



## wwPDB EM Validation Summary Report ⓘ

Sep 28, 2022 – 02:55 pm BST

PDB ID : 7Z86  
EMDB ID : EMD-14544  
Title : CRYO-EM STRUCTURE OF SARS-COV-2 SPIKE : H11-H4 Q98R H100E  
nanobody complex in 1Up2Down conformation  
Authors : Weckener, M.; Naismith, J.H.  
Deposited on : 2022-03-16  
Resolution : 3.40 Å(reported)  
Based on initial model : 6ZHD

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 1.8.4, 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

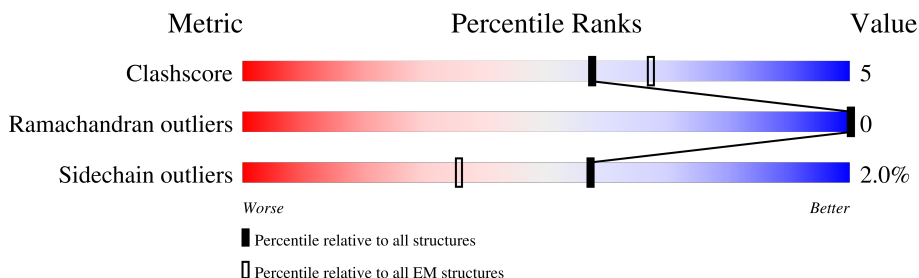
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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  $\geq 3$ , 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	1260	
1	B	1260	
1	C	1260	
2	X	127	
2	Y	127	
2	Z	127	
3	D	2	
3	E	2	

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Mol	Chain	Length	Quality of chain
3	F	2	
3	G	2	
3	H	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	M	1	X	-	-	-
4	NAG	C	1401	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 27071 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	987	7712	4924	1279	1474	35	0	0
1	B	992	7745	4951	1284	1475	35	0	0
1	C	991	7738	4941	1284	1478	35	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
A	1232	LEU	PHE	conflict	UNP P10104
A	1239	LEU	-	expression tag	UNP P10104
A	1240	LEU	-	expression tag	UNP P10104
A	1241	ASN	-	expression tag	UNP P10104
A	1242	ASP	-	expression tag	UNP P10104
A	1243	ILE	-	expression tag	UNP P10104
A	1244	PHE	-	expression tag	UNP P10104
A	1245	GLU	-	expression tag	UNP P10104
A	1246	ALA	-	expression tag	UNP P10104
A	1247	GLN	-	expression tag	UNP P10104
A	1248	LYS	-	expression tag	UNP P10104
A	1249	ILE	-	expression tag	UNP P10104
A	1250	GLU	-	expression tag	UNP P10104
A	1251	TRP	-	expression tag	UNP P10104
A	1252	HIS	-	expression tag	UNP P10104
A	1253	GLU	-	expression tag	UNP P10104
A	1254	LYS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	HIS	-	expression tag	UNP P10104
A	1256	HIS	-	expression tag	UNP P10104
A	1257	HIS	-	expression tag	UNP P10104
A	1258	HIS	-	expression tag	UNP P10104
A	1259	HIS	-	expression tag	UNP P10104
A	1260	HIS	-	expression tag	UNP P10104
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1232	LEU	PHE	conflict	UNP P10104
B	1239	LEU	-	expression tag	UNP P10104
B	1240	LEU	-	expression tag	UNP P10104
B	1241	ASN	-	expression tag	UNP P10104
B	1242	ASP	-	expression tag	UNP P10104
B	1243	ILE	-	expression tag	UNP P10104
B	1244	PHE	-	expression tag	UNP P10104
B	1245	GLU	-	expression tag	UNP P10104
B	1246	ALA	-	expression tag	UNP P10104
B	1247	GLN	-	expression tag	UNP P10104
B	1248	LYS	-	expression tag	UNP P10104
B	1249	ILE	-	expression tag	UNP P10104
B	1250	GLU	-	expression tag	UNP P10104
B	1251	TRP	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	GLU	-	expression tag	UNP P10104
B	1254	LYS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	HIS	-	expression tag	UNP P10104
B	1259	HIS	-	expression tag	UNP P10104
B	1260	HIS	-	expression tag	UNP P10104
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1210	SER	-	linker	UNP P0DTC2
C	1232	LEU	PHE	conflict	UNP P10104
C	1239	LEU	-	expression tag	UNP P10104
C	1240	LEU	-	expression tag	UNP P10104
C	1241	ASN	-	expression tag	UNP P10104
C	1242	ASP	-	expression tag	UNP P10104
C	1243	ILE	-	expression tag	UNP P10104
C	1244	PHE	-	expression tag	UNP P10104
C	1245	GLU	-	expression tag	UNP P10104
C	1246	ALA	-	expression tag	UNP P10104
C	1247	GLN	-	expression tag	UNP P10104
C	1248	LYS	-	expression tag	UNP P10104
C	1249	ILE	-	expression tag	UNP P10104
C	1250	GLU	-	expression tag	UNP P10104
C	1251	TRP	-	expression tag	UNP P10104
C	1252	HIS	-	expression tag	UNP P10104
C	1253	GLU	-	expression tag	UNP P10104
C	1254	LYS	-	expression tag	UNP P10104
C	1255	HIS	-	expression tag	UNP P10104
C	1256	HIS	-	expression tag	UNP P10104
C	1257	HIS	-	expression tag	UNP P10104
C	1258	HIS	-	expression tag	UNP P10104
C	1259	HIS	-	expression tag	UNP P10104
C	1260	HIS	-	expression tag	UNP P10104

- Molecule 2 is a protein called Nanobody H11-H4 Q98R H100E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	X	126	984	624	167	188	5	0	0
2	Y	126	984	624	167	188	5	0	0
2	Z	126	984	624	167	188	5	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	2	Total 28	C 16	N 2	O 10	0	0
3	E	2	Total 28	C 16	N 2	O 10	0	0
3	F	2	Total 28	C 16	N 2	O 10	0	0
3	G	2	Total 28	C 16	N 2	O 10	0	0
3	H	2	Total 28	C 16	N 2	O 10	0	0
3	I	2	Total 28	C 16	N 2	O 10	0	0
3	J	2	Total 28	C 16	N 2	O 10	0	0
3	K	2	Total 28	C 16	N 2	O 10	0	0
3	L	2	Total 28	C 16	N 2	O 10	0	0
3	M	2	Total 28	C 16	N 2	O 10	0	0
3	N	2	Total 28	C 16	N 2	O 10	0	0
3	O	2	Total 28	C 16	N 2	O 10	0	0
3	P	2	Total 28	C 16	N 2	O 10	0	0
3	Q	2	Total 28	C 16	N 2	O 10	0	0
3	R	2	Total 28	C 16	N 2	O 10	0	0
3	S	2	Total 28	C 16	N 2	O 10	0	0
3	T	2	Total 28	C 16	N 2	O 10	0	0
3	U	2	Total 28	C 16	N 2	O 10	0	0
3	V	2	Total 28	C 16	N 2	O 10	0	0
3	W	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	A	1	Total	C	N	O	0
			112	64	8	40	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	

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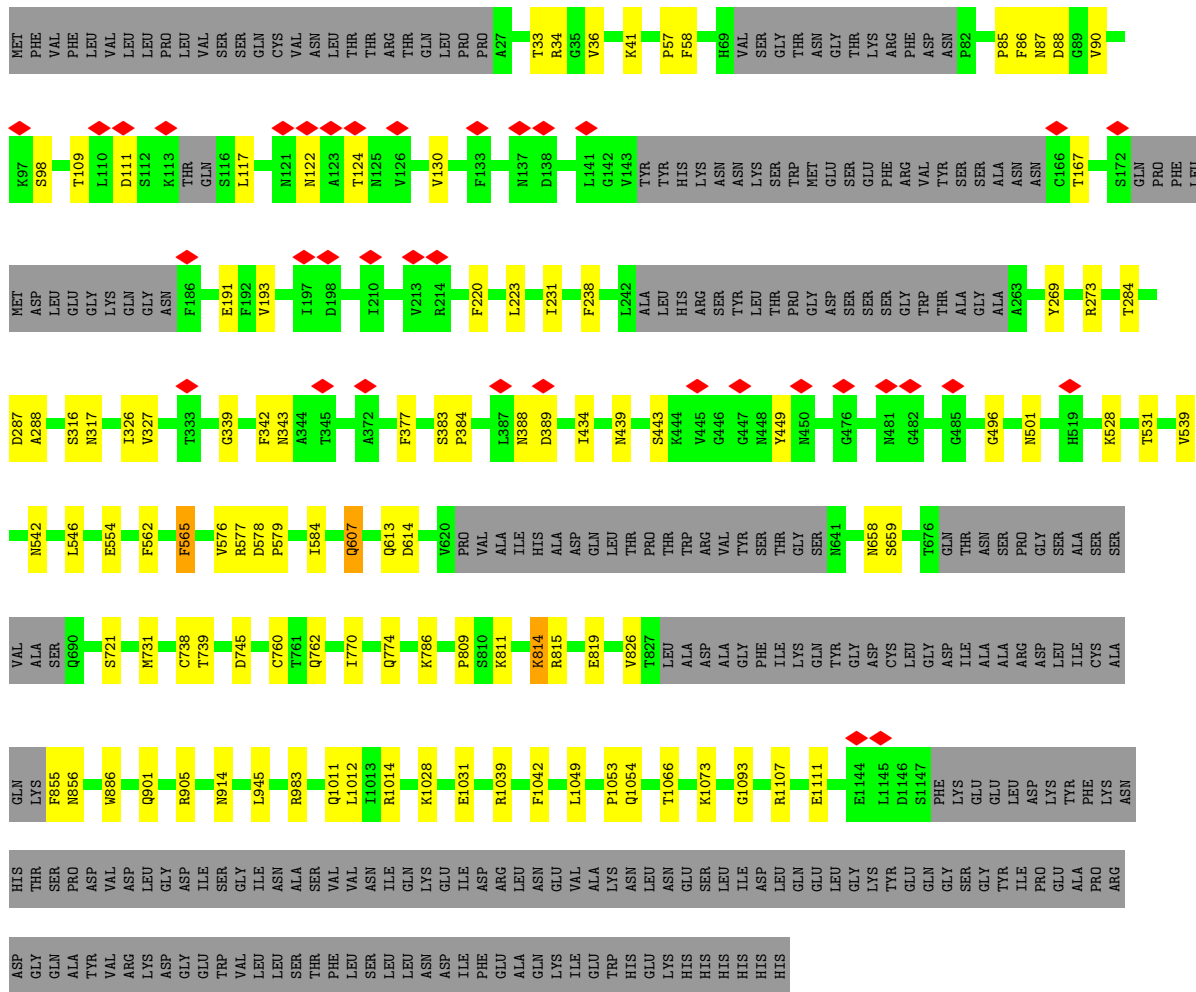
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	Total 140	80	10	50	0
4	B	1	Total 140	80	10	50	0
4	B	1	Total 140	80	10	50	0
4	B	1	Total 140	80	10	50	0
4	C	1	Total 112	64	8	40	0
4	C	1	Total 112	64	8	40	0
4	C	1	Total 112	64	8	40	0
4	C	1	Total 112	64	8	40	0
4	C	1	Total 112	64	8	40	0
4	C	1	Total 112	64	8	40	0
4	C	1	Total 112	64	8	40	0
4	C	1	Total 112	64	8	40	0
4	C	1	Total 112	64	8	40	0



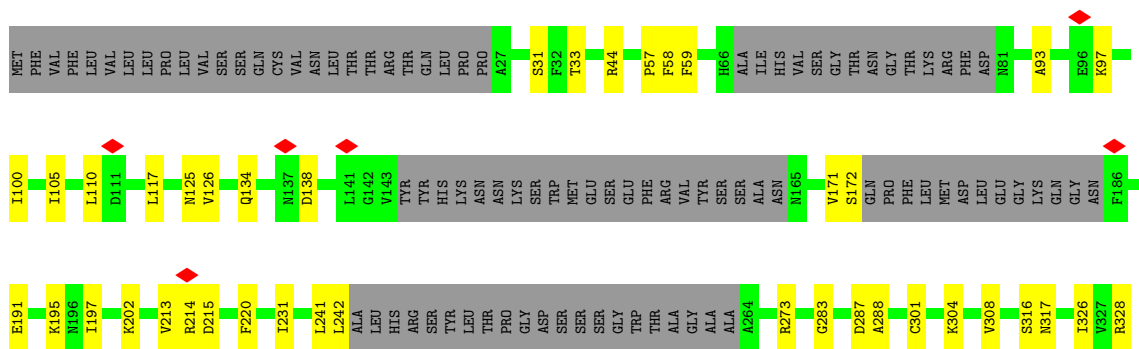
• Molecule 1: Spike glycoprotein,Fibrin

Chain B:

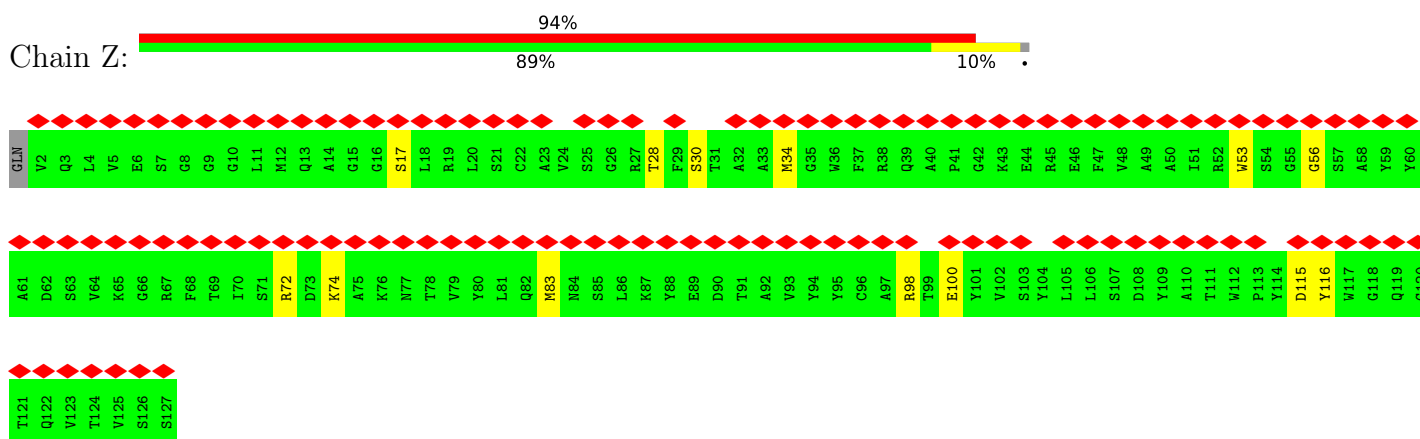


• Molecule 1: Spike glycoprotein,Fibrin

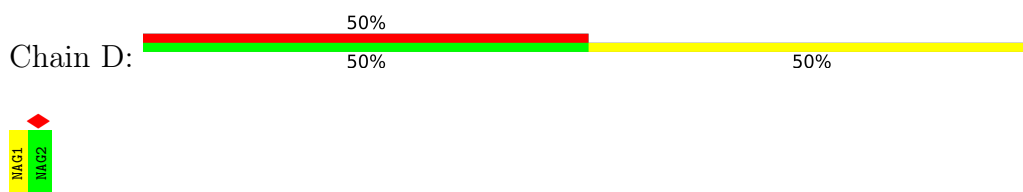
Chain C:



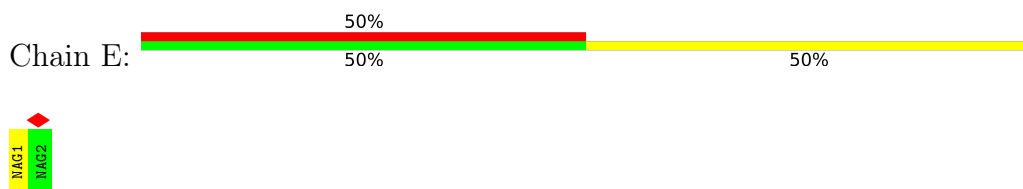




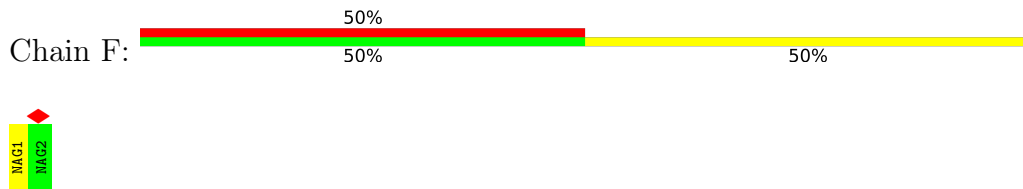
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



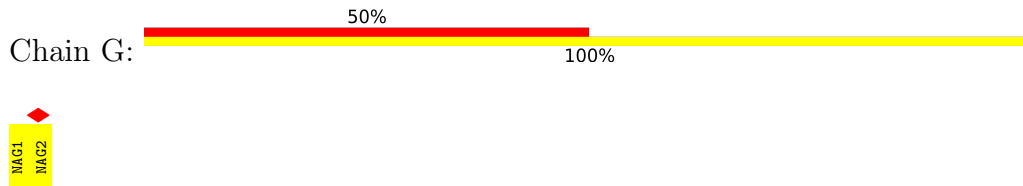
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



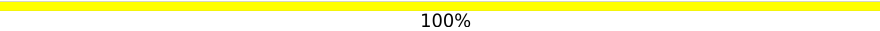
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain H:  100%

MAG1  
MAG2

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

Chain I:  50% 100%

MAG1  
MAG2

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

Chain J:  50% 100%

MAG1  
MAG2

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

Chain K:  50% 50% 50%

MAG1  
MAG2

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

Chain L:  100%

MAG1  
MAG2

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

Chain M:  50% 100%

MAG1  
MAG2

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



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



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



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



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



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



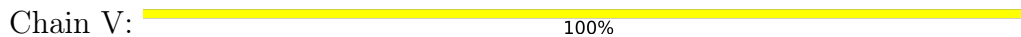
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	396910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.134	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	321.6, 321.6, 321.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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

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	0.36	0/7884	0.61	0/10725
1	B	0.37	0/7919	0.61	0/10774
1	C	0.36	0/7911	0.60	0/10766
2	X	0.31	0/1008	0.65	0/1365
2	Y	0.31	0/1008	0.65	0/1365
2	Z	0.31	0/1008	0.64	0/1365
All	All	0.36	0/26738	0.61	0/36360

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	7712	0	7504	65	0
1	B	7745	0	7555	74	0
1	C	7738	0	7542	78	0
2	X	984	0	939	21	0
2	Y	984	0	939	19	0
2	Z	984	0	939	19	0
3	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	2	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	2	0
3	K	28	0	25	6	0
3	L	28	0	25	0	0
3	M	28	0	25	1	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	2	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	1	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
4	A	112	0	104	0	0
4	B	140	0	130	5	0
4	C	112	0	104	10	0
All	All	27071	0	26256	266	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 5.

The worst 5 of 266 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:B:389:ASP:HB2	1:B:528:LYS:NZ	1.20	1.41
1:C:342:PHE:HB2	4:C:1401:NAG:C8	1.52	1.35
1:A:81:ASN:OD1	1:A:82:PRO:CD	1.86	1.23
1:A:81:ASN:OD1	1:A:82:PRO:HD3	0.99	1.14
1:B:342:PHE:HB2	4:B:1310:NAG:O7	1.47	1.13

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	967/1260 (77%)	937 (97%)	30 (3%)	0	100	100
1	B	974/1260 (77%)	942 (97%)	32 (3%)	0	100	100
1	C	975/1260 (77%)	943 (97%)	32 (3%)	0	100	100
2	X	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
2	Y	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
2	Z	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
All	All	3288/4161 (79%)	3191 (97%)	97 (3%)	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	865/1098 (79%)	840 (97%)	25 (3%)	42	69
1	B	867/1098 (79%)	848 (98%)	19 (2%)	52	75
1	C	868/1098 (79%)	855 (98%)	13 (2%)	65	82
2	X	100/101 (99%)	100 (100%)	0	100	100
2	Y	100/101 (99%)	100 (100%)	0	100	100
2	Z	100/101 (99%)	100 (100%)	0	100	100
All	All	2900/3597 (81%)	2843 (98%)	57 (2%)	57	77

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	98	SER
1	C	1146	ASP
1	B	745	ASP
1	C	988	GLU
1	C	215	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	ASN
1	C	87	ASN
1	C	1048	HIS
1	C	613	GLN
1	C	957	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](#)

40 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	$\# Z  > 2$
3	NAG	D	1	1,3	14,14,15	0.62	0	17,19,21	1.42	2 (11%)
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.75	0
3	NAG	E	1	1,3	14,14,15	0.52	0	17,19,21	1.12	1 (5%)
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	F	1	1,3	14,14,15	0.43	0	17,19,21	1.39	4 (23%)
3	NAG	F	2	3	14,14,15	0.40	0	17,19,21	0.75	0
3	NAG	G	1	1,3	14,14,15	0.48	0	17,19,21	1.34	2 (11%)
3	NAG	G	2	3	14,14,15	0.37	0	17,19,21	0.67	0
3	NAG	H	1	1,3	14,14,15	0.50	0	17,19,21	1.07	2 (11%)
3	NAG	H	2	3	14,14,15	0.41	0	17,19,21	0.92	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.54	0	17,19,21	1.27	2 (11%)
3	NAG	I	2	3	14,14,15	0.35	0	17,19,21	1.05	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.45	0	17,19,21	1.93	4 (23%)
3	NAG	J	2	3	14,14,15	0.30	0	17,19,21	0.77	0
3	NAG	K	1	1,3	14,14,15	0.47	0	17,19,21	0.76	1 (5%)
3	NAG	K	2	3	14,14,15	0.38	0	17,19,21	0.68	0
3	NAG	L	1	1,3	14,14,15	0.48	0	17,19,21	1.20	1 (5%)
3	NAG	L	2	3	14,14,15	0.40	0	17,19,21	0.85	1 (5%)
3	NAG	M	1	1,3	14,14,15	0.39	0	17,19,21	1.22	2 (11%)
3	NAG	M	2	3	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
3	NAG	N	1	1,3	14,14,15	0.38	0	17,19,21	1.56	3 (17%)
3	NAG	N	2	3	14,14,15	0.40	0	17,19,21	0.63	0
3	NAG	O	1	1,3	14,14,15	0.48	0	17,19,21	1.52	3 (17%)
3	NAG	O	2	3	14,14,15	0.38	0	17,19,21	0.75	0
3	NAG	P	1	1,3	14,14,15	0.52	0	17,19,21	1.68	3 (17%)
3	NAG	P	2	3	14,14,15	0.33	0	17,19,21	0.80	0
3	NAG	Q	1	1,3	14,14,15	0.43	0	17,19,21	1.56	3 (17%)
3	NAG	Q	2	3	14,14,15	0.34	0	17,19,21	0.57	0
3	NAG	R	1	1,3	14,14,15	0.44	0	17,19,21	1.02	1 (5%)
3	NAG	R	2	3	14,14,15	0.37	0	17,19,21	0.72	0
3	NAG	S	1	1,3	14,14,15	0.48	0	17,19,21	1.23	2 (11%)
3	NAG	S	2	3	14,14,15	0.35	0	17,19,21	0.99	1 (5%)
3	NAG	T	1	1,3	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
3	NAG	T	2	3	14,14,15	0.39	0	17,19,21	0.81	0
3	NAG	U	1	1,3	14,14,15	0.55	0	17,19,21	1.61	3 (17%)
3	NAG	U	2	3	14,14,15	0.36	0	17,19,21	0.61	0
3	NAG	V	1	1,3	14,14,15	0.38	0	17,19,21	1.45	2 (11%)
3	NAG	V	2	3	14,14,15	0.43	0	17,19,21	1.19	1 (5%)
3	NAG	W	1	1,3	14,14,15	0.52	0	17,19,21	0.86	1 (5%)
3	NAG	W	2	3	14,14,15	0.33	0	17,19,21	0.79	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
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	1,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	R	2	3	-	4/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	NAG	C3-C4-C5	4.67	118.57	110.24
3	J	1	NAG	C1-O5-C5	4.13	117.79	112.19
3	P	1	NAG	O5-C1-C2	-4.10	104.82	111.29
3	D	1	NAG	C3-C4-C5	4.08	117.52	110.24
3	Q	1	NAG	O5-C1-C2	-3.98	105.00	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	1	NAG	C1

5 of 126 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	2	0
3	J	2	NAG	2	0

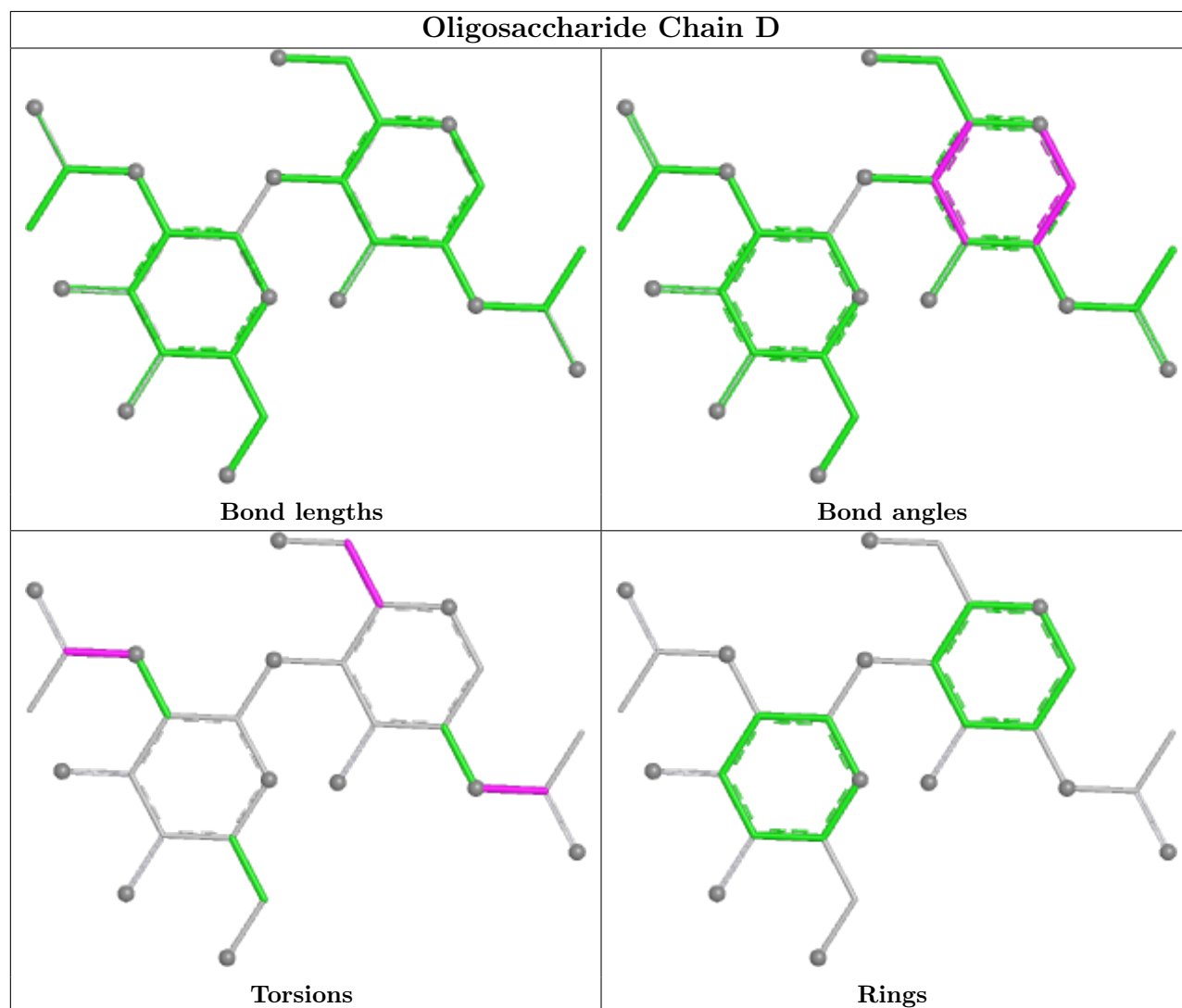
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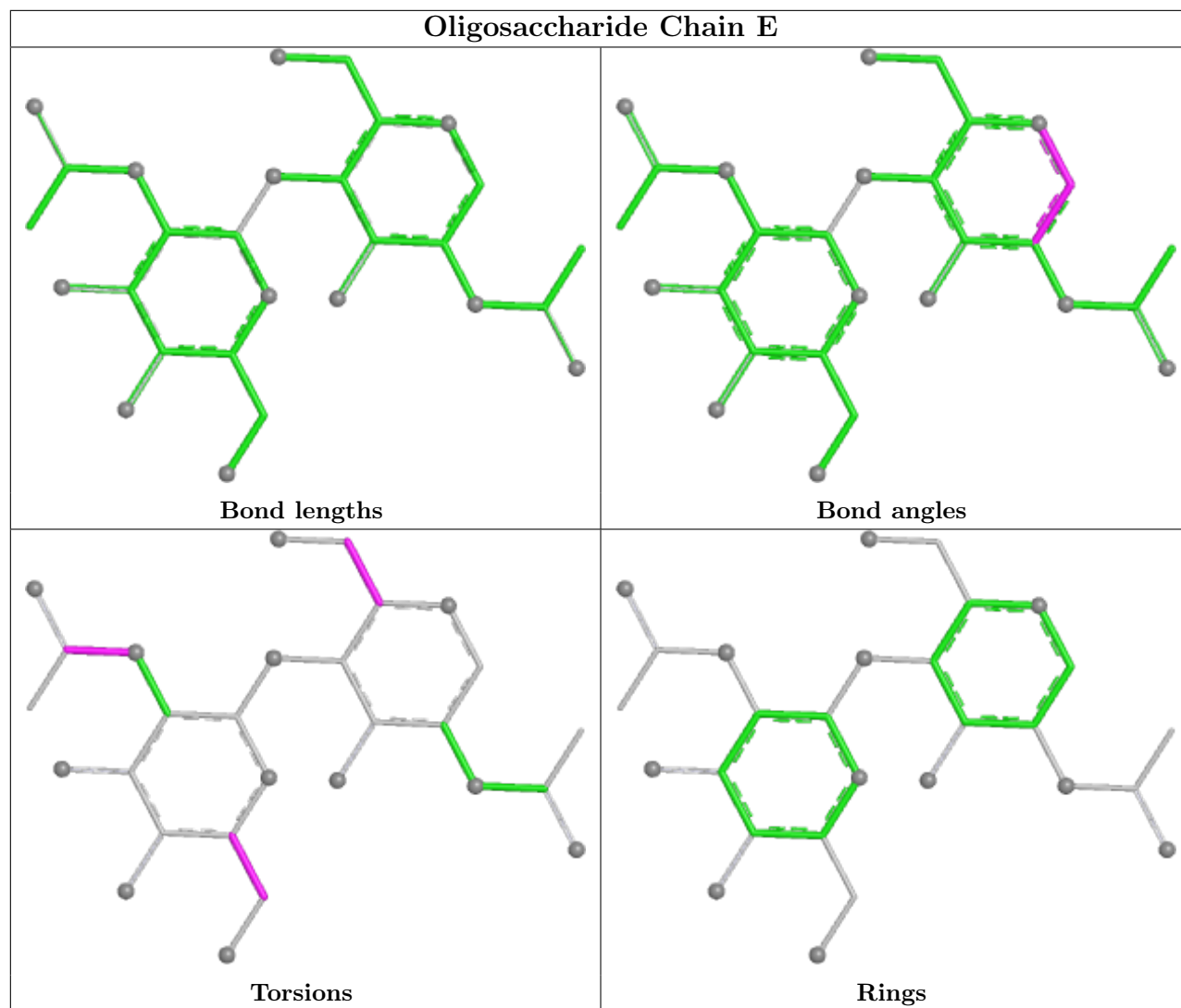


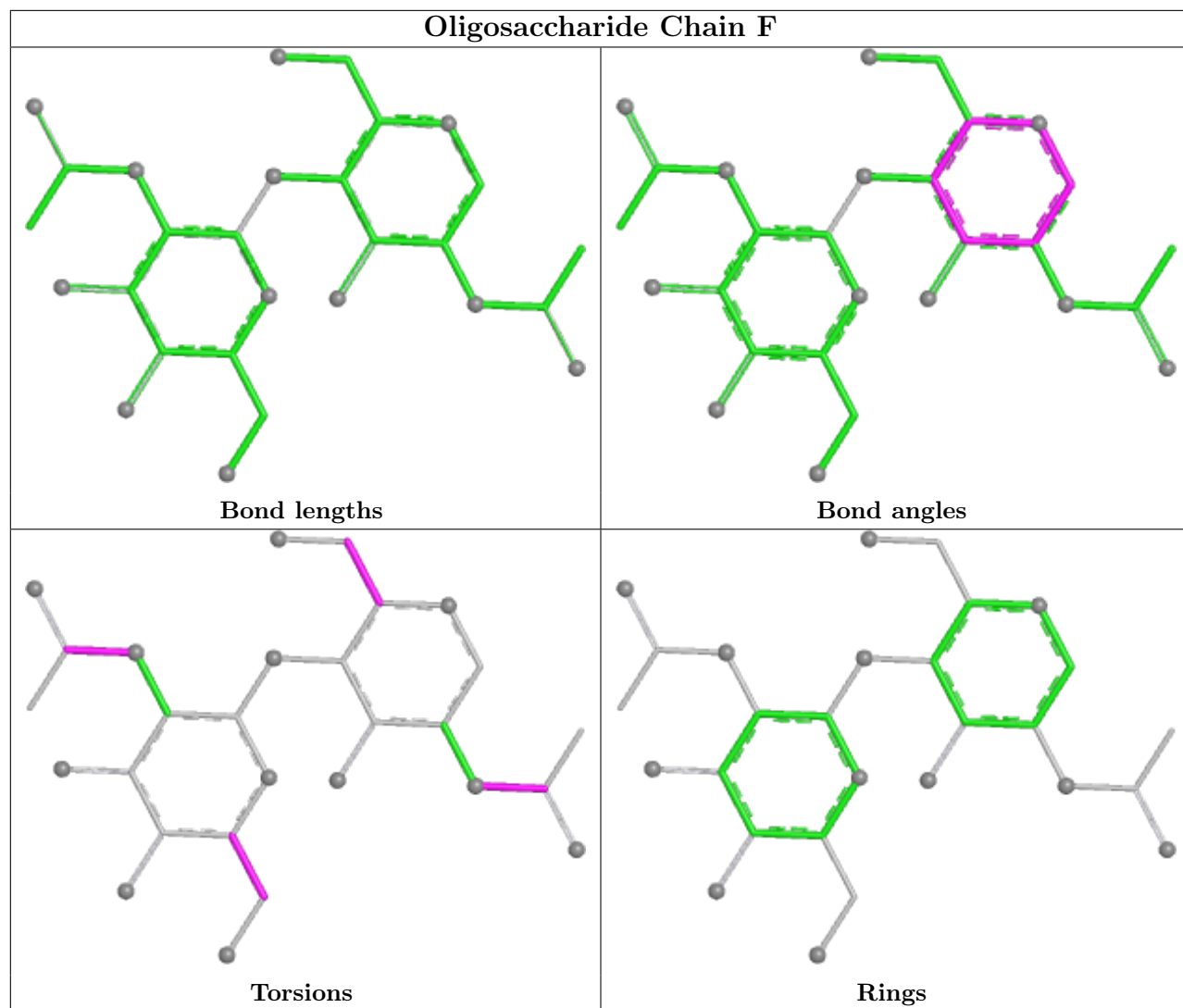
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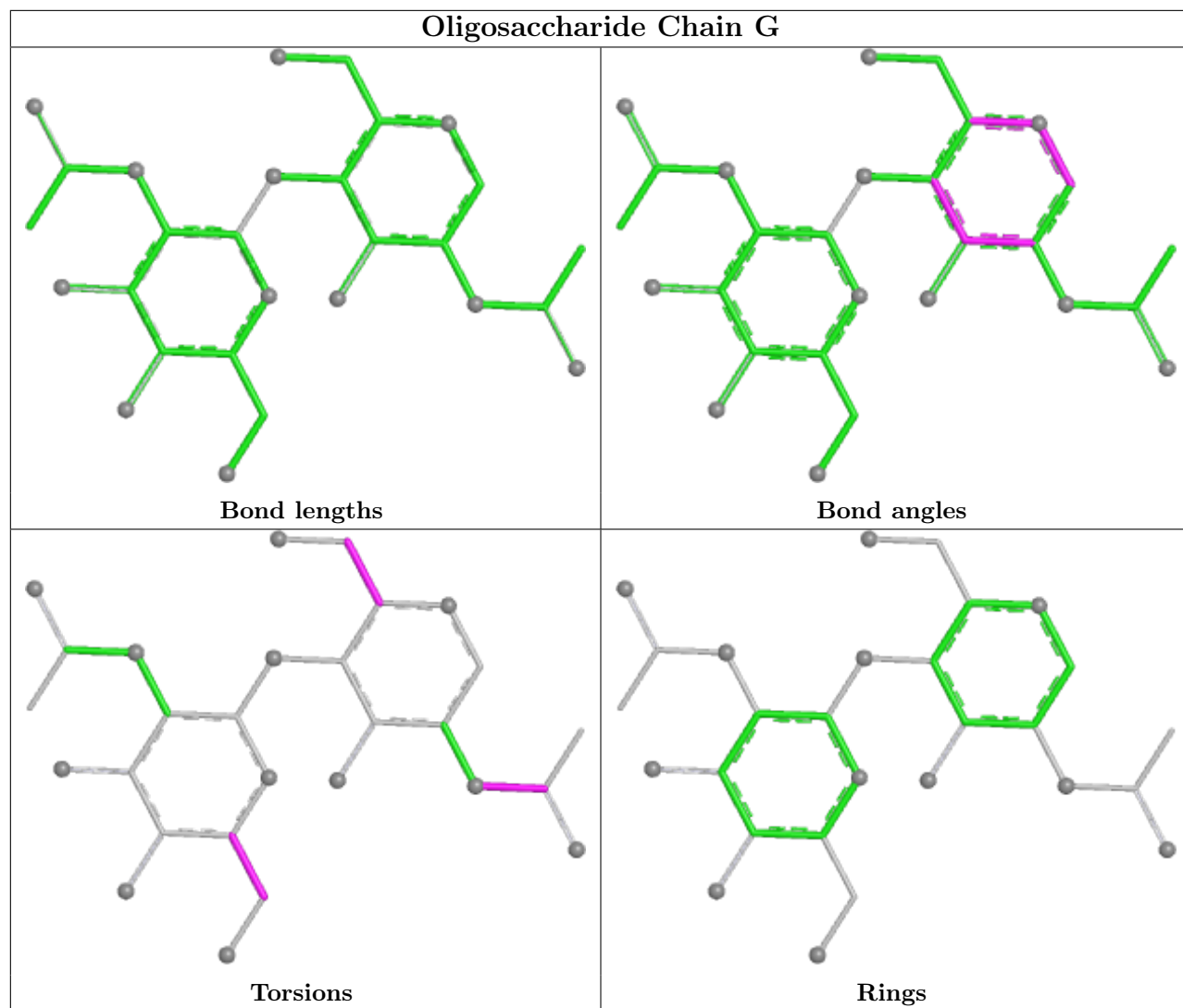
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	2	NAG	1	0
3	M	2	NAG	1	0
3	K	1	NAG	6	0
3	M	1	NAG	1	0
3	U	1	NAG	1	0
3	P	1	NAG	1	0

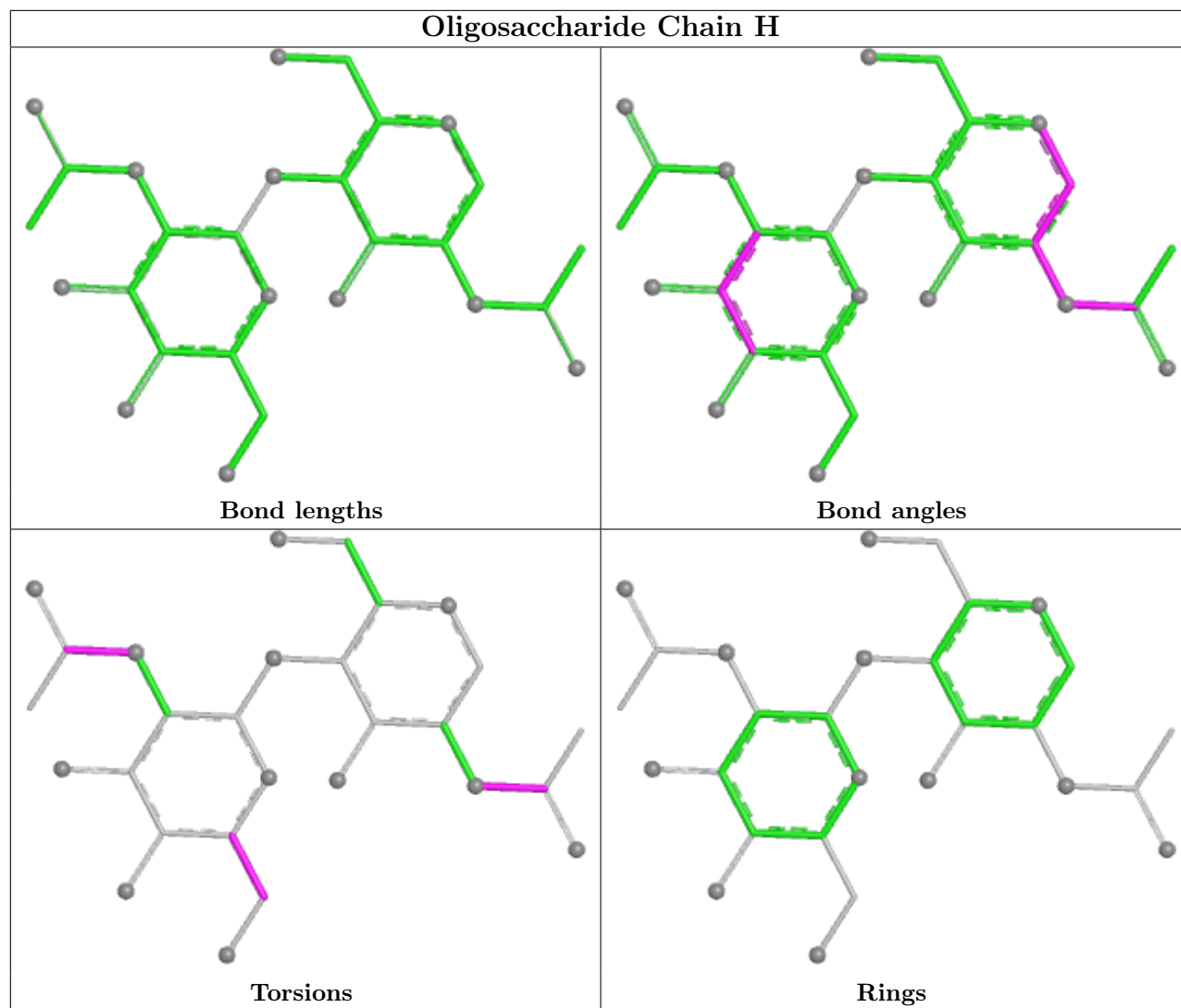
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

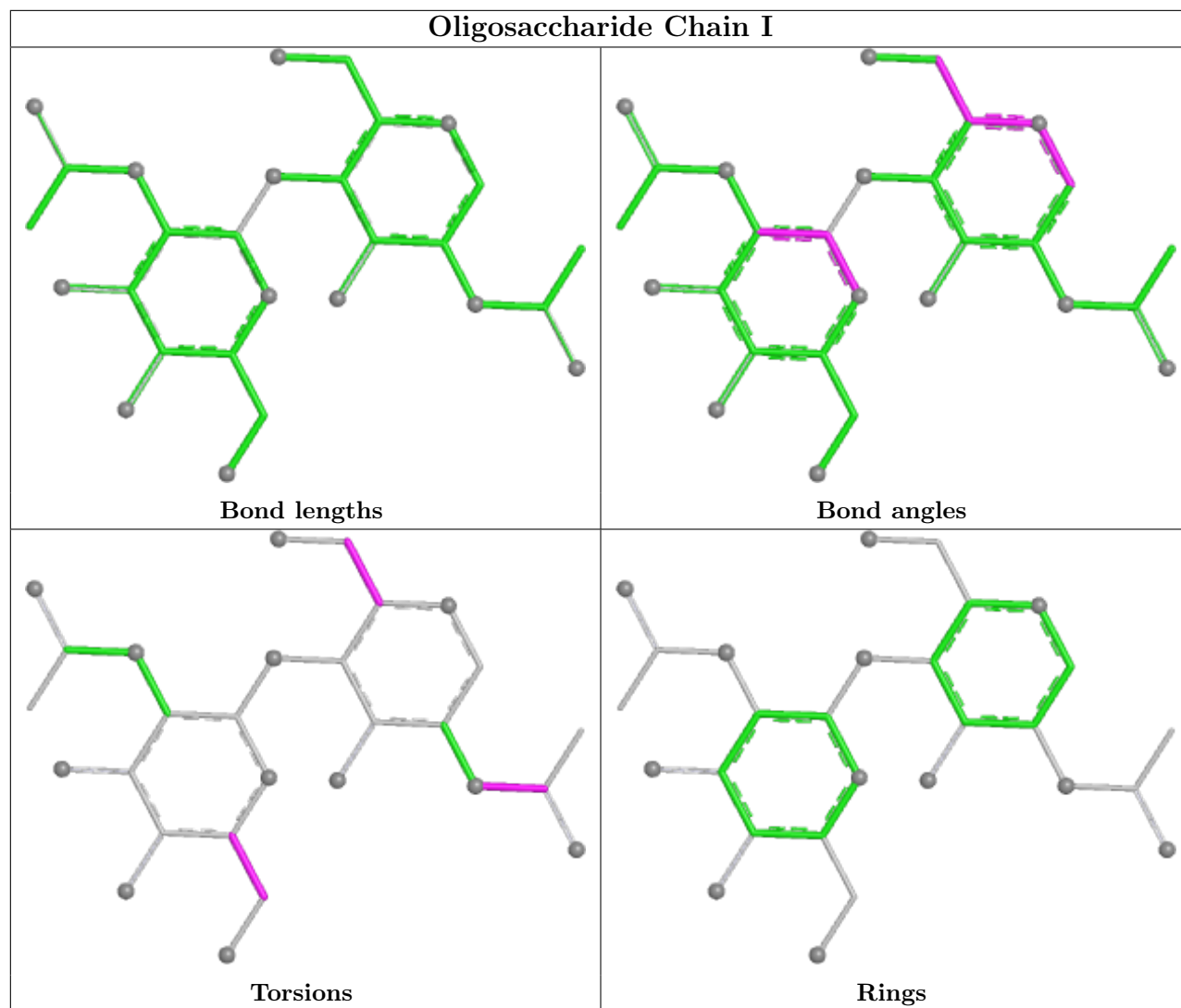


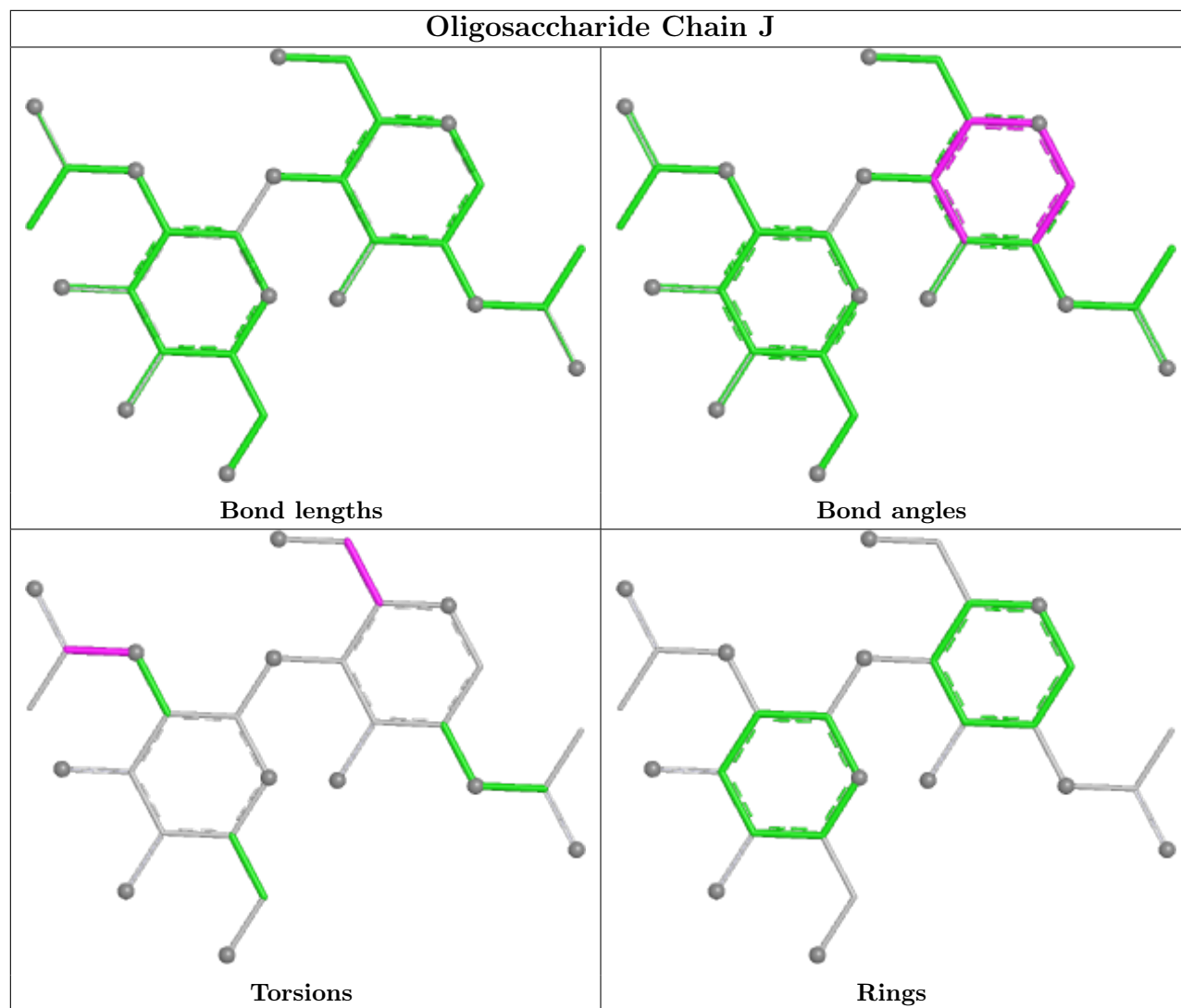


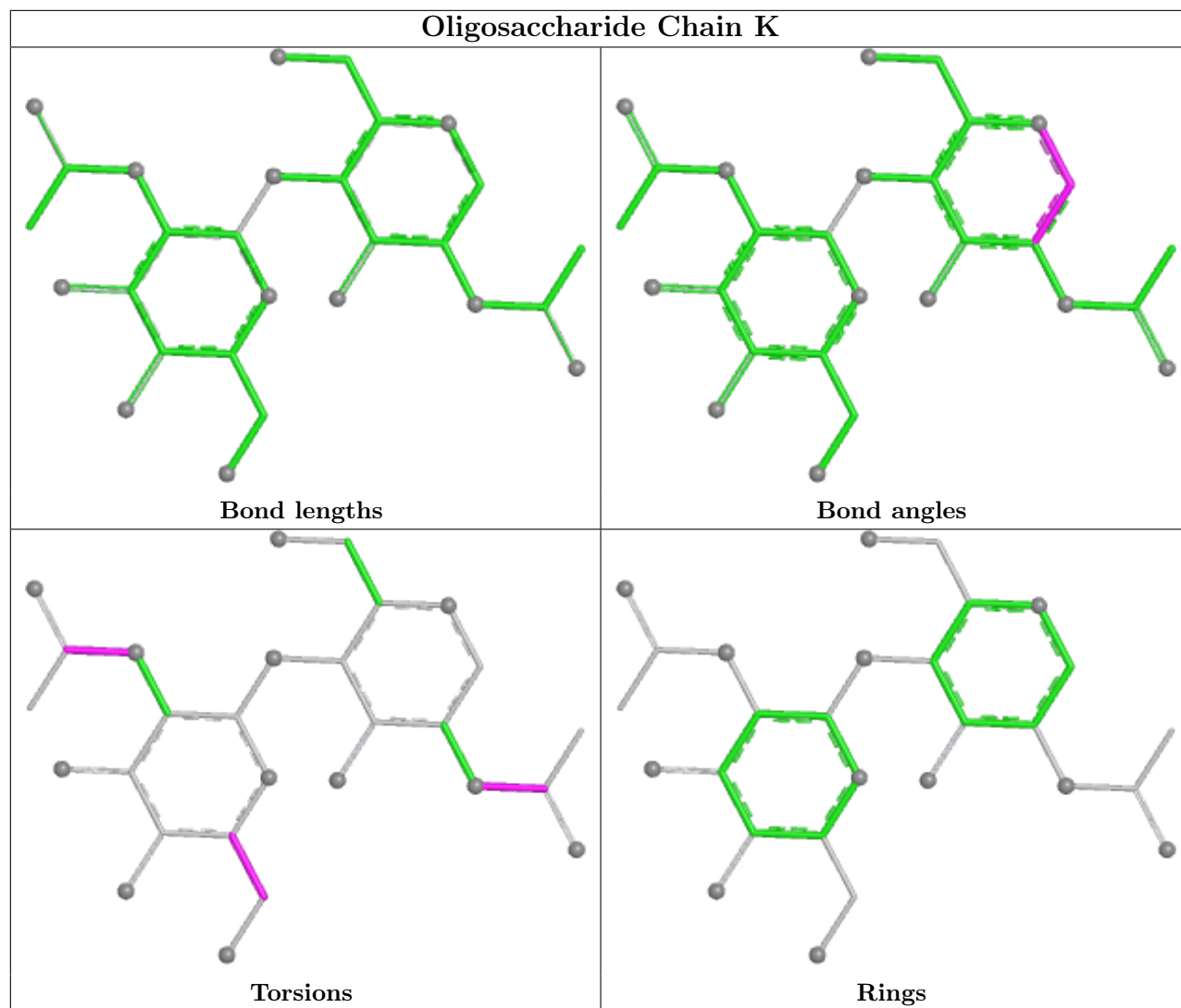




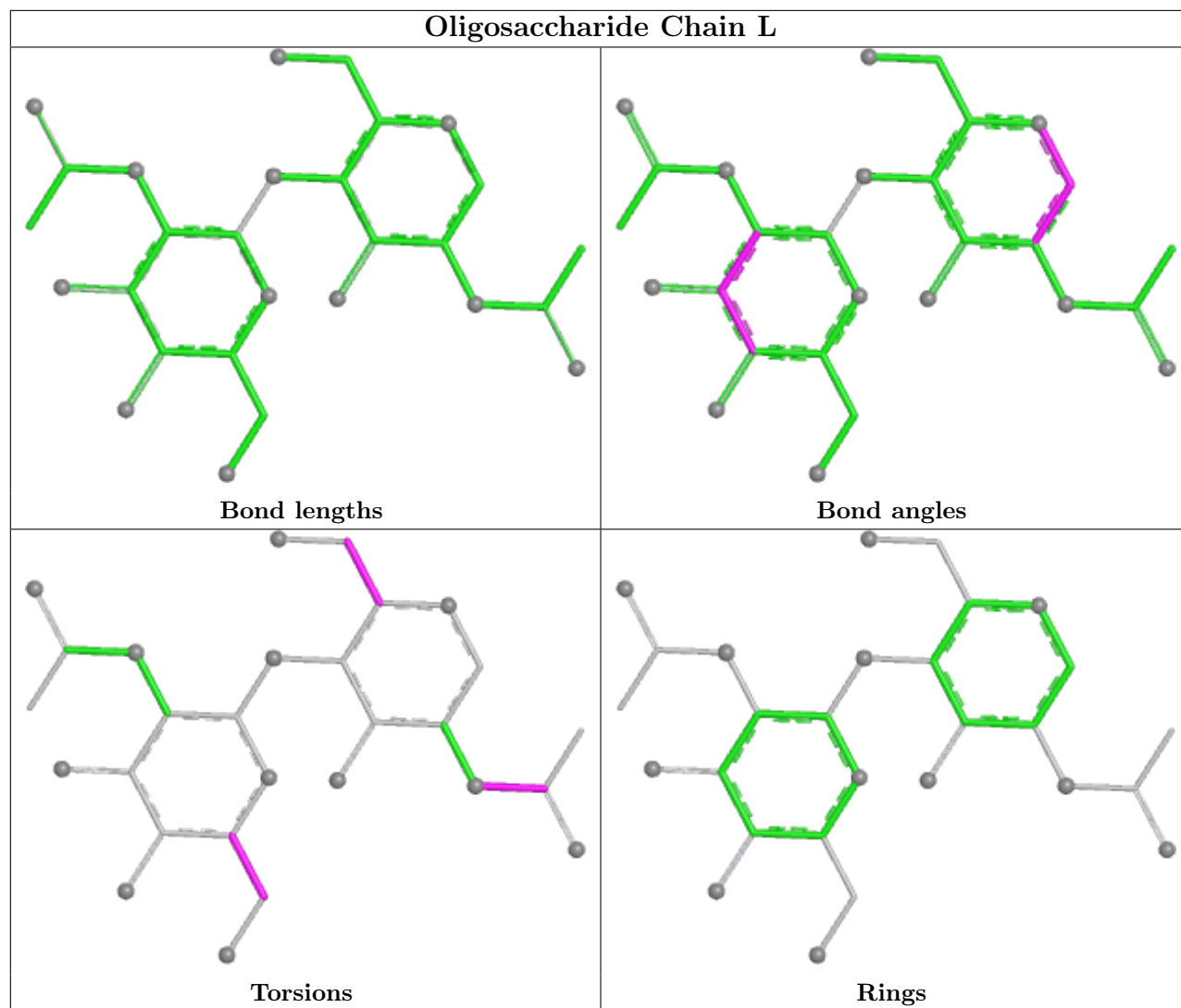


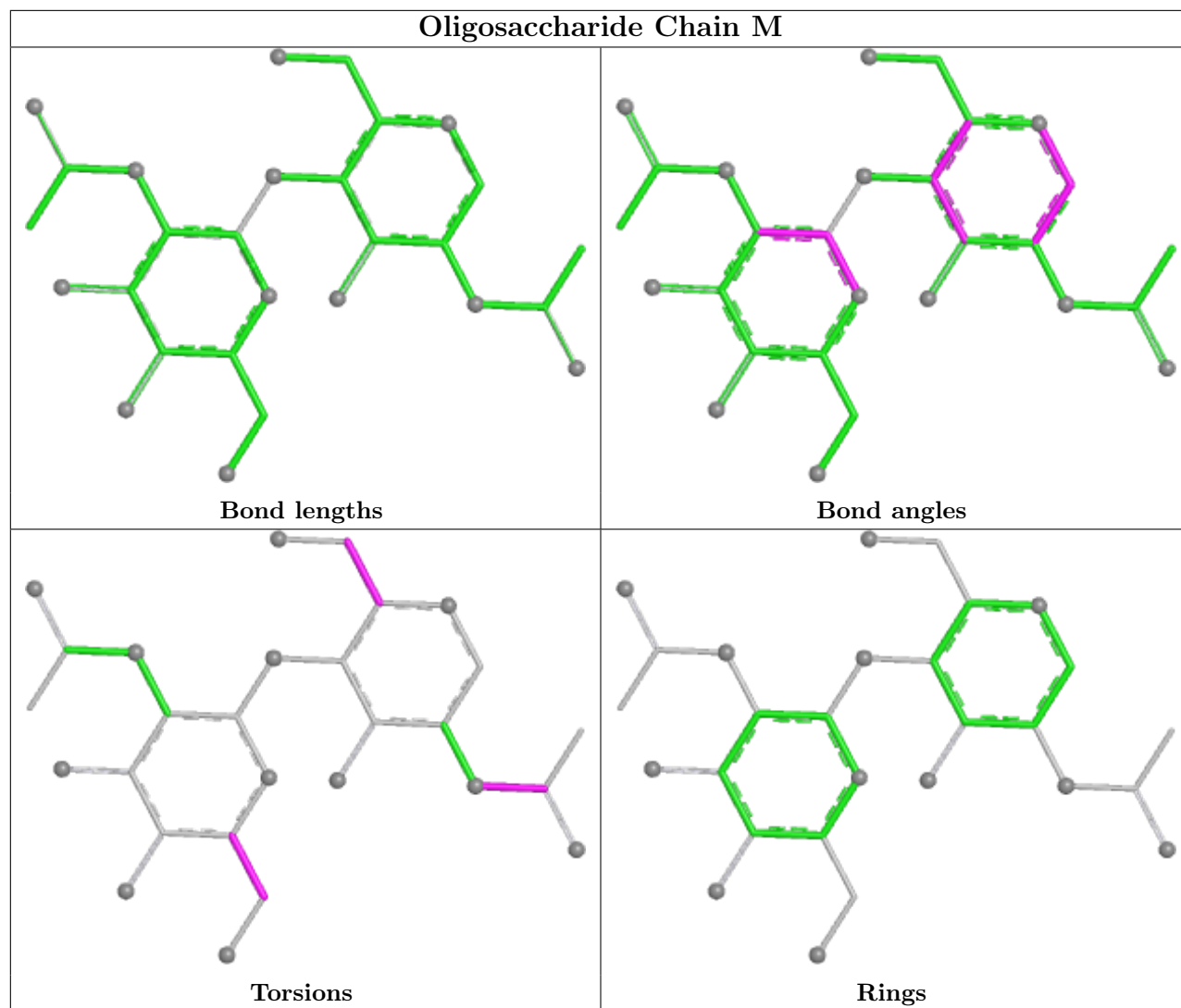


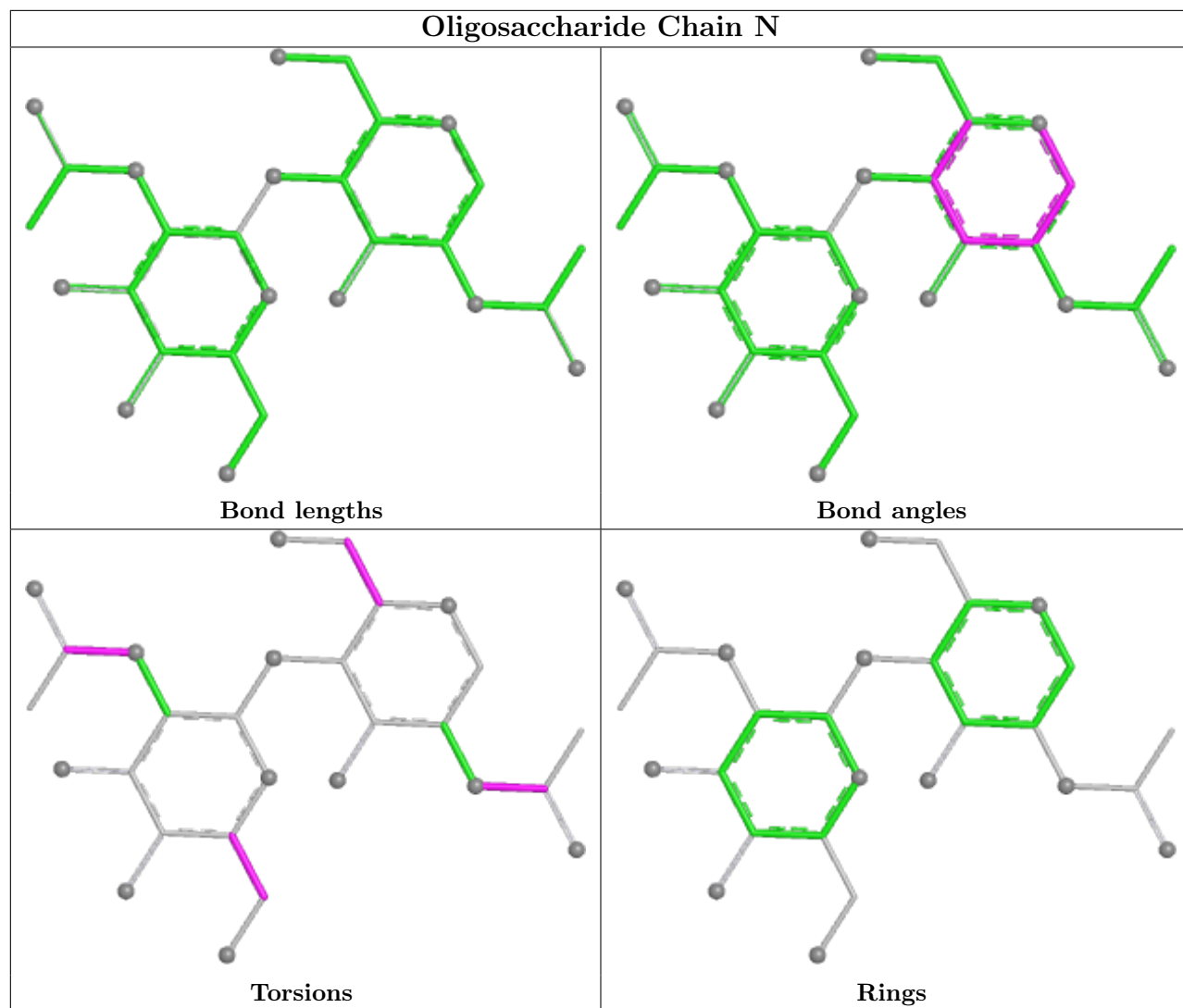


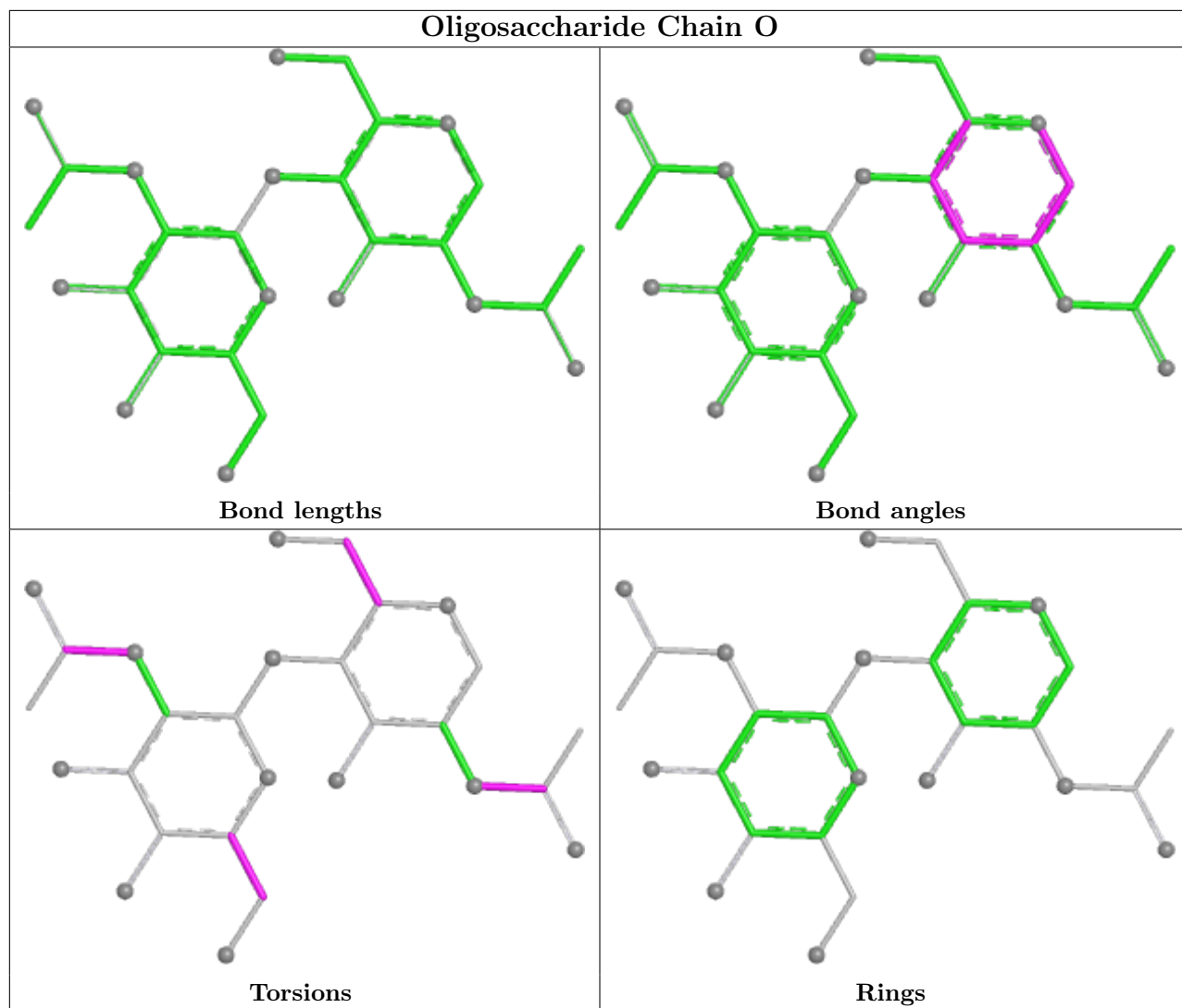


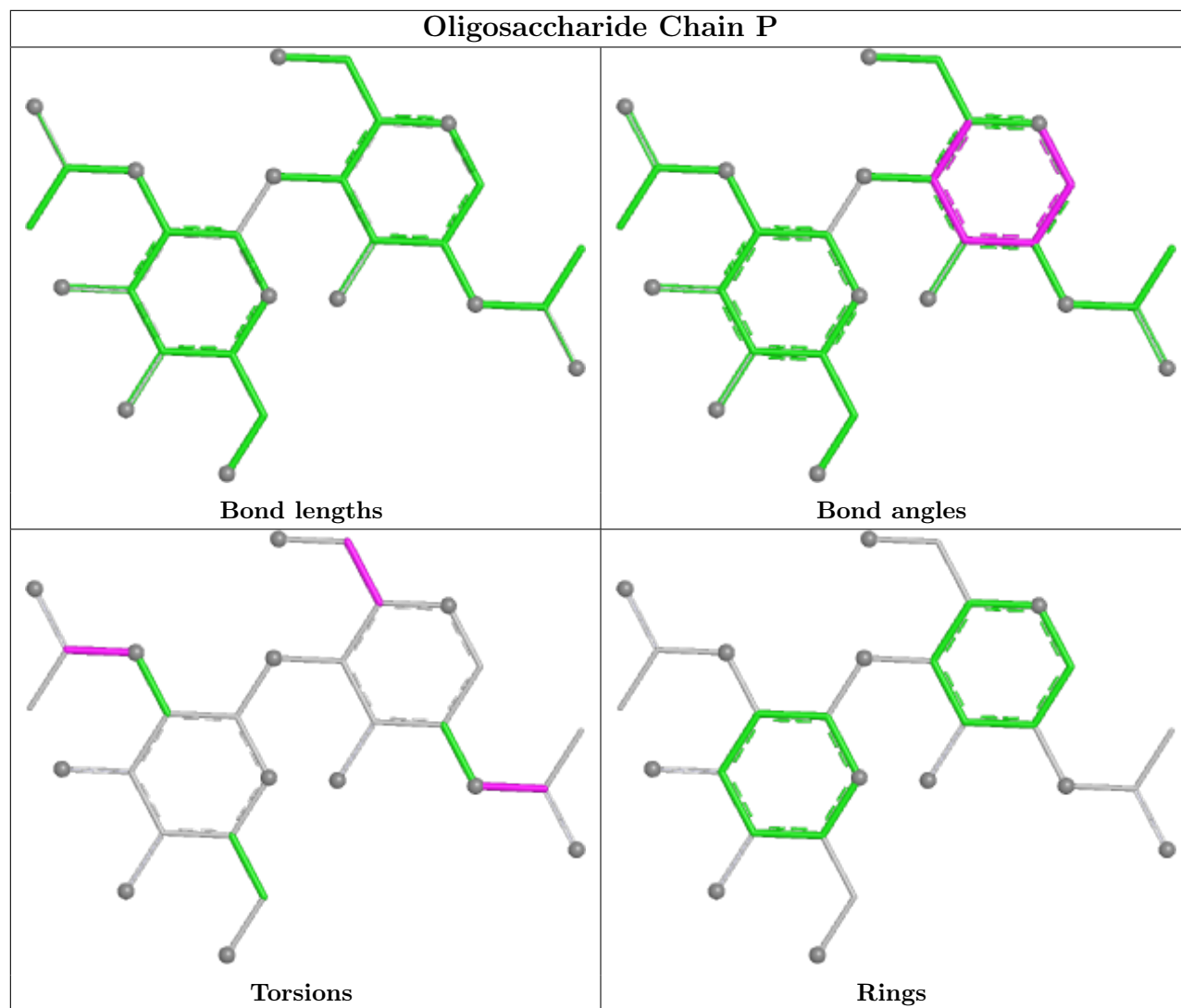


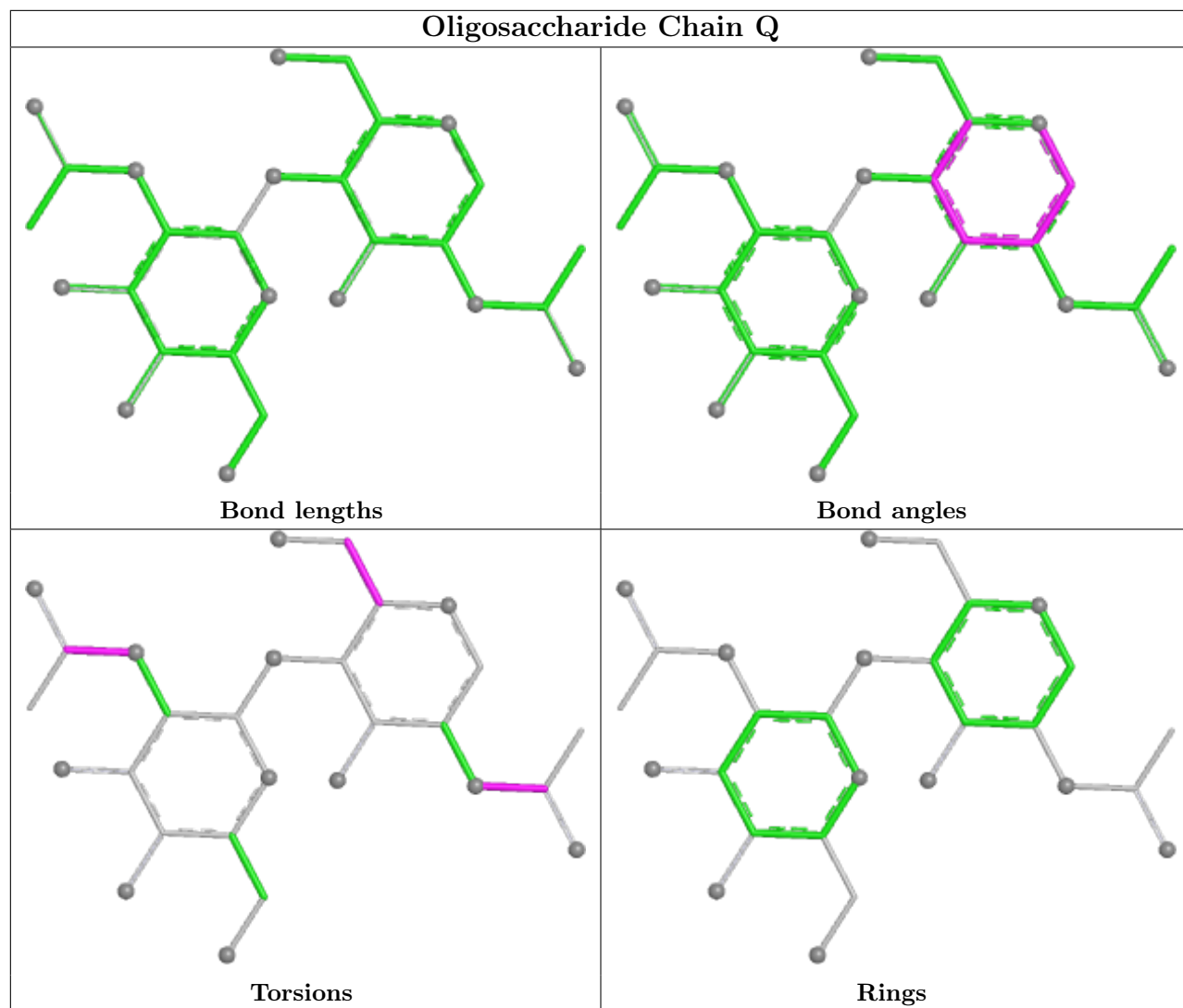


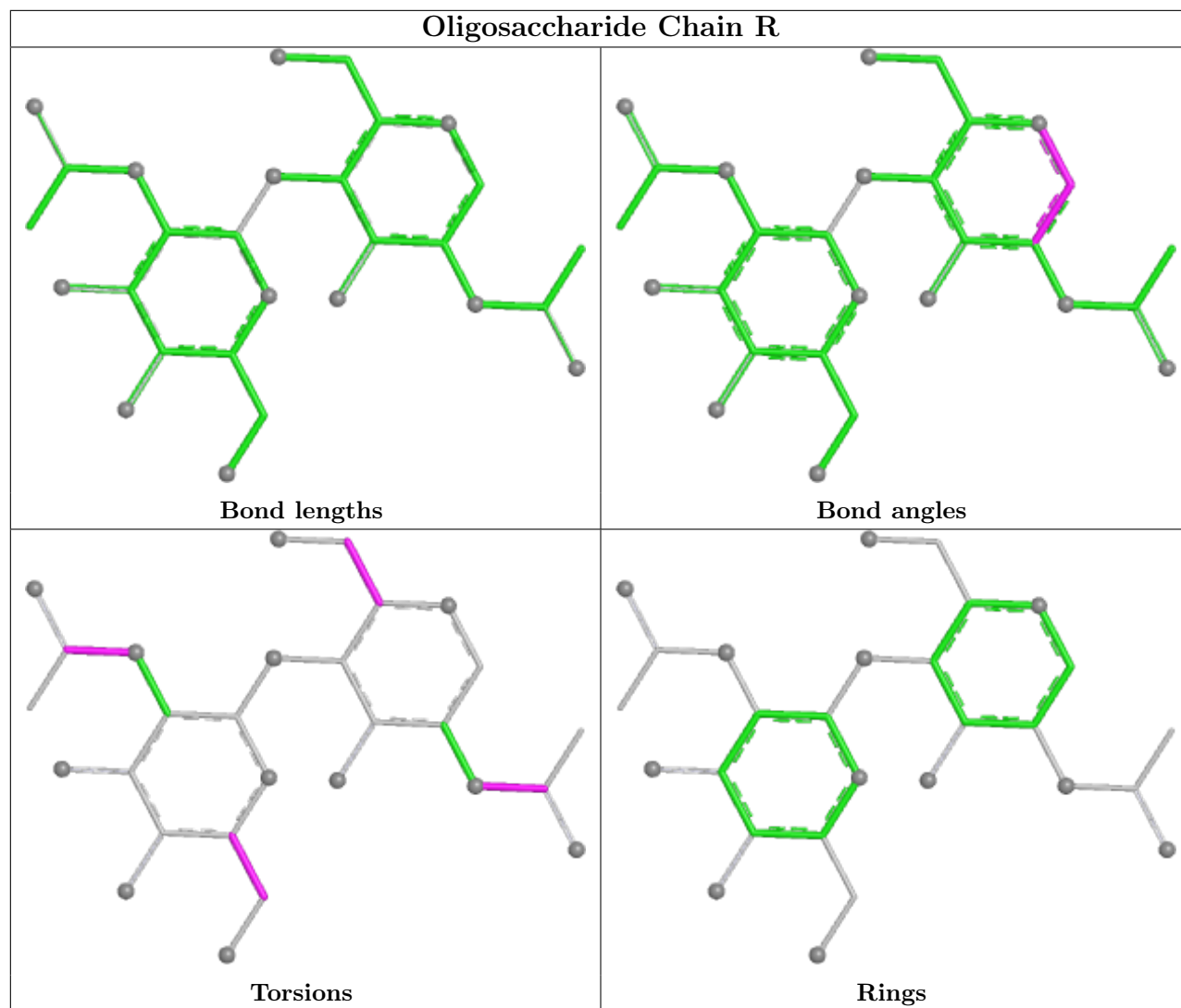


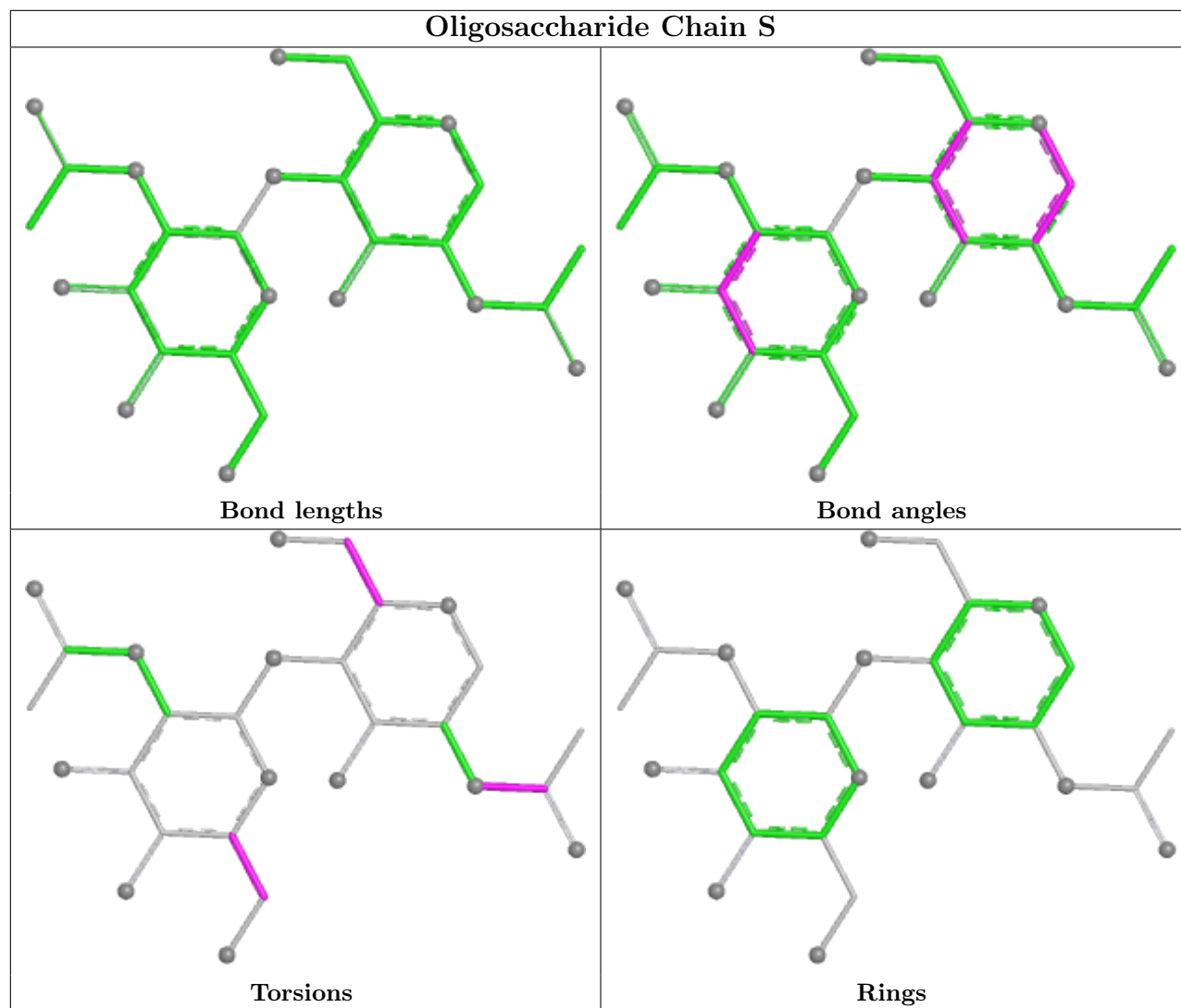




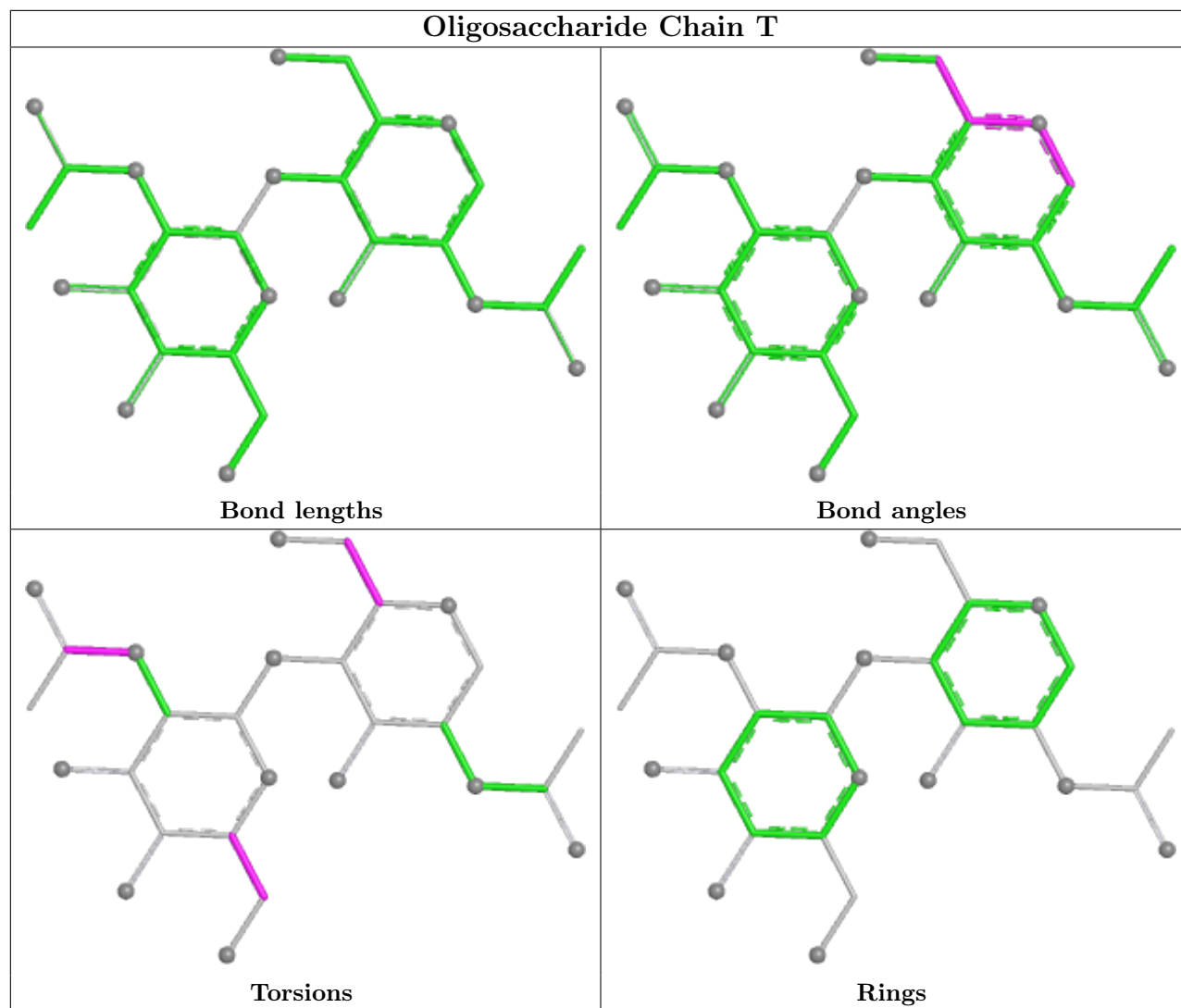


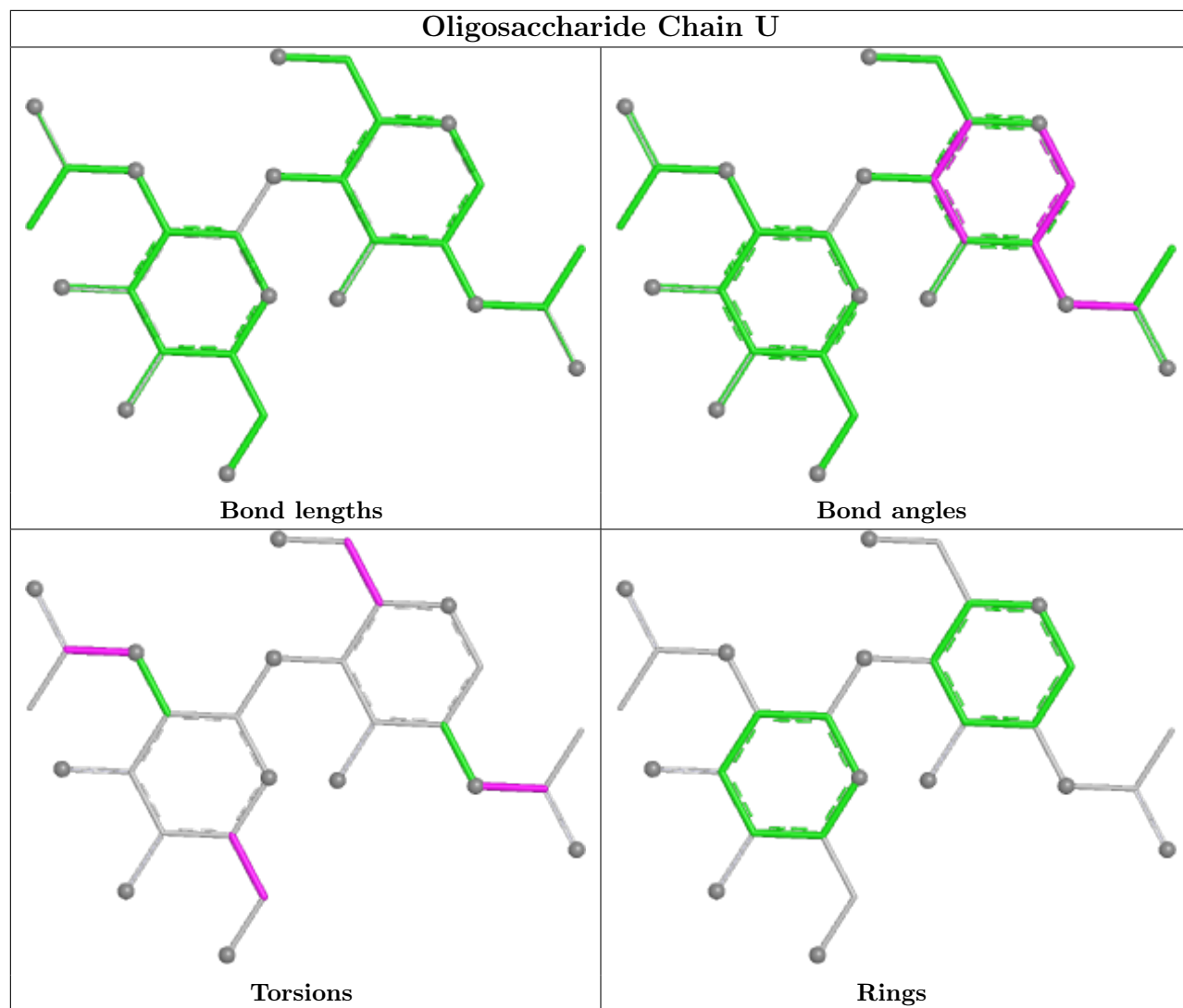


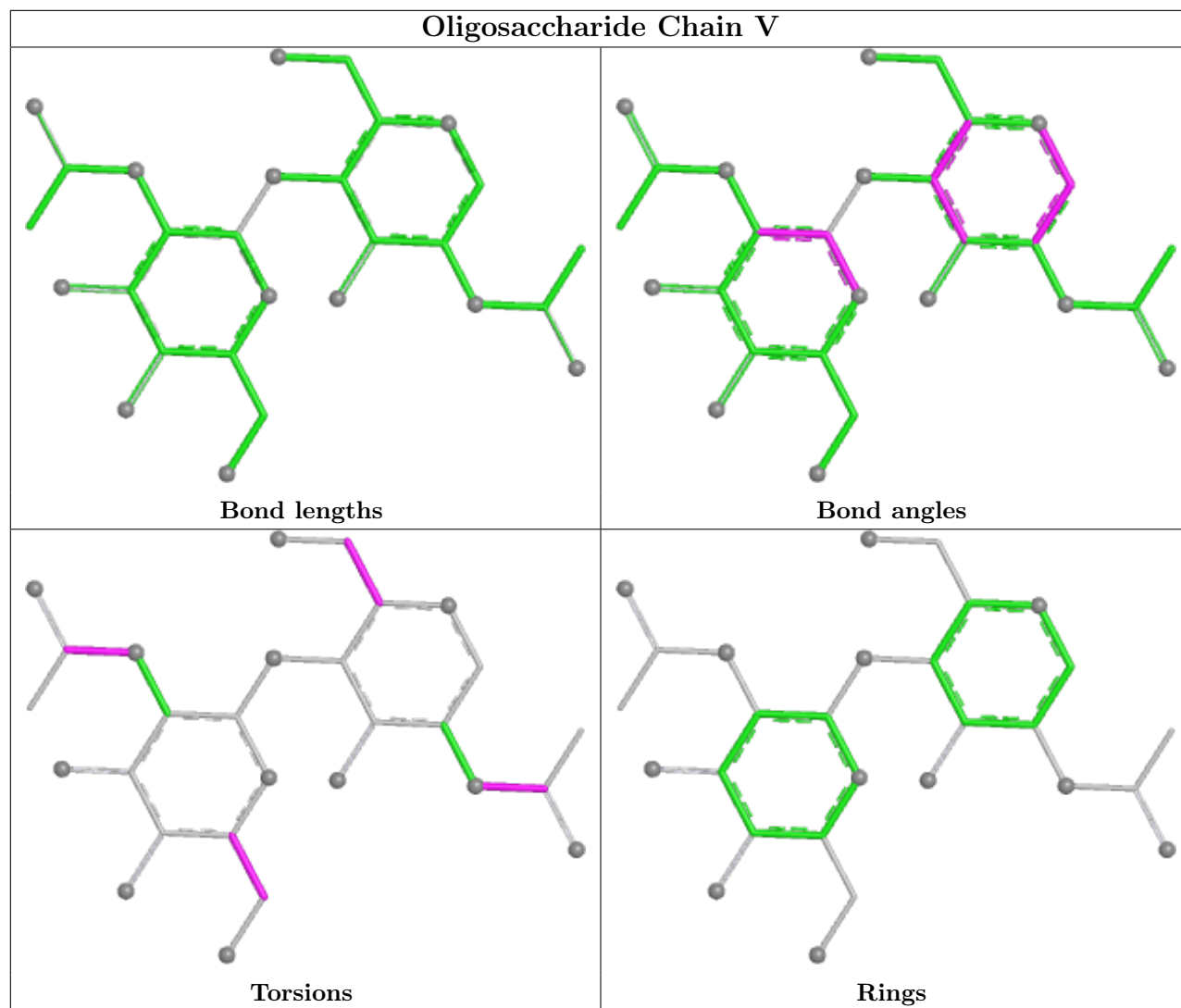


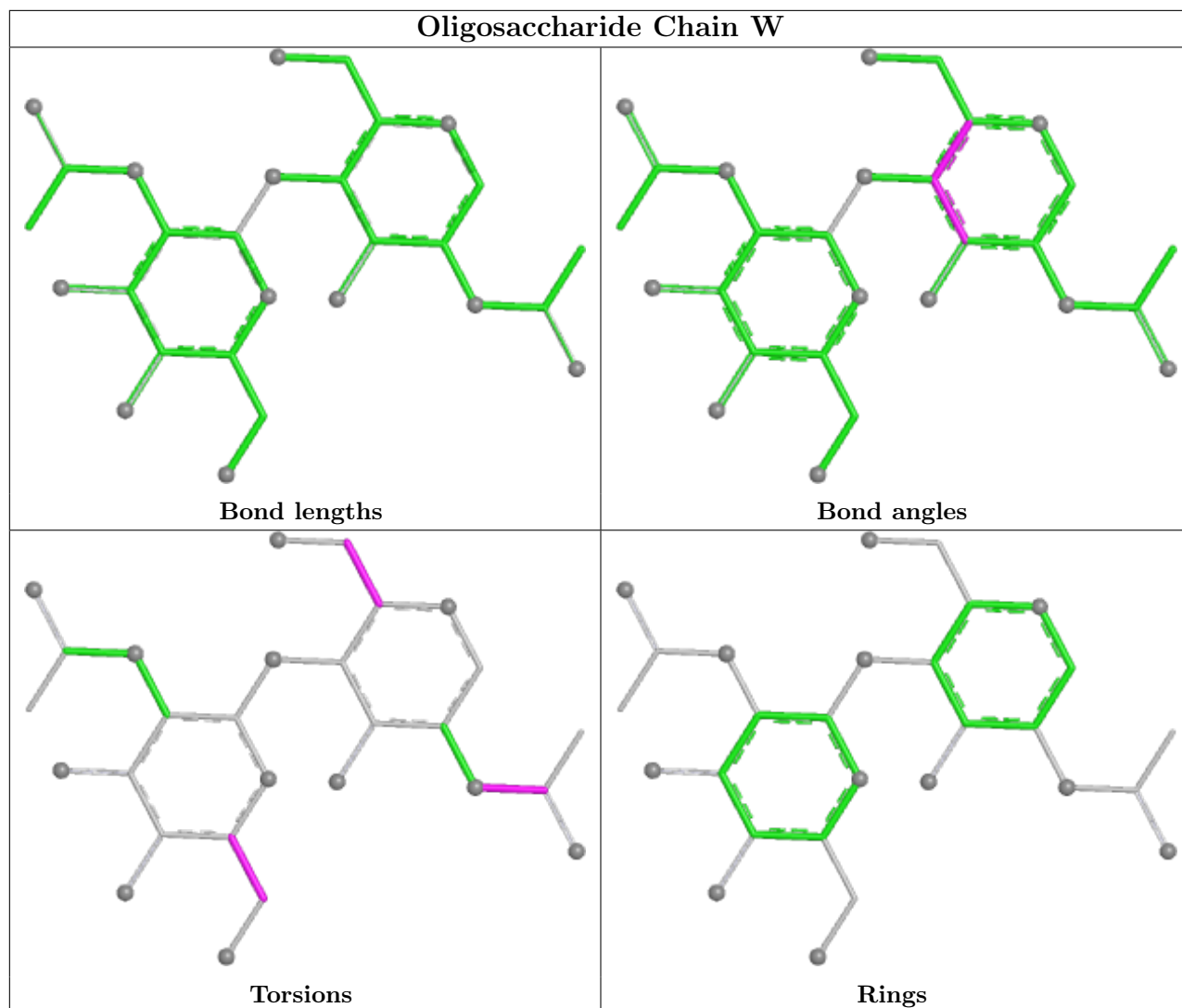












## 5.6 Ligand geometry [i](#)

26 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	$\# Z  > 2$
4	NAG	A	1306	1	14,14,15	0.36	0	17,19,21	0.81	0
4	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	0.59	0
4	NAG	B	1302	1	14,14,15	0.34	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1406	1	14,14,15	0.46	0	17,19,21	0.80	0
4	NAG	A	1307	1	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
4	NAG	A	1308	1	14,14,15	0.39	0	17,19,21	0.87	1 (5%)
4	NAG	B	1305	1	14,14,15	0.41	0	17,19,21	0.75	1 (5%)
4	NAG	B	1307	1	14,14,15	0.39	0	17,19,21	0.56	0
4	NAG	C	1405	1	14,14,15	0.61	1 (7%)	17,19,21	1.18	2 (11%)
4	NAG	C	1402	1	14,14,15	0.44	0	17,19,21	0.82	0
4	NAG	C	1403	1	14,14,15	0.42	0	17,19,21	0.62	0
4	NAG	A	1302	1	14,14,15	0.44	0	17,19,21	0.60	0
4	NAG	B	1308	1	14,14,15	0.55	0	17,19,21	0.89	0
4	NAG	B	1309	1	14,14,15	0.46	0	17,19,21	0.74	0
4	NAG	B	1306	1	14,14,15	0.42	0	17,19,21	0.62	0
4	NAG	C	1401	1	14,14,15	0.66	0	17,19,21	0.95	1 (5%)
4	NAG	C	1408	1	14,14,15	0.44	0	17,19,21	0.90	0
4	NAG	B	1304	1	14,14,15	0.35	0	17,19,21	1.25	2 (11%)
4	NAG	B	1310	1	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
4	NAG	B	1301	1	14,14,15	0.41	0	17,19,21	0.68	0
4	NAG	A	1305	1	14,14,15	0.41	0	17,19,21	0.73	0
4	NAG	C	1407	1	14,14,15	0.34	0	17,19,21	0.71	1 (5%)
4	NAG	B	1303	1	14,14,15	0.36	0	17,19,21	0.51	0
4	NAG	A	1301	1	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	A	1304	1	14,14,15	0.49	0	17,19,21	0.65	0
4	NAG	C	1404	1	14,14,15	0.35	0	17,19,21	1.18	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1402	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1405	NAG	C1-C2	2.04	1.55	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1405	NAG	C2-N2-C7	3.40	127.75	122.90
4	B	1304	NAG	O5-C1-C2	-3.34	106.01	111.29
4	C	1404	NAG	O5-C1-C2	-3.28	106.11	111.29
4	B	1304	NAG	C1-O5-C5	2.83	116.02	112.19
4	C	1404	NAG	C1-O5-C5	2.80	115.99	112.19

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1305	NAG	O7-C7-N2-C2
4	A	1306	NAG	C8-C7-N2-C2
4	A	1306	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	NAG	1	0
4	C	1401	NAG	10	0
4	B	1310	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.

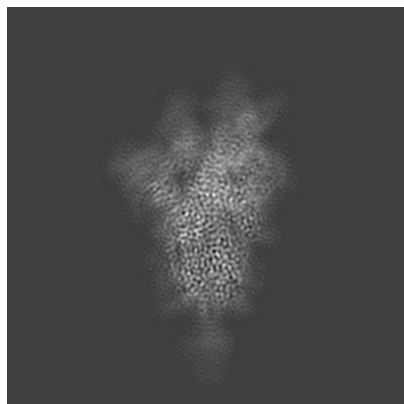
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14544. These allow visual inspection of the internal detail of the map and identification of artifacts.

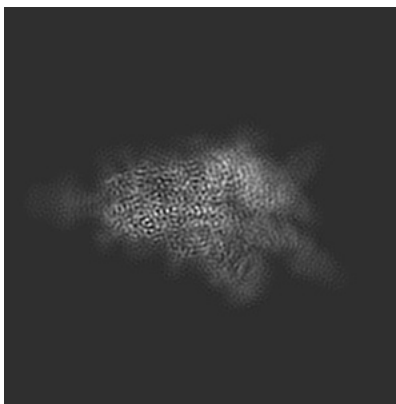
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

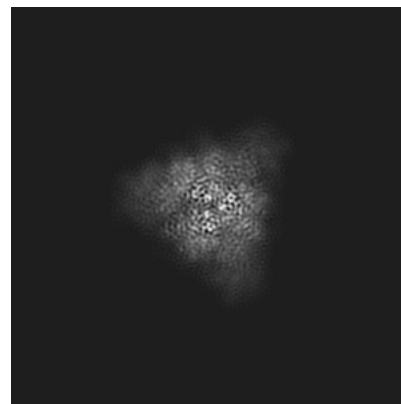
#### 6.1.1 Primary map



X

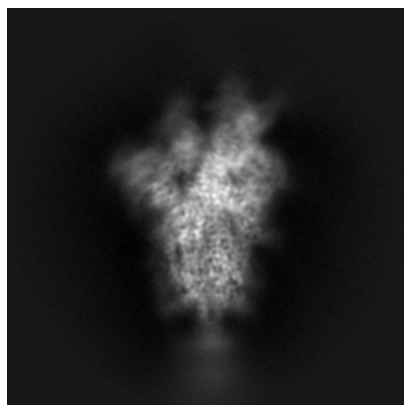


Y

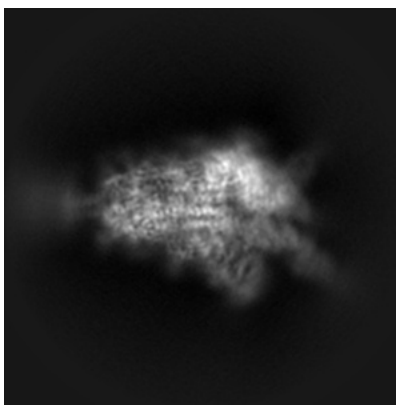


Z

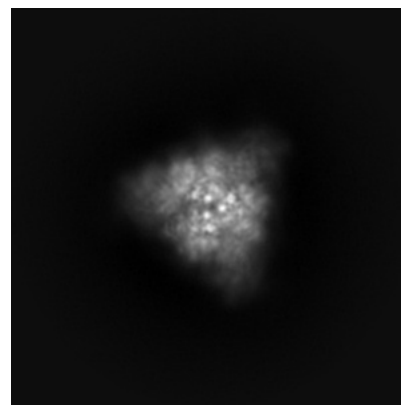
#### 6.1.2 Raw map



X



Y



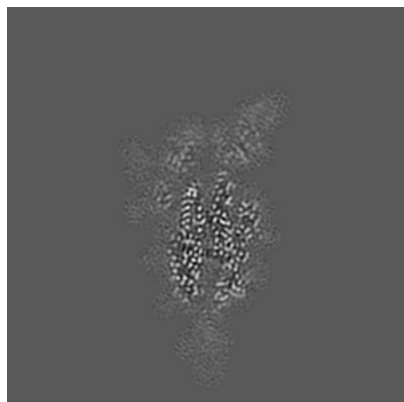
Z

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

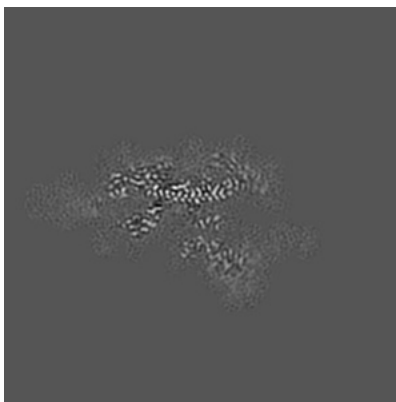


## 6.2 Central slices [i](#)

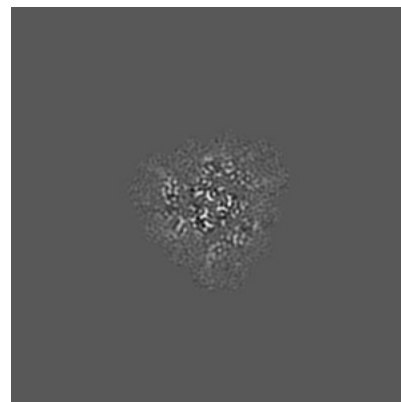
### 6.2.1 Primary map



X Index: 150

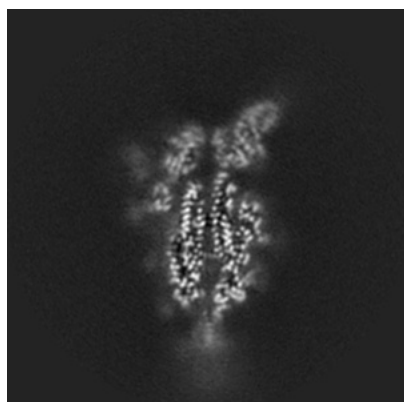


Y Index: 150

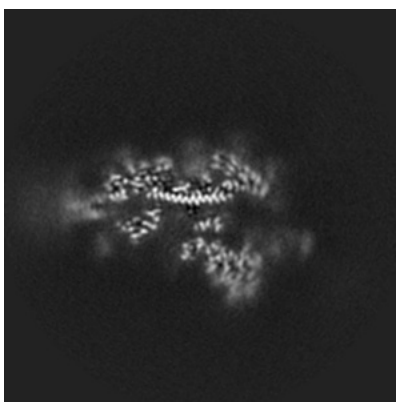


Z Index: 150

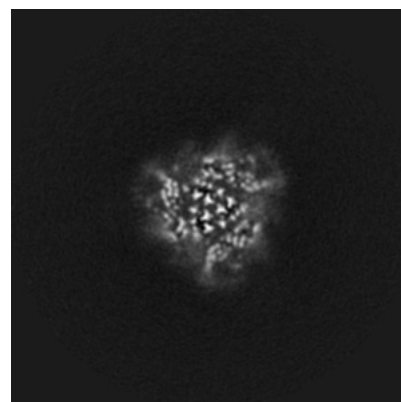
### 6.2.2 Raw map



X Index: 150



Y Index: 150

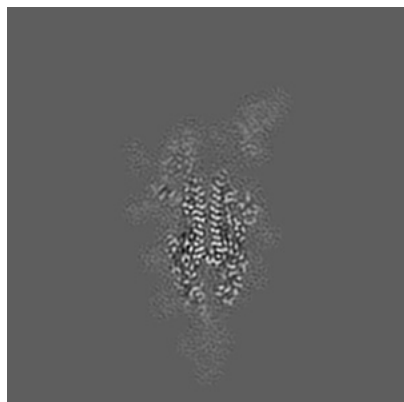


Z Index: 150

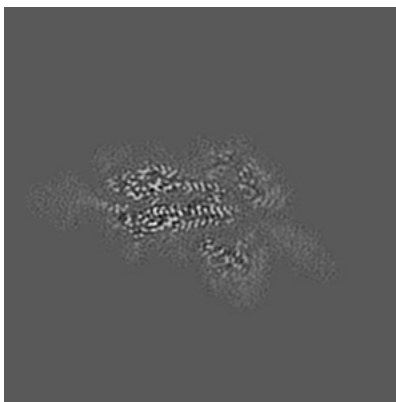
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

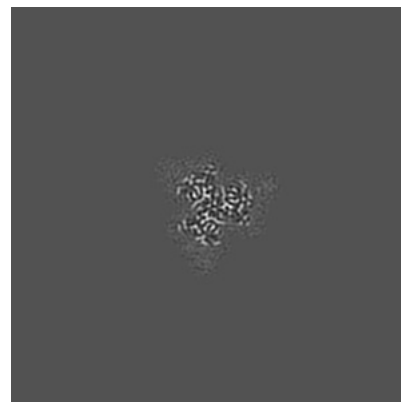
### 6.3.1 Primary map



X Index: 146

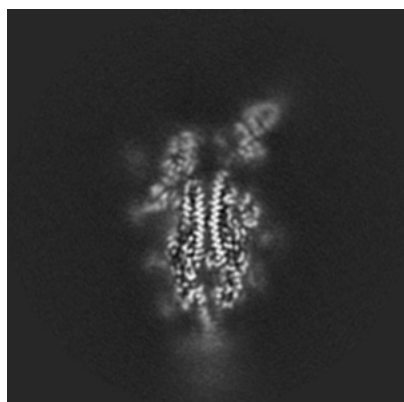


Y Index: 158

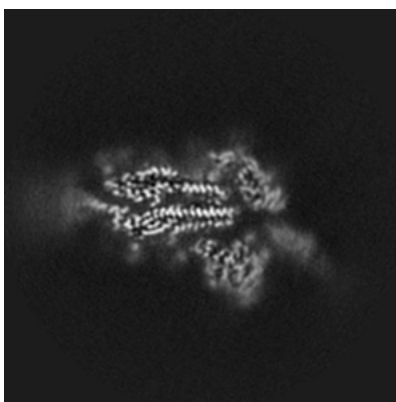


Z Index: 113

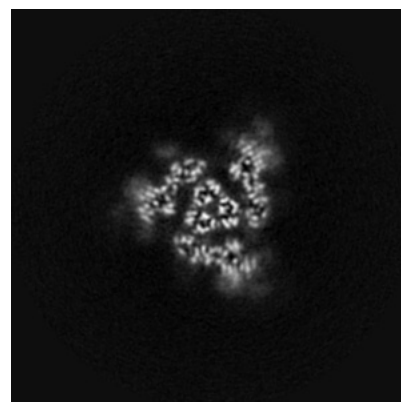
### 6.3.2 Raw map



X Index: 147



Y Index: 157

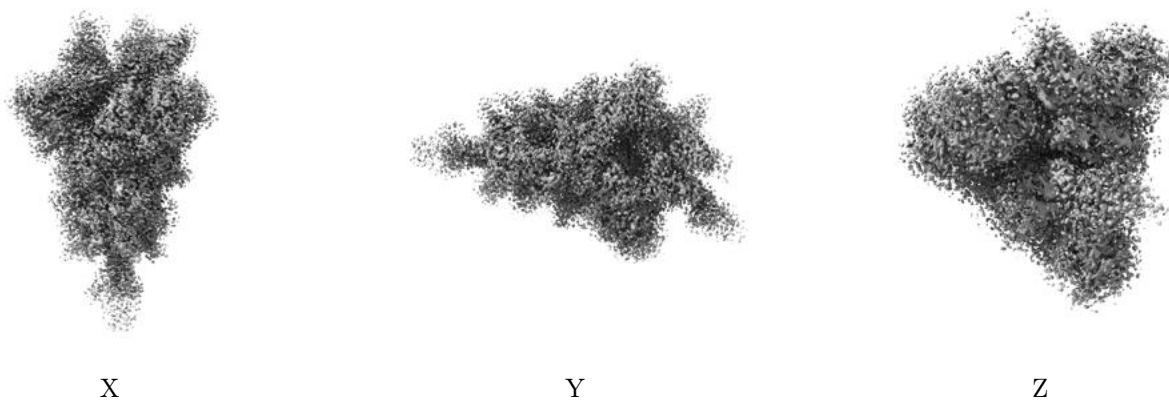


Z Index: 164

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 0.017. 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.

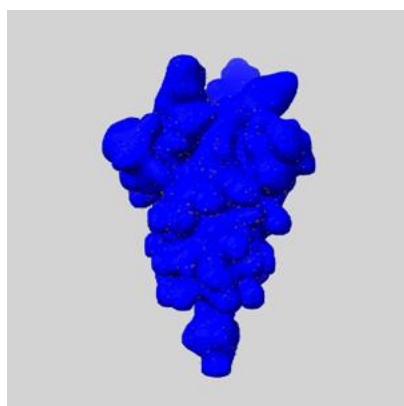
## 6.5 Mask visualisation [i](#)

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

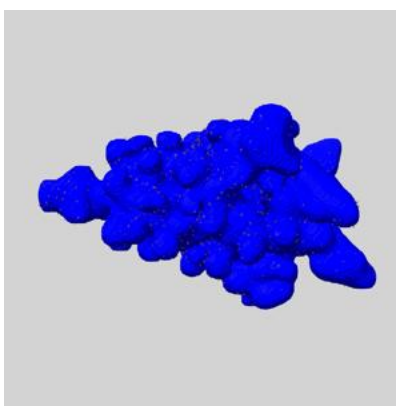
A mask typically either:

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

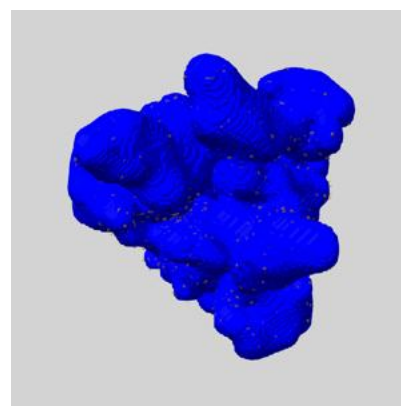
### 6.5.1 emd\_14544\_msk\_1.map [i](#)



X



Y

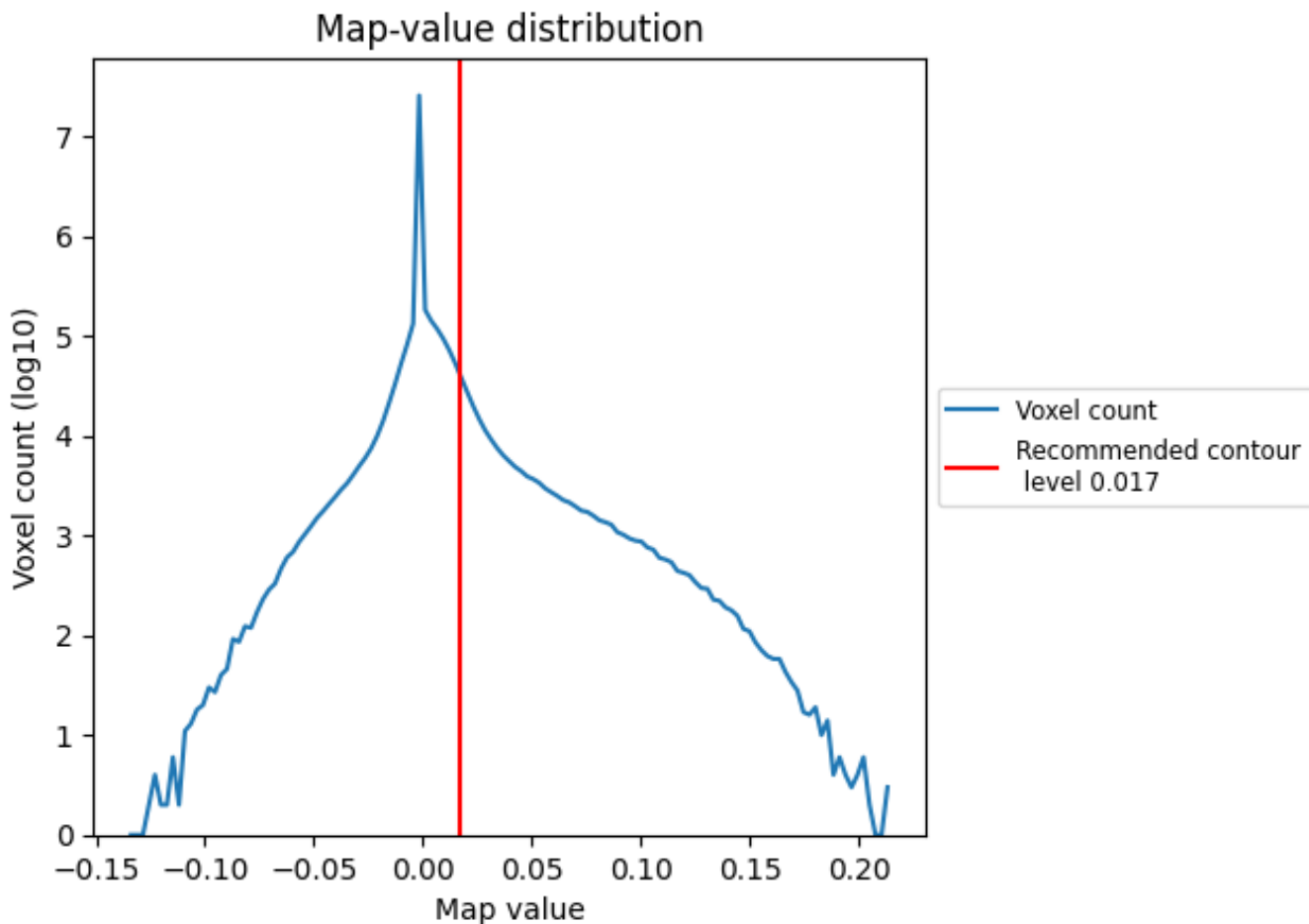


Z

## 7 Map analysis [i](#)

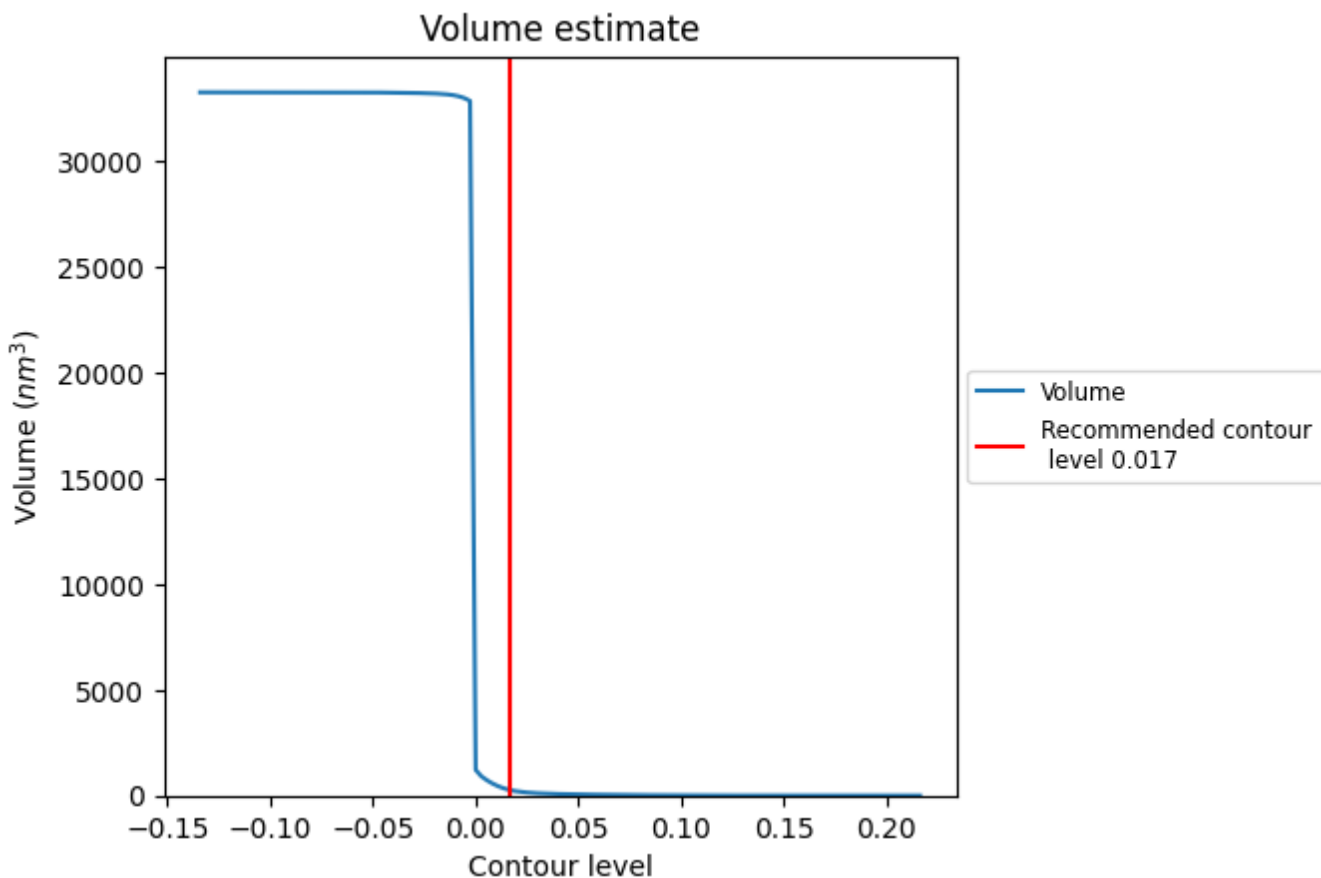
This section contains the results of statistical analysis of the map.

### 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.

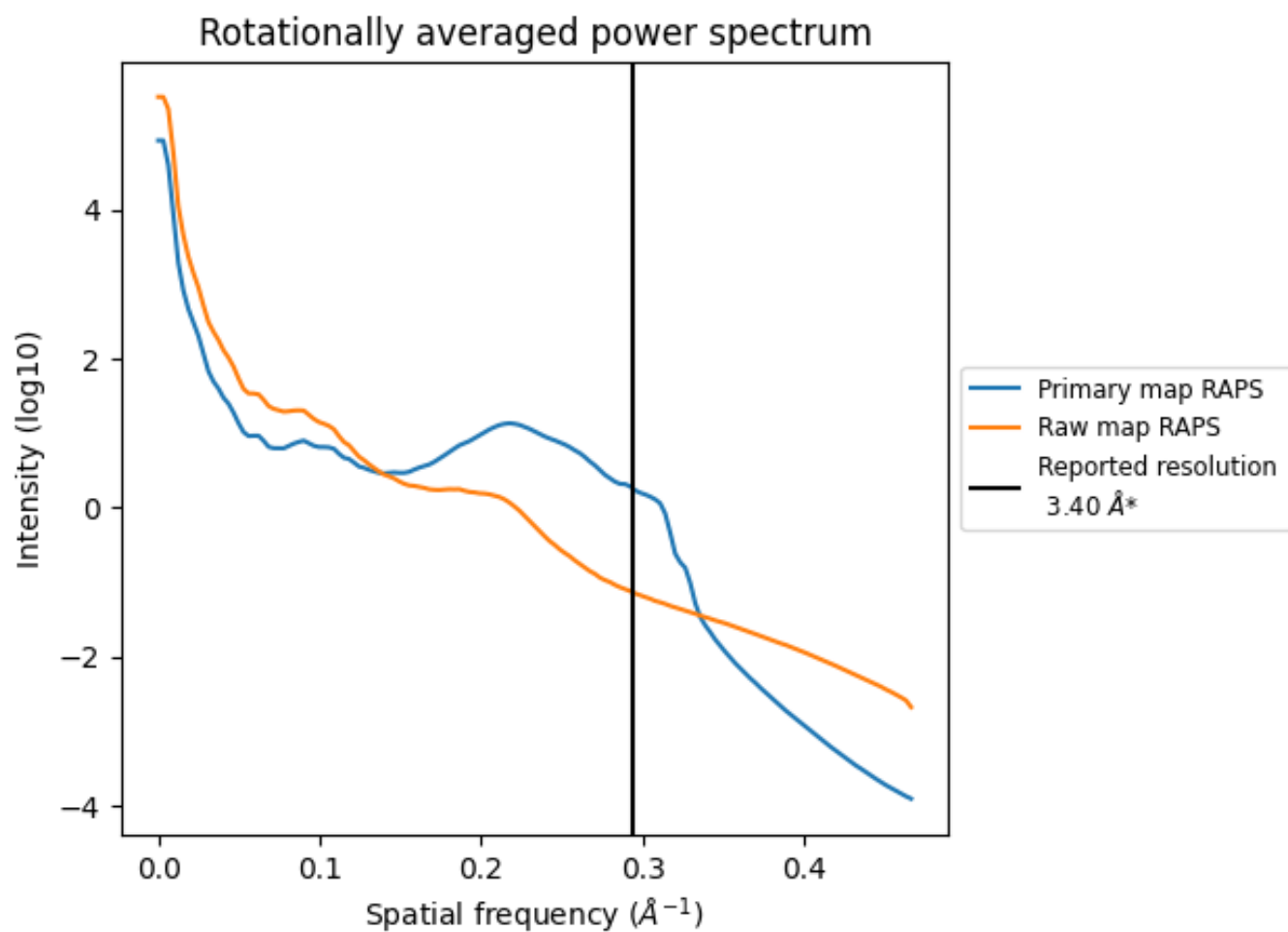
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm<sup>3</sup>; this corresponds to an approximate mass of 233 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

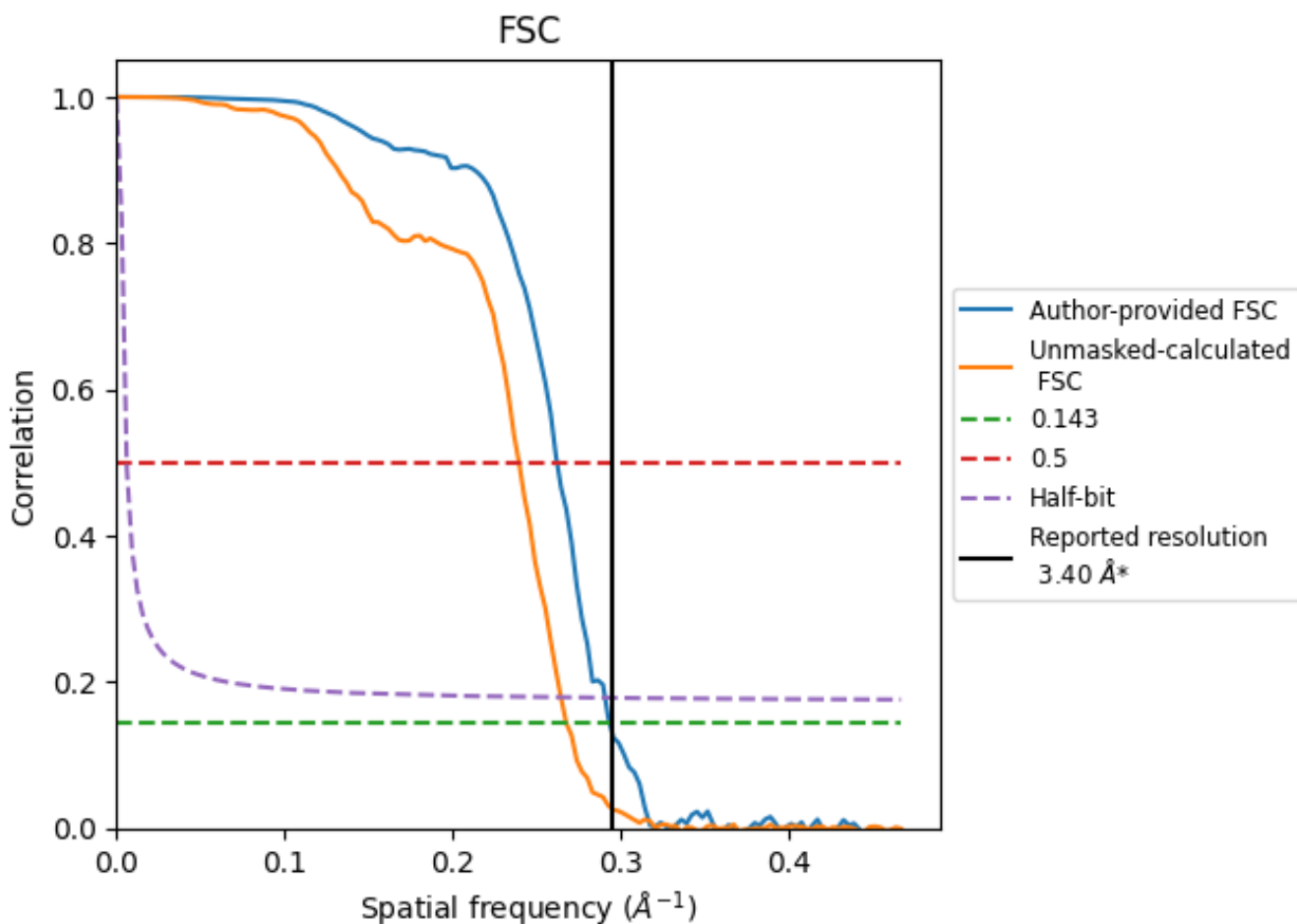


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 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 0.294 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

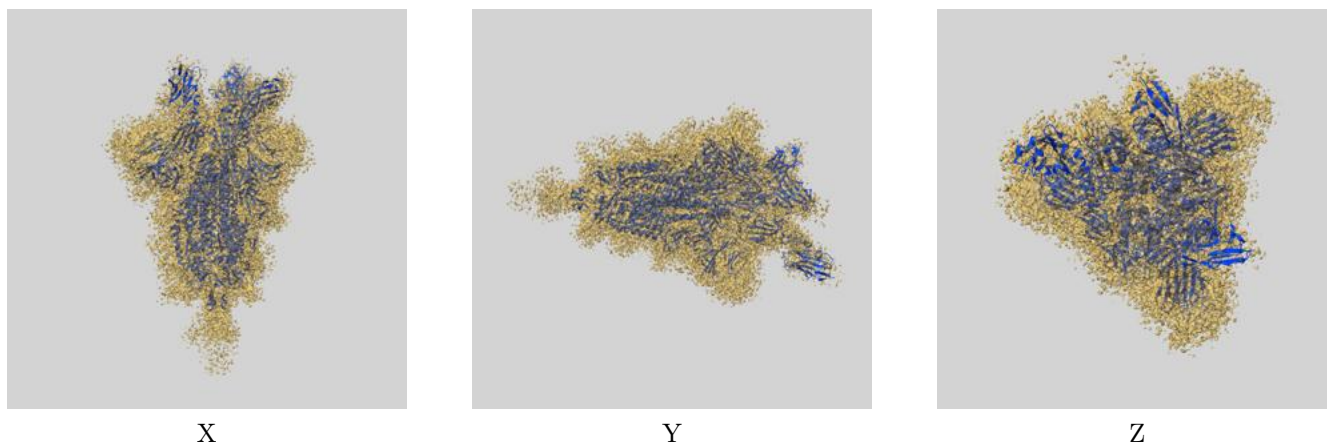
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	3.82	3.44
Unmasked-calculated*	3.74	4.18	3.79

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 3.4 by more than 10 %

## 9 Map-model fit [i](#)

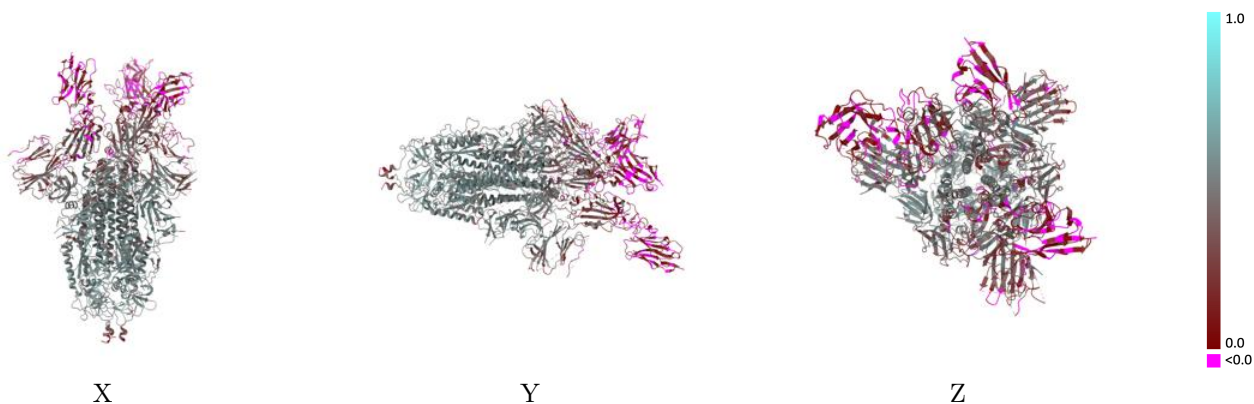
This section contains information regarding the fit between EMDB map EMD-14544 and PDB model 7Z86. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



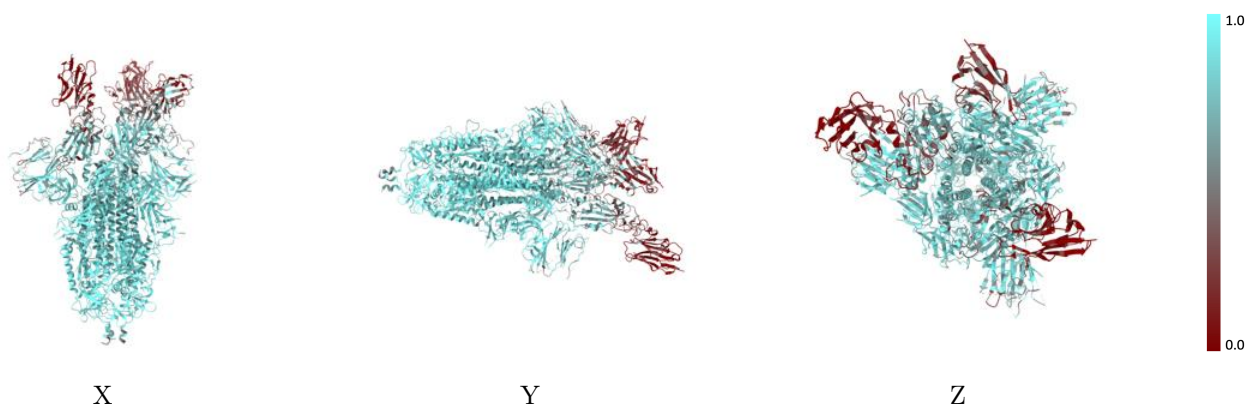
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



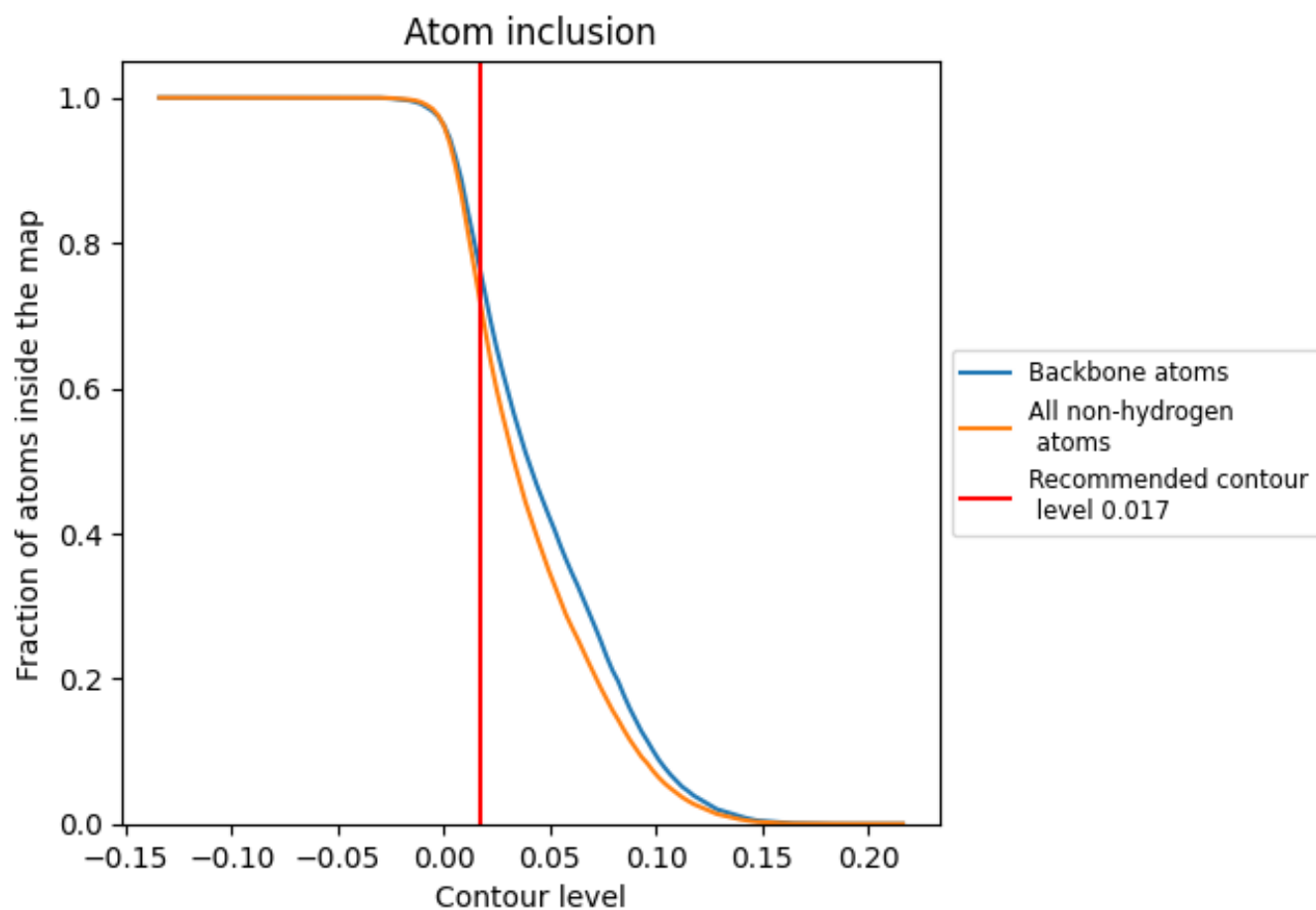
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7204	 0.3790
A	 0.7765	 0.4200
B	 0.8037	 0.4190
C	 0.7968	 0.4310
D	 0.2143	 0.0490
E	 0.4286	 0.1460
F	 0.3571	 0.0620
G	 0.3929	 0.1750
H	 0.5714	 0.2790
I	 0.3571	 0.1220
J	 0.5357	 0.2630
K	 0.5000	 0.2770
L	 0.7143	 0.4160
M	 0.3929	 0.1050
N	 0.5000	 0.1430
O	 0.3571	 0.1270
P	 0.5000	 0.3080
Q	 0.4286	 0.1800
R	 0.5357	 0.2130
S	 0.7500	 0.4070
T	 0.3571	 0.1160
U	 0.2500	 0.0180
V	 0.6429	 0.2470
W	 0.3929	 0.1410
X	 0.0955	 0.0480
Y	 0.3452	 0.0790
Z	 0.1207	 0.0440

