



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 09:58 PM JST

PDB ID : 7YBM
EMDB ID : EMD-33726
Title : SARS-CoV-2 C.1.2 variant spike (Close state)
Authors : Wang, X.; Fu, W.
Deposited on : 2022-06-29
Resolution : 3.45 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.39

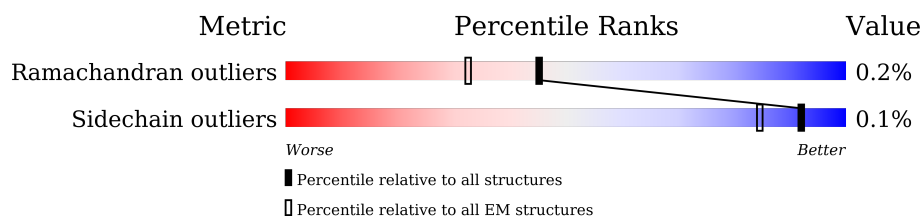
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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.



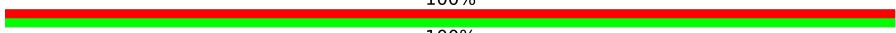

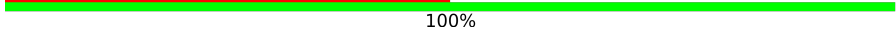



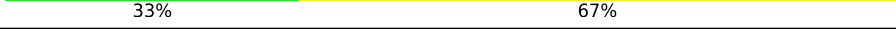

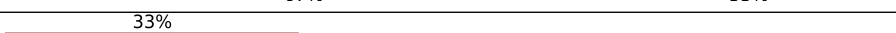
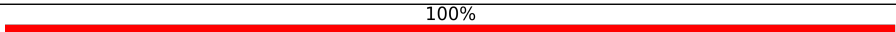





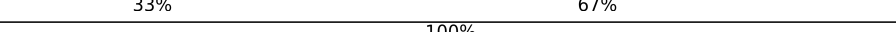
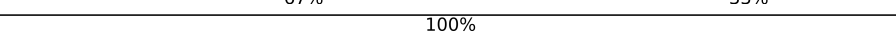








Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1271	<div> <div>20%</div> <div>86%</div> <div>13%</div> </div>
1	B	1271	<div> <div>20%</div> <div>86%</div> <div>13%</div> </div>
1	C	1271	<div> <div>21%</div> <div>86%</div> <div>13%</div> </div>
2	D	2	<div> <div>100%</div> <div>50%</div> <div>50%</div> </div>
2	F	2	<div> <div>100%</div> <div>100%</div> </div>
2	I	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>
2	O	2	<div> <div>100%</div> <div>100%</div> </div>
2	Q	2	<div> <div>100%</div> <div>100%</div> </div>
2	T	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	Z	2	100% 
2	b	2	100% 
2	e	2	50% 
3	E	3	100% 
3	G	3	67% 
3	H	3	67% 
3	J	3	33% 
3	K	3	67% 
3	M	3	33% 
3	N	3	33% 
3	P	3	100% 
3	R	3	67% 
3	S	3	67% 
3	U	3	33% 
3	V	3	67% 
3	X	3	67% 
3	Y	3	33% 
3	a	3	100% 
3	c	3	67% 
3	d	3	67% 
3	f	3	33% 
3	g	3	67% 
3	i	3	67% 
3	j	3	33% 
4	L	3	67% 

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Mol	Chain	Length	Quality of chain
4	W	3	<div><div></div><div>33%</div><div>67%</div><div>33%</div></div>
4	h	3	<div><div></div><div>67%</div><div>67%</div><div>33%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27456 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1103	Total	C	N	O	S	0	0
			8645	5525	1442	1640	38		
1	B	1103	Total	C	N	O	S	0	0
			8645	5525	1442	1640	38		
1	C	1103	Total	C	N	O	S	0	0
			8645	5525	1442	1640	38		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	136	PHE	CYS	conflict	UNP P0DTC2
A	190	SER	ARG	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	449	HIS	TYR	conflict	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	716	ILE	THR	variant	UNP P0DTC2
A	859	ASN	THR	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	136	PHE	CYS	conflict	UNP P0DTC2
B	190	SER	ARG	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	449	HIS	TYR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	716	ILE	THR	variant	UNP P0DTC2
B	859	ASN	THR	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	136	PHE	CYS	conflict	UNP P0DTC2
C	190	SER	ARG	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	449	HIS	TYR	conflict	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	716	ILE	THR	variant	UNP P0DTC2
C	859	ASN	THR	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		

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



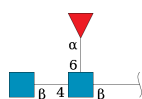
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	N	3	Total	C	N	O	0	0
			39	22	2	15		
3	P	3	Total	C	N	O	0	0
			39	22	2	15		
3	R	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	Y	3	Total	C	N	O	0	0
			39	22	2	15		
3	a	3	Total	C	N	O	0	0
			39	22	2	15		
3	c	3	Total	C	N	O	0	0
			39	22	2	15		
3	d	3	Total	C	N	O	0	0
			39	22	2	15		
3	f	3	Total	C	N	O	0	0
			39	22	2	15		
3	g	3	Total	C	N	O	0	0
			39	22	2	15		
3	i	3	Total	C	N	O	0	0
			39	22	2	15		
3	j	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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
4	L	3	Total	C	N	O	0	0
			38	22	2	14		
4	W	3	Total	C	N	O	0	0
			38	22	2	14		
4	h	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



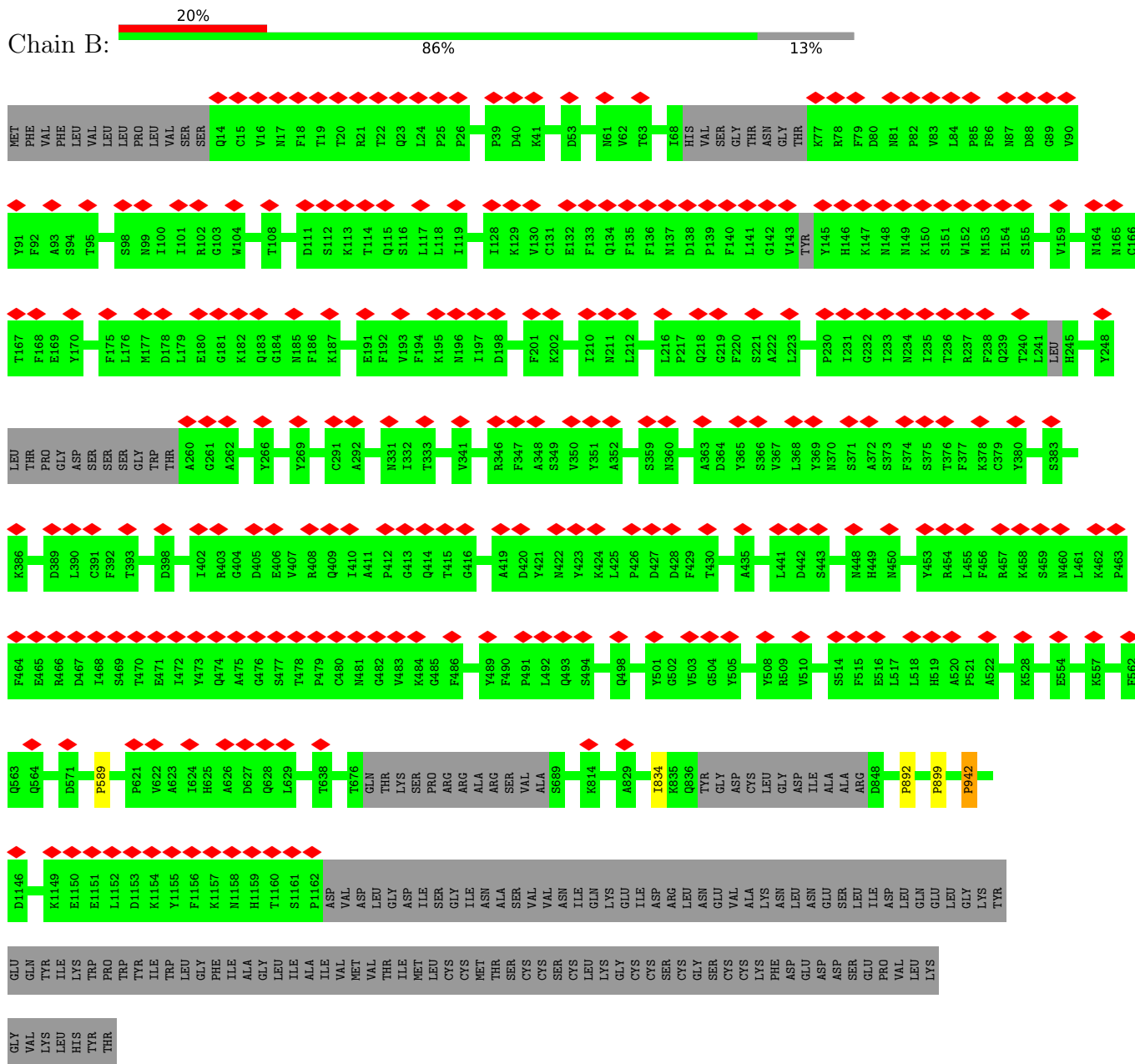
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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

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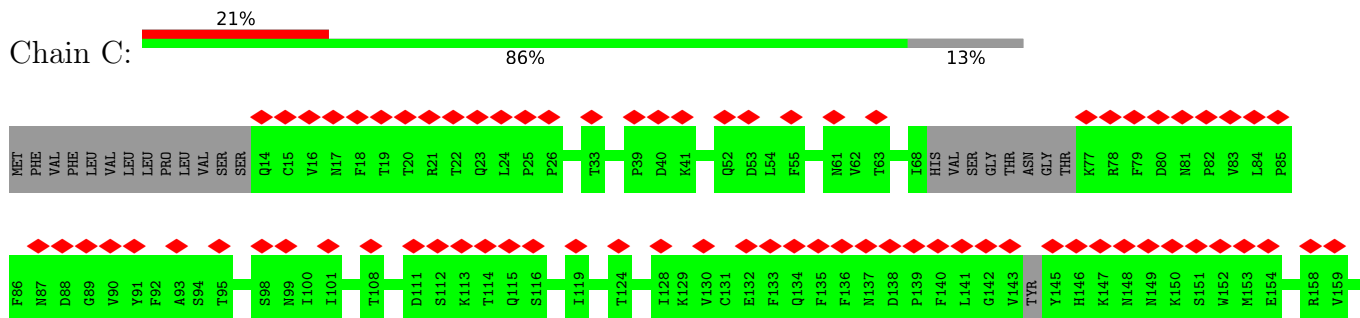
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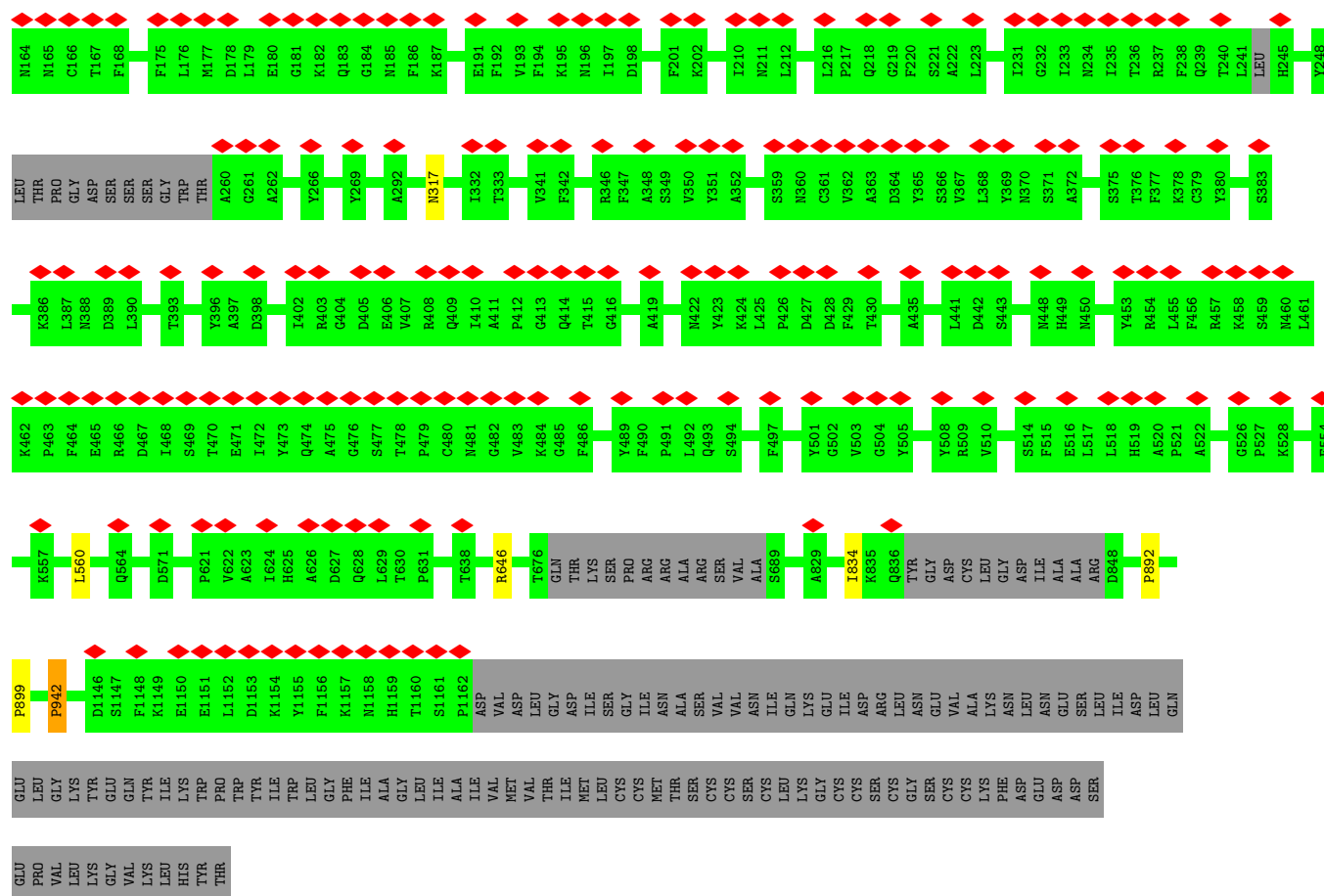
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

Chain B:



Chain C:





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



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



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





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



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



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



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



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



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



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



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



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



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



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



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

Chain V:  67% 33%



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

Chain X:  67% 33%



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

Chain Y:  33% 33% 67%



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

Chain a:  100% 67% 33%



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

Chain c:  100% 67% 33%



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

Chain d:  67% 67% 33%




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

Chain f: 



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

Chain g: 



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

Chain i: 



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

Chain j: 



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

Chain L: 



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

Chain W: 



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

Chain h: 67% 67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	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, FUC, MAN

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	0.26	0/8846	0.49	3/12028 (0.0%)
1	B	0.26	0/8846	0.50	4/12028 (0.0%)
1	C	0.26	0/8846	0.49	4/12028 (0.0%)
All	All	0.26	0/26538	0.50	11/36084 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	PRO	CA-N-CD	-7.56	100.92	111.50
1	C	892	PRO	N-CA-CB	5.95	110.44	103.30
1	B	892	PRO	N-CA-CB	5.93	110.42	103.30
1	C	899	PRO	N-CA-CB	5.79	110.25	103.30
1	A	892	PRO	N-CA-CB	5.77	110.23	103.30
1	A	899	PRO	N-CA-CB	5.75	110.20	103.30
1	B	942	PRO	N-CA-CB	5.63	110.05	103.30
1	B	899	PRO	N-CA-CB	5.63	110.05	103.30
1	A	942	PRO	N-CA-CB	5.61	110.03	103.30
1	C	560	LEU	CA-CB-CG	5.57	128.11	115.30
1	C	942	PRO	N-CA-CB	5.55	109.96	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1089/1271 (86%)	1037 (95%)	50 (5%)	2 (0%)	44	76
1	B	1089/1271 (86%)	1029 (94%)	58 (5%)	2 (0%)	44	76
1	C	1089/1271 (86%)	1040 (96%)	47 (4%)	2 (0%)	44	76
All	All	3267/3813 (86%)	3106 (95%)	155 (5%)	6 (0%)	45	76

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	942	PRO
1	A	834	ILE
1	A	942	PRO
1	B	834	ILE
1	C	834	ILE
1	C	942	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	963/1112 (87%)	962 (100%)	1 (0%)	92	97
1	B	963/1112 (87%)	963 (100%)	0	100	100
1	C	963/1112 (87%)	961 (100%)	2 (0%)	92	96
All	All	2889/3336 (87%)	2886 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	C	317	ASN
1	C	646	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	644	GLN
1	B	1159	HIS
1	C	613	GLN
1	C	644	GLN
1	C	658	ASN

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 ⓘ

90 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	0.62	1 (7%)	17,19,21	0.71	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	E	1	3,1	14,14,15	0.16	0	17,19,21	0.45	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	3	3	11,11,12	0.73	0	15,15,17	1.18	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.20	0	17,19,21	0.37	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	G	1	3,1	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	MAN	G	3	3	11,11,12	0.77	0	15,15,17	1.15	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.30	0	17,19,21	0.37	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	MAN	H	3	3	11,11,12	0.62	0	15,15,17	1.23	2 (13%)
2	NAG	I	1	1,2	14,14,15	0.38	0	17,19,21	0.64	1 (5%)
2	NAG	I	2	2	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	J	1	3,1	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
3	NAG	J	2	3	14,14,15	0.27	0	17,19,21	0.42	0
3	MAN	J	3	3	11,11,12	0.82	0	15,15,17	1.08	2 (13%)
3	NAG	K	1	3,1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	K	2	3	14,14,15	0.23	0	17,19,21	0.38	0
3	MAN	K	3	3	11,11,12	0.71	0	15,15,17	1.19	2 (13%)
4	NAG	L	1	1,4	14,14,15	0.36	0	17,19,21	0.89	1 (5%)
4	NAG	L	2	4	14,14,15	0.31	0	17,19,21	0.43	0
4	FUC	L	3	4	10,10,11	1.03	0	14,14,16	0.93	0
3	NAG	M	1	3,1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	M	2	3	14,14,15	0.20	0	17,19,21	0.36	0
3	MAN	M	3	3	11,11,12	0.75	0	15,15,17	1.24	2 (13%)
3	NAG	N	1	3,1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
3	NAG	N	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	MAN	N	3	3	11,11,12	0.78	0	15,15,17	1.14	2 (13%)
2	NAG	O	1	1,2	14,14,15	0.27	0	17,19,21	0.47	0
2	NAG	O	2	2	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	P	1	3,1	14,14,15	0.16	0	17,19,21	0.43	0
3	NAG	P	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	MAN	P	3	3	11,11,12	0.69	0	15,15,17	1.25	2 (13%)
2	NAG	Q	1	1,2	14,14,15	0.30	0	17,19,21	0.41	0
2	NAG	Q	2	2	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	R	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	R	2	3	14,14,15	0.22	0	17,19,21	0.39	0
3	MAN	R	3	3	11,11,12	0.74	0	15,15,17	1.15	2 (13%)
3	NAG	S	1	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	S	2	3	14,14,15	0.19	0	17,19,21	0.40	0
3	MAN	S	3	3	11,11,12	0.67	0	15,15,17	1.07	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	T	1	1,2	14,14,15	0.33	0	17,19,21	0.62	1 (5%)
2	NAG	T	2	2	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	U	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	0.90	0
3	NAG	U	2	3	14,14,15	0.34	0	17,19,21	0.43	0
3	MAN	U	3	3	11,11,12	0.83	0	15,15,17	1.30	2 (13%)
3	NAG	V	1	3,1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	V	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	MAN	V	3	3	11,11,12	0.68	0	15,15,17	1.27	2 (13%)
4	NAG	W	1	1,4	14,14,15	0.26	0	17,19,21	0.87	1 (5%)
4	NAG	W	2	4	14,14,15	0.28	0	17,19,21	0.44	0
4	FUC	W	3	4	10,10,11	0.90	0	14,14,16	0.94	0
3	NAG	X	1	3,1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	X	2	3	14,14,15	0.23	0	17,19,21	0.35	0
3	MAN	X	3	3	11,11,12	0.74	0	15,15,17	1.27	2 (13%)
3	NAG	Y	1	3,1	14,14,15	0.52	0	17,19,21	0.70	1 (5%)
3	NAG	Y	2	3	14,14,15	0.21	0	17,19,21	0.46	0
3	MAN	Y	3	3	11,11,12	0.80	0	15,15,17	1.14	2 (13%)
2	NAG	Z	1	1,2	14,14,15	0.31	0	17,19,21	0.51	0
2	NAG	Z	2	2	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	a	1	3,1	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	a	2	3	14,14,15	0.23	0	17,19,21	0.45	0
3	MAN	a	3	3	11,11,12	0.71	0	15,15,17	1.18	2 (13%)
2	NAG	b	1	1,2	14,14,15	0.21	0	17,19,21	0.38	0
2	NAG	b	2	2	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	c	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	c	2	3	14,14,15	0.22	0	17,19,21	0.39	0
3	MAN	c	3	3	11,11,12	0.75	0	15,15,17	1.16	2 (13%)
3	NAG	d	1	3,1	14,14,15	0.37	0	17,19,21	0.38	0
3	NAG	d	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	MAN	d	3	3	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
2	NAG	e	1	1,2	14,14,15	0.29	0	17,19,21	0.58	0
2	NAG	e	2	2	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	f	1	3,1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	f	2	3	14,14,15	0.21	0	17,19,21	0.40	0
3	MAN	f	3	3	11,11,12	0.71	0	15,15,17	1.08	2 (13%)
3	NAG	g	1	3,1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	g	2	3	14,14,15	0.23	0	17,19,21	0.39	0
3	MAN	g	3	3	11,11,12	0.68	0	15,15,17	1.26	2 (13%)
4	NAG	h	1	1,4	14,14,15	0.36	0	17,19,21	0.87	1 (5%)
4	NAG	h	2	4	14,14,15	0.33	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	h	3	4	10,10,11	0.86	0	14,14,16	0.85	0
3	NAG	i	1	3,1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	i	2	3	14,14,15	0.22	0	17,19,21	0.36	0
3	MAN	i	3	3	11,11,12	0.74	0	15,15,17	1.26	2 (13%)
3	NAG	j	1	3,1	14,14,15	0.53	0	17,19,21	0.69	1 (5%)
3	NAG	j	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	MAN	j	3	3	11,11,12	0.77	0	15,15,17	1.13	2 (13%)

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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	MAN	E	3	3	-	1/2/19/22	1/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	MAN	G	3	3	-	1/2/19/22	1/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	MAN	H	3	3	-	0/2/19/22	1/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	MAN	J	3	3	-	0/2/19/22	1/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	MAN	K	3	3	-	1/2/19/22	1/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	FUC	L	3	4	-	-	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	M	3	3	-	1/2/19/22	1/1/1/1
3	NAG	N	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	MAN	N	3	3	-	0/2/19/22	1/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	MAN	P	3	3	-	1/2/19/22	1/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	MAN	R	3	3	-	2/2/19/22	1/1/1/1
3	NAG	S	1	3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	MAN	S	3	3	-	0/2/19/22	1/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	MAN	U	3	3	-	0/2/19/22	1/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	MAN	V	3	3	-	1/2/19/22	1/1/1/1
4	NAG	W	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	FUC	W	3	4	-	-	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	MAN	X	3	3	-	1/2/19/22	1/1/1/1
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	MAN	Y	3	3	-	0/2/19/22	1/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
3	NAG	a	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	a	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	a	3	3	-	1/2/19/22	1/1/1/1
2	NAG	b	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
3	NAG	c	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	MAN	c	3	3	-	1/2/19/22	1/1/1/1
3	NAG	d	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	MAN	d	3	3	-	0/2/19/22	1/1/1/1
2	NAG	e	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
3	NAG	f	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	MAN	f	3	3	-	0/2/19/22	1/1/1/1
3	NAG	g	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	MAN	g	3	3	-	1/2/19/22	1/1/1/1
4	NAG	h	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	h	2	4	-	0/6/23/26	0/1/1/1
4	FUC	h	3	4	-	-	0/1/1/1
3	NAG	i	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	MAN	i	3	3	-	1/2/19/22	1/1/1/1
3	NAG	j	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1
3	MAN	j	3	3	-	0/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	1	NAG	O5-C1	-2.18	1.40	1.43
2	D	1	NAG	O5-C1	-2.16	1.40	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	3	MAN	C1-O5-C5	3.80	117.34	112.19
3	U	3	MAN	C1-O5-C5	3.77	117.30	112.19
3	X	3	MAN	C1-O5-C5	3.76	117.29	112.19
3	P	3	MAN	C1-O5-C5	3.74	117.26	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	g	3	MAN	C1-O5-C5	3.73	117.24	112.19
3	i	3	MAN	C1-O5-C5	3.72	117.23	112.19
3	H	3	MAN	C1-O5-C5	3.64	117.13	112.19
3	M	3	MAN	C1-O5-C5	3.62	117.10	112.19
3	a	3	MAN	C1-O5-C5	3.46	116.89	112.19
3	K	3	MAN	C1-O5-C5	3.44	116.85	112.19
3	E	3	MAN	C1-O5-C5	3.41	116.81	112.19
3	J	1	NAG	C1-O5-C5	3.34	116.72	112.19
3	c	3	MAN	C1-O5-C5	3.31	116.68	112.19
3	G	3	MAN	C1-O5-C5	3.26	116.61	112.19
3	R	3	MAN	C1-O5-C5	3.25	116.59	112.19
3	N	3	MAN	C1-O5-C5	3.21	116.54	112.19
4	L	1	NAG	C1-O5-C5	3.20	116.52	112.19
4	W	1	NAG	C1-O5-C5	3.19	116.51	112.19
3	Y	3	MAN	C1-O5-C5	3.18	116.50	112.19
4	h	1	NAG	C1-O5-C5	3.13	116.44	112.19
3	j	3	MAN	C1-O5-C5	3.13	116.43	112.19
3	f	3	MAN	C1-O5-C5	2.98	116.23	112.19
3	d	3	MAN	C1-O5-C5	2.97	116.22	112.19
3	J	3	MAN	C1-O5-C5	2.94	116.17	112.19
3	S	3	MAN	C1-O5-C5	2.94	116.17	112.19
3	N	1	NAG	C1-O5-C5	2.52	115.61	112.19
3	Y	1	NAG	C1-O5-C5	2.49	115.56	112.19
3	j	1	NAG	C1-O5-C5	2.41	115.46	112.19
3	H	3	MAN	O2-C2-C3	-2.30	105.53	110.14
3	U	3	MAN	O2-C2-C3	-2.28	105.56	110.14
3	j	3	MAN	O2-C2-C3	-2.28	105.57	110.14
3	K	3	MAN	O2-C2-C3	-2.27	105.59	110.14
3	R	3	MAN	O2-C2-C3	-2.26	105.61	110.14
3	Y	3	MAN	O2-C2-C3	-2.25	105.62	110.14
3	X	3	MAN	O2-C2-C3	-2.25	105.62	110.14
3	N	3	MAN	O2-C2-C3	-2.25	105.62	110.14
3	c	3	MAN	O2-C2-C3	-2.25	105.64	110.14
3	g	3	MAN	O2-C2-C3	-2.24	105.65	110.14
3	G	3	MAN	O2-C2-C3	-2.24	105.65	110.14
3	V	3	MAN	O2-C2-C3	-2.23	105.66	110.14
3	S	3	MAN	O2-C2-C3	-2.23	105.67	110.14
3	i	3	MAN	O2-C2-C3	-2.23	105.67	110.14
3	J	3	MAN	O2-C2-C3	-2.21	105.70	110.14
3	E	3	MAN	O2-C2-C3	-2.21	105.71	110.14
3	a	3	MAN	O2-C2-C3	-2.21	105.72	110.14
3	P	3	MAN	O2-C2-C3	-2.21	105.72	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	d	3	MAN	O2-C2-C3	-2.20	105.72	110.14
3	M	3	MAN	O2-C2-C3	-2.19	105.76	110.14
3	f	3	MAN	O2-C2-C3	-2.18	105.77	110.14
2	I	1	NAG	C1-O5-C5	2.13	115.08	112.19
2	T	1	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
4	h	1	NAG	O5-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	f	1	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
4	h	1	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	d	2	NAG	C4-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	f	1	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
3	K	3	MAN	O5-C5-C6-O6
3	M	3	MAN	O5-C5-C6-O6
3	X	3	MAN	O5-C5-C6-O6
3	R	3	MAN	C4-C5-C6-O6
3	i	3	MAN	O5-C5-C6-O6
3	E	3	MAN	O5-C5-C6-O6
3	a	3	MAN	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	V	3	MAN	O5-C5-C6-O6
3	g	3	MAN	O5-C5-C6-O6
3	P	3	MAN	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	G	3	MAN	C4-C5-C6-O6

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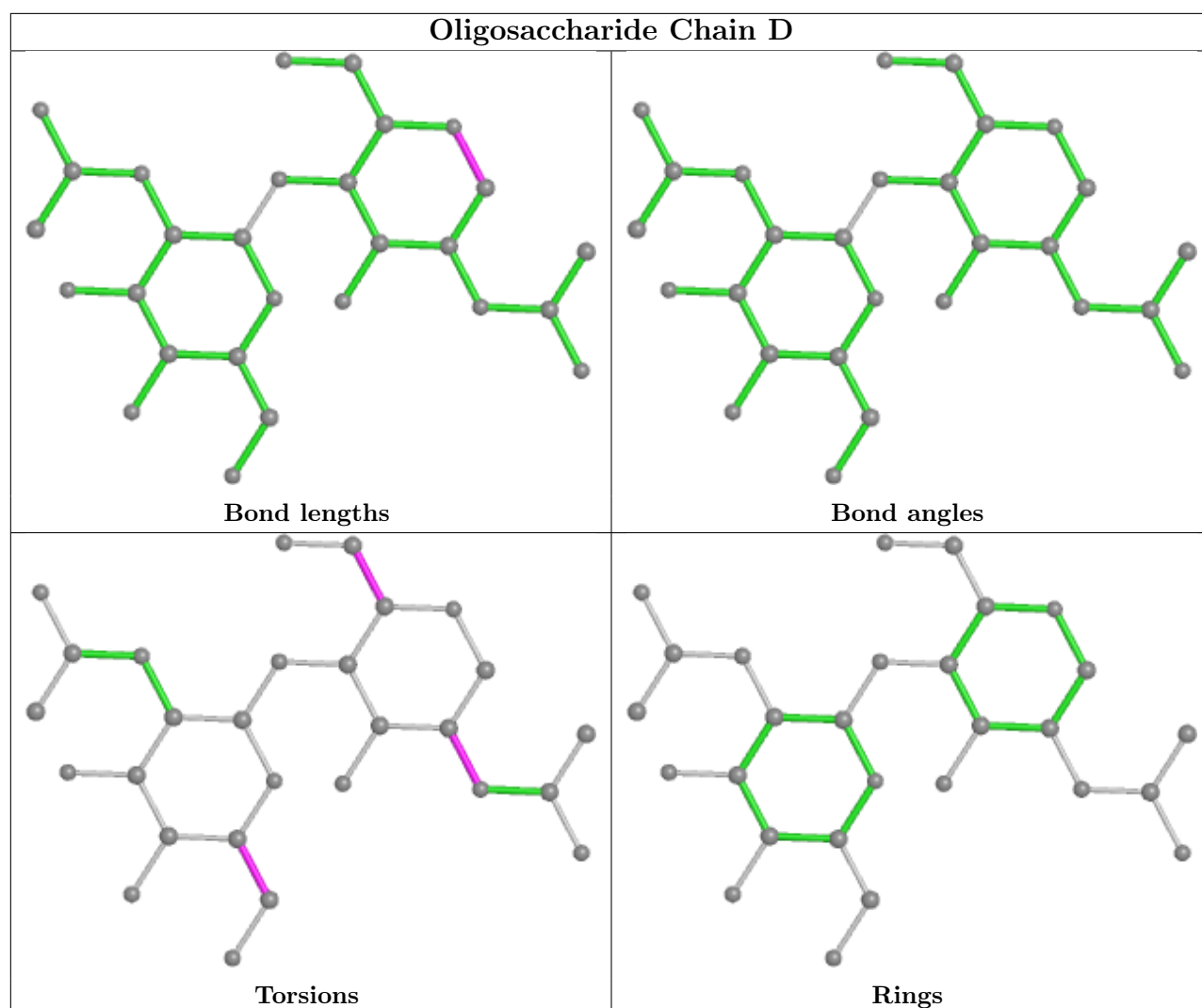
Mol	Chain	Res	Type	Atoms
3	R	2	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	R	3	MAN	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C1-C2-N2-C7
3	c	3	MAN	C4-C5-C6-O6

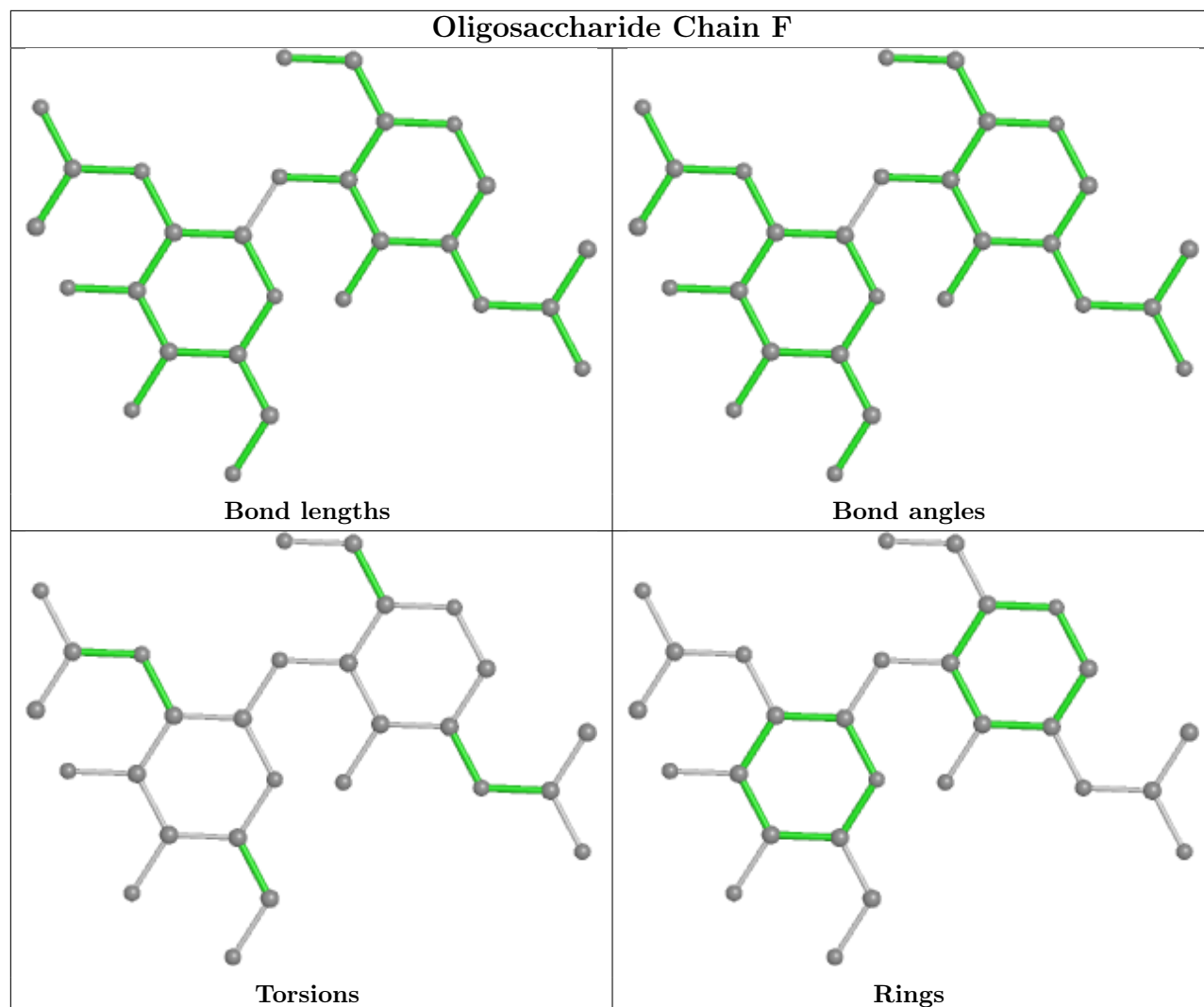
All (21) ring outliers are listed below:

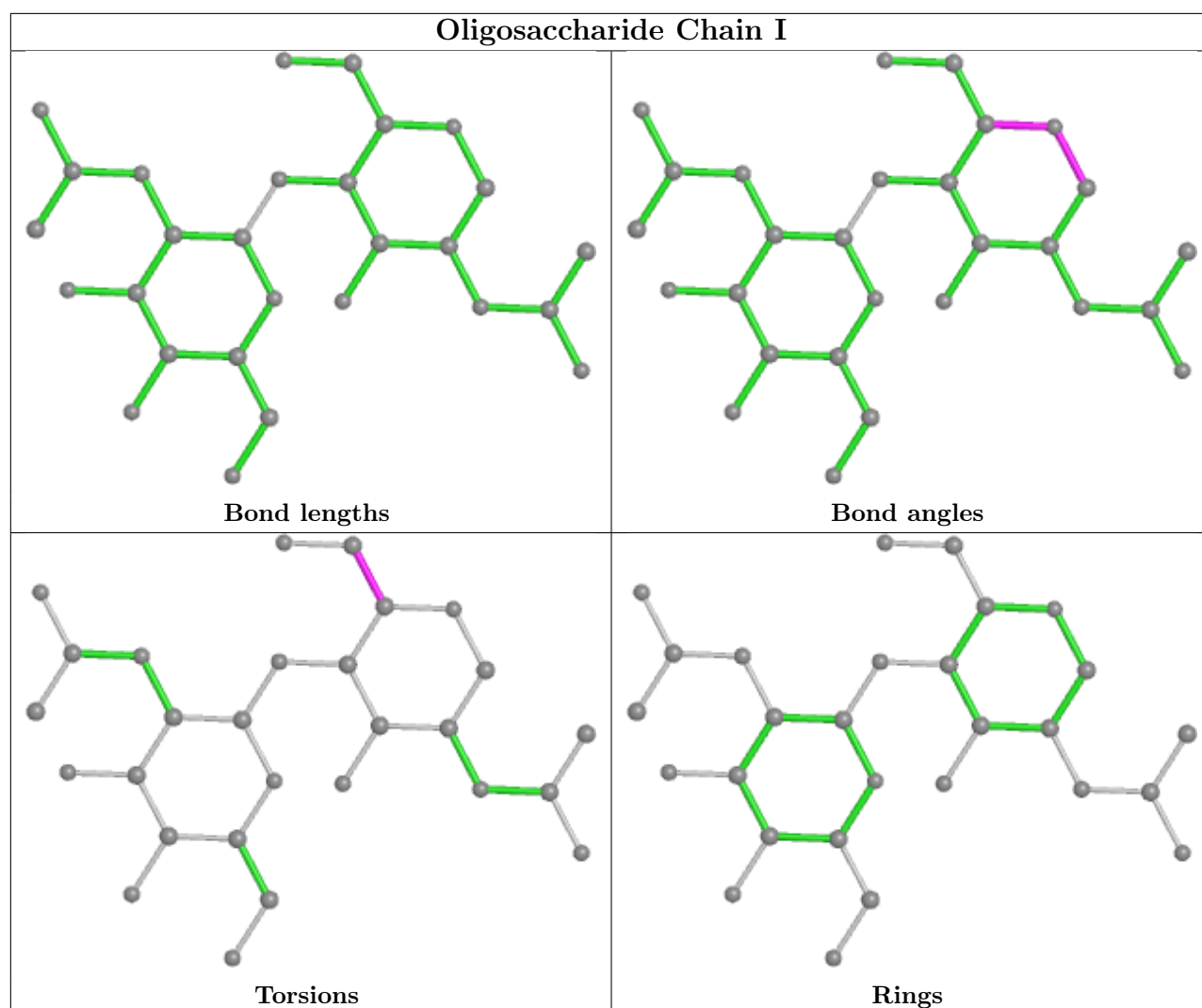
Mol	Chain	Res	Type	Atoms
3	d	3	MAN	C1-C2-C3-C4-C5-O5
3	J	3	MAN	C1-C2-C3-C4-C5-O5
3	f	3	MAN	C1-C2-C3-C4-C5-O5
3	S	3	MAN	C1-C2-C3-C4-C5-O5
3	Y	3	MAN	C1-C2-C3-C4-C5-O5
3	N	3	MAN	C1-C2-C3-C4-C5-O5
3	j	3	MAN	C1-C2-C3-C4-C5-O5
3	X	3	MAN	C1-C2-C3-C4-C5-O5
3	G	3	MAN	C1-C2-C3-C4-C5-O5
3	M	3	MAN	C1-C2-C3-C4-C5-O5
3	c	3	MAN	C1-C2-C3-C4-C5-O5
3	i	3	MAN	C1-C2-C3-C4-C5-O5
3	R	3	MAN	C1-C2-C3-C4-C5-O5
3	E	3	MAN	C1-C2-C3-C4-C5-O5
3	a	3	MAN	C1-C2-C3-C4-C5-O5
3	K	3	MAN	C1-C2-C3-C4-C5-O5
3	H	3	MAN	C1-C2-C3-C4-C5-O5
3	P	3	MAN	C1-C2-C3-C4-C5-O5
3	V	3	MAN	C1-C2-C3-C4-C5-O5
3	g	3	MAN	C1-C2-C3-C4-C5-O5
3	U	3	MAN	C1-C2-C3-C4-C5-O5

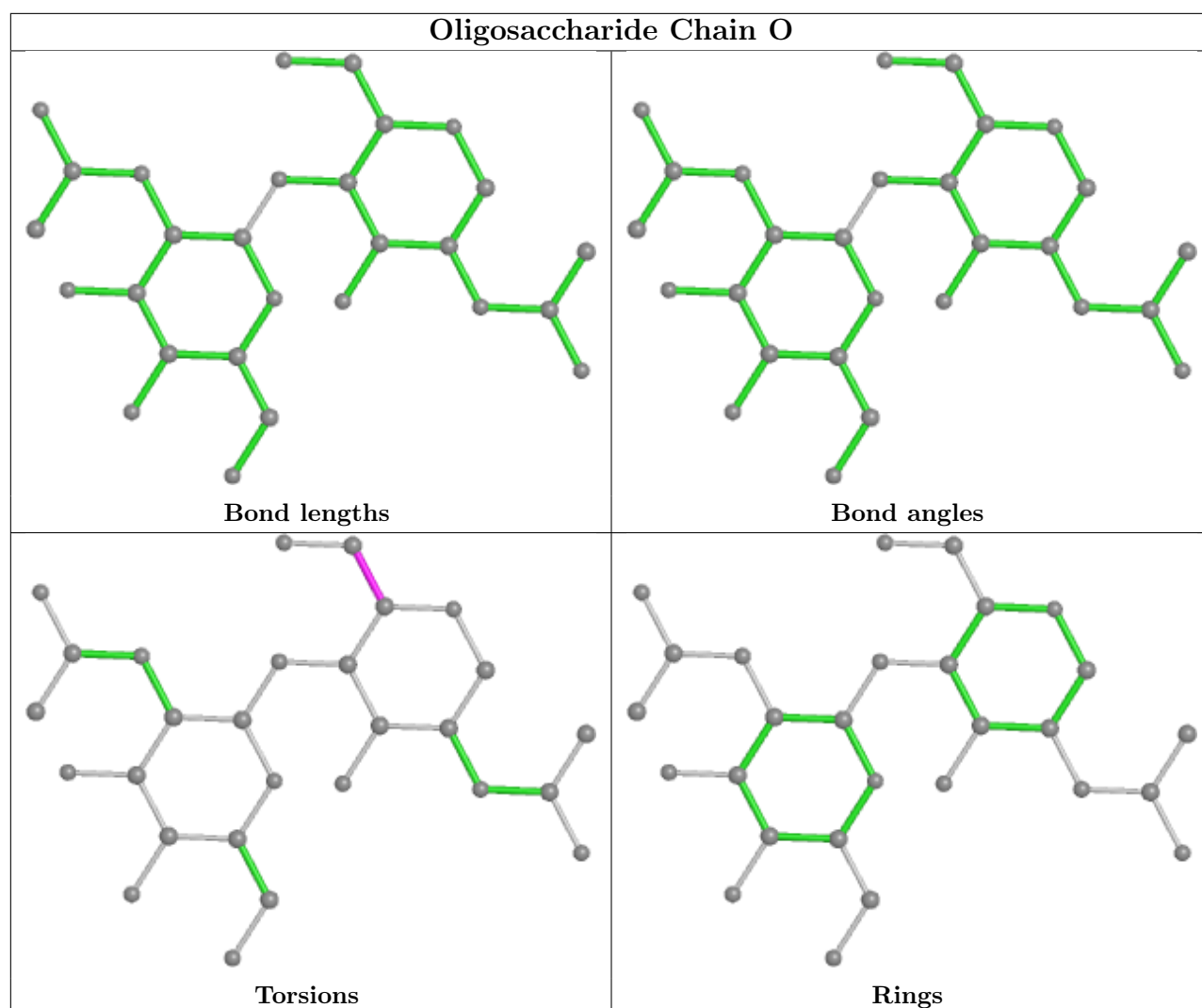
No monomer is involved in short contacts.

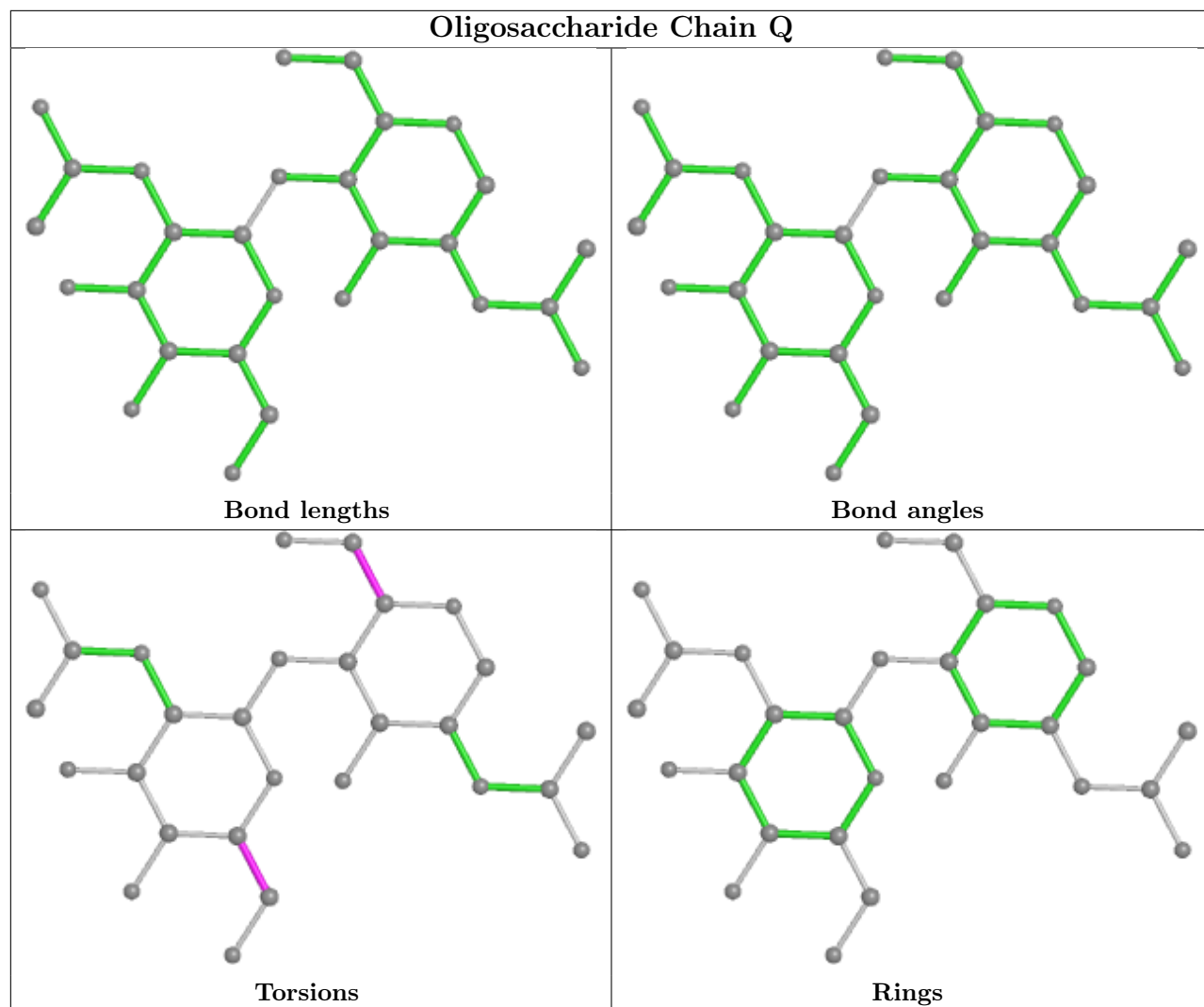
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

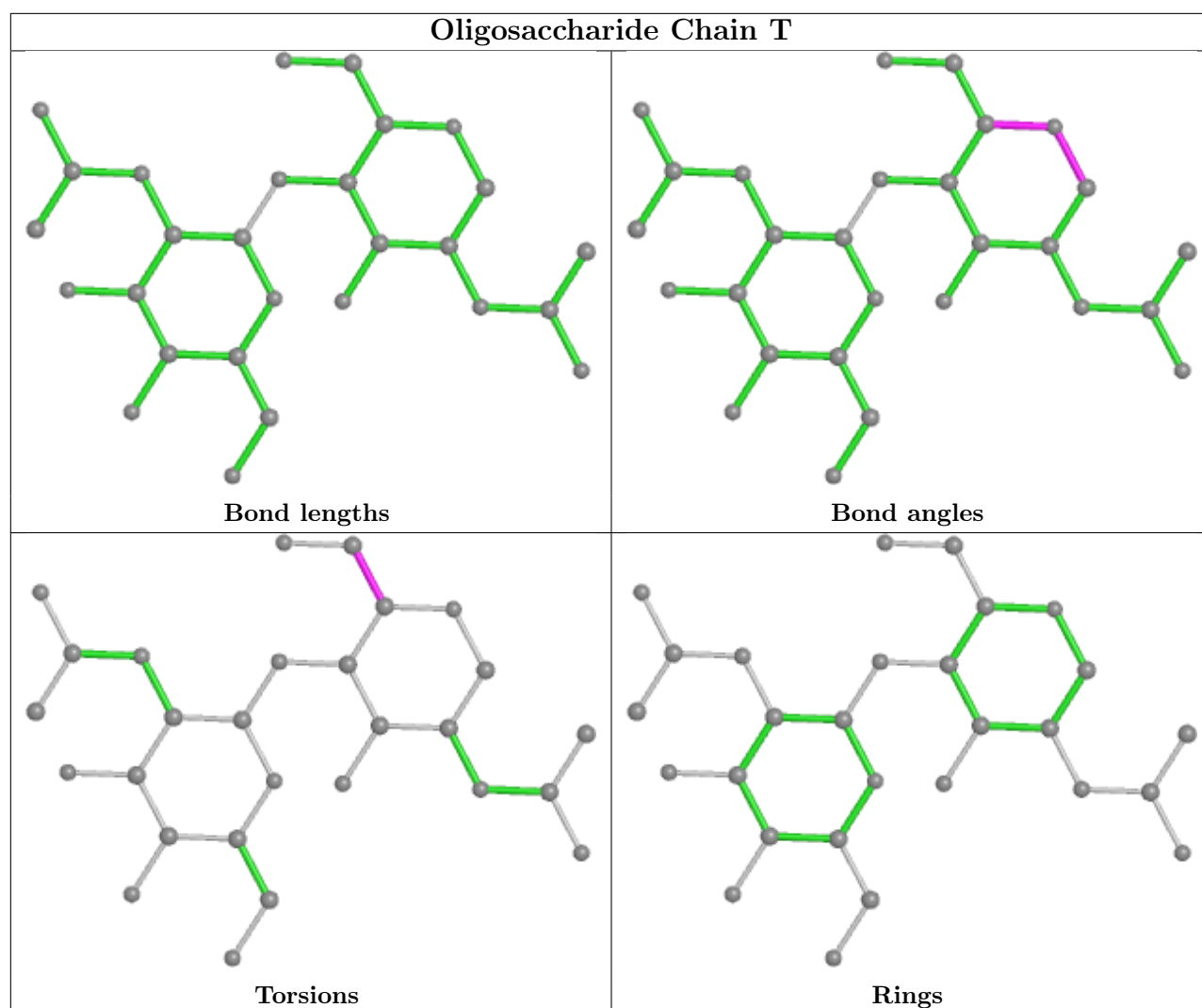


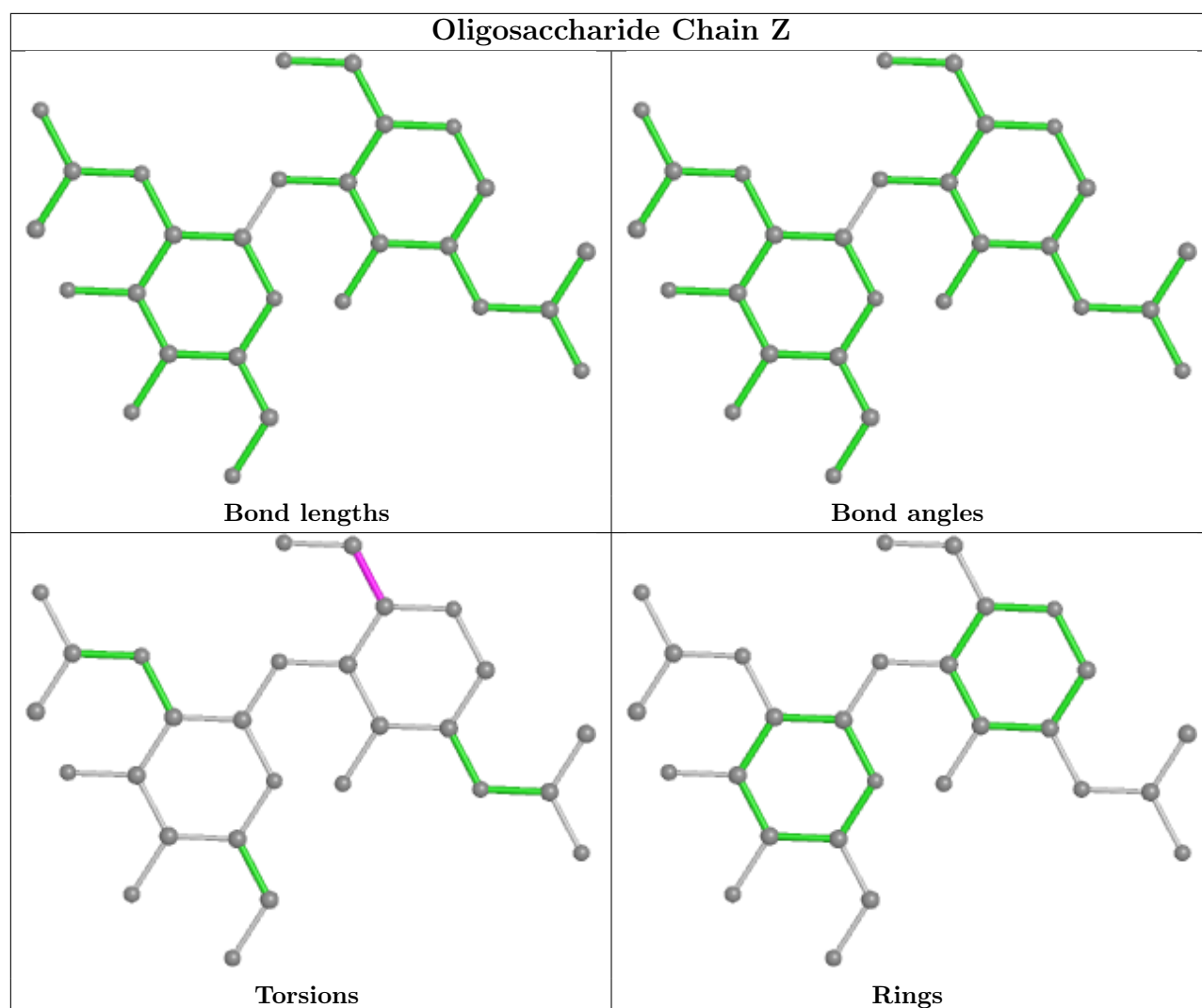


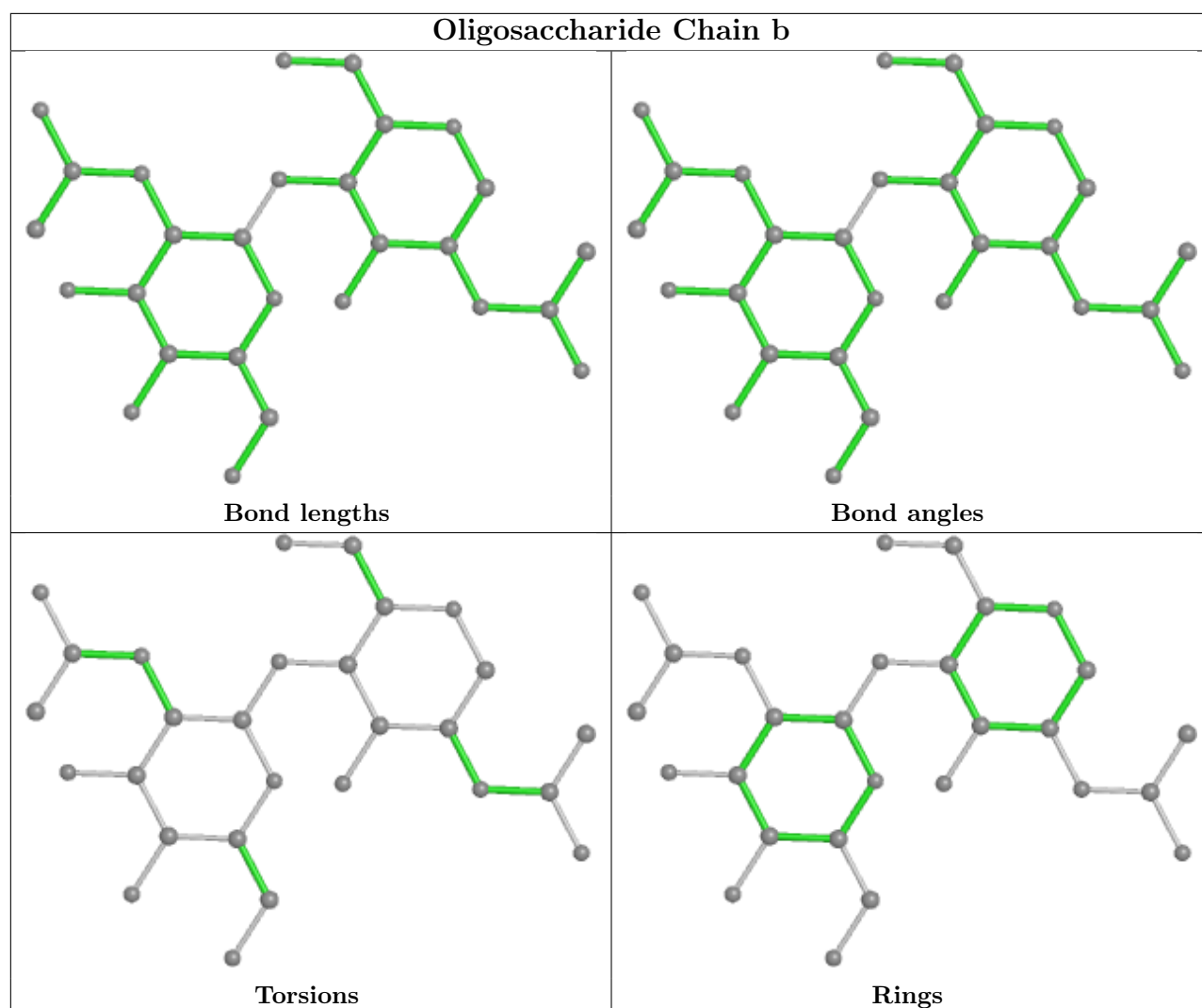


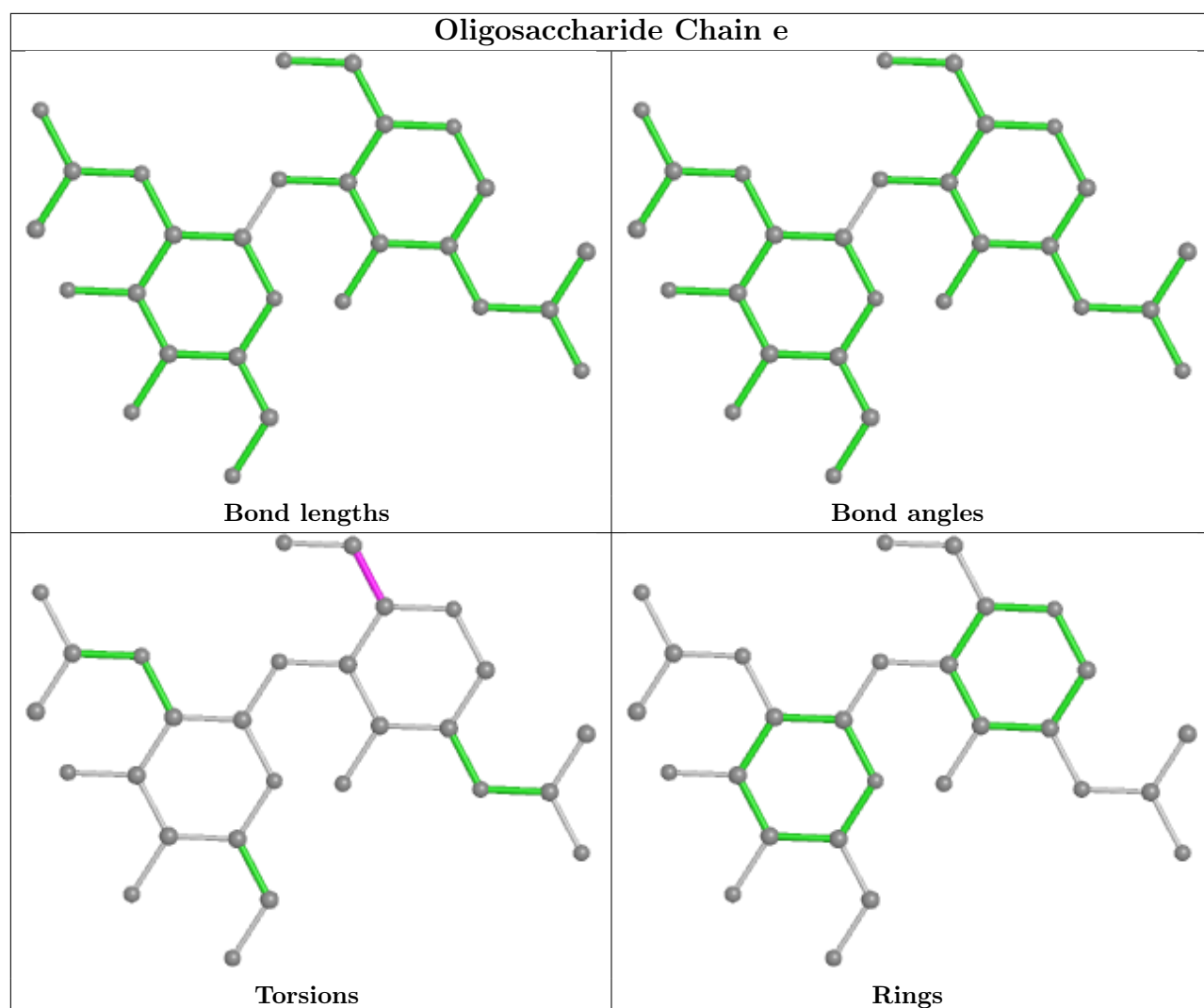


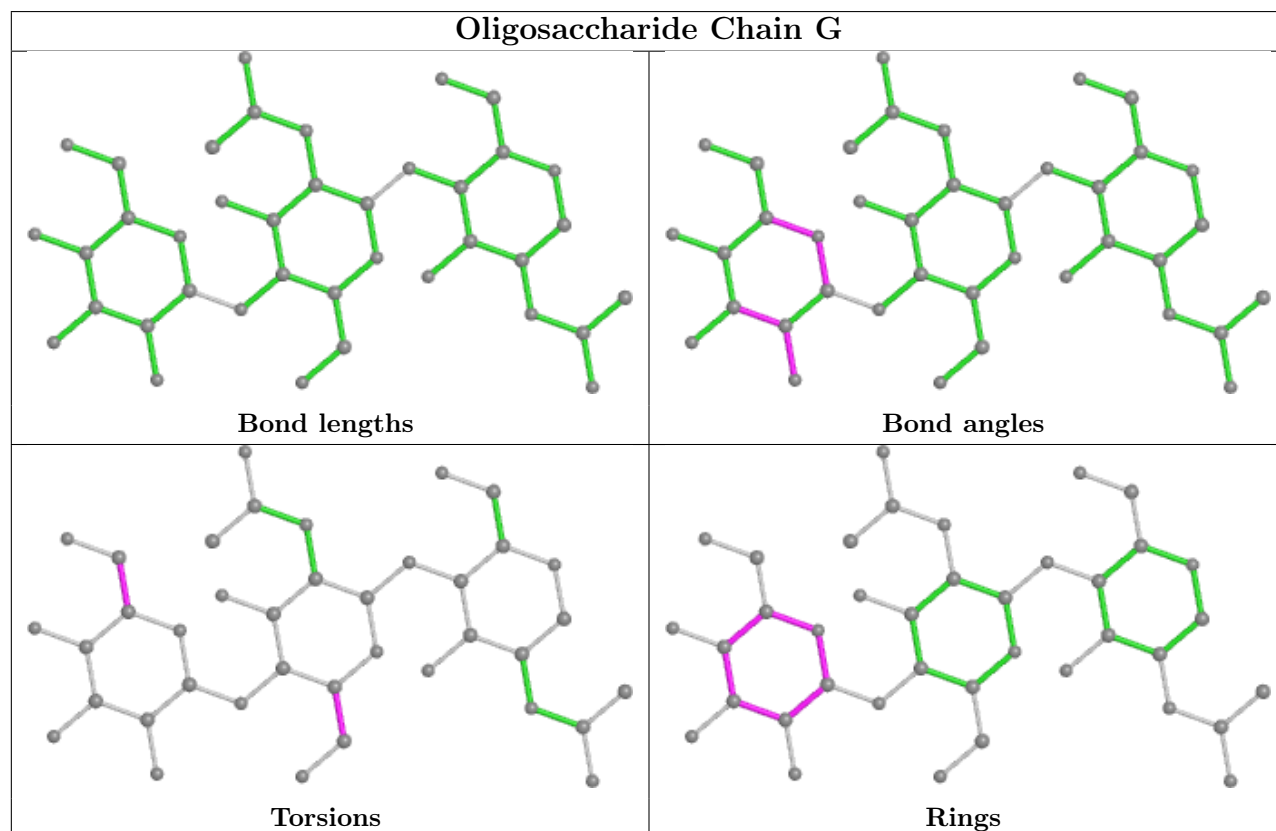
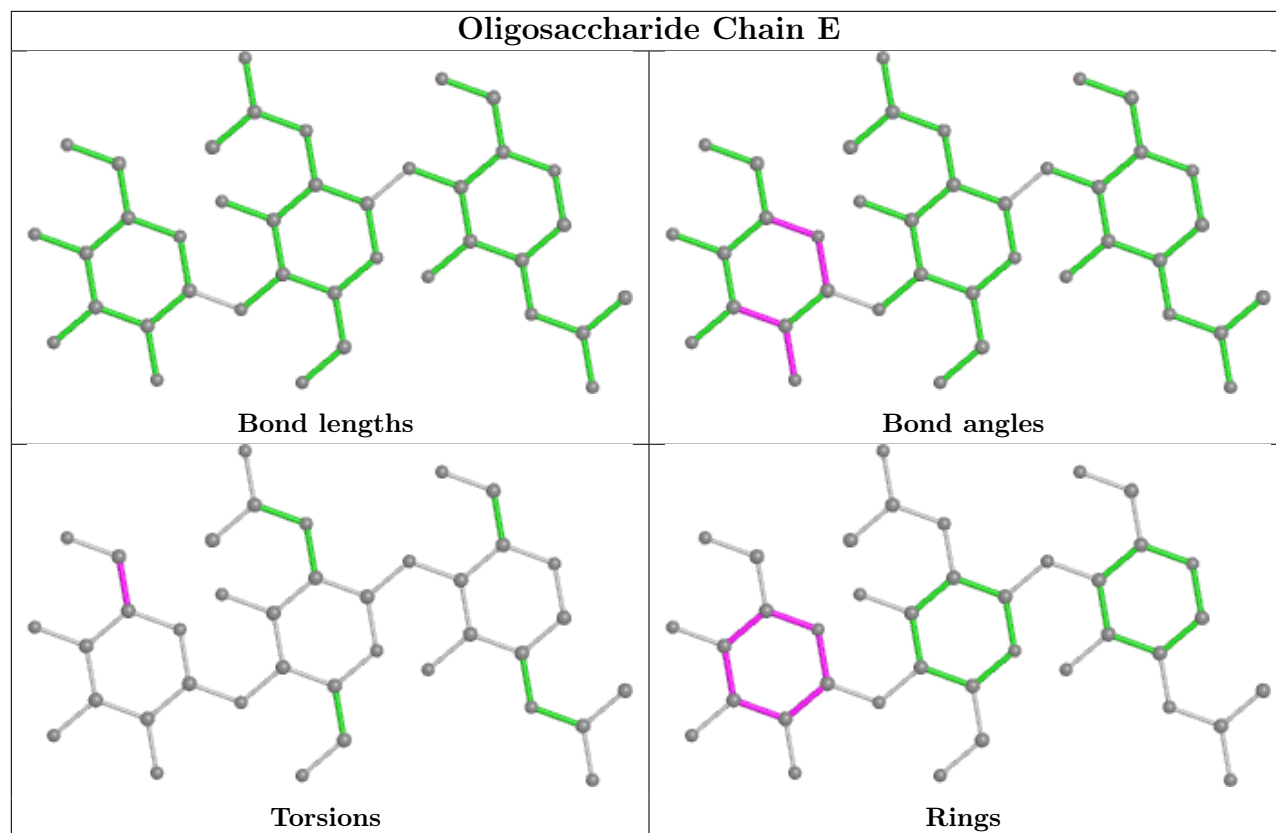


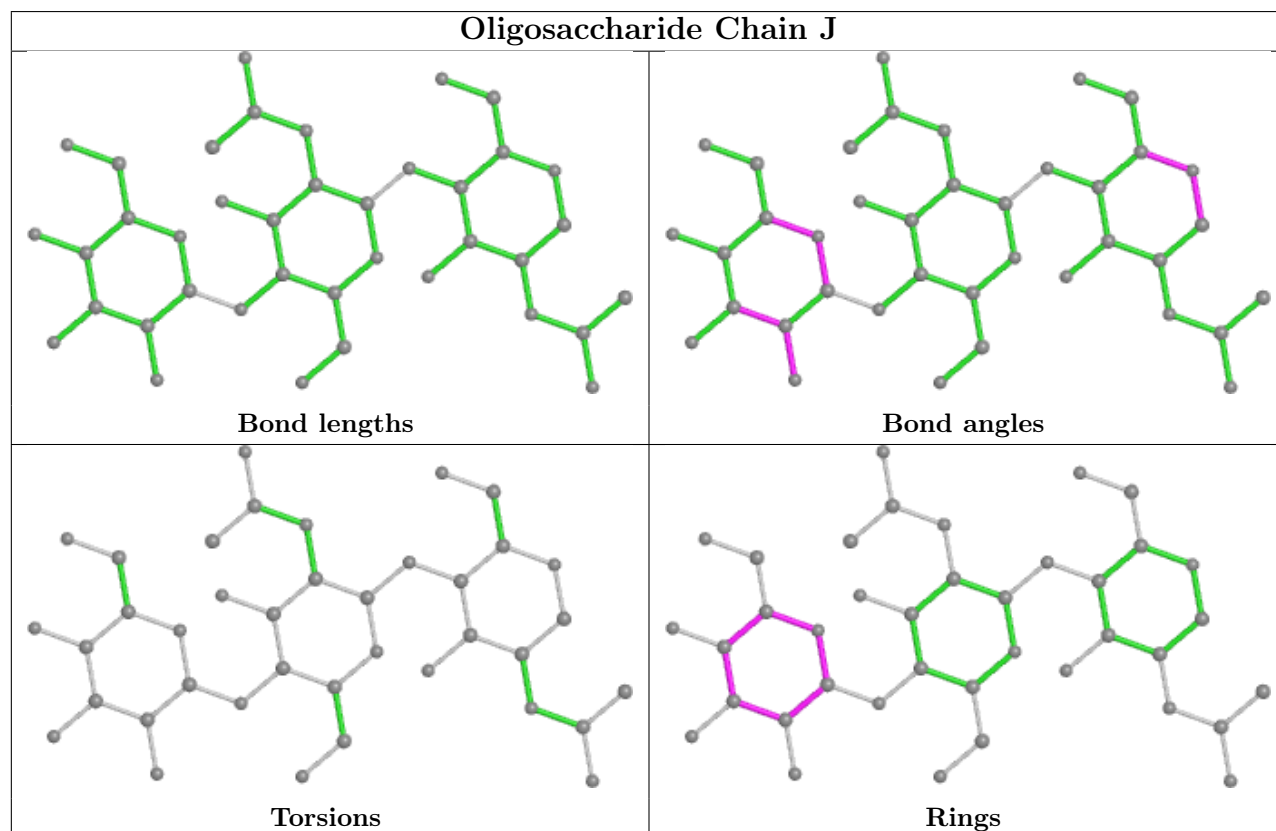
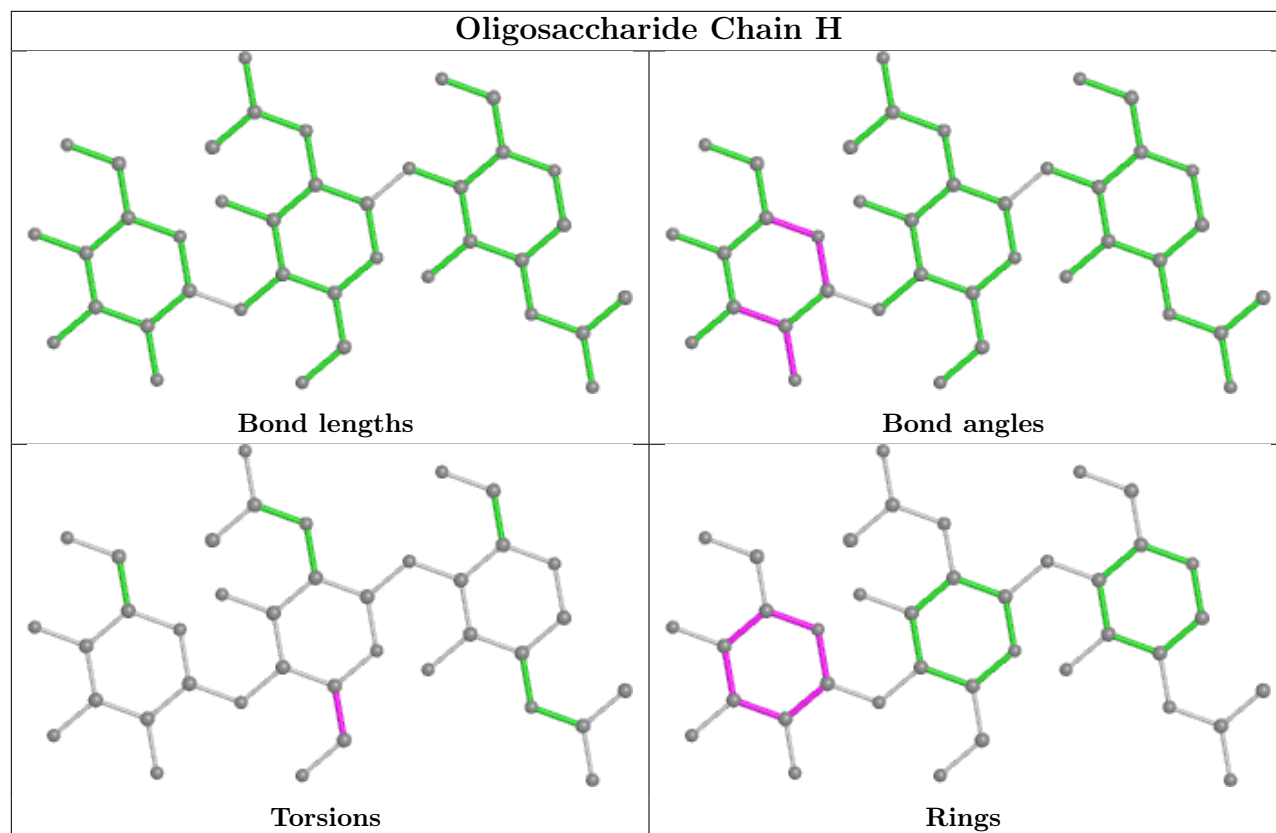


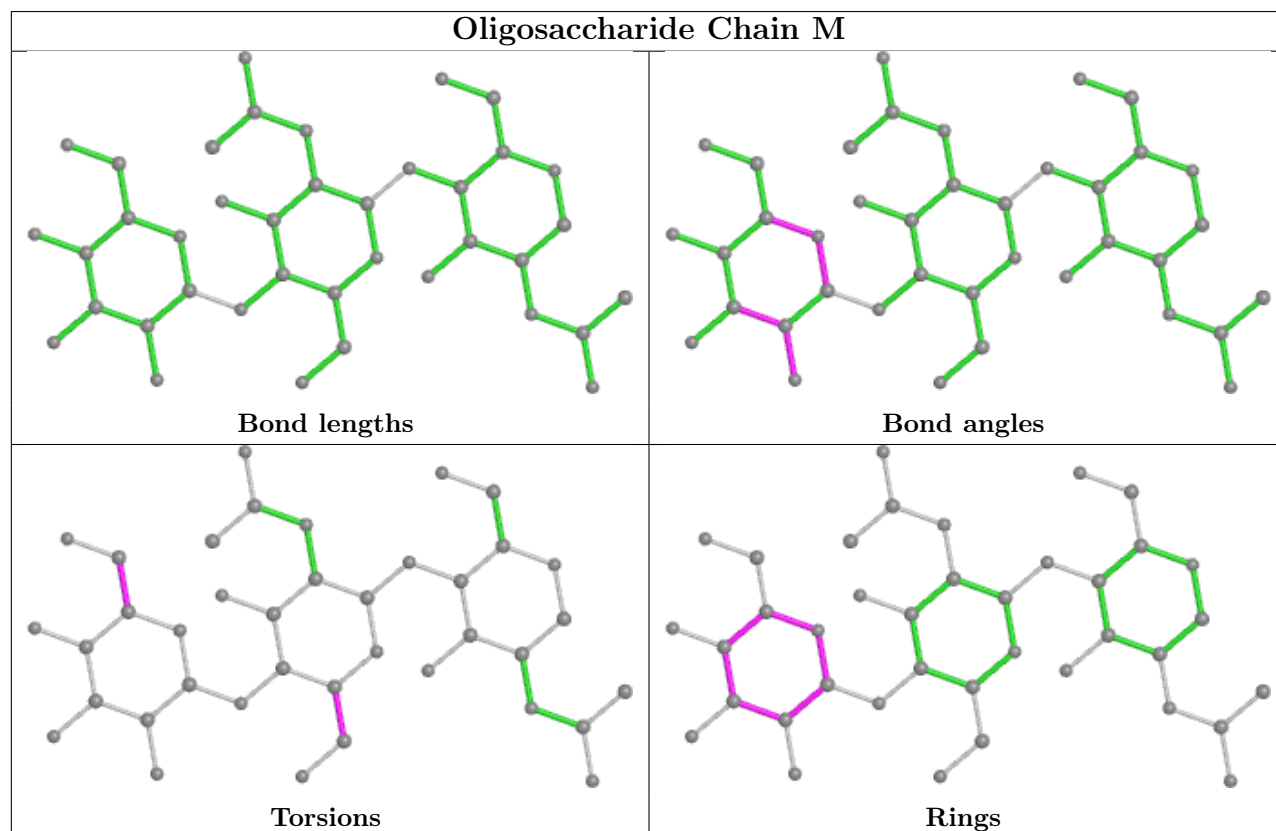
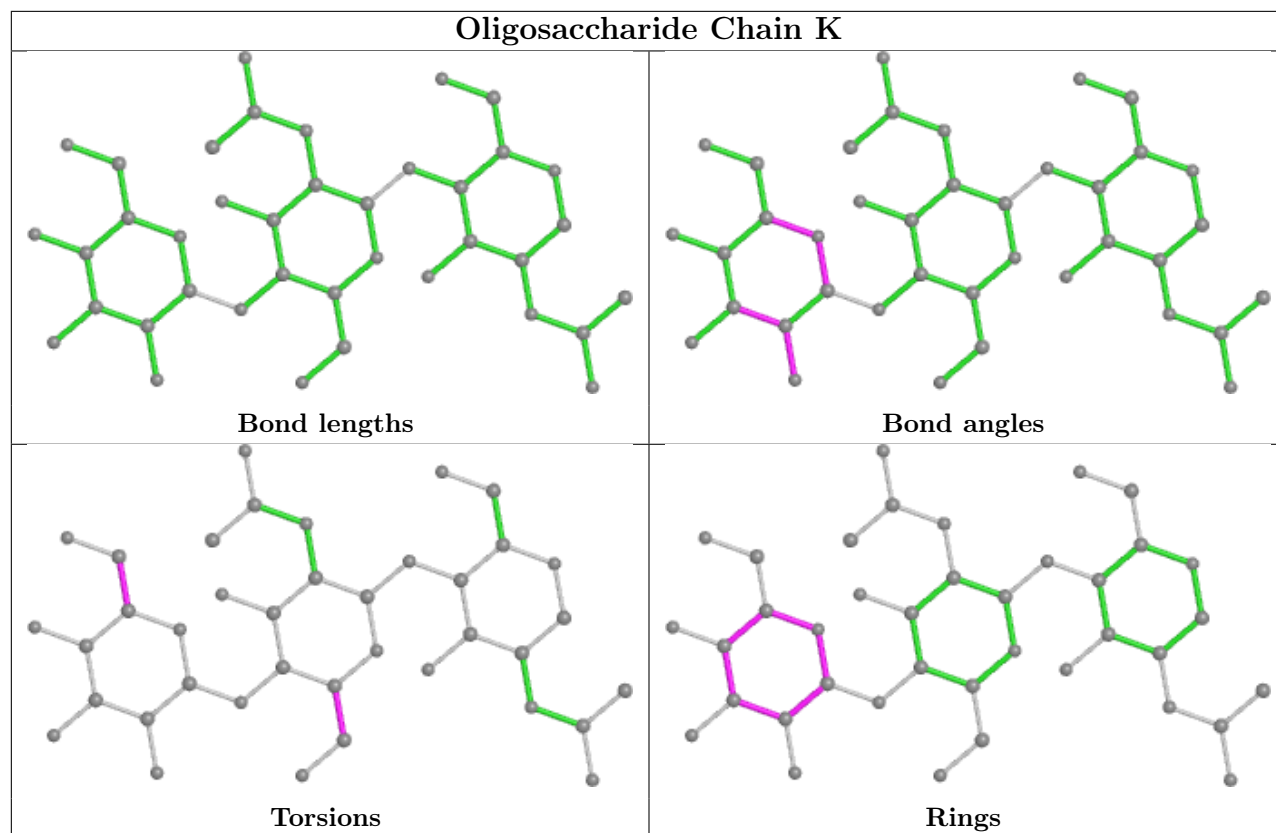


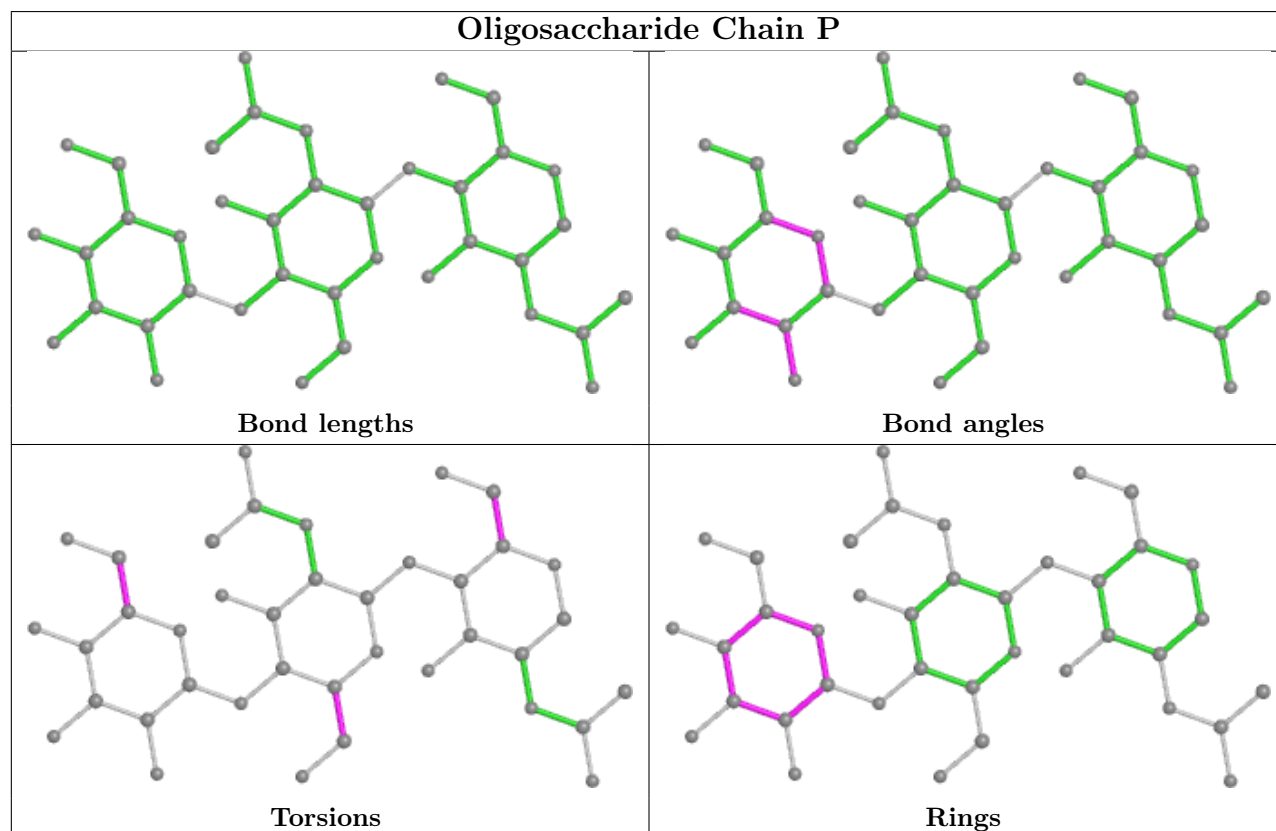
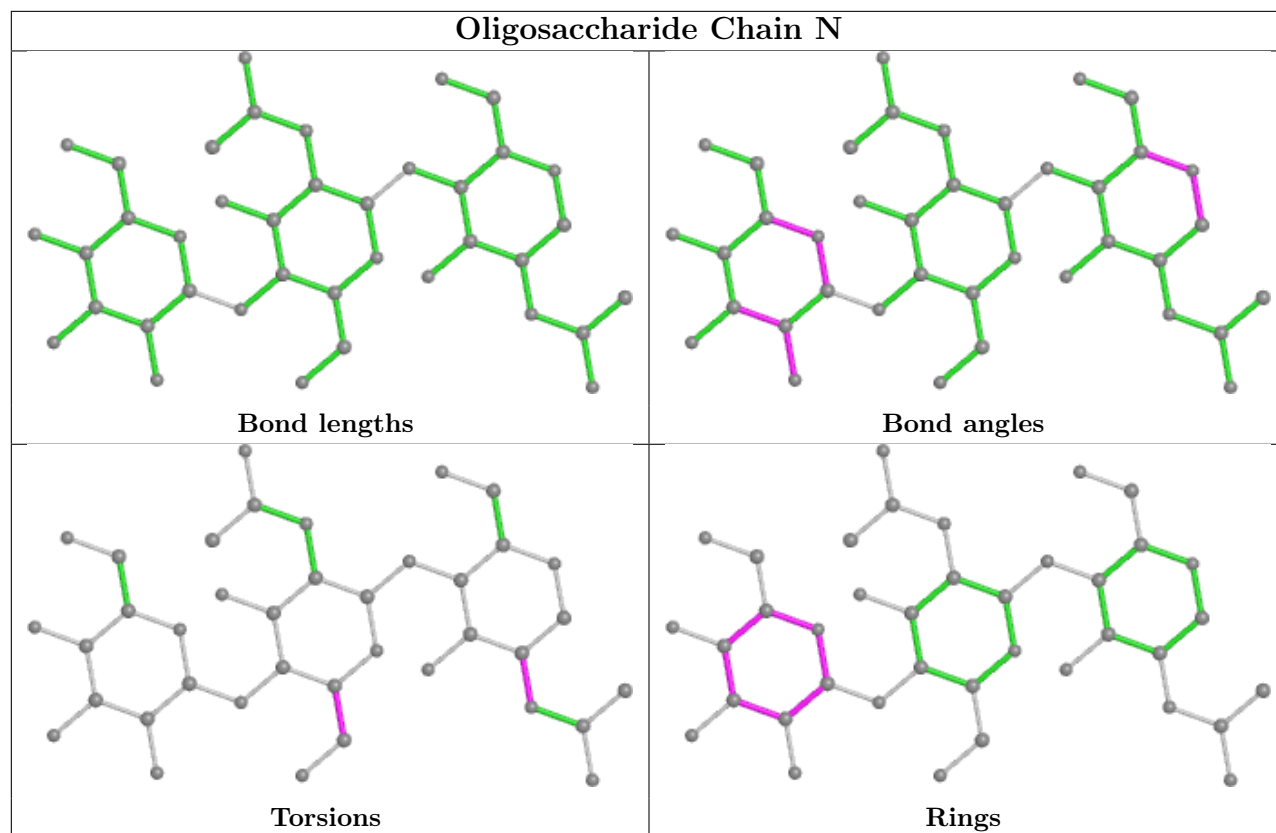


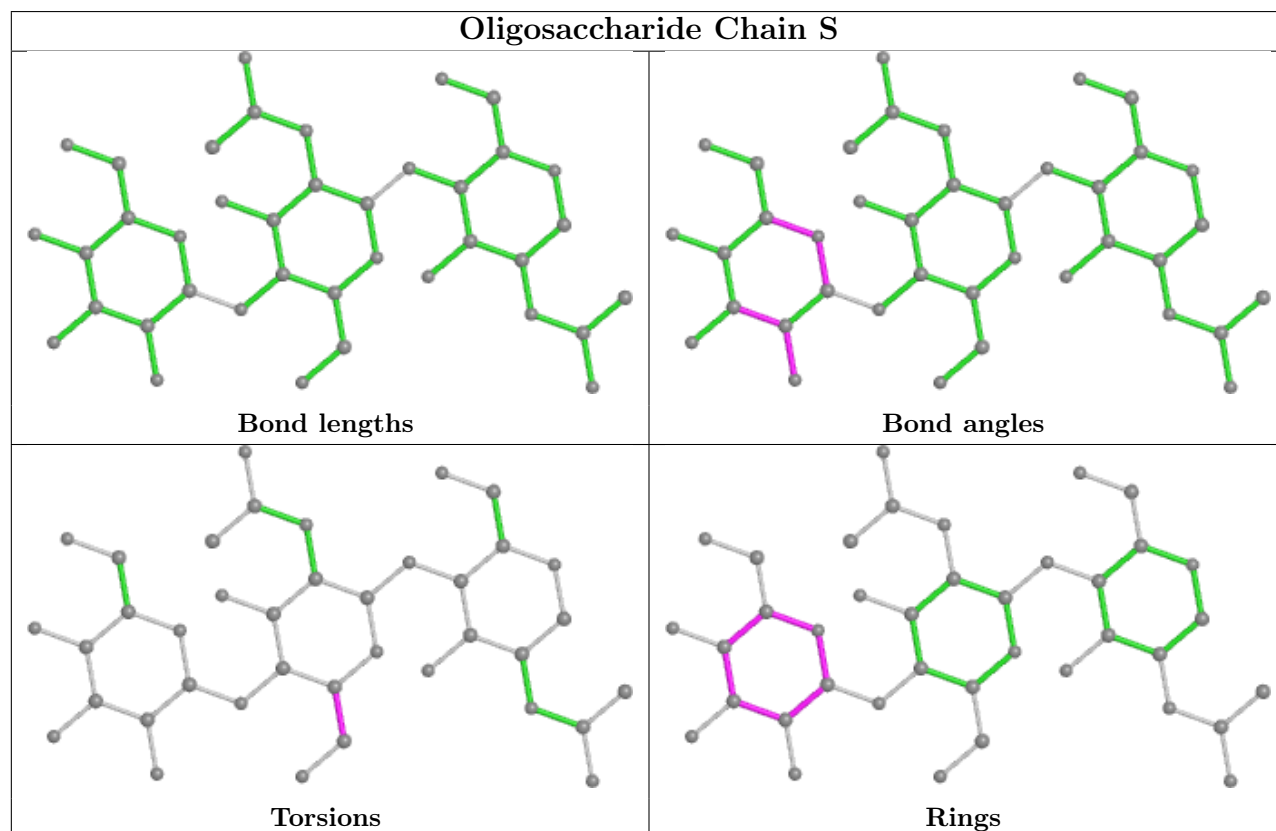
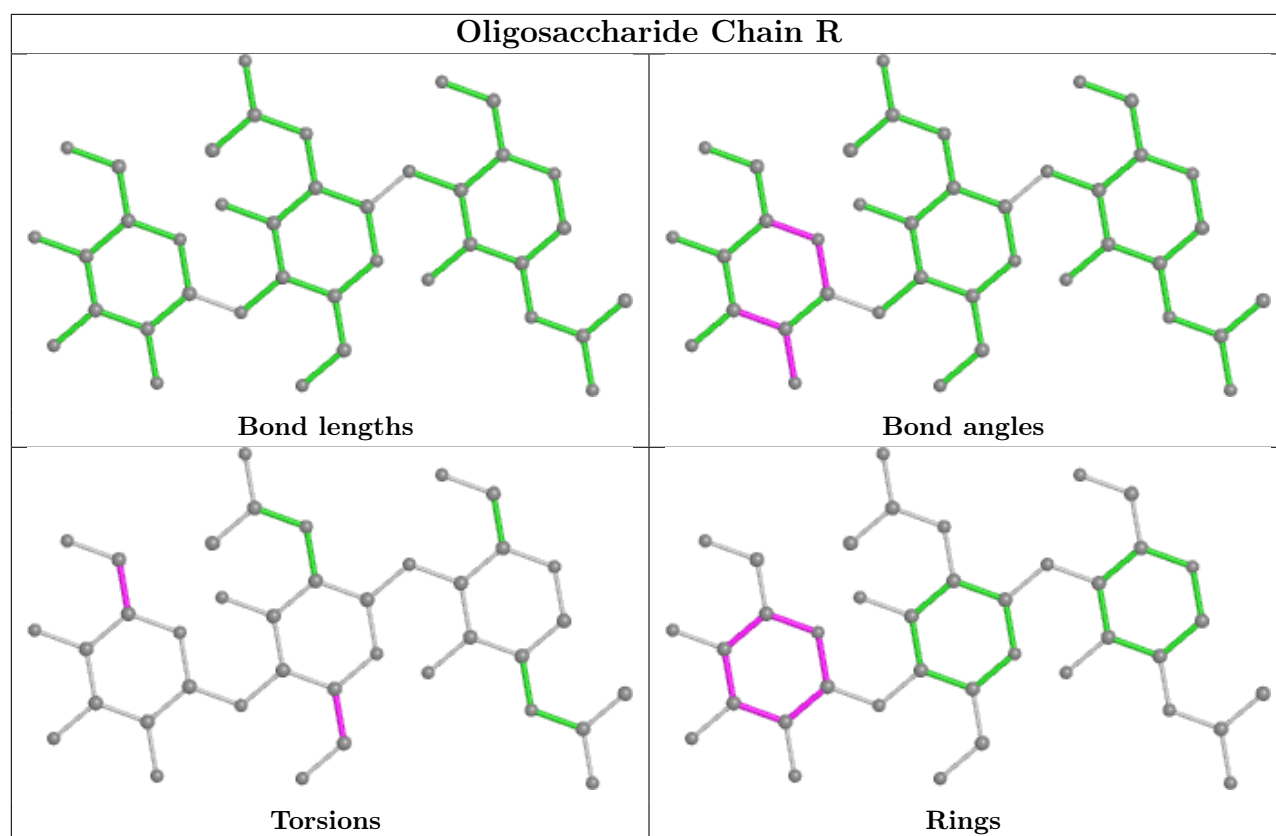


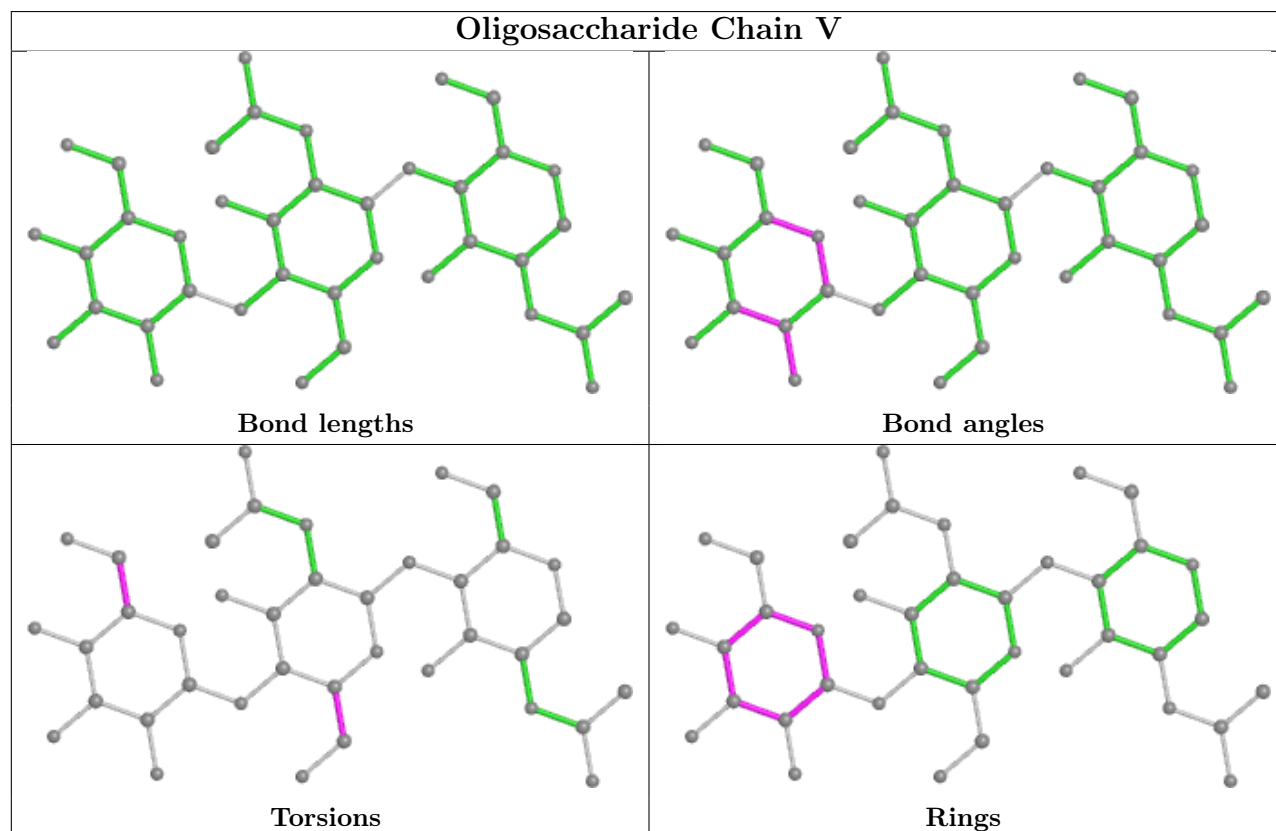
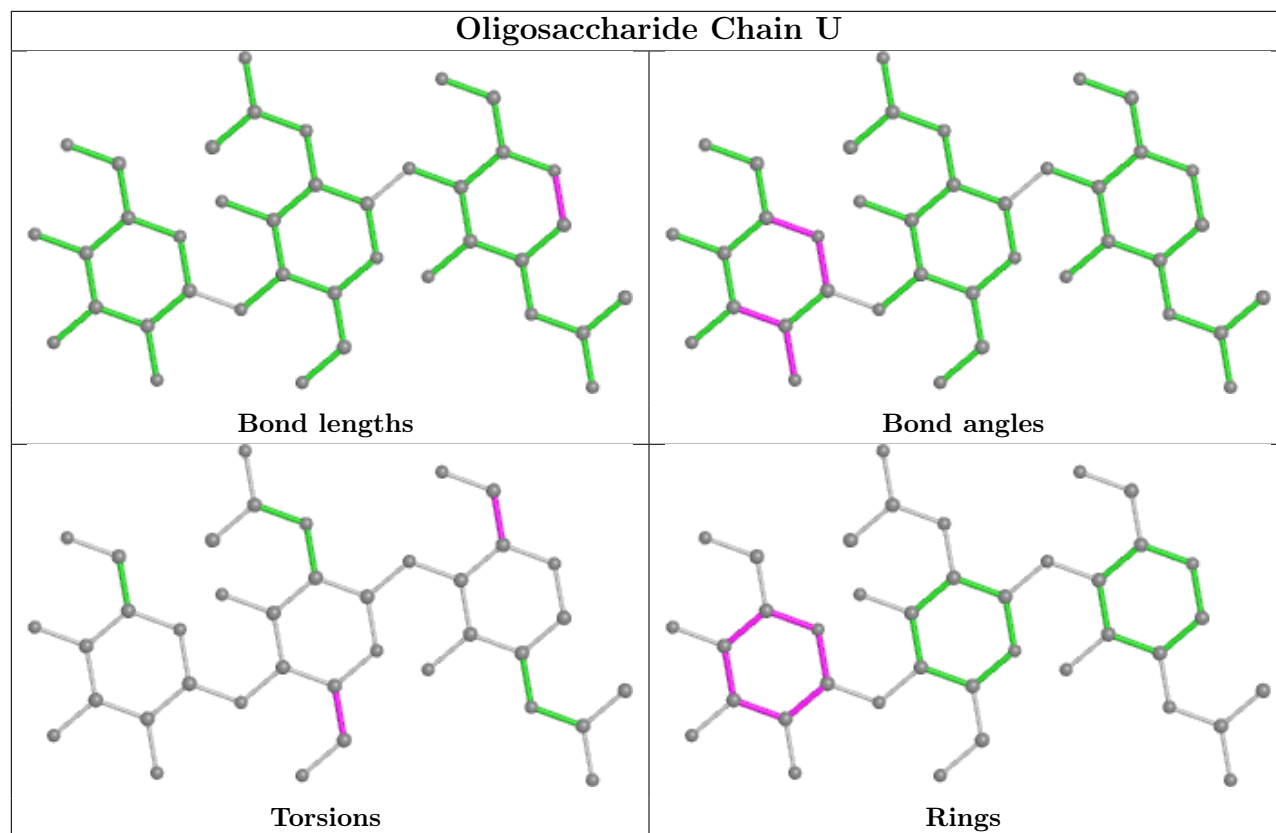


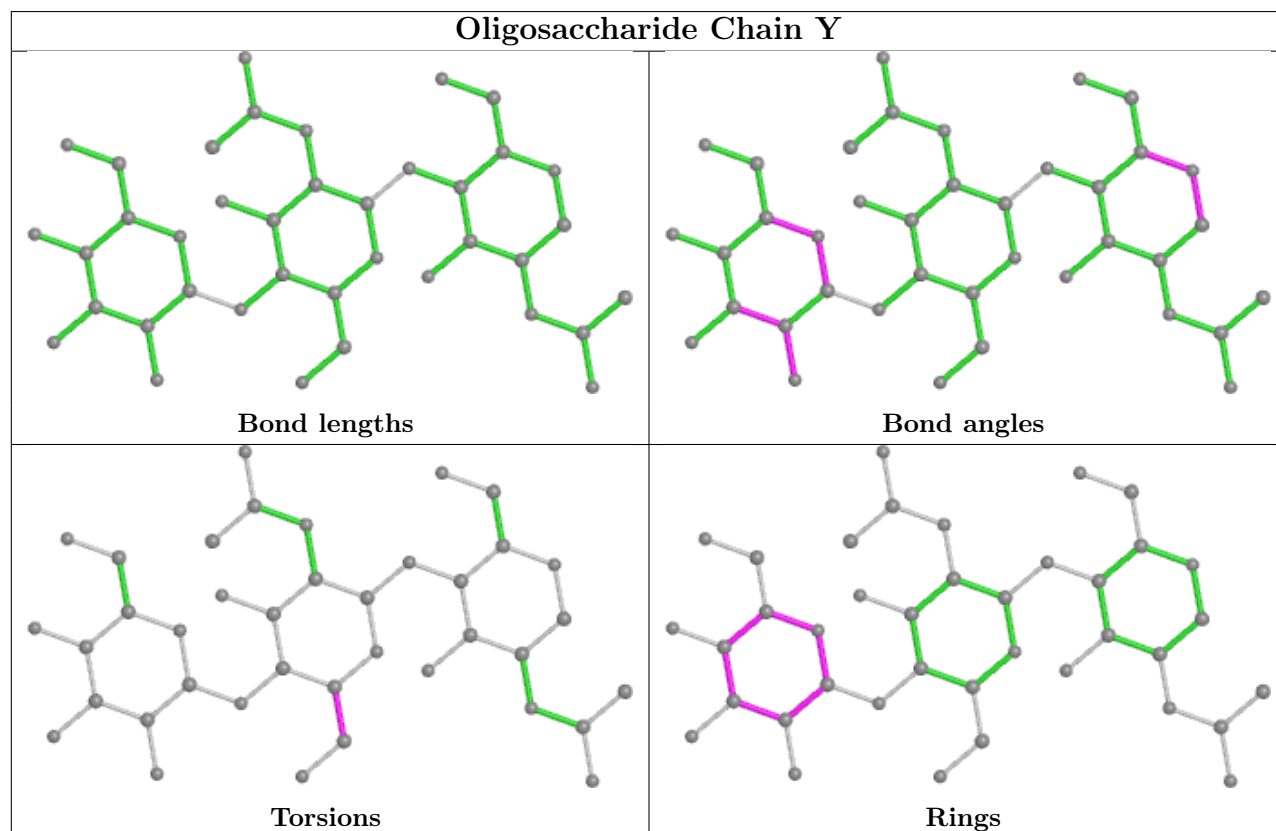
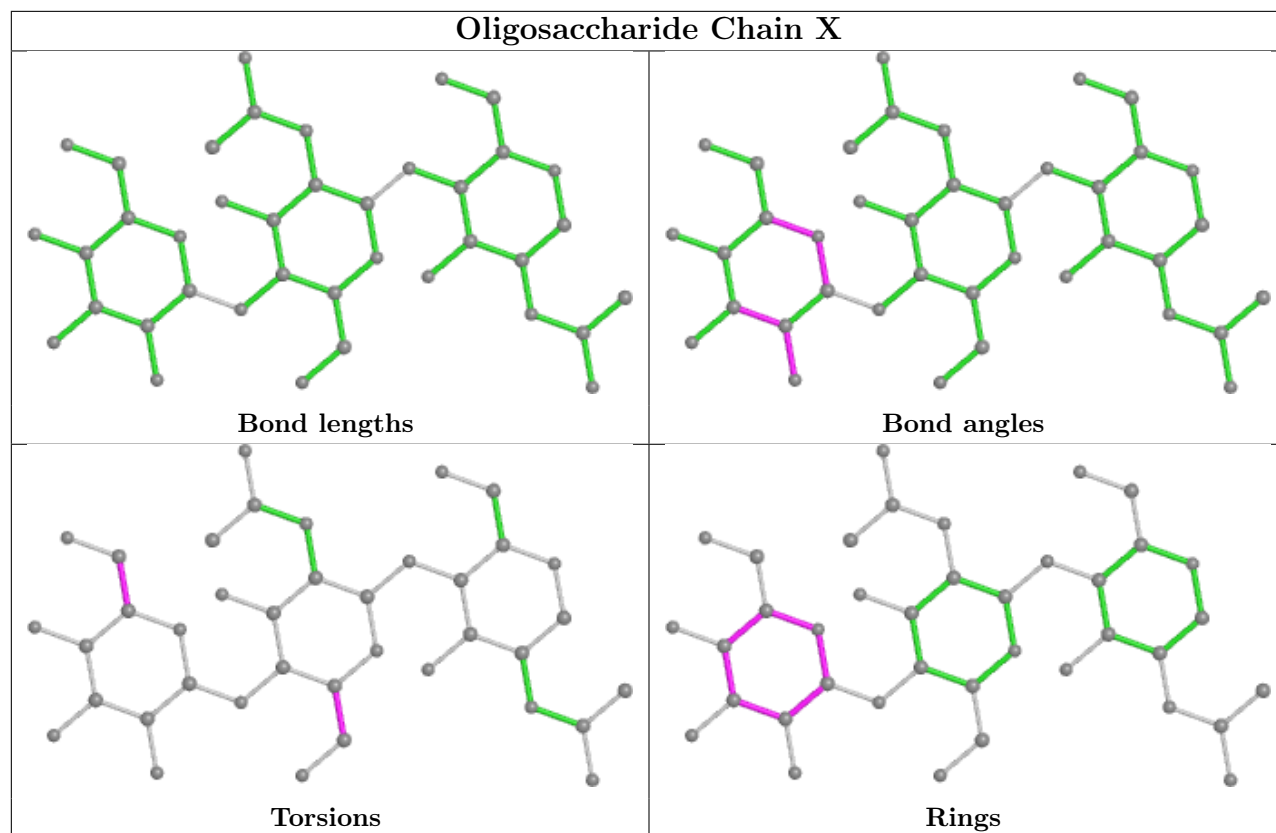


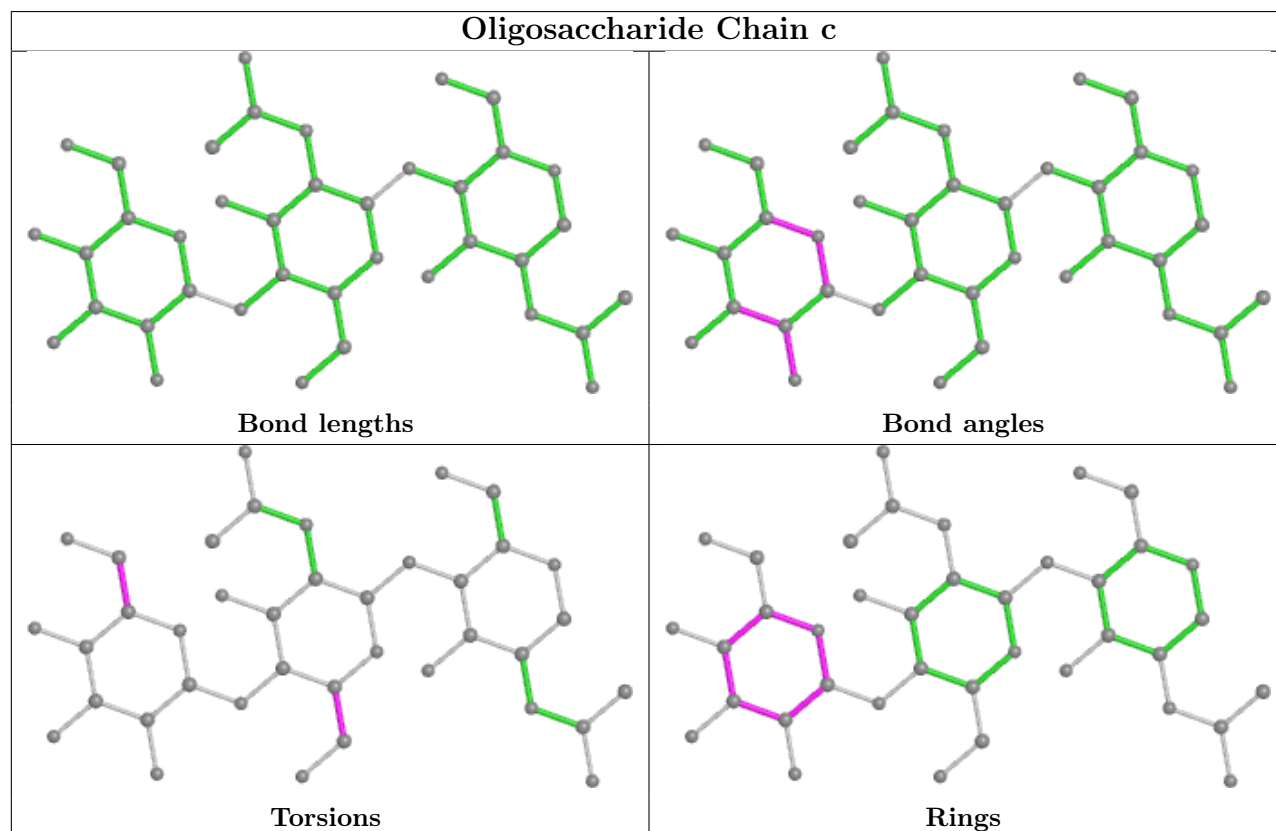
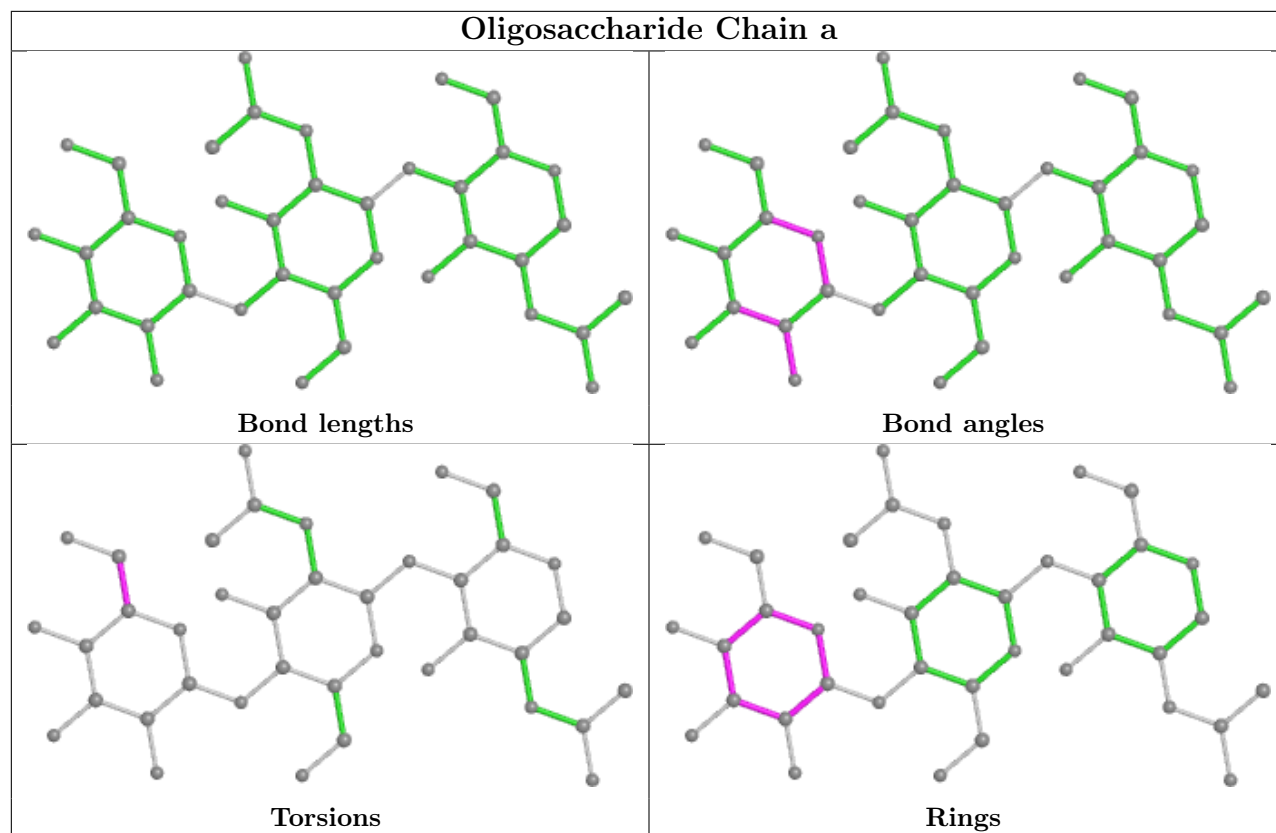


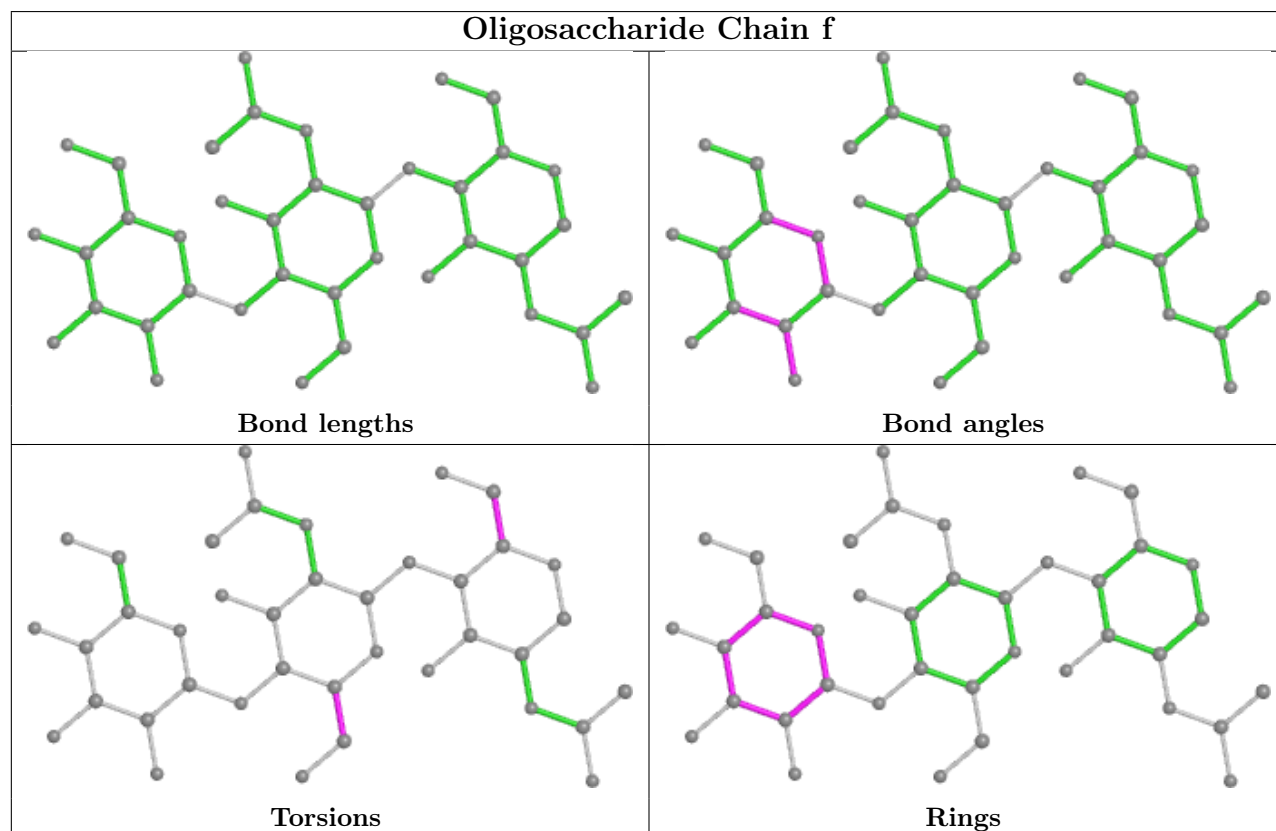
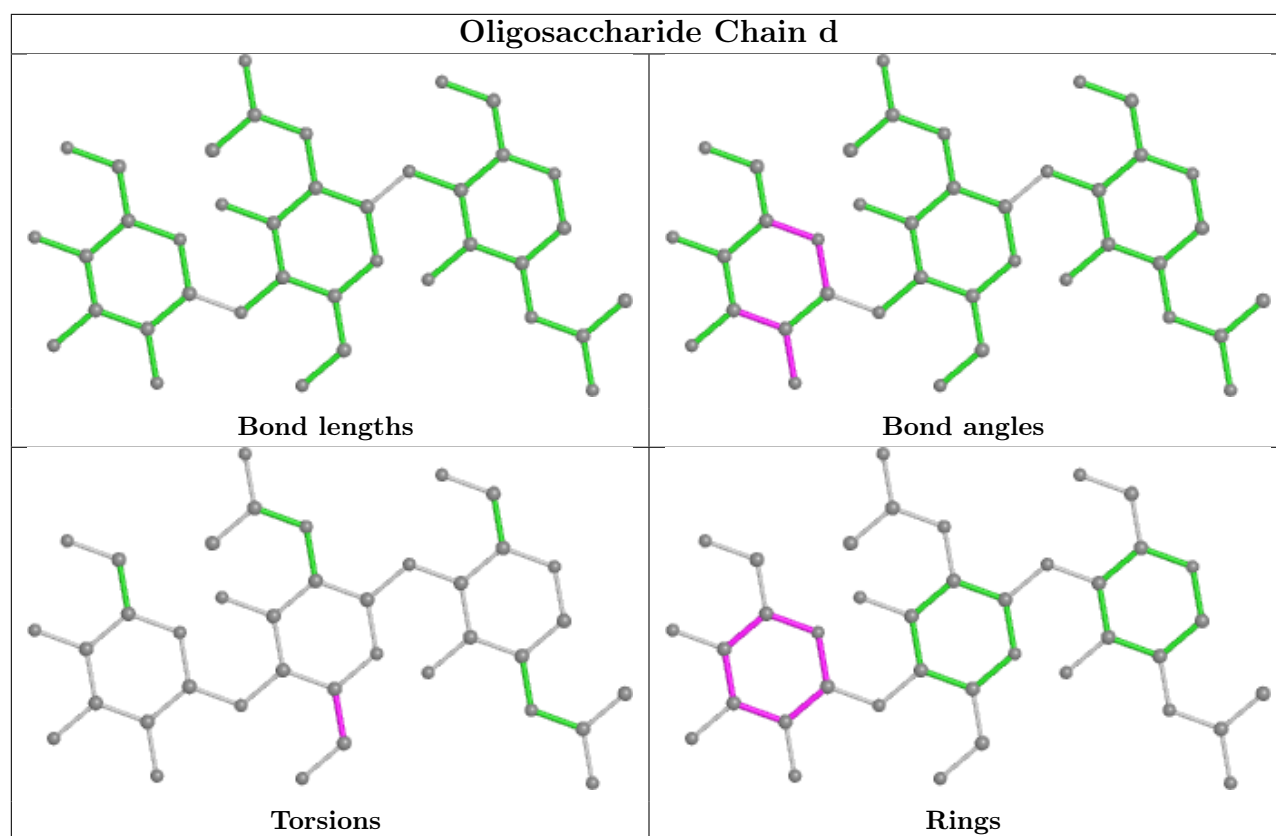


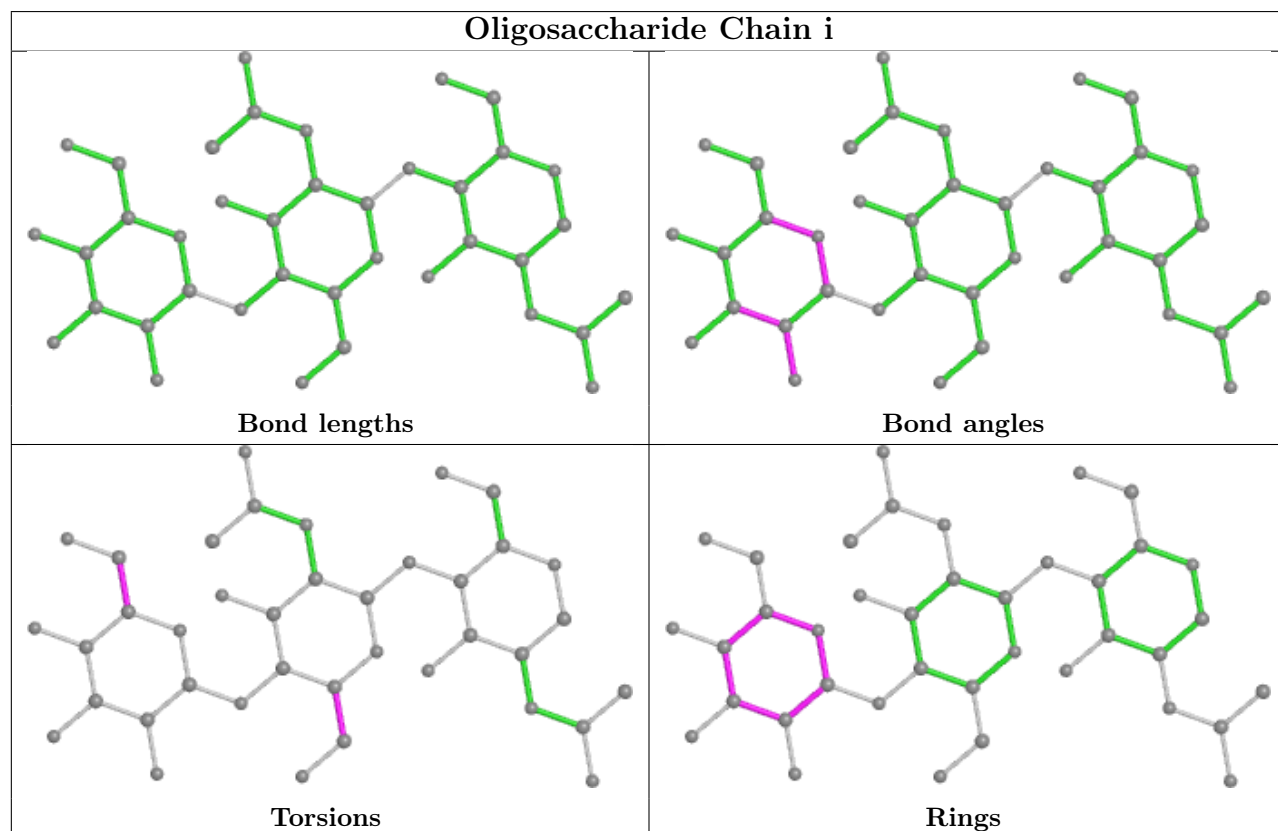
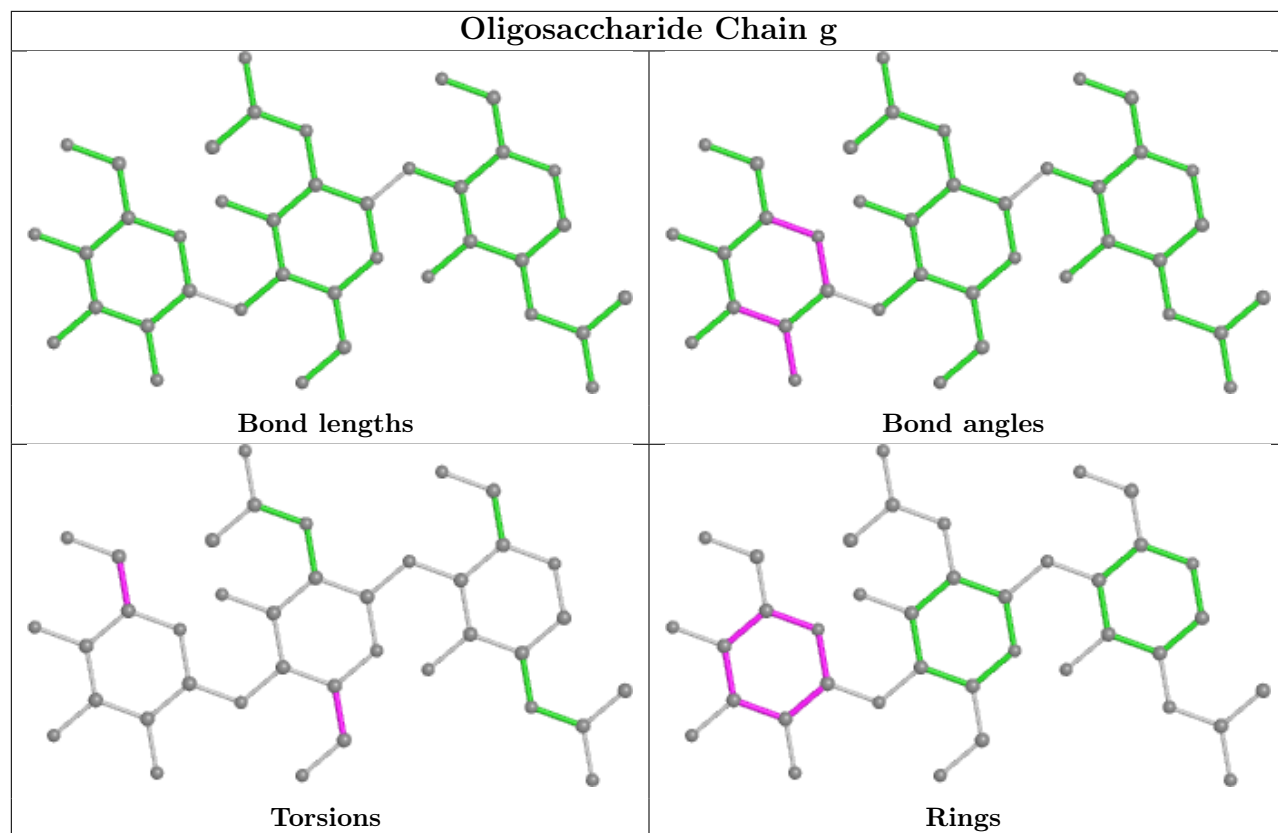


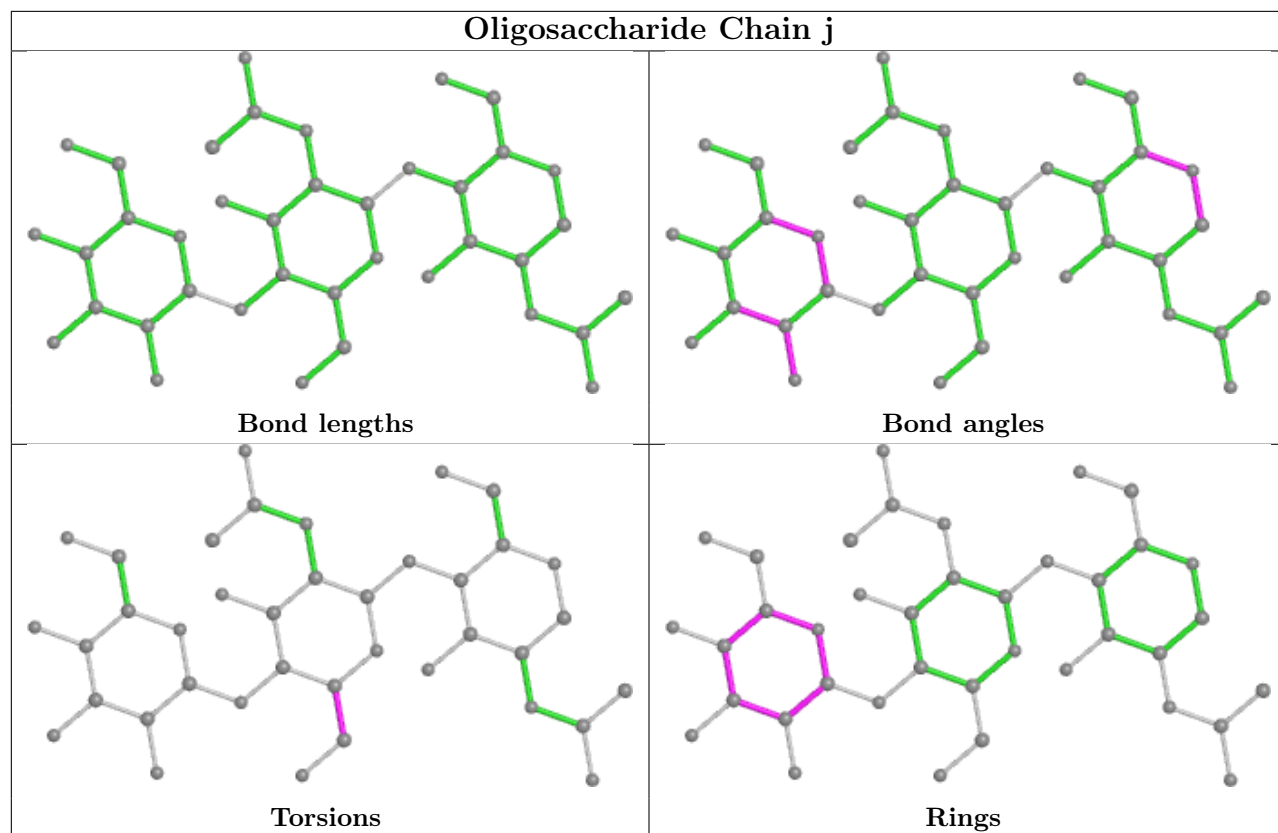


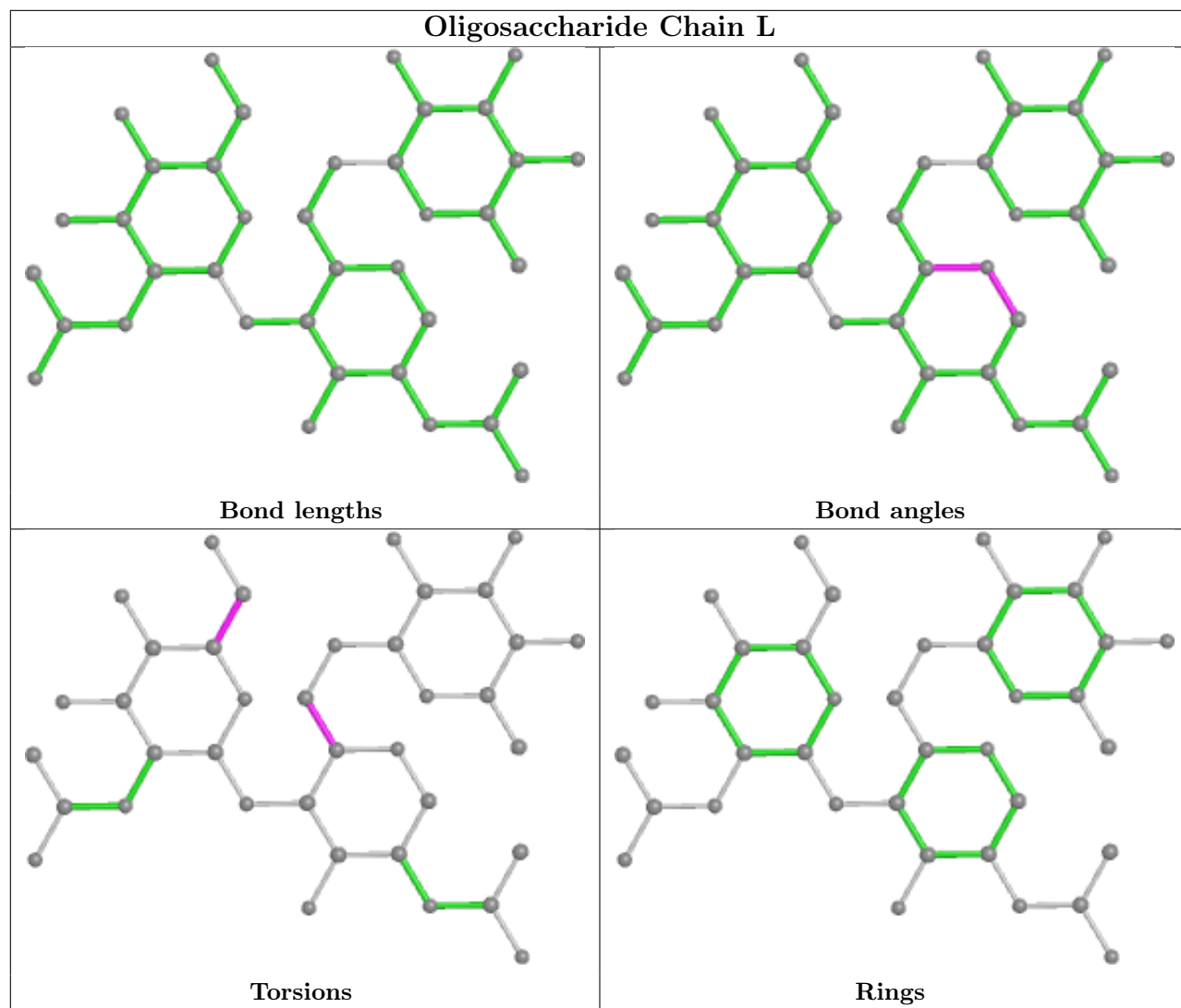


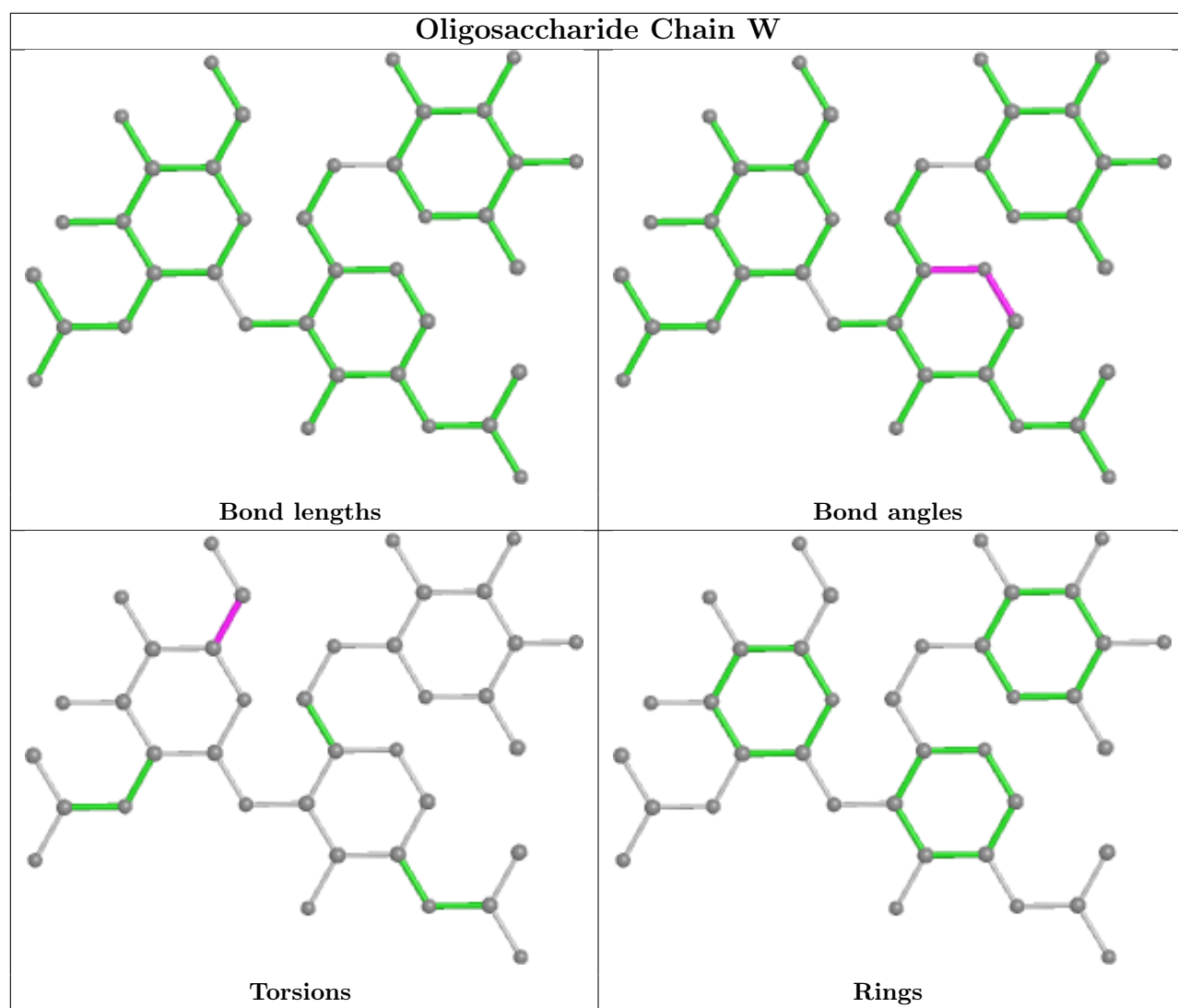


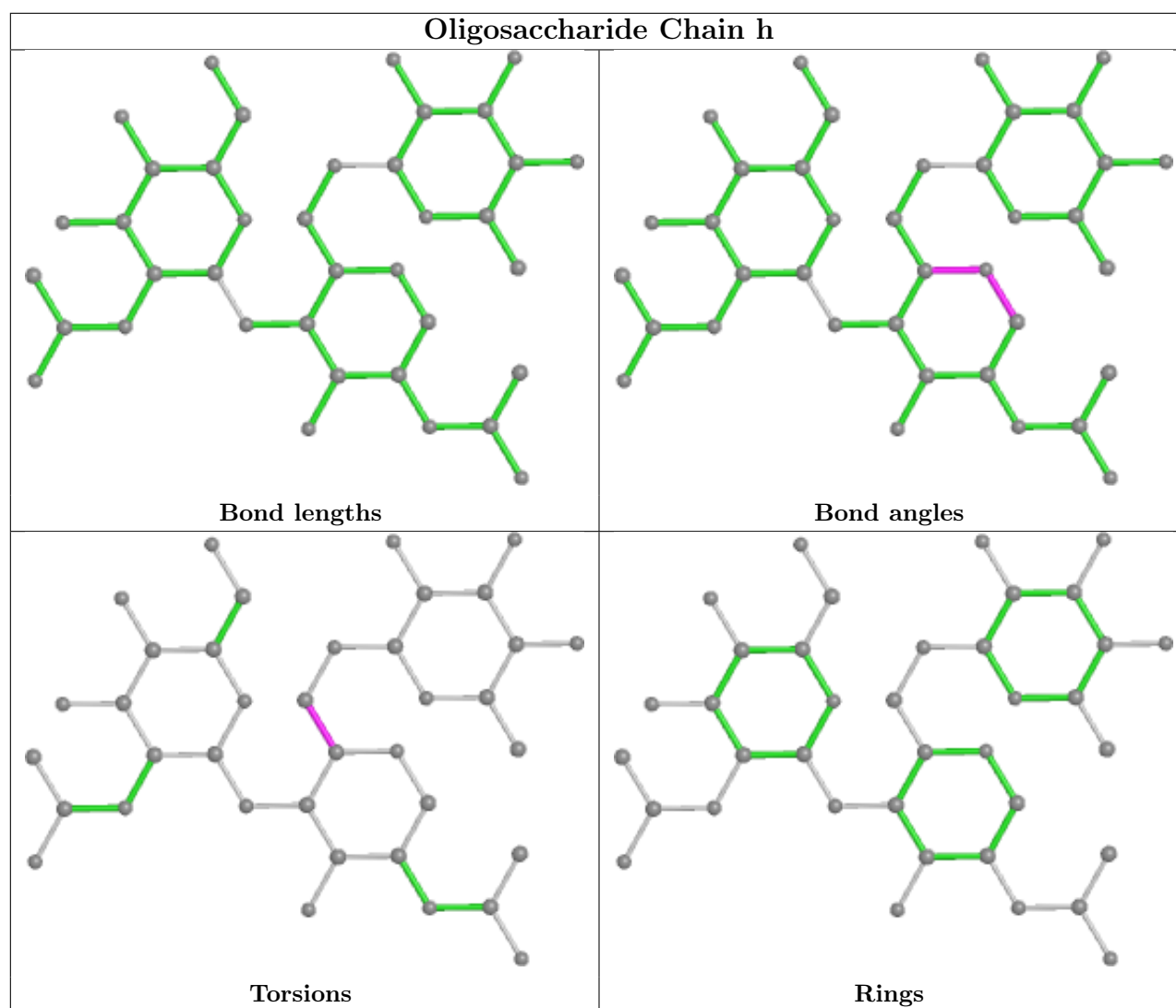












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
5	NAG	C	1405	1	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	B	1406	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	B	1407	1	14,14,15	0.19	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1405	1	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	B	1401	1	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	C	1408	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	C	1406	1	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	A	1402	1	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	A	1403	1	14,14,15	0.39	0	17,19,21	0.55	0
5	NAG	C	1403	1	14,14,15	0.36	0	17,19,21	0.43	0
5	NAG	C	1404	1	14,14,15	0.70	1 (7%)	17,19,21	0.70	1 (5%)
5	NAG	B	1403	1	14,14,15	0.36	0	17,19,21	0.44	0
5	NAG	C	1402	1	14,14,15	0.30	0	17,19,21	0.47	0
5	NAG	C	1407	1	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	A	1407	1	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	B	1402	1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	A	1401	1	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	A	1408	1	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	C	1401	1	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	B	1404	1	14,14,15	0.72	1 (7%)	17,19,21	0.71	1 (5%)
5	NAG	A	1404	1	14,14,15	0.73	1 (7%)	17,19,21	0.69	1 (5%)
5	NAG	B	1408	1	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	A	1406	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	A	1405	1	14,14,15	0.23	0	17,19,21	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1404	NAG	C1-C2	2.38	1.55	1.52
5	B	1404	NAG	C1-C2	2.37	1.55	1.52
5	C	1404	NAG	C1-C2	2.29	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1404	NAG	C1-O5-C5	2.43	115.48	112.19
5	C	1404	NAG	C1-O5-C5	2.42	115.47	112.19
5	A	1404	NAG	C1-O5-C5	2.34	115.36	112.19

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1405	NAG	O5-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	C	1406	NAG	O5-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1408	NAG	O5-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	A	1406	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1407	NAG	O5-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	C	1406	NAG	C4-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	C	1405	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	C	1405	NAG	C4-C5-C6-O6
5	A	1406	NAG	C4-C5-C6-O6
5	B	1408	NAG	C4-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	B	1407	NAG	O5-C5-C6-O6
5	A	1407	NAG	C4-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	B	1407	NAG	C4-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	B	1404	NAG	C1-C2-N2-C7
5	C	1407	NAG	O5-C5-C6-O6
5	C	1404	NAG	C1-C2-N2-C7
5	A	1404	NAG	C1-C2-N2-C7
5	A	1404	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

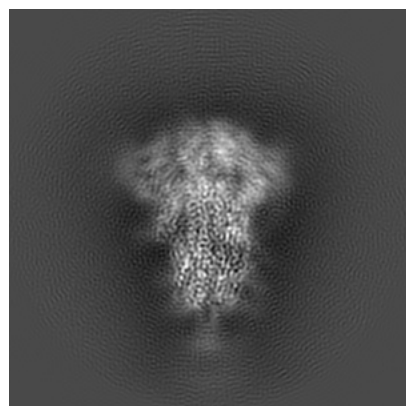
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33726. These allow visual inspection of the internal detail of the map and identification of artifacts.

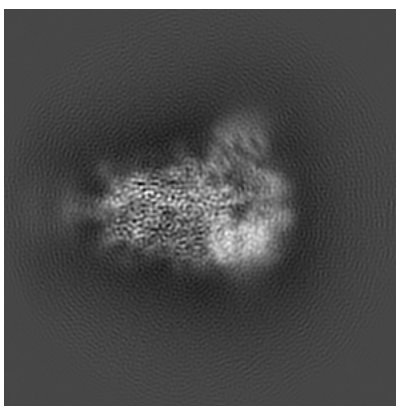
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

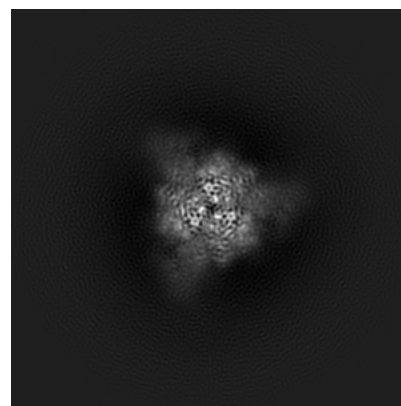
6.1.1 Primary map



X

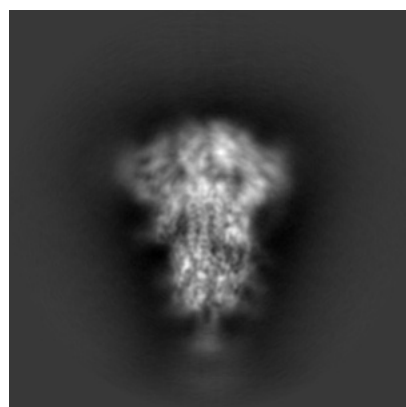


Y

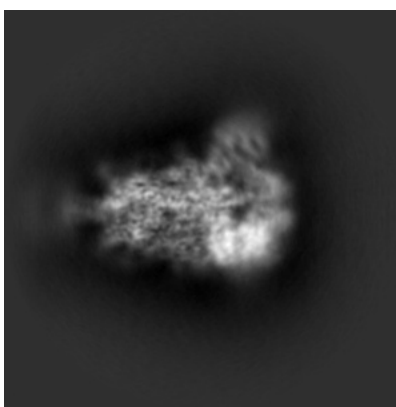


Z

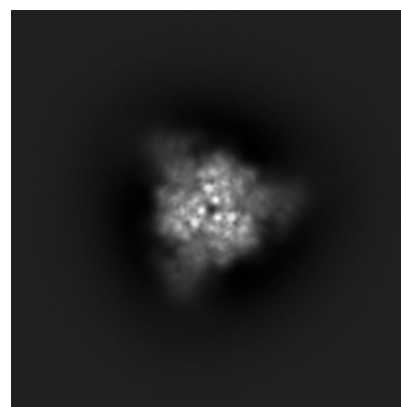
6.1.2 Raw map



X



Y

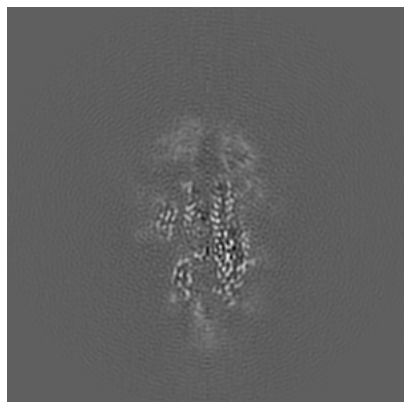


Z

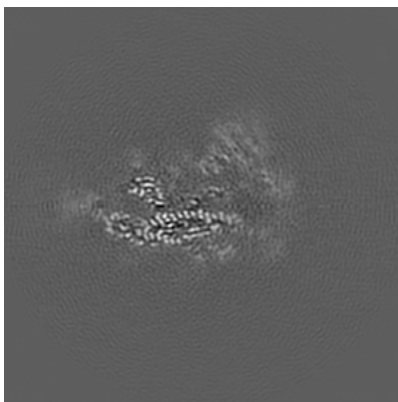
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

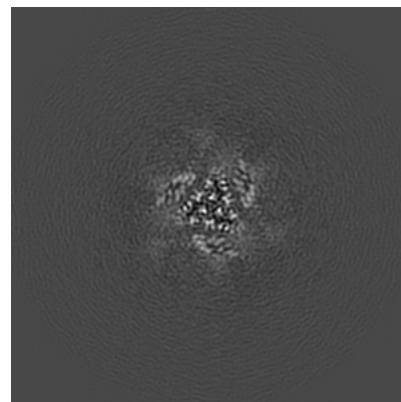
6.2.1 Primary map



X Index: 150

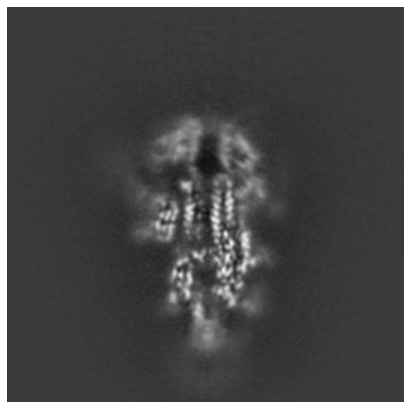


Y Index: 150

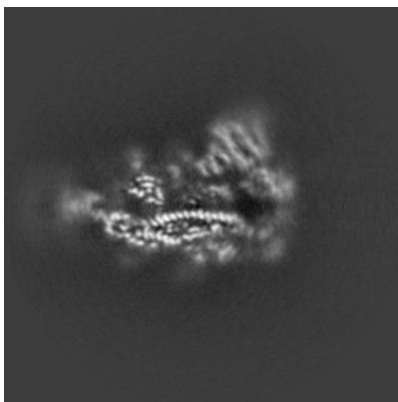


Z Index: 150

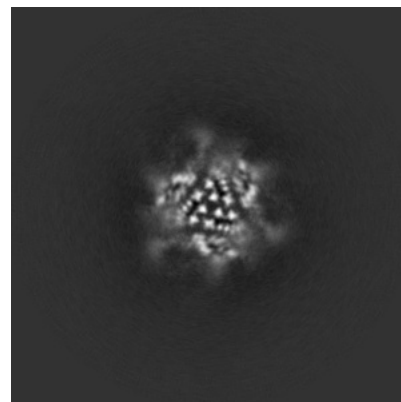
6.2.2 Raw map



X Index: 150



Y Index: 150

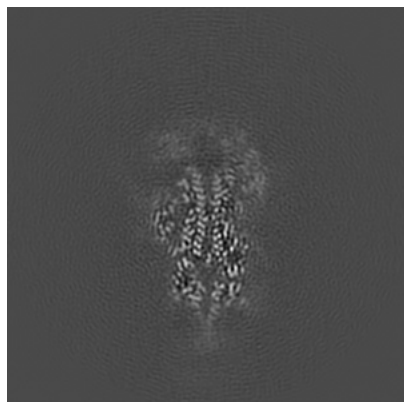


Z Index: 150

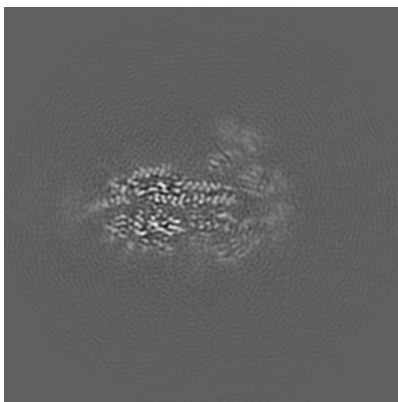
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

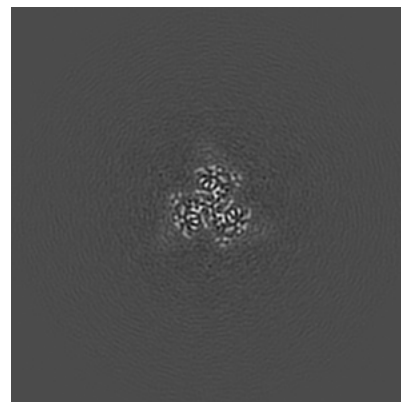
6.3.1 Primary map



X Index: 154

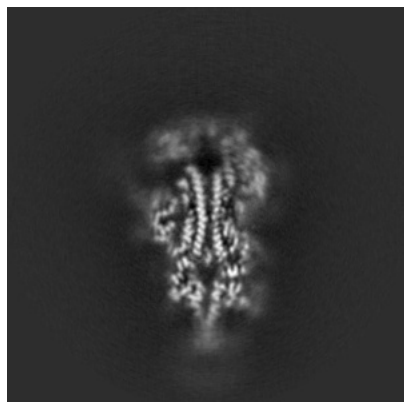


Y Index: 143

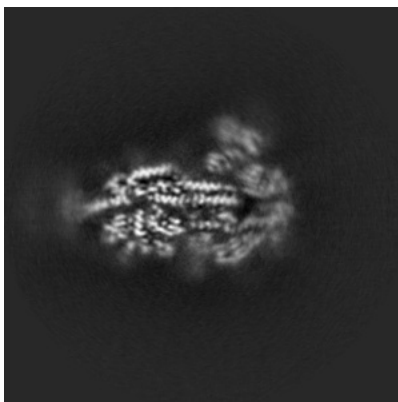


Z Index: 114

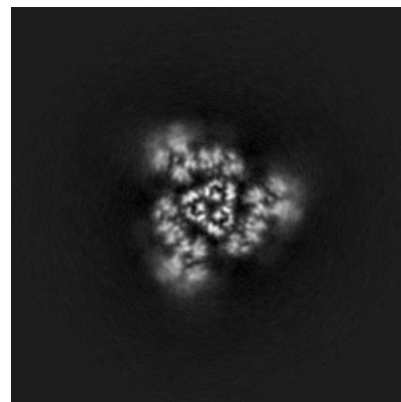
6.3.2 Raw map



X Index: 154



Y Index: 143

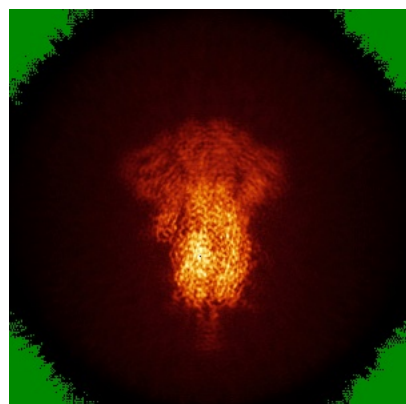


Z Index: 166

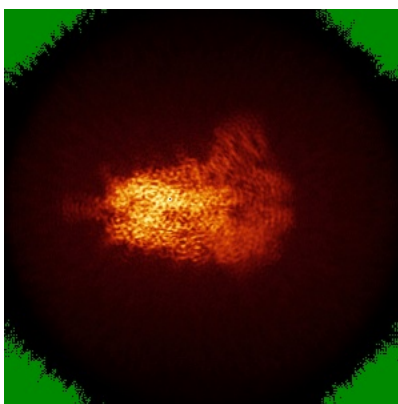
The images above show the largest variance slices of the map in three orthogonal directions.

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

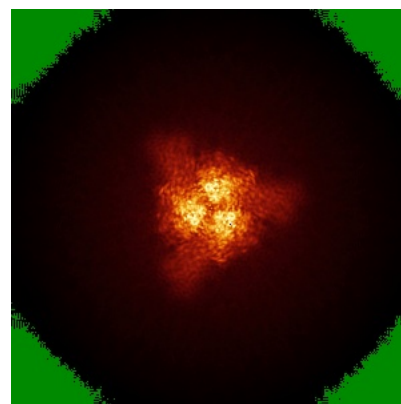
6.4.1 Primary map



X



Y

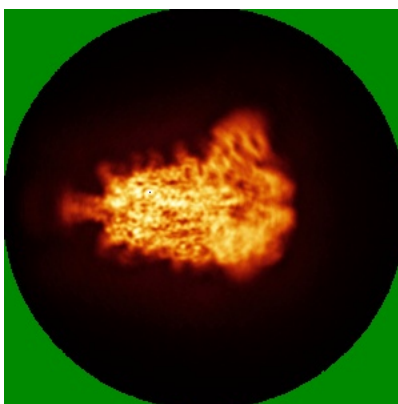


Z

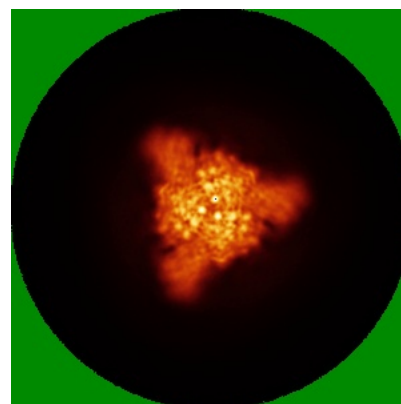
6.4.2 Raw map



X



Y

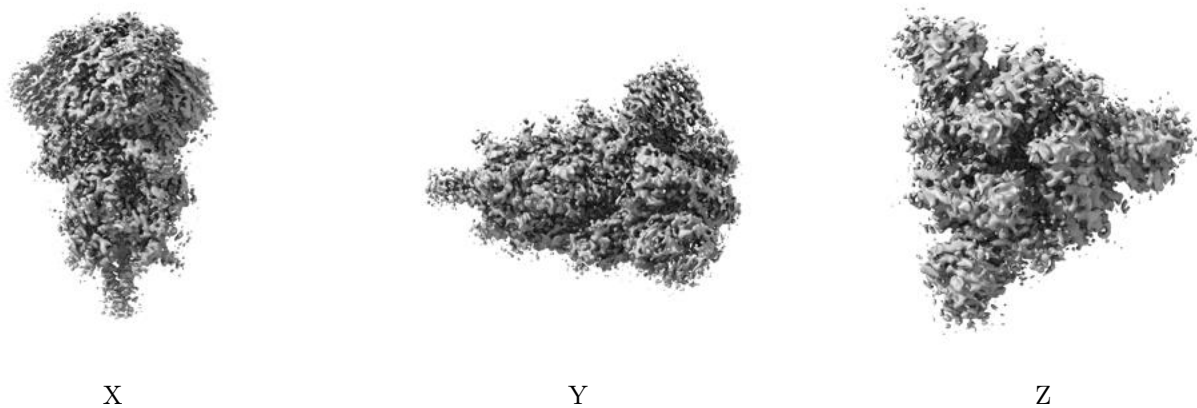


Z

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.

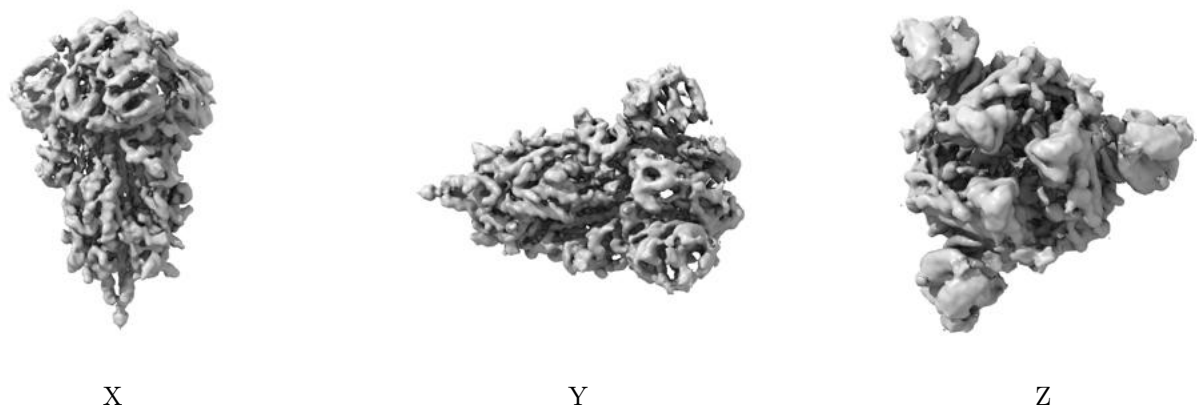
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

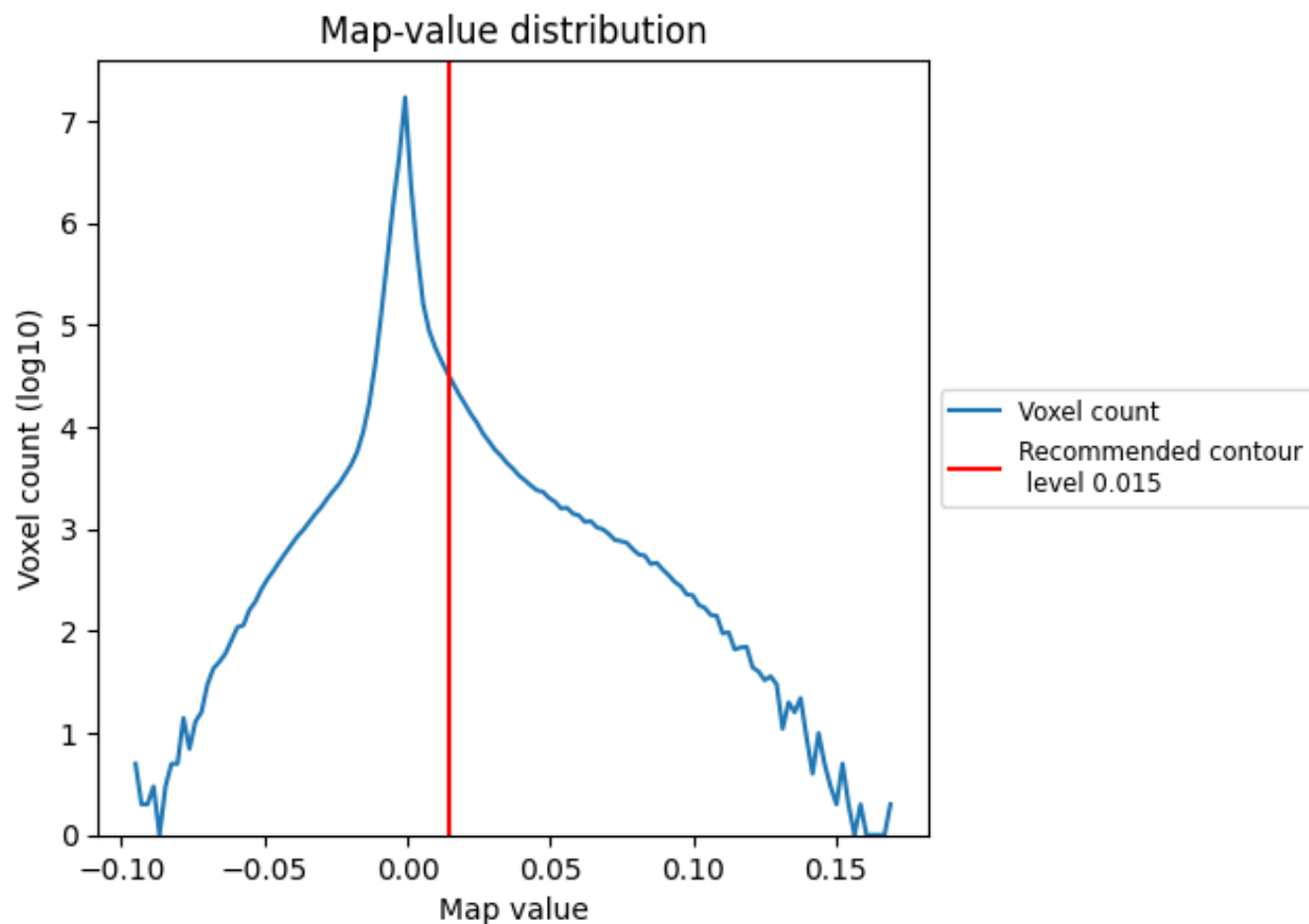
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

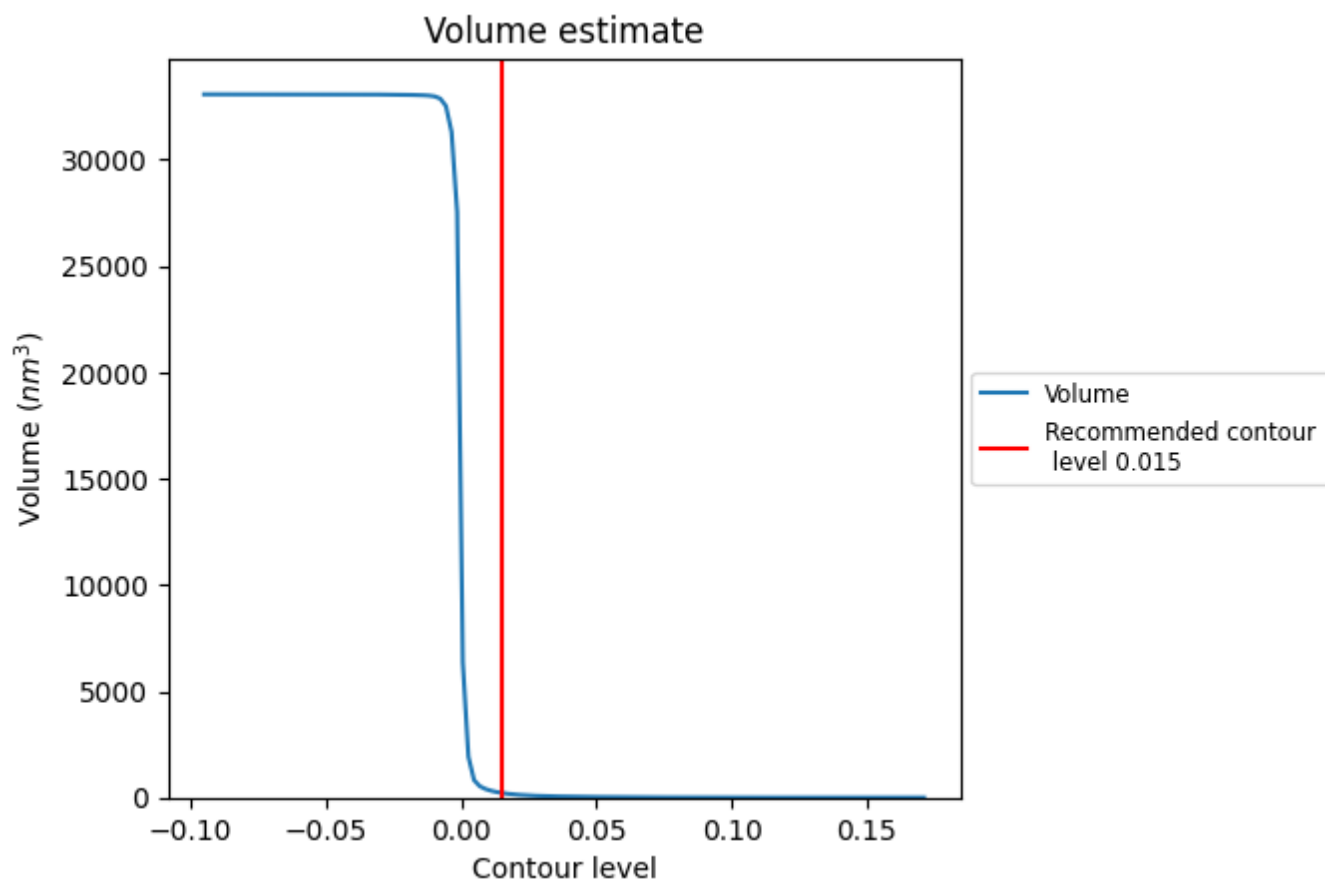
This section contains the results of statistical analysis of the map.

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.

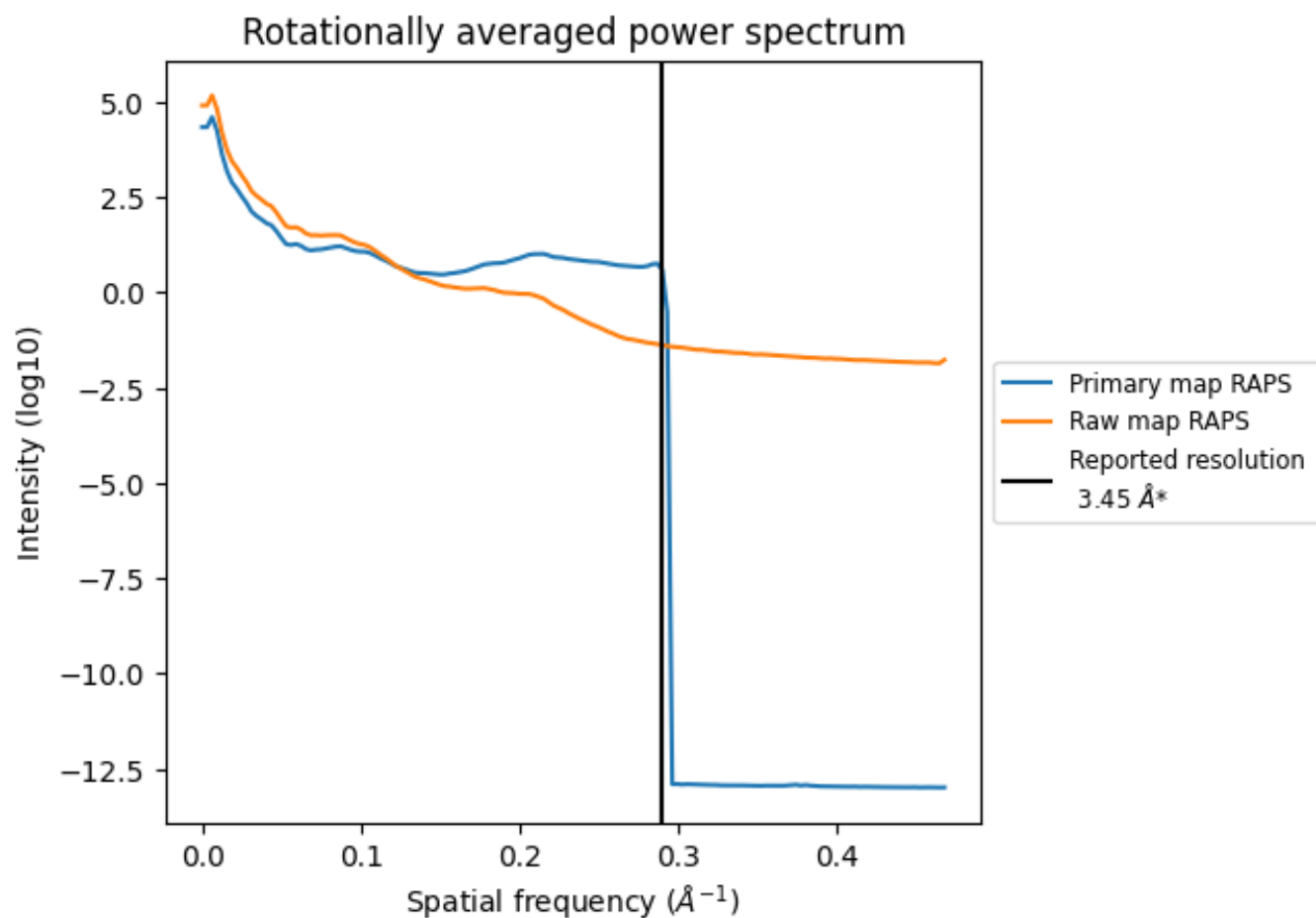
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 218 nm³; this corresponds to an approximate mass of 197 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 ⓘ

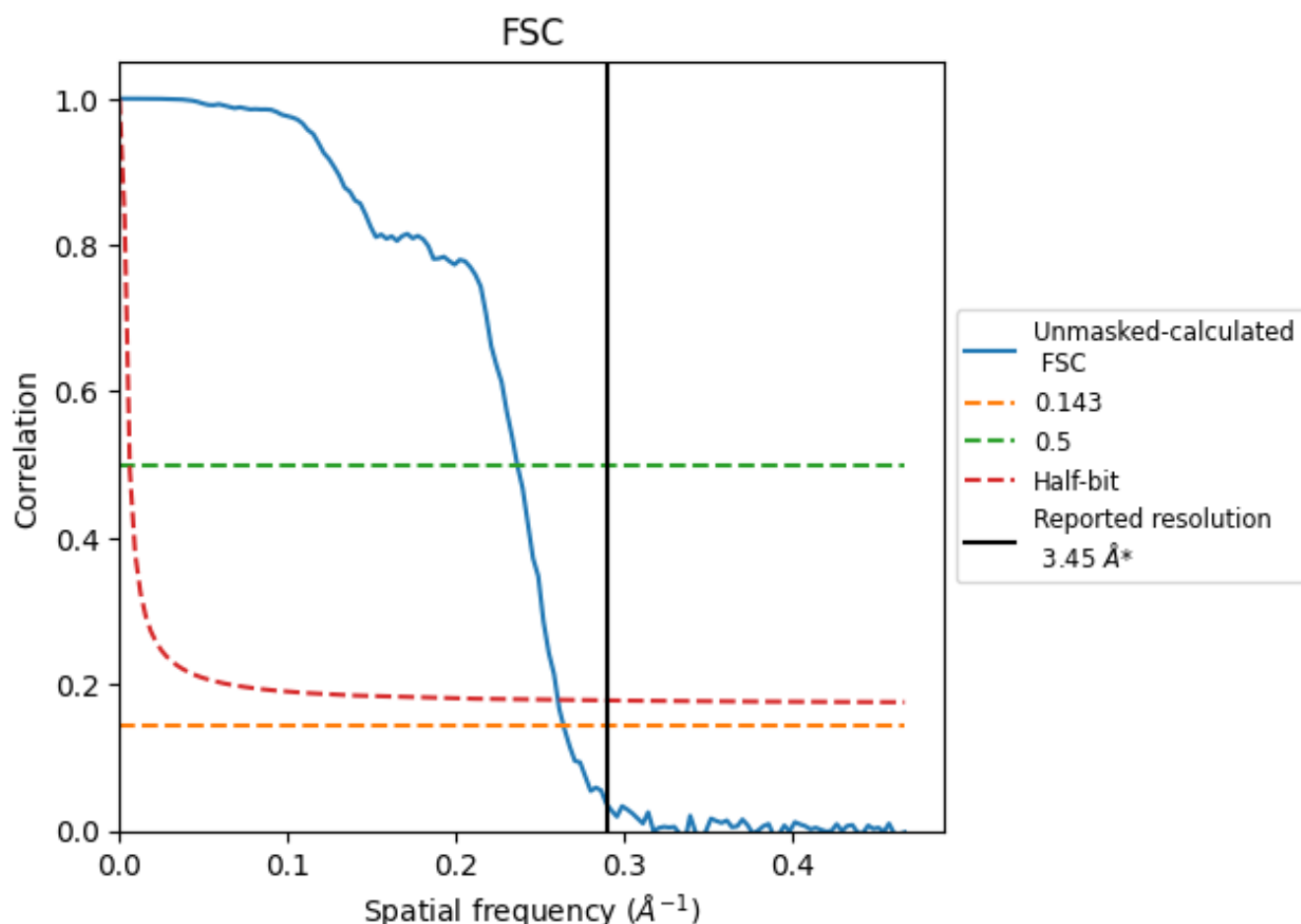


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

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 0.290 \AA^{-1}

8.2 Resolution estimates [i](#)

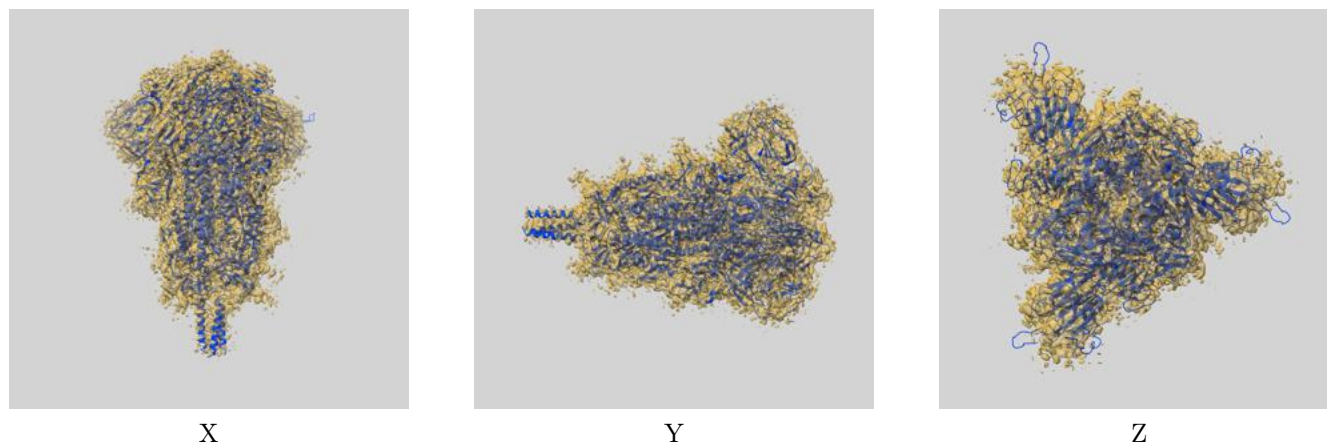
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.78	4.22	3.83

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

9 Map-model fit [i](#)

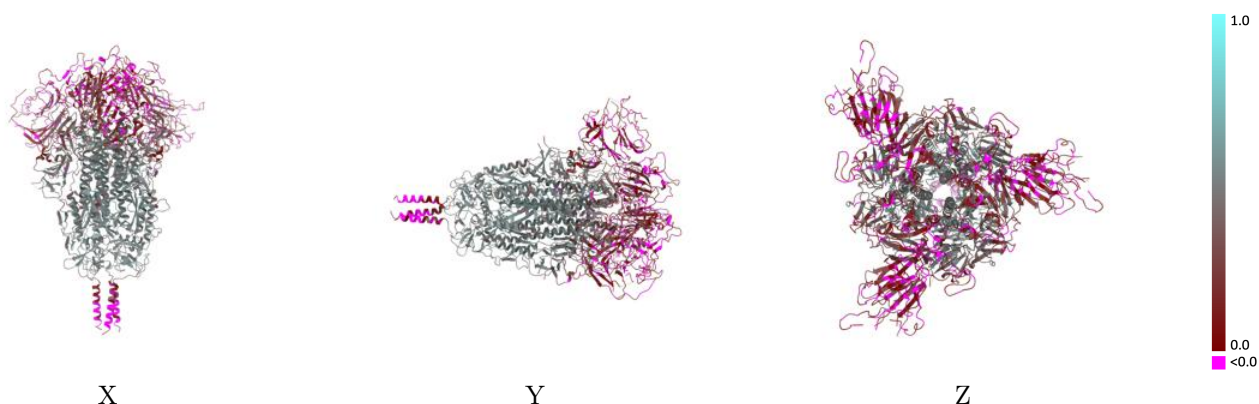
This section contains information regarding the fit between EMDB map EMD-33726 and PDB model 7YBM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



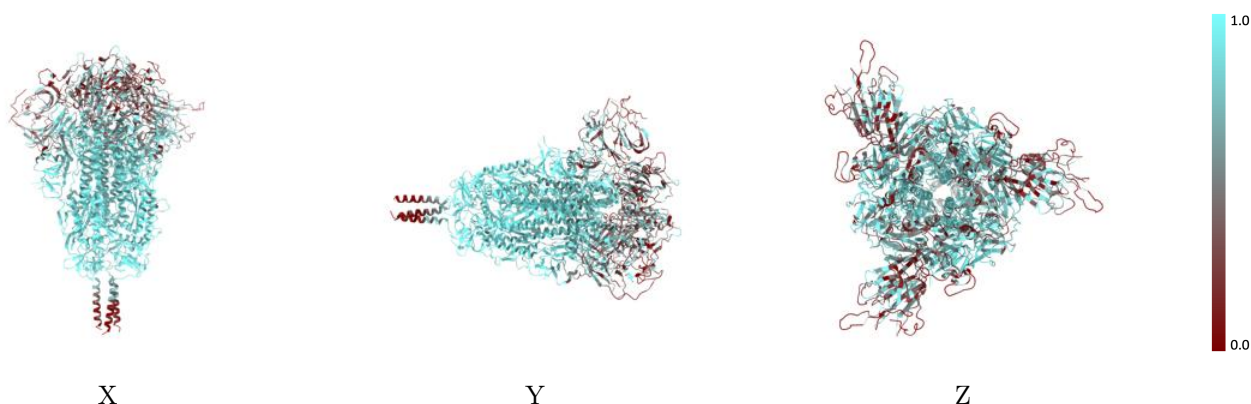
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



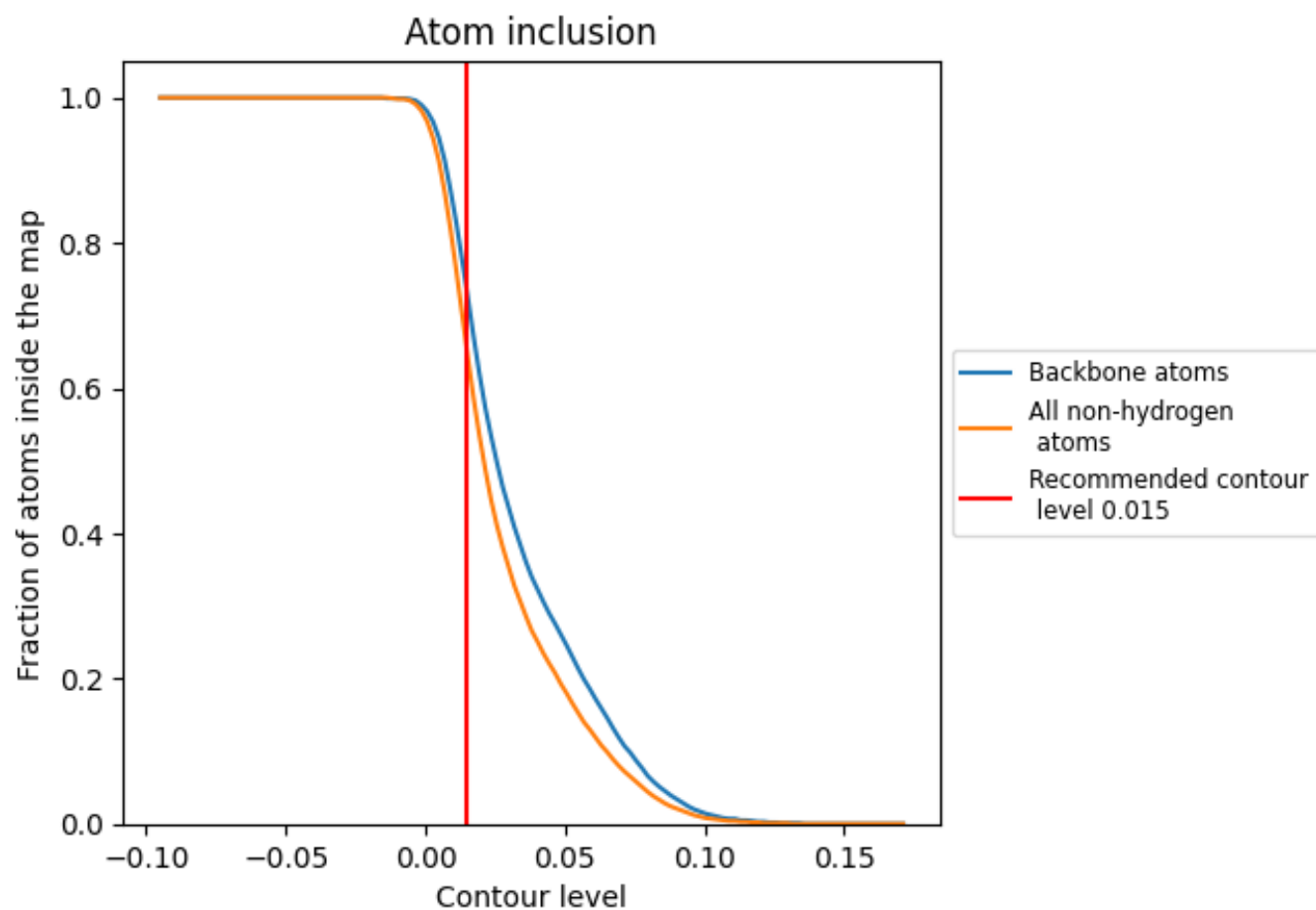
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6480	 0.3030
A	 0.6620	 0.3060
B	 0.6630	 0.3080
C	 0.6610	 0.3080
D	 0.0000	 0.1160
E	 0.0510	 0.0200
F	 0.0360	 0.1500
G	 0.0000	 -0.0670
H	 0.1540	 0.1230
I	 0.3930	 0.1750
J	 0.6670	 0.3570
K	 0.7440	 0.3850
L	 0.3680	 0.2340
M	 0.6410	 0.2410
N	 0.4870	 0.2270
O	 0.0000	 0.2300
P	 0.0510	 0.0470
Q	 0.0360	 0.1660
R	 0.0000	 -0.0260
S	 0.1790	 0.1650
T	 0.3930	 0.0730
U	 0.6150	 0.2650
V	 0.7690	 0.4000
W	 0.4470	 0.2910
X	 0.6670	 0.3260
Y	 0.5380	 0.2520
Z	 0.0000	 0.2380
a	 0.0510	 0.0160
b	 0.0360	 0.1480
c	 0.0000	 -0.0390
d	 0.2310	 0.1490
e	 0.4290	 0.1630
f	 0.6410	 0.4200
g	 0.7440	 0.3880
h	 0.3420	 0.2340



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Chain	Atom inclusion	Q-score
i	 0.6920	 0.3430
j	 0.5900	 0.2870