



## wwPDB EM Validation Summary Report ⓘ

May 4, 2026 – 01:29 PM EDT

PDB ID : 9Z9L / pdb\_00009z9l  
EMDB ID : EMD-73949  
Title : Q23.MD39 in Complex with Fabs from antibodies CH01 and 35O22  
Authors : Lin, Z.J.; Cui, J.; Du, J.; Habib, R.; Kulp, D.; Pallesen, J.  
Deposited on : 2025-11-18  
Resolution : 3.49 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

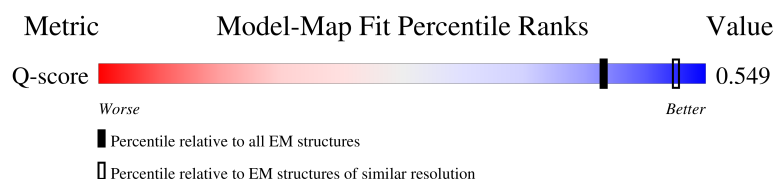
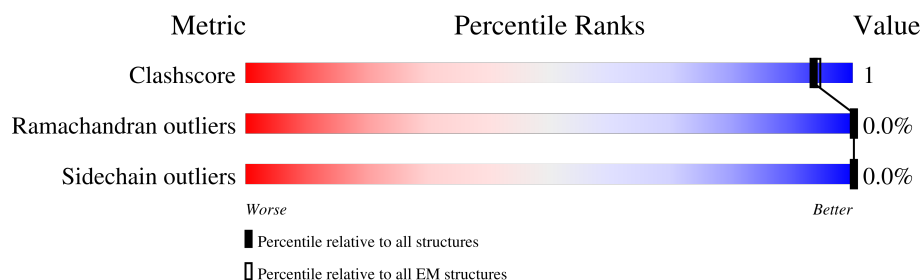
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 3.49 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.




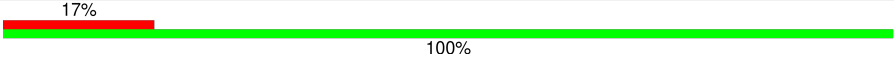


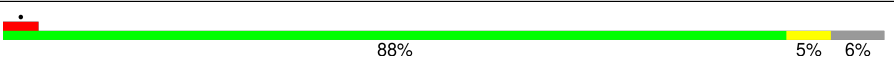
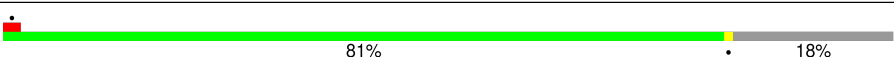
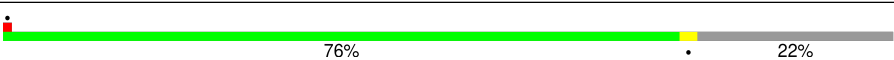
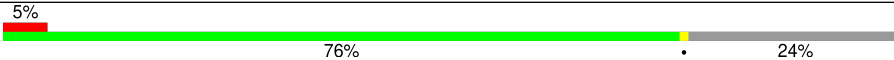
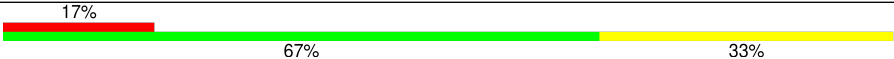
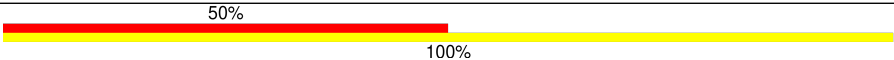

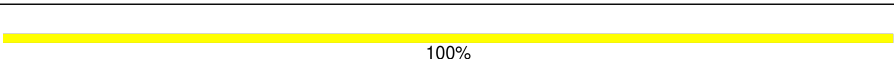
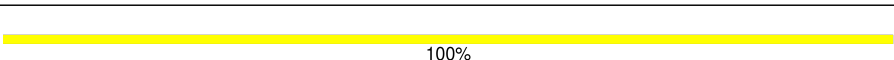
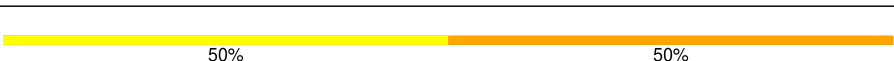
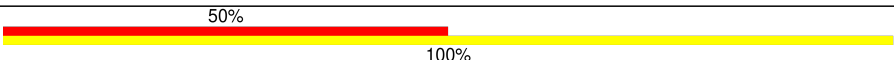
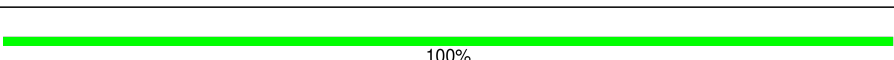
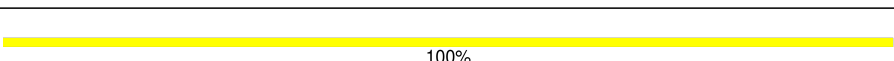

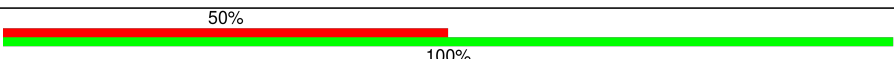

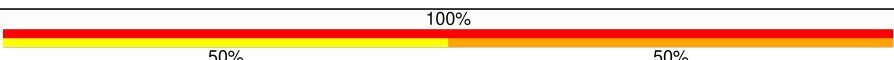
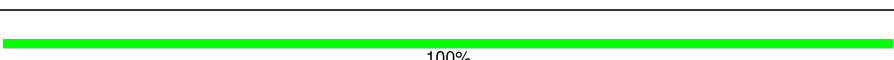

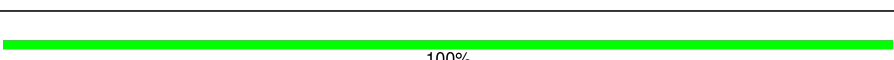

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13600 ( 2.99 - 3.99 )

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

Mol	Chain	Length	Quality of chain
1	E	243	
1	H	243	
2	F	216	
2	L	216	

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Mol	Chain	Length	Quality of chain
3	J	108	
4	K	133	
5	A	467	
5	C	467	
5	G	467	
6	B	153	
6	D	153	
6	I	153	
7	M	6	
8	N	2	
8	O	2	
8	P	2	
8	R	2	
8	T	2	
8	a	2	
8	b	2	
8	d	2	
8	e	2	
8	f	2	
8	g	2	
8	i	2	
8	k	2	
8	m	2	
8	n	2	
8	o	2	

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Mol	Chain	Length	Quality of chain
8	p	2	
8	q	2	
9	Q	7	
10	S	3	
10	U	3	
10	c	3	
11	V	3	
12	W	4	
13	X	7	
14	Y	7	
14	h	7	
15	Z	5	
15	l	5	
16	j	5	
17	r	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	NAG	W	1	-	-	X	-
12	NAG	W	2	-	-	X	-

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 20495 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 Antibody 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	130	Total	C	N	O	S	0	0
			1015	649	171	190	5		
1	H	130	Total	C	N	O	S	0	0
			1015	649	171	190	5		

- Molecule 2 is a protein called Antibody 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	110	Total	C	N	O	S	0	0
			836	525	138	167	6		
2	L	100	Total	C	N	O	S	0	0
			769	487	125	153	4		

- Molecule 3 is a protein called Antibody CH01 variable domain light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	105	Total	C	N	O	S	0	0
			796	505	137	152	2		

- Molecule 4 is a protein called Antibody CH01 variable domain heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	133	Total	C	N	O	S	0	0
			1049	664	184	197	4		

- Molecule 5 is a protein called Q23.MD39 Surface protein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	440	Total	C	N	O	S	0	0
			3486	2200	613	647	26		
5	C	441	Total	C	N	O	S	1	0
			3504	2214	615	649	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	438	Total	C	N	O	S	0	0
			3469	2191	610	642	26		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLU	THR	engineered mutation	UNP O55774
A	271	ILE	THR	engineered mutation	UNP O55774
A	304	VAL	ARG	engineered mutation	UNP O55774
A	319	TYR	ALA	engineered mutation	UNP O55774
A	363	GLN	ASN	engineered mutation	UNP O55774
A	473	SER	GLY	engineered mutation	UNP O55774
A	501	CYS	ALA	engineered mutation	UNP O55774
C	106	GLU	THR	engineered mutation	UNP O55774
C	271	ILE	THR	engineered mutation	UNP O55774
C	304	VAL	ARG	engineered mutation	UNP O55774
C	319	TYR	ALA	engineered mutation	UNP O55774
C	363	GLN	ASN	engineered mutation	UNP O55774
C	473	SER	GLY	engineered mutation	UNP O55774
C	501	CYS	ALA	engineered mutation	UNP O55774
G	106	GLU	THR	engineered mutation	UNP O55774
G	271	ILE	THR	engineered mutation	UNP O55774
G	304	VAL	ARG	engineered mutation	UNP O55774
G	319	TYR	ALA	engineered mutation	UNP O55774
G	363	GLN	ASN	engineered mutation	UNP O55774
G	473	SER	GLY	engineered mutation	UNP O55774
G	501	CYS	ALA	engineered mutation	UNP O55774

- Molecule 6 is a protein called Q23.MD39 Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	126	Total	C	N	O	S	0	0
			1012	639	175	193	5		
6	D	120	Total	C	N	O	S	0	0
			973	614	169	185	5		
6	I	117	Total	C	N	O	S	0	0
			946	598	166	177	5		

There are 24 discrepancies between the modelled and reference sequences:

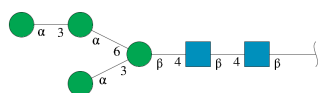
Chain	Residue	Modelled	Actual	Comment	Reference
B	519	SER	PHE	engineered mutation	UNP O55774

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Chain	Residue	Modelled	Actual	Comment	Reference
B	533	ALA	THR	engineered mutation	UNP O55774
B	559	PRO	ILE	engineered mutation	UNP O55774
B	561	PRO	ALA	engineered mutation	UNP O55774
B	568	ASP	LEU	engineered mutation	UNP O55774
B	570	HIS	VAL	engineered mutation	UNP O55774
B	585	HIS	ARG	engineered mutation	UNP O55774
B	605	CYS	THR	engineered mutation	UNP O55774
D	519	SER	PHE	engineered mutation	UNP O55774
D	533	ALA	THR	engineered mutation	UNP O55774
D	559	PRO	ILE	engineered mutation	UNP O55774
D	561	PRO	ALA	engineered mutation	UNP O55774
D	568	ASP	LEU	engineered mutation	UNP O55774
D	570	HIS	VAL	engineered mutation	UNP O55774
D	585	HIS	ARG	engineered mutation	UNP O55774
D	605	CYS	THR	engineered mutation	UNP O55774
I	519	SER	PHE	engineered mutation	UNP O55774
I	533	ALA	THR	engineered mutation	UNP O55774
I	559	PRO	ILE	engineered mutation	UNP O55774
I	561	PRO	ALA	engineered mutation	UNP O55774
I	568	ASP	LEU	engineered mutation	UNP O55774
I	570	HIS	VAL	engineered mutation	UNP O55774
I	585	HIS	ARG	engineered mutation	UNP O55774
I	605	CYS	THR	engineered mutation	UNP O55774

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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
7	M	6	Total	C	N	O	0	0
			72	40	2	30		

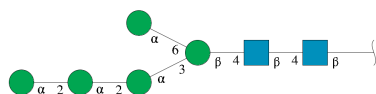
- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	2	Total 28	C 16	N 2	O 10	0	0
8	O	2	Total 28	C 16	N 2	O 10	0	0
8	P	2	Total 28	C 16	N 2	O 10	0	0
8	R	2	Total 28	C 16	N 2	O 10	0	0
8	T	2	Total 28	C 16	N 2	O 10	0	0
8	a	2	Total 28	C 16	N 2	O 10	0	0
8	b	2	Total 28	C 16	N 2	O 10	0	0
8	d	2	Total 28	C 16	N 2	O 10	0	0
8	e	2	Total 28	C 16	N 2	O 10	0	0
8	f	2	Total 28	C 16	N 2	O 10	0	0
8	g	2	Total 28	C 16	N 2	O 10	0	0
8	i	2	Total 28	C 16	N 2	O 10	0	0
8	k	2	Total 28	C 16	N 2	O 10	0	0
8	m	2	Total 28	C 16	N 2	O 10	0	0
8	n	2	Total 28	C 16	N 2	O 10	0	0
8	o	2	Total 28	C 16	N 2	O 10	0	0
8	p	2	Total 28	C 16	N 2	O 10	0	0
8	q	2	Total 28	C 16	N 2	O 10	0	0

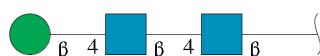
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





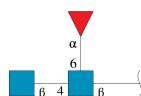
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 10 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.



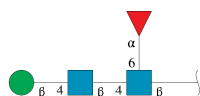
Mol	Chain	Residues	Atoms				AltConf	Trace
10	S	3	Total	C	N	O	0	0
			39	22	2	15		
10	U	3	Total	C	N	O	0	0
			39	22	2	15		
10	c	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 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.



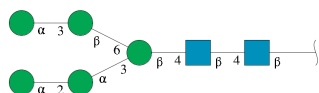
Mol	Chain	Residues	Atoms				AltConf	Trace
11	V	3	Total	C	N	O	0	0
			38	22	2	14		

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



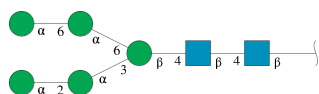
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-beta-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.



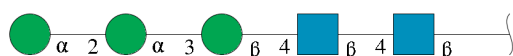
Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
14	Y	7	Total	C	N	O	0	0
			83	46	2	35		
14	h	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 15 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.



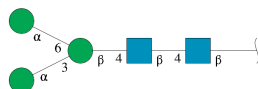
Mol	Chain	Residues	Atoms				AltConf	Trace
15	Z	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				AltConf	Trace
15	1	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 16 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
16	j	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 17 is an oligosaccharide called 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
17	r	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

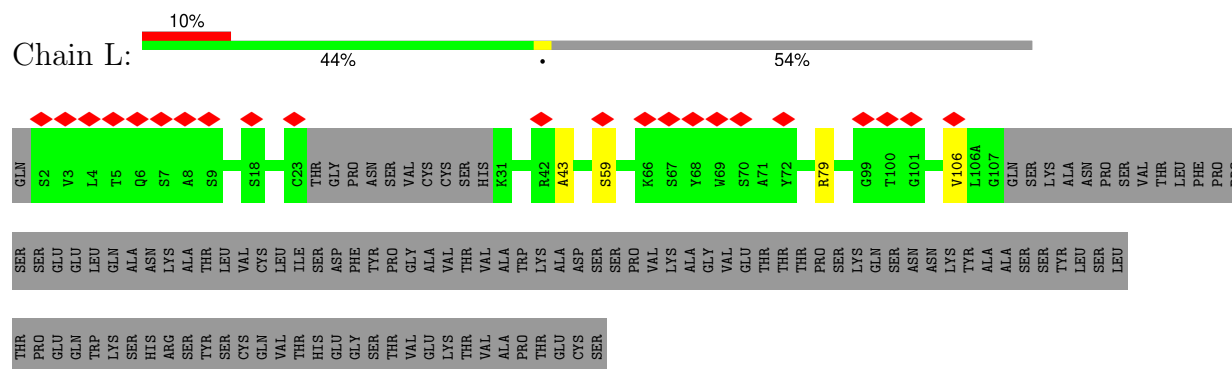
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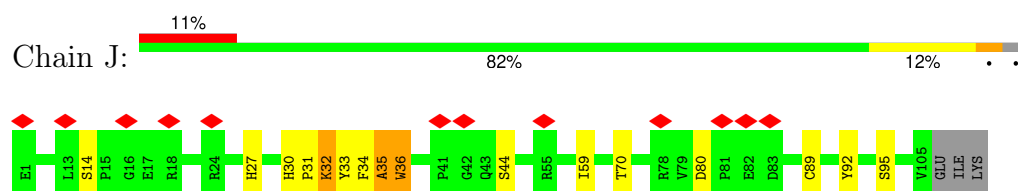
Mol	Chain	Residues	Atoms				AltConf
18	C	1	Total	C	N	O	0
			14	8	1	5	
18	G	1	Total	C	N	O	0
			14	8	1	5	
18	G	1	Total	C	N	O	0
			14	8	1	5	
18	G	1	Total	C	N	O	0
			14	8	1	5	
18	G	1	Total	C	N	O	0
			14	8	1	5	
18	G	1	Total	C	N	O	0
			14	8	1	5	



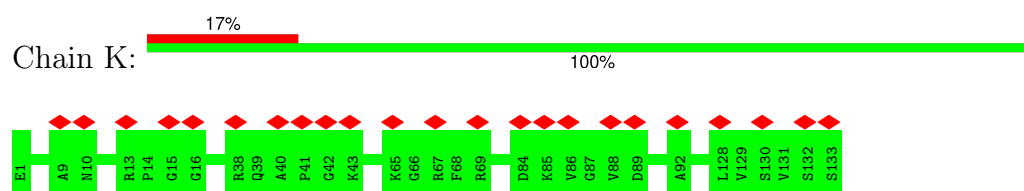
- Molecule 2: Antibody 35O22 Fab light chain



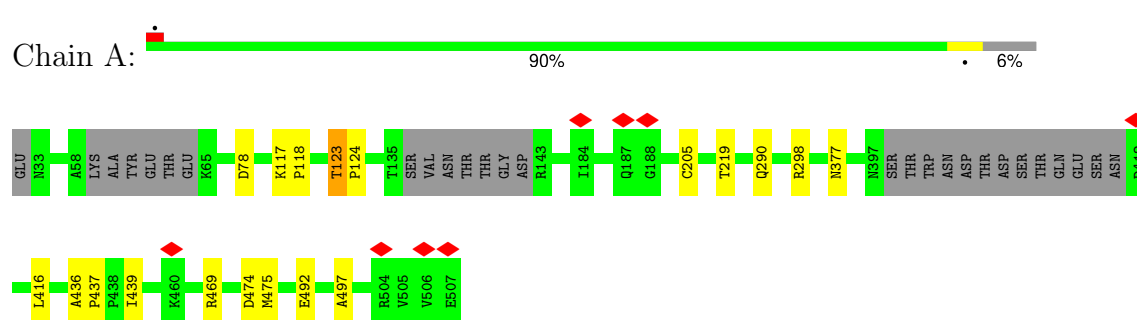
- Molecule 3: Antibody CH01 variable domain light chain



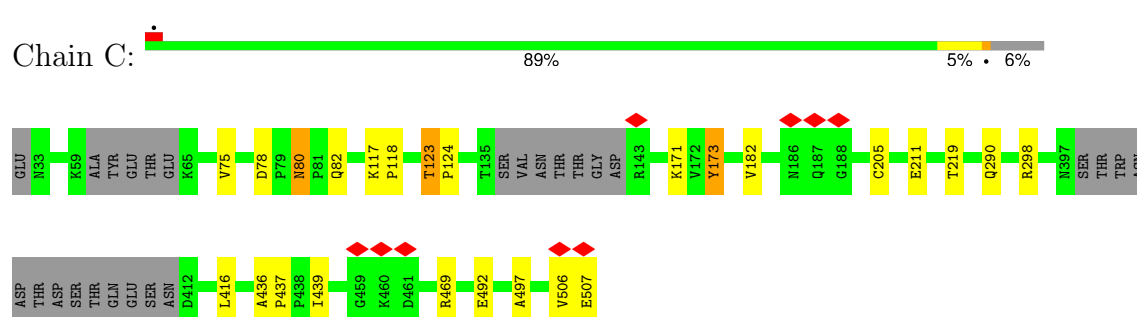
- Molecule 4: Antibody CH01 variable domain heavy chain



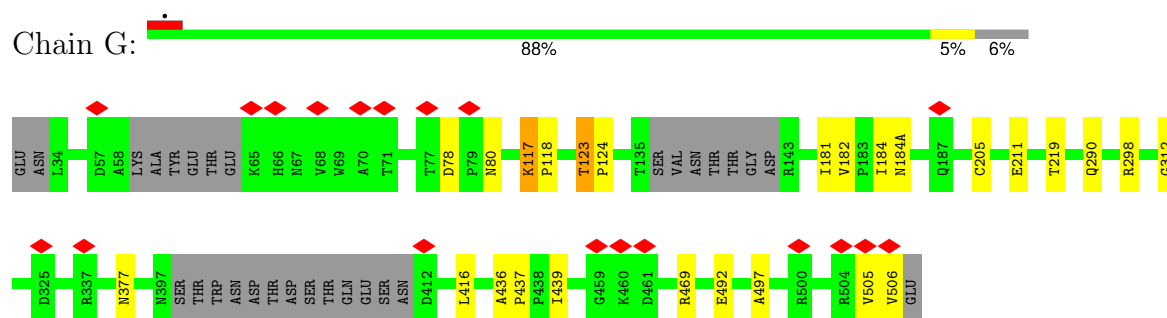
- Molecule 5: Q23.MD39 Surface protein gp120



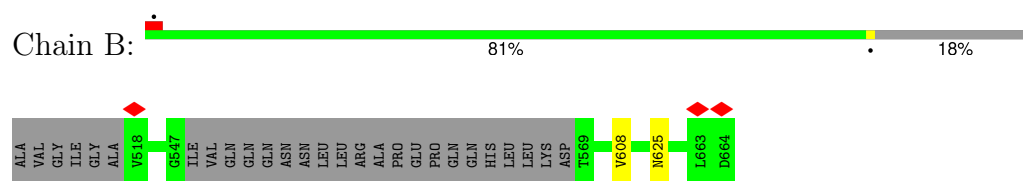
- Molecule 5: Q23.MD39 Surface protein gp120



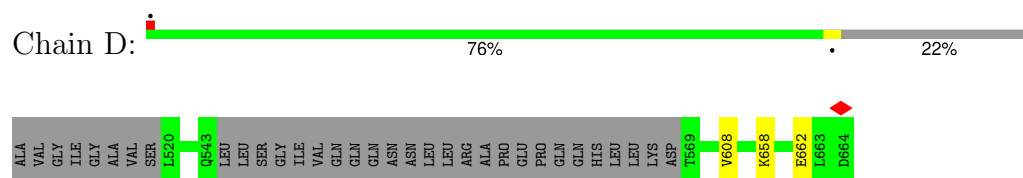
- Molecule 5: Q23.MD39 Surface protein gp120



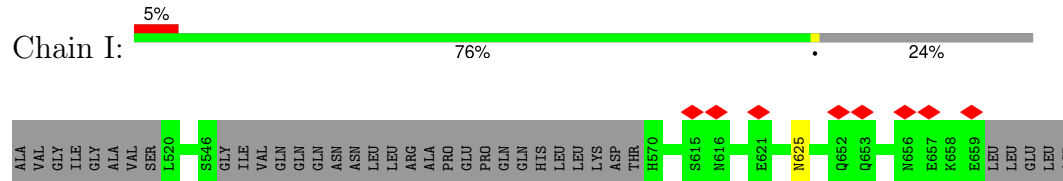
- Molecule 6: Q23.MD39 Transmembrane protein gp41



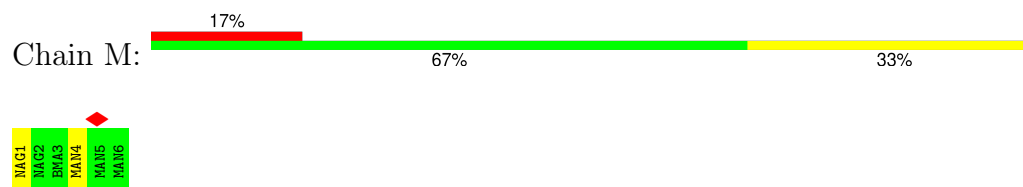
- Molecule 6: Q23.MD39 Transmembrane protein gp41



- Molecule 6: Q23.MD39 Transmembrane protein gp41



- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



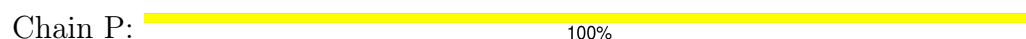




- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 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 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 d:  100%



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

Chain e:  50% 50%



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

Chain f:  50% 100%



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

Chain g:  100%



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

Chain i:  100% 50%



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

Chain k:  100%



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

Chain m:  50% 50%



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

Chain n:  100%



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

Chain o:  50% 50% 50%



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

Chain p:  50% 50% 100%



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

Chain q:  50% 50% 50%



- Molecule 9: alpha-D-mannopyranose-(1-2)-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

Chain Q:  57% 43% 43% 14%



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



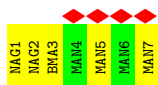
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  71% 29%



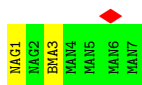
- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  29% 57% 71%



- Molecule 14: alpha-D-mannopyranose-(1-2)-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

Chain h:  14% 71% 29%




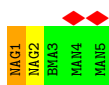
- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  20% 100%




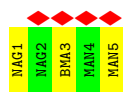
- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  40% 60% 20% 20%

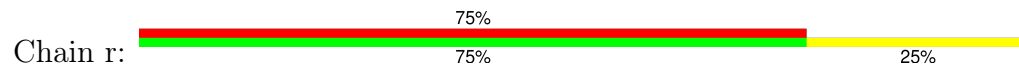


- Molecule 16: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  40% 80% 60%



- Molecule 17: 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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248110	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	16.767	Depositor
Minimum map value	-0.116	Depositor
Average map value	-0.052	Depositor
Map value standard deviation	0.387	Depositor
Recommended contour level	4.29	Depositor
Map size ( $\text{\AA}$ )	378.4, 378.4, 378.4	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.86, 0.86, 0.86	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, BMA, 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	E	0.69	0/1043	0.93	5/1416 (0.4%)
1	H	0.65	0/1043	0.91	5/1416 (0.4%)
2	F	0.65	0/860	1.07	10/1175 (0.9%)
2	L	0.70	0/790	1.07	6/1077 (0.6%)
3	J	0.78	0/819	1.16	13/1112 (1.2%)
4	K	0.70	0/1077	0.91	0/1455
5	A	0.69	0/3560	1.01	26/4835 (0.5%)
5	C	0.68	0/3582	1.01	36/4864 (0.7%)
5	G	0.68	0/3543	1.01	37/4812 (0.8%)
6	B	0.66	0/1031	0.70	2/1396 (0.1%)
6	D	0.66	0/992	0.66	2/1343 (0.1%)
6	I	0.64	0/965	0.68	0/1307
All	All	0.68	0/19305	0.96	142/26208 (0.5%)

There are no bond length outliers.

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	469	ARG	CA-C-N	8.16	128.36	119.87
5	A	469	ARG	C-N-CA	8.16	128.36	119.87
5	G	492	GLU	CA-C-N	8.16	127.88	119.56
5	G	492	GLU	C-N-CA	8.16	127.88	119.56
5	C	492	GLU	CA-C-N	8.11	127.83	119.56

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	E	1015	0	985	1	0
1	H	1015	0	985	0	0
2	F	836	0	785	0	0
2	L	769	0	727	0	0
3	J	796	0	766	13	0
4	K	1049	0	980	0	0
5	A	3486	0	3432	5	0
5	C	3504	0	3455	5	0
5	G	3469	0	3422	5	0
6	B	1012	0	986	1	0
6	D	973	0	942	1	0
6	I	946	0	921	1	0
7	M	72	0	61	0	0
8	N	28	0	25	0	0
8	O	28	0	25	0	0
8	P	28	0	25	0	0
8	R	28	0	25	0	0
8	T	28	0	25	1	0
8	a	28	0	25	0	0
8	b	28	0	25	0	0
8	d	28	0	25	0	0
8	e	28	0	25	0	0
8	f	28	0	25	0	0
8	g	28	0	25	0	0
8	i	28	0	25	2	0
8	k	28	0	25	0	0
8	m	28	0	25	0	0
8	n	28	0	25	0	0
8	o	28	0	25	0	0
8	p	28	0	25	0	0
8	q	28	0	25	0	0
9	Q	83	0	70	1	0
10	S	39	0	34	0	0
10	U	39	0	34	0	0
10	c	39	0	34	0	0
11	V	38	0	34	5	0
12	W	49	0	43	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	X	83	0	70	0	0
14	Y	83	0	70	3	0
14	h	83	0	70	0	0
15	Z	61	0	52	1	0
15	l	61	0	52	1	0
16	j	61	0	52	1	0
17	r	50	0	43	0	0
18	A	98	0	91	1	0
18	B	28	0	26	0	0
18	C	42	0	39	0	0
18	D	28	0	26	0	0
18	G	70	0	65	1	0
18	I	14	0	13	0	0
All	All	20495	0	19815	52	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 1.

The worst 5 of 52 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)
11:V:2:NAG:O7	11:V:2:NAG:C3	2.25	0.83
12:W:1:NAG:H61	12:W:2:NAG:N2	1.96	0.81
18:A:602:NAG:H81	9:Q:1:NAG:H62	1.65	0.78
3:J:27:HIS:O	3:J:70:THR:HG22	1.86	0.75
3:J:36:TRP:CZ3	3:J:89:CYS:HB3	2.22	0.74

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	128/243 (53%)	127 (99%)	1 (1%)	0	100	100
1	H	128/243 (53%)	127 (99%)	1 (1%)	0	100	100
2	F	108/216 (50%)	106 (98%)	2 (2%)	0	100	100
2	L	96/216 (44%)	94 (98%)	1 (1%)	1 (1%)	12	44
3	J	103/108 (95%)	100 (97%)	3 (3%)	0	100	100
4	K	131/133 (98%)	131 (100%)	0	0	100	100
5	A	432/467 (92%)	427 (99%)	5 (1%)	0	100	100
5	C	434/467 (93%)	424 (98%)	10 (2%)	0	100	100
5	G	430/467 (92%)	421 (98%)	9 (2%)	0	100	100
6	B	122/153 (80%)	122 (100%)	0	0	100	100
6	D	116/153 (76%)	116 (100%)	0	0	100	100
6	I	113/153 (74%)	113 (100%)	0	0	100	100
All	All	2341/3019 (78%)	2308 (99%)	32 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	106	VAL

### 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	E	108/206 (52%)	108 (100%)	0	100	100
1	H	108/206 (52%)	108 (100%)	0	100	100
2	F	96/189 (51%)	95 (99%)	1 (1%)	68	75
2	L	87/189 (46%)	87 (100%)	0	100	100
3	J	84/87 (97%)	84 (100%)	0	100	100
4	K	107/107 (100%)	107 (100%)	0	100	100
5	A	394/419 (94%)	394 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	396/419 (94%)	396 (100%)	0	100	100
5	G	392/419 (94%)	392 (100%)	0	100	100
6	B	110/132 (83%)	110 (100%)	0	100	100
6	D	105/132 (80%)	105 (100%)	0	100	100
6	I	102/132 (77%)	102 (100%)	0	100	100
All	All	2089/2637 (79%)	2088 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	54	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
6	I	575	GLN
6	I	616	ASN
5	G	356	ASN
5	C	425	ASN
5	G	330	HIS

### 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 ⓘ

105 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	$\# Z  > 2$
7	NAG	M	1	7,5	14,14,15	0.49	0	17,19,21	1.12	2 (11%)
7	NAG	M	2	7	14,14,15	0.45	0	17,19,21	0.64	0
7	BMA	M	3	7	11,11,12	0.62	0	15,15,17	0.61	0
7	MAN	M	4	7	11,11,12	0.44	0	15,15,17	1.07	2 (13%)
7	MAN	M	5	7	11,11,12	0.37	0	15,15,17	0.65	0
7	MAN	M	6	7	11,11,12	0.47	0	15,15,17	0.57	0
8	NAG	N	1	8,5	14,14,15	0.49	0	17,19,21	1.04	2 (11%)
8	NAG	N	2	8	14,14,15	0.44	0	17,19,21	0.97	1 (5%)
8	NAG	O	1	8,5	14,14,15	0.55	0	17,19,21	1.28	2 (11%)
8	NAG	O	2	8	14,14,15	0.35	0	17,19,21	0.82	0
8	NAG	P	1	8,5	14,14,15	0.63	0	17,19,21	1.34	1 (5%)
8	NAG	P	2	8	14,14,15	0.37	0	17,19,21	1.02	1 (5%)
9	NAG	Q	1	9,5	14,14,15	0.49	0	17,19,21	1.99	5 (29%)
9	NAG	Q	2	9	14,14,15	0.59	0	17,19,21	1.20	1 (5%)
9	BMA	Q	3	9	11,11,12	0.50	0	15,15,17	1.26	2 (13%)
9	MAN	Q	4	9	11,11,12	0.42	0	15,15,17	0.89	1 (6%)
9	MAN	Q	5	9	11,11,12	0.27	0	15,15,17	0.65	0
9	MAN	Q	6	9	11,11,12	0.19	0	15,15,17	0.64	0
9	MAN	Q	7	9	11,11,12	0.30	0	15,15,17	0.62	0
8	NAG	R	1	8,5	14,14,15	0.74	0	17,19,21	2.04	4 (23%)
8	NAG	R	2	8	14,14,15	0.60	0	17,19,21	1.11	2 (11%)
10	NAG	S	1	5,10	14,14,15	0.56	0	17,19,21	1.68	4 (23%)
10	NAG	S	2	10	14,14,15	0.62	0	17,19,21	0.98	1 (5%)
10	BMA	S	3	10	11,11,12	0.23	0	15,15,17	0.53	0
8	NAG	T	1	8,5	14,14,15	0.63	0	17,19,21	1.51	4 (23%)
8	NAG	T	2	8	14,14,15	0.46	0	17,19,21	1.52	4 (23%)
10	NAG	U	1	5,10	14,14,15	0.40	0	17,19,21	0.49	0
10	NAG	U	2	10	14,14,15	0.41	0	17,19,21	0.50	0
10	BMA	U	3	10	11,11,12	0.31	0	15,15,17	0.50	0
11	NAG	V	1	6,11	14,14,15	0.48	0	17,19,21	1.54	3 (17%)
11	NAG	V	2	11	14,14,15	0.35	0	17,19,21	0.71	0
11	FUC	V	3	11	10,10,11	0.34	0	14,14,16	0.87	0
12	NAG	W	1	6,12	14,14,15	0.62	0	17,19,21	1.39	4 (23%)
12	NAG	W	2	12	14,14,15	0.44	0	17,19,21	0.96	1 (5%)
12	BMA	W	3	12	11,11,12	0.25	0	15,15,17	0.61	0
12	FUC	W	4	12	10,10,11	0.51	0	14,14,16	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	NAG	X	1	13,5	14,14,15	0.47	0	17,19,21	1.23	2 (11%)
13	NAG	X	2	13	14,14,15	0.41	0	17,19,21	0.97	0
13	BMA	X	3	13	11,11,12	0.49	0	15,15,17	1.02	1 (6%)
13	MAN	X	4	13	11,11,12	0.37	0	15,15,17	1.11	0
13	MAN	X	5	13	11,11,12	0.30	0	15,15,17	0.57	0
13	BMA	X	6	13	11,11,12	0.28	0	15,15,17	0.72	0
13	MAN	X	7	13	11,11,12	0.24	0	15,15,17	0.77	0
14	NAG	Y	1	14,5	14,14,15	0.53	0	17,19,21	1.91	5 (29%)
14	NAG	Y	2	14	14,14,15	0.91	0	17,19,21	2.38	5 (29%)
14	BMA	Y	3	14	11,11,12	0.57	0	15,15,17	0.69	0
14	MAN	Y	4	14	11,11,12	0.37	0	15,15,17	0.57	0
14	MAN	Y	5	14	11,11,12	0.27	0	15,15,17	0.61	0
14	MAN	Y	6	14	11,11,12	0.28	0	15,15,17	0.81	0
14	MAN	Y	7	14	11,11,12	0.23	0	15,15,17	0.73	0
15	NAG	Z	1	5,15	14,14,15	0.49	0	17,19,21	2.03	5 (29%)
15	NAG	Z	2	15	14,14,15	0.57	0	17,19,21	1.52	4 (23%)
15	BMA	Z	3	15	11,11,12	0.52	0	15,15,17	1.14	1 (6%)
15	MAN	Z	4	15	11,11,12	0.27	0	15,15,17	1.16	0
15	MAN	Z	5	15	11,11,12	0.24	0	15,15,17	0.64	0
8	NAG	a	1	8,5	14,14,15	0.71	0	17,19,21	1.23	3 (17%)
8	NAG	a	2	8	14,14,15	0.50	0	17,19,21	1.06	2 (11%)
8	NAG	b	1	8,5	14,14,15	0.56	0	17,19,21	0.84	0
8	NAG	b	2	8	14,14,15	0.43	0	17,19,21	0.76	0
10	NAG	c	1	5,10	14,14,15	0.52	0	17,19,21	1.23	1 (5%)
10	NAG	c	2	10	14,14,15	0.60	0	17,19,21	1.28	2 (11%)
10	BMA	c	3	10	11,11,12	0.26	0	15,15,17	0.63	0
8	NAG	d	1	8,5	14,14,15	0.55	0	17,19,21	1.34	3 (17%)
8	NAG	d	2	8	14,14,15	0.52	0	17,19,21	1.05	1 (5%)
8	NAG	e	1	8,5	14,14,15	0.64	0	17,19,21	1.67	5 (29%)
8	NAG	e	2	8	14,14,15	0.55	0	17,19,21	0.89	0
8	NAG	f	1	8,5	14,14,15	0.44	0	17,19,21	0.81	0
8	NAG	f	2	8	14,14,15	0.33	0	17,19,21	0.68	0
8	NAG	g	1	8,5	14,14,15	0.34	0	17,19,21	0.77	0
8	NAG	g	2	8	14,14,15	0.39	0	17,19,21	0.84	0
14	NAG	h	1	14,5	14,14,15	0.48	0	17,19,21	1.29	3 (17%)
14	NAG	h	2	14	14,14,15	0.40	0	17,19,21	0.86	0
14	BMA	h	3	14	11,11,12	0.38	0	15,15,17	0.98	1 (6%)
14	MAN	h	4	14	11,11,12	0.35	0	15,15,17	0.95	0
14	MAN	h	5	14	11,11,12	0.30	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	MAN	h	6	14	11,11,12	0.24	0	15,15,17	0.73	0
14	MAN	h	7	14	11,11,12	0.28	0	15,15,17	0.56	0
8	NAG	i	1	8,5	14,14,15	0.42	0	17,19,21	1.20	1 (5%)
8	NAG	i	2	8	14,14,15	0.28	0	17,19,21	0.68	0
16	NAG	j	1	16,5	14,14,15	0.43	0	17,19,21	1.23	1 (5%)
16	NAG	j	2	16	14,14,15	0.30	0	17,19,21	0.69	0
16	BMA	j	3	16	11,11,12	0.27	0	15,15,17	0.66	0
16	MAN	j	4	16	11,11,12	0.23	0	15,15,17	0.63	0
16	MAN	j	5	16	11,11,12	0.22	0	15,15,17	0.59	0
8	NAG	k	1	8,5	14,14,15	0.41	0	17,19,21	0.85	0
8	NAG	k	2	8	14,14,15	0.34	0	17,19,21	0.63	0
15	NAG	l	1	5,15	14,14,15	0.43	0	17,19,21	1.20	2 (11%)
15	NAG	l	2	15	14,14,15	0.43	0	17,19,21	0.92	1 (5%)
15	BMA	l	3	15	11,11,12	0.31	0	15,15,17	0.71	0
15	MAN	l	4	15	11,11,12	0.24	0	15,15,17	0.56	0
15	MAN	l	5	15	11,11,12	0.26	0	15,15,17	0.64	0
8	NAG	m	1	8,5	14,14,15	0.43	0	17,19,21	1.06	2 (11%)
8	NAG	m	2	8	14,14,15	0.34	0	17,19,21	0.74	0
8	NAG	n	1	8,5	14,14,15	0.40	0	17,19,21	0.74	0
8	NAG	n	2	8	14,14,15	0.37	0	17,19,21	0.77	0
8	NAG	o	1	8,5	14,14,15	0.44	0	17,19,21	1.03	1 (5%)
8	NAG	o	2	8	14,14,15	0.37	0	17,19,21	0.77	0
8	NAG	p	1	8,5	14,14,15	0.41	0	17,19,21	1.00	2 (11%)
8	NAG	p	2	8	14,14,15	0.32	0	17,19,21	0.85	1 (5%)
8	NAG	q	1	8,5	14,14,15	0.48	0	17,19,21	0.93	1 (5%)
8	NAG	q	2	8	14,14,15	0.28	0	17,19,21	0.75	0
17	NAG	r	1	17,5	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
17	NAG	r	2	17	14,14,15	0.44	0	17,19,21	0.91	0
17	BMA	r	3	17	11,11,12	0.35	0	15,15,17	0.71	0
17	MAN	r	4	17	11,11,12	0.20	0	15,15,17	0.62	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
7	NAG	M	1	7,5	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	1/6/23/26	0/1/1/1
7	BMA	M	3	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	M	4	7	-	0/2/19/22	0/1/1/1
7	MAN	M	5	7	-	0/2/19/22	0/1/1/1
7	MAN	M	6	7	-	0/2/19/22	0/1/1/1
8	NAG	N	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	N	2	8	-	1/6/23/26	0/1/1/1
8	NAG	O	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	1/6/23/26	0/1/1/1
8	NAG	P	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	1/6/23/26	0/1/1/1
9	NAG	Q	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	1/6/23/26	0/1/1/1
9	BMA	Q	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Q	4	9	-	0/2/19/22	0/1/1/1
9	MAN	Q	5	9	-	0/2/19/22	0/1/1/1
9	MAN	Q	6	9	-	1/2/19/22	0/1/1/1
9	MAN	Q	7	9	-	0/2/19/22	0/1/1/1
8	NAG	R	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	R	2	8	-	1/6/23/26	0/1/1/1
10	NAG	S	1	5,10	-	0/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
10	BMA	S	3	10	-	0/2/19/22	0/1/1/1
8	NAG	T	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	1/6/23/26	0/1/1/1
10	NAG	U	1	5,10	-	0/6/23/26	0/1/1/1
10	NAG	U	2	10	-	0/6/23/26	0/1/1/1
10	BMA	U	3	10	-	0/2/19/22	0/1/1/1
11	NAG	V	1	6,11	-	0/6/23/26	0/1/1/1
11	NAG	V	2	11	-	1/6/23/26	0/1/1/1
11	FUC	V	3	11	-	-	0/1/1/1
12	NAG	W	1	6,12	-	0/6/23/26	0/1/1/1
12	NAG	W	2	12	-	0/6/23/26	0/1/1/1
12	BMA	W	3	12	-	1/2/19/22	0/1/1/1
12	FUC	W	4	12	-	-	0/1/1/1
13	NAG	X	1	13,5	-	0/6/23/26	0/1/1/1
13	NAG	X	2	13	-	0/6/23/26	0/1/1/1
13	BMA	X	3	13	-	1/2/19/22	0/1/1/1
13	MAN	X	4	13	-	0/2/19/22	0/1/1/1
13	MAN	X	5	13	-	0/2/19/22	0/1/1/1
13	BMA	X	6	13	-	1/2/19/22	0/1/1/1
13	MAN	X	7	13	-	1/2/19/22	0/1/1/1
14	NAG	Y	1	14,5	-	2/6/23/26	0/1/1/1
14	NAG	Y	2	14	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BMA	Y	3	14	-	0/2/19/22	0/1/1/1
14	MAN	Y	4	14	-	0/2/19/22	0/1/1/1
14	MAN	Y	5	14	-	1/2/19/22	0/1/1/1
14	MAN	Y	6	14	-	0/2/19/22	0/1/1/1
14	MAN	Y	7	14	-	0/2/19/22	0/1/1/1
15	NAG	Z	1	5,15	-	0/6/23/26	0/1/1/1
15	NAG	Z	2	15	-	0/6/23/26	0/1/1/1
15	BMA	Z	3	15	-	1/2/19/22	0/1/1/1
15	MAN	Z	4	15	-	0/2/19/22	0/1/1/1
15	MAN	Z	5	15	-	0/2/19/22	0/1/1/1
8	NAG	a	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	a	2	8	-	1/6/23/26	0/1/1/1
8	NAG	b	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	1/6/23/26	0/1/1/1
10	NAG	c	1	5,10	-	0/6/23/26	0/1/1/1
10	NAG	c	2	10	-	0/6/23/26	0/1/1/1
10	BMA	c	3	10	-	1/2/19/22	0/1/1/1
8	NAG	d	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	d	2	8	-	0/6/23/26	0/1/1/1
8	NAG	e	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	1/6/23/26	0/1/1/1
8	NAG	f	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	0/6/23/26	0/1/1/1
8	NAG	g	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	g	2	8	-	1/6/23/26	0/1/1/1
14	NAG	h	1	14,5	-	0/6/23/26	0/1/1/1
14	NAG	h	2	14	-	0/6/23/26	0/1/1/1
14	BMA	h	3	14	-	0/2/19/22	0/1/1/1
14	MAN	h	4	14	-	0/2/19/22	0/1/1/1
14	MAN	h	5	14	-	0/2/19/22	0/1/1/1
14	MAN	h	6	14	-	0/2/19/22	0/1/1/1
14	MAN	h	7	14	-	1/2/19/22	0/1/1/1
8	NAG	i	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	i	2	8	-	0/6/23/26	0/1/1/1
16	NAG	j	1	16,5	-	0/6/23/26	0/1/1/1
16	NAG	j	2	16	-	0/6/23/26	0/1/1/1
16	BMA	j	3	16	-	1/2/19/22	0/1/1/1
16	MAN	j	4	16	-	1/2/19/22	0/1/1/1
16	MAN	j	5	16	-	1/2/19/22	0/1/1/1
8	NAG	k	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	k	2	8	-	0/6/23/26	0/1/1/1
15	NAG	l	1	5,15	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	l	2	15	-	1/6/23/26	0/1/1/1
15	BMA	l	3	15	-	0/2/19/22	0/1/1/1
15	MAN	l	4	15	-	1/2/19/22	0/1/1/1
15	MAN	l	5	15	-	0/2/19/22	0/1/1/1
8	NAG	m	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	m	2	8	-	1/6/23/26	0/1/1/1
8	NAG	n	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	n	2	8	-	1/6/23/26	0/1/1/1
8	NAG	o	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	o	2	8	-	1/6/23/26	0/1/1/1
8	NAG	p	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	p	2	8	-	1/6/23/26	0/1/1/1
8	NAG	q	1	8,5	-	1/6/23/26	0/1/1/1
8	NAG	q	2	8	-	1/6/23/26	0/1/1/1
17	NAG	r	1	17,5	-	2/6/23/26	0/1/1/1
17	NAG	r	2	17	-	2/6/23/26	0/1/1/1
17	BMA	r	3	17	-	0/2/19/22	0/1/1/1
17	MAN	r	4	17	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Y	2	NAG	C1-C2-N2	5.99	119.87	110.43
14	Y	2	NAG	O4-C4-C3	-5.31	97.87	110.38
15	Z	1	NAG	C1-O5-C5	5.13	119.07	112.19
9	Q	1	NAG	C1-O5-C5	4.95	118.81	112.19
8	R	1	NAG	C1-C2-N2	4.73	117.88	110.43

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

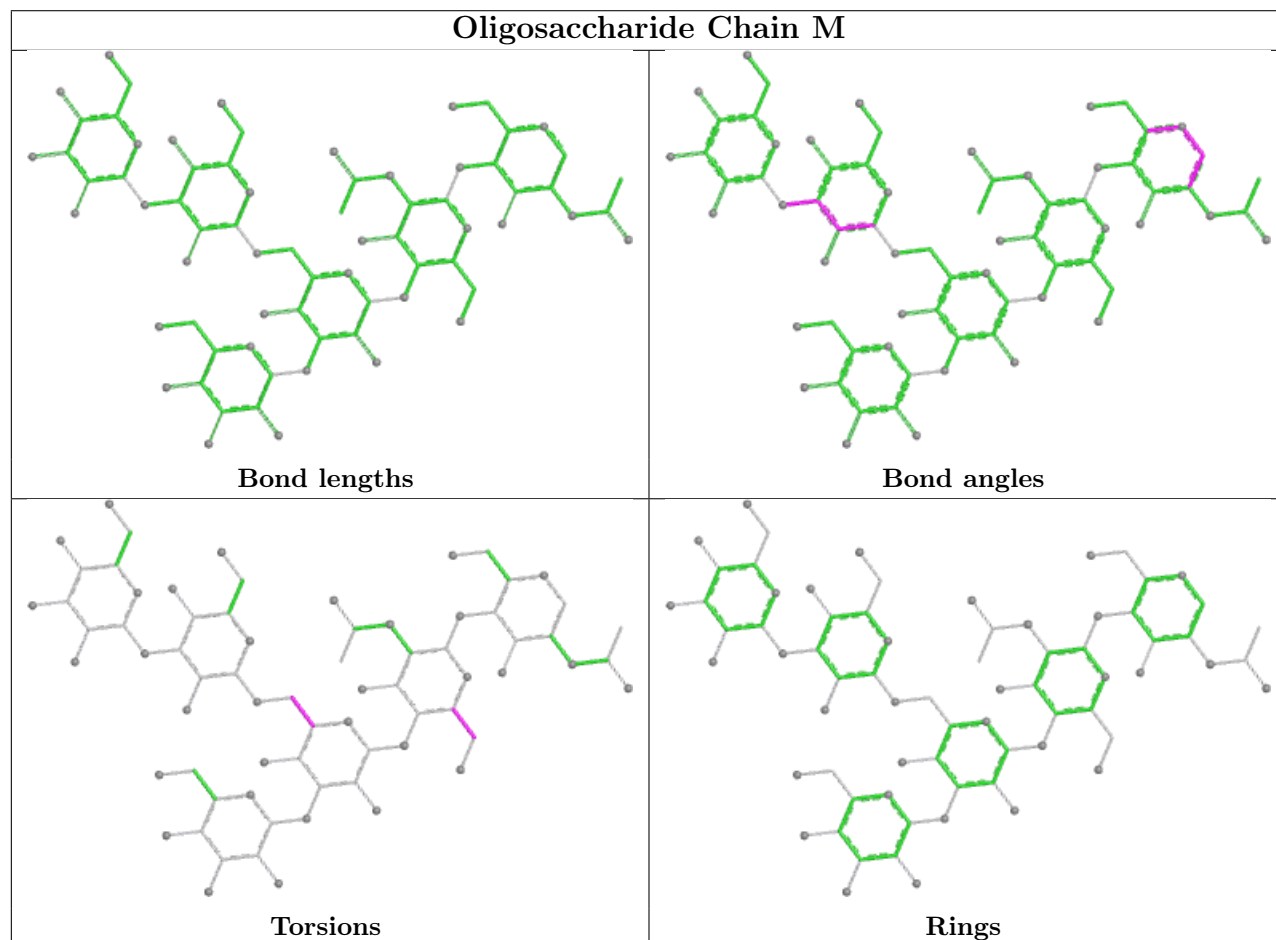
Mol	Chain	Res	Type	Atoms
11	V	2	NAG	C3-C2-N2-C7
17	r	1	NAG	O7-C7-N2-C2
17	r	2	NAG	C8-C7-N2-C2
17	r	2	NAG	O7-C7-N2-C2
17	r	1	NAG	C8-C7-N2-C2

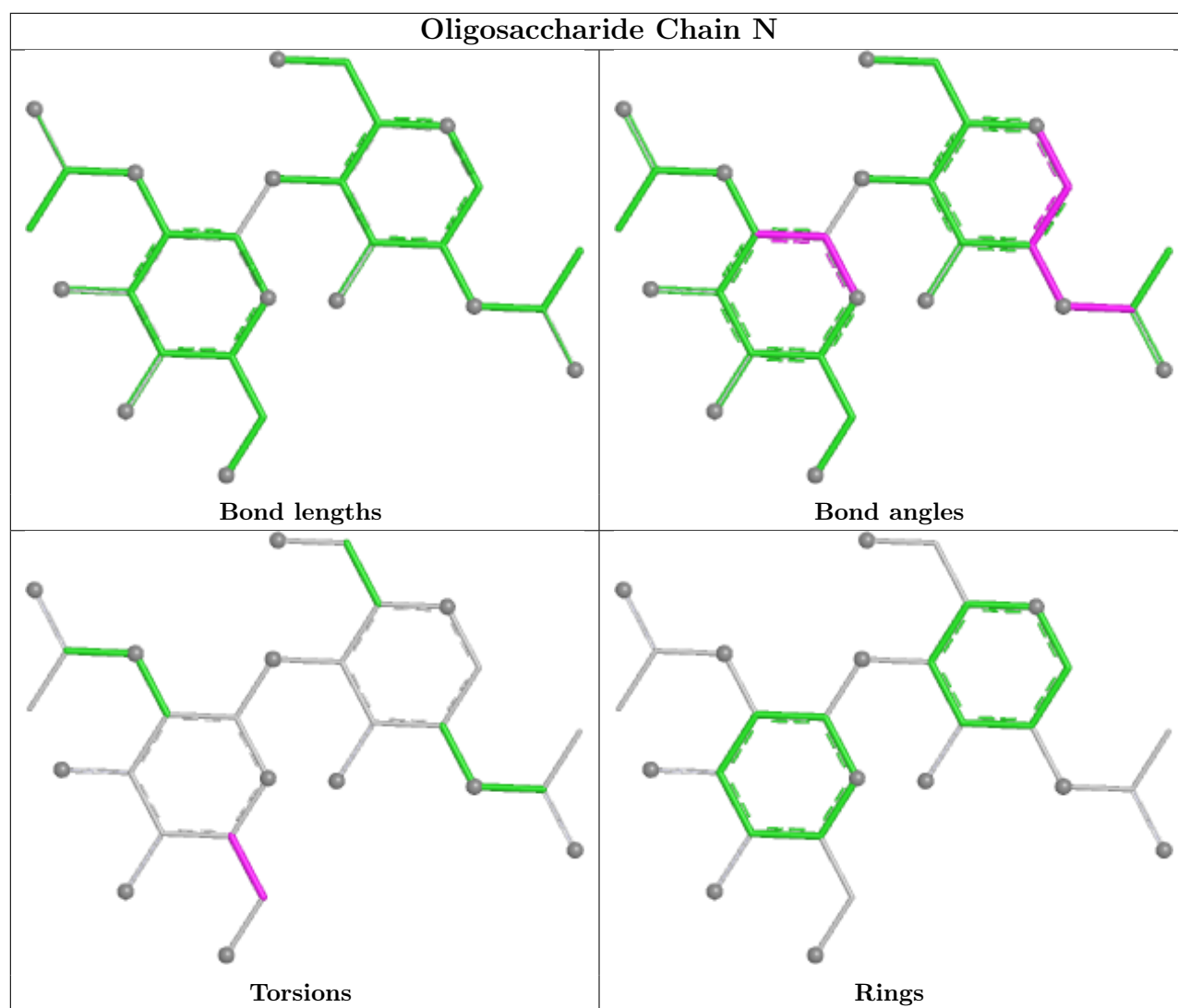
There are no ring outliers.

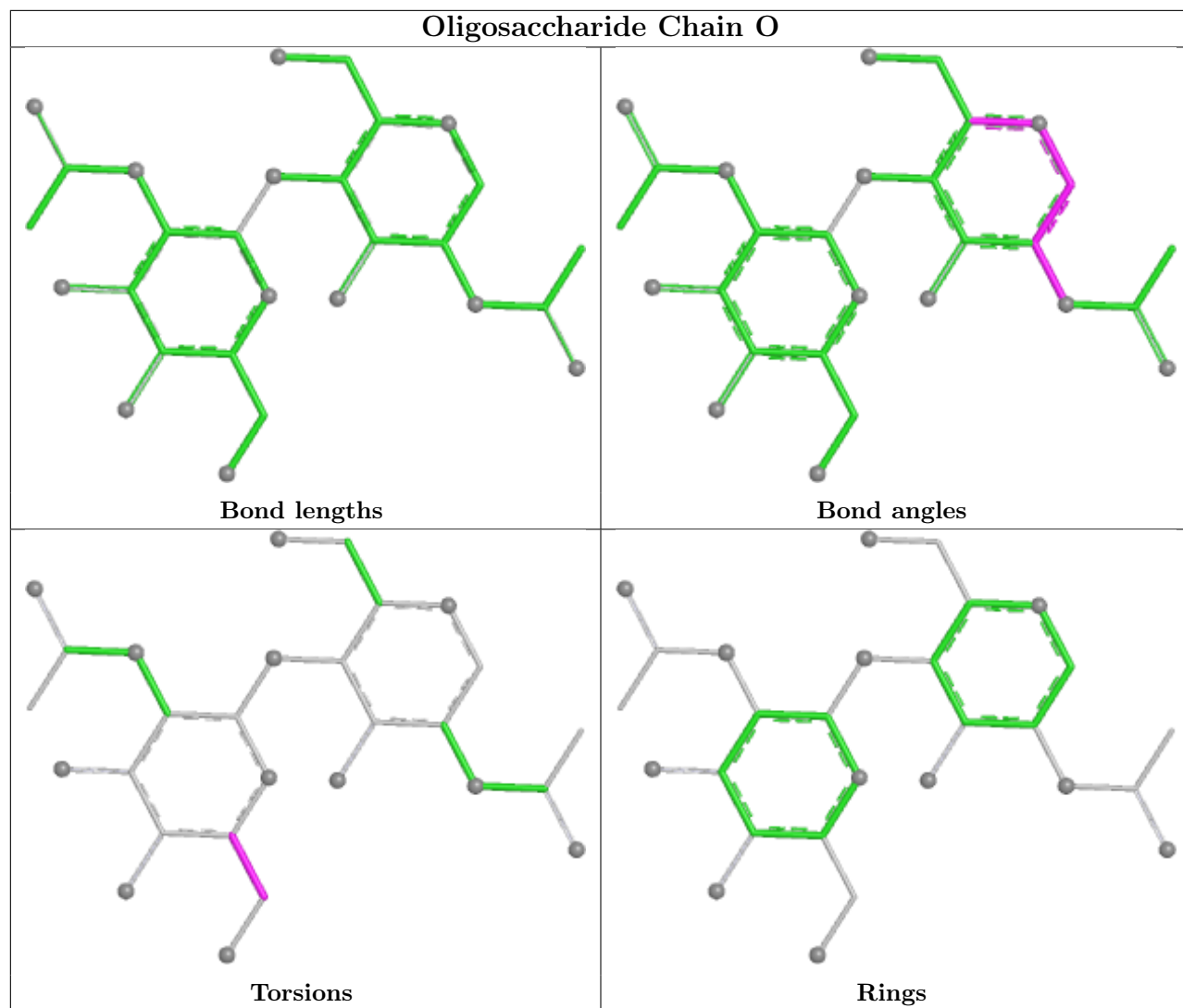
16 monomers are involved in 22 short contacts:

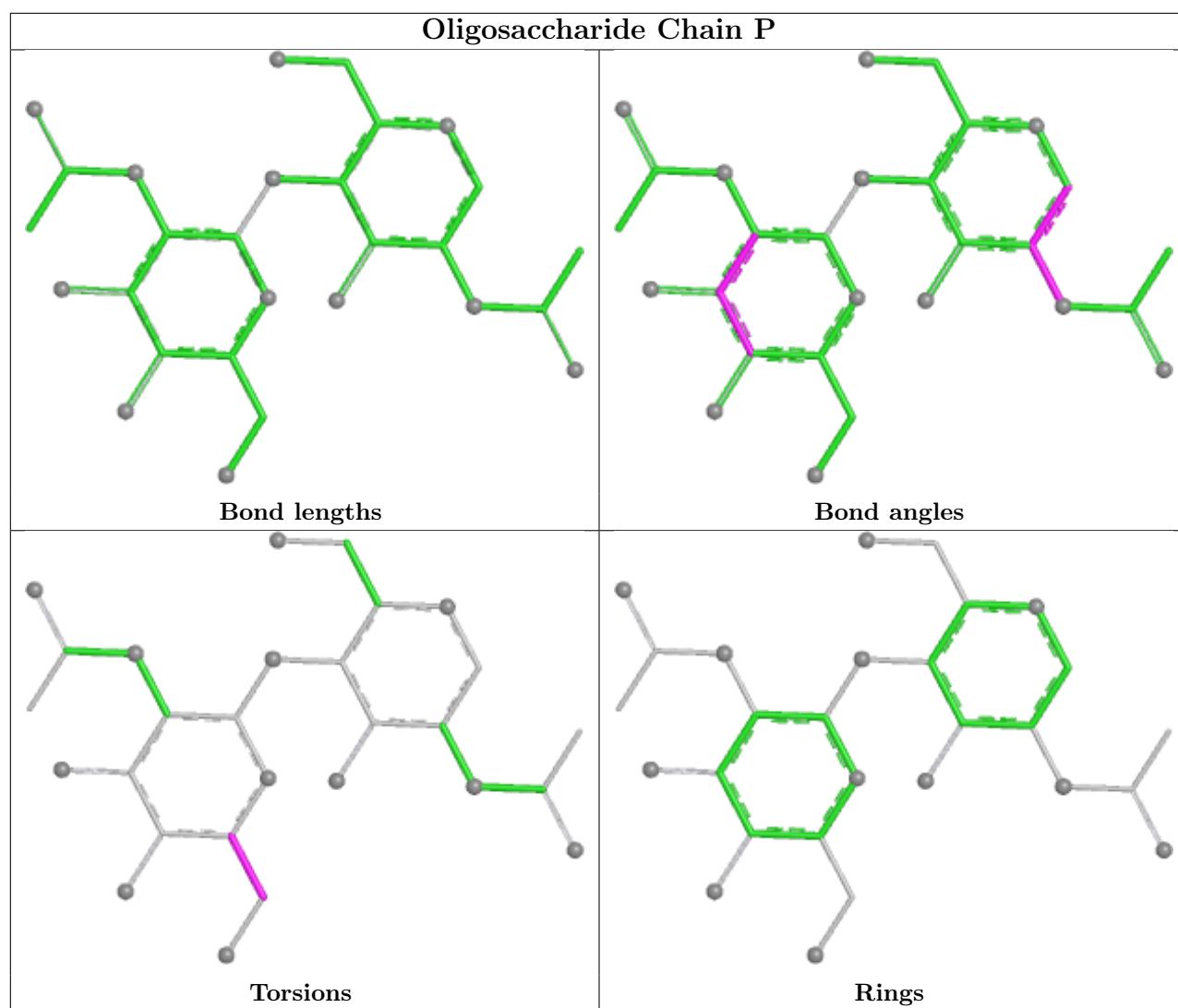
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	1	NAG	1	0
15	Z	5	MAN	1	0
11	V	3	FUC	1	0
8	i	2	NAG	2	0
14	Y	7	MAN	2	0
16	j	3	BMA	1	0
12	W	1	NAG	7	0
8	T	2	NAG	1	0
12	W	2	NAG	7	0
14	Y	3	BMA	3	0
15	l	1	NAG	1	0
15	Z	4	MAN	1	0
16	j	5	MAN	1	0
11	V	2	NAG	4	0
14	Y	5	MAN	1	0
8	i	1	NAG	2	0

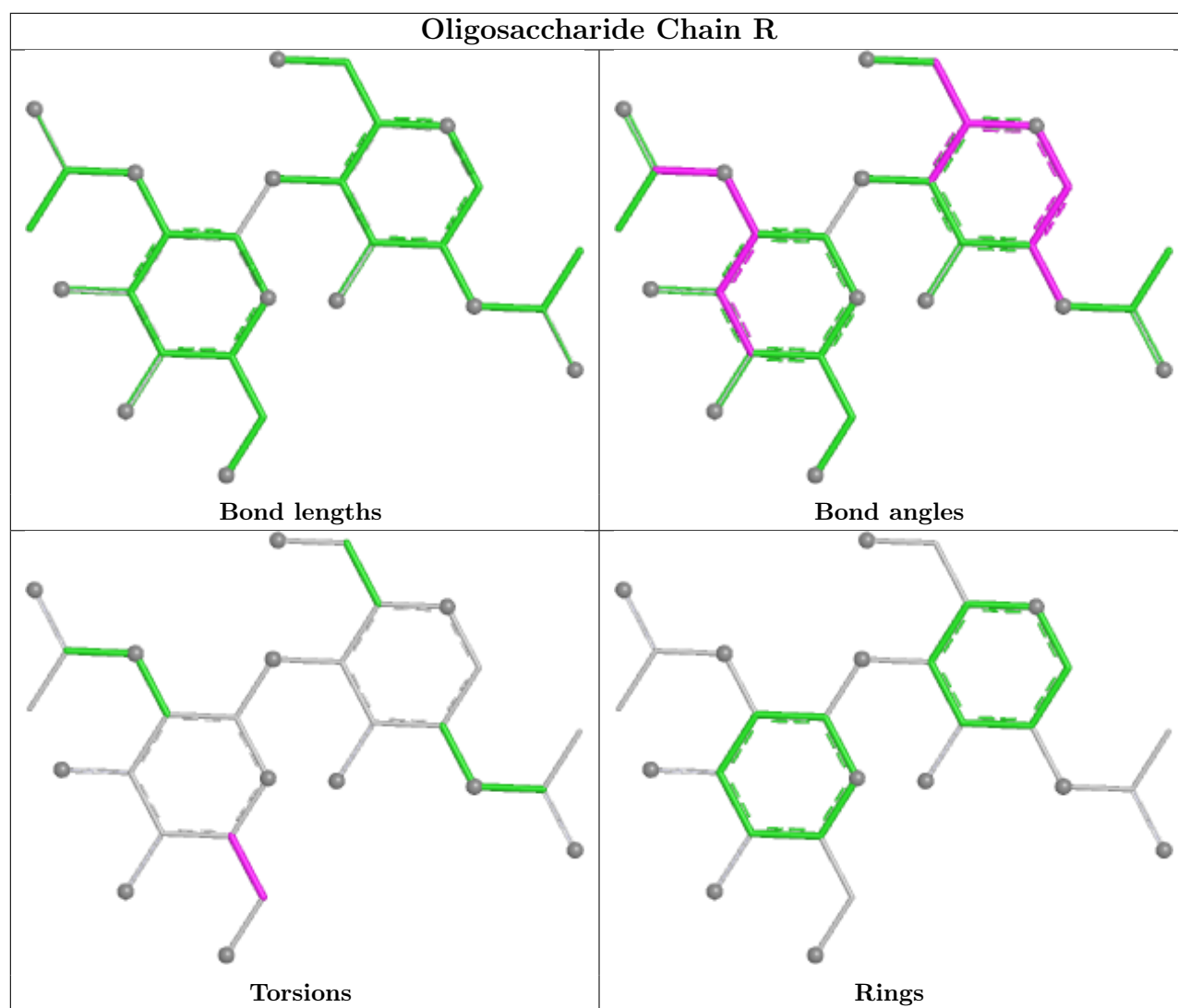
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

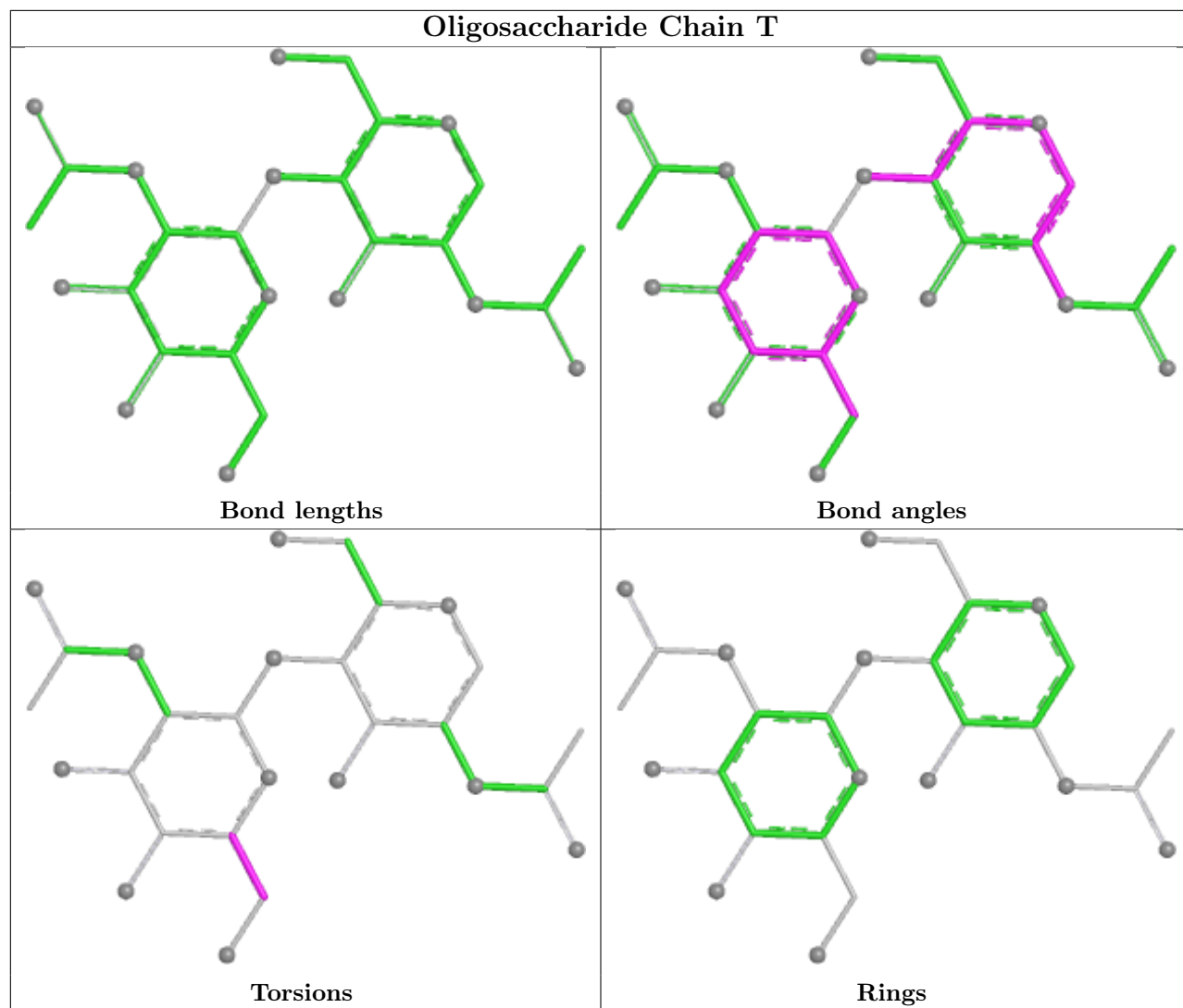




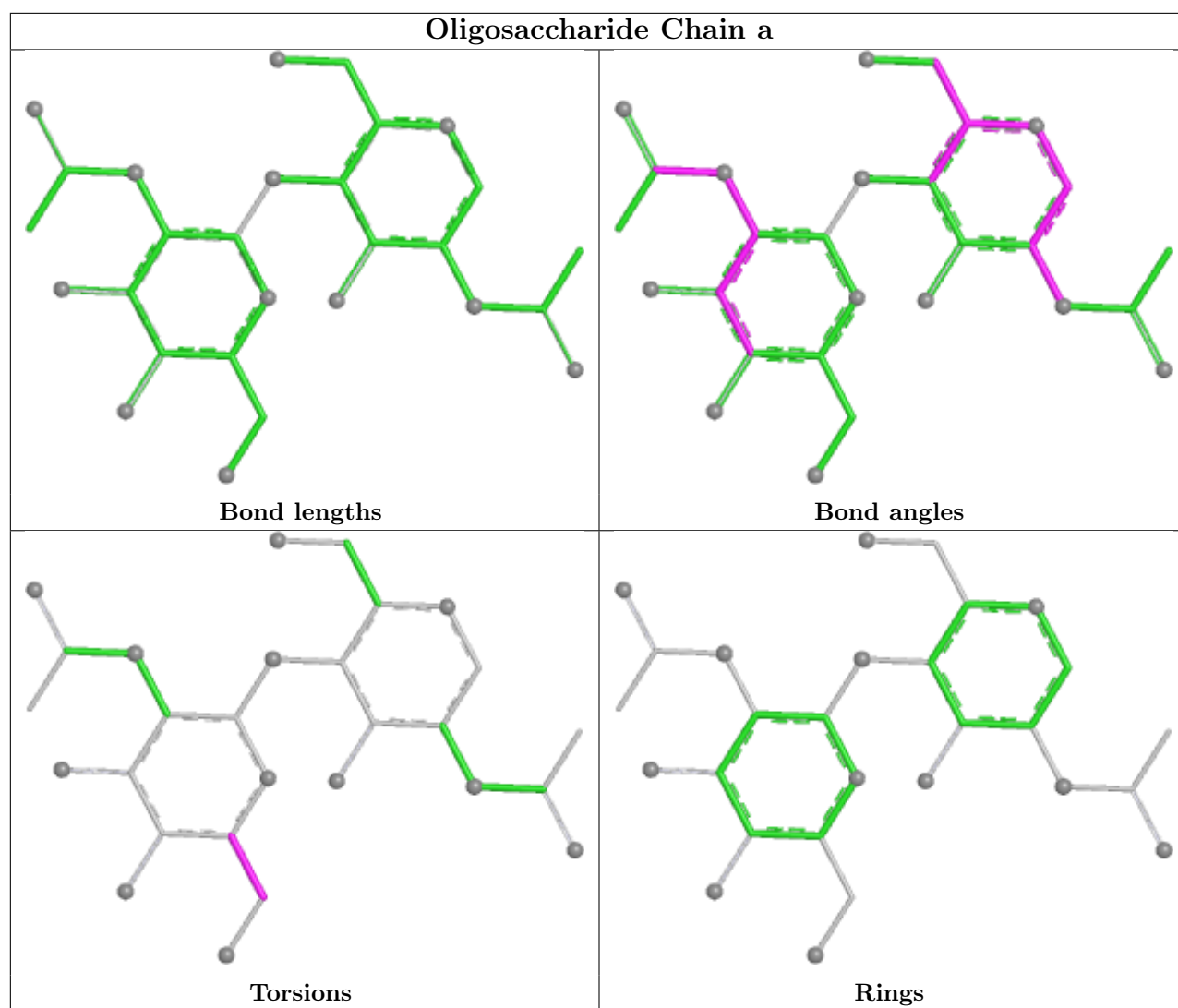


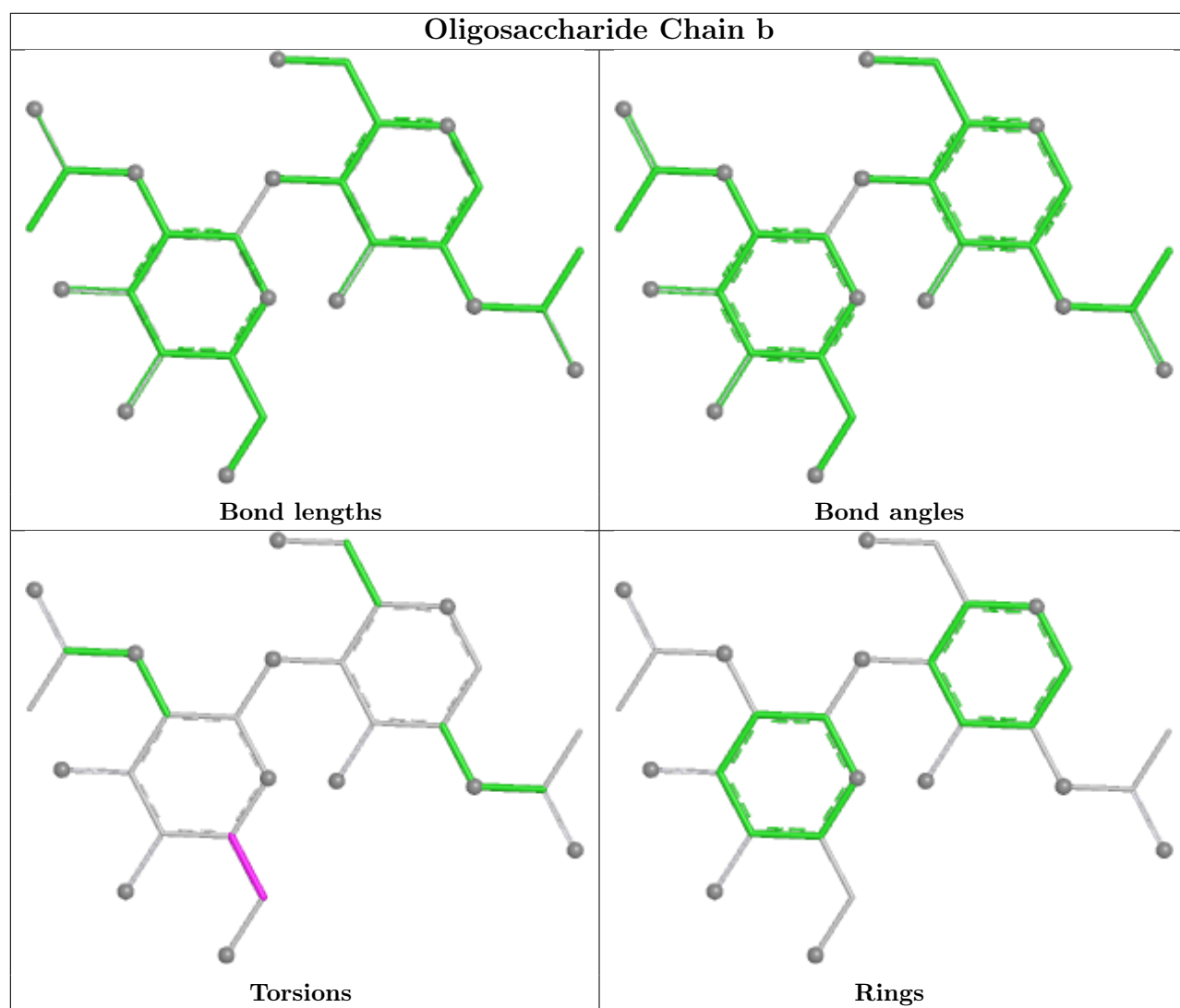


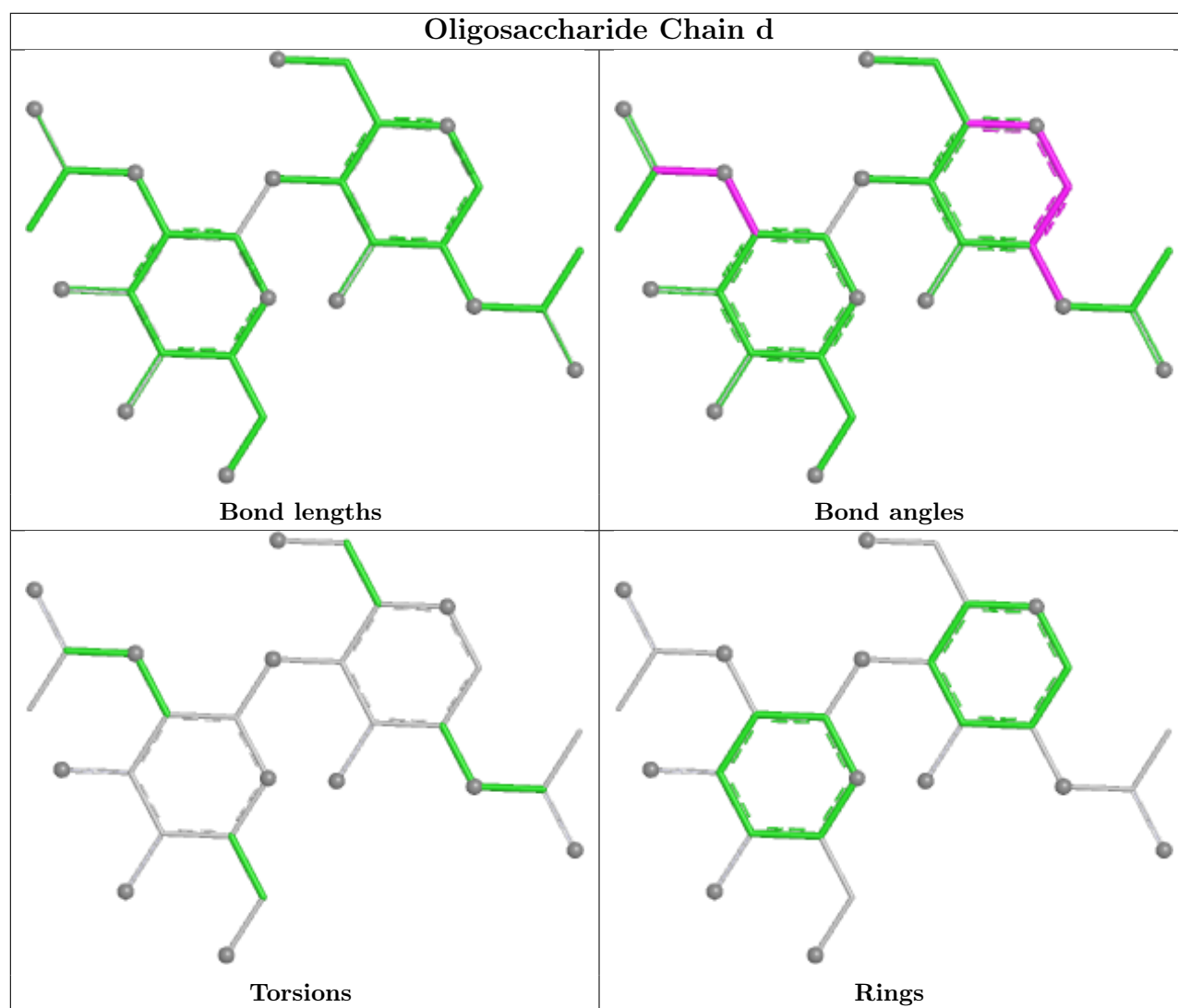


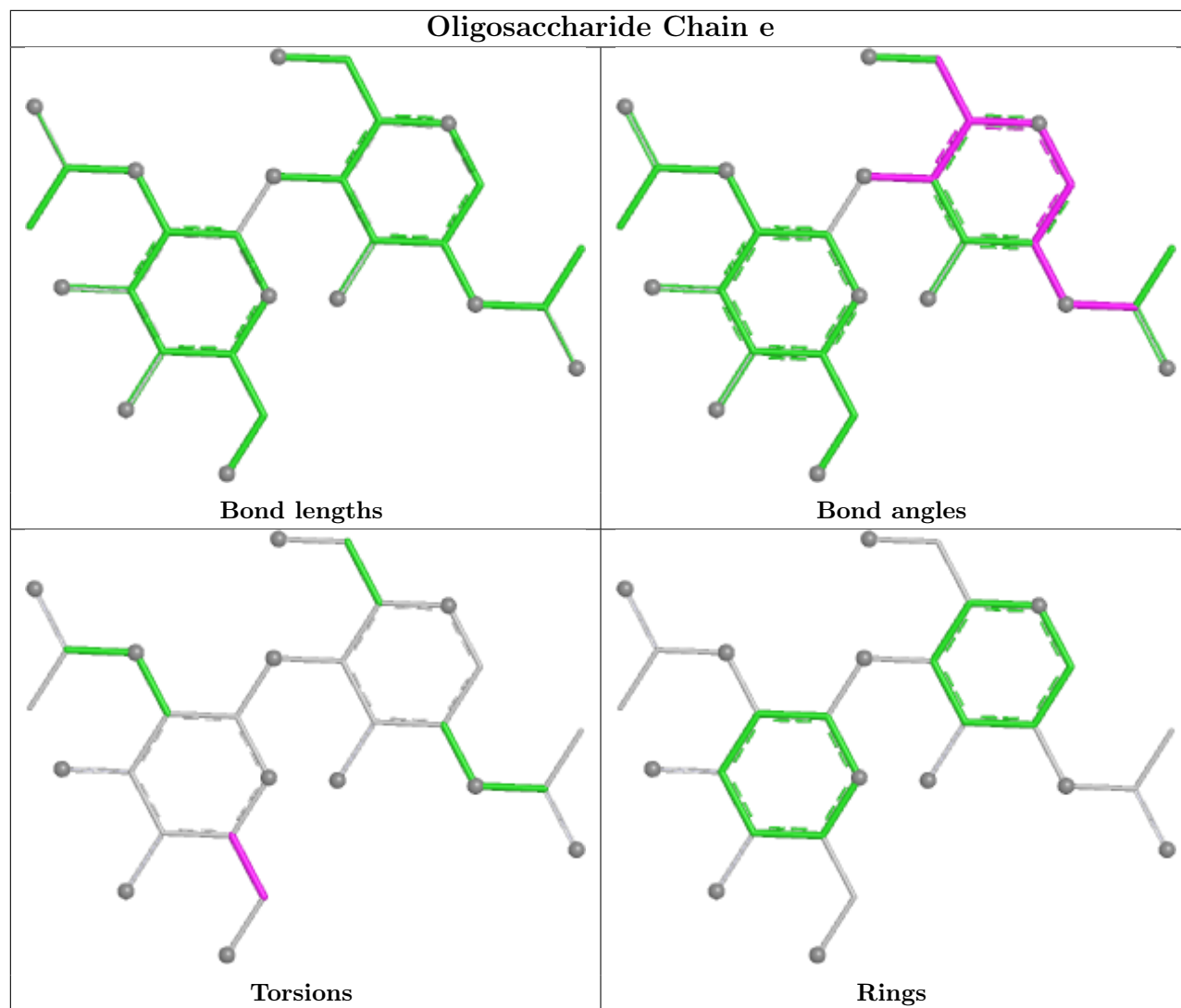


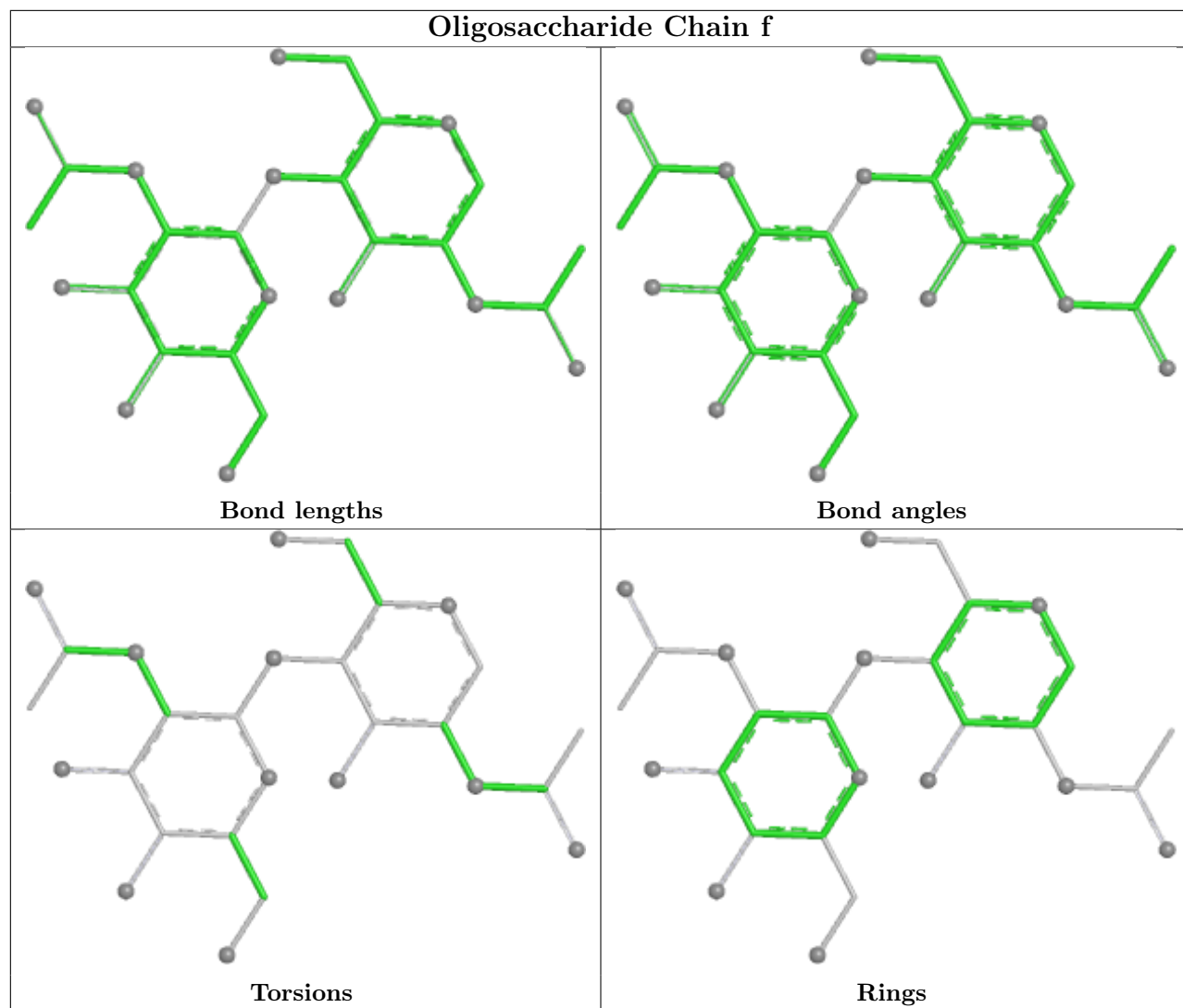


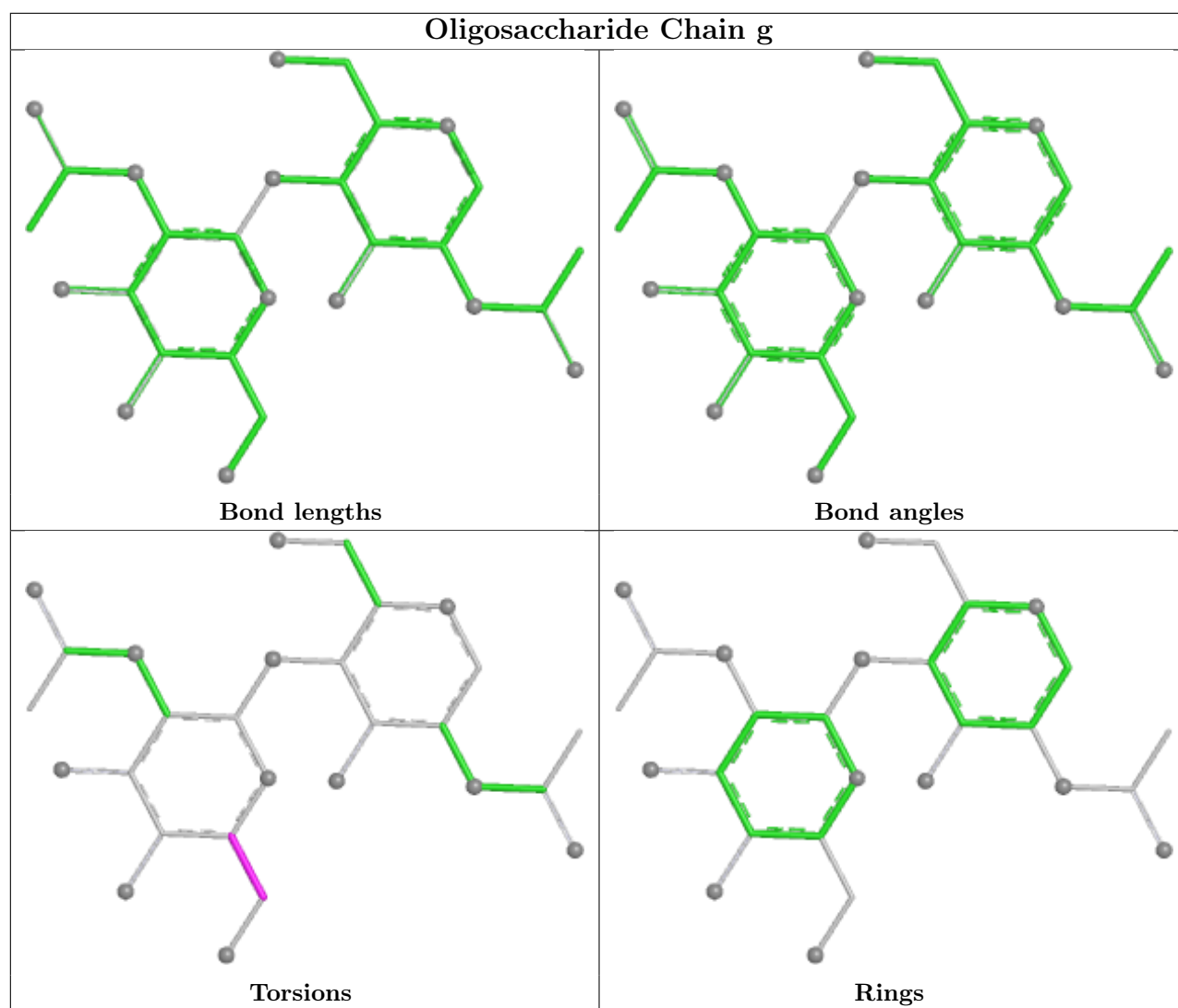


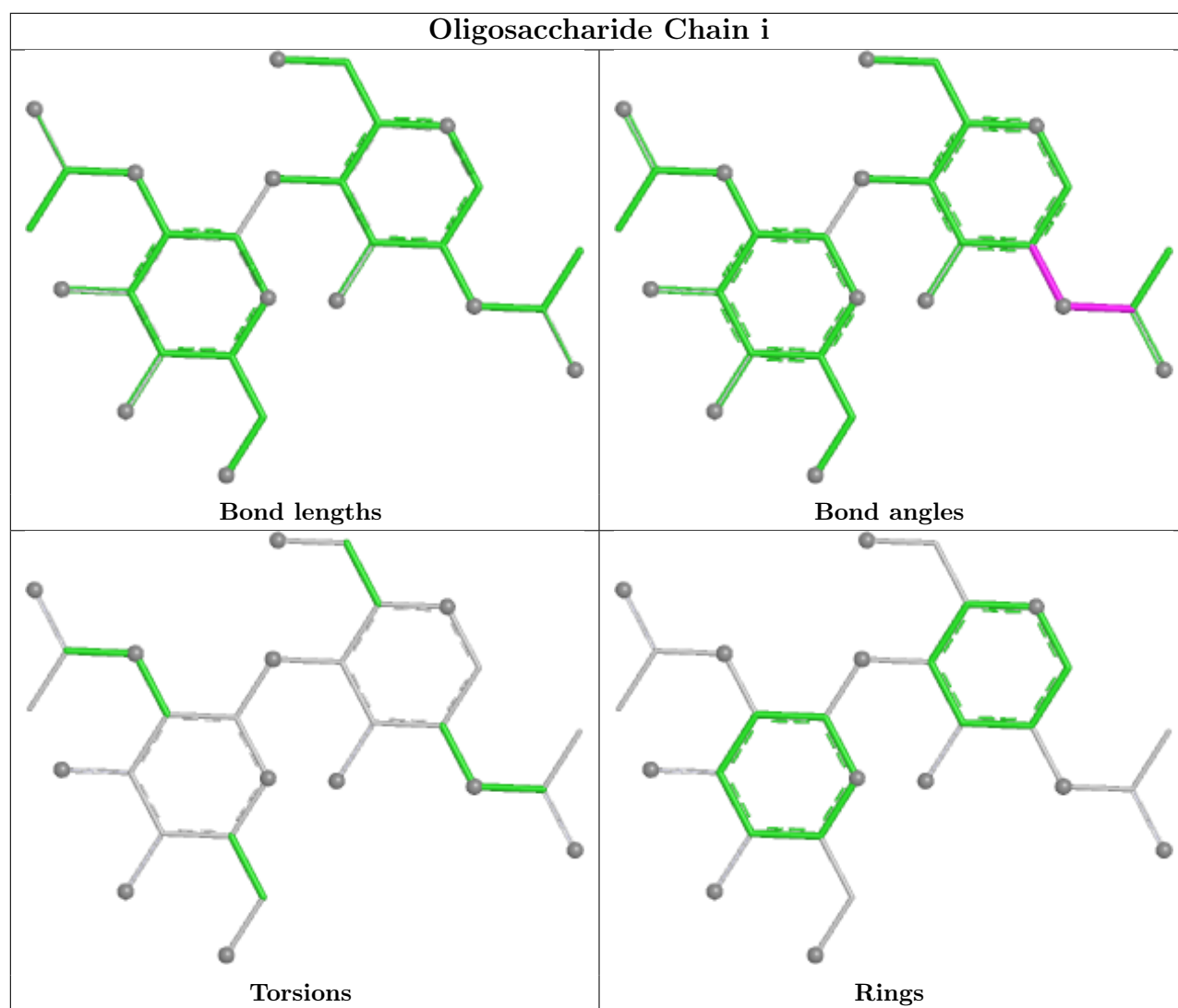


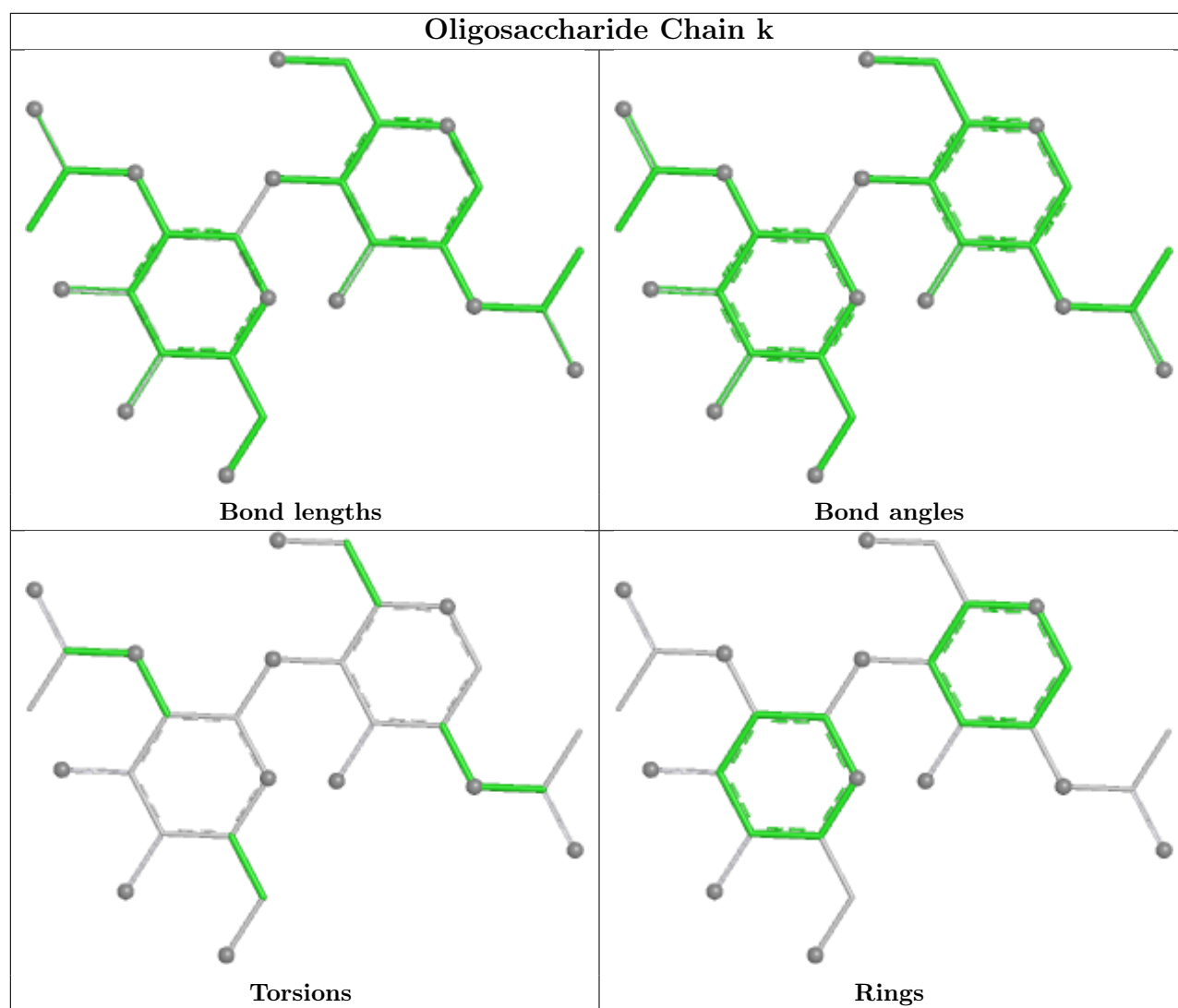




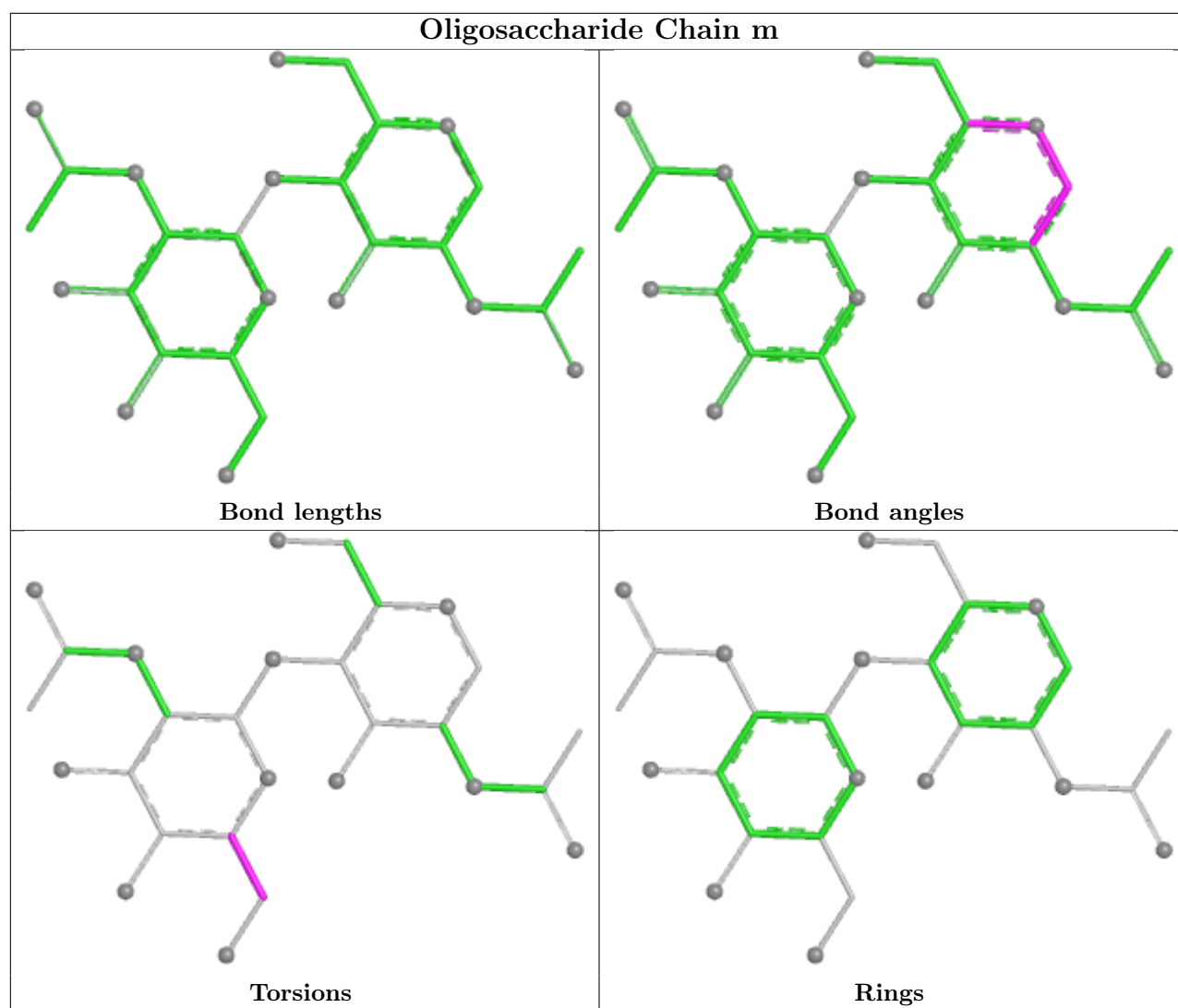


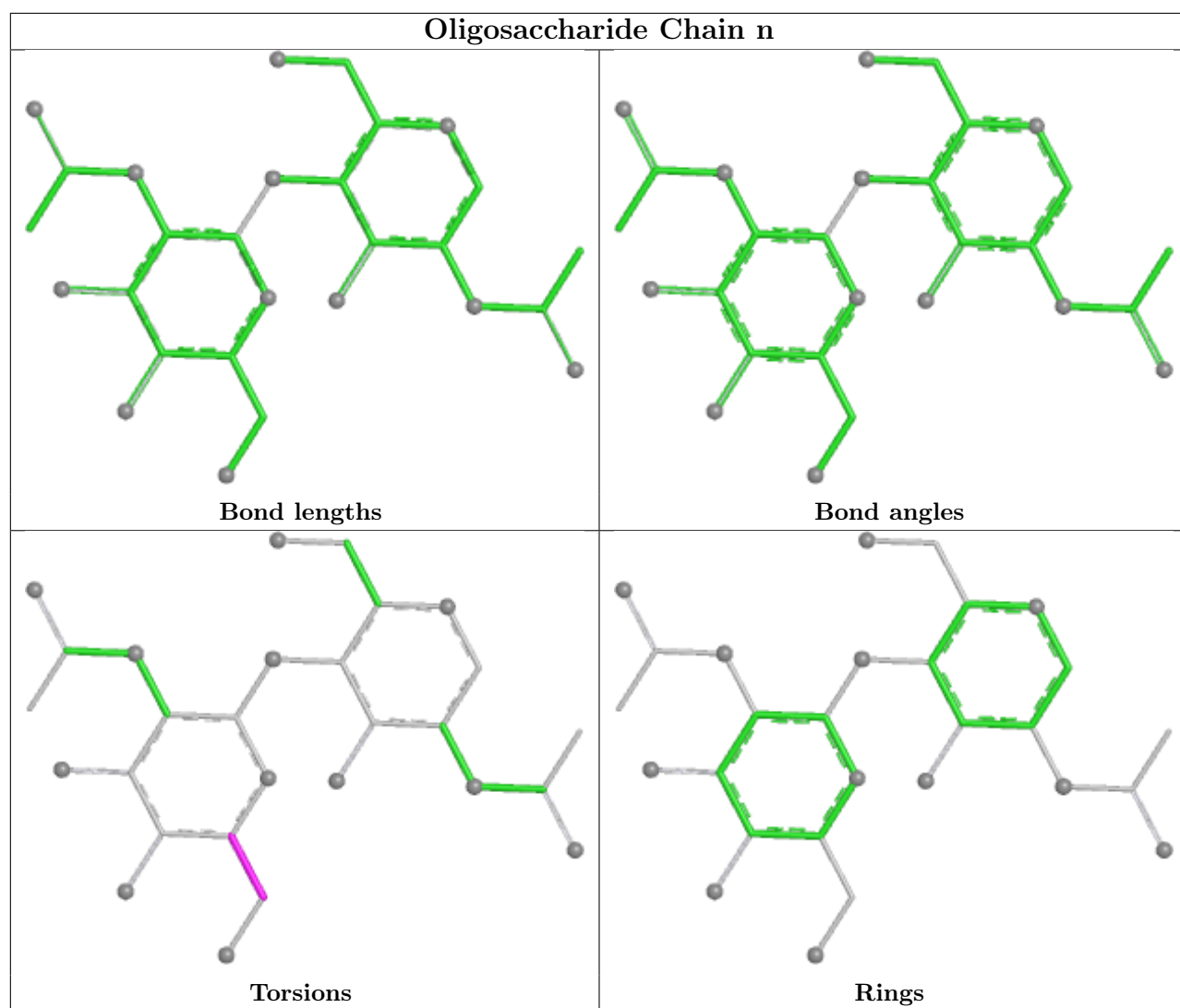


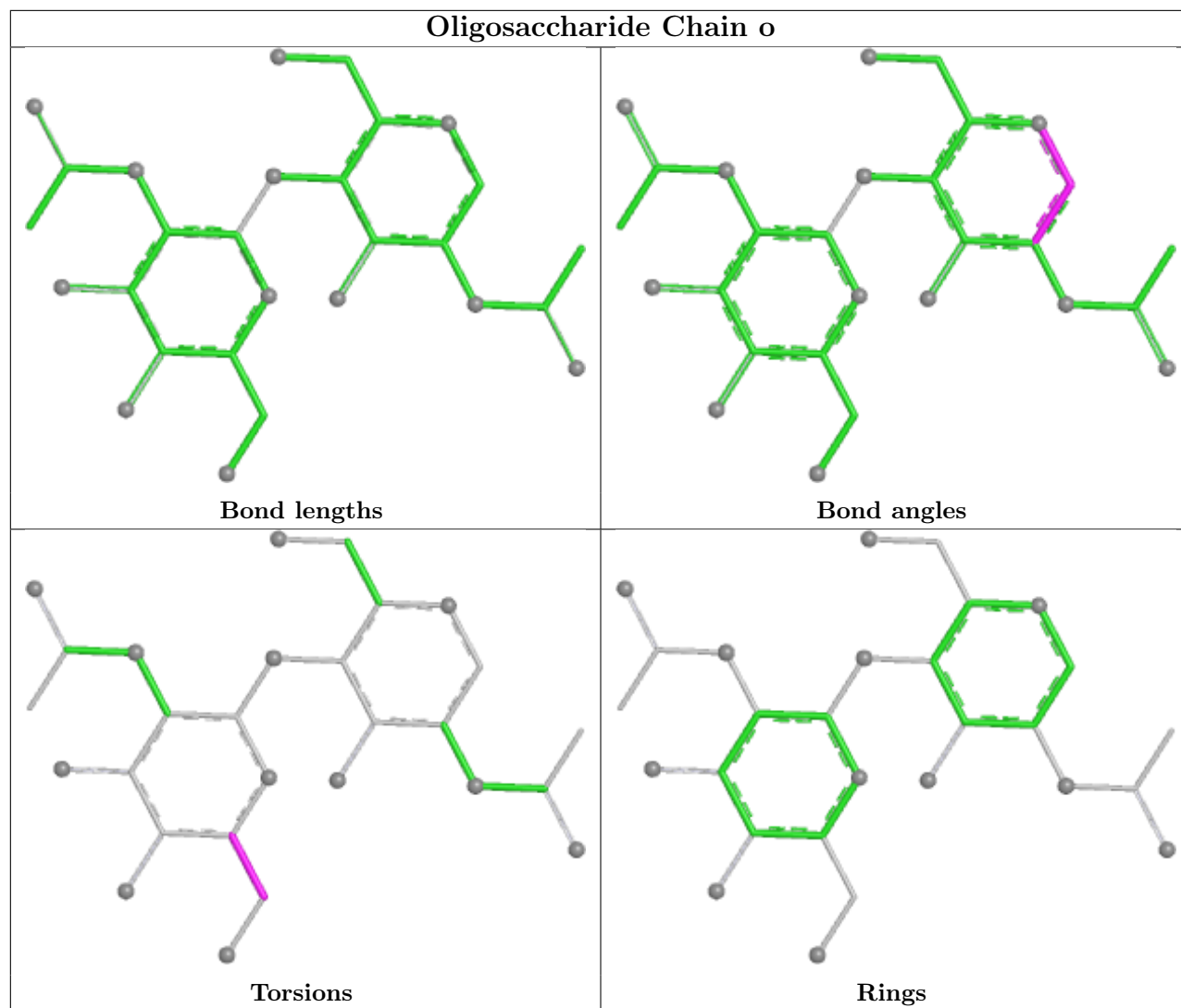


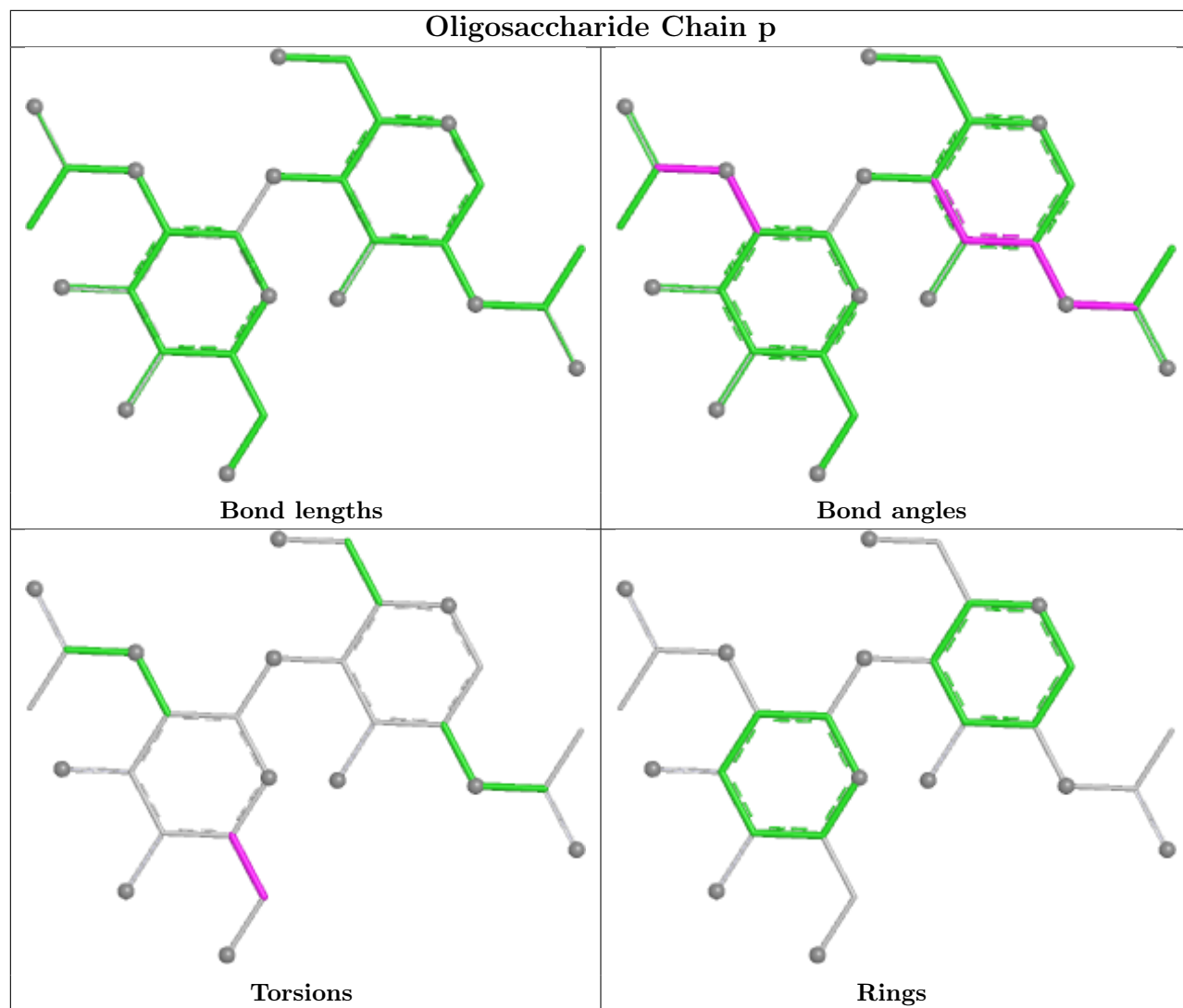


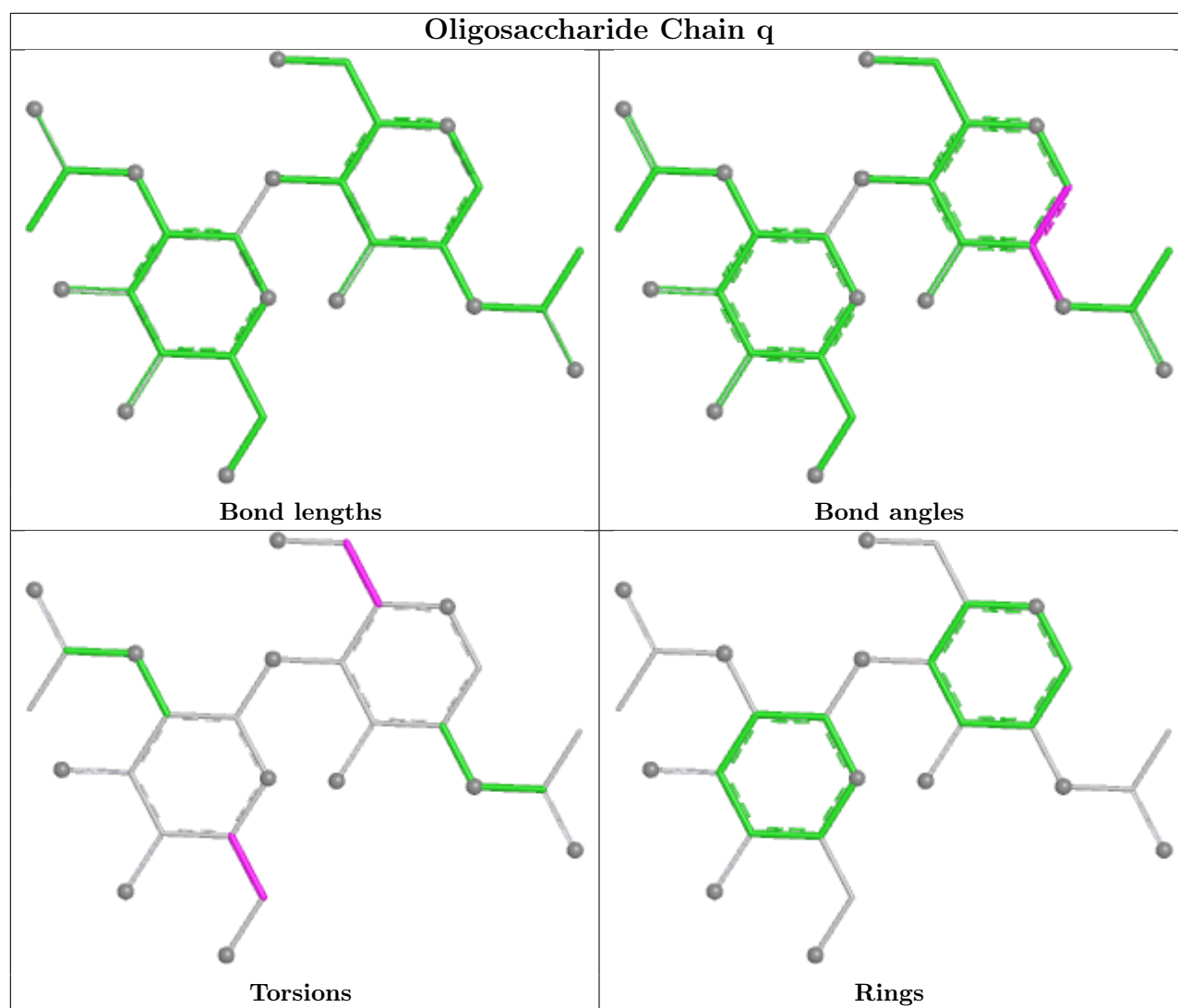


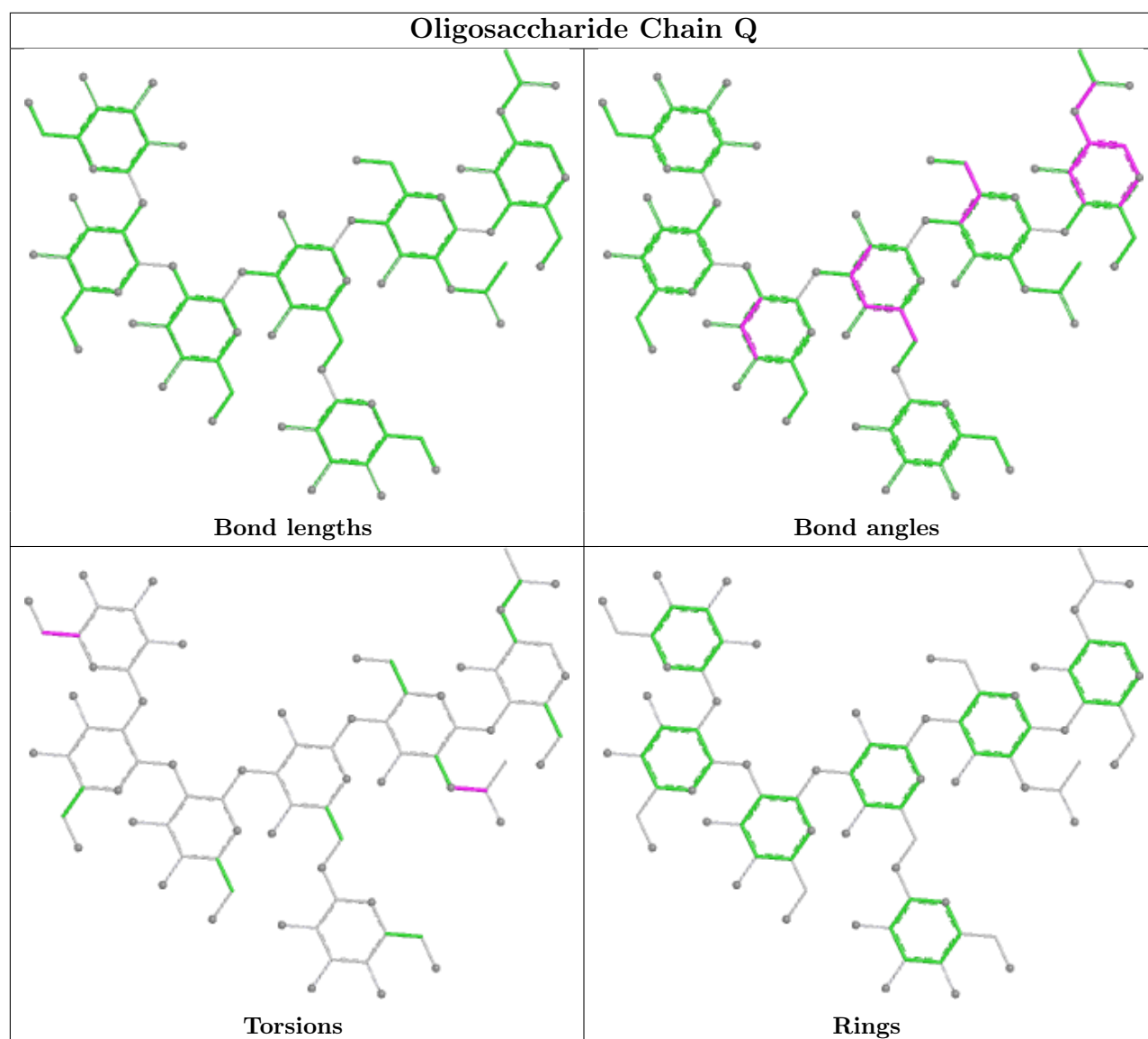


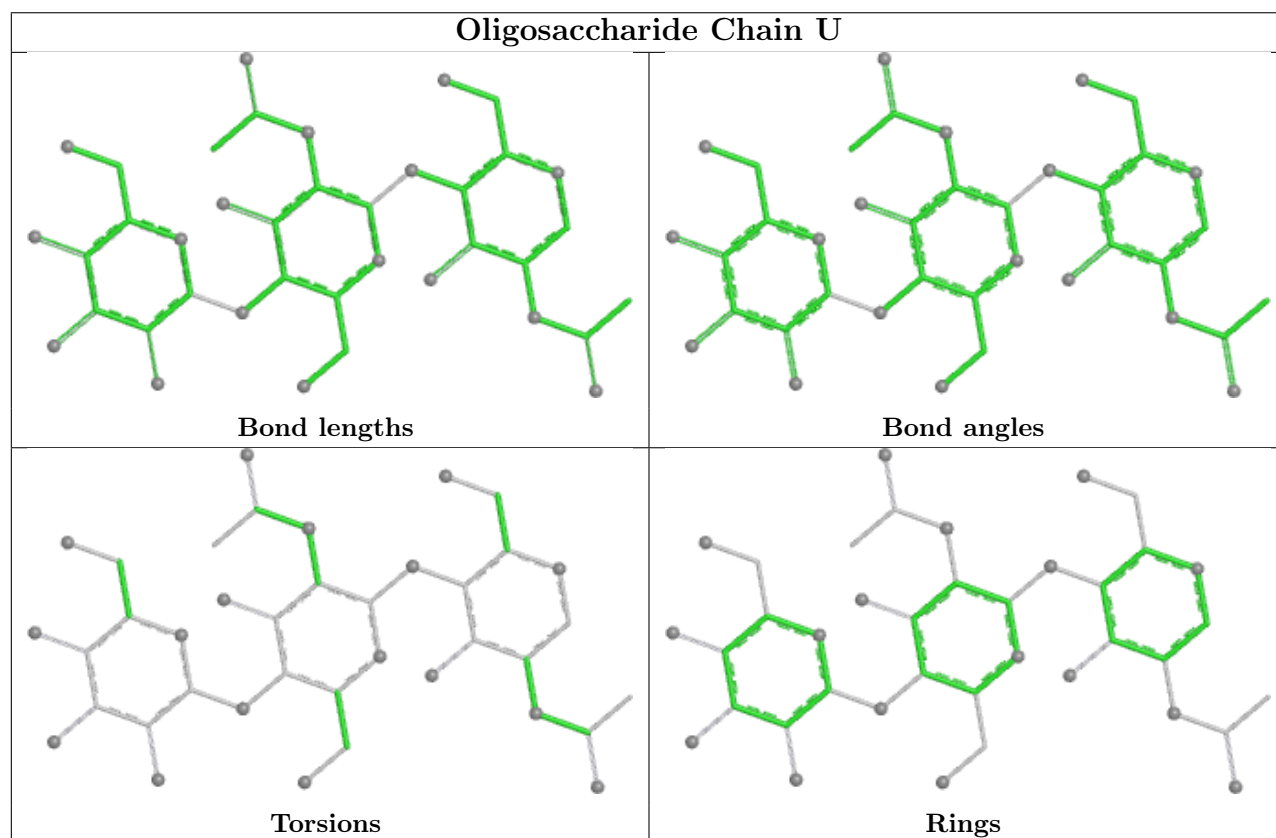
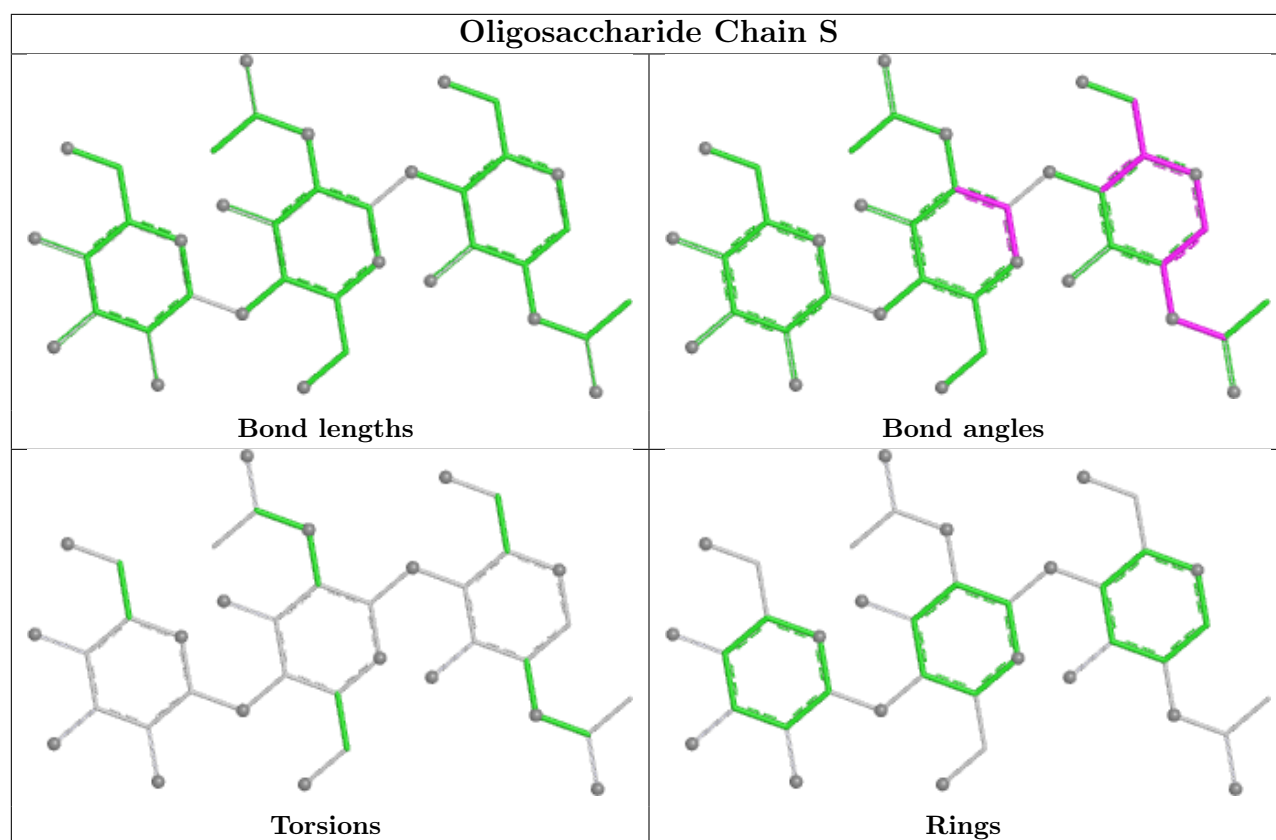


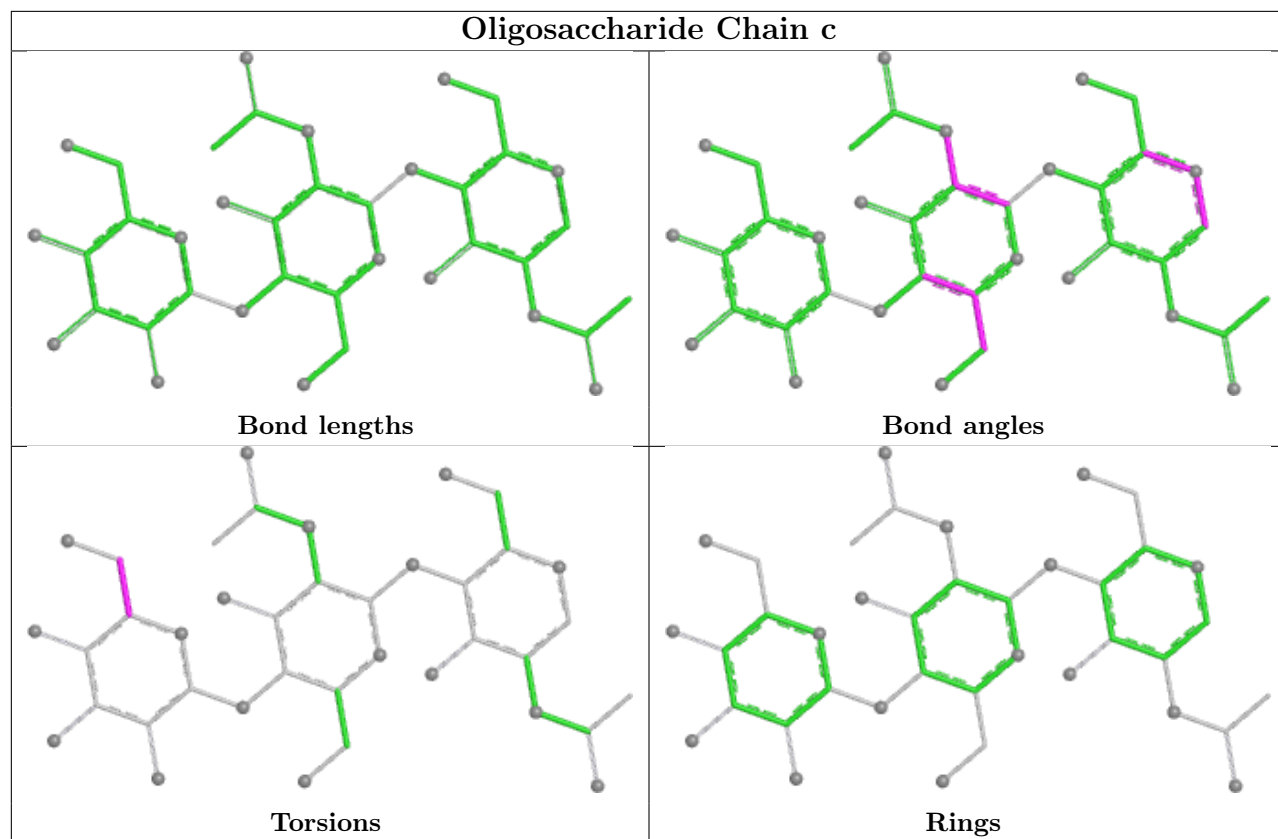




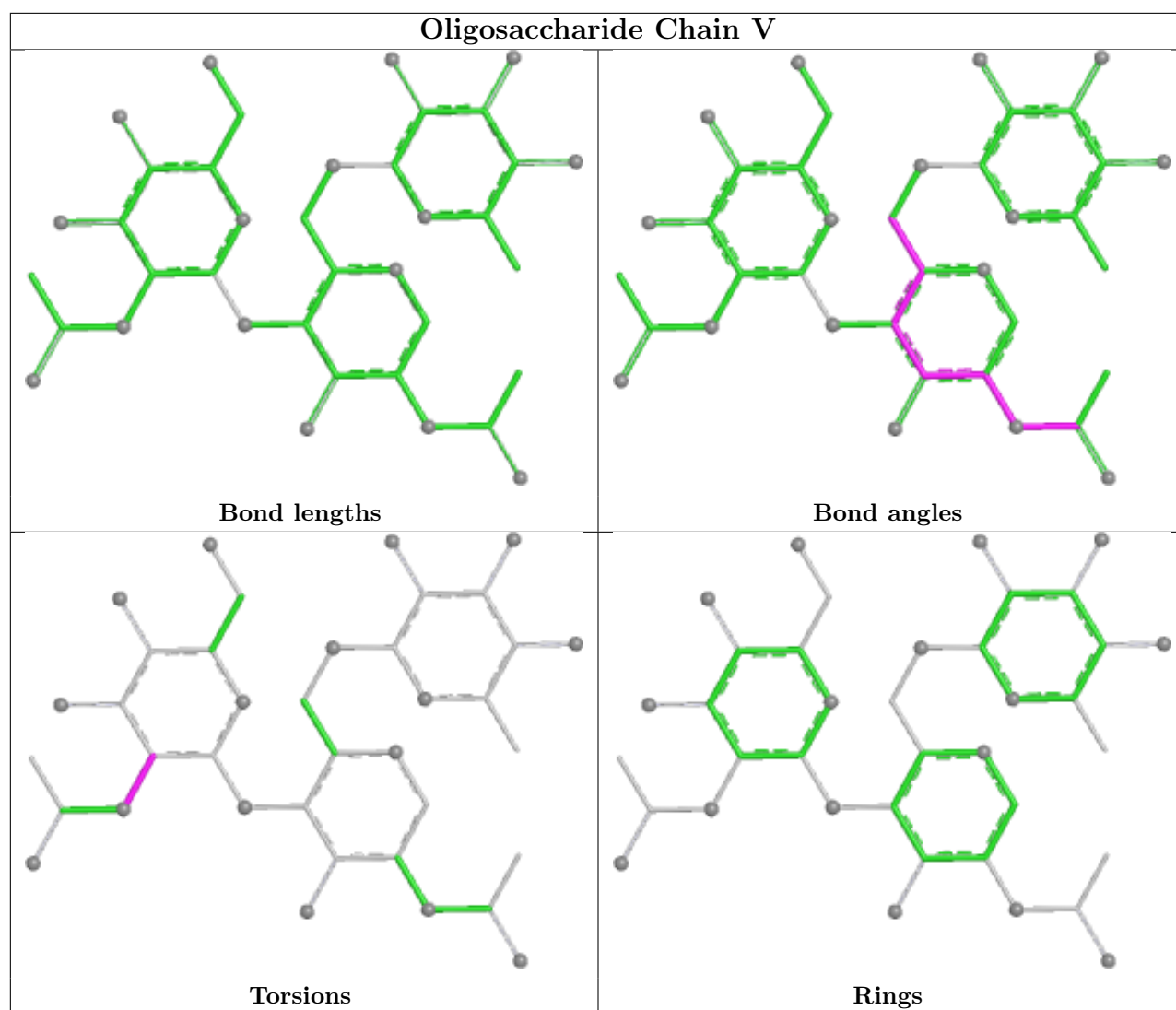


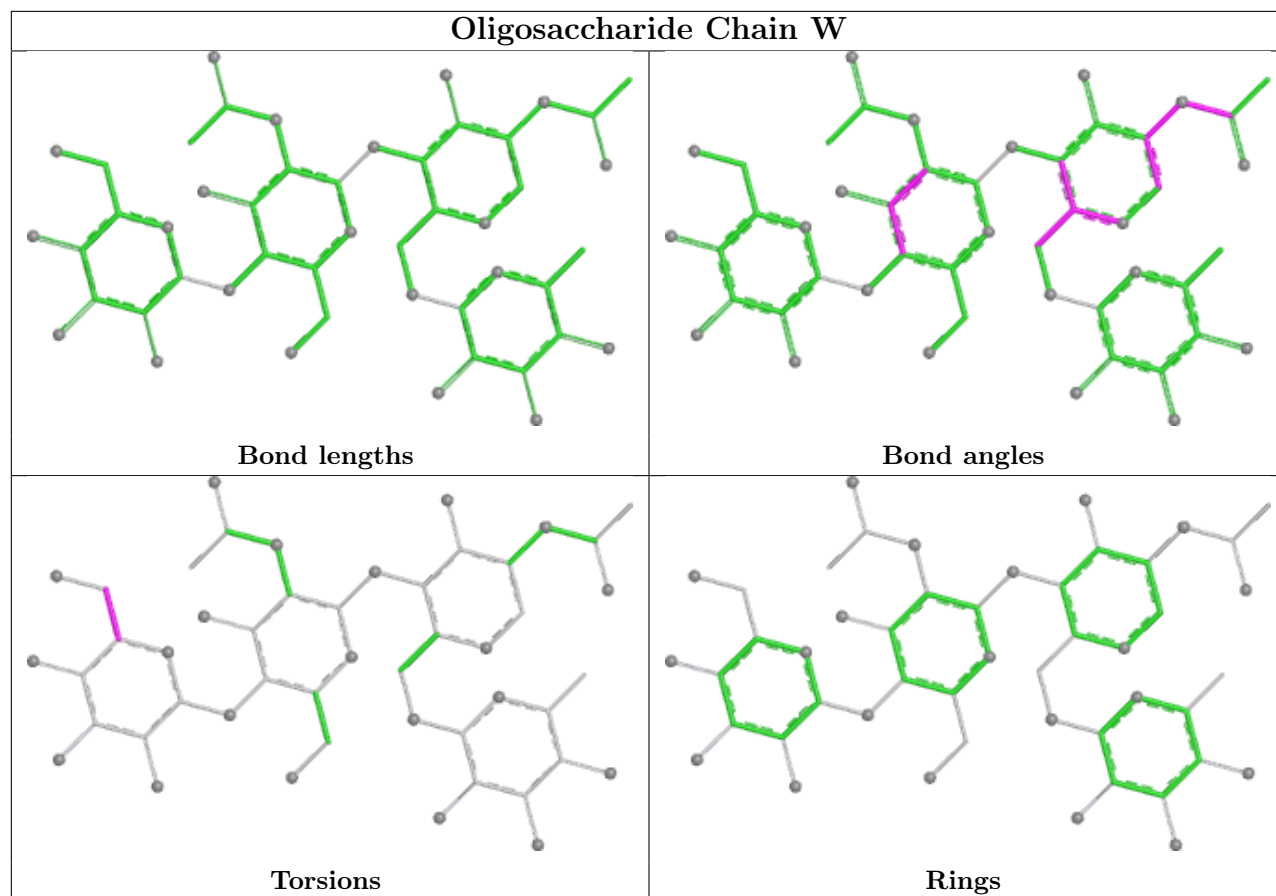


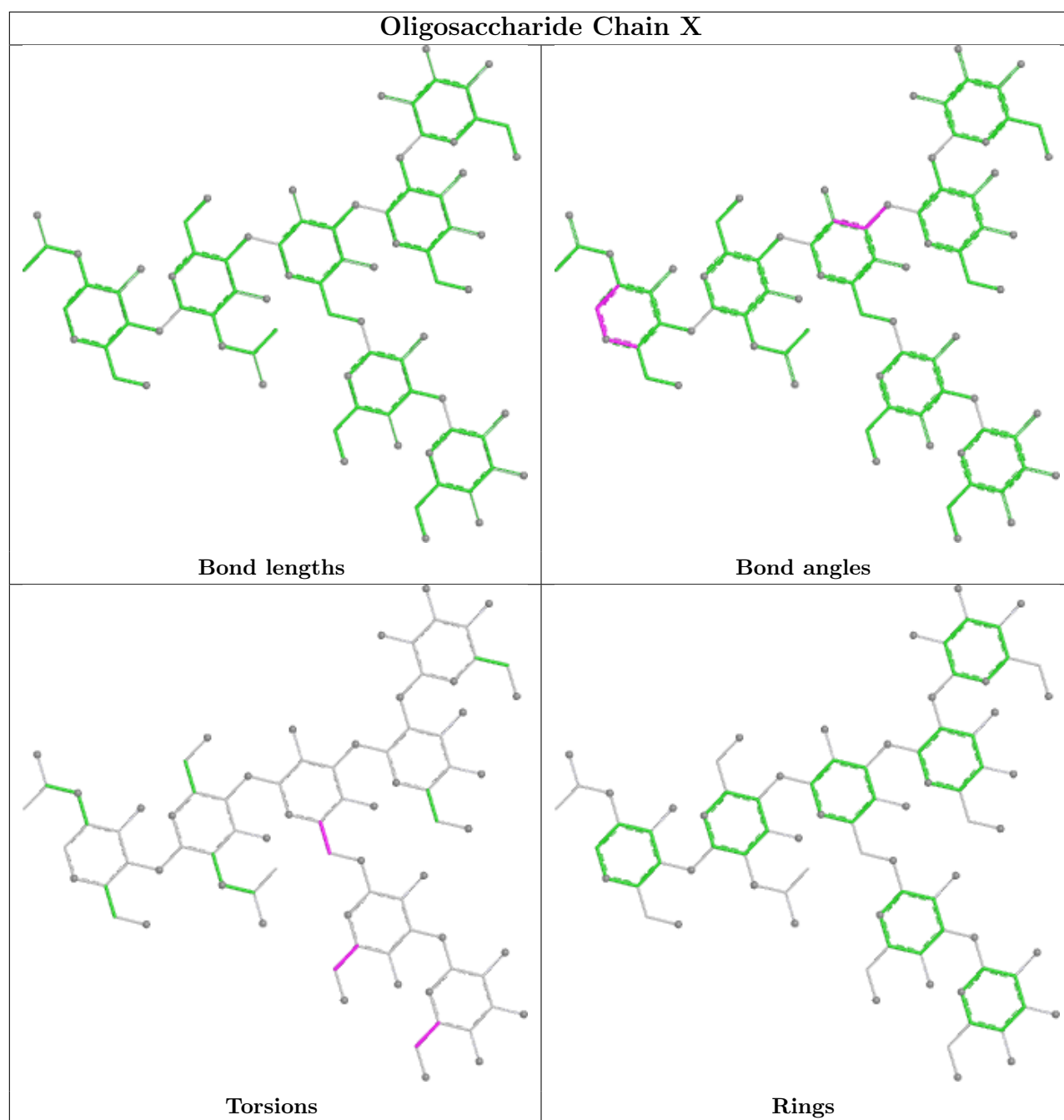


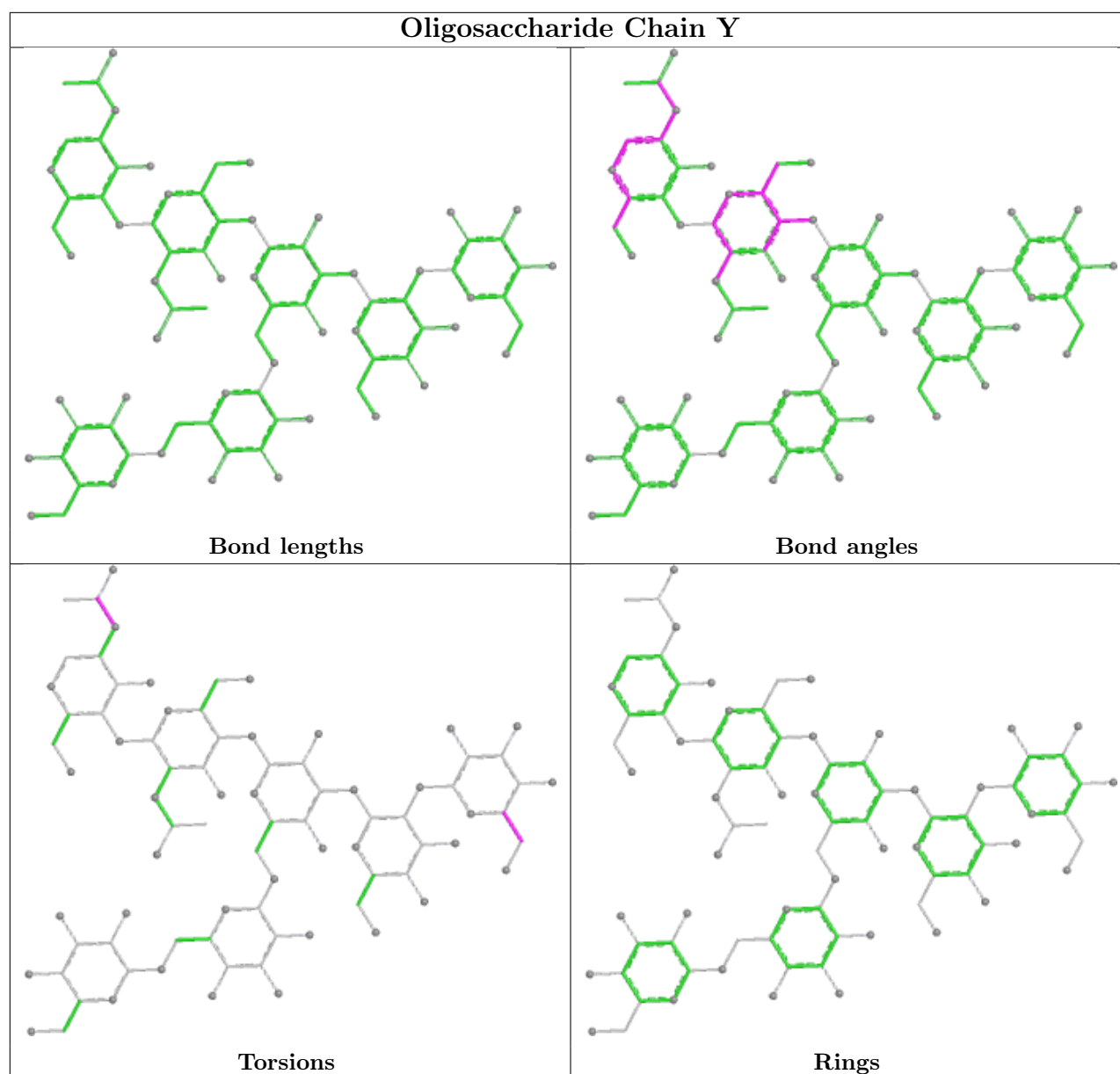


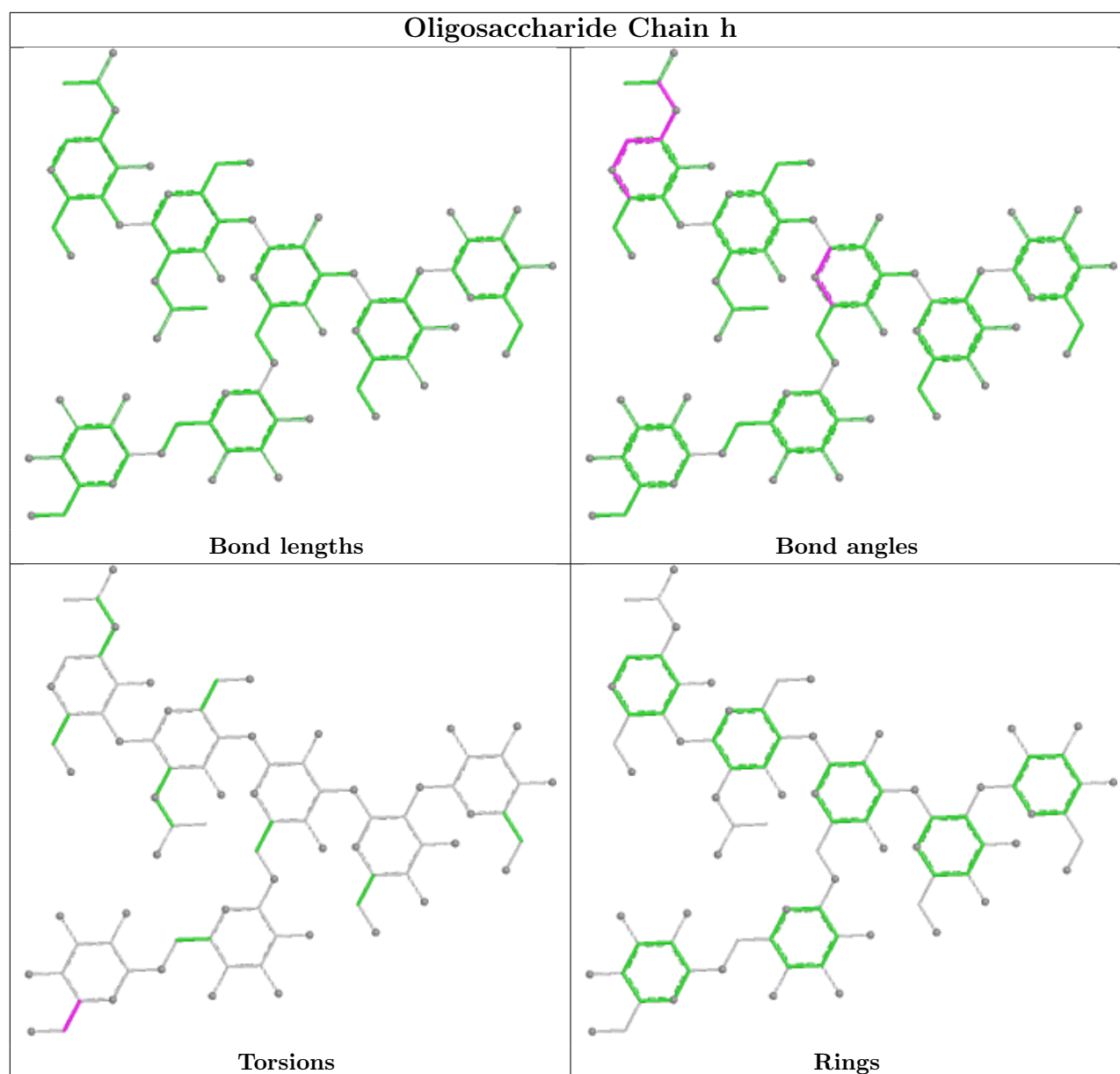


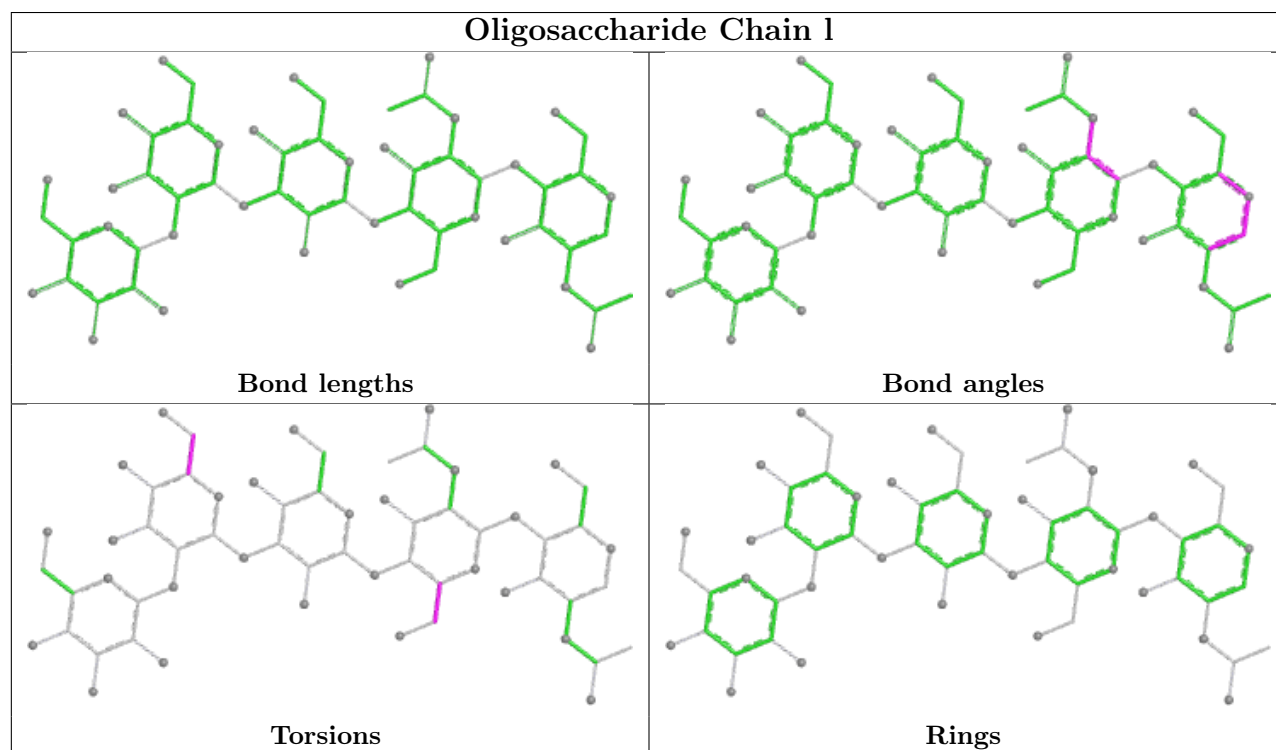
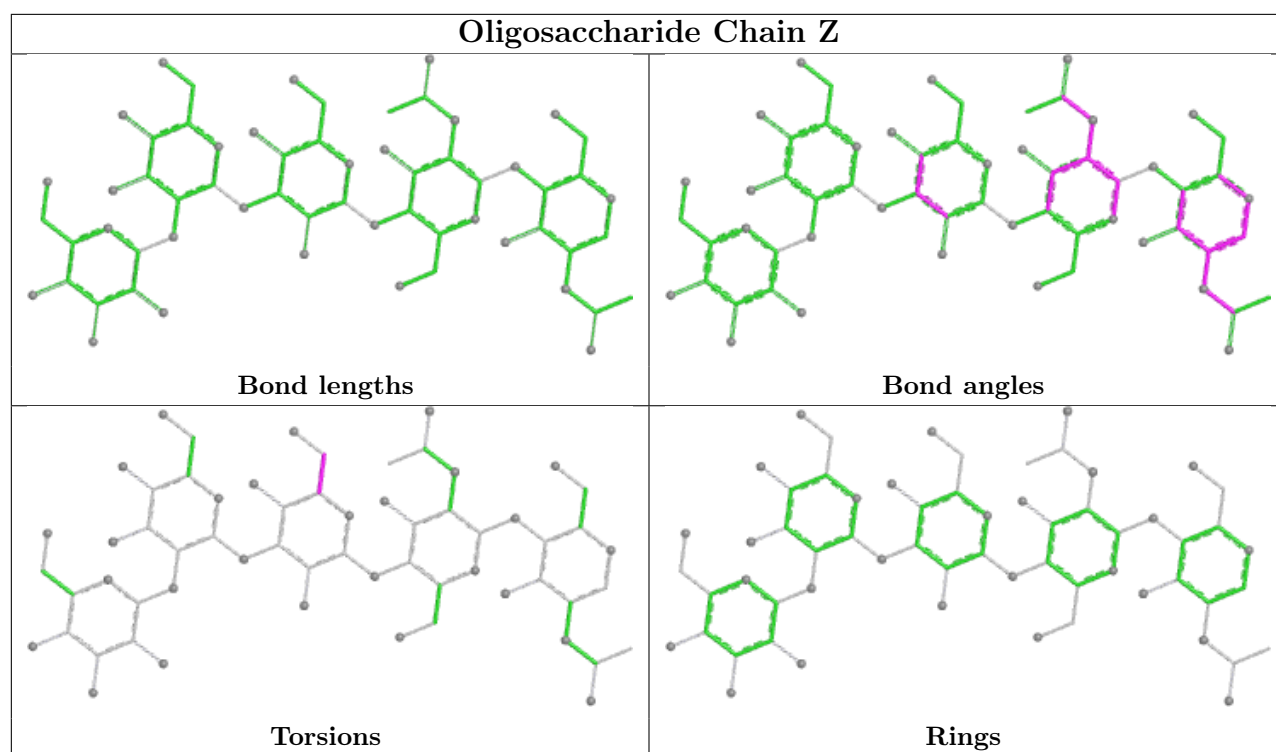


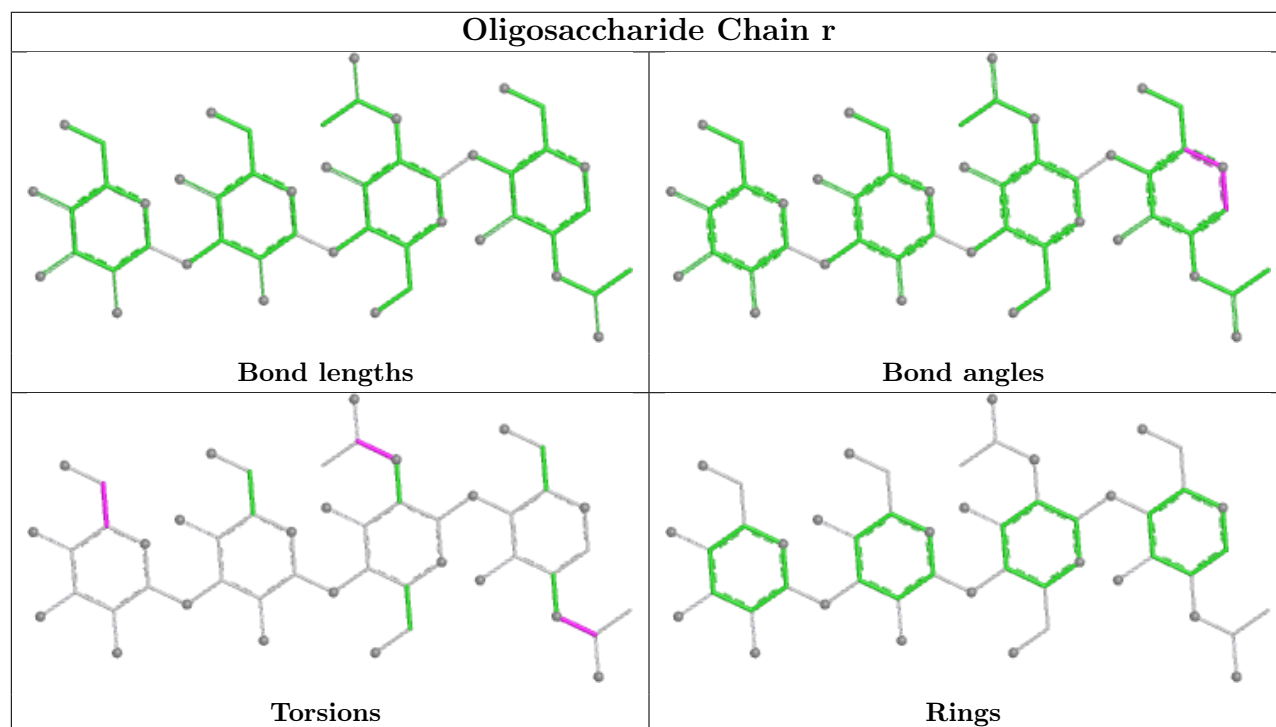
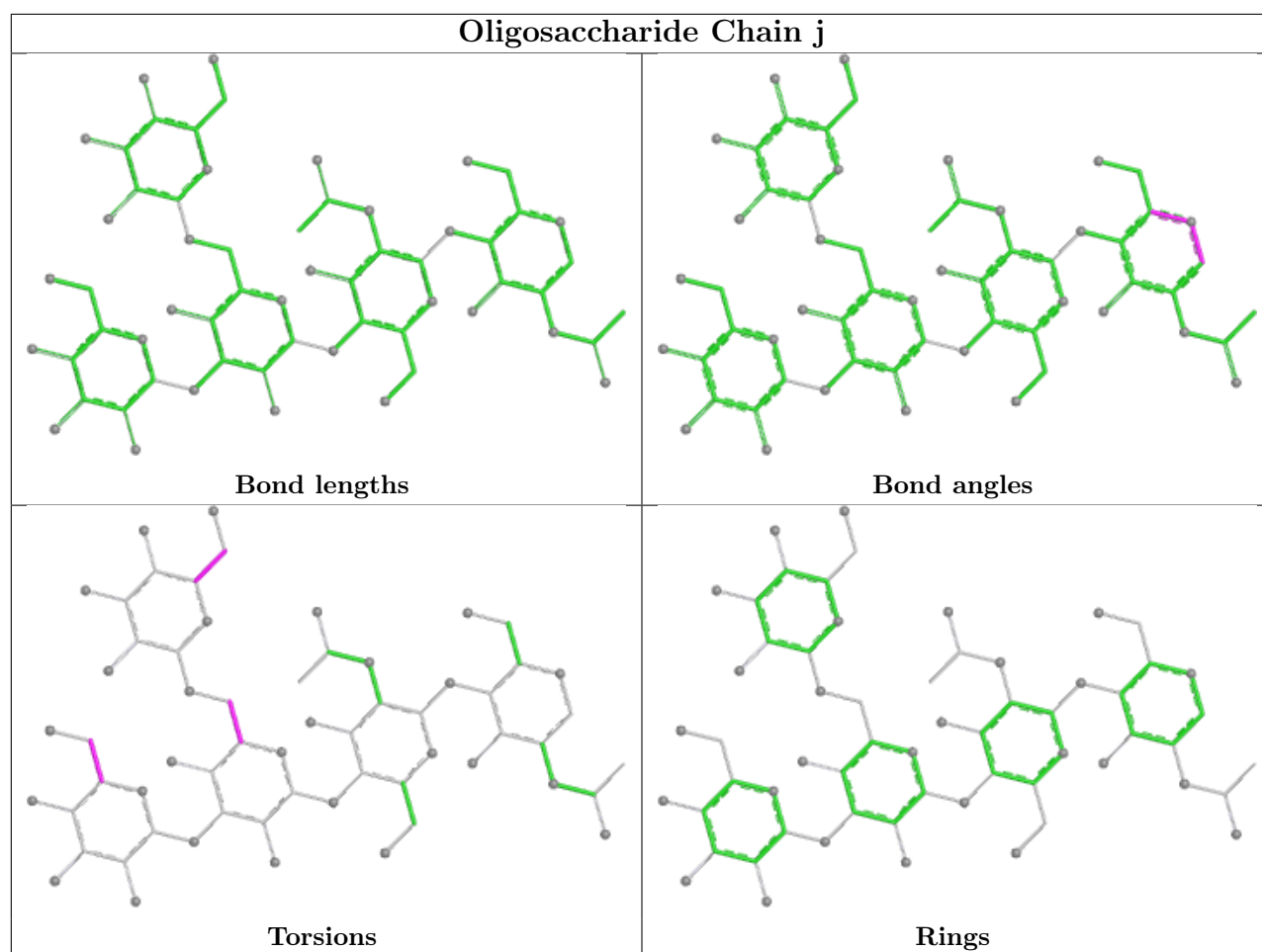












## 5.6 Ligand geometry

20 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	$\# Z  > 2$
18	NAG	G	601	5	14,14,15	0.40	0	17,19,21	0.84	0
18	NAG	A	603	5	14,14,15	0.56	0	17,19,21	1.26	3 (17%)
18	NAG	D	702	6	14,14,15	0.34	0	17,19,21	0.63	0
18	NAG	B	702	6	14,14,15	0.27	0	17,19,21	0.76	0
18	NAG	G	604	5	14,14,15	0.28	0	17,19,21	0.87	1 (5%)
18	NAG	G	603	5	14,14,15	0.39	0	17,19,21	0.92	0
18	NAG	C	602	5	14,14,15	0.55	0	17,19,21	1.17	2 (11%)
18	NAG	G	602	5	14,14,15	0.38	0	17,19,21	0.91	0
18	NAG	C	601	5	14,14,15	0.46	0	17,19,21	1.15	2 (11%)
18	NAG	I	701	6	14,14,15	0.37	0	17,19,21	0.69	0
18	NAG	A	607	5	14,14,15	0.51	0	17,19,21	1.17	2 (11%)
18	NAG	A	602	5	14,14,15	0.52	0	17,19,21	1.33	2 (11%)
18	NAG	A	604	5	14,14,15	0.49	0	17,19,21	1.41	2 (11%)
18	NAG	A	606	5	14,14,15	0.38	0	17,19,21	1.26	3 (17%)
18	NAG	B	701	6	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
18	NAG	G	605	5	14,14,15	0.31	0	17,19,21	0.80	0
18	NAG	D	701	6	14,14,15	0.39	0	17,19,21	1.08	2 (11%)
18	NAG	A	601	5	14,14,15	0.52	0	17,19,21	1.21	2 (11%)
18	NAG	A	605	5	14,14,15	0.62	0	17,19,21	0.81	0
18	NAG	C	603	5	14,14,15	0.32	0	17,19,21	1.39	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
18	NAG	G	601	5	-	1/6/23/26	0/1/1/1
18	NAG	A	603	5	-	1/6/23/26	0/1/1/1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	NAG	D	702	6	-	0/6/23/26	0/1/1/1
18	NAG	B	702	6	-	0/6/23/26	0/1/1/1
18	NAG	G	604	5	-	0/6/23/26	0/1/1/1
18	NAG	G	603	5	-	0/6/23/26	0/1/1/1
18	NAG	C	602	5	-	0/6/23/26	0/1/1/1
18	NAG	G	602	5	-	0/6/23/26	0/1/1/1
18	NAG	C	601	5	-	1/6/23/26	0/1/1/1
18	NAG	I	701	6	-	1/6/23/26	0/1/1/1
18	NAG	A	607	5	-	0/6/23/26	0/1/1/1
18	NAG	A	602	5	-	1/6/23/26	0/1/1/1
18	NAG	A	604	5	-	0/6/23/26	0/1/1/1
18	NAG	A	606	5	-	0/6/23/26	0/1/1/1
18	NAG	B	701	6	-	0/6/23/26	0/1/1/1
18	NAG	G	605	5	-	1/6/23/26	0/1/1/1
18	NAG	D	701	6	-	1/6/23/26	0/1/1/1
18	NAG	A	601	5	-	1/6/23/26	0/1/1/1
18	NAG	A	605	5	-	1/6/23/26	0/1/1/1
18	NAG	C	603	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	604	NAG	C2-N2-C7	-4.18	117.30	122.90
18	A	602	NAG	C1-O5-C5	4.12	117.71	112.19
18	C	603	NAG	C1-O5-C5	4.06	117.63	112.19
18	D	701	NAG	C1-O5-C5	3.04	116.25	112.19
18	A	606	NAG	C2-N2-C7	-3.02	118.86	122.90

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	601	NAG	O5-C5-C6-O6
18	A	605	NAG	O5-C5-C6-O6
18	C	601	NAG	O5-C5-C6-O6
18	A	603	NAG	O5-C5-C6-O6
18	D	701	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	604	NAG	1	0
18	A	602	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.

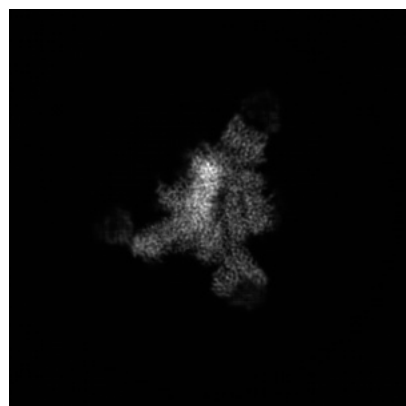
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73949. These allow visual inspection of the internal detail of the map and identification of artifacts.

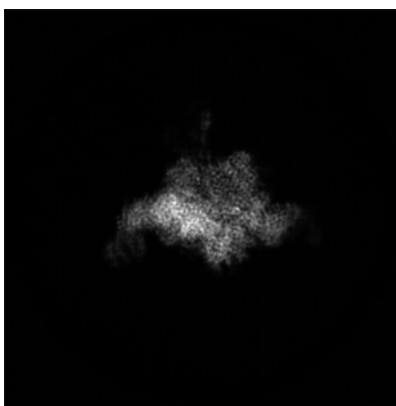
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

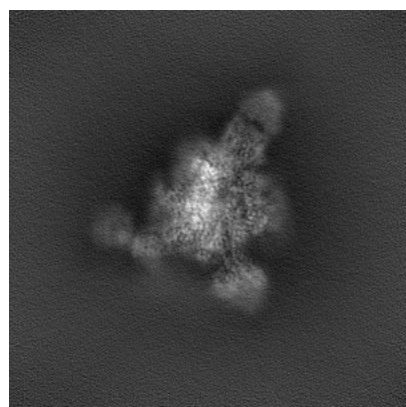


Y

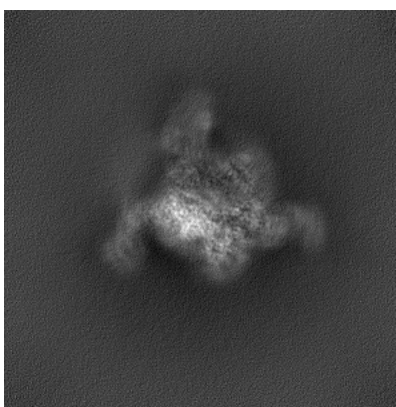


Z

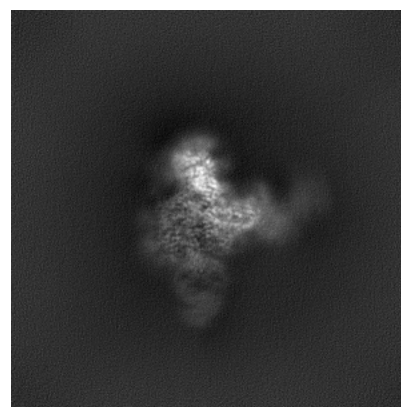
#### 6.1.2 Raw map



X



Y

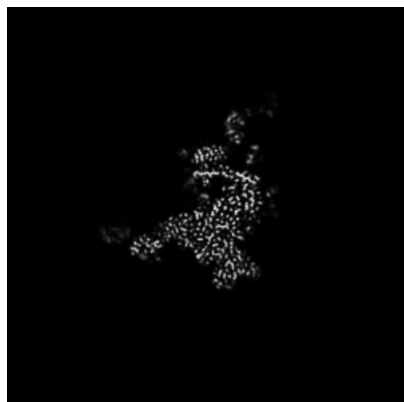


Z

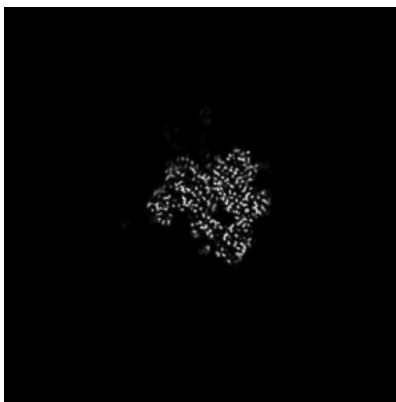
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 220

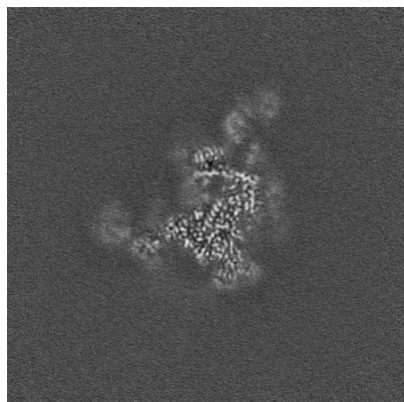


Y Index: 220

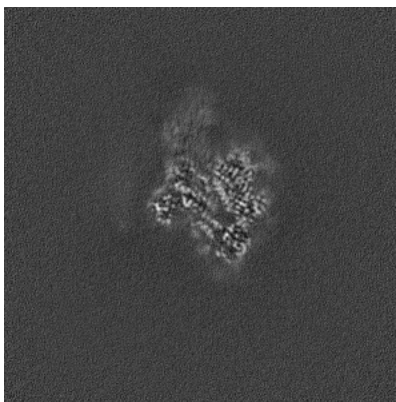


Z Index: 220

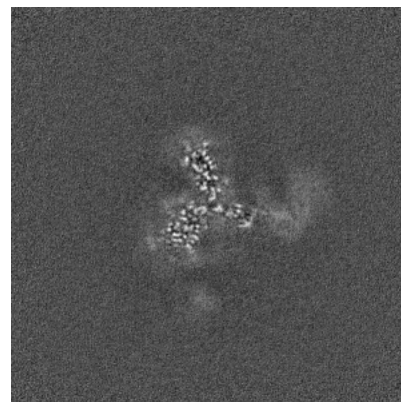
### 6.2.2 Raw map



X Index: 220



Y Index: 220



Z Index: 220

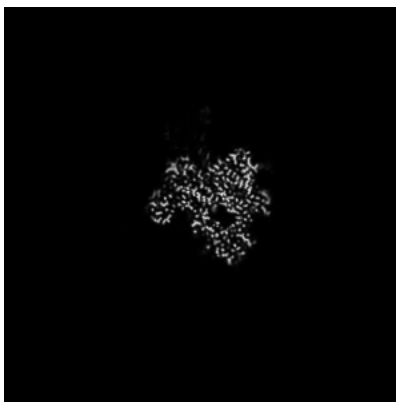
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 205

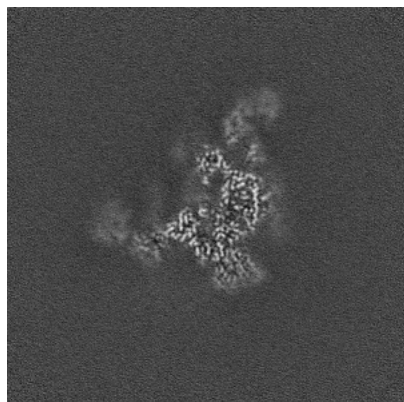


Y Index: 218

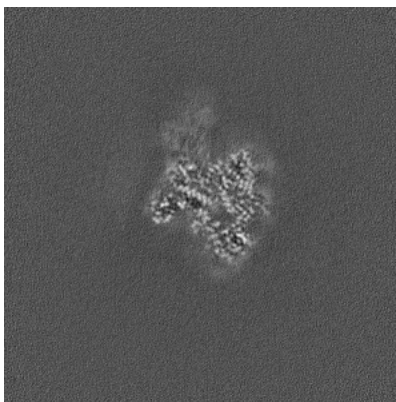


Z Index: 224

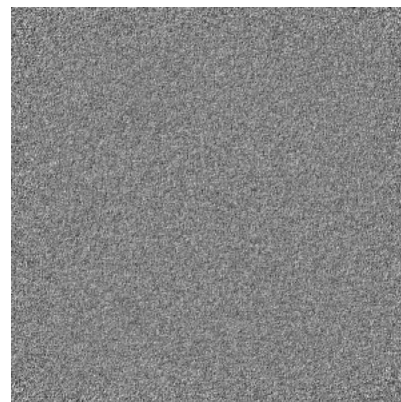
### 6.3.2 Raw map



X Index: 216



Y Index: 217

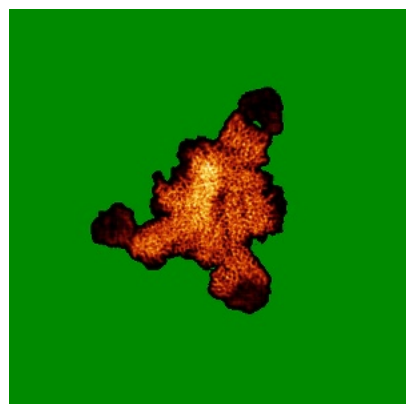


Z Index: 439

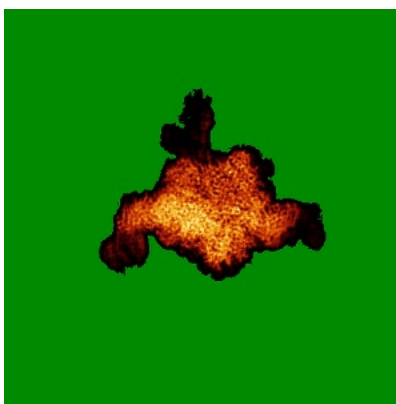
The images above show the largest variance slices of the map in three orthogonal directions.

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

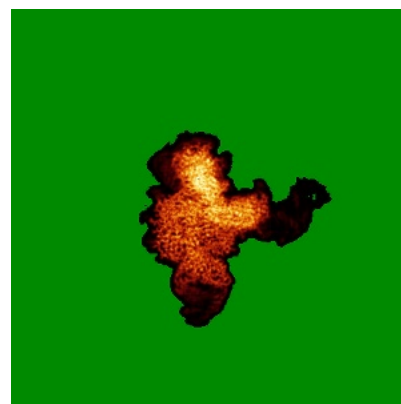
### 6.4.1 Primary map



X

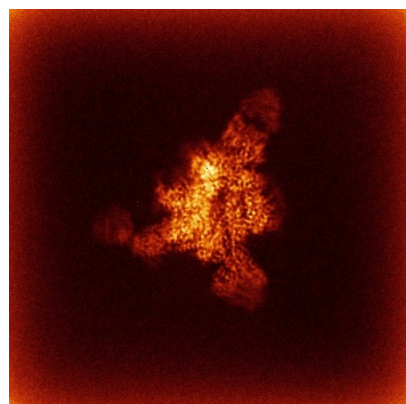


Y

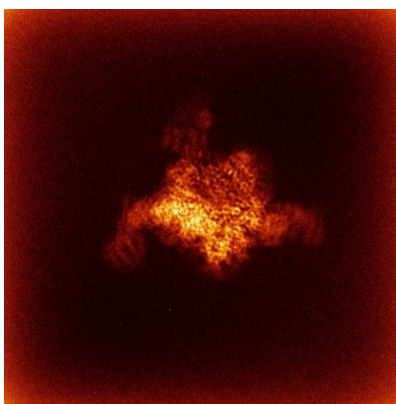


Z

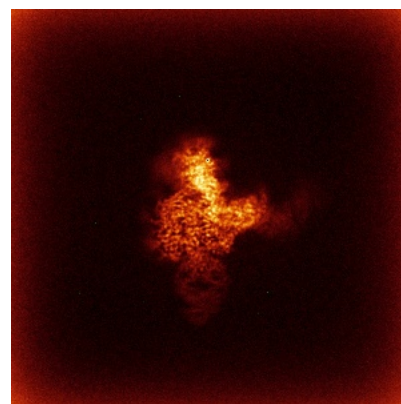
### 6.4.2 Raw map



X



Y



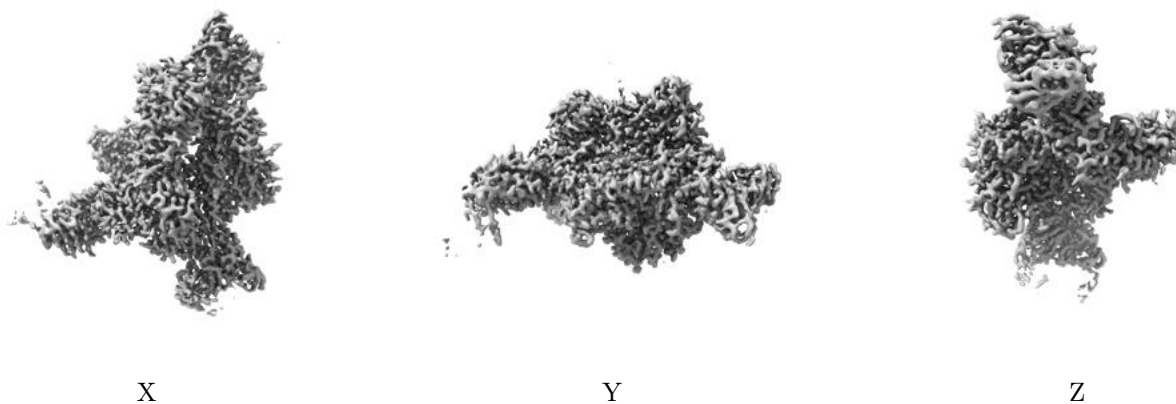
Z

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.



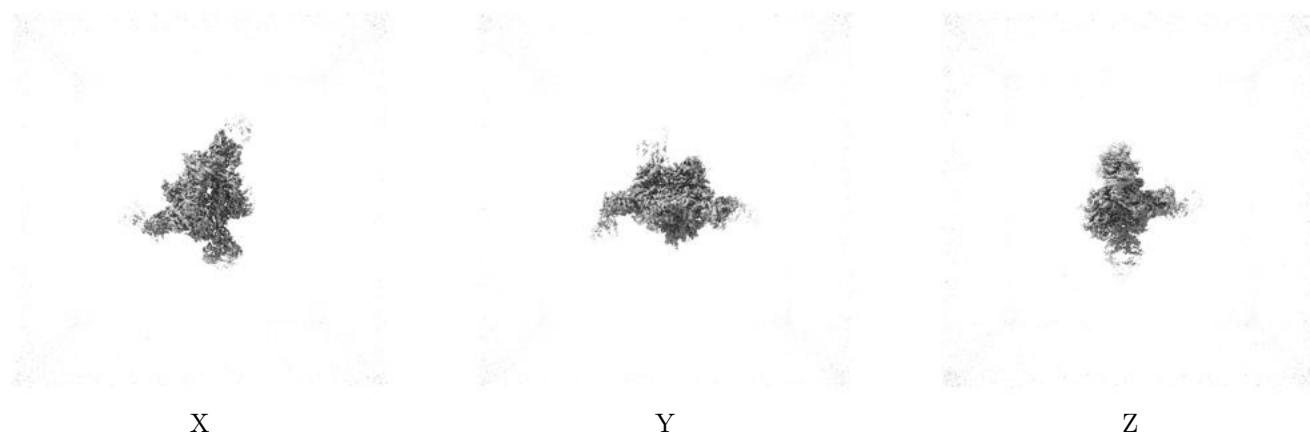
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

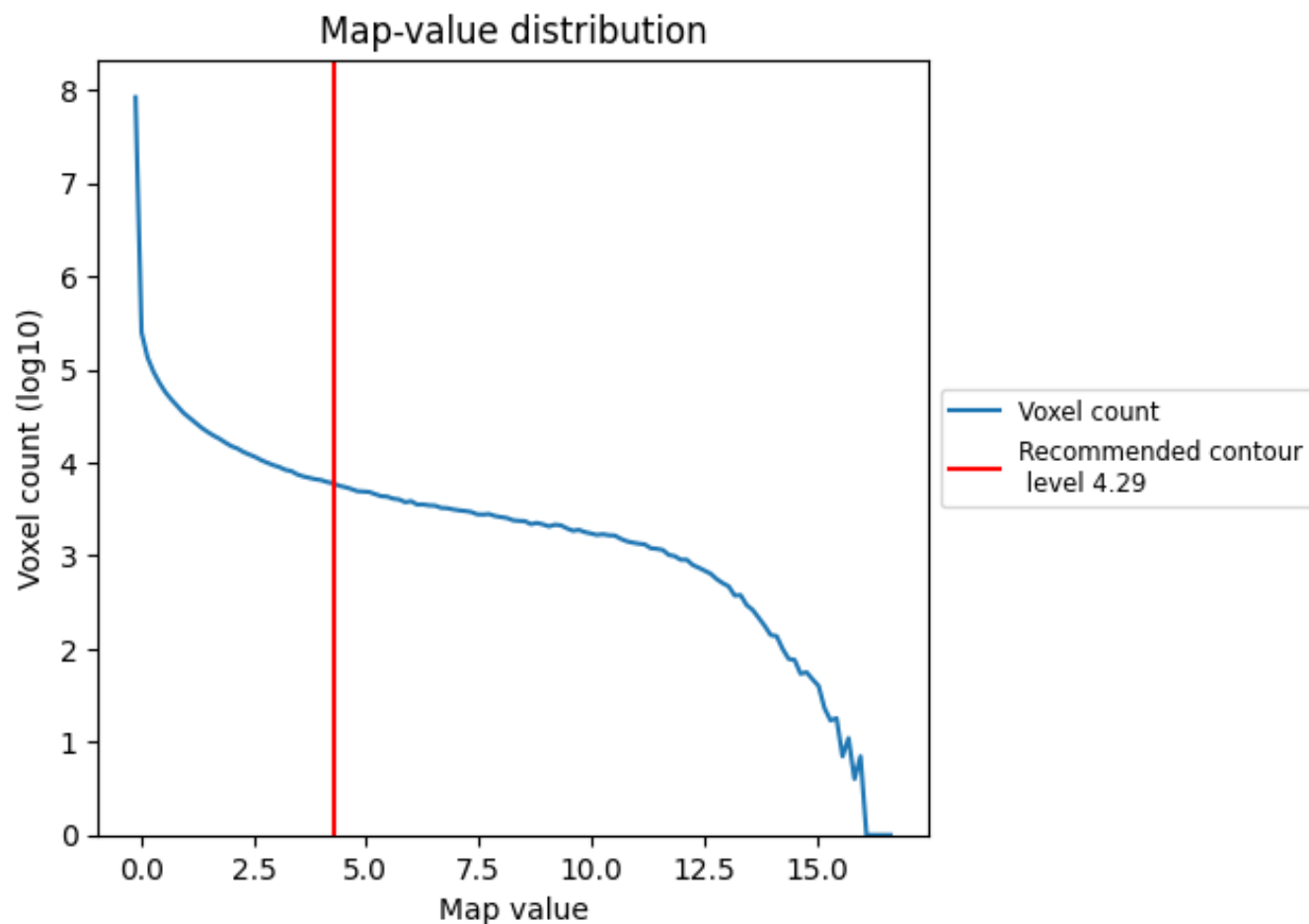
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

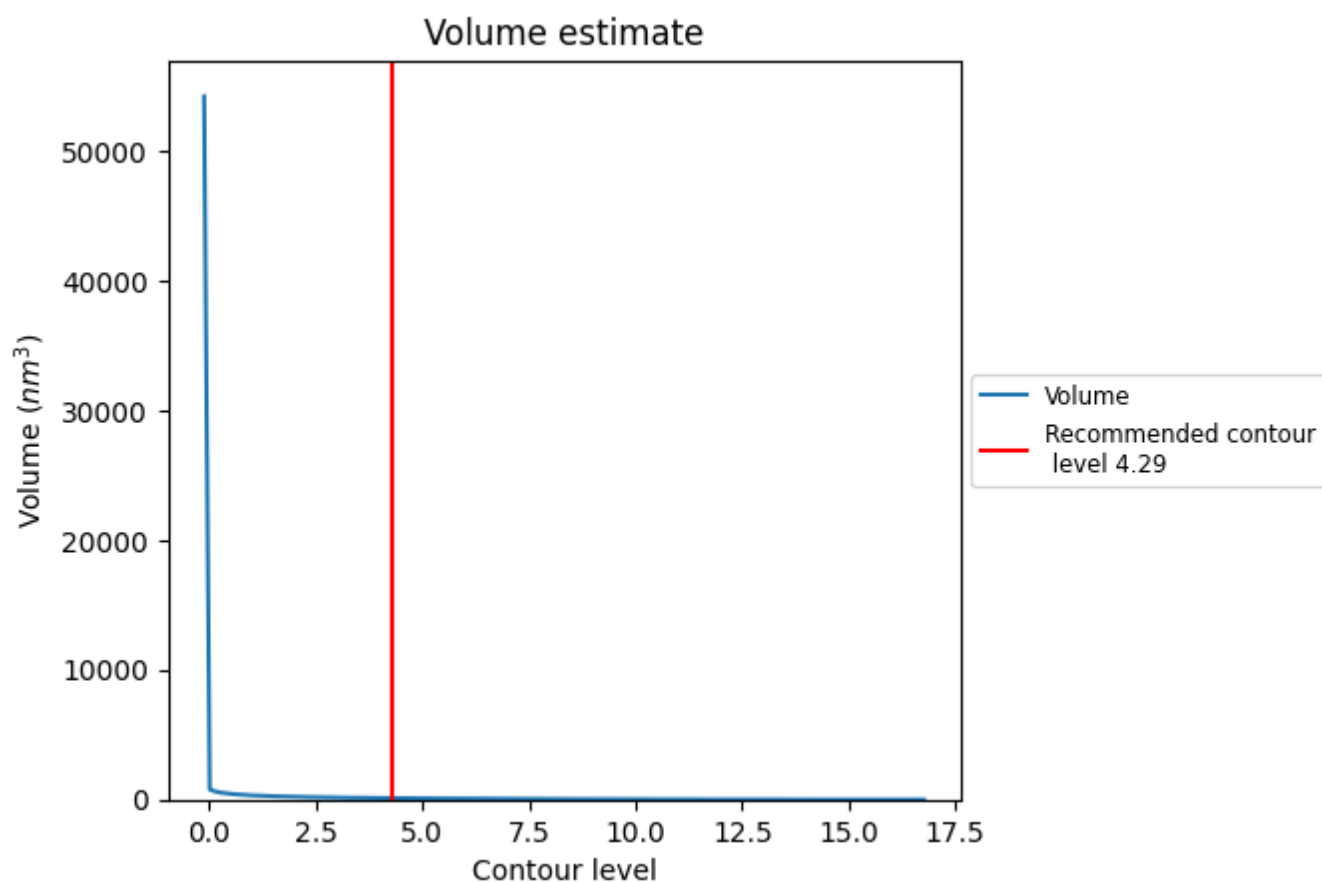
### 7.1 Map-value distribution [i](#)



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



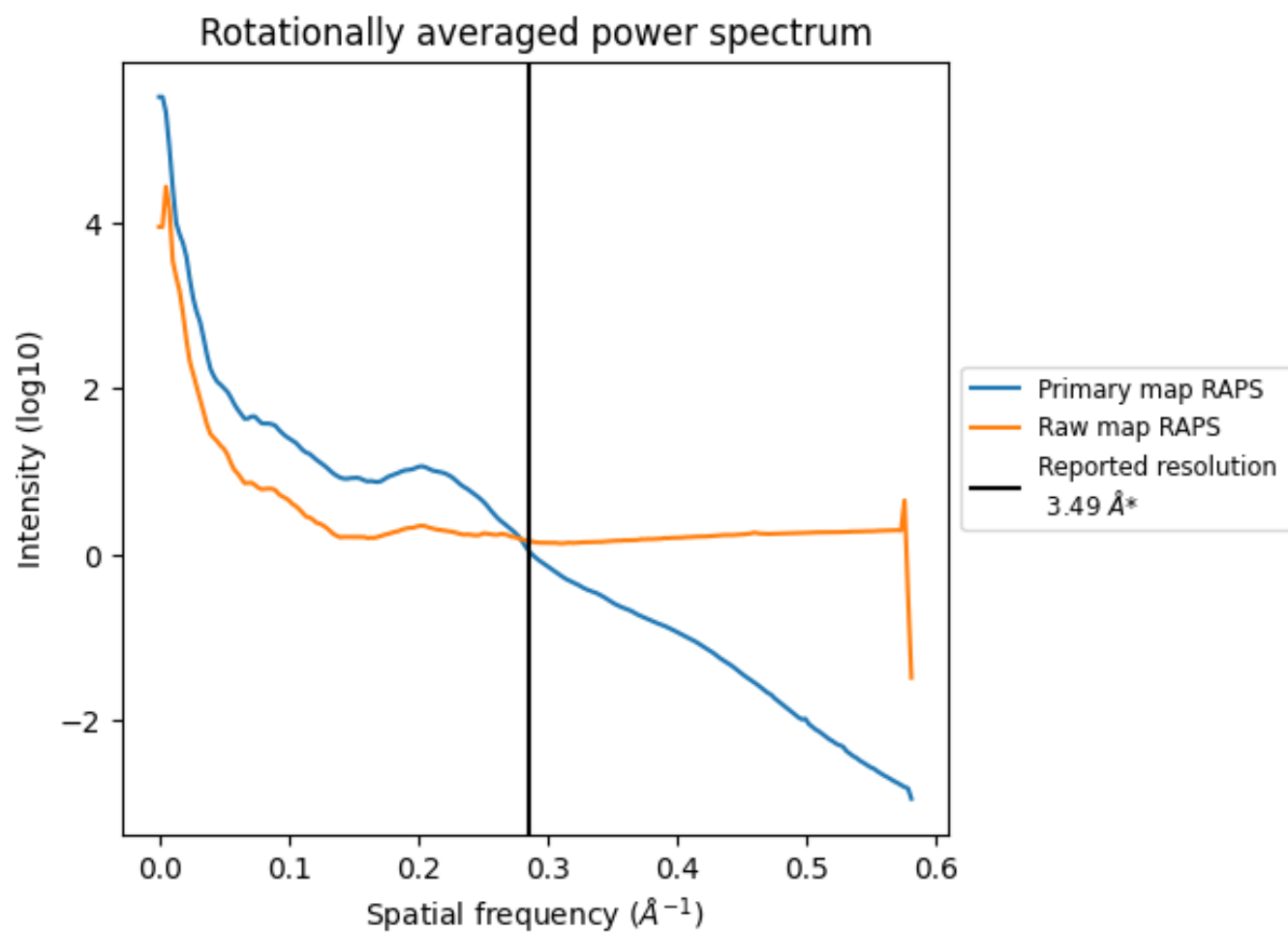
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109  $\text{nm}^3$ ; this corresponds to an approximate mass of 98 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 ⓘ

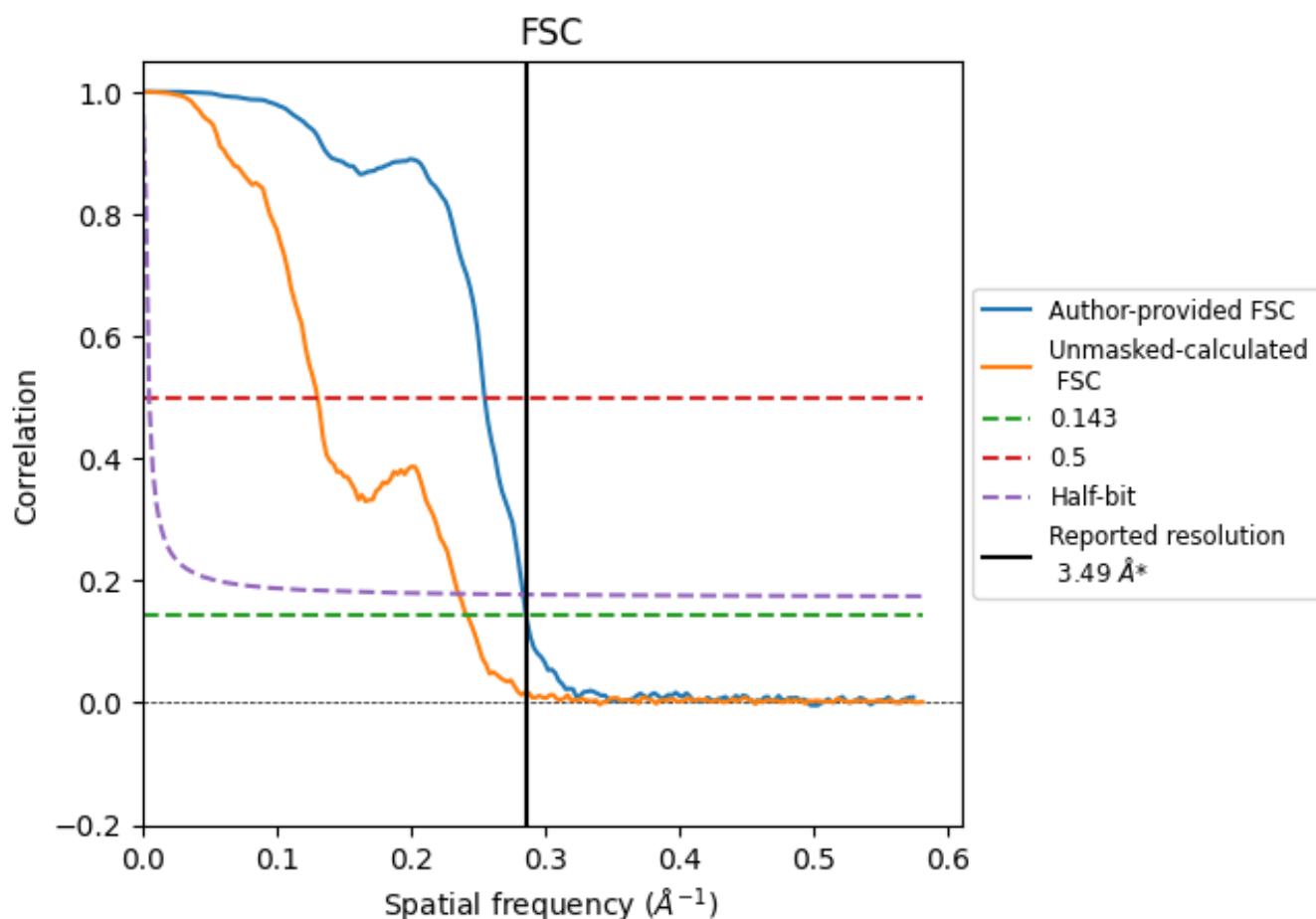


\*Reported resolution corresponds to spatial frequency of 0.287  $\text{\AA}^{-1}$

## 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  $0.287 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

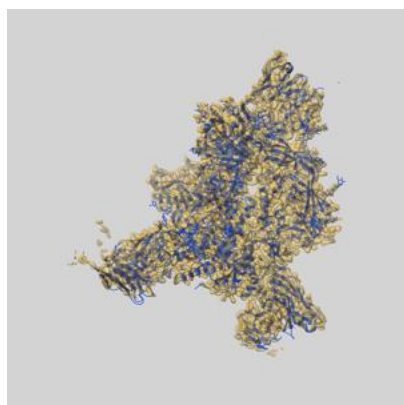
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	3.92	3.52
Unmasked-calculated*	4.13	7.66	4.24

\*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 4.13 differs from the reported value 3.49 by more than 10 %

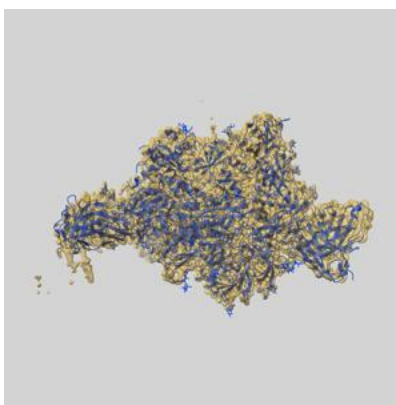
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73949 and PDB model 9Z9L. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

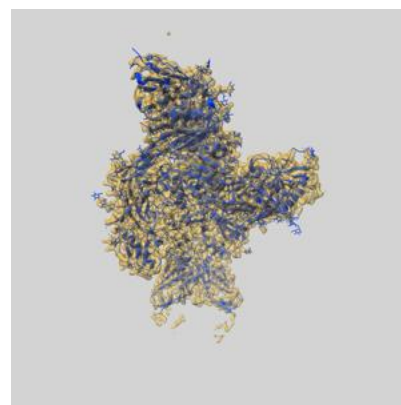
### 9.1 Map-model overlay [i](#)



X



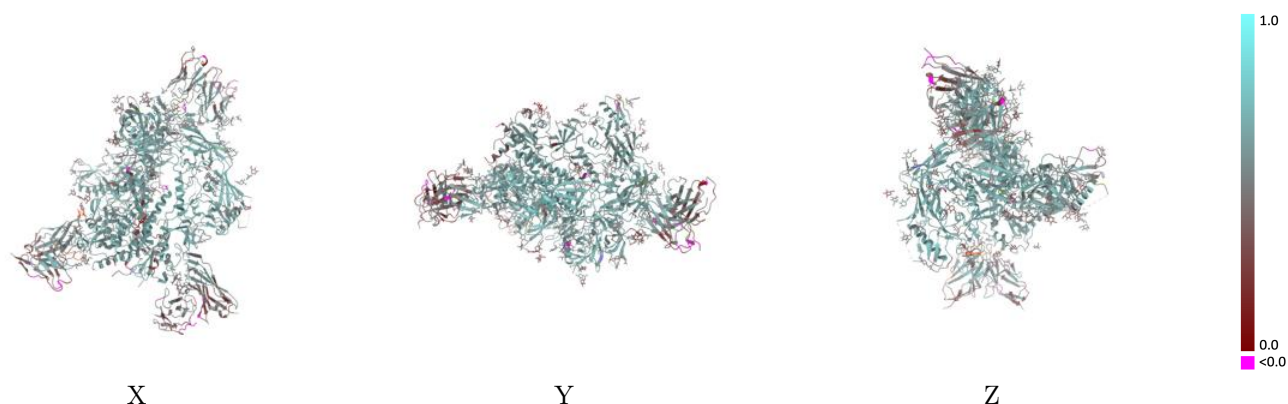
Y



Z

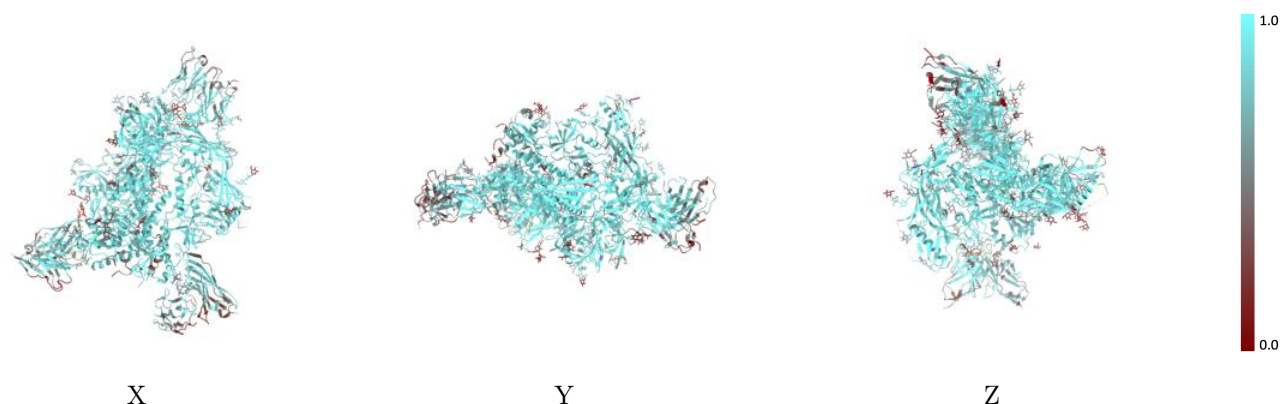
The images above show the 3D surface view of the map at the recommended contour level 4.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



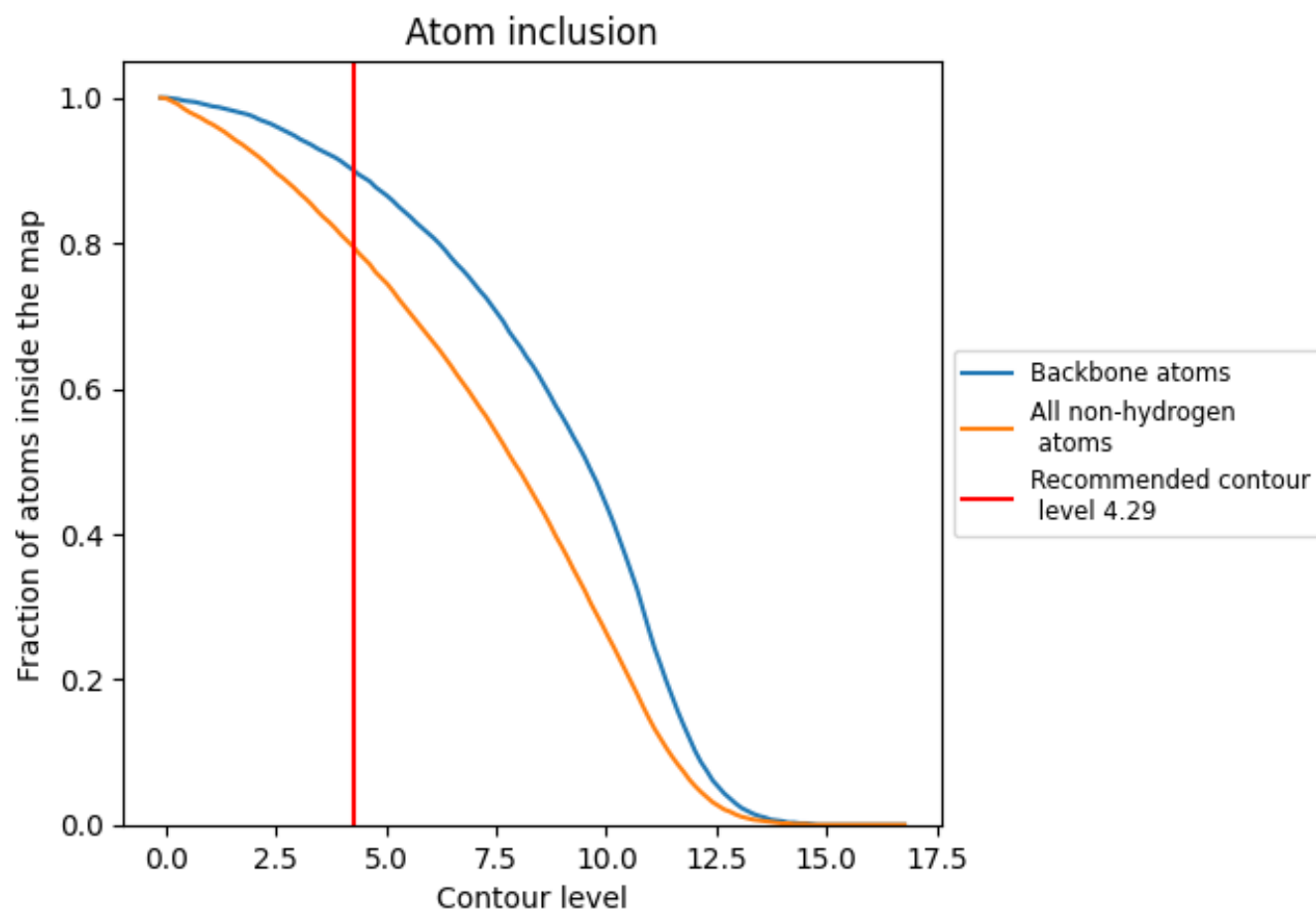
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.29).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 79% 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 (4.29) and Q-score for the entire model and for each chain.





















Chain	Atom inclusion	Q-score
All	 0.7930	 0.5490
A	 0.8890	 0.6160
B	 0.8450	 0.6200
C	 0.9030	 0.6260
D	 0.8800	 0.6410
E	 0.7410	 0.4890
F	 0.6070	 0.3940
G	 0.8350	 0.5620
H	 0.6810	 0.4560
I	 0.7770	 0.5480
J	 0.6750	 0.4370
K	 0.7220	 0.4850
L	 0.5920	 0.3760
M	 0.6940	 0.4500
N	 0.4290	 0.4340
O	 0.5000	 0.4100
P	 0.6430	 0.4250
Q	 0.4700	 0.4000
R	 0.7500	 0.5140
S	 0.6150	 0.4700
T	 0.7500	 0.5210
U	 0.2310	 0.1880
V	 0.2630	 0.3620
W	 0.5100	 0.4530
X	 0.6390	 0.4410
Y	 0.4460	 0.4390
Z	 0.6890	 0.4630
a	 0.5710	 0.4480
b	 0.6430	 0.5160
c	 0.5640	 0.4660
d	 0.6790	 0.5250
e	 0.7500	 0.5200
f	 0.2500	 0.4480
g	 0.7140	 0.4930
h	 0.6990	 0.4850



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Chain	Atom inclusion	Q-score
i	 0.1790	 0.3580
j	 0.1640	 0.3930
k	 0.5360	 0.4240
l	 0.4750	 0.4040
m	 0.6430	 0.4090
n	 0.6430	 0.4890
o	 0.6430	 0.5010
p	 0.4290	 0.3940
q	 0.4290	 0.4220
r	 0.2800	 0.2670