



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:12 AM UTC

PDB ID : 5FUU / pdb_00005fuu
EMDB ID : EMD-3308
Title : Ectodomain of cleaved wild type JR-FL EnvDCT trimer in complex with PGT151 Fab
Authors : Lee, J.H.; Ward, A.B.
Deposited on : 2016-01-29
Resolution : 4.19 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:

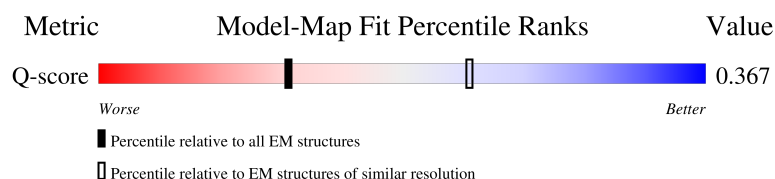
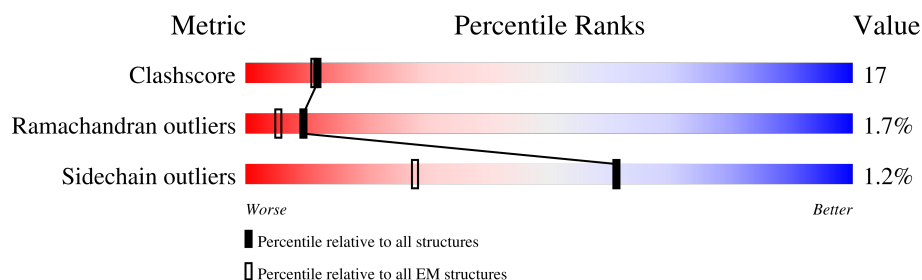
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 4.19 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.



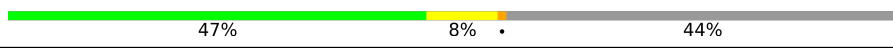
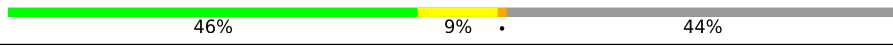
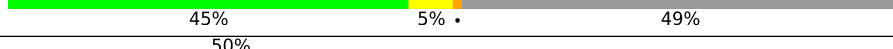
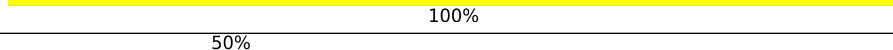
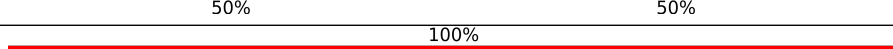
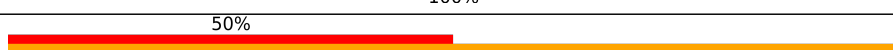
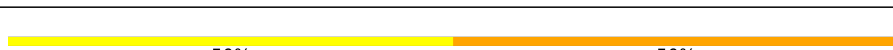
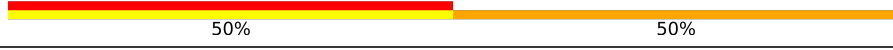
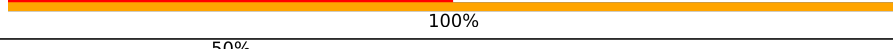
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5310 (3.70 - 4.69)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	473	 78% 15% • 5%
1	C	473	 74% 16% • 6%
1	E	473	 75% 16% • • 5%
2	B	153	 77% 11% 5% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	153	
2	F	153	
3	H	240	
3	M	240	
4	L	219	
4	N	219	
5	0	2	
5	1	2	
5	3	2	
5	4	2	
5	5	2	
5	AA	2	
5	G	2	
5	Q	2	
5	R	2	
5	T	2	
5	X	2	
5	b	2	
5	c	2	
5	h	2	
5	k	2	
5	l	2	
5	o	2	
5	r	2	
5	s	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	u	2	50% 100%
5	w	2	100%
5	z	2	50% 100%
6	2	3	33% 100%
6	7	3	67% 100%
6	I	3	33% 33% 67%
6	J	3	33% 33% 67%
6	K	3	33% 67% 33%
6	P	3	33% 67%
6	S	3	33% 100%
6	U	3	67% 100%
6	V	3	67% 33%
6	W	3	33% 100%
6	a	3	33% 100%
6	d	3	67% 33% 67%
6	g	3	33% 33% 67%
6	i	3	33% 100%
6	j	3	33% 67% 33%
6	m	3	33% 100%
6	n	3	33% 67%
6	t	3	100%
6	v	3	33% 33% 67%
7	O	7	43% 57%
7	f	7	29% 29% 57% 14%
7	y	7	57% 43%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	9	11	
8	Y	11	
9	Z	13	
10	e	5	
11	8	8	
11	p	8	
12	q	3	
13	x	6	
14	6	4	
15	BA	12	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	e	1	-	-	X	-
12	FUC	q	3	-	-	X	-
15	NAG	BA	2	-	-	X	-
16	NAG	E	1397	-	-	X	-
5	NAG	3	1	-	-	X	-
5	NAG	4	1	-	-	X	-
5	NAG	G	1	-	-	X	-
5	NAG	T	1	-	-	X	-
5	NAG	c	1	-	-	X	-
5	NAG	c	2	-	-	X	-
5	NAG	o	1	-	-	X	-
5	NAG	w	1	-	-	X	-
6	NAG	I	1	-	-	X	-
6	NAG	d	1	-	-	X	-
6	NAG	i	1	-	-	X	-
8	FUC	9	11	-	-	X	-
9	NAG	Z	2	-	-	X	-
9	NAG	Z	7	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 20735 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HIV-1 ENVELOPE GLYCOPROTEIN GP160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	449	Total	C	N	O	S	0	0
			3553	2233	624	671	25		
1	C	444	Total	C	N	O	S	0	0
			3506	2208	613	660	25		
1	E	448	Total	C	N	O	S	0	0
			3537	2224	620	668	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	THR	VAL	engineered mutation	UNP Q75760
C	31	THR	VAL	engineered mutation	UNP Q75760
E	31	THR	VAL	engineered mutation	UNP Q75760

- Molecule 2 is a protein called HIV-1 ENVELOPE GLYCOPROTEIN GP160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			1150	722	200	221	7		
2	D	147	Total	C	N	O	S	0	0
			1159	731	203	218	7		
2	F	153	Total	C	N	O	S	0	0
			1209	763	209	230	7		

- Molecule 3 is a protein called IMMUNOGLOBULIN G PGT151.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	135	Total	C	N	O	S	0	0
			1073	682	188	197	6		
3	M	135	Total	C	N	O	S	0	0
			1067	679	185	197	6		

- Molecule 4 is a protein called IMMUNOGLOBULIN G PGT151.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	114	Total	C	N	O	S	0	0
			881	553	151	173	4		
4	N	112	Total	C	N	O	S	0	0
			866	545	149	168	4		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



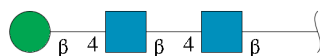
Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	2	Total	C	N	O		0	0
			28	16	2	10			
5	Q	2	Total	C	N	O		0	0
			28	16	2	10			
5	R	2	Total	C	N	O		0	0
			28	16	2	10			
5	T	2	Total	C	N	O		0	0
			28	16	2	10			
5	X	2	Total	C	N	O		0	0
			28	16	2	10			
5	b	2	Total	C	N	O		0	0
			28	16	2	10			
5	c	2	Total	C	N	O		0	0
			28	16	2	10			
5	h	2	Total	C	N	O		0	0
			28	16	2	10			
5	k	2	Total	C	N	O		0	0
			28	16	2	10			
5	l	2	Total	C	N	O		0	0
			28	16	2	10			
5	o	2	Total	C	N	O		0	0
			28	16	2	10			
5	r	2	Total	C	N	O		0	0
			28	16	2	10			
5	s	2	Total	C	N	O		0	0
			28	16	2	10			
5	u	2	Total	C	N	O		0	0
			28	16	2	10			
5	w	2	Total	C	N	O		0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
5	z	2	Total	C	N	O	0	0
			28	16	2	10		
5	0	2	Total	C	N	O	0	0
			28	16	2	10		
5	1	2	Total	C	N	O	0	0
			28	16	2	10		
5	3	2	Total	C	N	O	0	0
			28	16	2	10		
5	4	2	Total	C	N	O	0	0
			28	16	2	10		
5	5	2	Total	C	N	O	0	0
			28	16	2	10		
5	AA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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.



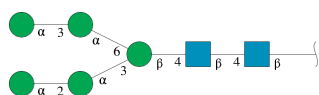
Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	3	Total	C	N	O	0	0
			39	22	2	15		
6	J	3	Total	C	N	O	0	0
			39	22	2	15		
6	K	3	Total	C	N	O	0	0
			39	22	2	15		
6	P	3	Total	C	N	O	0	0
			39	22	2	15		
6	S	3	Total	C	N	O	0	0
			39	22	2	15		
6	U	3	Total	C	N	O	0	0
			39	22	2	15		
6	V	3	Total	C	N	O	0	0
			39	22	2	15		
6	W	3	Total	C	N	O	0	0
			39	22	2	15		
6	a	3	Total	C	N	O	0	0
			39	22	2	15		
6	d	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

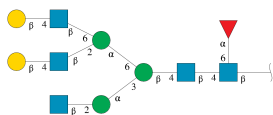
Mol	Chain	Residues	Atoms				AltConf	Trace
6	g	3	Total	C	N	O	0	0
			39	22	2	15		
6	i	3	Total	C	N	O	0	0
			39	22	2	15		
6	j	3	Total	C	N	O	0	0
			39	22	2	15		
6	m	3	Total	C	N	O	0	0
			39	22	2	15		
6	n	3	Total	C	N	O	0	0
			39	22	2	15		
6	t	3	Total	C	N	O	0	0
			39	22	2	15		
6	v	3	Total	C	N	O	0	0
			39	22	2	15		
6	2	3	Total	C	N	O	0	0
			39	22	2	15		
6	7	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



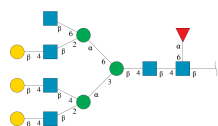
Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	7	Total	C	N	O	0	0
			83	46	2	35		
7	f	7	Total	C	N	O	0	0
			83	46	2	35		
7	y	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 8 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



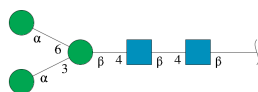
Mol	Chain	Residues	Atoms				AltConf	Trace
8	Y	11	Total 135	C 76	N 5	O 54	0	0
8	9	11	Total 135	C 76	N 5	O 54	0	0

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



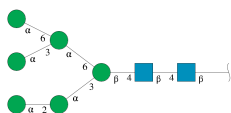
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	13	Total	C	N	O	0	0
			160	90	6	64		

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



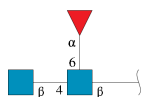
Mol	Chain	Residues	Atoms				AltConf	Trace
10	e	5	Total	C	N	O	0	0
			61	34	2	25		

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



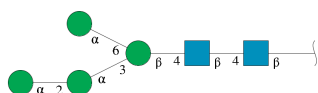
Mol	Chain	Residues	Atoms				AltConf	Trace
11	p	8	Total	C	N	O	0	0
			94	52	2	40		
11	8	8	Total	C	N	O	0	0
			94	52	2	40		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
12	q	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 13 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.



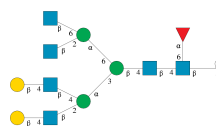
Mol	Chain	Residues	Atoms				AltConf	Trace
13	x	6	Total	C	N	O	0	0
			72	40	2	30		

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



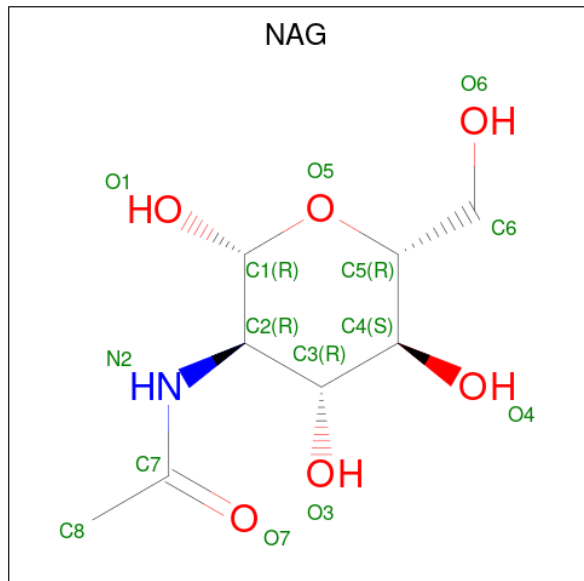
Mol	Chain	Residues	Atoms				AltConf	Trace
14	6	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 15 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
15	BA	12	Total	C	N	O	0	0
			149	84	6	59		

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

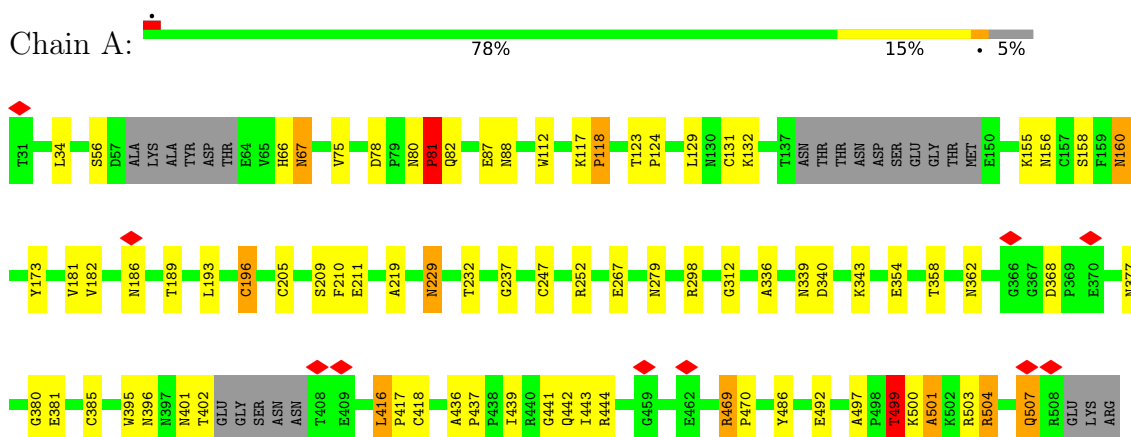
Continued from previous page...

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

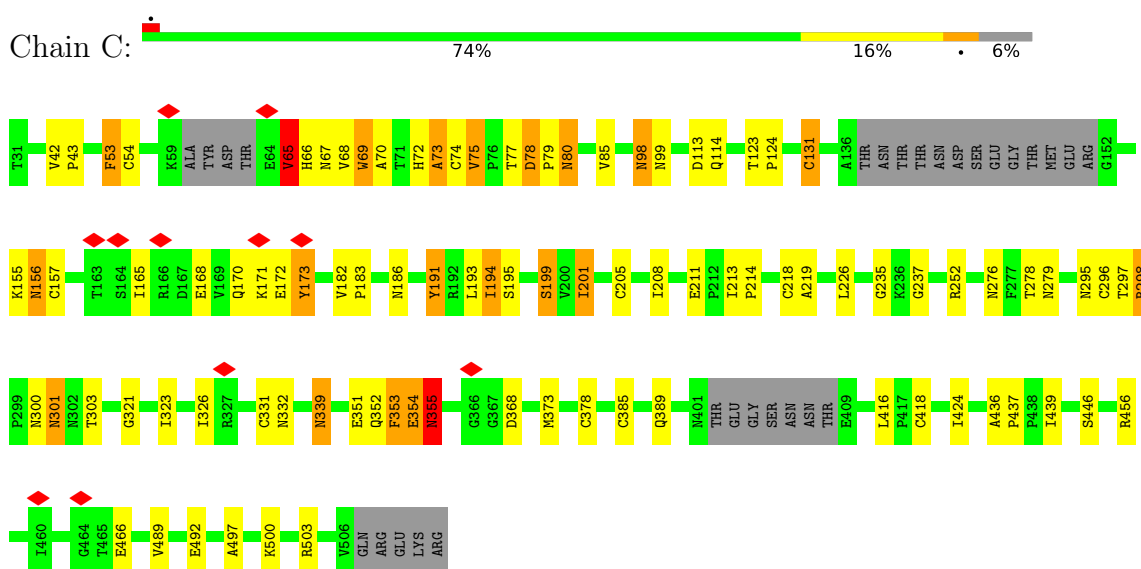
3 Residue-property plots

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

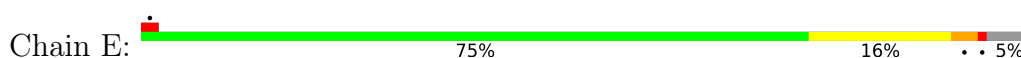
- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160

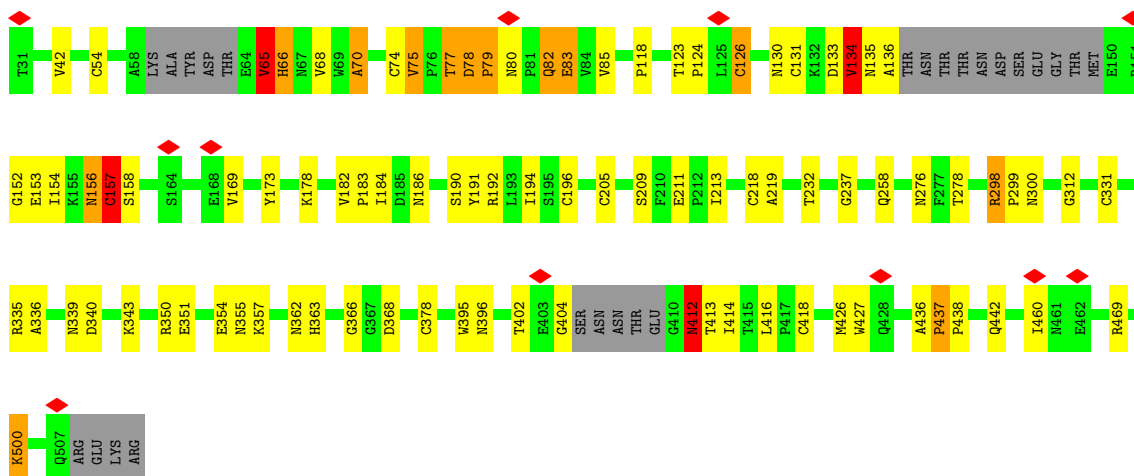


- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160

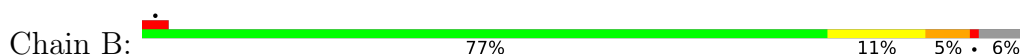


- Molecule 1: HIV-1 ENVELOPE GLYCOPROTEIN GP160

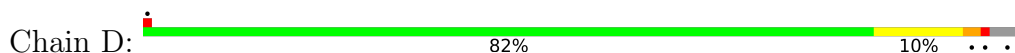




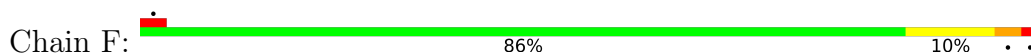
• Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN GP160



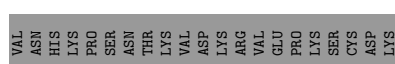
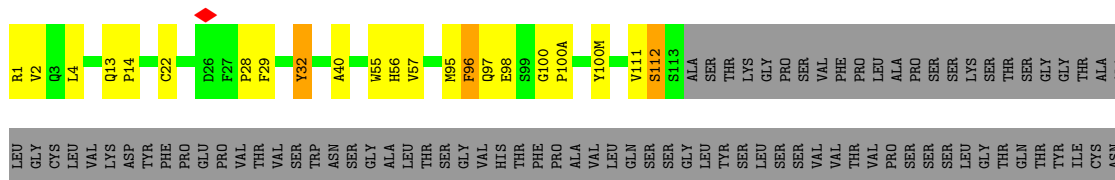
• Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN GP160



• Molecule 2: HIV-1 ENVELOPE GLYCOPROTEIN GP160



• Molecule 3: IMMUNOGLOBULIN G PGT151



• Molecule 3: IMMUNOGLOBULIN G PGT151

[illegible]

Chain L: 47% 48%

Position	Residue	Conservation	Annotations
1	PHE	0.00	
2	TYR	0.00	
3	PRO	0.00	
4	ARG	0.00	
5	GLU	0.00	
6	ALA	0.00	
7	LYS	0.00	
8	VAL	0.00	
9	THR	0.00	
10	LYS	0.00	
11	TRP	0.00	
12	LYS	0.00	
13	PHE	0.00	
14	ASN	0.00	
15	ARG	0.00	
16	ASP	0.00	
17	VAL	0.00	
18	ASN	0.00	
19	ALA	0.00	
20	LEU	0.00	
21	GLN	0.00	
22	SER	0.00	
23	GLY	0.00	
24	ASN	0.00	
25	SER	0.00	
26	GLN	0.00	
27	GLU	0.00	
28	SER	0.00	
29	VAL	0.00	
30	THR	0.00	
31	GLU	0.00	
32	GLN	0.00	
33	ASP	0.00	
34	SER	0.00	
35	LYS	0.00	
36	ASP	0.00	
37	SER	0.00	
38	THR	0.00	
39	TYR	0.00	
40	ALA	0.00	
41	ALA	0.00	
42	PRO	0.00	
43	LEU	0.00	
44	SER	0.00	
45	SER	0.00	
46	VAL	0.00	
47	THR	0.00	
48	PHE	0.00	
49	ILE	0.00	
50	GLY	0.00	
51	THR	0.00	
52	LEU	0.00	
53	SER	0.00	
54	LYS	0.00	
55	ALA	0.00	
56	ASP	0.00	
57	GLU	0.00	
58	THR	0.00	
59	GLY	0.00	
60	LYS	0.00	
61	HIS	0.00	
62	VAL	0.00	
63	THR	0.00	
64	ALA	0.00	
65	SER	0.00	
66	VAL	0.00	
67	CYS	0.00	
68	GLU	0.00	
69	VAL	0.00	
70	CYS	0.00	
71	THR	0.00	
72	LEU	0.00	
73	LEU	0.00	
74	ASN	0.00	
75	ASP	0.00	

Chain N: 45% 5% 49%

HIS	ASN	ASP
GLN	PHE	I2
GLY	TYR	V3
LEU	PRO	M4
SER	ARG	
SER	GLU	Tt14
PRO	ALA	
VAL	LYS	C23
THR	VAL	
LYS	GLN	N28
SER	TRP	G29
PHE	LYS	
ASN	VAL	Y36
ARG	ASP	
GLY	ASN	K39
GLU	ALA	
CYS	LEU	S43
	GLN	
	SER	L46
	GLY	
	ASN	F49
	GLN	E50
	GLU	V51
	SER	S52
	VAL	N53
	THR	R54
	GLN	F55
	GLU	
	ASP	R77
	SER	
	LYS	R108
	ASP	THR
	SER	VAL
	THR	ALA
	TYR	PRO
	SER	SER
	LEU	VAL
	SER	PHE
	SER	ILE
	THR	PHE
	GLY	THR
	LEU	PRO
	THR	PRO
	LEU	SER
	SER	SER
	LYS	ASP
	THR	GLU
	ASP	GLN
	TYR	LEU
	GLU	LYS
	LYS	SER
	HIS	GLY
	LYS	THR
	VAL	ALA
	TYR	SER
	ALA	VAL
	CYS	VAL
	GLU	CYS
	VAL	LEU
	THR	LEU

Chain G: 50% 100%

NAG1
NAG2

Chain Q: 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  50% 50%

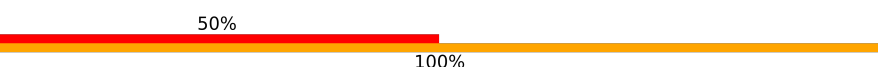


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 100%

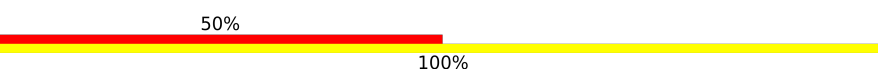


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  50% 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  50% 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



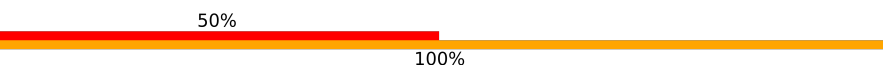


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:  50% 100%

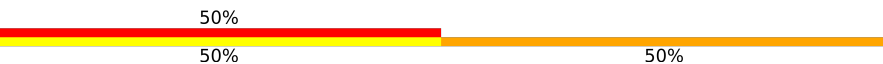


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  50% 100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:  50% 50% 50%

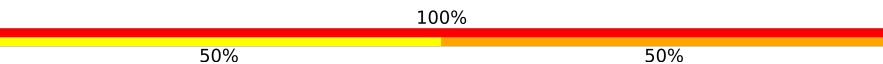


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:  100% 50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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

Chain S:  33% 100%



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

Chain U:  67% 100%



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

Chain V:  67% 33%



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

Chain W:  33% 100%



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

Chain a:  33% 100%



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



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



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



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



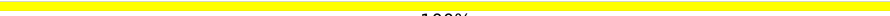
- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain t:  100%

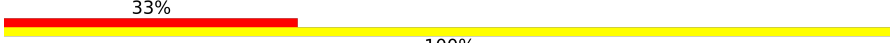
NAG1
NAG2
BMA3

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

Chain v:  33% 67%

NAG1
NAG2
BMA3

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

Chain 2:  33% 100%

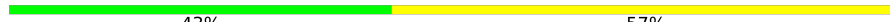
NAG1
NAG2
BMA3

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

Chain 7:  67% 100%

NAG1
NAG2
BMA3

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  43% 57%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  29% 29% 57% 14%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7

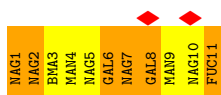
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:  57% 43%



- Molecule 8: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  18% 45% 55%



- Molecule 8: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:  18% 73% 27%



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

Chain Z:  15% 31% 69%



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

Chain e: 



- Molecule 11: 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 p: 



- Molecule 11: 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 8: 



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

Chain q: 



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

Chain x: 



- Molecule 14: 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 6: 



- Molecule 15: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	201386	Depositor
Resolution determination method	Not provided	
CTF correction method	WHOLE MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.034	Depositor
Map size ($\text{\AA}$)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	2/3625 (0.1%)	1.18	49/4921 (1.0%)
1	C	0.85	0/3578	1.21	52/4857 (1.1%)
1	E	0.84	1/3609 (0.0%)	1.18	49/4899 (1.0%)
2	B	0.89	0/1168	0.95	4/1583 (0.3%)
2	D	0.85	0/1178	1.01	11/1597 (0.7%)
2	F	0.91	1/1228 (0.1%)	1.09	10/1665 (0.6%)
3	H	0.82	0/1102	1.12	12/1496 (0.8%)
3	M	0.86	0/1096	1.05	5/1489 (0.3%)
4	L	0.78	0/899	1.03	8/1213 (0.7%)
4	N	0.75	0/884	1.05	8/1192 (0.7%)
All	All	0.84	4/18367 (0.0%)	1.13	208/24912 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	2
1	E	0	5
2	B	0	1
2	D	0	3
2	F	0	2
All	All	0	17

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	ASN	CA-CB	-7.15	1.41	1.53
1	E	118	PRO	N-CD	5.70	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	PRO	N-CD	5.40	1.55	1.47
2	F	599	SER	CA-C	-5.08	1.46	1.52

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	ASN	CA-C-N	9.71	130.47	119.99
1	C	80	ASN	C-N-CA	9.71	130.47	119.99
1	C	237	GLY	CA-C-N	9.10	128.86	119.76
1	C	237	GLY	C-N-CA	9.10	128.86	119.76
1	A	492	GLU	CA-C-N	8.74	129.28	119.32
1	A	492	GLU	C-N-CA	8.74	129.28	119.32
1	C	436	ALA	CA-C-N	8.70	125.92	119.66
1	C	436	ALA	C-N-CA	8.70	125.92	119.66
1	C	75	VAL	CA-C-N	8.62	128.21	119.24
1	C	75	VAL	C-N-CA	8.62	128.21	119.24
3	M	27	PHE	N-CA-C	8.56	115.84	108.13
1	C	352	GLN	N-CA-C	8.42	123.33	112.89
1	C	182	VAL	CA-C-N	8.35	128.86	119.93
1	C	182	VAL	C-N-CA	8.35	128.86	119.93
1	E	65	VAL	N-CA-C	8.21	118.79	110.82
1	C	219	ALA	CA-C-N	8.21	128.09	120.21
1	C	219	ALA	C-N-CA	8.21	128.09	120.21
1	C	368	ASP	CA-C-N	8.17	128.95	119.47
1	C	368	ASP	C-N-CA	8.17	128.95	119.47
1	C	298	ARG	CA-C-N	8.11	129.98	119.84
1	C	298	ARG	C-N-CA	8.11	129.98	119.84
3	H	96	PHE	N-CA-C	8.09	119.72	111.07
2	F	608	VAL	CA-C-N	8.07	127.83	119.76
2	F	608	VAL	C-N-CA	8.07	127.83	119.76
1	E	412	ASN	CA-C-O	-8.07	112.33	120.80
2	D	528	SER	CA-C-O	-7.96	112.88	121.56
4	L	43	SER	CA-C-N	7.88	127.94	119.90
4	L	43	SER	C-N-CA	7.88	127.94	119.90
1	A	237	GLY	CA-C-N	7.86	128.16	119.90
1	A	237	GLY	C-N-CA	7.86	128.16	119.90
1	A	368	ASP	CA-C-N	7.85	128.57	119.47
1	A	368	ASP	C-N-CA	7.85	128.57	119.47
1	E	219	ALA	CA-C-N	7.78	127.73	120.03
1	E	219	ALA	C-N-CA	7.78	127.73	120.03
1	E	500	LYS	N-CA-C	-7.69	101.04	110.88
1	A	78	ASP	CA-C-N	7.67	127.31	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASP	C-N-CA	7.67	127.31	119.56
1	E	368	ASP	CA-C-N	7.64	128.34	119.47
1	E	368	ASP	C-N-CA	7.64	128.34	119.47
1	A	205	CYS	CA-C-N	7.60	128.29	119.47
1	A	205	CYS	C-N-CA	7.60	128.29	119.47
1	A	437	PRO	CA-C-N	7.51	127.44	119.85
1	A	437	PRO	C-N-CA	7.51	127.44	119.85
1	E	205	CYS	CA-C-N	7.50	128.17	119.47
1	E	205	CYS	C-N-CA	7.50	128.17	119.47
1	E	157	CYS	CA-C-O	-7.50	112.44	121.28
1	E	182	VAL	CA-C-N	7.42	127.46	119.90
1	E	182	VAL	C-N-CA	7.42	127.46	119.90
1	C	205	CYS	CA-C-N	7.39	127.74	119.32
1	C	205	CYS	C-N-CA	7.39	127.74	119.32
1	C	353	PHE	N-CA-CB	-7.36	99.24	112.27
1	E	437	PRO	CA-C-N	7.31	127.34	119.89
1	E	437	PRO	C-N-CA	7.31	127.34	119.89
1	E	194	ILE	N-CA-C	7.29	121.23	111.17
1	A	436	ALA	CA-C-N	7.29	127.89	120.38
1	A	436	ALA	C-N-CA	7.29	127.89	120.38
1	C	252	ARG	CA-C-N	7.27	128.92	119.84
1	C	252	ARG	C-N-CA	7.27	128.92	119.84
1	C	492	GLU	CA-C-N	7.26	127.27	119.28
1	C	492	GLU	C-N-CA	7.26	127.27	119.28
1	A	416	LEU	CA-C-N	7.19	127.11	119.85
1	A	416	LEU	C-N-CA	7.19	127.11	119.85
2	F	600	GLY	CA-C-O	-7.11	114.22	121.90
1	A	81	PRO	CA-C-O	-7.11	113.00	121.67
2	F	554	ASN	N-CA-C	7.09	120.04	111.82
3	H	32	TYR	CA-C-N	7.09	127.05	120.03
3	H	32	TYR	C-N-CA	7.09	127.05	120.03
3	H	40	ALA	CA-C-N	6.99	127.14	119.87
3	H	40	ALA	C-N-CA	6.99	127.14	119.87
2	F	617	LYS	N-CA-C	6.97	120.11	110.35
2	B	636	ASP	N-CA-C	6.87	119.35	111.11
1	E	75	VAL	CA-C-N	6.82	126.34	119.24
1	E	75	VAL	C-N-CA	6.82	126.34	119.24
1	E	65	VAL	CA-C-O	-6.82	112.85	120.96
1	C	42	VAL	CA-C-N	6.82	128.36	119.84
1	C	42	VAL	C-N-CA	6.82	128.36	119.84
2	F	616	ASN	CB-CA-C	6.81	121.68	109.29
1	A	219	ALA	CA-C-N	6.79	126.70	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ALA	C-N-CA	6.79	126.70	119.85
1	C	437	PRO	CA-C-N	6.78	127.33	120.14
1	C	437	PRO	C-N-CA	6.78	127.33	120.14
2	D	518	VAL	CA-C-O	-6.76	112.81	121.40
3	H	13	GLN	CA-C-N	6.71	126.67	119.76
3	H	13	GLN	C-N-CA	6.71	126.67	119.76
1	E	237	GLY	CA-C-N	6.64	128.39	120.23
1	E	237	GLY	C-N-CA	6.64	128.39	120.23
1	E	412	ASN	CA-C-N	6.59	134.13	121.54
1	E	412	ASN	C-N-CA	6.59	134.13	121.54
1	A	80	ASN	CA-C-N	6.57	126.49	119.85
1	A	80	ASN	C-N-CA	6.57	126.49	119.85
1	C	497	ALA	CA-C-N	6.52	127.05	120.14
1	C	497	ALA	C-N-CA	6.52	127.05	120.14
1	A	252	ARG	CA-C-N	6.50	126.41	119.85
1	A	252	ARG	C-N-CA	6.50	126.41	119.85
1	C	191	TYR	N-CA-C	6.46	116.99	107.88
1	A	385	CYS	N-CA-CB	-6.46	100.90	110.85
2	D	608	VAL	CA-C-N	6.43	126.19	119.76
2	D	608	VAL	C-N-CA	6.43	126.19	119.76
1	A	186	ASN	CB-CA-C	-6.40	109.18	116.54
1	A	182	VAL	CA-C-N	6.34	126.10	119.76
1	A	182	VAL	C-N-CA	6.34	126.10	119.76
1	E	42	VAL	N-CA-C	6.32	114.14	107.76
1	A	507	GLN	CA-C-O	-6.29	114.01	121.11
2	F	546	SER	N-CA-C	6.27	116.14	107.73
2	F	598	CYS	N-CA-CB	-6.23	102.29	111.51
1	C	157	CYS	N-CA-CB	-6.22	100.86	110.56
2	F	518	VAL	CA-C-O	-6.19	113.04	120.78
1	E	157	CYS	CA-C-N	6.17	132.81	121.70
1	E	157	CYS	C-N-CA	6.17	132.81	121.70
1	C	211	GLU	CA-C-N	6.12	126.32	119.90
1	C	211	GLU	C-N-CA	6.12	126.32	119.90
2	D	518	VAL	O-C-N	-6.09	116.65	122.98
1	C	65	VAL	CA-C-O	-6.07	113.20	120.78
1	E	416	LEU	CA-C-N	6.03	126.23	119.90
1	E	416	LEU	C-N-CA	6.03	126.23	119.90
1	E	213	ILE	CA-C-N	6.01	125.77	119.76
1	E	213	ILE	C-N-CA	6.01	125.77	119.76
1	A	470	PRO	CA-C-N	-6.01	117.53	122.16
1	A	470	PRO	C-N-CA	-6.01	117.53	122.16
3	H	95	MET	CA-C-N	5.99	128.23	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	95	MET	C-N-CA	5.99	128.23	120.44
1	E	131	CYS	N-CA-C	5.95	116.26	107.88
3	H	22	CYS	N-CA-CB	-5.89	101.53	110.77
1	C	78	ASP	CA-C-N	5.88	127.19	119.84
1	C	78	ASP	C-N-CA	5.88	127.19	119.84
2	D	528	SER	CA-C-N	5.86	132.25	121.70
2	D	528	SER	C-N-CA	5.86	132.25	121.70
1	A	312	GLY	CA-C-N	5.80	127.09	119.84
1	A	312	GLY	C-N-CA	5.80	127.09	119.84
1	C	416	LEU	CA-C-N	5.77	126.06	119.83
1	C	416	LEU	C-N-CA	5.77	126.06	119.83
1	C	131	CYS	N-CA-CB	-5.75	101.71	111.31
4	N	36	TYR	N-CA-C	5.71	115.93	107.88
1	A	196	CYS	N-CA-CB	-5.70	101.44	110.22
1	A	418	CYS	N-CA-CB	-5.67	102.43	111.62
4	L	9	LEU	N-CA-C	5.67	118.23	111.71
2	D	528	SER	O-C-N	-5.65	116.19	122.86
1	C	218	CYS	N-CA-CB	-5.65	102.45	111.43
4	N	14	THR	CA-C-N	5.64	126.53	119.98
4	N	14	THR	C-N-CA	5.64	126.53	119.98
2	F	604	CYS	N-CA-CB	-5.62	102.85	111.56
4	N	39	LYS	CA-C-N	5.62	126.86	119.84
4	N	39	LYS	C-N-CA	5.62	126.86	119.84
1	A	186	ASN	N-CA-C	5.61	116.83	108.31
1	E	131	CYS	N-CA-CB	-5.58	101.67	111.49
1	C	201	ILE	CA-C-N	-5.57	115.01	122.42
1	C	201	ILE	C-N-CA	-5.57	115.01	122.42
3	M	40	ALA	CA-C-N	5.55	126.78	119.84
3	M	40	ALA	C-N-CA	5.55	126.78	119.84
1	E	82	GLN	CA-C-O	5.54	121.16	117.94
1	E	54	CYS	N-CA-CB	-5.52	101.42	110.52
2	D	604	CYS	N-CA-CB	-5.51	102.30	110.90
1	E	312	GLY	CA-C-N	5.51	126.73	119.84
1	E	312	GLY	C-N-CA	5.51	126.73	119.84
4	L	23	CYS	N-CA-CB	-5.51	102.31	110.90
1	E	436	ALA	CA-C-N	5.46	126.01	120.38
1	E	436	ALA	C-N-CA	5.46	126.01	120.38
2	B	608	VAL	CA-C-N	5.46	125.77	119.93
2	B	608	VAL	C-N-CA	5.46	125.77	119.93
1	E	218	CYS	N-CA-CB	-5.45	102.77	111.43
1	E	77	THR	N-CA-C	5.44	118.49	109.46
1	A	88	ASN	N-CA-C	5.40	119.03	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	13	GLN	CA-C-N	5.40	125.33	119.76
3	M	13	GLN	C-N-CA	5.40	125.33	119.76
1	A	81	PRO	CA-C-N	5.39	131.40	121.70
1	A	81	PRO	C-N-CA	5.39	131.40	121.70
1	E	80	ASN	CA-C-N	-5.37	114.06	120.13
1	E	80	ASN	C-N-CA	-5.37	114.06	120.13
1	E	412	ASN	O-C-N	-5.37	115.88	122.11
1	C	385	CYS	N-CA-CB	-5.35	102.28	110.85
1	C	131	CYS	N-CA-C	5.34	116.39	108.86
1	A	469	ARG	CA-C-N	5.32	126.49	119.84
1	A	469	ARG	C-N-CA	5.32	126.49	119.84
1	A	181	VAL	N-CA-C	5.29	117.25	108.99
1	A	486	TYR	N-CA-C	5.29	118.37	109.95
1	E	331	CYS	N-CA-CB	-5.27	102.74	110.85
2	B	598	CYS	N-CA-CB	-5.26	102.79	110.47
1	E	186	ASN	CB-CA-C	-5.25	110.09	117.23
3	H	100	GLY	N-CA-C	-5.24	105.89	112.23
1	C	98	ASN	N-CA-C	5.22	117.46	107.75
1	E	366	GLY	N-CA-C	-5.21	106.02	112.33
1	E	196	CYS	N-CA-CB	-5.20	101.75	110.39
4	N	43	SER	CA-C-N	-5.20	114.41	119.76
4	N	43	SER	C-N-CA	-5.20	114.41	119.76
1	A	385	CYS	N-CA-C	5.18	118.17	110.14
1	C	113	ASP	N-CA-C	-5.18	105.53	111.07
1	A	81	PRO	O-C-N	-5.16	116.71	123.06
1	C	418	CYS	N-CA-CB	-5.16	102.26	111.08
1	C	424	ILE	N-CA-C	5.15	115.27	107.80
4	L	17	GLN	CA-C-N	5.14	125.07	119.78
4	L	17	GLN	C-N-CA	5.14	125.07	119.78
1	E	418	CYS	N-CA-CB	-5.12	102.32	111.08
1	A	267	GLU	N-CA-C	5.10	116.65	111.14
1	A	56	SER	N-CA-C	5.09	114.96	108.24
4	N	23	CYS	N-CA-CB	-5.09	102.78	110.77
4	L	14	THR	CA-C-N	5.08	126.19	119.84
4	L	14	THR	C-N-CA	5.08	126.19	119.84
1	C	186	ASN	CB-CA-C	-5.06	110.34	117.23
1	A	497	ALA	CA-C-N	5.06	126.39	120.98
1	A	497	ALA	C-N-CA	5.06	126.39	120.98
1	C	157	CYS	N-CA-C	5.05	118.24	110.42
1	A	247	CYS	N-CA-CB	-5.04	102.58	111.39
1	C	235	GLY	N-CA-C	-5.03	108.38	114.92
1	E	298	ARG	CA-C-N	5.03	126.13	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	298	ARG	C-N-CA	5.03	126.13	119.84
3	H	100(A)	PRO	N-CA-C	-5.02	104.57	110.70
2	D	518	VAL	CA-C-N	5.01	130.72	121.70
2	D	518	VAL	C-N-CA	5.01	130.72	121.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	THR	Mainchain
1	A	507	GLN	Mainchain
1	A	81	PRO	Mainchain,Peptide
2	B	600	GLY	Mainchain
1	C	65	VAL	Mainchain,Peptide
2	D	518	VAL	Mainchain
2	D	528	SER	Mainchain
2	D	600	GLY	Mainchain
1	E	157	CYS	Mainchain
1	E	412	ASN	Mainchain,Peptide
1	E	65	VAL	Mainchain
1	E	66	HIS	Mainchain
2	F	518	VAL	Mainchain
2	F	600	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3553	0	3481	130	0
1	C	3506	0	3441	161	0
1	E	3537	0	3463	157	0
2	B	1150	0	1132	46	0
2	D	1159	0	1148	42	0
2	F	1209	0	1197	39	0
3	H	1073	0	1040	39	0
3	M	1067	0	1029	42	0
4	L	881	0	868	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	866	0	854	15	0
5	0	28	0	25	0	0
5	1	28	0	25	2	0
5	3	28	0	25	13	0
5	4	28	0	25	15	0
5	5	28	0	25	5	0
5	AA	28	0	25	0	0
5	G	28	0	25	9	0
5	Q	28	0	25	3	0
5	R	28	0	25	6	0
5	T	28	0	25	12	0
5	X	28	0	25	2	0
5	b	28	0	25	0	0
5	c	28	0	25	20	0
5	h	28	0	25	0	0
5	k	28	0	25	0	0
5	l	28	0	25	6	0
5	o	28	0	25	13	0
5	r	28	0	25	1	0
5	s	28	0	25	2	0
5	u	28	0	25	0	0
5	w	28	0	25	14	0
5	z	28	0	25	3	0
6	2	39	0	34	0	0
6	7	39	0	34	7	0
6	I	39	0	34	26	0
6	J	39	0	34	1	0
6	K	39	0	34	5	0
6	P	39	0	34	3	0
6	S	39	0	34	0	0
6	U	39	0	34	0	0
6	V	39	0	34	4	0
6	W	39	0	34	9	0
6	a	39	0	34	0	0
6	d	39	0	34	14	0
6	g	39	0	34	3	0
6	i	39	0	34	18	0
6	j	39	0	34	6	0
6	m	39	0	34	0	0
6	n	39	0	34	7	0
6	t	39	0	34	0	0
6	v	39	0	34	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	83	0	70	3	0
7	f	83	0	70	7	0
7	y	83	0	70	1	0
8	9	135	0	115	12	0
8	Y	135	0	115	8	0
9	Z	160	0	136	32	0
10	e	61	0	52	15	0
11	8	94	0	79	4	0
11	p	94	0	79	3	0
12	q	38	0	34	14	0
13	x	72	0	61	4	0
14	6	50	0	43	6	0
15	BA	149	0	127	18	0
16	A	42	0	39	6	0
16	B	28	0	26	0	0
16	C	14	0	13	0	0
16	D	14	0	13	0	0
16	E	28	0	26	11	0
16	F	14	0	13	0	0
All	All	20735	0	20030	713	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 17.

All (713) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:TYR:CD1	6:I:1:NAG:H82	1.21	1.65
1:A:173:TYR:CG	6:I:1:NAG:H82	1.30	1.60
1:A:210:PHE:CD2	1:A:380:GLY:HA2	1.35	1.56
1:E:183:PRO:CA	1:E:191:TYR:CD1	1.87	1.56
3:H:98:GLU:CD	15:BA:2:NAG:H62	1.31	1.55
1:A:395:TRP:HH2	5:T:1:NAG:C8	1.20	1.54
14:6:2:NAG:C8	6:7:1:NAG:H83	1.37	1.52
1:A:210:PHE:CE2	1:A:380:GLY:HA2	1.44	1.52
1:E:183:PRO:HA	1:E:191:TYR:CD1	1.00	1.52
2:B:522:PHE:CD1	2:B:544:LEU:HD13	1.47	1.46
1:A:298:ARG:HE	1:A:443:ILE:CD1	1.28	1.43
1:A:395:TRP:CH2	5:T:1:NAG:H81	1.54	1.40
1:C:323:ILE:CD1	6:i:1:NAG:H83	1.50	1.39
1:A:87:GLU:CD	5:G:1:NAG:H81	1.50	1.37

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:THR:HG22	6:j:1:NAG:C8	1.52	1.36
1:E:169:VAL:CG1	5:w:1:NAG:H82	1.55	1.36
1:A:298:ARG:NE	1:A:443:ILE:CD1	1.86	1.35
1:A:173:TYR:CD1	6:I:1:NAG:C8	2.10	1.35
2:D:638:TYR:CE1	12:q:3:FUC:C6	2.11	1.32
3:H:55:TRP:CD1	3:H:100(M):TYR:HH	1.47	1.31
1:E:351:GLU:CA	5:4:1:NAG:H81	1.59	1.31
1:A:298:ARG:NE	1:A:443:ILE:HD12	1.00	1.30
1:C:301:ASN:OD1	1:C:323:ILE:HB	1.22	1.30
1:A:173:TYR:CG	6:I:1:NAG:C8	2.14	1.30
1:E:183:PRO:HA	1:E:191:TYR:CE1	1.67	1.29
1:A:401:ASN:HB2	16:A:1397:NAG:O6	1.15	1.29
1:E:183:PRO:CA	1:E:191:TYR:CE1	2.16	1.28
14:6:2:NAG:H81	6:7:1:NAG:C8	1.62	1.28
1:A:395:TRP:CH2	5:T:1:NAG:C8	2.12	1.27
2:D:638:TYR:CE1	12:q:3:FUC:H63	1.66	1.27
3:M:98:GLU:CD	9:Z:2:NAG:H62	1.59	1.26
3:M:98:GLU:OE2	9:Z:2:NAG:H62	1.35	1.25
1:E:134:VAL:HG12	1:E:135:ASN:ND2	1.49	1.25
1:E:183:PRO:HB3	1:E:191:TYR:CE1	1.72	1.23
2:D:638:TYR:CD1	12:q:3:FUC:C6	2.21	1.22
1:E:169:VAL:HB	5:w:1:NAG:C8	1.70	1.22
1:A:210:PHE:CD2	1:A:380:GLY:CA	2.23	1.22
1:E:134:VAL:CG1	1:E:135:ASN:HD22	1.51	1.22
1:C:173:TYR:CD2	5:c:1:NAG:H4	1.76	1.20
1:E:355:ASN:HB2	1:E:357:LYS:CG	1.72	1.20
1:E:351:GLU:N	5:4:1:NAG:H81	1.55	1.20
2:D:638:TYR:CD1	12:q:3:FUC:H62	1.76	1.19
14:6:2:NAG:C8	6:7:1:NAG:C8	2.19	1.19
1:C:170:GLN:OE1	6:d:1:NAG:H2	1.40	1.18
1:C:323:ILE:CG1	6:i:1:NAG:H83	1.73	1.18
1:E:183:PRO:CB	1:E:191:TYR:CE1	2.26	1.18
1:E:183:PRO:HA	1:E:191:TYR:CG	1.80	1.17
1:C:53:PHE:CE1	1:C:75:VAL:HG21	1.80	1.15
1:E:184:ILE:N	1:E:191:TYR:HD1	1.42	1.15
1:A:87:GLU:OE2	5:G:1:NAG:H81	1.47	1.15
1:E:169:VAL:HG12	5:w:1:NAG:H82	1.26	1.14
1:C:297:THR:CG2	6:j:1:NAG:H82	1.76	1.14
1:C:323:ILE:HG13	6:i:1:NAG:N2	1.61	1.13
1:E:395:TRP:CH2	5:3:1:NAG:H81	1.84	1.13
1:C:323:ILE:HG13	6:i:1:NAG:C8	1.77	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ILE:CG1	6:i:1:NAG:C8	2.28	1.12
1:E:351:GLU:HA	5:4:1:NAG:H81	1.16	1.12
1:A:210:PHE:CE2	1:A:380:GLY:CA	2.32	1.12
1:A:336:ALA:HB2	5:T:1:NAG:O6	1.49	1.11
1:A:173:TYR:HB3	6:I:1:NAG:HN2	1.12	1.11
1:E:350:ARG:C	5:4:1:NAG:C8	2.22	1.11
1:C:323:ILE:HD11	6:i:1:NAG:H83	1.17	1.10
1:A:87:GLU:CD	5:G:1:NAG:C8	2.25	1.10
6:V:2:NAG:C8	6:W:1:NAG:H83	1.82	1.09
1:E:355:ASN:HB2	1:E:357:LYS:HG2	1.26	1.09
6:V:2:NAG:H82	6:W:1:NAG:H83	1.33	1.09
3:H:98:GLU:CD	15:BA:2:NAG:C6	2.26	1.07
1:C:168:GLU:CG	6:d:1:NAG:H82	1.83	1.07
1:E:343:LYS:HE3	5:3:1:NAG:H82	1.36	1.07
1:C:85:VAL:CG2	10:e:2:NAG:H82	1.84	1.07
1:C:389:GLN:NE2	5:o:1:NAG:H81	1.69	1.05
1:C:173:TYR:CE1	5:c:1:NAG:O3	2.09	1.04
1:E:184:ILE:N	1:E:191:TYR:CD1	2.17	1.04
1:E:190:SER:O	1:E:191:TYR:CD1	2.10	1.04
1:E:350:ARG:C	5:4:1:NAG:H81	1.82	1.03
3:H:98:GLU:OE1	15:BA:2:NAG:H62	1.56	1.03
1:A:339:ASN:OD1	1:A:340:ASP:N	1.90	1.02
1:C:323:ILE:HG13	6:i:1:NAG:C7	1.89	1.02
1:A:229:ASN:HB3	6:K:1:NAG:O6	1.59	1.02
1:E:169:VAL:CB	5:w:1:NAG:H82	1.88	1.02
1:A:173:TYR:CD2	6:I:1:NAG:C7	2.43	1.01
1:A:229:ASN:CB	6:K:1:NAG:O6	2.08	1.01
1:E:183:PRO:C	1:E:191:TYR:CD1	2.37	1.01
1:A:401:ASN:CB	16:A:1397:NAG:O6	2.08	1.01
1:E:357:LYS:HD2	16:E:1397:NAG:C8	1.89	1.01
1:C:53:PHE:HE1	1:C:75:VAL:CG2	1.74	1.00
2:B:522:PHE:CD1	2:B:544:LEU:CD1	2.44	1.00
1:C:173:TYR:CD1	5:c:1:NAG:H2	1.96	1.00
1:C:173:TYR:CZ	5:c:1:NAG:O3	2.15	1.00
13:x:3:BMA:H4	11:8:5:MAN:O2	1.60	1.00
1:C:53:PHE:CE1	1:C:75:VAL:CG2	2.44	1.00
1:E:169:VAL:CB	5:w:1:NAG:C8	2.38	1.00
1:C:323:ILE:HD11	6:i:1:NAG:C8	1.92	0.99
1:A:442:GLN:NE2	5:R:1:NAG:C8	2.25	0.99
1:E:395:TRP:CH2	5:3:1:NAG:C8	2.45	0.99
3:M:98:GLU:HG3	9:Z:2:NAG:H5	1.44	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:PHE:H	2:B:544:LEU:CD1	1.75	0.99
1:E:500:LYS:HE3	2:F:619:LEU:HD12	1.43	0.99
1:A:395:TRP:HH2	5:T:1:NAG:H82	1.25	0.99
1:C:85:VAL:HG21	10:e:2:NAG:H82	1.44	0.98
1:E:350:ARG:C	5:4:1:NAG:H82	1.88	0.98
1:C:323:ILE:CD1	6:i:1:NAG:C8	2.42	0.98
1:C:500:LYS:HE3	2:F:663:LEU:HD11	1.42	0.98
1:A:442:GLN:NE2	5:R:1:NAG:H82	1.79	0.97
1:A:395:TRP:HH2	5:T:1:NAG:H81	0.81	0.97
7:f:1:NAG:H61	7:f:2:NAG:H82	1.47	0.97
1:E:158:SER:OG	6:v:1:NAG:H83	1.63	0.96
1:E:351:GLU:HA	5:4:1:NAG:C8	1.93	0.96
2:D:638:TYR:HE1	12:q:3:FUC:H63	1.05	0.96
1:A:298:ARG:CZ	1:A:443:ILE:CD1	2.44	0.96
7:O:1:NAG:H61	7:O:2:NAG:H82	1.47	0.96
1:E:350:ARG:O	5:4:1:NAG:C8	2.13	0.95
2:F:641:GLU:OE1	8:9:11:FUC:H62	1.65	0.95
1:C:295:ASN:OD1	1:C:446:SER:HB2	1.66	0.95
1:C:301:ASN:OD1	1:C:323:ILE:CB	2.13	0.95
1:E:343:LYS:CE	5:3:1:NAG:H82	1.97	0.95
1:C:168:GLU:HG3	6:d:1:NAG:H82	1.47	0.94
1:C:323:ILE:HG13	6:i:1:NAG:HN2	1.17	0.94
2:D:638:TYR:HD1	12:q:3:FUC:H62	1.30	0.94
2:B:522:PHE:HD1	2:B:544:LEU:HD13	1.16	0.93
7:y:1:NAG:H61	7:y:2:NAG:H82	1.47	0.93
1:A:298:ARG:CZ	1:A:443:ILE:HD12	1.99	0.93
1:C:354:GLU:O	1:C:355:ASN:ND2	2.02	0.93
3:M:100(C):ARG:NH1	3:M:100(E):ASP:OD1	2.01	0.93
6:n:2:NAG:C8	5:o:1:NAG:H83	1.98	0.92
1:C:297:THR:HG22	6:j:1:NAG:H82	0.95	0.92
1:E:134:VAL:HB	1:E:135:ASN:HB2	1.51	0.92
1:E:395:TRP:HH2	5:3:1:NAG:C8	1.80	0.92
4:N:55:PHE:HZ	9:Z:5:NAG:H62	1.34	0.92
1:E:169:VAL:O	5:w:1:NAG:H81	1.69	0.92
2:B:522:PHE:H	2:B:544:LEU:HD12	1.33	0.92
1:A:354:GLU:HB3	16:A:1355:NAG:H82	1.51	0.91
1:A:210:PHE:HD2	1:A:380:GLY:HA2	1.32	0.91
1:C:353:PHE:CZ	1:C:456:ARG:NH1	2.37	0.91
1:C:354:GLU:C	1:C:355:ASN:ND2	2.28	0.91
1:C:500:LYS:HG3	2:F:663:LEU:CD1	2.01	0.90
3:M:28:PRO:CD	9:Z:7:NAG:O7	2.19	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:98:GLU:OE1	15:BA:2:NAG:C6	2.17	0.90
3:M:98:GLU:CG	9:Z:2:NAG:H62	2.02	0.90
1:A:173:TYR:CG	6:I:1:NAG:C7	2.55	0.90
1:A:444:ARG:NH2	5:Q:1:NAG:O6	2.05	0.89
1:E:183:PRO:C	1:E:191:TYR:HD1	1.75	0.89
1:A:87:GLU:OE1	5:G:1:NAG:C7	2.20	0.88
1:A:210:PHE:CD1	1:A:377:ASN:ND2	2.40	0.88
9:Z:4:MAN:H62	9:Z:7:NAG:HN2	1.38	0.88
1:E:357:LYS:CD	16:E:1397:NAG:C8	2.52	0.88
1:A:87:GLU:OE1	5:G:1:NAG:H81	1.71	0.88
1:E:169:VAL:CG1	5:w:1:NAG:C8	2.49	0.88
3:H:98:GLU:HB2	15:BA:2:NAG:H5	1.56	0.88
3:H:32:TYR:CE1	3:H:98:GLU:HG2	2.10	0.87
1:C:351:GLU:HA	5:l:1:NAG:H81	1.53	0.87
1:C:172:GLU:C	1:C:173:TYR:HD1	1.83	0.86
1:A:298:ARG:CD	1:A:443:ILE:HD12	2.05	0.86
15:BA:4:MAN:H62	15:BA:7:NAG:N2	1.90	0.86
1:C:295:ASN:OD1	1:C:446:SER:CB	2.23	0.86
1:C:297:THR:CG2	6:j:1:NAG:C8	2.43	0.86
1:C:168:GLU:HG3	6:d:1:NAG:C8	2.04	0.86
1:C:500:LYS:HG3	2:F:663:LEU:HD13	1.55	0.86
3:H:55:TRP:CD1	3:H:100(M):TYR:OH	2.27	0.86
4:N:55:PHE:HE2	9:Z:6:GAL:O2	1.58	0.86
1:E:357:LYS:HD2	16:E:1397:NAG:H83	1.58	0.86
1:C:323:ILE:CG1	6:i:1:NAG:HN2	1.88	0.86
1:E:183:PRO:HB3	1:E:191:TYR:CZ	2.10	0.86
1:E:357:LYS:CD	16:E:1397:NAG:H83	2.05	0.85
1:C:297:THR:HG22	6:j:1:NAG:H83	1.56	0.85
1:A:210:PHE:HD2	1:A:380:GLY:CA	1.86	0.85
14:6:2:NAG:H82	6:7:1:NAG:C8	2.06	0.85
1:C:389:GLN:HE22	5:o:1:NAG:H81	1.39	0.84
1:A:395:TRP:CH2	5:T:1:NAG:H82	2.03	0.84
1:E:355:ASN:CB	1:E:357:LYS:HG2	2.06	0.84
3:H:98:GLU:OE2	15:BA:2:NAG:H62	1.76	0.84
2:B:542:ARG:CZ	2:B:542:ARG:HB2	2.06	0.84
1:A:442:GLN:HE21	5:R:1:NAG:H82	1.42	0.84
2:D:638:TYR:CE1	12:q:3:FUC:H61	2.09	0.84
1:A:87:GLU:OE1	5:G:1:NAG:C8	2.23	0.84
1:E:469:ARG:NH2	5:5:1:NAG:O6	2.11	0.84
1:C:389:GLN:HE22	5:o:1:NAG:C7	1.90	0.84
3:M:98:GLU:HG3	9:Z:2:NAG:C5	2.08	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:GLU:CD	8:Y:11:FUC:H4	2.02	0.83
3:H:2:VAL:HG12	3:H:2:VAL:O	1.76	0.83
3:M:100(N):TYR:HE2	4:N:28:ASN:ND2	1.75	0.83
1:C:500:LYS:HE3	2:F:663:LEU:CD1	2.09	0.83
1:C:353:PHE:CE1	1:C:456:ARG:NH1	2.47	0.83
9:Z:4:MAN:H62	9:Z:7:NAG:N2	1.93	0.83
1:A:210:PHE:CE1	1:A:377:ASN:ND2	2.46	0.83
1:E:336:ALA:O	1:E:339:ASN:OD1	1.97	0.82
3:M:98:GLU:CD	9:Z:2:NAG:C6	2.48	0.82
1:A:401:ASN:HB2	16:A:1397:NAG:HO6	1.01	0.82
1:C:500:LYS:CE	2:F:663:LEU:HD11	2.10	0.82
3:H:55:TRP:HD1	3:H:100(M):TYR:OH	1.61	0.81
1:C:168:GLU:CD	6:d:1:NAG:H82	2.04	0.81
3:M:28:PRO:HD3	9:Z:7:NAG:O7	1.79	0.81
15:BA:4:MAN:H62	15:BA:7:NAG:HN2	1.46	0.81
3:H:57:VAL:O	8:9:6:GAL:H61	1.80	0.81
1:C:389:GLN:HE22	5:o:1:NAG:C8	1.92	0.80
1:A:87:GLU:OE1	5:G:1:NAG:O7	2.00	0.80
3:H:55:TRP:CZ3	8:9:2:NAG:O3	2.34	0.80
1:A:298:ARG:NH2	1:A:443:ILE:HD11	1.96	0.80
1:A:173:TYR:CB	6:I:1:NAG:HN2	1.93	0.80
3:M:98:GLU:OE2	9:Z:2:NAG:C6	2.26	0.80
1:C:389:GLN:NE2	5:o:1:NAG:C8	2.44	0.79
1:C:173:TYR:CG	5:c:1:NAG:H2	2.18	0.79
1:C:168:GLU:OE2	6:d:1:NAG:H82	1.83	0.79
1:C:500:LYS:HE3	2:F:663:LEU:HD21	1.65	0.79
1:A:173:TYR:CE1	6:I:1:NAG:C8	2.66	0.78
1:C:173:TYR:OH	5:c:2:NAG:H5	1.84	0.78
1:A:173:TYR:HB3	6:I:1:NAG:N2	1.95	0.78
1:E:169:VAL:HB	5:w:1:NAG:H81	1.66	0.78
1:A:173:TYR:CE1	6:I:1:NAG:H82	2.11	0.78
1:C:85:VAL:HG13	10:e:1:NAG:O6	1.85	0.77
1:E:351:GLU:N	5:4:1:NAG:C8	2.36	0.77
3:M:100(G):TRP:O	3:M:100(G):TRP:CE3	2.38	0.76
4:N:55:PHE:CZ	9:Z:5:NAG:H62	2.20	0.76
1:A:298:ARG:CZ	1:A:443:ILE:HD11	2.14	0.76
1:C:173:TYR:CG	5:c:1:NAG:H4	2.21	0.76
1:E:355:ASN:CB	1:E:357:LYS:CG	2.60	0.75
1:A:401:ASN:CB	16:A:1397:NAG:HO6	1.92	0.75
1:A:298:ARG:NH2	1:A:443:ILE:CD1	2.50	0.75
2:B:522:PHE:N	2:B:544:LEU:CD1	2.50	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:VAL:HG23	10:e:2:NAG:H82	1.69	0.74
1:C:339:ASN:OD1	1:C:339:ASN:C	2.29	0.74
1:A:343:LYS:HE3	5:T:1:NAG:H82	1.68	0.74
1:E:173:TYR:CG	6:v:1:NAG:H2	2.23	0.74
2:F:641:GLU:OE1	8:9:11:FUC:C6	2.35	0.74
2:B:641:GLU:OE2	8:Y:11:FUC:H4	1.87	0.74
1:E:190:SER:O	1:E:191:TYR:CG	2.40	0.74
1:C:173:TYR:CE2	5:c:1:NAG:H4	2.22	0.74
1:A:156:ASN:OD1	6:I:1:NAG:O7	2.05	0.74
1:A:173:TYR:CD2	6:I:1:NAG:C8	2.71	0.74
3:M:98:GLU:CG	9:Z:2:NAG:C6	2.65	0.74
3:M:98:GLU:HG3	9:Z:2:NAG:C6	2.18	0.73
6:V:2:NAG:H81	6:W:1:NAG:H83	1.67	0.73
1:A:173:TYR:CD2	6:I:1:NAG:N2	2.56	0.73
1:A:442:GLN:NE2	5:R:1:NAG:H81	2.02	0.73
1:C:168:GLU:CG	6:d:1:NAG:C8	2.62	0.73
1:E:156:ASN:CG	1:E:156:ASN:O	2.30	0.73
1:E:343:LYS:HE3	5:3:1:NAG:C8	2.17	0.73
1:C:354:GLU:O	1:C:355:ASN:CG	2.31	0.73
1:A:298:ARG:HE	1:A:443:ILE:CG1	2.00	0.73
1:E:500:LYS:HE3	2:F:619:LEU:CD1	2.18	0.73
6:n:2:NAG:C8	5:o:1:NAG:C8	2.67	0.73
3:H:55:TRP:HD1	3:H:100(M):TYR:HH	0.78	0.73
8:Y:6:GAL:O3	13:x:6:MAN:O2	2.00	0.73
1:E:134:VAL:CB	1:E:135:ASN:HB2	2.19	0.72
1:E:442:GLN:OE1	5:1:1:NAG:C8	2.36	0.72
4:N:55:PHE:CE2	9:Z:6:GAL:O2	2.38	0.72
5:z:1:NAG:H62	5:z:2:NAG:H82	1.71	0.72
3:H:1:ARG:HA	3:H:2:VAL:HB	1.71	0.72
1:A:354:GLU:CB	16:A:1355:NAG:H82	2.19	0.72
1:C:85:VAL:CG2	10:e:2:NAG:C8	2.67	0.72
3:H:32:TYR:CZ	3:H:98:GLU:HG2	2.24	0.72
1:E:78:ASP:HB2	1:E:79:PRO:HA	1.72	0.72
1:E:134:VAL:HG12	1:E:135:ASN:HD22	0.65	0.72
6:P:1:NAG:H62	6:P:2:NAG:H82	1.71	0.72
2:B:522:PHE:HD1	2:B:544:LEU:CD1	1.96	0.71
1:E:339:ASN:OD1	1:E:340:ASP:N	2.23	0.71
6:g:1:NAG:H62	6:g:2:NAG:H82	1.71	0.71
1:E:395:TRP:HH2	5:3:1:NAG:H82	1.56	0.70
1:A:209:SER:OG	7:O:4:MAN:H61	1.91	0.70
1:C:85:VAL:HG22	10:e:1:NAG:O6	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:6:2:NAG:H81	6:7:1:NAG:H83	0.72	0.70
1:E:357:LYS:NZ	16:E:1397:NAG:H83	2.07	0.70
1:C:354:GLU:C	1:C:355:ASN:HD22	1.97	0.70
1:C:172:GLU:C	1:C:173:TYR:CD1	2.69	0.69
3:M:98:GLU:HG2	9:Z:2:NAG:O4	1.92	0.69
1:A:336:ALA:HB2	5:T:1:NAG:HO6	1.57	0.69
1:C:389:GLN:HE21	5:o:1:NAG:H81	1.54	0.69
1:E:355:ASN:HB2	1:E:357:LYS:CA	2.23	0.69
6:V:2:NAG:H82	6:W:1:NAG:C8	2.18	0.69
1:E:133:ASP:C	1:E:134:VAL:HG22	2.16	0.69
3:H:98:GLU:HB2	15:BA:2:NAG:C5	2.22	0.69
1:C:353:PHE:CE2	1:C:466:GLU:OE2	2.45	0.69
3:H:56:HIS:CD2	8:9:6:GAL:H2	2.28	0.69
1:E:184:ILE:N	1:E:191:TYR:CE1	2.61	0.69
1:E:350:ARG:O	5:4:1:NAG:H82	1.85	0.69
1:A:343:LYS:CE	5:T:1:NAG:H82	2.21	0.69
2:F:518:VAL:O	2:F:518:VAL:HG23	1.92	0.69
1:E:354:GLU:O	1:E:355:ASN:CG	2.36	0.68
1:E:173:TYR:CE2	6:v:1:NAG:H61	2.29	0.68
1:E:395:TRP:CH2	5:3:1:NAG:H82	2.29	0.68
6:W:2:NAG:H3	6:W:3:BMA:O5	1.92	0.68
1:C:500:LYS:CD	2:F:663:LEU:HD11	2.24	0.68
3:H:98:GLU:CB	15:BA:2:NAG:H5	2.24	0.67
6:7:2:NAG:O3	6:7:3:BMA:O5	2.11	0.67
1:E:357:LYS:CD	16:E:1397:NAG:H82	2.22	0.67
1:C:172:GLU:O	1:C:173:TYR:HD1	1.77	0.67
1:E:169:VAL:HG11	5:w:1:NAG:H82	1.72	0.67
1:E:343:LYS:CE	5:3:1:NAG:C8	2.72	0.67
1:E:169:VAL:HB	5:w:1:NAG:H83	1.71	0.67
1:E:395:TRP:CZ3	5:3:1:NAG:H81	2.30	0.67
1:C:500:LYS:HE3	2:F:663:LEU:CD2	2.25	0.66
1:E:469:ARG:NH2	5:5:1:NAG:O5	2.27	0.66
1:A:336:ALA:CB	5:T:1:NAG:O6	2.36	0.66
1:C:303:THR:OG1	6:i:1:NAG:H82	1.95	0.66
1:C:351:GLU:OE2	5:l:1:NAG:C8	2.44	0.66
1:E:133:ASP:O	1:E:134:VAL:HG13	1.95	0.66
1:C:65:VAL:HB	1:C:66:HIS:HA	1.78	0.65
2:D:565:MET:O	2:D:565:MET:HG3	1.96	0.65
1:A:298:ARG:HH21	1:A:443:ILE:HG13	1.60	0.65
1:A:210:PHE:HE2	1:A:380:GLY:CA	2.04	0.65
1:A:442:GLN:HE21	5:R:1:NAG:C8	2.00	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ILE:CG2	7:f:5:MAN:O6	2.44	0.65
1:E:395:TRP:CZ3	5:3:1:NAG:C8	2.79	0.65
6:n:2:NAG:H82	5:o:1:NAG:C8	2.27	0.65
1:E:169:VAL:HG12	5:w:1:NAG:C8	2.16	0.65
6:W:2:NAG:C3	6:W:3:BMA:O5	2.44	0.65
7:f:3:BMA:H61	7:f:6:MAN:C5	2.26	0.65
2:B:540:GLN:O	2:B:542:ARG:N	2.30	0.65
2:D:638:TYR:CD1	12:q:3:FUC:H63	2.09	0.64
1:A:173:TYR:CG	6:I:1:NAG:N2	2.65	0.64
1:C:373:MET:HE3	6:n:1:NAG:C8	2.26	0.64
15:BA:7:NAG:H62	15:BA:8:GAL:O2	1.97	0.64
1:C:85:VAL:HG21	10:e:1:NAG:H62	1.79	0.64
1:C:297:THR:HG21	6:j:1:NAG:HN2	1.61	0.64
1:C:85:VAL:CG2	10:e:1:NAG:H62	2.28	0.64
9:Z:7:NAG:H62	9:Z:8:GAL:O2	1.97	0.64
6:n:2:NAG:H82	5:o:1:NAG:H83	1.79	0.64
1:A:279:ASN:ND2	6:P:1:NAG:O6	2.32	0.63
1:C:85:VAL:HG21	10:e:2:NAG:C8	2.24	0.63
3:M:100(C):ARG:HD3	9:Z:13:FUC:H4	1.80	0.63
1:A:81:PRO:HA	1:A:82:GLN:HB2	1.78	0.63
7:f:3:BMA:H61	7:f:6:MAN:H5	1.81	0.63
1:C:353:PHE:CD2	1:C:466:GLU:OE2	2.52	0.63
2:D:616:ASN:OD1	2:D:616:ASN:O	2.17	0.63
1:E:355:ASN:HB2	1:E:357:LYS:HA	1.80	0.63
1:A:298:ARG:HH21	1:A:443:ILE:CD1	2.11	0.63
3:M:100(N):TYR:HD1	3:M:100(O):TYR:N	1.95	0.63
1:E:183:PRO:HB3	1:E:191:TYR:HE1	1.56	0.62
3:M:55:TRP:CD1	8:Y:2:NAG:HO3	2.17	0.62
1:E:68:VAL:HG12	1:E:68:VAL:O	1.99	0.62
1:E:232:THR:O	1:E:232:THR:HG22	1.98	0.62
1:A:66:HIS:O	1:A:67:ASN:HB2	2.00	0.62
1:C:85:VAL:HG22	10:e:1:NAG:C6	2.29	0.62
3:H:98:GLU:OE1	15:BA:2:NAG:O6	2.17	0.62
1:E:469:ARG:NH2	5:5:1:NAG:C6	2.63	0.62
2:F:641:GLU:OE1	8:9:11:FUC:H4	1.98	0.62
6:W:2:NAG:O3	6:W:3:BMA:C1	2.47	0.62
1:A:298:ARG:HH21	1:A:443:ILE:CG1	2.11	0.62
1:E:357:LYS:HD2	16:E:1397:NAG:H82	1.78	0.62
2:B:522:PHE:CE1	2:B:544:LEU:HD22	2.35	0.61
1:E:355:ASN:CB	1:E:357:LYS:HA	2.30	0.61
1:E:82:GLN:O	1:E:83:GLU:CB	2.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:GLN:HG3	1:C:171:LYS:N	2.14	0.61
3:H:1:ARG:HA	3:H:2:VAL:C	2.26	0.61
2:F:551:GLN:O	2:F:552:GLN:CB	2.48	0.61
1:C:170:GLN:OE1	6:d:1:NAG:C2	2.34	0.61
1:A:156:ASN:OD1	6:I:1:NAG:C7	2.49	0.60
1:E:355:ASN:HB2	1:E:357:LYS:CB	2.30	0.60
14:6:2:NAG:H82	6:7:1:NAG:H81	1.83	0.60
1:C:156:ASN:OD1	5:c:1:NAG:O7	2.19	0.60
1:C:173:TYR:CD1	1:C:173:TYR:N	2.69	0.60
1:C:323:ILE:CG1	6:i:1:NAG:H82	2.26	0.60
1:C:171:LYS:CE	5:c:2:NAG:H62	2.31	0.60
1:E:65:VAL:HG12	1:E:65:VAL:O	1.99	0.60
2:F:600:GLY:HA2	2:F:601:LYS:HB2	1.84	0.60
1:C:503:ARG:HD2	2:D:605:THR:O	2.01	0.60
2:D:518:VAL:HG23	2:D:518:VAL:O	2.02	0.60
1:C:323:ILE:HG13	6:i:1:NAG:H83	1.49	0.60
1:E:350:ARG:O	5:4:1:NAG:C7	2.50	0.60
1:E:355:ASN:HB2	1:E:357:LYS:HG3	1.74	0.60
1:A:173:TYR:CB	6:I:1:NAG:H82	2.23	0.59
5:w:1:NAG:O3	5:w:2:NAG:O5	2.19	0.59
1:C:53:PHE:CZ	1:C:75:VAL:HG21	2.34	0.59
1:A:499:THR:O	1:A:499:THR:CG2	2.50	0.59
3:H:98:GLU:OE2	15:BA:3:BMA:H2	2.03	0.59
1:E:78:ASP:CB	1:E:79:PRO:HA	2.32	0.59
1:C:85:VAL:HG23	10:e:2:NAG:C8	2.29	0.59
1:A:75:VAL:CG2	2:B:556:LEU:HD13	2.33	0.59
4:L:109:THR:HG22	4:L:109:THR:O	2.02	0.59
6:d:1:NAG:O3	6:d:2:NAG:O5	2.20	0.59
6:n:2:NAG:H83	5:o:1:NAG:H83	1.85	0.59
1:A:75:VAL:HG21	2:B:556:LEU:HD13	1.85	0.59
1:C:354:GLU:O	5:l:1:NAG:C7	2.51	0.59
1:C:173:TYR:CD1	5:c:1:NAG:C2	2.82	0.59
1:E:65:VAL:O	1:E:65:VAL:CG1	2.50	0.58
2:B:564:ARG:NH1	2:D:574:LYS:NZ	2.50	0.58
1:E:442:GLN:OE1	5:1:1:NAG:H82	2.03	0.58
1:A:112:TRP:HH2	1:A:210:PHE:CE1	2.20	0.58
2:F:600:GLY:HA2	2:F:601:LYS:O	2.03	0.58
1:C:389:GLN:NE2	5:o:1:NAG:C7	2.66	0.58
1:A:298:ARG:HH22	1:A:441:GLY:H	1.50	0.58
1:C:353:PHE:CD2	1:C:466:GLU:OE1	2.57	0.57
3:M:98:GLU:CG	9:Z:2:NAG:C5	2.80	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ASN:OD1	1:C:446:SER:HB3	2.02	0.57
1:C:439:ILE:HG22	7:f:5:MAN:O6	2.05	0.57
1:E:133:ASP:O	1:E:134:VAL:HG22	2.04	0.57
3:H:98:GLU:HG3	15:BA:3:BMA:O2	2.05	0.57
2:B:637:ASN:OD1	2:B:637:ASN:N	2.38	0.56
1:C:351:GLU:CD	5:l:1:NAG:C8	2.78	0.56
1:E:355:ASN:OD1	1:E:357:LYS:HG3	2.04	0.56
2:B:542:ARG:HB2	2:B:542:ARG:NH1	2.20	0.56
2:D:616:ASN:OD1	2:D:616:ASN:C	2.47	0.56
3:M:100(G):TRP:O	3:M:100(G):TRP:HE3	1.84	0.56
1:A:229:ASN:CG	6:K:1:NAG:O6	2.48	0.56
1:A:298:ARG:HH21	1:A:443:ILE:HD11	1.71	0.56
1:E:412:ASN:HB2	1:E:413:THR:O	2.06	0.56
3:M:100(N):TYR:HE2	4:N:28:ASN:HD21	1.49	0.56
1:A:298:ARG:HB2	1:A:443:ILE:HB	1.86	0.56
1:C:173:TYR:CE2	5:c:2:NAG:C1	2.89	0.56
2:D:528:SER:HA	2:D:529:THR:CB	2.36	0.56
1:E:460:ILE:C	1:E:460:ILE:HD12	2.31	0.56
1:A:81:PRO:HA	1:A:82:GLN:CB	2.35	0.56
1:C:170:GLN:HB3	6:d:1:NAG:O7	2.06	0.56
1:E:82:GLN:O	1:E:83:GLU:HB2	2.05	0.56
1:E:157:CYS:HA	1:E:158:SER:HB2	1.89	0.55
6:i:1:NAG:O7	6:i:1:NAG:O3	2.24	0.55
1:C:53:PHE:CE1	1:C:75:VAL:HG23	2.39	0.55
1:E:276:ASN:OD1	1:E:276:ASN:C	2.49	0.55
1:E:500:LYS:CE	2:F:619:LEU:HD12	2.27	0.55
2:B:600:GLY:HA2	2:B:601:LYS:CB	2.35	0.55
1:E:133:ASP:OD1	1:E:134:VAL:N	2.39	0.55
3:M:32:TYR:CE1	3:M:98:GLU:HB3	2.41	0.55
1:E:152:GLY:O	1:E:178:LYS:HD2	2.06	0.55
3:H:1:ARG:HA	3:H:2:VAL:CB	2.33	0.55
1:A:499:THR:OG1	1:A:500:LYS:HA	2.06	0.55
1:E:357:LYS:HD3	16:E:1397:NAG:H82	1.87	0.55
1:E:157:CYS:HA	1:E:158:SER:CB	2.37	0.55
1:C:68:VAL:HB	1:C:69:TRP:HA	1.89	0.55
2:F:518:VAL:HA	2:F:519:PHE:HB2	1.88	0.55
1:C:131:CYS:SG	1:C:155:LYS:HB3	2.47	0.55
2:F:517:ALA:O	2:F:519:PHE:HD2	1.89	0.55
1:E:343:LYS:HE2	5:3:1:NAG:H82	1.84	0.55
3:M:100(N):TYR:CD1	3:M:100(O):TYR:N	2.75	0.55
2:B:522:PHE:CE1	2:B:544:LEU:HD13	2.27	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:VAL:CG2	10:e:1:NAG:C6	2.84	0.55
1:C:171:LYS:NZ	5:c:2:NAG:H61	2.22	0.55
3:M:100(N):TYR:CD1	3:M:100(N):TYR:C	2.85	0.55
1:C:85:VAL:CG1	10:e:1:NAG:O6	2.54	0.54
3:H:2:VAL:O	3:H:2:VAL:CG1	2.49	0.54
1:C:373:MET:HE3	6:n:1:NAG:H81	1.89	0.54
1:E:65:VAL:HB	1:E:66:HIS:HA	1.88	0.54
1:C:114:GLN:NE2	2:D:568:LEU:HD22	2.22	0.54
1:C:351:GLU:OE2	5:l:1:NAG:H83	2.07	0.54
1:C:65:VAL:HB	1:C:66:HIS:CA	2.36	0.54
1:E:351:GLU:HA	5:4:1:NAG:C7	2.38	0.54
1:A:129:LEU:C	1:A:129:LEU:HD12	2.33	0.54
1:A:173:TYR:CE1	6:I:1:NAG:H81	2.41	0.54
2:B:522:PHE:CD2	2:B:540:GLN:OE1	2.60	0.54
1:C:72:HIS:O	1:C:73:ALA:HB2	2.08	0.54
5:c:1:NAG:O3	5:c:2:NAG:O5	2.26	0.54
4:N:53:ASN:ND2	9:Z:12:NAG:HN2	2.06	0.54
2:B:564:ARG:HH11	2:D:574:LYS:NZ	2.05	0.54
6:v:1:NAG:O3	6:v:2:NAG:O5	2.26	0.54
1:E:413:THR:CG2	1:E:414:ILE:N	2.71	0.53
2:B:570:VAL:O	2:B:573:ILE:N	2.42	0.53
1:C:173:TYR:OH	5:c:2:NAG:C5	2.54	0.53
4:N:53:ASN:CG	9:Z:12:NAG:HN2	2.16	0.53
6:I:1:NAG:O3	6:I:2:NAG:O5	2.26	0.53
3:M:100(N):TYR:HD1	3:M:100(N):TYR:C	2.16	0.53
1:A:442:GLN:CD	5:R:1:NAG:H82	2.33	0.53
1:A:503:ARG:O	1:A:504:ARG:HB3	2.08	0.53
1:E:354:GLU:C	1:E:355:ASN:CG	2.76	0.53
1:A:499:THR:O	1:A:499:THR:HG22	2.09	0.53
1:C:53:PHE:CD1	1:C:53:PHE:C	2.85	0.53
1:C:389:GLN:NE2	5:o:1:NAG:O7	2.35	0.53
2:F:641:GLU:OE1	8:9:11:FUC:C4	2.56	0.53
9:Z:1:NAG:C1	9:Z:1:NAG:O7	2.57	0.53
2:D:528:SER:HA	2:D:529:THR:HB	1.91	0.53
3:H:56:HIS:HD2	8:9:6:GAL:H2	1.74	0.53
9:Z:1:NAG:O3	9:Z:2:NAG:O5	2.25	0.53
1:A:229:ASN:CB	6:K:1:NAG:HO6	2.20	0.53
2:D:613:SER:OG	12:q:1:NAG:C5	2.56	0.53
2:D:641:GLU:OE2	12:q:3:FUC:H4	2.09	0.53
2:F:600:GLY:CA	2:F:601:LYS:O	2.57	0.53
15:BA:1:NAG:C1	15:BA:1:NAG:O7	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BA:1:NAG:O3	15:BA:2:NAG:O5	2.25	0.52
2:B:564:ARG:HG2	2:D:574:LYS:HE2	1.91	0.52
2:D:549:VAL:O	2:D:550:GLN:HB2	2.08	0.52
5:s:1:NAG:O3	5:s:2:NAG:O5	2.25	0.52
3:H:28:PRO:O	3:H:29:PHE:HB2	2.10	0.52
7:f:3:BMA:C6	7:f:6:MAN:C5	2.88	0.52
1:C:114:GLN:HE22	2:D:568:LEU:HD22	1.74	0.52
1:C:65:VAL:H	1:C:66:HIS:HB3	1.75	0.52
1:C:353:PHE:CD2	1:C:466:GLU:CD	2.87	0.52
2:D:518:VAL:HA	2:D:519:PHE:HB2	1.91	0.52
5:s:1:NAG:C1	5:s:1:NAG:O7	2.57	0.52
1:C:276:ASN:OD1	1:C:278:THR:HB	2.09	0.52
2:F:637:ASN:N	2:F:637:ASN:OD1	2.42	0.52
1:C:78:ASP:N	1:C:79:PRO:CD	2.73	0.51
2:D:613:SER:OG	12:q:1:NAG:H5	2.10	0.51
1:C:303:THR:OG1	6:i:1:NAG:C8	2.58	0.51
1:C:500:LYS:CG	2:F:663:LEU:CD1	2.83	0.51
1:C:170:GLN:HG3	1:C:171:LYS:H	1.75	0.51
2:B:531:GLY:O	2:B:532:ALA:CB	2.58	0.51
1:A:173:TYR:CB	6:I:1:NAG:C8	2.85	0.51
2:B:542:ARG:NH1	2:B:542:ARG:CB	2.74	0.51
2:B:570:VAL:O	2:B:571:TRP:C	2.54	0.51
3:H:98:GLU:HB2	15:BA:2:NAG:O4	2.10	0.51
1:E:357:LYS:HD3	16:E:1397:NAG:C8	2.37	0.51
7:f:3:BMA:C6	7:f:6:MAN:H5	2.39	0.51
3:H:111:VAL:O	3:H:112:SER:CB	2.58	0.50
2:F:551:GLN:C	2:F:553:ASN:HA	2.36	0.50
1:E:135:ASN:O	1:E:136:ALA:HB3	2.11	0.50
1:A:117:LYS:CB	1:A:118:PRO:CD	2.90	0.50
1:A:503:ARG:O	1:A:504:ARG:CB	2.59	0.50
2:D:528:SER:HB2	2:D:529:THR:HB	1.93	0.50
1:E:460:ILE:HD12	1:E:460:ILE:O	2.12	0.50
1:C:279:ASN:ND2	6:g:1:NAG:O6	2.45	0.50
1:C:500:LYS:HG3	2:F:663:LEU:HD11	1.90	0.49
4:L:50:GLU:HB2	4:L:53:ASN:HB3	1.95	0.49
3:M:4:LEU:HD23	3:M:4:LEU:C	2.37	0.49
1:A:339:ASN:OD1	1:A:339:ASN:C	2.51	0.49
1:C:500:LYS:CE	2:F:663:LEU:HD21	2.40	0.49
1:E:351:GLU:HA	5:4:1:NAG:O7	2.12	0.49
1:E:362:ASN:OD1	1:E:363:HIS:O	2.30	0.49
13:x:3:BMA:C4	11:8:5:MAN:O2	2.49	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:613:SER:HB3	12:q:1:NAG:H62	1.94	0.49
2:F:552:GLN:N	2:F:553:ASN:HA	2.27	0.49
1:A:358:THR:HG23	1:A:396:ASN:HB3	1.94	0.49
1:A:298:ARG:CB	1:A:443:ILE:HB	2.43	0.49
1:E:413:THR:HG22	1:E:414:ILE:N	2.27	0.49
3:M:98:GLU:CG	9:Z:2:NAG:H5	2.30	0.49
1:C:85:VAL:CG2	10:e:1:NAG:O6	2.59	0.49
6:J:1:NAG:O3	6:J:2:NAG:O5	2.26	0.49
1:A:173:TYR:CB	6:I:1:NAG:N2	2.63	0.49
1:E:75:VAL:HA	2:F:562:GLN:HG3	1.95	0.48
2:B:641:GLU:OE1	8:Y:11:FUC:H62	2.13	0.48
1:E:134:VAL:HG12	1:E:135:ASN:CG	2.30	0.48
2:D:569:THR:O	2:D:570:VAL:HB	2.13	0.48
3:H:1:ARG:CA	3:H:2:VAL:HB	2.43	0.48
1:C:339:ASN:OD1	1:C:339:ASN:O	2.31	0.48
2:D:528:SER:HB2	2:D:529:THR:O	2.13	0.48
1:A:34:LEU:HA	1:A:499:THR:HB	1.96	0.48
3:H:32:TYR:OH	3:H:98:GLU:HG2	2.13	0.48
2:B:542:ARG:CZ	2:B:542:ARG:CB	2.86	0.48
1:E:355:ASN:CB	1:E:357:LYS:HG3	2.39	0.48
2:B:613:SER:OG	8:Y:1:NAG:C1	2.62	0.48
1:E:357:LYS:HZ3	16:E:1397:NAG:H83	1.78	0.48
2:F:641:GLU:OE2	8:9:11:FUC:O4	2.22	0.48
3:H:96:PHE:CD2	3:H:97:GLN:HG3	2.49	0.48
8:Y:7:NAG:H62	8:Y:8:GAL:O2	2.13	0.48
1:E:169:VAL:C	5:w:1:NAG:H81	2.36	0.48
1:E:183:PRO:C	1:E:191:TYR:CE1	2.77	0.48
3:M:97:GLN:NE2	9:Z:2:NAG:O3	2.46	0.48
1:E:153:GLU:HG3	1:E:154:ILE:HG13	1.96	0.47
3:M:100(N):TYR:CE2	4:N:28:ASN:ND2	2.67	0.47
6:P:1:NAG:C6	6:P:2:NAG:H82	2.44	0.47
1:A:173:TYR:HE2	6:I:2:NAG:H62	1.79	0.47
1:A:211:GLU:OE2	7:O:4:MAN:O6	2.30	0.47
2:B:568:LEU:HD13	2:D:573:ILE:HD13	1.96	0.47
1:C:173:TYR:CD1	5:c:1:NAG:O3	2.63	0.47
1:A:160:ASN:OD1	1:A:160:ASN:N	2.47	0.47
2:B:564:ARG:NH1	2:D:574:LYS:HZ1	2.11	0.47
2:F:551:GLN:O	2:F:552:GLN:HB2	2.15	0.47
3:H:14:PRO:HD3	3:H:112:SER:HA	1.96	0.47
1:A:117:LYS:CB	1:A:118:PRO:HD3	2.44	0.47
1:A:210:PHE:CD2	1:A:380:GLY:N	2.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ASN:CB	1:E:413:THR:HB	2.44	0.47
3:H:1:ARG:CA	3:H:2:VAL:C	2.87	0.47
2:B:600:GLY:CA	2:B:601:LYS:O	2.62	0.47
1:A:132:LYS:NZ	1:A:189:THR:HG21	2.29	0.47
1:A:173:TYR:CE2	6:I:1:NAG:C7	2.97	0.47
1:C:500:LYS:HG3	1:C:500:LYS:O	2.14	0.47
2:D:600:GLY:HA2	2:D:601:LYS:CB	2.43	0.47
1:E:426:MET:HB3	1:E:427:TRP:CE3	2.50	0.47
5:G:1:NAG:O3	5:G:2:NAG:O5	2.32	0.47
1:E:134:VAL:CG1	1:E:135:ASN:ND2	2.35	0.47
2:F:519:PHE:O	2:F:520:LEU:C	2.57	0.47
1:C:353:PHE:HE1	1:C:456:ARG:HH12	1.58	0.47
2:F:519:PHE:HE2	3:M:100(K):ASN:HD21	1.59	0.47
1:E:354:GLU:C	1:E:355:ASN:ND2	2.72	0.47
1:A:173:TYR:HD2	6:I:1:NAG:O3	1.99	0.46
2:B:568:LEU:HD11	2:B:573:ILE:CG1	2.45	0.46
1:C:170:GLN:HB3	6:d:1:NAG:C7	2.46	0.46
1:C:193:LEU:O	1:C:194:ILE:C	2.57	0.46
2:B:521:GLY:HA2	2:B:544:LEU:HD11	1.97	0.46
1:C:53:PHE:HE1	1:C:75:VAL:CB	2.28	0.46
1:A:381:GLU:HG3	1:A:443:ILE:HD13	1.97	0.46
1:C:78:ASP:N	1:C:79:PRO:HD3	2.30	0.46
11:8:1:NAG:O7	11:8:1:NAG:C3	2.64	0.46
1:A:336:ALA:O	1:A:339:ASN:OD1	2.34	0.46
1:E:357:LYS:CE	16:E:1397:NAG:H83	2.45	0.46
4:N:53:ASN:OD1	9:Z:12:NAG:H3	2.15	0.46
5:Q:1:NAG:H62	5:Q:2:NAG:H82	1.96	0.46
1:E:85:VAL:CG2	13:x:2:NAG:H82	2.46	0.46
11:p:1:NAG:O7	11:p:1:NAG:H3	2.16	0.46
1:C:70:ALA:O	1:C:74:CYS:HB3	2.16	0.46
11:8:1:NAG:O7	11:8:1:NAG:H3	2.16	0.46
2:B:568:LEU:HD11	2:B:573:ILE:HD11	1.97	0.46
2:B:568:LEU:HD11	2:B:573:ILE:HG12	1.98	0.46
1:E:209:SER:OG	1:E:211:GLU:HG3	2.15	0.46
4:N:4:MET:SD	4:N:23:CYS:SG	3.14	0.46
1:E:412:ASN:HB3	1:E:413:THR:HB	1.97	0.46
1:A:343:LYS:HE2	5:T:1:NAG:H82	1.95	0.45
2:B:522:PHE:O	2:B:522:PHE:CG	2.69	0.45
1:E:126:CYS:SG	1:E:192:ARG:HB2	2.56	0.45
3:M:28:PRO:CG	9:Z:7:NAG:O7	2.64	0.45
1:A:81:PRO:CA	1:A:82:GLN:HB2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LYS:HE2	5:c:2:NAG:H62	1.97	0.45
1:C:500:LYS:CG	2:F:663:LEU:HD11	2.45	0.45
1:E:396:ASN:O	1:E:404:GLY:N	2.49	0.45
3:M:111:VAL:O	3:M:112:SER:CB	2.64	0.45
1:A:444:ARG:NH2	5:Q:1:NAG:C6	2.79	0.45
2:B:541:ALA:HA	2:B:602:LEU:HD11	1.97	0.45
1:E:134:VAL:CG1	1:E:135:ASN:HB2	2.46	0.45
3:M:28:PRO:HD2	9:Z:7:NAG:O7	2.12	0.45
10:e:3:BMA:H4	11:p:5:MAN:O2	2.17	0.45
1:E:343:LYS:HE2	5:3:1:NAG:C8	2.45	0.45
1:A:210:PHE:CE2	1:A:380:GLY:C	2.92	0.45
1:A:381:GLU:HG3	1:A:443:ILE:CD1	2.47	0.45
1:A:499:THR:CB	1:A:500:LYS:HA	2.47	0.45
1:C:98:ASN:OD1	1:C:98:ASN:C	2.59	0.45
2:F:518:VAL:O	2:F:518:VAL:CG2	2.60	0.45
3:M:13:GLN:HG2	3:M:113:SER:HA	1.98	0.45
5:X:1:NAG:O7	5:X:1:NAG:C3	2.64	0.45
5:X:1:NAG:O7	5:X:1:NAG:H3	2.16	0.45
1:E:355:ASN:CG	1:E:357:LYS:HG3	2.42	0.45
6:g:1:NAG:C6	6:g:2:NAG:H82	2.44	0.45
3:H:4:LEU:N	3:H:4:LEU:HD12	2.32	0.45
11:p:1:NAG:O7	11:p:1:NAG:C3	2.64	0.45
1:C:54:CYS:C	1:C:74:CYS:SG	3.00	0.44
5:z:1:NAG:C6	5:z:2:NAG:H82	2.43	0.44
1:A:416:LEU:HA	1:A:417:PRO:HD2	1.91	0.44
1:C:170:GLN:OE1	6:d:1:NAG:O7	2.35	0.44
1:C:226:LEU:HD13	1:C:489:VAL:HG22	1.98	0.44
2:D:600:GLY:HA2	2:D:601:LYS:HB2	2.00	0.44
4:N:36:TYR:HB3	4:N:46:LEU:HA	2.00	0.44
2:B:600:GLY:HA2	2:B:601:LYS:HB2	1.99	0.44
1:C:68:VAL:HA	1:C:69:TRP:O	2.18	0.44
2:D:638:TYR:HD1	12:q:3:FUC:C6	1.96	0.44
1:E:336:ALA:O	1:E:339:ASN:CG	2.61	0.44
1:C:199:SER:O	1:C:201:ILE:HG23	2.17	0.44
5:w:1:NAG:C3	5:w:2:NAG:O5	2.66	0.44
3:M:100(E):ASP:HB2	3:M:100(I):GLY:HA3	2.00	0.44
3:M:100(N):TYR:HE2	4:N:28:ASN:HD22	1.60	0.44
1:A:66:HIS:O	1:A:67:ASN:CB	2.66	0.44
1:C:123:THR:HB	1:C:124:PRO:HD3	2.00	0.44
1:E:133:ASP:C	1:E:134:VAL:CG2	2.85	0.44
2:B:568:LEU:HD22	2:D:573:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ILE:HG12	6:i:1:NAG:H82	2.00	0.44
1:C:353:PHE:O	1:C:355:ASN:N	2.51	0.44
2:F:641:GLU:CD	8:9:11:FUC:HO4	2.19	0.44
3:M:111:VAL:O	3:M:112:SER:HB3	2.17	0.44
6:d:1:NAG:C3	6:d:2:NAG:O5	2.66	0.44
6:i:2:NAG:O3	6:i:3:BMA:O5	2.31	0.44
1:C:194:ILE:HG22	1:C:195:SER:N	2.33	0.43
6:W:1:NAG:C6	6:W:2:NAG:H82	2.48	0.43
1:A:229:ASN:HB2	6:K:1:NAG:O6	2.10	0.43
1:C:213:ILE:HB	1:C:214:PRO:HD2	2.00	0.43
2:B:564:ARG:NH1	2:D:574:LYS:HZ3	2.15	0.43
1:C:131:CYS:SG	1:C:155:LYS:CB	3.06	0.43
1:C:171:LYS:NZ	5:c:2:NAG:C6	2.82	0.43
1:C:321:GLY:O	5:c:1:NAG:O6	2.23	0.43
4:L:7:THR:HB	4:L:8:PRO:HD2	2.00	0.43
1:A:123:THR:N	1:A:124:PRO:CD	2.81	0.43
1:E:123:THR:HA	1:E:124:PRO:C	2.44	0.43
1:E:278:THR:OG1	5:z:1:NAG:C1	2.66	0.43
4:N:53:ASN:HD21	9:Z:12:NAG:HN2	1.66	0.43
6:I:1:NAG:C3	6:I:2:NAG:O5	2.67	0.43
5:c:1:NAG:C3	5:c:2:NAG:O5	2.67	0.43
2:F:641:GLU:CD	8:9:11:FUC:H4	2.43	0.43
4:N:49:PHE:O	4:N:50:GLU:C	2.61	0.43
1:A:500:LYS:O	1:A:501:ALA:CB	2.67	0.43
3:H:98:GLU:HG3	15:BA:3:BMA:C2	2.49	0.43
1:A:439:ILE:HD11	1:A:443:ILE:HG12	2.01	0.43
1:C:168:GLU:HG3	6:d:1:NAG:H81	1.95	0.43
1:E:130:ASN:OD1	1:E:130:ASN:C	2.62	0.43
1:E:134:VAL:HG12	1:E:135:ASN:CB	2.48	0.43
3:H:55:TRP:CG	3:H:55:TRP:O	2.71	0.43
6:W:1:NAG:H61	6:W:2:NAG:H82	2.00	0.43
1:A:210:PHE:O	1:A:211:GLU:C	2.61	0.43
2:B:522:PHE:HE1	2:B:544:LEU:HD22	1.83	0.43
5:r:1:NAG:O3	5:r:2:NAG:O5	2.30	0.43
1:E:350:ARG:HB3	5:4:1:NAG:H82	2.01	0.42
3:M:33:PRO:HG2	3:M:95:MET:SD	2.59	0.42
1:C:183:PRO:HA	1:C:191:TYR:CD2	2.54	0.42
1:C:131:CYS:SG	1:C:156:ASN:C	3.03	0.42
1:E:298:ARG:O	1:E:300:ASN:N	2.53	0.42
3:H:55:TRP:HD1	3:H:100(M):TYR:CZ	2.37	0.42
1:A:131:CYS:SG	1:A:155:LYS:HB3	2.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:PHE:N	2:B:544:LEU:HD12	2.17	0.42
1:C:300:ASN:HB3	1:C:326:ILE:HA	1.99	0.42
1:E:469:ARG:HH21	5:5:1:NAG:C6	2.32	0.42
1:E:437:PRO:HA	1:E:438:PRO:HD3	1.87	0.42
1:E:134:VAL:HA	1:E:135:ASN:HA	1.84	0.42
1:E:335:ARG:O	1:E:336:ALA:C	2.61	0.42
2:B:531:GLY:O	2:B:532:ALA:HB3	2.20	0.42
1:A:87:GLU:OE2	5:G:1:NAG:C8	2.40	0.42
1:E:190:SER:C	1:E:191:TYR:CG	2.97	0.42
1:C:65:VAL:HB	1:C:66:HIS:HB3	2.02	0.42
1:E:350:ARG:CB	5:4:1:NAG:H82	2.50	0.42
2:F:616:ASN:C	2:F:616:ASN:OD1	2.63	0.42
2:D:638:TYR:HE1	12:q:3:FUC:C6	1.78	0.41
1:A:158:SER:HB3	6:I:1:NAG:C8	2.50	0.41
2:B:564:ARG:HH11	2:D:574:LYS:HZ3	1.67	0.41
1:C:351:GLU:CD	5:l:1:NAG:H83	2.45	0.41
3:M:4:LEU:C	3:M:4:LEU:CD2	2.93	0.41
3:M:25:SER:O	3:M:26:ASP:HB2	2.19	0.41
1:E:70:ALA:O	1:E:74:CYS:N	2.53	0.41
1:E:77:THR:O	1:E:78:ASP:HB3	2.20	0.41
2:D:565:MET:O	2:D:565:MET:CG	2.68	0.41
1:A:112:TRP:HH2	1:A:210:PHE:HE1	1.65	0.41
1:E:183:PRO:CB	1:E:191:TYR:CZ	2.83	0.41
6:v:1:NAG:C3	6:v:2:NAG:O5	2.67	0.41
1:C:67:ASN:HB3	1:C:208:ILE:HD13	2.02	0.41
2:F:641:GLU:CD	8:9:11:FUC:C4	2.94	0.41
2:B:641:GLU:OE2	8:Y:11:FUC:C4	2.64	0.41
2:D:528:SER:CA	2:D:529:THR:HB	2.50	0.41
2:D:528:SER:CA	2:D:529:THR:CB	2.99	0.41
3:M:4:LEU:HD21	3:M:92:CYS:SG	2.61	0.41
3:M:100:GLY:HA3	9:Z:1:NAG:H2	2.03	0.41
1:A:362:ASN:HB3	1:A:469:ARG:HD3	2.02	0.41
1:A:499:THR:HG23	1:A:500:LYS:HA	2.03	0.41
1:E:173:TYR:CD2	6:v:1:NAG:O5	2.74	0.41
1:E:153:GLU:C	1:E:154:ILE:HG13	2.47	0.40
1:E:298:ARG:HD3	1:E:298:ARG:C	2.47	0.40
1:E:469:ARG:HH21	5:5:1:NAG:C5	2.34	0.40
3:H:111:VAL:O	3:H:112:SER:HB3	2.19	0.40
1:A:193:LEU:HB2	1:A:196:CYS:SG	2.61	0.40
1:C:66:HIS:HB2	1:C:67:ASN:HB2	2.03	0.40
1:C:77:THR:OG1	1:C:79:PRO:HD3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:CYS:HA	1:C:331:CYS:HA	2.02	0.40
2:D:549:VAL:O	2:D:550:GLN:CB	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/473 (93%)	409 (93%)	28 (6%)	4 (1%)	14	49
1	C	436/473 (92%)	395 (91%)	31 (7%)	10 (2%)	5	29
1	E	440/473 (93%)	405 (92%)	27 (6%)	8 (2%)	6	33
2	B	142/153 (93%)	127 (89%)	8 (6%)	7 (5%)	1	16
2	D	145/153 (95%)	136 (94%)	7 (5%)	2 (1%)	9	39
2	F	151/153 (99%)	137 (91%)	11 (7%)	3 (2%)	6	32
3	H	133/240 (55%)	125 (94%)	7 (5%)	1 (1%)	16	52
3	M	133/240 (55%)	124 (93%)	7 (5%)	2 (2%)	8	38
4	L	112/219 (51%)	105 (94%)	7 (6%)	0	100	100
4	N	110/219 (50%)	104 (94%)	5 (4%)	1 (1%)	14	49
All	All	2243/2796 (80%)	2067 (92%)	138 (6%)	38 (2%)	9	35

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
2	B	532	ALA
2	B	541	ALA
2	B	545	LEU
2	B	570	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	73	ALA
1	C	80	ASN
1	C	99	ASN
1	C	194	ILE
1	C	355	ASN
1	E	78	ASP
1	E	83	GLU
1	E	258	GLN
2	F	520	LEU
2	F	552	GLN
3	H	112	SER
3	M	112	SER
2	B	543	LEU
2	B	567	GLN
1	C	69	TRP
2	D	550	GLN
1	E	134	VAL
1	E	402	THR
4	N	51	VAL
1	A	504	ARG
1	C	354	GLU
1	E	70	ALA
2	F	601	LYS
3	M	100(K)	ASN
2	B	601	LYS
1	C	199	SER
1	E	79	PRO
1	A	67	ASN
1	A	232	THR
1	C	165	ILE
1	E	299	PRO
1	C	43	PRO
2	D	570	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	A	404/424 (95%)	401 (99%)	3 (1%)	76	78
1	C	398/424 (94%)	389 (98%)	9 (2%)	44	64
1	E	401/424 (95%)	397 (99%)	4 (1%)	68	75
2	B	123/128 (96%)	118 (96%)	5 (4%)	27	49
2	D	122/128 (95%)	122 (100%)	0	100	100
2	F	128/128 (100%)	126 (98%)	2 (2%)	55	69
3	H	116/207 (56%)	116 (100%)	0	100	100
3	M	115/207 (56%)	115 (100%)	0	100	100
4	L	101/195 (52%)	100 (99%)	1 (1%)	68	75
4	N	99/195 (51%)	99 (100%)	0	100	100
All	All	2007/2460 (82%)	1983 (99%)	24 (1%)	61	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	402	THR
1	A	499	THR
2	B	522	PHE
2	B	542	ARG
2	B	543	LEU
2	B	570	VAL
2	B	637	ASN
1	C	53	PHE
1	C	156	ASN
1	C	173	TYR
1	C	298	ARG
1	C	301	ASN
1	C	332	ASN
1	C	339	ASN
1	C	355	ASN
1	C	378	CYS
1	E	126	CYS
1	E	134	VAL
1	E	156	ASN
1	E	378	CYS
2	F	616	ASN
2	F	637	ASN
4	L	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	308	HIS
1	A	352	GLN
1	A	442	GLN
2	B	652	GLN
2	B	653	GLN
1	C	114	GLN
1	C	130	ASN
1	C	389	GLN
2	D	650	GLN
2	D	653	GLN
1	E	352	GLN
1	E	377	ASN
1	E	507	GLN
2	F	562	GLN
3	M	82(A)	ASN
3	M	100(K)	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

203 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
5	NAG	0	1	1,5	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
5	NAG	0	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
5	NAG	1	1	1,5	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
5	NAG	1	2	5	14,14,15	0.50	0	17,19,21	1.32	3 (17%)
6	NAG	2	1	1,6	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
6	NAG	2	2	6	14,14,15	0.52	0	17,19,21	1.32	3 (17%)
6	BMA	2	3	6	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
5	NAG	3	1	1,5	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
5	NAG	3	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
5	NAG	4	1	1,5	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
5	NAG	4	2	5	14,14,15	0.50	0	17,19,21	1.32	3 (17%)
5	NAG	5	1	1,5	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
5	NAG	5	2	5	14,14,15	0.48	0	17,19,21	1.34	3 (17%)
14	NAG	6	1	14,1	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
14	NAG	6	2	14	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
14	BMA	6	3	14	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
14	MAN	6	4	14	11,11,12	0.60	0	15,15,17	2.21	3 (20%)
6	NAG	7	1	1,6	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
6	NAG	7	2	6	14,14,15	0.50	0	17,19,21	1.34	3 (17%)
6	BMA	7	3	6	11,11,12	0.63	0	15,15,17	1.43	3 (20%)
11	NAG	8	1	1,11	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
11	NAG	8	2	11	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
11	BMA	8	3	11	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
11	MAN	8	4	11	11,11,12	0.55	0	15,15,17	1.48	2 (13%)
11	MAN	8	5	11	11,11,12	0.58	0	15,15,17	2.32	5 (33%)
11	MAN	8	6	11	11,11,12	0.61	0	15,15,17	2.22	3 (20%)
11	MAN	8	7	11	11,11,12	0.57	0	15,15,17	1.92	5 (33%)
11	MAN	8	8	11	11,11,12	0.58	0	15,15,17	2.26	7 (46%)
8	NAG	9	1	2,8	14,14,15	1.52	4 (28%)	17,19,21	1.10	1 (5%)
8	NAG	9	10	8	14,14,15	1.37	3 (21%)	17,19,21	1.22	1 (5%)
8	FUC	9	11	8	10,10,11	1.51	2 (20%)	14,14,16	0.86	0
8	NAG	9	2	8	14,14,15	1.34	2 (14%)	17,19,21	1.31	1 (5%)
8	BMA	9	3	8	11,11,12	1.34	2 (18%)	15,15,17	1.20	1 (6%)
8	MAN	9	4	8	11,11,12	1.53	3 (27%)	15,15,17	1.27	2 (13%)
8	NAG	9	5	8	14,14,15	1.43	3 (21%)	17,19,21	1.35	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GAL	9	6	8	11,11,12	1.33	2 (18%)	15,15,17	1.08	1 (6%)
8	NAG	9	7	8	14,14,15	1.43	3 (21%)	17,19,21	1.16	1 (5%)
8	GAL	9	8	8	11,11,12	1.34	2 (18%)	15,15,17	1.07	1 (6%)
8	MAN	9	9	8	11,11,12	1.70	4 (36%)	15,15,17	1.43	2 (13%)
5	NAG	AA	1	2,5	14,14,15	0.51	0	17,19,21	2.26	3 (17%)
5	NAG	AA	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
15	NAG	BA	1	2,15	14,14,15	1.52	3 (21%)	17,19,21	1.07	1 (5%)
15	NAG	BA	10	15	14,14,15	1.41	3 (21%)	17,19,21	1.32	1 (5%)
15	NAG	BA	11	15	14,14,15	1.40	3 (21%)	17,19,21	1.17	2 (11%)
15	FUC	BA	12	15	10,10,11	1.51	2 (20%)	14,14,16	0.86	0
15	NAG	BA	2	15	14,14,15	1.35	2 (14%)	17,19,21	1.31	1 (5%)
15	BMA	BA	3	15	11,11,12	1.35	2 (18%)	15,15,17	1.22	1 (6%)
15	MAN	BA	4	15	11,11,12	1.71	4 (36%)	15,15,17	1.42	2 (13%)
15	NAG	BA	5	15	14,14,15	1.36	3 (21%)	17,19,21	1.20	1 (5%)
15	GAL	BA	6	15	11,11,12	1.33	2 (18%)	15,15,17	1.06	1 (6%)
15	NAG	BA	7	15	14,14,15	1.36	3 (21%)	17,19,21	1.31	1 (5%)
15	GAL	BA	8	15	11,11,12	1.31	2 (18%)	15,15,17	1.10	1 (6%)
15	MAN	BA	9	15	11,11,12	1.53	3 (27%)	15,15,17	1.28	2 (13%)
5	NAG	G	1	1,5	14,14,15	0.49	0	17,19,21	2.28	3 (17%)
5	NAG	G	2	5	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
6	NAG	I	1	1,6	14,14,15	0.50	0	17,19,21	2.26	3 (17%)
6	NAG	I	2	6	14,14,15	0.49	0	17,19,21	1.32	3 (17%)
6	BMA	I	3	6	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
6	NAG	J	1	1,6	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
6	NAG	J	2	6	14,14,15	0.54	0	17,19,21	1.32	3 (17%)
6	BMA	J	3	6	11,11,12	0.65	0	15,15,17	1.42	3 (20%)
6	NAG	K	1	1,6	14,14,15	0.51	0	17,19,21	2.29	3 (17%)
6	NAG	K	2	6	14,14,15	0.48	0	17,19,21	1.37	3 (17%)
6	BMA	K	3	6	11,11,12	0.63	0	15,15,17	1.43	3 (20%)
7	NAG	O	1	7,1	14,14,15	0.61	0	17,19,21	0.66	0
7	NAG	O	2	7	14,14,15	0.55	0	17,19,21	0.86	0
7	BMA	O	3	7	11,11,12	0.65	0	15,15,17	0.71	0
7	MAN	O	4	7	11,11,12	0.58	0	15,15,17	0.58	0
7	MAN	O	5	7	11,11,12	0.51	0	15,15,17	0.64	0
7	MAN	O	6	7	11,11,12	0.64	0	15,15,17	0.93	2 (13%)
7	MAN	O	7	7	11,11,12	0.63	0	15,15,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	P	1	1,6	14,14,15	0.48	0	17,19,21	2.27	3 (17%)
6	NAG	P	2	6	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
6	BMA	P	3	6	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
5	NAG	Q	1	1,5	14,14,15	0.48	0	17,19,21	2.27	3 (17%)
5	NAG	Q	2	5	14,14,15	0.49	0	17,19,21	1.32	3 (17%)
5	NAG	R	1	1,5	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
5	NAG	R	2	5	14,14,15	0.51	0	17,19,21	1.32	3 (17%)
6	NAG	S	1	1,6	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
6	NAG	S	2	6	14,14,15	0.52	0	17,19,21	1.32	3 (17%)
6	BMA	S	3	6	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
5	NAG	T	1	1,5	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
5	NAG	T	2	5	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
6	NAG	U	1	1,6	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
6	NAG	U	2	6	14,14,15	0.49	0	17,19,21	1.33	3 (17%)
6	BMA	U	3	6	11,11,12	0.63	0	15,15,17	1.41	3 (20%)
6	NAG	V	1	1,6	14,14,15	0.51	0	17,19,21	2.29	3 (17%)
6	NAG	V	2	6	14,14,15	0.51	0	17,19,21	1.34	3 (17%)
6	BMA	V	3	6	11,11,12	0.63	0	15,15,17	1.43	3 (20%)
6	NAG	W	1	1,6	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
6	NAG	W	2	6	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
6	BMA	W	3	6	11,11,12	0.65	0	15,15,17	1.43	3 (20%)
5	NAG	X	1	1,5	14,14,15	0.48	0	17,19,21	2.25	3 (17%)
5	NAG	X	2	5	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
8	NAG	Y	1	2,8	14,14,15	1.52	3 (21%)	17,19,21	1.10	1 (5%)
8	NAG	Y	10	8	14,14,15	1.37	3 (21%)	17,19,21	1.23	1 (5%)
8	FUC	Y	11	8	10,10,11	1.51	2 (20%)	14,14,16	0.86	0
8	NAG	Y	2	8	14,14,15	1.33	2 (14%)	17,19,21	1.31	1 (5%)
8	BMA	Y	3	8	11,11,12	1.35	2 (18%)	15,15,17	1.20	1 (6%)
8	MAN	Y	4	8	11,11,12	1.53	3 (27%)	15,15,17	1.27	2 (13%)
8	NAG	Y	5	8	14,14,15	1.43	3 (21%)	17,19,21	1.34	1 (5%)
8	GAL	Y	6	8	11,11,12	1.32	2 (18%)	15,15,17	1.07	1 (6%)
8	NAG	Y	7	8	14,14,15	1.43	3 (21%)	17,19,21	1.15	1 (5%)
8	GAL	Y	8	8	11,11,12	1.33	2 (18%)	15,15,17	1.07	1 (6%)
8	MAN	Y	9	8	11,11,12	1.69	4 (36%)	15,15,17	1.43	2 (13%)
9	NAG	Z	1	2,9	14,14,15	1.53	3 (21%)	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	Z	10	9	14,14,15	1.40	3 (21%)	17,19,21	1.33	1 (5%)
9	GAL	Z	11	9	11,11,12	1.32	2 (18%)	15,15,17	1.08	1 (6%)
9	NAG	Z	12	9	14,14,15	1.41	3 (21%)	17,19,21	1.19	2 (11%)
9	FUC	Z	13	9	10,10,11	1.51	2 (20%)	14,14,16	0.87	0
9	NAG	Z	2	9	14,14,15	1.35	2 (14%)	17,19,21	1.31	1 (5%)
9	BMA	Z	3	9	11,11,12	1.36	2 (18%)	15,15,17	1.22	1 (6%)
9	MAN	Z	4	9	11,11,12	1.71	4 (36%)	15,15,17	1.41	2 (13%)
9	NAG	Z	5	9	14,14,15	1.36	3 (21%)	17,19,21	1.20	1 (5%)
9	GAL	Z	6	9	11,11,12	1.33	2 (18%)	15,15,17	1.06	1 (6%)
9	NAG	Z	7	9	14,14,15	1.35	3 (21%)	17,19,21	1.30	1 (5%)
9	GAL	Z	8	9	11,11,12	1.31	2 (18%)	15,15,17	1.09	1 (6%)
9	MAN	Z	9	9	11,11,12	1.54	3 (27%)	15,15,17	1.28	2 (13%)
6	NAG	a	1	1,6	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
6	NAG	a	2	6	14,14,15	0.52	0	17,19,21	1.31	3 (17%)
6	BMA	a	3	6	11,11,12	0.64	0	15,15,17	1.42	3 (20%)
5	NAG	b	1	1,5	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
5	NAG	b	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
5	NAG	c	1	1,5	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
5	NAG	c	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
6	NAG	d	1	1,6	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
6	NAG	d	2	6	14,14,15	0.53	0	17,19,21	1.33	3 (17%)
6	BMA	d	3	6	11,11,12	0.63	0	15,15,17	1.43	3 (20%)
10	NAG	e	1	1,10	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
10	NAG	e	2	10	14,14,15	0.49	0	17,19,21	1.37	3 (17%)
10	BMA	e	3	10	11,11,12	0.63	0	15,15,17	1.43	3 (20%)
10	MAN	e	4	10	11,11,12	0.54	0	15,15,17	1.48	2 (13%)
10	MAN	e	5	10	11,11,12	0.57	0	15,15,17	2.22	3 (20%)
7	NAG	f	1	7,1	14,14,15	0.60	0	17,19,21	0.66	0
7	NAG	f	2	7	14,14,15	0.57	0	17,19,21	0.86	0
7	BMA	f	3	7	11,11,12	0.64	0	15,15,17	0.71	0
7	MAN	f	4	7	11,11,12	0.59	0	15,15,17	0.58	0
7	MAN	f	5	7	11,11,12	0.51	0	15,15,17	0.63	0
7	MAN	f	6	7	11,11,12	0.65	0	15,15,17	0.92	2 (13%)
7	MAN	f	7	7	11,11,12	0.63	0	15,15,17	0.54	0
6	NAG	g	1	1,6	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
6	NAG	g	2	6	14,14,15	0.50	0	17,19,21	1.33	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	g	3	6	11,11,12	0.63	0	15,15,17	1.43	3 (20%)
5	NAG	h	1	1,5	14,14,15	0.49	0	17,19,21	2.26	3 (17%)
5	NAG	h	2	5	14,14,15	0.51	0	17,19,21	1.32	3 (17%)
6	NAG	i	1	1,6	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
6	NAG	i	2	6	14,14,15	0.50	0	17,19,21	1.31	3 (17%)
6	BMA	i	3	6	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
6	NAG	j	1	1,6	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
6	NAG	j	2	6	14,14,15	0.51	0	17,19,21	1.31	3 (17%)
6	BMA	j	3	6	11,11,12	0.64	0	15,15,17	1.43	3 (20%)
5	NAG	k	1	1,5	14,14,15	0.52	0	17,19,21	2.27	3 (17%)
5	NAG	k	2	5	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
5	NAG	l	1	1,5	14,14,15	0.48	0	17,19,21	2.28	3 (17%)
5	NAG	l	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
6	NAG	m	1	1,6	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
6	NAG	m	2	6	14,14,15	0.50	0	17,19,21	1.33	3 (17%)
6	BMA	m	3	6	11,11,12	0.62	0	15,15,17	1.41	3 (20%)
6	NAG	n	1	1,6	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
6	NAG	n	2	6	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
6	BMA	n	3	6	11,11,12	0.65	0	15,15,17	1.43	3 (20%)
5	NAG	o	1	1,5	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
5	NAG	o	2	5	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
11	NAG	p	1	1,11	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
11	NAG	p	2	11	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
11	BMA	p	3	11	11,11,12	0.63	0	15,15,17	1.42	3 (20%)
11	MAN	p	4	11	11,11,12	0.52	0	15,15,17	1.48	2 (13%)
11	MAN	p	5	11	11,11,12	0.59	0	15,15,17	2.33	5 (33%)
11	MAN	p	6	11	11,11,12	0.61	0	15,15,17	2.22	3 (20%)
11	MAN	p	7	11	11,11,12	0.58	0	15,15,17	1.93	5 (33%)
11	MAN	p	8	11	11,11,12	0.58	0	15,15,17	2.25	7 (46%)
12	NAG	q	1	2,12	14,14,15	1.52	4 (28%)	17,19,21	1.10	1 (5%)
12	NAG	q	2	12	14,14,15	1.36	2 (14%)	17,19,21	1.30	1 (5%)
12	FUC	q	3	12	10,10,11	1.50	2 (20%)	14,14,16	0.86	0
5	NAG	r	1	2,5	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
5	NAG	r	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
5	NAG	s	1	2,5	14,14,15	1.53	3 (21%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	s	2	5	14,14,15	1.35	2 (14%)	17,19,21	1.31	1 (5%)
6	NAG	t	1	1,6	14,14,15	0.49	0	17,19,21	2.28	3 (17%)
6	NAG	t	2	6	14,14,15	0.52	0	17,19,21	1.32	3 (17%)
6	BMA	t	3	6	11,11,12	0.61	0	15,15,17	1.43	3 (20%)
5	NAG	u	1	1,5	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
5	NAG	u	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)
6	NAG	v	1	1,6	14,14,15	0.51	0	17,19,21	2.26	3 (17%)
6	NAG	v	2	6	14,14,15	0.52	0	17,19,21	1.32	3 (17%)
6	BMA	v	3	6	11,11,12	0.65	0	15,15,17	1.43	3 (20%)
5	NAG	w	1	1,5	14,14,15	0.50	0	17,19,21	2.28	3 (17%)
5	NAG	w	2	5	14,14,15	0.52	0	17,19,21	1.33	3 (17%)
13	NAG	x	1	1,13	14,14,15	0.51	0	17,19,21	2.28	3 (17%)
13	NAG	x	2	13	14,14,15	0.49	0	17,19,21	1.35	3 (17%)
13	BMA	x	3	13	11,11,12	0.64	0	15,15,17	1.44	3 (20%)
13	MAN	x	4	13	11,11,12	0.53	0	15,15,17	1.50	3 (20%)
13	MAN	x	5	13	11,11,12	0.57	0	15,15,17	2.34	5 (33%)
13	MAN	x	6	13	11,11,12	0.59	0	15,15,17	2.22	3 (20%)
7	NAG	y	1	7,1	14,14,15	0.60	0	17,19,21	0.66	0
7	NAG	y	2	7	14,14,15	0.56	0	17,19,21	0.86	0
7	BMA	y	3	7	11,11,12	0.65	0	15,15,17	0.71	0
7	MAN	y	4	7	11,11,12	0.59	0	15,15,17	0.58	0
7	MAN	y	5	7	11,11,12	0.51	0	15,15,17	0.64	0
7	MAN	y	6	7	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
7	MAN	y	7	7	11,11,12	0.62	0	15,15,17	0.54	0
5	NAG	z	1	1,5	14,14,15	0.49	0	17,19,21	2.27	3 (17%)
5	NAG	z	2	5	14,14,15	0.51	0	17,19,21	1.33	3 (17%)

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	2	2	6	-	0/6/23/26	0/1/1/1
6	BMA	2	3	6	-	2/2/19/22	0/1/1/1
5	NAG	3	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	3	2	5	-	0/6/23/26	0/1/1/1
5	NAG	4	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	4	2	5	-	0/6/23/26	0/1/1/1
5	NAG	5	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	5	2	5	-	0/6/23/26	0/1/1/1
14	NAG	6	1	14,1	-	1/6/23/26	0/1/1/1
14	NAG	6	2	14	-	0/6/23/26	0/1/1/1
14	BMA	6	3	14	-	2/2/19/22	0/1/1/1
14	MAN	6	4	14	-	0/2/19/22	0/1/1/1
6	NAG	7	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	7	2	6	-	0/6/23/26	0/1/1/1
6	BMA	7	3	6	-	2/2/19/22	0/1/1/1
11	NAG	8	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	8	2	11	-	0/6/23/26	0/1/1/1
11	BMA	8	3	11	-	0/2/19/22	0/1/1/1
11	MAN	8	4	11	-	0/2/19/22	0/1/1/1
11	MAN	8	5	11	-	0/2/19/22	0/1/1/1
11	MAN	8	6	11	-	0/2/19/22	0/1/1/1
11	MAN	8	7	11	-	0/2/19/22	0/1/1/1
11	MAN	8	8	11	-	0/2/19/22	0/1/1/1
8	NAG	9	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	9	10	8	-	0/6/23/26	0/1/1/1
8	FUC	9	11	8	-	-	0/1/1/1
8	NAG	9	2	8	-	0/6/23/26	0/1/1/1
8	BMA	9	3	8	-	2/2/19/22	0/1/1/1
8	MAN	9	4	8	-	0/2/19/22	0/1/1/1
8	NAG	9	5	8	-	0/6/23/26	0/1/1/1
8	GAL	9	6	8	-	0/2/19/22	0/1/1/1
8	NAG	9	7	8	-	0/6/23/26	0/1/1/1
8	GAL	9	8	8	-	0/2/19/22	0/1/1/1
8	MAN	9	9	8	-	0/2/19/22	0/1/1/1
5	NAG	AA	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	AA	2	5	-	0/6/23/26	0/1/1/1
15	NAG	BA	1	2,15	-	1/6/23/26	0/1/1/1
15	NAG	BA	10	15	-	0/6/23/26	0/1/1/1
15	NAG	BA	11	15	-	0/6/23/26	0/1/1/1
15	FUC	BA	12	15	-	-	0/1/1/1
15	NAG	BA	2	15	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BMA	BA	3	15	-	0/2/19/22	0/1/1/1
15	MAN	BA	4	15	-	0/2/19/22	0/1/1/1
15	NAG	BA	5	15	-	0/6/23/26	0/1/1/1
15	GAL	BA	6	15	-	0/2/19/22	0/1/1/1
15	NAG	BA	7	15	-	0/6/23/26	0/1/1/1
15	GAL	BA	8	15	-	0/2/19/22	0/1/1/1
15	MAN	BA	9	15	-	1/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	NAG	K	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
7	NAG	O	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
7	MAN	O	4	7	-	0/2/19/22	0/1/1/1
7	MAN	O	5	7	-	2/2/19/22	0/1/1/1
7	MAN	O	6	7	-	2/2/19/22	0/1/1/1
7	MAN	O	7	7	-	0/2/19/22	0/1/1/1
6	NAG	P	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	2/2/19/22	0/1/1/1
5	NAG	Q	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
5	NAG	T	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	V	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
6	BMA	V	3	6	-	2/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	W	2	6	-	0/6/23/26	0/1/1/1
6	BMA	W	3	6	-	2/2/19/22	0/1/1/1
5	NAG	X	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
8	NAG	Y	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	10	8	-	0/6/23/26	0/1/1/1
8	FUC	Y	11	8	-	-	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1
8	NAG	Y	5	8	-	0/6/23/26	0/1/1/1
8	GAL	Y	6	8	-	0/2/19/22	0/1/1/1
8	NAG	Y	7	8	-	0/6/23/26	0/1/1/1
8	GAL	Y	8	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	9	8	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	Z	10	9	-	0/6/23/26	0/1/1/1
9	GAL	Z	11	9	-	0/2/19/22	0/1/1/1
9	NAG	Z	12	9	-	0/6/23/26	0/1/1/1
9	FUC	Z	13	9	-	-	0/1/1/1
9	NAG	Z	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	0/2/19/22	0/1/1/1
9	NAG	Z	5	9	-	0/6/23/26	0/1/1/1
9	GAL	Z	6	9	-	0/2/19/22	0/1/1/1
9	NAG	Z	7	9	-	0/6/23/26	0/1/1/1
9	GAL	Z	8	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	9	9	-	1/2/19/22	0/1/1/1
6	NAG	a	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	a	2	6	-	0/6/23/26	0/1/1/1
6	BMA	a	3	6	-	2/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	b	2	5	-	0/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
6	NAG	d	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	d	2	6	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	d	3	6	-	2/2/19/22	0/1/1/1
10	NAG	e	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	e	2	10	-	0/6/23/26	0/1/1/1
10	BMA	e	3	10	-	0/2/19/22	0/1/1/1
10	MAN	e	4	10	-	0/2/19/22	0/1/1/1
10	MAN	e	5	10	-	0/2/19/22	0/1/1/1
7	NAG	f	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	f	2	7	-	2/6/23/26	0/1/1/1
7	BMA	f	3	7	-	0/2/19/22	0/1/1/1
7	MAN	f	4	7	-	0/2/19/22	0/1/1/1
7	MAN	f	5	7	-	2/2/19/22	0/1/1/1
7	MAN	f	6	7	-	2/2/19/22	0/1/1/1
7	MAN	f	7	7	-	0/2/19/22	0/1/1/1
6	NAG	g	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	g	2	6	-	0/6/23/26	0/1/1/1
6	BMA	g	3	6	-	2/2/19/22	0/1/1/1
5	NAG	h	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	h	2	5	-	0/6/23/26	0/1/1/1
6	NAG	i	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	i	2	6	-	0/6/23/26	0/1/1/1
6	BMA	i	3	6	-	2/2/19/22	0/1/1/1
6	NAG	j	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	j	2	6	-	0/6/23/26	0/1/1/1
6	BMA	j	3	6	-	2/2/19/22	0/1/1/1
5	NAG	k	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	k	2	5	-	0/6/23/26	0/1/1/1
5	NAG	l	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	l	2	5	-	0/6/23/26	0/1/1/1
6	NAG	m	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	m	2	6	-	0/6/23/26	0/1/1/1
6	BMA	m	3	6	-	2/2/19/22	0/1/1/1
6	NAG	n	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	n	2	6	-	0/6/23/26	0/1/1/1
6	BMA	n	3	6	-	2/2/19/22	0/1/1/1
5	NAG	o	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	o	2	5	-	0/6/23/26	0/1/1/1
11	NAG	p	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	p	2	11	-	0/6/23/26	0/1/1/1
11	BMA	p	3	11	-	0/2/19/22	0/1/1/1
11	MAN	p	4	11	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	p	5	11	-	0/2/19/22	0/1/1/1
11	MAN	p	6	11	-	0/2/19/22	0/1/1/1
11	MAN	p	7	11	-	0/2/19/22	0/1/1/1
11	MAN	p	8	11	-	0/2/19/22	0/1/1/1
12	NAG	q	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	q	2	12	-	0/6/23/26	0/1/1/1
12	FUC	q	3	12	-	-	0/1/1/1
5	NAG	r	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	r	2	5	-	0/6/23/26	0/1/1/1
5	NAG	s	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	s	2	5	-	0/6/23/26	0/1/1/1
6	NAG	t	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	t	2	6	-	0/6/23/26	0/1/1/1
6	BMA	t	3	6	-	2/2/19/22	0/1/1/1
5	NAG	u	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	u	2	5	-	0/6/23/26	0/1/1/1
6	NAG	v	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	v	2	6	-	0/6/23/26	0/1/1/1
6	BMA	v	3	6	-	2/2/19/22	0/1/1/1
5	NAG	w	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	w	2	5	-	0/6/23/26	0/1/1/1
13	NAG	x	1	1,13	-	1/6/23/26	0/1/1/1
13	NAG	x	2	13	-	0/6/23/26	0/1/1/1
13	BMA	x	3	13	-	0/2/19/22	0/1/1/1
13	MAN	x	4	13	-	0/2/19/22	0/1/1/1
13	MAN	x	5	13	-	0/2/19/22	0/1/1/1
13	MAN	x	6	13	-	0/2/19/22	0/1/1/1
7	NAG	y	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	y	2	7	-	2/6/23/26	0/1/1/1
7	BMA	y	3	7	-	0/2/19/22	0/1/1/1
7	MAN	y	4	7	-	0/2/19/22	0/1/1/1
7	MAN	y	5	7	-	2/2/19/22	0/1/1/1
7	MAN	y	6	7	-	2/2/19/22	0/1/1/1
7	MAN	y	7	7	-	0/2/19/22	0/1/1/1
5	NAG	z	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	z	2	5	-	0/6/23/26	0/1/1/1

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	9	MAN	O5-C1	3.43	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	9	MAN	O5-C1	3.36	1.49	1.43
15	BA	4	MAN	O5-C1	3.33	1.49	1.43
9	Z	4	MAN	O5-C1	3.33	1.49	1.43
5	s	1	NAG	O5-C1	3.09	1.48	1.43
15	BA	1	NAG	O5-C1	3.07	1.48	1.43
9	Z	1	NAG	O5-C1	3.06	1.48	1.43
12	q	1	NAG	O5-C1	3.01	1.48	1.43
8	Y	1	NAG	O5-C1	3.01	1.48	1.43
8	9	1	NAG	O5-C1	3.00	1.48	1.43
15	BA	10	NAG	O5-C1	2.98	1.48	1.43
9	Z	10	NAG	O5-C1	2.92	1.48	1.43
8	9	5	NAG	O5-C1	2.89	1.48	1.43
12	q	2	NAG	O5-C1	2.89	1.48	1.43
9	Z	13	FUC	O5-C1	2.86	1.48	1.43
8	9	11	FUC	O5-C1	2.85	1.48	1.43
15	BA	12	FUC	O5-C1	2.85	1.48	1.43
8	Y	5	NAG	O5-C1	2.85	1.48	1.43
8	Y	11	FUC	O5-C1	2.83	1.48	1.43
8	Y	2	NAG	O5-C1	2.82	1.48	1.43
8	9	8	GAL	O5-C1	2.81	1.48	1.43
8	9	2	NAG	O5-C1	2.81	1.48	1.43
8	9	7	NAG	O5-C1	2.81	1.48	1.43
12	q	3	FUC	O5-C1	2.80	1.48	1.43
8	Y	4	MAN	O5-C5	2.79	1.48	1.43
15	BA	11	NAG	O5-C1	2.79	1.48	1.43
8	9	4	MAN	O5-C5	2.79	1.48	1.43
8	Y	7	NAG	O5-C1	2.77	1.48	1.43
9	Z	12	NAG	O5-C1	2.77	1.48	1.43
8	9	10	NAG	O5-C1	2.77	1.48	1.43
8	Y	10	NAG	O5-C1	2.76	1.48	1.43
9	Z	7	NAG	O5-C1	2.75	1.48	1.43
15	BA	6	GAL	O5-C1	2.75	1.48	1.43
15	BA	2	NAG	O5-C1	2.75	1.48	1.43
15	BA	5	NAG	O5-C1	2.75	1.48	1.43
8	Y	8	GAL	O5-C1	2.74	1.48	1.43
15	BA	4	MAN	O5-C5	2.74	1.48	1.43
15	BA	7	NAG	O5-C1	2.73	1.48	1.43
9	Z	4	MAN	O5-C5	2.73	1.48	1.43
9	Z	2	NAG	O5-C1	2.72	1.48	1.43
5	s	2	NAG	O5-C1	2.72	1.48	1.43
9	Z	6	GAL	O5-C1	2.72	1.48	1.43
5	s	1	NAG	O5-C5	2.71	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Y	9	MAN	O5-C5	2.71	1.48	1.43
15	BA	12	FUC	O5-C5	2.70	1.48	1.43
9	Z	5	NAG	O5-C1	2.70	1.48	1.43
9	Z	9	MAN	O5-C1	2.69	1.48	1.43
8	9	6	GAL	O5-C1	2.68	1.48	1.43
9	Z	13	FUC	O5-C5	2.68	1.48	1.43
9	Z	1	NAG	O5-C5	2.68	1.48	1.43
15	BA	9	MAN	O5-C1	2.67	1.48	1.43
9	Z	11	GAL	O5-C1	2.67	1.48	1.43
8	9	9	MAN	O5-C5	2.67	1.48	1.43
8	Y	11	FUC	O5-C5	2.66	1.48	1.43
9	Z	9	MAN	O5-C5	2.66	1.48	1.43
15	BA	1	NAG	O5-C5	2.66	1.48	1.43
8	9	11	FUC	O5-C5	2.65	1.48	1.43
15	BA	8	GAL	O5-C1	2.65	1.48	1.43
12	q	1	NAG	O5-C5	2.65	1.48	1.43
15	BA	9	MAN	O5-C5	2.65	1.48	1.43
8	Y	6	GAL	O5-C1	2.63	1.48	1.43
8	Y	3	BMA	O5-C1	2.63	1.48	1.43
8	Y	1	NAG	O5-C5	2.62	1.48	1.43
9	Z	3	BMA	O5-C1	2.62	1.48	1.43
12	q	3	FUC	O5-C5	2.61	1.48	1.43
9	Z	8	GAL	O5-C1	2.61	1.48	1.43
8	9	1	NAG	O5-C5	2.61	1.48	1.43
8	9	3	BMA	O5-C1	2.60	1.48	1.43
15	BA	3	BMA	O5-C1	2.56	1.48	1.43
8	9	4	MAN	O5-C1	2.54	1.48	1.43
8	Y	4	MAN	O5-C1	2.53	1.47	1.43
15	BA	11	NAG	O5-C5	2.51	1.48	1.43
15	BA	3	BMA	O5-C5	2.50	1.48	1.43
9	Z	3	BMA	O5-C5	2.49	1.48	1.43
9	Z	12	NAG	O5-C5	2.48	1.48	1.43
8	Y	7	NAG	O5-C5	2.47	1.48	1.43
8	Y	6	GAL	O5-C5	2.46	1.48	1.43
9	Z	11	GAL	O5-C5	2.46	1.48	1.43
8	Y	3	BMA	O5-C5	2.45	1.48	1.43
8	9	3	BMA	O5-C5	2.45	1.48	1.43
8	9	6	GAL	O5-C5	2.44	1.48	1.43
8	Y	4	MAN	O2-C2	2.44	1.48	1.43
9	Z	8	GAL	O5-C5	2.43	1.48	1.43
15	BA	9	MAN	O2-C2	2.41	1.48	1.43
9	Z	4	MAN	O2-C2	2.41	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BA	8	GAL	O5-C5	2.41	1.48	1.43
8	9	4	MAN	O2-C2	2.41	1.48	1.43
15	BA	4	MAN	O2-C2	2.41	1.48	1.43
8	9	7	NAG	O5-C5	2.40	1.48	1.43
8	Y	9	MAN	O2-C2	2.40	1.48	1.43
9	Z	9	MAN	O2-C2	2.39	1.48	1.43
8	Y	5	NAG	O5-C5	2.39	1.48	1.43
8	Y	8	GAL	O5-C5	2.38	1.48	1.43
8	9	9	MAN	O2-C2	2.37	1.48	1.43
8	9	5	NAG	O5-C5	2.37	1.48	1.43
9	Z	5	NAG	O5-C5	2.37	1.48	1.43
8	Y	10	NAG	O5-C5	2.36	1.48	1.43
8	9	10	NAG	O5-C5	2.36	1.48	1.43
9	Z	6	GAL	O5-C5	2.36	1.48	1.43
15	BA	5	NAG	O5-C5	2.35	1.48	1.43
8	9	8	GAL	O5-C5	2.34	1.48	1.43
15	BA	6	GAL	O5-C5	2.34	1.48	1.43
5	s	2	NAG	O5-C5	2.30	1.47	1.43
9	Z	2	NAG	O5-C5	2.29	1.47	1.43
15	BA	2	NAG	O5-C5	2.27	1.47	1.43
15	BA	10	NAG	O5-C5	2.27	1.47	1.43
9	Z	10	NAG	O5-C5	2.27	1.47	1.43
12	q	2	NAG	O5-C5	2.23	1.47	1.43
15	BA	4	MAN	O4-C4	2.21	1.48	1.43
15	BA	7	NAG	O5-C5	2.21	1.47	1.43
8	9	2	NAG	O5-C5	2.20	1.47	1.43
8	Y	2	NAG	O5-C5	2.20	1.47	1.43
9	Z	4	MAN	O4-C4	2.20	1.48	1.43
8	Y	5	NAG	O4-C4	2.19	1.48	1.43
8	9	7	NAG	O4-C4	2.19	1.48	1.43
8	9	5	NAG	O4-C4	2.17	1.48	1.43
9	Z	7	NAG	O5-C5	2.16	1.47	1.43
8	Y	7	NAG	O4-C4	2.15	1.48	1.43
8	9	10	NAG	O4-C4	2.15	1.48	1.43
8	Y	10	NAG	O4-C4	2.13	1.48	1.43
15	BA	10	NAG	O4-C4	2.13	1.48	1.43
9	Z	10	NAG	O4-C4	2.13	1.48	1.43
5	s	1	NAG	O4-C4	2.09	1.48	1.43
9	Z	12	NAG	O4-C4	2.08	1.48	1.43
8	Y	1	NAG	O4-C4	2.08	1.48	1.43
15	BA	7	NAG	O4-C4	2.08	1.48	1.43
15	BA	11	NAG	O4-C4	2.07	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Z	7	NAG	O4-C4	2.07	1.48	1.43
8	Y	9	MAN	O4-C4	2.07	1.48	1.43
9	Z	1	NAG	O4-C4	2.07	1.48	1.43
15	BA	1	NAG	O4-C4	2.06	1.48	1.43
8	9	9	MAN	O4-C4	2.06	1.48	1.43
8	9	1	NAG	O4-C4	2.05	1.48	1.43
12	q	1	NAG	O4-C4	2.05	1.48	1.43
8	9	1	NAG	C8-C7	2.04	1.54	1.50
12	q	1	NAG	C8-C7	2.03	1.54	1.50
9	Z	5	NAG	O4-C4	2.02	1.48	1.43
15	BA	5	NAG	O4-C4	2.01	1.47	1.43

All (467) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	O5-C1-C2	-7.58	99.56	111.29
6	t	1	NAG	O5-C1-C2	-7.57	99.57	111.29
6	V	1	NAG	O5-C1-C2	-7.57	99.59	111.29
6	a	1	NAG	O5-C1-C2	-7.57	99.59	111.29
5	G	1	NAG	O5-C1-C2	-7.56	99.59	111.29
6	U	1	NAG	O5-C1-C2	-7.56	99.59	111.29
5	5	1	NAG	O5-C1-C2	-7.55	99.61	111.29
5	T	1	NAG	O5-C1-C2	-7.55	99.61	111.29
5	l	1	NAG	O5-C1-C2	-7.55	99.61	111.29
5	k	1	NAG	O5-C1-C2	-7.55	99.62	111.29
6	n	1	NAG	O5-C1-C2	-7.54	99.62	111.29
5	4	1	NAG	O5-C1-C2	-7.54	99.63	111.29
14	6	1	NAG	O5-C1-C2	-7.53	99.63	111.29
6	i	1	NAG	O5-C1-C2	-7.53	99.64	111.29
5	3	1	NAG	O5-C1-C2	-7.53	99.64	111.29
13	x	1	NAG	O5-C1-C2	-7.53	99.64	111.29
6	d	1	NAG	O5-C1-C2	-7.53	99.65	111.29
5	u	1	NAG	O5-C1-C2	-7.52	99.66	111.29
5	w	1	NAG	O5-C1-C2	-7.52	99.66	111.29
11	p	1	NAG	O5-C1-C2	-7.52	99.66	111.29
6	m	1	NAG	O5-C1-C2	-7.52	99.66	111.29
11	8	1	NAG	O5-C1-C2	-7.52	99.66	111.29
6	J	1	NAG	O5-C1-C2	-7.51	99.66	111.29
10	e	1	NAG	O5-C1-C2	-7.51	99.67	111.29
5	o	1	NAG	O5-C1-C2	-7.51	99.68	111.29
5	1	1	NAG	O5-C1-C2	-7.51	99.68	111.29
6	2	1	NAG	O5-C1-C2	-7.51	99.68	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	1	NAG	O5-C1-C2	-7.51	99.68	111.29
5	R	1	NAG	O5-C1-C2	-7.50	99.69	111.29
6	j	1	NAG	O5-C1-C2	-7.50	99.69	111.29
6	7	1	NAG	O5-C1-C2	-7.49	99.70	111.29
6	W	1	NAG	O5-C1-C2	-7.49	99.70	111.29
5	r	1	NAG	O5-C1-C2	-7.49	99.70	111.29
5	b	1	NAG	O5-C1-C2	-7.49	99.70	111.29
6	S	1	NAG	O5-C1-C2	-7.49	99.70	111.29
5	z	1	NAG	O5-C1-C2	-7.49	99.71	111.29
5	0	1	NAG	O5-C1-C2	-7.49	99.71	111.29
5	Q	1	NAG	O5-C1-C2	-7.48	99.72	111.29
6	P	1	NAG	O5-C1-C2	-7.48	99.72	111.29
6	g	1	NAG	O5-C1-C2	-7.47	99.73	111.29
5	h	1	NAG	O5-C1-C2	-7.46	99.74	111.29
6	v	1	NAG	O5-C1-C2	-7.46	99.74	111.29
5	AA	1	NAG	O5-C1-C2	-7.46	99.76	111.29
6	I	1	NAG	O5-C1-C2	-7.43	99.79	111.29
5	X	1	NAG	O5-C1-C2	-7.39	99.85	111.29
11	p	6	MAN	C1-C2-C3	5.95	118.31	109.64
10	e	5	MAN	C1-C2-C3	5.95	118.30	109.64
11	8	6	MAN	C1-C2-C3	5.92	118.27	109.64
13	x	6	MAN	C1-C2-C3	5.91	118.25	109.64
14	6	4	MAN	C1-C2-C3	5.89	118.22	109.64
13	x	5	MAN	C1-O5-C5	4.94	118.81	112.19
11	p	5	MAN	C1-O5-C5	4.86	118.70	112.19
11	8	5	MAN	C1-O5-C5	4.85	118.69	112.19
11	8	8	MAN	C6-C5-C4	-4.82	101.19	113.02
11	p	8	MAN	C6-C5-C4	-4.80	101.24	113.02
8	Y	9	MAN	C1-O5-C5	4.59	118.34	112.19
8	9	9	MAN	C1-O5-C5	4.58	118.33	112.19
15	BA	4	MAN	C1-O5-C5	4.56	118.30	112.19
9	Z	4	MAN	C1-O5-C5	4.53	118.25	112.19
11	8	5	MAN	O2-C2-C1	4.51	119.54	109.22
13	x	5	MAN	O2-C2-C1	4.50	119.53	109.22
11	p	5	MAN	O2-C2-C1	4.50	119.53	109.22
8	Y	5	NAG	C1-O5-C5	4.24	117.87	112.19
8	9	5	NAG	C1-O5-C5	4.24	117.86	112.19
9	Z	10	NAG	C1-O5-C5	4.19	117.80	112.19
15	BA	10	NAG	C1-O5-C5	4.14	117.73	112.19
8	9	2	NAG	C1-O5-C5	4.13	117.73	112.19
9	Z	2	NAG	C1-O5-C5	4.10	117.69	112.19
8	Y	2	NAG	C1-O5-C5	4.10	117.68	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BA	2	NAG	C1-O5-C5	4.09	117.67	112.19
5	s	2	NAG	C1-O5-C5	4.08	117.66	112.19
12	q	2	NAG	C1-O5-C5	4.06	117.63	112.19
13	x	6	MAN	C2-C3-C4	-4.04	103.75	110.86
10	e	5	MAN	C2-C3-C4	-4.03	103.77	110.86
13	x	5	MAN	O2-C2-C3	-4.03	101.80	110.15
11	8	6	MAN	C2-C3-C4	-4.02	103.79	110.86
9	Z	7	NAG	C1-O5-C5	4.02	117.57	112.19
15	BA	7	NAG	C1-O5-C5	4.01	117.56	112.19
14	6	4	MAN	C2-C3-C4	-4.01	103.81	110.86
11	p	6	MAN	C2-C3-C4	-4.01	103.82	110.86
11	p	5	MAN	O2-C2-C3	-3.99	101.89	110.15
11	8	5	MAN	O2-C2-C3	-3.97	101.93	110.15
15	BA	3	BMA	C1-O5-C5	3.91	117.42	112.19
9	Z	3	BMA	C1-O5-C5	3.87	117.38	112.19
11	8	7	MAN	O4-C4-C3	-3.86	101.27	110.38
11	p	7	MAN	O4-C4-C3	-3.86	101.27	110.38
8	9	3	BMA	C1-O5-C5	3.82	117.30	112.19
8	Y	3	BMA	C1-O5-C5	3.80	117.28	112.19
8	Y	10	NAG	C1-O5-C5	3.66	117.09	112.19
8	9	10	NAG	C1-O5-C5	3.64	117.07	112.19
15	BA	9	MAN	C1-O5-C5	3.58	116.99	112.19
9	Z	9	MAN	C1-O5-C5	3.57	116.97	112.19
9	Z	5	NAG	C1-O5-C5	3.57	116.97	112.19
8	Y	4	MAN	C1-O5-C5	3.51	116.89	112.19
15	BA	5	NAG	C1-O5-C5	3.50	116.88	112.19
11	8	8	MAN	O4-C4-C3	-3.48	102.17	110.38
8	9	4	MAN	C1-O5-C5	3.48	116.85	112.19
11	p	8	MAN	O4-C4-C3	-3.48	102.18	110.38
8	Y	1	NAG	C1-O5-C5	3.41	116.76	112.19
12	q	1	NAG	C1-O5-C5	3.41	116.76	112.19
8	9	1	NAG	C1-O5-C5	3.40	116.75	112.19
9	Z	12	NAG	C1-O5-C5	3.35	116.67	112.19
15	BA	11	NAG	C1-O5-C5	3.34	116.66	112.19
9	Z	1	NAG	C1-O5-C5	3.33	116.65	112.19
5	s	1	NAG	C1-O5-C5	3.31	116.62	112.19
15	BA	1	NAG	C1-O5-C5	3.29	116.60	112.19
8	9	7	NAG	C1-O5-C5	3.28	116.59	112.19
11	p	7	MAN	O4-C4-C5	3.25	117.34	109.32
8	Y	7	NAG	C1-O5-C5	3.24	116.53	112.19
11	8	7	MAN	O4-C4-C5	3.23	117.27	109.32
15	BA	8	GAL	C1-O5-C5	3.12	116.36	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	2	NAG	O5-C5-C6	-3.11	101.60	107.66
5	5	2	NAG	O5-C5-C6	-3.11	101.61	107.66
5	X	2	NAG	O5-C5-C6	-3.11	101.62	107.66
11	8	2	NAG	O5-C5-C6	-3.10	101.62	107.66
5	Q	2	NAG	O5-C5-C6	-3.10	101.63	107.66
6	V	2	NAG	O5-C5-C6	-3.09	101.64	107.66
11	8	8	MAN	C3-C4-C5	-3.09	104.63	110.23
11	p	2	NAG	O5-C5-C6	-3.09	101.65	107.66
9	Z	11	GAL	C1-O5-C5	3.08	116.32	112.19
6	P	2	NAG	O5-C5-C6	-3.08	101.67	107.66
5	z	2	NAG	O5-C5-C6	-3.08	101.67	107.66
5	b	2	NAG	O5-C5-C6	-3.08	101.67	107.66
5	u	2	NAG	O5-C5-C6	-3.08	101.67	107.66
11	p	8	MAN	C3-C4-C5	-3.07	104.66	110.23
6	W	2	NAG	O5-C5-C6	-3.07	101.68	107.66
6	U	2	NAG	O5-C5-C6	-3.07	101.68	107.66
5	1	2	NAG	O5-C5-C6	-3.07	101.68	107.66
5	AA	2	NAG	O5-C5-C6	-3.07	101.68	107.66
6	m	2	NAG	O5-C5-C6	-3.07	101.68	107.66
6	v	2	NAG	O5-C5-C6	-3.07	101.69	107.66
6	7	2	NAG	O5-C5-C6	-3.07	101.69	107.66
5	o	2	NAG	O5-C5-C6	-3.07	101.69	107.66
5	c	2	NAG	O5-C5-C6	-3.07	101.69	107.66
9	Z	8	GAL	C1-O5-C5	3.07	116.30	112.19
6	2	2	NAG	O5-C5-C6	-3.07	101.69	107.66
5	l	2	NAG	O5-C5-C6	-3.07	101.70	107.66
5	0	2	NAG	O5-C5-C6	-3.06	101.70	107.66
5	T	2	NAG	O5-C5-C6	-3.06	101.71	107.66
5	4	2	NAG	O5-C5-C6	-3.06	101.71	107.66
6	g	2	NAG	O5-C5-C6	-3.06	101.71	107.66
8	9	6	GAL	C1-O5-C5	3.06	116.29	112.19
5	h	2	NAG	O5-C5-C6	-3.06	101.71	107.66
6	S	2	NAG	O5-C5-C6	-3.06	101.71	107.66
10	e	2	NAG	O5-C5-C6	-3.05	101.72	107.66
6	j	2	NAG	O5-C5-C6	-3.05	101.72	107.66
5	r	2	NAG	O5-C5-C6	-3.05	101.72	107.66
14	6	2	NAG	O5-C5-C6	-3.05	101.72	107.66
5	w	2	NAG	O5-C5-C6	-3.05	101.72	107.66
6	i	2	NAG	O5-C5-C6	-3.05	101.73	107.66
6	J	2	NAG	O5-C5-C6	-3.05	101.73	107.66
8	Y	6	GAL	C1-O5-C5	3.05	116.27	112.19
6	K	2	NAG	O5-C5-C6	-3.04	101.74	107.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	k	2	NAG	O5-C5-C6	-3.04	101.74	107.66
6	I	2	NAG	O5-C5-C6	-3.04	101.75	107.66
6	d	2	NAG	O5-C5-C6	-3.04	101.75	107.66
13	x	2	NAG	O5-C5-C6	-3.04	101.75	107.66
5	3	2	NAG	O5-C5-C6	-3.04	101.75	107.66
5	G	2	NAG	O5-C5-C6	-3.03	101.76	107.66
6	t	2	NAG	O5-C5-C6	-3.03	101.77	107.66
6	n	2	NAG	O5-C5-C6	-3.03	101.77	107.66
6	a	2	NAG	O5-C5-C6	-3.01	101.81	107.66
15	BA	6	GAL	C1-O5-C5	2.99	116.19	112.19
8	Y	8	GAL	C1-O5-C5	2.98	116.18	112.19
9	Z	6	GAL	C1-O5-C5	2.97	116.17	112.19
8	9	8	GAL	C1-O5-C5	2.96	116.16	112.19
6	V	1	NAG	O7-C7-C8	-2.94	116.83	122.05
5	o	1	NAG	O7-C7-C8	-2.93	116.84	122.05
6	W	1	NAG	O7-C7-C8	-2.93	116.84	122.05
14	6	1	NAG	O7-C7-C8	-2.92	116.85	122.05
6	n	1	NAG	O7-C7-C8	-2.92	116.85	122.05
6	j	1	NAG	O7-C7-C8	-2.91	116.87	122.05
6	7	1	NAG	O7-C7-C8	-2.91	116.87	122.05
5	Q	1	NAG	O7-C7-C8	-2.91	116.87	122.05
5	T	1	NAG	O7-C7-C8	-2.91	116.88	122.05
5	0	1	NAG	O7-C7-C8	-2.91	116.88	122.05
13	x	1	NAG	O7-C7-C8	-2.90	116.88	122.05
10	e	1	NAG	O7-C7-C8	-2.90	116.89	122.05
6	K	1	NAG	O7-C7-C8	-2.90	116.90	122.05
6	I	3	BMA	O2-C2-C3	2.89	116.14	110.15
6	J	1	NAG	O7-C7-C8	-2.89	116.90	122.05
5	u	1	NAG	O7-C7-C8	-2.89	116.91	122.05
5	b	1	NAG	O7-C7-C8	-2.89	116.91	122.05
6	d	1	NAG	O7-C7-C8	-2.89	116.91	122.05
5	w	1	NAG	O7-C7-C8	-2.89	116.91	122.05
6	S	1	NAG	O7-C7-C8	-2.88	116.92	122.05
6	2	1	NAG	O7-C7-C8	-2.88	116.92	122.05
6	i	1	NAG	O7-C7-C8	-2.88	116.93	122.05
6	a	3	BMA	O2-C2-C3	2.88	116.11	110.15
5	3	1	NAG	O7-C7-C8	-2.88	116.93	122.05
6	v	3	BMA	O2-C2-C3	2.88	116.11	110.15
5	1	1	NAG	O7-C7-C8	-2.88	116.93	122.05
6	j	3	BMA	O2-C2-C3	2.88	116.11	110.15
5	5	1	NAG	O7-C7-C8	-2.87	116.94	122.05
6	I	1	NAG	O7-C7-C8	-2.87	116.94	122.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	l	1	NAG	O7-C7-C8	-2.87	116.94	122.05
6	t	3	BMA	O2-C2-C3	2.87	116.09	110.15
5	r	1	NAG	O7-C7-C8	-2.87	116.95	122.05
5	AA	1	NAG	O7-C7-C8	-2.87	116.95	122.05
6	g	3	BMA	O2-C2-C3	2.87	116.09	110.15
5	c	1	NAG	O7-C7-C8	-2.86	116.96	122.05
5	z	1	NAG	O7-C7-C8	-2.86	116.96	122.05
5	h	1	NAG	O7-C7-C8	-2.86	116.96	122.05
6	7	3	BMA	O2-C2-C3	2.86	116.07	110.15
6	W	3	BMA	O2-C2-C3	2.86	116.07	110.15
6	i	3	BMA	O2-C2-C3	2.85	116.06	110.15
5	X	1	NAG	O7-C7-C8	-2.85	116.97	122.05
6	v	1	NAG	O7-C7-C8	-2.85	116.97	122.05
14	6	3	BMA	O2-C2-C3	2.85	116.06	110.15
6	P	1	NAG	O7-C7-C8	-2.85	116.97	122.05
5	4	1	NAG	O7-C7-C8	-2.85	116.98	122.05
6	P	3	BMA	O2-C2-C3	2.85	116.06	110.15
6	n	3	BMA	O2-C2-C3	2.85	116.06	110.15
11	8	1	NAG	O7-C7-C8	-2.85	116.98	122.05
11	8	8	MAN	O2-C2-C3	-2.85	104.25	110.15
5	k	1	NAG	O7-C7-C8	-2.85	116.99	122.05
5	R	1	NAG	O7-C7-C8	-2.84	116.99	122.05
6	d	3	BMA	O2-C2-C3	2.84	116.04	110.15
13	x	3	BMA	O2-C2-C3	2.84	116.04	110.15
6	J	3	BMA	O2-C2-C3	2.84	116.03	110.15
6	V	3	BMA	O2-C2-C3	2.84	116.03	110.15
11	8	3	BMA	O2-C2-C3	2.84	116.03	110.15
5	G	1	NAG	O7-C7-C8	-2.84	117.00	122.05
11	p	3	BMA	O2-C2-C3	2.84	116.03	110.15
6	m	1	NAG	O7-C7-C8	-2.83	117.01	122.05
6	g	1	NAG	O7-C7-C8	-2.83	117.01	122.05
6	K	3	BMA	O2-C2-C3	2.83	116.02	110.15
6	t	1	NAG	O7-C7-C8	-2.83	117.01	122.05
11	p	8	MAN	O2-C2-C3	-2.83	104.29	110.15
6	2	3	BMA	O2-C2-C3	2.83	116.01	110.15
11	p	1	NAG	O7-C7-C8	-2.83	117.01	122.05
6	S	3	BMA	O2-C2-C3	2.83	116.01	110.15
6	a	1	NAG	O7-C7-C8	-2.82	117.03	122.05
6	U	1	NAG	O7-C7-C8	-2.82	117.04	122.05
10	e	3	BMA	O2-C2-C3	2.82	115.99	110.15
6	U	3	BMA	O2-C2-C3	2.80	115.96	110.15
6	m	3	BMA	O2-C2-C3	2.80	115.95	110.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	8	5	MAN	O4-C4-C3	-2.73	103.94	110.38
11	p	5	MAN	O4-C4-C3	-2.73	103.95	110.38
13	x	5	MAN	O4-C4-C3	-2.72	103.96	110.38
5	c	1	NAG	C4-C3-C2	-2.72	107.04	111.02
6	W	1	NAG	C4-C3-C2	-2.71	107.04	111.02
6	v	1	NAG	C4-C3-C2	-2.71	107.05	111.02
6	t	3	BMA	O4-C4-C5	-2.70	102.67	109.32
5	R	1	NAG	C4-C3-C2	-2.70	107.06	111.02
6	I	1	NAG	C4-C3-C2	-2.70	107.06	111.02
5	5	1	NAG	C4-C3-C2	-2.70	107.07	111.02
5	o	1	NAG	C4-C3-C2	-2.69	107.07	111.02
6	2	3	BMA	O4-C4-C5	-2.69	102.69	109.32
6	7	1	NAG	C4-C3-C2	-2.69	107.08	111.02
5	h	1	NAG	C4-C3-C2	-2.69	107.08	111.02
6	m	1	NAG	C4-C3-C2	-2.69	107.08	111.02
6	J	3	BMA	O4-C4-C5	-2.68	102.72	109.32
6	S	3	BMA	O4-C4-C5	-2.68	102.73	109.32
6	t	1	NAG	C4-C3-C2	-2.67	107.10	111.02
6	j	3	BMA	O4-C4-C5	-2.67	102.74	109.32
11	8	1	NAG	C4-C3-C2	-2.67	107.10	111.02
6	W	3	BMA	O4-C4-C5	-2.67	102.74	109.32
5	u	1	NAG	C4-C3-C2	-2.67	107.10	111.02
5	4	1	NAG	C4-C3-C2	-2.67	107.10	111.02
11	8	3	BMA	O4-C4-C5	-2.67	102.75	109.32
6	a	3	BMA	O4-C4-C5	-2.67	102.75	109.32
6	V	1	NAG	C4-C3-C2	-2.67	107.11	111.02
11	p	3	BMA	O4-C4-C5	-2.67	102.75	109.32
6	n	1	NAG	C4-C3-C2	-2.67	107.11	111.02
6	a	1	NAG	C4-C3-C2	-2.66	107.11	111.02
6	V	3	BMA	O4-C4-C5	-2.66	102.77	109.32
5	0	1	NAG	C4-C3-C2	-2.66	107.12	111.02
6	d	3	BMA	O4-C4-C5	-2.66	102.77	109.32
5	G	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	l	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	k	1	NAG	C4-C3-C2	-2.66	107.12	111.02
6	U	1	NAG	C4-C3-C2	-2.66	107.12	111.02
13	x	1	NAG	C4-C3-C2	-2.66	107.12	111.02
6	7	3	BMA	O4-C4-C5	-2.66	102.77	109.32
6	i	3	BMA	O4-C4-C5	-2.66	102.78	109.32
6	g	3	BMA	O4-C4-C5	-2.66	102.78	109.32
6	I	3	BMA	O4-C4-C5	-2.66	102.78	109.32
5	AA	1	NAG	C4-C3-C2	-2.65	107.13	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1	NAG	C4-C3-C2	-2.65	107.13	111.02
6	m	3	BMA	O4-C4-C5	-2.65	102.79	109.32
5	z	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	1	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	r	1	NAG	C4-C3-C2	-2.65	107.13	111.02
14	6	3	BMA	O4-C4-C5	-2.65	102.80	109.32
5	b	1	NAG	C4-C3-C2	-2.65	107.14	111.02
6	v	3	BMA	O4-C4-C5	-2.65	102.80	109.32
6	i	1	NAG	C4-C3-C2	-2.65	107.14	111.02
6	n	3	BMA	O4-C4-C5	-2.65	102.80	109.32
5	T	1	NAG	C4-C3-C2	-2.65	107.14	111.02
5	w	1	NAG	C4-C3-C2	-2.65	107.14	111.02
14	6	1	NAG	C4-C3-C2	-2.65	107.14	111.02
6	P	3	BMA	O4-C4-C5	-2.64	102.82	109.32
5	X	1	NAG	C4-C3-C2	-2.64	107.15	111.02
6	d	1	NAG	C4-C3-C2	-2.64	107.15	111.02
6	U	3	BMA	O4-C4-C5	-2.64	102.83	109.32
5	Q	1	NAG	C4-C3-C2	-2.63	107.16	111.02
6	j	1	NAG	C4-C3-C2	-2.63	107.16	111.02
11	p	1	NAG	C4-C3-C2	-2.63	107.16	111.02
5	3	1	NAG	C4-C3-C2	-2.63	107.16	111.02
10	e	1	NAG	C4-C3-C2	-2.63	107.17	111.02
6	g	1	NAG	C4-C3-C2	-2.63	107.17	111.02
6	2	1	NAG	C4-C3-C2	-2.62	107.18	111.02
6	K	3	BMA	O4-C4-C5	-2.62	102.87	109.32
13	x	3	BMA	O4-C4-C5	-2.62	102.87	109.32
6	S	1	NAG	C4-C3-C2	-2.62	107.18	111.02
10	e	3	BMA	O4-C4-C5	-2.61	102.89	109.32
6	K	1	NAG	C4-C3-C2	-2.61	107.19	111.02
6	J	1	NAG	C4-C3-C2	-2.61	107.19	111.02
11	p	7	MAN	O5-C5-C6	-2.53	102.75	107.66
11	8	7	MAN	O5-C5-C6	-2.51	102.77	107.66
15	BA	9	MAN	C1-C2-C3	2.51	113.30	109.64
11	p	8	MAN	O5-C5-C6	2.51	112.54	107.66
11	8	8	MAN	O5-C5-C6	2.50	112.54	107.66
9	Z	9	MAN	C1-C2-C3	2.50	113.28	109.64
8	9	4	MAN	C1-C2-C3	2.49	113.27	109.64
8	Y	4	MAN	C1-C2-C3	2.49	113.27	109.64
11	8	4	MAN	O5-C5-C6	2.48	112.50	107.66
6	K	2	NAG	O5-C1-C2	-2.48	107.45	111.29
11	p	4	MAN	O5-C5-C6	2.46	112.45	107.66
13	x	2	NAG	O5-C1-C2	-2.42	107.54	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	x	4	MAN	O5-C5-C6	2.41	112.35	107.66
10	e	2	NAG	O5-C1-C2	-2.40	107.57	111.29
10	e	4	MAN	O5-C5-C6	2.40	112.34	107.66
5	G	2	NAG	O5-C1-C2	-2.36	107.64	111.29
5	3	2	NAG	O5-C1-C2	-2.36	107.64	111.29
6	K	3	BMA	C6-C5-C4	-2.36	107.23	113.02
13	x	3	BMA	C6-C5-C4	-2.36	107.24	113.02
10	e	2	NAG	C4-C3-C2	-2.35	107.57	111.02
6	n	2	NAG	O5-C1-C2	-2.35	107.66	111.29
6	t	2	NAG	O5-C1-C2	-2.34	107.67	111.29
10	e	3	BMA	C6-C5-C4	-2.34	107.27	113.02
6	V	2	NAG	O5-C1-C2	-2.34	107.67	111.29
5	5	2	NAG	O5-C1-C2	-2.34	107.67	111.29
5	Q	2	NAG	O5-C1-C2	-2.34	107.68	111.29
5	T	2	NAG	O5-C1-C2	-2.33	107.68	111.29
14	6	2	NAG	O5-C1-C2	-2.33	107.68	111.29
6	J	3	BMA	C6-C5-C4	-2.33	107.30	113.02
6	W	2	NAG	O5-C1-C2	-2.33	107.69	111.29
6	7	3	BMA	C6-C5-C4	-2.33	107.31	113.02
6	W	3	BMA	C6-C5-C4	-2.33	107.31	113.02
6	j	3	BMA	C6-C5-C4	-2.32	107.31	113.02
5	h	2	NAG	O5-C1-C2	-2.32	107.70	111.29
5	w	2	NAG	O5-C1-C2	-2.32	107.70	111.29
6	7	2	NAG	O5-C1-C2	-2.32	107.70	111.29
5	b	2	NAG	O5-C1-C2	-2.32	107.70	111.29
5	k	2	NAG	O5-C1-C2	-2.32	107.70	111.29
5	0	2	NAG	O5-C1-C2	-2.32	107.70	111.29
6	P	3	BMA	C6-C5-C4	-2.32	107.33	113.02
6	d	3	BMA	C6-C5-C4	-2.32	107.33	113.02
5	o	2	NAG	O5-C1-C2	-2.32	107.71	111.29
6	n	3	BMA	C6-C5-C4	-2.31	107.33	113.02
6	I	2	NAG	O5-C1-C2	-2.31	107.71	111.29
6	d	2	NAG	O5-C1-C2	-2.31	107.71	111.29
6	v	3	BMA	C6-C5-C4	-2.31	107.34	113.02
6	U	3	BMA	C6-C5-C4	-2.31	107.34	113.02
5	c	2	NAG	O5-C1-C2	-2.31	107.72	111.29
6	I	3	BMA	C6-C5-C4	-2.31	107.35	113.02
14	6	3	BMA	C6-C5-C4	-2.31	107.35	113.02
6	2	3	BMA	C6-C5-C4	-2.31	107.35	113.02
6	m	3	BMA	C6-C5-C4	-2.31	107.35	113.02
6	m	2	NAG	O5-C1-C2	-2.31	107.72	111.29
11	p	2	NAG	O5-C1-C2	-2.31	107.72	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	8	3	BMA	C6-C5-C4	-2.30	107.36	113.02
6	U	2	NAG	O5-C1-C2	-2.30	107.73	111.29
6	g	3	BMA	C6-C5-C4	-2.30	107.37	113.02
6	i	3	BMA	C6-C5-C4	-2.30	107.37	113.02
11	p	3	BMA	C6-C5-C4	-2.30	107.37	113.02
5	z	2	NAG	O5-C1-C2	-2.30	107.73	111.29
6	V	3	BMA	C6-C5-C4	-2.30	107.37	113.02
11	8	5	MAN	O6-C6-C5	2.30	119.16	111.33
8	9	9	MAN	C1-C2-C3	2.29	112.98	109.64
5	u	2	NAG	O5-C1-C2	-2.29	107.74	111.29
6	S	3	BMA	C6-C5-C4	-2.29	107.39	113.02
6	J	2	NAG	O5-C1-C2	-2.29	107.74	111.29
11	8	2	NAG	O5-C1-C2	-2.29	107.74	111.29
11	p	5	MAN	O6-C6-C5	2.29	119.14	111.33
5	l	2	NAG	O5-C1-C2	-2.29	107.75	111.29
5	X	2	NAG	O5-C1-C2	-2.29	107.75	111.29
6	a	3	BMA	C6-C5-C4	-2.29	107.40	113.02
5	l	2	NAG	O5-C1-C2	-2.29	107.75	111.29
6	t	3	BMA	C6-C5-C4	-2.28	107.41	113.02
5	4	2	NAG	O5-C1-C2	-2.28	107.76	111.29
6	g	2	NAG	O5-C1-C2	-2.28	107.76	111.29
6	i	2	NAG	O5-C1-C2	-2.28	107.76	111.29
5	R	2	NAG	O5-C1-C2	-2.28	107.77	111.29
5	r	2	NAG	O5-C1-C2	-2.28	107.77	111.29
6	P	2	NAG	O5-C1-C2	-2.28	107.77	111.29
13	x	5	MAN	O6-C6-C5	2.28	119.09	111.33
5	AA	2	NAG	O5-C1-C2	-2.27	107.77	111.29
8	Y	9	MAN	C1-C2-C3	2.27	112.95	109.64
6	2	2	NAG	O5-C1-C2	-2.27	107.78	111.29
6	K	2	NAG	C4-C3-C2	-2.27	107.69	111.02
10	e	5	MAN	O5-C1-C2	-2.27	105.39	110.79
5	r	2	NAG	C4-C3-C2	-2.26	107.70	111.02
13	x	2	NAG	C4-C3-C2	-2.26	107.70	111.02
6	j	2	NAG	O5-C1-C2	-2.26	107.79	111.29
6	v	2	NAG	O5-C1-C2	-2.26	107.80	111.29
6	S	2	NAG	O5-C1-C2	-2.26	107.80	111.29
6	a	2	NAG	O5-C1-C2	-2.25	107.81	111.29
6	7	2	NAG	C4-C3-C2	-2.25	107.72	111.02
11	p	6	MAN	O5-C1-C2	-2.24	105.43	110.79
14	6	4	MAN	O5-C1-C2	-2.24	105.44	110.79
11	8	7	MAN	C1-O5-C5	2.23	115.18	112.19
5	u	2	NAG	C4-C3-C2	-2.23	107.75	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	l	2	NAG	C4-C3-C2	-2.23	107.75	111.02
11	8	6	MAN	O5-C1-C2	-2.23	105.48	110.79
6	W	2	NAG	C4-C3-C2	-2.23	107.76	111.02
5	G	2	NAG	C4-C3-C2	-2.22	107.76	111.02
13	x	6	MAN	O5-C1-C2	-2.22	105.49	110.79
6	d	2	NAG	C4-C3-C2	-2.22	107.77	111.02
5	o	2	NAG	C4-C3-C2	-2.22	107.77	111.02
11	p	7	MAN	C1-O5-C5	2.21	115.15	112.19
6	2	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	AA	2	NAG	C4-C3-C2	-2.21	107.78	111.02
5	k	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	0	2	NAG	C4-C3-C2	-2.20	107.79	111.02
6	P	2	NAG	C4-C3-C2	-2.20	107.79	111.02
6	g	2	NAG	C4-C3-C2	-2.20	107.79	111.02
14	6	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	w	2	NAG	C4-C3-C2	-2.20	107.79	111.02
5	3	2	NAG	C4-C3-C2	-2.20	107.80	111.02
5	5	2	NAG	C4-C3-C2	-2.20	107.80	111.02
5	z	2	NAG	C4-C3-C2	-2.20	107.80	111.02
6	m	2	NAG	C4-C3-C2	-2.20	107.80	111.02
5	b	2	NAG	C4-C3-C2	-2.20	107.80	111.02
6	I	2	NAG	C4-C3-C2	-2.19	107.80	111.02
5	X	2	NAG	C4-C3-C2	-2.19	107.81	111.02
11	8	2	NAG	C4-C3-C2	-2.19	107.81	111.02
5	4	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	a	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	n	2	NAG	C4-C3-C2	-2.19	107.81	111.02
5	c	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	J	2	NAG	C4-C3-C2	-2.19	107.81	111.02
6	S	2	NAG	C4-C3-C2	-2.19	107.81	111.02
11	p	2	NAG	C4-C3-C2	-2.18	107.82	111.02
6	V	2	NAG	C4-C3-C2	-2.18	107.82	111.02
5	T	2	NAG	C4-C3-C2	-2.18	107.82	111.02
6	t	2	NAG	C4-C3-C2	-2.18	107.82	111.02
6	U	2	NAG	C4-C3-C2	-2.17	107.83	111.02
6	j	2	NAG	C4-C3-C2	-2.17	107.83	111.02
15	BA	4	MAN	C1-C2-C3	2.17	112.81	109.64
5	h	2	NAG	C4-C3-C2	-2.17	107.84	111.02
6	v	2	NAG	C4-C3-C2	-2.16	107.85	111.02
5	Q	2	NAG	C4-C3-C2	-2.16	107.86	111.02
11	8	7	MAN	O3-C3-C2	-2.15	105.67	110.05
5	1	2	NAG	C4-C3-C2	-2.14	107.88	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	i	2	NAG	C4-C3-C2	-2.14	107.88	111.02
9	Z	4	MAN	C1-C2-C3	2.14	112.76	109.64
11	8	8	MAN	O2-C2-C1	2.13	114.10	109.22
13	x	4	MAN	O3-C3-C4	2.13	115.39	110.38
5	R	2	NAG	C4-C3-C2	-2.13	107.90	111.02
11	p	7	MAN	O3-C3-C2	-2.12	105.73	110.05
11	p	8	MAN	O2-C2-C1	2.12	114.07	109.22
11	8	8	MAN	C2-C3-C4	2.11	114.58	110.86
11	p	8	MAN	C2-C3-C4	2.11	114.58	110.86
10	e	4	MAN	O3-C3-C4	2.09	115.30	110.38
7	y	6	MAN	C1-O5-C5	-2.08	109.40	112.19
11	8	4	MAN	O3-C3-C4	2.07	115.26	110.38
11	p	4	MAN	O3-C3-C4	2.06	115.24	110.38
9	Z	12	NAG	O5-C1-C2	-2.05	108.12	111.29
7	O	6	MAN	O5-C5-C6	2.03	111.61	107.66
7	O	6	MAN	C1-O5-C5	-2.02	109.47	112.19
13	x	4	MAN	O4-C4-C3	-2.02	105.61	110.38
7	f	6	MAN	C1-O5-C5	-2.02	109.48	112.19
15	BA	11	NAG	O5-C1-C2	-2.02	108.17	111.29
7	f	6	MAN	O5-C5-C6	2.01	111.58	107.66

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	X	1	NAG	C3-C2-N2-C7
5	s	1	NAG	C1-C2-N2-C7
9	Z	1	NAG	C1-C2-N2-C7
11	p	1	NAG	C3-C2-N2-C7
11	8	1	NAG	C3-C2-N2-C7
15	BA	1	NAG	C1-C2-N2-C7
8	Y	3	BMA	C4-C5-C6-O6
8	9	3	BMA	C4-C5-C6-O6
7	f	5	MAN	O5-C5-C6-O6
7	y	5	MAN	O5-C5-C6-O6
7	O	5	MAN	O5-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
8	9	3	BMA	O5-C5-C6-O6
7	O	2	NAG	C8-C7-N2-C2
7	f	2	NAG	C8-C7-N2-C2
7	y	2	NAG	C8-C7-N2-C2
7	O	6	MAN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	f	6	MAN	C4-C5-C6-O6
7	y	6	MAN	C4-C5-C6-O6
7	O	6	MAN	O5-C5-C6-O6
7	f	6	MAN	O5-C5-C6-O6
15	BA	9	MAN	O5-C5-C6-O6
7	y	6	MAN	O5-C5-C6-O6
7	y	2	NAG	O7-C7-N2-C2
9	Z	9	MAN	O5-C5-C6-O6
7	O	2	NAG	O7-C7-N2-C2
7	f	2	NAG	O7-C7-N2-C2
5	c	1	NAG	C3-C2-N2-C7
6	I	1	NAG	C3-C2-N2-C7
6	v	1	NAG	C3-C2-N2-C7
6	U	3	BMA	C4-C5-C6-O6
6	V	3	BMA	C4-C5-C6-O6
6	I	3	BMA	C4-C5-C6-O6
6	P	3	BMA	C4-C5-C6-O6
6	g	3	BMA	C4-C5-C6-O6
6	v	3	BMA	C4-C5-C6-O6
6	7	3	BMA	C4-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6
6	W	3	BMA	C4-C5-C6-O6
6	a	3	BMA	C4-C5-C6-O6
6	d	3	BMA	C4-C5-C6-O6
6	i	3	BMA	C4-C5-C6-O6
6	j	3	BMA	C4-C5-C6-O6
6	m	3	BMA	C4-C5-C6-O6
14	6	3	BMA	C4-C5-C6-O6
6	S	3	BMA	C4-C5-C6-O6
6	n	3	BMA	C4-C5-C6-O6
6	2	3	BMA	C4-C5-C6-O6
6	t	3	BMA	C4-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	m	3	BMA	O5-C5-C6-O6
6	g	3	BMA	O5-C5-C6-O6
6	v	3	BMA	O5-C5-C6-O6
6	7	3	BMA	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
6	W	3	BMA	O5-C5-C6-O6
6	i	3	BMA	O5-C5-C6-O6
6	2	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	J	3	BMA	O5-C5-C6-O6
6	d	3	BMA	O5-C5-C6-O6
6	j	3	BMA	O5-C5-C6-O6
6	t	3	BMA	O5-C5-C6-O6
14	6	3	BMA	O5-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
6	a	3	BMA	O5-C5-C6-O6
6	n	3	BMA	O5-C5-C6-O6
6	i	1	NAG	C3-C2-N2-C7
7	f	5	MAN	C4-C5-C6-O6
7	y	5	MAN	C4-C5-C6-O6
7	O	5	MAN	C4-C5-C6-O6
10	e	1	NAG	O7-C7-N2-C2
5	c	1	NAG	O7-C7-N2-C2
6	7	1	NAG	O7-C7-N2-C2
13	x	1	NAG	O7-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	l	1	NAG	O7-C7-N2-C2
5	0	1	NAG	O7-C7-N2-C2
5	3	1	NAG	O7-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
6	g	1	NAG	O7-C7-N2-C2
6	t	1	NAG	O7-C7-N2-C2
6	v	1	NAG	O7-C7-N2-C2
11	p	1	NAG	O7-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	b	1	NAG	O7-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
5	k	1	NAG	O7-C7-N2-C2
5	o	1	NAG	O7-C7-N2-C2
5	r	1	NAG	O7-C7-N2-C2
5	u	1	NAG	O7-C7-N2-C2
5	w	1	NAG	O7-C7-N2-C2
5	z	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	1	1	NAG	O7-C7-N2-C2
5	4	1	NAG	O7-C7-N2-C2
5	5	1	NAG	O7-C7-N2-C2
5	AA	1	NAG	O7-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	P	1	NAG	O7-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
6	a	1	NAG	O7-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
6	i	1	NAG	O7-C7-N2-C2
6	j	1	NAG	O7-C7-N2-C2
6	m	1	NAG	O7-C7-N2-C2
6	n	1	NAG	O7-C7-N2-C2
6	2	1	NAG	O7-C7-N2-C2
11	8	1	NAG	O7-C7-N2-C2
14	6	1	NAG	O7-C7-N2-C2

There are no ring outliers.

96 monomers are involved in 343 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	2	NAG	1	0
9	Z	7	NAG	7	0
8	9	6	GAL	3	0
8	9	11	FUC	8	0
8	Y	11	FUC	4	0
5	z	1	NAG	3	0
6	7	1	NAG	6	0
6	V	2	NAG	4	0
6	i	1	NAG	17	0
5	c	1	NAG	13	0
9	Z	4	MAN	2	0
9	Z	13	FUC	1	0
13	x	2	NAG	1	0
5	G	1	NAG	9	0
6	W	3	BMA	3	0
6	n	2	NAG	5	0
5	l	1	NAG	6	0
5	o	1	NAG	13	0
9	Z	5	NAG	2	0
12	q	1	NAG	3	0
5	5	1	NAG	5	0

Continued on next page...

Continued from previous page...

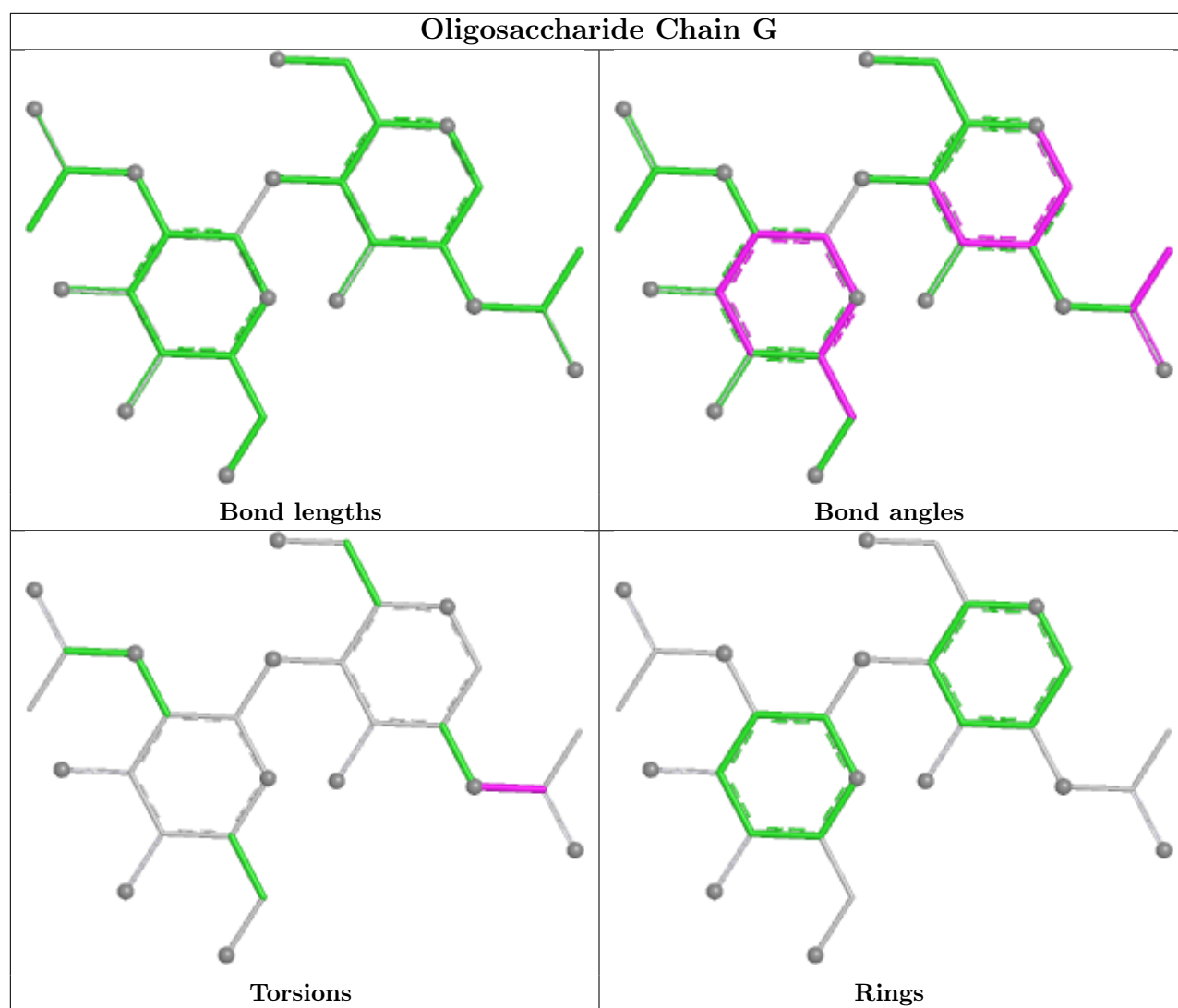
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	2	NAG	3	0
15	BA	2	NAG	11	0
7	O	2	NAG	1	0
5	1	1	NAG	2	0
15	BA	1	NAG	2	0
10	e	3	BMA	1	0
5	w	2	NAG	2	0
6	n	1	NAG	2	0
5	4	1	NAG	15	0
5	s	2	NAG	1	0
7	f	3	BMA	4	0
6	7	2	NAG	1	0
5	T	1	NAG	12	0
9	Z	12	NAG	4	0
12	q	3	FUC	11	0
6	I	1	NAG	25	0
7	y	2	NAG	1	0
7	f	6	MAN	4	0
15	BA	8	GAL	1	0
5	X	1	NAG	2	0
9	Z	8	GAL	1	0
5	r	2	NAG	1	0
5	G	2	NAG	1	0
7	y	1	NAG	1	0
11	p	5	MAN	1	0
5	s	1	NAG	2	0
7	f	5	MAN	2	0
11	p	1	NAG	2	0
7	f	1	NAG	1	0
15	BA	4	MAN	2	0
6	P	1	NAG	3	0
8	9	2	NAG	1	0
6	J	1	NAG	1	0
11	8	1	NAG	2	0
13	x	6	MAN	1	0
6	W	2	NAG	5	0
6	i	2	NAG	1	0
6	K	1	NAG	5	0
5	r	1	NAG	1	0
6	v	1	NAG	6	0
6	i	3	BMA	1	0
5	Q	2	NAG	1	0

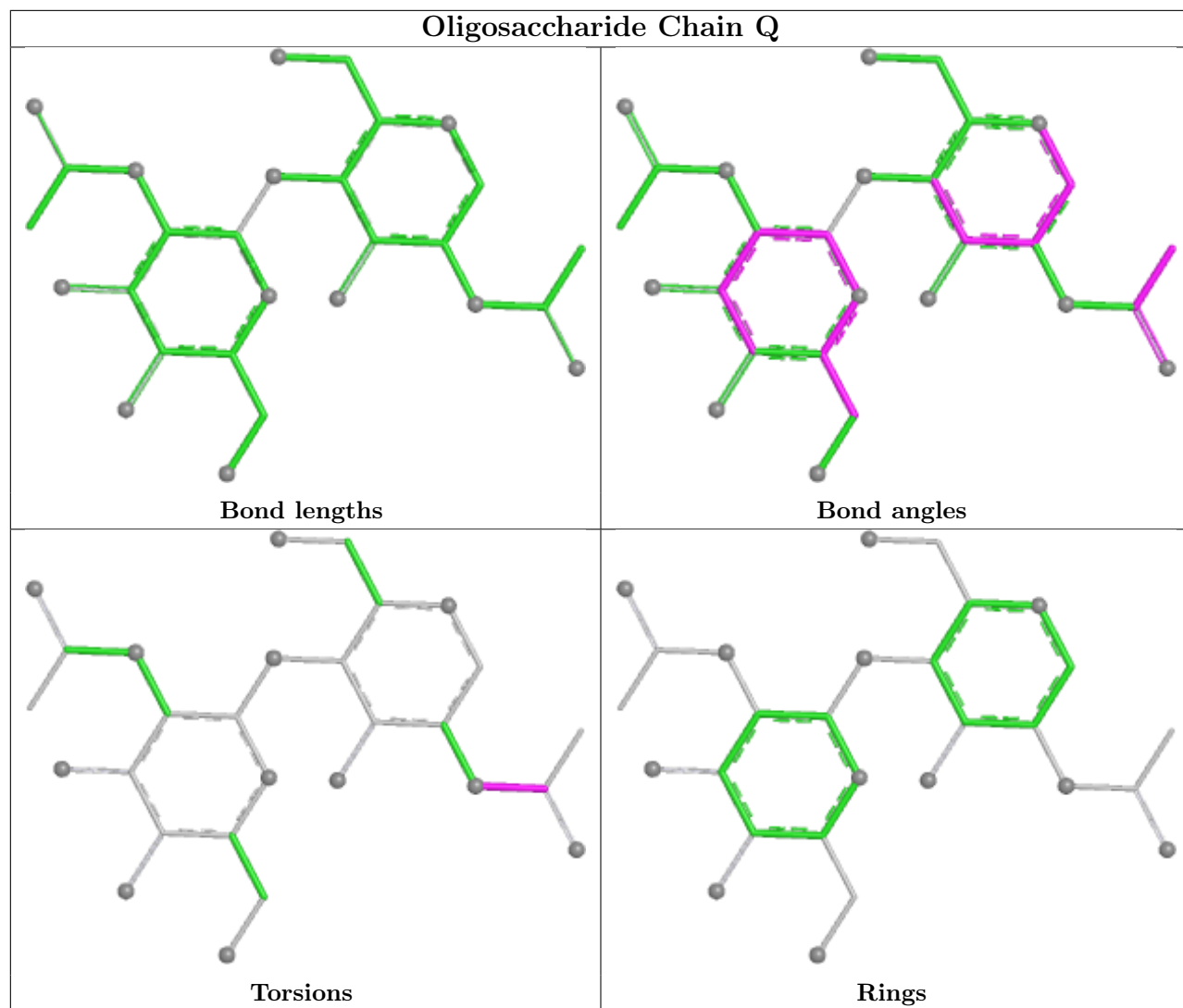
Continued on next page...

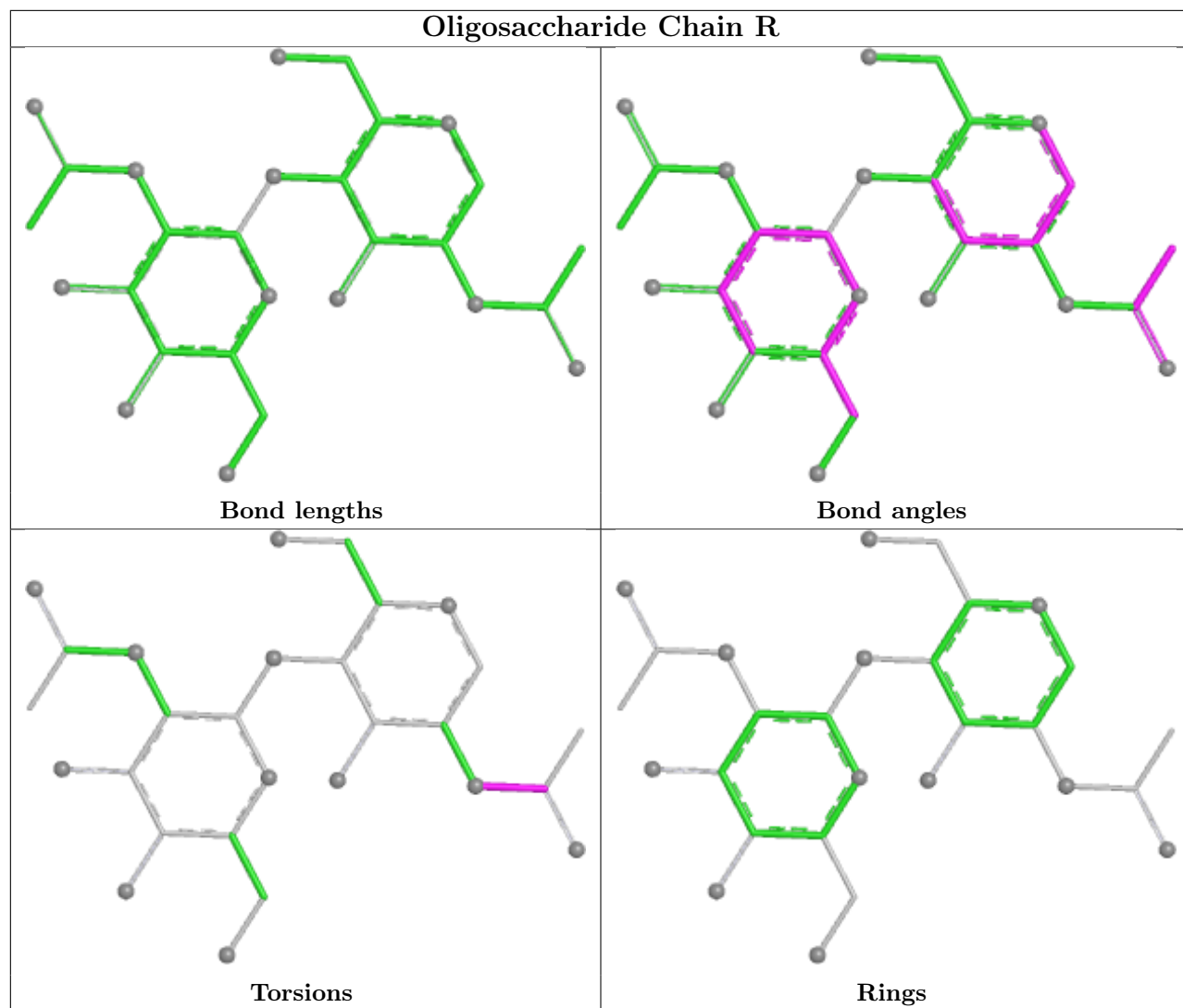
Continued from previous page...

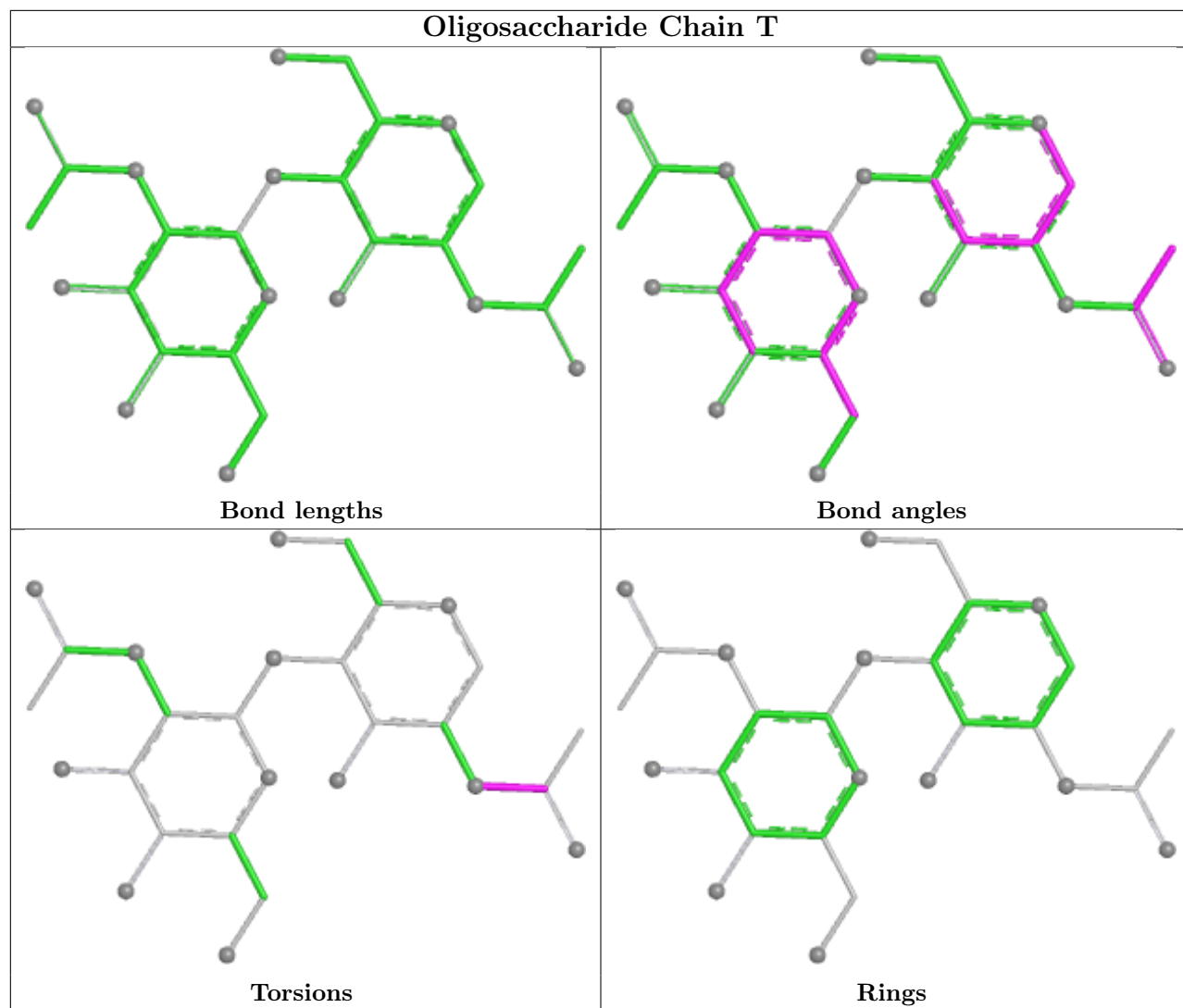
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	g	2	NAG	2	0
5	w	1	NAG	14	0
5	Q	1	NAG	3	0
7	O	4	MAN	2	0
10	e	1	NAG	8	0
5	c	2	NAG	9	0
7	f	2	NAG	1	0
5	3	1	NAG	13	0
11	8	5	MAN	2	0
13	x	3	BMA	2	0
14	6	2	NAG	6	0
8	Y	8	GAL	1	0
6	7	3	BMA	1	0
9	Z	2	NAG	14	0
8	Y	7	NAG	1	0
15	BA	7	NAG	3	0
6	d	2	NAG	2	0
6	P	2	NAG	2	0
6	W	1	NAG	6	0
5	R	1	NAG	6	0
5	z	2	NAG	2	0
6	g	1	NAG	3	0
9	Z	6	GAL	2	0
8	Y	6	GAL	1	0
8	Y	2	NAG	1	0
7	O	1	NAG	1	0
9	Z	1	NAG	3	0
15	BA	3	BMA	3	0
6	d	1	NAG	14	0
6	v	2	NAG	2	0
6	j	1	NAG	6	0
10	e	2	NAG	6	0
8	Y	1	NAG	1	0

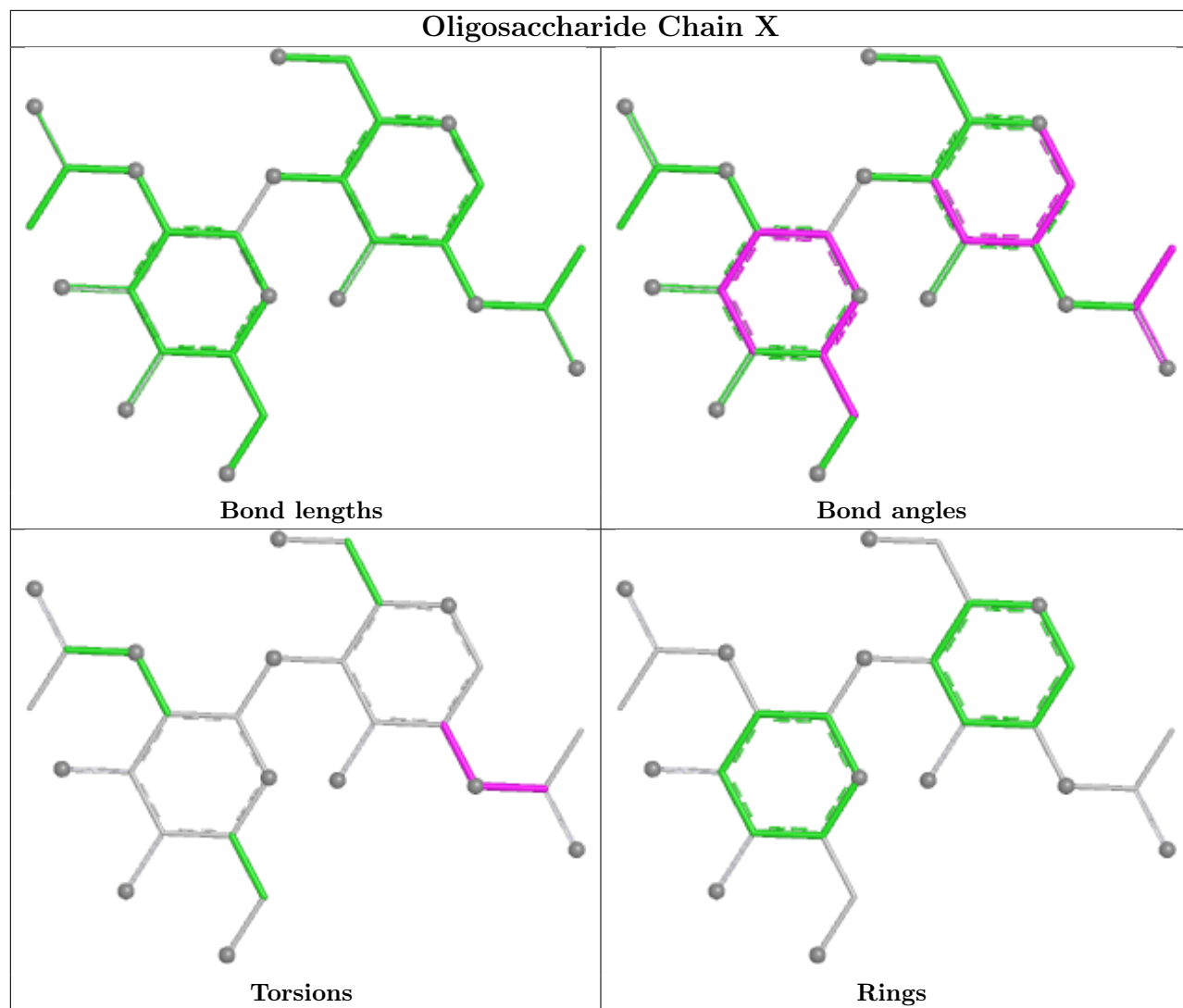
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

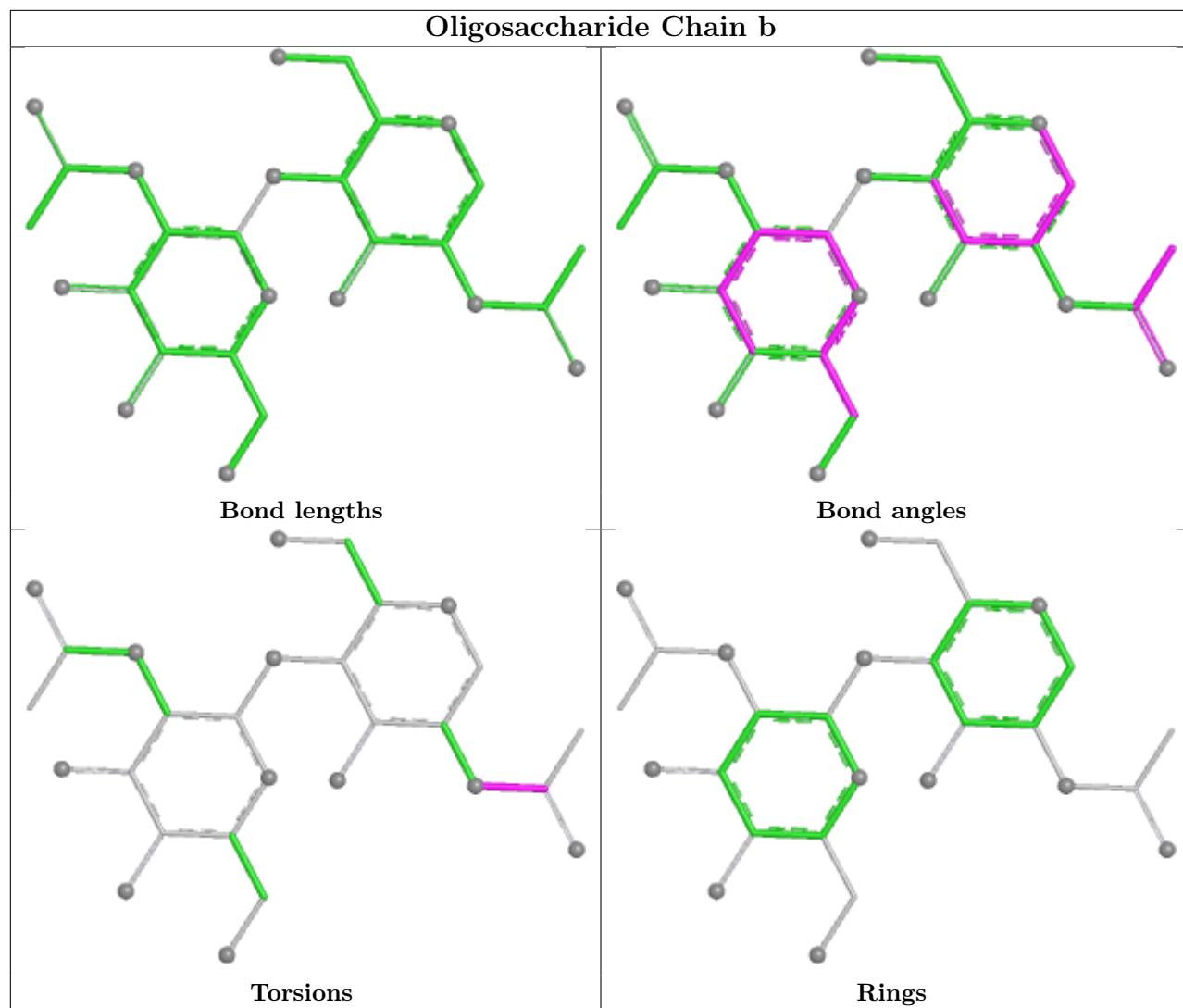


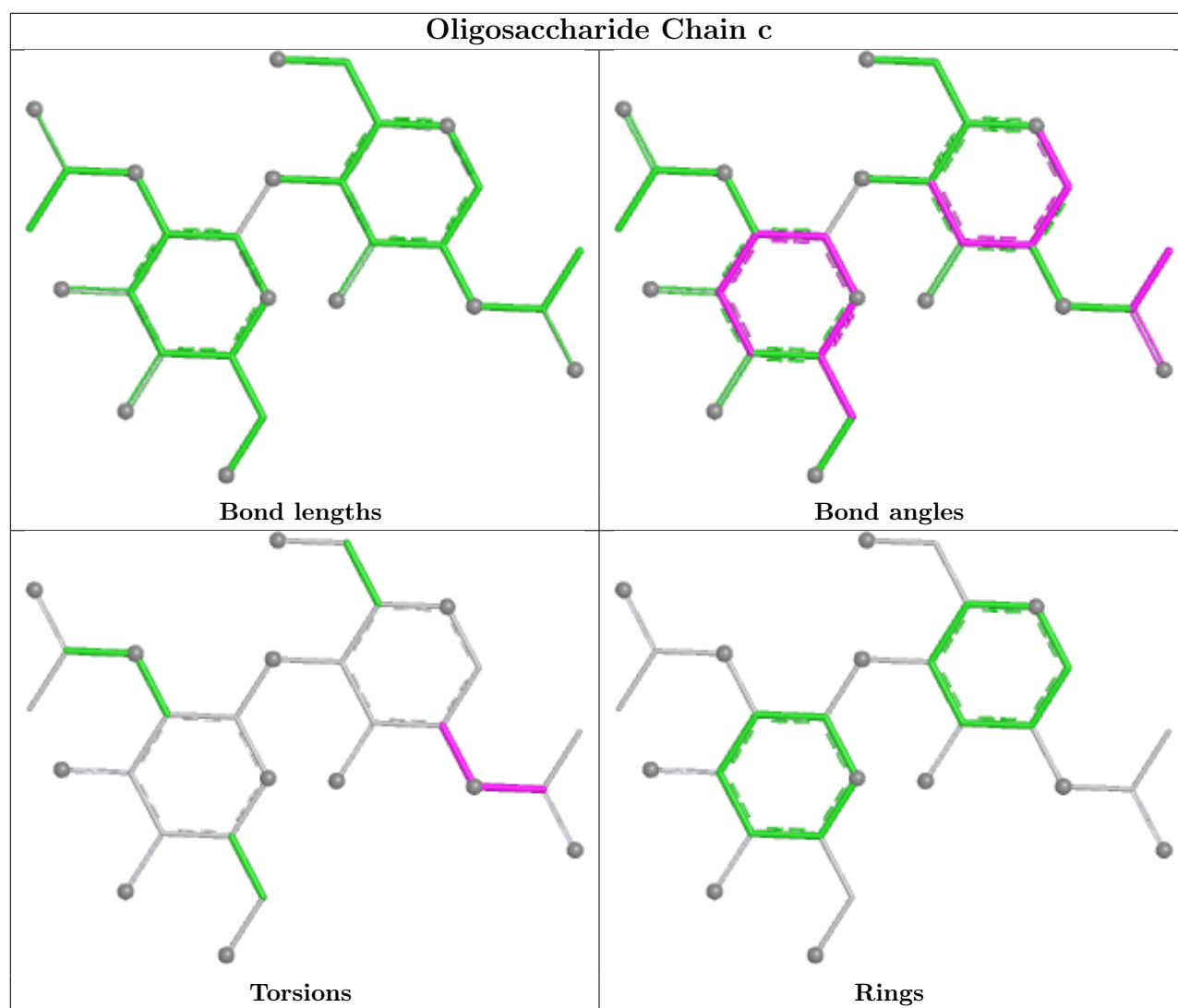


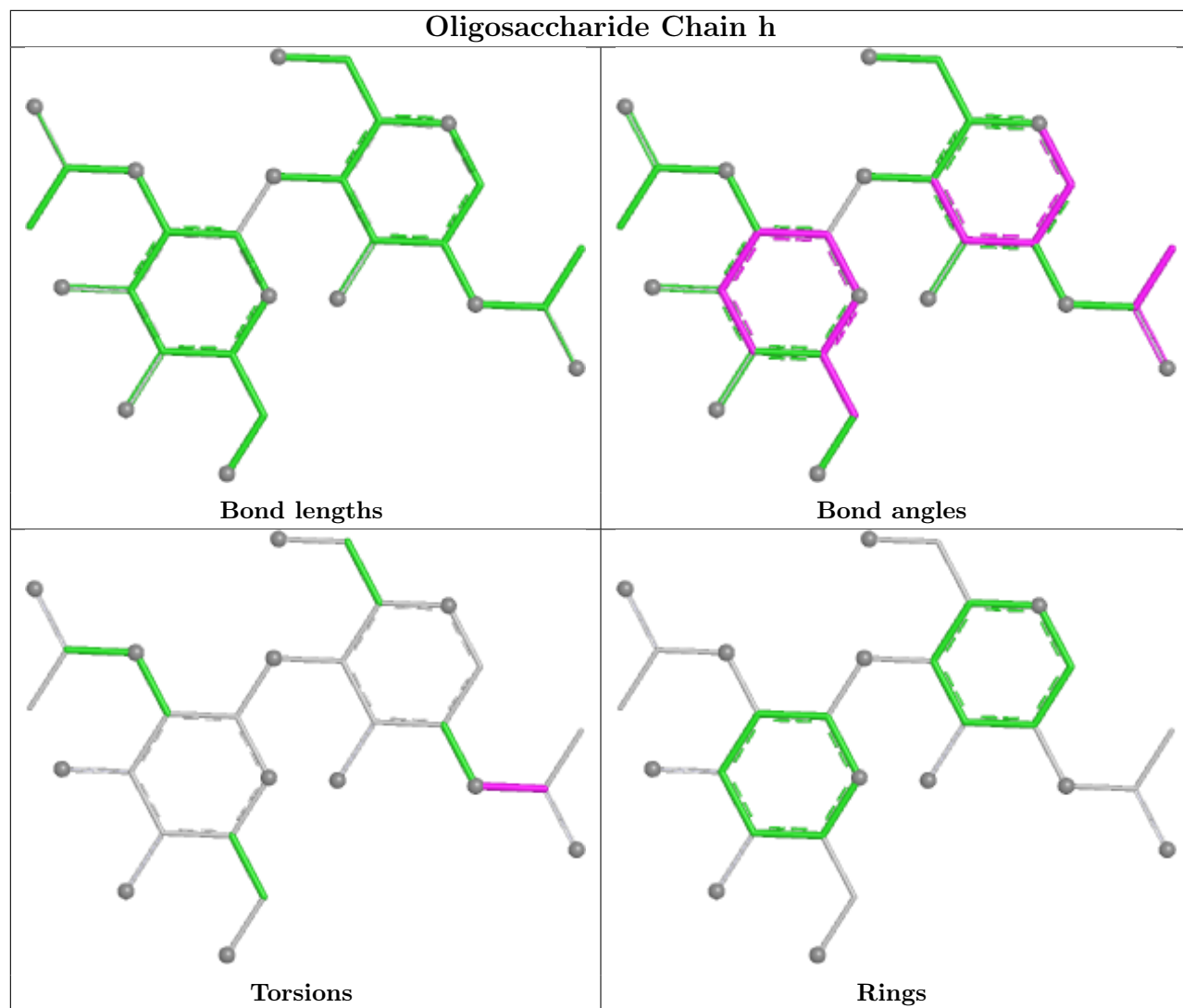


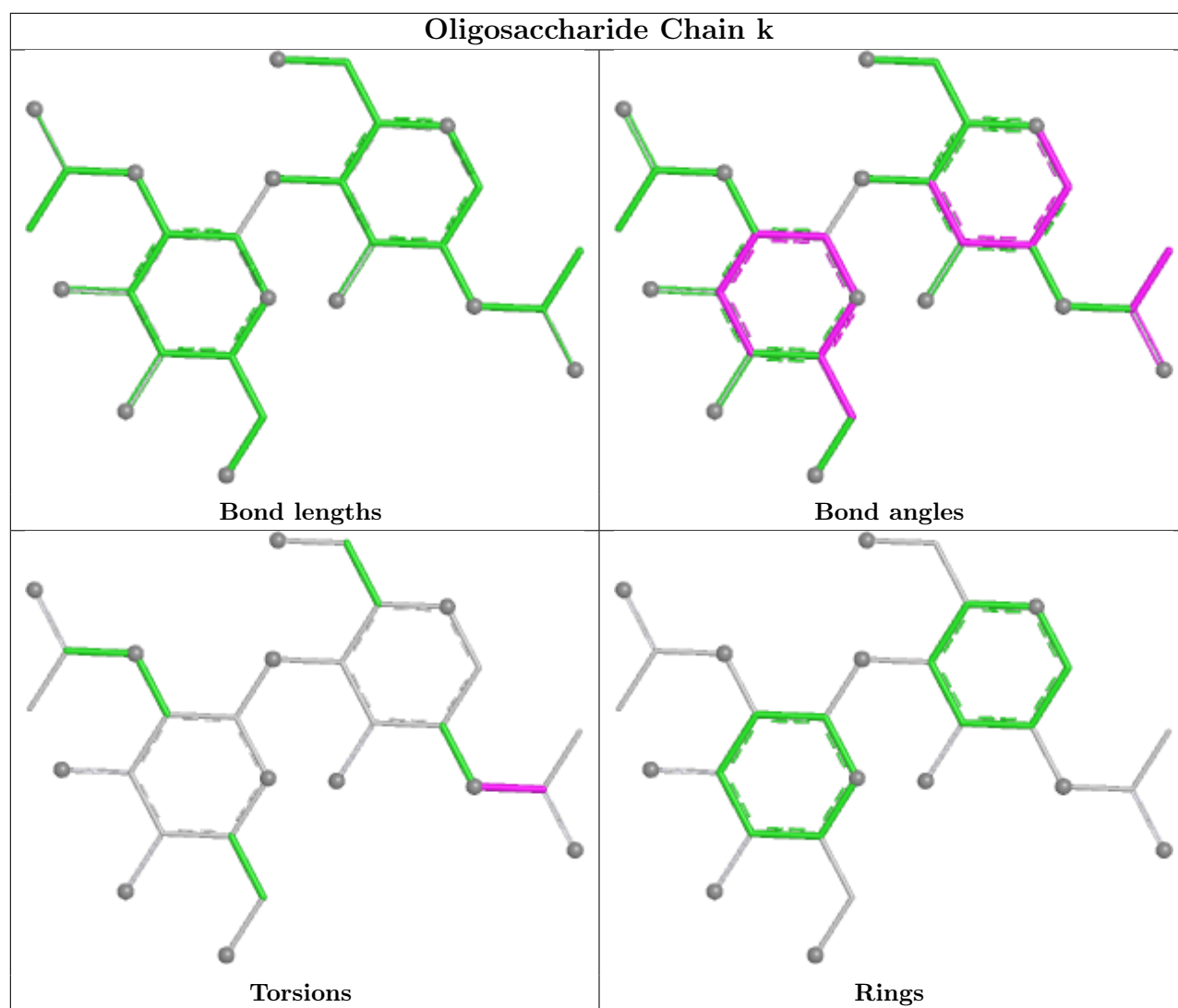


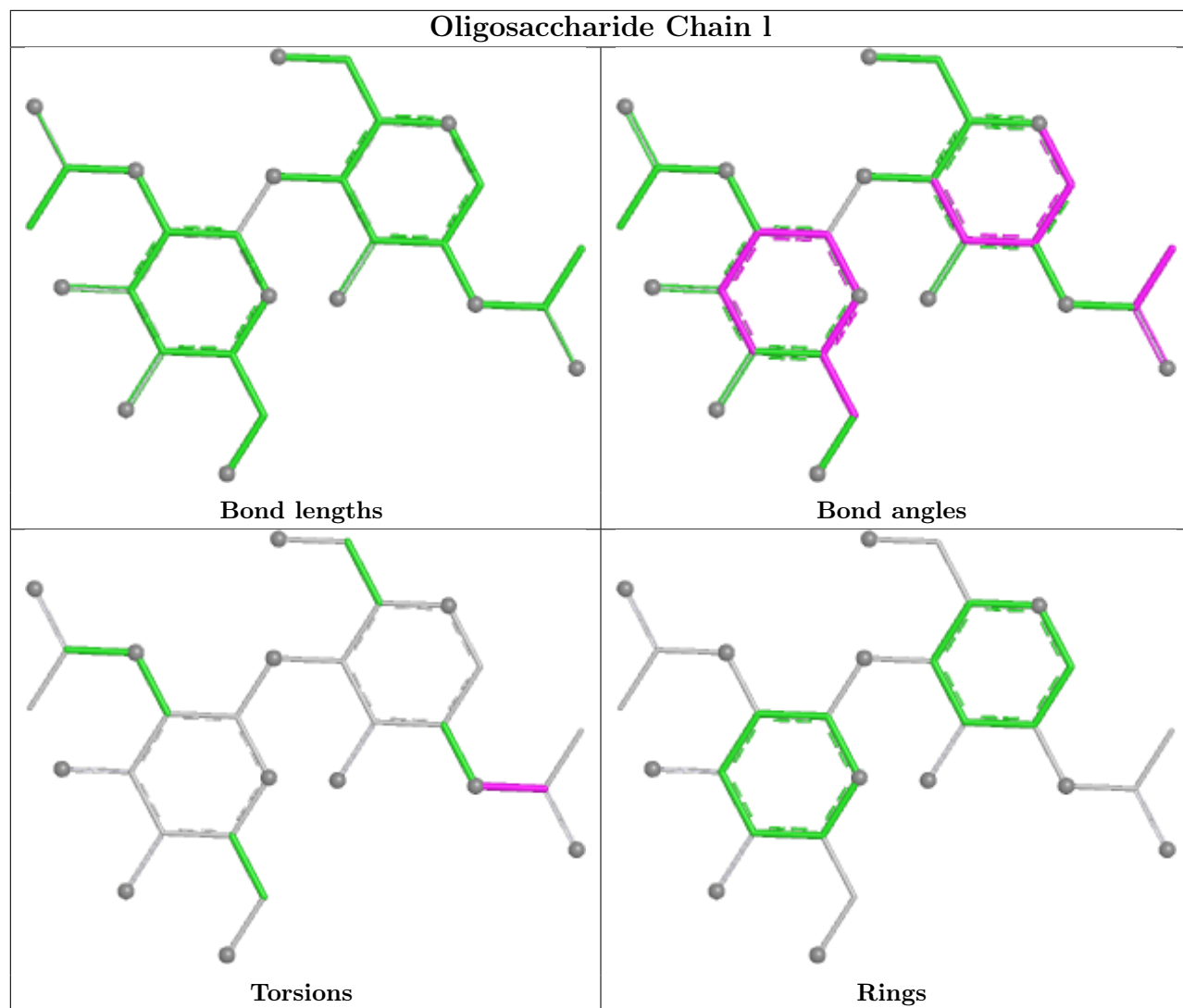


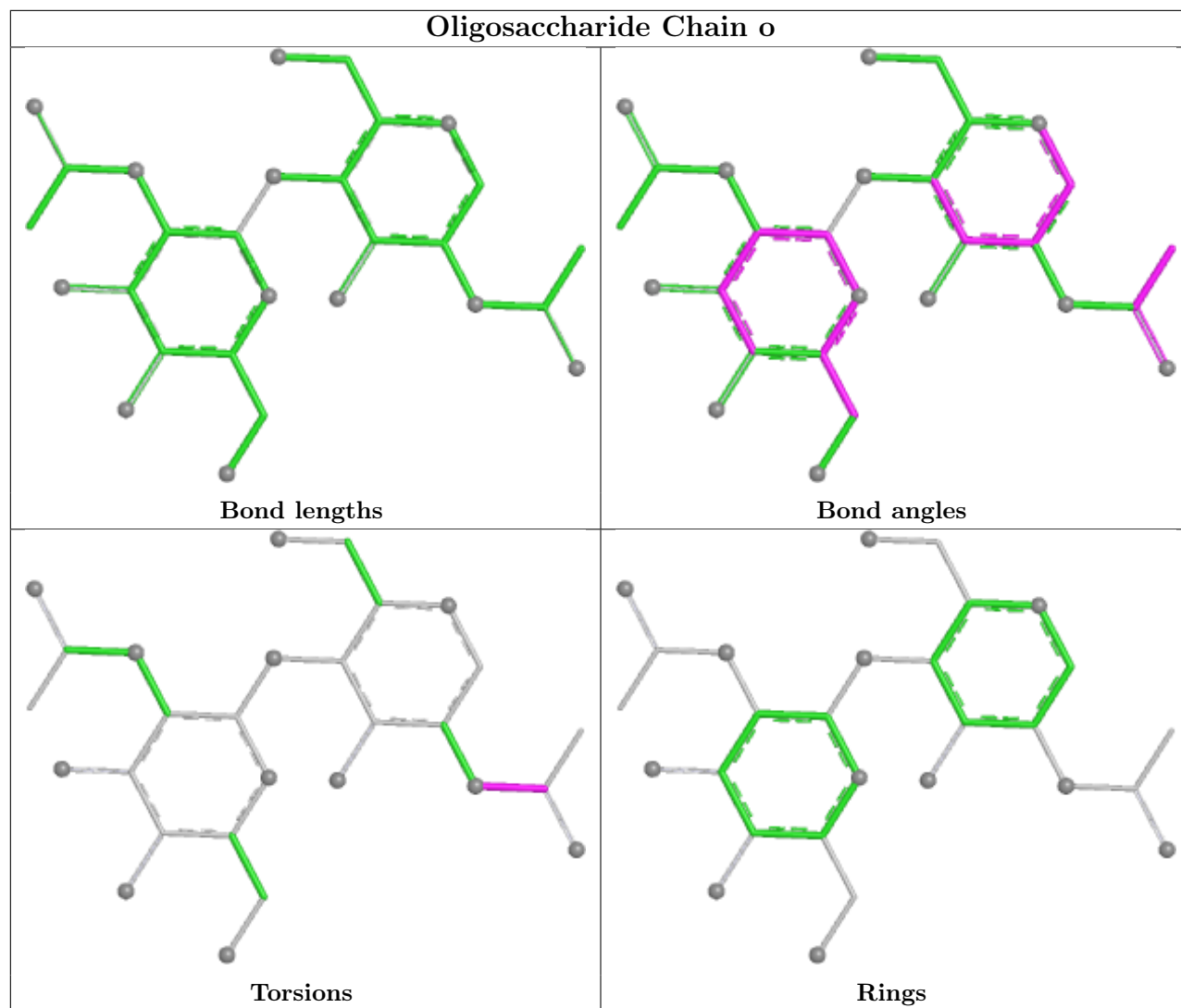


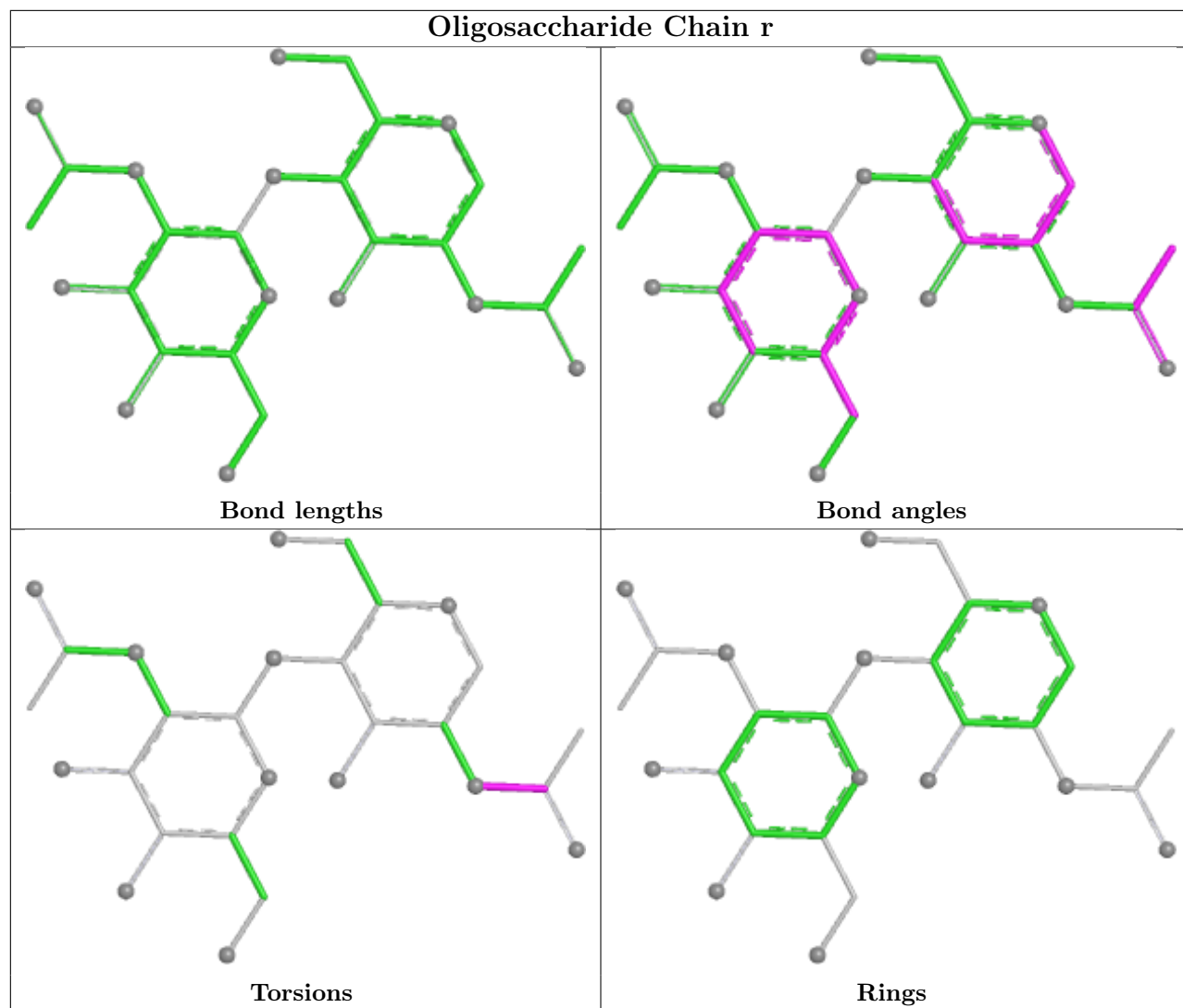


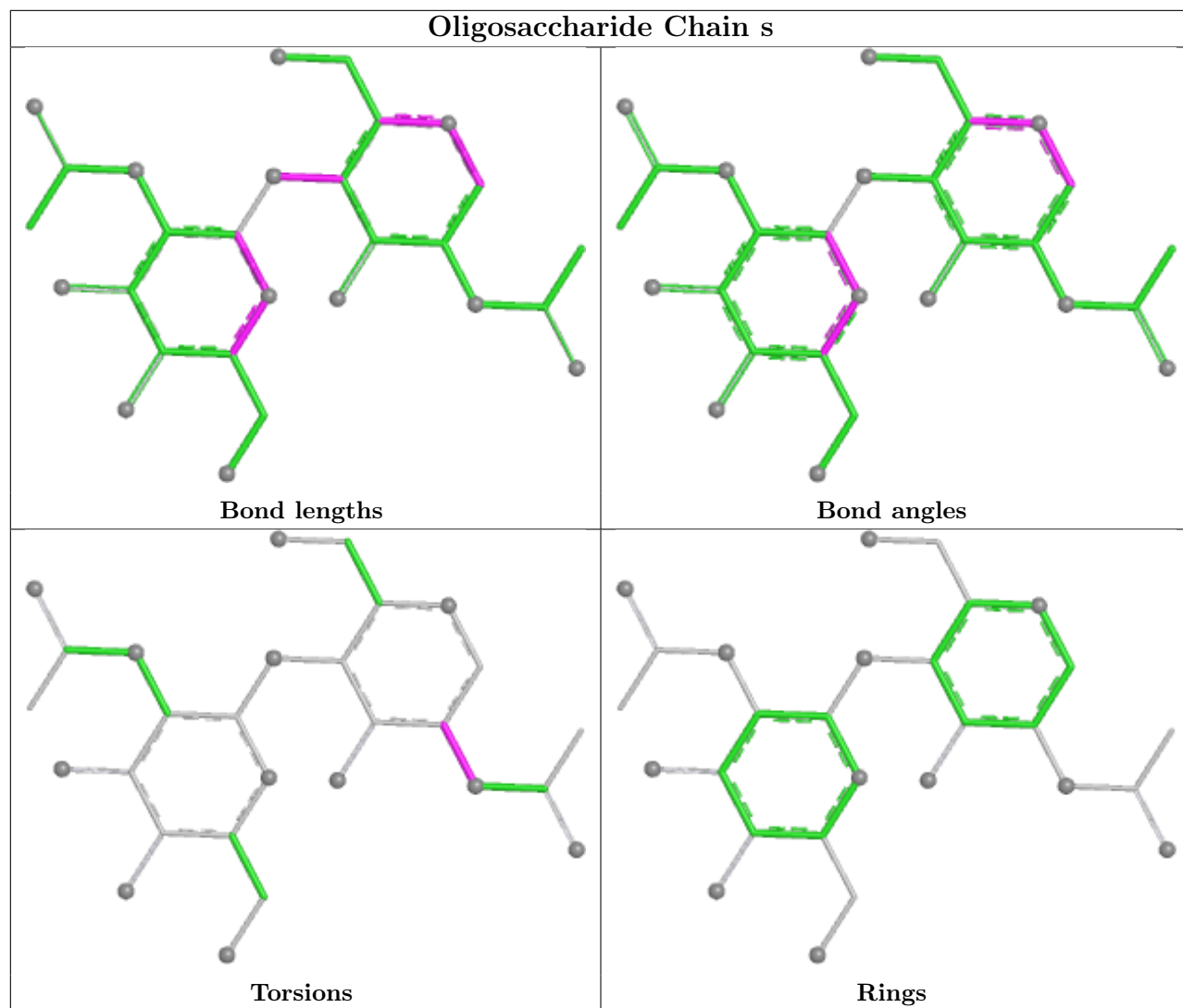


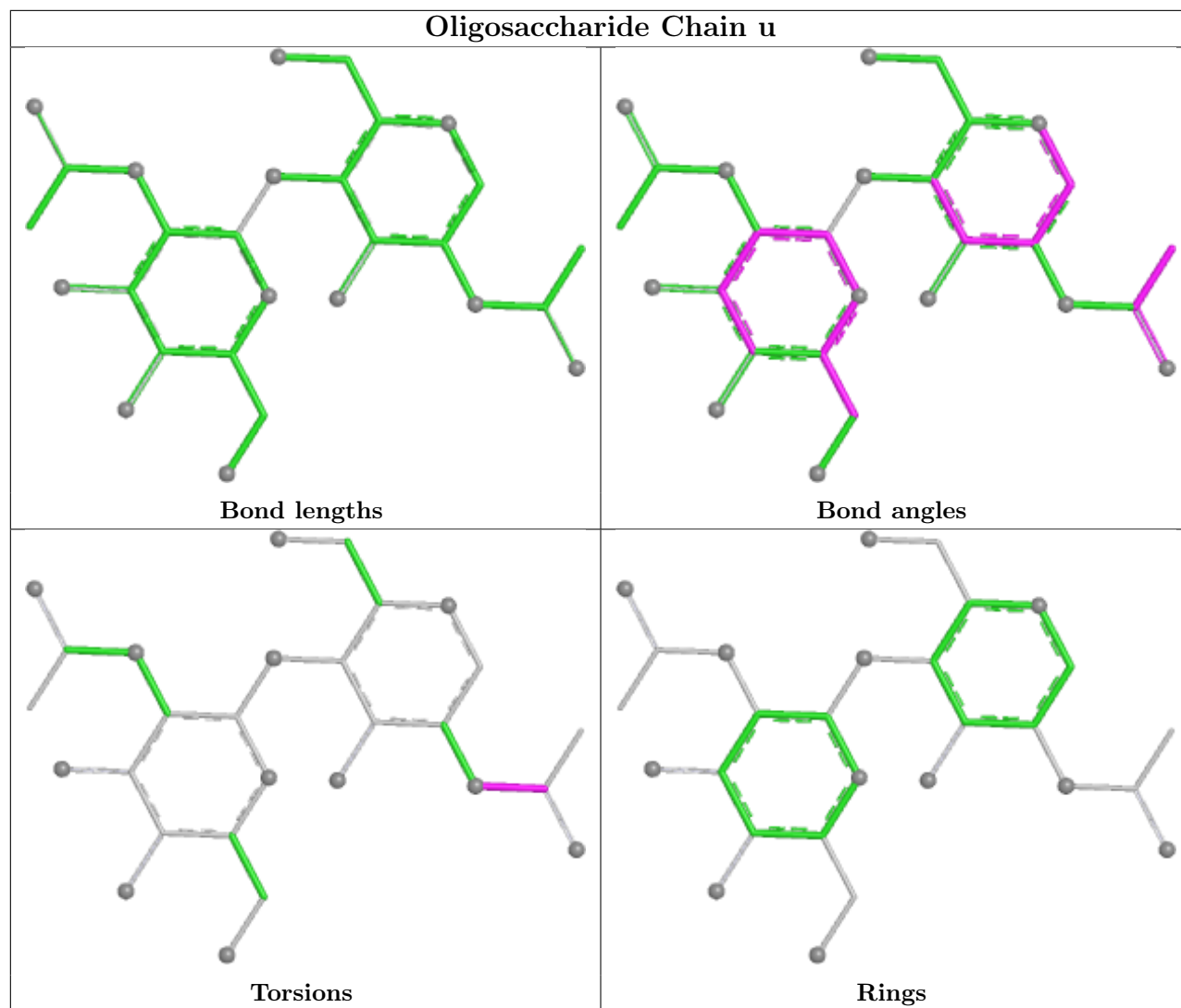


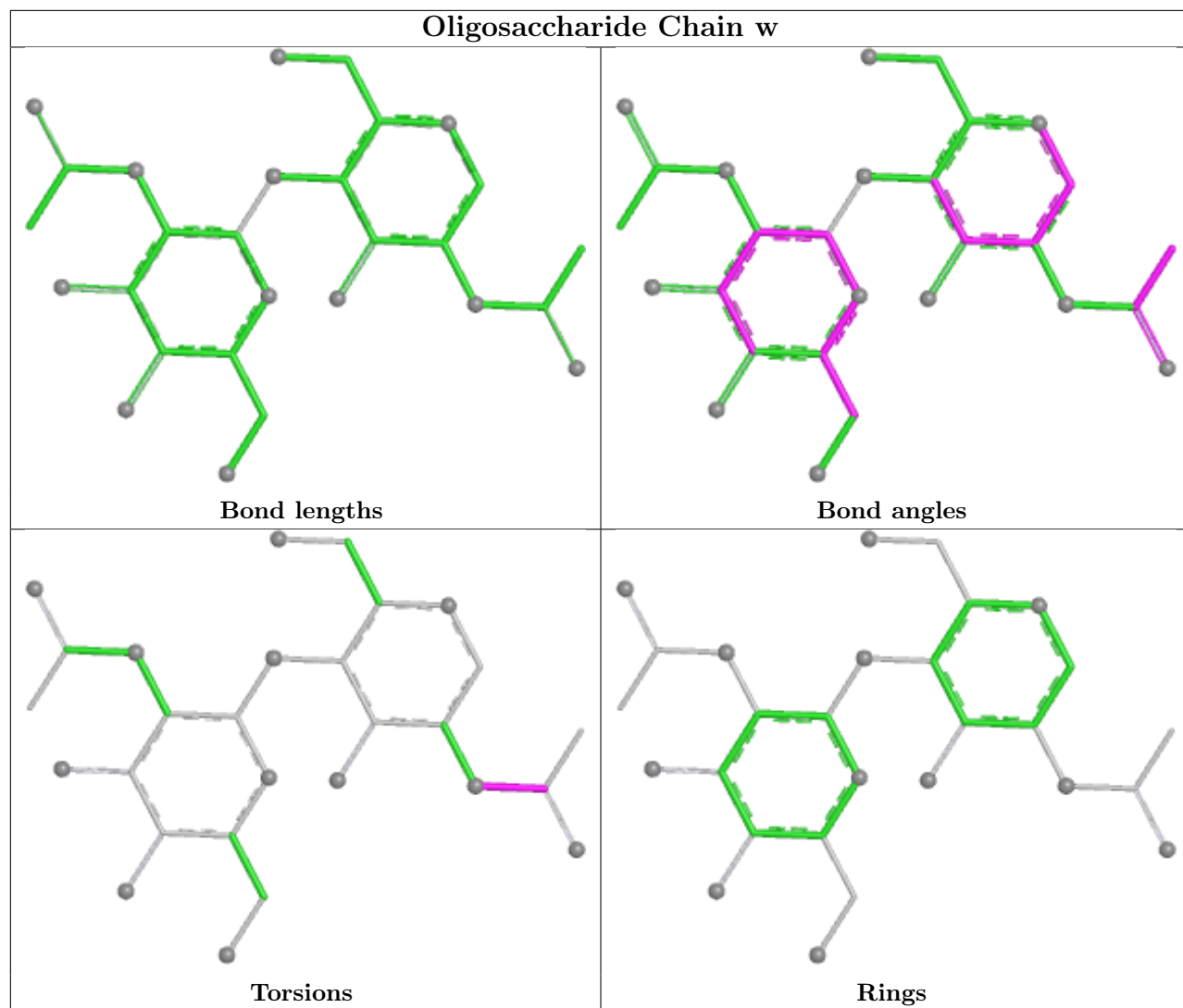


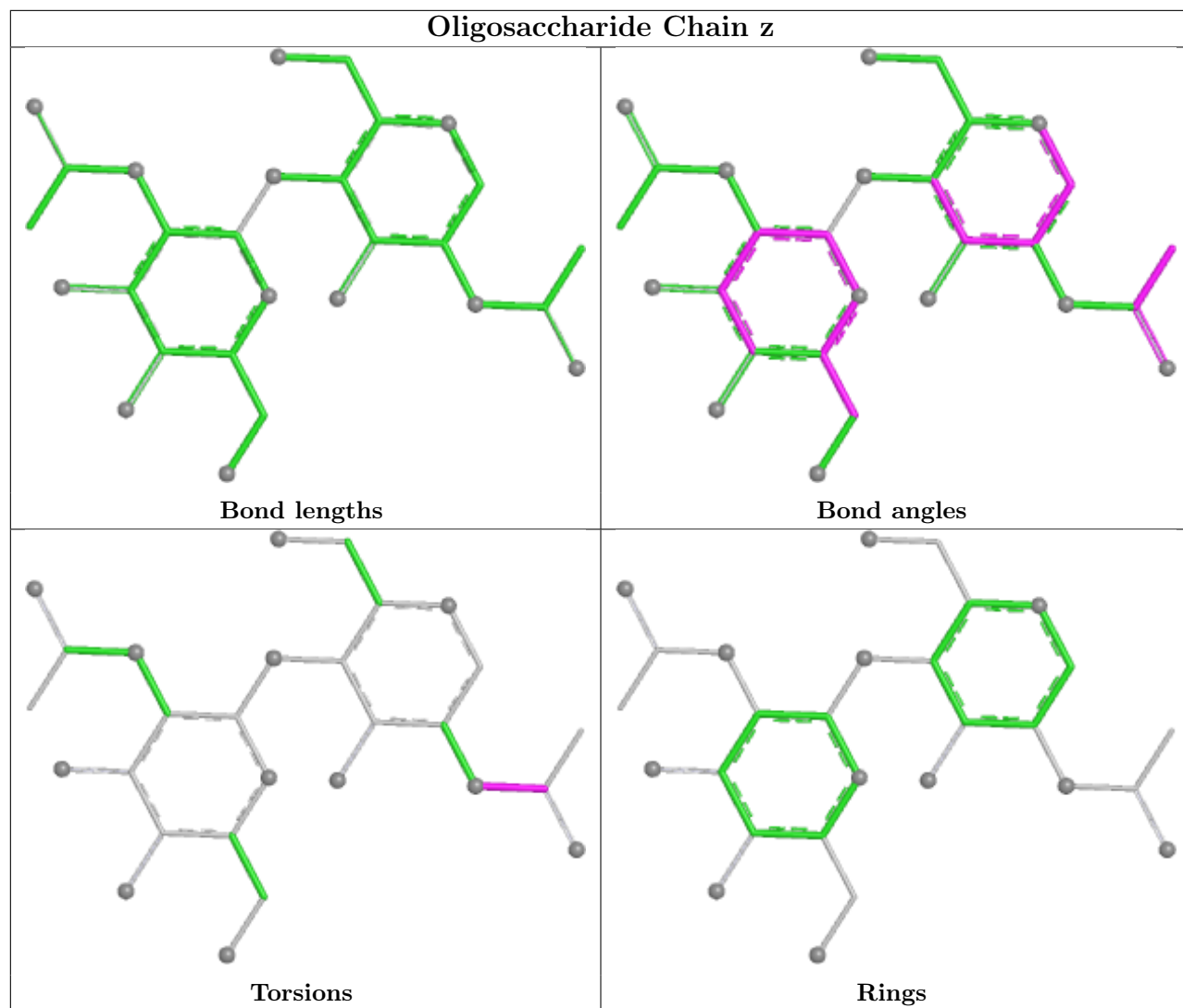


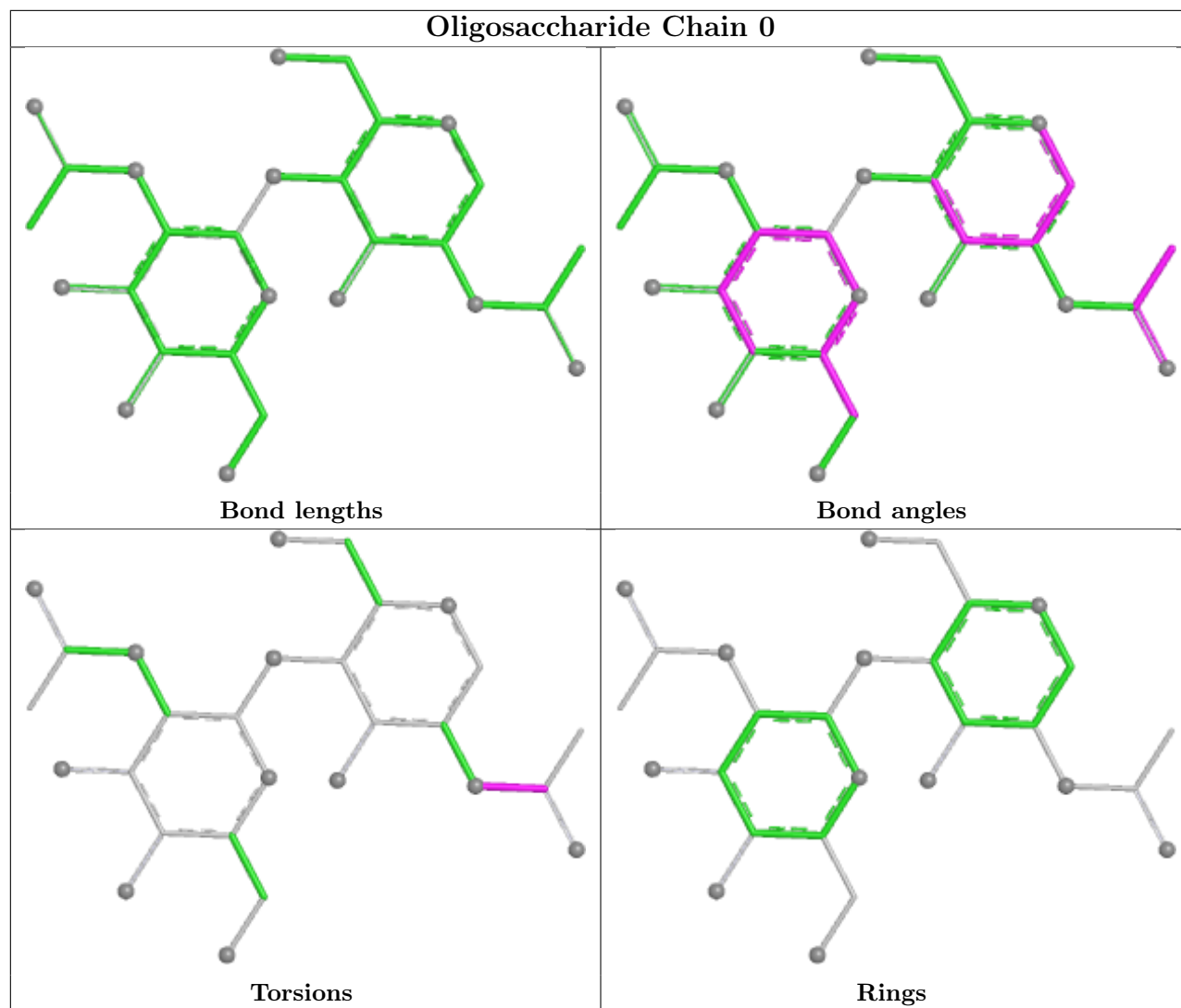


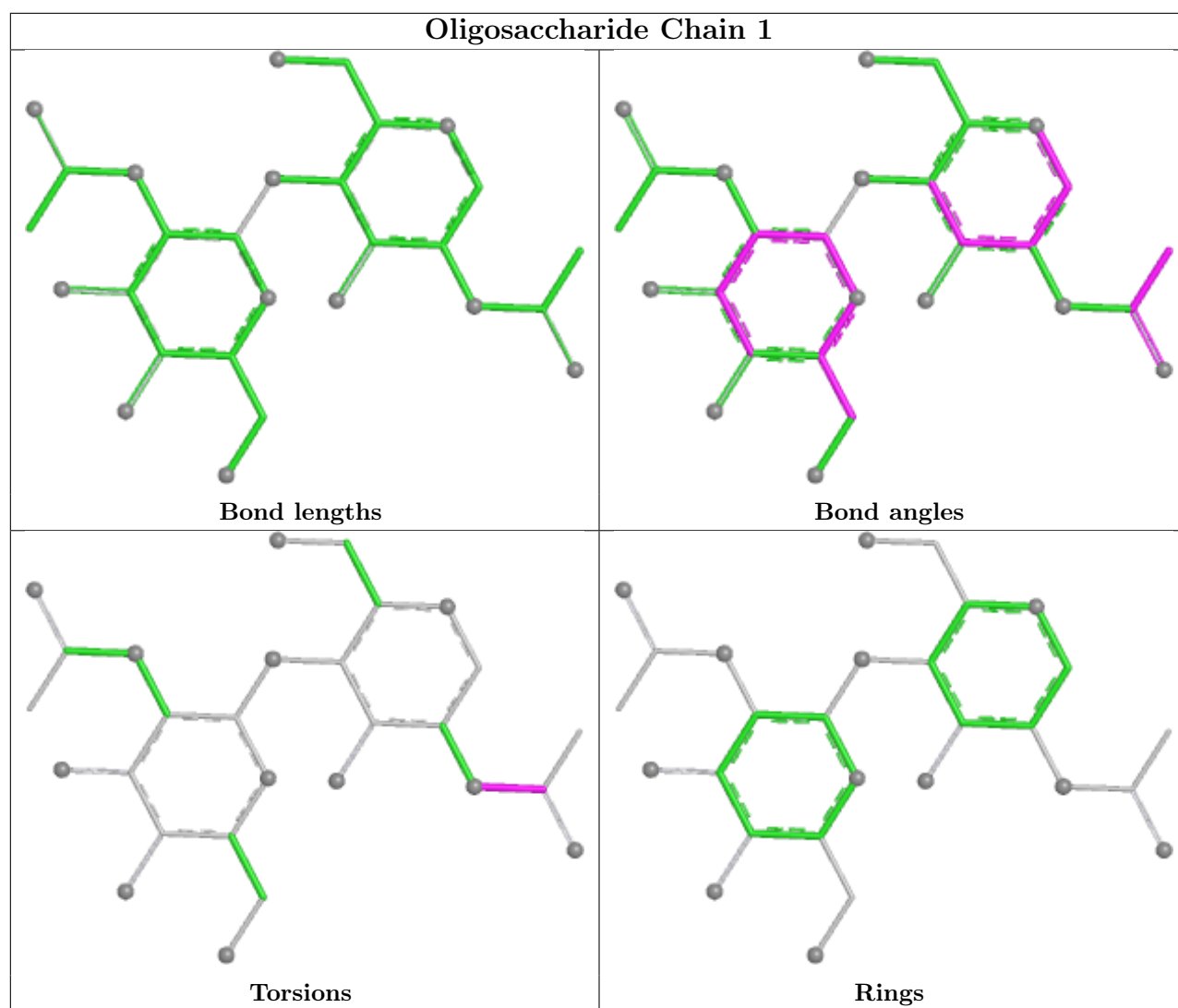


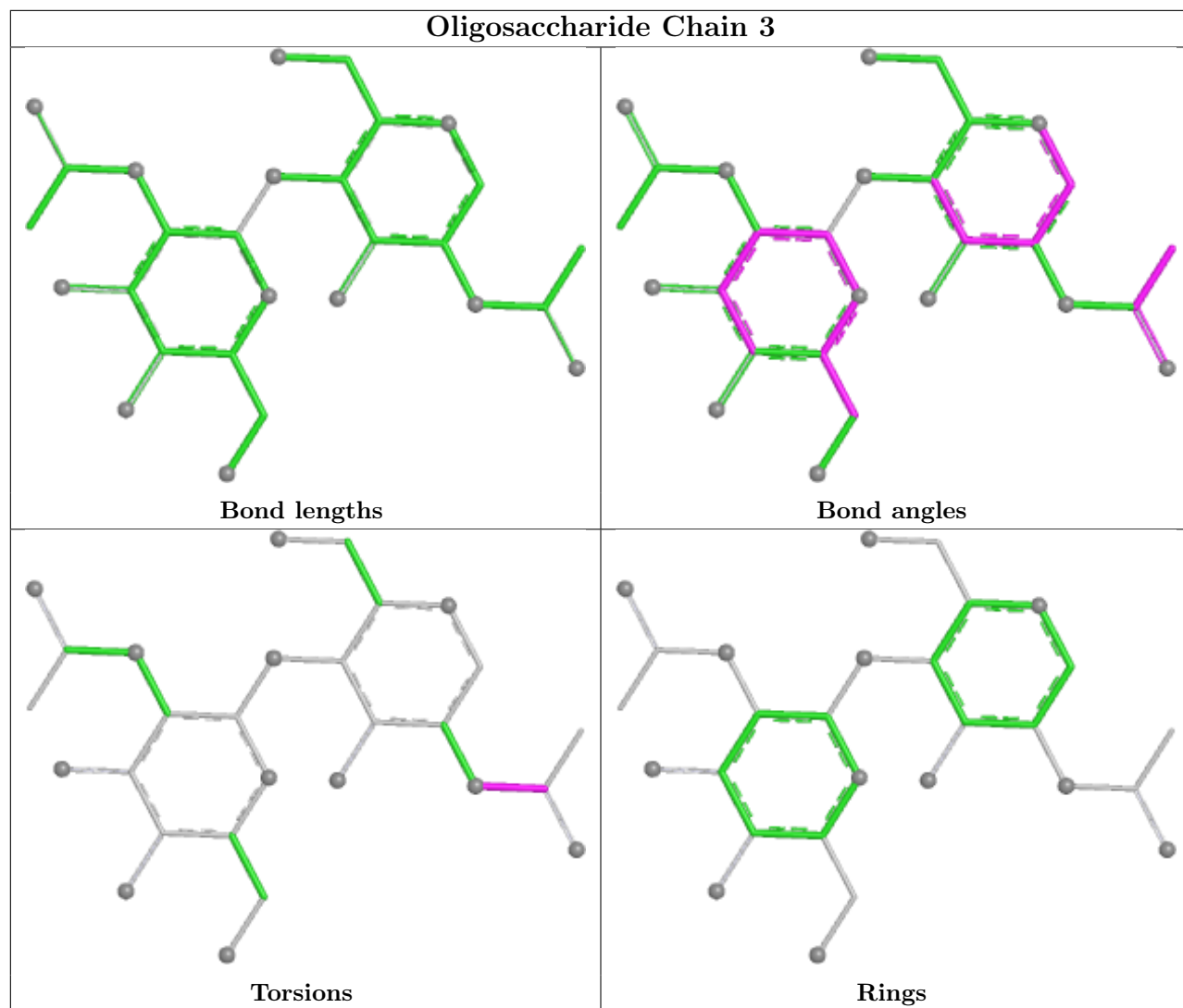


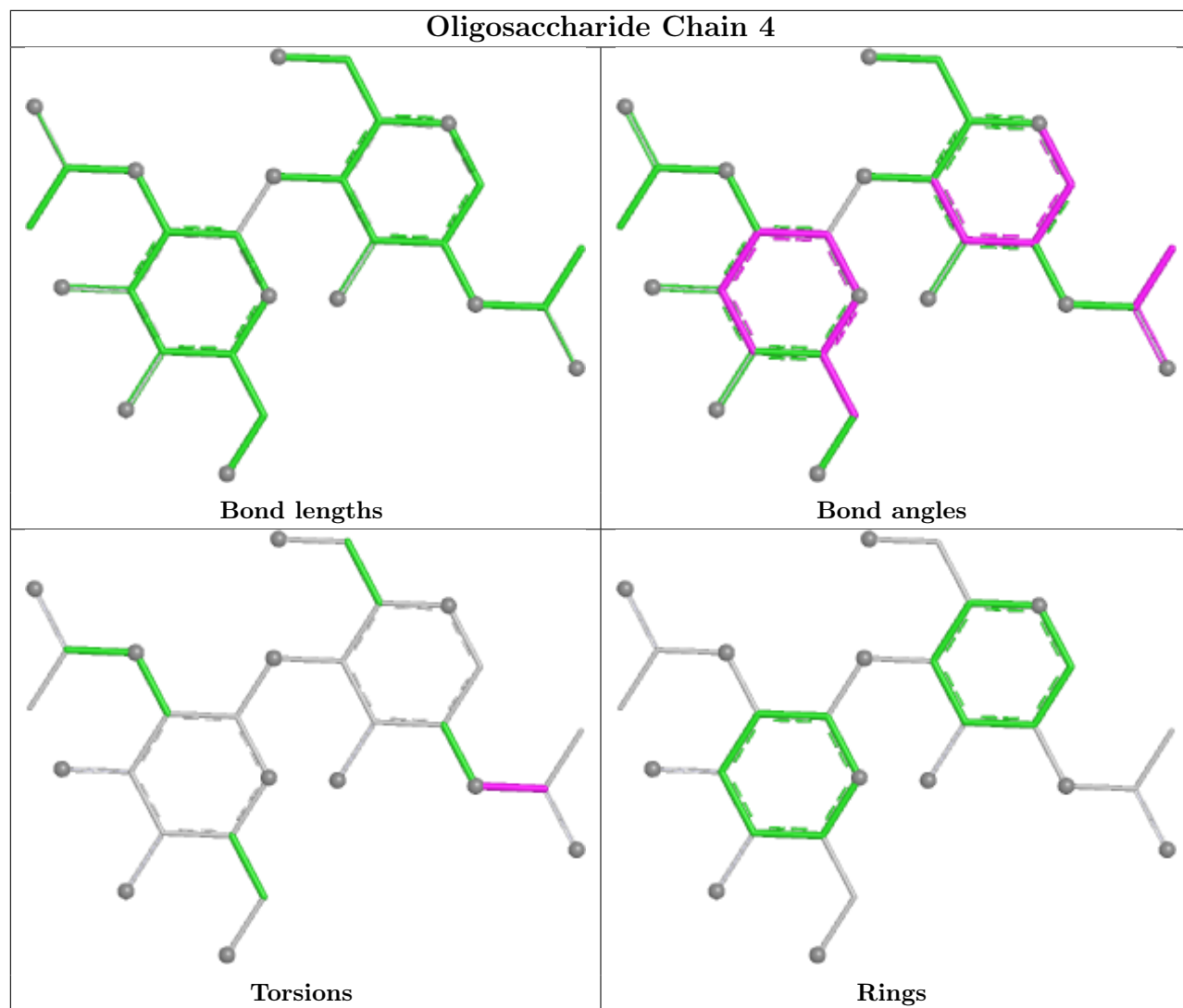


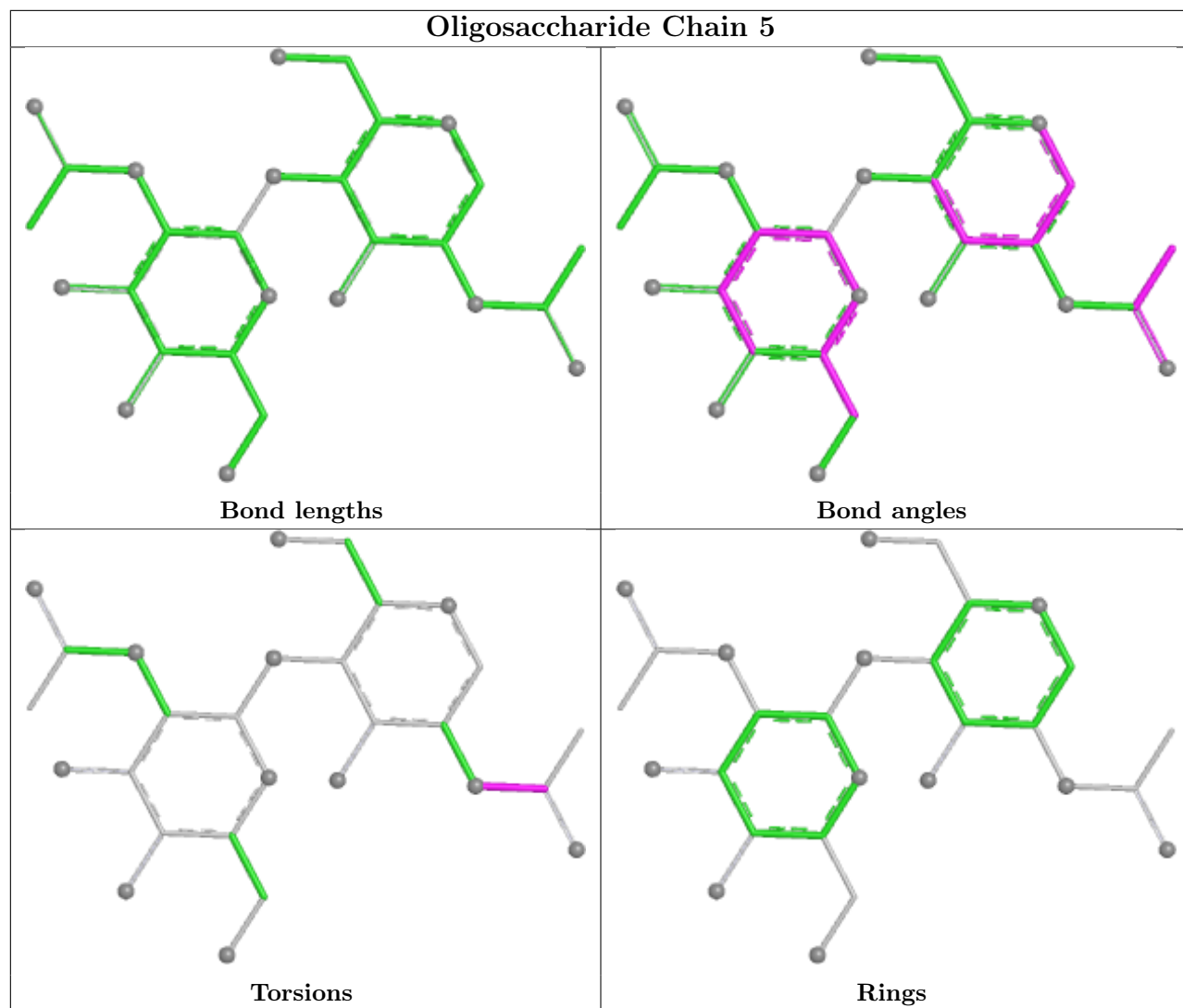


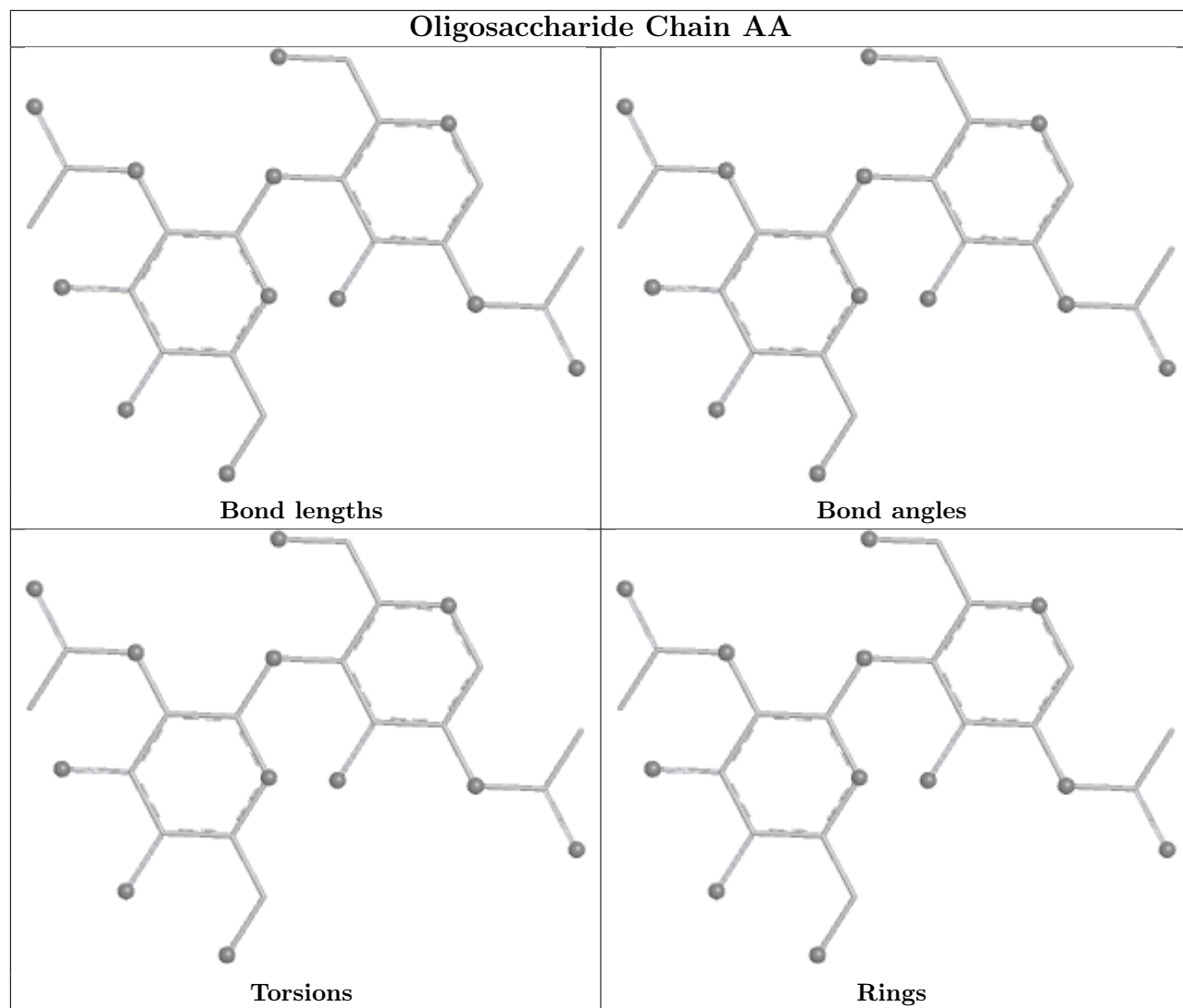


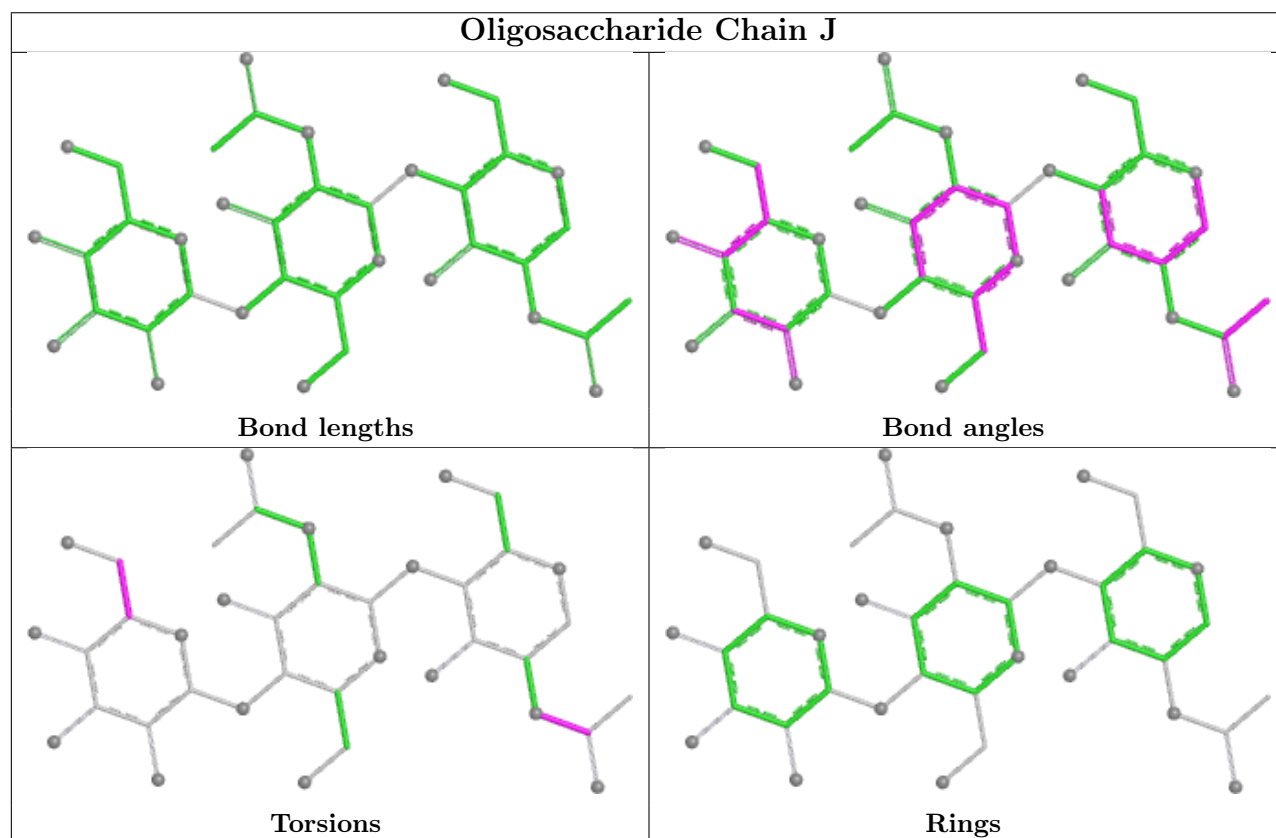
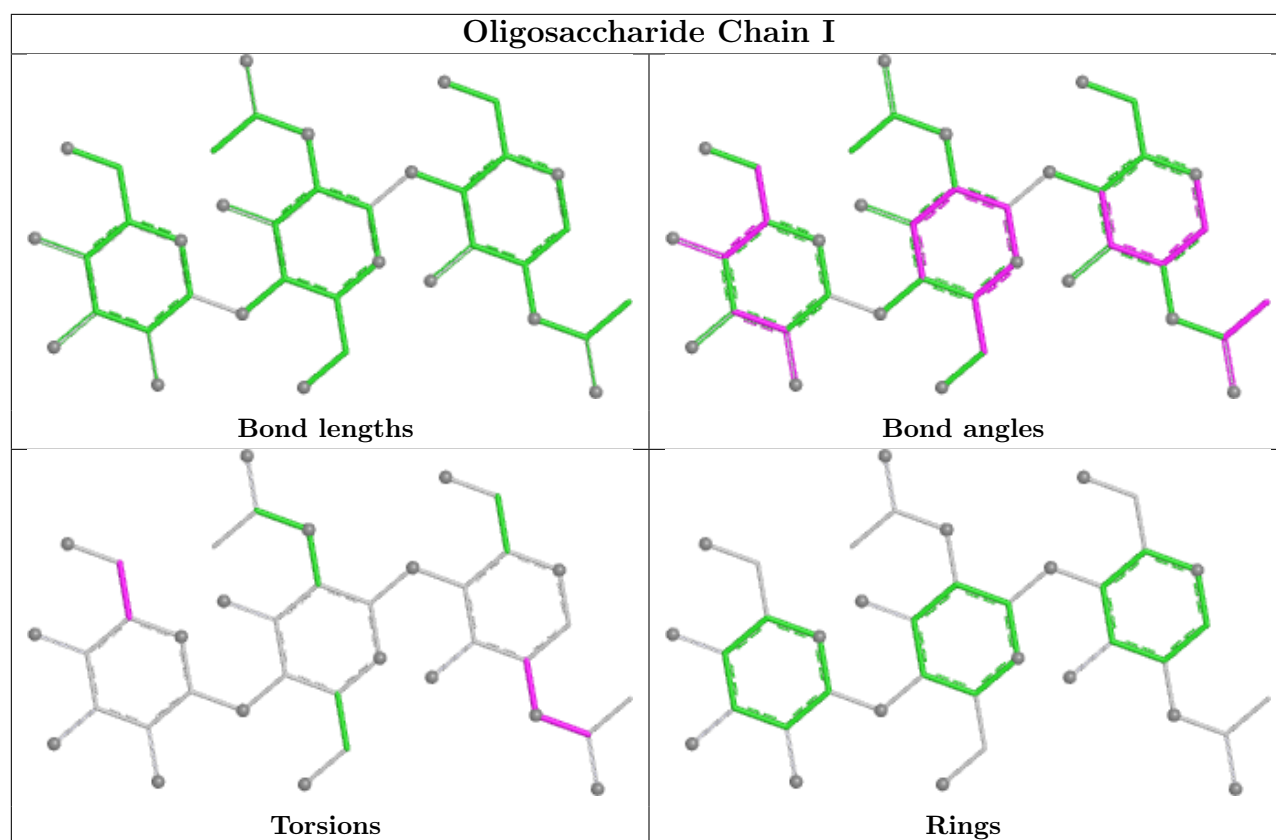


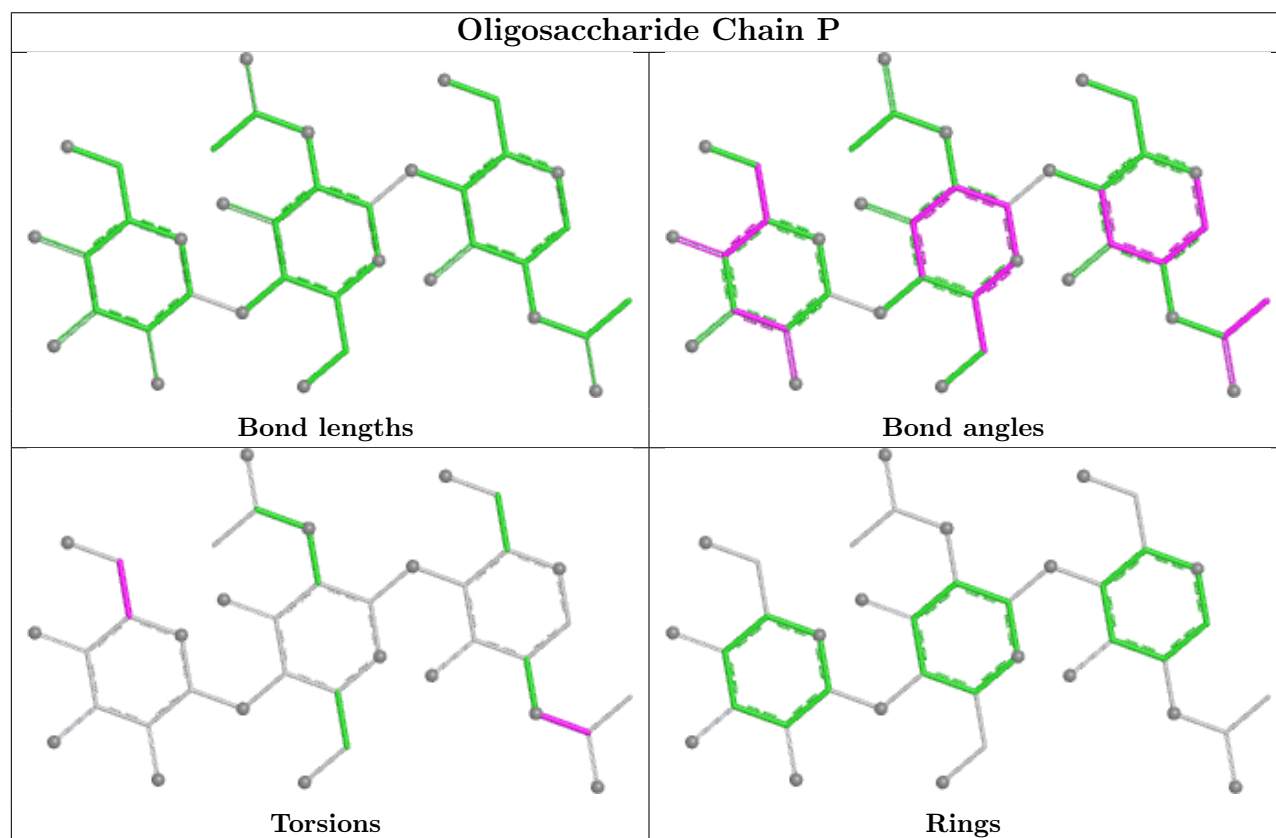
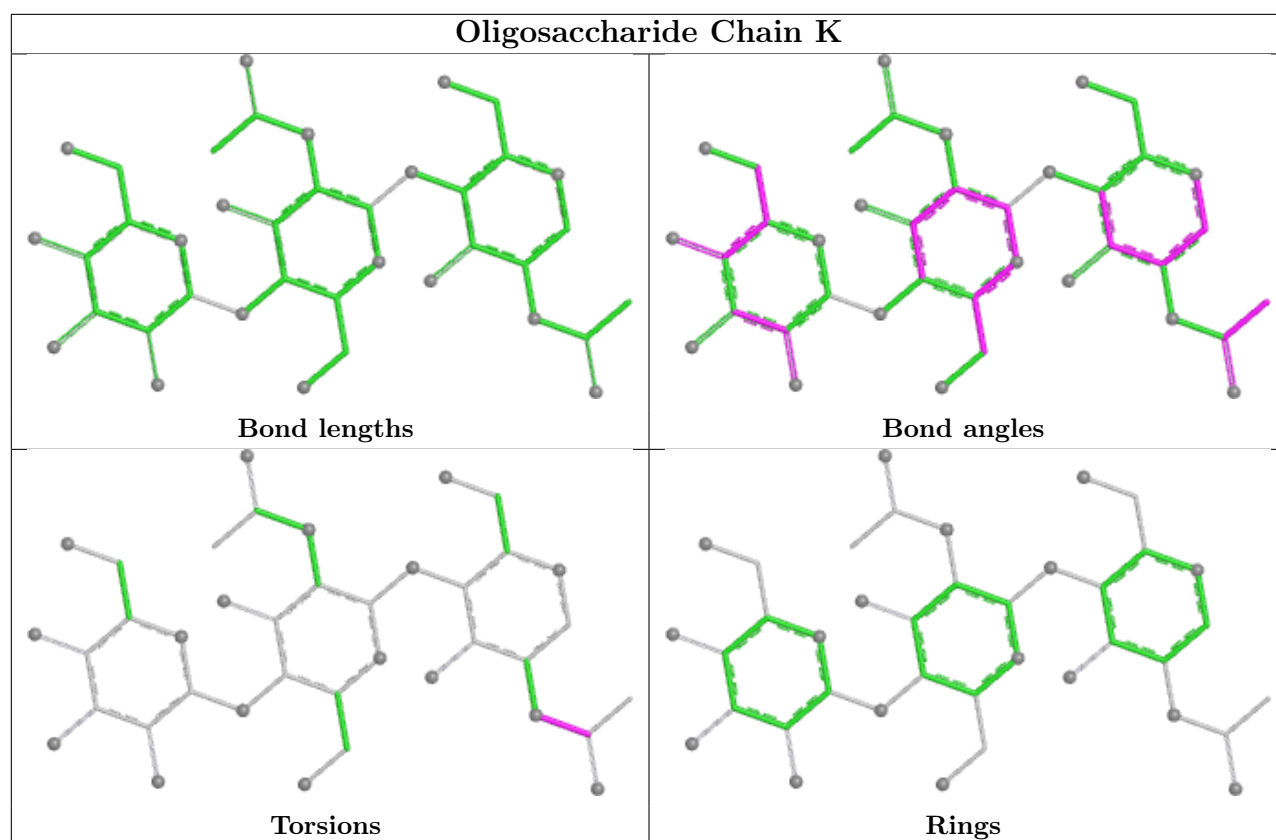


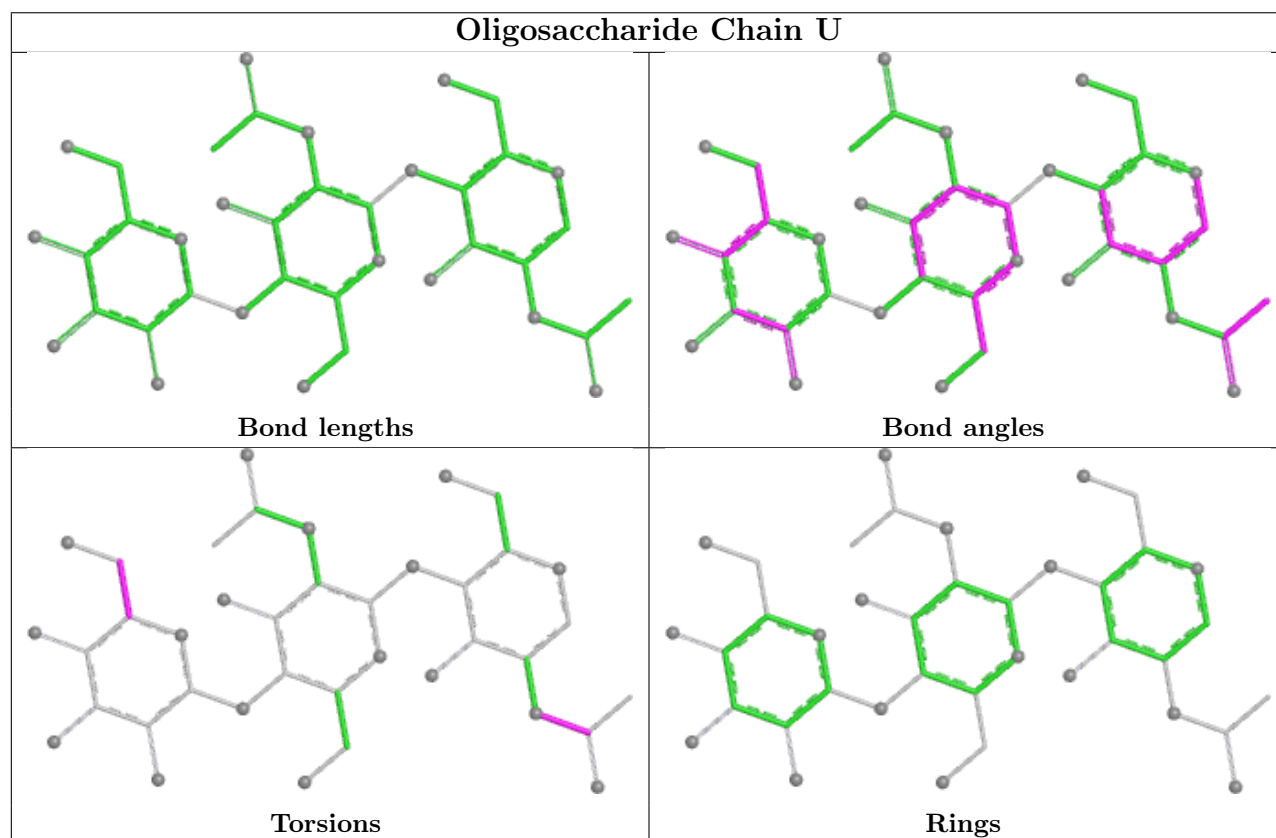
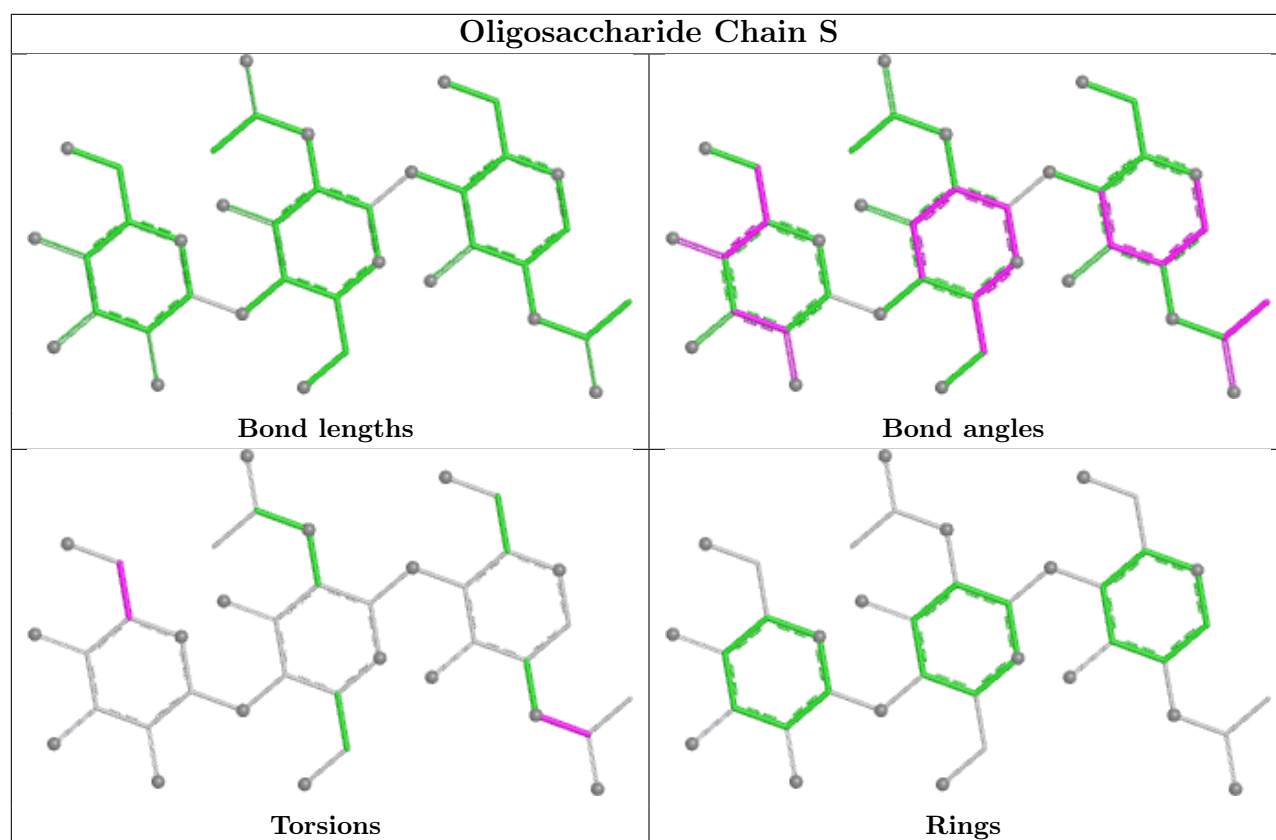


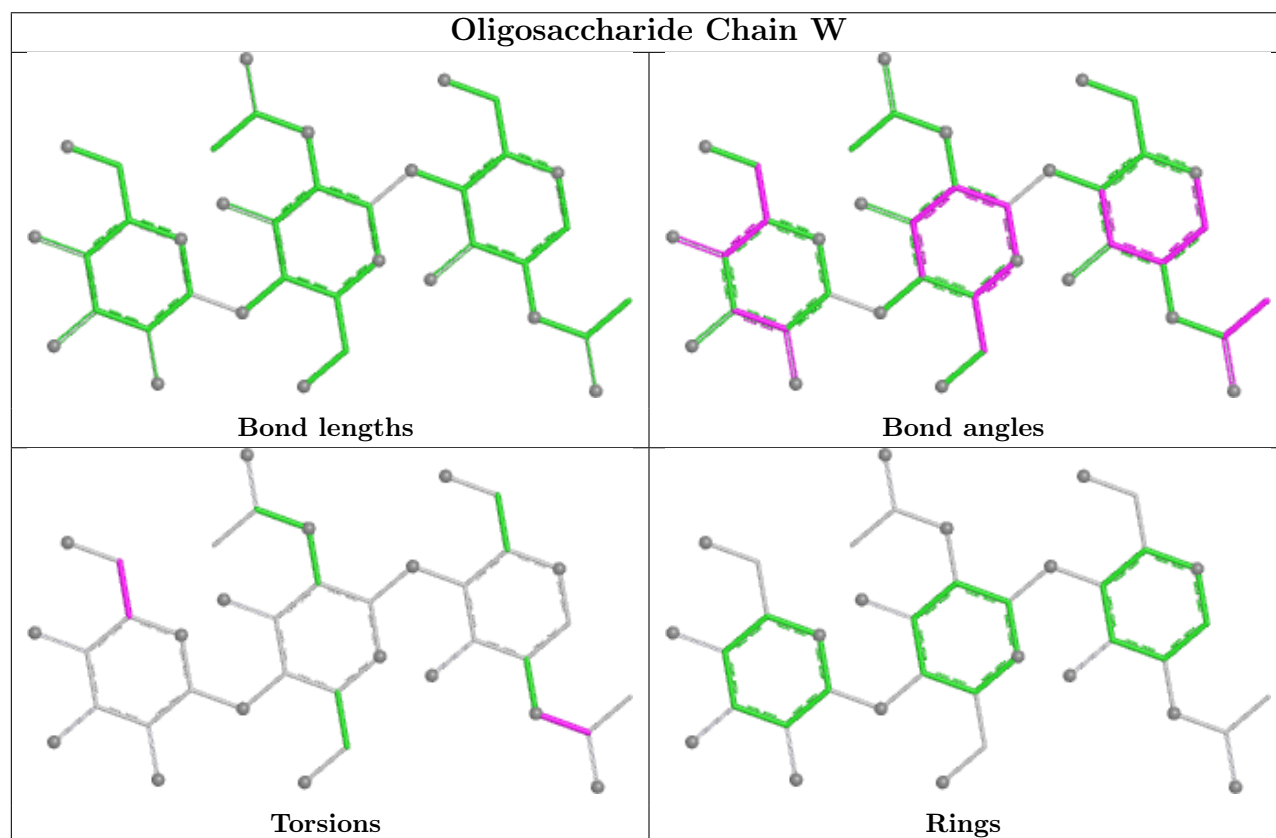
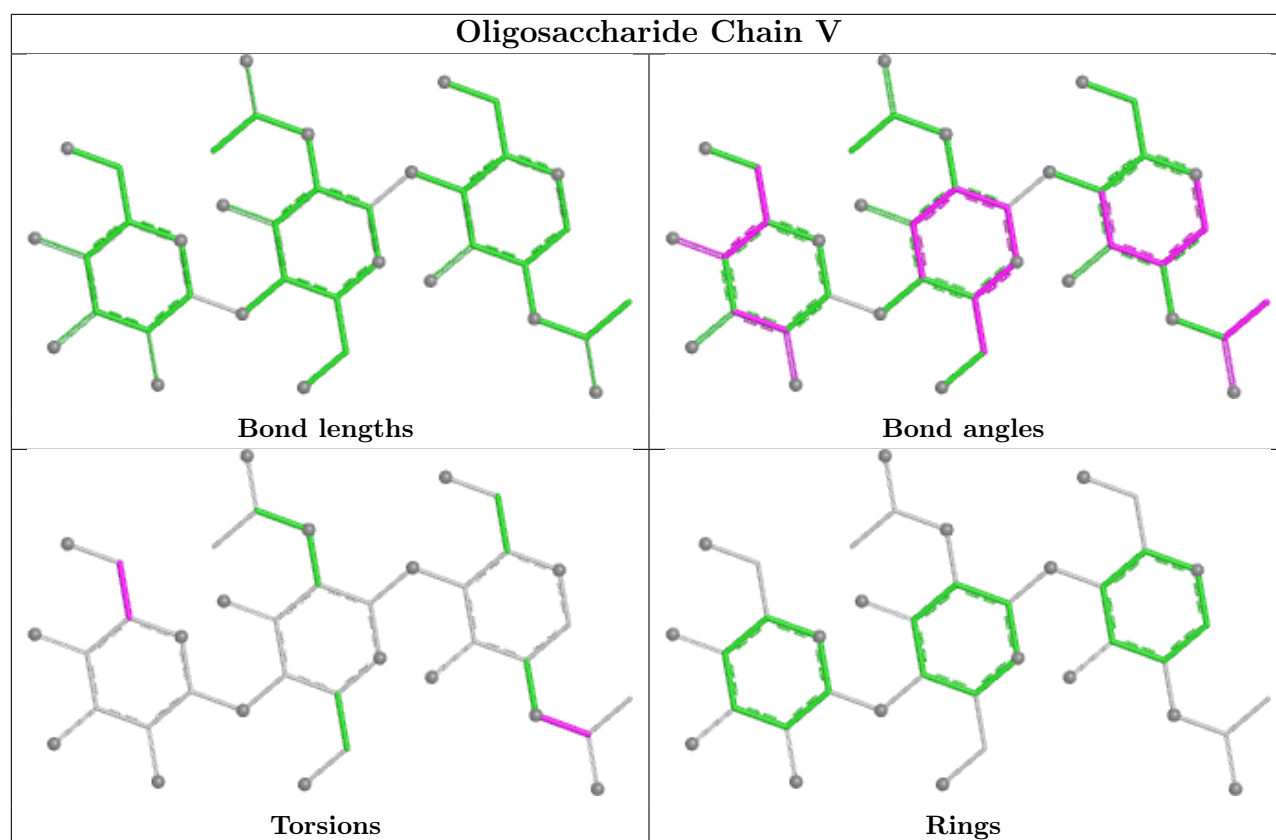


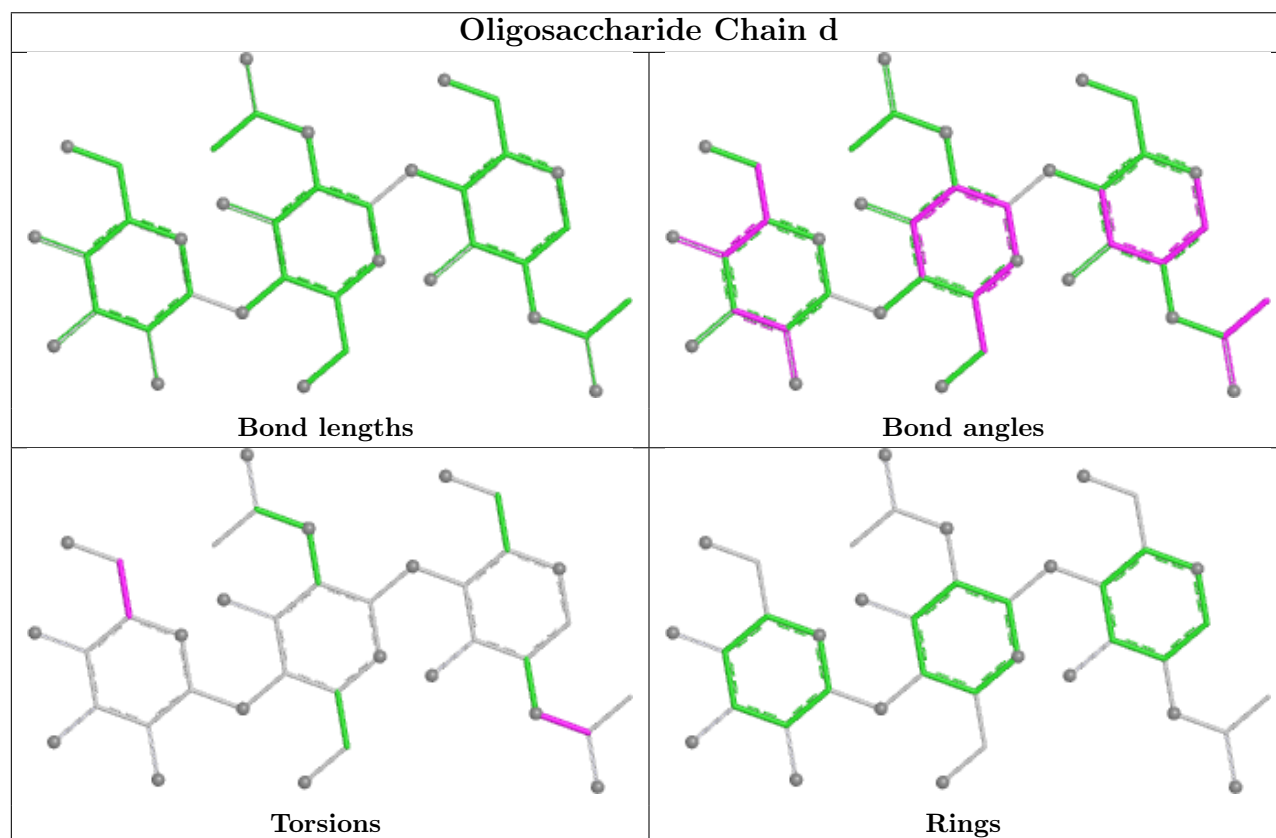
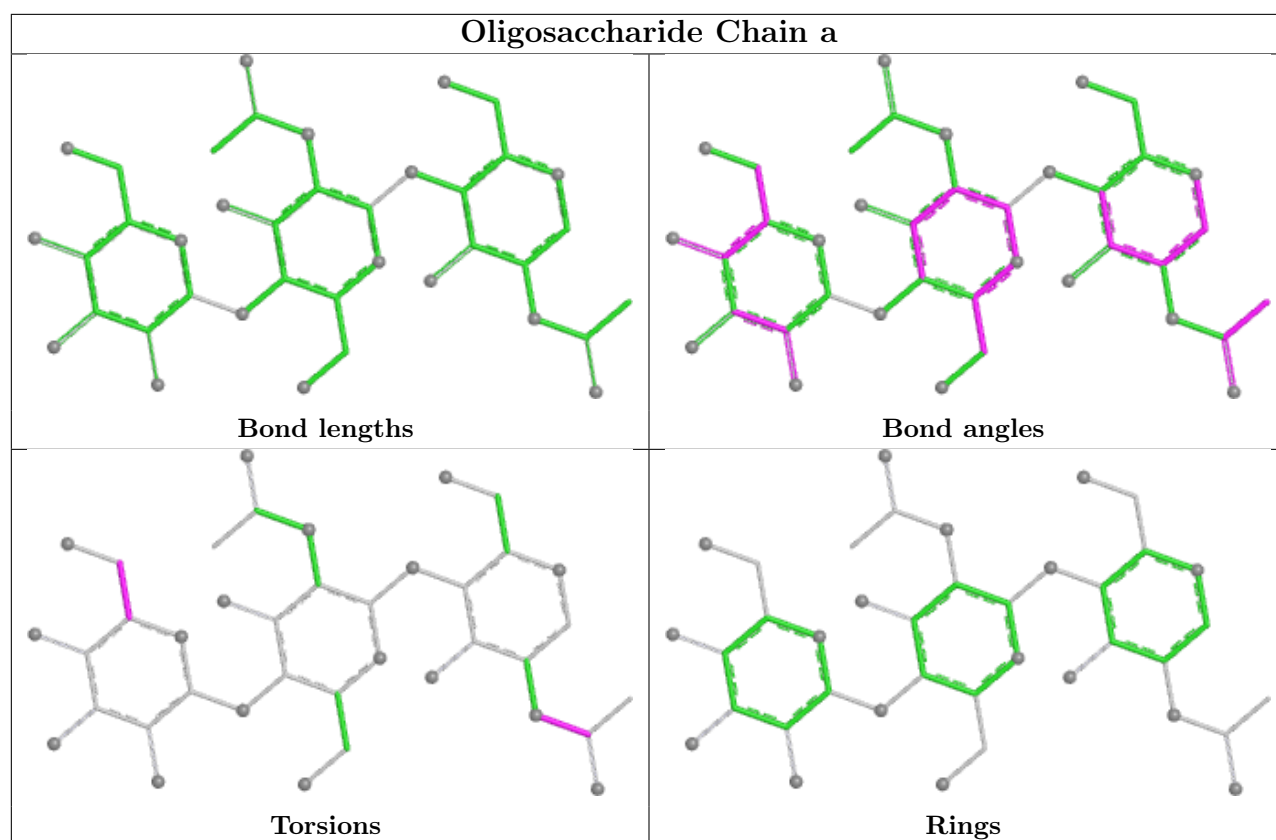


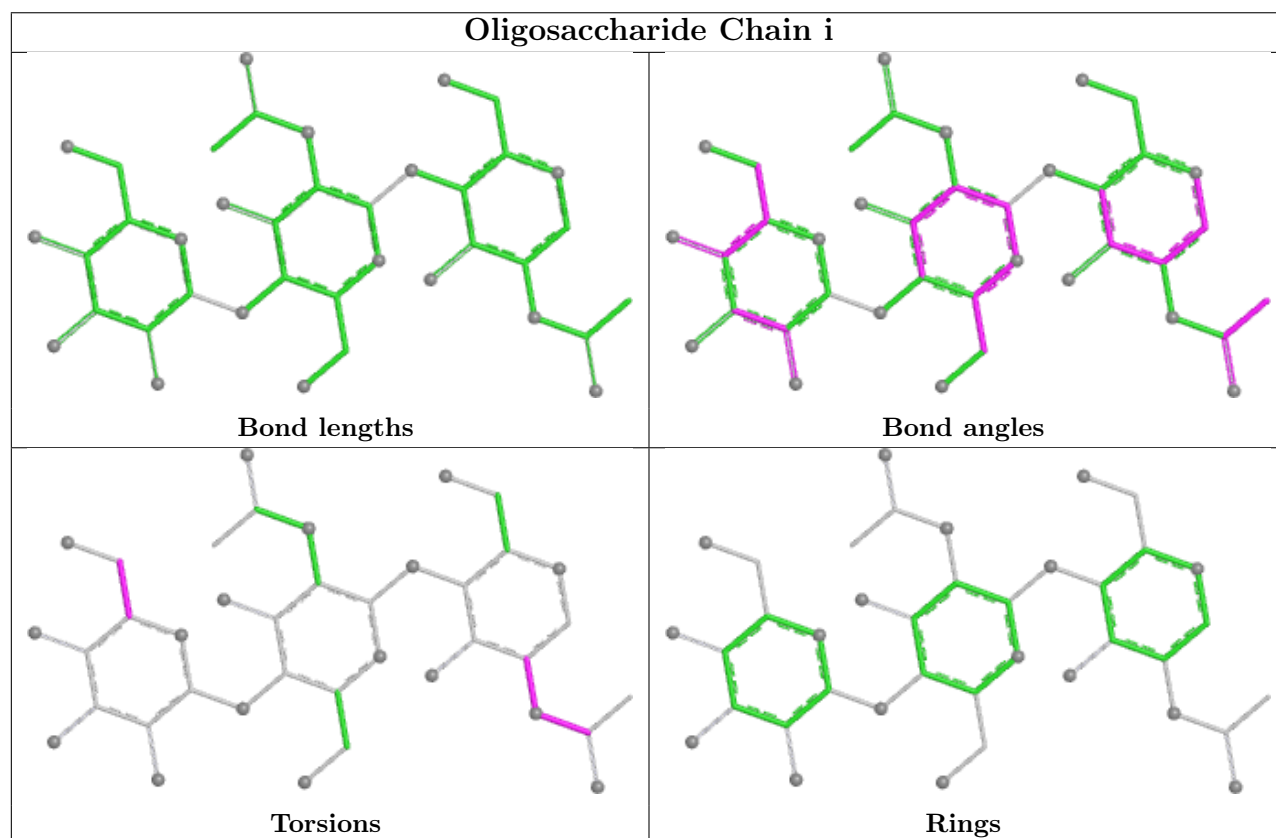
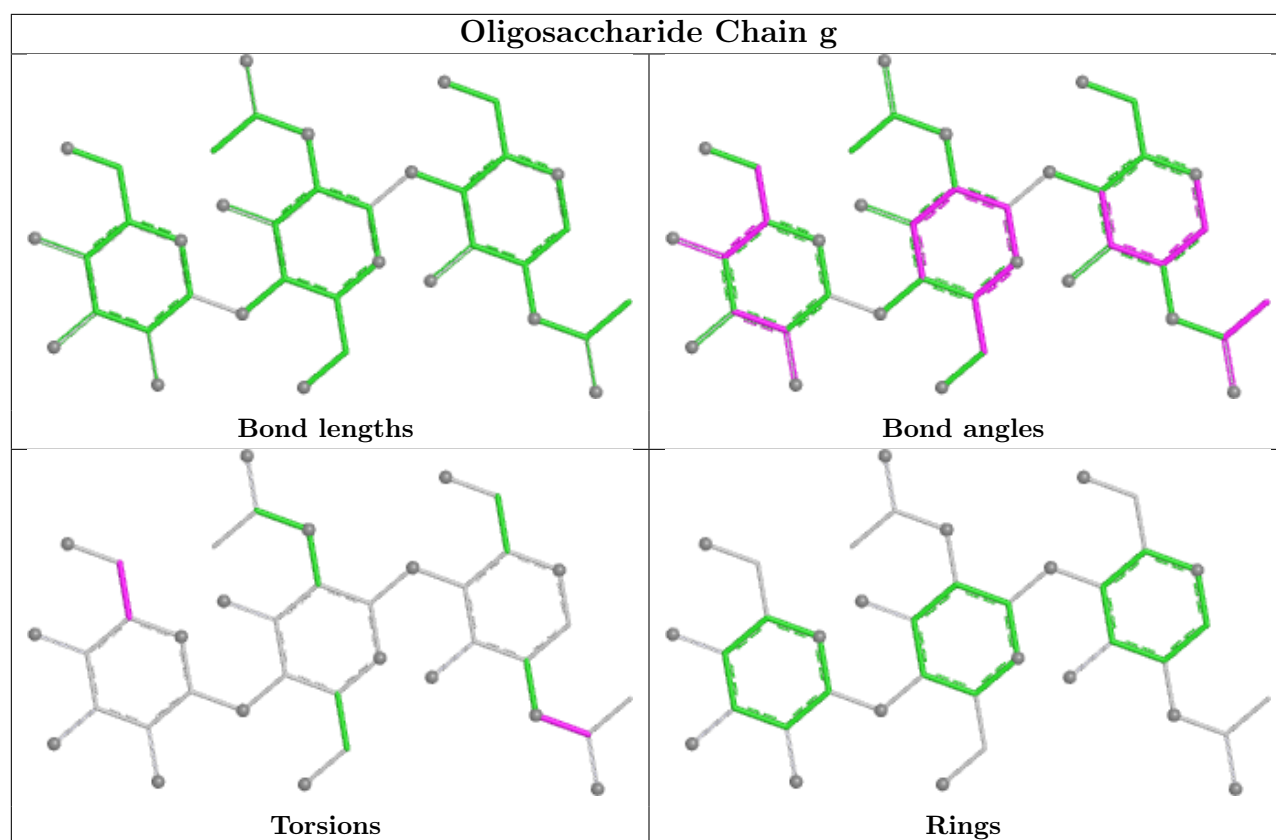


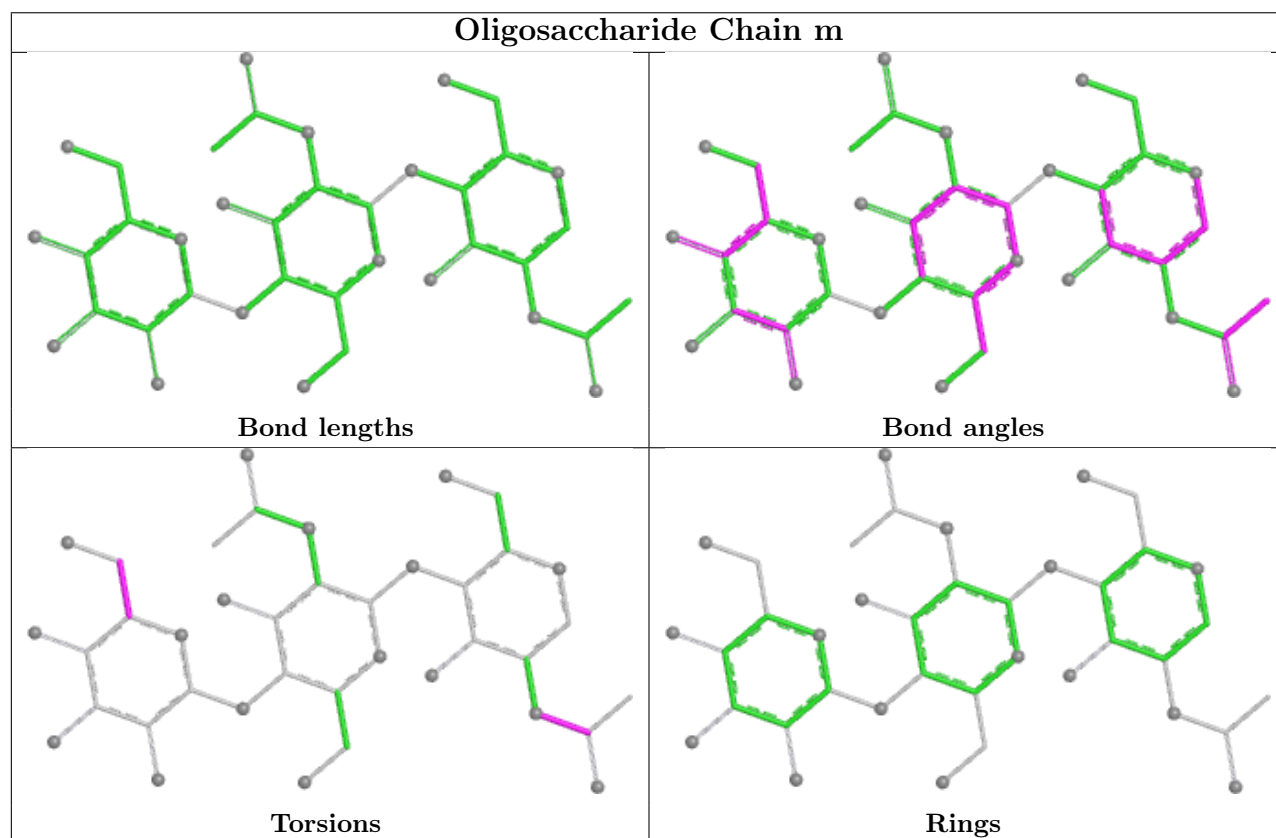
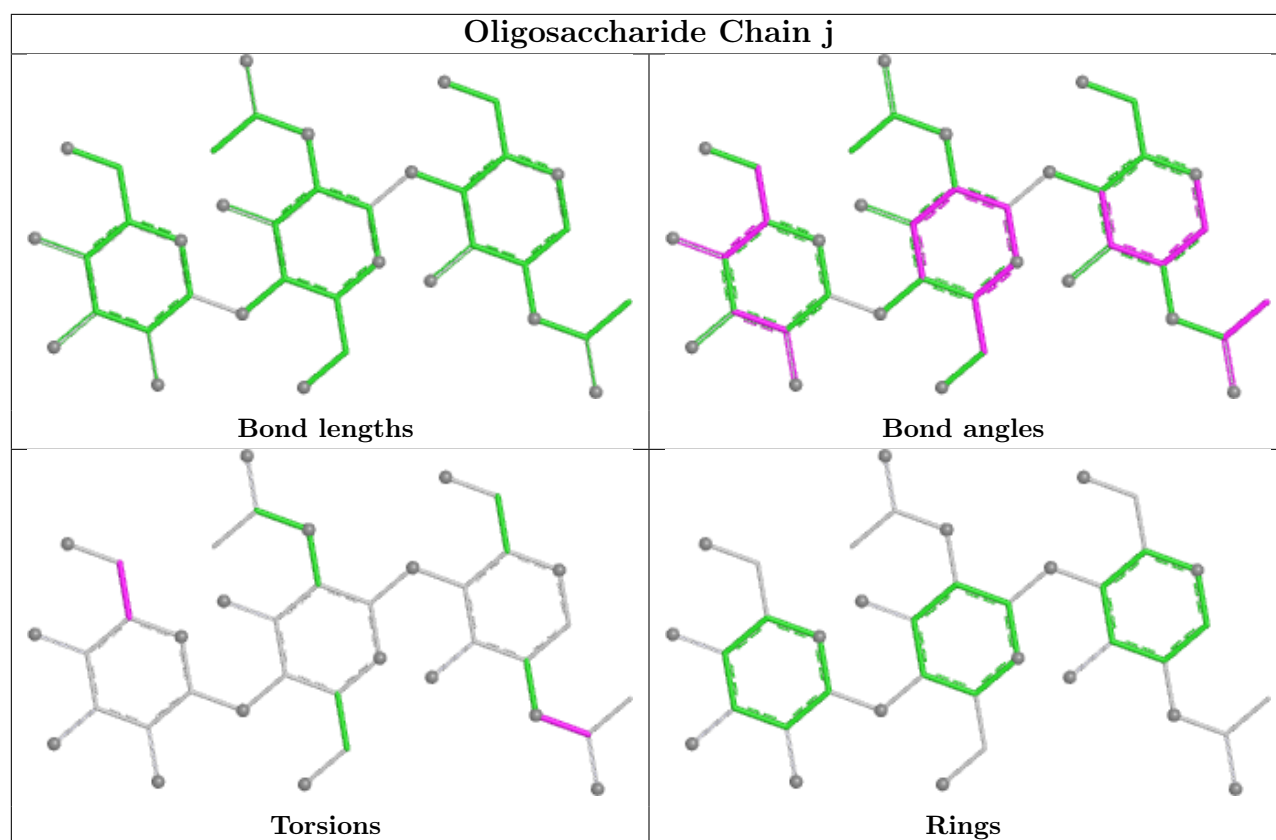


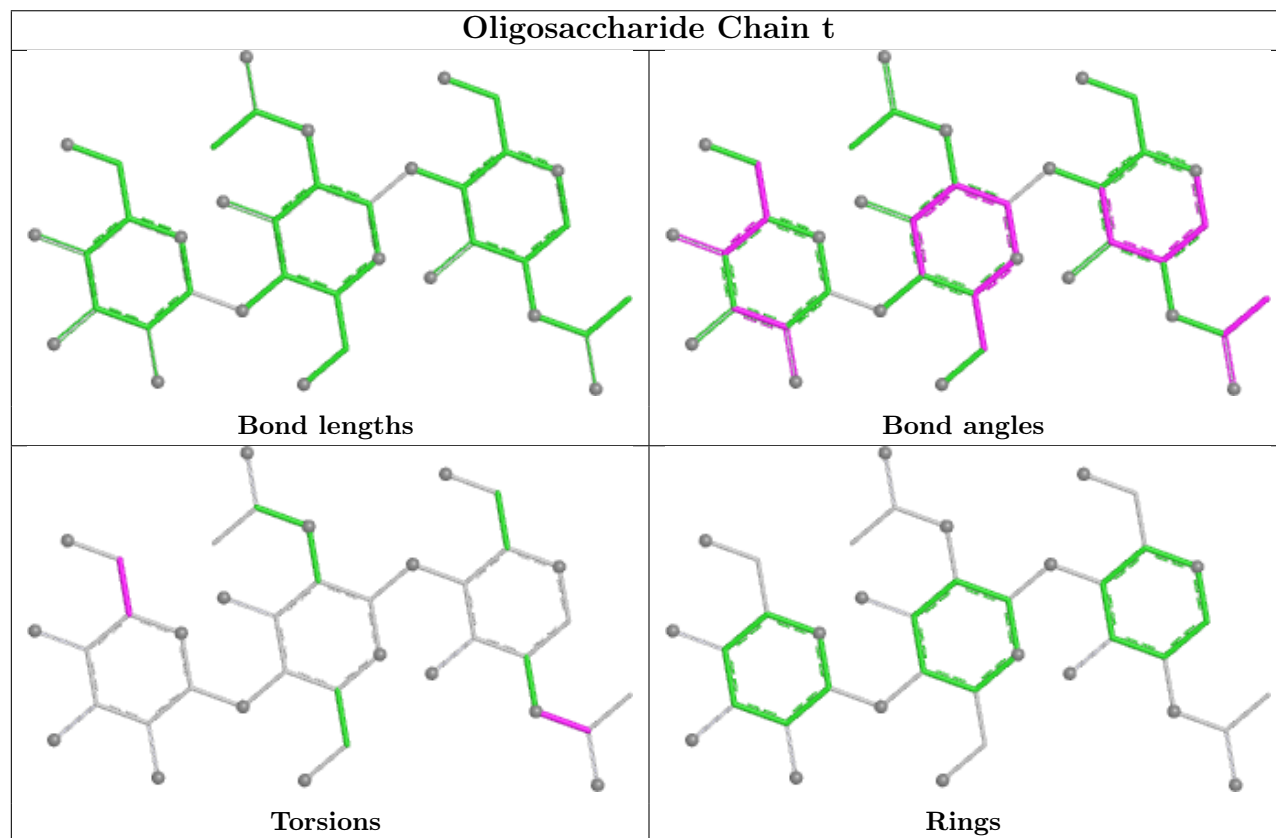
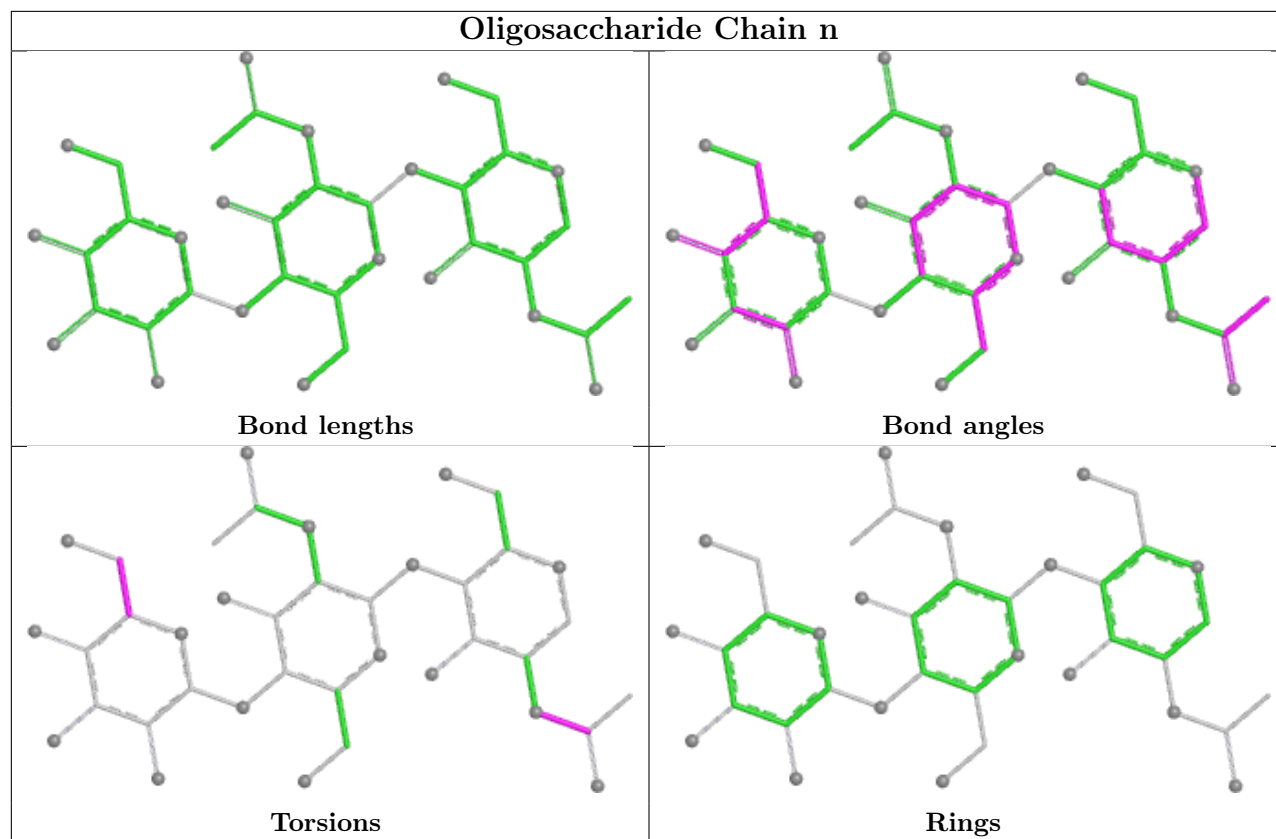


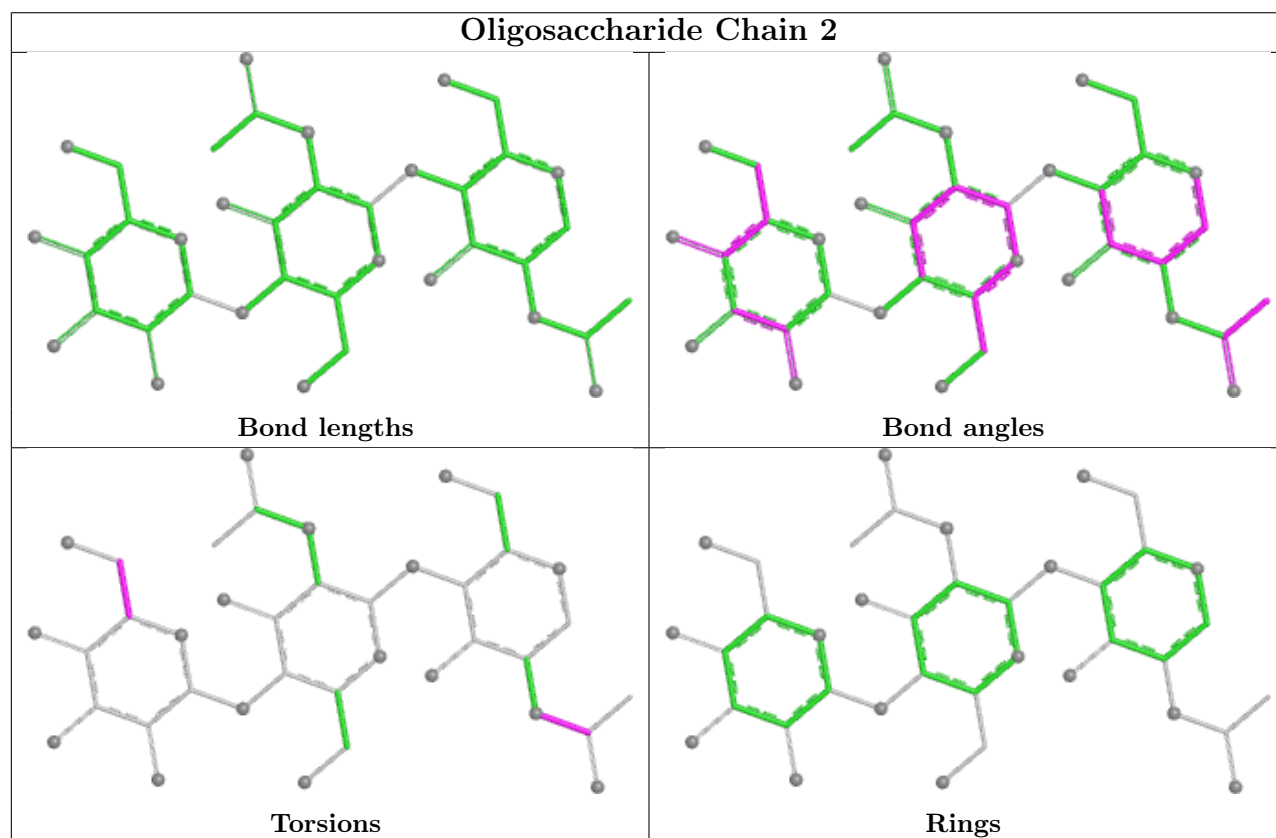
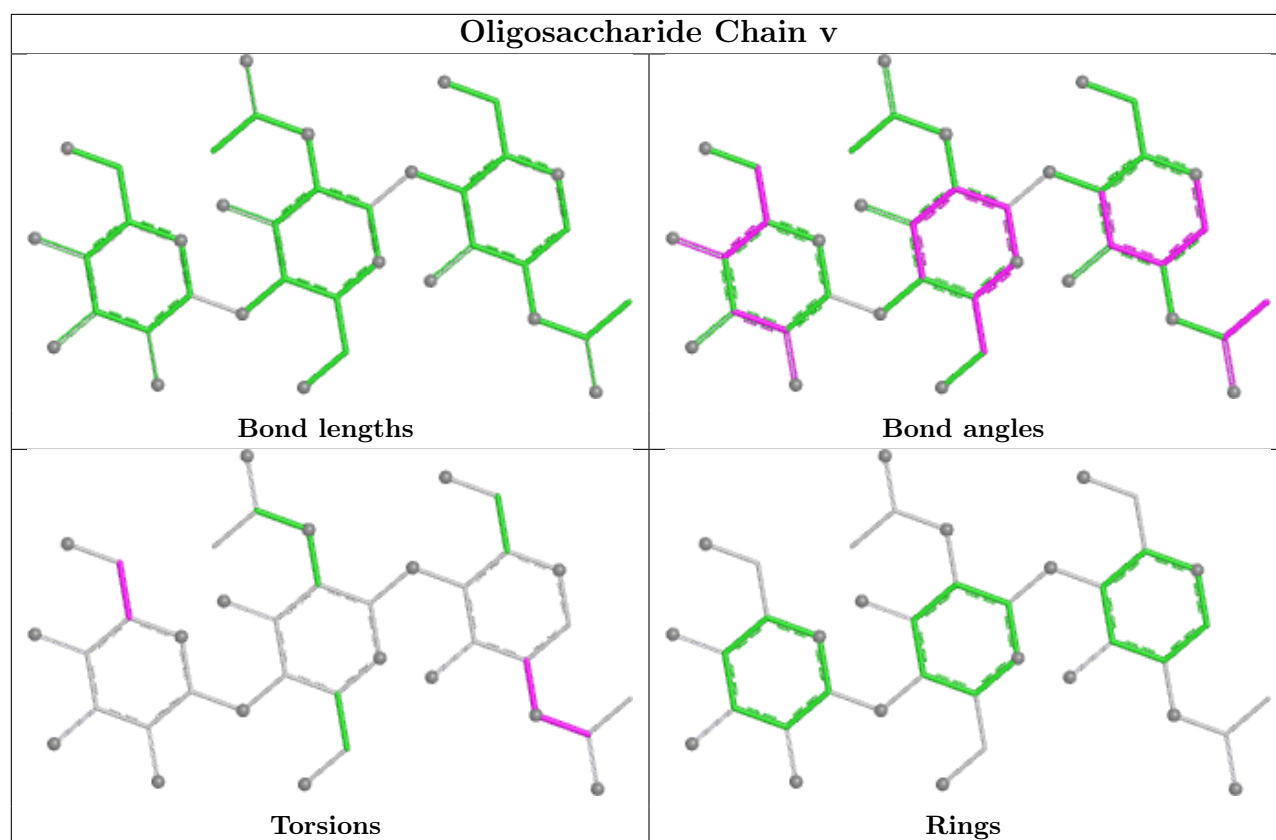


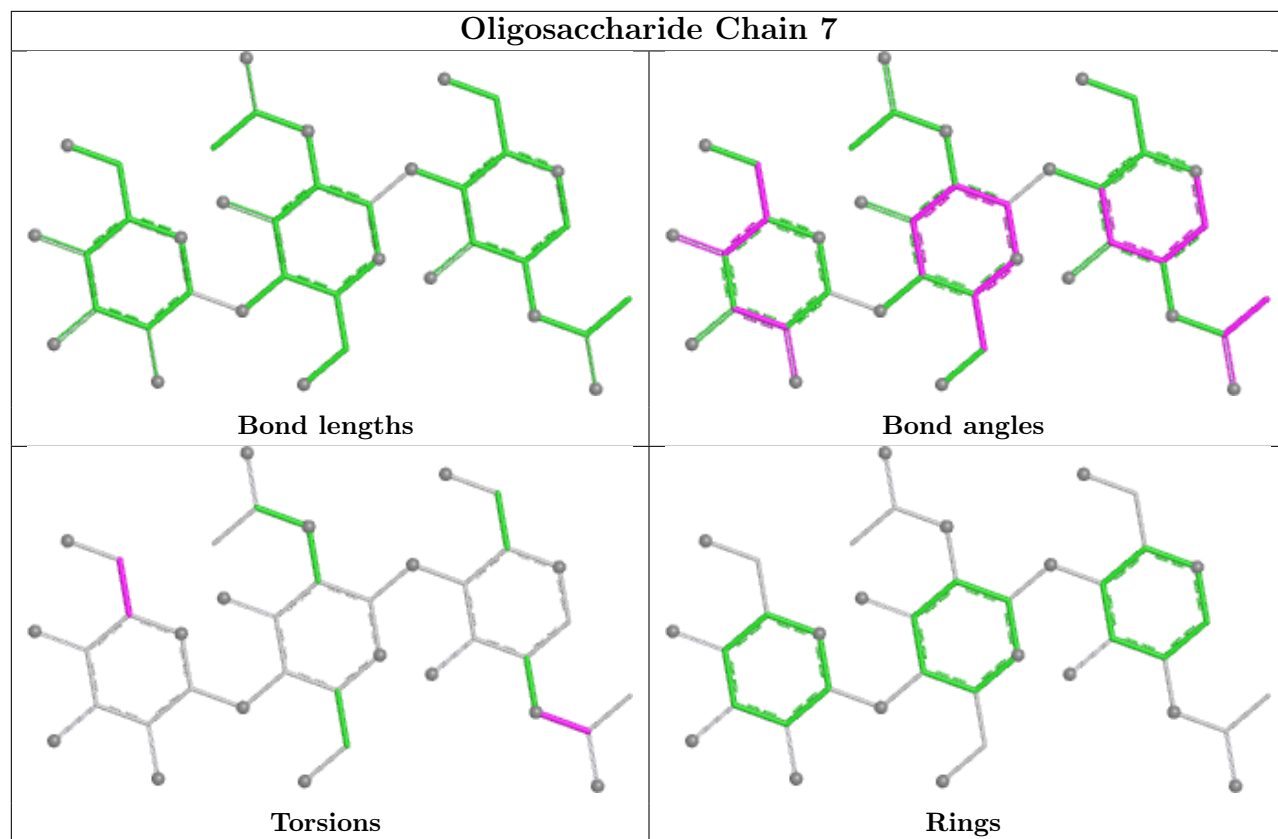


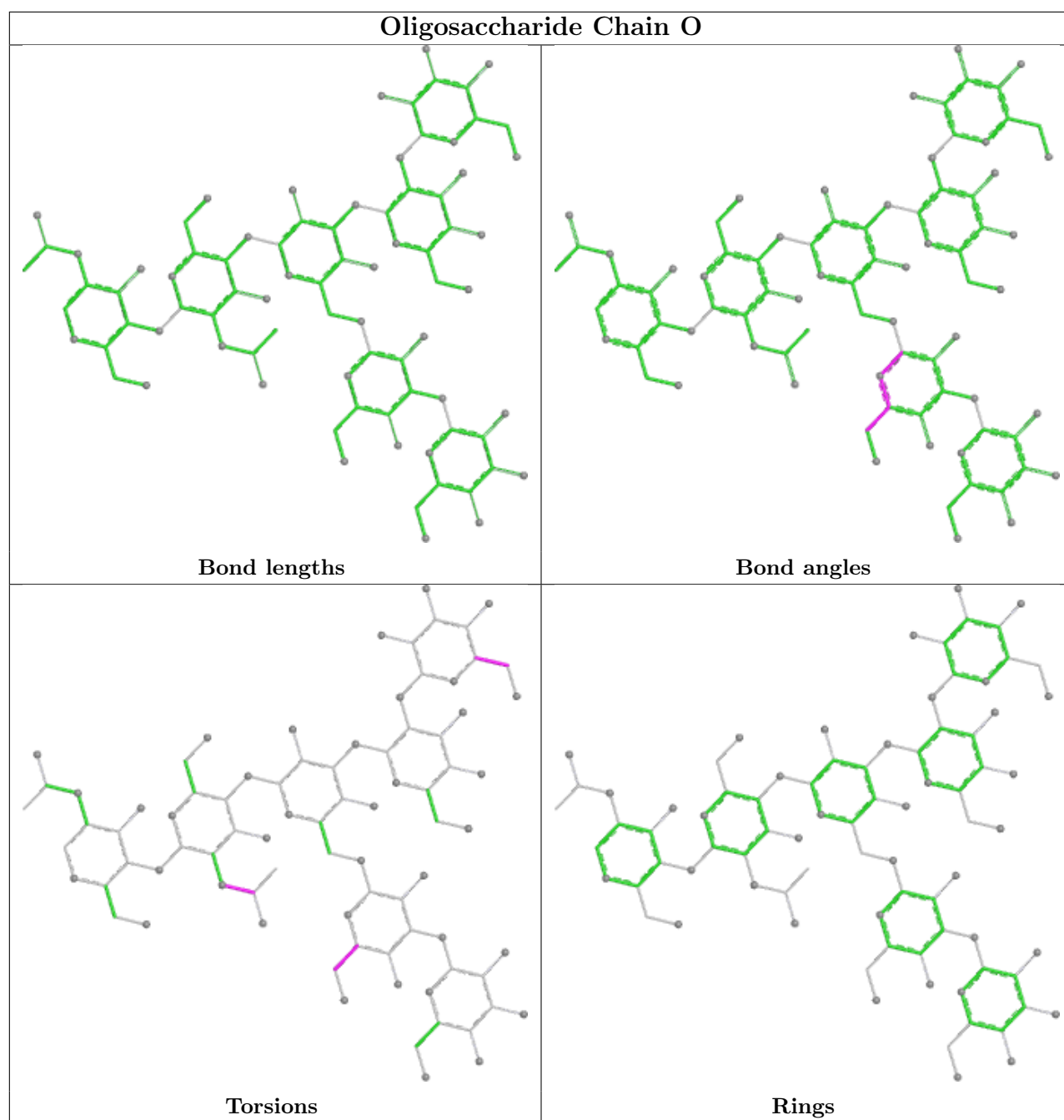


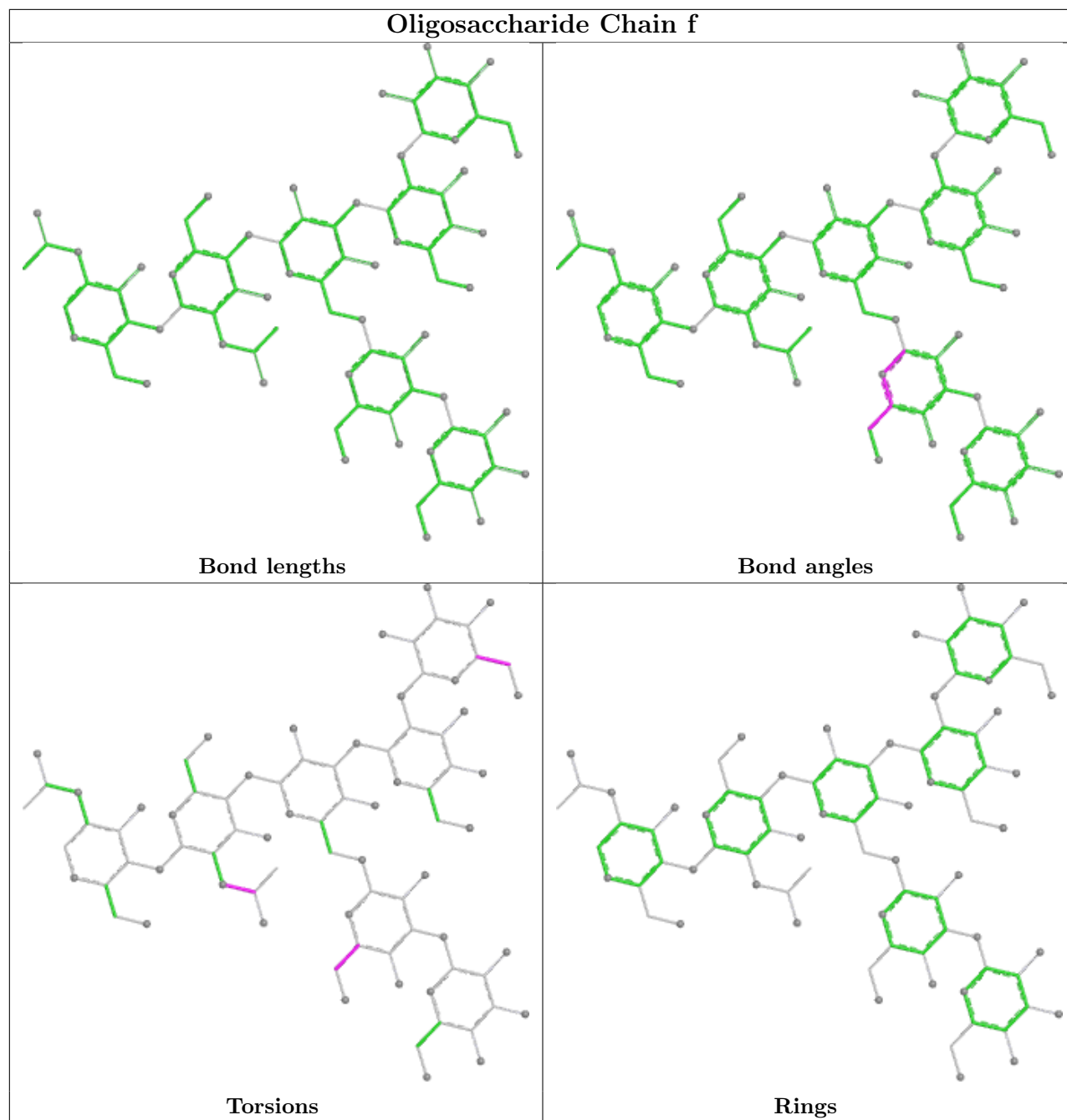


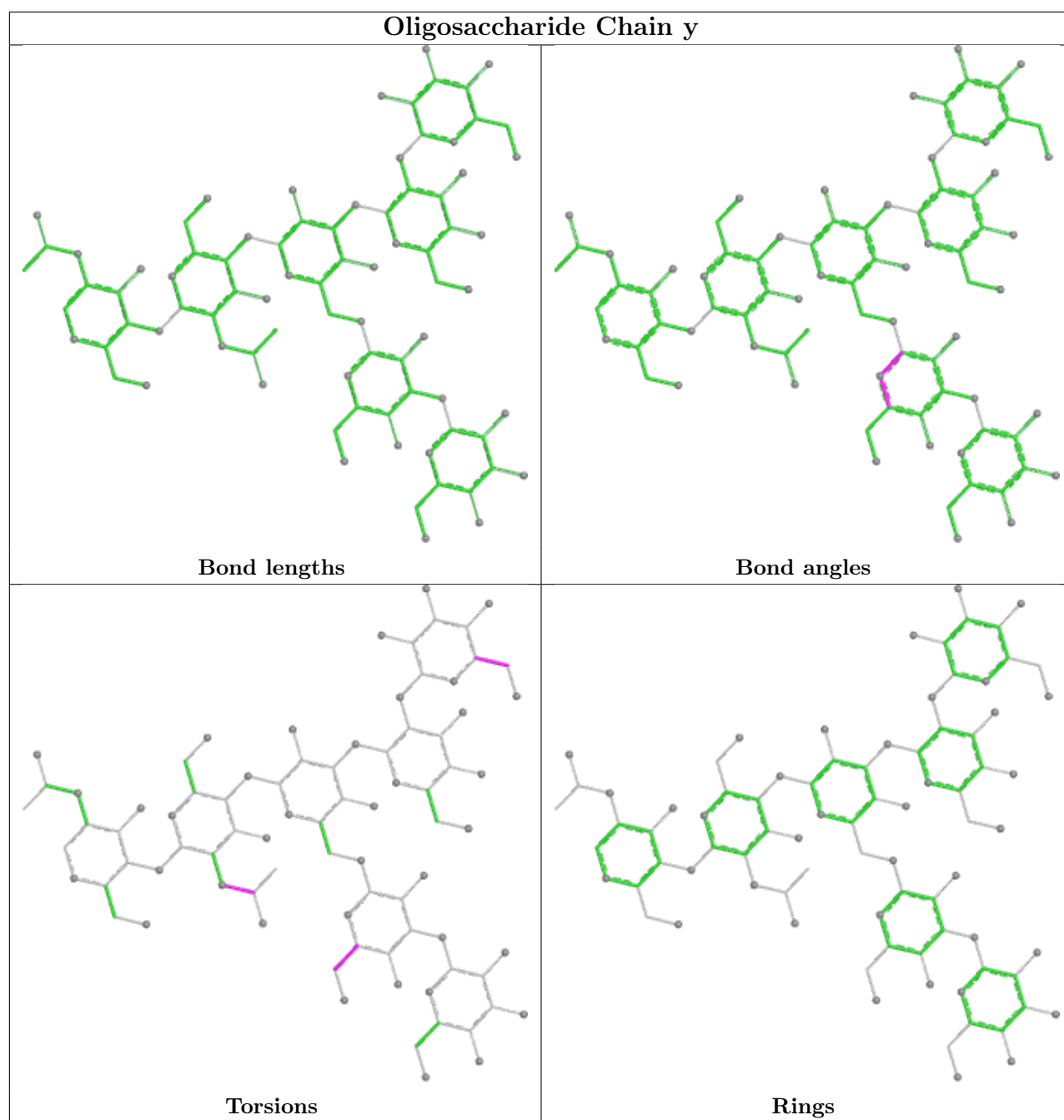


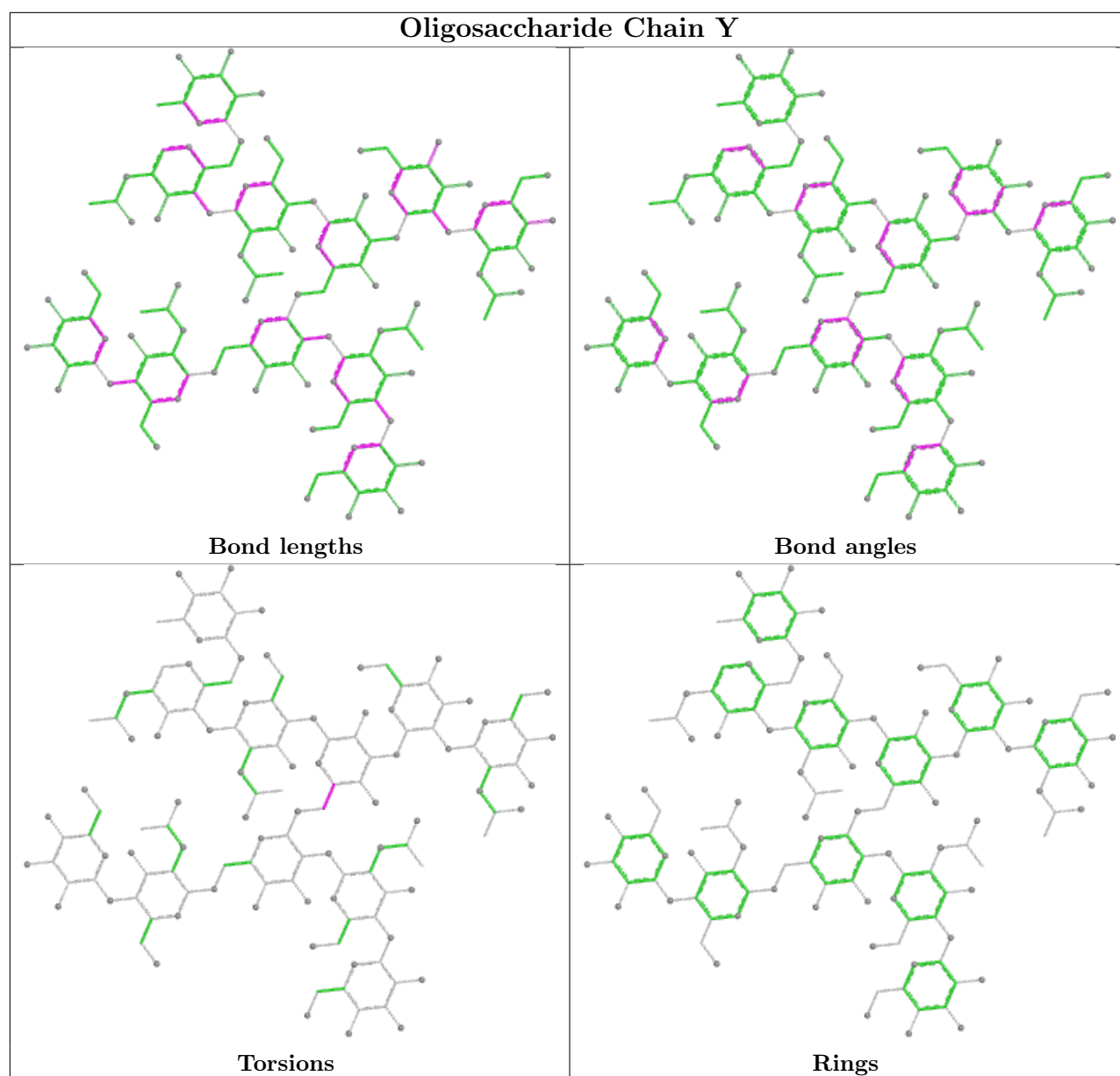


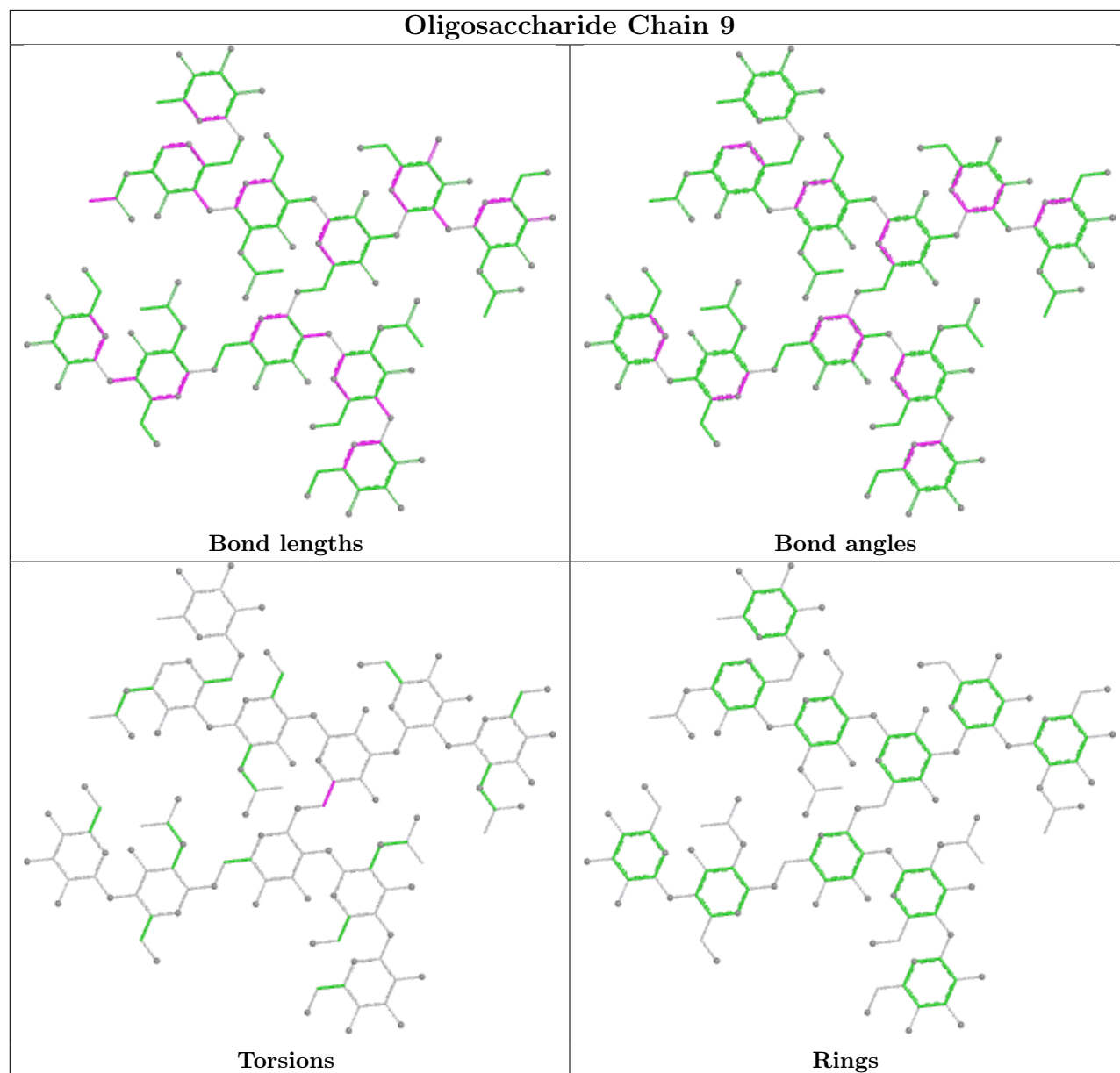


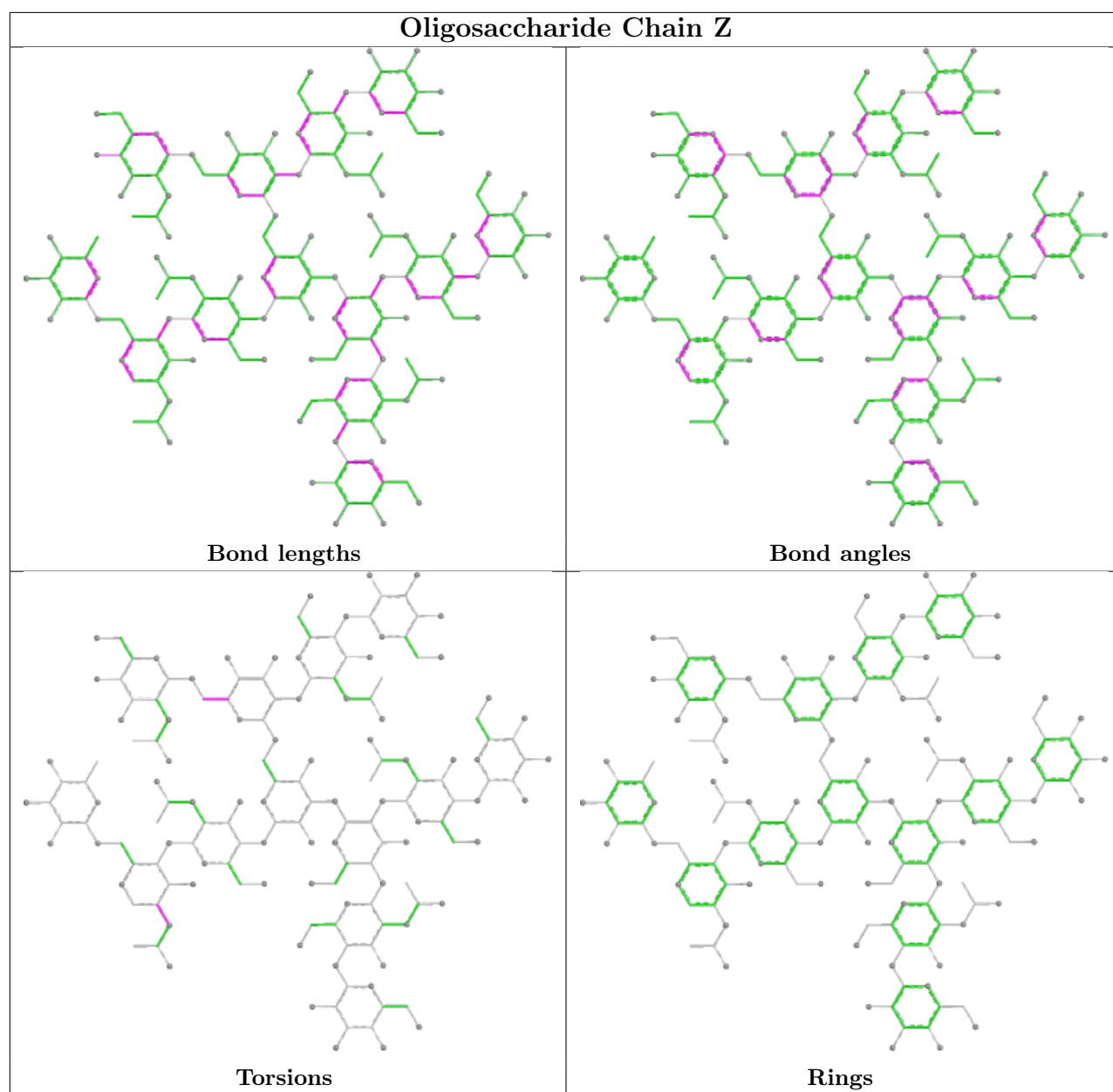


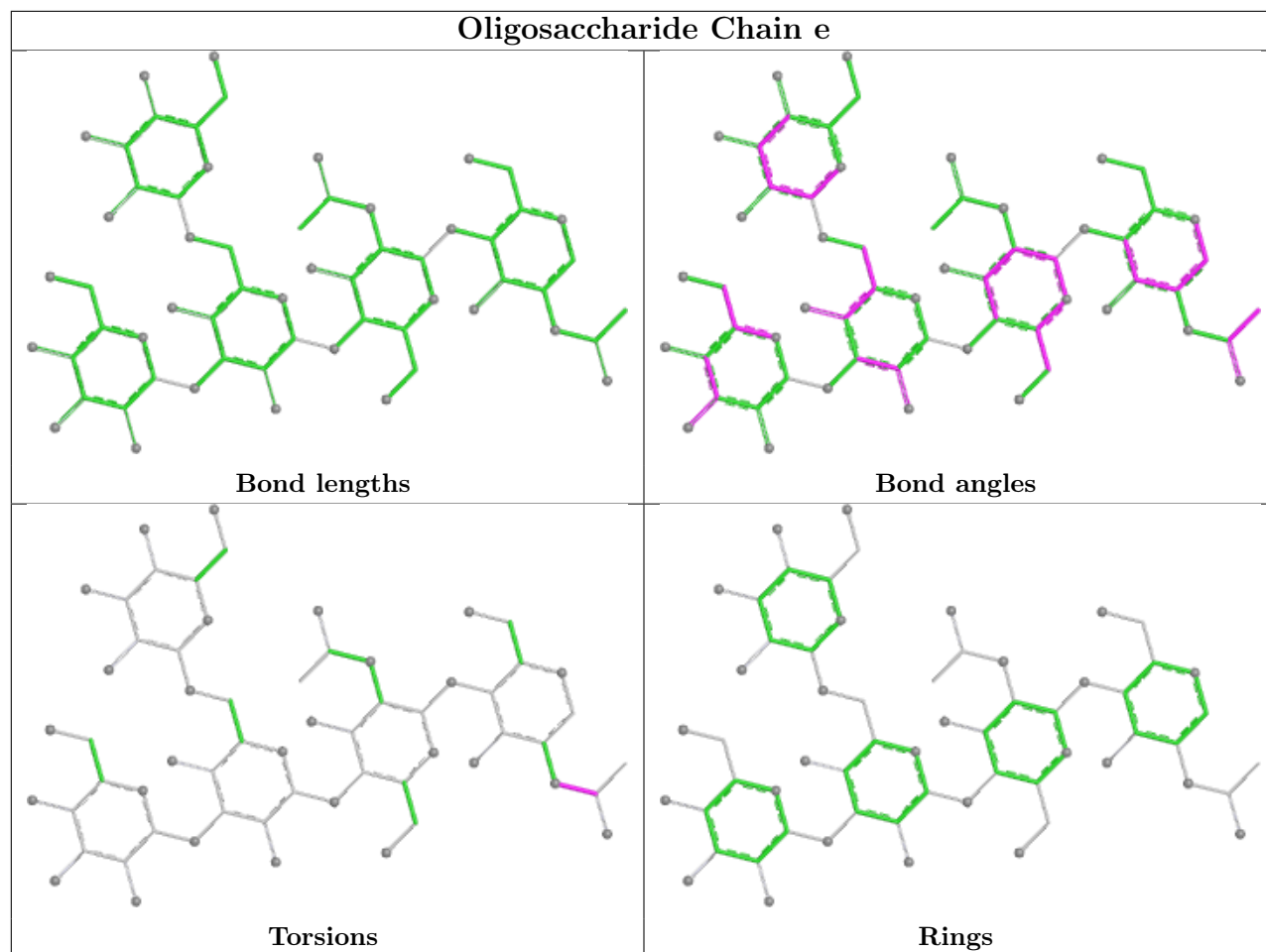


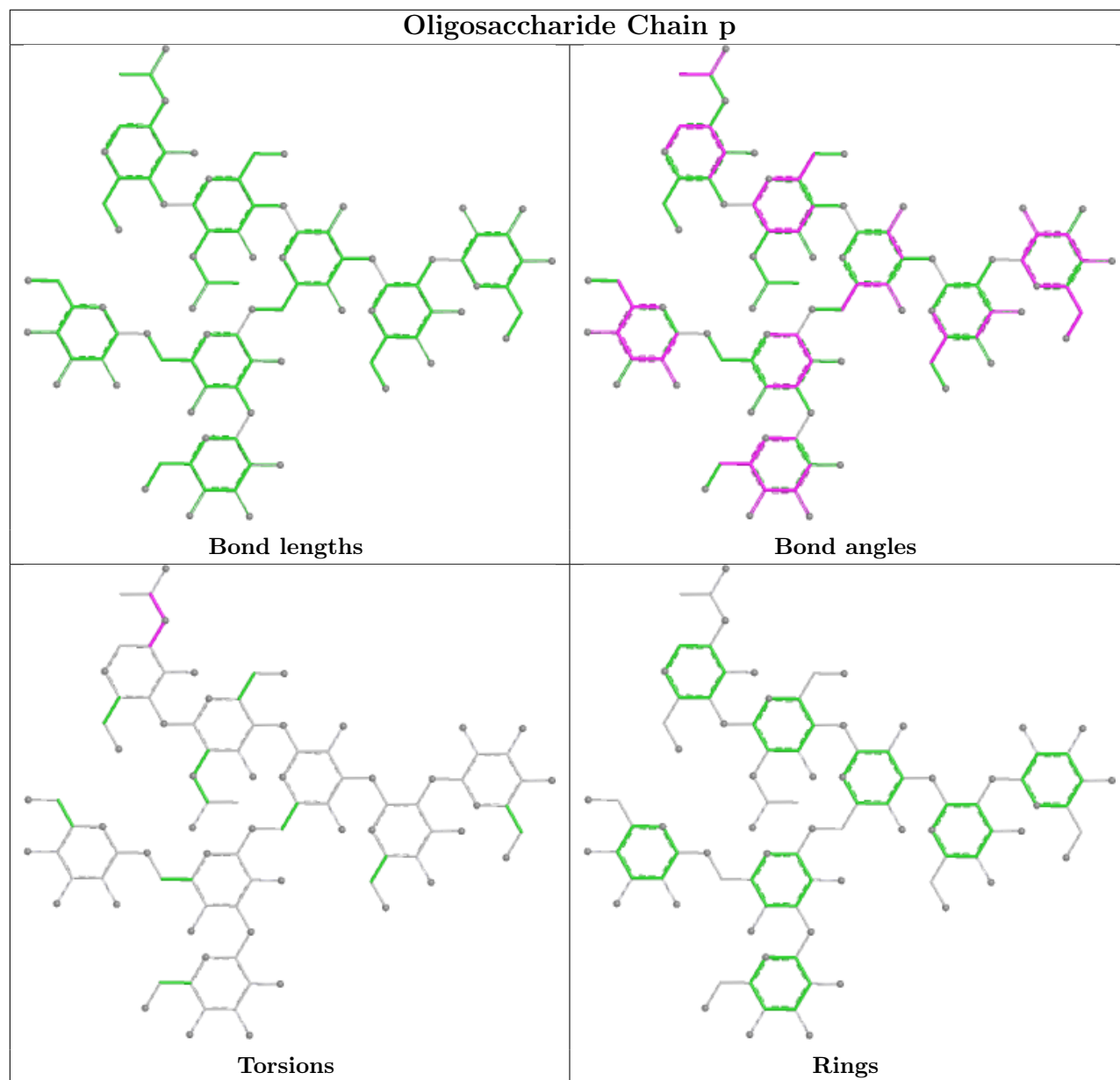


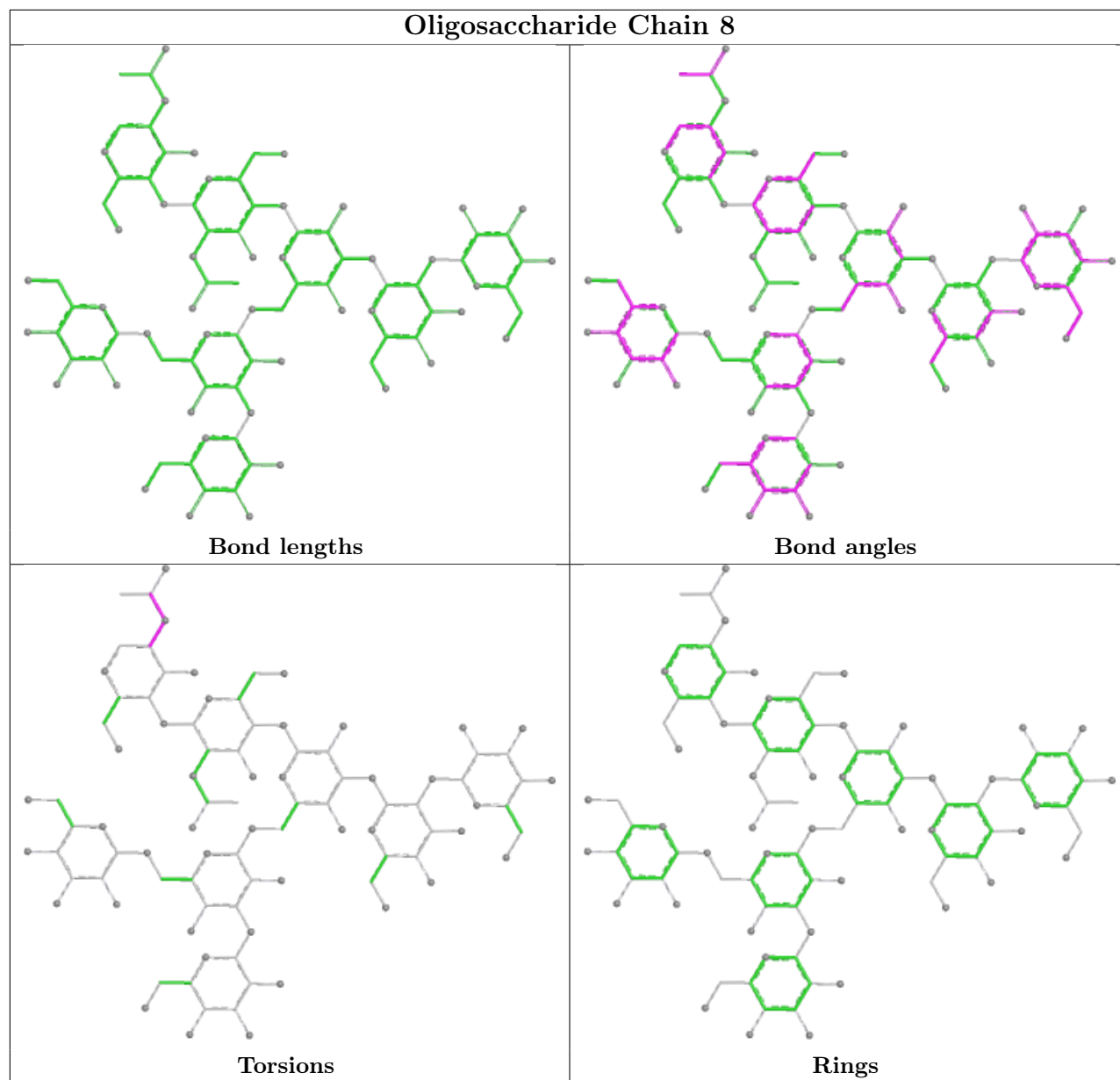


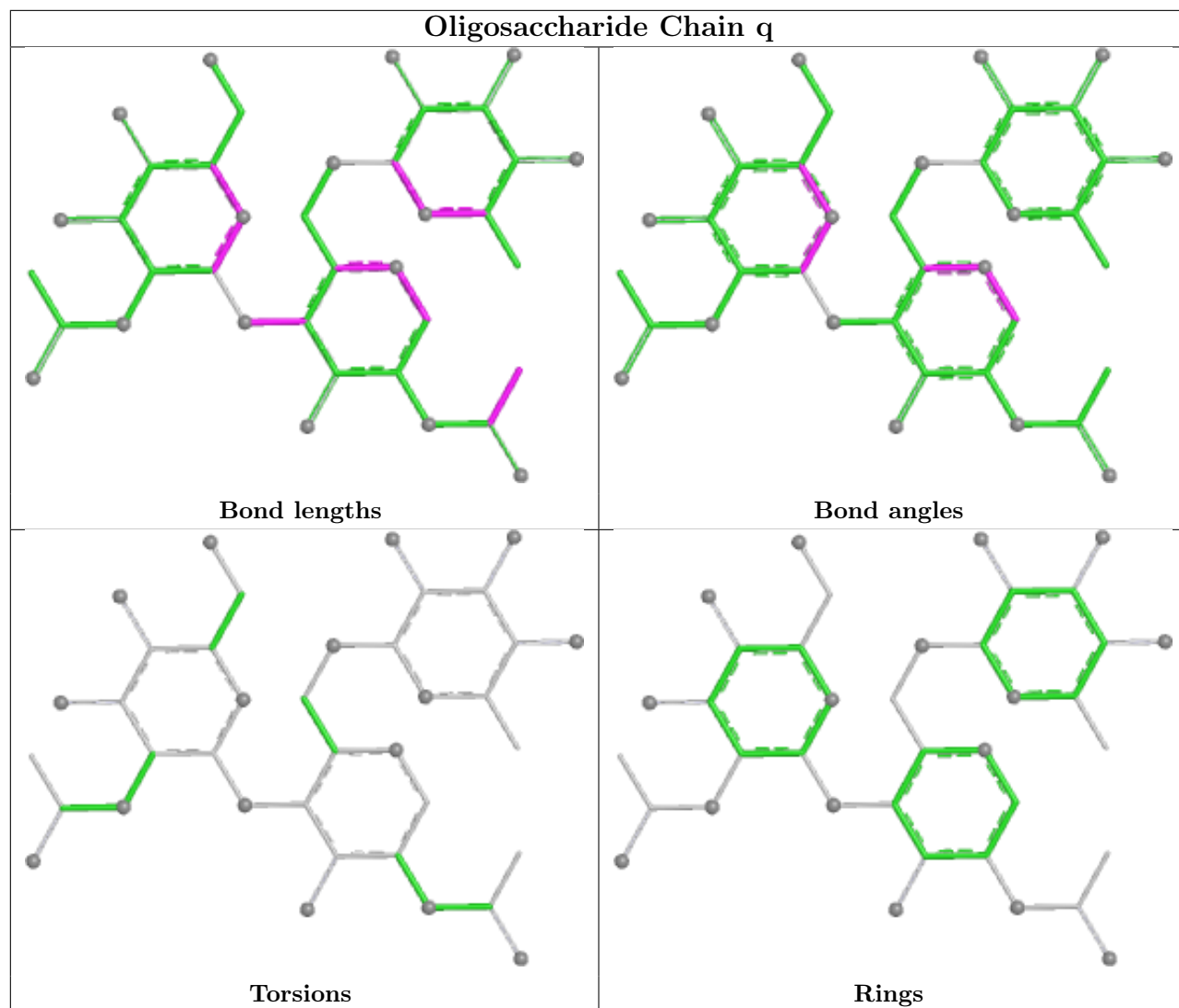


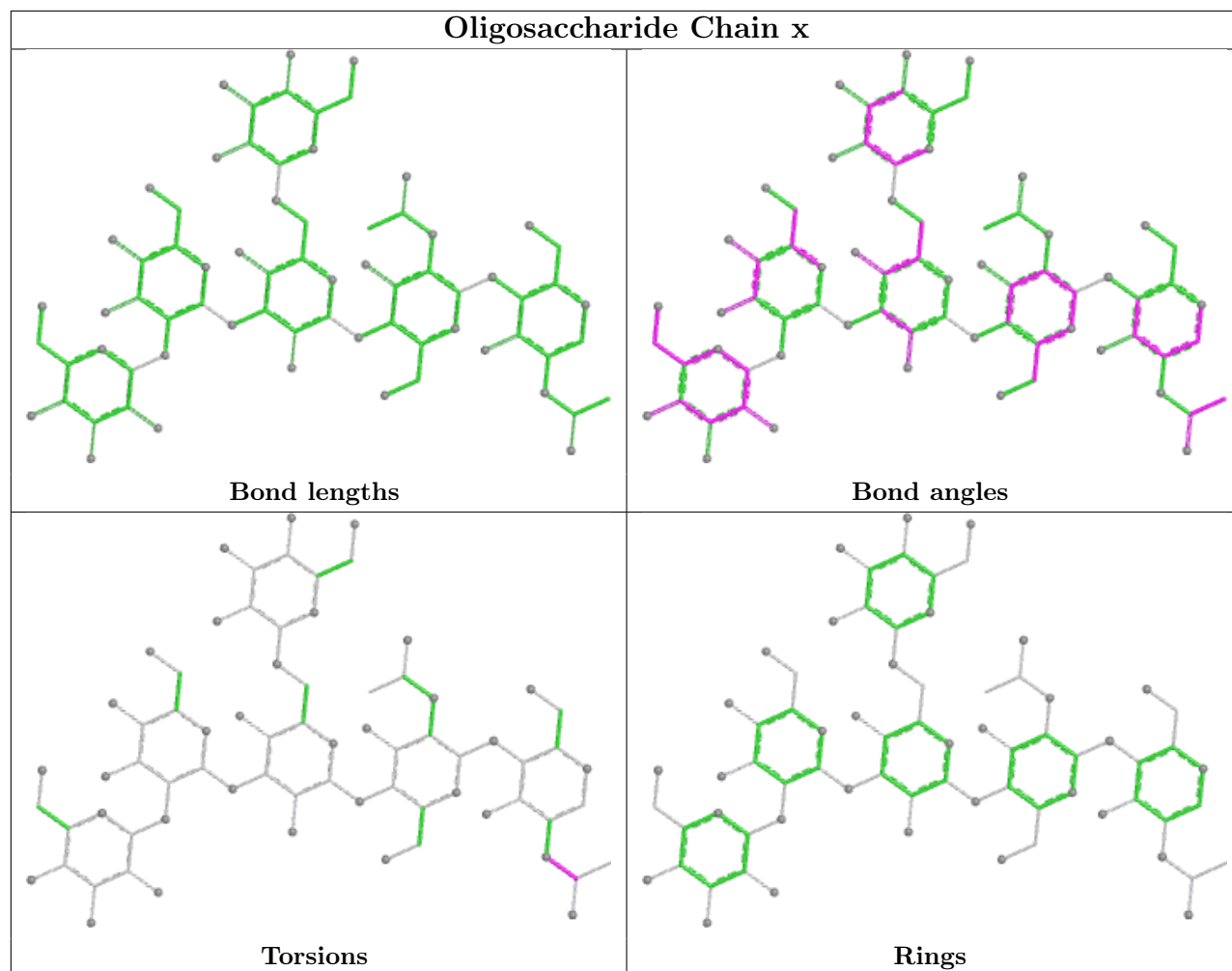


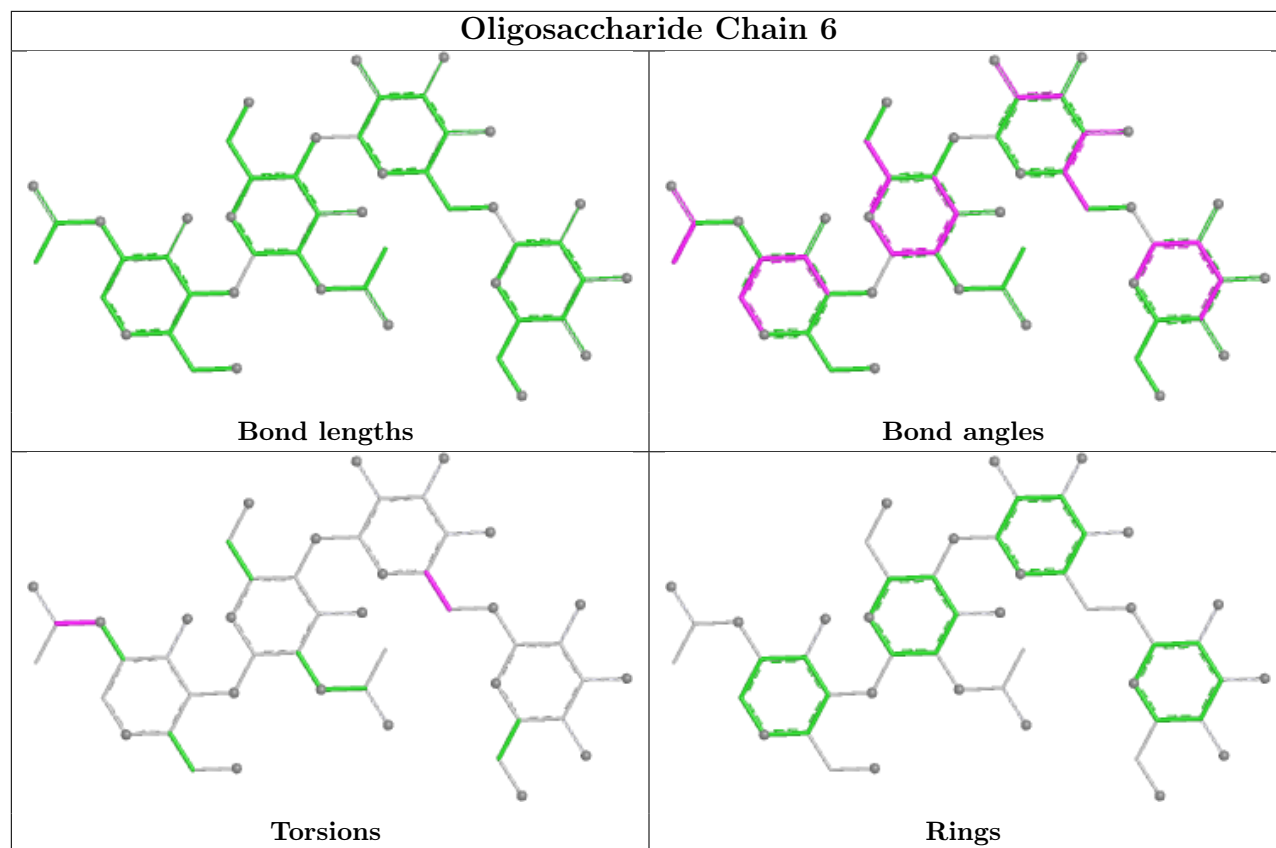


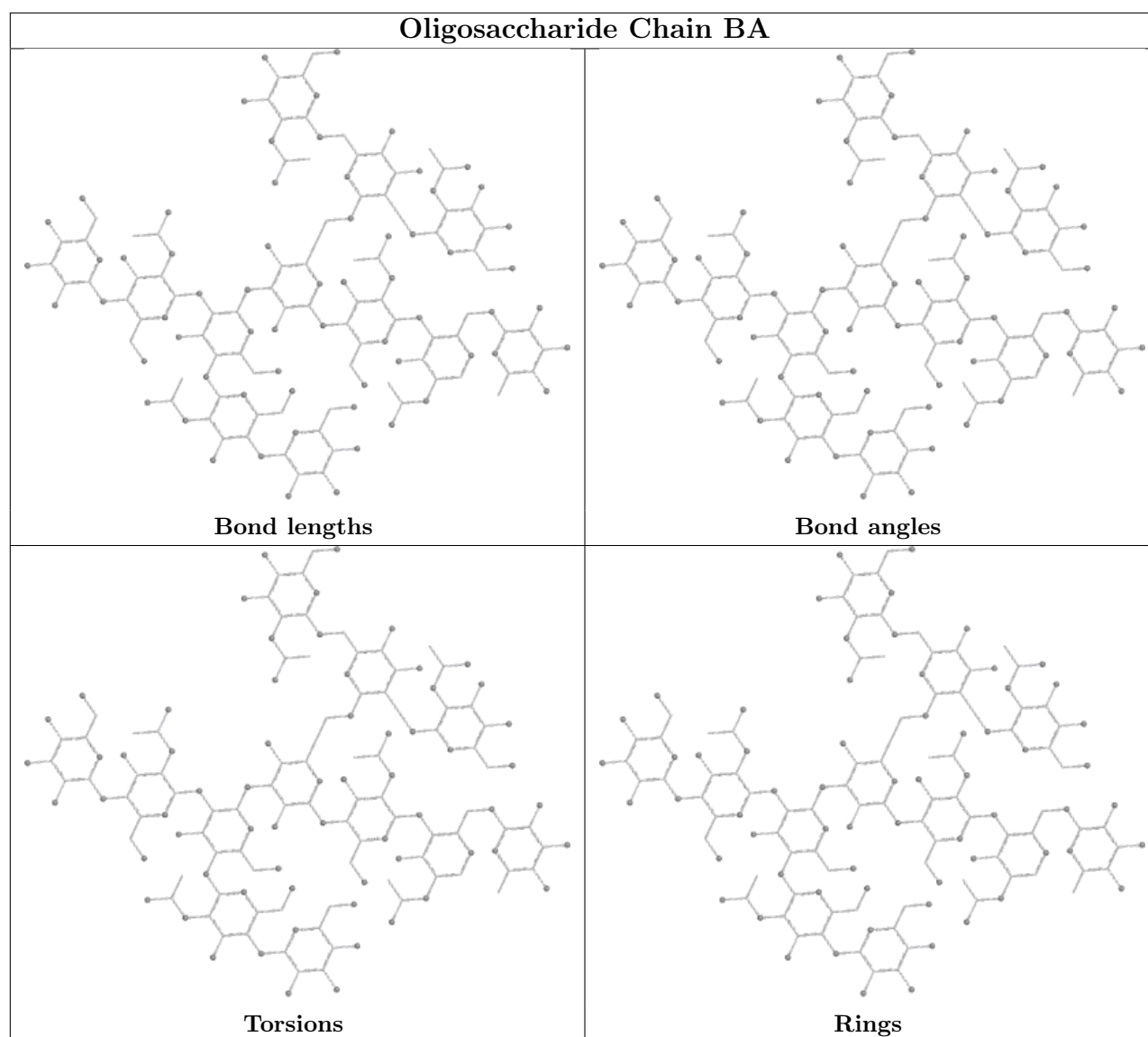












5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
16	NAG	C	1397	1	14,14,15	0.50	0	17,19,21	2.28	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	NAG	D	1600	2	14,14,15	0.52	0	17,19,21	2.29	3 (17%)
16	NAG	A	1135	1	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
16	NAG	A	1355	1	14,14,15	0.49	0	17,19,21	2.28	3 (17%)
16	NAG	A	1397	1	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
16	NAG	E	1187	1	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
16	NAG	F	1600	2	14,14,15	0.52	0	17,19,21	2.27	3 (17%)
16	NAG	B	1600	2	14,14,15	0.51	0	17,19,21	2.27	3 (17%)
16	NAG	E	1397	1	14,14,15	0.50	0	17,19,21	2.27	3 (17%)
16	NAG	B	1625	2	14,14,15	0.50	0	17,19,21	2.27	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	C	1397	1	-	1/6/23/26	0/1/1/1
16	NAG	D	1600	2	-	1/6/23/26	0/1/1/1
16	NAG	A	1135	1	-	1/6/23/26	0/1/1/1
16	NAG	A	1355	1	-	1/6/23/26	0/1/1/1
16	NAG	A	1397	1	-	1/6/23/26	0/1/1/1
16	NAG	E	1187	1	-	1/6/23/26	0/1/1/1
16	NAG	F	1600	2	-	1/6/23/26	0/1/1/1
16	NAG	B	1600	2	-	1/6/23/26	0/1/1/1
16	NAG	E	1397	1	-	1/6/23/26	0/1/1/1
16	NAG	B	1625	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	1600	NAG	O5-C1-C2	-7.55	99.61	111.29
16	C	1397	NAG	O5-C1-C2	-7.53	99.63	111.29
16	F	1600	NAG	O5-C1-C2	-7.53	99.64	111.29
16	A	1355	NAG	O5-C1-C2	-7.53	99.64	111.29
16	A	1135	NAG	O5-C1-C2	-7.52	99.65	111.29
16	B	1600	NAG	O5-C1-C2	-7.51	99.66	111.29
16	B	1625	NAG	O5-C1-C2	-7.50	99.69	111.29
16	E	1397	NAG	O5-C1-C2	-7.50	99.69	111.29
16	E	1187	NAG	O5-C1-C2	-7.50	99.69	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1397	NAG	O5-C1-C2	-7.48	99.72	111.29
16	D	1600	NAG	O7-C7-C8	-2.95	116.79	122.05
16	A	1397	NAG	O7-C7-C8	-2.93	116.84	122.05
16	C	1397	NAG	O7-C7-C8	-2.93	116.84	122.05
16	E	1397	NAG	O7-C7-C8	-2.92	116.85	122.05
16	B	1600	NAG	O7-C7-C8	-2.91	116.87	122.05
16	E	1187	NAG	O7-C7-C8	-2.89	116.90	122.05
16	F	1600	NAG	O7-C7-C8	-2.89	116.91	122.05
16	B	1625	NAG	O7-C7-C8	-2.88	116.92	122.05
16	A	1135	NAG	O7-C7-C8	-2.88	116.92	122.05
16	A	1355	NAG	O7-C7-C8	-2.87	116.95	122.05
16	D	1600	NAG	C4-C3-C2	-2.72	107.03	111.02
16	A	1355	NAG	C4-C3-C2	-2.68	107.09	111.02
16	A	1135	NAG	C4-C3-C2	-2.67	107.10	111.02
16	B	1600	NAG	C4-C3-C2	-2.67	107.11	111.02
16	F	1600	NAG	C4-C3-C2	-2.67	107.11	111.02
16	B	1625	NAG	C4-C3-C2	-2.66	107.11	111.02
16	E	1187	NAG	C4-C3-C2	-2.66	107.12	111.02
16	C	1397	NAG	C4-C3-C2	-2.66	107.12	111.02
16	A	1397	NAG	C4-C3-C2	-2.63	107.16	111.02
16	E	1397	NAG	C4-C3-C2	-2.62	107.18	111.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	D	1600	NAG	O7-C7-N2-C2
16	A	1135	NAG	O7-C7-N2-C2
16	A	1355	NAG	O7-C7-N2-C2
16	A	1397	NAG	O7-C7-N2-C2
16	B	1600	NAG	O7-C7-N2-C2
16	B	1625	NAG	O7-C7-N2-C2
16	C	1397	NAG	O7-C7-N2-C2
16	E	1187	NAG	O7-C7-N2-C2
16	E	1397	NAG	O7-C7-N2-C2
16	F	1600	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	1355	NAG	2	0
16	A	1397	NAG	4	0
16	E	1397	NAG	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

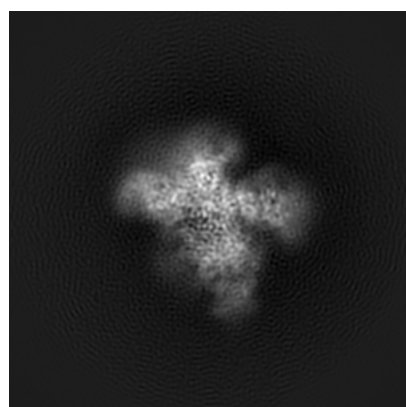
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3308. These allow visual inspection of the internal detail of the map and identification of artifacts.

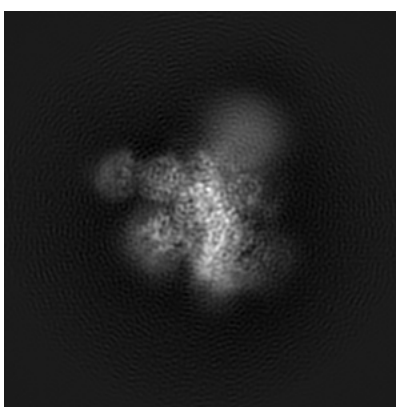
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

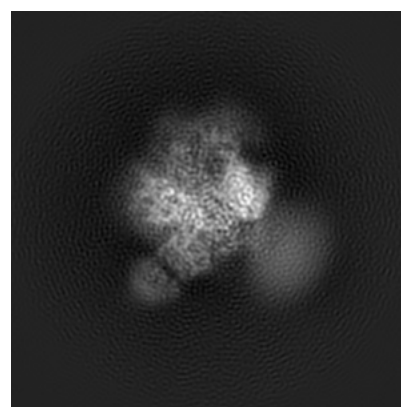
6.1.1 Primary map



X



Y

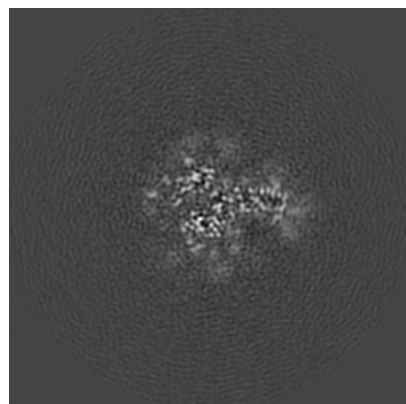


Z

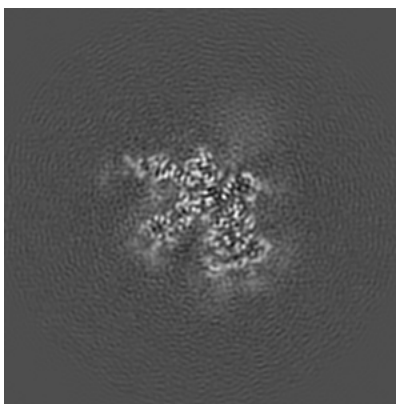
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

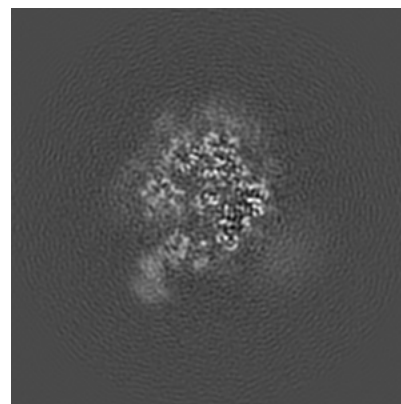
6.2.1 Primary map



X Index: 128



Y Index: 128

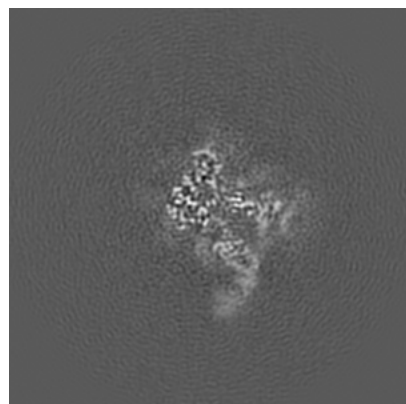


Z Index: 128

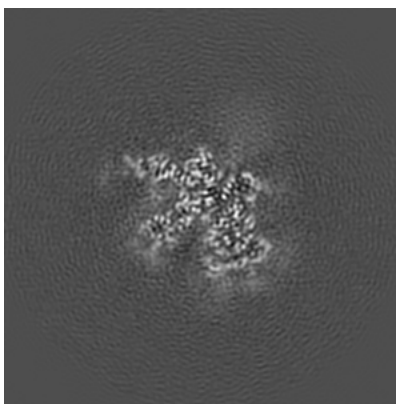
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

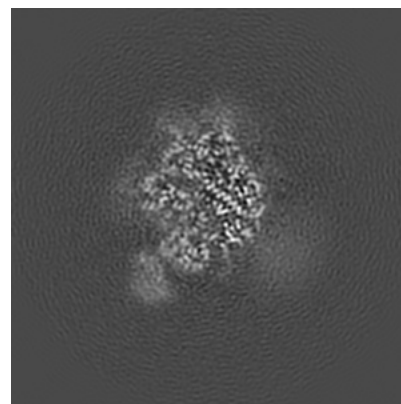
6.3.1 Primary map



X Index: 141



Y Index: 128

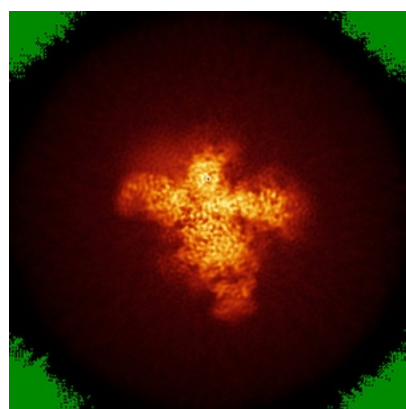


Z Index: 132

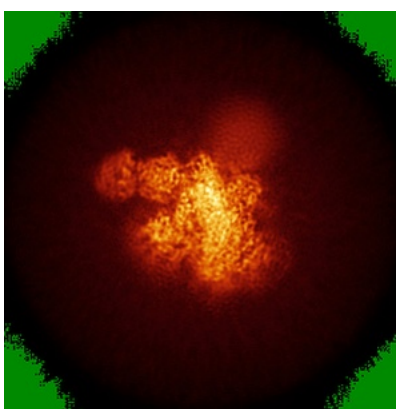
The images above show the largest variance slices of the map in three orthogonal directions.

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

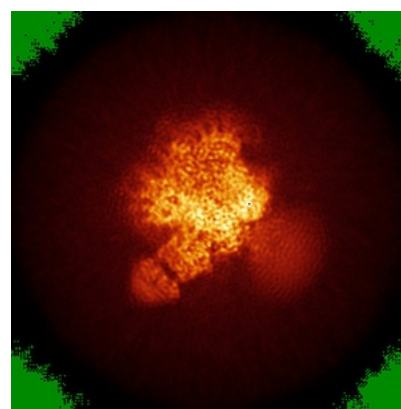
6.4.1 Primary map



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.

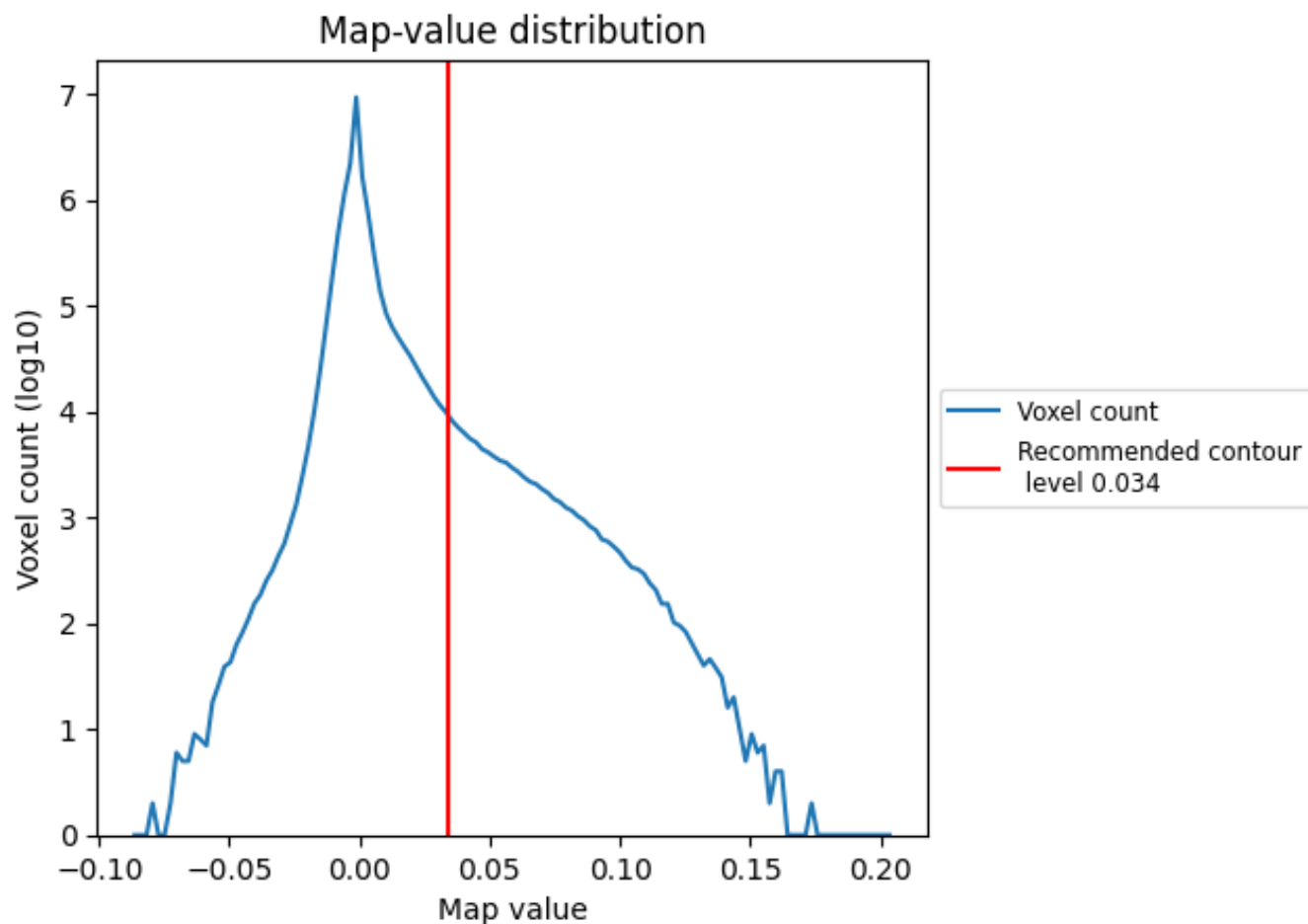
6.6 Mask visualisation

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

7 Map analysis [i](#)

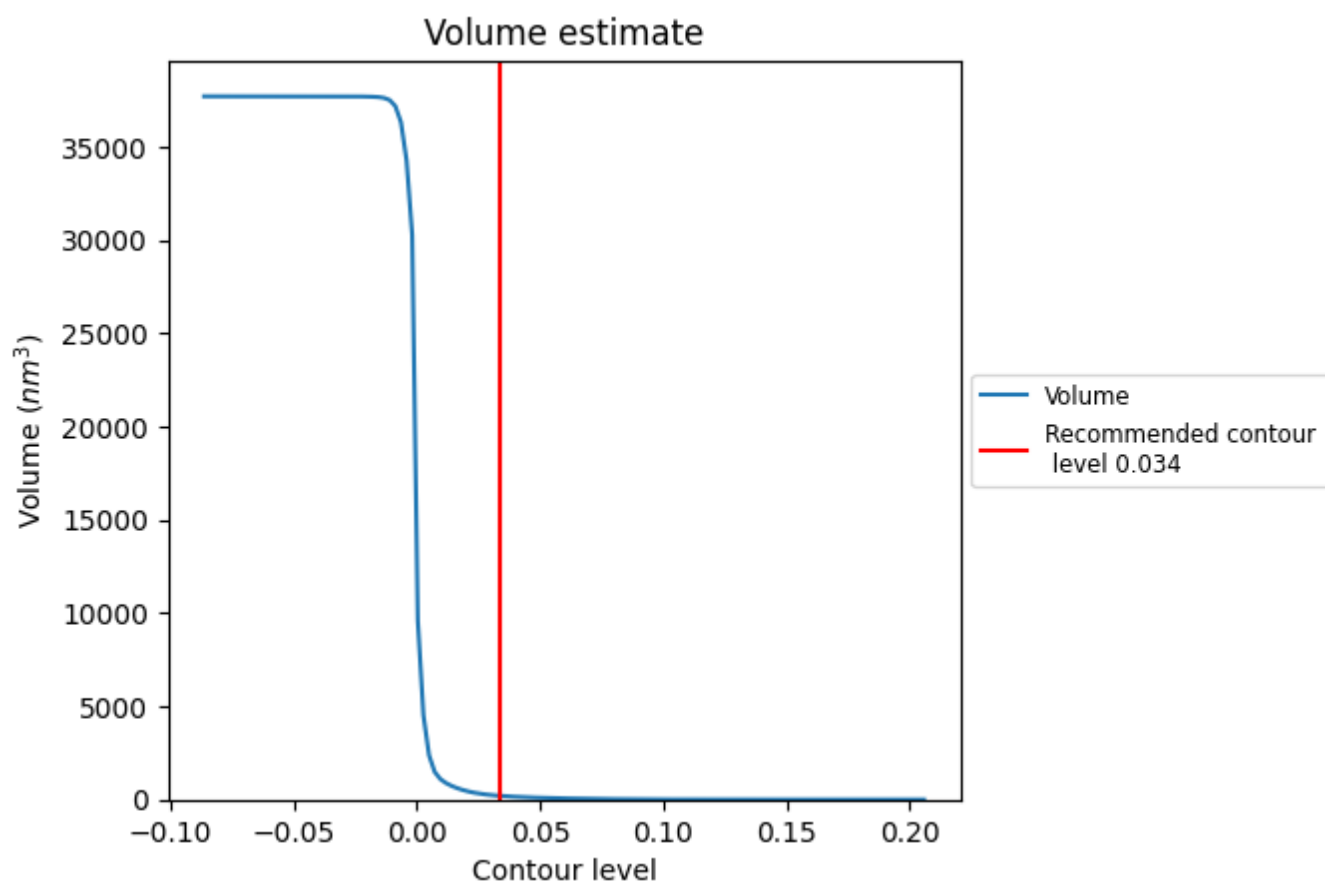
This section contains the results of statistical analysis of the map.

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.

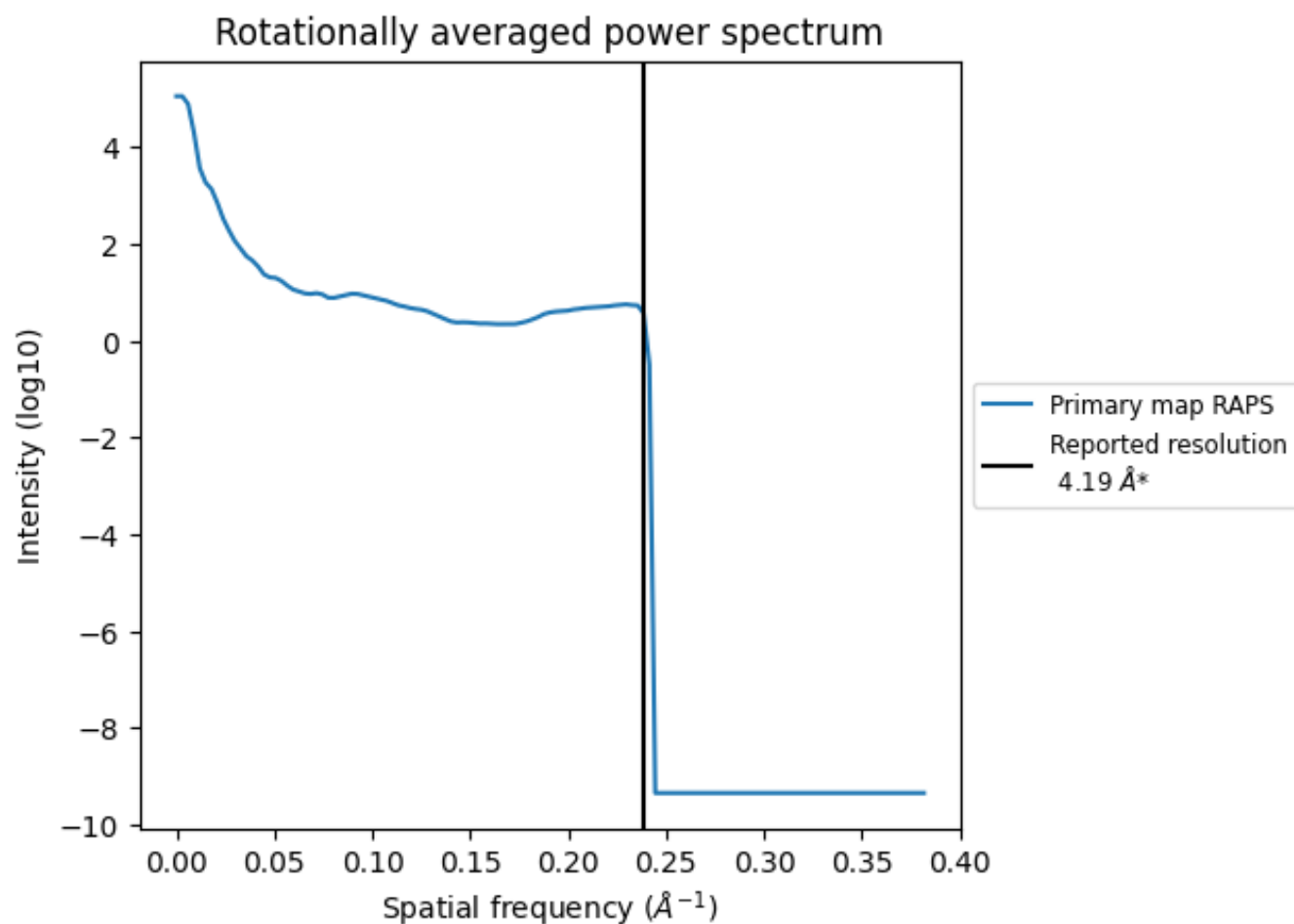
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm³; this corresponds to an approximate mass of 178 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 0.239 Å⁻¹

8 Fourier-Shell correlation

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

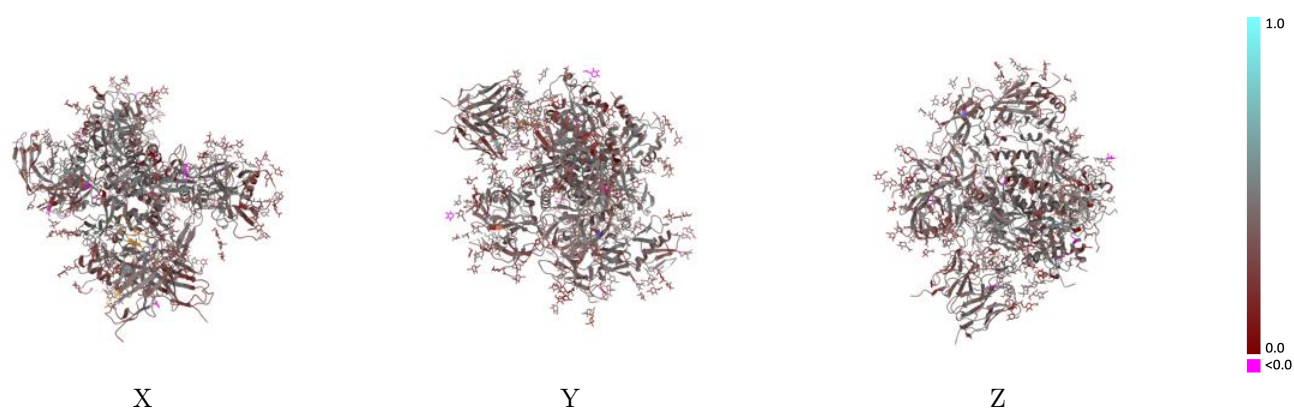
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3308 and PDB model 5FUU. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

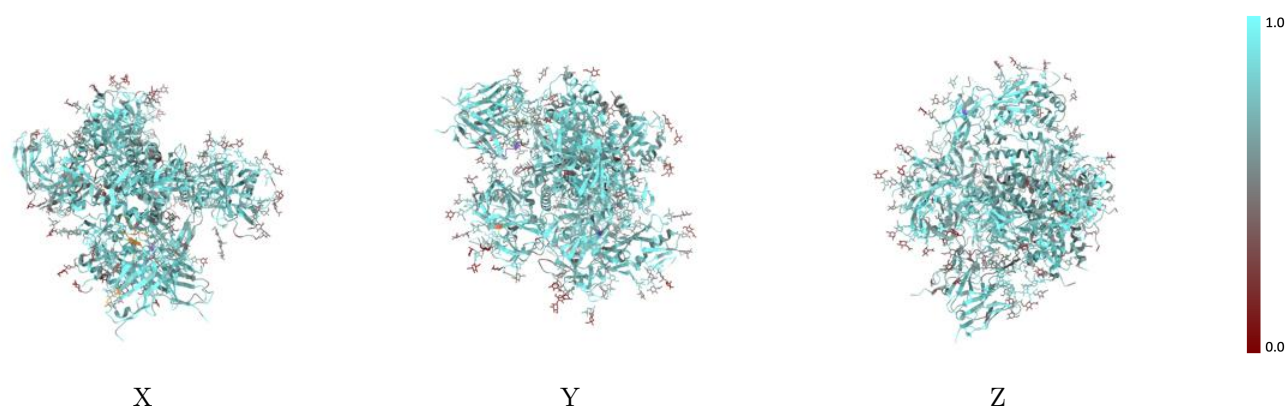
This section was not generated.

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



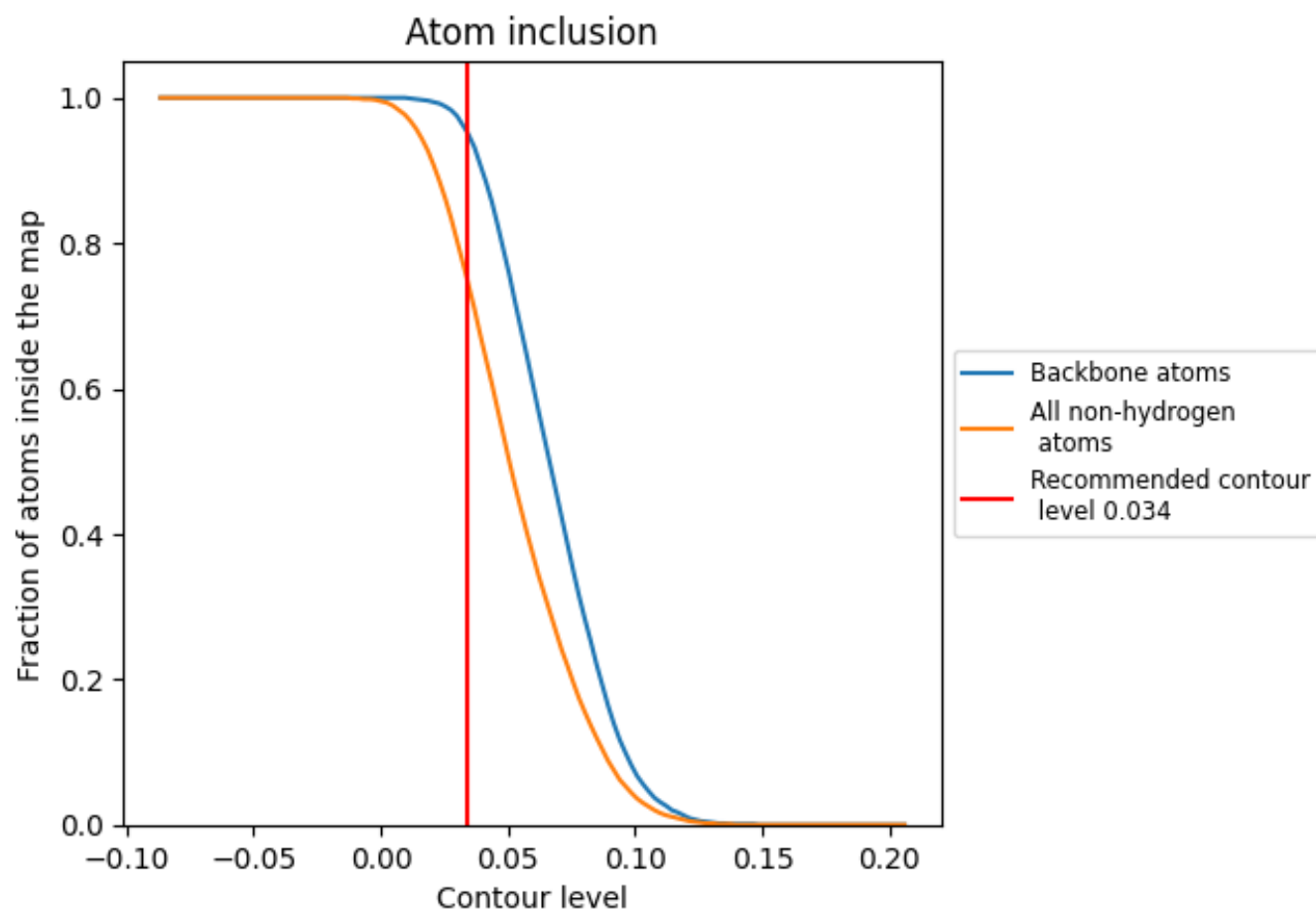
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7510	 0.3670
0	 0.4640	 0.2010
1	 0.4640	 0.1470
2	 0.5900	 0.1880
3	 0.6070	 0.2680
4	 0.1790	 0.1680
5	 0.5710	 0.2330
6	 0.5600	 0.2810
7	 0.4870	 0.2990
8	 0.5320	 0.3290
9	 0.6890	 0.3110
A	 0.7770	 0.3800
AA	 0.3570	 0.2390
B	 0.7610	 0.3620
BA	 0.5570	 0.2290
C	 0.7850	 0.3860
D	 0.7610	 0.3860
E	 0.7860	 0.3860
F	 0.7710	 0.3890
G	 0.5360	 0.2070
H	 0.8020	 0.3890
I	 0.5640	 0.2900
J	 0.4100	 0.3180
K	 0.4620	 0.2500
L	 0.7220	 0.3370
M	 0.8270	 0.3950
N	 0.7690	 0.3370
O	 0.7230	 0.3550
P	 0.4870	 0.2400
Q	 0.6070	 0.2900
R	 0.7140	 0.3680
S	 0.6150	 0.2730
T	 0.5710	 0.2050
U	 0.5130	 0.2210
V	 0.6670	 0.3260



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
W	 0.4870	 0.3550
X	 0.5360	 0.2820
Y	 0.6960	 0.3470
Z	 0.6440	 0.3150
a	 0.5130	 0.2100
b	 0.3930	 0.2500
c	 0.4290	 0.1540
d	 0.3080	 0.1950
e	 0.5570	 0.3060
f	 0.6510	 0.3170
g	 0.5130	 0.2020
h	 0.5710	 0.3400
i	 0.4620	 0.2990
j	 0.5640	 0.2570
k	 0.4640	 0.3430
l	 0.2860	 0.2700
m	 0.5130	 0.2590
n	 0.6670	 0.3450
o	 0.5710	 0.2520
p	 0.4890	 0.3700
q	 0.5000	 0.2570
r	 0.3210	 0.2000
s	 0.4640	 0.3000
t	 0.5900	 0.2520
u	 0.3930	 0.3080
v	 0.4870	 0.2680
w	 0.6070	 0.3000
x	 0.4720	 0.2700
y	 0.7350	 0.3250
z	 0.4290	 0.2030