



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 06:50 AM EST

PDB ID : 6OLP
EMDB ID : EMD-20118
Title : Full length HIV-1 Env AMC011 in complex with PGT151 Fab
Authors : Rantalainen, K.; Cottrell, C.A.
Deposited on : 2019-04-16
Resolution : 4.20 Å (reported)

This is a wwPDB EM Validation Summary 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

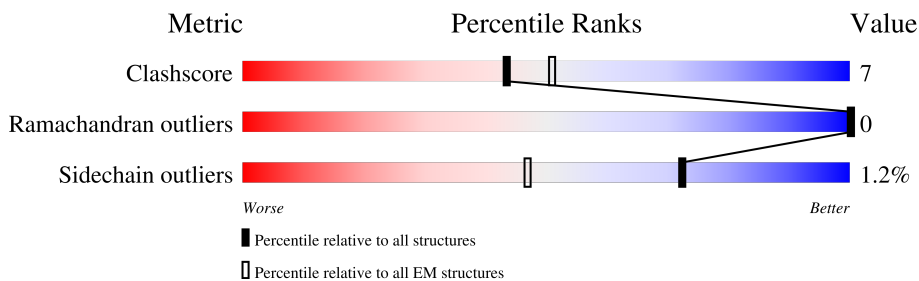
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	506	
1	C	506	
1	E	506	
2	B	345	
2	D	345	
2	F	345	
3	G	240	
3	H	240	

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Mol	Chain	Length	Quality of chain
4	I	219	8% 40% 10% 50%
4	L	219	13% 42% 9% 49%
5	J	2	50% 50% 50%
5	M	2	50% 100%
5	N	2	100%
5	O	2	50% 50% 50%
5	Q	2	50% 100%
5	S	2	50% 100%
5	T	2	100%
5	U	2	50% 50% 50%
5	Y	2	50% 100%
5	Z	2	50% 50% 50%
5	a	2	100% 100%
5	d	2	50% 100%
5	g	2	100%
5	h	2	50% 100%
6	K	2	50% 100%
7	P	4	25% 75% 25%
8	R	3	67% 33% 67%
8	i	3	67% 33%
9	V	9	22% 11% 89%
10	W	8	12% 50% 38% 12%
11	X	2	50% 100%
11	c	2	50% 50%
12	b	5	20% 40% 60%

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Mol	Chain	Length	Quality of chain
13	e	9	
14	f	10	

2 Entry composition i

There are 15 unique types of molecules in this entry. The entry contains 18868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	430	Total	C	N	O	S	1	0
			3392	2148	586	632	26		
1	C	438	Total	C	N	O	S	0	0
			3454	2185	600	643	26		
1	E	419	Total	C	N	O	S	0	0
			3298	2092	573	607	26		

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	143	Total	C	N	O	S	0	0
			1152	728	198	220	6		
2	D	129	Total	C	N	O	S	0	0
			1014	643	170	195	6		
2	F	134	Total	C	N	O	S	0	0
			1063	674	183	200	6		

- Molecule 3 is a protein called Immunoglobulin G PGT151 Fab, Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	134	Total	C	N	O	S	0	0
			1062	676	184	196	6		
3	H	135	Total	C	N	O	S	0	0
			1073	682	188	197	6		

- Molecule 4 is a protein called Immunoglobulin G PGT151 Fab, Light chain.

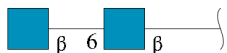
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	109	Total	C	N	O	S	0	0
			838	527	142	165	4		
4	L	111	Total	C	N	O	S	0	0
			854	537	144	169	4		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	J	2	28	16	2	10	0	0
5	M	2	28	16	2	10	0	0
5	N	2	28	16	2	10	0	0
5	O	2	28	16	2	10	0	0
5	Q	2	28	16	2	10	0	0
5	S	2	28	16	2	10	0	0
5	T	2	28	16	2	10	0	0
5	U	2	28	16	2	10	0	0
5	Y	2	28	16	2	10	0	0
5	Z	2	28	16	2	10	0	0
5	a	2	28	16	2	10	0	0
5	d	2	28	16	2	10	0	0
5	g	2	28	16	2	10	0	0
5	h	2	28	16	2	10	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	K	2	28	16	2	10	0	0

- Molecule 7 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.



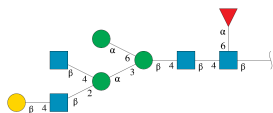
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	P	4	50	28	2	20	0	0

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



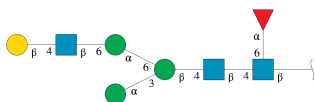
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	R	3	39	22	2	15	0	0
8	i	3	39	22	2	15	0	0

- Molecule 9 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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
			Total	C	N	O		
9	V	9	110	62	4	44	0	0

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



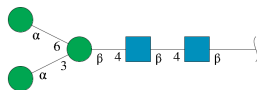
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	W	8	96	54	3	39	0	0

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



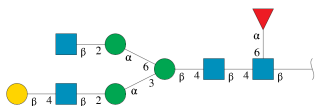
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	X	2	24	14	1	9	0	0
11	c	2	24	14	1	9	0	0

- Molecule 12 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.



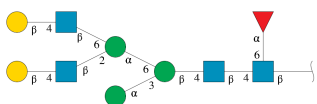
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	b	5	61	34	2	25	0	0

- Molecule 13 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.



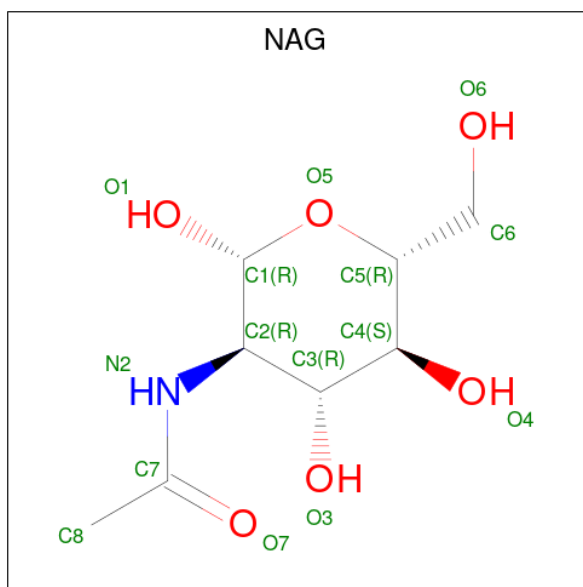
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
13	e	9	110	62	4	44	0	0

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



Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
14	f	10	121	68	4	49	0	0

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

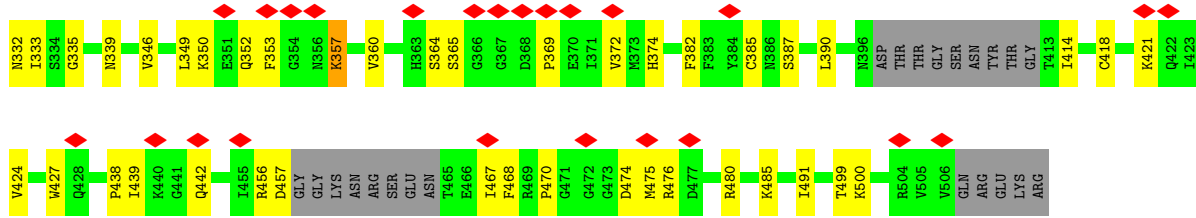


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	D	1	14	8	1	5	0

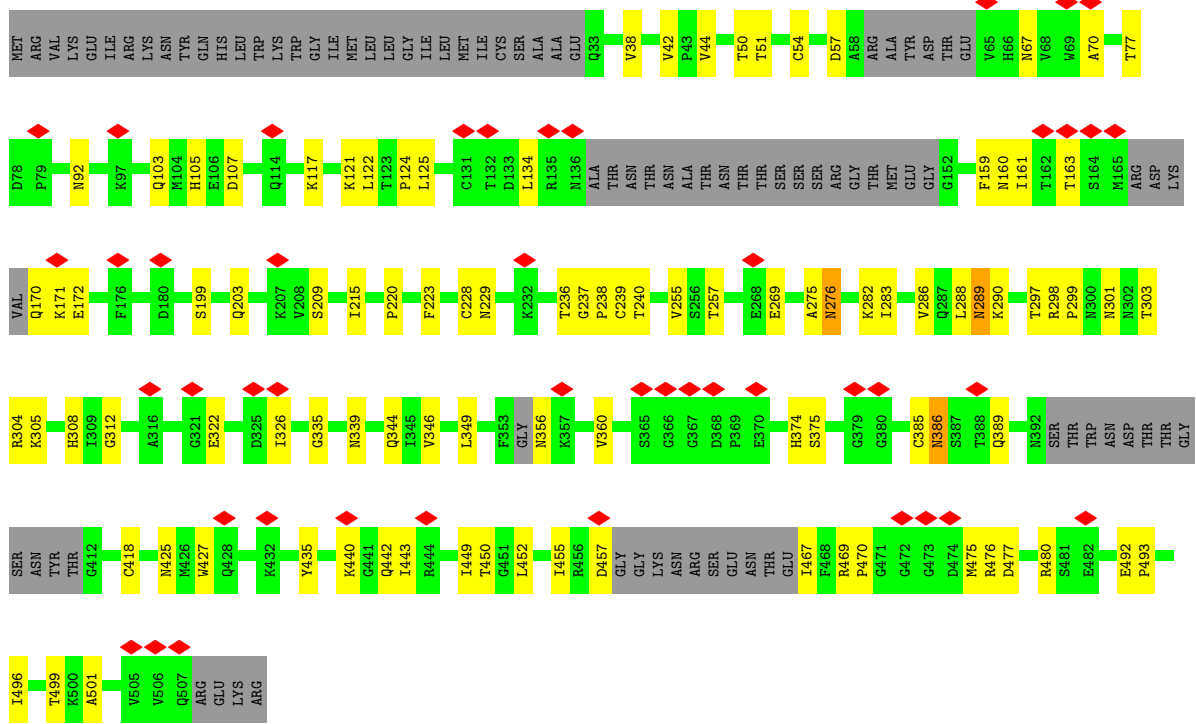
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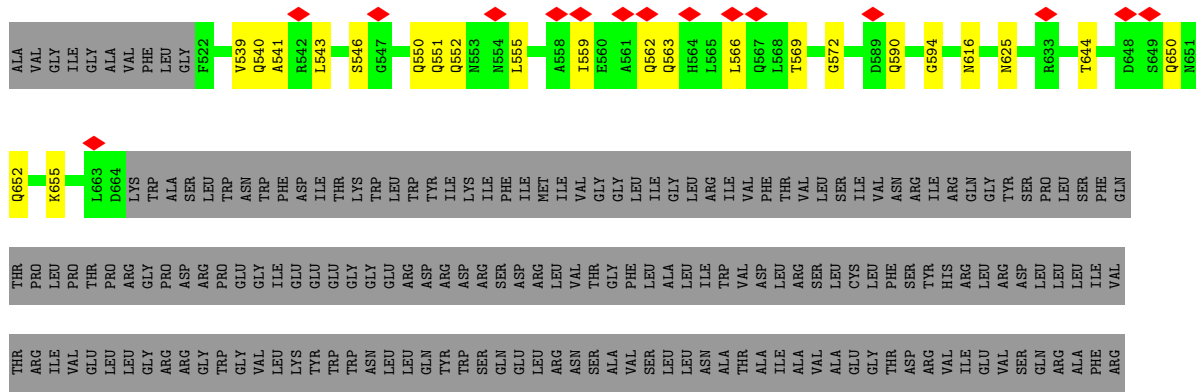
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	E	1	Total 210	C 120	N 15	O 75	0
15	F	1	Total 56	C 32	N 4	O 20	0
15	F	1	Total 56	C 32	N 4	O 20	0
15	F	1	Total 56	C 32	N 4	O 20	0
15	F	1	Total 56	C 32	N 4	O 20	0



• Molecule 1: Envelope glycoprotein gp120



• Molecule 2: Envelope glycoprotein gp41



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● Molecule 2: Envelope glycoprotein gp41



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● Molecule 2: Envelope glycoprotein gp41



A512
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● Molecule 3: Immunoglobulin G PGT151 Fab, Heavy chain



ARG
V2
Q3
E7
S7
G8
G9
R19
C22
S25
D26
F29
A40
K43
W47
I51
S52
H57
V58
V59
L69
V70
S71
R72
K76
L79
E82
R110
G113
D123
T129
S134
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- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



MAG1
MAG2

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

MAG1
MAG2

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

MAG1
MAG2

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

MAG1
MAG2

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

MAG1
MAG2

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

MAG1
MAG2

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



MAG1
MAG2

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



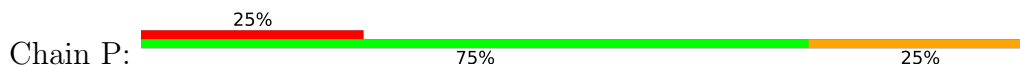
MAG1
MAG2

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



MAG1
MAG2

- Molecule 7: 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



MAG1
MAG2
BMA3
BMA4

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



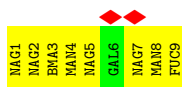
MAG1
MAG2
BMA3

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

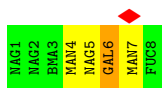


MAG1
MAG2
BMA3

- Molecule 9: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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



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



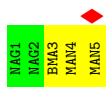
- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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

Chain f: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74889	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0218	Depositor
Map size (Å)	360.5, 360.5, 360.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	0/3462	0.61	0/4699
1	C	0.41	0/3527	0.60	0/4790
1	E	0.41	0/3365	0.58	0/4565
2	B	0.47	0/1172	0.62	0/1592
2	D	0.50	0/1031	0.58	0/1397
2	F	0.45	0/1081	0.58	0/1464
3	G	0.48	0/1091	0.56	0/1482
3	H	0.47	0/1102	0.55	0/1496
4	I	0.44	0/856	0.64	1/1156 (0.1%)
4	L	0.37	0/872	0.55	0/1178
All	All	0.43	0/17559	0.59	1/23819 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	96	LEU	CA-CB-CG	5.79	128.61	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3392	0	3345	50	0
1	C	3454	0	3406	63	0
1	E	3298	0	3269	63	0
2	B	1152	0	1136	14	0
2	D	1014	0	995	11	0
2	F	1063	0	1043	11	0
3	G	1062	0	1024	14	0
3	H	1073	0	1040	19	0
4	I	838	0	817	12	0
4	L	854	0	835	11	0
5	J	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	Q	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	1	0
5	Y	28	0	25	0	0
5	Z	28	0	25	1	0
5	a	28	0	25	0	0
5	d	28	0	25	0	0
5	g	28	0	25	0	0
5	h	28	0	25	0	0
6	K	28	0	25	0	0
7	P	50	0	43	2	0
8	R	39	0	34	0	0
8	i	39	0	34	0	0
9	V	110	0	94	0	0
10	W	96	0	82	1	0
11	X	24	0	22	0	0
11	c	24	0	22	0	0
12	b	61	0	52	0	0
13	e	110	0	94	0	0
14	f	121	0	103	0	0
15	A	112	0	104	0	0
15	C	182	0	169	0	0
15	D	14	0	13	0	0
15	E	210	0	195	4	0
15	F	56	0	52	1	0
All	All	18868	0	18398	259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 259 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:LEU:HD11	1:E:452:LEU:CD1	2.20	0.70
1:E:288:LEU:HD11	1:E:452:LEU:HD11	1.77	0.66
4:I:61:ARG:HH22	4:I:79:GLU:HB2	1.62	0.63
3:H:29:PHE:O	3:H:72:ARG:NH2	2.33	0.62
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.82	0.62

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/506 (83%)	370 (88%)	49 (12%)	0	100	100
1	C	430/506 (85%)	371 (86%)	59 (14%)	0	100	100
1	E	405/506 (80%)	358 (88%)	47 (12%)	0	100	100
2	B	141/345 (41%)	129 (92%)	12 (8%)	0	100	100
2	D	125/345 (36%)	113 (90%)	12 (10%)	0	100	100
2	F	128/345 (37%)	108 (84%)	20 (16%)	0	100	100
3	G	132/240 (55%)	118 (89%)	14 (11%)	0	100	100
3	H	133/240 (55%)	119 (90%)	14 (10%)	0	100	100
4	I	107/219 (49%)	95 (89%)	12 (11%)	0	100	100
4	L	109/219 (50%)	98 (90%)	11 (10%)	0	100	100
All	All	2129/3471 (61%)	1879 (88%)	250 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	386/450 (86%)	379 (98%)	7 (2%)	59	76
1	C	392/450 (87%)	388 (99%)	4 (1%)	76	86
1	E	376/450 (84%)	370 (98%)	6 (2%)	62	79
2	B	125/298 (42%)	123 (98%)	2 (2%)	62	79
2	D	108/298 (36%)	108 (100%)	0	100	100
2	F	113/298 (38%)	110 (97%)	3 (3%)	44	66
3	G	115/207 (56%)	115 (100%)	0	100	100
3	H	116/207 (56%)	114 (98%)	2 (2%)	60	78
4	I	96/195 (49%)	96 (100%)	0	100	100
4	L	98/195 (50%)	98 (100%)	0	100	100
All	All	1925/3048 (63%)	1901 (99%)	24 (1%)	72	83

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	289	ASN
1	E	386	ASN
1	E	356	ASN
1	E	425	ASN
1	A	425	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	105	HIS
1	E	386	ASN
1	E	344	GLN
1	E	422	GLN
2	B	550	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

85 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	1	1,5	14,14,15	0.53	0	17,19,21	1.00	1 (5%)
5	NAG	J	2	5	14,14,15	0.32	0	17,19,21	0.42	0
6	NAG	K	1	1,6	14,14,15	0.46	0	17,19,21	0.67	1 (5%)
6	NAG	K	2	6	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
5	NAG	M	1	1,5	14,14,15	0.27	0	17,19,21	0.65	0
5	NAG	M	2	5	14,14,15	0.33	0	17,19,21	0.43	0
5	NAG	N	1	1,5	14,14,15	0.41	0	17,19,21	0.62	0
5	NAG	N	2	5	14,14,15	0.47	0	17,19,21	0.44	0
5	NAG	O	1	1,5	14,14,15	0.27	0	17,19,21	1.00	1 (5%)
5	NAG	O	2	5	14,14,15	0.39	0	17,19,21	0.58	0
7	NAG	P	1	1,7	14,14,15	0.38	0	17,19,21	0.46	0
7	NAG	P	2	7	14,14,15	0.24	0	17,19,21	0.56	0
7	BMA	P	3	7	11,11,12	0.79	0	15,15,17	1.02	0
7	MAN	P	4	7	11,11,12	0.88	1 (9%)	15,15,17	1.53	2 (13%)
5	NAG	Q	1	1,5	14,14,15	0.45	0	17,19,21	0.61	0
5	NAG	Q	2	5	14,14,15	0.24	0	17,19,21	0.56	0
8	NAG	R	1	1,8	14,14,15	0.31	0	17,19,21	0.54	0
8	NAG	R	2	8	14,14,15	0.24	0	17,19,21	0.86	1 (5%)
8	BMA	R	3	8	11,11,12	0.70	0	15,15,17	0.80	1 (6%)
5	NAG	S	1	1,5	14,14,15	0.70	1 (7%)	17,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	S	2	5	14,14,15	0.37	0	17,19,21	0.91	1 (5%)
5	NAG	T	1	1,5	14,14,15	0.51	0	17,19,21	1.02	1 (5%)
5	NAG	T	2	5	14,14,15	0.21	0	17,19,21	0.74	1 (5%)
5	NAG	U	1	1,5	14,14,15	0.63	0	17,19,21	0.94	1 (5%)
5	NAG	U	2	5	14,14,15	0.44	0	17,19,21	0.96	1 (5%)
9	NAG	V	1	9,2	14,14,15	0.67	1 (7%)	17,19,21	0.82	0
9	NAG	V	2	9	14,14,15	0.48	0	17,19,21	1.04	1 (5%)
9	BMA	V	3	9	11,11,12	1.08	1 (9%)	15,15,17	1.75	4 (26%)
9	MAN	V	4	9	11,11,12	0.99	1 (9%)	15,15,17	1.76	2 (13%)
9	NAG	V	5	9	14,14,15	0.21	0	17,19,21	0.75	1 (5%)
9	GAL	V	6	9	11,11,12	0.65	0	15,15,17	1.14	0
9	NAG	V	7	9	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
9	MAN	V	8	9	11,11,12	0.97	1 (9%)	15,15,17	1.00	1 (6%)
9	FUC	V	9	9	10,10,11	1.00	1 (10%)	14,14,16	0.96	0
10	NAG	W	1	2,10	14,14,15	0.57	0	17,19,21	0.50	0
10	NAG	W	2	10	14,14,15	0.34	0	17,19,21	0.67	0
10	BMA	W	3	10	11,11,12	0.89	0	15,15,17	0.90	0
10	MAN	W	4	10	11,11,12	0.90	0	15,15,17	1.39	2 (13%)
10	NAG	W	5	10	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
10	GAL	W	6	10	11,11,12	0.86	0	15,15,17	1.19	2 (13%)
10	MAN	W	7	10	11,11,12	1.04	1 (9%)	15,15,17	1.43	3 (20%)
10	FUC	W	8	10	10,10,11	0.67	0	14,14,16	0.74	0
11	NAG	X	1	11,2	14,14,15	0.77	1 (7%)	17,19,21	2.29	4 (23%)
11	FUC	X	2	11	10,10,11	1.40	2 (20%)	14,14,16	1.64	3 (21%)
5	NAG	Y	1	1,5	14,14,15	0.19	0	17,19,21	0.58	0
5	NAG	Y	2	5	14,14,15	0.22	0	17,19,21	0.58	0
5	NAG	Z	1	1,5	14,14,15	0.33	0	17,19,21	0.63	0
5	NAG	Z	2	5	14,14,15	0.24	0	17,19,21	0.57	0
5	NAG	a	1	1,5	14,14,15	0.54	0	17,19,21	1.09	2 (11%)
5	NAG	a	2	5	14,14,15	0.41	0	17,19,21	0.62	1 (5%)
12	NAG	b	1	1,12	14,14,15	0.46	0	17,19,21	0.63	0
12	NAG	b	2	12	14,14,15	0.21	0	17,19,21	0.62	0
12	BMA	b	3	12	11,11,12	0.70	0	15,15,17	1.16	2 (13%)
12	MAN	b	4	12	11,11,12	1.14	1 (9%)	15,15,17	1.60	3 (20%)
12	MAN	b	5	12	11,11,12	0.86	1 (9%)	15,15,17	1.32	2 (13%)
11	NAG	c	1	1,11	14,14,15	0.42	0	17,19,21	0.57	0
11	FUC	c	2	11	10,10,11	0.86	0	14,14,16	1.25	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	d	1	1,5	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
5	NAG	d	2	5	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
13	NAG	e	1	13,2	14,14,15	0.42	0	17,19,21	0.63	0
13	NAG	e	2	13	14,14,15	0.66	1 (7%)	17,19,21	0.71	0
13	BMA	e	3	13	11,11,12	0.87	0	15,15,17	1.01	2 (13%)
13	MAN	e	4	13	11,11,12	0.84	1 (9%)	15,15,17	1.46	1 (6%)
13	NAG	e	5	13	14,14,15	0.21	0	17,19,21	0.52	0
13	GAL	e	6	13	11,11,12	1.08	1 (9%)	15,15,17	1.36	1 (6%)
13	MAN	e	7	13	11,11,12	0.73	0	15,15,17	1.38	1 (6%)
13	NAG	e	8	13	14,14,15	0.48	0	17,19,21	0.41	0
13	FUC	e	9	13	10,10,11	0.75	0	14,14,16	1.11	1 (7%)
14	NAG	f	1	14,2	14,14,15	0.77	1 (7%)	17,19,21	1.23	1 (5%)
14	FUC	f	10	14	10,10,11	1.06	1 (10%)	14,14,16	0.98	1 (7%)
14	NAG	f	2	14	14,14,15	0.21	0	17,19,21	0.43	0
14	BMA	f	3	14	11,11,12	0.88	0	15,15,17	1.09	1 (6%)
14	MAN	f	4	14	11,11,12	1.01	1 (9%)	15,15,17	1.66	3 (20%)
14	NAG	f	5	14	14,14,15	0.58	1 (7%)	17,19,21	0.57	0
14	GAL	f	6	14	11,11,12	0.72	0	15,15,17	0.92	0
14	NAG	f	7	14	14,14,15	0.19	0	17,19,21	0.62	1 (5%)
14	GAL	f	8	14	11,11,12	0.71	0	15,15,17	1.36	2 (13%)
14	MAN	f	9	14	11,11,12	0.87	0	15,15,17	1.07	2 (13%)
5	NAG	g	1	1,5	14,14,15	0.86	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	g	2	5	14,14,15	0.57	0	17,19,21	0.73	1 (5%)
5	NAG	h	1	1,5	14,14,15	0.50	0	17,19,21	0.63	0
5	NAG	h	2	5	14,14,15	0.37	0	17,19,21	0.45	0
8	NAG	i	1	1,8	14,14,15	0.35	0	17,19,21	0.58	0
8	NAG	i	2	8	14,14,15	0.37	0	17,19,21	0.76	0
8	BMA	i	3	8	11,11,12	0.69	0	15,15,17	1.01	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
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	W	7	10	-	2/2/19/22	0/1/1/1
10	FUC	W	8	10	-	-	0/1/1/1
11	NAG	X	1	11,2	-	5/6/23/26	0/1/1/1
11	FUC	X	2	11	-	-	0/1/1/1
5	NAG	Y	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Z	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	4/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
12	NAG	b	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	b	2	12	-	3/6/23/26	0/1/1/1
12	BMA	b	3	12	-	2/2/19/22	0/1/1/1
12	MAN	b	4	12	-	2/2/19/22	0/1/1/1
12	MAN	b	5	12	-	1/2/19/22	0/1/1/1
11	NAG	c	1	1,11	-	4/6/23/26	0/1/1/1
11	FUC	c	2	11	-	-	0/1/1/1
5	NAG	d	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	d	2	5	-	3/6/23/26	0/1/1/1
13	NAG	e	1	13,2	-	1/6/23/26	0/1/1/1
13	NAG	e	2	13	-	2/6/23/26	0/1/1/1
13	BMA	e	3	13	-	1/2/19/22	0/1/1/1
13	MAN	e	4	13	-	1/2/19/22	0/1/1/1
13	NAG	e	5	13	-	2/6/23/26	0/1/1/1
13	GAL	e	6	13	-	0/2/19/22	0/1/1/1
13	MAN	e	7	13	-	2/2/19/22	0/1/1/1
13	NAG	e	8	13	-	1/6/23/26	0/1/1/1
13	FUC	e	9	13	-	-	0/1/1/1
14	NAG	f	1	14,2	-	0/6/23/26	0/1/1/1
14	FUC	f	10	14	-	-	0/1/1/1
14	NAG	f	2	14	-	4/6/23/26	0/1/1/1
14	BMA	f	3	14	-	2/2/19/22	0/1/1/1
14	MAN	f	4	14	-	0/2/19/22	0/1/1/1
14	NAG	f	5	14	-	1/6/23/26	0/1/1/1
14	GAL	f	6	14	-	0/2/19/22	0/1/1/1
14	NAG	f	7	14	-	1/6/23/26	0/1/1/1
14	GAL	f	8	14	-	2/2/19/22	0/1/1/1
14	MAN	f	9	14	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	g	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	1/6/23/26	0/1/1/1
5	NAG	h	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	h	2	5	-	2/6/23/26	0/1/1/1
8	NAG	i	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	i	2	8	-	2/6/23/26	0/1/1/1
8	BMA	i	3	8	-	1/2/19/22	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	4	MAN	C1-C2	3.49	1.60	1.52
10	W	7	MAN	C1-C2	2.85	1.58	1.52
13	e	6	GAL	C1-C2	2.82	1.58	1.52
5	g	1	NAG	O5-C1	2.77	1.48	1.43
14	f	10	FUC	C1-C2	2.74	1.58	1.52

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	1	NAG	C2-N2-C7	7.96	134.24	122.90
9	V	4	MAN	C1-O5-C5	4.78	118.67	112.19
7	P	4	MAN	C1-O5-C5	4.43	118.19	112.19
13	e	7	MAN	C1-O5-C5	4.02	117.63	112.19
14	f	4	MAN	O2-C2-C3	-3.93	102.26	110.14

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

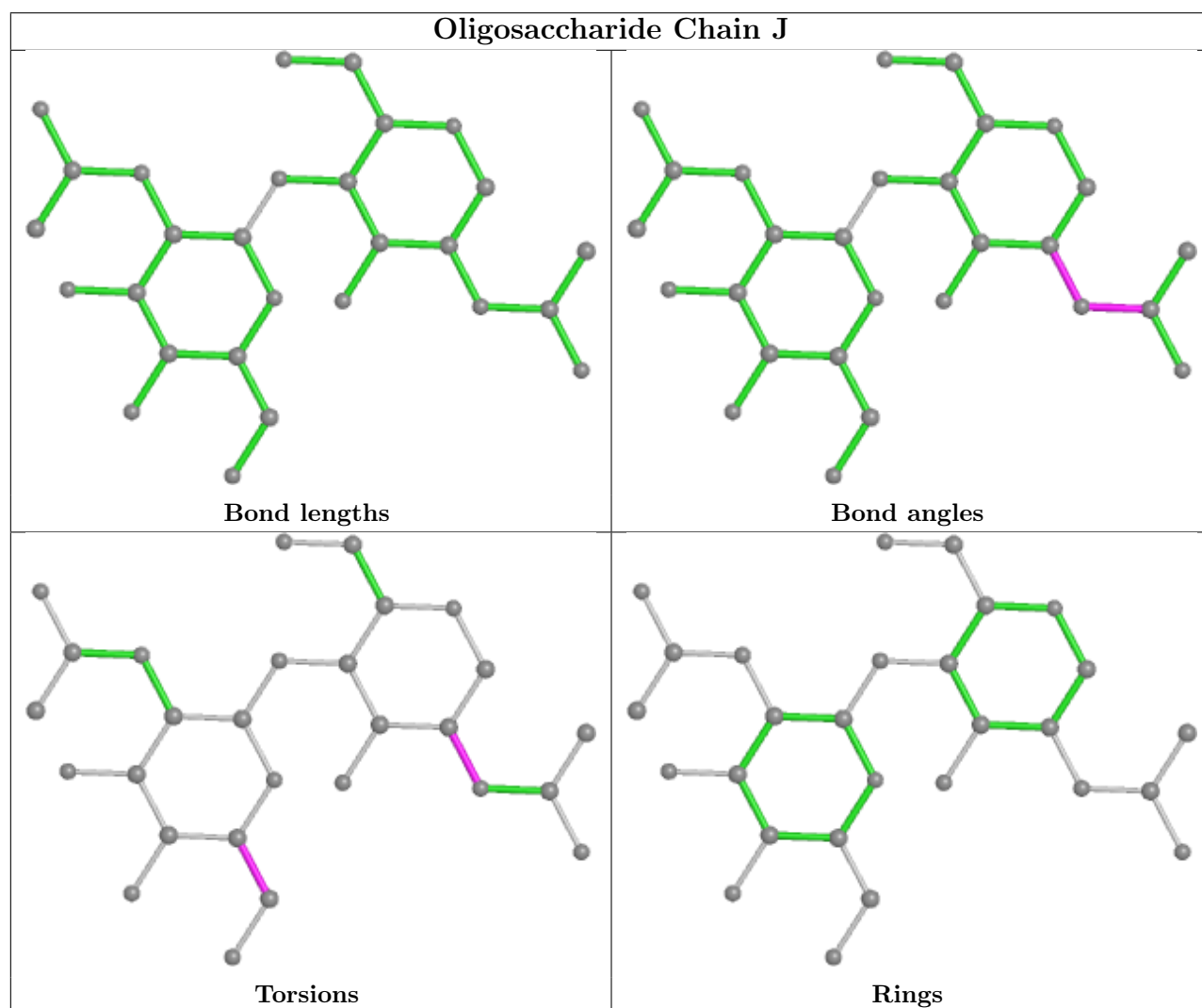
Mol	Chain	Res	Type	Atoms
5	a	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
12	b	1	NAG	O5-C5-C6-O6
9	V	8	MAN	O5-C5-C6-O6

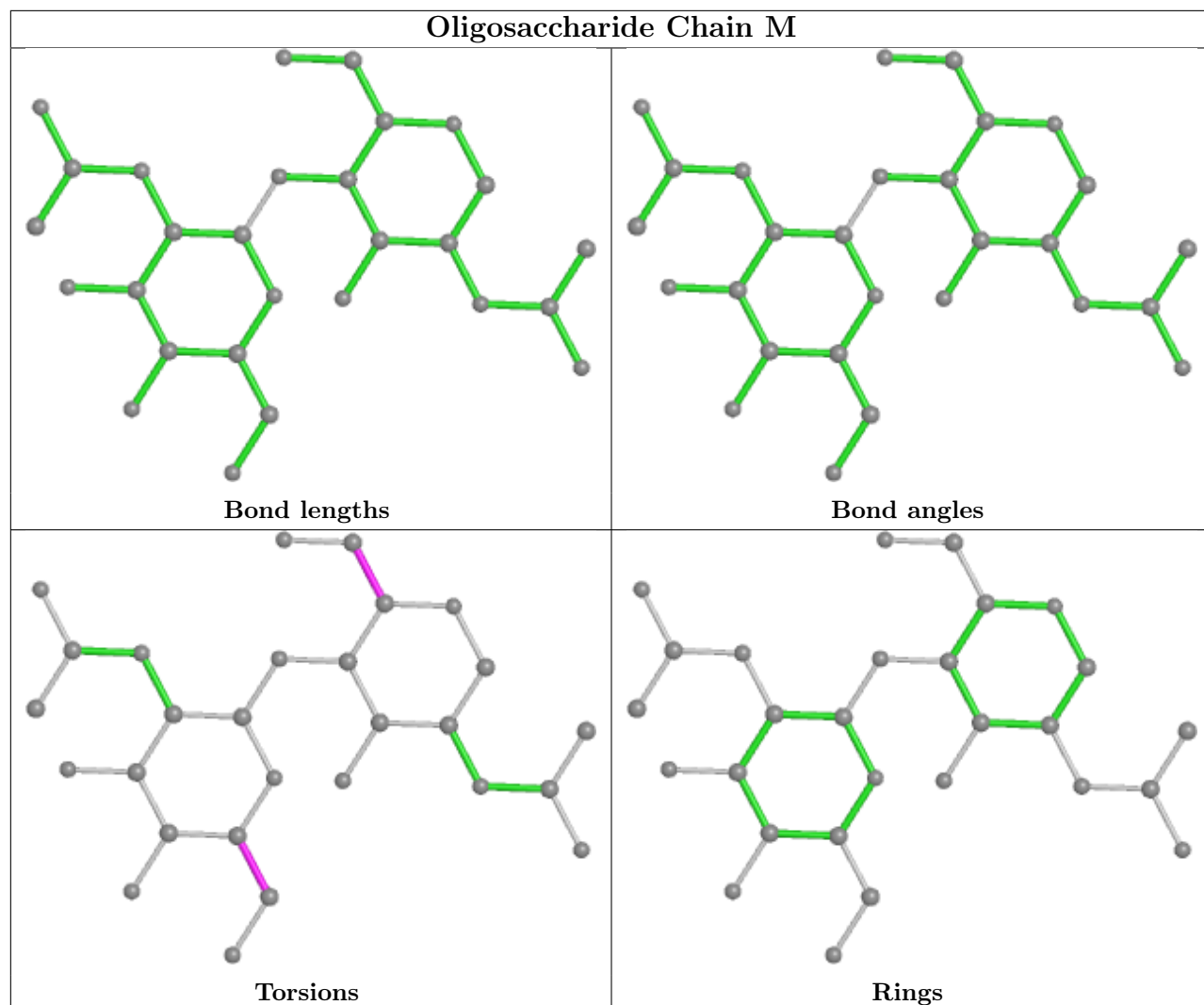
There are no ring outliers.

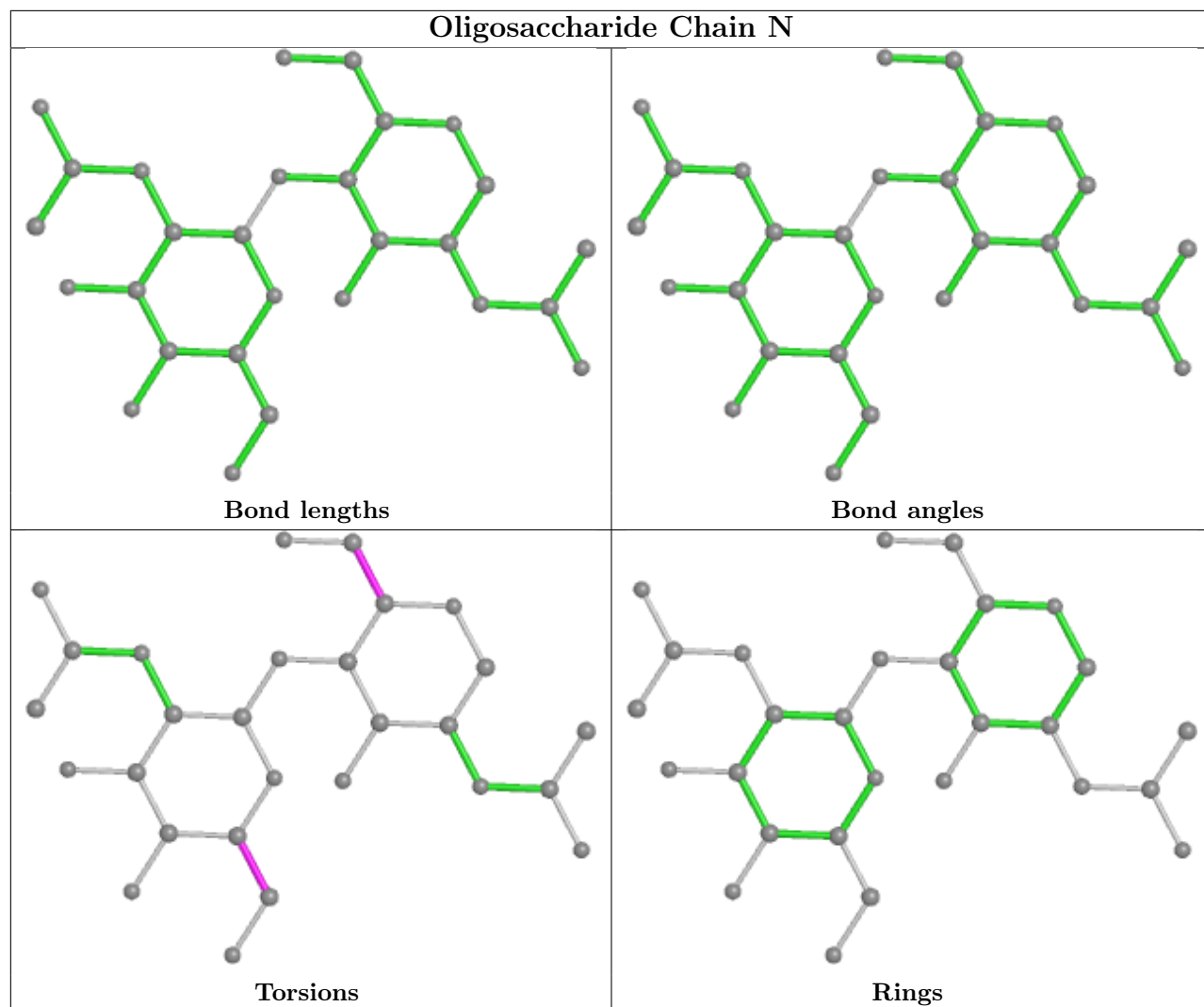
4 monomers are involved in 5 short contacts:

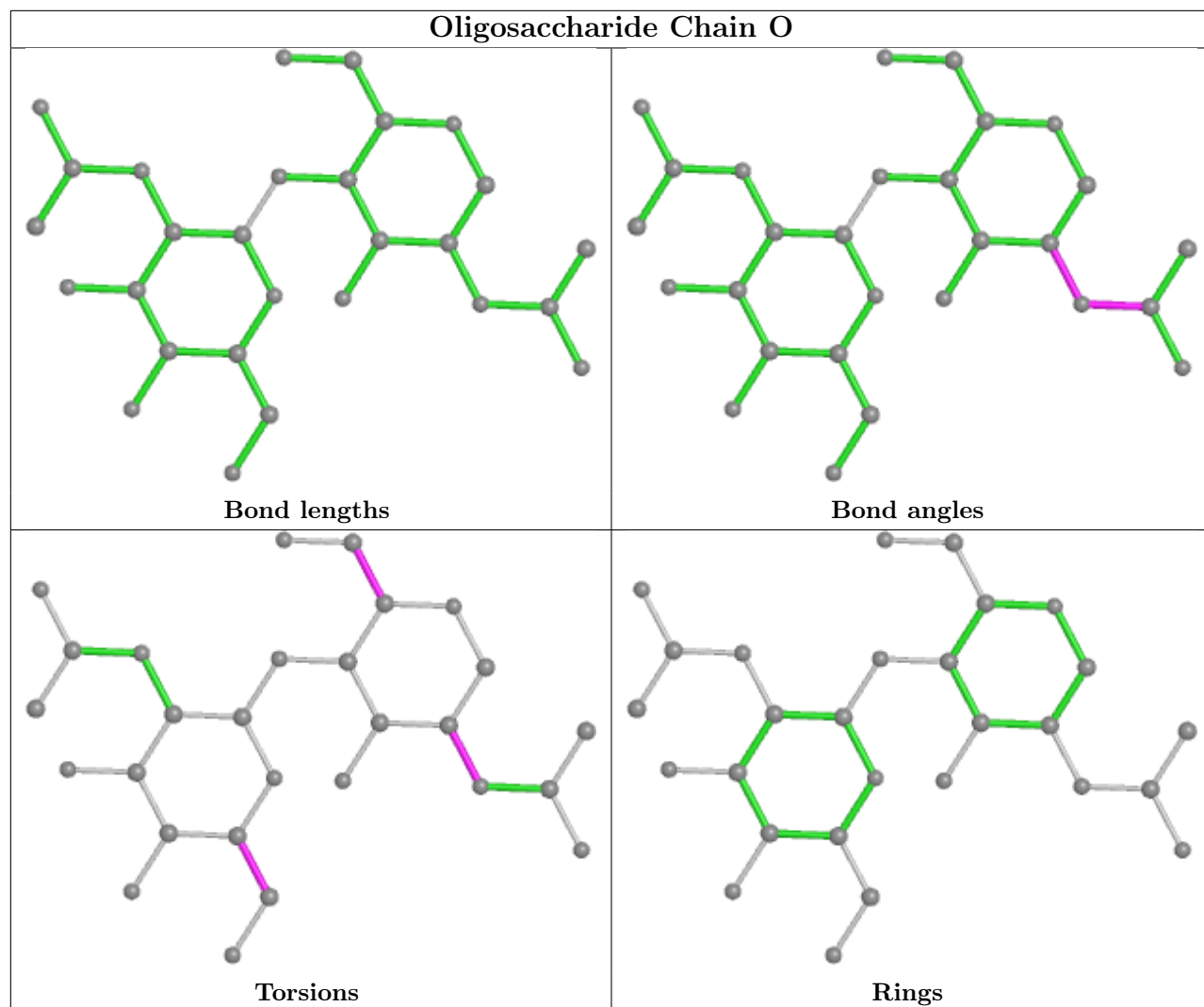
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	W	6	GAL	1	0
7	P	4	MAN	2	0
5	U	1	NAG	1	0
5	Z	1	NAG	1	0

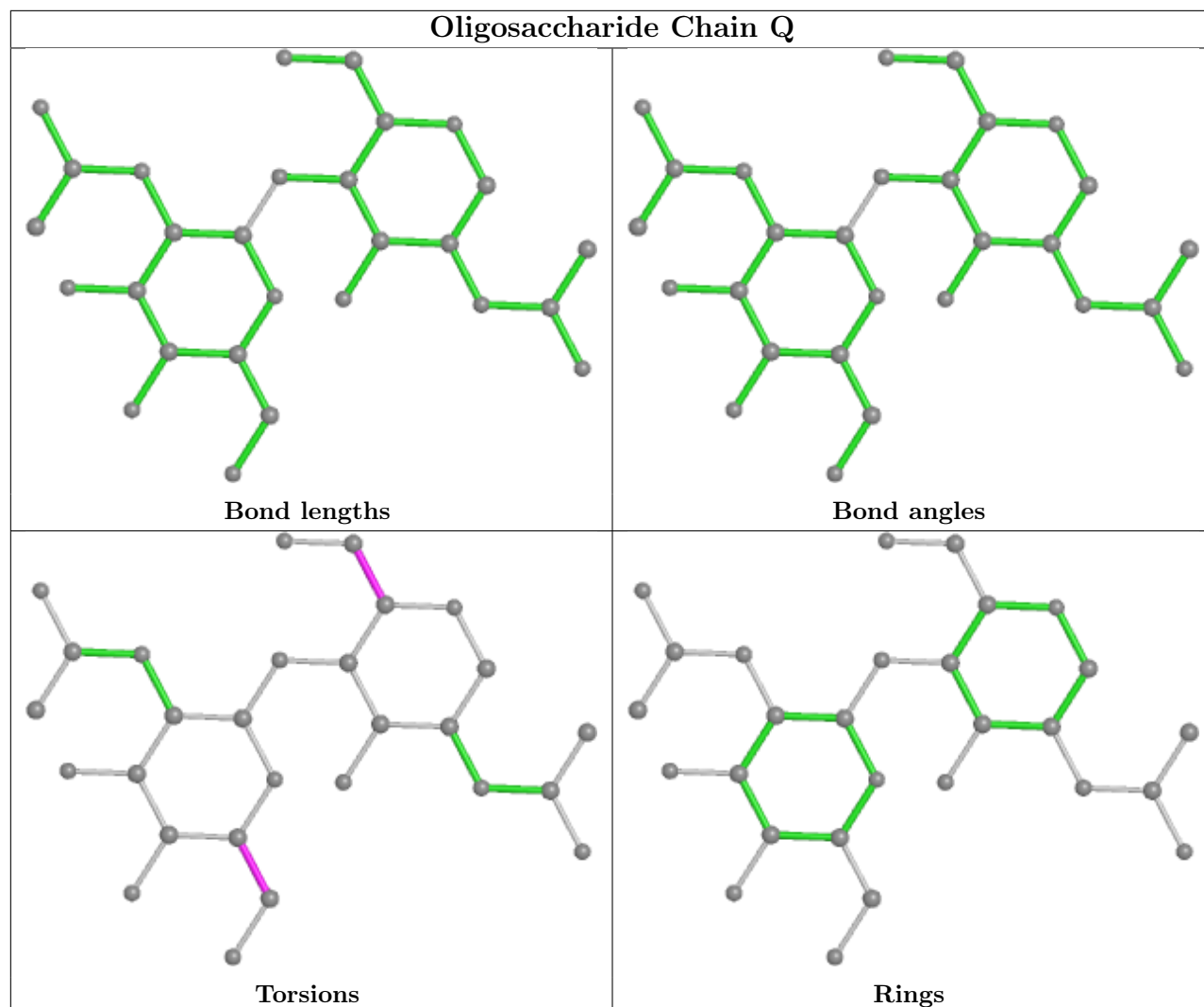
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

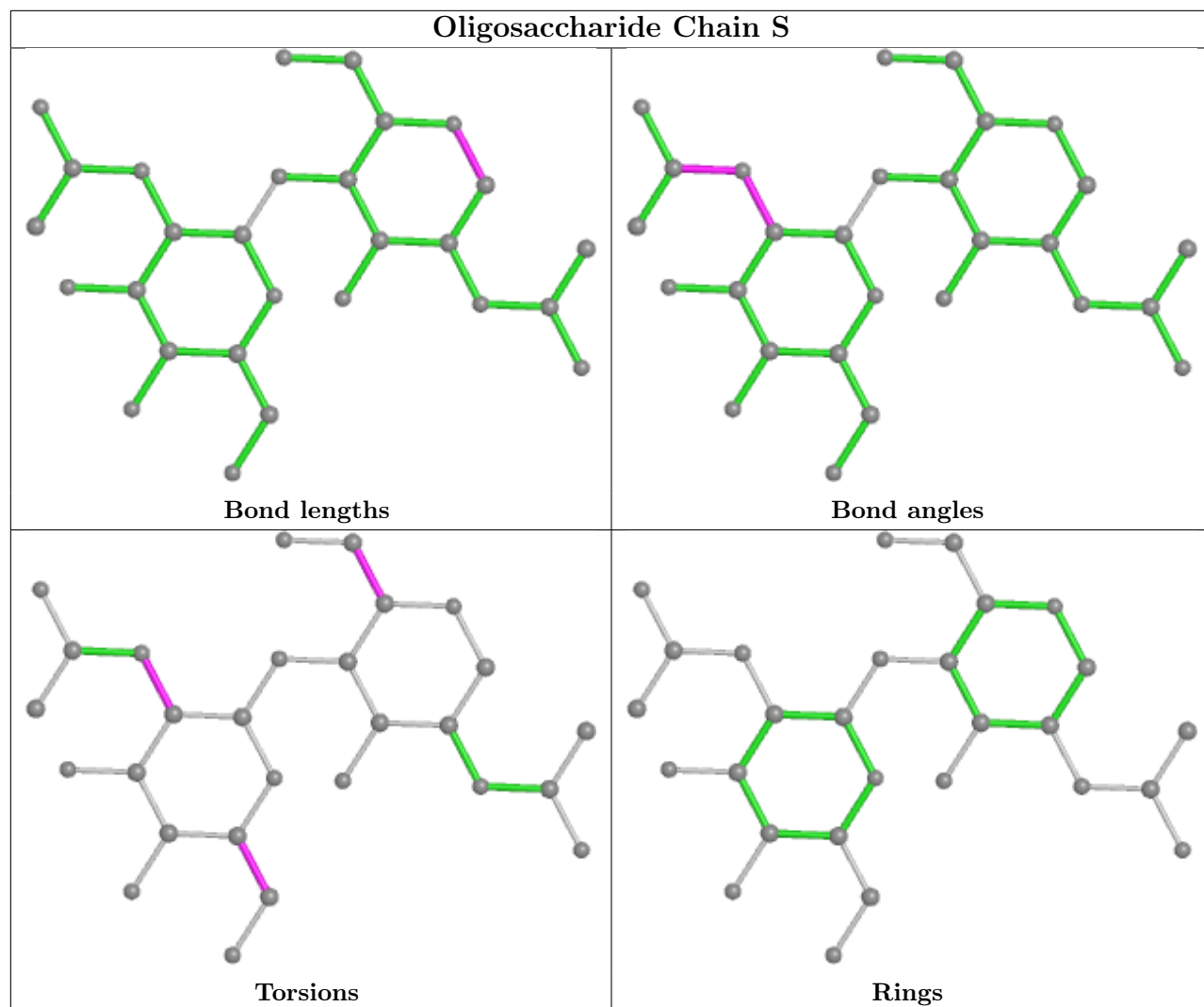


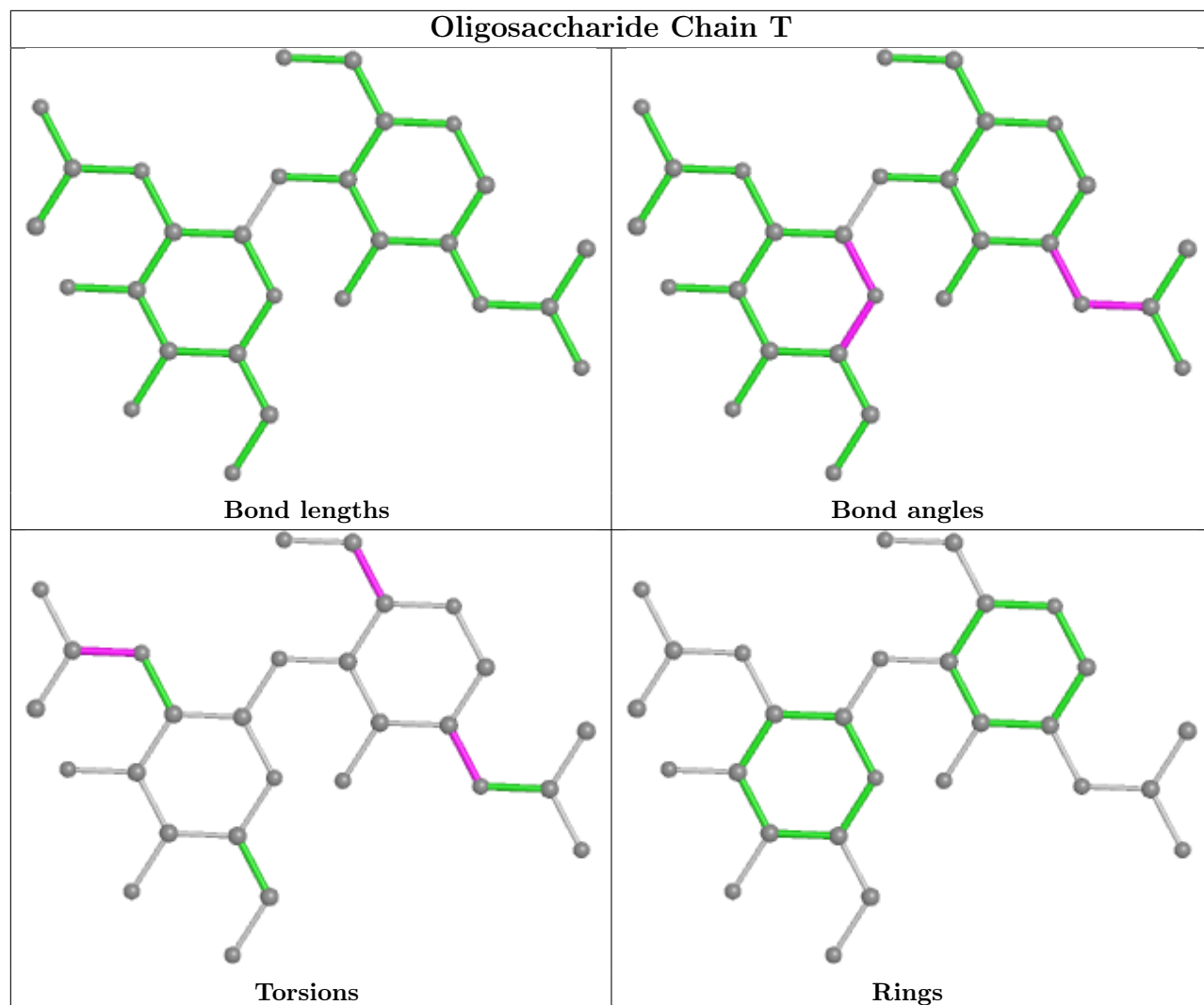


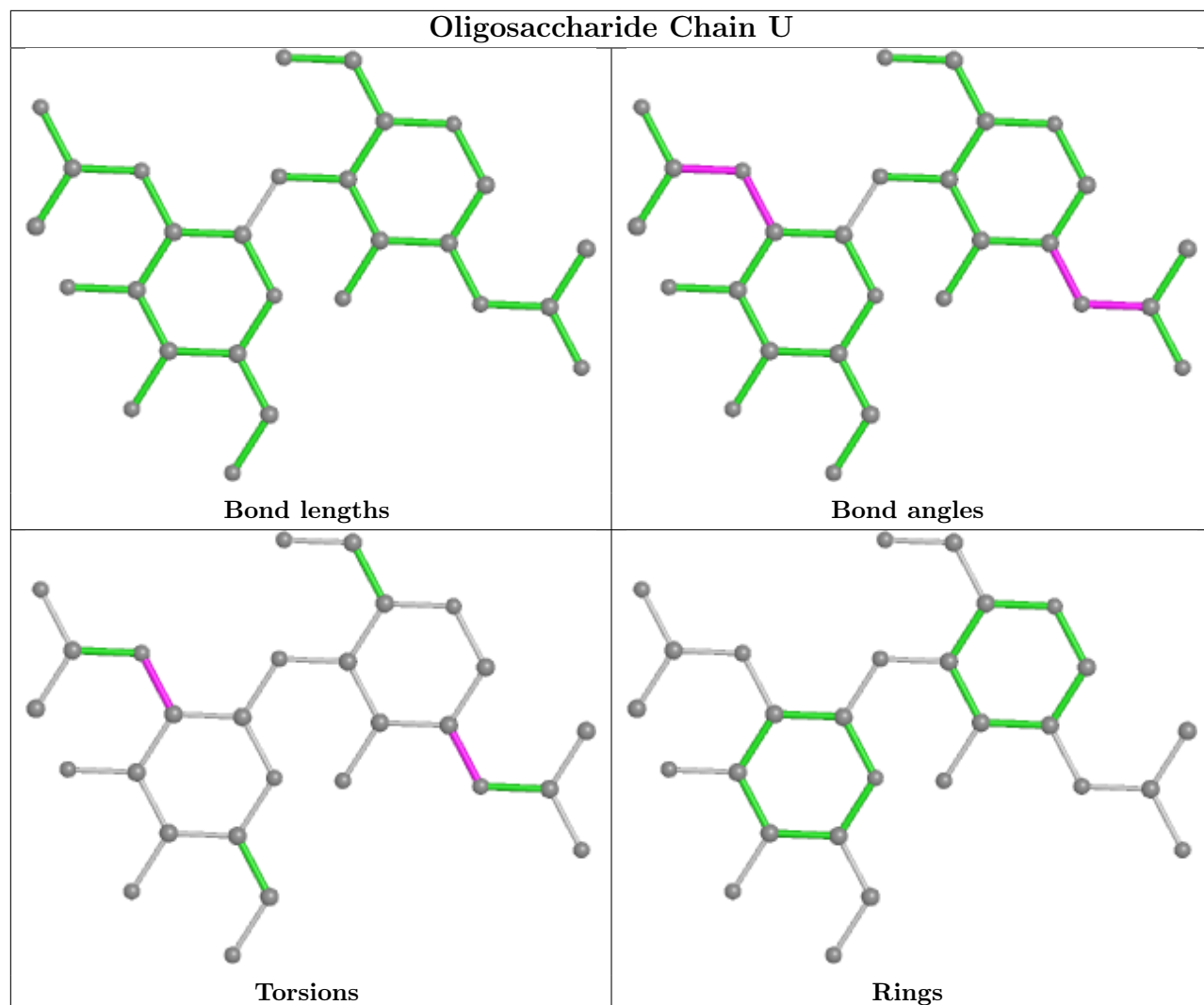


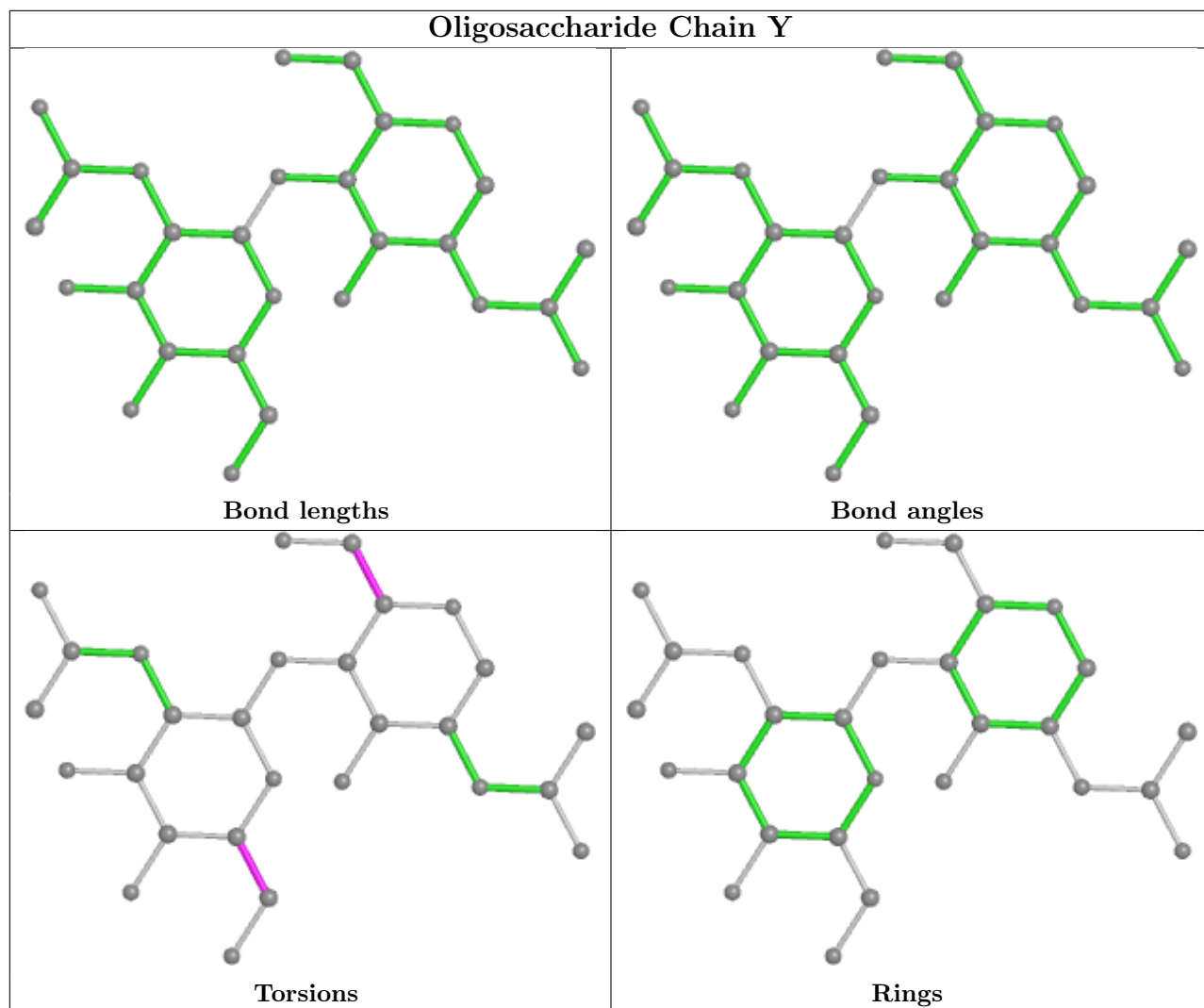


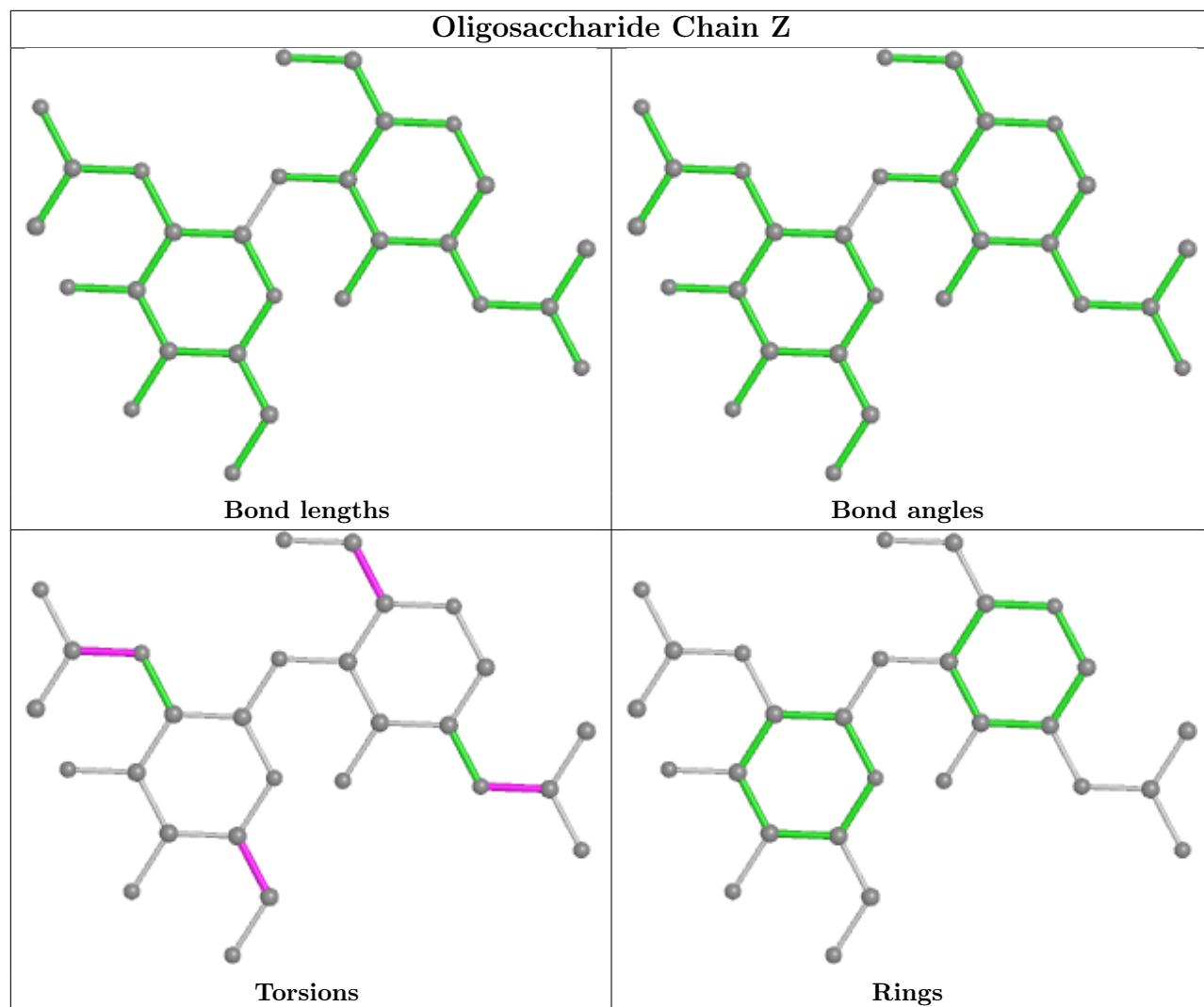


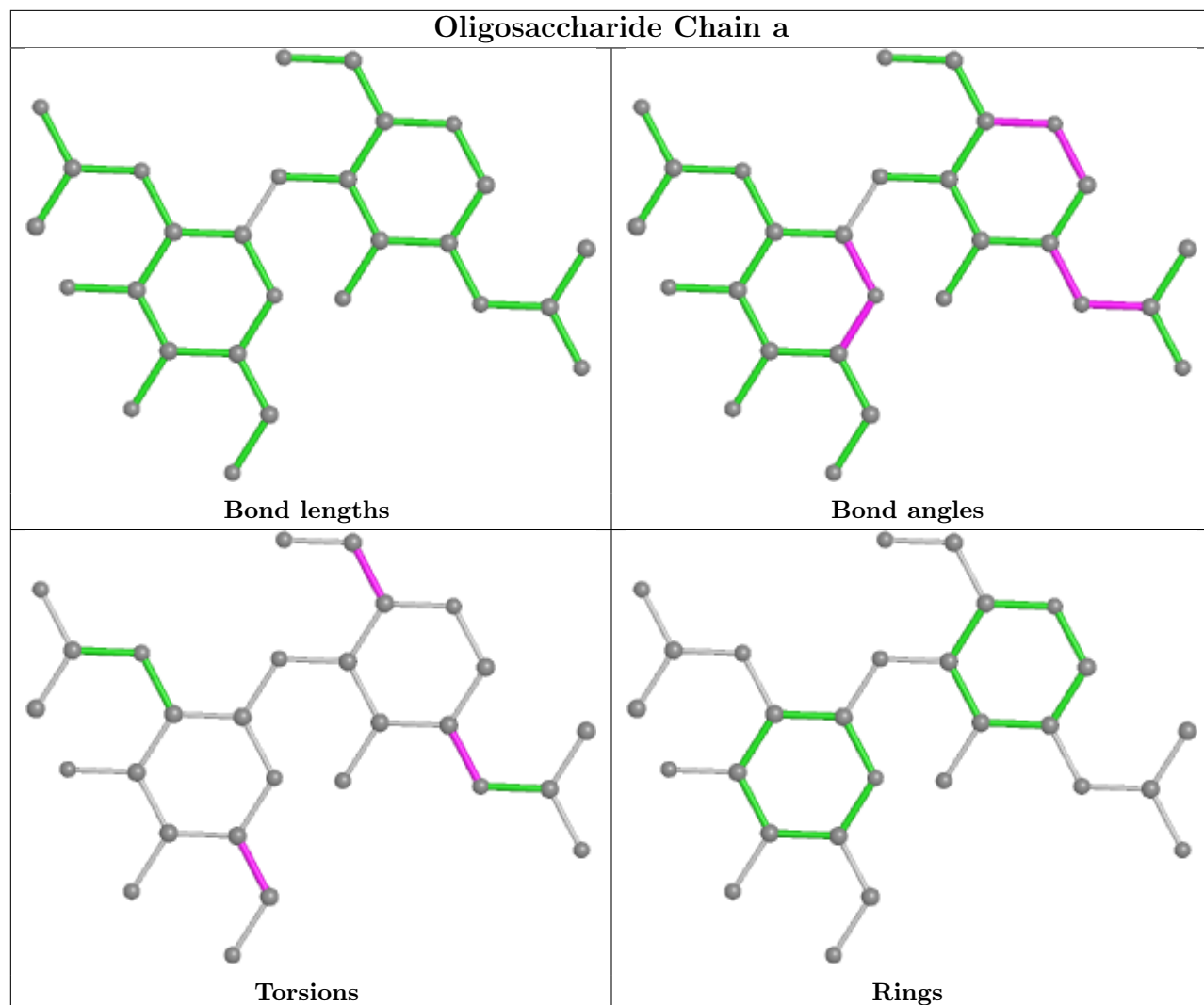


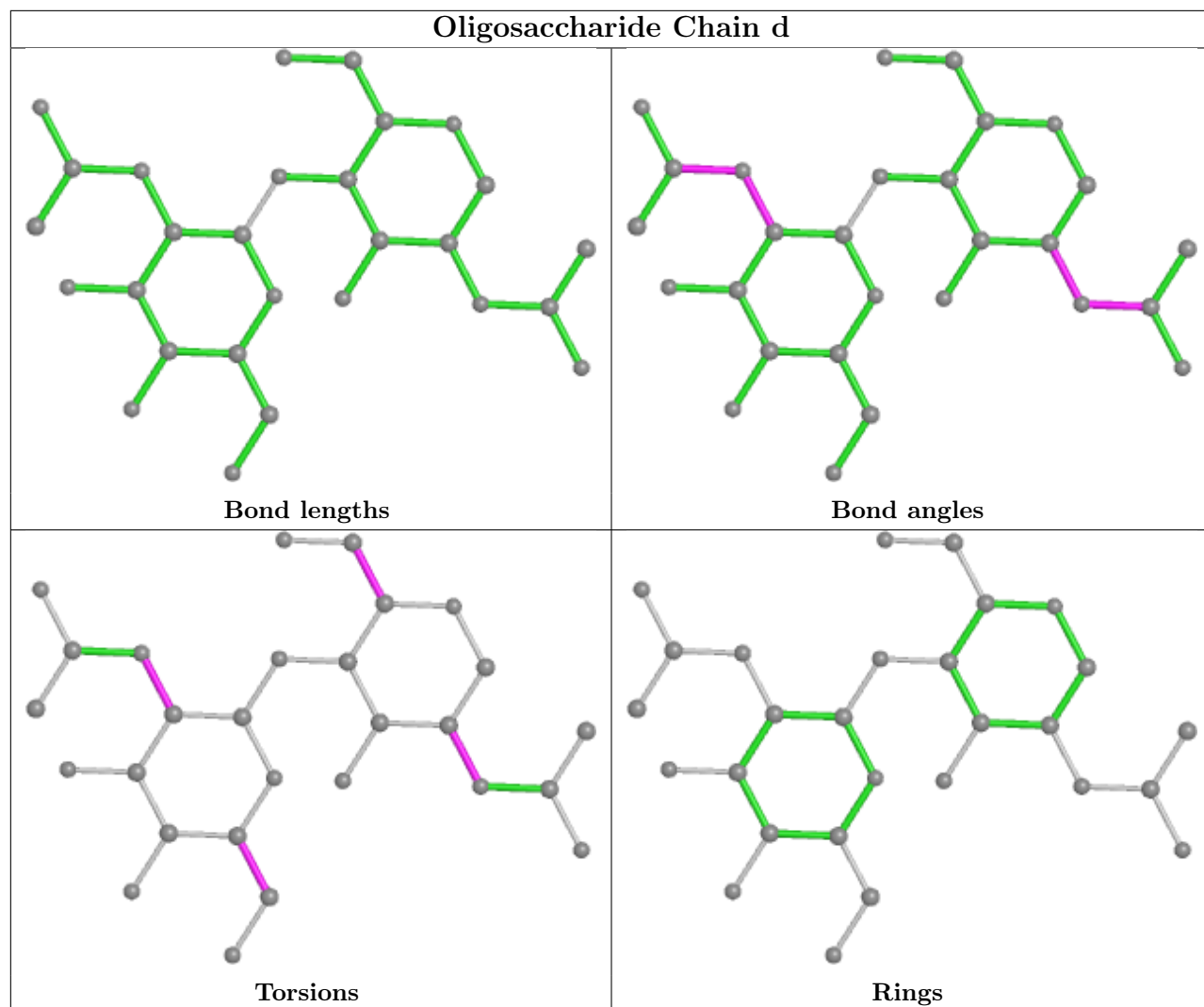


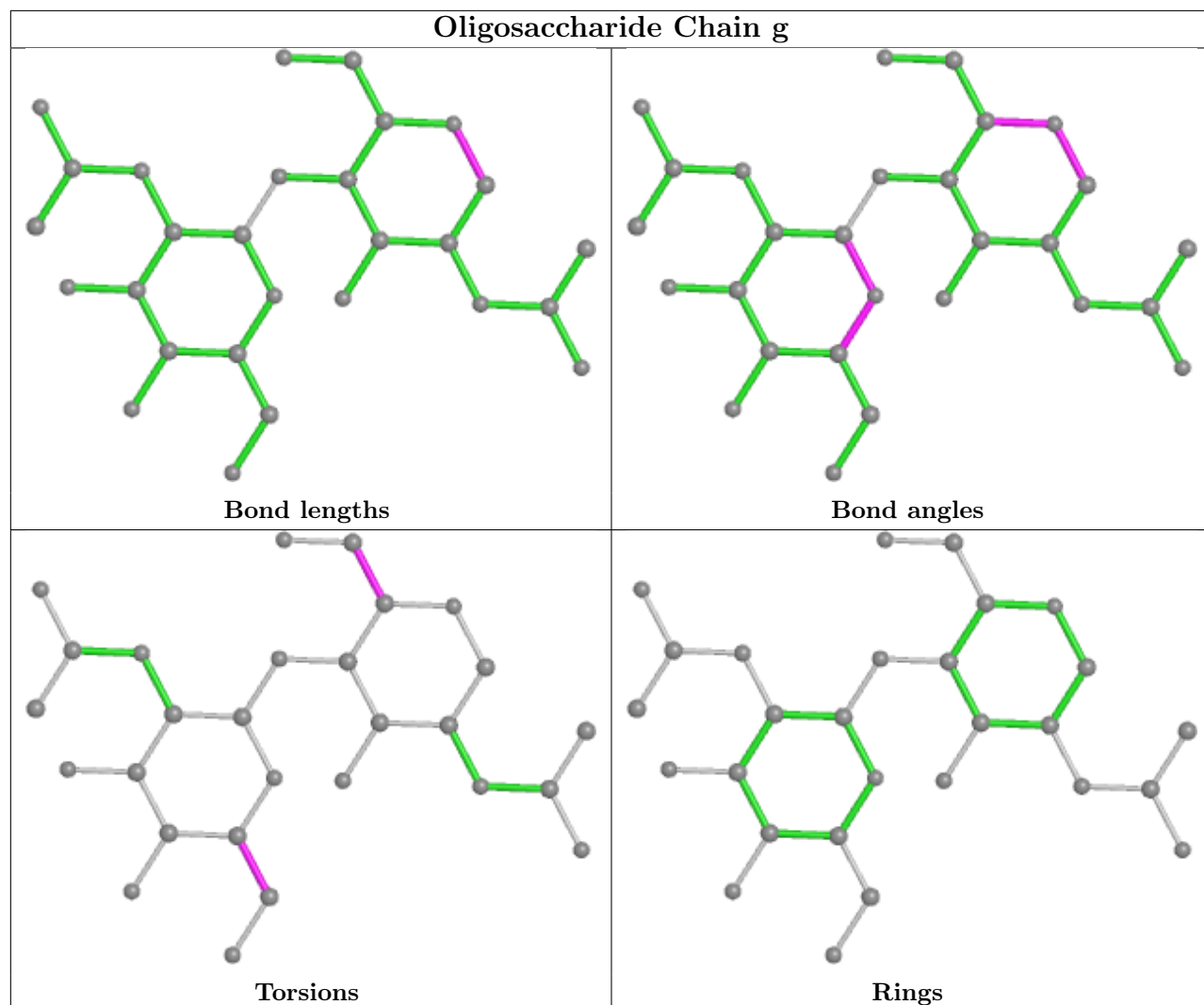


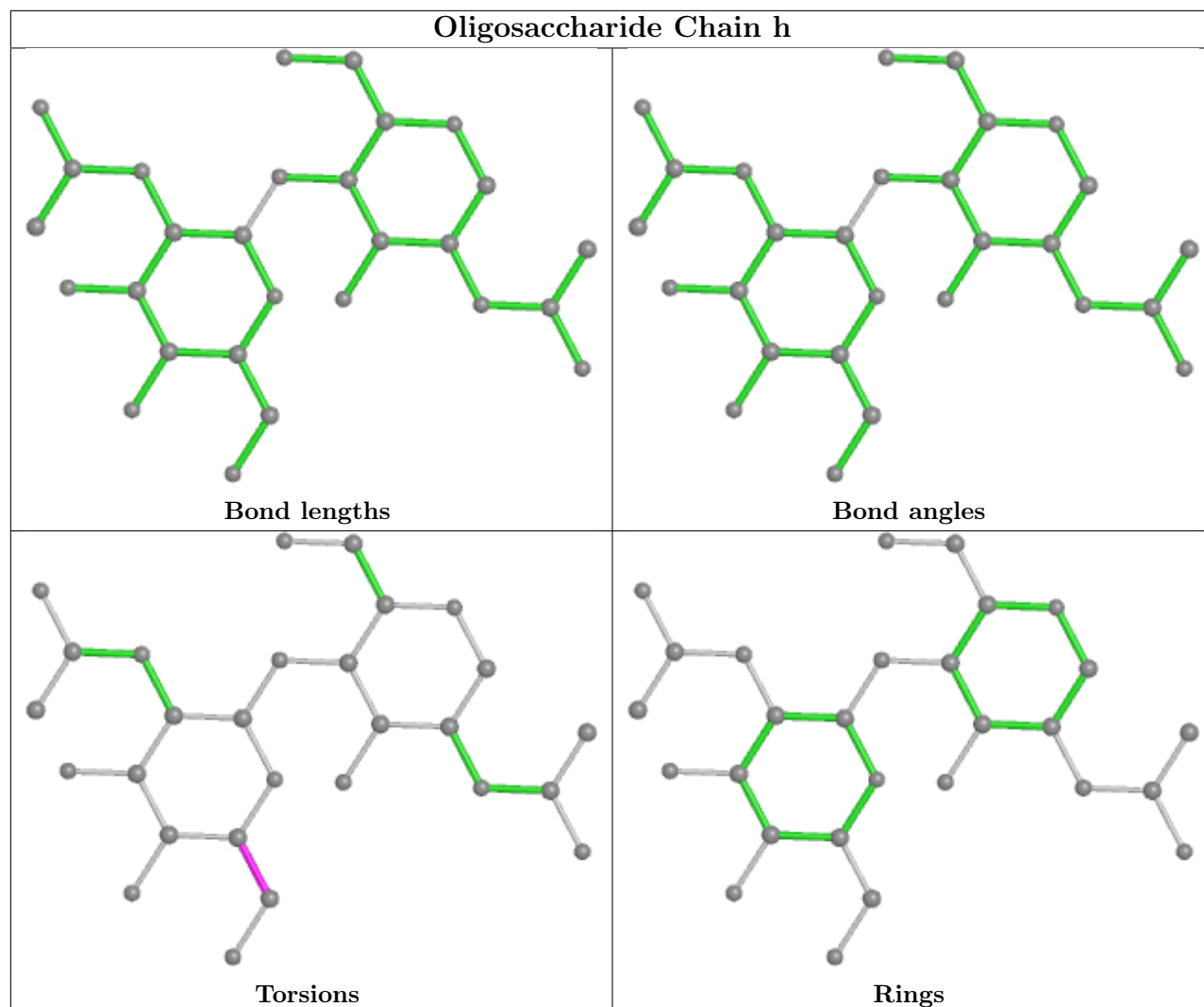


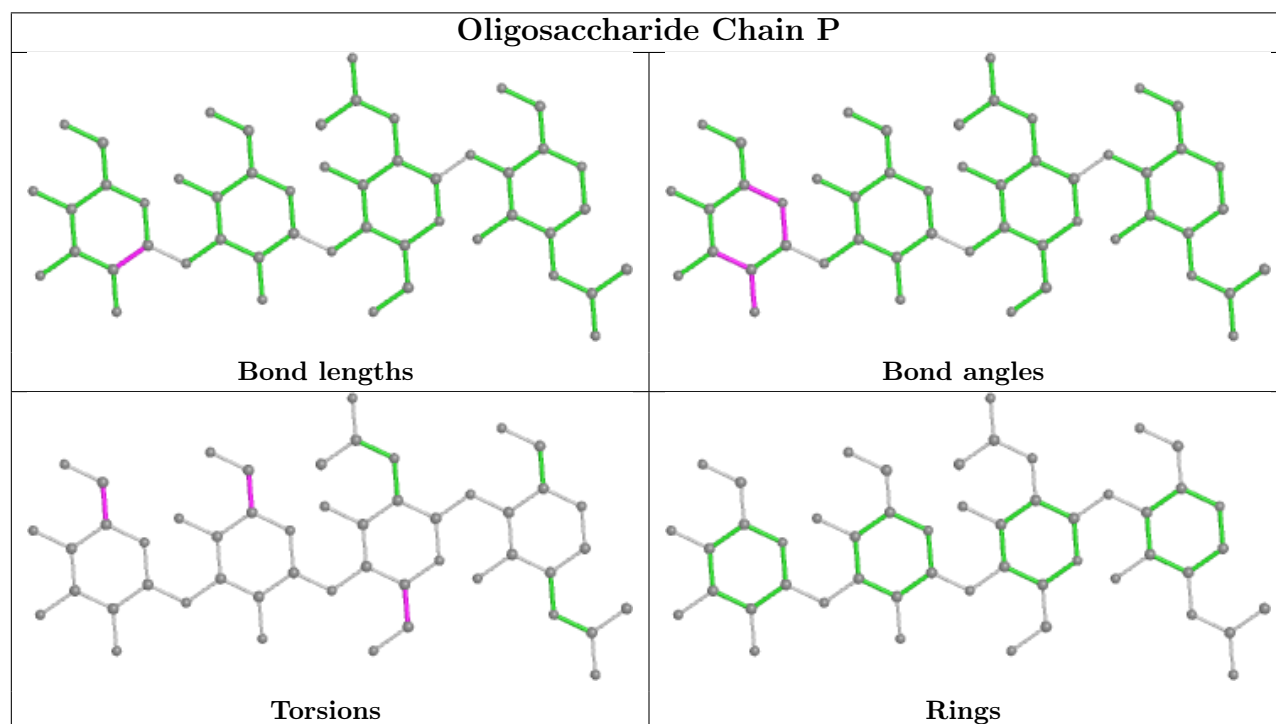
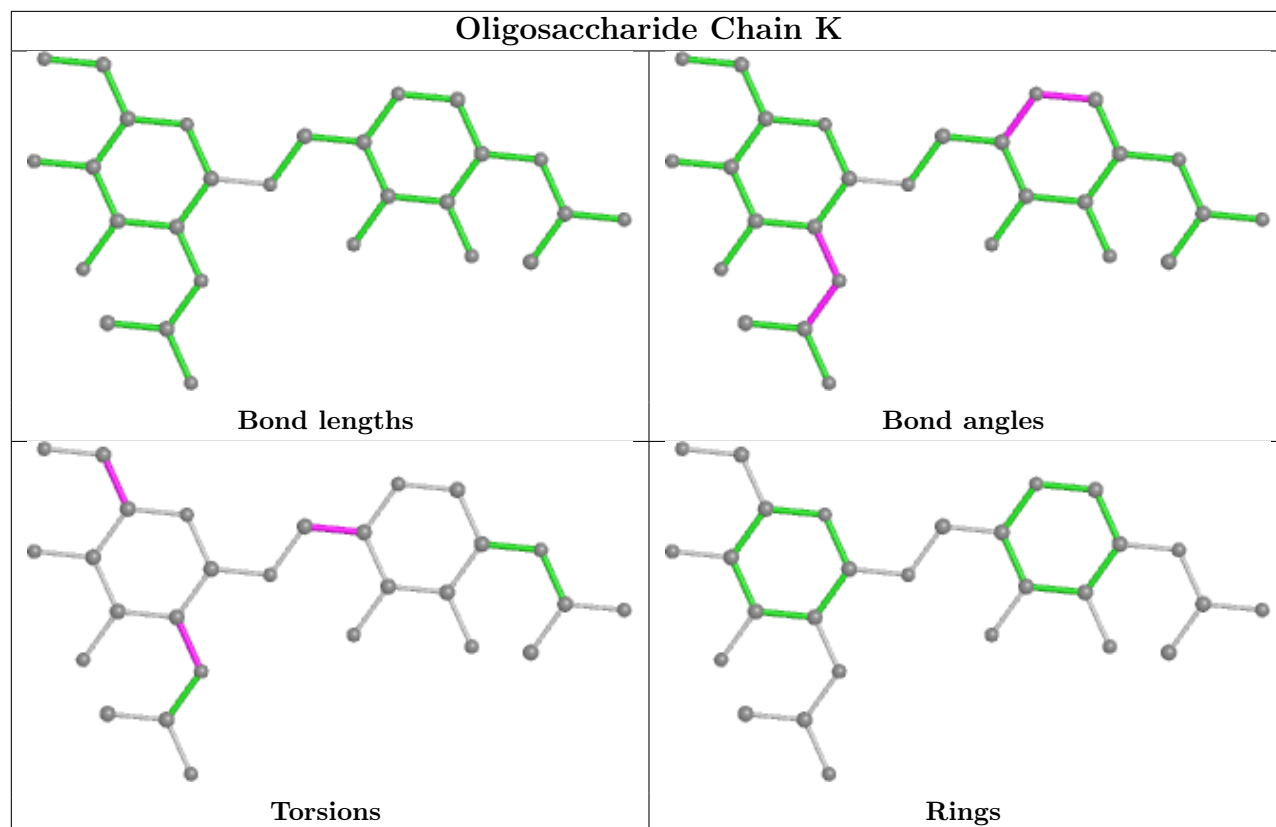


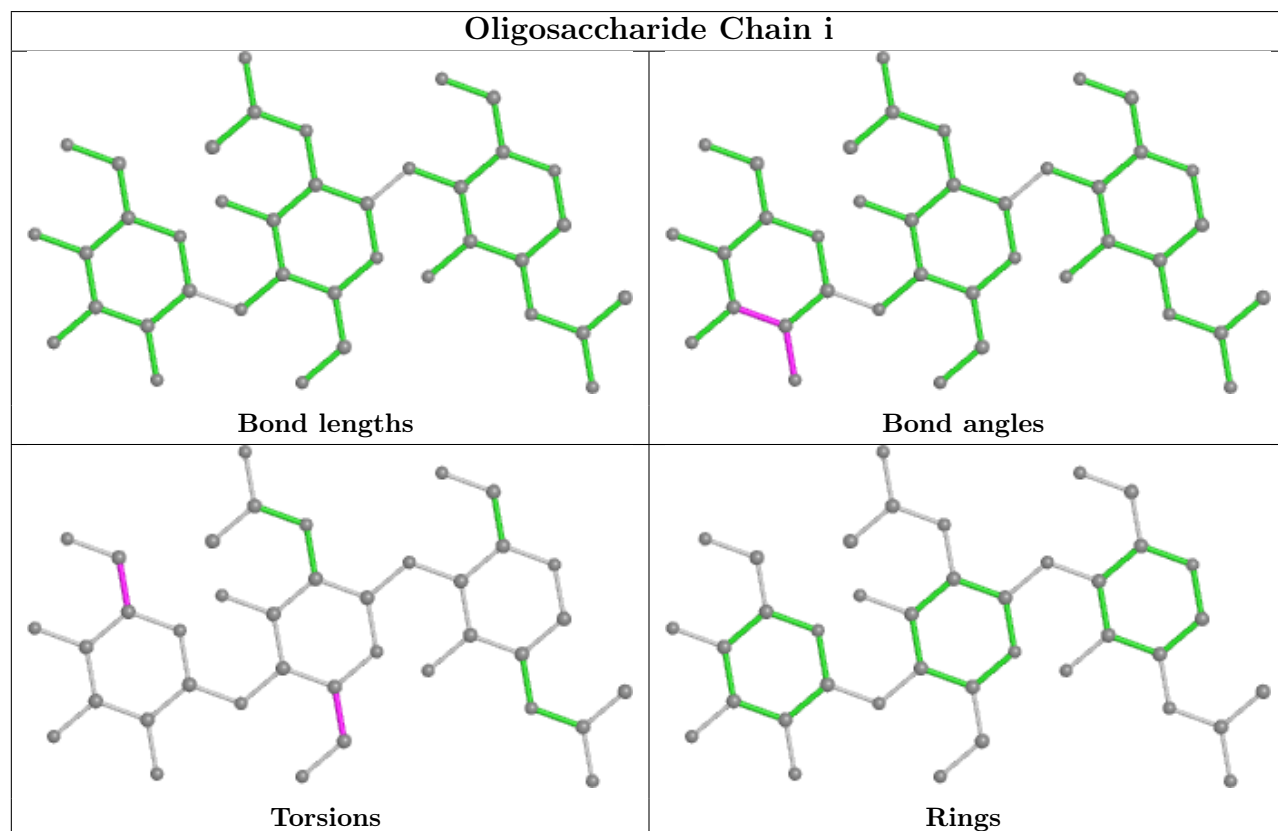
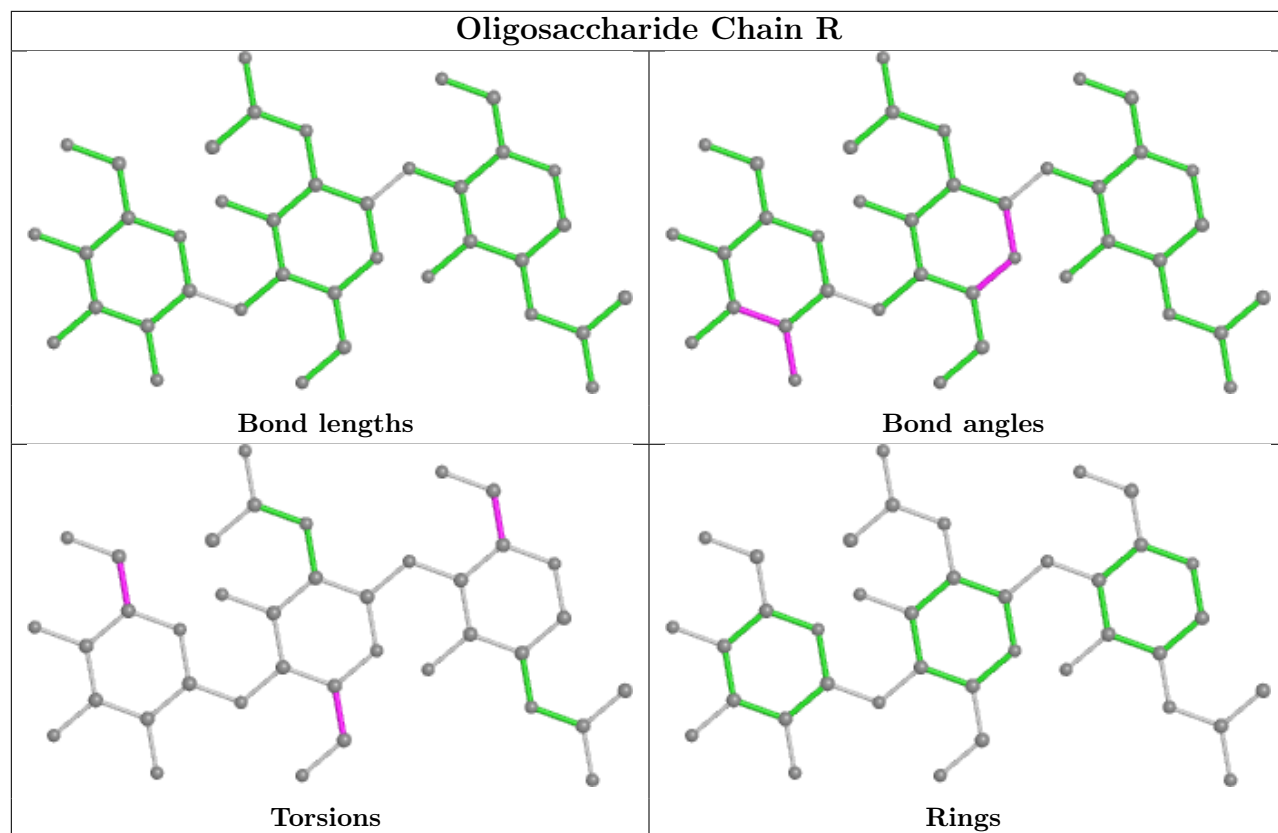


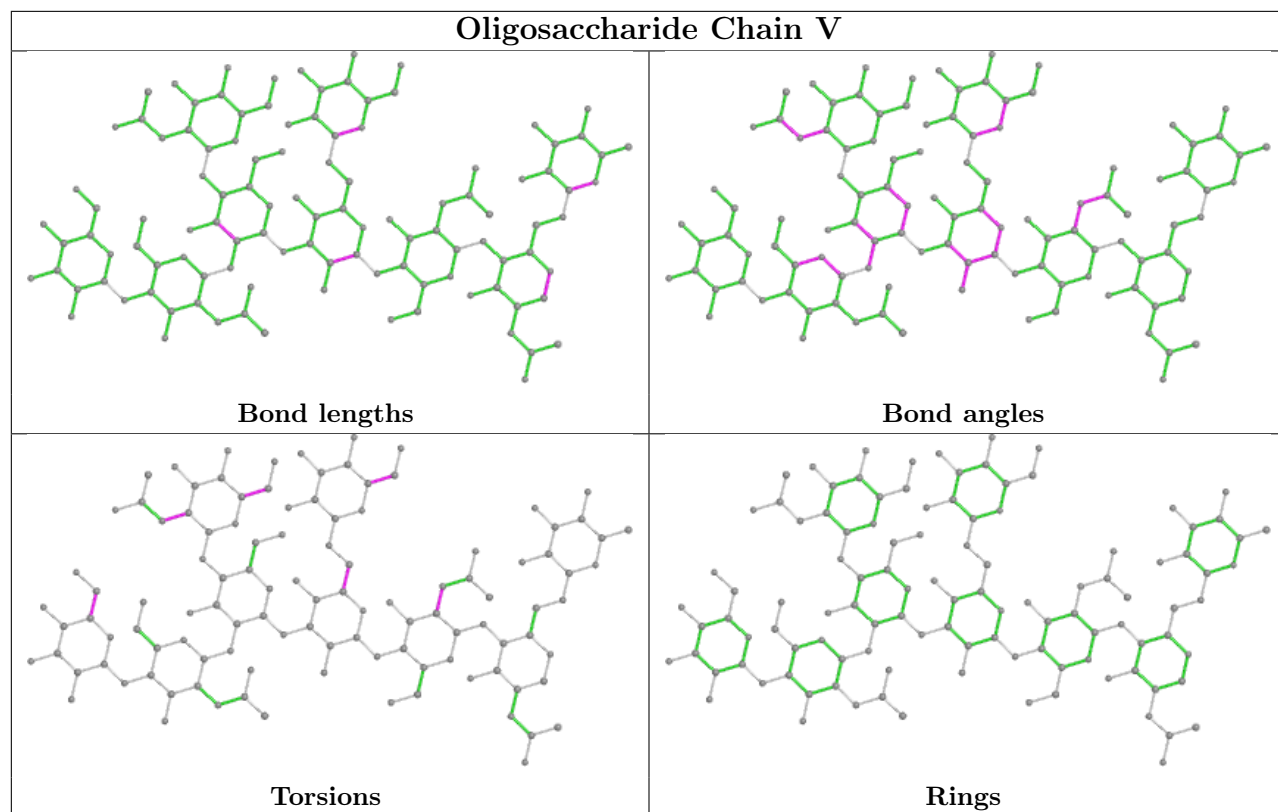


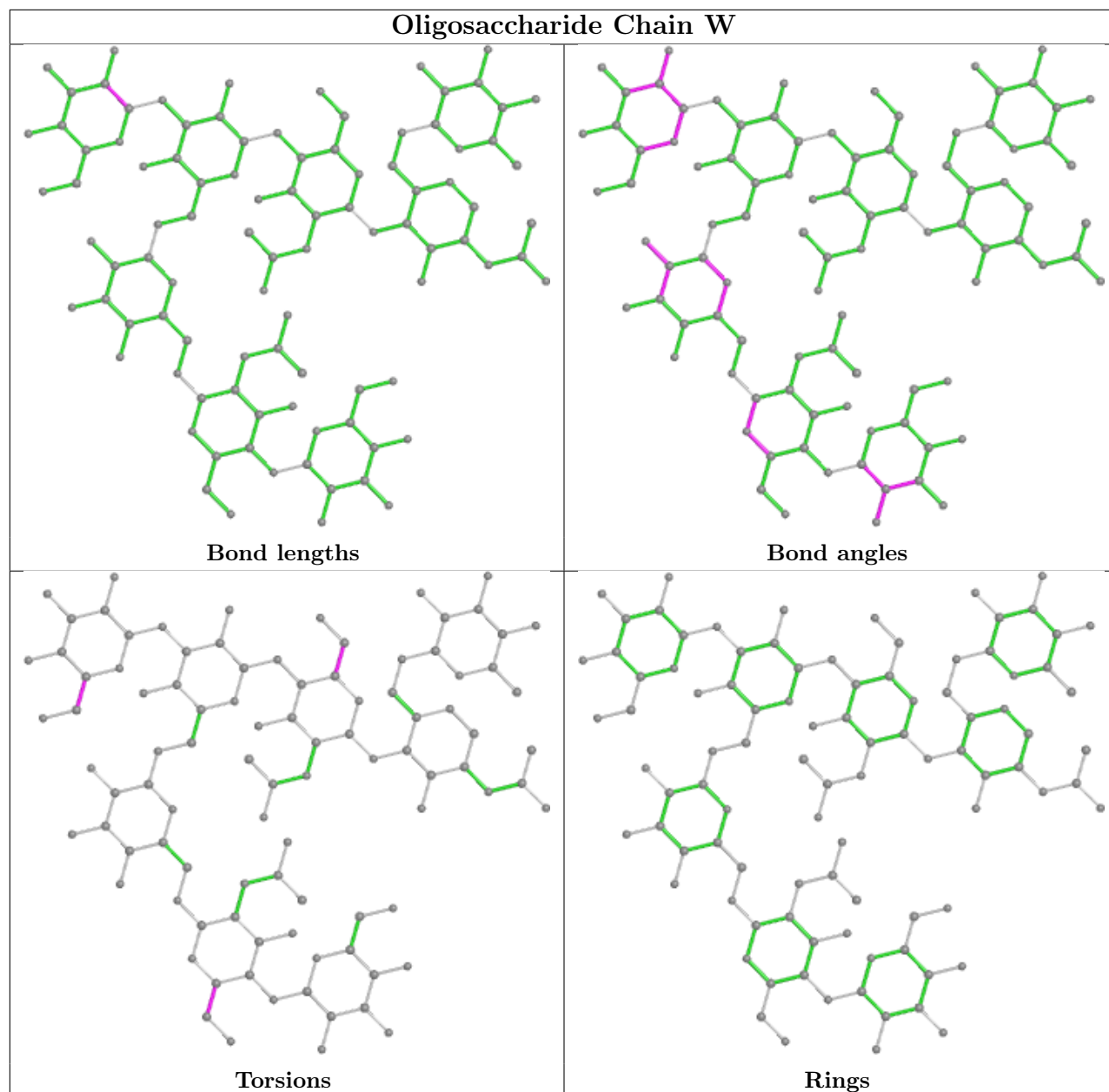


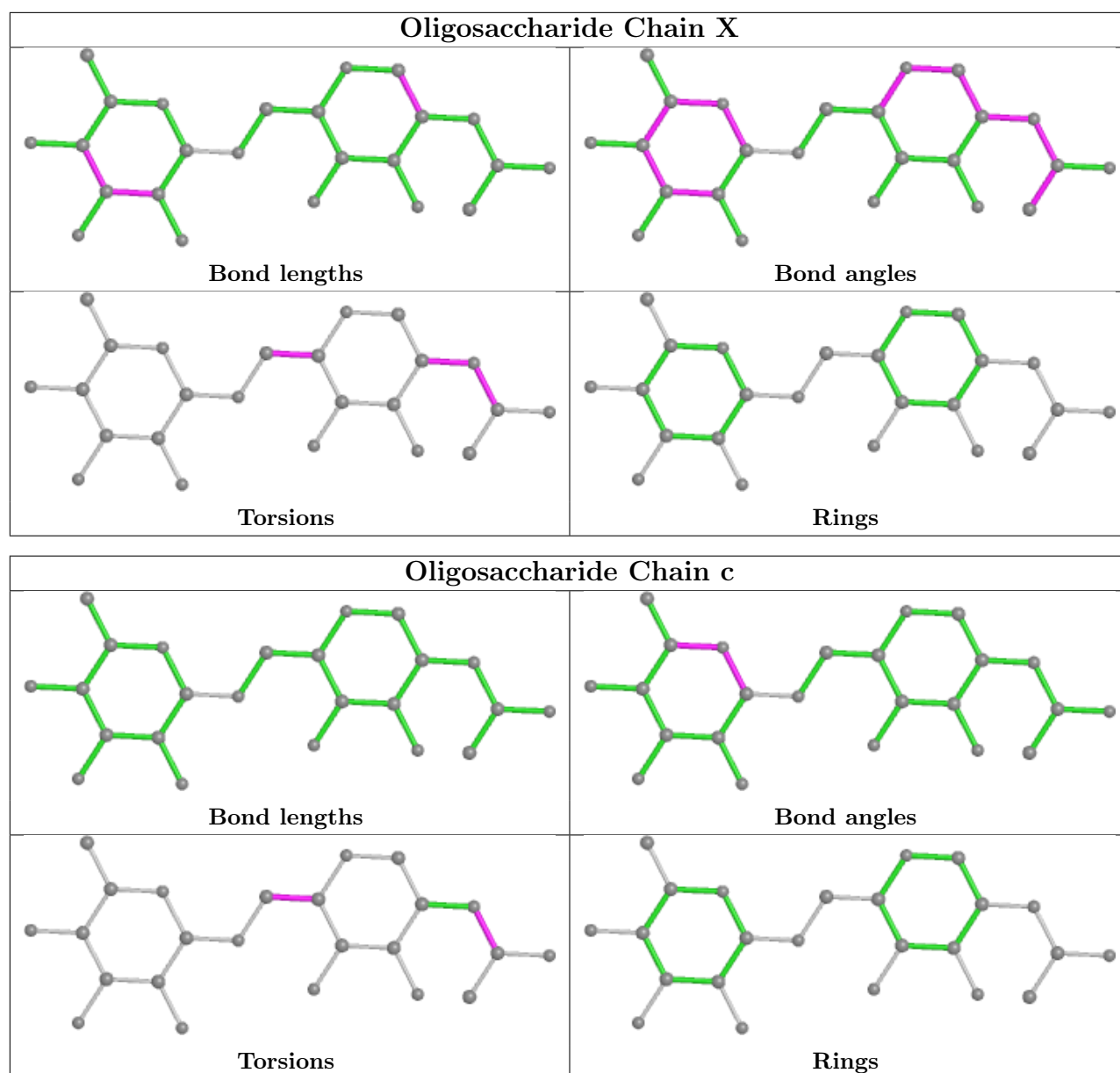


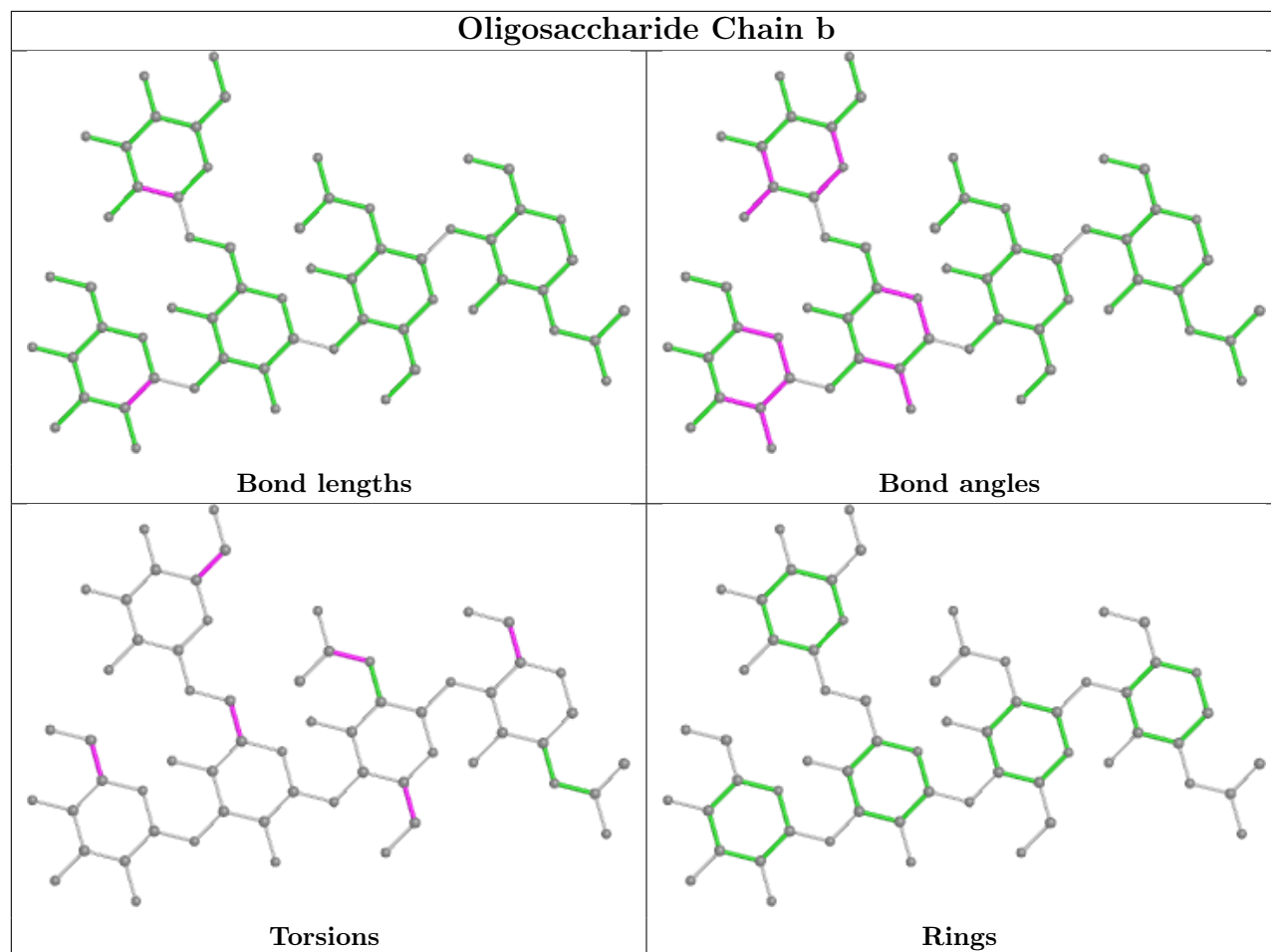


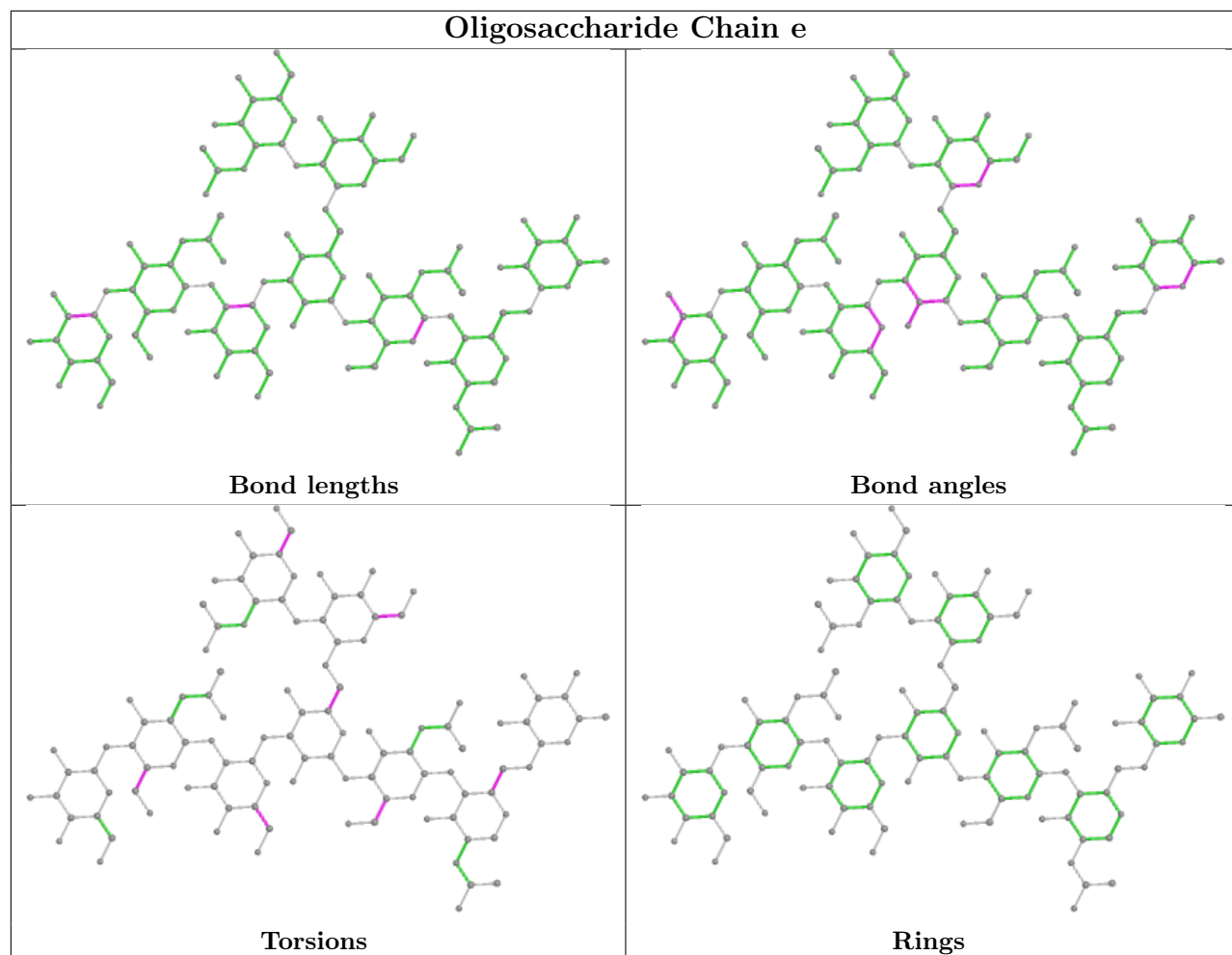


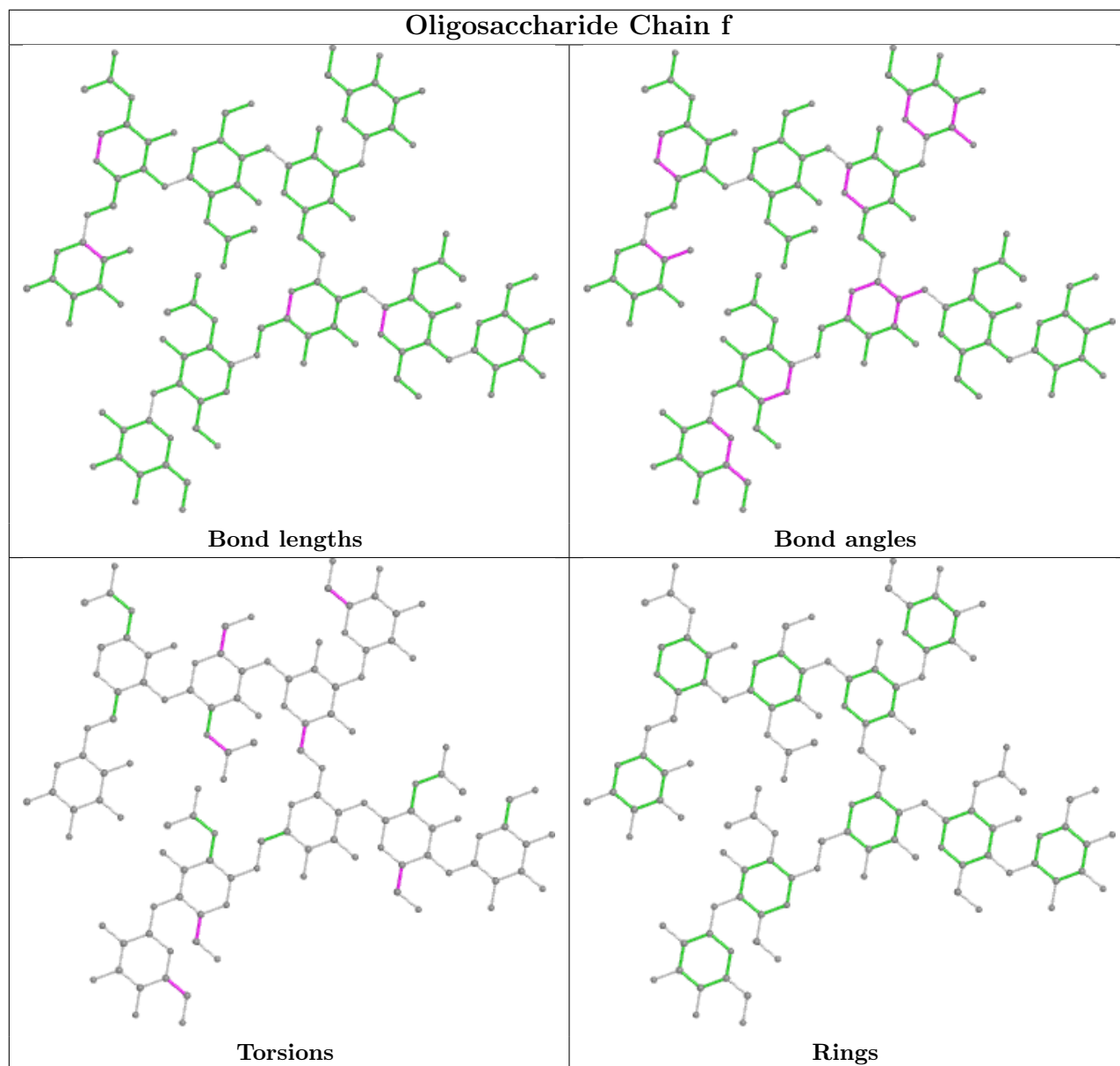












5.6 Ligand geometry [i](#)

41 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	E	612	1	14,14,15	0.78	1 (7%)	17,19,21	2.24	3 (17%)
15	NAG	E	614	1	14,14,15	0.37	0	17,19,21	0.50	0
15	NAG	F	901	2	14,14,15	0.20	0	17,19,21	0.67	1 (5%)
15	NAG	F	903	2	14,14,15	0.43	0	17,19,21	0.83	1 (5%)
15	NAG	F	902	2	14,14,15	0.34	0	17,19,21	0.38	0
15	NAG	C	627	1	14,14,15	0.32	0	17,19,21	0.53	0
15	NAG	C	624	1	14,14,15	0.68	1 (7%)	17,19,21	0.89	1 (5%)
15	NAG	C	622	1	14,14,15	0.26	0	17,19,21	0.44	0
15	NAG	C	606	1	14,14,15	0.18	0	17,19,21	0.39	0
15	NAG	C	603	1	14,14,15	0.44	0	17,19,21	0.59	1 (5%)
15	NAG	C	623	1	14,14,15	0.32	0	17,19,21	0.42	0
15	NAG	D	901	2	14,14,15	0.47	0	17,19,21	0.46	0
15	NAG	C	617	1	14,14,15	0.29	0	17,19,21	0.58	0
15	NAG	E	608	1	14,14,15	0.28	0	17,19,21	0.45	0
15	NAG	C	628	1	14,14,15	0.44	0	17,19,21	0.65	1 (5%)
15	NAG	A	619	1	14,14,15	0.45	0	17,19,21	0.52	0
15	NAG	E	610	1	14,14,15	0.32	0	17,19,21	0.39	0
15	NAG	A	604	1	14,14,15	0.41	0	17,19,21	0.60	0
15	NAG	E	622	1	14,14,15	0.48	0	17,19,21	0.70	1 (5%)
15	NAG	C	615	1	14,14,15	1.28	1 (7%)	17,19,21	1.61	1 (5%)
15	NAG	E	618	1	14,14,15	0.62	1 (7%)	17,19,21	1.66	1 (5%)
15	NAG	E	621	1	14,14,15	0.30	0	17,19,21	0.40	0
15	NAG	E	611	1	14,14,15	0.92	1 (7%)	17,19,21	0.62	0
15	NAG	C	614	1	14,14,15	0.62	0	17,19,21	0.68	1 (5%)
15	NAG	C	621	1	14,14,15	0.35	0	17,19,21	0.55	0
15	NAG	A	603	1	14,14,15	0.29	0	17,19,21	0.52	0
15	NAG	E	616	1	14,14,15	0.51	0	17,19,21	1.02	2 (11%)
15	NAG	A	605	1	14,14,15	0.48	0	17,19,21	0.81	1 (5%)
15	NAG	A	629	1	14,14,15	0.21	0	17,19,21	0.57	0
15	NAG	E	615	1	14,14,15	0.26	0	17,19,21	0.43	0
15	NAG	E	617	1	14,14,15	0.27	0	17,19,21	0.41	0
15	NAG	E	619	1	14,14,15	0.78	1 (7%)	17,19,21	2.18	3 (17%)
15	NAG	A	632	1	14,14,15	0.53	0	17,19,21	0.60	1 (5%)
15	NAG	C	616	1	14,14,15	0.44	0	17,19,21	0.35	0
15	NAG	E	609	1	14,14,15	0.25	0	17,19,21	0.61	0
15	NAG	F	904	2	14,14,15	0.60	0	17,19,21	0.48	0
15	NAG	E	620	1	14,14,15	0.52	0	17,19,21	0.63	1 (5%)
15	NAG	A	633	1	14,14,15	0.64	1 (7%)	17,19,21	0.96	1 (5%)
15	NAG	A	618	1	14,14,15	0.19	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	NAG	E	613	1	14,14,15	0.26	0	17,19,21	0.51	0
15	NAG	C	620	1	14,14,15	0.25	0	17,19,21	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	E	612	1	-	5/6/23/26	0/1/1/1
15	NAG	E	614	1	-	1/6/23/26	0/1/1/1
15	NAG	F	901	2	-	2/6/23/26	0/1/1/1
15	NAG	F	903	2	-	0/6/23/26	0/1/1/1
15	NAG	F	902	2	-	2/6/23/26	0/1/1/1
15	NAG	C	627	1	-	2/6/23/26	0/1/1/1
15	NAG	C	624	1	-	2/6/23/26	0/1/1/1
15	NAG	C	622	1	-	2/6/23/26	0/1/1/1
15	NAG	C	606	1	-	2/6/23/26	0/1/1/1
15	NAG	C	603	1	-	1/6/23/26	0/1/1/1
15	NAG	C	623	1	-	1/6/23/26	0/1/1/1
15	NAG	D	901	2	-	2/6/23/26	0/1/1/1
15	NAG	C	617	1	-	4/6/23/26	0/1/1/1
15	NAG	E	608	1	-	2/6/23/26	0/1/1/1
15	NAG	C	628	1	-	0/6/23/26	0/1/1/1
15	NAG	A	619	1	-	4/6/23/26	0/1/1/1
15	NAG	E	610	1	-	2/6/23/26	0/1/1/1
15	NAG	A	604	1	-	2/6/23/26	0/1/1/1
15	NAG	E	622	1	-	2/6/23/26	0/1/1/1
15	NAG	C	615	1	-	4/6/23/26	0/1/1/1
15	NAG	E	618	1	-	4/6/23/26	0/1/1/1
15	NAG	E	621	1	-	2/6/23/26	0/1/1/1
15	NAG	E	611	1	-	3/6/23/26	0/1/1/1
15	NAG	C	614	1	-	2/6/23/26	0/1/1/1
15	NAG	C	621	1	-	2/6/23/26	0/1/1/1
15	NAG	A	603	1	-	2/6/23/26	0/1/1/1
15	NAG	E	616	1	-	2/6/23/26	0/1/1/1
15	NAG	A	605	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	A	629	1	-	2/6/23/26	0/1/1/1
15	NAG	E	615	1	-	2/6/23/26	0/1/1/1
15	NAG	E	617	1	-	1/6/23/26	0/1/1/1
15	NAG	E	619	1	-	5/6/23/26	0/1/1/1
15	NAG	A	632	1	-	2/6/23/26	0/1/1/1
15	NAG	C	616	1	-	2/6/23/26	0/1/1/1
15	NAG	E	609	1	-	4/6/23/26	0/1/1/1
15	NAG	F	904	2	-	0/6/23/26	0/1/1/1
15	NAG	E	620	1	-	1/6/23/26	0/1/1/1
15	NAG	A	633	1	-	3/6/23/26	0/1/1/1
15	NAG	A	618	1	-	2/6/23/26	0/1/1/1
15	NAG	E	613	1	-	2/6/23/26	0/1/1/1
15	NAG	C	620	1	-	4/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	615	NAG	O5-C1	4.65	1.51	1.43
15	E	611	NAG	C1-C2	3.09	1.57	1.52
15	C	624	NAG	C1-C2	2.27	1.55	1.52
15	E	619	NAG	C1-C2	2.22	1.55	1.52
15	A	633	NAG	C1-C2	2.14	1.55	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	619	NAG	C2-N2-C7	7.86	134.09	122.90
15	E	612	NAG	C2-N2-C7	7.70	133.86	122.90
15	C	615	NAG	C1-O5-C5	6.41	120.88	112.19
15	E	618	NAG	C1-O5-C5	6.21	120.61	112.19
15	E	612	NAG	C1-C2-N2	3.79	116.96	110.49

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	615	NAG	C4-C5-C6-O6
15	E	609	NAG	O5-C5-C6-O6
15	E	608	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	D	901	NAG	O5-C5-C6-O6
15	E	615	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	901	NAG	1	0
15	E	611	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

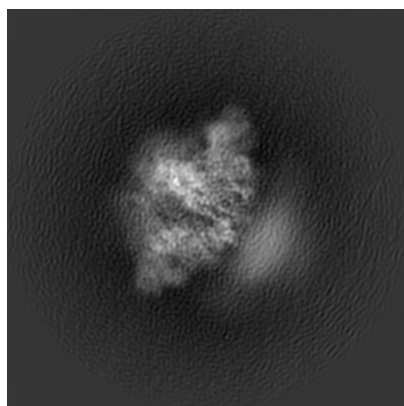
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20118. These allow visual inspection of the internal detail of the map and identification of artifacts.

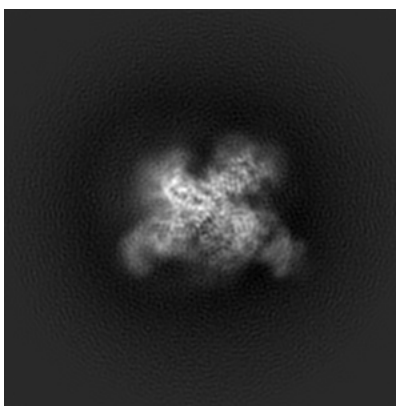
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

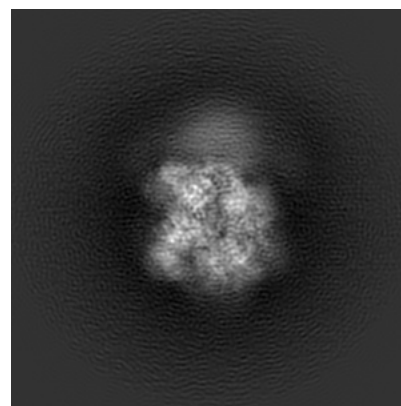
6.1.1 Primary map



X

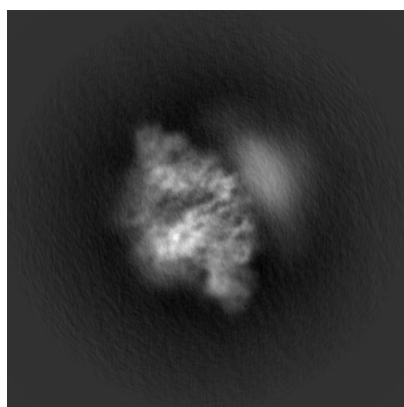


Y

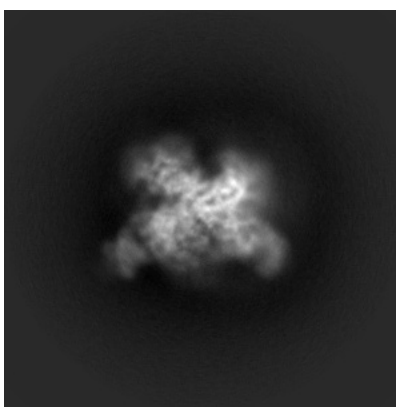


Z

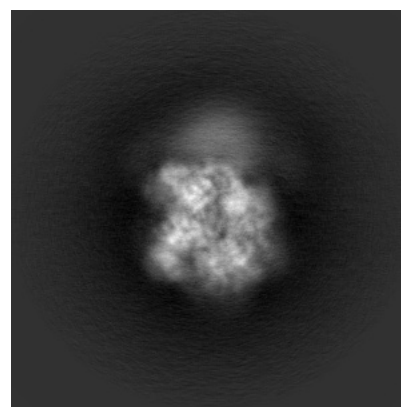
6.1.2 Raw map



X



Y

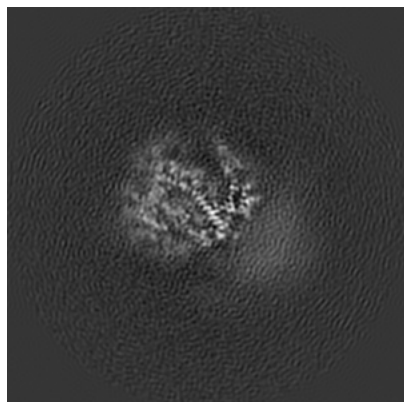


Z

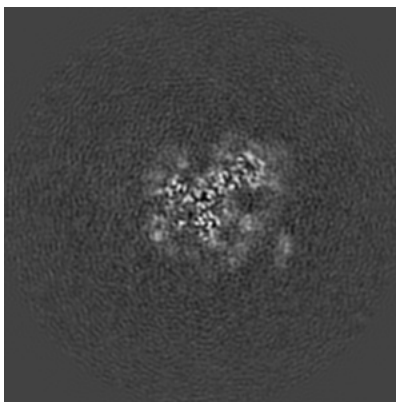
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

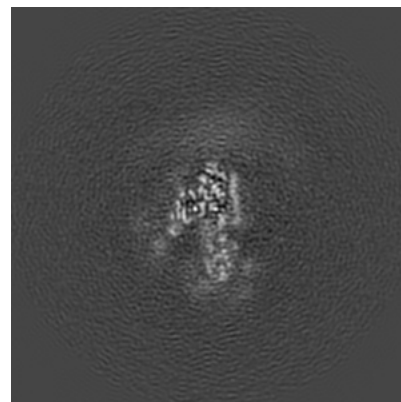
6.2.1 Primary map



X Index: 175

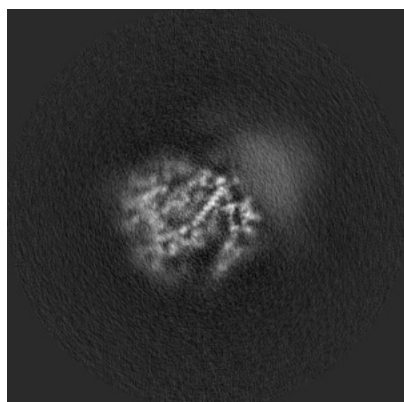


Y Index: 175

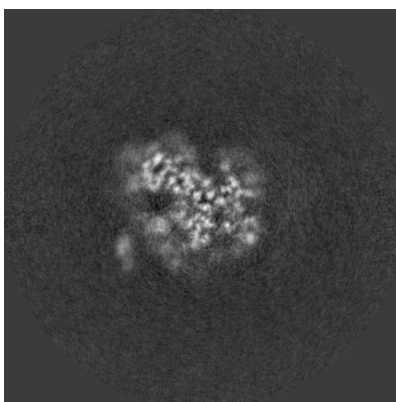


Z Index: 175

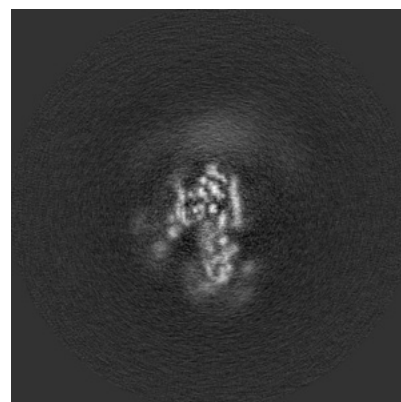
6.2.2 Raw map



X Index: 175



Y Index: 175

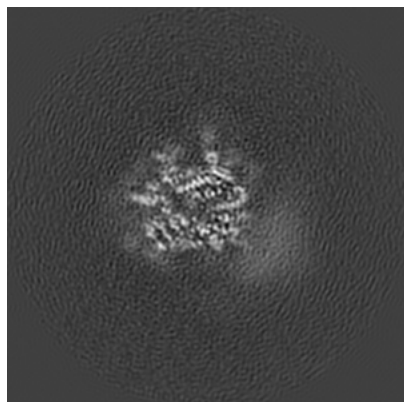


Z Index: 175

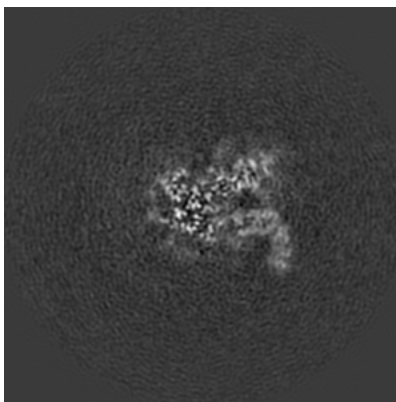
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

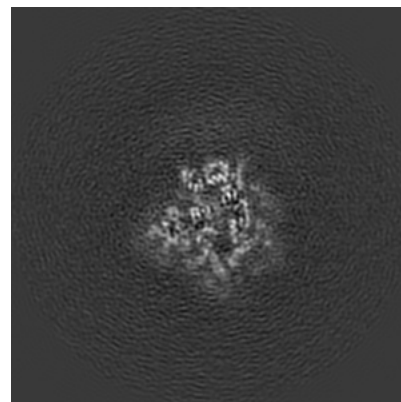
6.3.1 Primary map



X Index: 193

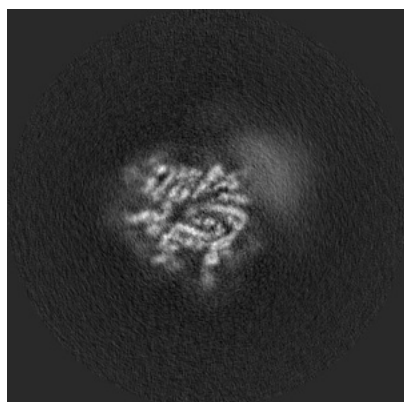


Y Index: 181

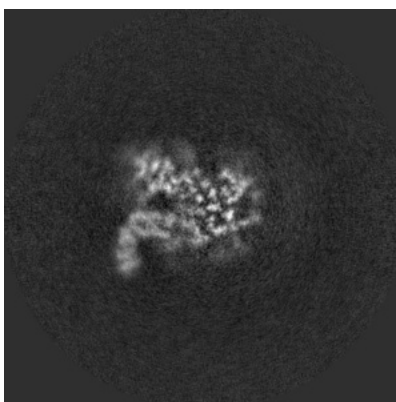


Z Index: 192

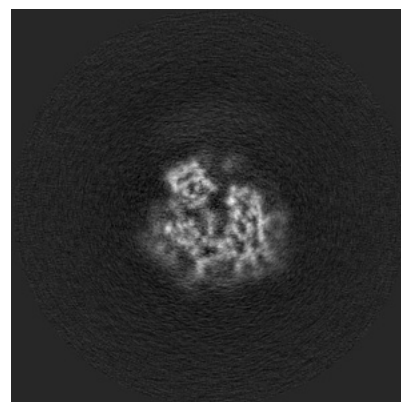
6.3.2 Raw map



X Index: 194



Y Index: 181

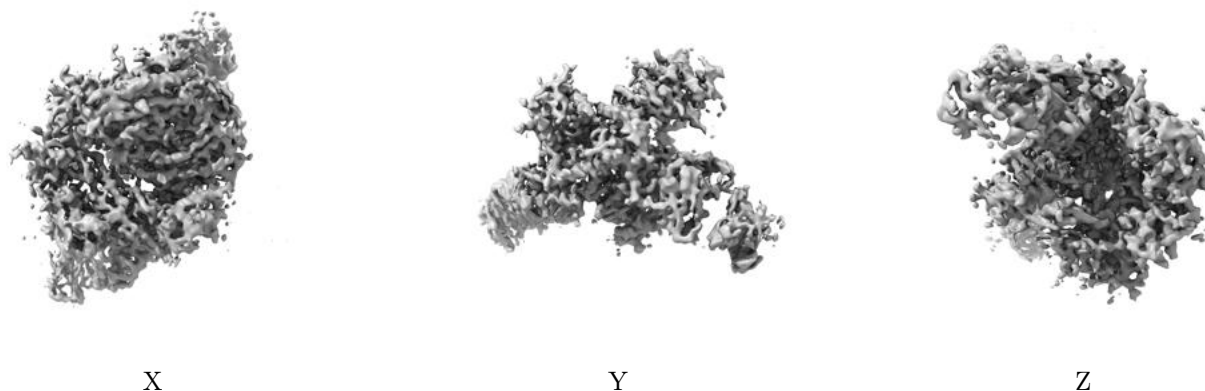


Z Index: 144

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

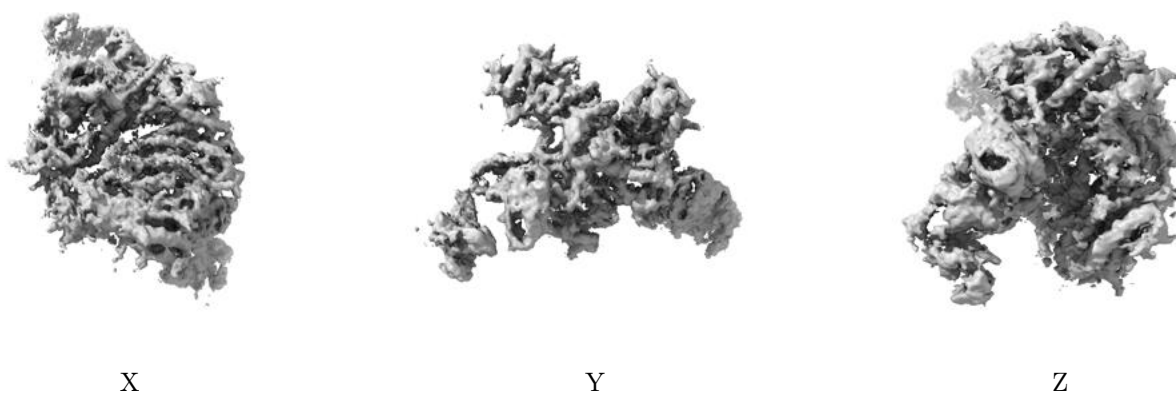
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0218. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

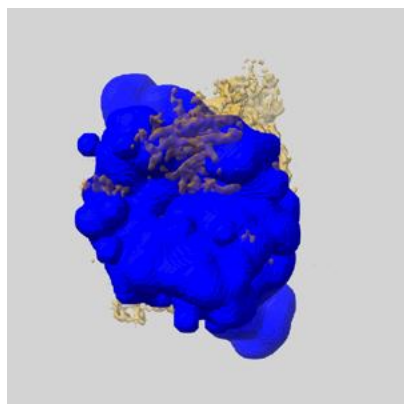
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

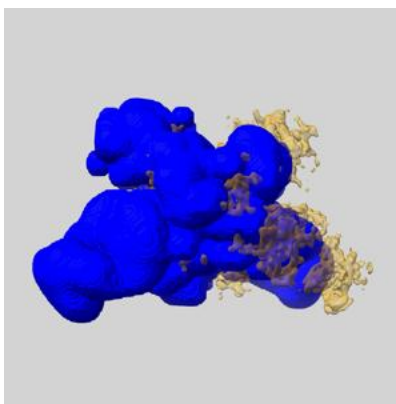
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

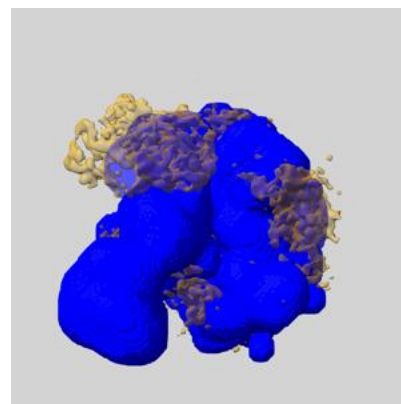
6.5.1 emd_20118_msk_1.map [i](#)



X



Y

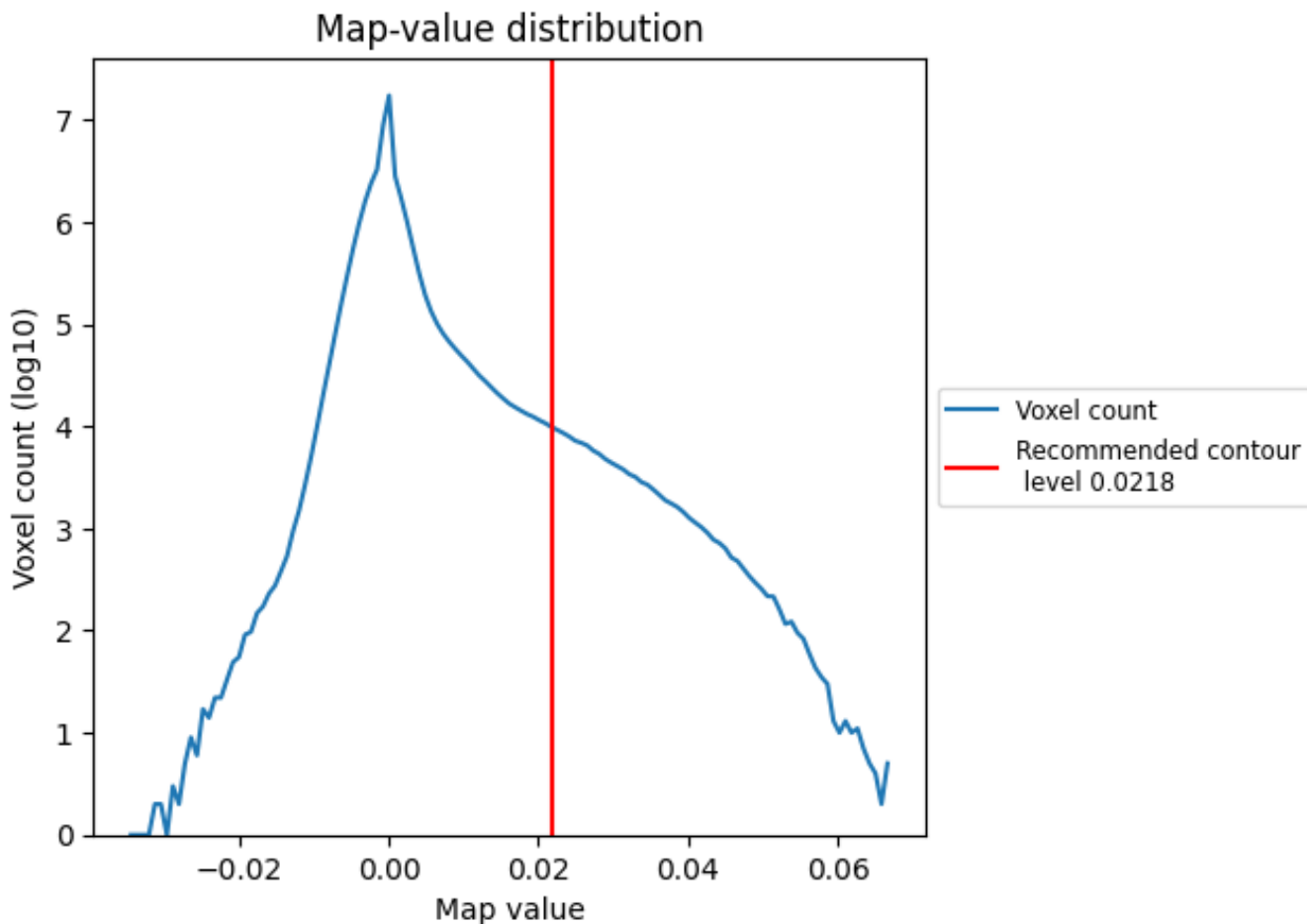


Z

7 Map analysis [i](#)

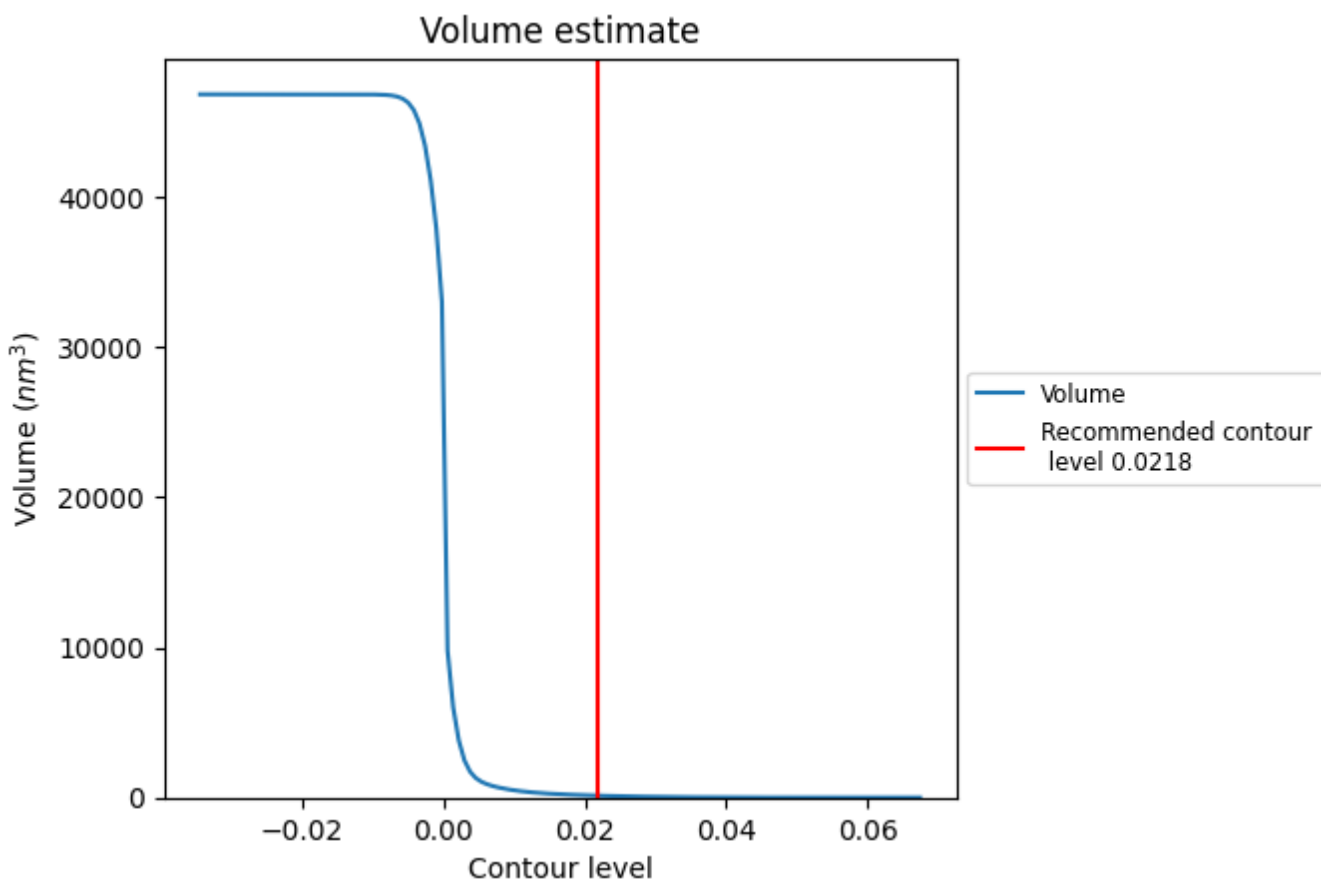
This section contains the results of statistical analysis of the map.

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.

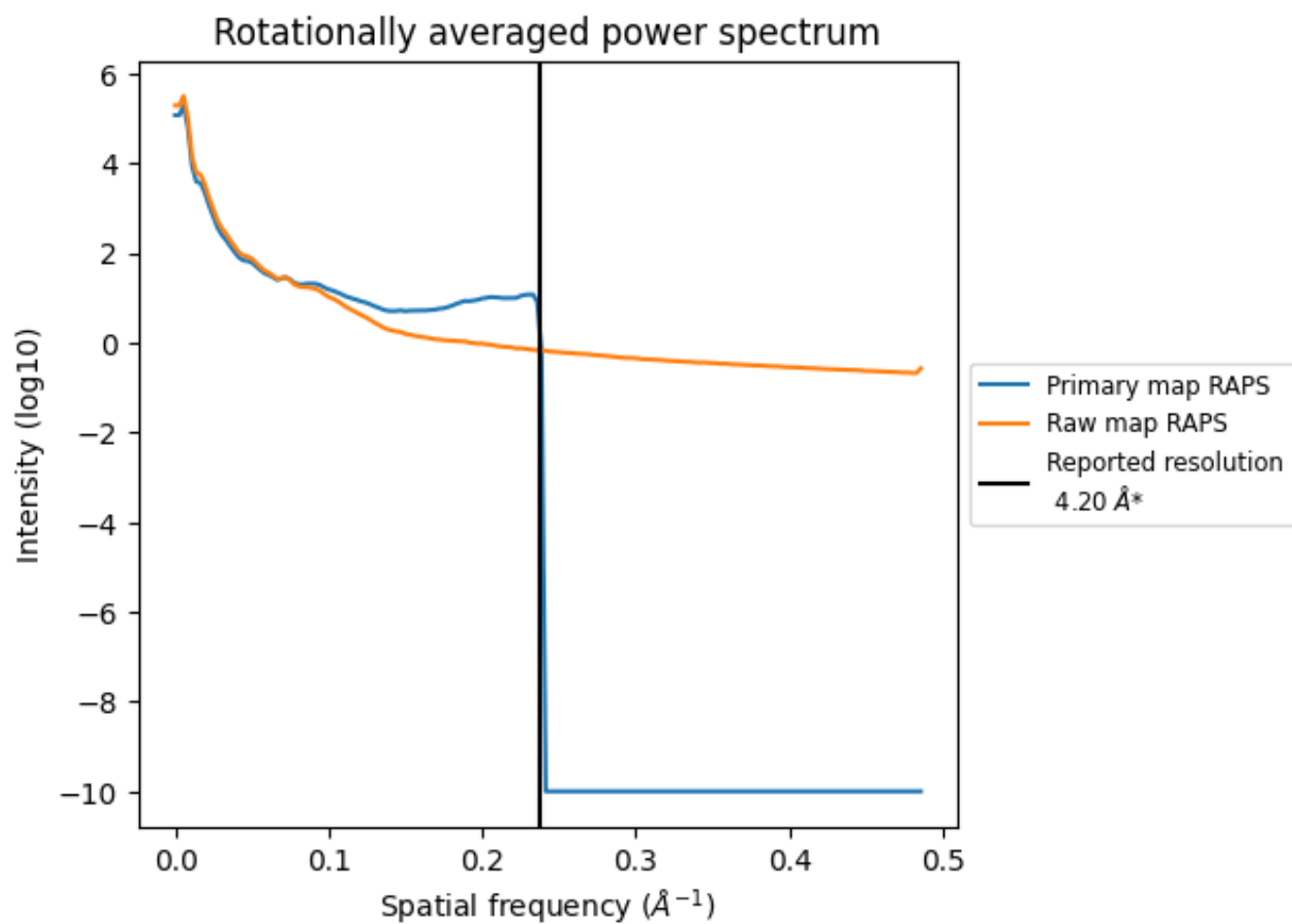
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 127 nm³; this corresponds to an approximate mass of 115 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 [i](#)

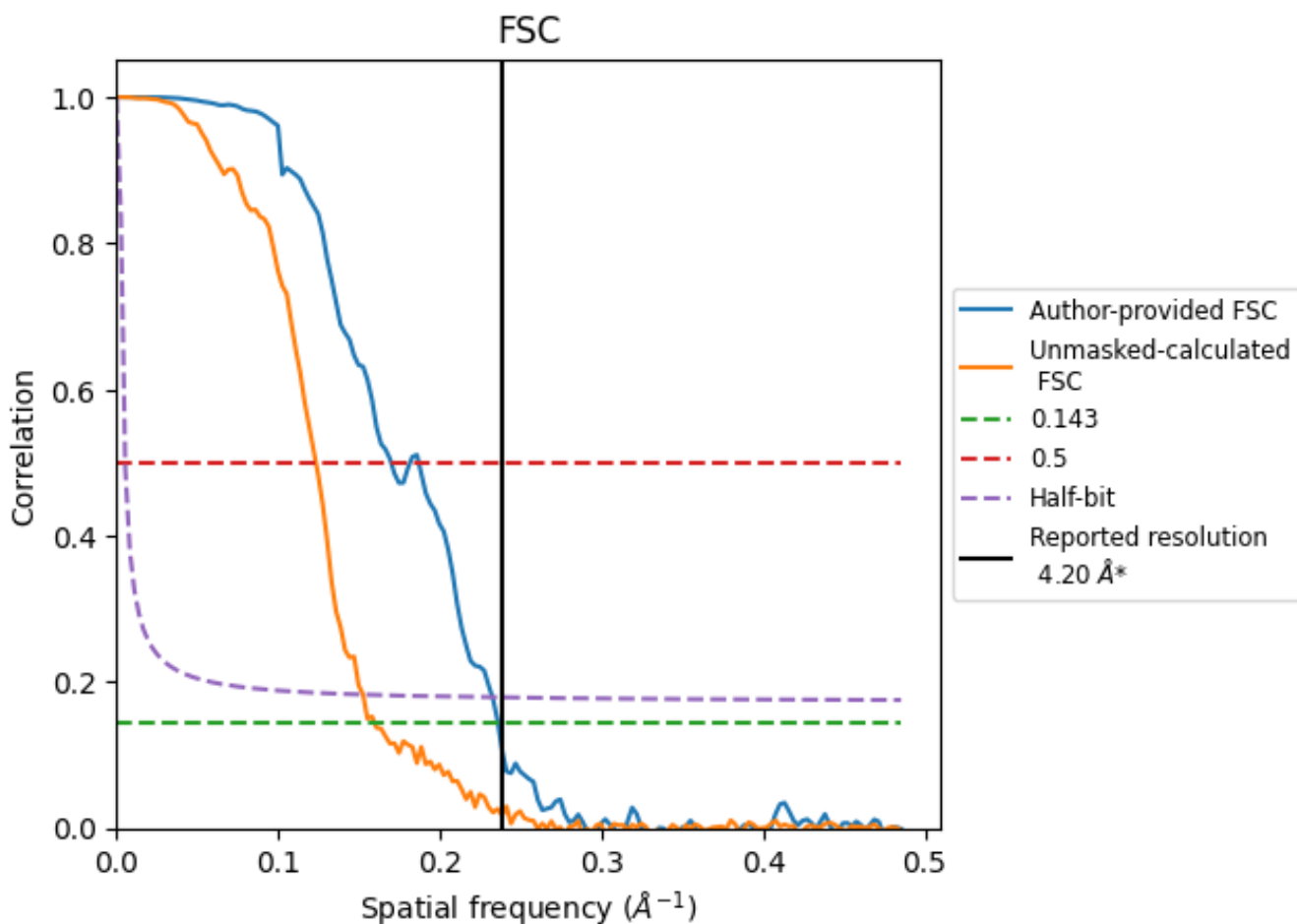


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

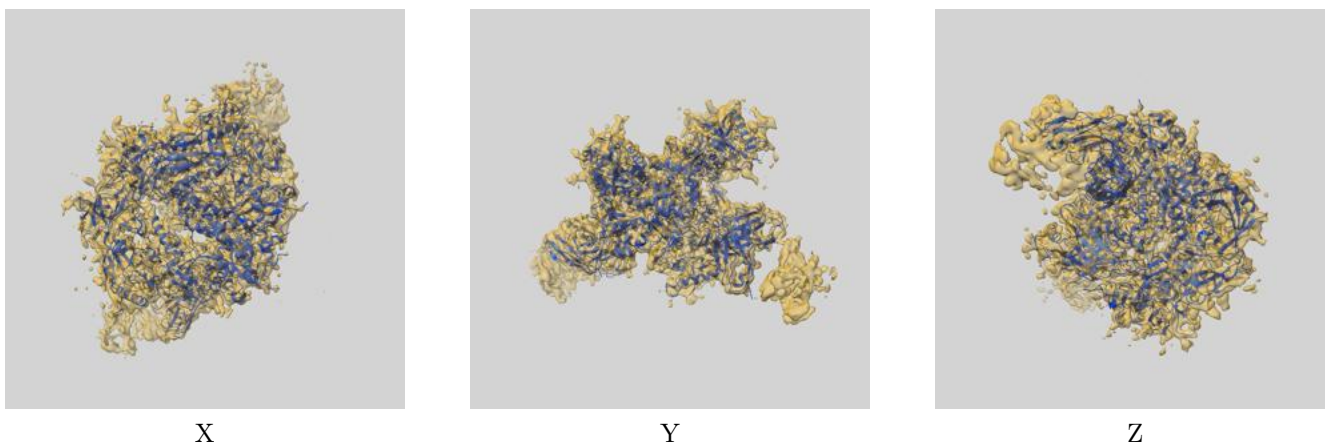
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.24	5.89	4.30
Unmasked-calculated*	6.26	8.10	6.56

*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 6.26 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

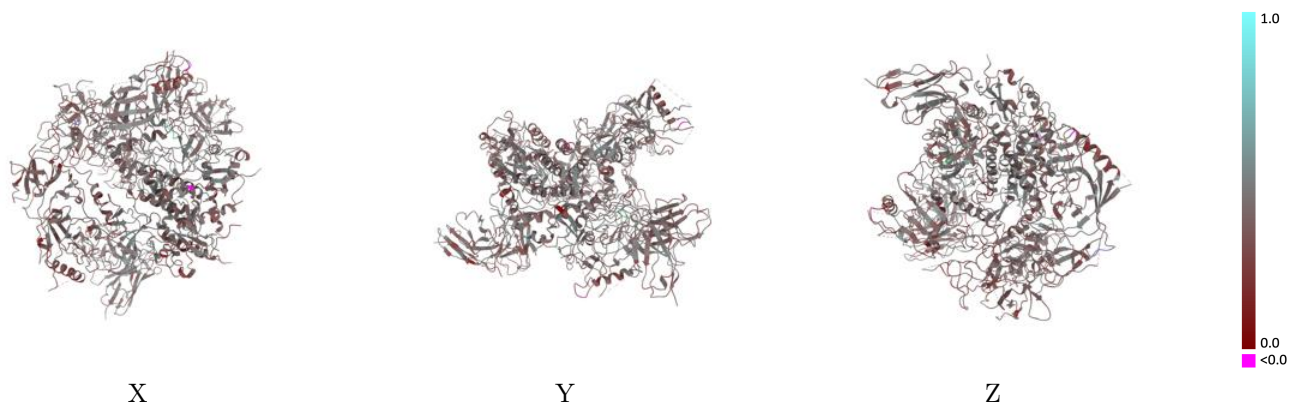
This section contains information regarding the fit between EMDB map EMD-20118 and PDB model 6OLP. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



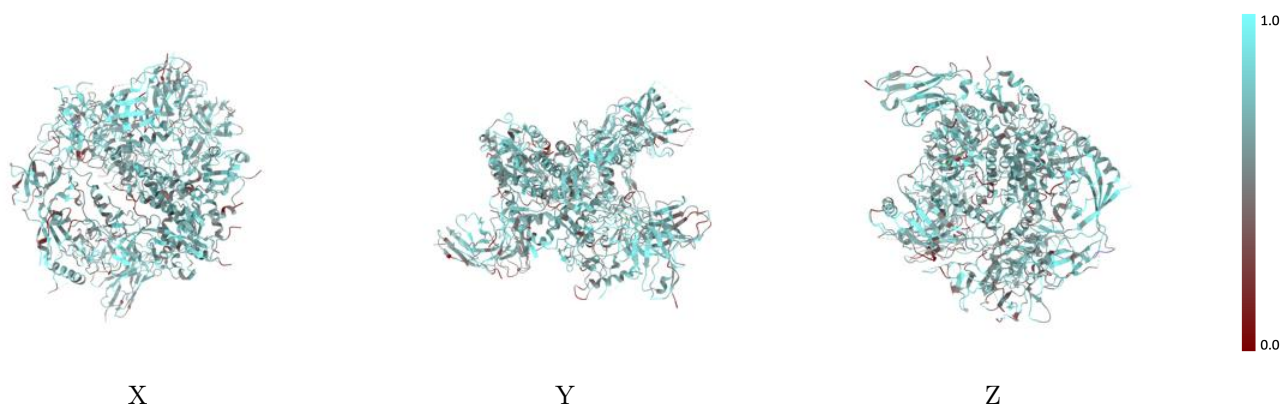
The images above show the 3D surface view of the map at the recommended contour level 0.0218 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



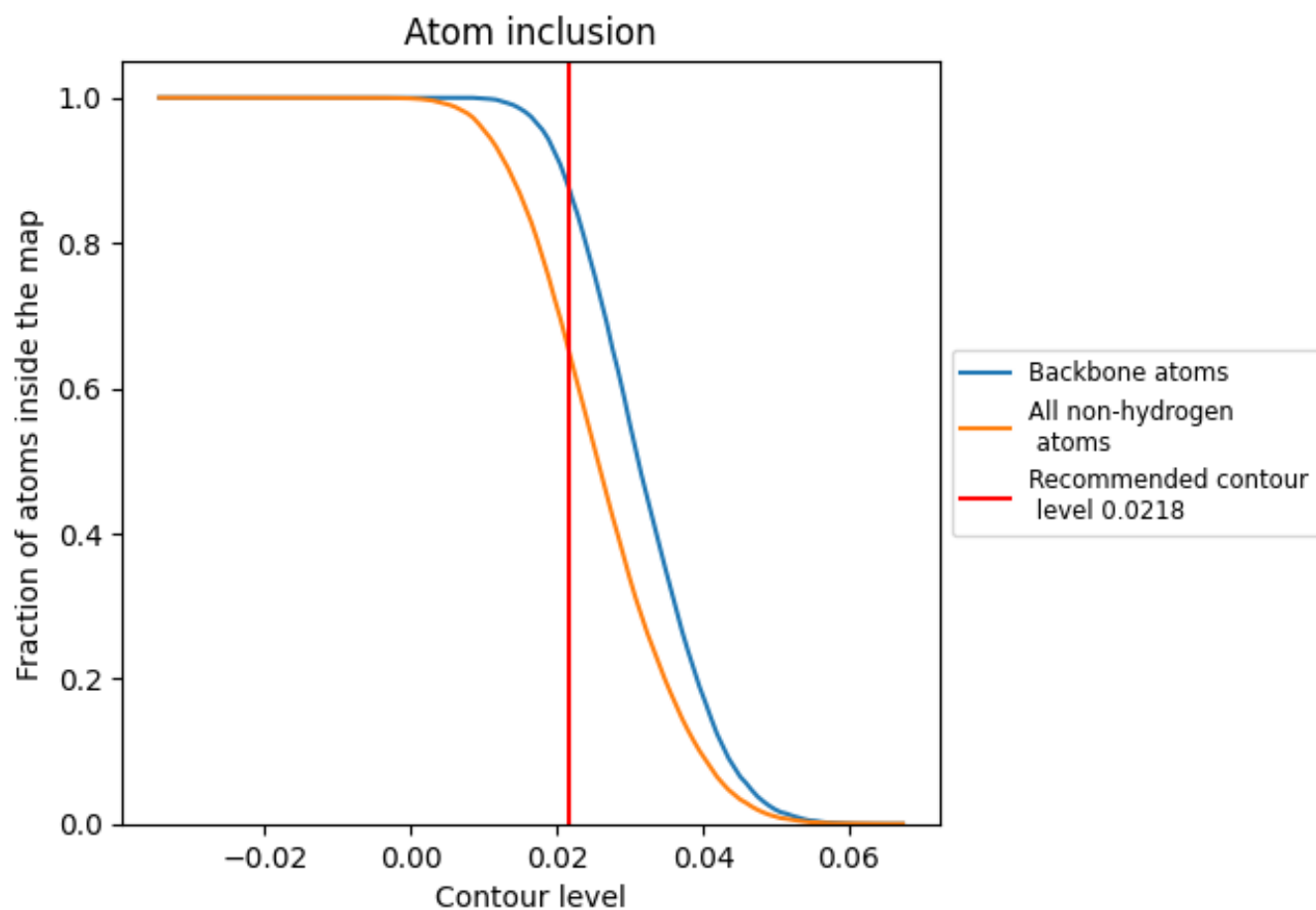
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0218).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 65% 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 (0.0218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6459	 0.3990
A	 0.6849	 0.4110
B	 0.6587	 0.3910
C	 0.6382	 0.3880
D	 0.6960	 0.4240
E	 0.6445	 0.3860
F	 0.6211	 0.4020
G	 0.7340	 0.4170
H	 0.6910	 0.4060
I	 0.5956	 0.3790
J	 0.4643	 0.4100
K	 0.3214	 0.4210
L	 0.5293	 0.3670
M	 0.3571	 0.3750
N	 0.6071	 0.4390
O	 0.4643	 0.4010
P	 0.6400	 0.4760
Q	 0.5357	 0.4370
R	 0.3846	 0.4180
S	 0.3571	 0.2910
T	 0.4643	 0.3390
U	 0.4286	 0.3760
V	 0.6182	 0.4150
W	 0.6458	 0.4480
X	 0.3750	 0.4150
Y	 0.4643	 0.4760
Z	 0.3571	 0.3950
a	 0.1786	 0.3980
b	 0.5902	 0.4770
c	 0.7500	 0.4510
d	 0.3929	 0.4700
e	 0.6182	 0.4840
f	 0.5041	 0.4680
g	 0.4643	 0.4070
h	 0.3214	 0.4310
i	 0.6667	 0.4330

