



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 05:00 PM UTC

PDB ID : 6EDU / pdb_00006edu
EMDB ID : EMD-9038
Title : B41 SOSIP.664 in complex with soluble CD4 (D1-D2), the co-receptor mimicking antibody 21c and the broadly neutralizing antibody 8ANC195
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2018-08-11
Resolution : 4.06 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:

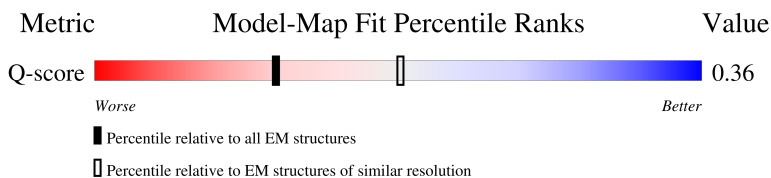
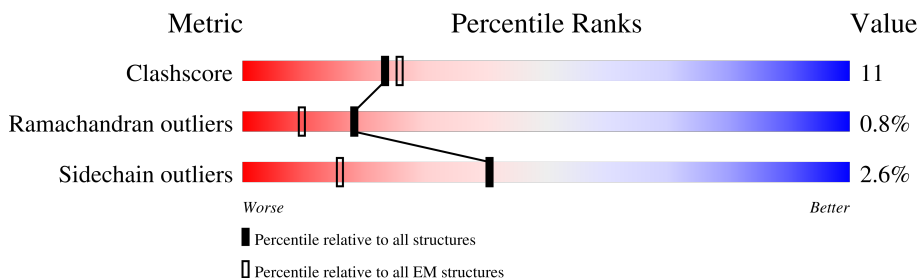
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.06 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6515 (3.56 - 4.56)

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	153	
1	B	153	
1	C	153	
2	D	516	

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Mol	Chain	Length	Quality of chain
2	E	516	16% 58% 16% 22%
2	F	516	15% 56% 18% 22%
3	G	185	7% 43% 9% 48%
3	H	185	9% 42% 10% 48%
3	I	185	9% 44% 8% 48%
4	J	231	27% 39% 13% 46%
4	L	231	27% 39% 13% 46%
4	N	231	24% 41% 12% 46%
5	K	217	29% 39% 12% 49%
5	M	217	29% 38% 12% 49%
5	O	217	28% 37% 12% 49%
6	P	244	7% 39% 15% 46%
6	R	244	7% 39% 14% 46%
6	T	244	7% 38% 16% 46%
7	Q	215	10% 40% 9% 50%
7	S	215	11% 40% 9% 50%
7	U	215	10% 41% 9% 50%
8	V	2	50% 50% 50%
8	W	2	50% 50% 50%
8	X	2	50% 50% 50%
8	Y	2	50% 100% 50%
8	c	2	50% 50% 50%
8	d	2	50% 50% 50%
8	e	2	100% 100%
8	f	2	50% 100% 100%

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Mol	Chain	Length	Quality of chain
8	j	2	50%
8	k	2	50%
8	l	2	50%
8	m	2	50%
8	q	2	50%
8	r	2	50%
8	s	2	50%
9	Z	5	80%
9	g	5	80%
9	n	5	80%
10	a	5	40%
10	h	5	40%
10	o	5	40%
11	b	3	100%
11	i	3	33%
11	p	3	33%
12	t	9	33%
12	u	9	22%
12	v	9	22%

2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 26271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	116	884	564	152	161	7	0	0
1	B	116	884	564	152	161	7	0	0
1	C	116	884	564	152	161	7	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	conflict	UNP B3UEZ6
A	605	CYS	THR	conflict	UNP B3UEZ6
B	559	PRO	ILE	conflict	UNP B3UEZ6
B	605	CYS	THR	conflict	UNP B3UEZ6
C	559	PRO	ILE	conflict	UNP B3UEZ6
C	605	CYS	THR	conflict	UNP B3UEZ6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	401	2989	1874	531	559	25	0	0
2	E	401	2989	1874	531	559	25	0	0
2	F	401	2989	1874	531	559	25	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	MET	-	initiating methionine	UNP B3UES2
D	-3	ASP	-	expression tag	UNP B3UES2
D	-2	ALA	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	expression tag	UNP B3UES2
D	0	LYS	-	expression tag	UNP B3UES2
D	1	ARG	-	expression tag	UNP B3UES2
D	2	GLY	-	expression tag	UNP B3UES2
D	3	LEU	-	expression tag	UNP B3UES2
D	4	CYS	-	expression tag	UNP B3UES2
D	5	CYS	-	expression tag	UNP B3UES2
D	6	VAL	-	expression tag	UNP B3UES2
D	7	LEU	-	expression tag	UNP B3UES2
D	8	LEU	-	expression tag	UNP B3UES2
D	9	LEU	-	expression tag	UNP B3UES2
D	10	CYS	-	expression tag	UNP B3UES2
D	11	GLY	-	expression tag	UNP B3UES2
D	12	ALA	-	expression tag	UNP B3UES2
D	13	VAL	-	expression tag	UNP B3UES2
D	14	PHE	-	expression tag	UNP B3UES2
D	15	VAL	-	expression tag	UNP B3UES2
D	16	SER	-	expression tag	UNP B3UES2
D	17	PRO	-	expression tag	UNP B3UES2
D	18	SER	-	expression tag	UNP B3UES2
D	19	GLN	-	expression tag	UNP B3UES2
D	20	GLU	-	expression tag	UNP B3UES2
D	21	ILE	-	expression tag	UNP B3UES2
D	22	HIS	-	expression tag	UNP B3UES2
D	23	ALA	-	expression tag	UNP B3UES2
D	24	ARG	-	expression tag	UNP B3UES2
D	25	PHE	-	expression tag	UNP B3UES2
D	26	ARG	-	expression tag	UNP B3UES2
D	27	ARG	-	expression tag	UNP B3UES2
D	28	GLY	-	expression tag	UNP B3UES2
D	29	ALA	-	expression tag	UNP B3UES2
D	30	ARG	-	expression tag	UNP B3UES2
D	501	CYS	ALA	conflict	UNP B3UES2
E	-4	MET	-	initiating methionine	UNP B3UES2
E	-3	ASP	-	expression tag	UNP B3UES2
E	-2	ALA	-	expression tag	UNP B3UES2
E	-1	MET	-	expression tag	UNP B3UES2
E	0	LYS	-	expression tag	UNP B3UES2
E	1	ARG	-	expression tag	UNP B3UES2
E	2	GLY	-	expression tag	UNP B3UES2
E	3	LEU	-	expression tag	UNP B3UES2
E	4	CYS	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	5	CYS	-	expression tag	UNP B3UES2
E	6	VAL	-	expression tag	UNP B3UES2
E	7	LEU	-	expression tag	UNP B3UES2
E	8	LEU	-	expression tag	UNP B3UES2
E	9	LEU	-	expression tag	UNP B3UES2
E	10	CYS	-	expression tag	UNP B3UES2
E	11	GLY	-	expression tag	UNP B3UES2
E	12	ALA	-	expression tag	UNP B3UES2
E	13	VAL	-	expression tag	UNP B3UES2
E	14	PHE	-	expression tag	UNP B3UES2
E	15	VAL	-	expression tag	UNP B3UES2
E	16	SER	-	expression tag	UNP B3UES2
E	17	PRO	-	expression tag	UNP B3UES2
E	18	SER	-	expression tag	UNP B3UES2
E	19	GLN	-	expression tag	UNP B3UES2
E	20	GLU	-	expression tag	UNP B3UES2
E	21	ILE	-	expression tag	UNP B3UES2
E	22	HIS	-	expression tag	UNP B3UES2
E	23	ALA	-	expression tag	UNP B3UES2
E	24	ARG	-	expression tag	UNP B3UES2
E	25	PHE	-	expression tag	UNP B3UES2
E	26	ARG	-	expression tag	UNP B3UES2
E	27	ARG	-	expression tag	UNP B3UES2
E	28	GLY	-	expression tag	UNP B3UES2
E	29	ALA	-	expression tag	UNP B3UES2
E	30	ARG	-	expression tag	UNP B3UES2
E	501	CYS	ALA	conflict	UNP B3UES2
F	-4	MET	-	initiating methionine	UNP B3UES2
F	-3	ASP	-	expression tag	UNP B3UES2
F	-2	ALA	-	expression tag	UNP B3UES2
F	-1	MET	-	expression tag	UNP B3UES2
F	0	LYS	-	expression tag	UNP B3UES2
F	1	ARG	-	expression tag	UNP B3UES2
F	2	GLY	-	expression tag	UNP B3UES2
F	3	LEU	-	expression tag	UNP B3UES2
F	4	CYS	-	expression tag	UNP B3UES2
F	5	CYS	-	expression tag	UNP B3UES2
F	6	VAL	-	expression tag	UNP B3UES2
F	7	LEU	-	expression tag	UNP B3UES2
F	8	LEU	-	expression tag	UNP B3UES2
F	9	LEU	-	expression tag	UNP B3UES2
F	10	CYS	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	11	GLY	-	expression tag	UNP B3UES2
F	12	ALA	-	expression tag	UNP B3UES2
F	13	VAL	-	expression tag	UNP B3UES2
F	14	PHE	-	expression tag	UNP B3UES2
F	15	VAL	-	expression tag	UNP B3UES2
F	16	SER	-	expression tag	UNP B3UES2
F	17	PRO	-	expression tag	UNP B3UES2
F	18	SER	-	expression tag	UNP B3UES2
F	19	GLN	-	expression tag	UNP B3UES2
F	20	GLU	-	expression tag	UNP B3UES2
F	21	ILE	-	expression tag	UNP B3UES2
F	22	HIS	-	expression tag	UNP B3UES2
F	23	ALA	-	expression tag	UNP B3UES2
F	24	ARG	-	expression tag	UNP B3UES2
F	25	PHE	-	expression tag	UNP B3UES2
F	26	ARG	-	expression tag	UNP B3UES2
F	27	ARG	-	expression tag	UNP B3UES2
F	28	GLY	-	expression tag	UNP B3UES2
F	29	ALA	-	expression tag	UNP B3UES2
F	30	ARG	-	expression tag	UNP B3UES2
F	501	CYS	ALA	conflict	UNP B3UES2

- Molecule 3 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	97	775	487	136	150	2	0	0
3	H	97	775	487	136	150	2	0	0
3	I	97	775	487	136	150	2	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	184	ASN	-	expression tag	UNP P01730
G	185	THR	-	expression tag	UNP P01730
H	184	ASN	-	expression tag	UNP P01730
H	185	THR	-	expression tag	UNP P01730
I	184	ASN	-	expression tag	UNP P01730
I	185	THR	-	expression tag	UNP P01730

- Molecule 4 is a protein called 21c Fab VH domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	124	Total	C	N	O	S	0	0
			958	609	158	186	5		
4	L	124	Total	C	N	O	S	0	0
			958	609	158	186	5		
4	N	124	Total	C	N	O	S	0	0
			958	609	158	186	5		

- Molecule 5 is a protein called 21c Fab VL domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	111	Total	C	N	O	S	0	0
			802	501	133	166	2		
5	M	111	Total	C	N	O	S	0	0
			802	501	133	166	2		
5	O	111	Total	C	N	O	S	0	0
			802	501	133	166	2		

- Molecule 6 is a protein called 8ANC195 G52K5 Fab VH domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	131	Total	C	N	O	S	0	0
			1007	639	173	192	3		
6	R	131	Total	C	N	O	S	0	0
			1007	639	173	192	3		
6	T	131	Total	C	N	O	S	0	0
			1007	639	173	192	3		

- Molecule 7 is a protein called 8ANC195 G52K5 Fab VL domain.

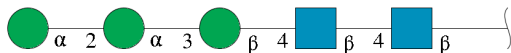
Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	107	Total	C	N	O	S	0	0
			810	509	140	158	3		
7	S	107	Total	C	N	O	S	0	0
			810	509	140	158	3		
7	U	107	Total	C	N	O	S	0	0
			810	509	140	158	3		

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



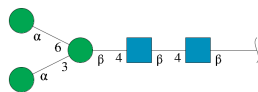
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	V	2	28	16	2	10	0	0
8	W	2	28	16	2	10	0	0
8	X	2	28	16	2	10	0	0
8	Y	2	28	16	2	10	0	0
8	c	2	28	16	2	10	0	0
8	d	2	28	16	2	10	0	0
8	e	2	28	16	2	10	0	0
8	f	2	28	16	2	10	0	0
8	j	2	28	16	2	10	0	0
8	k	2	28	16	2	10	0	0
8	l	2	28	16	2	10	0	0
8	m	2	28	16	2	10	0	0
8	q	2	28	16	2	10	0	0
8	r	2	28	16	2	10	0	0
8	s	2	28	16	2	10	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	5	Total	C	N	O	0	0
			61	34	2	25		
9	g	5	Total	C	N	O	0	0
			61	34	2	25		
9	n	5	Total	C	N	O	0	0
			61	34	2	25		

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



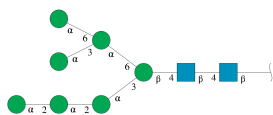
Mol	Chain	Residues	Atoms				AltConf	Trace
10	a	5	Total	C	N	O	0	0
			61	34	2	25		
10	h	5	Total	C	N	O	0	0
			61	34	2	25		
10	o	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 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.



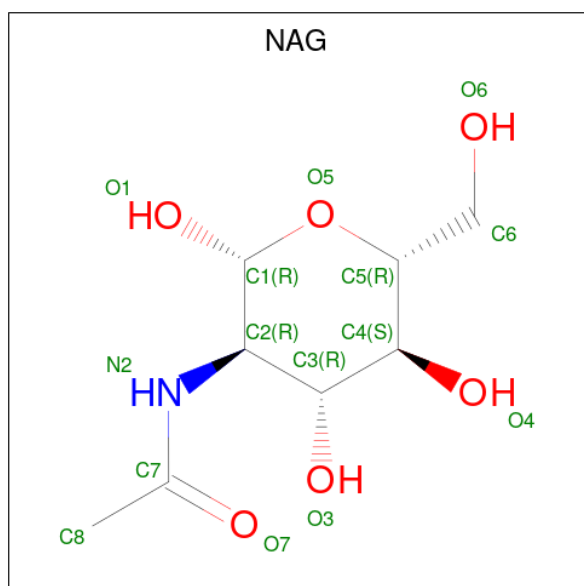
Mol	Chain	Residues	Atoms				AltConf	Trace
11	b	3	Total	C	N	O	0	0
			39	22	2	15		
11	i	3	Total	C	N	O	0	0
			39	22	2	15		
11	p	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	t	9	Total	C	N	O	0	0
			105	58	2	45		
12	u	9	Total	C	N	O	0	0
			105	58	2	45		
12	v	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
13	D	1	Total 14	C 8	N 1	O 5	0
13	D	1	Total 14	C 8	N 1	O 5	0
13	D	1	Total 14	C 8	N 1	O 5	0
13	D	1	Total 14	C 8	N 1	O 5	0
13	D	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	E	1	Total 14	C 8	N 1	O 5	0
13	F	1	Total 14	C 8	N 1	O 5	0
13	F	1	Total 14	C 8	N 1	O 5	0
13	F	1	Total 14	C 8	N 1	O 5	0
13	F	1	Total 14	C 8	N 1	O 5	0
13	F	1	Total 14	C 8	N 1	O 5	0
13	F	1	Total 14	C 8	N 1	O 5	0
13	F	1	Total 14	C 8	N 1	O 5	0
13	F	1	Total 14	C 8	N 1	O 5	0



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



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



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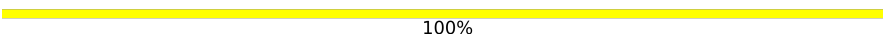
- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain e:  100%


NAG1
NAG2

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

Chain f:  50%
100%


NAG1
NAG2

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

Chain j:  50%
50% 50%


NAG1
NAG2

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

Chain k:  50%
50% 50%


NAG1
NAG2

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

Chain l:  50% 50%


NAG1
NAG2

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

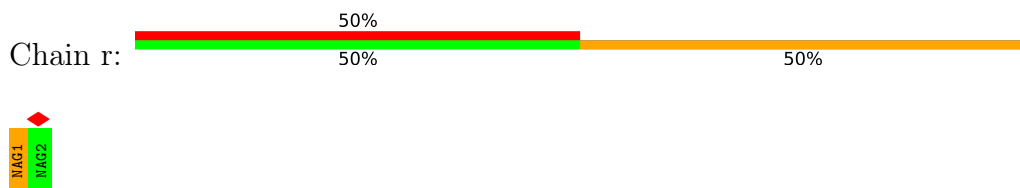
Chain m:  50%
100%


NAG1
NAG2

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



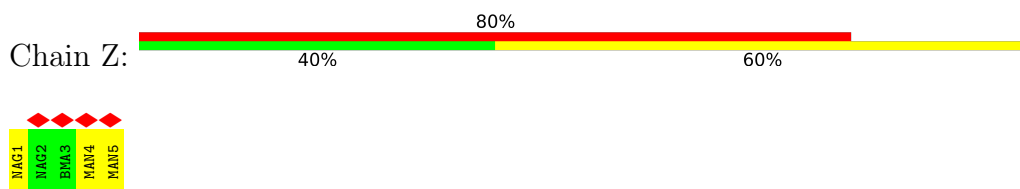
- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



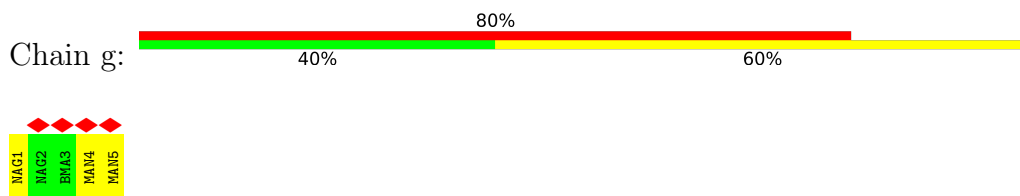
- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



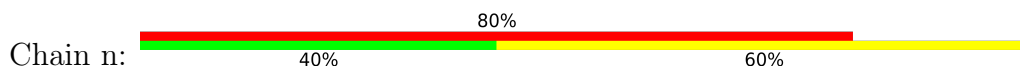
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

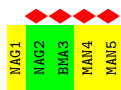


- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

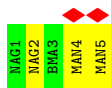


- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

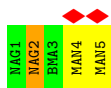




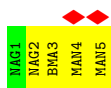
- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



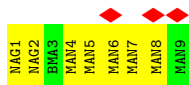
- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	305469	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)	1700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.041	Depositor
Map size (Å)	377.27997, 377.27997, 377.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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, 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	0.41	0/901	1.00	6/1228 (0.5%)
1	B	0.26	0/901	0.62	0/1228
1	C	0.26	0/901	0.62	0/1228
2	D	0.49	0/3049	0.94	18/4156 (0.4%)
2	E	0.56	1/3049 (0.0%)	1.12	24/4156 (0.6%)
2	F	0.47	1/3049 (0.0%)	1.23	26/4156 (0.6%)
3	G	0.25	0/785	0.61	1/1053 (0.1%)
3	H	0.25	0/785	0.61	1/1053 (0.1%)
3	I	0.25	0/785	0.61	1/1053 (0.1%)
4	J	0.31	0/982	0.65	1/1335 (0.1%)
4	L	0.33	0/982	0.71	1/1335 (0.1%)
4	N	0.37	0/982	0.69	0/1335
5	K	0.23	0/819	0.67	1/1115 (0.1%)
5	M	0.23	0/819	0.67	1/1115 (0.1%)
5	O	0.31	0/819	0.67	1/1115 (0.1%)
6	P	0.24	0/1034	0.58	0/1408
6	R	0.24	0/1034	0.58	0/1408
6	T	0.24	0/1034	0.58	0/1408
7	Q	0.21	0/828	0.51	0/1125
7	S	0.20	0/828	0.51	0/1125
7	U	0.20	0/828	0.50	0/1125
All	All	0.38	2/25194 (0.0%)	0.84	82/34260 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	6
2	E	0	6
2	F	0	6
3	G	0	1
3	H	0	1
3	I	0	1
5	K	0	3
5	M	0	3
5	O	0	3
All	All	0	33

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	204	ALA	C-N	18.24	1.54	1.33
2	F	204	ALA	C-N	-6.79	1.27	1.33

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	204	ALA	CA-C-N	-28.74	90.97	122.00
2	F	204	ALA	O-C-N	28.74	157.71	122.65
2	F	204	ALA	C-N-CA	-28.74	90.97	122.00
2	E	204	ALA	O-C-N	24.78	152.88	122.65
2	E	204	ALA	CA-C-N	-20.74	96.91	122.42

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	610	TRP	Peptide
1	B	610	TRP	Peptide
1	C	610	TRP	Peptide
2	D	166	ARG	Sidechain
2	D	192	ARG	Sidechain

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	884	0	843	25	0
1	B	884	0	841	21	0
1	C	884	0	841	8	0
2	D	2989	0	2792	101	0
2	E	2989	0	2792	85	0
2	F	2989	0	2792	91	0
3	G	775	0	795	7	0
3	H	775	0	795	9	0
3	I	775	0	795	8	0
4	J	958	0	919	38	0
4	L	958	0	919	36	0
4	N	958	0	919	40	0
5	K	802	0	780	21	0
5	M	802	0	780	18	0
5	O	802	0	780	21	0
6	P	1007	0	979	22	0
6	R	1007	0	979	19	0
6	T	1007	0	979	21	0
7	Q	810	0	783	11	0
7	S	810	0	783	11	0
7	U	810	0	783	10	0
8	V	28	0	25	1	0
8	W	28	0	25	1	0
8	X	28	0	25	0	0
8	Y	28	0	25	0	0
8	c	28	0	25	0	0
8	d	28	0	25	1	0
8	e	28	0	25	4	0
8	f	28	0	25	0	0
8	j	28	0	25	0	0
8	k	28	0	25	1	0
8	l	28	0	25	2	0
8	m	28	0	25	0	0
8	q	28	0	25	0	0
8	r	28	0	25	1	0
8	s	28	0	25	4	0
9	Z	61	0	52	0	0
9	g	61	0	52	0	0
9	n	61	0	52	0	0
10	a	61	0	52	0	0
10	h	61	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	o	61	0	52	1	0
11	b	39	0	34	0	0
11	i	39	0	34	0	0
11	p	39	0	34	0	0
12	t	105	0	87	0	0
12	u	105	0	87	0	0
12	v	105	0	87	0	0
13	A	14	0	13	0	0
13	B	14	0	13	0	0
13	C	14	0	13	0	0
13	D	112	0	104	2	0
13	E	112	0	104	2	0
13	F	112	0	104	2	0
All	All	26271	0	25070	560	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 11.

The worst 5 of 560 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)
4:N:97:ALA:CB	4:N:112:LEU:HD13	1.40	1.50
2:E:198:THR:CG2	4:N:103:TYR:HA	1.50	1.39
4:L:102:TYR:OH	4:L:111:PRO:HD2	1.44	1.18
2:F:198:THR:HG21	4:J:104:ASN:O	1.40	1.18
4:N:97:ALA:HB1	4:N:112:LEU:HD13	1.17	1.14

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	112/153 (73%)	106 (95%)	5 (4%)	1 (1%)	14	49
1	B	112/153 (73%)	107 (96%)	5 (4%)	0	100	100
1	C	112/153 (73%)	107 (96%)	5 (4%)	0	100	100
2	D	389/516 (75%)	324 (83%)	59 (15%)	6 (2%)	8	39
2	E	389/516 (75%)	326 (84%)	55 (14%)	8 (2%)	5	32
2	F	389/516 (75%)	326 (84%)	53 (14%)	10 (3%)	4	29
3	G	95/185 (51%)	79 (83%)	16 (17%)	0	100	100
3	H	95/185 (51%)	78 (82%)	17 (18%)	0	100	100
3	I	95/185 (51%)	78 (82%)	17 (18%)	0	100	100
4	J	122/231 (53%)	109 (89%)	12 (10%)	1 (1%)	16	52
4	L	122/231 (53%)	109 (89%)	13 (11%)	0	100	100
4	N	122/231 (53%)	110 (90%)	12 (10%)	0	100	100
5	K	109/217 (50%)	93 (85%)	16 (15%)	0	100	100
5	M	109/217 (50%)	93 (85%)	16 (15%)	0	100	100
5	O	109/217 (50%)	93 (85%)	16 (15%)	0	100	100
6	P	129/244 (53%)	115 (89%)	14 (11%)	0	100	100
6	R	129/244 (53%)	115 (89%)	14 (11%)	0	100	100
6	T	129/244 (53%)	115 (89%)	14 (11%)	0	100	100
7	Q	105/215 (49%)	96 (91%)	9 (9%)	0	100	100
7	S	105/215 (49%)	96 (91%)	9 (9%)	0	100	100
7	U	105/215 (49%)	96 (91%)	9 (9%)	0	100	100
All	All	3183/5283 (60%)	2771 (87%)	386 (12%)	26 (1%)	18	52

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	163	THR
2	D	179	LEU
2	E	156	ASN
2	E	163	THR
2	E	179	LEU

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	89/130 (68%)	87 (98%)	2 (2%)	45	65
1	B	89/130 (68%)	87 (98%)	2 (2%)	45	65
1	C	89/130 (68%)	87 (98%)	2 (2%)	45	65
2	D	314/453 (69%)	303 (96%)	11 (4%)	32	54
2	E	314/453 (69%)	306 (98%)	8 (2%)	42	62
2	F	314/453 (69%)	306 (98%)	8 (2%)	42	62
3	G	89/167 (53%)	85 (96%)	4 (4%)	24	48
3	H	89/167 (53%)	85 (96%)	4 (4%)	24	48
3	I	89/167 (53%)	85 (96%)	4 (4%)	24	48
4	J	101/194 (52%)	98 (97%)	3 (3%)	36	57
4	L	101/194 (52%)	98 (97%)	3 (3%)	36	57
4	N	101/194 (52%)	96 (95%)	5 (5%)	22	45
5	K	89/180 (49%)	88 (99%)	1 (1%)	65	74
5	M	89/180 (49%)	88 (99%)	1 (1%)	65	74
5	O	89/180 (49%)	87 (98%)	2 (2%)	45	65
6	P	112/210 (53%)	110 (98%)	2 (2%)	51	68
6	R	112/210 (53%)	110 (98%)	2 (2%)	51	68
6	T	112/210 (53%)	110 (98%)	2 (2%)	51	68
7	Q	85/182 (47%)	84 (99%)	1 (1%)	63	73
7	S	85/182 (47%)	84 (99%)	1 (1%)	63	73
7	U	85/182 (47%)	84 (99%)	1 (1%)	63	73
All	All	2637/4548 (58%)	2568 (97%)	69 (3%)	41	61

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	N	104	ASN
5	O	97	LEU

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Mol	Chain	Res	Type
7	S	89	CYS
2	E	413	ASN
2	E	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	101	ASN
4	N	39	GLN
5	K	40	GLN
4	L	101	ASN
5	O	40	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

96 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
8	NAG	V	1	1,8	14,14,15	1.19	1 (7%)	17,19,21	1.14	3 (17%)
8	NAG	V	2	8	14,14,15	0.61	0	17,19,21	0.33	0
8	NAG	W	1	1,8	14,14,15	1.20	1 (7%)	17,19,21	1.14	3 (17%)
8	NAG	W	2	8	14,14,15	0.62	0	17,19,21	0.33	0
8	NAG	X	1	1,8	14,14,15	1.19	1 (7%)	17,19,21	1.14	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	X	2	8	14,14,15	0.61	0	17,19,21	0.33	0
8	NAG	Y	1	2,8	14,14,15	0.29	0	17,19,21	0.49	0
8	NAG	Y	2	8	14,14,15	0.33	0	17,19,21	0.48	0
9	NAG	Z	1	2,9	14,14,15	0.21	0	17,19,21	0.63	1 (5%)
9	NAG	Z	2	9	14,14,15	0.27	0	17,19,21	0.55	0
9	BMA	Z	3	9	11,11,12	0.66	0	15,15,17	0.79	0
9	MAN	Z	4	9	11,11,12	0.70	0	15,15,17	1.34	2 (13%)
9	MAN	Z	5	9	11,11,12	0.82	0	15,15,17	1.14	2 (13%)
10	NAG	a	1	2,10	14,14,15	0.25	0	17,19,21	0.62	0
10	NAG	a	2	10	14,14,15	0.40	0	17,19,21	0.80	1 (5%)
10	BMA	a	3	10	11,11,12	0.67	0	15,15,17	0.89	0
10	MAN	a	4	10	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
10	MAN	a	5	10	11,11,12	0.78	0	15,15,17	1.06	2 (13%)
11	NAG	b	1	2,11	14,14,15	0.32	0	17,19,21	0.49	0
11	NAG	b	2	11	14,14,15	0.21	0	17,19,21	0.62	0
11	BMA	b	3	11	11,11,12	0.88	0	15,15,17	0.74	0
8	NAG	c	1	2,8	14,14,15	0.39	0	17,19,21	0.80	0
8	NAG	c	2	8	14,14,15	0.86	1 (7%)	17,19,21	0.97	1 (5%)
8	NAG	d	1	2,8	14,14,15	0.44	0	17,19,21	0.98	1 (5%)
8	NAG	d	2	8	14,14,15	0.45	0	17,19,21	0.45	0
8	NAG	e	1	2,8	14,14,15	0.58	0	17,19,21	1.76	4 (23%)
8	NAG	e	2	8	14,14,15	0.27	0	17,19,21	0.57	0
8	NAG	f	1	2,8	14,14,15	0.30	0	17,19,21	0.49	0
8	NAG	f	2	8	14,14,15	0.31	0	17,19,21	0.49	0
9	NAG	g	1	2,9	14,14,15	0.21	0	17,19,21	0.63	1 (5%)
9	NAG	g	2	9	14,14,15	0.27	0	17,19,21	0.55	0
9	BMA	g	3	9	11,11,12	0.66	0	15,15,17	0.80	0
9	MAN	g	4	9	11,11,12	0.69	0	15,15,17	1.33	2 (13%)
9	MAN	g	5	9	11,11,12	0.80	0	15,15,17	1.14	2 (13%)
10	NAG	h	1	2,10	14,14,15	0.25	0	17,19,21	0.63	0
10	NAG	h	2	10	14,14,15	0.42	0	17,19,21	0.80	1 (5%)
10	BMA	h	3	10	11,11,12	0.68	0	15,15,17	0.89	0
10	MAN	h	4	10	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
10	MAN	h	5	10	11,11,12	0.78	0	15,15,17	1.07	2 (13%)
11	NAG	i	1	2,11	14,14,15	0.31	0	17,19,21	0.48	0
11	NAG	i	2	11	14,14,15	0.21	0	17,19,21	0.62	0
11	BMA	i	3	11	11,11,12	0.88	0	15,15,17	0.74	0
8	NAG	j	1	2,8	14,14,15	0.39	0	17,19,21	0.81	0
8	NAG	j	2	8	14,14,15	0.86	1 (7%)	17,19,21	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	k	1	2,8	14,14,15	0.44	0	17,19,21	0.98	1 (5%)
8	NAG	k	2	8	14,14,15	0.45	0	17,19,21	0.46	0
8	NAG	l	1	2,8	14,14,15	0.51	0	17,19,21	1.54	4 (23%)
8	NAG	l	2	8	14,14,15	0.27	0	17,19,21	0.57	0
8	NAG	m	1	2,8	14,14,15	0.29	0	17,19,21	0.50	0
8	NAG	m	2	8	14,14,15	0.33	0	17,19,21	0.48	0
9	NAG	n	1	2,9	14,14,15	0.21	0	17,19,21	0.64	1 (5%)
9	NAG	n	2	9	14,14,15	0.27	0	17,19,21	0.55	0
9	BMA	n	3	9	11,11,12	0.66	0	15,15,17	0.80	0
9	MAN	n	4	9	11,11,12	0.70	0	15,15,17	1.33	2 (13%)
9	MAN	n	5	9	11,11,12	0.81	0	15,15,17	1.14	2 (13%)
10	NAG	o	1	2,10	14,14,15	0.25	0	17,19,21	0.62	0
10	NAG	o	2	10	14,14,15	0.42	0	17,19,21	0.80	1 (5%)
10	BMA	o	3	10	11,11,12	0.67	0	15,15,17	0.89	0
10	MAN	o	4	10	11,11,12	0.73	0	15,15,17	1.05	2 (13%)
10	MAN	o	5	10	11,11,12	0.77	0	15,15,17	1.07	2 (13%)
11	NAG	p	1	2,11	14,14,15	0.31	0	17,19,21	0.48	0
11	NAG	p	2	11	14,14,15	0.21	0	17,19,21	0.62	0
11	BMA	p	3	11	11,11,12	0.88	0	15,15,17	0.74	0
8	NAG	q	1	2,8	14,14,15	0.39	0	17,19,21	0.80	0
8	NAG	q	2	8	14,14,15	0.87	1 (7%)	17,19,21	0.98	1 (5%)
8	NAG	r	1	2,8	14,14,15	0.43	0	17,19,21	0.98	1 (5%)
8	NAG	r	2	8	14,14,15	0.45	0	17,19,21	0.46	0
8	NAG	s	1	2,8	14,14,15	0.36	0	17,19,21	1.09	2 (11%)
8	NAG	s	2	8	14,14,15	0.30	0	17,19,21	0.73	0
12	NAG	t	1	2,12	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
12	NAG	t	2	12	14,14,15	0.35	0	17,19,21	0.65	1 (5%)
12	BMA	t	3	12	11,11,12	0.72	0	15,15,17	0.77	0
12	MAN	t	4	12	11,11,12	0.68	0	15,15,17	1.31	2 (13%)
12	MAN	t	5	12	11,11,12	0.86	1 (9%)	15,15,17	1.16	1 (6%)
12	MAN	t	6	12	11,11,12	0.88	0	15,15,17	0.89	1 (6%)
12	MAN	t	7	12	11,11,12	0.78	0	15,15,17	1.39	2 (13%)
12	MAN	t	8	12	11,11,12	0.89	1 (9%)	15,15,17	1.30	2 (13%)
12	MAN	t	9	12	11,11,12	0.23	0	15,15,17	0.72	0
12	NAG	u	1	2,12	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
12	NAG	u	2	12	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
12	BMA	u	3	12	11,11,12	0.73	0	15,15,17	0.77	0
12	MAN	u	4	12	11,11,12	0.68	0	15,15,17	1.31	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	u	5	12	11,11,12	0.86	1 (9%)	15,15,17	1.17	1 (6%)
12	MAN	u	6	12	11,11,12	0.88	0	15,15,17	0.89	1 (6%)
12	MAN	u	7	12	11,11,12	0.79	0	15,15,17	1.40	2 (13%)
12	MAN	u	8	12	11,11,12	0.88	1 (9%)	15,15,17	1.30	2 (13%)
12	MAN	u	9	12	11,11,12	0.24	0	15,15,17	0.73	0
12	NAG	v	1	2,12	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
12	NAG	v	2	12	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
12	BMA	v	3	12	11,11,12	0.71	0	15,15,17	0.77	0
12	MAN	v	4	12	11,11,12	0.68	0	15,15,17	1.31	2 (13%)
12	MAN	v	5	12	11,11,12	0.87	1 (9%)	15,15,17	1.16	1 (6%)
12	MAN	v	6	12	11,11,12	0.89	0	15,15,17	0.89	1 (6%)
12	MAN	v	7	12	11,11,12	0.78	0	15,15,17	1.39	2 (13%)
12	MAN	v	8	12	11,11,12	0.88	1 (9%)	15,15,17	1.31	2 (13%)
12	MAN	v	9	12	11,11,12	0.25	0	15,15,17	0.74	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
8	NAG	V	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	NAG	W	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
8	NAG	X	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	NAG	Y	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
9	NAG	Z	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	2/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	5	9	-	2/2/19/22	0/1/1/1
10	NAG	a	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	a	2	10	-	2/6/23/26	0/1/1/1
10	BMA	a	3	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	a	4	10	-	0/2/19/22	0/1/1/1
10	MAN	a	5	10	-	2/2/19/22	0/1/1/1
11	NAG	b	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	b	2	11	-	1/6/23/26	0/1/1/1
11	BMA	b	3	11	-	1/2/19/22	0/1/1/1
8	NAG	c	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	3/6/23/26	0/1/1/1
8	NAG	d	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	d	2	8	-	1/6/23/26	0/1/1/1
8	NAG	e	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	e	2	8	-	2/6/23/26	0/1/1/1
8	NAG	f	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
9	NAG	g	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	g	2	9	-	2/6/23/26	0/1/1/1
9	BMA	g	3	9	-	2/2/19/22	0/1/1/1
9	MAN	g	4	9	-	0/2/19/22	0/1/1/1
9	MAN	g	5	9	-	2/2/19/22	0/1/1/1
10	NAG	h	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	h	2	10	-	2/6/23/26	0/1/1/1
10	BMA	h	3	10	-	0/2/19/22	0/1/1/1
10	MAN	h	4	10	-	0/2/19/22	0/1/1/1
10	MAN	h	5	10	-	2/2/19/22	0/1/1/1
11	NAG	i	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	i	2	11	-	1/6/23/26	0/1/1/1
11	BMA	i	3	11	-	1/2/19/22	0/1/1/1
8	NAG	j	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	3/6/23/26	0/1/1/1
8	NAG	k	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	k	2	8	-	1/6/23/26	0/1/1/1
8	NAG	l	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	l	2	8	-	3/6/23/26	0/1/1/1
8	NAG	m	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	m	2	8	-	2/6/23/26	0/1/1/1
9	NAG	n	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	2/6/23/26	0/1/1/1
9	BMA	n	3	9	-	2/2/19/22	0/1/1/1
9	MAN	n	4	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	n	5	9	-	2/2/19/22	0/1/1/1
10	NAG	o	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	o	2	10	-	2/6/23/26	0/1/1/1
10	BMA	o	3	10	-	0/2/19/22	0/1/1/1
10	MAN	o	4	10	-	0/2/19/22	0/1/1/1
10	MAN	o	5	10	-	2/2/19/22	0/1/1/1
11	NAG	p	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	p	2	11	-	1/6/23/26	0/1/1/1
11	BMA	p	3	11	-	1/2/19/22	0/1/1/1
8	NAG	q	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	q	2	8	-	3/6/23/26	0/1/1/1
8	NAG	r	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	r	2	8	-	1/6/23/26	0/1/1/1
8	NAG	s	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	s	2	8	-	4/6/23/26	0/1/1/1
12	NAG	t	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	t	2	12	-	2/6/23/26	0/1/1/1
12	BMA	t	3	12	-	2/2/19/22	0/1/1/1
12	MAN	t	4	12	-	2/2/19/22	0/1/1/1
12	MAN	t	5	12	-	1/2/19/22	0/1/1/1
12	MAN	t	6	12	-	0/2/19/22	0/1/1/1
12	MAN	t	7	12	-	2/2/19/22	0/1/1/1
12	MAN	t	8	12	-	0/2/19/22	0/1/1/1
12	MAN	t	9	12	-	0/2/19/22	0/1/1/1
12	NAG	u	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	u	2	12	-	2/6/23/26	0/1/1/1
12	BMA	u	3	12	-	2/2/19/22	0/1/1/1
12	MAN	u	4	12	-	2/2/19/22	0/1/1/1
12	MAN	u	5	12	-	1/2/19/22	0/1/1/1
12	MAN	u	6	12	-	0/2/19/22	0/1/1/1
12	MAN	u	7	12	-	0/2/19/22	0/1/1/1
12	MAN	u	8	12	-	0/2/19/22	0/1/1/1
12	MAN	u	9	12	-	0/2/19/22	0/1/1/1
12	NAG	v	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	v	2	12	-	2/6/23/26	0/1/1/1
12	BMA	v	3	12	-	2/2/19/22	0/1/1/1
12	MAN	v	4	12	-	2/2/19/22	0/1/1/1
12	MAN	v	5	12	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	v	6	12	-	0/2/19/22	0/1/1/1
12	MAN	v	7	12	-	0/2/19/22	0/1/1/1
12	MAN	v	8	12	-	0/2/19/22	0/1/1/1
12	MAN	v	9	12	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	1	NAG	O5-C1	-4.27	1.36	1.43
8	V	1	NAG	O5-C1	-4.24	1.36	1.43
8	X	1	NAG	O5-C1	-4.24	1.36	1.43
8	q	2	NAG	C1-C2	2.63	1.55	1.52
8	j	2	NAG	C1-C2	2.60	1.55	1.52

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	1	NAG	O5-C1-C2	-4.76	103.93	111.29
9	Z	4	MAN	C1-O5-C5	4.16	117.76	112.19
9	g	4	MAN	C1-O5-C5	4.12	117.71	112.19
9	n	4	MAN	C1-O5-C5	4.11	117.69	112.19
8	l	1	NAG	O5-C1-C2	-4.02	105.07	111.29

There are no chirality outliers.

5 of 126 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	e	1	NAG	C8-C7-N2-C2
8	l	1	NAG	C8-C7-N2-C2
8	l	1	NAG	O7-C7-N2-C2
8	l	2	NAG	C3-C2-N2-C7
8	l	2	NAG	C8-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 17 short contacts:

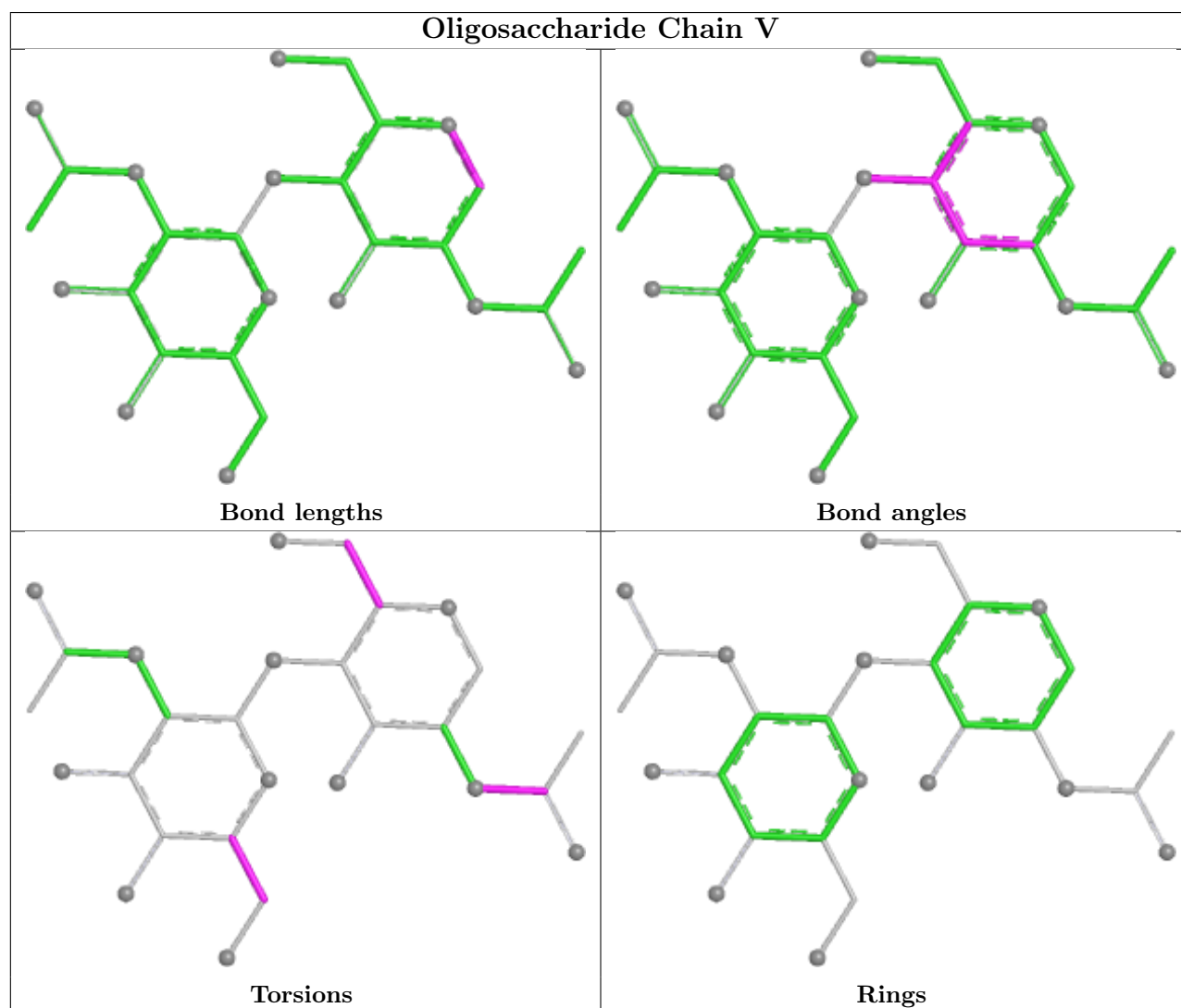
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	l	2	NAG	1	0
8	W	1	NAG	1	0
8	e	2	NAG	4	0
8	l	1	NAG	1	0

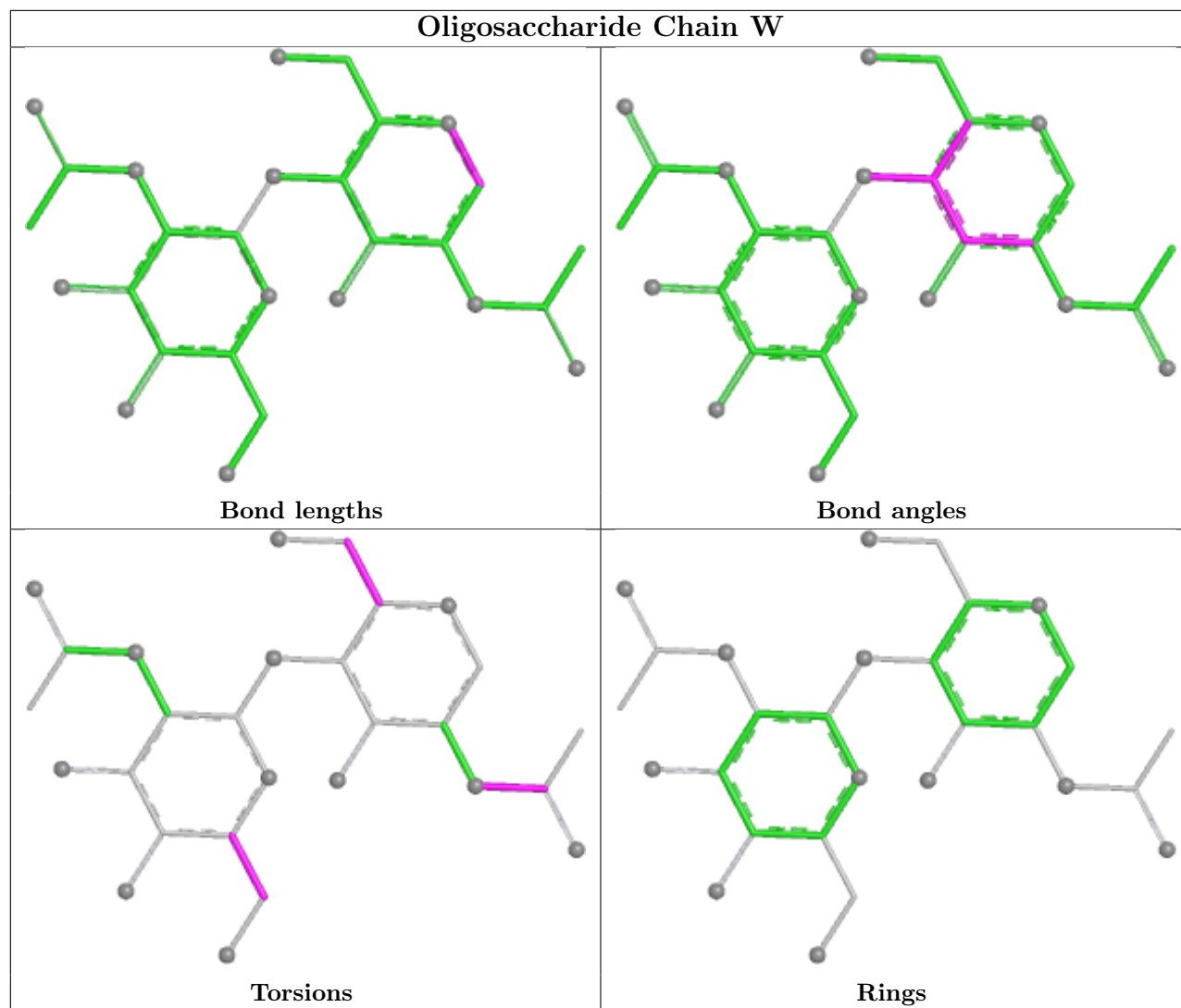
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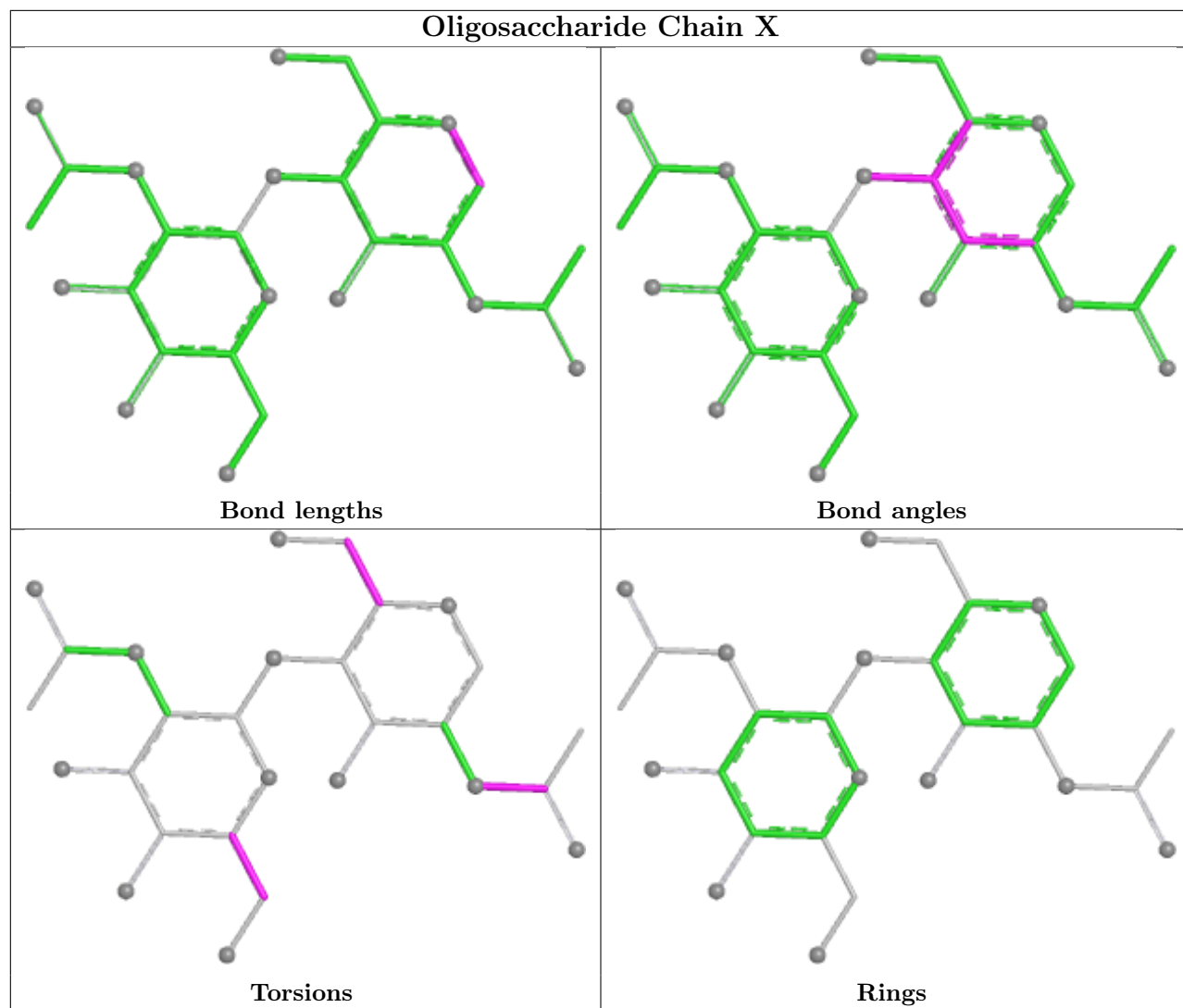
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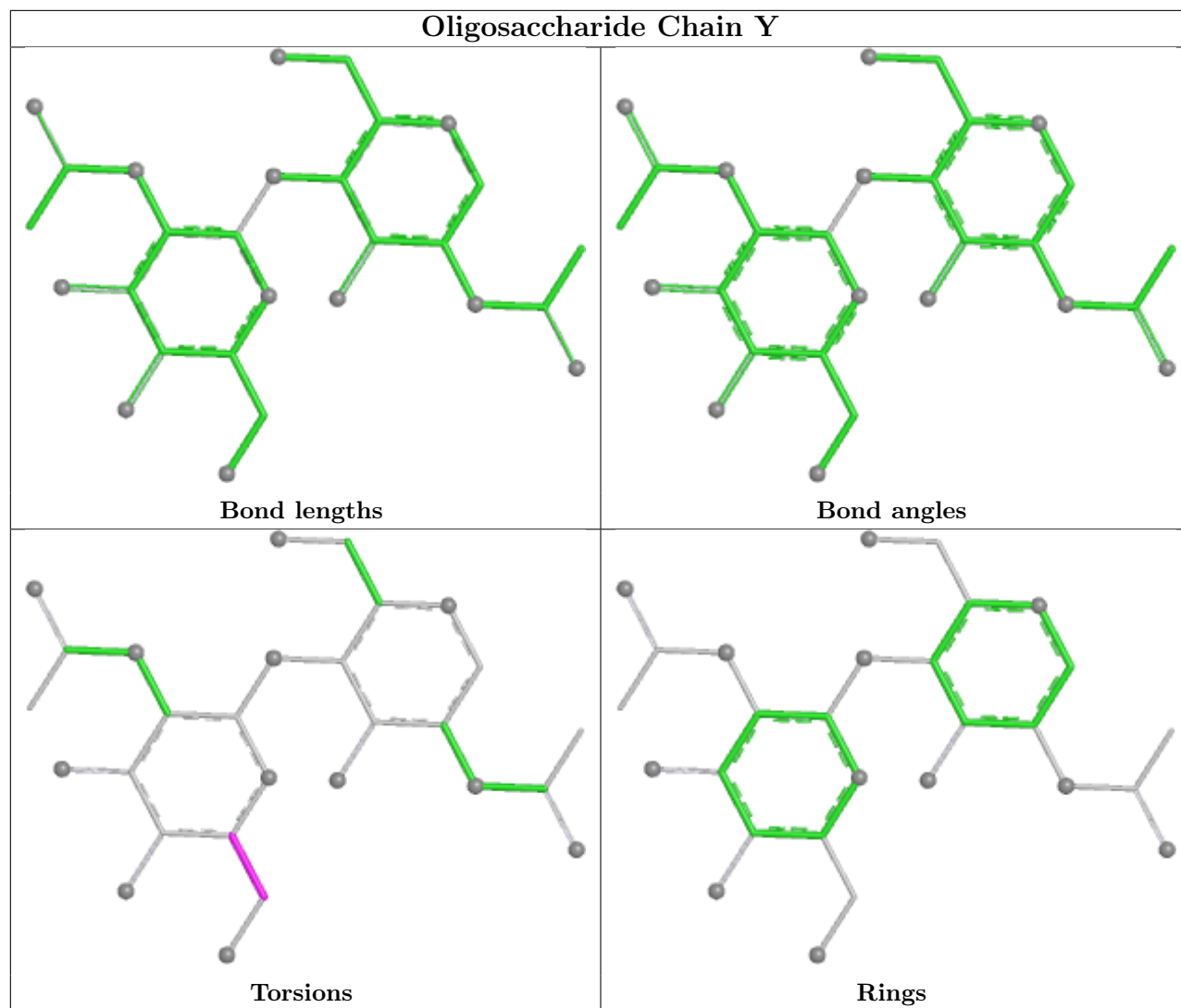
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	o	3	BMA	1	0
10	h	2	NAG	1	0
8	k	1	NAG	1	0
8	s	1	NAG	1	0
8	d	1	NAG	1	0
8	s	2	NAG	3	0
8	r	1	NAG	1	0
8	V	1	NAG	1	0

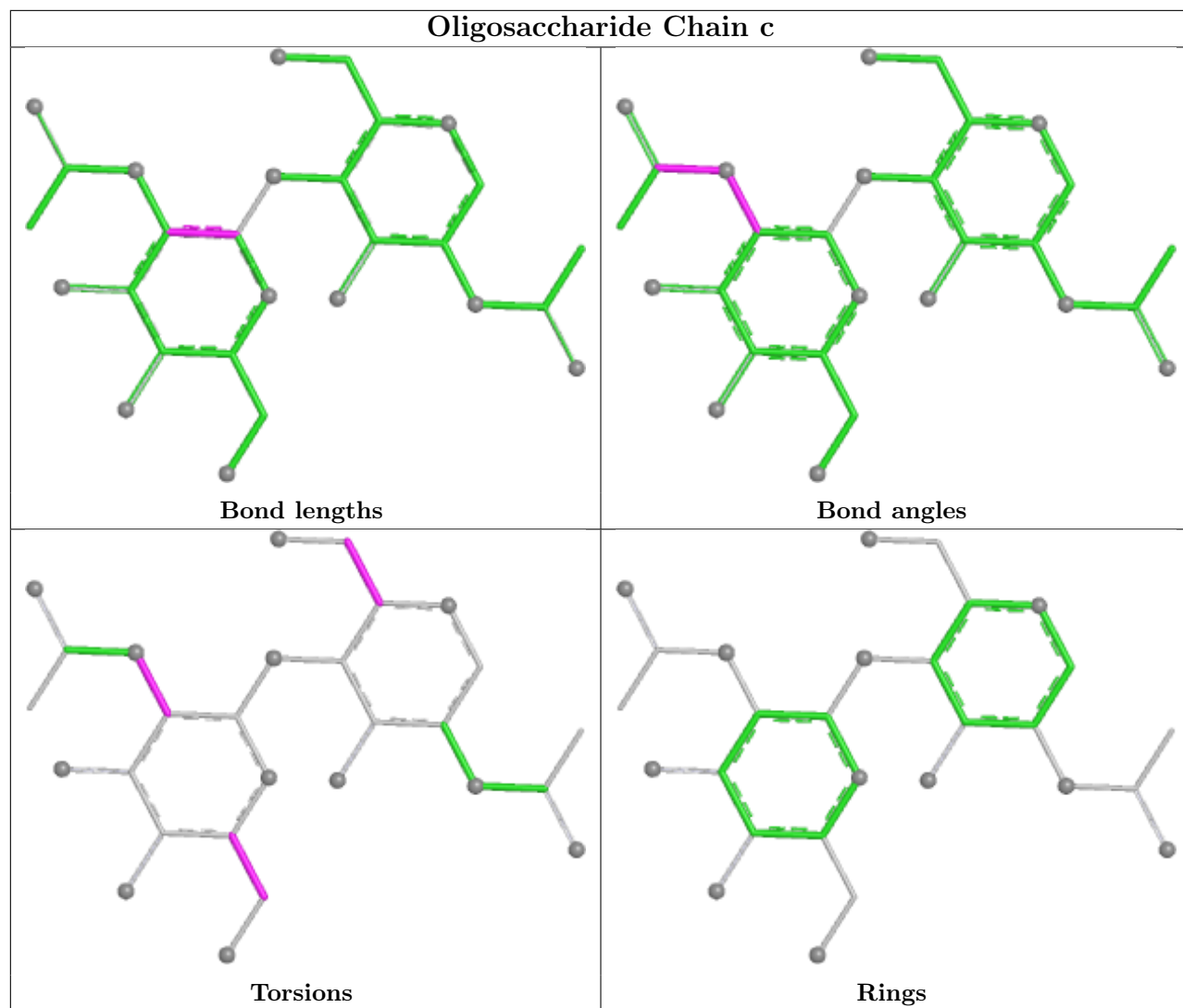
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

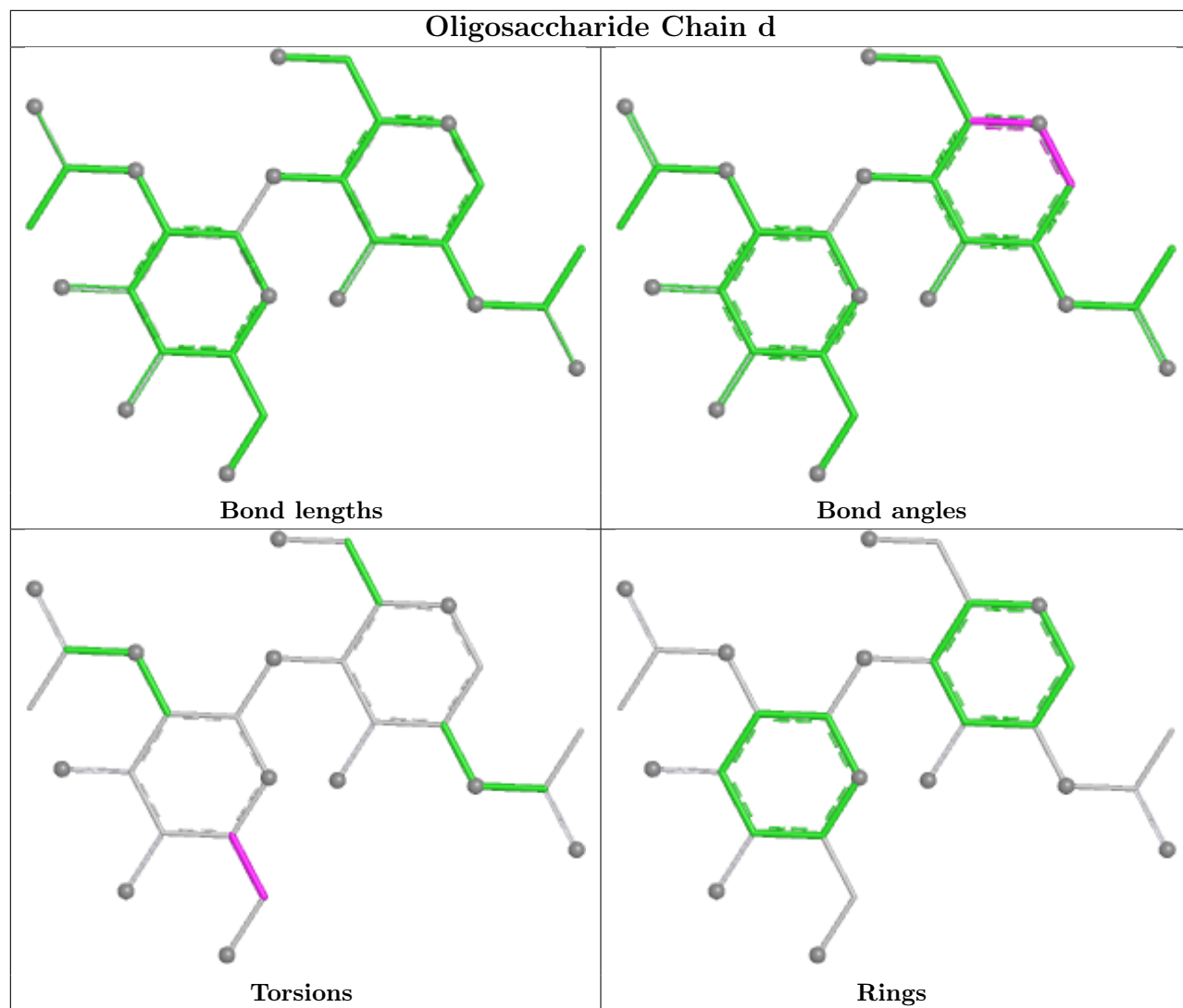


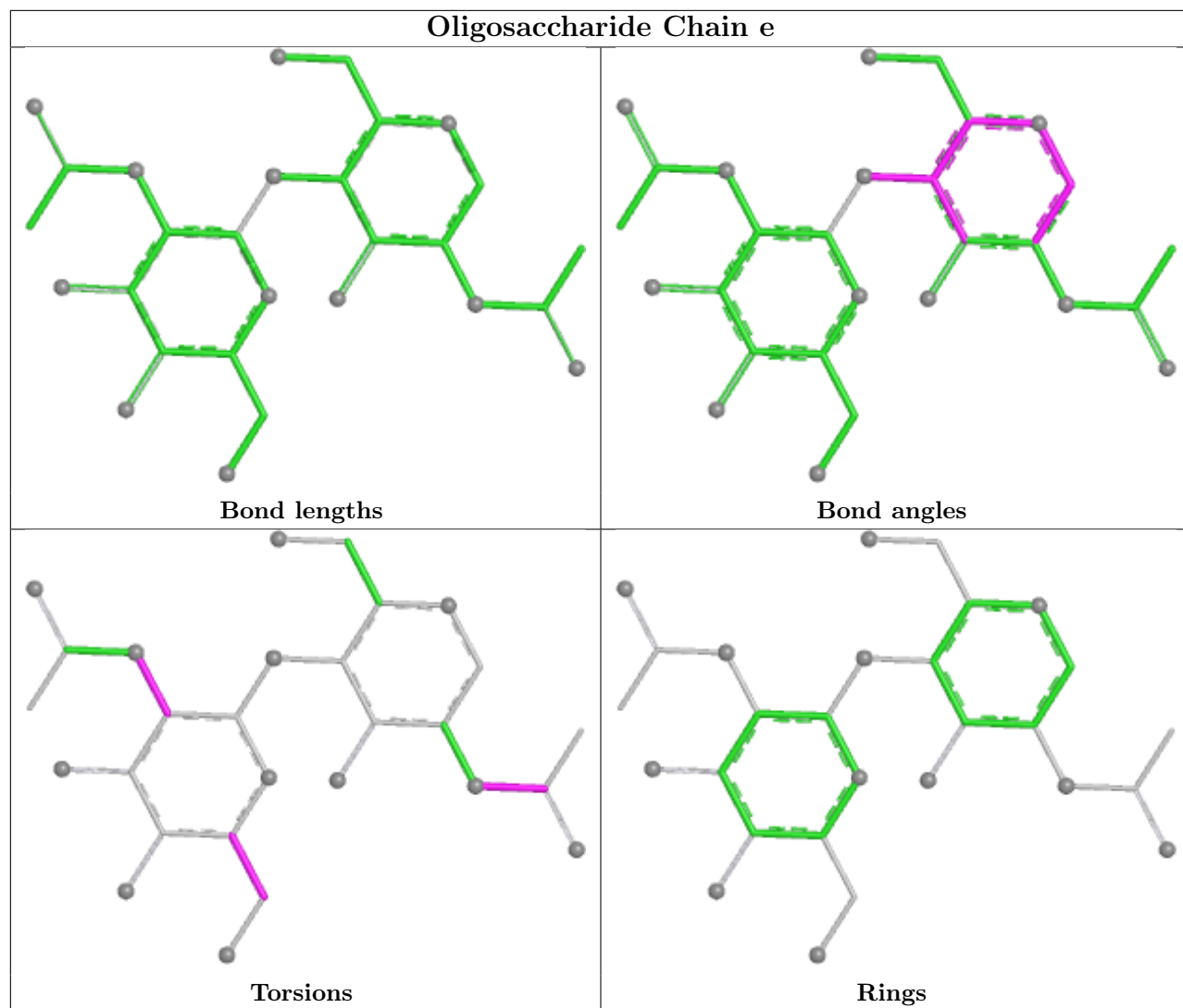


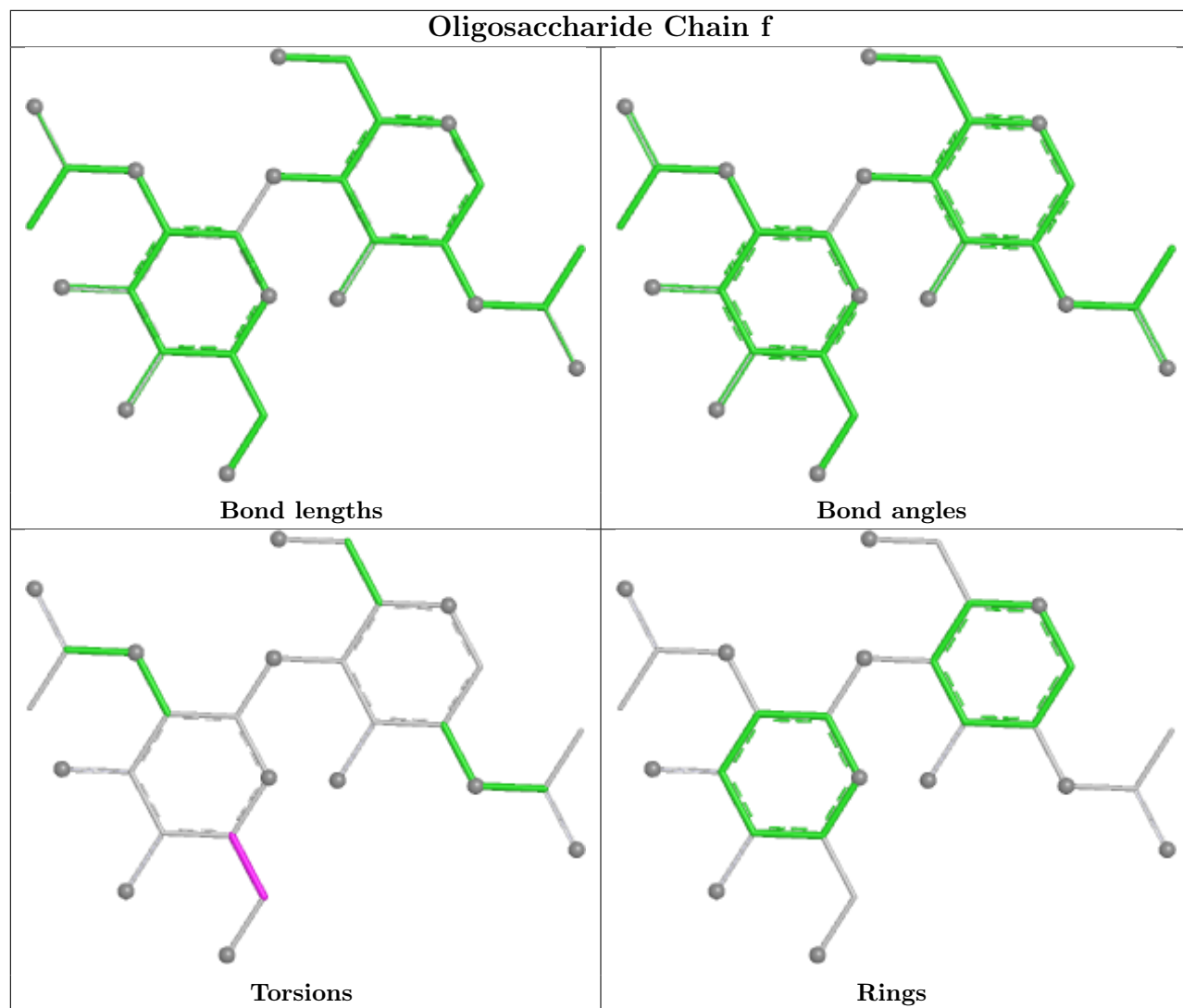


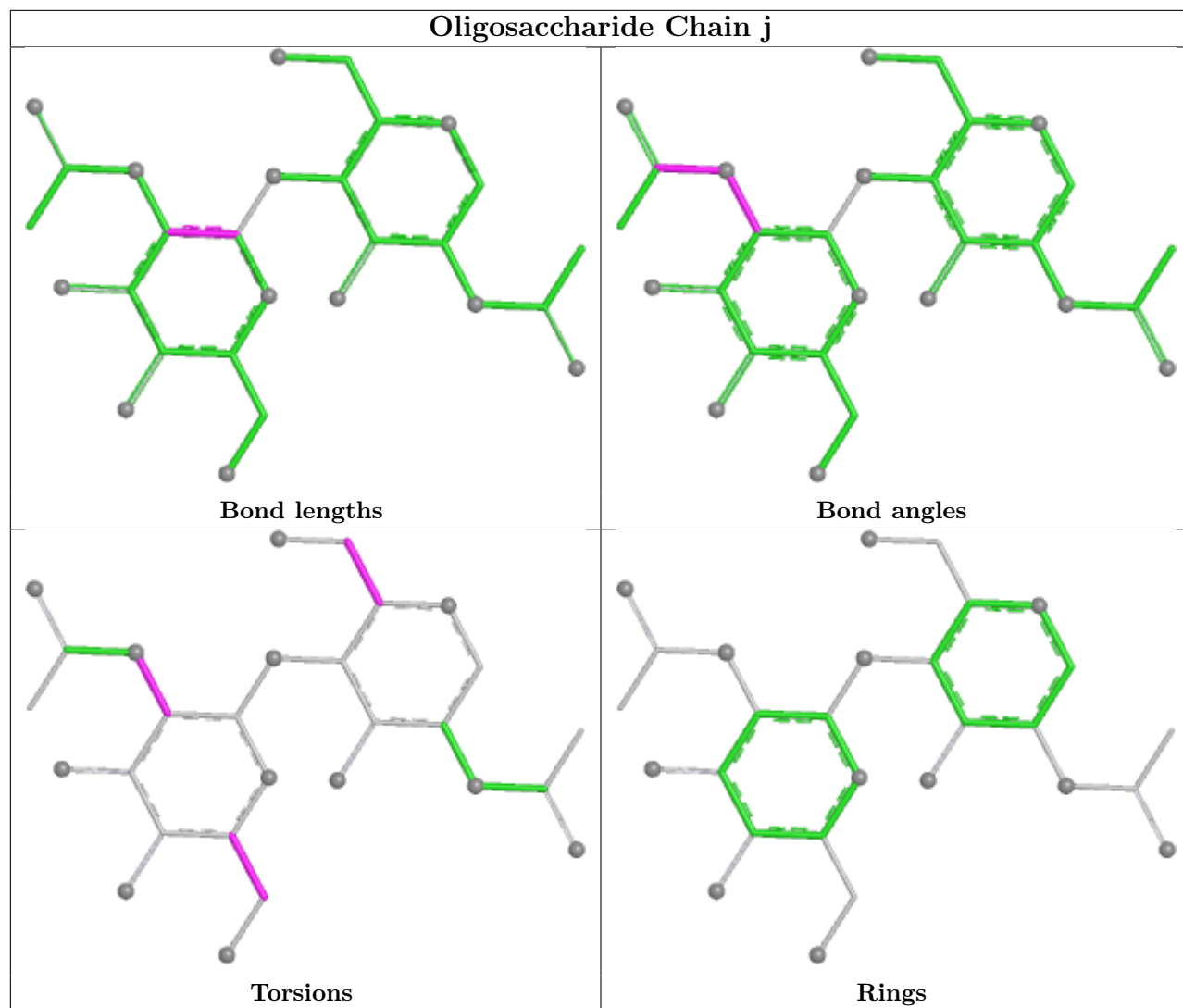


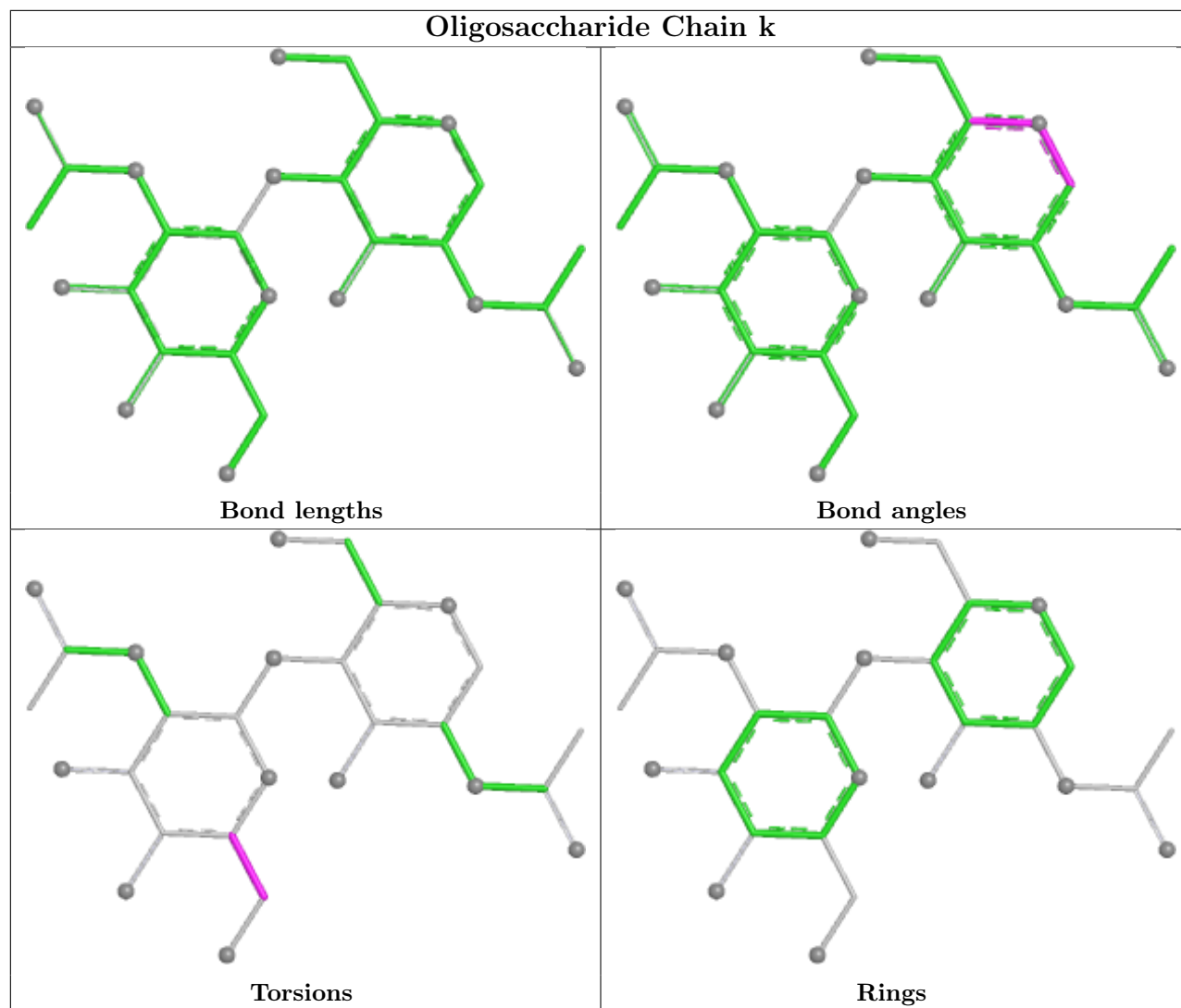


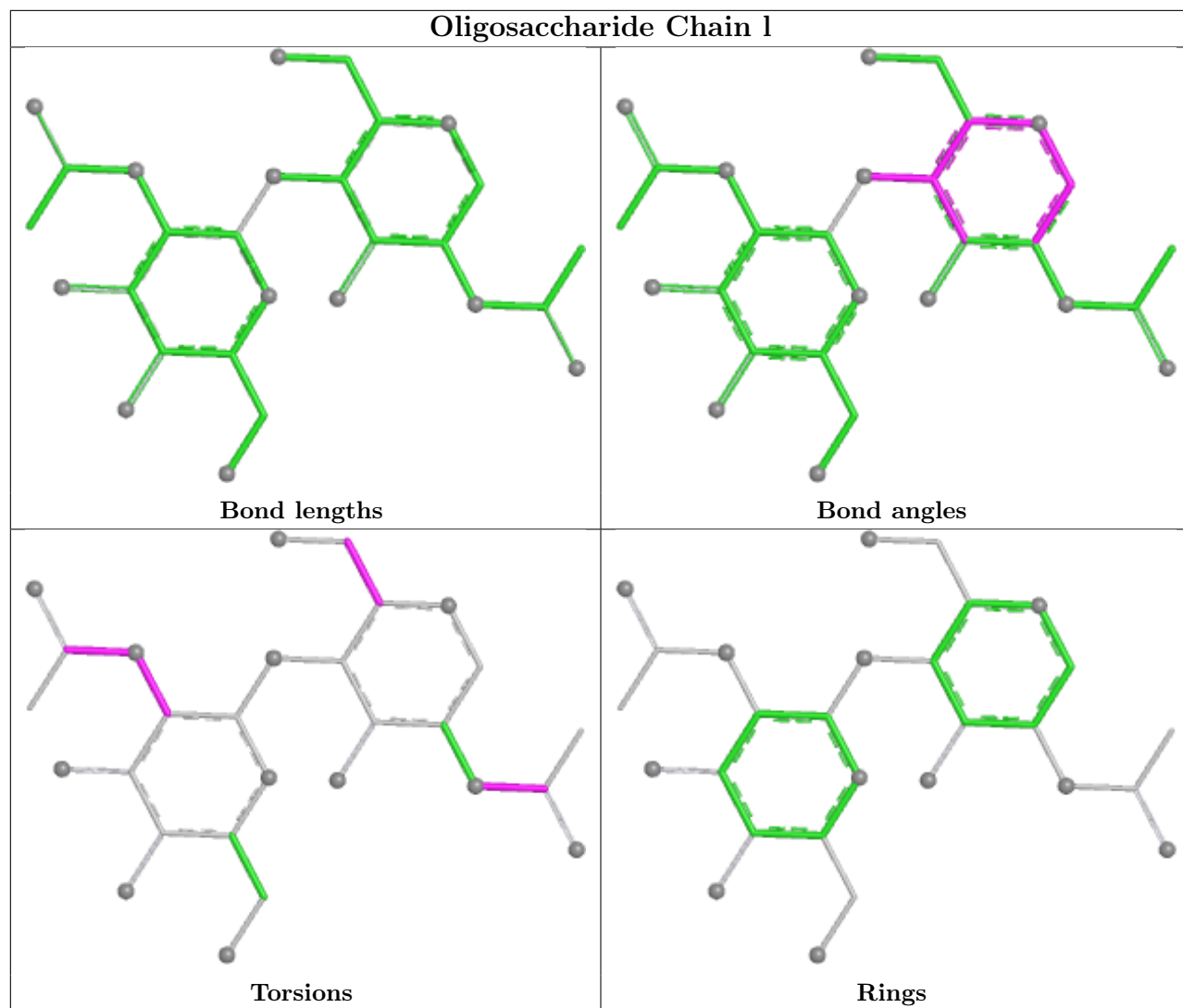


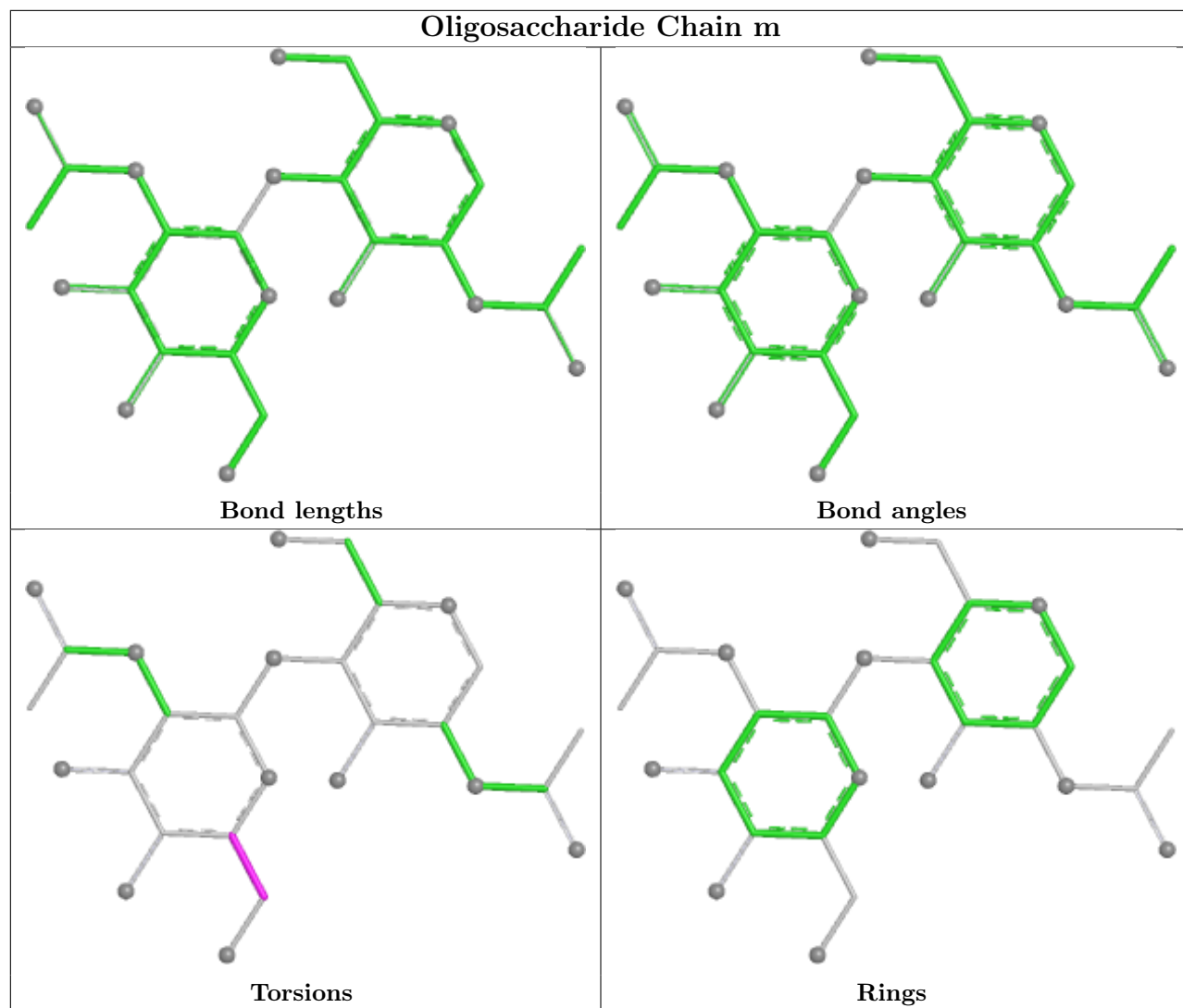


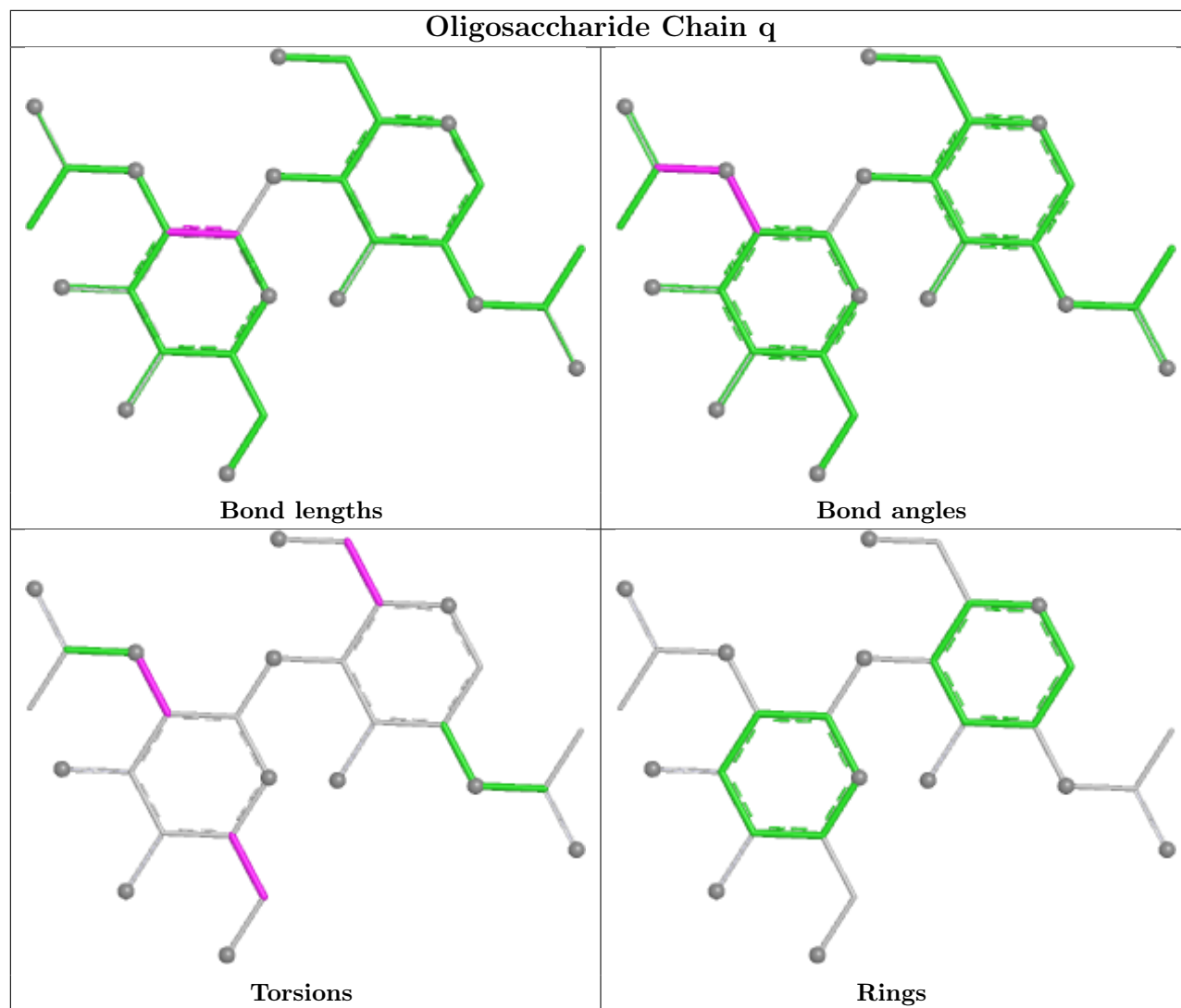


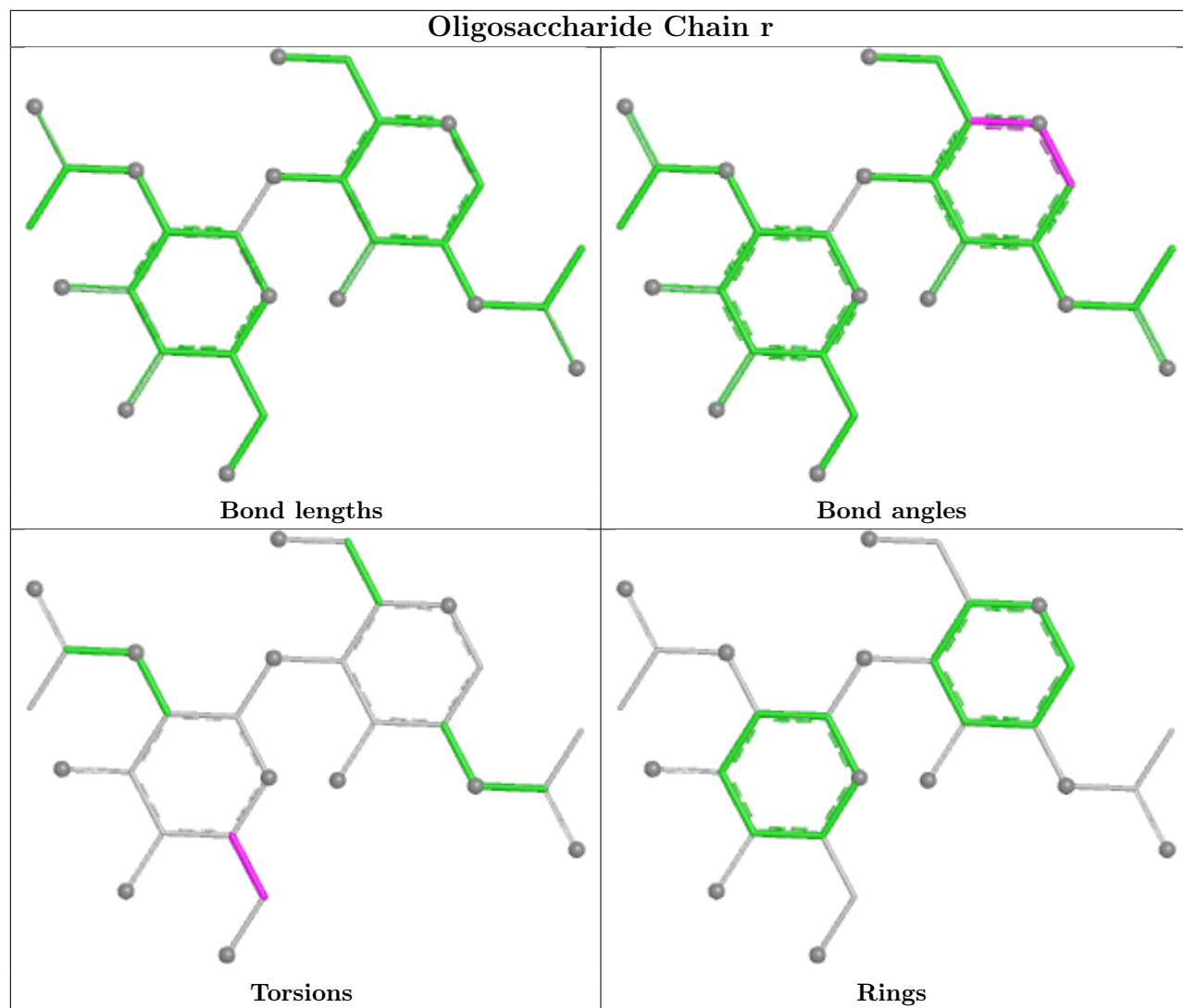


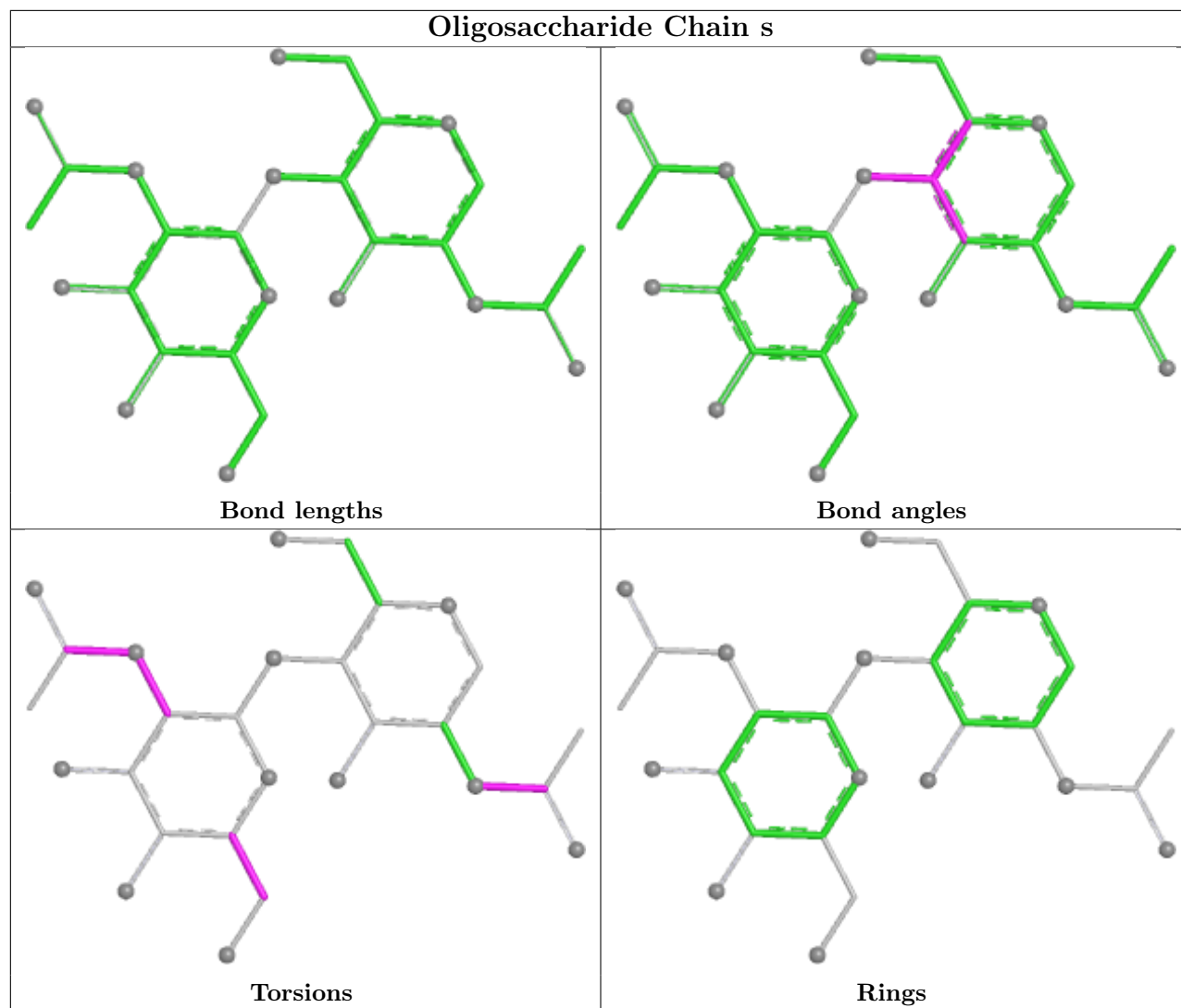


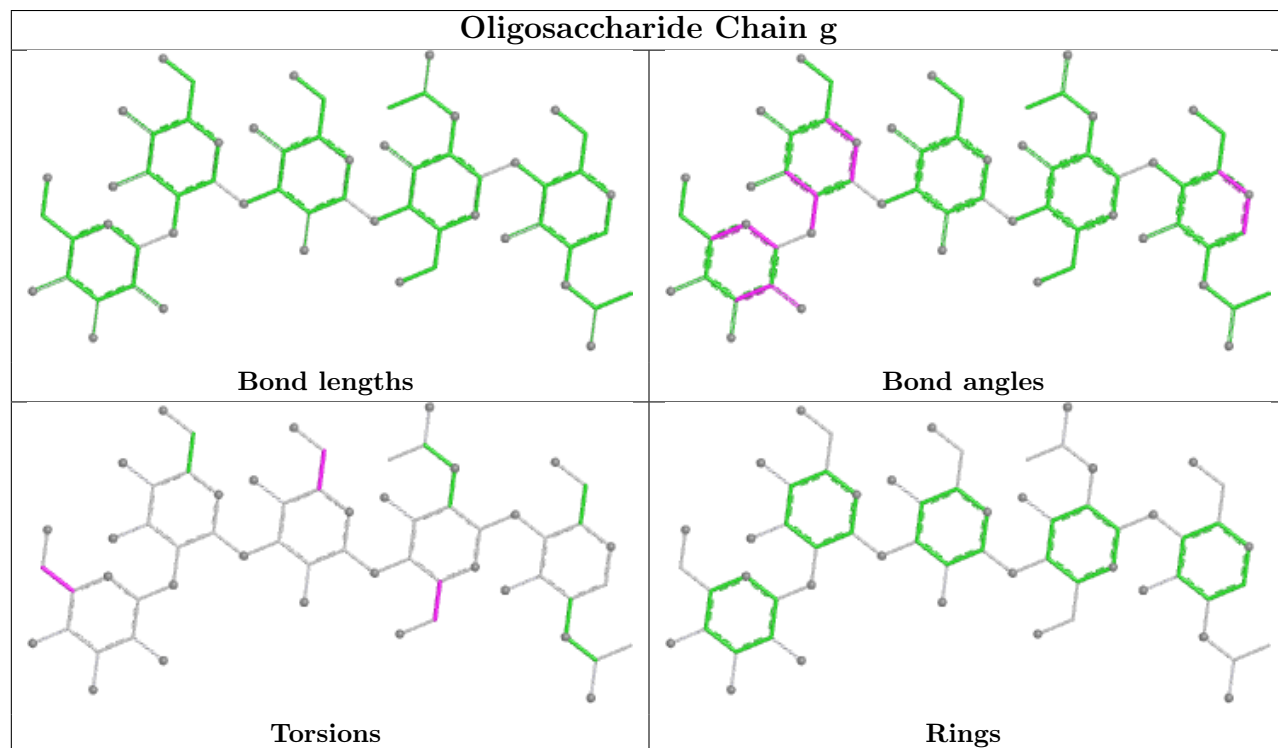
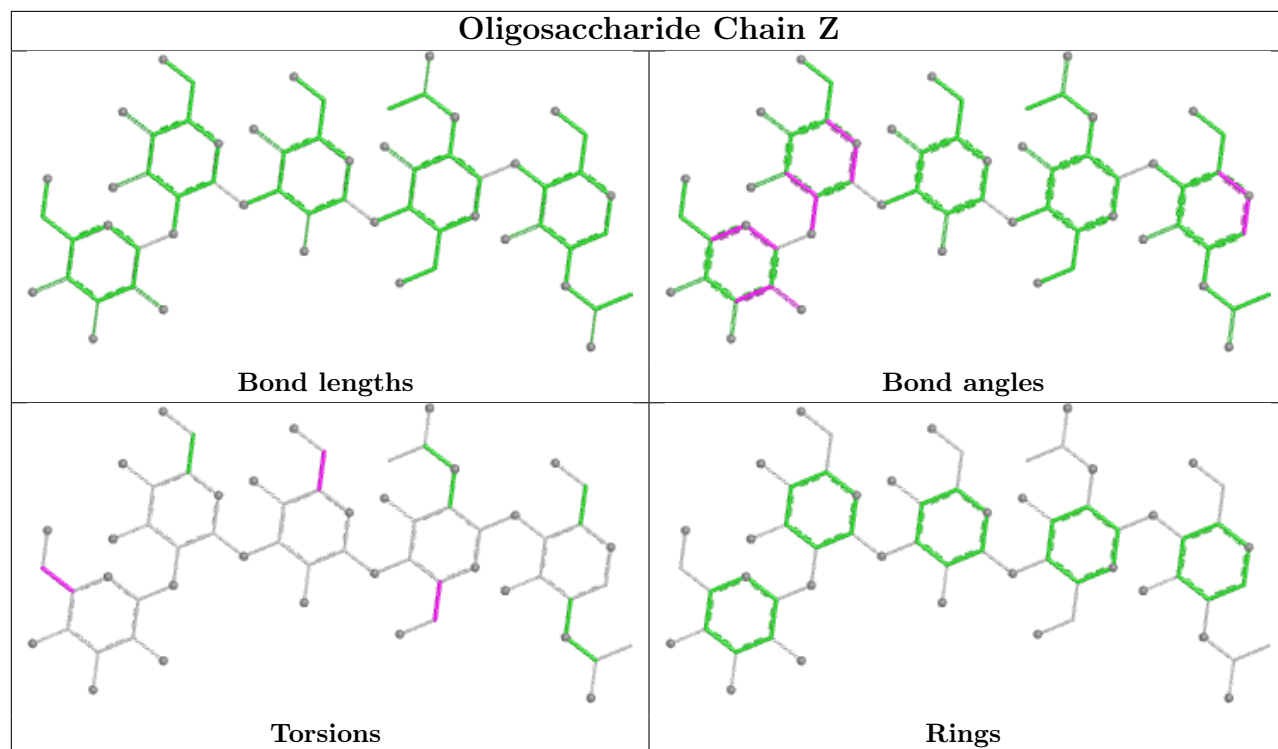


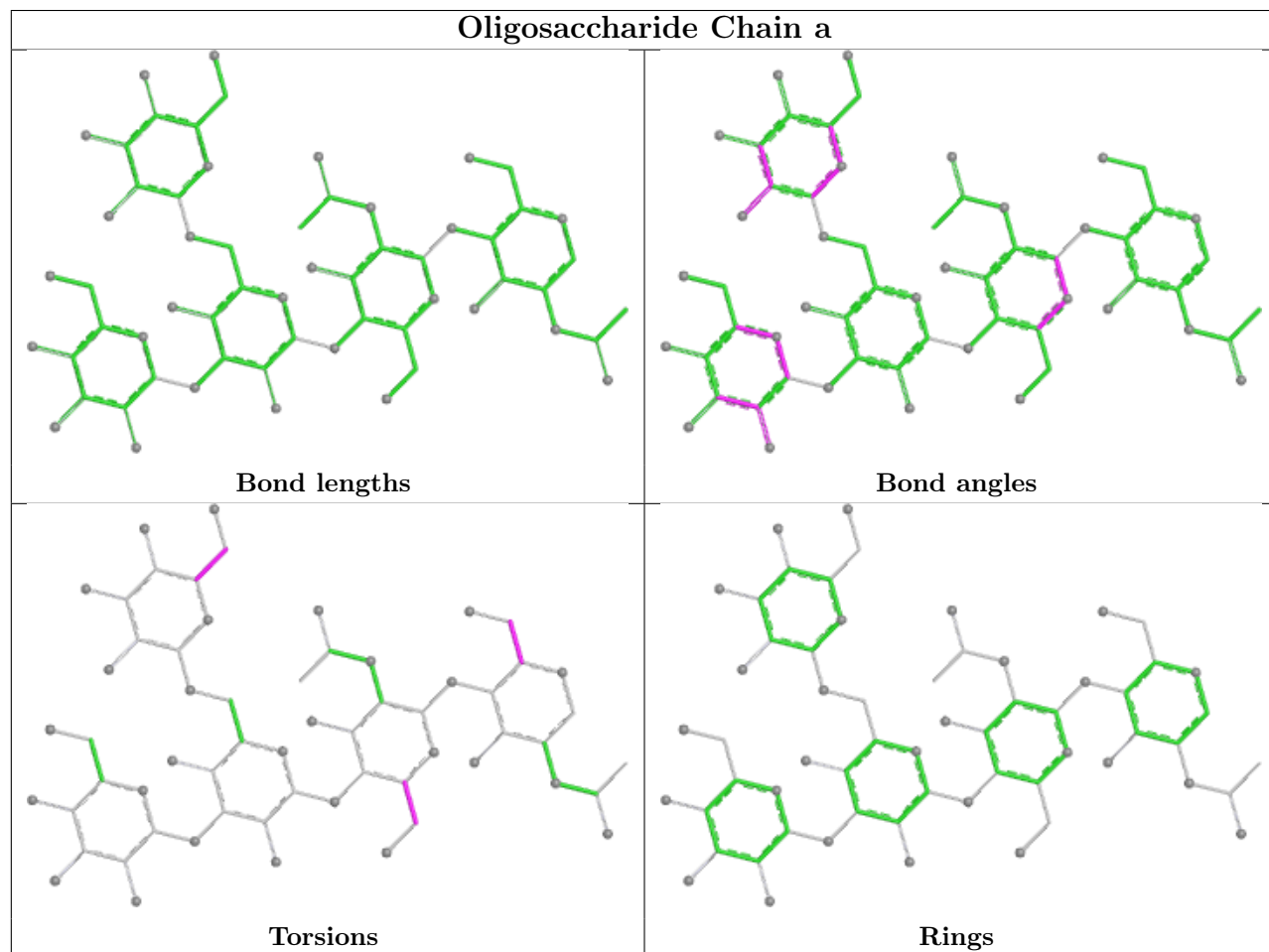
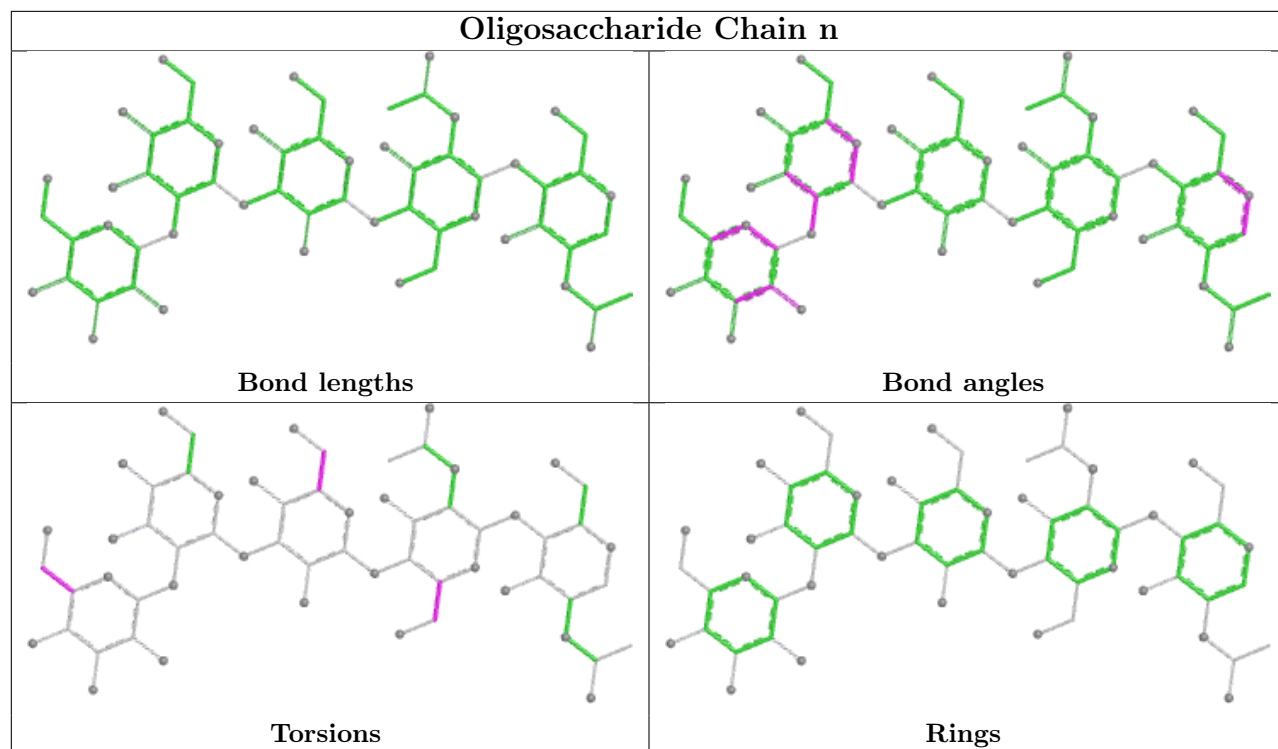


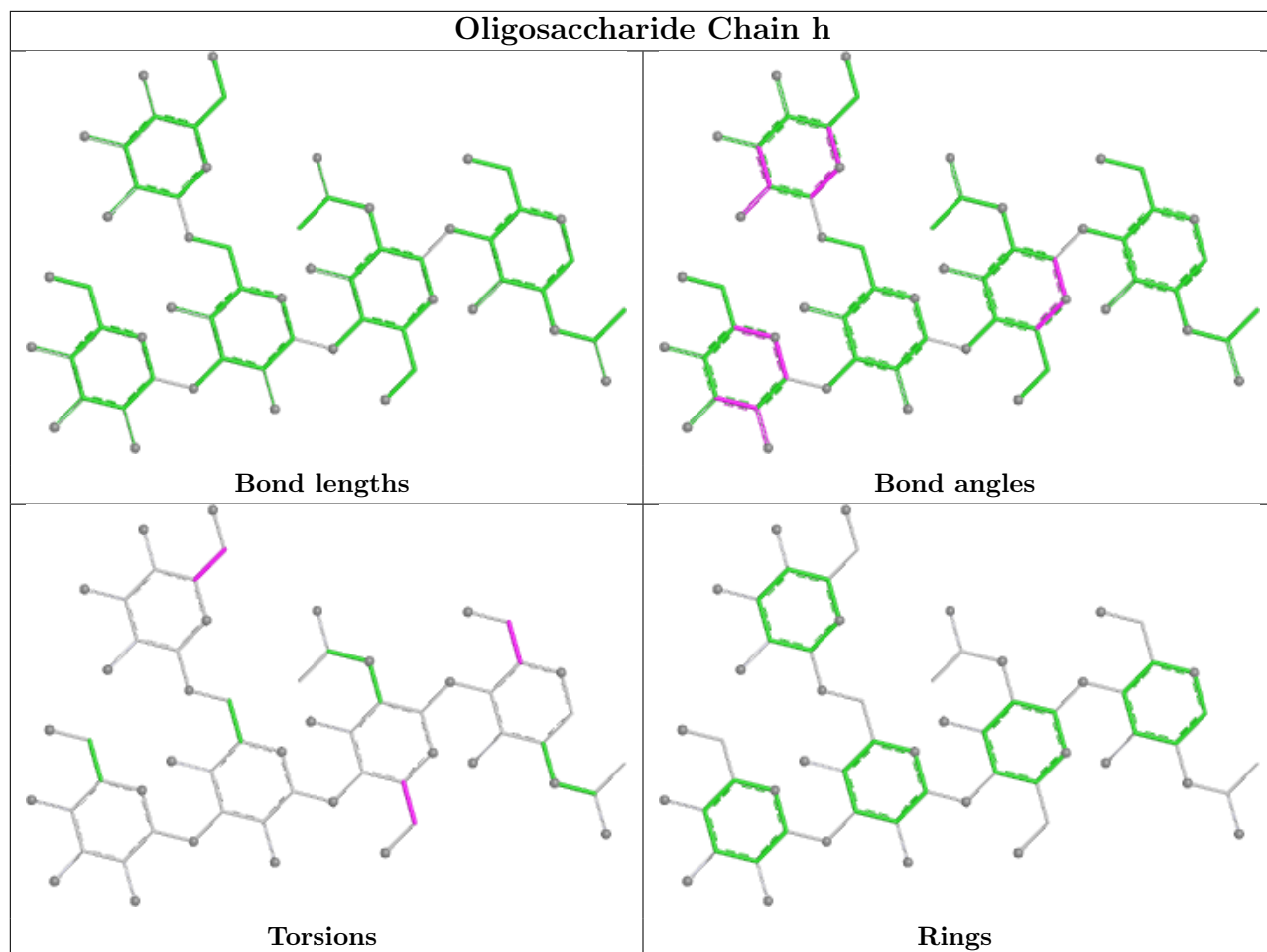


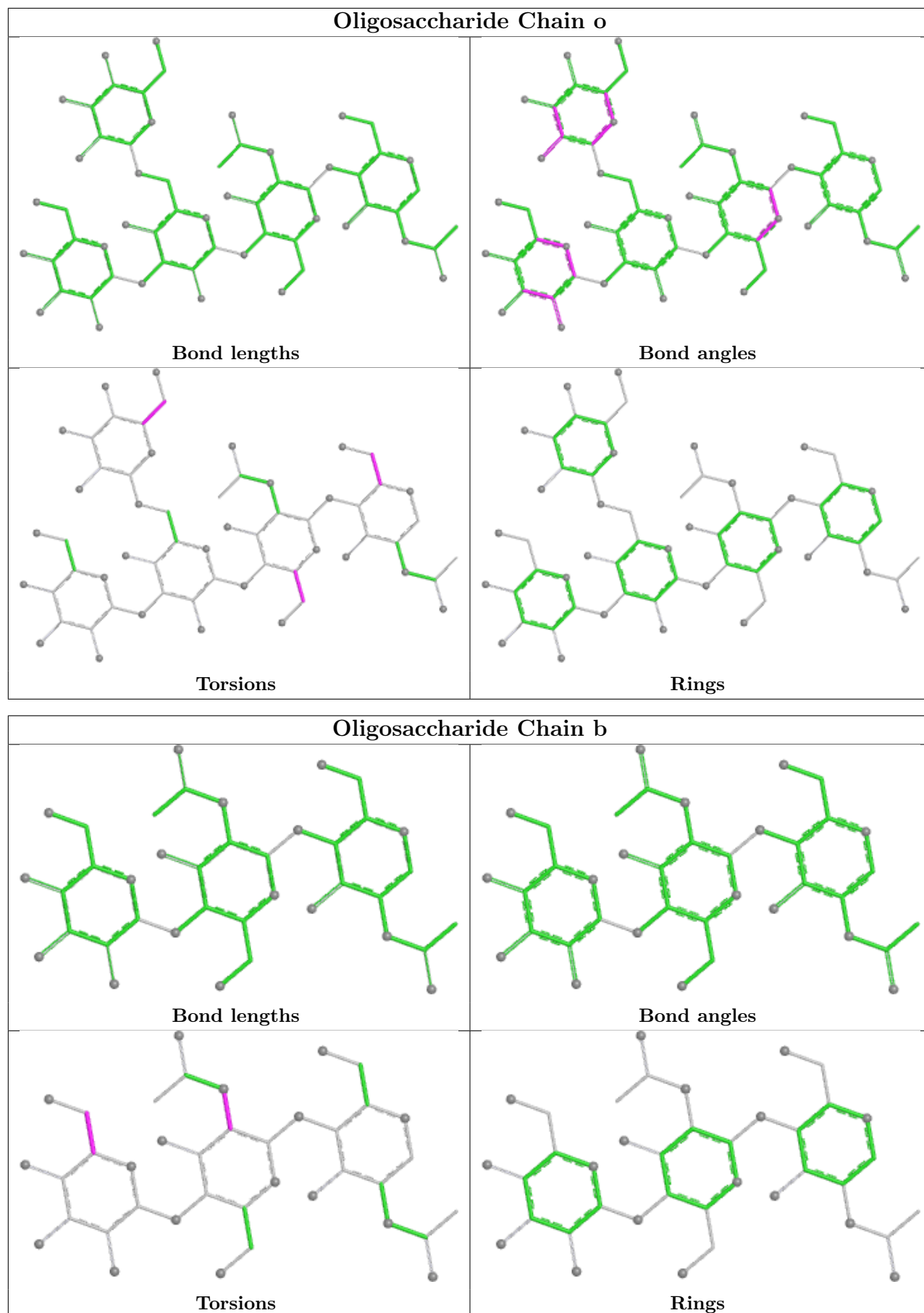


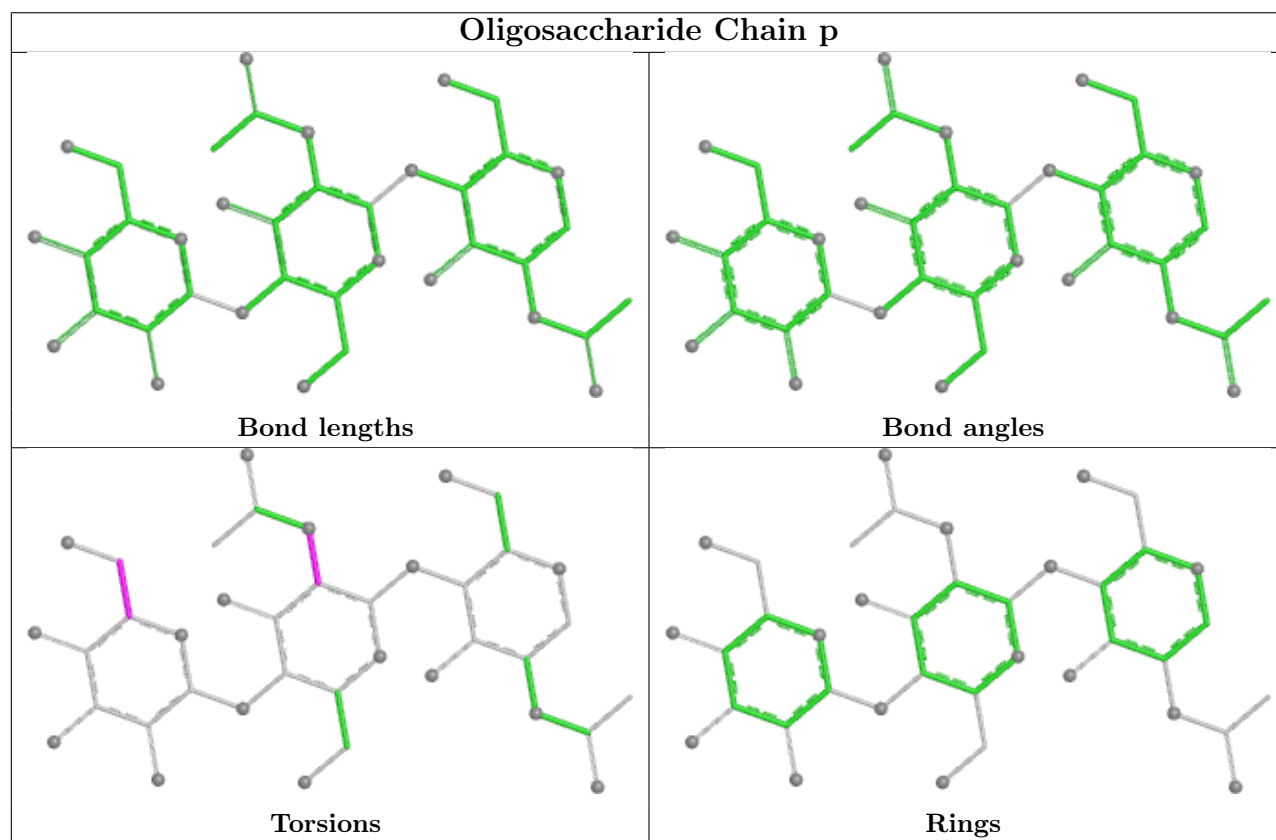
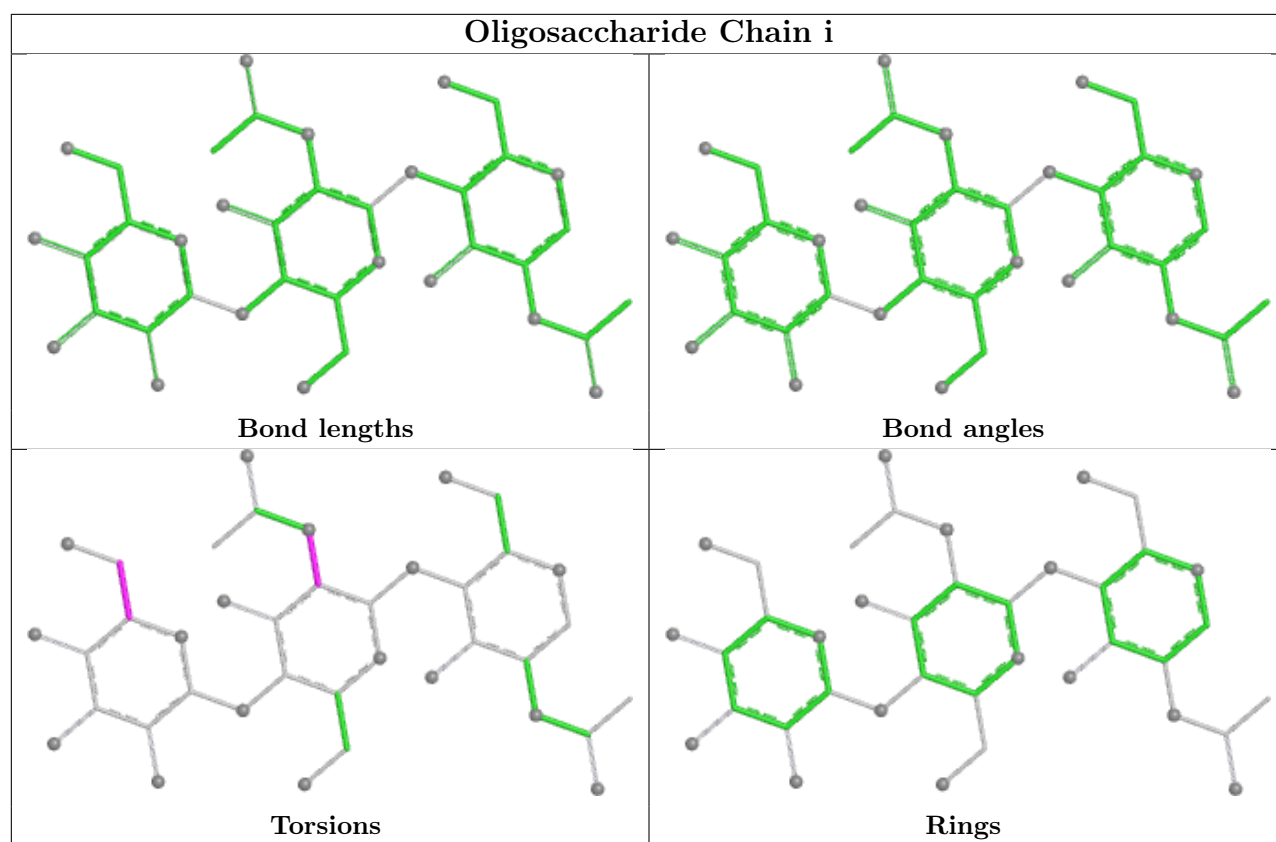


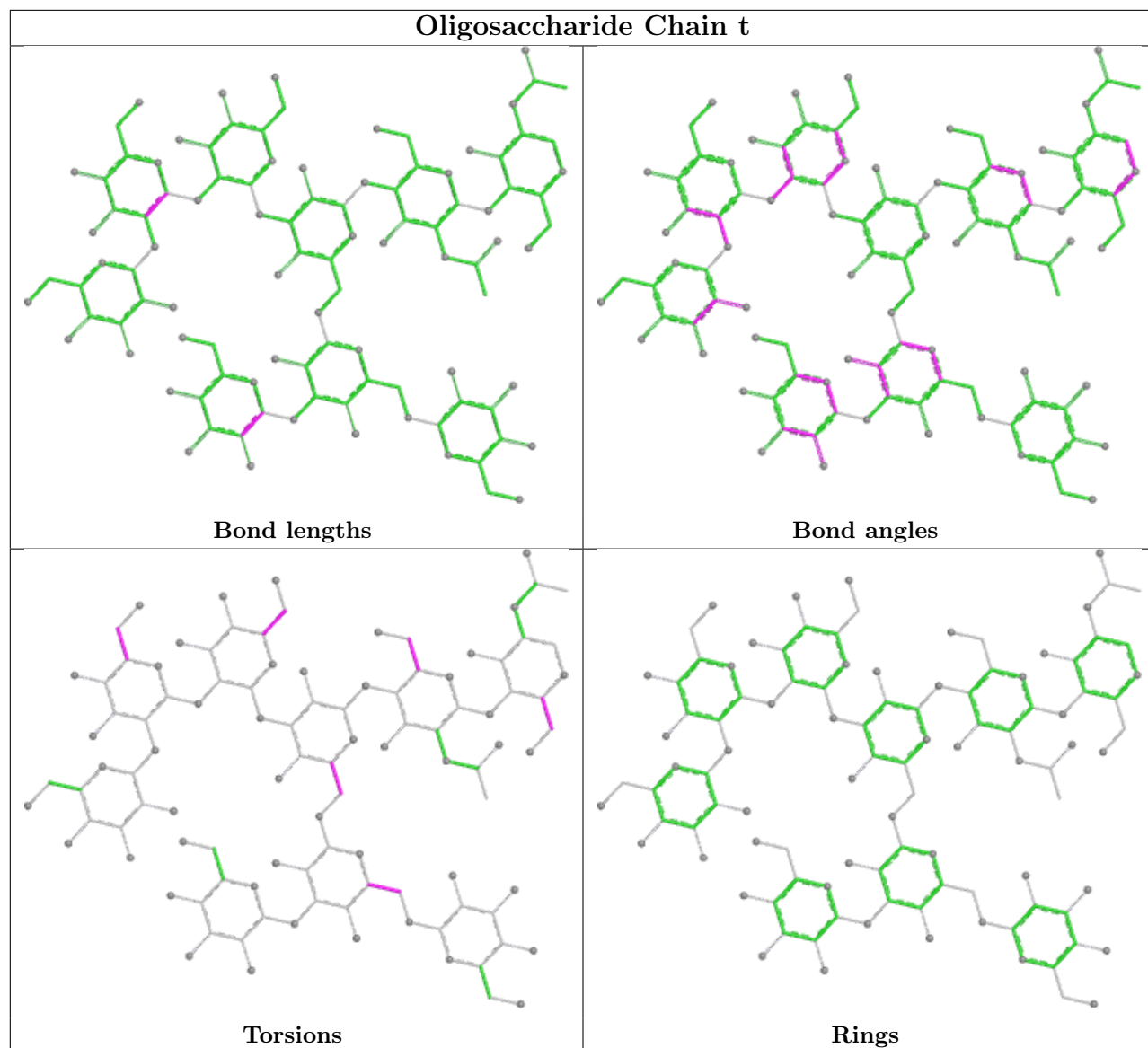


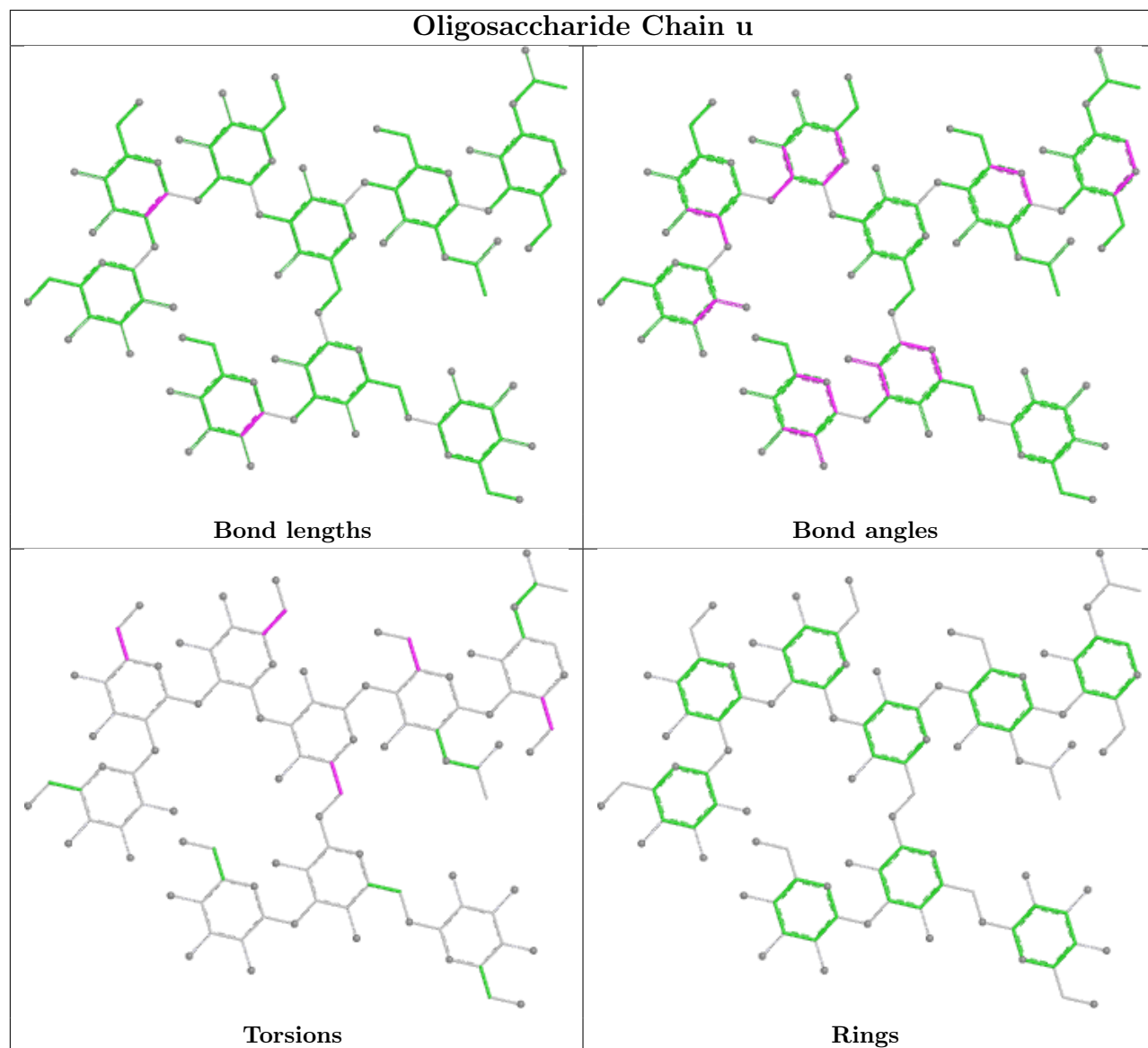


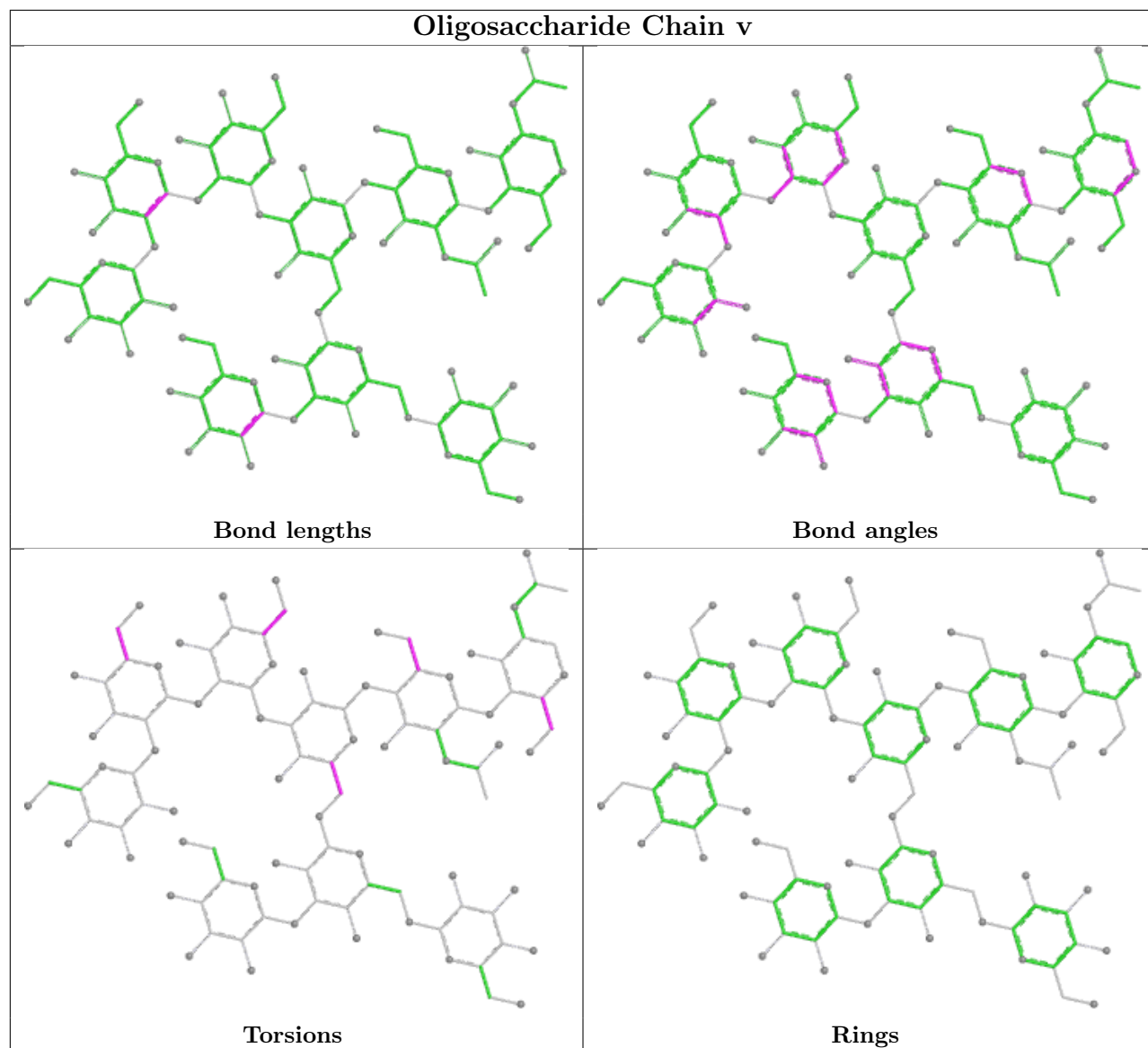












5.6 Ligand geometry [i](#)

27 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	$\# Z > 2$
13	NAG	E	601	2	14,14,15	0.26	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	NAG	E	603	2	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
13	NAG	F	607	2	14,14,15	0.29	0	17,19,21	0.58	0
13	NAG	F	608	2	14,14,15	0.32	0	17,19,21	0.64	0
13	NAG	D	602	2	14,14,15	0.38	0	17,19,21	0.52	0
13	NAG	C	701	1	14,14,15	0.54	0	17,19,21	0.45	0
13	NAG	E	602	2	14,14,15	0.38	0	17,19,21	0.52	0
13	NAG	D	601	2	14,14,15	0.25	0	17,19,21	0.46	0
13	NAG	D	607	2	14,14,15	0.29	0	17,19,21	0.59	0
13	NAG	D	605	2	14,14,15	0.43	0	17,19,21	0.58	0
13	NAG	E	607	2	14,14,15	0.30	0	17,19,21	0.59	0
13	NAG	F	604	2	14,14,15	0.46	0	17,19,21	0.52	0
13	NAG	F	606	2	14,14,15	0.52	0	17,19,21	0.42	0
13	NAG	A	701	1	14,14,15	0.27	0	17,19,21	0.59	0
13	NAG	D	604	2	14,14,15	0.47	0	17,19,21	0.53	0
13	NAG	D	608	2	14,14,15	0.33	0	17,19,21	0.64	0
13	NAG	E	606	2	14,14,15	0.53	0	17,19,21	0.42	0
13	NAG	F	602	2	14,14,15	0.37	0	17,19,21	0.52	0
13	NAG	D	603	2	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
13	NAG	B	701	1	14,14,15	0.54	0	17,19,21	0.45	0
13	NAG	F	605	2	14,14,15	0.44	0	17,19,21	0.58	0
13	NAG	D	606	2	14,14,15	0.52	0	17,19,21	0.41	0
13	NAG	E	608	2	14,14,15	0.33	0	17,19,21	0.64	0
13	NAG	F	601	2	14,14,15	0.25	0	17,19,21	0.46	0
13	NAG	E	604	2	14,14,15	0.47	0	17,19,21	0.53	0
13	NAG	E	605	2	14,14,15	0.41	0	17,19,21	0.58	0
13	NAG	F	603	2	14,14,15	0.31	0	17,19,21	0.67	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
13	NAG	E	601	2	-	2/6/23/26	0/1/1/1
13	NAG	E	603	2	-	0/6/23/26	0/1/1/1
13	NAG	F	607	2	-	0/6/23/26	0/1/1/1
13	NAG	F	608	2	-	4/6/23/26	0/1/1/1
13	NAG	D	602	2	-	2/6/23/26	0/1/1/1
13	NAG	C	701	1	-	2/6/23/26	0/1/1/1
13	NAG	E	602	2	-	2/6/23/26	0/1/1/1
13	NAG	D	601	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	D	607	2	-	0/6/23/26	0/1/1/1
13	NAG	D	605	2	-	2/6/23/26	0/1/1/1
13	NAG	E	607	2	-	0/6/23/26	0/1/1/1
13	NAG	F	604	2	-	2/6/23/26	0/1/1/1
13	NAG	F	606	2	-	2/6/23/26	0/1/1/1
13	NAG	A	701	1	-	2/6/23/26	0/1/1/1
13	NAG	D	604	2	-	2/6/23/26	0/1/1/1
13	NAG	D	608	2	-	4/6/23/26	0/1/1/1
13	NAG	E	606	2	-	2/6/23/26	0/1/1/1
13	NAG	F	602	2	-	2/6/23/26	0/1/1/1
13	NAG	D	603	2	-	0/6/23/26	0/1/1/1
13	NAG	B	701	1	-	2/6/23/26	0/1/1/1
13	NAG	F	605	2	-	2/6/23/26	0/1/1/1
13	NAG	D	606	2	-	2/6/23/26	0/1/1/1
13	NAG	E	608	2	-	4/6/23/26	0/1/1/1
13	NAG	F	601	2	-	2/6/23/26	0/1/1/1
13	NAG	E	604	2	-	2/6/23/26	0/1/1/1
13	NAG	E	605	2	-	2/6/23/26	0/1/1/1
13	NAG	F	603	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	E	603	NAG	C1-O5-C5	2.12	115.02	112.19
13	F	603	NAG	C1-O5-C5	2.12	115.02	112.19
13	D	603	NAG	C1-O5-C5	2.11	115.02	112.19

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	701	NAG	C1-C2-N2-C7
13	D	608	NAG	C4-C5-C6-O6
13	E	608	NAG	C4-C5-C6-O6
13	F	608	NAG	C4-C5-C6-O6
13	D	602	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	601	NAG	1	0
13	E	603	NAG	1	0
13	D	601	NAG	1	0
13	D	603	NAG	1	0
13	F	601	NAG	1	0
13	F	603	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

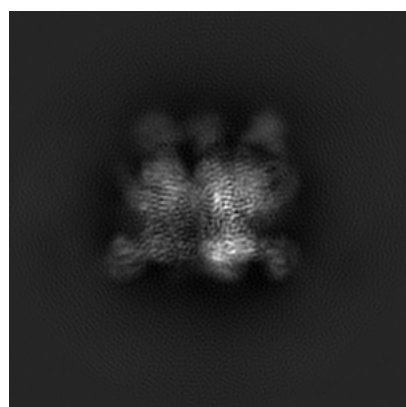
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9038. These allow visual inspection of the internal detail of the map and identification of artifacts.

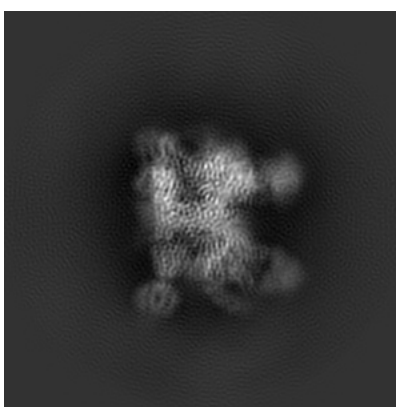
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

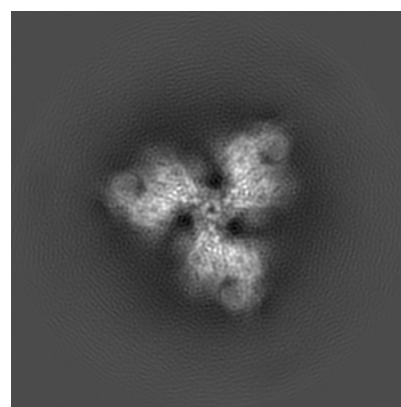
6.1.1 Primary map



X



Y

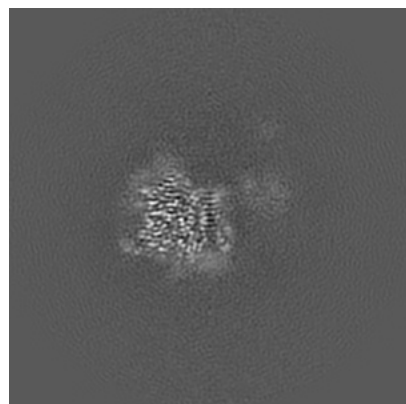


Z

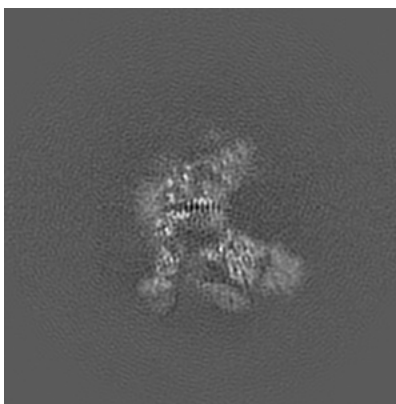
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

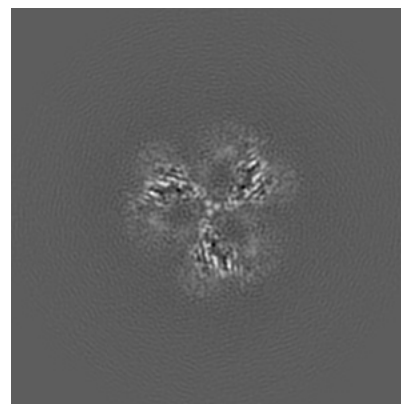
6.2.1 Primary map



X Index: 144



Y Index: 144

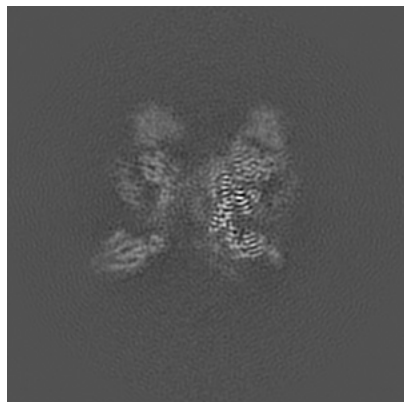


Z Index: 144

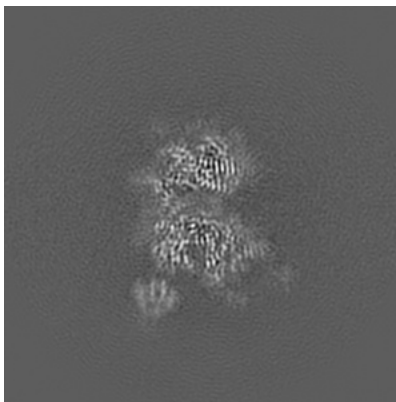
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

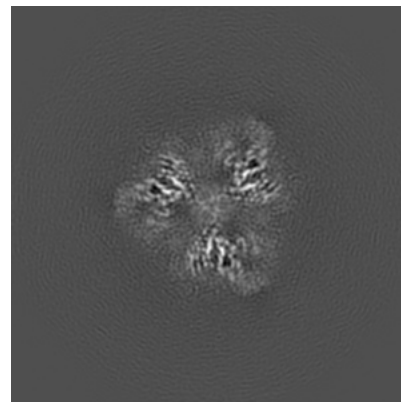
6.3.1 Primary map



X Index: 169



Y Index: 157

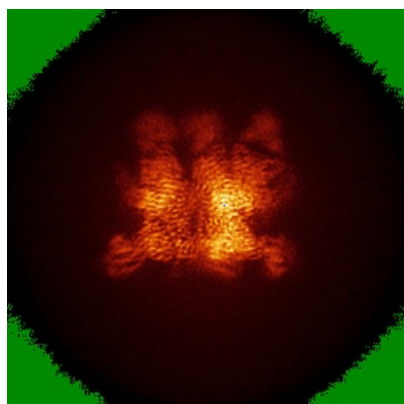


Z Index: 153

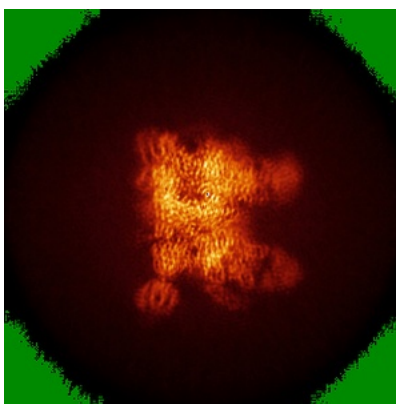
The images above show the largest variance slices of the map in three orthogonal directions.

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

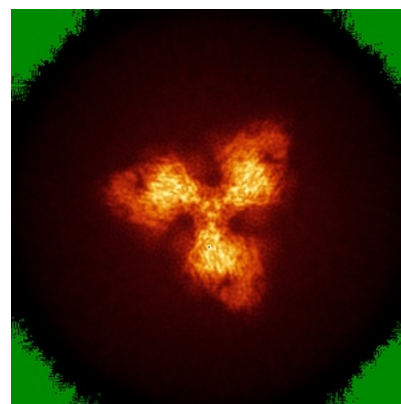
6.4.1 Primary map



X



Y

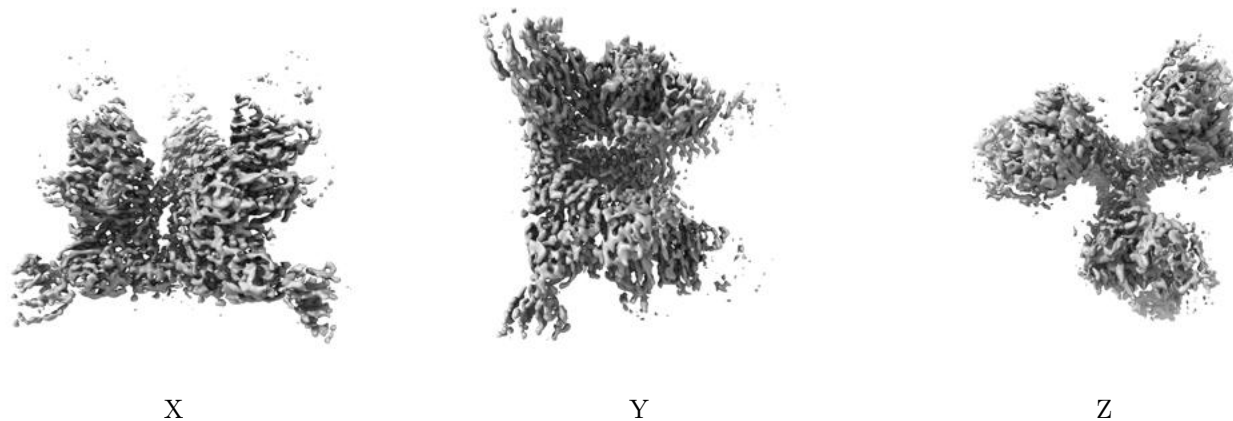


Z

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 0.041. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

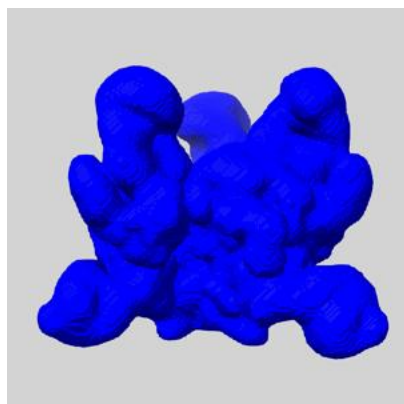
6.6 Mask visualisation [i](#)

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

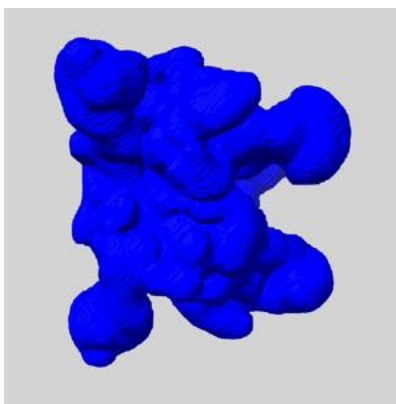
A mask typically either:

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

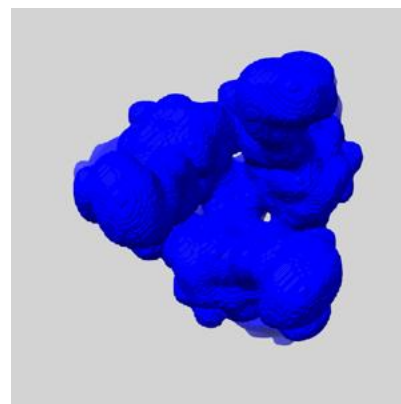
6.6.1 emd_9038_msk_1.map [i](#)



X

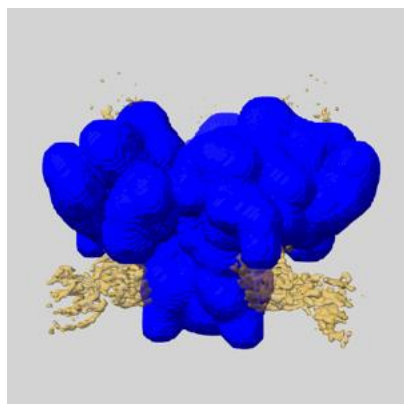


Y

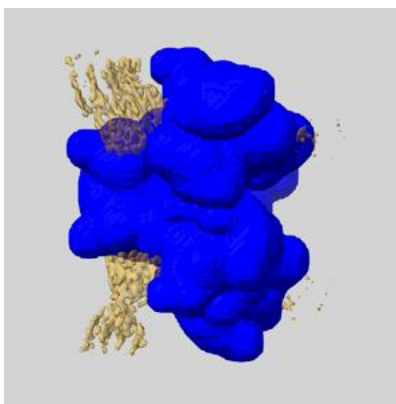


Z

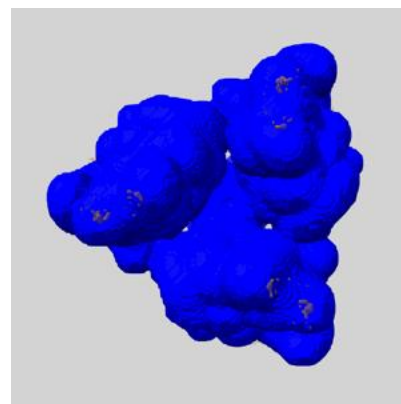
6.6.2 emd_9038_msk_2.map [i](#)



X



Y

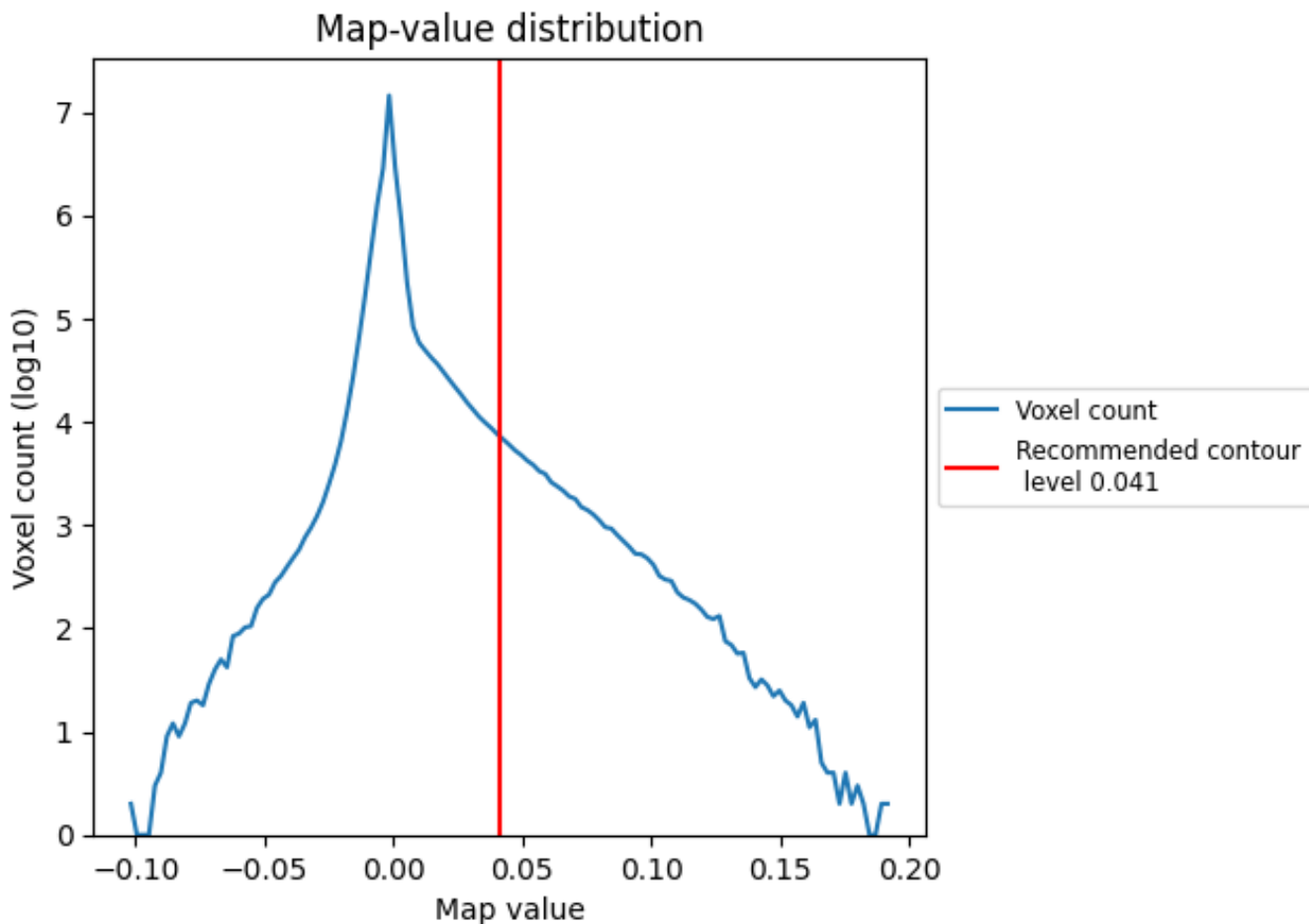


Z

7 Map analysis [i](#)

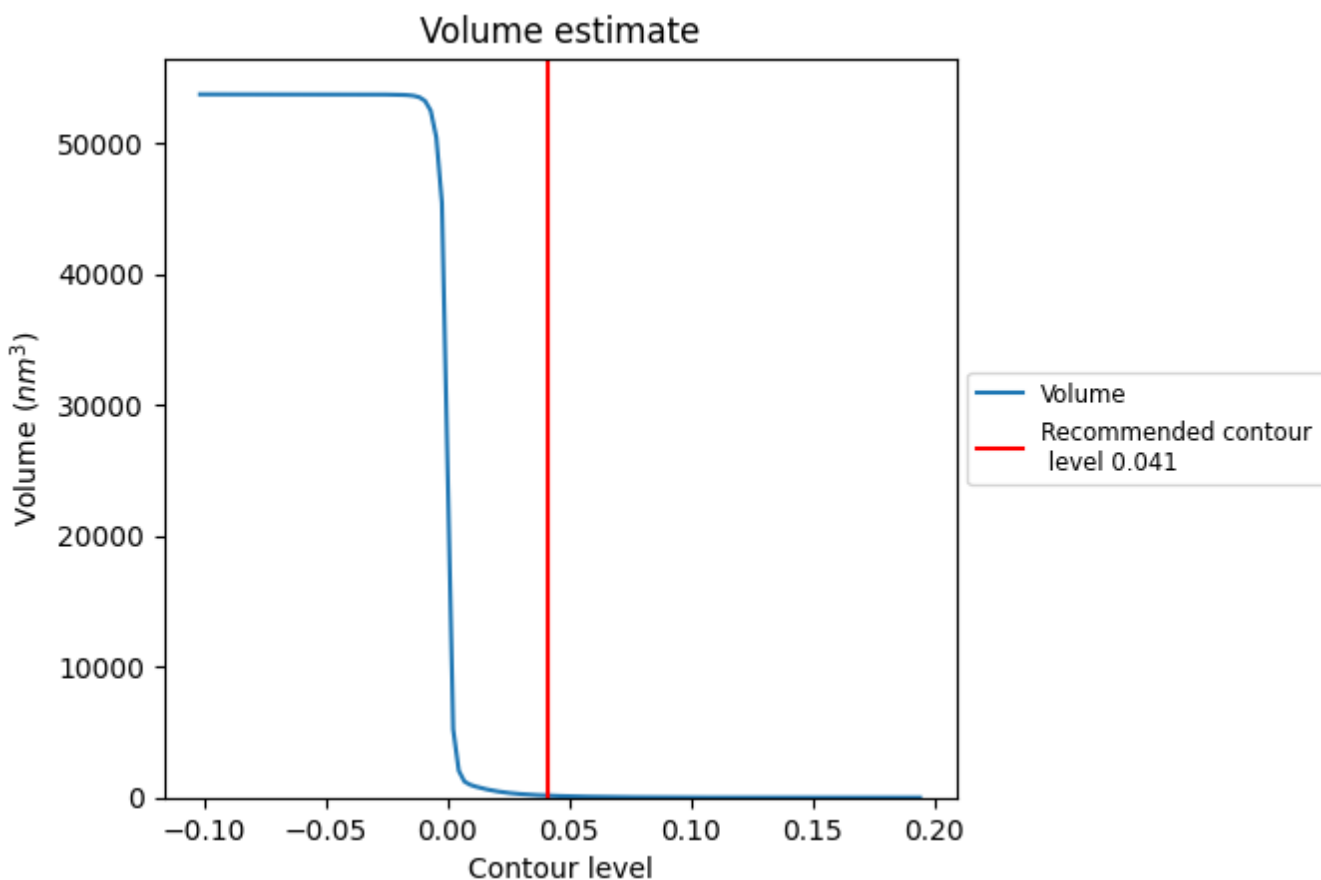
This section contains the results of statistical analysis of the map.

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.

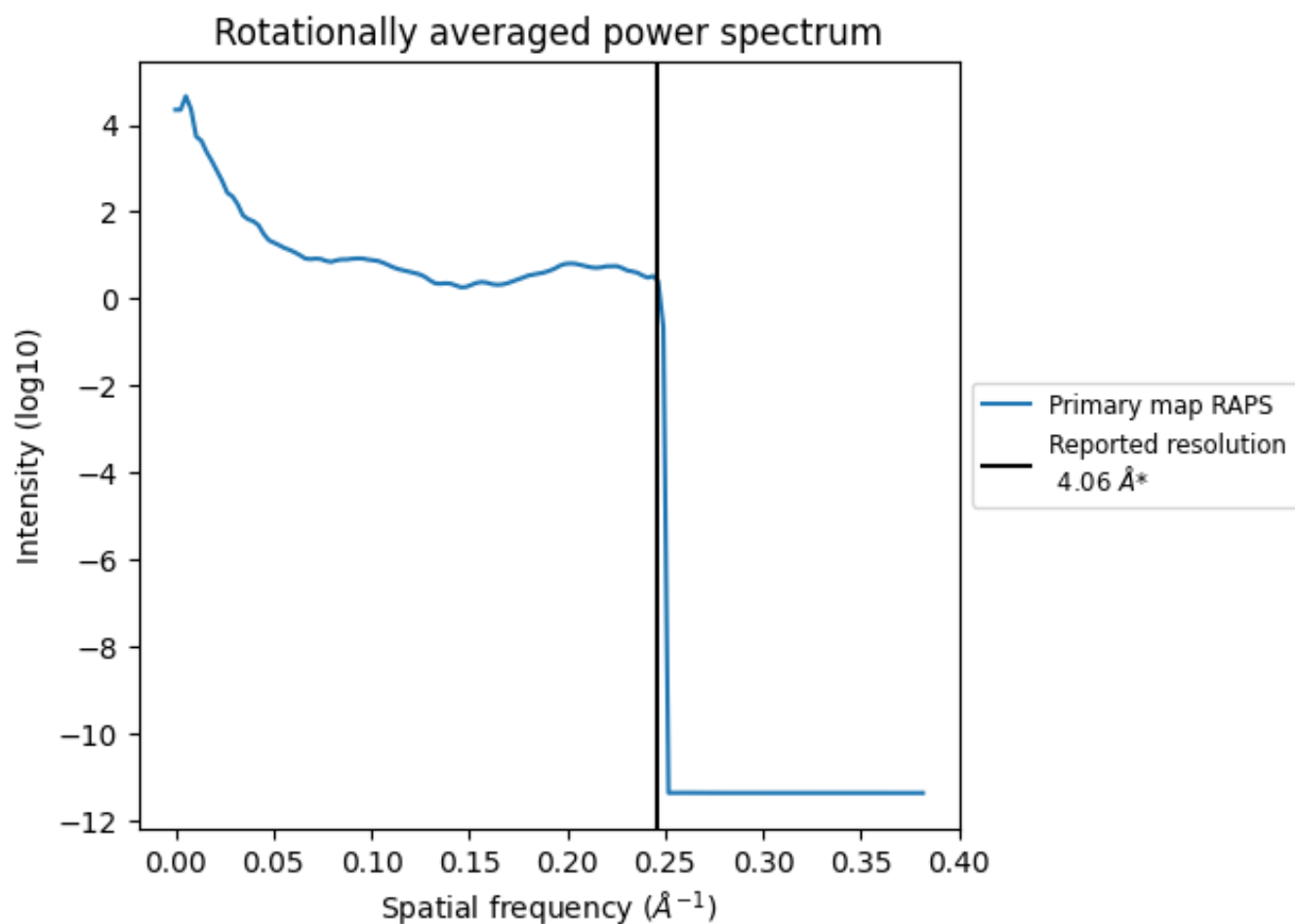
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 138 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 [\(i\)](#)

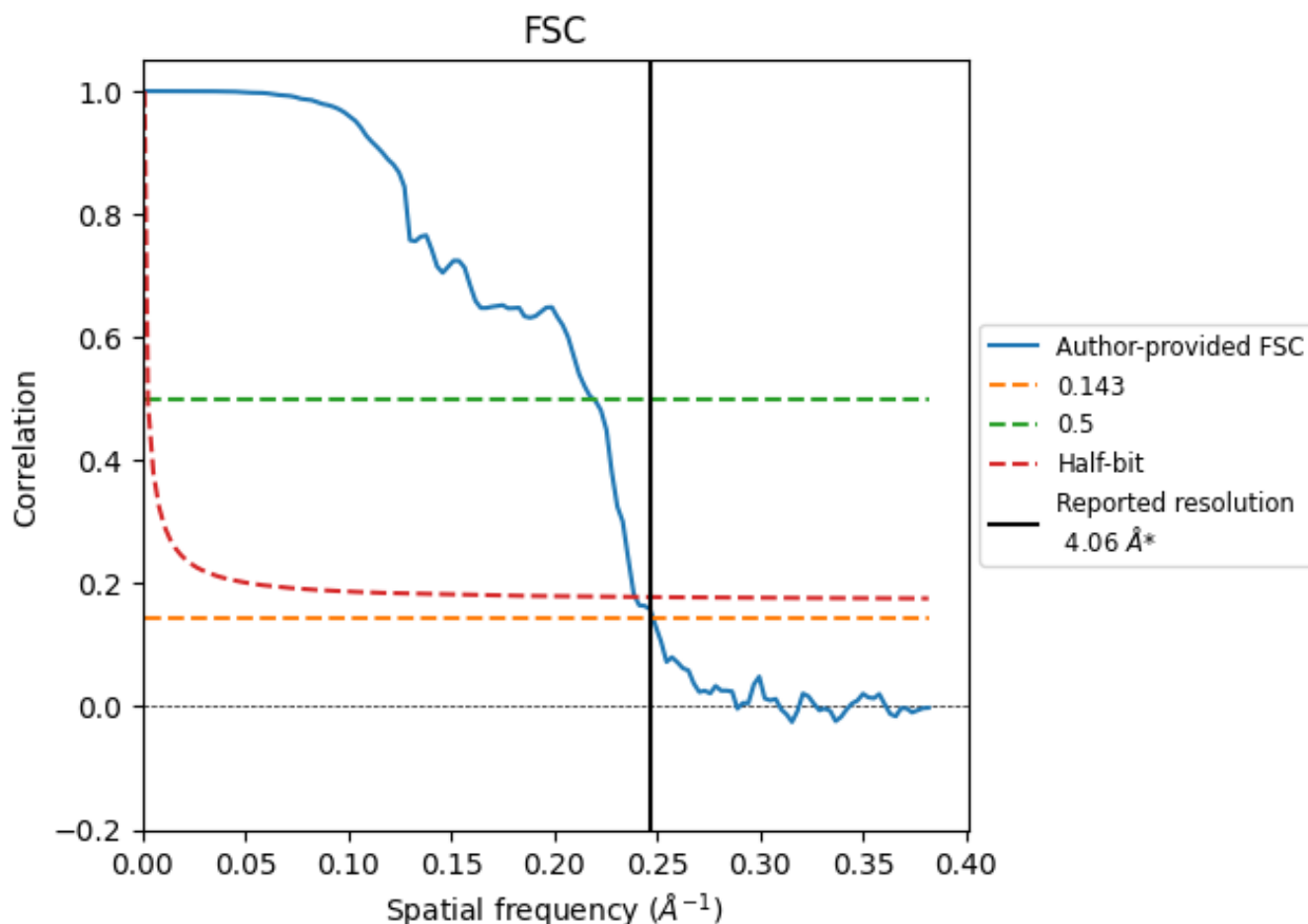


*Reported resolution corresponds to spatial frequency of 0.246 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.246 Å⁻¹

8.2 Resolution estimates [i](#)

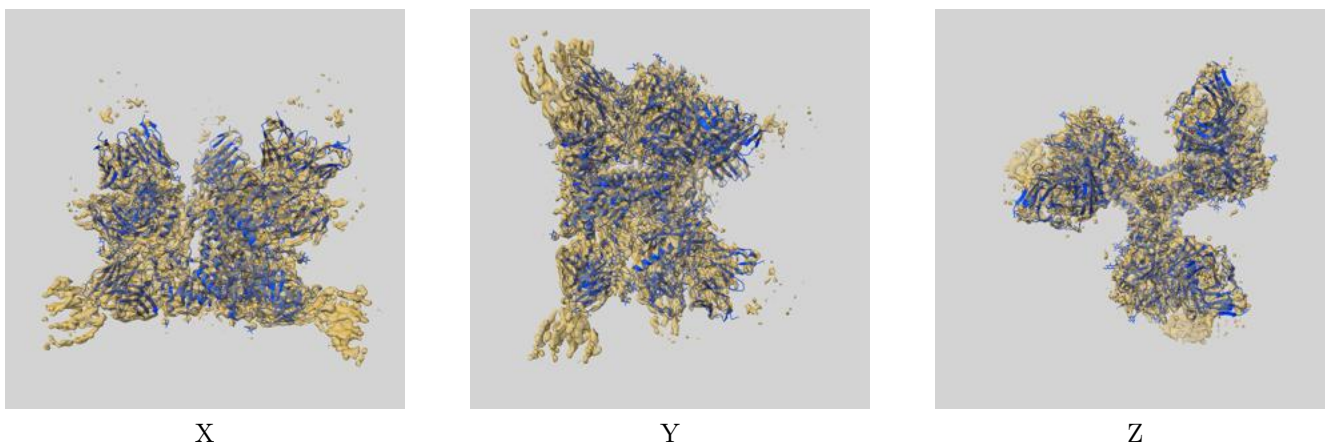
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.06	-	-
Author-provided FSC curve	4.03	4.57	4.18
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

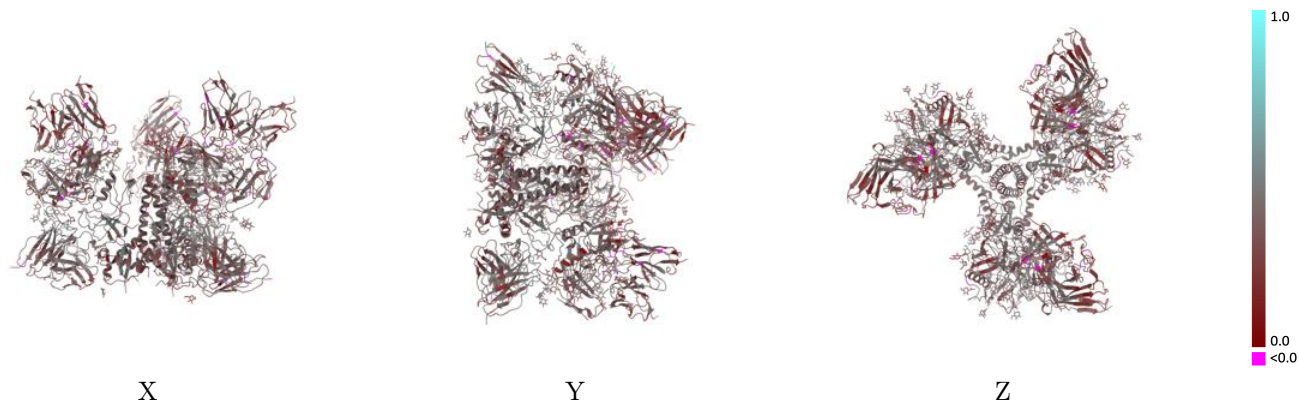
This section contains information regarding the fit between EMDB map EMD-9038 and PDB model 6EDU. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



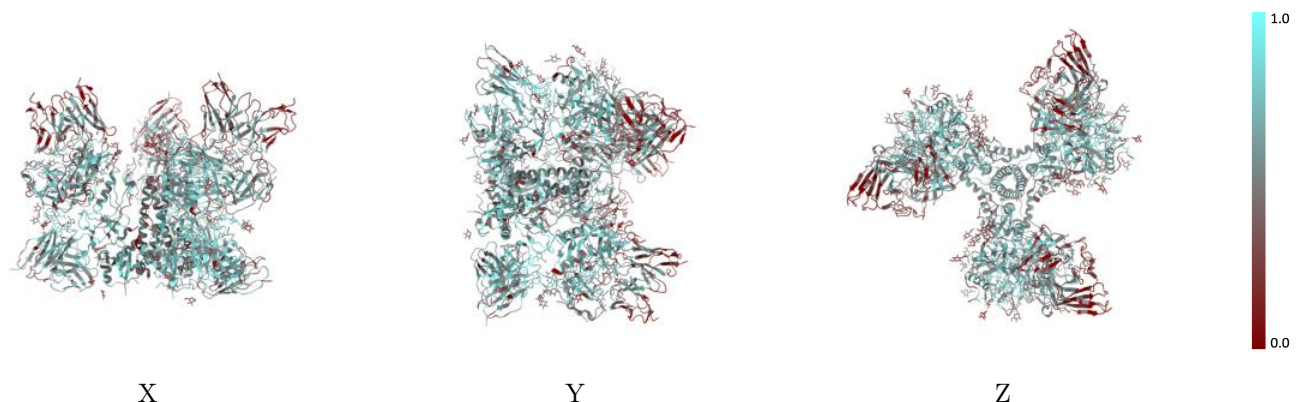
The images above show the 3D surface view of the map at the recommended contour level 0.041 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



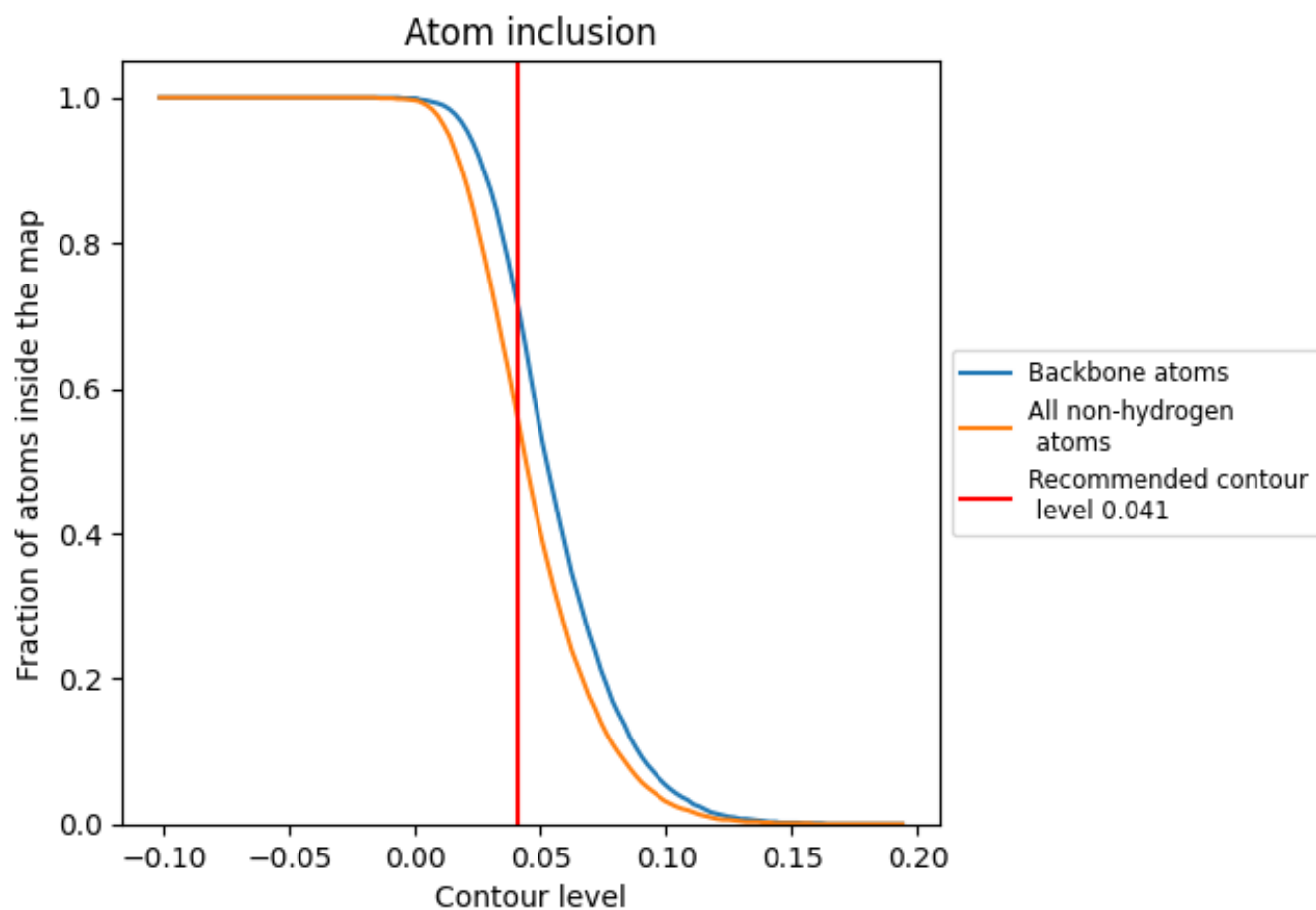
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.041).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 55% 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 (0.041) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.3600
A	 0.5990	 0.3560
B	 0.5830	 0.3420
C	 0.5950	 0.3550
D	 0.5930	 0.3650
E	 0.5960	 0.3650
F	 0.5950	 0.3620
G	 0.6020	 0.4000
H	 0.6120	 0.4030
I	 0.6150	 0.4040
J	 0.4060	 0.3030
K	 0.3590	 0.3190
L	 0.4050	 0.3000
M	 0.3830	 0.3230
N	 0.4160	 0.3060
O	 0.3670	 0.3160
P	 0.6290	 0.3790
Q	 0.5970	 0.3890
R	 0.6230	 0.3870
S	 0.5970	 0.3900
T	 0.6280	 0.3890
U	 0.5840	 0.3830
V	 0.4290	 0.3140
W	 0.4290	 0.3080
X	 0.4290	 0.3270
Y	 0.2500	 0.3640
Z	 0.3110	 0.3200
a	 0.5250	 0.4100
b	 0.5640	 0.3790
c	 0.5360	 0.3710
d	 0.2860	 0.2420
e	 0.5710	 0.3120
f	 0.2500	 0.3960
g	 0.2460	 0.3030
h	 0.5410	 0.4170



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Chain	Atom inclusion	Q-score
i	 0.5380	 0.3850
j	 0.5360	 0.3640
k	 0.2860	 0.2060
l	 0.6430	 0.3020
m	 0.2500	 0.3750
n	 0.2620	 0.3090
o	 0.5900	 0.3970
p	 0.5130	 0.4020
q	 0.5360	 0.3660
r	 0.2500	 0.1720
s	 0.6430	 0.2760
t	 0.5810	 0.4290
u	 0.6480	 0.4360
v	 0.6290	 0.4310