



Full wwPDB EM Validation Report ⓘ

Apr 9, 2025 – 06:43 PM EDT

PDB ID : 9BD9 / pdb_00009bd9
EMDB ID : EMD-44447
Title : SARS CoV-2 full-length WT spike protein, 1RBD-up conformation (SPIKE-WT)
Authors : Singh, S.; Hasan, S.S.
Deposited on : 2024-04-11
Resolution : 2.95 Å(reported)
Based on initial model : 7KRR

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:

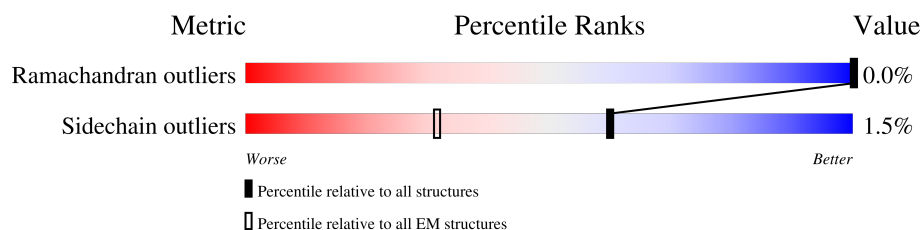
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY






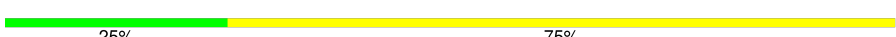
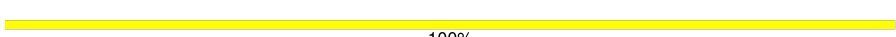


The reported resolution of this entry is 2.95 Å.

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.



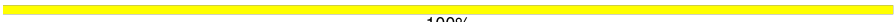
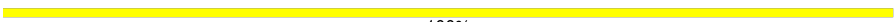
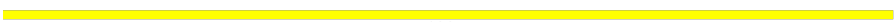
















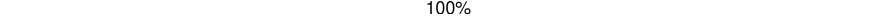

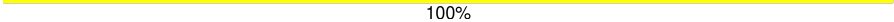
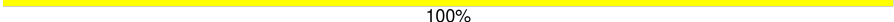

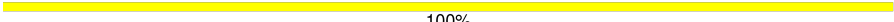
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1312	
1	B	1312	
1	C	1312	
2	D	4	
2	K	4	
2	e	4	
3	E	2	
3	F	2	
3	I	2	


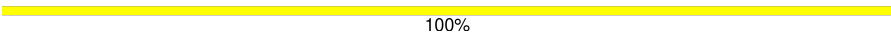

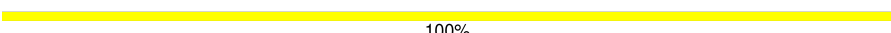
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Mol	Chain	Length	Quality of chain
3	O	2	 100%
3	Q	2	 100%
3	R	2	 100%
3	S	2	 100%
3	a	2	 100%
3	b	2	 100%
3	c	2	 100%
3	d	2	 100%
3	f	2	 100%
4	G	3	 33% 67%
4	H	3	 33% 67%
4	J	3	 33% 67%
4	N	3	 33% 67%
4	P	3	 33% 67%
4	T	3	 33% 67%
4	U	3	 33% 67%
4	g	3	 33% 67%
5	L	3	 33% 67%
5	X	3	 100%
5	i	3	 33% 67%
6	M	5	 100%
7	V	4	 100%
7	W	4	 25% 75%
7	h	4	 100%
7	j	4	 25% 75%

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Mol	Chain	Length	Quality of chain
8	Y	5	 20%80%
9	Z	6	 100%
10	k	2	 50%50%
11	l	2	 100%

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	k	1	X	-	-	-
12	NAG	A	1404	X	-	-	-
3	NAG	F	1	X	-	-	-
7	NAG	h	1	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 51610 atoms, of which 25066 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1032	Total	C	H	N	O	S	0	0
			15871	5148	7822	1337	1528	36		
1	B	1080	Total	C	H	N	O	S	0	0
			16544	5366	8140	1399	1601	38		
1	C	1091	Total	C	H	N	O	S	0	0
			16767	5435	8254	1418	1622	38		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	SER	-	insertion	UNP P0DTC2
A	-19	ALA	-	insertion	UNP P0DTC2
A	-18	TRP	-	insertion	UNP P0DTC2
A	-17	SER	-	insertion	UNP P0DTC2
A	-16	HIS	-	insertion	UNP P0DTC2
A	-15	PRO	-	insertion	UNP P0DTC2
A	-14	GLN	-	insertion	UNP P0DTC2
A	-13	PHE	-	insertion	UNP P0DTC2
A	-12	GLU	-	insertion	UNP P0DTC2
A	-11	LYS	-	insertion	UNP P0DTC2
A	-10	GLY	-	insertion	UNP P0DTC2
A	-9	GLY	-	insertion	UNP P0DTC2
A	-8	GLY	-	insertion	UNP P0DTC2
A	-7	SER	-	insertion	UNP P0DTC2
A	-6	GLY	-	insertion	UNP P0DTC2
A	-5	GLY	-	insertion	UNP P0DTC2
A	-4	GLY	-	insertion	UNP P0DTC2
A	-3	SER	-	insertion	UNP P0DTC2
A	-2	GLY	-	insertion	UNP P0DTC2
A	-1	GLY	-	insertion	UNP P0DTC2
A	0	SER	-	insertion	UNP P0DTC2
A	1	SER	-	insertion	UNP P0DTC2
A	2	ALA	-	insertion	UNP P0DTC2
A	3	TRP	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	-	insertion	UNP P0DTC2
A	5	HIS	-	insertion	UNP P0DTC2
A	6	PRO	-	insertion	UNP P0DTC2
A	7	GLN	-	insertion	UNP P0DTC2
A	8	PHE	-	insertion	UNP P0DTC2
A	9	GLU	-	insertion	UNP P0DTC2
A	10	LYS	-	insertion	UNP P0DTC2
A	11	SER	-	insertion	UNP P0DTC2
A	12	ALA	-	insertion	UNP P0DTC2
A	13	LEU	-	insertion	UNP P0DTC2
A	14	VAL	-	insertion	UNP P0DTC2
A	15	PRO	-	insertion	UNP P0DTC2
A	16	ARG	-	insertion	UNP P0DTC2
A	17	GLY	-	insertion	UNP P0DTC2
A	18	SER	-	insertion	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	-20	SER	-	insertion	UNP P0DTC2
B	-19	ALA	-	insertion	UNP P0DTC2
B	-18	TRP	-	insertion	UNP P0DTC2
B	-17	SER	-	insertion	UNP P0DTC2
B	-16	HIS	-	insertion	UNP P0DTC2
B	-15	PRO	-	insertion	UNP P0DTC2
B	-14	GLN	-	insertion	UNP P0DTC2
B	-13	PHE	-	insertion	UNP P0DTC2
B	-12	GLU	-	insertion	UNP P0DTC2
B	-11	LYS	-	insertion	UNP P0DTC2
B	-10	GLY	-	insertion	UNP P0DTC2
B	-9	GLY	-	insertion	UNP P0DTC2
B	-8	GLY	-	insertion	UNP P0DTC2
B	-7	SER	-	insertion	UNP P0DTC2
B	-6	GLY	-	insertion	UNP P0DTC2
B	-5	GLY	-	insertion	UNP P0DTC2
B	-4	GLY	-	insertion	UNP P0DTC2
B	-3	SER	-	insertion	UNP P0DTC2
B	-2	GLY	-	insertion	UNP P0DTC2
B	-1	GLY	-	insertion	UNP P0DTC2
B	0	SER	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	insertion	UNP P0DTC2
B	2	ALA	-	insertion	UNP P0DTC2
B	3	TRP	-	insertion	UNP P0DTC2
B	4	SER	-	insertion	UNP P0DTC2
B	5	HIS	-	insertion	UNP P0DTC2
B	6	PRO	-	insertion	UNP P0DTC2
B	7	GLN	-	insertion	UNP P0DTC2
B	8	PHE	-	insertion	UNP P0DTC2
B	9	GLU	-	insertion	UNP P0DTC2
B	10	LYS	-	insertion	UNP P0DTC2
B	11	SER	-	insertion	UNP P0DTC2
B	12	ALA	-	insertion	UNP P0DTC2
B	13	LEU	-	insertion	UNP P0DTC2
B	14	VAL	-	insertion	UNP P0DTC2
B	15	PRO	-	insertion	UNP P0DTC2
B	16	ARG	-	insertion	UNP P0DTC2
B	17	GLY	-	insertion	UNP P0DTC2
B	18	SER	-	insertion	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
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B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	-20	SER	-	insertion	UNP P0DTC2
C	-19	ALA	-	insertion	UNP P0DTC2
C	-18	TRP	-	insertion	UNP P0DTC2
C	-17	SER	-	insertion	UNP P0DTC2
C	-16	HIS	-	insertion	UNP P0DTC2
C	-15	PRO	-	insertion	UNP P0DTC2
C	-14	GLN	-	insertion	UNP P0DTC2
C	-13	PHE	-	insertion	UNP P0DTC2
C	-12	GLU	-	insertion	UNP P0DTC2
C	-11	LYS	-	insertion	UNP P0DTC2
C	-10	GLY	-	insertion	UNP P0DTC2
C	-9	GLY	-	insertion	UNP P0DTC2
C	-8	GLY	-	insertion	UNP P0DTC2
C	-7	SER	-	insertion	UNP P0DTC2
C	-6	GLY	-	insertion	UNP P0DTC2
C	-5	GLY	-	insertion	UNP P0DTC2
C	-4	GLY	-	insertion	UNP P0DTC2
C	-3	SER	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	insertion	UNP P0DTC2
C	-1	GLY	-	insertion	UNP P0DTC2
C	0	SER	-	insertion	UNP P0DTC2
C	1	SER	-	insertion	UNP P0DTC2
C	2	ALA	-	insertion	UNP P0DTC2
C	3	TRP	-	insertion	UNP P0DTC2
C	4	SER	-	insertion	UNP P0DTC2
C	5	HIS	-	insertion	UNP P0DTC2
C	6	PRO	-	insertion	UNP P0DTC2
C	7	GLN	-	insertion	UNP P0DTC2
C	8	PHE	-	insertion	UNP P0DTC2
C	9	GLU	-	insertion	UNP P0DTC2
C	10	LYS	-	insertion	UNP P0DTC2
C	11	SER	-	insertion	UNP P0DTC2
C	12	ALA	-	insertion	UNP P0DTC2
C	13	LEU	-	insertion	UNP P0DTC2
C	14	VAL	-	insertion	UNP P0DTC2
C	15	PRO	-	insertion	UNP P0DTC2
C	16	ARG	-	insertion	UNP P0DTC2
C	17	GLY	-	insertion	UNP P0DTC2
C	18	SER	-	insertion	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

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



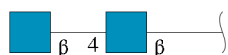
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	4	Total	C	H	N	O	0	0
			93	28	43	2	20		
2	K	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

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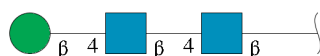
Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	4	Total	C	H	N	O	0	0
			93	28	43	2	20		

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



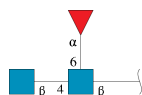
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	2	Total	C	H	N	O	0	0
			40	16	12	2	10		
3	F	2	Total	C	H	N	O	0	0
			39	16	11	2	10		
3	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	O	2	Total	C	H	N	O	0	0
			40	16	12	2	10		
3	Q	2	Total	C	H	N	O	0	0
			40	16	12	2	10		
3	R	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	S	2	Total	C	N	O		0	0
			28	16	2	10			
3	a	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	b	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	c	2	Total	C	H	N	O	0	0
			40	16	12	2	10		
3	d	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	f	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 4 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.



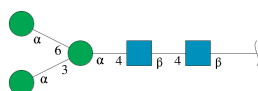
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
4	H	3	Total	C	H	N	O	0	0
			63	22	24	2	15		
4	J	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
4	N	3	Total	C	N	O		0	0
			39	22	2	15			
4	P	3	Total	C	H	N	O	0	0
			73	22	34	2	15		
4	T	3	Total	C	N	O		0	0
			39	22	2	15			
4	U	3	Total	C	N	O		0	0
			39	22	2	15			
4	g	3	Total	C	H	N	O	0	0
			73	22	34	2	15		

- Molecule 5 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
5	L	3	Total	C	H	N	O	0	0
			59	22	21	2	14		
5	X	3	Total	C	N	O		0	0
			38	22	2	14			
5	i	3	Total	C	H	N	O	0	0
			72	22	34	2	14		

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



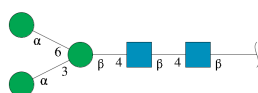
Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 7 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.



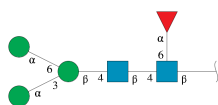
Mol	Chain	Residues	Atoms				AltConf	Trace
7	V	4	Total	C	N	O	0	0
			50	28	2	20		
7	W	4	Total	C	N	O	0	0
			50	28	2	20		
7	h	4	Total	C	H	N	0	0
			93	28	43	2		
7	j	4	Total	C	H	N	0	0
			74	28	24	2		

- Molecule 8 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
8	Y	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 10 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



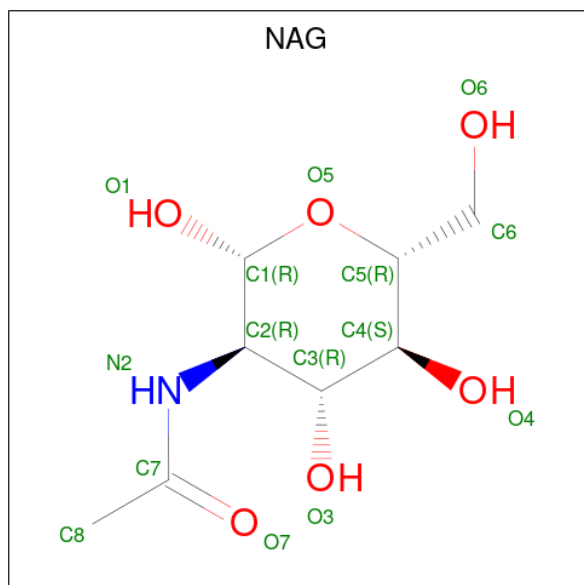
Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	2	Total	C	H	N	O	0	0
			34	14	10	1	9		

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	l	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	A	1	Total	C	H	N	O	0
			26	8	12	1	5	
12	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	A	1	Total	C	N	O		0
			14	8	1	5		
12	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	B	1	Total	C	N	O		0
			14	8	1	5		
12	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
12	C	1	Total	C	N	O		0
			14	8	1	5		

ILE
ALA
ILE
VAL
MET
VAL
THR
MET
LEU
CYS
CYS
MET
THR
SER
CYS
CYS
SER
LEU
GLY
CYS
CYS
SER
CYS
GLY
SER
CYS
CYS
PHE
ASP
GLU
ASP
ASP
SER
SER
GLU
PRO
VAL
LEU
LYS
GLY
VAL
LYS
HIS
HIS
TYR
THR

• Molecule 1: Spike glycoprotein

Chain C:



MET
PHE
VAL
PHE
PRO
LEU
VAL
LEU
LEU
PRO
VAL
SER
SER
GLN
CYS
VAL
ASN
LEU
SER
ALA
TRP
HIS
HIS
CYS
PRO
GLN
PHE
GLU
LYS
GLY
GLY
GLY
SER
GLY
GLY
GLY
SER
GLY
SER
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS
SER
ALA
VAL
PRO
ARG
GLY
SER
THR
ARG

THR
GLN
PRO
PRO
A27
H69
VAL
GLY
THR
ASN
GLY
K77
C196
N137
D138
F139
F140
M153
M165
Y170
M177
G184
N185
Y200
L244
HIS
ARG
SER
TYR
LEU
THR
PRO
GLY
ASP
S254
C301
N317
D586
V622
A626
D627
Q628

N679
SER
PRO
GLY
SER
ALA
SER
S686
Q836
TYR
GLY
ASP
CYS
LEU
GLY
ASP
ILE
ALA
ALA
ARG
D848
P887
E1150
GLU
LEU
ASP
LYS
TYR
PHE
LYS
ASN
HIS
THR
SER
PRO
ASP
VAL
ASP
LEU
LEU
GLY
ASP
ILE
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GLY
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ASN
ALA
SER
VAL
VAL
ASN
ILE
GLN
LYS
GLU
ILE
ASP

ARG
LEU
ASN
GLU
VAL
ALA
LYS
ASN
LEU
CYS
ASN
SER
PHE
ILE
ASP
GLU
ASP
SER
GLN
GLU
LEU
LEU
GLY
LYS
TYR
GLY
VAL
GLN
TYR
ILE
LYS
TRP
TRP
TRP
ILE
TRP
LEU
GLY
PHE
ILE
ALA
GLY
ILE
LEU
ILE
VAL
MET
VAL
THR
THR
ILE
MET
LEU
CYS
CYS
MET
THR
SER
CYS
CYS
SER
GLU
ILE
ASP

LYS
GLY
CYS
CYS
SER
CYS
GLY
SER
SER
CYS
LYS
PHE
ASP
GLU
ASP
SER
GLU
PRO
VAL
LEU
LYS
GLY
VAL
LYS
LEU
HIS
TYR
THR

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

Chain D:



MAG1
MAG2
BMA3
MAN4

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

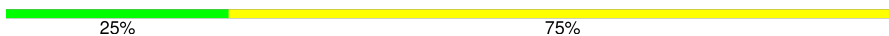
Chain K:



MAG1
MAG2
BMA3
MAN4

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

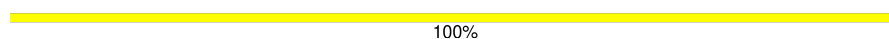
Chain e:



MAG1
MAG2
BMA3
MAN4

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



MAG1
MAG2

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

Chain F:  100%MAG1
MAG2

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

Chain I:  100%MAG1
MAG2

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

Chain O:  100%MAG1
MAG2

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

Chain Q:  100%MAG1
MAG2

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

Chain R:  100%MAG1
MAG2

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

Chain S:  100%MAG1
MAG2

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

Chain a:  100%

MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain d:  100%

MAG1
MAG2

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

Chain f:  100%

MAG1
MAG2

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

Chain G:  33%  67%

MAG1
MAG2
BWA3

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

Chain H:  33%  67%



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

Chain J:



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

Chain N:



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

Chain P:



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

Chain T:



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

Chain U:



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

Chain g:



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33% 67%

MAG1
MAG2
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1
MAG2
FUC3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  33% 67%

MAG1
MAG2
FUC3

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

Chain M:  100%

MAG1
MAG2
MAN3
MAN4
MAN5

- Molecule 7: 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 V:  100%

MAG1
MAG2
EMAN3
MAN4

- Molecule 7: 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 W:  25% 75%

MAG1
MAG2
EMAN3
MAN4

- Molecule 7: 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 h:  100%

MAG1
MAG2
BMA3
MAN4

- Molecule 7: 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 j:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 8: 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:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 9: alpha-D-mannopyranose-(1-3)-[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:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 10: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  50% 50%

MAG1
FUC2

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

Chain l:  100%

MAG1
BMA2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.924	Depositor
Minimum map value	-0.303	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	350.01, 350.01, 350.01	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1667, 1.1667, 1.1667	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, MAN, NAG, FUC

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	0.29	0/8231	0.47	0/11196
1	B	0.29	0/8596	0.47	0/11696
1	C	0.29	0/8711	0.47	0/11854
All	All	0.29	0/25538	0.47	0/34746

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	1014/1312 (77%)	964 (95%)	50 (5%)	0	100	100
1	B	1066/1312 (81%)	1007 (94%)	59 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1081/1312 (82%)	1017 (94%)	63 (6%)	1 (0%)	48	72
All	All	3161/3936 (80%)	2988 (94%)	172 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	987	PRO

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	895/1137 (79%)	877 (98%)	18 (2%)	50	72
1	B	930/1137 (82%)	916 (98%)	14 (2%)	60	78
1	C	946/1137 (83%)	937 (99%)	9 (1%)	73	85
All	All	2771/3411 (81%)	2730 (98%)	41 (2%)	60	78

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASP
1	A	144	TYR
1	A	153	MET
1	A	168	PHE
1	A	282	ASN
1	A	315	THR
1	A	318	PHE
1	A	466	ARG
1	A	530	SER
1	A	571	ASP
1	A	602	THR
1	A	657	ASN
1	A	855	PHE
1	A	937	SER

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Mol	Chain	Res	Type
1	A	955	ASN
1	A	1002	GLN
1	A	1097	SER
1	A	1148	PHE
1	B	28	TYR
1	B	140	PHE
1	B	147	LYS
1	B	186	PHE
1	B	214	ARG
1	B	319	ARG
1	B	427	ASP
1	B	449	TYR
1	B	473	TYR
1	B	505	TYR
1	B	567	ARG
1	B	578	ASP
1	B	848	ASP
1	B	1148	PHE
1	C	140	PHE
1	C	153	MET
1	C	165	ASN
1	C	170	TYR
1	C	177	MET
1	C	200	TYR
1	C	301	CYS
1	C	317	ASN
1	C	586	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	ASN
1	A	762	GLN
1	B	919	ASN
1	C	519	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

105 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$
2	NAG	D	1	1,2	14,14,15	2.02	5 (35%)	17,19,21	1.18	1 (5%)
2	NAG	D	2	2	14,14,15	1.99	4 (28%)	17,19,21	1.01	2 (11%)
2	BMA	D	3	2	11,11,12	0.52	0	15,15,17	0.61	0
2	MAN	D	4	2	11,11,12	0.55	0	15,15,17	1.03	2 (13%)
3	NAG	E	1	1,3	14,14,15	1.95	4 (28%)	17,19,21	2.61	7 (41%)
3	NAG	E	2	3	14,14,15	2.05	4 (28%)	17,19,21	1.09	1 (5%)
3	NAG	F	1	1,3	14,14,15	1.94	4 (28%)	17,19,21	2.74	8 (47%)
3	NAG	F	2	3	14,14,15	2.00	4 (28%)	17,19,21	1.39	2 (11%)
4	NAG	G	1	1,4	14,14,15	2.06	5 (35%)	17,19,21	1.14	2 (11%)
4	NAG	G	2	4	14,14,15	2.01	4 (28%)	17,19,21	1.18	2 (11%)
4	BMA	G	3	4	11,11,12	0.75	0	15,15,17	0.73	0
4	NAG	H	1	1,4	14,14,15	1.98	5 (35%)	17,19,21	1.66	4 (23%)
4	NAG	H	2	4	14,14,15	1.98	4 (28%)	17,19,21	1.32	2 (11%)
4	BMA	H	3	4	11,11,12	0.54	0	15,15,17	0.65	0
3	NAG	I	1	1,3	14,14,15	2.06	5 (35%)	17,19,21	1.16	1 (5%)
3	NAG	I	2	3	14,14,15	2.02	4 (28%)	17,19,21	0.87	1 (5%)
4	NAG	J	1	1,4	14,14,15	1.90	3 (21%)	17,19,21	1.21	2 (11%)
4	NAG	J	2	4	14,14,15	1.92	3 (21%)	17,19,21	1.07	2 (11%)
4	BMA	J	3	4	11,11,12	0.50	0	15,15,17	0.64	0
2	NAG	K	1	1,2	14,14,15	1.89	3 (21%)	17,19,21	1.11	2 (11%)
2	NAG	K	2	2	14,14,15	2.04	4 (28%)	17,19,21	0.84	0
2	BMA	K	3	2	11,11,12	0.56	0	15,15,17	0.67	0
2	MAN	K	4	2	11,11,12	1.19	1 (9%)	15,15,17	1.87	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	L	1	1,5	14,14,15	1.89	3 (21%)	17,19,21	1.55	5 (29%)
5	NAG	L	2	5	14,14,15	1.99	4 (28%)	17,19,21	1.32	2 (11%)
5	FUC	L	3	5	10,10,11	0.56	0	14,14,16	0.69	0
6	NAG	M	1	1,6	14,14,15	1.93	4 (28%)	17,19,21	1.11	2 (11%)
6	NAG	M	2	6	14,14,15	1.86	3 (21%)	17,19,21	1.51	4 (23%)
6	MAN	M	3	6	11,11,12	0.99	1 (9%)	15,15,17	1.01	1 (6%)
6	MAN	M	4	6	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
6	MAN	M	5	6	11,11,12	0.65	0	15,15,17	0.89	1 (6%)
4	NAG	N	1	1,4	14,14,15	2.12	4 (28%)	17,19,21	2.03	5 (29%)
4	NAG	N	2	4	14,14,15	2.09	4 (28%)	17,19,21	1.14	1 (5%)
4	BMA	N	3	4	11,11,12	0.76	0	15,15,17	0.75	0
3	NAG	O	1	1,3	14,14,15	1.96	4 (28%)	17,19,21	1.02	1 (5%)
3	NAG	O	2	3	14,14,15	2.04	4 (28%)	17,19,21	1.14	2 (11%)
4	NAG	P	1	1,4	14,14,15	1.97	4 (28%)	17,19,21	1.23	2 (11%)
4	NAG	P	2	4	14,14,15	2.02	4 (28%)	17,19,21	0.96	1 (5%)
4	BMA	P	3	4	11,11,12	0.52	0	15,15,17	0.67	0
3	NAG	Q	1	1,3	14,14,15	1.92	3 (21%)	17,19,21	1.62	3 (17%)
3	NAG	Q	2	3	14,14,15	1.98	4 (28%)	17,19,21	1.11	2 (11%)
3	NAG	R	1	1,3	14,14,15	1.96	4 (28%)	17,19,21	1.18	2 (11%)
3	NAG	R	2	3	14,14,15	2.01	4 (28%)	17,19,21	1.04	2 (11%)
3	NAG	S	1	1,3	14,14,15	2.42	4 (28%)	17,19,21	1.99	5 (29%)
3	NAG	S	2	3	14,14,15	2.13	4 (28%)	17,19,21	1.26	2 (11%)
4	NAG	T	1	1,4	14,14,15	1.94	3 (21%)	17,19,21	1.20	2 (11%)
4	NAG	T	2	4	14,14,15	2.01	4 (28%)	17,19,21	1.00	1 (5%)
4	BMA	T	3	4	11,11,12	0.54	0	15,15,17	0.71	0
4	NAG	U	1	1,4	14,14,15	2.04	4 (28%)	17,19,21	1.63	3 (17%)
4	NAG	U	2	4	14,14,15	1.99	4 (28%)	17,19,21	1.19	2 (11%)
4	BMA	U	3	4	11,11,12	0.51	0	15,15,17	0.66	0
7	NAG	V	1	1,7	14,14,15	1.94	5 (35%)	17,19,21	1.14	2 (11%)
7	NAG	V	2	7	14,14,15	1.98	4 (28%)	17,19,21	1.22	2 (11%)
7	BMA	V	3	7	11,11,12	0.87	0	15,15,17	1.31	2 (13%)
7	MAN	V	4	7	11,11,12	0.56	0	15,15,17	0.95	2 (13%)
7	NAG	W	1	1,7	14,14,15	1.90	3 (21%)	17,19,21	1.17	2 (11%)
7	NAG	W	2	7	14,14,15	1.99	4 (28%)	17,19,21	0.96	1 (5%)
7	BMA	W	3	7	11,11,12	0.59	0	15,15,17	0.67	0
7	MAN	W	4	7	11,11,12	1.08	1 (9%)	15,15,17	1.65	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	X	1	1,5	14,14,15	2.05	4 (28%)	17,19,21	1.09	1 (5%)
5	NAG	X	2	5	14,14,15	1.99	4 (28%)	17,19,21	1.12	2 (11%)
5	FUC	X	3	5	10,10,11	0.80	0	14,14,16	0.91	1 (7%)
8	NAG	Y	1	1,8	14,14,15	2.00	5 (35%)	17,19,21	1.25	2 (11%)
8	NAG	Y	2	8	14,14,15	2.04	4 (28%)	17,19,21	1.24	3 (17%)
8	BMA	Y	3	8	11,11,12	0.72	0	15,15,17	0.92	0
8	MAN	Y	4	8	11,11,12	0.66	0	15,15,17	0.91	2 (13%)
8	MAN	Y	5	8	11,11,12	1.03	1 (9%)	15,15,17	1.31	3 (20%)
9	NAG	Z	1	1,9	14,14,15	1.93	4 (28%)	17,19,21	1.31	4 (23%)
9	NAG	Z	2	9	14,14,15	1.94	4 (28%)	17,19,21	1.27	2 (11%)
9	BMA	Z	3	9	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
9	MAN	Z	4	9	11,11,12	0.62	0	15,15,17	1.03	2 (13%)
9	MAN	Z	5	9	11,11,12	0.57	0	15,15,17	0.99	2 (13%)
9	FUC	Z	6	9	10,10,11	1.17	1 (10%)	14,14,16	1.63	3 (21%)
3	NAG	a	1	1,3	14,14,15	2.02	4 (28%)	17,19,21	1.10	2 (11%)
3	NAG	a	2	3	14,14,15	1.99	4 (28%)	17,19,21	1.03	1 (5%)
3	NAG	b	1	1,3	14,14,15	1.93	4 (28%)	17,19,21	1.21	2 (11%)
3	NAG	b	2	3	14,14,15	2.03	4 (28%)	17,19,21	1.07	1 (5%)
3	NAG	c	1	1,3	14,14,15	2.07	4 (28%)	17,19,21	2.32	5 (29%)
3	NAG	c	2	3	14,14,15	1.99	4 (28%)	17,19,21	1.16	2 (11%)
3	NAG	d	1	1,3	14,14,15	1.97	3 (21%)	17,19,21	1.40	1 (5%)
3	NAG	d	2	3	14,14,15	1.97	3 (21%)	17,19,21	1.52	2 (11%)
2	NAG	e	1	1,2	14,14,15	1.95	4 (28%)	17,19,21	1.20	2 (11%)
2	NAG	e	2	2	14,14,15	1.93	4 (28%)	17,19,21	1.94	5 (29%)
2	BMA	e	3	2	11,11,12	0.61	0	15,15,17	0.77	0
2	MAN	e	4	2	11,11,12	0.71	0	15,15,17	1.53	2 (13%)
3	NAG	f	1	1,3	14,14,15	1.96	4 (28%)	17,19,21	1.50	2 (11%)
3	NAG	f	2	3	14,14,15	1.97	4 (28%)	17,19,21	1.26	1 (5%)
4	NAG	g	1	1,4	14,14,15	1.93	4 (28%)	17,19,21	1.15	2 (11%)
4	NAG	g	2	4	14,14,15	1.93	4 (28%)	17,19,21	1.15	1 (5%)
4	BMA	g	3	4	11,11,12	0.50	0	15,15,17	0.69	0
7	NAG	h	1	1,7	14,14,15	1.95	3 (21%)	17,19,21	2.50	7 (41%)
7	NAG	h	2	7	14,14,15	2.00	4 (28%)	17,19,21	1.58	2 (11%)
7	BMA	h	3	7	11,11,12	1.02	1 (9%)	15,15,17	0.90	1 (6%)
7	MAN	h	4	7	11,11,12	0.64	0	15,15,17	0.91	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	i	1	1,5	14,14,15	1.92	4 (28%)	17,19,21	1.81	4 (23%)
5	NAG	i	2	5	14,14,15	1.99	4 (28%)	17,19,21	1.17	2 (11%)
5	FUC	i	3	5	10,10,11	0.83	0	14,14,16	0.72	0
7	NAG	j	1	1,7	14,14,15	1.91	3 (21%)	17,19,21	1.19	2 (11%)
7	NAG	j	2	7	14,14,15	1.93	4 (28%)	17,19,21	1.20	2 (11%)
7	BMA	j	3	7	11,11,12	0.53	0	15,15,17	0.73	0
7	MAN	j	4	7	11,11,12	1.05	1 (9%)	15,15,17	1.35	3 (20%)
10	NAG	k	1	1,10	14,14,15	2.19	4 (28%)	17,19,21	3.05	11 (64%)
10	FUC	k	2	10	10,10,11	0.62	0	14,14,16	0.81	0
11	NAG	l	1	11	14,14,15	2.11	5 (35%)	17,19,21	1.76	3 (17%)
11	BMA	l	2	11	11,11,12	0.60	0	15,15,17	1.00	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	F	1	1,3	1/1/6/7	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	BMA	H	3	4	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	MAN	K	4	2	-	2/2/19/22	0/1/1/1
5	NAG	L	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1
6	NAG	M	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	M	2	6	-	1/6/23/26	0/1/1/1
6	MAN	M	3	6	-	2/2/19/22	1/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	MAN	M	5	6	-	2/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	1/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	3/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	4/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
4	NAG	U	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1
4	BMA	U	3	4	-	0/2/19/22	0/1/1/1
7	NAG	V	1	1,7	-	3/6/23/26	0/1/1/1
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
7	BMA	V	3	7	-	1/2/19/22	0/1/1/1
7	MAN	V	4	7	-	0/2/19/22	1/1/1/1
7	NAG	W	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	W	2	7	-	4/6/23/26	0/1/1/1
7	BMA	W	3	7	-	2/2/19/22	0/1/1/1
7	MAN	W	4	7	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	X	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	1/6/23/26	0/1/1/1
5	FUC	X	3	5	-	-	0/1/1/1
8	NAG	Y	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	1/1/1/1
8	MAN	Y	5	8	-	2/2/19/22	0/1/1/1
9	NAG	Z	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	2/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	0/2/19/22	1/1/1/1
9	MAN	Z	5	9	-	0/2/19/22	0/1/1/1
9	FUC	Z	6	9	-	-	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	1/6/23/26	0/1/1/1
3	NAG	c	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1
2	BMA	e	3	2	-	1/2/19/22	0/1/1/1
2	MAN	e	4	2	-	0/2/19/22	1/1/1/1
3	NAG	f	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
4	NAG	g	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	BMA	g	3	4	-	1/2/19/22	0/1/1/1
7	NAG	h	1	1,7	1/1/6/7	1/6/23/26	0/1/1/1
7	NAG	h	2	7	-	1/6/23/26	0/1/1/1
7	BMA	h	3	7	-	2/2/19/22	0/1/1/1
7	MAN	h	4	7	-	0/2/19/22	0/1/1/1
5	NAG	i	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	i	2	5	-	2/6/23/26	0/1/1/1
5	FUC	i	3	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	j	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	j	2	7	-	2/6/23/26	0/1/1/1
7	BMA	j	3	7	-	0/2/19/22	0/1/1/1
7	MAN	j	4	7	-	0/2/19/22	0/1/1/1
10	NAG	k	1	1,10	1/1/6/7	4/6/23/26	0/1/1/1
10	FUC	k	2	10	-	-	0/1/1/1
11	NAG	l	1	11	-	5/6/23/26	0/1/1/1
11	BMA	l	2	11	-	1/2/19/22	0/1/1/1

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	1	NAG	O5-C1	5.38	1.52	1.43
10	k	1	NAG	O5-C1	4.67	1.51	1.43
4	N	2	NAG	O5-C1	4.62	1.51	1.43
4	N	1	NAG	O5-C1	4.62	1.51	1.43
5	X	1	NAG	O5-C1	4.57	1.51	1.43
3	b	2	NAG	O5-C1	4.56	1.51	1.43
3	O	2	NAG	O5-C1	4.55	1.51	1.43
3	S	2	NAG	O5-C1	4.54	1.51	1.43
3	E	2	NAG	O5-C1	4.53	1.51	1.43
4	G	1	NAG	O5-C1	4.44	1.51	1.43
3	I	1	NAG	O5-C1	4.43	1.51	1.43
4	G	2	NAG	O5-C1	4.42	1.51	1.43
8	Y	2	NAG	O5-C1	4.42	1.51	1.43
2	K	2	NAG	O5-C1	4.41	1.51	1.43
7	h	1	NAG	O5-C1	4.40	1.51	1.43
3	c	1	NAG	O5-C1	4.40	1.51	1.43
4	U	1	NAG	O5-C1	4.38	1.51	1.43
2	D	2	NAG	O5-C1	4.34	1.51	1.43
11	l	1	NAG	O5-C1	4.34	1.51	1.43
3	I	2	NAG	O5-C1	4.34	1.51	1.43
4	T	2	NAG	O5-C1	4.33	1.51	1.43
4	P	2	NAG	O5-C1	4.33	1.51	1.43
3	R	2	NAG	O5-C1	4.32	1.51	1.43
3	a	1	NAG	O5-C1	4.32	1.51	1.43
4	H	2	NAG	O5-C1	4.32	1.50	1.43
8	Y	1	NAG	O5-C1	4.29	1.50	1.43
5	L	2	NAG	O5-C1	4.29	1.50	1.43
2	D	1	NAG	O5-C1	4.28	1.50	1.43
3	c	2	NAG	O5-C1	4.28	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	2	NAG	O5-C1	4.27	1.50	1.43
3	a	2	NAG	O5-C1	4.26	1.50	1.43
7	h	2	NAG	O5-C1	4.26	1.50	1.43
7	V	2	NAG	O5-C1	4.25	1.50	1.43
2	e	1	NAG	O5-C1	4.25	1.50	1.43
7	W	2	NAG	O5-C1	4.24	1.50	1.43
4	P	1	NAG	O5-C1	4.22	1.50	1.43
5	i	2	NAG	O5-C1	4.21	1.50	1.43
3	R	1	NAG	O5-C1	4.21	1.50	1.43
4	U	2	NAG	O5-C1	4.20	1.50	1.43
3	f	1	NAG	O5-C1	4.19	1.50	1.43
5	X	2	NAG	O5-C1	4.19	1.50	1.43
3	d	2	NAG	O5-C1	4.16	1.50	1.43
3	f	2	NAG	O5-C1	4.14	1.50	1.43
3	F	2	NAG	O5-C1	4.14	1.50	1.43
3	d	1	NAG	O5-C1	4.13	1.50	1.43
9	Z	2	NAG	O5-C1	4.13	1.50	1.43
7	W	1	NAG	O5-C1	4.13	1.50	1.43
3	E	1	NAG	C7-N2	4.10	1.47	1.34
3	b	1	NAG	O5-C1	4.09	1.50	1.43
9	Z	1	NAG	O5-C1	4.09	1.50	1.43
7	j	2	NAG	O5-C1	4.08	1.50	1.43
4	T	1	NAG	O5-C1	4.08	1.50	1.43
7	V	1	NAG	O5-C1	4.08	1.50	1.43
10	k	1	NAG	C7-N2	4.08	1.47	1.34
3	O	1	NAG	O5-C1	4.08	1.50	1.43
6	M	1	NAG	O5-C1	4.07	1.50	1.43
4	g	1	NAG	O5-C1	4.06	1.50	1.43
3	c	1	NAG	C7-N2	4.04	1.47	1.34
7	j	1	NAG	O5-C1	4.03	1.50	1.43
4	N	1	NAG	C7-N2	4.03	1.47	1.34
4	g	2	NAG	O5-C1	4.02	1.50	1.43
3	S	2	NAG	C7-N2	4.02	1.47	1.34
4	J	2	NAG	O5-C1	4.01	1.50	1.43
4	H	1	NAG	O5-C1	4.00	1.50	1.43
4	J	1	NAG	O5-C1	4.00	1.50	1.43
3	d	1	NAG	C7-N2	3.99	1.47	1.34
3	S	1	NAG	O5-C5	3.99	1.51	1.43
4	U	1	NAG	C7-N2	3.97	1.47	1.34
3	S	1	NAG	C7-N2	3.96	1.47	1.34
3	I	1	NAG	C7-N2	3.96	1.47	1.34
11	l	1	NAG	C7-N2	3.95	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	NAG	C7-N2	3.94	1.47	1.34
3	d	2	NAG	C7-N2	3.94	1.47	1.34
2	e	2	NAG	C7-N2	3.93	1.47	1.34
3	Q	1	NAG	O5-C1	3.92	1.50	1.43
3	O	1	NAG	C7-N2	3.92	1.47	1.34
4	U	2	NAG	C7-N2	3.92	1.47	1.34
2	K	1	NAG	O5-C1	3.92	1.50	1.43
2	D	1	NAG	C7-N2	3.91	1.47	1.34
3	F	1	NAG	C7-N2	3.91	1.47	1.34
3	R	2	NAG	C7-N2	3.91	1.47	1.34
8	Y	2	NAG	C7-N2	3.90	1.46	1.34
3	a	1	NAG	C7-N2	3.90	1.46	1.34
4	N	2	NAG	C7-N2	3.90	1.46	1.34
5	X	2	NAG	C7-N2	3.90	1.46	1.34
3	a	2	NAG	C7-N2	3.90	1.46	1.34
3	F	2	NAG	C7-N2	3.89	1.46	1.34
3	I	2	NAG	C7-N2	3.89	1.46	1.34
4	P	2	NAG	C7-N2	3.88	1.46	1.34
5	X	1	NAG	C7-N2	3.88	1.46	1.34
3	E	2	NAG	C7-N2	3.88	1.46	1.34
3	c	2	NAG	C7-N2	3.87	1.46	1.34
3	f	2	NAG	C7-N2	3.87	1.46	1.34
7	W	2	NAG	C7-N2	3.87	1.46	1.34
5	L	2	NAG	C7-N2	3.87	1.46	1.34
4	T	1	NAG	C7-N2	3.86	1.46	1.34
3	R	1	NAG	C7-N2	3.86	1.46	1.34
3	O	2	NAG	C7-N2	3.86	1.46	1.34
5	i	1	NAG	C7-N2	3.86	1.46	1.34
5	i	2	NAG	C7-N2	3.86	1.46	1.34
7	h	2	NAG	C7-N2	3.85	1.46	1.34
3	Q	2	NAG	C7-N2	3.85	1.46	1.34
4	G	2	NAG	C7-N2	3.85	1.46	1.34
4	H	1	NAG	C7-N2	3.85	1.46	1.34
4	P	1	NAG	C7-N2	3.85	1.46	1.34
2	D	2	NAG	C7-N2	3.85	1.46	1.34
3	b	2	NAG	C7-N2	3.84	1.46	1.34
5	i	1	NAG	O5-C1	3.84	1.50	1.43
4	T	2	NAG	C7-N2	3.83	1.46	1.34
4	g	2	NAG	C7-N2	3.83	1.46	1.34
4	G	1	NAG	C7-N2	3.83	1.46	1.34
9	Z	2	NAG	C7-N2	3.83	1.46	1.34
6	M	2	NAG	C7-N2	3.83	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NAG	C7-N2	3.82	1.46	1.34
4	J	2	NAG	C7-N2	3.81	1.46	1.34
7	V	2	NAG	C7-N2	3.81	1.46	1.34
7	j	2	NAG	C7-N2	3.81	1.46	1.34
3	f	1	NAG	C7-N2	3.81	1.46	1.34
5	L	1	NAG	C7-N2	3.80	1.46	1.34
6	M	1	NAG	C7-N2	3.79	1.46	1.34
8	Y	1	NAG	C7-N2	3.78	1.46	1.34
4	J	1	NAG	C7-N2	3.78	1.46	1.34
3	b	1	NAG	C7-N2	3.78	1.46	1.34
4	g	1	NAG	C7-N2	3.78	1.46	1.34
3	Q	1	NAG	C7-N2	3.78	1.46	1.34
2	e	1	NAG	C7-N2	3.77	1.46	1.34
9	Z	1	NAG	C7-N2	3.77	1.46	1.34
7	j	1	NAG	C7-N2	3.77	1.46	1.34
7	h	1	NAG	C7-N2	3.76	1.46	1.34
2	K	1	NAG	C7-N2	3.75	1.46	1.34
7	W	1	NAG	C7-N2	3.72	1.46	1.34
5	L	1	NAG	O5-C1	3.72	1.49	1.43
6	M	2	NAG	O5-C1	3.71	1.49	1.43
7	V	1	NAG	C7-N2	3.70	1.46	1.34
3	F	1	NAG	O5-C1	3.67	1.49	1.43
2	e	2	NAG	O5-C1	3.61	1.49	1.43
3	E	1	NAG	O5-C1	3.56	1.49	1.43
10	k	1	NAG	C2-N2	3.33	1.51	1.46
7	j	4	MAN	C1-C2	3.17	1.59	1.52
9	Z	6	FUC	C1-C2	3.15	1.59	1.52
7	h	3	BMA	C1-C2	3.07	1.59	1.52
8	Y	5	MAN	C1-C2	3.03	1.59	1.52
2	K	4	MAN	C1-C2	3.01	1.59	1.52
3	S	2	NAG	C2-N2	2.88	1.51	1.46
3	Q	1	NAG	C2-N2	2.84	1.51	1.46
11	l	1	NAG	C2-N2	2.83	1.50	1.46
4	N	1	NAG	O5-C5	2.76	1.48	1.43
3	E	1	NAG	C2-N2	2.70	1.50	1.46
4	U	1	NAG	C2-N2	2.67	1.50	1.46
2	K	2	NAG	C2-N2	2.63	1.50	1.46
4	N	2	NAG	O5-C5	2.63	1.48	1.43
3	c	1	NAG	C2-N2	2.61	1.50	1.46
2	e	2	NAG	C2-N2	2.60	1.50	1.46
5	L	1	NAG	C2-N2	2.57	1.50	1.46
3	I	2	NAG	C2-N2	2.57	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	f	2	NAG	C2-N2	2.55	1.50	1.46
3	O	1	NAG	C2-N2	2.54	1.50	1.46
3	F	1	NAG	O5-C5	2.53	1.48	1.43
3	d	1	NAG	C2-N2	2.53	1.50	1.46
4	P	2	NAG	C2-N2	2.53	1.50	1.46
7	W	4	MAN	C1-C2	2.51	1.58	1.52
8	Y	2	NAG	C2-N2	2.51	1.50	1.46
3	d	2	NAG	C2-N2	2.50	1.50	1.46
5	X	2	NAG	C2-N2	2.50	1.50	1.46
3	E	2	NAG	C2-N2	2.50	1.50	1.46
4	U	2	NAG	C2-N2	2.50	1.50	1.46
3	F	2	NAG	C2-N2	2.49	1.50	1.46
11	l	1	NAG	O5-C5	2.49	1.48	1.43
3	R	2	NAG	C2-N2	2.49	1.50	1.46
7	W	2	NAG	C2-N2	2.49	1.50	1.46
3	a	2	NAG	C2-N2	2.48	1.50	1.46
7	h	2	NAG	C2-N2	2.48	1.50	1.46
3	I	1	NAG	C2-N2	2.48	1.50	1.46
4	G	2	NAG	C2-N2	2.47	1.50	1.46
3	S	1	NAG	C2-N2	2.47	1.50	1.46
3	a	1	NAG	C2-N2	2.46	1.50	1.46
5	L	2	NAG	C2-N2	2.46	1.50	1.46
3	c	2	NAG	C2-N2	2.45	1.50	1.46
3	O	2	NAG	C2-N2	2.44	1.50	1.46
4	T	2	NAG	C2-N2	2.44	1.50	1.46
2	D	1	NAG	C2-N2	2.43	1.50	1.46
5	i	2	NAG	C2-N2	2.43	1.50	1.46
3	Q	2	NAG	C2-N2	2.41	1.50	1.46
4	T	1	NAG	C2-N2	2.40	1.50	1.46
3	b	2	NAG	C2-N2	2.40	1.50	1.46
2	D	2	NAG	C2-N2	2.39	1.50	1.46
4	J	2	NAG	C2-N2	2.39	1.50	1.46
3	F	2	NAG	O5-C5	2.39	1.48	1.43
9	Z	2	NAG	C2-N2	2.39	1.50	1.46
3	R	1	NAG	C2-N2	2.38	1.50	1.46
3	c	1	NAG	O5-C5	2.38	1.48	1.43
4	P	1	NAG	C2-N2	2.37	1.50	1.46
4	g	2	NAG	C2-N2	2.37	1.50	1.46
7	V	2	NAG	C2-N2	2.37	1.50	1.46
5	X	1	NAG	C2-N2	2.37	1.50	1.46
4	H	1	NAG	C2-N2	2.36	1.50	1.46
3	F	1	NAG	C2-N2	2.36	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	2	NAG	C2-N2	2.36	1.50	1.46
4	G	1	NAG	O5-C5	2.35	1.48	1.43
4	G	1	NAG	C2-N2	2.33	1.50	1.46
3	b	1	NAG	C2-N2	2.32	1.50	1.46
8	Y	1	NAG	O5-C5	2.32	1.48	1.43
3	f	1	NAG	C2-N2	2.32	1.50	1.46
5	X	1	NAG	O5-C5	2.32	1.48	1.43
4	H	2	NAG	C2-N2	2.32	1.50	1.46
7	j	2	NAG	C2-N2	2.32	1.50	1.46
2	e	1	NAG	C2-N2	2.32	1.50	1.46
5	i	1	NAG	O5-C5	2.31	1.47	1.43
4	T	2	NAG	O5-C5	2.30	1.47	1.43
5	i	1	NAG	C2-N2	2.29	1.50	1.46
3	a	1	NAG	O5-C5	2.28	1.47	1.43
3	E	2	NAG	O5-C5	2.27	1.47	1.43
3	S	2	NAG	O5-C5	2.27	1.47	1.43
3	I	1	NAG	O5-C5	2.27	1.47	1.43
4	P	2	NAG	O5-C5	2.26	1.47	1.43
4	N	2	NAG	C2-N2	2.26	1.50	1.46
3	I	2	NAG	O5-C5	2.26	1.47	1.43
5	i	2	NAG	O5-C5	2.26	1.47	1.43
4	G	2	NAG	O5-C5	2.25	1.47	1.43
6	M	1	NAG	C2-N2	2.25	1.50	1.46
3	R	2	NAG	O5-C5	2.25	1.47	1.43
7	h	1	NAG	C2-N2	2.24	1.50	1.46
2	K	1	NAG	C2-N2	2.24	1.50	1.46
2	e	2	NAG	O5-C5	2.24	1.47	1.43
3	f	1	NAG	O5-C5	2.23	1.47	1.43
7	V	1	NAG	C2-N2	2.23	1.49	1.46
5	L	2	NAG	O5-C5	2.22	1.47	1.43
7	j	1	NAG	C2-N2	2.21	1.49	1.46
3	c	2	NAG	O5-C5	2.21	1.47	1.43
4	U	2	NAG	O5-C5	2.21	1.47	1.43
4	J	1	NAG	C2-N2	2.21	1.49	1.46
4	g	1	NAG	C2-N2	2.20	1.49	1.46
3	f	2	NAG	O5-C5	2.20	1.47	1.43
4	P	1	NAG	O5-C5	2.20	1.47	1.43
4	N	1	NAG	C2-N2	2.19	1.49	1.46
9	Z	1	NAG	C2-N2	2.19	1.49	1.46
8	Y	1	NAG	C3-C2	-2.19	1.47	1.52
8	Y	1	NAG	C2-N2	2.18	1.49	1.46
4	H	1	NAG	O5-C5	2.18	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	k	1	NAG	O5-C5	2.17	1.47	1.43
3	I	1	NAG	C3-C2	-2.17	1.48	1.52
4	H	1	NAG	C3-C2	-2.16	1.48	1.52
7	V	1	NAG	O5-C5	2.16	1.47	1.43
11	l	1	NAG	C3-C2	-2.16	1.48	1.52
3	a	2	NAG	O5-C5	2.15	1.47	1.43
5	X	2	NAG	O5-C5	2.15	1.47	1.43
7	W	1	NAG	C2-N2	2.15	1.49	1.46
3	Q	2	NAG	O5-C5	2.15	1.47	1.43
3	b	2	NAG	O5-C5	2.15	1.47	1.43
7	V	1	NAG	C3-C2	-2.14	1.48	1.52
7	V	2	NAG	O5-C5	2.14	1.47	1.43
3	O	2	NAG	O5-C5	2.13	1.47	1.43
2	D	1	NAG	C3-C2	-2.13	1.48	1.52
2	K	2	NAG	O5-C5	2.12	1.47	1.43
6	M	3	MAN	C1-C2	2.11	1.57	1.52
3	R	1	NAG	O5-C5	2.10	1.47	1.43
4	H	2	NAG	O5-C5	2.10	1.47	1.43
8	Y	2	NAG	O5-C5	2.09	1.47	1.43
7	W	2	NAG	O5-C5	2.08	1.47	1.43
2	D	2	NAG	O5-C5	2.08	1.47	1.43
6	M	1	NAG	O5-C5	2.07	1.47	1.43
3	b	1	NAG	O5-C5	2.06	1.47	1.43
3	O	1	NAG	O5-C5	2.06	1.47	1.43
4	G	1	NAG	C3-C2	-2.05	1.48	1.52
4	g	2	NAG	O5-C5	2.05	1.47	1.43
9	Z	1	NAG	O5-C5	2.05	1.47	1.43
9	Z	2	NAG	O5-C5	2.04	1.47	1.43
3	E	1	NAG	O5-C5	2.04	1.47	1.43
7	j	2	NAG	O5-C5	2.03	1.47	1.43
7	h	2	NAG	O5-C5	2.03	1.47	1.43
2	D	1	NAG	O5-C5	2.03	1.47	1.43
4	U	1	NAG	O5-C5	2.02	1.47	1.43
4	g	1	NAG	O5-C5	2.02	1.47	1.43
2	e	1	NAG	O5-C5	2.02	1.47	1.43

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	4	MAN	C1-O5-C5	6.29	120.62	112.19
10	k	1	NAG	C3-C4-C5	5.98	121.07	110.23
3	F	1	NAG	C1-O5-C5	-5.95	104.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	W	4	MAN	C1-O5-C5	5.51	119.58	112.19
3	c	1	NAG	O5-C5-C6	5.36	118.10	107.66
4	N	1	NAG	C1-O5-C5	5.34	119.34	112.19
3	E	1	NAG	C1-O5-C5	-5.29	105.09	112.19
3	F	1	NAG	O5-C5-C6	5.29	117.96	107.66
7	h	1	NAG	C4-C3-C2	5.29	118.77	111.02
7	h	1	NAG	O3-C3-C2	5.08	119.95	109.40
5	i	1	NAG	C1-O5-C5	-5.05	105.41	112.19
3	E	1	NAG	C3-C4-C5	5.00	119.30	110.23
2	e	2	NAG	C3-C4-C5	4.95	119.21	110.23
2	e	4	MAN	C1-O5-C5	4.83	118.66	112.19
10	k	1	NAG	C8-C7-N2	4.82	124.11	116.12
3	c	1	NAG	O5-C5-C4	4.67	122.18	110.83
3	E	1	NAG	C8-C7-N2	4.61	123.77	116.12
3	S	1	NAG	O5-C5-C6	4.53	116.48	107.66
3	F	1	NAG	O5-C5-C4	4.42	121.58	110.83
10	k	1	NAG	C1-O5-C5	4.34	118.00	112.19
3	Q	1	NAG	C1-C2-N2	4.28	117.18	110.43
7	h	2	NAG	C4-C3-C2	4.20	117.18	111.02
10	k	1	NAG	O5-C1-C2	4.19	117.78	111.29
3	f	1	NAG	C1-O5-C5	-4.11	106.68	112.19
7	h	1	NAG	O3-C3-C4	4.09	120.01	110.38
4	U	1	NAG	C8-C7-N2	4.05	122.84	116.12
3	d	1	NAG	C8-C7-N2	4.00	122.76	116.12
10	k	1	NAG	O4-C4-C5	3.83	118.76	109.32
3	S	1	NAG	C1-O5-C5	-3.79	107.11	112.19
3	E	1	NAG	C4-C3-C2	3.77	116.54	111.02
11	l	1	NAG	C8-C7-N2	3.58	122.06	116.12
3	F	1	NAG	C3-C4-C5	3.57	116.71	110.23
10	k	1	NAG	O4-C4-C3	3.54	118.73	110.38
9	Z	6	FUC	C1-O5-C5	3.53	121.30	112.97
4	H	1	NAG	C1-O5-C5	3.45	116.81	112.19
3	d	2	NAG	C1-O5-C5	-3.44	107.57	112.19
4	U	1	NAG	C2-N2-C7	3.41	127.47	122.90
3	c	1	NAG	C8-C7-N2	3.38	121.72	116.12
7	V	3	BMA	C1-O5-C5	3.36	116.68	112.19
4	G	1	NAG	C8-C7-N2	3.32	121.62	116.12
2	D	1	NAG	C8-C7-N2	3.22	121.45	116.12
4	H	2	NAG	C2-N2-C7	-3.20	118.61	122.90
8	Y	1	NAG	C2-N2-C7	-3.14	118.70	122.90
3	F	2	NAG	C8-C7-N2	3.10	121.26	116.12
7	j	4	MAN	C1-O5-C5	3.09	116.32	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1	NAG	O5-C1-C2	-3.08	106.53	111.29
3	I	1	NAG	C8-C7-N2	3.06	121.20	116.12
2	e	2	NAG	C4-C3-C2	3.04	115.48	111.02
8	Y	5	MAN	C1-O5-C5	3.03	116.25	112.19
3	d	2	NAG	C8-C7-N2	3.00	121.09	116.12
5	i	1	NAG	C3-C4-C5	2.92	115.53	110.23
11	l	1	NAG	O4-C4-C5	2.90	116.47	109.32
4	H	2	NAG	C8-C7-N2	2.85	120.84	116.12
2	D	4	MAN	C1-O5-C5	2.85	116.00	112.19
9	Z	1	NAG	C2-N2-C7	-2.85	119.08	122.90
9	Z	6	FUC	C1-C2-C3	2.84	113.79	109.64
4	H	1	NAG	O4-C4-C3	-2.83	103.69	110.38
9	Z	4	MAN	C1-O5-C5	2.81	115.95	112.19
10	k	1	NAG	C2-N2-C7	2.81	126.66	122.90
4	N	1	NAG	C8-C7-N2	2.80	120.76	116.12
6	M	4	MAN	C1-O5-C5	2.80	115.93	112.19
9	Z	3	BMA	C1-O5-C5	2.79	115.92	112.19
3	S	1	NAG	C8-C7-N2	2.78	120.73	116.12
7	V	2	NAG	C2-N2-C7	-2.77	119.19	122.90
7	j	4	MAN	C1-C2-C3	2.74	113.63	109.64
8	Y	2	NAG	C2-N2-C7	-2.68	119.31	122.90
2	e	1	NAG	C2-N2-C7	-2.67	119.32	122.90
2	e	2	NAG	O5-C5-C4	2.64	117.24	110.83
9	Z	2	NAG	C2-N2-C7	-2.63	119.38	122.90
6	M	2	NAG	C4-C3-C2	2.62	114.86	111.02
3	F	1	NAG	C4-C3-C2	2.59	114.82	111.02
3	c	1	NAG	C4-C3-C2	2.59	114.82	111.02
6	M	3	MAN	C1-O5-C5	2.59	115.66	112.19
3	O	2	NAG	C2-N2-C7	-2.59	119.43	122.90
3	S	2	NAG	C8-C7-N2	2.58	120.39	116.12
4	J	1	NAG	C2-N2-C7	-2.57	119.46	122.90
4	N	1	NAG	C6-C5-C4	-2.56	106.74	113.02
8	Y	5	MAN	C1-C2-C3	2.55	113.36	109.64
4	P	1	NAG	C2-N2-C7	-2.55	119.49	122.90
5	X	2	NAG	C2-N2-C7	-2.53	119.51	122.90
7	j	2	NAG	C2-N2-C7	-2.53	119.51	122.90
3	E	1	NAG	O5-C1-C2	-2.51	107.40	111.29
9	Z	2	NAG	C8-C7-N2	2.50	120.27	116.12
7	W	1	NAG	C2-N2-C7	-2.50	119.55	122.90
5	X	2	NAG	C8-C7-N2	2.49	120.25	116.12
6	M	2	NAG	C8-C7-N2	2.49	120.25	116.12
9	Z	5	MAN	C1-O5-C5	2.47	115.50	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	1	NAG	C2-N2-C7	-2.47	119.58	122.90
3	a	1	NAG	C8-C7-N2	2.47	120.22	116.12
4	J	1	NAG	C8-C7-N2	2.47	120.22	116.12
7	j	2	NAG	C8-C7-N2	2.47	120.22	116.12
3	Q	1	NAG	C2-N2-C7	-2.46	119.60	122.90
2	e	1	NAG	C8-C7-N2	2.46	120.19	116.12
4	T	1	NAG	C8-C7-N2	2.45	120.18	116.12
4	P	1	NAG	C8-C7-N2	2.45	120.17	116.12
3	S	1	NAG	O4-C4-C5	2.44	115.34	109.32
2	e	4	MAN	O2-C2-C3	-2.44	105.10	110.15
8	Y	1	NAG	C8-C7-N2	2.43	120.15	116.12
3	O	2	NAG	C8-C7-N2	2.43	120.14	116.12
8	Y	2	NAG	C8-C7-N2	2.43	120.14	116.12
3	b	1	NAG	C8-C7-N2	2.42	120.13	116.12
3	R	1	NAG	C8-C7-N2	2.41	120.12	116.12
5	i	2	NAG	C2-N2-C7	-2.41	119.67	122.90
3	b	1	NAG	C2-N2-C7	-2.41	119.67	122.90
3	F	2	NAG	C6-C5-C4	-2.40	107.12	113.02
5	L	2	NAG	C8-C7-N2	2.40	120.10	116.12
7	V	2	NAG	C8-C7-N2	2.40	120.09	116.12
5	i	2	NAG	C8-C7-N2	2.39	120.09	116.12
3	c	1	NAG	C1-O5-C5	2.39	115.39	112.19
3	S	1	NAG	C3-C4-C5	-2.39	105.90	110.23
9	Z	1	NAG	C8-C7-N2	2.38	120.07	116.12
11	l	2	BMA	C1-C2-C3	-2.38	106.18	109.64
4	g	1	NAG	C8-C7-N2	2.37	120.05	116.12
6	M	2	NAG	C2-N2-C7	-2.37	119.73	122.90
3	c	2	NAG	C8-C7-N2	2.36	120.04	116.12
7	V	4	MAN	C1-O5-C5	2.36	115.35	112.19
3	R	2	NAG	C8-C7-N2	2.36	120.03	116.12
3	E	2	NAG	C8-C7-N2	2.35	120.02	116.12
4	G	2	NAG	C1-C2-N2	-2.34	106.75	110.43
4	H	1	NAG	C8-C7-N2	2.34	120.00	116.12
3	F	1	NAG	C6-C5-C4	2.33	118.75	113.02
4	g	1	NAG	C2-N2-C7	-2.33	119.77	122.90
2	K	4	MAN	O2-C2-C3	-2.33	105.32	110.15
4	J	2	NAG	C8-C7-N2	2.33	119.98	116.12
7	j	4	MAN	O2-C2-C3	-2.32	105.34	110.15
3	Q	2	NAG	C8-C7-N2	2.32	119.96	116.12
5	L	1	NAG	O4-C4-C3	-2.32	104.91	110.38
3	F	1	NAG	C8-C7-N2	2.32	119.96	116.12
3	c	2	NAG	C2-N2-C7	-2.31	119.81	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1	NAG	O5-C5-C6	-2.30	103.19	107.66
10	k	1	NAG	O7-C7-C8	-2.30	117.96	122.05
6	M	2	NAG	C1-O5-C5	-2.30	109.11	112.19
10	k	1	NAG	O7-C7-N2	-2.30	117.92	121.98
4	U	2	NAG	C2-N2-C7	-2.29	119.83	122.90
4	U	2	NAG	C8-C7-N2	2.29	119.92	116.12
3	Q	1	NAG	C8-C7-N2	2.29	119.91	116.12
5	L	2	NAG	C2-N2-C7	-2.28	119.85	122.90
3	f	2	NAG	C8-C7-N2	2.26	119.86	116.12
8	Y	5	MAN	O2-C2-C3	-2.25	105.49	110.15
2	e	2	NAG	C6-C5-C4	-2.25	107.50	113.02
4	H	1	NAG	O5-C5-C6	-2.25	103.29	107.66
3	a	1	NAG	C2-N2-C7	-2.24	119.89	122.90
3	f	1	NAG	C8-C7-N2	2.24	119.83	116.12
7	W	2	NAG	C8-C7-N2	2.23	119.82	116.12
6	M	1	NAG	C2-N2-C7	-2.23	119.91	122.90
3	a	2	NAG	C8-C7-N2	2.23	119.82	116.12
6	M	1	NAG	C8-C7-N2	2.23	119.82	116.12
4	g	2	NAG	C8-C7-N2	2.23	119.81	116.12
2	D	2	NAG	C8-C7-N2	2.22	119.81	116.12
8	Y	4	MAN	C1-O5-C5	2.22	115.16	112.19
3	E	1	NAG	O7-C7-N2	-2.22	118.06	121.98
7	h	1	NAG	C8-C7-N2	2.22	119.79	116.12
3	F	1	NAG	O4-C4-C3	-2.21	105.16	110.38
7	V	1	NAG	C8-C7-N2	2.21	119.78	116.12
4	N	1	NAG	O5-C5-C4	2.21	116.20	110.83
4	T	2	NAG	C8-C7-N2	2.21	119.78	116.12
11	l	1	NAG	C3-C4-C5	2.21	114.24	110.23
4	G	2	NAG	C8-C7-N2	2.20	119.77	116.12
2	e	2	NAG	C8-C7-N2	2.20	119.77	116.12
2	K	1	NAG	C8-C7-N2	2.20	119.76	116.12
3	O	1	NAG	C8-C7-N2	2.19	119.75	116.12
10	k	1	NAG	C1-C2-N2	2.18	113.87	110.43
3	E	1	NAG	O7-C7-C8	-2.18	118.17	122.05
7	W	4	MAN	O2-C2-C3	-2.18	105.64	110.15
7	h	1	NAG	C3-C4-C5	-2.17	106.29	110.23
5	X	3	FUC	O2-C2-C1	2.17	114.20	109.22
2	K	1	NAG	C2-N2-C7	-2.17	119.99	122.90
7	h	1	NAG	C2-N2-C7	-2.17	120.00	122.90
5	X	1	NAG	C8-C7-N2	2.16	119.70	116.12
10	k	1	NAG	C4-C3-C2	2.16	114.18	111.02
3	S	2	NAG	C6-C5-C4	-2.16	107.72	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	1	NAG	C2-N2-C7	-2.16	120.01	122.90
4	P	2	NAG	C8-C7-N2	2.16	119.69	116.12
9	Z	4	MAN	O2-C2-C3	-2.15	105.69	110.15
3	Q	2	NAG	C2-N2-C7	-2.15	120.01	122.90
5	i	1	NAG	C8-C7-N2	2.15	119.69	116.12
9	Z	6	FUC	O5-C1-C2	2.15	115.92	110.79
4	G	1	NAG	O7-C7-N2	-2.15	118.19	121.98
6	M	5	MAN	O2-C2-C3	-2.15	105.70	110.15
9	Z	5	MAN	O2-C2-C3	-2.15	105.70	110.15
7	W	1	NAG	C8-C7-N2	2.14	119.67	116.12
7	h	2	NAG	C8-C7-N2	2.14	119.67	116.12
4	N	1	NAG	O5-C1-C2	-2.14	107.98	111.29
4	U	1	NAG	C1-C2-N2	2.13	113.79	110.43
2	D	4	MAN	O2-C2-C3	-2.13	105.75	110.15
4	J	2	NAG	C2-N2-C7	-2.12	120.06	122.90
6	M	4	MAN	O2-C2-C3	-2.12	105.75	110.15
7	h	1	NAG	O5-C1-C2	2.12	114.57	111.29
8	Y	2	NAG	C1-O5-C5	2.11	115.01	112.19
9	Z	1	NAG	C3-C4-C5	2.10	114.04	110.23
7	h	4	MAN	O2-C2-C3	-2.10	105.80	110.15
5	L	1	NAG	C4-C3-C2	2.10	114.09	111.02
7	h	3	BMA	O2-C2-C3	-2.08	105.84	110.15
9	Z	1	NAG	C6-C5-C4	-2.08	107.91	113.02
8	Y	4	MAN	O2-C2-C3	-2.06	105.87	110.15
3	I	2	NAG	C8-C7-N2	2.06	119.54	116.12
7	j	1	NAG	C8-C7-N2	2.06	119.54	116.12
3	b	2	NAG	C8-C7-N2	2.06	119.53	116.12
7	V	4	MAN	O2-C2-C3	-2.05	105.91	110.15
7	V	3	BMA	C3-C4-C5	2.02	113.89	110.23
4	T	1	NAG	C2-N2-C7	-2.02	120.19	122.90
2	D	2	NAG	C2-N2-C7	-2.02	120.19	122.90
5	L	1	NAG	C3-C4-C5	2.02	113.89	110.23
5	i	1	NAG	C2-N2-C7	-2.02	120.20	122.90
3	R	2	NAG	C2-N2-C7	-2.01	120.20	122.90
7	j	1	NAG	C2-N2-C7	-2.01	120.20	122.90
4	N	2	NAG	C8-C7-N2	2.01	119.45	116.12

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	1	NAG	C5
7	h	1	NAG	C3

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Mol	Chain	Res	Type	Atom
10	k	1	NAG	C4

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	C1-C2-N2-C7
2	e	2	NAG	C1-C2-N2-C7
3	E	1	NAG	C1-C2-N2-C7
3	I	2	NAG	C1-C2-N2-C7
3	O	1	NAG	C1-C2-N2-C7
4	P	2	NAG	C1-C2-N2-C7
4	U	1	NAG	C1-C2-N2-C7
4	U	2	NAG	C1-C2-N2-C7
10	k	1	NAG	C1-C2-N2-C7
11	l	1	NAG	C1-C2-N2-C7
5	i	1	NAG	C4-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
6	M	3	MAN	O5-C5-C6-O6
9	Z	1	NAG	O5-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
6	M	3	MAN	C4-C5-C6-O6
11	l	1	NAG	O5-C5-C6-O6
9	Z	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
7	j	2	NAG	O5-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
9	Z	3	BMA	C4-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
7	h	3	BMA	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C4-C5-C6-O6
9	Z	1	NAG	C4-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
7	h	3	BMA	C4-C5-C6-O6
11	l	1	NAG	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
5	i	2	NAG	C4-C5-C6-O6
9	Z	3	BMA	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	c	1	NAG	C8-C7-N2-C2
3	c	1	NAG	O7-C7-N2-C2
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	d	2	NAG	C8-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
7	W	1	NAG	C8-C7-N2-C2
7	W	1	NAG	O7-C7-N2-C2
10	k	1	NAG	C8-C7-N2-C2
10	k	1	NAG	O7-C7-N2-C2
11	l	1	NAG	C8-C7-N2-C2
11	l	1	NAG	O7-C7-N2-C2
7	W	4	MAN	O5-C5-C6-O6
7	j	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	Z	2	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
4	N	3	BMA	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	c	1	NAG	C4-C5-C6-O6
6	M	5	MAN	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
10	k	1	NAG	O5-C5-C6-O6
7	j	2	NAG	C4-C5-C6-O6
2	e	3	BMA	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
7	W	3	BMA	C4-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
7	h	1	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
7	V	3	BMA	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
4	g	3	BMA	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
4	U	2	NAG	C3-C2-N2-C7
5	X	1	NAG	C3-C2-N2-C7
4	H	3	BMA	O5-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
8	Y	5	MAN	O5-C5-C6-O6
2	K	4	MAN	C4-C5-C6-O6
3	f	2	NAG	C1-C2-N2-C7
4	T	2	NAG	C1-C2-N2-C7
7	V	1	NAG	C1-C2-N2-C7
5	L	1	NAG	C4-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6

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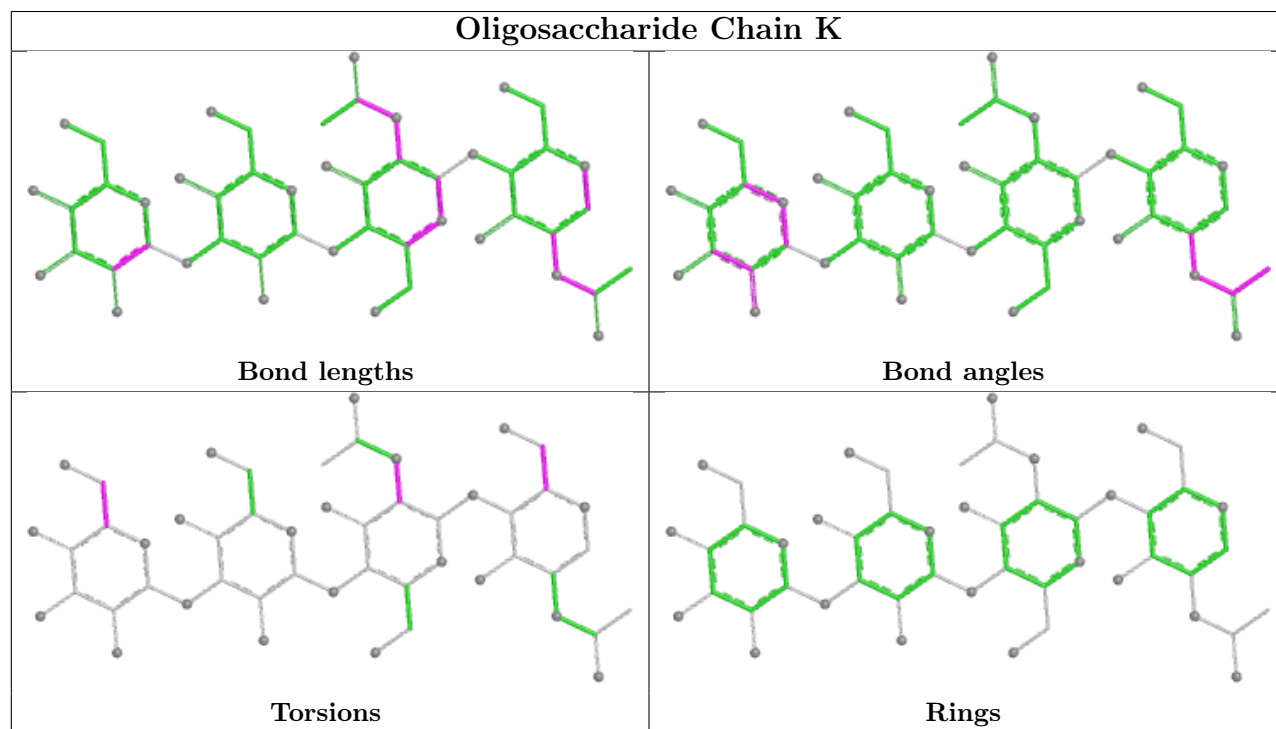
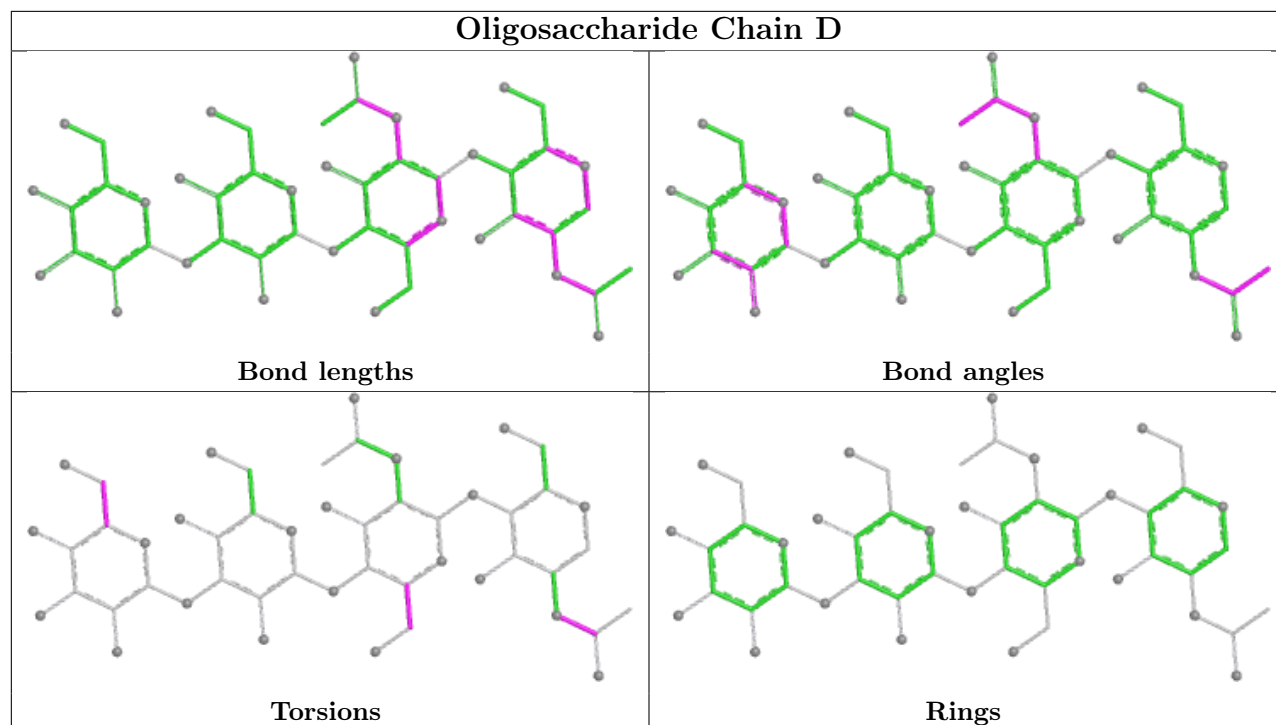
Mol	Chain	Res	Type	Atoms
7	j	1	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
6	M	5	MAN	C4-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
3	S	1	NAG	C3-C2-N2-C7
4	T	2	NAG	C3-C2-N2-C7
5	L	1	NAG	C3-C2-N2-C7
7	V	1	NAG	C3-C2-N2-C7
7	W	2	NAG	C3-C2-N2-C7
2	K	4	MAN	O5-C5-C6-O6
7	W	4	MAN	C4-C5-C6-O6
3	E	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
5	L	1	NAG	C1-C2-N2-C7
6	M	2	NAG	C1-C2-N2-C7
7	W	2	NAG	C1-C2-N2-C7
7	V	1	NAG	C4-C5-C6-O6
2	e	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
3	O	1	NAG	C3-C2-N2-C7
3	f	1	NAG	C3-C2-N2-C7
3	f	2	NAG	C3-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
3	S	1	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
11	l	2	BMA	C4-C5-C6-O6
8	Y	5	MAN	C4-C5-C6-O6

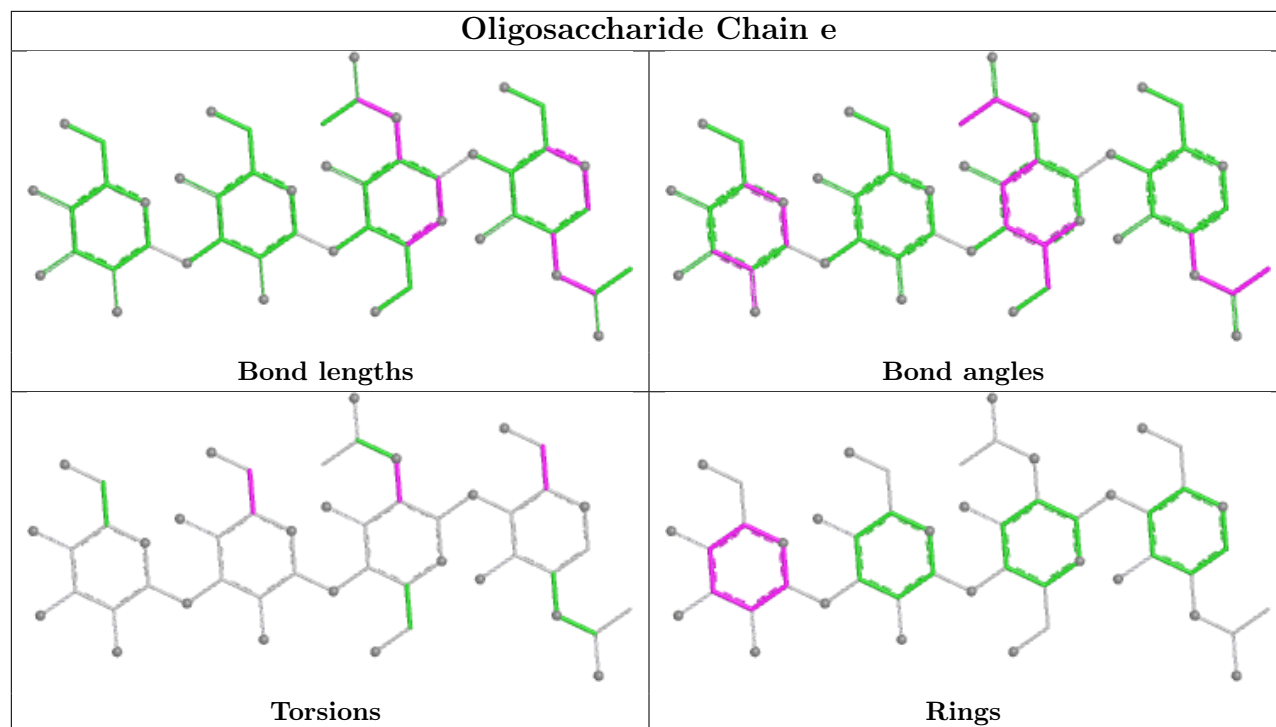
All (5) ring outliers are listed below:

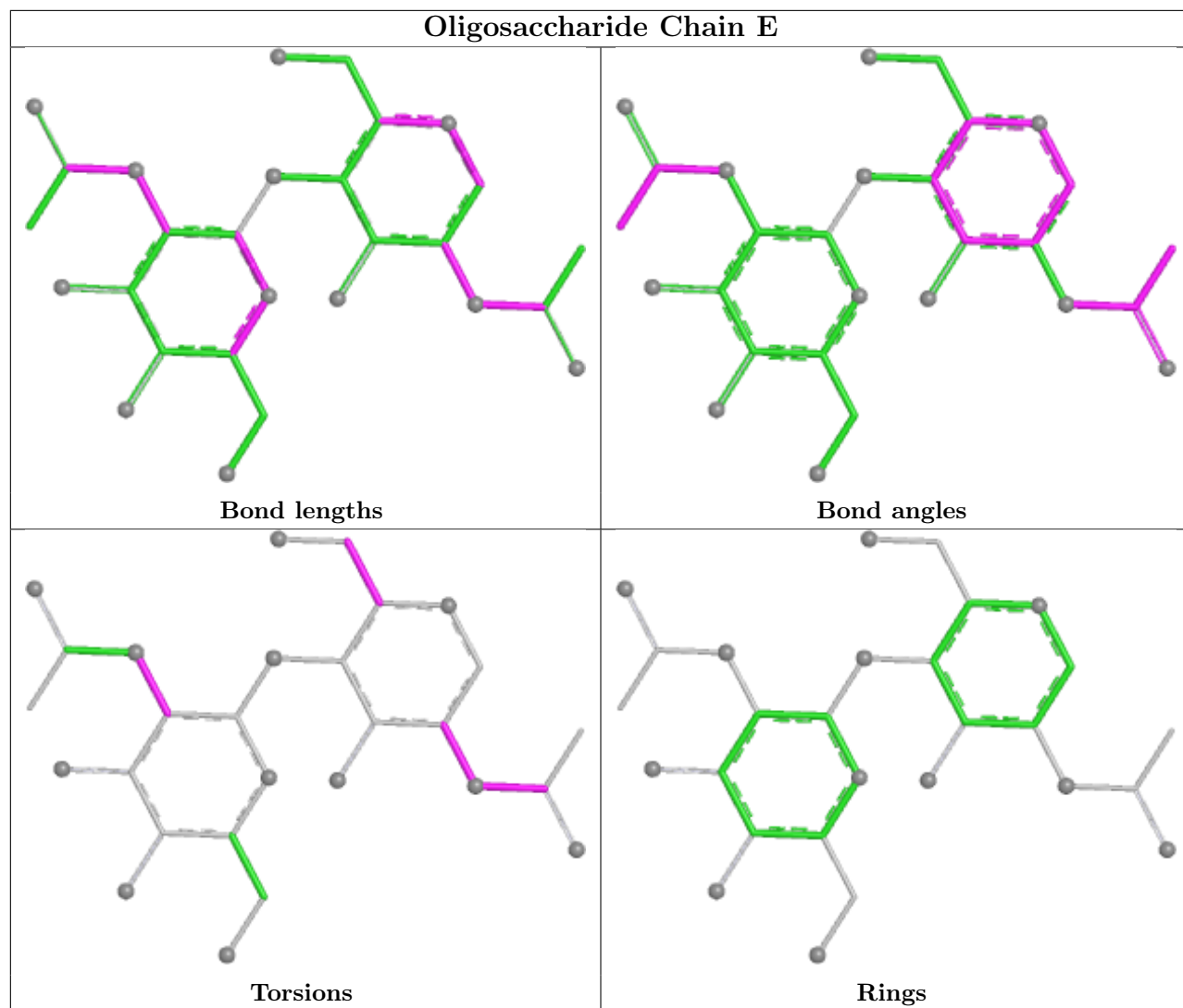
Mol	Chain	Res	Type	Atoms
2	e	4	MAN	C1-C2-C3-C4-C5-O5
8	Y	4	MAN	C1-C2-C3-C4-C5-O5
7	V	4	MAN	C1-C2-C3-C4-C5-O5
9	Z	4	MAN	C1-C2-C3-C4-C5-O5
6	M	3	MAN	C1-C2-C3-C4-C5-O5

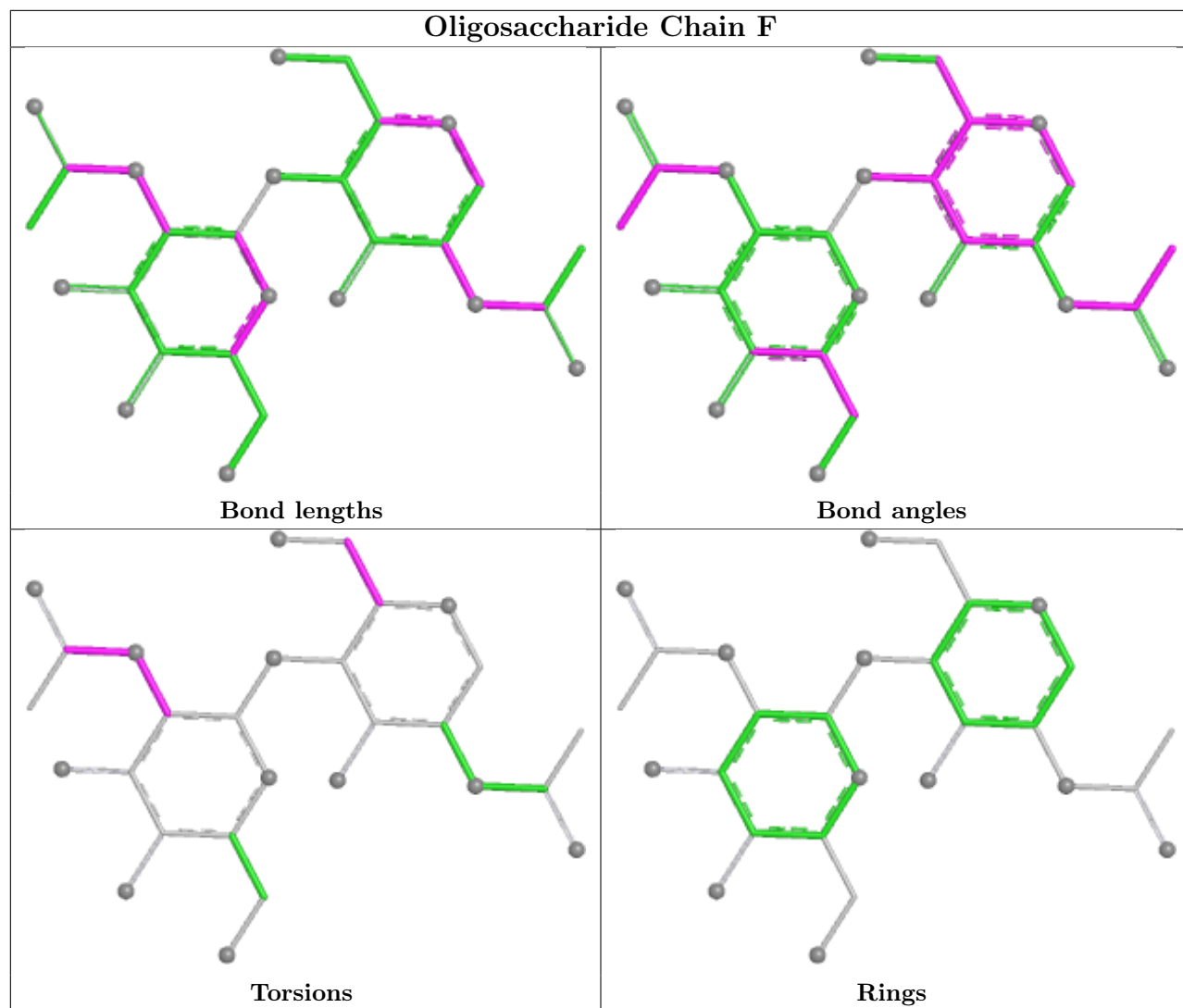
No monomer is involved in short contacts.

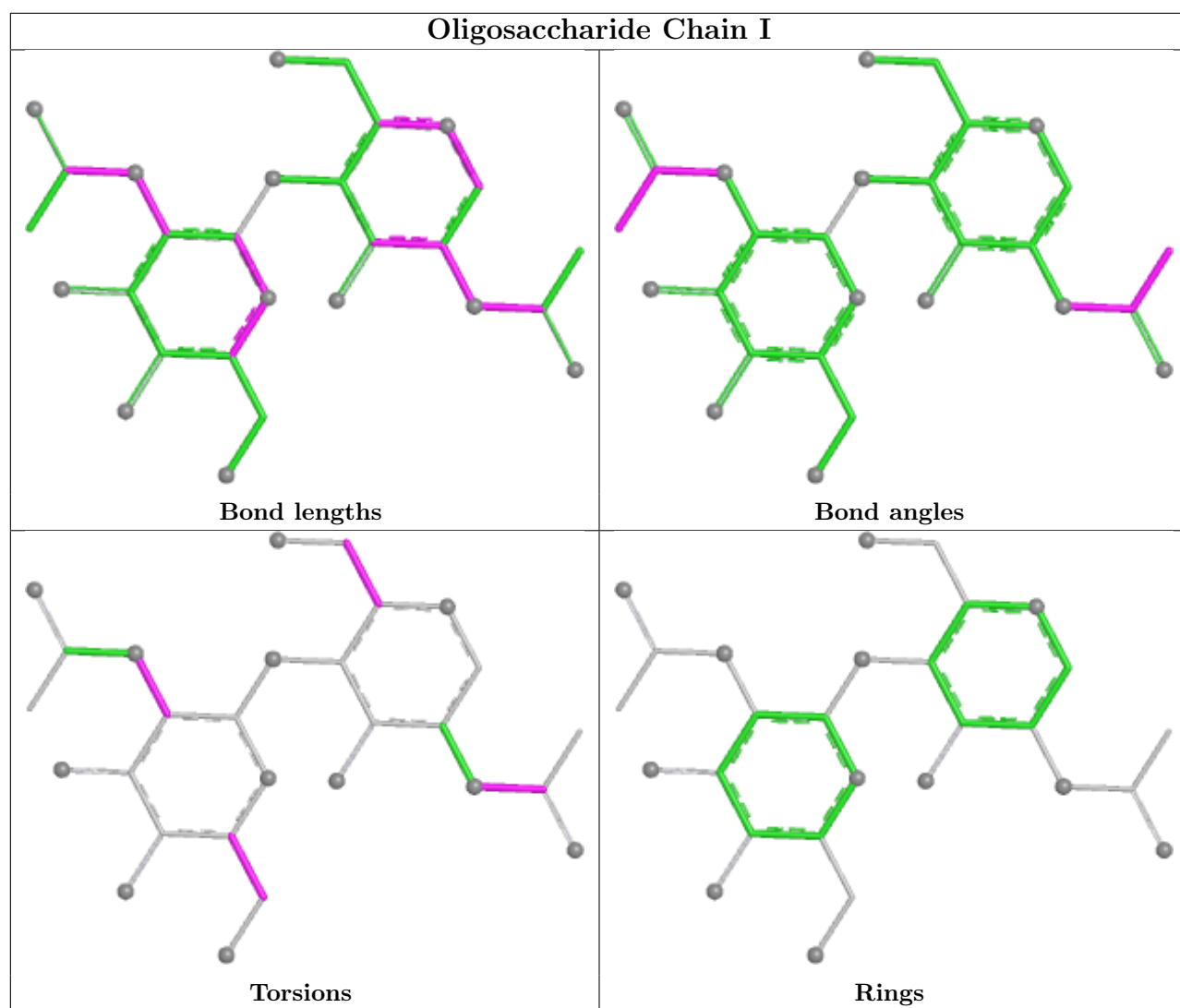
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

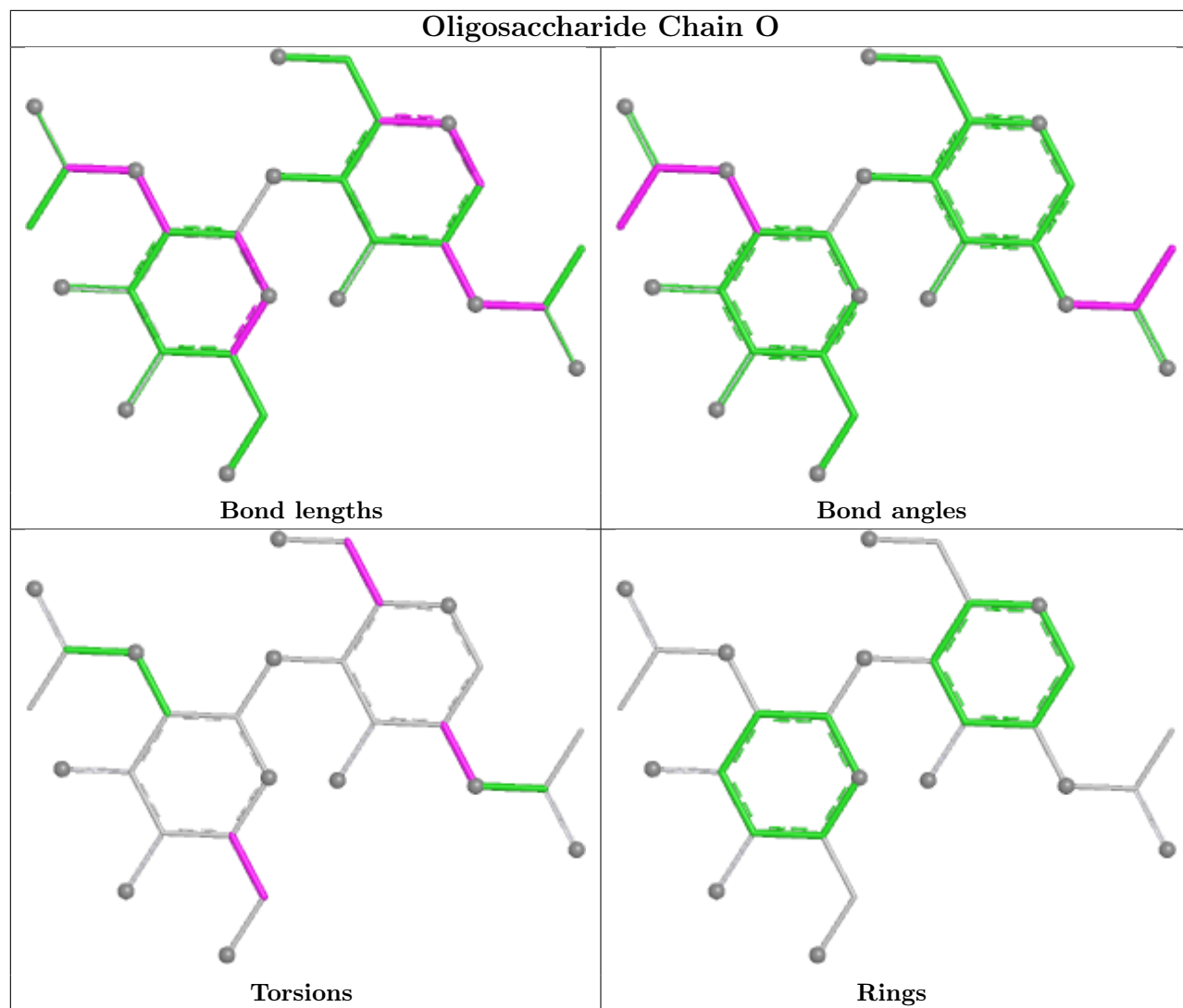


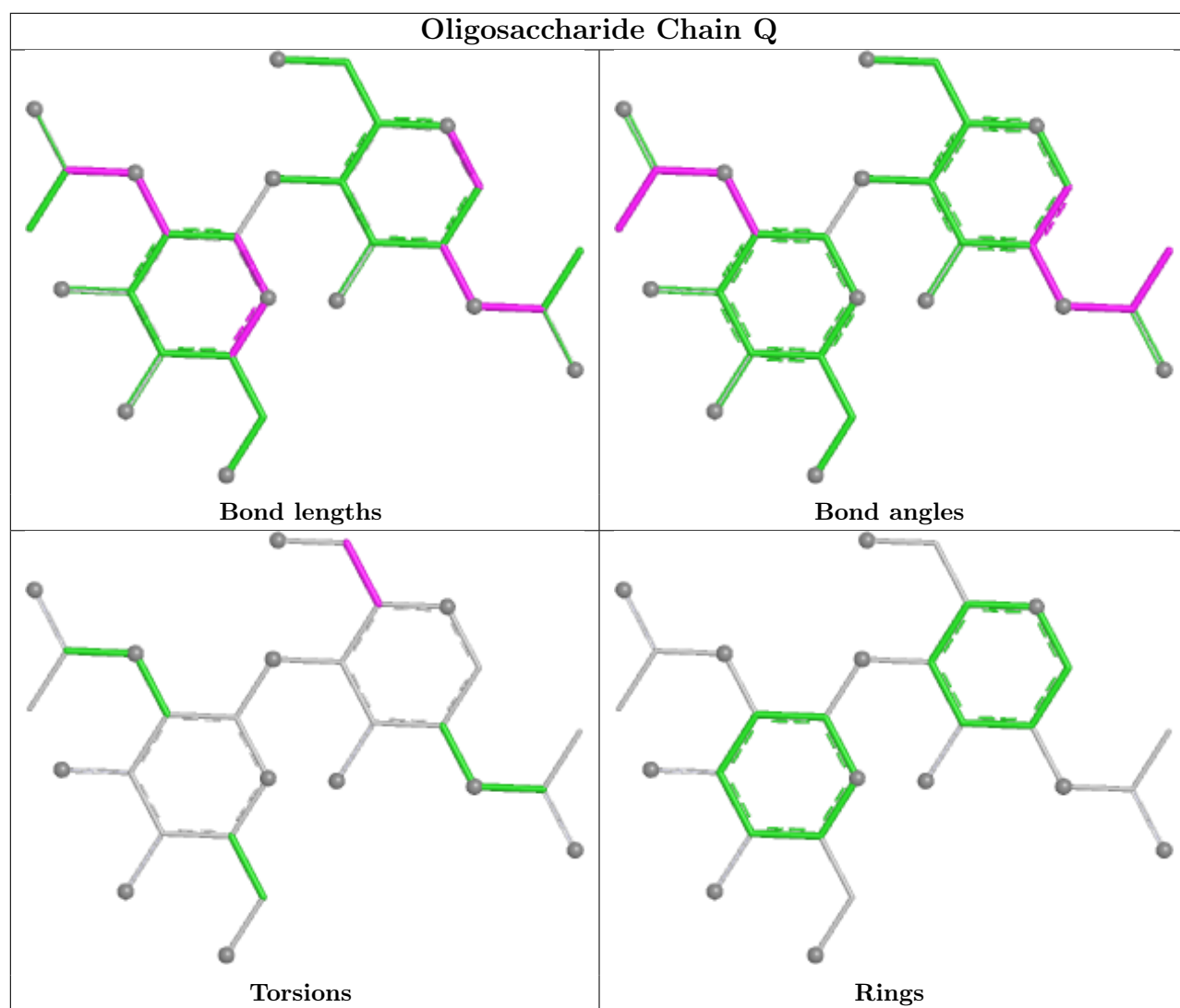


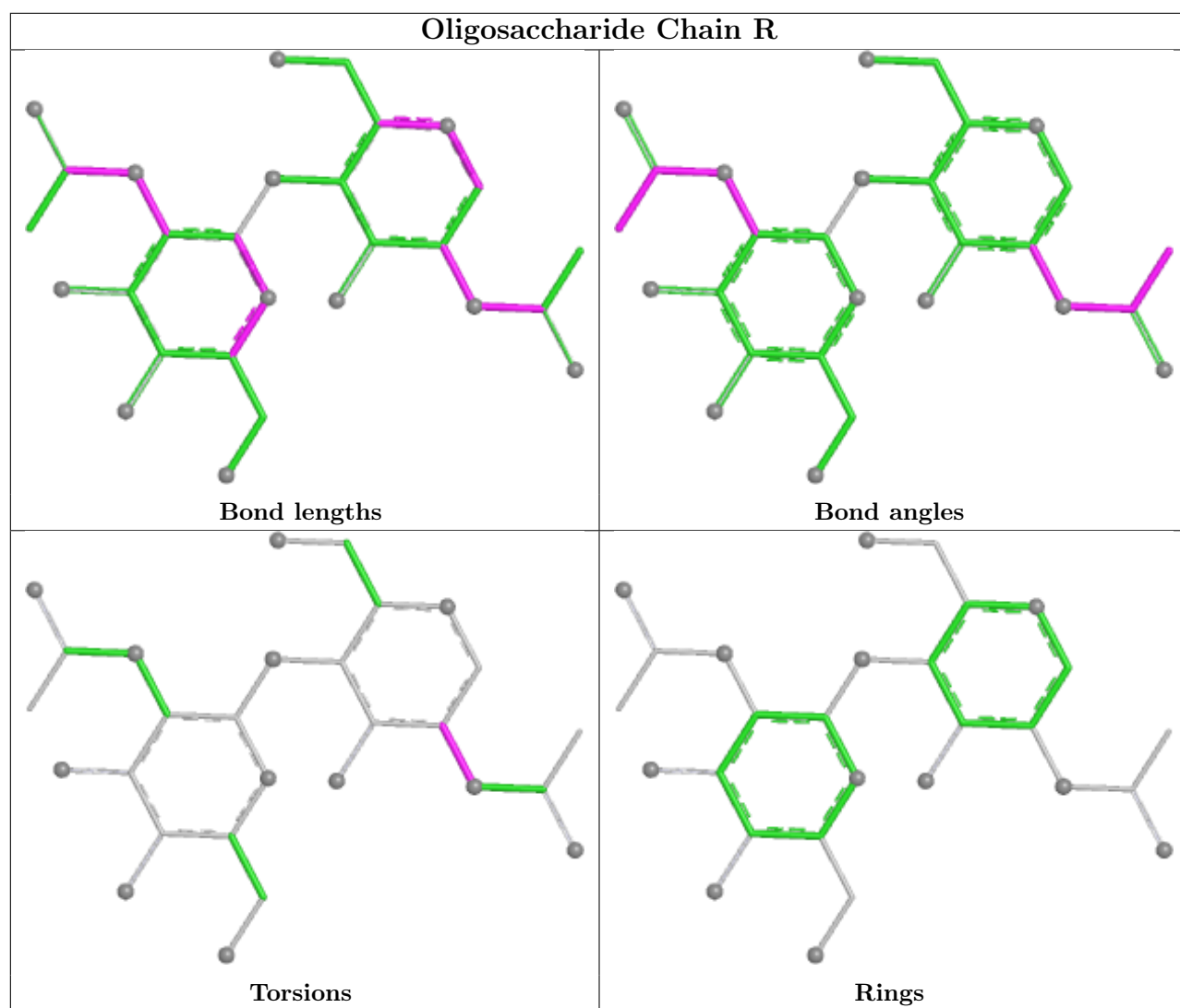


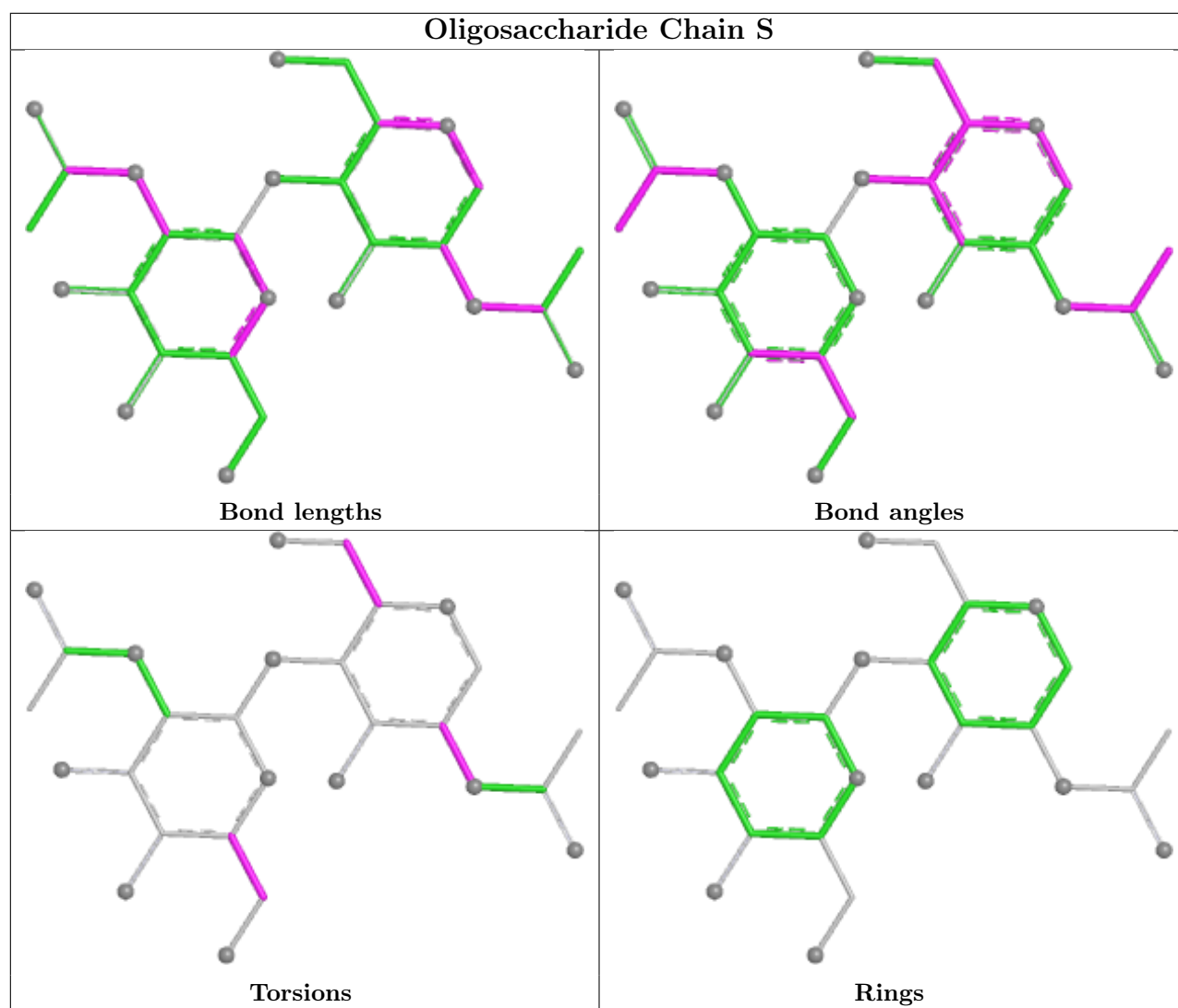


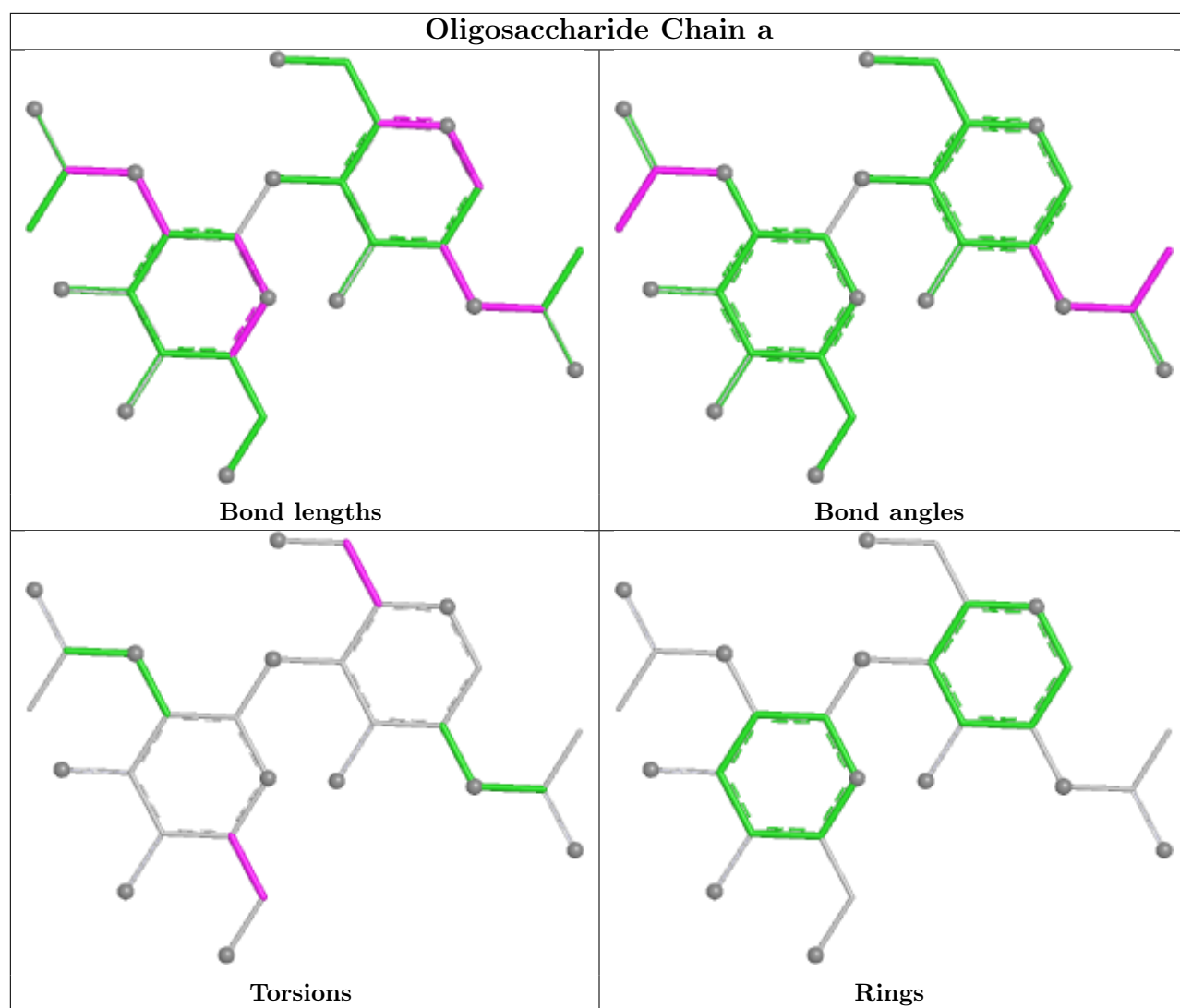


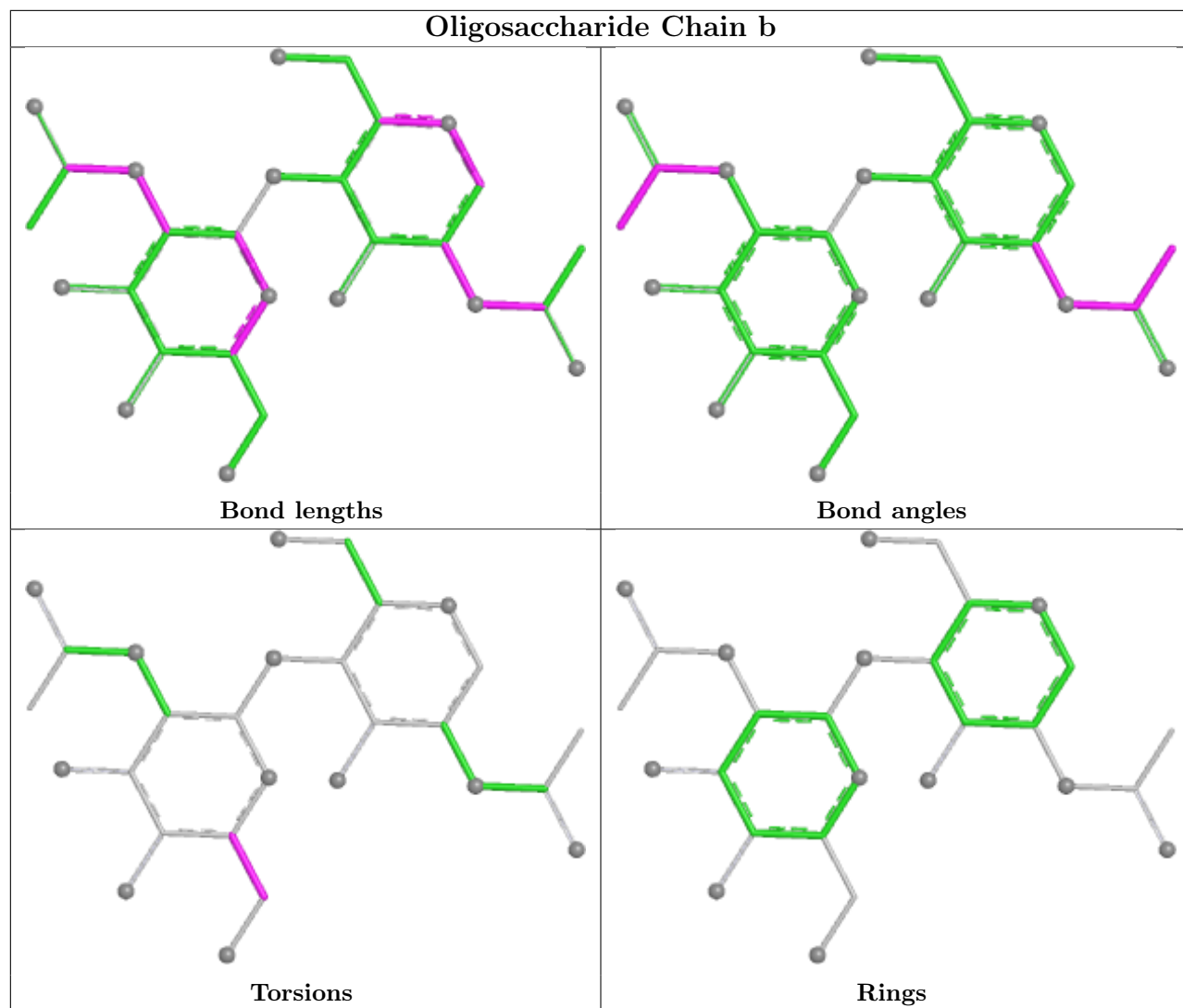


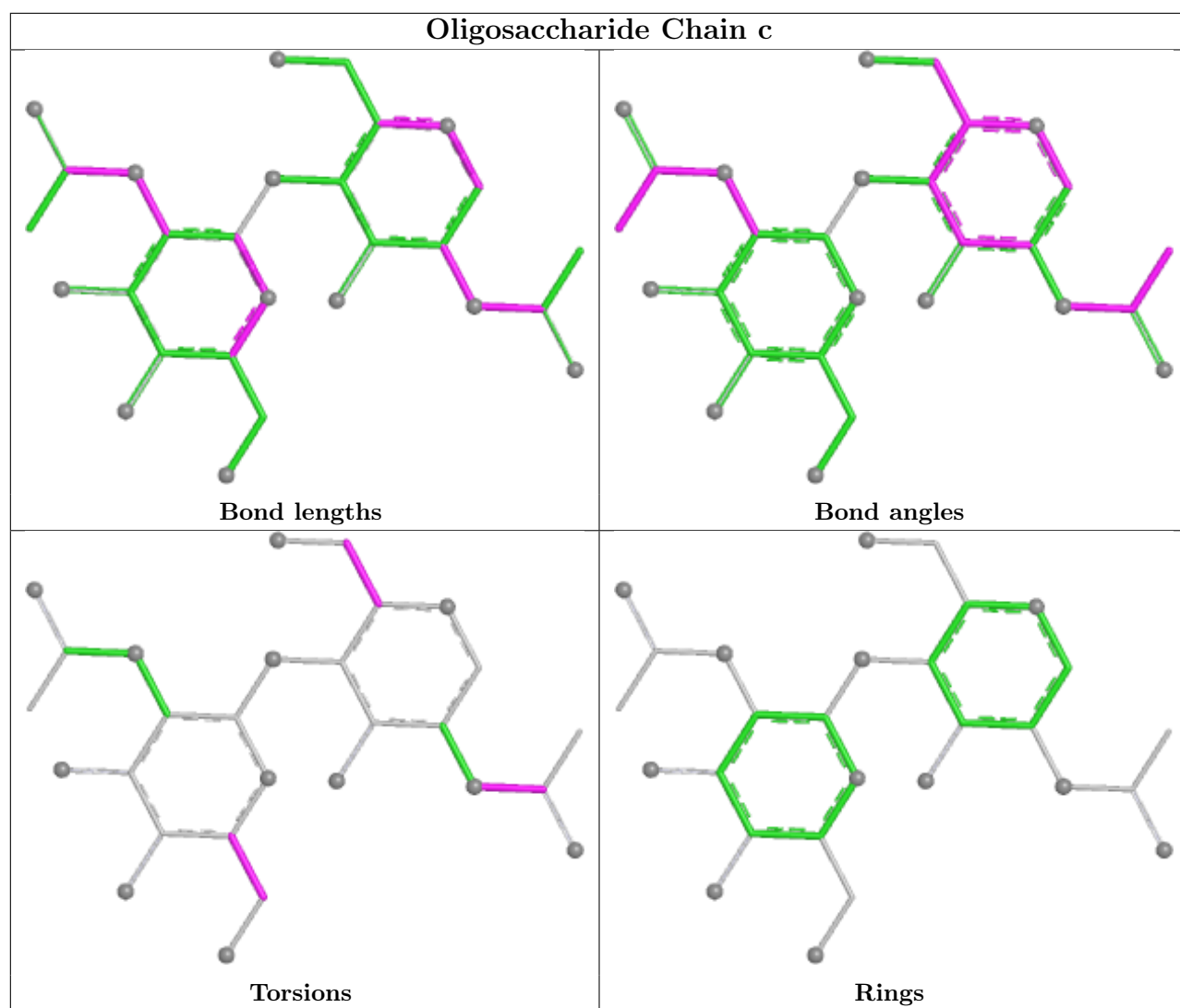


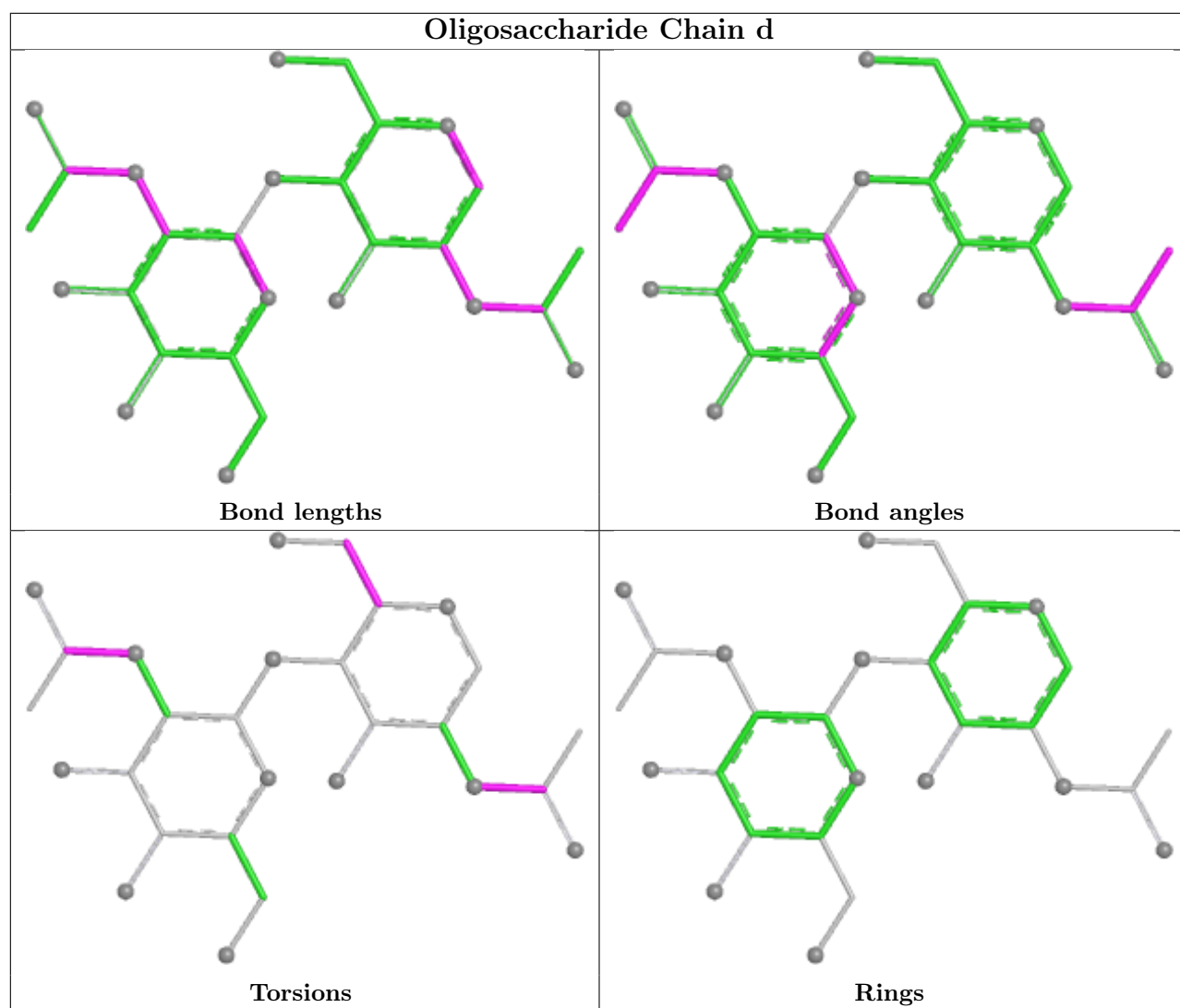


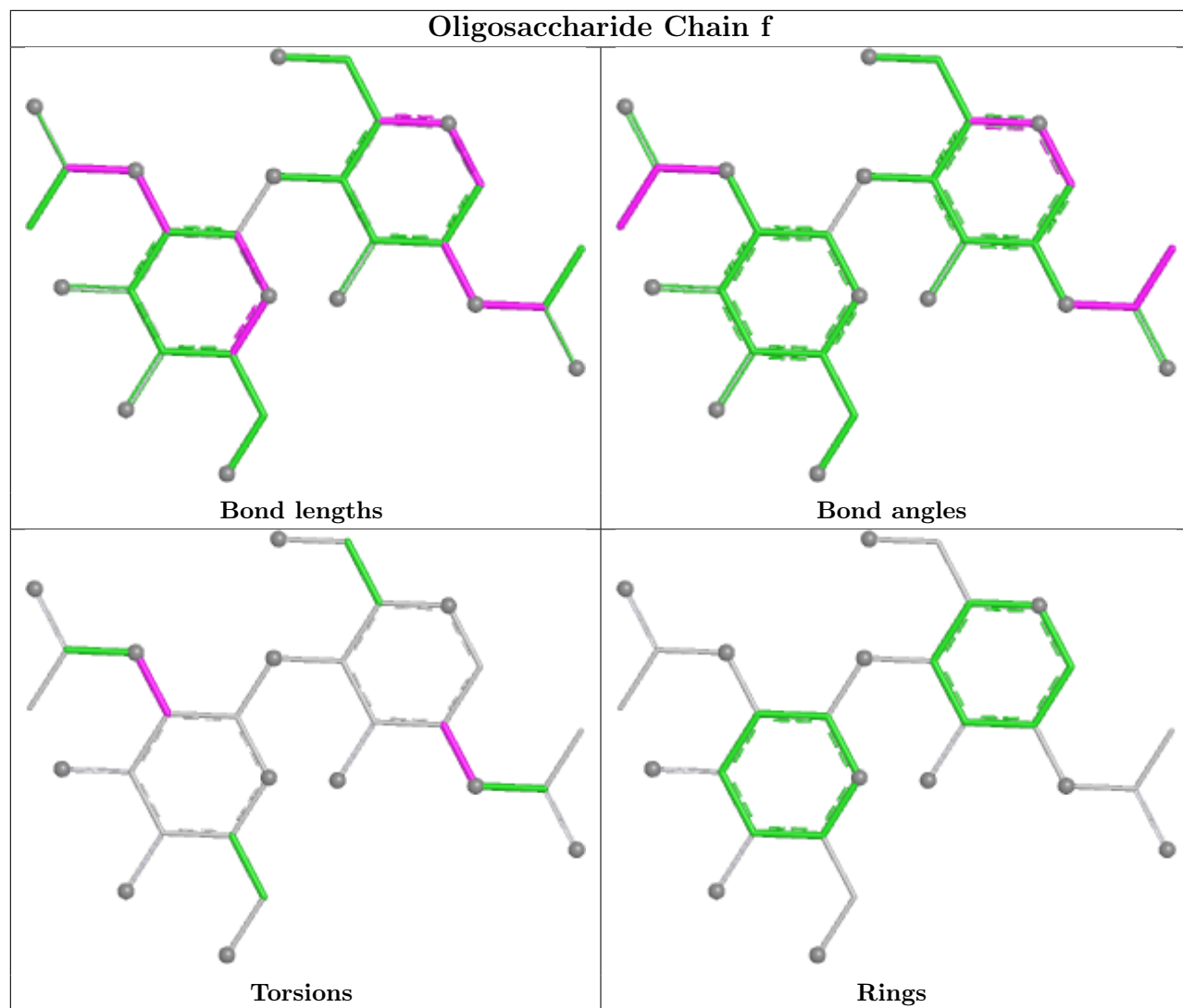


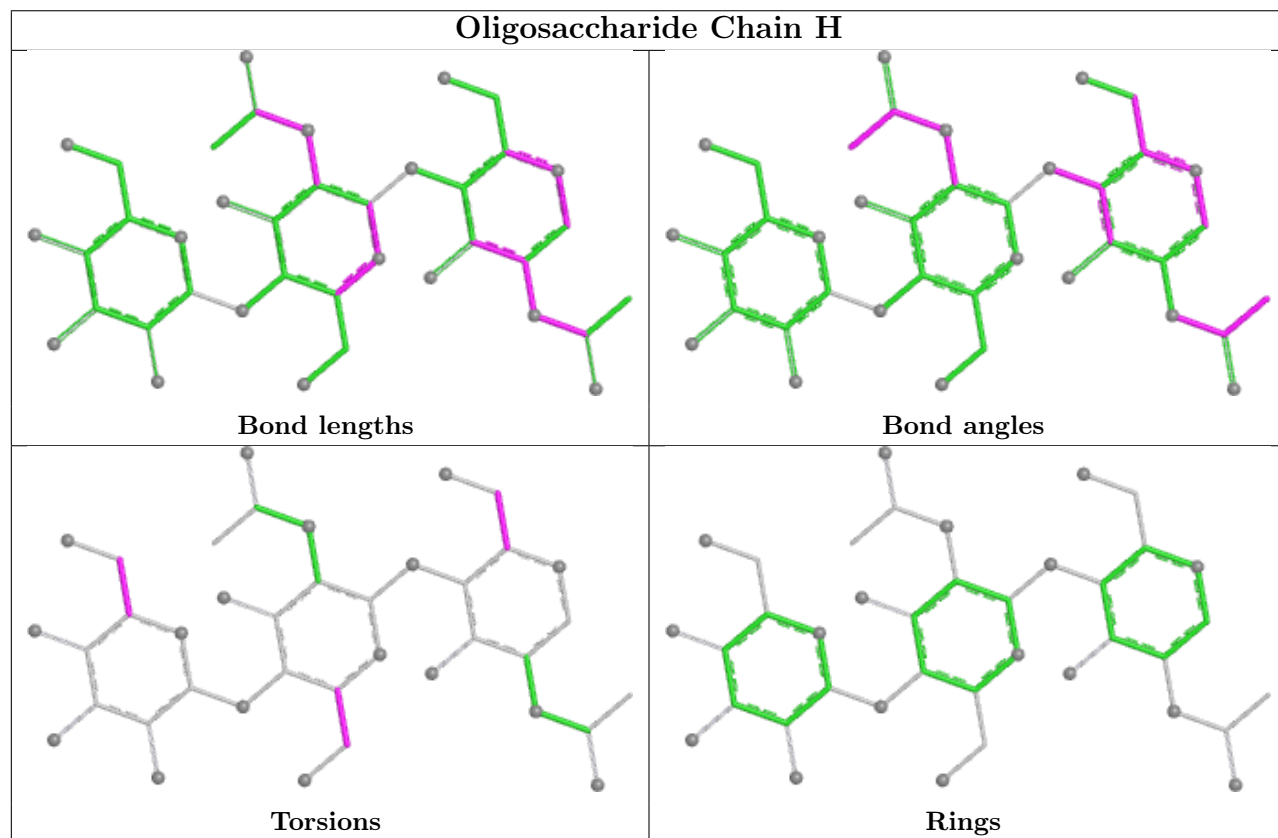
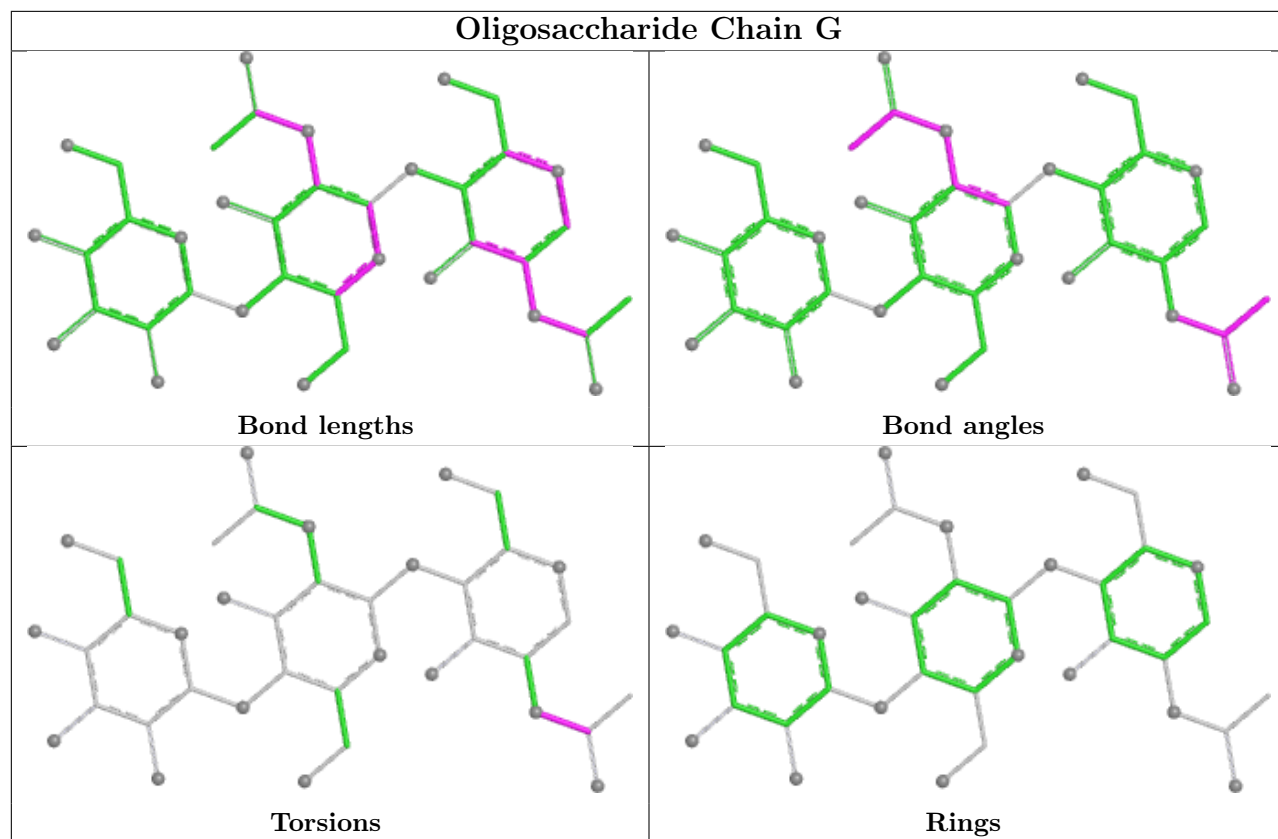


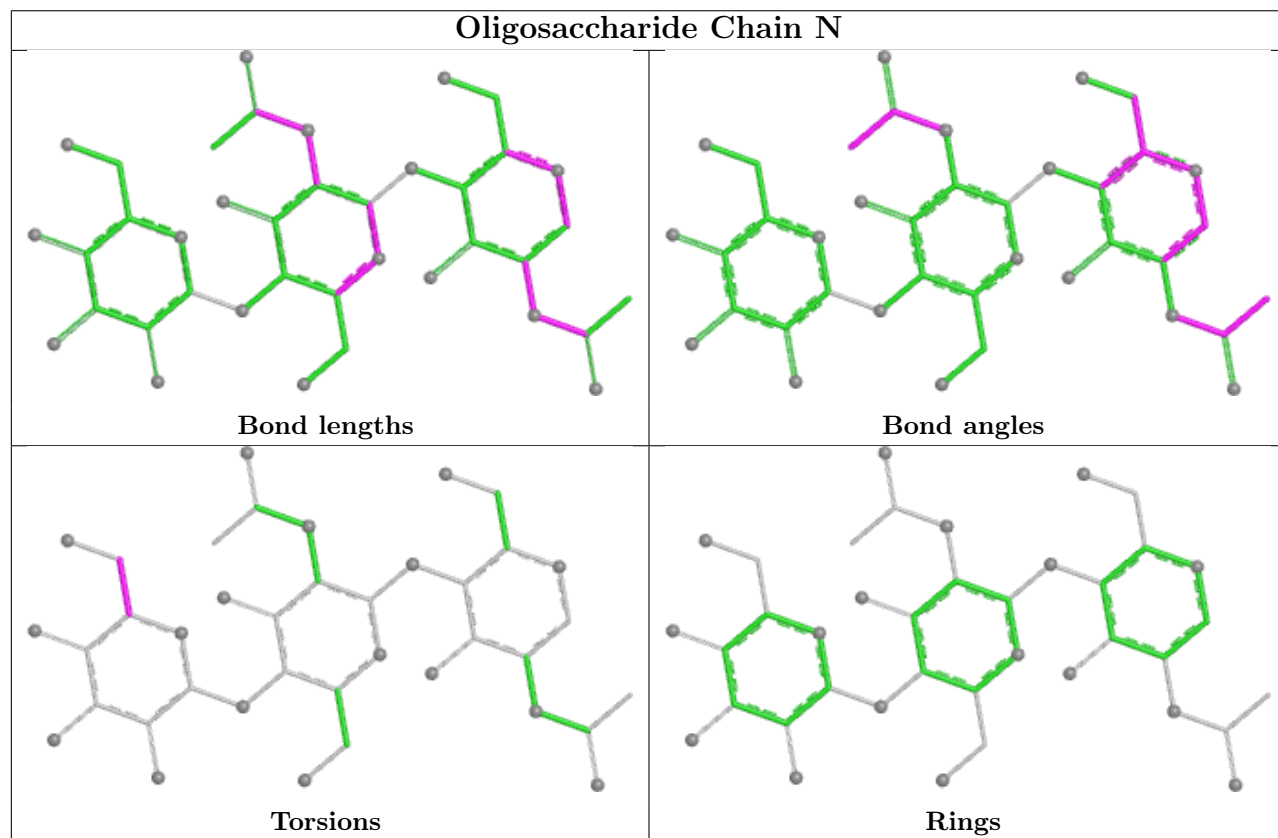
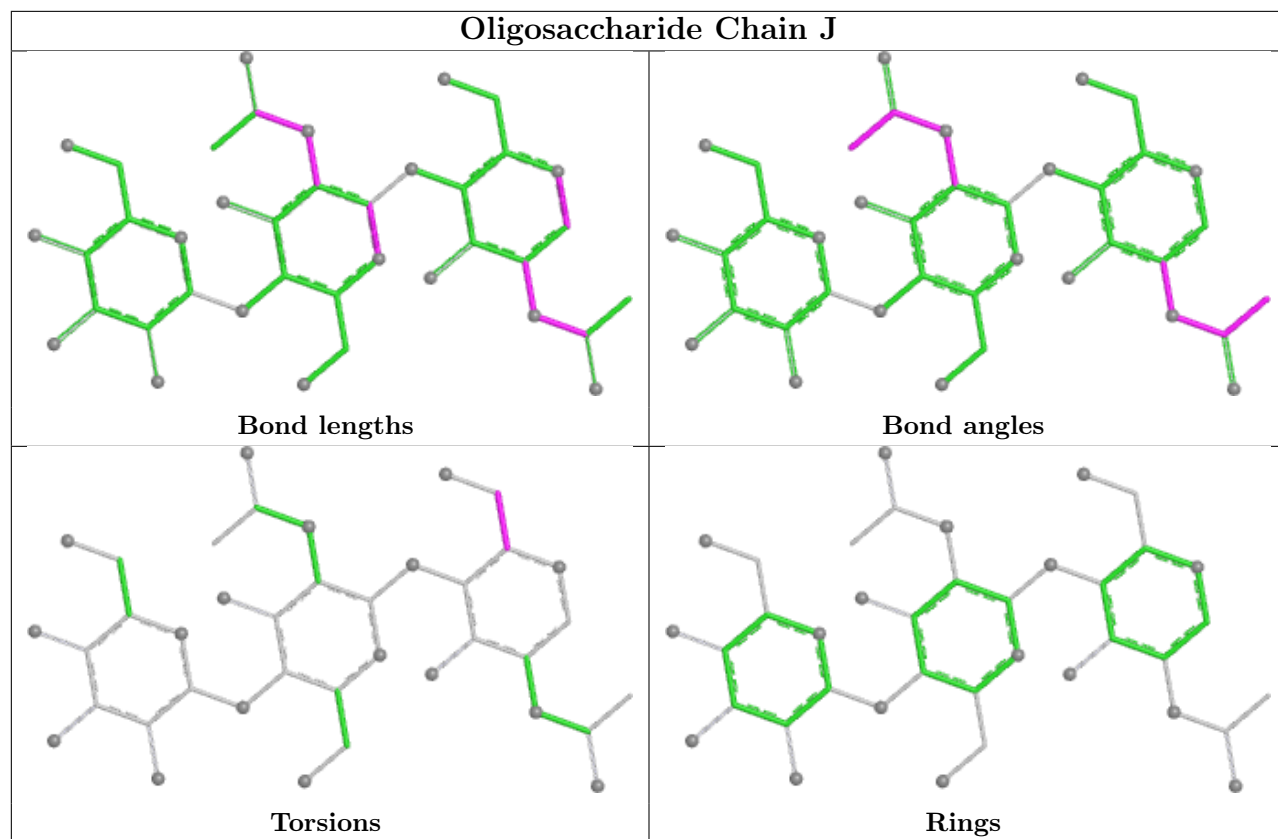


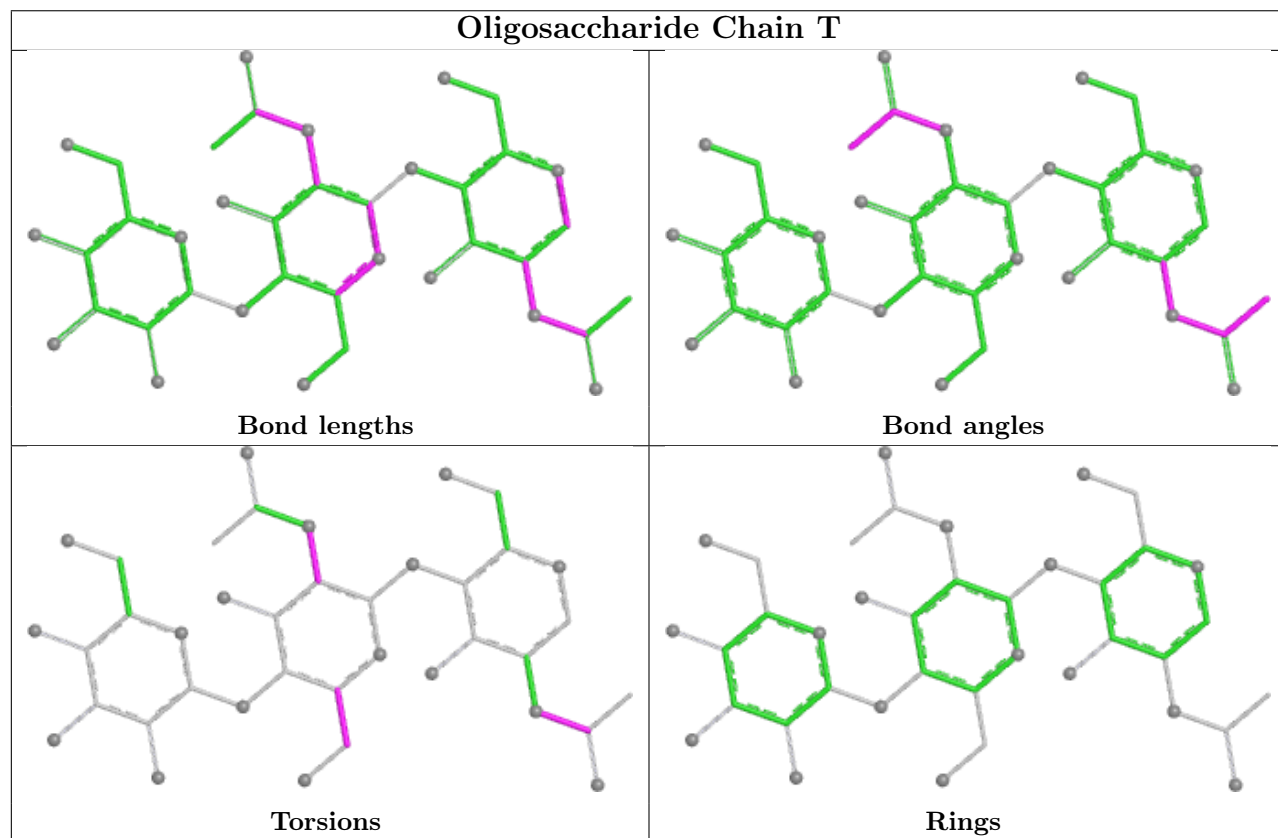
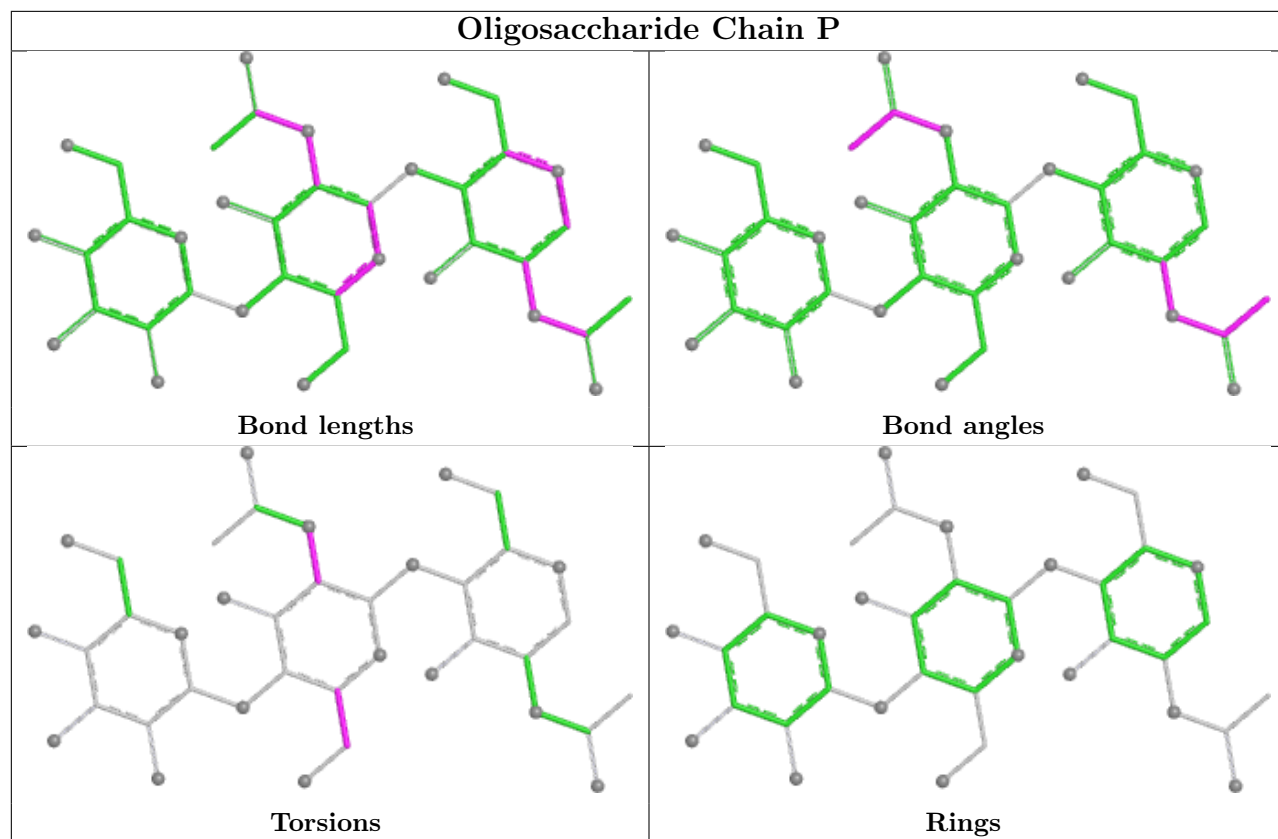


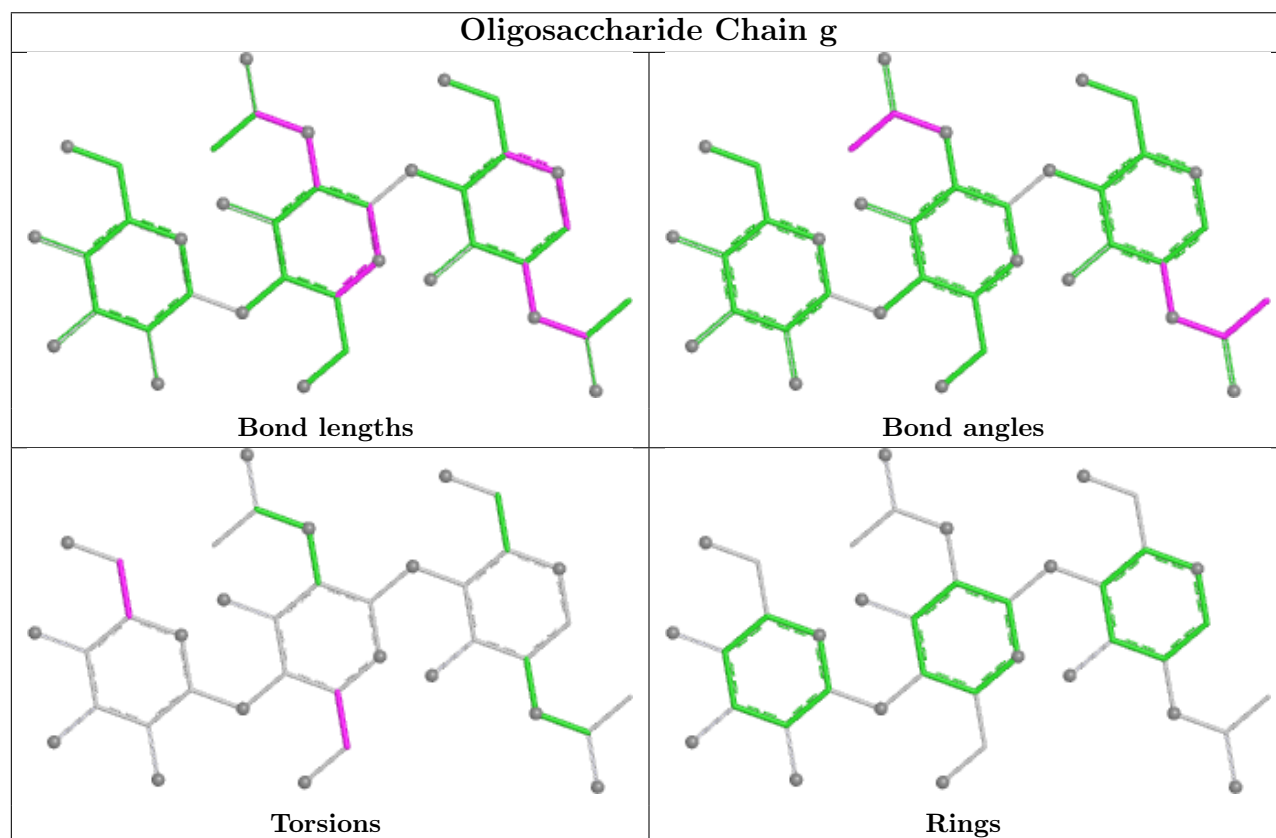
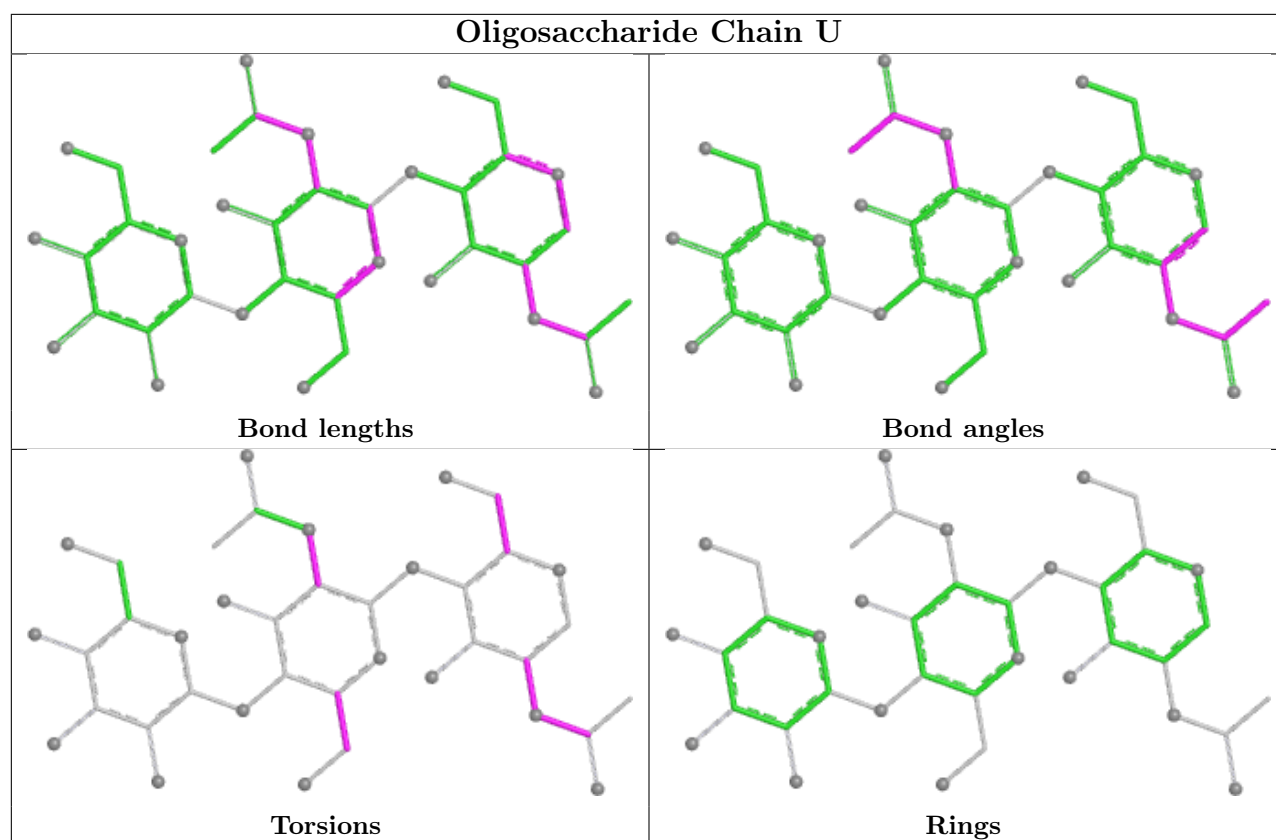


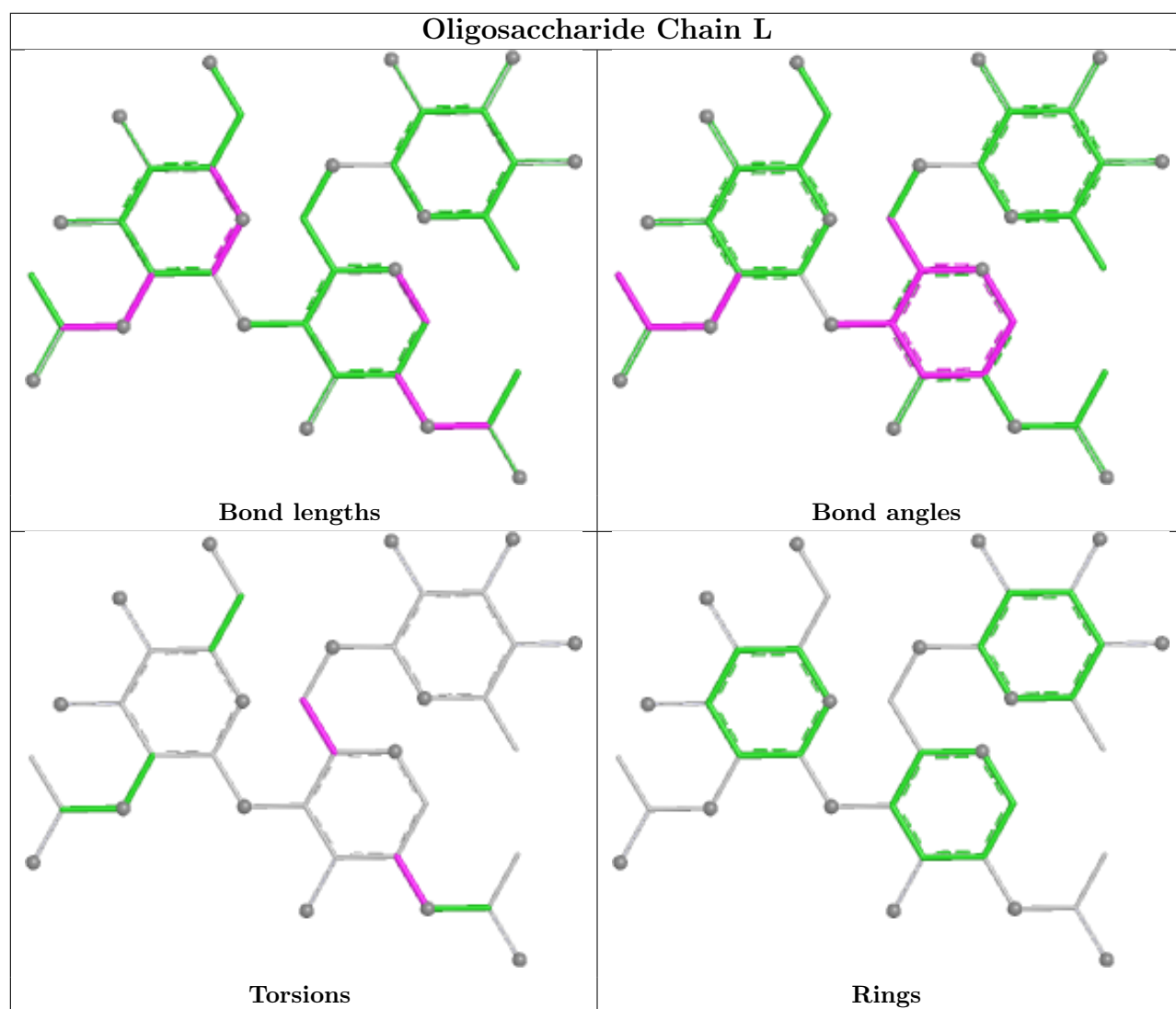


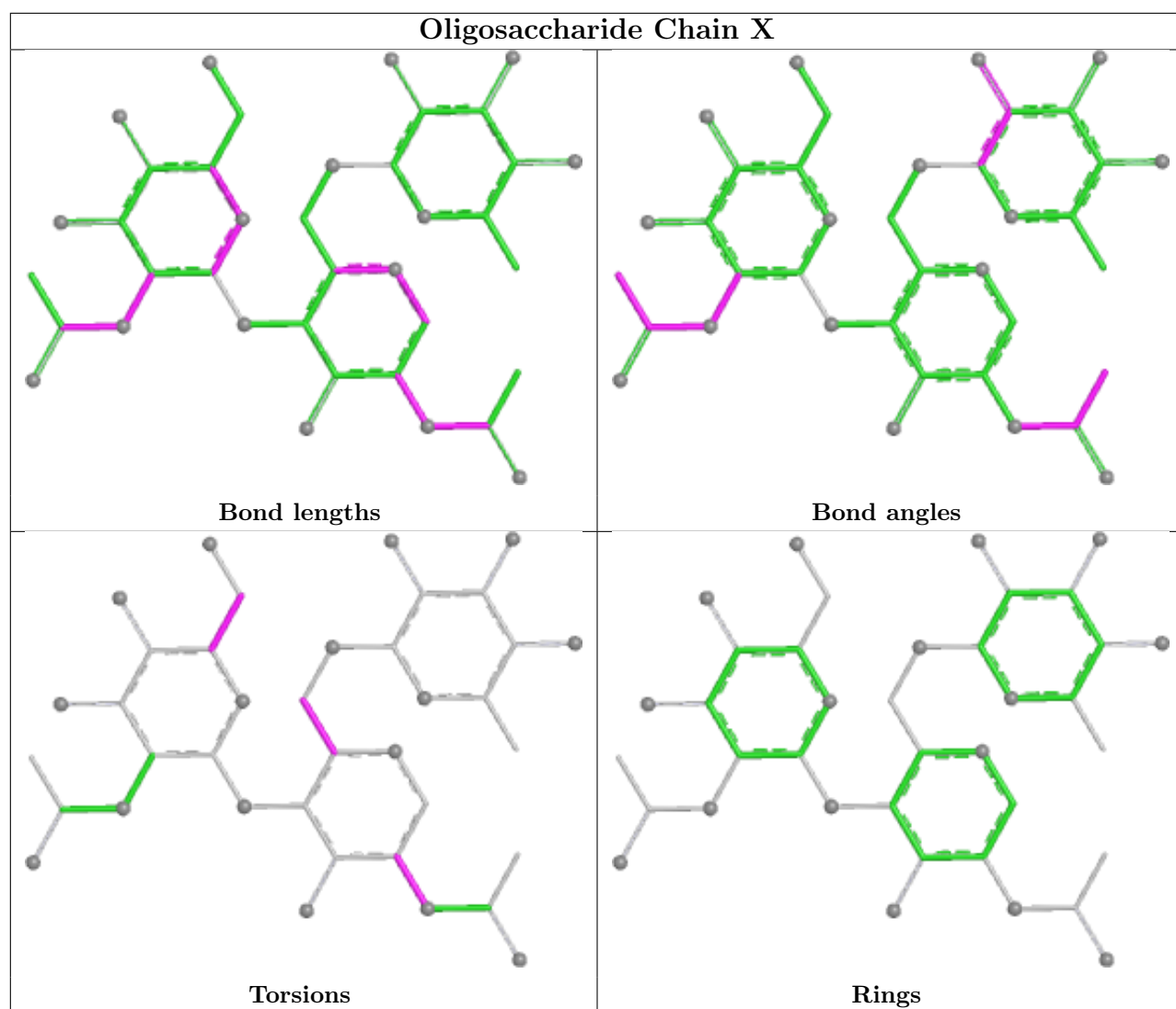


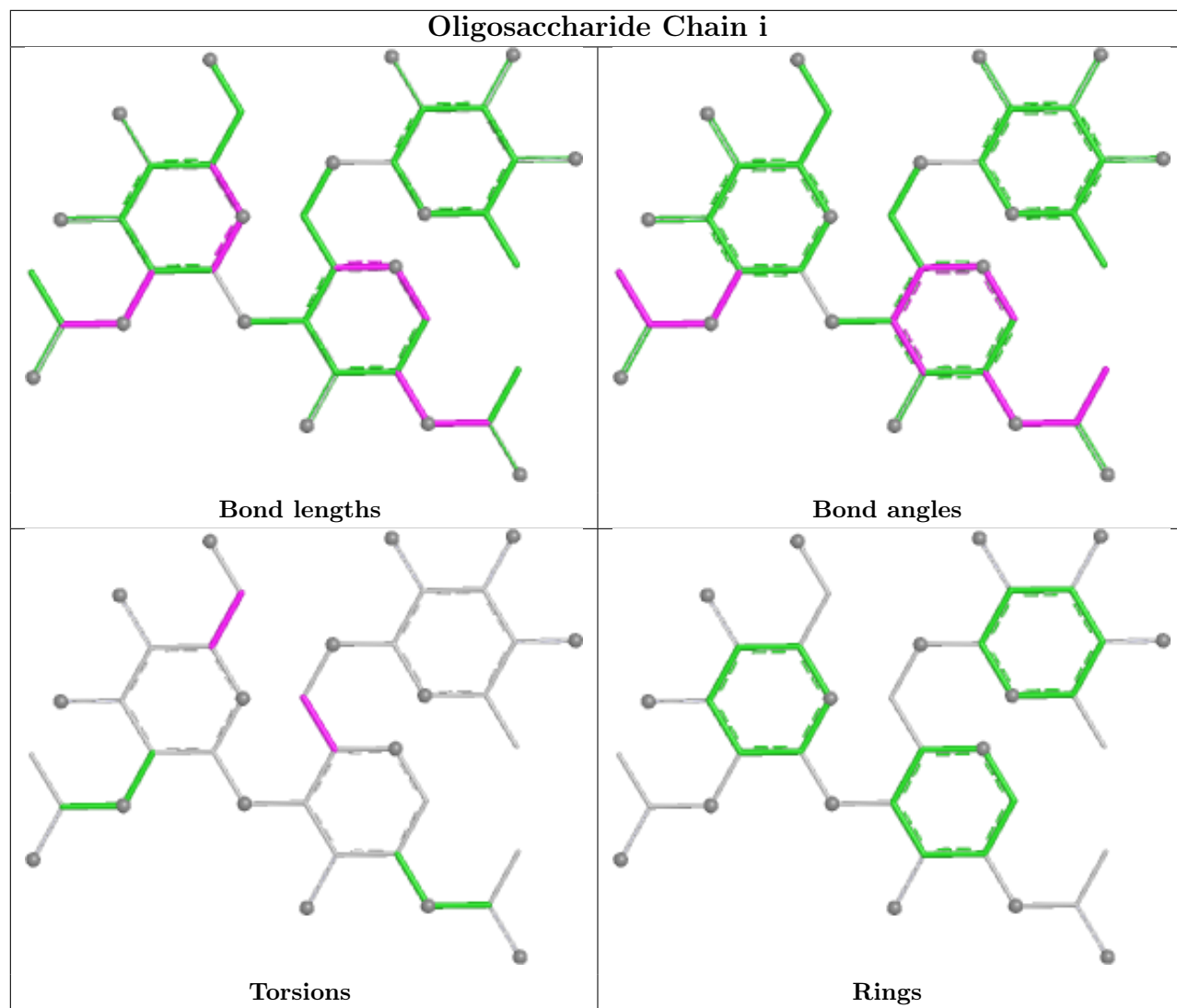


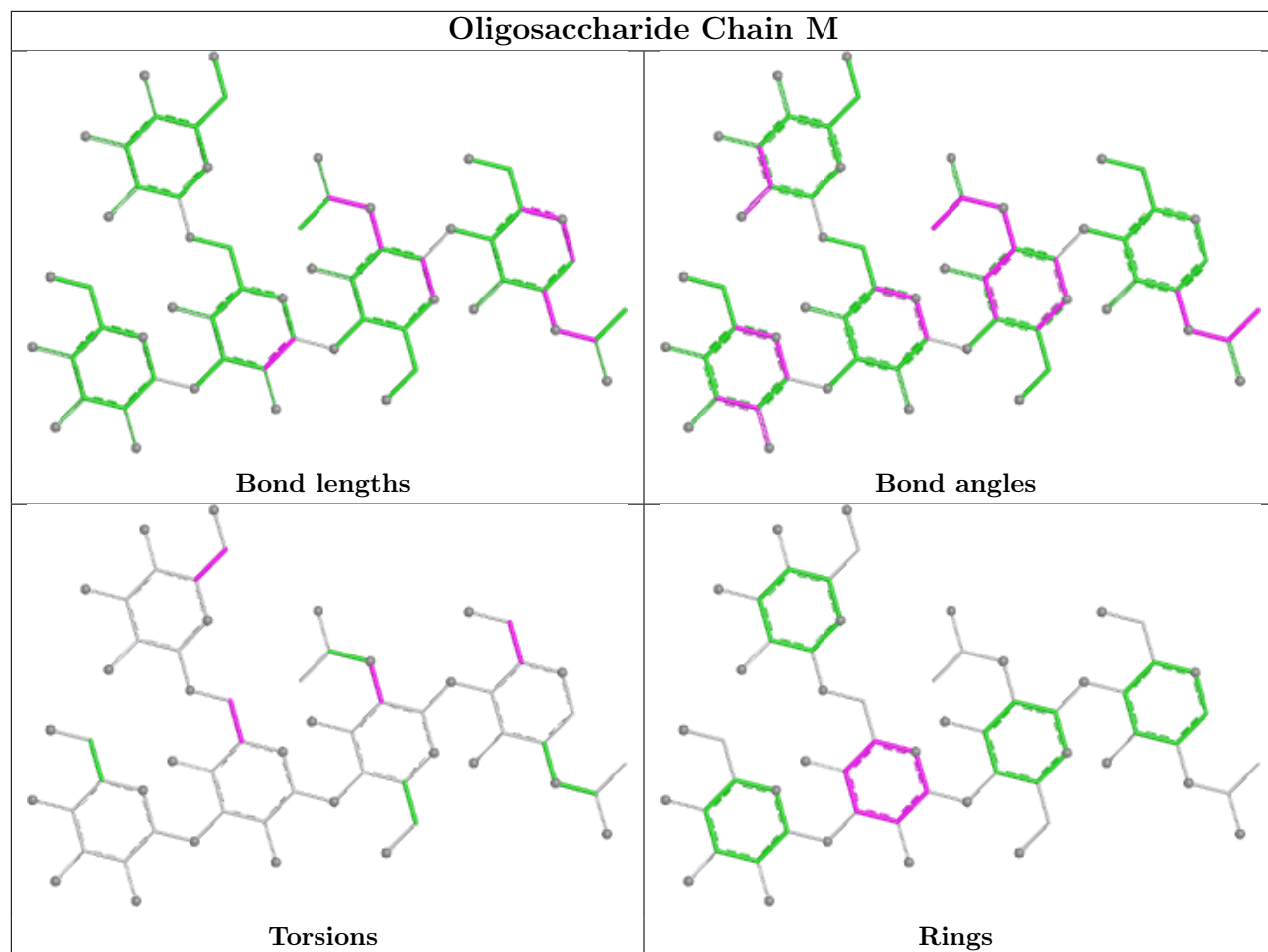


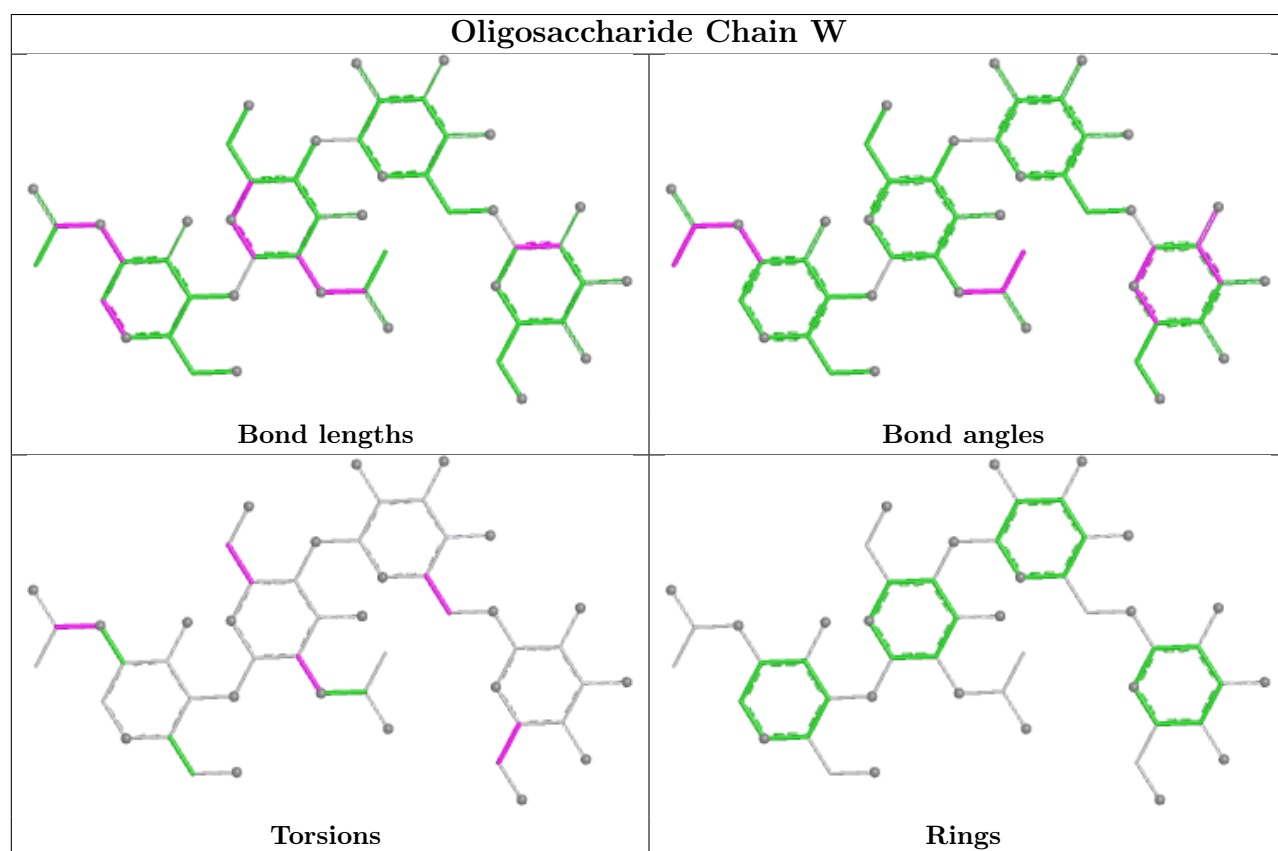
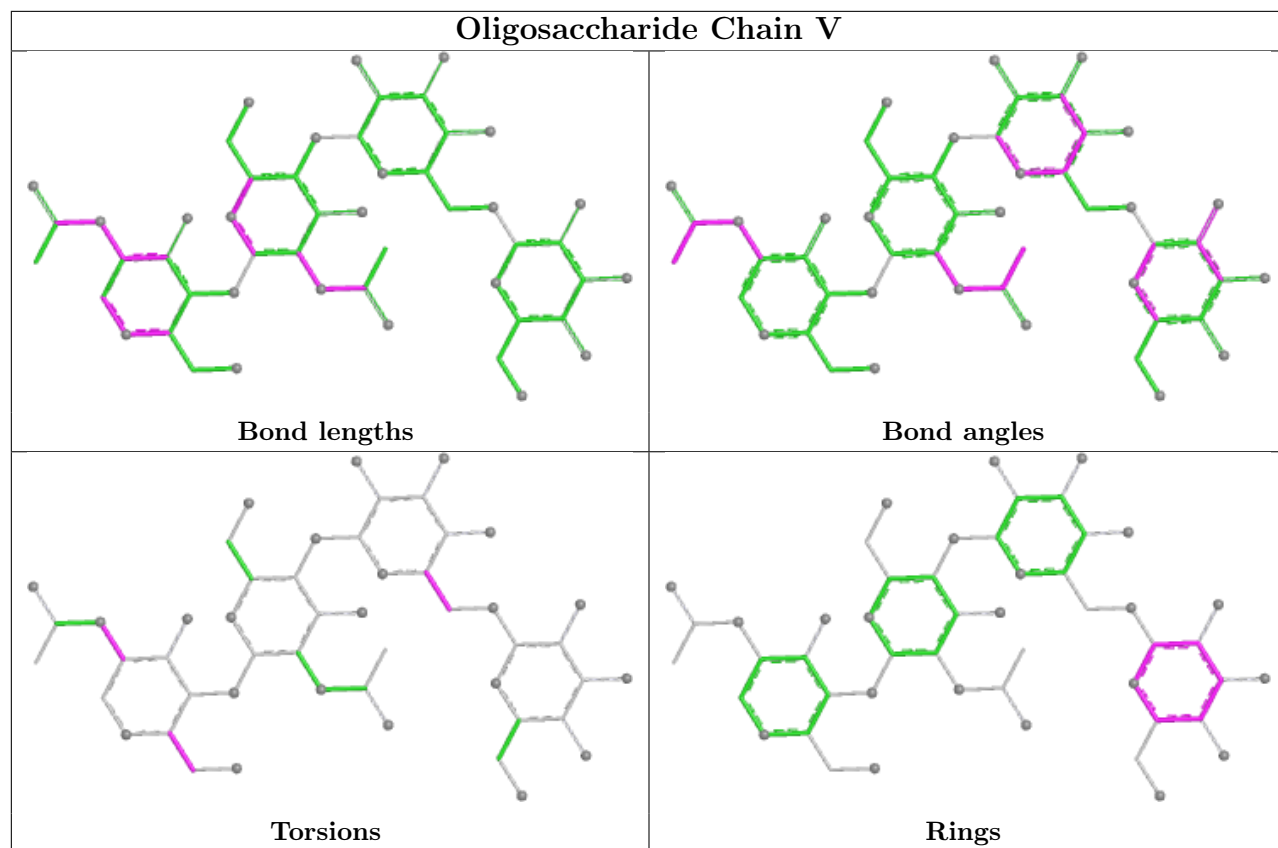


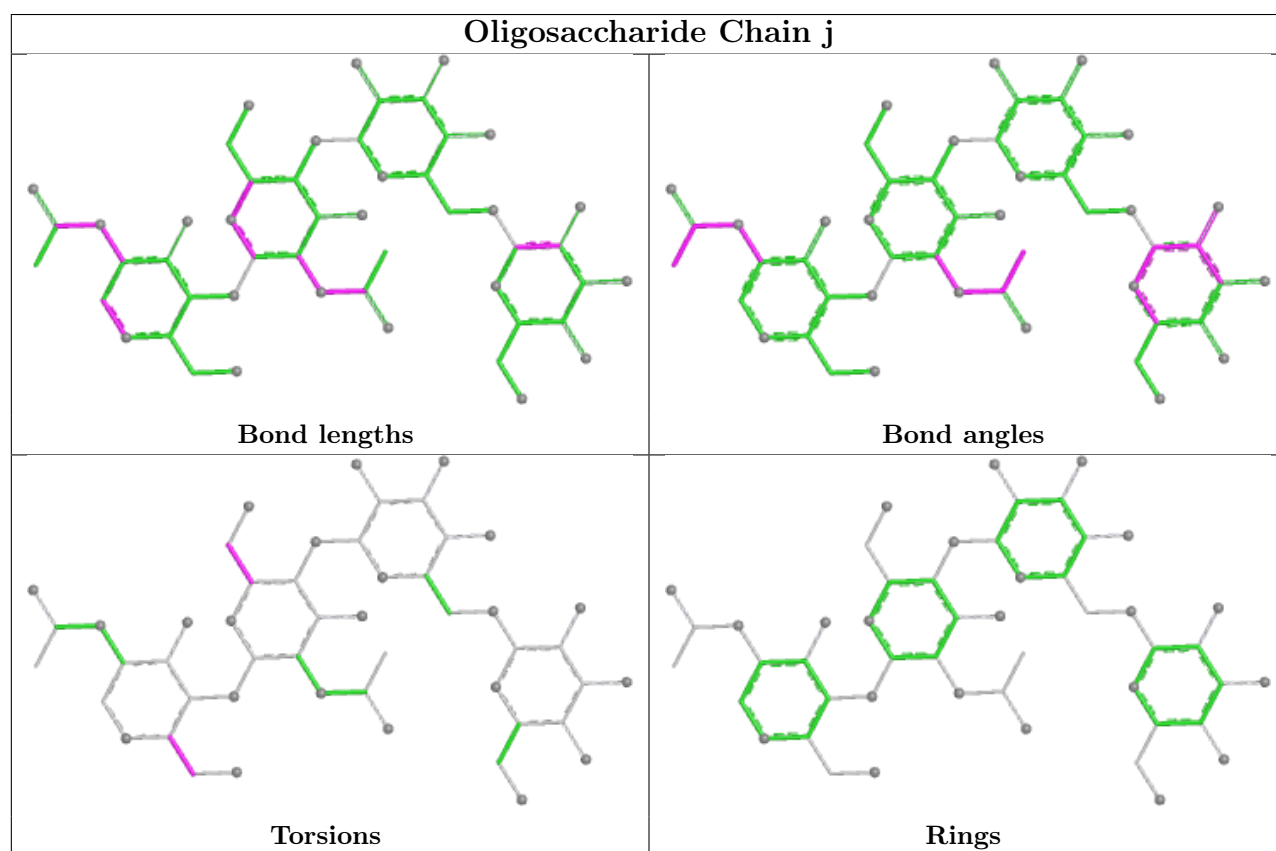
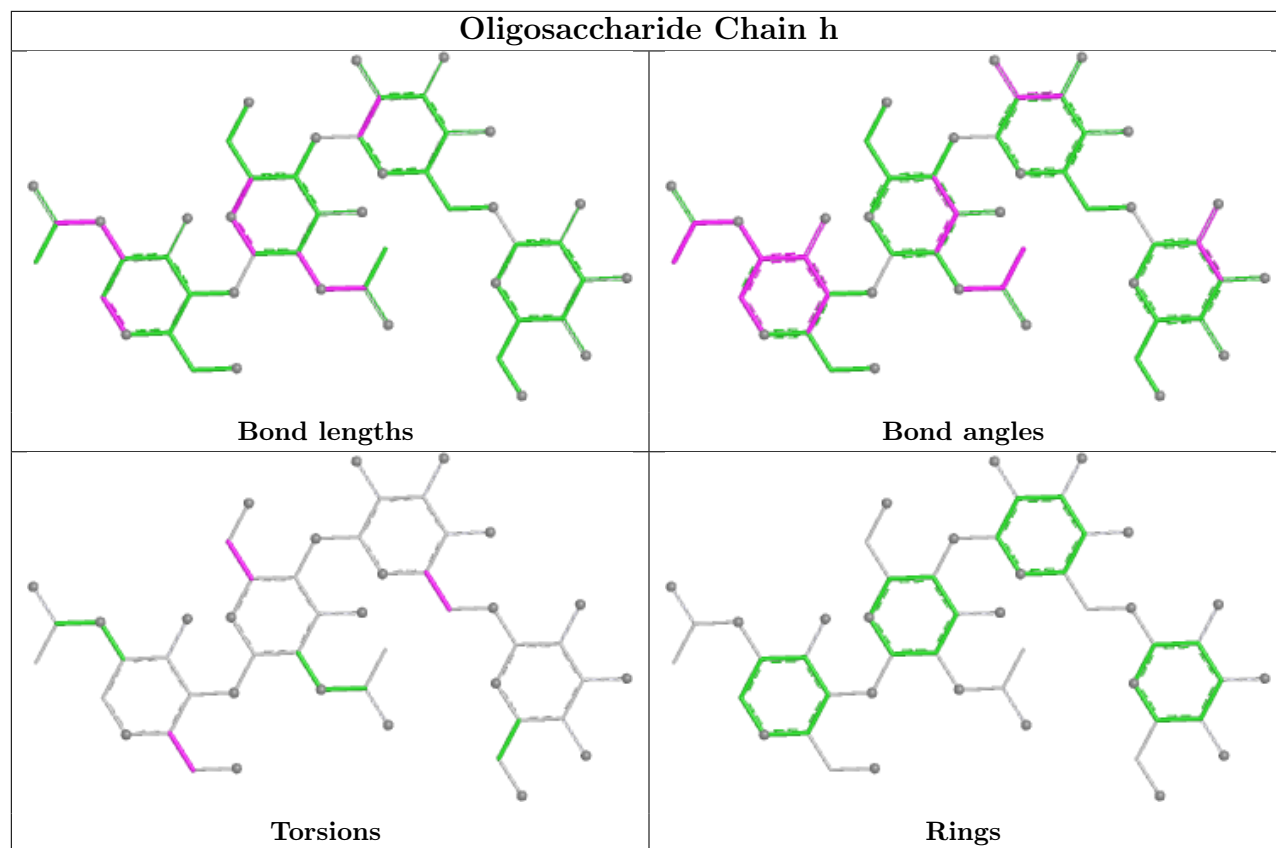


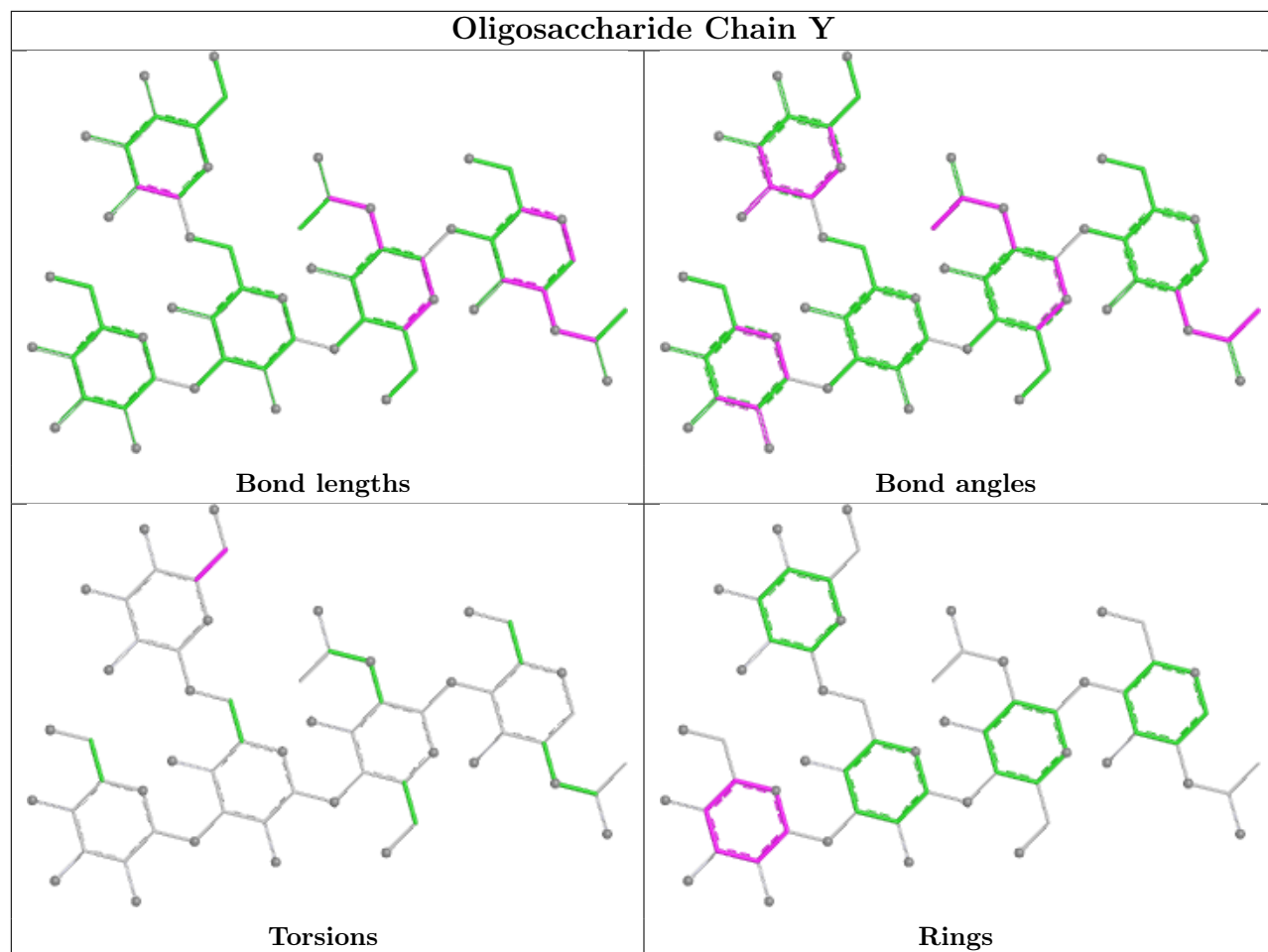


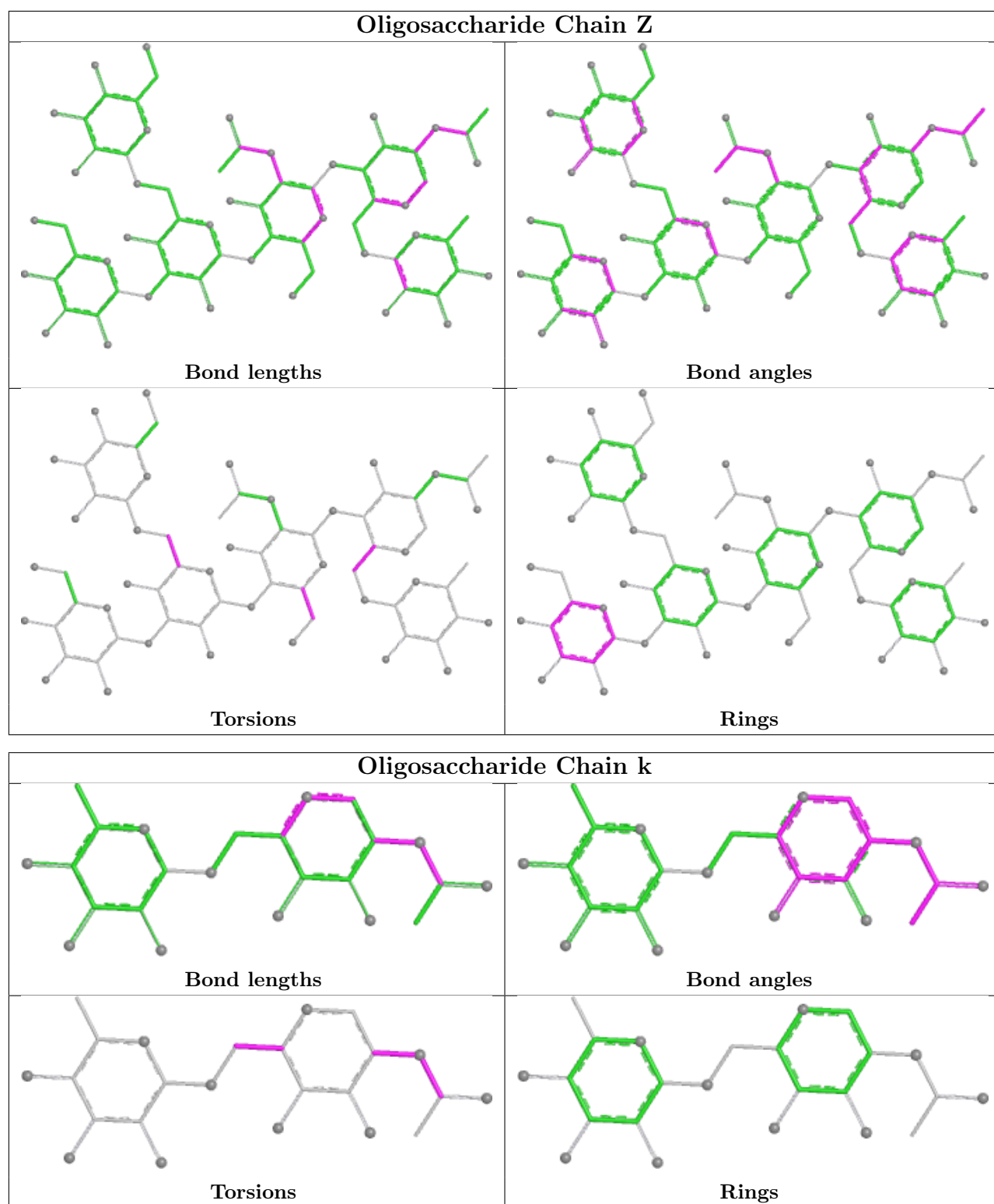


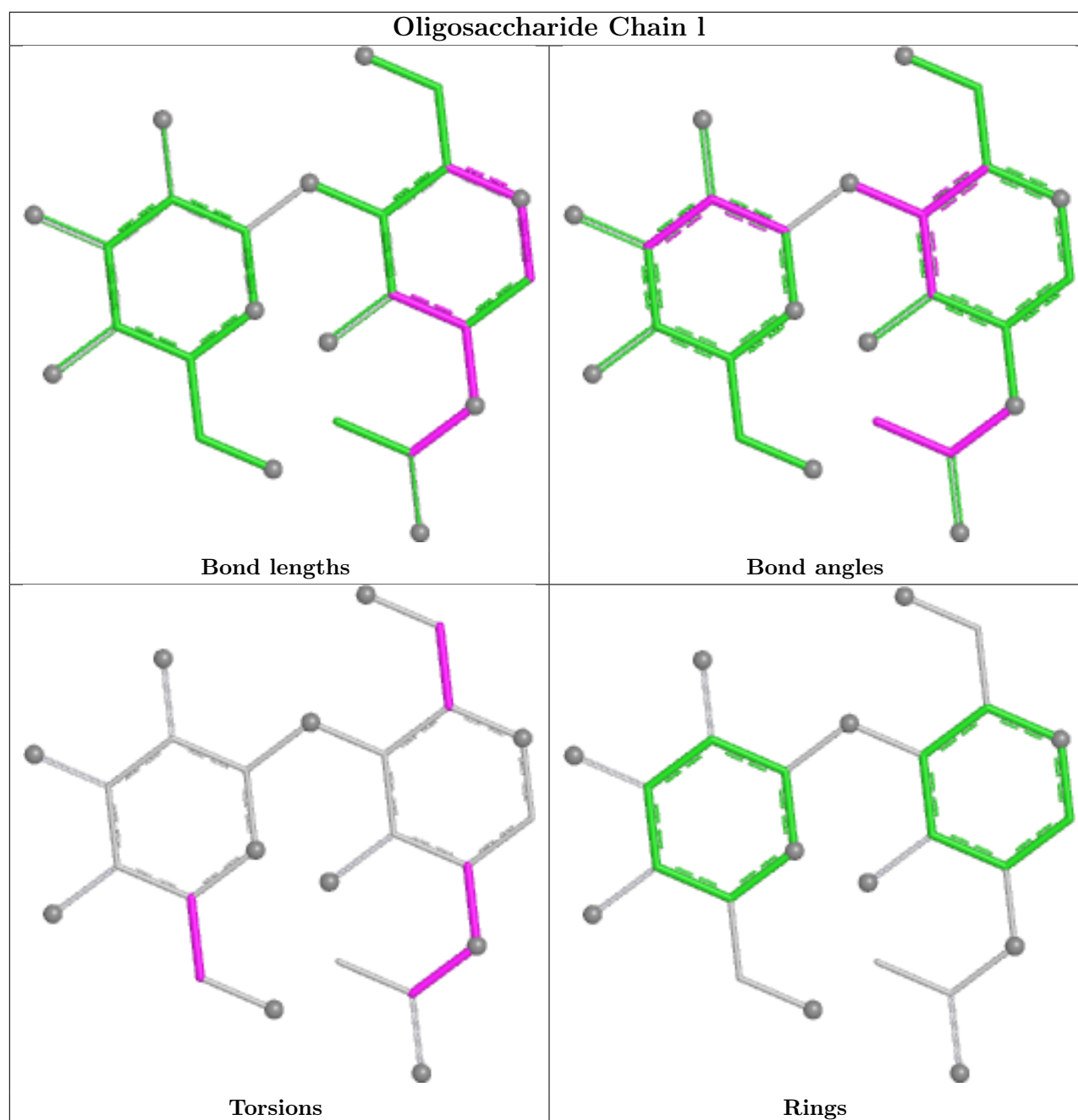












5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	A	1406	-	14,14,15	1.99	4 (28%)	17,19,21	0.91	1 (5%)
12	NAG	B	1404	1	14,14,15	1.98	4 (28%)	17,19,21	1.21	2 (11%)
12	NAG	C	1403	1	14,14,15	2.02	4 (28%)	17,19,21	1.15	1 (5%)
12	NAG	B	1401	1	14,14,15	2.00	4 (28%)	17,19,21	1.02	1 (5%)
12	NAG	B	1403	1	14,14,15	1.98	4 (28%)	17,19,21	1.09	2 (11%)
12	NAG	C	1402	1	14,14,15	2.02	4 (28%)	17,19,21	1.13	2 (11%)
12	NAG	A	1402	1	14,14,15	2.01	4 (28%)	17,19,21	1.15	2 (11%)
12	NAG	C	1405	1	14,14,15	1.99	4 (28%)	17,19,21	0.97	1 (5%)
12	NAG	A	1404	1	14,14,15	2.07	4 (28%)	17,19,21	2.57	7 (41%)
12	NAG	A	1405	1	14,14,15	2.05	4 (28%)	17,19,21	1.19	1 (5%)
12	NAG	B	1402	1	14,14,15	1.99	4 (28%)	17,19,21	1.06	2 (11%)
12	NAG	A	1401	1	14,14,15	1.98	4 (28%)	17,19,21	1.13	2 (11%)
12	NAG	B	1405	1	14,14,15	1.94	3 (21%)	17,19,21	1.65	3 (17%)
12	NAG	C	1404	1	14,14,15	2.05	4 (28%)	17,19,21	1.20	2 (11%)
12	NAG	C	1401	1	14,14,15	2.01	4 (28%)	17,19,21	1.32	1 (5%)
12	NAG	A	1403	1	14,14,15	1.99	4 (28%)	17,19,21	1.14	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	1406	-	-	4/6/23/26	0/1/1/1
12	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
12	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
12	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
12	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
12	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
12	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
12	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
12	NAG	A	1404	1	1/1/6/7	5/6/23/26	0/1/1/1
12	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
12	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
12	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
12	NAG	B	1405	1	-	4/6/23/26	0/1/1/1
12	NAG	C	1404	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	C	1401	1	-	3/6/23/26	0/1/1/1
12	NAG	A	1403	1	-	2/6/23/26	0/1/1/1

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1404	NAG	O5-C1	4.51	1.51	1.43
12	C	1402	NAG	O5-C1	4.41	1.51	1.43
12	A	1405	NAG	O5-C1	4.39	1.51	1.43
12	C	1405	NAG	O5-C1	4.37	1.51	1.43
12	A	1402	NAG	O5-C1	4.33	1.51	1.43
12	A	1404	NAG	O5-C1	4.33	1.51	1.43
12	B	1401	NAG	O5-C1	4.30	1.50	1.43
12	A	1401	NAG	O5-C1	4.30	1.50	1.43
12	B	1402	NAG	O5-C1	4.29	1.50	1.43
12	A	1403	NAG	O5-C1	4.29	1.50	1.43
12	C	1401	NAG	O5-C1	4.28	1.50	1.43
12	C	1403	NAG	O5-C1	4.28	1.50	1.43
12	B	1404	NAG	O5-C1	4.27	1.50	1.43
12	A	1406	NAG	O5-C1	4.21	1.50	1.43
12	B	1403	NAG	O5-C1	4.19	1.50	1.43
12	B	1405	NAG	O5-C1	4.13	1.50	1.43
12	A	1404	NAG	C7-N2	4.07	1.47	1.34
12	C	1403	NAG	C7-N2	3.98	1.47	1.34
12	C	1401	NAG	C7-N2	3.97	1.47	1.34
12	A	1405	NAG	C7-N2	3.95	1.47	1.34
12	B	1401	NAG	C7-N2	3.90	1.46	1.34
12	B	1405	NAG	C7-N2	3.90	1.46	1.34
12	C	1402	NAG	C7-N2	3.89	1.46	1.34
12	A	1403	NAG	C7-N2	3.89	1.46	1.34
12	A	1406	NAG	C7-N2	3.88	1.46	1.34
12	B	1403	NAG	C7-N2	3.87	1.46	1.34
12	C	1404	NAG	C7-N2	3.87	1.46	1.34
12	B	1402	NAG	C7-N2	3.87	1.46	1.34
12	B	1404	NAG	C7-N2	3.86	1.46	1.34
12	A	1402	NAG	C7-N2	3.86	1.46	1.34
12	A	1401	NAG	C7-N2	3.86	1.46	1.34
12	C	1405	NAG	C7-N2	3.79	1.46	1.34
12	A	1404	NAG	C2-N2	2.72	1.50	1.46
12	B	1405	NAG	C2-N2	2.61	1.50	1.46
12	C	1403	NAG	C2-N2	2.57	1.50	1.46
12	C	1401	NAG	C2-N2	2.55	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1405	NAG	C2-N2	2.53	1.50	1.46
12	A	1406	NAG	C2-N2	2.48	1.50	1.46
12	B	1401	NAG	C2-N2	2.47	1.50	1.46
12	C	1402	NAG	C2-N2	2.45	1.50	1.46
12	A	1403	NAG	C2-N2	2.44	1.50	1.46
12	A	1402	NAG	C2-N2	2.44	1.50	1.46
12	B	1404	NAG	C2-N2	2.43	1.50	1.46
12	B	1403	NAG	C2-N2	2.43	1.50	1.46
12	B	1402	NAG	C2-N2	2.41	1.50	1.46
12	C	1404	NAG	O5-C5	2.41	1.48	1.43
12	C	1404	NAG	C2-N2	2.39	1.50	1.46
12	A	1401	NAG	C2-N2	2.35	1.50	1.46
12	A	1402	NAG	O5-C5	2.34	1.48	1.43
12	A	1405	NAG	O5-C5	2.32	1.47	1.43
12	C	1405	NAG	C2-N2	2.30	1.50	1.46
12	A	1404	NAG	O5-C5	2.24	1.47	1.43
12	C	1405	NAG	O5-C5	2.23	1.47	1.43
12	B	1402	NAG	O5-C5	2.22	1.47	1.43
12	B	1401	NAG	O5-C5	2.20	1.47	1.43
12	B	1403	NAG	O5-C5	2.18	1.47	1.43
12	B	1404	NAG	O5-C5	2.18	1.47	1.43
12	C	1403	NAG	O5-C5	2.18	1.47	1.43
12	C	1402	NAG	O5-C5	2.17	1.47	1.43
12	A	1406	NAG	O5-C5	2.17	1.47	1.43
12	C	1401	NAG	O5-C5	2.15	1.47	1.43
12	A	1403	NAG	O5-C5	2.15	1.47	1.43
12	A	1401	NAG	O5-C5	2.12	1.47	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1404	NAG	C3-C4-C5	6.03	121.17	110.23
12	A	1404	NAG	C8-C7-N2	4.43	123.47	116.12
12	A	1404	NAG	O4-C4-C5	3.82	118.74	109.32
12	A	1404	NAG	C1-O5-C5	-3.76	107.14	112.19
12	B	1405	NAG	C4-C3-C2	3.75	116.52	111.02
12	A	1404	NAG	O4-C4-C3	3.50	118.62	110.38
12	B	1405	NAG	C2-N2-C7	-3.45	118.27	122.90
12	C	1401	NAG	C8-C7-N2	3.34	121.65	116.12
12	A	1405	NAG	C8-C7-N2	3.21	121.44	116.12
12	C	1403	NAG	C8-C7-N2	3.14	121.33	116.12
12	A	1401	NAG	C2-N2-C7	-2.60	119.42	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1401	NAG	C8-C7-N2	2.38	120.07	116.12
12	C	1402	NAG	C8-C7-N2	2.36	120.04	116.12
12	A	1402	NAG	C8-C7-N2	2.36	120.03	116.12
12	A	1402	NAG	C2-N2-C7	-2.34	119.76	122.90
12	A	1403	NAG	C8-C7-N2	2.33	119.99	116.12
12	C	1404	NAG	C8-C7-N2	2.32	119.97	116.12
12	B	1403	NAG	C8-C7-N2	2.32	119.96	116.12
12	B	1403	NAG	C2-N2-C7	-2.31	119.80	122.90
12	B	1401	NAG	C8-C7-N2	2.25	119.85	116.12
12	B	1402	NAG	C8-C7-N2	2.23	119.82	116.12
12	B	1404	NAG	C8-C7-N2	2.23	119.81	116.12
12	C	1402	NAG	C2-N2-C7	-2.20	119.95	122.90
12	C	1404	NAG	C2-N2-C7	-2.20	119.95	122.90
12	B	1402	NAG	C2-N2-C7	-2.16	120.00	122.90
12	A	1404	NAG	O7-C7-C8	-2.13	118.26	122.05
12	A	1404	NAG	O7-C7-N2	-2.10	118.27	121.98
12	B	1405	NAG	C8-C7-N2	2.05	119.52	116.12
12	A	1406	NAG	C8-C7-N2	2.04	119.51	116.12
12	A	1403	NAG	C2-N2-C7	-2.03	120.18	122.90
12	C	1405	NAG	C6-C5-C4	-2.02	108.06	113.02
12	B	1404	NAG	C2-N2-C7	-2.01	120.20	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1404	NAG	C4

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1404	NAG	C1-C2-N2-C7
12	A	1406	NAG	C1-C2-N2-C7
12	A	1404	NAG	C4-C5-C6-O6
12	A	1403	NAG	O5-C5-C6-O6
12	B	1401	NAG	O5-C5-C6-O6
12	A	1404	NAG	O5-C5-C6-O6
12	B	1405	NAG	O5-C5-C6-O6
12	C	1403	NAG	O5-C5-C6-O6
12	A	1402	NAG	O5-C5-C6-O6
12	A	1402	NAG	C4-C5-C6-O6
12	A	1406	NAG	O5-C5-C6-O6
12	A	1403	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	B	1405	NAG	C4-C5-C6-O6
12	B	1401	NAG	C4-C5-C6-O6
12	A	1406	NAG	C4-C5-C6-O6
12	C	1403	NAG	C4-C5-C6-O6
12	A	1404	NAG	C8-C7-N2-C2
12	A	1404	NAG	O7-C7-N2-C2
12	A	1405	NAG	C8-C7-N2-C2
12	A	1405	NAG	O7-C7-N2-C2
12	B	1405	NAG	C8-C7-N2-C2
12	B	1405	NAG	O7-C7-N2-C2
12	C	1401	NAG	C8-C7-N2-C2
12	C	1401	NAG	O7-C7-N2-C2
12	C	1403	NAG	C8-C7-N2-C2
12	C	1403	NAG	O7-C7-N2-C2
12	C	1401	NAG	O5-C5-C6-O6
12	A	1406	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

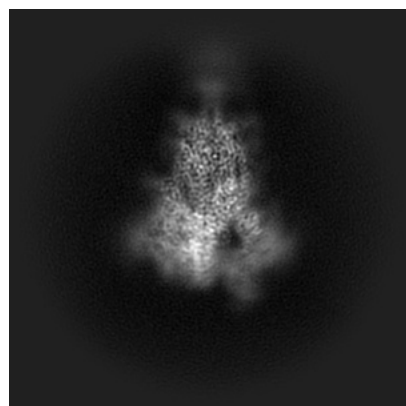
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44447. These allow visual inspection of the internal detail of the map and identification of artifacts.

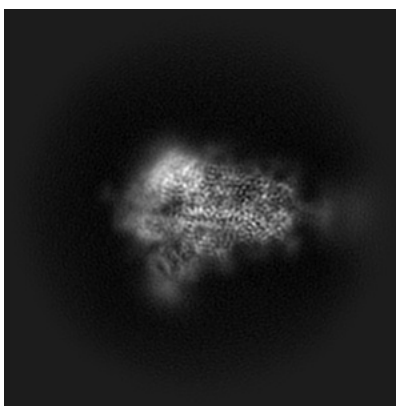
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

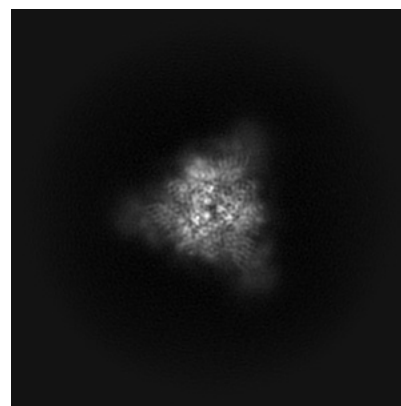
6.1.1 Primary map



X

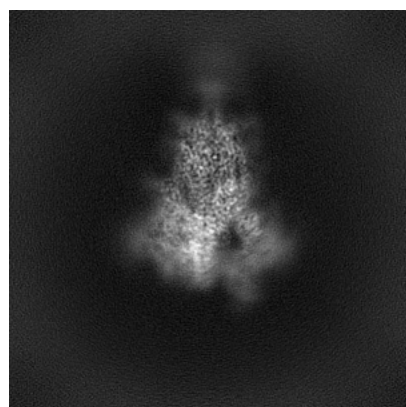


Y

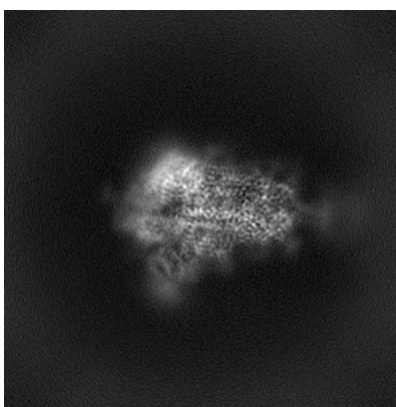


Z

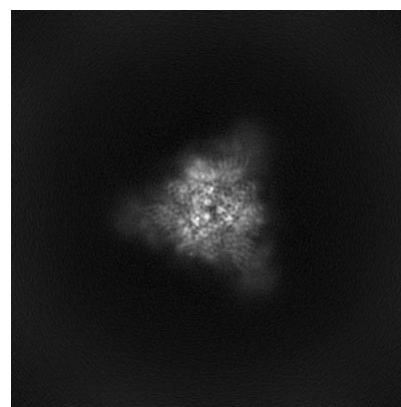
6.1.2 Raw map



X



Y

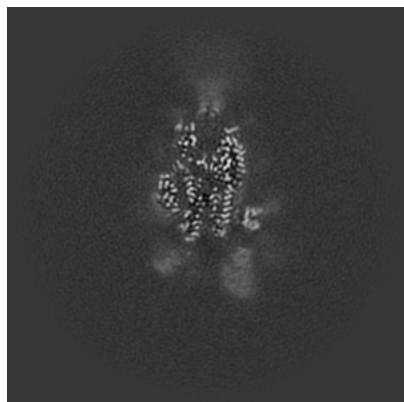


Z

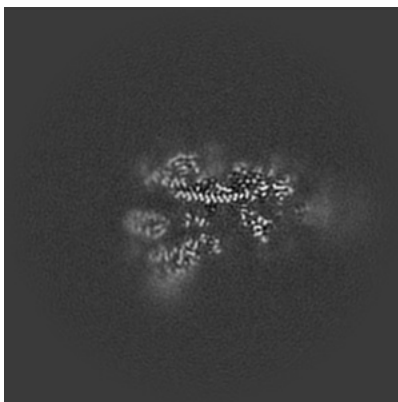
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

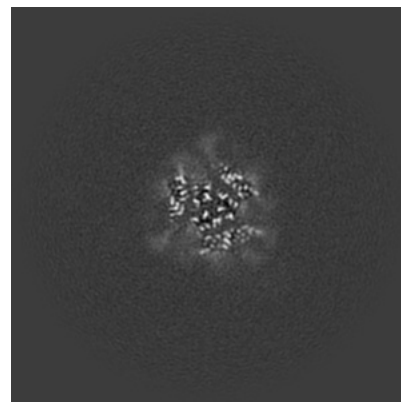
6.2.1 Primary map



X Index: 150

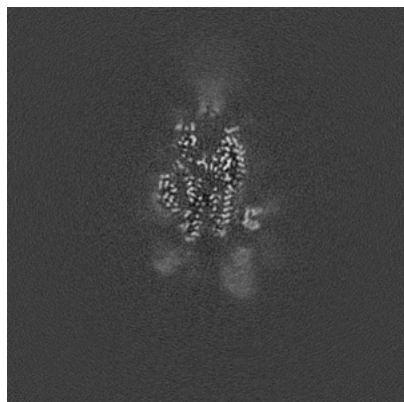


Y Index: 150

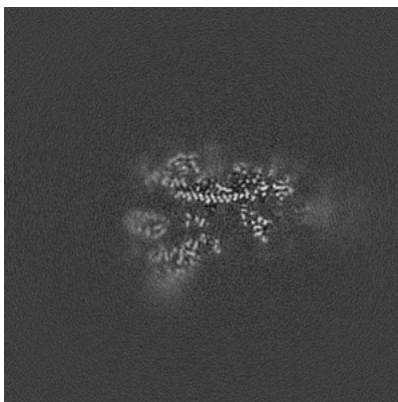


Z Index: 150

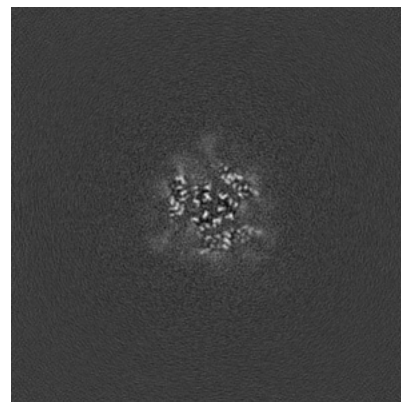
6.2.2 Raw map



X Index: 150



Y Index: 150

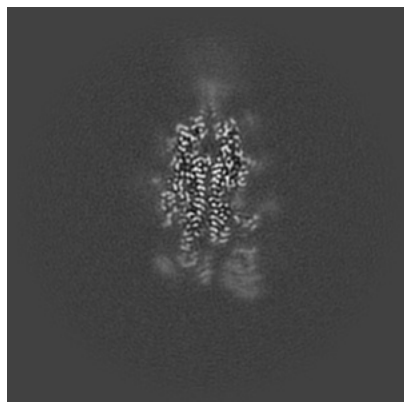


Z Index: 150

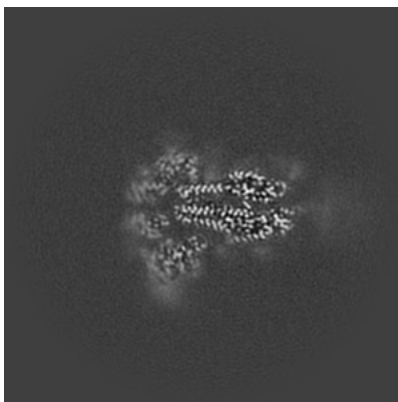
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

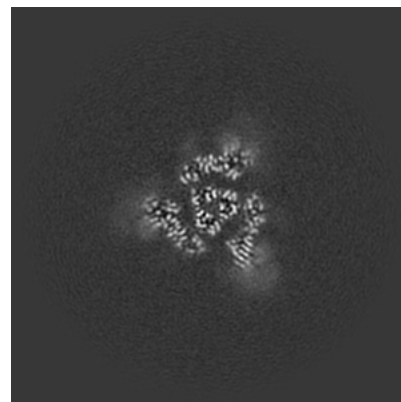
6.3.1 Primary map



X Index: 145

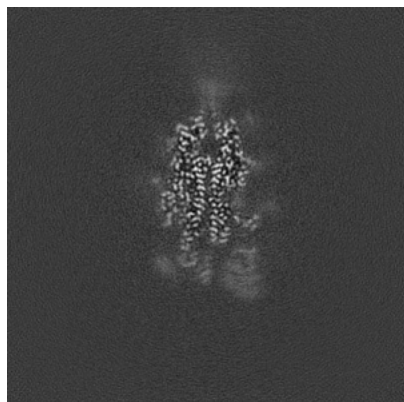


Y Index: 143

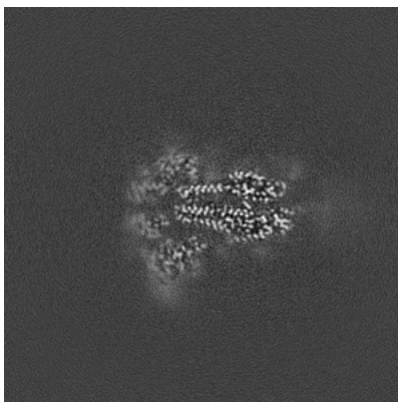


Z Index: 135

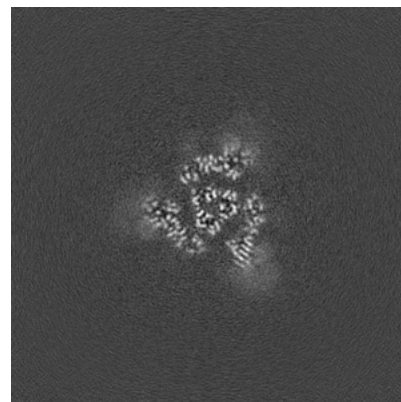
6.3.2 Raw map



X Index: 145



Y Index: 143

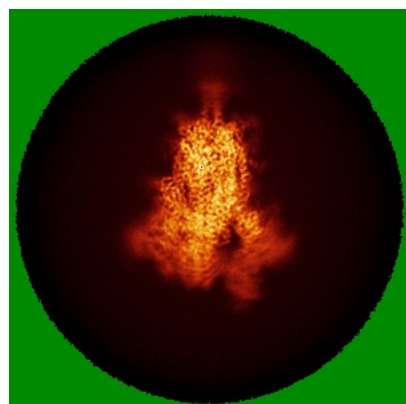


Z Index: 135

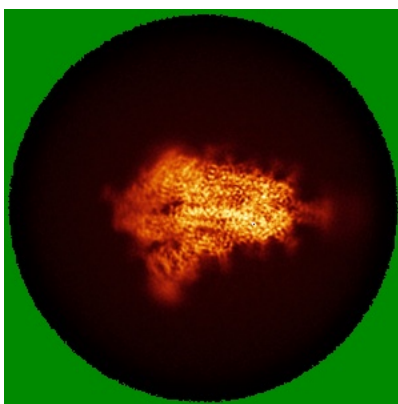
The images above show the largest variance slices of the map in three orthogonal directions.

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

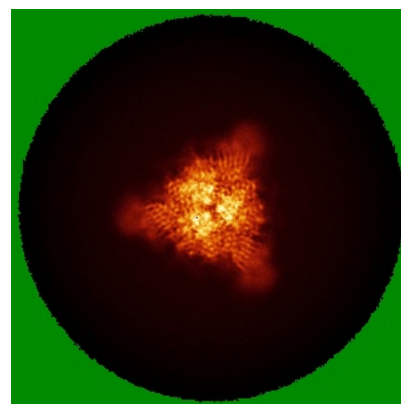
6.4.1 Primary map



X

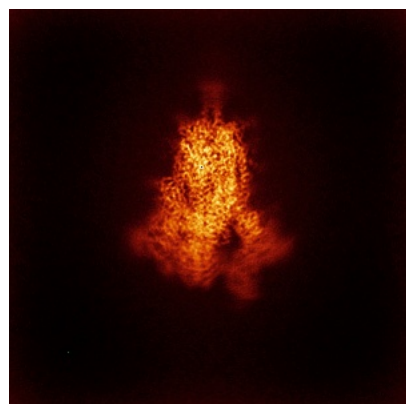


Y

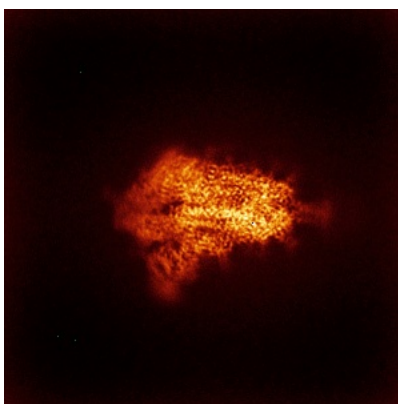


Z

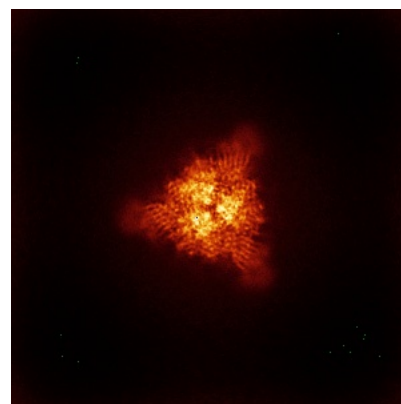
6.4.2 Raw map



X



Y

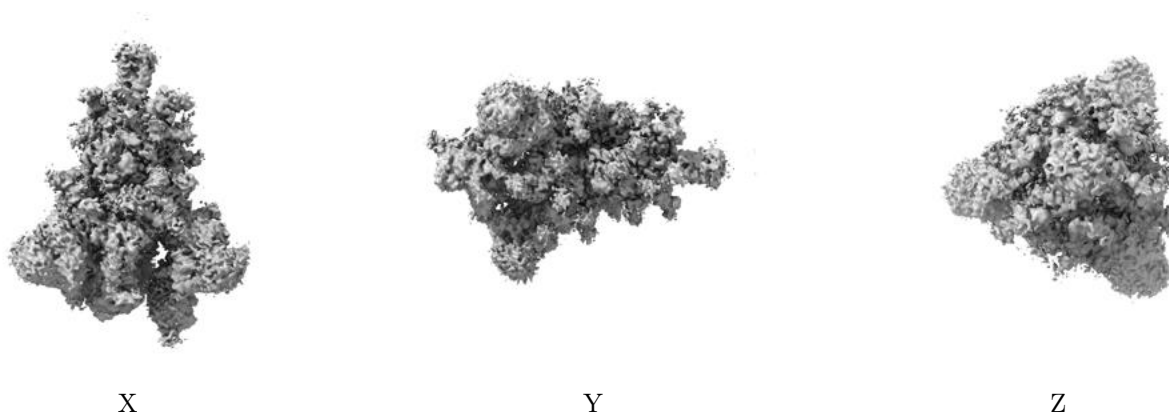


Z

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

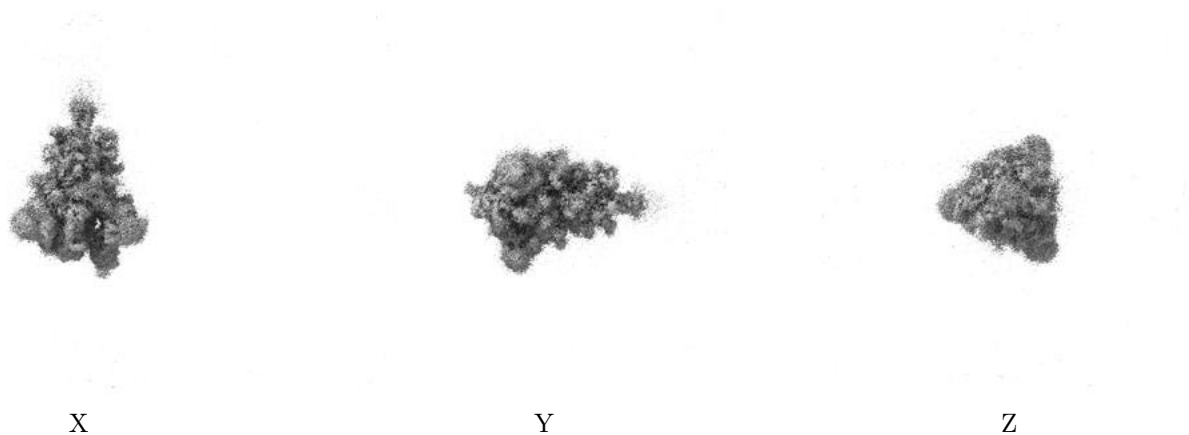
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

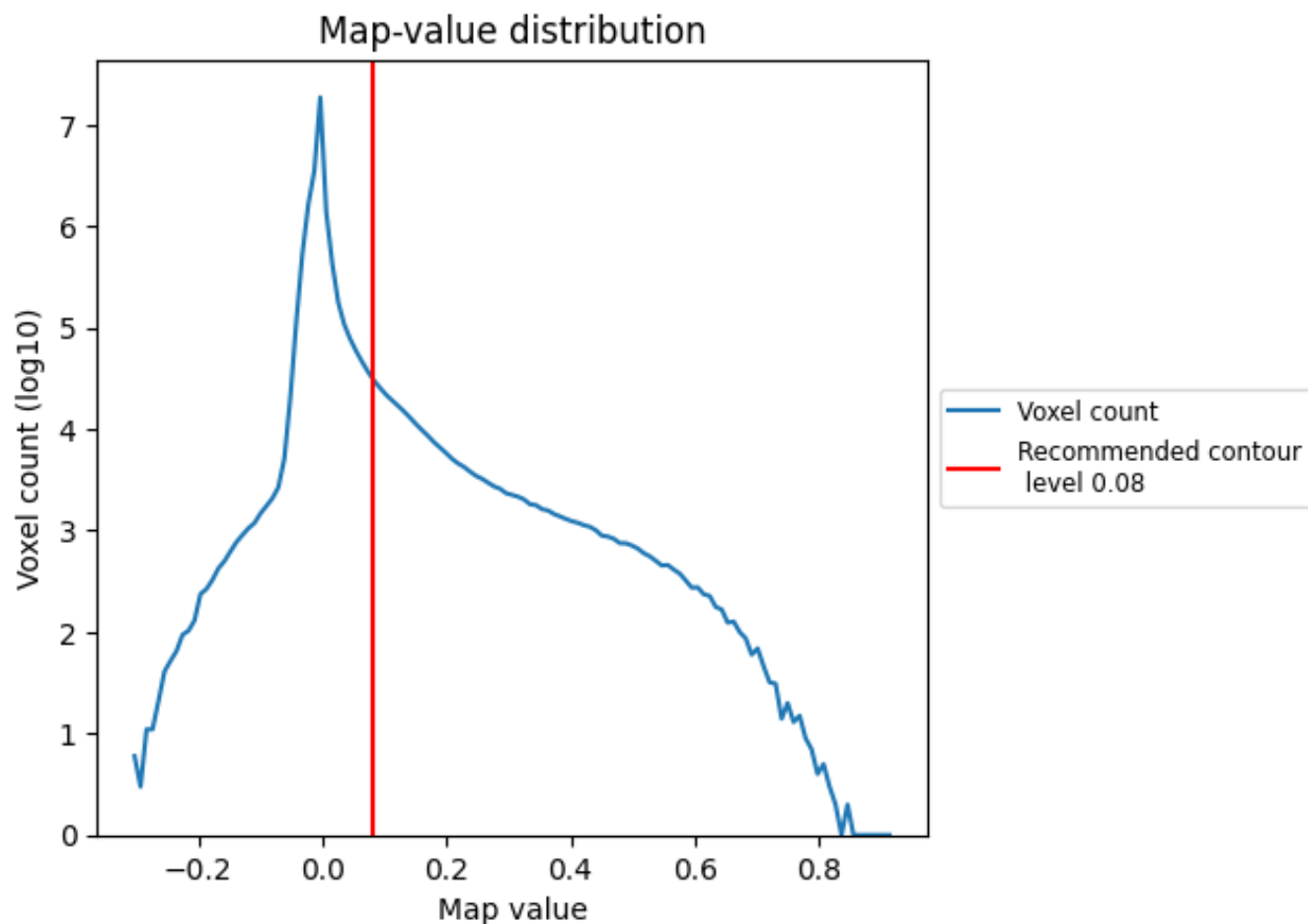
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

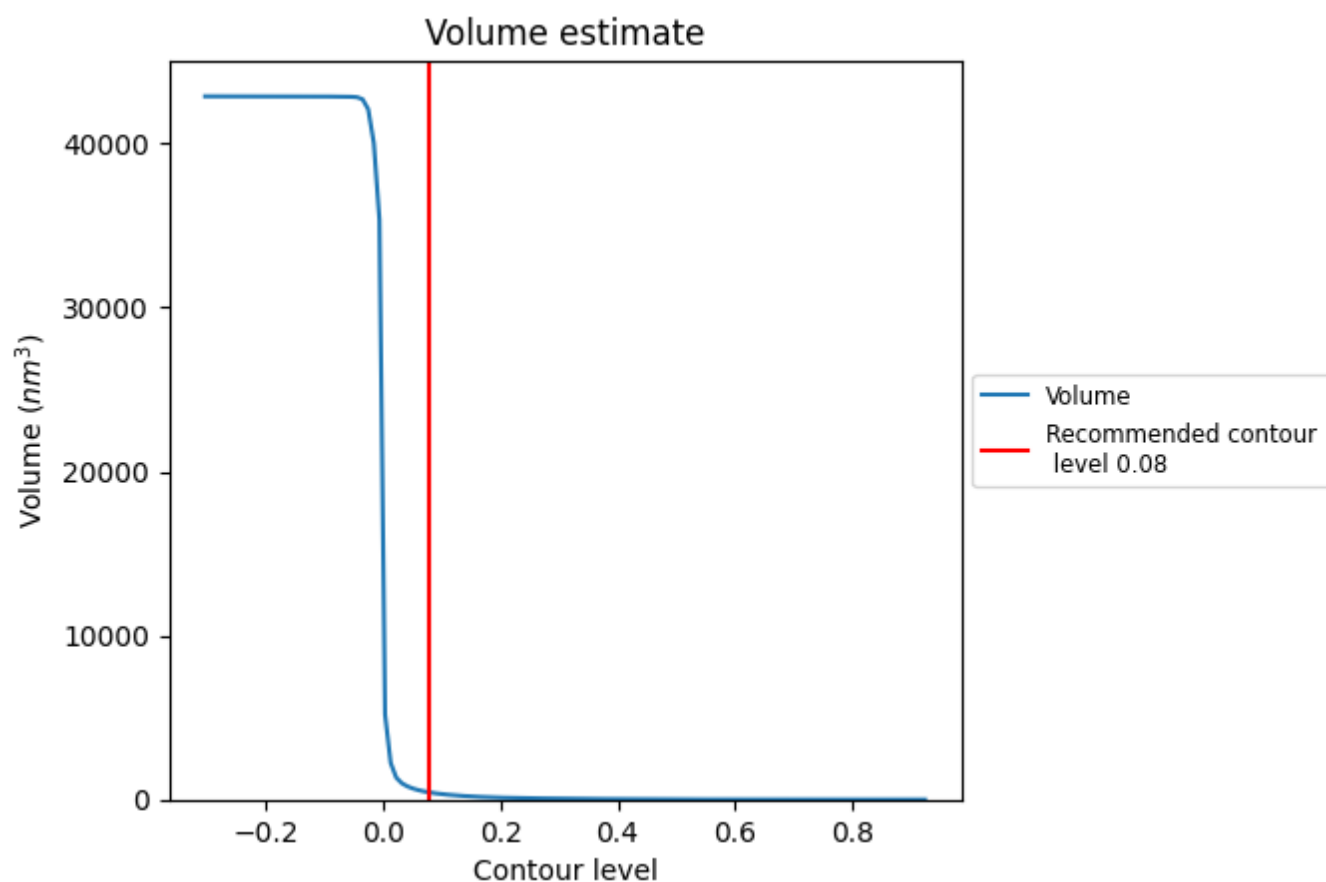
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

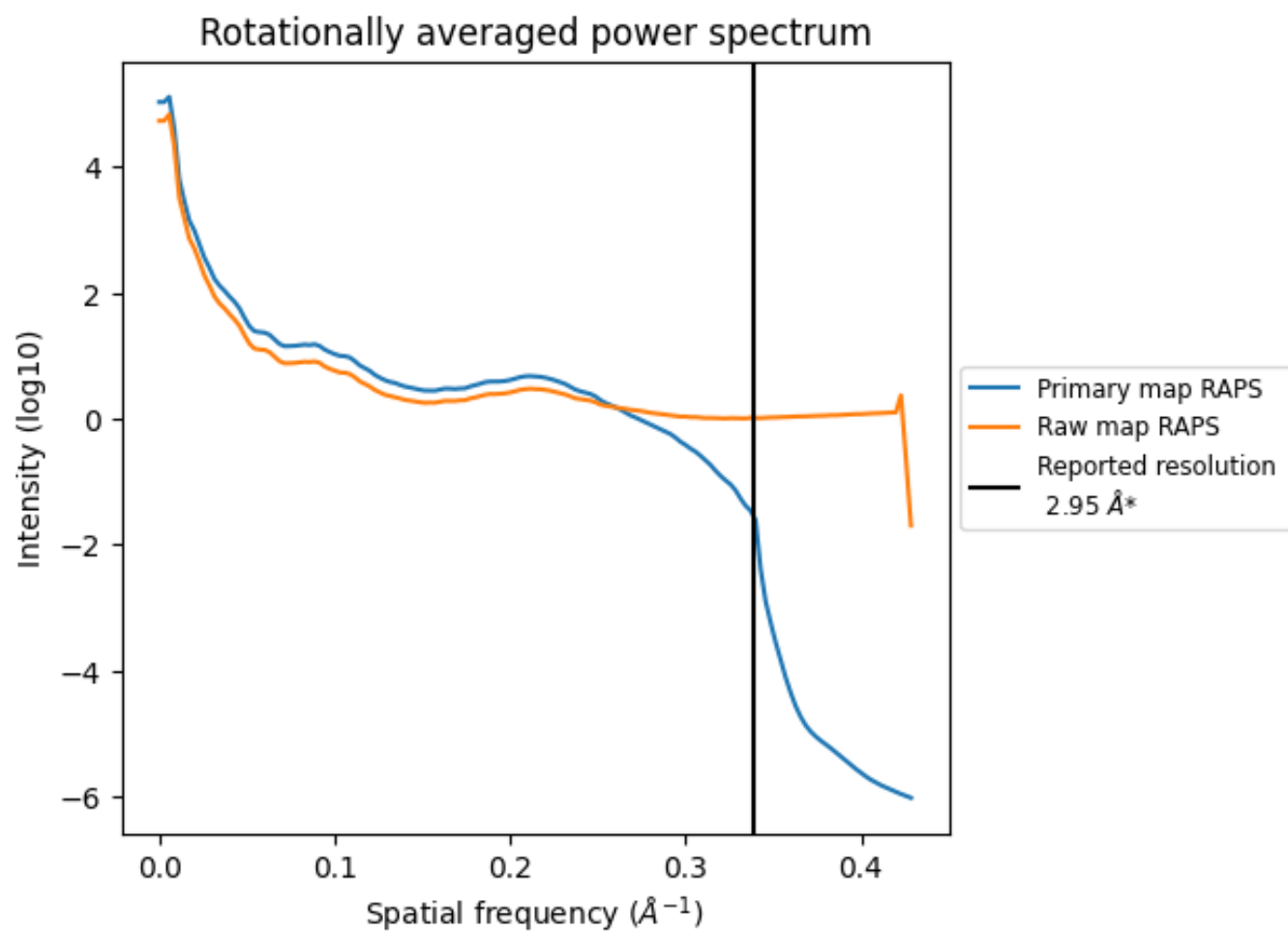
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 432 nm³; this corresponds to an approximate mass of 390 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 ⓘ

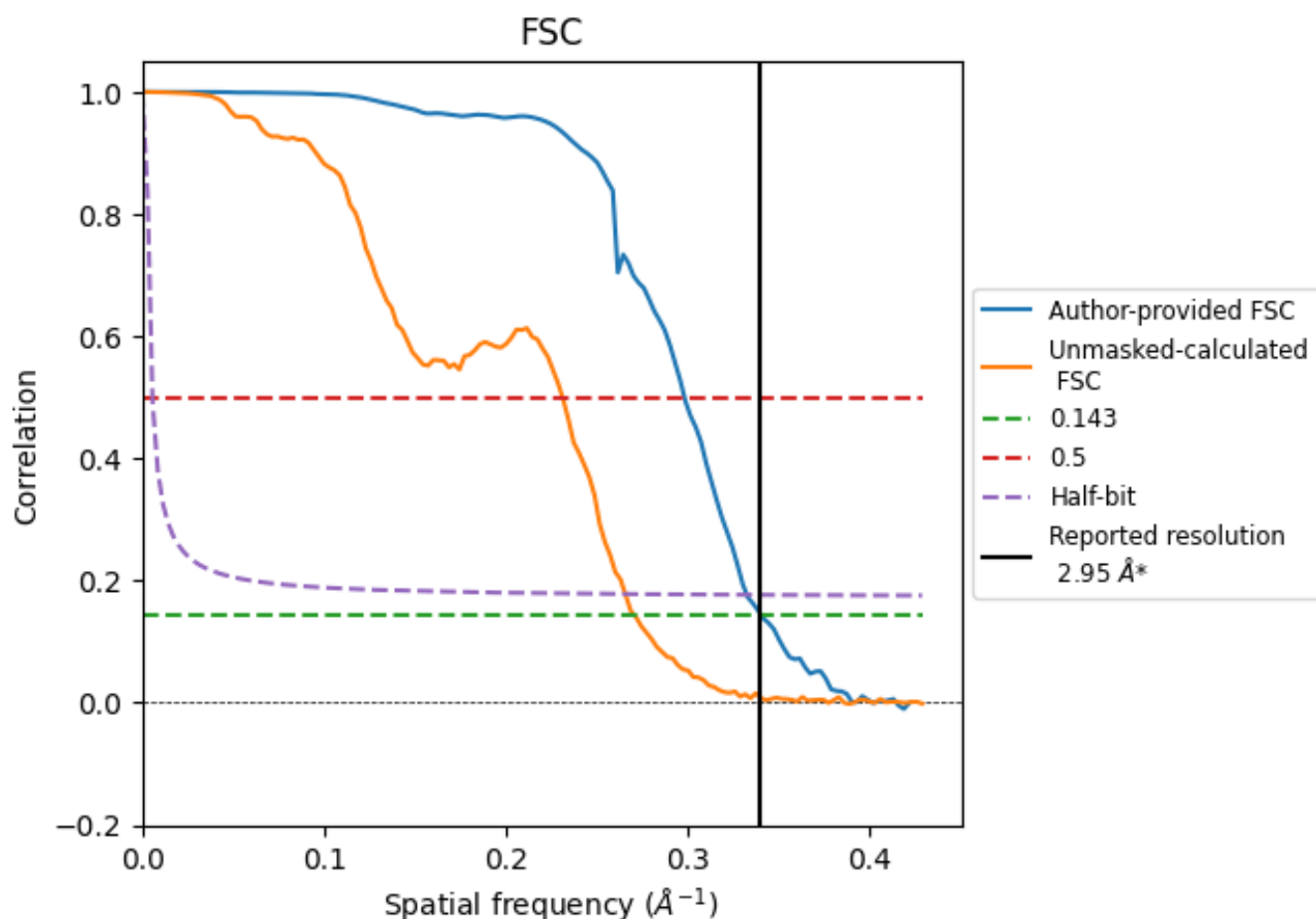


*Reported resolution corresponds to spatial frequency of 0.339 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.339 \AA^{-1}

8.2 Resolution estimates [i](#)

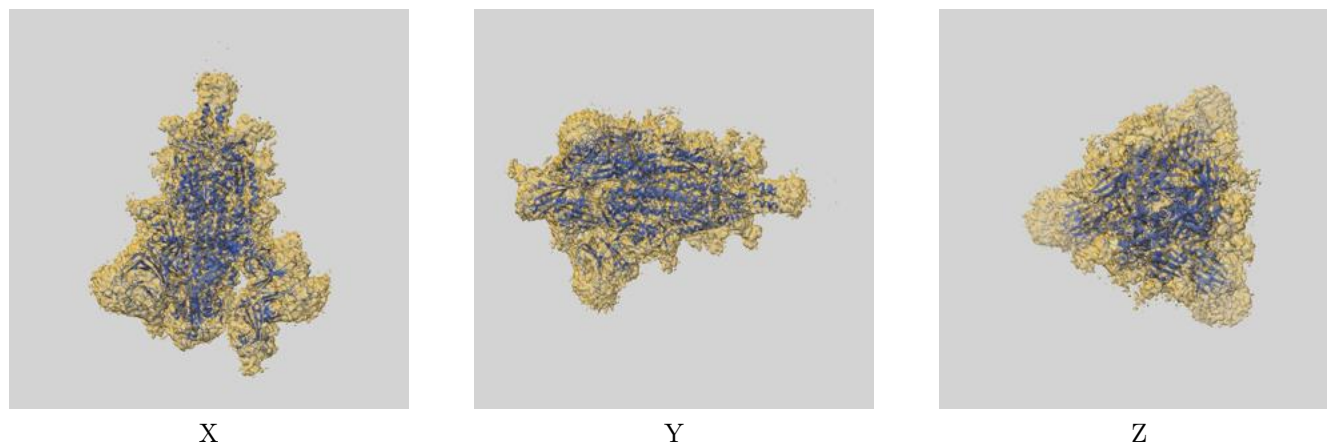
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.94	3.36	3.01
Unmasked-calculated*	3.70	4.33	3.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 2.95 by more than 10 %

9 Map-model fit [i](#)

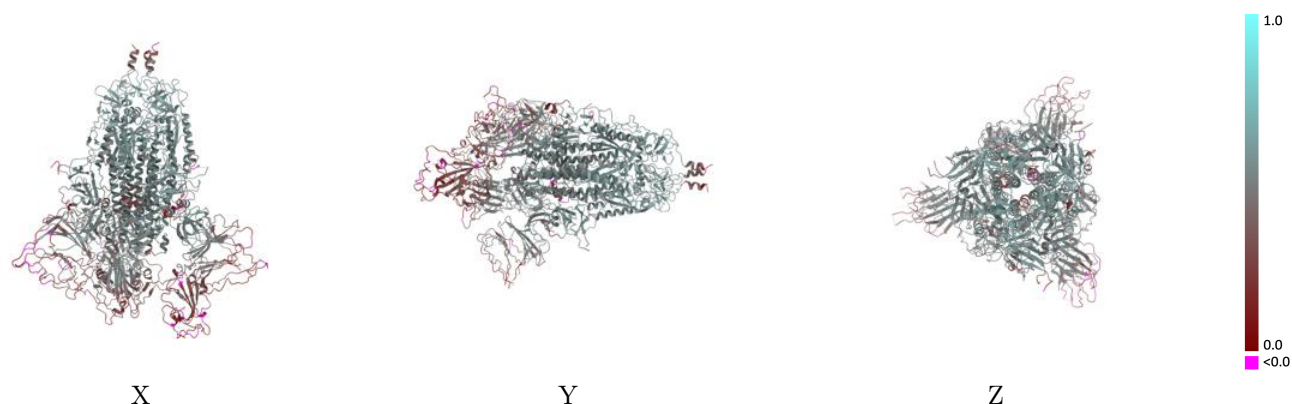
This section contains information regarding the fit between EMDB map EMD-44447 and PDB model 9BD9. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



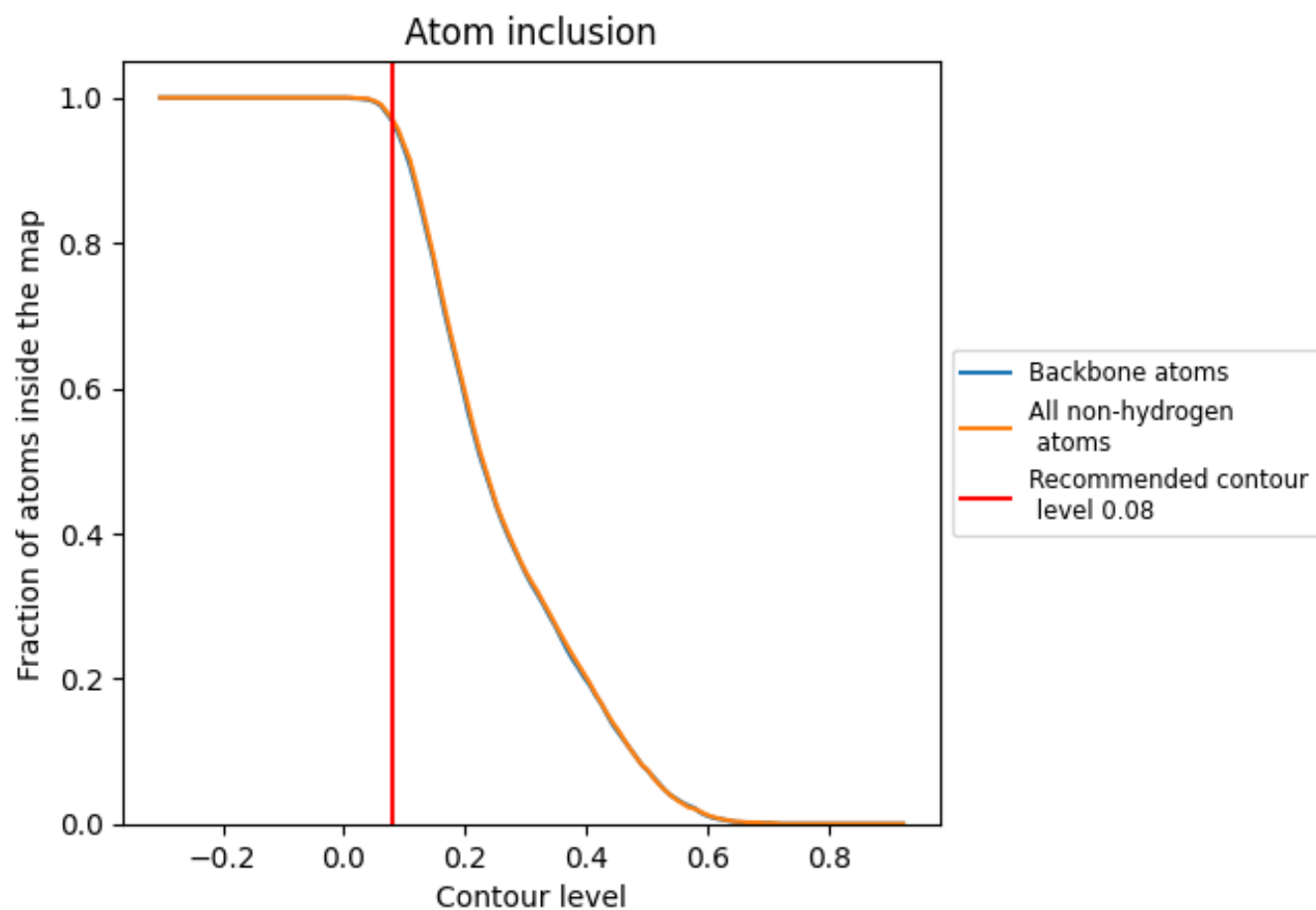
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9710	 0.4470
A	 0.9730	 0.4480
B	 0.9800	 0.4580
C	 0.9750	 0.4550
D	 0.9200	 0.3150
E	 0.8210	 0.2270
F	 0.8570	 0.2860
G	 0.8970	 0.1270
H	 0.9230	 0.2680
I	 0.9640	 0.2960
J	 1.0000	 0.4800
K	 0.8800	 0.3450
L	 0.8950	 0.2660
M	 0.9020	 0.3530
N	 0.9740	 0.4280
O	 0.8210	 0.2380
P	 0.9230	 0.2570
Q	 0.9290	 0.3840
R	 0.7860	 0.2590
S	 0.9640	 0.2880
T	 0.9230	 0.3670
U	 0.9230	 0.2870
V	 0.9600	 0.3690
W	 0.9200	 0.3710
X	 0.9210	 0.3950
Y	 0.9340	 0.2700
Z	 0.9010	 0.3180
a	 0.8210	 0.2890
b	 0.9290	 0.3910
c	 0.7140	 0.2500
d	 0.7500	 0.2590
e	 0.9400	 0.3150
f	 0.9640	 0.2680
g	 1.0000	 0.5000
h	 0.8200	 0.2610



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Chain	Atom inclusion	Q-score
i	 0.9740	 0.4340
j	 0.9400	 0.3780
k	 0.8330	 0.2780
l	 0.8000	 0.1860