



## wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 07:17 PM EST

PDB ID : 7KDE  
EMDB ID : EMD-22820  
Title : BG505 SOSIP.664 in complex with the V3-targeting rhesus macaque antibody 1485 and human gp120-gp41 interface antibody 8ANC195  
Authors : Barnes, C.O.; Bjorkman, P.J.  
Deposited on : 2020-10-08  
Resolution : 3.55 Å(reported)  
Based on initial model : 6UDJ

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

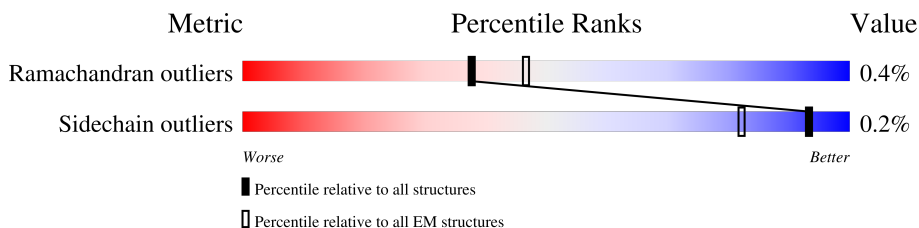
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.55 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	153	80% 20%
1	B	153	80% 20%
1	C	153	80% 20%
2	E	479	89% 10%
2	F	479	88% 10%
2	G	479	88% 10%
3	H	233	54% 45%
3	J	233	55% 45%
3	M	233	55% 45%

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Mol	Chain	Length	Quality of chain
4	O	244	54% 46%
4	Q	244	54% 46%
4	S	244	54% 46%
5	P	215	50% 50%
5	R	215	50% 50%
5	T	215	50% 50%
6	I	216	10% 46% 52%
6	L	216	10% 46% 52%
6	N	216	10% 46% 52%
7	D	4	25% 50% 75%
8	K	3	33% 67%
9	U	3	100%
9	X	3	67% 33%
9	Y	3	100%
10	V	4	50% 50%
10	b	4	50% 50%
11	W	9	33% 67%
12	Z	7	14% 86%
12	f	7	14% 86%
13	a	2	100%
13	d	2	100%
13	g	2	100%
13	h	2	100%
13	k	2	100%
13	m	2	100%

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Mol	Chain	Length	Quality of chain
13	o	2	 100%
13	p	2	 100%
14	c	8	 100%
14	j	8	 25%  75%
15	e	5	 100%
15	i	5	 40%  60%
15	l	5	 80%  20%
16	n	6	 17%  83%

## 2 Entry composition i

There are 17 unique types of molecules in this entry. The entry contains 25487 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 HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	123	982	622	169	185	6	0	0
1	B	123	982	622	169	185	6	0	0
1	C	123	982	622	169	185	6	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	engineered mutation	UNP Q2N0S6
A	605	CYS	THR	engineered mutation	UNP Q2N0S6
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
C	559	PRO	ILE	engineered mutation	UNP Q2N0S6
C	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	429	3378	2126	597	628	27	0	0
2	F	429	3378	2126	597	628	27	0	0
2	G	429	3378	2126	597	628	27	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	510	ARG	-	expression tag	UNP Q2N0S6
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6
F	332	ASN	THR	conflict	UNP Q2N0S6
F	501	CYS	ALA	conflict	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	511	ARG	-	expression tag	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called Ab 1485 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	129	Total	C	N	O	S	0	0
			1023	650	173	198	2		
3	J	129	Total	C	N	O	S	0	0
			1023	650	173	198	2		
3	M	129	Total	C	N	O	S	0	0
			1023	650	173	198	2		

- Molecule 4 is a protein called 8ANC195 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	132	Total	C	N	O	S	0	0
			970	614	162	191	3		
4	Q	132	Total	C	N	O	S	0	0
			970	614	162	191	3		
4	S	132	Total	C	N	O	S	0	0
			970	614	162	191	3		

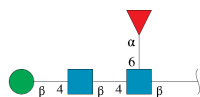
- Molecule 5 is a protein called 8ANC195 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	107	Total	C	N	O	S	0	0
			790	496	135	156	3		
5	R	107	Total	C	N	O	S	0	0
			790	496	135	156	3		
5	T	107	Total	C	N	O	S	0	0
			790	496	135	156	3		

- Molecule 6 is a protein called Ab 1485 Light Chain.

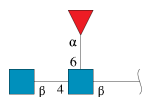
Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	103	Total	C	N	O	S	0	0
			780	483	135	159	3		
6	L	103	Total	C	N	O	S	0	0
			780	483	135	159	3		
6	N	103	Total	C	N	O	S	0	0
			780	483	135	159	3		

- Molecule 7 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.



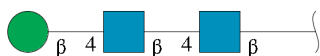
Mol	Chain	Residues	Atoms				AltConf	Trace
7	D	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



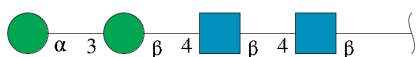
Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	3	Total	C	N	O	0	0
			38	22	2	14		

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



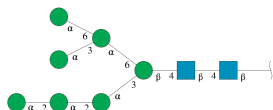
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	U	3	39	22	2	15	0	0
9	X	3	39	22	2	15	0	0
9	Y	3	39	22	2	15	0	0

- Molecule 10 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
			Total	C	N	O		
10	V	4	50	28	2	20	0	0
10	b	4	50	28	2	20	0	0

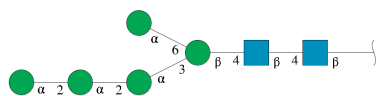
- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	W	9	105	58	2	45	0	0

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





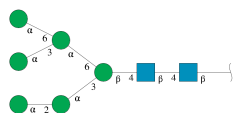
Mol	Chain	Residues	Atoms				AltConf	Trace
12	Z	7	Total	C	N	O	0	0
			83	46	2	35		
12	f	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 13 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



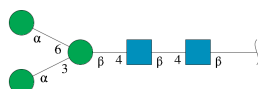
Mol	Chain	Residues	Atoms				AltConf	Trace
13	a	2	Total	C	N	O	0	0
			28	16	2	10		
13	d	2	Total	C	N	O	0	0
			28	16	2	10		
13	g	2	Total	C	N	O	0	0
			28	16	2	10		
13	h	2	Total	C	N	O	0	0
			28	16	2	10		
13	k	2	Total	C	N	O	0	0
			28	16	2	10		
13	m	2	Total	C	N	O	0	0
			28	16	2	10		
13	o	2	Total	C	N	O	0	0
			28	16	2	10		
13	p	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 14 is an oligosaccharide called 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.



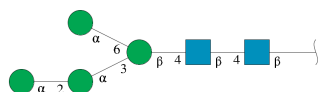
Mol	Chain	Residues	Atoms				AltConf	Trace
14	c	8	Total	C	N	O	0	0
			94	52	2	40		
14	j	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 15 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
15	e	5	Total	C	N	O	0	0
			61	34	2	25		
15	i	5	Total	C	N	O	0	0
			61	34	2	25		
15	l	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
16	n	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
17	A	1	28	16	2	10	0
17	A	1	28	16	2	10	0
17	B	1	28	16	2	10	0
17	B	1	28	16	2	10	0
17	C	1	28	16	2	10	0
17	C	1	28	16	2	10	0
17	E	1	140	80	10	50	0
17	E	1	140	80	10	50	0
17	E	1	140	80	10	50	0
17	E	1	140	80	10	50	0
17	E	1	140	80	10	50	0
17	E	1	140	80	10	50	0
17	E	1	140	80	10	50	0
17	E	1	140	80	10	50	0

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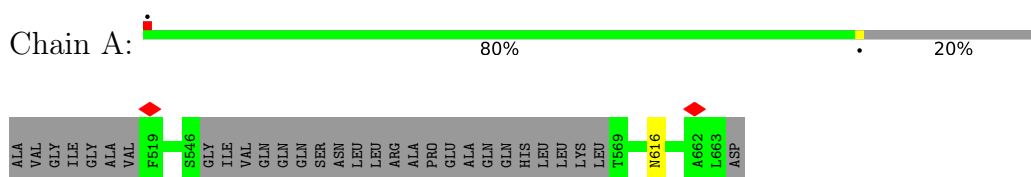
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	E	1	Total 140	C 80	N 10	O 50	0
17	E	1	Total 140	C 80	N 10	O 50	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	F	1	Total 154	C 88	N 11	O 55	0
17	G	1	Total 98	C 56	N 7	O 35	0
17	G	1	Total 98	C 56	N 7	O 35	0
17	G	1	Total 98	C 56	N 7	O 35	0
17	G	1	Total 98	C 56	N 7	O 35	0
17	G	1	Total 98	C 56	N 7	O 35	0
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17	G	1	Total 98	C 56	N 7	O 35	0

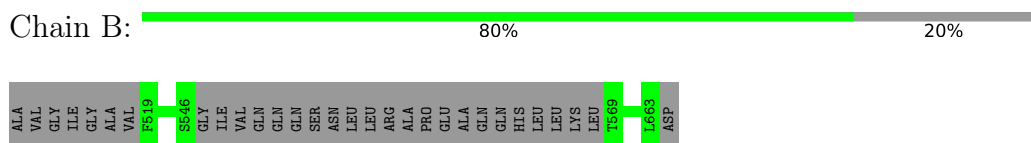
### 3 Residue-property plots [i](#)

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

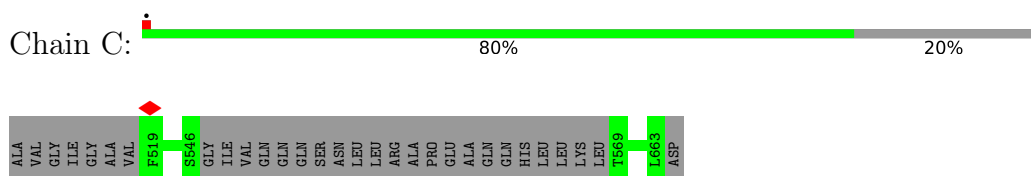
- Molecule 1: HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp41



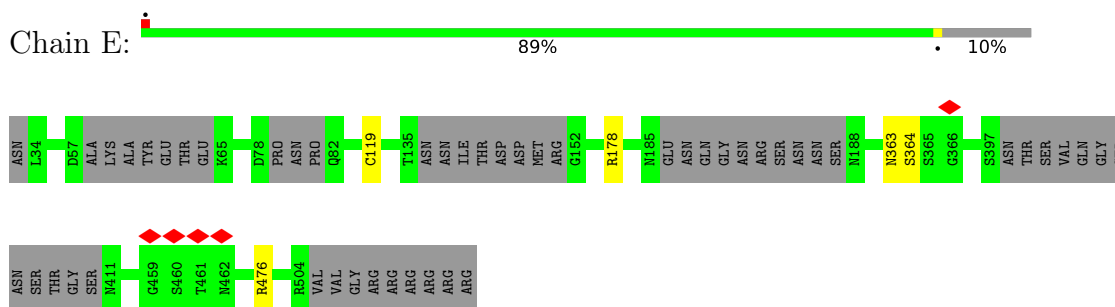
- Molecule 1: HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp41



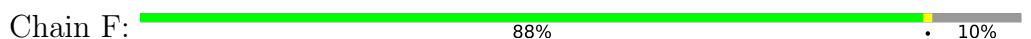
- Molecule 1: HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp41

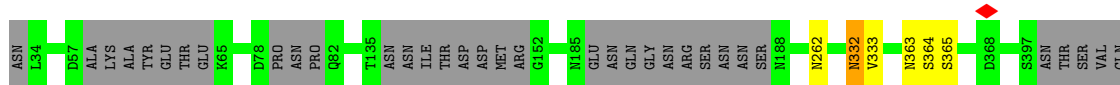


- Molecule 2: Envelope glycoprotein gp120

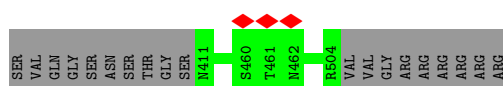
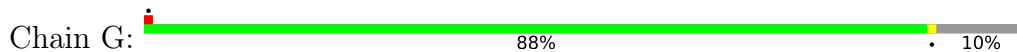


- Molecule 2: Envelope glycoprotein gp120

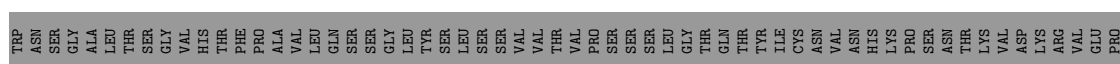
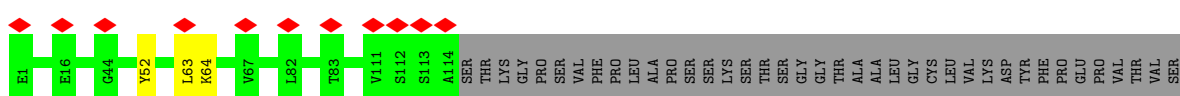




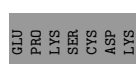
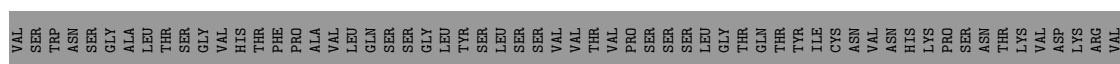
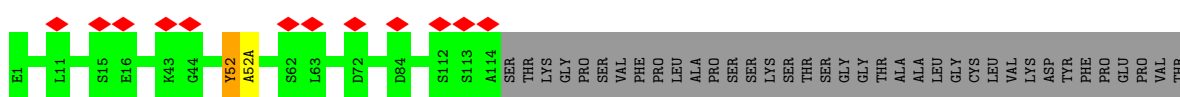
• Molecule 2: Envelope glycoprotein gp120



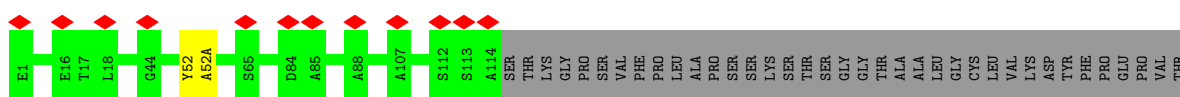
• Molecule 3: Ab 1485 Heavy Chain



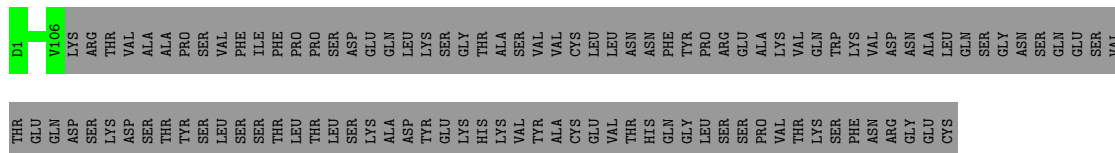
• Molecule 3: Ab 1485 Heavy Chain



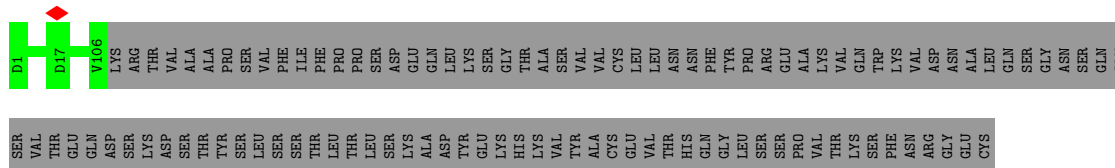
• Molecule 3: Ab 1485 Heavy Chain



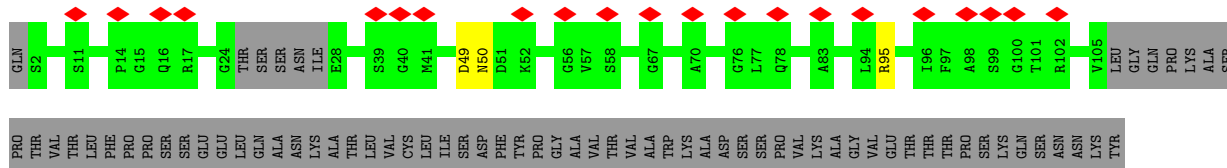




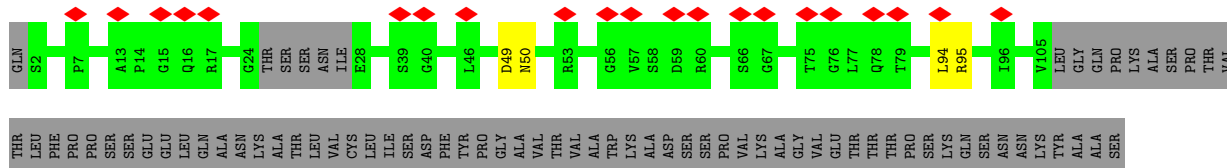
Molecule 5: 8ANC195 Fab Light Chain



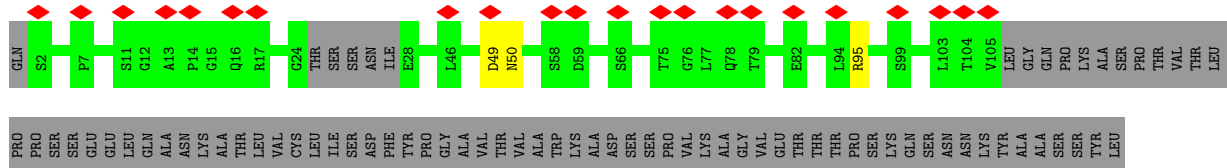
Molecule 6: Ab 1485 Light Chain



Molecule 6: Ab 1485 Light Chain



Molecule 6: Ab 1485 Light Chain





SER LEU THR PRO GLU GLN TRP LYS SER HIS ARG ARG SER TYR SER CYS GLN VAL THR HIS GLY THR SER VAL GLU LYS THR VAL ALA PRO THR GLU CYS SER

- Molecule 7: 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



MAG1  
MAG2  
BMA3  
FUC4

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



MAG1  
MAG2  
FUC3

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



MAG1  
MAG2  
BMA3

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



MAG1  
MAG2  
BMA3

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



MAG1  
MAG2  
BMA3

- Molecule 10: 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



MAG1  
MAG2  
BMA3  
MAN4

- Molecule 10: 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 b:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 11: 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

Chain W:  33% 67%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

- Molecule 12: 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

Chain Z:  14% 86%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 12: 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

Chain f:  14% 86%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1  
MAG2

- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

MAG1  
MAG2

- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  100%



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%



- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%




- Molecule 13: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%




- Molecule 14: 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

Chain c:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

- Molecule 14: 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

Chain j:  25% 75%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

- Molecule 15: 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 e:  100%


MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 15: 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 i:  40% 60%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 15: 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 l:  80% 20%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain n:  17% 83%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	405519	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.057	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	279.864, 279.864, 279.864	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.897, 0.897, 0.897	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA, FUC

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	0.45	0/1000	0.53	0/1356
1	B	0.43	0/1000	0.49	0/1356
1	C	0.43	0/1000	0.49	0/1356
2	E	0.48	0/3446	0.57	0/4672
2	F	0.47	0/3446	0.59	0/4672
2	G	0.50	0/3446	0.58	2/4672 (0.0%)
3	H	0.37	0/1052	0.58	0/1434
3	J	0.35	0/1052	0.56	0/1434
3	M	0.37	0/1052	0.62	0/1434
4	O	0.41	0/995	0.51	0/1365
4	Q	0.38	0/995	0.51	0/1365
4	S	0.39	0/995	0.49	0/1365
5	P	0.39	0/808	0.54	0/1103
5	R	0.37	0/808	0.56	0/1103
5	T	0.35	0/808	0.55	0/1103
6	I	0.31	0/796	0.52	0/1077
6	L	0.33	0/796	0.62	1/1077 (0.1%)
6	N	0.31	0/796	0.54	0/1077
All	All	0.43	0/24291	0.56	3/33021 (0.0%)

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
2	E	0	2
2	F	0	4
2	G	0	4
3	H	0	2
3	J	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	1
6	I	0	2
6	L	0	2
6	N	0	2
All	All	0	20

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	94	LEU	CA-CB-CG	6.87	131.11	115.30
2	G	333	VAL	CG1-CB-CG2	-6.29	100.84	110.90
2	G	204	ALA	C-N-CA	-5.60	107.69	121.70

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	119	CYS	Peptide
2	E	363	ASN	Peptide
2	F	262	ASN	Peptide
2	F	332	ASN	Peptide
2	F	363	ASN	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	119/153 (78%)	109 (92%)	10 (8%)	0	100	100
1	B	119/153 (78%)	115 (97%)	4 (3%)	0	100	100
1	C	119/153 (78%)	115 (97%)	4 (3%)	0	100	100
2	E	417/479 (87%)	376 (90%)	40 (10%)	1 (0%)	47	80
2	F	417/479 (87%)	366 (88%)	48 (12%)	3 (1%)	22	62
2	G	417/479 (87%)	373 (89%)	42 (10%)	2 (0%)	29	67
3	H	127/233 (54%)	88 (69%)	39 (31%)	0	100	100
3	J	127/233 (54%)	97 (76%)	28 (22%)	2 (2%)	9	46
3	M	127/233 (54%)	99 (78%)	27 (21%)	1 (1%)	19	59
4	O	130/244 (53%)	111 (85%)	19 (15%)	0	100	100
4	Q	130/244 (53%)	119 (92%)	11 (8%)	0	100	100
4	S	130/244 (53%)	117 (90%)	13 (10%)	0	100	100
5	P	105/215 (49%)	92 (88%)	13 (12%)	0	100	100
5	R	105/215 (49%)	92 (88%)	13 (12%)	0	100	100
5	T	105/215 (49%)	88 (84%)	17 (16%)	0	100	100
6	I	99/216 (46%)	85 (86%)	13 (13%)	1 (1%)	15	55
6	L	99/216 (46%)	81 (82%)	17 (17%)	1 (1%)	15	55
6	N	99/216 (46%)	83 (84%)	15 (15%)	1 (1%)	15	55
All	All	2991/4620 (65%)	2606 (87%)	373 (12%)	12 (0%)	38	71

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	333	VAL
2	G	333	VAL
2	E	364	SER
2	F	332	ASN
2	F	364	SER

### 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	106/129 (82%)	105 (99%)	1 (1%)	78	90
1	B	106/129 (82%)	106 (100%)	0	100	100
1	C	106/129 (82%)	106 (100%)	0	100	100
2	E	383/427 (90%)	381 (100%)	2 (0%)	88	95
2	F	383/427 (90%)	383 (100%)	0	100	100
2	G	383/427 (90%)	383 (100%)	0	100	100
3	H	111/202 (55%)	110 (99%)	1 (1%)	78	90
3	J	111/202 (55%)	111 (100%)	0	100	100
3	M	111/202 (55%)	111 (100%)	0	100	100
4	O	102/210 (49%)	102 (100%)	0	100	100
4	Q	102/210 (49%)	102 (100%)	0	100	100
4	S	102/210 (49%)	102 (100%)	0	100	100
5	P	80/182 (44%)	80 (100%)	0	100	100
5	R	80/182 (44%)	80 (100%)	0	100	100
5	T	80/182 (44%)	80 (100%)	0	100	100
6	I	85/184 (46%)	85 (100%)	0	100	100
6	L	85/184 (46%)	85 (100%)	0	100	100
6	N	85/184 (46%)	85 (100%)	0	100	100
All	All	2601/4002 (65%)	2597 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	616	ASN
2	E	178	ARG
2	E	476	ARG
3	H	64	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
6	I	6	GLN
6	N	6	GLN
6	N	16	GLN
2	G	425	ASN
1	B	658	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](#)

100 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	D	1	7,1	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
7	NAG	D	2	7	14,14,15	0.34	0	17,19,21	0.45	0
7	BMA	D	3	7	11,11,12	0.62	0	15,15,17	0.86	1 (6%)
7	FUC	D	4	7	10,10,11	0.72	0	14,14,16	1.08	1 (7%)
8	NAG	K	1	8,1	14,14,15	0.67	1 (7%)	17,19,21	0.73	1 (5%)
8	NAG	K	2	8	14,14,15	0.30	0	17,19,21	0.42	0
8	FUC	K	3	8	10,10,11	0.98	1 (10%)	14,14,16	1.17	2 (14%)
9	NAG	U	1	9,1	14,14,15	0.43	0	17,19,21	0.63	0
9	NAG	U	2	9	14,14,15	0.34	0	17,19,21	0.46	0
9	BMA	U	3	9	11,11,12	0.67	0	15,15,17	0.77	0
10	NAG	V	1	2,10	14,14,15	0.64	1 (7%)	17,19,21	0.49	0
10	NAG	V	2	10	14,14,15	0.26	0	17,19,21	0.46	0
10	BMA	V	3	10	11,11,12	0.43	0	15,15,17	0.85	0
10	MAN	V	4	10	11,11,12	0.75	1 (9%)	15,15,17	1.09	2 (13%)
11	NAG	W	1	2,11	14,14,15	0.29	0	17,19,21	0.58	0
11	NAG	W	2	11	14,14,15	0.26	0	17,19,21	0.68	0
11	BMA	W	3	11	11,11,12	0.65	0	15,15,17	0.71	0
11	MAN	W	4	11	11,11,12	0.54	0	15,15,17	1.10	2 (13%)
11	MAN	W	5	11	11,11,12	0.99	1 (9%)	15,15,17	1.58	2 (13%)
11	MAN	W	6	11	11,11,12	0.55	0	15,15,17	1.17	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	MAN	W	7	11	11,11,12	0.90	1 (9%)	15,15,17	0.93	1 (6%)
11	MAN	W	8	11	11,11,12	0.45	0	15,15,17	1.09	2 (13%)
11	MAN	W	9	11	11,11,12	0.59	0	15,15,17	1.15	2 (13%)
9	NAG	X	1	2,9	14,14,15	0.24	0	17,19,21	0.47	0
9	NAG	X	2	9	14,14,15	0.25	0	17,19,21	0.45	0
9	BMA	X	3	9	11,11,12	0.57	0	15,15,17	0.75	1 (6%)
9	NAG	Y	1	2,9	14,14,15	0.40	0	17,19,21	0.47	0
9	NAG	Y	2	9	14,14,15	0.36	0	17,19,21	0.57	0
9	BMA	Y	3	9	11,11,12	0.64	0	15,15,17	0.69	0
12	NAG	Z	1	2,12	14,14,15	0.75	1 (7%)	17,19,21	0.44	0
12	NAG	Z	2	12	14,14,15	0.22	0	17,19,21	0.41	0
12	BMA	Z	3	12	11,11,12	0.98	0	15,15,17	1.28	2 (13%)
12	MAN	Z	4	12	11,11,12	0.43	0	15,15,17	1.21	2 (13%)
12	MAN	Z	5	12	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
12	MAN	Z	6	12	11,11,12	0.76	0	15,15,17	1.23	2 (13%)
12	MAN	Z	7	12	11,11,12	0.56	0	15,15,17	1.13	2 (13%)
13	NAG	a	1	2,13	14,14,15	0.27	0	17,19,21	0.49	0
13	NAG	a	2	13	14,14,15	0.22	0	17,19,21	0.51	0
10	NAG	b	1	2,10	14,14,15	0.65	1 (7%)	17,19,21	0.48	0
10	NAG	b	2	10	14,14,15	0.42	0	17,19,21	0.46	0
10	BMA	b	3	10	11,11,12	0.72	0	15,15,17	0.80	0
10	MAN	b	4	10	11,11,12	0.94	1 (9%)	15,15,17	1.16	3 (20%)
14	NAG	c	1	2,14	14,14,15	0.17	0	17,19,21	0.86	1 (5%)
14	NAG	c	2	14	14,14,15	0.39	0	17,19,21	0.69	1 (5%)
14	BMA	c	3	14	11,11,12	0.97	1 (9%)	15,15,17	0.98	0
14	MAN	c	4	14	11,11,12	0.86	0	15,15,17	1.33	2 (13%)
14	MAN	c	5	14	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
14	MAN	c	6	14	11,11,12	0.80	1 (9%)	15,15,17	1.16	2 (13%)
14	MAN	c	7	14	11,11,12	0.64	0	15,15,17	1.07	2 (13%)
14	MAN	c	8	14	11,11,12	0.69	0	15,15,17	1.18	2 (13%)
13	NAG	d	1	2,13	14,14,15	0.24	0	17,19,21	0.41	0
13	NAG	d	2	13	14,14,15	0.29	0	17,19,21	0.49	0
15	NAG	e	1	2,15	14,14,15	0.44	0	17,19,21	1.25	1 (5%)
15	NAG	e	2	15	14,14,15	0.55	0	17,19,21	0.75	1 (5%)
15	BMA	e	3	15	11,11,12	1.24	2 (18%)	15,15,17	0.99	0
15	MAN	e	4	15	11,11,12	0.55	0	15,15,17	1.05	2 (13%)
15	MAN	e	5	15	11,11,12	1.06	1 (9%)	15,15,17	1.48	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	NAG	f	1	2,12	14,14,15	0.62	1 (7%)	17,19,21	0.58	0
12	NAG	f	2	12	14,14,15	0.22	0	17,19,21	0.45	0
12	BMA	f	3	12	11,11,12	1.16	1 (9%)	15,15,17	1.01	1 (6%)
12	MAN	f	4	12	11,11,12	0.66	0	15,15,17	0.93	1 (6%)
12	MAN	f	5	12	11,11,12	0.64	0	15,15,17	1.04	2 (13%)
12	MAN	f	6	12	11,11,12	0.68	0	15,15,17	1.43	2 (13%)
12	MAN	f	7	12	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
13	NAG	g	1	2,13	14,14,15	0.24	0	17,19,21	0.43	0
13	NAG	g	2	13	14,14,15	0.34	0	17,19,21	0.38	0
13	NAG	h	1	2,13	14,14,15	0.27	0	17,19,21	0.49	0
13	NAG	h	2	13	14,14,15	0.23	0	17,19,21	0.47	0
15	NAG	i	1	2,15	14,14,15	0.61	1 (7%)	17,19,21	0.46	0
15	NAG	i	2	15	14,14,15	0.30	0	17,19,21	0.59	0
15	BMA	i	3	15	11,11,12	0.48	0	15,15,17	0.97	0
15	MAN	i	4	15	11,11,12	0.81	0	15,15,17	1.04	1 (6%)
15	MAN	i	5	15	11,11,12	0.57	0	15,15,17	1.12	2 (13%)
14	NAG	j	1	2,14	14,14,15	0.44	0	17,19,21	0.64	0
14	NAG	j	2	14	14,14,15	0.50	0	17,19,21	0.60	0
14	BMA	j	3	14	11,11,12	0.82	1 (9%)	15,15,17	0.84	0
14	MAN	j	4	14	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
14	MAN	j	5	14	11,11,12	0.76	0	15,15,17	0.99	2 (13%)
14	MAN	j	6	14	11,11,12	0.75	0	15,15,17	1.11	2 (13%)
14	MAN	j	7	14	11,11,12	0.87	0	15,15,17	1.15	1 (6%)
14	MAN	j	8	14	11,11,12	0.91	1 (9%)	15,15,17	0.98	1 (6%)
13	NAG	k	1	2,13	14,14,15	0.32	0	17,19,21	0.40	0
13	NAG	k	2	13	14,14,15	0.23	0	17,19,21	0.45	0
15	NAG	l	1	2,15	14,14,15	0.27	0	17,19,21	0.56	0
15	NAG	l	2	15	14,14,15	0.47	0	17,19,21	0.51	0
15	BMA	l	3	15	11,11,12	0.81	0	15,15,17	0.91	0
15	MAN	l	4	15	11,11,12	0.77	0	15,15,17	1.03	2 (13%)
15	MAN	l	5	15	11,11,12	0.64	0	15,15,17	0.96	0
13	NAG	m	1	2,13	14,14,15	0.54	0	17,19,21	0.41	0
13	NAG	m	2	13	14,14,15	0.21	0	17,19,21	0.43	0
16	NAG	n	1	2,16	14,14,15	0.61	1 (7%)	17,19,21	0.46	0
16	NAG	n	2	16	14,14,15	0.23	0	17,19,21	0.45	0
16	BMA	n	3	16	11,11,12	1.11	0	15,15,17	1.34	2 (13%)
16	MAN	n	4	16	11,11,12	0.50	0	15,15,17	1.13	2 (13%)
16	MAN	n	5	16	11,11,12	0.56	0	15,15,17	1.04	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	MAN	n	6	16	11,11,12	0.80	1 (9%)	15,15,17	0.85	1 (6%)
13	NAG	o	1	2,13	14,14,15	0.58	1 (7%)	17,19,21	0.75	0
13	NAG	o	2	13	14,14,15	0.38	0	17,19,21	1.30	2 (11%)
13	NAG	p	1	2,13	14,14,15	0.38	0	17,19,21	0.42	0
13	NAG	p	2	13	14,14,15	0.30	0	17,19,21	0.49	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	D	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	D	2	7	-	1/6/23/26	0/1/1/1
7	BMA	D	3	7	-	0/2/19/22	0/1/1/1
7	FUC	D	4	7	-	-	0/1/1/1
8	NAG	K	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	K	2	8	-	3/6/23/26	0/1/1/1
8	FUC	K	3	8	-	-	0/1/1/1
9	NAG	U	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	U	2	9	-	2/6/23/26	0/1/1/1
9	BMA	U	3	9	-	2/2/19/22	0/1/1/1
10	NAG	V	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	V	2	10	-	2/6/23/26	0/1/1/1
10	BMA	V	3	10	-	0/2/19/22	0/1/1/1
10	MAN	V	4	10	-	2/2/19/22	0/1/1/1
11	NAG	W	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	W	2	11	-	3/6/23/26	0/1/1/1
11	BMA	W	3	11	-	0/2/19/22	0/1/1/1
11	MAN	W	4	11	-	2/2/19/22	0/1/1/1
11	MAN	W	5	11	-	2/2/19/22	0/1/1/1
11	MAN	W	6	11	-	2/2/19/22	0/1/1/1
11	MAN	W	7	11	-	0/2/19/22	0/1/1/1
11	MAN	W	8	11	-	2/2/19/22	0/1/1/1
11	MAN	W	9	11	-	2/2/19/22	0/1/1/1
9	NAG	X	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	0/6/23/26	0/1/1/1
9	BMA	X	3	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	Y	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	2/2/19/22	0/1/1/1
12	NAG	Z	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	Z	2	12	-	2/6/23/26	0/1/1/1
12	BMA	Z	3	12	-	0/2/19/22	0/1/1/1
12	MAN	Z	4	12	-	2/2/19/22	0/1/1/1
12	MAN	Z	5	12	-	2/2/19/22	0/1/1/1
12	MAN	Z	6	12	-	0/2/19/22	0/1/1/1
12	MAN	Z	7	12	-	0/2/19/22	0/1/1/1
13	NAG	a	1	2,13	-	4/6/23/26	0/1/1/1
13	NAG	a	2	13	-	0/6/23/26	0/1/1/1
10	NAG	b	1	2,10	-	3/6/23/26	0/1/1/1
10	NAG	b	2	10	-	2/6/23/26	0/1/1/1
10	BMA	b	3	10	-	2/2/19/22	0/1/1/1
10	MAN	b	4	10	-	0/2/19/22	0/1/1/1
14	NAG	c	1	2,14	-	2/6/23/26	0/1/1/1
14	NAG	c	2	14	-	1/6/23/26	0/1/1/1
14	BMA	c	3	14	-	2/2/19/22	0/1/1/1
14	MAN	c	4	14	-	0/2/19/22	0/1/1/1
14	MAN	c	5	14	-	2/2/19/22	1/1/1/1
14	MAN	c	6	14	-	0/2/19/22	0/1/1/1
14	MAN	c	7	14	-	1/2/19/22	0/1/1/1
14	MAN	c	8	14	-	2/2/19/22	0/1/1/1
13	NAG	d	1	2,13	-	0/6/23/26	0/1/1/1
13	NAG	d	2	13	-	2/6/23/26	0/1/1/1
15	NAG	e	1	2,15	-	2/6/23/26	0/1/1/1
15	NAG	e	2	15	-	2/6/23/26	0/1/1/1
15	BMA	e	3	15	-	0/2/19/22	0/1/1/1
15	MAN	e	4	15	-	0/2/19/22	0/1/1/1
15	MAN	e	5	15	-	1/2/19/22	0/1/1/1
12	NAG	f	1	2,12	-	3/6/23/26	0/1/1/1
12	NAG	f	2	12	-	2/6/23/26	0/1/1/1
12	BMA	f	3	12	-	2/2/19/22	0/1/1/1
12	MAN	f	4	12	-	2/2/19/22	0/1/1/1
12	MAN	f	5	12	-	2/2/19/22	0/1/1/1
12	MAN	f	6	12	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	f	7	12	-	2/2/19/22	0/1/1/1
13	NAG	g	1	2,13	-	3/6/23/26	0/1/1/1
13	NAG	g	2	13	-	0/6/23/26	0/1/1/1
13	NAG	h	1	2,13	-	1/6/23/26	0/1/1/1
13	NAG	h	2	13	-	2/6/23/26	0/1/1/1
15	NAG	i	1	2,15	-	3/6/23/26	0/1/1/1
15	NAG	i	2	15	-	3/6/23/26	0/1/1/1
15	BMA	i	3	15	-	2/2/19/22	0/1/1/1
15	MAN	i	4	15	-	2/2/19/22	0/1/1/1
15	MAN	i	5	15	-	2/2/19/22	0/1/1/1
14	NAG	j	1	2,14	-	2/6/23/26	0/1/1/1
14	NAG	j	2	14	-	2/6/23/26	0/1/1/1
14	BMA	j	3	14	-	2/2/19/22	0/1/1/1
14	MAN	j	4	14	-	2/2/19/22	0/1/1/1
14	MAN	j	5	14	-	2/2/19/22	0/1/1/1
14	MAN	j	6	14	-	0/2/19/22	0/1/1/1
14	MAN	j	7	14	-	2/2/19/22	0/1/1/1
14	MAN	j	8	14	-	1/2/19/22	0/1/1/1
13	NAG	k	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	k	2	13	-	2/6/23/26	0/1/1/1
15	NAG	l	1	2,15	-	2/6/23/26	0/1/1/1
15	NAG	l	2	15	-	3/6/23/26	0/1/1/1
15	BMA	l	3	15	-	0/2/19/22	0/1/1/1
15	MAN	l	4	15	-	0/2/19/22	0/1/1/1
15	MAN	l	5	15	-	1/2/19/22	0/1/1/1
13	NAG	m	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	m	2	13	-	2/6/23/26	0/1/1/1
16	NAG	n	1	2,16	-	0/6/23/26	0/1/1/1
16	NAG	n	2	16	-	3/6/23/26	0/1/1/1
16	BMA	n	3	16	-	1/2/19/22	0/1/1/1
16	MAN	n	4	16	-	2/2/19/22	0/1/1/1
16	MAN	n	5	16	-	2/2/19/22	1/1/1/1
16	MAN	n	6	16	-	1/2/19/22	0/1/1/1
13	NAG	o	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	o	2	13	-	3/6/23/26	0/1/1/1
13	NAG	p	1	2,13	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	p	2	13	-	3/6/23/26	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	e	5	MAN	C1-C2	3.36	1.59	1.52
15	e	3	BMA	C1-C2	2.96	1.58	1.52
11	W	5	MAN	C2-C3	-2.86	1.48	1.52
8	K	3	FUC	O5-C1	-2.67	1.39	1.43
12	Z	1	NAG	O5-C1	-2.64	1.39	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	e	1	NAG	C1-O5-C5	4.84	118.75	112.19
13	o	2	NAG	C2-N2-C7	4.50	129.32	122.90
12	f	6	MAN	C1-O5-C5	4.33	118.06	112.19
11	W	5	MAN	C1-O5-C5	4.02	117.64	112.19
11	W	5	MAN	O2-C2-C3	-3.61	102.91	110.14

There are no chirality outliers.

5 of 156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	j	1	NAG	C4-C5-C6-O6
13	d	2	NAG	C4-C5-C6-O6
14	c	3	BMA	C4-C5-C6-O6
13	p	2	NAG	C4-C5-C6-O6
9	X	1	NAG	O5-C5-C6-O6

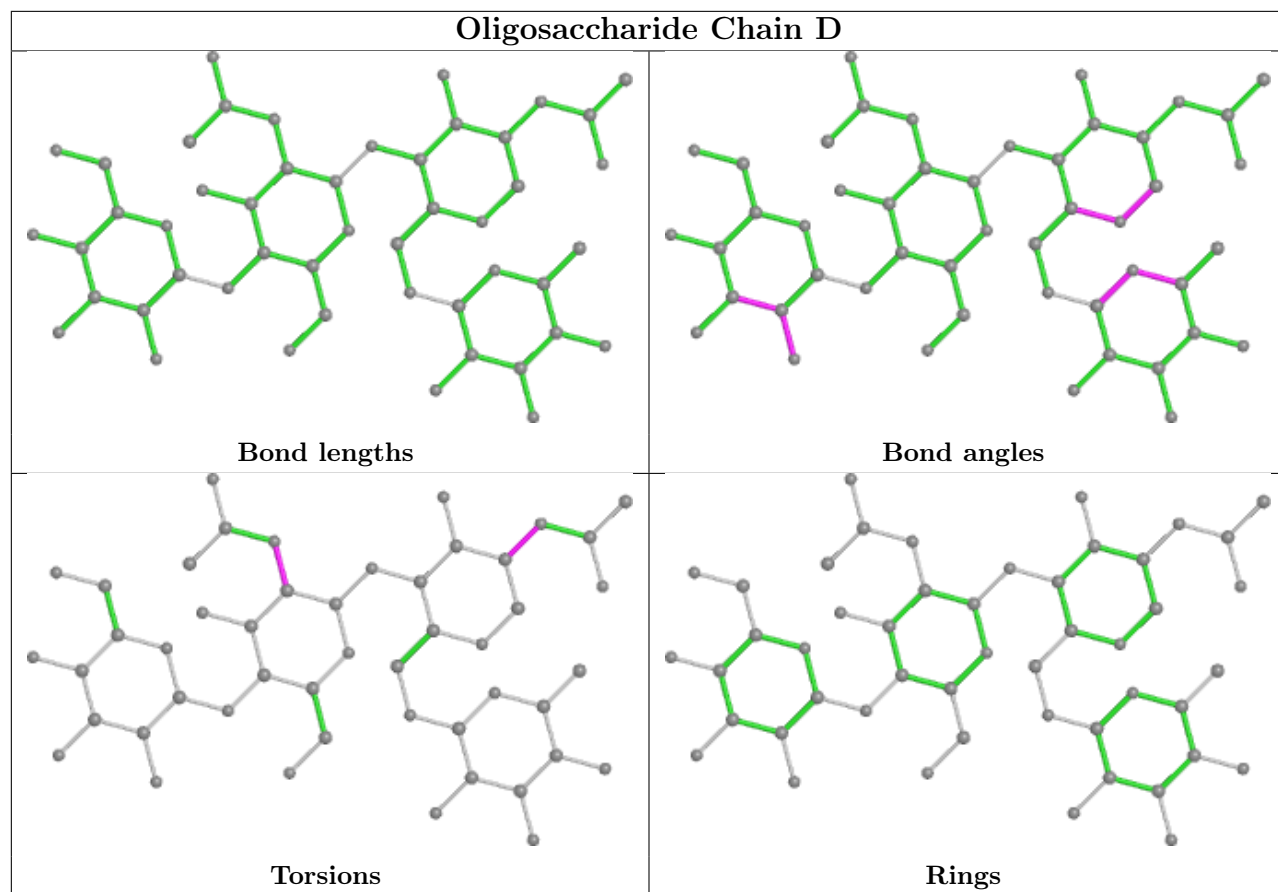
All (2) ring outliers are listed below:

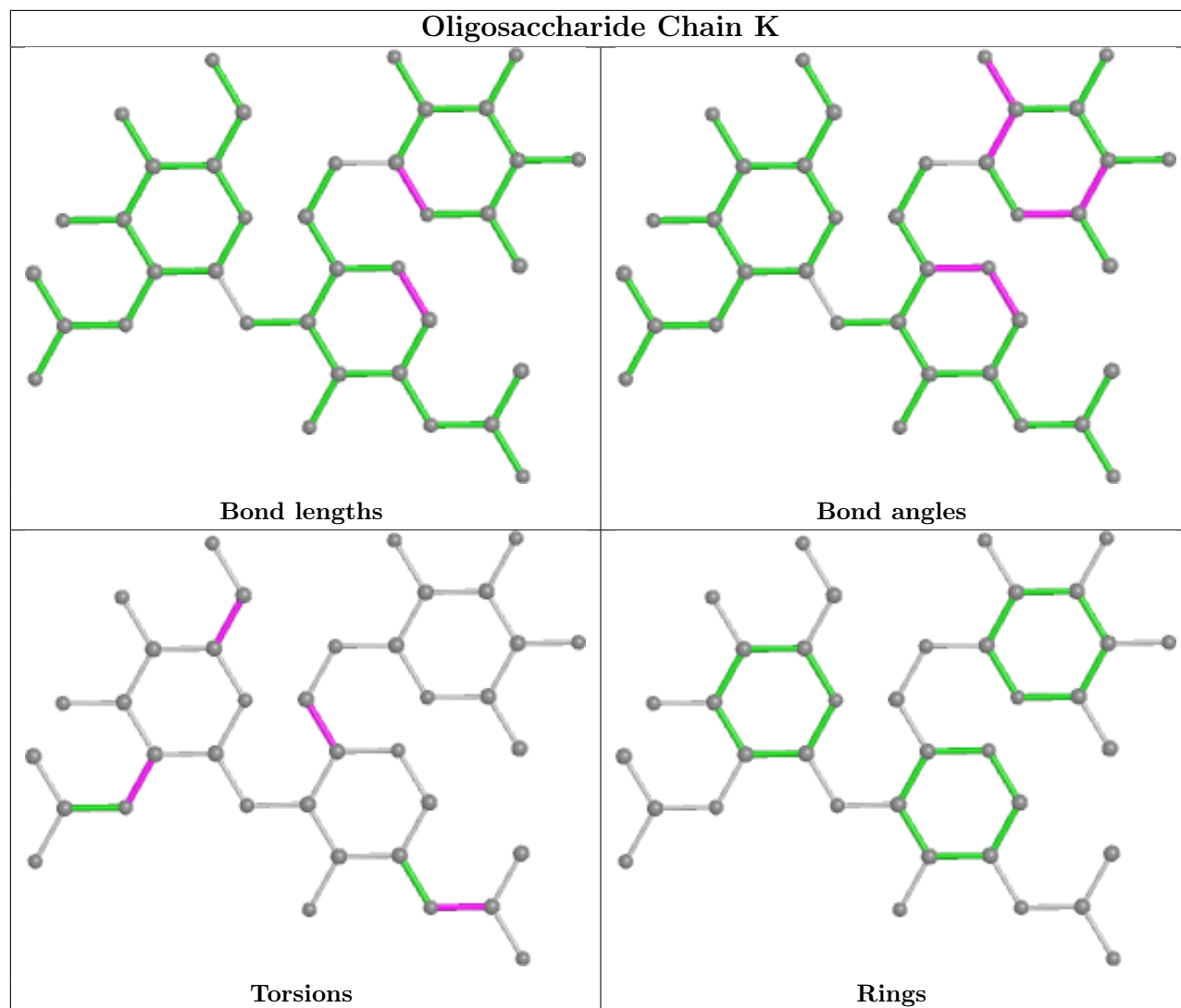
Mol	Chain	Res	Type	Atoms
14	c	5	MAN	C1-C2-C3-C4-C5-O5
16	n	5	MAN	C1-C2-C3-C4-C5-O5

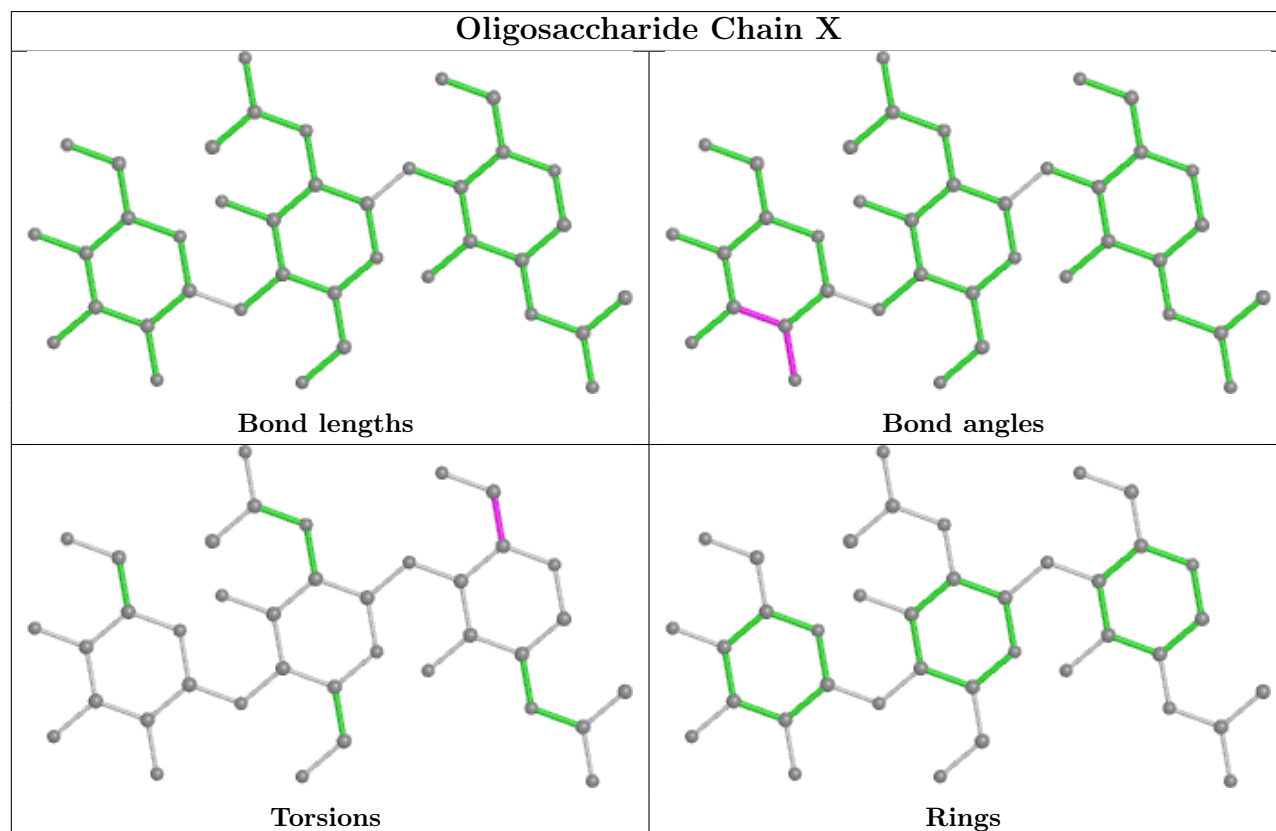
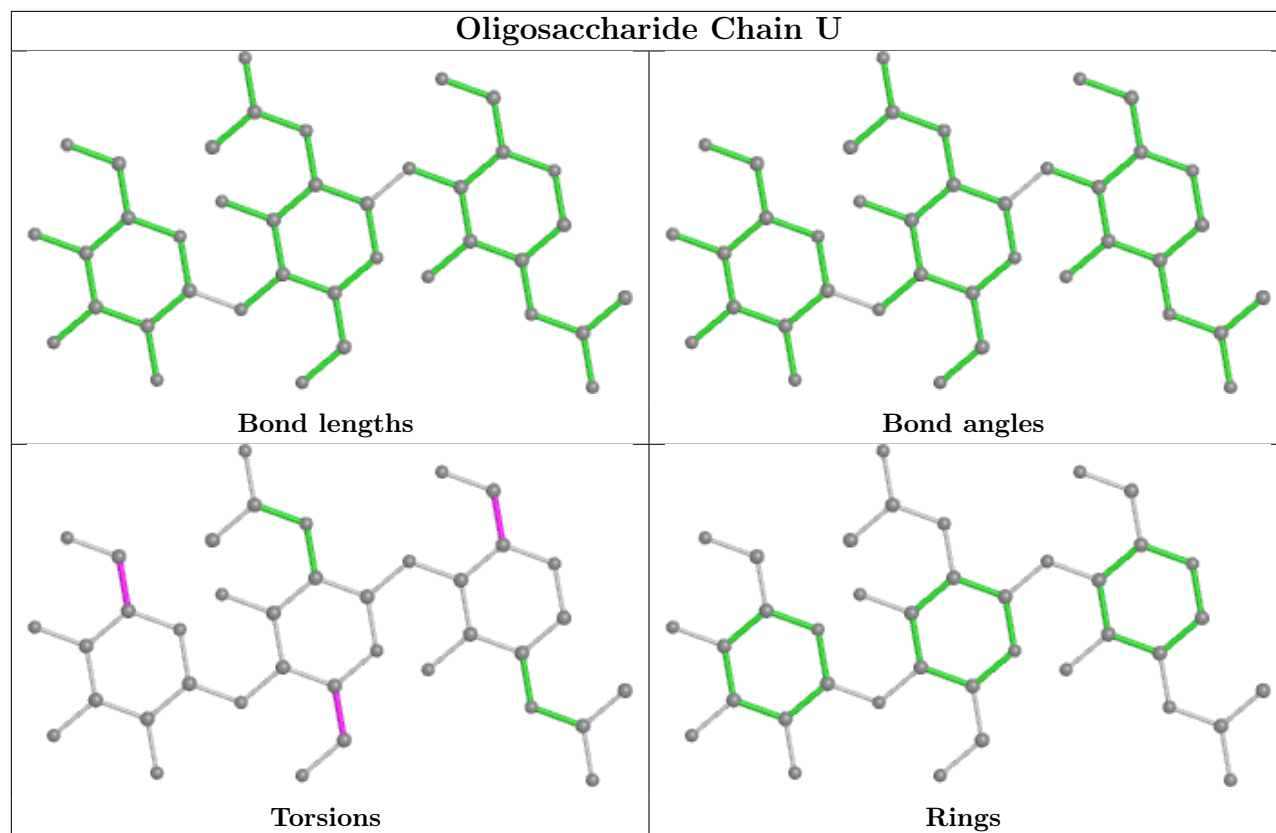
No monomer is involved in short contacts.

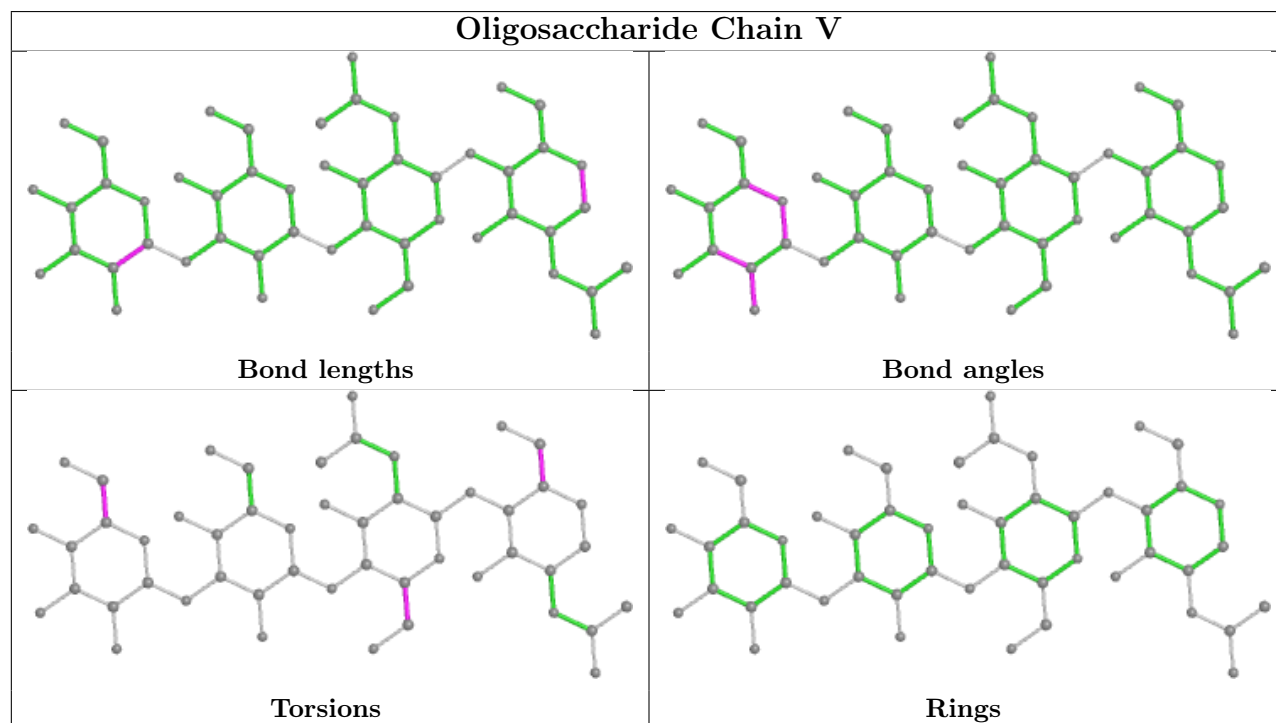
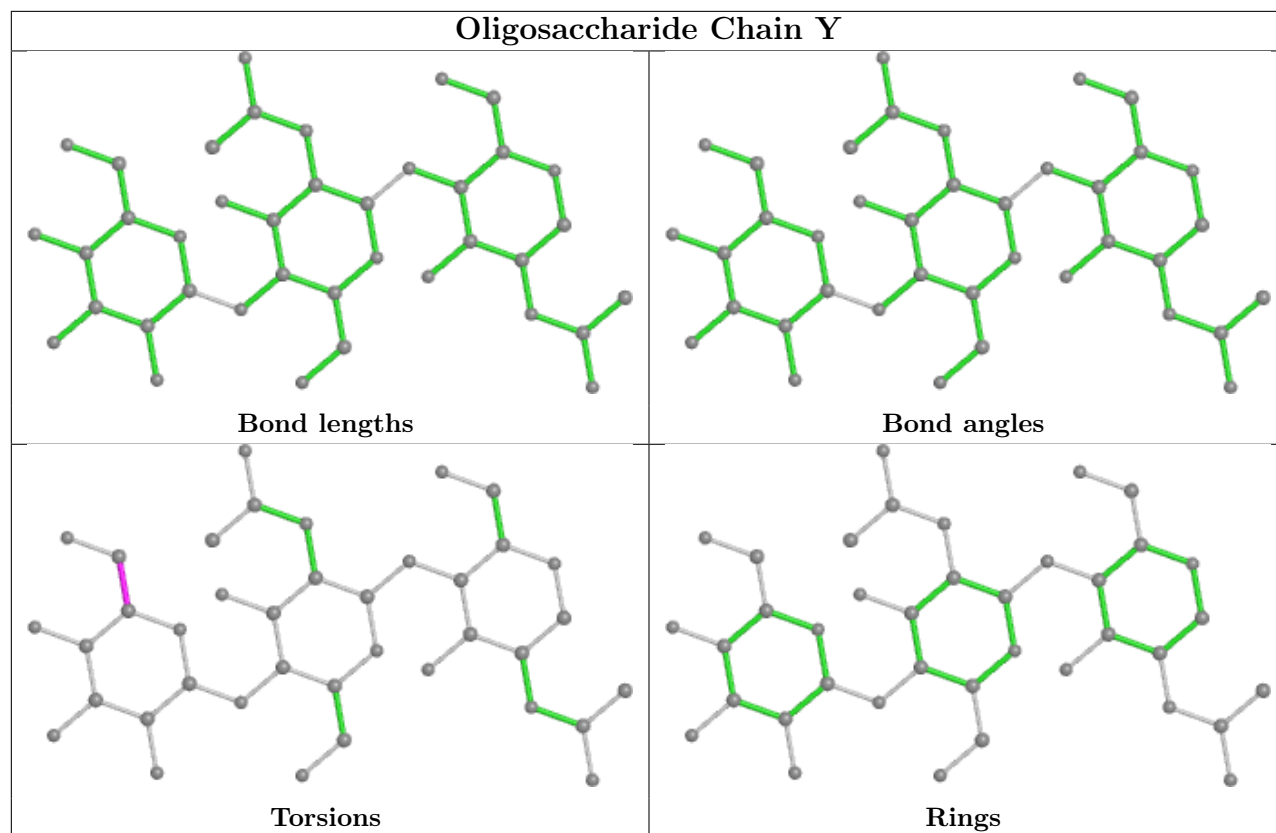
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

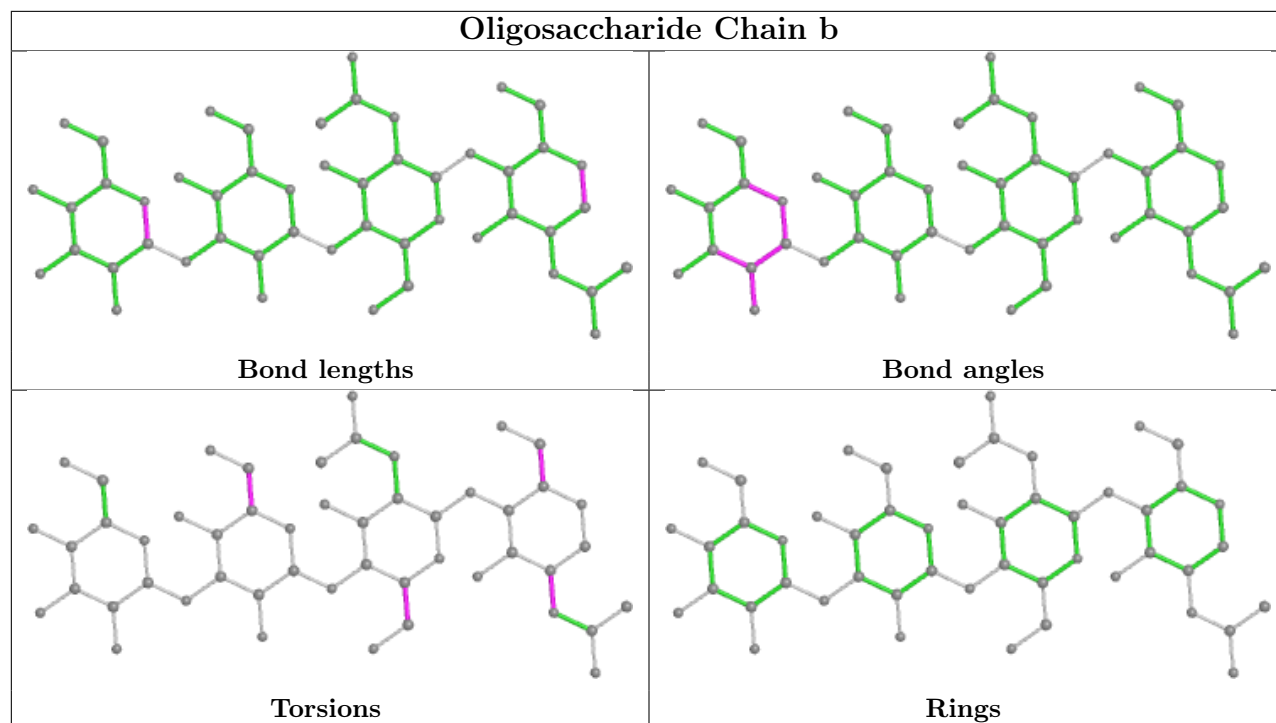


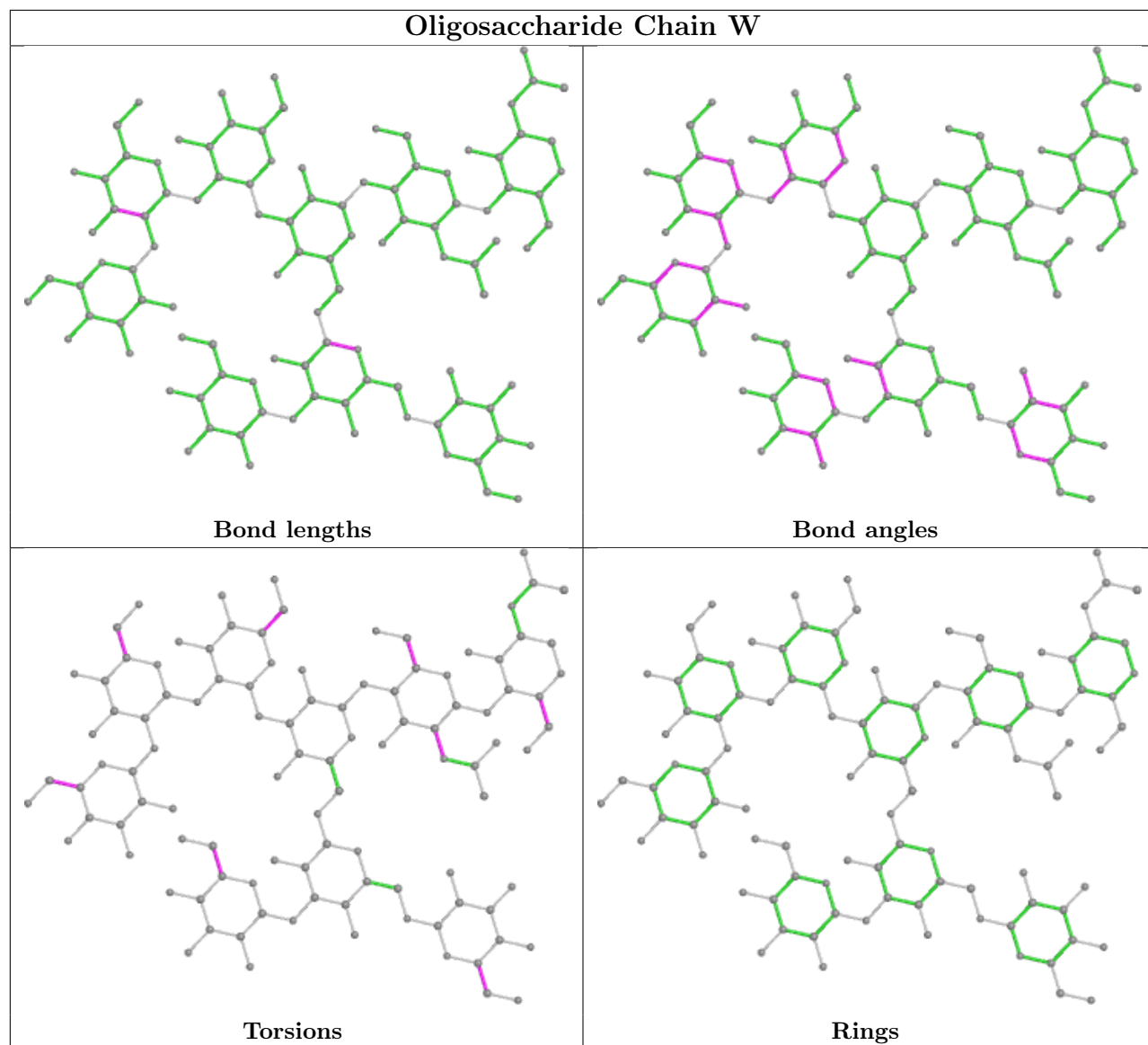


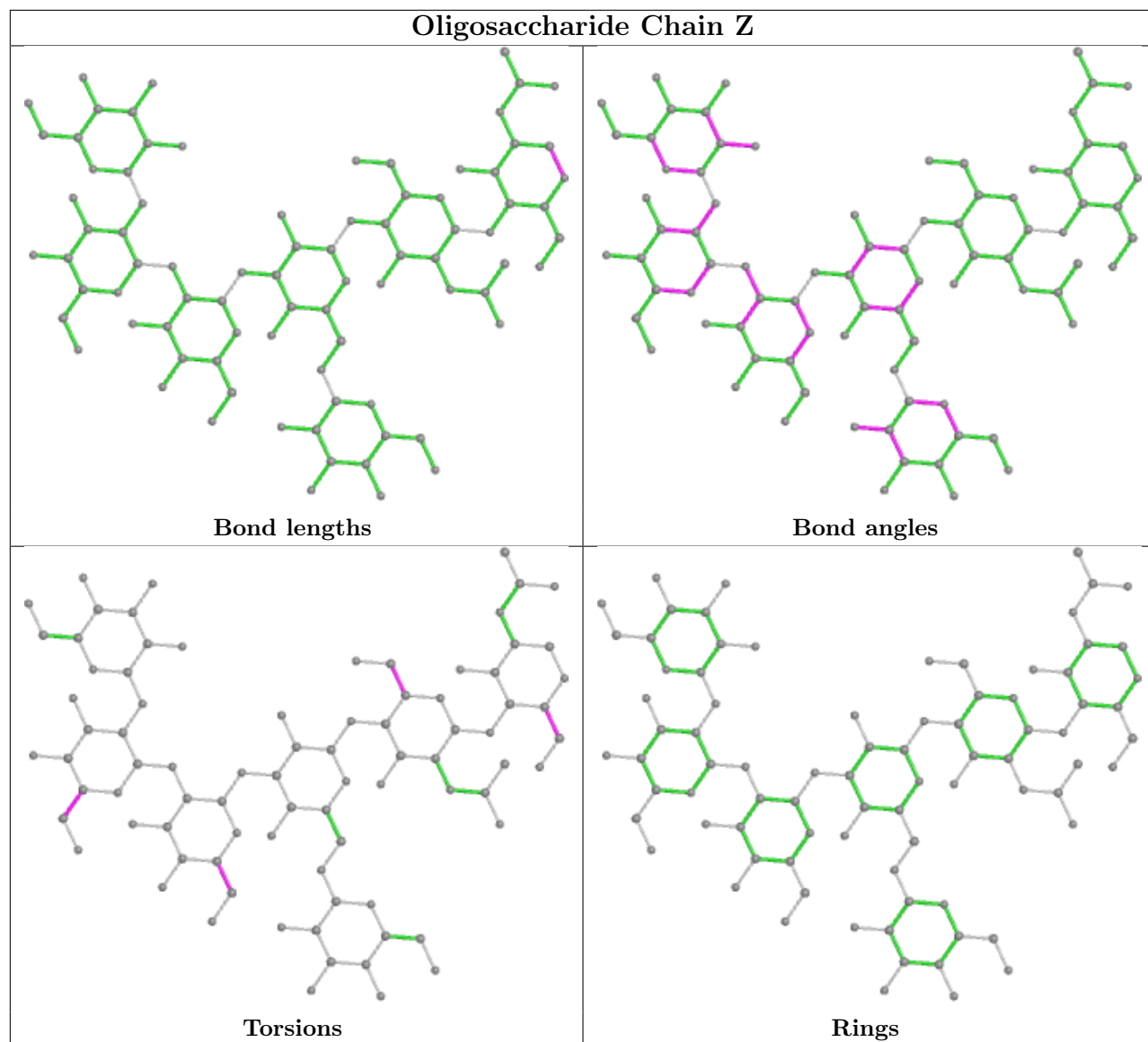


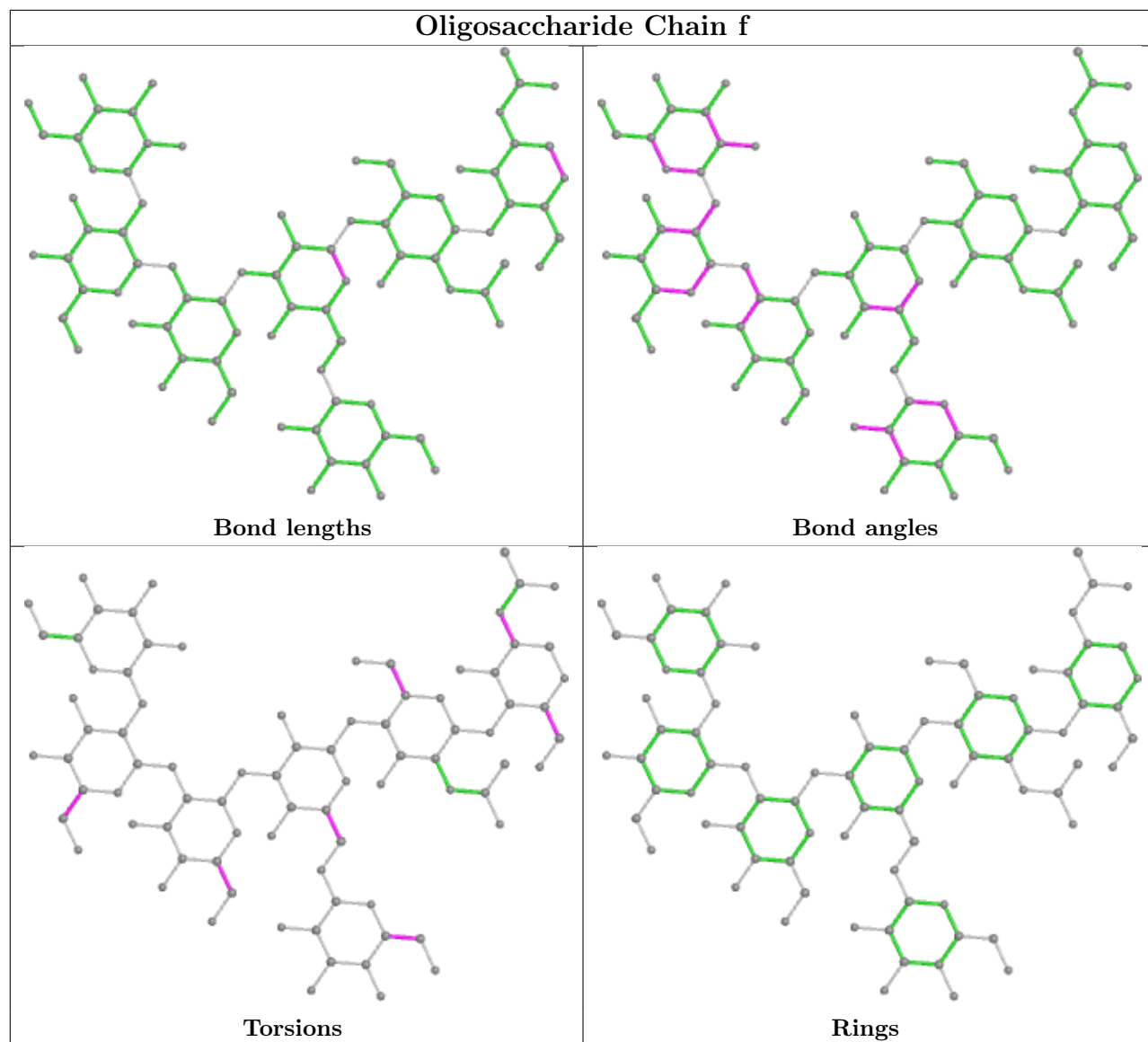




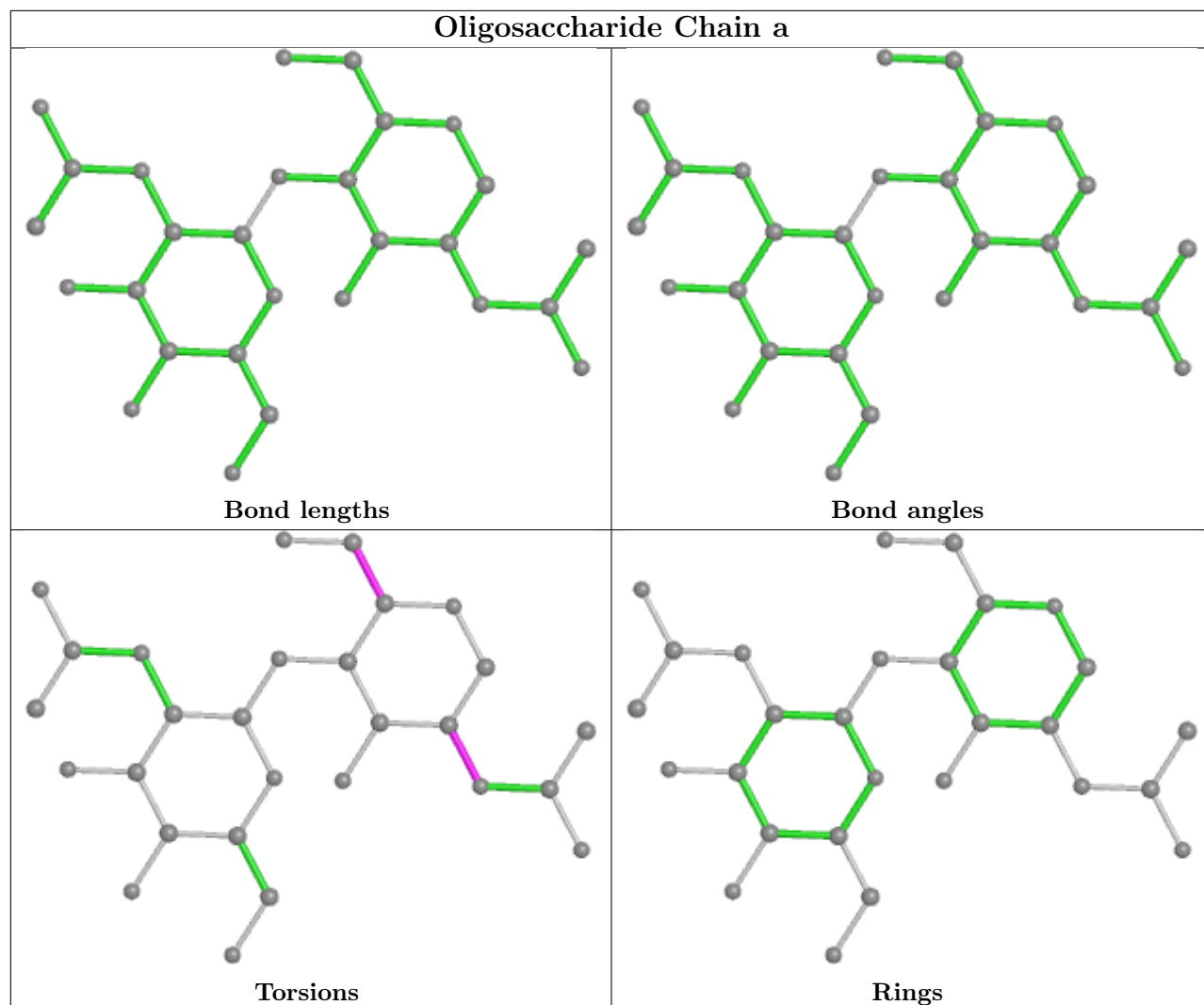


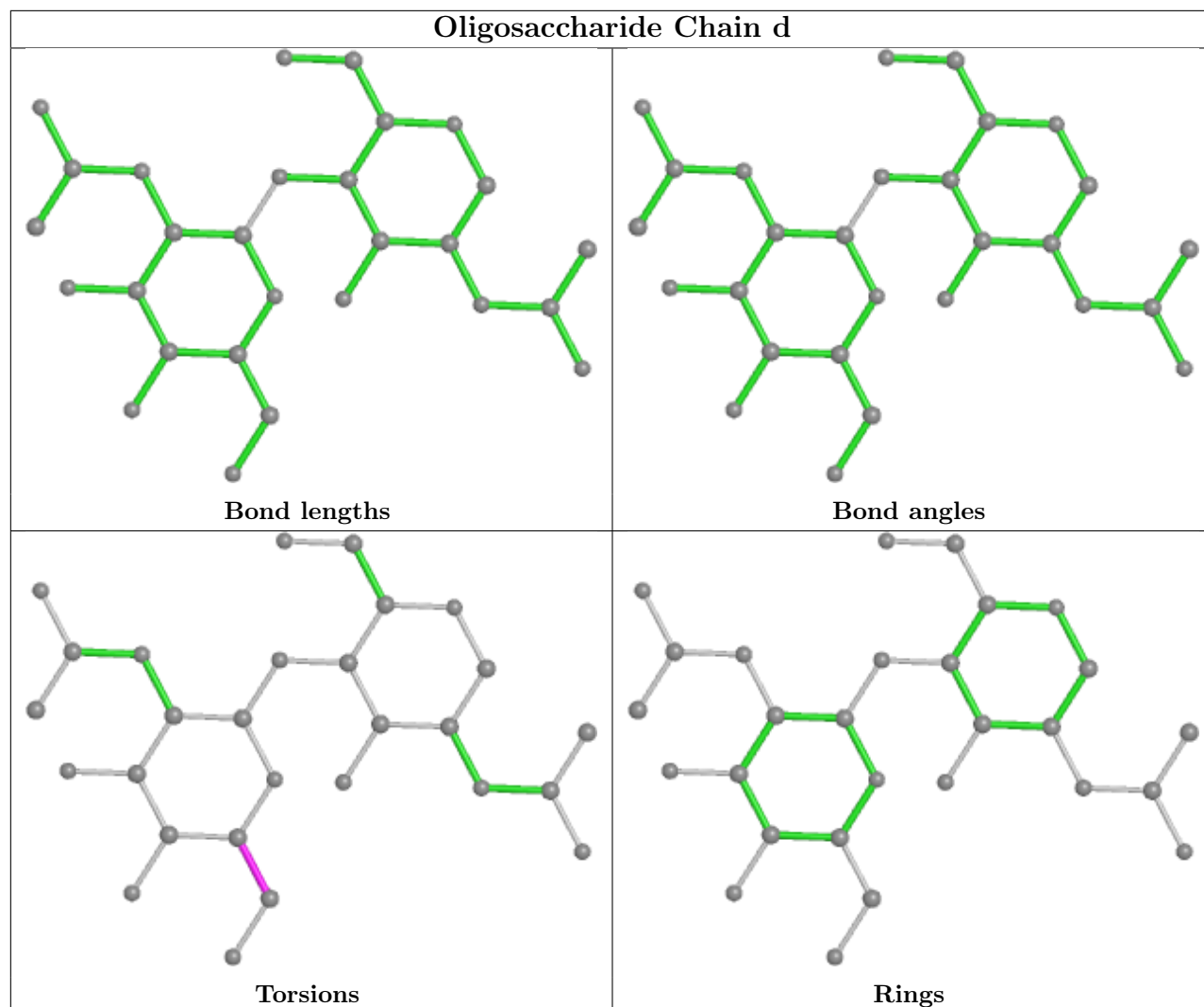


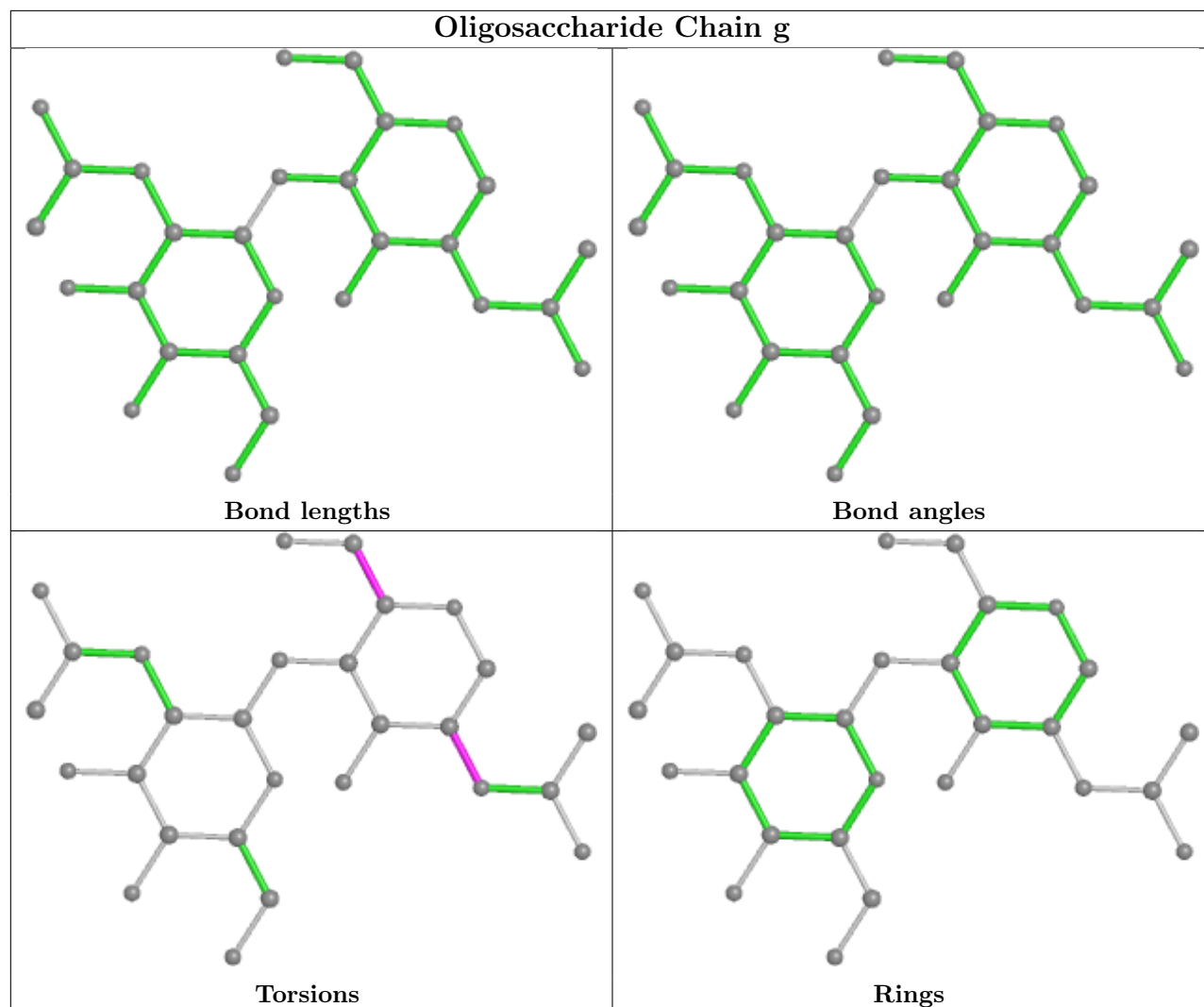


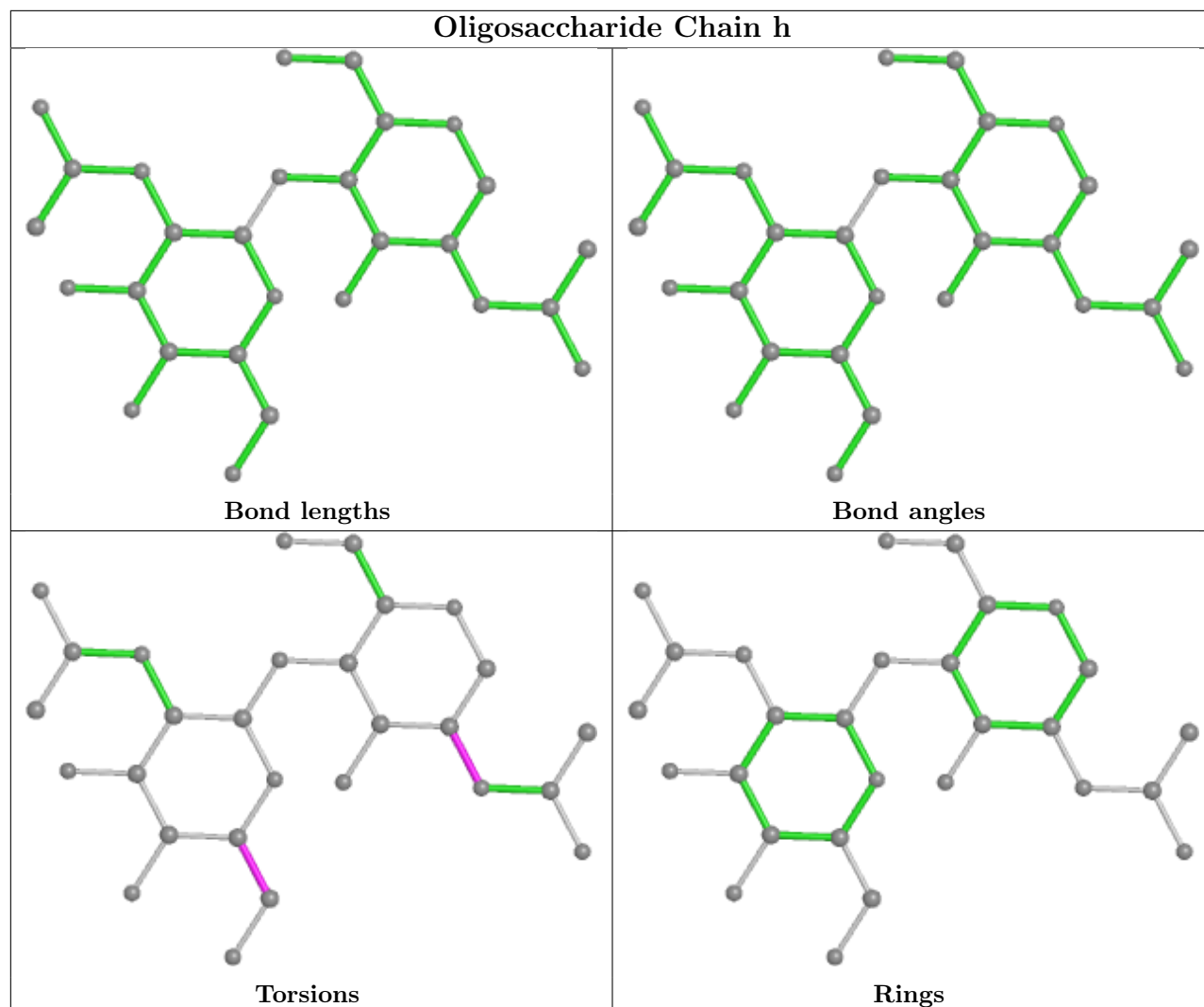


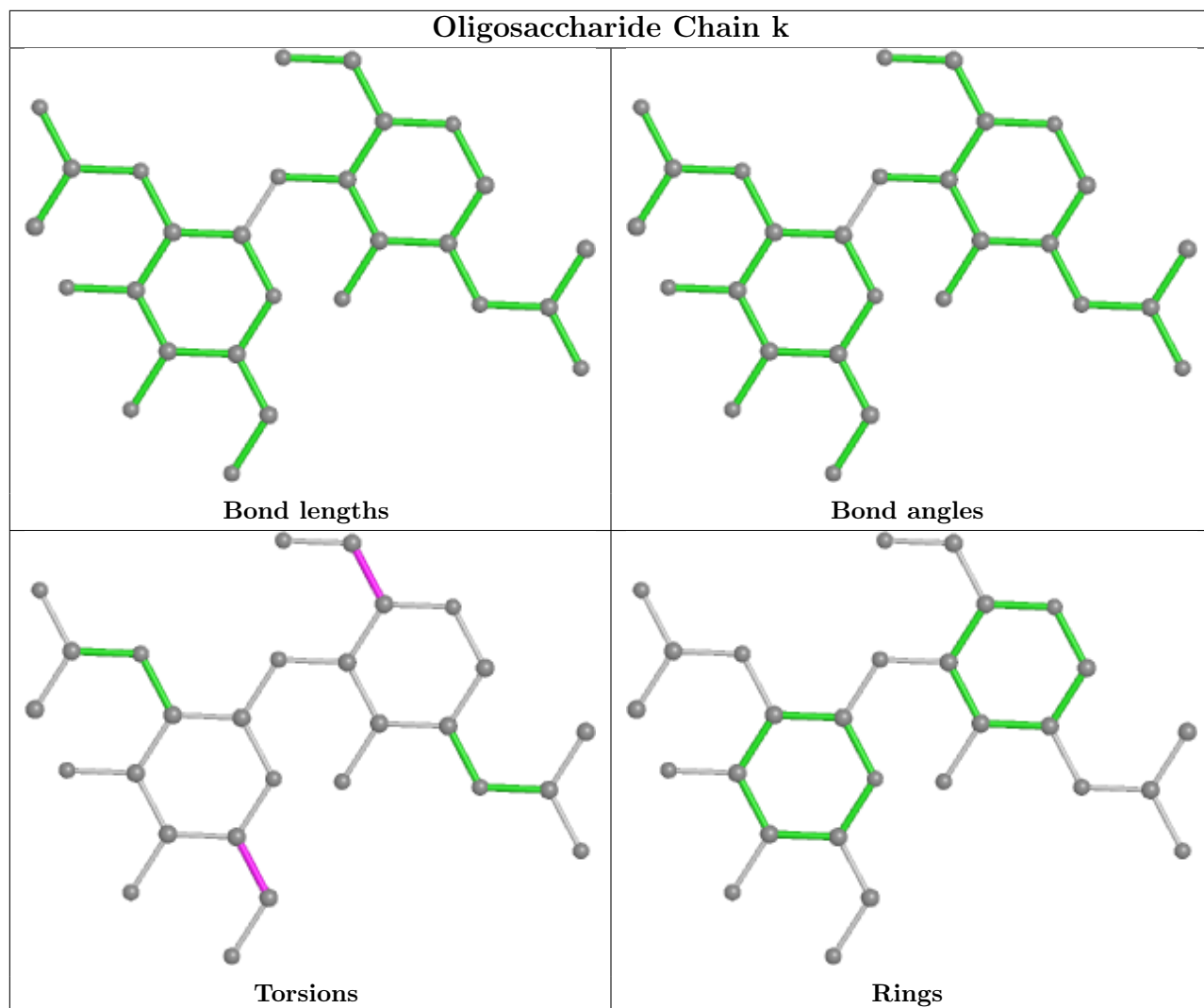


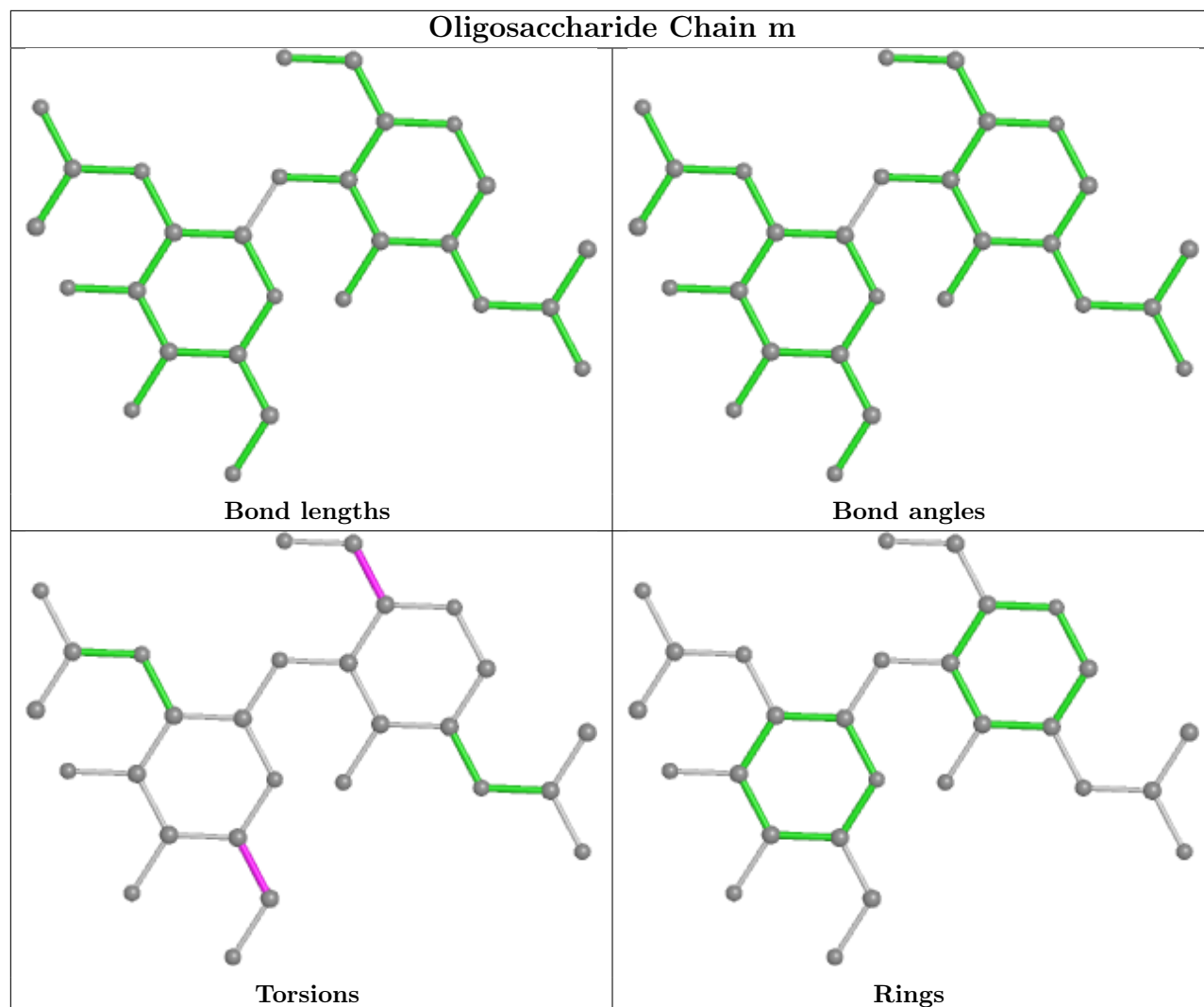


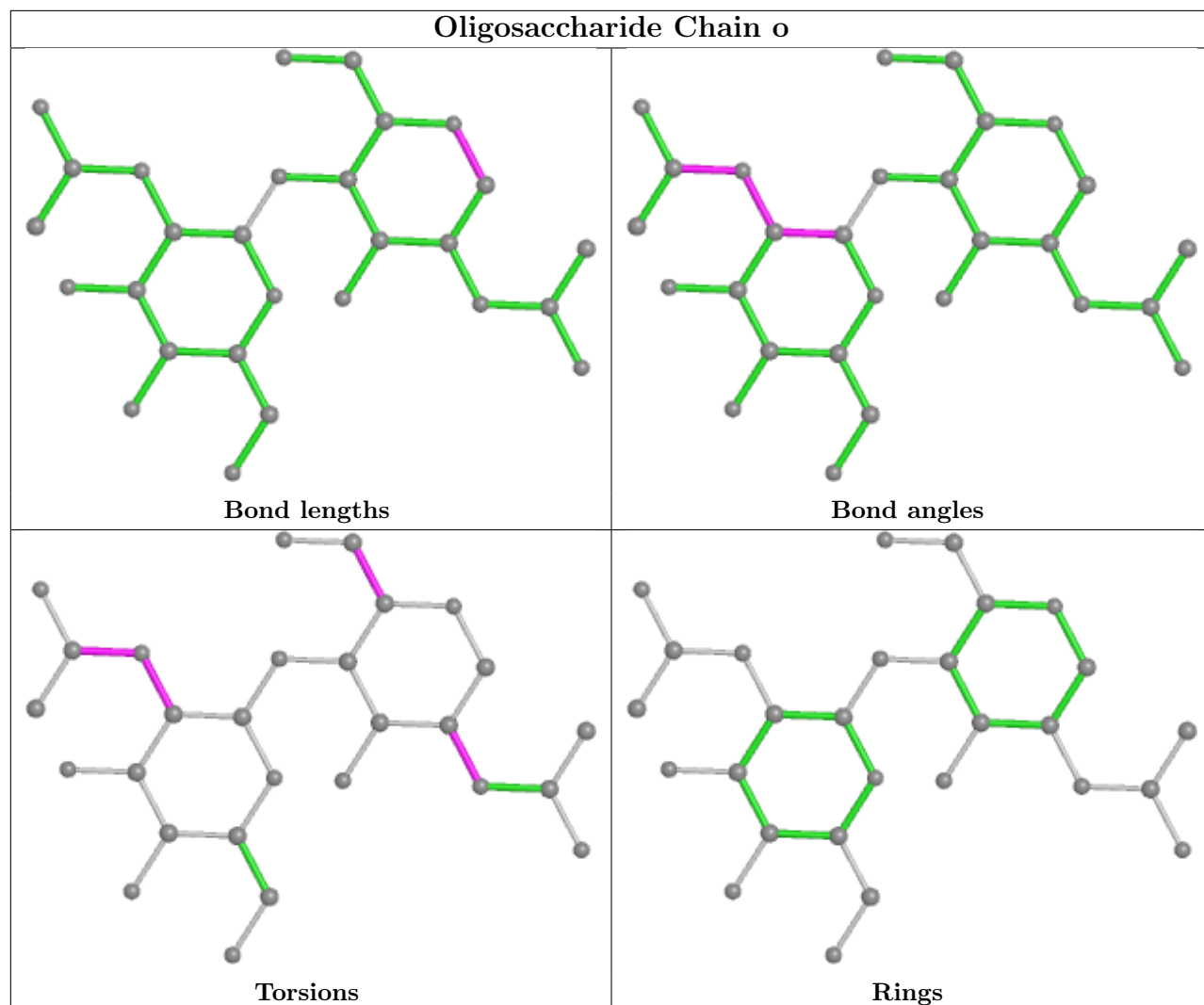


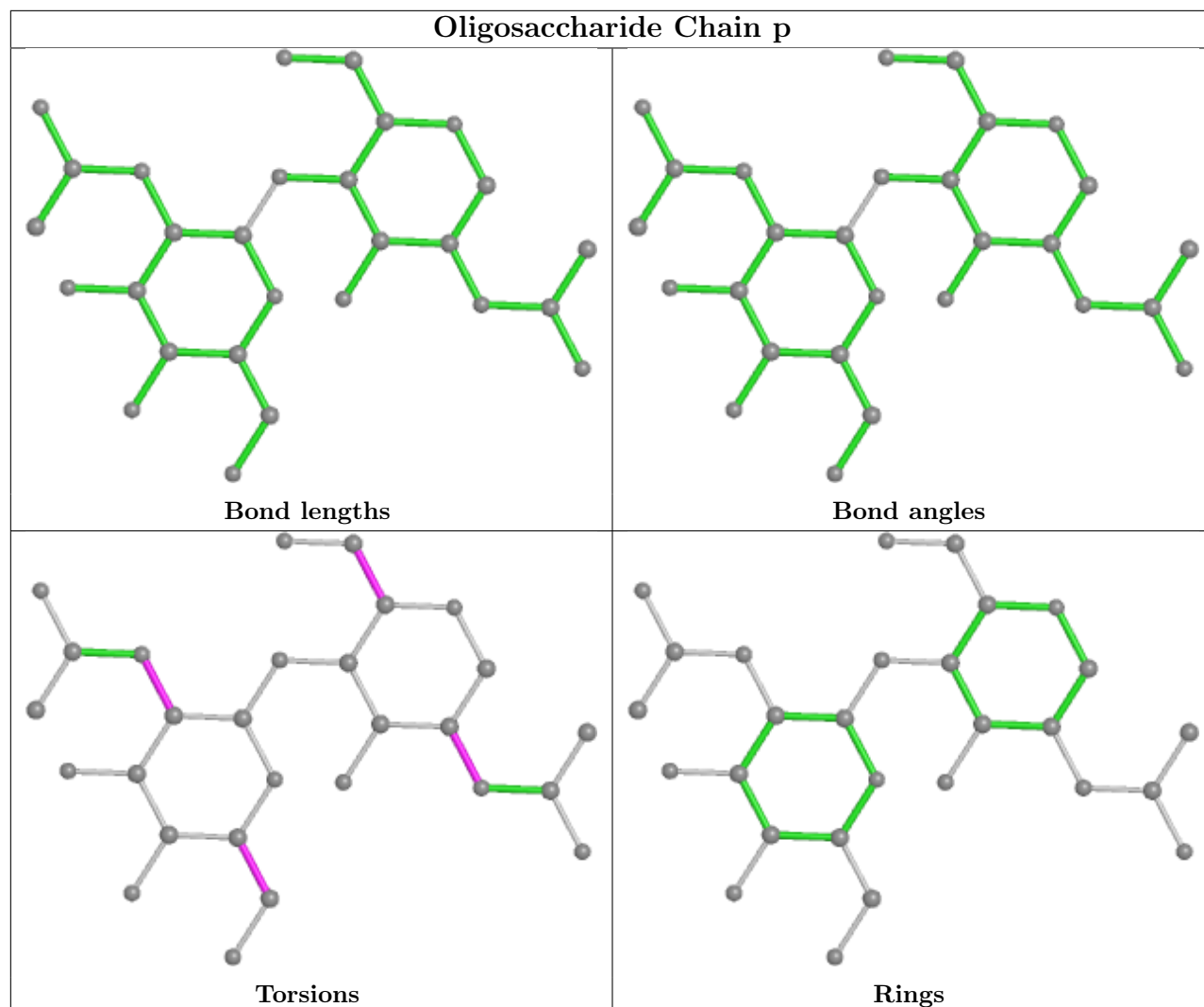




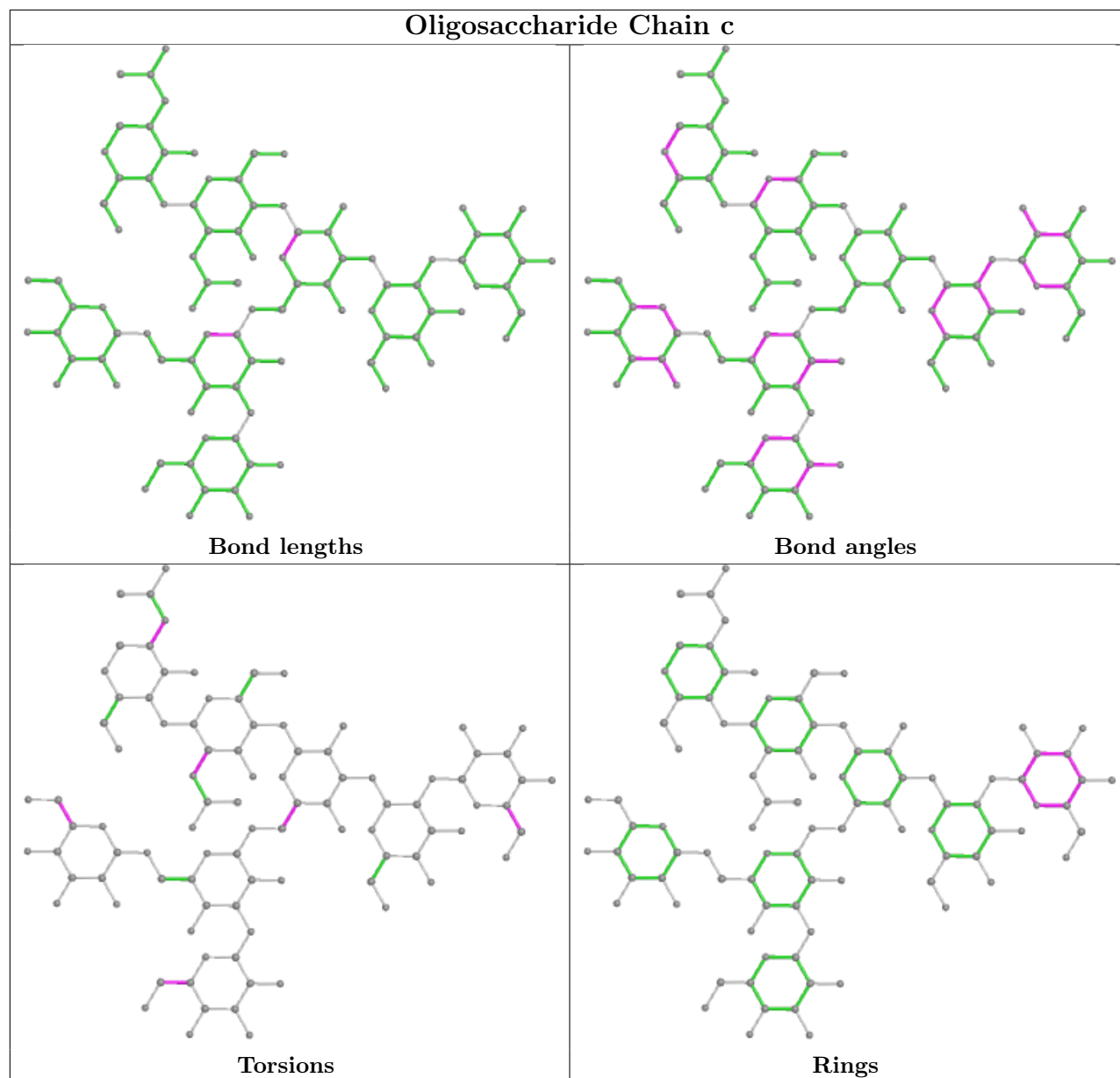


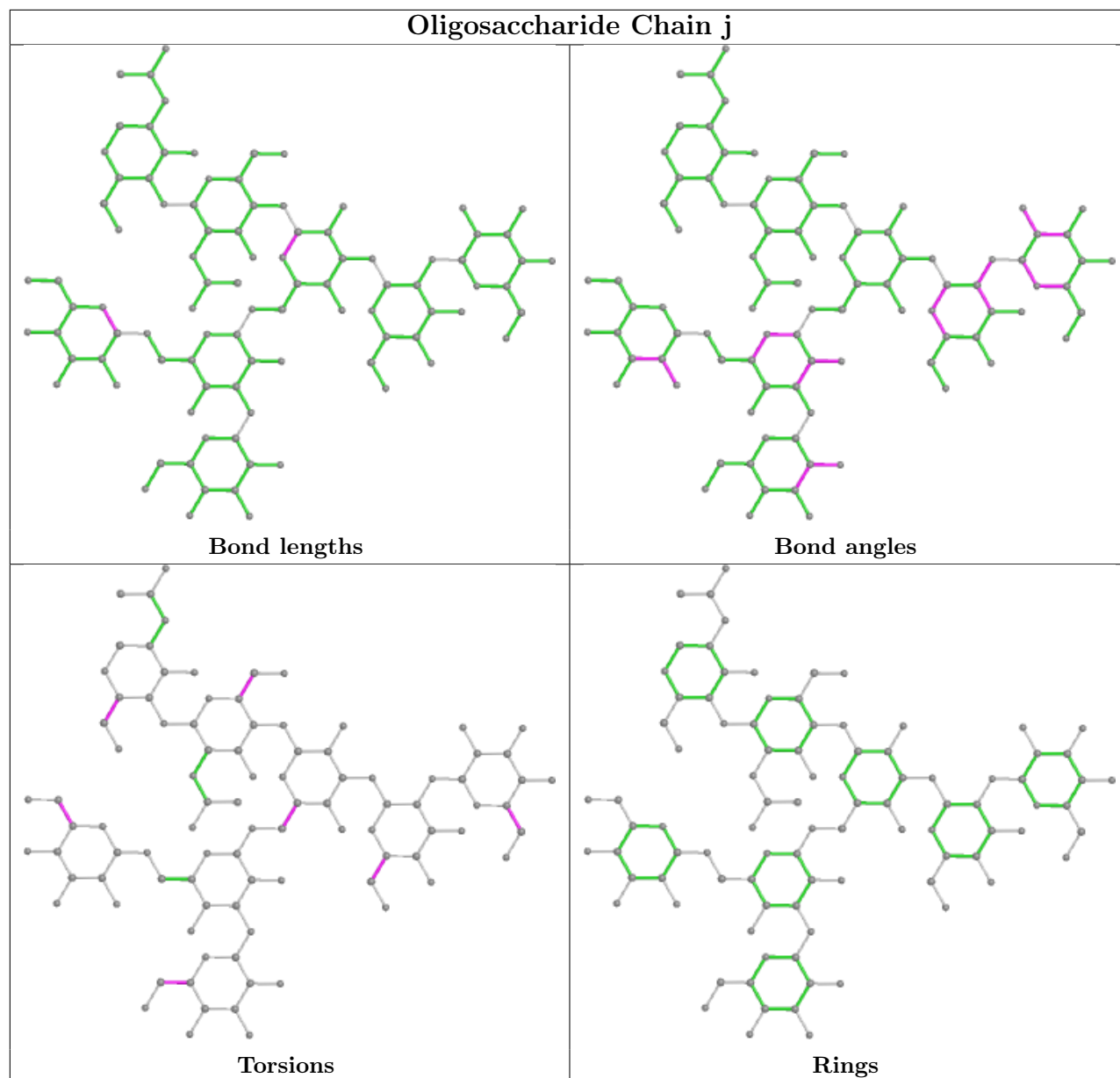


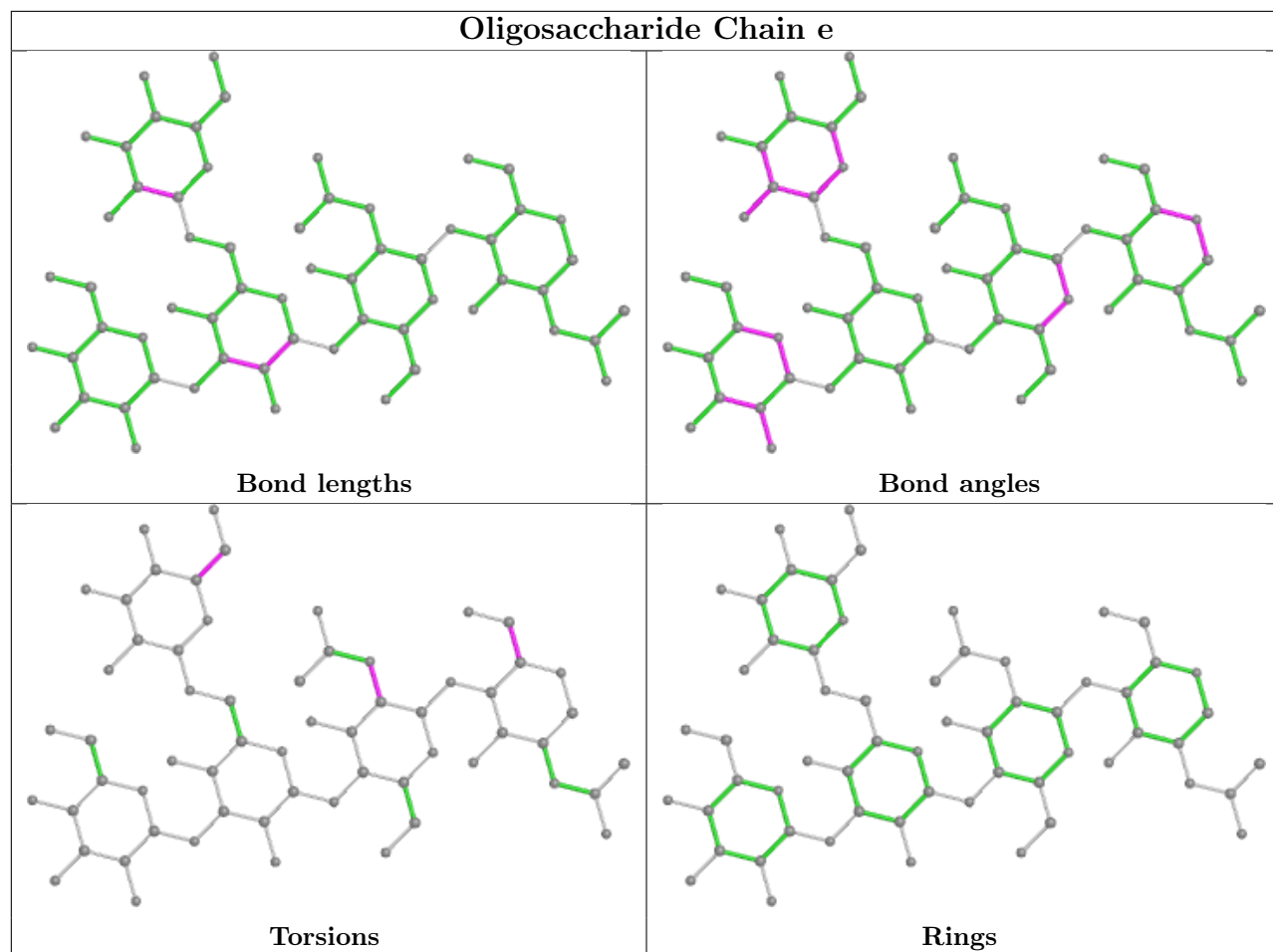


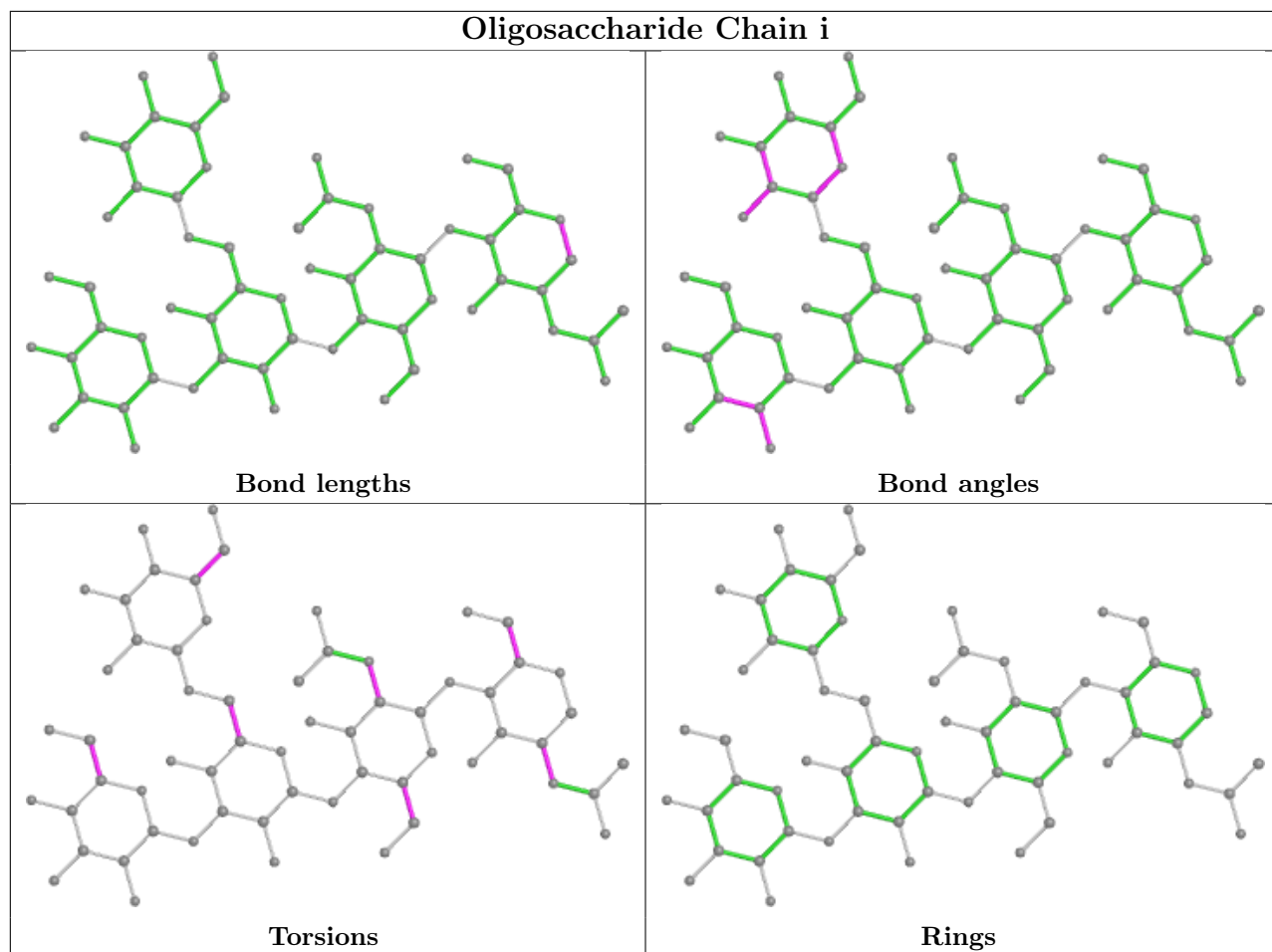


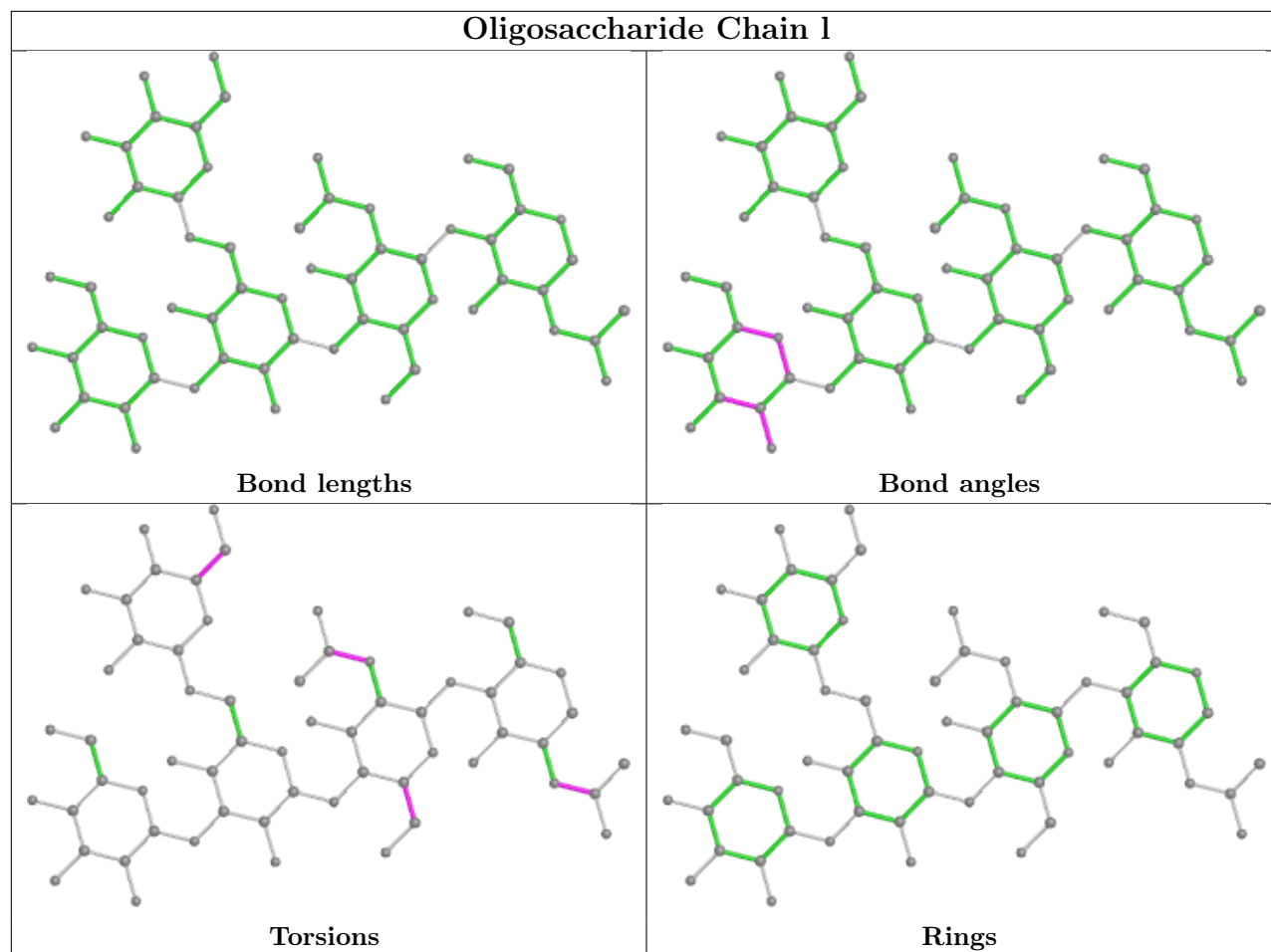


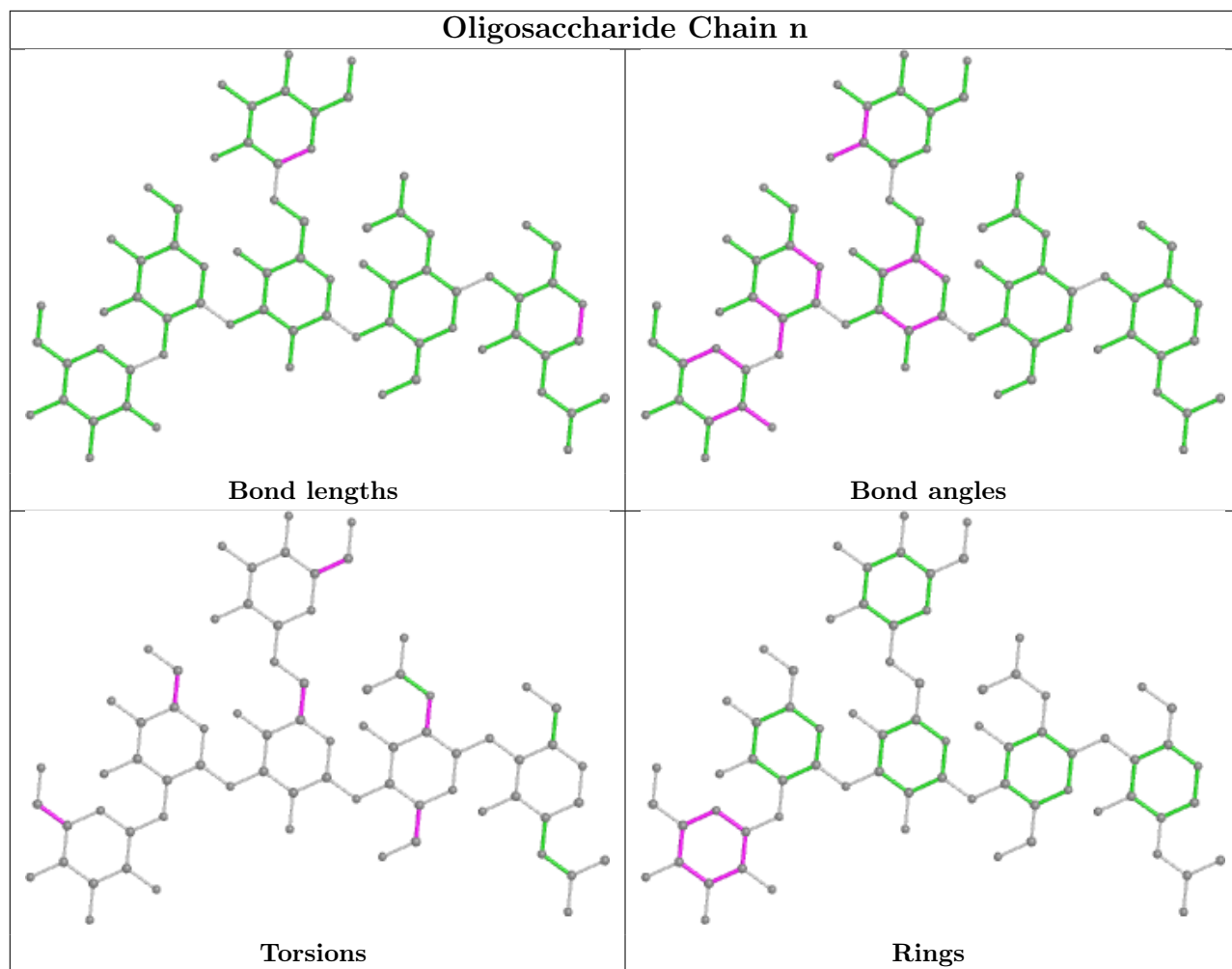












## 5.6 Ligand geometry [i](#)

34 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
17	NAG	E	605	2	14,14,15	0.24	0	17,19,21	0.46	0
17	NAG	E	606	2	14,14,15	0.34	0	17,19,21	0.45	0
17	NAG	G	602	2	14,14,15	0.25	0	17,19,21	0.54	0
17	NAG	F	602	2	14,14,15	0.19	0	17,19,21	0.42	0
17	NAG	E	607	2	14,14,15	0.25	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	NAG	F	605	2	14,14,15	0.32	0	17,19,21	0.41	0
17	NAG	F	610	2	14,14,15	0.34	0	17,19,21	0.52	0
17	NAG	G	603	2	14,14,15	0.26	0	17,19,21	0.61	0
17	NAG	C	702	1	14,14,15	0.17	0	17,19,21	0.32	0
17	NAG	C	701	1	14,14,15	0.28	0	17,19,21	0.40	0
17	NAG	E	602	2	14,14,15	0.29	0	17,19,21	0.44	0
17	NAG	F	601	2	14,14,15	0.31	0	17,19,21	0.38	0
17	NAG	E	604	2	14,14,15	0.28	0	17,19,21	0.81	1 (5%)
17	NAG	E	609	2	14,14,15	0.26	0	17,19,21	0.35	0
17	NAG	F	604	2	14,14,15	0.16	0	17,19,21	0.62	0
17	NAG	B	702	1	14,14,15	0.24	0	17,19,21	0.56	0
17	NAG	F	609	2	14,14,15	0.21	0	17,19,21	0.58	0
17	NAG	F	611	2	14,14,15	0.36	0	17,19,21	0.44	0
17	NAG	G	606	2	14,14,15	0.33	0	17,19,21	0.44	0
17	NAG	F	603	2	14,14,15	0.29	0	17,19,21	0.50	0
17	NAG	A	701	1	14,14,15	0.24	0	17,19,21	0.53	0
17	NAG	F	606	2	14,14,15	0.37	0	17,19,21	0.82	1 (5%)
17	NAG	E	610	2	14,14,15	0.35	0	17,19,21	0.44	0
17	NAG	A	702	1	14,14,15	0.34	0	17,19,21	0.56	0
17	NAG	E	608	2	14,14,15	0.47	0	17,19,21	0.63	0
17	NAG	F	608	2	14,14,15	0.22	0	17,19,21	0.42	0
17	NAG	G	607	2	14,14,15	0.24	0	17,19,21	0.63	0
17	NAG	F	607	2	14,14,15	0.20	0	17,19,21	0.44	0
17	NAG	G	601	2	14,14,15	0.45	0	17,19,21	0.55	0
17	NAG	B	701	1	14,14,15	0.26	0	17,19,21	0.57	0
17	NAG	E	603	2	14,14,15	0.32	0	17,19,21	0.63	0
17	NAG	G	605	2	14,14,15	0.34	0	17,19,21	0.55	0
17	NAG	G	604	2	14,14,15	0.44	0	17,19,21	0.41	0
17	NAG	E	601	2	14,14,15	0.38	0	17,19,21	0.38	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
17	NAG	E	605	2	-	0/6/23/26	0/1/1/1
17	NAG	E	606	2	-	0/6/23/26	0/1/1/1
17	NAG	G	602	2	-	2/6/23/26	0/1/1/1
17	NAG	F	602	2	-	2/6/23/26	0/1/1/1
17	NAG	E	607	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	F	605	2	-	2/6/23/26	0/1/1/1
17	NAG	F	610	2	-	0/6/23/26	0/1/1/1
17	NAG	G	603	2	-	3/6/23/26	0/1/1/1
17	NAG	C	702	1	-	2/6/23/26	0/1/1/1
17	NAG	C	701	1	-	2/6/23/26	0/1/1/1
17	NAG	E	602	2	-	0/6/23/26	0/1/1/1
17	NAG	F	601	2	-	3/6/23/26	0/1/1/1
17	NAG	E	604	2	-	3/6/23/26	0/1/1/1
17	NAG	E	609	2	-	4/6/23/26	0/1/1/1
17	NAG	F	604	2	-	1/6/23/26	0/1/1/1
17	NAG	B	702	1	-	2/6/23/26	0/1/1/1
17	NAG	F	609	2	-	2/6/23/26	0/1/1/1
17	NAG	F	611	2	-	2/6/23/26	0/1/1/1
17	NAG	G	606	2	-	2/6/23/26	0/1/1/1
17	NAG	F	603	2	-	1/6/23/26	0/1/1/1
17	NAG	A	701	1	-	4/6/23/26	0/1/1/1
17	NAG	F	606	2	-	3/6/23/26	0/1/1/1
17	NAG	E	610	2	-	4/6/23/26	0/1/1/1
17	NAG	A	702	1	-	0/6/23/26	0/1/1/1
17	NAG	E	608	2	-	1/6/23/26	0/1/1/1
17	NAG	F	608	2	-	0/6/23/26	0/1/1/1
17	NAG	G	607	2	-	1/6/23/26	0/1/1/1
17	NAG	F	607	2	-	2/6/23/26	0/1/1/1
17	NAG	G	601	2	-	1/6/23/26	0/1/1/1
17	NAG	B	701	1	-	3/6/23/26	0/1/1/1
17	NAG	E	603	2	-	2/6/23/26	0/1/1/1
17	NAG	G	605	2	-	1/6/23/26	0/1/1/1
17	NAG	G	604	2	-	1/6/23/26	0/1/1/1
17	NAG	E	601	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	606	NAG	C1-O5-C5	2.75	115.92	112.19
17	E	604	NAG	C1-O5-C5	2.41	115.46	112.19

There are no chirality outliers.



5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	E	604	NAG	C4-C5-C6-O6
17	F	601	NAG	O5-C5-C6-O6
17	G	602	NAG	O5-C5-C6-O6
17	E	604	NAG	O5-C5-C6-O6
17	F	602	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

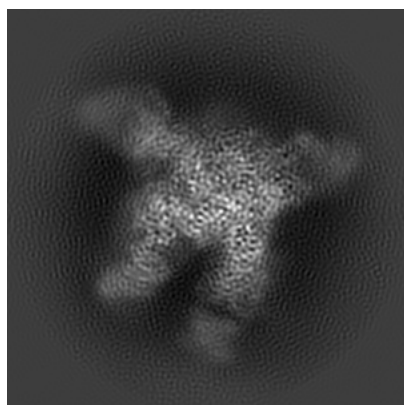
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22820. These allow visual inspection of the internal detail of the map and identification of artifacts.

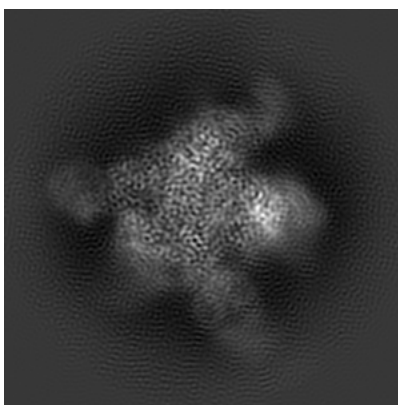
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

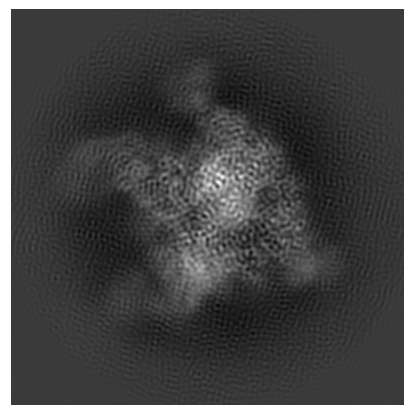
#### 6.1.1 Primary map



X



Y

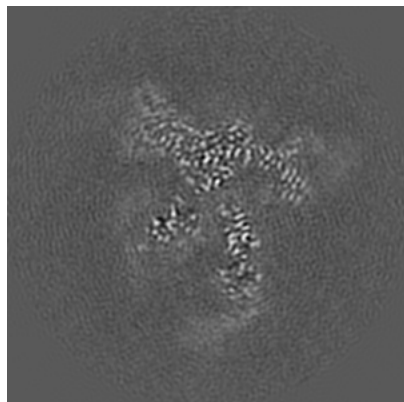


Z

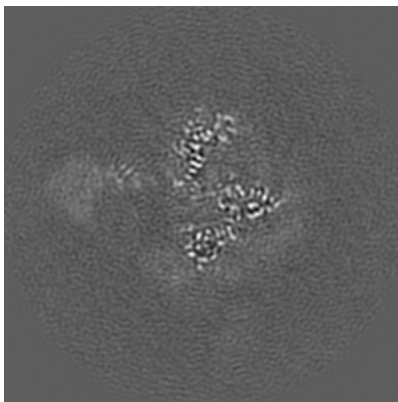
The images above show the map projected in three orthogonal directions.

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

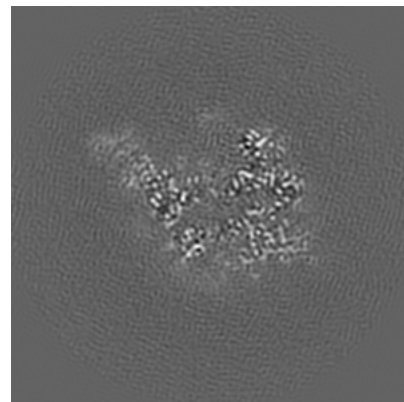
#### 6.2.1 Primary map



X Index: 156



Y Index: 156

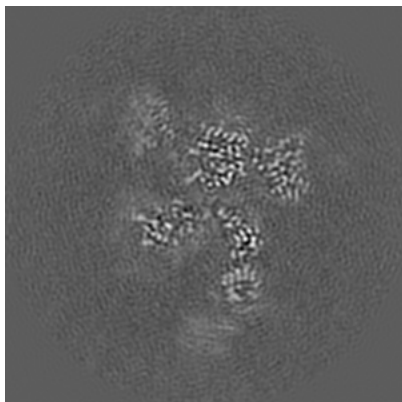


Z Index: 156

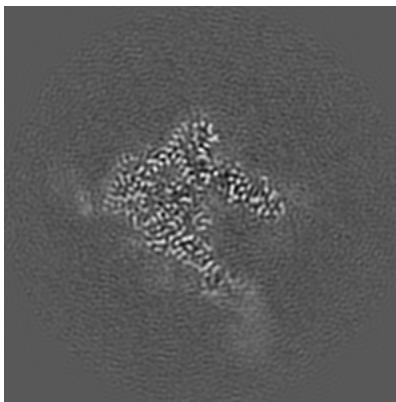
The images above show central slices of the map in three orthogonal directions.

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

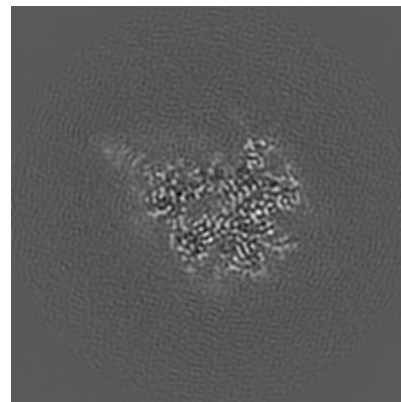
### 6.3.1 Primary map



X Index: 162



Y Index: 176



Z Index: 149

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

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

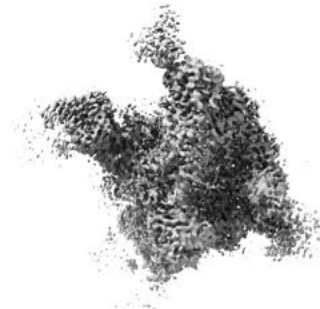
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

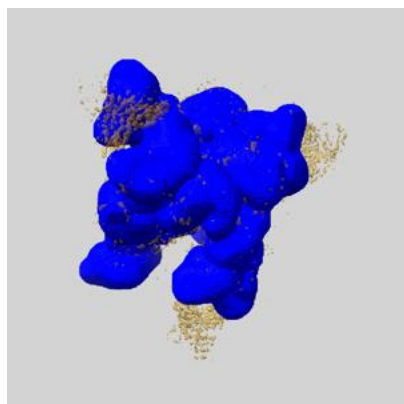
## 6.5 Mask visualisation [i](#)

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

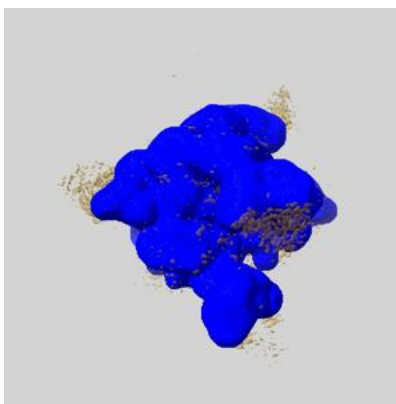
A mask typically either:

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

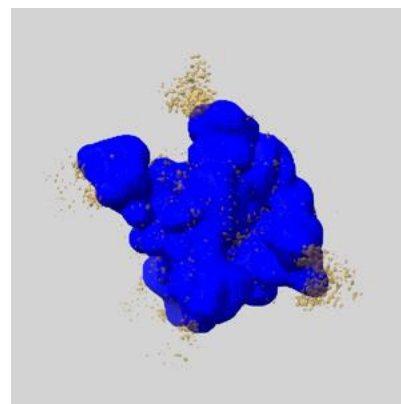
### 6.5.1 emd\_22820\_msk\_1.map [i](#)



X



Y

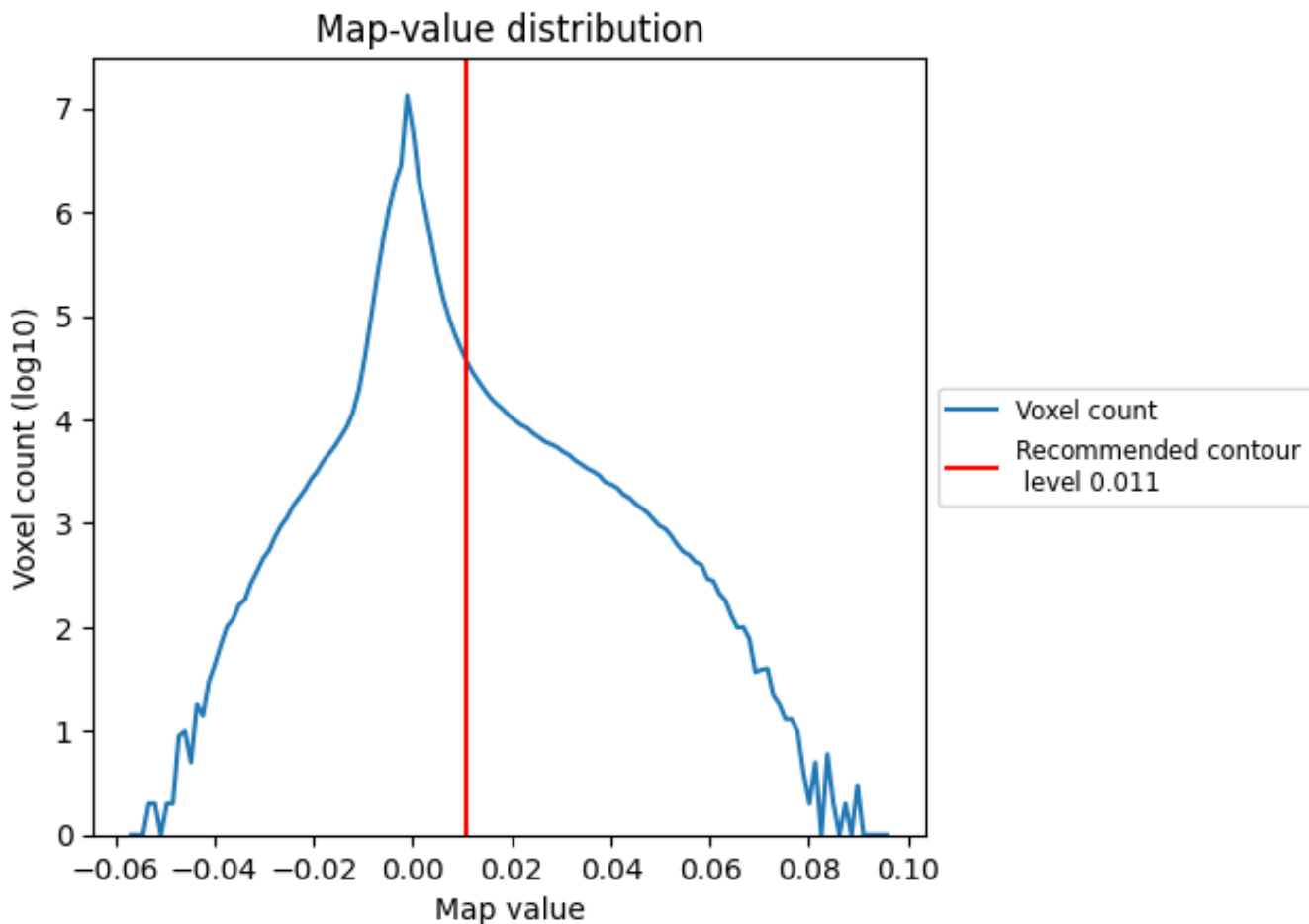


Z

## 7 Map analysis [i](#)

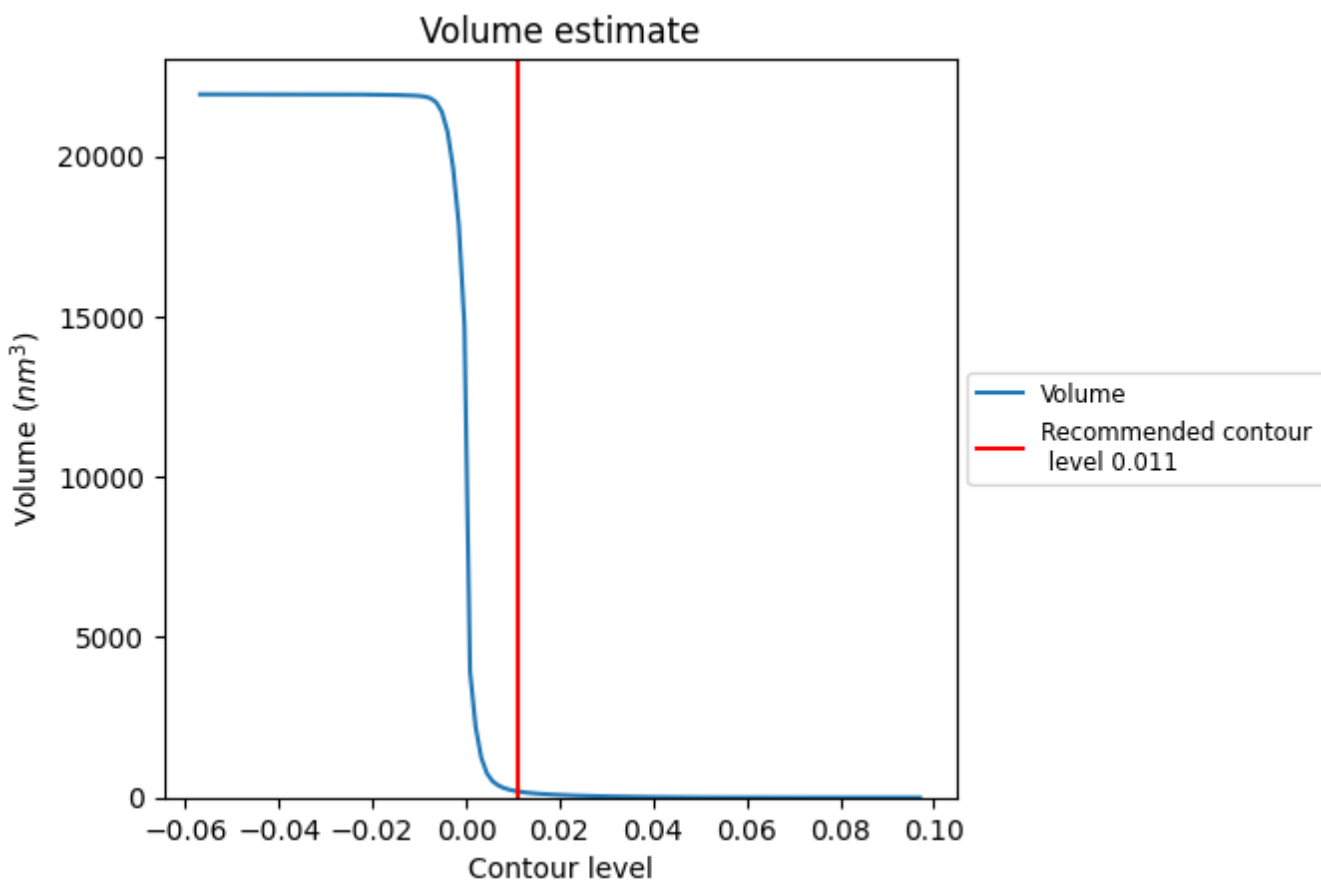
This section contains the results of statistical analysis of the map.

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



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

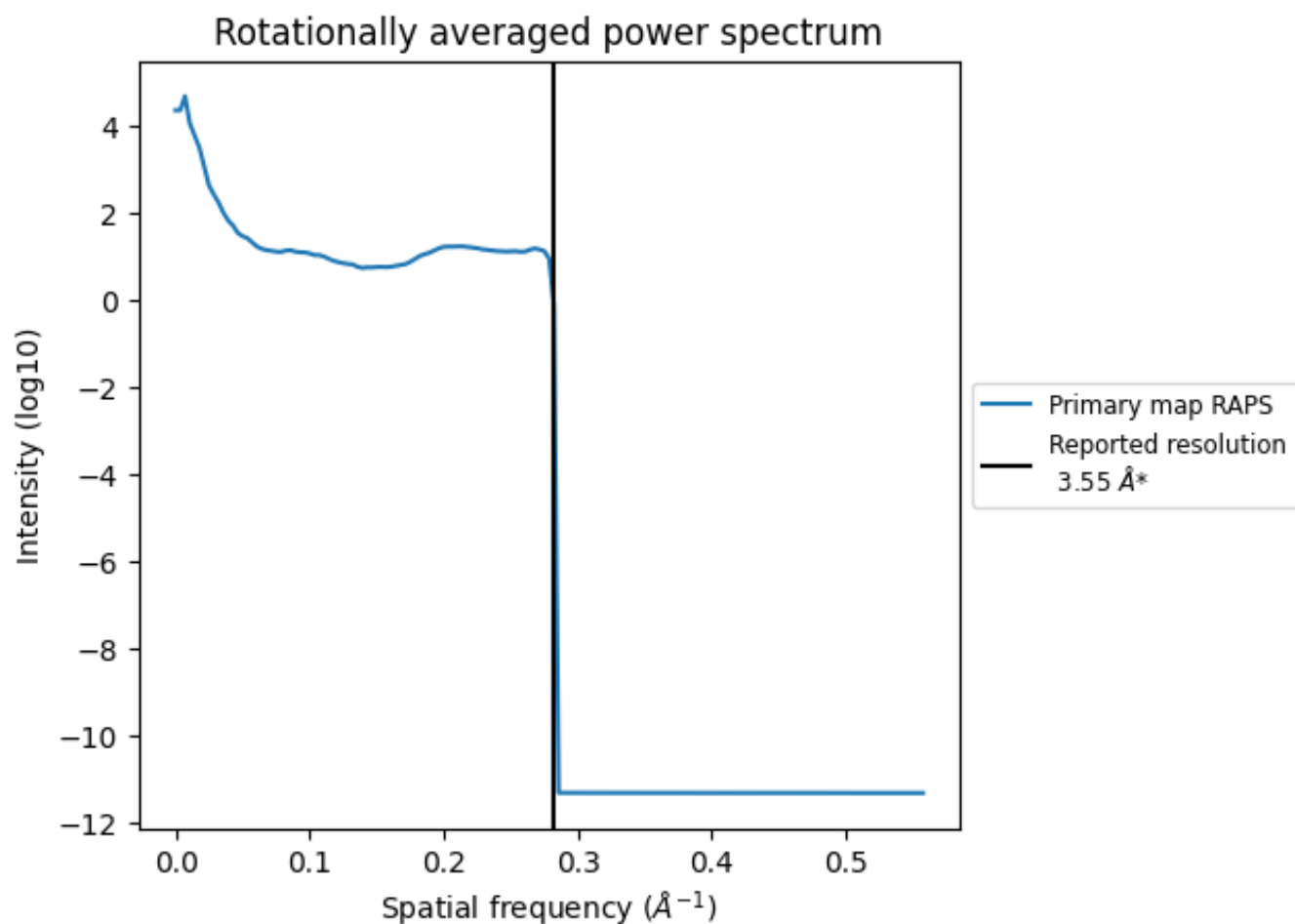
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194  $\text{nm}^3$ ; this corresponds to an approximate mass of 175 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 [\(i\)](#)

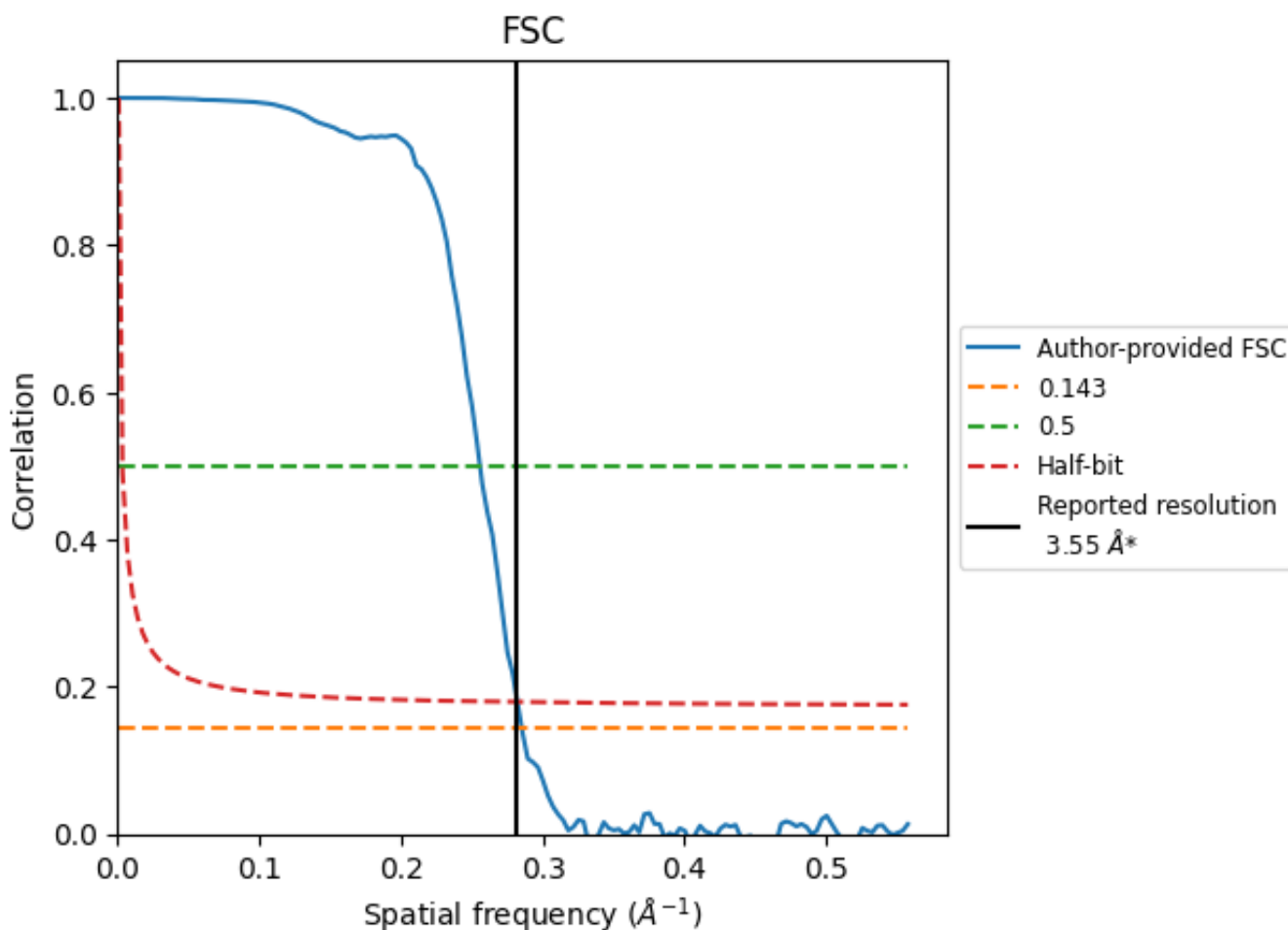


\*Reported resolution corresponds to spatial frequency of  $0.282 \text{\AA}^{-1}$

## 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 0.282 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

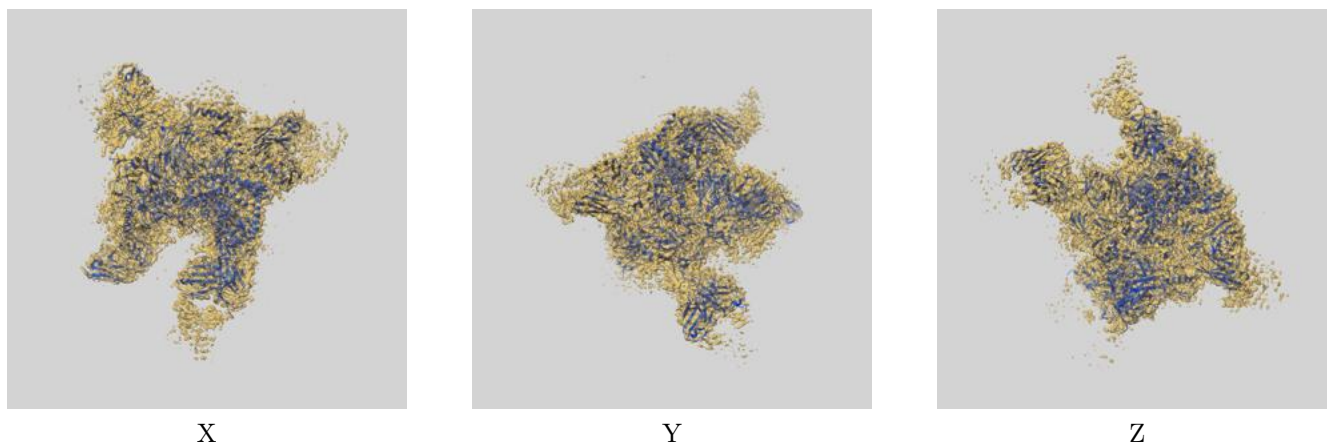
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	3.51	3.91	3.54
Unmasked-calculated*	-	-	-

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

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

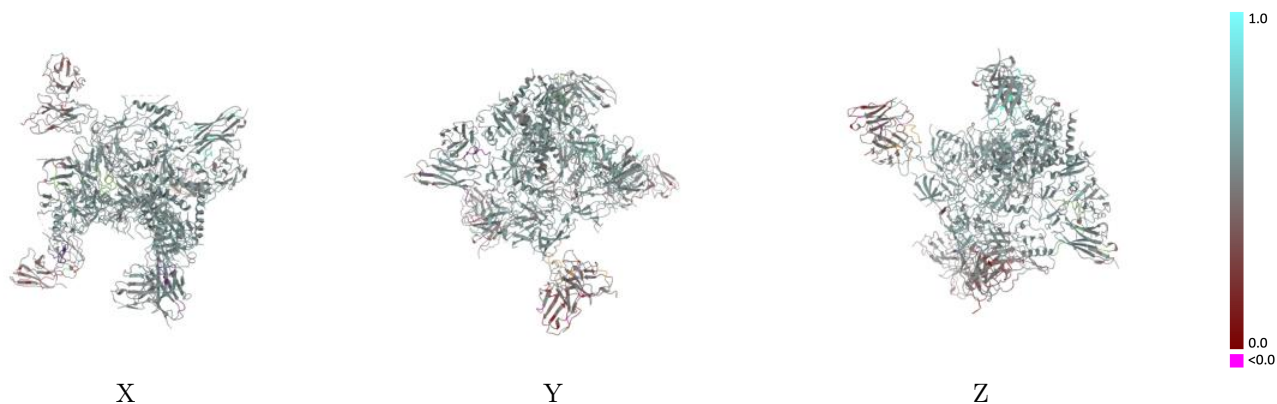
This section contains information regarding the fit between EMDB map EMD-22820 and PDB model 7KDE. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



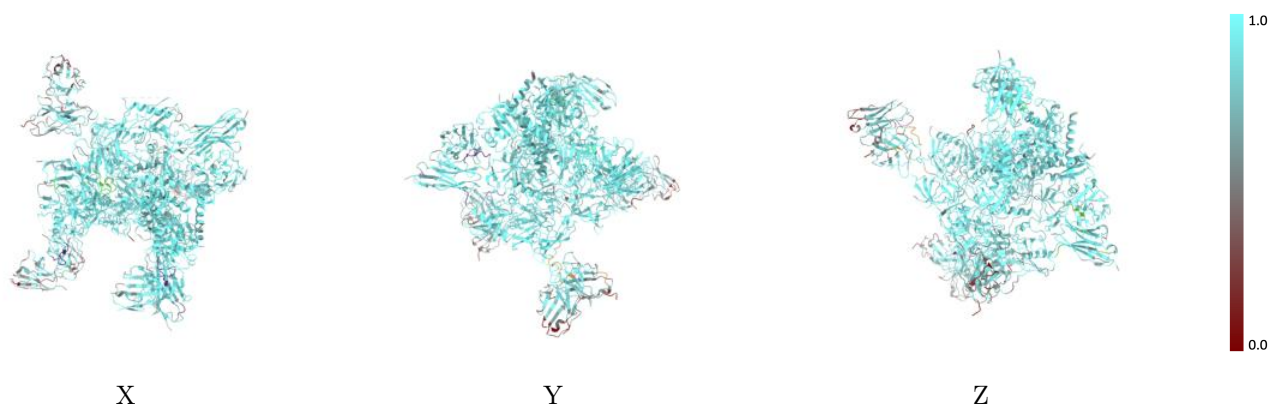
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



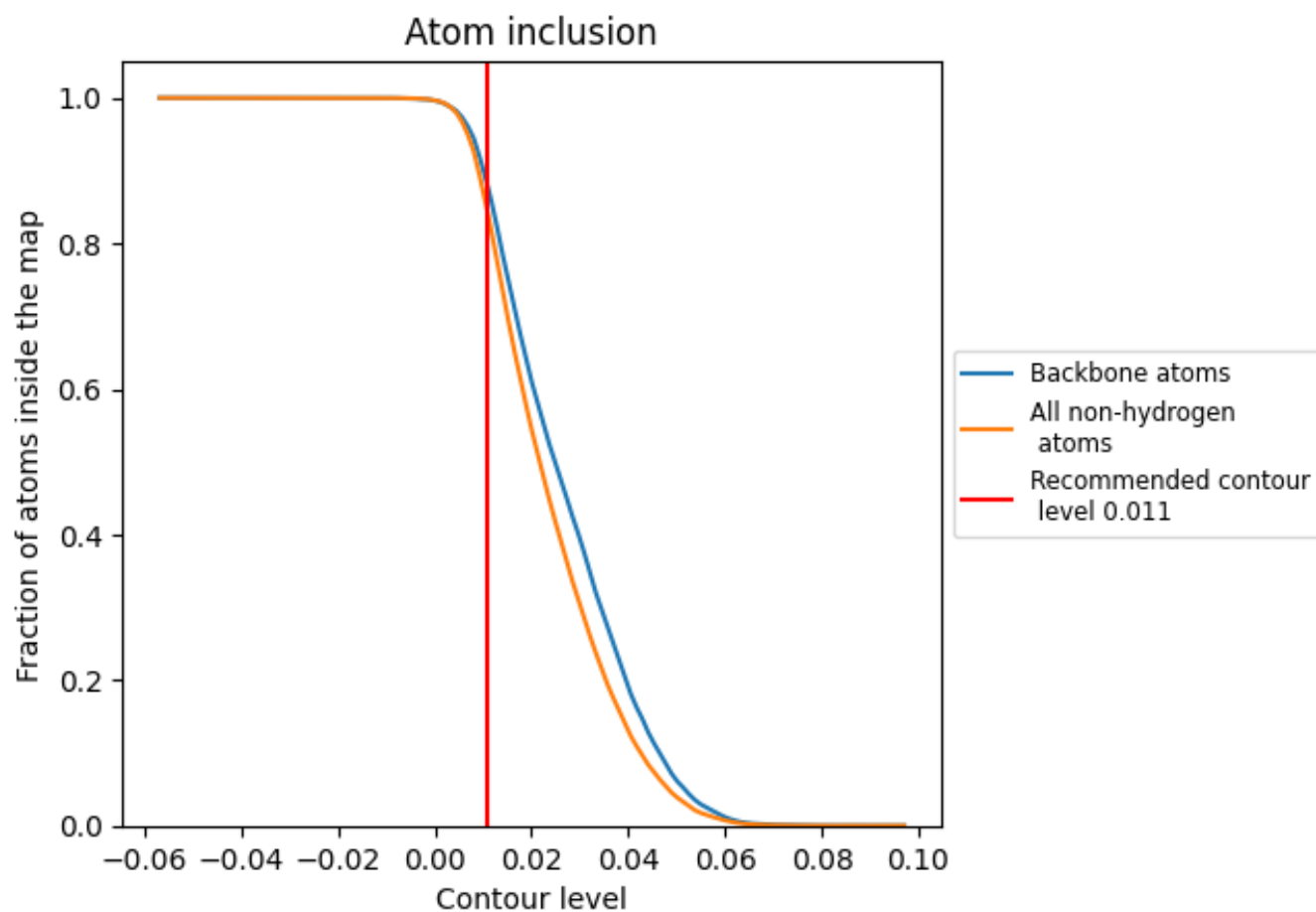
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8418	 0.5140
A	 0.8798	 0.5440
B	 0.8990	 0.5490
C	 0.8778	 0.5500
D	 0.6327	 0.4670
E	 0.8858	 0.5430
F	 0.8848	 0.5410
G	 0.8923	 0.5460
H	 0.7528	 0.4620
I	 0.6202	 0.3960
J	 0.7568	 0.4500
K	 0.8684	 0.5360
L	 0.6360	 0.4110
M	 0.7538	 0.4560
N	 0.6058	 0.3690
O	 0.8908	 0.5420
P	 0.8823	 0.5270
Q	 0.8782	 0.5270
R	 0.8745	 0.5100
S	 0.8782	 0.5320
T	 0.8344	 0.5200
U	 0.8205	 0.4940
V	 0.8200	 0.5330
W	 0.9143	 0.5360
X	 0.9487	 0.5470
Y	 0.8462	 0.5570
Z	 0.8916	 0.5410
a	 0.8571	 0.5060
b	 0.8200	 0.4430
c	 0.8191	 0.5100
d	 0.9643	 0.5600
e	 0.7869	 0.4740
f	 0.8554	 0.5070
g	 0.7857	 0.4840
h	 0.5357	 0.3840



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Chain	Atom inclusion	Q-score
i	 0.8033	 0.5130
j	 0.9149	 0.5180
k	 1.0000	 0.5670
l	 0.7705	 0.4630
m	 0.8214	 0.5180
n	 0.9444	 0.5450
o	 0.7143	 0.3630
p	 0.6786	 0.4810