



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:32 PM UTC

PDB ID : 5V8L / pdb_00005v8l
EMDB ID : EMD-8643
Title : BG505 SOSIP.664 trimer in complex with broadly neutralizing HIV antibodies
3BNC117 and PGT145
Authors : Lee, J.H.; Ward, A.B.
Deposited on : 2017-03-22
Resolution : 4.30 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

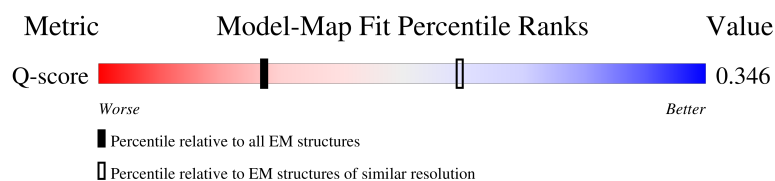
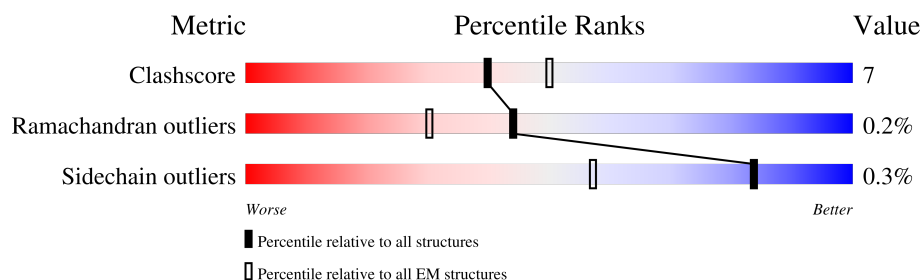
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.



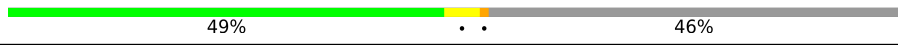
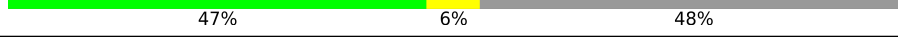
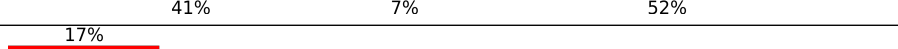
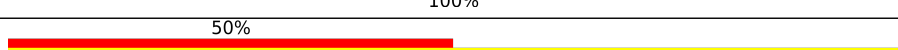
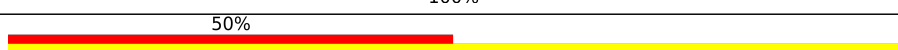
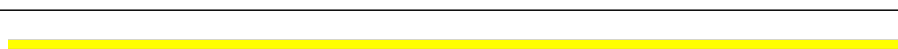
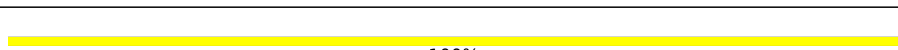
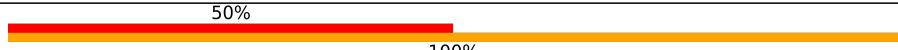
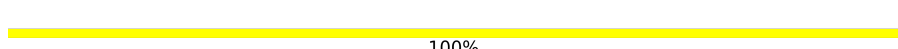
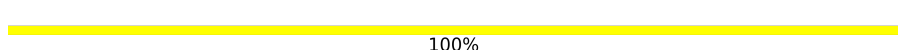
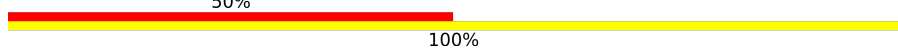
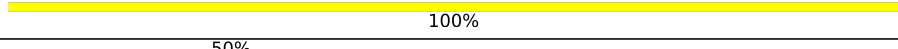
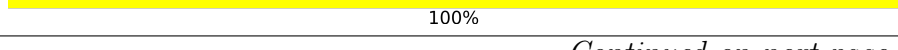
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	 83% 10% • 6%
1	C	481	 84% 9% 6%
1	D	481	 83% 10% • 6%
2	B	153	 77% • • 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	153	
2	F	153	
3	G	226	
3	H	226	
3	I	226	
4	J	267	
5	K	206	
5	L	206	
5	M	206	
6	N	219	
7	0	2	
7	1	2	
7	2	2	
7	3	2	
7	4	2	
7	O	2	
7	P	2	
7	Q	2	
7	R	2	
7	V	2	
7	W	2	
7	Z	2	
7	a	2	
7	b	2	
7	c	2	

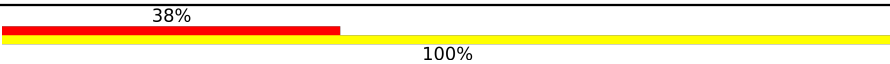
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	e	2	100%
7	h	2	50%
7	i	2	100%
7	j	2	50%
7	m	2	100%
7	n	2	100%
7	o	2	50%
7	p	2	100%
7	r	2	100%
7	u	2	50%
7	v	2	100%
7	w	2	50%
7	z	2	100%
8	S	3	33%
8	X	3	33%
8	d	3	67%
8	l	3	33%
8	y	3	67%
9	T	6	100%
10	U	7	86%
11	Y	5	20%
11	k	5	20%
11	x	5	20%
11	x	5	80%
12	f	7	14%
12	s	7	29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	g	8	
13	q	8	
13	t	8	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	NAG	q	1	-	-	X	-
13	NAG	q	2	-	-	X	-
13	MAN	q	4	-	-	X	-
14	NAG	D	639	X	-	-	-
7	NAG	Q	1	-	-	X	-
7	NAG	h	1	-	-	X	-
7	NAG	j	1	-	-	X	-
7	NAG	u	1	-	-	X	-
7	NAG	w	1	-	-	X	-
8	NAG	l	1	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22934 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 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	450	Total	C	N	O	S	0	0
			3545	2227	625	665	28		
1	C	451	Total	C	N	O	S	0	0
			3553	2231	627	667	28		
1	D	452	Total	C	N	O	S	0	0
			3562	2236	628	670	28		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	-	expression tag	UNP Q2N0S6
C	510	ARG	-	expression tag	UNP Q2N0S6
C	511	ARG	-	expression tag	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6
D	332	ASN	THR	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6
D	509	ARG	-	expression tag	UNP Q2N0S6
D	510	ARG	-	expression tag	UNP Q2N0S6
D	511	ARG	-	expression tag	UNP Q2N0S6
D	512	ARG	-	expression tag	UNP Q2N0S6
D	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			1004	635	173	190	6		
2	E	124	Total	C	N	O	S	0	0
			987	623	170	188	6		
2	F	123	Total	C	N	O	S	0	0
			981	620	169	186	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
E	559	PRO	ILE	conflict	UNP Q2N0S6
E	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called 3BNC117 antibody, heavy chain.

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

- Molecule 4 is a protein called PGT145 antibody, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	140	Total	C	N	O	S	0	0
			1094	685	191	213	5		

- Molecule 5 is a protein called 3BNC117 antibody, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
5	L	98	Total	C	N	O	S	0	0
			783	493	137	150	3		
5	M	98	Total	C	N	O	S	0	0
			783	493	137	150	3		

- Molecule 6 is a protein called PGT145 antibody, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	112	Total	C	N	O	S	0	0
			859	542	153	160	4		

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



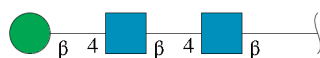
Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	2	Total	C	N	O		0	0
			28	16	2	10			
7	P	2	Total	C	N	O		0	0
			28	16	2	10			
7	Q	2	Total	C	N	O		0	0
			28	16	2	10			
7	R	2	Total	C	N	O		0	0
			28	16	2	10			
7	V	2	Total	C	N	O		0	0
			28	16	2	10			
7	W	2	Total	C	N	O		0	0
			28	16	2	10			
7	Z	2	Total	C	N	O		0	0
			28	16	2	10			
7	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	e	2	Total	C	N	O		0	0
			28	16	2	10			
7	h	2	Total	C	N	O		0	0
			28	16	2	10			
7	i	2	Total	C	N	O		0	0
			28	16	2	10			
7	j	2	Total	C	N	O		0	0
			28	16	2	10			
7	m	2	Total	C	N	O		0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
7	n	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	2	Total	C	N	O	0	0
			28	16	2	10		
7	p	2	Total	C	N	O	0	0
			28	16	2	10		
7	r	2	Total	C	N	O	0	0
			28	16	2	10		
7	u	2	Total	C	N	O	0	0
			28	16	2	10		
7	v	2	Total	C	N	O	0	0
			28	16	2	10		
7	w	2	Total	C	N	O	0	0
			28	16	2	10		
7	z	2	Total	C	N	O	0	0
			28	16	2	10		
7	0	2	Total	C	N	O	0	0
			28	16	2	10		
7	1	2	Total	C	N	O	0	0
			28	16	2	10		
7	2	2	Total	C	N	O	0	0
			28	16	2	10		
7	3	2	Total	C	N	O	0	0
			28	16	2	10		
7	4	2	Total	C	N	O	0	0
			28	16	2	10		

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



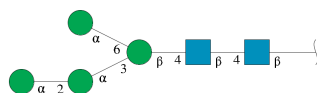
Mol	Chain	Residues	Atoms				AltConf	Trace
8	S	3	Total	C	N	O	0	0
			39	22	2	15		
8	X	3	Total	C	N	O	0	0
			39	22	2	15		
8	d	3	Total	C	N	O	0	0
			39	22	2	15		
8	l	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

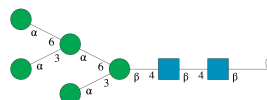
Mol	Chain	Residues	Atoms				AltConf	Trace
8	y	3	Total	C	N	O	0	0
			39	22	2	15		

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



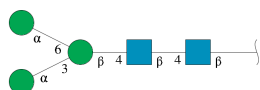
Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



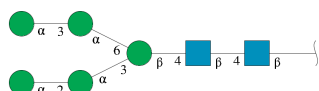
Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	5	Total	C	N	O	0	0
			61	34	2	25		
11	k	5	Total	C	N	O	0	0
			61	34	2	25		

Continued on next page...

Continued from previous page...

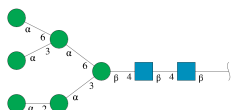
Mol	Chain	Residues	Atoms				AltConf	Trace
11	x	5	Total	C	N	O	0	0
			61	34	2	25		

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



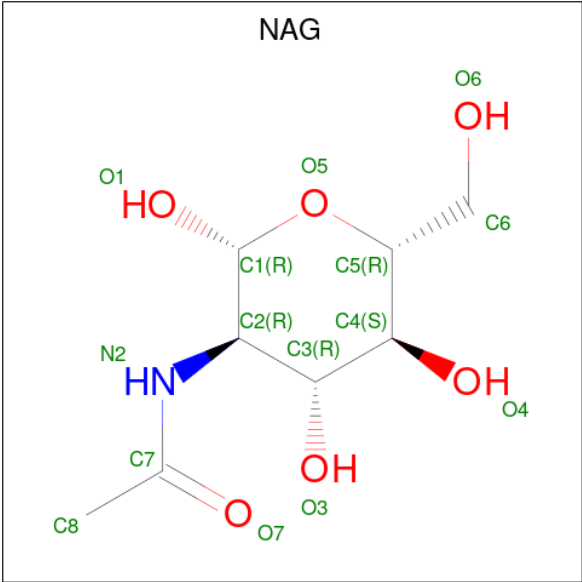
Mol	Chain	Residues	Atoms				AltConf	Trace
12	f	7	Total	C	N	O	0	0
			83	46	2	35		
12	s	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 13 is an oligosaccharide called 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
13	g	8	Total	C	N	O	0	0
			94	52	2	40		
13	q	8	Total	C	N	O	0	0
			94	52	2	40		
13	t	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

Continued on next page...

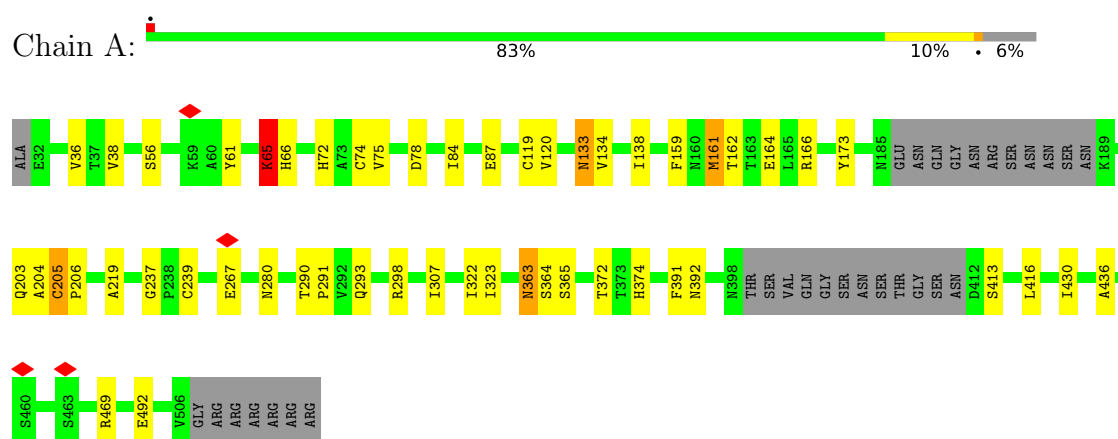
Continued from previous page...

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

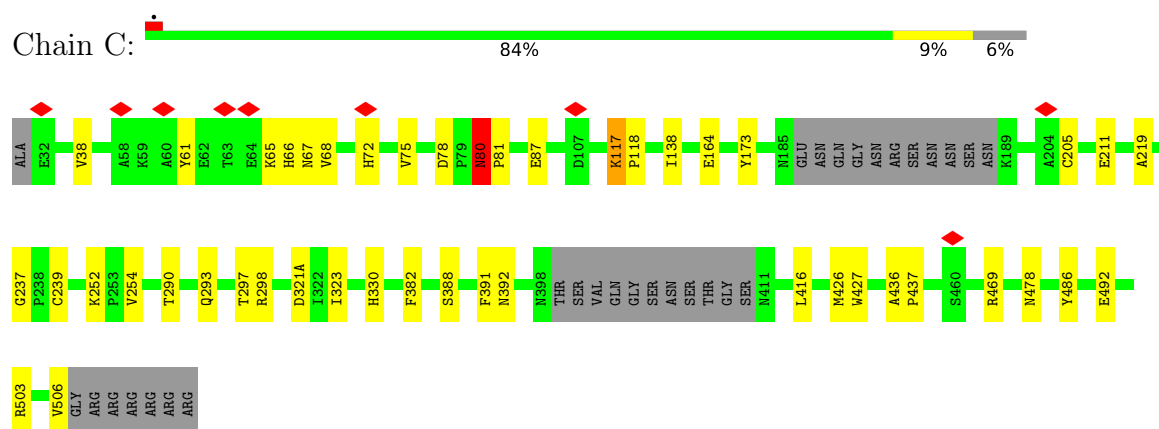
3 Residue-property plots

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.

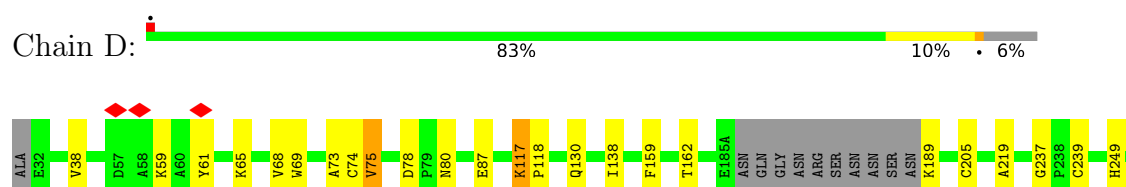
• Molecule 1: gp120

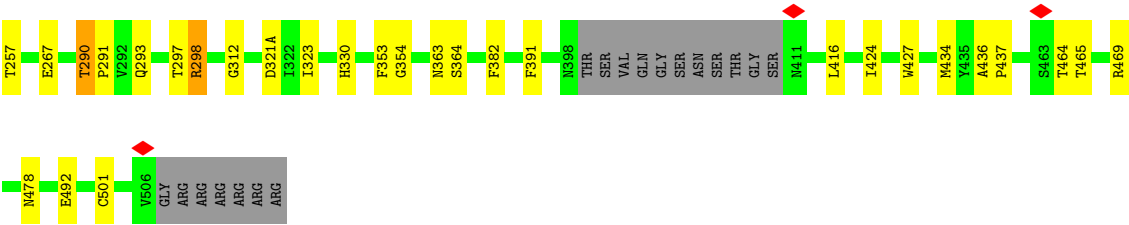


• Molecule 1: gp120

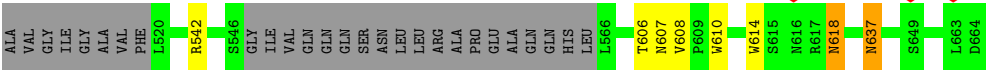
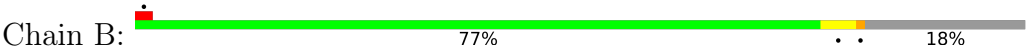


• Molecule 1: gp120

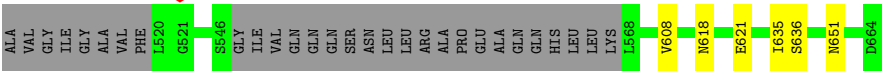
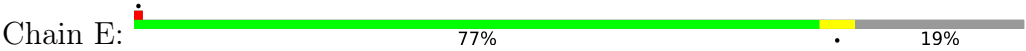




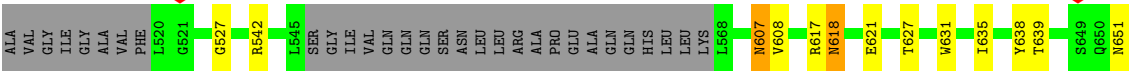
• Molecule 2: gp41



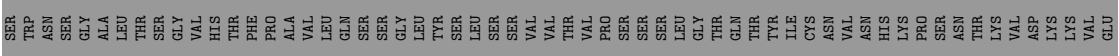
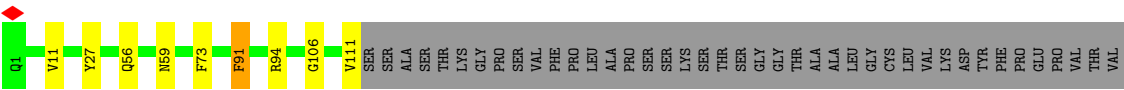
• Molecule 2: gp41



• Molecule 2: gp41

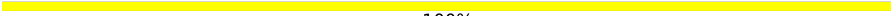


• Molecule 3: 3BNC117 antibody, heavy chain



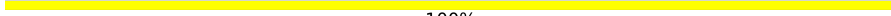
• Molecule 3: 3BNC117 antibody, heavy chain



Chain P:  100%

NAG1
NAG2

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

Chain Q:  100%

NAG1
NAG2

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

Chain R:  100%

NAG1
NAG2

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

Chain V:  50%

NAG1
NAG2

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

Chain W:  100%

NAG1
NAG2

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

Chain Z:  50%

NAG1
NAG2

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

Chain a:  50%



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

Chain b:  100%



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

Chain c:  50% 100%



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

Chain e:  100%



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

Chain h:  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 j:  50% 50%



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

Chain m:  100%

NAG1
NAG2

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

Chain n:  100%

NAG1
NAG2

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

Chain o:  50%
100%

♦
NAG1
NAG2

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

Chain p:  100%

NAG1
NAG2

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

Chain r:  100%

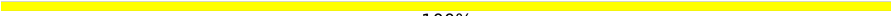
NAG1
NAG2

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

Chain u:  50% 50%

NAG1
NAG2

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

Chain v:  100%

NAG1
NAG2

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

Chain w:  50%  50%

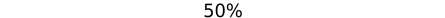
NAG1
NAG2

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

Chain z:  100%

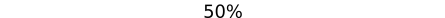
NAG1
NAG2

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

Chain 0:  50%  100%

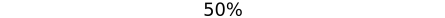
♦
NAG1
NAG2

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

Chain 1:  50%  100%

♦
NAG1
NAG2

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

Chain 2:  50%  100%

♦
NAG1
NAG2

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

Chain 3:  100%

MAG1
MAG2

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

Chain 4:  100%

MAG1
MAG2

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

Chain S:  33% 100%

MAG1
MAG2
BMA3

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

Chain X:  33% 100%

MAG1
MAG2
BMA3

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

Chain d:  67% 100%

MAG1
MAG2
BMA3

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

Chain l:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain y:  67% 33%



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

Chain T:



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

Chain U:



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

Chain Y:



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

Chain k:

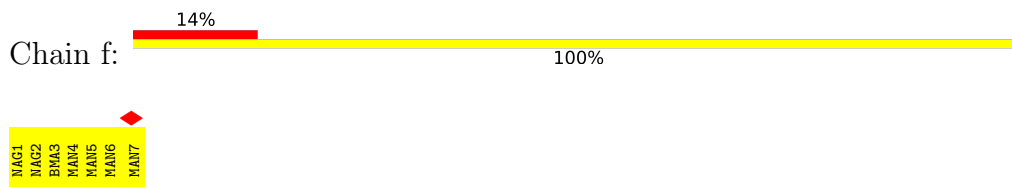


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

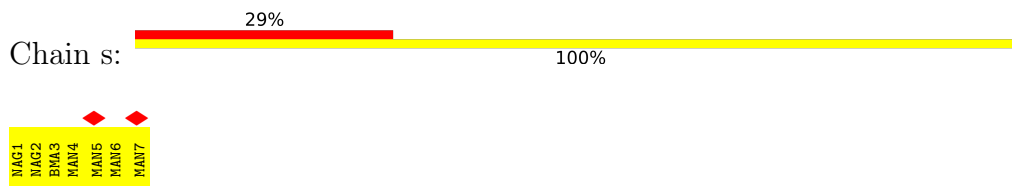
Chain x:



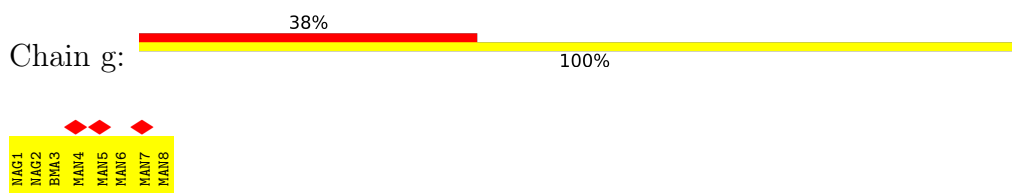
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



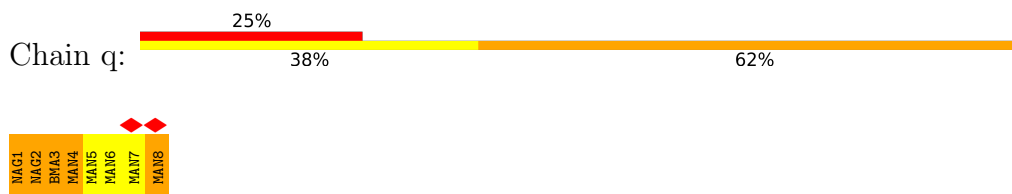
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



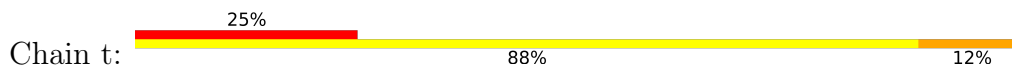
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 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 13: 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



MAG1	
MAG2	
BMA3	
MAN4	
MAN5	
MAN6	
MAN7	
MAN8	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	377.27997, 377.27997, 377.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.90	0/3619	1.29	35/4914 (0.7%)
1	C	0.92	0/3627	1.32	40/4925 (0.8%)
1	D	0.93	0/3636	1.31	46/4937 (0.9%)
2	B	0.98	0/1021	1.11	3/1384 (0.2%)
2	E	0.98	0/1004	1.11	5/1362 (0.4%)
2	F	1.01	0/998	1.09	8/1354 (0.6%)
3	G	0.98	0/1017	1.26	6/1386 (0.4%)
3	H	0.97	0/1017	1.28	7/1386 (0.5%)
3	I	1.01	0/1017	1.31	8/1386 (0.6%)
4	J	0.82	0/1121	1.15	2/1519 (0.1%)
5	K	0.82	0/800	1.28	7/1086 (0.6%)
5	L	0.82	0/800	1.31	5/1086 (0.5%)
5	M	0.81	0/800	1.29	7/1086 (0.6%)
6	N	0.75	0/882	1.23	8/1199 (0.7%)
All	All	0.92	0/21359	1.26	187/29010 (0.6%)

There are no bond length outliers.

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	LYS	CA-C-N	10.06	131.29	120.12
1	C	252	LYS	C-N-CA	10.06	131.29	120.12
1	A	436	ALA	CA-C-N	9.49	126.49	119.66
1	A	436	ALA	C-N-CA	9.49	126.49	119.66
1	C	298	ARG	CA-C-N	9.26	129.01	119.56
1	C	298	ARG	C-N-CA	9.26	129.01	119.56
1	D	239	CYS	CA-C-N	9.09	128.83	119.56
1	D	239	CYS	C-N-CA	9.09	128.83	119.56
2	B	608	VAL	CA-C-N	9.09	129.03	119.85
2	B	608	VAL	C-N-CA	9.09	129.03	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	56	GLN	CA-C-N	9.03	128.97	119.85
3	I	56	GLN	C-N-CA	9.03	128.97	119.85
5	M	43	ALA	CA-C-N	8.79	128.73	120.03
5	M	43	ALA	C-N-CA	8.79	128.73	120.03
2	F	608	VAL	CA-C-N	8.75	128.69	119.85
2	F	608	VAL	C-N-CA	8.75	128.69	119.85
1	D	205	CYS	CA-C-N	8.74	128.47	119.56
1	D	205	CYS	C-N-CA	8.74	128.47	119.56
1	D	298	ARG	CA-C-N	8.69	128.43	119.56
1	D	298	ARG	C-N-CA	8.69	128.43	119.56
1	D	237	GLY	CA-C-N	8.59	128.53	119.85
1	D	237	GLY	C-N-CA	8.59	128.53	119.85
1	A	239	CYS	CA-C-N	8.53	128.26	119.56
1	A	239	CYS	C-N-CA	8.53	128.26	119.56
1	C	239	CYS	CA-C-N	8.46	128.19	119.56
1	C	239	CYS	C-N-CA	8.46	128.19	119.56
3	G	56	GLN	CA-C-N	8.37	128.31	119.85
3	G	56	GLN	C-N-CA	8.37	128.31	119.85
3	H	56	GLN	CA-C-N	8.33	128.26	119.85
3	H	56	GLN	C-N-CA	8.33	128.26	119.85
2	E	608	VAL	CA-C-N	8.22	128.16	119.85
2	E	608	VAL	C-N-CA	8.22	128.16	119.85
1	A	298	ARG	CA-C-N	8.12	127.84	119.56
1	A	298	ARG	C-N-CA	8.12	127.84	119.56
1	C	436	ALA	CA-C-N	8.08	125.48	119.66
1	C	436	ALA	C-N-CA	8.08	125.48	119.66
1	C	78	ASP	CA-C-N	8.06	128.25	119.87
1	C	78	ASP	C-N-CA	8.06	128.25	119.87
1	C	75	VAL	CA-C-N	8.05	127.98	119.85
1	C	75	VAL	C-N-CA	8.05	127.98	119.85
6	N	43	THR	CA-C-N	7.98	128.00	119.78
6	N	43	THR	C-N-CA	7.98	128.00	119.78
1	D	354	GLY	N-CA-C	-7.89	102.86	111.93
3	H	59	ASN	CA-C-N	7.88	127.90	119.78
3	H	59	ASN	C-N-CA	7.88	127.90	119.78
1	C	416	LEU	CA-C-N	7.84	127.77	119.85
1	C	416	LEU	C-N-CA	7.84	127.77	119.85
1	C	492	GLU	CA-C-N	7.83	127.89	119.28
1	C	492	GLU	C-N-CA	7.83	127.89	119.28
1	D	78	ASP	CA-C-N	7.83	127.55	119.56
1	D	78	ASP	C-N-CA	7.83	127.55	119.56
1	C	237	GLY	CA-C-N	7.83	127.84	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	GLY	C-N-CA	7.83	127.84	119.78
1	A	492	GLU	CA-C-N	7.82	127.89	119.28
1	A	492	GLU	C-N-CA	7.82	127.89	119.28
1	C	219	ALA	CA-C-N	7.59	127.52	119.85
1	C	219	ALA	C-N-CA	7.59	127.52	119.85
3	I	59	ASN	CA-C-N	7.56	127.48	119.85
3	I	59	ASN	C-N-CA	7.56	127.48	119.85
5	K	43	ALA	CA-C-N	7.39	127.40	119.78
5	K	43	ALA	C-N-CA	7.39	127.40	119.78
1	A	161	MET	CB-CA-C	-7.29	107.12	115.79
1	A	219	ALA	CA-C-N	7.27	127.27	119.78
1	A	219	ALA	C-N-CA	7.27	127.27	119.78
1	A	78	ASP	CA-C-N	7.23	126.94	119.56
1	A	78	ASP	C-N-CA	7.23	126.94	119.56
5	L	43	ALA	CA-C-N	7.20	127.62	119.92
5	L	43	ALA	C-N-CA	7.20	127.62	119.92
1	C	290	THR	CA-C-N	7.07	126.98	119.85
1	C	290	THR	C-N-CA	7.07	126.98	119.85
1	D	427	TRP	CB-CA-C	-7.07	108.43	116.63
1	D	219	ALA	CA-C-N	7.05	126.97	119.85
1	D	219	ALA	C-N-CA	7.05	126.97	119.85
1	A	205	CYS	CA-C-N	7.01	126.71	119.56
1	A	205	CYS	C-N-CA	7.01	126.71	119.56
1	C	254	VAL	N-CA-C	6.99	118.81	109.37
1	A	237	GLY	CA-C-N	6.95	126.94	119.78
1	A	237	GLY	C-N-CA	6.95	126.94	119.78
3	G	91	PHE	N-CA-C	6.88	119.53	109.07
1	D	117	LYS	CA-C-N	6.86	126.49	119.56
1	D	117	LYS	C-N-CA	6.86	126.49	119.56
1	C	211	GLU	CA-C-N	6.86	126.78	119.85
1	C	211	GLU	C-N-CA	6.86	126.78	119.85
5	L	79	GLN	CA-C-N	6.82	126.78	119.28
5	L	79	GLN	C-N-CA	6.82	126.78	119.28
1	A	38	VAL	N-CA-C	6.80	118.35	109.58
4	J	13	LYS	CA-C-N	6.79	126.77	119.78
4	J	13	LYS	C-N-CA	6.79	126.77	119.78
1	C	117	LYS	CA-C-N	6.76	126.39	119.56
1	C	117	LYS	C-N-CA	6.76	126.39	119.56
1	A	391	PHE	CA-CB-CG	-6.74	107.06	113.80
3	I	104	GLY	N-CA-C	-6.73	103.92	112.54
1	D	492	GLU	CA-C-N	6.70	126.39	119.56
1	D	492	GLU	C-N-CA	6.70	126.39	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	LEU	CA-C-N	6.68	126.60	119.85
1	A	416	LEU	C-N-CA	6.68	126.60	119.85
1	D	416	LEU	CA-C-N	6.68	126.60	119.85
1	D	416	LEU	C-N-CA	6.68	126.60	119.85
2	E	608	VAL	N-CA-C	6.67	114.15	107.55
1	A	290	THR	CA-C-N	6.59	126.51	119.85
1	A	290	THR	C-N-CA	6.59	126.51	119.85
1	D	80	ASN	CA-C-N	6.54	126.51	119.78
1	D	80	ASN	C-N-CA	6.54	126.51	119.78
1	D	437	PRO	CA-C-N	6.54	126.45	119.85
1	D	437	PRO	C-N-CA	6.54	126.45	119.85
1	C	205	CYS	CA-C-N	6.42	126.11	119.56
1	C	205	CYS	C-N-CA	6.42	126.11	119.56
5	M	79	GLN	CA-C-N	6.41	126.33	119.28
5	M	79	GLN	C-N-CA	6.41	126.33	119.28
1	A	65	LYS	N-CA-C	6.39	118.83	108.41
1	D	75	VAL	CA-C-N	6.32	126.23	119.85
1	D	75	VAL	C-N-CA	6.32	126.23	119.85
3	I	91	PHE	N-CA-C	6.27	118.60	109.07
1	D	162	THR	N-CA-C	6.24	118.83	110.35
1	C	38	VAL	N-CA-C	6.23	117.62	109.58
1	D	159	PHE	N-CA-C	6.14	118.11	108.96
5	L	103	ARG	N-CA-C	6.10	118.34	109.07
1	D	290	THR	CA-C-N	6.09	126.00	119.85
1	D	290	THR	C-N-CA	6.09	126.00	119.85
3	G	73	PHE	CA-CB-CG	-6.08	107.72	113.80
2	F	607	ASN	CA-C-N	-6.07	118.22	122.59
2	F	607	ASN	C-N-CA	-6.07	118.22	122.59
1	C	469	ARG	CA-C-N	5.99	125.94	119.78
1	C	469	ARG	C-N-CA	5.99	125.94	119.78
3	H	91	PHE	N-CA-C	5.98	118.15	109.07
1	D	68	VAL	CB-CA-C	-5.94	104.23	112.02
1	C	68	VAL	CB-CA-C	-5.91	104.40	111.97
1	D	353	PHE	CA-C-N	-5.83	114.56	120.10
1	D	353	PHE	C-N-CA	-5.83	114.56	120.10
1	D	257	THR	N-CA-C	5.72	121.30	113.97
3	H	104	GLY	N-CA-C	-5.68	105.27	112.54
3	G	59	ASN	CA-C-N	5.67	125.62	119.78
3	G	59	ASN	C-N-CA	5.67	125.62	119.78
1	D	382	PHE	CA-CB-CG	-5.63	108.17	113.80
1	A	267	GLU	N-CA-C	5.55	117.41	111.36
1	D	249	HIS	CA-CB-CG	-5.49	108.31	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	58	VAL	CA-C-N	5.49	125.44	119.78
6	N	58	VAL	C-N-CA	5.49	125.44	119.78
5	K	82	ASP	CA-C-N	-5.47	114.14	121.80
5	K	82	ASP	C-N-CA	-5.47	114.14	121.80
6	N	92	LEU	N-CA-C	5.46	117.31	111.36
2	B	542	ARG	N-CA-C	5.44	117.21	111.28
1	C	478	ASN	N-CA-C	-5.44	104.77	111.40
2	F	608	VAL	N-CA-C	5.43	113.25	107.76
5	M	9	SER	CB-CA-C	-5.42	109.34	115.79
1	D	436	ALA	CA-C-N	5.41	123.56	119.66
1	D	436	ALA	C-N-CA	5.41	123.56	119.66
1	D	267	GLU	N-CA-C	5.40	117.25	111.36
1	C	80	ASN	N-CA-C	5.39	121.72	109.81
1	C	437	PRO	CA-C-N	5.39	125.33	119.78
1	C	437	PRO	C-N-CA	5.39	125.33	119.78
2	F	542	ARG	N-CA-C	5.38	117.14	111.28
1	A	75	VAL	CA-C-N	5.36	125.26	119.85
1	A	75	VAL	C-N-CA	5.36	125.26	119.85
1	D	469	ARG	CA-C-N	5.36	125.26	119.85
1	D	469	ARG	C-N-CA	5.36	125.26	119.85
1	C	486	TYR	N-CA-C	5.35	118.46	109.95
2	F	651	ASN	N-CA-C	5.35	118.27	111.69
3	I	99	TYR	N-CA-C	-5.34	106.35	112.92
1	D	38	VAL	N-CA-C	5.34	116.47	109.21
1	A	322	ILE	N-CA-C	5.30	116.33	108.23
2	E	636	SER	N-CA-C	5.29	119.22	112.34
1	A	469	ARG	CA-C-N	5.26	125.20	119.78
1	A	469	ARG	C-N-CA	5.26	125.20	119.78
6	N	13	VAL	N-CA-C	5.21	115.63	108.12
1	D	424	ILE	N-CA-C	5.19	115.38	108.11
1	C	391	PHE	CA-CB-CG	-5.18	108.62	113.80
5	M	37	GLN	CA-C-N	-5.16	114.79	122.74
5	M	37	GLN	C-N-CA	-5.16	114.79	122.74
1	C	382	PHE	CA-CB-CG	-5.12	108.69	113.80
5	K	7	SER	N-CA-C	5.09	121.07	109.81
1	D	478	ASN	N-CA-C	-5.08	105.82	111.36
2	E	651	ASN	N-CA-C	5.08	116.90	111.36
1	A	120	VAL	N-CA-C	5.08	115.64	109.30
1	A	374	HIS	CA-C-N	-5.08	114.70	122.62
1	A	374	HIS	C-N-CA	-5.08	114.70	122.62
1	D	312	GLY	N-CA-C	-5.08	101.99	112.34
1	A	413	SER	CA-C-N	5.06	128.90	122.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	SER	C-N-CA	5.06	128.90	122.37
3	I	3	GLN	N-CA-C	5.05	117.53	109.96
1	D	391	PHE	CA-CB-CG	-5.03	108.77	113.80
2	F	627	THR	N-CA-C	-5.03	103.75	110.55
6	N	11	LEU	CA-C-N	5.03	124.93	119.85
6	N	11	LEU	C-N-CA	5.03	124.93	119.85
5	K	7	SER	CA-C-N	5.02	124.81	119.28
5	K	7	SER	C-N-CA	5.02	124.81	119.28
3	H	21	SER	N-CA-C	5.01	116.42	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3545	0	3481	66	0
1	C	3553	0	3488	56	0
1	D	3562	0	3494	53	0
2	B	1004	0	989	6	0
2	E	987	0	965	2	0
2	F	981	0	960	19	0
3	G	985	0	919	4	0
3	H	985	0	919	7	0
3	I	985	0	919	6	0
4	J	1094	0	1033	31	0
5	K	783	0	763	7	0
5	L	783	0	763	16	0
5	M	783	0	763	11	0
6	N	859	0	841	8	0
7	0	28	0	25	0	0
7	1	28	0	25	0	0
7	2	28	0	25	0	0
7	3	28	0	25	0	0
7	4	28	0	25	0	0
7	O	28	0	25	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	28	0	25	0	0
7	Q	28	0	25	15	0
7	R	28	0	25	0	0
7	V	28	0	25	6	0
7	W	28	0	25	3	0
7	Z	28	0	25	0	0
7	a	28	0	25	4	0
7	b	28	0	25	0	0
7	c	28	0	25	4	0
7	e	28	0	25	0	0
7	h	28	0	25	13	0
7	i	28	0	25	2	0
7	j	28	0	25	12	0
7	m	28	0	25	0	0
7	n	28	0	25	2	0
7	o	28	0	25	5	0
7	p	28	0	25	5	0
7	r	28	0	25	0	0
7	u	28	0	25	9	0
7	v	28	0	25	4	0
7	w	28	0	25	9	0
7	z	28	0	25	2	0
8	S	39	0	34	0	0
8	X	39	0	34	0	0
8	d	39	0	34	0	0
8	l	39	0	34	5	0
8	y	39	0	34	4	0
9	T	72	0	61	0	0
10	U	83	0	70	6	0
11	Y	61	0	52	6	0
11	k	61	0	52	2	0
11	x	61	0	52	2	0
12	f	83	0	70	0	0
12	s	83	0	70	0	0
13	g	94	0	79	2	0
13	q	94	0	79	34	0
13	t	94	0	79	6	0
14	A	56	0	52	0	0
14	B	42	0	39	0	0
14	C	56	0	52	5	0
14	D	70	0	65	3	0
14	E	28	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	28	0	26	0	0
All	All	22934	0	22091	305	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 7.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG11	7:Q:1:NAG:O7	1.16	1.28
1:C:330:HIS:HE1	7:j:1:NAG:N2	1.29	1.28
1:C:330:HIS:CE1	7:j:1:NAG:HN2	1.56	1.23
1:A:173:TYR:OH	7:Q:1:NAG:H3	1.38	1.20
1:C:87:GLU:CG	14:C:601:NAG:H82	1.72	1.19
1:A:291:PRO:HG3	7:a:1:NAG:C6	1.77	1.14
1:D:87:GLU:CD	7:o:1:NAG:H81	1.74	1.13
1:C:293:GLN:CD	7:h:1:NAG:HN2	1.59	1.11
1:A:173:TYR:CZ	7:Q:1:NAG:H3	1.84	1.11
1:A:161:MET:HG3	1:A:162:THR:H	0.96	1.09
1:A:291:PRO:HG3	7:a:1:NAG:H62	1.13	1.09
2:F:631:TRP:CZ3	2:F:635:ILE:HG21	1.87	1.08
1:C:87:GLU:HG2	14:C:601:NAG:C8	1.84	1.08
1:C:330:HIS:CE1	7:j:1:NAG:N2	2.15	1.07
1:D:323:ILE:HD13	7:v:1:NAG:O6	1.52	1.07
6:N:53:HIS:HE1	13:q:8:MAN:O2	1.40	1.05
2:F:617:ARG:NH2	2:F:621:GLU:HG3	1.72	1.03
1:A:134:VAL:CG1	7:Q:1:NAG:O7	2.09	1.01
5:L:22:THR:HG22	5:L:72:ASN:OD1	1.59	1.01
6:N:53:HIS:CE1	13:q:8:MAN:O2	2.16	0.99
1:C:61:TYR:OH	1:C:66:HIS:C	2.04	0.99
1:D:321(A):ASP:OD1	7:p:1:NAG:C8	2.12	0.97
5:L:32:TYR:CD2	10:U:1:NAG:O6	2.18	0.96
1:A:161:MET:HG3	1:A:162:THR:N	1.78	0.96
4:J:52(A):HIS:HD2	4:J:97:LYS:HZ3	1.13	0.96
1:C:293:GLN:NE2	7:h:1:NAG:HN2	1.63	0.96
1:A:372:THR:CG2	11:Y:1:NAG:C8	2.45	0.95
1:D:321(A):ASP:OD1	7:p:1:NAG:H83	1.67	0.95
1:A:173:TYR:CE2	7:Q:1:NAG:H5	2.02	0.94
1:A:372:THR:HG23	11:Y:1:NAG:H82	1.48	0.94
1:C:293:GLN:HE22	7:h:1:NAG:H3	1.33	0.93
4:J:52(A):HIS:CD2	4:J:97:LYS:HZ3	1.87	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLU:OE1	7:o:1:NAG:H81	1.66	0.92
1:C:87:GLU:HG2	14:C:601:NAG:H82	0.94	0.92
4:J:98:HIS:CE1	13:q:3:BMA:H61	2.04	0.92
2:F:617:ARG:HH21	2:F:621:GLU:HG3	1.34	0.90
4:J:100(A):ARG:NH2	4:J:100(N):GLU:OE2	2.03	0.90
4:J:100:LEU:HD21	13:q:2:NAG:O3	1.71	0.89
1:D:61:TYR:OH	1:D:73:ALA:HA	1.71	0.89
1:D:130:GLN:HE21	13:q:1:NAG:H81	1.37	0.89
1:C:392:ASN:O	1:C:392:ASN:OD1	1.90	0.89
1:A:372:THR:HG23	11:Y:1:NAG:C8	2.02	0.89
5:L:32:TYR:CE2	10:U:1:NAG:O6	2.27	0.88
1:A:291:PRO:CG	7:a:1:NAG:H62	2.00	0.87
1:C:173:TYR:CZ	7:c:1:NAG:H3	2.09	0.86
1:A:161:MET:CG	1:A:162:THR:H	1.75	0.86
1:D:321(A):ASP:CG	7:p:1:NAG:H83	2.02	0.85
1:A:173:TYR:OH	7:Q:1:NAG:C3	2.24	0.85
1:C:293:GLN:NE2	7:h:1:NAG:N2	2.23	0.84
1:A:372:THR:CG2	11:Y:1:NAG:H82	2.05	0.84
1:A:61:TYR:OH	1:A:74:CYS:N	2.11	0.83
1:D:293:GLN:HE22	7:u:1:NAG:H3	1.43	0.83
7:n:1:NAG:H61	7:n:2:NAG:HN2	1.43	0.83
5:M:66:ARG:NH2	13:t:2:NAG:O7	2.13	0.82
7:z:1:NAG:H61	7:z:2:NAG:HN2	1.43	0.82
1:D:297:THR:HG23	7:w:1:NAG:H81	1.62	0.81
5:L:22:THR:CG2	5:L:72:ASN:OD1	2.28	0.81
1:A:65:LYS:HG2	1:A:66:HIS:HB3	1.62	0.81
1:A:372:THR:HG21	11:Y:1:NAG:H81	1.63	0.80
1:C:330:HIS:CE1	7:j:1:NAG:H82	2.17	0.80
4:J:52(A):HIS:CD2	4:J:97:LYS:NZ	2.50	0.80
6:N:28:THR:HG21	13:q:2:NAG:C8	2.10	0.80
1:C:330:HIS:HE1	7:j:1:NAG:C7	1.93	0.79
1:A:173:TYR:CZ	7:Q:1:NAG:C3	2.65	0.79
4:J:100(A):ARG:HG2	4:J:100(P):TRP:CH2	2.18	0.77
1:C:323:ILE:HD13	7:i:1:NAG:O6	1.83	0.77
1:C:65:LYS:HG2	1:C:72:HIS:CE1	2.19	0.76
1:A:372:THR:CG2	11:Y:1:NAG:H81	2.11	0.76
1:D:293:GLN:CD	7:u:1:NAG:HN2	1.93	0.76
2:F:618:ASN:OD1	2:F:621:GLU:CB	2.34	0.76
4:J:100:LEU:CD2	13:q:2:NAG:O3	2.34	0.76
4:J:100:LEU:HD23	13:q:2:NAG:H3	1.69	0.75
6:N:28:THR:HG21	13:q:2:NAG:H83	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:THR:HG21	7:j:1:NAG:H83	1.69	0.75
1:C:65:LYS:HG2	1:C:72:HIS:ND1	2.01	0.74
1:A:173:TYR:CZ	7:Q:1:NAG:H5	2.21	0.74
4:J:52(A):HIS:NE2	13:q:4:MAN:H4	2.02	0.74
11:k:1:NAG:H2	8:l:1:NAG:H5	1.70	0.73
1:D:323:ILE:HD13	7:v:1:NAG:HO6	1.51	0.73
1:C:330:HIS:CE1	7:j:1:NAG:C8	2.71	0.73
1:A:173:TYR:CE1	7:Q:1:NAG:C1	2.71	0.73
2:B:618:ASN:OD1	2:B:618:ASN:N	2.14	0.73
2:F:617:ARG:NH2	2:F:621:GLU:CG	2.50	0.73
4:J:100:LEU:CD2	13:q:2:NAG:C3	2.66	0.73
4:J:97:LYS:HE2	13:q:4:MAN:O4	1.89	0.71
1:C:297:THR:CG2	7:j:1:NAG:C8	2.69	0.71
4:J:100:LEU:CD2	13:q:2:NAG:H3	2.19	0.71
1:C:61:TYR:HH	1:C:66:HIS:C	1.99	0.70
3:H:111:VAL:HG12	3:H:111:VAL:O	1.89	0.70
4:J:52(A):HIS:CD2	13:q:4:MAN:O4	2.43	0.70
1:C:293:GLN:HE22	7:h:1:NAG:C3	2.05	0.70
1:A:293:GLN:HB2	7:V:1:NAG:H83	1.73	0.70
3:I:111:VAL:HG12	3:I:111:VAL:O	1.90	0.70
1:A:173:TYR:CE1	7:Q:1:NAG:H3	2.26	0.70
2:F:618:ASN:OD1	2:F:621:GLU:HB2	1.92	0.69
2:F:635:ILE:HD12	2:F:638:TYR:HD2	1.58	0.69
1:C:173:TYR:OH	7:c:1:NAG:H3	1.93	0.68
1:C:388:SER:CB	8:l:1:NAG:HO6	2.05	0.68
1:A:161:MET:HG3	1:A:162:THR:O	1.94	0.68
1:C:293:GLN:NE2	7:h:1:NAG:C2	2.57	0.67
1:D:130:GLN:NE2	13:q:1:NAG:H81	2.07	0.67
1:A:293:GLN:HB2	7:V:1:NAG:C8	2.24	0.67
1:C:330:HIS:CE1	7:j:1:NAG:C7	2.73	0.67
1:D:323:ILE:CD1	7:v:1:NAG:O6	2.38	0.67
1:A:173:TYR:CD2	7:Q:1:NAG:H5	2.30	0.66
1:C:164:GLU:N	1:C:164:GLU:OE1	2.28	0.66
14:C:601:NAG:O7	2:F:527:GLY:O	2.14	0.65
4:J:98:HIS:CD2	13:q:3:BMA:H4	2.32	0.65
1:A:365:SER:OG	3:H:56:GLN:NE2	2.29	0.65
2:F:618:ASN:OD1	2:F:618:ASN:N	2.30	0.65
14:D:648:NAG:O7	8:y:2:NAG:H81	1.96	0.64
1:C:297:THR:HG22	7:j:1:NAG:H82	1.79	0.64
4:J:96:SER:O	4:J:102:LEU:HD12	1.98	0.64
1:C:87:GLU:CB	14:C:601:NAG:H82	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HD3	1:A:72:HIS:CE1	2.33	0.63
5:K:22:THR:HB	5:K:72:ASN:OD1	1.98	0.63
4:J:97:LYS:CE	13:q:4:MAN:O4	2.47	0.63
1:D:130:GLN:HG2	13:q:1:NAG:C8	2.28	0.63
2:F:631:TRP:CZ3	2:F:635:ILE:CG2	2.75	0.63
6:N:28:THR:CG2	13:q:2:NAG:C8	2.76	0.63
2:F:631:TRP:CH2	2:F:635:ILE:HG21	2.32	0.63
5:M:66:ARG:O	5:M:67:TRP:HE3	1.82	0.63
14:D:648:NAG:O7	8:y:2:NAG:C8	2.46	0.62
1:C:392:ASN:OD1	1:C:392:ASN:C	2.43	0.62
1:D:189:LYS:HD2	1:D:189:LYS:N	2.14	0.62
2:F:618:ASN:OD1	2:F:621:GLU:HB3	2.00	0.62
1:D:130:GLN:CG	13:q:1:NAG:H83	2.29	0.62
3:G:111:VAL:HG12	3:G:111:VAL:O	2.00	0.61
1:A:323:ILE:CD1	7:W:1:NAG:O6	2.48	0.61
1:C:293:GLN:HB3	7:h:1:NAG:C8	2.30	0.61
2:F:635:ILE:O	2:F:635:ILE:HG13	2.00	0.61
4:J:98:HIS:CE1	13:q:3:BMA:C6	2.83	0.61
1:C:388:SER:CB	8:l:1:NAG:O6	2.48	0.60
4:J:52(A):HIS:NE2	13:q:4:MAN:C4	2.64	0.60
2:F:635:ILE:HD12	2:F:638:TYR:CD2	2.37	0.60
1:C:61:TYR:OH	1:C:66:HIS:CA	2.50	0.60
1:C:61:TYR:CZ	1:C:67:ASN:HB2	2.37	0.59
1:D:330:HIS:CD2	7:w:1:NAG:H82	2.37	0.59
1:D:293:GLN:NE2	7:u:1:NAG:H3	2.14	0.59
1:D:297:THR:CG2	7:w:1:NAG:H81	2.32	0.59
5:K:66:ARG:NH2	13:g:2:NAG:O7	2.35	0.59
1:C:297:THR:HG22	7:j:1:NAG:C8	2.33	0.58
1:D:330:HIS:NE2	7:w:1:NAG:C8	2.67	0.58
1:D:321(A):ASP:OD1	7:p:1:NAG:H82	2.01	0.58
5:M:66:ARG:CZ	13:t:2:NAG:O7	2.52	0.57
1:C:65:LYS:CG	1:C:72:HIS:CE1	2.88	0.57
4:J:97:LYS:NZ	13:q:4:MAN:O4	2.38	0.57
1:A:87:GLU:OE2	7:O:1:NAG:O7	2.24	0.56
5:M:27:GLY:HA2	13:t:1:NAG:H61	1.87	0.56
1:C:293:GLN:CD	7:h:1:NAG:N2	2.44	0.56
2:F:617:ARG:CZ	2:F:621:GLU:HG3	2.35	0.56
1:C:293:GLN:HB3	7:h:1:NAG:H82	1.88	0.55
1:D:330:HIS:CD2	7:w:1:NAG:HN2	2.24	0.55
4:J:52(A):HIS:CD2	13:q:4:MAN:C4	2.89	0.55
4:J:98:HIS:HA	13:q:3:BMA:O2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:100(A):ARG:HG2	4:J:100(P):TRP:CZ3	2.41	0.55
1:C:293:GLN:NE2	7:h:1:NAG:C1	2.69	0.55
1:D:293:GLN:NE2	7:u:1:NAG:HN2	2.04	0.55
1:D:87:GLU:OE1	7:o:1:NAG:C8	2.49	0.54
1:A:173:TYR:CZ	7:Q:1:NAG:C4	2.91	0.54
11:x:1:NAG:H2	8:y:1:NAG:H5	1.91	0.53
1:A:363:ASN:OD1	1:A:364:SER:O	2.27	0.53
1:A:56:SER:HG	1:A:61:TYR:HE2	1.56	0.53
1:A:307:ILE:C	1:A:307:ILE:HD12	2.34	0.53
1:D:297:THR:OG1	7:w:1:NAG:H83	2.09	0.52
1:A:203:GLN:C	1:A:203:GLN:CD	2.77	0.52
1:C:173:TYR:CE2	7:c:1:NAG:H3	2.45	0.52
1:D:290:THR:HB	1:D:291:PRO:HD2	1.92	0.52
1:D:130:GLN:HE21	13:q:1:NAG:C8	2.17	0.52
1:D:293:GLN:NE2	7:u:1:NAG:C1	2.72	0.52
5:L:32:TYR:CD2	10:U:1:NAG:C6	2.93	0.52
1:C:506:VAL:HG12	1:C:506:VAL:O	2.09	0.52
2:F:618:ASN:CG	2:F:621:GLU:HB2	2.35	0.52
1:D:130:GLN:NE2	13:q:1:NAG:C8	2.72	0.51
1:C:293:GLN:NE2	7:h:1:NAG:H3	2.15	0.51
1:D:130:GLN:CG	13:q:1:NAG:C8	2.87	0.51
5:K:7:SER:N	5:K:8:PRO:CD	2.73	0.51
1:C:65:LYS:CE	1:C:66:HIS:HD2	2.23	0.51
1:D:293:GLN:HB3	7:u:1:NAG:C8	2.41	0.51
3:H:5:LEU:HB2	3:H:23:GLU:HB2	1.93	0.51
7:O:2:NAG:H83	7:O:2:NAG:H3	1.92	0.50
11:x:1:NAG:O3	11:x:2:NAG:O5	2.26	0.50
1:A:323:ILE:HD12	7:W:1:NAG:O6	2.11	0.50
1:D:363:ASN:OD1	1:D:364:SER:N	2.45	0.50
7:o:2:NAG:H3	7:o:2:NAG:H83	1.92	0.50
1:A:164:GLU:H	1:A:164:GLU:CD	2.20	0.50
4:J:59:GLN:OE1	4:J:59:GLN:N	2.39	0.50
5:L:7:SER:N	5:L:8:PRO:CD	2.75	0.49
1:D:293:GLN:NE2	7:u:1:NAG:N2	2.61	0.49
2:B:607:ASN:C	2:B:607:ASN:OD1	2.53	0.49
1:C:321(A):ASP:CG	7:c:1:NAG:H83	2.37	0.49
1:A:61:TYR:HH	1:A:74:CYS:H	1.58	0.49
1:A:133:ASN:OD1	1:A:133:ASN:N	2.44	0.48
1:D:434:MET:SD	1:D:434:MET:C	2.96	0.48
5:K:22:THR:CB	5:K:72:ASN:OD1	2.60	0.48
5:M:27:GLY:CA	13:t:1:NAG:H61	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:O	1:A:84:ILE:HG13	2.13	0.48
2:B:637:ASN:OD1	2:B:637:ASN:N	2.46	0.48
1:D:297:THR:OG1	7:w:1:NAG:C8	2.61	0.48
1:A:87:GLU:HG3	7:O:1:NAG:O7	2.13	0.48
1:A:173:TYR:CZ	7:Q:1:NAG:C5	2.93	0.48
1:D:69:TRP:HA	1:D:69:TRP:CE3	2.49	0.48
5:K:67:TRP:HA	5:K:67:TRP:CE3	2.47	0.48
11:k:1:NAG:O7	8:l:1:NAG:H3	2.13	0.48
1:C:293:GLN:HB3	7:h:1:NAG:H83	1.95	0.48
5:M:69:GLN:OE1	5:M:69:GLN:N	2.36	0.48
5:L:32:TYR:CE2	10:U:1:NAG:C6	2.96	0.47
1:A:293:GLN:O	7:V:1:NAG:H82	2.13	0.47
1:C:388:SER:OG	8:l:1:NAG:O5	2.32	0.47
4:J:100(H):GLU:H	4:J:100(H):GLU:CD	2.19	0.47
3:H:111:VAL:O	3:H:111:VAL:CG1	2.61	0.47
13:g:2:NAG:O7	13:g:2:NAG:O3	2.28	0.47
1:A:291:PRO:HG3	7:a:1:NAG:O6	2.14	0.47
7:z:1:NAG:H61	7:z:2:NAG:N2	2.22	0.47
1:D:293:GLN:NE2	7:u:1:NAG:C2	2.77	0.47
3:G:11:VAL:O	3:G:11:VAL:HG13	2.14	0.47
4:J:52(A):HIS:CD2	13:q:4:MAN:HO4	2.33	0.47
1:C:297:THR:CG2	7:j:1:NAG:H83	2.33	0.46
4:J:52(A):HIS:HD2	13:q:4:MAN:O4	1.93	0.46
5:M:32:TYR:CD2	13:t:1:NAG:O6	2.56	0.46
1:A:392:ASN:OD1	1:A:392:ASN:C	2.58	0.46
3:H:100:TRP:CD1	3:H:100:TRP:N	2.83	0.46
5:L:32:TYR:CE2	10:U:1:NAG:H4	2.50	0.46
4:J:98:HIS:ND1	13:q:3:BMA:H61	2.30	0.46
5:K:91:TYR:N	5:K:91:TYR:CD1	2.84	0.46
2:B:610:TRP:N	2:B:610:TRP:CD1	2.84	0.46
1:D:293:GLN:HB3	7:u:1:NAG:H82	1.97	0.46
5:L:66:ARG:NH2	10:U:2:NAG:O7	2.49	0.46
1:C:65:LYS:HE3	1:C:66:HIS:HD2	1.80	0.45
3:I:96:ARG:O	3:I:96:ARG:HG2	2.16	0.45
1:A:293:GLN:CB	7:V:1:NAG:H82	2.46	0.45
3:I:91:PHE:HB3	3:I:106:GLY:HA2	1.99	0.45
1:A:173:TYR:CD1	7:Q:1:NAG:C1	2.99	0.45
7:v:1:NAG:H61	7:v:2:NAG:N2	2.32	0.45
4:J:93:LEU:C	4:J:93:LEU:HD12	2.41	0.45
1:D:464:THR:OG1	1:D:465:THR:N	2.50	0.45
1:A:363:ASN:OD1	1:A:363:ASN:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:CYS:HB3	1:A:204:ALA:HB3	2.00	0.44
7:i:1:NAG:H61	7:i:2:NAG:N2	2.32	0.44
1:C:426:MET:HB3	1:C:427:TRP:CE3	2.52	0.44
5:M:27:GLY:HA2	13:t:1:NAG:C6	2.47	0.44
6:N:28:THR:CG2	13:q:2:NAG:H81	2.46	0.44
5:L:106:LEU:HD23	5:L:106:LEU:N	2.32	0.44
1:A:293:GLN:CB	7:V:1:NAG:C8	2.96	0.44
1:D:138:ILE:HG23	1:D:138:ILE:O	2.18	0.44
7:n:1:NAG:H61	7:n:2:NAG:N2	2.22	0.44
1:D:465:THR:O	1:D:465:THR:HG22	2.17	0.44
5:M:97:PHE:CD1	5:M:97:PHE:N	2.85	0.44
2:F:635:ILE:O	2:F:639:THR:HG23	2.18	0.44
7:W:1:NAG:H61	7:W:2:NAG:N2	2.32	0.43
1:C:61:TYR:OH	1:C:66:HIS:O	2.23	0.43
5:M:73:LEU:C	5:M:73:LEU:HD23	2.43	0.43
1:D:59:LYS:CE	1:D:61:TYR:OH	2.67	0.43
3:G:91:PHE:HB3	3:G:106:GLY:HA2	2.00	0.43
5:L:73:LEU:C	5:L:73:LEU:HD23	2.44	0.43
1:A:166:ARG:HA	1:A:166:ARG:HD3	1.89	0.43
1:A:173:TYR:CE1	7:Q:1:NAG:C3	2.98	0.43
1:D:59:LYS:HE3	1:D:61:TYR:OH	2.19	0.43
2:E:635:ILE:HG13	2:E:635:ILE:O	2.19	0.43
1:A:430:ILE:C	1:A:430:ILE:HD12	2.44	0.43
2:E:621:GLU:O	2:E:621:GLU:HG2	2.18	0.42
4:J:100(A):ARG:HH21	4:J:100(N):GLU:CD	2.17	0.42
5:L:4:MET:HE2	5:L:99:VAL:HG13	2.01	0.42
5:L:11:LEU:O	5:L:105:ASP:N	2.52	0.42
1:D:321(A):ASP:OD1	7:p:1:NAG:N2	2.50	0.42
1:D:330:HIS:NE2	7:w:1:NAG:H83	2.34	0.42
3:I:91:PHE:HB3	3:I:106:GLY:CA	2.48	0.42
1:A:65:LYS:HD3	1:A:72:HIS:ND1	2.34	0.42
1:C:80:ASN:N	1:C:81:PRO:CD	2.83	0.42
1:D:298:ARG:O	1:D:298:ARG:HD2	2.19	0.42
1:A:65:LYS:HA	1:A:66:HIS:HA	1.79	0.42
1:A:161:MET:CG	1:A:162:THR:O	2.66	0.42
1:A:293:GLN:C	7:V:1:NAG:H82	2.44	0.42
5:L:1:ASP:OD1	5:L:1:ASP:C	2.61	0.42
5:L:52:SER:OG	5:L:53:LYS:N	2.51	0.42
1:D:117:LYS:HB3	1:D:118:PRO:HD3	2.02	0.42
1:D:330:HIS:NE2	7:w:1:NAG:H82	2.35	0.42
3:I:100:TRP:N	3:I:100:TRP:CD1	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:O	2:B:606:THR:OG1	2.36	0.41
1:A:138:ILE:O	1:A:138:ILE:HG23	2.20	0.41
1:C:503:ARG:HB3	2:F:607:ASN:HB2	2.01	0.41
1:D:61:TYR:HH	1:D:73:ALA:HA	1.81	0.41
1:A:280:ASN:C	1:A:280:ASN:OD1	2.63	0.41
1:C:138:ILE:O	1:C:138:ILE:HG13	2.20	0.41
14:D:648:NAG:O7	8:y:2:NAG:H82	2.18	0.41
3:G:27:TYR:OH	3:G:94:ARG:NH1	2.53	0.41
3:H:56:GLN:HA	3:H:57:PRO:HD2	1.90	0.41
3:H:91:PHE:HB3	3:H:106:GLY:HA2	2.01	0.41
5:K:73:LEU:HD23	5:K:73:LEU:C	2.46	0.41
6:N:28:THR:HG21	13:q:2:NAG:H81	1.95	0.41
1:D:74:CYS:SG	1:D:75:VAL:N	2.94	0.41
6:N:28:THR:HB	13:q:2:NAG:H81	2.03	0.41
1:A:159:PHE:CD1	1:A:159:PHE:N	2.89	0.41
3:I:28:ASN:OD1	3:I:28:ASN:C	2.63	0.41
1:D:501:CYS:SG	2:F:662:ALA:HB1	2.61	0.41
2:B:614:TRP:N	2:B:614:TRP:CD1	2.88	0.40
1:C:293:GLN:CB	7:h:1:NAG:H82	2.49	0.40
5:M:7:SER:N	5:M:8:PRO:CD	2.84	0.40
1:A:205:CYS:N	1:A:206:PRO:CD	2.84	0.40
1:C:117:LYS:N	1:C:118:PRO:CD	2.84	0.40
1:A:204:ALA:O	1:A:205:CYS:HB2	2.21	0.40
1:D:87:GLU:OE1	7:o:1:NAG:O7	2.40	0.40
4:J:5:VAL:O	4:J:22:CYS:HA	2.21	0.40
5:L:55:GLU:HA	5:L:55:GLU:OE1	2.21	0.40
1:A:203:GLN:OE1	1:A:203:GLN:O	2.40	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	444/481 (92%)	433 (98%)	11 (2%)	0	100	100
1	C	445/481 (92%)	434 (98%)	10 (2%)	1 (0%)	43	77
1	D	446/481 (93%)	439 (98%)	7 (2%)	0	100	100
2	B	122/153 (80%)	122 (100%)	0	0	100	100
2	E	120/153 (78%)	118 (98%)	2 (2%)	0	100	100
2	F	119/153 (78%)	117 (98%)	2 (2%)	0	100	100
3	G	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	H	119/226 (53%)	117 (98%)	2 (2%)	0	100	100
3	I	119/226 (53%)	119 (100%)	0	0	100	100
4	J	138/267 (52%)	137 (99%)	1 (1%)	0	100	100
5	K	96/206 (47%)	93 (97%)	2 (2%)	1 (1%)	12	47
5	L	96/206 (47%)	92 (96%)	2 (2%)	2 (2%)	5	30
5	M	96/206 (47%)	93 (97%)	2 (2%)	1 (1%)	12	47
6	N	110/219 (50%)	108 (98%)	2 (2%)	0	100	100
All	All	2589/3684 (70%)	2539 (98%)	45 (2%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	52	SER
1	C	80	ASN
5	M	52	SER
5	K	7	SER
5	L	7	SER

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	402/428 (94%)	399 (99%)	3 (1%)	76	79
1	C	403/428 (94%)	403 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	404/428 (94%)	403 (100%)	1 (0%)	87	85
2	B	109/129 (84%)	107 (98%)	2 (2%)	51	67
2	E	107/129 (83%)	106 (99%)	1 (1%)	70	76
2	F	106/129 (82%)	105 (99%)	1 (1%)	70	76
3	G	102/193 (53%)	102 (100%)	0	100	100
3	H	102/193 (53%)	102 (100%)	0	100	100
3	I	102/193 (53%)	102 (100%)	0	100	100
4	J	115/223 (52%)	115 (100%)	0	100	100
5	K	86/183 (47%)	86 (100%)	0	100	100
5	L	86/183 (47%)	86 (100%)	0	100	100
5	M	86/183 (47%)	86 (100%)	0	100	100
6	N	95/191 (50%)	95 (100%)	0	100	100
All	All	2305/3213 (72%)	2297 (100%)	8 (0%)	84	84

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

Mol	Chain	Res	Type
1	A	65	LYS
1	A	133	ASN
1	A	363	ASN
2	B	618	ASN
2	B	637	ASN
1	D	65	LYS
2	E	618	ASN
2	F	618	ASN

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

Mol	Chain	Res	Type
1	A	72	HIS
1	A	293	GLN
2	B	658	GLN
1	C	66	HIS
1	C	72	HIS
1	C	293	GLN
1	C	330	HIS
1	D	105	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	130	GLN
1	D	293	GLN
1	D	356	ASN
1	D	377	ASN
1	D	422	GLN
3	G	56	GLN
3	H	56	GLN
3	I	6	GLN
3	I	46	GLN
4	J	52(A)	HIS
4	J	98	HIS
5	K	76	ASN
5	L	37	GLN
5	M	37	GLN
6	N	53	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

137 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	0	1	7,2	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	0	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
7	NAG	1	1	7,2	14,14,15	0.51	0	17,19,21	2.28	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	1	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
7	NAG	2	1	7,5	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	2	2	7	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
7	NAG	3	1	7,5	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	3	2	7	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
7	NAG	4	1	7,5	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
7	NAG	4	2	7	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
7	NAG	O	1	1,7	14,14,15	0.78	1 (7%)	17,19,21	0.92	2 (11%)
7	NAG	O	2	7	14,14,15	0.45	0	17,19,21	1.55	3 (17%)
7	NAG	P	1	1,7	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
7	NAG	P	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
7	NAG	Q	1	1,7	14,14,15	0.26	0	17,19,21	0.56	0
7	NAG	Q	2	7	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
7	NAG	R	1	1,7	14,14,15	0.48	0	17,19,21	2.27	3 (17%)
7	NAG	R	2	7	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
8	NAG	S	1	1,8	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
8	NAG	S	2	8	14,14,15	0.51	0	17,19,21	1.34	3 (17%)
8	BMA	S	3	8	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
9	NAG	T	1	1,9	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
9	NAG	T	2	9	14,14,15	0.50	0	17,19,21	1.32	3 (17%)
9	BMA	T	3	9	11,11,12	0.67	0	15,15,17	1.43	3 (20%)
9	MAN	T	4	9	11,11,12	0.55	0	15,15,17	1.49	2 (13%)
9	MAN	T	5	9	11,11,12	0.59	0	15,15,17	2.31	5 (33%)
9	MAN	T	6	9	11,11,12	0.60	0	15,15,17	2.22	3 (20%)
10	NAG	U	1	1,10	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
10	NAG	U	2	10	14,14,15	0.41	0	17,19,21	0.47	0
10	BMA	U	3	10	11,11,12	1.65	4 (36%)	15,15,17	1.79	2 (13%)
10	MAN	U	4	10	11,11,12	0.61	0	15,15,17	2.21	3 (20%)
10	MAN	U	5	10	11,11,12	0.57	0	15,15,17	1.92	5 (33%)
10	MAN	U	6	10	11,11,12	0.60	0	15,15,17	2.27	6 (40%)
10	MAN	U	7	10	11,11,12	1.65	3 (27%)	15,15,17	1.28	2 (13%)
7	NAG	V	1	1,7	14,14,15	0.31	0	17,19,21	0.72	0
7	NAG	V	2	7	14,14,15	0.67	0	17,19,21	0.54	0
7	NAG	W	1	1,7	14,14,15	0.46	0	17,19,21	0.43	0
7	NAG	W	2	7	14,14,15	0.61	0	17,19,21	0.57	0
8	NAG	X	1	1,8	14,14,15	0.50	0	17,19,21	2.27	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	X	2	8	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
8	BMA	X	3	8	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
11	NAG	Y	1	1,11	14,14,15	0.32	0	17,19,21	0.60	0
11	NAG	Y	2	11	14,14,15	0.35	0	17,19,21	0.84	1 (5%)
11	BMA	Y	3	11	11,11,12	0.65	0	15,15,17	1.43	3 (20%)
11	MAN	Y	4	11	11,11,12	0.53	0	15,15,17	1.47	2 (13%)
11	MAN	Y	5	11	11,11,12	0.63	0	15,15,17	2.19	3 (20%)
7	NAG	Z	1	1,7	14,14,15	0.99	1 (7%)	17,19,21	1.05	1 (5%)
7	NAG	Z	2	7	14,14,15	0.50	0	17,19,21	0.56	0
7	NAG	a	1	1,7	14,14,15	0.49	0	17,19,21	0.56	0
7	NAG	a	2	7	14,14,15	0.41	0	17,19,21	0.45	0
7	NAG	b	1	1,7	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
7	NAG	b	2	7	14,14,15	0.50	0	17,19,21	1.32	3 (17%)
7	NAG	c	1	1,7	14,14,15	0.27	0	17,19,21	0.55	0
7	NAG	c	2	7	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
8	NAG	d	1	1,8	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
8	NAG	d	2	8	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
8	BMA	d	3	8	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
7	NAG	e	1	1,7	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
7	NAG	e	2	7	14,14,15	0.53	0	17,19,21	1.33	3 (17%)
12	NAG	f	1	1,12	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
12	NAG	f	2	12	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
12	BMA	f	3	12	11,11,12	0.67	0	15,15,17	1.43	3 (20%)
12	MAN	f	4	12	11,11,12	0.57	0	15,15,17	1.50	2 (13%)
12	MAN	f	5	12	11,11,12	0.60	0	15,15,17	2.31	5 (33%)
12	MAN	f	6	12	11,11,12	0.59	0	15,15,17	2.21	3 (20%)
12	MAN	f	7	12	11,11,12	0.55	0	15,15,17	1.92	5 (33%)
13	NAG	g	1	1,13	14,14,15	0.76	1 (7%)	17,19,21	0.69	0
13	NAG	g	2	13	14,14,15	0.41	0	17,19,21	0.45	0
13	BMA	g	3	13	11,11,12	1.66	3 (27%)	15,15,17	1.81	2 (13%)
13	MAN	g	4	13	11,11,12	1.67	3 (27%)	15,15,17	1.27	2 (13%)
13	MAN	g	5	13	11,11,12	2.27	4 (36%)	15,15,17	1.68	3 (20%)
13	MAN	g	6	13	11,11,12	0.58	0	15,15,17	2.22	3 (20%)
13	MAN	g	7	13	11,11,12	0.58	0	15,15,17	1.93	5 (33%)
13	MAN	g	8	13	11,11,12	0.62	0	15,15,17	2.27	7 (46%)
7	NAG	h	1	1,7	14,14,15	0.32	0	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	h	2	7	14,14,15	0.67	0	17,19,21	0.54	0
7	NAG	i	1	1,7	14,14,15	0.44	0	17,19,21	0.43	0
7	NAG	i	2	7	14,14,15	0.61	0	17,19,21	0.58	0
7	NAG	j	1	1,7	14,14,15	0.40	0	17,19,21	0.76	1 (5%)
7	NAG	j	2	7	14,14,15	0.53	0	17,19,21	0.55	0
11	NAG	k	1	1,11	14,14,15	0.34	0	17,19,21	0.59	0
11	NAG	k	2	11	14,14,15	0.36	0	17,19,21	0.85	1 (5%)
11	BMA	k	3	11	11,11,12	0.66	0	15,15,17	1.45	3 (20%)
11	MAN	k	4	11	11,11,12	0.55	0	15,15,17	1.48	2 (13%)
11	MAN	k	5	11	11,11,12	0.63	0	15,15,17	2.20	3 (20%)
8	NAG	l	1	1,8	14,14,15	0.96	1 (7%)	17,19,21	1.05	1 (5%)
8	NAG	l	2	8	14,14,15	0.52	0	17,19,21	0.56	0
8	BMA	l	3	8	11,11,12	0.62	0	15,15,17	1.42	3 (20%)
7	NAG	m	1	1,7	14,14,15	0.49	0	17,19,21	2.28	3 (17%)
7	NAG	m	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
7	NAG	n	1	1,7	14,14,15	0.49	0	17,19,21	0.57	0
7	NAG	n	2	7	14,14,15	0.40	0	17,19,21	0.44	0
7	NAG	o	1	1,7	14,14,15	0.79	1 (7%)	17,19,21	0.91	2 (11%)
7	NAG	o	2	7	14,14,15	0.45	0	17,19,21	1.55	3 (17%)
7	NAG	p	1	1,7	14,14,15	0.27	0	17,19,21	0.55	0
7	NAG	p	2	7	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
13	NAG	q	1	1,13	14,14,15	1.48	4 (28%)	17,19,21	1.04	1 (5%)
13	NAG	q	2	13	14,14,15	1.35	2 (14%)	17,19,21	1.26	2 (11%)
13	BMA	q	3	13	11,11,12	1.40	2 (18%)	15,15,17	0.95	1 (6%)
13	MAN	q	4	13	11,11,12	1.50	3 (27%)	15,15,17	1.59	2 (13%)
13	MAN	q	5	13	11,11,12	1.55	3 (27%)	15,15,17	1.61	2 (13%)
13	MAN	q	6	13	11,11,12	1.64	3 (27%)	15,15,17	1.44	1 (6%)
13	MAN	q	7	13	11,11,12	1.55	3 (27%)	15,15,17	1.33	1 (6%)
13	MAN	q	8	13	11,11,12	1.45	2 (18%)	15,15,17	1.39	1 (6%)
7	NAG	r	1	1,7	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
7	NAG	r	2	7	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
12	NAG	s	1	1,12	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
12	NAG	s	2	12	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
12	BMA	s	3	12	11,11,12	0.67	0	15,15,17	1.43	3 (20%)
12	MAN	s	4	12	11,11,12	0.57	0	15,15,17	1.50	3 (20%)
12	MAN	s	5	12	11,11,12	0.59	0	15,15,17	2.30	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	s	6	12	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
12	MAN	s	7	12	11,11,12	0.56	0	15,15,17	1.92	5 (33%)
13	NAG	t	1	1,13	14,14,15	0.77	1 (7%)	17,19,21	0.69	0
13	NAG	t	2	13	14,14,15	0.41	0	17,19,21	0.47	0
13	BMA	t	3	13	11,11,12	1.66	4 (36%)	15,15,17	1.80	2 (13%)
13	MAN	t	4	13	11,11,12	1.66	3 (27%)	15,15,17	1.27	2 (13%)
13	MAN	t	5	13	11,11,12	2.28	4 (36%)	15,15,17	1.68	3 (20%)
13	MAN	t	6	13	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
13	MAN	t	7	13	11,11,12	0.58	0	15,15,17	1.93	5 (33%)
13	MAN	t	8	13	11,11,12	0.60	0	15,15,17	2.26	7 (46%)
7	NAG	u	1	1,7	14,14,15	0.30	0	17,19,21	0.73	0
7	NAG	u	2	7	14,14,15	0.66	0	17,19,21	0.54	0
7	NAG	v	1	1,7	14,14,15	0.44	0	17,19,21	0.42	0
7	NAG	v	2	7	14,14,15	0.60	0	17,19,21	0.57	0
7	NAG	w	1	1,7	14,14,15	0.39	0	17,19,21	0.76	1 (5%)
7	NAG	w	2	7	14,14,15	0.54	0	17,19,21	0.55	0
11	NAG	x	1	1,11	14,14,15	0.33	0	17,19,21	0.59	0
11	NAG	x	2	11	14,14,15	0.37	0	17,19,21	0.84	1 (5%)
11	BMA	x	3	11	11,11,12	0.65	0	15,15,17	1.44	3 (20%)
11	MAN	x	4	11	11,11,12	0.53	0	15,15,17	1.47	2 (13%)
11	MAN	x	5	11	11,11,12	0.60	0	15,15,17	2.19	3 (20%)
8	NAG	y	1	1,8	14,14,15	0.97	1 (7%)	17,19,21	1.06	1 (5%)
8	NAG	y	2	8	14,14,15	0.51	0	17,19,21	0.56	0
8	BMA	y	3	8	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
7	NAG	z	1	1,7	14,14,15	0.51	0	17,19,21	0.57	0
7	NAG	z	2	7	14,14,15	0.40	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	0	1	7,2	-	1/6/23/26	0/1/1/1
7	NAG	0	2	7	-	0/6/23/26	0/1/1/1
7	NAG	1	1	7,2	-	1/6/23/26	0/1/1/1
7	NAG	1	2	7	-	0/6/23/26	0/1/1/1
7	NAG	2	1	7,5	-	1/6/23/26	0/1/1/1
7	NAG	2	2	7	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	u	2	7	-	0/6/23/26	0/1/1/1
7	NAG	v	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	v	2	7	-	2/6/23/26	0/1/1/1
7	NAG	w	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	w	2	7	-	2/6/23/26	0/1/1/1
11	NAG	x	1	1,11	-	3/6/23/26	0/1/1/1
11	NAG	x	2	11	-	2/6/23/26	0/1/1/1
11	BMA	x	3	11	-	2/2/19/22	0/1/1/1
11	MAN	x	4	11	-	0/2/19/22	0/1/1/1
11	MAN	x	5	11	-	0/2/19/22	0/1/1/1
8	NAG	y	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	y	3	8	-	2/2/19/22	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

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	5	MAN	C4-C5	4.33	1.62	1.53
13	t	5	MAN	C4-C5	4.32	1.62	1.53
13	t	5	MAN	C4-C3	3.69	1.61	1.52
13	g	5	MAN	C4-C3	3.67	1.61	1.52
7	Z	1	NAG	O5-C1	3.49	1.49	1.43
8	y	1	NAG	O5-C1	3.42	1.49	1.43
8	l	1	NAG	O5-C1	3.39	1.49	1.43
13	q	6	MAN	O5-C1	3.35	1.49	1.43
13	g	4	MAN	O5-C5	3.21	1.49	1.43
10	U	7	MAN	O5-C5	3.20	1.49	1.43
13	t	4	MAN	O5-C5	3.15	1.49	1.43
13	q	5	MAN	O5-C1	3.08	1.48	1.43
13	q	4	MAN	O5-C1	3.07	1.48	1.43
13	q	8	MAN	O5-C1	3.07	1.48	1.43
13	q	7	MAN	O5-C1	3.04	1.48	1.43
13	t	5	MAN	C2-C3	2.94	1.57	1.52
13	q	8	MAN	O5-C5	2.88	1.49	1.43
13	q	1	NAG	O5-C1	2.87	1.48	1.43
13	g	5	MAN	C2-C3	2.86	1.56	1.52
13	q	2	NAG	O5-C1	2.85	1.48	1.43
13	q	3	BMA	O5-C1	2.85	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	q	5	MAN	O5-C5	2.79	1.48	1.43
13	q	6	MAN	O5-C5	2.75	1.48	1.43
13	q	4	MAN	O5-C5	2.68	1.48	1.43
13	q	7	MAN	O5-C5	2.66	1.48	1.43
13	q	1	NAG	O5-C5	2.57	1.48	1.43
13	t	4	MAN	C4-C5	2.49	1.58	1.53
13	t	4	MAN	C4-C3	2.46	1.58	1.52
10	U	7	MAN	C4-C5	2.45	1.58	1.53
13	g	4	MAN	C4-C5	2.45	1.58	1.53
10	U	7	MAN	C4-C3	2.45	1.58	1.52
13	q	3	BMA	O5-C5	2.43	1.48	1.43
13	g	3	BMA	O5-C5	2.43	1.48	1.43
13	t	3	BMA	O5-C5	2.42	1.48	1.43
13	g	3	BMA	C2-C3	2.41	1.56	1.52
13	g	4	MAN	C4-C3	2.40	1.58	1.52
13	t	3	BMA	C2-C3	2.40	1.56	1.52
10	U	3	BMA	C2-C3	2.38	1.56	1.52
10	U	3	BMA	O5-C5	2.38	1.48	1.43
13	q	7	MAN	O2-C2	2.36	1.48	1.43
13	t	5	MAN	O5-C5	2.33	1.48	1.43
13	q	1	NAG	O4-C4	2.30	1.48	1.43
10	U	1	NAG	O5-C1	-2.29	1.39	1.43
13	g	5	MAN	O5-C5	2.28	1.47	1.43
13	t	1	NAG	O5-C1	-2.28	1.39	1.43
13	g	1	NAG	O5-C1	-2.25	1.39	1.43
13	g	3	BMA	C4-C5	2.21	1.57	1.53
13	q	6	MAN	O3-C3	2.21	1.48	1.43
7	o	1	NAG	O5-C1	-2.19	1.40	1.43
13	q	5	MAN	O2-C2	2.19	1.47	1.43
13	t	3	BMA	C4-C5	2.18	1.57	1.53
7	O	1	NAG	O5-C1	-2.17	1.40	1.43
10	U	3	BMA	C4-C5	2.14	1.57	1.53
13	q	4	MAN	O2-C2	2.11	1.47	1.43
13	q	2	NAG	O5-C5	2.08	1.47	1.43
13	t	3	BMA	O2-C2	2.05	1.47	1.43
10	U	3	BMA	O2-C2	2.04	1.47	1.43
13	q	1	NAG	C8-C7	2.00	1.54	1.50

All (285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	1	NAG	O5-C1-C2	-7.54	99.63	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4	1	NAG	O5-C1-C2	-7.54	99.63	111.29
7	b	1	NAG	O5-C1-C2	-7.54	99.63	111.29
7	m	1	NAG	O5-C1-C2	-7.54	99.63	111.29
12	s	1	NAG	O5-C1-C2	-7.53	99.64	111.29
7	1	1	NAG	O5-C1-C2	-7.53	99.64	111.29
7	2	1	NAG	O5-C1-C2	-7.52	99.66	111.29
12	f	1	NAG	O5-C1-C2	-7.51	99.67	111.29
8	S	1	NAG	O5-C1-C2	-7.51	99.67	111.29
7	0	1	NAG	O5-C1-C2	-7.51	99.67	111.29
8	d	1	NAG	O5-C1-C2	-7.51	99.68	111.29
7	e	1	NAG	O5-C1-C2	-7.51	99.68	111.29
7	3	1	NAG	O5-C1-C2	-7.50	99.68	111.29
7	R	1	NAG	O5-C1-C2	-7.50	99.69	111.29
8	X	1	NAG	O5-C1-C2	-7.49	99.70	111.29
7	r	1	NAG	O5-C1-C2	-7.49	99.71	111.29
7	P	1	NAG	O5-C1-C2	-7.49	99.71	111.29
13	t	6	MAN	C1-C2-C3	5.92	118.27	109.64
9	T	6	MAN	C1-C2-C3	5.91	118.25	109.64
13	g	6	MAN	C1-C2-C3	5.90	118.23	109.64
12	s	6	MAN	C1-C2-C3	5.89	118.22	109.64
10	U	4	MAN	C1-C2-C3	5.88	118.20	109.64
12	f	6	MAN	C1-C2-C3	5.87	118.19	109.64
11	k	5	MAN	C1-C2-C3	5.85	118.17	109.64
11	x	5	MAN	C1-C2-C3	5.84	118.14	109.64
11	Y	5	MAN	C1-C2-C3	5.82	118.12	109.64
13	g	3	BMA	C1-O5-C5	5.79	119.94	112.19
13	t	3	BMA	C1-O5-C5	5.70	119.83	112.19
10	U	3	BMA	C1-O5-C5	5.70	119.82	112.19
13	q	5	MAN	C1-O5-C5	5.13	119.06	112.19
13	q	4	MAN	C1-O5-C5	4.94	118.80	112.19
12	f	5	MAN	C1-O5-C5	4.85	118.68	112.19
9	T	5	MAN	C1-O5-C5	4.84	118.68	112.19
13	g	8	MAN	C6-C5-C4	-4.83	101.16	113.02
10	U	6	MAN	C6-C5-C4	-4.83	101.16	113.02
12	s	5	MAN	C1-O5-C5	4.81	118.64	112.19
13	t	8	MAN	C6-C5-C4	-4.81	101.22	113.02
7	o	2	NAG	C2-N2-C7	4.74	129.25	122.90
7	O	2	NAG	C2-N2-C7	4.72	129.22	122.90
13	q	8	MAN	C1-O5-C5	4.66	118.44	112.19
12	s	5	MAN	O2-C2-C1	4.47	119.47	109.22
9	T	5	MAN	O2-C2-C1	4.46	119.44	109.22
12	f	5	MAN	O2-C2-C1	4.45	119.41	109.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	q	6	MAN	C1-O5-C5	4.16	117.77	112.19
12	s	6	MAN	C2-C3-C4	-4.07	103.69	110.86
9	T	6	MAN	C2-C3-C4	-4.07	103.70	110.86
13	g	6	MAN	C2-C3-C4	-4.04	103.75	110.86
13	t	6	MAN	C2-C3-C4	-4.04	103.76	110.86
12	f	6	MAN	C2-C3-C4	-4.03	103.78	110.86
10	U	4	MAN	C2-C3-C4	-4.02	103.78	110.86
12	f	5	MAN	O2-C2-C3	-3.97	101.94	110.15
11	k	5	MAN	C2-C3-C4	-3.96	103.89	110.86
11	Y	5	MAN	C2-C3-C4	-3.96	103.90	110.86
9	T	5	MAN	O2-C2-C3	-3.95	101.96	110.15
11	x	5	MAN	C2-C3-C4	-3.95	103.91	110.86
13	g	5	MAN	C1-O5-C5	3.95	117.47	112.19
13	q	7	MAN	C1-O5-C5	3.93	117.46	112.19
12	s	5	MAN	O2-C2-C3	-3.93	102.02	110.15
13	q	2	NAG	C1-O5-C5	3.92	117.45	112.19
13	t	5	MAN	C1-O5-C5	3.90	117.42	112.19
12	s	7	MAN	O4-C4-C3	-3.89	101.19	110.38
12	f	7	MAN	O4-C4-C3	-3.87	101.26	110.38
13	g	7	MAN	O4-C4-C3	-3.86	101.28	110.38
13	t	7	MAN	O4-C4-C3	-3.86	101.28	110.38
10	U	5	MAN	O4-C4-C3	-3.85	101.31	110.38
10	U	7	MAN	C1-O5-C5	3.76	117.23	112.19
13	g	4	MAN	C1-O5-C5	3.74	117.20	112.19
13	t	4	MAN	C1-O5-C5	3.73	117.19	112.19
13	g	8	MAN	O4-C4-C3	-3.55	102.02	110.38
10	U	6	MAN	O4-C4-C3	-3.53	102.07	110.38
13	t	8	MAN	O4-C4-C3	-3.52	102.09	110.38
12	s	7	MAN	O4-C4-C5	3.25	117.33	109.32
12	f	7	MAN	O4-C4-C5	3.22	117.26	109.32
13	g	7	MAN	O4-C4-C5	3.22	117.25	109.32
13	t	7	MAN	O4-C4-C5	3.21	117.23	109.32
10	U	5	MAN	O4-C4-C5	3.20	117.21	109.32
8	y	1	NAG	C1-O5-C5	3.17	116.43	112.19
8	l	1	NAG	C1-O5-C5	3.15	116.41	112.19
7	Z	1	NAG	C1-O5-C5	3.15	116.40	112.19
12	s	2	NAG	O5-C5-C6	-3.13	101.57	107.66
13	t	8	MAN	C3-C4-C5	-3.11	104.59	110.23
12	f	2	NAG	O5-C5-C6	-3.10	101.62	107.66
13	g	8	MAN	C3-C4-C5	-3.10	104.62	110.23
8	S	2	NAG	O5-C5-C6	-3.10	101.64	107.66
7	P	2	NAG	O5-C5-C6	-3.09	101.66	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1	2	NAG	O5-C5-C6	-3.08	101.67	107.66
8	X	2	NAG	O5-C5-C6	-3.08	101.67	107.66
7	3	2	NAG	O5-C5-C6	-3.07	101.68	107.66
7	b	2	NAG	O5-C5-C6	-3.07	101.69	107.66
7	m	2	NAG	O5-C5-C6	-3.07	101.69	107.66
7	4	2	NAG	O5-C5-C6	-3.07	101.69	107.66
10	U	6	MAN	C3-C4-C5	-3.07	104.67	110.23
9	T	2	NAG	O5-C5-C6	-3.07	101.69	107.66
7	R	2	NAG	O5-C5-C6	-3.06	101.70	107.66
7	2	2	NAG	O5-C5-C6	-3.06	101.70	107.66
7	r	2	NAG	O5-C5-C6	-3.05	101.73	107.66
7	0	2	NAG	O5-C5-C6	-3.05	101.73	107.66
7	e	2	NAG	O5-C5-C6	-3.04	101.76	107.66
8	d	2	NAG	O5-C5-C6	-3.03	101.77	107.66
13	q	1	NAG	C1-O5-C5	3.00	116.20	112.19
12	s	3	BMA	O2-C2-C3	2.93	116.23	110.15
11	k	3	BMA	O2-C2-C3	2.93	116.22	110.15
12	f	3	BMA	O2-C2-C3	2.92	116.20	110.15
7	b	1	NAG	O7-C7-C8	-2.91	116.86	122.05
9	T	3	BMA	O2-C2-C3	2.91	116.19	110.15
11	x	3	BMA	O2-C2-C3	2.91	116.19	110.15
11	Y	3	BMA	O2-C2-C3	2.91	116.17	110.15
7	2	1	NAG	O7-C7-C8	-2.90	116.88	122.05
7	P	1	NAG	O7-C7-C8	-2.90	116.89	122.05
7	4	1	NAG	O7-C7-C8	-2.89	116.90	122.05
8	d	1	NAG	O7-C7-C8	-2.89	116.91	122.05
7	3	1	NAG	O7-C7-C8	-2.89	116.92	122.05
8	X	1	NAG	O7-C7-C8	-2.88	116.92	122.05
7	1	1	NAG	O7-C7-C8	-2.88	116.93	122.05
8	S	1	NAG	O7-C7-C8	-2.88	116.93	122.05
9	T	1	NAG	O7-C7-C8	-2.87	116.94	122.05
7	0	1	NAG	O7-C7-C8	-2.87	116.94	122.05
8	X	3	BMA	O2-C2-C3	2.87	116.09	110.15
7	m	1	NAG	O7-C7-C8	-2.87	116.95	122.05
7	R	1	NAG	O7-C7-C8	-2.87	116.95	122.05
13	t	8	MAN	O2-C2-C3	-2.86	104.22	110.15
10	U	6	MAN	O2-C2-C3	-2.86	104.23	110.15
8	d	3	BMA	O2-C2-C3	2.86	116.07	110.15
12	f	1	NAG	O7-C7-C8	-2.84	116.99	122.05
8	S	3	BMA	O2-C2-C3	2.84	116.04	110.15
12	s	1	NAG	O7-C7-C8	-2.84	117.00	122.05
8	l	3	BMA	O2-C2-C3	2.84	116.03	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	1	NAG	O7-C7-C8	-2.83	117.01	122.05
8	y	3	BMA	O2-C2-C3	2.83	116.02	110.15
7	e	1	NAG	O7-C7-C8	-2.83	117.02	122.05
13	g	8	MAN	O2-C2-C3	-2.82	104.30	110.15
13	t	5	MAN	C1-C2-C3	-2.79	105.58	109.64
13	g	5	MAN	C1-C2-C3	-2.75	105.64	109.64
8	S	1	NAG	C4-C3-C2	-2.72	107.03	111.02
7	e	1	NAG	C4-C3-C2	-2.71	107.05	111.02
12	f	5	MAN	O4-C4-C3	-2.69	104.03	110.38
7	4	1	NAG	C4-C3-C2	-2.69	107.08	111.02
9	T	5	MAN	O4-C4-C3	-2.69	104.03	110.38
8	X	1	NAG	C4-C3-C2	-2.69	107.08	111.02
12	f	1	NAG	C4-C3-C2	-2.69	107.08	111.02
7	m	1	NAG	C4-C3-C2	-2.68	107.08	111.02
8	S	3	BMA	O4-C4-C5	-2.68	102.72	109.32
11	k	3	BMA	O4-C4-C5	-2.68	102.73	109.32
7	0	1	NAG	C4-C3-C2	-2.68	107.09	111.02
7	r	1	NAG	C4-C3-C2	-2.68	107.09	111.02
8	d	3	BMA	O4-C4-C5	-2.67	102.74	109.32
7	2	1	NAG	C4-C3-C2	-2.67	107.11	111.02
7	1	1	NAG	C4-C3-C2	-2.67	107.11	111.02
7	P	1	NAG	C4-C3-C2	-2.67	107.11	111.02
9	T	1	NAG	C4-C3-C2	-2.67	107.11	111.02
7	b	1	NAG	C4-C3-C2	-2.67	107.11	111.02
8	l	3	BMA	O4-C4-C5	-2.66	102.76	109.32
12	s	5	MAN	O4-C4-C3	-2.66	104.10	110.38
11	x	3	BMA	O4-C4-C5	-2.66	102.77	109.32
8	X	3	BMA	O4-C4-C5	-2.66	102.78	109.32
12	s	1	NAG	C4-C3-C2	-2.66	107.12	111.02
11	Y	3	BMA	O4-C4-C5	-2.65	102.79	109.32
8	d	1	NAG	C4-C3-C2	-2.65	107.13	111.02
8	y	3	BMA	O4-C4-C5	-2.64	102.83	109.32
7	3	1	NAG	C4-C3-C2	-2.63	107.17	111.02
9	T	3	BMA	O4-C4-C5	-2.63	102.85	109.32
12	s	3	BMA	O4-C4-C5	-2.62	102.86	109.32
7	o	2	NAG	C1-C2-N2	2.62	114.56	110.43
7	O	2	NAG	C1-C2-N2	2.62	114.56	110.43
12	f	3	BMA	O4-C4-C5	-2.62	102.88	109.32
7	R	1	NAG	C4-C3-C2	-2.61	107.19	111.02
10	U	5	MAN	O5-C5-C6	-2.58	102.64	107.66
10	U	6	MAN	O5-C5-C6	2.54	112.61	107.66
13	g	7	MAN	O5-C5-C6	-2.54	102.72	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	s	4	MAN	O5-C5-C6	2.53	112.59	107.66
13	t	7	MAN	O5-C5-C6	-2.53	102.75	107.66
13	g	8	MAN	O5-C5-C6	2.52	112.57	107.66
12	f	4	MAN	O5-C5-C6	2.52	112.56	107.66
12	f	7	MAN	O5-C5-C6	-2.51	102.78	107.66
12	s	7	MAN	O5-C5-C6	-2.51	102.79	107.66
9	T	4	MAN	O5-C5-C6	2.50	112.53	107.66
13	t	8	MAN	O5-C5-C6	2.47	112.47	107.66
11	k	4	MAN	O5-C5-C6	2.44	112.42	107.66
11	Y	4	MAN	O5-C5-C6	2.43	112.40	107.66
11	x	4	MAN	O5-C5-C6	2.42	112.36	107.66
13	q	3	BMA	C1-O5-C5	2.41	115.42	112.19
12	f	3	BMA	C6-C5-C4	-2.37	107.19	113.02
9	T	3	BMA	C6-C5-C4	-2.36	107.22	113.02
8	S	2	NAG	O5-C1-C2	-2.36	107.64	111.29
7	r	2	NAG	O5-C1-C2	-2.35	107.66	111.29
7	e	2	NAG	O5-C1-C2	-2.34	107.67	111.29
12	s	3	BMA	C6-C5-C4	-2.34	107.27	113.02
7	0	2	NAG	O5-C1-C2	-2.32	107.69	111.29
8	d	2	NAG	O5-C1-C2	-2.32	107.69	111.29
8	S	3	BMA	C6-C5-C4	-2.32	107.31	113.02
13	g	5	MAN	O3-C3-C4	2.32	115.84	110.38
13	t	5	MAN	O3-C3-C4	2.32	115.84	110.38
7	m	2	NAG	O5-C1-C2	-2.32	107.71	111.29
8	X	3	BMA	C6-C5-C4	-2.31	107.34	113.02
11	k	3	BMA	C6-C5-C4	-2.31	107.34	113.02
11	Y	2	NAG	C1-O5-C5	2.31	115.28	112.19
8	y	3	BMA	C6-C5-C4	-2.31	107.34	113.02
7	4	2	NAG	O5-C1-C2	-2.31	107.72	111.29
7	1	2	NAG	O5-C1-C2	-2.31	107.72	111.29
7	3	2	NAG	O5-C1-C2	-2.30	107.72	111.29
7	P	2	NAG	O5-C1-C2	-2.30	107.73	111.29
9	T	2	NAG	O5-C1-C2	-2.30	107.73	111.29
8	d	3	BMA	C6-C5-C4	-2.30	107.37	113.02
8	l	3	BMA	C6-C5-C4	-2.30	107.38	113.02
8	X	2	NAG	O5-C1-C2	-2.30	107.74	111.29
11	k	2	NAG	C1-O5-C5	2.30	115.26	112.19
11	x	3	BMA	C6-C5-C4	-2.29	107.39	113.02
12	f	5	MAN	O6-C6-C5	2.29	119.14	111.33
12	f	2	NAG	O5-C1-C2	-2.29	107.74	111.29
7	2	2	NAG	O5-C1-C2	-2.29	107.75	111.29
7	b	2	NAG	O5-C1-C2	-2.29	107.75	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	5	MAN	O6-C6-C5	2.28	119.11	111.33
13	t	7	MAN	C1-O5-C5	2.28	115.24	112.19
12	s	5	MAN	O6-C6-C5	2.28	119.09	111.33
12	s	2	NAG	O5-C1-C2	-2.28	107.77	111.29
7	R	2	NAG	O5-C1-C2	-2.28	107.77	111.29
11	Y	3	BMA	C6-C5-C4	-2.26	107.46	113.02
11	x	2	NAG	C1-O5-C5	2.26	115.22	112.19
7	o	1	NAG	C3-C4-C5	2.25	114.31	110.23
9	T	6	MAN	O5-C1-C2	-2.25	105.43	110.79
7	O	1	NAG	C3-C4-C5	2.25	114.31	110.23
12	s	6	MAN	O5-C1-C2	-2.23	105.46	110.79
7	2	2	NAG	C4-C3-C2	-2.23	107.75	111.02
8	S	2	NAG	C4-C3-C2	-2.23	107.75	111.02
13	g	7	MAN	C1-O5-C5	2.23	115.17	112.19
12	f	7	MAN	C1-O5-C5	2.22	115.17	112.19
12	s	7	MAN	C1-O5-C5	2.22	115.16	112.19
7	1	2	NAG	C4-C3-C2	-2.22	107.77	111.02
12	f	6	MAN	O5-C1-C2	-2.22	105.50	110.79
10	U	7	MAN	O2-C2-C3	-2.22	105.56	110.15
7	r	2	NAG	C4-C3-C2	-2.22	107.77	111.02
13	q	4	MAN	C1-C2-C3	2.22	112.87	109.64
13	t	6	MAN	O5-C1-C2	-2.22	105.50	110.79
13	g	3	BMA	O2-C2-C1	2.22	114.30	109.22
13	t	3	BMA	O2-C2-C1	2.22	114.30	109.22
8	d	2	NAG	C4-C3-C2	-2.21	107.78	111.02
8	X	2	NAG	C4-C3-C2	-2.21	107.78	111.02
13	g	4	MAN	O2-C2-C3	-2.21	105.57	110.15
7	m	2	NAG	C4-C3-C2	-2.21	107.78	111.02
10	U	3	BMA	O2-C2-C1	2.20	114.26	109.22
12	f	2	NAG	C4-C3-C2	-2.20	107.80	111.02
11	k	5	MAN	O5-C1-C2	-2.20	105.55	110.79
7	R	2	NAG	C4-C3-C2	-2.20	107.80	111.02
12	s	2	NAG	C4-C3-C2	-2.20	107.80	111.02
7	e	2	NAG	C4-C3-C2	-2.20	107.80	111.02
10	U	4	MAN	O5-C1-C2	-2.20	105.55	110.79
7	O	2	NAG	O4-C4-C5	-2.19	103.92	109.32
9	T	2	NAG	C4-C3-C2	-2.19	107.80	111.02
7	P	2	NAG	C4-C3-C2	-2.19	107.80	111.02
7	0	2	NAG	C4-C3-C2	-2.19	107.80	111.02
7	o	2	NAG	O4-C4-C5	-2.19	103.92	109.32
13	g	6	MAN	O5-C1-C2	-2.19	105.56	110.79
13	t	4	MAN	O2-C2-C3	-2.19	105.61	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4	2	NAG	C4-C3-C2	-2.18	107.83	111.02
7	3	2	NAG	C4-C3-C2	-2.17	107.83	111.02
11	Y	5	MAN	O5-C1-C2	-2.17	105.61	110.79
7	w	1	NAG	O4-C4-C5	-2.17	103.99	109.32
7	b	2	NAG	C4-C3-C2	-2.17	107.84	111.02
13	t	8	MAN	O2-C2-C1	2.16	114.18	109.22
11	x	5	MAN	O5-C1-C2	-2.16	105.63	110.79
10	U	5	MAN	C1-O5-C5	2.16	115.09	112.19
10	U	6	MAN	O2-C2-C1	2.16	114.17	109.22
13	g	8	MAN	O2-C2-C1	2.15	114.15	109.22
7	j	1	NAG	O4-C4-C5	-2.15	104.02	109.32
12	s	7	MAN	O3-C3-C2	-2.15	105.66	110.05
13	q	5	MAN	C1-C2-C3	2.14	112.76	109.64
13	t	7	MAN	O3-C3-C2	-2.14	105.69	110.05
12	f	7	MAN	O3-C3-C2	-2.14	105.69	110.05
13	g	7	MAN	O3-C3-C2	-2.13	105.71	110.05
13	q	2	NAG	O5-C5-C4	-2.13	105.65	110.83
12	s	4	MAN	O3-C3-C4	2.12	115.38	110.38
12	f	4	MAN	O3-C3-C4	2.11	115.36	110.38
10	U	5	MAN	O3-C3-C2	-2.11	105.74	110.05
11	x	4	MAN	O3-C3-C4	2.09	115.31	110.38
9	T	4	MAN	O3-C3-C4	2.09	115.30	110.38
11	Y	4	MAN	O3-C3-C4	2.08	115.28	110.38
11	k	4	MAN	O3-C3-C4	2.07	115.25	110.38
7	Q	2	NAG	C1-O5-C5	2.04	114.92	112.19
7	p	2	NAG	C1-O5-C5	2.03	114.91	112.19
7	c	2	NAG	C1-O5-C5	2.02	114.90	112.19
13	t	8	MAN	C2-C3-C4	2.02	114.42	110.86
7	O	1	NAG	O4-C4-C5	-2.01	104.37	109.32
12	s	4	MAN	O4-C4-C3	-2.01	105.64	110.38
7	o	1	NAG	O4-C4-C5	-2.00	104.39	109.32
13	g	8	MAN	C2-C3-C4	2.00	114.38	110.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	l	1	NAG	C1

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	V	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	h	1	NAG	O5-C5-C6-O6
7	u	1	NAG	O5-C5-C6-O6
7	v	1	NAG	O5-C5-C6-O6
7	W	1	NAG	O5-C5-C6-O6
7	i	1	NAG	O5-C5-C6-O6
10	U	1	NAG	C4-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
10	U	1	NAG	O5-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
7	w	2	NAG	O5-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6
7	w	1	NAG	O5-C5-C6-O6
10	U	2	NAG	O5-C5-C6-O6
13	g	2	NAG	O5-C5-C6-O6
13	t	2	NAG	O5-C5-C6-O6
7	V	1	NAG	C4-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
7	h	1	NAG	C4-C5-C6-O6
7	i	1	NAG	C4-C5-C6-O6
7	u	1	NAG	C4-C5-C6-O6
7	v	1	NAG	C4-C5-C6-O6
13	g	1	NAG	C4-C5-C6-O6
13	t	1	NAG	C4-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	o	2	NAG	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	c	1	NAG	O5-C5-C6-O6
7	p	1	NAG	O5-C5-C6-O6
11	Y	1	NAG	O5-C5-C6-O6
11	k	1	NAG	O5-C5-C6-O6
11	x	1	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
7	v	2	NAG	O5-C5-C6-O6
11	Y	1	NAG	C4-C5-C6-O6
11	k	1	NAG	C4-C5-C6-O6
11	x	1	NAG	C4-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6
7	j	1	NAG	C4-C5-C6-O6
7	o	2	NAG	C4-C5-C6-O6
7	w	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	U	2	NAG	C4-C5-C6-O6
13	g	2	NAG	C4-C5-C6-O6
13	t	2	NAG	C4-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
7	i	2	NAG	C4-C5-C6-O6
7	j	2	NAG	C4-C5-C6-O6
7	v	2	NAG	C4-C5-C6-O6
7	w	2	NAG	C4-C5-C6-O6
10	U	7	MAN	O5-C5-C6-O6
13	g	4	MAN	O5-C5-C6-O6
13	t	4	MAN	O5-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
11	k	2	NAG	O5-C5-C6-O6
11	x	2	NAG	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
7	p	2	NAG	O5-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
7	o	1	NAG	C4-C5-C6-O6
11	Y	2	NAG	C4-C5-C6-O6
11	k	2	NAG	C4-C5-C6-O6
11	x	2	NAG	C4-C5-C6-O6
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
7	o	2	NAG	C8-C7-N2-C2
7	o	2	NAG	O7-C7-N2-C2
7	a	2	NAG	O5-C5-C6-O6
7	n	2	NAG	O5-C5-C6-O6
7	z	2	NAG	O5-C5-C6-O6
11	Y	3	BMA	O5-C5-C6-O6
11	k	3	BMA	O5-C5-C6-O6
11	x	3	BMA	O5-C5-C6-O6
7	Q	2	NAG	C4-C5-C6-O6
7	c	2	NAG	C4-C5-C6-O6
7	p	2	NAG	C4-C5-C6-O6
11	Y	3	BMA	C4-C5-C6-O6
11	k	3	BMA	C4-C5-C6-O6
11	x	3	BMA	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
7	n	2	NAG	C4-C5-C6-O6
7	z	2	NAG	C4-C5-C6-O6
13	g	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	t	1	NAG	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
8	l	1	NAG	O5-C5-C6-O6
8	y	1	NAG	O5-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
7	p	1	NAG	C4-C5-C6-O6
10	U	7	MAN	C4-C5-C6-O6
13	t	4	MAN	C4-C5-C6-O6
13	g	4	MAN	C4-C5-C6-O6
8	l	2	NAG	C4-C5-C6-O6
8	y	2	NAG	C4-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
8	y	3	BMA	C4-C5-C6-O6
8	X	3	BMA	C4-C5-C6-O6
8	l	3	BMA	C4-C5-C6-O6
8	S	3	BMA	C4-C5-C6-O6
8	d	3	BMA	C4-C5-C6-O6
8	y	3	BMA	O5-C5-C6-O6
8	l	3	BMA	O5-C5-C6-O6
8	S	3	BMA	O5-C5-C6-O6
8	X	3	BMA	O5-C5-C6-O6
8	d	3	BMA	O5-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
8	l	1	NAG	C4-C5-C6-O6
8	y	1	NAG	C4-C5-C6-O6
8	l	2	NAG	O5-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6
8	y	2	NAG	O5-C5-C6-O6
7	O	2	NAG	C1-C2-N2-C7
7	o	2	NAG	C1-C2-N2-C7
7	O	2	NAG	C3-C2-N2-C7
7	o	2	NAG	C3-C2-N2-C7
11	Y	1	NAG	C3-C2-N2-C7
11	k	1	NAG	C3-C2-N2-C7
11	x	1	NAG	C3-C2-N2-C7
13	g	2	NAG	C3-C2-N2-C7
13	t	2	NAG	C3-C2-N2-C7
8	d	1	NAG	O7-C7-N2-C2
12	s	1	NAG	O7-C7-N2-C2
7	b	1	NAG	O7-C7-N2-C2
7	e	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	m	1	NAG	O7-C7-N2-C2
7	3	1	NAG	O7-C7-N2-C2
8	X	1	NAG	O7-C7-N2-C2
12	f	1	NAG	O7-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	R	1	NAG	O7-C7-N2-C2
7	r	1	NAG	O7-C7-N2-C2
7	0	1	NAG	O7-C7-N2-C2
7	1	1	NAG	O7-C7-N2-C2
7	2	1	NAG	O7-C7-N2-C2
7	4	1	NAG	O7-C7-N2-C2
8	S	1	NAG	O7-C7-N2-C2
9	T	1	NAG	O7-C7-N2-C2

There are no ring outliers.

40 monomers are involved in 162 short contacts:

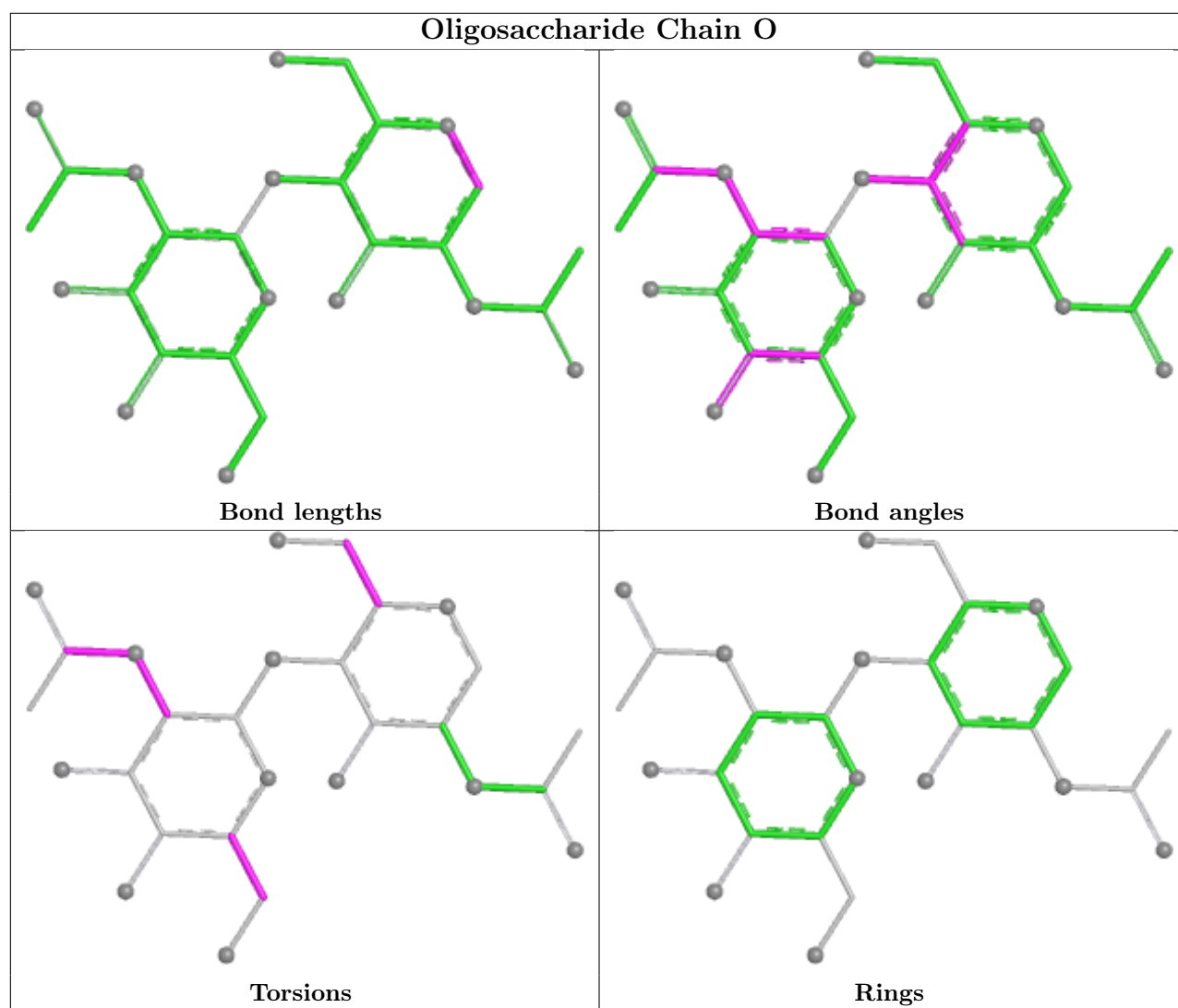
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	u	1	NAG	9	0
7	o	1	NAG	4	0
7	v	2	NAG	1	0
7	z	1	NAG	2	0
11	Y	1	NAG	6	0
7	n	2	NAG	2	0
11	x	2	NAG	1	0
11	k	1	NAG	2	0
7	w	1	NAG	9	0
10	U	1	NAG	5	0
7	O	2	NAG	1	0
7	v	1	NAG	4	0
7	W	2	NAG	1	0
13	q	1	NAG	7	0
7	i	2	NAG	1	0
7	p	1	NAG	5	0
13	q	3	BMA	5	0
7	n	1	NAG	2	0
13	q	4	MAN	9	0
7	o	2	NAG	1	0
8	l	1	NAG	5	0
7	z	2	NAG	2	0
10	U	2	NAG	1	0
13	g	2	NAG	2	0

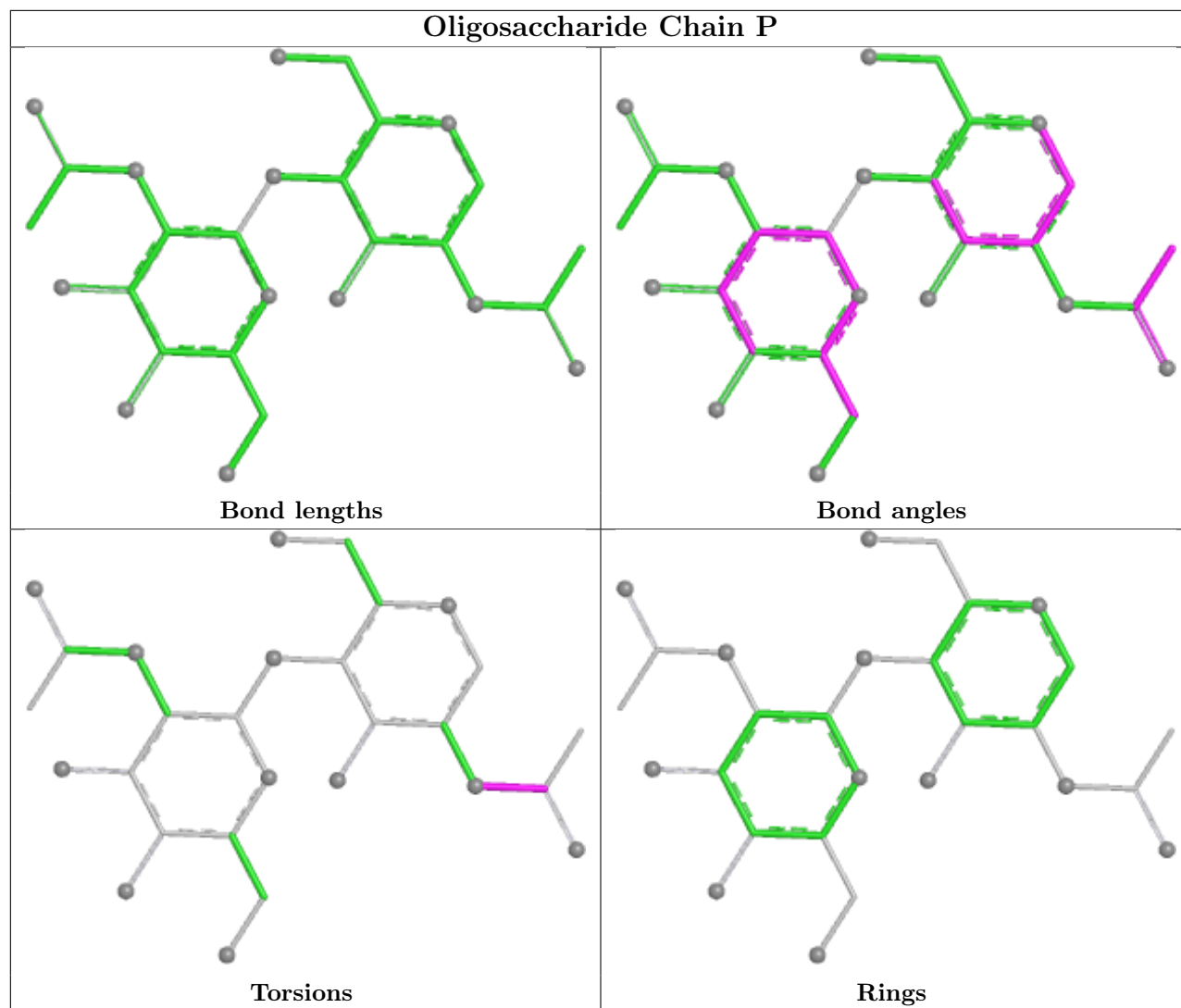
Continued on next page...

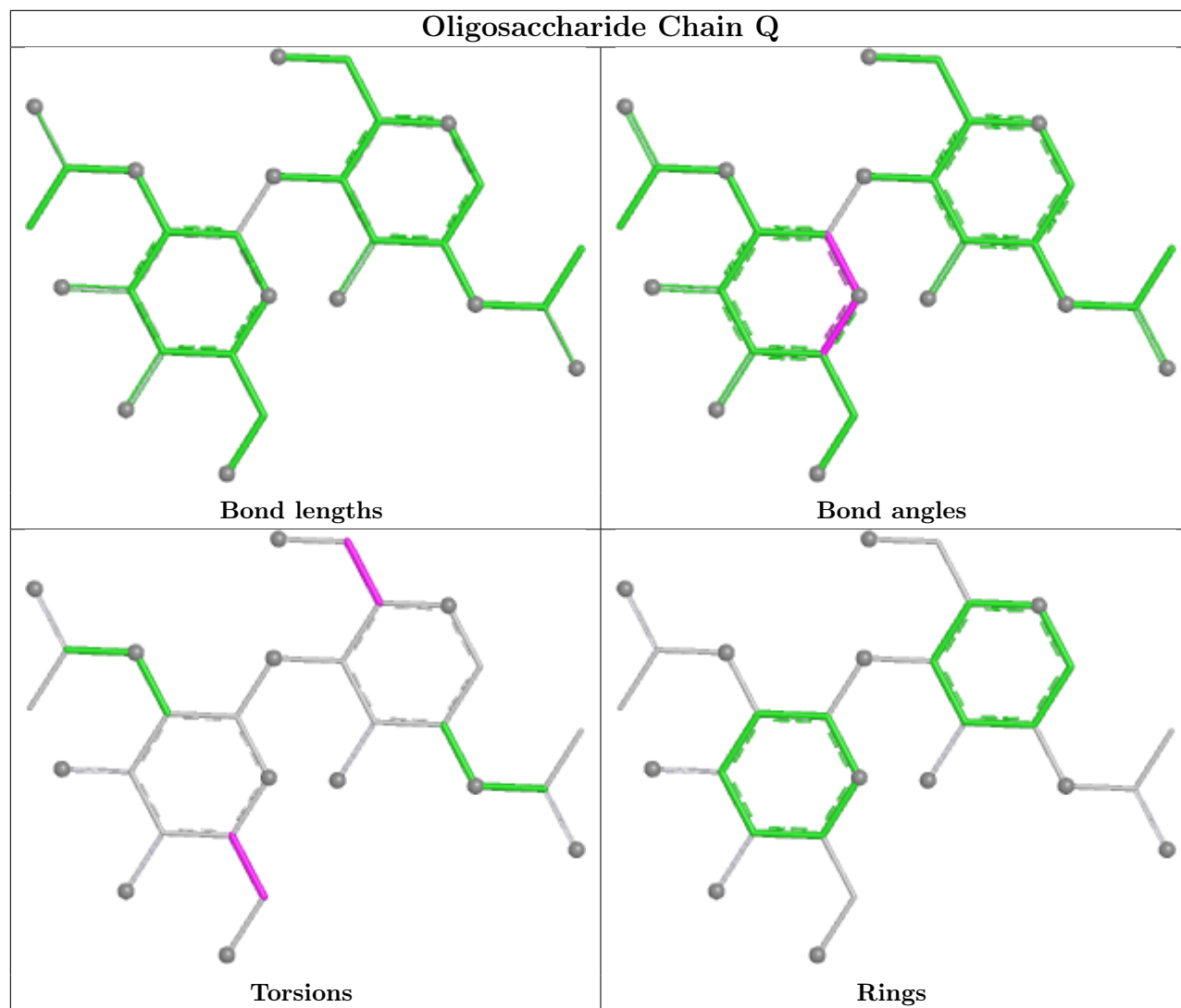
Continued from previous page...

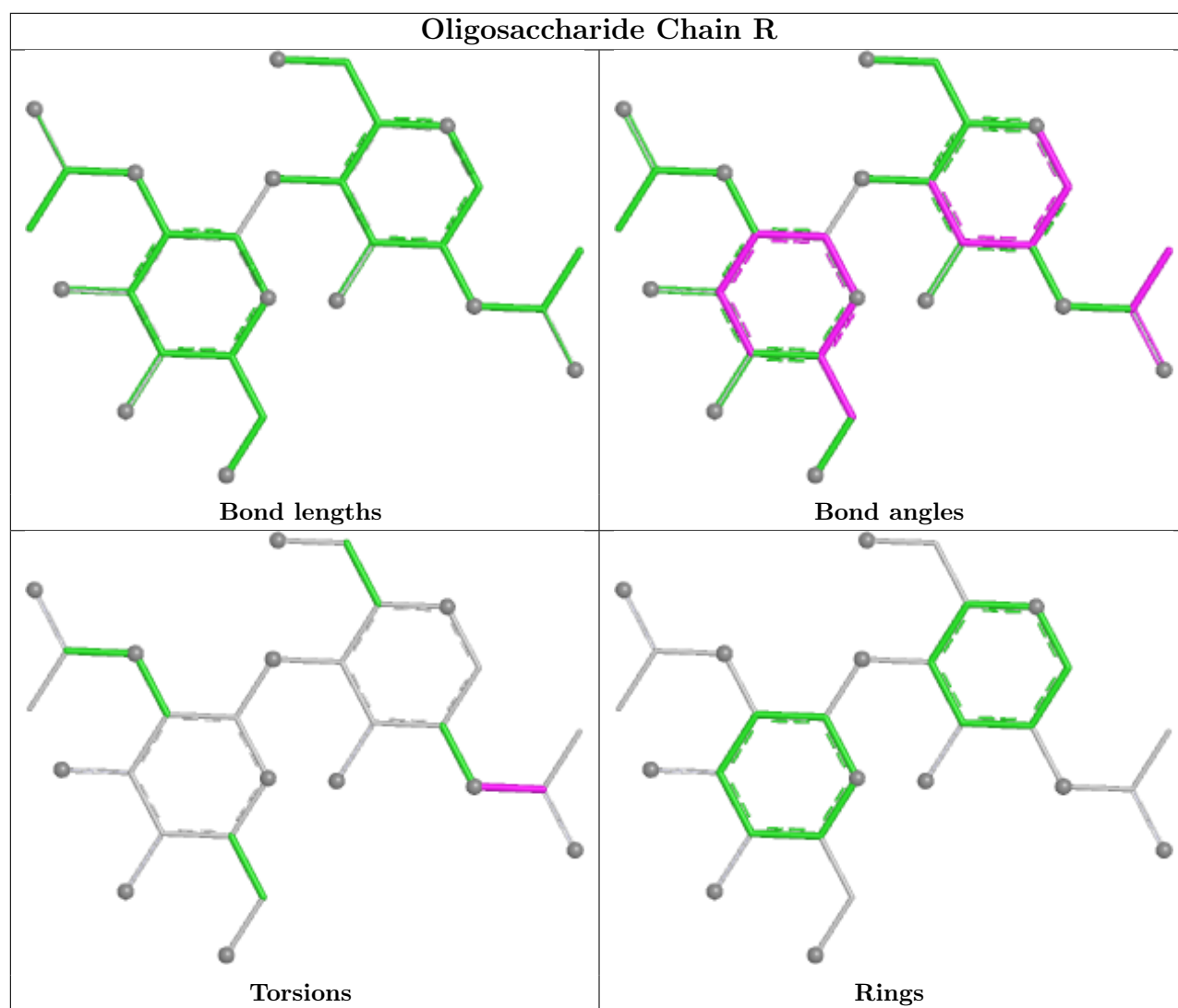
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	c	1	NAG	4	0
7	a	1	NAG	4	0
7	O	1	NAG	2	0
8	y	2	NAG	3	0
7	W	1	NAG	3	0
8	y	1	NAG	1	0
7	h	1	NAG	13	0
13	q	2	NAG	11	0
11	x	1	NAG	2	0
7	j	1	NAG	12	0
13	q	8	MAN	2	0
13	t	1	NAG	4	0
7	Q	1	NAG	15	0
7	V	1	NAG	6	0
13	t	2	NAG	2	0
7	i	1	NAG	2	0

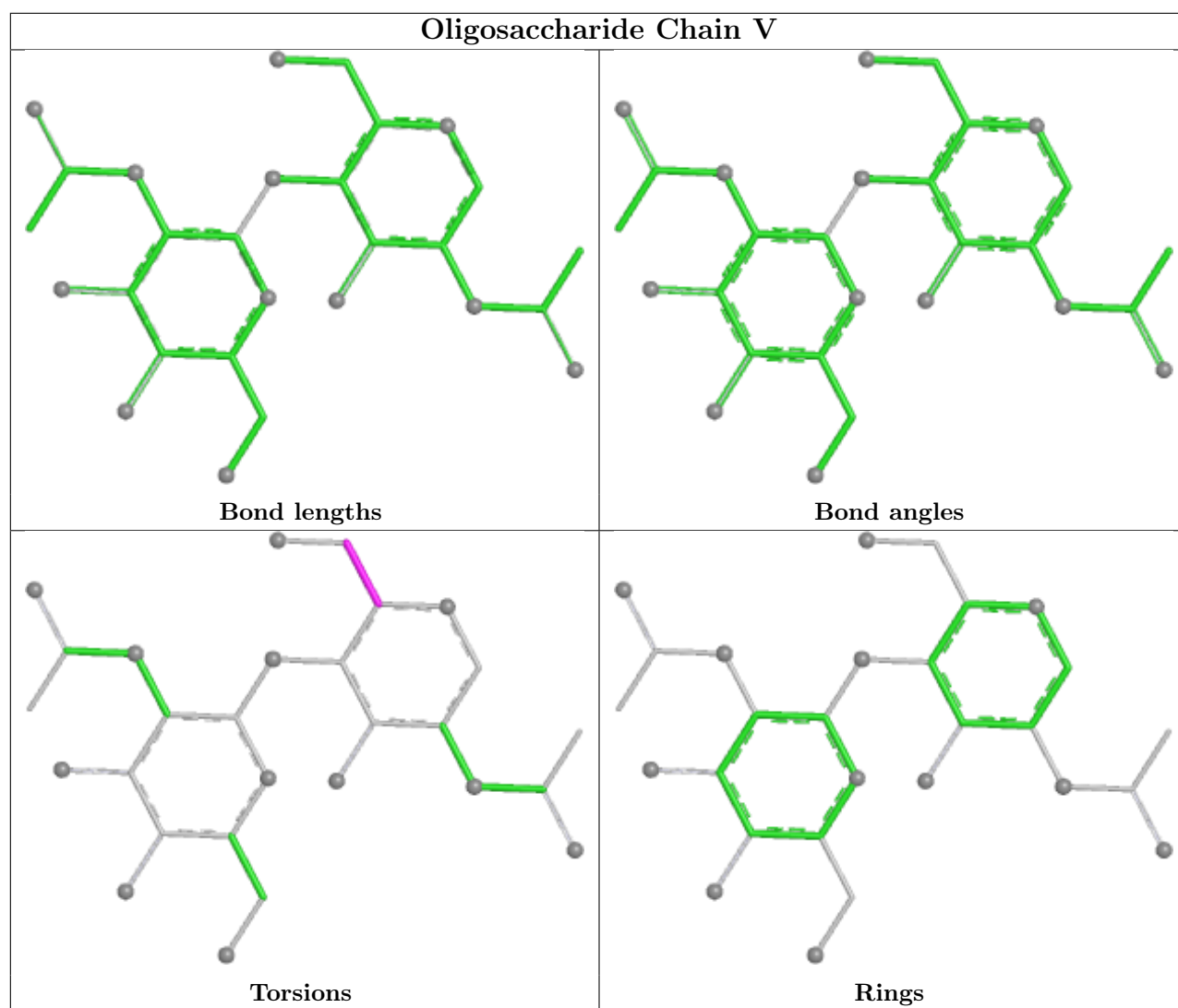
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

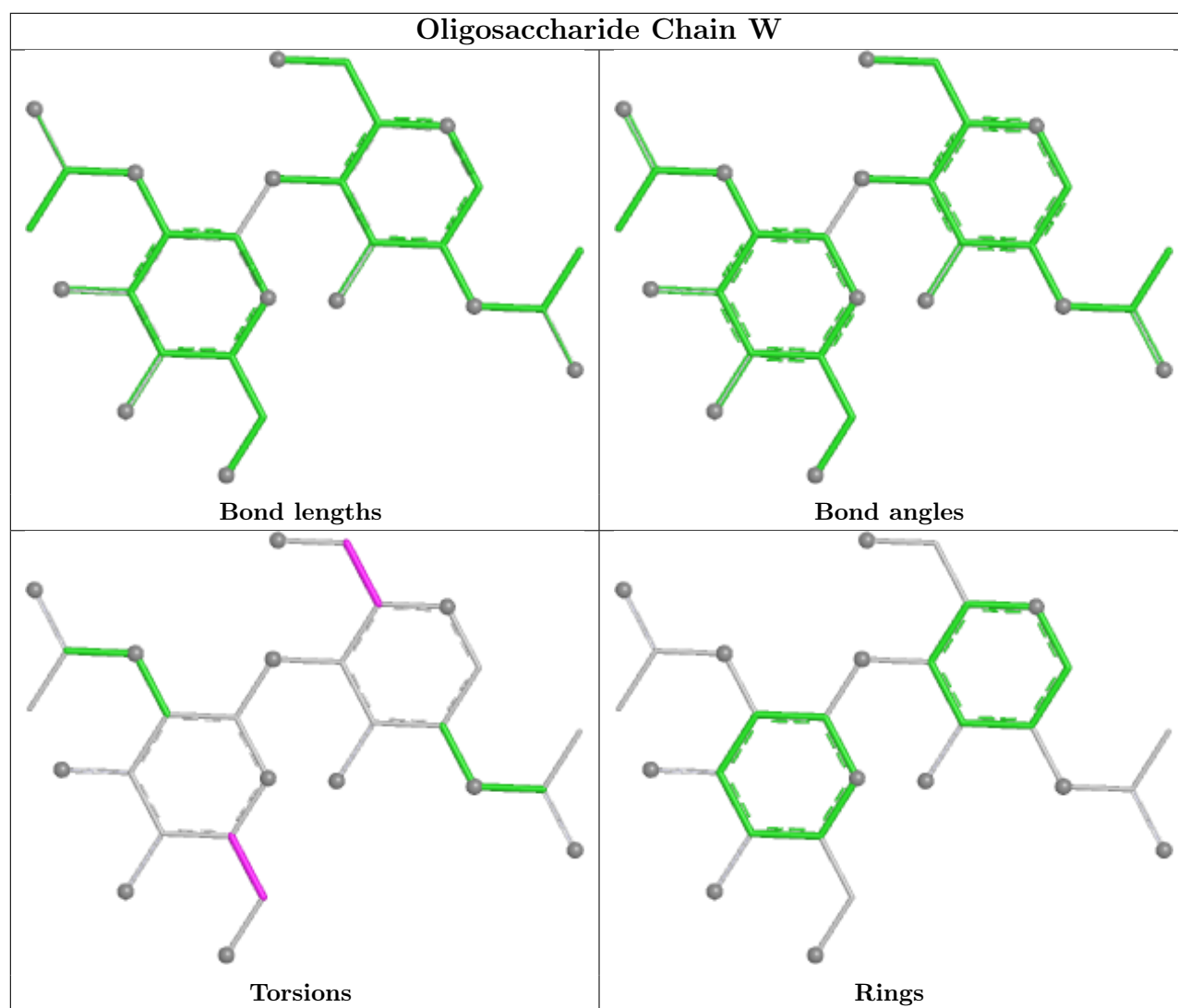


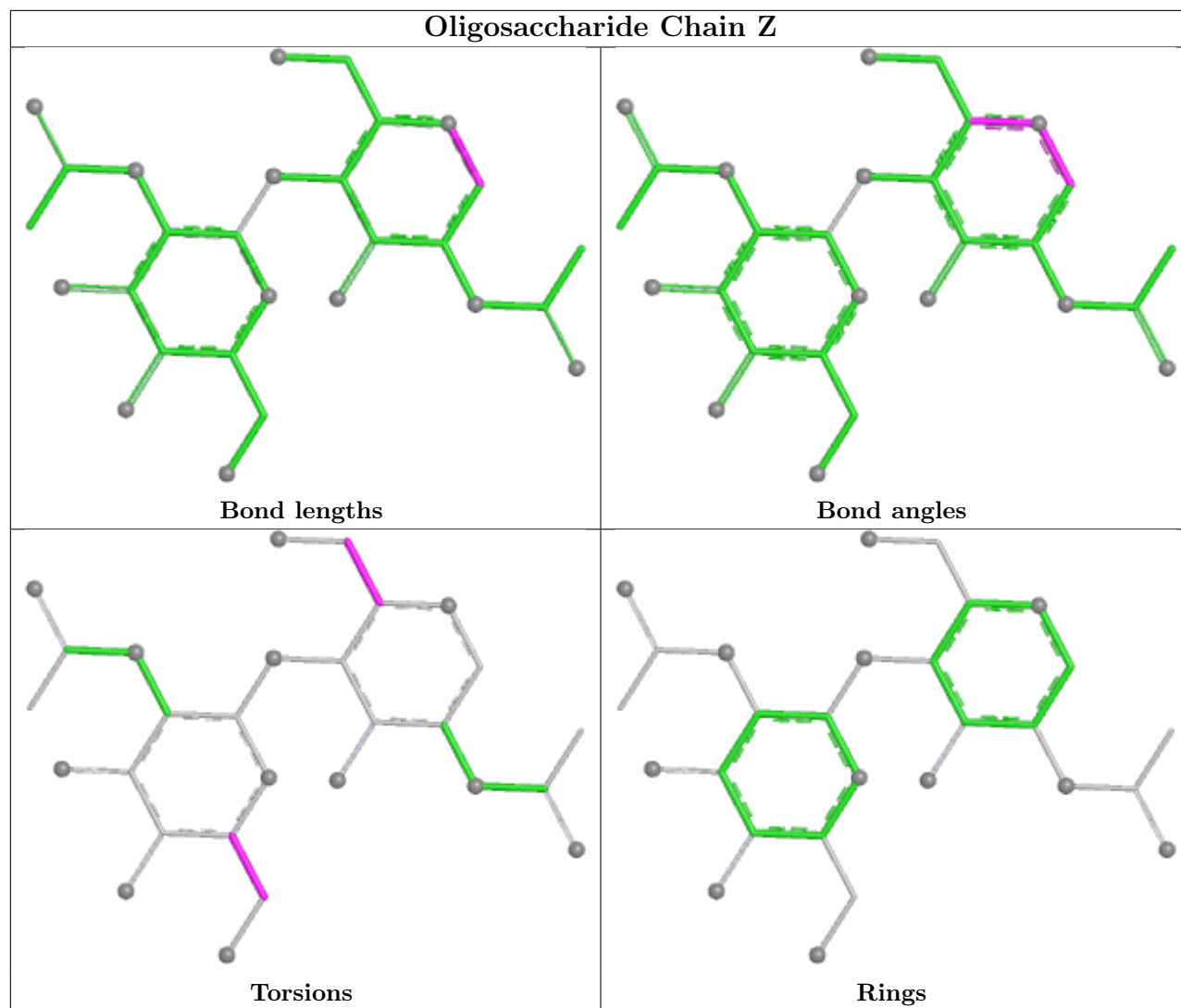


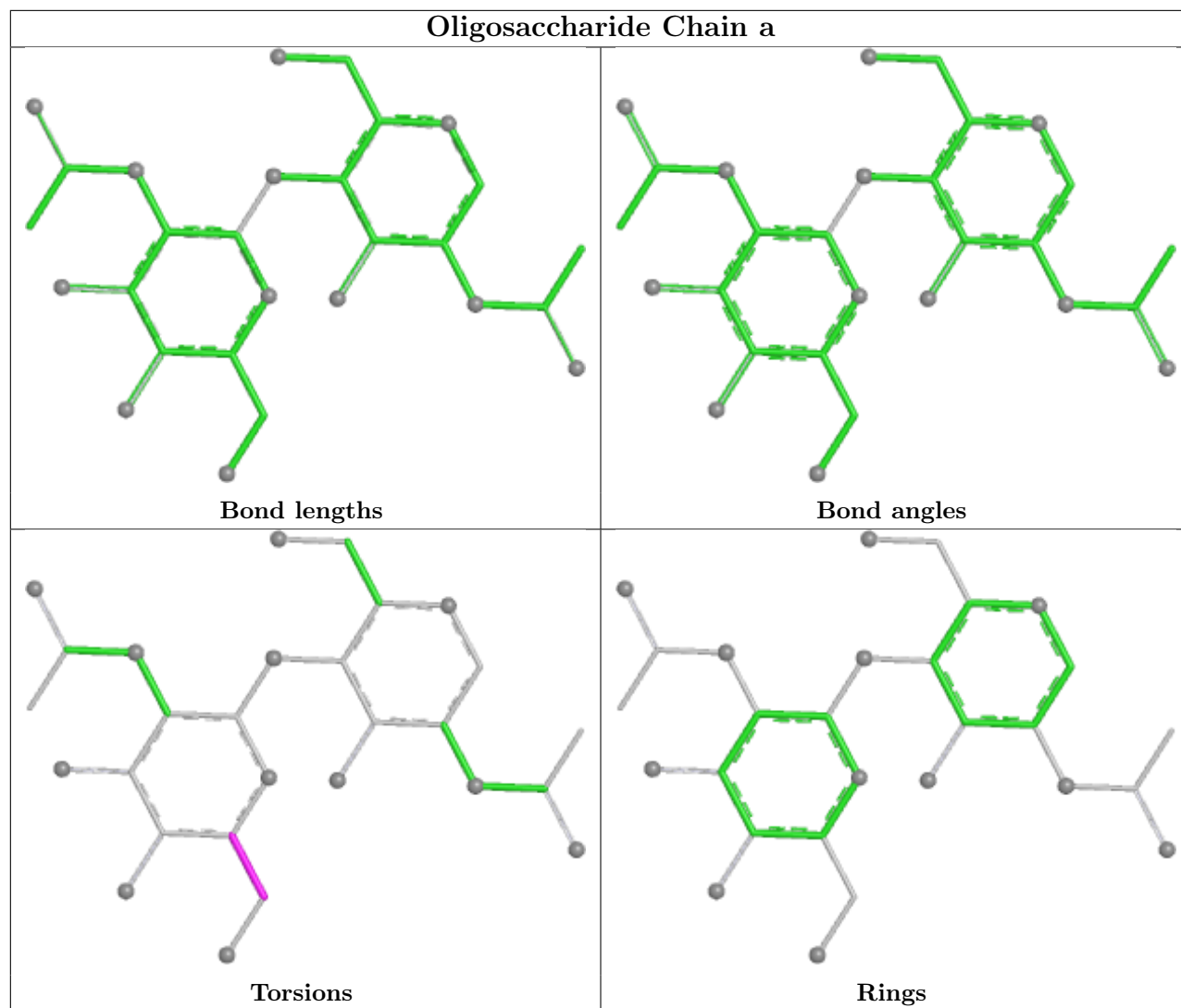


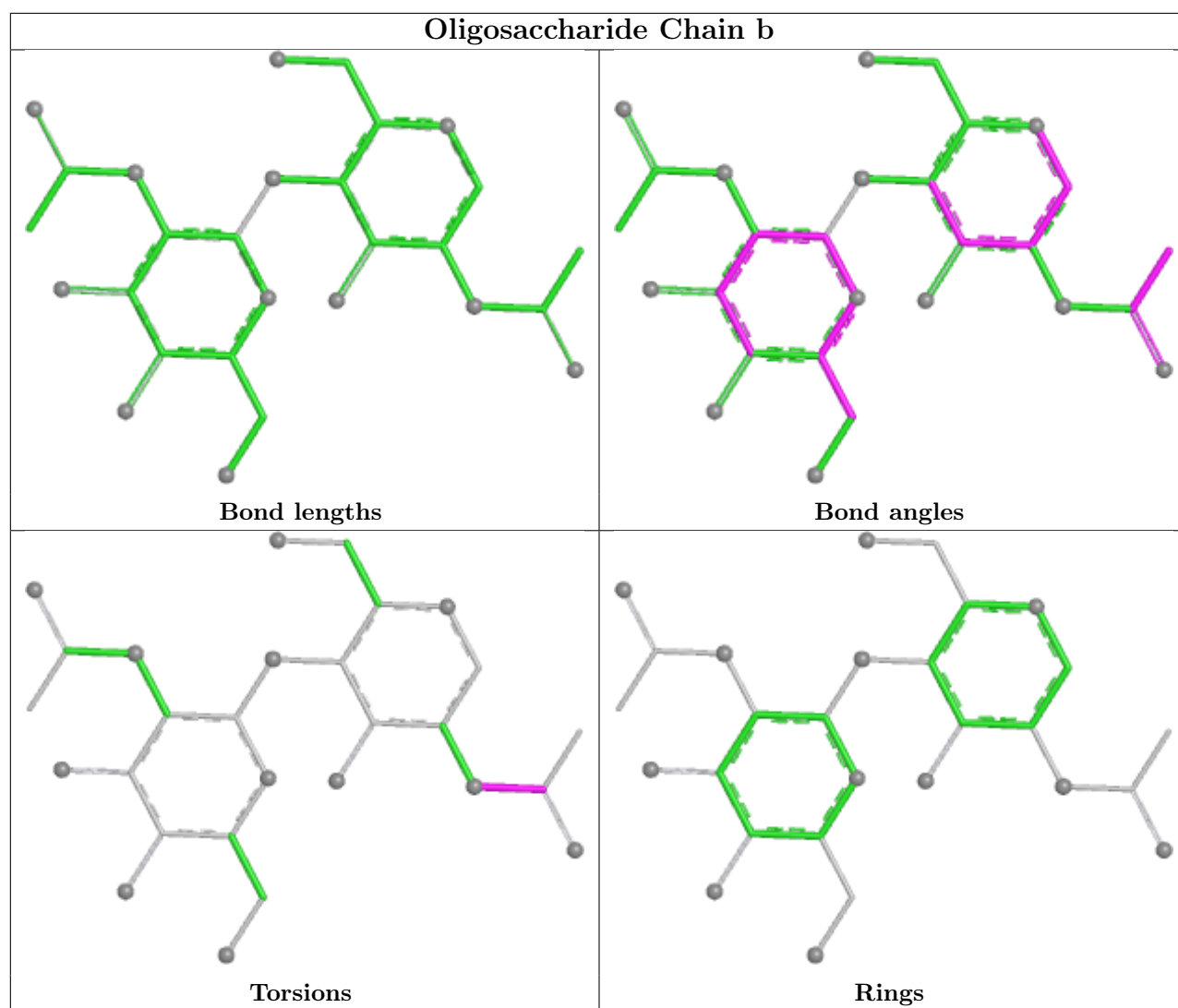


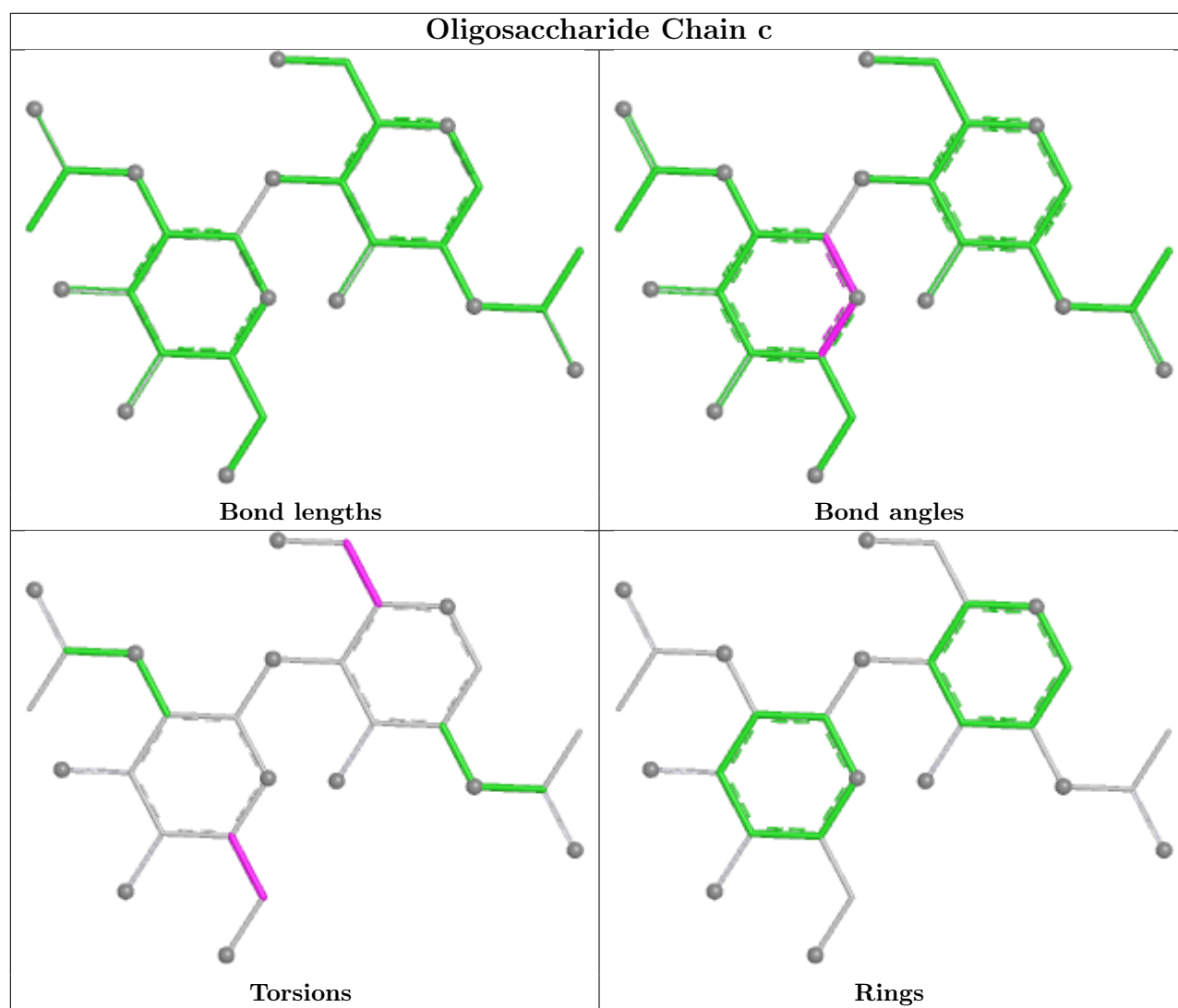


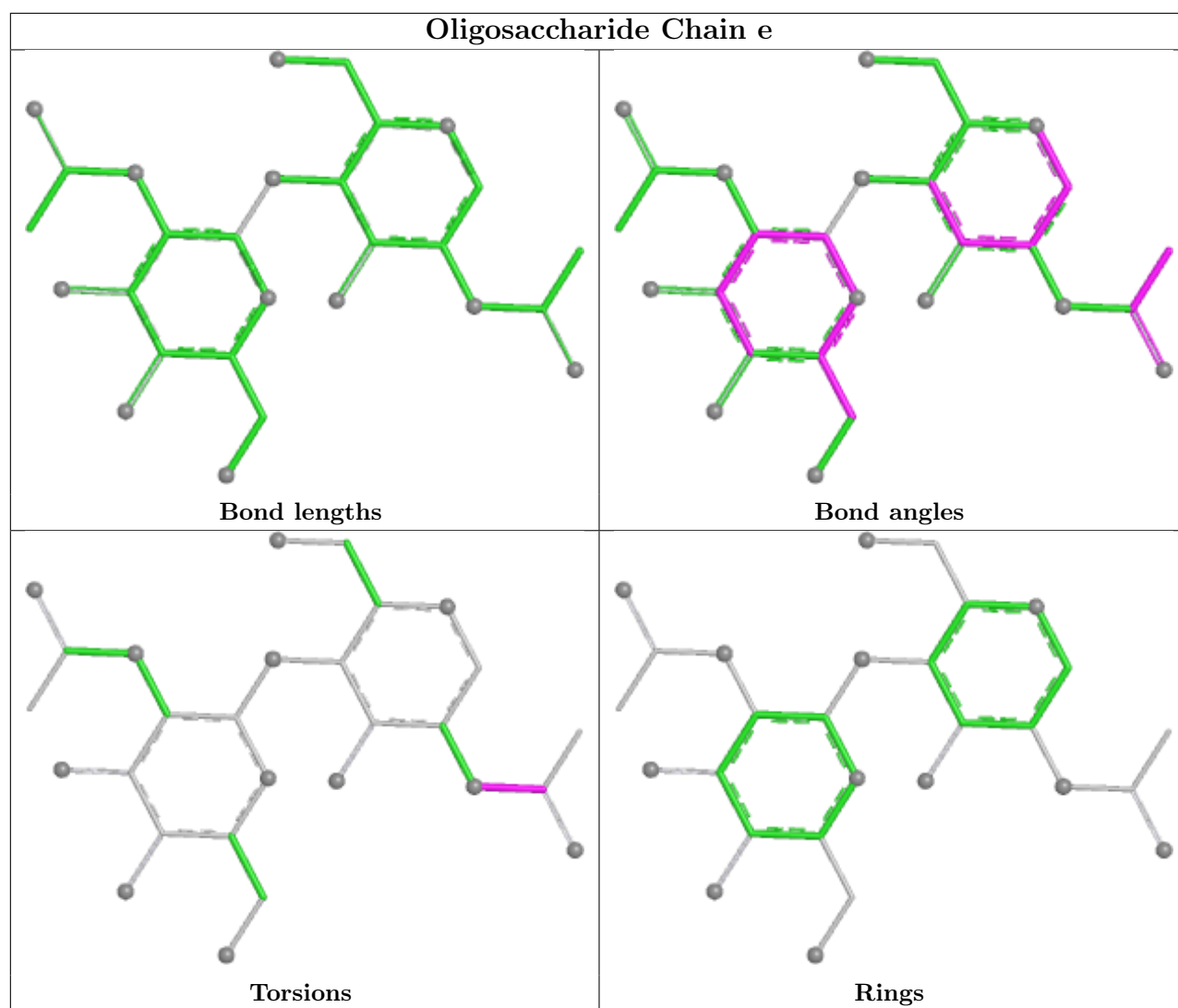


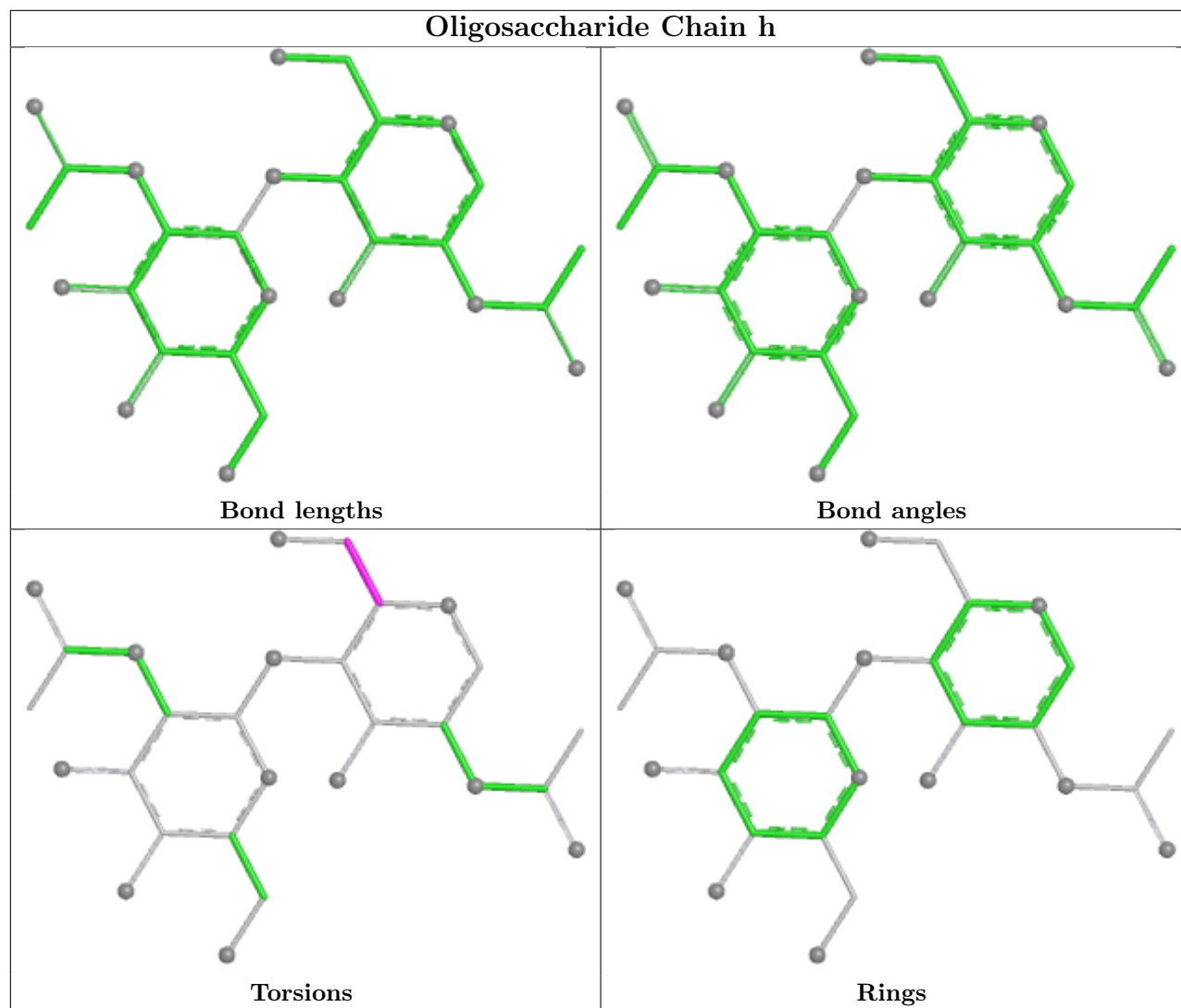


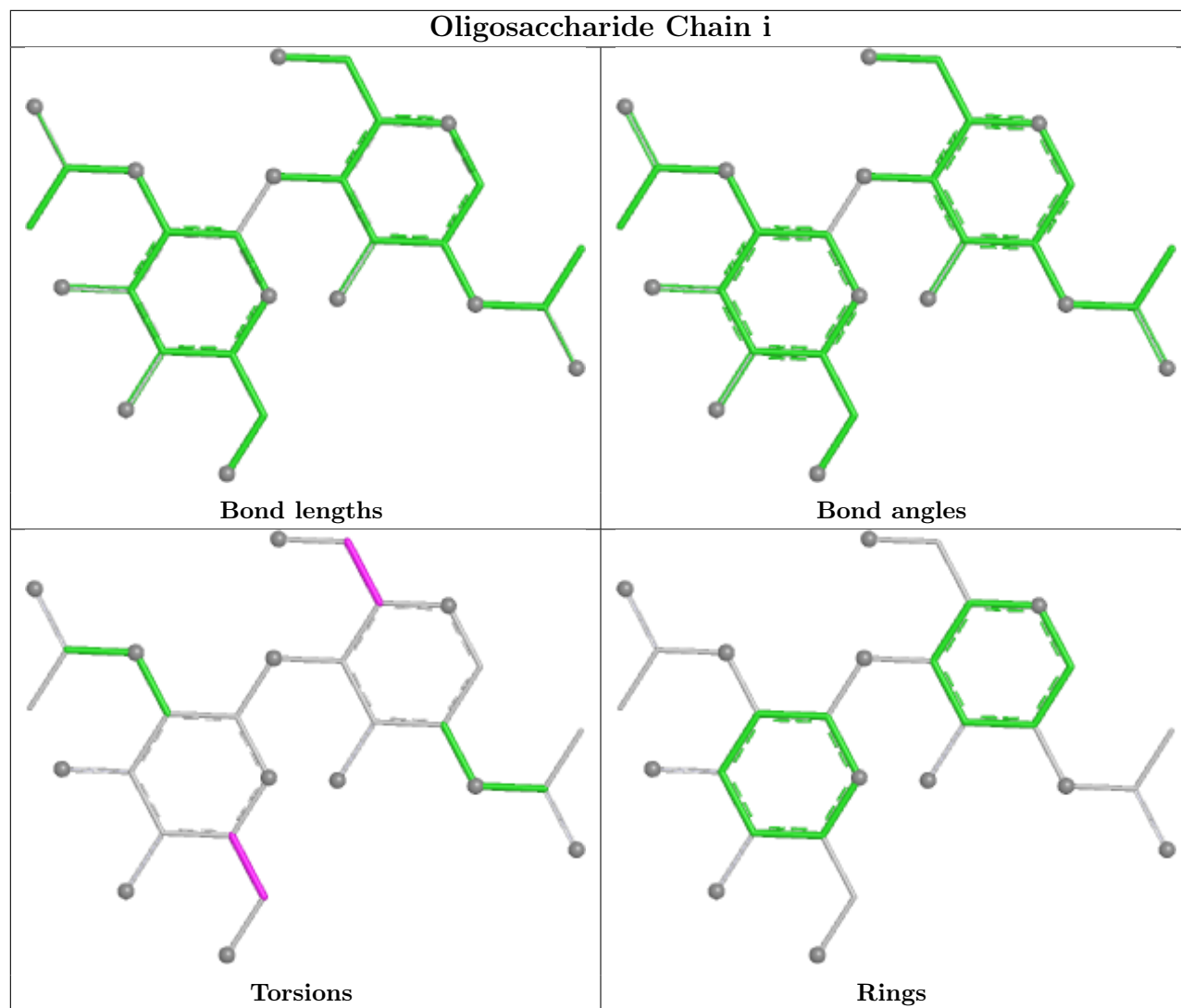


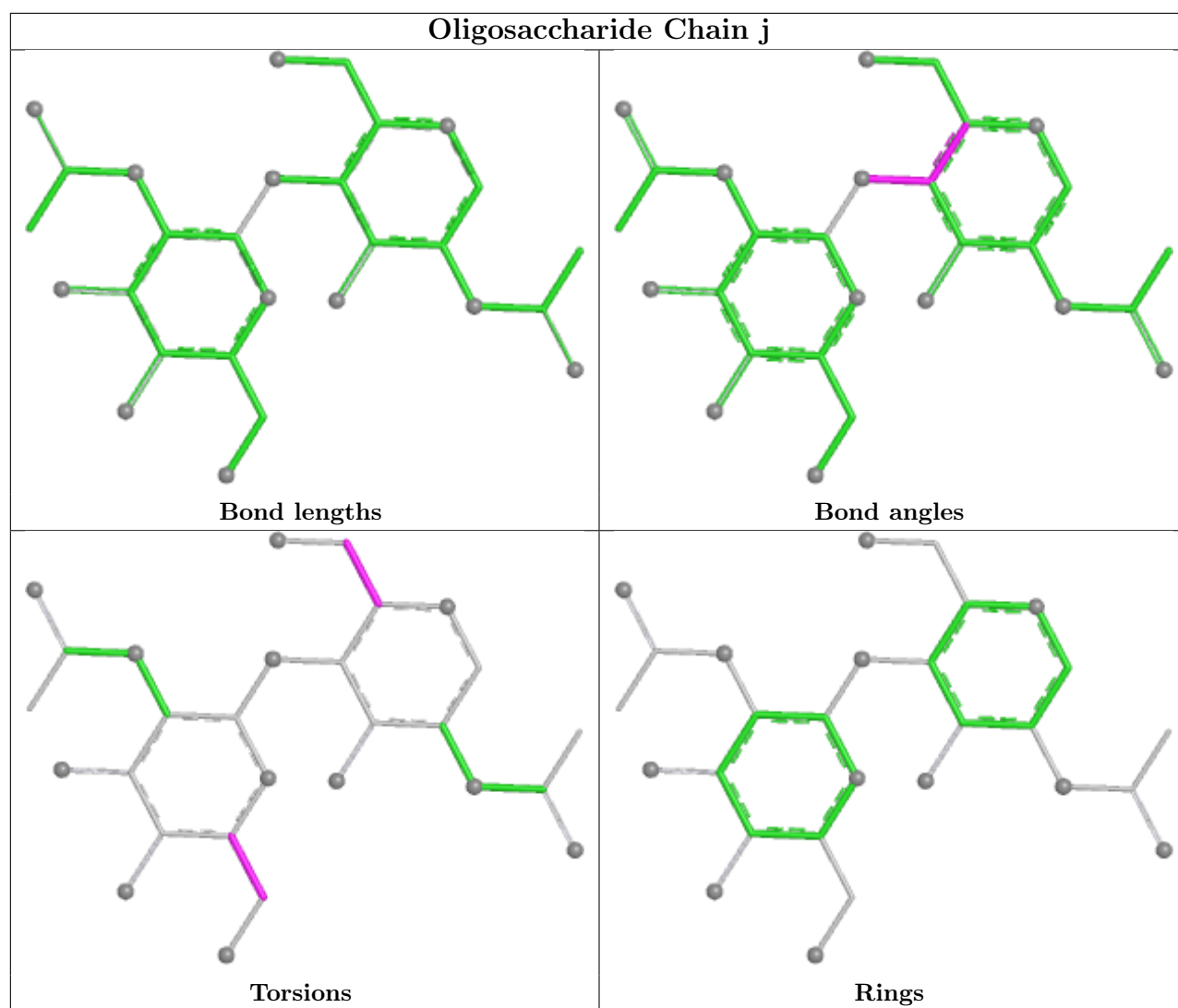


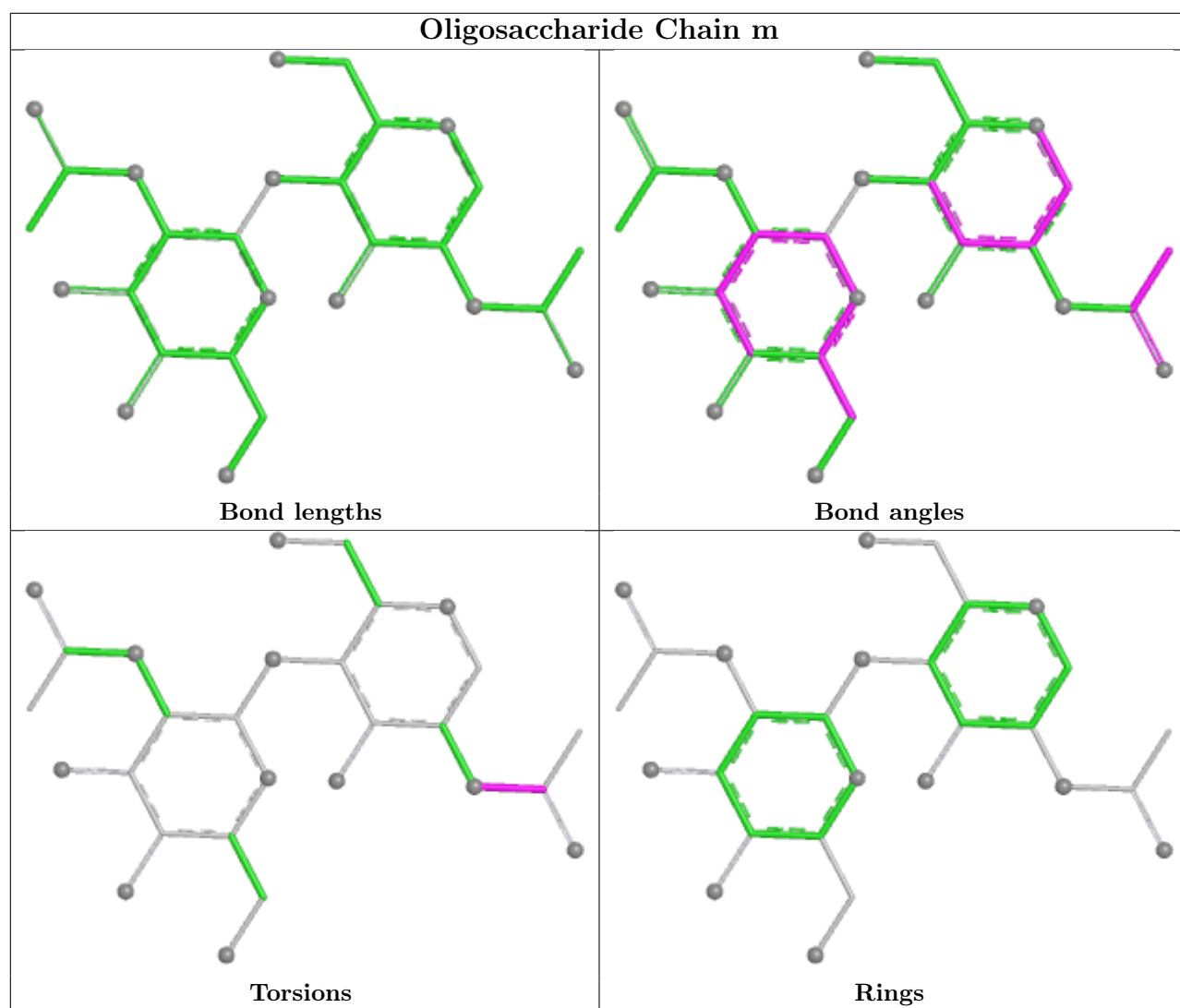


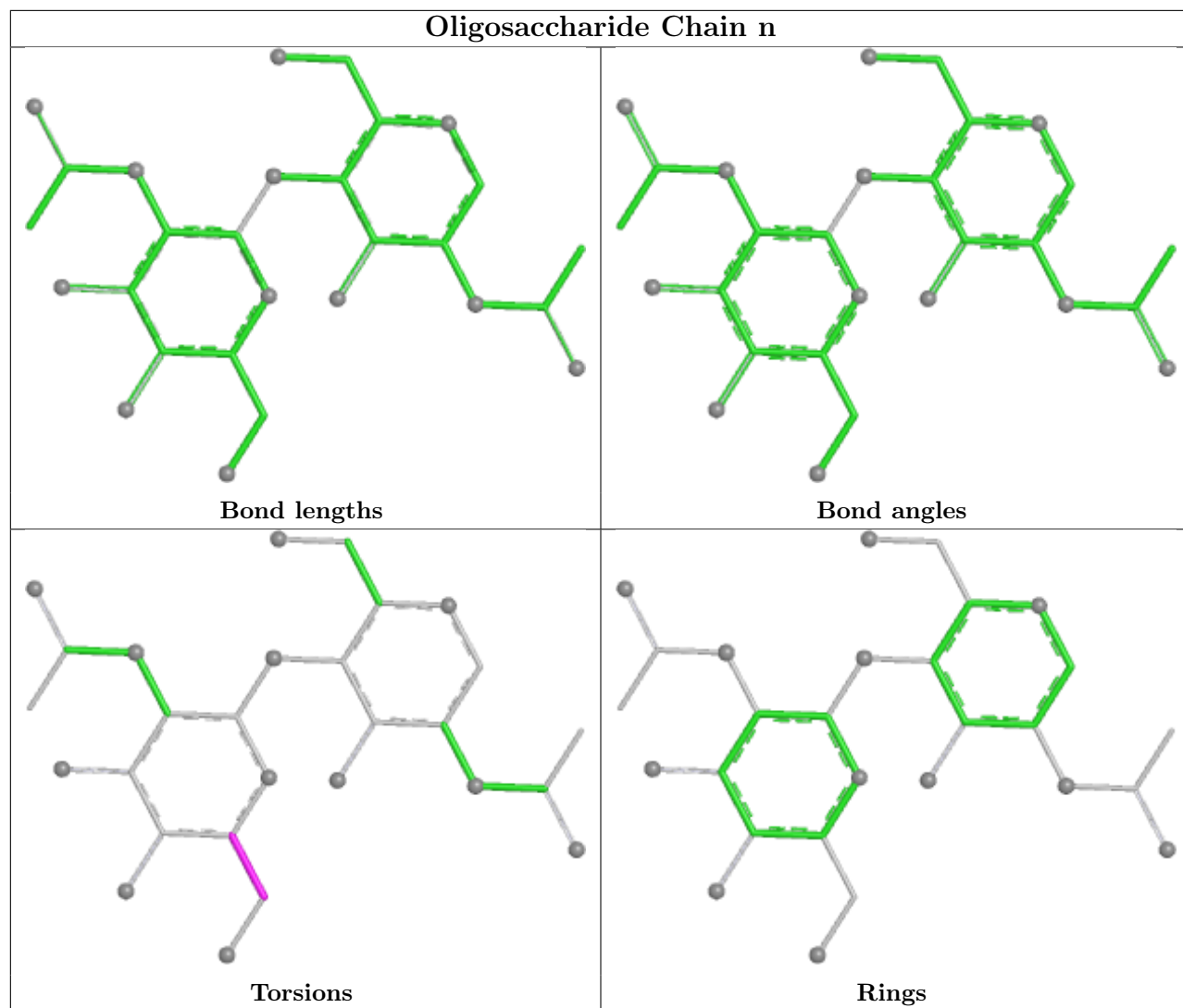


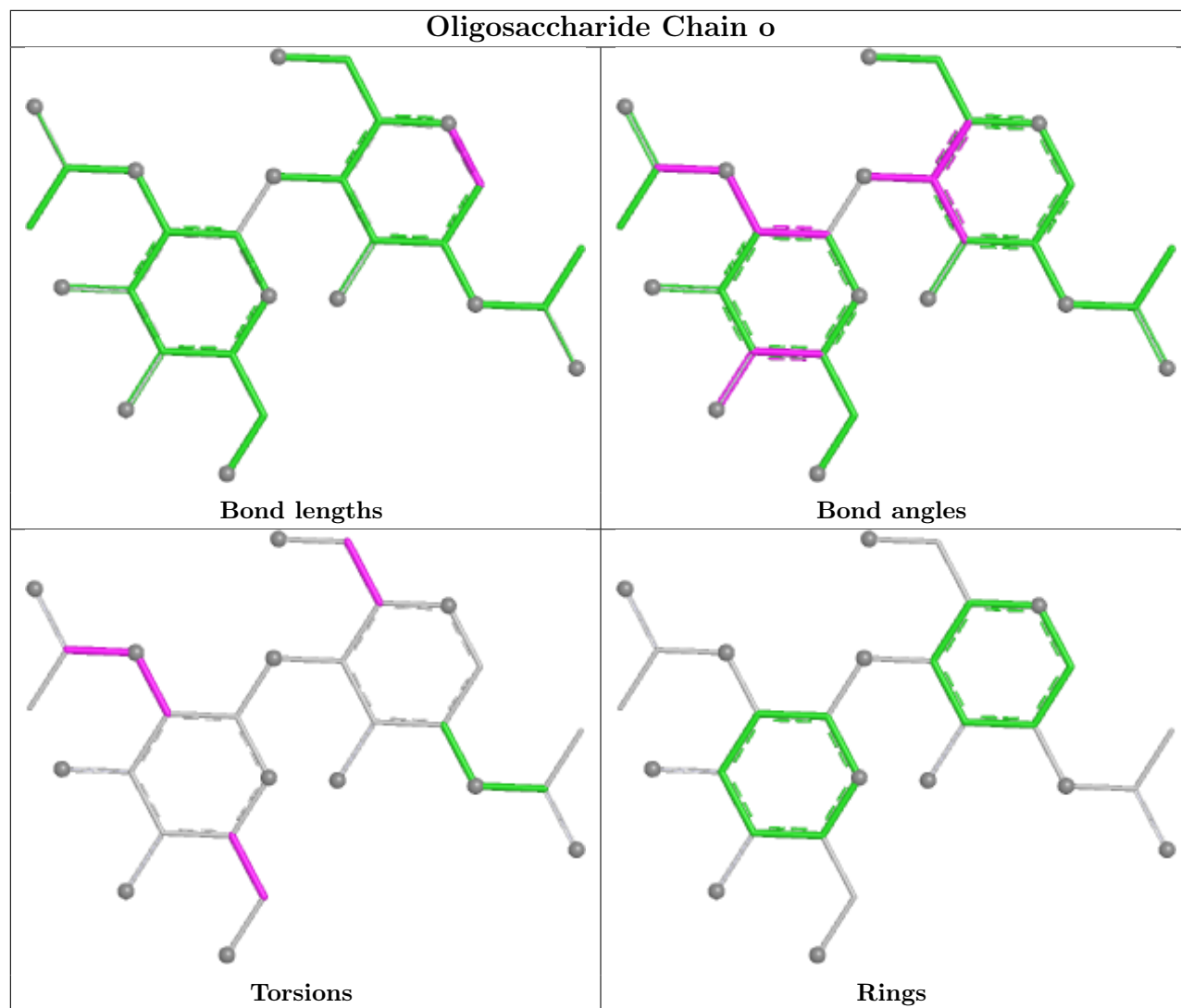


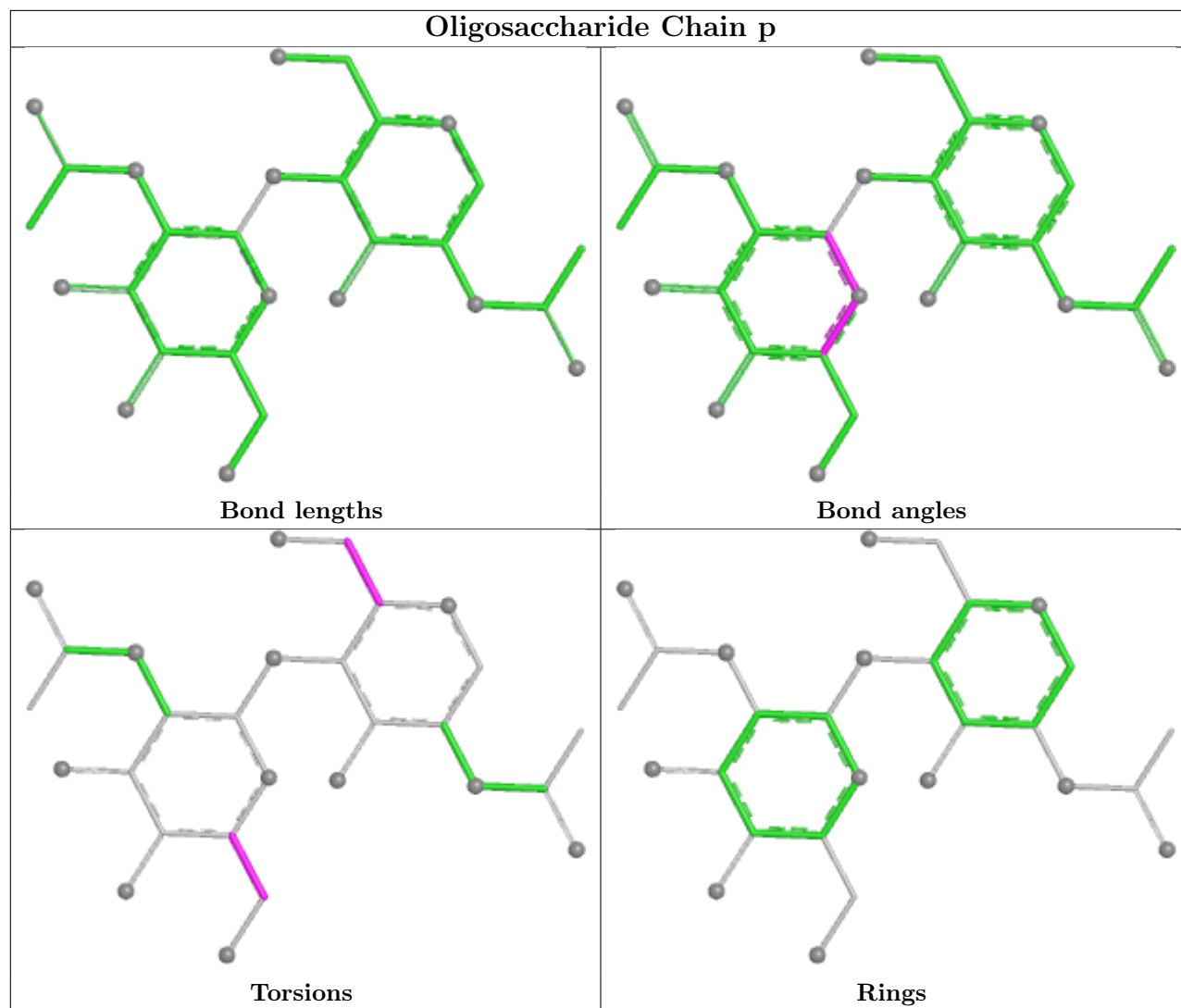


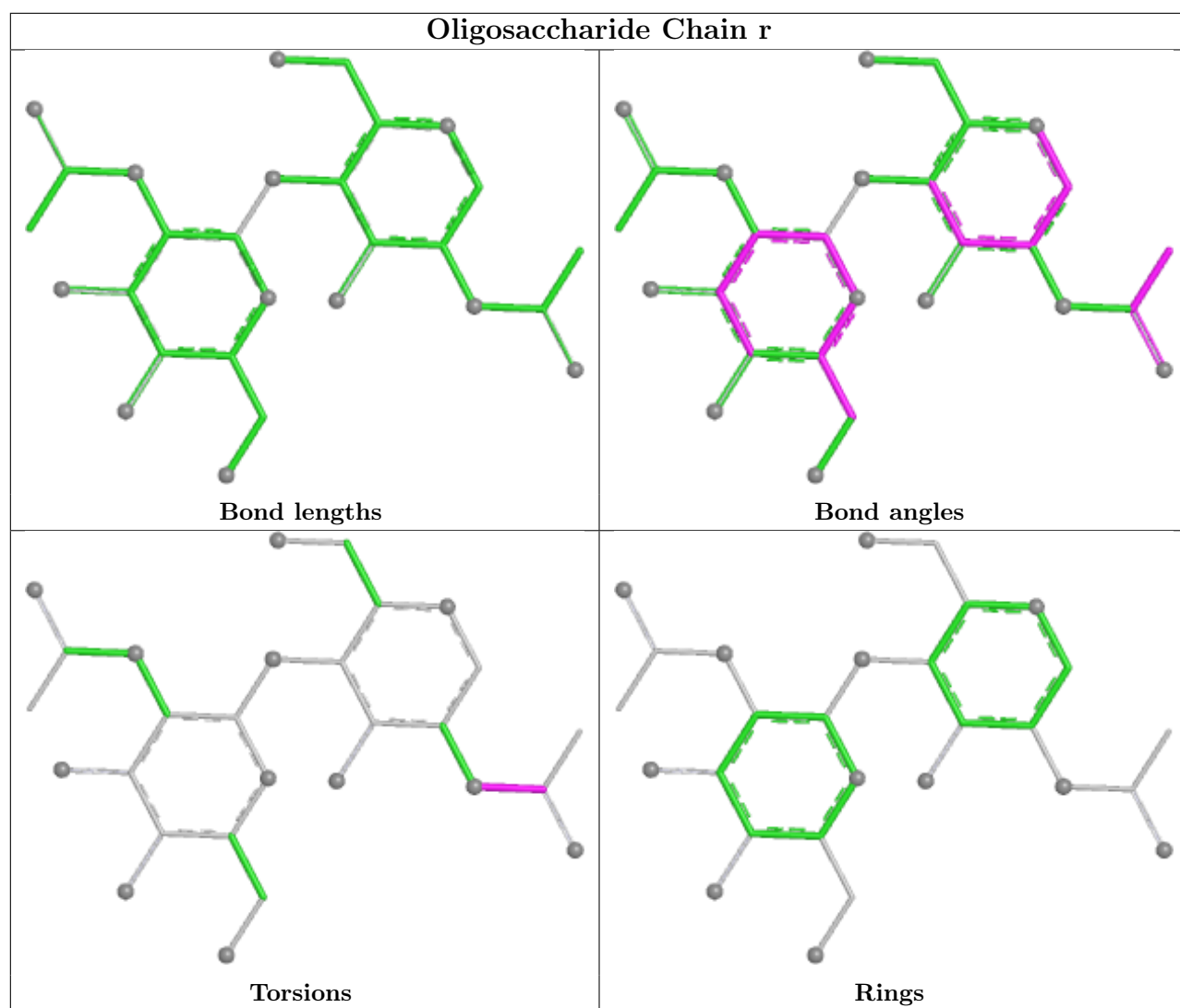


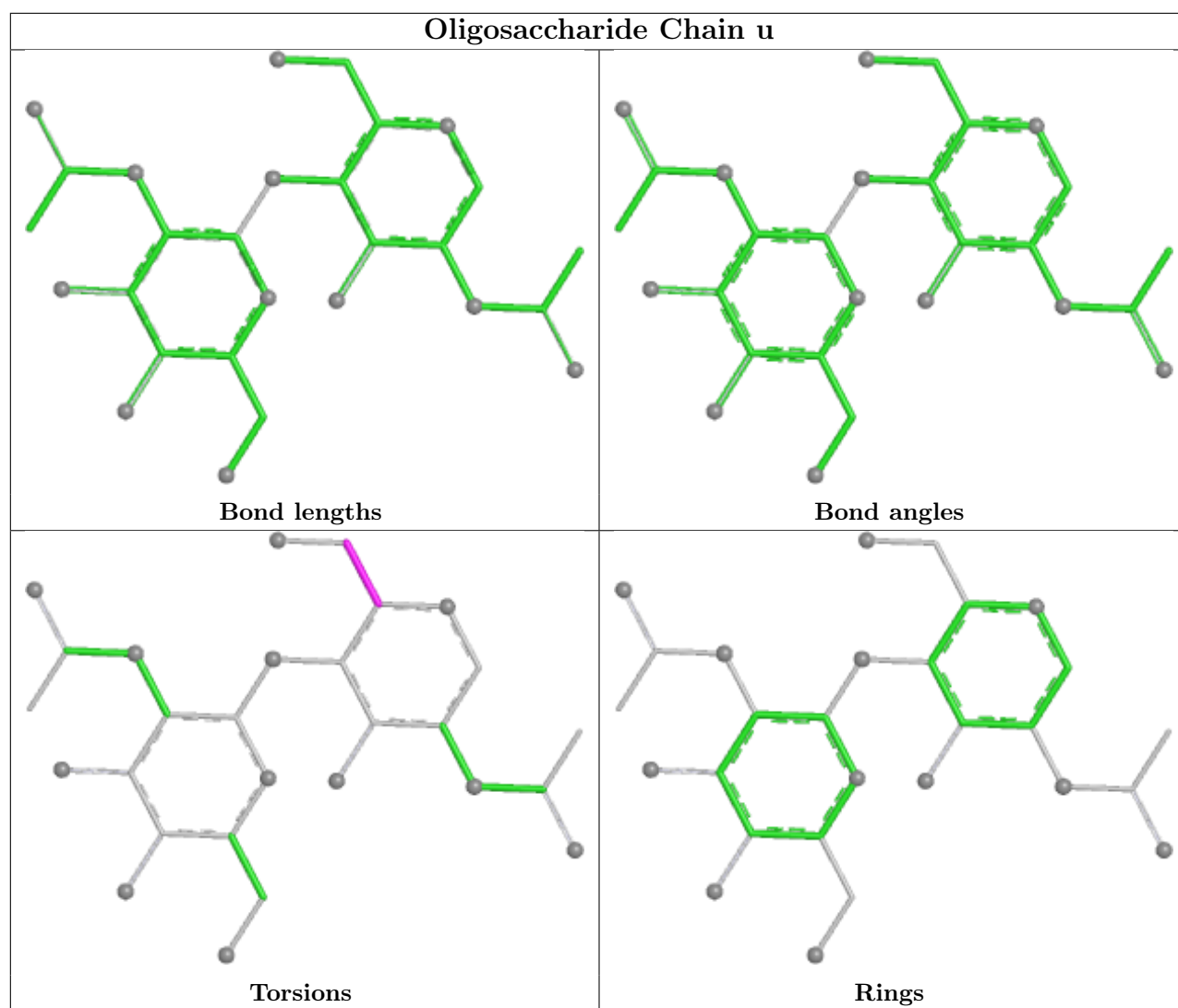


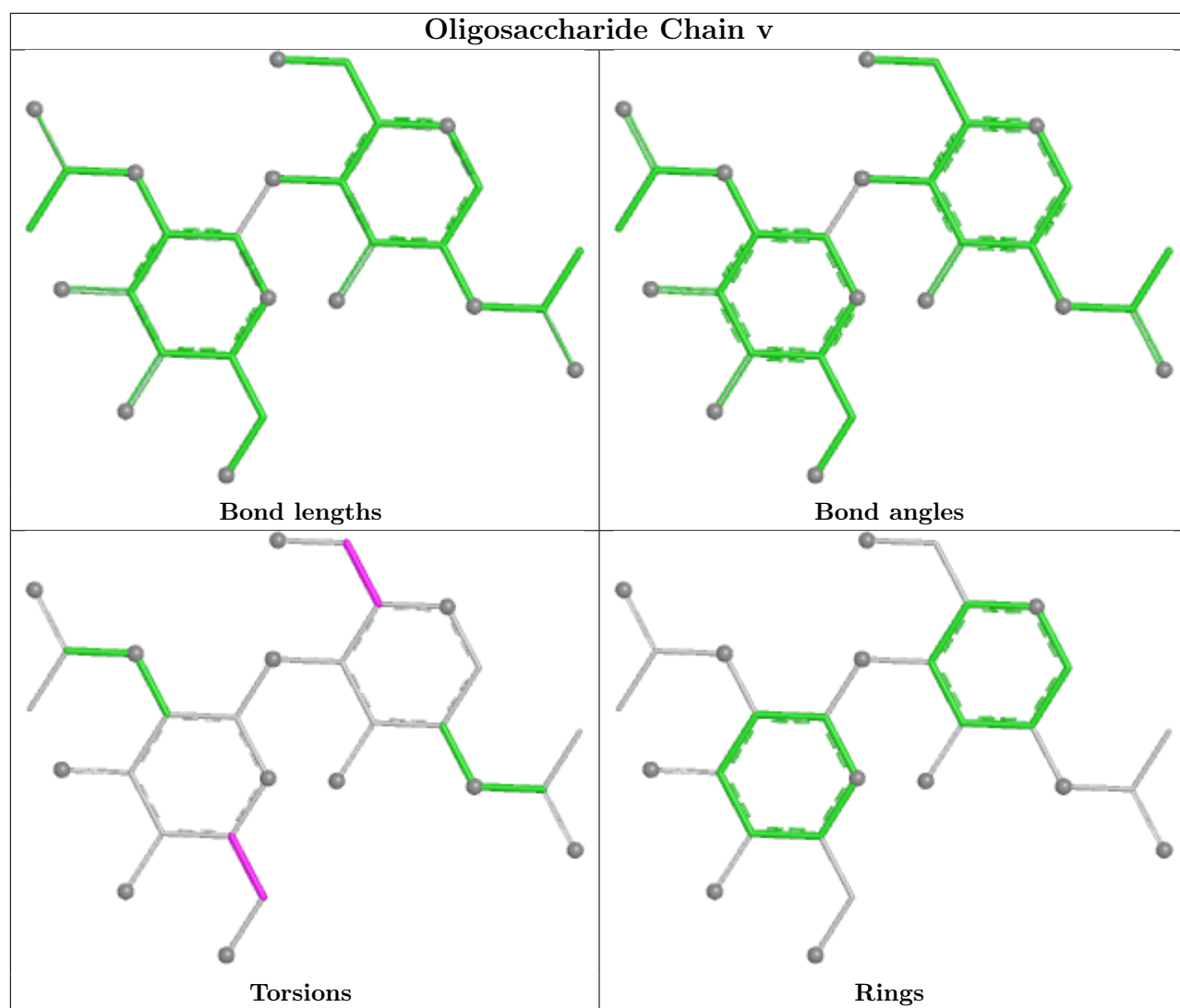


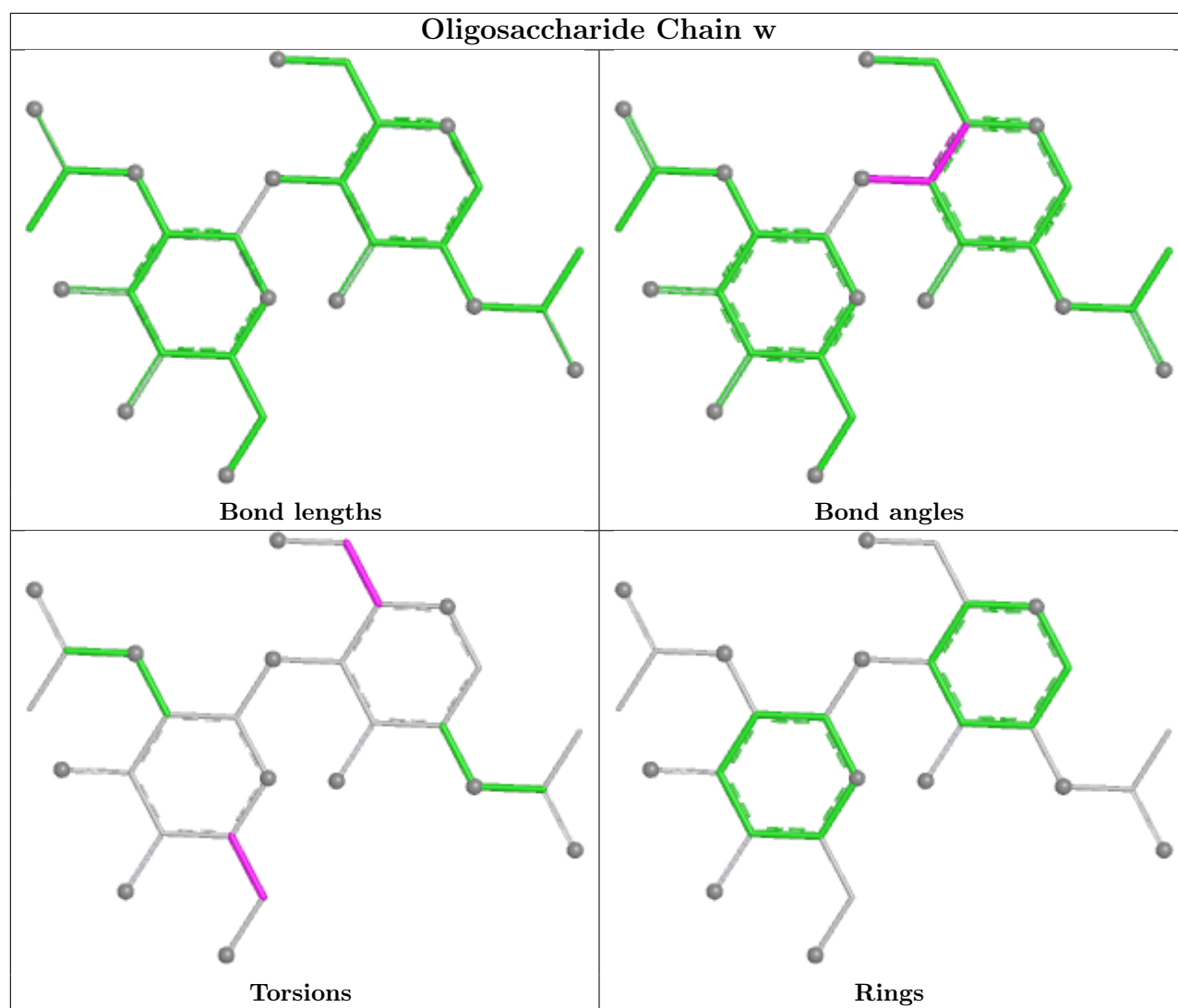


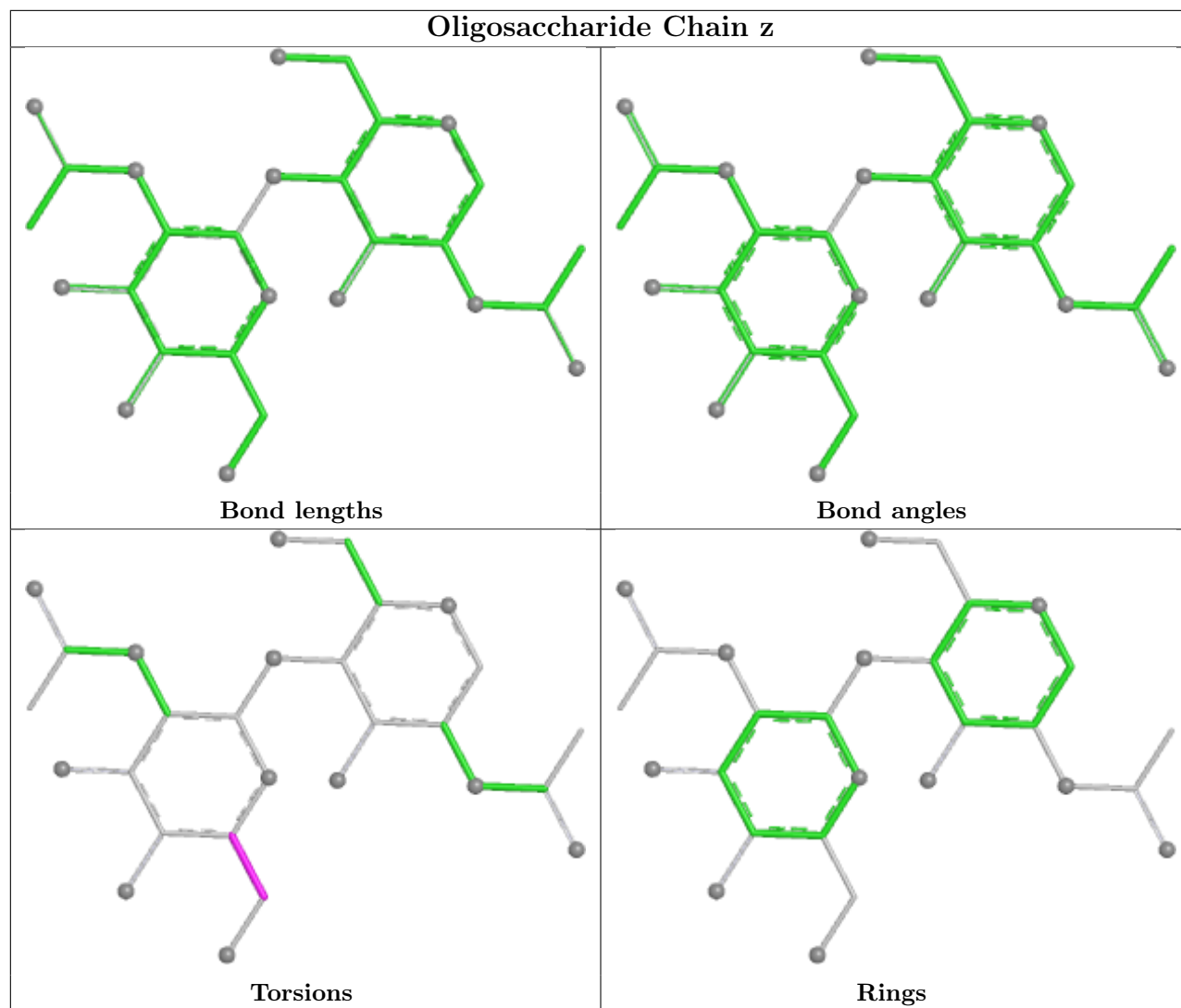


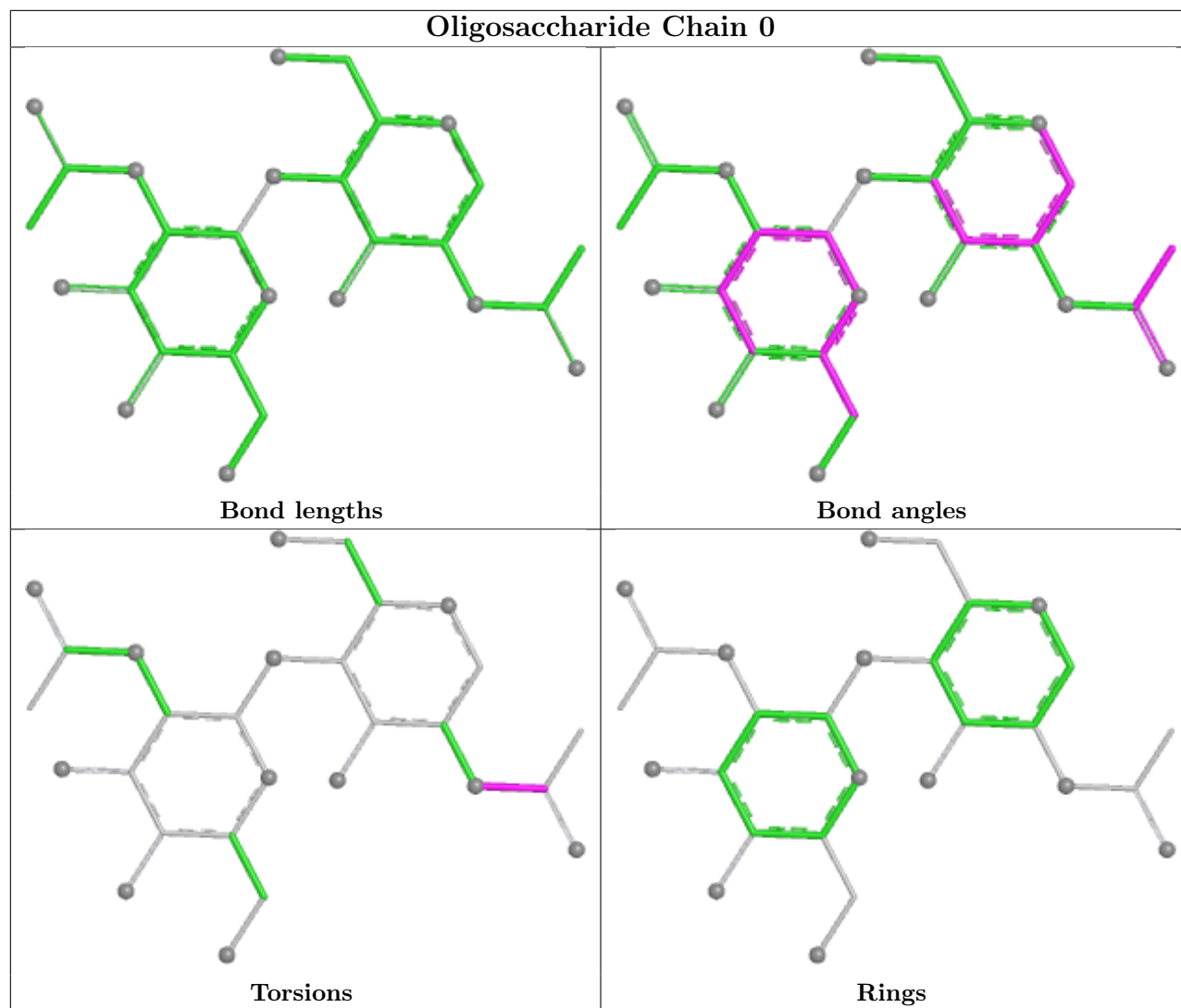


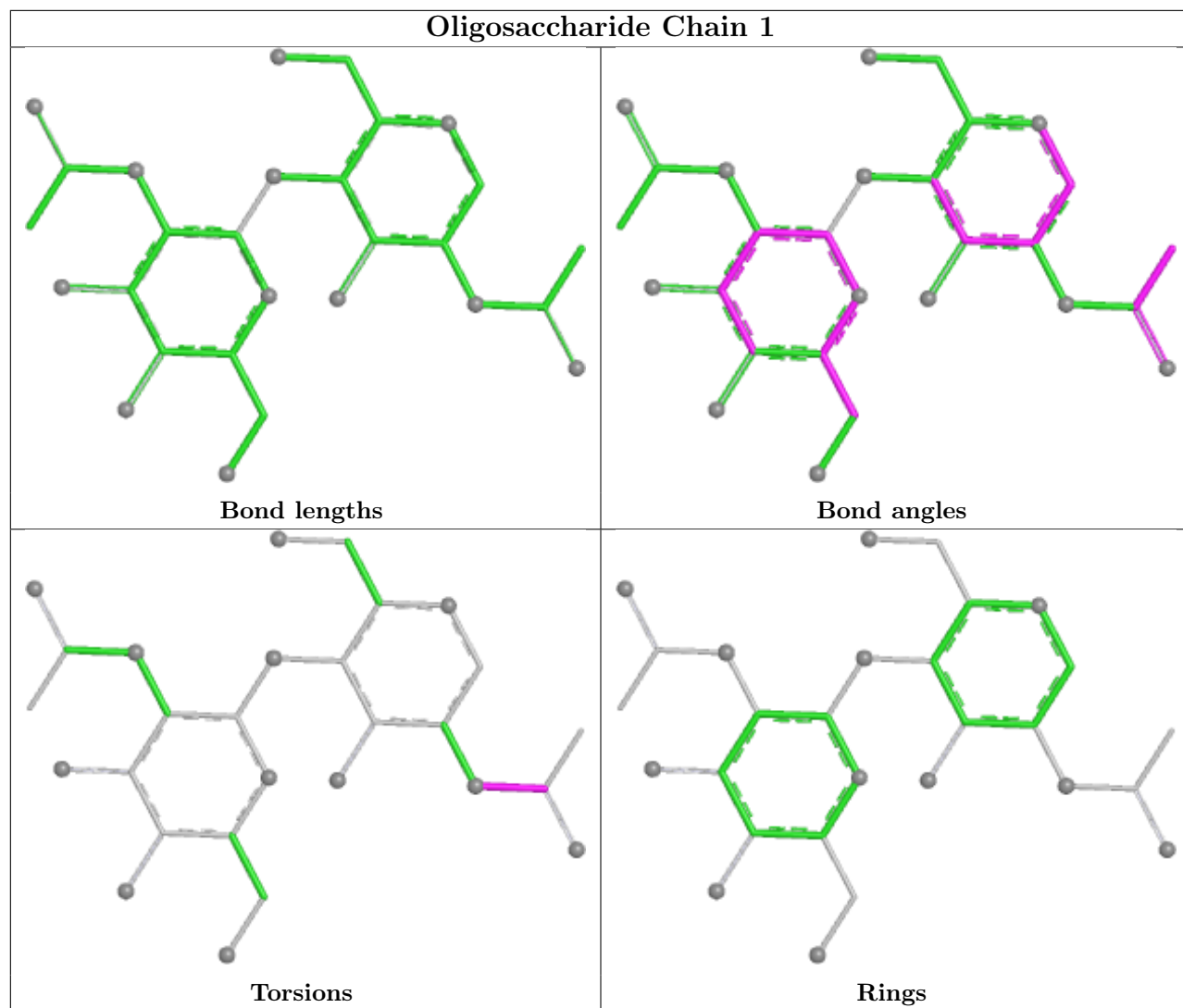


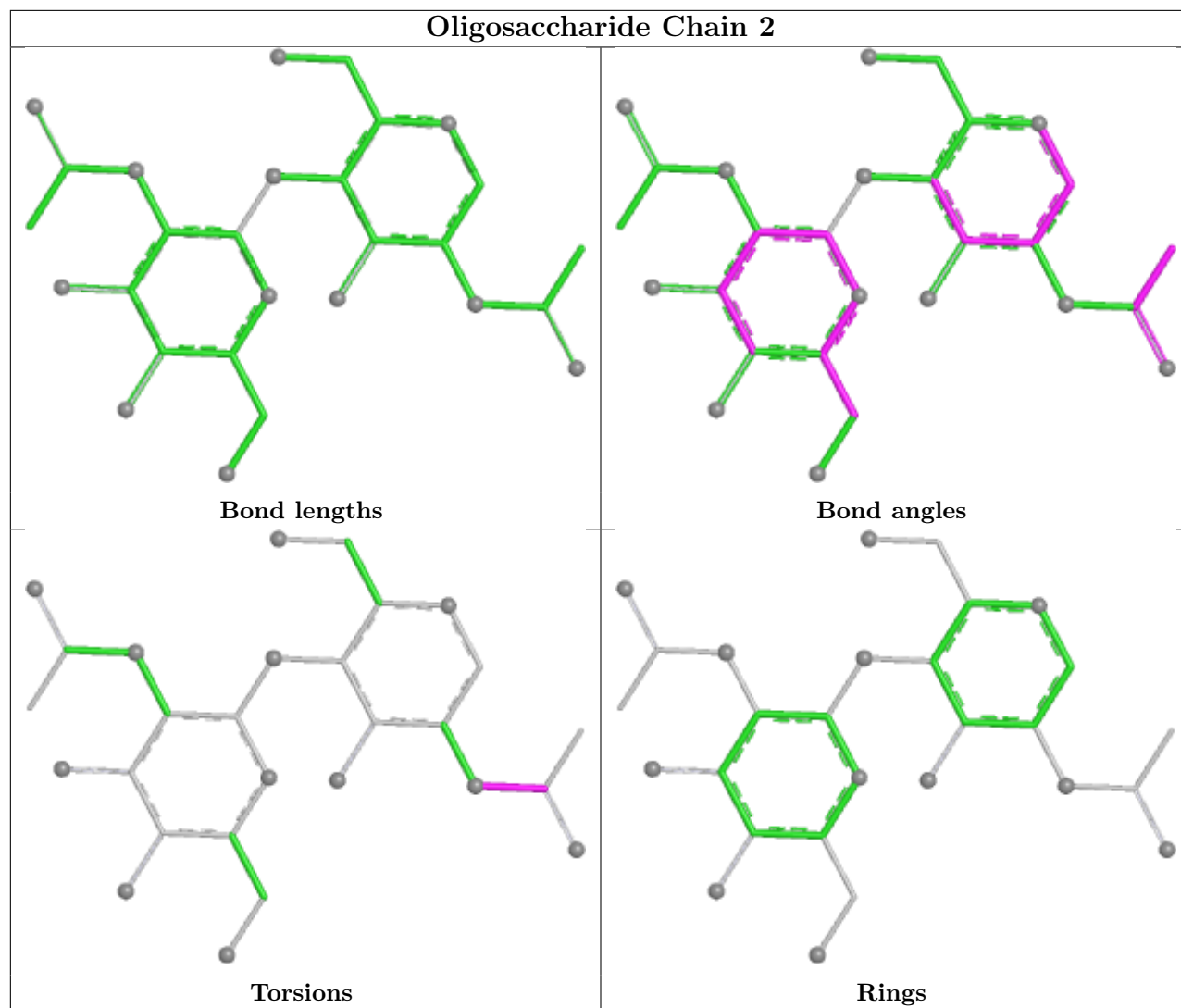


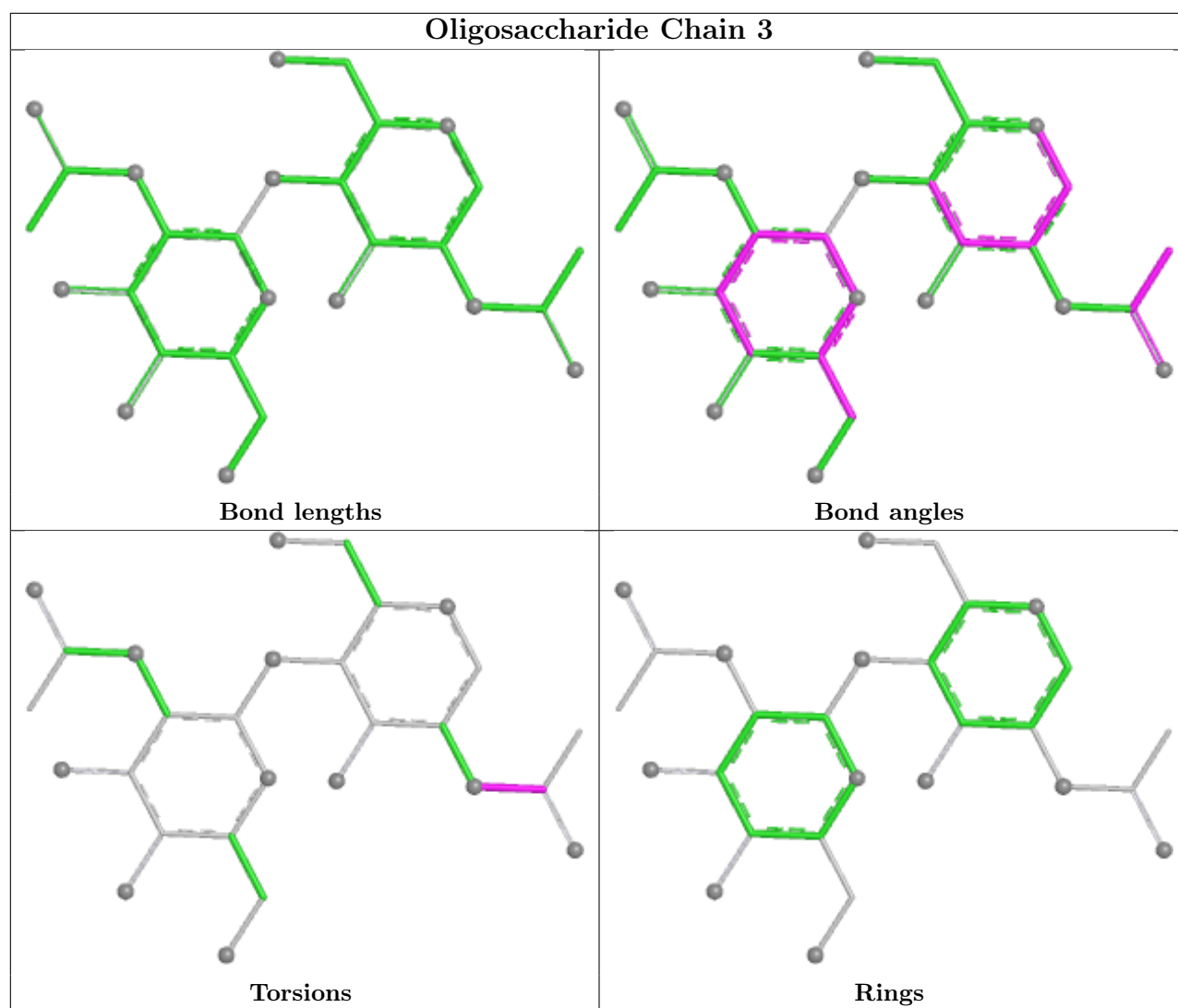


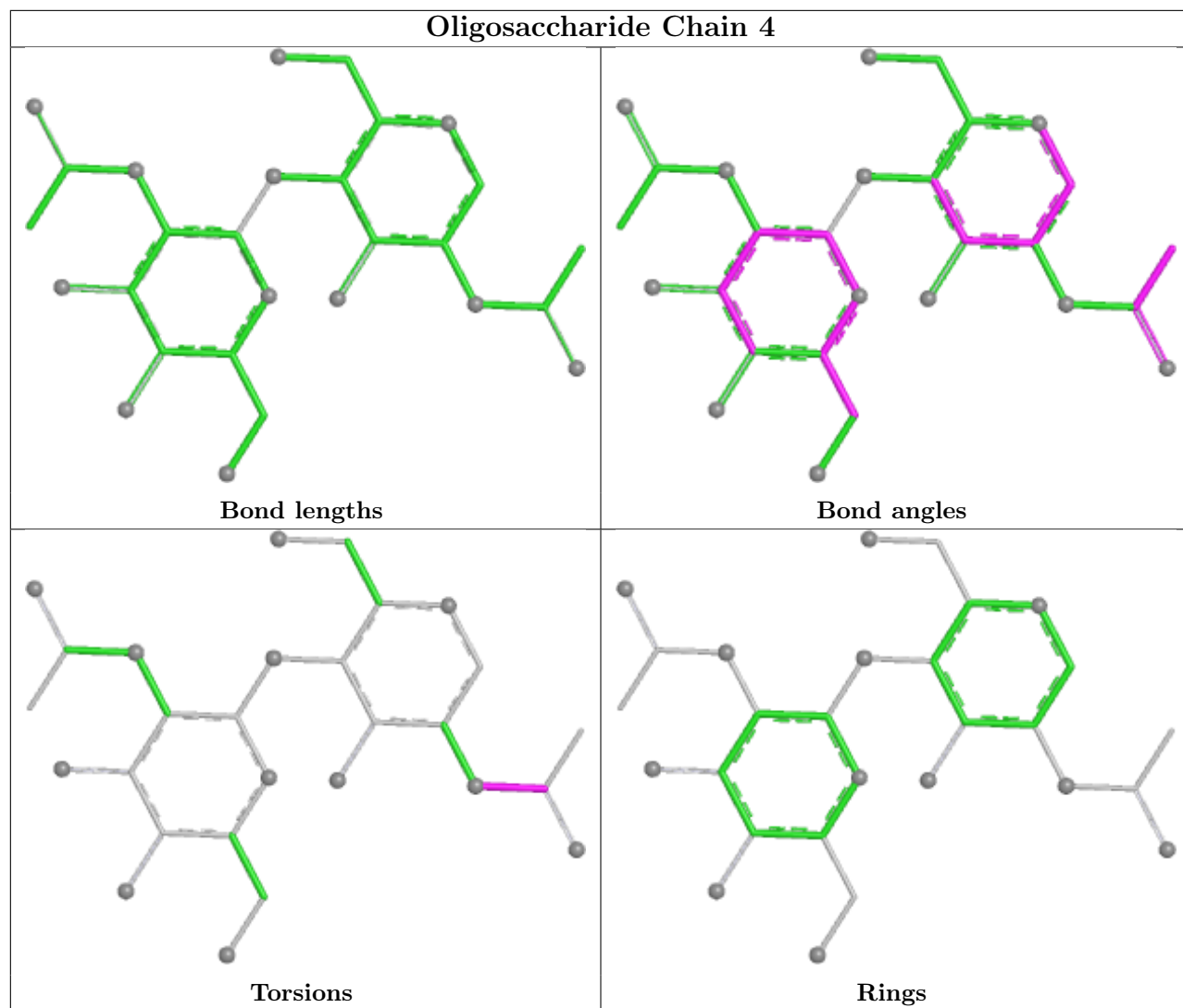


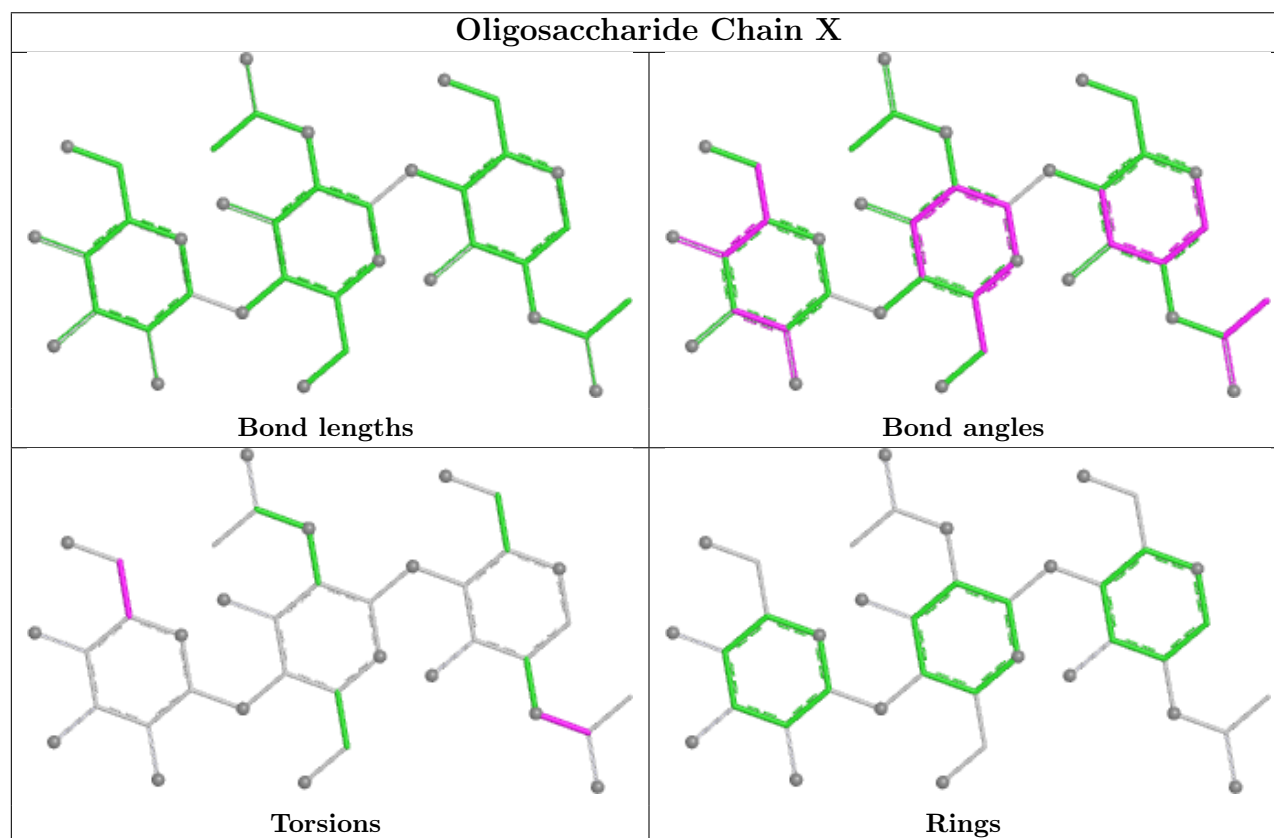
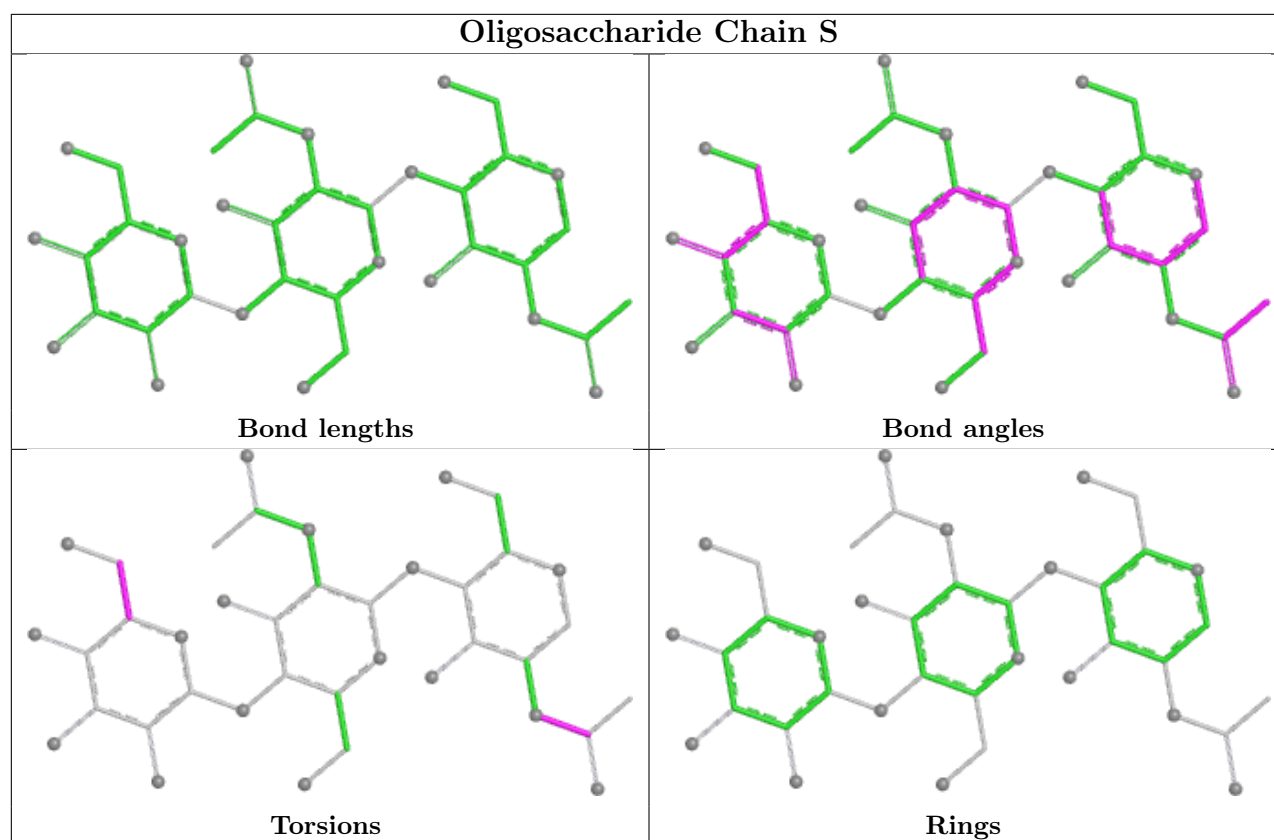


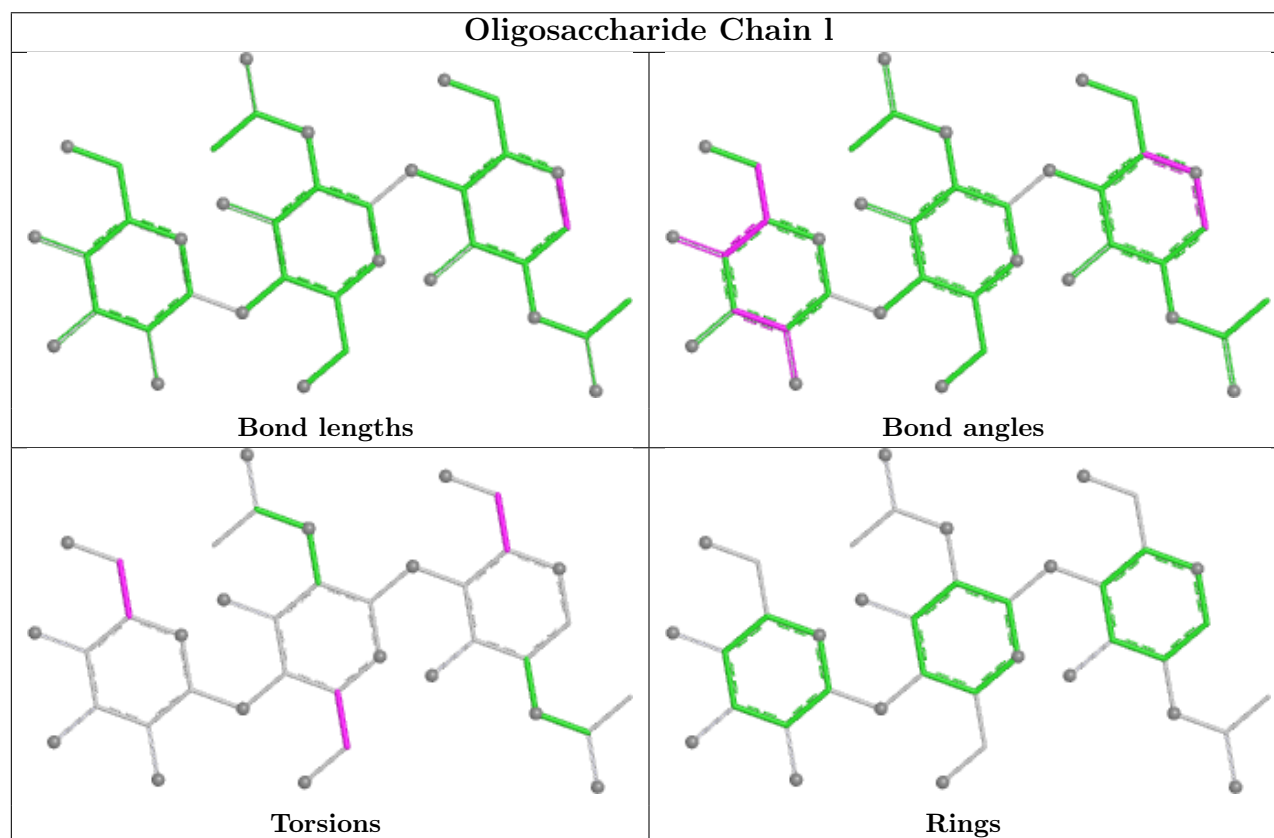
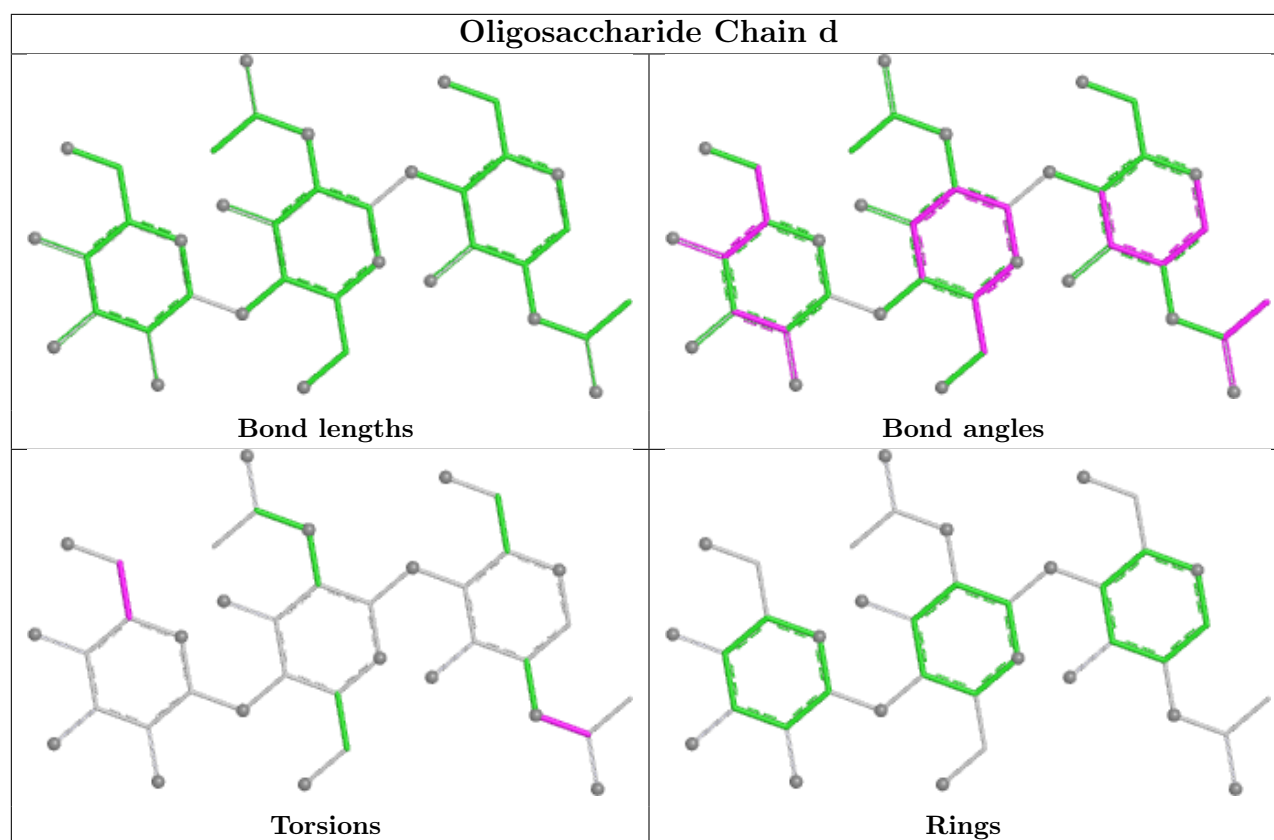


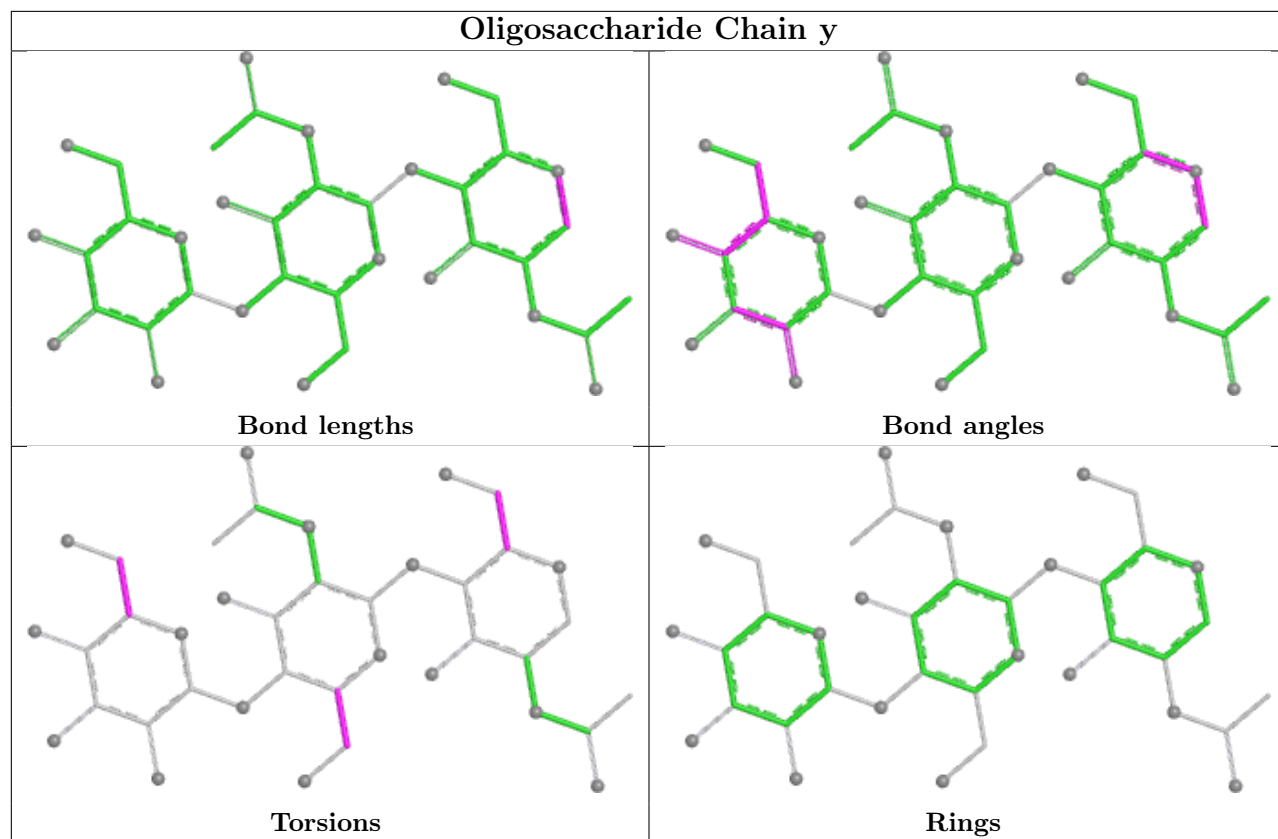


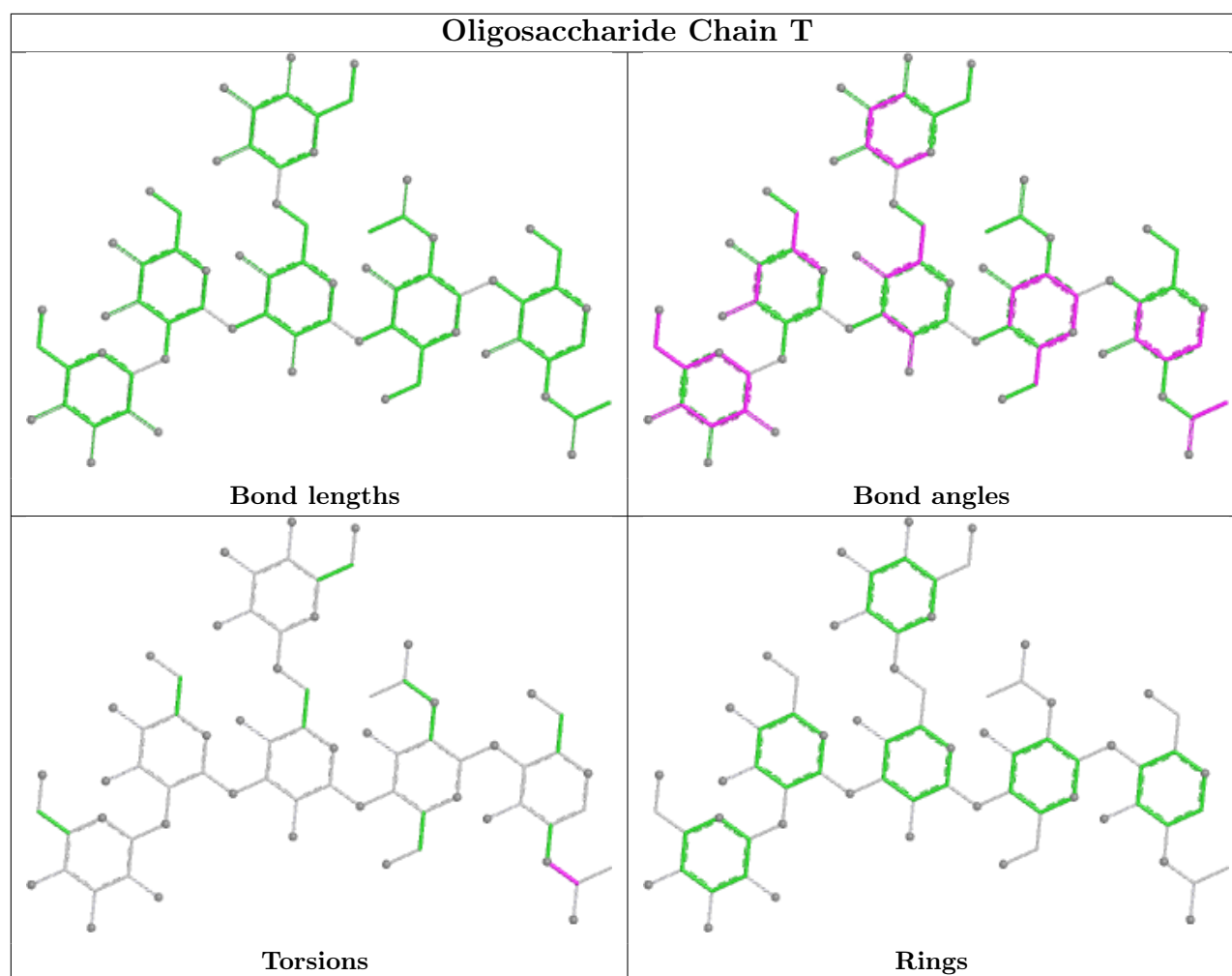


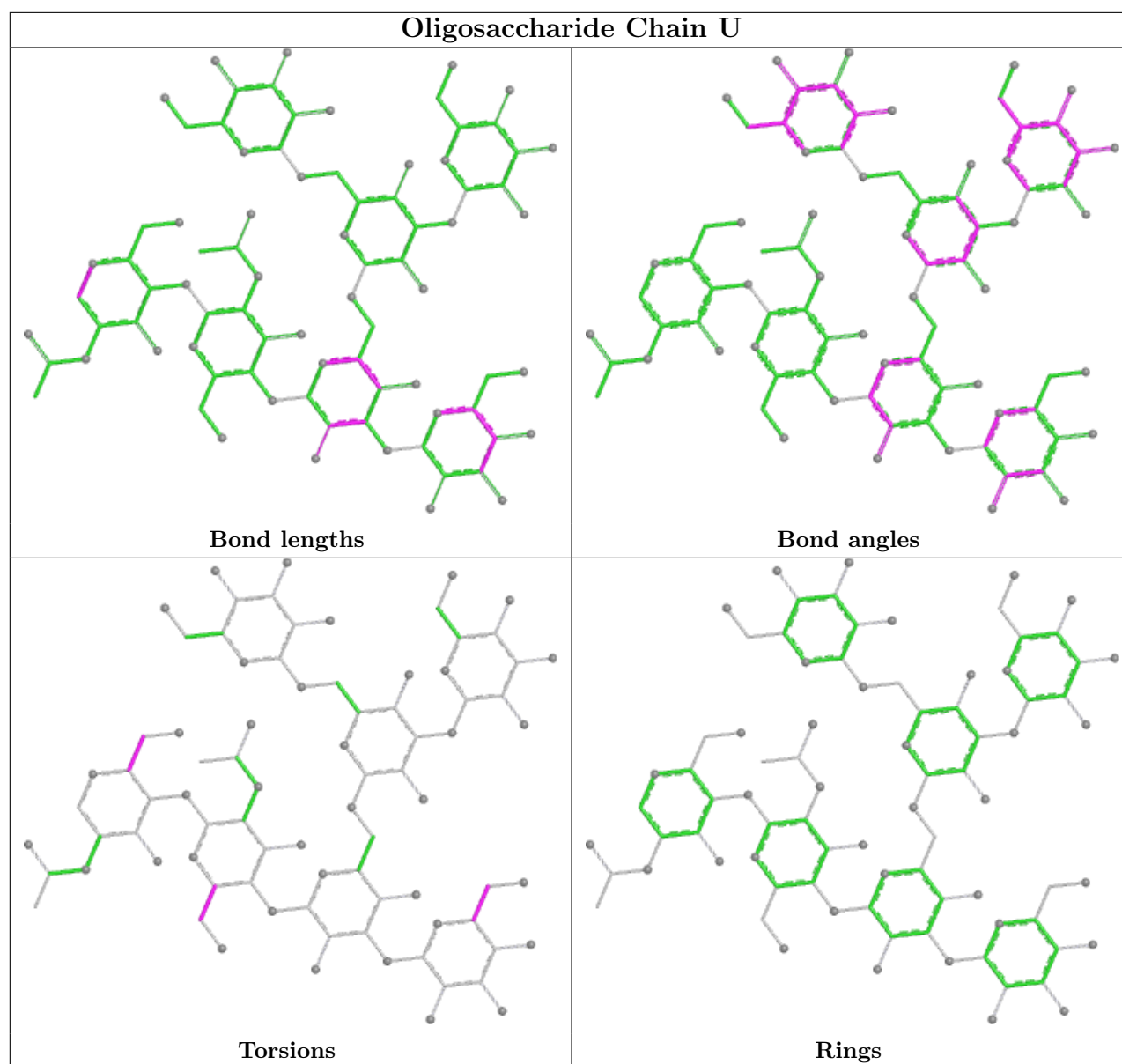


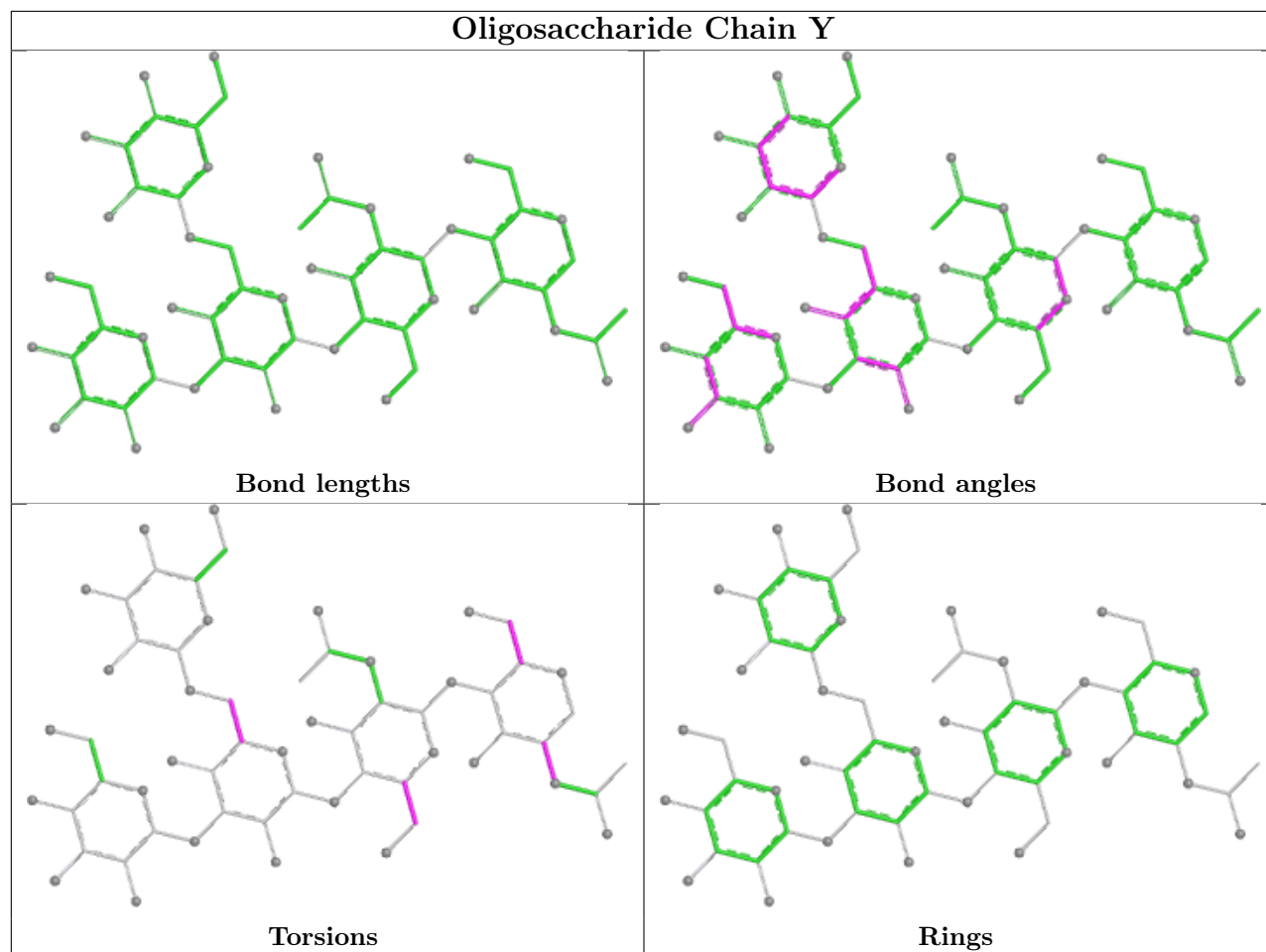


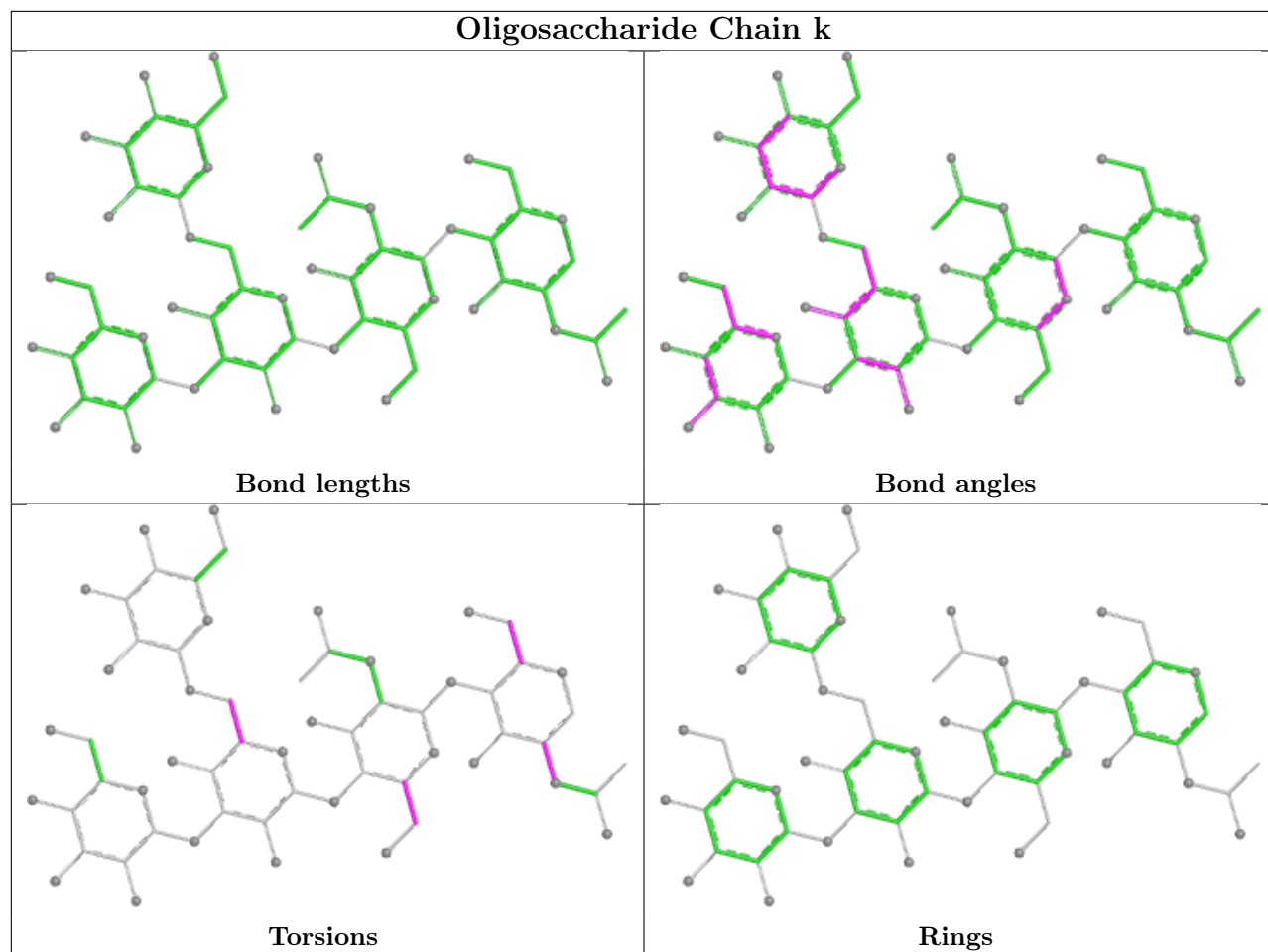


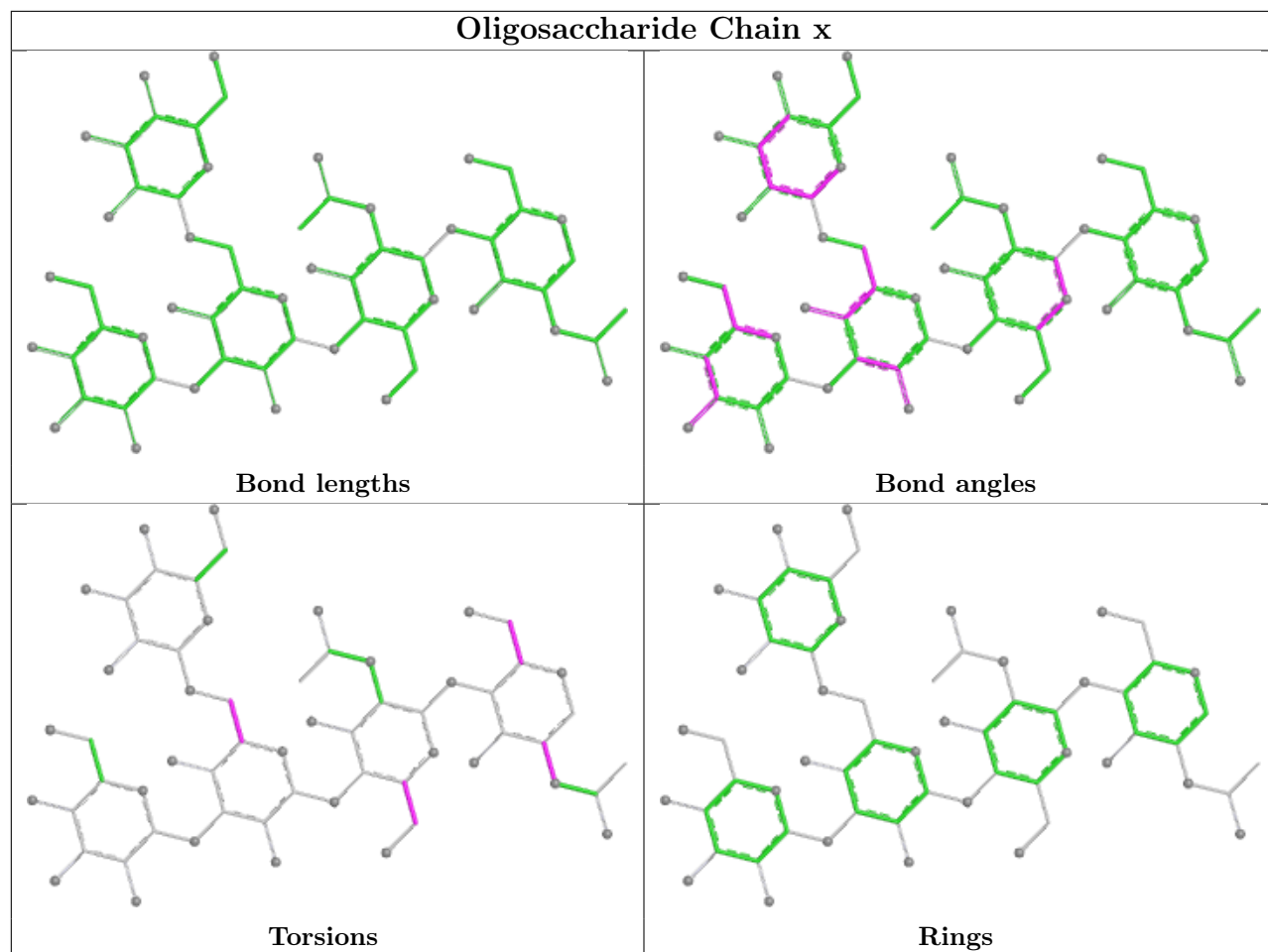


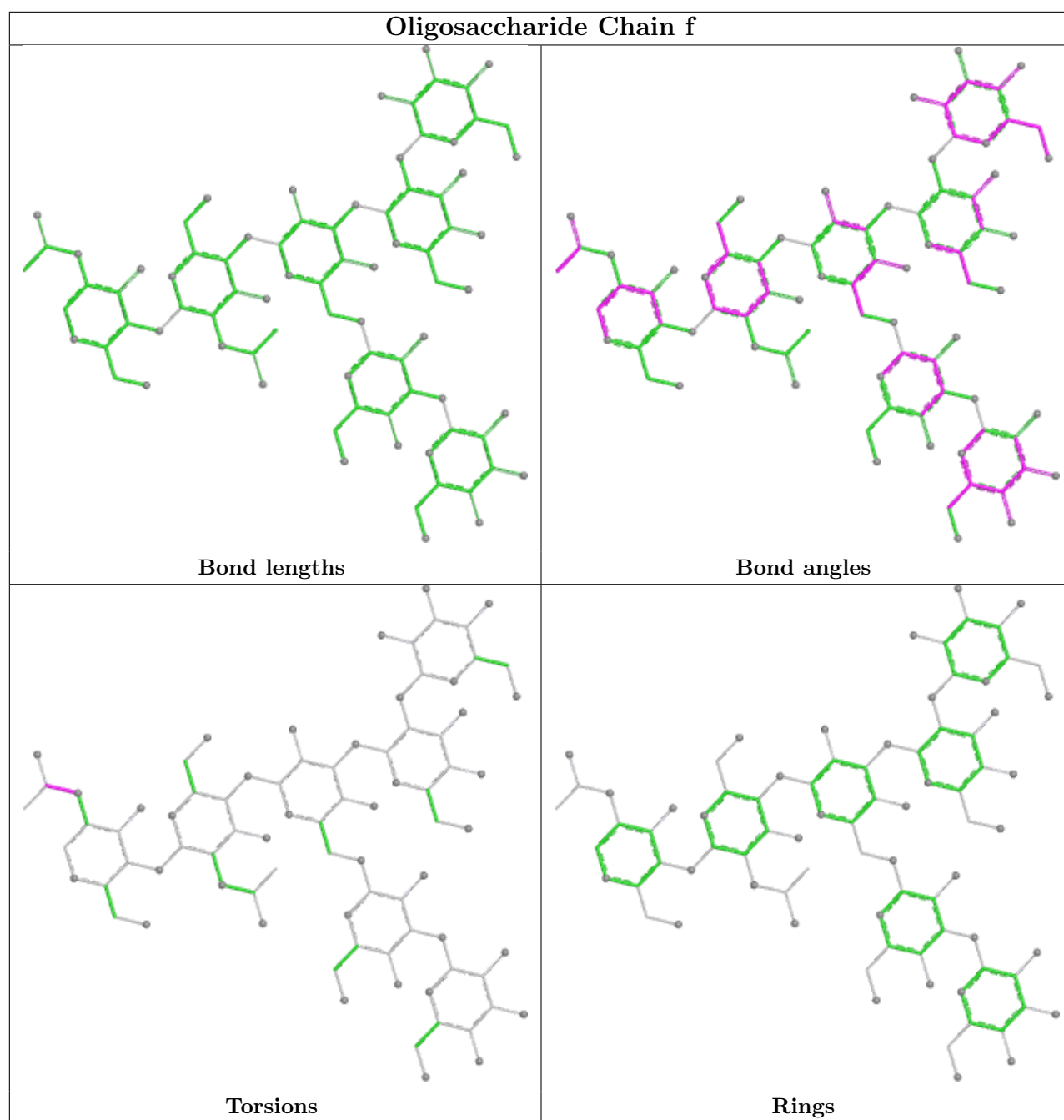


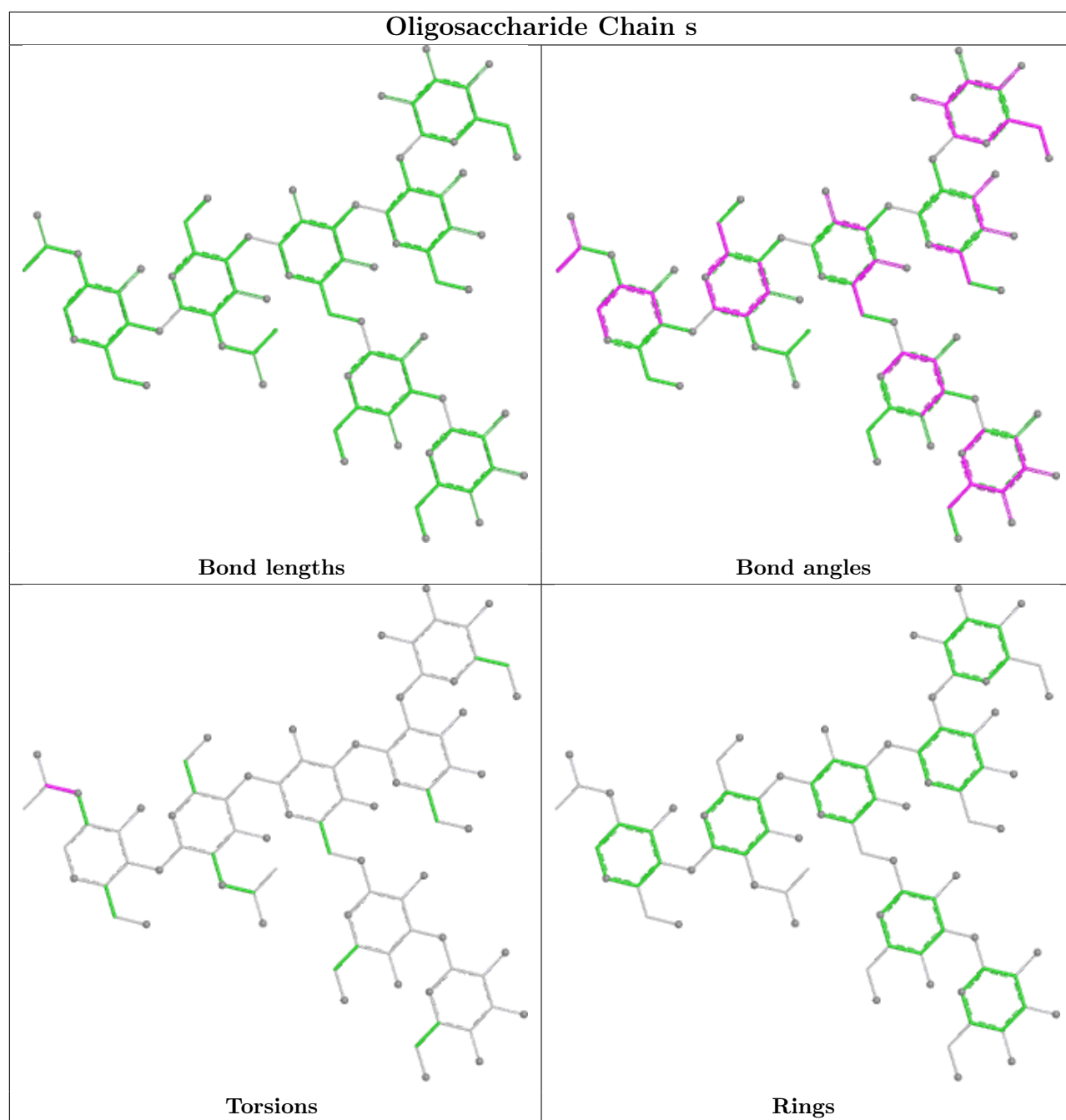


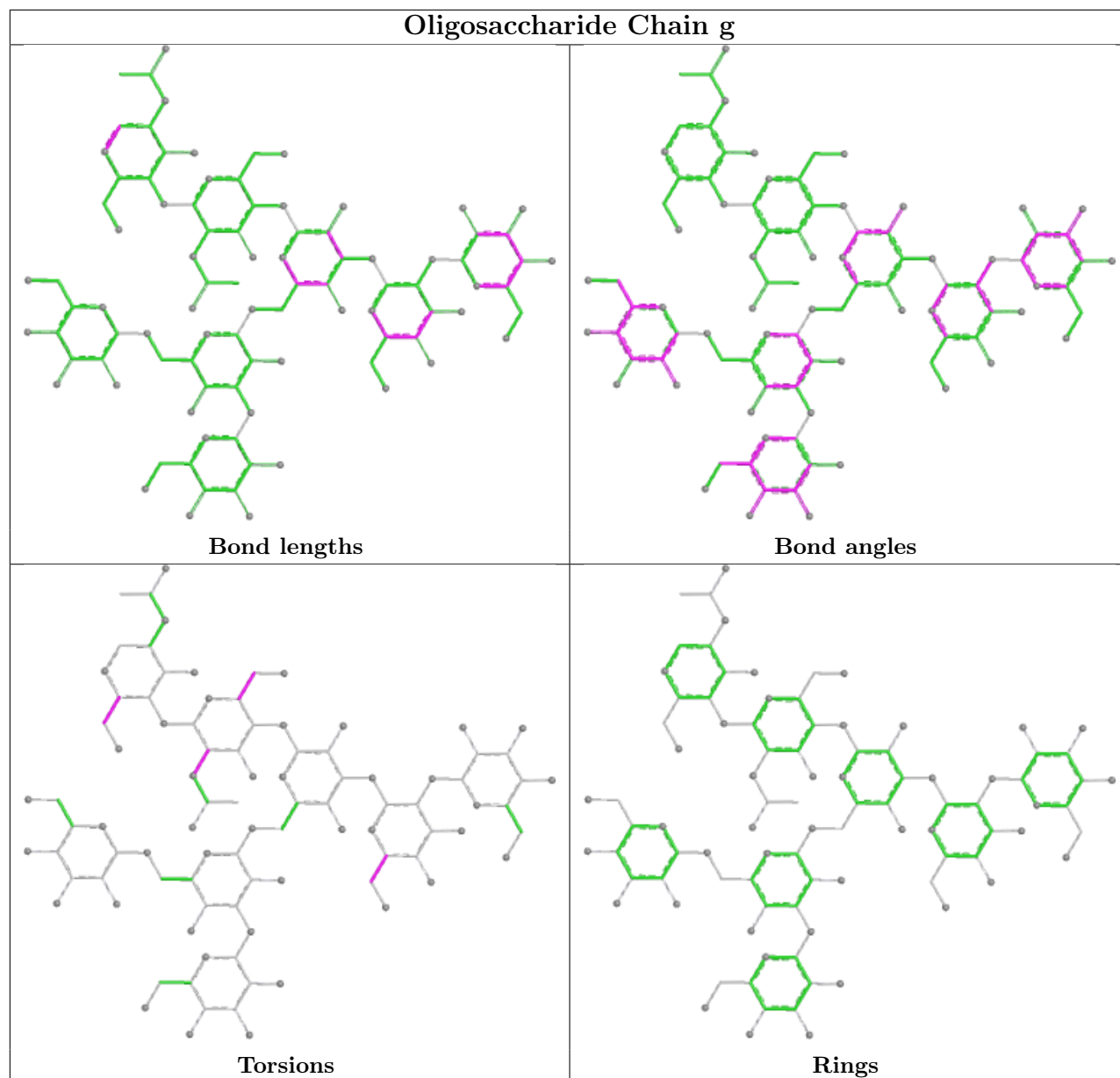


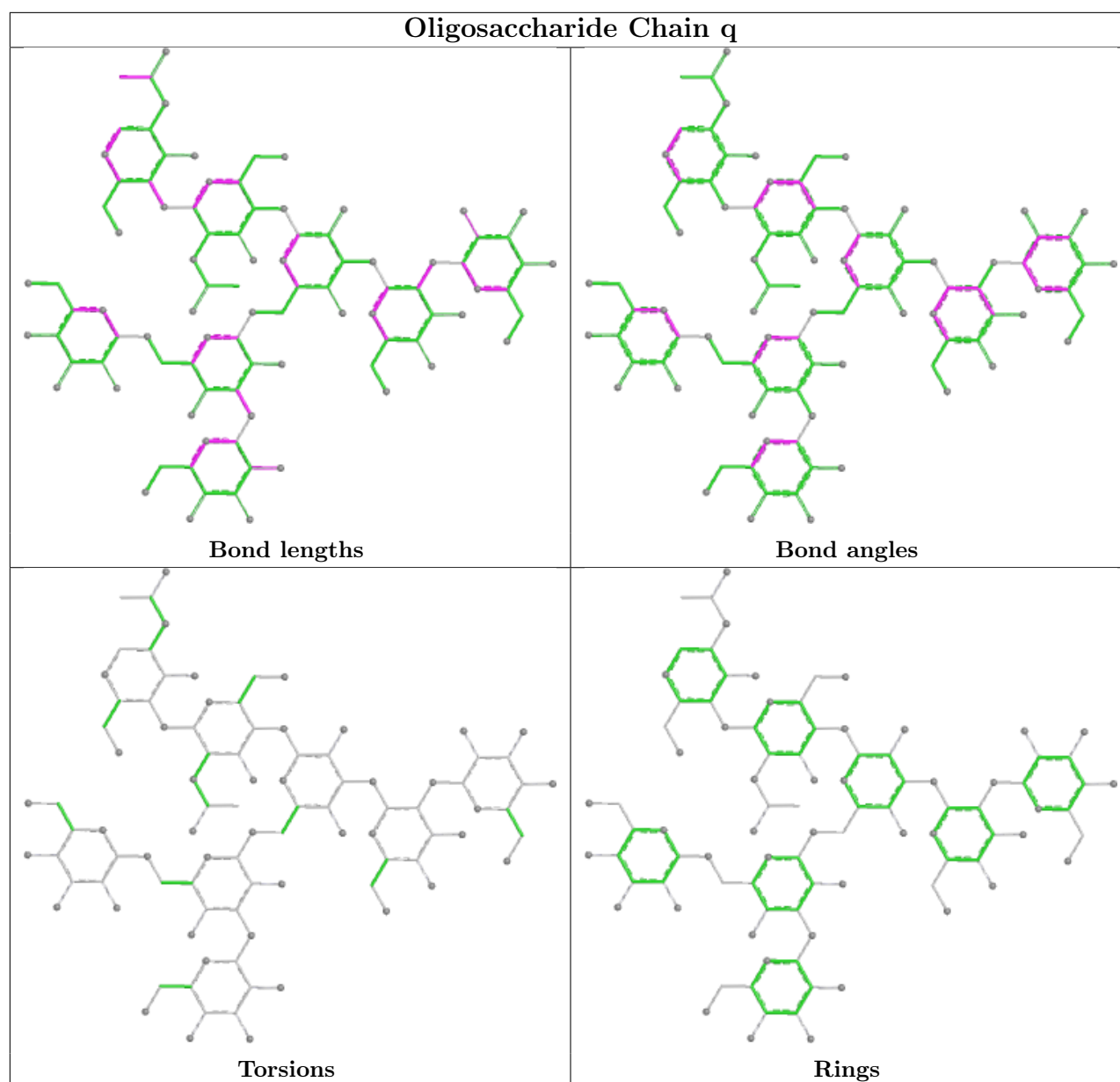


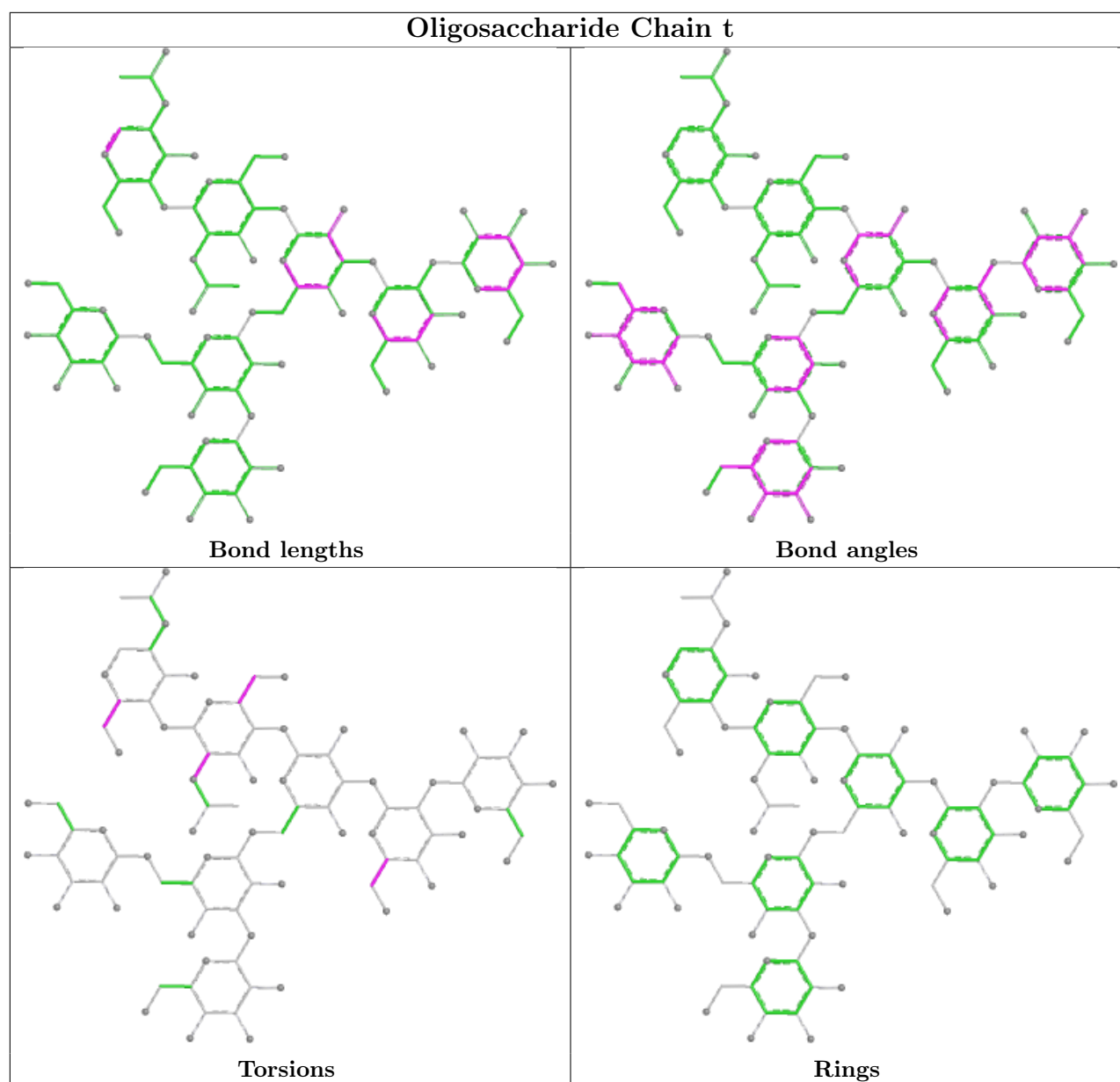












5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	D	639	1	14,14,15	0.51	0	17,19,21	0.42	0
14	NAG	F	704	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
14	NAG	A	633	1	14,14,15	0.30	0	17,19,21	0.41	0
14	NAG	C	611	1	14,14,15	0.51	0	17,19,21	0.52	0
14	NAG	D	603	1	14,14,15	0.41	0	17,19,21	0.66	1 (5%)
14	NAG	C	634	1	14,14,15	0.51	0	17,19,21	0.42	0
14	NAG	C	633	1	14,14,15	0.33	0	17,19,21	0.42	0
14	NAG	E	701	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
14	NAG	A	642	1	14,14,15	0.47	0	17,19,21	0.56	0
14	NAG	D	616	1	14,14,15	0.53	0	17,19,21	0.52	0
14	NAG	A	612	1	14,14,15	0.52	0	17,19,21	0.51	0
14	NAG	D	648	1	14,14,15	0.48	0	17,19,21	0.55	0
14	NAG	C	601	1	14,14,15	0.79	1 (7%)	17,19,21	0.92	2 (11%)
14	NAG	A	634	1	14,14,15	0.51	0	17,19,21	0.41	0
14	NAG	D	638	1	14,14,15	0.33	0	17,19,21	0.40	0
14	NAG	F	703	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
14	NAG	B	703	2	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
14	NAG	B	701	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
14	NAG	B	702	2	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
14	NAG	E	702	2	14,14,15	0.51	0	17,19,21	2.27	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	D	639	1	1/1/5/7	2/6/23/26	0/1/1/1
14	NAG	F	704	2	-	1/6/23/26	0/1/1/1
14	NAG	A	633	1	-	2/6/23/26	0/1/1/1
14	NAG	C	611	1	-	2/6/23/26	0/1/1/1
14	NAG	D	603	1	-	2/6/23/26	0/1/1/1
14	NAG	C	634	1	-	2/6/23/26	0/1/1/1
14	NAG	C	633	1	-	2/6/23/26	0/1/1/1
14	NAG	E	701	2	-	1/6/23/26	0/1/1/1
14	NAG	A	642	1	-	0/6/23/26	0/1/1/1
14	NAG	D	616	1	-	2/6/23/26	0/1/1/1
14	NAG	A	612	1	-	2/6/23/26	0/1/1/1
14	NAG	D	648	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	C	601	1	-	2/6/23/26	0/1/1/1
14	NAG	A	634	1	-	2/6/23/26	0/1/1/1
14	NAG	D	638	1	-	2/6/23/26	0/1/1/1
14	NAG	F	703	2	-	1/6/23/26	0/1/1/1
14	NAG	B	703	2	-	1/6/23/26	0/1/1/1
14	NAG	B	701	2	-	1/6/23/26	0/1/1/1
14	NAG	B	702	2	-	1/6/23/26	0/1/1/1
14	NAG	E	702	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	601	NAG	O5-C1	-2.19	1.40	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	703	NAG	O5-C1-C2	-7.52	99.65	111.29
14	B	702	NAG	O5-C1-C2	-7.52	99.66	111.29
14	F	703	NAG	O5-C1-C2	-7.51	99.67	111.29
14	E	702	NAG	O5-C1-C2	-7.51	99.67	111.29
14	F	704	NAG	O5-C1-C2	-7.51	99.68	111.29
14	E	701	NAG	O5-C1-C2	-7.49	99.71	111.29
14	B	701	NAG	O5-C1-C2	-7.48	99.71	111.29
14	B	702	NAG	O7-C7-C8	-2.90	116.88	122.05
14	B	701	NAG	O7-C7-C8	-2.90	116.89	122.05
14	F	703	NAG	O7-C7-C8	-2.90	116.89	122.05
14	B	703	NAG	O7-C7-C8	-2.89	116.92	122.05
14	E	702	NAG	O7-C7-C8	-2.88	116.92	122.05
14	F	704	NAG	O7-C7-C8	-2.88	116.93	122.05
14	E	701	NAG	O7-C7-C8	-2.87	116.94	122.05
14	B	703	NAG	C4-C3-C2	-2.69	107.08	111.02
14	E	701	NAG	C4-C3-C2	-2.68	107.08	111.02
14	B	702	NAG	C4-C3-C2	-2.67	107.10	111.02
14	B	701	NAG	C4-C3-C2	-2.66	107.12	111.02
14	E	702	NAG	C4-C3-C2	-2.66	107.12	111.02
14	F	703	NAG	C4-C3-C2	-2.66	107.12	111.02
14	F	704	NAG	C4-C3-C2	-2.64	107.15	111.02
14	C	601	NAG	C3-C4-C5	2.26	114.32	110.23
14	D	603	NAG	C1-O5-C5	2.08	114.97	112.19
14	C	601	NAG	O4-C4-C5	-2.00	104.39	109.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	D	639	NAG	C1

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	633	NAG	O5-C5-C6-O6
14	A	634	NAG	O5-C5-C6-O6
14	C	601	NAG	O5-C5-C6-O6
14	C	633	NAG	O5-C5-C6-O6
14	C	634	NAG	O5-C5-C6-O6
14	D	638	NAG	O5-C5-C6-O6
14	D	639	NAG	O5-C5-C6-O6
14	A	634	NAG	C4-C5-C6-O6
14	C	634	NAG	C4-C5-C6-O6
14	D	639	NAG	C4-C5-C6-O6
14	D	603	NAG	O5-C5-C6-O6
14	A	612	NAG	O5-C5-C6-O6
14	C	611	NAG	O5-C5-C6-O6
14	D	616	NAG	O5-C5-C6-O6
14	A	633	NAG	C4-C5-C6-O6
14	C	633	NAG	C4-C5-C6-O6
14	D	638	NAG	C4-C5-C6-O6
14	C	601	NAG	C4-C5-C6-O6
14	A	612	NAG	C4-C5-C6-O6
14	C	611	NAG	C4-C5-C6-O6
14	D	616	NAG	C4-C5-C6-O6
14	D	603	NAG	C4-C5-C6-O6
14	E	702	NAG	O7-C7-N2-C2
14	F	703	NAG	O7-C7-N2-C2
14	B	701	NAG	O7-C7-N2-C2
14	B	702	NAG	O7-C7-N2-C2
14	B	703	NAG	O7-C7-N2-C2
14	E	701	NAG	O7-C7-N2-C2
14	F	704	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	648	NAG	3	0
14	C	601	NAG	5	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.

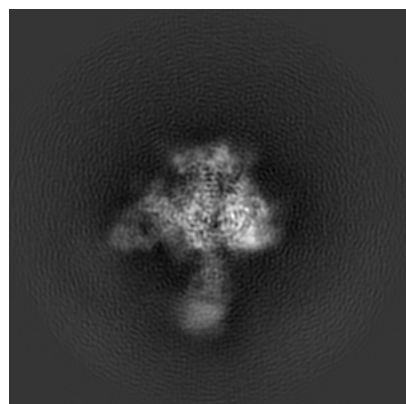
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8643. These allow visual inspection of the internal detail of the map and identification of artifacts.

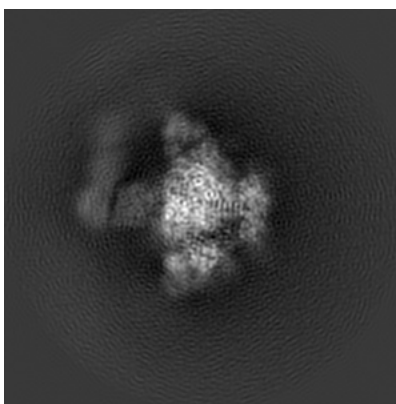
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

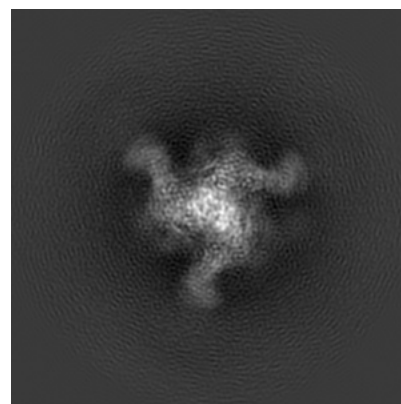
6.1.1 Primary map



X

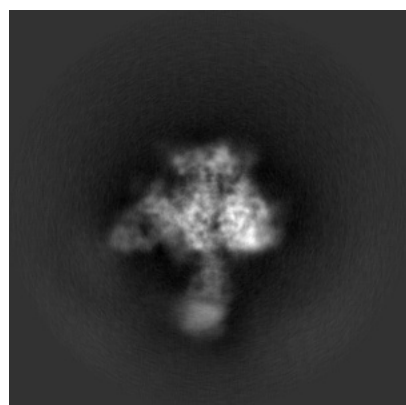


Y

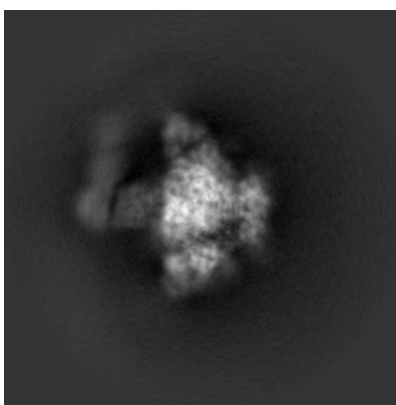


Z

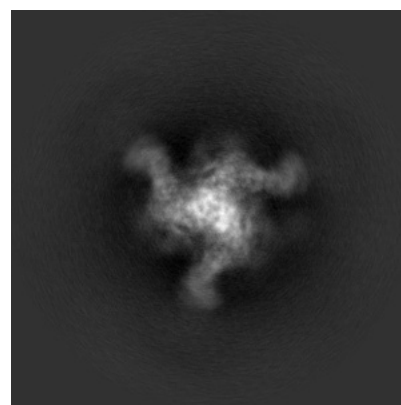
6.1.2 Raw map



X



Y

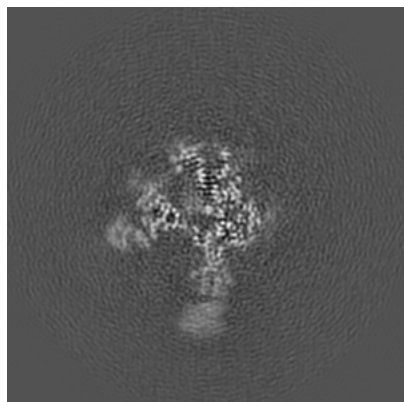


Z

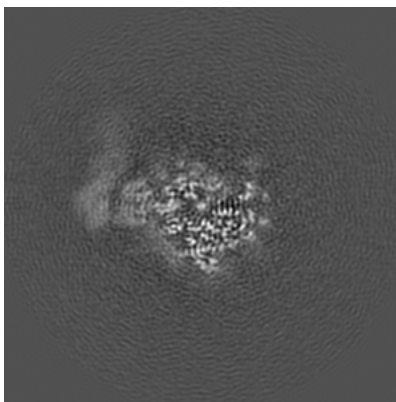
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

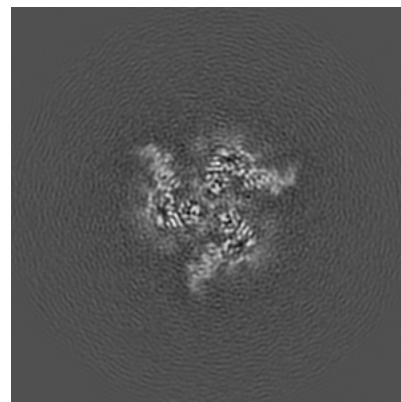
6.2.1 Primary map



X Index: 144

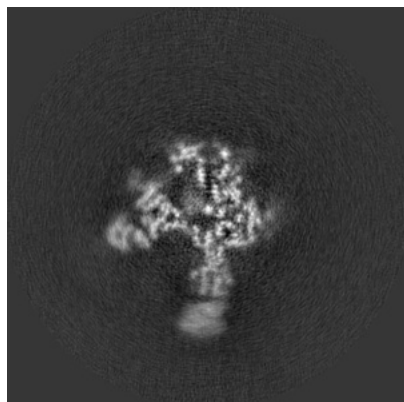


Y Index: 144

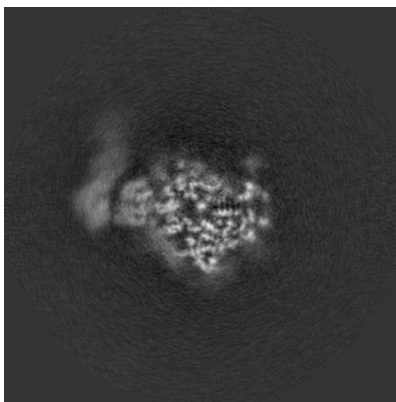


Z Index: 144

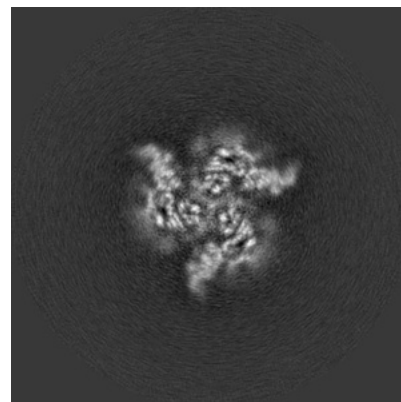
6.2.2 Raw map



X Index: 144



Y Index: 144

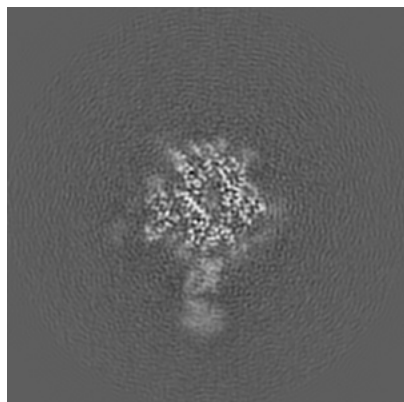


Z Index: 144

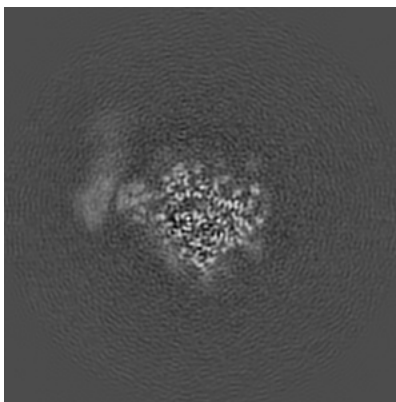
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

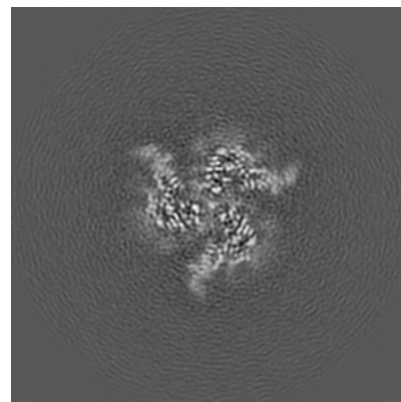
6.3.1 Primary map



X Index: 152

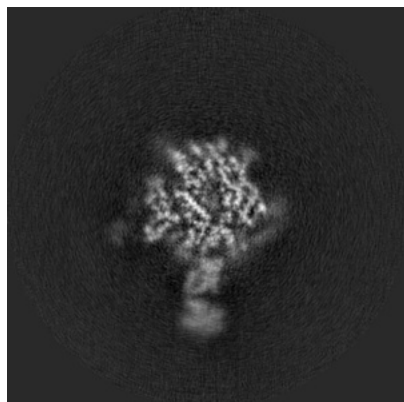


Y Index: 140

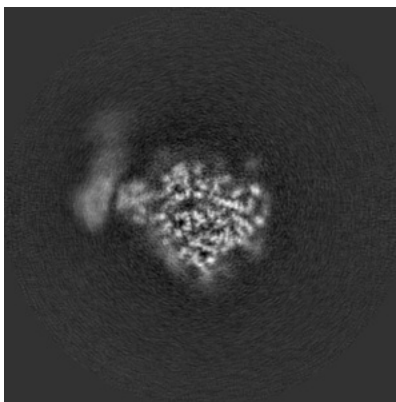


Z Index: 143

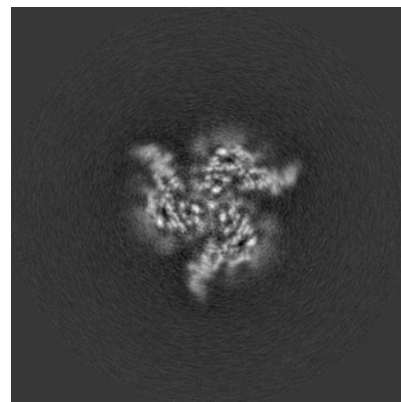
6.3.2 Raw map



X Index: 152



Y Index: 140

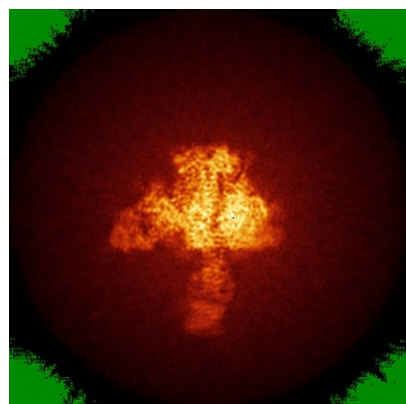


Z Index: 143

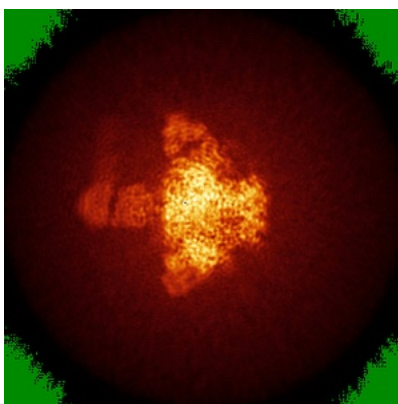
The images above show the largest variance slices of the map in three orthogonal directions.

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

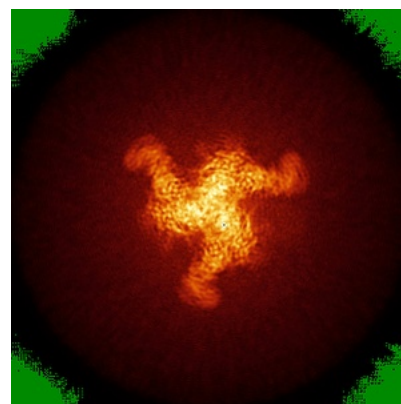
6.4.1 Primary map



X



Y

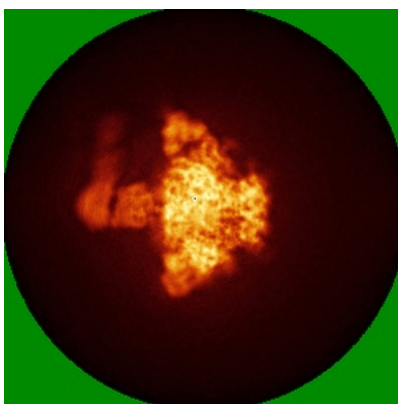


Z

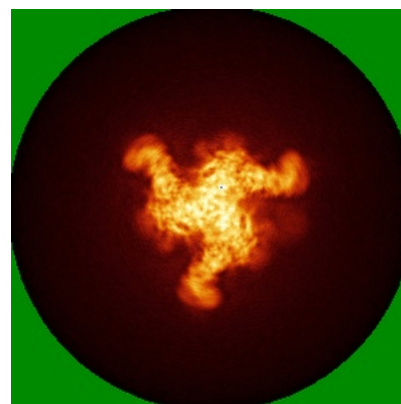
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

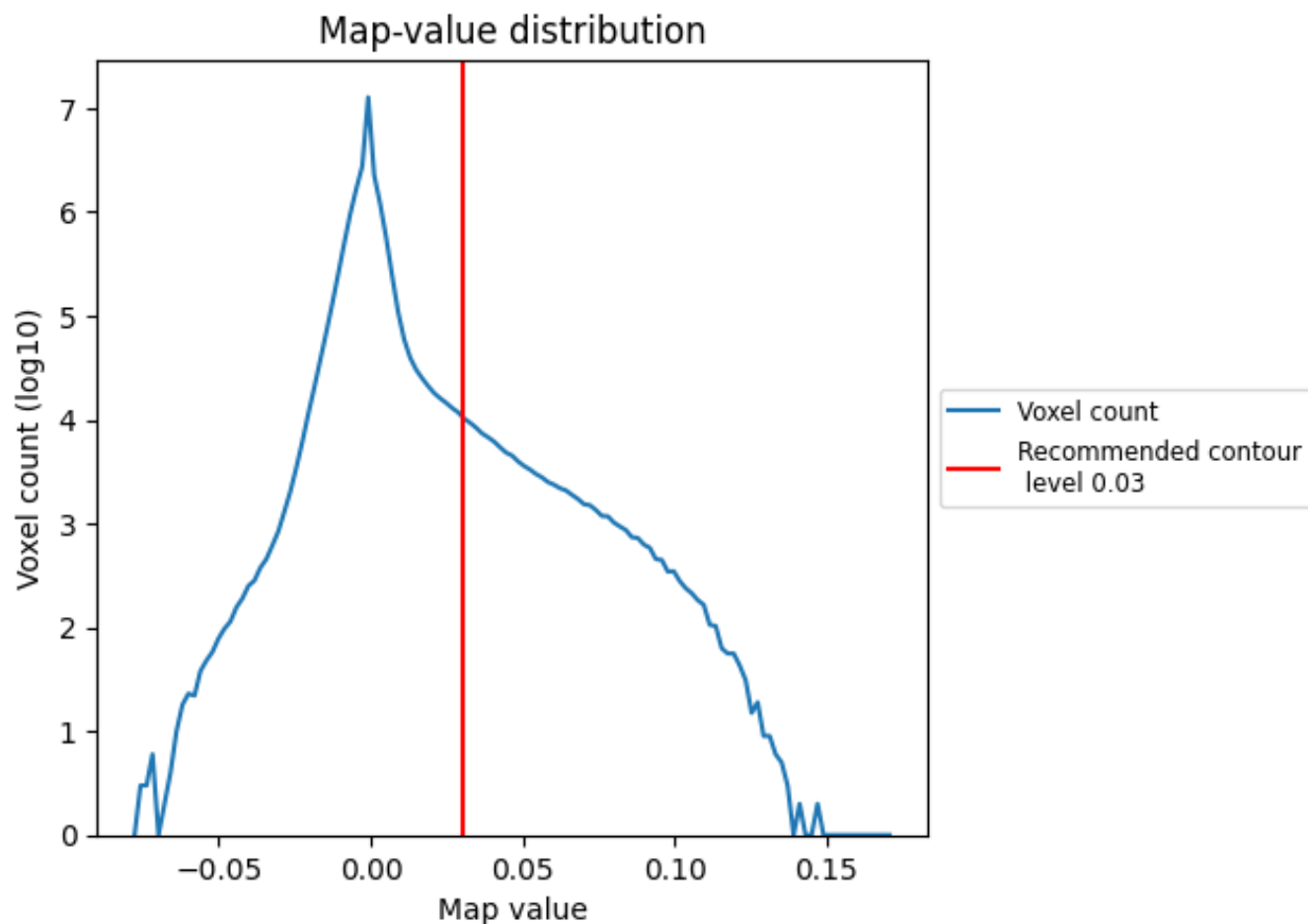
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

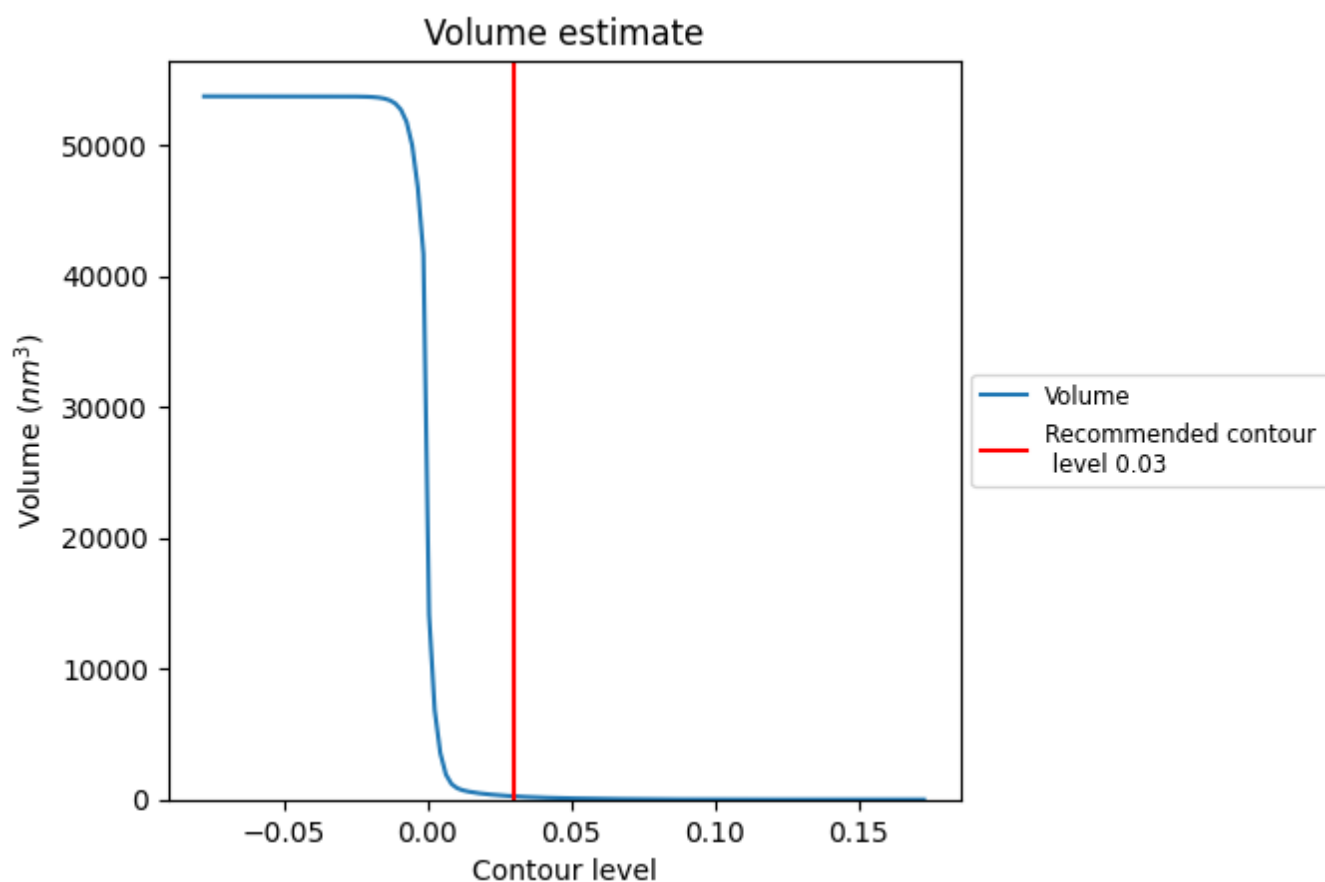
This section contains the results of statistical analysis of the map.

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.

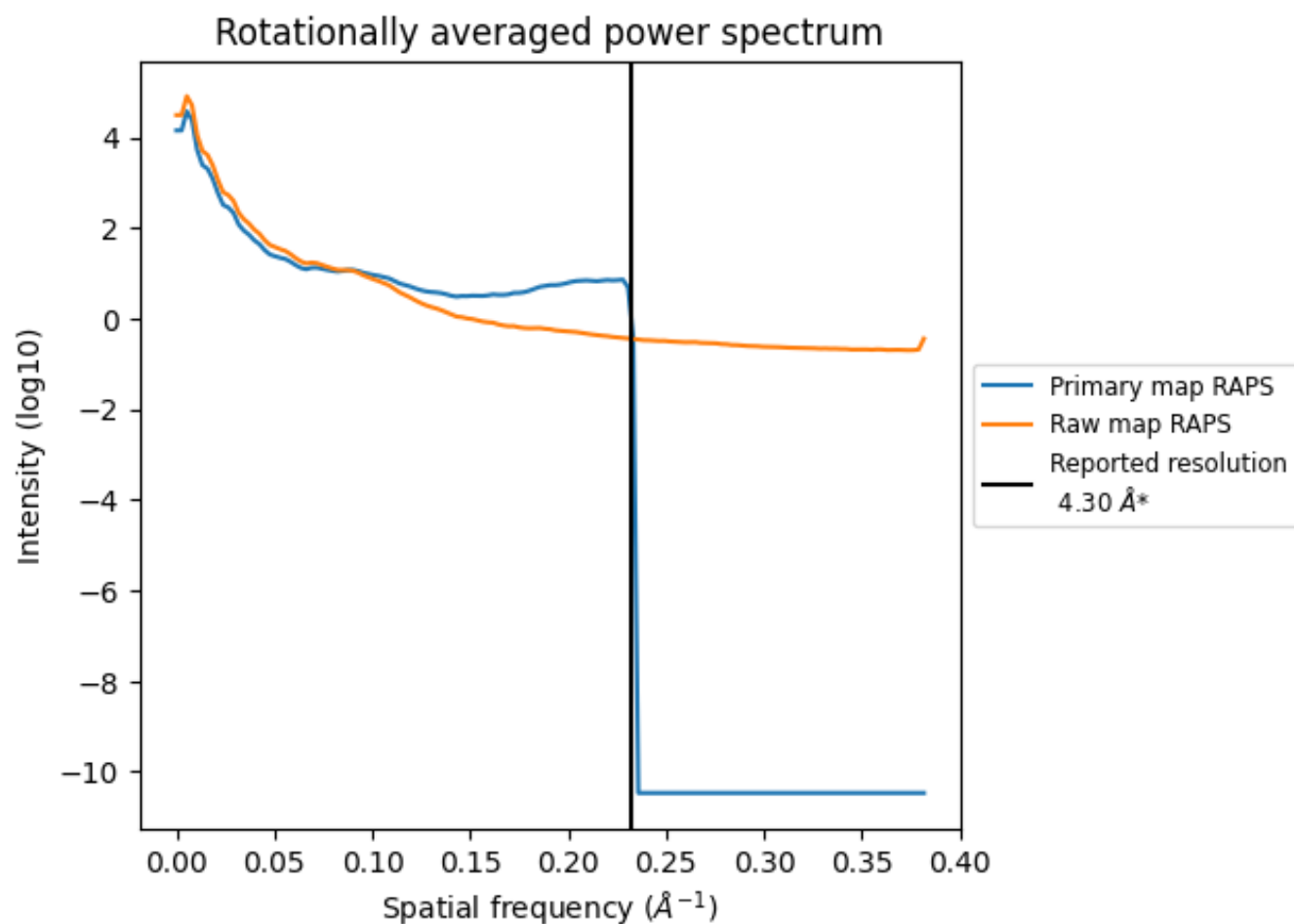
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 252 nm³; this corresponds to an approximate mass of 228 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 ⓘ

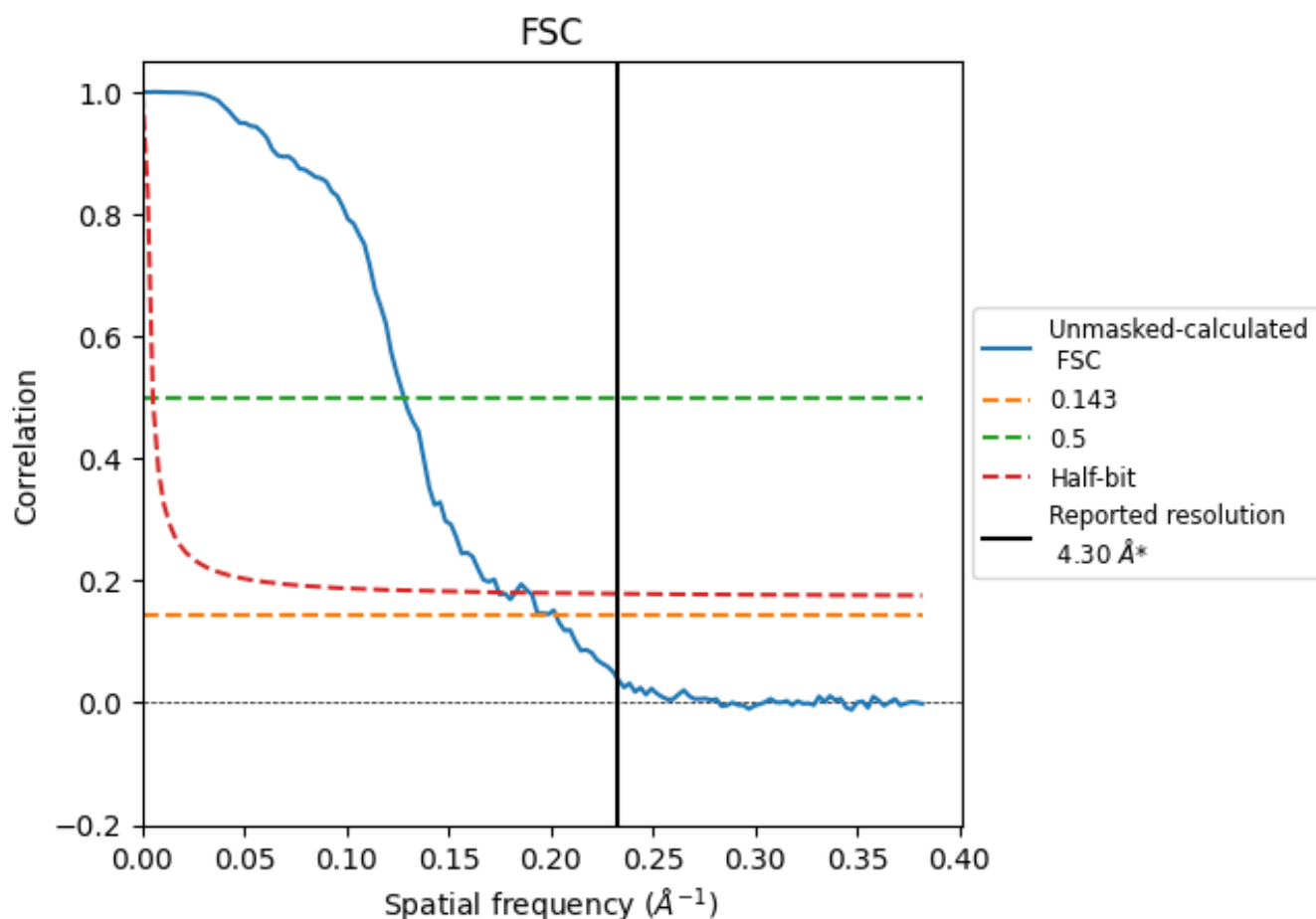


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

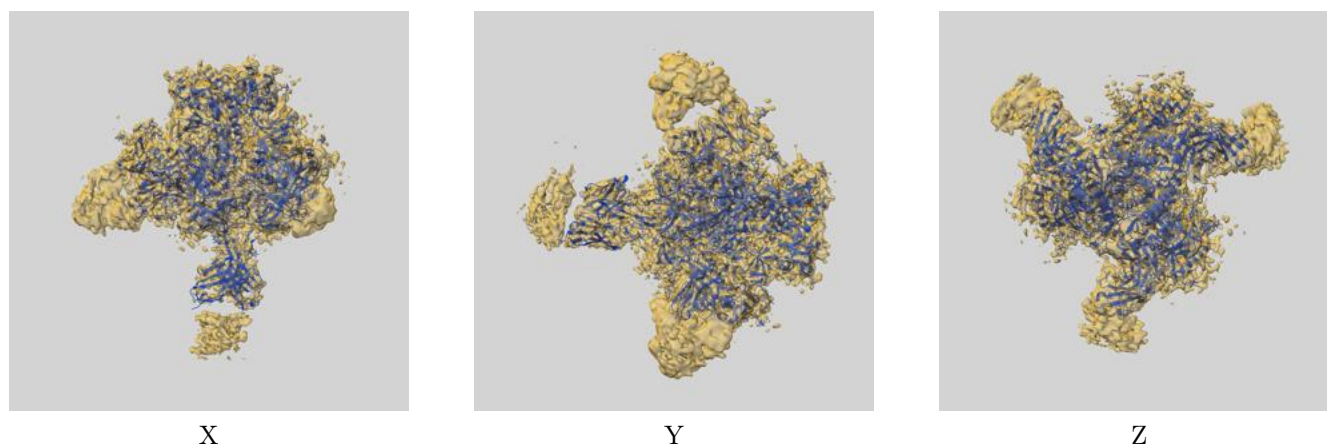
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.94	7.81	5.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.94 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

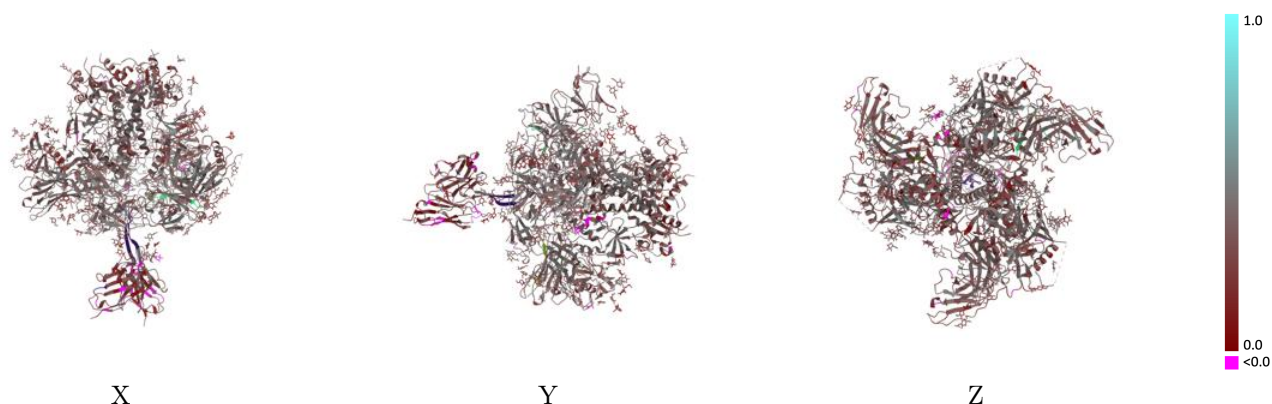
This section contains information regarding the fit between EMDB map EMD-8643 and PDB model 5V8L. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



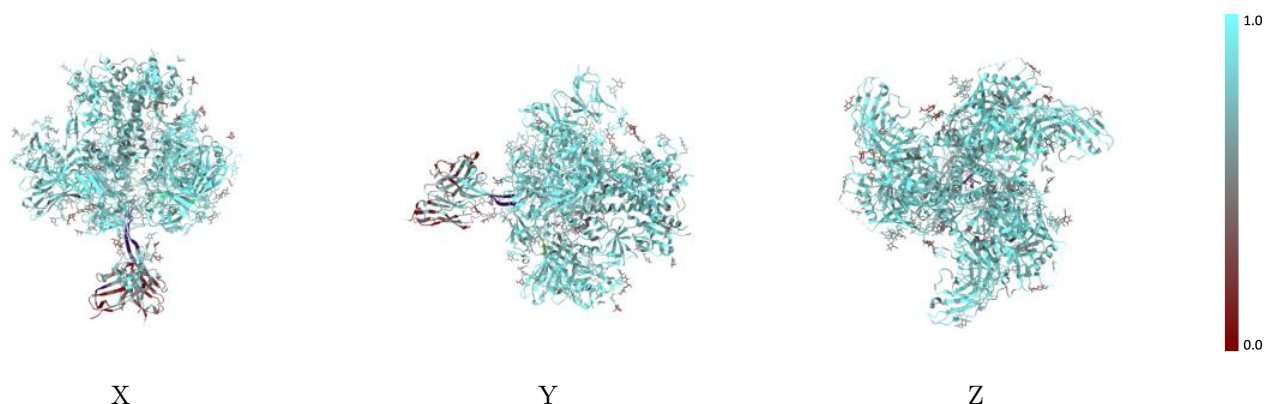
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



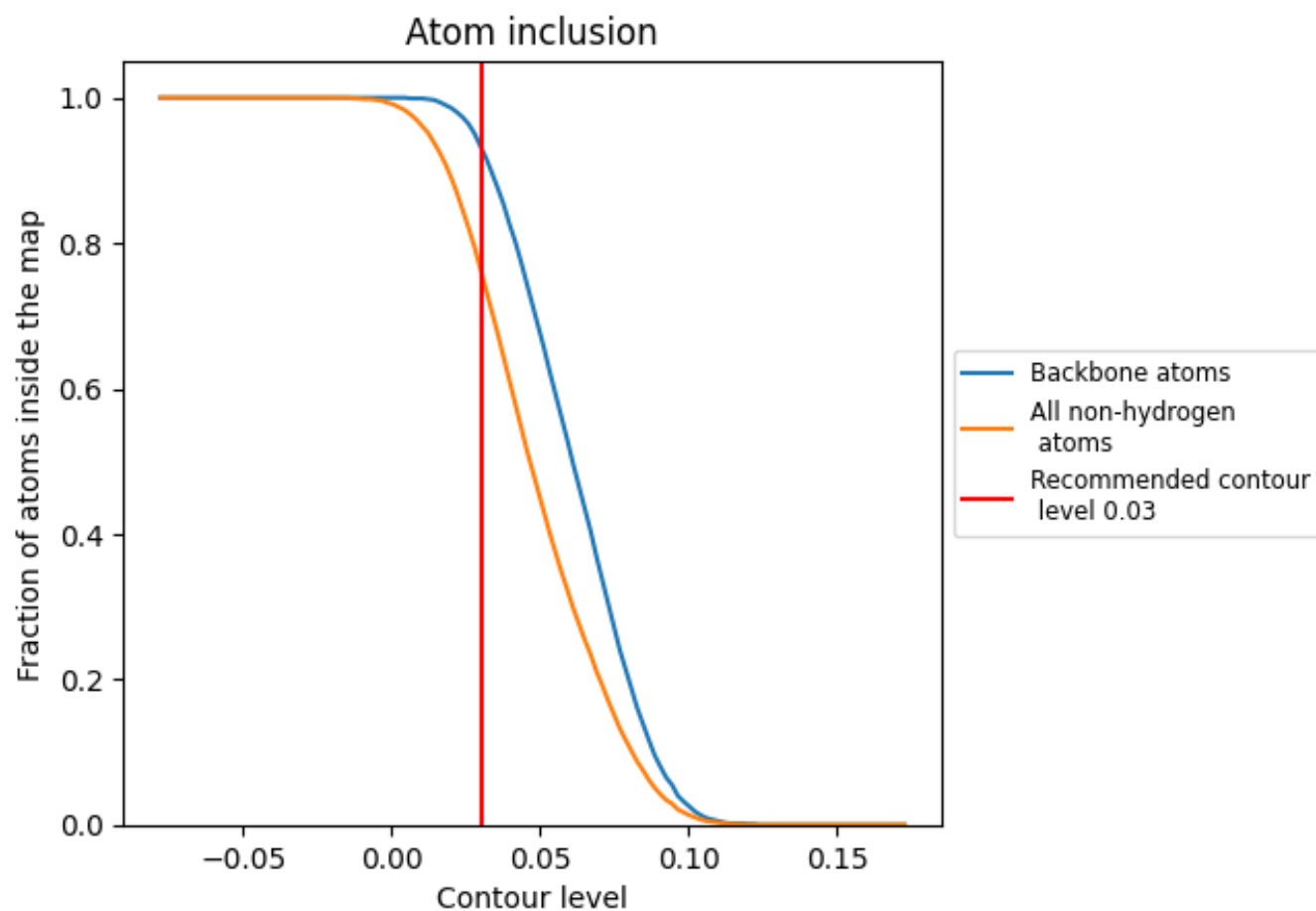
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.3460
0	 0.2860	 0.2220
1	 0.4290	 0.3450
2	 0.5000	 0.2110
3	 0.5710	 0.2220
4	 0.6070	 0.2580
A	 0.8040	 0.3640
B	 0.7760	 0.3180
C	 0.8030	 0.3750
D	 0.8080	 0.3780
E	 0.7920	 0.3380
F	 0.7730	 0.3250
G	 0.8370	 0.3810
H	 0.8260	 0.3880
I	 0.8390	 0.3930
J	 0.5450	 0.2580
K	 0.7840	 0.3320
L	 0.7740	 0.3170
M	 0.7870	 0.3500
N	 0.5230	 0.2360
O	 0.4290	 0.2690
P	 0.7140	 0.3160
Q	 0.7140	 0.3470
R	 0.3930	 0.2490
S	 0.4620	 0.2450
T	 0.7640	 0.3690
U	 0.7350	 0.2970
V	 0.5360	 0.2690
W	 0.3930	 0.2590
X	 0.6410	 0.3410
Y	 0.6070	 0.2530
Z	 0.6790	 0.2220
a	 0.6430	 0.3340
b	 0.7860	 0.3430
c	 0.5710	 0.2820



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.4870	 0.1400
e	 0.5360	 0.3290
f	 0.5900	 0.3040
g	 0.5960	 0.2670
h	 0.5710	 0.3390
i	 0.5710	 0.3070
j	 0.6430	 0.3270
k	 0.5410	 0.1720
l	 0.7690	 0.2240
m	 0.5360	 0.2690
n	 0.6070	 0.2970
o	 0.3930	 0.3060
p	 0.6790	 0.3370
q	 0.5320	 0.2030
r	 0.5710	 0.2350
s	 0.5900	 0.2890
t	 0.6920	 0.2980
u	 0.6070	 0.2960
v	 0.5710	 0.2530
w	 0.6070	 0.2310
x	 0.6560	 0.2690
y	 0.6670	 0.1470
z	 0.5360	 0.3120