



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 11:34 AM JST

PDB ID : 8ZHF
EMDB ID : EMD-60101
Title : SARS-CoV-2 spike trimer (6P) in complex with R1-26 Fab, head-to-head aggregate
Authors : Yan, Q.; Gao, X.; Liu, B.; Hou, R.; He, P.; Li, Z.; Chen, Q.; Wang, J.; He, J.; Chen, L.; Zhao, J.; Xiong, X.
Deposited on : 2024-05-10
Resolution : 5.26 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

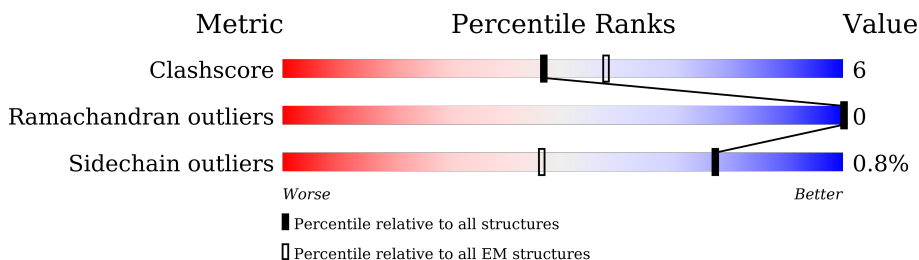
EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.














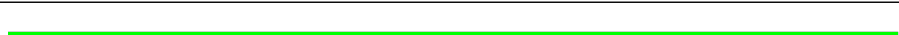

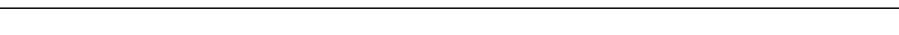
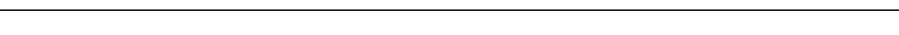
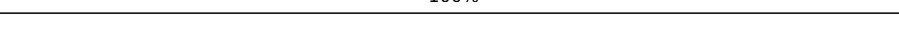

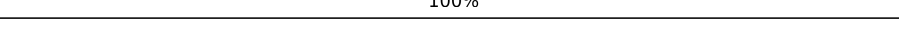
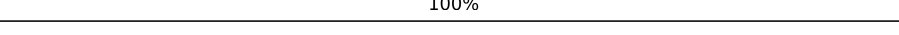
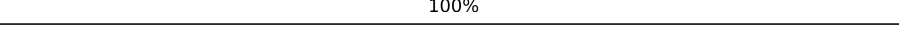
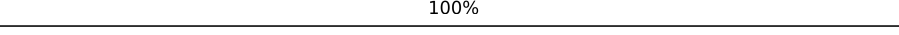
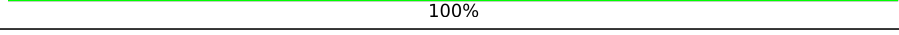
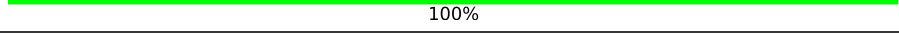
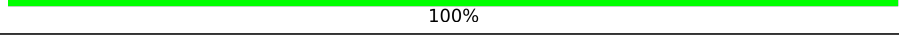
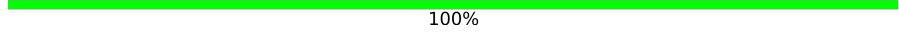
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1278	
1	B	1278	
1	C	1278	
1	D	1278	
1	E	1278	
1	I	1278	
2	F	243	
2	H	243	
2	J	243	

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Mol	Chain	Length	Quality of chain
2	M	243	 79% 12% 9%
2	R	243	 79% 12% 9%
2	S	243	 76% 14% 9%
3	G	240	 76% 13% 11%
3	K	240	 78% 11% 11%
3	L	240	 73% 16% 11%
3	N	240	 76% 13% 11%
3	T	240	 77% 12% 11%
3	U	240	 72% 17% 11%
4	O	2	 100%
4	P	2	 100%
4	Q	2	 100%
4	V	2	 100%
4	W	2	 100%
4	X	2	 100%
4	Y	2	 50% 50%
4	Z	2	 100%
4	a	2	 100%
4	b	2	 100%
4	c	2	 100%
4	d	2	 100%
4	e	2	 100%
4	f	2	 100%
4	g	2	 100%
4	h	2	 100%

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Mol	Chain	Length	Quality of chain
4	i	2	 100%
4	j	2	 100%
4	k	2	 100%
4	l	2	 100%
4	m	2	 100%
4	n	2	 100%
4	o	2	 100%
4	p	2	 100%
4	q	2	 100%
4	r	2	 100%
4	s	2	 100%
4	t	2	 100%
4	u	2	 100%
4	v	2	 100%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 70929 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 Spike glycoprotein,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1066	8320	5307	1388	1587	38	0	0
1	B	1045	8167	5211	1364	1556	36	0	0
1	C	1066	8320	5307	1388	1587	38	0	0
1	D	1066	8320	5307	1388	1587	38	0	0
1	E	1066	8320	5307	1388	1587	38	0	0
1	I	1066	8320	5307	1388	1587	38	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
D	682	GLY	ARG	conflict	UNP P0DTC2
D	683	SER	ARG	conflict	UNP P0DTC2
D	685	SER	ARG	conflict	UNP P0DTC2
D	817	PRO	PHE	conflict	UNP P0DTC2
D	892	PRO	ALA	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1209	GLY	-	linker	UNP P0DTC2
D	1210	SER	-	linker	UNP P0DTC2
E	682	GLY	ARG	conflict	UNP P0DTC2
E	683	SER	ARG	conflict	UNP P0DTC2
E	685	SER	ARG	conflict	UNP P0DTC2
E	817	PRO	PHE	conflict	UNP P0DTC2
E	892	PRO	ALA	conflict	UNP P0DTC2
E	899	PRO	ALA	conflict	UNP P0DTC2
E	942	PRO	ALA	conflict	UNP P0DTC2
E	986	PRO	LYS	variant	UNP P0DTC2
E	987	PRO	VAL	variant	UNP P0DTC2
E	1209	GLY	-	linker	UNP P0DTC2
E	1210	SER	-	linker	UNP P0DTC2
I	682	GLY	ARG	conflict	UNP P0DTC2
I	683	SER	ARG	conflict	UNP P0DTC2
I	685	SER	ARG	conflict	UNP P0DTC2
I	817	PRO	PHE	conflict	UNP P0DTC2
I	892	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	899	PRO	ALA	conflict	UNP P0DTC2
I	942	PRO	ALA	conflict	UNP P0DTC2
I	986	PRO	LYS	variant	UNP P0DTC2
I	987	PRO	VAL	variant	UNP P0DTC2
I	1209	GLY	-	linker	UNP P0DTC2
I	1210	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of R1-26 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	221	1656	1048	279	323	6	0	0
2	F	221	1656	1048	279	323	6	0	0
2	J	221	1656	1048	279	323	6	0	0
2	R	221	1656	1048	279	323	6	0	0
2	M	221	1656	1048	279	323	6	0	0
2	S	221	1656	1048	279	323	6	0	0

- Molecule 3 is a protein called Light chain of R1-26 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	214	1591	987	260	339	5	0	0
3	G	214	1591	987	260	339	5	0	0
3	K	214	1591	987	260	339	5	0	0
3	U	214	1591	987	260	339	5	0	0
3	N	214	1591	987	260	339	5	0	0
3	T	214	1591	987	260	339	5	0	0

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



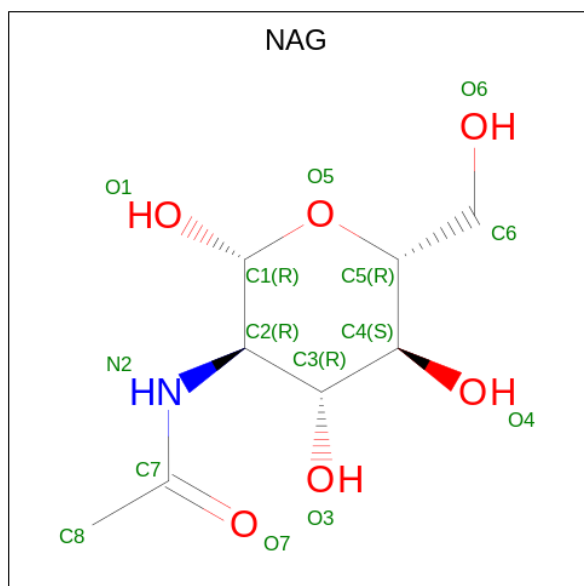
Mol	Chain	Residues	Atoms				AltConf	Trace
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	j	2	Total	C	N	O	0	0
			28	16	2	10		
4	k	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	l	2	Total 28	C 16	N 2	O 10	0	0
4	m	2	Total 28	C 16	N 2	O 10	0	0
4	n	2	Total 28	C 16	N 2	O 10	0	0
4	o	2	Total 28	C 16	N 2	O 10	0	0
4	p	2	Total 28	C 16	N 2	O 10	0	0
4	q	2	Total 28	C 16	N 2	O 10	0	0
4	r	2	Total 28	C 16	N 2	O 10	0	0
4	s	2	Total 28	C 16	N 2	O 10	0	0
4	t	2	Total 28	C 16	N 2	O 10	0	0
4	u	2	Total 28	C 16	N 2	O 10	0	0
4	v	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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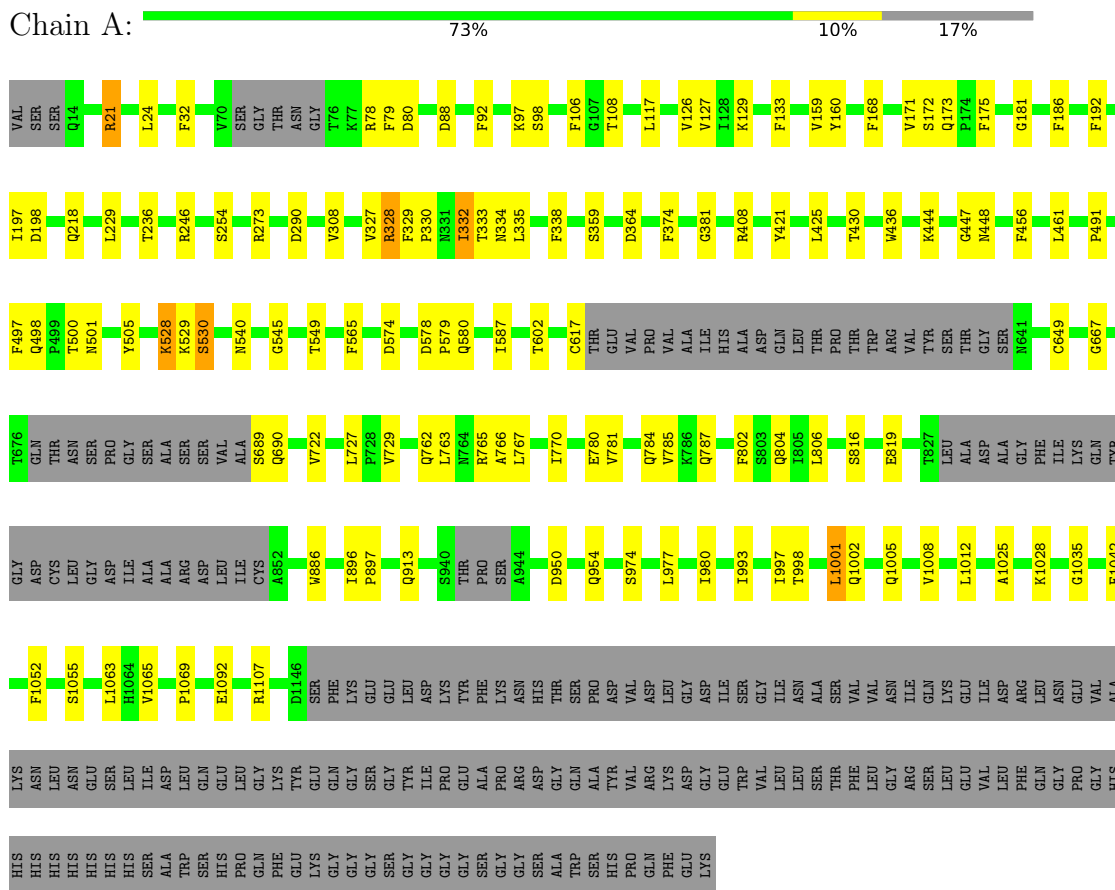
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	E	1	Total 14	8	1	5	0
5	E	1	Total 14	8	1	5	0
5	E	1	Total 14	8	1	5	0
5	E	1	Total 14	8	1	5	0
5	E	1	Total 14	8	1	5	0
5	E	1	Total 14	8	1	5	0
5	E	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	0
5	I	1	Total 14	8	1	5	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. 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. 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.

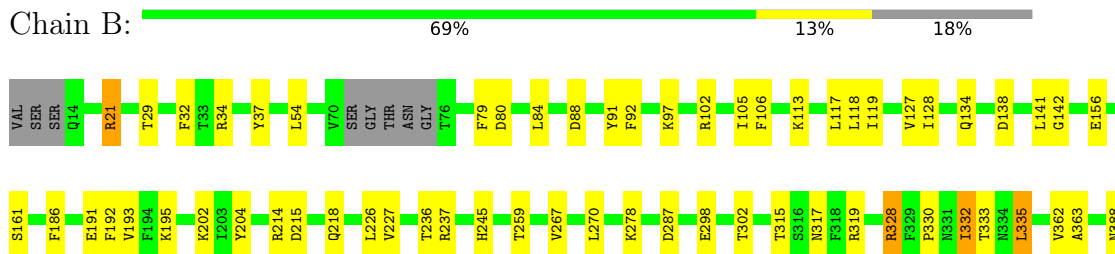
- Molecule 1: Spike glycoprotein,Fibrin,Expression Tag

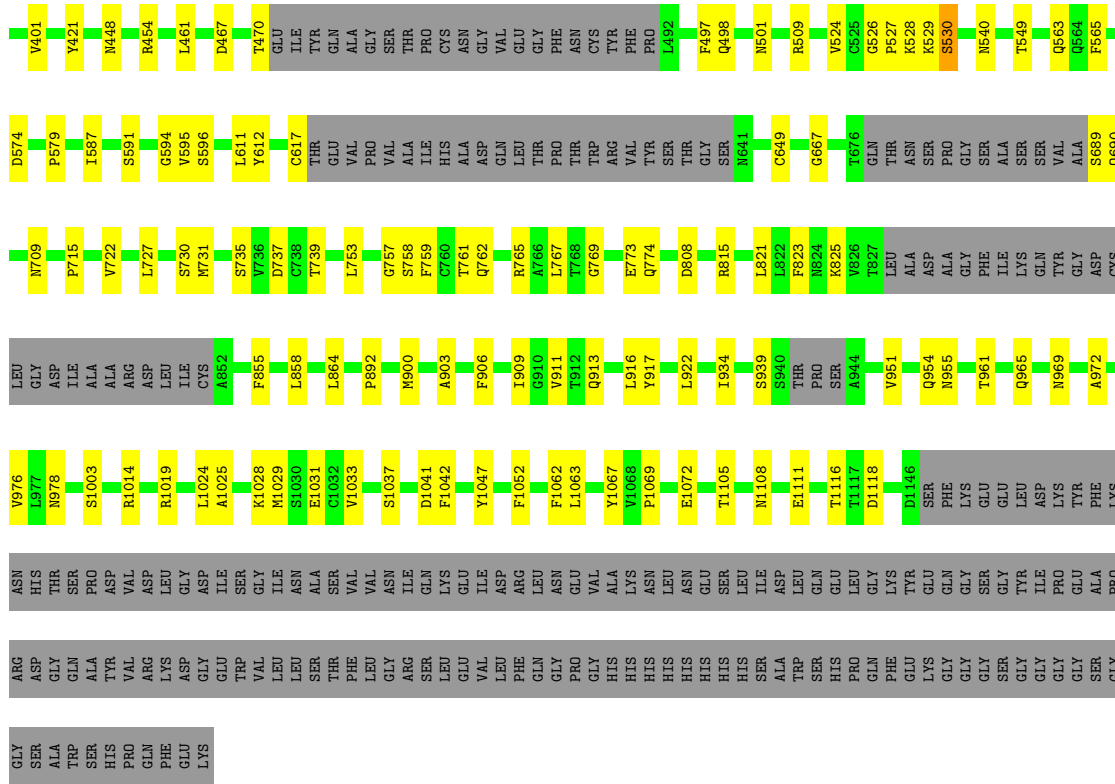
Chain A:



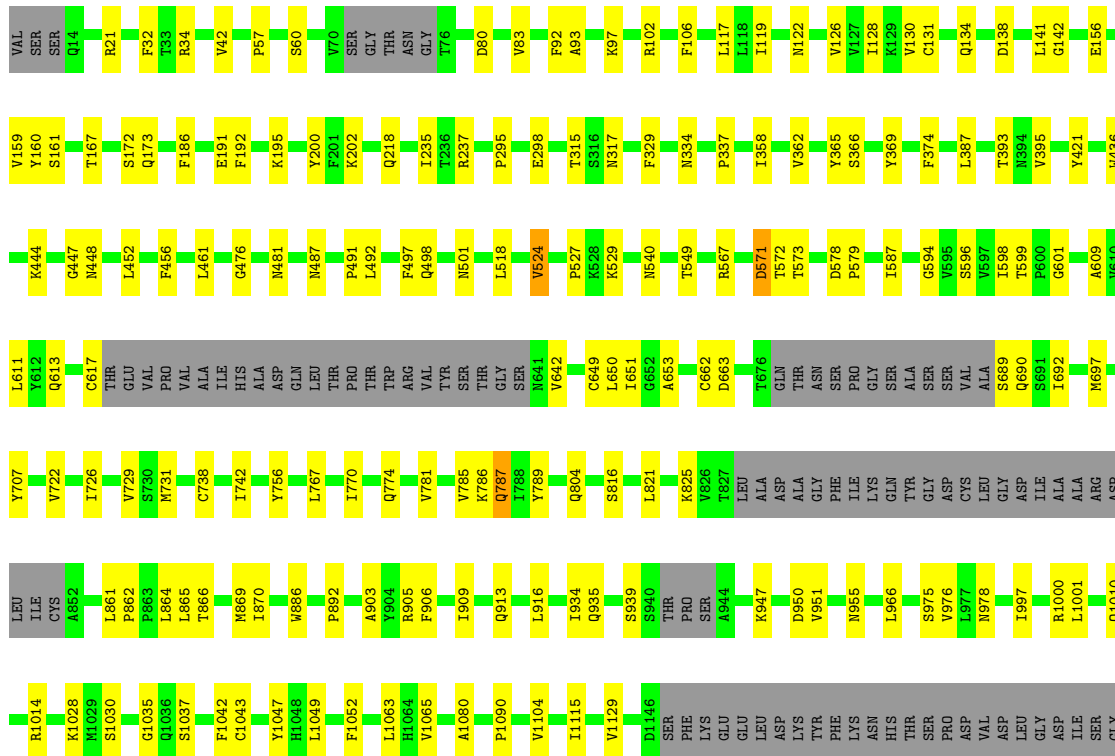
- Molecule 1: Spike glycoprotein,Fibrin,Expression Tag

Chain B:





● Molecule 1: Spike glycoprotein, Fibrin, Expression Tag



ILE	ASN	ALA	SER	VAL	VAL	ASN	ILE	GLN	LYS	GLY	LEU	ASP	ARG	LEU	LEU	LEU	GLY	VAL	ALA	LYS	ASN	HIS	HIS	HIS	HIS	ASN	GLY	LEU	ILE	LEU	ILE	ASP	ARG	LEU	LEU	ASN	GLY	PRO	GLY	VAL	ALA	LYS	ASN	HIS	HIS	HIS	HIS	ASN	GLY	LEU	ASP	ARG	LEU	LEU	ASP	GLY	TRP	TRP	VAL
LEU	LEU	THR	PHE	LEU	GLY	ARG	SER	GLN	LYS	GLY	LEU	VAL	VAL	LEU	LEU	VAL	ASP	GLY	PHE	GLN	ASN	GLY	PRO	GLY	HIS	HIS	HIS	HIS	ASN	GLY	LEU	ASP	ARG	LEU	LEU	ASN	GLY	PRO	GLY	VAL	ALA	LYS	ASN	HIS	HIS	HIS	HIS	ASN	GLY	LEU	ASP	ARG	LEU	LEU	ASP	GLY	TRP	TRP	VAL

• Molecule 1: Spike glycoprotein, Fibritin, Expression Tag


Chain D:  73% 10% 17%

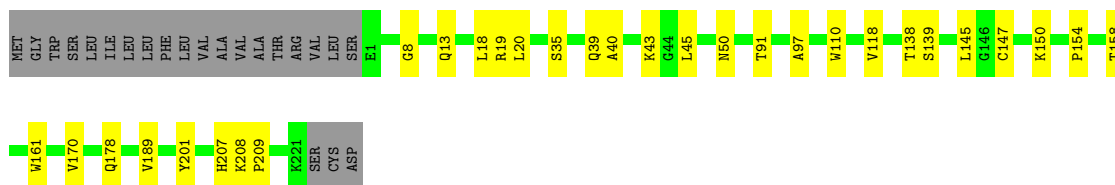
VAL	SER	Q14	R21	L24	F32	V70	GLY	THR	ASN	GLY	T76	K77	R78	F79	D80	D88	F92	K97	S98	F106	L117	A123	V126	K129	F133	V159	Y160	F168	S172	Q173	M177	G181	F186	F192	L216	P217								
Q218	L229	Q239	T240	R246	S254	L276	L277	K278	V289	D290	C291	F306	K310	N317	R328	L332	T333	N334	L335	C336	F337	F338	V341	C361	V362	D364	S366	F374	C381	V395	R403	Y421	T430	W436	K444									
G447	L452	L461	L492	Y495	P521	L524	F543	Q563	Q566	D574	D578	Q580	P579	T581	E583	L587	G594	V595	V610	Q613	C617	THR	GLU	VAL	PRO	VAL	ALA	ILE	HIS	ASP	GLN	LEU	THR	PRO	THR	TRP	VAL	TYR	SER	THR				
GLY	SER	M641	C649	C662	D663	P665	I666	G667	C671	T676	GLN	THR	ASN	SER	PRO	ILE	CYS	LEU	ALA	ALA	A852	M699	P715	T719	V722	V729	I742	R765	L767	I770	W777	T778	V781	Q965	S974	F602								
L806	V826	T827	ALA	ASP	ALA	PHE	ILE	LYS	GLN	GLY	CYS	LEU	GLY	ASP	ILE	ALA	ALA	A852	W886	P897	Q913	I931	I934	S940	PRO	PRO	A944	L945	L948	V951	Q954	V963	K964	Q965	S974	V976								
L977	M978	D979	I980	I987	Q1005	T1009	R1014	K1028	M1029	S1030	L1034	G1035	R1039	F1042	Y1047	Y1067	V1068	P1069	A1070	B1146	SER	PHE	LYS	GLY	GLY	GLY	ASP	THR	THR	ALA	PRO	ASP	VAL	ASP	LEU	GLY	ASP	GLY	ASN	ALA				
SER	VAL	ASN	ILE	GLN	LYS	ILE	ARG	LEU	ASN	GLY	VAL	ALA	ASN	ASN	ASP	GLN	GLU	LEU	GLY	LYS	TRP	GLY	TYR	ILE	PRO	GLY	ALA	GLY	GLN	ALA	TYR	VAL	ARG	LYS	LEU	GLY	ASP	GLY	ASP	TRP	VAL	LEU	LEU	SER
THR	PHE	LEU	GLY	ARG	LEU	LEU	VAL	PHE	GLN	PRO	HIS	GLY	HIS	HIS	HIS	HIS	THR	PRO	GLN	PHE	GLY	GLY	SER	GLY	GLY	GLY	GLY	ALA	ALA	SER	HIS	PRO	GLN	ARG	PHE	GLY	LYS							

• Molecule 1: Spike glycoprotein, Fibritin, Expression Tag

Chain E:  71% 12% 17%

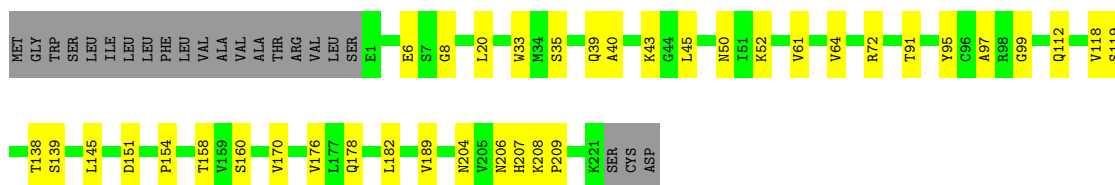
VAL	SER	Q14	R21	F32	T33	R34	Y37	V42	L54	H66	V70	SER	GLY	THR	Y204	R214	D215	Q218	F79	D80	L84	D88	F92	K97	R102	I105	F106	L117	L118	I119	V127	I128	K129	V130	Q134	D138	L141	G142			
E156	S161	M164	F168	E169	F186	K444	E191	F192	V193	F194	K195	G199	Y200	F201	K202	Y204	R214	D215	Q218	F79	D80	L84	D88	F92	K97	R102	I105	F106	L117	L118	I119	V127	I128	K129	V130	Q134	D138	L141	G142		
C391	F392	T393	V401	Y421	L425	K444	G447	Y451	R454	L461	D467	I468	Q474	P479	Q493	R509	A522	T523	V524	C525	G232	L233	H234	T236	R237	H245	T259	F565	G566	D574	P579	I687	F329	P330	S349	L387	L390				
A609	V610	L611	C617	THR	GLU	PRO	VAL	ALA	ILE	HIS	ALA	ASP	GLN	ASN	GLY	THR	THR	GLY	M641	C649	L650	A653	T676	GLN	THR	ASN	SER	PRO	GLY	SER	ALA	SER	SER	VAL	ALA	Q690	M697	A701	S711	P715	D737

Chain H:  79% 12% 9%



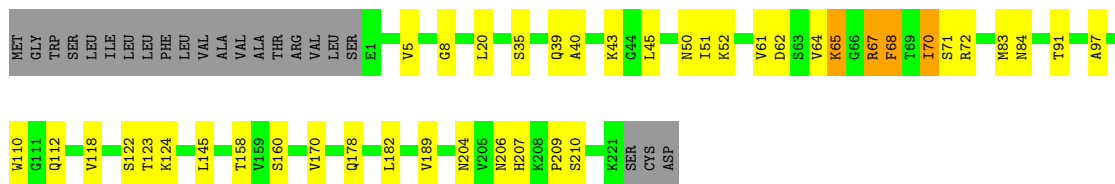
- Molecule 2: Heavy chain of R1-26 Fab

Chain F:  75% 16% 9%




- Molecule 2: Heavy chain of R1-26 Fab

Chain J:  74% 16% 9%




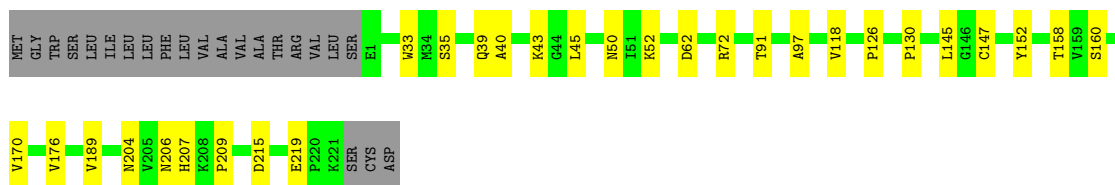
- Molecule 2: Heavy chain of R1-26 Fab

Chain R:  79% 12% 9%



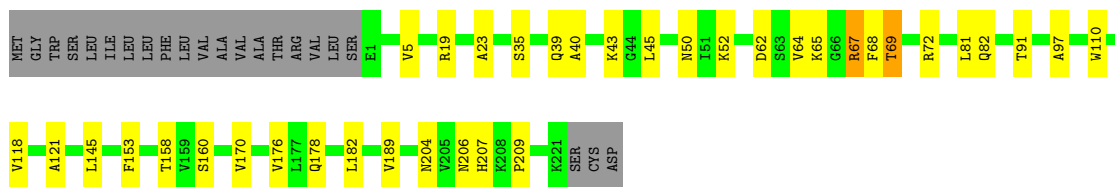
- Molecule 2: Heavy chain of R1-26 Fab

Chain M:  79% 12% 9%



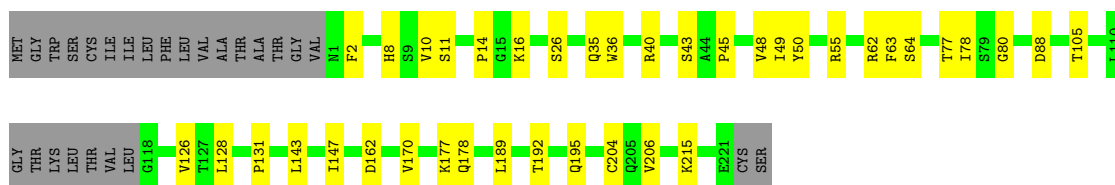
- Molecule 2: Heavy chain of R1-26 Fab

Chain S:  76% 14% 9%



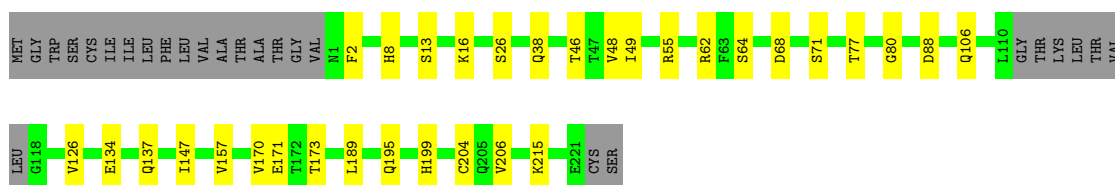
• Molecule 3: Light chain of R1-26 Fab

Chain L:  73% 16% 11%




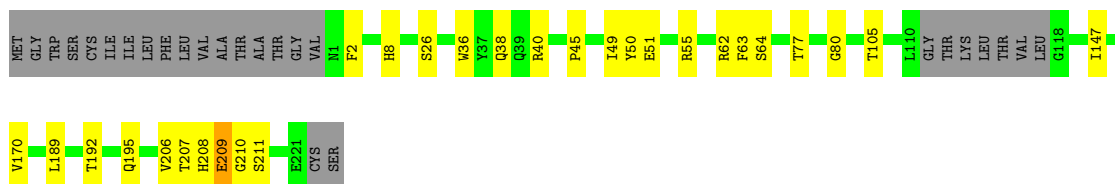
• Molecule 3: Light chain of R1-26 Fab

Chain G:  76% 13% 11%



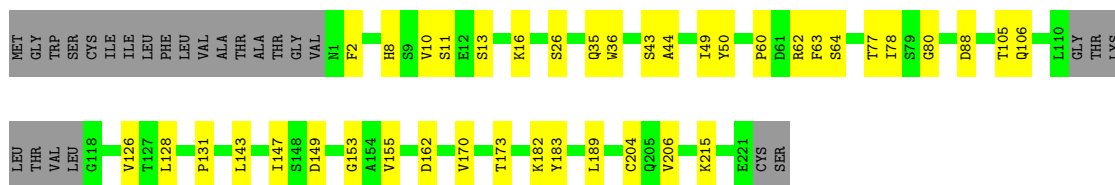
• Molecule 3: Light chain of R1-26 Fab

Chain K:  78% 11% 11%




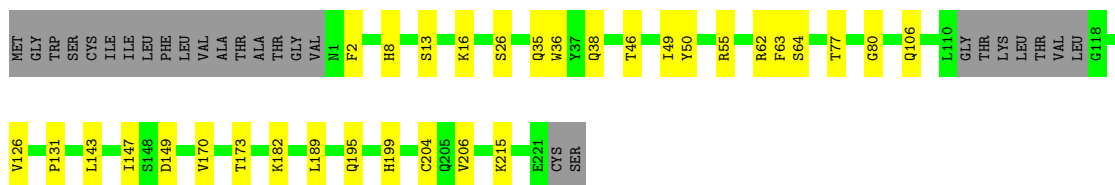
• Molecule 3: Light chain of R1-26 Fab

Chain U:  72% 17% 11%




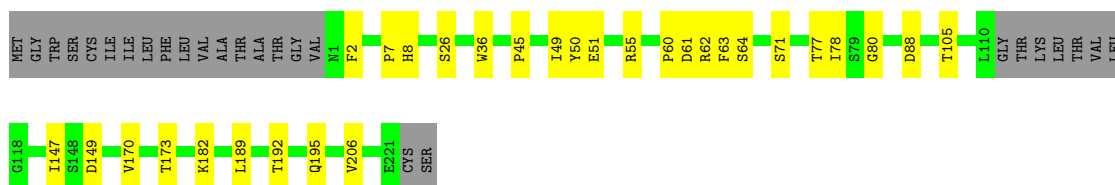
• Molecule 3: Light chain of R1-26 Fab

Chain N:  76% 13% 11%



- Molecule 3: Light chain of R1-26 Fab

Chain T:  77% 12% 11%



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

Chain O:  100%



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

Chain P:  100%



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

Chain Q:  100%



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

Chain V:  100%



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

Chain W:  100%

MAG1
MAG2

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

Chain X:  100%

MAG1
MAG2

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

Chain Y:  50% 50%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain a:  100%

MAG1
MAG2

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

Chain b:  100%

MAG1
MAG2

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

Chain c:  100%

MAG1
MAG2

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

Chain d:  100%MAG1
MAG2

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

Chain e:  100%MAG1
MAG2

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

Chain f:  100%MAG1
MAG2

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

Chain g:  100%MAG1
MAG2

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

Chain h:  100%MAG1
MAG2

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

Chain i:  100%MAG1
MAG2

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

Chain j:  100%



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

Chain k:  100%



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

Chain l:  100%



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

Chain m:  100%



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

Chain n:  100%



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

Chain o:  100%



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

Chain p:  100%

MAG1
MAG2

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

Chain q:  100%MAG1
MAG2

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

Chain r:  100%MAG1
MAG2

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

Chain s:  100%MAG1
MAG2

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

Chain t:  100%MAG1
MAG2

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

Chain u:  100%MAG1
MAG2

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

Chain v:  100%MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	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

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	0.27	0/8515	0.49	0/11595
1	B	0.27	0/8356	0.50	0/11376
1	C	0.26	0/8515	0.49	0/11595
1	D	0.25	0/8515	0.50	0/11595
1	E	0.26	0/8515	0.50	0/11595
1	I	0.26	0/8515	0.52	0/11595
2	F	0.25	0/1697	0.52	0/2311
2	H	0.25	0/1697	0.51	0/2311
2	J	0.25	0/1697	0.49	0/2311
2	M	0.25	0/1697	0.51	0/2311
2	R	0.25	0/1697	0.51	0/2311
2	S	0.25	0/1697	0.51	0/2311
3	G	0.25	0/1630	0.48	0/2232
3	K	0.25	0/1630	0.48	0/2232
3	L	0.26	0/1630	0.50	0/2232
3	N	0.25	0/1630	0.49	0/2232
3	T	0.25	0/1630	0.49	0/2232
3	U	0.25	0/1630	0.49	0/2232
All	All	0.26	0/70893	0.50	0/96609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8320	0	8074	87	0
1	B	8167	0	7944	104	0
1	C	8320	0	8074	102	0
1	D	8320	0	8074	97	0
1	E	8320	0	8074	100	0
1	I	8320	0	8074	124	0
2	F	1656	0	1626	24	0
2	H	1656	0	1626	17	0
2	J	1656	0	1626	26	0
2	M	1656	0	1626	19	0
2	R	1656	0	1626	17	0
2	S	1656	0	1626	20	0
3	G	1591	0	1482	20	0
3	K	1591	0	1482	14	0
3	L	1591	0	1482	26	0
3	N	1591	0	1482	18	0
3	T	1591	0	1482	21	0
3	U	1591	0	1482	24	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	1	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	c	28	0	25	0	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
4	h	28	0	25	0	0
4	i	28	0	25	0	0
4	j	28	0	25	0	0
4	k	28	0	25	0	0
4	l	28	0	25	0	0
4	m	28	0	25	0	0
4	n	28	0	25	0	0
4	o	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	p	28	0	25	0	0
4	q	28	0	25	0	0
4	r	28	0	25	0	0
4	s	28	0	25	0	0
4	t	28	0	25	0	0
4	u	28	0	25	0	0
4	v	28	0	25	0	0
5	A	140	0	130	0	0
5	B	140	0	130	1	0
5	C	140	0	130	0	0
5	D	140	0	130	0	0
5	E	140	0	130	1	0
5	I	140	0	130	0	0
All	All	70929	0	68492	815	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 6.

The worst 5 of 815 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:THR:HA	1:A:1001:LEU:CD2	1.27	1.58
1:A:998:THR:CA	1:A:1001:LEU:HD21	1.41	1.51
1:A:998:THR:O	1:A:1001:LEU:CG	1.82	1.27
1:A:998:THR:O	1:A:1001:LEU:HG	1.00	1.17
1:A:997:ILE:O	1:A:1001:LEU:HD23	1.44	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1054/1278 (82%)	1013 (96%)	41 (4%)	0	100	100
1	B	1031/1278 (81%)	994 (96%)	37 (4%)	0	100	100
1	C	1054/1278 (82%)	1014 (96%)	40 (4%)	0	100	100
1	D	1054/1278 (82%)	1019 (97%)	35 (3%)	0	100	100
1	E	1054/1278 (82%)	1015 (96%)	39 (4%)	0	100	100
1	I	1054/1278 (82%)	1012 (96%)	42 (4%)	0	100	100
2	F	219/243 (90%)	203 (93%)	16 (7%)	0	100	100
2	H	219/243 (90%)	204 (93%)	15 (7%)	0	100	100
2	J	219/243 (90%)	205 (94%)	14 (6%)	0	100	100
2	M	219/243 (90%)	206 (94%)	13 (6%)	0	100	100
2	R	219/243 (90%)	205 (94%)	14 (6%)	0	100	100
2	S	219/243 (90%)	201 (92%)	18 (8%)	0	100	100
3	G	210/240 (88%)	199 (95%)	11 (5%)	0	100	100
3	K	210/240 (88%)	198 (94%)	12 (6%)	0	100	100
3	L	210/240 (88%)	199 (95%)	11 (5%)	0	100	100
3	N	210/240 (88%)	196 (93%)	14 (7%)	0	100	100
3	T	210/240 (88%)	194 (92%)	16 (8%)	0	100	100
3	U	210/240 (88%)	195 (93%)	15 (7%)	0	100	100
All	All	8875/10566 (84%)	8472 (96%)	403 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	929/1106 (84%)	915 (98%)	14 (2%)	60	75
1	B	913/1106 (82%)	904 (99%)	9 (1%)	73	82
1	C	929/1106 (84%)	922 (99%)	7 (1%)	79	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	929/1106 (84%)	921 (99%)	8 (1%)	75	83
1	E	929/1106 (84%)	919 (99%)	10 (1%)	70	80
1	I	929/1106 (84%)	926 (100%)	3 (0%)	91	92
2	F	184/203 (91%)	184 (100%)	0	100	100
2	H	184/203 (91%)	183 (100%)	1 (0%)	86	90
2	J	184/203 (91%)	179 (97%)	5 (3%)	40	59
2	M	184/203 (91%)	184 (100%)	0	100	100
2	R	184/203 (91%)	183 (100%)	1 (0%)	86	90
2	S	184/203 (91%)	181 (98%)	3 (2%)	58	74
3	G	181/206 (88%)	181 (100%)	0	100	100
3	K	181/206 (88%)	179 (99%)	2 (1%)	70	80
3	L	181/206 (88%)	181 (100%)	0	100	100
3	N	181/206 (88%)	181 (100%)	0	100	100
3	T	181/206 (88%)	181 (100%)	0	100	100
3	U	181/206 (88%)	181 (100%)	0	100	100
All	All	7748/9090 (85%)	7685 (99%)	63 (1%)	77	85

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	786	LYS
1	E	529	LYS
2	J	71	SER
1	E	528	LYS
2	R	19	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	178	GLN
2	S	206	ASN
2	S	178	GLN
1	D	613	GLN
1	I	1011	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](#)

60 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	$\# Z > 2$
4	NAG	O	1	4,1	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	O	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	P	1	4,1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	P	2	4	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	Q	1	4,1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	Q	2	4	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	V	1	4,1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.43	0
4	NAG	W	1	4,1	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	W	2	4	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	X	1	4,1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	X	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	Y	1	4,1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	Y	2	4	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	Z	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	Z	2	4	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	a	1	4,1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	a	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	b	1	4,1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	b	2	4	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	c	1	4,1	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	c	2	4	14,14,15	0.26	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	d	1	4,1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	d	2	4	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	e	1	4,1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	e	2	4	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	f	1	4,1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	f	2	4	14,14,15	0.27	0	17,19,21	0.43	0
4	NAG	g	1	4,1	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	g	2	4	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	h	1	4,1	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	h	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	i	1	4,1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	i	2	4	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	j	1	4,1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	j	2	4	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	k	1	4,1	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	k	2	4	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	l	1	4,1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	l	2	4	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	m	1	4,1	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	m	2	4	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	n	1	4,1	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	n	2	4	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	o	1	4,1	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	o	2	4	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	p	1	4,1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	p	2	4	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	q	1	4,1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	q	2	4	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	r	1	4,1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	r	2	4	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	s	1	4,1	14,14,15	0.16	0	17,19,21	0.49	0
4	NAG	s	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	t	1	4,1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	t	2	4	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	u	1	4,1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	u	2	4	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	v	1	4,1	14,14,15	0.22	0	17,19,21	0.46	0
4	NAG	v	2	4	14,14,15	0.25	0	17,19,21	0.44	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
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	1/6/23/26	0/1/1/1
4	NAG	d	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	2/6/23/26	0/1/1/1
4	NAG	e	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
4	NAG	f	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	NAG	h	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	1/6/23/26	0/1/1/1
4	NAG	i	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	i	2	4	-	2/6/23/26	0/1/1/1
4	NAG	j	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	j	2	4	-	2/6/23/26	0/1/1/1
4	NAG	k	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	k	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	l	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	l	2	4	-	2/6/23/26	0/1/1/1
4	NAG	m	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	m	2	4	-	1/6/23/26	0/1/1/1
4	NAG	n	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	n	2	4	-	2/6/23/26	0/1/1/1
4	NAG	o	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	o	2	4	-	2/6/23/26	0/1/1/1
4	NAG	p	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	p	2	4	-	2/6/23/26	0/1/1/1
4	NAG	q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	r	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	r	2	4	-	1/6/23/26	0/1/1/1
4	NAG	s	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	s	2	4	-	2/6/23/26	0/1/1/1
4	NAG	t	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	t	2	4	-	2/6/23/26	0/1/1/1
4	NAG	u	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	u	2	4	-	2/6/23/26	0/1/1/1
4	NAG	v	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	v	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

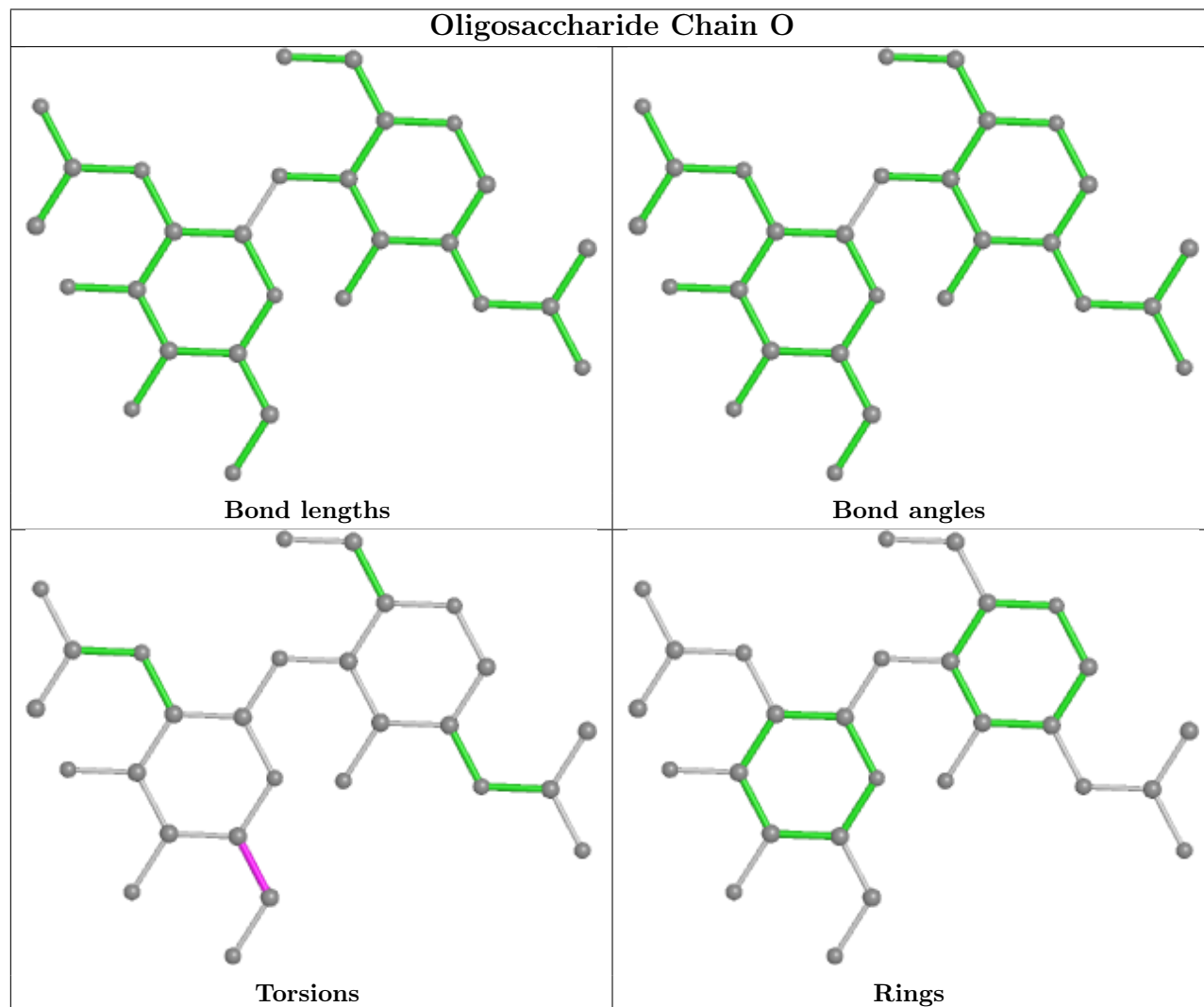
Mol	Chain	Res	Type	Atoms
4	a	2	NAG	C4-C5-C6-O6
4	p	2	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6

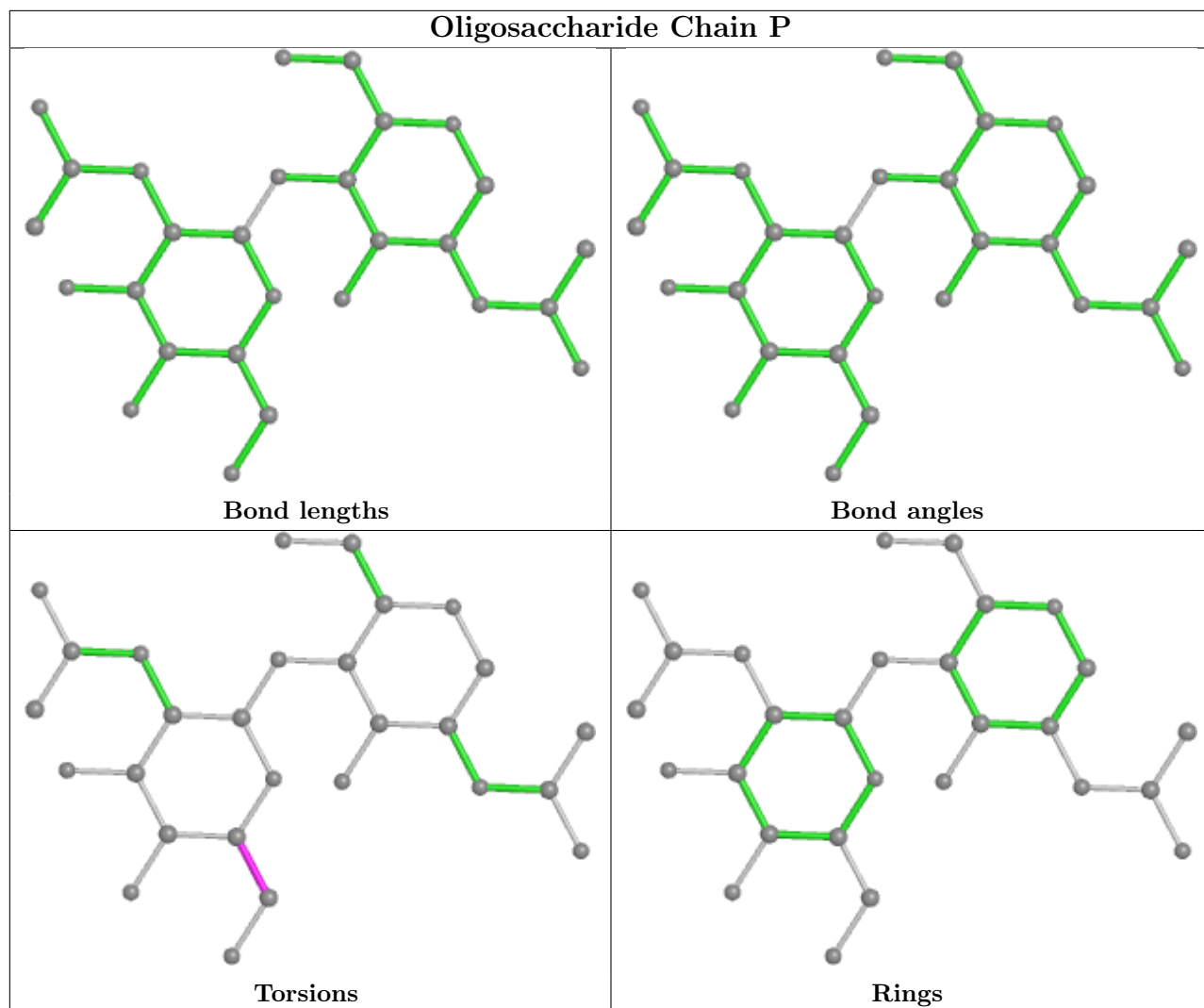
There are no ring outliers.

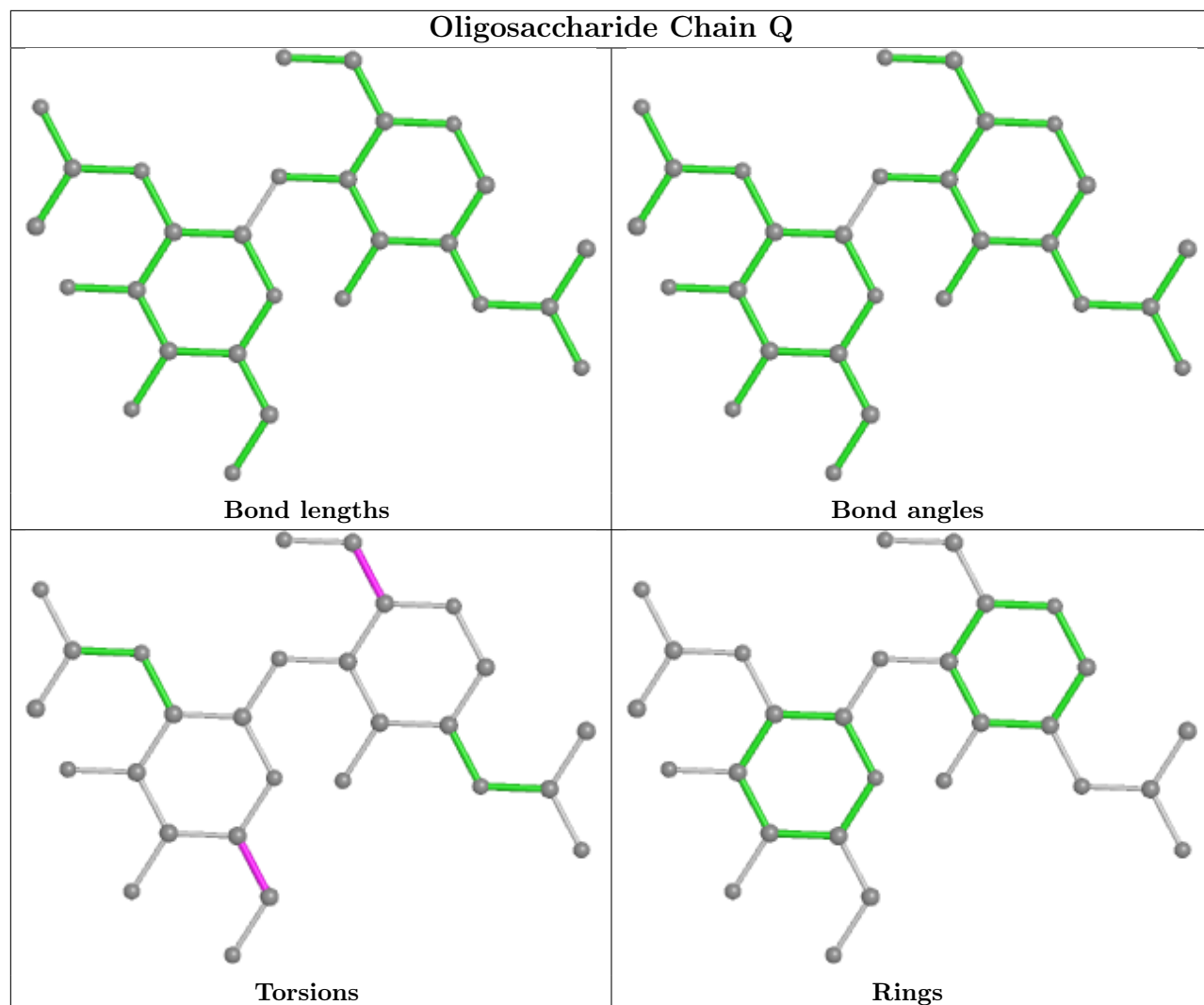
1 monomer is involved in 1 short contact:

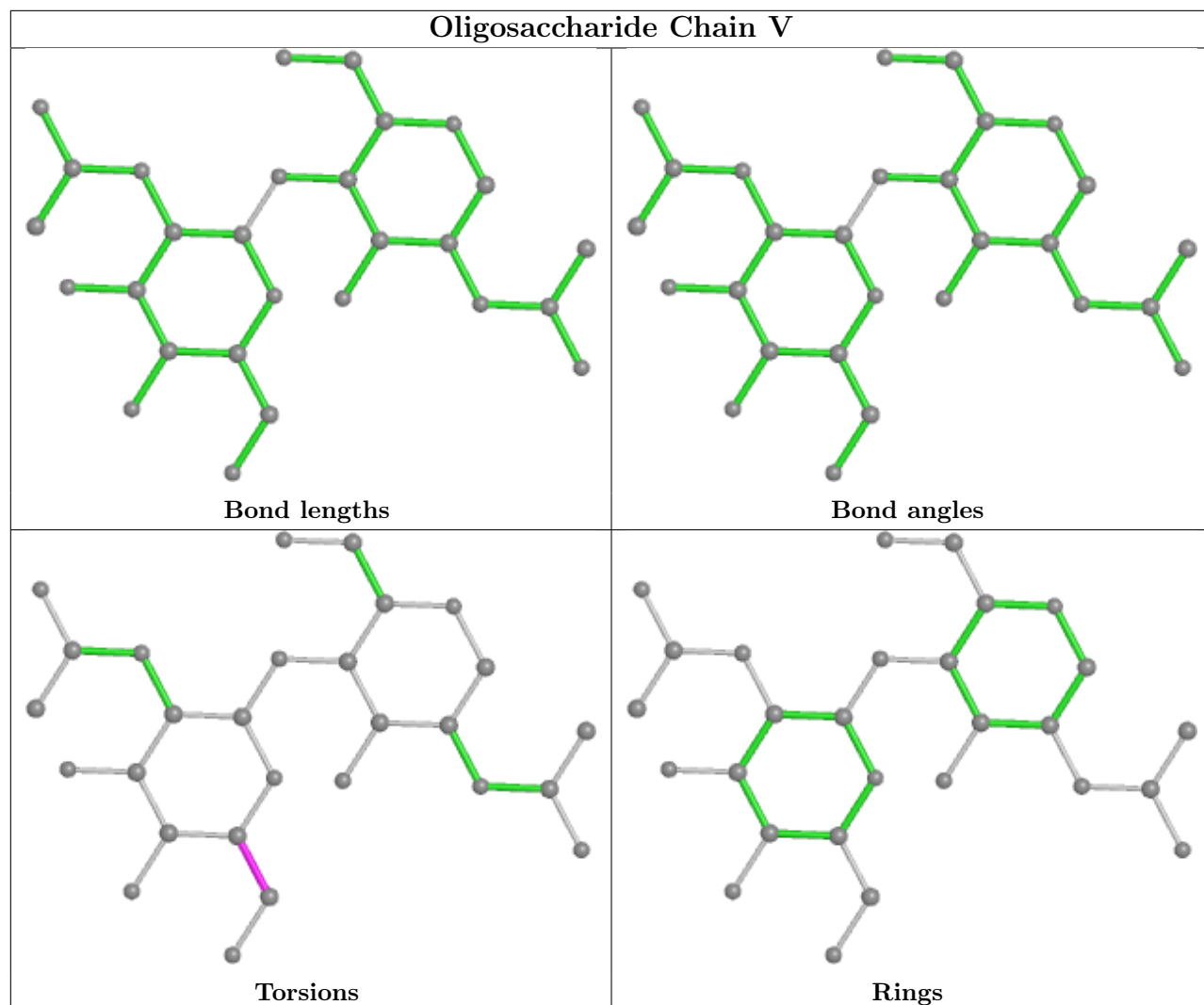
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	1	NAG	1	0

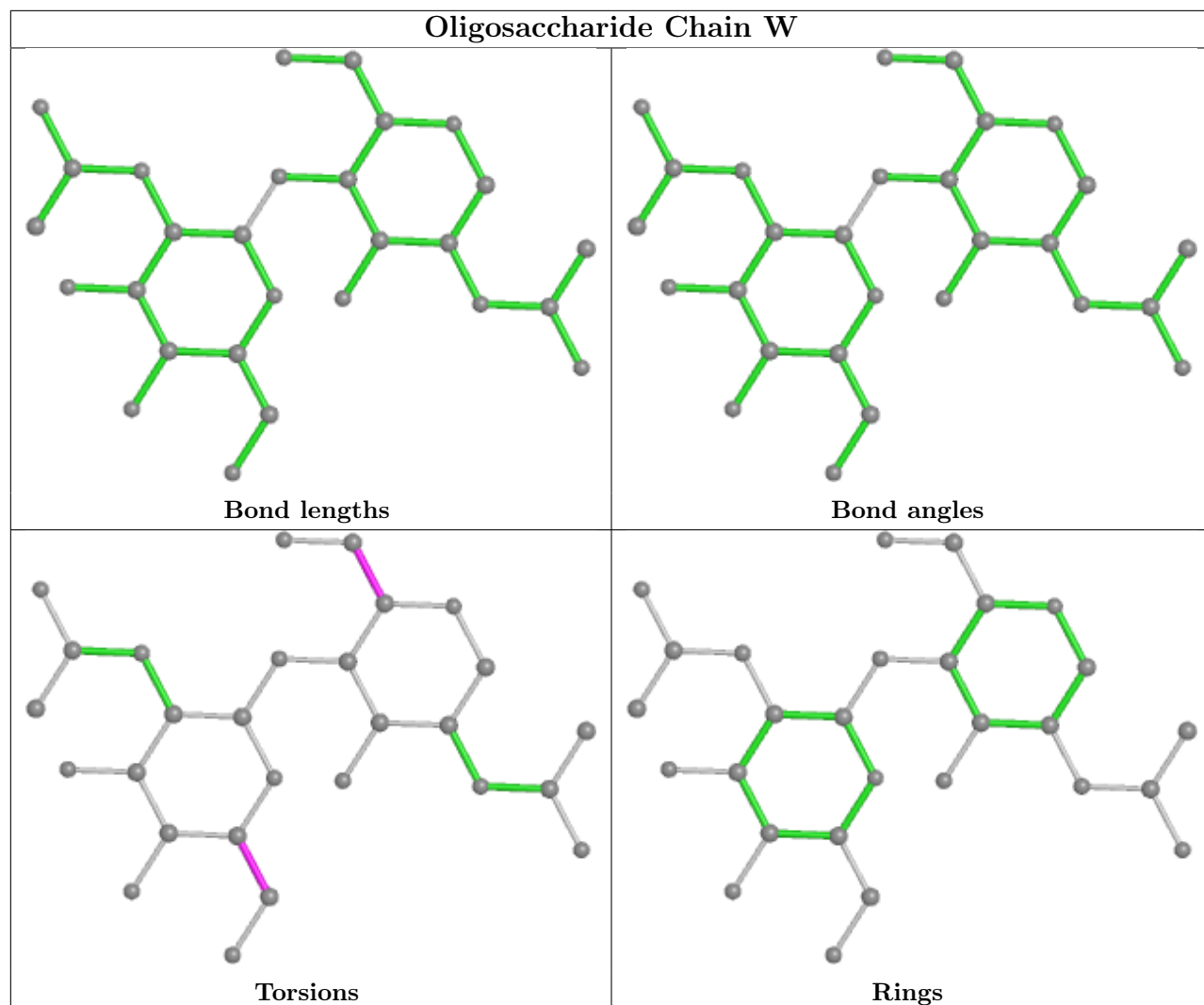
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

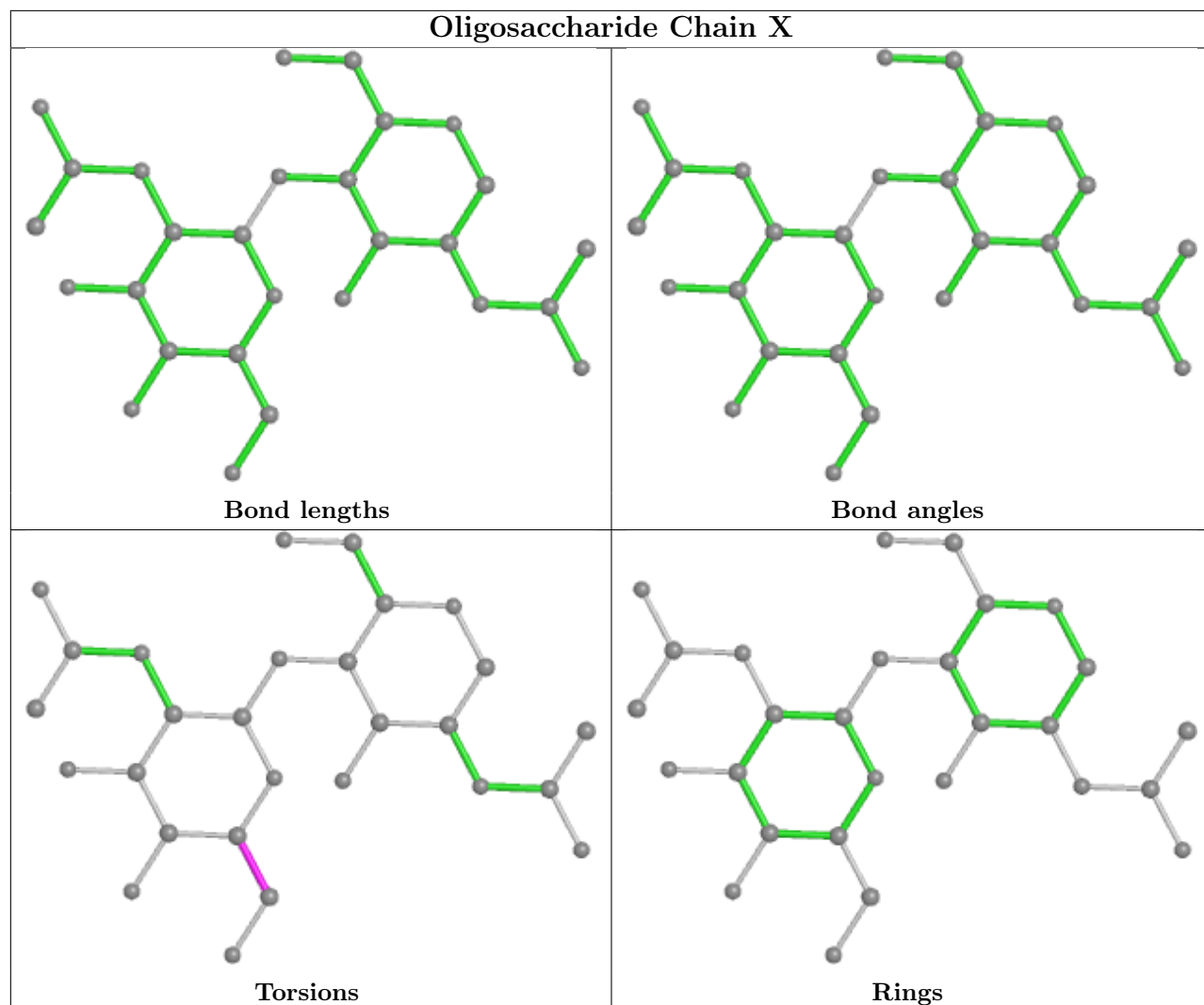


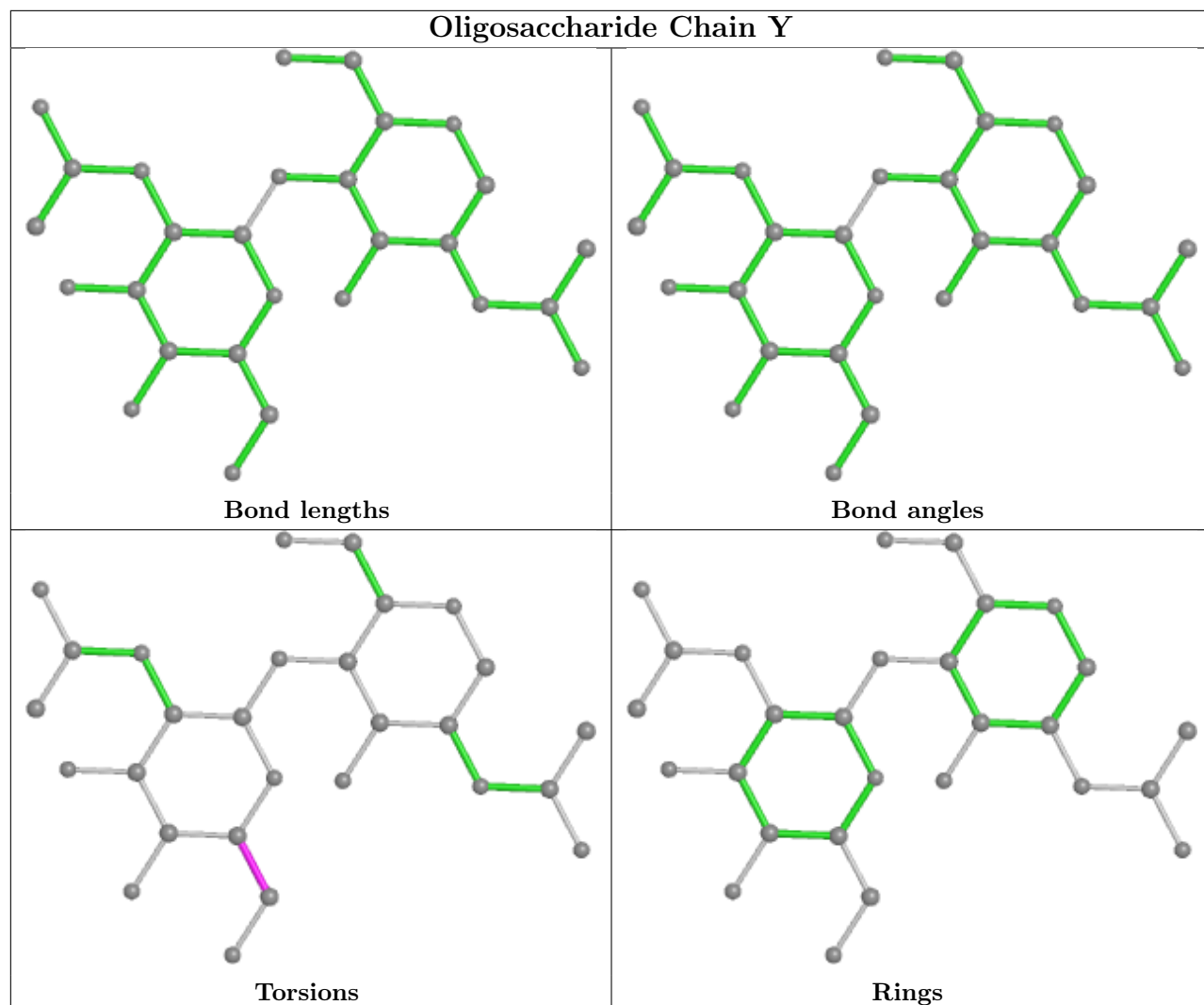


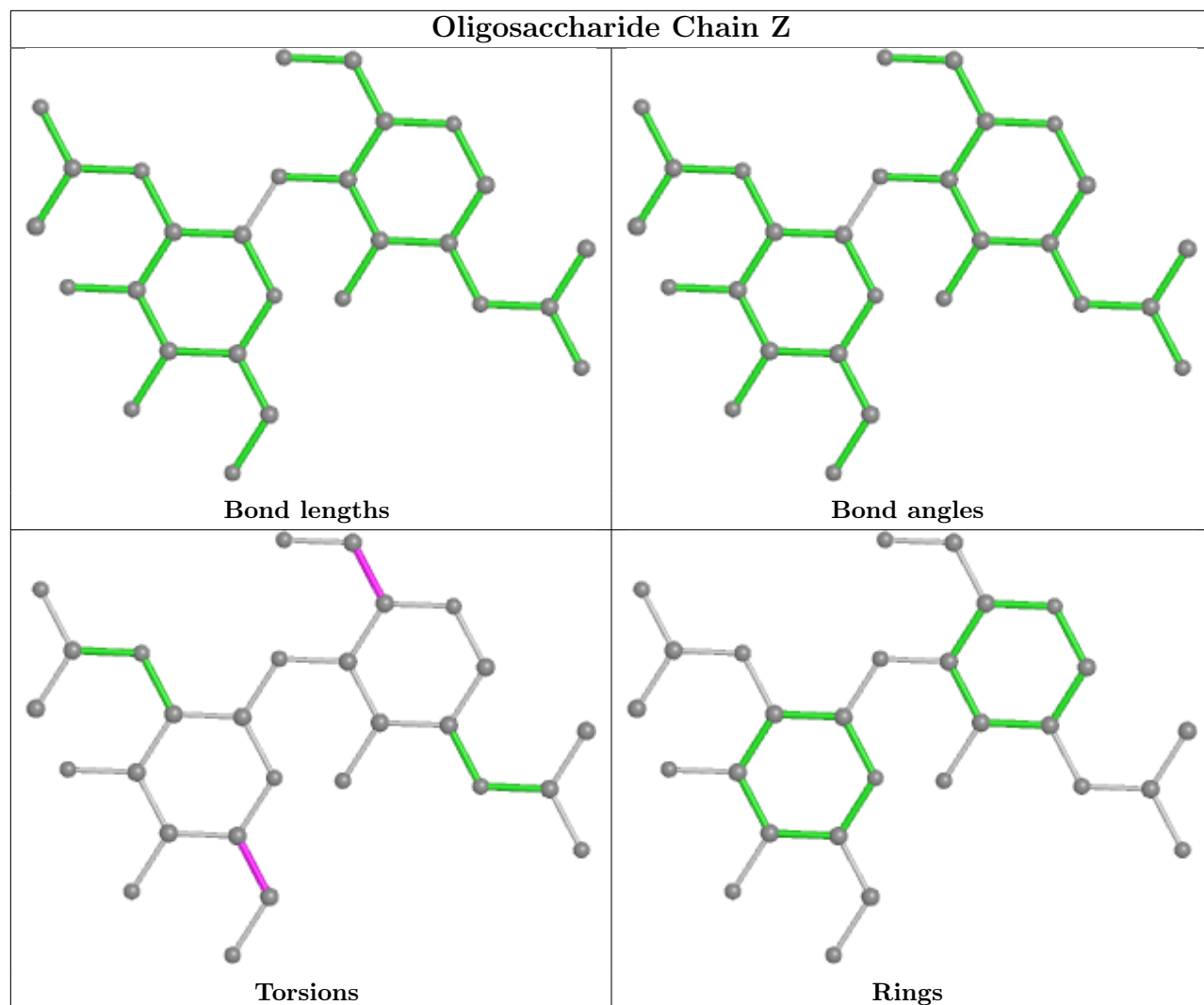


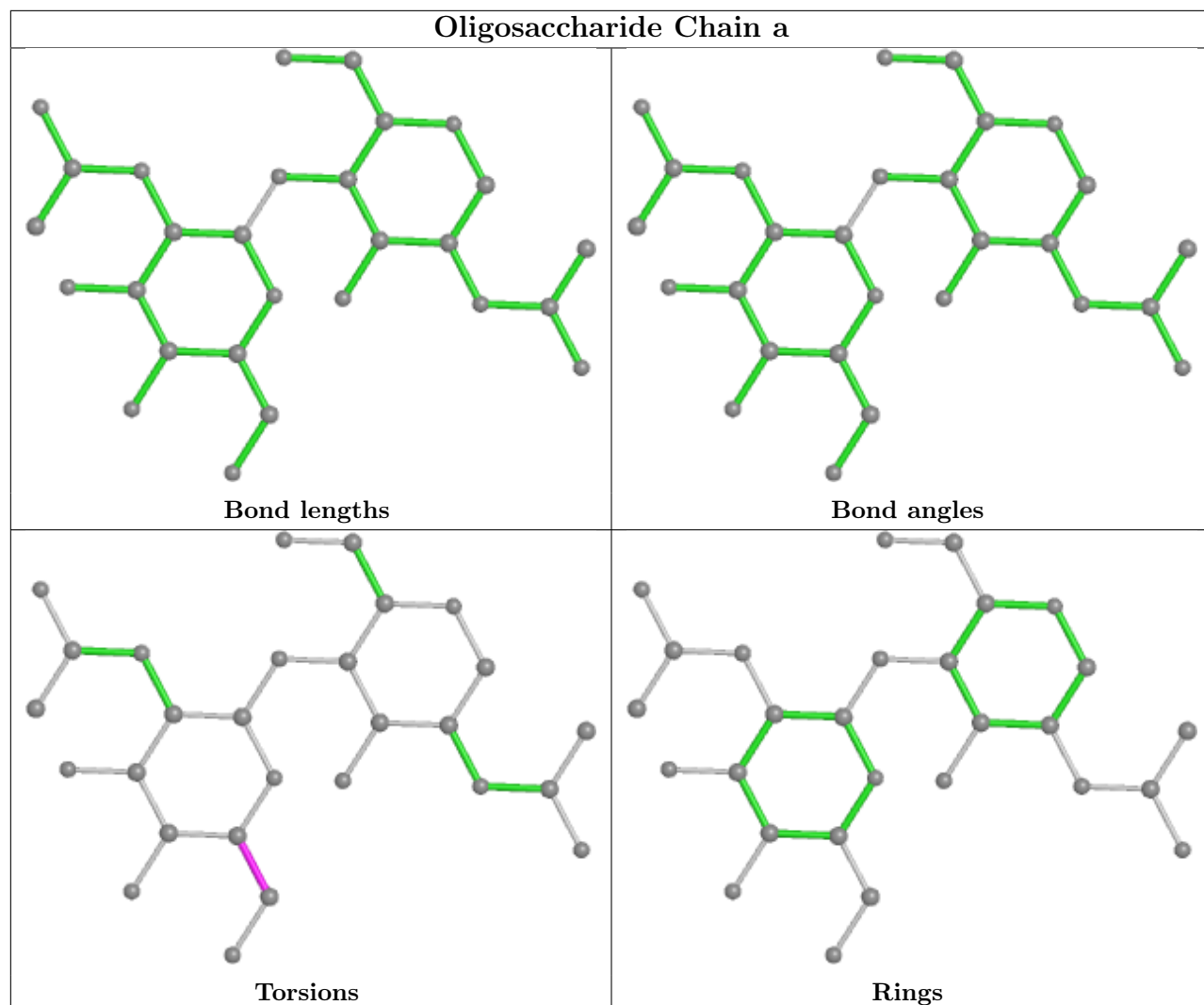


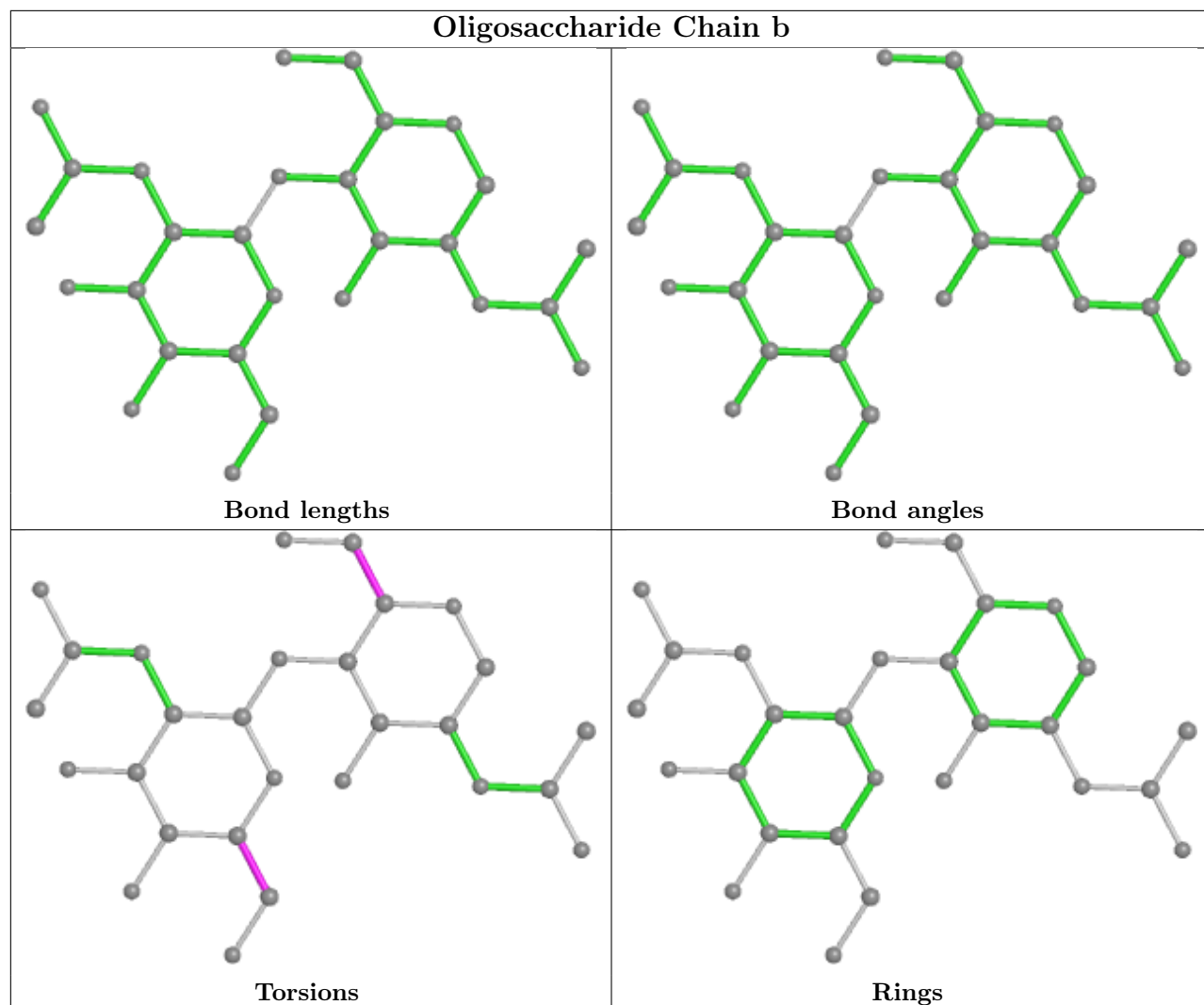


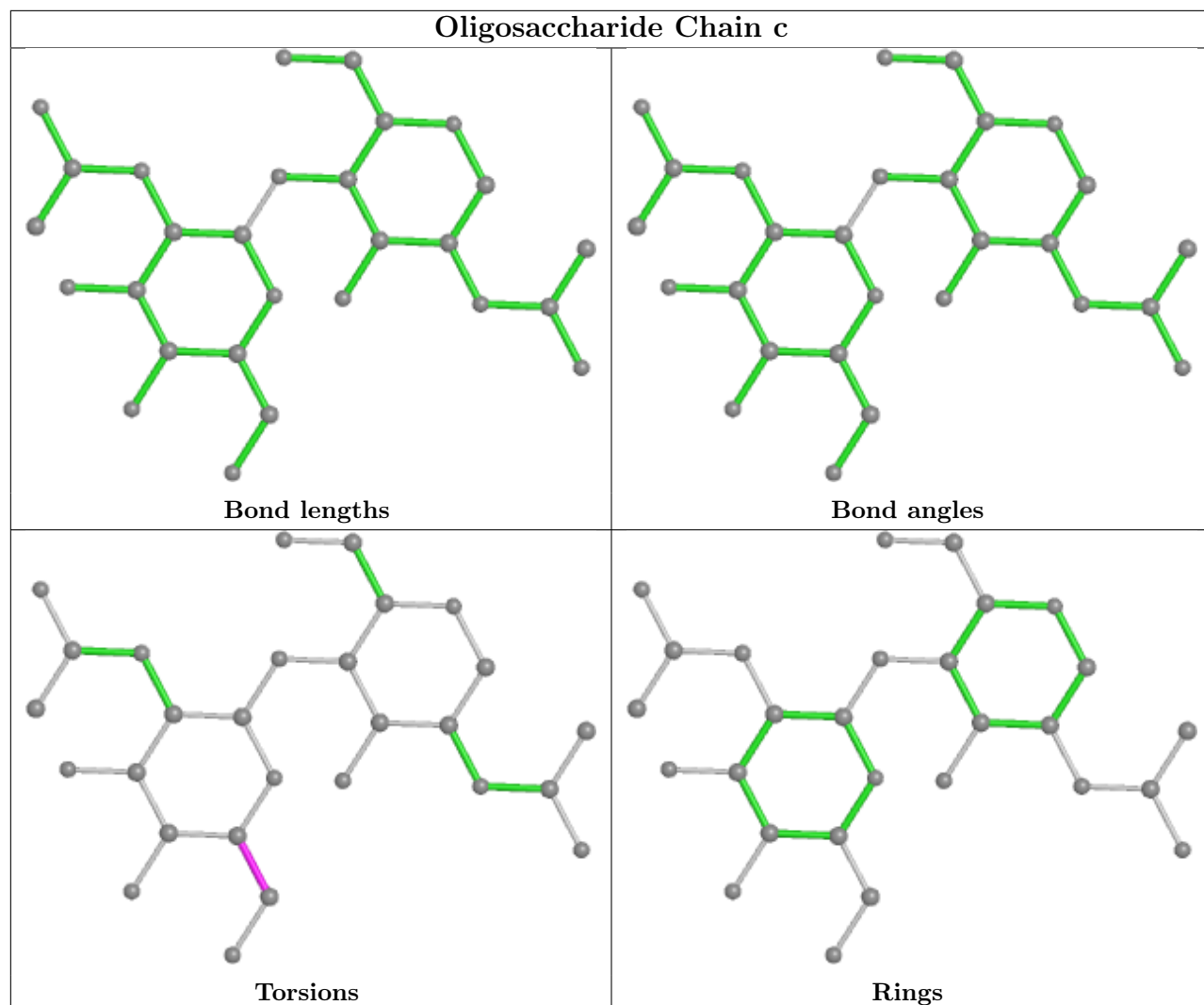


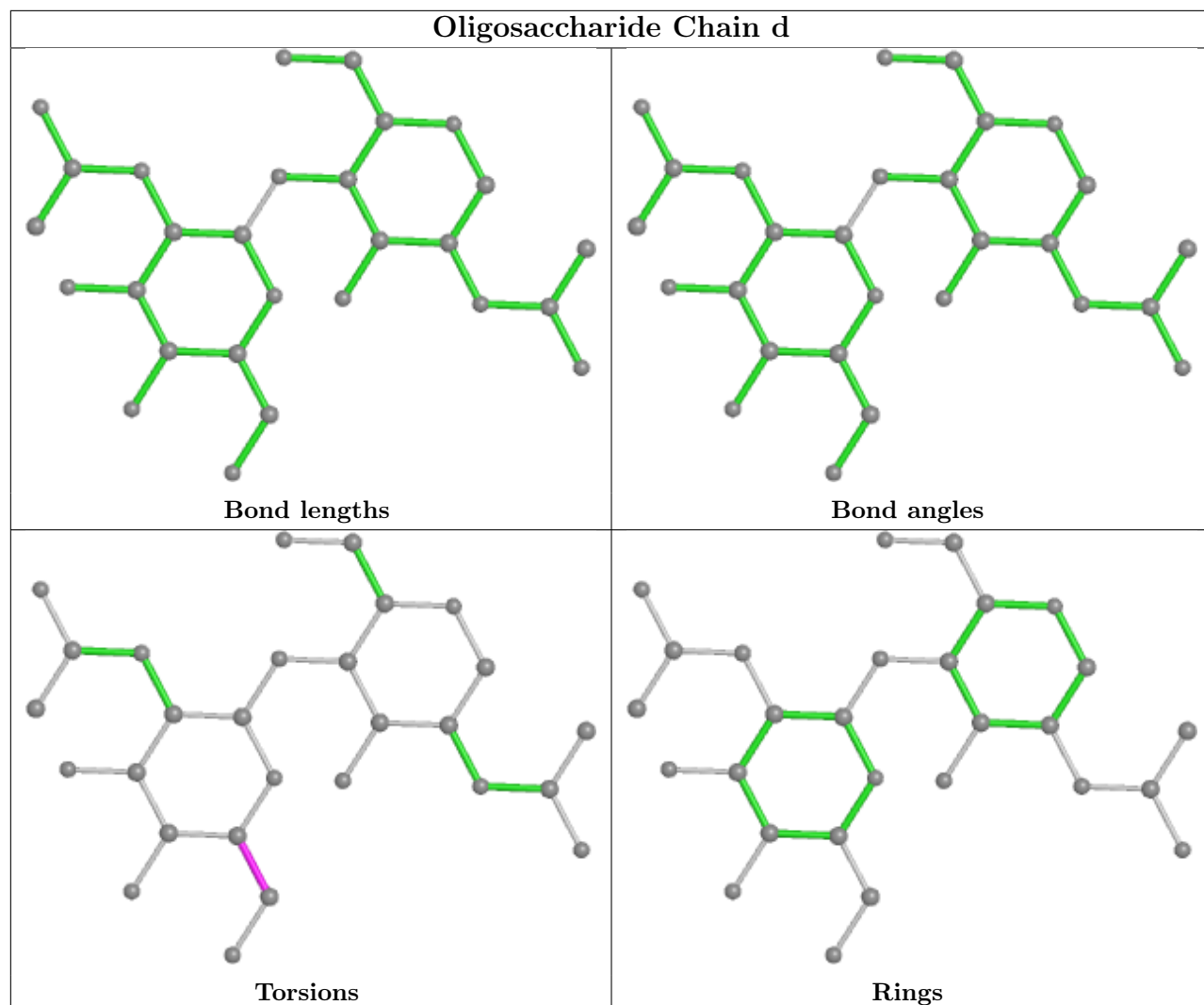


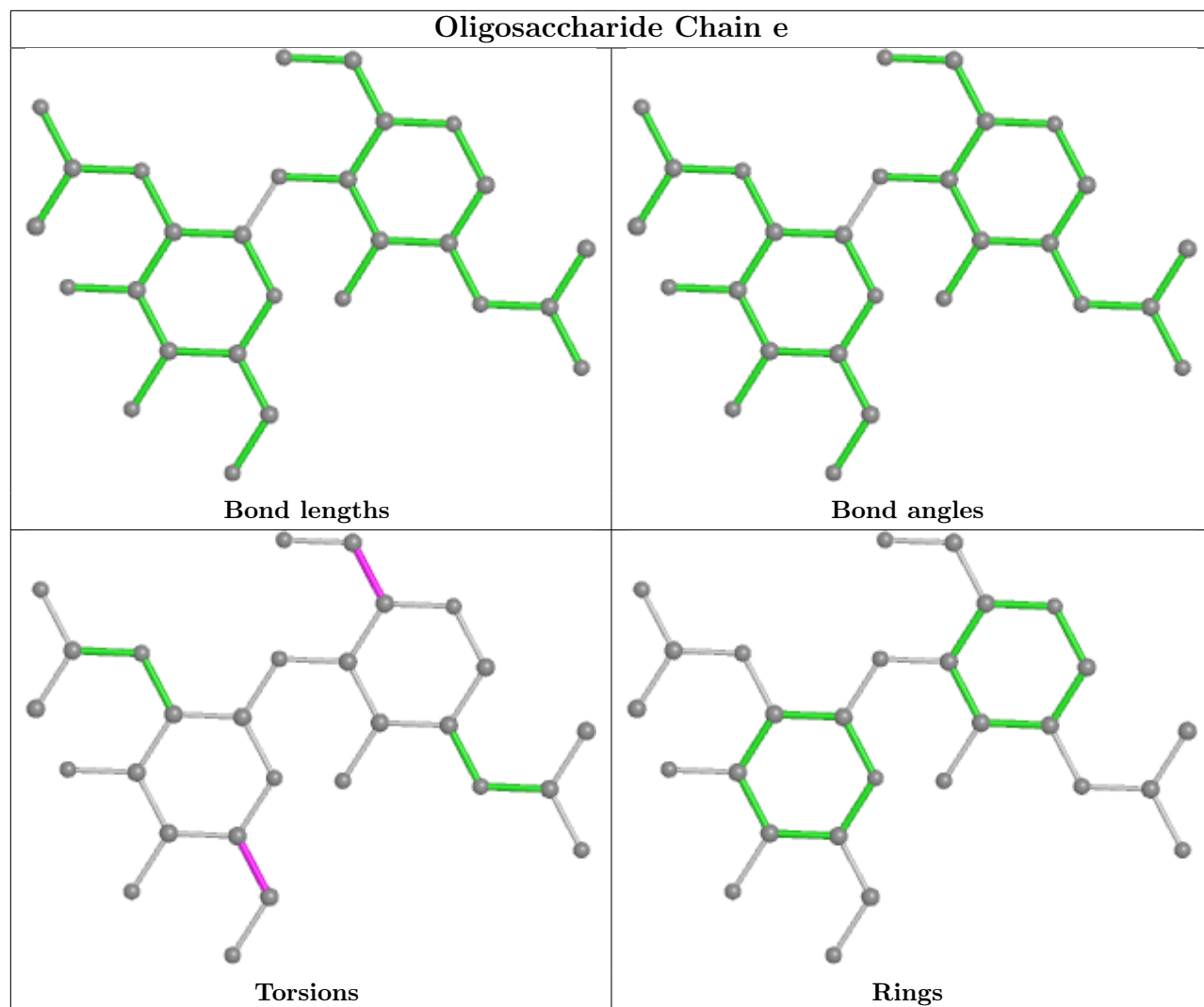


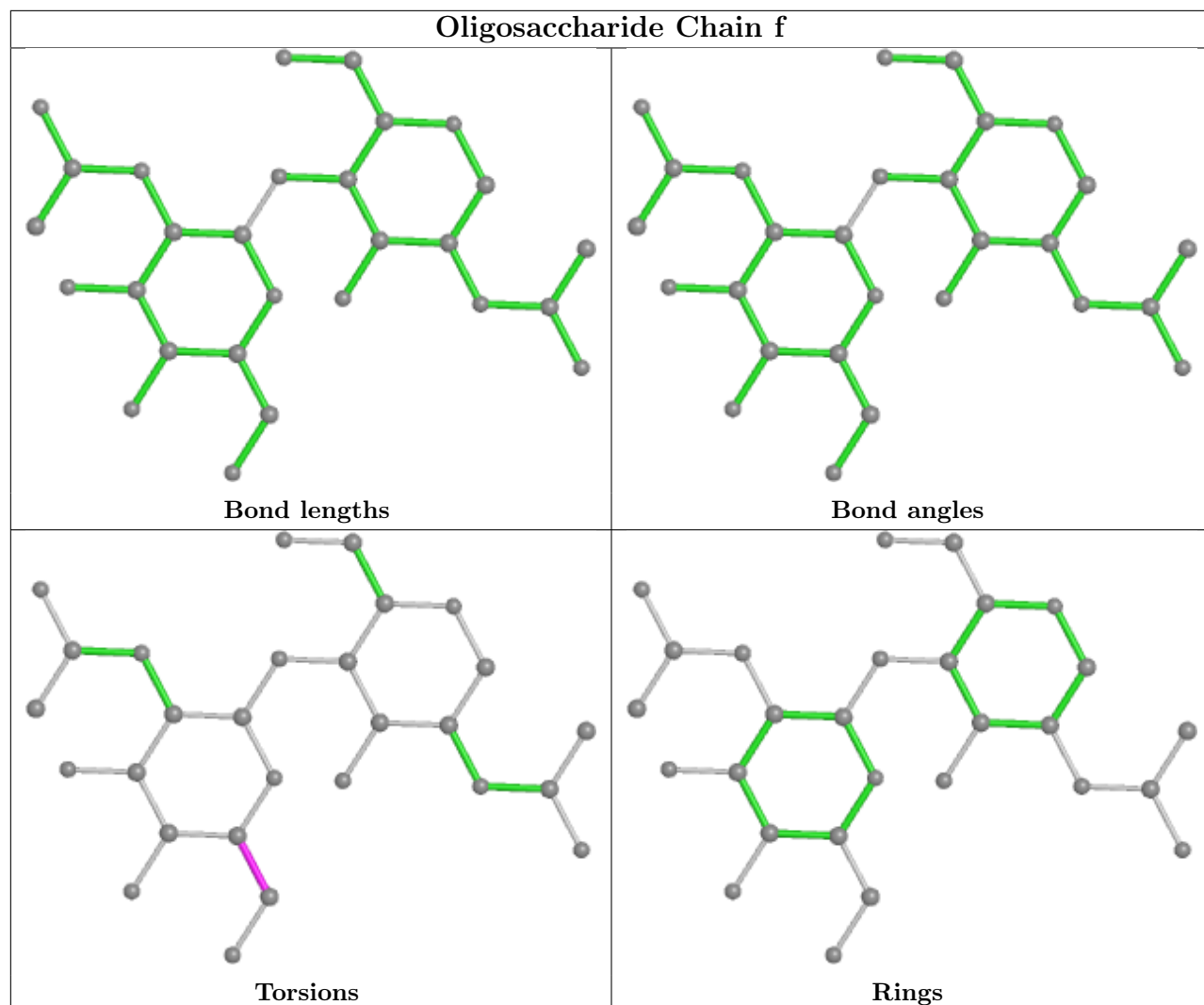


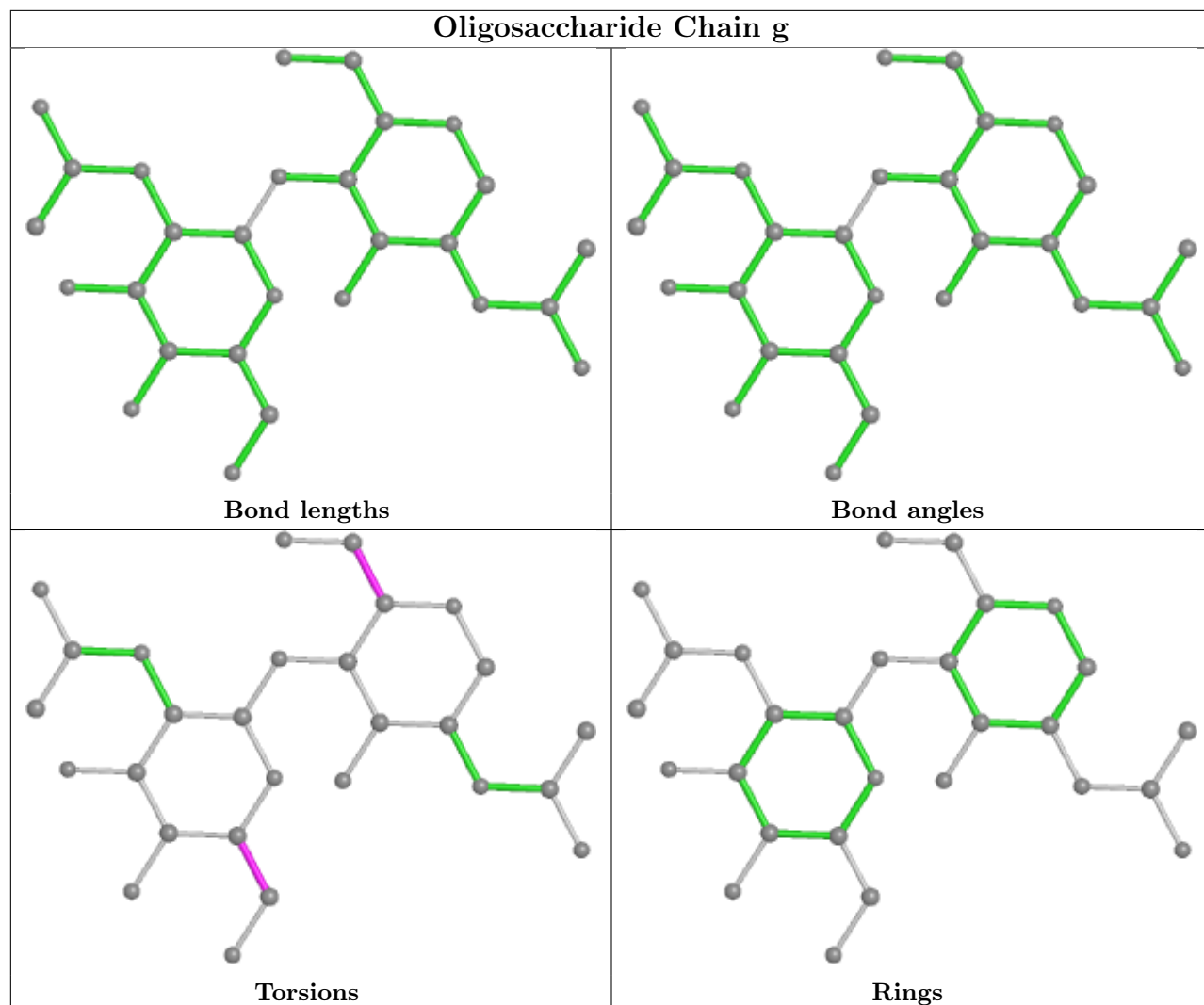


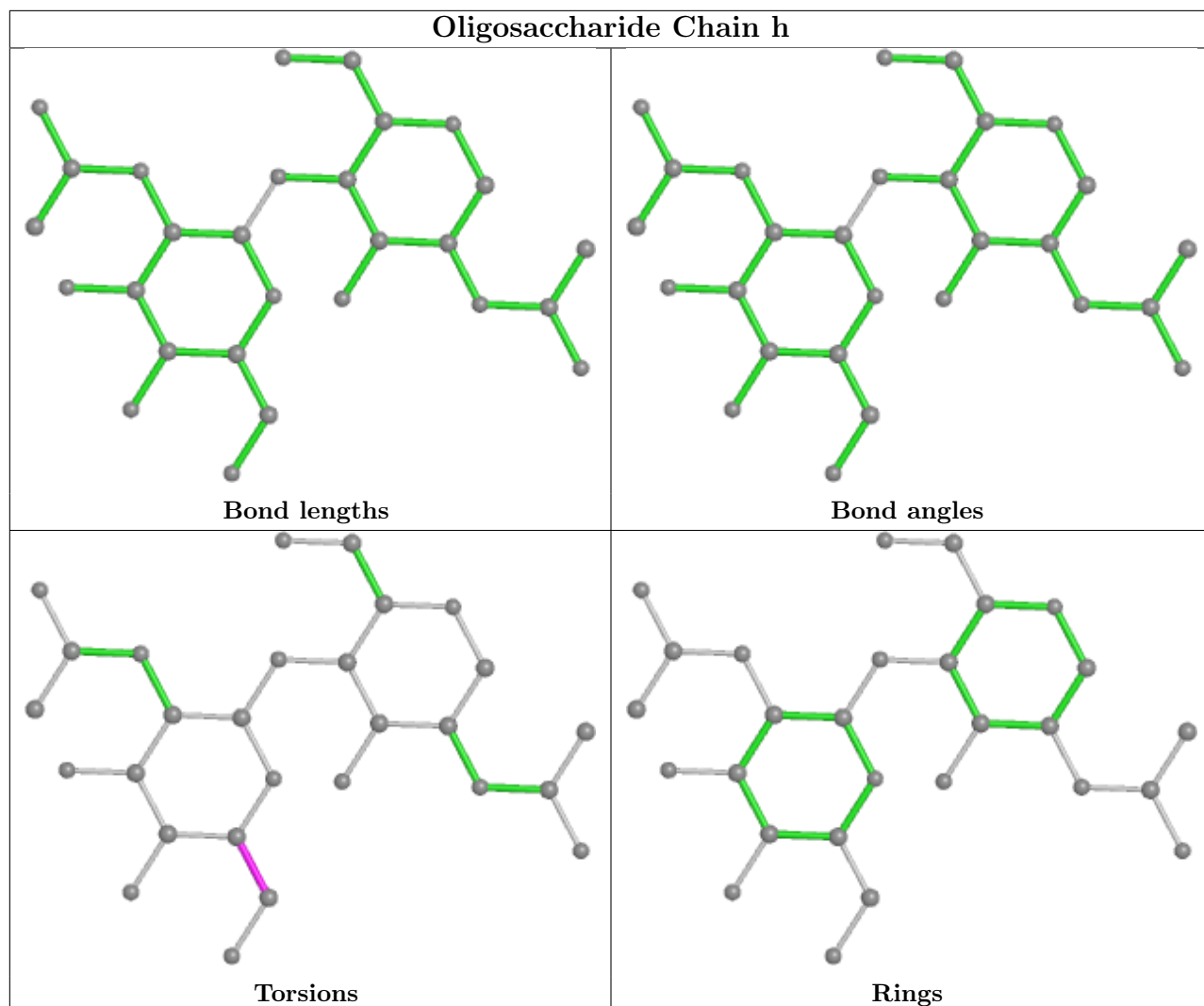


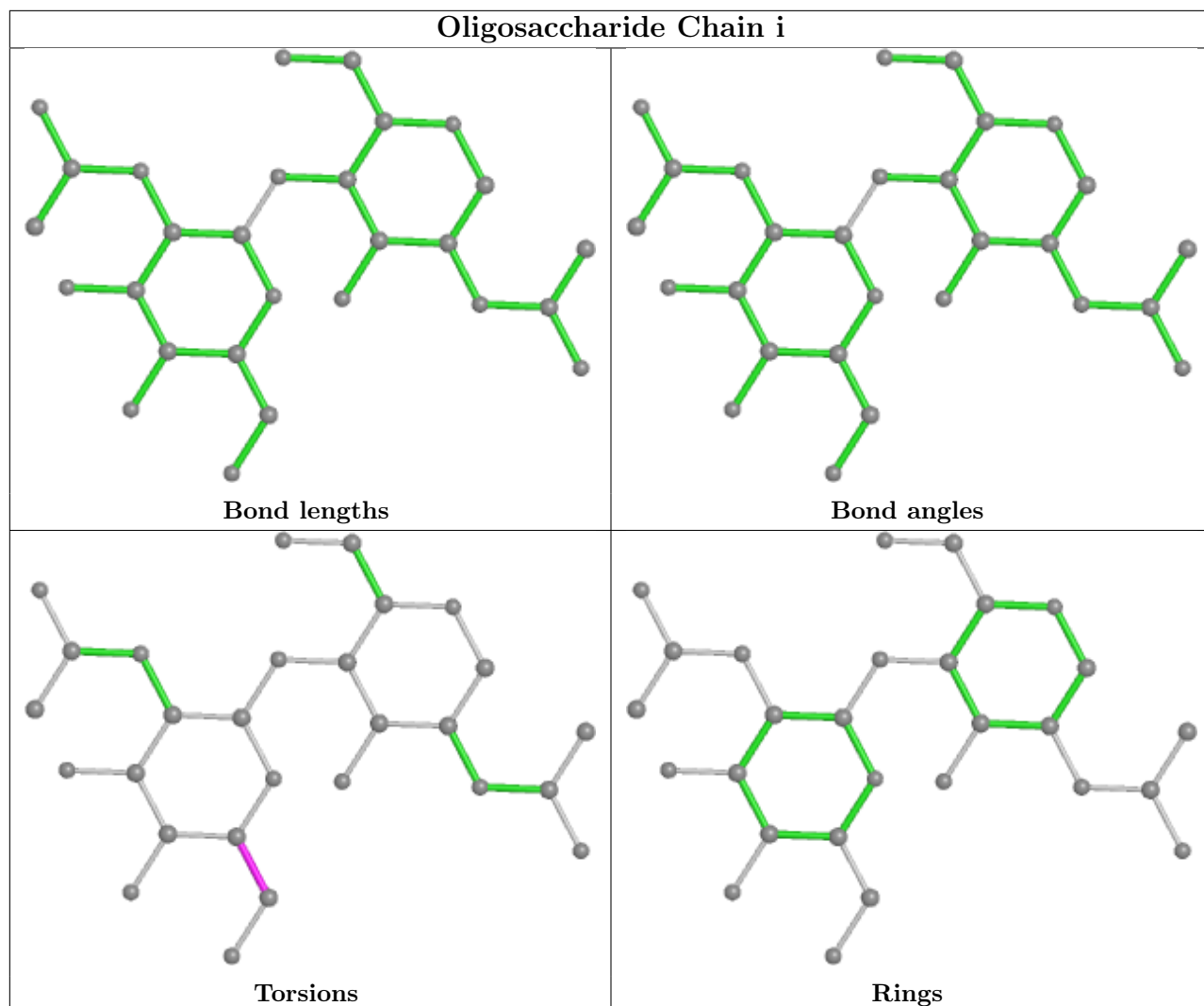


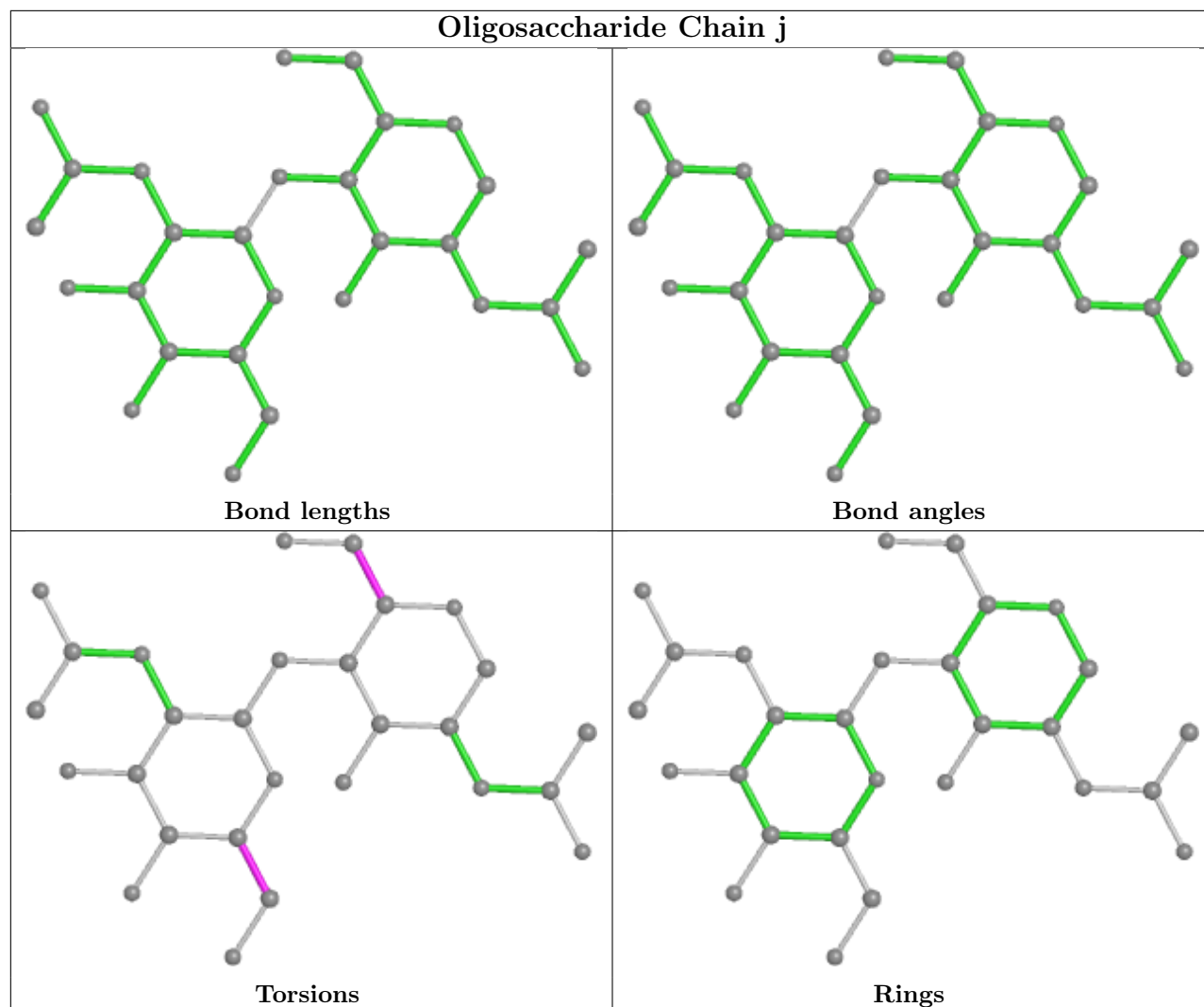


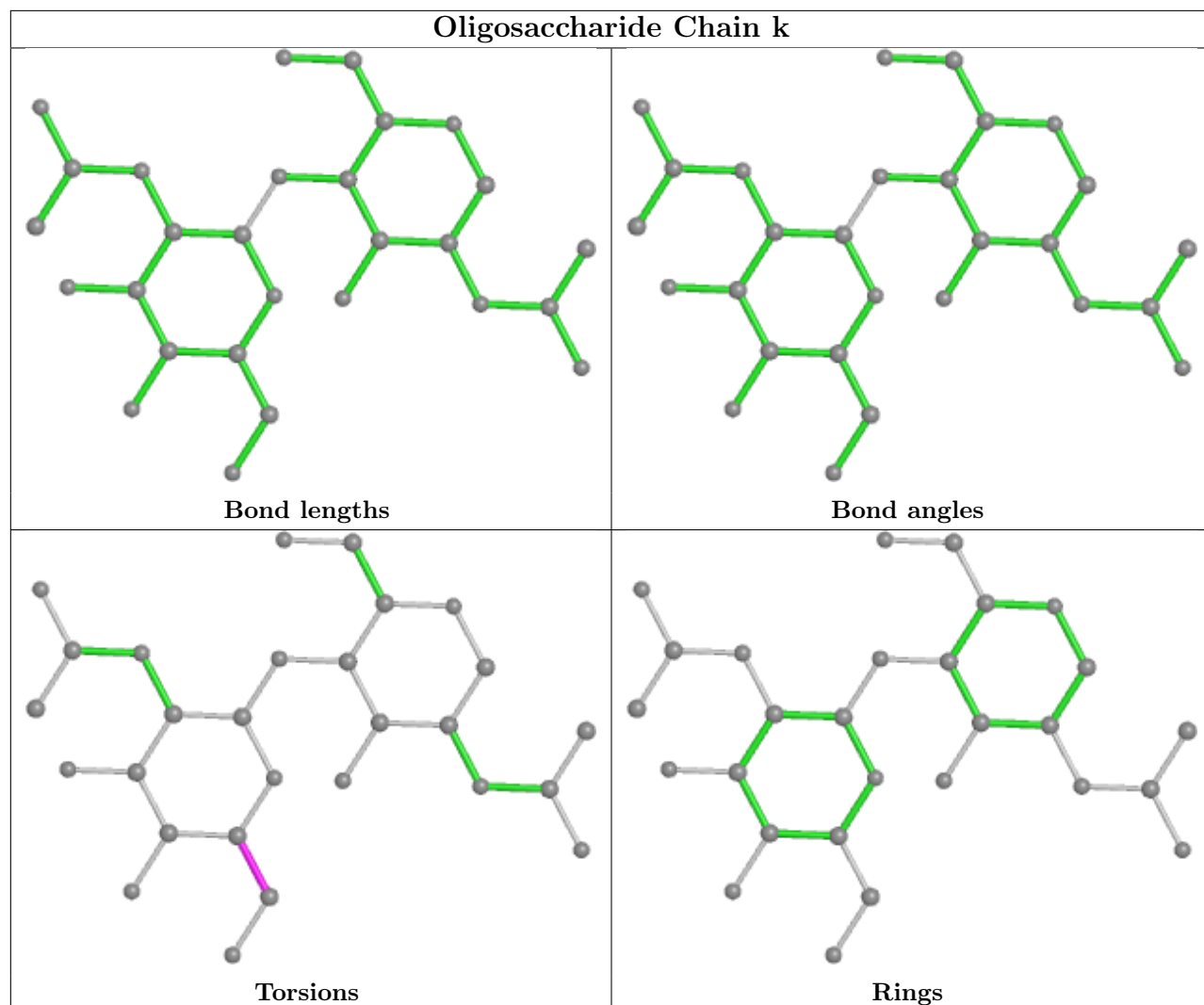


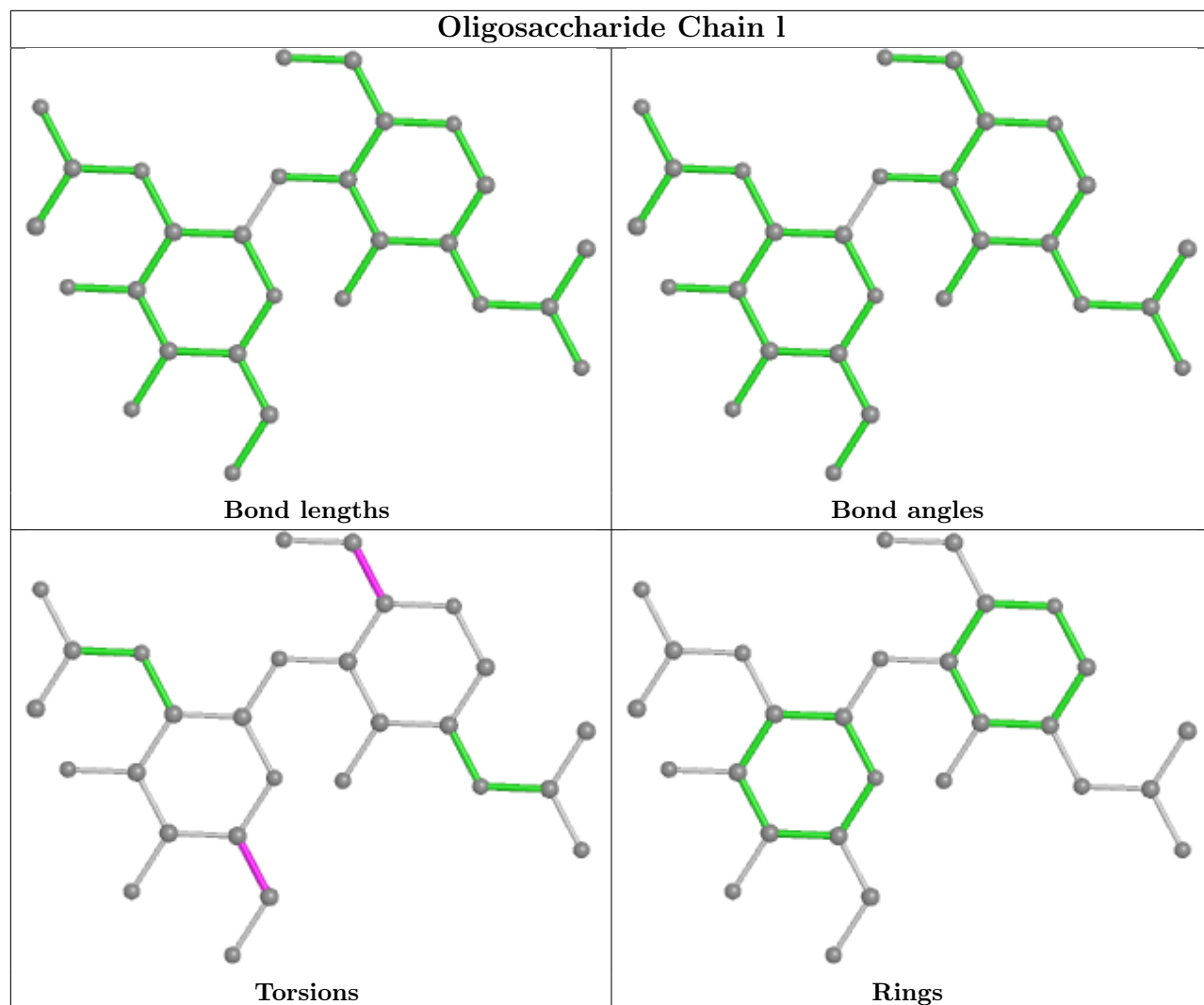


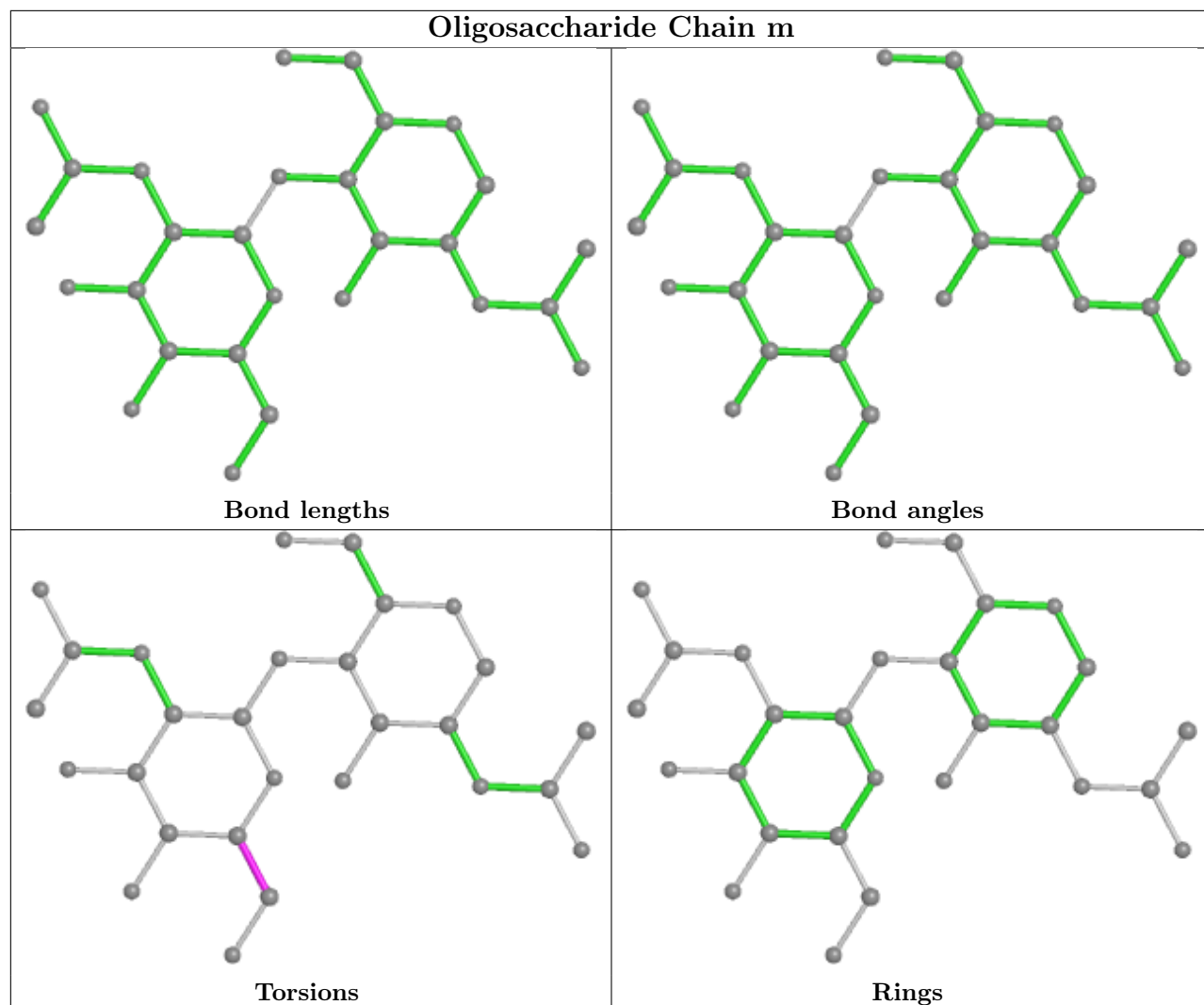


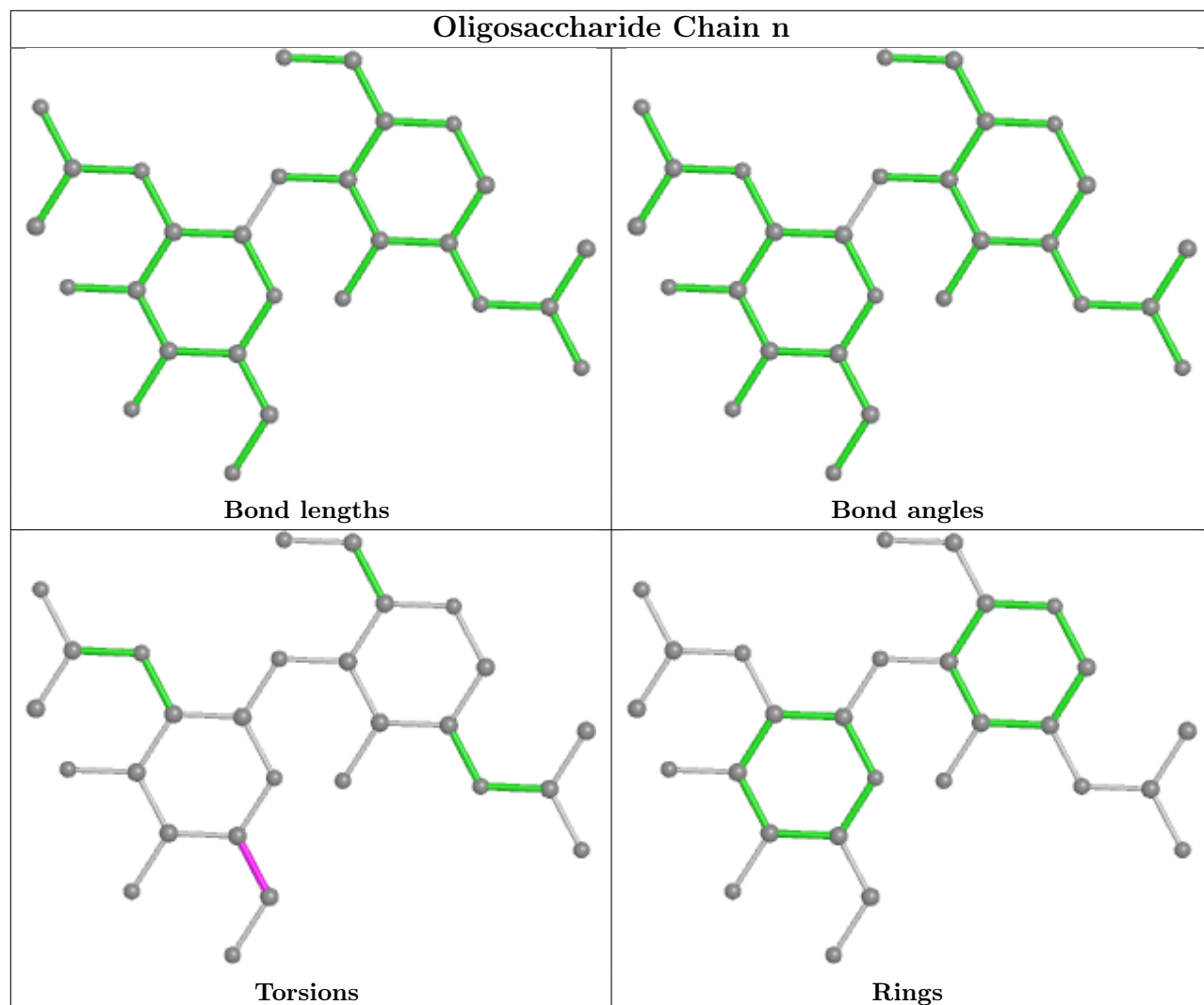


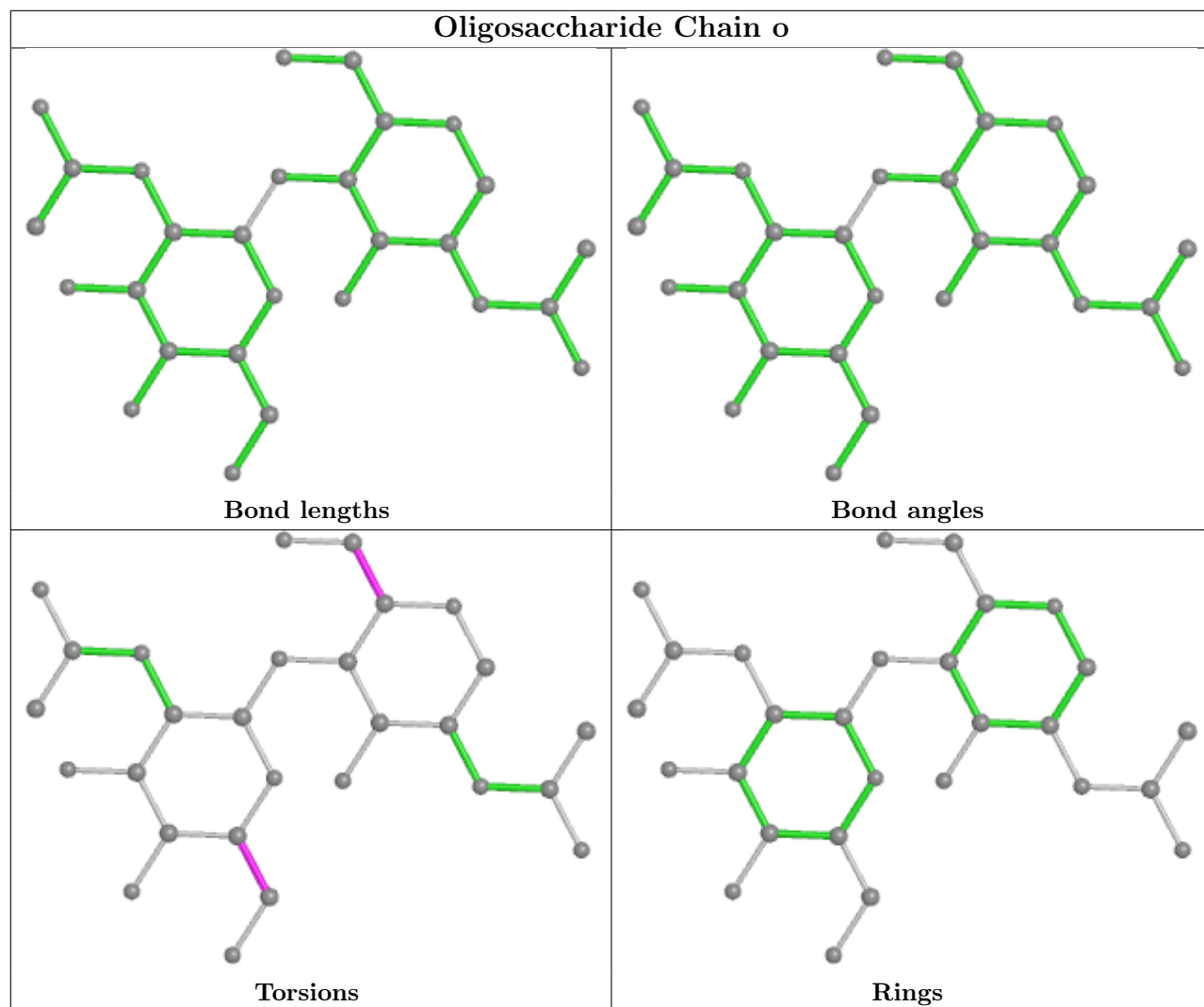


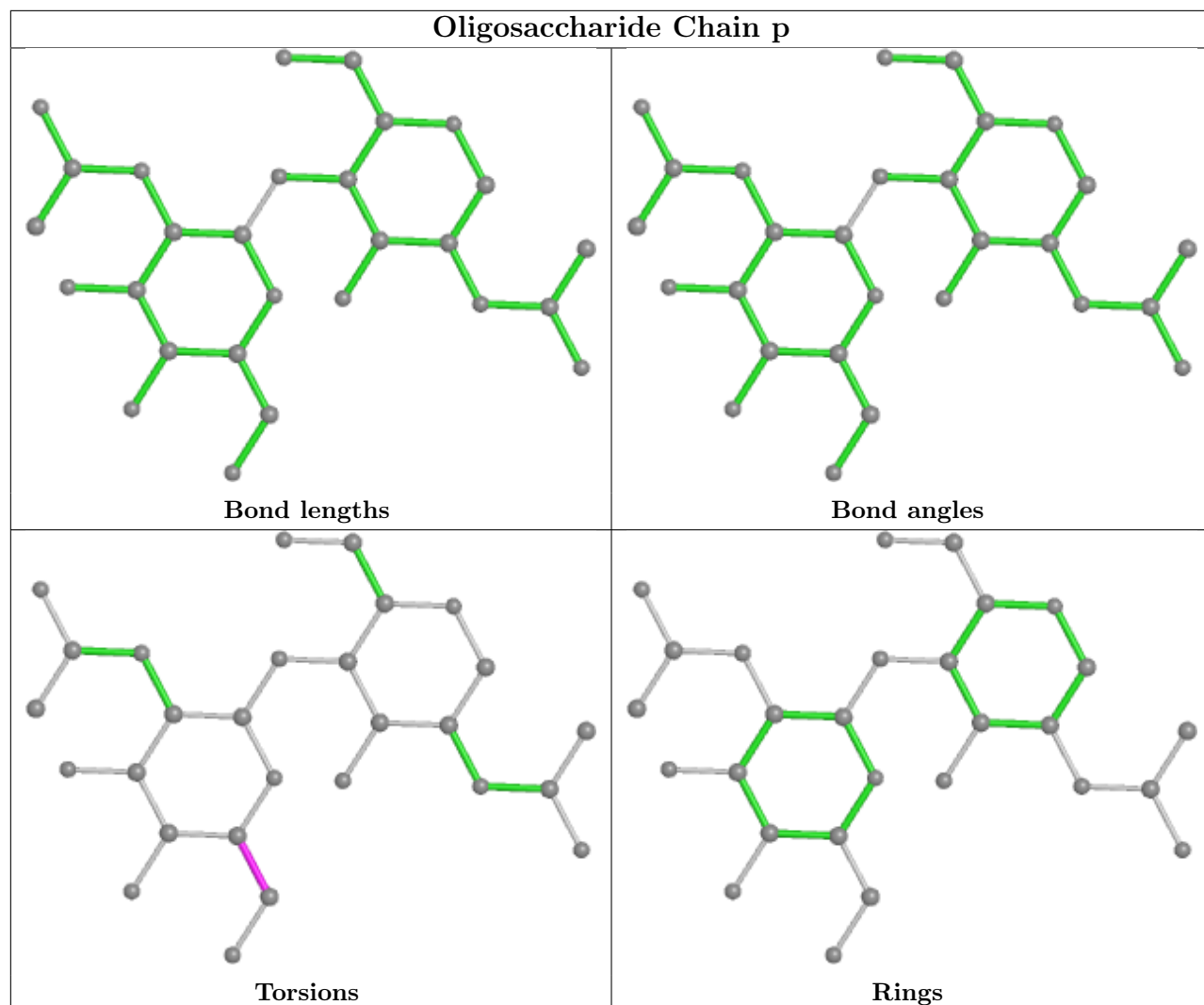


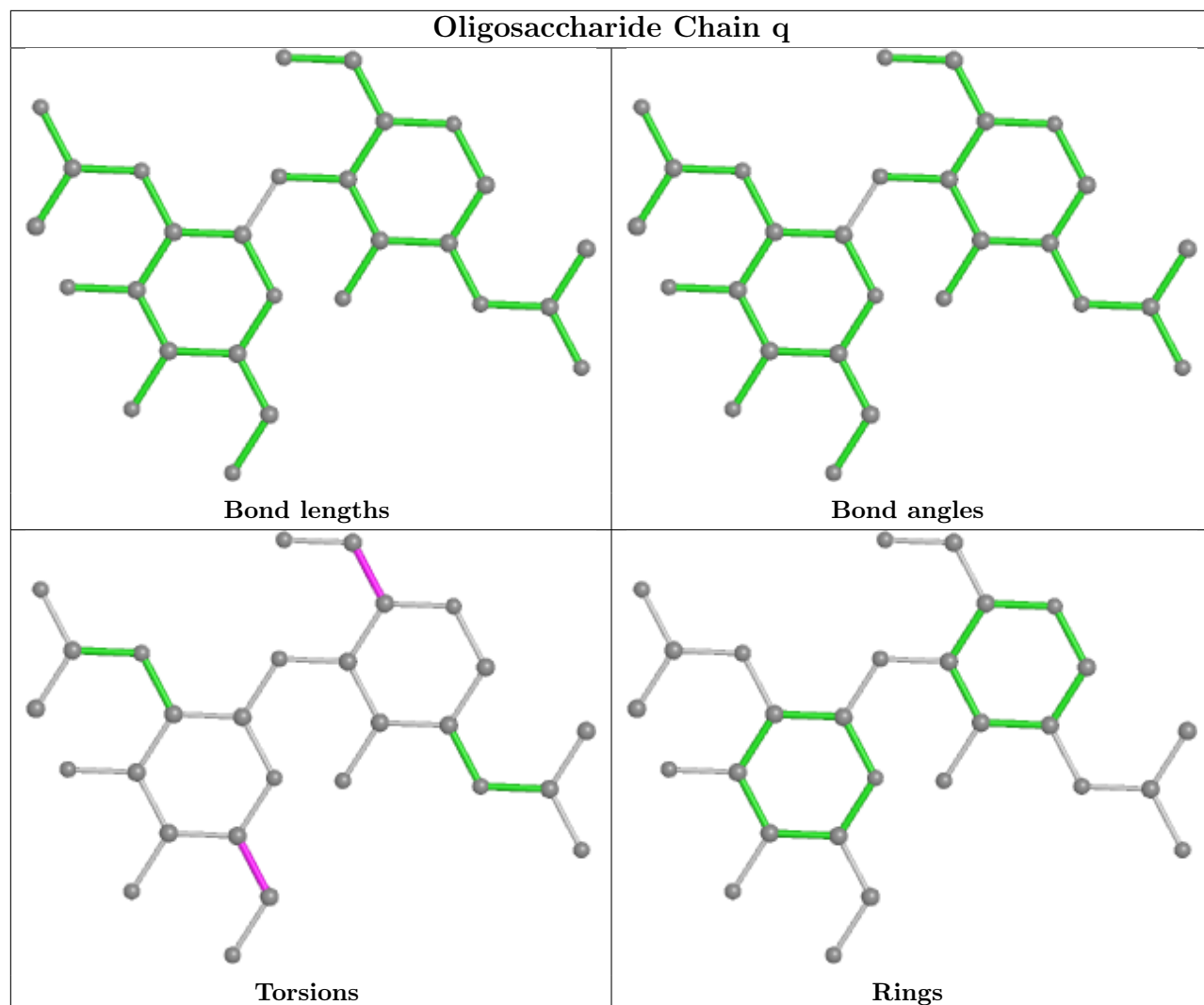


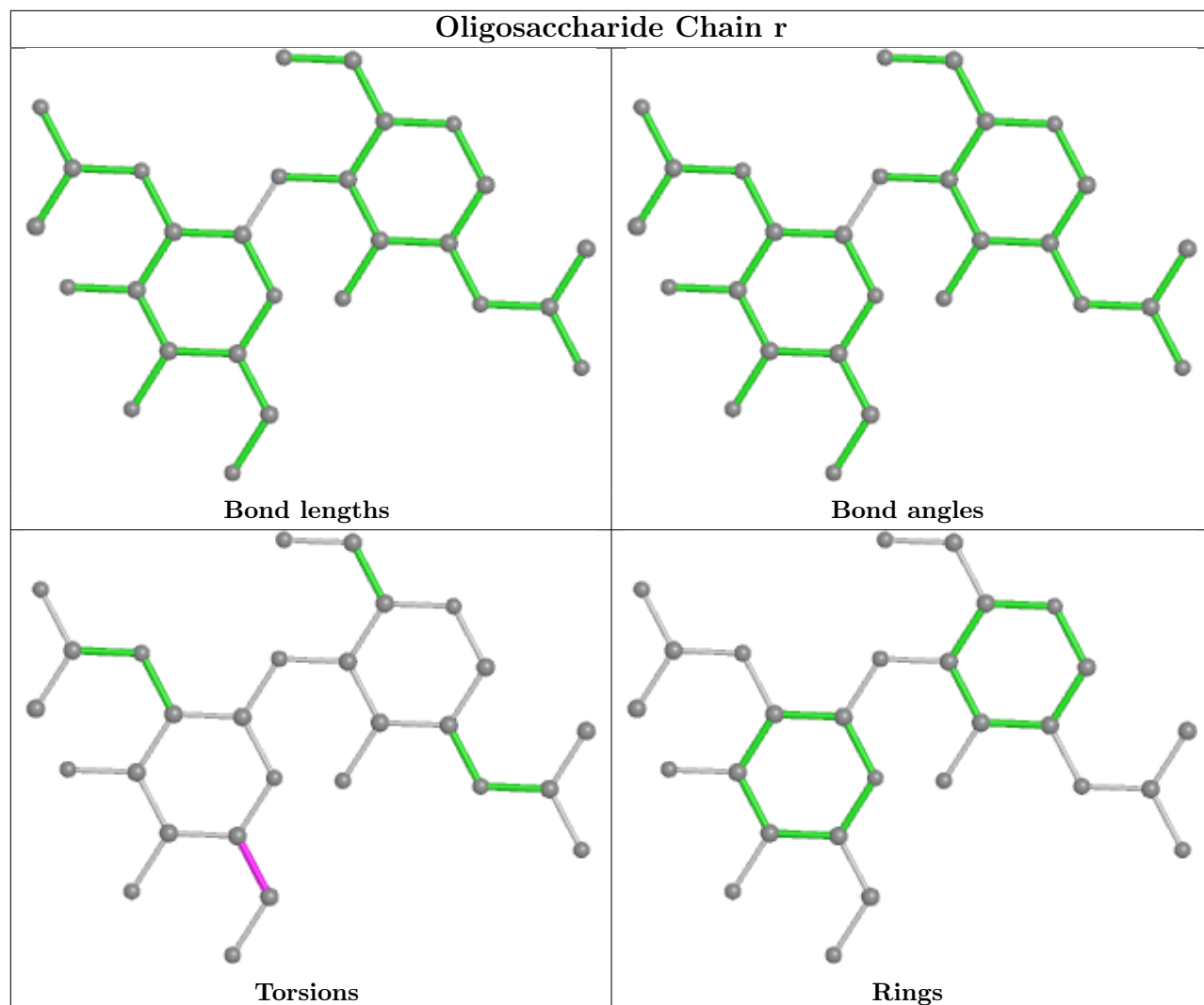


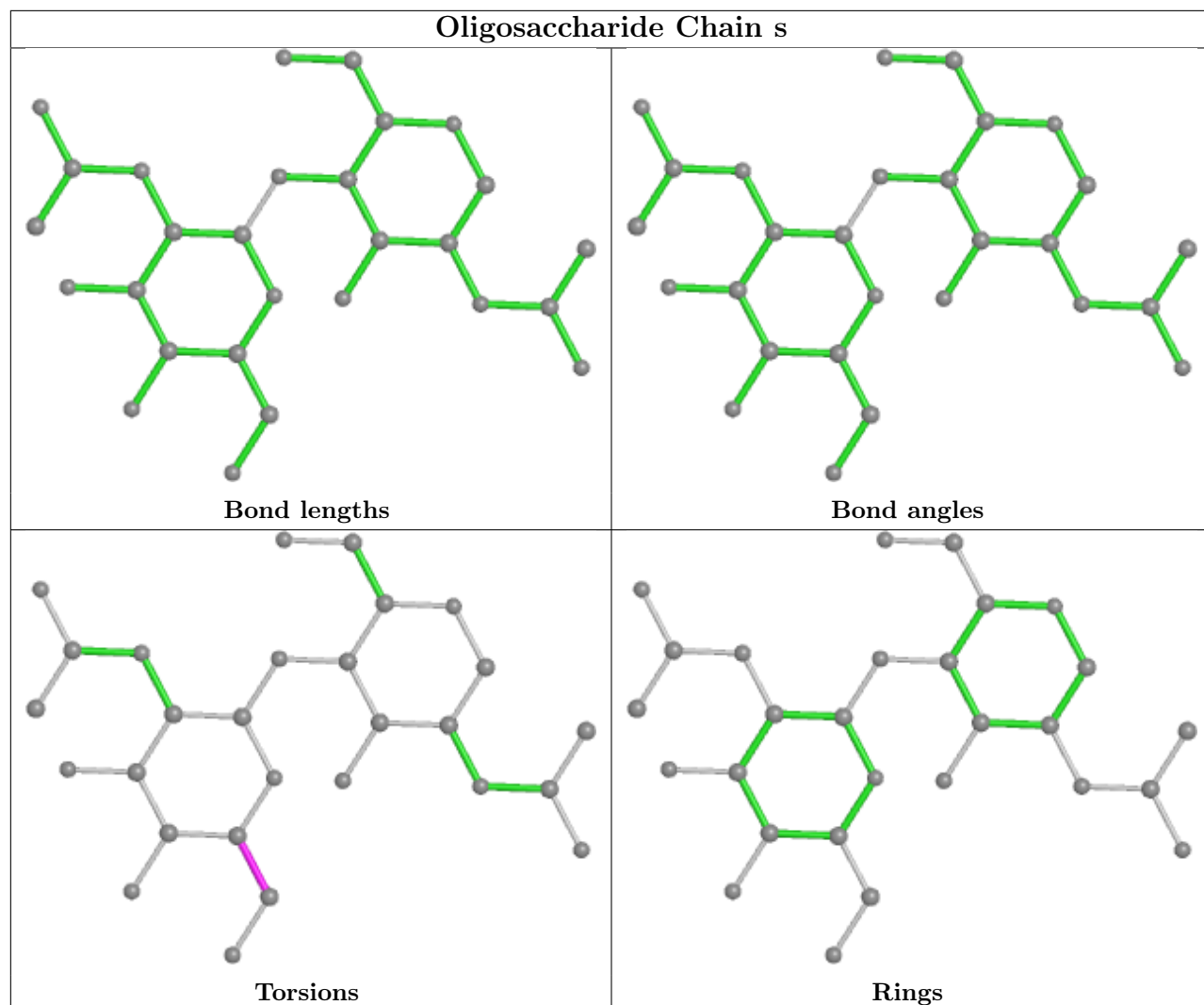


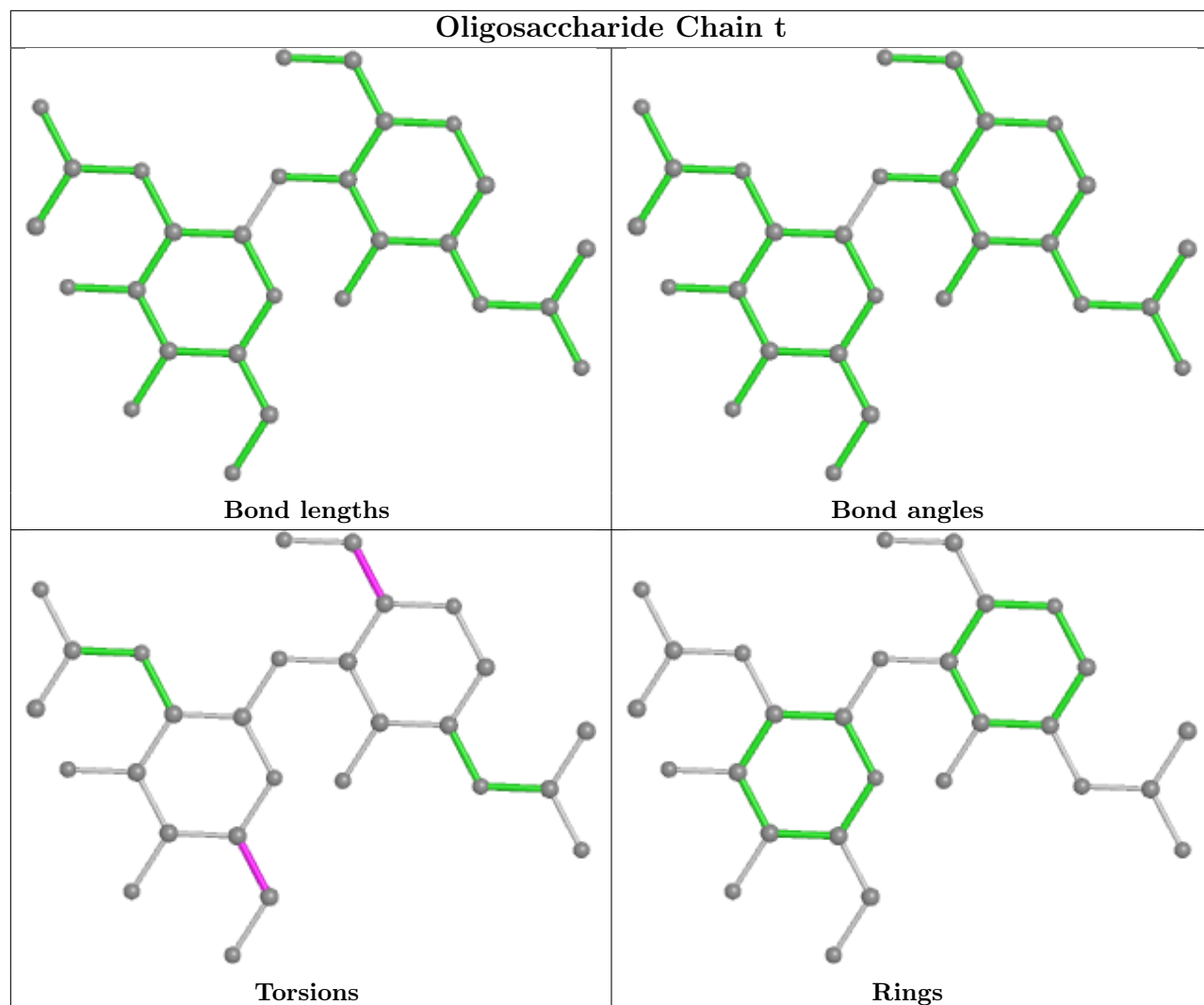


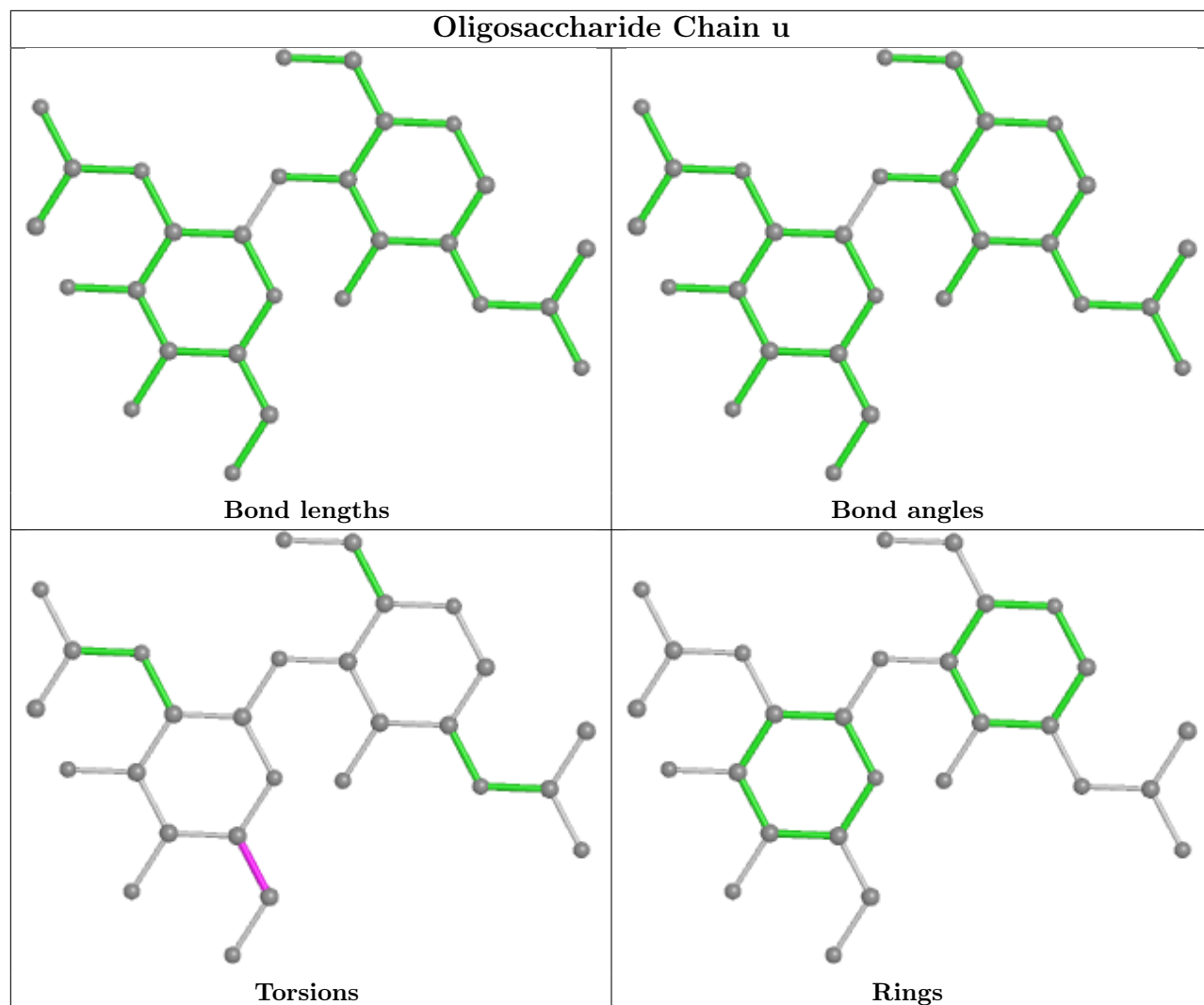


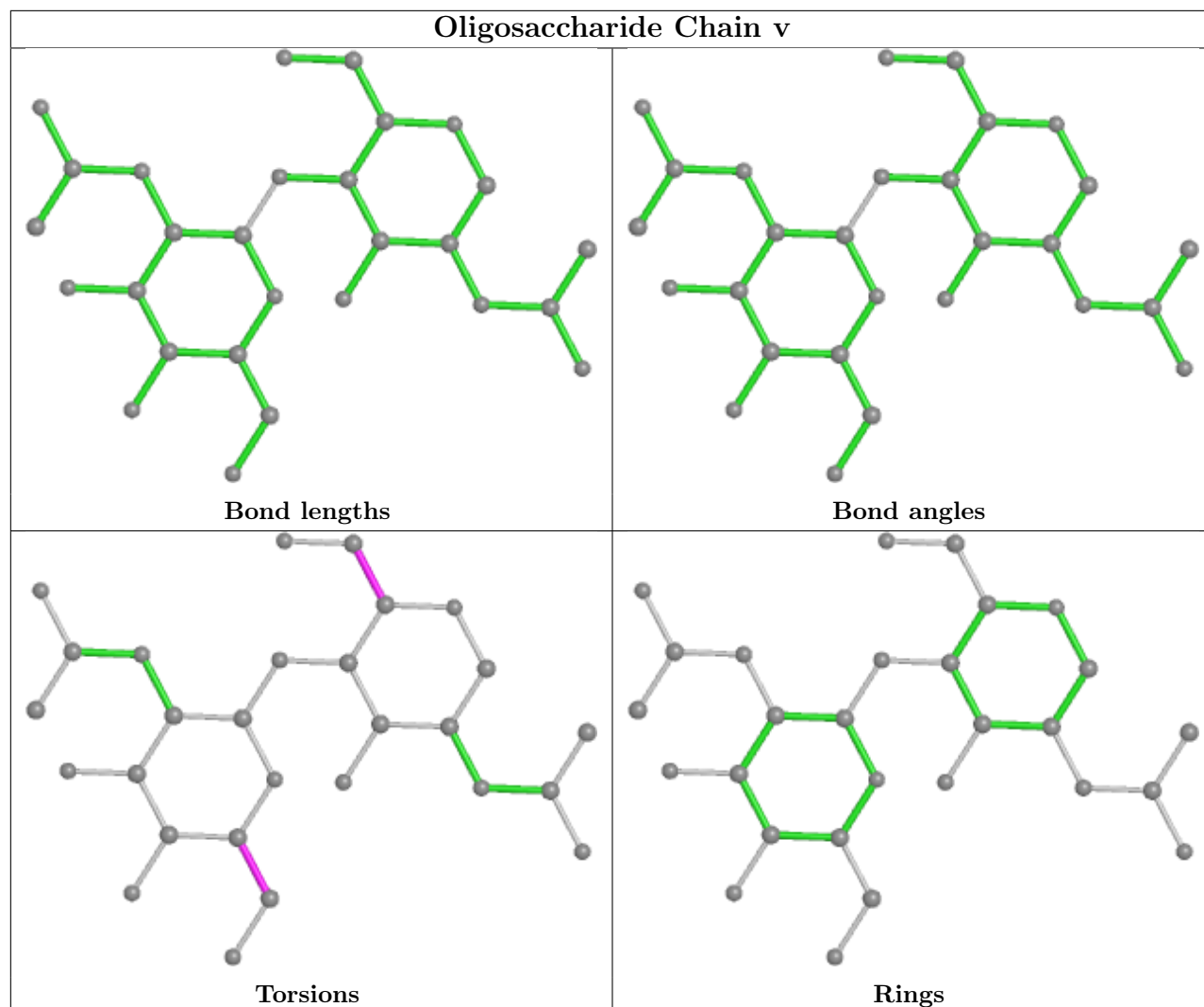












5.6 Ligand geometry [i](#)

60 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	$\# Z > 2$
5	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	E	1308	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	A	1309	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	1303	1	14,14,15	0.31	0	17,19,21	0.41	0
5	NAG	E	1306	1	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	B	1307	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	E	1307	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	D	1301	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	B	1301	1	14,14,15	0.40	0	17,19,21	0.39	0
5	NAG	D	1304	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	I	1303	1	14,14,15	0.35	0	17,19,21	0.48	0
5	NAG	B	1310	1	14,14,15	0.40	0	17,19,21	0.54	0
5	NAG	E	1304	1	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	A	1306	1	14,14,15	0.17	0	17,19,21	0.40	0
5	NAG	I	1305	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	I	1310	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	B	1303	1	14,14,15	0.24	0	17,19,21	0.39	0
5	NAG	A	1301	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	C	1310	1	14,14,15	0.45	0	17,19,21	0.46	0
5	NAG	D	1307	1	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	C	1309	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	B	1302	1	14,14,15	0.24	0	17,19,21	0.50	0
5	NAG	D	1303	1	14,14,15	0.49	0	17,19,21	0.54	0
5	NAG	D	1305	1	14,14,15	0.19	0	17,19,21	0.37	0
5	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.40	0
5	NAG	I	1304	1	14,14,15	0.31	0	17,19,21	0.44	0
5	NAG	D	1309	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	E	1305	1	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	E	1310	1	14,14,15	0.40	0	17,19,21	0.55	0
5	NAG	D	1302	1	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	E	1309	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	C	1306	1	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	E	1302	1	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	I	1301	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	D	1308	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	I	1306	1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	C	1304	1	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	D	1306	1	14,14,15	0.18	0	17,19,21	0.43	0
5	NAG	B	1306	1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	A	1308	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	I	1302	1	14,14,15	0.55	0	17,19,21	0.52	0
5	NAG	A	1304	1	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	A	1303	1	14,14,15	0.48	0	17,19,21	0.54	0
5	NAG	E	1301	1	14,14,15	0.41	0	17,19,21	0.38	0
5	NAG	C	1307	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	A	1307	1	14,14,15	0.26	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	C	1305	1	14,14,15	0.29	0	17,19,21	0.45	0
5	NAG	I	1309	1	14,14,15	0.37	0	17,19,21	0.37	0
5	NAG	A	1310	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	A	1305	1	14,14,15	0.19	0	17,19,21	0.36	0
5	NAG	B	1309	1	14,14,15	0.33	0	17,19,21	0.53	0
5	NAG	B	1308	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	C	1302	1	14,14,15	0.54	0	17,19,21	0.45	0
5	NAG	I	1308	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	D	1310	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	I	1307	1	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.45	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
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1306	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1305	1	-	4/6/23/26	0/1/1/1
5	NAG	I	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
5	NAG	E	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	I	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	I	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	I	1302	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1309	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
5	NAG	I	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1310	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1305	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	D	1302	NAG	C4-C5-C6-O6
5	B	1310	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
5	B	1302	NAG	1	0
5	E	1302	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.