



## Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 12:46 PM EST

PDB ID : 6V0R  
EMDB ID : EMD-20396  
Title : BG505 SOSIP.664 Trimer  
Authors : Nogal, B.; Cottrell, C.A.; Ward, A.B.  
Deposited on : 2019-11-19  
Resolution : 3.87 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](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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

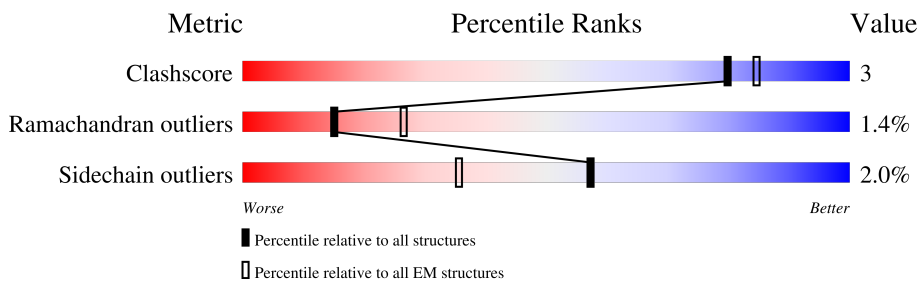
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.87 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.



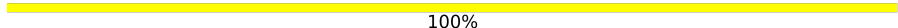

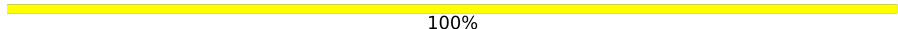
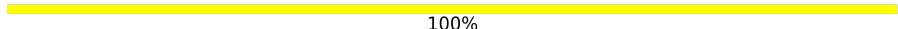
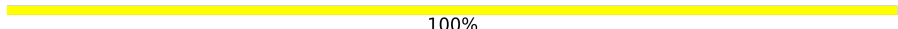

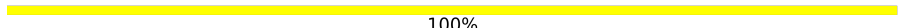
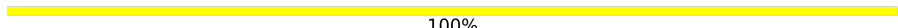
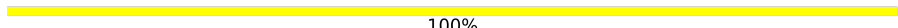

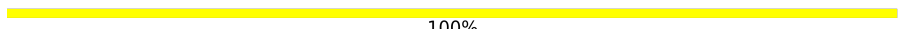
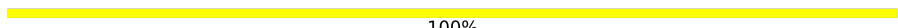
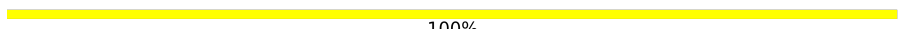

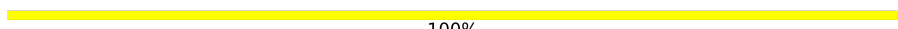

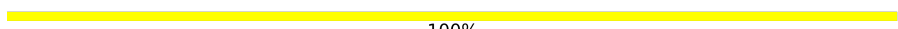
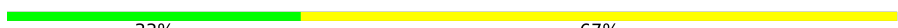
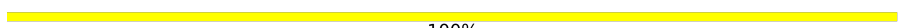
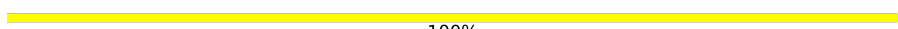
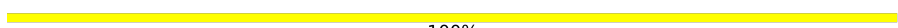
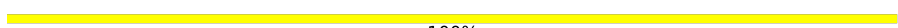
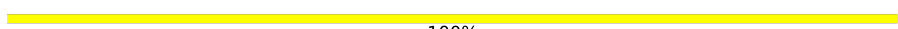
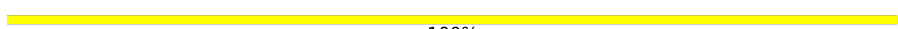

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	475	
1	C	475	
1	D	475	
2	B	153	
2	E	153	
2	F	153	
3	G	2	
3	H	2	

Continued on next page...

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Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	N	2	 50% 50%
3	P	2	 100%
3	Q	2	 100%
3	R	2	 100%
3	W	2	 50% 50%
3	Y	2	 100%
3	Z	2	 100%
3	a	2	 100%
3	f	2	 50% 50%
4	J	6	 100%
4	S	6	 100%
4	b	6	 100%
5	K	3	 33% 67%
5	L	3	 100%
5	T	3	 33% 67%
5	U	3	 100%
5	c	3	 33% 67%
5	d	3	 100%
6	M	3	 100%
6	V	3	 100%
6	e	3	 100%
7	O	2	 100%
7	X	2	 100%
7	g	2	 100%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14910 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 BG505 SOSIPv5.2 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	439	3462	2177	610	646	29	0	0
1	C	439	3462	2177	610	646	29	0	0
1	D	439	3462	2177	610	646	29	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	CYS	ALA	conflict	UNP Q2N0S6
A	316	TRP	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
C	73	CYS	ALA	conflict	UNP Q2N0S6
C	316	TRP	ALA	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
D	73	CYS	ALA	conflict	UNP Q2N0S6
D	316	TRP	ALA	conflict	UNP Q2N0S6
D	332	ASN	THR	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIPv5.2 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	129	1030	650	180	193	7	0	0
2	E	129	1030	650	180	193	7	0	0
2	F	129	1030	650	180	193	7	0	0

There are 9 discrepancies between the modelled and reference sequences:

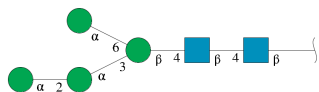
Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	561	CYS	ALA	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
E	559	PRO	ILE	conflict	UNP Q2N0S6
E	561	CYS	ALA	conflict	UNP Q2N0S6
E	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	561	CYS	ALA	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

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



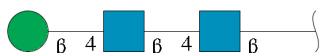
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0
3	I	2	28	16	2	10	0	0
3	N	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0
3	Q	2	28	16	2	10	0	0
3	R	2	28	16	2	10	0	0
3	W	2	28	16	2	10	0	0
3	Y	2	28	16	2	10	0	0
3	Z	2	28	16	2	10	0	0
3	a	2	28	16	2	10	0	0
3	f	2	28	16	2	10	0	0

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



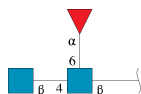
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	J	6	72	40	2	30	0	0
4	S	6	72	40	2	30	0	0
4	b	6	72	40	2	30	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	K	3	39	22	2	15	0	0
5	L	3	39	22	2	15	0	0
5	T	3	39	22	2	15	0	0
5	U	3	39	22	2	15	0	0
5	c	3	39	22	2	15	0	0
5	d	3	39	22	2	15	0	0

- Molecule 6 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.



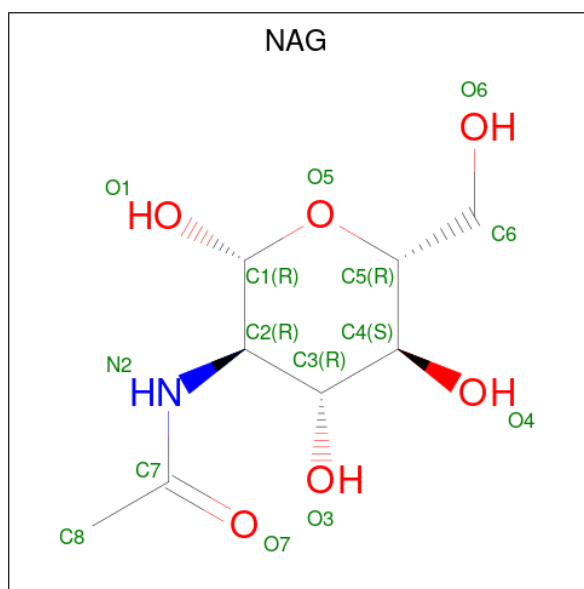
Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	3	Total	C	N	O	0	0
			38	22	2	14		
6	V	3	Total	C	N	O	0	0
			38	22	2	14		
6	e	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	B	1	Total	C	N	O	0
			28	16	2	10	
8	B	1	Total	C	N	O	0
			28	16	2	10	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	C	1	Total	C	N	O	0
			126	72	9	45	
8	E	1	Total	C	N	O	0
			28	16	2	10	
8	E	1	Total	C	N	O	0
			28	16	2	10	

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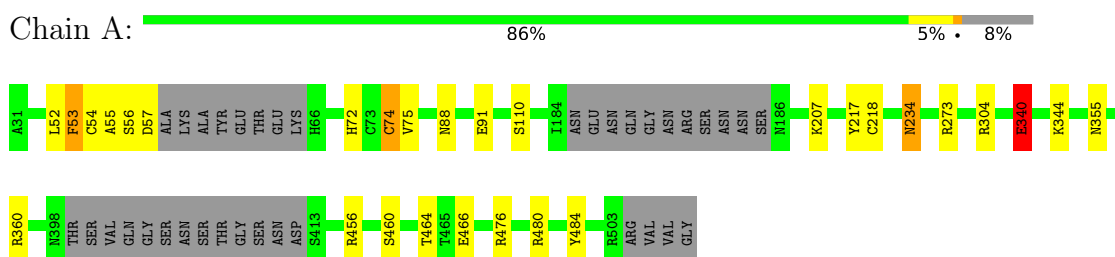
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>
8	D	1	Total	C	N	O	0
			126	72	9	45	
8	D	1	Total	C	N	O	0
			126	72	9	45	
8	D	1	Total	C	N	O	0
			126	72	9	45	
8	D	1	Total	C	N	O	0
			126	72	9	45	
8	D	1	Total	C	N	O	0
			126	72	9	45	
8	D	1	Total	C	N	O	0
			126	72	9	45	
8	D	1	Total	C	N	O	0
			126	72	9	45	
8	F	1	Total	C	N	O	0
			28	16	2	10	
8	F	1	Total	C	N	O	0
			28	16	2	10	

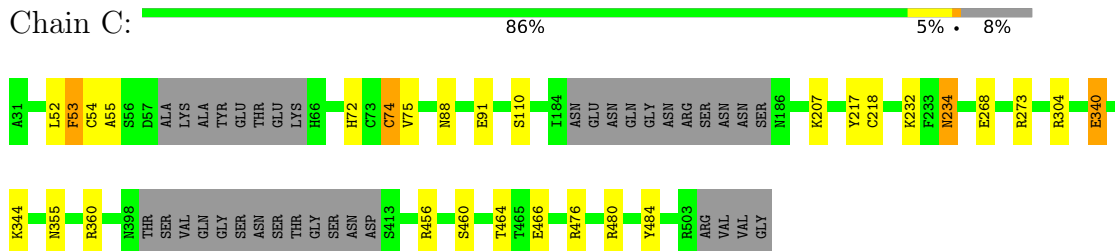
### 3 Residue-property plots [i](#)

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

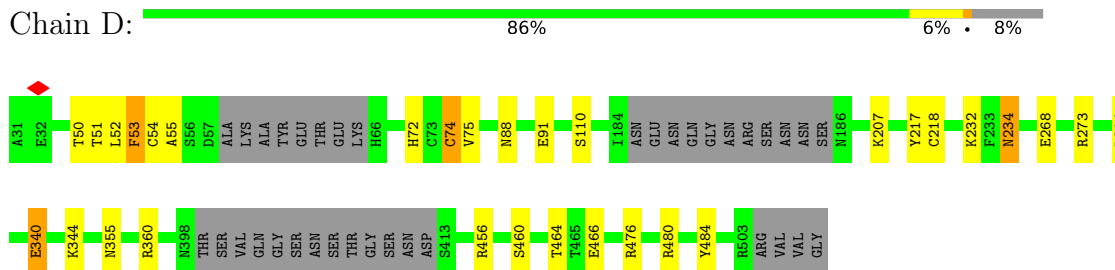
- Molecule 1: BG505 SOSIPv5.2 gp120



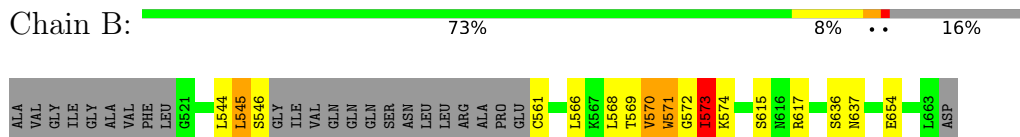
- Molecule 1: BG505 SOSIPv5.2 gp120



- Molecule 1: BG505 SOSIPv5.2 gp120

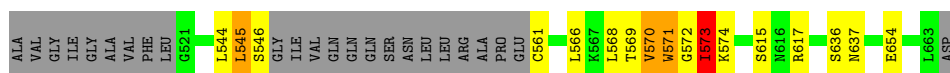


- Molecule 2: BG505 SOSIPv5.2 gp41



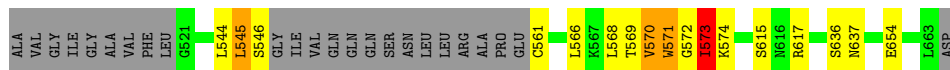
- Molecule 2: BG505 SOSIPv5.2 gp41

Chain E:  73% 8% .. 16%

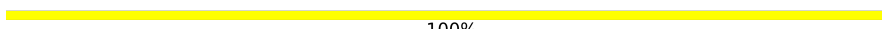


- Molecule 2: BG505 SOSIPv5.2 gp41

Chain F:  73% 8% .. 16%

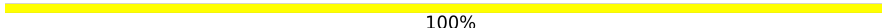


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

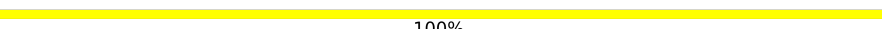
MAG1  
MAG2

- 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:  100%

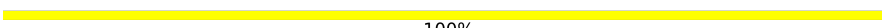
MAG1  
MAG2

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

Chain N:  50% 50%

MAG1  
MAG2

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


Chain P:  100%

MAG1  
MAG2

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

Chain Q:  100%MAG1  
MAG2


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

Chain R:  100%MAG1  
MAG2


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

Chain W:  50% 50%MAG1  
MAG2


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

Chain Y:  100%MAG1  
MAG2

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

Chain Z:  100%MAG1  
MAG2

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

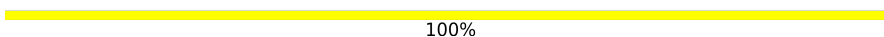
Chain a:  100%MAG1  
MAG2

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

Chain f:  50% 50%

MAG1  
MAG2

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

Chain J:  100%

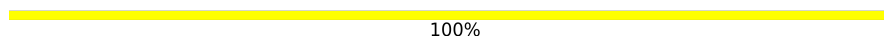
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain S:  100%

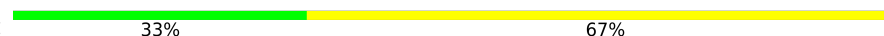
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain b:  100%

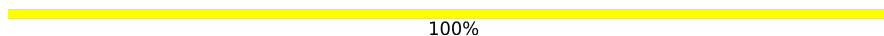
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain K:  33% 67%

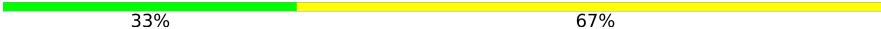
MAG1  
MAG2  
BMA3

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

Chain L:  100%

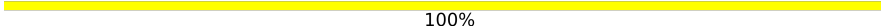
MAG1  
MAG2  
BMA3

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

Chain T:  33% 67%


MAG1  
MAG2  
BMA3

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

Chain U:  100%

MAG1  
MAG2  
BMA3

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

Chain c:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain d:  100%

MAG1  
MAG2  
BMA3

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

Chain M:  100%

MAG1  
MAG2  
FUC3

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

Chain V:  100%


MAG1  
MAG2  
FUC3

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

Chain e:  100%

MAG1  
MAG2  
FUC3

- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%MAG1  
FUC2

- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%MAG1  
FUC2

- Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%MAG1  
FUC2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	155394	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.195	Depositor
Minimum map value	-1.938	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.275	Depositor
Map size ( $\text{\AA}$ )	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.03, 1.03, 1.03	Depositor



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUC, NAG, 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	1.03	8/3536 (0.2%)	0.91	7/4802 (0.1%)
1	C	1.03	7/3536 (0.2%)	0.91	7/4802 (0.1%)
1	D	1.03	7/3536 (0.2%)	0.91	7/4802 (0.1%)
2	B	1.00	1/1048 (0.1%)	0.83	2/1420 (0.1%)
2	E	1.00	1/1048 (0.1%)	0.83	2/1420 (0.1%)
2	F	1.00	1/1048 (0.1%)	0.83	2/1420 (0.1%)
All	All	1.02	25/13752 (0.2%)	0.89	27/18666 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	TYR	CB-CG	-8.46	1.39	1.51
1	C	484	TYR	CB-CG	-8.44	1.39	1.51
1	D	484	TYR	CB-CG	-8.41	1.39	1.51
1	C	217	TYR	CB-CG	-6.81	1.41	1.51
1	A	217	TYR	CB-CG	-6.81	1.41	1.51
1	D	217	TYR	CB-CG	-6.81	1.41	1.51
1	D	484	TYR	CG-CD1	-6.69	1.30	1.39
1	C	484	TYR	CG-CD1	-6.69	1.30	1.39
1	A	484	TYR	CG-CD1	-6.68	1.30	1.39
1	C	91	GLU	CG-CD	-6.39	1.42	1.51
1	D	91	GLU	CG-CD	-6.36	1.42	1.51
1	A	91	GLU	CG-CD	-6.35	1.42	1.51
1	D	484	TYR	CD1-CE1	-5.76	1.30	1.39
1	C	484	TYR	CD1-CE1	-5.73	1.30	1.39
1	A	484	TYR	CD1-CE1	-5.71	1.30	1.39
1	C	466	GLU	CD-OE1	-5.38	1.19	1.25
1	D	466	GLU	CD-OE1	-5.36	1.19	1.25
1	A	466	GLU	CD-OE1	-5.35	1.19	1.25
2	E	654	GLU	CD-OE1	-5.17	1.20	1.25
2	B	654	GLU	CD-OE1	-5.12	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	654	GLU	CD-OE1	-5.12	1.20	1.25
1	A	91	GLU	CD-OE2	-5.08	1.20	1.25
1	C	91	GLU	CD-OE2	-5.06	1.20	1.25
1	D	91	GLU	CD-OE2	-5.05	1.20	1.25
1	A	340	GLU	CD-OE1	-5.00	1.20	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	D	480	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	C	480	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	476	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	476	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	D	476	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	D	304	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	304	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	C	304	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	273	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	273	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	273	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	456	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	C	456	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	456	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	484	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	A	484	TYR	CB-CG-CD1	-6.50	117.10	121.00
1	D	484	TYR	CB-CG-CD1	-6.49	117.10	121.00
2	B	617	ARG	NE-CZ-NH2	-6.33	117.13	120.30
2	F	617	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	E	617	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	360	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	360	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	360	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	E	617	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	F	617	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	B	617	ARG	NE-CZ-NH1	5.30	122.95	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3462	0	3395	15	0
1	C	3462	0	3395	15	0
1	D	3462	0	3395	17	0
2	B	1030	0	1013	13	0
2	E	1030	0	1013	12	0
2	F	1030	0	1013	12	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	N	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	W	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	f	28	0	25	0	0
4	J	72	0	58	0	0
4	S	72	0	58	0	0
4	b	72	0	58	0	0
5	K	39	0	33	0	0
5	L	39	0	33	0	0
5	T	39	0	33	0	0
5	U	39	0	33	0	0
5	c	39	0	33	0	0
5	d	39	0	33	0	0
6	M	38	0	34	0	0
6	V	38	0	34	0	0
6	e	38	0	34	0	0
7	O	24	0	22	0	0
7	X	24	0	22	0	0
7	g	24	0	22	0	0
8	A	126	0	117	0	0
8	B	28	0	26	0	0
8	C	126	0	117	0	0
8	D	126	0	117	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	28	0	26	0	0
8	F	28	0	26	0	0
All	All	14910	0	14493	74	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 3.

All (74) 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)
2:B:568:LEU:HD21	2:B:571:TRP:CE3	2.33	0.64
2:E:568:LEU:HD21	2:E:571:TRP:CE3	2.33	0.64
2:F:568:LEU:HD21	2:F:571:TRP:CE3	2.33	0.63
1:D:53:PHE:CE1	1:D:218:CYS:HB2	2.34	0.62
1:A:53:PHE:CE1	1:A:218:CYS:HB2	2.34	0.62
1:C:72:HIS:O	1:C:72:HIS:CG	2.53	0.62
1:A:72:HIS:CG	1:A:72:HIS:O	2.53	0.62
1:C:53:PHE:CE1	1:C:218:CYS:HB2	2.34	0.62
1:D:72:HIS:CG	1:D:72:HIS:O	2.53	0.61
1:D:74:CYS:HG	2:F:561:CYS:HG	0.96	0.60
2:E:568:LEU:C	2:E:570:VAL:H	2.05	0.60
2:F:568:LEU:C	2:F:570:VAL:H	2.05	0.59
2:B:568:LEU:C	2:B:570:VAL:H	2.05	0.58
1:A:54:CYS:SG	1:A:55:ALA:N	2.77	0.58
1:C:54:CYS:SG	1:C:55:ALA:N	2.77	0.58
1:D:54:CYS:SG	1:D:55:ALA:N	2.77	0.58
1:C:53:PHE:C	1:C:53:PHE:CD1	2.81	0.55
1:D:53:PHE:C	1:D:53:PHE:CD1	2.81	0.55
1:D:74:CYS:CB	2:F:561:CYS:SG	2.96	0.54
1:A:74:CYS:CB	2:B:561:CYS:SG	2.96	0.54
1:C:74:CYS:CB	2:E:561:CYS:SG	2.96	0.53
1:C:53:PHE:C	1:C:53:PHE:HD1	2.12	0.53
1:A:53:PHE:CD1	1:A:53:PHE:C	2.81	0.53
1:D:53:PHE:C	1:D:53:PHE:HD1	2.12	0.52
1:A:53:PHE:C	1:A:53:PHE:HD1	2.12	0.52
1:C:52:LEU:HD22	1:C:52:LEU:N	2.26	0.51
1:A:52:LEU:N	1:A:52:LEU:HD22	2.26	0.50
1:D:52:LEU:HD22	1:D:52:LEU:N	2.26	0.50
1:A:53:PHE:CD1	1:A:53:PHE:O	2.66	0.49
1:D:53:PHE:CD1	1:D:53:PHE:O	2.66	0.49
1:D:52:LEU:N	1:D:52:LEU:CD2	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:PHE:CD1	1:C:53:PHE:O	2.66	0.48
1:C:52:LEU:N	1:C:52:LEU:CD2	2.77	0.48
1:A:52:LEU:N	1:A:52:LEU:CD2	2.77	0.47
2:B:545:LEU:HD23	2:B:545:LEU:HA	1.68	0.47
2:B:573:ILE:HD13	2:E:566:LEU:HD23	1.96	0.47
2:B:566:LEU:HD23	2:F:573:ILE:HD13	1.96	0.47
2:B:545:LEU:O	2:B:546:SER:HB3	2.16	0.46
2:E:572:GLY:C	2:E:574:LYS:H	2.19	0.46
2:E:573:ILE:HD13	2:F:566:LEU:HD23	1.96	0.46
2:F:545:LEU:O	2:F:546:SER:HB3	2.16	0.46
1:C:110:SER:HB3	2:E:571:TRP:CH2	2.51	0.46
2:F:572:GLY:C	2:F:574:LYS:H	2.19	0.46
1:A:110:SER:HB3	2:B:571:TRP:CH2	2.51	0.45
2:B:572:GLY:C	2:B:574:LYS:H	2.19	0.45
1:D:110:SER:HB3	2:F:571:TRP:CH2	2.51	0.45
1:A:340:GLU:OE2	1:A:344:LYS:NZ	2.50	0.45
2:E:545:LEU:O	2:E:546:SER:HB3	2.16	0.45
1:C:53:PHE:HD1	1:C:53:PHE:O	2.00	0.45
1:A:53:PHE:HD1	1:A:53:PHE:O	2.00	0.45
1:D:88:ASN:N	1:D:88:ASN:OD1	2.50	0.45
1:D:340:GLU:OE2	1:D:344:LYS:NZ	2.50	0.45
1:D:53:PHE:HD1	1:D:53:PHE:O	2.00	0.44
1:C:340:GLU:OE2	1:C:344:LYS:NZ	2.50	0.44
2:E:568:LEU:C	2:E:570:VAL:N	2.70	0.44
2:B:568:LEU:C	2:B:570:VAL:N	2.69	0.44
2:F:568:LEU:C	2:F:570:VAL:N	2.70	0.44
1:D:232:LYS:NZ	1:D:268:GLU:OE1	2.48	0.44
1:C:88:ASN:OD1	1:C:88:ASN:N	2.50	0.43
1:C:232:LYS:NZ	1:C:268:GLU:OE1	2.48	0.43
1:A:88:ASN:OD1	1:A:88:ASN:N	2.50	0.42
2:F:573:ILE:CG1	2:F:573:ILE:O	2.68	0.42
2:F:637:ASN:N	2:F:637:ASN:OD1	2.53	0.42
2:E:637:ASN:N	2:E:637:ASN:OD1	2.53	0.41
2:B:573:ILE:CG1	2:B:573:ILE:O	2.68	0.41
2:B:637:ASN:N	2:B:637:ASN:OD1	2.53	0.41
1:C:234:ASN:O	1:C:234:ASN:CG	2.59	0.41
2:E:573:ILE:O	2:E:573:ILE:CG1	2.68	0.41
2:B:568:LEU:HD21	2:B:571:TRP:HE3	1.85	0.41
1:A:234:ASN:O	1:A:234:ASN:CG	2.59	0.41
1:A:56:SER:OG	1:A:57:ASP:N	2.54	0.40
2:E:545:LEU:HD23	2:E:545:LEU:HA	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:THR:OG1	1:D:51:THR:N	2.55	0.40
1:D:234:ASN:CG	1:D:234:ASN:O	2.59	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/475 (91%)	405 (94%)	22 (5%)	4 (1%)	17	54
1	C	431/475 (91%)	405 (94%)	22 (5%)	4 (1%)	17	54
1	D	431/475 (91%)	405 (94%)	22 (5%)	4 (1%)	17	54
2	B	125/153 (82%)	119 (95%)	2 (2%)	4 (3%)	4	32
2	E	125/153 (82%)	119 (95%)	2 (2%)	4 (3%)	4	32
2	F	125/153 (82%)	119 (95%)	2 (2%)	4 (3%)	4	32
All	All	1668/1884 (88%)	1572 (94%)	72 (4%)	24 (1%)	15	46

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	569	THR
2	B	636	SER
2	E	569	THR
2	E	636	SER
2	F	569	THR
2	F	636	SER
1	A	340	GLU
1	C	340	GLU
1	D	340	GLU
1	A	207	LYS

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Mol	Chain	Res	Type
2	B	573	ILE
1	C	207	LYS
2	E	573	ILE
1	D	207	LYS
2	F	573	ILE
1	A	460	SER
2	B	615	SER
1	C	460	SER
2	E	615	SER
1	D	460	SER
2	F	615	SER
1	A	464	THR
1	C	464	THR
1	D	464	THR

### 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	394/424 (93%)	389 (99%)	5 (1%)	69 81
1	C	394/424 (93%)	389 (99%)	5 (1%)	69 81
1	D	394/424 (93%)	389 (99%)	5 (1%)	69 81
2	B	112/130 (86%)	107 (96%)	5 (4%)	27 56
2	E	112/130 (86%)	107 (96%)	5 (4%)	27 56
2	F	112/130 (86%)	107 (96%)	5 (4%)	27 56
All	All	1518/1662 (91%)	1488 (98%)	30 (2%)	57 74

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	74	CYS
1	A	75	VAL
1	A	234	ASN

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Mol	Chain	Res	Type
1	A	355	ASN
2	B	544	LEU
2	B	545	LEU
2	B	570	VAL
2	B	571	TRP
2	B	573	ILE
1	C	53	PHE
1	C	74	CYS
1	C	75	VAL
1	C	234	ASN
1	C	355	ASN
2	E	544	LEU
2	E	545	LEU
2	E	570	VAL
2	E	571	TRP
2	E	573	ILE
1	D	53	PHE
1	D	74	CYS
1	D	75	VAL
1	D	234	ASN
1	D	355	ASN
2	F	544	LEU
2	F	545	LEU
2	F	570	VAL
2	F	571	TRP
2	F	573	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	C	72	HIS
1	D	72	HIS

### 5.3.3 RNA

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](#)

75 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	G	1	3,1	14,14,15	0.81	0	17,19,21	1.24	1 (5%)
3	NAG	G	2	3	14,14,15	0.79	0	17,19,21	0.96	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.88	0	17,19,21	2.05	5 (29%)
3	NAG	H	2	3	14,14,15	0.75	0	17,19,21	0.91	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.77	0	17,19,21	1.03	1 (5%)
3	NAG	I	2	3	14,14,15	0.78	0	17,19,21	1.20	2 (11%)
4	NAG	J	1	4,1	14,14,15	0.75	0	17,19,21	1.16	1 (5%)
4	NAG	J	2	4	14,14,15	0.80	1 (7%)	17,19,21	1.19	2 (11%)
4	BMA	J	3	4	11,11,12	1.87	2 (18%)	15,15,17	1.13	1 (6%)
4	MAN	J	4	4	11,11,12	1.59	1 (9%)	15,15,17	1.08	2 (13%)
4	MAN	J	5	4	11,11,12	1.87	3 (27%)	15,15,17	1.18	2 (13%)
4	MAN	J	6	4	11,11,12	1.82	2 (18%)	15,15,17	1.13	2 (13%)
5	NAG	K	1	5,1	14,14,15	0.78	0	17,19,21	1.20	2 (11%)
5	NAG	K	2	5	14,14,15	0.81	0	17,19,21	0.81	0
5	BMA	K	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.88	1 (6%)
5	NAG	L	1	5,1	14,14,15	0.81	1 (7%)	17,19,21	1.36	2 (11%)
5	NAG	L	2	5	14,14,15	0.81	0	17,19,21	1.01	2 (11%)
5	BMA	L	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.99	1 (6%)
6	NAG	M	1	6,1	14,14,15	0.81	1 (7%)	17,19,21	1.03	0
6	NAG	M	2	6	14,14,15	0.80	0	17,19,21	1.17	1 (5%)
6	FUC	M	3	6	10,10,11	0.76	0	14,14,16	1.00	1 (7%)
3	NAG	N	1	3,1	14,14,15	0.80	0	17,19,21	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	N	2	3	14,14,15	0.79	0	17,19,21	1.22	2 (11%)
7	NAG	O	1	2,7	14,14,15	0.75	0	17,19,21	1.09	1 (5%)
7	FUC	O	2	7	10,10,11	1.35	1 (10%)	14,14,16	4.12	6 (42%)
3	NAG	P	1	3,1	14,14,15	0.81	0	17,19,21	1.24	1 (5%)
3	NAG	P	2	3	14,14,15	0.80	0	17,19,21	0.96	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.89	0	17,19,21	2.04	5 (29%)
3	NAG	Q	2	3	14,14,15	0.75	0	17,19,21	0.91	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.77	0	17,19,21	1.03	1 (5%)
3	NAG	R	2	3	14,14,15	0.77	0	17,19,21	1.20	2 (11%)
4	NAG	S	1	4,1	14,14,15	0.76	0	17,19,21	1.16	1 (5%)
4	NAG	S	2	4	14,14,15	0.80	1 (7%)	17,19,21	1.19	2 (11%)
4	BMA	S	3	4	11,11,12	1.86	2 (18%)	15,15,17	1.13	1 (6%)
4	MAN	S	4	4	11,11,12	1.59	1 (9%)	15,15,17	1.09	2 (13%)
4	MAN	S	5	4	11,11,12	1.87	3 (27%)	15,15,17	1.18	2 (13%)
4	MAN	S	6	4	11,11,12	1.82	2 (18%)	15,15,17	1.14	3 (20%)
5	NAG	T	1	5,1	14,14,15	0.77	0	17,19,21	1.20	2 (11%)
5	NAG	T	2	5	14,14,15	0.81	0	17,19,21	0.81	0
5	BMA	T	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.88	1 (6%)
5	NAG	U	1	5,1	14,14,15	0.83	1 (7%)	17,19,21	1.37	2 (11%)
5	NAG	U	2	5	14,14,15	0.81	0	17,19,21	1.01	2 (11%)
5	BMA	U	3	5	11,11,12	1.83	2 (18%)	15,15,17	1.00	1 (6%)
6	NAG	V	1	6,1	14,14,15	0.81	1 (7%)	17,19,21	1.03	0
6	NAG	V	2	6	14,14,15	0.79	0	17,19,21	1.17	1 (5%)
6	FUC	V	3	6	10,10,11	0.76	0	14,14,16	1.01	1 (7%)
3	NAG	W	1	3,1	14,14,15	0.79	0	17,19,21	0.94	0
3	NAG	W	2	3	14,14,15	0.79	0	17,19,21	1.22	2 (11%)
7	NAG	X	1	2,7	14,14,15	0.75	0	17,19,21	1.10	1 (5%)
7	FUC	X	2	7	10,10,11	1.35	1 (10%)	14,14,16	4.12	6 (42%)
3	NAG	Y	1	3,1	14,14,15	0.81	0	17,19,21	1.24	1 (5%)
3	NAG	Y	2	3	14,14,15	0.80	0	17,19,21	0.96	1 (5%)
3	NAG	Z	1	3,1	14,14,15	0.88	0	17,19,21	2.04	5 (29%)
3	NAG	Z	2	3	14,14,15	0.75	0	17,19,21	0.90	1 (5%)
3	NAG	a	1	3,1	14,14,15	0.77	0	17,19,21	1.03	1 (5%)
3	NAG	a	2	3	14,14,15	0.78	0	17,19,21	1.20	2 (11%)
4	NAG	b	1	4,1	14,14,15	0.75	0	17,19,21	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	b	2	4	14,14,15	0.79	1 (7%)	17,19,21	1.19	2 (11%)
4	BMA	b	3	4	11,11,12	1.87	2 (18%)	15,15,17	1.13	1 (6%)
4	MAN	b	4	4	11,11,12	1.59	2 (18%)	15,15,17	1.09	2 (13%)
4	MAN	b	5	4	11,11,12	1.87	3 (27%)	15,15,17	1.18	2 (13%)
4	MAN	b	6	4	11,11,12	1.82	2 (18%)	15,15,17	1.14	3 (20%)
5	NAG	c	1	5,1	14,14,15	0.77	0	17,19,21	1.20	2 (11%)
5	NAG	c	2	5	14,14,15	0.81	0	17,19,21	0.81	0
5	BMA	c	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.89	1 (6%)
5	NAG	d	1	5,1	14,14,15	0.82	1 (7%)	17,19,21	1.37	2 (11%)
5	NAG	d	2	5	14,14,15	0.80	0	17,19,21	1.00	2 (11%)
5	BMA	d	3	5	11,11,12	1.83	2 (18%)	15,15,17	1.00	1 (6%)
6	NAG	e	1	6,1	14,14,15	0.81	1 (7%)	17,19,21	1.03	0
6	NAG	e	2	6	14,14,15	0.80	0	17,19,21	1.16	1 (5%)
6	FUC	e	3	6	10,10,11	0.76	0	14,14,16	1.00	1 (7%)
3	NAG	f	1	3,1	14,14,15	0.80	0	17,19,21	0.94	0
3	NAG	f	2	3	14,14,15	0.79	0	17,19,21	1.22	2 (11%)
7	NAG	g	1	2,7	14,14,15	0.74	0	17,19,21	1.09	1 (5%)
7	FUC	g	2	7	10,10,11	1.36	1 (10%)	14,14,16	4.12	6 (42%)

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	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	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
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	1/2/19/22	0/1/1/1
4	MAN	J	5	4	-	2/2/19/22	0/1/1/1
4	MAN	J	6	4	-	1/2/19/22	0/1/1/1

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

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

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	5	MAN	O2-C2	-4.27	1.34	1.43
4	J	5	MAN	O2-C2	-4.26	1.34	1.43
4	b	5	MAN	O2-C2	-4.26	1.34	1.43
5	T	3	BMA	O2-C2	-4.18	1.34	1.43
5	c	3	BMA	O2-C2	-4.16	1.34	1.43
5	K	3	BMA	O2-C2	-4.16	1.34	1.43
4	J	3	BMA	O2-C2	-4.16	1.34	1.43
4	b	3	BMA	O2-C2	-4.15	1.34	1.43
4	S	3	BMA	O2-C2	-4.14	1.34	1.43
4	J	6	MAN	O2-C2	-4.10	1.34	1.43
4	b	6	MAN	O2-C2	-4.10	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	6	MAN	O2-C2	-4.07	1.34	1.43
5	d	3	BMA	O2-C2	-4.06	1.34	1.43
5	U	3	BMA	O2-C2	-4.05	1.34	1.43
5	L	3	BMA	O2-C2	-4.02	1.34	1.43
4	S	4	MAN	O2-C2	-3.16	1.36	1.43
4	J	4	MAN	O2-C2	-3.15	1.36	1.43
4	b	4	MAN	O2-C2	-3.15	1.36	1.43
7	g	2	FUC	O5-C1	3.06	1.48	1.43
7	X	2	FUC	O5-C1	3.04	1.48	1.43
7	O	2	FUC	O5-C1	3.01	1.48	1.43
5	L	3	BMA	C2-C3	-2.59	1.48	1.52
5	d	3	BMA	C2-C3	-2.58	1.48	1.52
5	U	3	BMA	C2-C3	-2.57	1.48	1.52
5	c	3	BMA	C2-C3	-2.42	1.48	1.52
5	K	3	BMA	C2-C3	-2.42	1.49	1.52
5	T	3	BMA	C2-C3	-2.39	1.49	1.52
4	b	3	BMA	C2-C3	-2.37	1.49	1.52
4	J	3	BMA	C2-C3	-2.35	1.49	1.52
4	S	3	BMA	C2-C3	-2.34	1.49	1.52
4	b	6	MAN	C2-C3	-2.20	1.49	1.52
4	S	6	MAN	C2-C3	-2.18	1.49	1.52
4	J	6	MAN	C2-C3	-2.18	1.49	1.52
4	J	5	MAN	C2-C3	-2.13	1.49	1.52
4	b	5	MAN	C2-C3	-2.12	1.49	1.52
4	S	5	MAN	C2-C3	-2.12	1.49	1.52
5	U	1	NAG	C3-C2	-2.10	1.48	1.52
4	J	2	NAG	C3-C2	-2.08	1.48	1.52
4	J	5	MAN	O5-C1	2.08	1.47	1.43
4	b	5	MAN	O5-C1	2.08	1.47	1.43
4	S	5	MAN	O5-C1	2.07	1.47	1.43
5	d	1	NAG	C3-C2	-2.07	1.48	1.52
4	S	2	NAG	C3-C2	-2.07	1.48	1.52
5	L	1	NAG	C3-C2	-2.06	1.48	1.52
6	V	1	NAG	C3-C2	-2.05	1.48	1.52
6	e	1	NAG	C3-C2	-2.05	1.48	1.52
6	M	1	NAG	C3-C2	-2.05	1.48	1.52
4	b	2	NAG	C3-C2	-2.04	1.48	1.52
4	b	4	MAN	O5-C1	2.00	1.46	1.43

All (122) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	2	FUC	C6-C5-C4	-11.52	91.79	113.07
7	O	2	FUC	C6-C5-C4	-11.51	91.80	113.07
7	g	2	FUC	C6-C5-C4	-11.51	91.80	113.07
7	g	2	FUC	C3-C4-C5	6.57	120.00	109.77
7	O	2	FUC	C3-C4-C5	6.56	120.00	109.77
7	X	2	FUC	C3-C4-C5	6.56	119.99	109.77
3	H	1	NAG	O4-C4-C3	-4.88	99.06	110.35
3	Q	1	NAG	O4-C4-C3	-4.88	99.07	110.35
7	g	2	FUC	O5-C5-C6	4.87	117.82	107.33
7	O	2	FUC	O5-C5-C6	4.87	117.82	107.33
7	X	2	FUC	O5-C5-C6	4.87	117.81	107.33
3	Z	1	NAG	O4-C4-C3	-4.87	99.09	110.35
3	H	1	NAG	O5-C5-C6	-4.68	99.87	107.20
3	Q	1	NAG	O5-C5-C6	-4.67	99.88	107.20
3	Z	1	NAG	O5-C5-C6	-4.67	99.88	107.20
7	g	2	FUC	C2-C3-C4	-4.25	103.55	110.89
7	O	2	FUC	C2-C3-C4	-4.24	103.56	110.89
7	X	2	FUC	C2-C3-C4	-4.23	103.57	110.89
7	g	2	FUC	O5-C5-C4	-3.60	103.07	109.52
7	X	2	FUC	O5-C5-C4	-3.59	103.08	109.52
7	O	2	FUC	O5-C5-C4	-3.59	103.08	109.52
6	V	2	NAG	C4-C3-C2	-3.46	105.95	111.02
6	M	2	NAG	C4-C3-C2	-3.44	105.97	111.02
6	e	2	NAG	C4-C3-C2	-3.44	105.97	111.02
3	R	2	NAG	C4-C3-C2	-3.37	106.08	111.02
3	a	2	NAG	C4-C3-C2	-3.37	106.08	111.02
3	I	2	NAG	C4-C3-C2	-3.36	106.09	111.02
7	X	1	NAG	C4-C3-C2	-3.16	106.38	111.02
7	g	1	NAG	C4-C3-C2	-3.16	106.39	111.02
7	O	1	NAG	C4-C3-C2	-3.15	106.41	111.02
3	N	2	NAG	C4-C3-C2	-2.97	106.66	111.02
3	f	2	NAG	C4-C3-C2	-2.97	106.66	111.02
3	W	2	NAG	C4-C3-C2	-2.96	106.68	111.02
4	b	1	NAG	C3-C4-C5	-2.88	105.10	110.24
4	S	1	NAG	C3-C4-C5	-2.88	105.11	110.24
4	J	1	NAG	C3-C4-C5	-2.87	105.12	110.24
5	T	1	NAG	O5-C5-C6	-2.85	102.73	107.20
5	K	1	NAG	O5-C5-C6	-2.85	102.73	107.20
5	c	1	NAG	O5-C5-C6	-2.85	102.73	107.20
3	H	1	NAG	C3-C4-C5	-2.79	105.26	110.24
3	G	2	NAG	C4-C3-C2	-2.79	106.93	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	1	NAG	C3-C4-C5	-2.78	105.27	110.24
3	Q	1	NAG	C3-C4-C5	-2.78	105.28	110.24
3	P	2	NAG	C4-C3-C2	-2.77	106.95	111.02
4	J	3	BMA	C2-C3-C4	-2.77	106.10	110.89
3	Y	2	NAG	C4-C3-C2	-2.77	106.96	111.02
4	b	3	BMA	C2-C3-C4	-2.77	106.11	110.89
4	S	3	BMA	C2-C3-C4	-2.76	106.13	110.89
5	d	1	NAG	C8-C7-N2	2.70	120.67	116.10
5	U	1	NAG	C8-C7-N2	2.69	120.65	116.10
5	L	1	NAG	C8-C7-N2	2.68	120.64	116.10
3	R	1	NAG	C3-C4-C5	-2.55	105.69	110.24
3	a	1	NAG	C3-C4-C5	-2.55	105.69	110.24
3	I	1	NAG	C3-C4-C5	-2.55	105.69	110.24
5	T	1	NAG	C3-C4-C5	-2.52	105.74	110.24
5	c	1	NAG	C3-C4-C5	-2.52	105.74	110.24
3	Q	2	NAG	C4-C3-C2	-2.52	107.32	111.02
5	K	1	NAG	C3-C4-C5	-2.52	105.75	110.24
3	H	2	NAG	C4-C3-C2	-2.50	107.35	111.02
3	Z	2	NAG	C4-C3-C2	-2.50	107.36	111.02
3	Z	1	NAG	O4-C4-C5	2.49	115.47	109.30
4	J	5	MAN	C1-C2-C3	2.48	112.72	109.67
4	b	5	MAN	C1-C2-C3	2.48	112.72	109.67
4	S	5	MAN	C1-C2-C3	2.48	112.71	109.67
3	Q	1	NAG	O4-C4-C5	2.48	115.45	109.30
3	H	1	NAG	O4-C4-C5	2.48	115.45	109.30
5	U	3	BMA	C2-C3-C4	-2.40	106.75	110.89
3	G	1	NAG	C4-C3-C2	-2.40	107.51	111.02
3	Y	1	NAG	C4-C3-C2	-2.39	107.51	111.02
3	P	1	NAG	C4-C3-C2	-2.38	107.53	111.02
4	S	5	MAN	C2-C3-C4	-2.38	106.78	110.89
5	d	3	BMA	C2-C3-C4	-2.38	106.78	110.89
4	b	5	MAN	C2-C3-C4	-2.37	106.79	110.89
4	J	5	MAN	C2-C3-C4	-2.37	106.80	110.89
4	S	2	NAG	O5-C5-C6	-2.37	103.50	107.20
4	b	2	NAG	O5-C5-C6	-2.36	103.50	107.20
5	L	3	BMA	C2-C3-C4	-2.36	106.81	110.89
4	b	2	NAG	O5-C1-C2	-2.36	107.56	111.29
4	J	2	NAG	O5-C1-C2	-2.36	107.57	111.29
4	J	2	NAG	O5-C5-C6	-2.35	103.52	107.20
4	S	2	NAG	O5-C1-C2	-2.35	107.58	111.29
3	f	2	NAG	O5-C1-C2	-2.34	107.59	111.29
3	W	2	NAG	O5-C1-C2	-2.34	107.59	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	2	NAG	O5-C1-C2	-2.33	107.61	111.29
5	U	1	NAG	O5-C1-C2	-2.25	107.74	111.29
5	d	1	NAG	O5-C1-C2	-2.23	107.77	111.29
5	L	1	NAG	O5-C1-C2	-2.22	107.78	111.29
4	S	6	MAN	O5-C1-C2	-2.21	107.37	110.77
4	b	6	MAN	O5-C1-C2	-2.21	107.37	110.77
4	J	6	MAN	O5-C1-C2	-2.20	107.37	110.77
5	T	3	BMA	C2-C3-C4	-2.18	107.13	110.89
5	c	3	BMA	C2-C3-C4	-2.17	107.14	110.89
5	K	3	BMA	C2-C3-C4	-2.16	107.15	110.89
6	V	3	FUC	C2-C3-C4	-2.12	107.23	110.89
6	e	3	FUC	C2-C3-C4	-2.12	107.23	110.89
6	M	3	FUC	C2-C3-C4	-2.11	107.25	110.89
4	J	6	MAN	C2-C3-C4	-2.09	107.27	110.89
4	b	6	MAN	C2-C3-C4	-2.09	107.28	110.89
4	S	6	MAN	C2-C3-C4	-2.08	107.29	110.89
5	L	2	NAG	O5-C5-C6	-2.07	103.97	107.20
4	S	4	MAN	C2-C3-C4	-2.06	107.33	110.89
3	I	2	NAG	O5-C1-C2	-2.06	108.04	111.29
5	U	2	NAG	O5-C5-C6	-2.06	103.98	107.20
4	J	4	MAN	C2-C3-C4	-2.05	107.34	110.89
4	b	4	MAN	C2-C3-C4	-2.05	107.34	110.89
3	H	1	NAG	C4-C3-C2	2.05	114.02	111.02
5	d	2	NAG	O5-C5-C6	-2.05	104.00	107.20
3	a	2	NAG	O5-C1-C2	-2.04	108.06	111.29
7	X	2	FUC	O4-C4-C3	-2.04	105.63	110.35
3	Q	1	NAG	C4-C3-C2	2.04	114.00	111.02
3	Z	1	NAG	C4-C3-C2	2.03	114.00	111.02
7	g	2	FUC	O4-C4-C3	-2.03	105.66	110.35
5	U	2	NAG	C3-C4-C5	-2.02	106.63	110.24
3	R	2	NAG	O5-C1-C2	-2.02	108.09	111.29
7	O	2	FUC	O4-C4-C3	-2.02	105.67	110.35
5	L	2	NAG	C3-C4-C5	-2.02	106.63	110.24
4	S	6	MAN	C1-C2-C3	2.02	112.15	109.67
4	S	4	MAN	O2-C2-C1	-2.02	105.02	109.15
4	b	4	MAN	O2-C2-C1	-2.01	105.03	109.15
5	d	2	NAG	C3-C4-C5	-2.01	106.65	110.24
4	J	4	MAN	O2-C2-C1	-2.01	105.04	109.15
4	b	6	MAN	C1-C2-C3	2.01	112.14	109.67

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
4	J	5	MAN	O5-C5-C6-O6
4	S	5	MAN	O5-C5-C6-O6
4	b	5	MAN	O5-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
7	X	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
7	X	1	NAG	C4-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
5	L	1	NAG	C8-C7-N2-C2
5	L	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
5	d	1	NAG	C8-C7-N2-C2
5	d	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	P	1	NAG	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
4	J	6	MAN	O5-C5-C6-O6
4	S	6	MAN	O5-C5-C6-O6
4	b	6	MAN	O5-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
4	S	4	MAN	O5-C5-C6-O6
4	b	4	MAN	O5-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
4	S	3	BMA	C4-C5-C6-O6
4	b	3	BMA	C4-C5-C6-O6
5	L	3	BMA	O5-C5-C6-O6
5	U	3	BMA	O5-C5-C6-O6
5	d	3	BMA	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
4	J	5	MAN	C4-C5-C6-O6
4	S	5	MAN	C4-C5-C6-O6
4	b	5	MAN	C4-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	e	2	NAG	C4-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
4	J	3	BMA	O5-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6
4	b	3	BMA	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6

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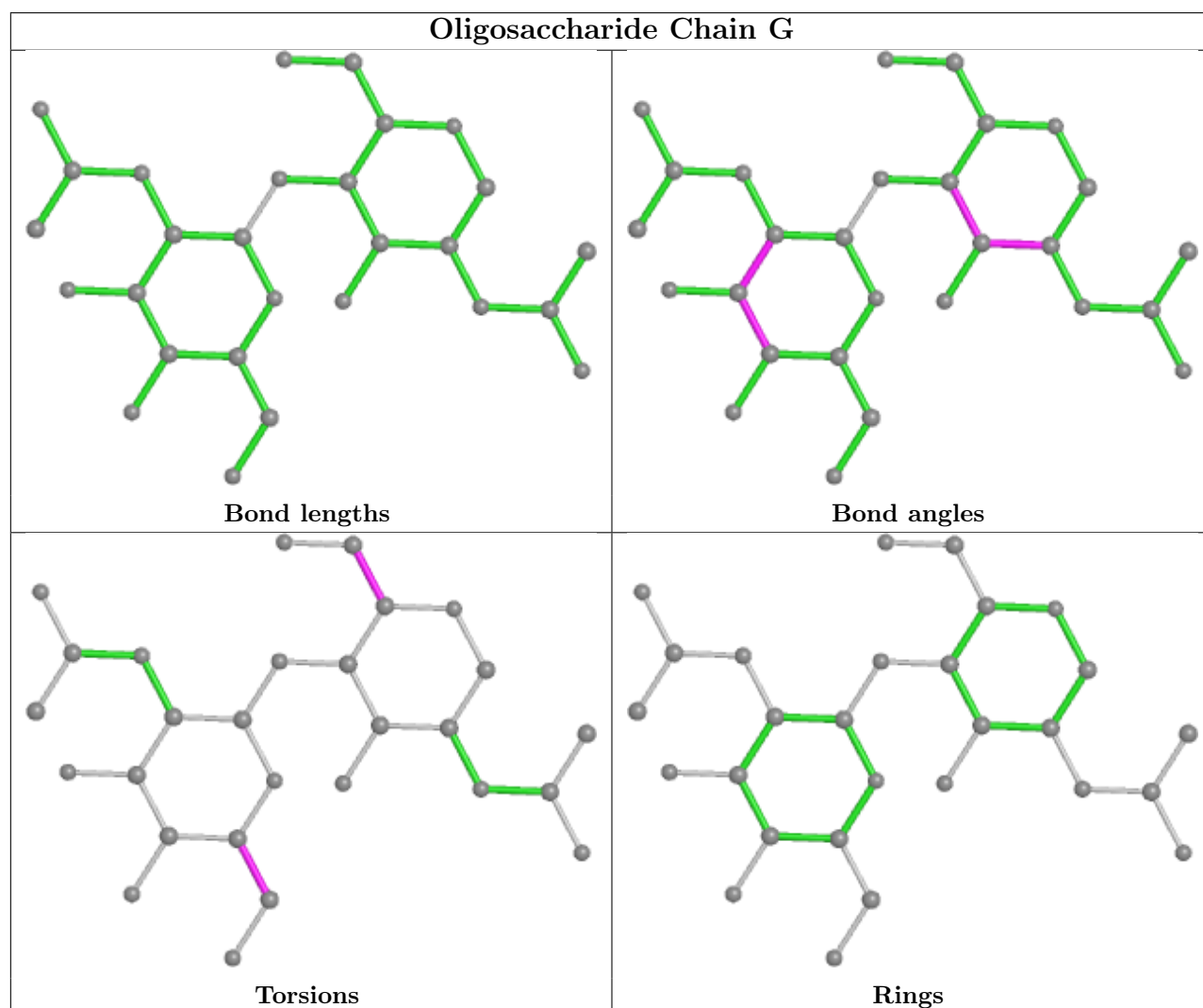
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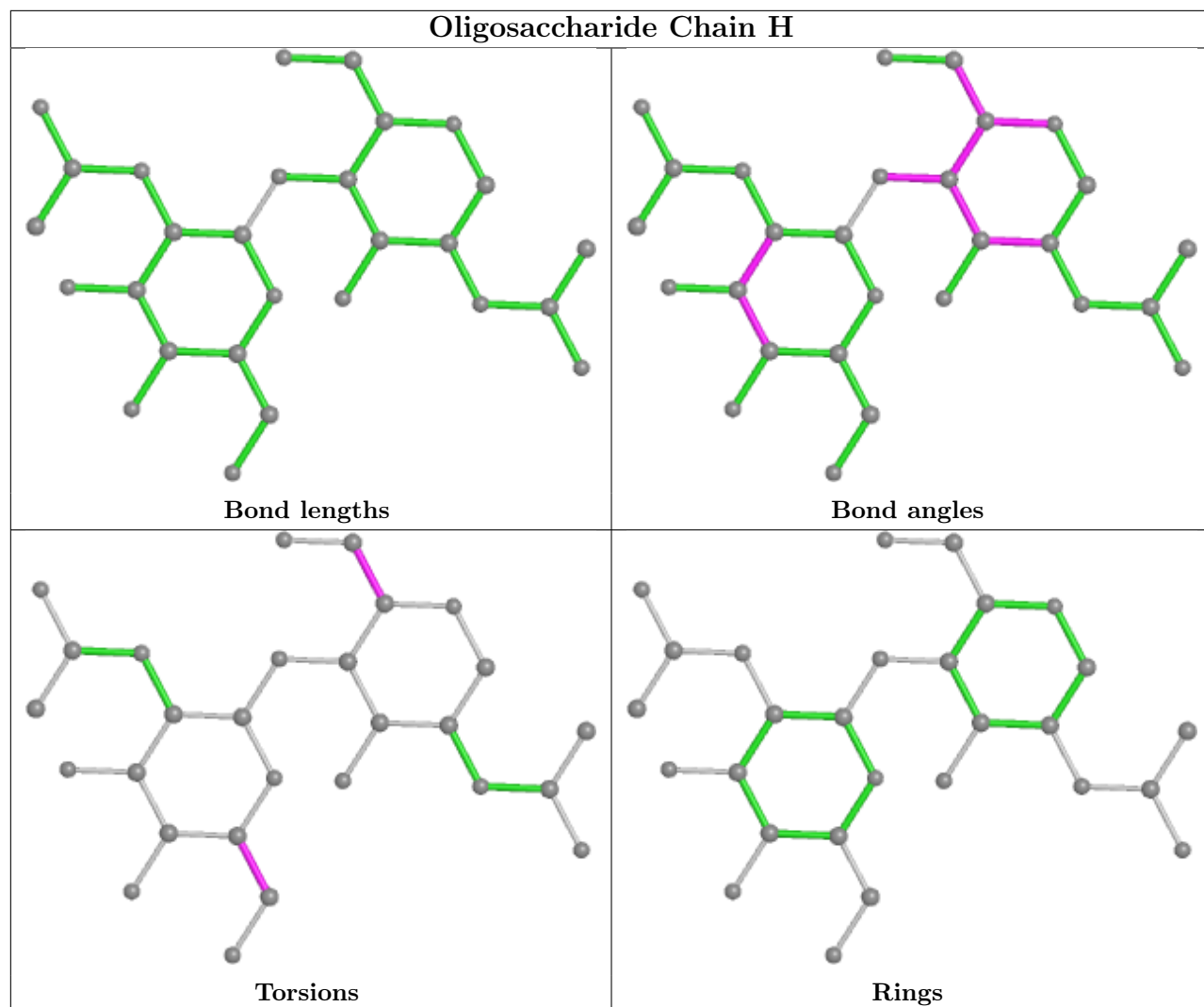
Mol	Chain	Res	Type	Atoms
3	P	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

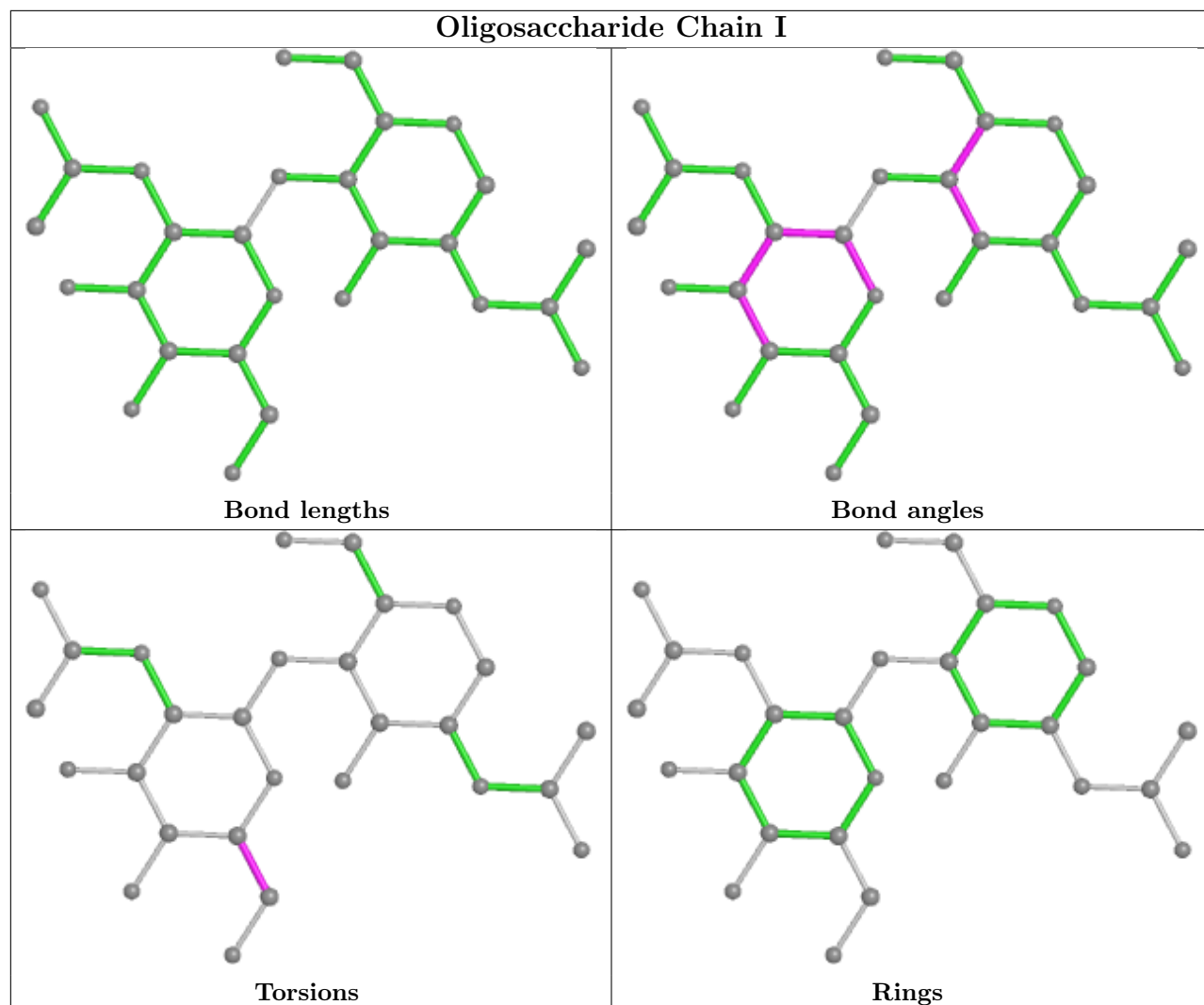
There are no ring outliers.

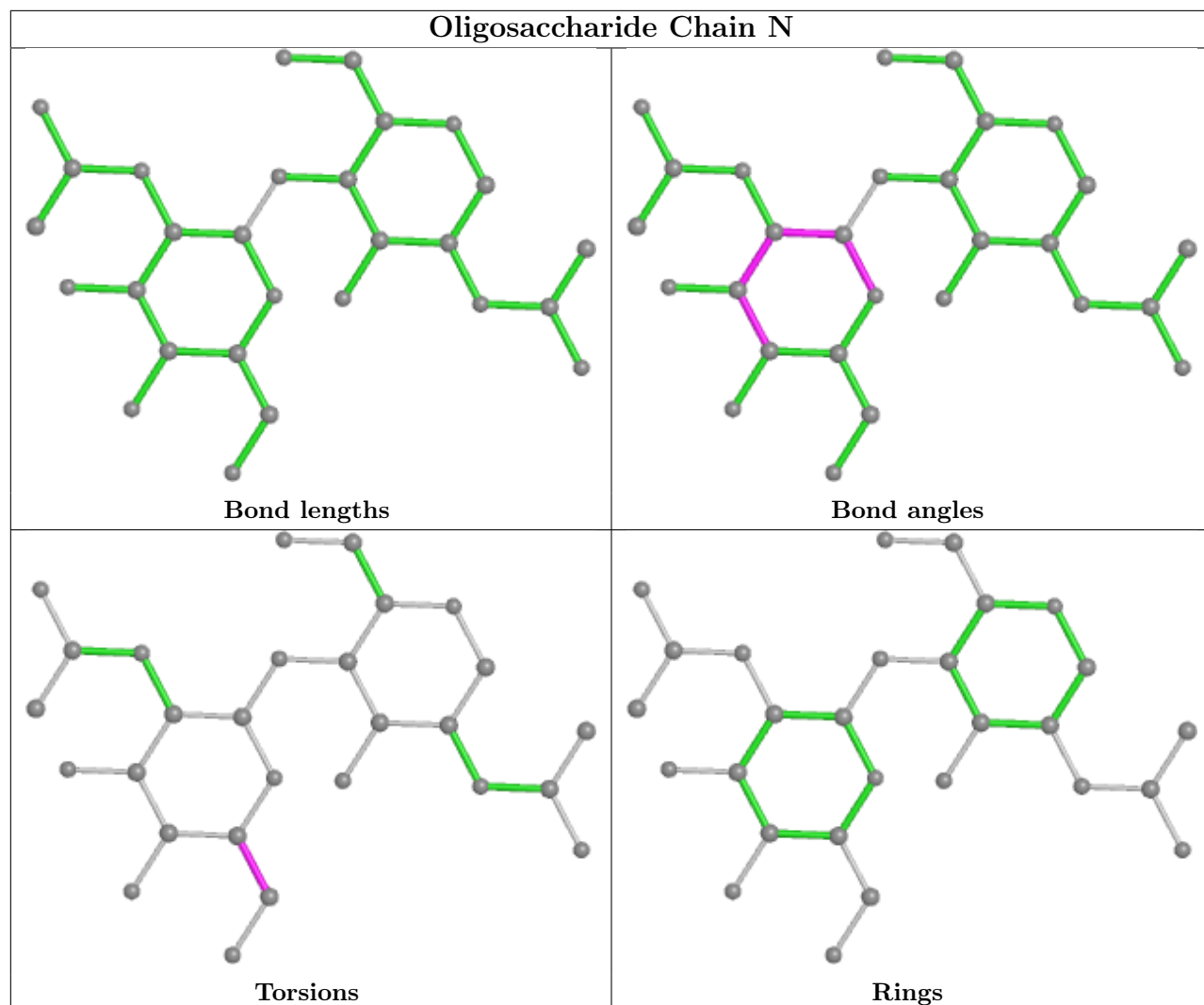
No monomer is involved in short contacts.

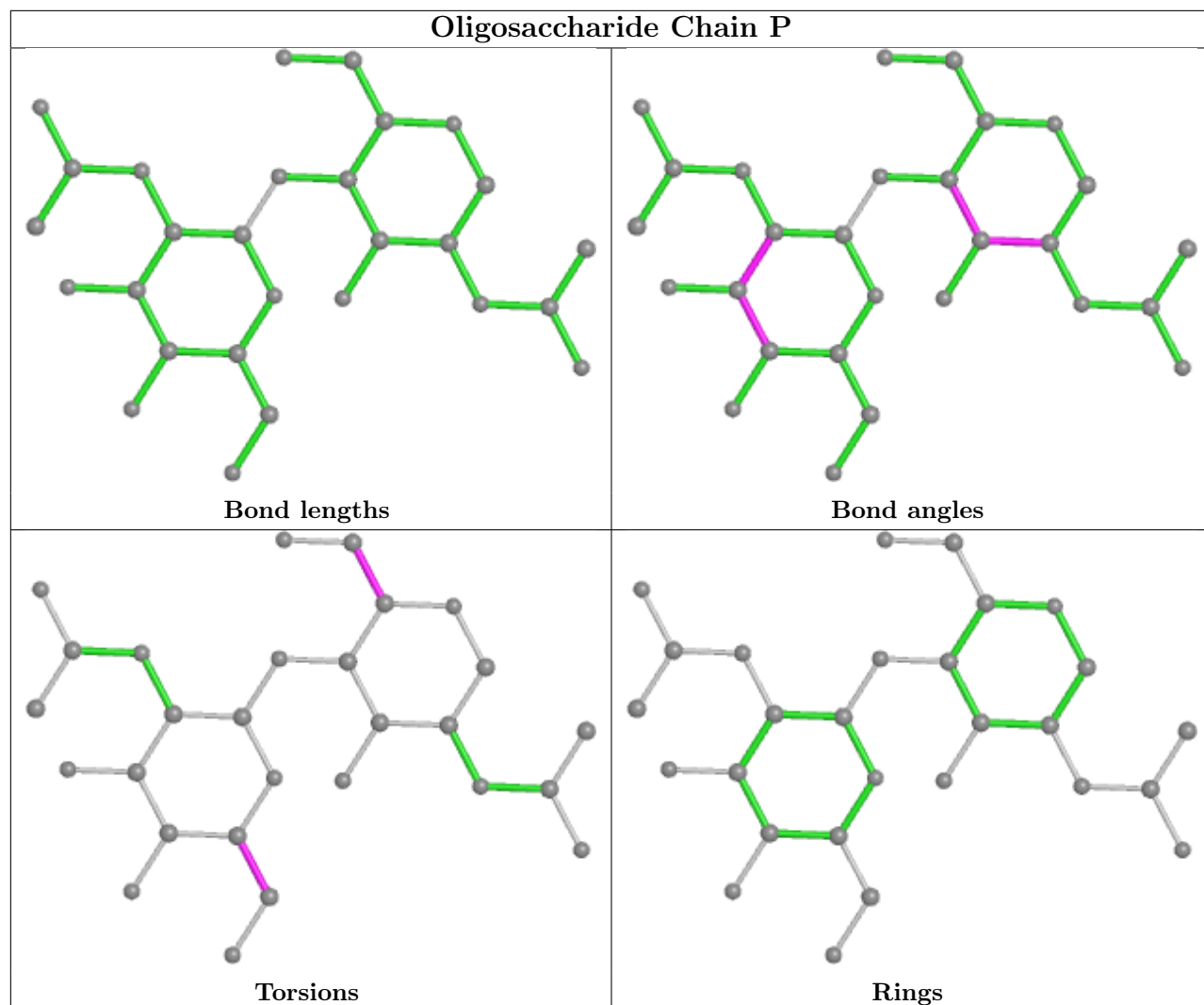
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



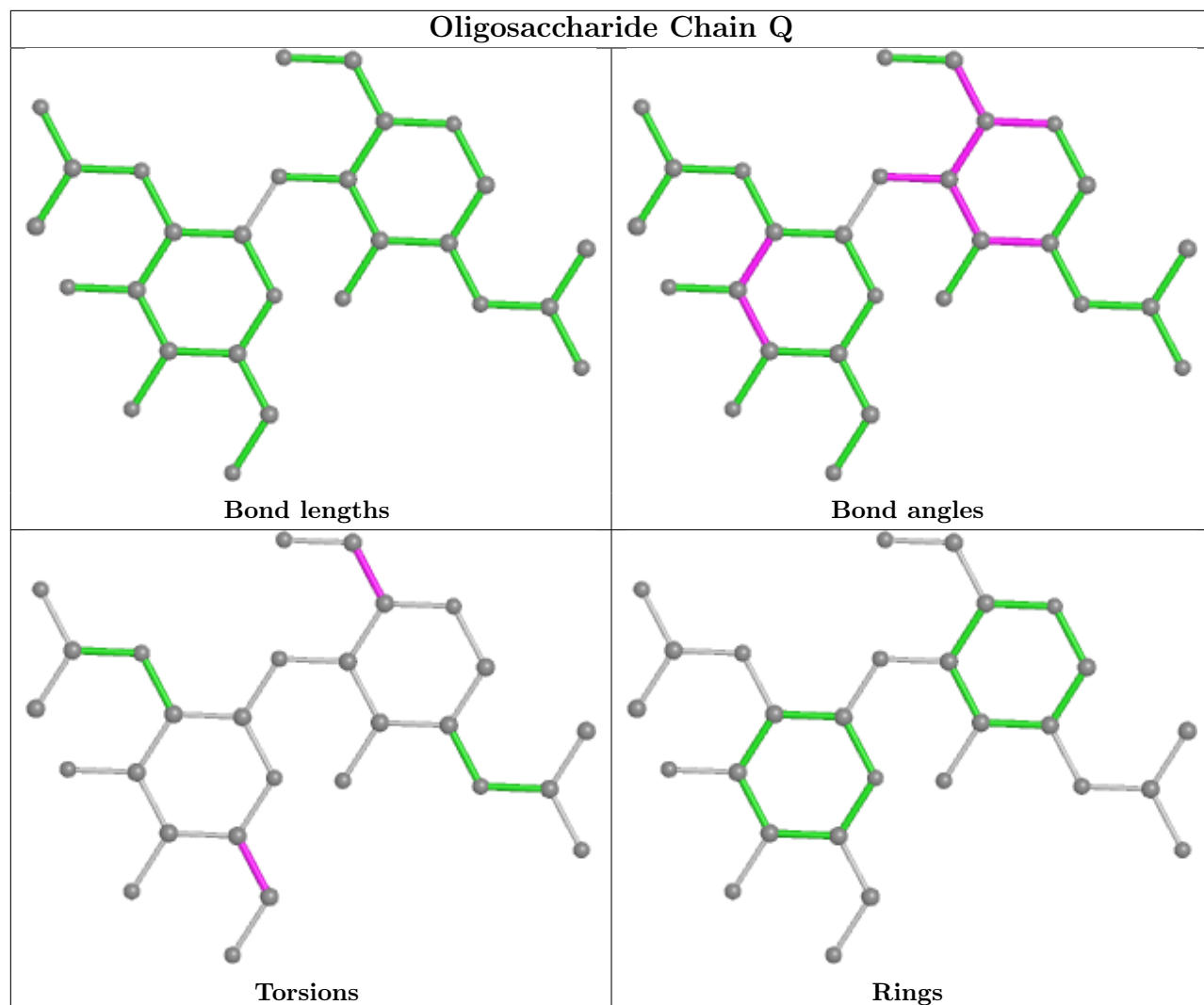


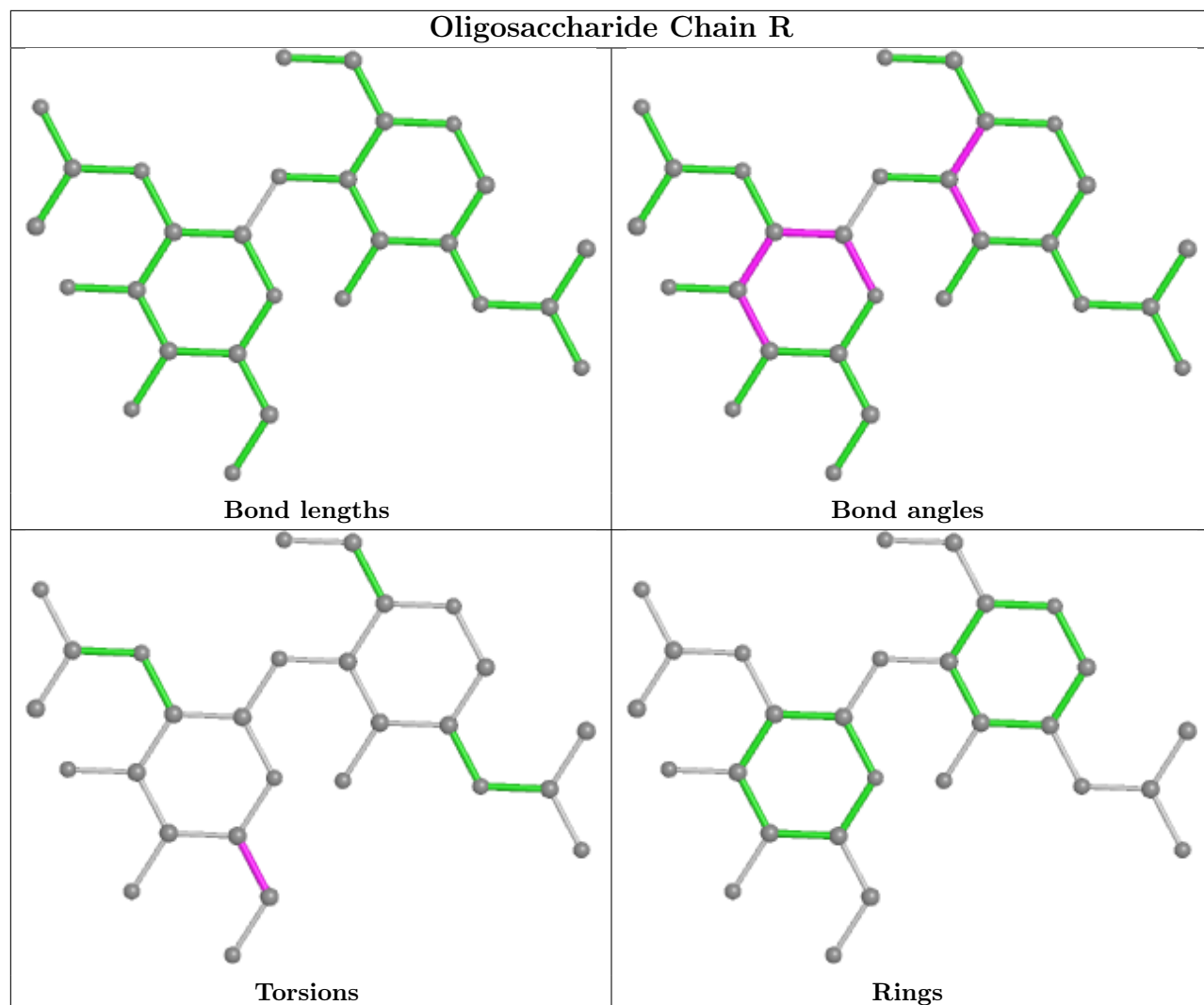


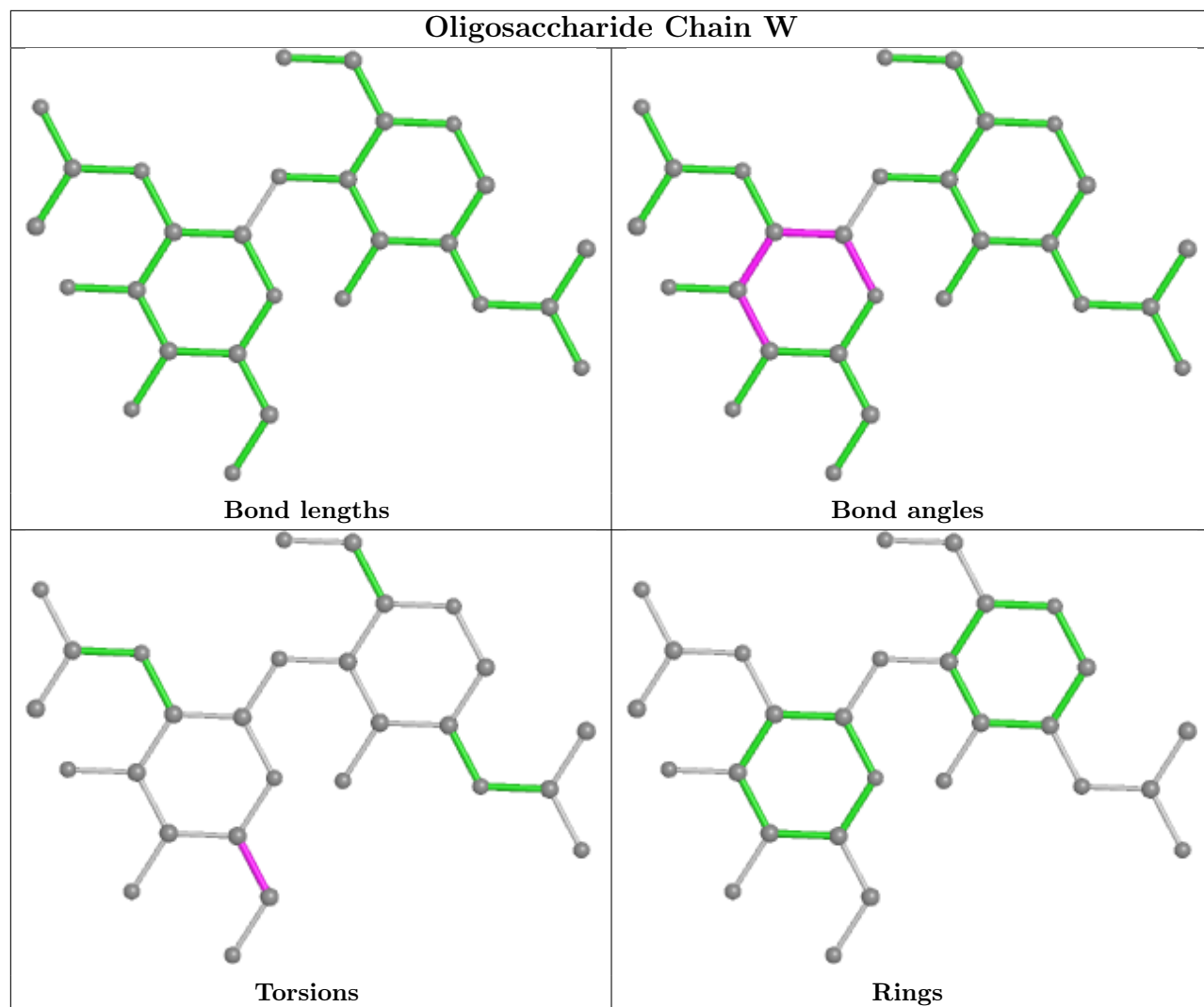


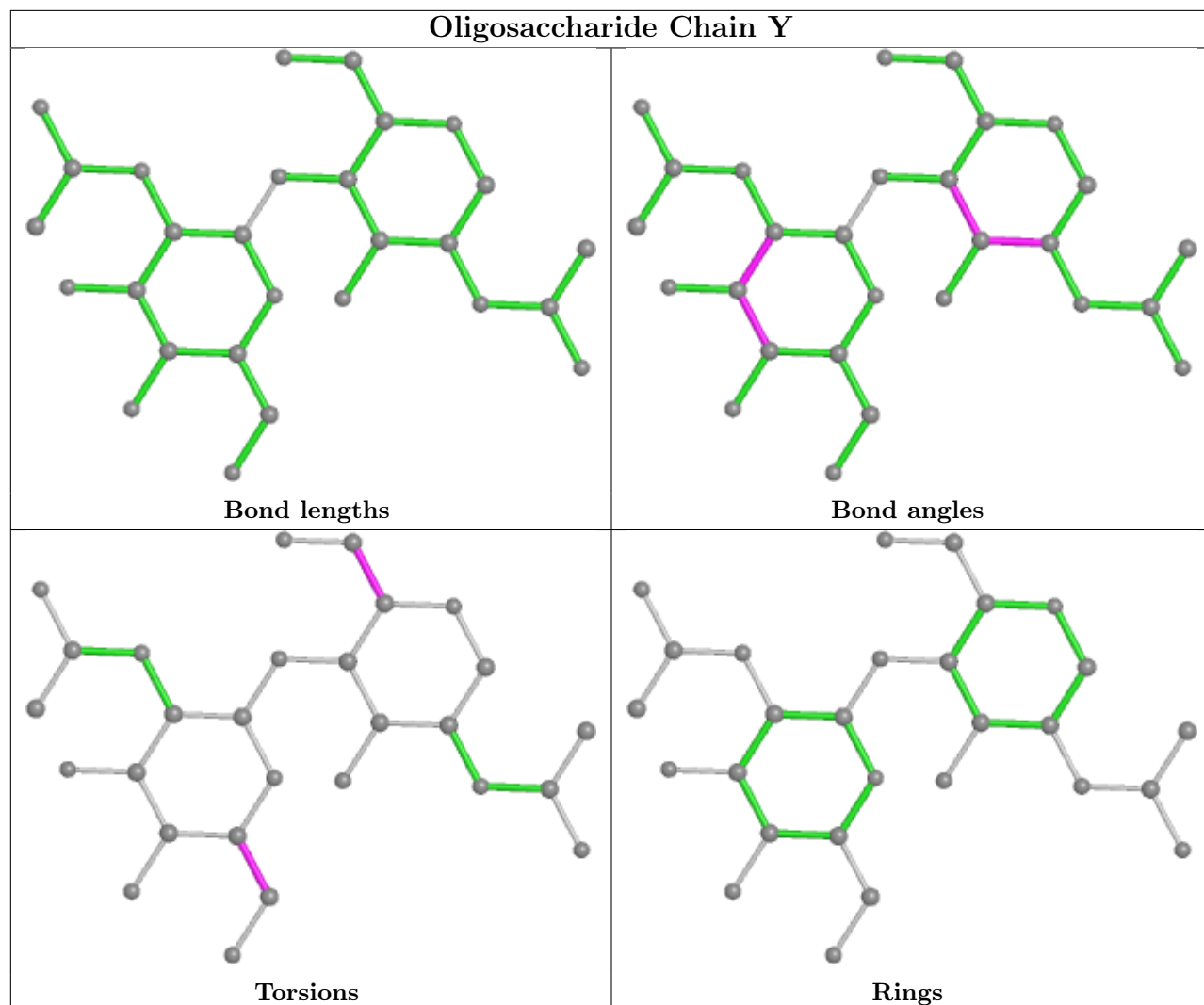


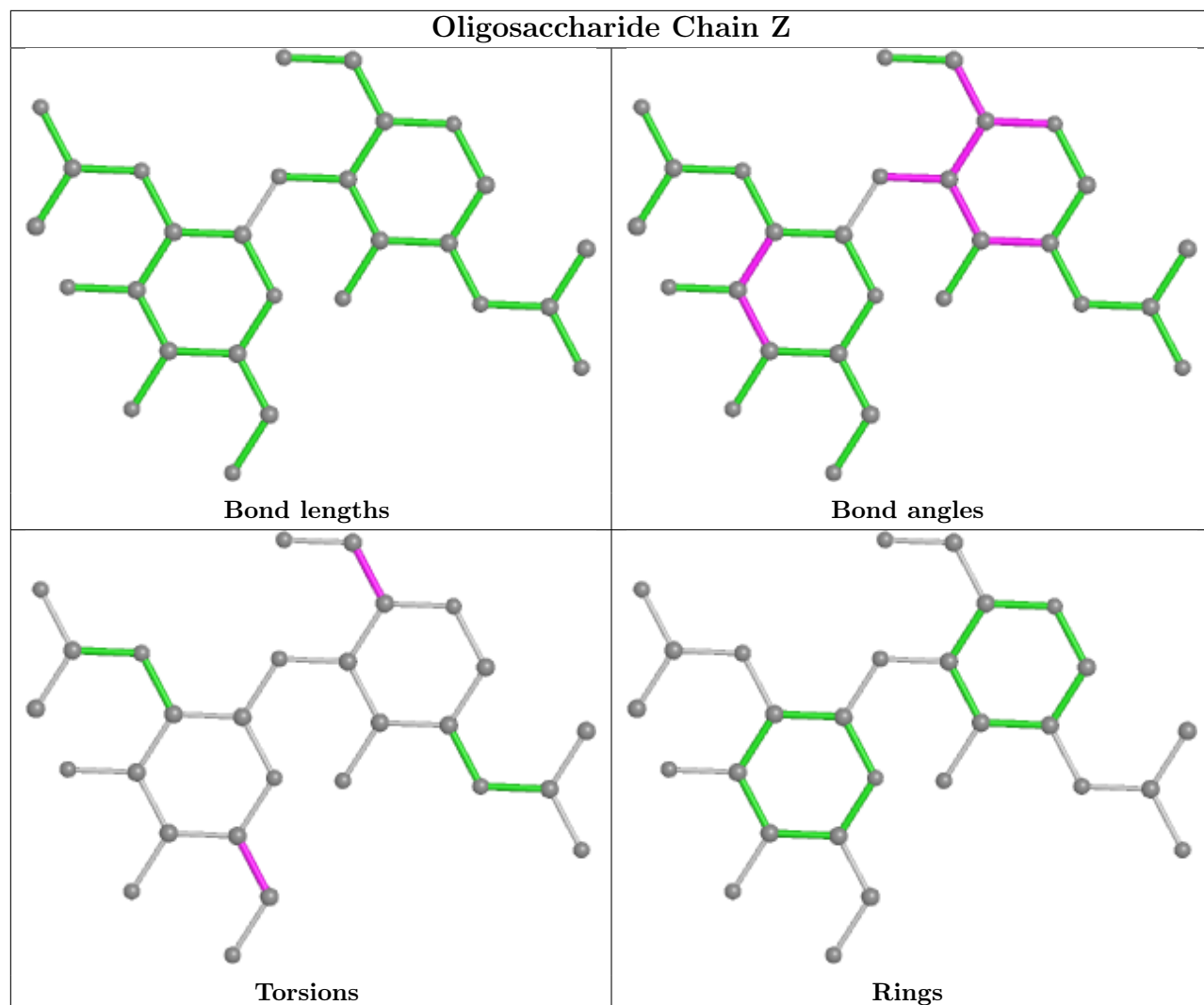


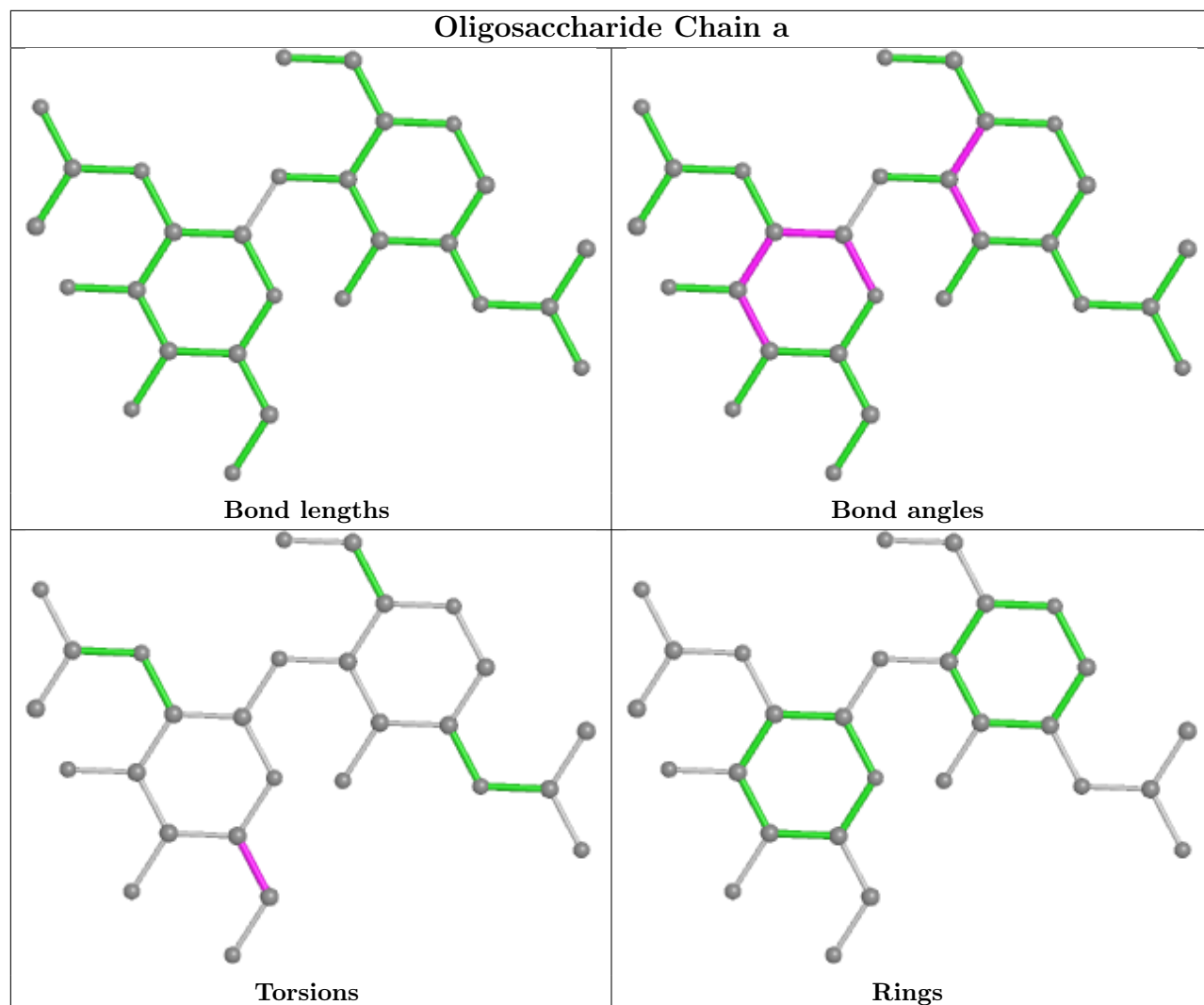


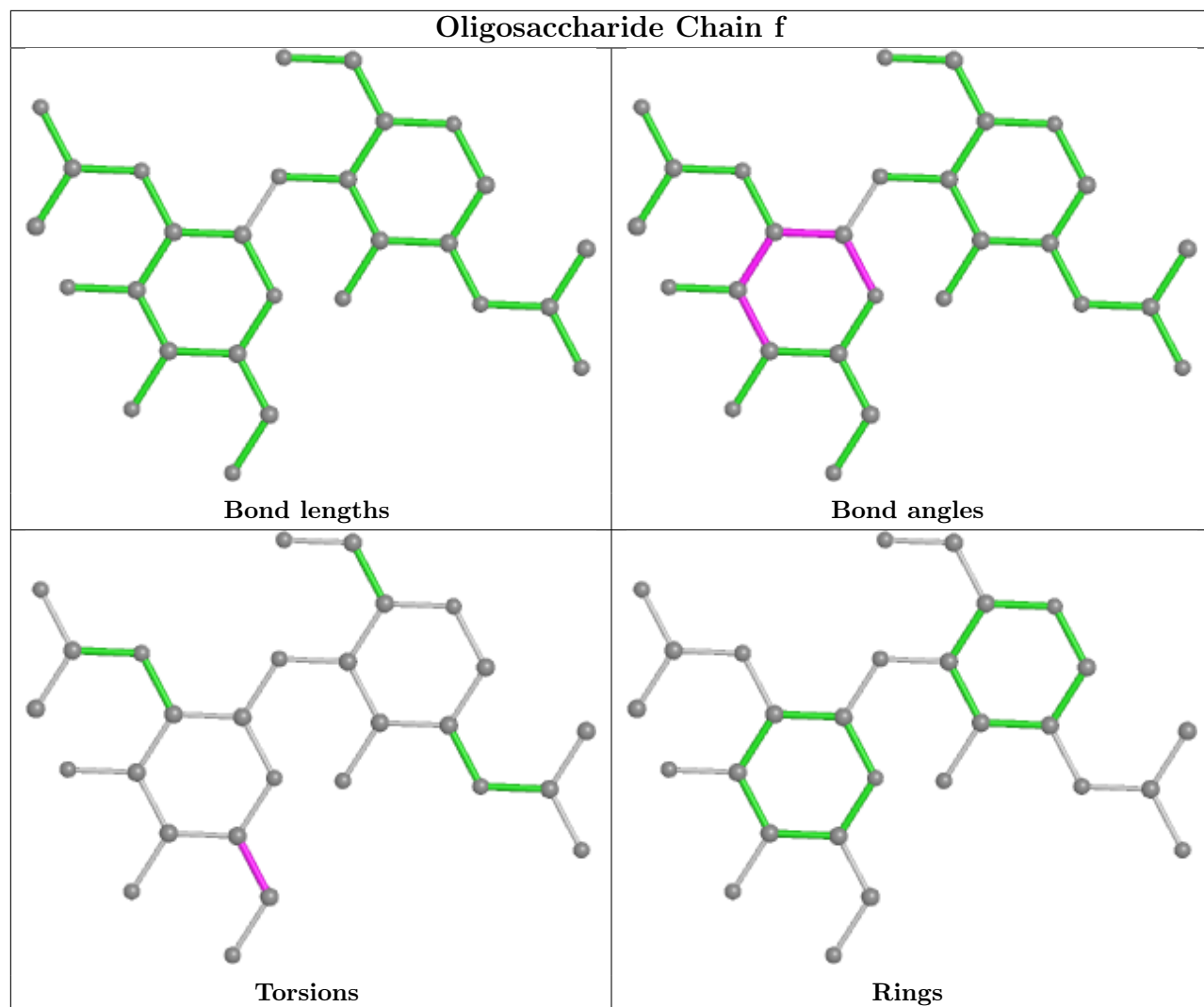


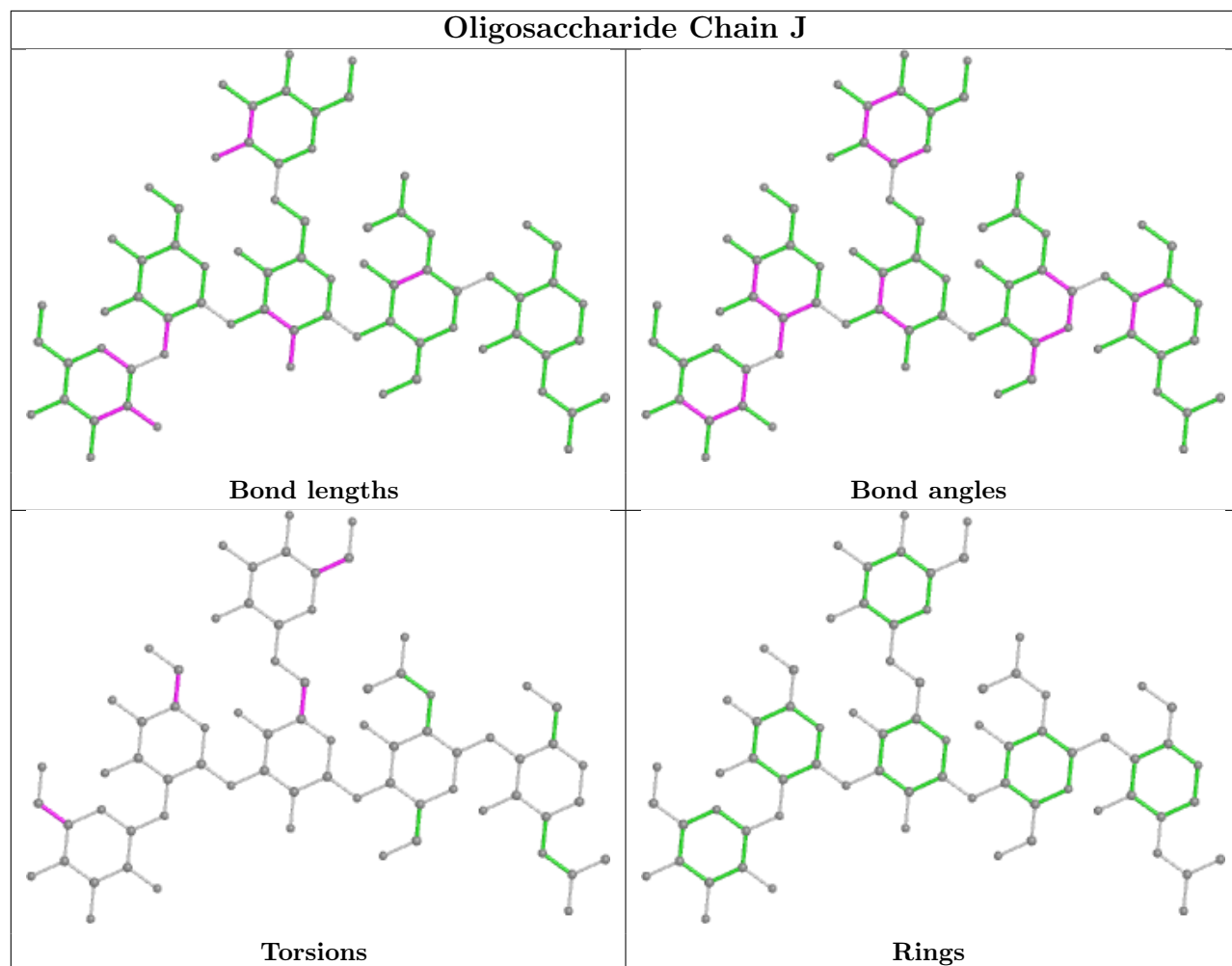




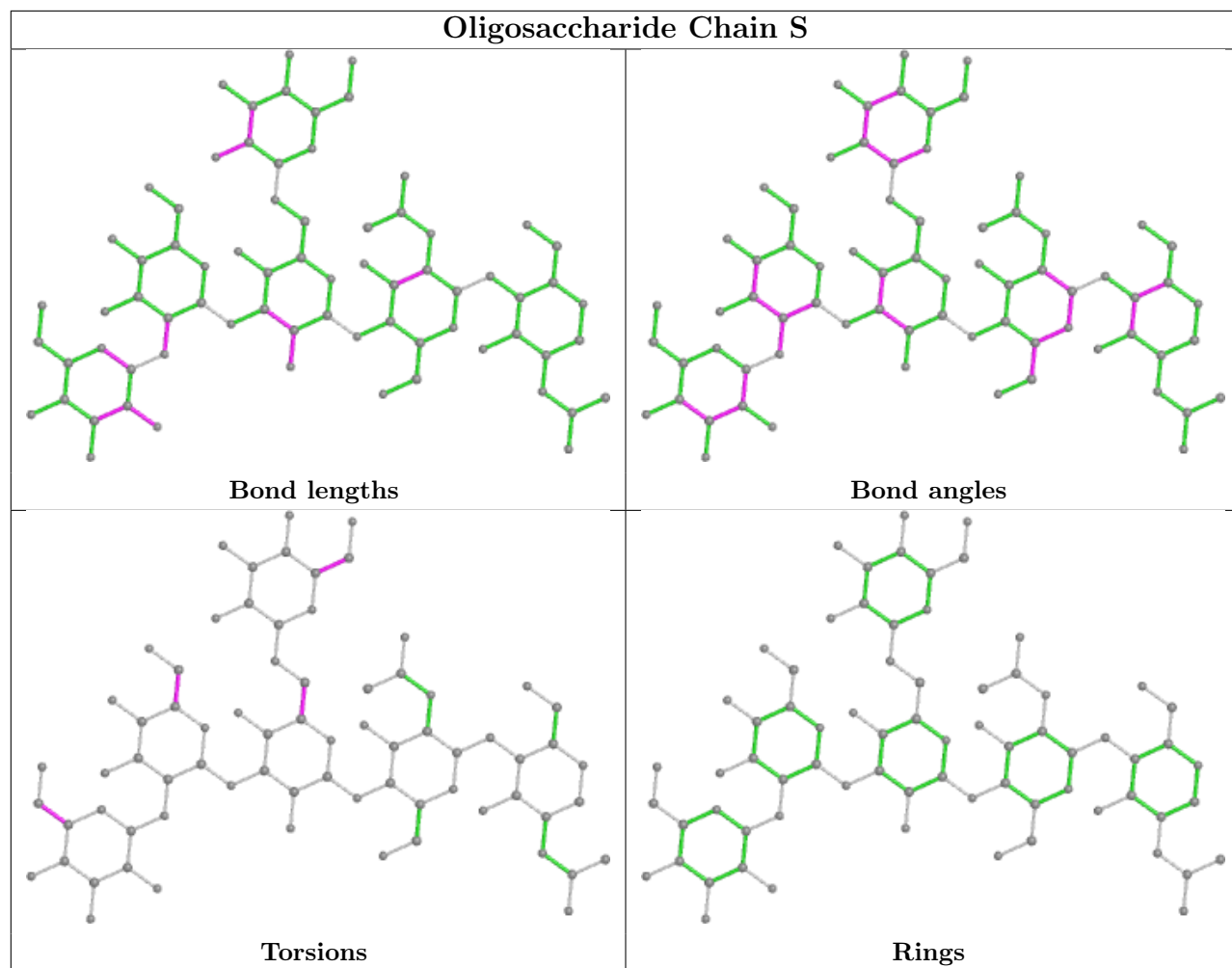


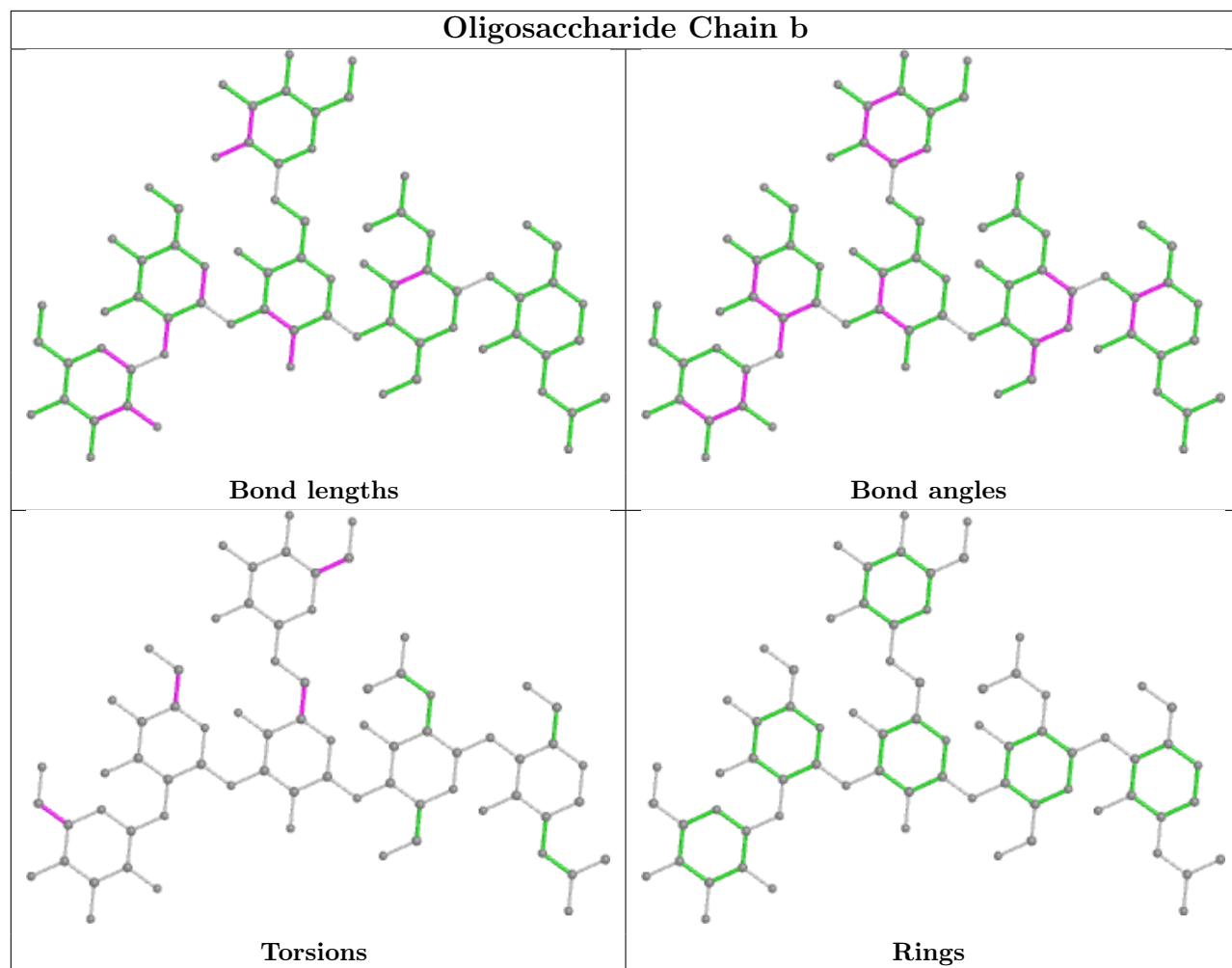


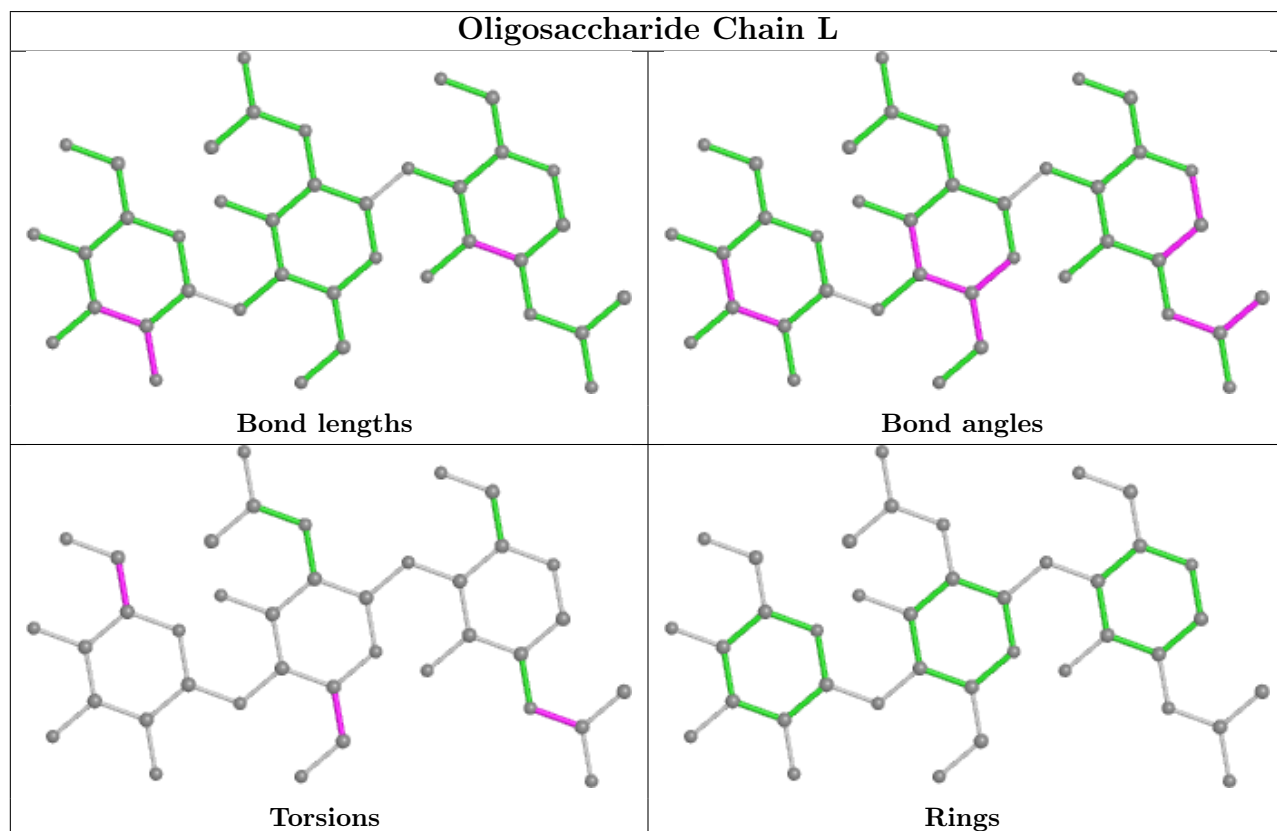
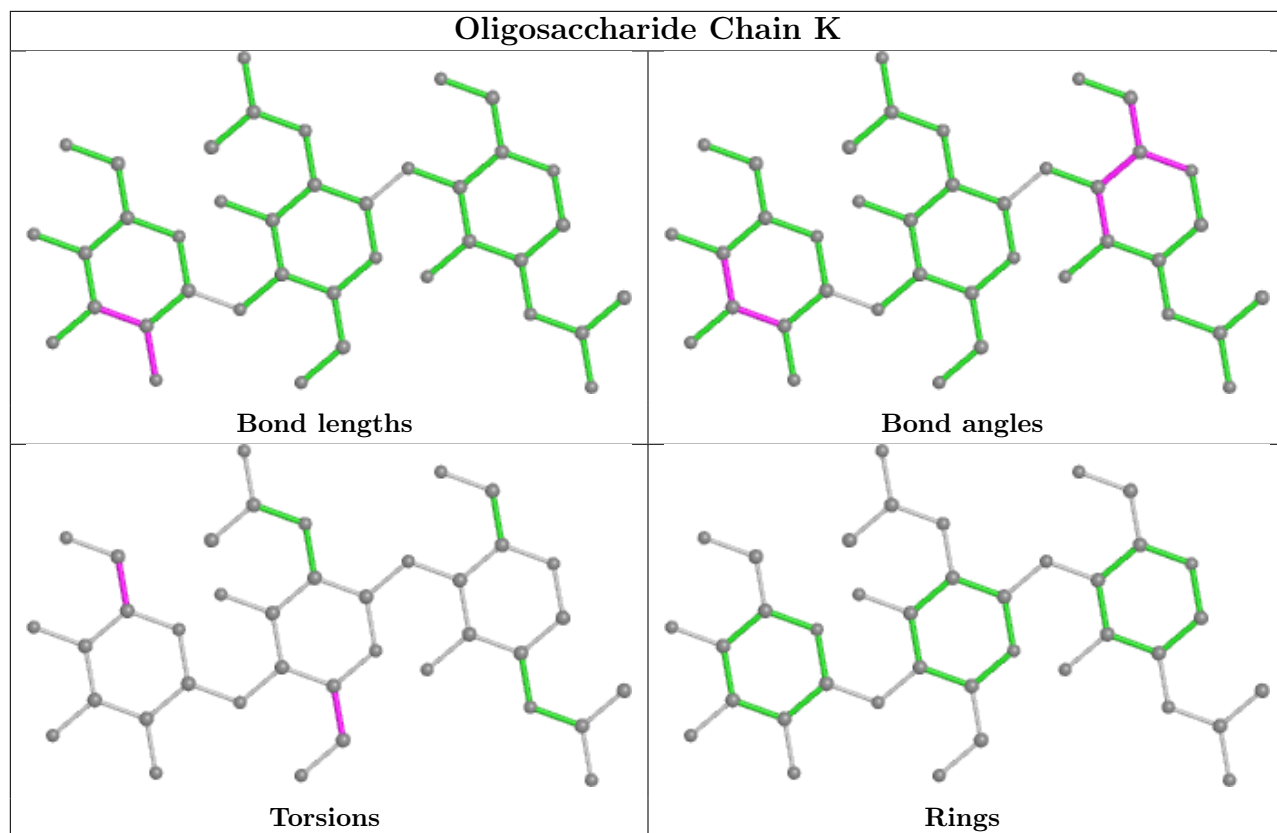


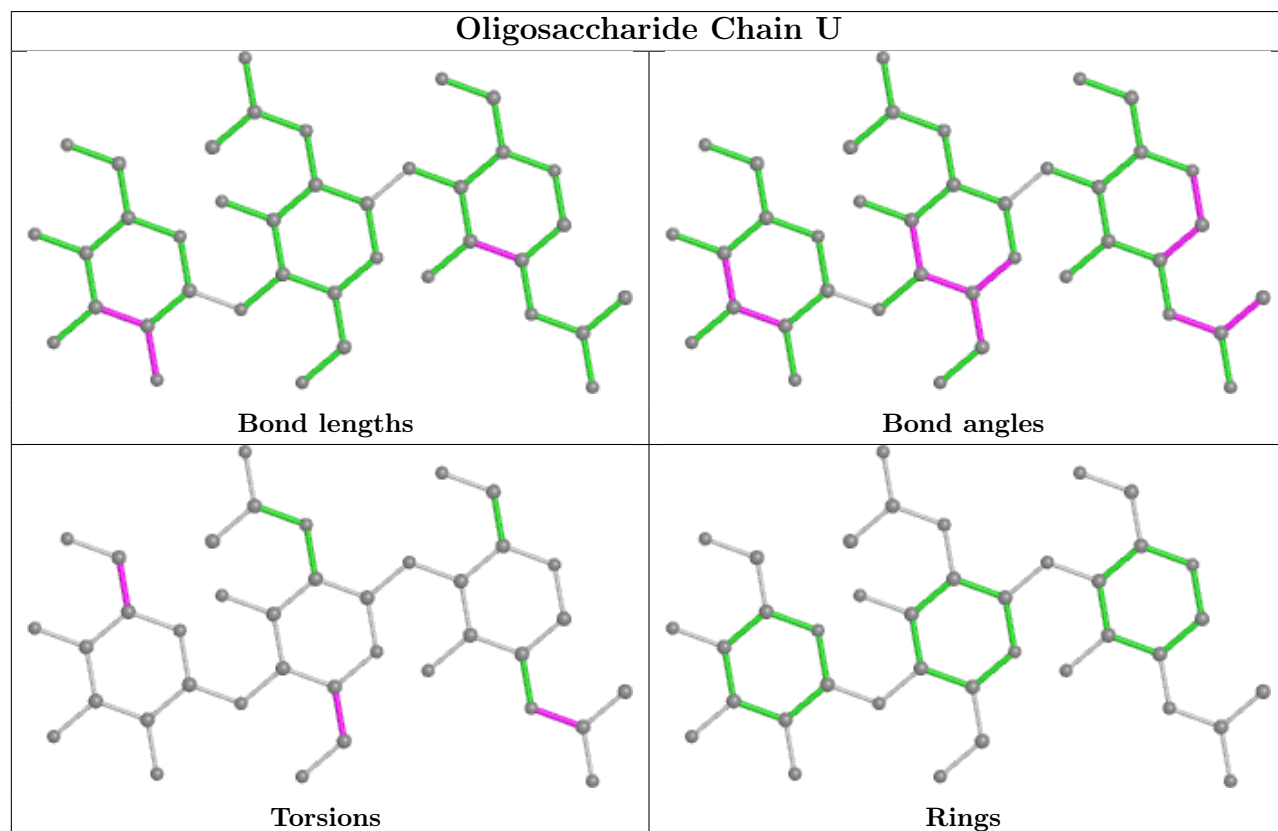
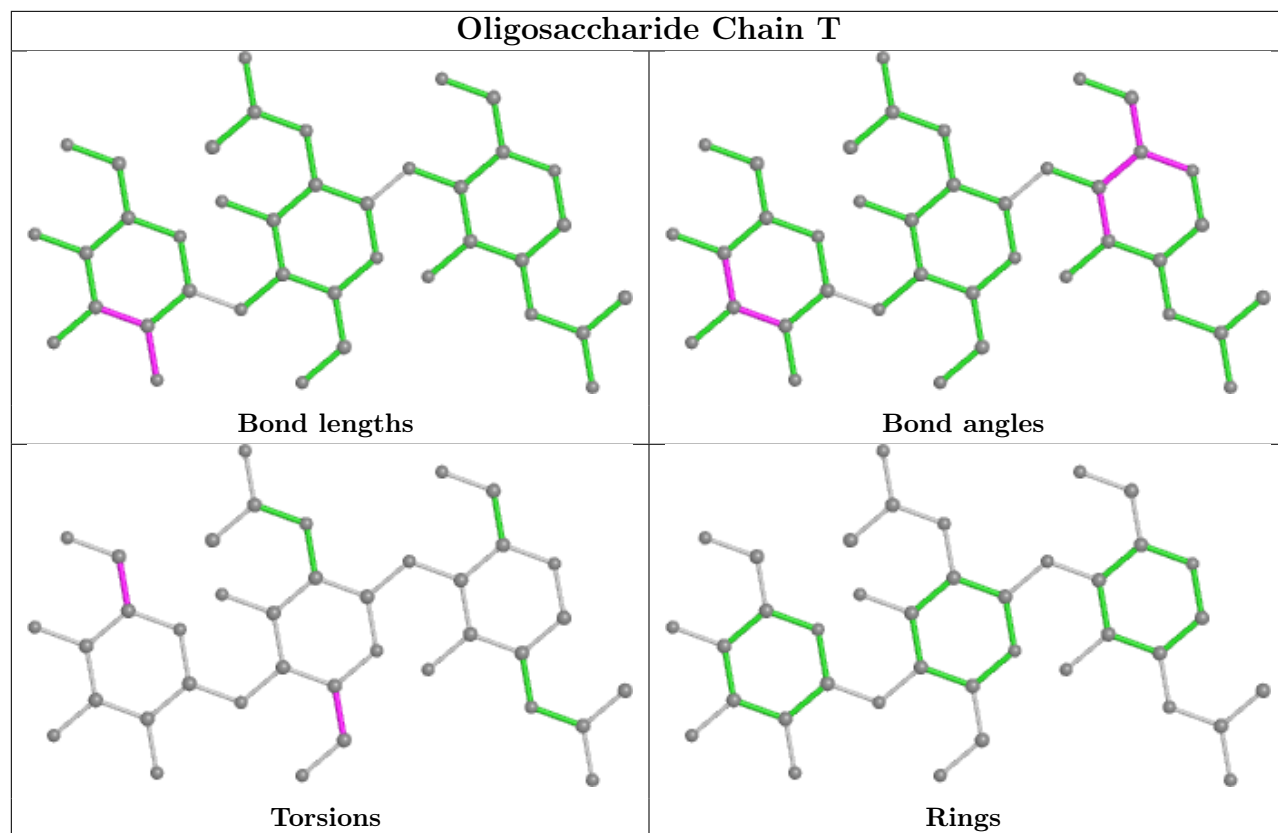


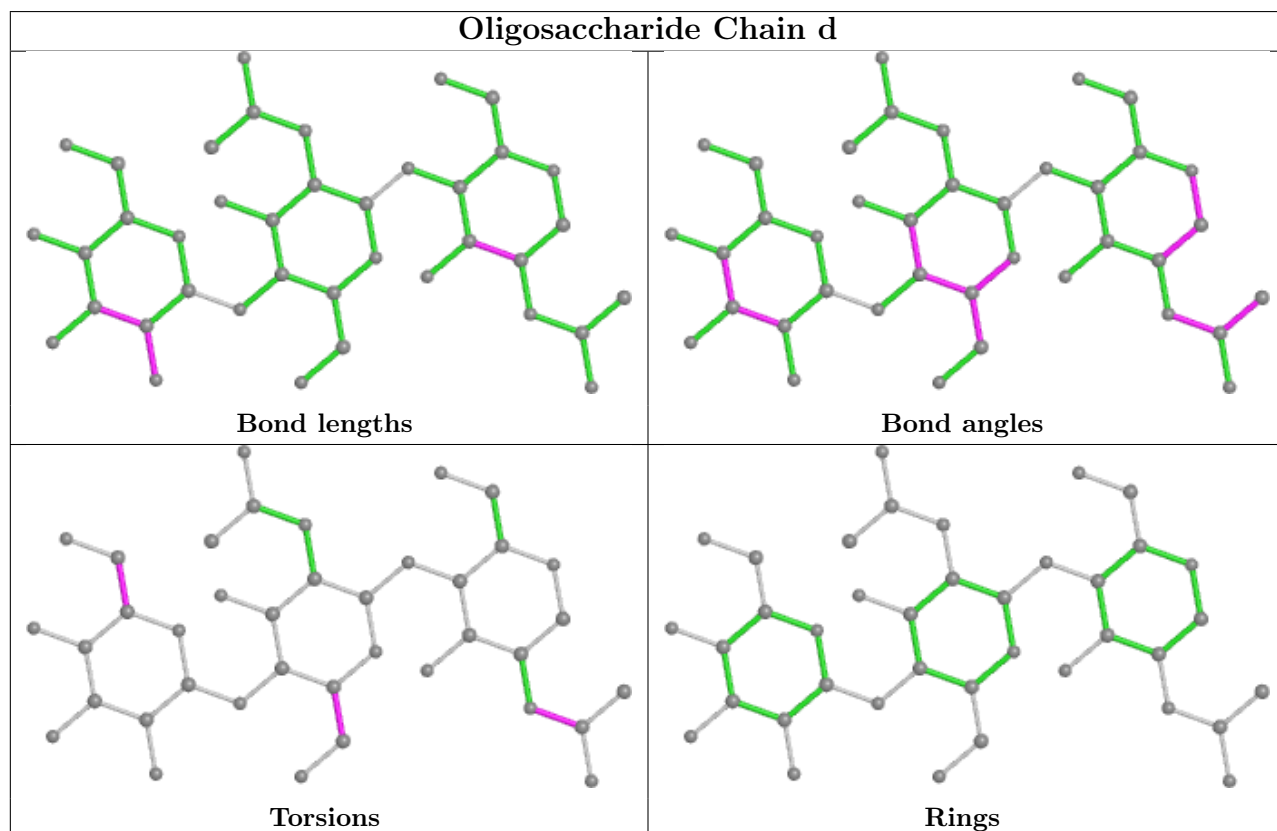
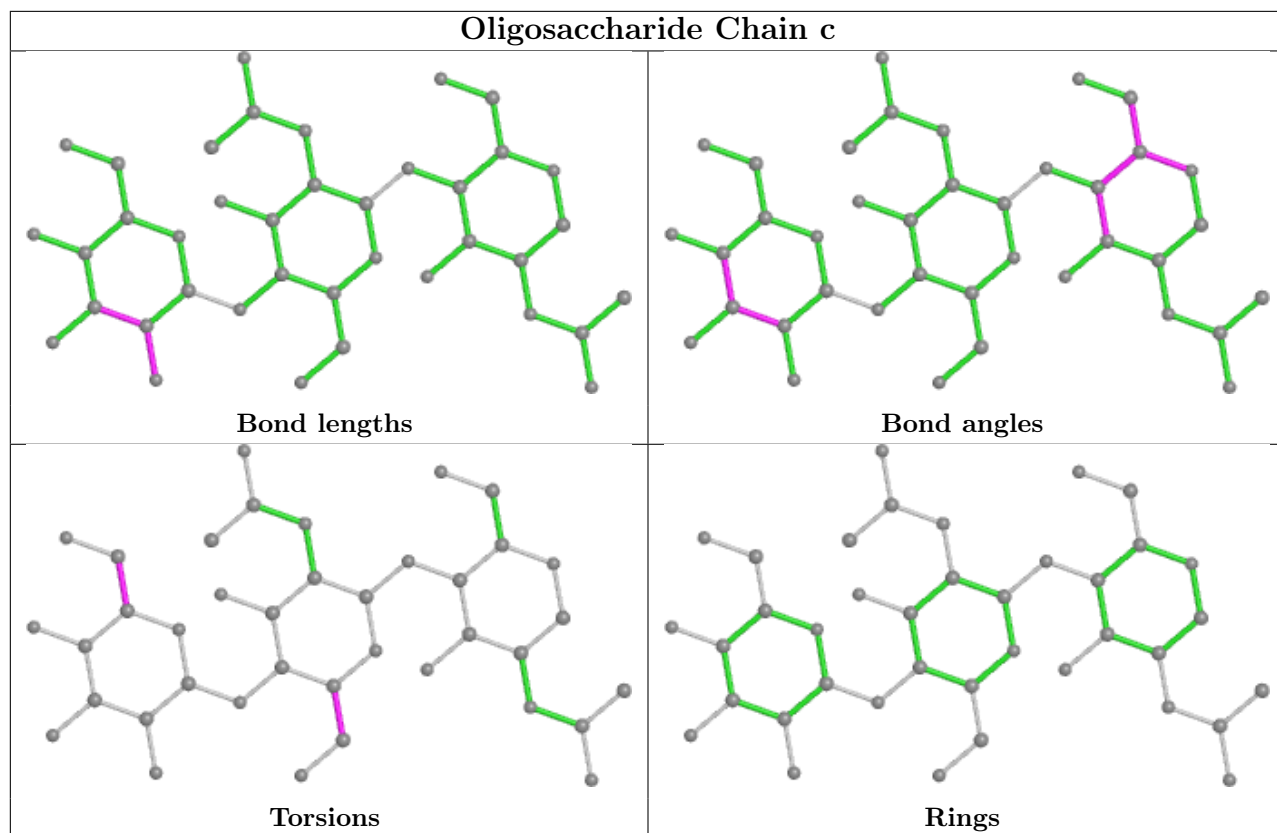


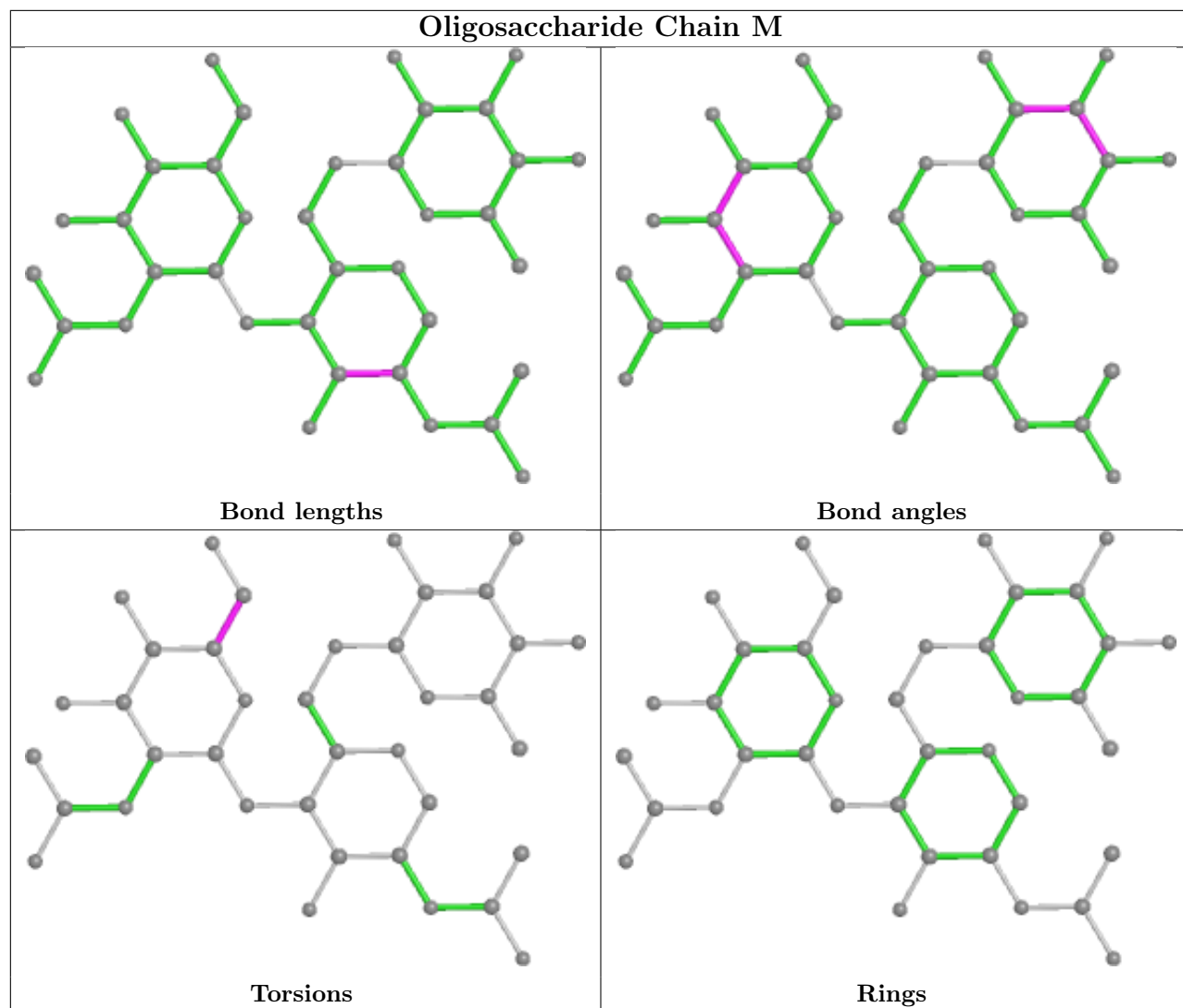


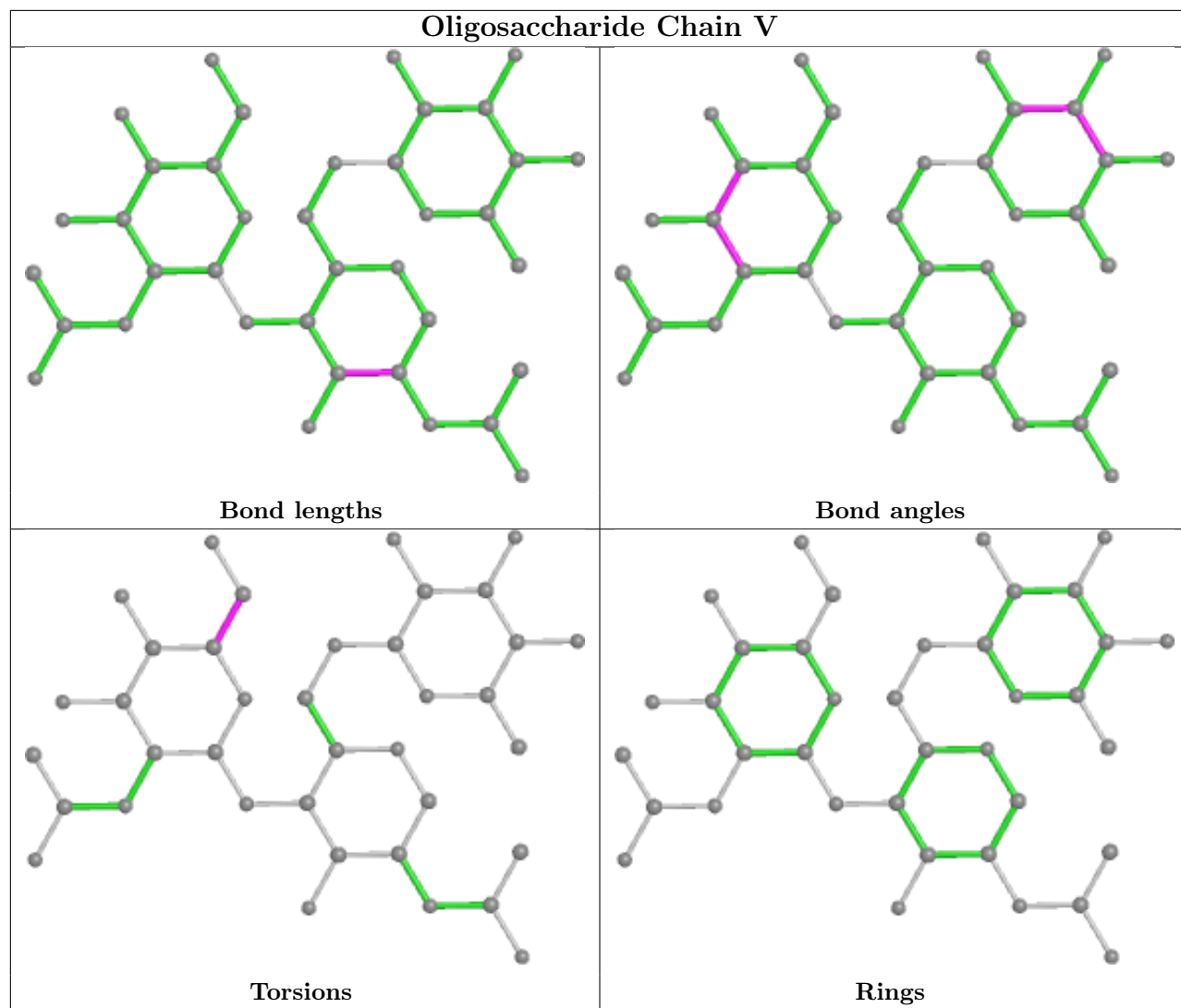


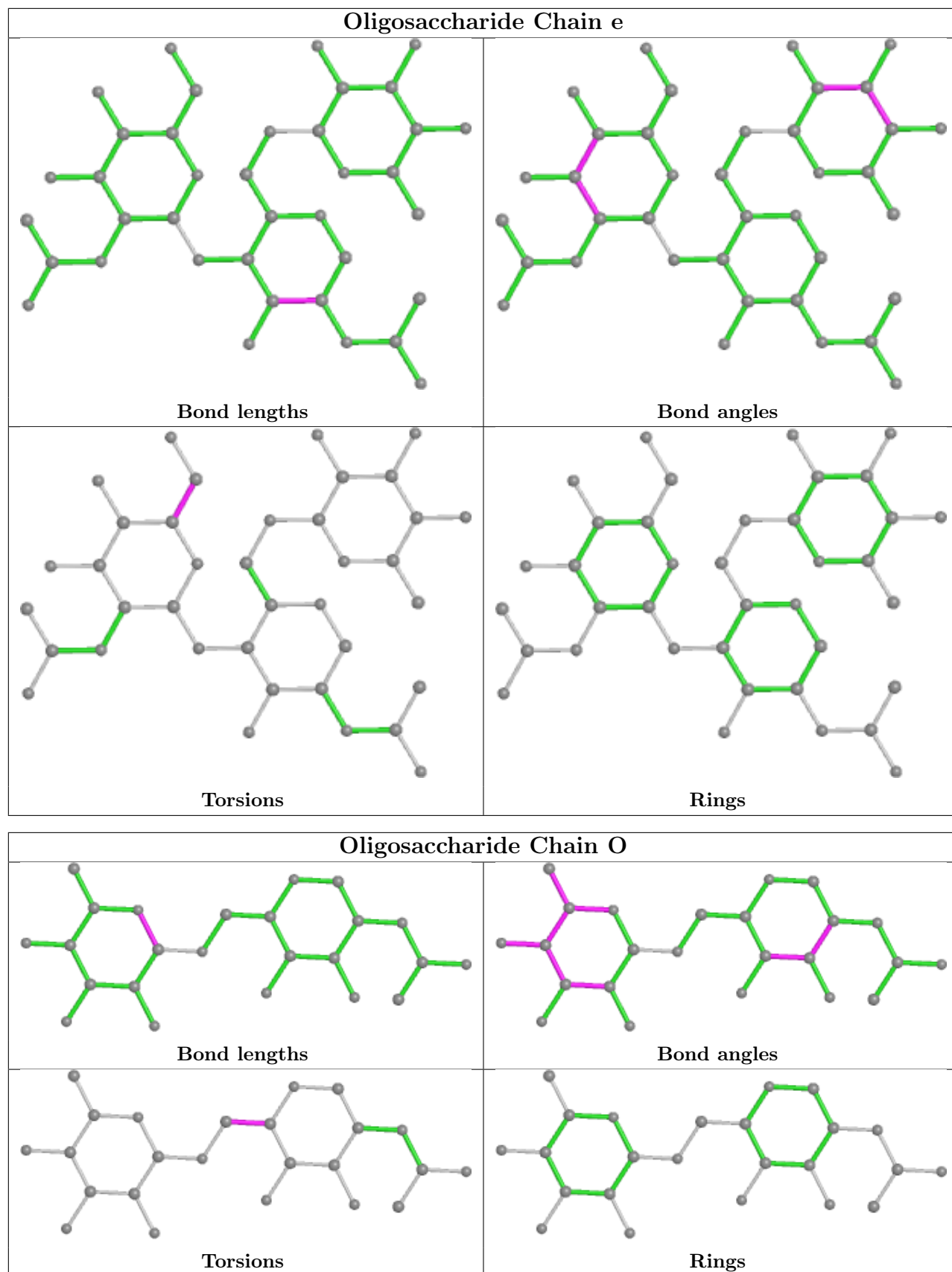




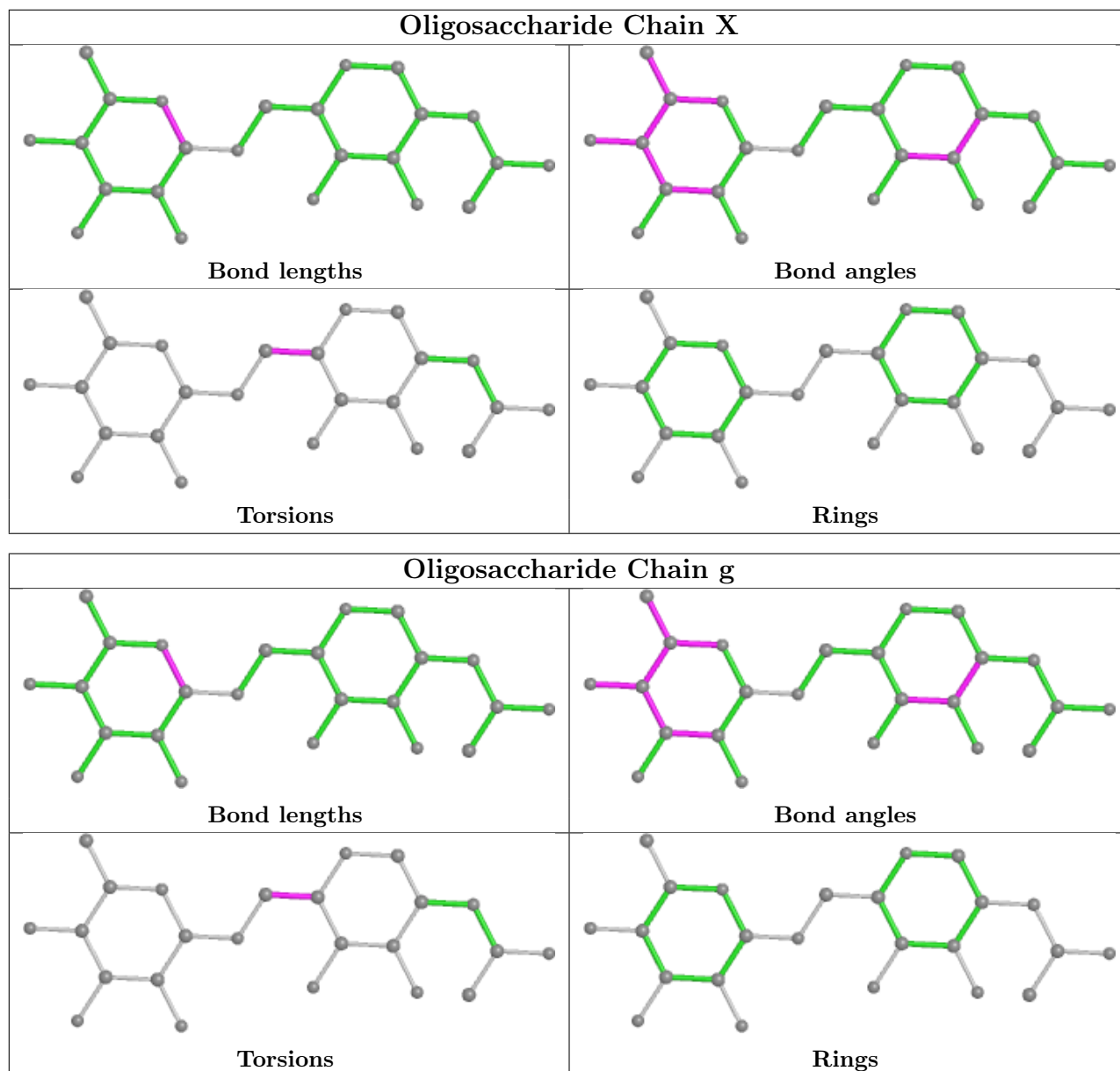












## 5.6 Ligand geometry [i](#)

33 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
8	NAG	C	609	1	14,14,15	0.86	0	17,19,21	1.25	1 (5%)
8	NAG	A	609	1	14,14,15	0.85	0	17,19,21	1.25	1 (5%)
8	NAG	E	704	2	14,14,15	0.90	0	17,19,21	0.96	1 (5%)
8	NAG	D	603	1	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
8	NAG	D	606	1	14,14,15	0.78	0	17,19,21	0.89	1 (5%)
8	NAG	C	632	1	14,14,15	0.81	0	17,19,21	1.08	1 (5%)
8	NAG	F	703	2	14,14,15	0.86	0	17,19,21	0.82	1 (5%)
8	NAG	A	603	1	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
8	NAG	D	618	1	14,14,15	0.89	1 (7%)	17,19,21	1.03	2 (11%)
8	NAG	A	606	1	14,14,15	0.78	0	17,19,21	0.90	1 (5%)
8	NAG	C	603	1	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
8	NAG	D	610	1	14,14,15	0.82	0	17,19,21	0.98	1 (5%)
8	NAG	C	611	1	14,14,15	0.88	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	C	622	1	14,14,15	0.83	0	17,19,21	0.75	0
8	NAG	F	704	2	14,14,15	0.90	0	17,19,21	0.96	1 (5%)
8	NAG	D	609	1	14,14,15	0.86	0	17,19,21	1.25	1 (5%)
8	NAG	A	623	1	14,14,15	0.88	0	17,19,21	0.88	1 (5%)
8	NAG	A	618	1	14,14,15	0.89	1 (7%)	17,19,21	1.03	2 (11%)
8	NAG	A	611	1	14,14,15	0.88	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	A	622	1	14,14,15	0.83	0	17,19,21	0.75	0
8	NAG	D	623	1	14,14,15	0.89	0	17,19,21	0.88	1 (5%)
8	NAG	A	610	1	14,14,15	0.83	0	17,19,21	0.98	1 (5%)
8	NAG	C	606	1	14,14,15	0.78	0	17,19,21	0.90	1 (5%)
8	NAG	D	611	1	14,14,15	0.88	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	D	632	1	14,14,15	0.81	0	17,19,21	1.07	1 (5%)
8	NAG	C	623	1	14,14,15	0.89	0	17,19,21	0.88	1 (5%)
8	NAG	E	703	2	14,14,15	0.86	0	17,19,21	0.82	1 (5%)
8	NAG	B	703	2	14,14,15	0.86	0	17,19,21	0.82	1 (5%)
8	NAG	A	632	1	14,14,15	0.81	0	17,19,21	1.07	1 (5%)
8	NAG	C	618	1	14,14,15	0.89	1 (7%)	17,19,21	1.03	2 (11%)
8	NAG	B	704	2	14,14,15	0.91	0	17,19,21	0.96	1 (5%)
8	NAG	D	622	1	14,14,15	0.83	0	17,19,21	0.75	0
8	NAG	C	610	1	14,14,15	0.83	0	17,19,21	0.98	1 (5%)

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
8	NAG	C	609	1	-	1/6/23/26	0/1/1/1
8	NAG	A	609	1	-	1/6/23/26	0/1/1/1
8	NAG	E	704	2	-	1/6/23/26	0/1/1/1
8	NAG	D	603	1	-	1/6/23/26	0/1/1/1
8	NAG	D	606	1	-	2/6/23/26	0/1/1/1
8	NAG	C	632	1	-	2/6/23/26	0/1/1/1
8	NAG	F	703	2	-	1/6/23/26	0/1/1/1
8	NAG	A	603	1	-	1/6/23/26	0/1/1/1
8	NAG	D	618	1	-	1/6/23/26	0/1/1/1
8	NAG	A	606	1	-	2/6/23/26	0/1/1/1
8	NAG	C	603	1	-	1/6/23/26	0/1/1/1
8	NAG	D	610	1	-	1/6/23/26	0/1/1/1
8	NAG	C	611	1	-	2/6/23/26	0/1/1/1
8	NAG	C	622	1	-	2/6/23/26	0/1/1/1
8	NAG	F	704	2	-	1/6/23/26	0/1/1/1
8	NAG	D	609	1	-	1/6/23/26	0/1/1/1
8	NAG	A	623	1	-	2/6/23/26	0/1/1/1
8	NAG	A	618	1	-	1/6/23/26	0/1/1/1
8	NAG	A	611	1	-	2/6/23/26	0/1/1/1
8	NAG	A	622	1	-	2/6/23/26	0/1/1/1
8	NAG	D	623	1	-	2/6/23/26	0/1/1/1
8	NAG	A	610	1	-	1/6/23/26	0/1/1/1
8	NAG	C	606	1	-	2/6/23/26	0/1/1/1
8	NAG	D	611	1	-	2/6/23/26	0/1/1/1
8	NAG	D	632	1	-	2/6/23/26	0/1/1/1
8	NAG	C	623	1	-	2/6/23/26	0/1/1/1
8	NAG	E	703	2	-	1/6/23/26	0/1/1/1
8	NAG	B	703	2	-	1/6/23/26	0/1/1/1
8	NAG	A	632	1	-	2/6/23/26	0/1/1/1
8	NAG	C	618	1	-	1/6/23/26	0/1/1/1
8	NAG	B	704	2	-	1/6/23/26	0/1/1/1
8	NAG	D	622	1	-	2/6/23/26	0/1/1/1
8	NAG	C	610	1	-	1/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	618	NAG	C3-C2	-2.03	1.48	1.52
8	D	611	NAG	C3-C2	-2.02	1.48	1.52
8	A	611	NAG	C3-C2	-2.01	1.48	1.52
8	C	618	NAG	C3-C2	-2.01	1.48	1.52
8	C	611	NAG	C3-C2	-2.01	1.48	1.52
8	A	618	NAG	C3-C2	-2.00	1.48	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	609	NAG	C4-C3-C2	-4.04	105.10	111.02
8	D	609	NAG	C4-C3-C2	-4.04	105.10	111.02
8	C	609	NAG	C4-C3-C2	-4.03	105.11	111.02
8	C	632	NAG	C4-C3-C2	-3.35	106.11	111.02
8	A	632	NAG	C4-C3-C2	-3.35	106.11	111.02
8	D	632	NAG	C4-C3-C2	-3.34	106.12	111.02
8	A	611	NAG	C4-C3-C2	-3.21	106.31	111.02
8	D	611	NAG	C4-C3-C2	-3.20	106.32	111.02
8	C	611	NAG	C4-C3-C2	-3.20	106.33	111.02
8	B	704	NAG	C4-C3-C2	-2.83	106.87	111.02
8	F	704	NAG	C4-C3-C2	-2.83	106.87	111.02
8	E	704	NAG	C4-C3-C2	-2.83	106.88	111.02
8	C	618	NAG	C4-C3-C2	-2.79	106.94	111.02
8	D	618	NAG	C4-C3-C2	-2.78	106.94	111.02
8	A	618	NAG	C4-C3-C2	-2.78	106.95	111.02
8	A	610	NAG	C4-C3-C2	-2.75	106.99	111.02
8	D	610	NAG	C4-C3-C2	-2.75	106.99	111.02
8	C	610	NAG	C4-C3-C2	-2.74	107.00	111.02
8	C	606	NAG	C4-C3-C2	-2.50	107.35	111.02
8	A	606	NAG	C4-C3-C2	-2.49	107.36	111.02
8	D	606	NAG	C4-C3-C2	-2.49	107.37	111.02
8	D	611	NAG	O5-C1-C2	-2.46	107.41	111.29
8	C	611	NAG	O5-C1-C2	-2.44	107.44	111.29
8	A	611	NAG	O5-C1-C2	-2.44	107.44	111.29
8	A	603	NAG	C4-C3-C2	-2.43	107.46	111.02
8	D	603	NAG	C4-C3-C2	-2.43	107.46	111.02
8	C	603	NAG	C4-C3-C2	-2.42	107.47	111.02
8	C	618	NAG	O5-C1-C2	-2.30	107.66	111.29
8	D	618	NAG	O5-C1-C2	-2.29	107.67	111.29
8	A	618	NAG	O5-C1-C2	-2.28	107.68	111.29
8	F	703	NAG	C4-C3-C2	-2.14	107.89	111.02
8	B	703	NAG	C4-C3-C2	-2.11	107.93	111.02
8	E	703	NAG	C4-C3-C2	-2.11	107.93	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	623	NAG	C4-C3-C2	-2.05	108.01	111.02
8	C	623	NAG	C4-C3-C2	-2.04	108.03	111.02
8	D	623	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	632	NAG	O5-C5-C6-O6
8	C	632	NAG	O5-C5-C6-O6
8	D	632	NAG	O5-C5-C6-O6
8	A	623	NAG	O5-C5-C6-O6
8	C	623	NAG	O5-C5-C6-O6
8	D	623	NAG	O5-C5-C6-O6
8	A	611	NAG	O5-C5-C6-O6
8	A	622	NAG	O5-C5-C6-O6
8	C	611	NAG	O5-C5-C6-O6
8	C	622	NAG	O5-C5-C6-O6
8	D	611	NAG	O5-C5-C6-O6
8	D	622	NAG	O5-C5-C6-O6
8	A	606	NAG	O5-C5-C6-O6
8	C	606	NAG	O5-C5-C6-O6
8	D	606	NAG	O5-C5-C6-O6
8	A	609	NAG	O5-C5-C6-O6
8	C	609	NAG	O5-C5-C6-O6
8	D	609	NAG	O5-C5-C6-O6
8	B	704	NAG	O5-C5-C6-O6
8	E	704	NAG	O5-C5-C6-O6
8	F	704	NAG	O5-C5-C6-O6
8	A	610	NAG	O5-C5-C6-O6
8	C	610	NAG	O5-C5-C6-O6
8	D	610	NAG	O5-C5-C6-O6
8	A	618	NAG	O5-C5-C6-O6
8	C	618	NAG	O5-C5-C6-O6
8	D	618	NAG	O5-C5-C6-O6
8	E	703	NAG	O5-C5-C6-O6
8	B	703	NAG	O5-C5-C6-O6
8	F	703	NAG	O5-C5-C6-O6
8	A	632	NAG	C4-C5-C6-O6
8	C	632	NAG	C4-C5-C6-O6
8	D	632	NAG	C4-C5-C6-O6
8	A	603	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	603	NAG	O5-C5-C6-O6
8	D	603	NAG	O5-C5-C6-O6
8	C	611	NAG	C4-C5-C6-O6
8	A	611	NAG	C4-C5-C6-O6
8	D	611	NAG	C4-C5-C6-O6
8	A	623	NAG	C4-C5-C6-O6
8	C	623	NAG	C4-C5-C6-O6
8	D	623	NAG	C4-C5-C6-O6
8	C	606	NAG	C4-C5-C6-O6
8	A	606	NAG	C4-C5-C6-O6
8	D	606	NAG	C4-C5-C6-O6
8	D	622	NAG	C4-C5-C6-O6
8	A	622	NAG	C4-C5-C6-O6
8	C	622	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.

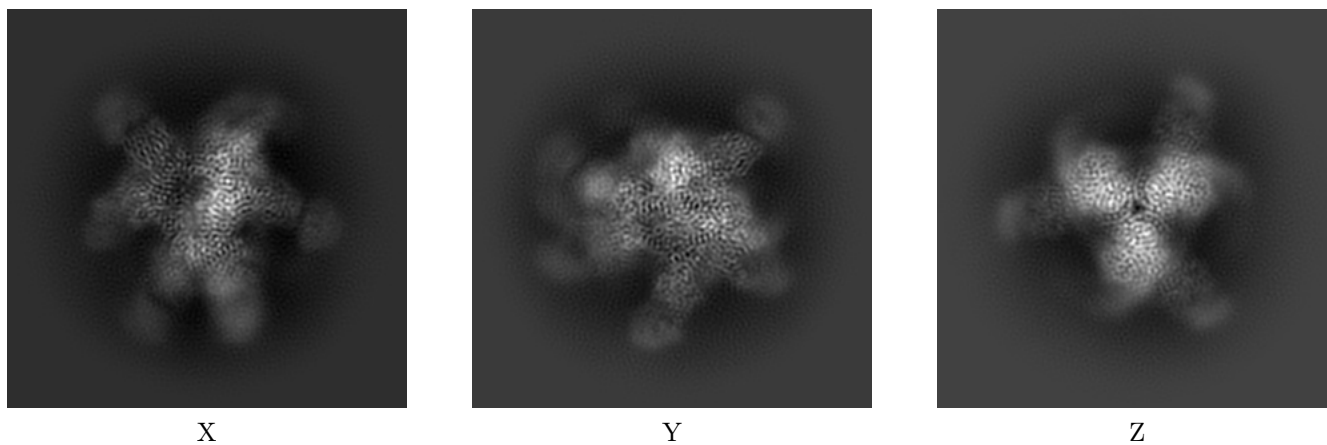
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20396. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

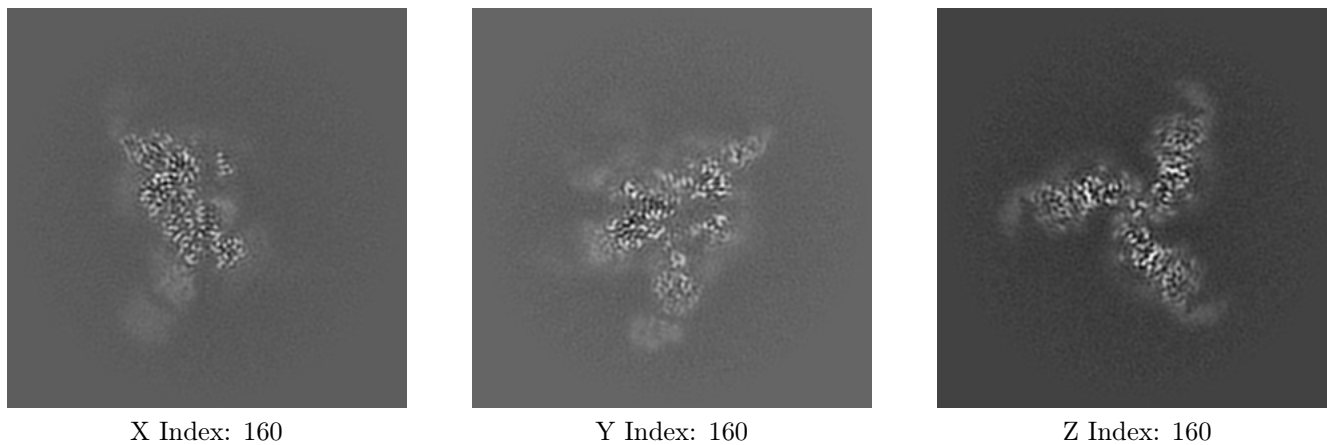
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

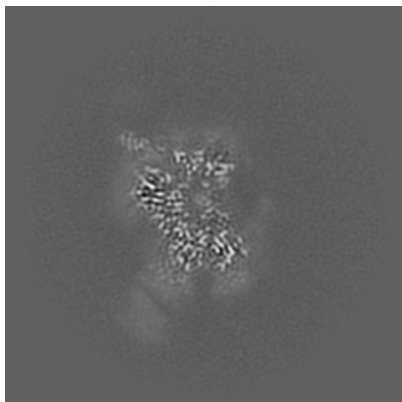
#### 6.2.1 Primary map



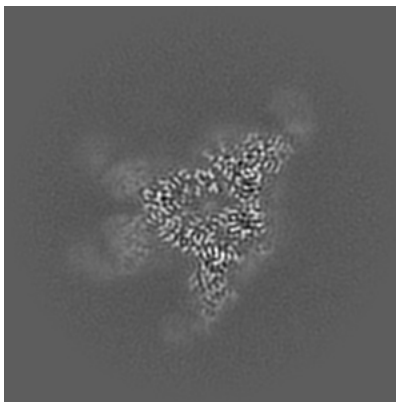
The images above show central slices of the map in three orthogonal directions.

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

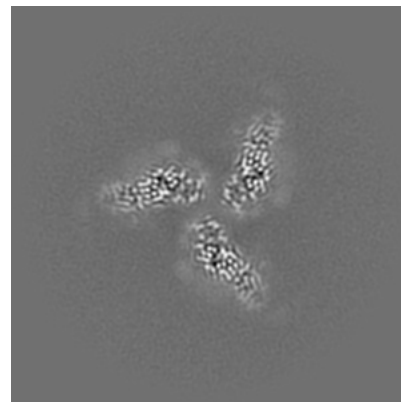
### 6.3.1 Primary map



X Index: 168



Y Index: 170



Z Index: 170

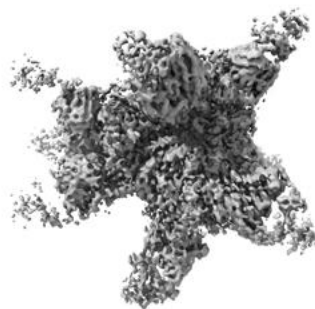
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.275. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



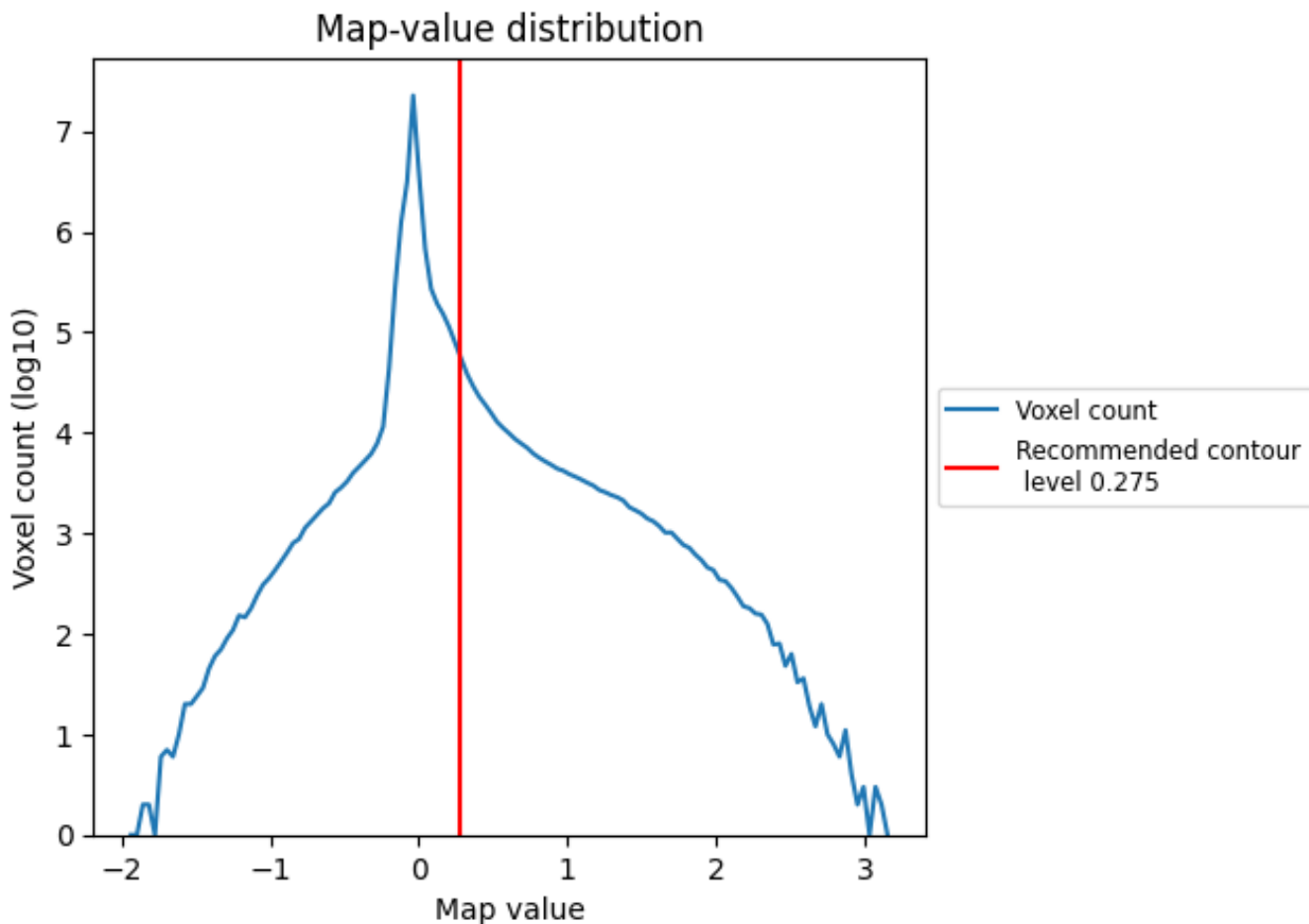
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

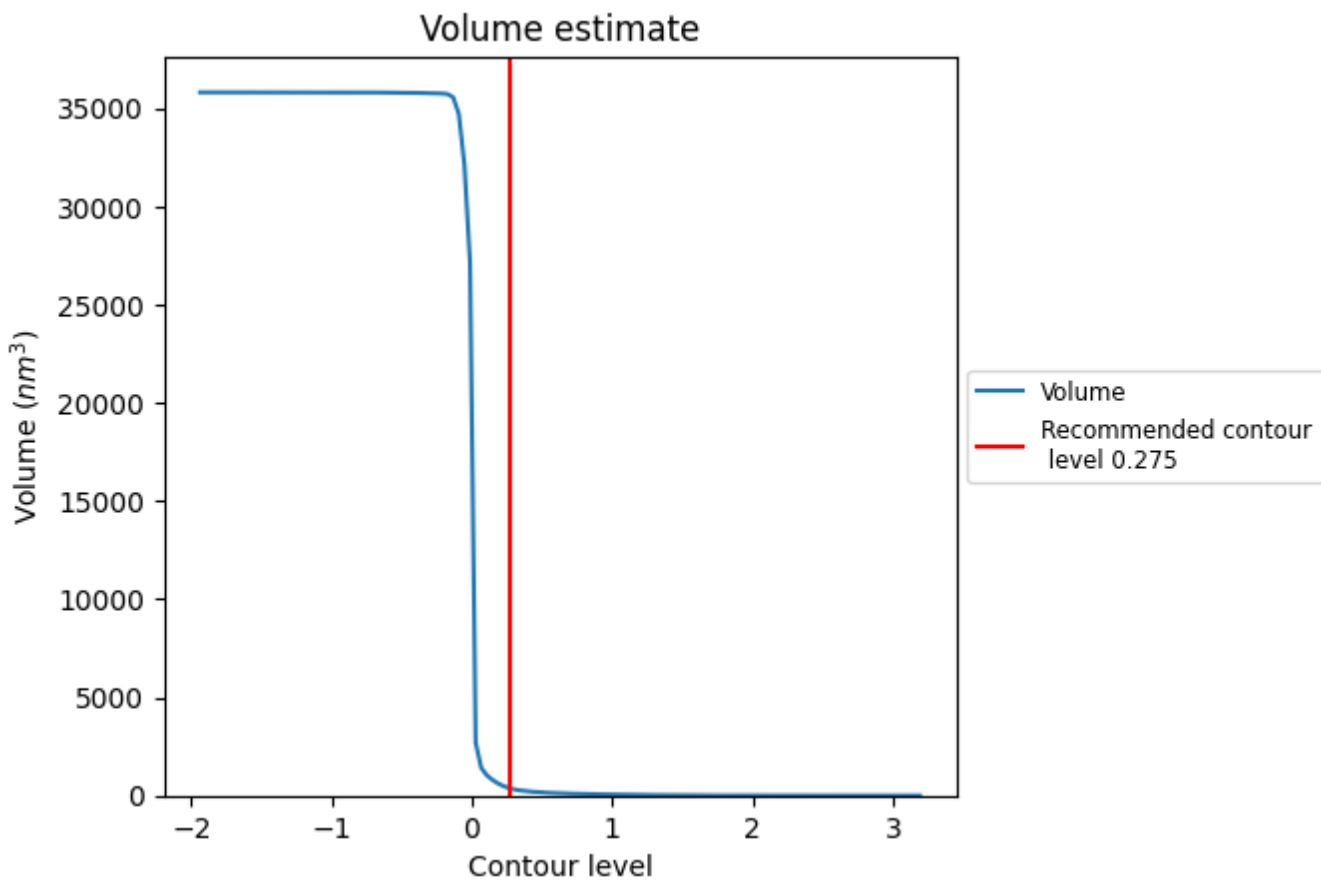
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

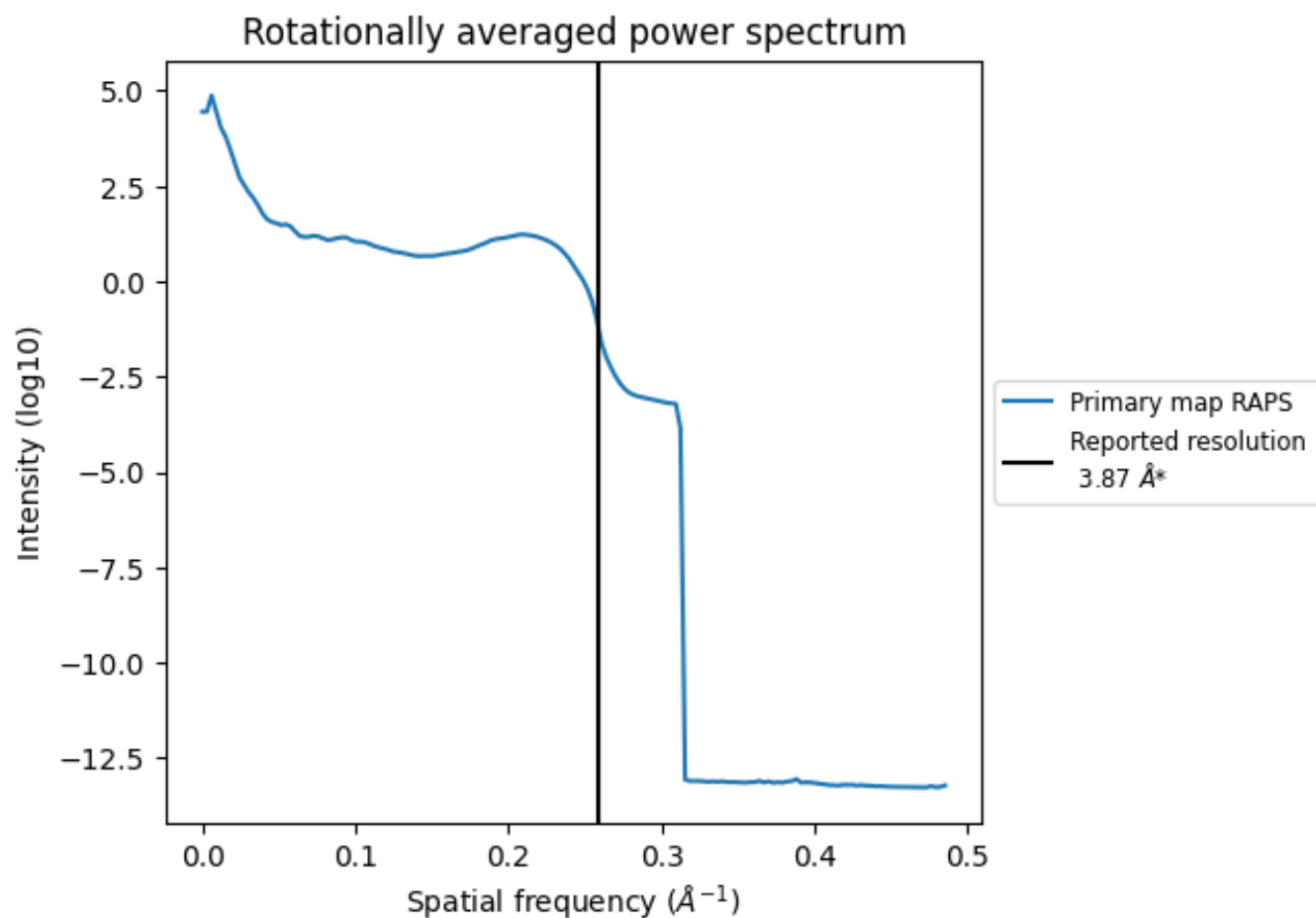
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm<sup>3</sup>; this corresponds to an approximate mass of 328 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 0.258 Å<sup>-1</sup>

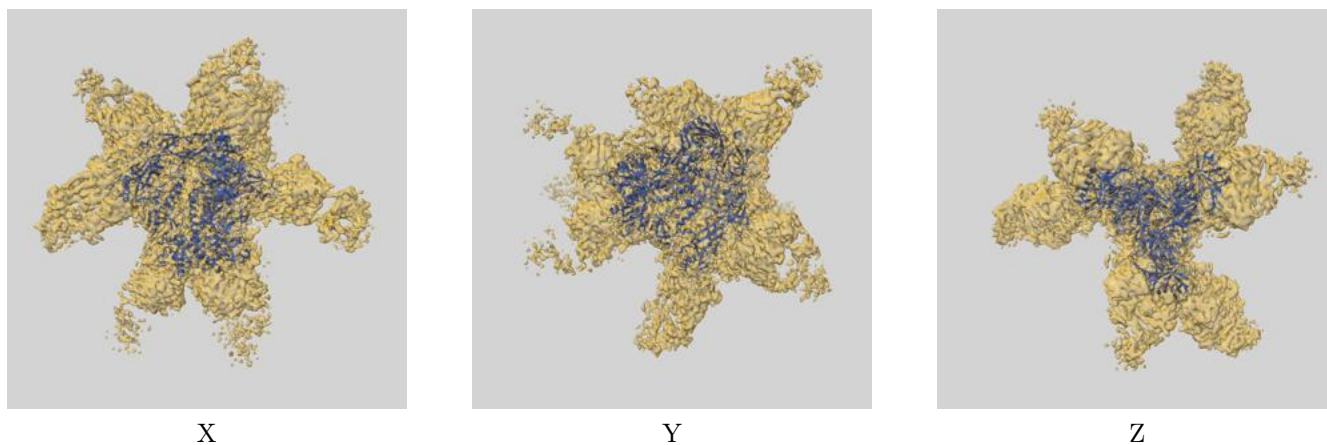
## 8 Fourier-Shell correlation

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

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

This section contains information regarding the fit between EMDB map EMD-20396 and PDB model 6V0R. Per-residue inclusion information can be found in section 3 on page 10.

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



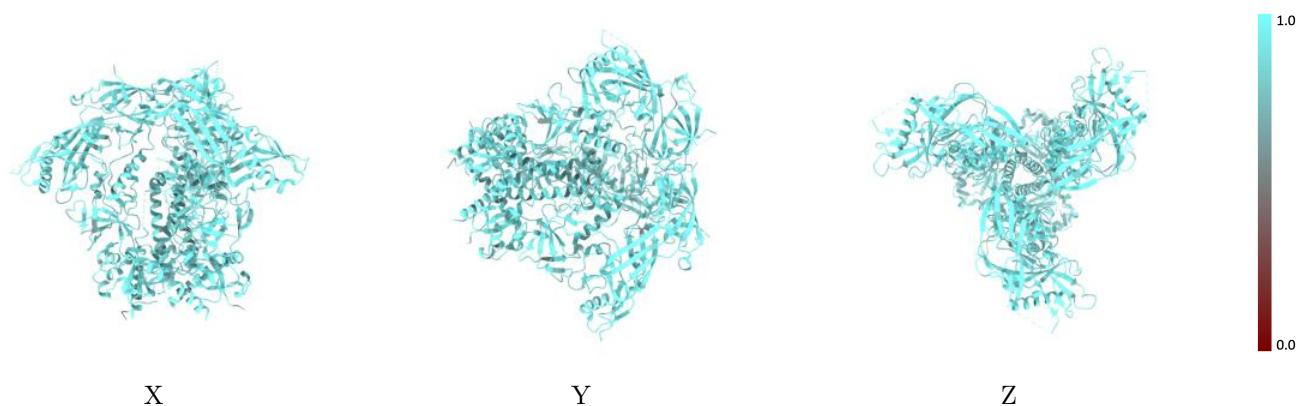
The images above show the 3D surface view of the map at the recommended contour level 0.275 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



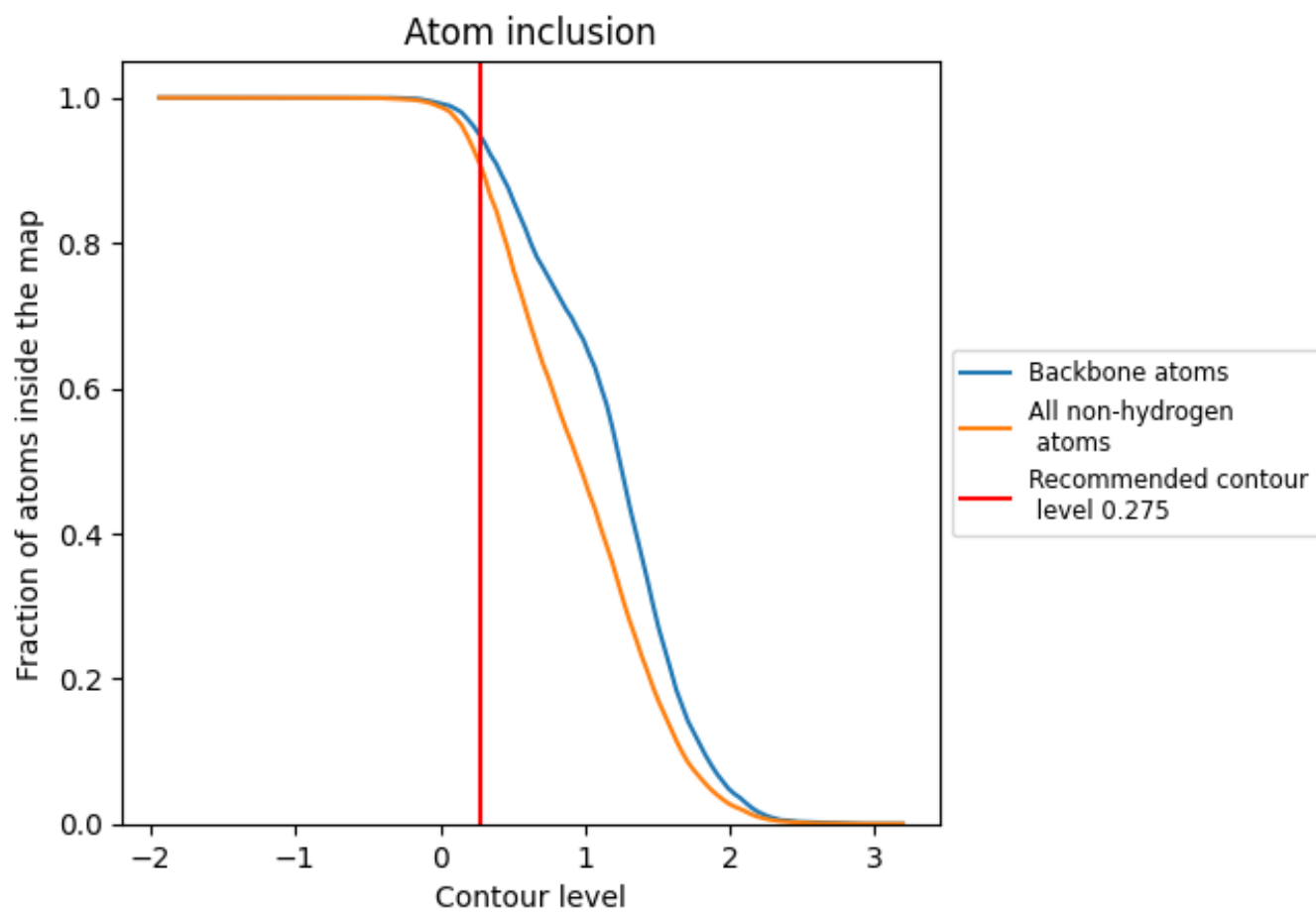
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.275).

## 9.4 Atom inclusion [i](#)







































































At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.275) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9082	 0.4500
A	 0.9135	 0.4610
B	 0.8979	 0.4260
C	 0.9149	 0.4600
D	 0.9149	 0.4600
E	 0.8960	 0.4250
F	 0.9017	 0.4230
G	 0.6786	 0.3420
H	 0.8571	 0.3620
I	 1.0000	 0.4780
J	 0.9306	 0.4510
K	 0.8974	 0.4390
L	 0.9487	 0.4620
M	 0.7368	 0.3740
N	 0.9286	 0.4090
O	 0.7917	 0.3270
P	 0.6786	 0.3380
Q	 0.8571	 0.3540
R	 0.9643	 0.4820
S	 0.9306	 0.4410
T	 0.8974	 0.4280
U	 0.9487	 0.4600
V	 0.7632	 0.3760
W	 0.9286	 0.4040
X	 0.7917	 0.3240
Y	 0.6786	 0.3500
Z	 0.8571	 0.3540
a	 1.0000	 0.4660
b	 0.9306	 0.4520
c	 0.8974	 0.4360
d	 0.9487	 0.4560
e	 0.7105	 0.3830
f	 0.8929	 0.3990
g	 0.7917	 0.3240

