



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:33 AM UTC

PDB ID : 6CUF / pdb_00006cuf
EMDB ID : EMD-7622
Title : Cryo-EM structure at 4.2 Å resolution of vaccine-elicited antibody vFP1.01 in complex with HIV-1 Env BG505 DS-SOSIP, and antibodies VRC03 and PGT122
Authors : Acharya, P.; Carragher, B.; Potter, C.S.; Kwong, P.D.
Deposited on : 2018-03-26
Resolution : 4.00 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:

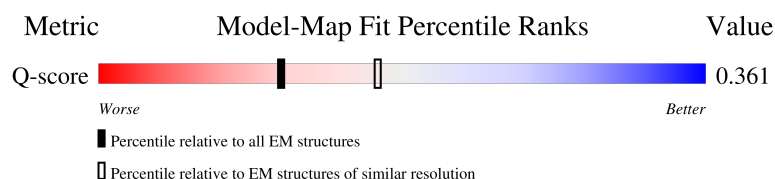
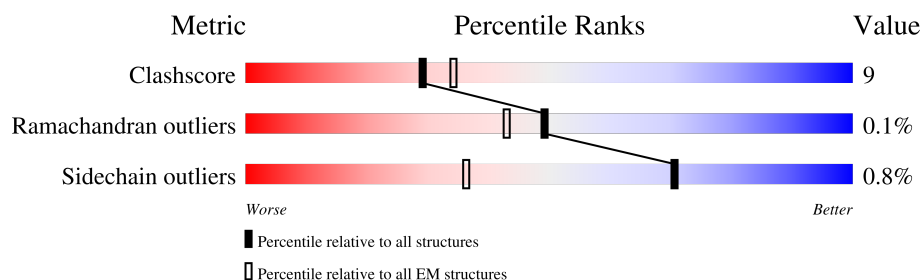
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 4.00 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	7587 (3.50 - 4.50)

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	3	211	14% 43% 12% 45%
1	H	211	13% 41% 14% 45%
1	h	211	14% 41% 14% 45%
2	4	219	36% 33% 18% 48%

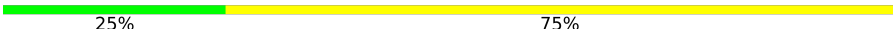
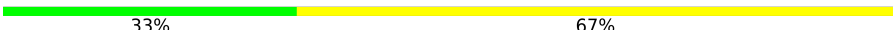
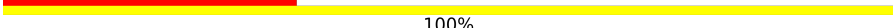
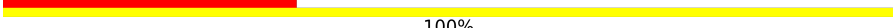
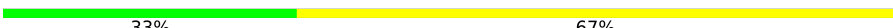
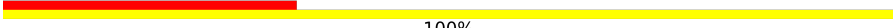
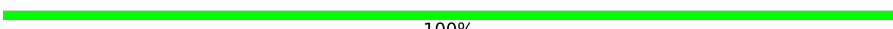
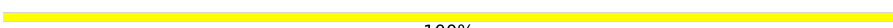
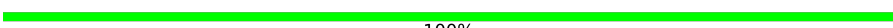
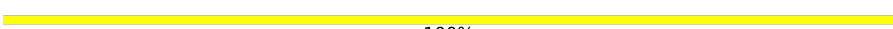
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Mol	Chain	Length	Quality of chain
2	L	219	
2	l	219	
3	5	132	
3	M	132	
3	m	132	
4	6	105	
4	N	105	
4	n	105	
5	7	102	
5	R	102	
5	r	102	
6	8	128	
6	Q	128	
6	q	128	
7	2	473	
7	C	473	
7	d	473	
8	A	153	
8	D	153	
8	c	153	
9	B	4	
9	DA	4	
9	E	4	
9	W	4	
9	X	4	

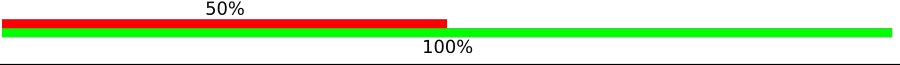
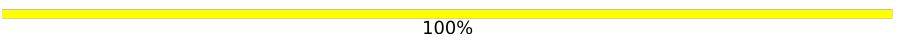
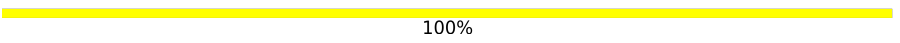
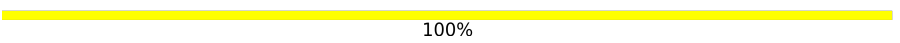
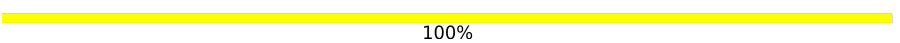
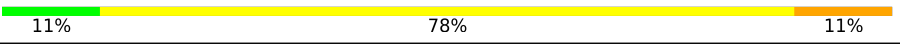
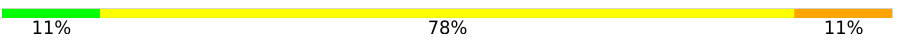
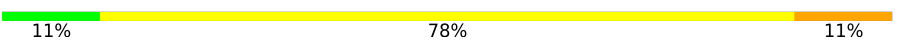
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Mol	Chain	Length	Quality of chain
9	Y	4	 75% 25%
9	s	4	 75% 25%
9	t	4	 25% 75%
9	u	4	 75% 25%
10	l	3	 33% 67%
10	F	3	 33% 100%
10	I	3	 33% 67%
10	P	3	 33% 67%
10	Z	3	 33% 100%
10	b	3	 33% 67%
10	i	3	 33% 67%
10	v	3	 33% 100%
10	x	3	 33% 67%
11	0	2	 100%
11	AA	2	 50% 50%
11	CA	2	 50% 50%
11	G	2	 50% 100%
11	K	2	 100%
11	O	2	 100%
11	T	2	 50% 50%
11	V	2	 50% 50%
11	a	2	 50% 100%
11	f	2	 100%
11	g	2	 100%
11	k	2	 50% 50%

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Mol	Chain	Length	Quality of chain
11	p	2	 50%50%
11	w	2	 50%100%
11	z	2	 100%
12	J	6	 17%33%67%
12	e	6	 17%33%67%
12	y	6	 17%33%67%
13	9	5	 100%
13	S	5	 100%
13	j	5	 100%
14	BA	9	 11%78%11%
14	U	9	 11%78%11%
14	o	9	 11%78%11%

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 32325 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 vFP1.01 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	116	Total	C	N	O	S	0	0
			930	597	154	176	3		
1	H	116	Total	C	N	O	S	0	0
			930	597	154	176	3		
1	h	116	Total	C	N	O	S	0	0
			930	597	154	176	3		

- Molecule 2 is a protein called vFP1.01 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	113	Total	C	N	O	S	0	0
			882	560	149	170	3		
2	L	113	Total	C	N	O	S	0	0
			882	560	149	170	3		
2	l	113	Total	C	N	O	S	0	0
			882	560	149	170	3		

- Molecule 3 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
3	M	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		
3	m	132	Total	C	N	O	S	0	0
			1047	669	180	195	3		

- Molecule 4 is a protein called PGT122 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	105	Total	C	N	O	S	0	0
			805	504	139	160	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	105	Total	C	N	O	S	0	0
			805	504	139	160	2		
4	n	105	Total	C	N	O	S	0	0
			805	504	139	160	2		

- Molecule 5 is a protein called VRC03 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	102	Total	C	N	O	S	0	0
			802	510	137	152	3		
5	R	102	Total	C	N	O	S	0	0
			802	510	137	152	3		
5	r	102	Total	C	N	O	S	0	0
			802	510	137	152	3		

- Molecule 6 is a protein called VRC03 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		
6	Q	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		
6	q	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		

- Molecule 7 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	453	Total	C	N	O	S	0	0
			3565	2236	630	671	28		
7	2	453	Total	C	N	O	S	0	0
			3565	2236	630	671	28		
7	d	453	Total	C	N	O	S	0	0
			3565	2236	630	671	28		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
2	332	ASN	THR	conflict	UNP Q2N0S6
2	501	CYS	ALA	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
d	332	ASN	THR	conflict	UNP Q2N0S6
d	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 8 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
8	A	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
8	c	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	605	CYS	THR	conflict	UNP Q2N0S7
A	605	CYS	THR	conflict	UNP Q2N0S7
c	605	CYS	THR	conflict	UNP Q2N0S7

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



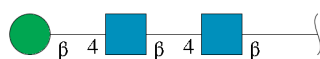
Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	4	Total	C	N	O		0	0
			50	28	2	20			
9	E	4	Total	C	N	O		0	0
			50	28	2	20			
9	W	4	Total	C	N	O		0	0
			50	28	2	20			
9	X	4	Total	C	N	O		0	0
			50	28	2	20			
9	Y	4	Total	C	N	O		0	0
			50	28	2	20			
9	s	4	Total	C	N	O		0	0
			50	28	2	20			

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	t	4	Total	C	N	O	0	0
			50	28	2	20		
9	u	4	Total	C	N	O	0	0
			50	28	2	20		
9	DA	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 10 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.



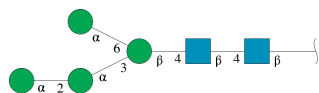
Mol	Chain	Residues	Atoms				AltConf	Trace
10	F	3	Total	C	N	O	0	0
			39	22	2	15		
10	I	3	Total	C	N	O	0	0
			39	22	2	15		
10	P	3	Total	C	N	O	0	0
			39	22	2	15		
10	Z	3	Total	C	N	O	0	0
			39	22	2	15		
10	b	3	Total	C	N	O	0	0
			39	22	2	15		
10	i	3	Total	C	N	O	0	0
			39	22	2	15		
10	v	3	Total	C	N	O	0	0
			39	22	2	15		
10	x	3	Total	C	N	O	0	0
			39	22	2	15		
10	1	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 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
11	G	2	Total	C	N	O	0	0
			28	16	2	10		
11	K	2	Total	C	N	O	0	0
			28	16	2	10		
11	O	2	Total	C	N	O	0	0
			28	16	2	10		
11	T	2	Total	C	N	O	0	0
			28	16	2	10		
11	V	2	Total	C	N	O	0	0
			28	16	2	10		
11	a	2	Total	C	N	O	0	0
			28	16	2	10		
11	f	2	Total	C	N	O	0	0
			28	16	2	10		
11	g	2	Total	C	N	O	0	0
			28	16	2	10		
11	k	2	Total	C	N	O	0	0
			28	16	2	10		
11	p	2	Total	C	N	O	0	0
			28	16	2	10		
11	w	2	Total	C	N	O	0	0
			28	16	2	10		
11	z	2	Total	C	N	O	0	0
			28	16	2	10		
11	0	2	Total	C	N	O	0	0
			28	16	2	10		
11	AA	2	Total	C	N	O	0	0
			28	16	2	10		
11	CA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 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.



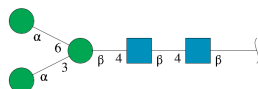
Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	6	Total	C	N	O	0	0
			72	40	2	30		
12	e	6	Total	C	N	O	0	0
			72	40	2	30		

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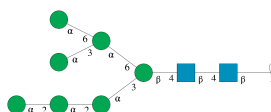
Mol	Chain	Residues	Atoms				AltConf	Trace
12	y	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 13 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.



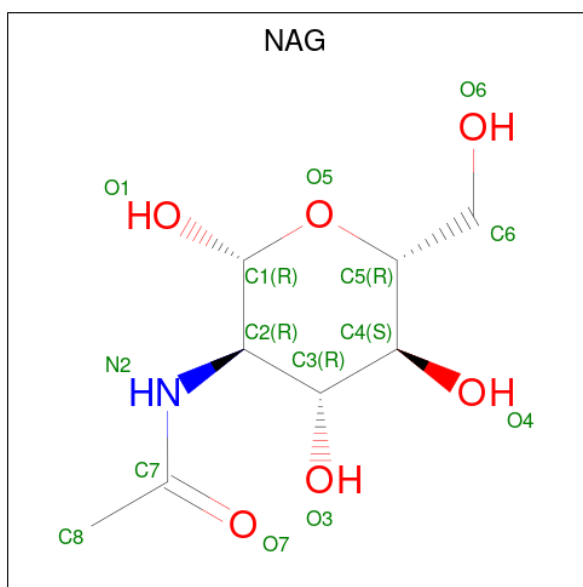
Mol	Chain	Residues	Atoms				AltConf	Trace
13	S	5	Total	C	N	O	0	0
			61	34	2	25		
13	j	5	Total	C	N	O	0	0
			61	34	2	25		
13	9	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	9	Total	C	N	O	0	0
			105	58	2	45		
14	o	9	Total	C	N	O	0	0
			105	58	2	45		
14	BA	9	Total	C	N	O	0	0
			105	58	2	45		

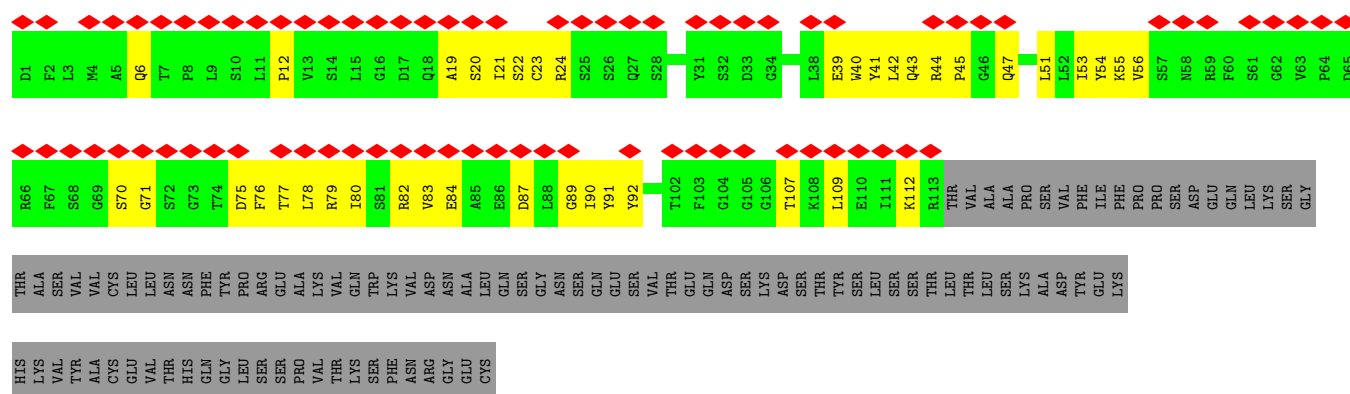
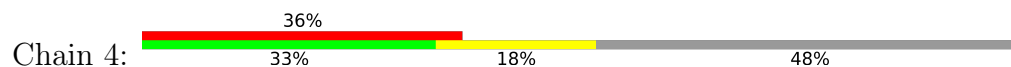
- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



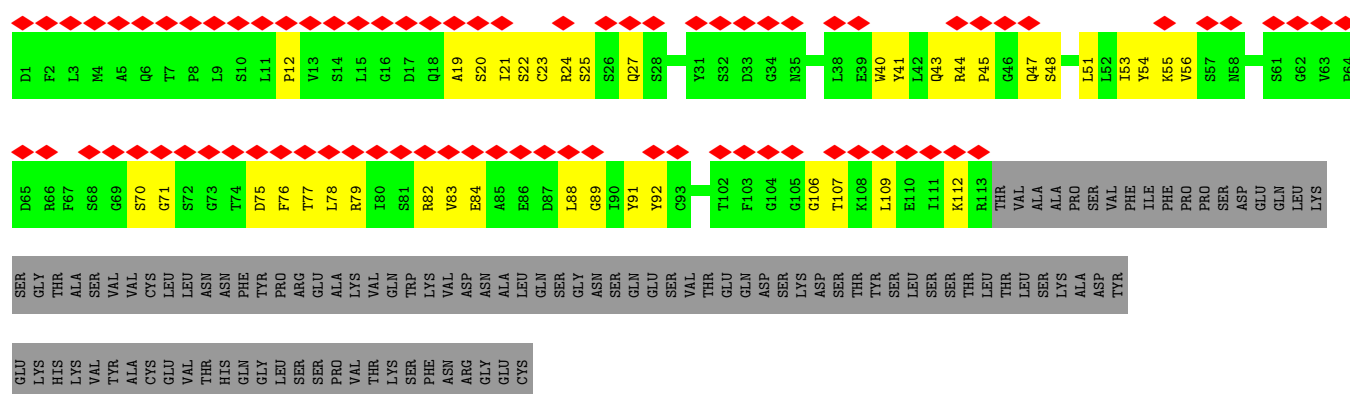
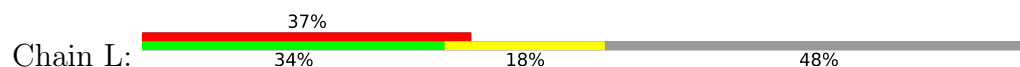
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	C	1	Total	C	N	O	0
			14	8	1	5	
15	D	1	Total	C	N	O	0
			14	8	1	5	
15	2	1	Total	C	N	O	0
			14	8	1	5	
15	2	1	Total	C	N	O	0
			14	8	1	5	
15	A	1	Total	C	N	O	0
			14	8	1	5	
15	c	1	Total	C	N	O	0
			14	8	1	5	
15	d	1	Total	C	N	O	0
			14	8	1	5	
15	d	1	Total	C	N	O	0
			14	8	1	5	

THR PRO ALA VAL LEU GLN SER SER GLY TYR SER LEU SER SER VAL VAL THR VAL VAL PRO PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO

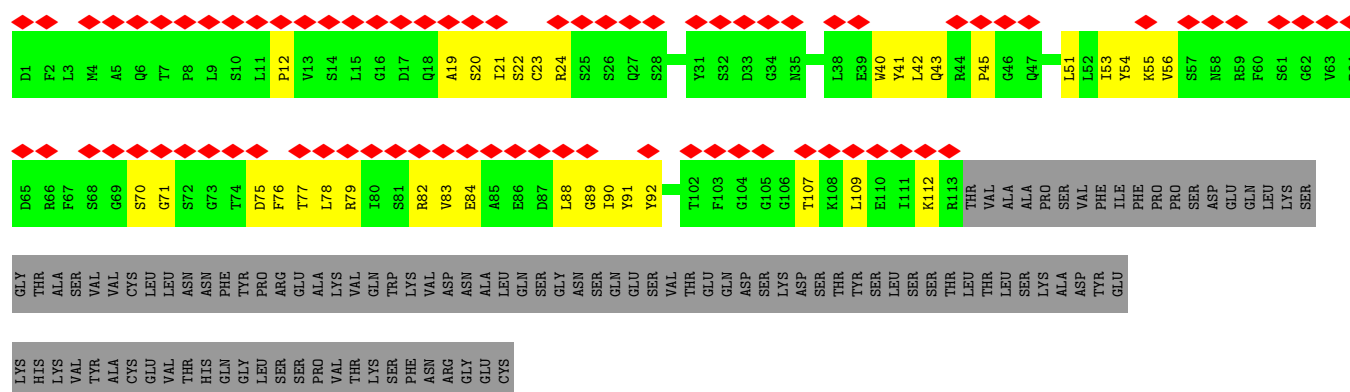
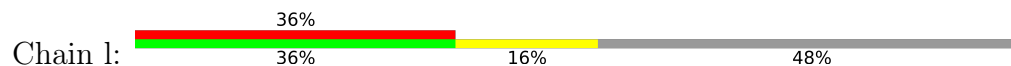
• Molecule 2: vFP1.01 Light chain



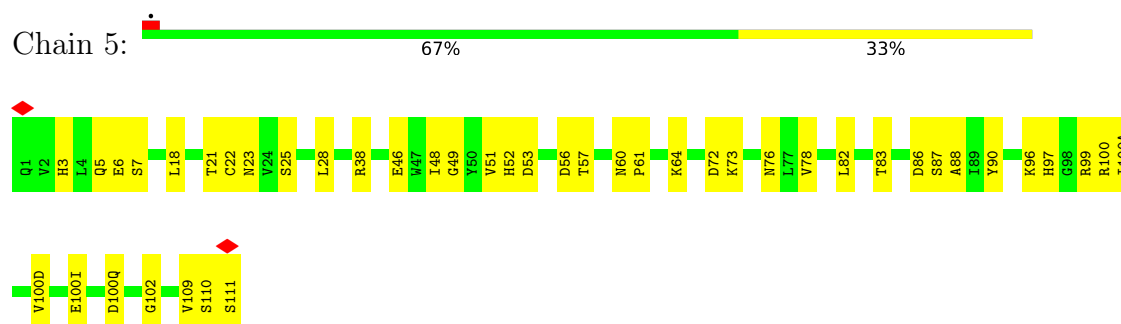
• Molecule 2: vFP1.01 Light chain



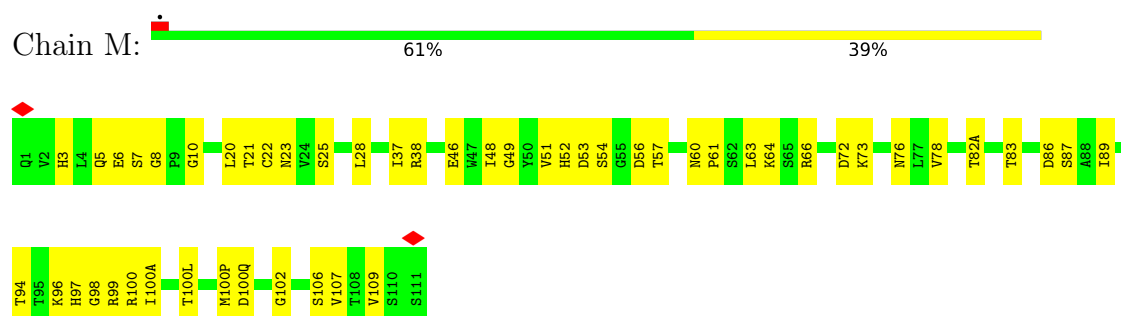
• Molecule 2: vFP1.01 Light chain



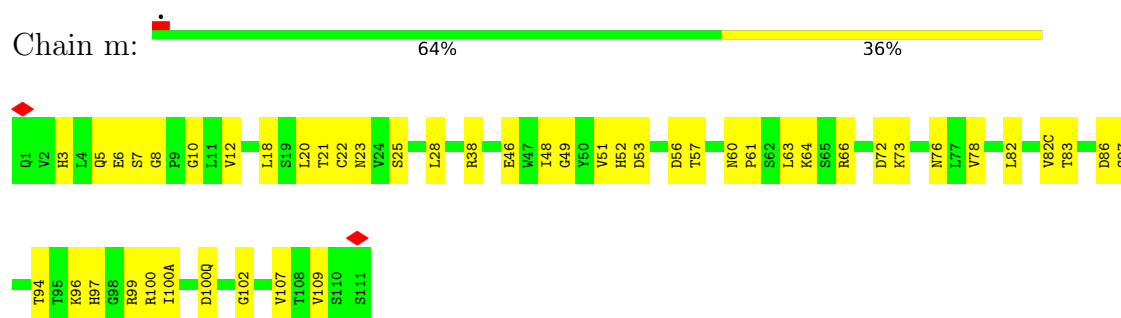
- Molecule 3: PGT122 Heavy chain



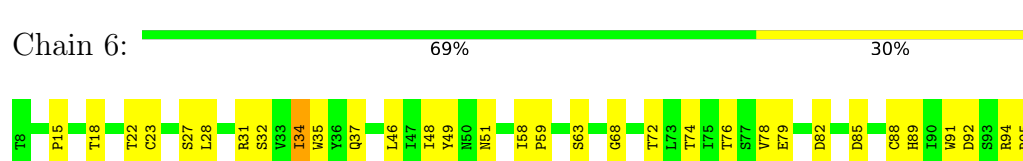
- Molecule 3: PGT122 Heavy chain



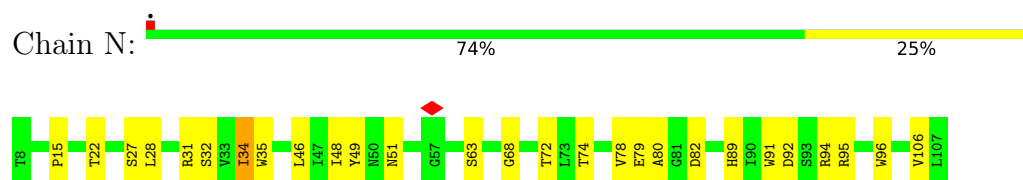
- Molecule 3: PGT122 Heavy chain



- Molecule 4: PGT122 light chain

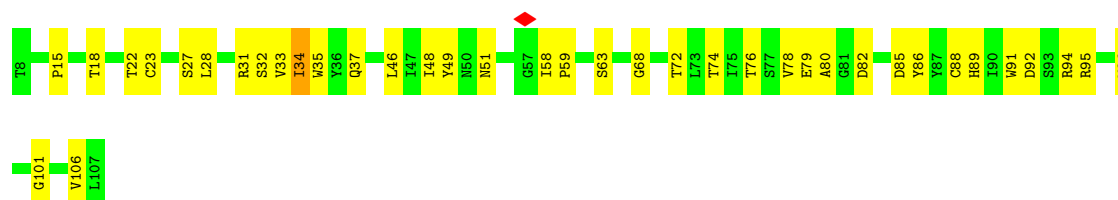


- Molecule 4: PGT122 light chain



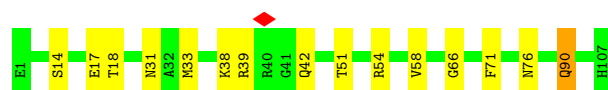
- Molecule 4: PGT122 light chain

Chain n:  64% 35%



- Molecule 5: VRC03 light chain

Chain 7:  85% 14%



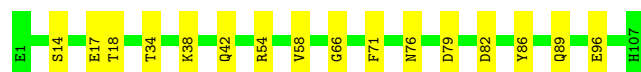
- Molecule 5: VRC03 light chain

Chain R:  87% 13%



- Molecule 5: VRC03 light chain

Chain r:  84% 16%



- Molecule 6: VRC03 heavy chain

Chain 8:  77% 23%



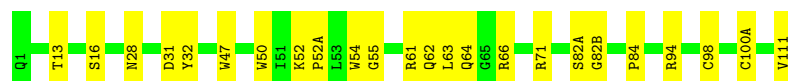
- Molecule 6: VRC03 heavy chain

Chain Q:  84% 16%

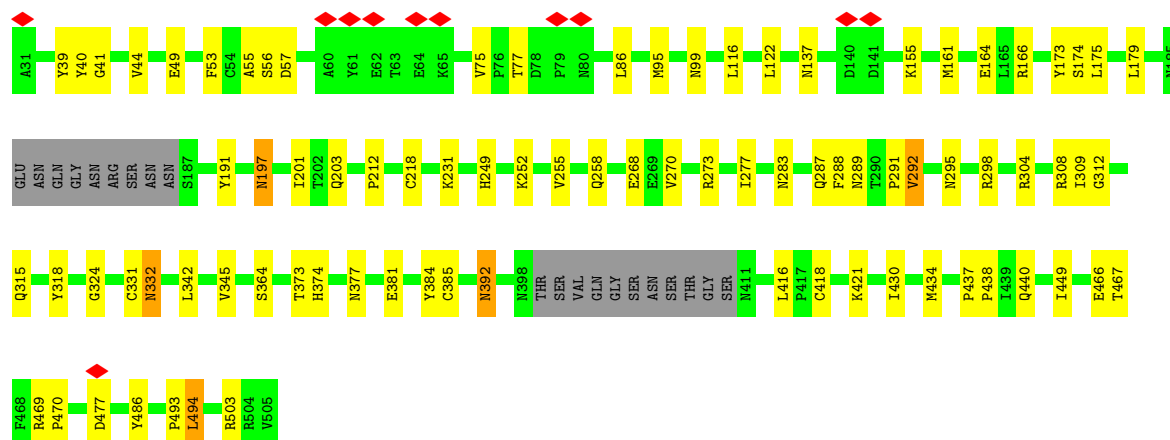
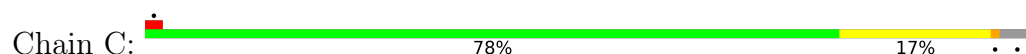


- Molecule 6: VRC03 heavy chain

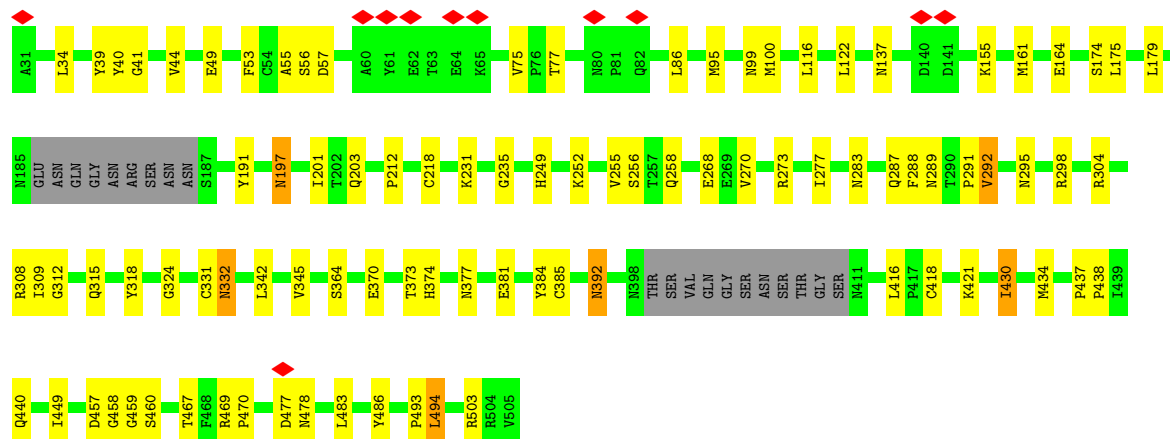
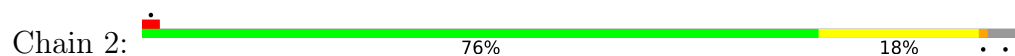
Chain q:  81% 19%



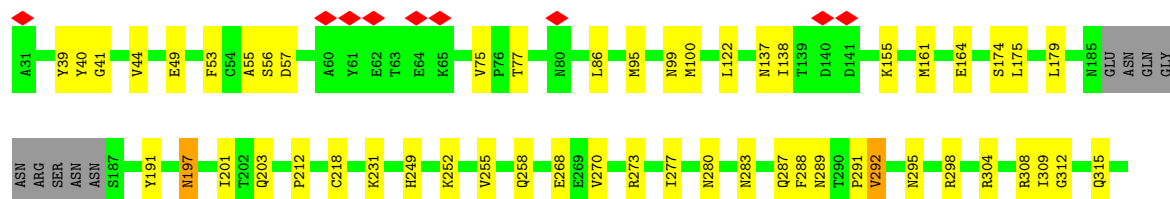
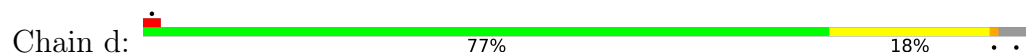
• Molecule 7: Envelope glycoprotein gp120



• Molecule 7: Envelope glycoprotein gp120



• Molecule 7: Envelope glycoprotein gp120



Chain E:  50% 50%



- Molecule 9: 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 W:  75% 25%



- Molecule 9: 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 X:  25% 75%



- Molecule 9: 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 Y:  75% 25%

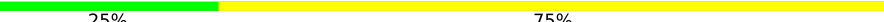


- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  75% 25%



- Molecule 9: 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 t:  25% 75%



- Molecule 9: 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:  75% 25%



- Molecule 9: 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 DA:  75% 25%

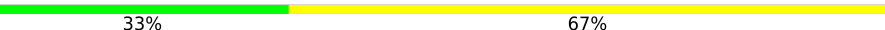


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  33% 100%

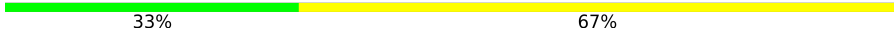


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%



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

Chain P:  33% 67%



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

Chain Z:  33% 100%

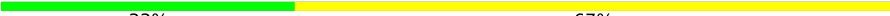


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  33% 67%

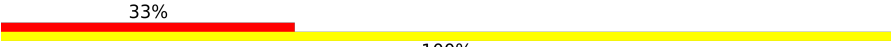


- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  33% 67%



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

Chain v:  33% 100%



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

Chain x:  33% 67%



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

Chain 1:  33% 67%

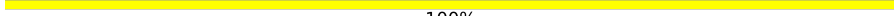


- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 100%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%

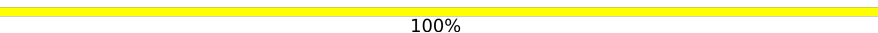


- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 100%

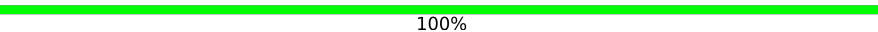


- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  50% 50%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  50% 50%

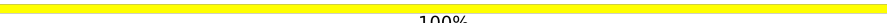


- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  50% 100%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:  100%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  100%



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:  50% 50% 50%



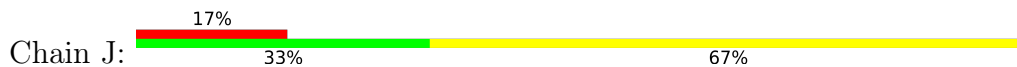
- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:  50% 50%



- Molecule 12: 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-aceta

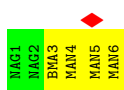
mido-2-deoxy-beta-D-glucopyranose



• Molecule 12: 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



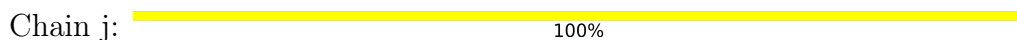
• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 13: 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-(1-3)-[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

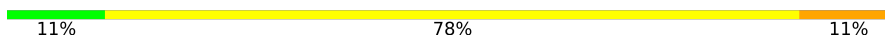


• Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



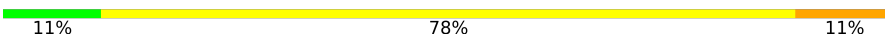


- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  11% 78% 11%

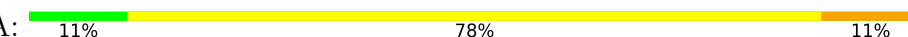


- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  11% 78% 11%



- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:  11% 78% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	44652	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 ($e^-/\text{\AA}^2$)	70.28	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.565	Depositor
Minimum map value	-1.291	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	1	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, NAG, BMA

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	3	0.21	0/956	0.49	0/1305
1	H	0.22	0/956	0.47	0/1305
1	h	0.22	0/956	0.47	0/1305
2	4	0.22	0/903	0.52	0/1221
2	L	0.22	0/903	0.51	0/1221
2	l	0.22	0/903	0.52	0/1221
3	5	0.27	0/1076	0.54	0/1465
3	M	0.27	0/1076	0.53	0/1465
3	m	0.26	0/1076	0.53	0/1465
4	6	0.29	0/826	0.48	0/1130
4	N	0.29	0/826	0.49	0/1130
4	n	0.29	0/826	0.48	0/1130
5	7	0.30	0/820	0.57	0/1107
5	R	0.30	0/820	0.58	0/1107
5	r	0.30	0/820	0.56	0/1107
6	8	0.37	0/1056	0.51	0/1439
6	Q	0.37	0/1056	0.49	0/1439
6	q	0.36	0/1056	0.48	0/1439
7	2	0.37	0/3639	0.59	1/4941 (0.0%)
7	C	0.37	0/3639	0.59	1/4941 (0.0%)
7	d	0.37	0/3639	0.59	1/4941 (0.0%)
8	A	0.37	0/1052	0.64	0/1427
8	D	0.37	0/1052	0.64	0/1427
8	c	0.37	0/1052	0.64	0/1427
All	All	0.33	0/30984	0.56	3/42105 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	4	0	1
2	L	0	1
2	1	0	1
5	7	0	1
5	R	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	494	LEU	CA-CB-CG	5.22	134.56	116.30
7	d	494	LEU	CA-CB-CG	5.21	134.54	116.30
7	C	494	LEU	CA-CB-CG	5.21	134.53	116.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	55	LYS	Peptide
5	7	90	GLN	Peptide
2	L	55	LYS	Peptide
5	R	90	GLN	Peptide
2	1	55	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	930	0	900	15	0
1	H	930	0	900	20	0
1	h	930	0	900	21	0
2	4	882	0	860	28	0
2	L	882	0	860	28	0
2	1	882	0	860	26	0
3	5	1047	0	1026	24	0
3	M	1047	0	1026	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	m	1047	0	1026	27	0
4	6	805	0	761	21	0
4	N	805	0	761	17	0
4	n	805	0	761	23	0
5	7	802	0	780	8	0
5	R	802	0	780	6	0
5	r	802	0	780	9	0
6	8	1023	0	971	24	0
6	Q	1023	0	971	14	0
6	q	1023	0	971	19	0
7	2	3565	0	3494	83	0
7	C	3565	0	3494	74	0
7	d	3565	0	3494	80	0
8	A	1034	0	1014	18	0
8	D	1034	0	1014	19	0
8	c	1034	0	1014	19	0
9	B	50	0	43	0	0
9	DA	50	0	43	0	0
9	E	50	0	43	1	0
9	W	50	0	43	0	0
9	X	50	0	43	0	0
9	Y	50	0	43	0	0
9	s	50	0	43	0	0
9	t	50	0	43	0	0
9	u	50	0	43	0	0
10	l	39	0	34	0	0
10	F	39	0	34	0	0
10	I	39	0	34	1	0
10	P	39	0	34	0	0
10	Z	39	0	34	0	0
10	b	39	0	34	1	0
10	i	39	0	34	0	0
10	v	39	0	34	0	0
10	x	39	0	34	1	0
11	0	28	0	25	0	0
11	AA	28	0	25	1	0
11	CA	28	0	25	1	0
11	G	28	0	25	0	0
11	K	28	0	25	6	0
11	O	28	0	25	0	0
11	T	28	0	25	1	0
11	V	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	a	28	0	25	0	0
11	f	28	0	25	6	0
11	g	28	0	25	0	0
11	k	28	0	25	1	0
11	p	28	0	25	1	0
11	w	28	0	25	0	0
11	z	28	0	25	6	0
12	J	72	0	61	0	0
12	e	72	0	61	0	0
12	y	72	0	61	0	0
13	9	61	0	52	1	0
13	S	61	0	52	1	0
13	j	61	0	52	1	0
14	BA	105	0	88	1	0
14	U	105	0	88	2	0
14	o	105	0	88	1	0
15	2	28	0	25	0	0
15	A	14	0	13	0	0
15	C	28	0	25	0	0
15	D	14	0	13	0	0
15	c	14	0	13	0	0
15	d	28	0	25	0	0
All	All	32325	0	31203	590	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 9.

All (590) 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)
7:2:295:ASN:HD21	11:f:1:NAG:C1	1.28	1.47
7:C:295:ASN:HD21	11:K:1:NAG:C1	1.28	1.47
7:d:295:ASN:HD21	11:z:1:NAG:C1	1.28	1.46
7:C:295:ASN:ND2	11:K:1:NAG:C1	1.85	1.39
7:d:295:ASN:ND2	11:z:1:NAG:C1	1.85	1.36
7:2:295:ASN:ND2	11:f:1:NAG:C1	1.85	1.34
7:d:295:ASN:CG	11:z:1:NAG:C1	2.23	1.12
7:2:295:ASN:CG	11:f:1:NAG:C1	2.23	1.11
7:C:295:ASN:CG	11:K:1:NAG:C1	2.23	1.11
7:C:295:ASN:OD1	11:K:1:NAG:C1	2.12	0.98
7:d:295:ASN:OD1	11:z:1:NAG:C1	2.12	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:295:ASN:OD1	11:f:1:NAG:C1	2.12	0.95
7:d:164:GLU:OE2	7:d:308:ARG:NH1	2.02	0.93
7:2:164:GLU:OE2	7:2:308:ARG:NH1	2.02	0.92
7:C:164:GLU:OE2	7:C:308:ARG:NH1	2.02	0.91
1:3:87:SER:HA	1:3:109:VAL:O	1.72	0.90
1:h:87:SER:HA	1:h:109:VAL:O	1.73	0.88
2:L:70:SER:OG	2:L:79:ARG:NH1	2.08	0.87
2:4:70:SER:OG	2:4:79:ARG:NH1	2.09	0.85
1:H:87:SER:HA	1:H:109:VAL:O	1.75	0.85
2:l:70:SER:OG	2:l:79:ARG:NH1	2.09	0.84
7:2:197:ASN:OD1	7:2:197:ASN:O	1.98	0.81
7:d:197:ASN:OD1	7:d:197:ASN:O	1.98	0.80
7:C:197:ASN:OD1	7:C:197:ASN:O	1.98	0.80
3:m:46:GLU:OE2	3:m:60:ASN:ND2	2.15	0.79
6:8:64:GLN:HE22	7:2:469:ARG:HH12	1.28	0.79
7:C:392:ASN:O	7:C:392:ASN:ND2	2.17	0.78
2:L:40:TRP:HA	2:L:92:TYR:O	1.82	0.78
6:q:64:GLN:HE22	7:d:469:ARG:HH12	1.29	0.78
5:r:54:ARG:NH1	5:r:58:VAL:O	2.17	0.77
7:d:392:ASN:ND2	7:d:392:ASN:O	2.17	0.77
7:2:392:ASN:O	7:2:392:ASN:ND2	2.17	0.77
5:R:54:ARG:NH1	5:R:58:VAL:O	2.18	0.76
3:5:53:ASP:OD2	3:5:73:LYS:NZ	2.19	0.75
2:l:40:TRP:HA	2:l:92:TYR:O	1.86	0.75
7:C:308:ARG:NH1	7:2:197:ASN:OD1	2.20	0.75
7:2:308:ARG:NH1	7:d:197:ASN:OD1	2.20	0.74
7:C:197:ASN:OD1	7:d:308:ARG:NH1	2.20	0.74
8:A:542:ARG:NH2	8:c:647:GLU:OE2	2.22	0.73
5:7:54:ARG:NH1	5:7:58:VAL:O	2.23	0.72
5:r:96:GLU:OE2	7:d:280:ASN:ND2	2.23	0.72
2:L:91:TYR:O	2:L:106:GLY:HA2	1.89	0.72
1:H:35:HIS:HD2	1:H:47:TRP:HE1	1.38	0.72
7:C:469:ARG:HH12	6:Q:64:GLN:HE22	1.38	0.71
8:c:627:THR:H	8:c:630:GLN:HE21	1.38	0.71
8:A:627:THR:H	8:A:630:GLN:HE21	1.38	0.71
8:D:627:THR:H	8:D:630:GLN:HE21	1.38	0.71
8:D:647:GLU:OE2	8:c:542:ARG:NH2	2.23	0.70
4:6:51:ASN:ND2	14:o:5:MAN:O4	2.24	0.70
2:4:40:TRP:HA	2:4:92:TYR:O	1.93	0.69
8:D:542:ARG:NH2	8:A:647:GLU:OE2	2.24	0.68
4:n:51:ASN:ND2	14:BA:5:MAN:O4	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:295:ASN:HD21	11:f:1:NAG:C2	2.07	0.68
7:C:295:ASN:HD21	11:K:1:NAG:C2	2.07	0.68
3:M:46:GLU:OE2	3:M:60:ASN:ND2	2.26	0.67
3:M:53:ASP:OD2	3:M:73:LYS:NZ	2.27	0.67
1:h:35:HIS:HD2	1:h:47:TRP:HE1	1.43	0.67
7:2:332:ASN:OD1	7:2:332:ASN:N	2.28	0.66
7:d:332:ASN:N	7:d:332:ASN:OD1	2.28	0.66
7:d:197:ASN:OD1	7:d:197:ASN:C	2.38	0.66
7:d:231:LYS:NZ	7:d:268:GLU:OE1	2.25	0.66
7:2:197:ASN:OD1	7:2:197:ASN:C	2.38	0.66
4:n:86:TYR:O	4:n:101:GLY:HA2	1.95	0.66
3:5:100:ARG:NH1	3:5:100(A):ILE:O	2.28	0.66
7:2:392:ASN:O	7:2:392:ASN:CG	2.39	0.66
1:h:2:VAL:HA	1:h:25:SER:O	1.96	0.65
2:l:12:PRO:HB2	2:l:112:LYS:HZ1	1.59	0.65
7:C:197:ASN:OD1	7:C:197:ASN:C	2.38	0.65
3:5:7:SER:HG	3:5:21:THR:HG1	1.42	0.65
7:d:392:ASN:O	7:d:392:ASN:CG	2.39	0.65
7:C:231:LYS:NZ	7:C:268:GLU:OE1	2.25	0.65
7:2:95:MET:HE1	7:2:273:ARG:HD3	1.79	0.65
2:l:45:PRO:HD3	2:l:89:GLY:HA2	1.79	0.65
7:C:95:MET:HE1	7:C:273:ARG:HD3	1.79	0.65
7:C:332:ASN:OD1	7:C:332:ASN:N	2.28	0.65
7:C:469:ARG:HH12	6:Q:64:GLN:NE2	1.95	0.65
7:C:392:ASN:O	7:C:392:ASN:CG	2.39	0.64
6:q:64:GLN:NE2	7:d:469:ARG:HH12	1.94	0.64
2:L:45:PRO:HD3	2:L:89:GLY:HA2	1.79	0.64
7:d:95:MET:HE1	7:d:273:ARG:HD3	1.79	0.64
1:3:35:HIS:HD2	1:3:47:TRP:HE1	1.44	0.64
3:5:52:HIS:HB3	3:5:56:ASP:HB3	1.81	0.63
3:5:5:GLN:HB3	3:5:23:ASN:HB2	1.79	0.63
2:L:70:SER:HG	2:L:79:ARG:HH12	1.45	0.63
6:8:64:GLN:NE2	7:2:469:ARG:HH12	1.95	0.63
2:L:82:ARG:NH1	2:L:84:GLU:OE2	2.32	0.63
2:l:82:ARG:NH1	2:l:84:GLU:OE2	2.32	0.63
3:m:5:GLN:HB3	3:m:23:ASN:HB2	1.82	0.62
4:6:94:ARG:O	7:2:137:ASN:N	2.33	0.62
2:4:45:PRO:HD3	2:4:89:GLY:HA2	1.81	0.62
3:m:83:THR:N	3:m:86:ASP:OD2	2.19	0.62
3:5:51:VAL:HG23	3:5:57:THR:HG23	1.81	0.61
3:m:53:ASP:OD2	3:m:73:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:295:ASN:ND2	11:f:1:NAG:O5	2.33	0.61
7:2:231:LYS:NZ	7:2:268:GLU:OE1	2.25	0.61
7:d:155:LYS:HZ3	7:d:191:TYR:HE2	1.48	0.61
5:7:38:LYS:NZ	5:7:42:GLN:O	2.34	0.61
2:4:12:PRO:HB2	2:4:112:LYS:HZ1	1.65	0.61
3:m:52:HIS:HB3	3:m:56:ASP:HB3	1.83	0.61
7:2:155:LYS:HZ3	7:2:191:TYR:HE2	1.48	0.61
4:6:94:ARG:NH2	7:2:324:GLY:O	2.33	0.61
7:d:295:ASN:ND2	11:z:1:NAG:O5	2.33	0.60
13:j:1:NAG:H62	11:k:1:NAG:H81	1.83	0.60
7:d:295:ASN:HD21	11:z:1:NAG:C2	2.07	0.60
13:9:1:NAG:H62	11:AA:1:NAG:H81	1.83	0.60
3:M:5:GLN:HB3	3:M:23:ASN:HB2	1.82	0.60
2:4:91:TYR:HB2	2:4:107:THR:HB	1.82	0.60
1:3:39:GLN:HB3	1:3:89:VAL:HB	1.83	0.60
7:C:295:ASN:ND2	11:K:1:NAG:O5	2.33	0.60
3:m:22:CYS:HB3	3:m:78:VAL:HB	1.84	0.60
2:4:12:PRO:HB2	2:4:112:LYS:NZ	2.17	0.59
6:8:98:CYS:SG	6:8:100(A):CYS:N	2.75	0.59
4:N:32:SER:HB3	4:N:91:TRP:HB2	1.83	0.59
7:2:161:MET:HE2	7:2:309:ILE:HD12	1.84	0.59
13:S:1:NAG:H62	11:T:1:NAG:H81	1.82	0.59
2:L:22:SER:HA	2:L:76:PHE:O	2.02	0.59
1:h:3:GLN:O	1:h:25:SER:HB3	2.01	0.59
7:d:161:MET:HE2	7:d:309:ILE:HD12	1.84	0.59
6:8:28:ASN:ND2	6:8:31:ASP:OD2	2.35	0.59
1:H:2:VAL:HA	1:H:25:SER:O	2.02	0.59
3:m:51:VAL:HG23	3:m:57:THR:HG23	1.84	0.59
7:2:331:CYS:C	7:2:332:ASN:OD1	2.46	0.59
7:d:331:CYS:C	7:d:332:ASN:OD1	2.46	0.59
7:C:155:LYS:HZ3	7:C:191:TYR:HE2	1.49	0.59
7:C:161:MET:HE2	7:C:309:ILE:HD12	1.84	0.59
2:l:22:SER:HA	2:l:76:PHE:O	2.03	0.59
4:n:94:ARG:NH2	7:d:324:GLY:O	2.35	0.59
6:q:98:CYS:SG	6:q:100(A):CYS:N	2.76	0.59
7:C:331:CYS:C	7:C:332:ASN:OD1	2.46	0.58
2:L:12:PRO:HB2	2:L:112:LYS:HZ1	1.68	0.58
3:M:87:SER:HB2	3:M:109:VAL:HG12	1.85	0.58
4:n:94:ARG:O	7:d:137:ASN:N	2.36	0.58
7:C:137:ASN:N	4:N:94:ARG:O	2.36	0.58
2:L:23:CYS:O	2:L:76:PHE:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:52:HIS:HB3	3:M:56:ASP:HB3	1.84	0.58
2:l:91:TYR:HB2	2:l:107:THR:HB	1.85	0.58
4:N:34:ILE:HB	4:N:89:HIS:HB3	1.85	0.58
3:5:22:CYS:HB3	3:5:78:VAL:HB	1.86	0.58
6:q:28:ASN:ND2	6:q:31:ASP:OD2	2.37	0.58
2:4:22:SER:HA	2:4:76:PHE:O	2.02	0.58
1:H:5:GLN:HB3	1:H:23:LYS:HB2	1.86	0.58
2:L:12:PRO:HB2	2:L:112:LYS:NZ	2.19	0.58
6:Q:98:CYS:SG	6:Q:100(A):CYS:N	2.76	0.58
1:3:5:GLN:HB3	1:3:23:LYS:HB2	1.85	0.58
3:5:6:GLU:OE2	3:5:102:GLY:HA3	2.04	0.58
3:m:100:ARG:NH1	3:m:100(A):ILE:O	2.37	0.58
3:m:87:SER:HB2	3:m:109:VAL:HG12	1.86	0.57
7:2:373:THR:OG1	7:2:374:HIS:N	2.36	0.57
7:C:324:GLY:O	4:N:94:ARG:NH2	2.37	0.57
1:H:7:SER:HB3	1:H:21:SER:H	1.69	0.57
3:M:7:SER:HG	3:M:21:THR:HG1	1.53	0.57
3:M:51:VAL:HG23	3:M:57:THR:HG23	1.84	0.57
2:l:12:PRO:HB2	2:l:112:LYS:NZ	2.19	0.57
2:l:41:TYR:HB2	2:l:92:TYR:HB2	1.86	0.57
3:m:6:GLU:OE2	3:m:102:GLY:HA3	2.04	0.57
7:C:373:THR:OG1	7:C:374:HIS:N	2.36	0.57
3:M:100:ARG:NH1	3:M:100(A):ILE:O	2.38	0.57
7:C:467:THR:H	6:Q:61:ARG:HH12	1.51	0.57
3:m:3:HIS:H	3:m:25:SER:HB2	1.70	0.57
4:n:22:THR:HG22	4:n:72:THR:HG22	1.87	0.57
7:d:249:HIS:HD1	7:d:486:TYR:HH	1.52	0.57
7:C:270:VAL:HG11	7:C:345:VAL:HG12	1.86	0.57
7:d:270:VAL:HG11	7:d:345:VAL:HG12	1.85	0.57
4:6:22:THR:HG22	4:6:72:THR:HG22	1.86	0.57
7:2:270:VAL:HG11	7:2:345:VAL:HG12	1.85	0.57
7:2:283:ASN:ND2	7:2:477:ASP:OD2	2.38	0.57
7:2:249:HIS:HD1	7:2:486:TYR:HH	1.52	0.57
8:A:632:ASP:O	8:A:636:SER:HB3	2.05	0.56
7:d:268:GLU:O	7:d:289:ASN:ND2	2.39	0.56
1:H:91:TYR:OH	2:L:43:GLN:NE2	2.39	0.56
5:r:34:THR:HB	5:r:89:GLN:HB3	1.87	0.56
1:H:39:GLN:HB3	1:H:89:VAL:HB	1.87	0.56
6:8:61:ARG:HH12	7:2:467:THR:H	1.53	0.56
6:q:61:ARG:HH12	7:d:467:THR:H	1.53	0.56
7:2:39:TYR:O	7:2:494:LEU:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:268:GLU:O	7:2:289:ASN:ND2	2.39	0.56
7:C:268:GLU:O	7:C:289:ASN:ND2	2.38	0.56
6:q:66:ARG:NH2	6:q:82(B):GLY:O	2.39	0.56
8:c:632:ASP:O	8:c:636:SER:HB3	2.05	0.56
4:6:34:ILE:HB	4:6:89:HIS:HB3	1.88	0.56
7:C:249:HIS:HD1	7:C:486:TYR:HH	1.52	0.56
3:M:97:HIS:CE1	3:M:99:ARG:HH12	2.24	0.56
4:N:22:THR:HG22	4:N:72:THR:HG22	1.88	0.56
7:d:39:TYR:O	7:d:494:LEU:HA	2.06	0.56
7:C:283:ASN:ND2	7:C:477:ASP:OD2	2.38	0.56
8:D:632:ASP:O	8:D:636:SER:HB3	2.05	0.56
6:Q:28:ASN:ND2	6:Q:31:ASP:OD2	2.39	0.56
3:M:22:CYS:HB3	3:M:78:VAL:HB	1.88	0.55
7:d:373:THR:OG1	7:d:374:HIS:N	2.36	0.55
4:6:32:SER:HB3	4:6:91:TRP:HB2	1.88	0.55
1:h:5:GLN:HB3	1:h:23:LYS:HB2	1.88	0.55
3:m:7:SER:OG	3:m:21:THR:OG1	2.23	0.55
4:N:63:SER:HB2	4:N:74:THR:HB	1.88	0.55
4:n:35:TRP:HB2	4:n:48:ILE:HB	1.89	0.55
4:6:35:TRP:HB2	4:6:48:ILE:HB	1.89	0.55
6:8:66:ARG:NH2	6:8:82(B):GLY:O	2.39	0.55
2:4:41:TYR:HB2	2:4:92:TYR:HB2	1.88	0.55
3:5:3:HIS:H	3:5:25:SER:HB2	1.71	0.55
3:5:87:SER:HB2	3:5:109:VAL:HG12	1.88	0.55
7:C:39:TYR:O	7:C:494:LEU:HA	2.06	0.55
7:d:283:ASN:ND2	7:d:477:ASP:OD2	2.38	0.55
7:2:273:ARG:NH1	7:2:287:GLN:OE1	2.40	0.55
7:d:273:ARG:NH1	7:d:287:GLN:OE1	2.40	0.55
7:C:273:ARG:NH1	7:C:287:GLN:OE1	2.40	0.55
7:2:40:TYR:HB3	8:A:602:LEU:HD12	1.89	0.54
7:2:312:GLY:H	7:2:315:GLN:HB2	1.72	0.54
3:m:96:LYS:HE2	3:m:100(Q):ASP:OD2	2.08	0.54
3:5:96:LYS:HE2	3:5:100(Q):ASP:OD2	2.08	0.54
3:M:10:GLY:HA2	3:M:107:VAL:HA	1.90	0.54
4:N:35:TRP:HB2	4:N:48:ILE:HB	1.89	0.54
6:8:37:VAL:HG23	6:8:47:TRP:HA	1.90	0.54
3:M:3:HIS:H	3:M:25:SER:HB2	1.73	0.54
4:N:51:ASN:ND2	14:U:5:MAN:O4	2.35	0.54
2:l:71:GLY:HA3	2:l:76:PHE:HA	1.90	0.54
7:2:270:VAL:HG22	7:2:289:ASN:H	1.73	0.54
3:M:83:THR:O	3:M:86:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:19:ALA:O	2:l:79:ARG:HA	2.08	0.54
8:D:569:THR:HG23	8:D:570:VAL:HG23	1.90	0.54
6:Q:66:ARG:NH2	6:Q:82(B):GLY:O	2.40	0.54
4:n:34:ILE:HB	4:n:89:HIS:HB3	1.90	0.54
2:l:51:LEU:HD21	2:l:54:TYR:HB3	1.90	0.54
7:C:312:GLY:H	7:C:315:GLN:HB2	1.72	0.53
7:C:304:ARG:N	7:C:440:GLN:OE1	2.42	0.53
2:L:41:TYR:HB2	2:L:92:TYR:HB2	1.89	0.53
4:n:32:SER:HB3	4:n:91:TRP:HB2	1.90	0.53
3:M:96:LYS:HE2	3:M:100(Q):ASP:OD2	2.08	0.53
7:2:258:GLN:NE2	7:2:470:PRO:O	2.41	0.53
8:c:602:LEU:HD12	7:d:40:TYR:HB3	1.89	0.53
7:d:270:VAL:HG22	7:d:289:ASN:H	1.72	0.53
7:d:312:GLY:H	7:d:315:GLN:HB2	1.72	0.53
7:C:40:TYR:HB3	8:D:602:LEU:HD12	1.89	0.53
8:A:569:THR:HG23	8:A:570:VAL:HG23	1.90	0.53
2:4:83:VAL:HG13	2:4:109:LEU:HD21	1.89	0.53
3:M:7:SER:OG	3:M:21:THR:OG1	2.22	0.53
2:L:51:LEU:HD21	2:L:54:TYR:HB3	1.91	0.53
2:l:23:CYS:O	2:l:76:PHE:HB2	2.09	0.53
8:c:569:THR:HG23	8:c:570:VAL:HG23	1.90	0.53
7:d:258:GLN:NE2	7:d:470:PRO:O	2.41	0.53
7:2:364:SER:OG	7:2:470:PRO:O	2.25	0.52
7:C:258:GLN:NE2	7:C:470:PRO:O	2.41	0.52
7:C:364:SER:OG	7:C:470:PRO:O	2.25	0.52
6:q:98:CYS:N	6:q:100(A):CYS:SG	2.80	0.52
2:L:41:TYR:O	2:L:91:TYR:HA	2.09	0.52
7:d:304:ARG:N	7:d:440:GLN:OE1	2.42	0.52
4:6:27:SER:OG	4:6:68:GLY:N	2.42	0.52
2:L:71:GLY:HA3	2:L:76:PHE:HA	1.92	0.52
3:M:6:GLU:OE2	3:M:102:GLY:HA3	2.09	0.52
3:5:83:THR:N	3:5:86:ASP:OD2	2.21	0.52
7:C:385:CYS:HA	7:C:418:CYS:HA	1.91	0.52
1:3:91:TYR:OH	2:4:43:GLN:NE2	2.42	0.52
7:C:270:VAL:HG22	7:C:289:ASN:H	1.72	0.52
1:h:7:SER:HB3	1:h:21:SER:H	1.75	0.52
3:5:97:HIS:CE1	3:5:99:ARG:HH12	2.28	0.52
1:H:38:LYS:HG3	1:H:90:TYR:HE1	1.75	0.52
7:2:212:PRO:HB2	7:2:252:LYS:HB2	1.92	0.52
1:3:39:GLN:HG3	2:4:43:GLN:HE22	1.75	0.51
7:d:292:VAL:HG13	7:d:449:ILE:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:62:GLN:NE2	7:2:460:SER:OG	2.38	0.51
4:N:80:ALA:HA	4:N:106:VAL:HG11	1.92	0.51
7:C:373:THR:OG1	7:C:385:CYS:O	2.27	0.51
4:n:63:SER:HB2	4:n:74:THR:HB	1.92	0.51
7:2:385:CYS:HA	7:2:418:CYS:HA	1.91	0.51
3:5:46:GLU:OE2	3:5:60:ASN:ND2	2.44	0.51
7:C:212:PRO:HB2	7:C:252:LYS:HB2	1.92	0.51
5:R:18:THR:HG22	5:R:76:ASN:HA	1.91	0.51
7:d:385:CYS:HA	7:d:418:CYS:HA	1.92	0.51
2:4:84:GLU:N	2:4:87:ASP:OD2	2.42	0.51
7:2:304:ARG:N	7:2:440:GLN:OE1	2.42	0.51
1:3:7:SER:HB3	1:3:21:SER:H	1.76	0.51
3:5:49:GLY:HA2	4:6:96:TRP:HZ3	1.76	0.51
4:n:27:SER:OG	4:n:68:GLY:N	2.43	0.51
8:c:580:VAL:HA	8:c:583:VAL:HG22	1.93	0.51
6:8:66:ARG:NH2	6:8:86:ASP:OD2	2.43	0.50
7:C:503:ARG:NH2	8:D:653:GLN:OE1	2.44	0.50
7:2:292:VAL:HG13	7:2:449:ILE:HB	1.92	0.50
7:d:212:PRO:HB2	7:d:252:LYS:HB2	1.92	0.50
2:4:23:CYS:O	2:4:76:PHE:HB2	2.12	0.50
6:8:93:VAL:HG12	6:8:103:TRP:HA	1.93	0.50
8:c:653:GLN:OE1	7:d:503:ARG:NH2	2.44	0.50
7:d:373:THR:OG1	7:d:385:CYS:O	2.27	0.50
3:M:63:LEU:HD22	3:M:66:ARG:HE	1.77	0.50
3:M:94:THR:OG1	3:M:100(Q):ASP:OD1	2.30	0.50
2:4:82:ARG:NH1	2:4:84:GLU:OE2	2.45	0.50
5:r:38:LYS:NZ	5:r:42:GLN:O	2.45	0.50
7:C:56:SER:O	7:C:77:THR:N	2.41	0.50
7:C:292:VAL:HG13	7:C:449:ILE:HB	1.92	0.50
8:D:580:VAL:HA	8:D:583:VAL:HG22	1.93	0.50
1:H:88:ALA:O	1:H:108:THR:HA	2.11	0.50
3:M:28:LEU:HA	3:M:76:ASN:HD21	1.77	0.50
4:N:27:SER:OG	4:N:68:GLY:N	2.44	0.50
4:n:46:LEU:HD21	4:n:49:TYR:HB3	1.93	0.50
6:q:47:TRP:HZ2	6:q:50:TRP:HD1	1.60	0.50
8:A:580:VAL:HA	8:A:583:VAL:HG22	1.93	0.50
2:4:39:GLU:OE1	2:4:41:TYR:OH	2.26	0.50
2:L:91:TYR:HB2	2:L:107:THR:HB	1.94	0.50
1:h:38:LYS:O	1:h:45:LEU:HA	2.12	0.50
4:6:63:SER:HB2	4:6:74:THR:HB	1.94	0.49
2:4:51:LEU:HD21	2:4:54:TYR:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:44:VAL:HG23	8:D:629:LEU:HD23	1.94	0.49
2:L:83:VAL:HG13	2:L:109:LEU:HD21	1.93	0.49
5:r:18:THR:HG22	5:r:76:ASN:HA	1.92	0.49
7:2:503:ARG:NH2	8:A:653:GLN:OE1	2.44	0.49
8:c:629:LEU:HD23	7:d:44:VAL:HG23	1.94	0.49
6:8:54:TRP:CZ3	7:2:370:GLU:OE2	2.66	0.49
7:d:364:SER:OG	7:d:470:PRO:O	2.25	0.49
1:3:38:LYS:HG3	1:3:90:TYR:HE1	1.76	0.49
3:m:97:HIS:CE1	3:m:99:ARG:HH12	2.30	0.49
6:q:61:ARG:NH1	7:d:466:GLU:HA	2.27	0.49
2:l:42:LEU:HA	2:l:90:ILE:O	2.13	0.49
2:l:40:TRP:HB2	2:l:53:ILE:HB	1.94	0.49
4:n:33:VAL:HG12	4:n:51:ASN:HA	1.94	0.49
3:m:63:LEU:HD22	3:m:66:ARG:HE	1.78	0.49
4:6:79:GLU:N	4:6:82:ASP:OD2	2.45	0.49
4:n:80:ALA:HA	4:n:106:VAL:HG11	1.94	0.49
6:8:62:GLN:HE22	7:2:460:SER:HG	1.57	0.48
7:C:270:VAL:HG13	7:C:288:PHE:HA	1.95	0.48
7:2:44:VAL:HG23	8:A:629:LEU:HD23	1.95	0.48
7:2:270:VAL:HG13	7:2:288:PHE:HA	1.95	0.48
1:3:88:ALA:O	1:3:108:THR:HA	2.13	0.48
6:Q:98:CYS:N	6:Q:100(A):CYS:SG	2.82	0.48
7:d:270:VAL:HG13	7:d:288:PHE:HA	1.95	0.48
7:C:342:LEU:HA	7:C:345:VAL:HG22	1.95	0.48
7:C:503:ARG:HH12	8:D:650:GLN:NE2	2.12	0.48
3:m:28:LEU:HA	3:m:76:ASN:HD21	1.78	0.48
6:q:84:PRO:HA	6:q:111:VAL:HB	1.95	0.48
5:r:14:SER:HB2	5:r:17:GLU:OE2	2.13	0.48
7:d:342:LEU:HA	7:d:345:VAL:HG22	1.95	0.48
6:8:38:ARG:HB3	6:8:48:ILE:HD11	1.94	0.48
2:L:40:TRP:HB2	2:L:53:ILE:HB	1.96	0.48
5:R:14:SER:HB2	5:R:17:GLU:OE2	2.13	0.48
3:5:28:LEU:HA	3:5:76:ASN:HD21	1.79	0.48
5:7:14:SER:HB2	5:7:17:GLU:OE2	2.13	0.48
2:L:24:ARG:HG2	2:L:75:ASP:HA	1.96	0.48
7:d:53:PHE:HB3	7:d:218:CYS:HB2	1.95	0.48
1:h:38:LYS:HG3	1:h:90:TYR:HE1	1.78	0.48
1:h:82(A):ARG:NH2	1:h:82(B):ARG:HH12	2.12	0.48
1:3:80:MET:HE3	1:3:82:LEU:HD11	1.95	0.48
7:2:53:PHE:HB3	7:2:218:CYS:HB2	1.96	0.48
1:h:39:GLN:HB3	1:h:89:VAL:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:38:ARG:HB3	3:5:48:ILE:HD11	1.95	0.47
3:m:18:LEU:O	3:m:82:LEU:N	2.45	0.47
3:m:38:ARG:HB3	3:m:48:ILE:HD11	1.97	0.47
3:m:72:ASP:O	3:m:76:ASN:N	2.47	0.47
7:C:53:PHE:HB3	7:C:218:CYS:HB2	1.95	0.47
7:C:122:LEU:HD11	7:C:203:GLN:HB2	1.97	0.47
3:M:61:PRO:HA	3:M:64:LYS:HB2	1.97	0.47
3:5:72:ASP:O	3:5:76:ASN:N	2.48	0.47
6:8:32:TYR:CG	6:8:94:ARG:NH1	2.82	0.47
3:M:38:ARG:HB3	3:M:48:ILE:HD11	1.97	0.47
2:l:41:TYR:O	2:l:91:TYR:HA	2.15	0.47
3:m:61:PRO:HA	3:m:64:LYS:HB2	1.97	0.47
2:4:41:TYR:O	2:4:91:TYR:HA	2.15	0.47
5:7:66:GLY:HA3	5:7:71:PHE:HA	1.97	0.47
7:2:258:GLN:HB2	7:2:374:HIS:HB3	1.97	0.47
8:D:515:ILE:HD11	1:H:58:ALA:HB3	1.96	0.47
7:2:342:LEU:HA	7:2:345:VAL:HG22	1.95	0.47
7:d:258:GLN:HB2	7:d:374:HIS:HB3	1.97	0.47
7:2:155:LYS:NZ	7:2:191:TYR:HE2	2.13	0.47
8:c:650:GLN:NE2	7:d:503:ARG:HH12	2.12	0.47
5:7:18:THR:HG22	5:7:76:ASN:HA	1.96	0.46
1:H:39:GLN:HG3	2:L:43:GLN:HE22	1.80	0.46
7:2:122:LEU:HD11	7:2:203:GLN:HB2	1.97	0.46
3:5:100(D):VAL:N	3:5:100(I):GLU:OE1	2.45	0.46
8:A:577:GLN:HA	8:A:580:VAL:HG22	1.98	0.46
6:8:98:CYS:N	6:8:100(A):CYS:SG	2.84	0.46
3:M:8:GLY:HA3	3:M:20:LEU:HD22	1.97	0.46
7:2:56:SER:O	7:2:77:THR:N	2.41	0.46
2:4:42:LEU:HA	2:4:90:ILE:O	2.15	0.46
1:H:60:ASN:HB3	1:H:63:PHE:HD2	1.80	0.46
3:M:89:ILE:HG22	3:M:106:SER:HA	1.97	0.46
4:n:28:LEU:HB3	4:n:94:ARG:HD2	1.98	0.46
7:2:291:PRO:HG3	11:p:1:NAG:H61	1.98	0.46
8:A:572:GLY:O	8:A:576:LEU:HB2	2.16	0.46
5:r:82:ASP:O	5:r:86:TYR:OH	2.28	0.46
7:2:86:LEU:HD21	8:A:526:ALA:HB3	1.98	0.46
7:2:503:ARG:HH12	8:A:650:GLN:NE2	2.12	0.46
7:d:56:SER:O	7:d:77:THR:N	2.41	0.46
7:C:258:GLN:HB2	7:C:374:HIS:HB3	1.97	0.46
8:c:572:GLY:O	8:c:576:LEU:HB2	2.16	0.46
1:H:104:GLY:O	2:L:48:SER:OG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:47:TRP:HZ2	6:Q:50:TRP:HD1	1.64	0.46
3:m:49:GLY:HA2	4:n:96:TRP:HZ3	1.80	0.46
7:d:122:LEU:HD11	7:d:203:GLN:HB2	1.97	0.46
7:C:49:GLU:HB3	7:C:99:ASN:HD22	1.81	0.46
7:C:503:ARG:HB2	8:D:605:CYS:HB2	1.98	0.46
5:R:66:GLY:HA3	5:R:71:PHE:HA	1.98	0.46
2:l:83:VAL:HG13	2:l:109:LEU:HD21	1.97	0.46
4:6:79:GLU:O	4:6:82:ASP:HB2	2.16	0.46
4:N:28:LEU:HB3	4:N:94:ARG:HD2	1.98	0.46
7:2:49:GLU:HB3	7:2:99:ASN:HD22	1.81	0.46
8:c:577:GLN:HA	8:c:580:VAL:HG22	1.98	0.46
1:H:39:GLN:HA	1:H:44:GLY:O	2.16	0.45
2:L:21:ILE:O	2:L:77:THR:HA	2.17	0.45
4:N:46:LEU:HD21	4:N:49:TYR:HB3	1.97	0.45
6:q:52(A):PRO:HB3	6:q:71:ARG:HG3	1.98	0.45
6:8:47:TRP:HZ2	6:8:50:TRP:HD1	1.65	0.45
7:d:174:SER:OG	7:d:175:LEU:N	2.50	0.45
7:d:49:GLU:HB3	7:d:99:ASN:HD22	1.81	0.45
7:d:291:PRO:HG3	11:CA:1:NAG:H61	1.98	0.45
4:6:15:PRO:HA	4:6:78:VAL:HG23	1.98	0.45
7:C:86:LEU:HD21	8:D:526:ALA:HB3	1.98	0.45
8:D:577:GLN:HA	8:D:580:VAL:HG22	1.97	0.45
1:h:58:ALA:HB3	8:c:515:ILE:HD11	1.99	0.45
7:2:503:ARG:HB2	8:A:605:CYS:HB2	1.98	0.45
7:d:155:LYS:NZ	7:d:191:TYR:HE2	2.13	0.45
8:c:526:ALA:HB3	7:d:86:LEU:HD21	1.98	0.45
4:6:58:ILE:HD12	4:6:59:PRO:HD2	1.99	0.45
8:D:572:GLY:O	8:D:576:LEU:HB2	2.16	0.45
1:3:38:LYS:HB3	1:3:46:GLU:HB2	1.98	0.45
2:L:19:ALA:O	2:L:79:ARG:HA	2.17	0.45
3:M:37:ILE:HD11	3:M:100(P):MET:HG2	1.98	0.45
14:U:5:MAN:O4	14:U:5:MAN:O6	2.33	0.45
4:6:46:LEU:HD21	4:6:49:TYR:HB3	1.99	0.45
7:C:179:LEU:O	7:C:421:LYS:NZ	2.50	0.45
6:q:32:TYR:CG	6:q:94:ARG:NH1	2.85	0.45
3:5:52:HIS:N	3:5:56:ASP:O	2.50	0.45
4:n:79:GLU:N	4:n:82:ASP:OD2	2.50	0.45
8:c:605:CYS:HB2	7:d:503:ARG:HB2	1.98	0.45
2:4:40:TRP:HB2	2:4:53:ILE:HB	2.00	0.44
8:D:597:GLY:N	8:D:650:GLN:OE1	2.50	0.44
6:8:40:ILE:HB	6:8:43:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:62:GLN:NE2	7:2:460:SER:HG	2.14	0.44
7:C:174:SER:OG	7:C:175:LEU:N	2.50	0.44
1:H:80:MET:HE3	1:H:82:LEU:HD11	1.98	0.44
1:h:39:GLN:HG3	2:l:43:GLN:HE22	1.83	0.44
7:C:291:PRO:HG3	11:V:1:NAG:H61	1.98	0.44
3:M:49:GLY:HA2	4:N:96:TRP:HZ3	1.82	0.44
3:M:98:GLY:O	3:M:100(L):THR:HA	2.17	0.44
1:h:88:ALA:O	1:h:108:THR:HA	2.17	0.44
2:l:70:SER:HG	2:l:79:ARG:HH12	1.59	0.44
4:n:28:LEU:HD13	4:n:95:ARG:HE	1.82	0.44
1:h:10:GLU:HB2	1:h:109:VAL:HG22	2.00	0.44
4:n:31:ARG:HG2	4:n:92:ASP:HA	1.99	0.44
2:l:20:SER:HA	2:l:78:LEU:O	2.17	0.44
2:l:88:LEU:HA	2:l:109:LEU:HD23	2.00	0.44
7:d:179:LEU:O	7:d:421:LYS:NZ	2.50	0.44
1:3:3:GLN:O	1:3:25:SER:HB3	2.17	0.44
7:d:57:ASP:OD1	7:d:77:THR:OG1	2.32	0.44
7:C:173:TYR:CE2	9:E:1:NAG:H3	2.53	0.44
5:R:39:ARG:NE	5:R:42:GLN:OE1	2.50	0.44
3:m:94:THR:OG1	3:m:100(Q):ASP:OD1	2.35	0.44
6:q:62:GLN:HE22	7:d:460:SER:HG	1.59	0.44
7:2:55:ALA:HA	7:2:75:VAL:O	2.17	0.44
7:2:179:LEU:O	7:2:421:LYS:NZ	2.50	0.44
8:c:597:GLY:N	8:c:650:GLN:OE1	2.50	0.44
2:4:20:SER:HA	2:4:78:LEU:O	2.17	0.44
3:m:5:GLN:O	3:m:22:CYS:HA	2.18	0.44
1:3:2:VAL:HA	1:3:25:SER:O	2.18	0.44
6:Q:84:PRO:HA	6:Q:111:VAL:HB	2.00	0.44
5:r:66:GLY:HA3	5:r:71:PHE:HA	2.00	0.44
7:d:249:HIS:ND1	7:d:486:TYR:OH	2.41	0.44
2:4:19:ALA:O	2:4:79:ARG:HA	2.18	0.43
5:7:33:MET:N	5:7:51:THR:OG1	2.47	0.43
1:H:6:GLN:OE1	1:H:106:GLY:N	2.45	0.43
8:A:597:GLY:N	8:A:650:GLN:OE1	2.50	0.43
2:4:44:ARG:HB2	2:4:47:GLN:HB2	2.00	0.43
3:5:18:LEU:O	3:5:82:LEU:N	2.45	0.43
6:8:52(A):PRO:HB3	6:8:71:ARG:HG3	2.00	0.43
3:m:10:GLY:HA2	3:m:107:VAL:HA	2.00	0.43
7:C:55:ALA:HA	7:C:75:VAL:O	2.17	0.43
7:d:41:GLY:H	7:d:493:PRO:HB3	1.84	0.43
7:d:55:ALA:HA	7:d:75:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:6:GLN:OE1	1:3:106:GLY:N	2.46	0.43
1:H:38:LYS:HB3	1:H:46:GLU:HB2	2.00	0.43
1:h:80:MET:HE3	1:h:82:LEU:HD11	2.00	0.43
4:6:31:ARG:HG2	4:6:92:ASP:HA	1.99	0.43
6:8:84:PRO:HA	6:8:111:VAL:HB	2.00	0.43
4:n:58:ILE:HD12	4:n:59:PRO:HD2	2.01	0.43
7:2:203:GLN:HE22	7:2:318:TYR:H	1.66	0.43
4:6:18:THR:HA	4:6:76:THR:HA	2.01	0.43
7:C:466:GLU:HA	6:Q:61:ARG:NH1	2.33	0.43
6:Q:32:TYR:CG	6:Q:94:ARG:NH1	2.86	0.43
8:c:621:GLU:O	8:c:625:ASN:CB	2.67	0.43
5:7:39:ARG:NE	5:7:42:GLN:OE1	2.50	0.43
3:M:52:HIS:ND1	3:M:53:ASP:O	2.51	0.43
3:m:8:GLY:HA3	3:m:20:LEU:HD22	2.01	0.43
7:2:298:ARG:NH1	7:2:381:GLU:OE2	2.52	0.43
3:5:110:SER:OG	3:5:111:SER:N	2.52	0.43
7:2:174:SER:OG	7:2:175:LEU:N	2.50	0.43
7:C:203:GLN:HE22	7:C:318:TYR:H	1.66	0.43
7:2:377:ASN:OD1	7:2:381:GLU:N	2.52	0.43
2:4:21:ILE:O	2:4:77:THR:HA	2.19	0.43
7:C:298:ARG:NH1	7:C:381:GLU:OE2	2.52	0.43
3:M:100(Q):ASP:OD1	3:M:100(Q):ASP:N	2.52	0.43
1:h:33:GLU:CD	8:c:515:ILE:HG22	2.44	0.43
3:m:100(Q):ASP:OD1	3:m:100(Q):ASP:N	2.51	0.43
7:d:377:ASN:OD1	7:d:381:GLU:N	2.52	0.43
3:5:61:PRO:HA	3:5:64:LYS:HB2	2.01	0.42
7:C:155:LYS:NZ	7:C:191:TYR:HE2	2.14	0.42
7:C:288:PHE:HZ	7:C:449:ILE:HG22	1.83	0.42
7:C:308:ARG:HH12	7:2:197:ASN:CG	2.27	0.42
8:D:621:GLU:O	8:D:625:ASN:CB	2.67	0.42
6:Q:93:VAL:HG12	6:Q:103:TRP:HA	2.01	0.42
4:N:15:PRO:HA	4:N:78:VAL:HG23	2.01	0.42
7:2:430:ILE:H	7:2:430:ILE:HG13	1.55	0.42
8:c:606:THR:OG1	8:c:607:ASN:N	2.53	0.42
6:8:13:THR:OG1	6:8:16:SER:OG	2.34	0.42
6:8:47:TRP:HZ3	7:2:458:GLY:HA3	1.85	0.42
1:h:39:GLN:HE21	1:h:89:VAL:HB	1.84	0.42
4:n:23:CYS:HB3	4:n:88:CYS:HB3	1.81	0.42
7:2:288:PHE:HZ	7:2:449:ILE:HG22	1.83	0.42
7:C:41:GLY:H	7:C:493:PRO:HB3	1.84	0.42
1:H:10:GLU:HB2	1:H:109:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:52:LYS:O	6:Q:55:GLY:N	2.52	0.42
7:2:41:GLY:H	7:2:493:PRO:HB3	1.84	0.42
7:2:308:ARG:HH12	7:d:197:ASN:CG	2.28	0.42
7:d:277:ILE:HD12	10:x:1:NAG:H82	2.02	0.42
7:d:288:PHE:HZ	7:d:449:ILE:HG22	1.83	0.42
7:d:298:ARG:NH1	7:d:381:GLU:OE2	2.52	0.42
7:C:166:ARG:HA	7:C:166:ARG:HD3	1.91	0.42
7:C:197:ASN:CG	7:d:308:ARG:HH12	2.28	0.42
2:l:21:ILE:O	2:l:77:THR:HA	2.20	0.42
8:A:621:GLU:O	8:A:625:ASN:CB	2.67	0.42
2:4:71:GLY:HA3	2:4:76:PHE:HA	2.01	0.42
7:C:116:LEU:HD21	7:C:434:MET:HE2	2.02	0.42
7:C:377:ASN:OD1	7:C:381:GLU:N	2.52	0.42
8:D:514:GLY:HA3	1:H:97:ASN:HD22	1.85	0.42
6:q:52:LYS:O	6:q:55:GLY:N	2.53	0.42
7:d:203:GLN:HE22	7:d:318:TYR:H	1.66	0.42
2:4:6:GLN:NE2	2:4:91:TYR:O	2.45	0.42
2:4:40:TRP:CE2	2:4:78:LEU:HB2	2.55	0.42
8:D:606:THR:OG1	8:D:607:ASN:N	2.53	0.42
4:N:79:GLU:N	4:N:82:ASP:OD2	2.51	0.42
6:Q:87:THR:HA	6:Q:109:VAL:O	2.20	0.42
1:h:91:TYR:OH	2:l:43:GLN:NE2	2.53	0.42
4:n:18:THR:HA	4:n:76:THR:HA	2.01	0.42
8:A:606:THR:OG1	8:A:607:ASN:N	2.53	0.42
1:H:33:GLU:OE2	1:H:97:ASN:ND2	2.47	0.41
6:q:61:ARG:HE	7:d:459:GLY:HA3	1.85	0.41
7:2:122:LEU:HB2	7:2:201:ILE:HG23	2.02	0.41
4:6:28:LEU:HD13	4:6:95:ARG:HE	1.85	0.41
4:N:28:LEU:HD13	4:N:95:ARG:HE	1.85	0.41
7:2:116:LEU:HD21	7:2:434:MET:HE2	2.02	0.41
7:2:373:THR:OG1	7:2:385:CYS:O	2.27	0.41
4:6:23:CYS:HB3	4:6:88:CYS:HB3	1.78	0.41
5:7:31:ASN:HB2	5:7:90:GLN:NE2	2.35	0.41
3:M:72:ASP:O	3:M:76:ASN:N	2.52	0.41
2:l:40:TRP:CE2	2:l:78:LEU:HB2	2.55	0.41
4:n:15:PRO:HA	4:n:78:VAL:HG23	2.02	0.41
2:L:44:ARG:HB2	2:L:47:GLN:HB2	2.02	0.41
1:h:9:THR:HG23	1:h:108:THR:HB	2.01	0.41
7:2:277:ILE:HD12	10:b:1:NAG:H82	2.02	0.41
2:4:24:ARG:HG2	2:4:75:ASP:HA	2.02	0.41
7:C:57:ASP:OD1	7:C:77:THR:OG1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:384:TYR:HE2	7:C:421:LYS:HB2	1.85	0.41
3:M:66:ARG:HB2	3:M:82(A):THR:HB	2.02	0.41
4:n:37:GLN:HA	4:n:85:ASP:O	2.21	0.41
7:2:100:MET:HG3	7:2:483:LEU:HD13	2.03	0.41
7:d:122:LEU:HB2	7:d:201:ILE:HG23	2.02	0.41
7:d:430:ILE:H	7:d:430:ILE:HG13	1.55	0.41
4:N:31:ARG:HG2	4:N:92:ASP:HA	2.02	0.41
1:h:6:GLN:OE1	1:h:106:GLY:N	2.45	0.41
1:3:83:THR:O	1:3:86:ASP:HB2	2.20	0.41
7:2:384:TYR:HE2	7:2:421:LYS:HB2	1.85	0.41
7:2:457:ASP:OD2	7:2:469:ARG:NH1	2.54	0.41
4:6:37:GLN:HA	4:6:85:ASP:O	2.20	0.41
7:C:277:ILE:HD12	10:I:1:NAG:H82	2.02	0.41
2:L:88:LEU:HA	2:L:109:LEU:HD23	2.03	0.41
3:m:12:VAL:HG11	3:m:82(C):VAL:HG21	2.03	0.41
6:q:13:THR:OG1	6:q:16:SER:OG	2.32	0.41
7:d:100:MET:HG3	7:d:483:LEU:HD13	2.03	0.41
7:d:138:ILE:H	7:d:138:ILE:HG13	1.72	0.41
7:2:57:ASP:OD1	7:2:77:THR:OG1	2.32	0.41
7:d:457:ASP:OD2	7:d:469:ARG:NH1	2.54	0.41
5:r:79:ASP:O	5:r:82:ASP:HB2	2.20	0.40
7:2:95:MET:HE3	7:2:235:GLY:HA3	2.03	0.40
3:5:88:ALA:HB3	3:5:90:TYR:HE1	1.86	0.40
7:C:437:PRO:HA	7:C:438:PRO:HD3	1.97	0.40
2:L:20:SER:HA	2:L:78:LEU:O	2.21	0.40
2:L:40:TRP:CE2	2:L:78:LEU:HB2	2.56	0.40
3:M:53:ASP:OD1	3:M:54:SER:N	2.54	0.40
6:q:54:TRP:CZ3	7:d:370:GLU:OE2	2.74	0.40
6:q:66:ARG:O	6:q:82(A):SER:OG	2.37	0.40
7:d:384:TYR:HE2	7:d:421:LYS:HB2	1.85	0.40
7:d:436:ALA:HA	7:d:437:PRO:HD3	1.90	0.40
6:8:12:LYS:NZ	6:8:17:SER:O	2.54	0.40
6:8:61:ARG:HE	7:2:459:GLY:HA3	1.87	0.40
7:C:122:LEU:HB2	7:C:201:ILE:HG23	2.02	0.40
2:l:24:ARG:HG2	2:l:75:ASP:HA	2.04	0.40
7:2:34:LEU:HD13	7:2:34:LEU:HA	1.93	0.40
4:6:28:LEU:HB3	4:6:94:ARG:HD2	2.04	0.40
2:L:25:SER:OG	2:L:27:GLN:O	2.36	0.40
5:R:79:ASP:O	5:R:82:ASP:HB2	2.22	0.40
1:h:6:GLN:NE2	1:h:92:CYS:H	2.18	0.40
7:2:256:SER:O	7:2:478:ASN:ND2	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:437:PRO:HA	7:2:438:PRO:HD3	1.97	0.40
2:4:19:ALA:HB3	2:4:80:ILE:HB	2.04	0.40
2:l:42:LEU:HD13	2:l:91:TYR:CE1	2.57	0.40
6:q:62:GLN:HG2	6:q:63:LEU:HD12	2.04	0.40
8:A:576:LEU:HD12	8:A:576:LEU:HA	1.94	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	3	114/211 (54%)	106 (93%)	8 (7%)	0	100	100
1	H	114/211 (54%)	107 (94%)	7 (6%)	0	100	100
1	h	114/211 (54%)	105 (92%)	9 (8%)	0	100	100
2	4	111/219 (51%)	103 (93%)	7 (6%)	1 (1%)	14	48
2	L	111/219 (51%)	103 (93%)	7 (6%)	1 (1%)	14	48
2	l	111/219 (51%)	103 (93%)	7 (6%)	1 (1%)	14	48
3	5	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
3	M	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
3	m	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
4	6	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
4	N	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
4	n	103/105 (98%)	93 (90%)	10 (10%)	0	100	100
5	7	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
5	R	100/102 (98%)	91 (91%)	9 (9%)	0	100	100
5	r	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
6	8	126/128 (98%)	117 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Q	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
6	q	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
7	2	447/473 (94%)	413 (92%)	34 (8%)	0	100	100
7	C	447/473 (94%)	413 (92%)	34 (8%)	0	100	100
7	d	447/473 (94%)	413 (92%)	34 (8%)	0	100	100
8	A	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
8	D	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
8	c	128/153 (84%)	120 (94%)	8 (6%)	0	100	100
All	All	3777/4569 (83%)	3497 (93%)	277 (7%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	4	56	VAL
2	l	56	VAL
2	L	56	VAL

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	3	100/182 (55%)	100 (100%)	0	100	100
1	H	100/182 (55%)	100 (100%)	0	100	100
1	h	100/182 (55%)	100 (100%)	0	100	100
2	4	98/193 (51%)	98 (100%)	0	100	100
2	L	98/193 (51%)	98 (100%)	0	100	100
2	l	98/193 (51%)	98 (100%)	0	100	100
3	5	116/116 (100%)	116 (100%)	0	100	100
3	M	116/116 (100%)	116 (100%)	0	100	100
3	m	116/116 (100%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	6	88/88 (100%)	87 (99%)	1 (1%)	65	74
4	N	88/88 (100%)	87 (99%)	1 (1%)	65	74
4	n	88/88 (100%)	87 (99%)	1 (1%)	65	74
5	7	86/86 (100%)	86 (100%)	0	100	100
5	R	86/86 (100%)	86 (100%)	0	100	100
5	r	86/86 (100%)	86 (100%)	0	100	100
6	8	108/108 (100%)	108 (100%)	0	100	100
6	Q	108/108 (100%)	108 (100%)	0	100	100
6	q	108/108 (100%)	108 (100%)	0	100	100
7	2	404/421 (96%)	397 (98%)	7 (2%)	53	68
7	C	404/421 (96%)	397 (98%)	7 (2%)	53	68
7	d	404/421 (96%)	397 (98%)	7 (2%)	53	68
8	A	110/129 (85%)	109 (99%)	1 (1%)	70	76
8	D	110/129 (85%)	109 (99%)	1 (1%)	70	76
8	c	110/129 (85%)	109 (99%)	1 (1%)	70	76
All	All	3330/3969 (84%)	3303 (99%)	27 (1%)	70	77

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

Mol	Chain	Res	Type
4	6	34	ILE
7	C	197	ASN
7	C	255	VAL
7	C	292	VAL
7	C	332	ASN
7	C	392	ASN
7	C	416	LEU
7	C	430	ILE
8	D	577	GLN
4	N	34	ILE
4	n	34	ILE
7	2	197	ASN
7	2	255	VAL
7	2	292	VAL
7	2	332	ASN
7	2	392	ASN
7	2	416	LEU

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Mol	Chain	Res	Type
7	2	430	ILE
8	A	577	GLN
8	c	577	GLN
7	d	197	ASN
7	d	255	VAL
7	d	292	VAL
7	d	332	ASN
7	d	392	ASN
7	d	416	LEU
7	d	430	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	35	HIS
1	3	39	GLN
1	3	43	HIS
1	3	97	ASN
2	4	35	ASN
2	4	43	GLN
3	5	68	HIS
3	5	97	HIS
6	8	64	GLN
7	C	289	ASN
7	C	432	GLN
8	D	611	ASN
8	D	630	GLN
1	H	35	HIS
1	H	43	HIS
1	H	97	ASN
2	L	43	GLN
3	M	97	HIS
6	Q	64	GLN
1	h	35	HIS
1	h	39	GLN
1	h	43	HIS
2	l	43	GLN
3	m	76	ASN
4	n	51	ASN
6	q	64	GLN
7	2	374	HIS
7	2	432	GLN

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Mol	Chain	Res	Type
8	A	611	ASN
8	A	630	GLN
8	c	611	ASN
8	c	630	GLN
7	d	289	ASN
7	d	432	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

153 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	NAG	0	1	7,11	14,14,15	0.21	0	17,19,21	0.58	0
11	NAG	0	2	11	14,14,15	0.22	0	17,19,21	0.49	0
10	NAG	1	1	7,10	14,14,15	0.51	0	17,19,21	0.49	0
10	NAG	1	2	10	14,14,15	0.17	0	17,19,21	0.68	1 (5%)
10	BMA	1	3	10	11,11,12	1.17	1 (9%)	15,15,17	1.22	2 (13%)
13	NAG	9	1	7,13	14,14,15	0.29	0	17,19,21	0.55	0
13	NAG	9	2	13	14,14,15	0.40	0	17,19,21	1.16	1 (5%)
13	BMA	9	3	13	11,11,12	0.75	0	15,15,17	1.03	2 (13%)
13	MAN	9	4	13	11,11,12	0.80	0	15,15,17	0.94	2 (13%)
13	MAN	9	5	13	11,11,12	0.79	0	15,15,17	0.96	2 (13%)
11	NAG	AA	1	7,11	14,14,15	0.44	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	AA	2	11	14,14,15	0.49	0	17,19,21	0.57	0
9	NAG	B	1	9,7	14,14,15	0.27	0	17,19,21	0.47	0
9	NAG	B	2	9	14,14,15	0.38	0	17,19,21	1.12	2 (11%)
9	BMA	B	3	9	11,11,12	0.75	0	15,15,17	1.54	1 (6%)
9	MAN	B	4	9	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
14	NAG	BA	1	7,14	14,14,15	0.32	0	17,19,21	0.56	0
14	NAG	BA	2	14	14,14,15	0.38	0	17,19,21	1.25	2 (11%)
14	BMA	BA	3	14	11,11,12	1.07	1 (9%)	15,15,17	1.24	2 (13%)
14	MAN	BA	4	14	11,11,12	0.55	0	15,15,17	1.40	2 (13%)
14	MAN	BA	5	14	11,11,12	0.73	0	15,15,17	1.31	2 (13%)
14	MAN	BA	6	14	11,11,12	0.84	0	15,15,17	1.14	2 (13%)
14	MAN	BA	7	14	11,11,12	0.69	0	15,15,17	1.17	2 (13%)
14	MAN	BA	8	14	11,11,12	0.71	0	15,15,17	1.00	2 (13%)
14	MAN	BA	9	14	11,11,12	0.87	0	15,15,17	0.99	2 (13%)
11	NAG	CA	1	7,11	14,14,15	0.32	0	17,19,21	1.05	1 (5%)
11	NAG	CA	2	11	14,14,15	0.26	0	17,19,21	0.56	0
9	NAG	DA	1	9,7	14,14,15	0.56	0	17,19,21	0.57	0
9	NAG	DA	2	9	14,14,15	0.32	0	17,19,21	0.81	0
9	BMA	DA	3	9	11,11,12	1.14	0	15,15,17	0.91	0
9	MAN	DA	4	9	11,11,12	0.79	1 (9%)	15,15,17	1.28	2 (13%)
9	NAG	E	1	9,7	14,14,15	0.41	0	17,19,21	0.46	0
9	NAG	E	2	9	14,14,15	0.33	0	17,19,21	0.64	0
9	BMA	E	3	9	11,11,12	0.63	0	15,15,17	0.86	0
9	MAN	E	4	9	11,11,12	0.81	0	15,15,17	0.95	2 (13%)
10	NAG	F	1	7,10	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
10	NAG	F	2	10	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
10	BMA	F	3	10	11,11,12	0.77	0	15,15,17	0.83	1 (6%)
11	NAG	G	1	7,11	14,14,15	0.24	0	17,19,21	0.64	0
11	NAG	G	2	11	14,14,15	0.36	0	17,19,21	0.39	0
10	NAG	I	1	7,10	14,14,15	0.44	0	17,19,21	0.52	0
10	NAG	I	2	10	14,14,15	0.26	0	17,19,21	0.59	0
10	BMA	I	3	10	11,11,12	0.57	0	15,15,17	1.13	1 (6%)
12	NAG	J	1	12,7	14,14,15	0.31	0	17,19,21	0.58	0
12	NAG	J	2	12	14,14,15	0.21	0	17,19,21	0.49	0
12	BMA	J	3	12	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
12	MAN	J	4	12	11,11,12	0.80	1 (9%)	15,15,17	1.49	3 (20%)
12	MAN	J	5	12	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
12	MAN	J	6	12	11,11,12	0.70	0	15,15,17	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	K	1	11	14,14,15	0.36	0	17,19,21	0.68	0
11	NAG	K	2	11	14,14,15	0.40	0	17,19,21	0.60	1 (5%)
11	NAG	O	1	7,11	14,14,15	0.21	0	17,19,21	0.57	0
11	NAG	O	2	11	14,14,15	0.22	0	17,19,21	0.50	0
10	NAG	P	1	7,10	14,14,15	0.50	0	17,19,21	0.50	0
10	NAG	P	2	10	14,14,15	0.18	0	17,19,21	0.67	1 (5%)
10	BMA	P	3	10	11,11,12	1.17	1 (9%)	15,15,17	1.21	2 (13%)
13	NAG	S	1	7,13	14,14,15	0.29	0	17,19,21	0.56	0
13	NAG	S	2	13	14,14,15	0.39	0	17,19,21	1.16	1 (5%)
13	BMA	S	3	13	11,11,12	0.73	0	15,15,17	1.03	2 (13%)
13	MAN	S	4	13	11,11,12	0.80	0	15,15,17	0.94	2 (13%)
13	MAN	S	5	13	11,11,12	0.78	0	15,15,17	0.95	2 (13%)
11	NAG	T	1	7,11	14,14,15	0.44	0	17,19,21	0.69	0
11	NAG	T	2	11	14,14,15	0.48	0	17,19,21	0.57	0
14	NAG	U	1	7,14	14,14,15	0.31	0	17,19,21	0.56	0
14	NAG	U	2	14	14,14,15	0.38	0	17,19,21	1.25	2 (11%)
14	BMA	U	3	14	11,11,12	1.08	1 (9%)	15,15,17	1.24	2 (13%)
14	MAN	U	4	14	11,11,12	0.56	0	15,15,17	1.40	2 (13%)
14	MAN	U	5	14	11,11,12	0.72	0	15,15,17	1.30	2 (13%)
14	MAN	U	6	14	11,11,12	0.84	0	15,15,17	1.14	2 (13%)
14	MAN	U	7	14	11,11,12	0.70	0	15,15,17	1.18	2 (13%)
14	MAN	U	8	14	11,11,12	0.71	0	15,15,17	0.99	2 (13%)
14	MAN	U	9	14	11,11,12	0.88	0	15,15,17	0.99	2 (13%)
11	NAG	V	1	7,11	14,14,15	0.31	0	17,19,21	1.06	1 (5%)
11	NAG	V	2	11	14,14,15	0.25	0	17,19,21	0.56	0
9	NAG	W	1	9,7	14,14,15	0.56	0	17,19,21	0.56	0
9	NAG	W	2	9	14,14,15	0.32	0	17,19,21	0.81	0
9	BMA	W	3	9	11,11,12	1.14	0	15,15,17	0.91	0
9	MAN	W	4	9	11,11,12	0.79	1 (9%)	15,15,17	1.27	2 (13%)
9	NAG	X	1	9,7	14,14,15	0.27	0	17,19,21	0.46	0
9	NAG	X	2	9	14,14,15	0.38	0	17,19,21	1.12	2 (11%)
9	BMA	X	3	9	11,11,12	0.76	0	15,15,17	1.53	1 (6%)
9	MAN	X	4	9	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
9	NAG	Y	1	9,7	14,14,15	0.41	0	17,19,21	0.46	0
9	NAG	Y	2	9	14,14,15	0.33	0	17,19,21	0.63	0
9	BMA	Y	3	9	11,11,12	0.63	0	15,15,17	0.86	0
9	MAN	Y	4	9	11,11,12	0.81	0	15,15,17	0.95	2 (13%)
10	NAG	Z	1	7,10	14,14,15	0.51	0	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	Z	2	10	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
10	BMA	Z	3	10	11,11,12	0.78	0	15,15,17	0.83	1 (6%)
11	NAG	a	1	7,11	14,14,15	0.24	0	17,19,21	0.63	0
11	NAG	a	2	11	14,14,15	0.37	0	17,19,21	0.39	0
10	NAG	b	1	7,10	14,14,15	0.42	0	17,19,21	0.52	0
10	NAG	b	2	10	14,14,15	0.26	0	17,19,21	0.59	0
10	BMA	b	3	10	11,11,12	0.58	0	15,15,17	1.12	1 (6%)
12	NAG	e	1	12,7	14,14,15	0.30	0	17,19,21	0.58	0
12	NAG	e	2	12	14,14,15	0.21	0	17,19,21	0.48	0
12	BMA	e	3	12	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
12	MAN	e	4	12	11,11,12	0.80	1 (9%)	15,15,17	1.49	3 (20%)
12	MAN	e	5	12	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
12	MAN	e	6	12	11,11,12	0.70	0	15,15,17	1.28	2 (13%)
11	NAG	f	1	11	14,14,15	0.36	0	17,19,21	0.68	0
11	NAG	f	2	11	14,14,15	0.40	0	17,19,21	0.60	1 (5%)
11	NAG	g	1	7,11	14,14,15	0.19	0	17,19,21	0.57	0
11	NAG	g	2	11	14,14,15	0.22	0	17,19,21	0.50	0
10	NAG	i	1	7,10	14,14,15	0.50	0	17,19,21	0.50	0
10	NAG	i	2	10	14,14,15	0.18	0	17,19,21	0.67	1 (5%)
10	BMA	i	3	10	11,11,12	1.16	1 (9%)	15,15,17	1.21	2 (13%)
13	NAG	j	1	7,13	14,14,15	0.29	0	17,19,21	0.55	0
13	NAG	j	2	13	14,14,15	0.39	0	17,19,21	1.16	1 (5%)
13	BMA	j	3	13	11,11,12	0.74	0	15,15,17	1.02	2 (13%)
13	MAN	j	4	13	11,11,12	0.80	0	15,15,17	0.94	2 (13%)
13	MAN	j	5	13	11,11,12	0.78	0	15,15,17	0.96	2 (13%)
11	NAG	k	1	7,11	14,14,15	0.43	0	17,19,21	0.68	0
11	NAG	k	2	11	14,14,15	0.49	0	17,19,21	0.57	0
14	NAG	o	1	7,14	14,14,15	0.32	0	17,19,21	0.56	0
14	NAG	o	2	14	14,14,15	0.37	0	17,19,21	1.26	2 (11%)
14	BMA	o	3	14	11,11,12	1.08	1 (9%)	15,15,17	1.25	2 (13%)
14	MAN	o	4	14	11,11,12	0.56	0	15,15,17	1.41	2 (13%)
14	MAN	o	5	14	11,11,12	0.73	0	15,15,17	1.30	2 (13%)
14	MAN	o	6	14	11,11,12	0.83	0	15,15,17	1.13	2 (13%)
14	MAN	o	7	14	11,11,12	0.69	0	15,15,17	1.19	2 (13%)
14	MAN	o	8	14	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
14	MAN	o	9	14	11,11,12	0.88	0	15,15,17	0.99	2 (13%)
11	NAG	p	1	7,11	14,14,15	0.31	0	17,19,21	1.05	1 (5%)
11	NAG	p	2	11	14,14,15	0.26	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	s	1	9,7	14,14,15	0.57	0	17,19,21	0.57	0
9	NAG	s	2	9	14,14,15	0.33	0	17,19,21	0.81	0
9	BMA	s	3	9	11,11,12	1.14	0	15,15,17	0.91	0
9	MAN	s	4	9	11,11,12	0.79	1 (9%)	15,15,17	1.28	2 (13%)
9	NAG	t	1	9,7	14,14,15	0.27	0	17,19,21	0.46	0
9	NAG	t	2	9	14,14,15	0.38	0	17,19,21	1.12	2 (11%)
9	BMA	t	3	9	11,11,12	0.75	0	15,15,17	1.53	1 (6%)
9	MAN	t	4	9	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
9	NAG	u	1	9,7	14,14,15	0.40	0	17,19,21	0.47	0
9	NAG	u	2	9	14,14,15	0.33	0	17,19,21	0.63	0
9	BMA	u	3	9	11,11,12	0.64	0	15,15,17	0.86	0
9	MAN	u	4	9	11,11,12	0.81	0	15,15,17	0.95	2 (13%)
10	NAG	v	1	7,10	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
10	NAG	v	2	10	14,14,15	0.26	0	17,19,21	0.74	1 (5%)
10	BMA	v	3	10	11,11,12	0.77	0	15,15,17	0.83	1 (6%)
11	NAG	w	1	7,11	14,14,15	0.26	0	17,19,21	0.64	0
11	NAG	w	2	11	14,14,15	0.38	0	17,19,21	0.39	0
10	NAG	x	1	7,10	14,14,15	0.45	0	17,19,21	0.52	0
10	NAG	x	2	10	14,14,15	0.25	0	17,19,21	0.59	0
10	BMA	x	3	10	11,11,12	0.57	0	15,15,17	1.13	1 (6%)
12	NAG	y	1	12,7	14,14,15	0.31	0	17,19,21	0.59	0
12	NAG	y	2	12	14,14,15	0.21	0	17,19,21	0.48	0
12	BMA	y	3	12	11,11,12	0.78	0	15,15,17	1.15	2 (13%)
12	MAN	y	4	12	11,11,12	0.80	1 (9%)	15,15,17	1.50	3 (20%)
12	MAN	y	5	12	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
12	MAN	y	6	12	11,11,12	0.71	0	15,15,17	1.28	2 (13%)
11	NAG	z	1	11	14,14,15	0.37	0	17,19,21	0.69	0
11	NAG	z	2	11	14,14,15	0.40	0	17,19,21	0.60	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	0	1	7,11	-	1/6/23/26	0/1/1/1
11	NAG	0	2	11	-	2/6/23/26	0/1/1/1
10	NAG	1	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	1	2	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	1	3	10	-	1/2/19/22	0/1/1/1
13	NAG	9	1	7,13	-	2/6/23/26	0/1/1/1
13	NAG	9	2	13	-	2/6/23/26	0/1/1/1
13	BMA	9	3	13	-	0/2/19/22	0/1/1/1
13	MAN	9	4	13	-	0/2/19/22	0/1/1/1
13	MAN	9	5	13	-	0/2/19/22	0/1/1/1
11	NAG	AA	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	AA	2	11	-	2/6/23/26	0/1/1/1
9	NAG	B	1	9,7	-	2/6/23/26	0/1/1/1
9	NAG	B	2	9	-	2/6/23/26	0/1/1/1
9	BMA	B	3	9	-	2/2/19/22	0/1/1/1
9	MAN	B	4	9	-	2/2/19/22	0/1/1/1
14	NAG	BA	1	7,14	-	2/6/23/26	0/1/1/1
14	NAG	BA	2	14	-	2/6/23/26	0/1/1/1
14	BMA	BA	3	14	-	0/2/19/22	0/1/1/1
14	MAN	BA	4	14	-	2/2/19/22	0/1/1/1
14	MAN	BA	5	14	-	2/2/19/22	0/1/1/1
14	MAN	BA	6	14	-	0/2/19/22	0/1/1/1
14	MAN	BA	7	14	-	2/2/19/22	0/1/1/1
14	MAN	BA	8	14	-	2/2/19/22	0/1/1/1
14	MAN	BA	9	14	-	0/2/19/22	0/1/1/1
11	NAG	CA	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	CA	2	11	-	2/6/23/26	0/1/1/1
9	NAG	DA	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	DA	2	9	-	2/6/23/26	0/1/1/1
9	BMA	DA	3	9	-	2/2/19/22	0/1/1/1
9	MAN	DA	4	9	-	0/2/19/22	0/1/1/1
9	NAG	E	1	9,7	-	1/6/23/26	0/1/1/1
9	NAG	E	2	9	-	2/6/23/26	0/1/1/1
9	BMA	E	3	9	-	0/2/19/22	0/1/1/1
9	MAN	E	4	9	-	1/2/19/22	0/1/1/1
10	NAG	F	1	7,10	-	2/6/23/26	0/1/1/1
10	NAG	F	2	10	-	2/6/23/26	0/1/1/1
10	BMA	F	3	10	-	0/2/19/22	0/1/1/1
11	NAG	G	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	G	2	11	-	0/6/23/26	0/1/1/1
10	NAG	I	1	7,10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	2/2/19/22	0/1/1/1
12	NAG	J	1	12,7	-	2/6/23/26	0/1/1/1
12	NAG	J	2	12	-	2/6/23/26	0/1/1/1
12	BMA	J	3	12	-	2/2/19/22	0/1/1/1
12	MAN	J	4	12	-	2/2/19/22	0/1/1/1
12	MAN	J	5	12	-	0/2/19/22	0/1/1/1
12	MAN	J	6	12	-	2/2/19/22	0/1/1/1
11	NAG	K	1	11	-	2/6/23/26	0/1/1/1
11	NAG	K	2	11	-	0/6/23/26	0/1/1/1
11	NAG	O	1	7,11	-	1/6/23/26	0/1/1/1
11	NAG	O	2	11	-	2/6/23/26	0/1/1/1
10	NAG	P	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	BMA	P	3	10	-	1/2/19/22	0/1/1/1
13	NAG	S	1	7,13	-	2/6/23/26	0/1/1/1
13	NAG	S	2	13	-	2/6/23/26	0/1/1/1
13	BMA	S	3	13	-	0/2/19/22	0/1/1/1
13	MAN	S	4	13	-	0/2/19/22	0/1/1/1
13	MAN	S	5	13	-	0/2/19/22	0/1/1/1
11	NAG	T	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	T	2	11	-	2/6/23/26	0/1/1/1
14	NAG	U	1	7,14	-	2/6/23/26	0/1/1/1
14	NAG	U	2	14	-	2/6/23/26	0/1/1/1
14	BMA	U	3	14	-	0/2/19/22	0/1/1/1
14	MAN	U	4	14	-	2/2/19/22	0/1/1/1
14	MAN	U	5	14	-	2/2/19/22	0/1/1/1
14	MAN	U	6	14	-	0/2/19/22	0/1/1/1
14	MAN	U	7	14	-	2/2/19/22	0/1/1/1
14	MAN	U	8	14	-	2/2/19/22	0/1/1/1
14	MAN	U	9	14	-	0/2/19/22	0/1/1/1
11	NAG	V	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	V	2	11	-	2/6/23/26	0/1/1/1
9	NAG	W	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	W	2	9	-	2/6/23/26	0/1/1/1
9	BMA	W	3	9	-	2/2/19/22	0/1/1/1
9	MAN	W	4	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	X	1	9,7	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
9	MAN	X	4	9	-	2/2/19/22	0/1/1/1
9	NAG	Y	1	9,7	-	1/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	4	9	-	1/2/19/22	0/1/1/1
10	NAG	Z	1	7,10	-	2/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	2/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
11	NAG	a	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	a	2	11	-	0/6/23/26	0/1/1/1
10	NAG	b	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	b	2	10	-	2/6/23/26	0/1/1/1
10	BMA	b	3	10	-	2/2/19/22	0/1/1/1
12	NAG	e	1	12,7	-	2/6/23/26	0/1/1/1
12	NAG	e	2	12	-	2/6/23/26	0/1/1/1
12	BMA	e	3	12	-	2/2/19/22	0/1/1/1
12	MAN	e	4	12	-	2/2/19/22	0/1/1/1
12	MAN	e	5	12	-	0/2/19/22	0/1/1/1
12	MAN	e	6	12	-	2/2/19/22	0/1/1/1
11	NAG	f	1	11	-	2/6/23/26	0/1/1/1
11	NAG	f	2	11	-	0/6/23/26	0/1/1/1
11	NAG	g	1	7,11	-	1/6/23/26	0/1/1/1
11	NAG	g	2	11	-	2/6/23/26	0/1/1/1
10	NAG	i	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	i	2	10	-	0/6/23/26	0/1/1/1
10	BMA	i	3	10	-	1/2/19/22	0/1/1/1
13	NAG	j	1	7,13	-	2/6/23/26	0/1/1/1
13	NAG	j	2	13	-	2/6/23/26	0/1/1/1
13	BMA	j	3	13	-	0/2/19/22	0/1/1/1
13	MAN	j	4	13	-	0/2/19/22	0/1/1/1
13	MAN	j	5	13	-	0/2/19/22	0/1/1/1
11	NAG	k	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	k	2	11	-	2/6/23/26	0/1/1/1
14	NAG	o	1	7,14	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	o	2	14	-	2/6/23/26	0/1/1/1
14	BMA	o	3	14	-	0/2/19/22	0/1/1/1
14	MAN	o	4	14	-	2/2/19/22	0/1/1/1
14	MAN	o	5	14	-	2/2/19/22	0/1/1/1
14	MAN	o	6	14	-	0/2/19/22	0/1/1/1
14	MAN	o	7	14	-	2/2/19/22	0/1/1/1
14	MAN	o	8	14	-	2/2/19/22	0/1/1/1
14	MAN	o	9	14	-	0/2/19/22	0/1/1/1
11	NAG	p	1	7,11	-	3/6/23/26	0/1/1/1
11	NAG	p	2	11	-	2/6/23/26	0/1/1/1
9	NAG	s	1	9,7	-	0/6/23/26	0/1/1/1
9	NAG	s	2	9	-	2/6/23/26	0/1/1/1
9	BMA	s	3	9	-	2/2/19/22	0/1/1/1
9	MAN	s	4	9	-	0/2/19/22	0/1/1/1
9	NAG	t	1	9,7	-	2/6/23/26	0/1/1/1
9	NAG	t	2	9	-	2/6/23/26	0/1/1/1
9	BMA	t	3	9	-	2/2/19/22	0/1/1/1
9	MAN	t	4	9	-	2/2/19/22	0/1/1/1
9	NAG	u	1	9,7	-	1/6/23/26	0/1/1/1
9	NAG	u	2	9	-	2/6/23/26	0/1/1/1
9	BMA	u	3	9	-	0/2/19/22	0/1/1/1
9	MAN	u	4	9	-	1/2/19/22	0/1/1/1
10	NAG	v	1	7,10	-	2/6/23/26	0/1/1/1
10	NAG	v	2	10	-	2/6/23/26	0/1/1/1
10	BMA	v	3	10	-	0/2/19/22	0/1/1/1
11	NAG	w	1	7,11	-	2/6/23/26	0/1/1/1
11	NAG	w	2	11	-	0/6/23/26	0/1/1/1
10	NAG	x	1	7,10	-	0/6/23/26	0/1/1/1
10	NAG	x	2	10	-	2/6/23/26	0/1/1/1
10	BMA	x	3	10	-	2/2/19/22	0/1/1/1
12	NAG	y	1	12,7	-	2/6/23/26	0/1/1/1
12	NAG	y	2	12	-	2/6/23/26	0/1/1/1
12	BMA	y	3	12	-	2/2/19/22	0/1/1/1
12	MAN	y	4	12	-	2/2/19/22	0/1/1/1
12	MAN	y	5	12	-	0/2/19/22	0/1/1/1
12	MAN	y	6	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	z	1	11	-	2/6/23/26	0/1/1/1
11	NAG	z	2	11	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	3	BMA	C1-C2	2.63	1.58	1.52
10	P	3	BMA	C1-C2	2.62	1.58	1.52
10	i	3	BMA	C1-C2	2.61	1.58	1.52
12	J	4	MAN	O5-C5	2.13	1.47	1.43
12	y	4	MAN	O5-C5	2.13	1.47	1.43
12	e	4	MAN	O5-C5	2.13	1.47	1.43
9	W	4	MAN	C1-C2	2.09	1.57	1.52
9	DA	4	MAN	C1-C2	2.09	1.57	1.52
9	s	4	MAN	C1-C2	2.07	1.57	1.52
14	o	3	BMA	O5-C1	-2.04	1.40	1.43
14	U	3	BMA	O5-C1	-2.03	1.40	1.43
14	BA	3	BMA	O5-C1	-2.02	1.40	1.43

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	3	BMA	C1-O5-C5	4.96	118.84	112.19
9	t	3	BMA	C1-O5-C5	4.96	118.84	112.19
9	X	3	BMA	C1-O5-C5	4.94	118.81	112.19
14	U	4	MAN	C1-O5-C5	4.52	118.25	112.19
14	o	4	MAN	C1-O5-C5	4.51	118.23	112.19
14	BA	4	MAN	C1-O5-C5	4.50	118.22	112.19
12	y	4	MAN	C1-O5-C5	4.06	117.62	112.19
12	e	4	MAN	C1-O5-C5	4.06	117.62	112.19
12	J	4	MAN	C1-O5-C5	4.04	117.60	112.19
9	s	4	MAN	C1-O5-C5	3.66	117.09	112.19
13	9	2	NAG	C1-O5-C5	3.66	117.08	112.19
9	DA	4	MAN	C1-O5-C5	3.64	117.07	112.19
13	S	2	NAG	C1-O5-C5	3.64	117.07	112.19
9	W	4	MAN	C1-O5-C5	3.63	117.05	112.19
13	j	2	NAG	C1-O5-C5	3.61	117.03	112.19
12	J	6	MAN	C1-O5-C5	3.60	117.01	112.19
12	e	6	MAN	C1-O5-C5	3.58	116.98	112.19
12	y	6	MAN	C1-O5-C5	3.58	116.98	112.19
12	y	5	MAN	C1-O5-C5	3.52	116.90	112.19
12	J	5	MAN	C1-O5-C5	3.50	116.87	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	5	MAN	C1-O5-C5	3.50	116.87	112.19
12	J	3	BMA	C1-O5-C5	3.43	116.78	112.19
12	e	3	BMA	C1-O5-C5	3.40	116.74	112.19
12	y	3	BMA	C1-O5-C5	3.39	116.73	112.19
9	t	4	MAN	C1-O5-C5	3.38	116.71	112.19
9	B	4	MAN	C1-O5-C5	3.37	116.71	112.19
9	X	4	MAN	C1-O5-C5	3.37	116.70	112.19
14	BA	5	MAN	C1-O5-C5	3.32	116.63	112.19
14	U	5	MAN	C1-O5-C5	3.28	116.58	112.19
14	o	5	MAN	C1-O5-C5	3.28	116.58	112.19
11	V	1	NAG	C2-N2-C7	3.26	127.27	122.90
11	p	1	NAG	C2-N2-C7	3.24	127.24	122.90
11	CA	1	NAG	C2-N2-C7	3.23	127.23	122.90
14	o	2	NAG	C2-N2-C7	3.23	127.23	122.90
14	BA	2	NAG	C2-N2-C7	3.21	127.21	122.90
14	U	2	NAG	C2-N2-C7	3.20	127.19	122.90
14	BA	5	MAN	O2-C2-C3	-3.15	103.62	110.15
14	U	5	MAN	O2-C2-C3	-3.15	103.62	110.15
14	o	5	MAN	O2-C2-C3	-3.14	103.64	110.15
10	x	3	BMA	C1-O5-C5	3.14	116.40	112.19
10	I	3	BMA	C1-O5-C5	3.13	116.38	112.19
10	b	3	BMA	C1-O5-C5	3.11	116.36	112.19
9	t	2	NAG	C1-O5-C5	3.05	116.28	112.19
9	X	2	NAG	C1-O5-C5	3.05	116.27	112.19
9	B	2	NAG	C1-O5-C5	3.04	116.26	112.19
10	F	1	NAG	C2-N2-C7	3.04	126.97	122.90
10	Z	1	NAG	C2-N2-C7	3.04	126.97	122.90
10	v	1	NAG	C2-N2-C7	3.02	126.94	122.90
13	9	3	BMA	C1-O5-C5	2.94	116.13	112.19
14	BA	6	MAN	C1-O5-C5	2.94	116.12	112.19
14	U	6	MAN	C1-O5-C5	2.93	116.12	112.19
14	o	6	MAN	C1-O5-C5	2.93	116.11	112.19
13	S	3	BMA	C1-O5-C5	2.93	116.11	112.19
13	j	3	BMA	C1-O5-C5	2.92	116.10	112.19
10	1	3	BMA	O2-C2-C3	-2.87	104.20	110.15
10	P	3	BMA	O2-C2-C3	-2.87	104.20	110.15
10	i	3	BMA	O2-C2-C3	-2.86	104.22	110.15
14	o	7	MAN	C1-O5-C5	2.85	116.01	112.19
14	U	7	MAN	C1-O5-C5	2.83	115.97	112.19
14	BA	7	MAN	C1-O5-C5	2.81	115.95	112.19
14	o	3	BMA	C1-O5-C5	2.71	115.81	112.19
14	U	3	BMA	C1-O5-C5	2.69	115.79	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BA	3	BMA	C1-O5-C5	2.68	115.77	112.19
12	e	6	MAN	O2-C2-C3	-2.52	104.94	110.15
12	J	6	MAN	O2-C2-C3	-2.51	104.95	110.15
12	y	6	MAN	O2-C2-C3	-2.51	104.95	110.15
9	X	2	NAG	O4-C4-C5	2.49	115.46	109.32
9	X	4	MAN	O2-C2-C3	-2.48	105.02	110.15
9	B	2	NAG	O4-C4-C5	2.48	115.43	109.32
14	BA	7	MAN	O2-C2-C3	-2.48	105.02	110.15
9	B	4	MAN	O2-C2-C3	-2.47	105.03	110.15
14	U	7	MAN	O2-C2-C3	-2.47	105.03	110.15
14	o	7	MAN	O2-C2-C3	-2.47	105.03	110.15
9	t	2	NAG	O4-C4-C5	2.47	115.41	109.32
9	t	4	MAN	O2-C2-C3	-2.47	105.04	110.15
14	BA	8	MAN	C1-O5-C5	2.44	115.45	112.19
14	BA	8	MAN	O2-C2-C3	-2.41	105.17	110.15
14	o	8	MAN	O2-C2-C3	-2.41	105.17	110.15
14	U	8	MAN	O2-C2-C3	-2.40	105.19	110.15
14	U	8	MAN	C1-O5-C5	2.40	115.40	112.19
10	v	2	NAG	C1-O5-C5	2.39	115.39	112.19
9	s	4	MAN	O2-C2-C3	-2.36	105.26	110.15
10	F	2	NAG	C1-O5-C5	2.36	115.35	112.19
9	DA	4	MAN	O2-C2-C3	-2.36	105.27	110.15
14	o	8	MAN	C1-O5-C5	2.36	115.34	112.19
9	W	4	MAN	O2-C2-C3	-2.35	105.27	110.15
10	Z	2	NAG	C1-O5-C5	2.35	115.34	112.19
12	e	4	MAN	O3-C3-C2	2.35	114.84	110.05
12	J	4	MAN	O3-C3-C2	2.34	114.83	110.05
12	y	4	MAN	O3-C3-C2	2.34	114.83	110.05
13	j	5	MAN	C1-O5-C5	2.33	115.31	112.19
13	9	5	MAN	C1-O5-C5	2.32	115.29	112.19
13	S	5	MAN	C1-O5-C5	2.30	115.27	112.19
14	U	6	MAN	O2-C2-C3	-2.26	105.47	110.15
14	BA	6	MAN	O2-C2-C3	-2.26	105.48	110.15
14	U	3	BMA	O2-C2-C3	-2.26	105.48	110.15
14	BA	3	BMA	O2-C2-C3	-2.26	105.48	110.15
14	o	6	MAN	O2-C2-C3	-2.25	105.50	110.15
14	o	3	BMA	O2-C2-C3	-2.25	105.50	110.15
12	y	5	MAN	O2-C2-C3	-2.22	105.56	110.15
13	9	5	MAN	O2-C2-C3	-2.21	105.58	110.15
12	J	5	MAN	O2-C2-C3	-2.20	105.60	110.15
12	e	5	MAN	O2-C2-C3	-2.20	105.60	110.15
12	y	3	BMA	O2-C2-C3	-2.19	105.61	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	4	MAN	C1-C2-C3	-2.19	106.46	109.64
13	S	5	MAN	O2-C2-C3	-2.19	105.62	110.15
12	y	4	MAN	C1-C2-C3	-2.19	106.46	109.64
13	j	5	MAN	O2-C2-C3	-2.18	105.63	110.15
12	e	4	MAN	C1-C2-C3	-2.18	106.47	109.64
12	J	3	BMA	O2-C2-C3	-2.17	105.65	110.15
12	e	3	BMA	O2-C2-C3	-2.17	105.67	110.15
9	E	4	MAN	C1-O5-C5	2.16	115.09	112.19
9	Y	4	MAN	C1-O5-C5	2.16	115.08	112.19
10	l	3	BMA	C1-C2-C3	-2.16	106.50	109.64
10	P	3	BMA	C1-C2-C3	-2.15	106.52	109.64
9	u	4	MAN	C1-O5-C5	2.15	115.06	112.19
10	i	3	BMA	C1-C2-C3	-2.14	106.53	109.64
14	BA	2	NAG	C1-O5-C5	2.14	115.05	112.19
10	l	2	NAG	C1-O5-C5	2.14	115.05	112.19
14	o	2	NAG	C1-O5-C5	2.14	115.05	112.19
10	i	2	NAG	C1-O5-C5	2.13	115.05	112.19
13	S	4	MAN	O2-C2-C3	-2.13	105.73	110.15
13	9	4	MAN	O2-C2-C3	-2.13	105.73	110.15
13	S	4	MAN	C1-O5-C5	2.13	115.04	112.19
13	j	4	MAN	O2-C2-C3	-2.13	105.74	110.15
14	U	2	NAG	C1-O5-C5	2.12	115.03	112.19
13	j	4	MAN	C1-O5-C5	2.12	115.03	112.19
13	9	4	MAN	C1-O5-C5	2.11	115.02	112.19
10	P	2	NAG	C1-O5-C5	2.11	115.02	112.19
9	u	4	MAN	O2-C2-C3	-2.11	105.79	110.15
9	E	4	MAN	O2-C2-C3	-2.10	105.80	110.15
9	Y	4	MAN	O2-C2-C3	-2.09	105.82	110.15
14	U	9	MAN	O2-C2-C3	-2.09	105.83	110.15
14	o	9	MAN	O2-C2-C3	-2.08	105.85	110.15
14	BA	9	MAN	O2-C2-C3	-2.08	105.85	110.15
13	S	3	BMA	O2-C2-C3	-2.07	105.86	110.15
13	j	3	BMA	O2-C2-C3	-2.07	105.87	110.15
13	9	3	BMA	O2-C2-C3	-2.07	105.87	110.15
11	f	2	NAG	C1-O5-C5	2.06	114.95	112.19
11	K	2	NAG	C1-O5-C5	2.06	114.94	112.19
14	o	4	MAN	O2-C2-C3	-2.05	105.91	110.15
14	BA	4	MAN	O2-C2-C3	-2.05	105.91	110.15
11	z	2	NAG	C1-O5-C5	2.05	114.93	112.19
14	o	9	MAN	C1-O5-C5	2.04	114.92	112.19
14	U	9	MAN	C1-O5-C5	2.04	114.92	112.19
14	U	4	MAN	O2-C2-C3	-2.03	105.95	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	v	3	BMA	O2-C2-C3	-2.02	105.96	110.15
14	BA	9	MAN	C1-O5-C5	2.02	114.89	112.19
10	F	3	BMA	O2-C2-C3	-2.02	105.97	110.15
10	Z	3	BMA	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (201) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	S	2	NAG	O5-C5-C6-O6
13	j	2	NAG	O5-C5-C6-O6
13	9	2	NAG	O5-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
10	b	2	NAG	O5-C5-C6-O6
10	x	2	NAG	O5-C5-C6-O6
13	S	1	NAG	O5-C5-C6-O6
13	j	1	NAG	O5-C5-C6-O6
13	9	1	NAG	O5-C5-C6-O6
11	V	2	NAG	O5-C5-C6-O6
11	p	2	NAG	O5-C5-C6-O6
11	CA	2	NAG	O5-C5-C6-O6
9	W	2	NAG	O5-C5-C6-O6
9	s	2	NAG	O5-C5-C6-O6
9	DA	2	NAG	O5-C5-C6-O6
11	T	1	NAG	O5-C5-C6-O6
11	k	1	NAG	O5-C5-C6-O6
11	AA	1	NAG	O5-C5-C6-O6
13	S	2	NAG	C4-C5-C6-O6
13	j	2	NAG	C4-C5-C6-O6
13	9	2	NAG	C4-C5-C6-O6
12	J	4	MAN	O5-C5-C6-O6
12	e	4	MAN	O5-C5-C6-O6
12	y	4	MAN	O5-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
10	b	2	NAG	C4-C5-C6-O6
10	x	2	NAG	C4-C5-C6-O6
13	j	1	NAG	C4-C5-C6-O6
14	U	5	MAN	O5-C5-C6-O6
14	U	8	MAN	O5-C5-C6-O6
14	o	5	MAN	O5-C5-C6-O6
14	o	8	MAN	O5-C5-C6-O6
14	BA	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	BA	8	MAN	O5-C5-C6-O6
13	S	1	NAG	C4-C5-C6-O6
13	9	1	NAG	C4-C5-C6-O6
11	G	1	NAG	O5-C5-C6-O6
11	K	1	NAG	O5-C5-C6-O6
11	a	1	NAG	O5-C5-C6-O6
11	f	1	NAG	O5-C5-C6-O6
11	w	1	NAG	O5-C5-C6-O6
11	z	1	NAG	O5-C5-C6-O6
12	J	4	MAN	C4-C5-C6-O6
12	e	4	MAN	C4-C5-C6-O6
12	y	4	MAN	C4-C5-C6-O6
10	F	2	NAG	O5-C5-C6-O6
10	I	3	BMA	O5-C5-C6-O6
10	Z	2	NAG	O5-C5-C6-O6
10	b	3	BMA	O5-C5-C6-O6
10	v	2	NAG	O5-C5-C6-O6
10	x	3	BMA	O5-C5-C6-O6
11	T	2	NAG	O5-C5-C6-O6
11	k	2	NAG	O5-C5-C6-O6
11	AA	2	NAG	O5-C5-C6-O6
14	U	1	NAG	O5-C5-C6-O6
14	U	4	MAN	O5-C5-C6-O6
14	o	1	NAG	O5-C5-C6-O6
14	o	4	MAN	O5-C5-C6-O6
14	BA	1	NAG	O5-C5-C6-O6
14	BA	4	MAN	O5-C5-C6-O6
12	J	6	MAN	O5-C5-C6-O6
12	e	6	MAN	O5-C5-C6-O6
12	y	6	MAN	O5-C5-C6-O6
11	G	1	NAG	C4-C5-C6-O6
11	T	2	NAG	C4-C5-C6-O6
11	a	1	NAG	C4-C5-C6-O6
11	k	2	NAG	C4-C5-C6-O6
11	w	1	NAG	C4-C5-C6-O6
11	AA	2	NAG	C4-C5-C6-O6
9	B	2	NAG	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
9	t	2	NAG	O5-C5-C6-O6
10	F	2	NAG	C4-C5-C6-O6
10	Z	2	NAG	C4-C5-C6-O6
10	v	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	T	1	NAG	C4-C5-C6-O6
11	k	1	NAG	C4-C5-C6-O6
11	AA	1	NAG	C4-C5-C6-O6
11	O	2	NAG	O5-C5-C6-O6
11	g	2	NAG	O5-C5-C6-O6
11	0	2	NAG	O5-C5-C6-O6
10	I	3	BMA	C4-C5-C6-O6
10	b	3	BMA	C4-C5-C6-O6
10	x	3	BMA	C4-C5-C6-O6
11	K	1	NAG	C4-C5-C6-O6
11	V	2	NAG	C4-C5-C6-O6
11	f	1	NAG	C4-C5-C6-O6
11	p	2	NAG	C4-C5-C6-O6
11	z	1	NAG	C4-C5-C6-O6
11	CA	2	NAG	C4-C5-C6-O6
12	J	6	MAN	C4-C5-C6-O6
9	W	2	NAG	C4-C5-C6-O6
9	s	2	NAG	C4-C5-C6-O6
12	e	6	MAN	C4-C5-C6-O6
12	y	6	MAN	C4-C5-C6-O6
9	DA	2	NAG	C4-C5-C6-O6
9	B	1	NAG	O5-C5-C6-O6
9	X	1	NAG	O5-C5-C6-O6
9	t	1	NAG	O5-C5-C6-O6
11	O	2	NAG	C4-C5-C6-O6
11	g	2	NAG	C4-C5-C6-O6
11	0	2	NAG	C4-C5-C6-O6
9	B	2	NAG	C4-C5-C6-O6
9	X	2	NAG	C4-C5-C6-O6
9	t	2	NAG	C4-C5-C6-O6
12	J	2	NAG	O5-C5-C6-O6
12	e	2	NAG	O5-C5-C6-O6
12	y	2	NAG	O5-C5-C6-O6
12	J	2	NAG	C4-C5-C6-O6
12	e	2	NAG	C4-C5-C6-O6
12	y	2	NAG	C4-C5-C6-O6
14	U	1	NAG	C4-C5-C6-O6
14	o	1	NAG	C4-C5-C6-O6
14	BA	1	NAG	C4-C5-C6-O6
9	E	4	MAN	O5-C5-C6-O6
9	Y	4	MAN	O5-C5-C6-O6
9	u	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	P	3	BMA	O5-C5-C6-O6
10	i	3	BMA	O5-C5-C6-O6
10	l	3	BMA	O5-C5-C6-O6
9	E	1	NAG	O5-C5-C6-O6
9	Y	1	NAG	O5-C5-C6-O6
9	u	1	NAG	O5-C5-C6-O6
14	BA	7	MAN	O5-C5-C6-O6
14	U	7	MAN	O5-C5-C6-O6
14	o	7	MAN	O5-C5-C6-O6
9	B	3	BMA	C4-C5-C6-O6
9	X	3	BMA	C4-C5-C6-O6
9	t	3	BMA	C4-C5-C6-O6
14	BA	7	MAN	C4-C5-C6-O6
9	W	3	BMA	C4-C5-C6-O6
9	s	3	BMA	C4-C5-C6-O6
9	DA	3	BMA	C4-C5-C6-O6
14	U	7	MAN	C4-C5-C6-O6
14	o	7	MAN	C4-C5-C6-O6
14	BA	8	MAN	C4-C5-C6-O6
14	U	8	MAN	C4-C5-C6-O6
14	o	8	MAN	C4-C5-C6-O6
11	O	1	NAG	O5-C5-C6-O6
11	g	1	NAG	O5-C5-C6-O6
11	0	1	NAG	O5-C5-C6-O6
11	V	1	NAG	O5-C5-C6-O6
11	p	1	NAG	O5-C5-C6-O6
11	CA	1	NAG	O5-C5-C6-O6
9	s	3	BMA	O5-C5-C6-O6
9	DA	3	BMA	O5-C5-C6-O6
9	W	3	BMA	O5-C5-C6-O6
9	B	4	MAN	O5-C5-C6-O6
9	t	4	MAN	O5-C5-C6-O6
9	X	4	MAN	O5-C5-C6-O6
9	X	4	MAN	C4-C5-C6-O6
9	B	4	MAN	C4-C5-C6-O6
9	t	4	MAN	C4-C5-C6-O6
12	y	1	NAG	C4-C5-C6-O6
12	J	1	NAG	C4-C5-C6-O6
12	e	1	NAG	C4-C5-C6-O6
12	y	3	BMA	C4-C5-C6-O6
12	e	3	BMA	C4-C5-C6-O6
12	J	3	BMA	C4-C5-C6-O6

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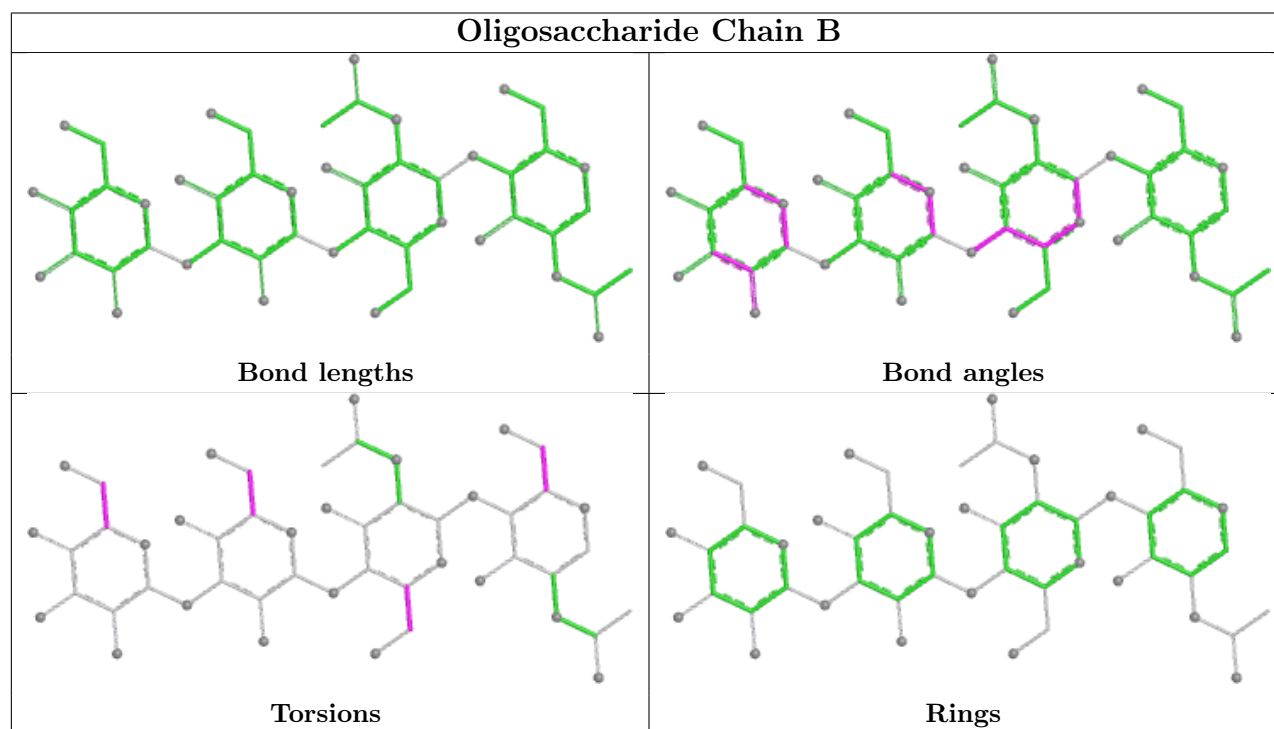
Mol	Chain	Res	Type	Atoms
9	E	2	NAG	C4-C5-C6-O6
9	Y	2	NAG	C4-C5-C6-O6
9	u	2	NAG	C4-C5-C6-O6
9	X	3	BMA	O5-C5-C6-O6
9	B	1	NAG	C4-C5-C6-O6
9	X	1	NAG	C4-C5-C6-O6
9	t	1	NAG	C4-C5-C6-O6
14	U	5	MAN	C4-C5-C6-O6
9	B	3	BMA	O5-C5-C6-O6
9	t	3	BMA	O5-C5-C6-O6
14	o	5	MAN	C4-C5-C6-O6
14	BA	5	MAN	C4-C5-C6-O6
14	U	4	MAN	C4-C5-C6-O6
14	BA	4	MAN	C4-C5-C6-O6
9	E	2	NAG	O5-C5-C6-O6
9	Y	2	NAG	O5-C5-C6-O6
9	u	2	NAG	O5-C5-C6-O6
14	o	4	MAN	C4-C5-C6-O6
14	U	2	NAG	C3-C2-N2-C7
14	o	2	NAG	C3-C2-N2-C7
14	BA	2	NAG	C3-C2-N2-C7
12	J	3	BMA	O5-C5-C6-O6
12	e	3	BMA	O5-C5-C6-O6
12	y	3	BMA	O5-C5-C6-O6
12	y	1	NAG	O5-C5-C6-O6
12	e	1	NAG	O5-C5-C6-O6
12	J	1	NAG	O5-C5-C6-O6
10	F	1	NAG	C1-C2-N2-C7
10	Z	1	NAG	C1-C2-N2-C7
10	v	1	NAG	C1-C2-N2-C7
11	V	1	NAG	C1-C2-N2-C7
11	p	1	NAG	C1-C2-N2-C7
11	CA	1	NAG	C1-C2-N2-C7
14	U	2	NAG	C1-C2-N2-C7
14	o	2	NAG	C1-C2-N2-C7
14	BA	2	NAG	C1-C2-N2-C7
10	F	1	NAG	C3-C2-N2-C7
10	Z	1	NAG	C3-C2-N2-C7
10	v	1	NAG	C3-C2-N2-C7
11	V	1	NAG	C3-C2-N2-C7
11	p	1	NAG	C3-C2-N2-C7
11	CA	1	NAG	C3-C2-N2-C7

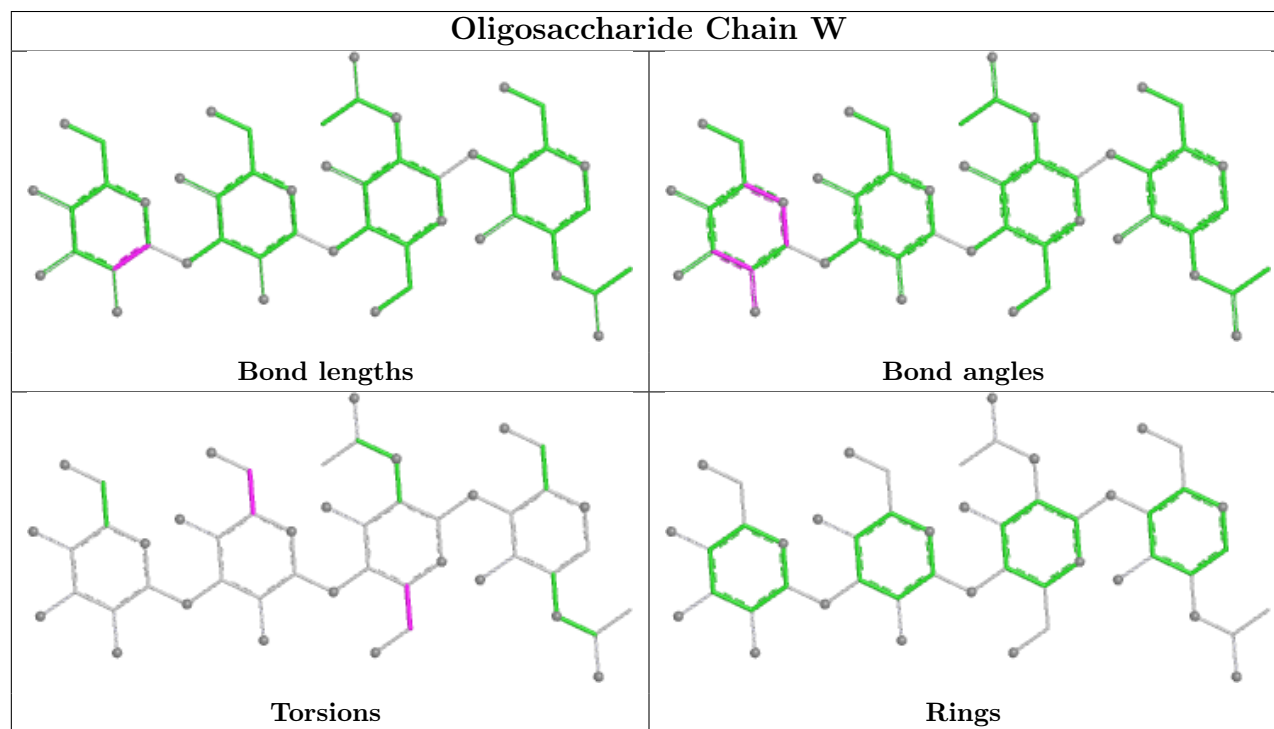
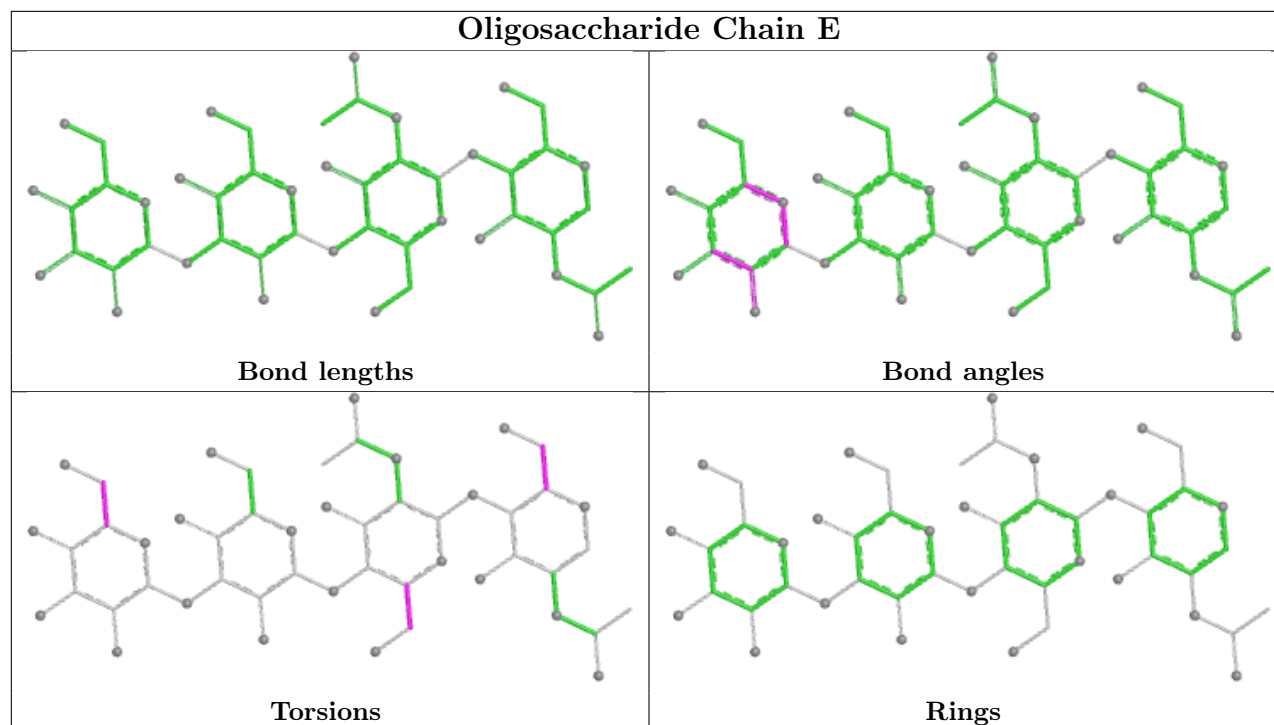
There are no ring outliers.

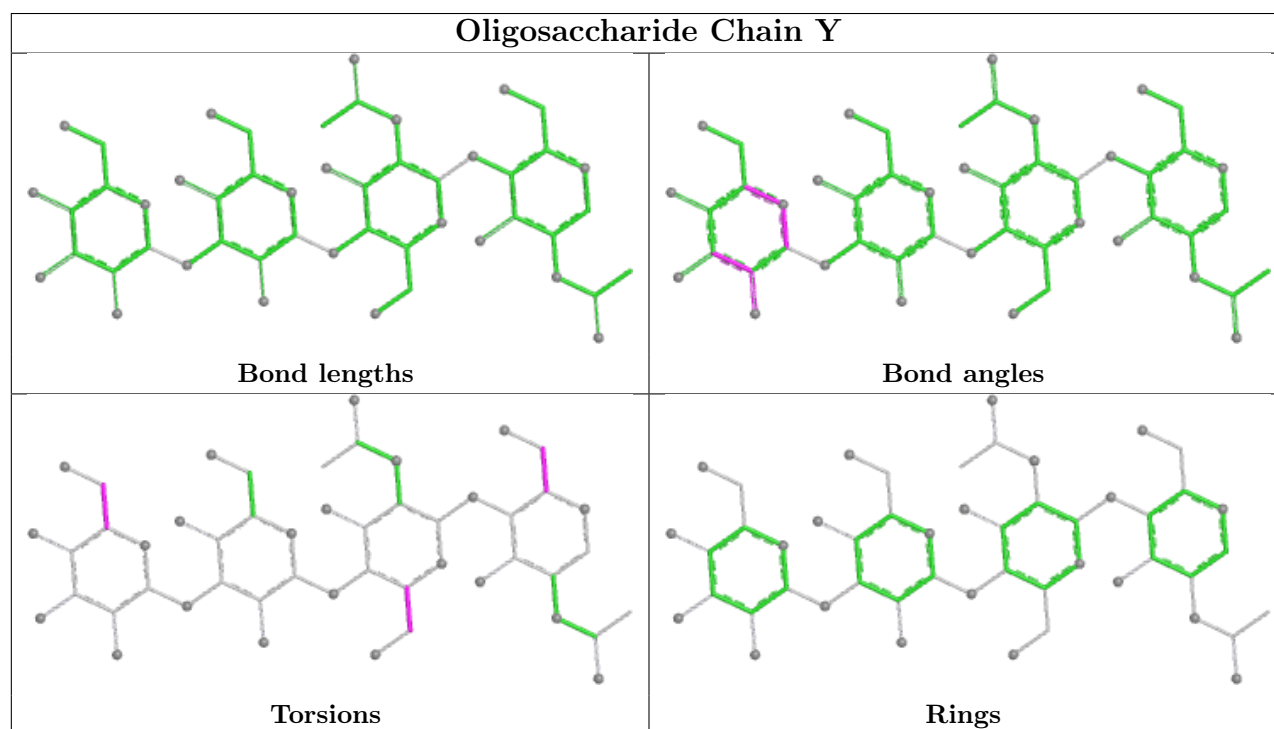
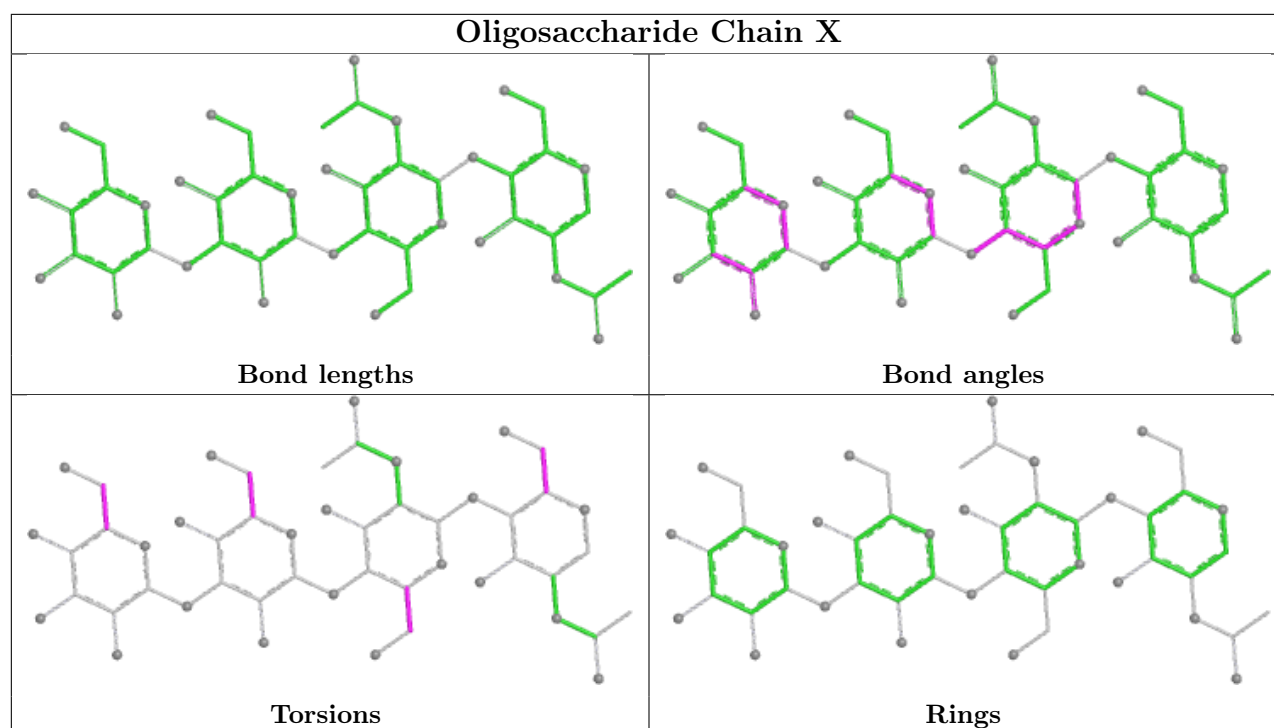
19 monomers are involved in 32 short contacts:

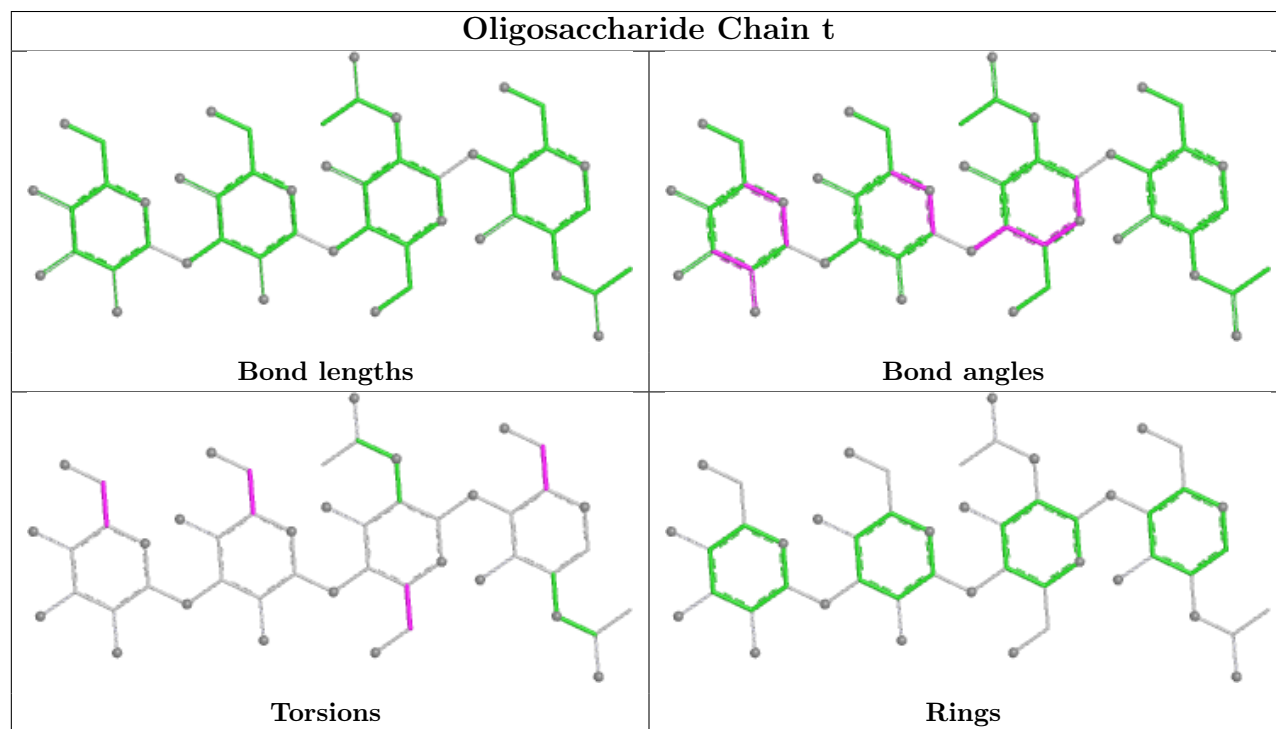
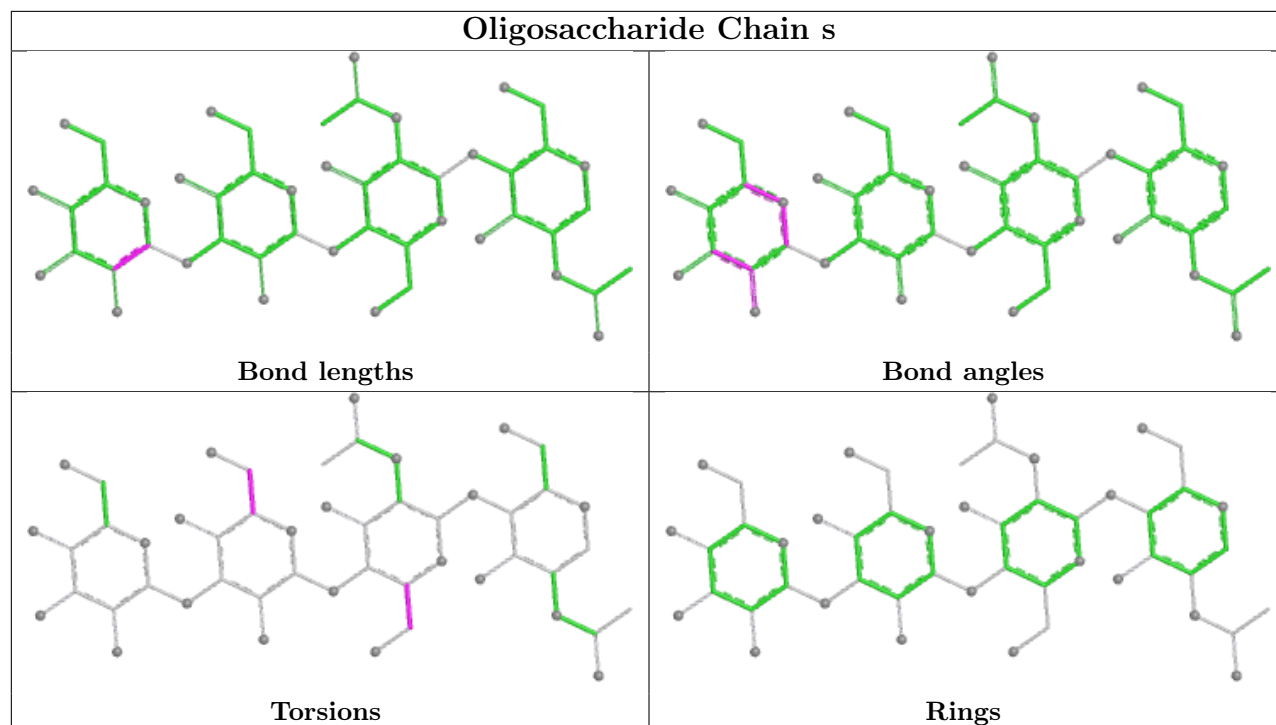
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	CA	1	NAG	1	0
10	I	1	NAG	1	0
11	K	1	NAG	6	0
11	V	1	NAG	1	0
11	AA	1	NAG	1	0
11	f	1	NAG	6	0
13	S	1	NAG	1	0
11	T	1	NAG	1	0
11	k	1	NAG	1	0
10	b	1	NAG	1	0
9	E	1	NAG	1	0
14	o	5	MAN	1	0
13	9	1	NAG	1	0
14	BA	5	MAN	1	0
13	j	1	NAG	1	0
11	p	1	NAG	1	0
10	x	1	NAG	1	0
14	U	5	MAN	2	0
11	z	1	NAG	6	0

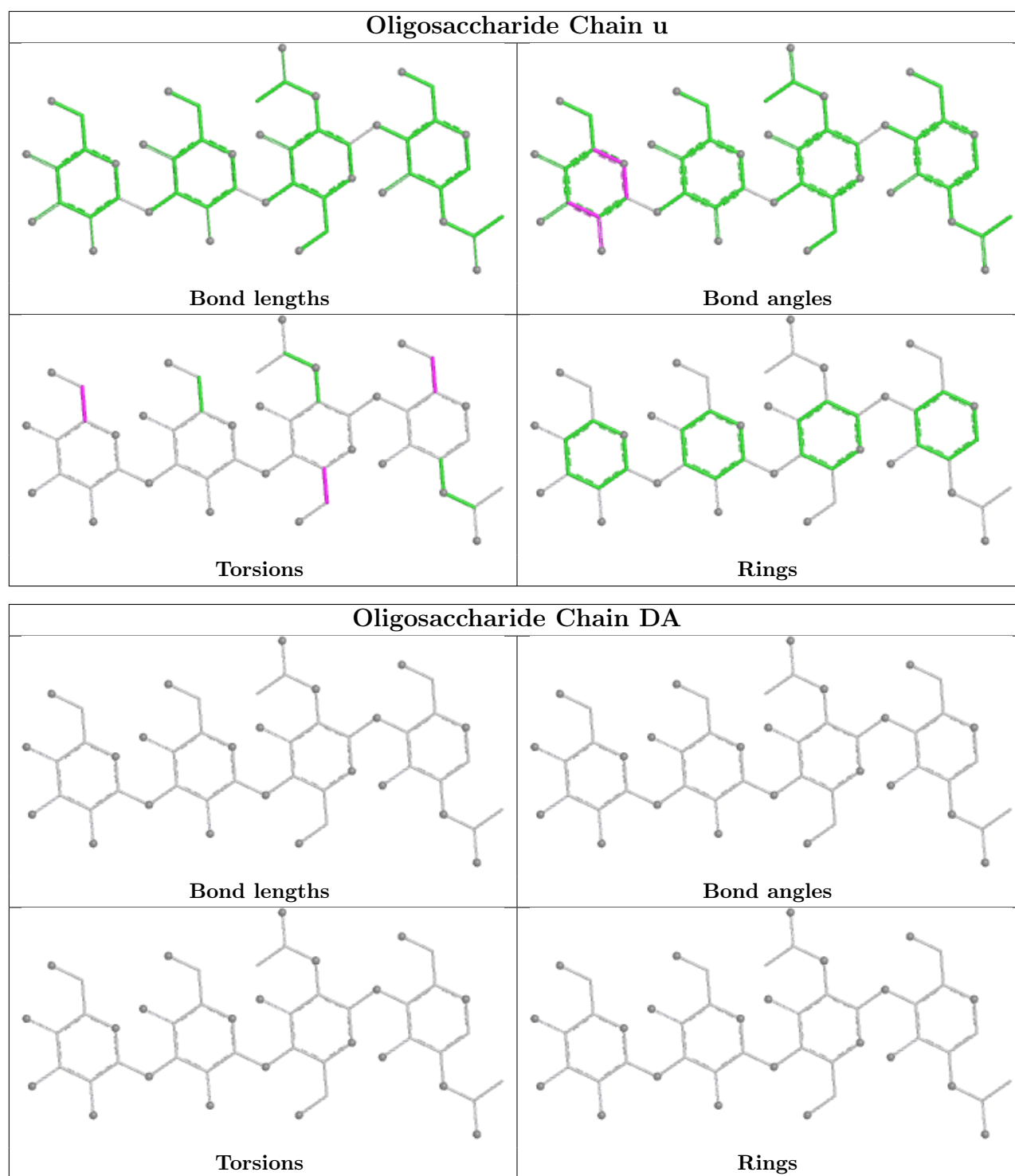
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

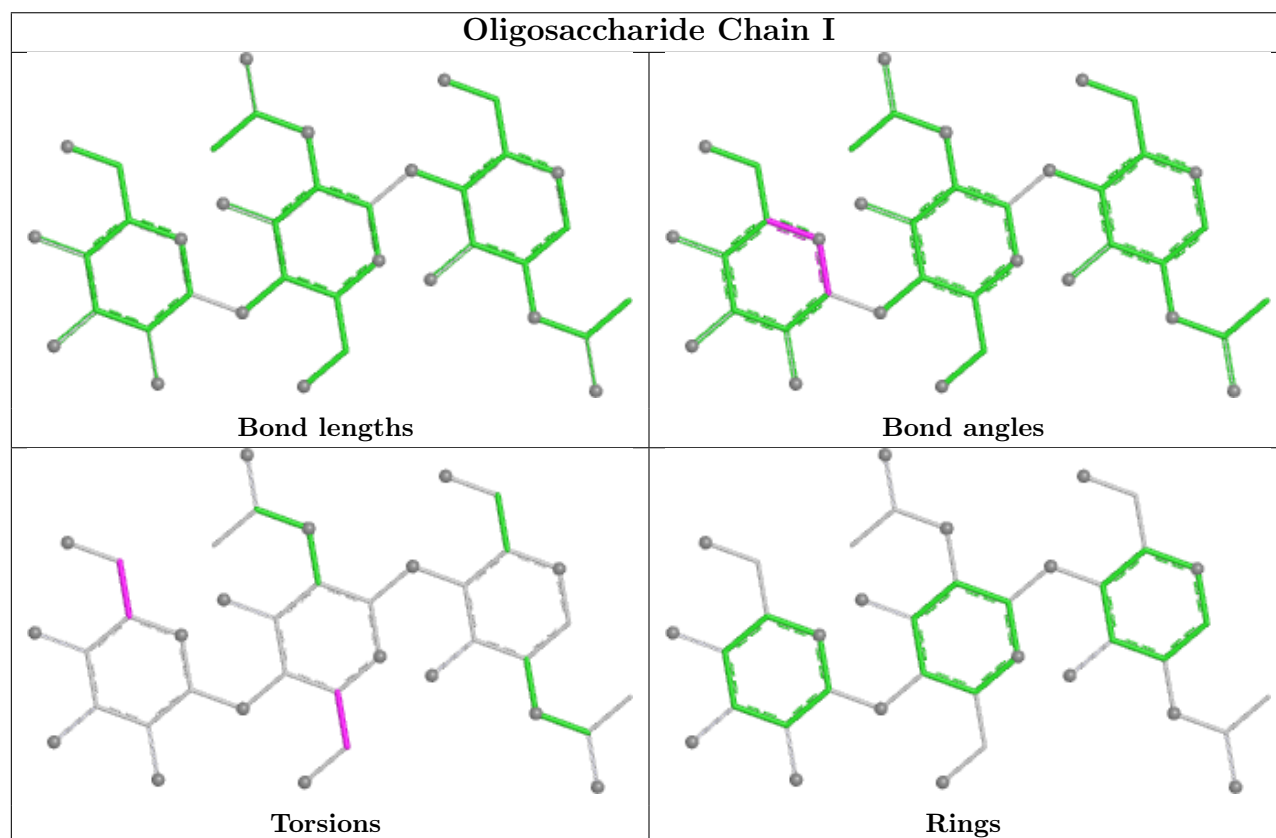
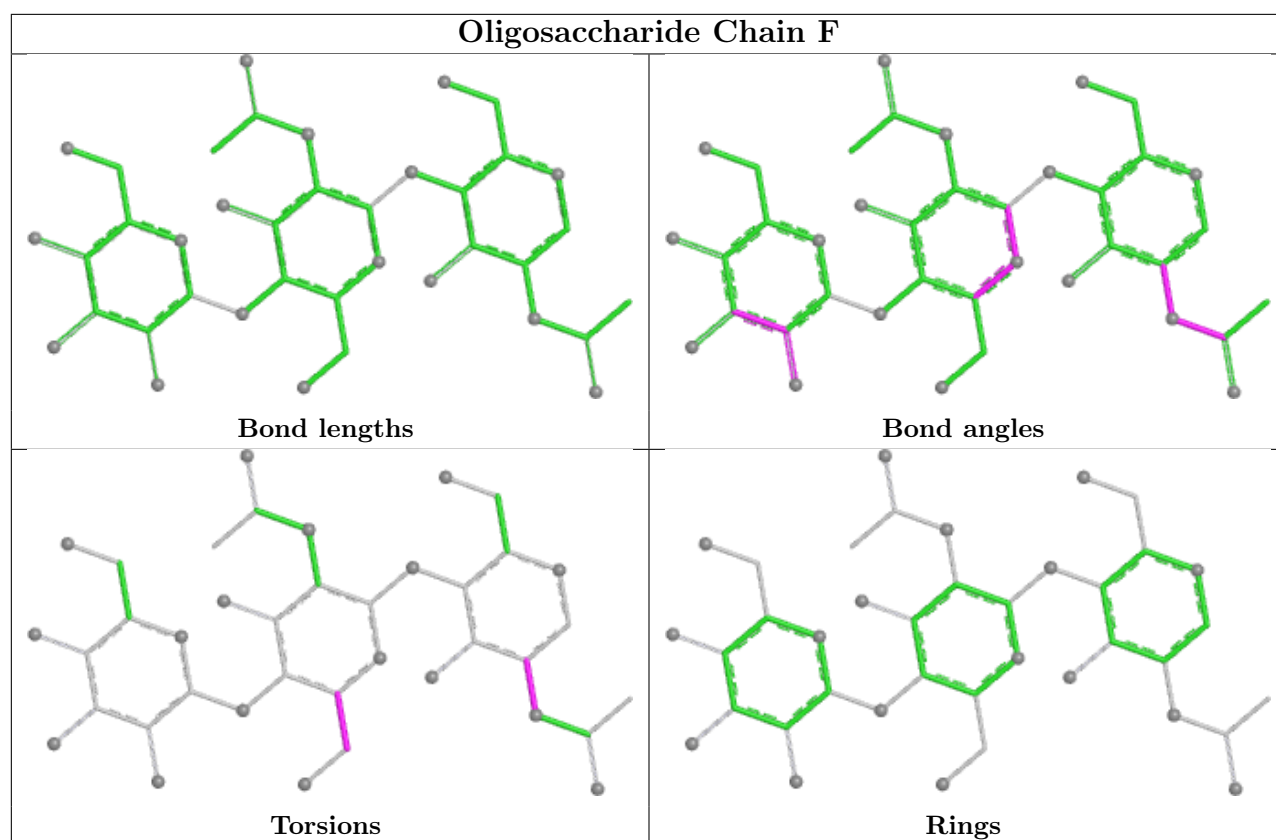


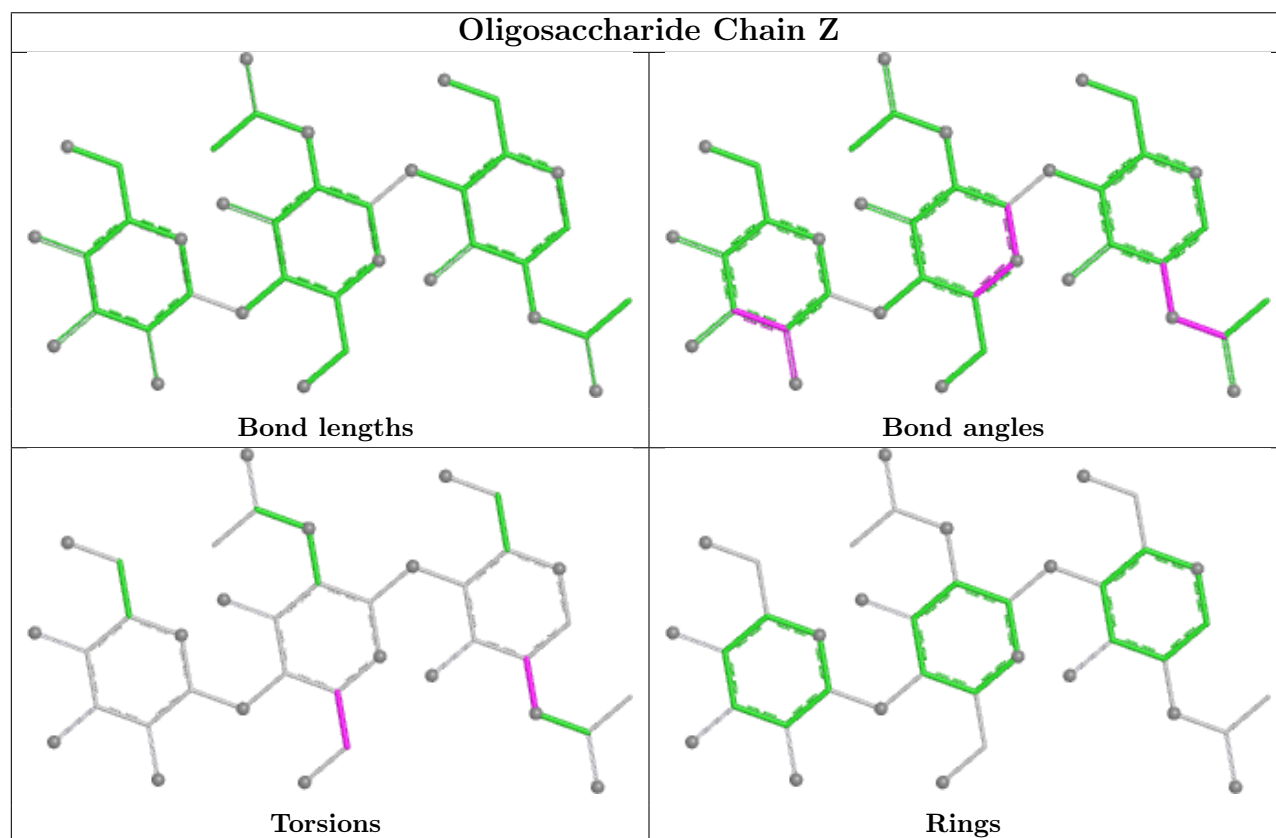
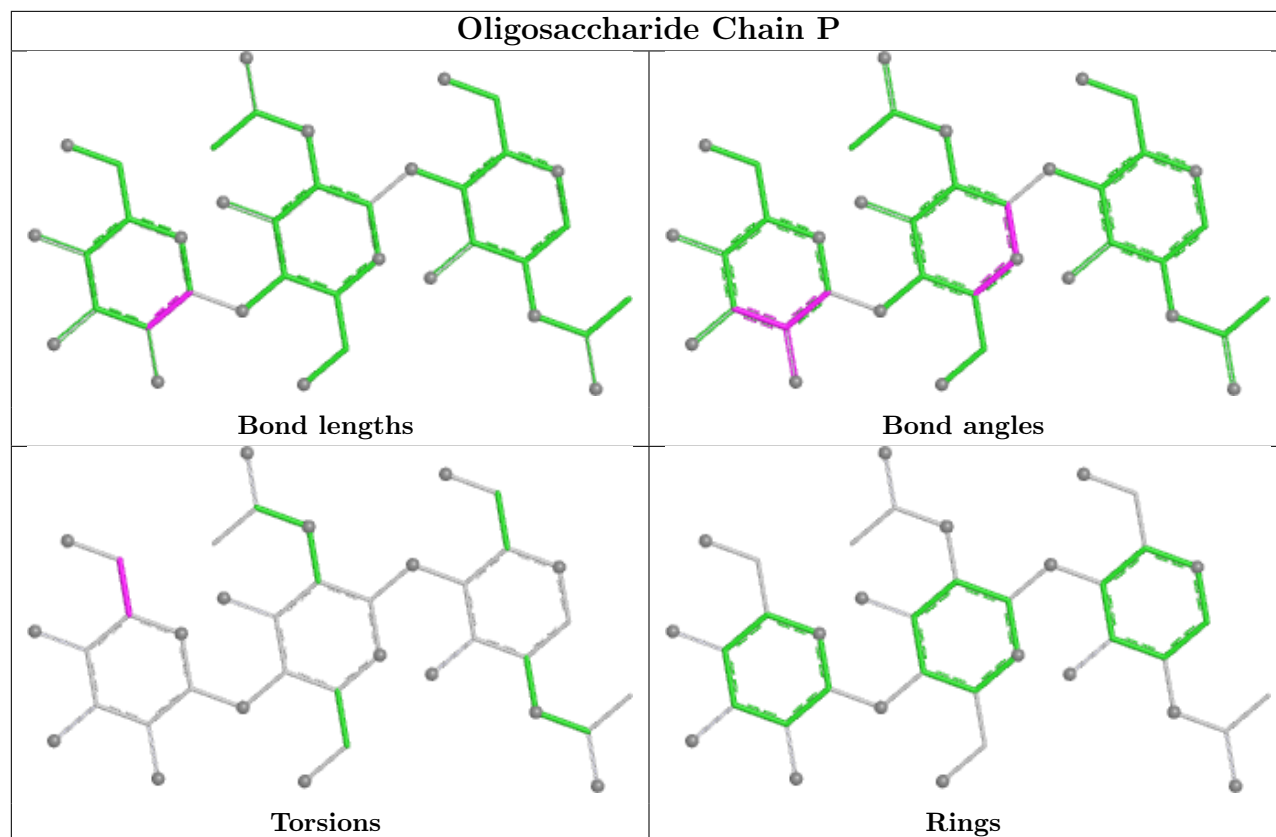


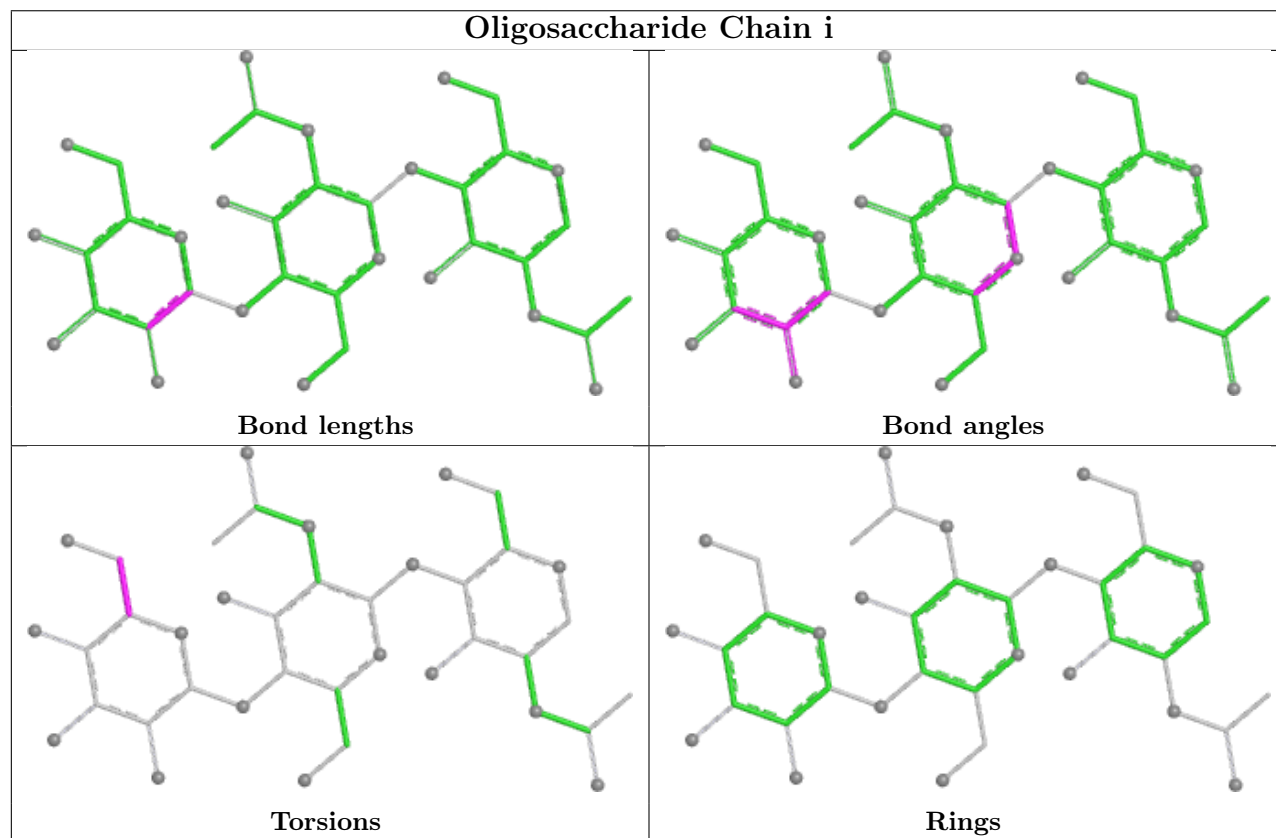
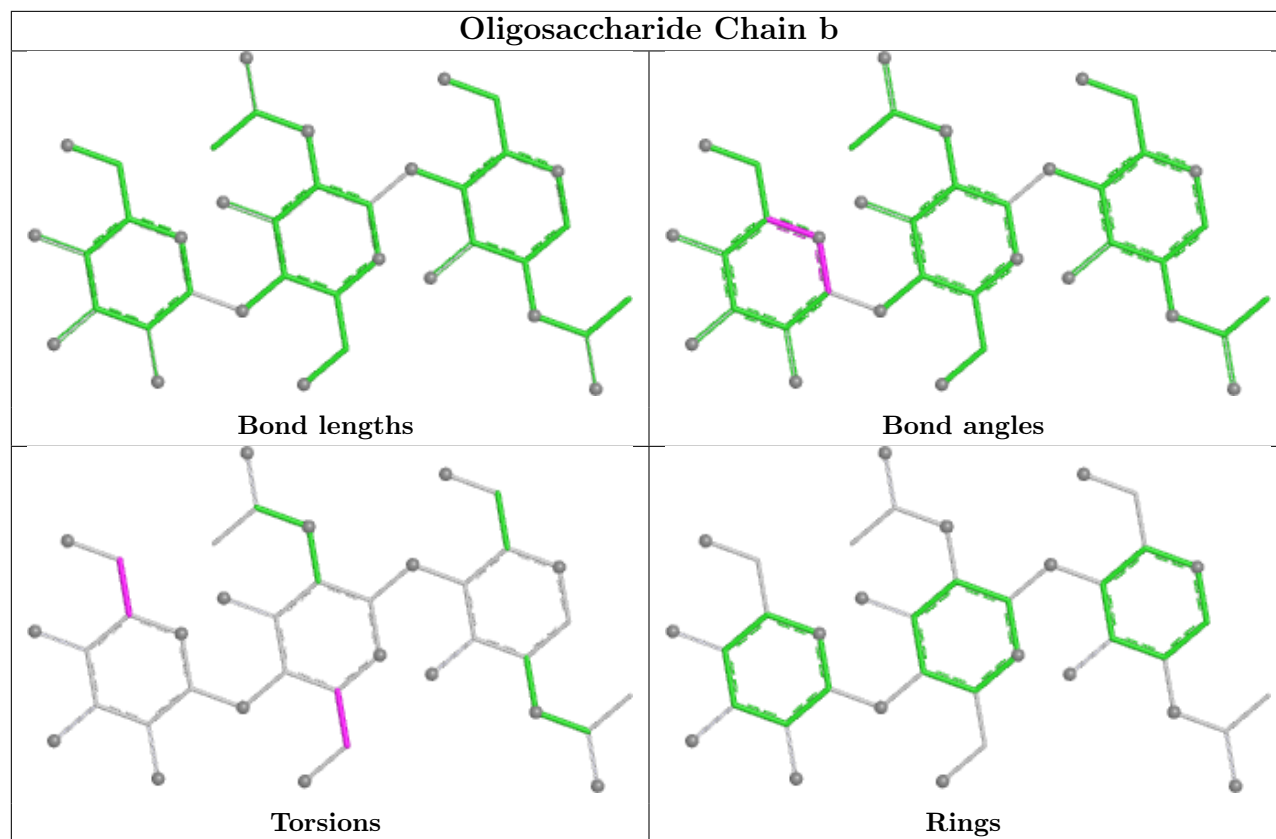


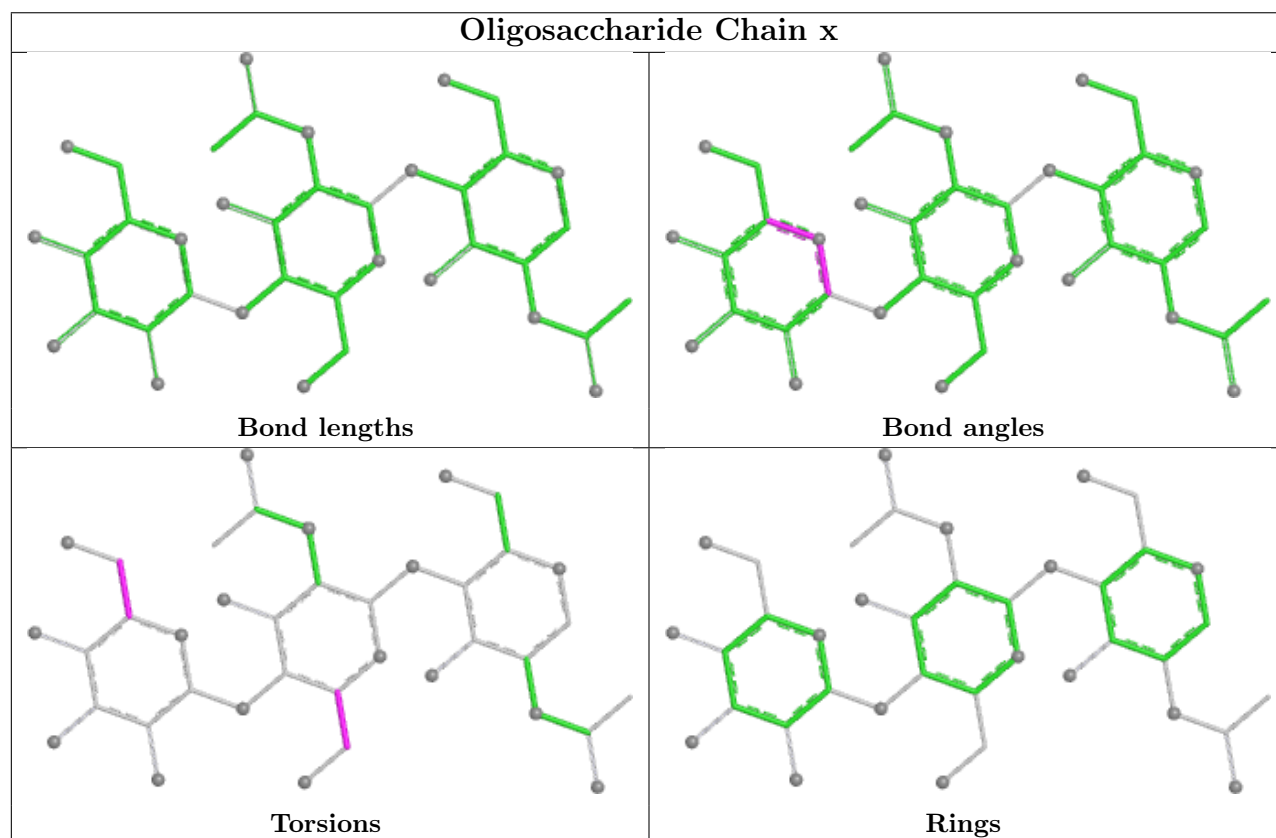
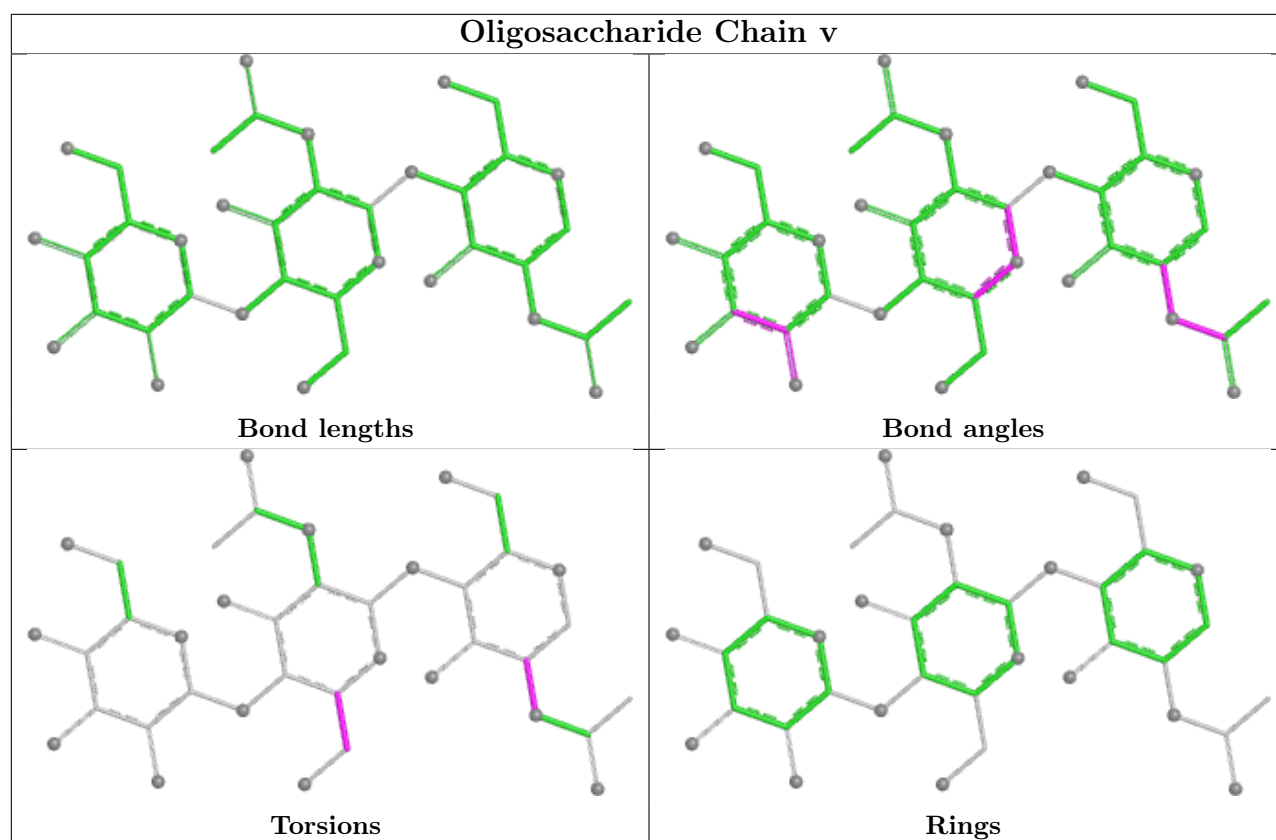


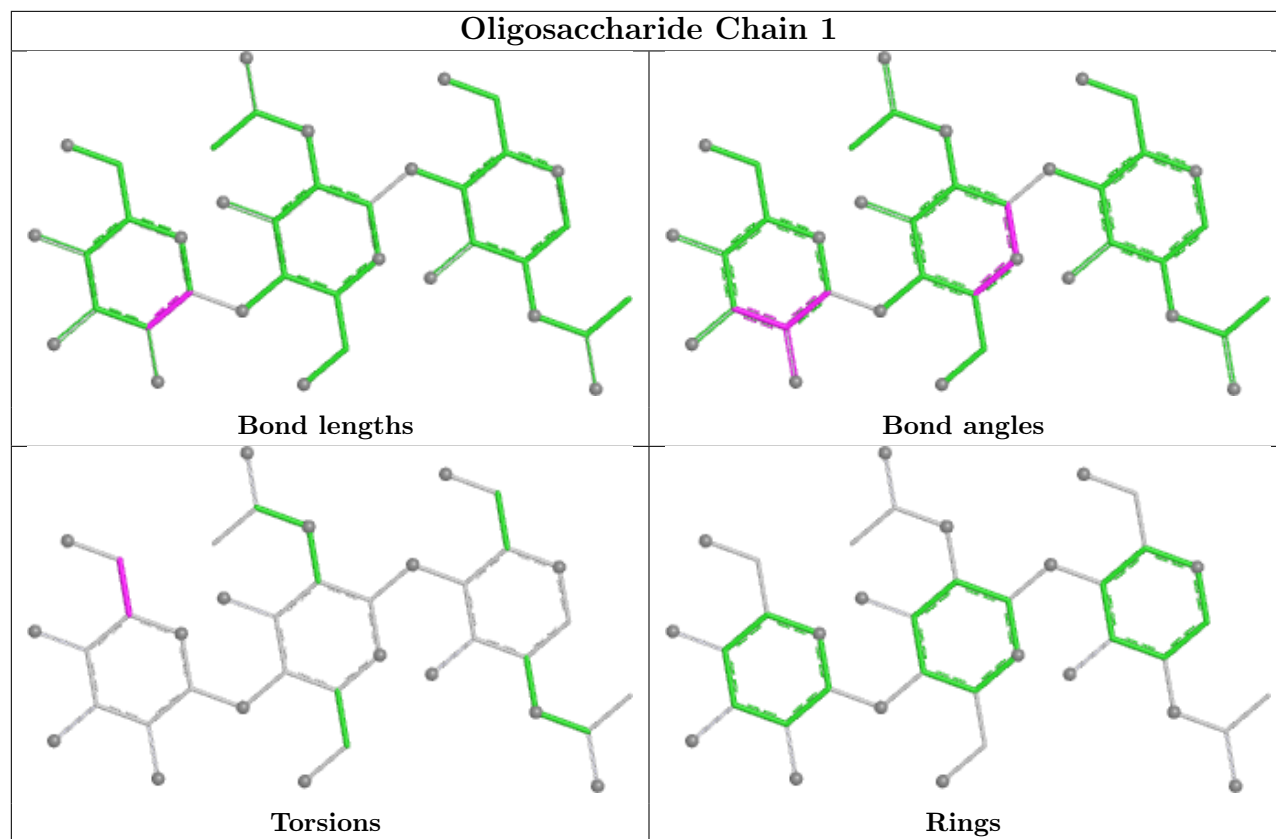


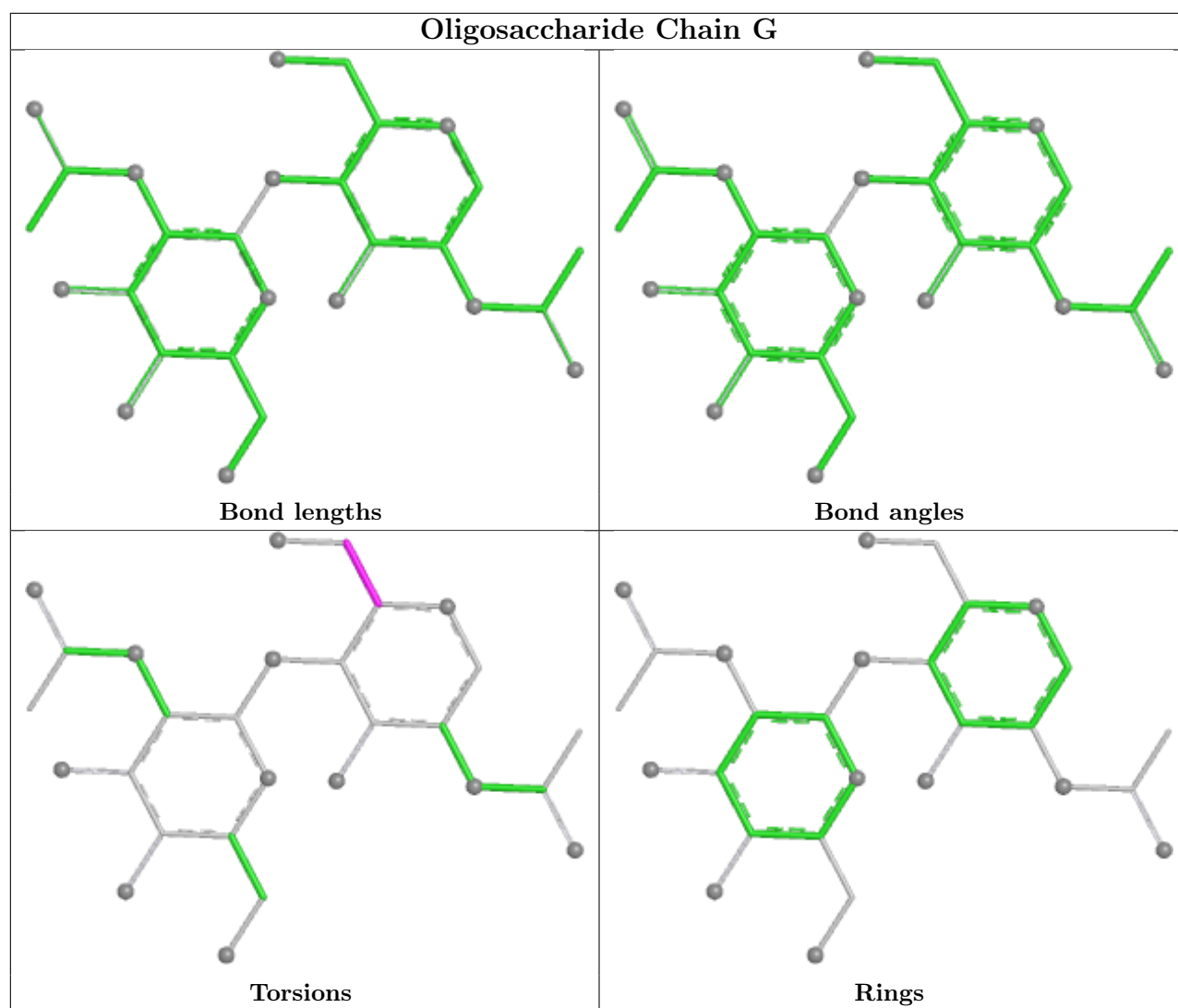


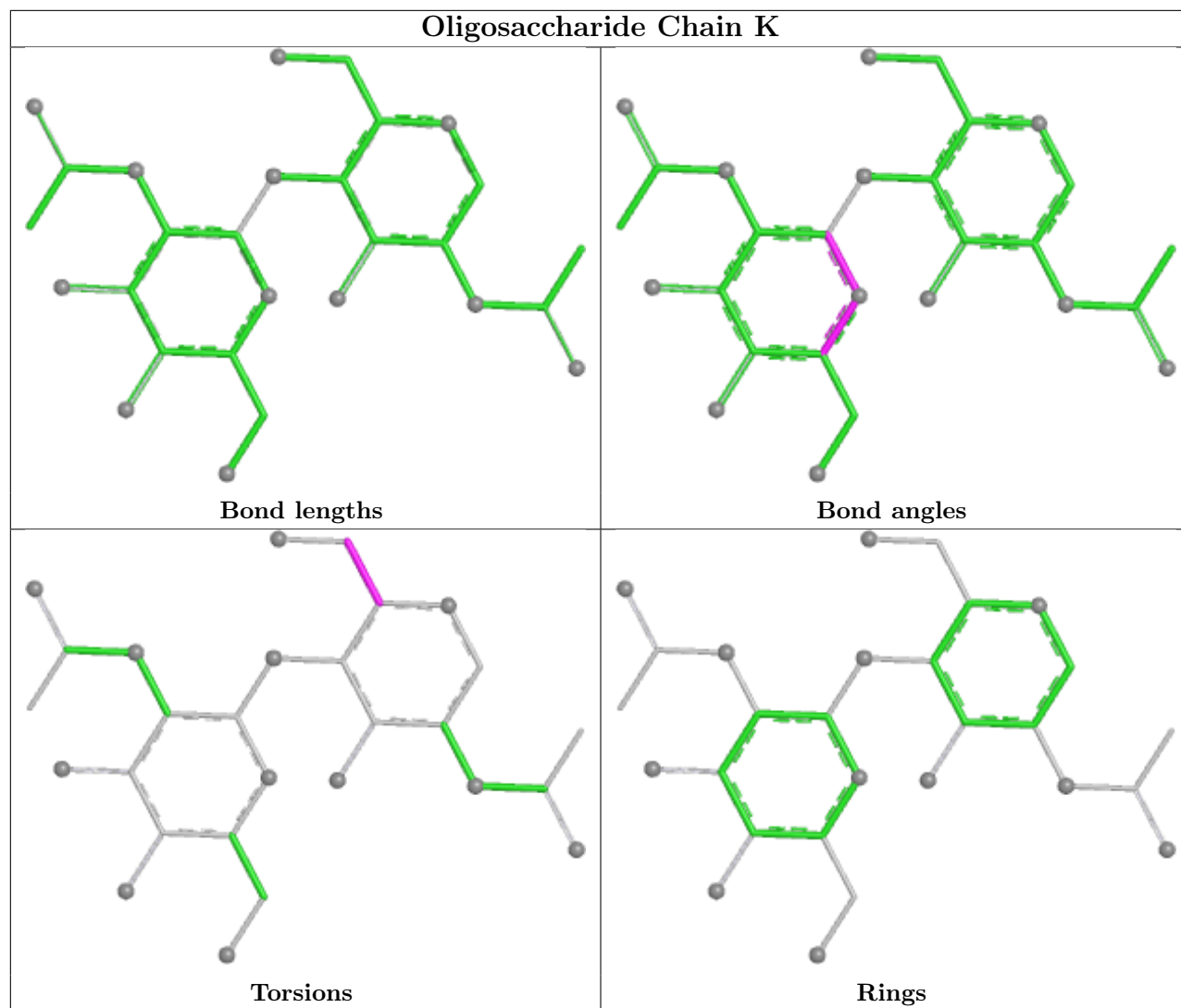


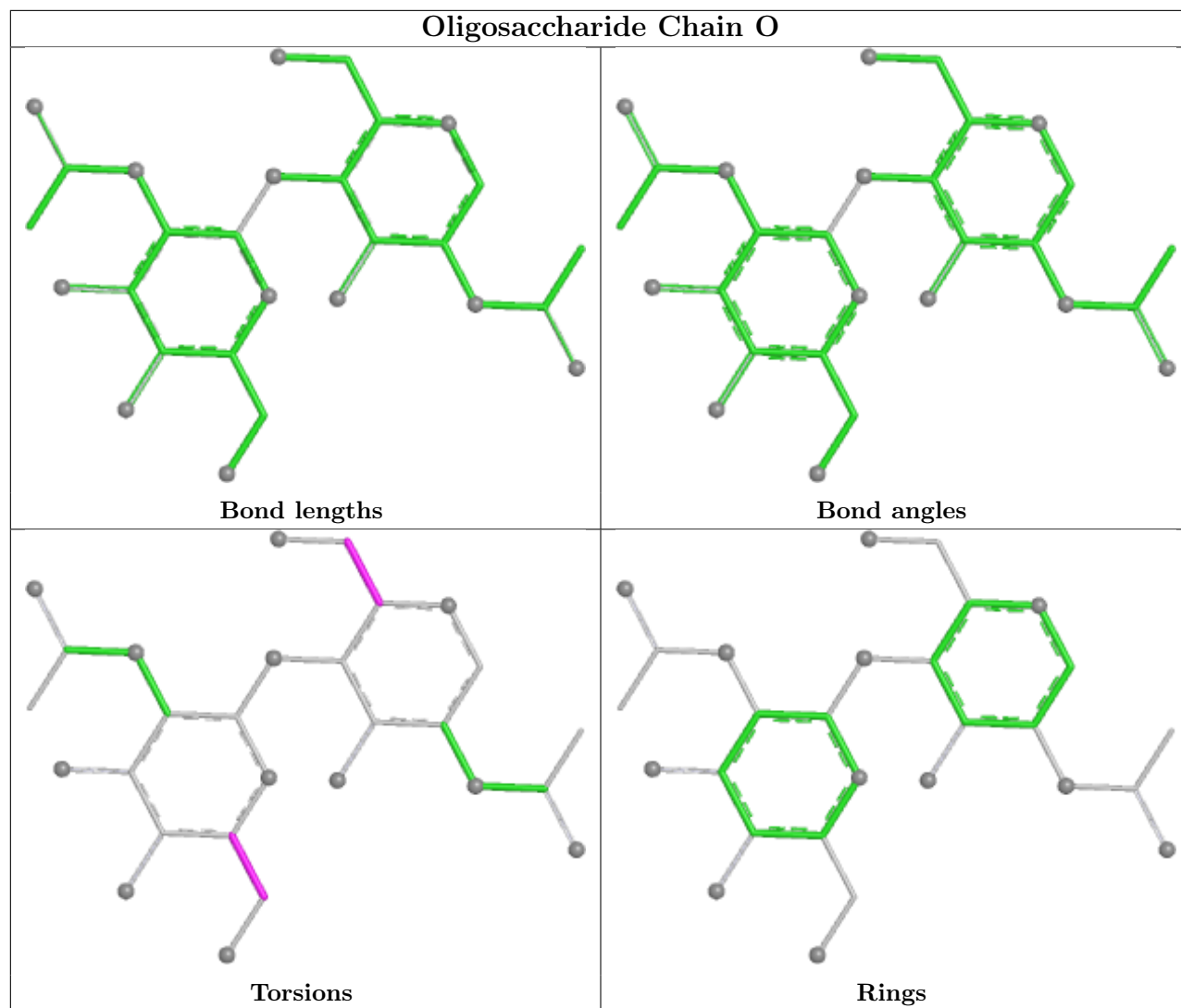


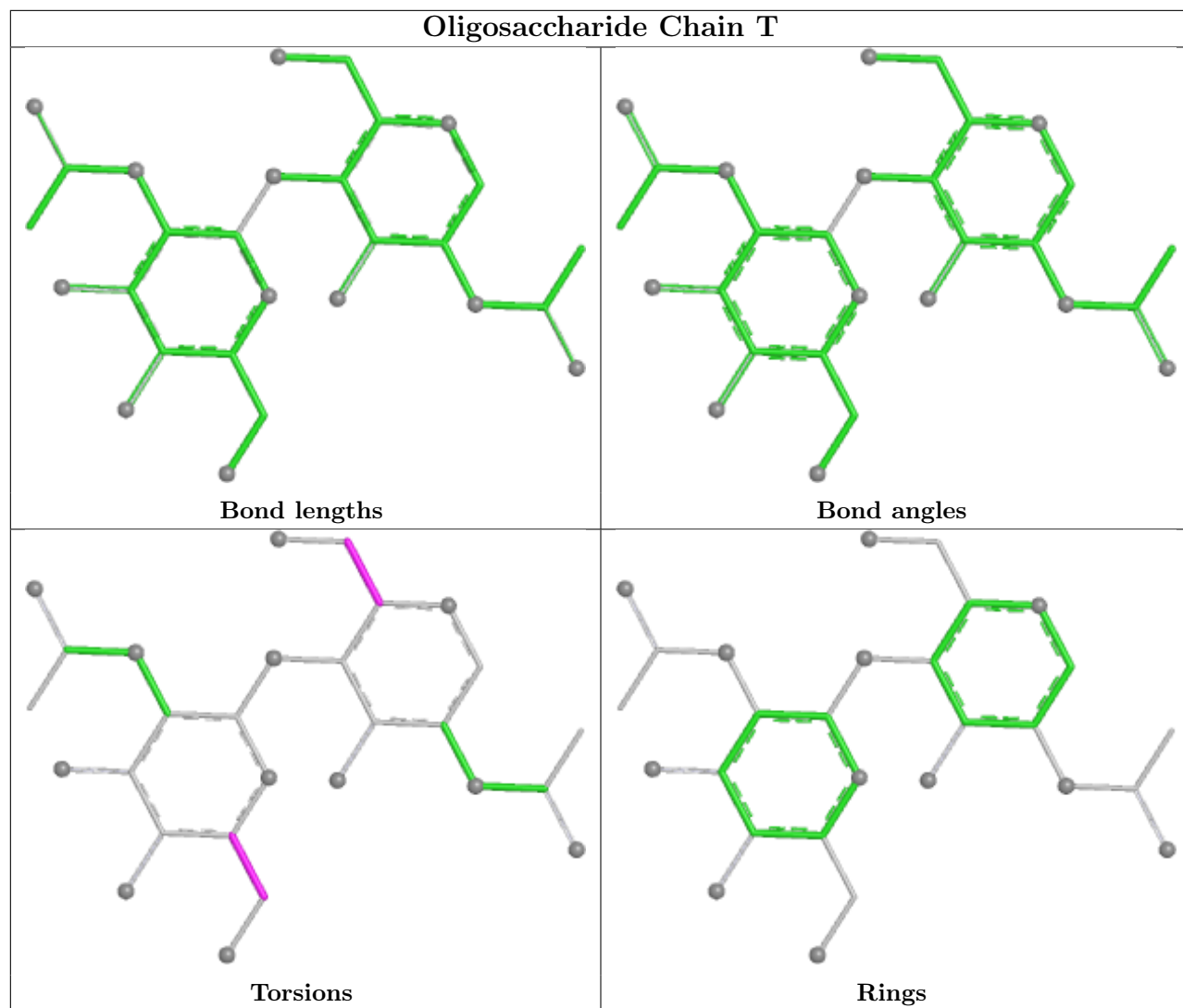


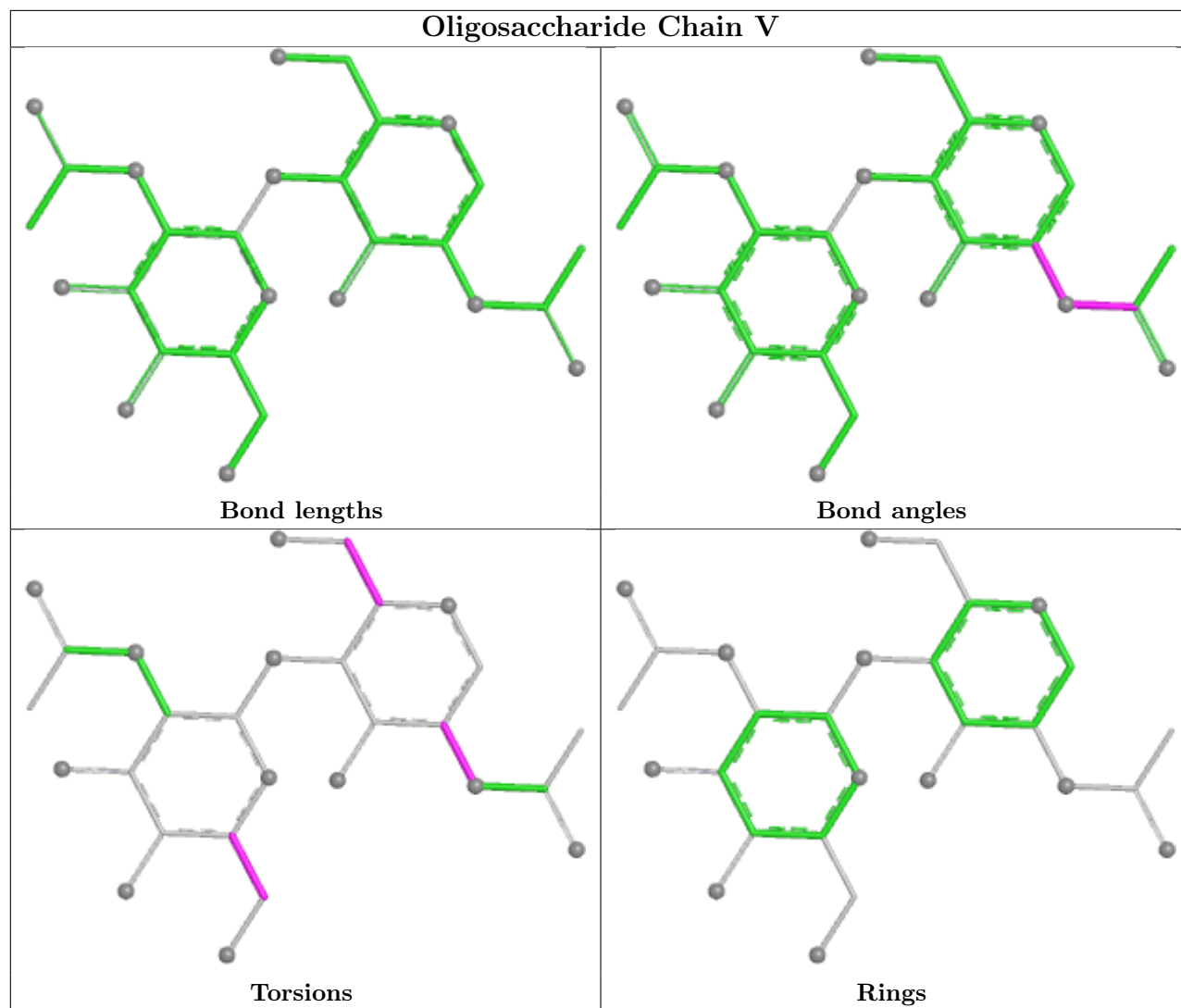


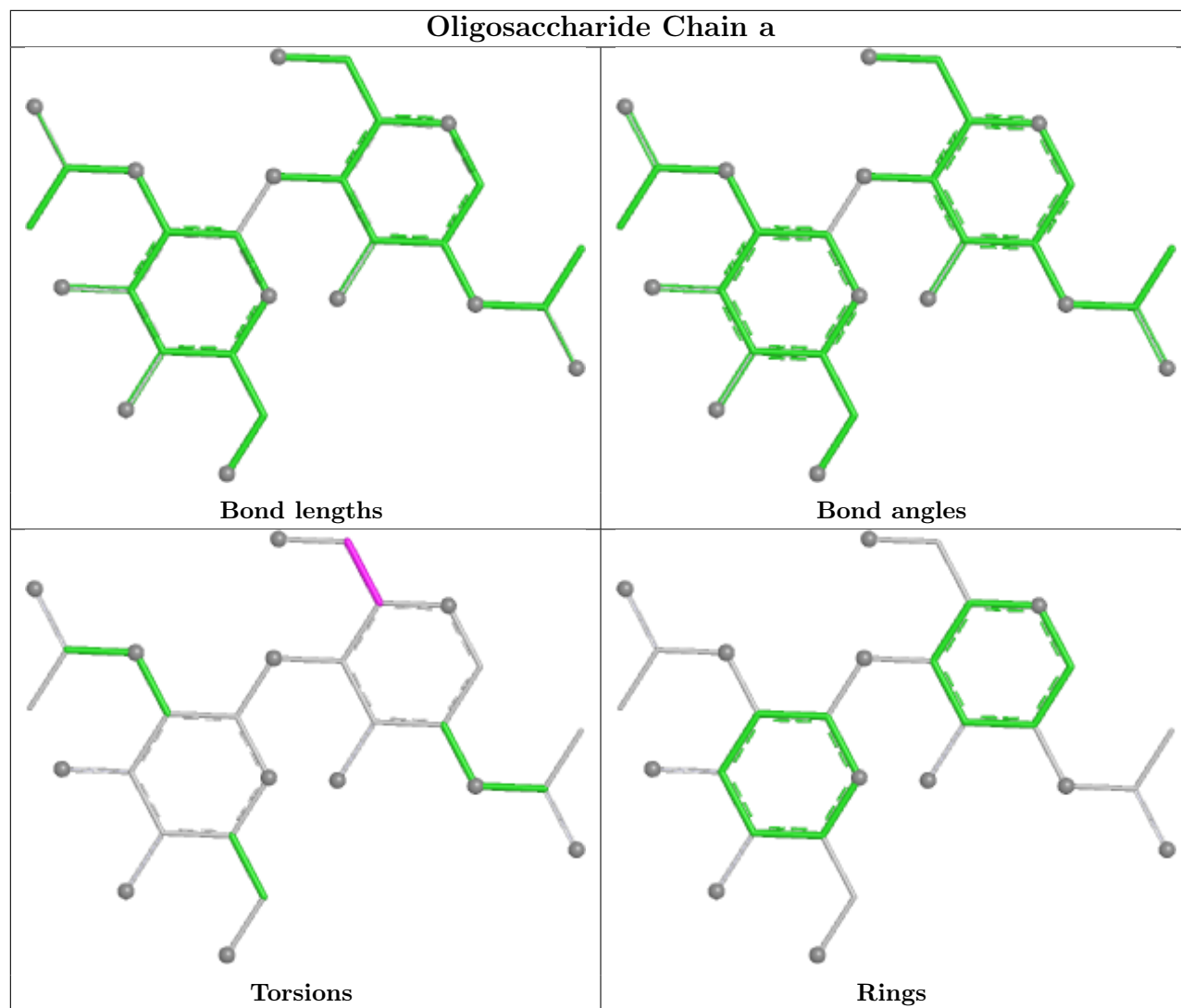


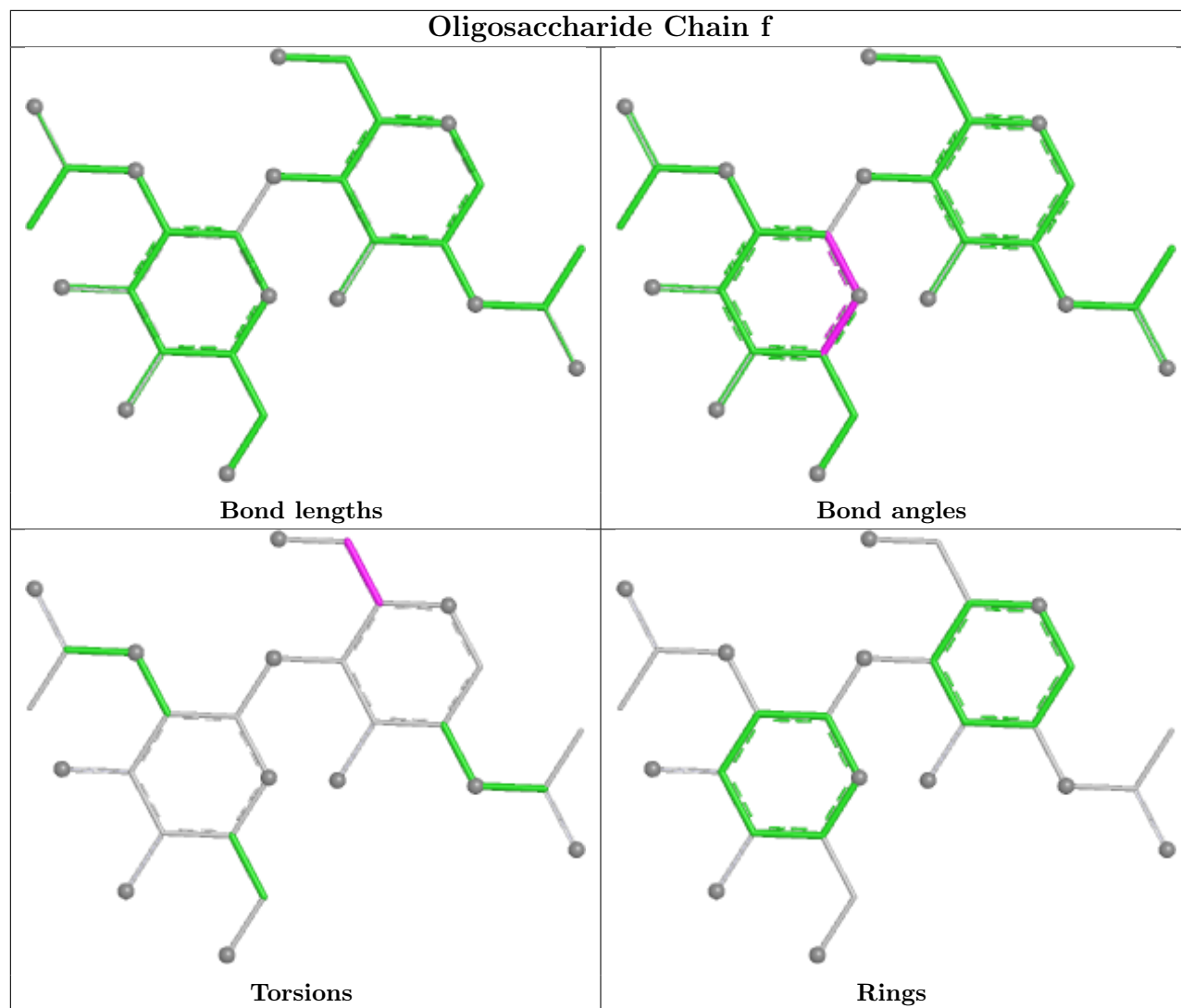


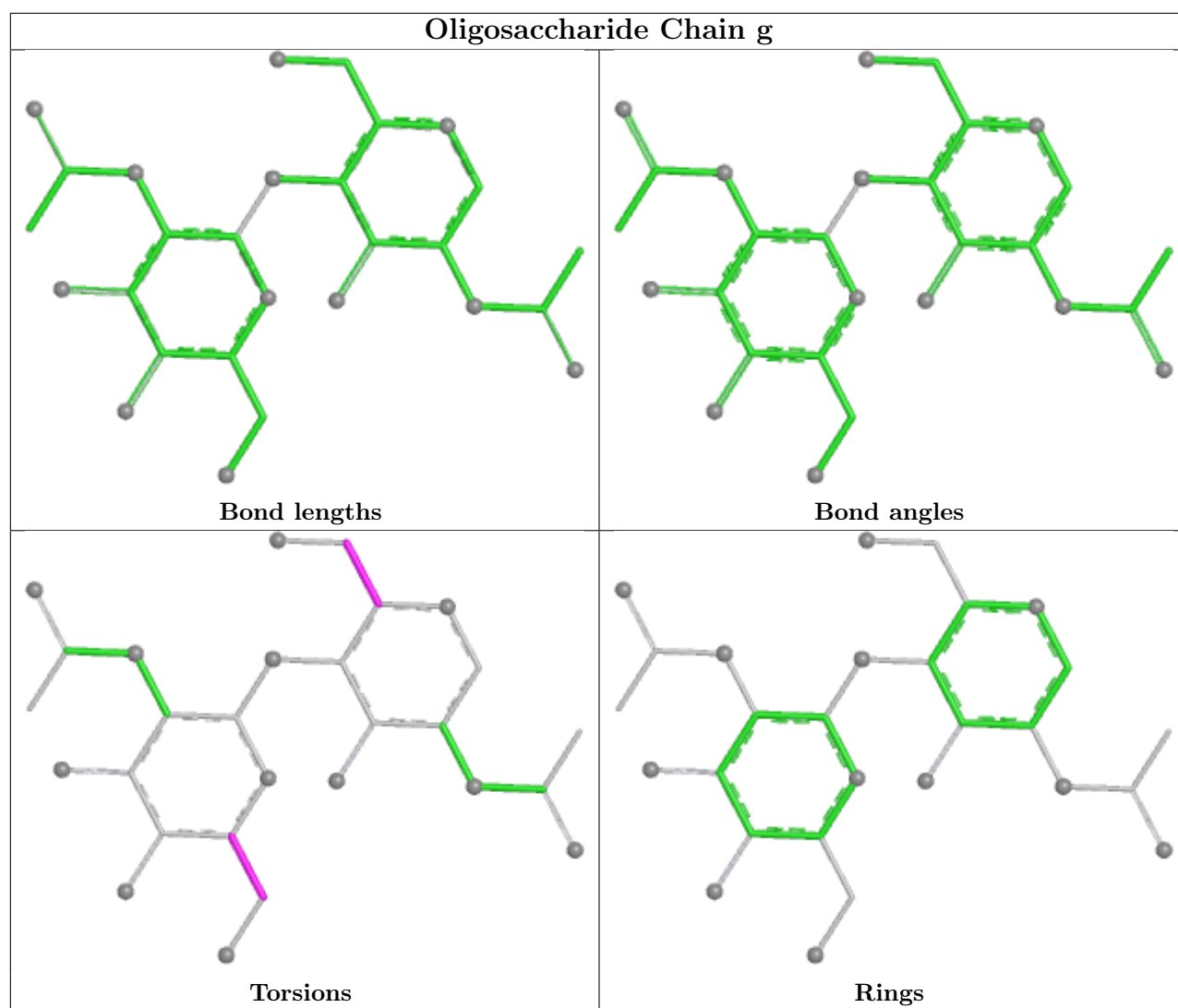


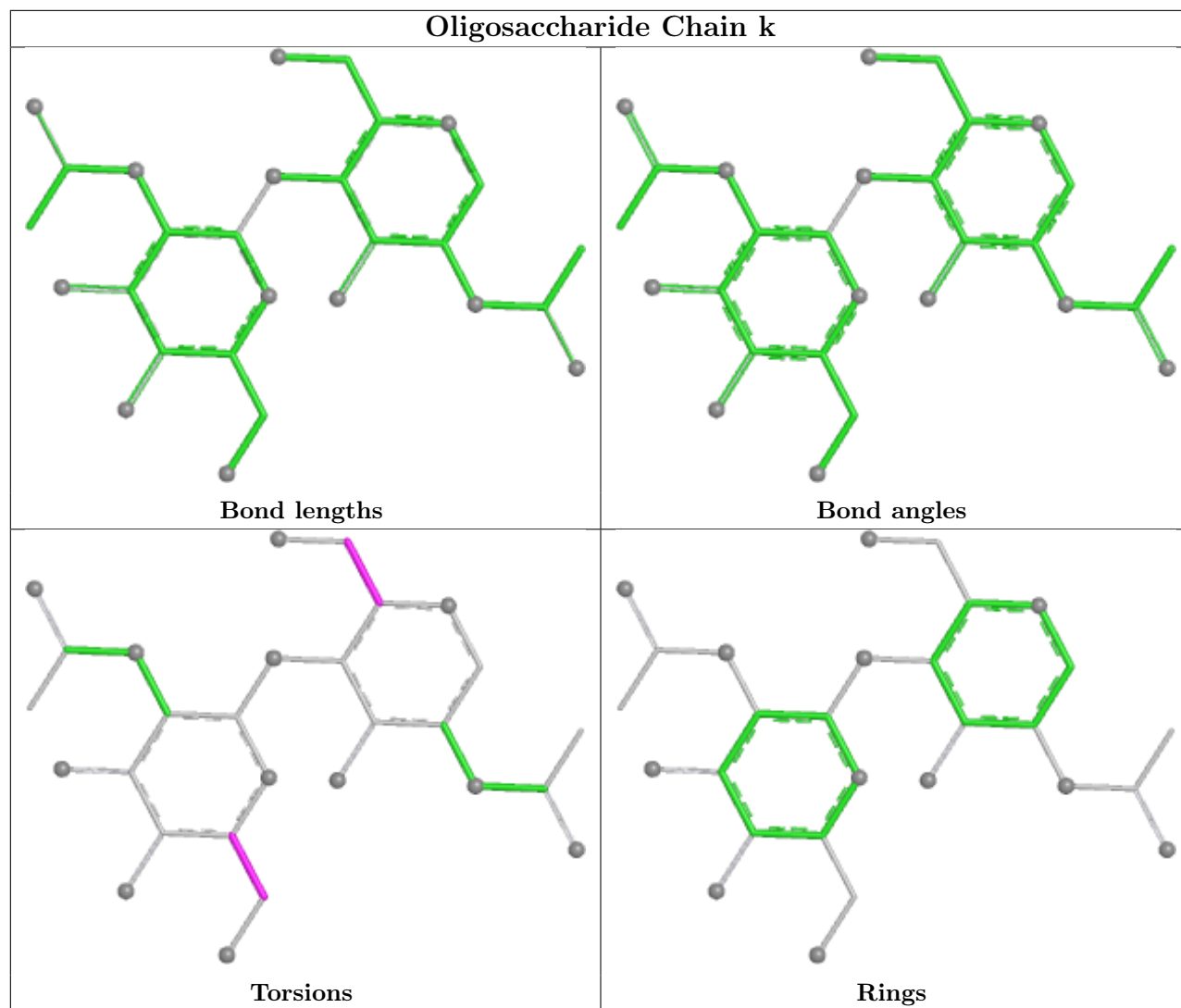


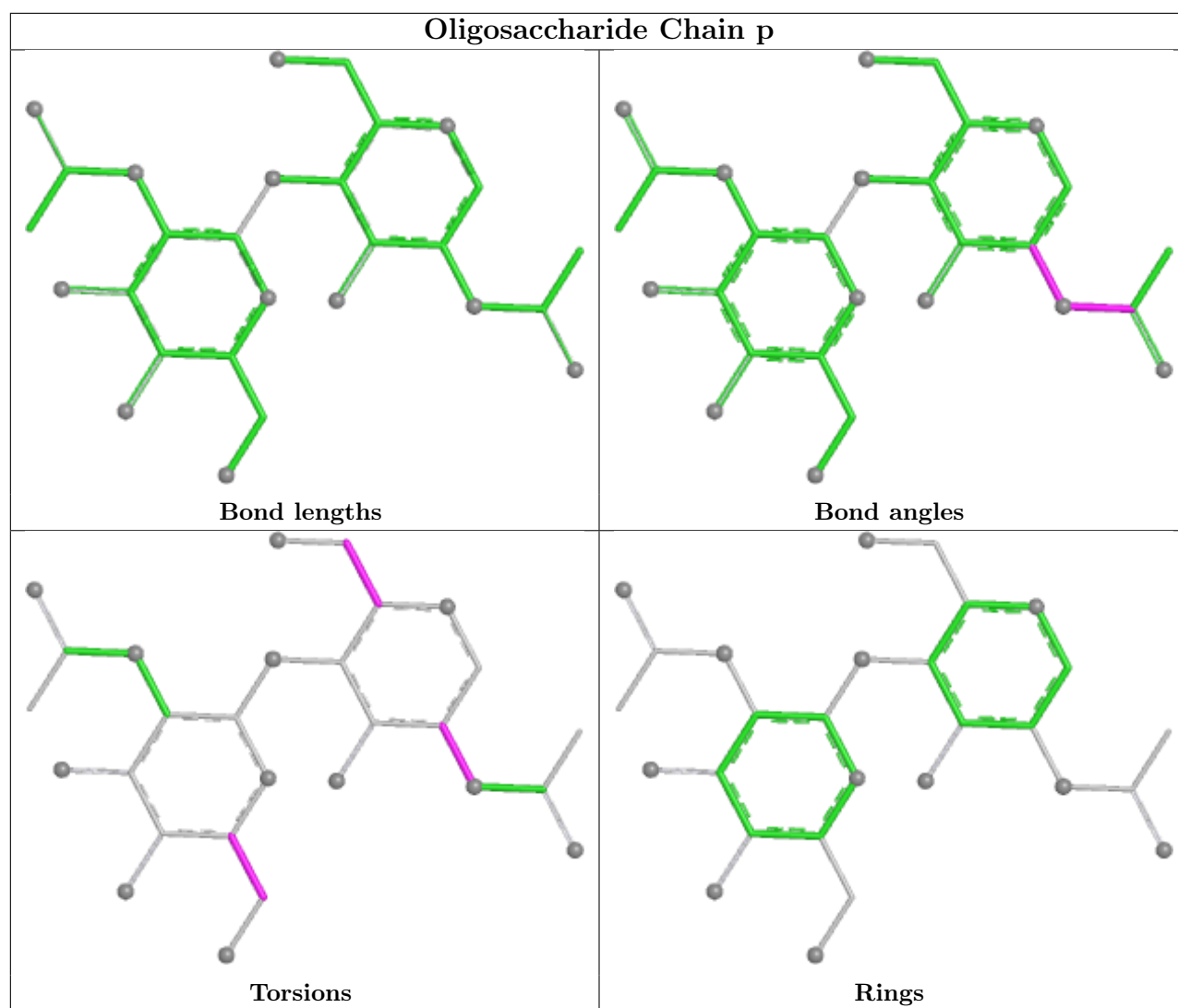


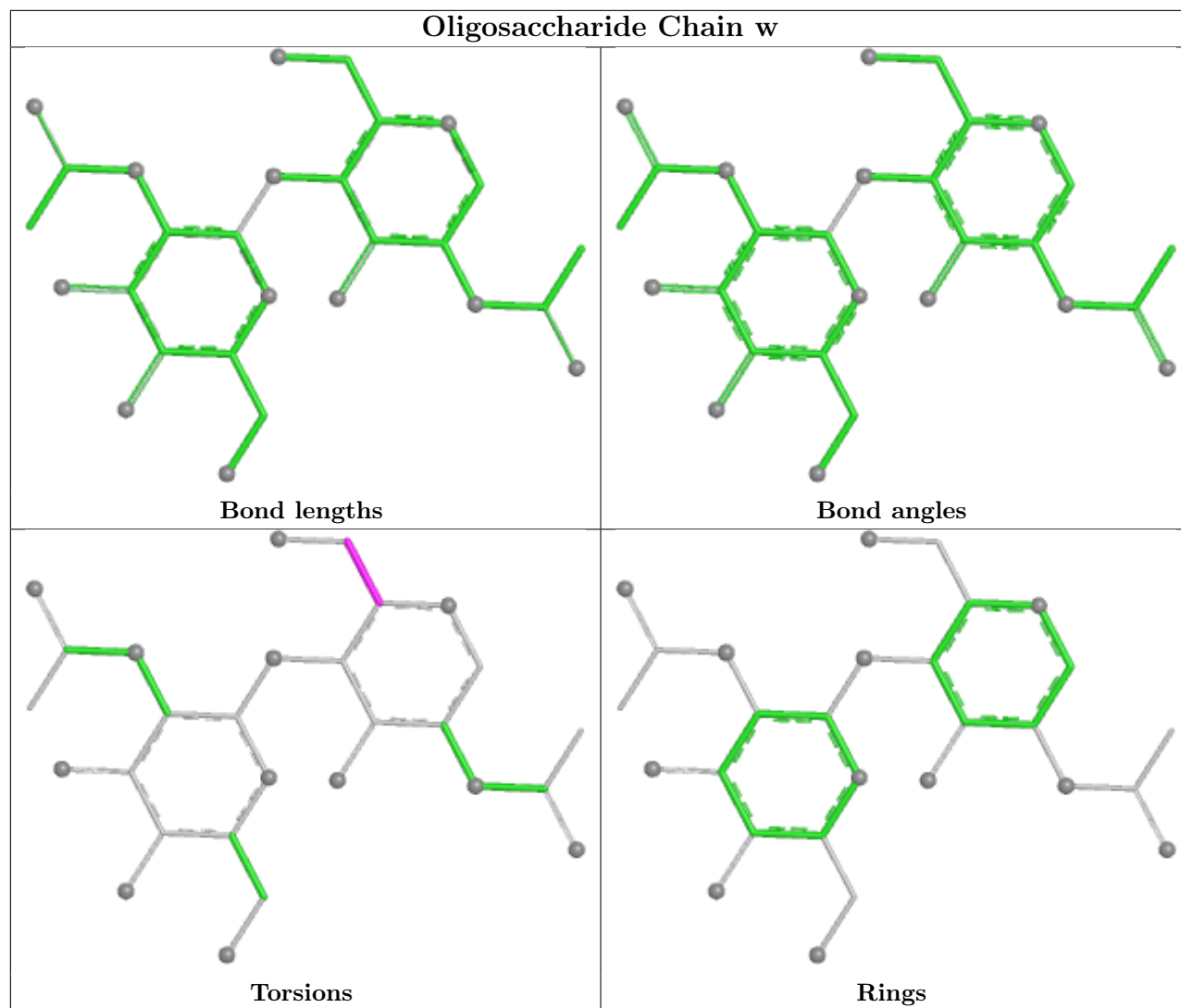


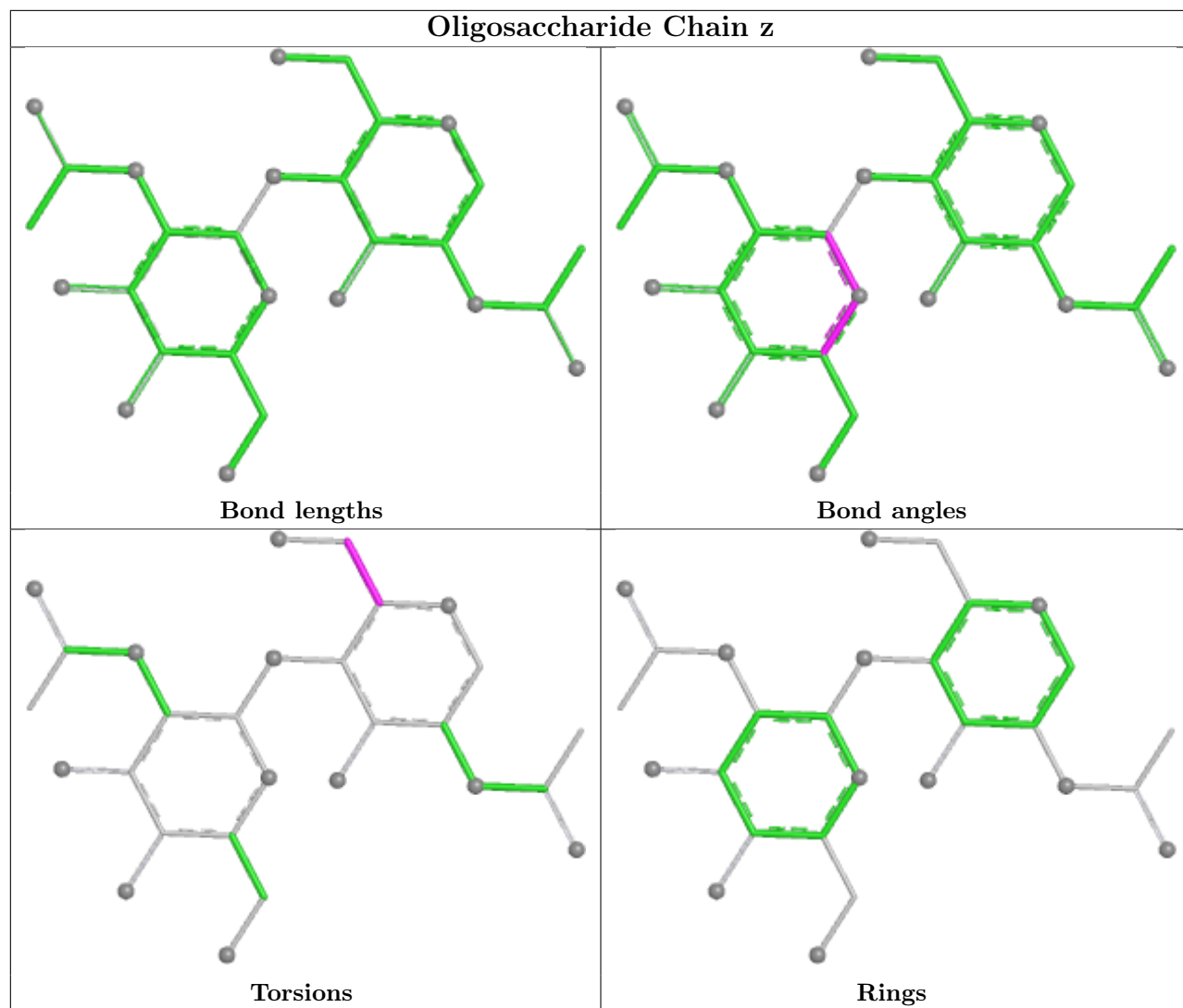


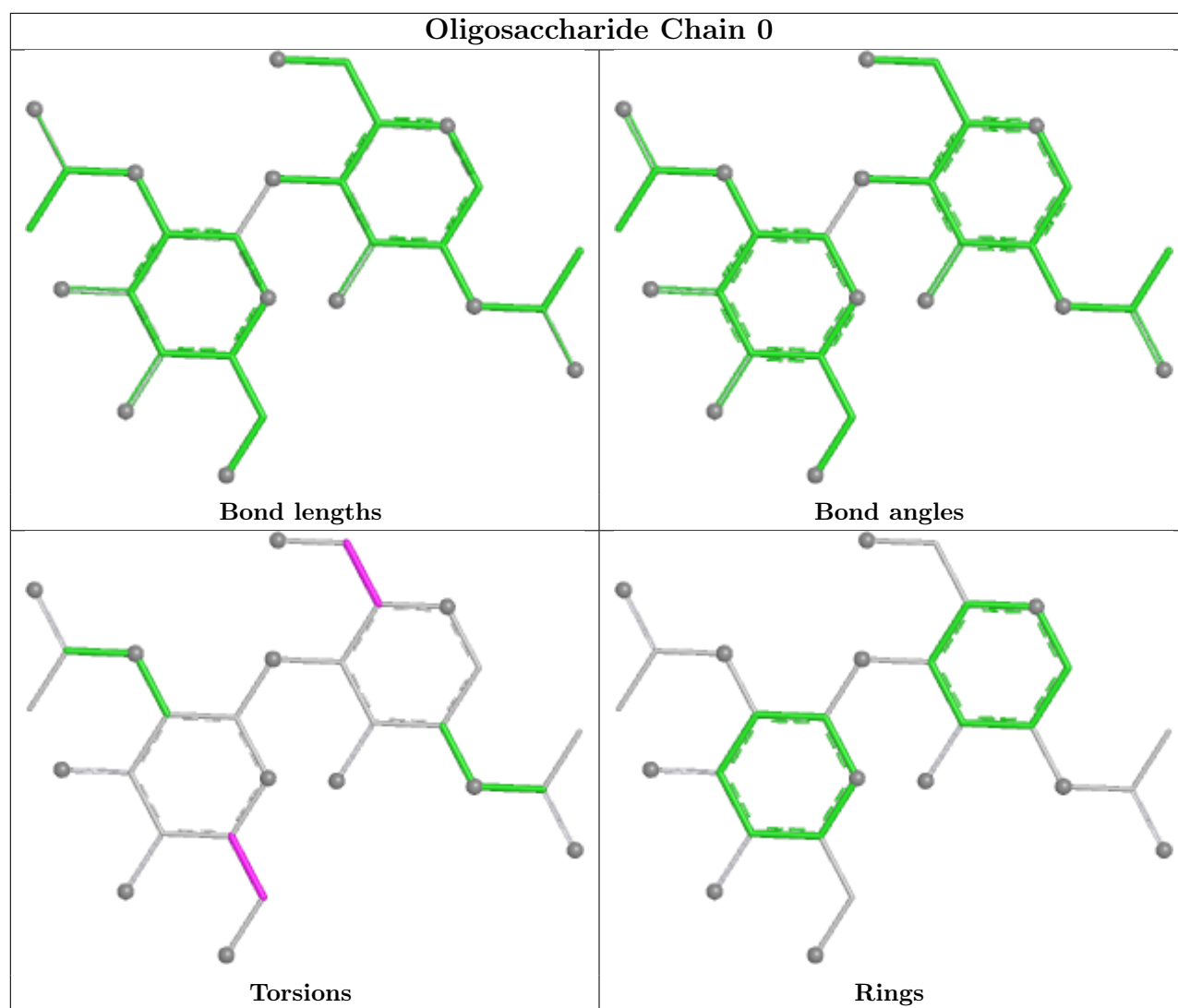


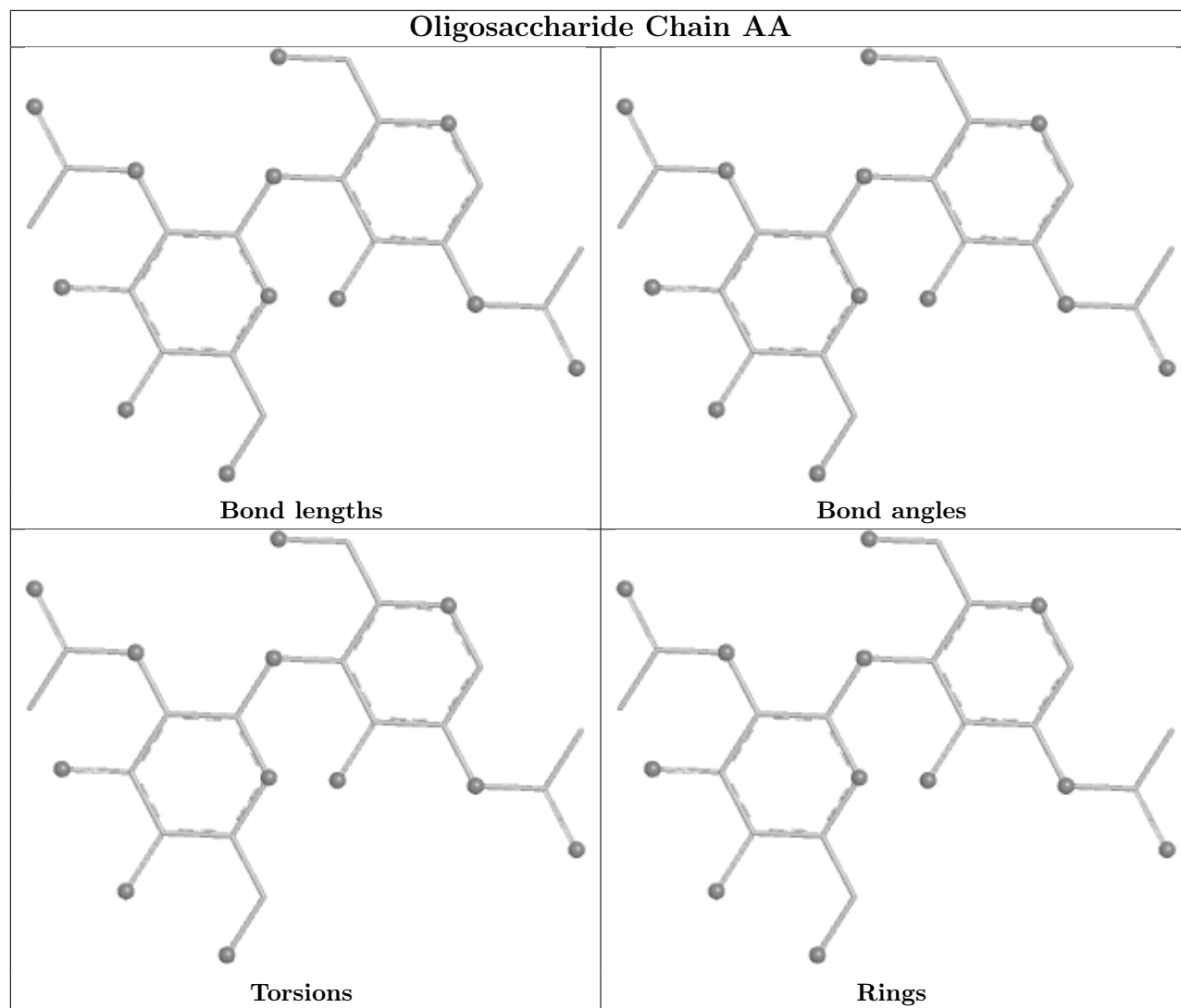


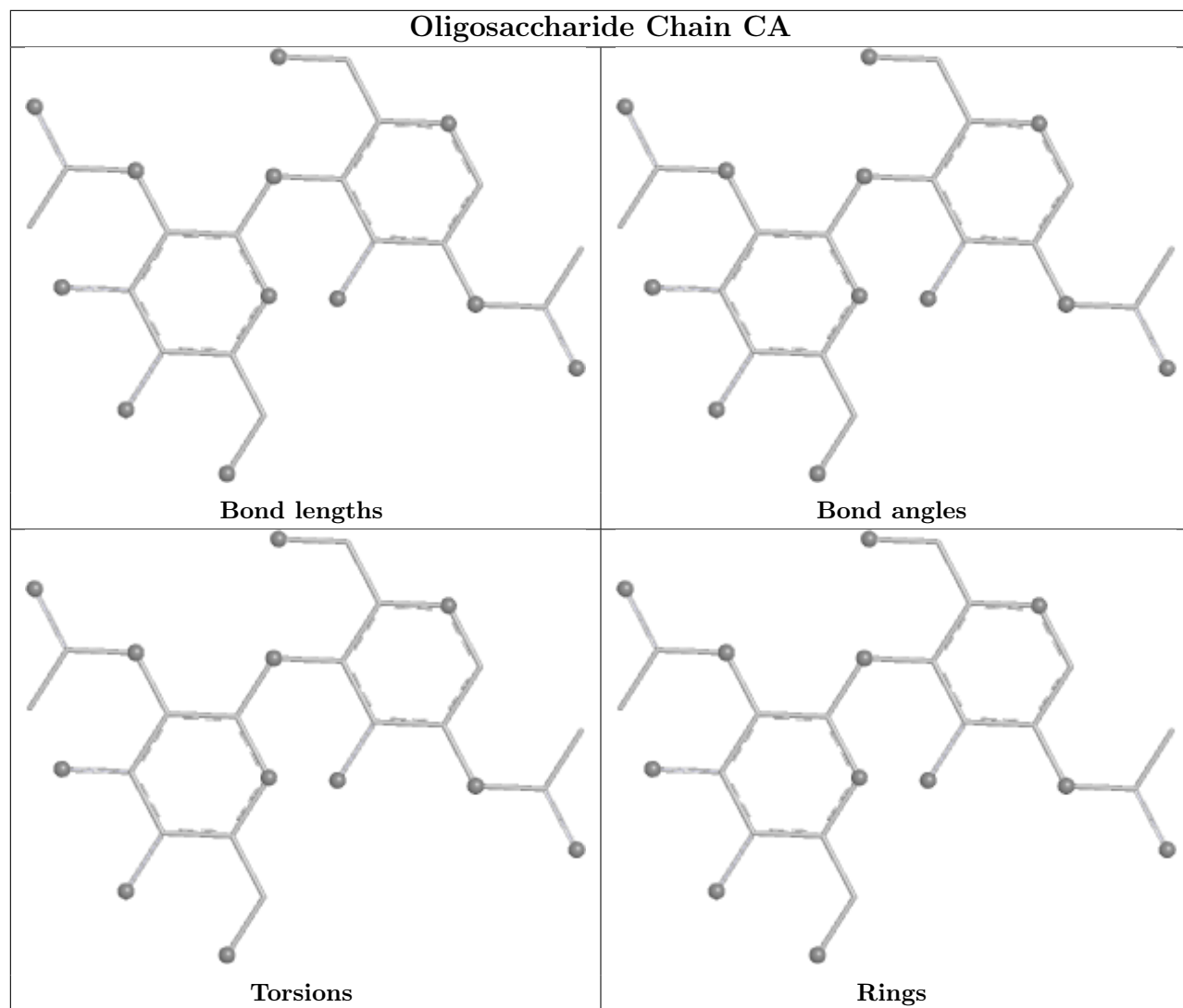


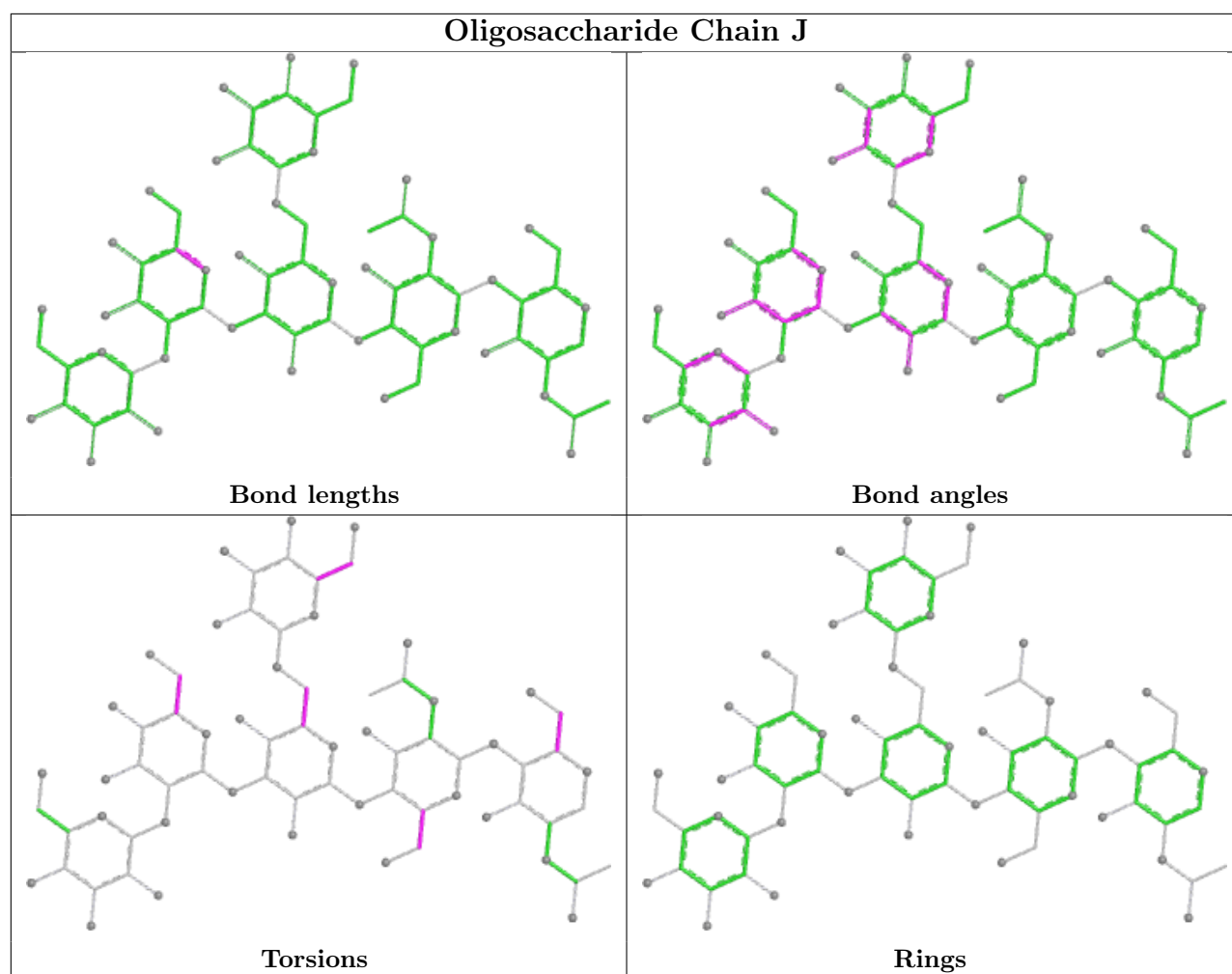


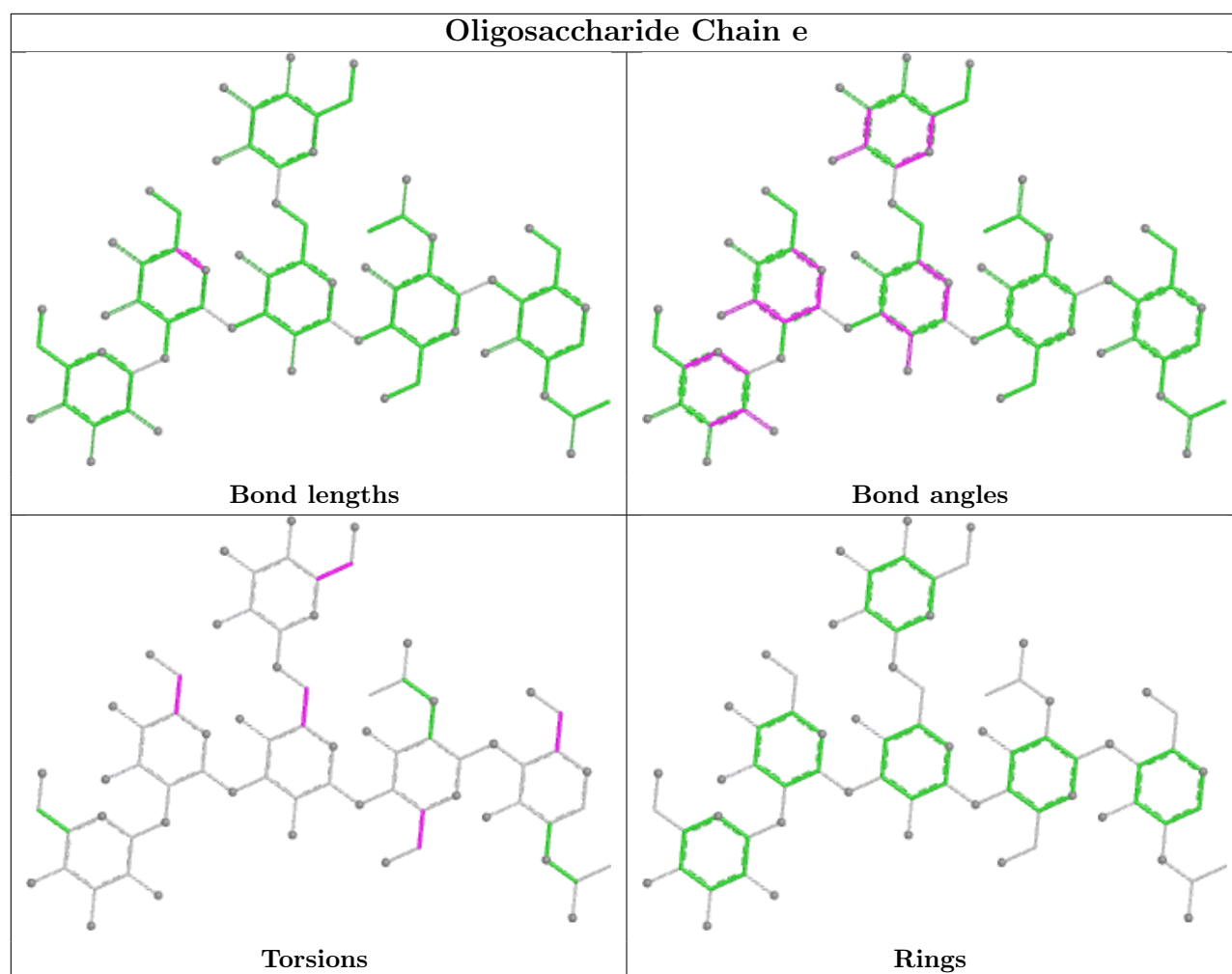


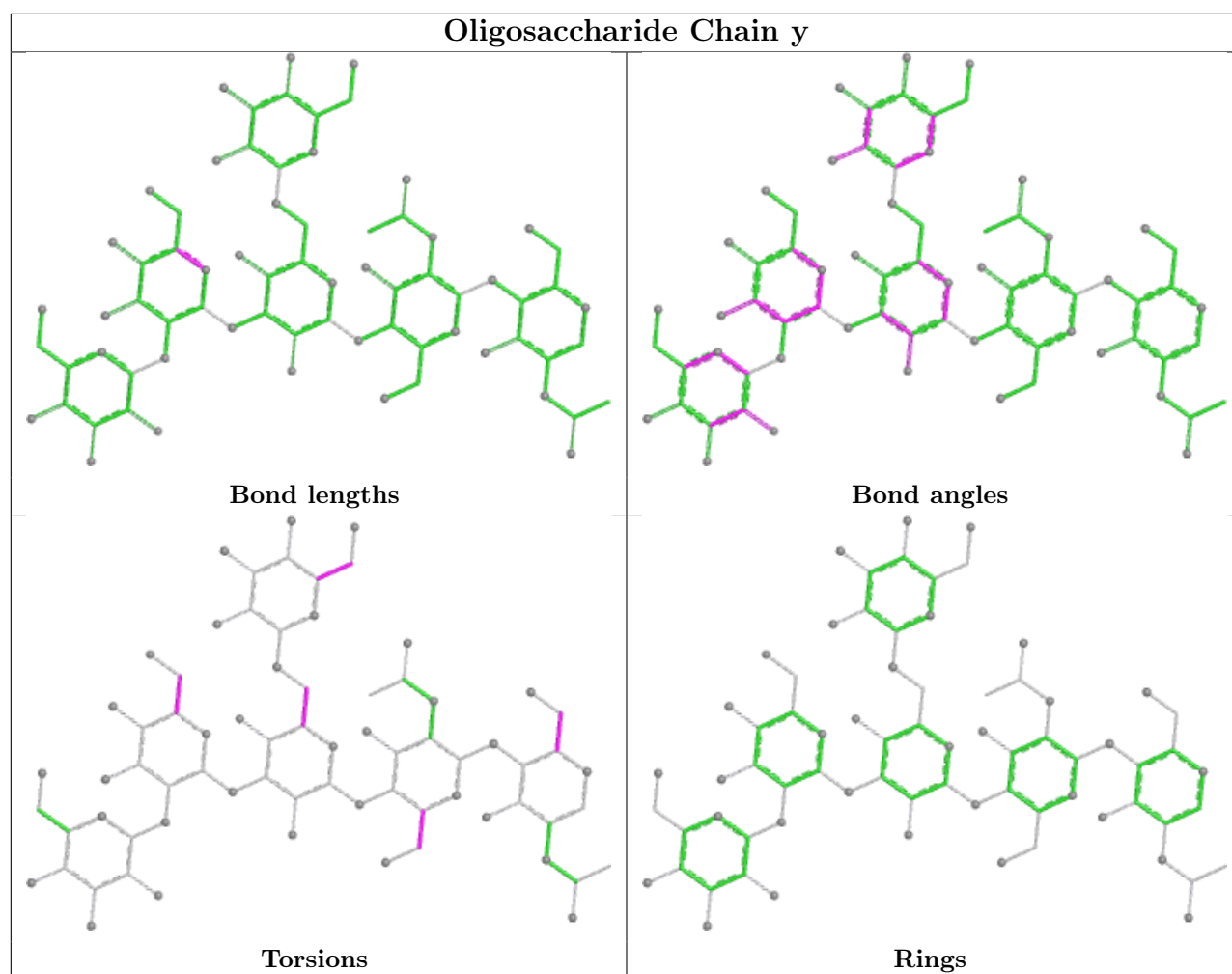


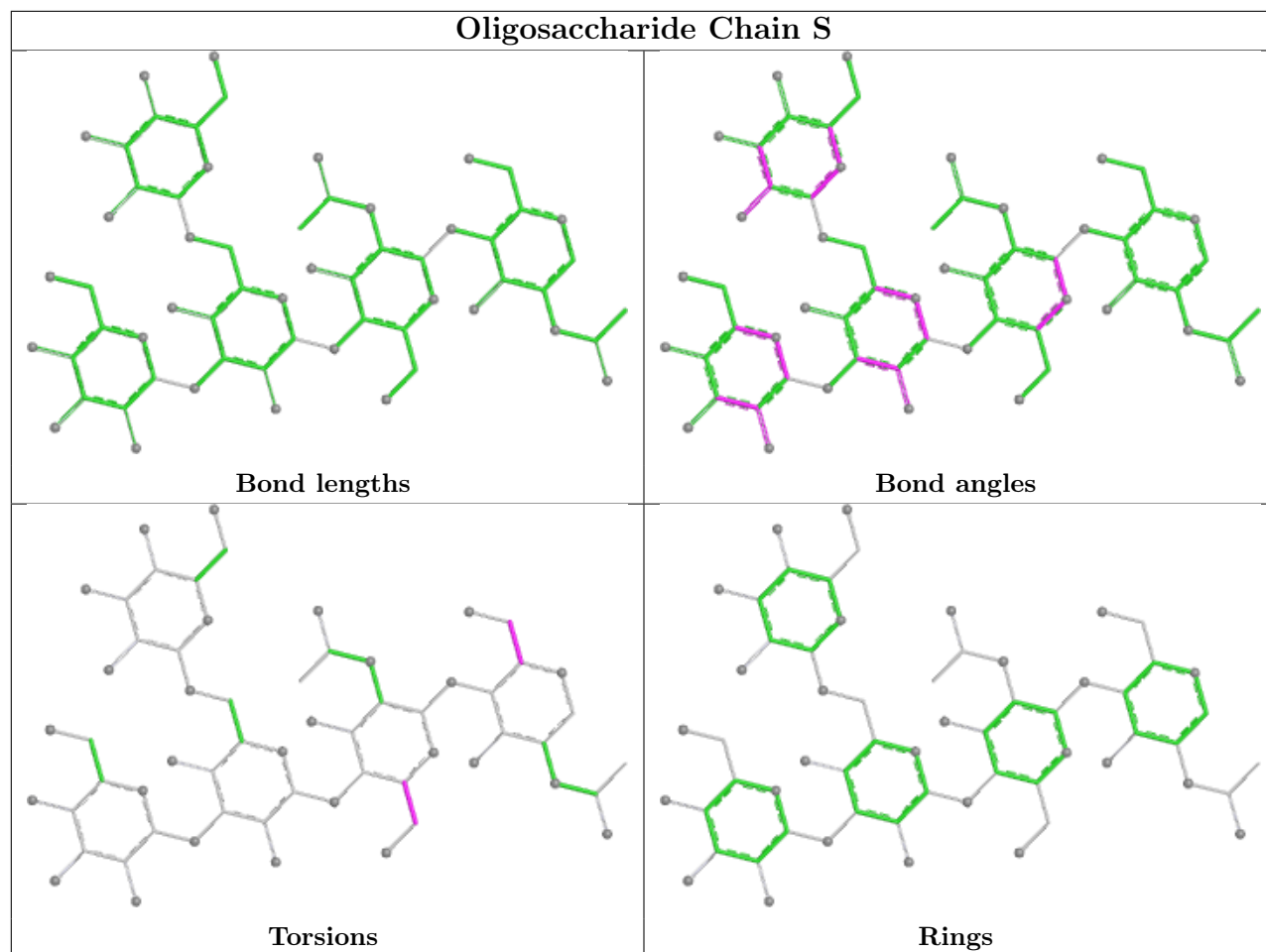


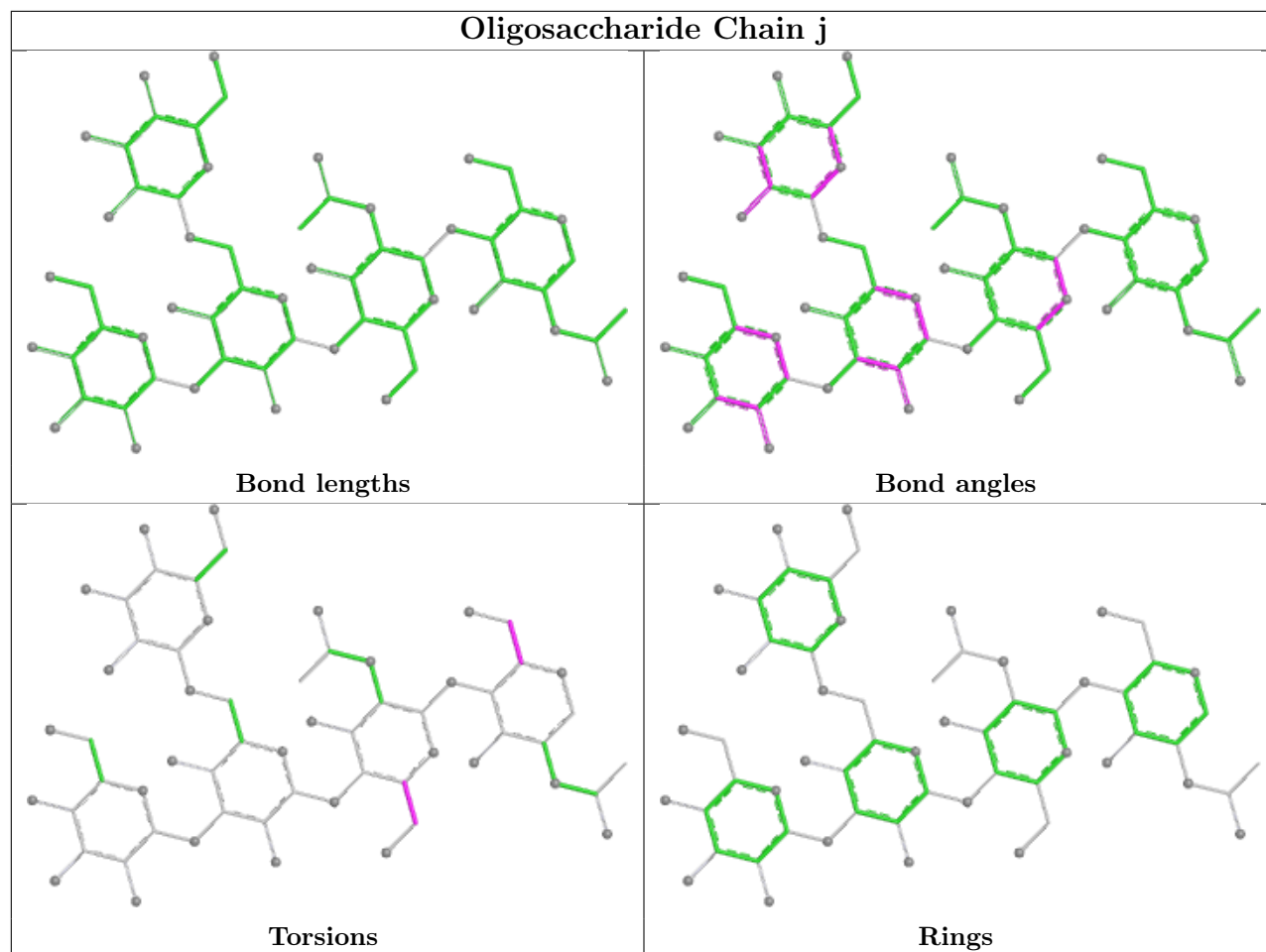


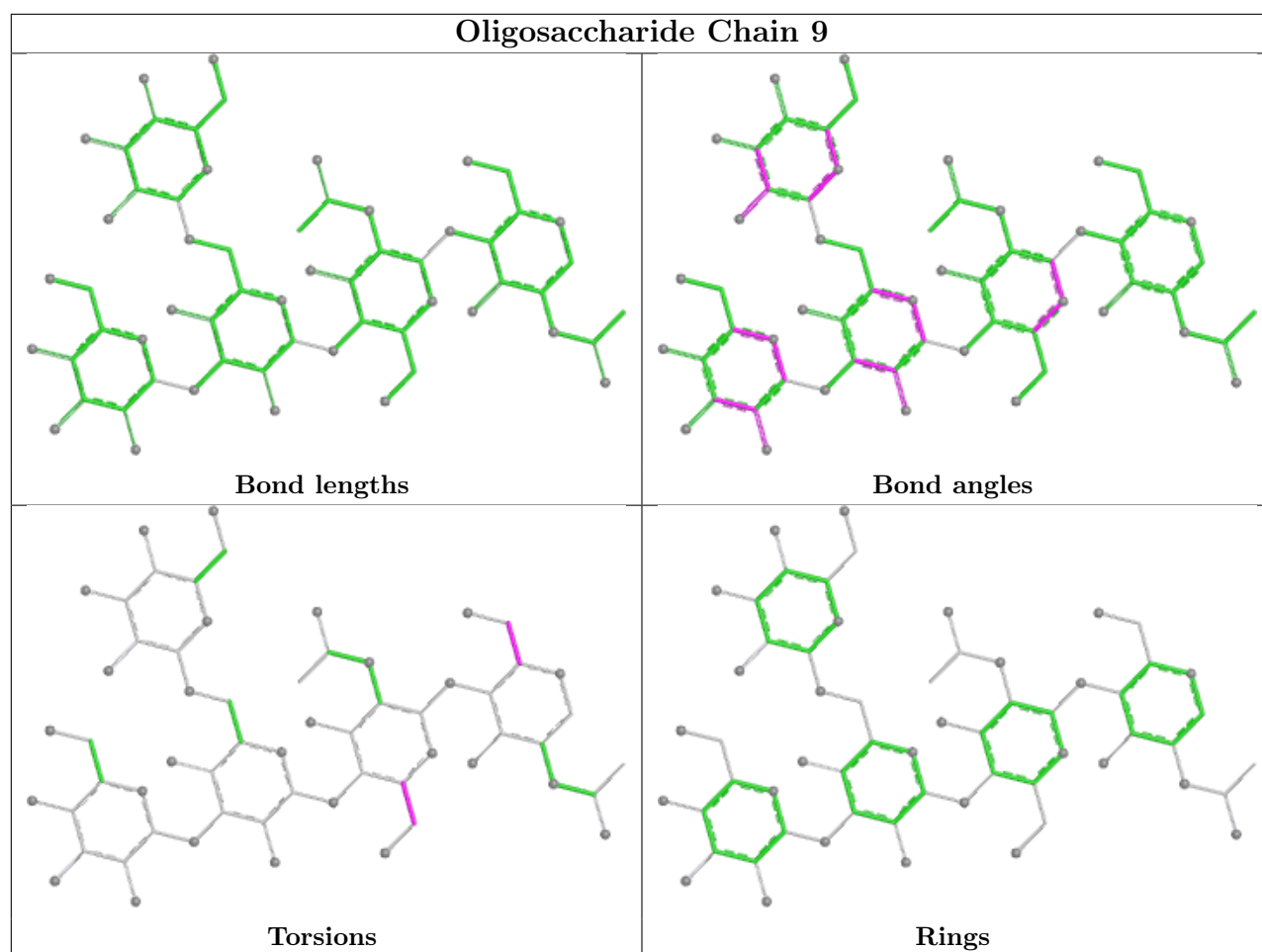


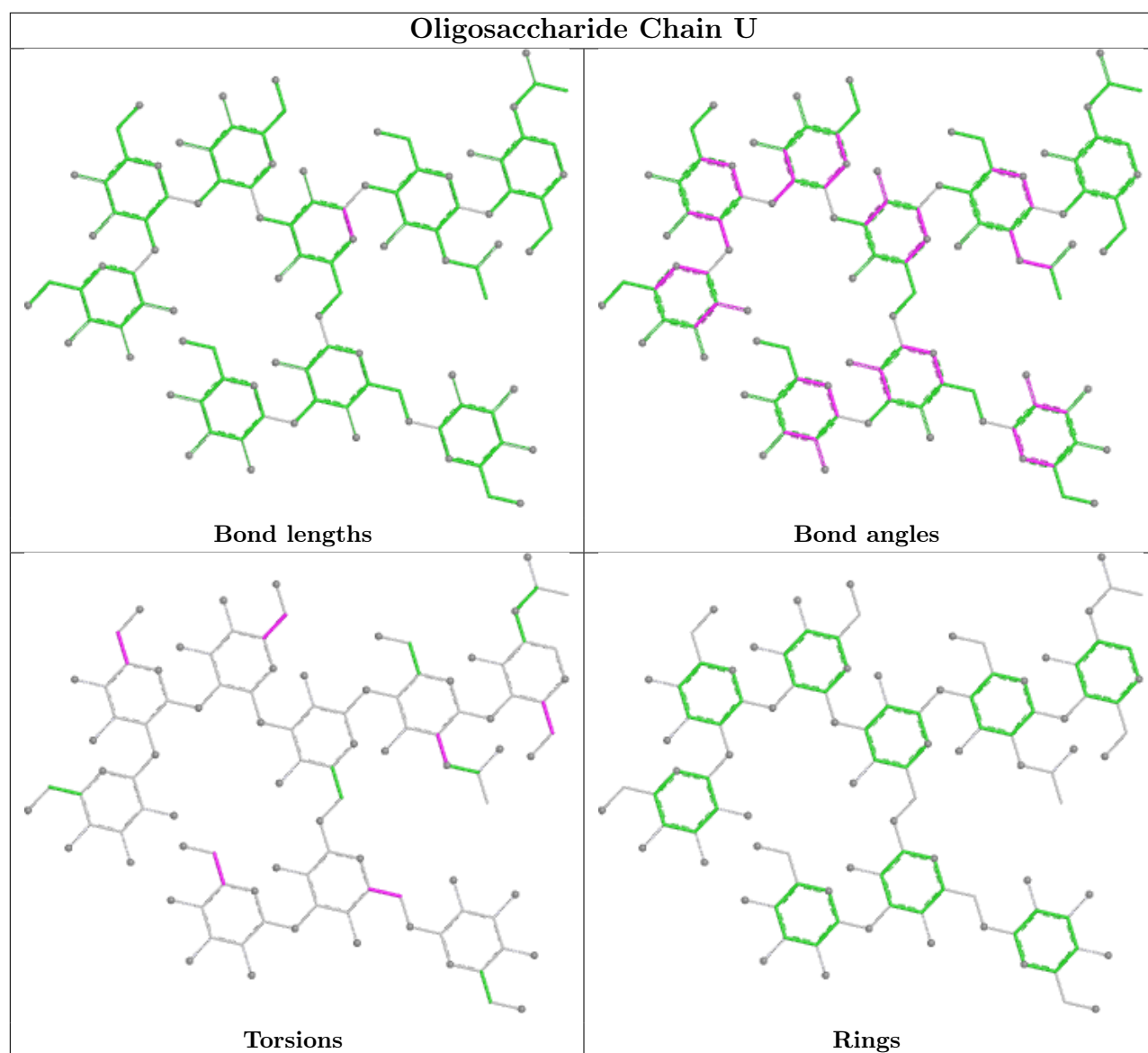


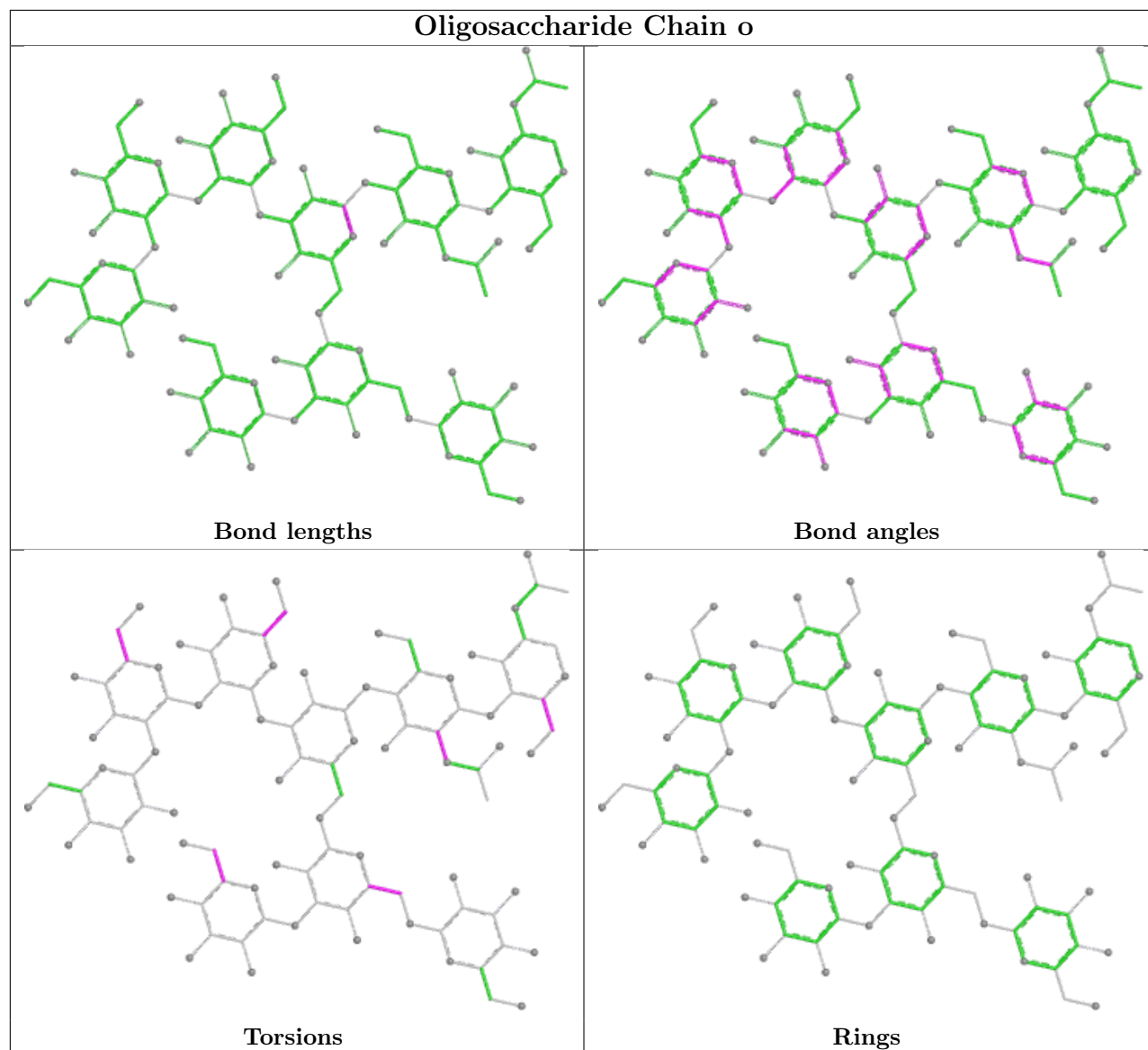


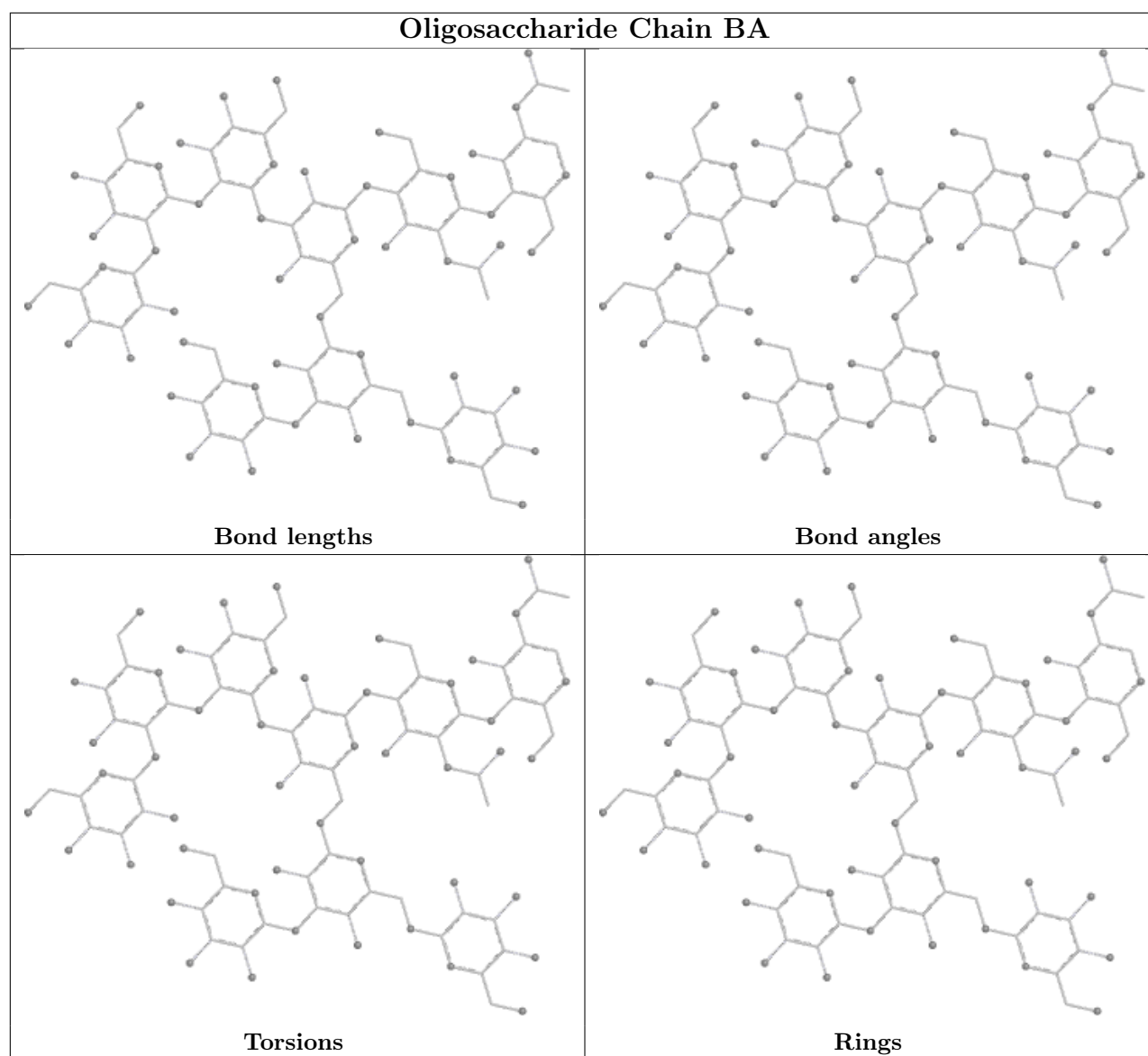












5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	NAG	A	701	8	14,14,15	0.19	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	d	601	7	14,14,15	0.32	0	17,19,21	1.09	1 (5%)
15	NAG	d	602	7	14,14,15	0.31	0	17,19,21	0.49	0
15	NAG	2	602	7	14,14,15	0.31	0	17,19,21	0.50	0
15	NAG	2	601	7	14,14,15	0.32	0	17,19,21	1.09	1 (5%)
15	NAG	D	701	8	14,14,15	0.19	0	17,19,21	0.47	0
15	NAG	C	601	7	14,14,15	0.32	0	17,19,21	1.09	1 (5%)
15	NAG	C	602	7	14,14,15	0.32	0	17,19,21	0.50	0
15	NAG	c	701	8	14,14,15	0.19	0	17,19,21	0.47	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
15	NAG	A	701	8	-	2/6/23/26	0/1/1/1
15	NAG	d	601	7	-	4/6/23/26	0/1/1/1
15	NAG	d	602	7	-	2/6/23/26	0/1/1/1
15	NAG	2	602	7	-	2/6/23/26	0/1/1/1
15	NAG	2	601	7	-	4/6/23/26	0/1/1/1
15	NAG	D	701	8	-	2/6/23/26	0/1/1/1
15	NAG	C	601	7	-	4/6/23/26	0/1/1/1
15	NAG	C	602	7	-	2/6/23/26	0/1/1/1
15	NAG	c	701	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	601	NAG	C2-N2-C7	3.29	127.30	122.90
15	2	601	NAG	C2-N2-C7	3.27	127.29	122.90
15	C	601	NAG	C2-N2-C7	3.26	127.27	122.90

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	D	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	A	701	NAG	O5-C5-C6-O6
15	c	701	NAG	O5-C5-C6-O6
15	D	701	NAG	C4-C5-C6-O6
15	A	701	NAG	C4-C5-C6-O6
15	c	701	NAG	C4-C5-C6-O6
15	C	602	NAG	O5-C5-C6-O6
15	2	602	NAG	O5-C5-C6-O6
15	d	602	NAG	O5-C5-C6-O6
15	d	601	NAG	C4-C5-C6-O6
15	C	601	NAG	C4-C5-C6-O6
15	2	601	NAG	C4-C5-C6-O6
15	d	601	NAG	O5-C5-C6-O6
15	C	601	NAG	O5-C5-C6-O6
15	2	601	NAG	O5-C5-C6-O6
15	C	601	NAG	C1-C2-N2-C7
15	2	601	NAG	C1-C2-N2-C7
15	d	601	NAG	C1-C2-N2-C7
15	C	601	NAG	C3-C2-N2-C7
15	2	601	NAG	C3-C2-N2-C7
15	d	601	NAG	C3-C2-N2-C7
15	d	602	NAG	C4-C5-C6-O6
15	C	602	NAG	C4-C5-C6-O6
15	2	602	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

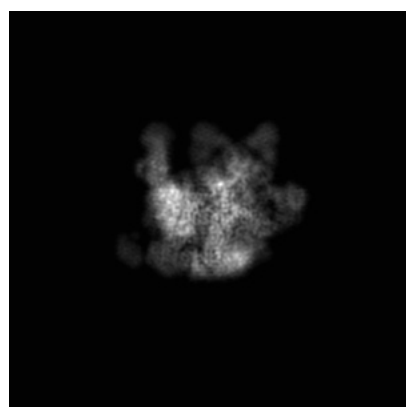
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7622. These allow visual inspection of the internal detail of the map and identification of artifacts.

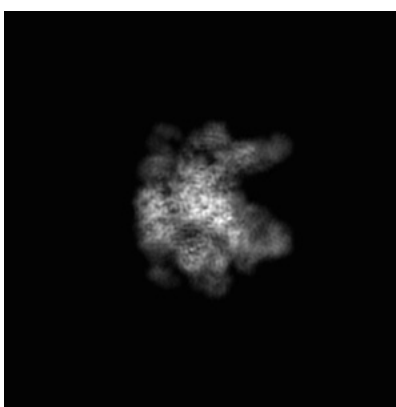
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

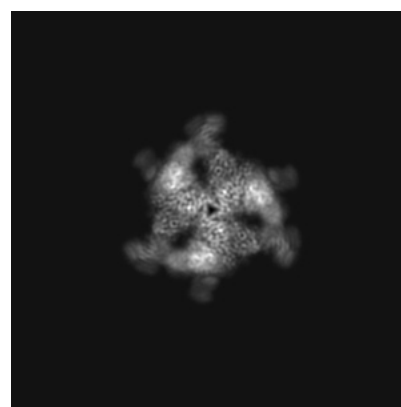
6.1.1 Primary map



X



Y

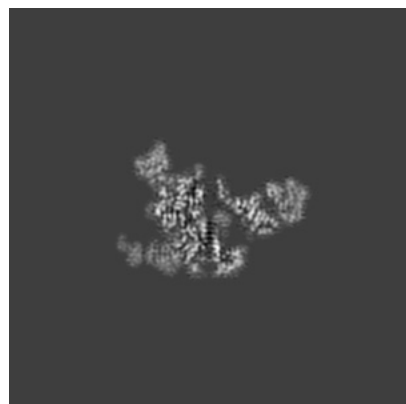


Z

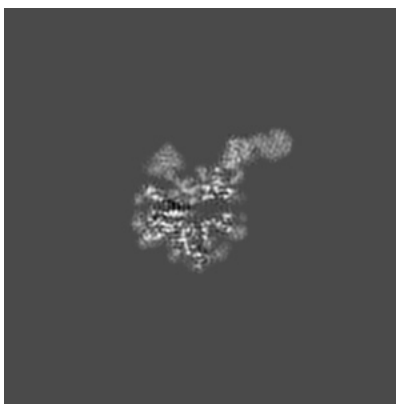
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

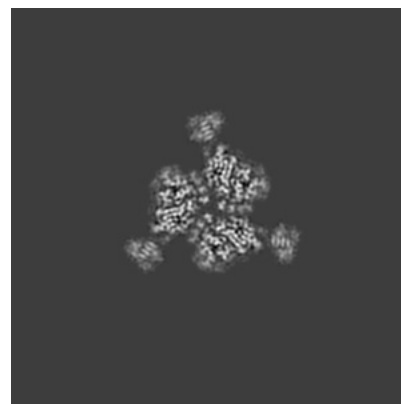
6.2.1 Primary map



X Index: 192



Y Index: 192

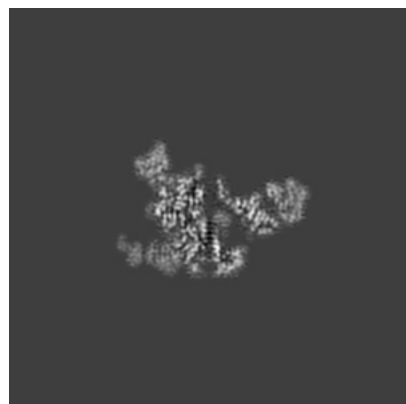


Z Index: 192

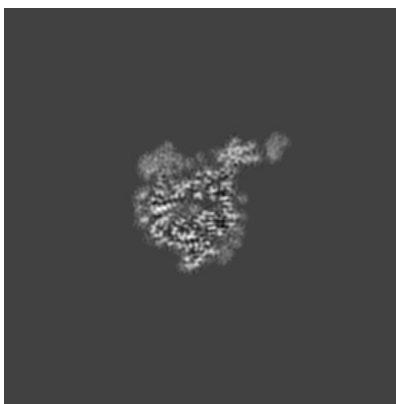
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

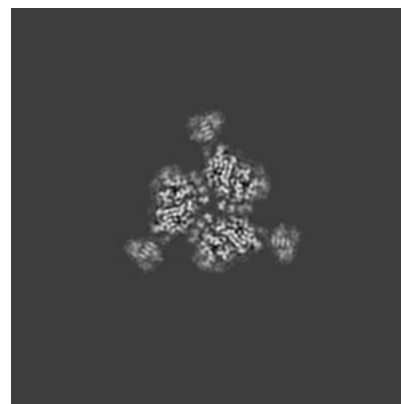
6.3.1 Primary map



X Index: 192



Y Index: 200

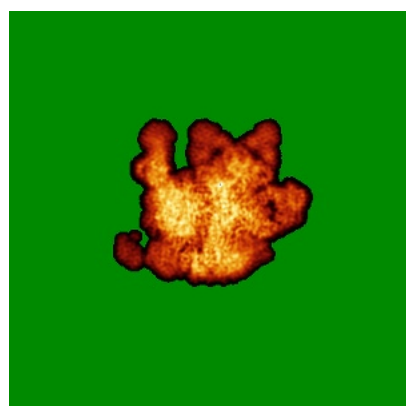


Z Index: 192

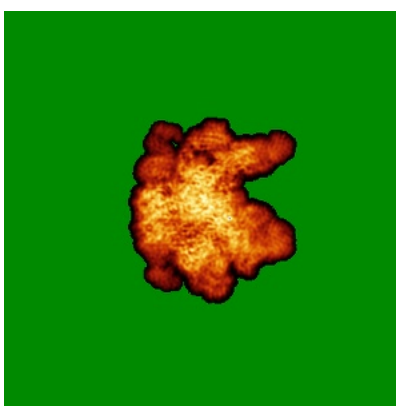
The images above show the largest variance slices of the map in three orthogonal directions.

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

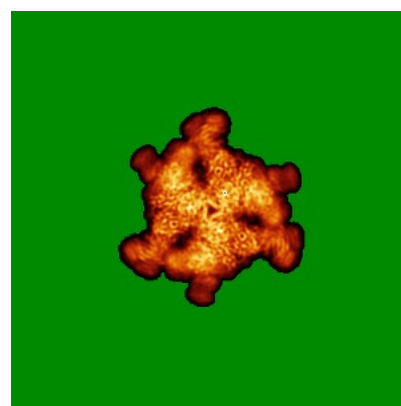
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

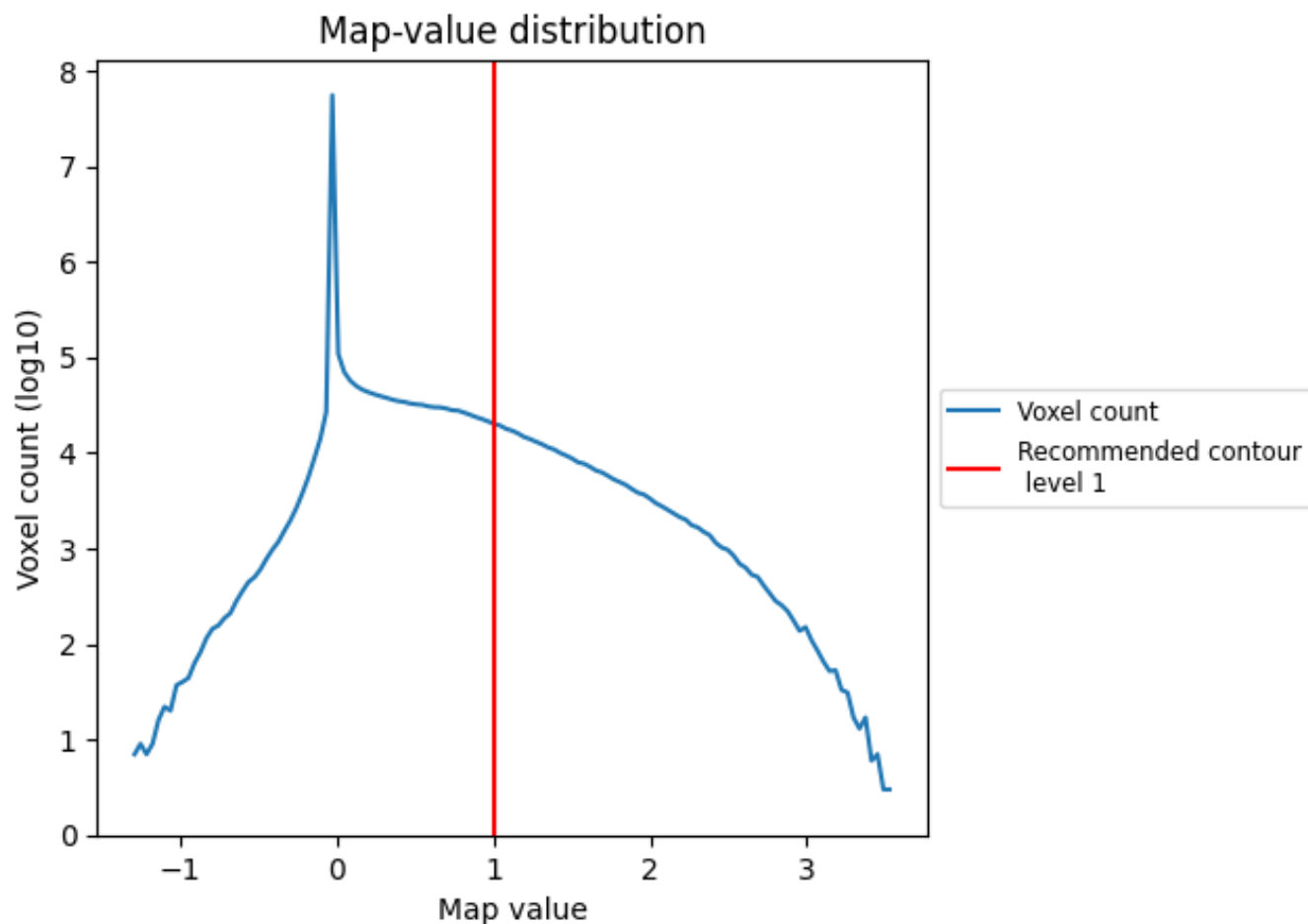
6.6 Mask visualisation

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

7 Map analysis [i](#)

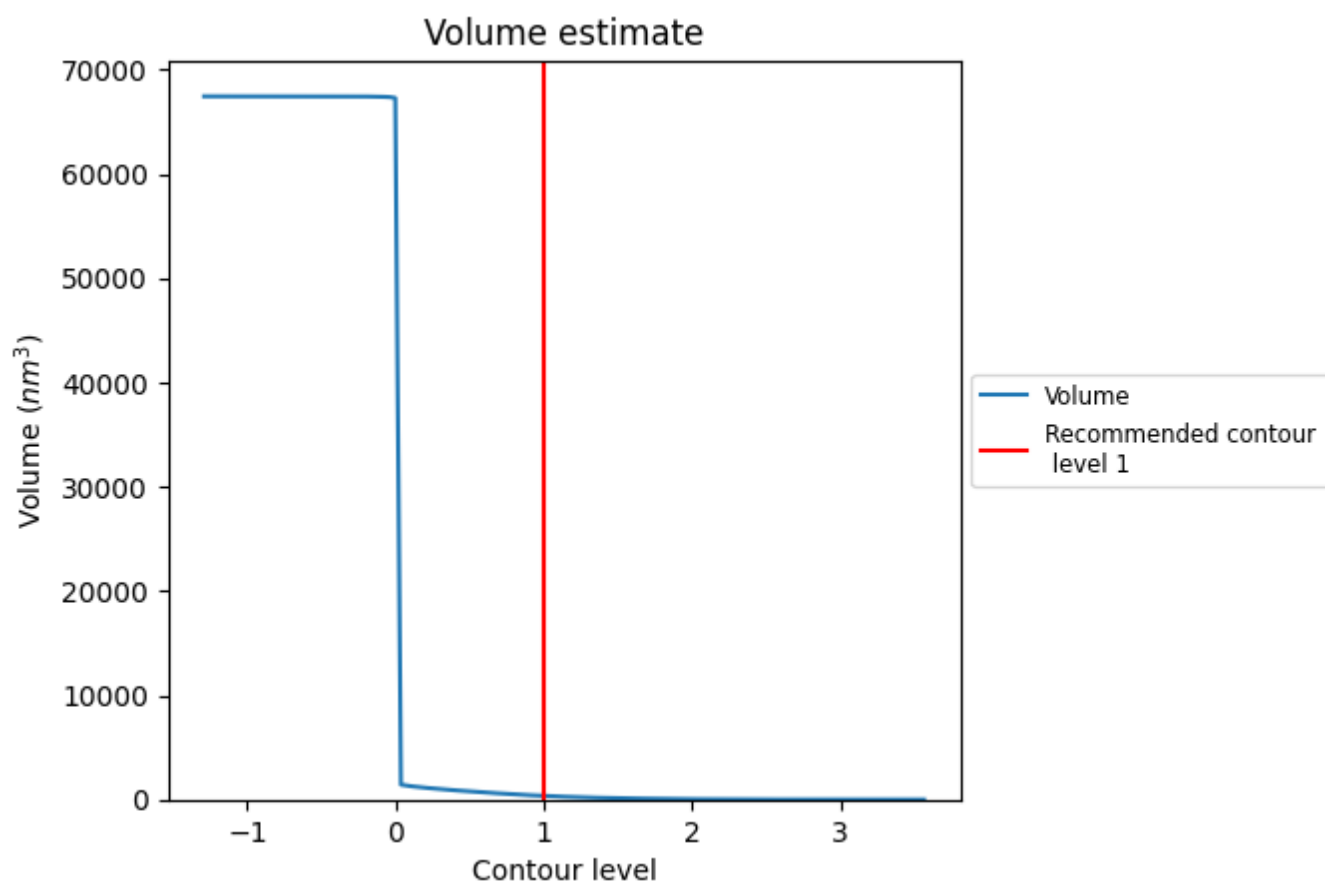
This section contains the results of statistical analysis of the map.

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.

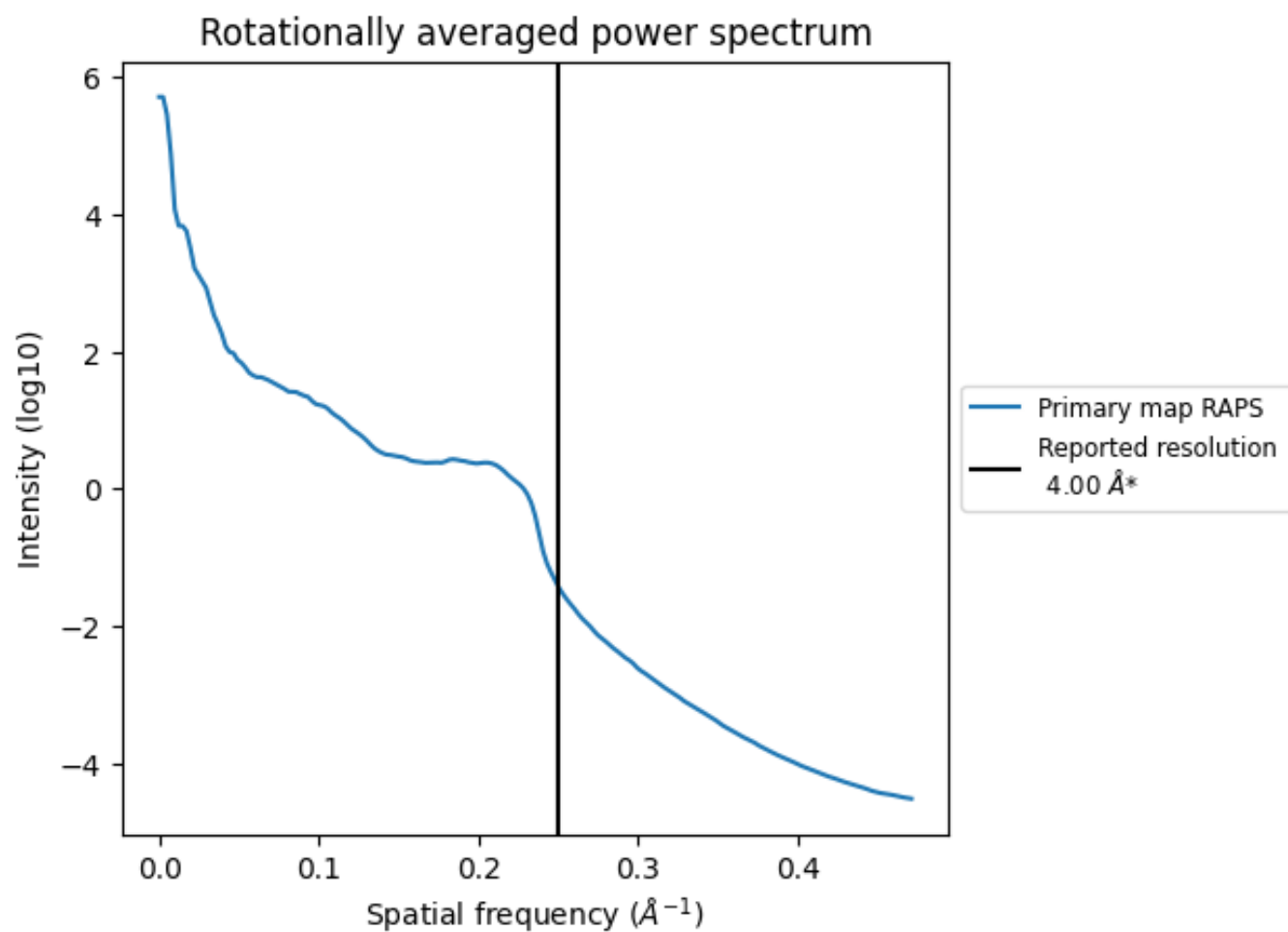
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 354 nm³; this corresponds to an approximate mass of 320 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 ⓘ

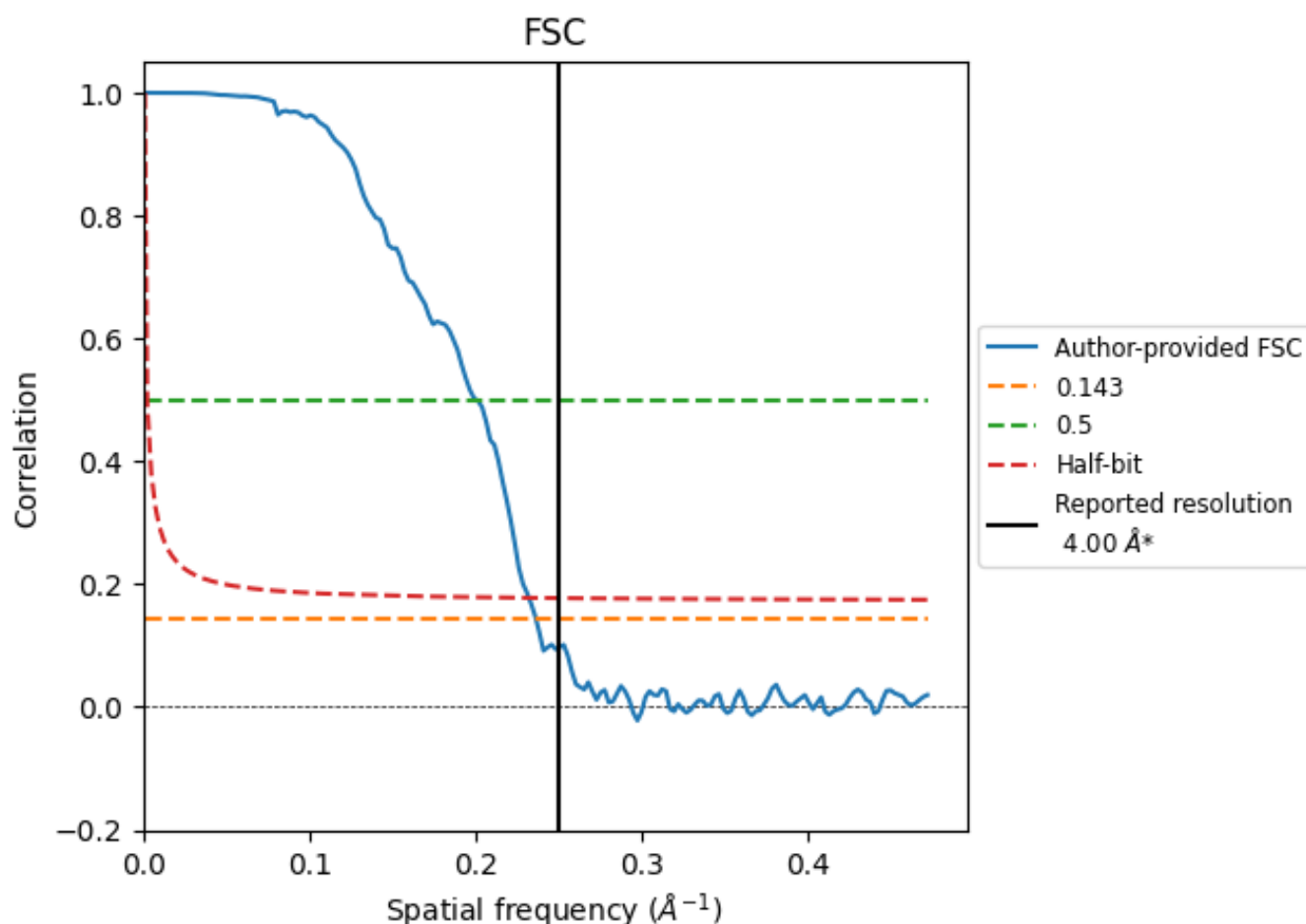


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.23	4.99	4.31
Unmasked-calculated*	-	-	-

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

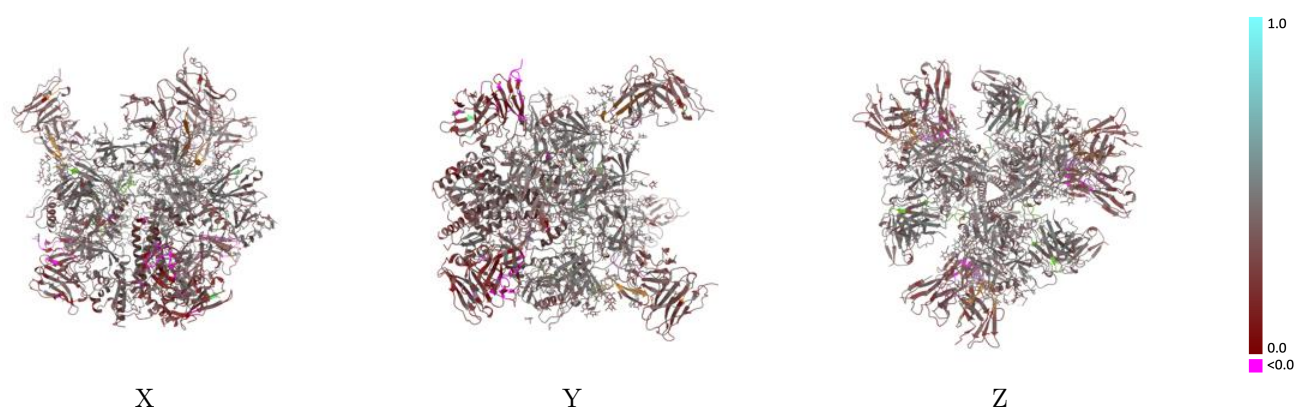
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7622 and PDB model 6CUF. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

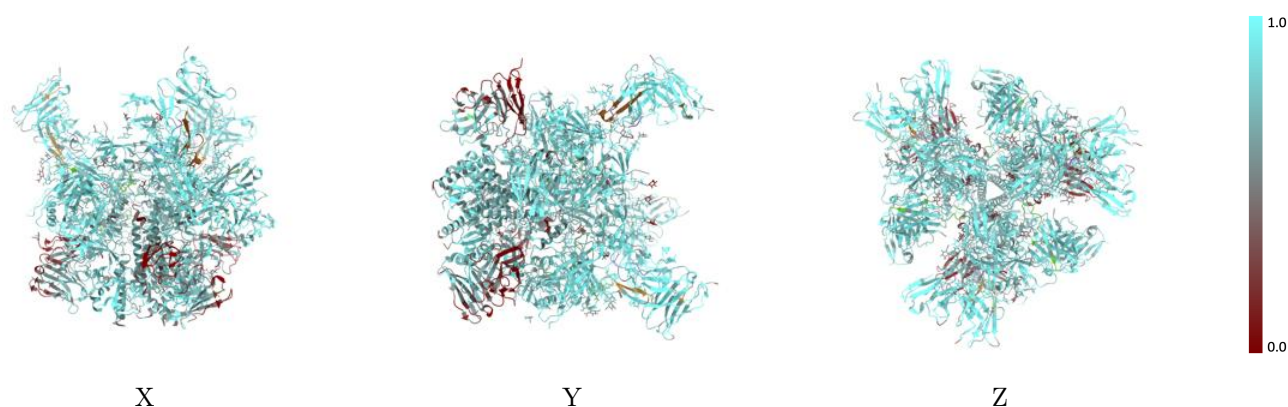
This section was not generated.

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



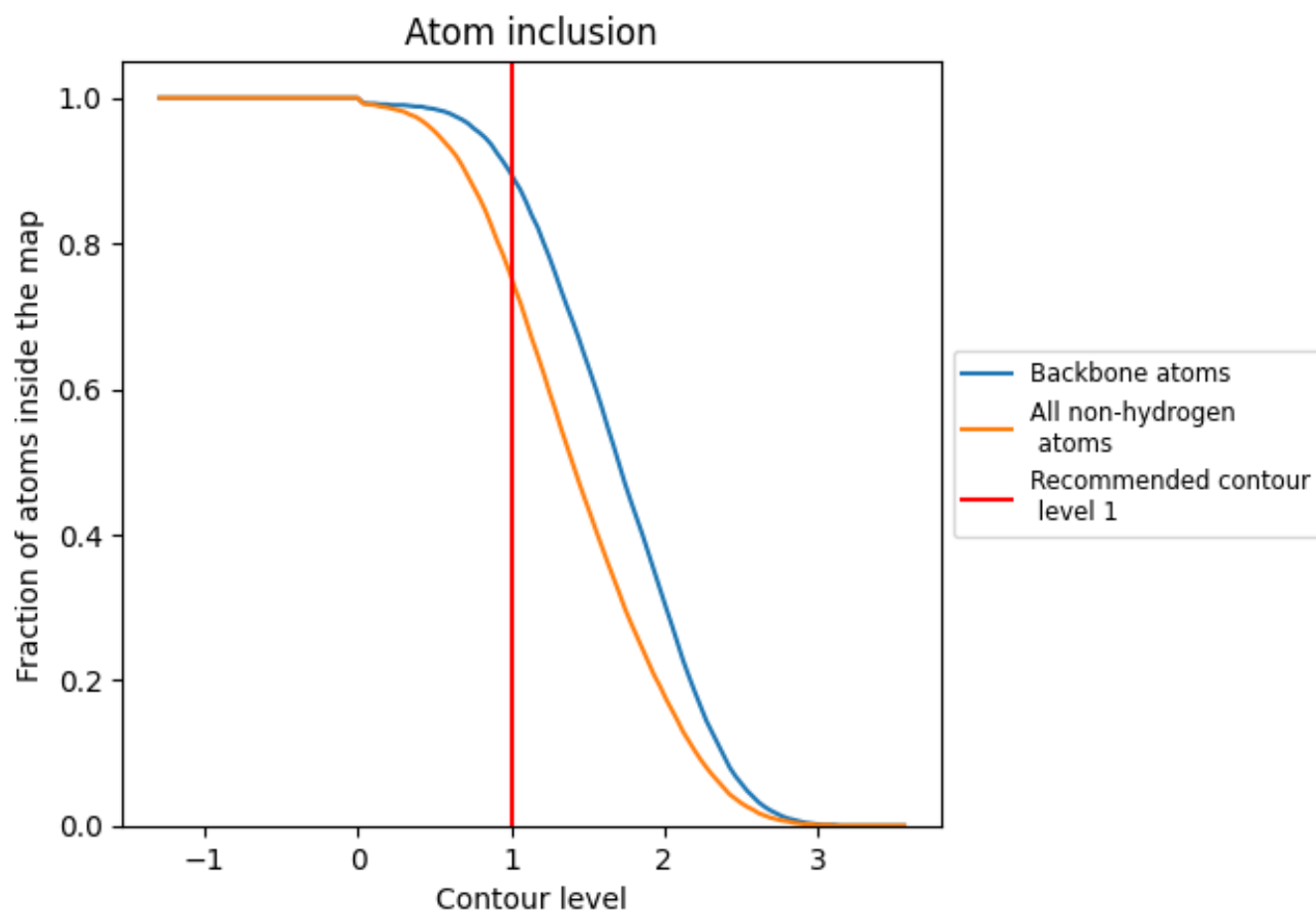
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.3610
0	 0.6790	 0.4260
1	 0.9490	 0.4560
2	 0.8070	 0.4080
3	 0.5750	 0.2560
4	 0.2880	 0.1720
5	 0.8470	 0.3370
6	 0.9060	 0.3640
7	 0.8280	 0.4010
8	 0.8530	 0.4230
9	 0.6720	 0.3740
A	 0.7970	 0.3550
AA	 0.5360	 0.3520
B	 0.8200	 0.4080
BA	 0.8760	 0.4310
C	 0.8100	 0.4090
CA	 0.6430	 0.3780
D	 0.7950	 0.3590
DA	 0.6600	 0.4040
E	 0.7600	 0.4350
F	 0.5380	 0.3540
G	 0.4290	 0.3670
H	 0.5760	 0.2580
I	 0.6920	 0.3770
J	 0.6940	 0.4310
K	 0.7500	 0.4430
L	 0.2810	 0.1700
M	 0.8480	 0.3370
N	 0.8920	 0.3620
O	 0.6430	 0.4190
P	 0.9490	 0.4660
Q	 0.8490	 0.4220
R	 0.8350	 0.4040
S	 0.6720	 0.3610
T	 0.5710	 0.3530



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Chain	Atom inclusion	Q-score
U	 0.8760	 0.4290
V	 0.6430	 0.3750
W	 0.6600	 0.4090
X	 0.8200	 0.4110
Y	 0.7400	 0.4330
Z	 0.5640	 0.3670
a	 0.3930	 0.3680
b	 0.6920	 0.3820
c	 0.7940	 0.3590
d	 0.8090	 0.4090
e	 0.6670	 0.4330
f	 0.7500	 0.4440
g	 0.6430	 0.4330
h	 0.5720	 0.2500
i	 0.9490	 0.4640
j	 0.6560	 0.3630
k	 0.5710	 0.3580
l	 0.2830	 0.1720
m	 0.8520	 0.3360
n	 0.8970	 0.3610
o	 0.8760	 0.4280
p	 0.6430	 0.3740
q	 0.8560	 0.4190
r	 0.8370	 0.4000
s	 0.6800	 0.4090
t	 0.8200	 0.4120
u	 0.7400	 0.4370
v	 0.5380	 0.3630
w	 0.4290	 0.3780
x	 0.6670	 0.3810
y	 0.6810	 0.4260
z	 0.7500	 0.4330