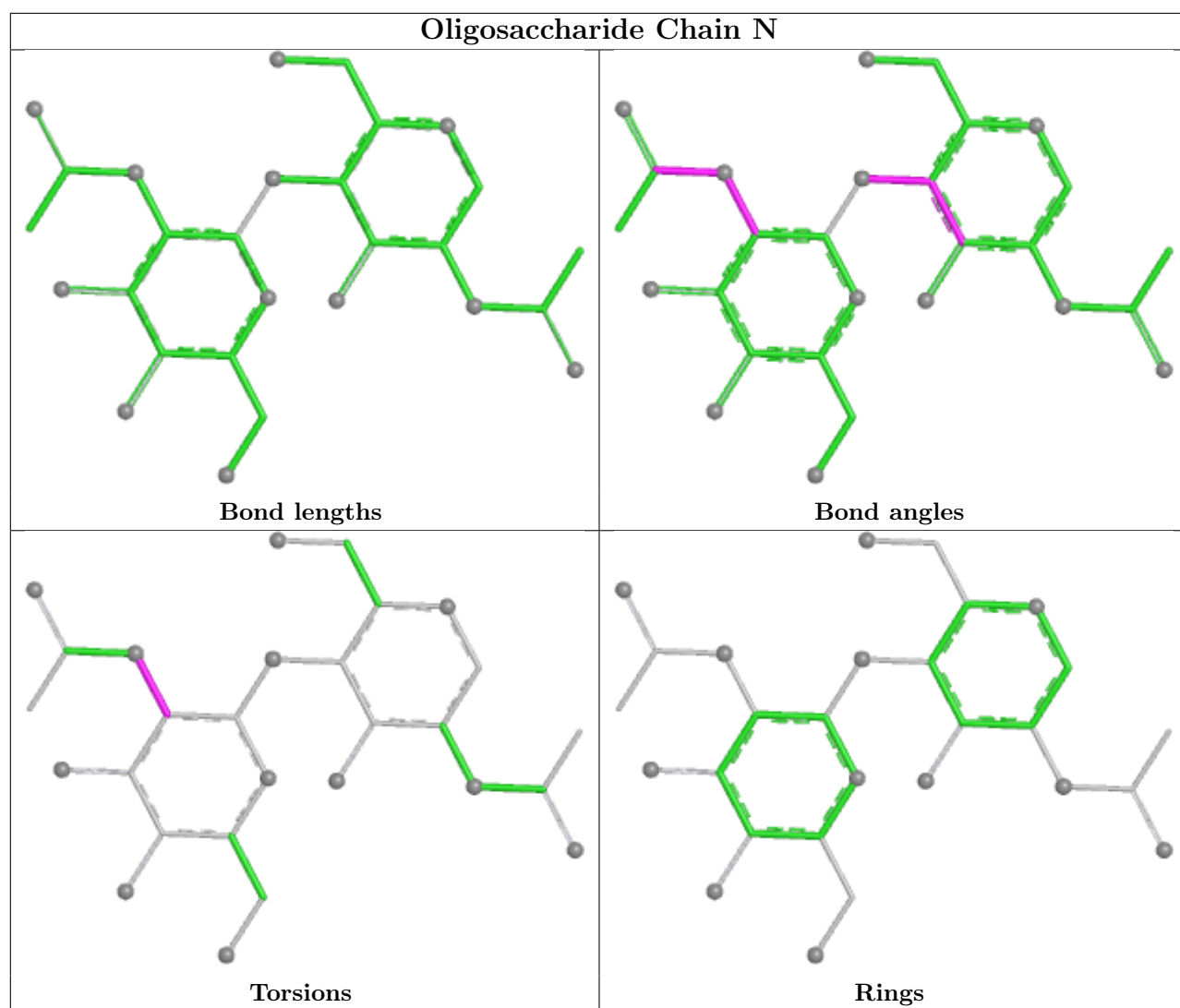


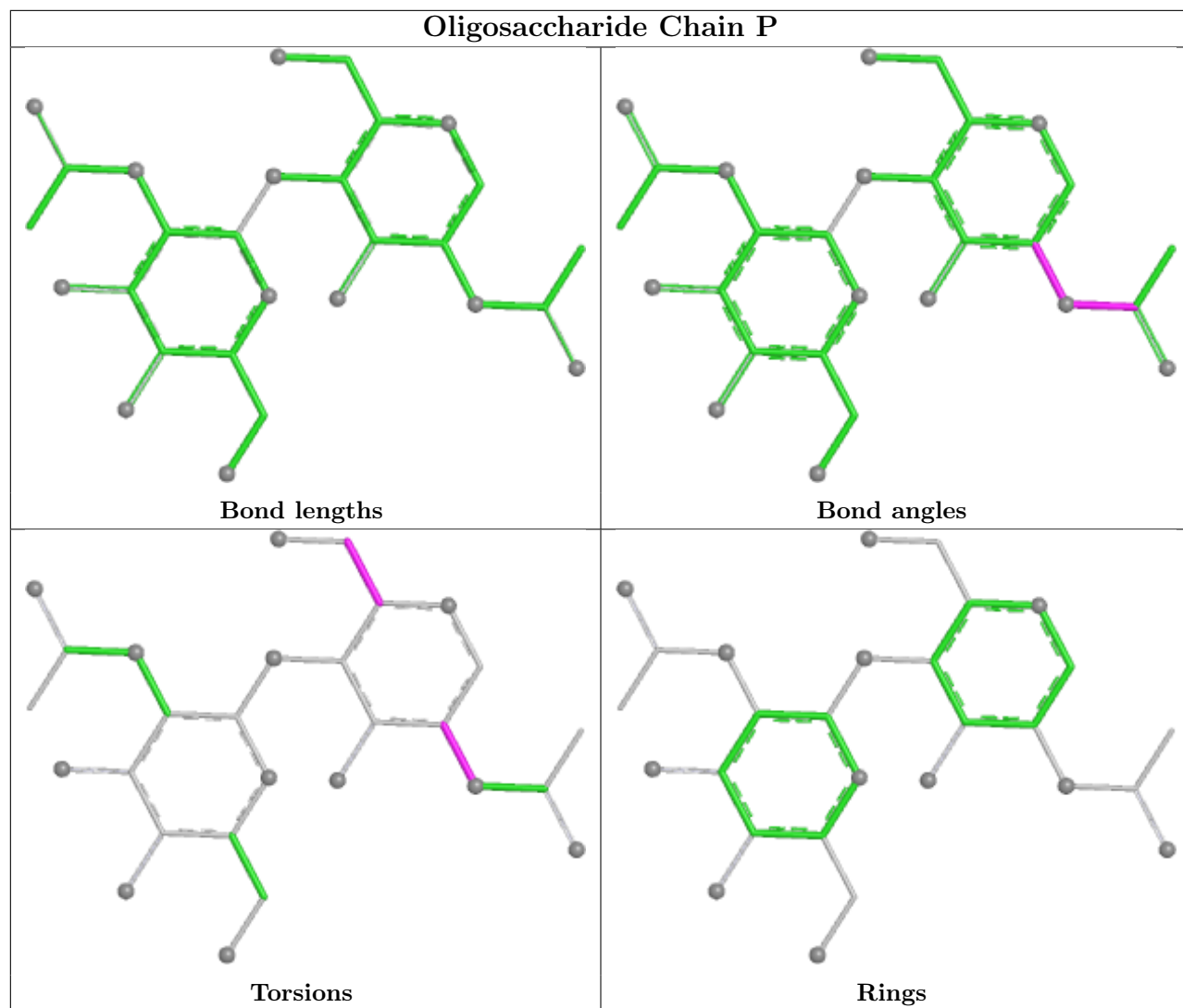


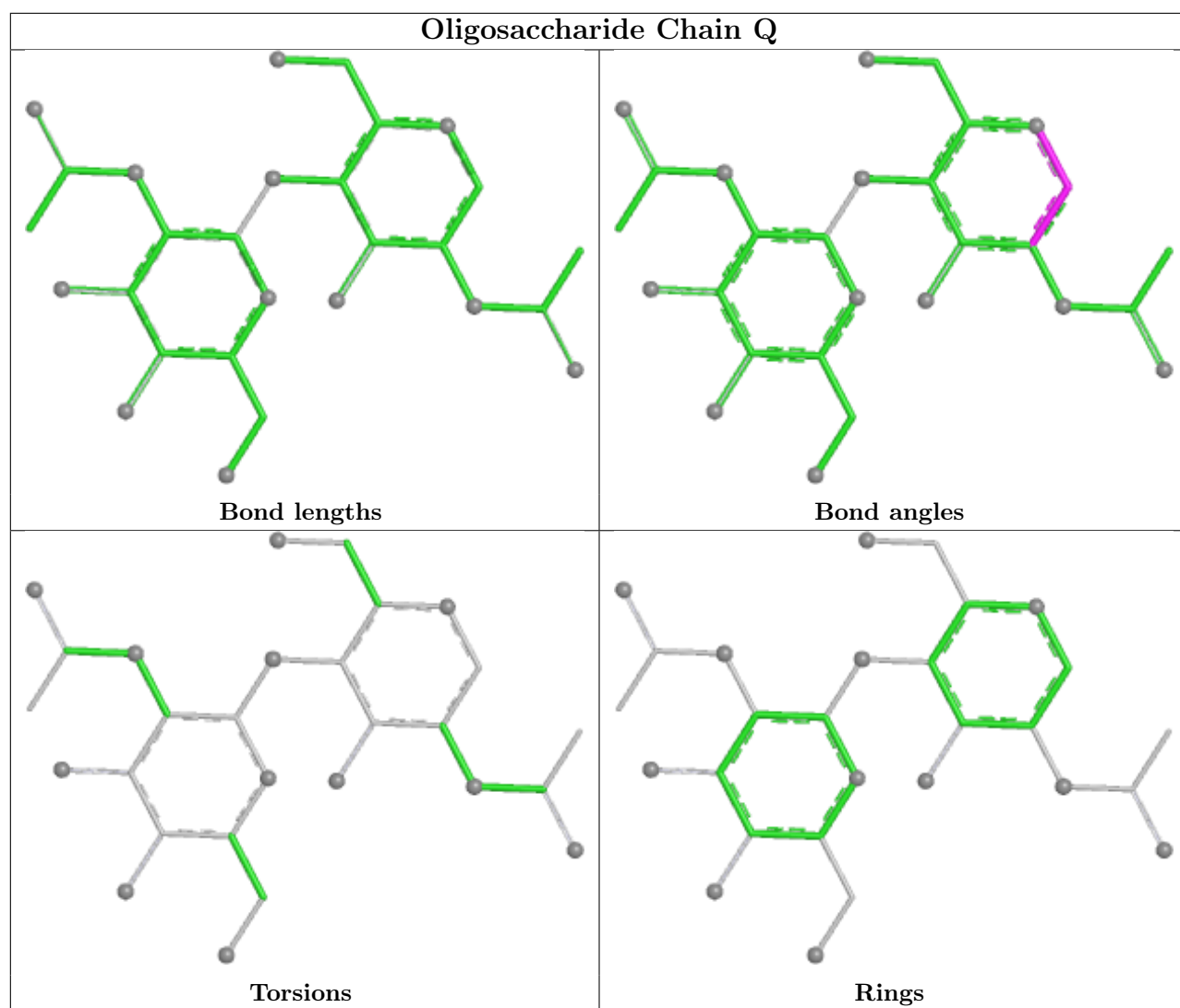


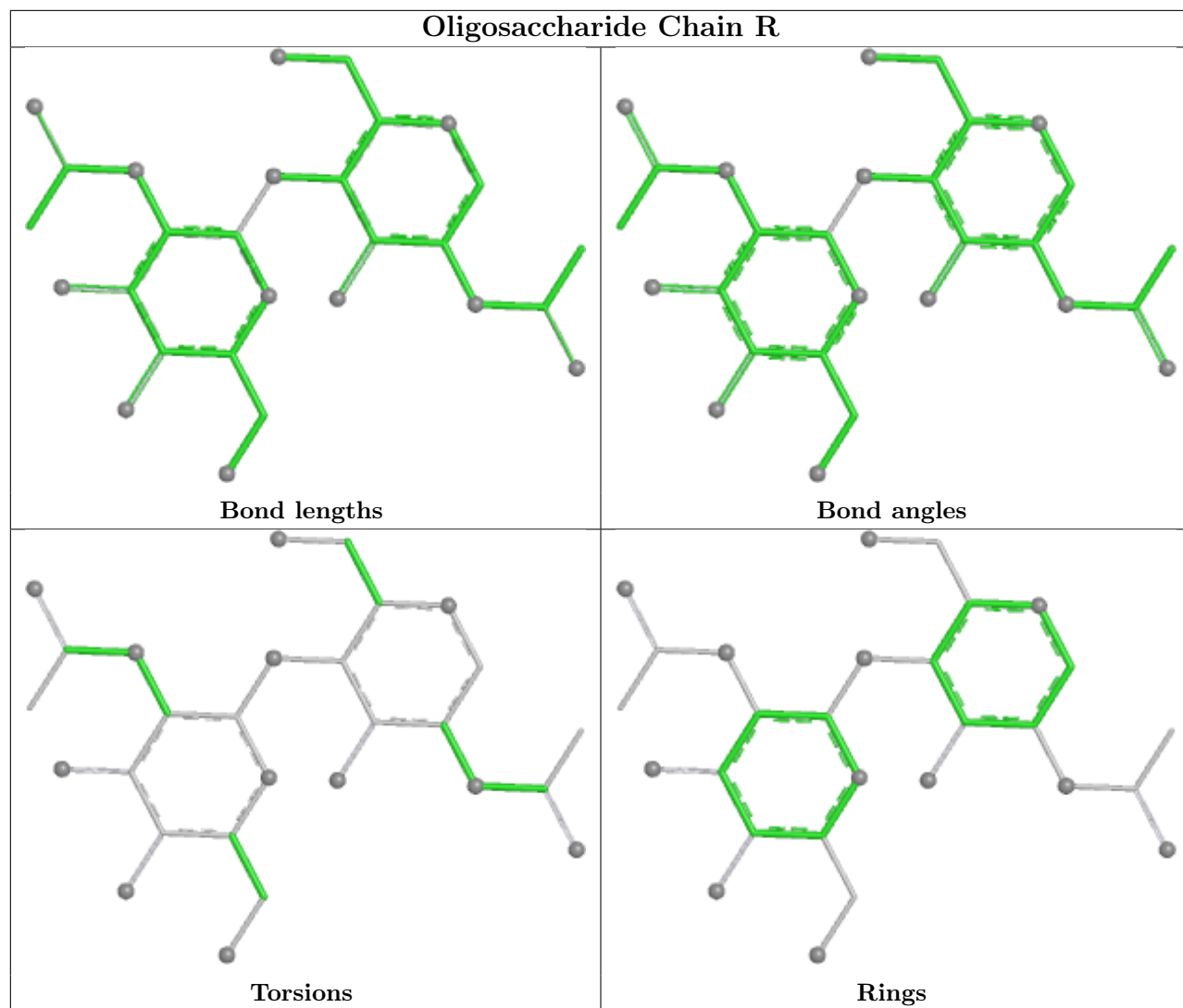


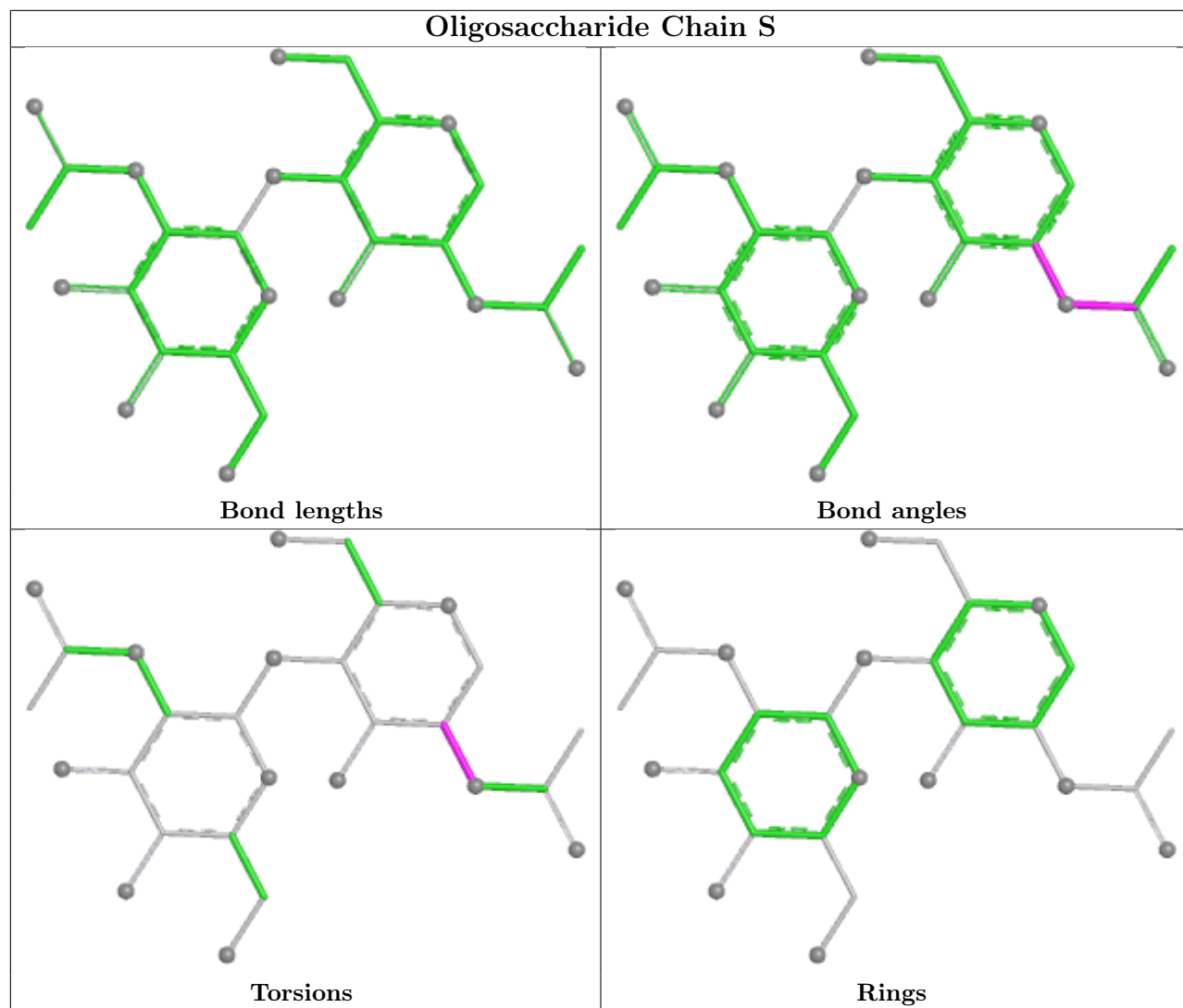


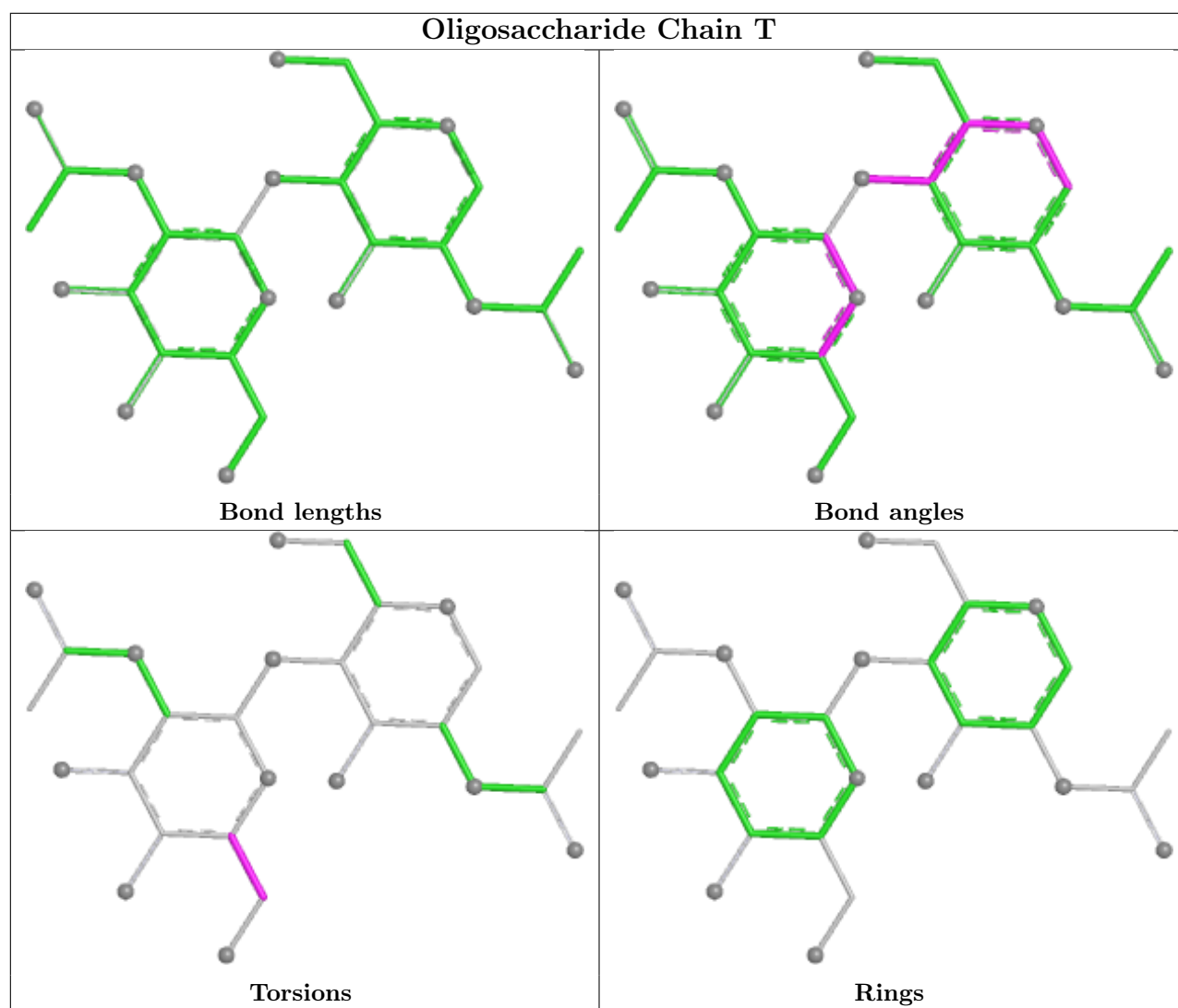


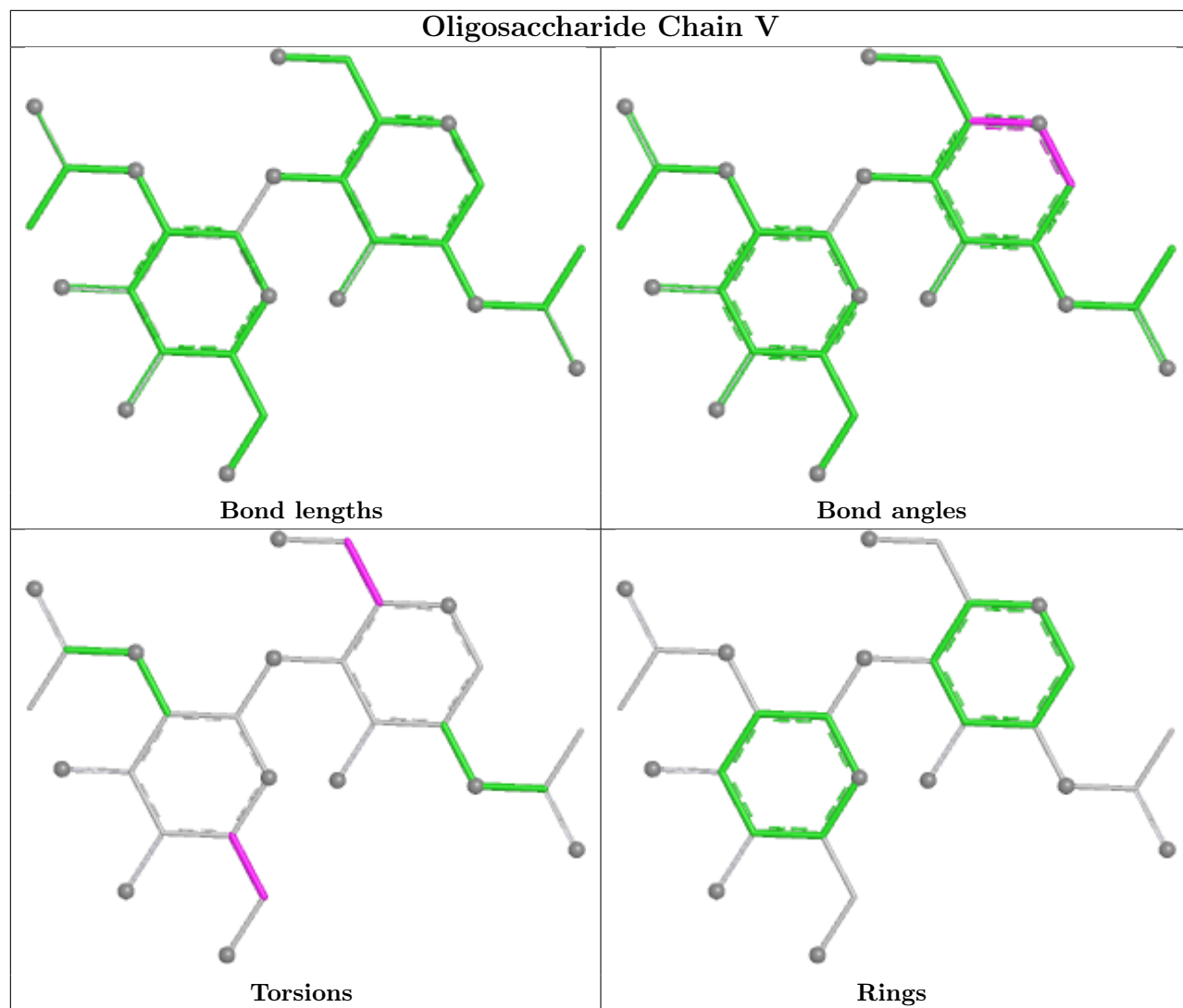


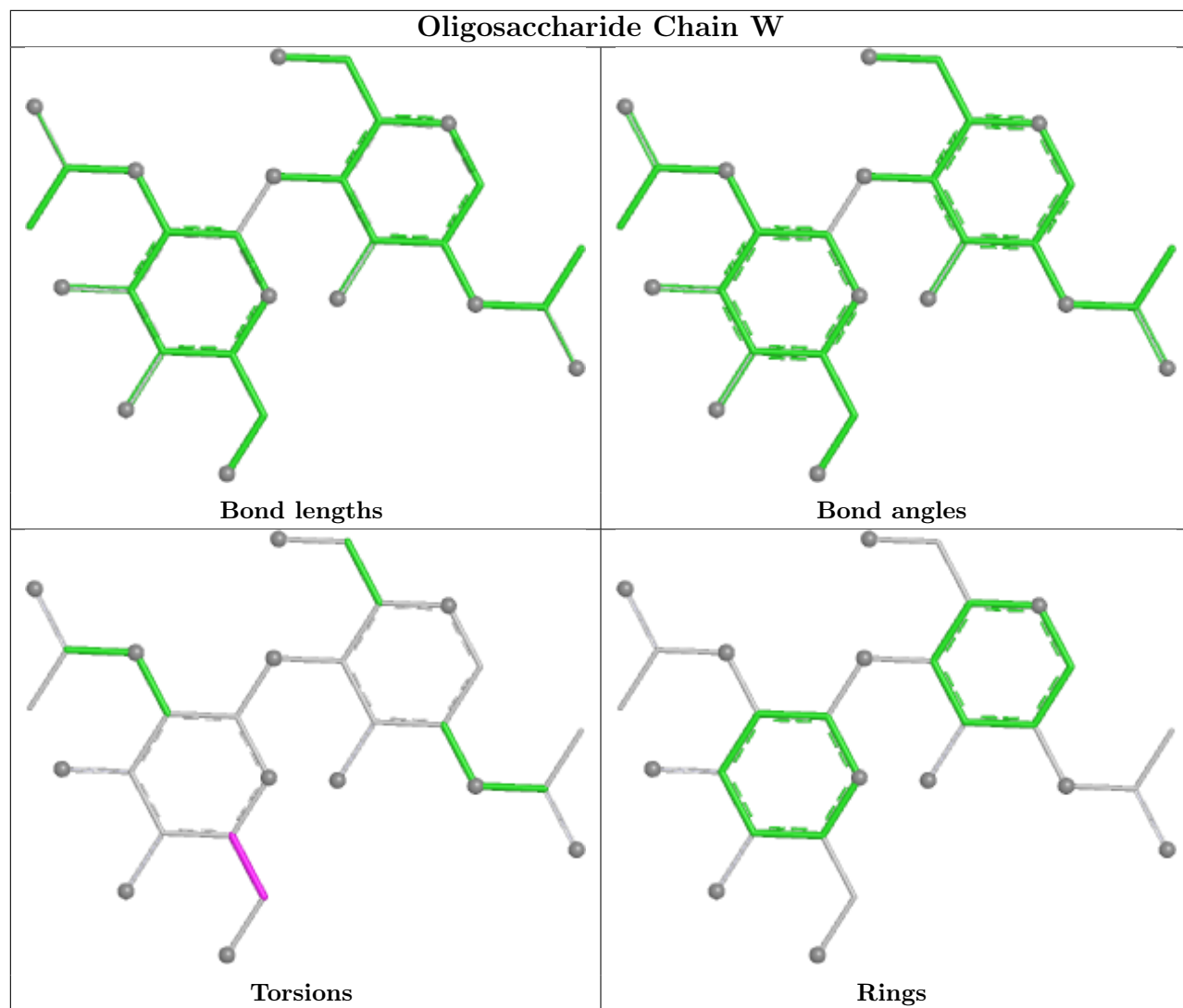


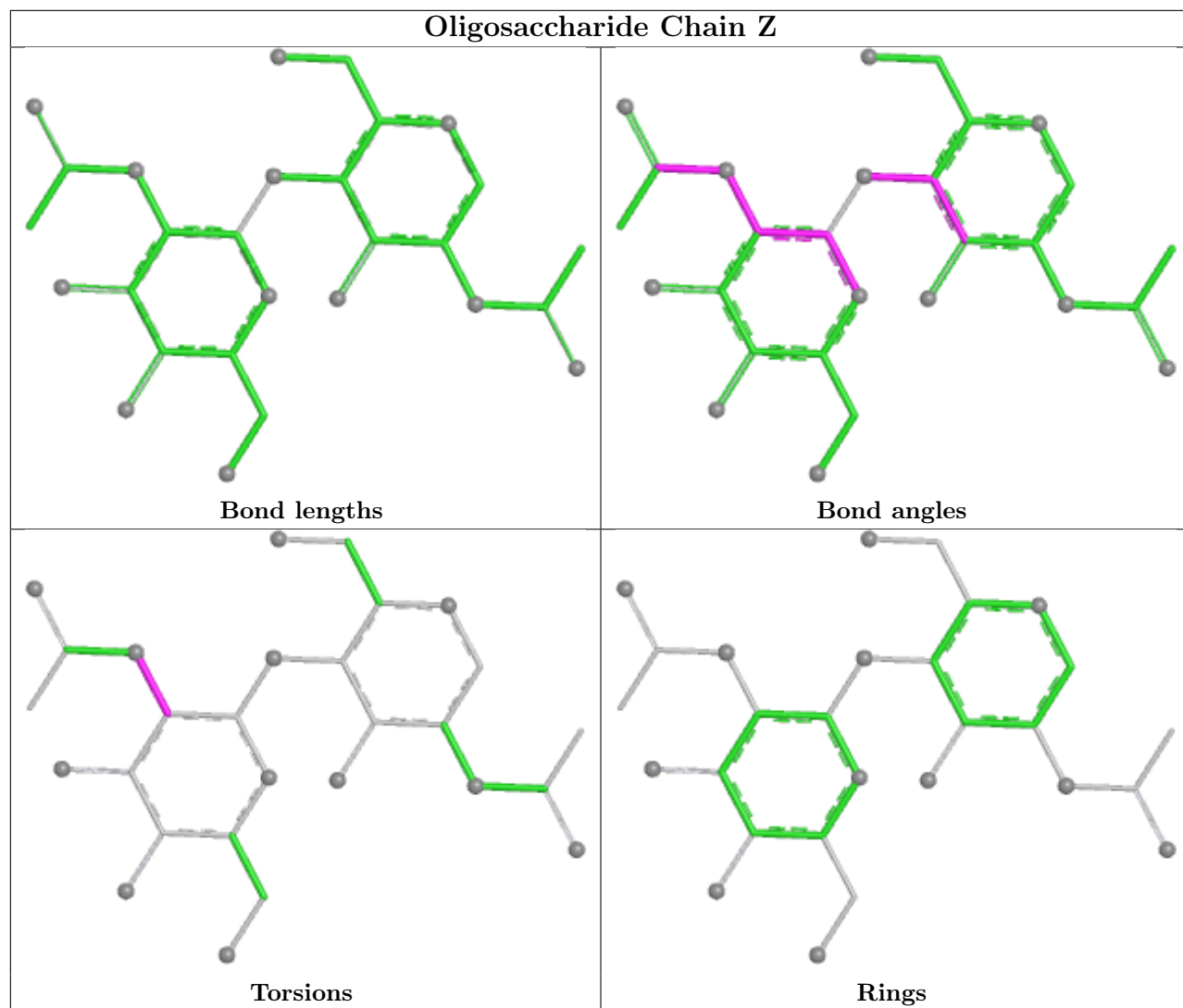


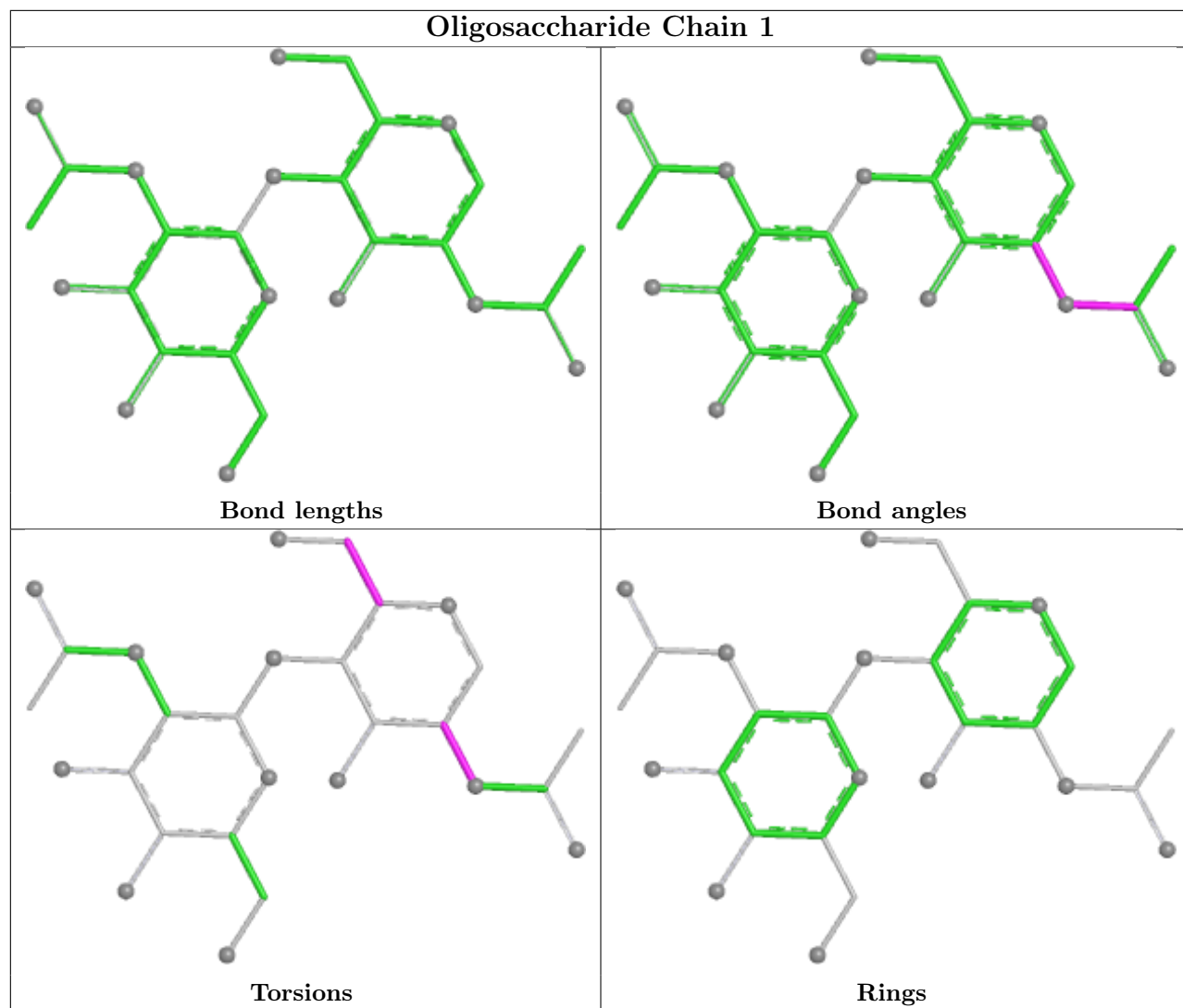


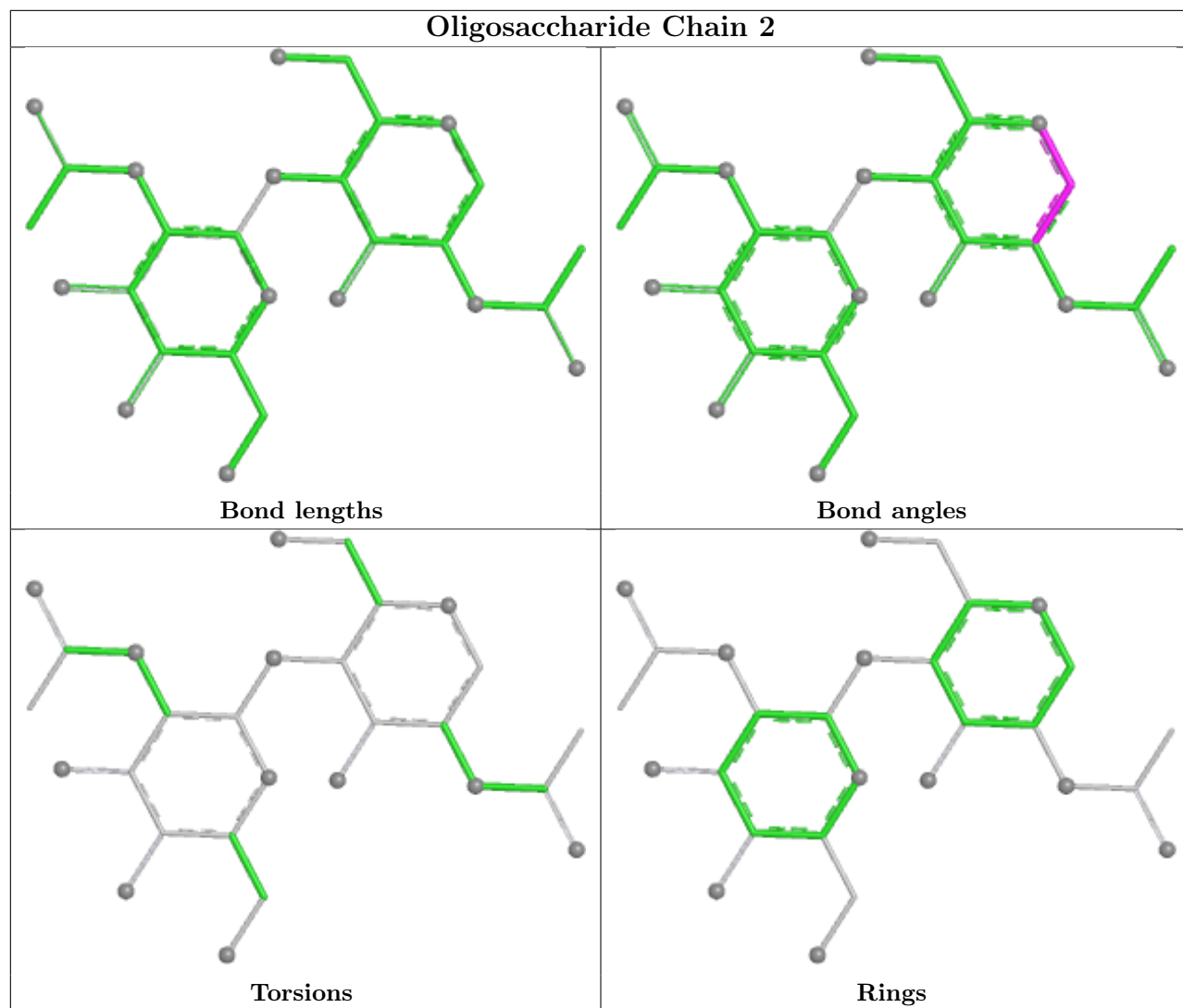


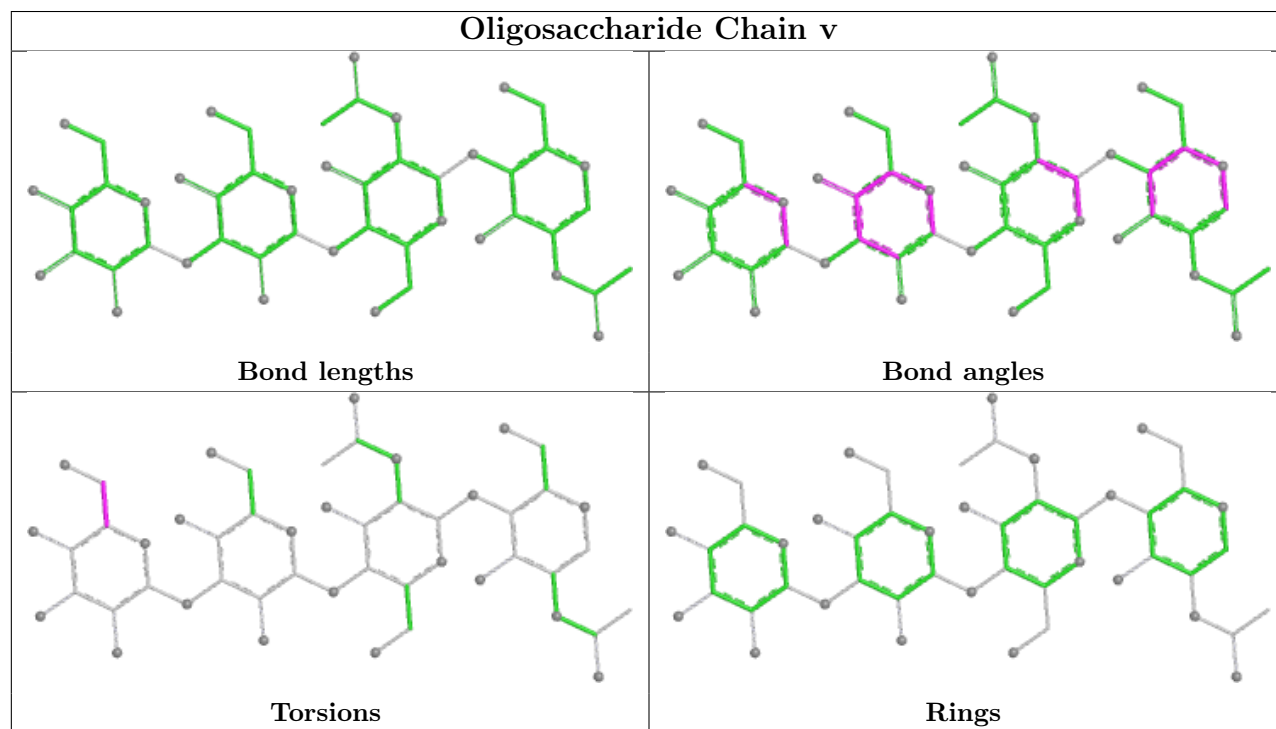
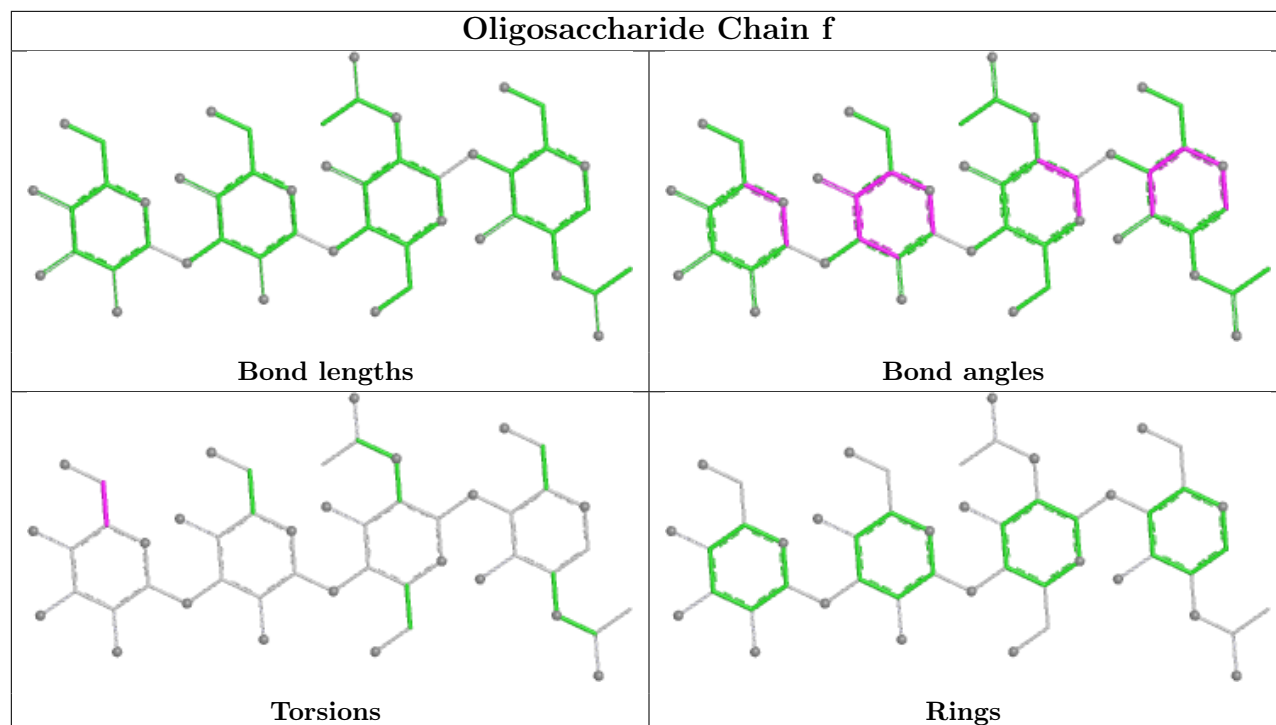


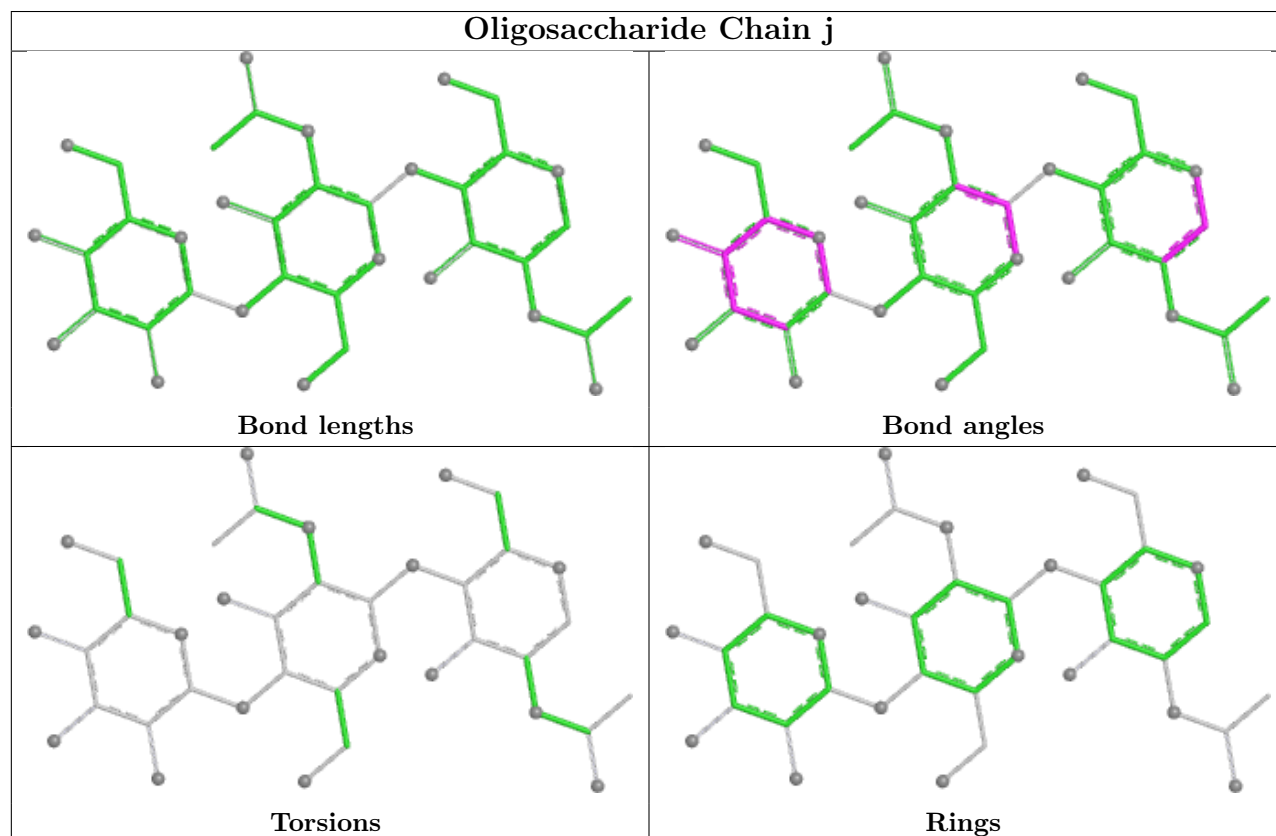
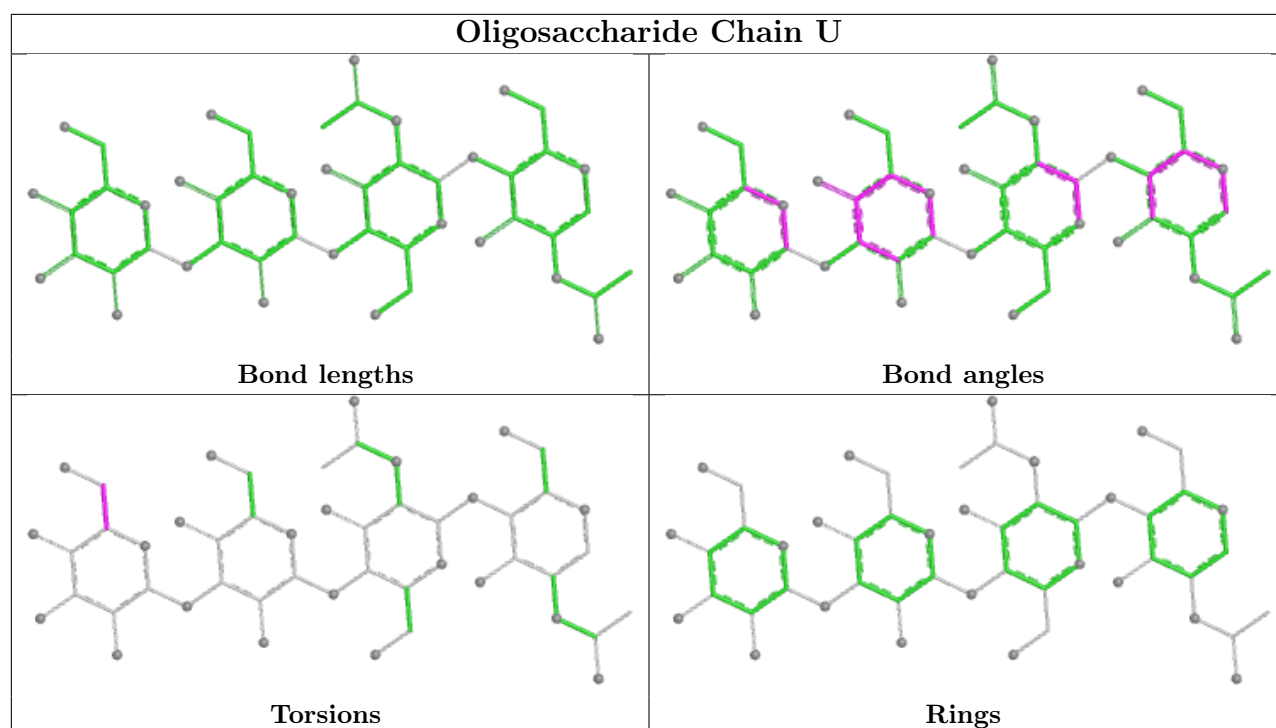


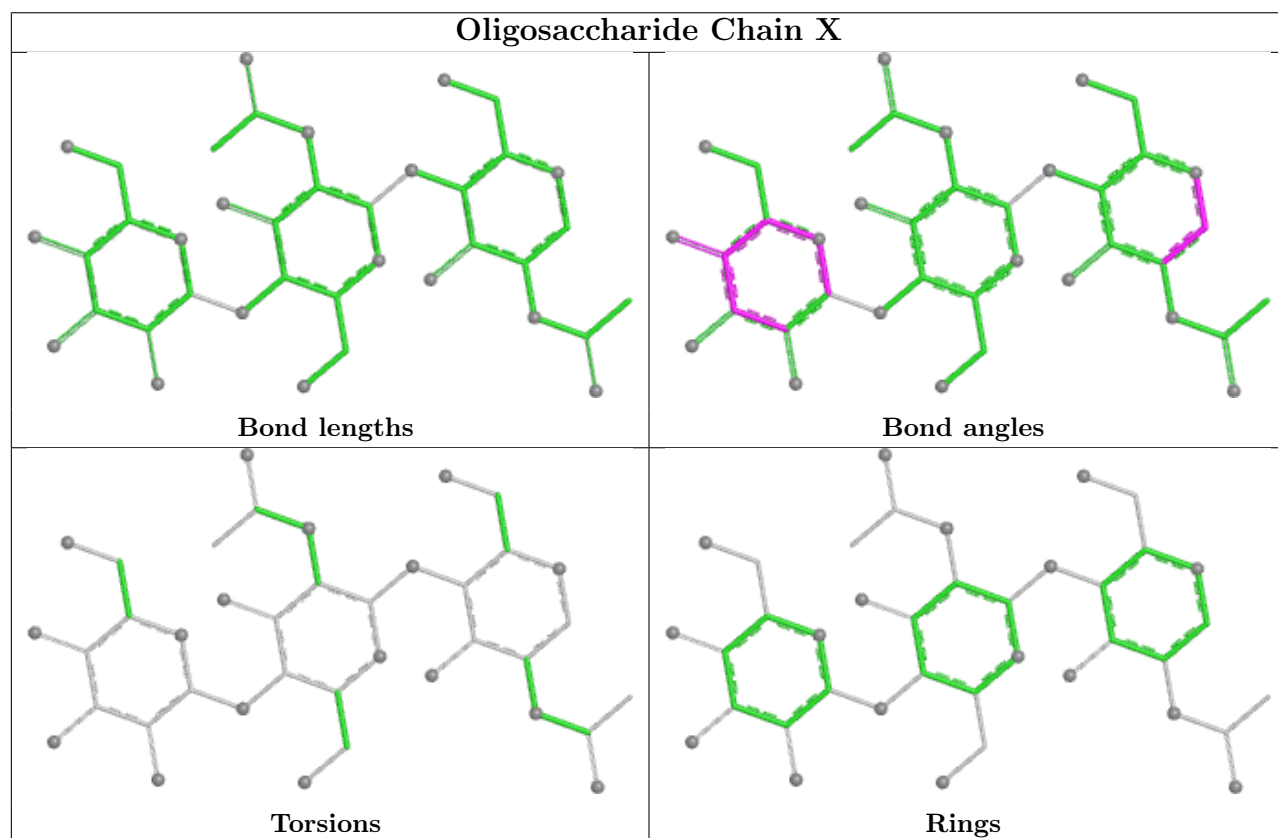
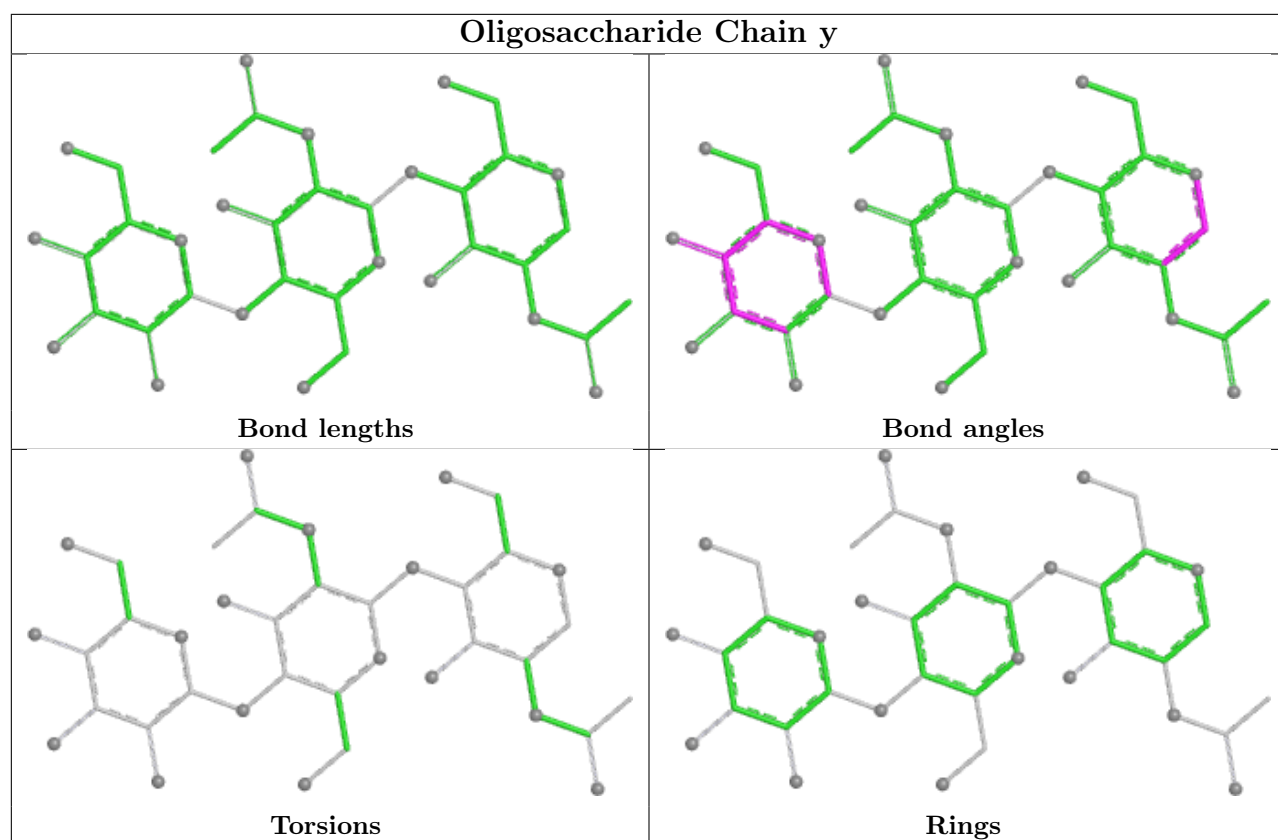


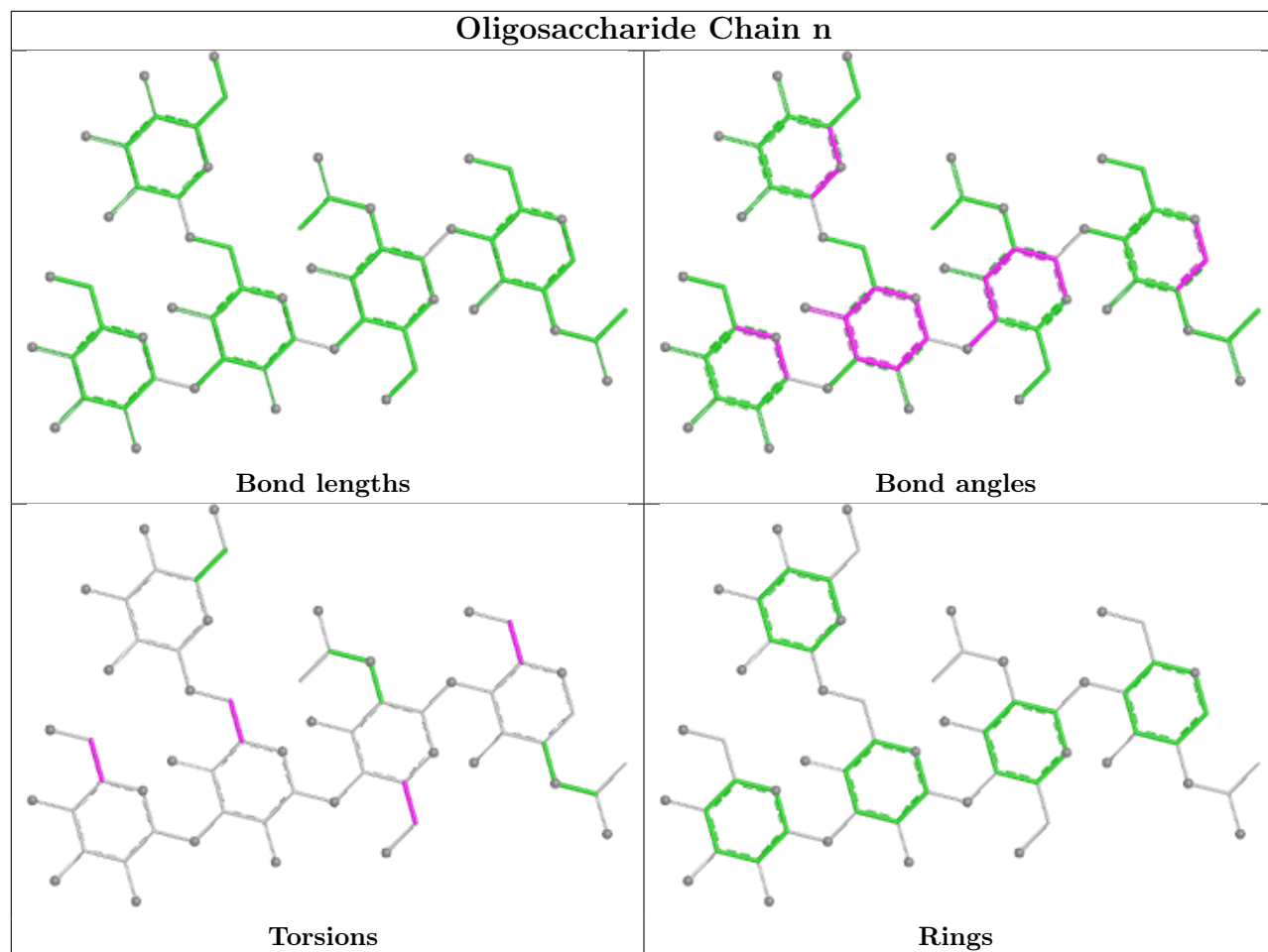


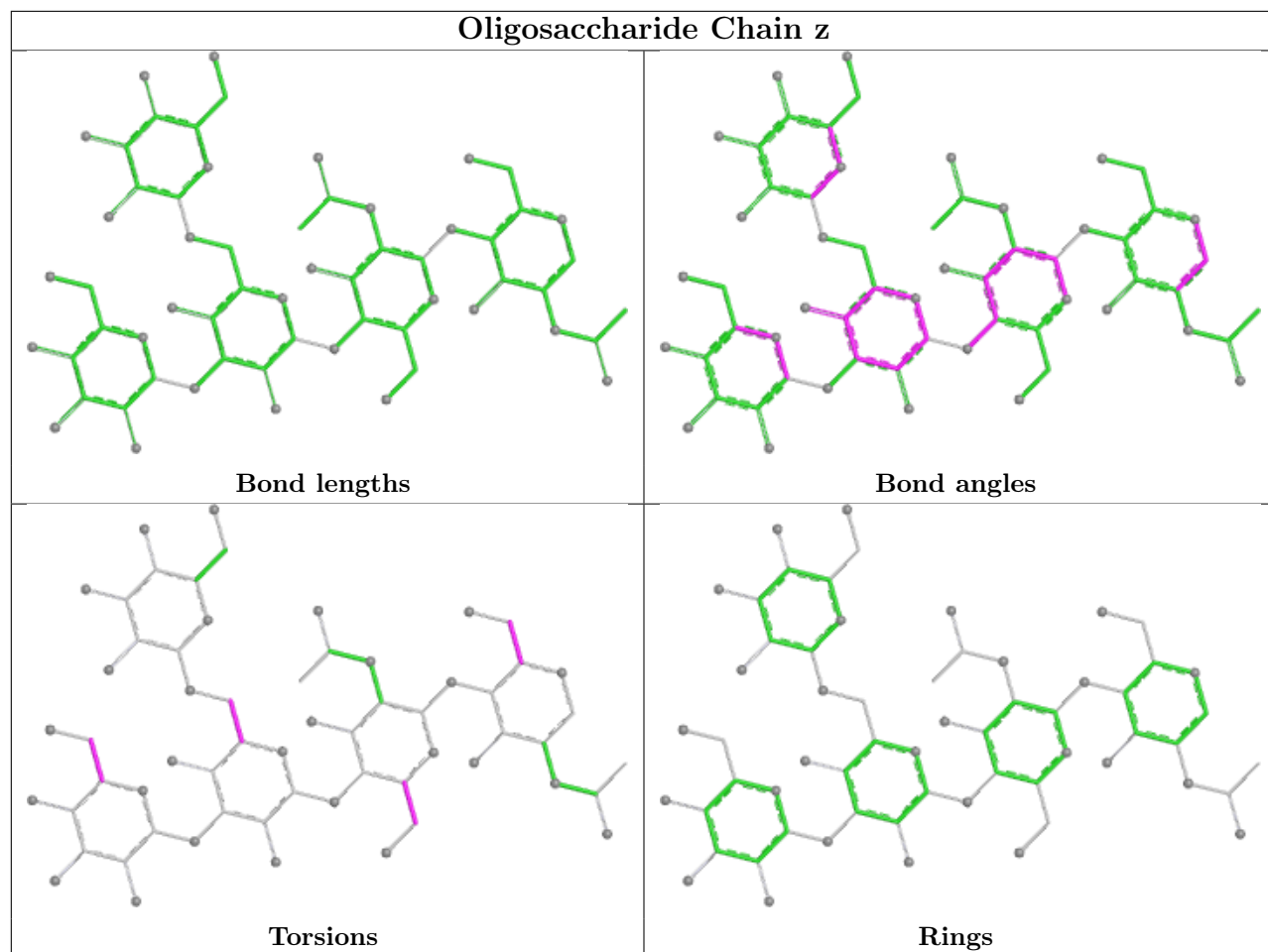


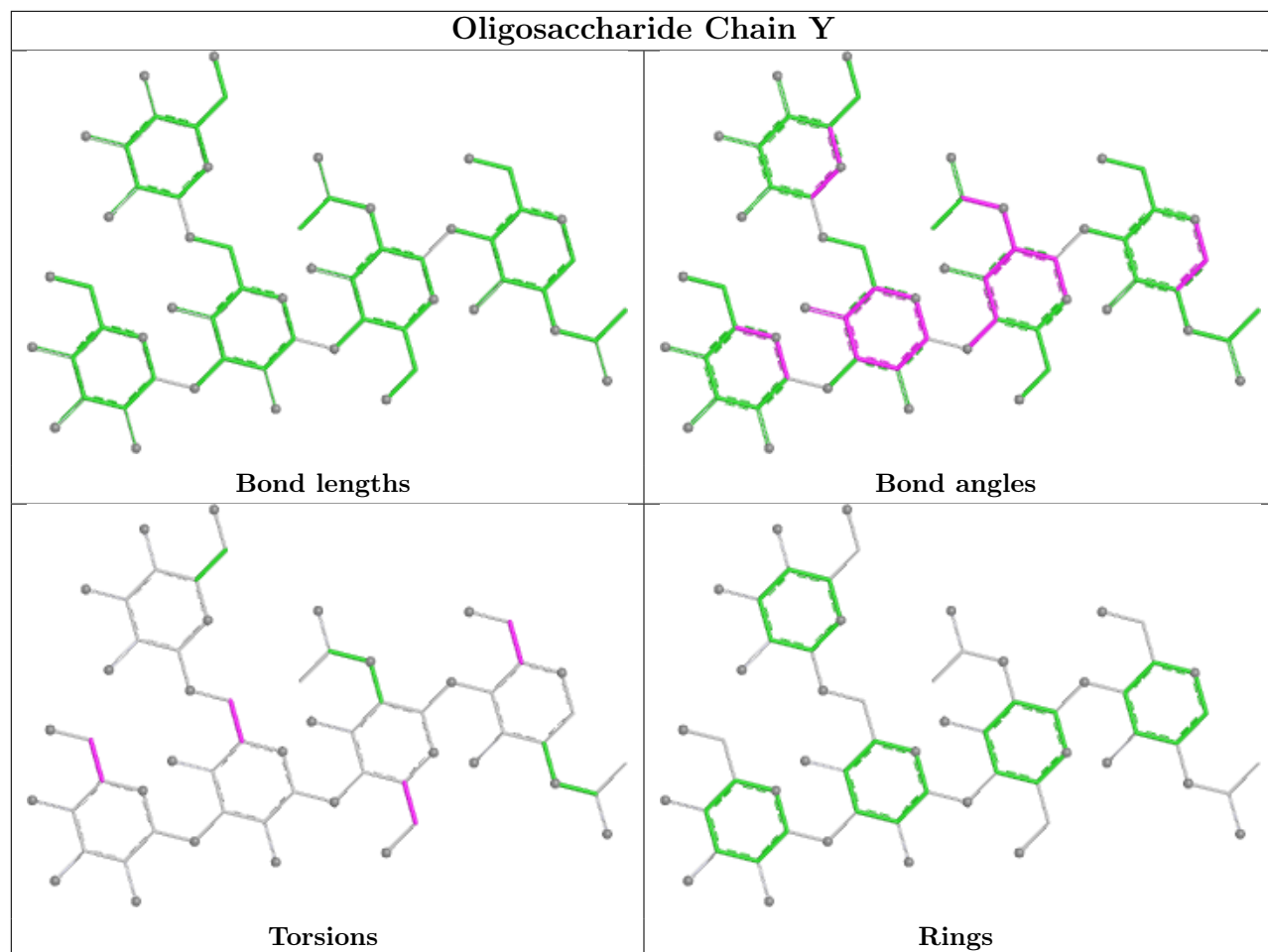


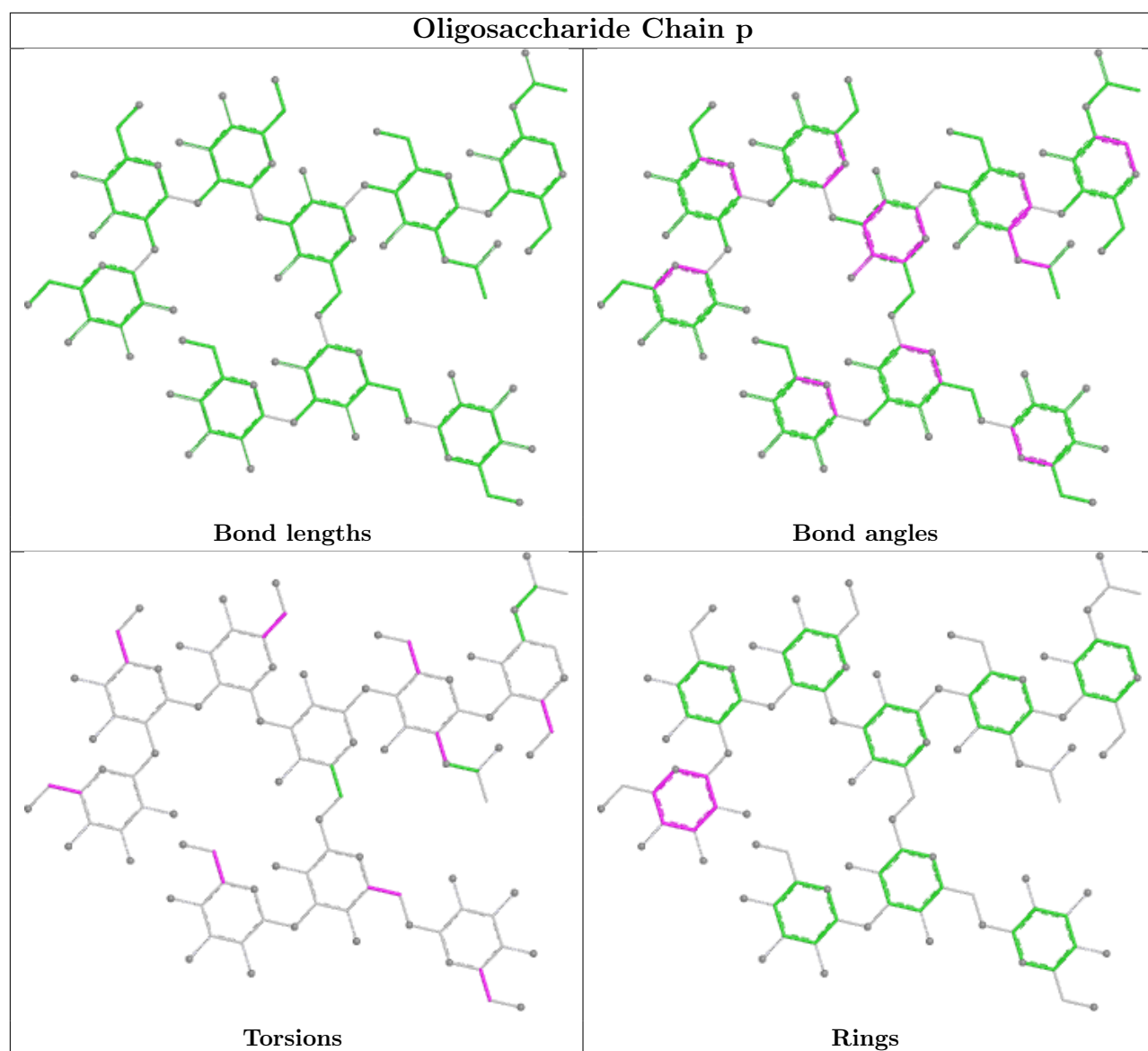


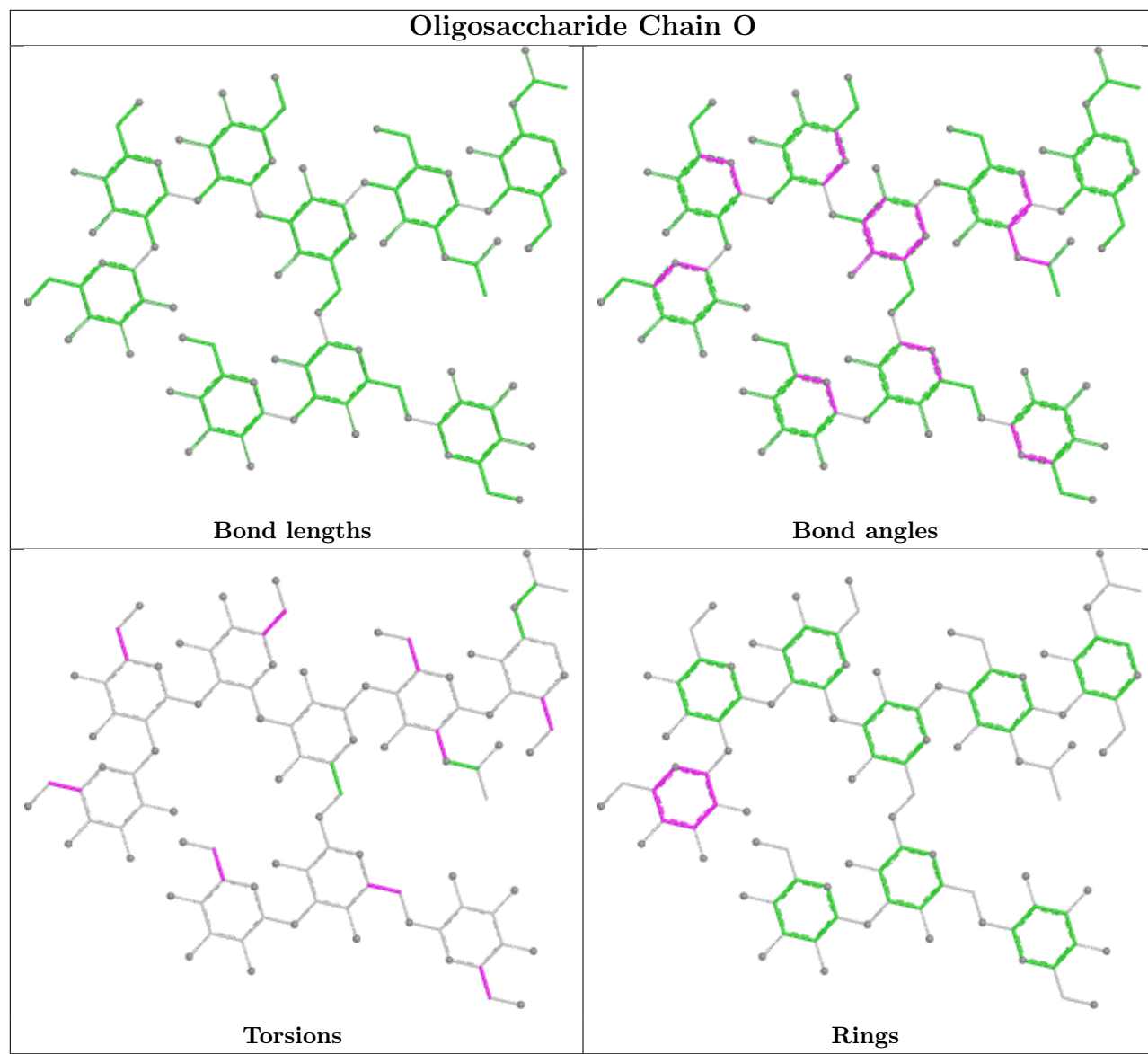


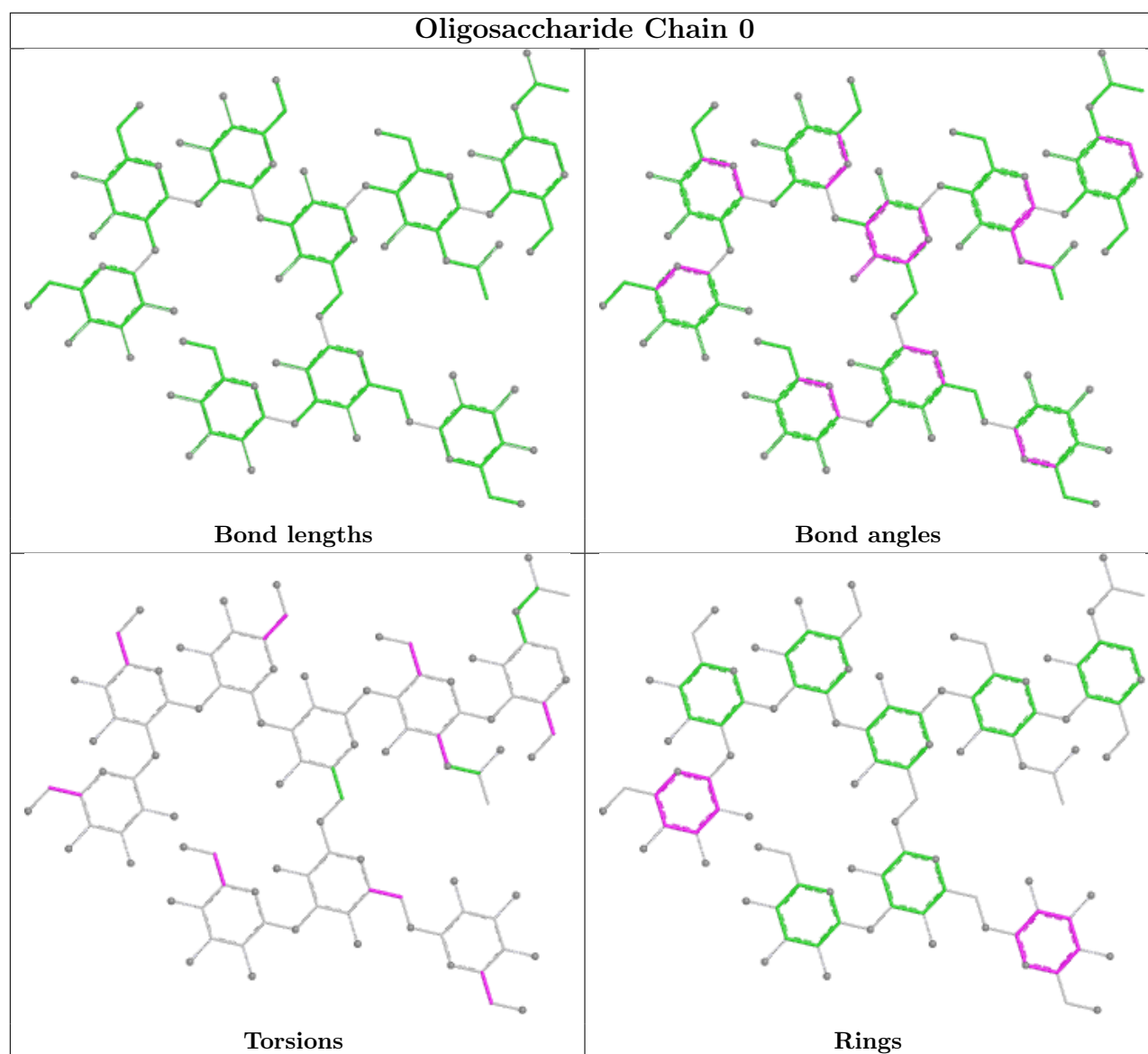












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
12	NAG	A	607	1	14,14,15	0.74	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	C	701	2	14,14,15	0.70	0	17,19,21	0.80	0
12	NAG	I	606	1	14,14,15	0.67	0	17,19,21	0.99	1 (5%)
12	NAG	I	602	1	14,14,15	0.74	0	17,19,21	0.84	0
12	NAG	I	607	1	14,14,15	0.74	0	17,19,21	0.82	0
12	NAG	A	605	1	14,14,15	0.69	0	17,19,21	0.80	0
12	NAG	I	605	1	14,14,15	0.70	0	17,19,21	0.79	0
12	NAG	G	607	1	14,14,15	0.72	0	17,19,21	0.78	0
12	NAG	G	606	1	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
12	NAG	G	602	1	14,14,15	0.74	0	17,19,21	0.83	0
12	NAG	G	604	1	14,14,15	0.73	0	17,19,21	1.04	1 (5%)
12	NAG	A	606	1	14,14,15	0.68	0	17,19,21	1.00	1 (5%)
12	NAG	J	701	2	14,14,15	0.70	0	17,19,21	0.81	0
12	NAG	A	601	1	14,14,15	0.70	0	17,19,21	0.83	0
12	NAG	A	603	1	14,14,15	0.73	0	17,19,21	1.41	2 (11%)
12	NAG	G	601	1	14,14,15	0.71	0	17,19,21	0.83	0
12	NAG	I	604	1	14,14,15	0.68	0	17,19,21	0.97	1 (5%)
12	NAG	B	701	2	14,14,15	0.70	0	17,19,21	0.80	0
12	NAG	I	601	1	14,14,15	0.71	0	17,19,21	0.82	0
12	NAG	G	605	1	14,14,15	0.70	0	17,19,21	0.81	0
12	NAG	G	603	1	14,14,15	0.72	0	17,19,21	1.43	2 (11%)
12	NAG	I	603	1	14,14,15	0.71	0	17,19,21	1.40	2 (11%)
12	NAG	A	602	1	14,14,15	0.72	0	17,19,21	0.80	0
12	NAG	A	604	1	14,14,15	0.69	0	17,19,21	0.92	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
12	NAG	A	607	1	-	1/6/23/26	0/1/1/1
12	NAG	C	701	2	-	0/6/23/26	0/1/1/1
12	NAG	I	606	1	-	0/6/23/26	0/1/1/1
12	NAG	I	602	1	-	1/6/23/26	0/1/1/1
12	NAG	I	607	1	-	1/6/23/26	0/1/1/1
12	NAG	A	605	1	-	0/6/23/26	0/1/1/1
12	NAG	I	605	1	-	0/6/23/26	0/1/1/1
12	NAG	G	607	1	-	1/6/23/26	0/1/1/1
12	NAG	G	606	1	-	0/6/23/26	0/1/1/1
12	NAG	G	602	1	-	1/6/23/26	0/1/1/1
12	NAG	G	604	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	606	1	-	0/6/23/26	0/1/1/1
12	NAG	J	701	2	-	0/6/23/26	0/1/1/1
12	NAG	A	601	1	-	1/6/23/26	0/1/1/1
12	NAG	A	603	1	-	1/6/23/26	0/1/1/1
12	NAG	G	601	1	-	1/6/23/26	0/1/1/1
12	NAG	I	604	1	-	1/6/23/26	0/1/1/1
12	NAG	B	701	2	-	0/6/23/26	0/1/1/1
12	NAG	I	601	1	-	1/6/23/26	0/1/1/1
12	NAG	G	605	1	-	0/6/23/26	0/1/1/1
12	NAG	G	603	1	-	1/6/23/26	0/1/1/1
12	NAG	I	603	1	-	1/6/23/26	0/1/1/1
12	NAG	A	602	1	-	1/6/23/26	0/1/1/1
12	NAG	A	604	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	603	NAG	C2-N2-C7	3.71	127.87	122.90
12	I	603	NAG	C2-N2-C7	3.71	127.87	122.90
12	G	603	NAG	C2-N2-C7	3.70	127.85	122.90
12	G	604	NAG	C1-O5-C5	2.90	116.08	112.19
12	G	603	NAG	C1-O5-C5	2.84	115.99	112.19
12	I	604	NAG	O5-C1-C2	-2.84	106.90	111.29
12	A	606	NAG	C1-O5-C5	2.77	115.89	112.19
12	A	603	NAG	C1-O5-C5	2.76	115.89	112.19
12	I	606	NAG	C1-O5-C5	2.70	115.80	112.19
12	G	606	NAG	C1-O5-C5	2.62	115.70	112.19
12	I	603	NAG	C1-O5-C5	2.57	115.63	112.19
12	A	604	NAG	O5-C1-C2	-2.21	107.87	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	607	NAG	O5-C5-C6-O6
12	G	601	NAG	O5-C5-C6-O6
12	A	601	NAG	O5-C5-C6-O6
12	A	607	NAG	O5-C5-C6-O6
12	I	601	NAG	O5-C5-C6-O6
12	I	607	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	G	602	NAG	O5-C5-C6-O6
12	A	602	NAG	O5-C5-C6-O6
12	I	602	NAG	O5-C5-C6-O6
12	I	604	NAG	C4-C5-C6-O6
12	G	603	NAG	C3-C2-N2-C7
12	A	603	NAG	C3-C2-N2-C7
12	I	603	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
12	I	606	NAG	1	0
12	G	606	NAG	1	0
12	A	606	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.

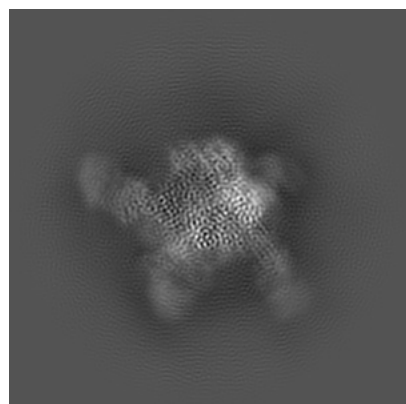
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72216. These allow visual inspection of the internal detail of the map and identification of artifacts.

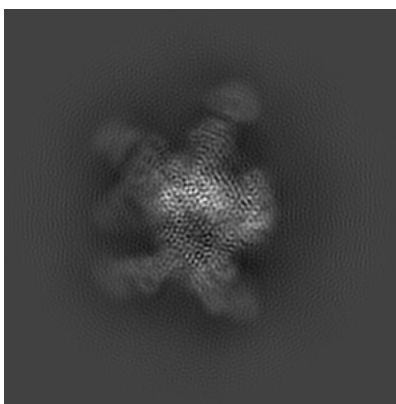
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

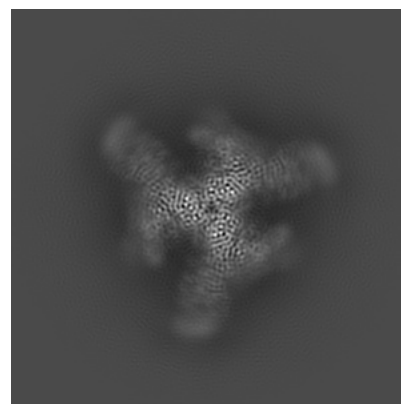
6.1.1 Primary map



X

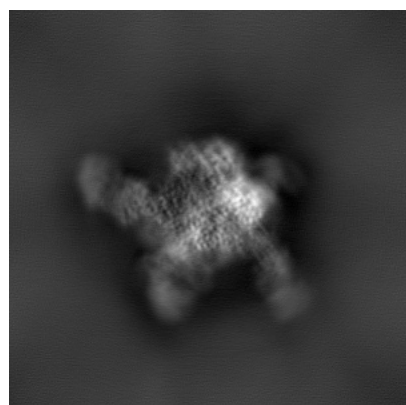


Y

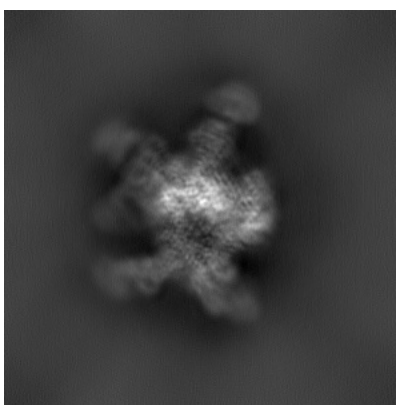


Z

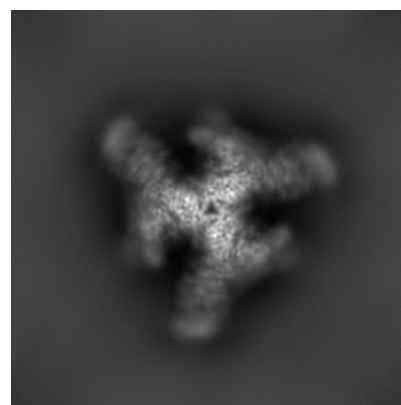
6.1.2 Raw map



X



Y

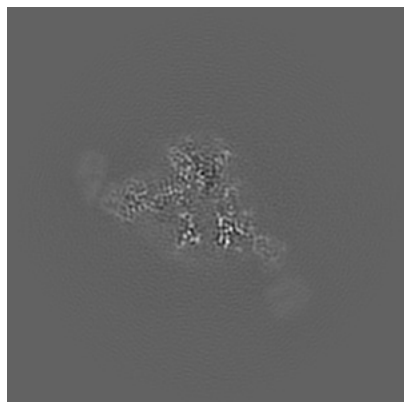


Z

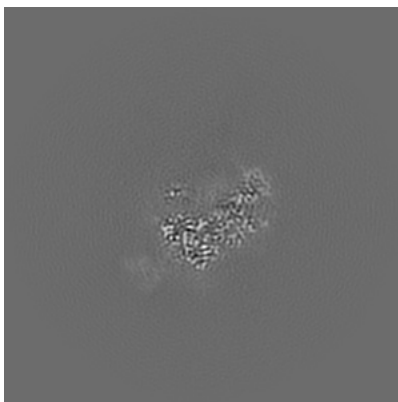
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

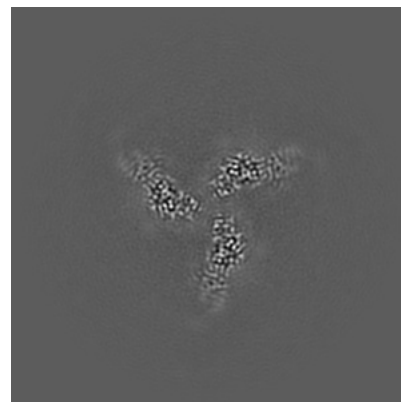
6.2.1 Primary map



X Index: 200

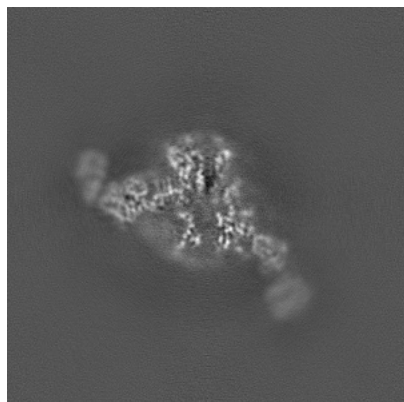


Y Index: 200

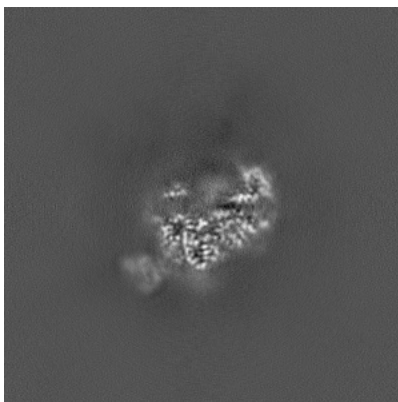


Z Index: 200

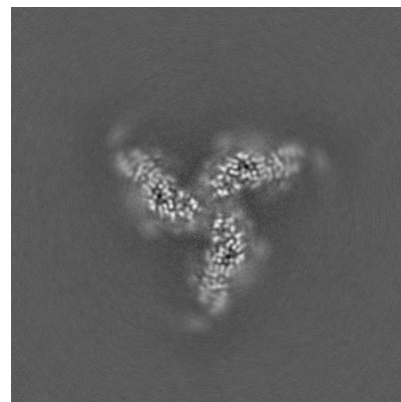
6.2.2 Raw map



X Index: 200



Y Index: 200

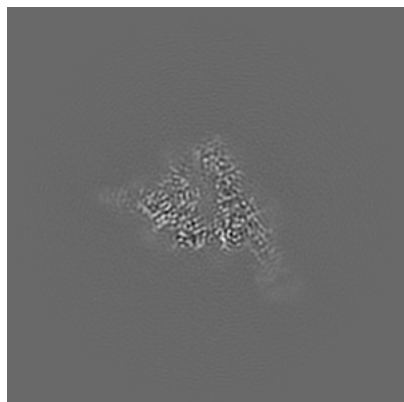


Z Index: 200

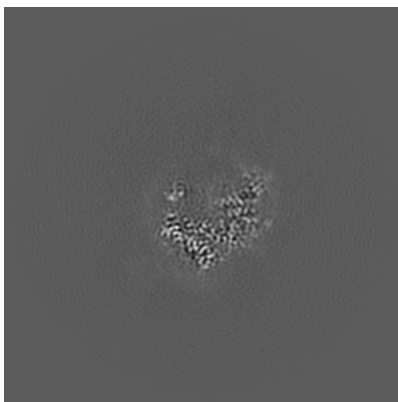
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

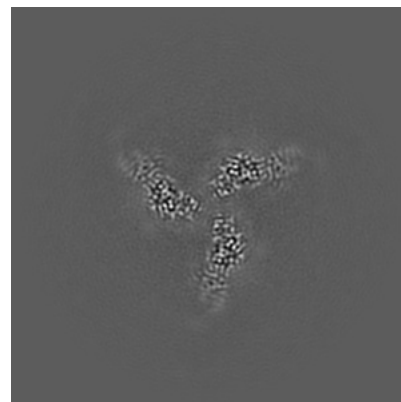
6.3.1 Primary map



X Index: 216

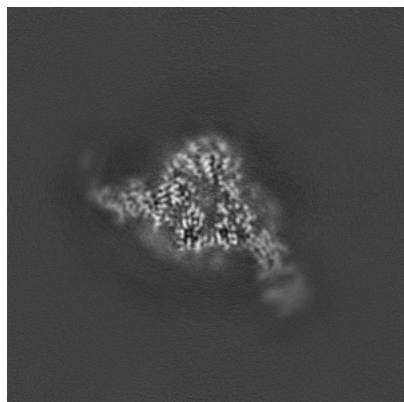


Y Index: 205

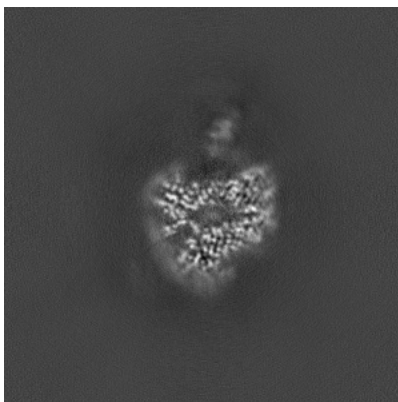


Z Index: 200

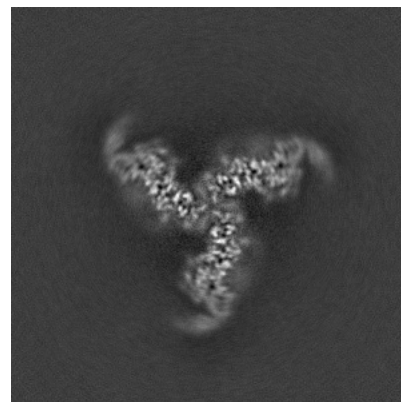
6.3.2 Raw map



X Index: 210



Y Index: 212

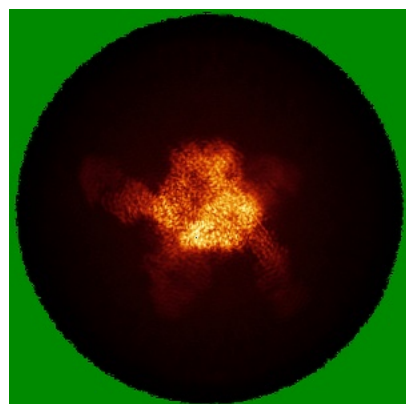


Z Index: 210

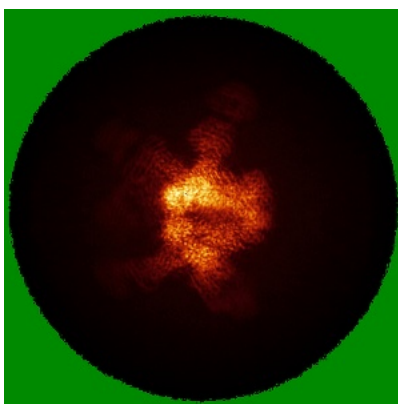
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

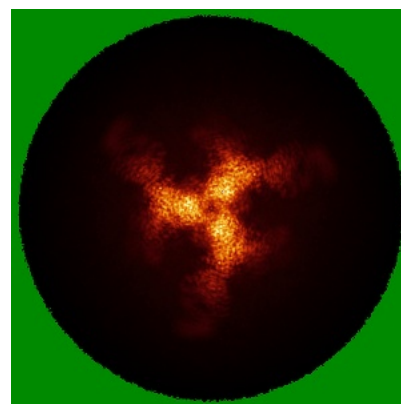
6.4.1 Primary map



X

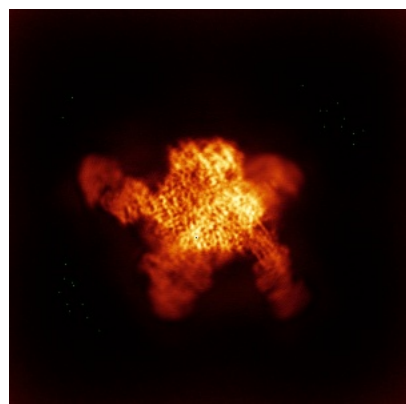


Y

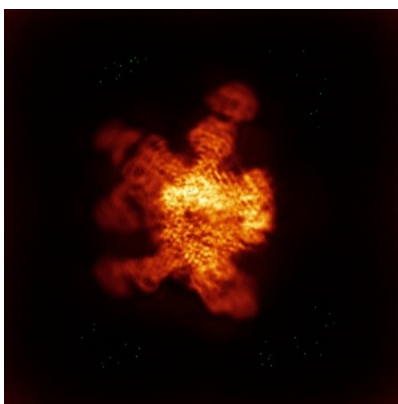


Z

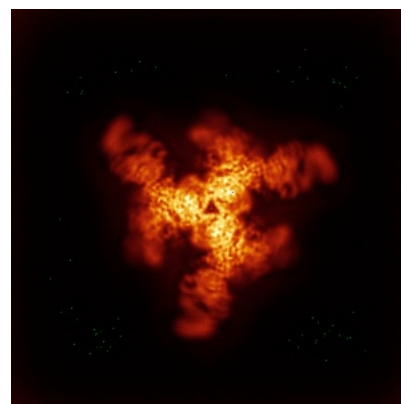
6.4.2 Raw map



X



Y

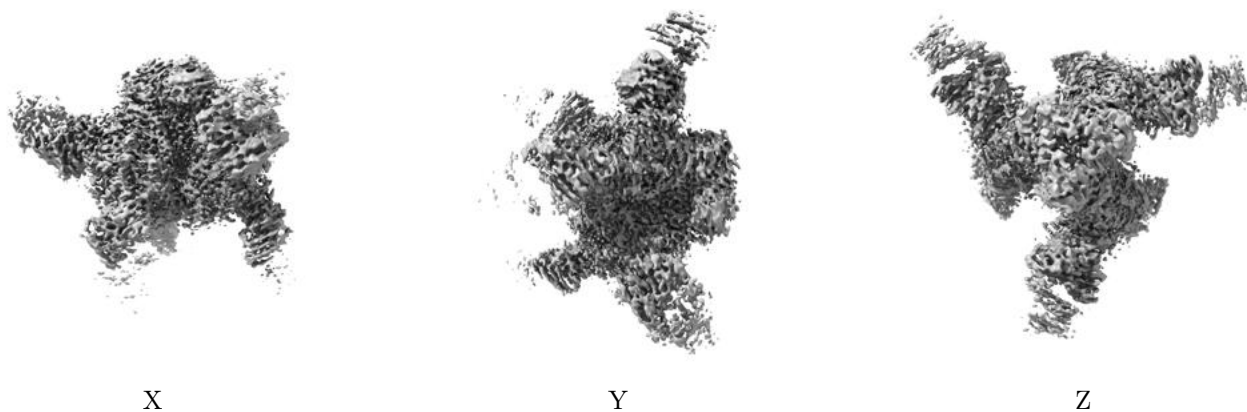


Z

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

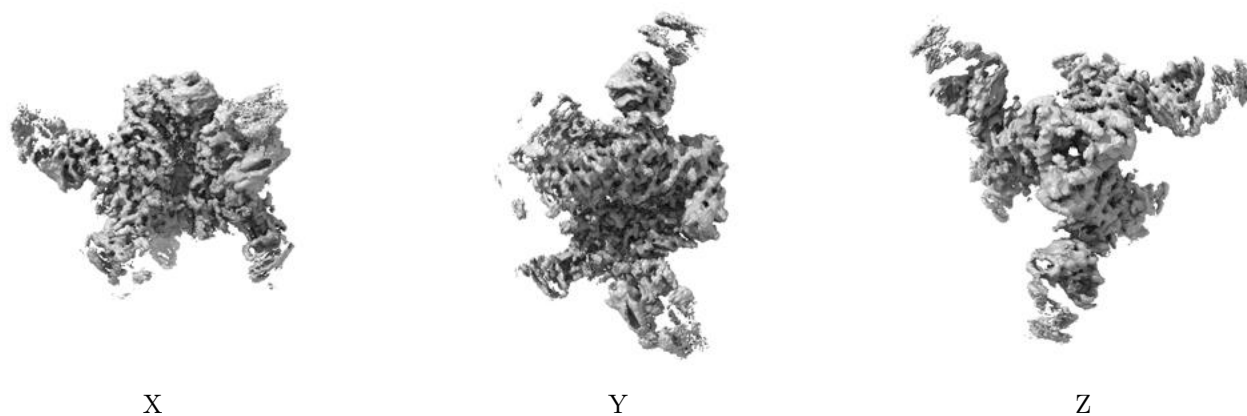
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.094. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

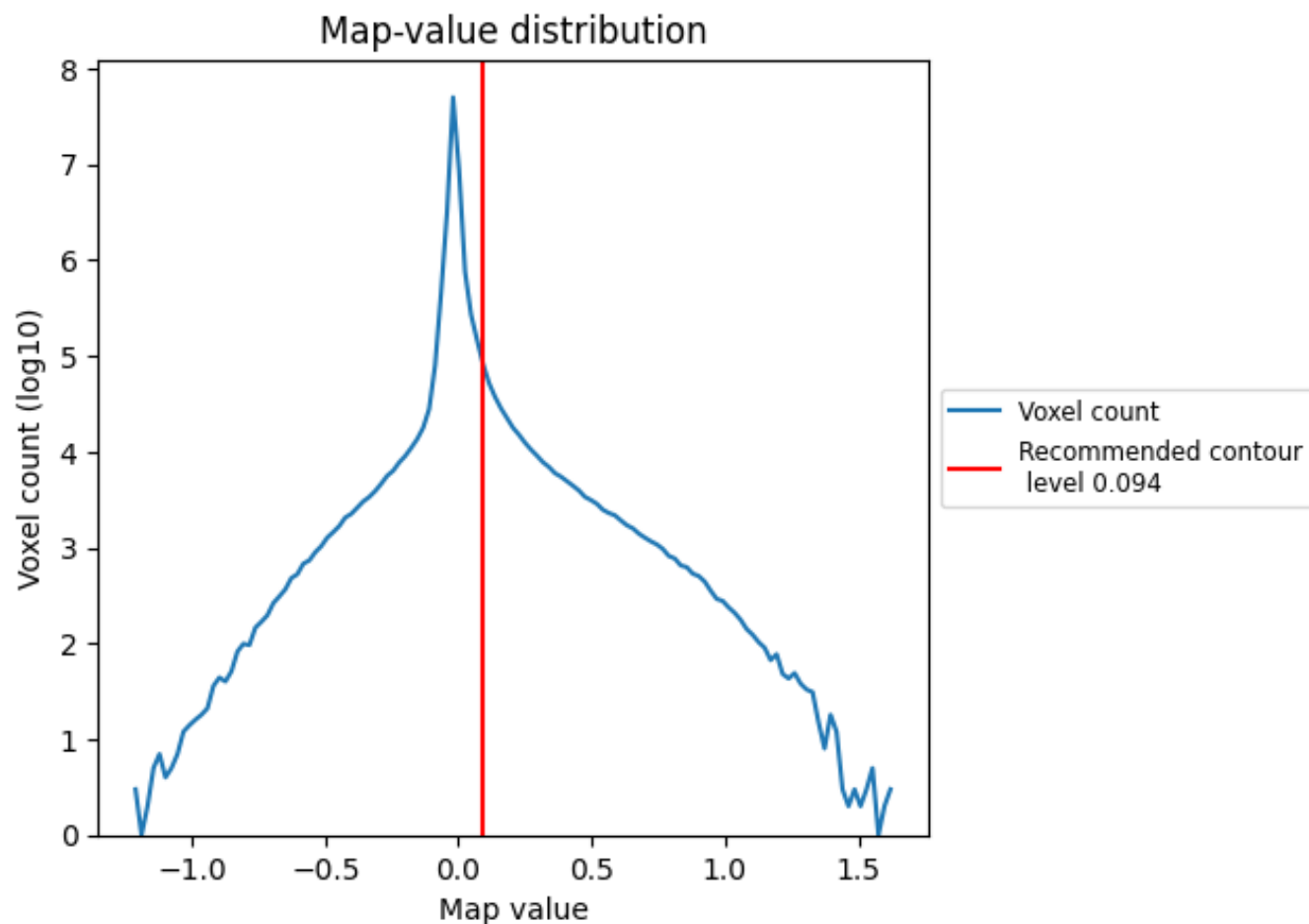
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

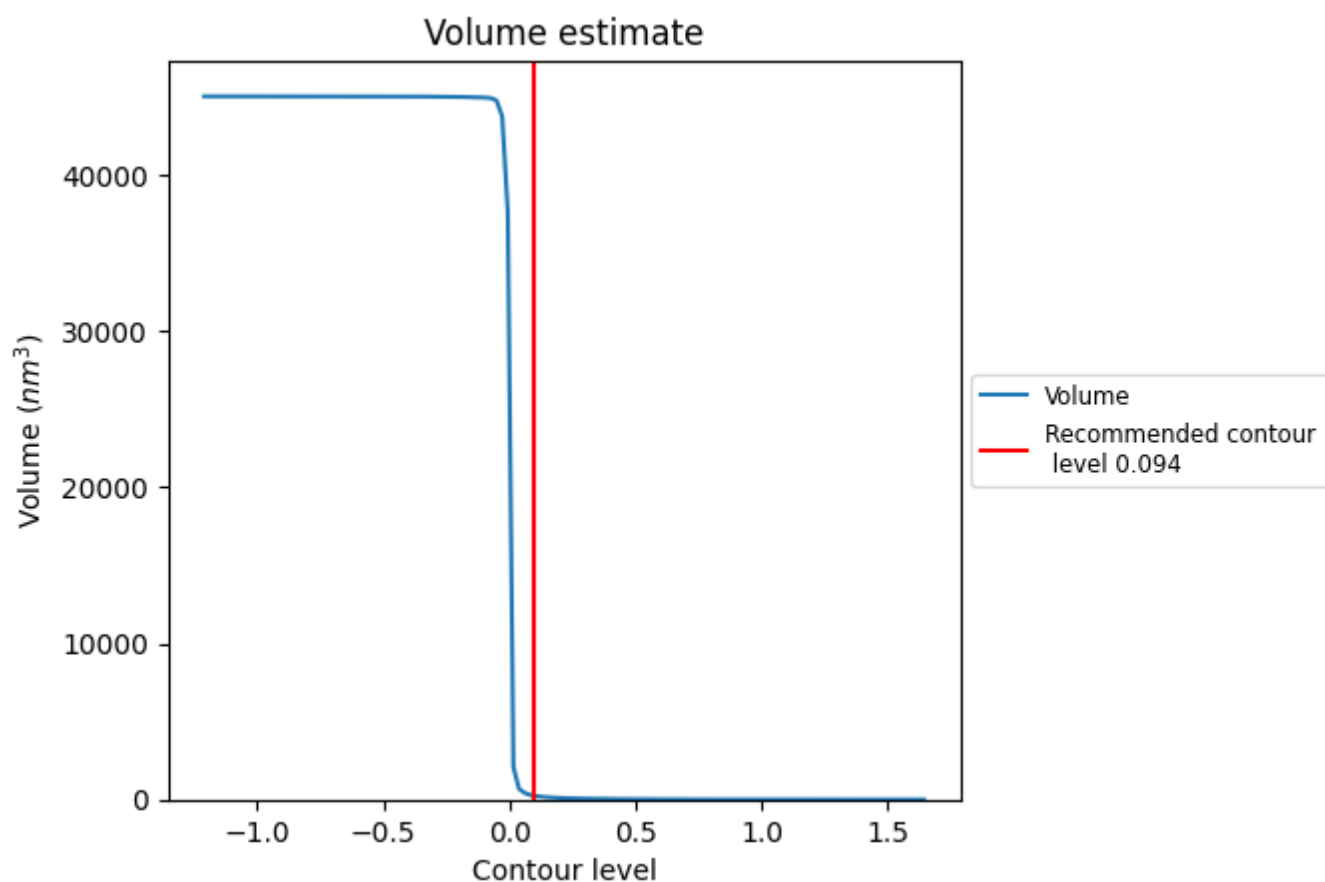
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

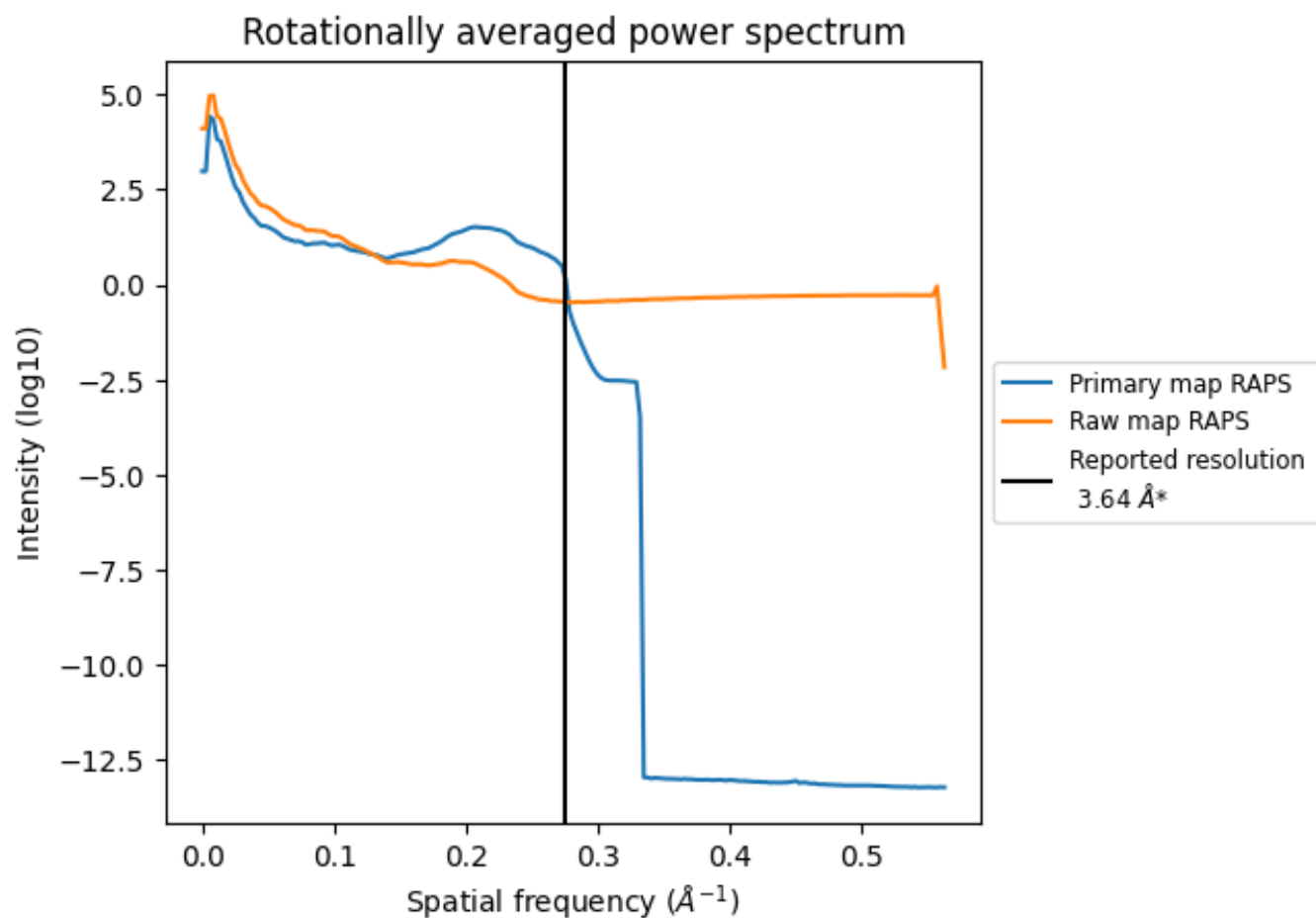
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 253 nm³; this corresponds to an approximate mass of 229 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 ⓘ

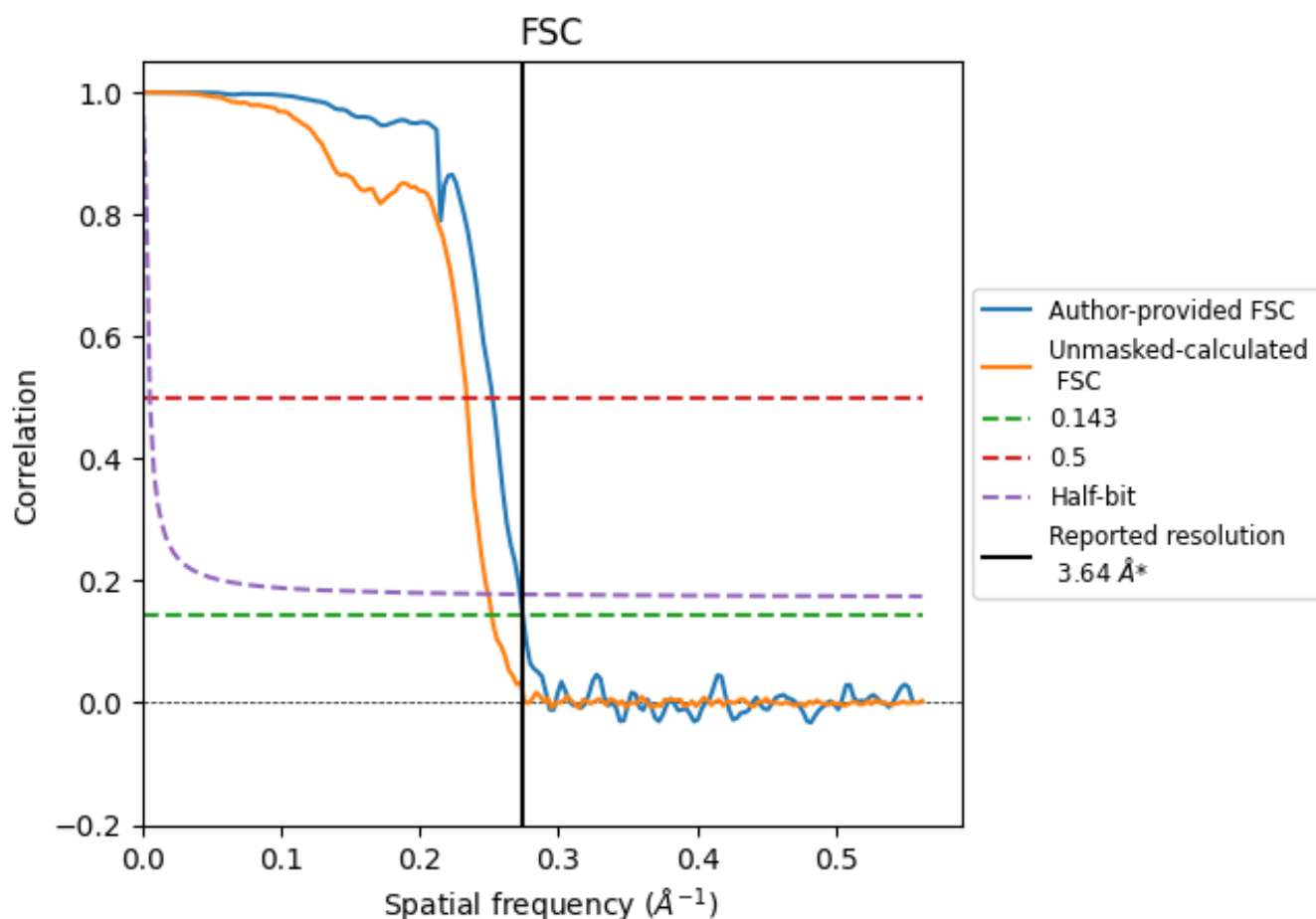


*Reported resolution corresponds to spatial frequency of 0.275 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.275 \AA^{-1}

8.2 Resolution estimates [i](#)

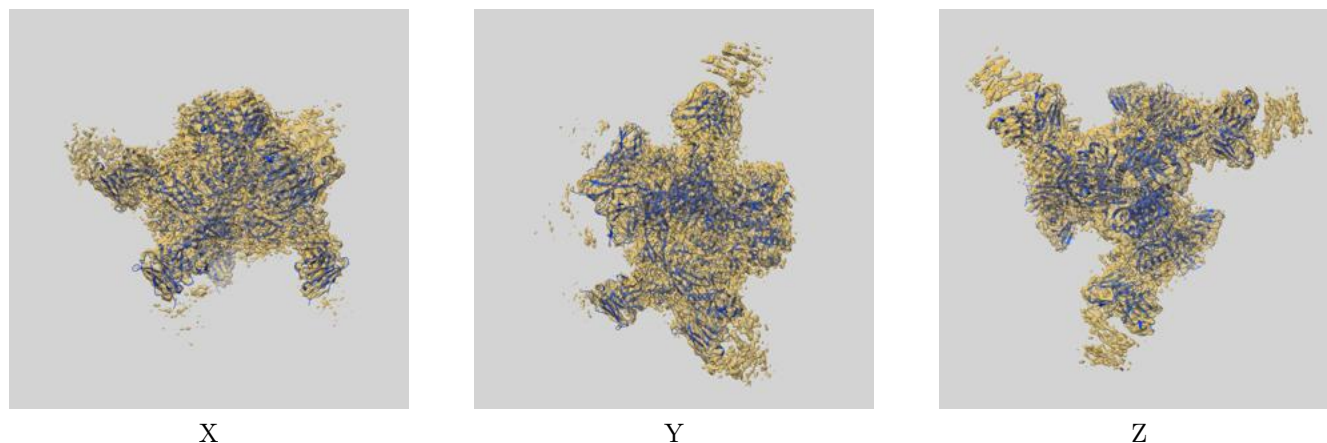
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	3.64	3.96	3.67
Unmasked-calculated*	3.97	4.28	4.01

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

9 Map-model fit [i](#)

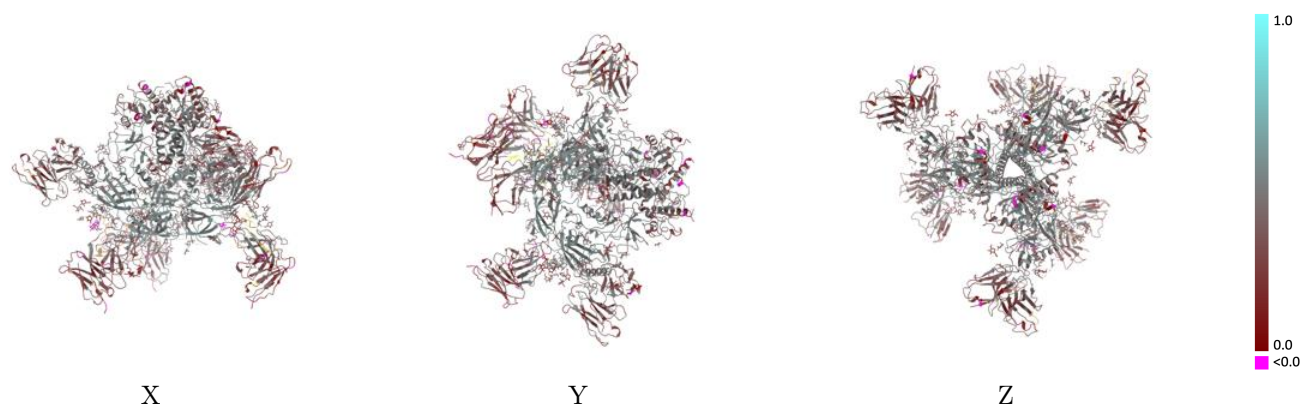
This section contains information regarding the fit between EMDB map EMD-72216 and PDB model 9Q3X. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



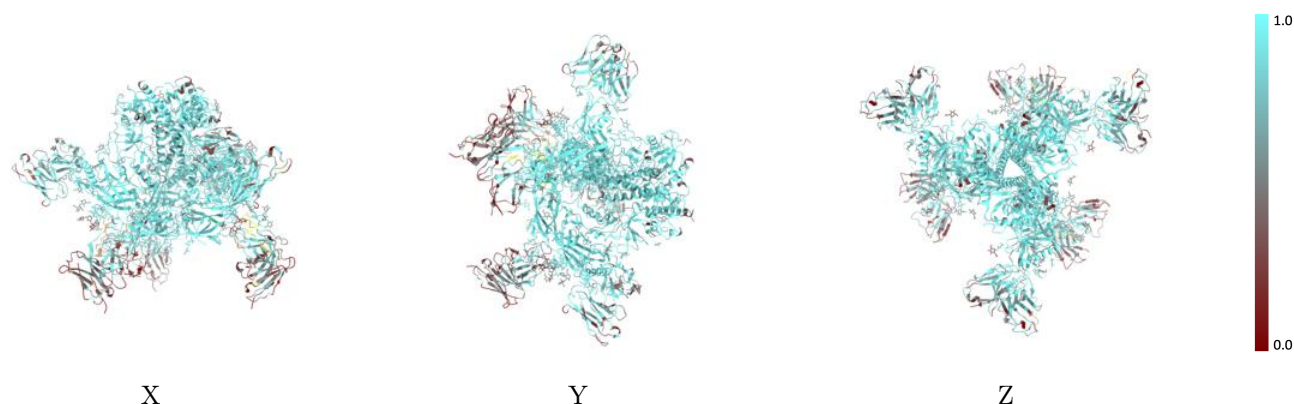
The images above show the 3D surface view of the map at the recommended contour level 0.094 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



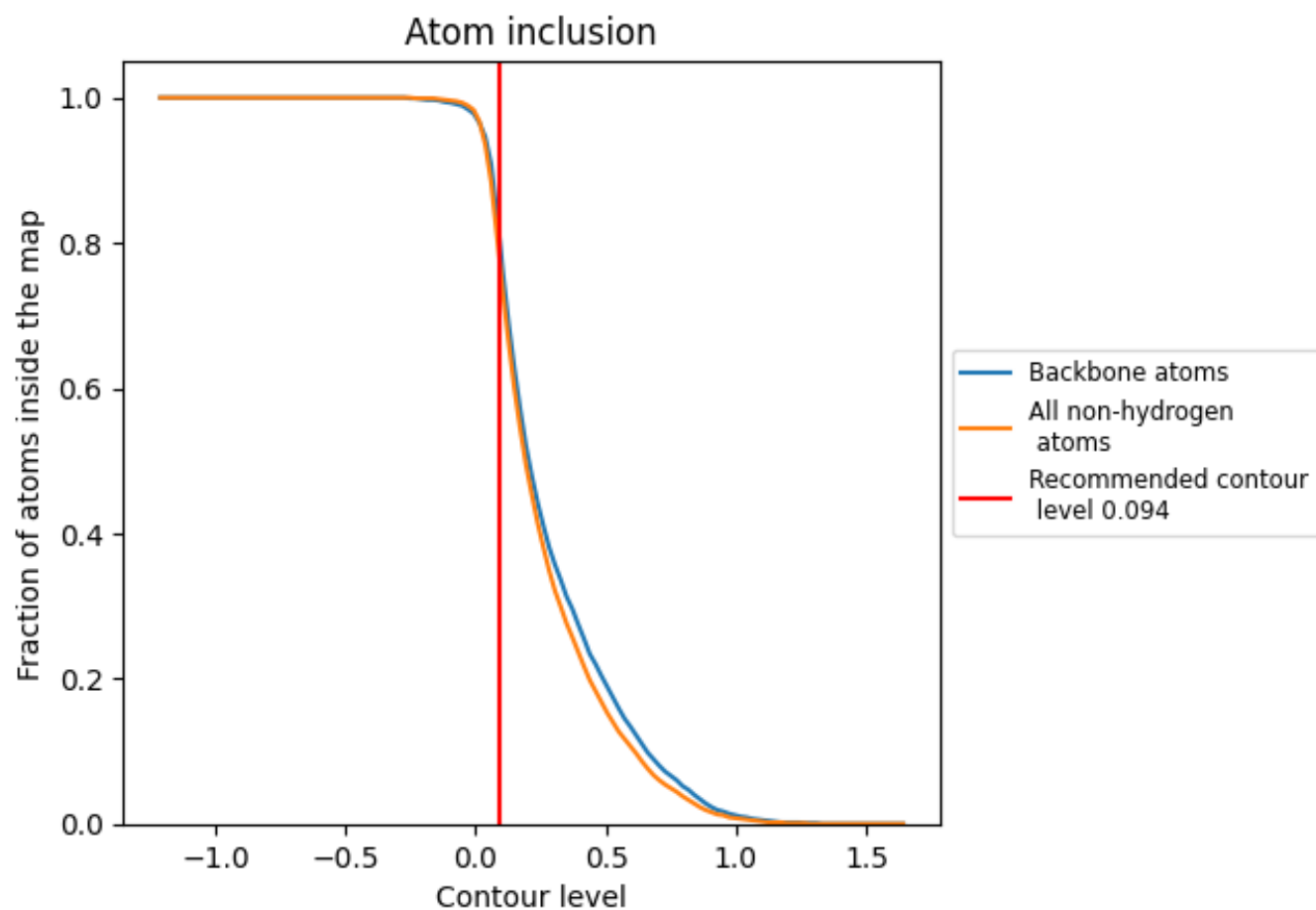
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.094).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ









































The table lists the average atom inclusion at the recommended contour level (0.094) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.3990
0	 0.7900	 0.4280
1	 0.7860	 0.3480
2	 0.6070	 0.2210
A	 0.9040	 0.4750
B	 0.8480	 0.3890
C	 0.8430	 0.3860
D	 0.6890	 0.3290
E	 0.7030	 0.3450
G	 0.9010	 0.4750
H	 0.6830	 0.3340
I	 0.8980	 0.4720
J	 0.8560	 0.3900
K	 0.6940	 0.3320
L	 0.7070	 0.3450
M	 0.6920	 0.3460
N	 0.5360	 0.2340
O	 0.8000	 0.4230
P	 0.7860	 0.3540
Q	 0.5710	 0.2050
R	 0.8570	 0.4590
S	 0.8570	 0.4360
T	 0.6790	 0.2800
U	 0.8200	 0.3950
V	 0.7860	 0.3890
W	 0.6430	 0.2730
X	 0.7440	 0.3360
Y	 0.5570	 0.2780
Z	 0.5360	 0.2210
a	 0.8570	 0.4620
b	 0.8570	 0.4270
c	 0.6430	 0.2730
d	 0.4980	 0.3000
e	 0.5980	 0.3480
f	 0.8200	 0.3960



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Chain	Atom inclusion	Q-score
g	 0.8210	 0.3940
h	 0.4960	 0.3000
i	 0.6790	 0.2440
j	 0.7440	 0.3420
k	 0.5010	 0.3010
l	 0.6110	 0.3480
m	 0.6060	 0.3520
n	 0.5740	 0.2670
o	 0.5360	 0.2260
p	 0.7810	 0.4210
q	 0.7860	 0.3440
r	 0.6070	 0.2190
s	 0.8570	 0.4720
t	 0.8570	 0.4130
u	 0.6430	 0.2770
v	 0.8200	 0.4010
w	 0.7860	 0.3940
x	 0.6430	 0.2660
y	 0.7440	 0.3240
z	 0.5900	 0.2630