



wwPDB EM Validation Summary Report ⓘ

Apr 2, 2025 – 12:16 PM EDT

PDB ID : 8TYC / pdb_00008tyc
EMDB ID : EMD-41713
Title : Lassa GPC (strain Josiah) bound to rabbit polyclonal base-targeting antibody Base-1
Authors : Perrett, H.R.; Brouwer, P.J.M.; Ward, A.B.
Deposited on : 2023-08-24
Resolution : 3.30 Å(reported)

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

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

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

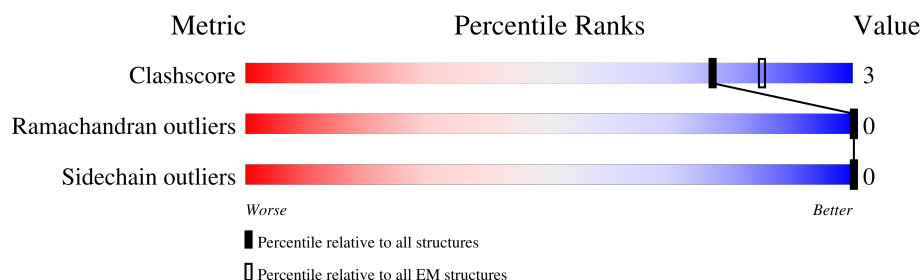
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



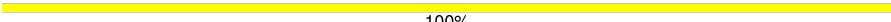
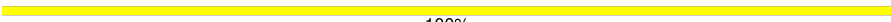
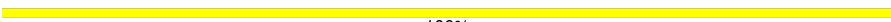
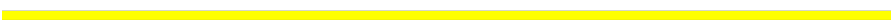









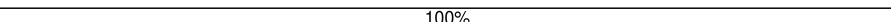

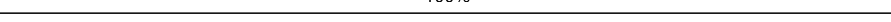
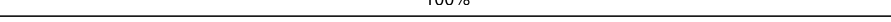
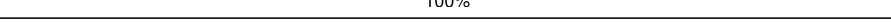
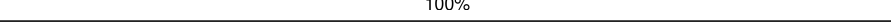
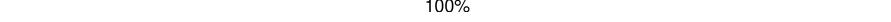
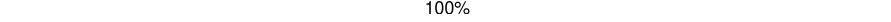
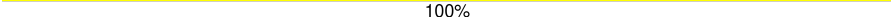
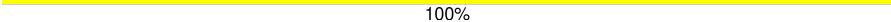
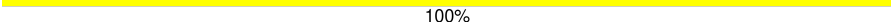
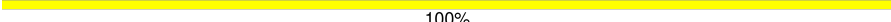
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	259	
1	B	259	
1	C	259	
2	H	108	
3	L	107	
4	a	406	
4	b	406	
4	c	406	

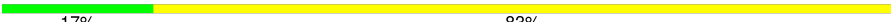

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Mol	Chain	Length	Quality of chain
5	D	2	 100%
5	F	2	 100%
5	G	2	 100%
5	I	2	 100%
5	J	2	 100%
5	K	2	 50% 50%
5	M	2	 50% 100%
5	P	2	 100%
5	R	2	 100%
5	T	2	 100%
5	V	2	 100%
5	Y	2	 100%
5	d	2	 50% 100%
5	g	2	 100% 100%
5	i	2	 50% 100%
6	E	3	 100%
6	N	3	 100%
6	O	3	 100%
6	S	3	 100%
6	U	3	 100%
6	X	3	 100%
6	e	3	 33% 100%
7	Q	2	 100%
8	W	3	 100%
9	Z	6	 100%

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Mol	Chain	Length	Quality of chain
9	f	6	 17%83%
9	h	6	 17%83%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10628 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 Glycoprotein G1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	193	Total	C	N	O	S	0	0
			1536	967	262	291	16		
1	B	200	Total	C	N	O	S	0	0
			1583	995	270	302	16		
1	C	194	Total	C	N	O	S	0	0
			1548	976	263	293	16		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	CYS	ARG	conflict	UNP P08669
B	207	CYS	ARG	conflict	UNP P08669
C	207	CYS	ARG	conflict	UNP P08669

- Molecule 2 is a protein called Polyclonal antibody Base-1 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	108	Total	C	N	O	0	0
			540	324	108	108		

- Molecule 3 is a protein called Polyclonal antibody Base-1 light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	107	Total	C	N	O	0	0
			535	321	107	107		

- Molecule 4 is a protein called Glycoprotein G2, 2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	154	Total	C	N	O	S	0	0
			1256	795	211	235	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	156	Total	C	N	O	S	0	0
			1269	803	213	238	15		
4	c	161	Total	C	N	O	S	0	0
			1306	824	219	248	15		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	329	PRO	GLU	conflict	UNP P08669
a	360	CYS	GLY	conflict	UNP P08669
a	424	GLY	-	linker	UNP P08669
a	425	GLY	-	linker	UNP P08669
a	426	SER	-	linker	UNP P08669
a	427	GLY	-	linker	UNP P08669
a	428	GLY	-	linker	UNP P08669
a	429	SER	-	linker	UNP P08669
a	430	GLY	-	linker	UNP P08669
a	431	GLY	-	linker	UNP P08669
a	432	SER	-	linker	UNP P08669
a	433	GLY	-	linker	UNP P08669
a	434	GLY	-	linker	UNP P08669
a	435	SER	-	linker	UNP P08669
a	436	GLY	-	linker	UNP P08669
a	437	GLY	-	linker	UNP P08669
a	438	SER	-	linker	UNP P08669
a	439	GLU	-	linker	UNP P08669
a	440	LYS	-	linker	UNP P08669
a	441	ALA	-	linker	UNP P08669
a	442	ALA	-	linker	UNP P08669
a	443	LYS	-	linker	UNP P08669
a	444	ALA	-	linker	UNP P08669
a	445	GLU	-	linker	UNP P08669
a	446	GLU	-	linker	UNP P08669
a	447	ALA	-	linker	UNP P08669
a	448	ALA	-	linker	UNP P08669
a	449	ARG	-	linker	UNP P08669
a	473	ILE	LYS	conflict	UNP Q9WXS1
a	477	VAL	LEU	conflict	UNP Q9WXS1
a	481	ALA	GLU	conflict	UNP Q9WXS1
a	502	ALA	GLU	conflict	UNP Q9WXS1
a	505	VAL	PHE	conflict	UNP Q9WXS1
a	574	ASP	THR	conflict	UNP Q9WXS1

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Chain	Residue	Modelled	Actual	Comment	Reference
a	587	GLU	GLN	conflict	UNP Q9WXS1
a	608	ASP	ASN	conflict	UNP Q9WXS1
a	617	ASP	LYS	conflict	UNP Q9WXS1
a	627	ASP	SER	conflict	UNP Q9WXS1
a	631	GLU	LYS	conflict	UNP Q9WXS1
a	633	ASP	THR	conflict	UNP Q9WXS1
a	643	GLU	ALA	conflict	UNP Q9WXS1
a	654	GLY	-	expression tag	UNP Q9WXS1
a	655	SER	-	expression tag	UNP Q9WXS1
a	656	LEU	-	expression tag	UNP Q9WXS1
a	657	GLU	-	expression tag	UNP Q9WXS1
a	658	TRP	-	expression tag	UNP Q9WXS1
a	659	SER	-	expression tag	UNP Q9WXS1
a	660	HIS	-	expression tag	UNP Q9WXS1
a	661	PRO	-	expression tag	UNP Q9WXS1
a	662	GLN	-	expression tag	UNP Q9WXS1
a	663	PHE	-	expression tag	UNP Q9WXS1
a	664	GLU	-	expression tag	UNP Q9WXS1
a	665	LYS	-	expression tag	UNP Q9WXS1
b	329	PRO	GLU	conflict	UNP P08669
b	360	CYS	GLY	conflict	UNP P08669
b	424	GLY	-	linker	UNP P08669
b	425	GLY	-	linker	UNP P08669
b	426	SER	-	linker	UNP P08669
b	427	GLY	-	linker	UNP P08669
b	428	GLY	-	linker	UNP P08669
b	429	SER	-	linker	UNP P08669
b	430	GLY	-	linker	UNP P08669
b	431	GLY	-	linker	UNP P08669
b	432	SER	-	linker	UNP P08669
b	433	GLY	-	linker	UNP P08669
b	434	GLY	-	linker	UNP P08669
b	435	SER	-	linker	UNP P08669
b	436	GLY	-	linker	UNP P08669
b	437	GLY	-	linker	UNP P08669
b	438	SER	-	linker	UNP P08669
b	439	GLU	-	linker	UNP P08669
b	440	LYS	-	linker	UNP P08669
b	441	ALA	-	linker	UNP P08669
b	442	ALA	-	linker	UNP P08669
b	443	LYS	-	linker	UNP P08669
b	444	ALA	-	linker	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	445	GLU	-	linker	UNP P08669
b	446	GLU	-	linker	UNP P08669
b	447	ALA	-	linker	UNP P08669
b	448	ALA	-	linker	UNP P08669
b	449	ARG	-	linker	UNP P08669
b	473	ILE	LYS	conflict	UNP Q9WXS1
b	477	VAL	LEU	conflict	UNP Q9WXS1
b	481	ALA	GLU	conflict	UNP Q9WXS1
b	502	ALA	GLU	conflict	UNP Q9WXS1
b	505	VAL	PHE	conflict	UNP Q9WXS1
b	574	ASP	THR	conflict	UNP Q9WXS1
b	587	GLU	GLN	conflict	UNP Q9WXS1
b	608	ASP	ASN	conflict	UNP Q9WXS1
b	617	ASP	LYS	conflict	UNP Q9WXS1
b	627	ASP	SER	conflict	UNP Q9WXS1
b	631	GLU	LYS	conflict	UNP Q9WXS1
b	633	ASP	THR	conflict	UNP Q9WXS1
b	643	GLU	ALA	conflict	UNP Q9WXS1
b	654	GLY	-	expression tag	UNP Q9WXS1
b	655	SER	-	expression tag	UNP Q9WXS1
b	656	LEU	-	expression tag	UNP Q9WXS1
b	657	GLU	-	expression tag	UNP Q9WXS1
b	658	TRP	-	expression tag	UNP Q9WXS1
b	659	SER	-	expression tag	UNP Q9WXS1
b	660	HIS	-	expression tag	UNP Q9WXS1
b	661	PRO	-	expression tag	UNP Q9WXS1
b	662	GLN	-	expression tag	UNP Q9WXS1
b	663	PHE	-	expression tag	UNP Q9WXS1
b	664	GLU	-	expression tag	UNP Q9WXS1
b	665	LYS	-	expression tag	UNP Q9WXS1
c	329	PRO	GLU	conflict	UNP P08669
c	360	CYS	GLY	conflict	UNP P08669
c	424	GLY	-	linker	UNP P08669
c	425	GLY	-	linker	UNP P08669
c	426	SER	-	linker	UNP P08669
c	427	GLY	-	linker	UNP P08669
c	428	GLY	-	linker	UNP P08669
c	429	SER	-	linker	UNP P08669
c	430	GLY	-	linker	UNP P08669
c	431	GLY	-	linker	UNP P08669
c	432	SER	-	linker	UNP P08669
c	433	GLY	-	linker	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	434	GLY	-	linker	UNP P08669
c	435	SER	-	linker	UNP P08669
c	436	GLY	-	linker	UNP P08669
c	437	GLY	-	linker	UNP P08669
c	438	SER	-	linker	UNP P08669
c	439	GLU	-	linker	UNP P08669
c	440	LYS	-	linker	UNP P08669
c	441	ALA	-	linker	UNP P08669
c	442	ALA	-	linker	UNP P08669
c	443	LYS	-	linker	UNP P08669
c	444	ALA	-	linker	UNP P08669
c	445	GLU	-	linker	UNP P08669
c	446	GLU	-	linker	UNP P08669
c	447	ALA	-	linker	UNP P08669
c	448	ALA	-	linker	UNP P08669
c	449	ARG	-	linker	UNP P08669
c	473	ILE	LYS	conflict	UNP Q9WXS1
c	477	VAL	LEU	conflict	UNP Q9WXS1
c	481	ALA	GLU	conflict	UNP Q9WXS1
c	502	ALA	GLU	conflict	UNP Q9WXS1
c	505	VAL	PHE	conflict	UNP Q9WXS1
c	574	ASP	THR	conflict	UNP Q9WXS1
c	587	GLU	GLN	conflict	UNP Q9WXS1
c	608	ASP	ASN	conflict	UNP Q9WXS1
c	617	ASP	LYS	conflict	UNP Q9WXS1
c	627	ASP	SER	conflict	UNP Q9WXS1
c	631	GLU	LYS	conflict	UNP Q9WXS1
c	633	ASP	THR	conflict	UNP Q9WXS1
c	643	GLU	ALA	conflict	UNP Q9WXS1
c	654	GLY	-	expression tag	UNP Q9WXS1
c	655	SER	-	expression tag	UNP Q9WXS1
c	656	LEU	-	expression tag	UNP Q9WXS1
c	657	GLU	-	expression tag	UNP Q9WXS1
c	658	TRP	-	expression tag	UNP Q9WXS1
c	659	SER	-	expression tag	UNP Q9WXS1
c	660	HIS	-	expression tag	UNP Q9WXS1
c	661	PRO	-	expression tag	UNP Q9WXS1
c	662	GLN	-	expression tag	UNP Q9WXS1
c	663	PHE	-	expression tag	UNP Q9WXS1
c	664	GLU	-	expression tag	UNP Q9WXS1
c	665	LYS	-	expression tag	UNP Q9WXS1

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

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		
5	i	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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.



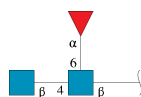
Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	3	Total	C	N	O	0	0
			39	22	2	15		
6	N	3	Total	C	N	O	0	0
			39	22	2	15		
6	O	3	Total	C	N	O	0	0
			39	22	2	15		
6	S	3	Total	C	N	O	0	0
			39	22	2	15		
6	U	3	Total	C	N	O	0	0
			39	22	2	15		
6	X	3	Total	C	N	O	0	0
			39	22	2	15		
6	e	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



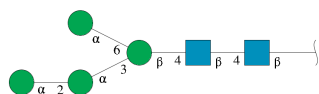
Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 8 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.



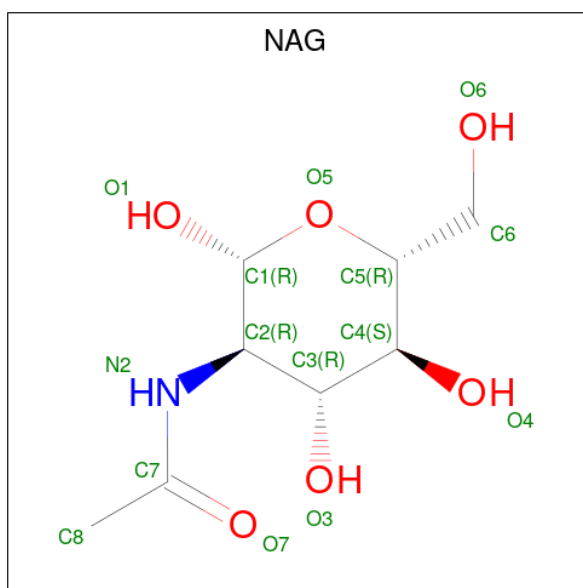
Mol	Chain	Residues	Atoms				AltConf	Trace
8	W	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 9 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
9	Z	6	Total	C	N	O	0	0
			72	40	2	30		
9	f	6	Total	C	N	O	0	0
			72	40	2	30		
9	h	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

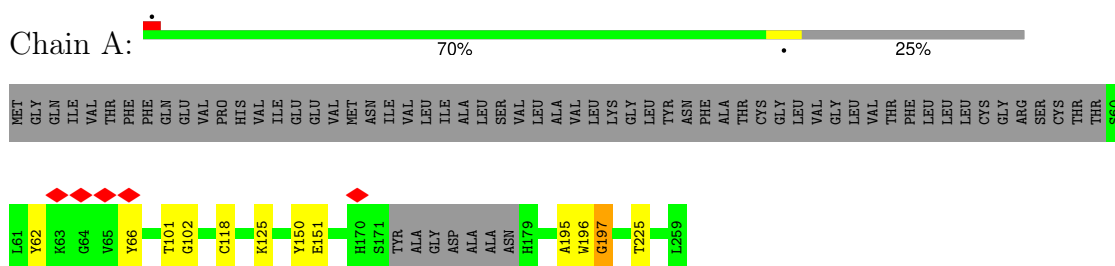


Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	N	O	0
			14	8	1	5	
10	a	1	Total	C	N	O	0
			14	8	1	5	
10	a	1	Total	C	N	O	0
			14	8	1	5	
10	b	1	Total	C	N	O	0
			14	8	1	5	
10	c	1	Total	C	N	O	0
			14	8	1	5	
10	c	1	Total	C	N	O	0
			14	8	1	5	

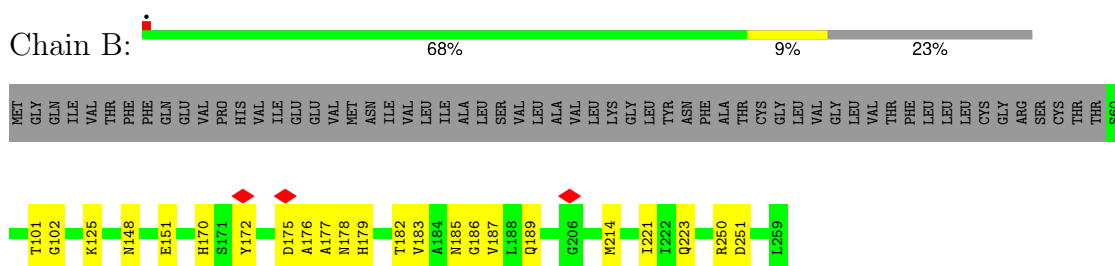
3 Residue-property plots [i](#)

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.

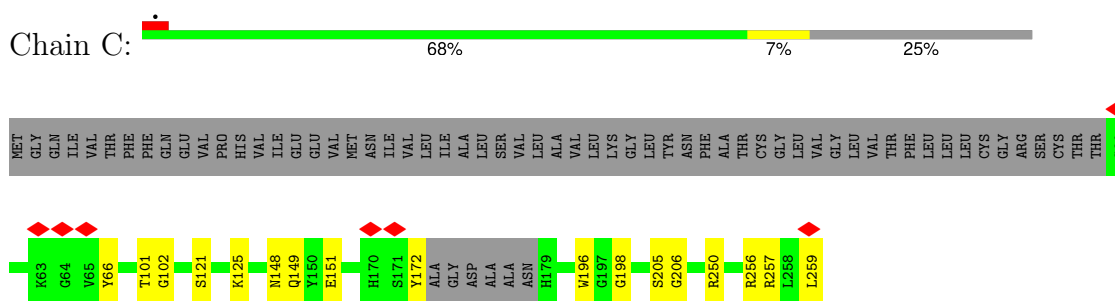
- Molecule 1: Glycoprotein G1



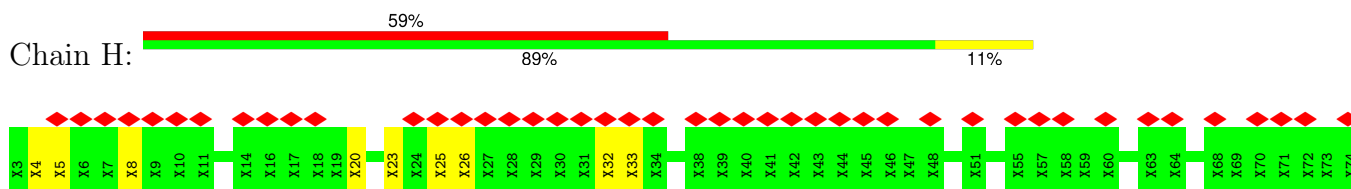
- Molecule 1: Glycoprotein G1

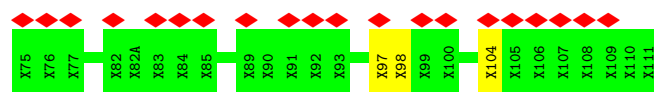


- Molecule 1: Glycoprotein G1

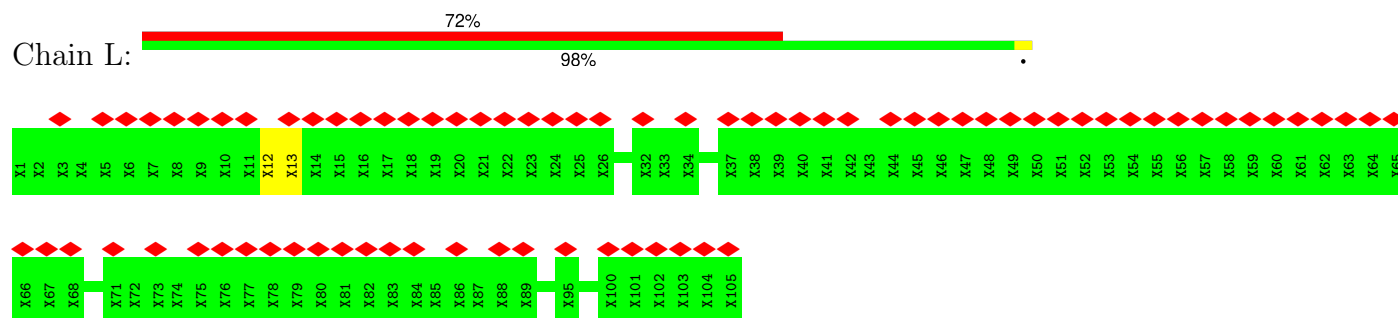


- Molecule 2: Polyclonal antibody Base-1 heavy chain

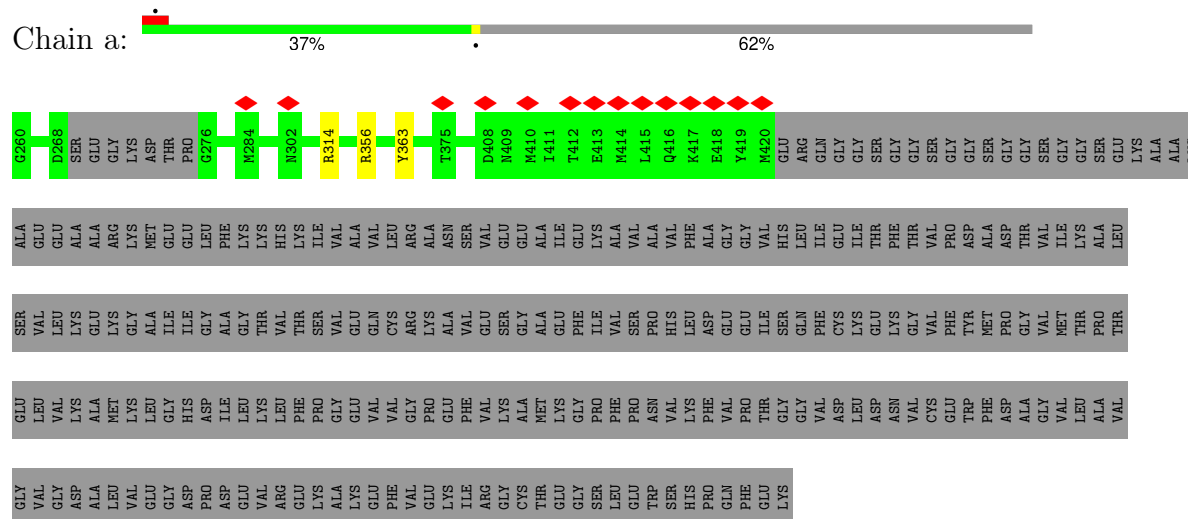




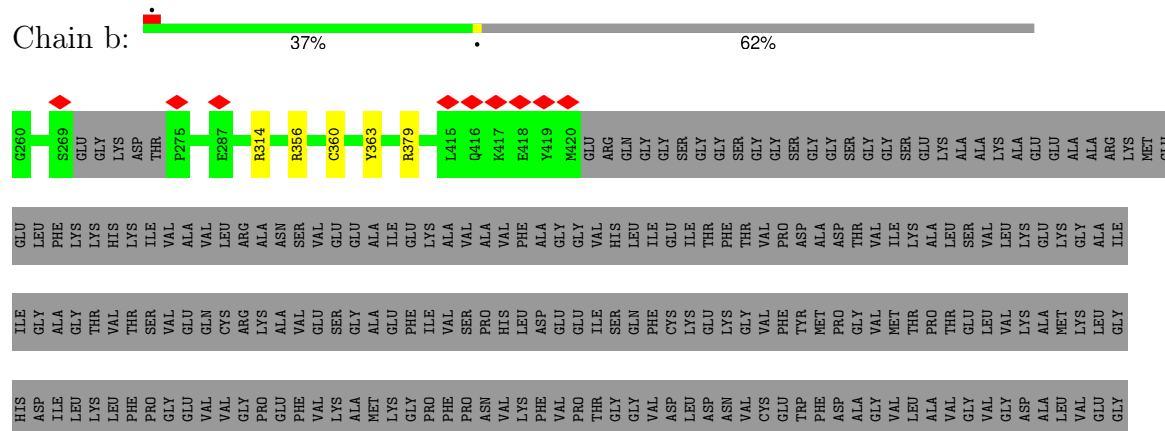
- Molecule 3: Polyclonal antibody Base-1 light chain



- Molecule 4: Glycoprotein G2, 2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase fusion protein



- Molecule 4: Glycoprotein G2, 2-dehydro-3-deoxyphosphogluconate aldolase/4-hydroxy-2-oxoglutarate aldolase fusion protein



MAG1
MAG2

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

Chain J:  100%MAG1
MAG2

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

Chain K:  50% 50%MAG1
MAG2

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

Chain M:  50% 100%MAG1
MAG2

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

Chain P:  100%MAG1
MAG2

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

Chain R:  100%MAG1
MAG2

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

Chain T:  100%MAG1
MAG2

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

Chain V:  100%

NAG1
NAG2

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

Chain Y:  100%

NAG1
NAG2

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

Chain d:  50%
100%

♦
NAG1
NAG2

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

Chain g:  100%
100%

♦ ♦
NAG1
NAG2

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

Chain i:  50%
100%

♦
NAG1
NAG2

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

NAG1
NAG2
EMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

MAG1
MAG2
BMA3

- Molecule 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

- Molecule 6: 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 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  33% 100%

MAG1
MAG2
BMA3

- Molecule 7: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

MAG1
FUC2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%MAG1
MAG2
FUC3

- Molecule 9: 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 Z:  100%MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 9: 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 f:  17%  83%MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 9: 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 h:  17%  83%MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30182	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 ($e^-/\text{\AA}^2$)	50.4	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.351	Depositor
Minimum map value	-0.650	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.253	Depositor
Map size (\AA)	266.56, 266.56, 266.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.833, 0.833, 0.833	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: FUC, NAG, MAN, BMA

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	0.98	1/1570 (0.1%)	0.88	2/2124 (0.1%)
1	B	1.00	0/1619	0.87	1/2193 (0.0%)
1	C	1.08	7/1583 (0.4%)	0.91	1/2142 (0.0%)
4	a	1.02	0/1282	0.87	3/1730 (0.2%)
4	b	1.03	2/1296 (0.2%)	0.90	3/1749 (0.2%)
4	c	1.01	1/1334 (0.1%)	0.88	4/1802 (0.2%)
All	All	1.02	11/8684 (0.1%)	0.89	14/11740 (0.1%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	172	TYR	CG-CD1	7.90	1.49	1.39
1	C	172	TYR	CG-CD2	7.71	1.49	1.39
1	C	172	TYR	CE2-CZ	7.18	1.47	1.38
1	C	172	TYR	CE1-CZ	7.16	1.47	1.38
1	C	121	SER	CA-CB	-6.55	1.43	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	314	ARG	NE-CZ-NH2	-8.91	115.84	120.30
4	c	314	ARG	NE-CZ-NH1	6.51	123.56	120.30
4	b	314	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	197	GLY	N-CA-C	-6.15	97.74	113.10
1	C	250	ARG	NE-CZ-NH1	6.11	123.36	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1536	0	1470	9	0
1	B	1583	0	1509	20	0
1	C	1548	0	1479	11	0
2	H	540	0	136	7	0
3	L	535	0	132	1	0
4	a	1256	0	1209	0	0
4	b	1269	0	1223	0	0
4	c	1306	0	1255	0	0
5	D	28	0	25	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	K	28	0	25	1	0
5	M	28	0	25	0	0
5	P	28	0	25	0	0
5	R	28	0	25	0	0
5	T	28	0	25	2	0
5	V	28	0	25	0	0
5	Y	28	0	25	0	0
5	d	28	0	25	0	0
5	g	28	0	25	0	0
5	i	28	0	25	0	0
6	E	39	0	34	0	0
6	N	39	0	34	0	0
6	O	39	0	34	0	0
6	S	39	0	34	0	0
6	U	39	0	34	0	0
6	X	39	0	34	0	0
6	e	39	0	34	0	0
7	Q	24	0	22	0	0
8	W	38	0	34	0	0
9	Z	72	0	61	0	0
9	f	72	0	61	0	0
9	h	72	0	61	0	0
10	C	14	0	13	0	0
10	a	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	b	14	0	13	0	0
10	c	28	0	26	0	0
All	All	10628	0	9343	44	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.

The worst 5 of 44 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:C:256:ARG:HG3	1:C:259:LEU:HB2	1.74	0.69
1:B:175:ASP:O	1:B:178:ASN:HB2	1.94	0.67
1:A:118:CYS:HB3	1:C:257:ARG:HH11	1.63	0.63
1:B:170:HIS:CD2	1:B:182:THR:HB	2.36	0.61
2:H:8:UNK:O	2:H:20:UNK:HA	2.01	0.61

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	189/259 (73%)	183 (97%)	6 (3%)	0	100	100
1	B	198/259 (76%)	186 (94%)	12 (6%)	0	100	100
1	C	190/259 (73%)	178 (94%)	12 (6%)	0	100	100
4	a	150/406 (37%)	149 (99%)	1 (1%)	0	100	100
4	b	152/406 (37%)	151 (99%)	1 (1%)	0	100	100
4	c	159/406 (39%)	159 (100%)	0	0	100	100
All	All	1038/1995 (52%)	1006 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/228 (76%)	174 (100%)	0	100	100
1	B	177/228 (78%)	177 (100%)	0	100	100
1	C	175/228 (77%)	175 (100%)	0	100	100
4	a	139/337 (41%)	139 (100%)	0	100	100
4	b	141/337 (42%)	141 (100%)	0	100	100
4	c	145/337 (43%)	145 (100%)	0	100	100
All	All	951/1695 (56%)	951 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	B	170	HIS
1	B	185	ASN
1	B	223	GLN
1	C	149	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

74 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	D	1	5,1	14,14,15	1.50	2 (14%)	17,19,21	1.03	1 (5%)
5	NAG	D	2	5	14,14,15	1.98	6 (42%)	17,19,21	0.90	0
6	NAG	E	1	6,1	14,14,15	1.90	4 (28%)	17,19,21	1.41	4 (23%)
6	NAG	E	2	6	14,14,15	1.96	4 (28%)	17,19,21	0.99	1 (5%)
6	BMA	E	3	6	11,11,12	1.85	5 (45%)	15,15,17	0.61	0
5	NAG	F	1	5,1	14,14,15	2.06	3 (21%)	17,19,21	1.29	2 (11%)
5	NAG	F	2	5	14,14,15	1.96	5 (35%)	17,19,21	0.91	1 (5%)
5	NAG	G	1	5,1	14,14,15	2.12	4 (28%)	17,19,21	0.94	1 (5%)
5	NAG	G	2	5	14,14,15	1.96	5 (35%)	17,19,21	0.91	1 (5%)
5	NAG	I	1	5,1	14,14,15	2.19	4 (28%)	17,19,21	1.26	3 (17%)
5	NAG	I	2	5	14,14,15	1.97	6 (42%)	17,19,21	0.97	2 (11%)
5	NAG	J	1	5,1	14,14,15	1.84	3 (21%)	17,19,21	1.25	2 (11%)
5	NAG	J	2	5	14,14,15	1.99	4 (28%)	17,19,21	1.03	2 (11%)
5	NAG	K	1	5,1	14,14,15	1.91	4 (28%)	17,19,21	1.26	2 (11%)
5	NAG	K	2	5	14,14,15	1.95	4 (28%)	17,19,21	0.95	2 (11%)
5	NAG	M	1	5,1	14,14,15	2.15	4 (28%)	17,19,21	0.97	1 (5%)
5	NAG	M	2	5	14,14,15	1.94	5 (35%)	17,19,21	0.92	1 (5%)
6	NAG	N	1	6,1	14,14,15	2.09	5 (35%)	17,19,21	1.09	1 (5%)
6	NAG	N	2	6	14,14,15	2.13	7 (50%)	17,19,21	1.20	2 (11%)
6	BMA	N	3	6	11,11,12	1.98	4 (36%)	15,15,17	0.91	1 (6%)
6	NAG	O	1	6,1	14,14,15	1.67	4 (28%)	17,19,21	1.24	1 (5%)
6	NAG	O	2	6	14,14,15	2.15	4 (28%)	17,19,21	1.22	3 (17%)
6	BMA	O	3	6	11,11,12	1.88	5 (45%)	15,15,17	0.64	0
5	NAG	P	1	5,1	14,14,15	1.55	2 (14%)	17,19,21	0.94	1 (5%)
5	NAG	P	2	5	14,14,15	2.16	6 (42%)	17,19,21	1.38	3 (17%)
7	NAG	Q	1	7,1	14,14,15	1.67	3 (21%)	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FUC	Q	2	7	10,10,11	1.89	4 (40%)	14,14,16	0.92	1 (7%)
5	NAG	R	1	5,1	14,14,15	1.61	2 (14%)	17,19,21	0.93	1 (5%)
5	NAG	R	2	5	14,14,15	2.11	4 (28%)	17,19,21	1.14	2 (11%)
6	NAG	S	1	6,1	14,14,15	1.91	4 (28%)	17,19,21	1.45	4 (23%)
6	NAG	S	2	6	14,14,15	2.04	5 (35%)	17,19,21	1.10	2 (11%)
6	BMA	S	3	6	11,11,12	1.88	5 (45%)	15,15,17	0.63	0
5	NAG	T	1	5,1	14,14,15	0.34	0	17,19,21	0.66	0
5	NAG	T	2	5	14,14,15	0.27	0	17,19,21	0.67	0
6	NAG	U	1	6,1	14,14,15	1.95	4 (28%)	17,19,21	1.46	5 (29%)
6	NAG	U	2	6	14,14,15	1.97	5 (35%)	17,19,21	1.00	1 (5%)
6	BMA	U	3	6	11,11,12	1.78	5 (45%)	15,15,17	0.66	0
5	NAG	V	1	5,1	14,14,15	2.03	3 (21%)	17,19,21	1.69	4 (23%)
5	NAG	V	2	5	14,14,15	2.04	5 (35%)	17,19,21	1.03	2 (11%)
8	NAG	W	1	8,1	14,14,15	1.47	2 (14%)	17,19,21	0.94	0
8	NAG	W	2	8	14,14,15	1.91	4 (28%)	17,19,21	0.98	1 (5%)
8	FUC	W	3	8	10,10,11	1.81	4 (40%)	14,14,16	0.74	0
6	NAG	X	1	6,1	14,14,15	1.96	3 (21%)	17,19,21	1.23	3 (17%)
6	NAG	X	2	6	14,14,15	2.01	5 (35%)	17,19,21	1.08	2 (11%)
6	BMA	X	3	6	11,11,12	1.83	5 (45%)	15,15,17	0.69	0
5	NAG	Y	1	5,1	14,14,15	1.90	4 (28%)	17,19,21	1.45	4 (23%)
5	NAG	Y	2	5	14,14,15	1.96	4 (28%)	17,19,21	0.84	1 (5%)
9	NAG	Z	1	9,4	14,14,15	2.09	4 (28%)	17,19,21	1.11	1 (5%)
9	NAG	Z	2	9	14,14,15	1.89	3 (21%)	17,19,21	1.08	1 (5%)
9	BMA	Z	3	9	11,11,12	1.32	2 (18%)	15,15,17	0.69	0
9	MAN	Z	4	9	11,11,12	0.76	0	15,15,17	1.14	1 (6%)
9	MAN	Z	5	9	11,11,12	1.80	4 (36%)	15,15,17	0.64	0
9	MAN	Z	6	9	11,11,12	1.80	4 (36%)	15,15,17	0.66	0
5	NAG	d	1	4,5	14,14,15	1.99	5 (35%)	17,19,21	1.17	3 (17%)
5	NAG	d	2	5	14,14,15	2.02	5 (35%)	17,19,21	1.99	3 (17%)
6	NAG	e	1	4,6	14,14,15	2.12	5 (35%)	17,19,21	1.15	2 (11%)
6	NAG	e	2	6	14,14,15	2.01	5 (35%)	17,19,21	0.94	1 (5%)
6	BMA	e	3	6	11,11,12	1.86	5 (45%)	15,15,17	0.67	0
9	NAG	f	1	9,4	14,14,15	2.00	2 (14%)	17,19,21	1.26	2 (11%)
9	NAG	f	2	9	14,14,15	1.83	3 (21%)	17,19,21	1.01	1 (5%)
9	BMA	f	3	9	11,11,12	1.33	1 (9%)	15,15,17	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	f	4	9	11,11,12	0.68	0	15,15,17	0.65	0
9	MAN	f	5	9	11,11,12	1.80	4 (36%)	15,15,17	0.66	0
9	MAN	f	6	9	11,11,12	1.84	4 (36%)	15,15,17	0.64	0
5	NAG	g	1	4,5	14,14,15	0.25	0	17,19,21	0.71	0
5	NAG	g	2	5	14,14,15	0.26	0	17,19,21	0.61	0
9	NAG	h	1	9,4	14,14,15	1.97	2 (14%)	17,19,21	1.30	2 (11%)
9	NAG	h	2	9	14,14,15	1.79	3 (21%)	17,19,21	1.12	2 (11%)
9	BMA	h	3	9	11,11,12	1.26	1 (9%)	15,15,17	0.62	0
9	MAN	h	4	9	11,11,12	0.72	0	15,15,17	0.87	0
9	MAN	h	5	9	11,11,12	1.81	4 (36%)	15,15,17	0.68	0
9	MAN	h	6	9	11,11,12	1.79	4 (36%)	15,15,17	0.65	0
5	NAG	i	1	4,5	14,14,15	2.02	5 (35%)	17,19,21	1.20	2 (11%)
5	NAG	i	2	5	14,14,15	2.02	5 (35%)	17,19,21	1.97	3 (17%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	O	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	1/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
7	NAG	Q	1	7,1	-	1/6/23/26	0/1/1/1
7	FUC	Q	2	7	-	-	0/1/1/1
5	NAG	R	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	BMA	S	3	6	-	1/2/19/22	0/1/1/1
5	NAG	T	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	T	2	5	-	3/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
8	NAG	W	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
8	FUC	W	3	8	-	-	0/1/1/1
6	NAG	X	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1
6	BMA	X	3	6	-	1/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	1/6/23/26	0/1/1/1
9	NAG	Z	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	5	9	-	1/2/19/22	0/1/1/1
9	MAN	Z	6	9	-	1/2/19/22	0/1/1/1
5	NAG	d	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1
6	NAG	e	1	4,6	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	BMA	e	3	6	-	1/2/19/22	0/1/1/1
9	NAG	f	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	f	3	9	-	0/2/19/22	0/1/1/1
9	MAN	f	4	9	-	0/2/19/22	0/1/1/1
9	MAN	f	5	9	-	0/2/19/22	0/1/1/1
9	MAN	f	6	9	-	1/2/19/22	0/1/1/1
5	NAG	g	1	4,5	-	3/6/23/26	0/1/1/1
5	NAG	g	2	5	-	4/6/23/26	0/1/1/1
9	NAG	h	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	h	2	9	-	0/6/23/26	0/1/1/1
9	BMA	h	3	9	-	0/2/19/22	0/1/1/1
9	MAN	h	4	9	-	0/2/19/22	0/1/1/1
9	MAN	h	5	9	-	0/2/19/22	0/1/1/1
9	MAN	h	6	9	-	1/2/19/22	0/1/1/1
5	NAG	i	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	i	2	5	-	3/6/23/26	0/1/1/1

The worst 5 of 269 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	1	NAG	C1-C2	5.92	1.60	1.52
9	h	1	NAG	C1-C2	5.81	1.60	1.52
6	e	1	NAG	C1-C2	5.78	1.60	1.52
9	Z	1	NAG	C1-C2	5.73	1.60	1.52
5	I	1	NAG	C1-C2	5.63	1.60	1.52

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	2	NAG	C8-C7-N2	6.27	126.52	116.12
5	i	2	NAG	C8-C7-N2	6.24	126.47	116.12
5	d	2	NAG	O7-C7-N2	-3.93	115.04	121.98
5	V	1	NAG	O4-C4-C3	-3.93	101.12	110.38
5	i	2	NAG	O7-C7-N2	-3.89	115.11	121.98

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	T	2	NAG	C1-C2-N2-C7
5	T	2	NAG	O7-C7-N2-C2

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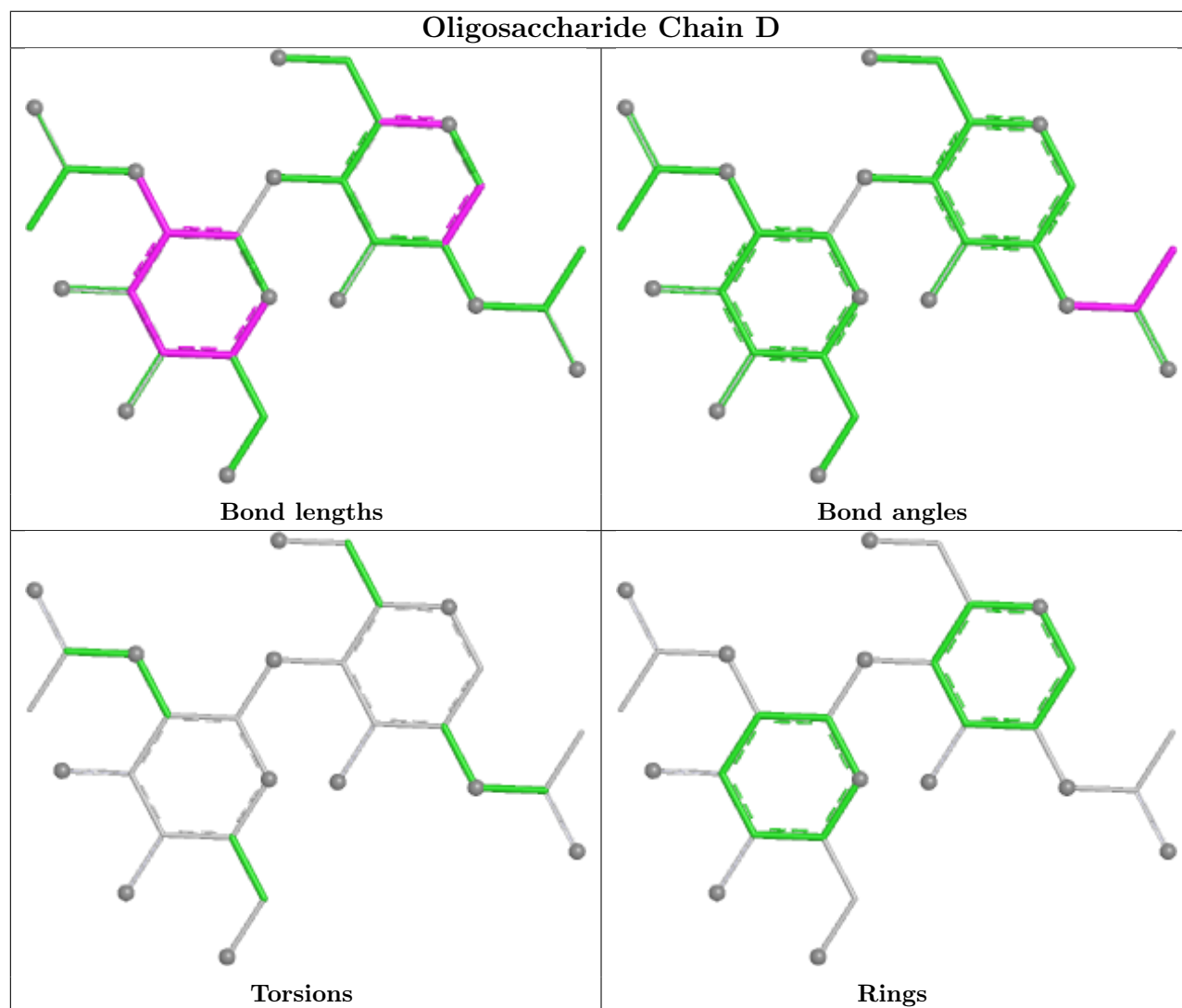
Mol	Chain	Res	Type	Atoms
5	g	1	NAG	C3-C2-N2-C7

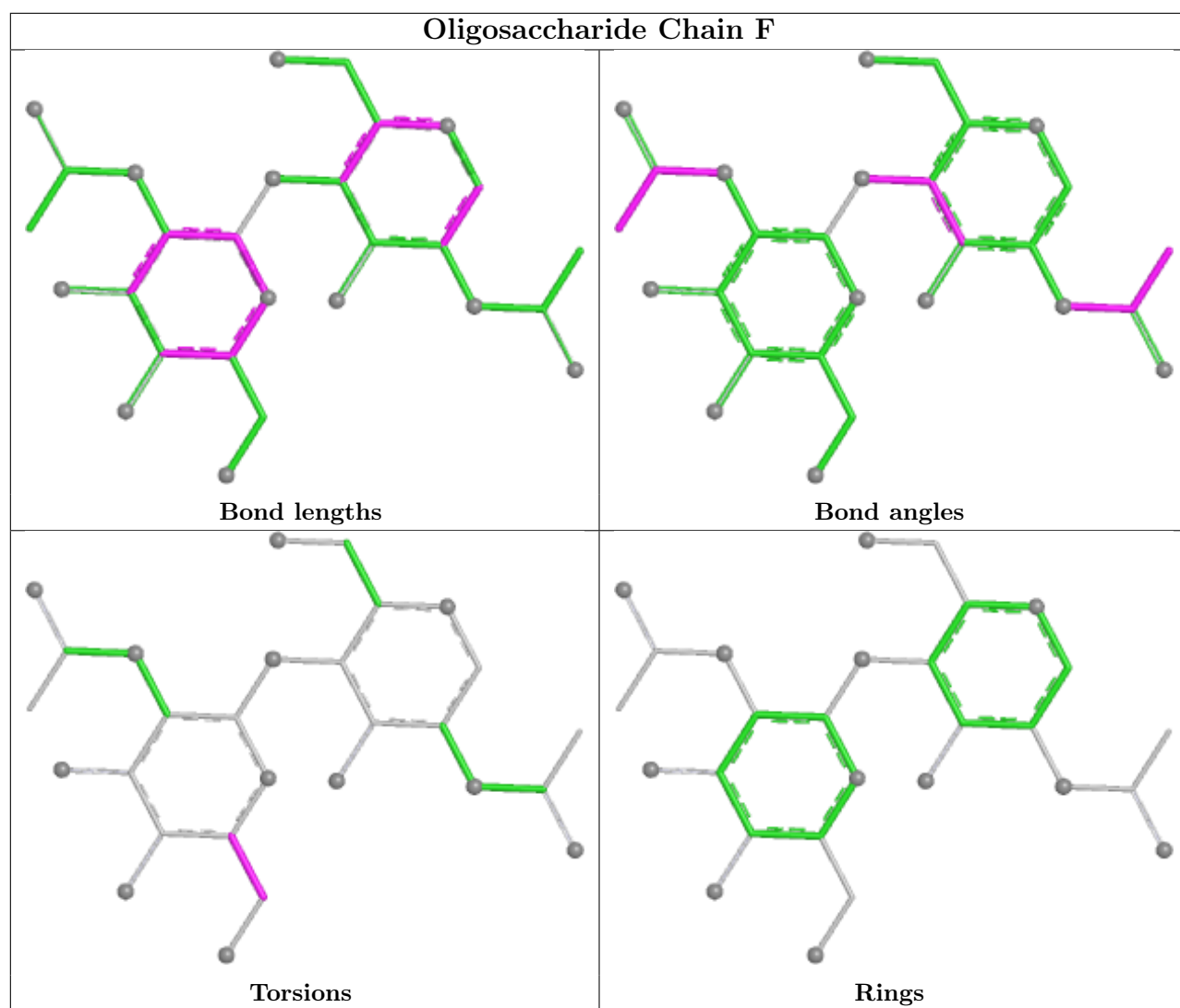
There are no ring outliers.

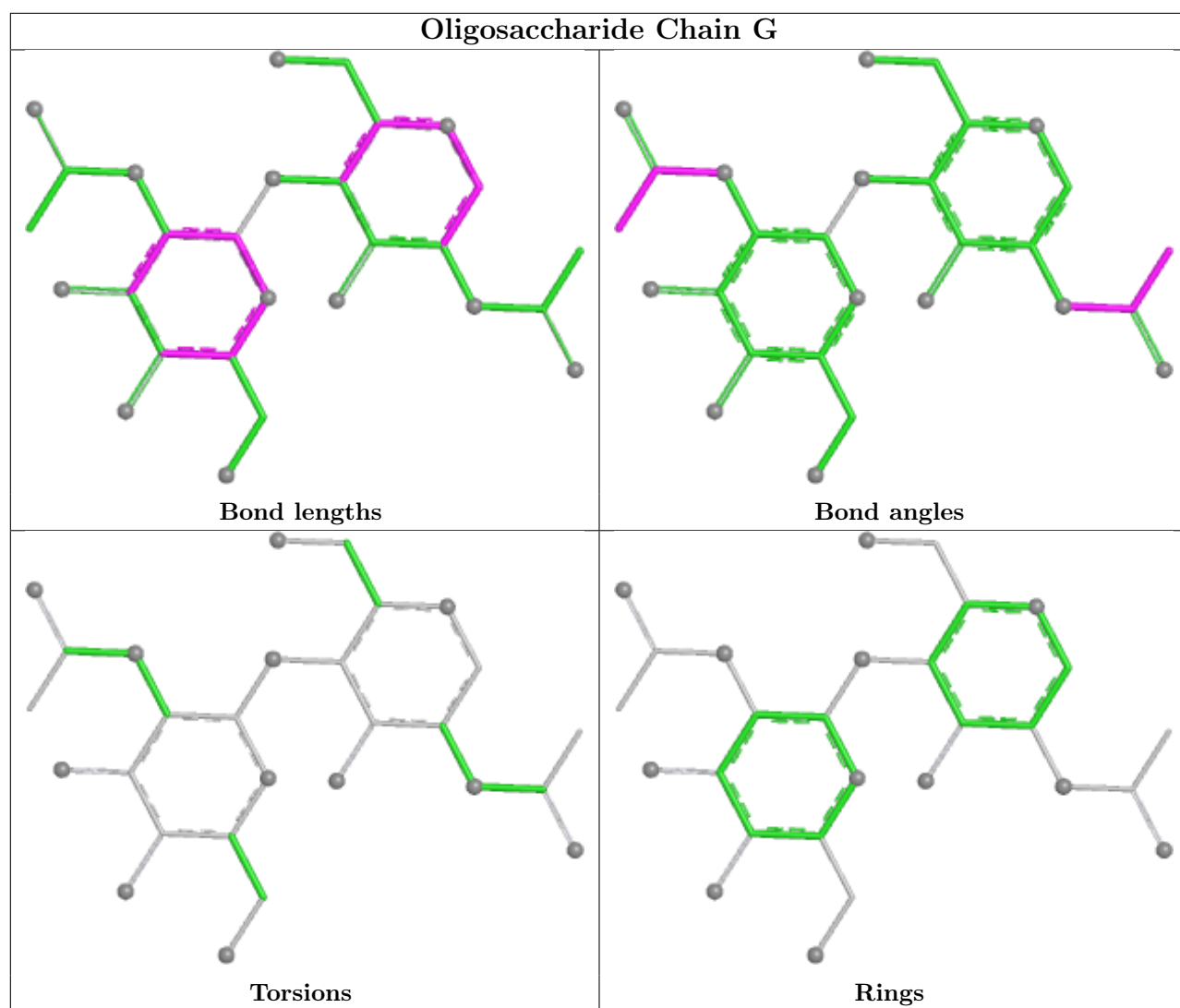
3 monomers are involved in 3 short contacts:

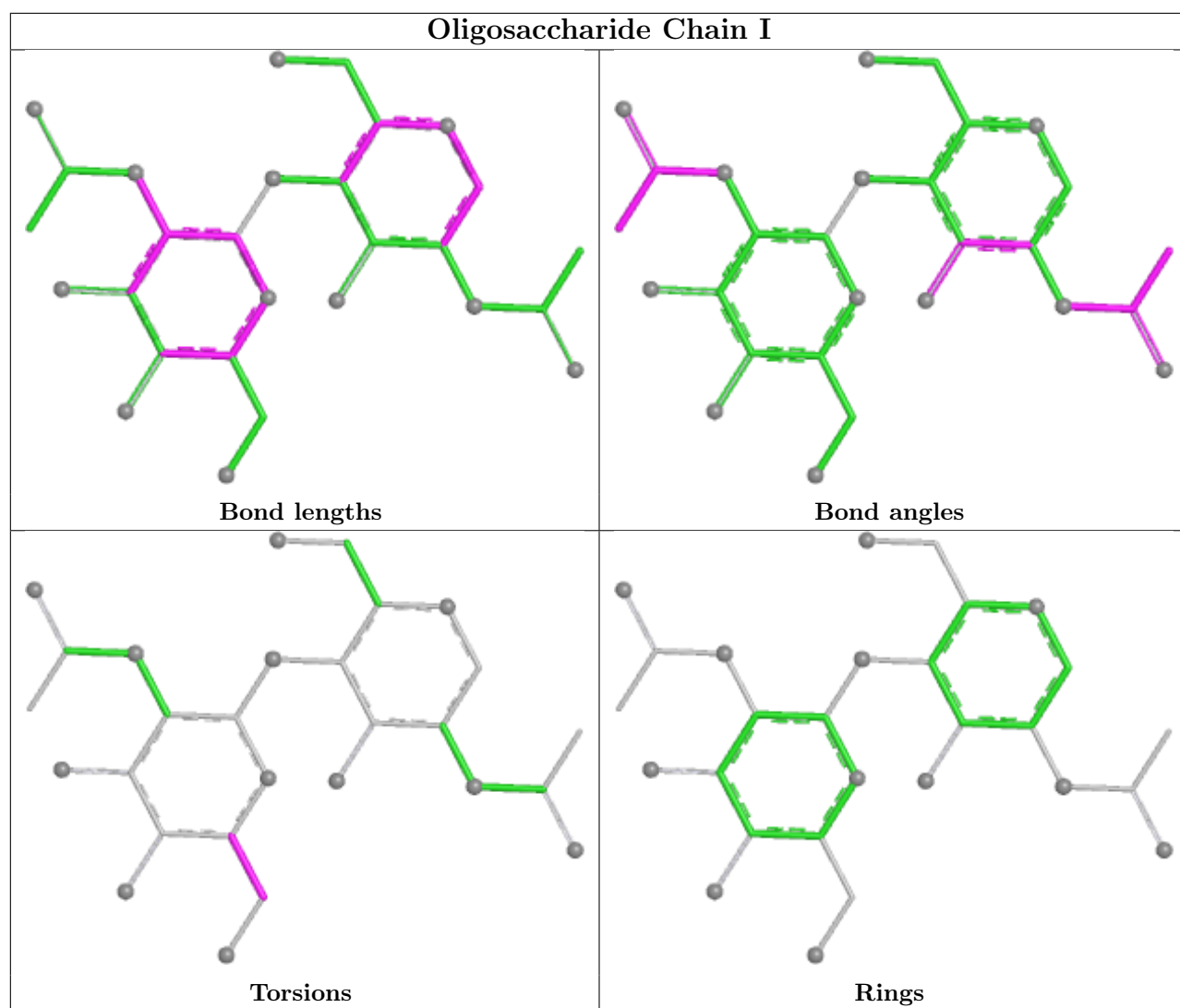
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	2	NAG	2	0
5	K	1	NAG	1	0
5	T	1	NAG	2	0

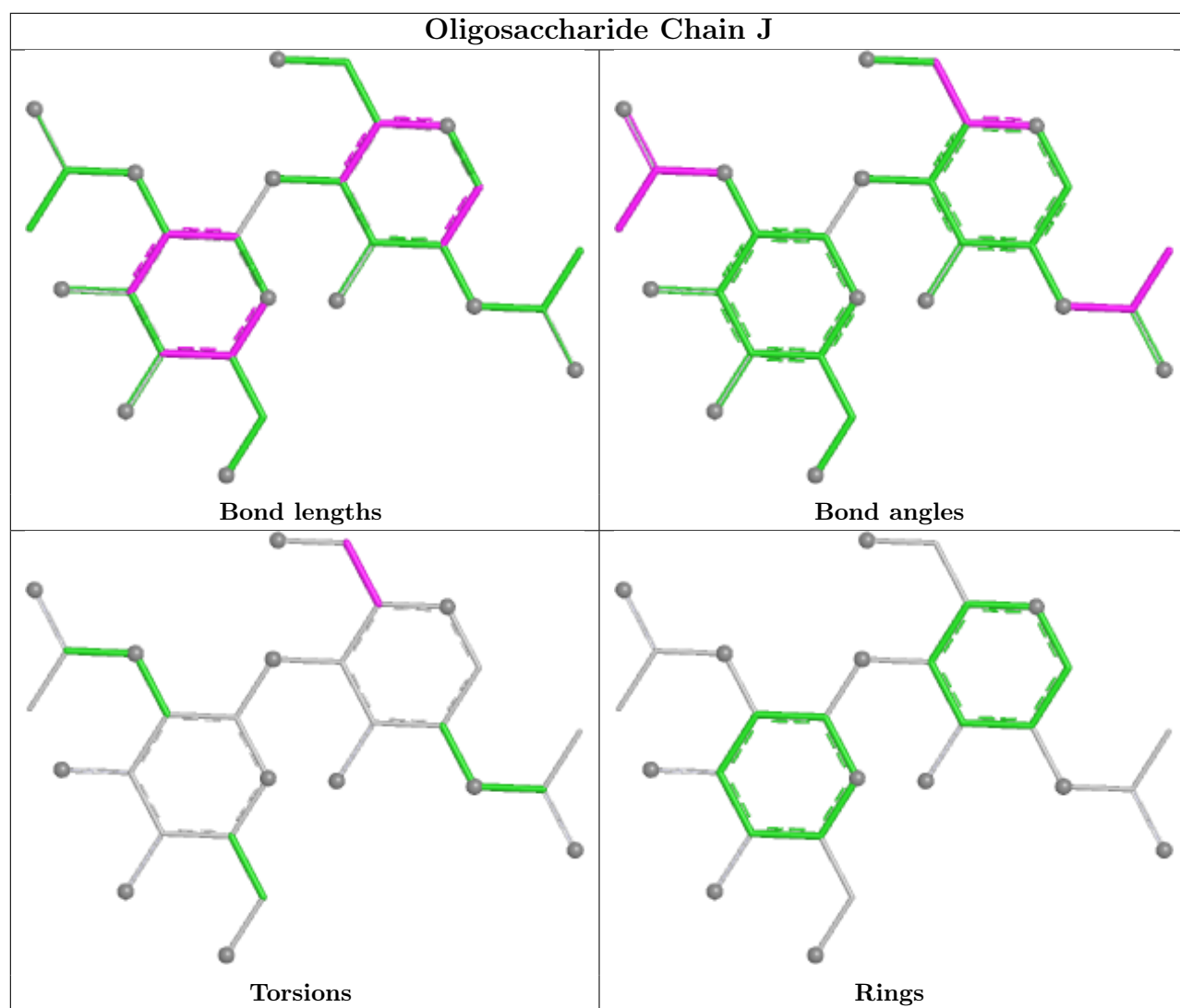
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

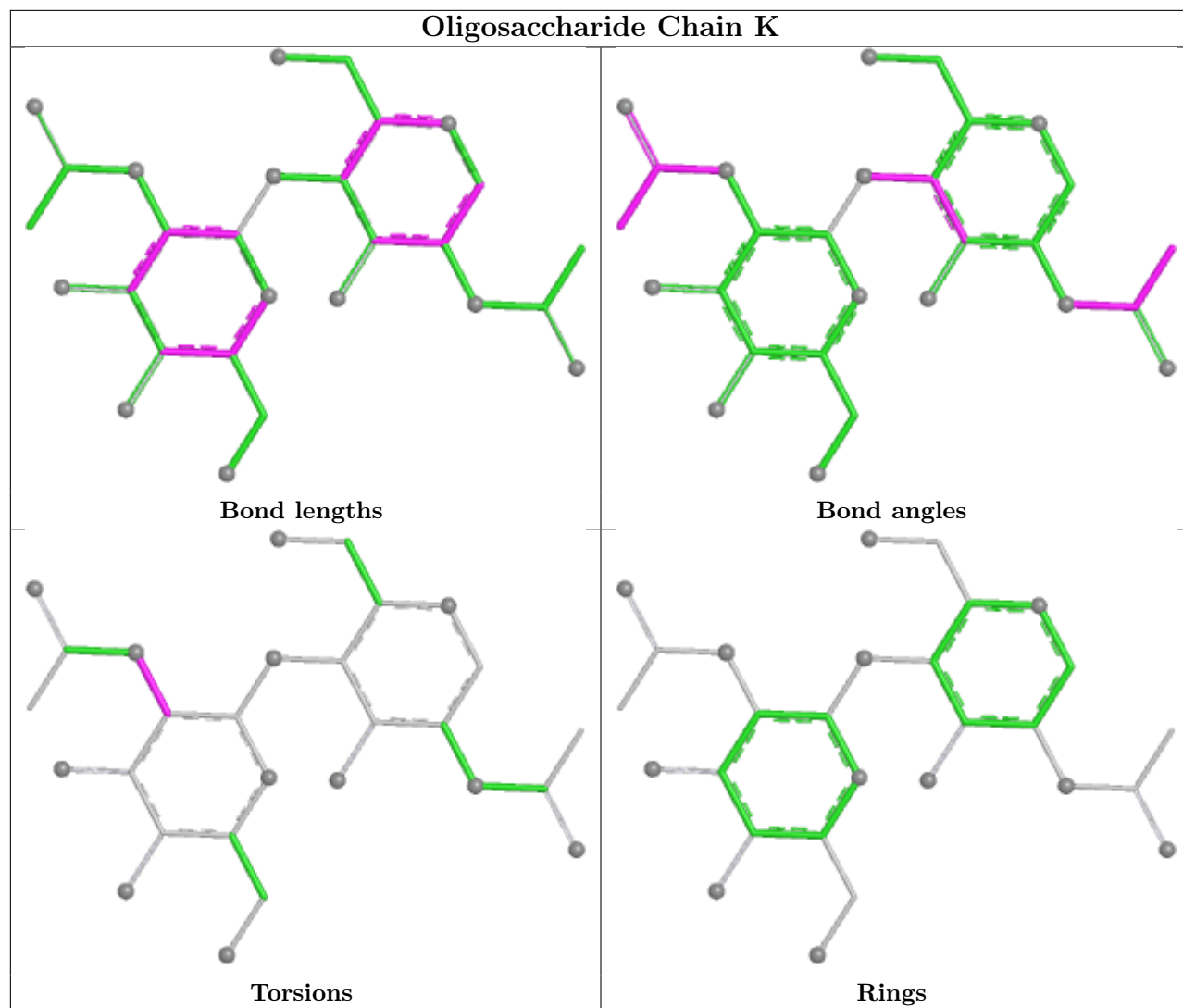


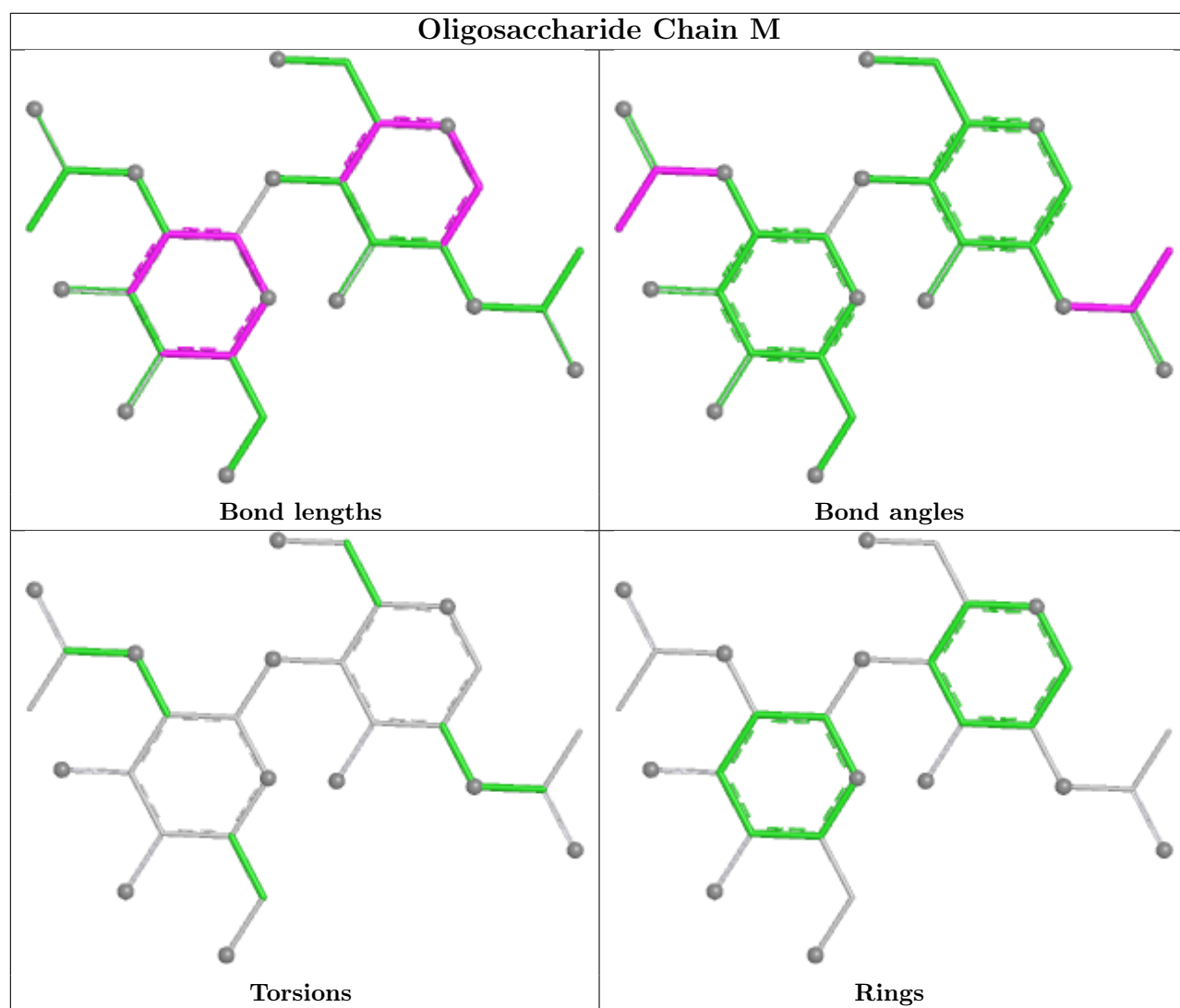


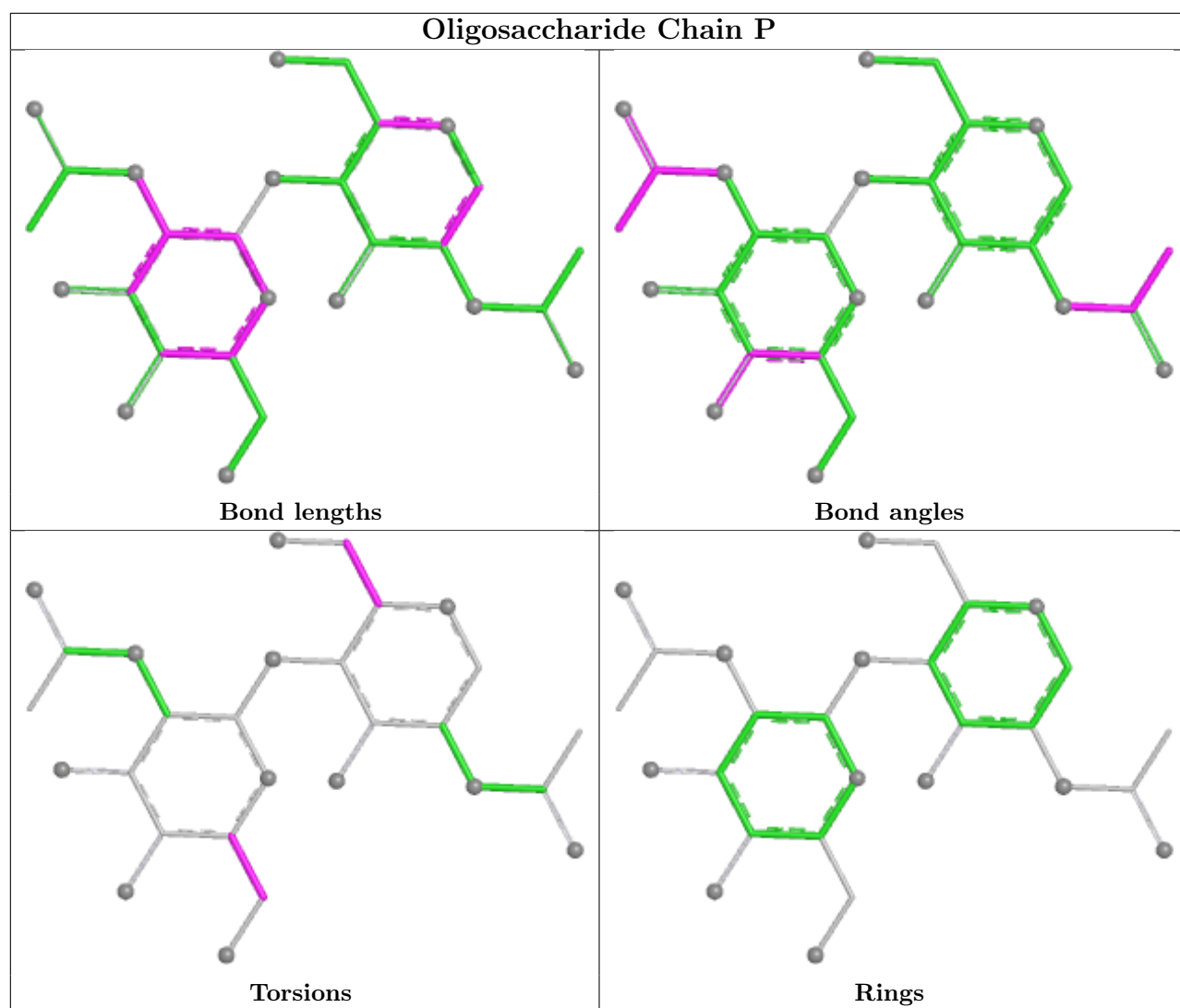


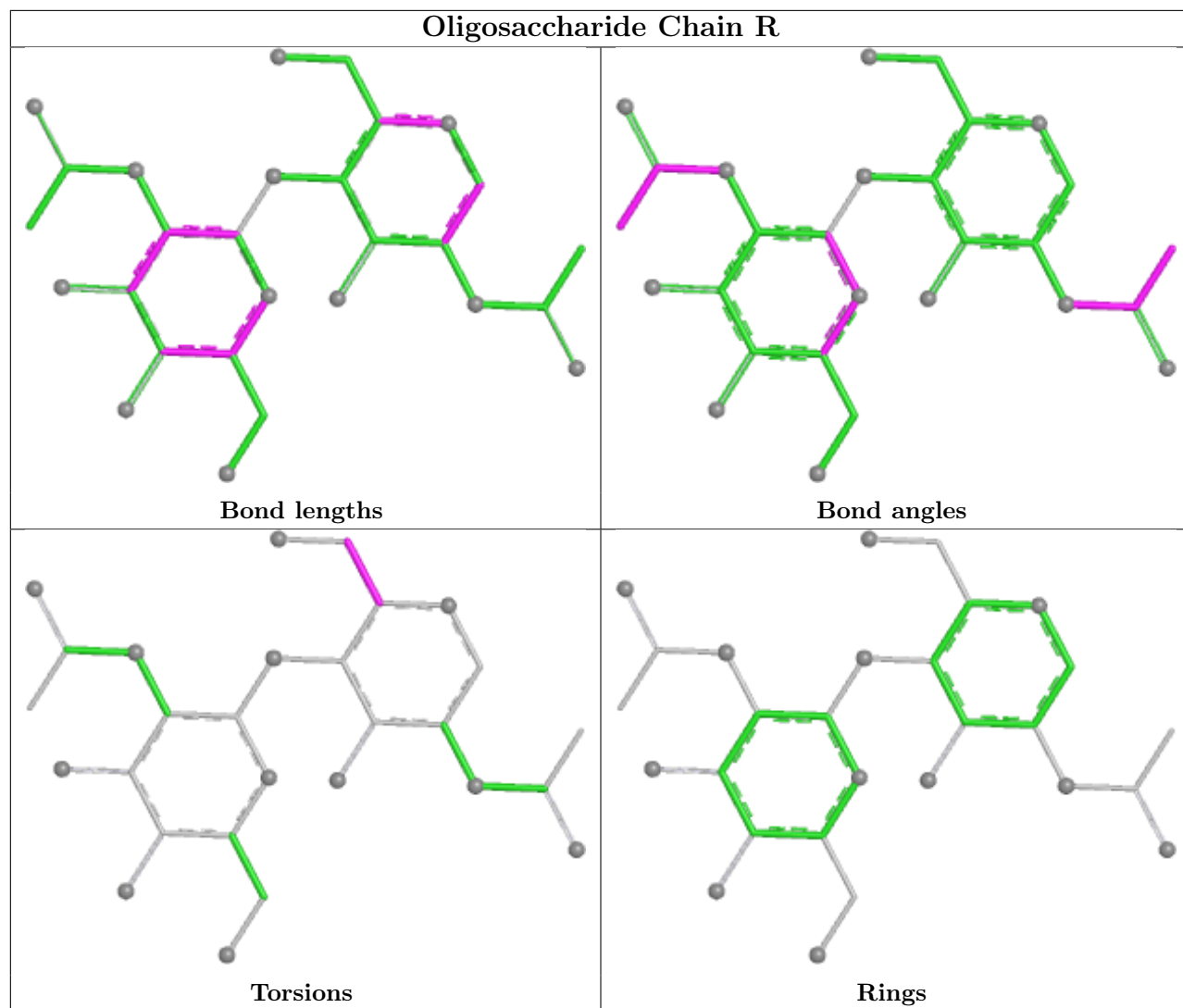


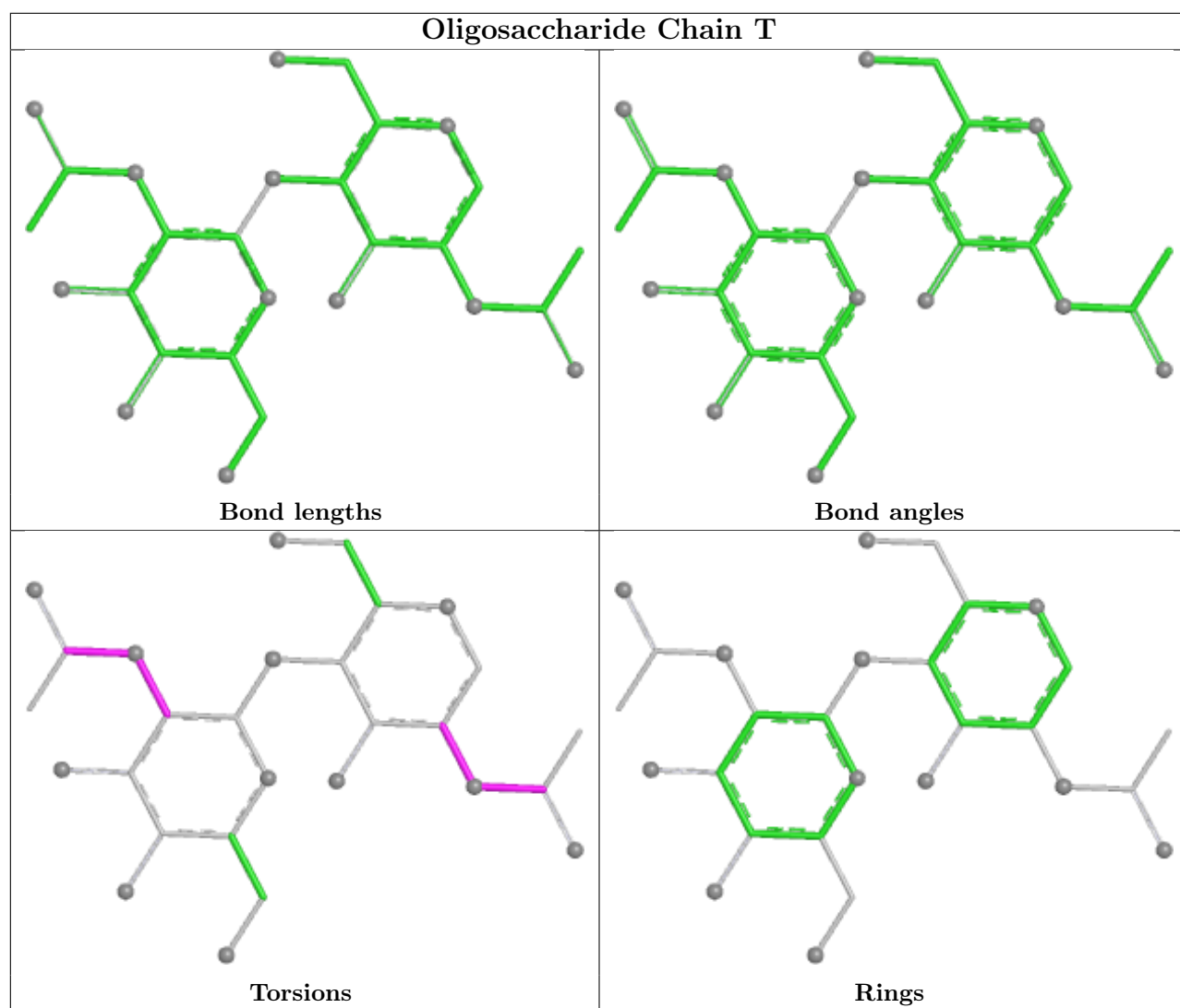


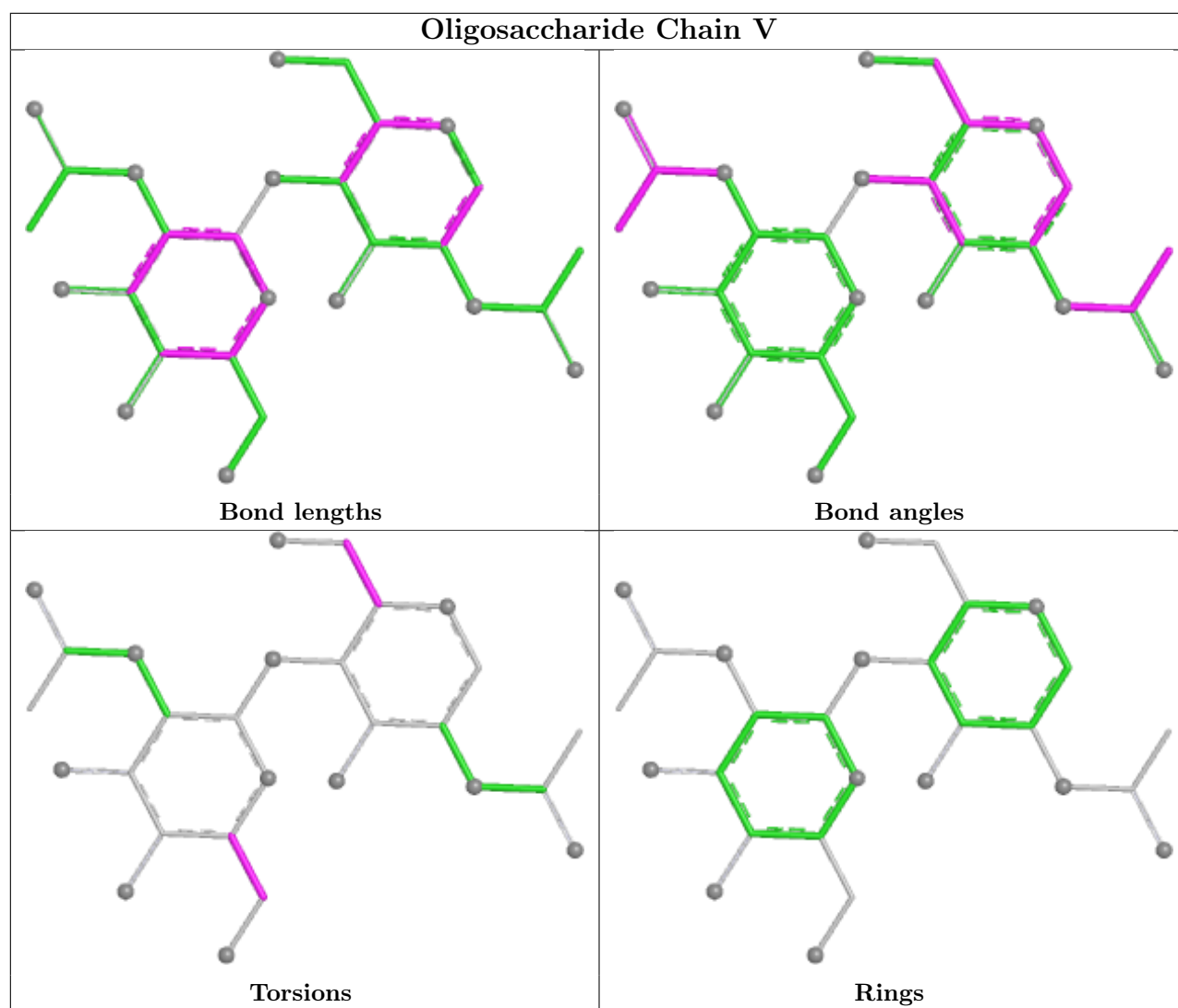


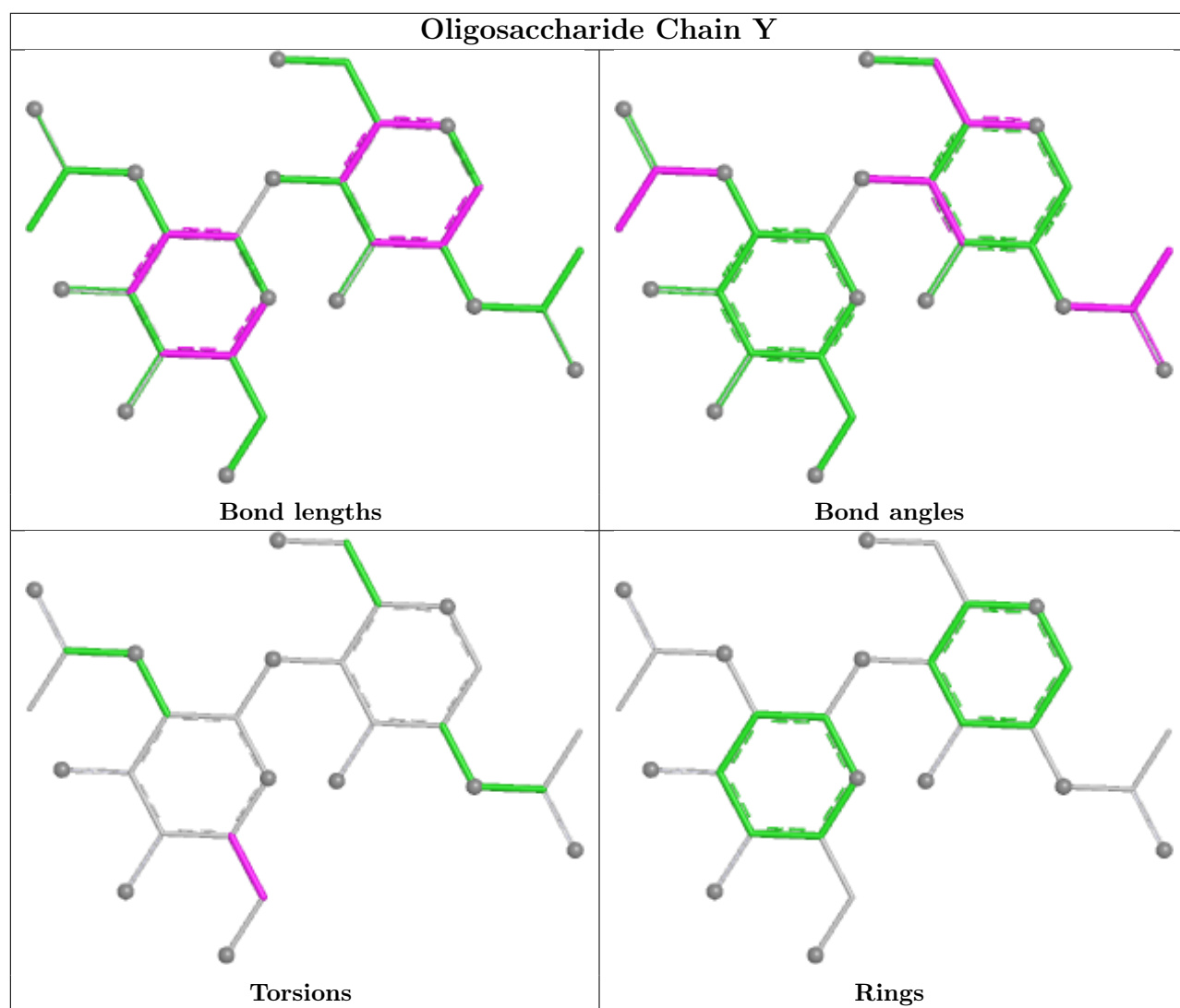


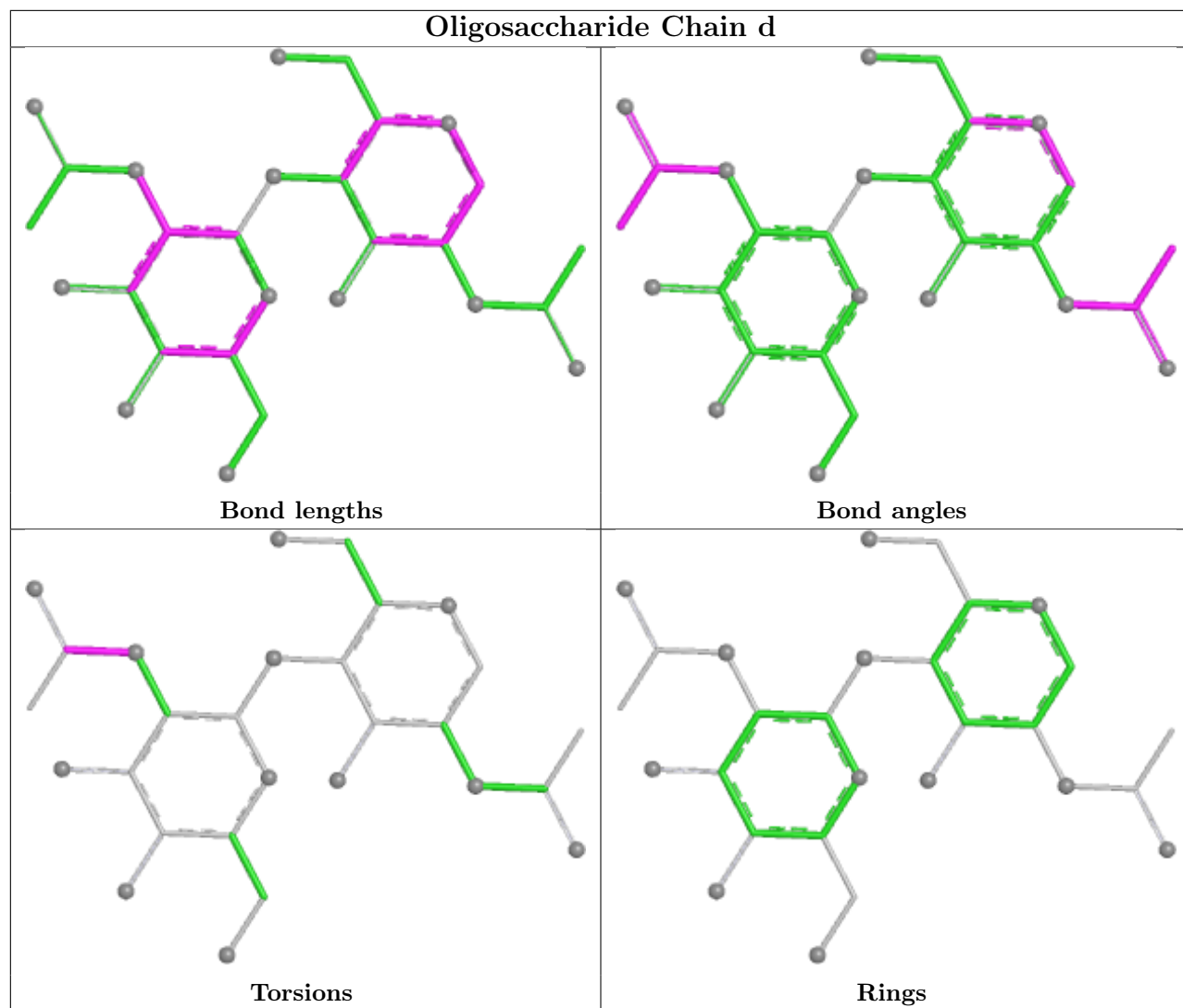


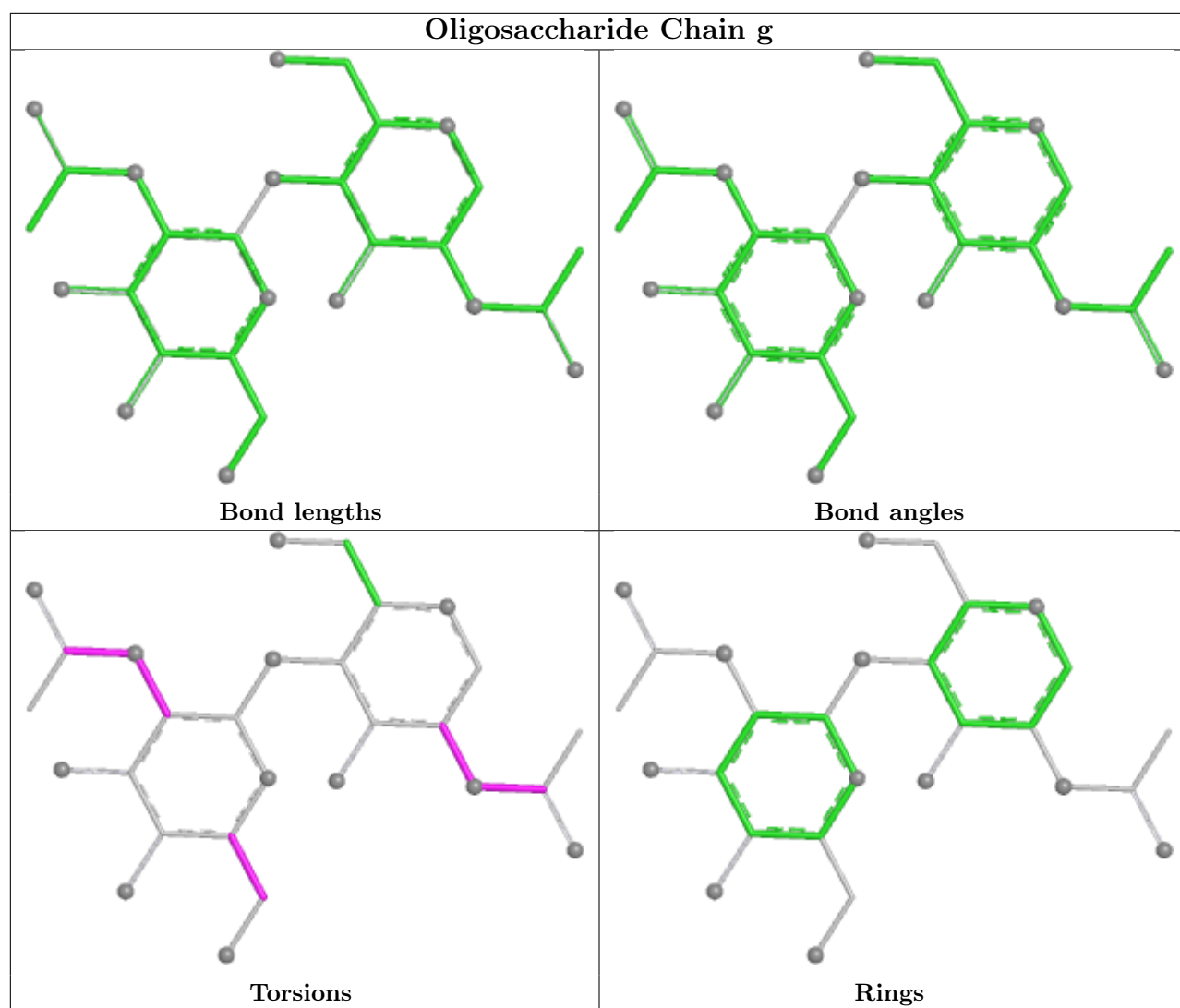


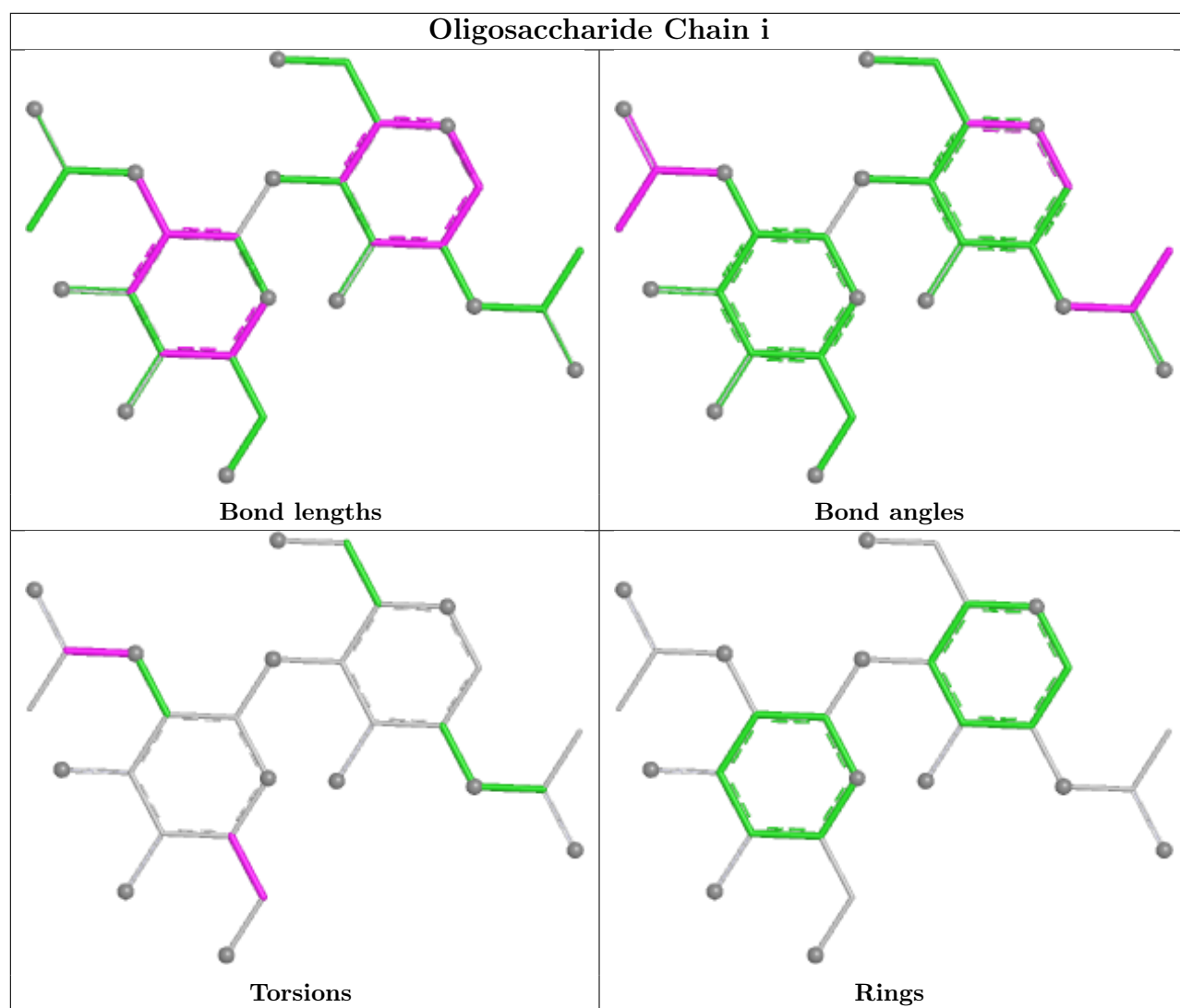


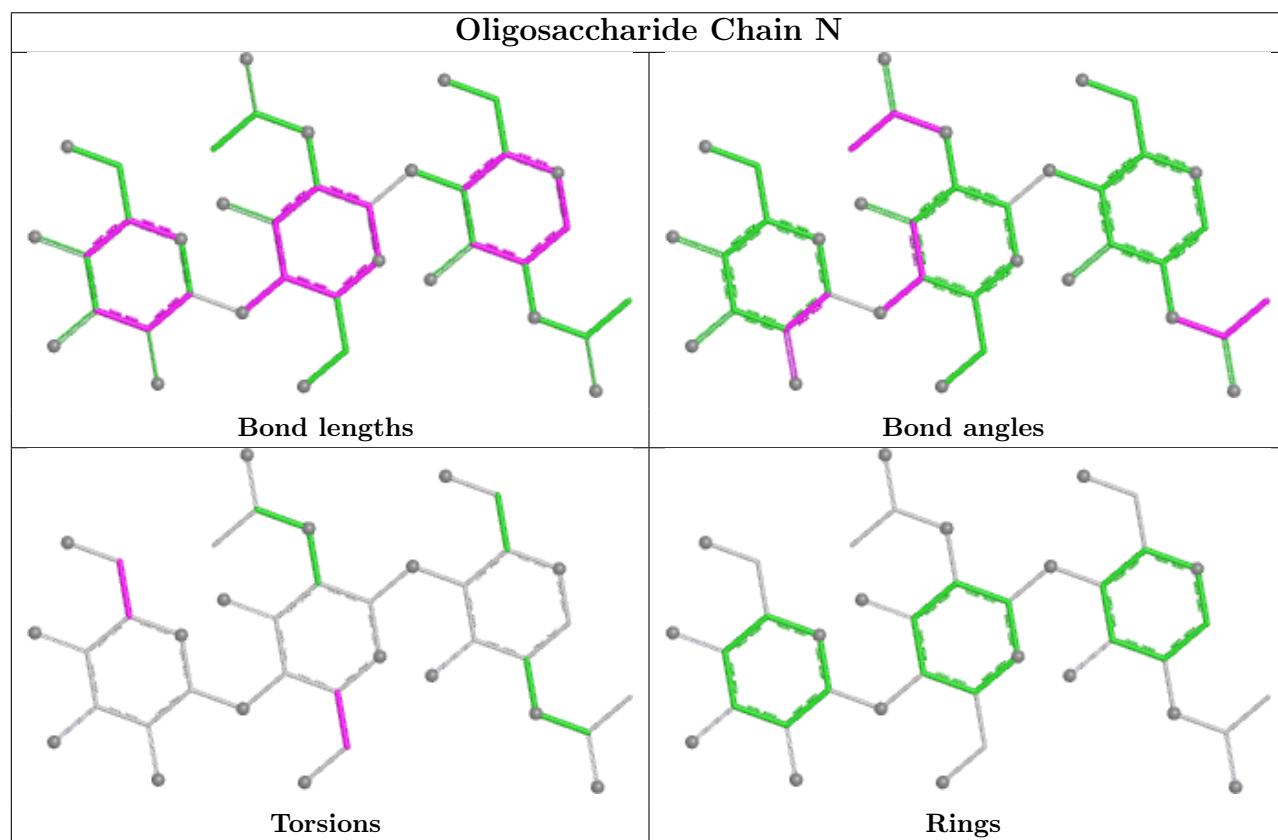
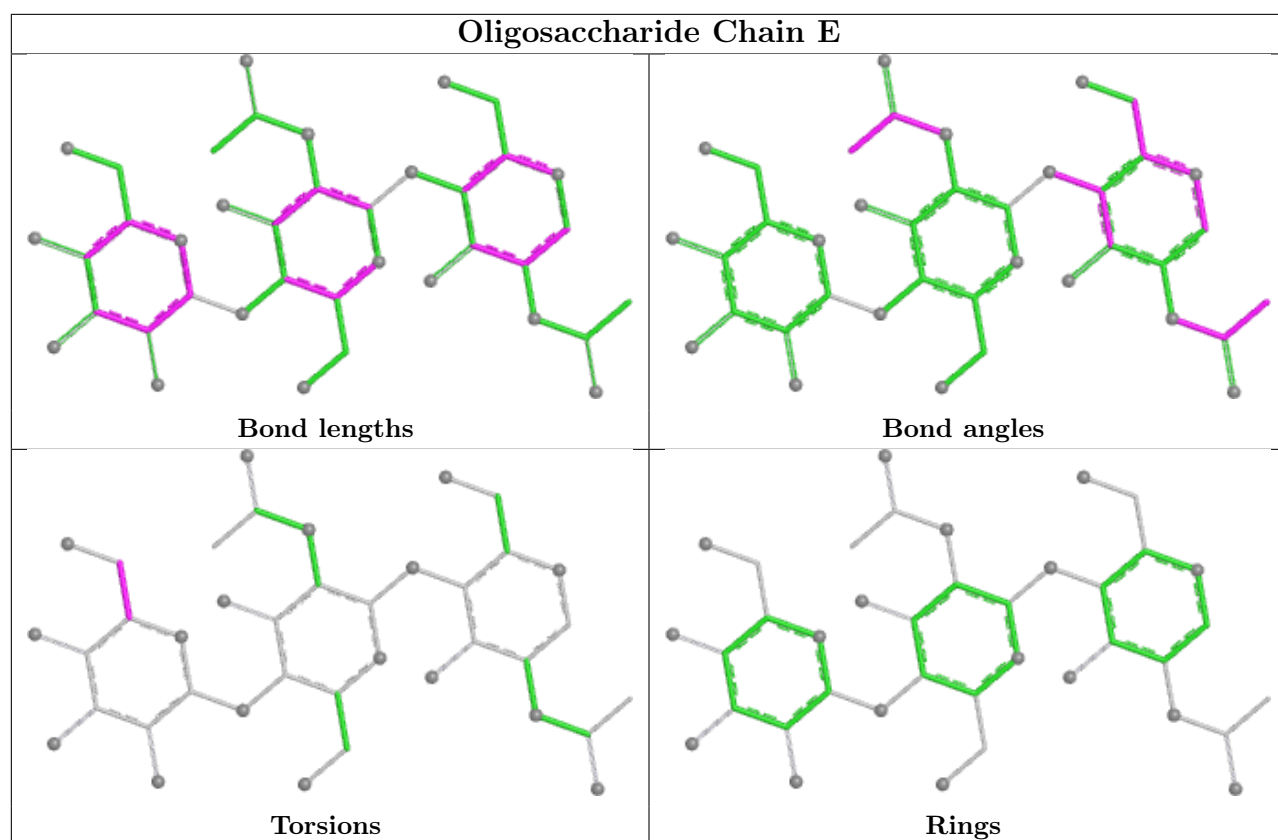


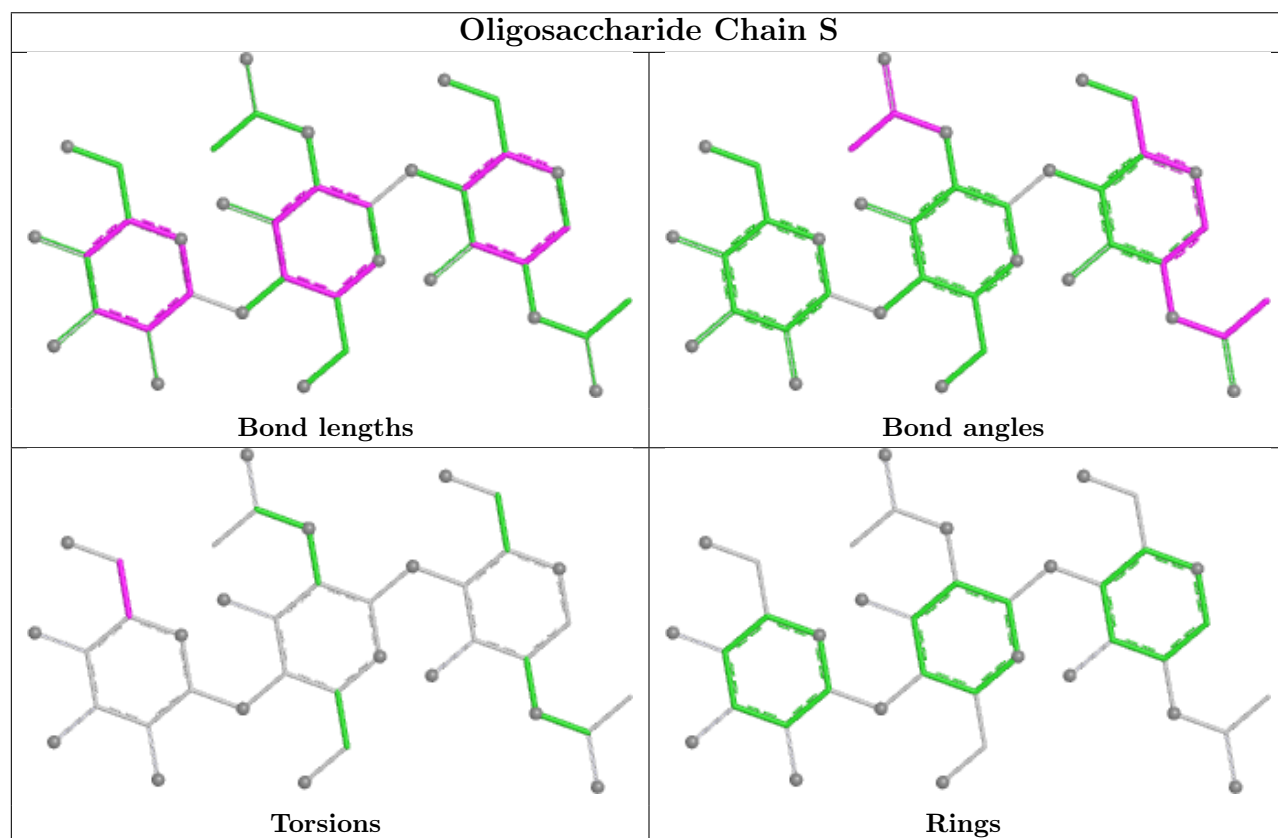
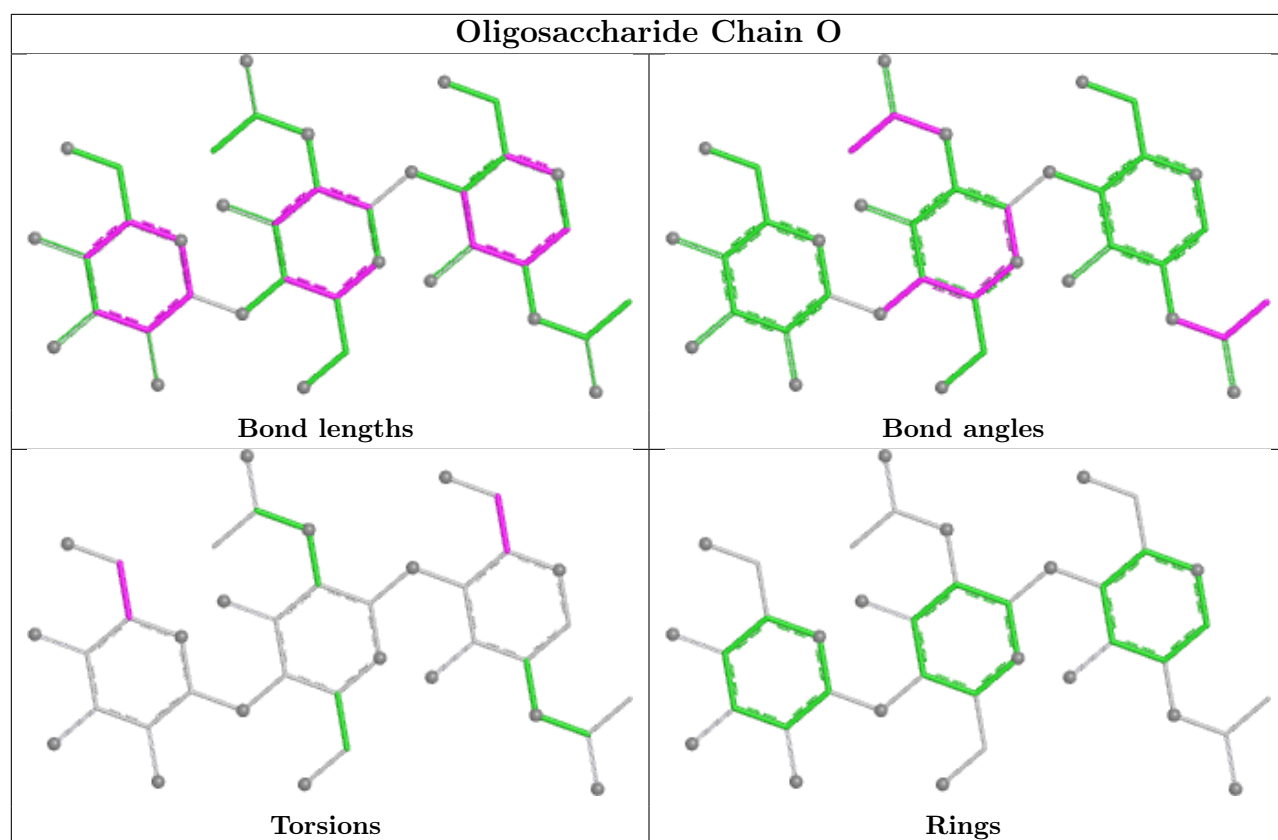


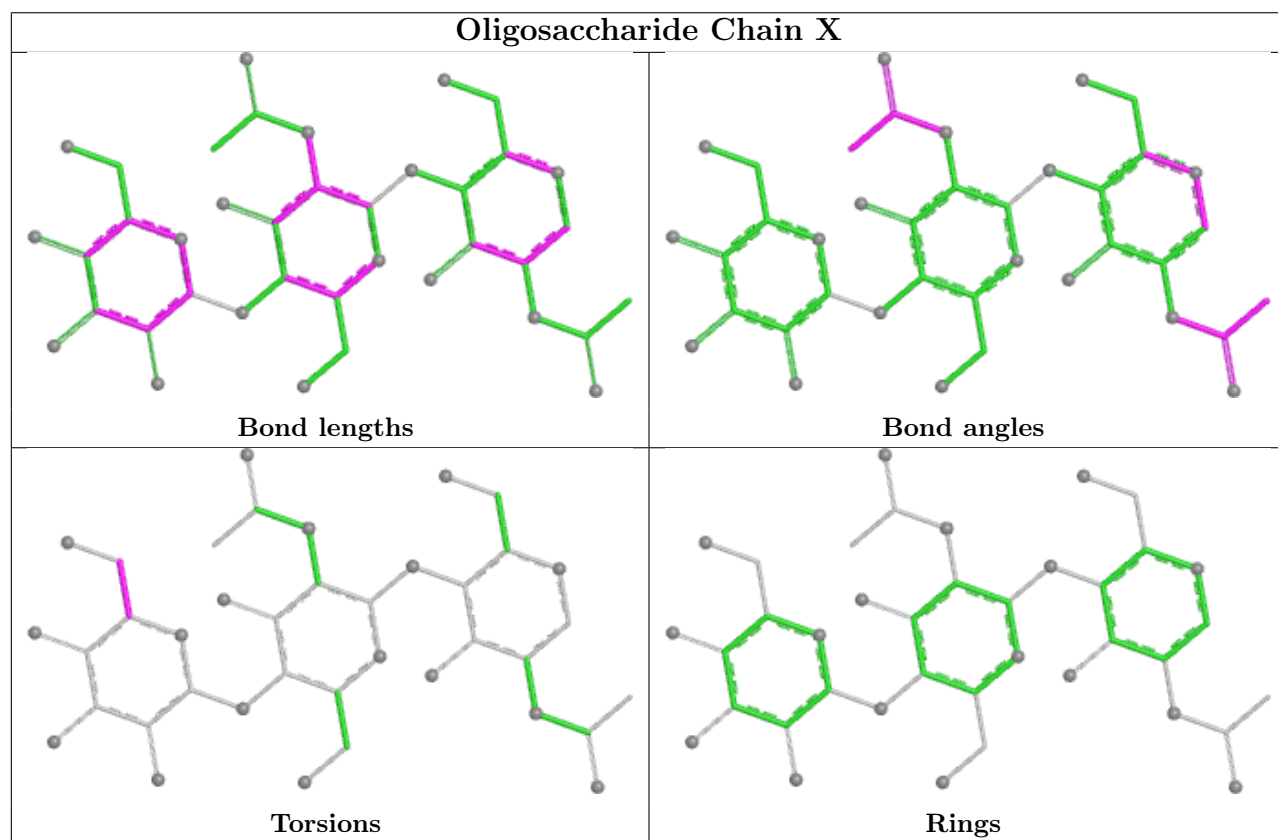
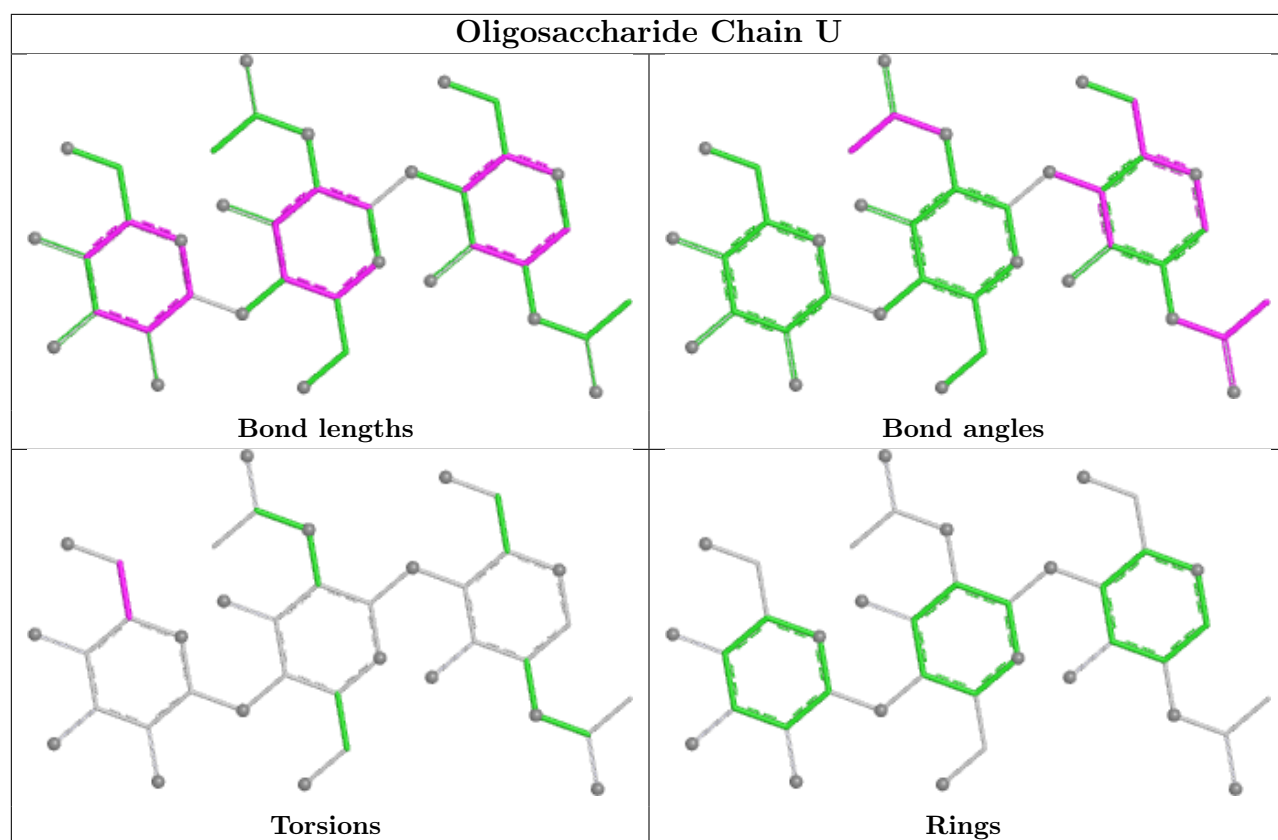


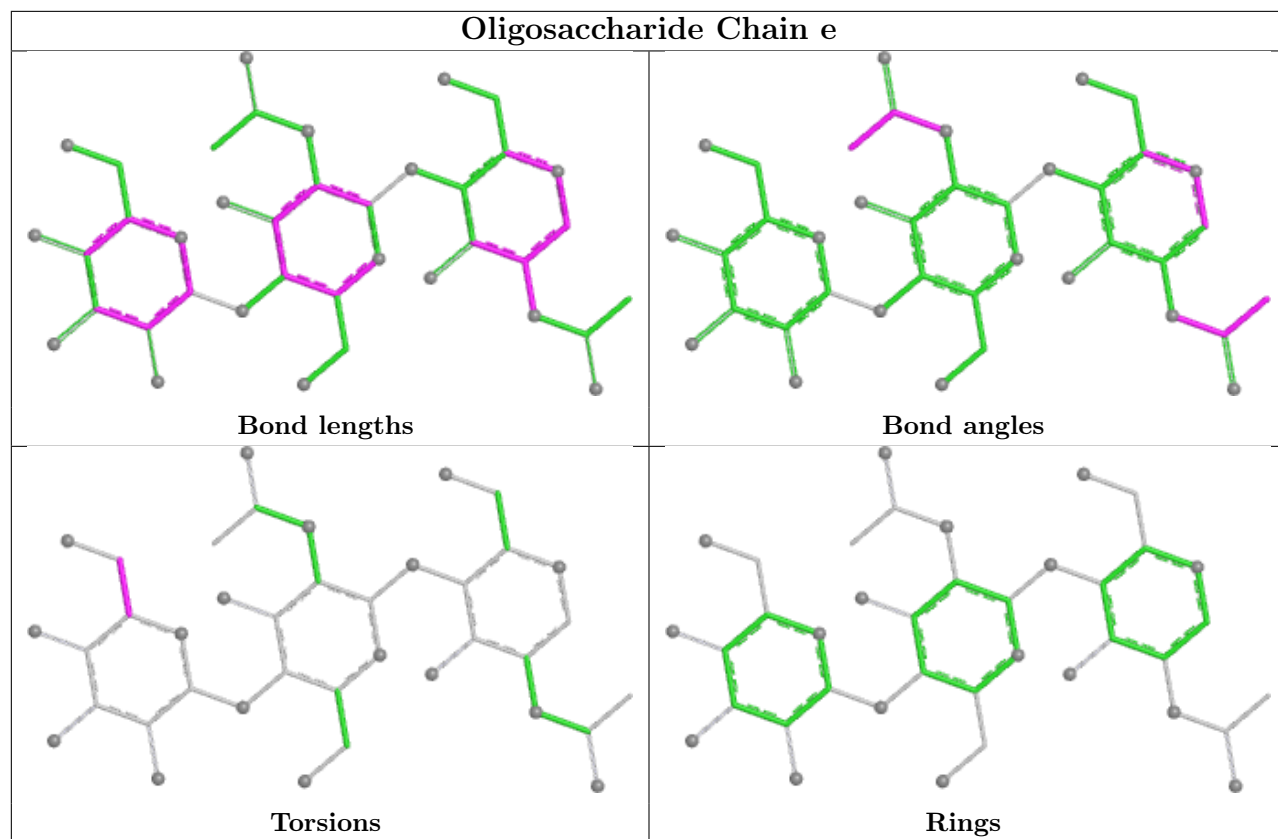


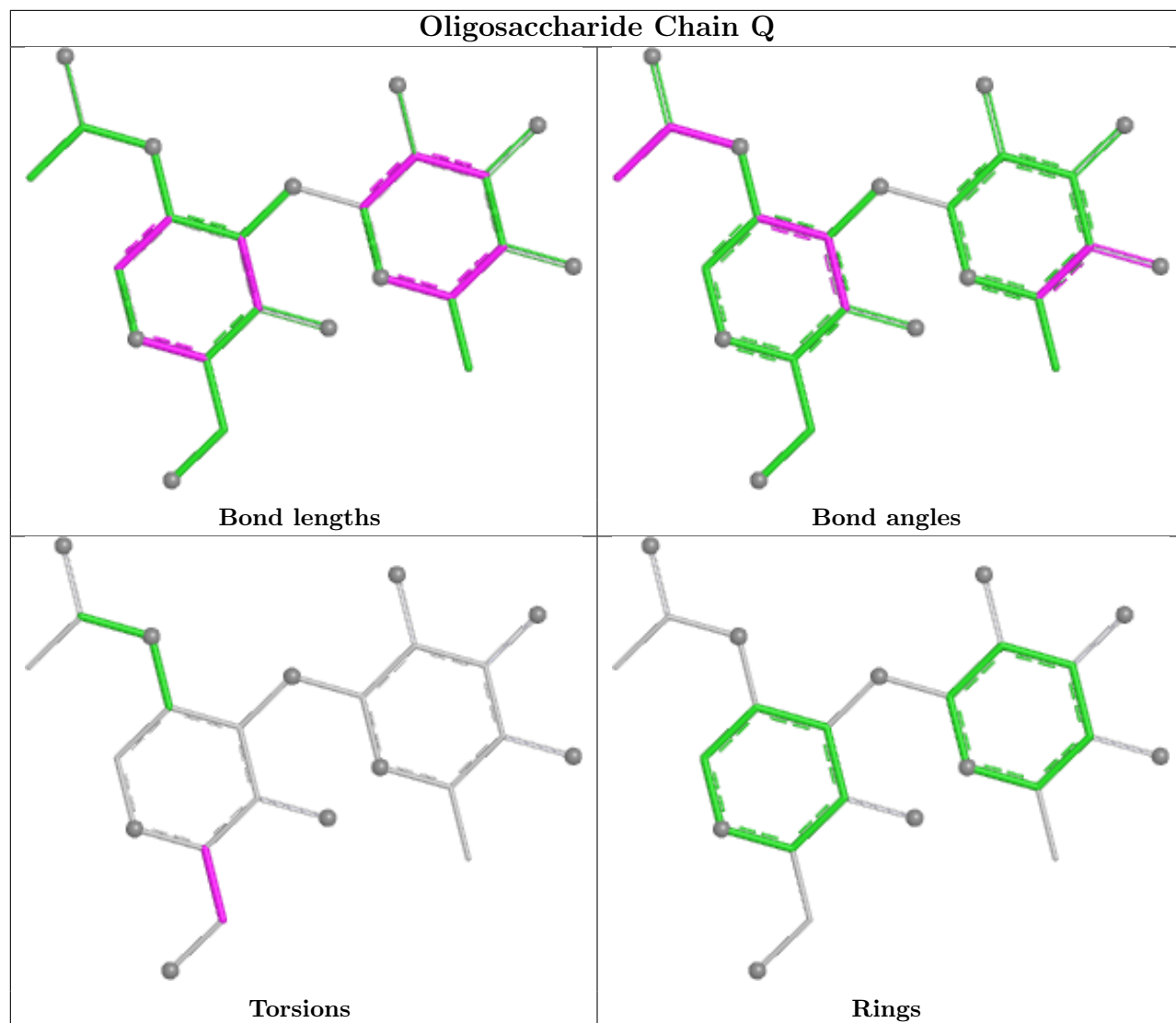


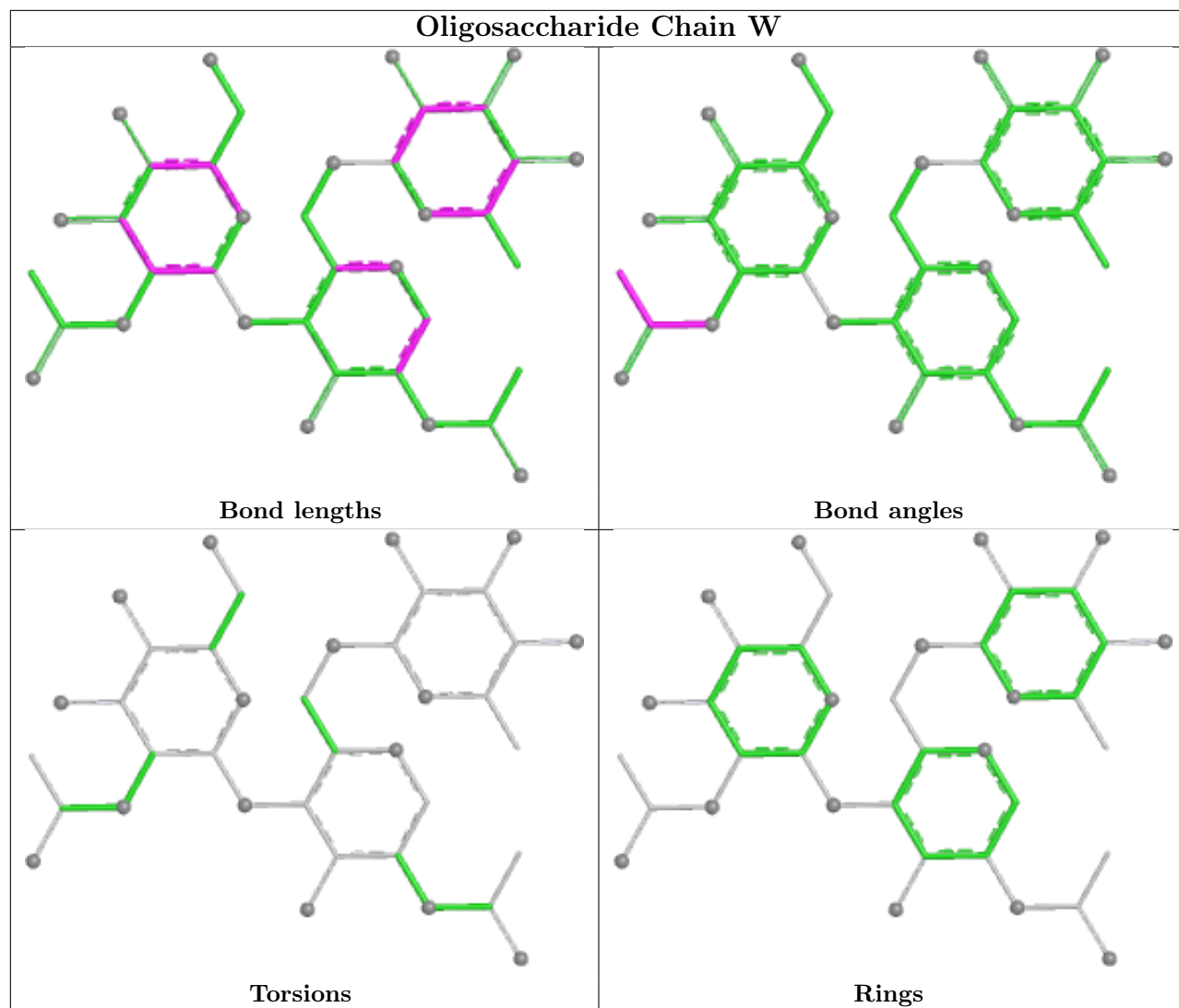


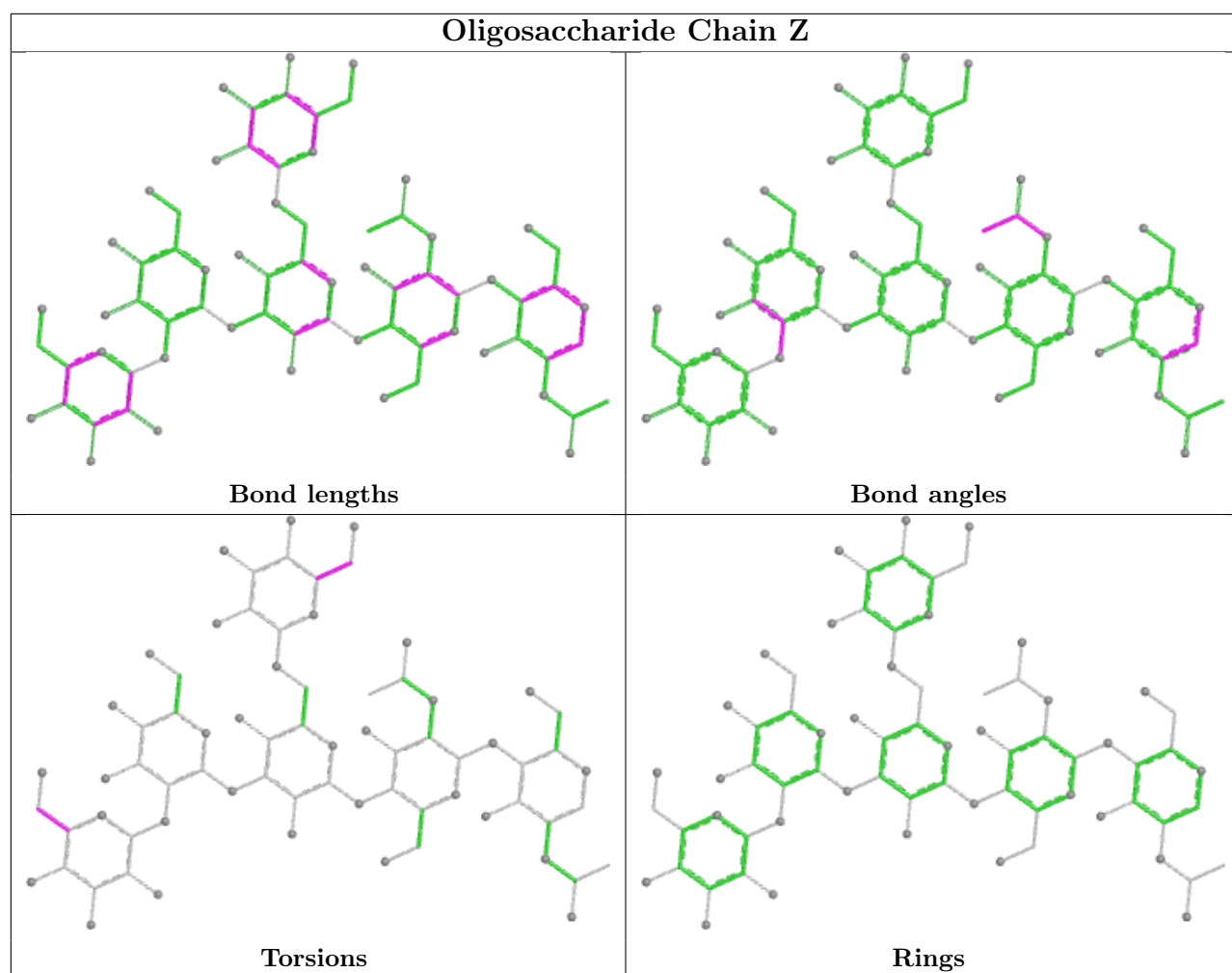


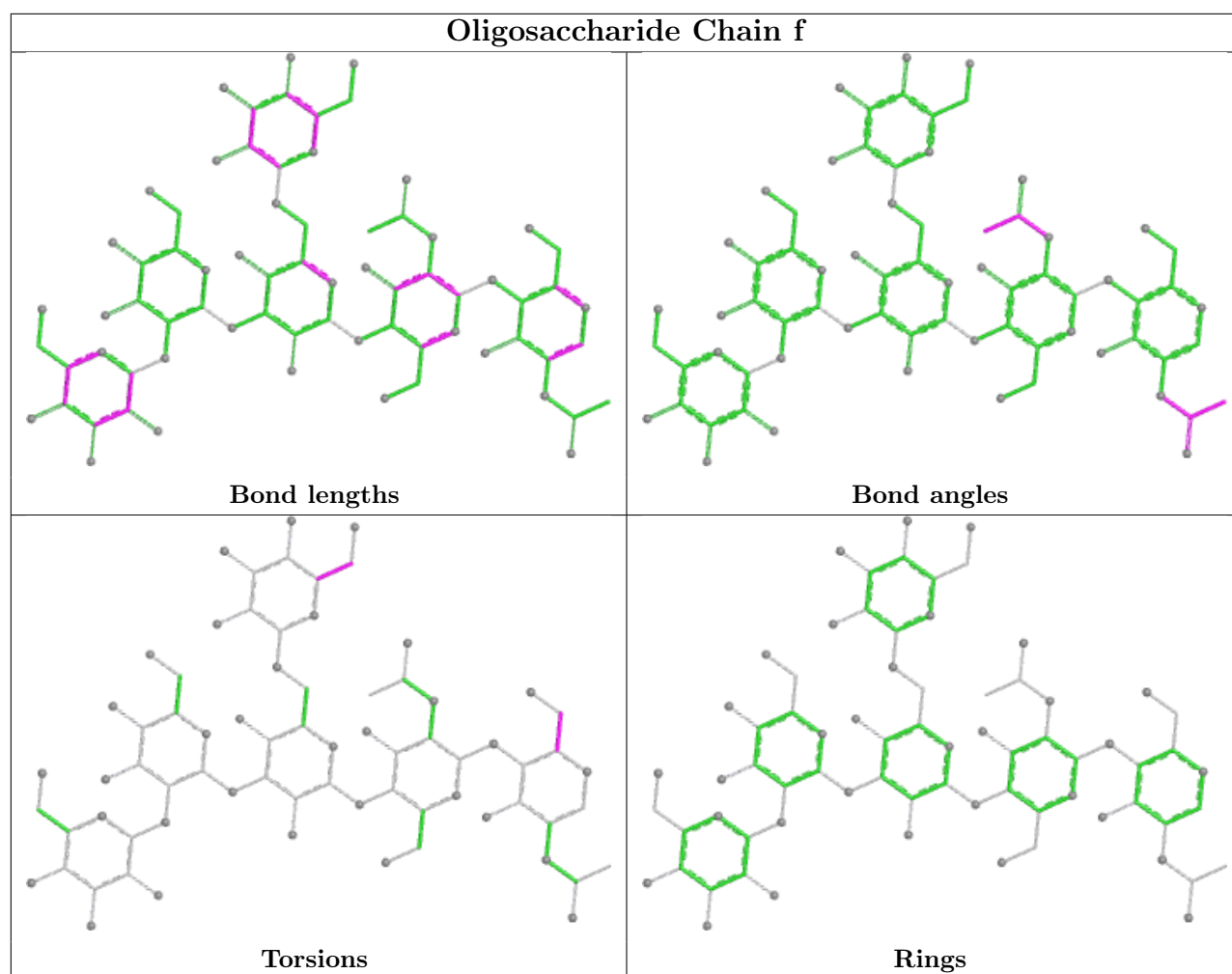


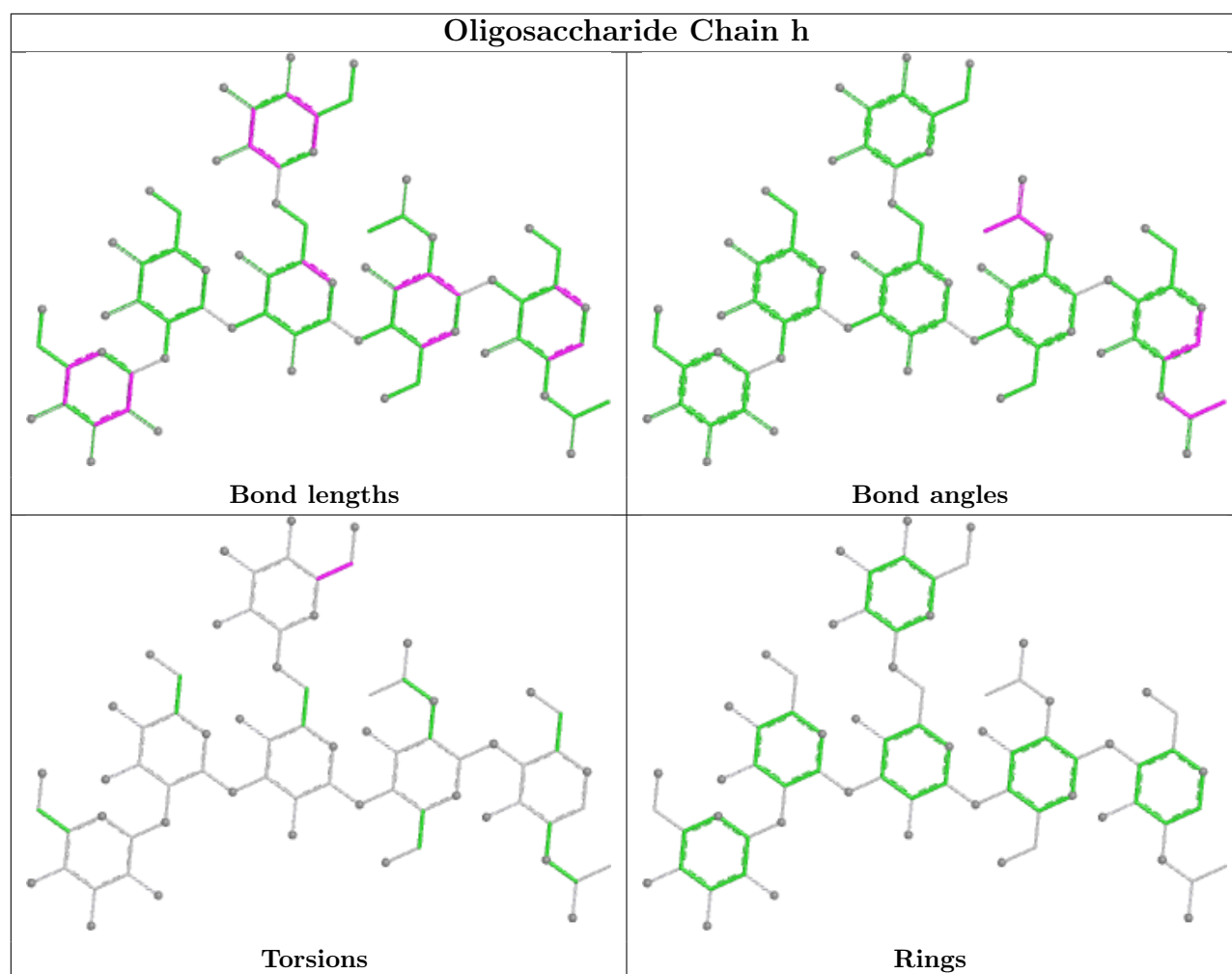












5.6 Ligand geometry [i](#)

6 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
10	NAG	b	701	4	14,14,15	2.52	6 (42%)	17,19,21	1.61	2 (11%)
10	NAG	a	702	4	14,14,15	2.27	6 (42%)	17,19,21	0.98	1 (5%)
10	NAG	c	701	4	14,14,15	2.25	6 (42%)	17,19,21	1.00	1 (5%)
10	NAG	c	702	4	14,14,15	2.24	5 (35%)	17,19,21	1.05	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	C	301	1	14,14,15	2.24	6 (42%)	17,19,21	1.06	2 (11%)
10	NAG	a	701	4	14,14,15	2.33	5 (35%)	17,19,21	0.98	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
10	NAG	b	701	4	-	2/6/23/26	0/1/1/1
10	NAG	a	702	4	-	0/6/23/26	0/1/1/1
10	NAG	c	701	4	-	1/6/23/26	0/1/1/1
10	NAG	c	702	4	-	1/6/23/26	0/1/1/1
10	NAG	C	301	1	-	0/6/23/26	0/1/1/1
10	NAG	a	701	4	-	0/6/23/26	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	701	NAG	C1-C2	7.29	1.62	1.52
10	a	701	NAG	C1-C2	6.41	1.61	1.52
10	a	702	NAG	C1-C2	6.05	1.60	1.52
10	c	702	NAG	C1-C2	5.88	1.60	1.52
10	C	301	NAG	C1-C2	5.83	1.60	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	b	701	NAG	C1-C2-N2	3.86	116.51	110.43
10	b	701	NAG	C2-N2-C7	3.61	127.74	122.90
10	C	301	NAG	C8-C7-N2	2.58	120.40	116.12
10	c	701	NAG	C8-C7-N2	2.53	120.32	116.12
10	c	702	NAG	C8-C7-N2	2.49	120.25	116.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	b	701	NAG	C1-C2-N2-C7
10	b	701	NAG	O5-C5-C6-O6
10	c	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	c	702	NAG	O5-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.

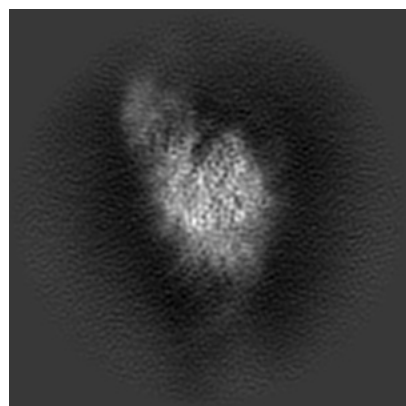
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41713. These allow visual inspection of the internal detail of the map and identification of artifacts.

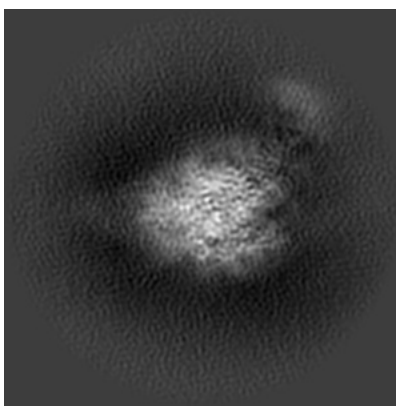
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

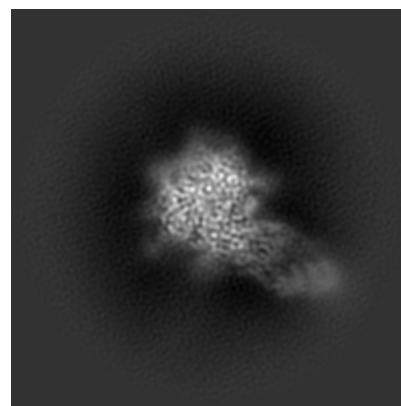
6.1.1 Primary map



X

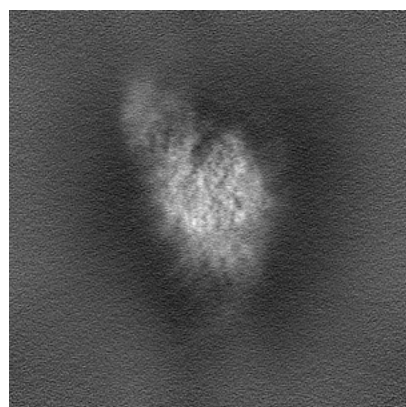


Y

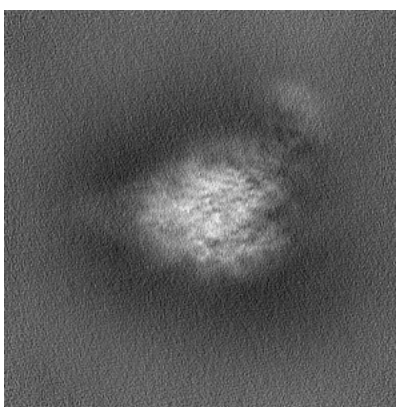


Z

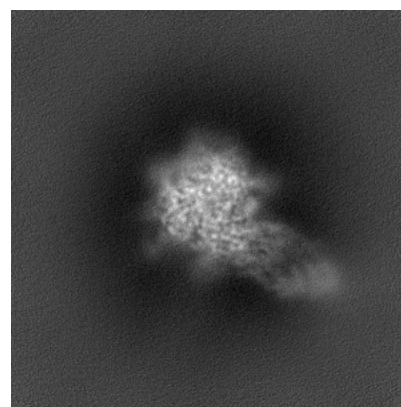
6.1.2 Raw map



X



Y

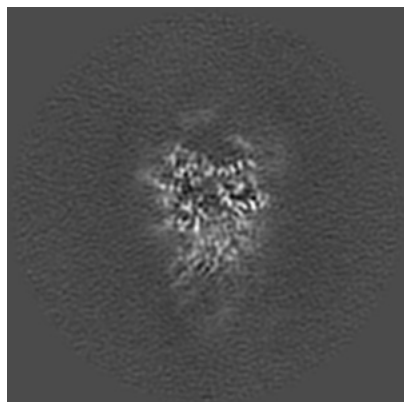


Z

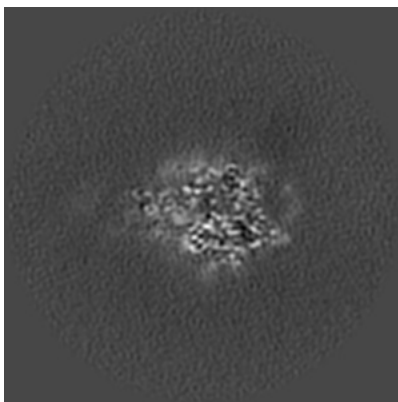
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

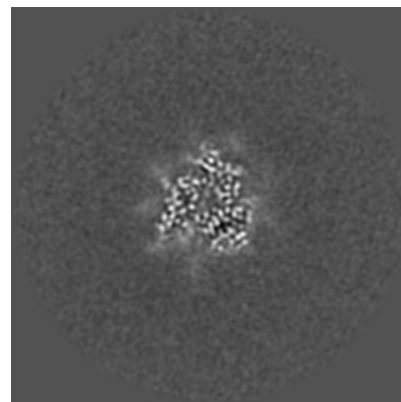
6.2.1 Primary map



X Index: 160

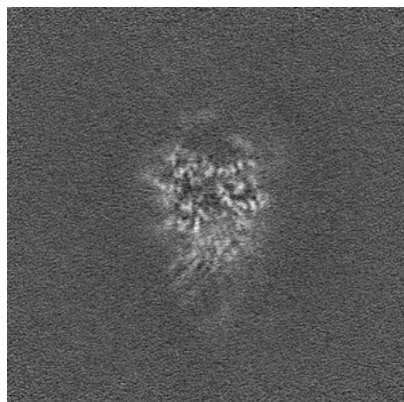


Y Index: 160

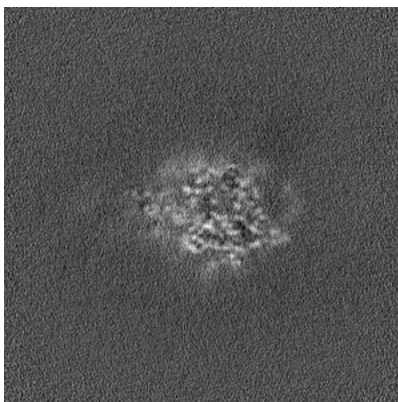


Z Index: 160

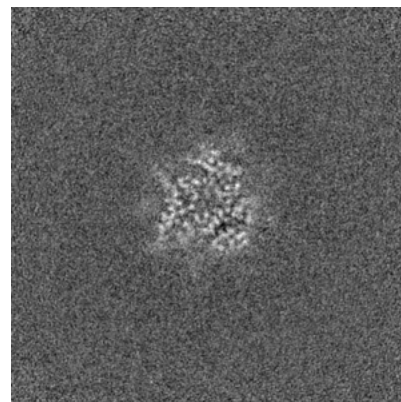
6.2.2 Raw map



X Index: 160



Y Index: 160

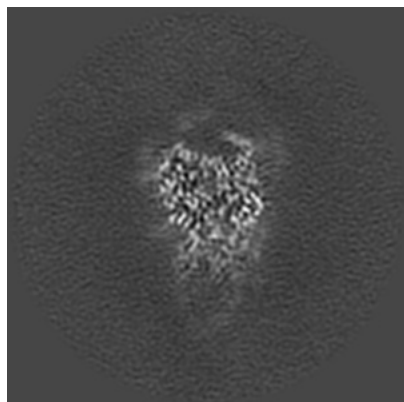


Z Index: 160

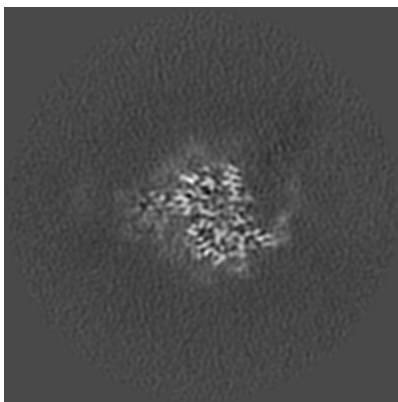
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

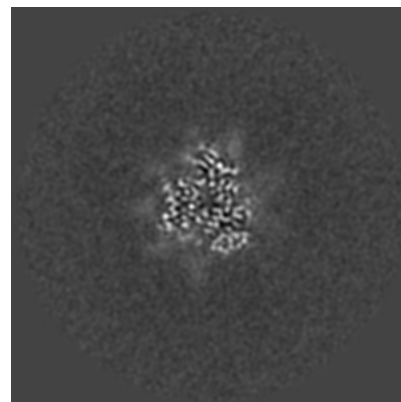
6.3.1 Primary map



X Index: 163

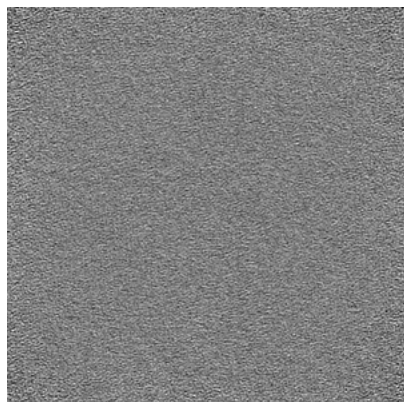


Y Index: 153

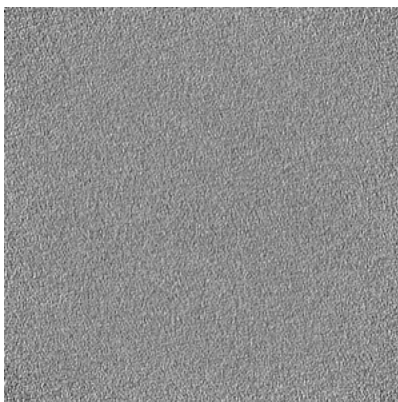


Z Index: 162

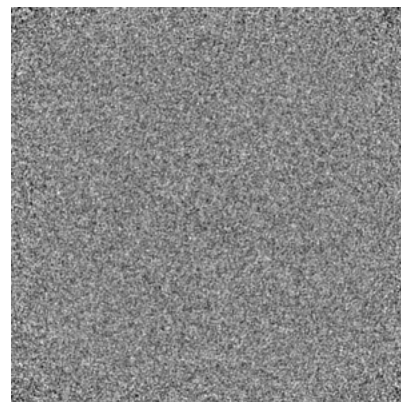
6.3.2 Raw map



X Index: 0



Y Index: 0

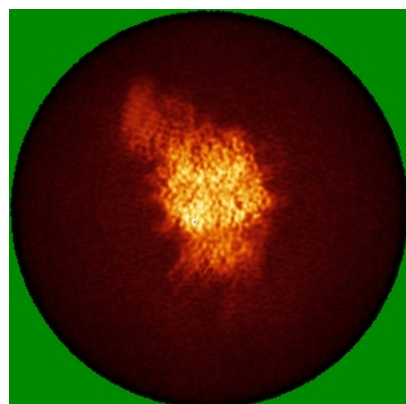


Z Index: 319

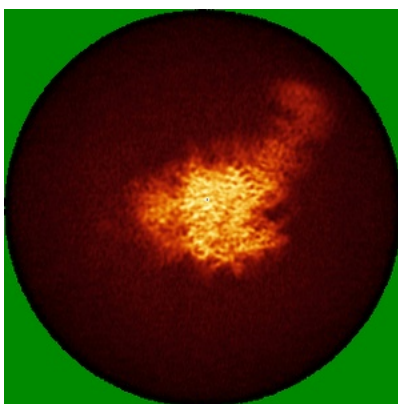
The images above show the largest variance slices of the map in three orthogonal directions.

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

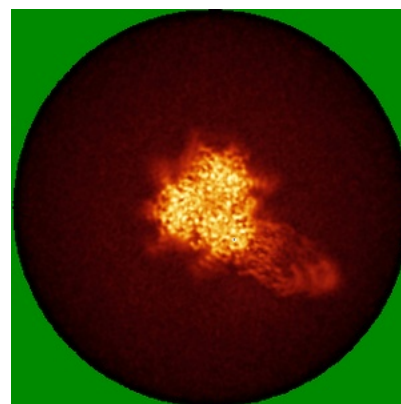
6.4.1 Primary map



X

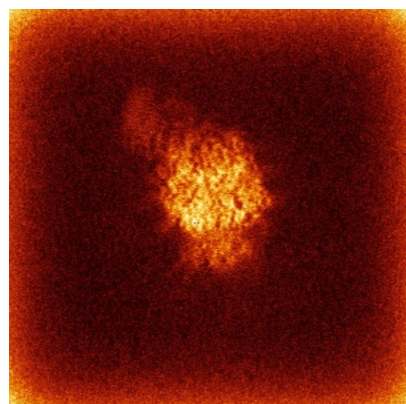


Y

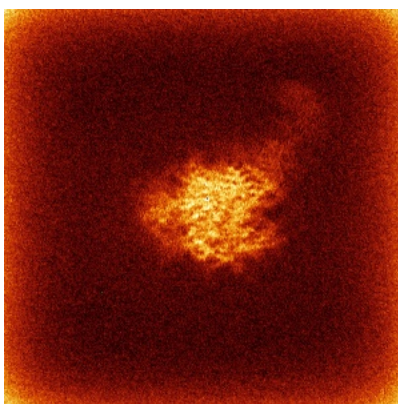


Z

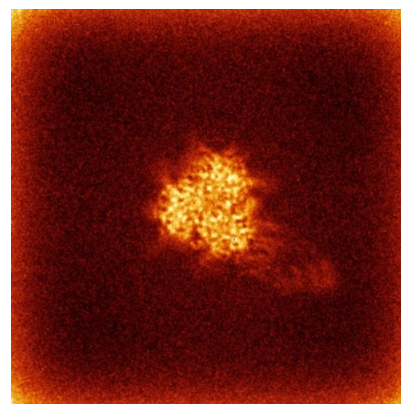
6.4.2 Raw map



X



Y



Z

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

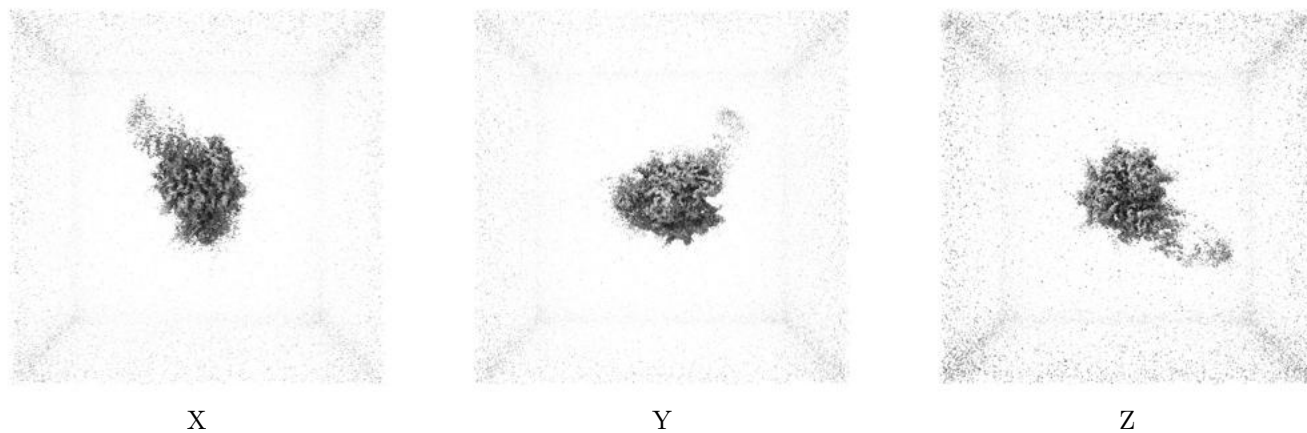
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.253. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

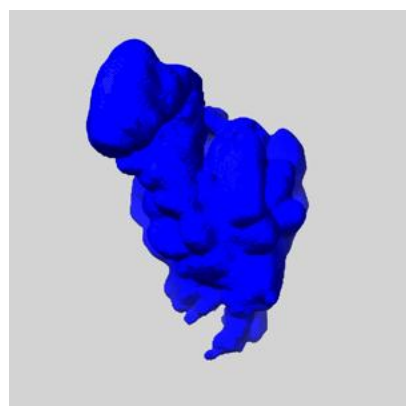
6.6 Mask visualisation [i](#)

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

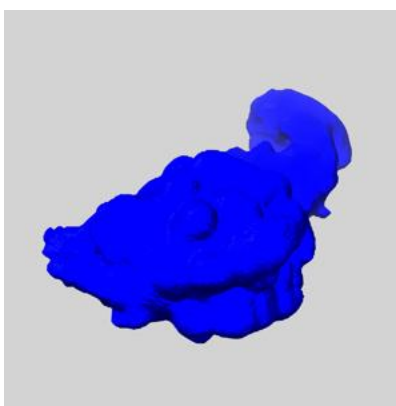
A mask typically either:

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

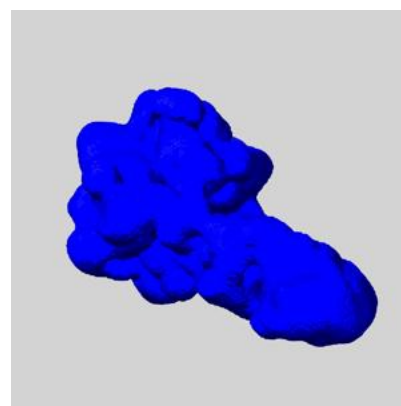
6.6.1 emd_41713_msk_1.map [i](#)



X



Y

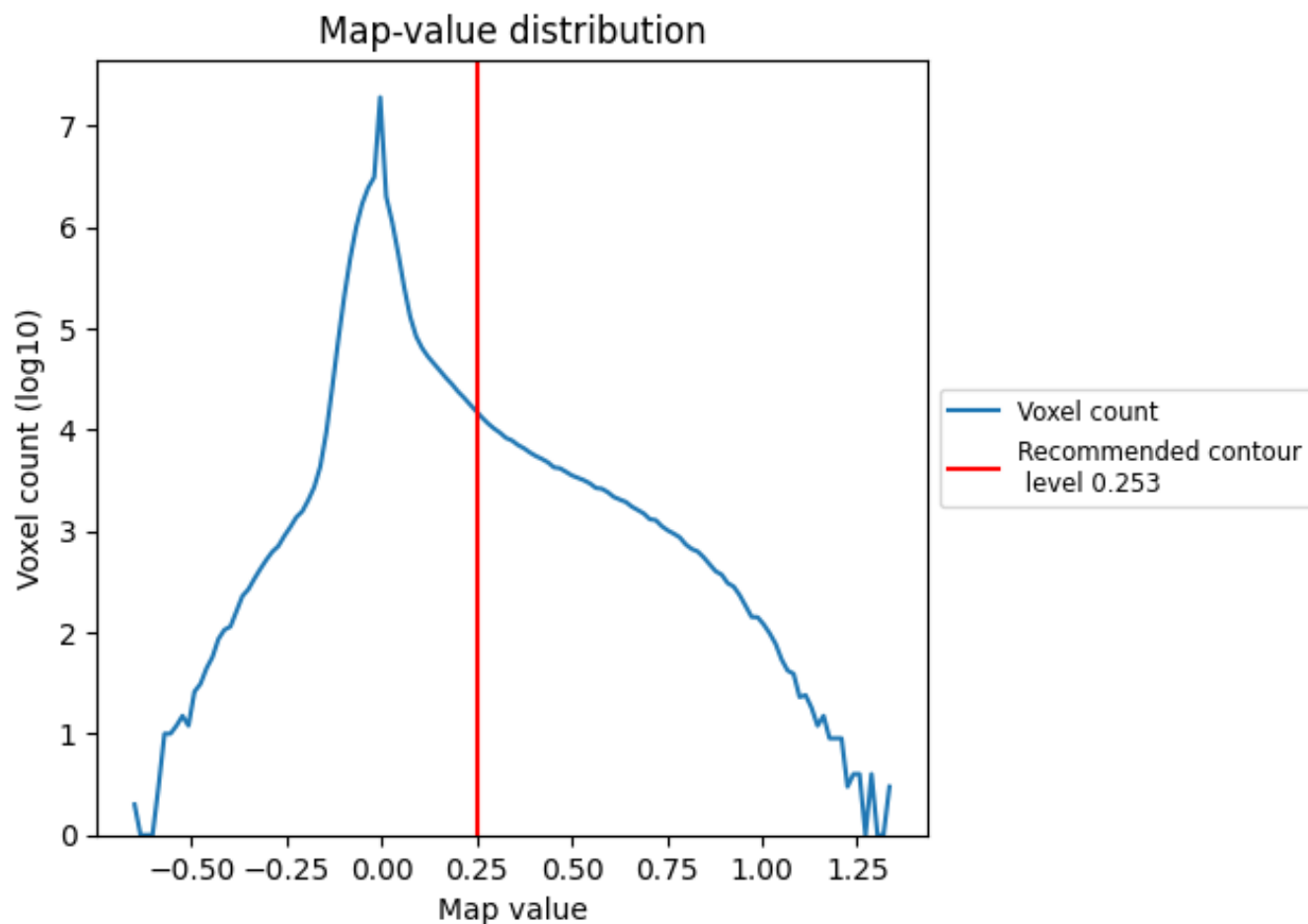


Z

7 Map analysis [i](#)

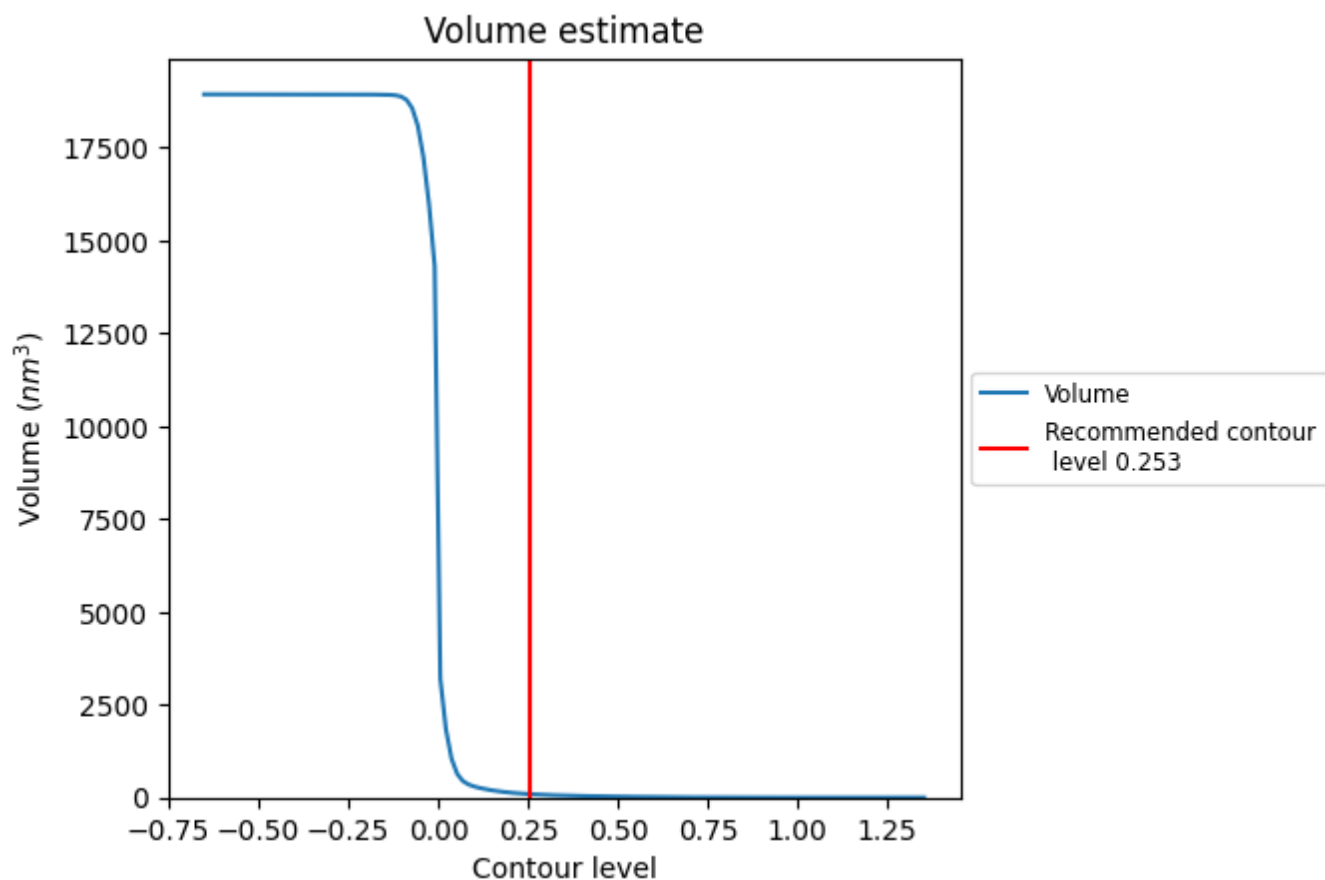
This section contains the results of statistical analysis of the map.

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.

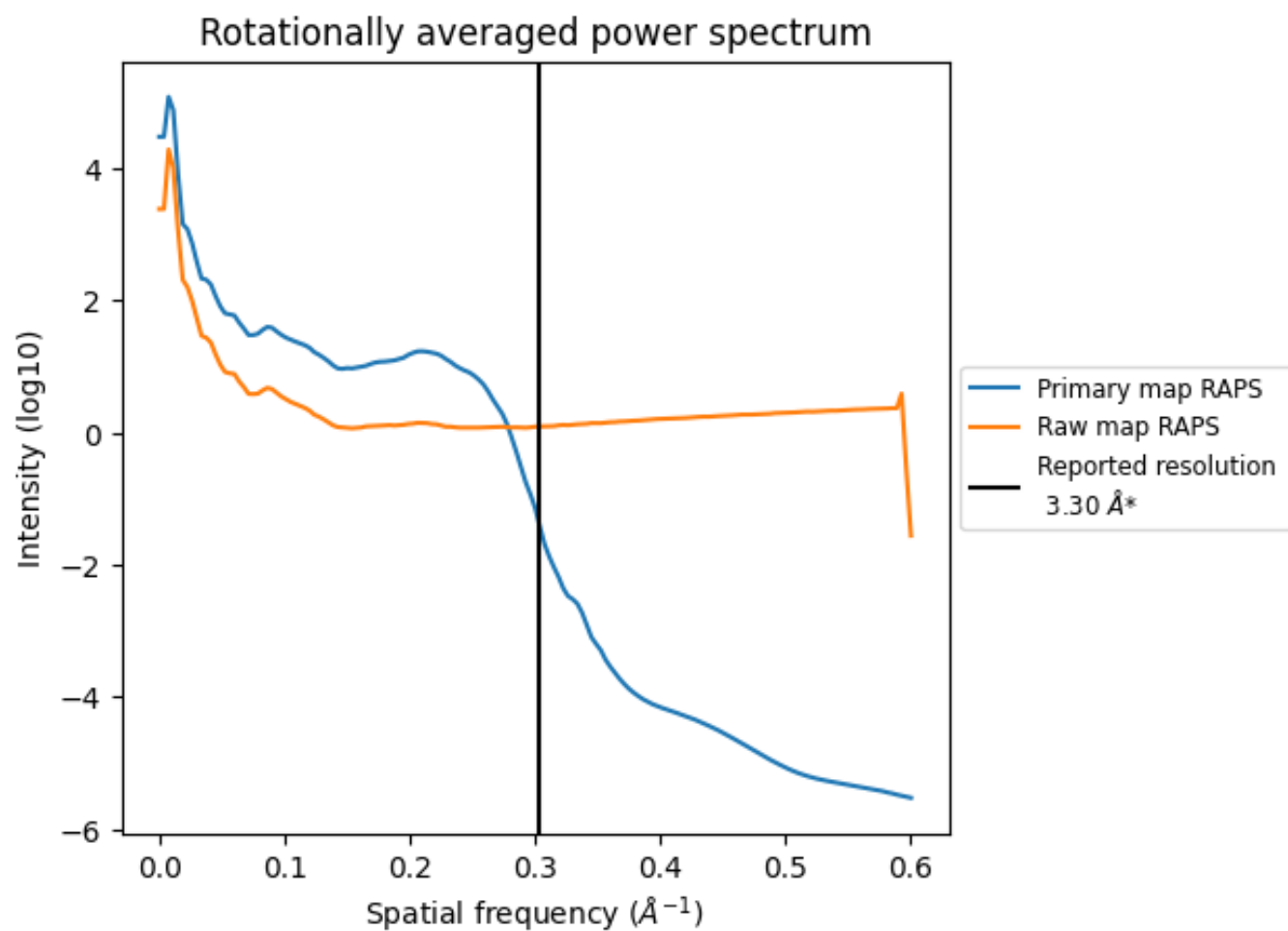
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94 nm³; this corresponds to an approximate mass of 85 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

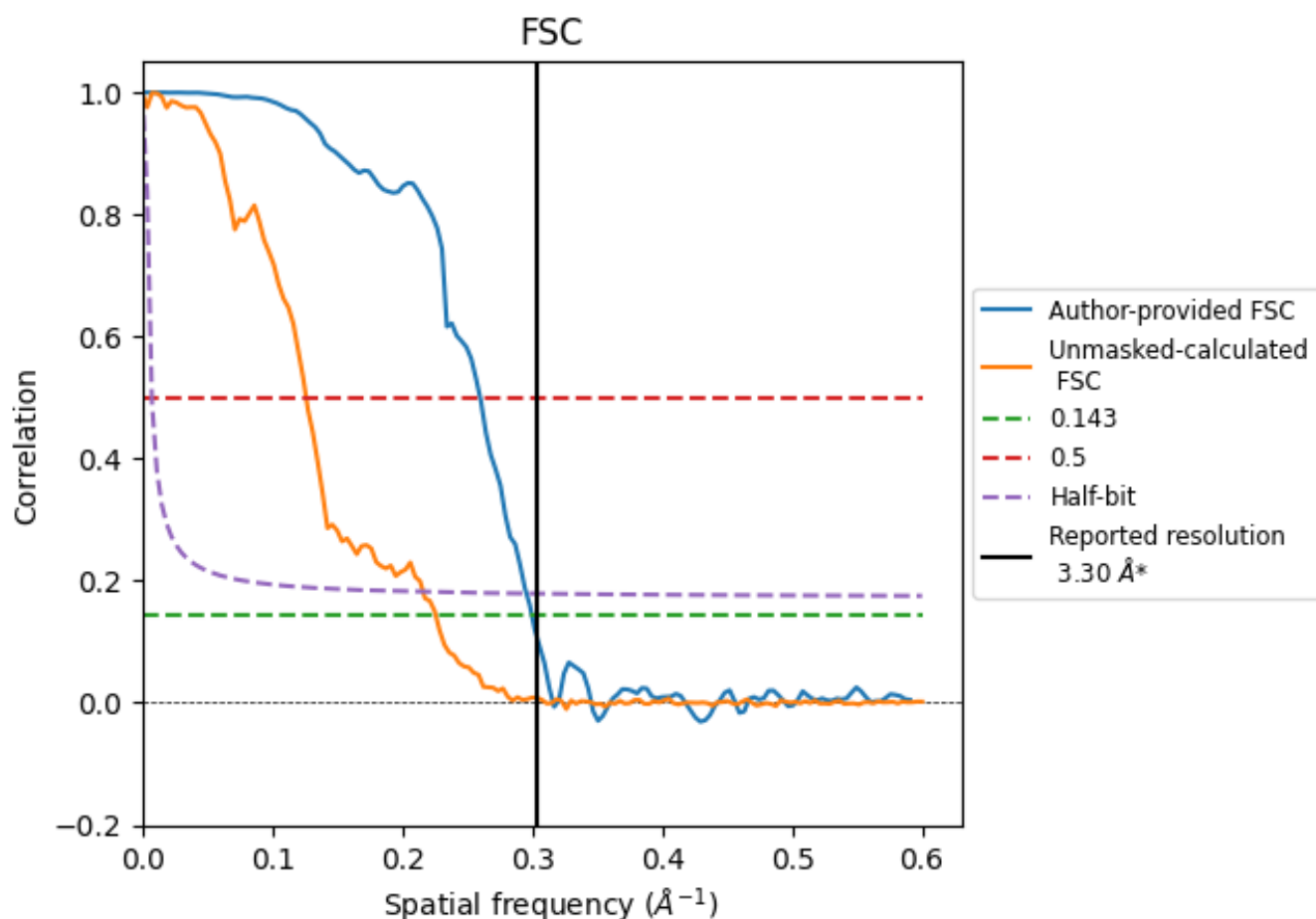


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

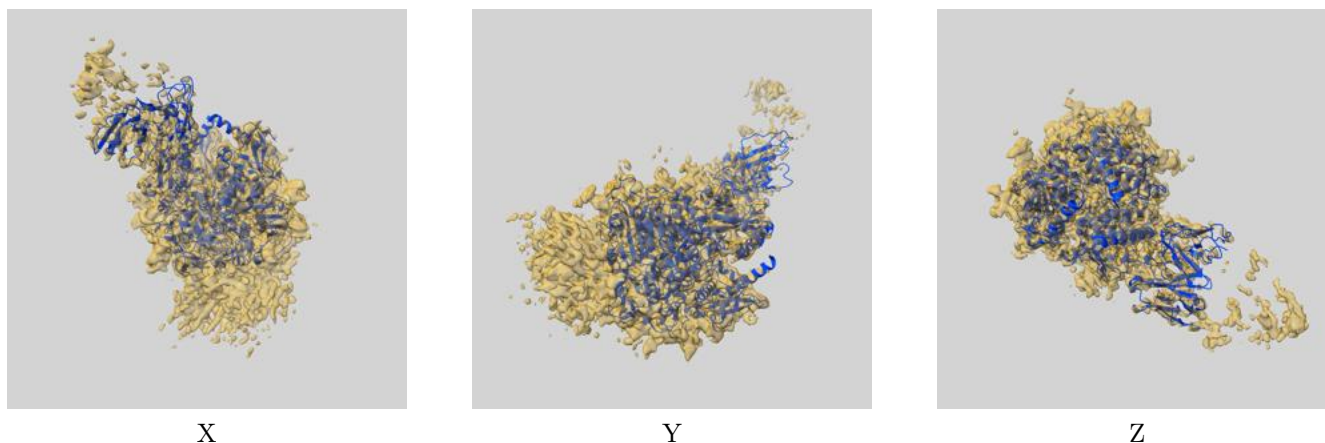
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.84	3.38
Unmasked-calculated*	4.43	7.93	4.63

*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 4.43 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

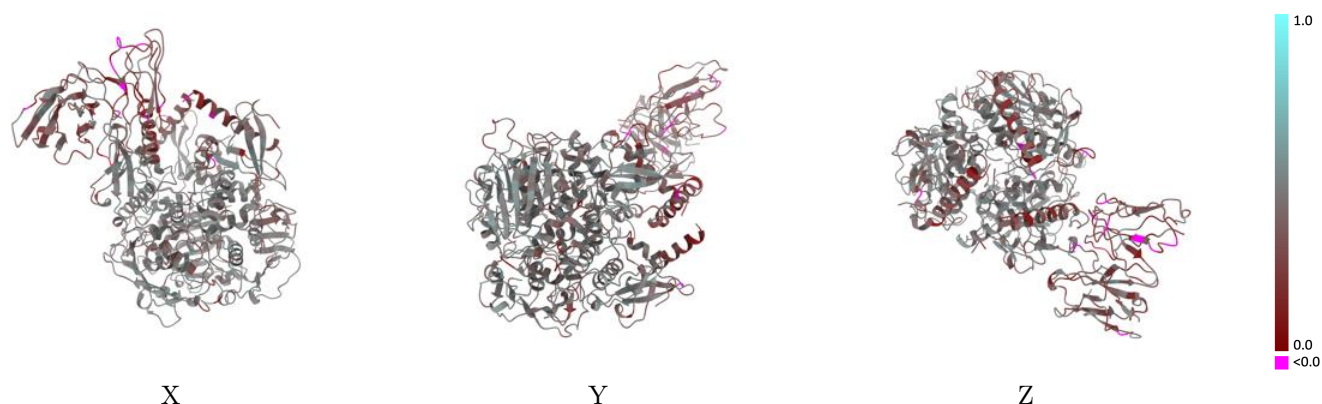
This section contains information regarding the fit between EMDB map EMD-41713 and PDB model 8TYC. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



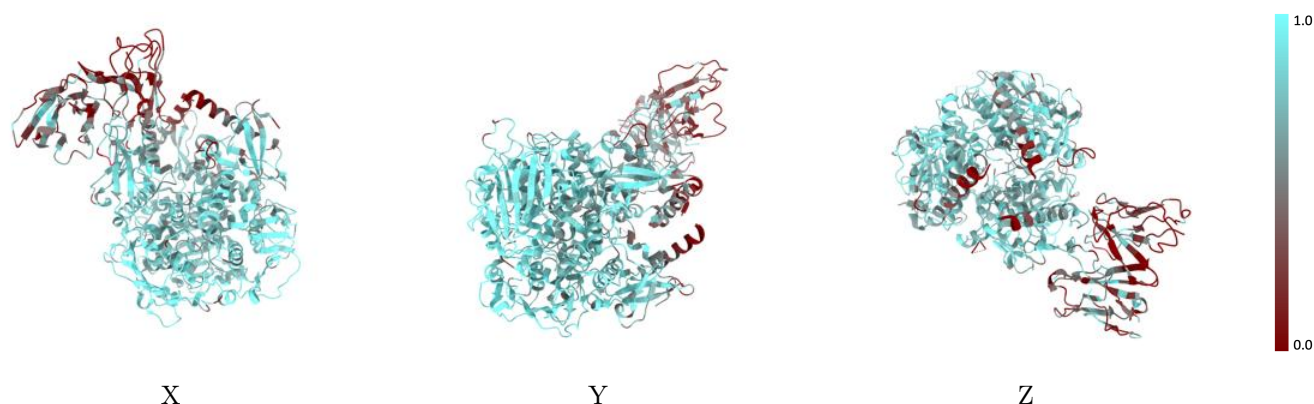
The images above show the 3D surface view of the map at the recommended contour level 0.253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



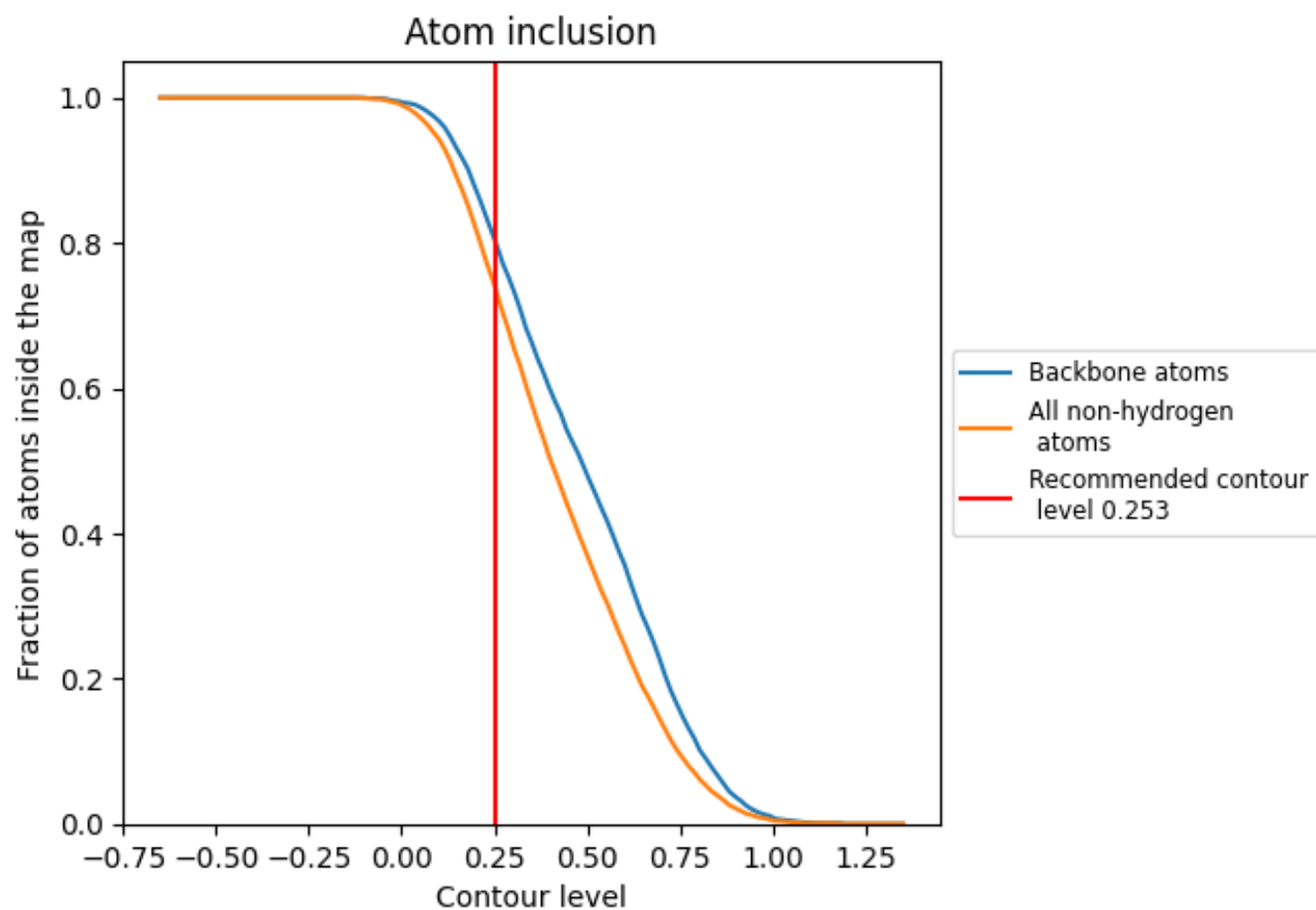
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.253).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.4140
A	 0.8520	 0.4450
B	 0.8540	 0.4540
C	 0.8350	 0.4420
D	 0.9290	 0.4460
E	 0.7440	 0.3560
F	 0.8210	 0.4390
G	 0.6070	 0.4180
H	 0.4280	 0.3380
I	 0.8210	 0.4300
J	 0.8930	 0.3820
K	 0.7140	 0.3460
L	 0.3050	 0.2770
M	 0.5710	 0.3880
N	 0.7440	 0.3400
O	 0.7690	 0.3120
P	 0.9640	 0.4620
Q	 0.7920	 0.3690
R	 0.7140	 0.2900
S	 0.8460	 0.4090
T	 0.8930	 0.3540
U	 0.8210	 0.3980
V	 0.7860	 0.3670
W	 0.8160	 0.4370
X	 0.8720	 0.4060
Y	 0.7140	 0.3310
Z	 0.8190	 0.4410
a	 0.7090	 0.4090
b	 0.7270	 0.4220
c	 0.6770	 0.4010
d	 0.5360	 0.3980
e	 0.4870	 0.4050
f	 0.7920	 0.4330
g	 0.3210	 0.0410
h	 0.8060	 0.4250
i	 0.5000	 0.3760

