



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 07:21 AM UTC

PDB ID : 8TRZ / pdb_00008trz
EMDB ID : EMD-41586
Title : Cryo-EM structure of N-glycosylated Pomacea canaliculata hemocyanin
Authors : Brola, T.R.; Chiumiento, I.R.; Gragera, M.; Carazo, J.M.; Heras, H.; Dreon, M.S.; Otero, L.H.
Deposited on : 2023-08-10
Resolution : 4.40 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

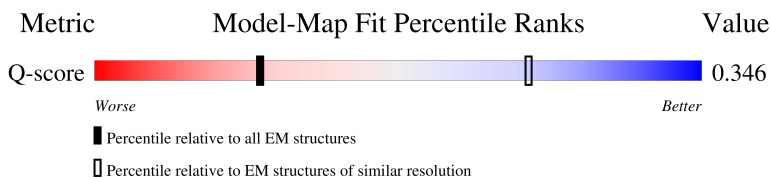
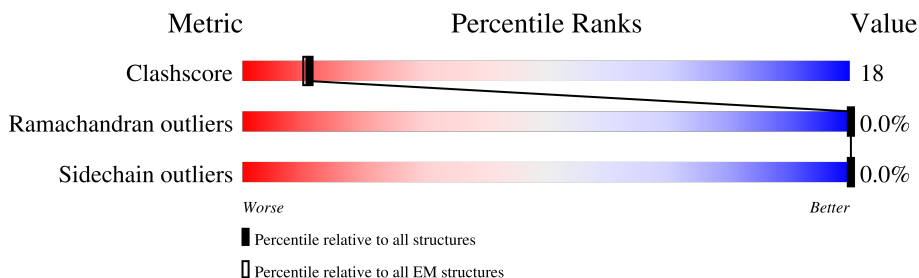
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 Å.

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



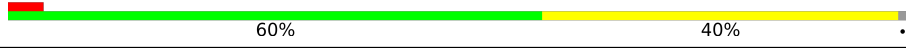
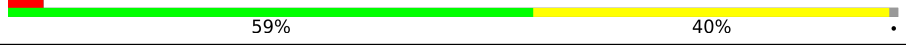
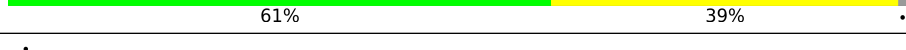
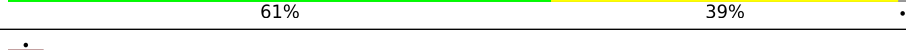
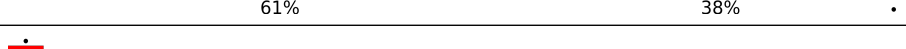
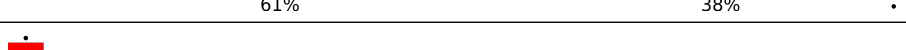
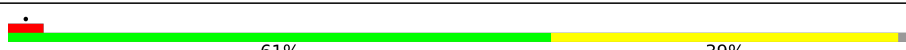
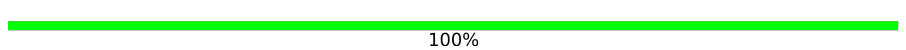
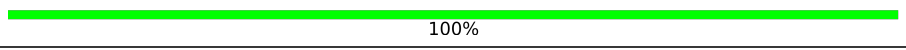
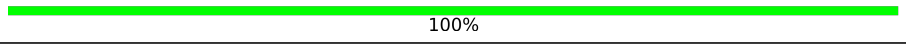
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	3408	 60% 39%
1	B	3408	 61% 38%
1	C	3408	 62% 38%
1	D	3408	 61% 38%

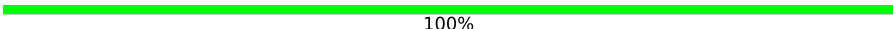
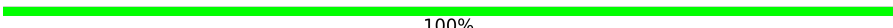
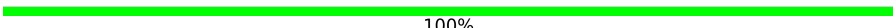
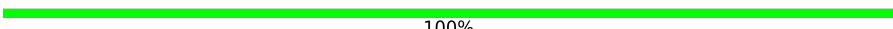
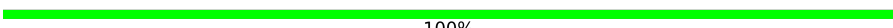
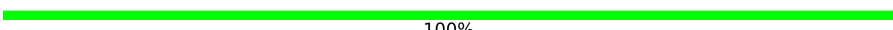
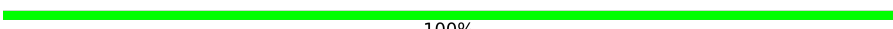
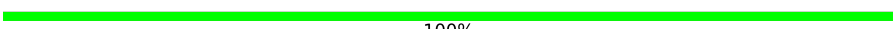
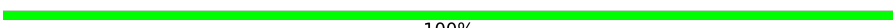
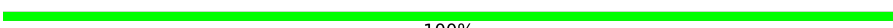
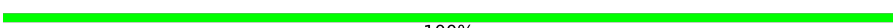
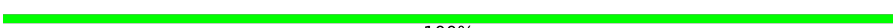
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Mol	Chain	Length	Quality of chain
1	E	3408	 61%39%
1	F	3408	 60%39%
1	G	3408	 60%40%
1	H	3408	 59%40%
1	I	3408	 61%39%
1	J	3408	 61%39%
1	K	3408	 61%39%
1	L	3408	 61%39%
1	M	3408	 61%38%
1	N	3408	 61%38%
1	O	3408	 61%38%
1	P	3408	 61%38%
1	Q	3408	 60%39%
1	R	3408	 59%41%
1	S	3408	 61%38%
1	T	3408	 61%39%
2	0	2	 50%50%
2	0A	2	 50%50%
2	2	2	 100%
2	5A	2	 50%50%
2	7	2	 50%50%
2	8	2	 100%
2	AA	2	 100%
2	CA	2	 50%50%
2	HA	2	 50%50%

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Mol	Chain	Length	Quality of chain
2	IA	2	 50% 50%
2	KA	2	 50% 50%
2	MA	2	 100%
2	RA	2	 50% 50%
2	SA	2	 50% 50%
2	U	2	 50% 50%
2	UA	2	 100%
2	W	2	 100%
2	WA	2	 50% 50%
2	Y	2	 100%
2	bA	2	 50% 50%
2	cA	2	 100%
2	d	2	 100%
2	e	2	 100%
2	eA	2	 100%
2	g	2	 100%
2	gA	2	 100%
2	i	2	 50% 50%
2	lA	2	 50% 50%
2	mA	2	 100%
2	n	2	 50% 50%
2	o	2	 100%
2	oA	2	 50% 50%
2	q	2	 50% 50%
2	qA	2	 100%

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Mol	Chain	Length	Quality of chain
2	s	2	100%
2	vA	2	50%
2	wA	2	100%
2	x	2	50%
2	y	2	100%
2	yA	2	50%
3	1	3	33%
3	1A	3	100%
3	2A	3	67%
3	3	3	67%
3	3A	3	100%
3	4	3	100%
3	4A	3	33%
3	5	3	100%
3	6	3	33%
3	9	3	67%
3	BA	3	33%
3	DA	3	67%
3	EA	3	67%
3	FA	3	100%
3	GA	3	33%
3	JA	3	67%
3	LA	3	33%
3	NA	3	67%
3	OA	3	100%

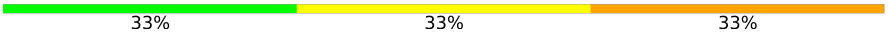
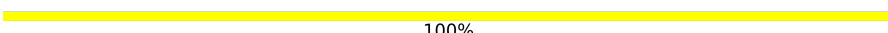
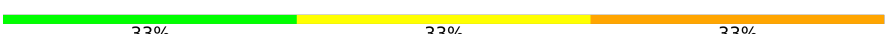
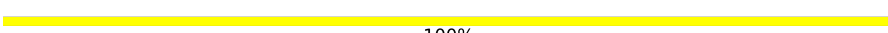
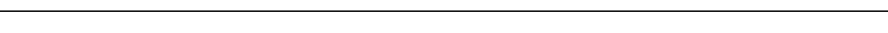
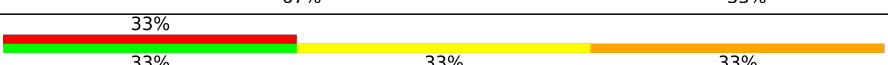
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Mol	Chain	Length	Quality of chain
3	PA	3	100%
3	QA	3	67% 33%
3	TA	3	100%
3	V	3	67% 33%
3	VA	3	100%
3	X	3	33% 33% 33%
3	XA	3	67% 33%
3	YA	3	67% 33%
3	Z	3	33% 67%
3	ZA	3	100%
3	a	3	67% 33%
3	aA	3	33% 67%
3	b	3	67% 33%
3	c	3	33% 33% 33%
3	dA	3	67% 33%
3	f	3	67% 33%
3	fA	3	33% 67%
3	h	3	67% 33%
3	hA	3	33% 67%
3	iA	3	100%
3	j	3	100%
3	jA	3	67% 33%
3	k	3	100%
3	kA	3	100%
3	l	3	100%

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Mol	Chain	Length	Quality of chain
3	m	3	 33%33%33%
3	nA	3	 67%33%
3	p	3	 67%33%
3	pA	3	 100%
3	r	3	 33%33%33%
3	rA	3	 100%
3	sA	3	 100%
3	t	3	 100%
3	tA	3	 100%
3	u	3	 100%
3	uA	3	 33%33%33%
3	v	3	 100%
3	w	3	 67%33%
3	xA	3	 100%
3	z	3	 67%33%
3	zA	3	 33%33%33%33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 549912 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 Hemocyanin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	B	3388	Total	C	N	O	S	0	0
			27308	17387	4689	5141	91		
1	C	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	D	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	E	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	F	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	G	3387	Total	C	N	O	S	0	0
			27307	17393	4686	5137	91		
1	H	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	I	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	J	3388	Total	C	N	O	S	0	0
			27309	17388	4689	5141	91		
1	K	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	L	3388	Total	C	N	O	S	0	0
			27308	17387	4689	5141	91		
1	M	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	N	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	O	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	P	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	Q	3387	Total	C	N	O	S	0	0
			27307	17393	4686	5137	91		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	S	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	T	3388	Total	C	N	O	S	0	0
			27309	17388	4689	5141	91		

- Molecule 2 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
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	i	2	Total	C	N	O	0	0
			28	16	2	10		
2	n	2	Total	C	N	O	0	0
			28	16	2	10		
2	o	2	Total	C	N	O	0	0
			28	16	2	10		
2	q	2	Total	C	N	O	0	0
			28	16	2	10		
2	s	2	Total	C	N	O	0	0
			28	16	2	10		
2	x	2	Total	C	N	O	0	0
			28	16	2	10		
2	y	2	Total	C	N	O	0	0
			28	16	2	10		
2	0	2	Total	C	N	O	0	0
			28	16	2	10		

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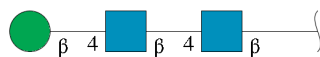
Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	2	Total	C	N	O	0	0
			28	16	2	10		
2	7	2	Total	C	N	O	0	0
			28	16	2	10		
2	8	2	Total	C	N	O	0	0
			28	16	2	10		
2	AA	2	Total	C	N	O	0	0
			28	16	2	10		
2	CA	2	Total	C	N	O	0	0
			28	16	2	10		
2	HA	2	Total	C	N	O	0	0
			28	16	2	10		
2	IA	2	Total	C	N	O	0	0
			28	16	2	10		
2	KA	2	Total	C	N	O	0	0
			28	16	2	10		
2	MA	2	Total	C	N	O	0	0
			28	16	2	10		
2	RA	2	Total	C	N	O	0	0
			28	16	2	10		
2	SA	2	Total	C	N	O	0	0
			28	16	2	10		
2	UA	2	Total	C	N	O	0	0
			28	16	2	10		
2	WA	2	Total	C	N	O	0	0
			28	16	2	10		
2	bA	2	Total	C	N	O	0	0
			28	16	2	10		
2	cA	2	Total	C	N	O	0	0
			28	16	2	10		
2	eA	2	Total	C	N	O	0	0
			28	16	2	10		
2	gA	2	Total	C	N	O	0	0
			28	16	2	10		
2	lA	2	Total	C	N	O	0	0
			28	16	2	10		
2	mA	2	Total	C	N	O	0	0
			28	16	2	10		
2	oA	2	Total	C	N	O	0	0
			28	16	2	10		
2	qA	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	vA	2	Total	C	N	O	0	0
			28	16	2	10		
2	wA	2	Total	C	N	O	0	0
			28	16	2	10		
2	yA	2	Total	C	N	O	0	0
			28	16	2	10		
2	0A	2	Total	C	N	O	0	0
			28	16	2	10		
2	5A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	Z	3	Total	C	N	O	0	0
			39	22	2	15		
3	a	3	Total	C	N	O	0	0
			39	22	2	15		
3	b	3	Total	C	N	O	0	0
			39	22	2	15		
3	c	3	Total	C	N	O	0	0
			39	22	2	15		
3	f	3	Total	C	N	O	0	0
			39	22	2	15		
3	h	3	Total	C	N	O	0	0
			39	22	2	15		
3	j	3	Total	C	N	O	0	0
			39	22	2	15		
3	k	3	Total	C	N	O	0	0
			39	22	2	15		
3	l	3	Total	C	N	O	0	0
			39	22	2	15		
3	m	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	p	3	Total 39	C 22	N 2	O 15	0	0
3	r	3	Total 39	C 22	N 2	O 15	0	0
3	t	3	Total 39	C 22	N 2	O 15	0	0
3	u	3	Total 39	C 22	N 2	O 15	0	0
3	v	3	Total 39	C 22	N 2	O 15	0	0
3	w	3	Total 39	C 22	N 2	O 15	0	0
3	z	3	Total 39	C 22	N 2	O 15	0	0
3	1	3	Total 39	C 22	N 2	O 15	0	0
3	3	3	Total 39	C 22	N 2	O 15	0	0
3	4	3	Total 39	C 22	N 2	O 15	0	0
3	5	3	Total 39	C 22	N 2	O 15	0	0
3	6	3	Total 39	C 22	N 2	O 15	0	0
3	9	3	Total 39	C 22	N 2	O 15	0	0
3	BA	3	Total 39	C 22	N 2	O 15	0	0
3	DA	3	Total 39	C 22	N 2	O 15	0	0
3	EA	3	Total 39	C 22	N 2	O 15	0	0
3	FA	3	Total 39	C 22	N 2	O 15	0	0
3	GA	3	Total 39	C 22	N 2	O 15	0	0
3	JA	3	Total 39	C 22	N 2	O 15	0	0
3	LA	3	Total 39	C 22	N 2	O 15	0	0
3	NA	3	Total 39	C 22	N 2	O 15	0	0

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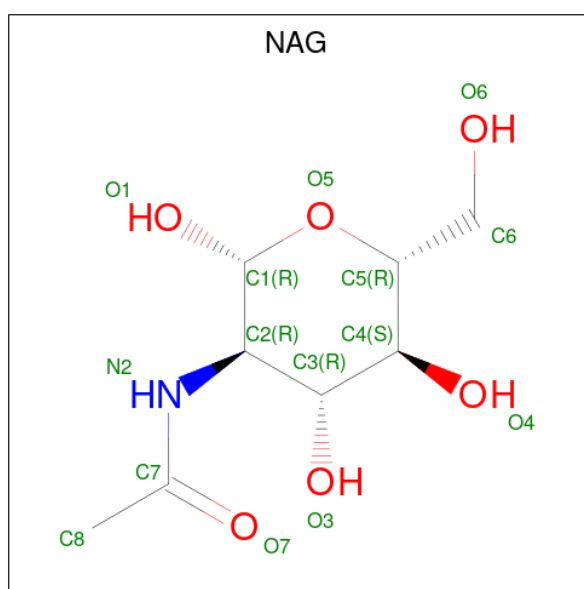
Mol	Chain	Residues	Atoms				AltConf	Trace
3	OA	3	Total	C	N	O	0	0
			39	22	2	15		
3	PA	3	Total	C	N	O	0	0
			39	22	2	15		
3	QA	3	Total	C	N	O	0	0
			39	22	2	15		
3	TA	3	Total	C	N	O	0	0
			39	22	2	15		
3	VA	3	Total	C	N	O	0	0
			39	22	2	15		
3	XA	3	Total	C	N	O	0	0
			39	22	2	15		
3	YA	3	Total	C	N	O	0	0
			39	22	2	15		
3	ZA	3	Total	C	N	O	0	0
			39	22	2	15		
3	aA	3	Total	C	N	O	0	0
			39	22	2	15		
3	dA	3	Total	C	N	O	0	0
			39	22	2	15		
3	fA	3	Total	C	N	O	0	0
			39	22	2	15		
3	hA	3	Total	C	N	O	0	0
			39	22	2	15		
3	iA	3	Total	C	N	O	0	0
			39	22	2	15		
3	jA	3	Total	C	N	O	0	0
			39	22	2	15		
3	kA	3	Total	C	N	O	0	0
			39	22	2	15		
3	nA	3	Total	C	N	O	0	0
			39	22	2	15		
3	pA	3	Total	C	N	O	0	0
			39	22	2	15		
3	rA	3	Total	C	N	O	0	0
			39	22	2	15		
3	sA	3	Total	C	N	O	0	0
			39	22	2	15		
3	tA	3	Total	C	N	O	0	0
			39	22	2	15		
3	uA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	xA	3	Total	C	N	O	0	0
			39	22	2	15		
3	zA	3	Total	C	N	O	0	0
			39	22	2	15		
3	1A	3	Total	C	N	O	0	0
			39	22	2	15		
3	2A	3	Total	C	N	O	0	0
			39	22	2	15		
3	3A	3	Total	C	N	O	0	0
			39	22	2	15		
3	4A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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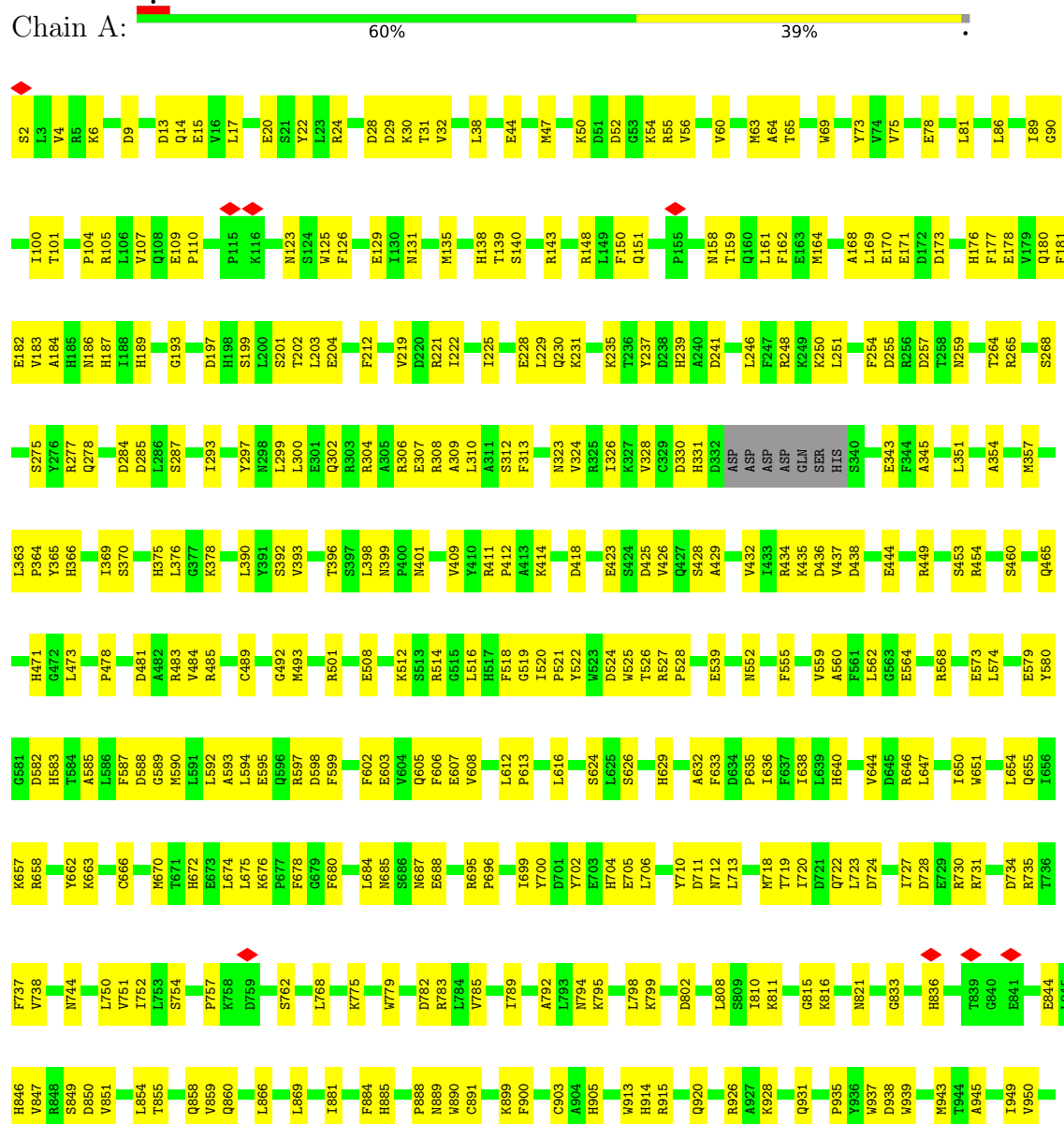
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Mol	Chain	Residues	Atoms				AltConf
4	F	1	Total 14	C 8	N 1	O 5	0
4	G	1	Total 14	C 8	N 1	O 5	0
4	H	1	Total 14	C 8	N 1	O 5	0
4	I	1	Total 14	C 8	N 1	O 5	0
4	J	1	Total 14	C 8	N 1	O 5	0
4	K	1	Total 14	C 8	N 1	O 5	0
4	L	1	Total 14	C 8	N 1	O 5	0
4	M	1	Total 14	C 8	N 1	O 5	0
4	N	1	Total 14	C 8	N 1	O 5	0
4	O	1	Total 14	C 8	N 1	O 5	0
4	P	1	Total 14	C 8	N 1	O 5	0
4	Q	1	Total 14	C 8	N 1	O 5	0
4	R	1	Total 14	C 8	N 1	O 5	0
4	S	1	Total 14	C 8	N 1	O 5	0
4	T	1	Total 14	C 8	N 1	O 5	0

3 Residue-property plots

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: Hemocyanin

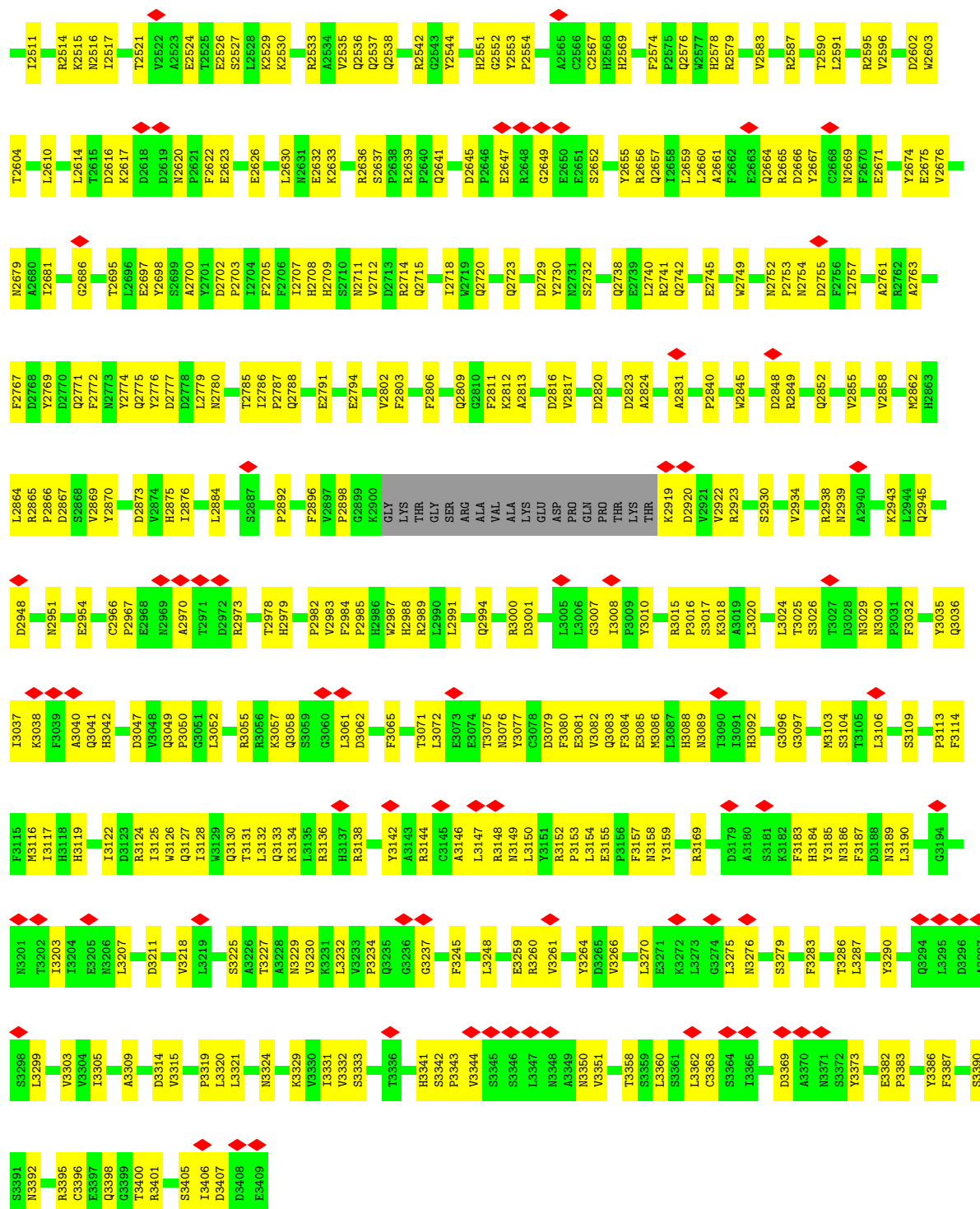






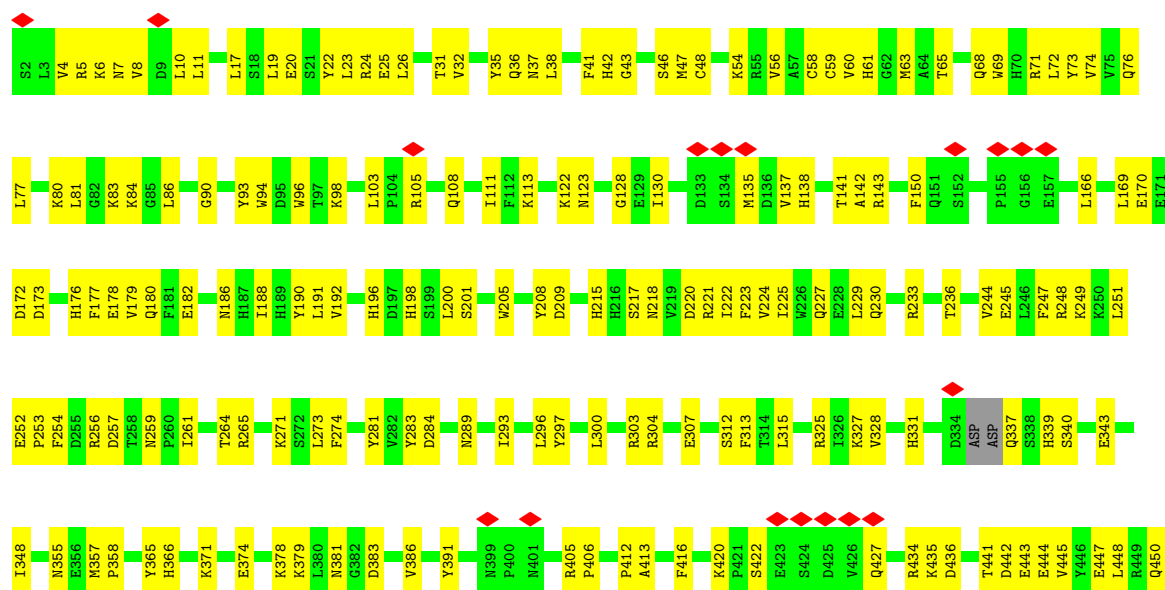


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C2413	D2302	L2208	E1959	P1776	T1884	G1580	R1466	A1372	K1280	R1196	T1103
E2415	D2303	E2209	D1878	F1777	E1687	N1581	T1467	Q1373	S1281	L1197	T1104
N2416	W2306	N2210	P1879	F1779	L1691	G1582	W1468	E1375	L1283	F1198	V1108
G2417	W2307	P2211	F1881	N1780	L1694	N1585	Q1475	T1374	R1284	T1203	P1109
A2424	Q2310	F2212	L1882	R1785	A1694	S1594	R1478	E1376	R1285	D1204	F1110
L2428	E2311	A1965	L1883	D1786	L1695	V1595	R1478	E1377	R1286	L1206	E1111
G2429	L2312	H1884	Q1696	F1787	S1697	L1596	S1485	N1378	Q1287	A1207	F1112
G2430	D2313	H1885	H1885	L1789	S1697	G1597	D1486	I1385	K1294	K1208	F1113
E2433	R2315	S1887	S1886	D1790	S1702	G1598	D1492	V1391	S1297	S1222	E1116
F2438	R2316	T1888	T1888	P1796	L1710	E1599	M1492	W1391	F1298	V1223	R1117
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D2448	L2232	I1891	I1891	K1814	H1714	M1602	N1500	L1400	F1301	D1225	H1121
T2449	L2235	W1895	Q1896	V1809	A1715	F1603	D1501	F1401	P1302	L1226	H1122
L2450	G2239	Q1897	L1898	E1810	W1716	F1604	Q1504	N1402	S1303	K1230	Y1123
R2456	K2240	L1901	L1901	R1817	P1717	L1609	P1516	N1408	C1305	I1231	D1124
L2453	V2243	C2001	P1906	L1818	E1724	S1627	D1521	E1415	T1306	S1232	D1125
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I2455	G2218	A2010	M1910	D1821	R1728	K1636	M1536	F1422	E1308	K1238	S1132
R2456	G2118	A2010	C1911	D1827	C1731	K1637	M1536	F1422	K1311	V1239	Q1135
V2460	Q2124	A2010	A1912	N1827	C1731	K1637	M1536	F1422	V1312	L1136	L1136
F2461	L2111	E2004	E1915	N1828	C1732	R1638	M1536	F1422	A1313	V1241	Q1137
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A2463	D2113	E2004	E1915	N1828	C1732	R1638	M1536	F1422	C1315	V1243	E1139
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F2467	Q2115	E2004	E1915	N1828	C1732	R1638	M1536	F1422	A1320	T1249	R1143
S2468	K2116	E2004	E1915	N1828	C1732	R1638	M1536	F1422	V1321	K1250	R1148
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V2476	D2120	E2004	E1915	N1828	C1732	R1638	M1536	F1422	V1325	I1254	T1165
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E2503	Q2130	E2004	E1915	N1828	C1732	R1638	M1536	F1422	T1352	Q1268	E1187
A2504	D2131	E2004	E1915	N1828	C1732	R1638	M1536	F1422	Q1353	D1270	Y1188
S2505	L2132	E2004	E1915	N1828	C1732	R1638	M1536	F1422	R1356	L1271	E1189
V2508	Q2133	E2004	E1915	N1828	C1732	R1638	M1536	F1422	T1362	D1272	S1272
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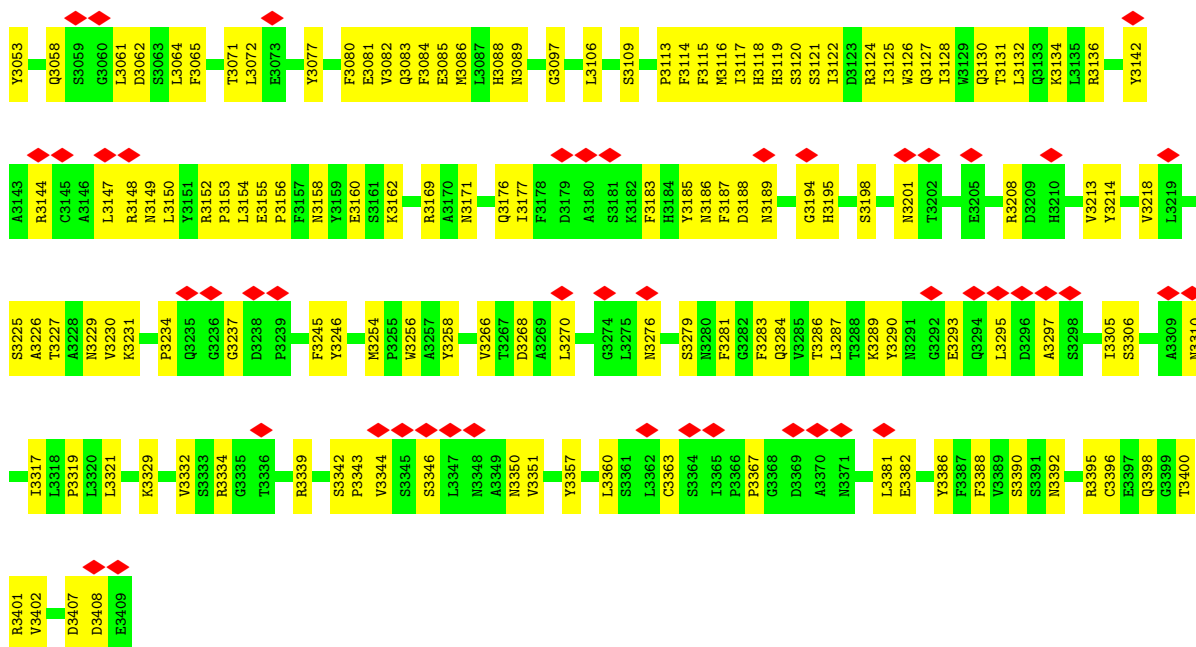




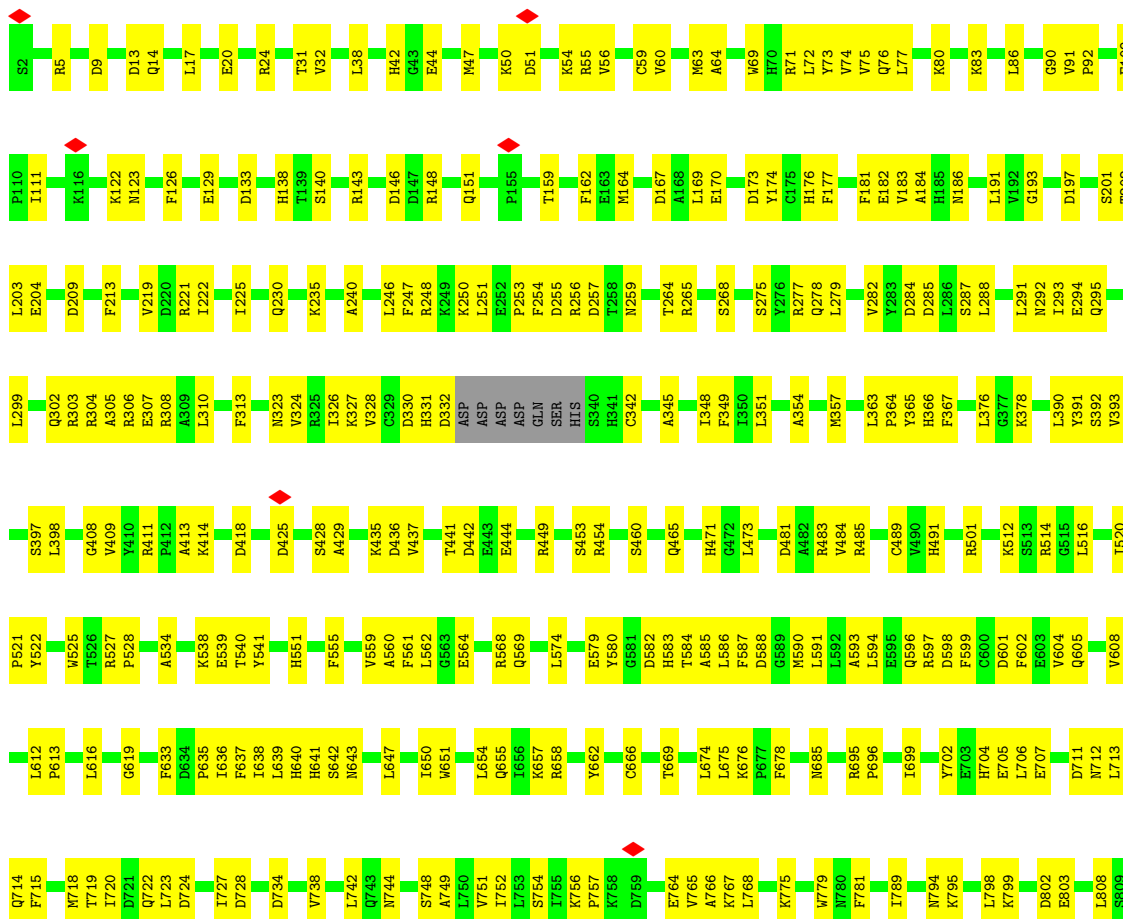


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S631	A632	F633	D634	P635	I636	F637	L638	L639	H640	H641	E729	S642	N643	P644	D645	W648	A649	I650	Q655	R658	L740	H741	L742	R658	Y662	K663	A664	H665	H668	T671	H672	E673	L674	L675	K676	P677	F678	E688	K689	R695	P696	T697	N698	P613	I699	Y700	F615	L616	V617	G618	G619	L625	S626	T627	A709	L628	H629	I535	Y630
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D802	D805	V806	V807	L808	S809	I810	E820	H825	I828	I829	H830	A831	H836	E837	E838	T839	G840	E841	H842	Q843	E844	H846	V847	R848	T855	R856	E857	Q858	V859	Q860	S861	L862	R863	E864	A865	L866	Q867	S868	N889	W890	C891	A896	E897	K898	K899														
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G2881	T2882	Q2883	L2884	S2887	P2892	K2899	G2900	GLY	L2989	THR	GLY	SER	ARG	ALA	VAL	ALA	LYS	GLU	ASP	PRO	GLN	PRG	THR	LYS	THR	K2919	T2920	V2921	R2922	L2923	Y2924	E2925	S2930	V2931	V2934	L2940	L2944	D2948	T2949	P2953	D2954	D2955	D2956	F2957	T2958	R2959	D2960	D2961	R2962	D2963	A2964	
N2773	D2777	L2778	L2779	H2782	G2783	L2784	T2785	T2786	P2787	Q2788	L2789	E2790	I2793	R2796	T2797	S2798	E2799	L2800	N2801	V2802	F2803	A2804	N2805	F2806	Q2809	K2812	V2817	D2820	A2831	G2832	T2833	P2840	W2845	R2849	L2850	V2855	D2856	D2857	F2858	L2859	L2860	E2863	Q2864	D2865	D2866	Y2867	C2868					
E2671	V2672	Q2673	Y2674	E2675	V2676	M2679	M2693	E2697	A2700	Y2701	D2702	F2706	L2707	H2708	H2709	S2710	E2711	N2712	D2713	Q2714	Q2715	L2718	W2719	Q2720	Q2723	D2729	Y2730	Q2738	E2739	L2740	R2741	Q2742	E2745	W2749	N2752	P2753	N2754	D2755	F2756	L2757	A2761	R2762	A2763	A2766								
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• Molecule 1: Hemocyanin





F3178	S3104	T3034	G2961	D2857	Y2774	R2656	W2577	P2495	E2407	N2328	D2246	C2147
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E3199	H3042	Q3043	A2970	T2882	L2784	L2585	T2585	A2504	T2420	N2338	E2254	F2154
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R3208	G3051	L3052	P2982	V2894	I2793	E2697	I2598	K2515	G2429	V2262	Q2263	T2162
D3209	L3052	L3052	H2986	V2900	E2795	W2601	W2601	R2518	W2436	L2353	V2266	H2172
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D3211	K3057	K3057	H2988	G2901	S2797	W2603	W2603	K2521	R2441	K2355	H2268	V2176
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V3213	S3059	S3059	L2990	THR	E2799	E2605	E2605	T2525	I2446	N2364	H2272	T2195
Y3214	S3060	G3060	R2993	GLY	D2800	S2606	S2606	E2526	T2447	R2365	Y2273	E2196
A3215	L3061	L3061	Q2994	SER	R2801	L2614	L2614	E2526	D2448	R2366	Q2197	Q2197
G3216	K3064	L3064	F2995	ALA	W2802	T2615	T2615	K2529	T2449	S2284	S2284	F2198
F3217	F3065	F3065	E2996	VAL	N2805	D2616	D2616	K2530	E2452	K2371	S2285	T2199
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D3238	T3075	T3075	A3004	T2918	D2820	E2624	E2624	Q2538	V2460	D2379	T2297	P2211
V3240	C3078	C3078	L3006	V2922	A2831	D2729	D2729	S2539	F2461	L2380	H2296	H2299
D3241	D3079	D3079	W3011	V2926	Q2839	Y2730	Y2730	G2540	N2462	E2381	T2300	F2301
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K3263	H3088	H3088	P3021	A2940	L2850	S2637	S2637	L2556	I2473	R2392	K2314	Y2223
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R3269	T3090	T3090	L3023	T2943	F2852	R2639	R2639	K2558	S2484	F2394	K2314	R2226
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D3268	L3094	L3094	T3027	V2854	V2854	Q2641	Q2641	N2560	K2488	H2400	P2319	K2234
E3269	V3095	V3095	D3028	T2855	T2855	S2644	S2644	V2564	P2489	G2401	A2323	D2238
L3270	G3096	G3096	H3029	A2955	A2955	D2645	D2645	C2567	T2491	T2404	D2324	G2239
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G3274	L3275	L3275	S3033	N2773	N2773	E2650	E2650	F2574	K2494	A2406	A2326	V2243
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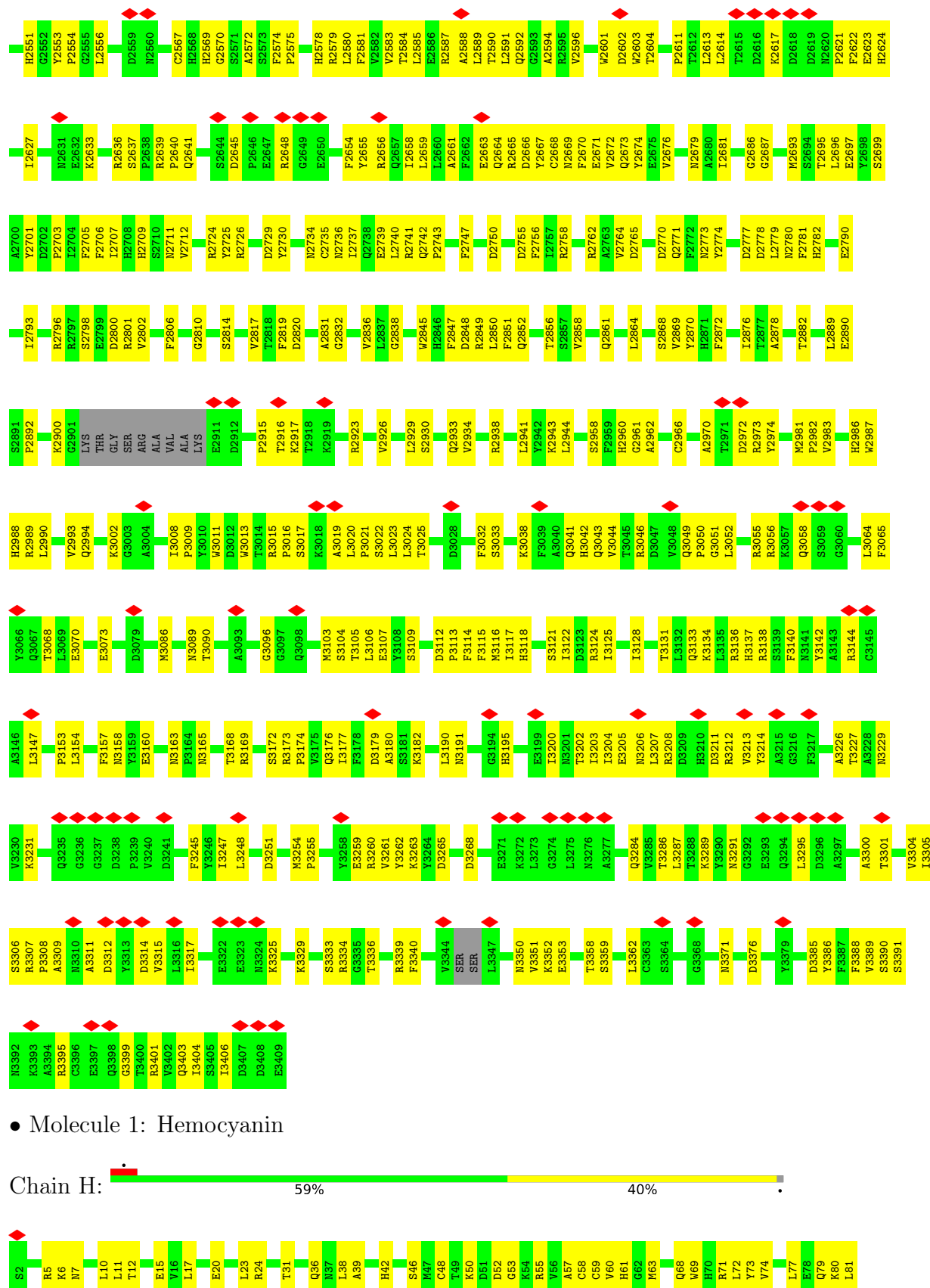
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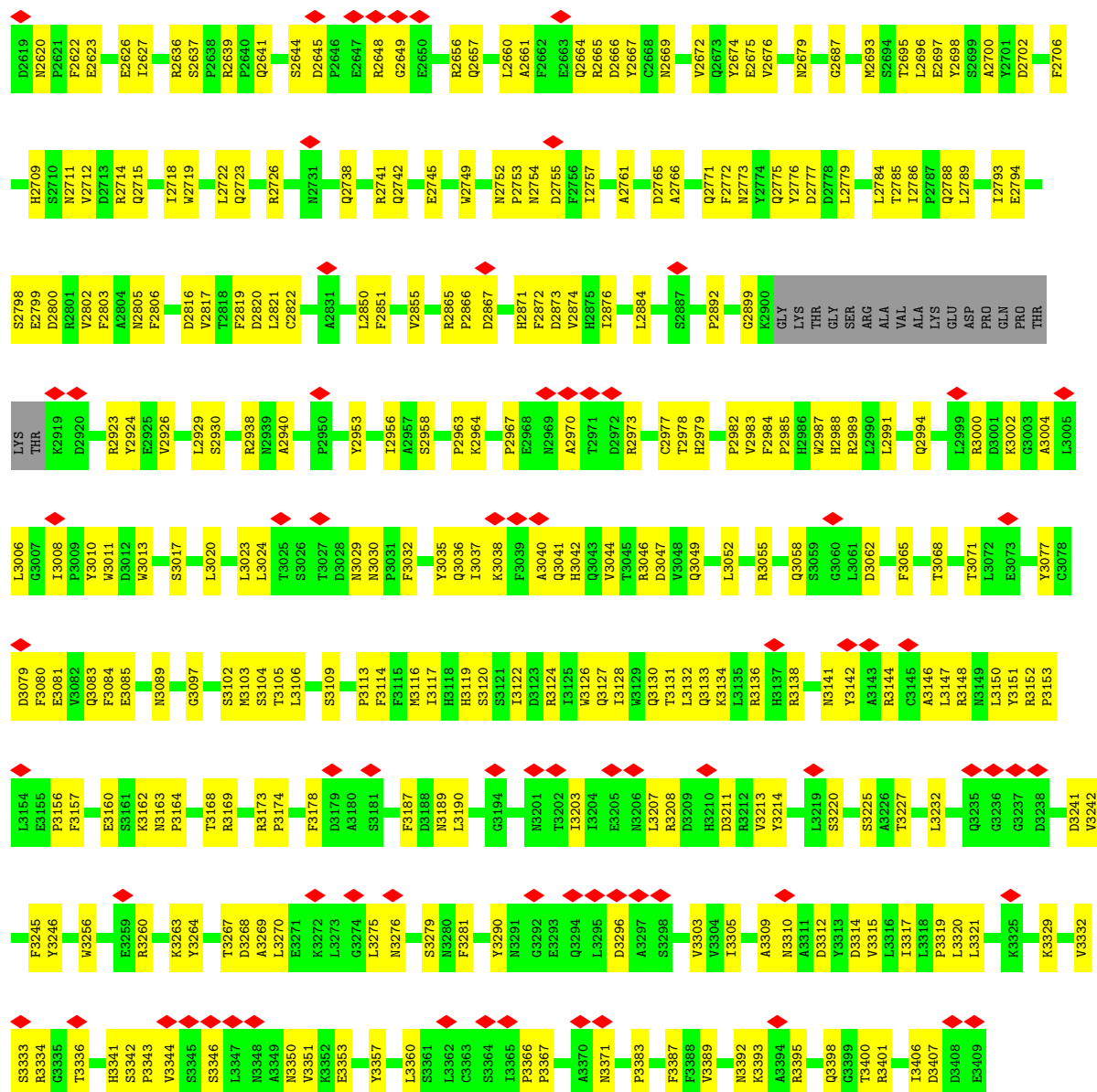






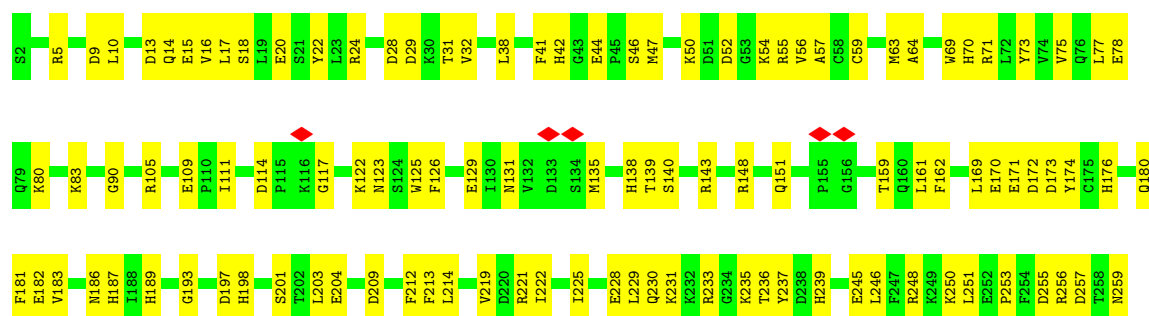
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E1234	E1147	P1073	F910	F910	L829	N744	B658	Q571	D481	R405	D284	W94	
K1237	R1148	N1074	G993	W913	H830	L750	Y662	Q571	A482	P406	D284	H196	
V1240	V1149	N1075	L955	H914	E831	L755	K663	S575	R483	P406	D285	D197	
F1238	F1153	C1078	K997	L917	E832	T755	A664	S575	V484	G408	Y297	H198	
V1239	C1079	K997	K997	L917	E832	T755	A664	S575	V484	G408	Y297	H198	
T1240	K997	K997	K997	L917	E832	T755	A664	S575	V484	G408	Y297	H198	
P1245	I1158	A1080	A999	T918	H836	T756	H665	Y580	R485	V409	L299	N208	
G1246	R1159	I1081	A999	T918	H836	T756	H665	Y580	R485	V409	L299	N208	
S1247	R1159	A1082	E1000	Q920	E838	K758	H665	F587	W499	D418	L310	F213	
E1248	A1162	L1084	M1001	A921	H842	T759	H665	D588	H500	P419	E301	L214	
T1249	L1163	K1085	L1004	A924	H842	T759	H665	D588	H500	P419	E301	L214	
K1250	V1164	P1087	Q1008	L925	H842	T759	H665	D588	H500	P419	E301	L214	
K1251	L1166	L1088	Q1008	A926	H842	T759	H665	D588	H500	P419	E301	L214	
G1252	E1187	Q1089	T1009	R926	H842	T759	H665	D588	H500	P419	E301	L214	
E1253	V1168	A1092	D1010	K928	H842	T759	H665	D588	H500	P419	E301	L214	
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K1256	S1172	T1094	C1012	G933	H842	T759	H665	D588	H500	P419	E301	L214	
K1257	C1175	S1095	E1015	L934	H842	T759	H665	D588	H500	P419	E301	L214	
I1258	N1098	Y1018	Y1018	W937	H842	T759	H665	D588	H500	P419	E301	L214	
L1268	G1179	E1180	E1019	D938	H842	T759	H665	D588	H500	P419	E301	L214	
Q1269	F1181	R1104	H1022	W939	H842	T759	H665	D588	H500	P419	E301	L214	
D1270	Y1182	Y1182	Y1024	L946	H842	T759	H665	D588	H500	P419	E301	L214	
S1271	L1183	P1109	L1028	V950	H842	T759	H665	D588	H500	P419	E301	L214	
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G1274	E1111	E1111	G1031	A952	H842	T759	H665	D588	H500	P419	E301	L214	
E1275	Y1188	F1112	G1031	E953	H842	T759	H665	D588	H500	P419	E301	L214	
V1276	W1192	F1113	S1036	T954	H842	T759	H665	D588	H500	P419	E301	L214	
Q1193	Q1193	E1116	R1041	Y955	H842	T759	H665	D588	H500	P419	E301	L214	
Y1194	Y1194	R1117	Y1042	Y956	H842	T759	H665	D588	H500	P419	E301	L214	
D1195	D1195	S1118	F1119	N957	H842	T759	H665	D588	H500	P419	E301	L214	
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A1282	A1282	Y1121	Y1045	N961	H842	T759	H665	D588	H500	P419	E301	L214	
L1283	L1283	D1125	D1046	N962	H842	T759	H665	D588	H500	P419	E301	L214	
R1284	R1284	Q1126	P1047	L962	H842	T759	H665	D588	H500	P419	E301	L214	
R1285	R1285	L1206	I1048	F963	H842	T759	H665	D588	H500	P419	E301	L214	
M1286	M1286	E1127	F1049	E964	H842	T759	H665	D588	H500	P419	E301	L214	
T1291	T1291	E1127	F1050	N965	H842	T759	H665	D588	H500	P419	E301	L214	
K1294	K1294	F1131	F1051	N966	H842	T759	H665	D588	H500	P419	E301	L214	
I1295	I1295	S1132	H1052	P967	H842	T759	H665	D588	H500	P419	E301	L214	
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S1297	S1297	L1136	S1054	H969	H842	T759	H665	D588	H500	P419	E301	L214	
F1298	F1298				H842	T759	H665	D588	H500	P419	E301	L214	
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T2521	L2432	G2239	H2130	L2043	F1945	A1870	A1777	L1695	C1586	F1508	M1376	G1300
V2522	E2433	K2240	H2130	S2044	D1946	H1871	F1778	Q1696	S1594	L1509	M1379	F1301
A2523	N2338	V2243	P2137	D2047	H1950	L1872	F1779	S1697	V1595	F1380	F1380	S1303
T2524	S2339	L2244	S2138	A2048	D1956	S1876	N1780	D1701	L1596	S1514	F1380	L1304
T2525	L2244	L2244	S2138	F2049	T1957	Y1877	E1781	S1702	E1516	R1515	M1402	L1305
E2526	V2340	E2247	K2143	T2050	L1958	D1878	P1782	G1706	G1597	P1516	E1415	T1306
S2527	V2341	E2247	Y2144	L2055	L1958	P1879	Y1784	E1599	G1598	I1517	E1415	H1307
L2342	N2342	V2251	C2147	L2055	E1959	F1881	Y1784	R1785	E1599	D1518	C1420	H1307
L2343	L2344	L2252	L2148	L2058	L1960	F1881	D1786	L1710	T1600	V1519	C1420	H1307
L2344	E2253	E2253	L2148	L2058	L1960	F1881	D1786	L1710	M1602	F1520	C1420	H1307
E2345	Q2254	Q2254	H2149	L2063	I1963	L1883	D1790	H1714	P1603	D1521	K1311	V1312
R2349	C2258	C2258	P2152	L2063	H1964	H1883	D1790	H1714	F1604	M1524	I1424	C1315
L2353	D2259	D2259	T2153	S2064	A1965	H1885	P1794	V1718	F1604	H1525	Q1425	C1315
P2354	F2260	F2260	T2153	S2065	E1966	S1886	N1795	P1717	D1607	F1426	Q1425	V1316
E2355	E2261	E2261	P2155	S2066	L1967	S1887	P1796	P1718	R1608	E1427	F1426	V1316
K2356	V2262	V2262	H2156	S2072	L1968	L1888	L1719	L1719	L1609	G1318	I1428	G1318
V2357	Q2263	Q2263	K2157	T2073	L1969	D1889	D1801	C1720	L1610	T1532	S1319	S1319
F2358	F2264	F2264	H2158	L2074	S1970	R1890	I1802	P1721	K1611	F1535	M1431	A1320
N2359	T2267	T2267	R2159	Y2075	L1971	I1891	I1802	Y1722	K1611	M1536	A1432	V1321
R2366	H2268	H2268	T2162	K2078	I1972	Y1892	E1805	P1723	T1614	S1537	L1433	H1324
Y2367	N2269	N2269	V2165	S2079	A1893	L1894	V1809	E1724	D1626	W1538	V1437	W1325
D2368	A2270	A2270	V2165	K2080	K1978	Q1896	E1810	A1725	S1627	T1539	L1448	H1326
D2369	I2271	I2271	V2165	R2080	I1990	E1897	R1811	Q1727	P1541	I1540	L1448	R1327
K2370	L2274	L2274	L2169	Q2085	I1990	L1898	R1817	R1728	Q1542	Q1542	A1482	Q1332
R2371	L2274	L2274	S2174	E2086	S1993	L1898	R1818	A1730	L1543	L1543	V1437	V1333
Q2374	L2283	L2283	V2176	L2087	A1994	N1910	E1820	C1731	E1544	L1456	L1456	L1338
L2375	D2292	D2292	D2182	R2090	H1995	Q1911	S1820	C1732	R1638	F1457	F1457	L1338
N2376	F2296	F2296	W2183	R2091	L1998	L1913	H1824	M1736	Y1644	H1460	H1460	R1340
D2378	T2297	T2297	W2183	R2092	K1999	E1914	D1827	A1737	R1651	H1461	H1461	G1341
E2379	H2298	H2298	P2191	L2093	C2001	M1916	M1828	T1738	R1651	A1462	A1462	S1345
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Q2388	D2302	D2302	E2209	S2097	A2010	L1920	A1837	L1745	N1663	R1555	D1350	D1350
Q2388	D2303	D2303	N2210	A2101	G2011	L1921	Y1843	Y1746	S1664	F1557	W1351	W1351
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V2393	E2311	E2311	A2213	M2105	F2013	G1926	E1847	F1750	D1666	G1559	S1485	R1356
F2397	L2312	L2312	R2214	K2108	G2018	A1927	V1848	E1751	Q1667	F1560	D1486	R1356
E2407	Q2314	Q2314	G2215	A2109	E2021	P1928	Q1849	Q1667	T1668	M1564	C1487	P1359
V2408	R2315	R2315	Y2216	A2110	M2022	Y1929	F1850	V1761	G1669	S1568	T1491	I1362
E2502	R2316	R2316	T2217	L2111	M2023	H1930	E1851	G1762	G1669	T1491	M1492	N1363
L2318	G2317	G2317	K2218	R2112	V2024	L1931	I1852	P1764	K1670	L1573	M1493	E1364
C2413	L2318	L2318	E2219	D2113	S2025	D1932	A1853	Y1765	T1671	C1576	L1496	A1365
Q2414	P2319	P2319	S2220	L2114	S2025	T1935	H1854	W1766	E1672	C1576	Y1367	S1366
E2415	K2221	K2221	Q2115	Q2115	D2027	E1937	N1855	W1766	R1673	T1579	K1497	F1368
N2416	Q2116	Q2116	Q2116	Q2116	R2028	I1857	A1856	V1769	R1673	T1579	L1496	S1366
G2417	E2231	E2231	E2231	G2117	L2038	K1865	K1865	Q1772	T1676	G1580	D1501	S1370
K2418	L2232	L2232	L2232	G2118	E2039	E1866	E1866	N1773	K1677	N1581	D1369	S1370
A2422	L2235	L2235	L2235	Q2124	K2040	R1867	R1867	S1774	S1679	G1582	Q1504	R1371
L2428	D2238	D2238	D2238	K2041	K2041	S1868	S1868	L1775	V1680	E1583	N1505	S1372
				L2126	G2042	M1869	M1869	P1776	L1683	R1584	F1507	T1374



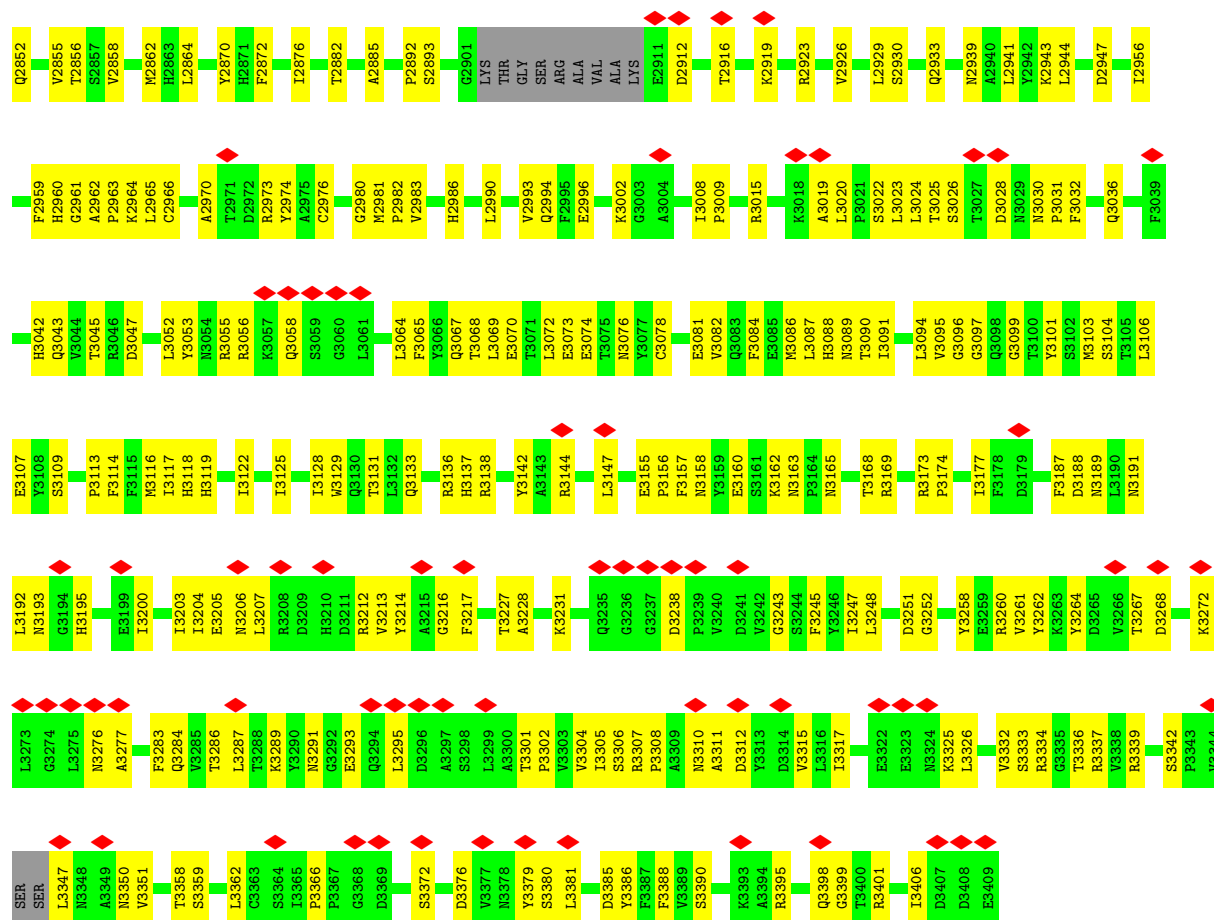
● Molecule 1: Hemocyanin

Chain I: 61% 39%



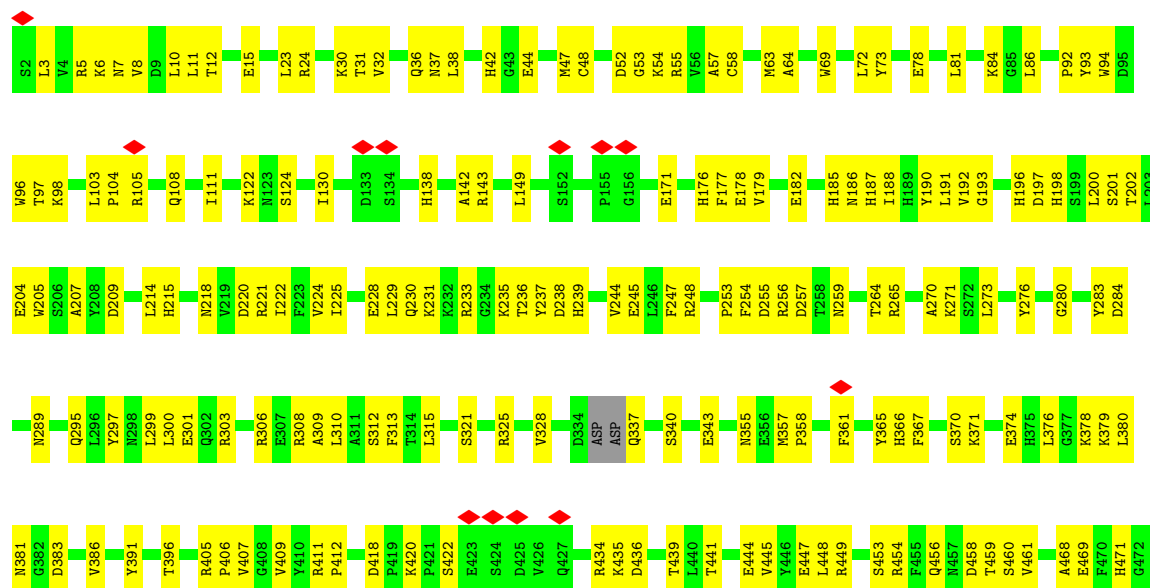






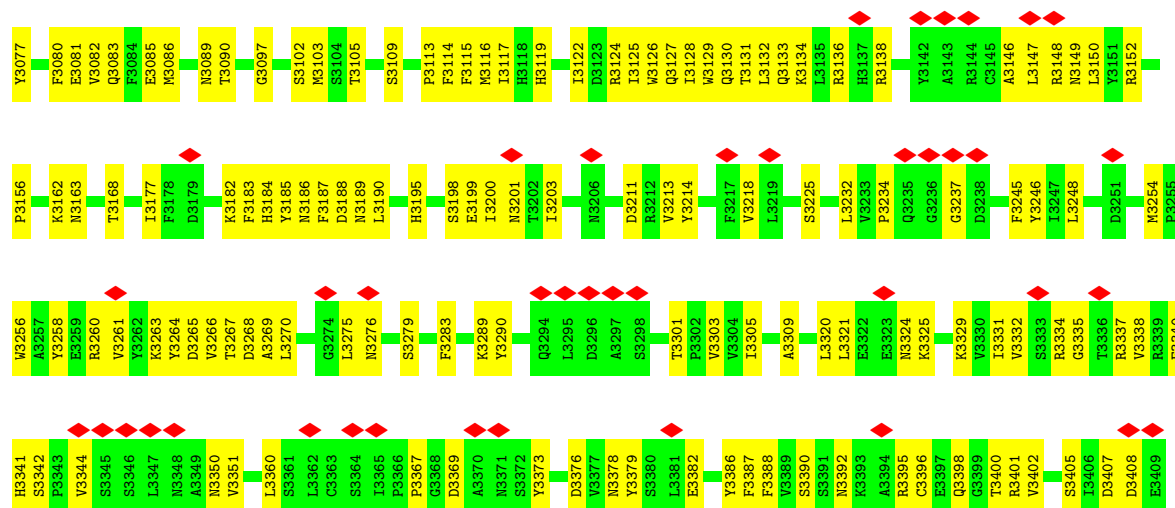
• Molecule 1: Hemocyanin

Chain J: 61% 39% .



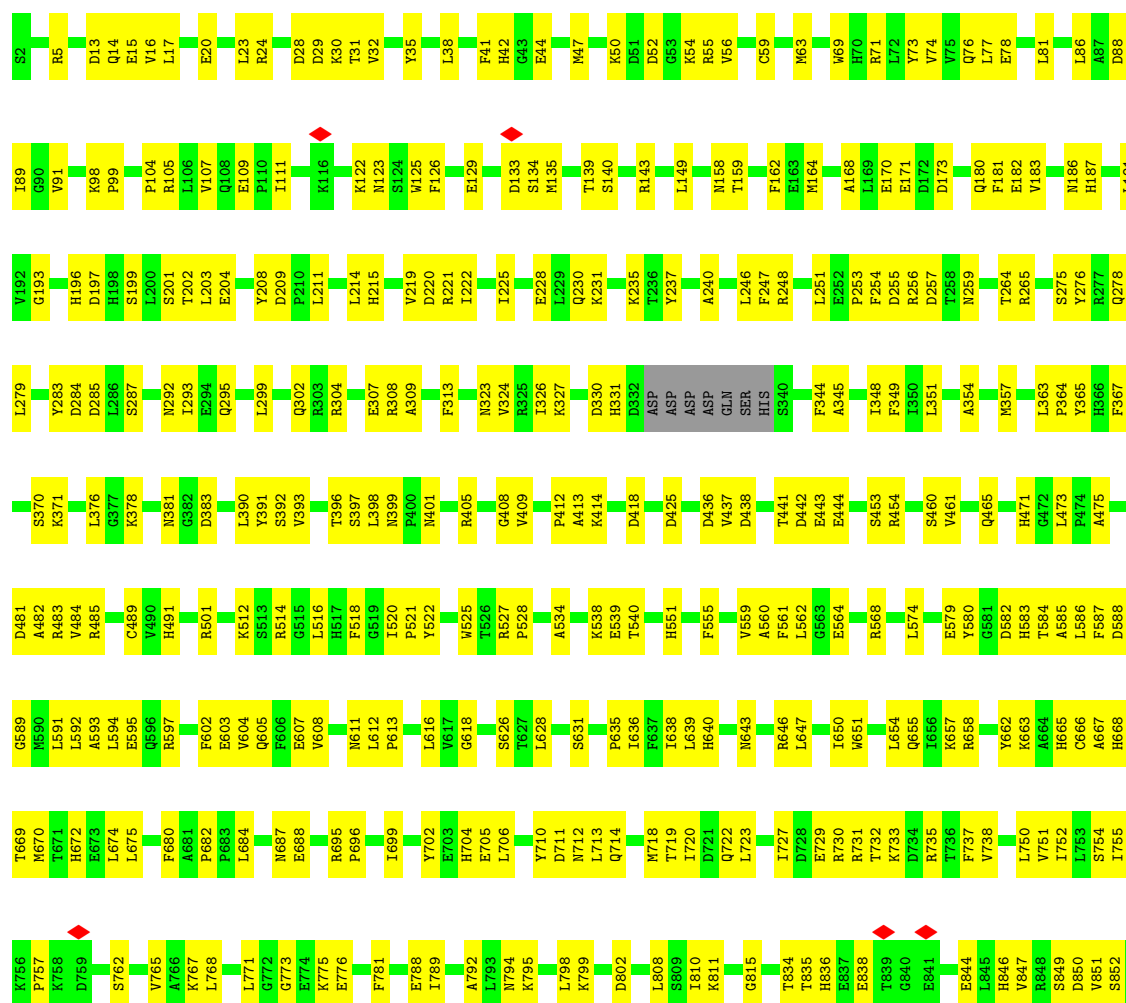
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H2986	H2987	H2988	R2989	L2990	L2991	W2997	A2998	L2999	R3000	R3001	K3002	K2919	D2920	L2921	G3007	L3008	P3009	Y3010	W3011	D3012	W3013	L3020	P3021	L3024	T3027	F3032	Y3035	Q3036	I3037	F3039	A3040	Q3041	H3042	Q3043	V3044	D3047	V3048	Q3049	L3052	Y3053	K3057	Q3058	S3059	G3060	L3061	D3062	F3065						
K2795	S2796	E2797	D2800	R2801	V2802	Q2809	K2812	D2816	V2817	D2820	L2821	C2822	R2823	A2824	S2829	F2830	A2831	G2832	T2833	P2840	W2845	D2848	R2849	L2850	V2855	R2865	P2866	D2867	S2868	V2869	Y2870	H2871	I2876	L2884	S2887	F2896	G2899	K2900	GLY	LYS	THR	GLY	SER										
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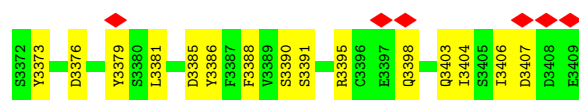
• Molecule 1: Hemocyanin

Chain K: 61% 39%.

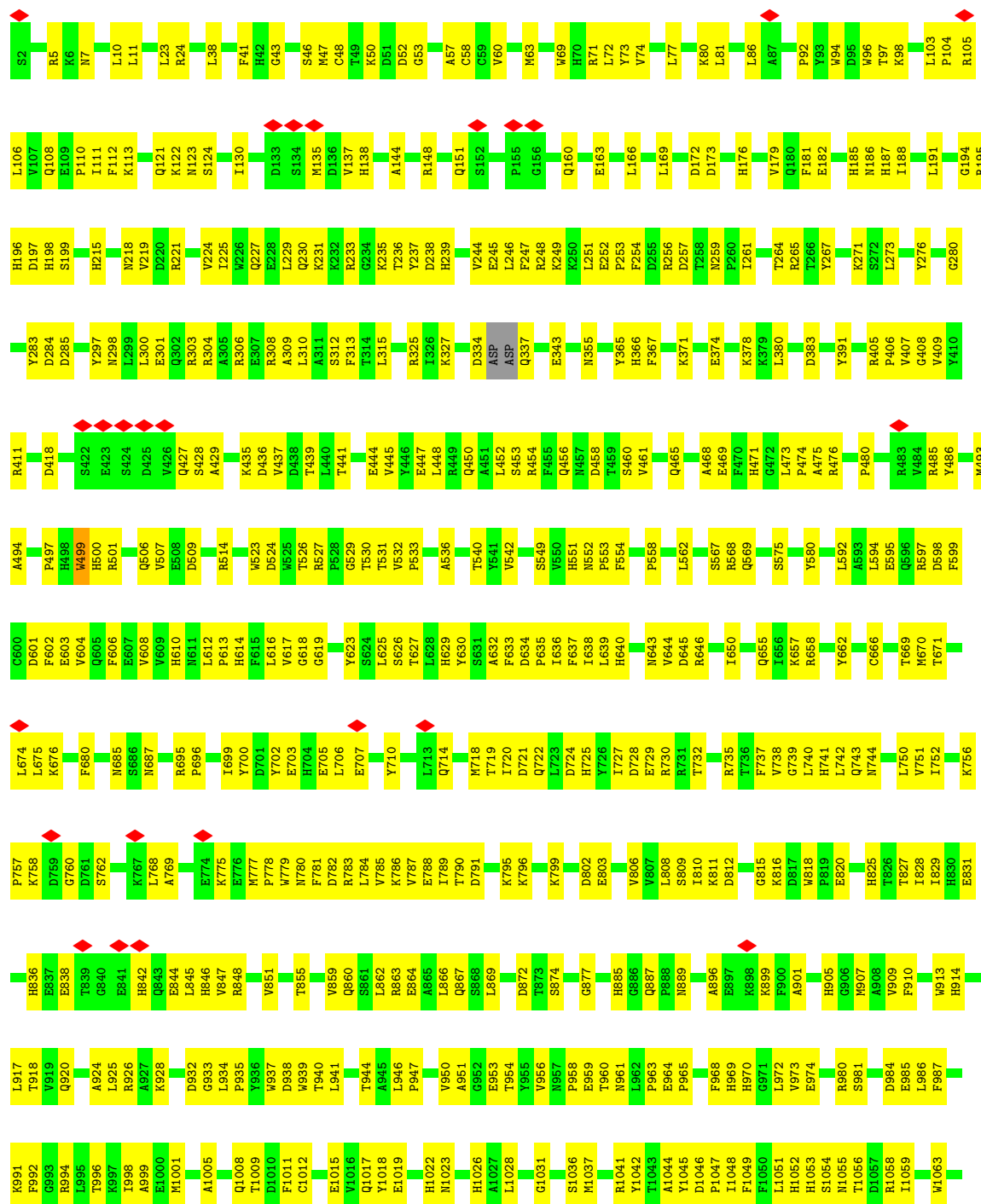




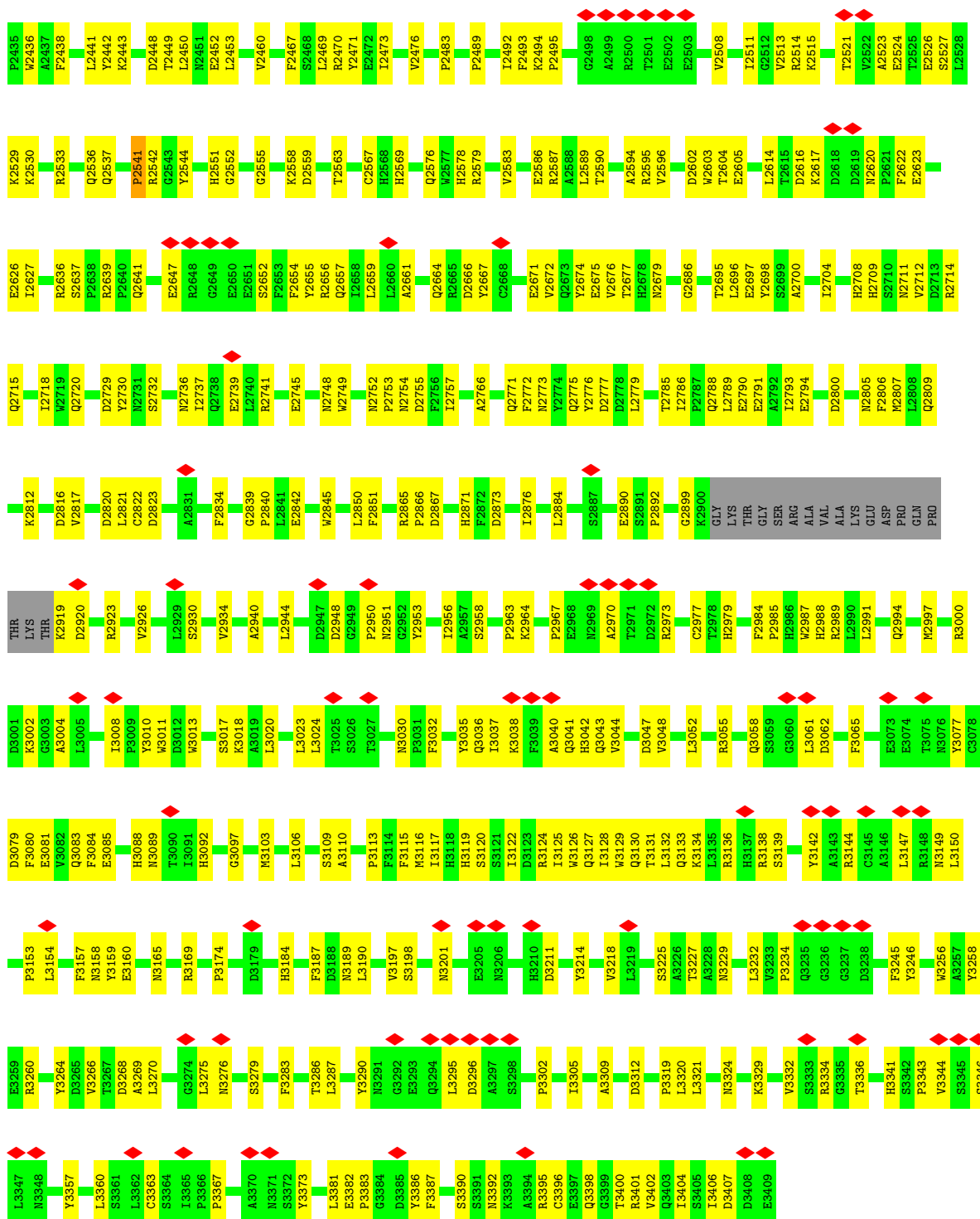
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● Molecule 1: Hemocyanin

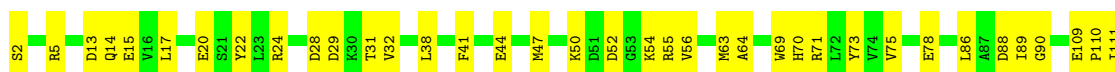


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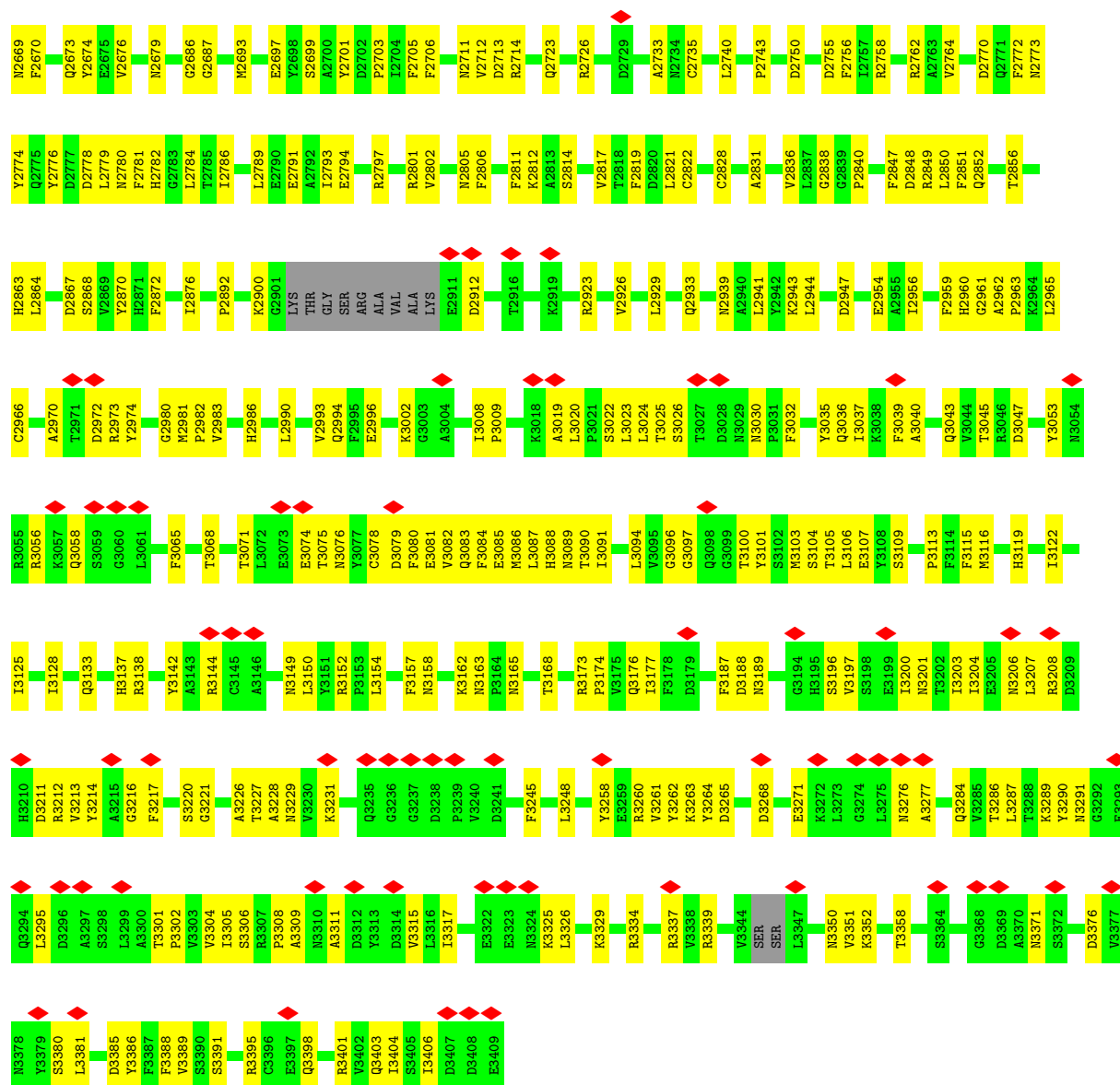
• Molecule 1: Hemocyanin

Chain M:



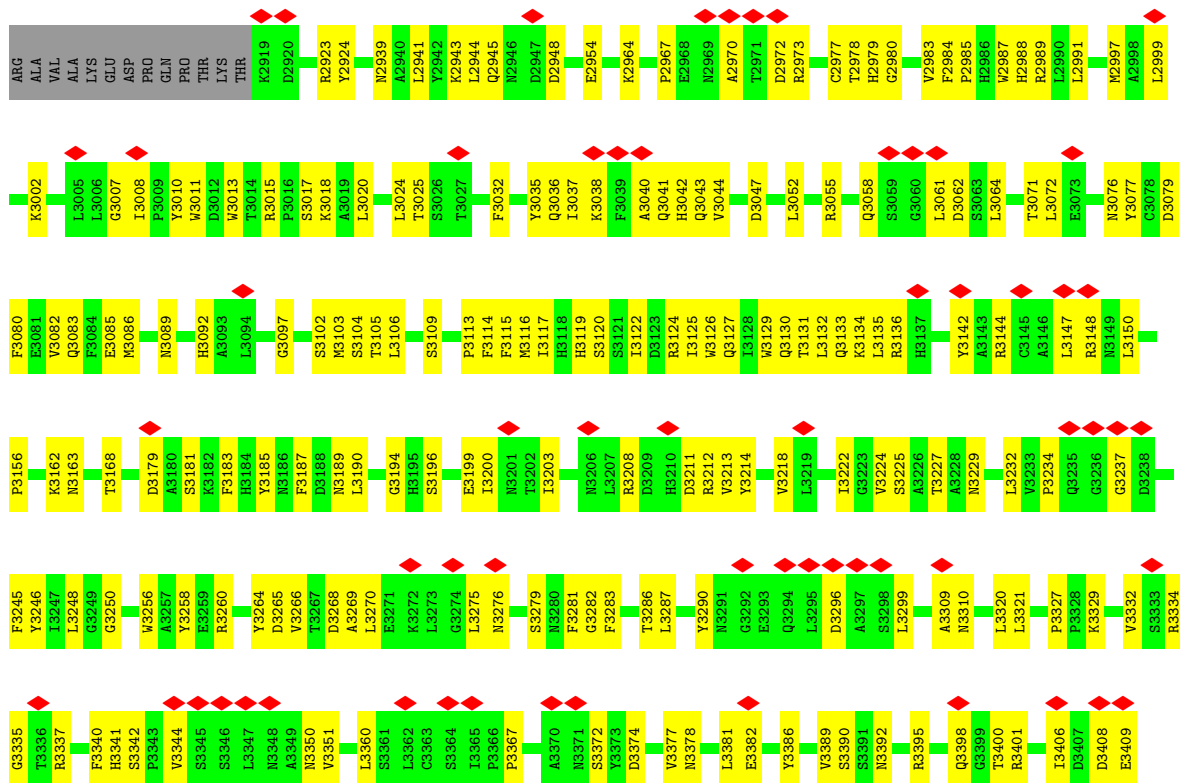


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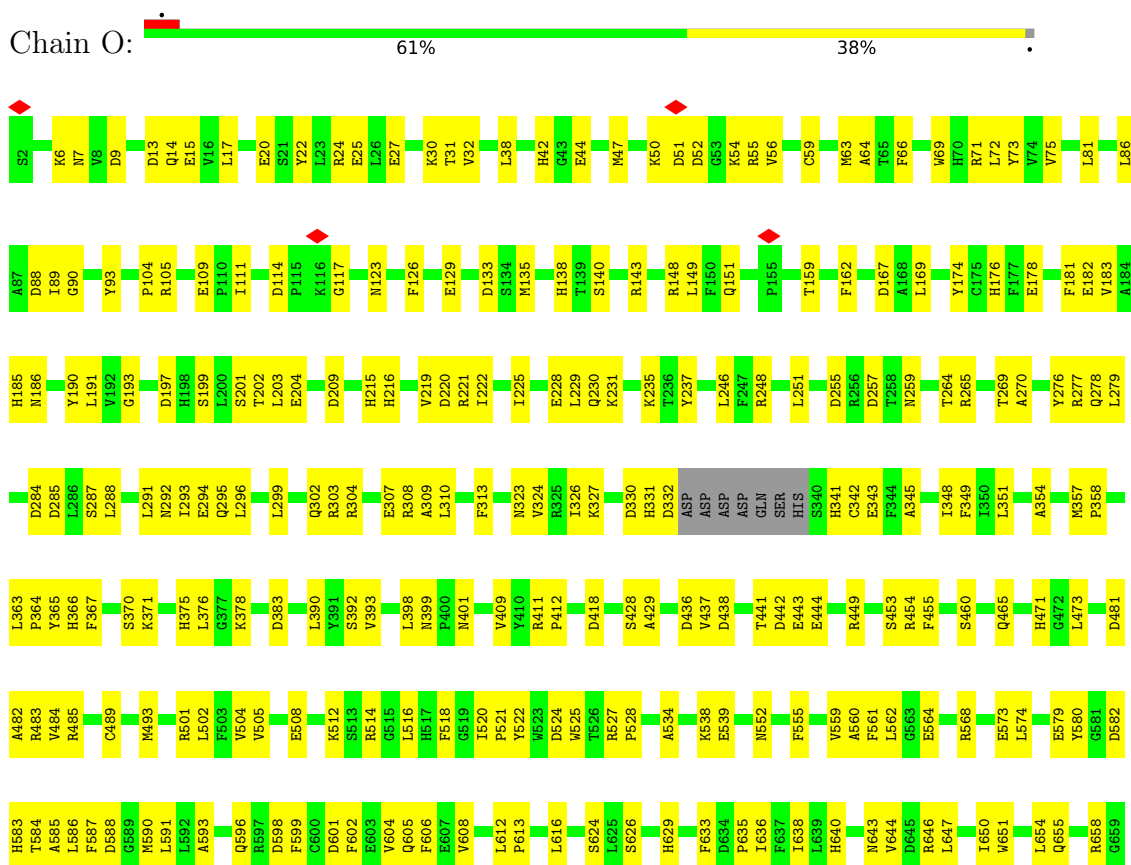


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D1518	I1428	H1300	L1226	S1132	I1048	Y955	R863	N780	Y700	D524	W523	K435	S312
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		F1401	R1284	I1205			Y935	E844	G760	P677	R597	F503	
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- Molecule 1: Hemocyanin

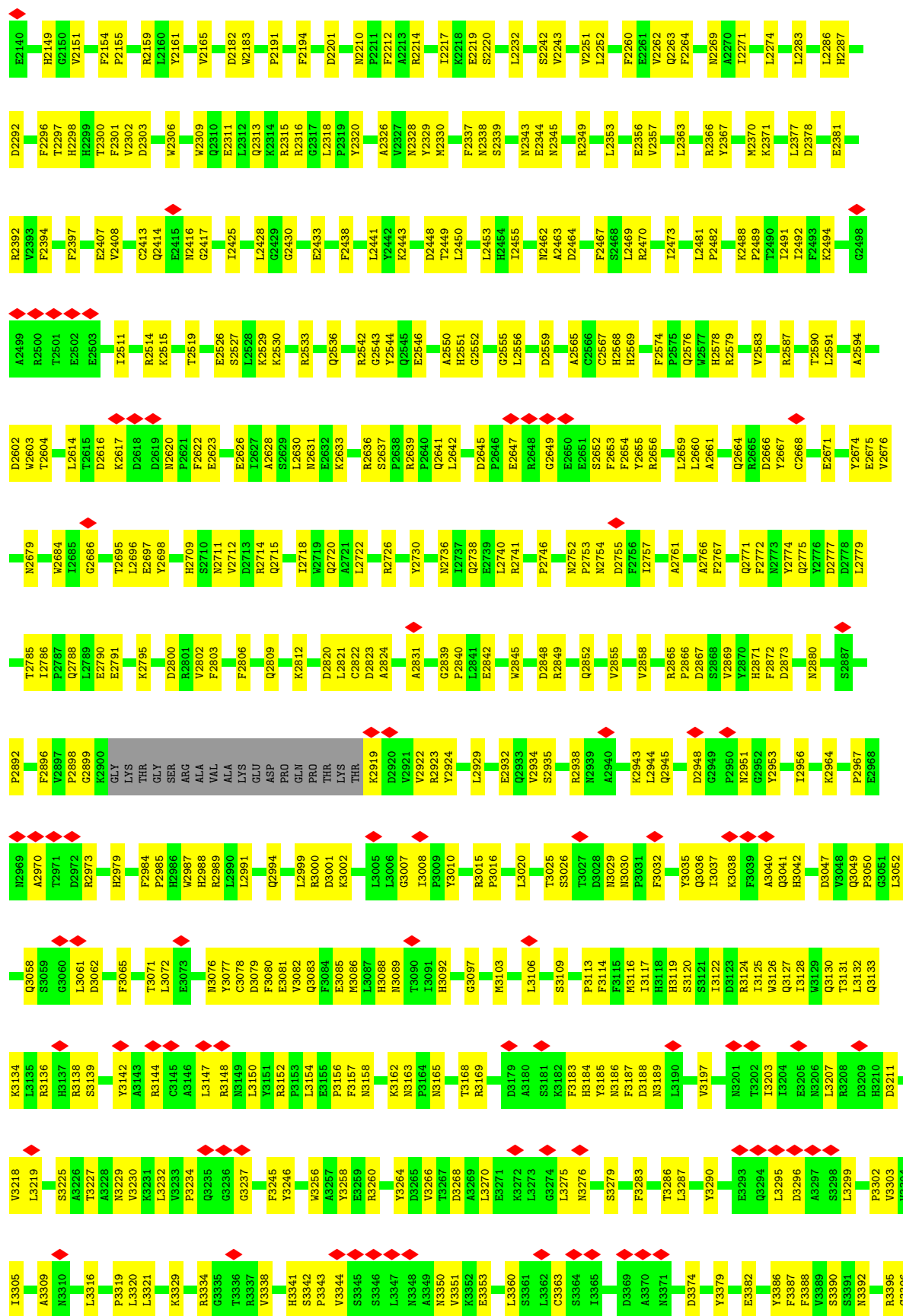


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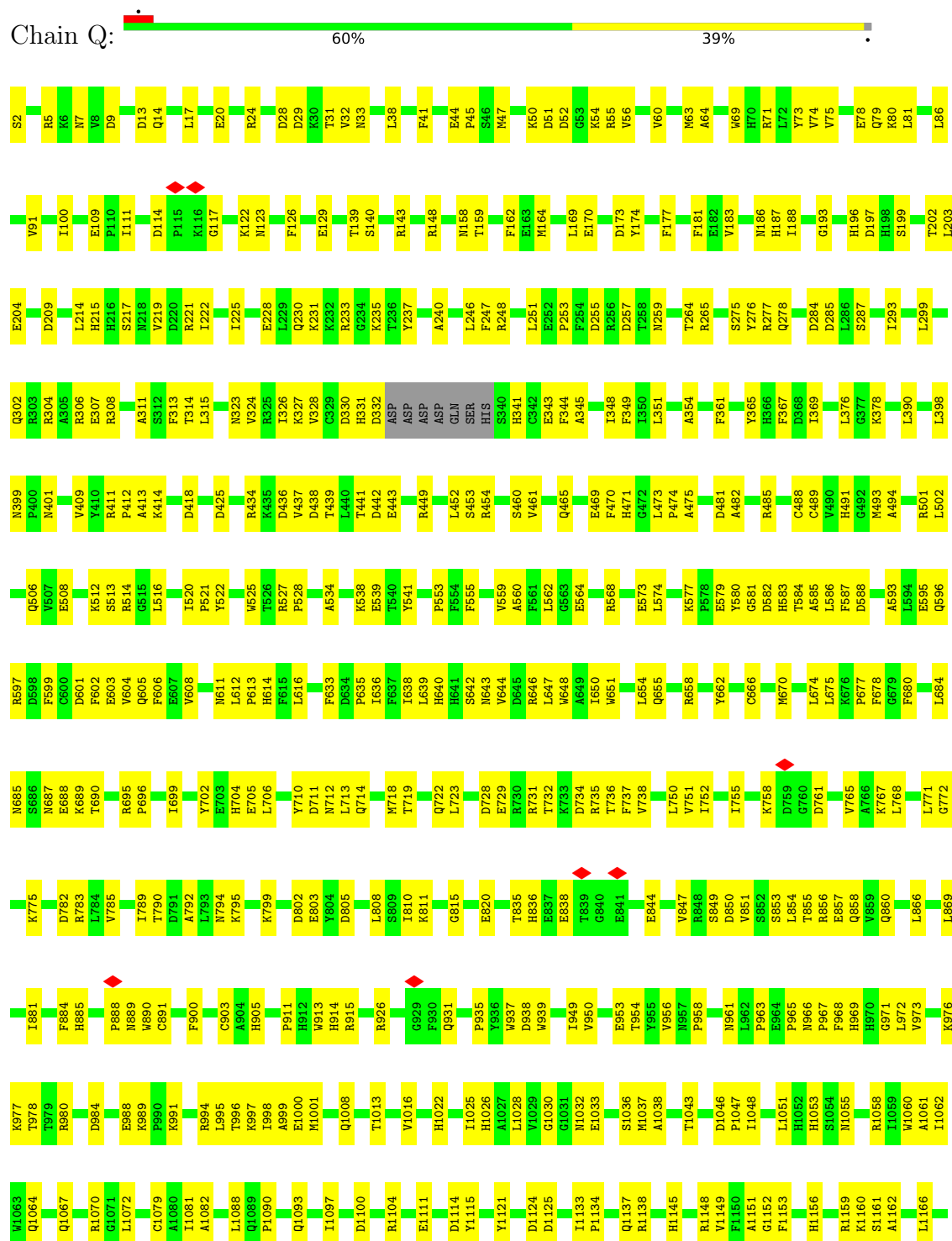
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S3104	T2856	T2856	T2856	Q2771	Q2771	E2663	L2585	R2500	K2304	D2201	D2201	D2201
S3104	S2857	S2857	S2857	F2772	F2772	Q2664	E2586	T2501	I2305	A2202	A2202	A2202
S3104	V2858	V2858	V2858	N2773	N2773	R2665	A2588	E2502	W2306	W2203	W2203	W2203
S3104	L2864	L2864	L2864	Y2774	Y2774	D2666	L2589	E2503	Q2313	L2208	L2208	L2208
S3104	R2865	R2865	R2865	Q2775	Q2775	N2669	T2590	A2504	R2314	E2209	E2209	E2209
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S3104	D2867	D2867	D2867	D2777	D2777	E2672	Q2592	T2507	R2316	P2211	P2211	P2211
S3104	S2868	S2868	S2868	L2778	L2778	V2672	A2594	V2508	Y2320	G2117	G2117	G2117
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S3104	Q2883	Q2883	Q2883	F2781	F2781	A2680	V2596	S2509	N2328	G2215	G2215	G2215
S3104	L2884	L2884	L2884	H2782	H2782	L2681	Q2597	T2420	W2330	Y2216	Y2216	Y2216
S3104	S2893	S2893	S2893	Q2783	Q2783	H2682	L2598	R2421	Y2329	T2224	T2224	T2224
S3104	K2900	K2900	K2900	L2784	L2784	I2685	W2601	A2424	W2331	V2225	V2225	V2225
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S3104	LYS	LYS	LYS	I2786	I2786	I2685	V2603	F2426	W2334	L2232	L2232	L2232
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S3104	THR	THR	THR	I2793	I2793	E2697	T2615	T2521	G2429			



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G2041	P1906	D1827	A1737	R1655	E1545	L1456	V1346	K1256	L1166	P1073	E985	A908
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		V1761	N1564	R1673	N1564	D1466	R1356	L1271	Y1182	T1009	Q1008	T918
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		W1766	G1580	R1673	G1580	S1485	A1365	E1275	G1185	D1100	A921	A921
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		Q1772	N1585	R1673	N1585	L1489	S1377	E1277	Y1188	R1104	L924	L924
		S1774	S1594	R1673	S1594	I1491	M1378	S1276	W1192	V1108	V1016	V1016
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		N1780	L1598	R1673	L1598	N1490		R1283	L1196	F1113	M1022	M1022
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		P1796	G1629	R1673	G1629	D1521		H1299	P1047	D1124	S1036	S1036
		W1797	D1630	R1673	D1630	H1526		G1300	M1037	D1125	M1037	M1037
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			P1717	R1673	P1717	D1531		P1303	Y1042	S1132	Y1042	Y1042
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			P1723	R1673	P1723	N1534		K1231	F1047	Q1137	F1047	F1047
			Y1722	R1673	Y1722	M1536		S1232	T1048	R1138	T1048	T1048
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			N1726	R1673	N1726	Y1538			L1051	L1141	L1051	L1051
			Q1727	R1673	Q1727	I1540			H1052	H1142	H1052	H1052
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				R1673					M1154	F1150	M1058	M1058
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				R1673					R1159	F1150	R1058	R1058
				R1673					V1063	G1152	V1063	V1063
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				R1673					V1063	F1153	V1063	V1063
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				R1673					R1159	F1153	R1058	R1058
				R1673					V1063	G1152	V1063	V1063
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				R1673					R1159	M1154	R1058	R1058
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				R1673					V1063	G1152	V1063	V1063
				R1673					T1067	F1153	T1067	T1067
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				R1673					V1063	F1153	V	



- Molecule 1: Hemocyanin

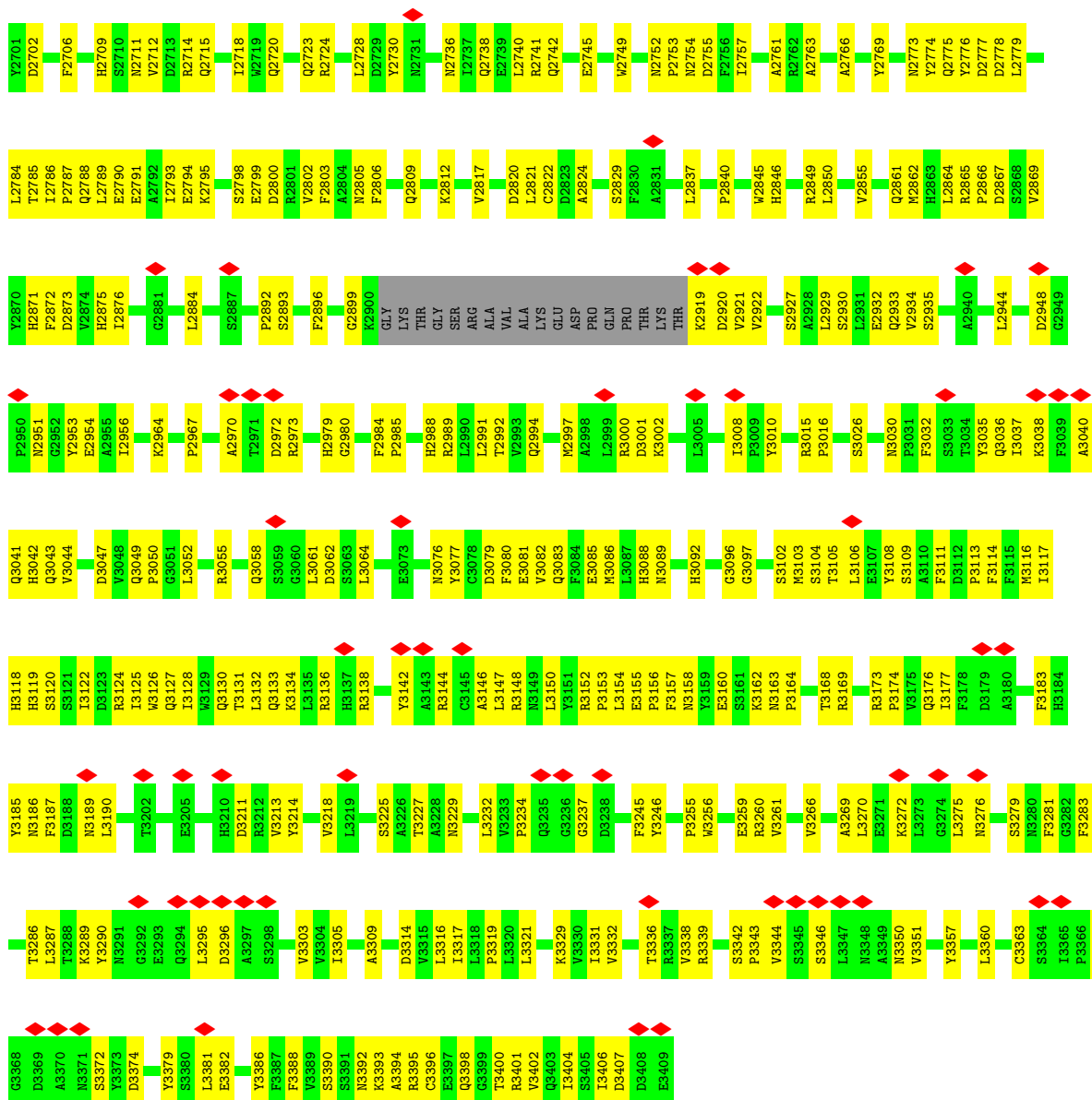


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L2382	D2292	L2384	D2292	F2194	R2102	V2015	P1933	A1356	R1756	N1663	D1570	N1463	A1361	H1263	D1186
L2385	L2386	L2387	H2298	T2195	T2104	G2017	I1934	H1858	L1760	S1664	F1571	D1465	I1362	Y1188	E1189
L2388	L2389	L2390	L2391	Y2200	N2105	T2019	K1940	H1860	P1764	Q1685	C1576	R1466	A1365	L1268	
L2392	L2393	L2394	D2303	D2201	K2108	A2020	D1943	V1861		D1666	C1577	Q1475	S1366	S1272	Q1193
L2395	L2396	L2397	K2304	A2202	A2109	W2024	D1946	S1862	P1770	T1667	A1578	Q1476	R1371	E1275	Y1194
L2398	L2399	L2400	W2305	K2204	L2111	S2025	Y1947	K1865	P1771	Q1668	T1579	D1482	S1377	R1196	R1196
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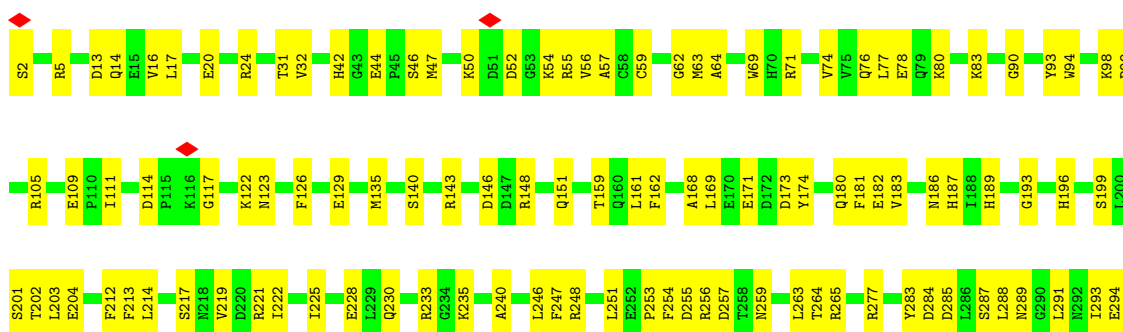


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L103	P104	R105	Q108	I111	F112	K113	L119	G120	Q121	K122	N123	S124	I130	D133	S134	M135	D136	V137	H138	A142	R143	A144	Q227	F313	E228	T314	Q230	Q231	L149	S152	V153	A154	P155	G156	E157	N158	T159	V165	L166	L169	E170	E171	H176	F177	E178	V179	E182	M186	H187								
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E374	H375	L376	G377	K378	K379	L380	N381	G382	D383	Y391	N399	P400	N401	L402	L403	P404	R405	P406	V407	G408	V409	Y410	R411	D418	P419	K420	P421	S422	E423	S424	D425	V426	Q427	R434	K435	D436	D442	E443	E444	E447	L448	R449	Q450	S453	F455	Q456	N457	T459	S460	V461							
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P558	S567	R568	Q569	V570	Q571	S575	Y580	G581	F587	D588	L591	E595	Q596	R597	D598	F599	C600	D601	F602	E603	V608	L612	P613	H614	F615	L616	V617	G618	G619	Y623	S624	L625	S626	T627	L628	H629	P633	A634	I635	D634	P635	I636	F637	I638	N643	V644	D645										
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G739	L740	H741	L742	Q743	N744	L750	V751	I752	K756	P757	K758	D759	G760	D761	S762	K767	L768	M777	P778	W779	N780	F781	D782	L783	L784	W785	K786	H787	E788	V789	Y710	L713	Q714	G717	W718	T719	Q722	L723	D724	H725	V726	I727	D728	E729	R730	R731	T732	R735	V736	F737	V738						
E837	E838	T839	G840	E841	H842	Q843	E844	L845	H846	V847	R848	T855	R856	V859	Q860	S861	L862	R863	L866	Q867	S868	L869	E870	F878	L881	P884	Q887	P888	N889	E897	K898	A901	H905	G906	N907	A908	F910	W913	H914	L917	T918	V919	Q920	E921	E922	N923											
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L1004	E1007	Q1008	T1009	D1010	F1011	C1012	T1013	F1014	E1015	Y1018	E1019	I1020	A1021	H1022	N1023	Y1024	L1028	A1051	G1031	S1036	L1040	R1041	Y1042	P1047	T1048	F1049	F1050	L1051	H1052	H1053	S1054	N1055	T1056	D1057	L1058	I1059	W1063	Q1067	R1070	G1071	L1072	P1073	A1077	A1080	T1081	A1082	S1083	L1084									
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E1167	V1168	C1169	F1174	C1175	H1176	F1177	E1178	G1179	Y1182	I1183	L1184	Y1188	Q1193	D1194	R1195	L1196	L1197	F1198	Q1199	Y1200	E1201	I1202	T1203	D1204	T1205	L1206	A1207	L1208	V1219	K1220	Y1221	S1222	V1223	G1283	K1294	I1295	A1296	S1297	K1229	K1230	I1231	S1232	S1233	E1234	V1239	T1240	V1241	V1242	P1245	G1246	V1316	H1317	G1318	S1319	A1320	V1321	
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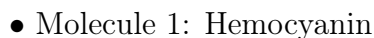


● Molecule 1: Hemocyanin





D2750	D2751	N2752	P2753	R2758	R2762	A2766	F2772	N2773	Y2774	D2777	Q2664	R2665	L2779	N2780	F2781	L2784	R2796	R2797	D2800	R2801	F2802	F2803	A2804	N2805	F2806	K2812	V2817	T2818	F2819	C2822	C2828	A2831	G2839	F2847	D2848	R2849	L2850	F2851	Q2852	V2855	S2857	Q2861											
S2644	D2645	P2646	E2647	R2648	Q2649	E2650	F2653	F2654	Y2655	R2656	E2663	Q2664	R2665	D2666	T2667	C2668	N2669	F2670	E2671	V2672	Q2673	Y2674	V2675	V2676	V2684	Q2687	L2696	S2699	A2700	P2703	I2704	F2705	H2709	S2710	N2711	V2712	R2714	R2726	D2729	N2734	C2735	R2741	P2746	N2749									
Q2570	F2574	Q2576	V2577	H2578	R2579	L2580	F2581	V2582	L2583	L2585	E2586	L2587	A2588	L2589	T2590	L2591	Q2592	G2593	A2594	R2595	V2596	I2597	L2598	W2601	D2602	W2603	T2604	E2605	S2606	P2611	L2614	T2615	D2616	K2617	D2618	D2619	N2620	F2621	F2622	E2623	H2624	N2631	E2632	K2633	R2636	F2637	R2638	R2639	P2640	Q2641			
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R2226	Q2229	L2232	F2233	K2234	D2238	G2239	V2243	V2248	L2249	P2250	H2251	W2252	E2253	Q2254	D2255	Y2257	C2258	Q2263	V2266	T2267	H2268	V2269	L2270	I2271	Y2272	Y2273	L2274	S2284	S2285	L2286	H2287	S2290	H2298	V2302	V2308	E2311	L2312	Q2313	K2314	R2315	R2316	Y2320	C2325										
H2130	C2136	Y2144	C2147	L2148	G2149	V2150	P2152	T2153	F2154	P2155	H2156	W2157	H2158	R2159	T2162	L2163	Q2164	V2165	H2172	G2173	S2174	T2175	P2179	L2190	R2191	Y2192	L2193	F2194	Q2197	T2198	F2199	Y2200	D2201	A2202	W2203	L2208	P2211	F2212	A2213	G2215	Y2216	E2219	Y2223	T2224	V2225								
V2053	R2056	A2057	L2058	N2059	G2060	S2061	S2064	S2065	S2066	L2067	I2068	P2069	T2070	P2071	S2072	V2073	K2078	S2079	R2080	S2083	E2086	L2087	P2088	P2089	N2090	R2091	Y2092	R2093	H2094	E2095	L2096	S2097	H2098	L2099	D2100	A2101	T2104	N2105	K2108	A2109	A2110	L2111	R2112	P2113	L2114	D2117	Q2118	T2119	W2123	Q2124			
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D1878	F1879	F1880	F1881	L1882	L1883	H1884	H1885	S1886	R1890	L1894	H1895	Q1896	E1897	L1898	Q1899	R1900	G1903	H1904	D1905	P1906	N1907	E1908	G1909	N1910	L1913	M1916	R1917	E1918	A2020	E2021	K1921	S1924	N1930	K1936	P1941	V1944	F1945	D1946	Y1955	D1956	T1957	L1958	L1969	V1969	G2118	D2046	V2051	K1978					
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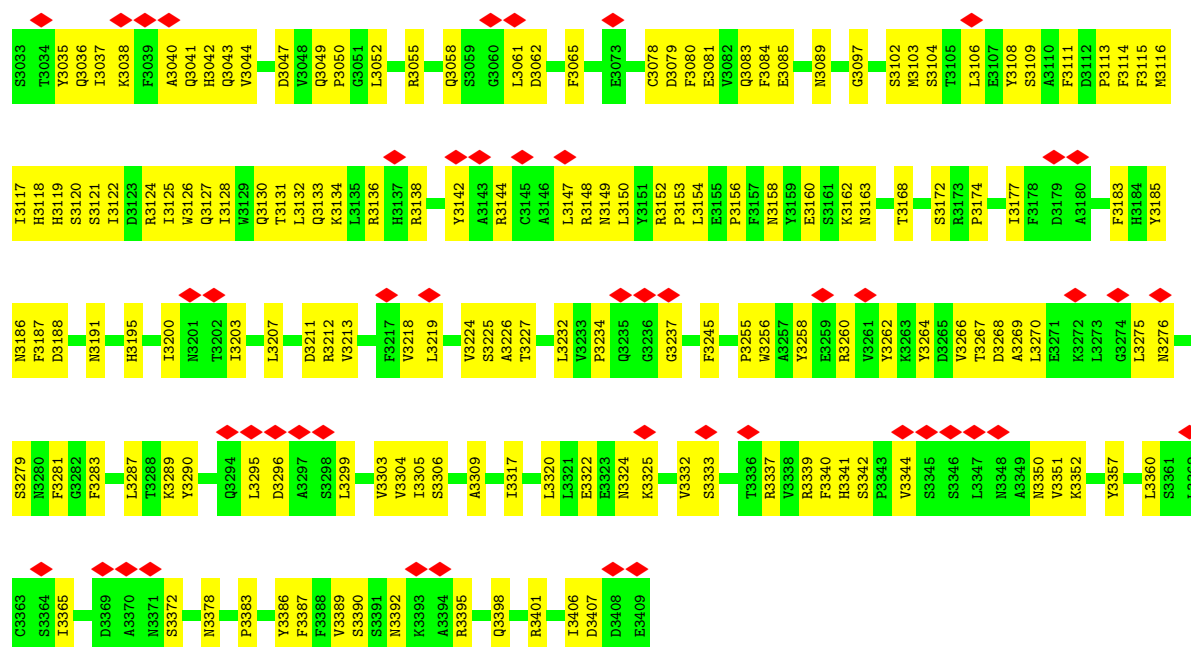


Frequency	Percentage
Often	61%
Sometimes	39%



K1611	Y1528	M1431	R1327	N1257	T1165	N1075	R994	T918	I828	T736	L562	C477
K1620	H1529	A1432	Q1332	I1258	L1166	S1076	L995	V919	I829	F737	L563	F478
L1625	Y1530	L1433	V1333	V1259	E1167	A1077	T996	Q920	H830	G738	G563	R479
D1626	D1531	L1436	L1338	S1262	C1169	A1081	K997	A924	E831	G739	E564	P480
S1627	T1532	V1437	L1338	H1263	C1175	I1082	A999	A924	H836	H741	S567	R483
	F1535	L1445	G1341	L1267	H1176	A1082	E1000	R926			R568	V484
T1631	W1538	L1448	S1342	L1268	P1177	L1084	M1001	A927		N744	Q569	R485
L1633	T1539	L1448	S1342	Q1269	E1178	R1085	V1002	R928			Q571	Y486
	I1540	A1452	S1345	L1270	K1179	K1086	L1003	G929		L750		
P1641	P1541	A1452	V1346	L1271	E1180	P1087	L1004	F930		I752		
	Q1542	P1455	P1347	S1272	F1181	Q1088	E1007	Q931			Y580	M493
L1543	L1543	P1456	Y1348	E1273	D1186	Q1089	Q1008	D932			G581	
E1544	E1544	L1456	W1349	G1274			G933	G933		P757	H688	F496
E1545	V1546	F1457	W1351	E1275	W1192	A1092	L845	L934		K758	L586	P497
V1547	L1547	H1460	W1351	V1276	Q1193	N1098	H846	P935		M670	F587	H498
K1548	K1548	H1461	R1356	E1277	Y1194	P1099	V947	Y936		G760	T671	W499
R1549	R1549	N1462	Q1357	S1278	D1195	D1100	R948	W937		D761	L591	H500
Q1550	Q1550	N1463	P1359	L1279	R1196	P1099	V947	D938			L594	R501
R1551	R1551	V1464	P1359	K1280	L1197	D1100	R948	T940		K767	E595	L502
		D1465	I1362	S1281	F1198	T1103	R856			L768	Q596	L502
R1555	R1555	R1466	I1363	L1283	I1205	V1108	Q860	T944			Q597	R514
L1556	L1556	D1465	E1364	R1284	L1206	P1109	S861	A945		K775	Q597	P621
F1557	F1557	I1470	A1365	R1285	K1208	F1110	L862	L946		M777	R597	D524
		Q1471	S1366	M1286		E1111	D872	P947		P778	D988	W525
F1560	F1560	Q1472	I1367	T1291	Y1221	V1112	G877			N885	F599	T526
N1564	N1564	Q1475	F1368	F1292	S1222	F1113	Q867	V950		K889	D801	R527
S1568	S1568	D1482	D1369	G1293	I1223	E1116	S869	G952		T690	Y604	
L1573	L1573	S1485	R1371	K1294	I1224	Q1120	L869	E953		R895	Q605	
C1576	C1576	A1488	S1372	L1295	D1225	H1122	E870	Y955		P696	H610	
		L1489	T1374	A1296	L1226	Y1121	D871	N957		T697	H614	
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G1580	G1580	I1491	E1376	H1299	G1230	D1124	I881	E959		I699	F615	
N1581	N1581	M1492	S1377	G1300	I1231	D1125	Q887	T960		D701	L616	
G1582	G1582	P1379	P1378	F1301	S1232	L1126	P888	N961		Y702	V617	
		L1496	F1380	S1302	E1233	T1133	N889	P964		E703	G618	
T1684	T1684	K1497	Q1397	L1304	E1234	P1134	F1050	P965		L706	G619	
		N1500	L1400	C1305	G1237	Q1137	E997			Y623	Y623	
E1687	E1687	D1501	F1401	T1306	K1238	R1138	K898	F968		D711	S824	
A1694	A1694	Q1504	N1402	H1307	V1239	E1139		H969		T719	S826	
S1697	S1697	N1505	Y1405	V1312	T1240	H1142	A901	E974		Q722	T627	
T1705	T1705	P1516	L1406	A1311	V1242	R1143	H905			L723	L628	
G1706	G1706	I1517	E1415	C1314	P1245	E1147	G906	R980		D724	H629	
A1709	A1709	D1518	E1415	C1315	T1249	R1148	M907			H725	Y630	
L1710	L1710	F1520	G1420	H1317	K1250	V1149	A908	R983		D728	L638	
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S1712	S1712	N1524	I1424	A1320	G1252	R1159	F910	W818		R731	R730	
F1713	F1713	H1525	E1427	V1321	E1253		N911	P819		T732	S842	
				H1324	I1254	P1073	H914	E820		R735	N643	
Y1722	Y1722				D1255	Y1074	L917	H825			W651	
E1724	E1724				K1256							
A1725	A1725											

K2964	P2967	E2968	N2969	A2970	T2971	T2972	R2973	C2976	C2977	T2978	H2979	G2980	F2984	P2985	H2986	V2987	H2988	R2989	L2990	L2991	T2992	V2993	Q2994	N2997	R3000	D3001	K3002	L3005	L3006	G3007	I3008	P3009	V3010	V3011	K3012	H3013	T3014	R3015	P3016	S3017	L3020	L3024	T3025	S3026	T3027	D3028	N3029	N3030	P3031	F3032
D2867	S2868	V2869	H2870	H2871	L2876	G2881	L2884	S2887	G2889	K2900	GLY	THR	LYS	THR	GLY	SER	ARG	ALA	VAL	ALA	LYS	GLU	ASP	PRO	GLN	PRO	THR	LYS	K2919	D2920	V2921	V2922	V2923	L2929	E2932	Q2933	V2934	R2938	K2943	L2944	Q2945	N2946	D2947	D2948	G2949	P2950	E2954	F2959		
Q2771	Q2775	D2776	D2777	D2778	L2779	T2785	L2786	P2787	Q2788	L2789	E2790	E2791	R2796	D2800	R2801	V2802	Q2809	K2812	V2817	D2820	L2821	C2822	D2823	A2824	S2829	F2830	T2833	L2837	G2838	P2840	W2845	D2848	R2849	V2855	T2856	S2857	N2860	Q2861	T2862	R2865	P2866									
E2875	N2879	G2886	M2893	S2894	T2895	L2896	E2897	Y2898	P2703	L2704	F2705	H2708	H2709	N2710	N2711	D2712	D2713	R2714	Q2715	I2718	Q2723	R2724	Y2725	R2726	D2729	Y2730	N2731	S2732	N2736	Q2738	E2739	L2740	R2741	Q2742	E2745	W2749	N2752	P2753	N2754	D2755	F2756	I2757	A2761	R2762	A2763					
H2578	F2581	T2584	L2585	E2586	D2587	L2589	T2590	L2591	Q2592	D2602	W2603	L2614	T2615	D2616	K2617	D2618	D2619	N2620	P2621	F2622	E2623	L2630	R2636	S2637	D2645	P2646	E2647	G2648	E2650	F2654	Y2655	R2656	Q2657	I2658	L2659	A2661	F2662	Q2664	R2665	D2666	Y2667	C2668	N2669	F2670	E2671	Y2674				
L3469	R3470	I2473	L2481	P2482	K2488	P2489	T2490	I2491	G2498	A2499	R2500	T2501	E2502	E2503	A2504	S2505	Y2506	V2513	R2514	K2515	N2516	I2517	N2518	V2522	A2523	E2526	S2527	K2529	R2533	Q2536	Q2537	Q2538	R2542	G2543	Y2544	G2552	Y2553	P2554	C2567	H2568	H2569	F2574	P2575							
D2368	G2374	L2375	N2376	L2377	D2378	E2379	L2380	E2381	V2393	L2398	L2399	V2408	V2412	C2413	Q2414	E2415	N2416	G2417	K2418	A2422	T2425	L2428	Q2429	G2430	S2431	L2432	E2433	F2438	D2439	R2440	L2441	K2443	T2449	L2450	L2453	H2454	R2456	V2460	F2461	N2462	P2463	D2464	F2467	S2468						
N2269	A2270	I2271	L2274	L2283	L2286	H2287	D2292	F2296	T2297	H2298	D2299	T2300	F2301	V2302	D2303	W2306	W2309	Q2310	E2311	L2312	Q2313	K2314	R2315	R2316	G2317	L2318	P2319	Y2320	V2327	N2328	Y2329	M2330	P2336	S2339	L2342	N2343	E2344	N2345	R2349	Q2353	P2354	K2355	F2365							
K2040	K2041	G2042	L2043	S2044	V2045	D2046	D2047	T2050	L2055	L2058	L2063	S2064	H2065	S2066	Y2075	K2078	S2079	R2080	P2088	P2089	N2090	E2095	L2096	T2097	A2101	R2102	M2105	A2109	L2111	R2112	D2113	L2114	Q2115	K2116	L2126	H2130	E2260	V2261	T2262	Q2263	F2264	E2265	V2266	T2267	H2149					
P2152	T2153	F2154	P2155	H2156	R2159	T2162	L2163	Q2164	V2165	L2169	L2182	W2183	F2194	L2208	N2210	P2211	F2212	A2213	T2217	K2218	E2219	S2220	R2226	E2231	L2232	L2235	Q2239	V2251	L2252	Q2254	Y2257	F2260	E2261	V2262	Q2263	F2264	E2265	V2266	T2267	H2268										
M1828	W1831	E1839	Q1840	E1841	H1842	Y1843	E1847	V1848	Q1849	F1850	E1851	I1852	H1853	H1854	N1855	A1856	I1857	K1865	T1867	E1866	H1867	Y1877	D1878	P1879	I1880	P1881	L1882	L1883	H1884	H1885	S1886	S1887	R1890	A1893	L1894	W1895	Q1896	E1897	L1898	R1902	D1905	E1908	S2025	F2026	M1916	R1917	L1920			
G1926	A1927	P1928	Y1929	N1930	L1931	K1936	E1937	Y1938	F1945	D1946	Y1947	K1948	S1949	H1950	E1959	A1965	E1966	L1967	L1968	K1978	S1979	L1987	I1990	K1991	T1992	S1993	P1762	H1995	I1998	K1999	V2000	C2001	E2004	D2005	V2006	C2007	K2008	D2009	A2010	F2013	W2024	S2025	F2026	R2027	R2028	L2038	E2039			
M1736	A1737	T1738	Q1741	H1742	H1743	T1747	F1750	E1751	R1757	E1847	V1848	Q1849	F1850	E1851	I1852	H1853	H1854	N1855	A1856	I1857	K1865	T1867	E1866	H1867	Y1877	D1878	P1879	I1880	P1881	L1882	L1883	H1884	H1885	S1886	S1887	R1890	A1893	L1894	W1895	Q1896	E1897	L1898	R1902	D1905	E1908	S2025	F2026	M1916	R1917	L1920



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

Chain U:  50%



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

Chain W:  100%



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

Chain Y:  100%



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

Chain d:  100%



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

Chain e:  100%



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

Chain g:  100%



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

Chain i:  50% 50%



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

Chain n:  50% 50% 50%



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

Chain o:  100%



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

Chain q:  50% 50%



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

Chain s:  100%

NAG1
NAG2

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

Chain x:  50% 50%

NAG1
NAG2

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

Chain y:  100%

NAG1
NAG2

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

Chain 0:  50% 50%

NAG1
NAG2

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

Chain 2:  100%

NAG1
NAG2

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

Chain 7:  50% 50%

NAG1
NAG2

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

Chain 8:  100%

NAG1
NAG2

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

Chain AA:  100%



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

Chain CA:  50% 50%



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

Chain HA:  50% 50%



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

Chain IA:  50% 50%



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

Chain KA:  50% 50%



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

Chain MA:  100%



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

Chain RA:  50% 50%



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

Chain SA:  50%  50%



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

Chain UA:  100%



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

Chain WA:  50%  50%



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

Chain bA:  50%  50%



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

Chain cA:  100%

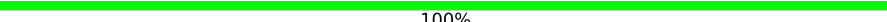


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain eA:  100%



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

Chain gA:  100%



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

Chain lA:  50% 50%



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

Chain mA:  100%

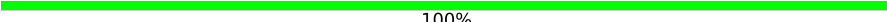


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain oA:  50% 50%



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

Chain qA:  100%



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

Chain vA:  50% 50%



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

Chain wA:  100%

MAG1
MAG2

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

Chain yA:  50% 50%

MAG1
MAG2

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

Chain 0A:  50% 50%

MAG1
MAG2

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

Chain 5A:  50% 50%

MAG1
MAG2

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

Chain V:  67% 33%

MAG1
MAG2
BMA3

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

Chain X:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain Z:  33% 67%

MAG1
MAG2
BMA3

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

Chain a:  67% 33%

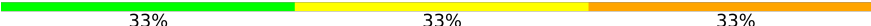


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  67% 33%



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

Chain c:  33% 33% 33%



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

Chain f:  67% 33%

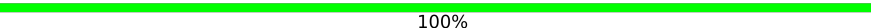


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  67% 33%

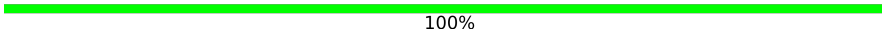


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%



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

Chain k:  100%



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

Chain l:  100%



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

Chain m:  33% 33% 33%



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

Chain p:  67% 33%



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

Chain r:  33% 33% 33%



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

Chain t:  100%



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

Chain u:  100%



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

Chain v:  100%

MAG1
MAG2
BMA3

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

Chain w:  67% 33%

MAG1
MAG2
BMA3

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

Chain z:  67% 33%

MAG1
MAG2
BMA3

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

Chain 1:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain 3:  67% 33%

MAG1
MAG2
BMA3

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

Chain 4:  100%

MAG1
MAG2
BMA3

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

Chain 5:  100%



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



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



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



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



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



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



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

Chain GA:  33% 67%



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

Chain JA:  67% 33%



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

Chain LA:  33% 67%

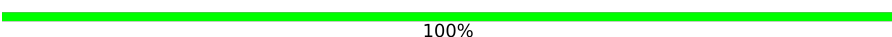


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:  67% 33%



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

Chain OA:  100%



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

Chain PA:  100%



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

Chain QA:  67% 33%



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

Chain TA:  100%



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

Chain VA:  100%



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

Chain XA:  67% 33%



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

Chain YA:  67% 33%



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

Chain ZA:  100%



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

Chain aA:  33% 67%

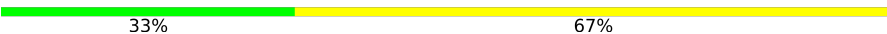


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain dA:  67% 33%



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

Chain fA:  33% 67%

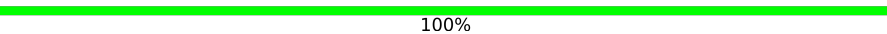


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain hA:  33% 67%



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

Chain iA:  100%

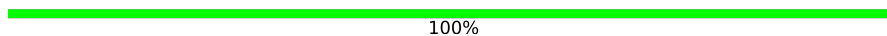


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain jA:  67% 33%



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

Chain kA:  100%



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

Chain nA:  67% 33%



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

Chain pA:  100%



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

Chain rA:  100%



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

Chain sA:  100%



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

Chain tA:  100%



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

Chain uA:  33% 33% 33%

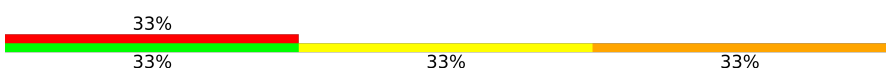


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain xA:  100%

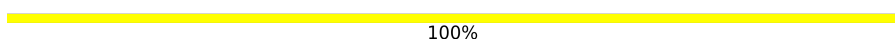


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain zA: 



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

Chain 1A: 

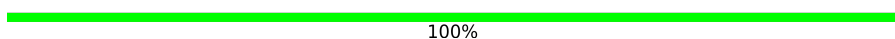


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2A: 



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

Chain 3A: 



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

Chain 4A: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	29935	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 ($e^-/\text{\AA}^2$)	36.75	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.862	Depositor
Minimum map value	-2.136	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.212	Depositor
Recommended contour level	0.637	Depositor
Map size (Å)	597.77997, 597.77997, 597.77997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.9925998, 1.9925998, 1.9925998	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, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/28074	0.36	0/38177
1	B	0.15	0/28072	0.34	0/38172
1	C	0.16	0/28074	0.35	0/38177
1	D	0.15	0/28077	0.35	1/38182 (0.0%)
1	E	0.16	0/28074	0.35	0/38177
1	F	0.15	0/28077	0.34	1/38182 (0.0%)
1	G	0.16	0/28073	0.35	0/38176
1	H	0.15	0/28077	0.36	2/38182 (0.0%)
1	I	0.16	0/28074	0.35	0/38177
1	J	0.15	0/28074	0.35	0/38175
1	K	0.16	0/28074	0.35	0/38177
1	L	0.16	0/28072	0.36	1/38172 (0.0%)
1	M	0.16	0/28074	0.35	0/38177
1	N	0.15	0/28077	0.35	1/38182 (0.0%)
1	O	0.16	0/28074	0.35	0/38177
1	P	0.15	0/28077	0.34	0/38182
1	Q	0.16	0/28073	0.35	0/38176
1	R	0.15	0/28077	0.35	1/38182 (0.0%)
1	S	0.16	0/28074	0.36	0/38177
1	T	0.15	0/28074	0.35	0/38175
All	All	0.16	0/561492	0.35	7/763554 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	2541	PRO	CA-N-CD	-6.58	102.78	112.00
1	H	3142	TYR	CA-CB-CG	5.96	124.63	113.90
1	N	1673	ARG	CB-CA-C	-5.33	110.45	116.63
1	F	745	ILE	N-CA-C	-5.31	108.33	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1673	ARG	CB-CA-C	-5.30	110.48	116.63

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	27308	0	26081	1005	0
1	B	27308	0	26066	1001	0
1	C	27308	0	26081	1000	0
1	D	27310	0	26071	1024	0
1	E	27308	0	26081	1001	0
1	F	27310	0	26071	1030	0
1	G	27307	0	26078	1041	0
1	H	27310	0	26071	1045	0
1	I	27308	0	26081	986	0
1	J	27309	0	26067	1015	0
1	K	27308	0	26081	995	0
1	L	27308	0	26066	1005	0
1	M	27308	0	26081	961	0
1	N	27310	0	26071	1001	0
1	O	27308	0	26081	960	0
1	P	27310	0	26071	1007	0
1	Q	27307	0	26078	1023	0
1	R	27310	0	26071	1075	0
1	S	27308	0	26081	985	0
1	T	27309	0	26068	1012	0
2	0	28	0	25	0	0
2	0A	28	0	25	1	0
2	2	28	0	25	0	0
2	5A	28	0	25	0	0
2	7	28	0	25	0	0
2	8	28	0	25	0	0
2	AA	28	0	25	0	0
2	CA	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	HA	28	0	25	0	0
2	IA	28	0	25	1	0
2	KA	28	0	25	1	0
2	MA	28	0	25	0	0
2	RA	28	0	25	0	0
2	SA	28	0	25	1	0
2	U	28	0	25	2	0
2	UA	28	0	25	0	0
2	W	28	0	25	0	0
2	WA	28	0	25	0	0
2	Y	28	0	25	0	0
2	bA	28	0	25	0	0
2	cA	28	0	25	0	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
2	eA	28	0	25	0	0
2	g	28	0	25	0	0
2	gA	28	0	25	0	0
2	i	28	0	25	0	0
2	lA	28	0	25	2	0
2	mA	28	0	25	0	0
2	n	28	0	25	0	0
2	o	28	0	25	0	0
2	oA	28	0	25	1	0
2	q	28	0	25	1	0
2	qA	28	0	25	0	0
2	s	28	0	25	0	0
2	vA	28	0	25	0	0
2	wA	28	0	25	0	0
2	x	28	0	25	0	0
2	y	28	0	25	0	0
2	yA	28	0	25	1	0
3	1	39	0	34	2	0
3	1A	39	0	34	1	0
3	2A	39	0	34	1	0
3	3	39	0	34	0	0
3	3A	39	0	34	0	0
3	4	39	0	34	0	0
3	4A	39	0	34	2	0
3	5	39	0	34	0	0
3	6	39	0	34	1	0
3	9	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BA	39	0	34	2	0
3	DA	39	0	34	0	0
3	EA	39	0	34	1	0
3	FA	39	0	34	0	0
3	GA	39	0	34	1	0
3	JA	39	0	34	1	0
3	LA	39	0	34	1	0
3	NA	39	0	34	0	0
3	OA	39	0	34	0	0
3	PA	39	0	34	0	0
3	QA	39	0	34	0	0
3	TA	39	0	34	0	0
3	V	39	0	34	1	0
3	VA	39	0	34	2	0
3	X	39	0	34	1	0
3	XA	39	0	34	0	0
3	YA	39	0	34	1	0
3	Z	39	0	34	1	0
3	ZA	39	0	34	0	0
3	a	39	0	34	1	0
3	aA	39	0	34	1	0
3	b	39	0	34	1	0
3	c	39	0	34	1	0
3	dA	39	0	34	1	0
3	f	39	0	34	1	0
3	fA	39	0	34	2	0
3	h	39	0	34	0	0
3	hA	39	0	34	1	0
3	iA	39	0	34	0	0
3	j	39	0	34	0	0
3	jA	39	0	34	1	0
3	k	39	0	34	0	0
3	kA	39	0	34	0	0
3	l	39	0	34	0	0
3	m	39	0	34	2	0
3	nA	39	0	34	1	0
3	p	39	0	34	2	0
3	pA	39	0	34	1	0
3	r	39	0	34	3	0
3	rA	39	0	34	2	0
3	sA	39	0	34	0	0
3	t	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	tA	39	0	34	0	0
3	u	39	0	34	0	0
3	uA	39	0	34	2	0
3	v	39	0	34	0	0
3	w	39	0	34	1	0
3	xA	39	0	34	0	0
3	z	39	0	34	1	0
3	zA	39	0	34	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	1	0
4	D	14	0	13	1	0
4	E	14	0	13	1	0
4	F	14	0	13	1	0
4	G	14	0	13	1	0
4	H	14	0	13	1	0
4	I	14	0	13	1	0
4	J	14	0	13	0	0
4	K	14	0	13	1	0
4	L	14	0	13	0	0
4	M	14	0	13	0	0
4	N	14	0	13	1	0
4	O	14	0	13	0	0
4	P	14	0	13	0	0
4	Q	14	0	13	0	0
4	R	14	0	13	1	0
4	S	14	0	13	0	0
4	T	14	0	13	3	0
All	All	549912	0	524797	19650	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 18.

The worst 5 of 19650 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:N:2720:GLN:HE22	1:N:2730:TYR:HB2	1.34	0.92
1:A:754:SER:HG	1:A:762:SER:HG	1.18	0.92
1:M:2533:ARG:NH2	1:M:2619:ASP:O	2.04	0.91
1:J:597:ARG:HH21	1:J:658:ARG:HB2	1.34	0.91
1:L:486:TYR:HB3	1:L:777:MET:HE1	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3377/3408 (99%)	3136 (93%)	241 (7%)	0	100	100
1	B	3382/3408 (99%)	3151 (93%)	231 (7%)	0	100	100
1	C	3377/3408 (99%)	3138 (93%)	238 (7%)	1 (0%)	100	100
1	D	3382/3408 (99%)	3141 (93%)	241 (7%)	0	100	100
1	E	3377/3408 (99%)	3143 (93%)	233 (7%)	1 (0%)	100	100
1	F	3382/3408 (99%)	3151 (93%)	231 (7%)	0	100	100
1	G	3377/3408 (99%)	3143 (93%)	234 (7%)	0	100	100
1	H	3382/3408 (99%)	3135 (93%)	247 (7%)	0	100	100
1	I	3377/3408 (99%)	3132 (93%)	244 (7%)	1 (0%)	100	100
1	J	3381/3408 (99%)	3128 (92%)	253 (8%)	0	100	100
1	K	3377/3408 (99%)	3146 (93%)	231 (7%)	0	100	100
1	L	3382/3408 (99%)	3147 (93%)	235 (7%)	0	100	100
1	M	3377/3408 (99%)	3130 (93%)	246 (7%)	1 (0%)	100	100
1	N	3382/3408 (99%)	3140 (93%)	242 (7%)	0	100	100
1	O	3377/3408 (99%)	3139 (93%)	238 (7%)	0	100	100
1	P	3382/3408 (99%)	3137 (93%)	245 (7%)	0	100	100
1	Q	3377/3408 (99%)	3139 (93%)	237 (7%)	1 (0%)	100	100
1	R	3382/3408 (99%)	3143 (93%)	239 (7%)	0	100	100
1	S	3377/3408 (99%)	3135 (93%)	241 (7%)	1 (0%)	100	100
1	T	3381/3408 (99%)	3159 (93%)	222 (7%)	0	100	100
All	All	67588/68160 (99%)	62813 (93%)	4769 (7%)	6 (0%)	100	100

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	1509	LEU
1	I	2477	ASN
1	E	2511	ILE
1	Q	2511	ILE
1	S	2511	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2965/2981 (100%)	2965 (100%)	0	100	100
1	B	2964/2981 (99%)	2963 (100%)	1 (0%)	100	100
1	C	2965/2981 (100%)	2965 (100%)	0	100	100
1	D	2965/2981 (100%)	2965 (100%)	0	100	100
1	E	2965/2981 (100%)	2965 (100%)	0	100	100
1	F	2965/2981 (100%)	2965 (100%)	0	100	100
1	G	2964/2981 (99%)	2964 (100%)	0	100	100
1	H	2965/2981 (100%)	2965 (100%)	0	100	100
1	I	2965/2981 (100%)	2965 (100%)	0	100	100
1	J	2964/2981 (99%)	2964 (100%)	0	100	100
1	K	2965/2981 (100%)	2965 (100%)	0	100	100
1	L	2964/2981 (99%)	2963 (100%)	1 (0%)	100	100
1	M	2965/2981 (100%)	2965 (100%)	0	100	100
1	N	2965/2981 (100%)	2965 (100%)	0	100	100
1	O	2965/2981 (100%)	2965 (100%)	0	100	100
1	P	2965/2981 (100%)	2965 (100%)	0	100	100
1	Q	2964/2981 (99%)	2964 (100%)	0	100	100
1	R	2965/2981 (100%)	2965 (100%)	0	100	100
1	S	2965/2981 (100%)	2965 (100%)	0	100	100
1	T	2964/2981 (99%)	2964 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	59294/59620 (100%)	59292 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	499	TRP
1	L	499	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1349 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	2752	ASN
1	R	61	HIS
1	O	914	HIS
1	N	2720	GLN
1	P	1490	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

260 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	$\# Z > 2$
2	NAG	0	1	1,2	14,14,15	1.05	1 (7%)	17,19,21	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	0	2	2	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	0A	1	1,2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	0A	2	2	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	1	1	1,3	14,14,15	1.06	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	1	2	3	14,14,15	0.22	0	17,19,21	0.57	0
3	BMA	1	3	3	11,11,12	0.46	0	15,15,17	0.78	0
3	NAG	1A	1	1,3	14,14,15	0.62	0	17,19,21	0.93	1 (5%)
3	NAG	1A	2	3	14,14,15	0.27	0	17,19,21	0.44	0
3	BMA	1A	3	3	11,11,12	0.59	0	15,15,17	0.73	0
2	NAG	2	1	1,2	14,14,15	0.26	0	17,19,21	0.54	0
2	NAG	2	2	2	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	2A	1	1,3	14,14,15	0.53	0	17,19,21	0.45	0
3	NAG	2A	2	3	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	2A	3	3	11,11,12	0.53	0	15,15,17	0.68	0
3	NAG	3	1	1,3	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
3	NAG	3	2	3	14,14,15	0.23	0	17,19,21	0.49	0
3	BMA	3	3	3	11,11,12	0.63	0	15,15,17	0.75	0
3	NAG	3A	1	1,3	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	3A	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	3A	3	3	11,11,12	0.55	0	15,15,17	0.78	0
3	NAG	4	1	1,3	14,14,15	0.45	0	17,19,21	0.43	0
3	NAG	4	2	3	14,14,15	0.30	0	17,19,21	0.51	0
3	BMA	4	3	3	11,11,12	0.57	0	15,15,17	0.77	0
3	NAG	4A	1	1,3	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
3	NAG	4A	2	3	14,14,15	0.86	1 (7%)	17,19,21	0.95	1 (5%)
3	BMA	4A	3	3	11,11,12	0.64	0	15,15,17	1.02	0
3	NAG	5	1	1,3	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	5	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	BMA	5	3	3	11,11,12	0.57	0	15,15,17	0.79	0
2	NAG	5A	1	1,2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	5A	2	2	14,14,15	0.51	0	17,19,21	1.25	1 (5%)
3	NAG	6	1	1,3	14,14,15	0.39	0	17,19,21	0.35	0
3	NAG	6	2	3	14,14,15	0.63	1 (7%)	17,19,21	1.41	1 (5%)
3	BMA	6	3	3	11,11,12	0.67	0	15,15,17	0.77	0
2	NAG	7	1	1,2	14,14,15	0.18	0	17,19,21	0.42	0
2	NAG	7	2	2	14,14,15	0.50	0	17,19,21	1.26	1 (5%)
2	NAG	8	1	1,2	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	8	2	2	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	9	1	1,3	14,14,15	0.54	0	17,19,21	0.76	1 (5%)
3	NAG	9	2	3	14,14,15	0.20	0	17,19,21	0.39	0
3	BMA	9	3	3	11,11,12	0.54	0	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	AA	1	1,2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	AA	2	2	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	BA	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	BA	2	3	14,14,15	0.23	0	17,19,21	0.60	0
3	BMA	BA	3	3	11,11,12	0.47	0	15,15,17	0.78	0
2	NAG	CA	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	1.43	1 (5%)
2	NAG	CA	2	2	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	DA	1	1,3	14,14,15	0.64	0	17,19,21	0.96	1 (5%)
3	NAG	DA	2	3	14,14,15	0.24	0	17,19,21	0.47	0
3	BMA	DA	3	3	11,11,12	0.59	0	15,15,17	0.81	0
3	NAG	EA	1	1,3	14,14,15	0.50	0	17,19,21	0.48	0
3	NAG	EA	2	3	14,14,15	0.27	0	17,19,21	0.49	0
3	BMA	EA	3	3	11,11,12	0.52	0	15,15,17	0.71	0
3	NAG	FA	1	1,3	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	FA	2	3	14,14,15	0.19	0	17,19,21	0.46	0
3	BMA	FA	3	3	11,11,12	0.51	0	15,15,17	0.81	0
3	NAG	GA	1	1,3	14,14,15	0.34	0	17,19,21	0.35	0
3	NAG	GA	2	3	14,14,15	0.60	1 (7%)	17,19,21	1.33	1 (5%)
3	BMA	GA	3	3	11,11,12	0.63	0	15,15,17	0.76	0
2	NAG	HA	1	1,2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	HA	2	2	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
2	NAG	IA	1	1,2	14,14,15	0.20	0	17,19,21	0.40	0
2	NAG	IA	2	2	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	JA	1	1,3	14,14,15	0.19	0	17,19,21	0.36	0
3	NAG	JA	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	BMA	JA	3	3	11,11,12	0.49	0	15,15,17	0.78	0
2	NAG	KA	1	1,2	14,14,15	0.38	0	17,19,21	0.65	1 (5%)
2	NAG	KA	2	2	14,14,15	0.27	0	17,19,21	0.47	0
3	NAG	LA	1	1,3	14,14,15	0.46	0	17,19,21	0.66	0
3	NAG	LA	2	3	14,14,15	0.18	0	17,19,21	0.49	0
3	BMA	LA	3	3	11,11,12	0.45	0	15,15,17	0.82	0
2	NAG	MA	1	1,2	14,14,15	0.26	0	17,19,21	0.53	0
2	NAG	MA	2	2	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	NA	1	1,3	14,14,15	0.61	0	17,19,21	0.95	1 (5%)
3	NAG	NA	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	BMA	NA	3	3	11,11,12	0.61	0	15,15,17	0.75	0
3	NAG	OA	1	1,3	14,14,15	0.44	0	17,19,21	0.41	0
3	NAG	OA	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	BMA	OA	3	3	11,11,12	0.58	0	15,15,17	0.77	0
3	NAG	PA	1	1,3	14,14,15	0.27	0	17,19,21	0.48	0
3	NAG	PA	2	3	14,14,15	0.19	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	PA	3	3	11,11,12	0.55	0	15,15,17	0.79	0
3	NAG	QA	1	1,3	14,14,15	0.28	0	17,19,21	0.40	0
3	NAG	QA	2	3	14,14,15	0.55	0	17,19,21	1.34	1 (5%)
3	BMA	QA	3	3	11,11,12	0.58	0	15,15,17	0.80	0
2	NAG	RA	1	1,2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	RA	2	2	14,14,15	0.50	0	17,19,21	1.25	1 (5%)
2	NAG	SA	1	1,2	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	SA	2	2	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	TA	1	1,3	14,14,15	0.18	0	17,19,21	0.39	0
3	NAG	TA	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	BMA	TA	3	3	11,11,12	0.54	0	15,15,17	0.76	0
2	NAG	U	1	1,2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	U	2	2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	UA	1	1,2	14,14,15	0.23	0	17,19,21	0.48	0
2	NAG	UA	2	2	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	V	1	1,3	14,14,15	0.14	0	17,19,21	0.39	0
3	NAG	V	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	BMA	V	3	3	11,11,12	0.49	0	15,15,17	0.78	0
3	NAG	VA	1	1,3	14,14,15	0.43	0	17,19,21	0.65	0
3	NAG	VA	2	3	14,14,15	0.17	0	17,19,21	0.50	0
3	BMA	VA	3	3	11,11,12	0.45	0	15,15,17	0.85	1 (6%)
2	NAG	W	1	1,2	14,14,15	0.21	0	17,19,21	0.50	0
2	NAG	W	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	WA	1	1,2	14,14,15	0.60	1 (7%)	17,19,21	0.69	0
2	NAG	WA	2	2	14,14,15	0.21	0	17,19,21	0.49	0
3	NAG	X	1	1,3	14,14,15	1.10	1 (7%)	17,19,21	0.96	1 (5%)
3	NAG	X	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	BMA	X	3	3	11,11,12	0.47	0	15,15,17	0.76	0
3	NAG	XA	1	1,3	14,14,15	0.62	0	17,19,21	0.93	1 (5%)
3	NAG	XA	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	BMA	XA	3	3	11,11,12	0.56	0	15,15,17	0.79	0
2	NAG	Y	1	1,2	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	Y	2	2	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	YA	1	1,3	14,14,15	0.54	0	17,19,21	0.47	0
3	NAG	YA	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	BMA	YA	3	3	11,11,12	0.54	0	15,15,17	0.72	0
3	NAG	Z	1	1,3	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	Z	2	3	14,14,15	0.25	0	17,19,21	0.45	0
3	BMA	Z	3	3	11,11,12	0.61	0	15,15,17	0.74	0
3	NAG	ZA	1	1,3	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	ZA	2	3	14,14,15	0.19	0	17,19,21	0.45	0
3	BMA	ZA	3	3	11,11,12	0.51	0	15,15,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	a	1	1,3	14,14,15	0.42	0	17,19,21	0.42	0
3	NAG	a	2	3	14,14,15	0.31	0	17,19,21	0.49	0
3	BMA	a	3	3	11,11,12	0.53	0	15,15,17	0.77	0
3	NAG	aA	1	1,3	14,14,15	0.36	0	17,19,21	0.37	0
3	NAG	aA	2	3	14,14,15	0.64	1 (7%)	17,19,21	1.33	1 (5%)
3	BMA	aA	3	3	11,11,12	0.63	0	15,15,17	0.77	0
3	NAG	b	1	1,3	14,14,15	0.32	0	17,19,21	0.48	0
3	NAG	b	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	BMA	b	3	3	11,11,12	0.56	0	15,15,17	0.83	0
2	NAG	bA	1	1,2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	bA	2	2	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
3	NAG	c	1	1,3	14,14,15	0.35	0	17,19,21	0.38	0
3	NAG	c	2	3	14,14,15	0.42	0	17,19,21	1.32	1 (5%)
3	BMA	c	3	3	11,11,12	0.62	0	15,15,17	0.78	0
2	NAG	cA	1	1,2	14,14,15	0.22	0	17,19,21	0.48	0
2	NAG	cA	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	NAG	d	1	1,2	14,14,15	0.45	0	17,19,21	0.56	0
2	NAG	d	2	2	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	dA	1	1,3	14,14,15	0.15	0	17,19,21	0.39	0
3	NAG	dA	2	3	14,14,15	0.22	0	17,19,21	0.40	0
3	BMA	dA	3	3	11,11,12	0.50	0	15,15,17	0.79	0
2	NAG	e	1	1,2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	e	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	eA	1	1,2	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	eA	2	2	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	f	1	1,3	14,14,15	0.18	0	17,19,21	0.38	0
3	NAG	f	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	BMA	f	3	3	11,11,12	0.52	0	15,15,17	0.77	0
3	NAG	fA	1	1,3	14,14,15	0.44	0	17,19,21	0.64	0
3	NAG	fA	2	3	14,14,15	0.19	0	17,19,21	0.47	0
3	BMA	fA	3	3	11,11,12	0.48	0	15,15,17	0.82	0
2	NAG	g	1	1,2	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	g	2	2	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	gA	1	1,2	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	gA	2	2	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	h	1	1,3	14,14,15	0.99	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	h	2	3	14,14,15	0.22	0	17,19,21	0.58	0
3	BMA	h	3	3	11,11,12	0.47	0	15,15,17	0.76	0
3	NAG	hA	1	1,3	14,14,15	0.18	0	17,19,21	0.48	0
3	NAG	hA	2	3	14,14,15	0.24	0	17,19,21	0.44	0
3	BMA	hA	3	3	11,11,12	0.62	0	15,15,17	0.74	0
2	NAG	i	1	1,2	14,14,15	0.63	1 (7%)	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	i	2	2	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	iA	1	1,3	14,14,15	0.43	0	17,19,21	0.41	0
3	NAG	iA	2	3	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	iA	3	3	11,11,12	0.53	0	15,15,17	0.78	0
3	NAG	j	1	1,3	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	j	2	3	14,14,15	0.26	0	17,19,21	0.44	0
3	BMA	j	3	3	11,11,12	0.62	0	15,15,17	0.78	0
3	NAG	jA	1	1,3	14,14,15	0.30	0	17,19,21	0.48	0
3	NAG	jA	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	jA	3	3	11,11,12	0.56	0	15,15,17	0.81	0
3	NAG	k	1	1,3	14,14,15	0.46	0	17,19,21	0.43	0
3	NAG	k	2	3	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	k	3	3	11,11,12	0.53	0	15,15,17	0.74	0
3	NAG	kA	1	1,3	14,14,15	0.25	0	17,19,21	0.38	0
3	NAG	kA	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	BMA	kA	3	3	11,11,12	0.55	0	15,15,17	0.71	0
3	NAG	l	1	1,3	14,14,15	0.32	0	17,19,21	0.50	0
3	NAG	l	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	BMA	l	3	3	11,11,12	0.56	0	15,15,17	0.78	0
2	NAG	lA	1	1,2	14,14,15	0.44	0	17,19,21	0.65	0
2	NAG	lA	2	2	14,14,15	0.59	1 (7%)	17,19,21	1.23	1 (5%)
3	NAG	m	1	1,3	14,14,15	0.28	0	17,19,21	0.37	0
3	NAG	m	2	3	14,14,15	0.51	0	17,19,21	1.37	1 (5%)
3	BMA	m	3	3	11,11,12	0.57	0	15,15,17	0.76	0
2	NAG	mA	1	1,2	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	mA	2	2	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	n	1	1,2	14,14,15	0.18	0	17,19,21	0.39	0
2	NAG	n	2	2	14,14,15	0.50	0	17,19,21	1.27	1 (5%)
3	NAG	nA	1	1,3	14,14,15	0.17	0	17,19,21	0.38	0
3	NAG	nA	2	3	14,14,15	0.25	0	17,19,21	0.43	0
3	BMA	nA	3	3	11,11,12	0.53	0	15,15,17	0.78	0
2	NAG	o	1	1,2	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	o	2	2	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	oA	1	1,2	14,14,15	0.19	0	17,19,21	0.50	0
2	NAG	oA	2	2	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	p	1	1,3	14,14,15	0.15	0	17,19,21	0.42	0
3	NAG	p	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	BMA	p	3	3	11,11,12	0.55	0	15,15,17	0.75	0
3	NAG	pA	1	1,3	14,14,15	0.46	0	17,19,21	0.66	0
3	NAG	pA	2	3	14,14,15	0.19	0	17,19,21	0.48	0
3	BMA	pA	3	3	11,11,12	0.47	0	15,15,17	0.88	1 (6%)
2	NAG	q	1	1,2	14,14,15	0.29	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	q	2	2	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	qA	1	1,2	14,14,15	0.28	0	17,19,21	0.55	0
2	NAG	qA	2	2	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	r	1	1,3	14,14,15	1.00	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	r	2	3	14,14,15	0.23	0	17,19,21	0.55	0
3	BMA	r	3	3	11,11,12	0.52	0	15,15,17	0.78	0
3	NAG	rA	1	1,3	14,14,15	0.21	0	17,19,21	0.49	0
3	NAG	rA	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	BMA	rA	3	3	11,11,12	0.56	0	15,15,17	0.84	0
2	NAG	s	1	1,2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	s	2	2	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	sA	1	1,3	14,14,15	0.47	0	17,19,21	0.42	0
3	NAG	sA	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	BMA	sA	3	3	11,11,12	0.54	0	15,15,17	0.74	0
3	NAG	t	1	1,3	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	t	2	3	14,14,15	0.28	0	17,19,21	0.48	0
3	BMA	t	3	3	11,11,12	0.63	0	15,15,17	0.72	0
3	NAG	tA	1	1,3	14,14,15	0.33	0	17,19,21	0.49	0
3	NAG	tA	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	BMA	tA	3	3	11,11,12	0.58	0	15,15,17	0.79	0
3	NAG	u	1	1,3	14,14,15	0.49	0	17,19,21	0.44	0
3	NAG	u	2	3	14,14,15	0.31	0	17,19,21	0.50	0
3	BMA	u	3	3	11,11,12	0.58	0	15,15,17	0.75	0
3	NAG	uA	1	1,3	14,14,15	0.30	0	17,19,21	0.36	0
3	NAG	uA	2	3	14,14,15	0.53	0	17,19,21	1.37	1 (5%)
3	BMA	uA	3	3	11,11,12	0.59	0	15,15,17	0.76	0
3	NAG	v	1	1,3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	v	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	v	3	3	11,11,12	0.56	0	15,15,17	0.78	0
2	NAG	vA	1	1,2	14,14,15	0.18	0	17,19,21	0.43	0
2	NAG	vA	2	2	14,14,15	0.54	0	17,19,21	1.26	1 (5%)
3	NAG	w	1	1,3	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
3	NAG	w	2	3	14,14,15	0.37	0	17,19,21	0.50	0
3	BMA	w	3	3	11,11,12	0.54	0	15,15,17	0.76	0
2	NAG	wA	1	1,2	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	wA	2	2	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	x	1	1,2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	x	2	2	14,14,15	0.51	0	17,19,21	1.24	1 (5%)
3	NAG	xA	1	1,3	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	xA	2	3	14,14,15	0.16	0	17,19,21	0.47	0
3	BMA	xA	3	3	11,11,12	0.58	0	15,15,17	0.76	0
2	NAG	y	1	1,2	14,14,15	0.25	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	y	2	2	14,14,15	0.27	0	17,19,21	0.47	0
2	NAG	yA	1	1,2	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	yA	2	2	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	z	1	1,3	14,14,15	0.17	0	17,19,21	0.39	0
3	NAG	z	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	BMA	z	3	3	11,11,12	0.51	0	15,15,17	0.75	0
3	NAG	zA	1	1,3	14,14,15	1.04	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	zA	2	3	14,14,15	0.22	0	17,19,21	0.53	0
3	BMA	zA	3	3	11,11,12	0.49	0	15,15,17	0.78	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
2	NAG	0	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	0	2	2	-	2/6/23/26	0/1/1/1
2	NAG	0A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	0A	2	2	-	2/6/23/26	0/1/1/1
3	NAG	1	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	1	2	3	-	2/6/23/26	0/1/1/1
3	BMA	1	3	3	-	2/2/19/22	0/1/1/1
3	NAG	1A	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	1A	2	3	-	2/6/23/26	0/1/1/1
3	BMA	1A	3	3	-	0/2/19/22	0/1/1/1
2	NAG	2	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	2	2	2	-	2/6/23/26	0/1/1/1
3	NAG	2A	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	2A	2	3	-	3/6/23/26	0/1/1/1
3	BMA	2A	3	3	-	1/2/19/22	0/1/1/1
3	NAG	3	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	3	2	3	-	3/6/23/26	0/1/1/1
3	BMA	3	3	3	-	0/2/19/22	0/1/1/1
3	NAG	3A	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	3A	2	3	-	2/6/23/26	0/1/1/1
3	BMA	3A	3	3	-	0/2/19/22	0/1/1/1
3	NAG	4	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	4	2	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	4	3	3	-	0/2/19/22	0/1/1/1
3	NAG	4A	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	4A	2	3	-	4/6/23/26	0/1/1/1
3	BMA	4A	3	3	-	2/2/19/22	0/1/1/1
3	NAG	5	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	5	2	3	-	2/6/23/26	0/1/1/1
3	BMA	5	3	3	-	0/2/19/22	0/1/1/1
2	NAG	5A	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	5A	2	2	-	2/6/23/26	0/1/1/1
3	NAG	6	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	6	2	3	-	2/6/23/26	0/1/1/1
3	BMA	6	3	3	-	1/2/19/22	0/1/1/1
2	NAG	7	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	7	2	2	-	2/6/23/26	0/1/1/1
2	NAG	8	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	8	2	2	-	0/6/23/26	0/1/1/1
3	NAG	9	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	9	2	3	-	2/6/23/26	0/1/1/1
3	BMA	9	3	3	-	0/2/19/22	0/1/1/1
2	NAG	AA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	BA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	BA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	BA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	CA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	CA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	DA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	DA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	DA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	EA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	EA	2	3	-	3/6/23/26	0/1/1/1
3	BMA	EA	3	3	-	1/2/19/22	0/1/1/1
3	NAG	FA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	FA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	FA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	GA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	GA	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	GA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	HA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	HA	2	2	-	3/6/23/26	0/1/1/1
2	NAG	IA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	IA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	JA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	JA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	JA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	KA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	KA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	LA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	LA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	LA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	MA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	NA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	NA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	NA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	OA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	OA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	OA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	PA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	PA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	PA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	QA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	QA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	QA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	RA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	RA	2	2	-	3/6/23/26	0/1/1/1
2	NAG	SA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	SA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	TA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	TA	2	3	-	0/6/23/26	0/1/1/1
3	BMA	TA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	U	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	U	2	2	-	1/6/23/26	0/1/1/1
2	NAG	UA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	UA	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	V	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
3	NAG	VA	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	VA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	VA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	WA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	WA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	NAG	XA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	XA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	XA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
3	NAG	YA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	YA	2	3	-	3/6/23/26	0/1/1/1
3	BMA	YA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	Z	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Z	3	3	-	0/2/19/22	0/1/1/1
3	NAG	ZA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	ZA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	ZA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	a	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	a	2	3	-	4/6/23/26	0/1/1/1
3	BMA	a	3	3	-	0/2/19/22	0/1/1/1
3	NAG	aA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	aA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	aA	3	3	-	1/2/19/22	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	BMA	b	3	3	-	0/2/19/22	0/1/1/1
2	NAG	bA	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	bA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	c	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	BMA	c	3	3	-	1/2/19/22	0/1/1/1
2	NAG	cA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	cA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	1/6/23/26	0/1/1/1
3	NAG	dA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	dA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	dA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	e	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	NAG	eA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	eA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	f	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	BMA	f	3	3	-	0/2/19/22	0/1/1/1
3	NAG	fA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	fA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	fA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	g	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	NAG	gA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	gA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	h	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
3	NAG	hA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	hA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	hA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	i	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	i	2	2	-	2/6/23/26	0/1/1/1
3	NAG	iA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	iA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	iA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	j	1	1,3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1
3	BMA	j	3	3	-	0/2/19/22	0/1/1/1
3	NAG	jA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	jA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	jA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	k	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	k	2	3	-	4/6/23/26	0/1/1/1
3	BMA	k	3	3	-	0/2/19/22	0/1/1/1
3	NAG	kA	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	kA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	kA	3	3	-	2/2/19/22	0/1/1/1
3	NAG	l	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	BMA	l	3	3	-	2/2/19/22	0/1/1/1
2	NAG	lA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	lA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	m	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	2/6/23/26	0/1/1/1
3	BMA	m	3	3	-	1/2/19/22	0/1/1/1
2	NAG	mA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	mA	2	2	-	0/6/23/26	0/1/1/1
2	NAG	n	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	n	2	2	-	2/6/23/26	0/1/1/1
3	NAG	nA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	nA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	nA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	o	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	o	2	2	-	1/6/23/26	0/1/1/1
2	NAG	oA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	oA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	p	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	p	2	3	-	2/6/23/26	0/1/1/1
3	BMA	p	3	3	-	0/2/19/22	0/1/1/1
3	NAG	pA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	pA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	pA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	q	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	qA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	qA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	r	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	2/6/23/26	0/1/1/1
3	BMA	r	3	3	-	0/2/19/22	0/1/1/1
3	NAG	rA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	rA	2	3	-	3/6/23/26	0/1/1/1
3	BMA	rA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	s	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	s	2	2	-	2/6/23/26	0/1/1/1
3	NAG	sA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	sA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	sA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	t	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	t	2	3	-	2/6/23/26	0/1/1/1
3	BMA	t	3	3	-	0/2/19/22	0/1/1/1
3	NAG	tA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	tA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	tA	3	3	-	2/2/19/22	0/1/1/1
3	NAG	u	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	u	2	3	-	4/6/23/26	0/1/1/1
3	BMA	u	3	3	-	0/2/19/22	0/1/1/1
3	NAG	uA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	uA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	uA	3	3	-	1/2/19/22	0/1/1/1
3	NAG	v	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	v	2	3	-	2/6/23/26	0/1/1/1
3	BMA	v	3	3	-	0/2/19/22	0/1/1/1
2	NAG	vA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	vA	2	2	-	4/6/23/26	0/1/1/1
3	NAG	w	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	w	2	3	-	2/6/23/26	0/1/1/1
3	BMA	w	3	3	-	1/2/19/22	0/1/1/1
2	NAG	wA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	wA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	x	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	x	2	2	-	2/6/23/26	0/1/1/1
3	NAG	xA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	xA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	xA	3	3	-	2/2/19/22	0/1/1/1
2	NAG	y	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	y	2	2	-	0/6/23/26	0/1/1/1
2	NAG	yA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	yA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	z	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	z	2	3	-	2/6/23/26	0/1/1/1
3	BMA	z	3	3	-	0/2/19/22	0/1/1/1
3	NAG	zA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	zA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	zA	3	3	-	0/2/19/22	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	1	NAG	O5-C1	-3.78	1.37	1.43
3	1	1	NAG	O5-C1	-3.68	1.37	1.43
3	BA	1	NAG	O5-C1	-3.66	1.37	1.43
3	zA	1	NAG	O5-C1	-3.57	1.37	1.43
2	0	1	NAG	O5-C1	-3.53	1.37	1.43

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	2	NAG	C1-O5-C5	5.32	119.32	112.19
3	m	2	NAG	C1-O5-C5	5.16	119.10	112.19
2	CA	1	NAG	C1-O5-C5	5.15	119.09	112.19
3	uA	2	NAG	C1-O5-C5	5.14	119.08	112.19
3	QA	2	NAG	C1-O5-C5	5.12	119.04	112.19

There are no chirality outliers.

5 of 421 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	pA	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	i	2	NAG	C4-C5-C6-O6
2	WA	2	NAG	C4-C5-C6-O6
3	fA	2	NAG	C4-C5-C6-O6

There are no ring outliers.

66 monomers are involved in 59 short contacts:

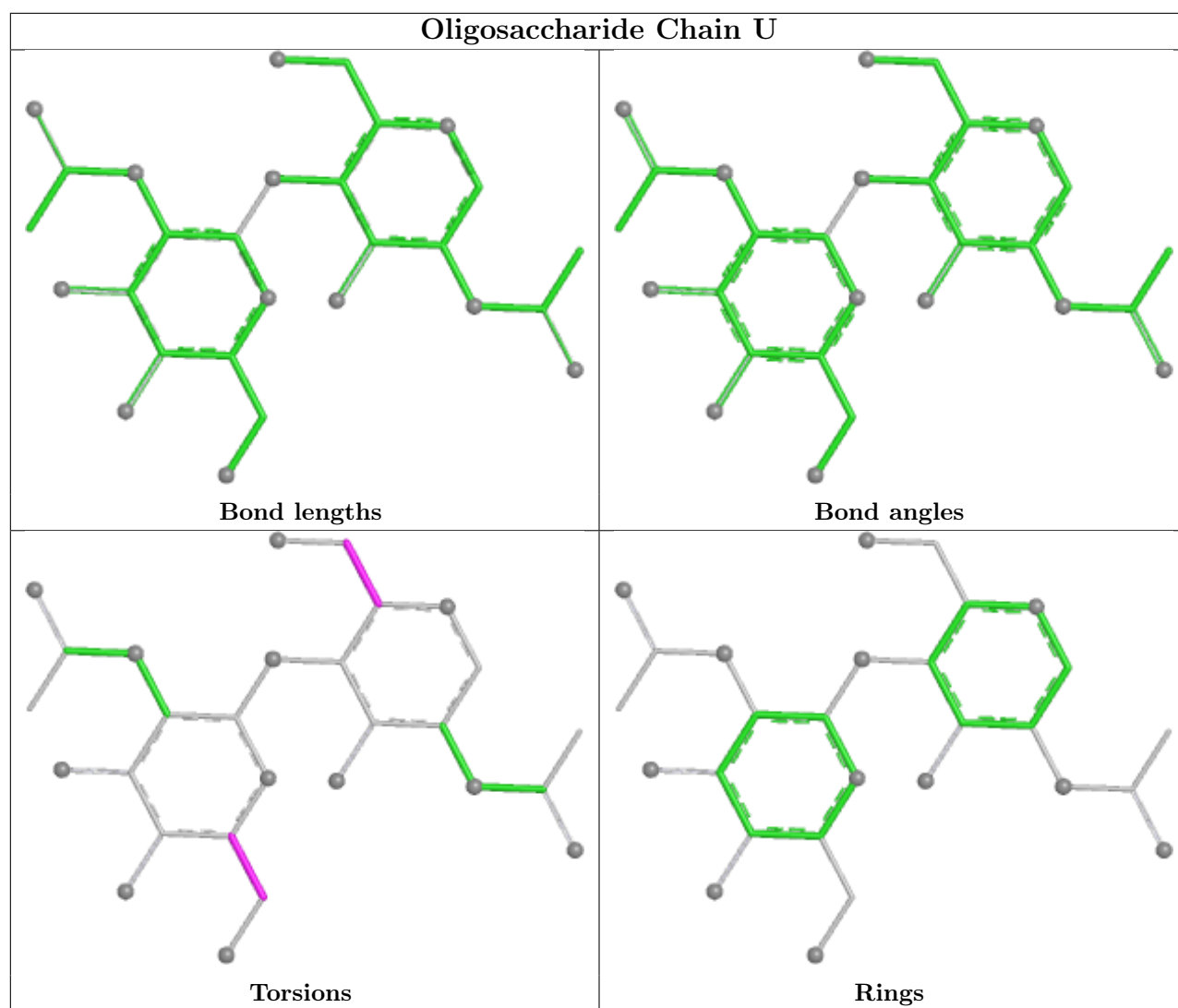
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4A	1	NAG	2	0
3	Z	2	NAG	1	0
3	rA	1	NAG	1	0
3	t	2	NAG	1	0
3	b	2	NAG	1	0
2	q	1	NAG	1	0
3	2A	1	NAG	1	0
3	1	1	NAG	2	0
3	LA	2	NAG	1	0
3	X	2	NAG	1	0
2	lA	1	NAG	2	0
3	zA	1	NAG	1	0
3	1A	2	NAG	1	0
3	r	2	NAG	1	0
3	r	1	NAG	3	0
3	VA	2	NAG	2	0
3	fA	2	NAG	2	0
3	m	2	NAG	1	0
3	V	1	NAG	1	0
3	t	1	NAG	1	0
3	BA	1	NAG	1	0
3	hA	3	BMA	1	0
3	JA	1	NAG	1	0
3	YA	1	NAG	1	0
3	jA	2	NAG	1	0
3	f	1	NAG	1	0
2	0A	1	NAG	1	0
3	LA	1	NAG	1	0
3	VA	1	NAG	2	0
3	p	1	NAG	2	0
3	X	1	NAG	1	0
3	1	2	NAG	1	0
2	oA	1	NAG	1	0
3	Z	3	BMA	1	0

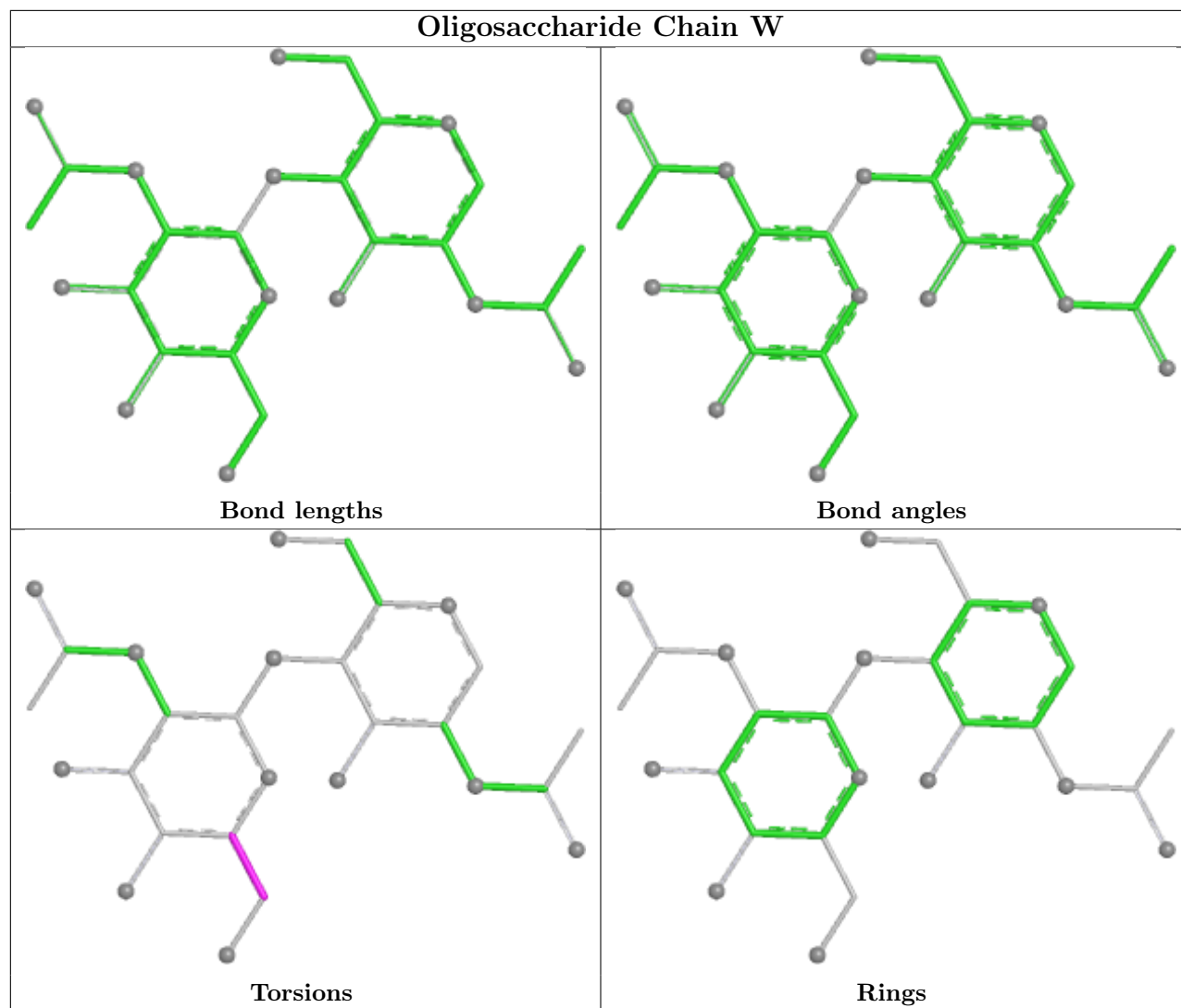
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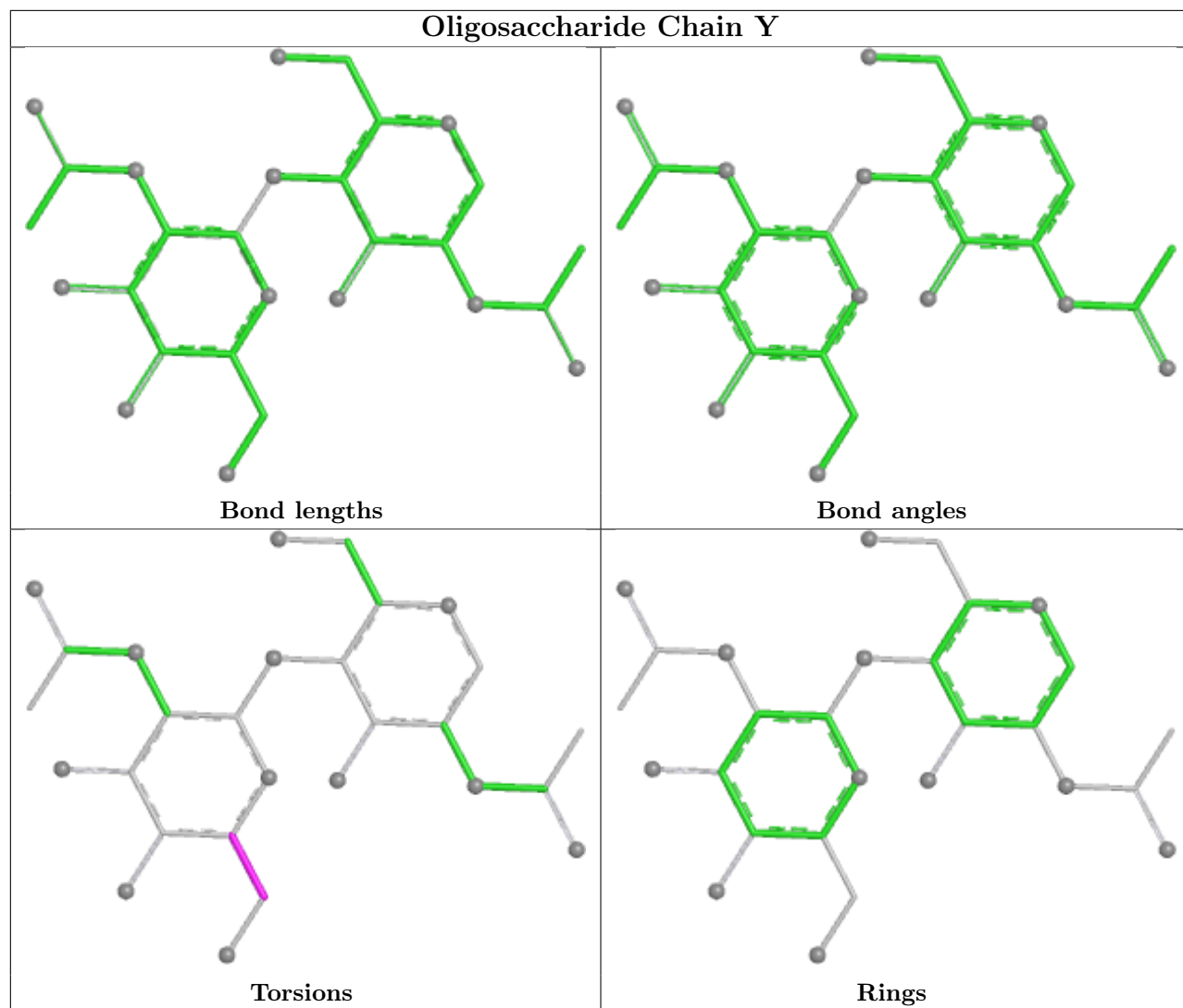
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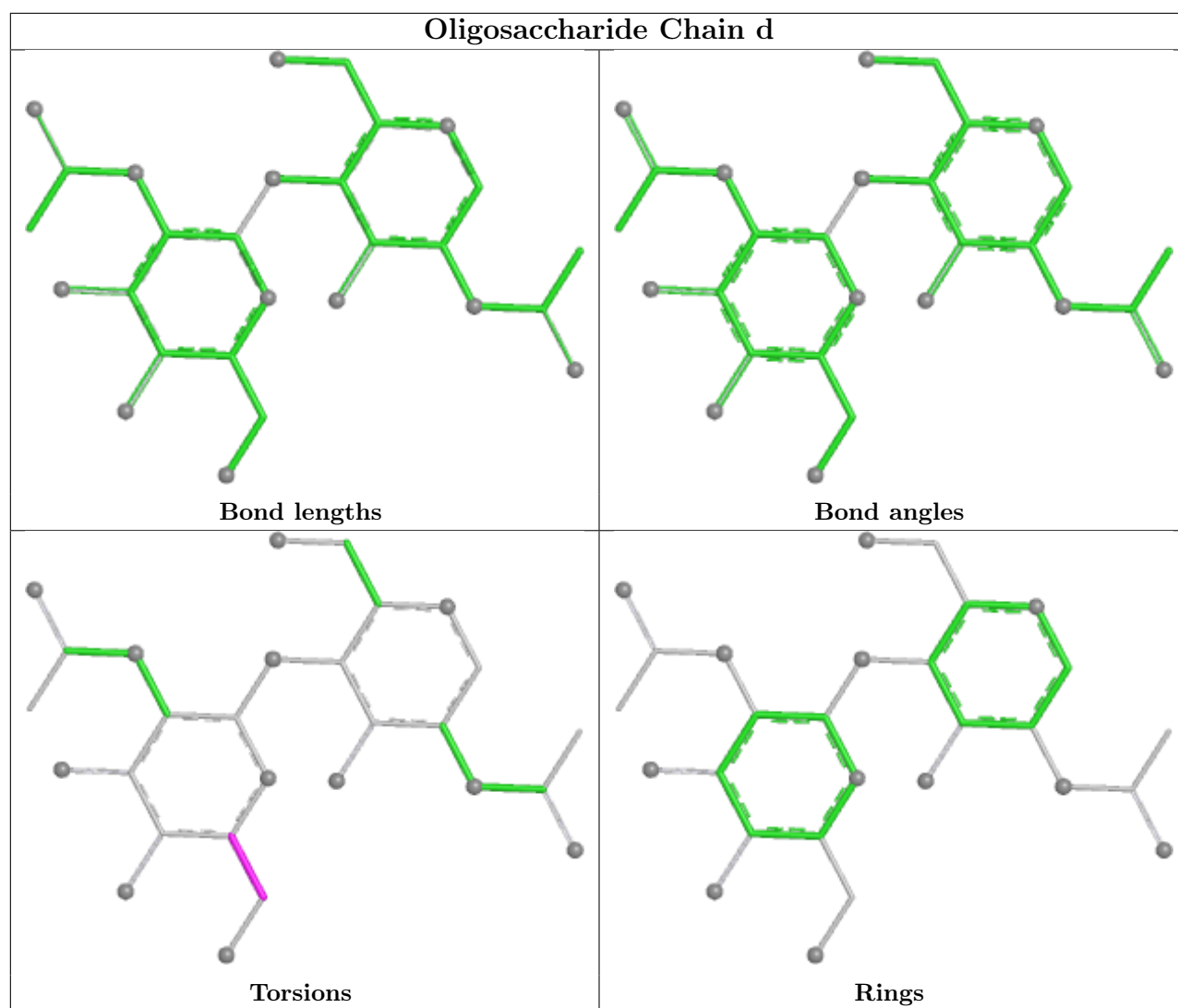
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	EA	1	NAG	1	0
3	aA	1	NAG	1	0
2	U	1	NAG	2	0
3	uA	1	NAG	2	0
3	zA	2	NAG	1	0
3	fA	1	NAG	2	0
2	SA	1	NAG	1	0
3	rA	3	BMA	1	0
3	z	1	NAG	1	0
3	t	3	BMA	1	0
3	hA	2	NAG	1	0
3	m	1	NAG	2	0
3	uA	2	NAG	1	0
2	yA	1	NAG	1	0
3	c	1	NAG	1	0
2	KA	1	NAG	1	0
3	4A	2	NAG	2	0
3	w	1	NAG	1	0
2	lA	2	NAG	1	0
2	CA	1	NAG	1	0
3	6	1	NAG	1	0
3	pA	1	NAG	1	0
3	c	2	NAG	1	0
3	BA	2	NAG	1	0
3	a	1	NAG	1	0
3	rA	2	NAG	1	0
3	nA	1	NAG	1	0
3	lA	3	BMA	1	0
3	pA	2	NAG	1	0
2	IA	1	NAG	1	0
3	dA	1	NAG	1	0
3	GA	1	NAG	1	0

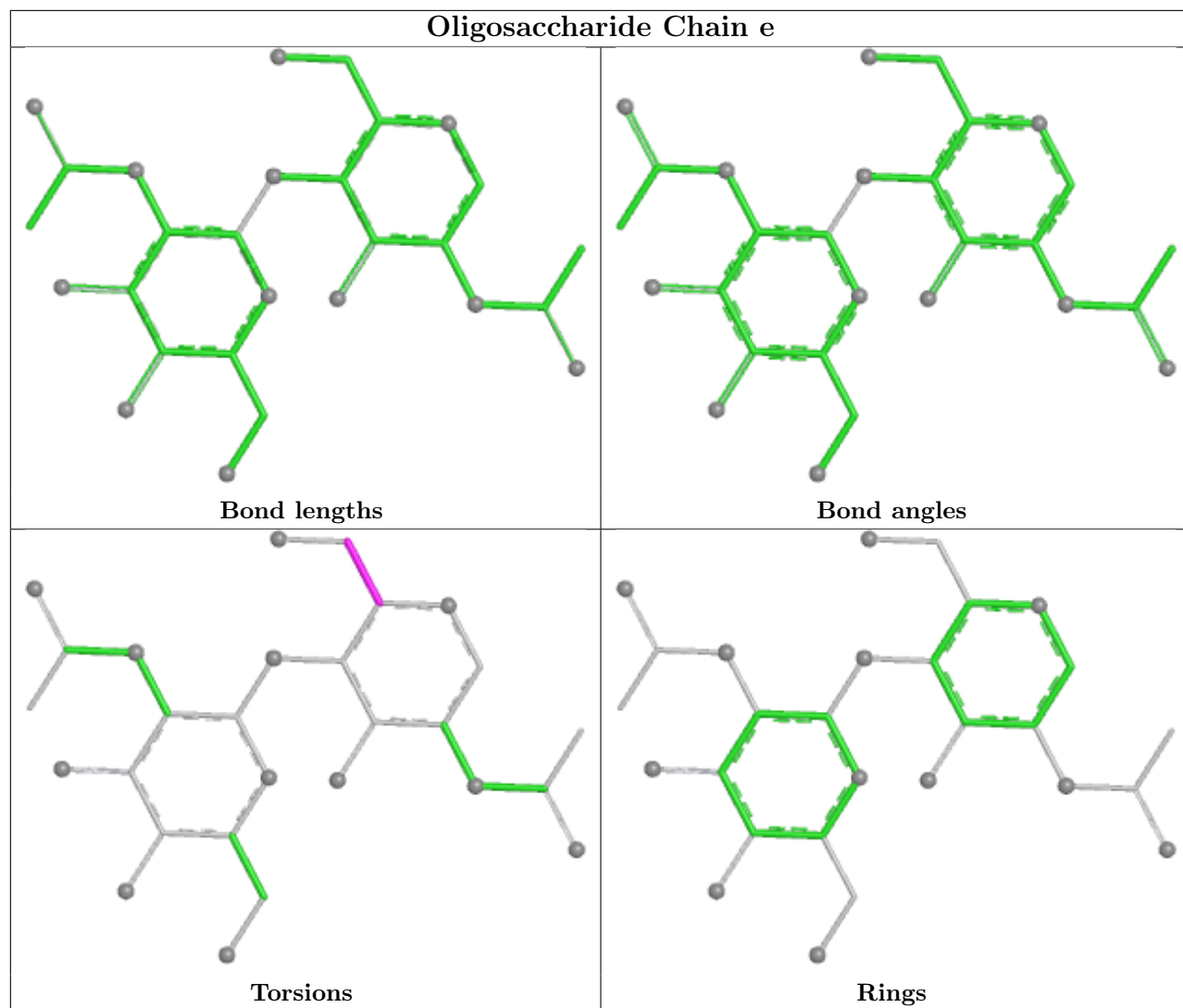
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

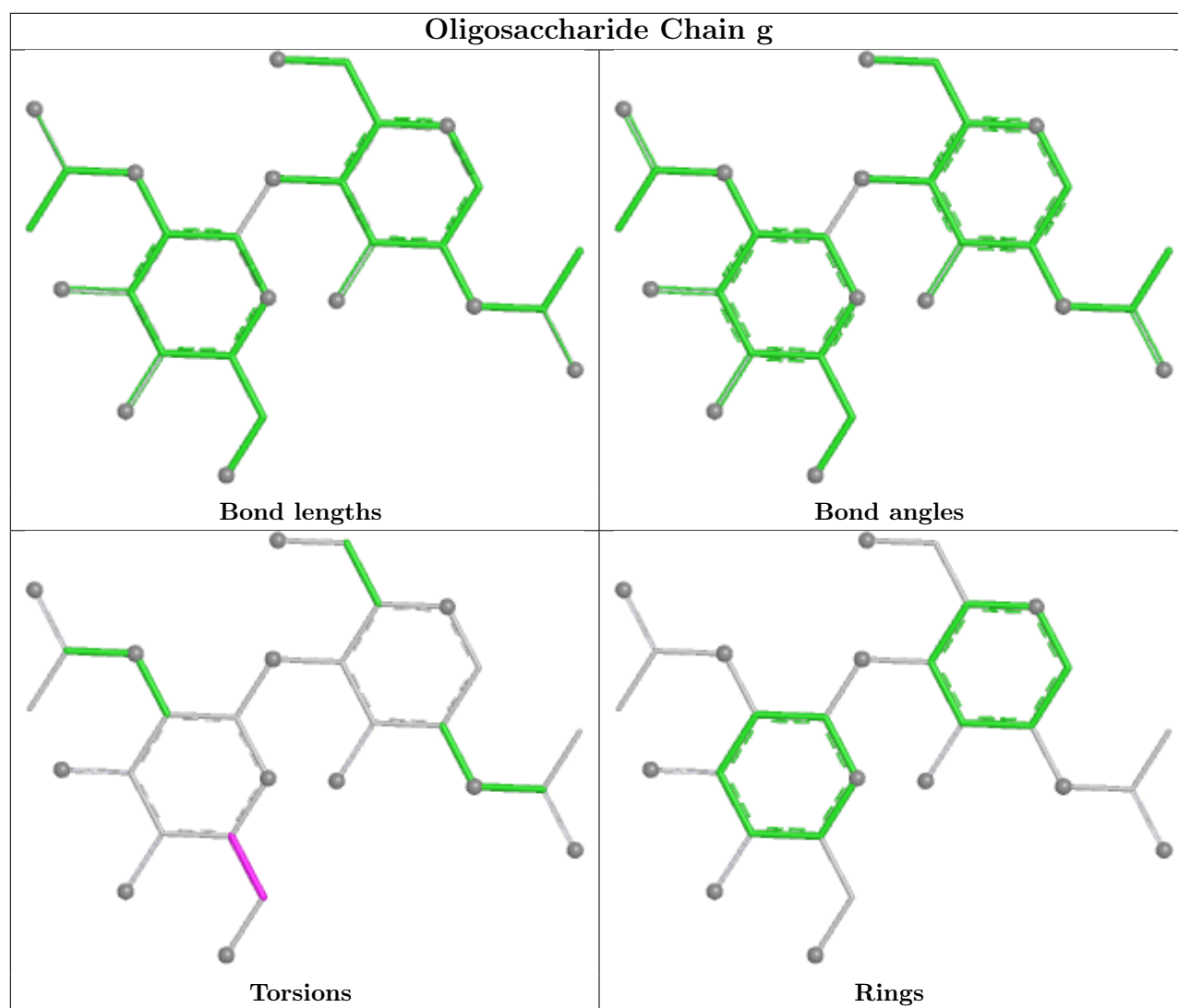


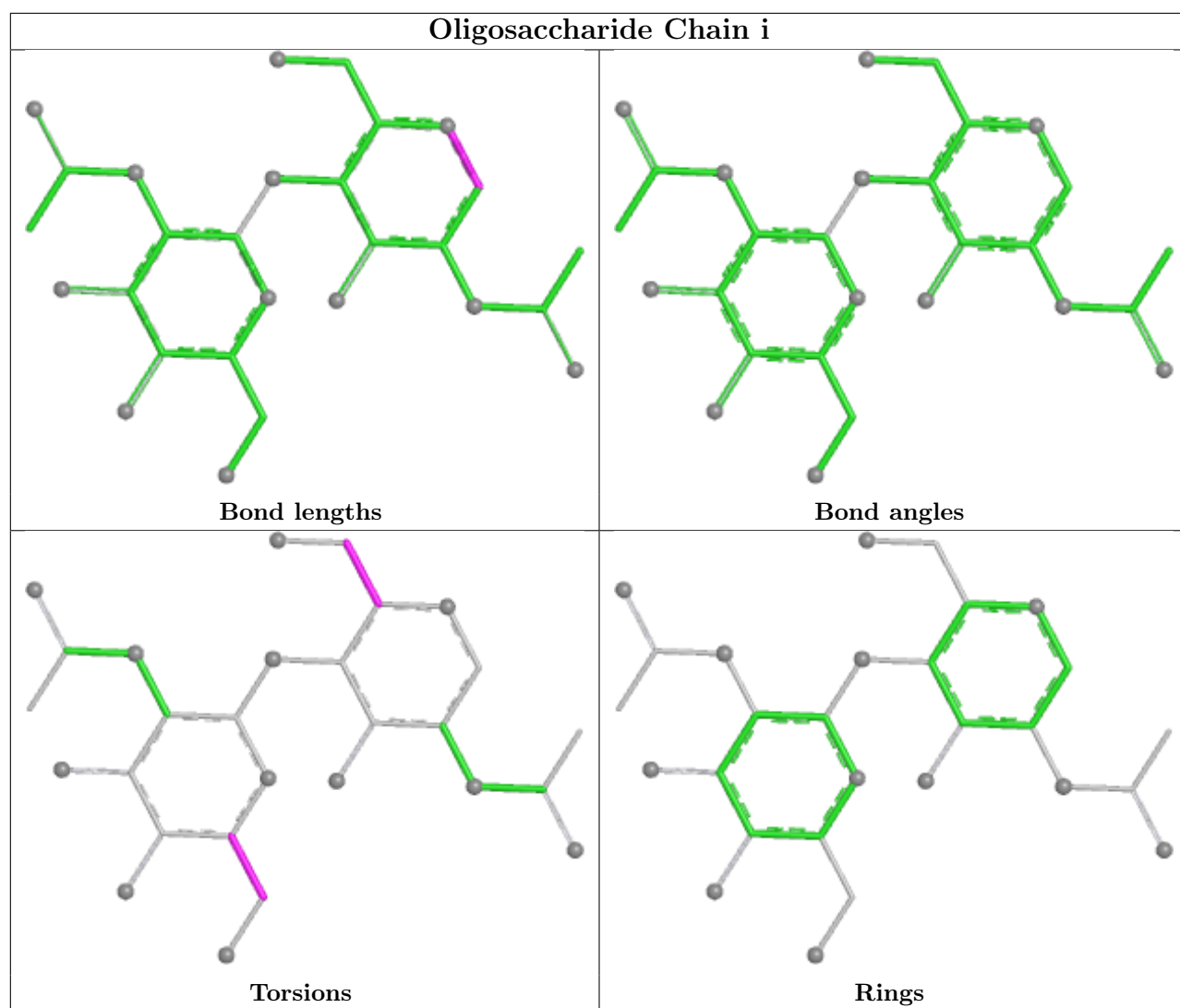


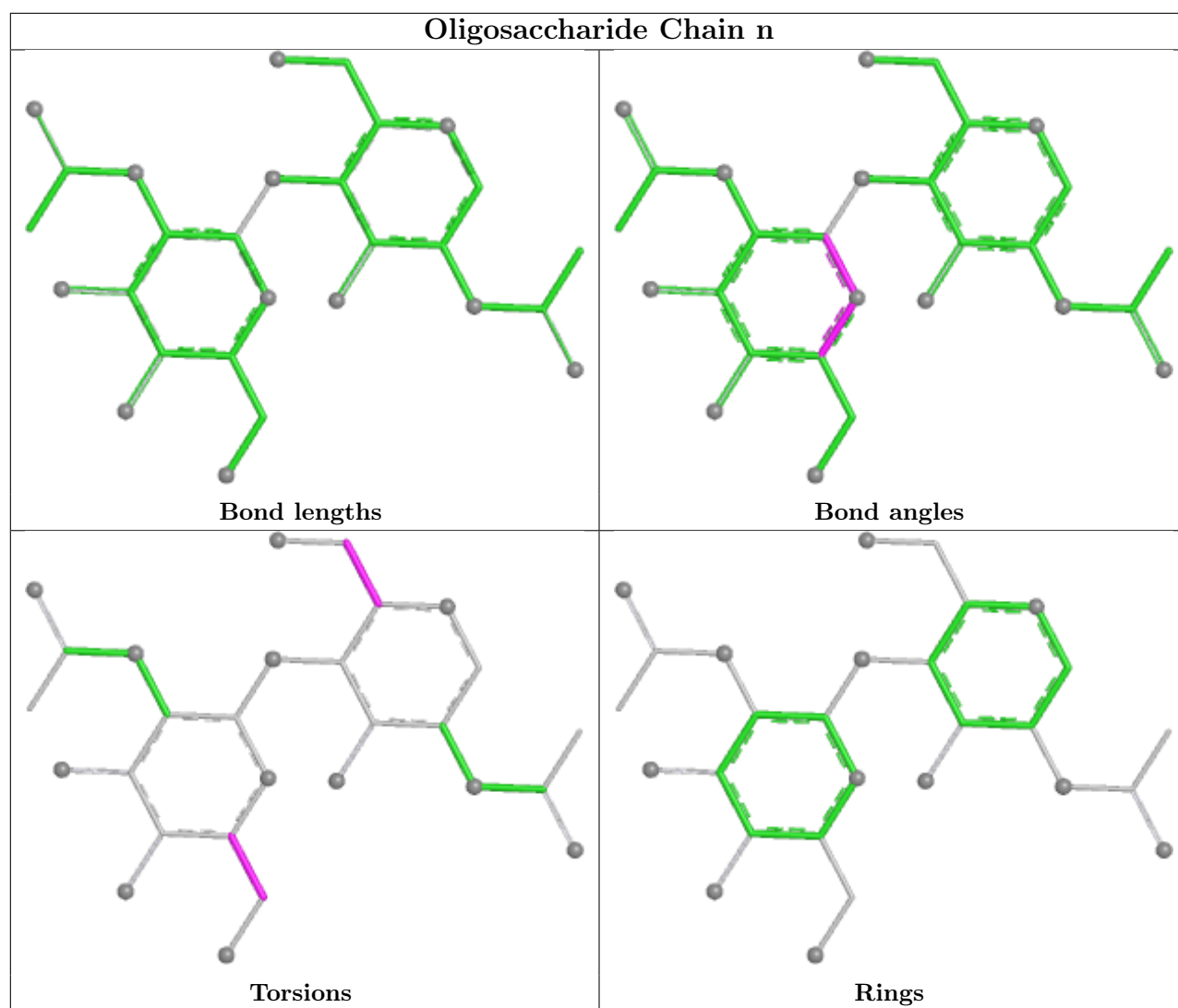


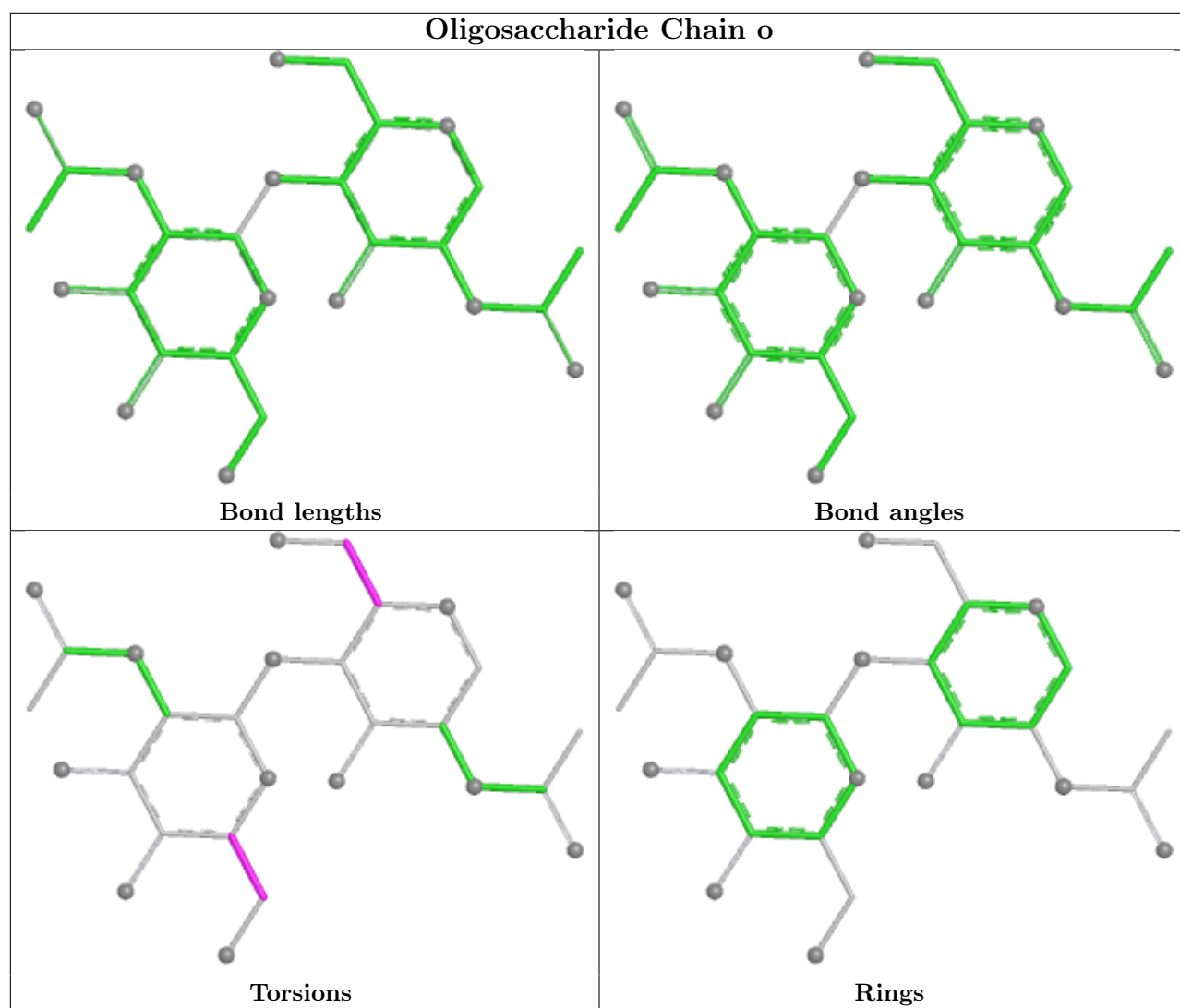


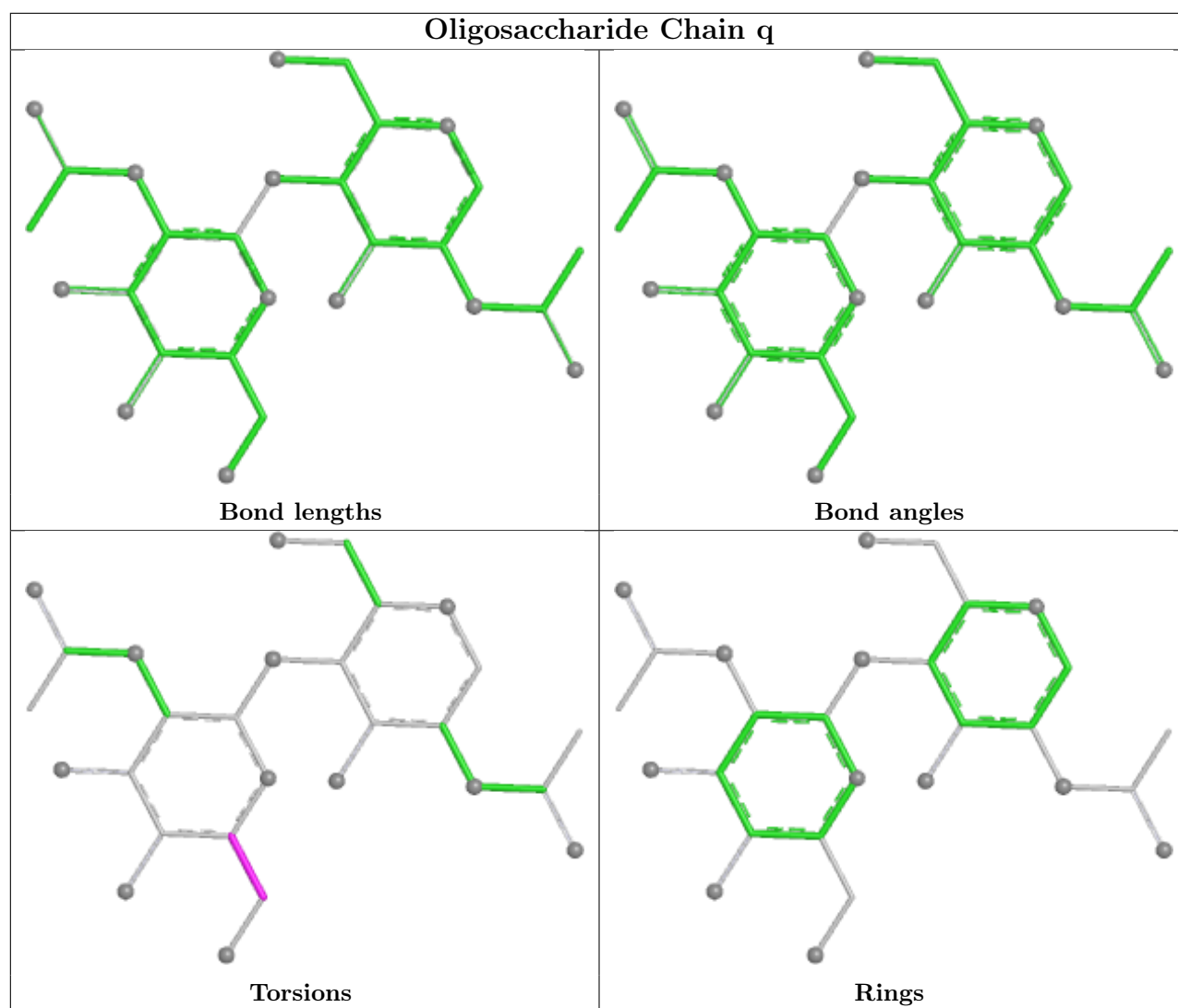


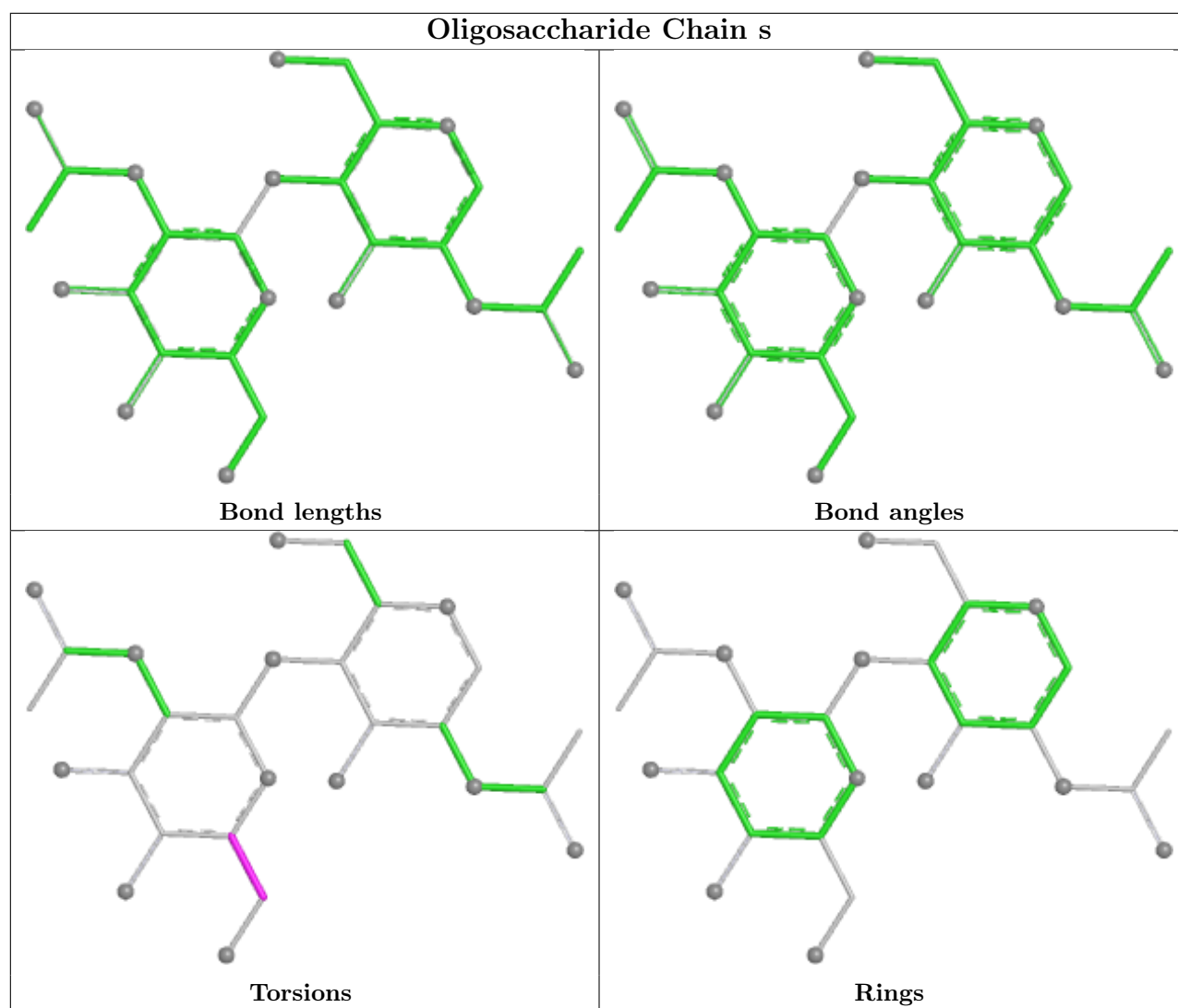


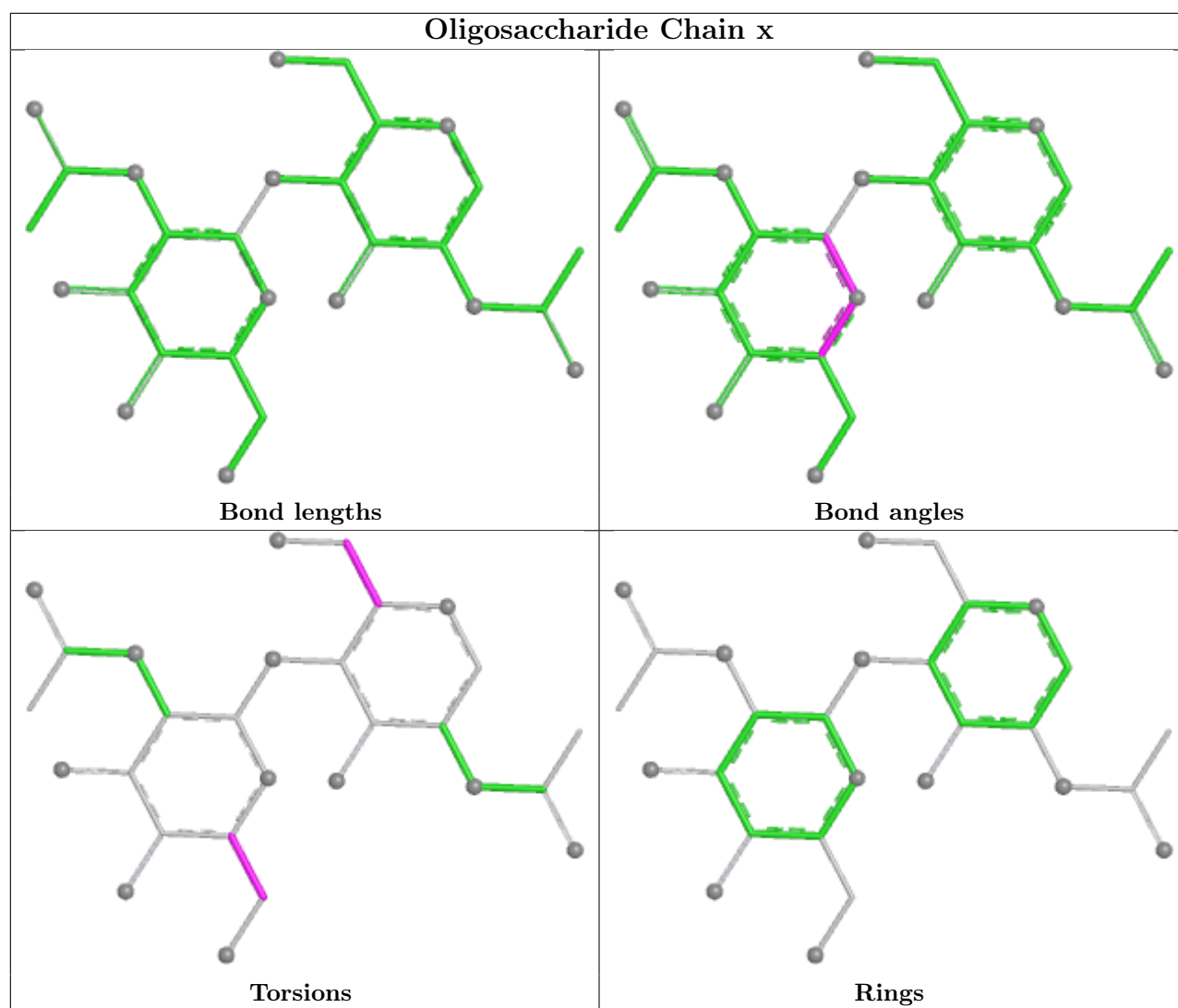


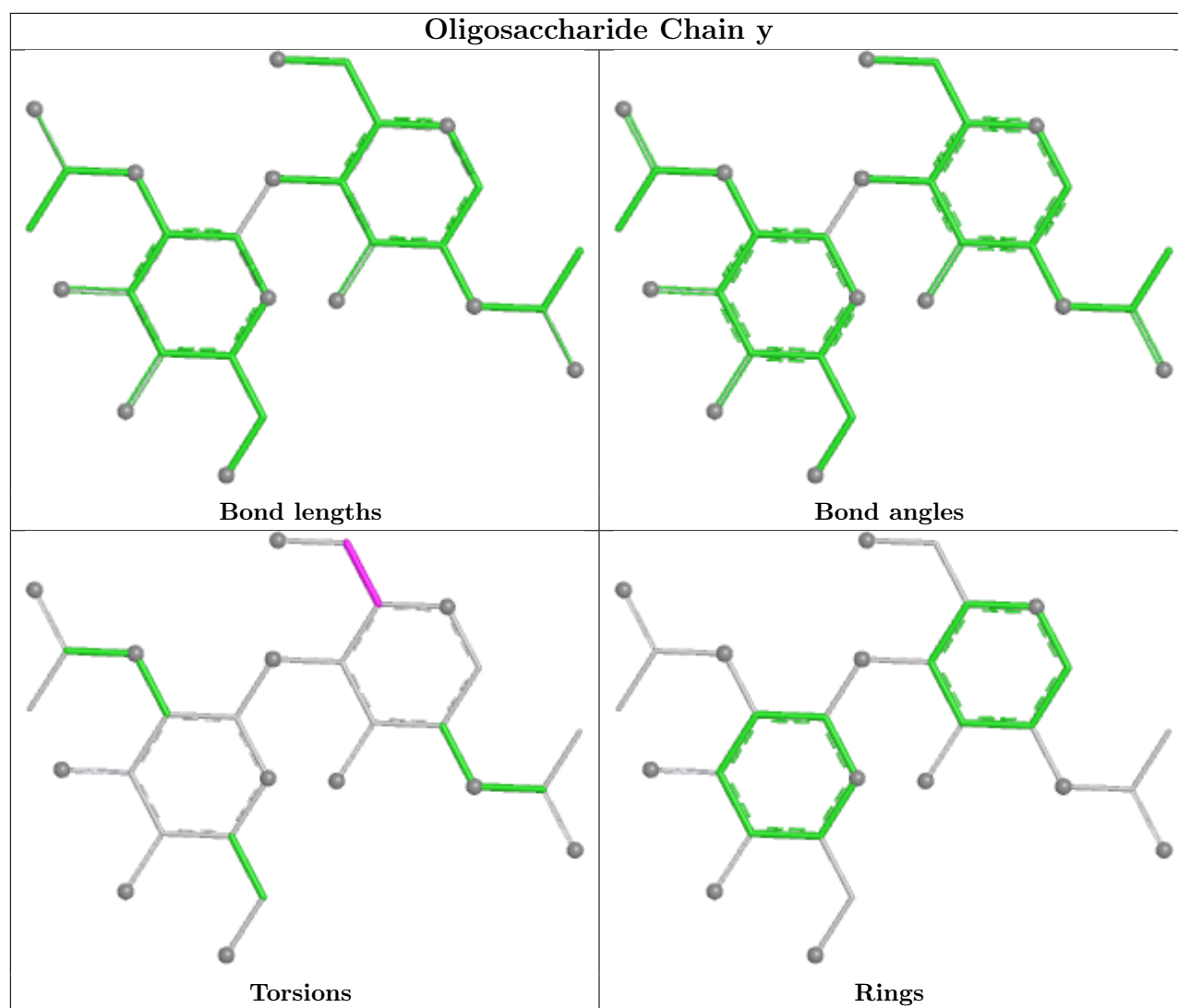


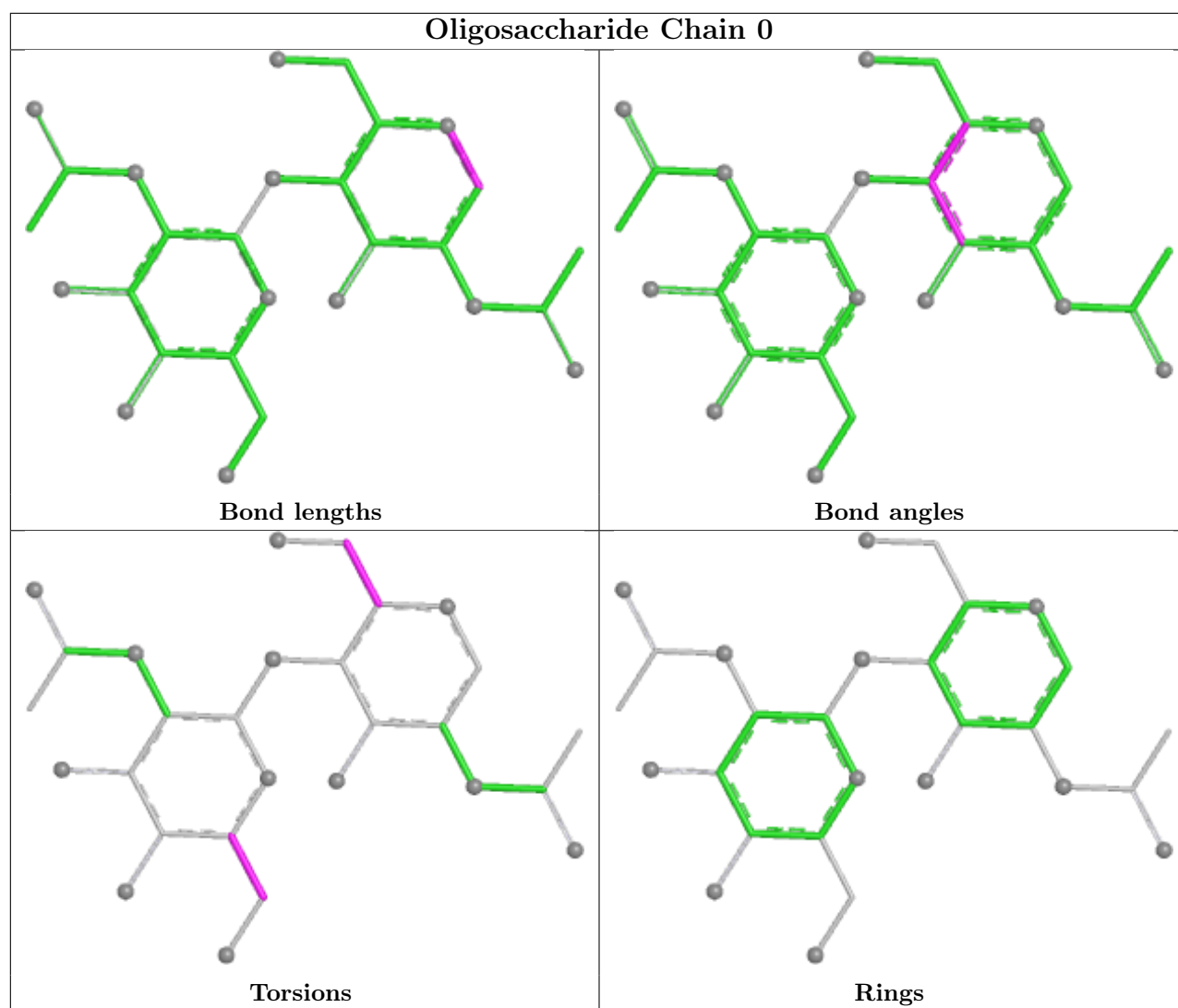


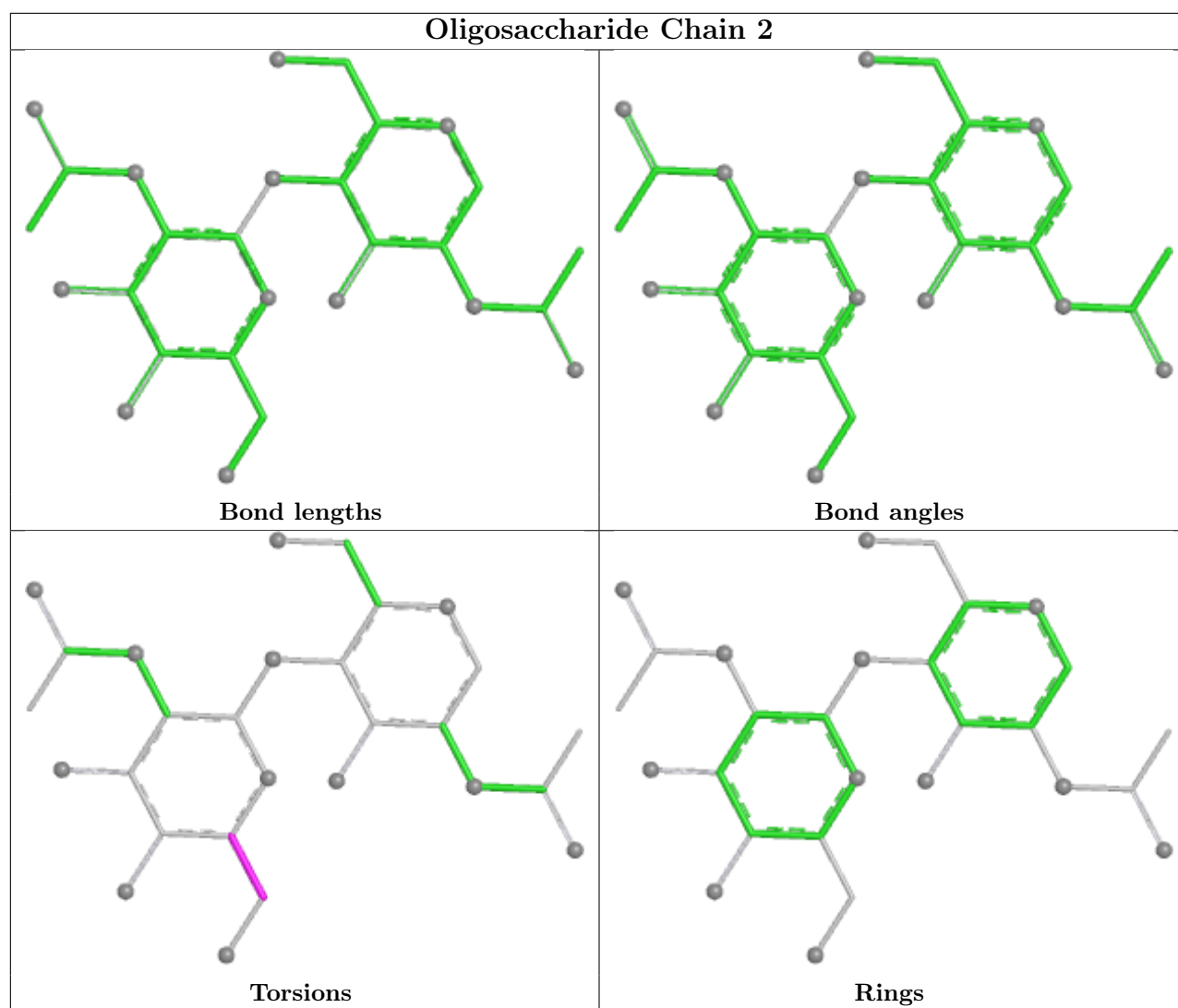


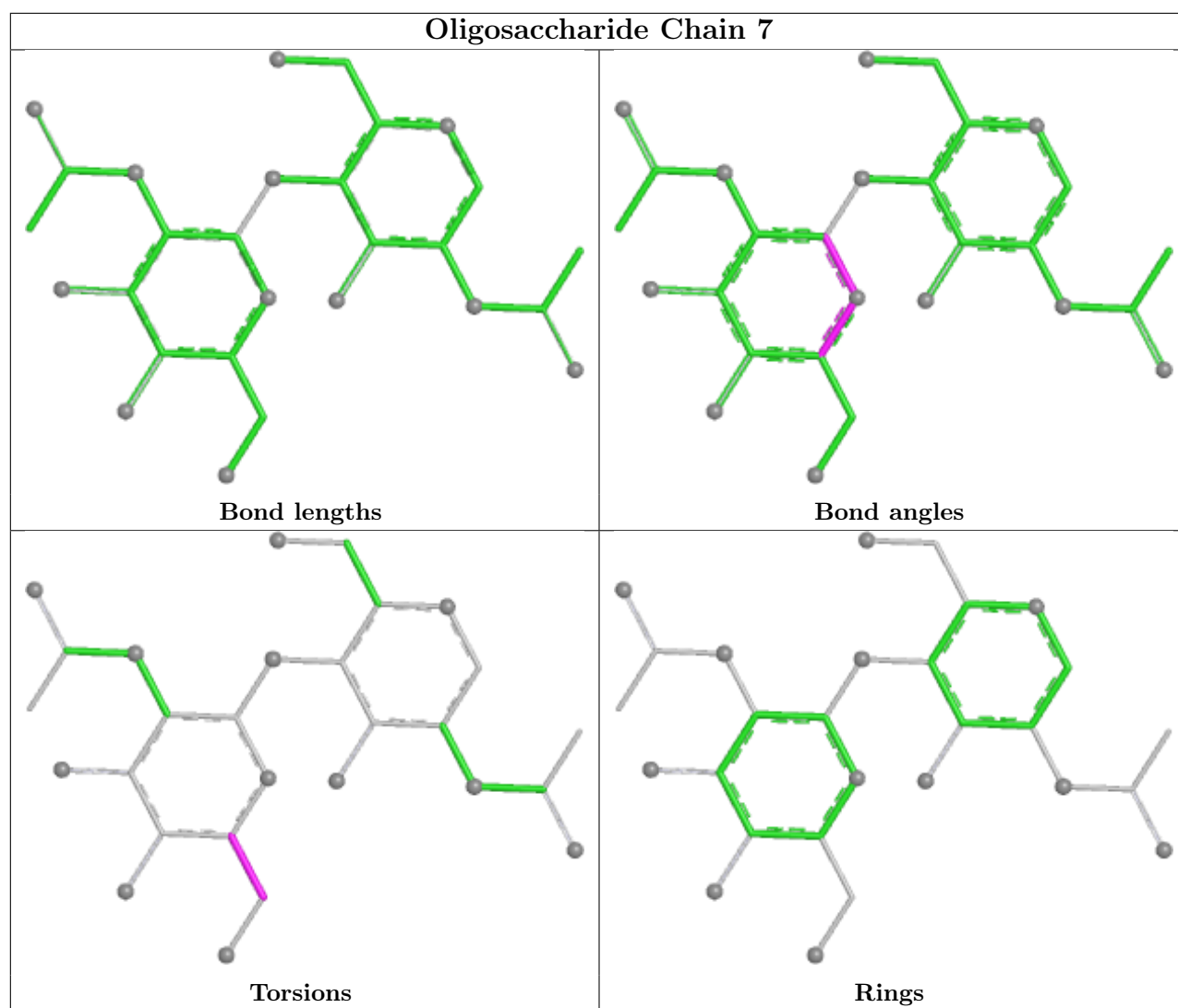


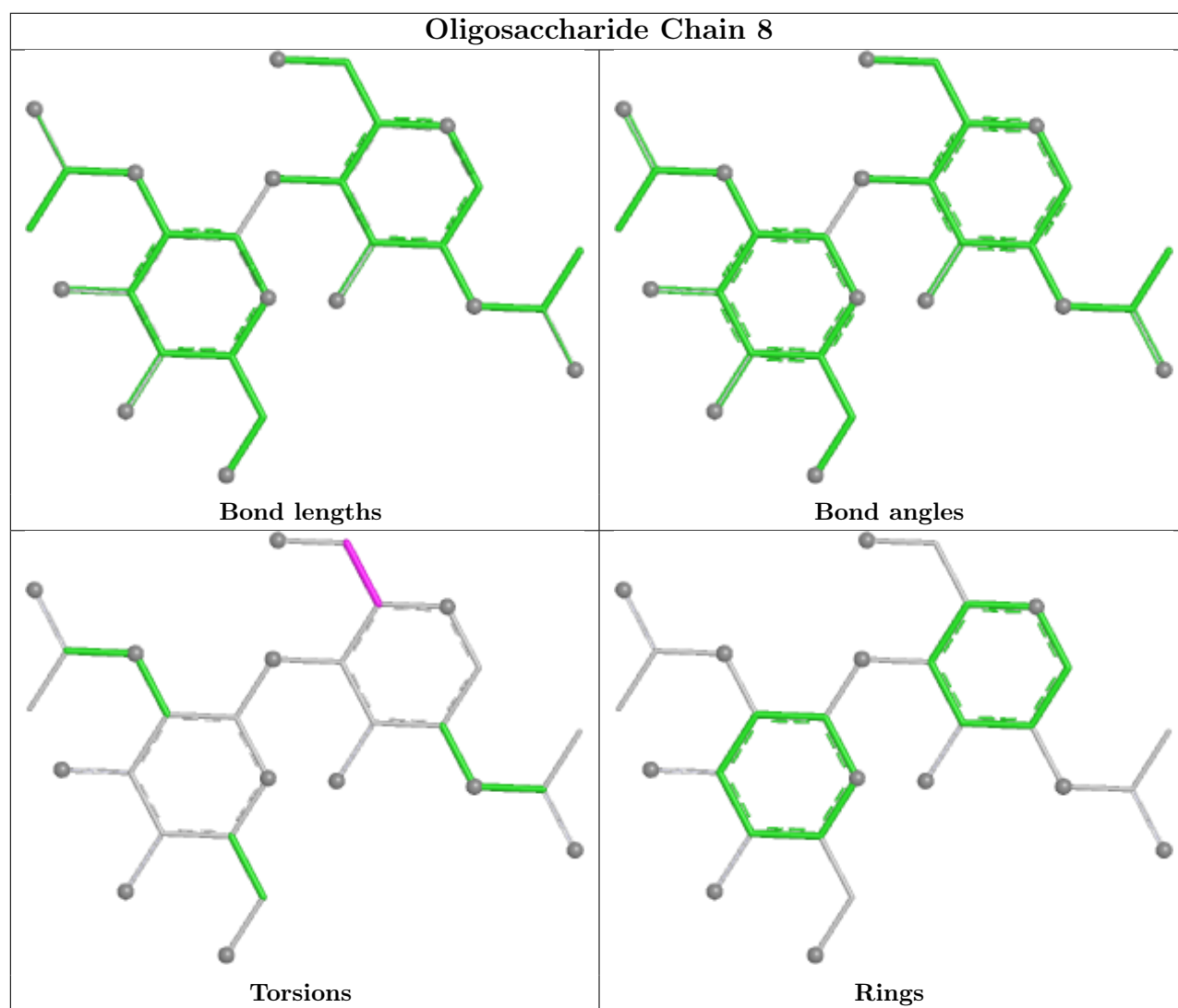


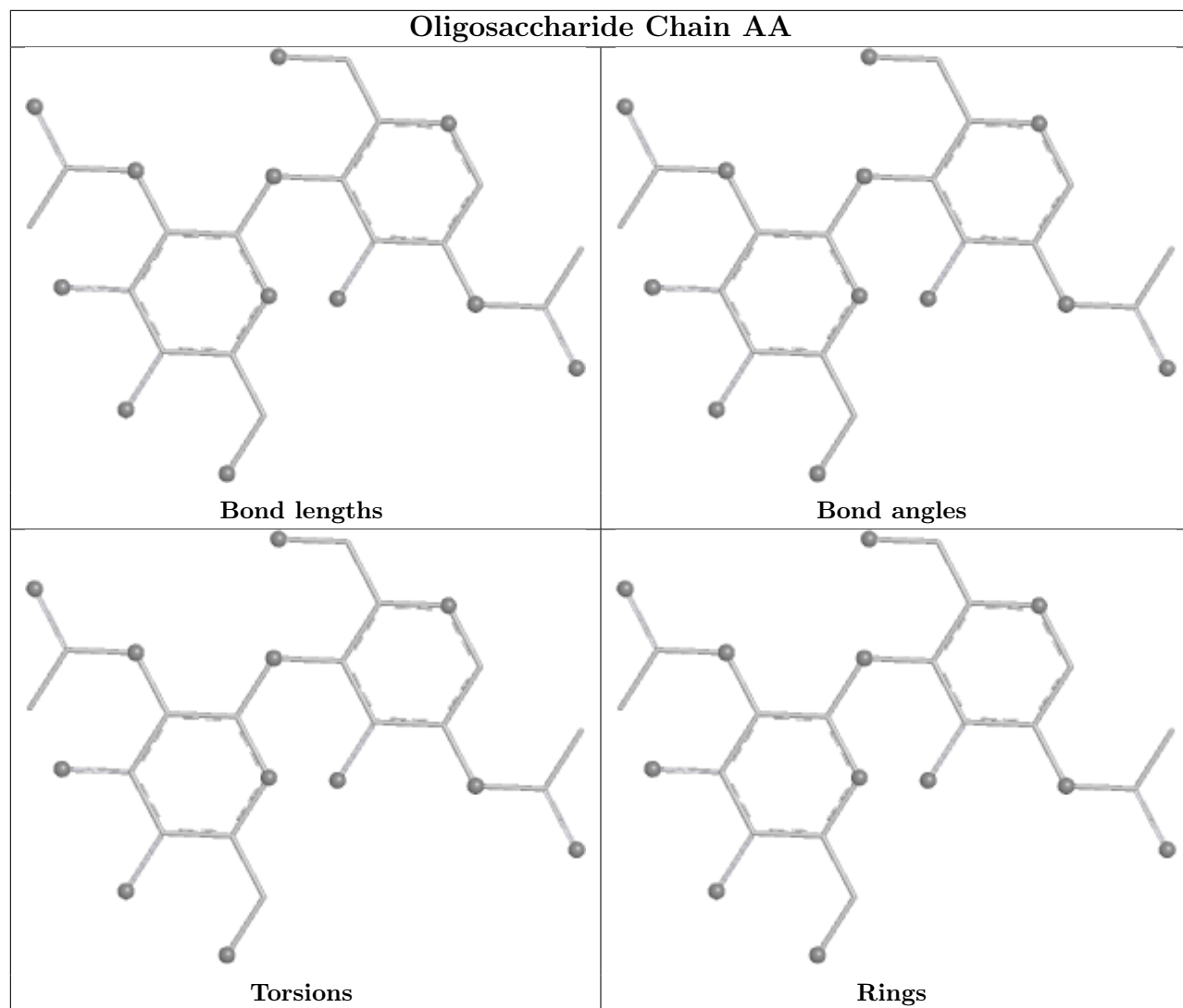


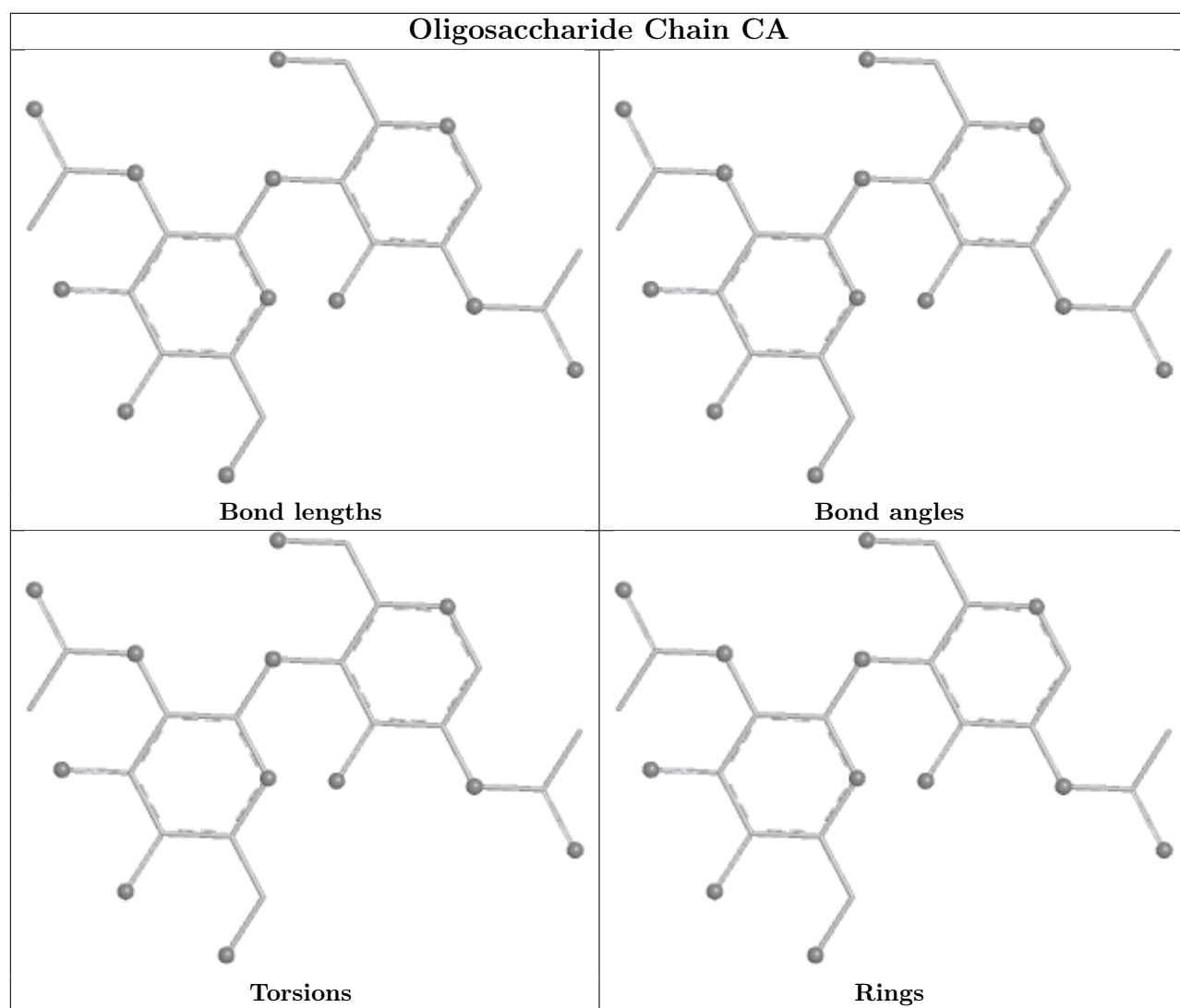


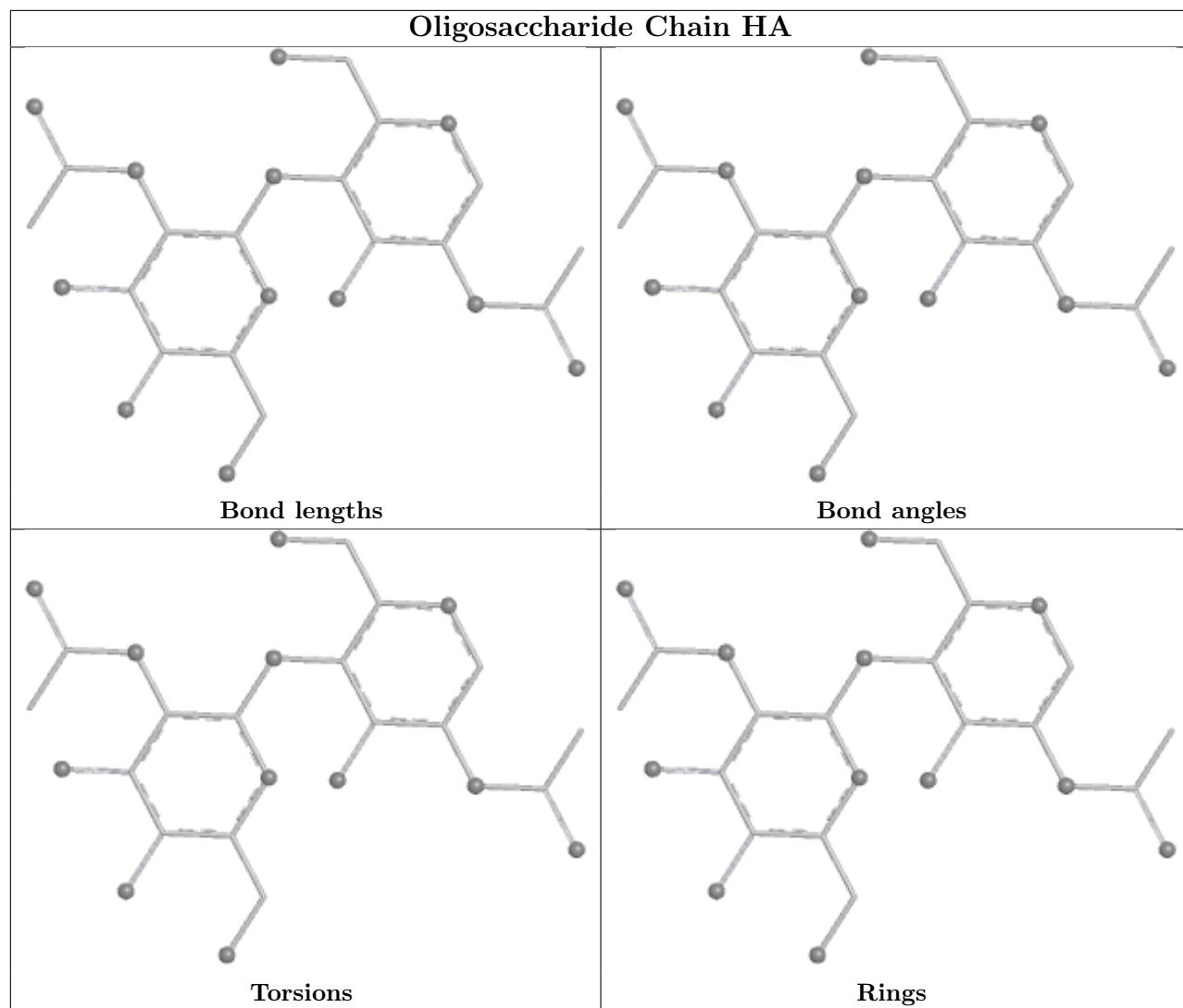


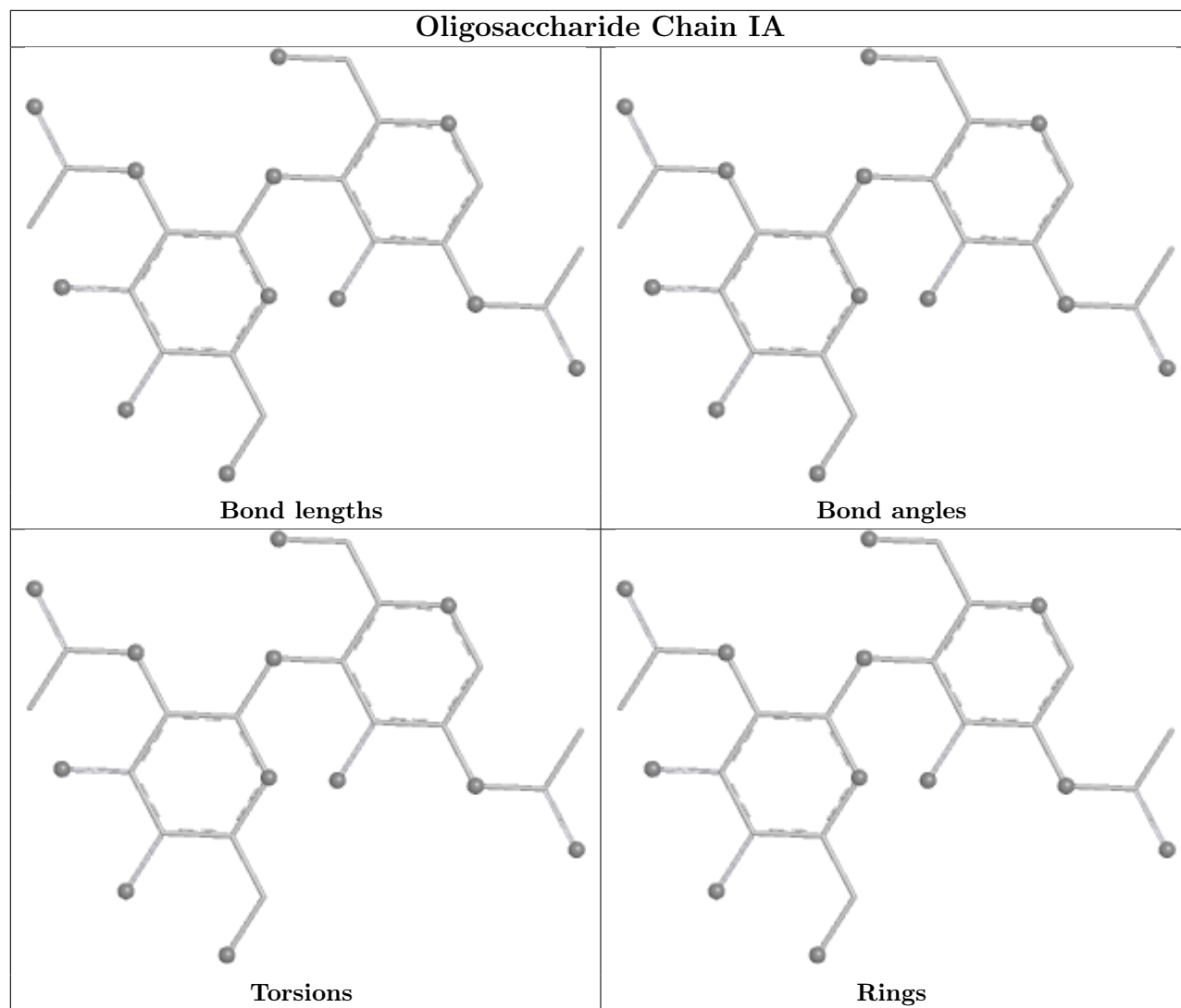


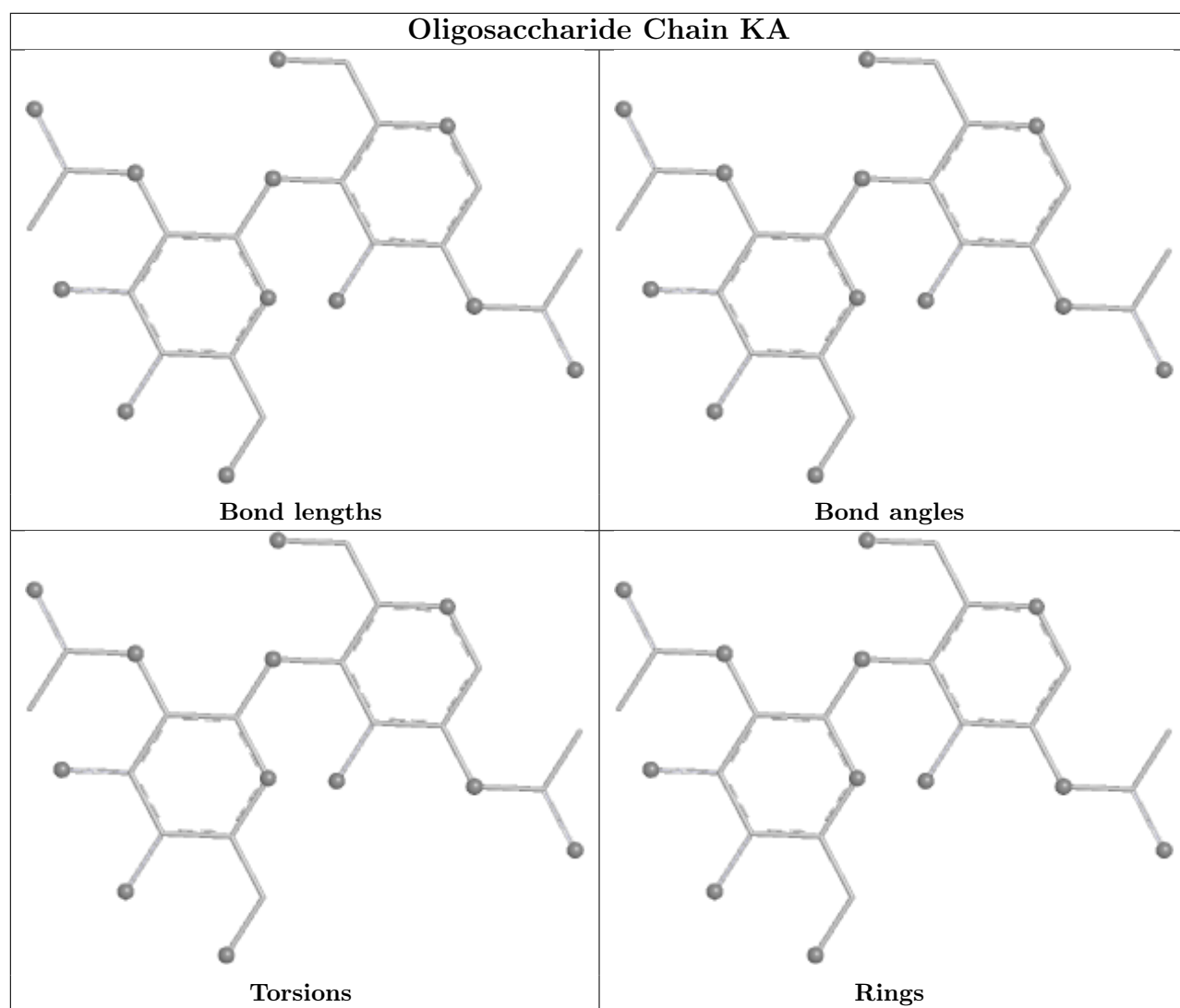


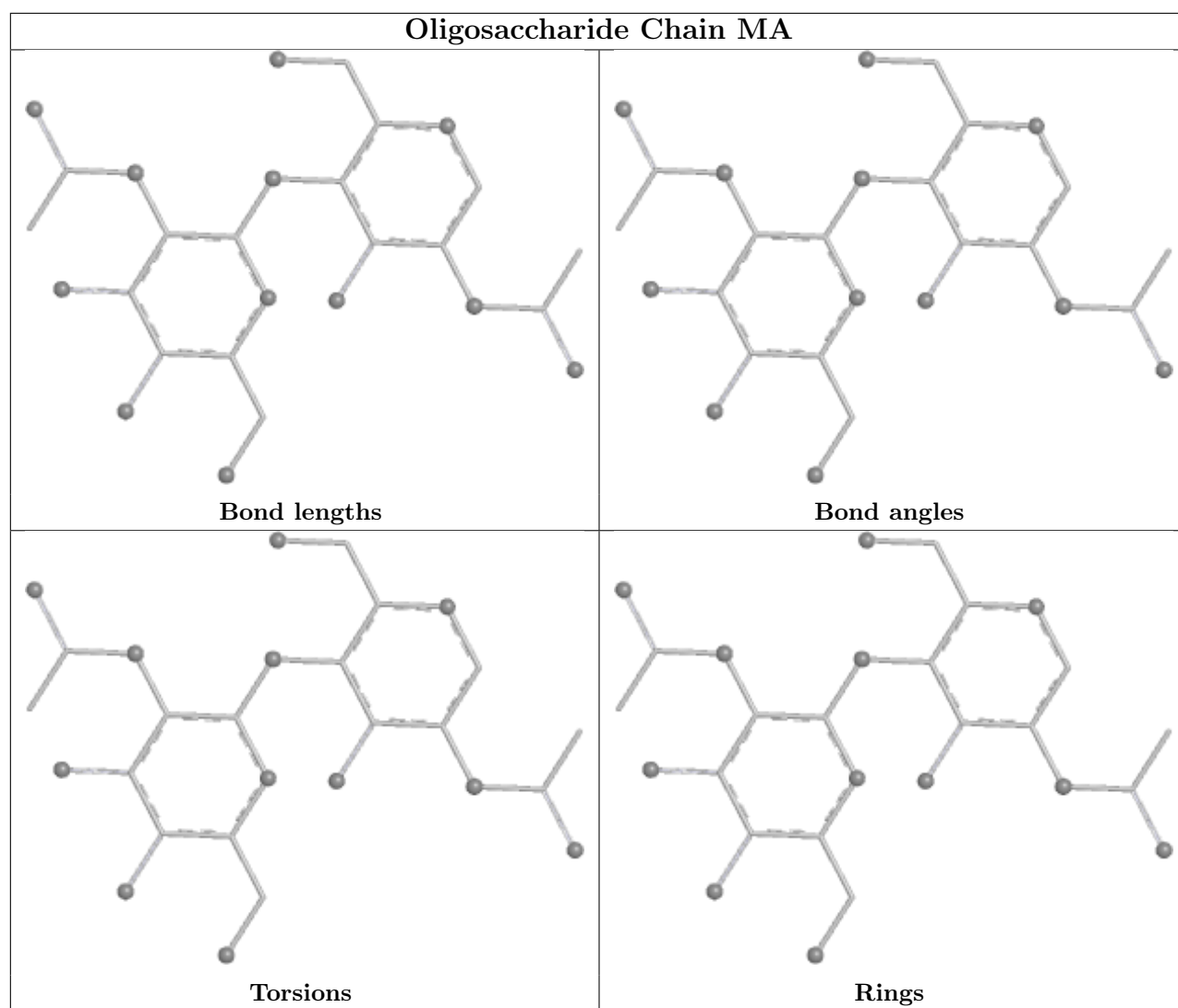


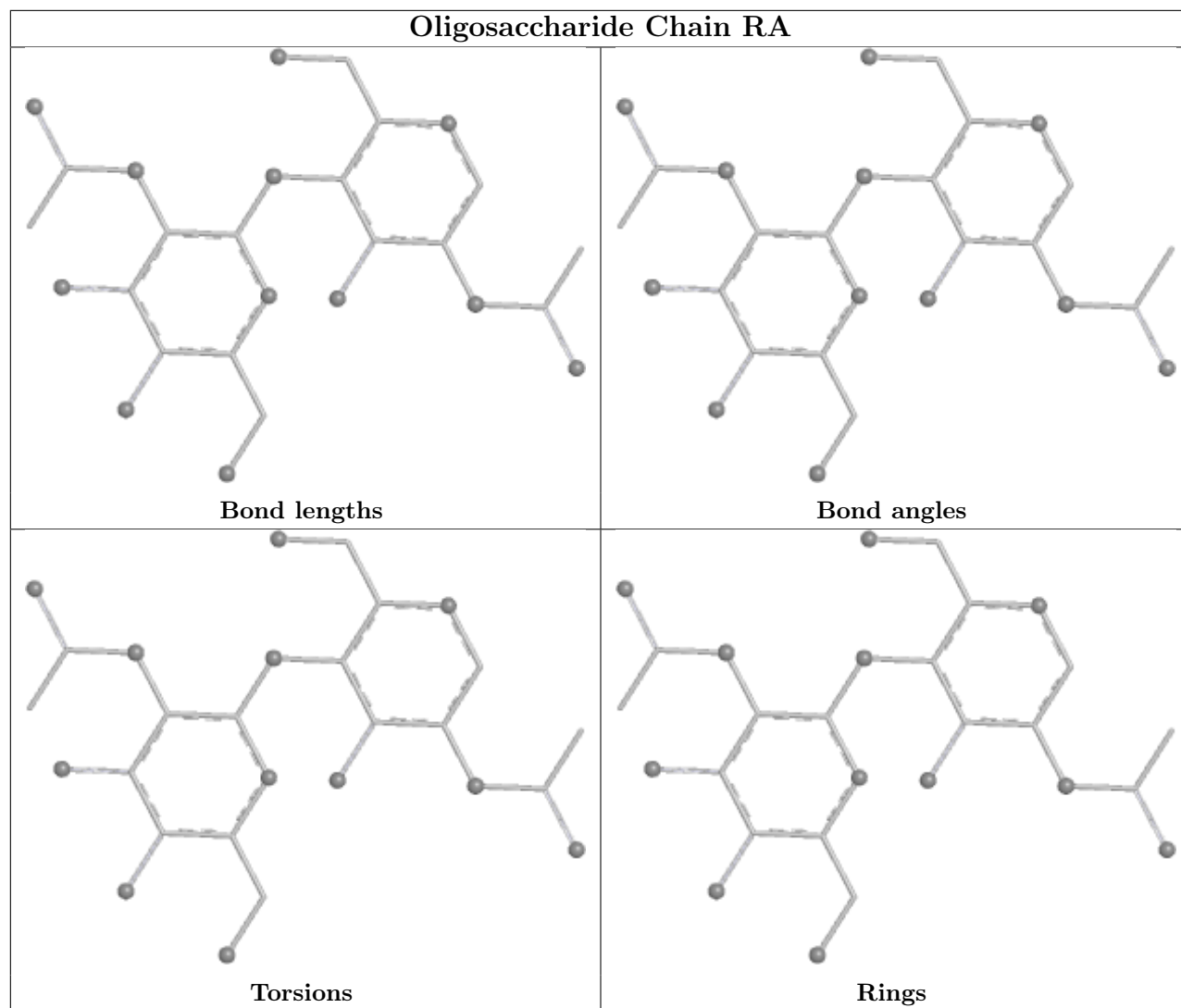


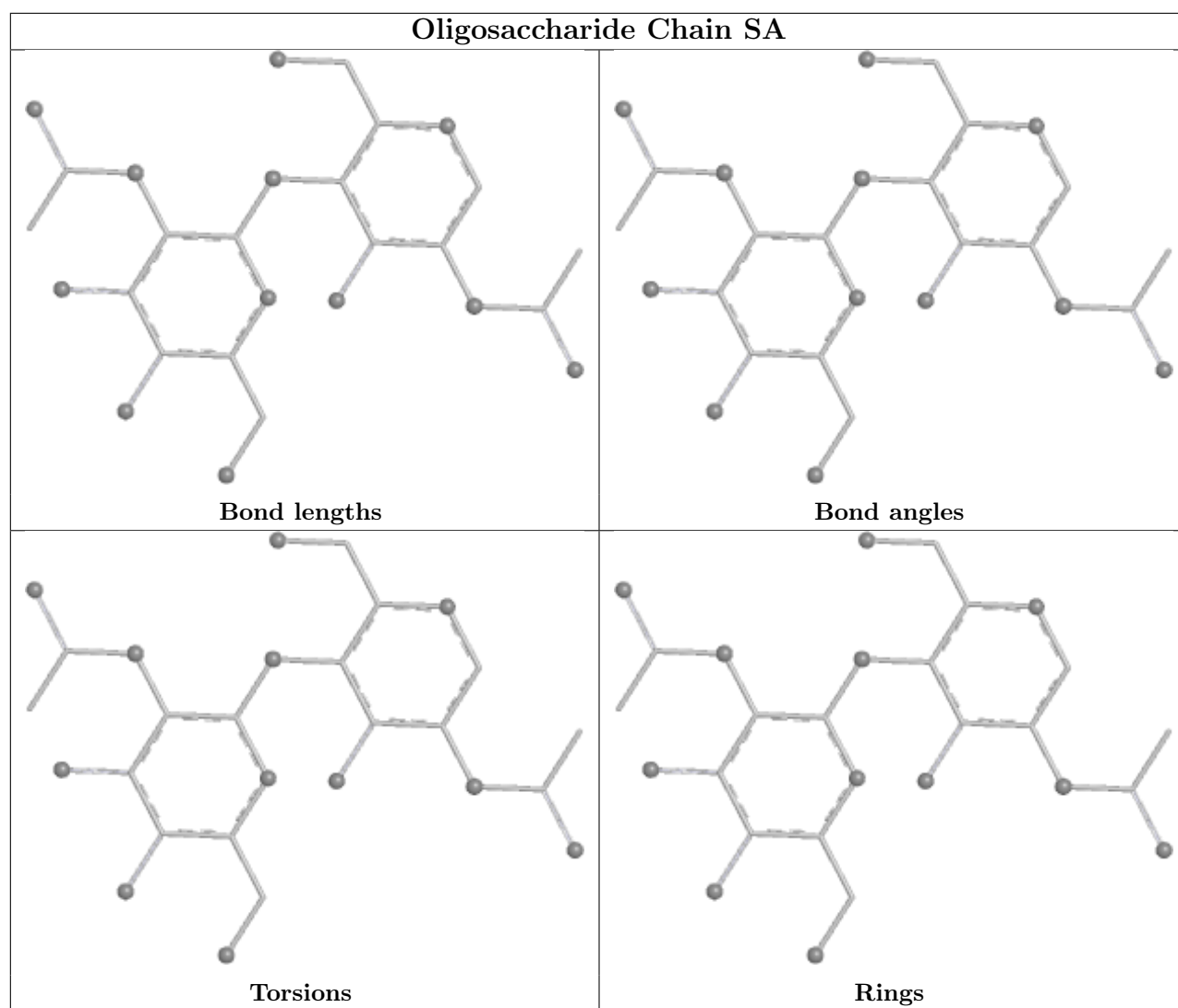


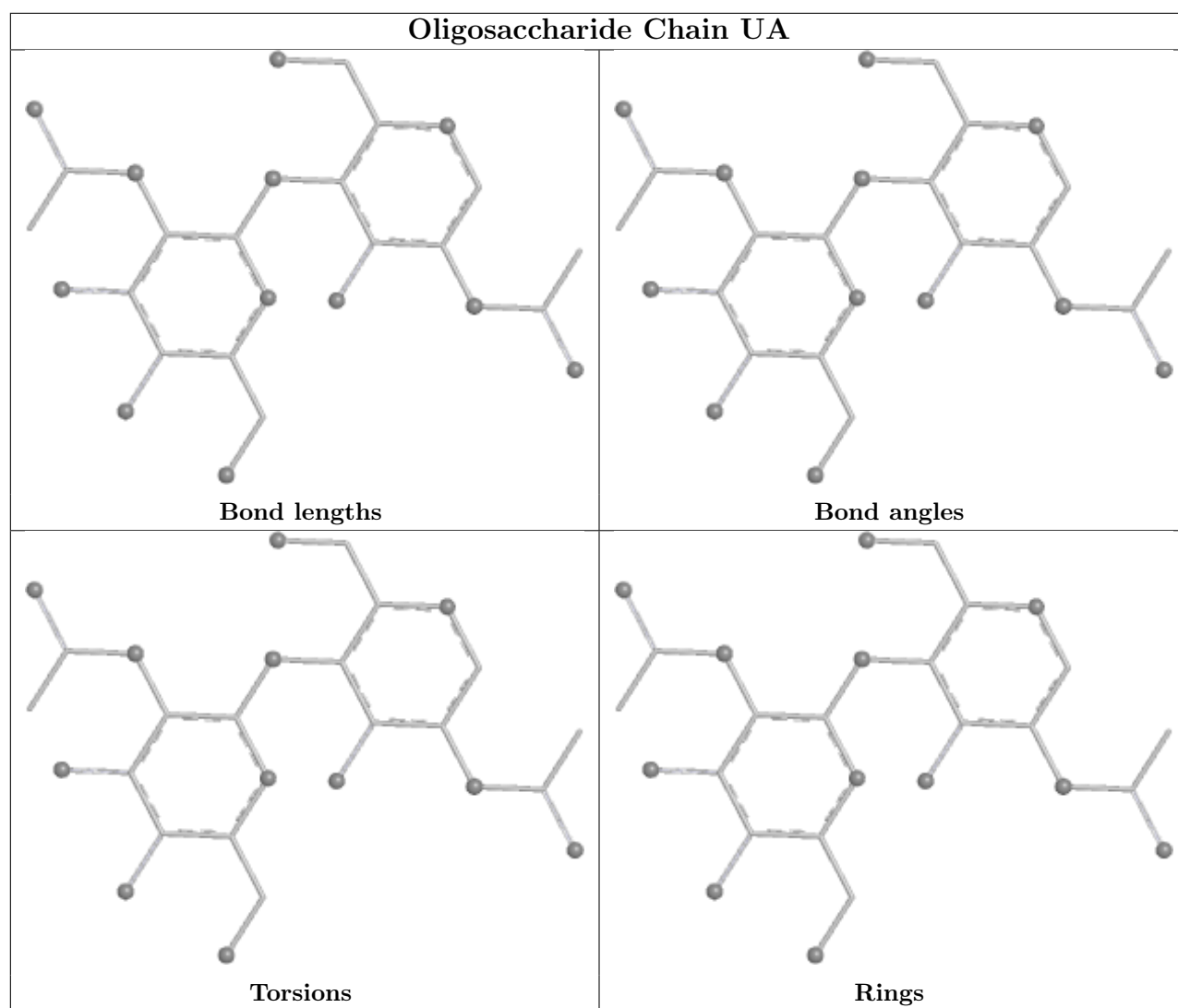


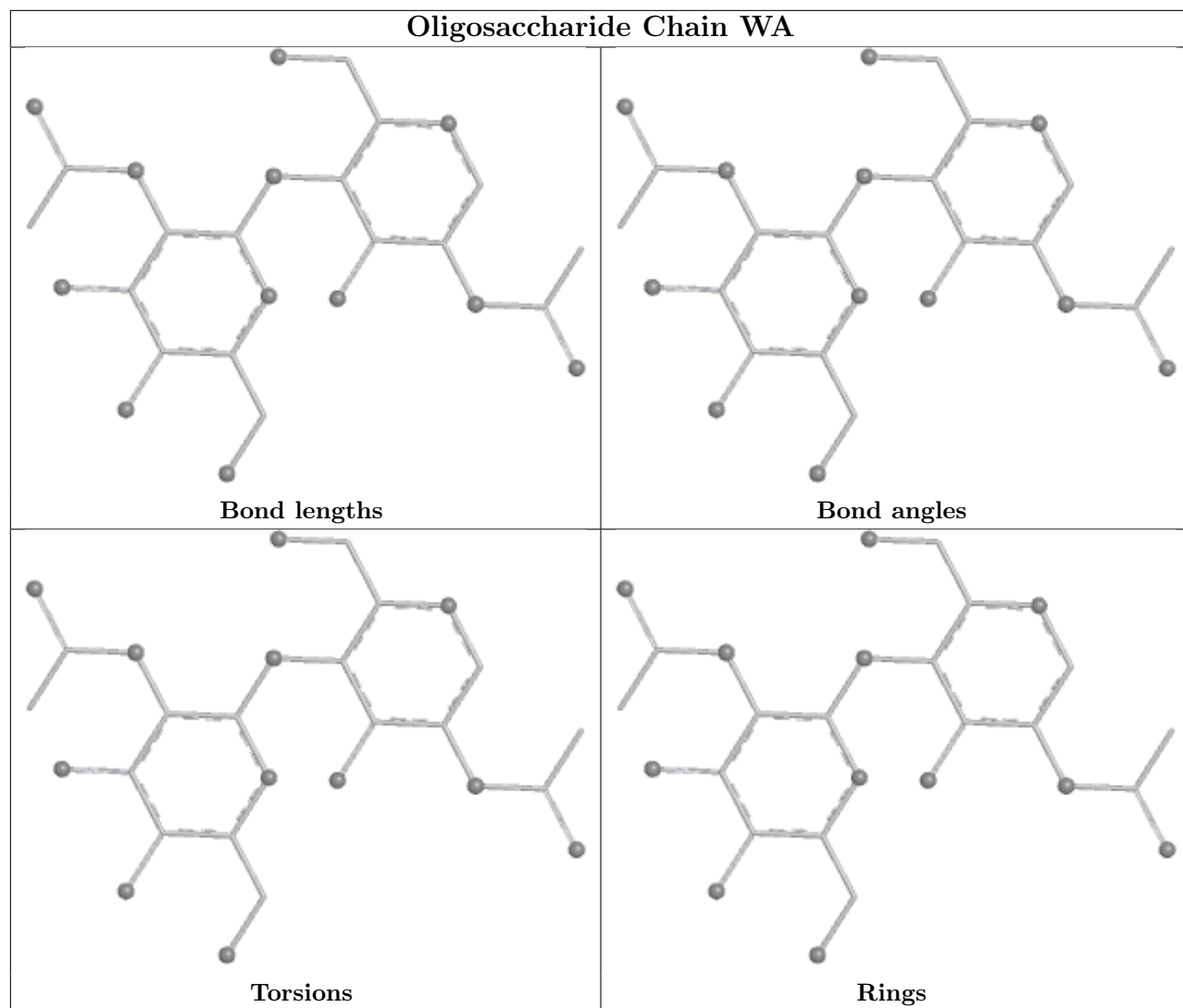


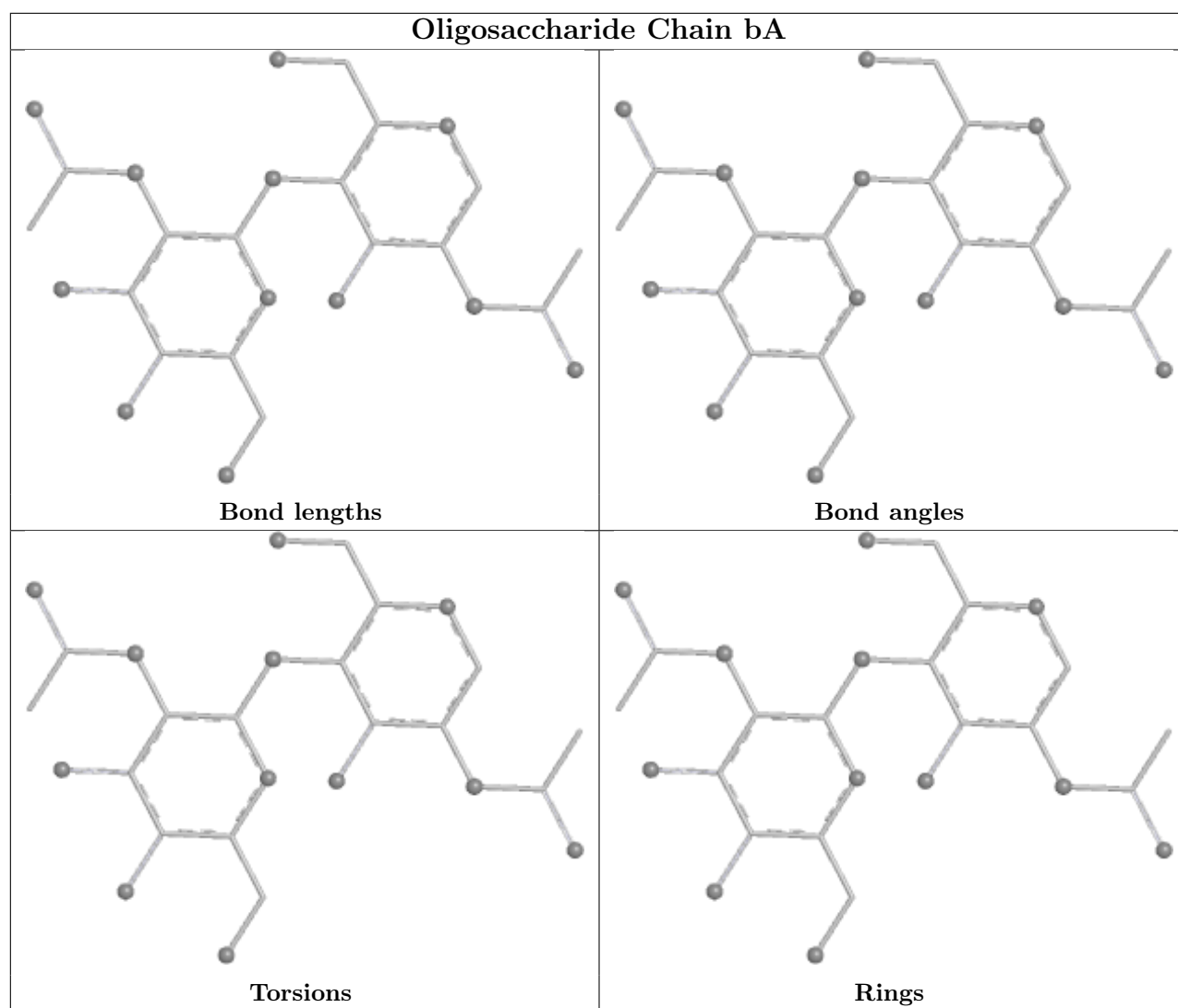


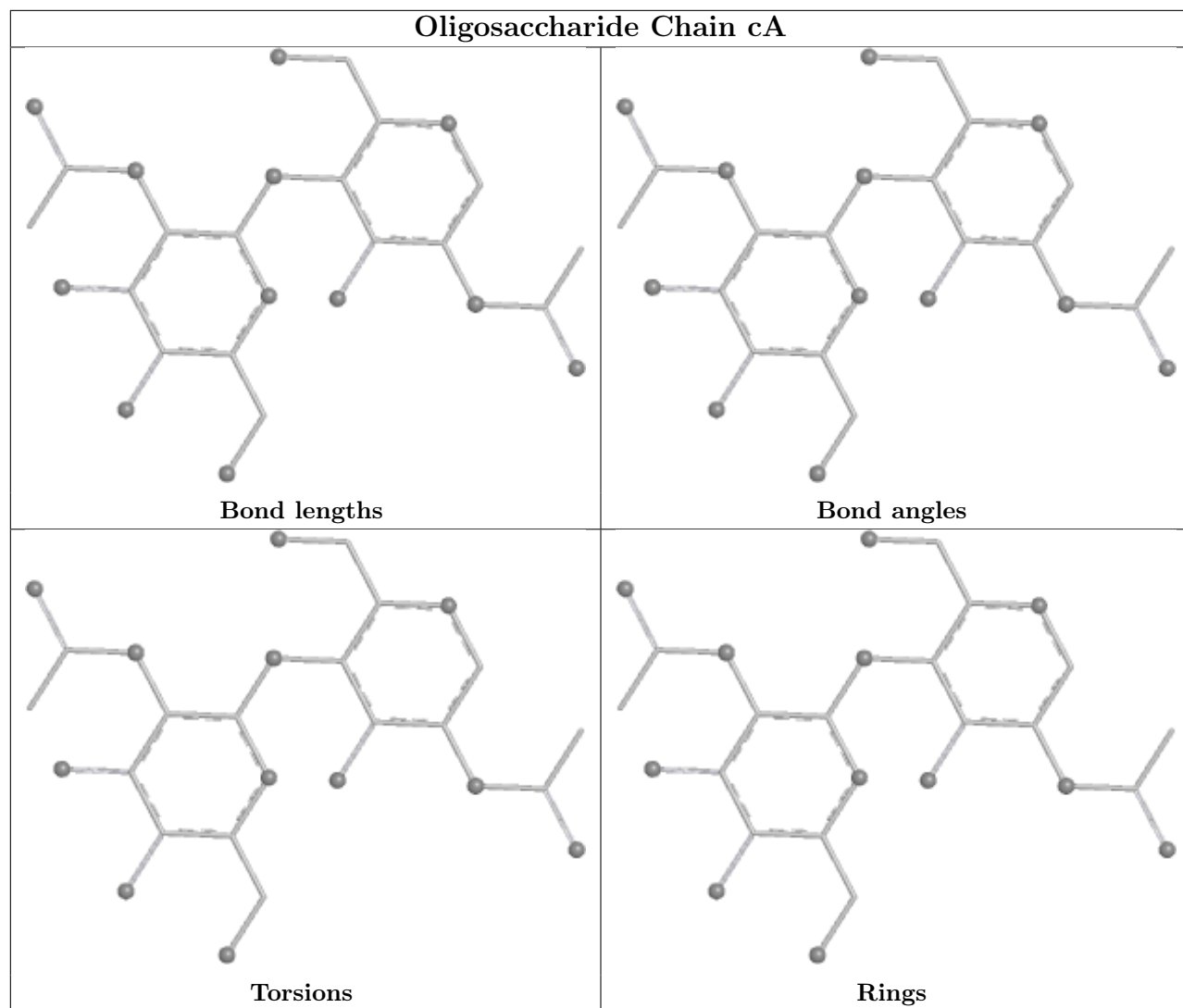


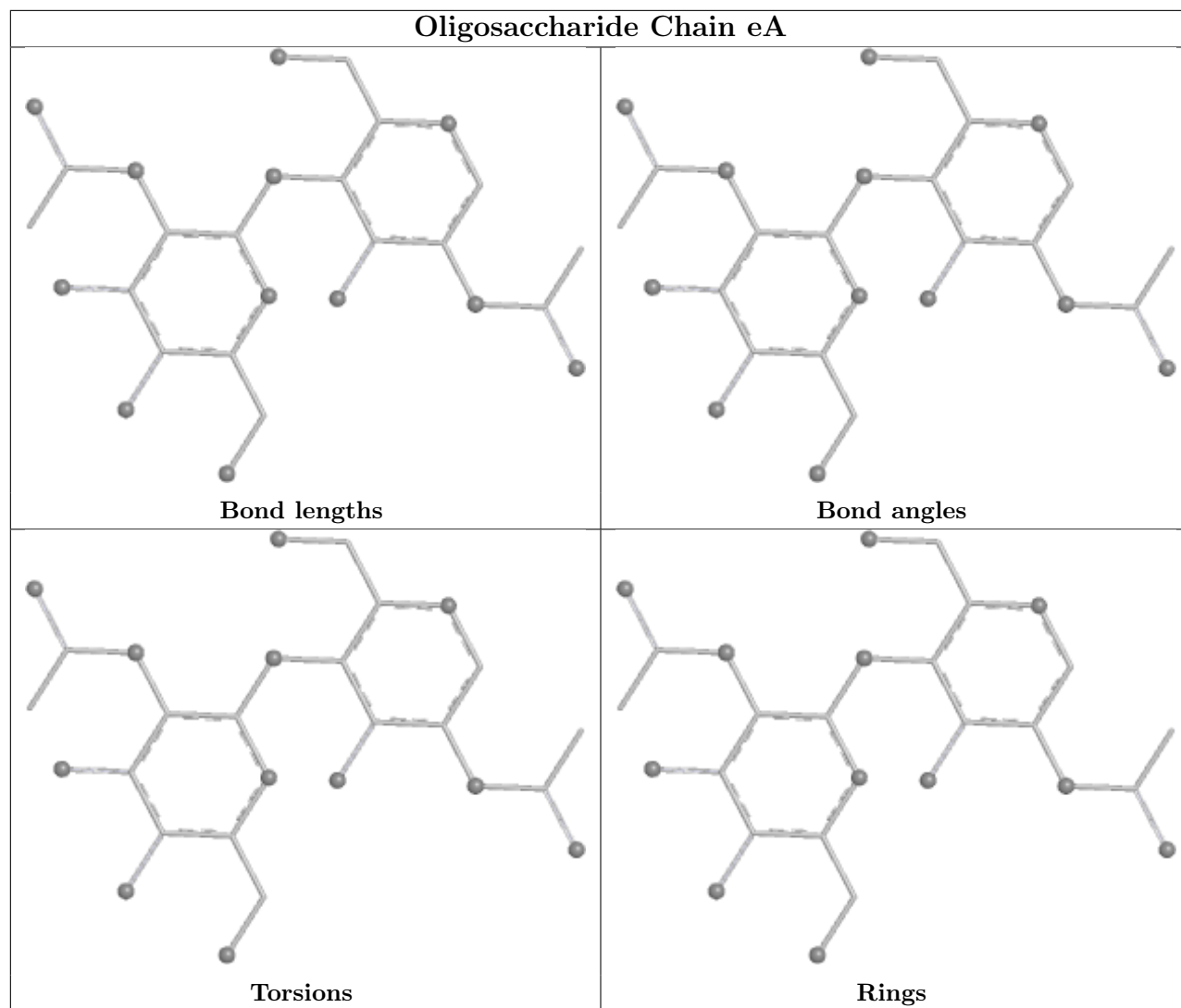


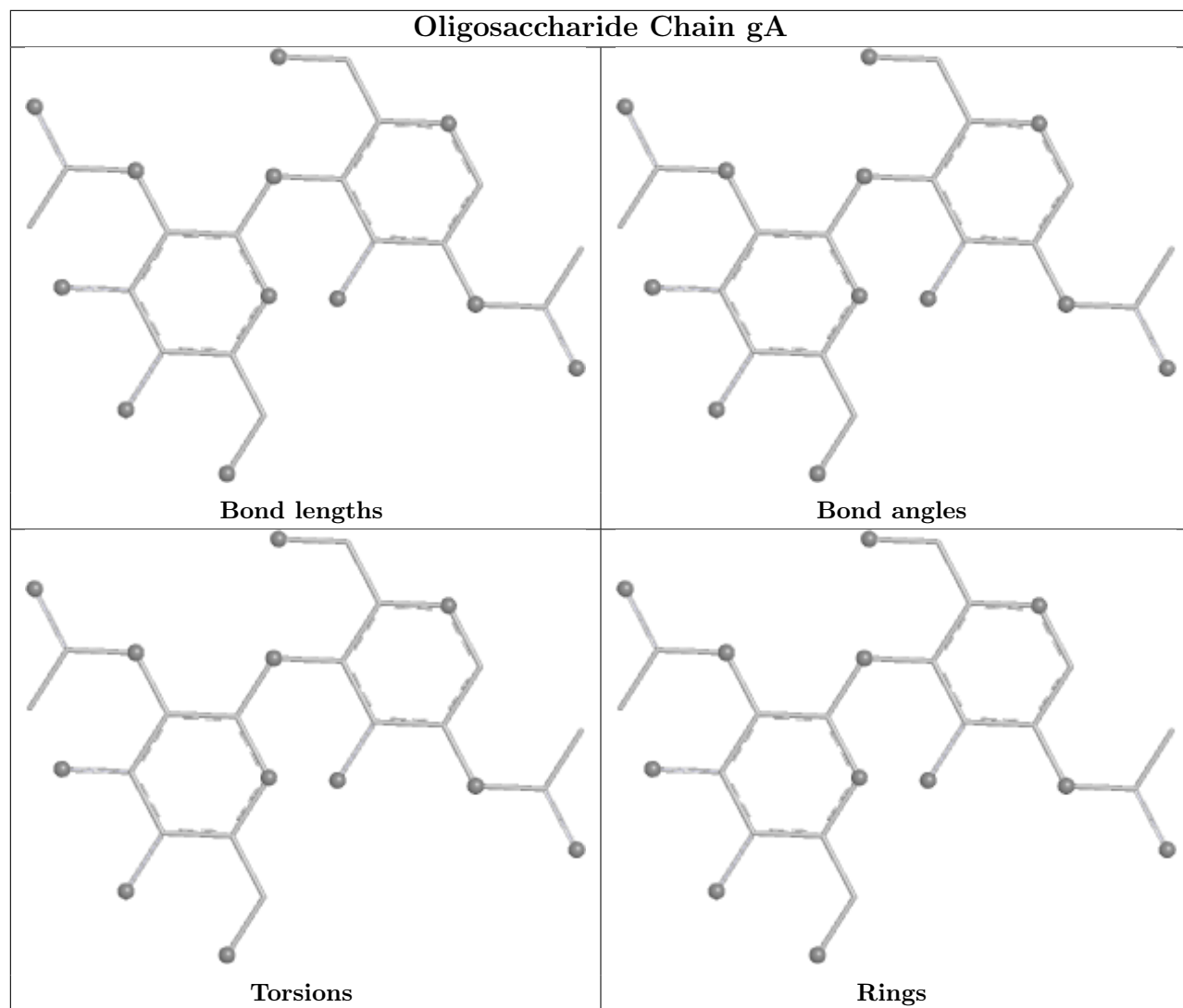


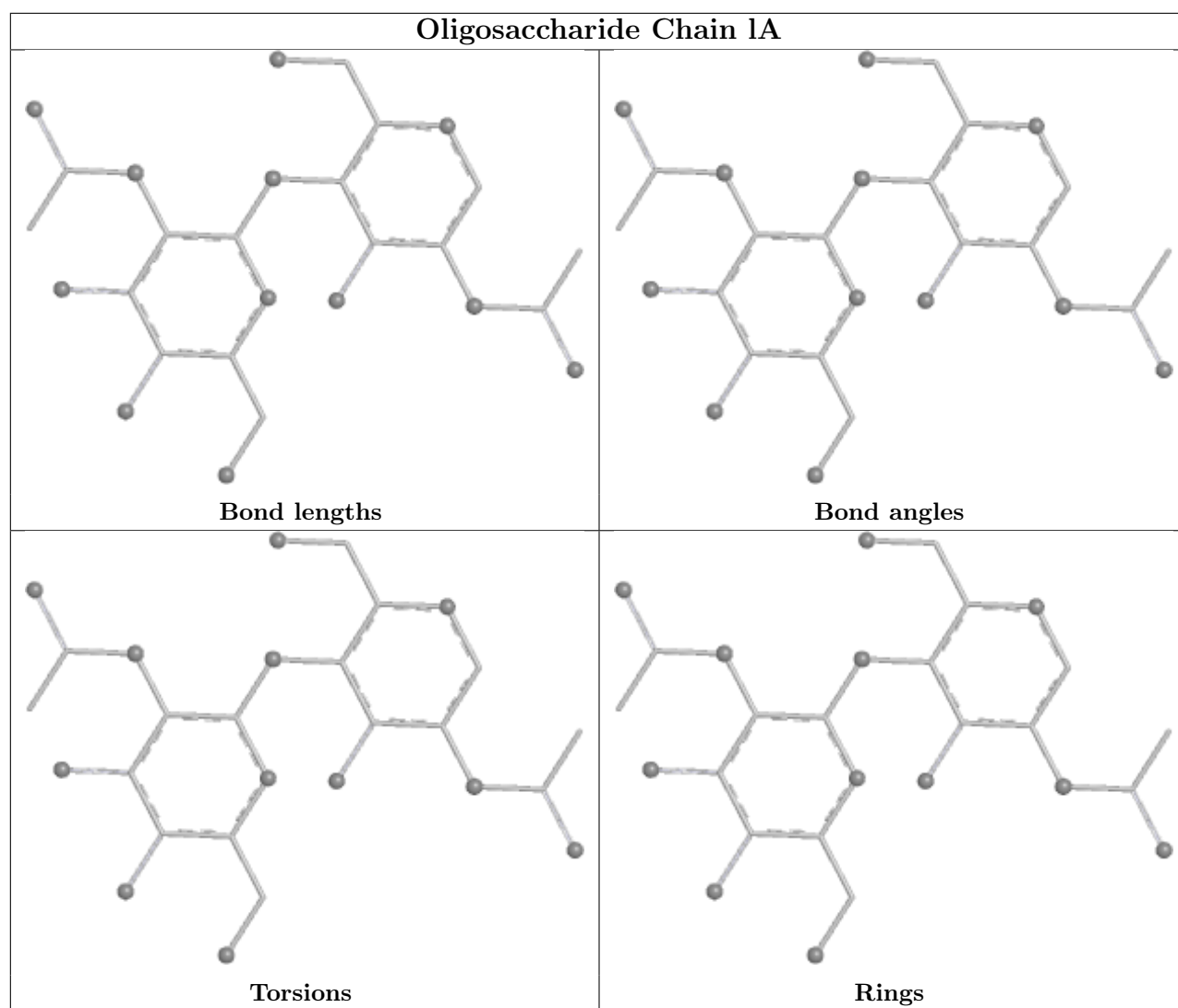


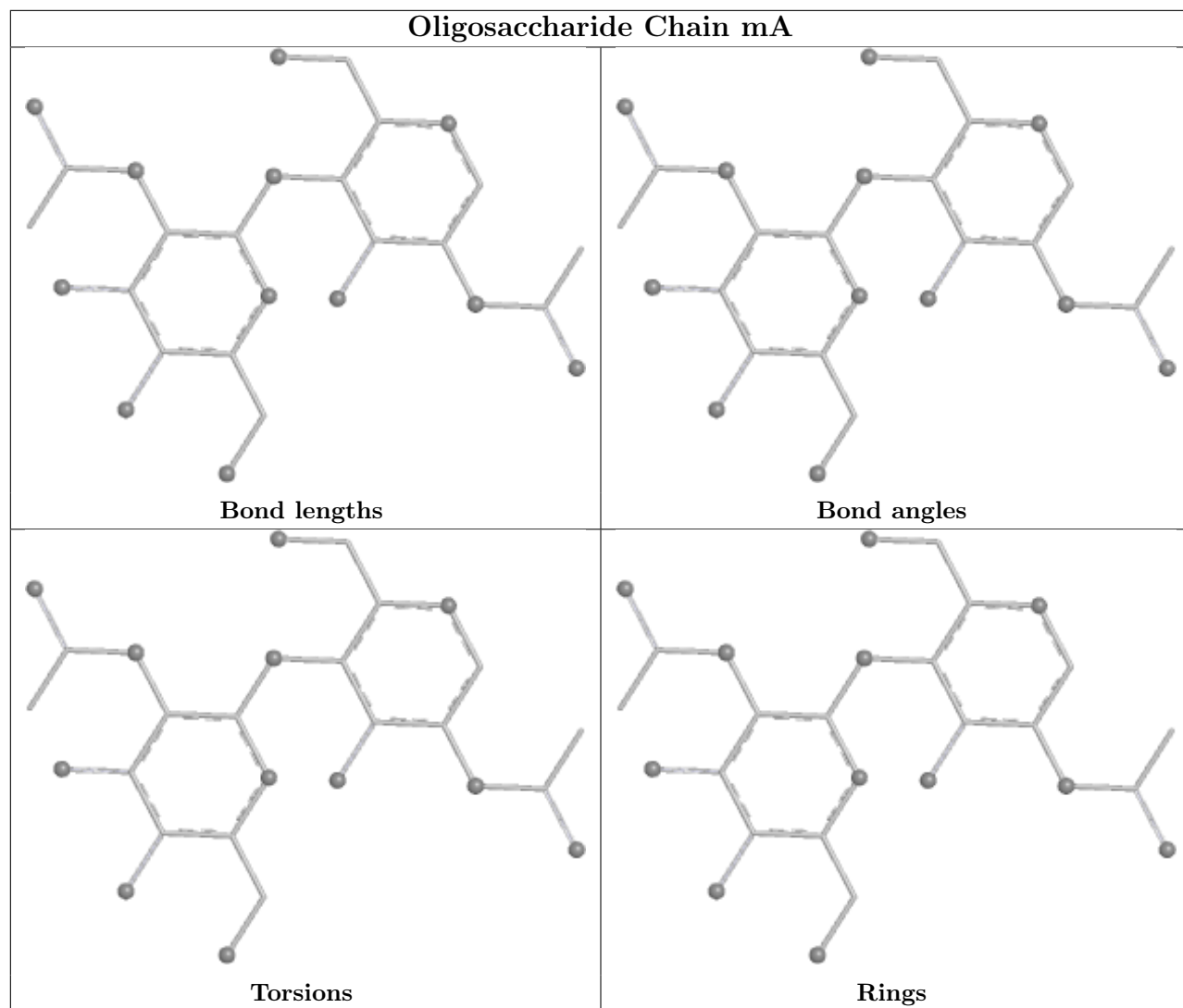


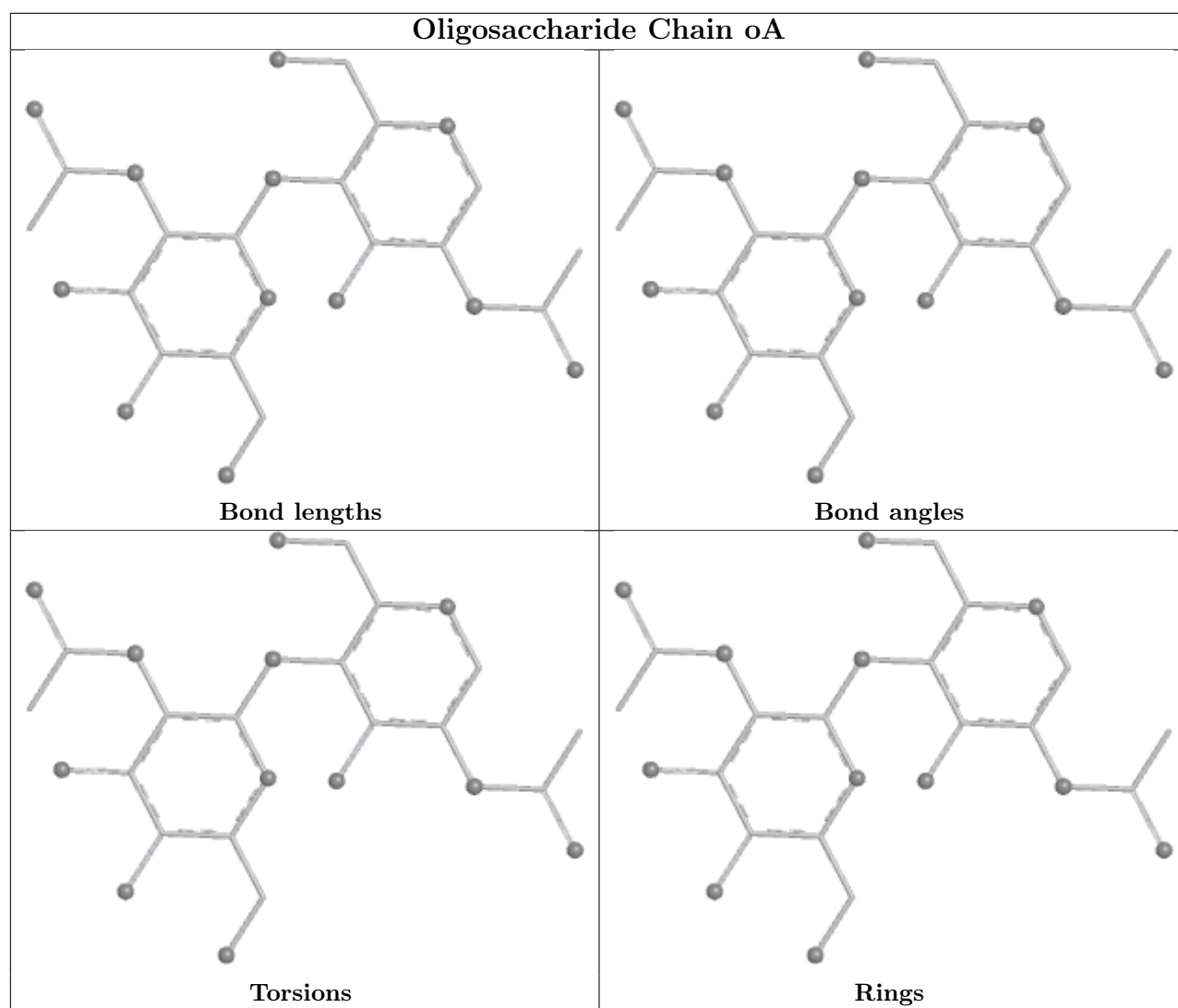


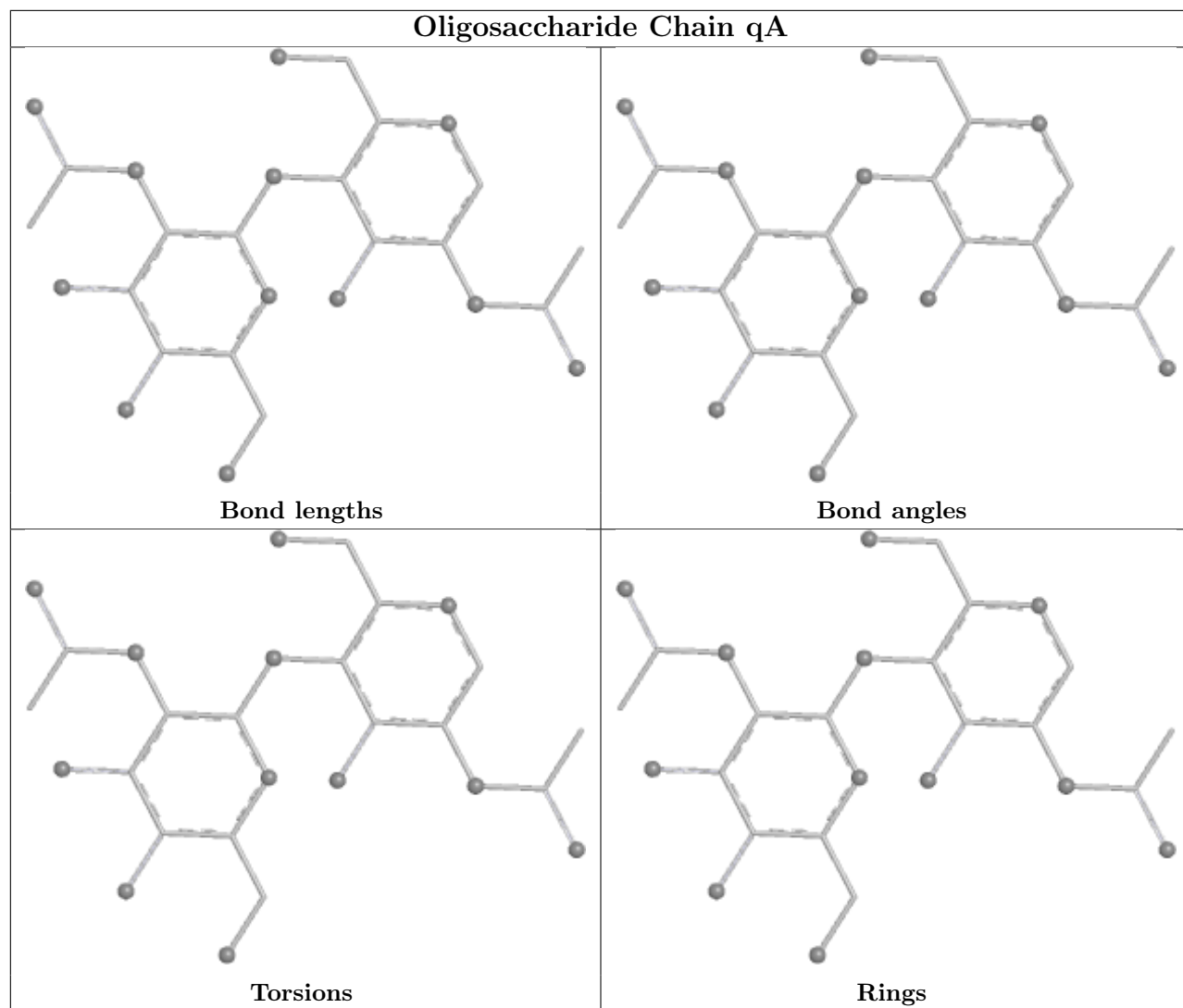


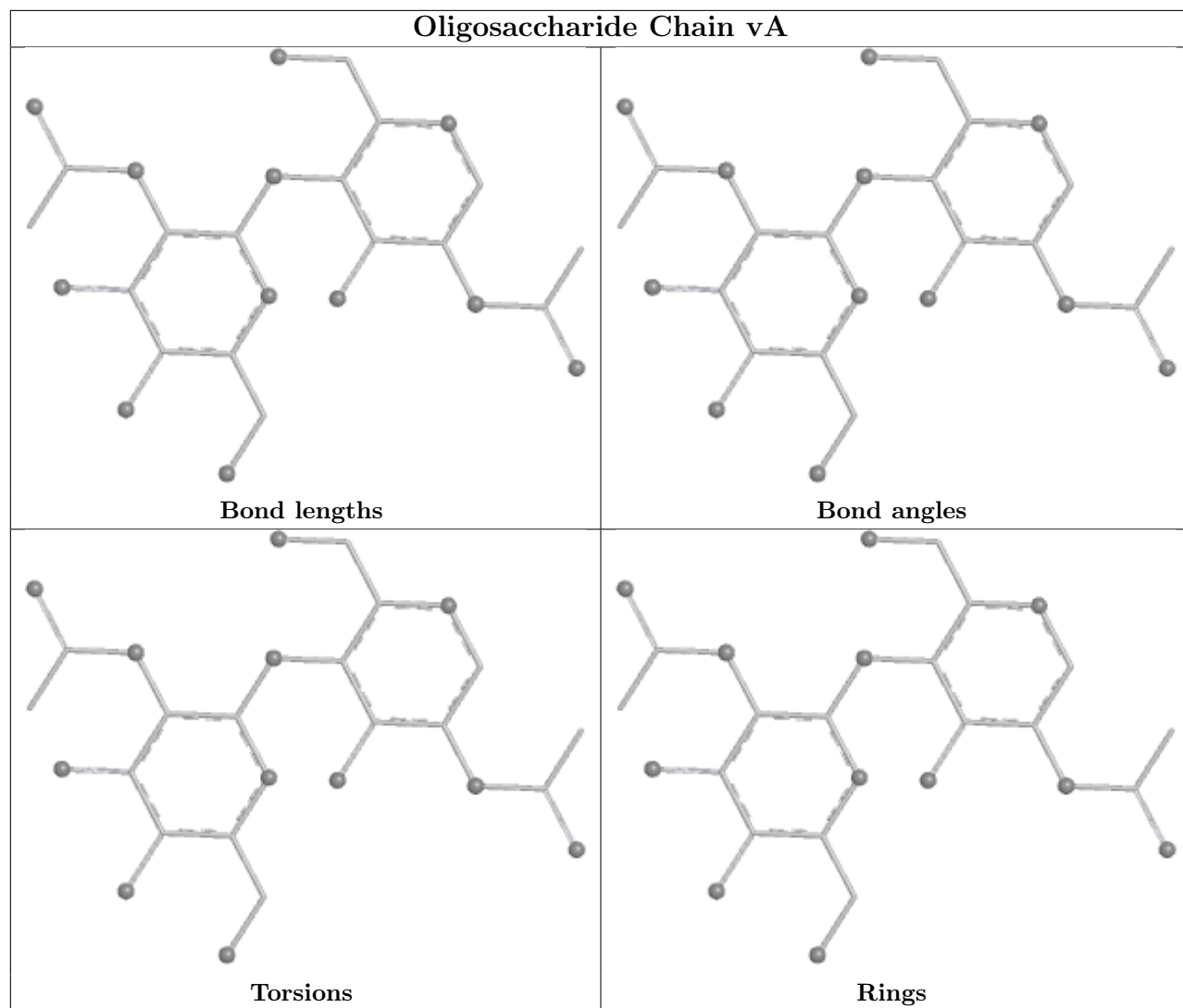


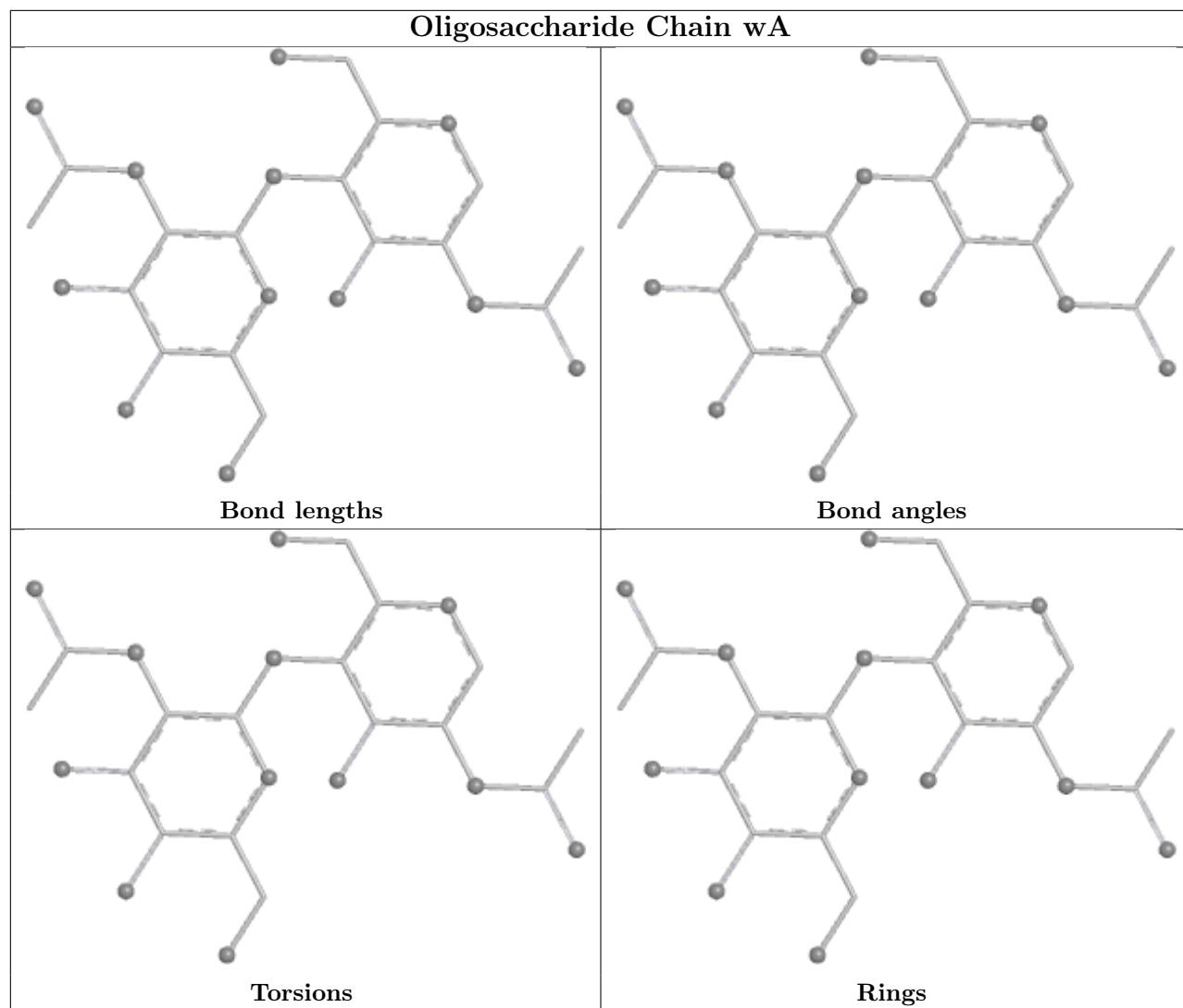


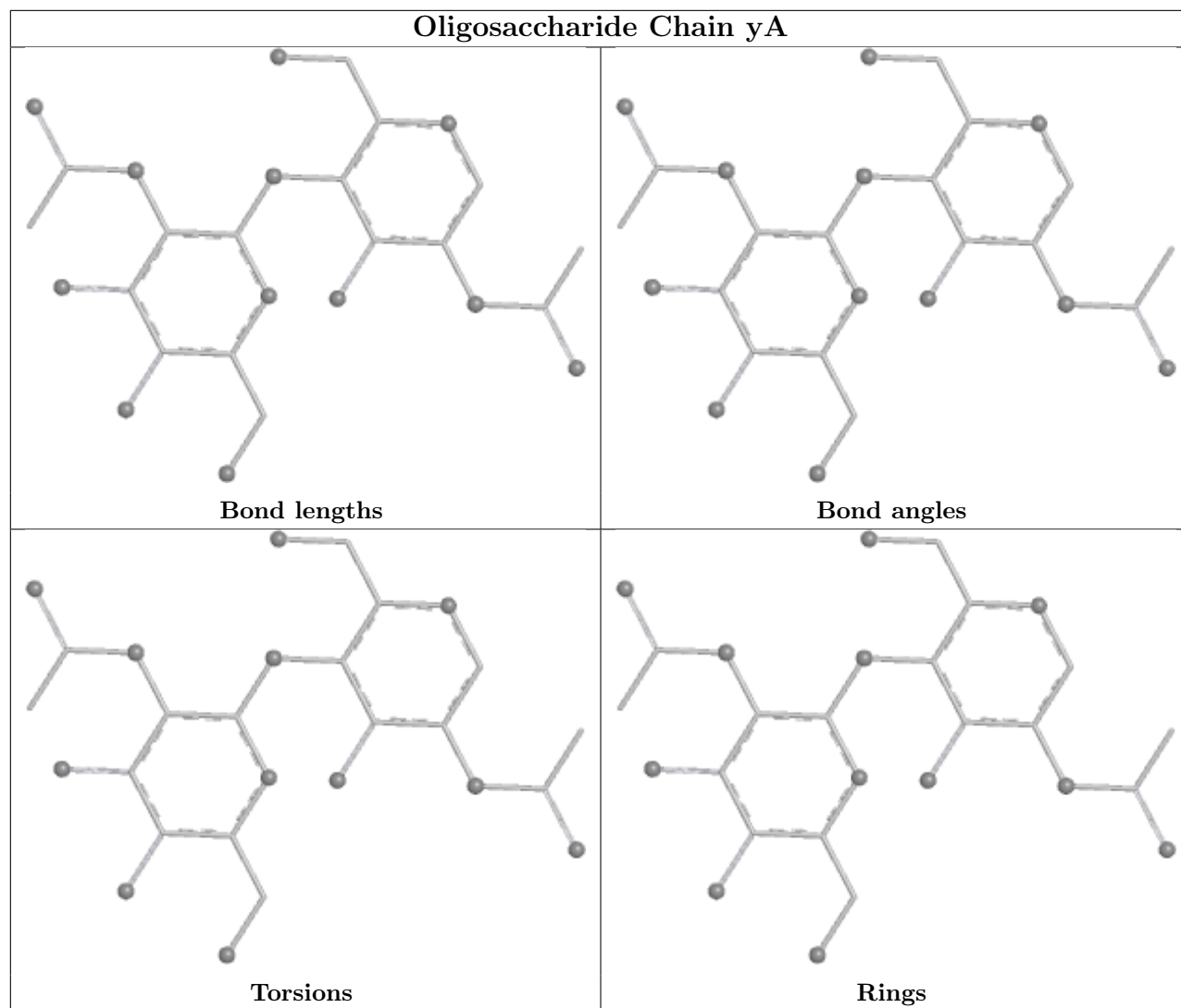


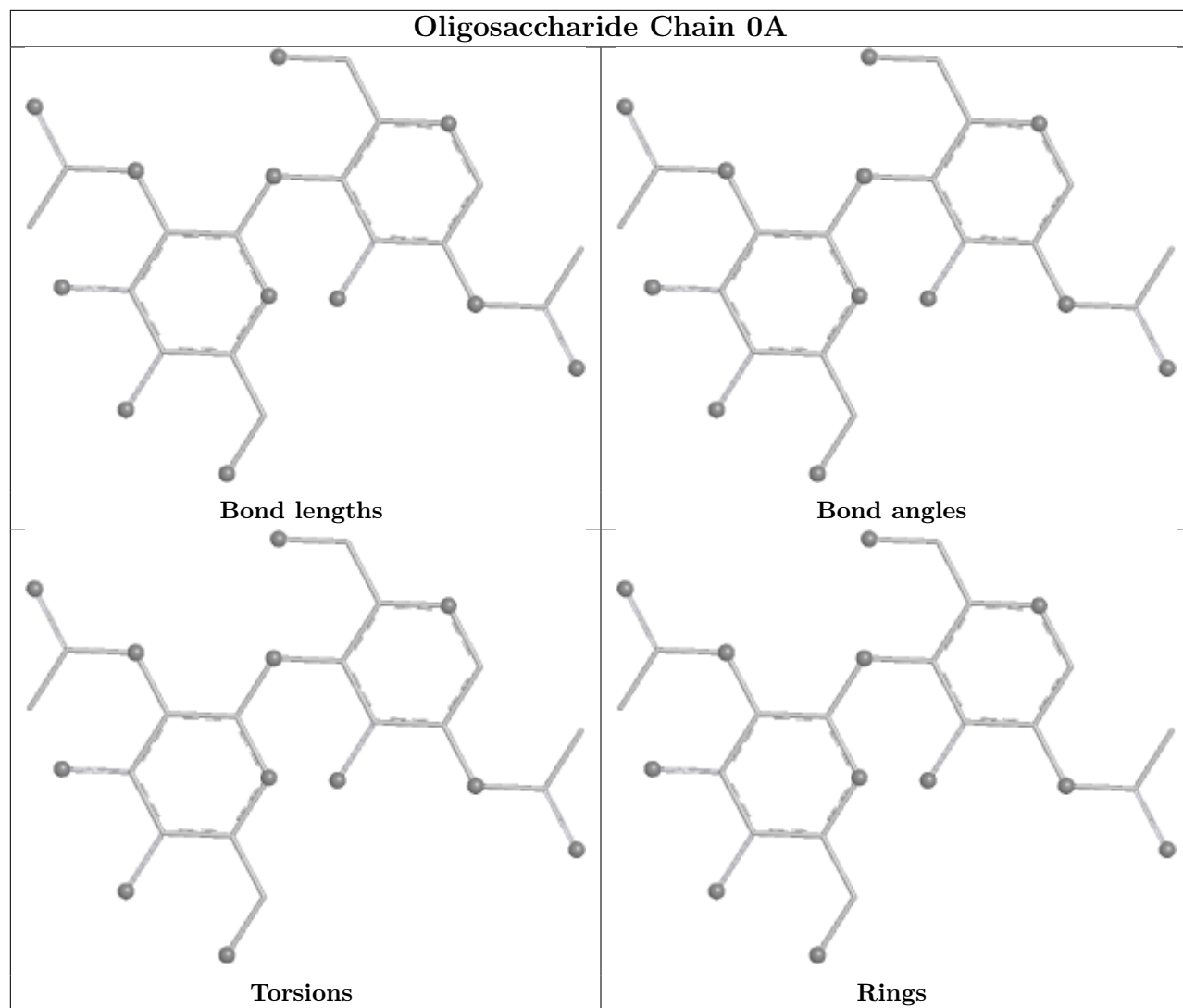


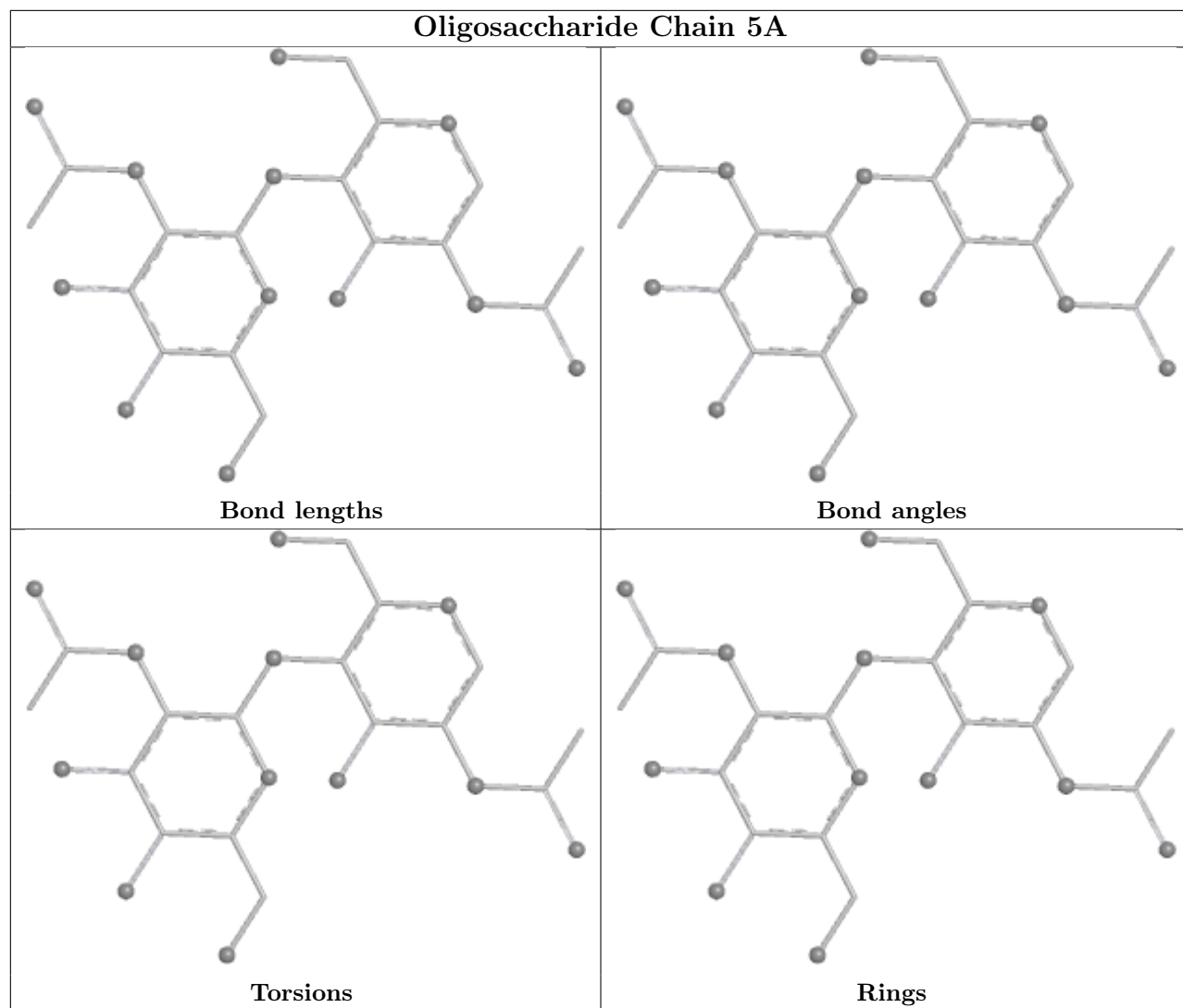


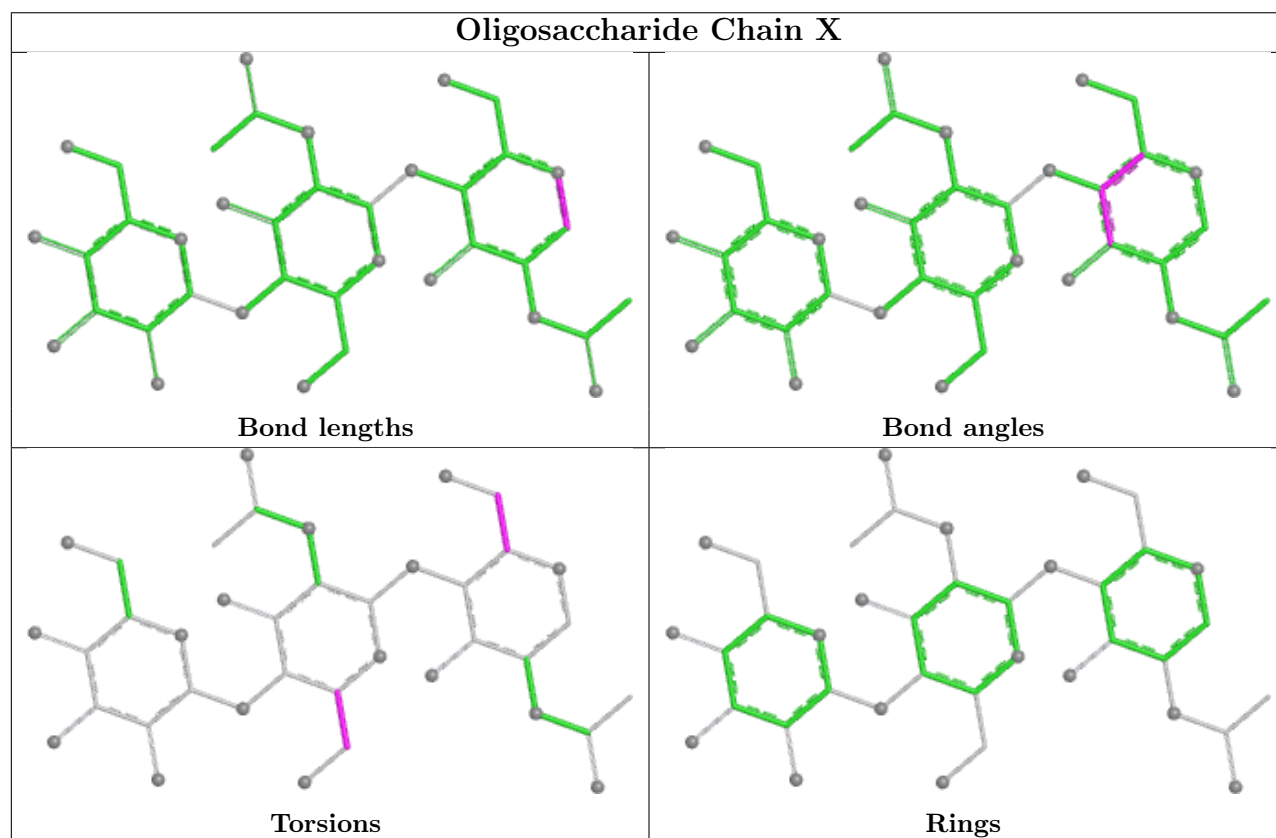
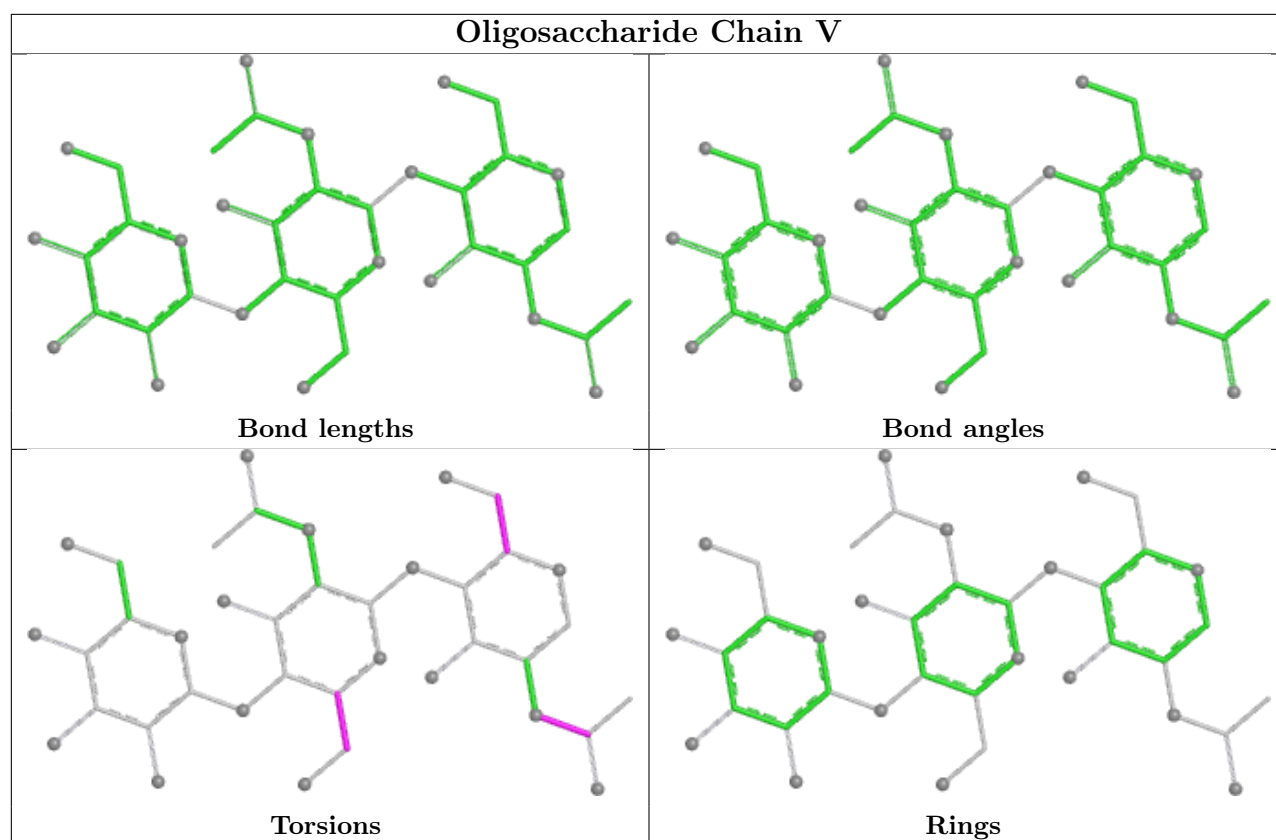


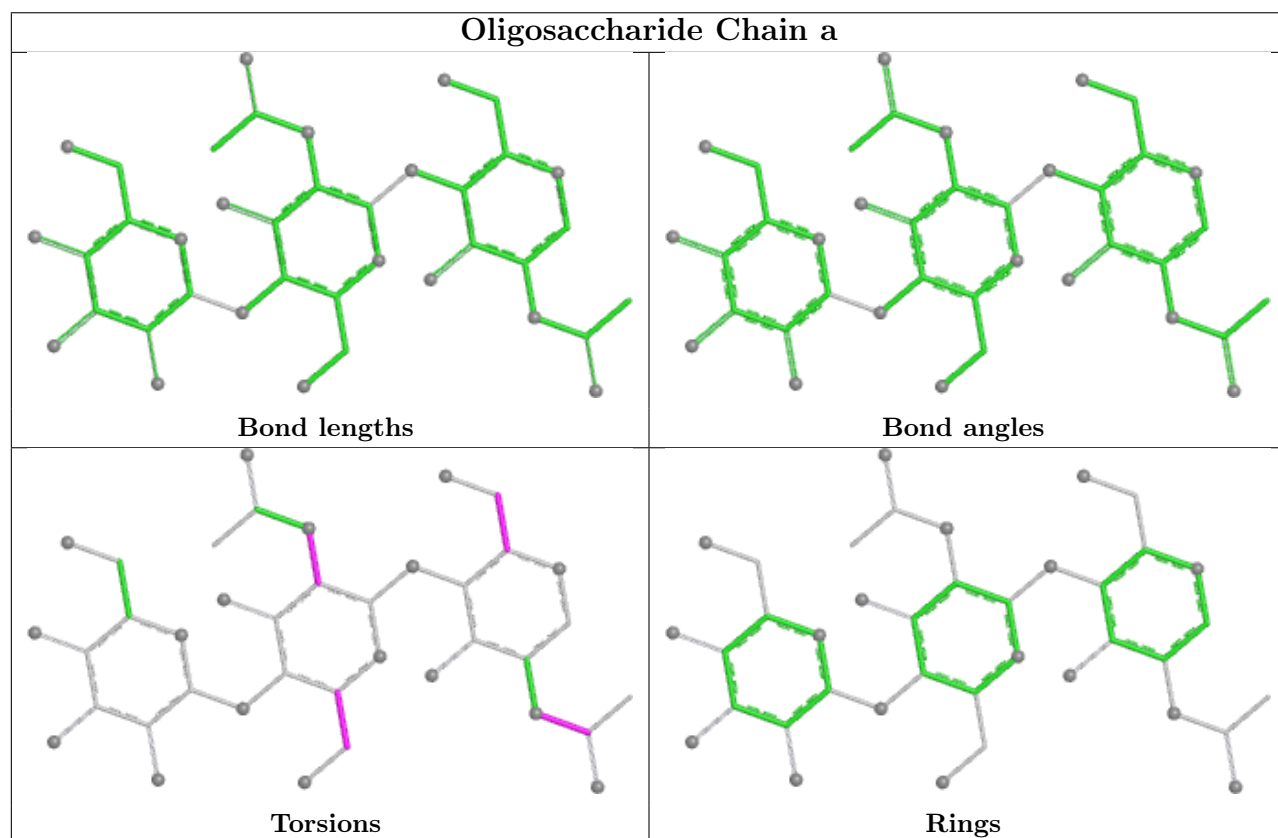
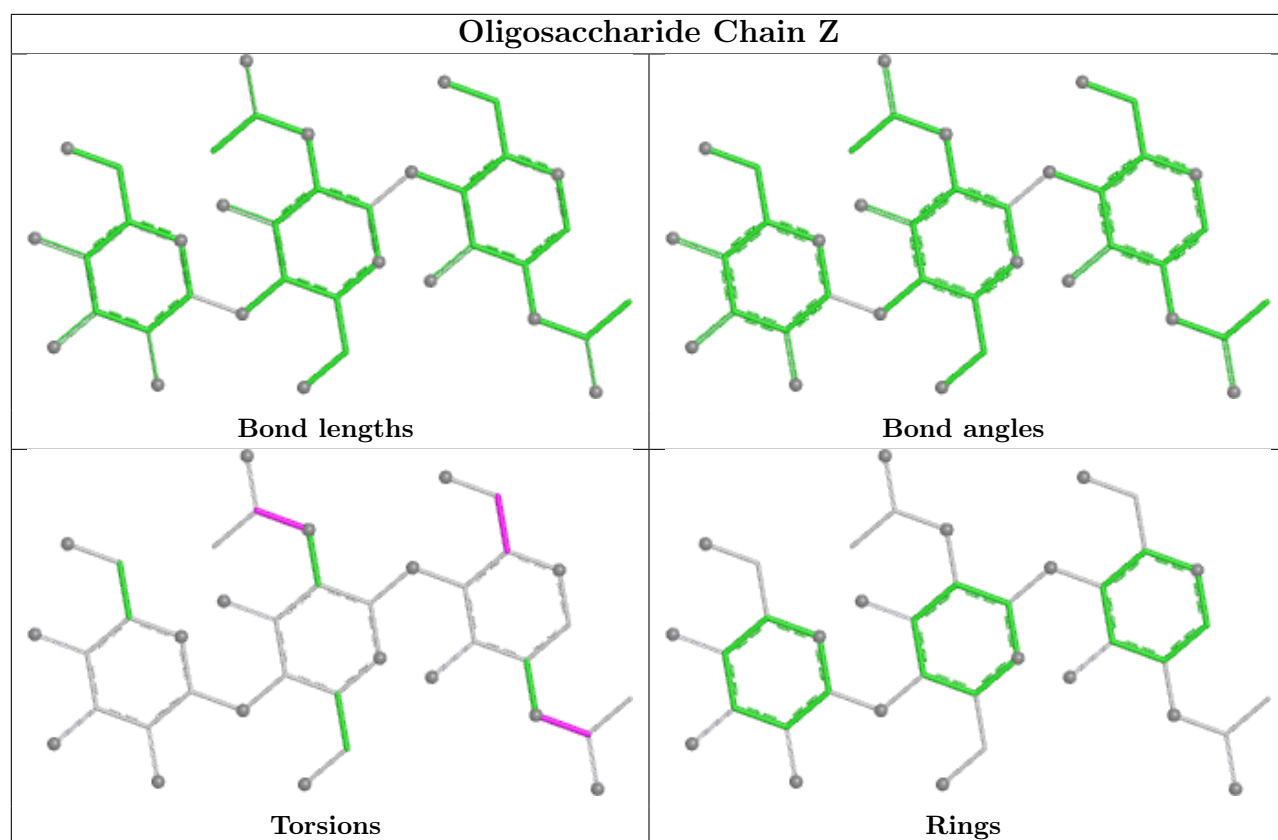


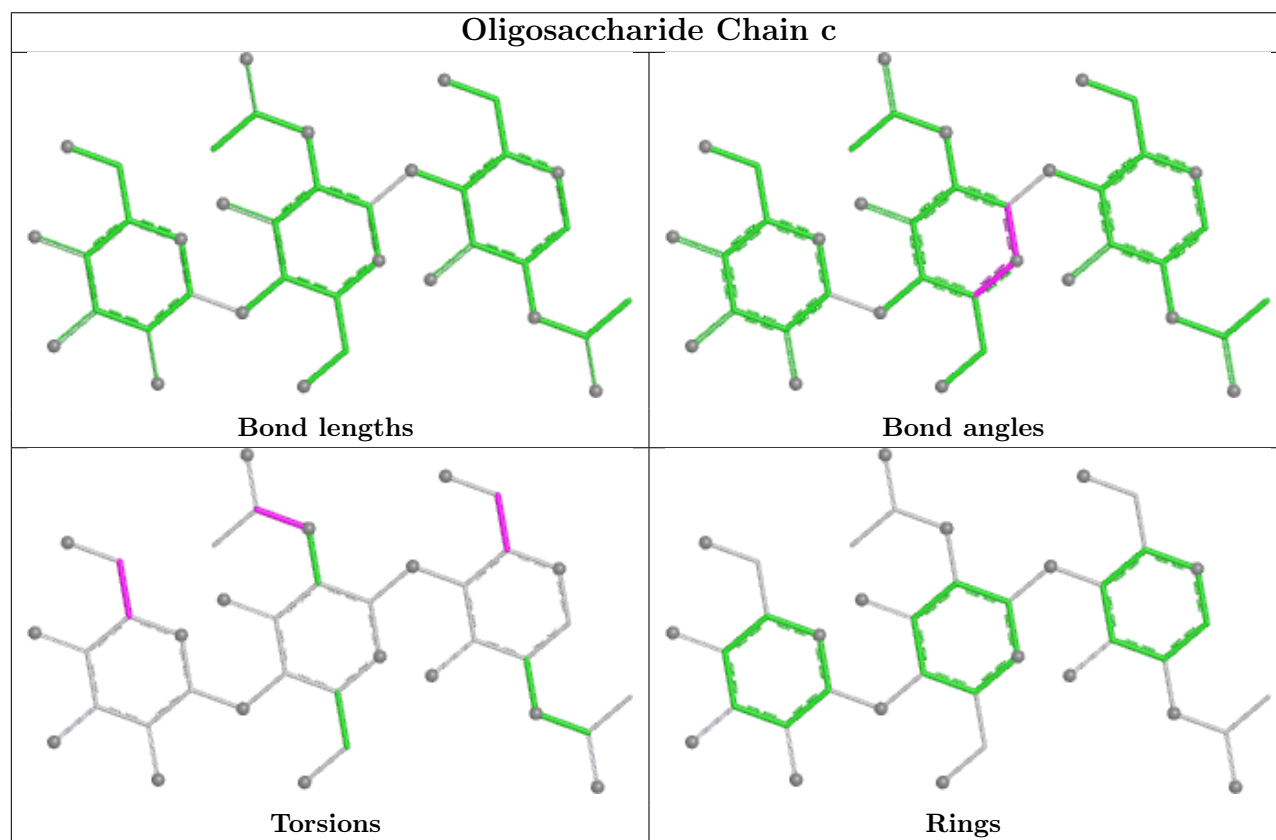
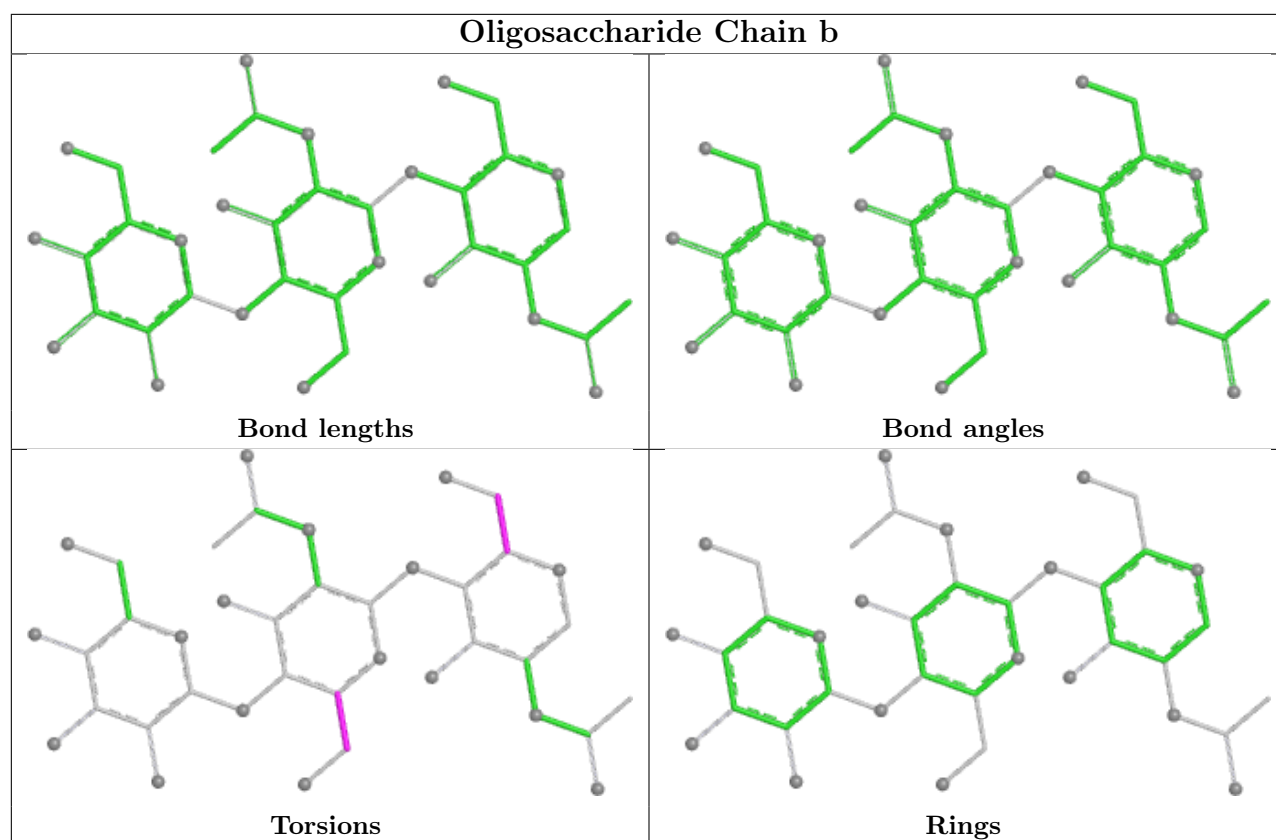


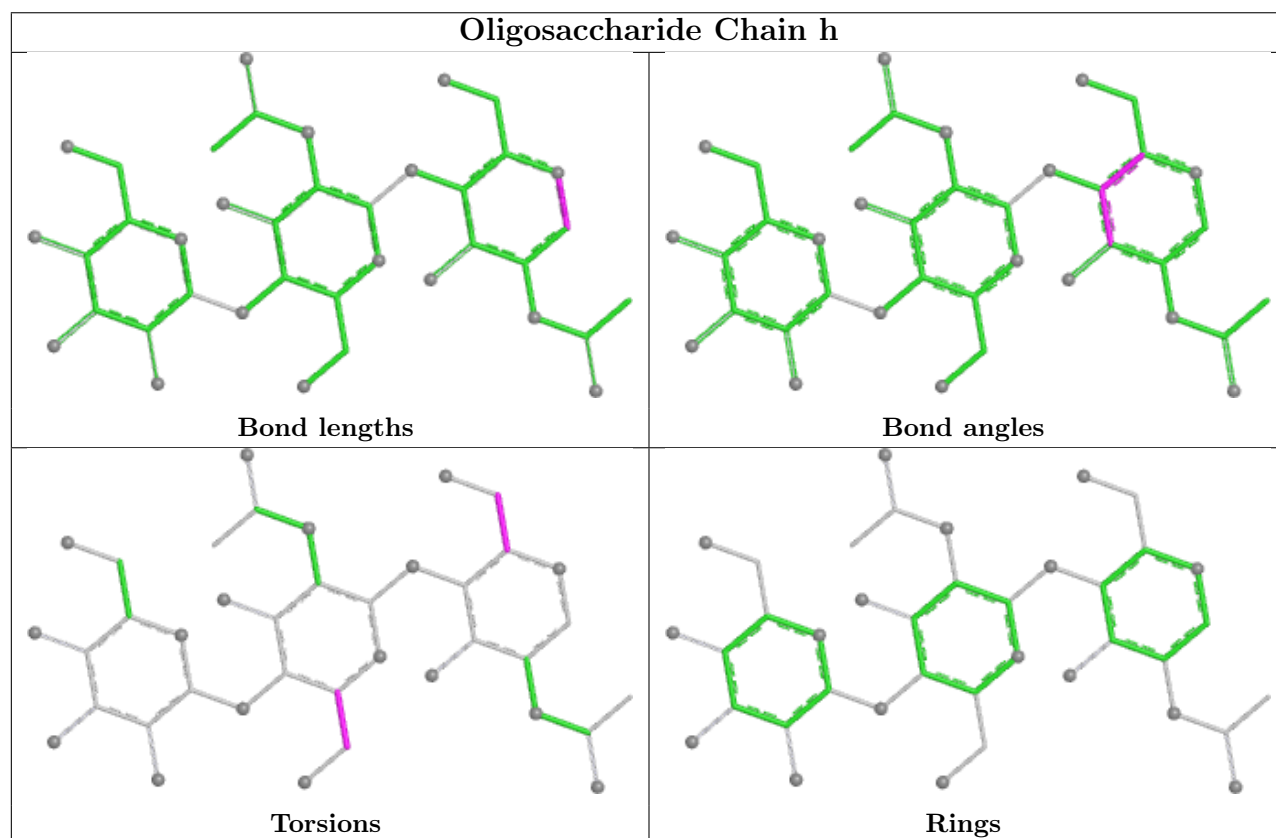
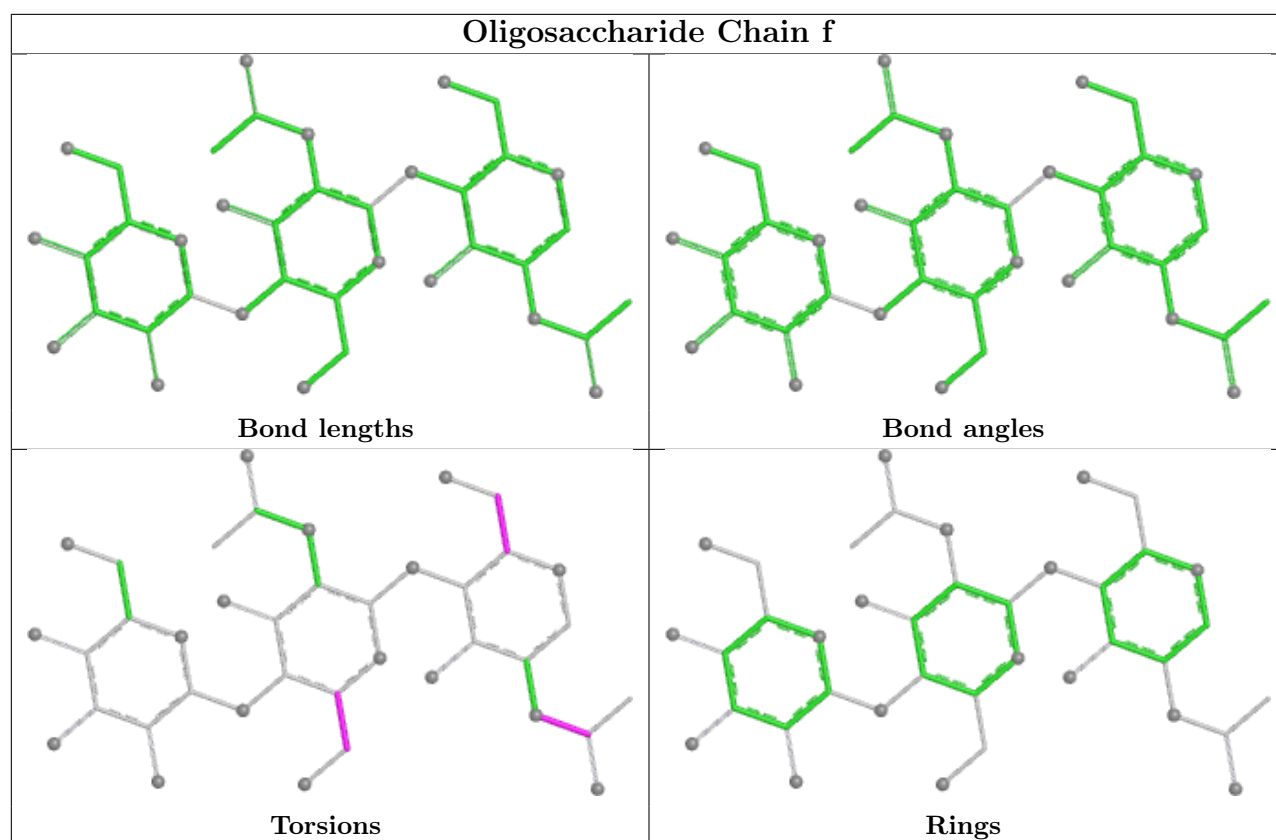


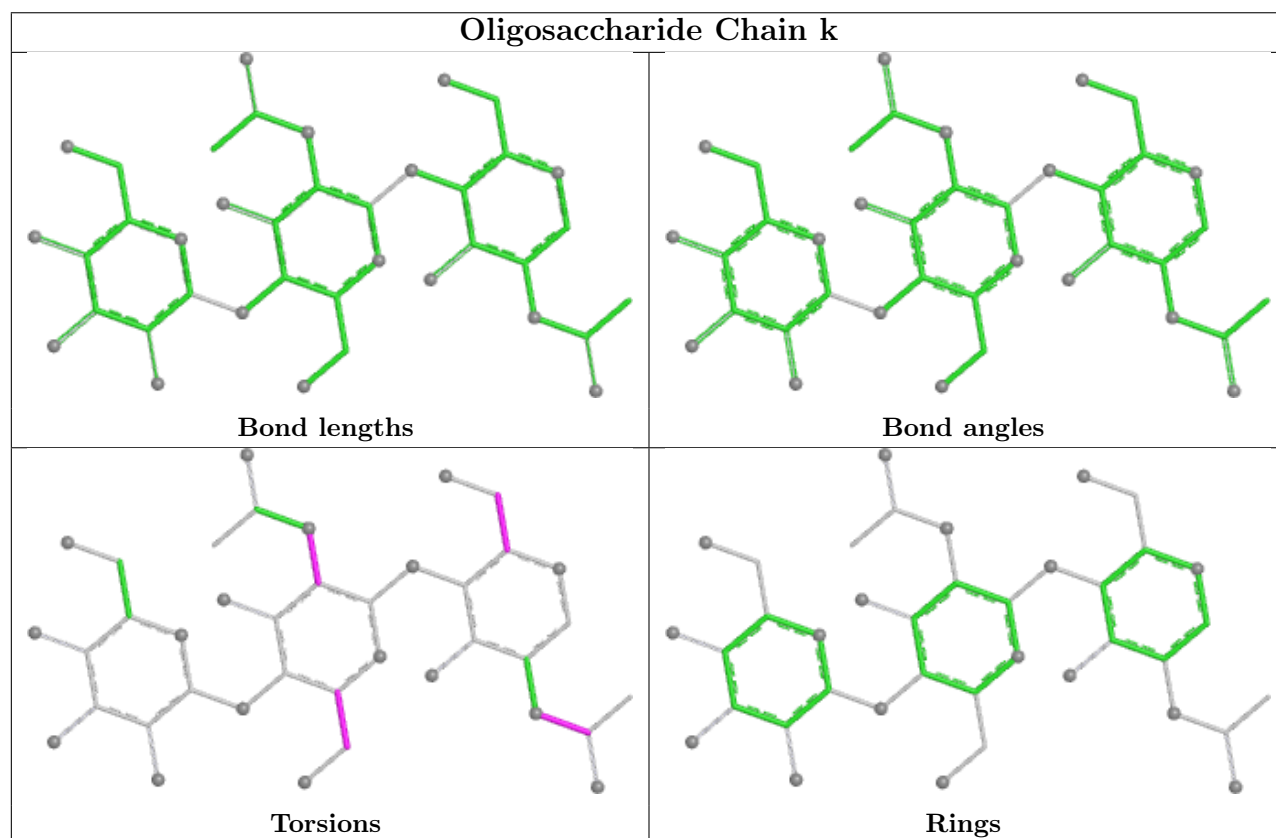
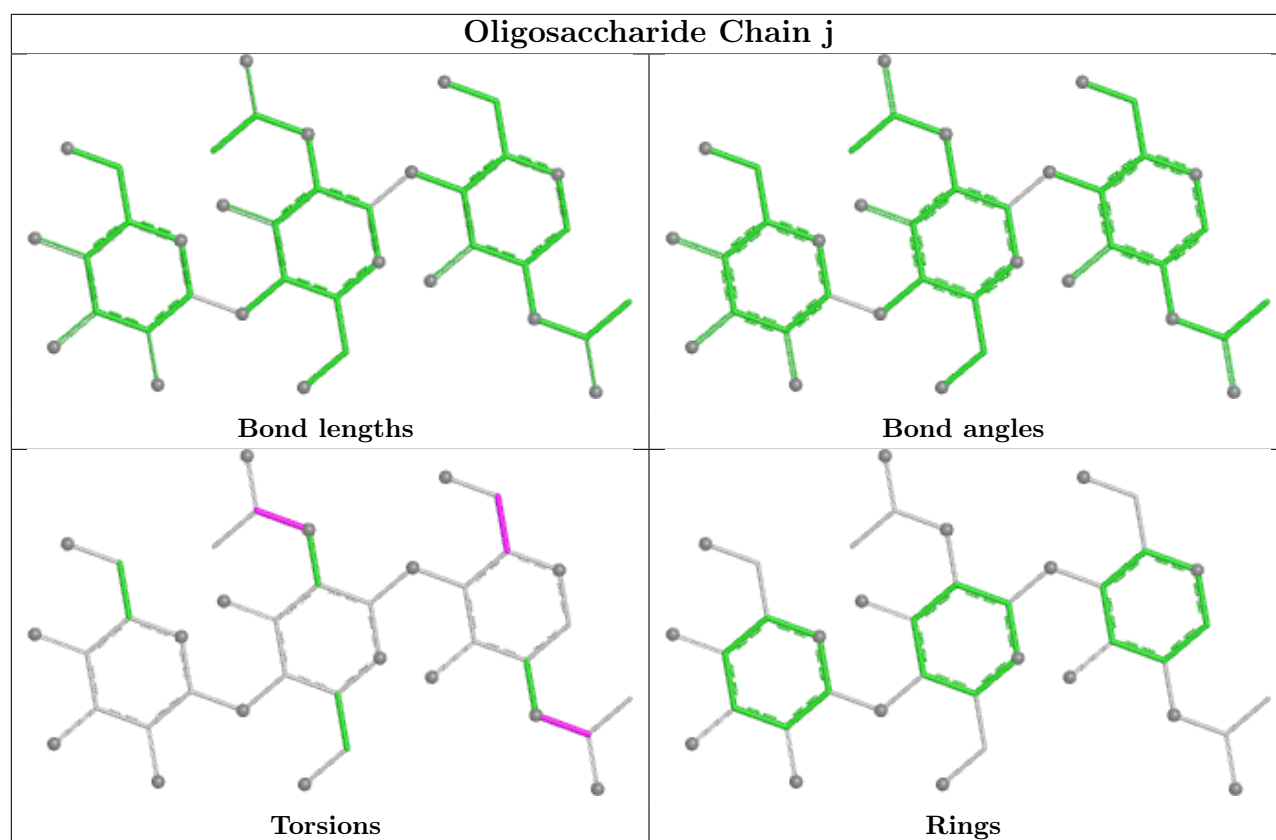


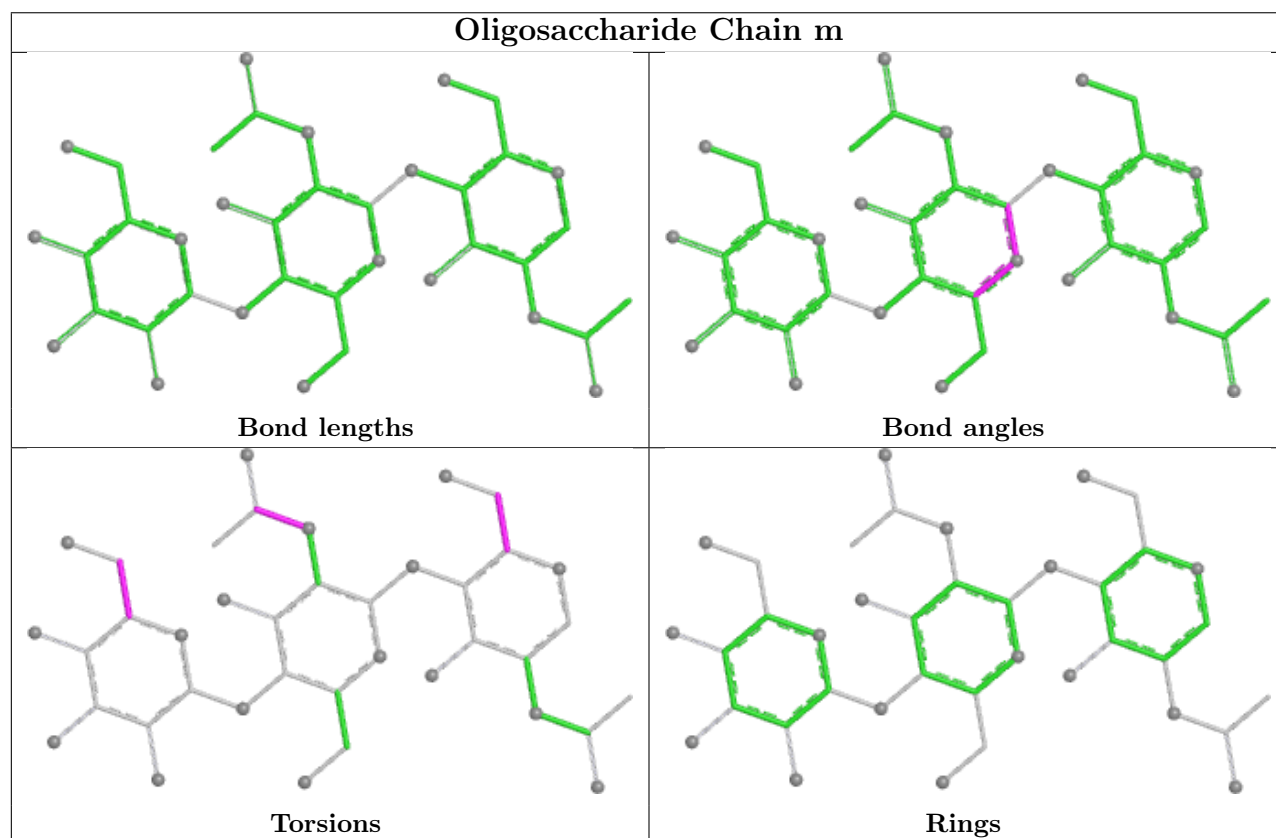
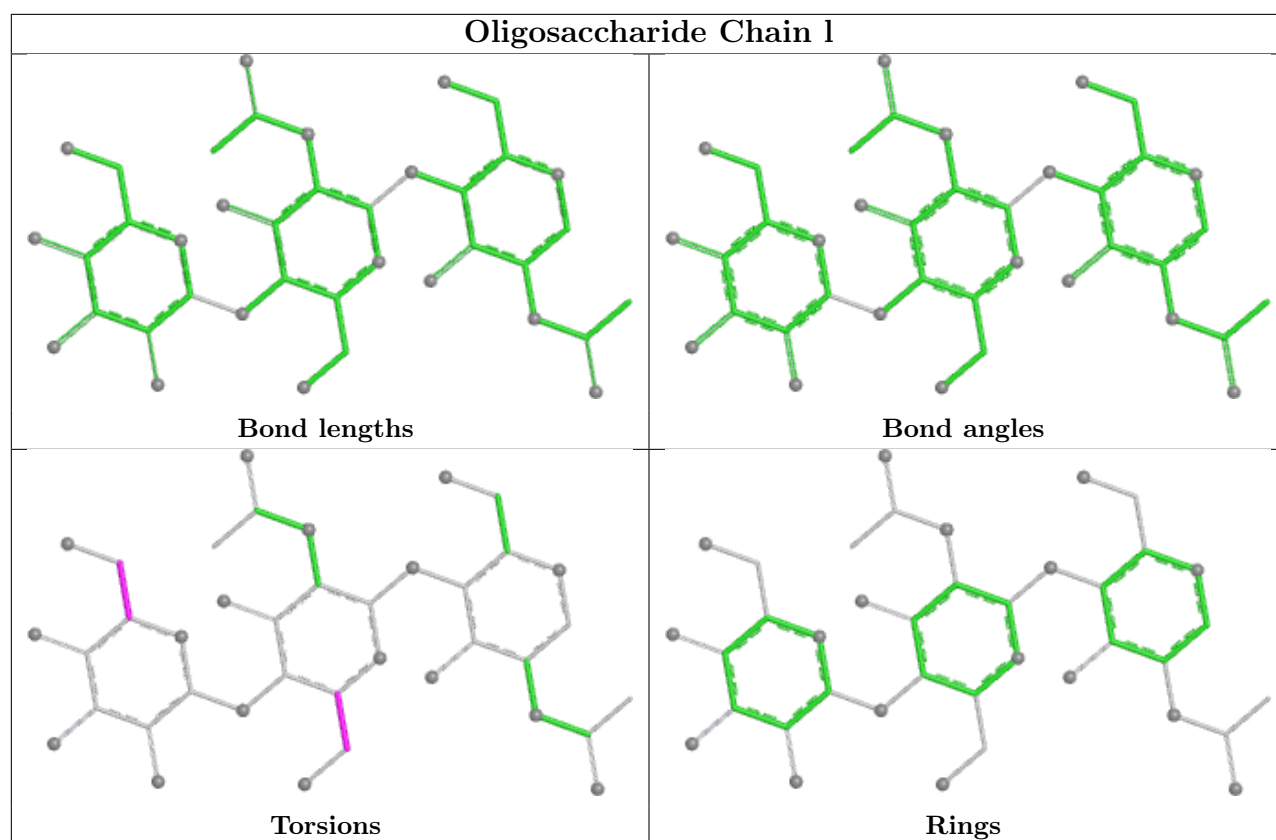


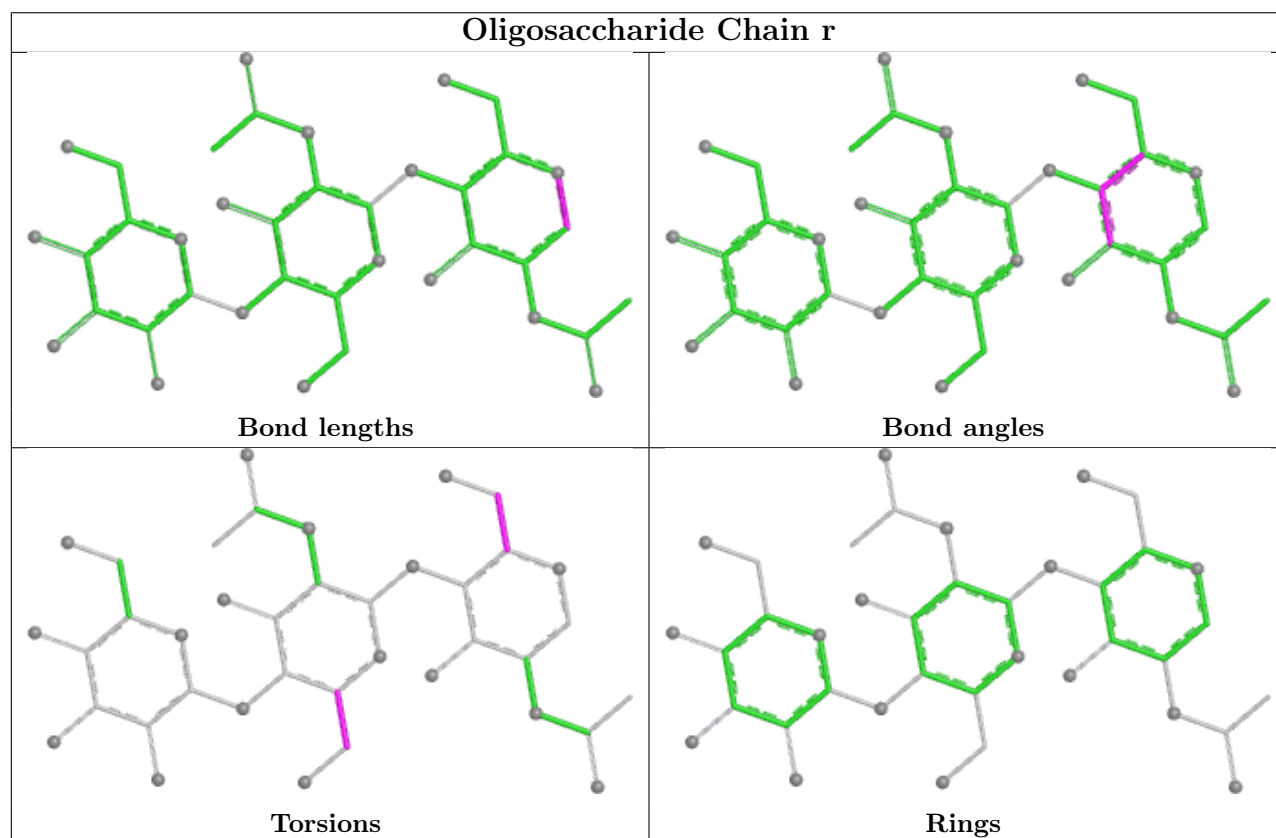
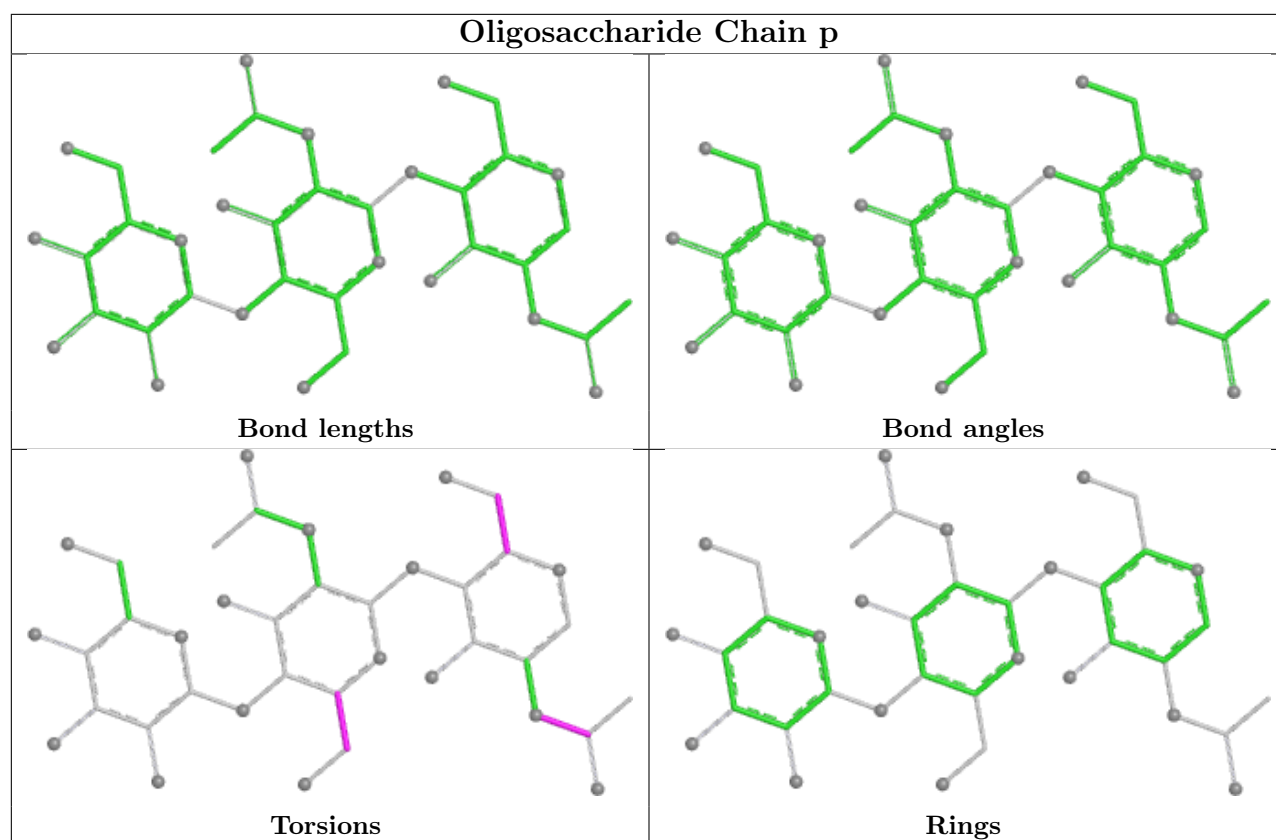


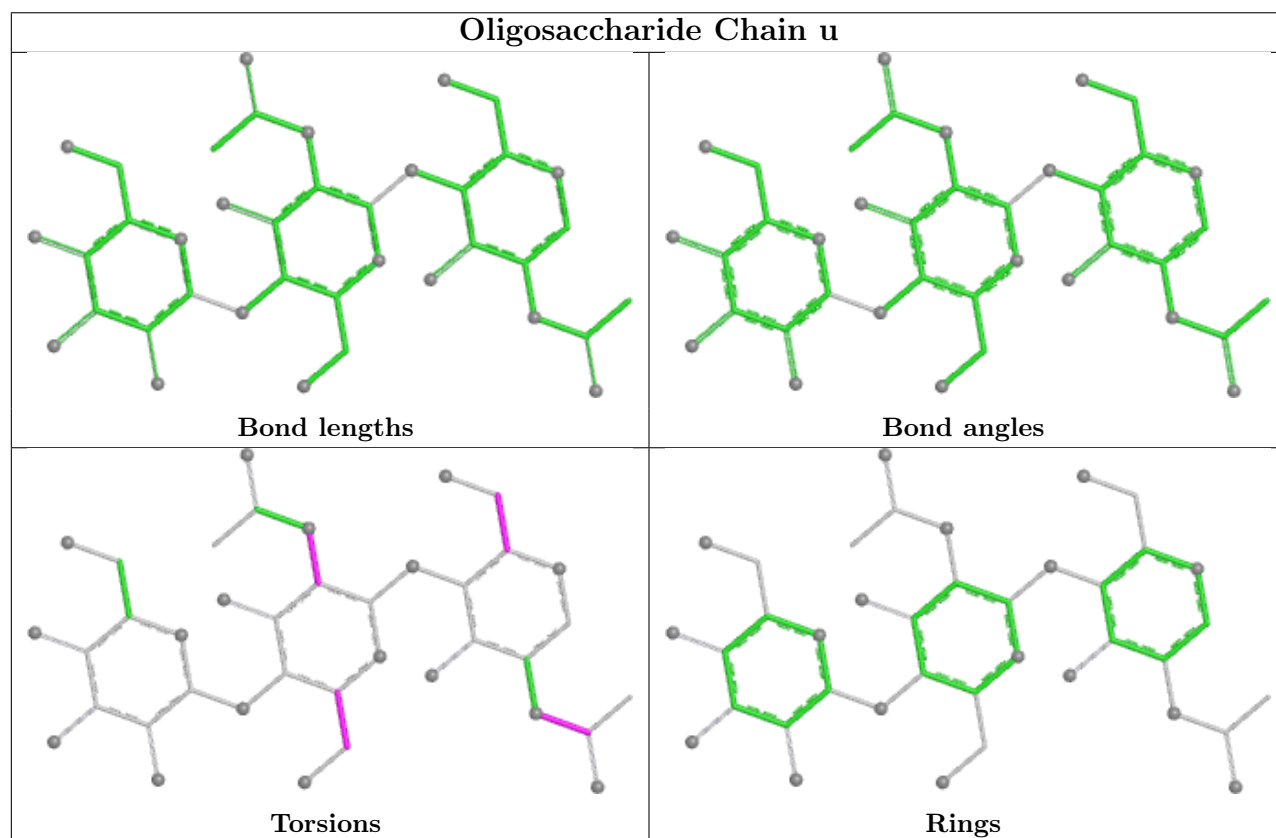
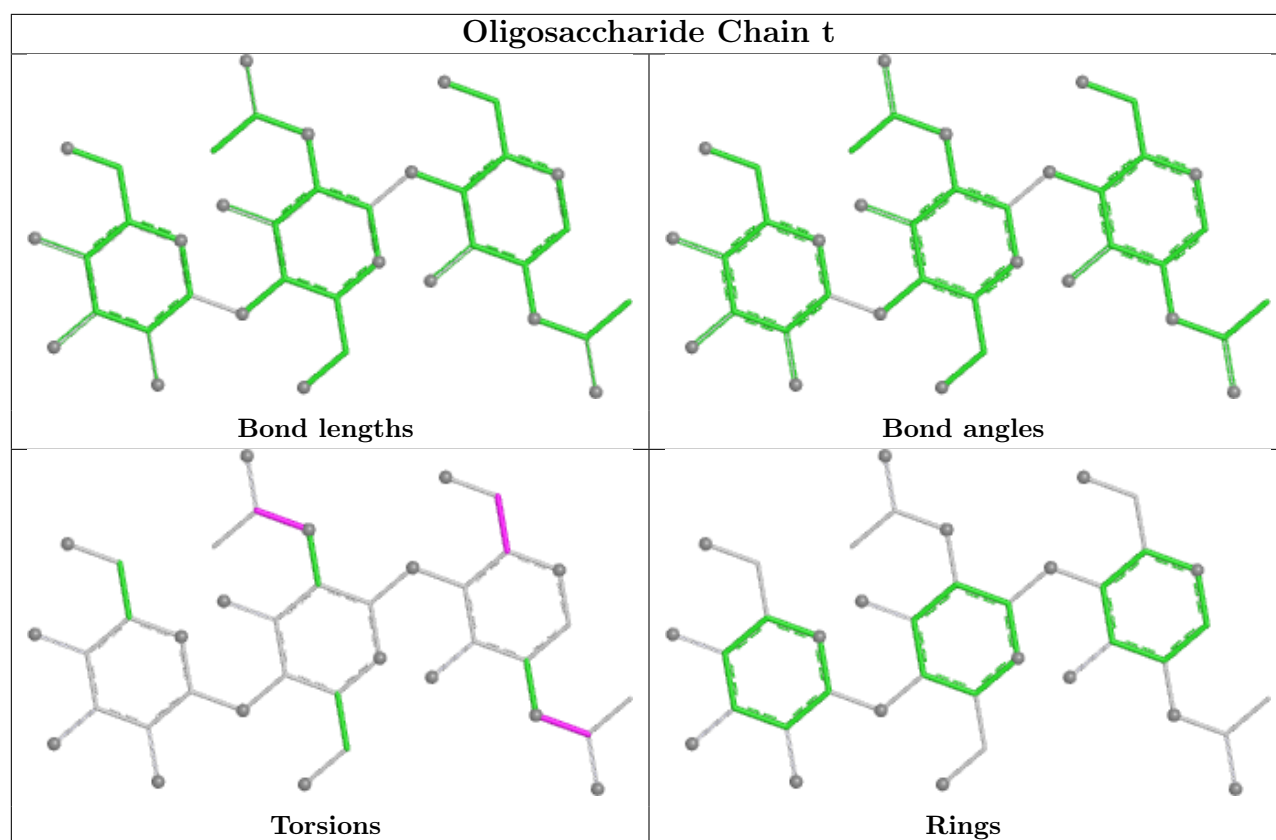


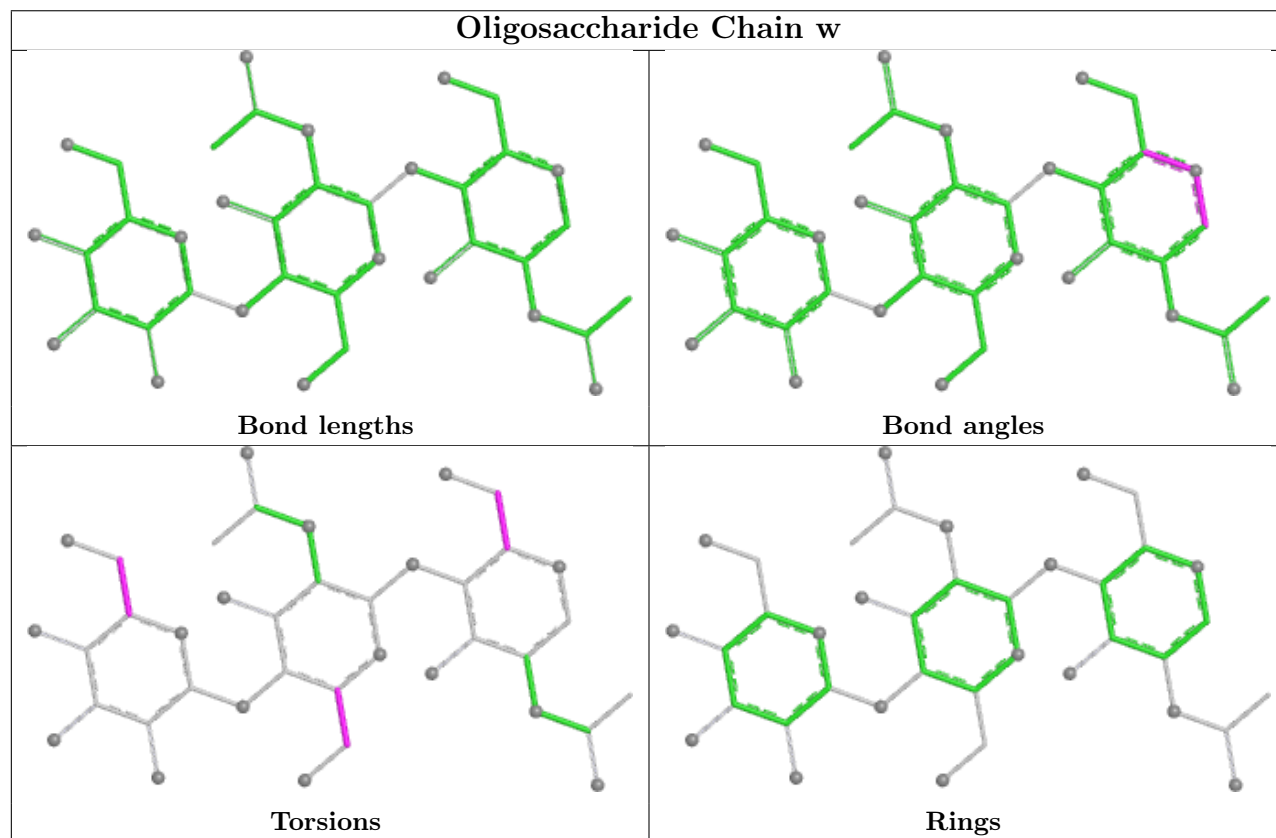
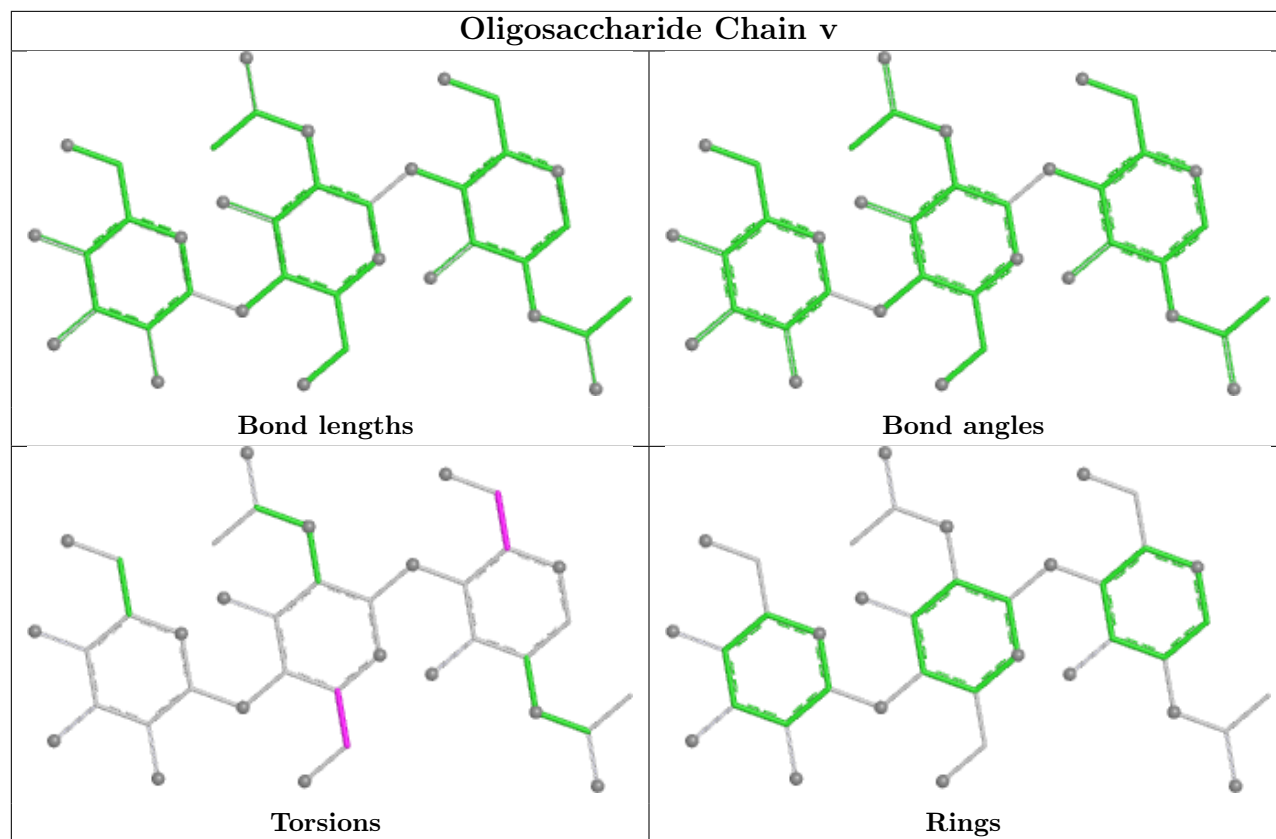


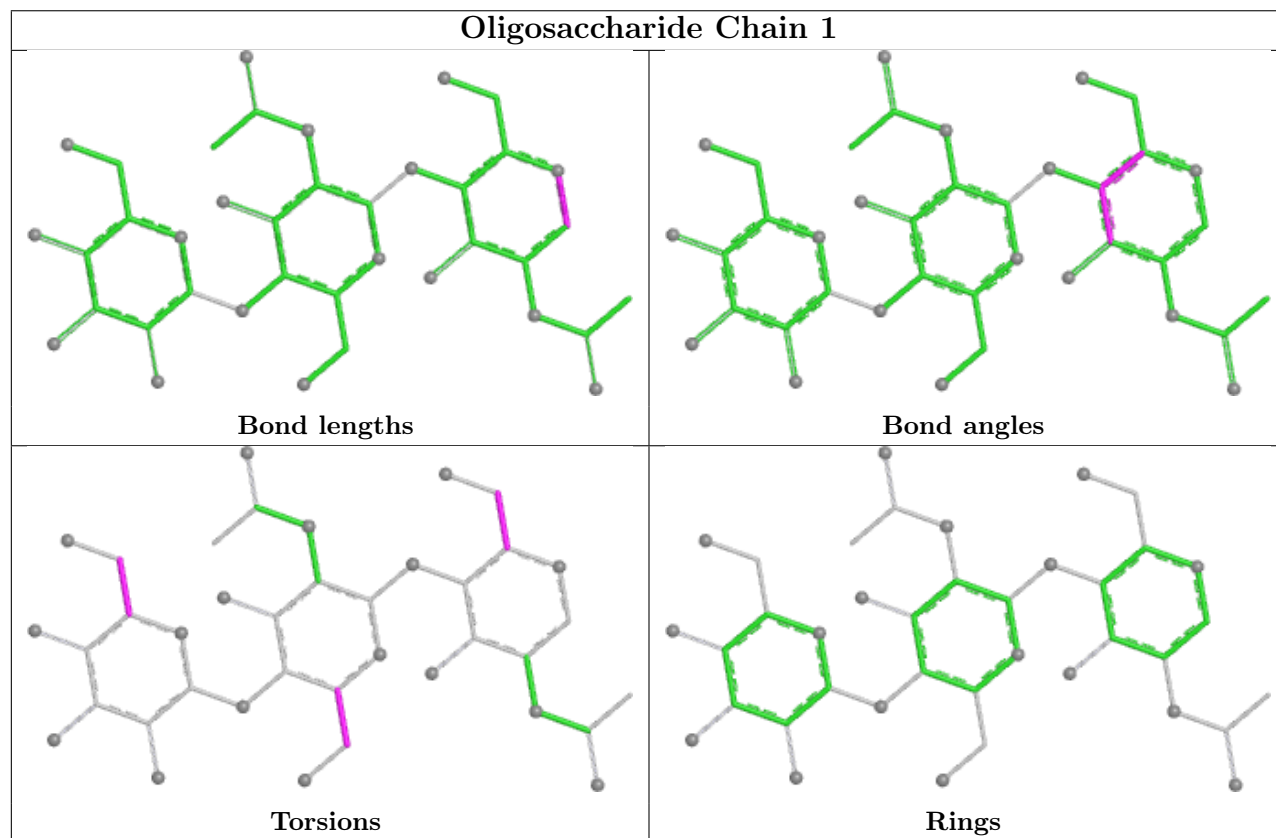
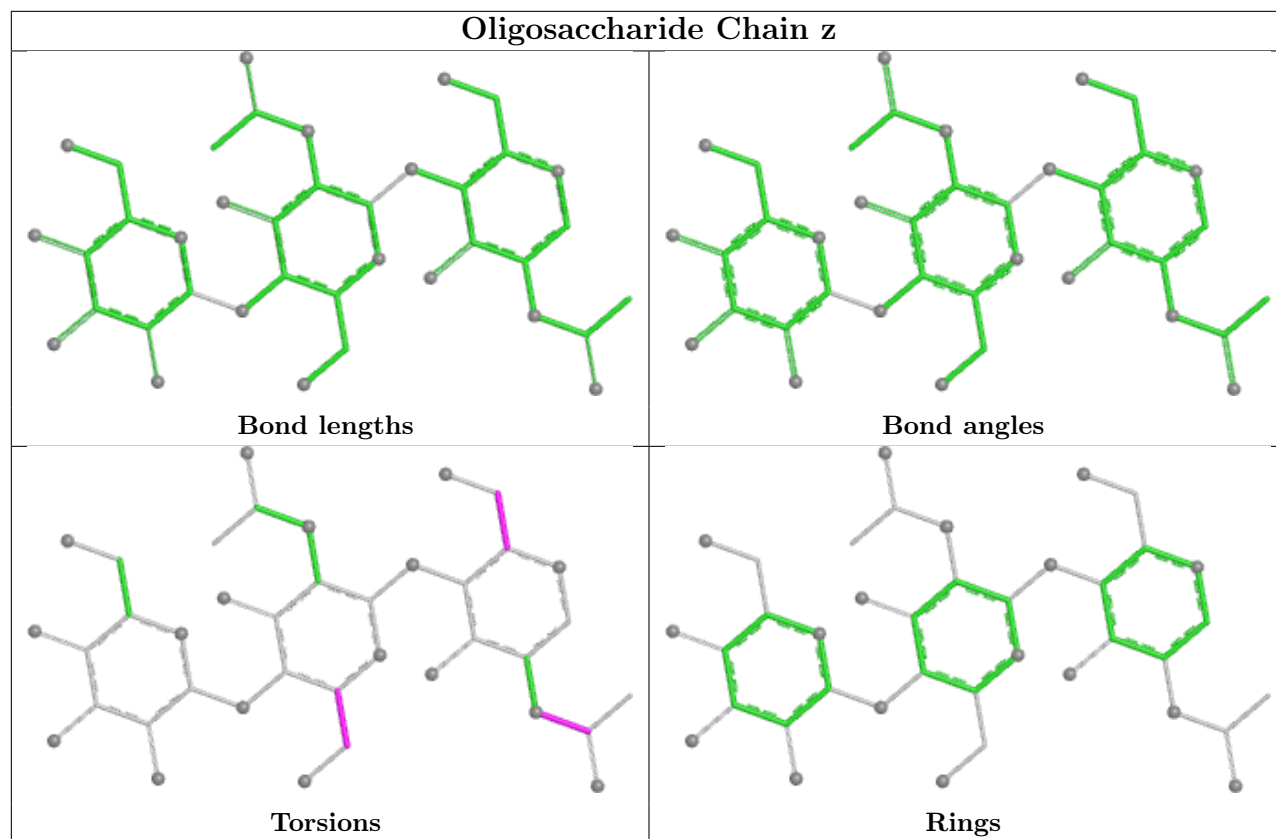


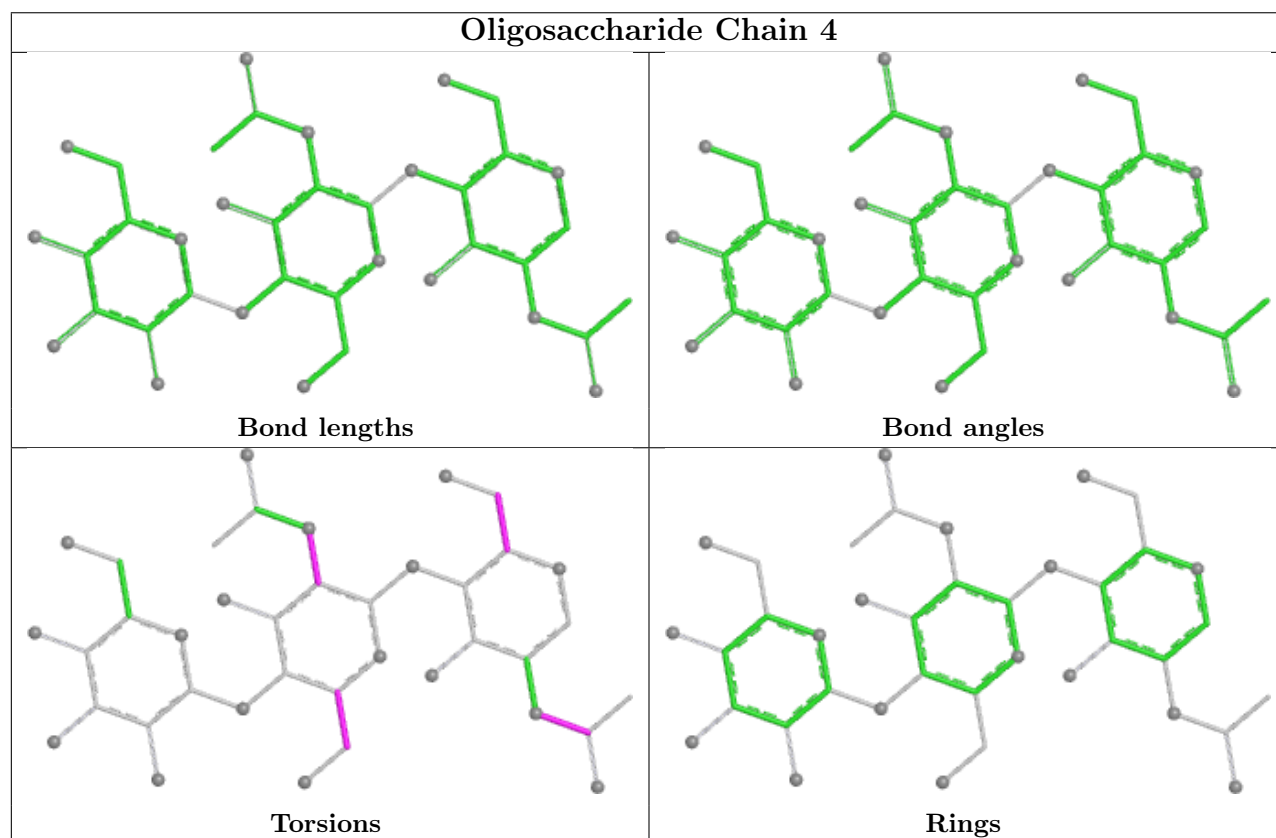
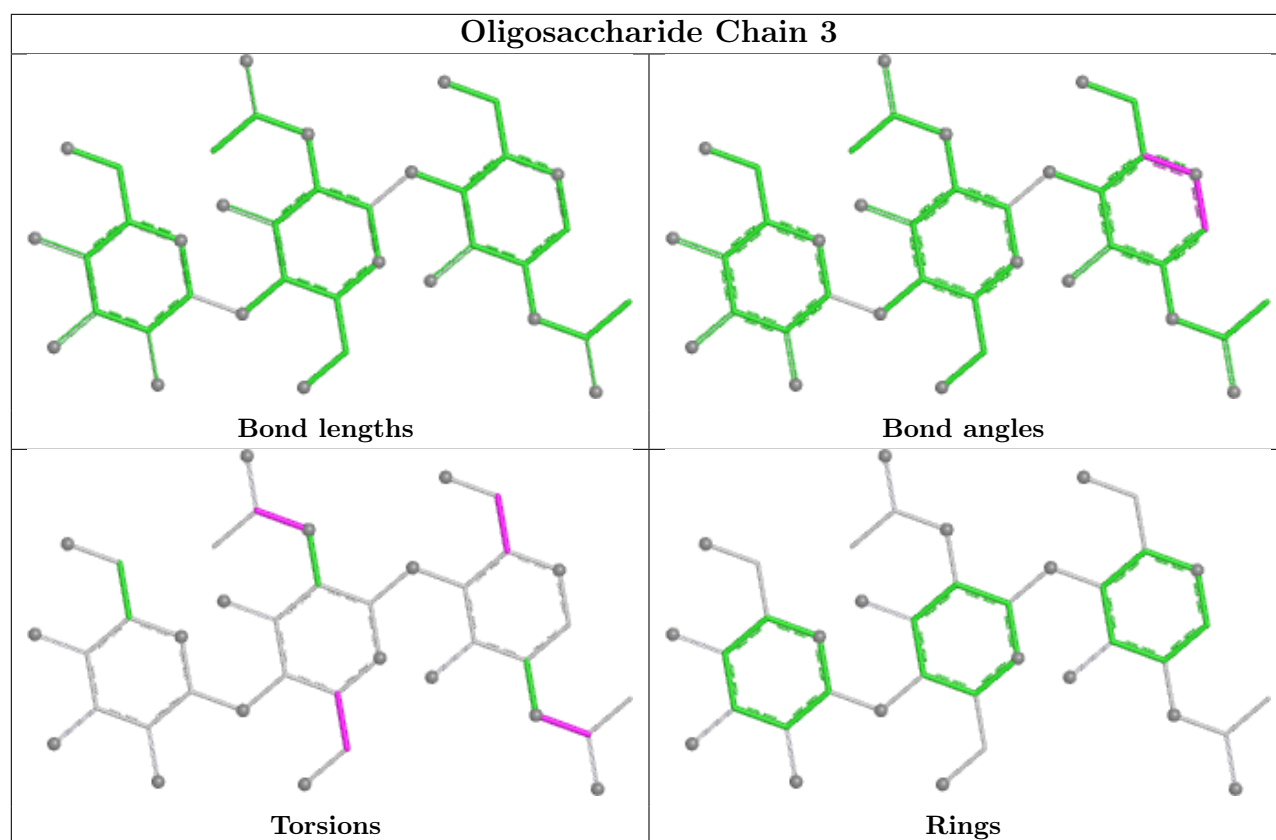




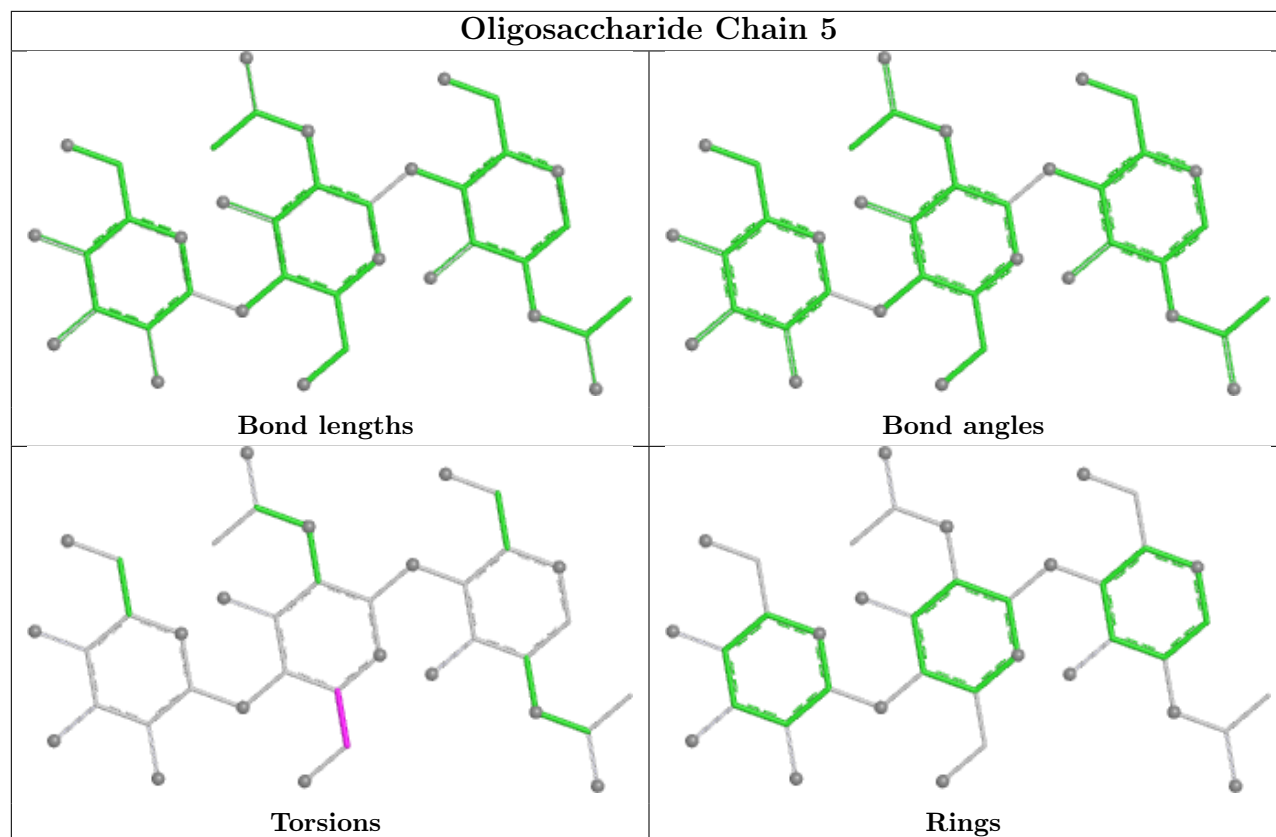




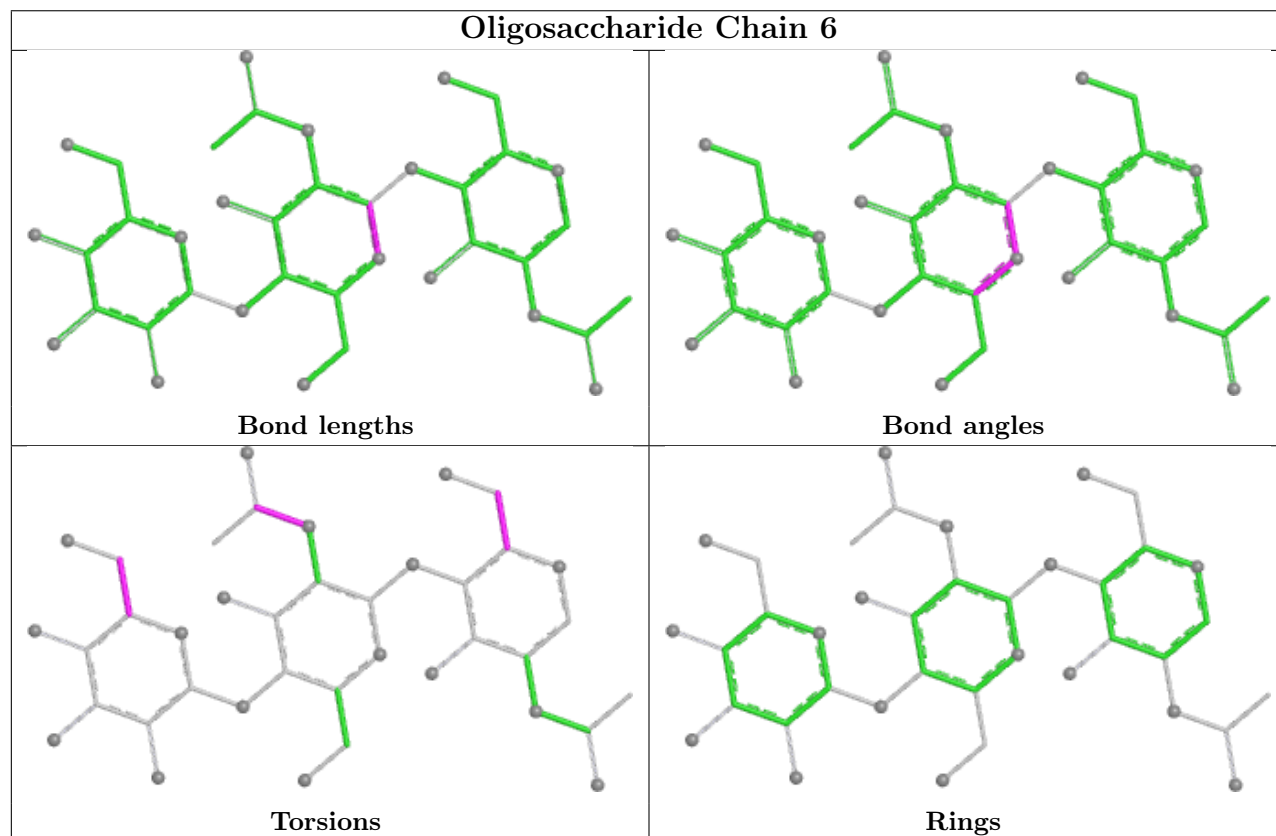


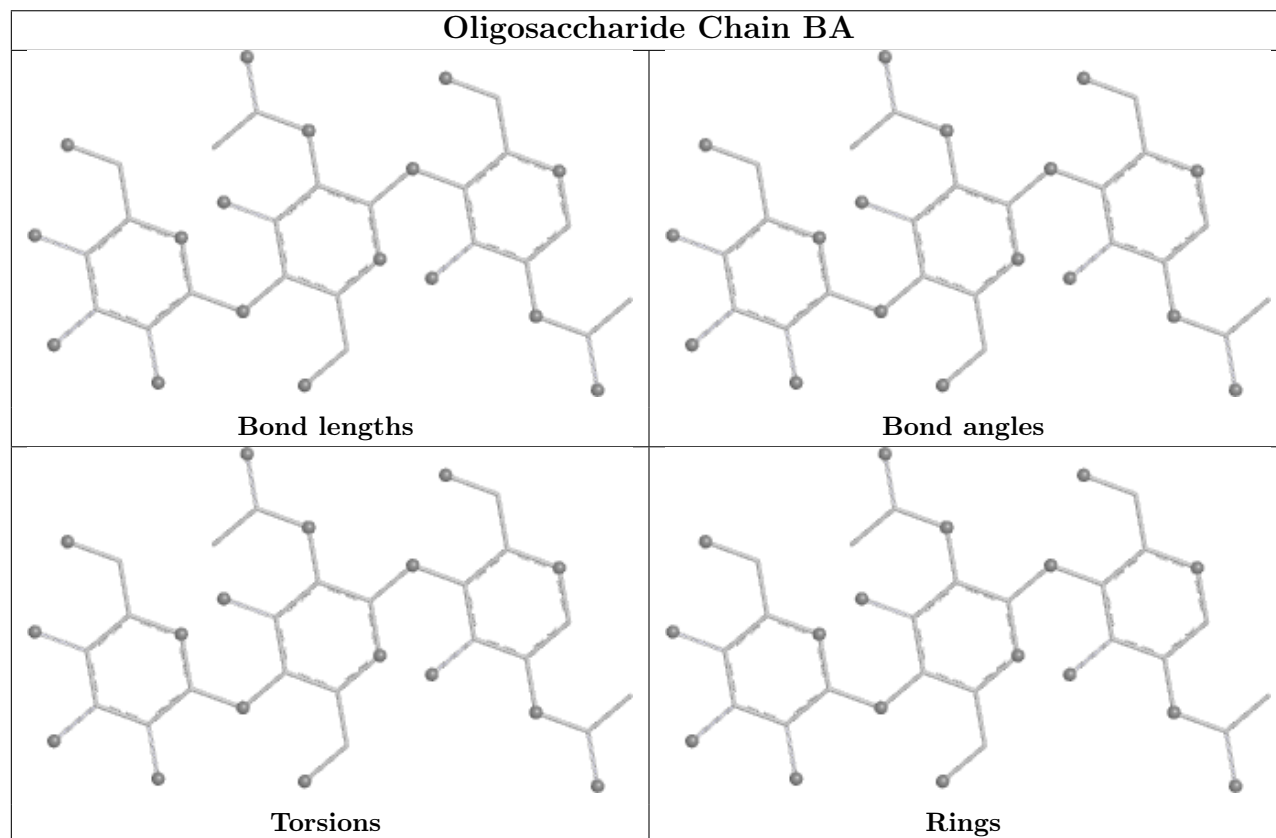
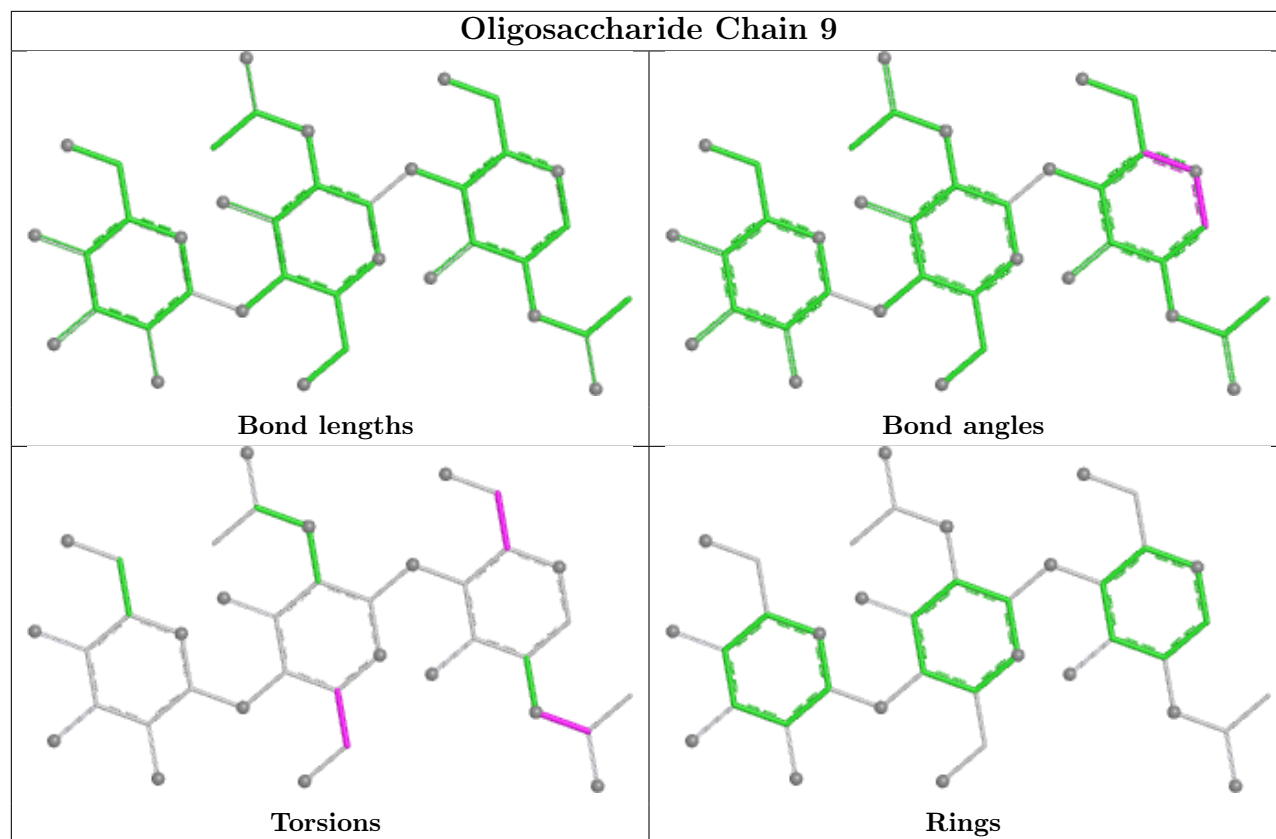


Oligosaccharide Chain 5

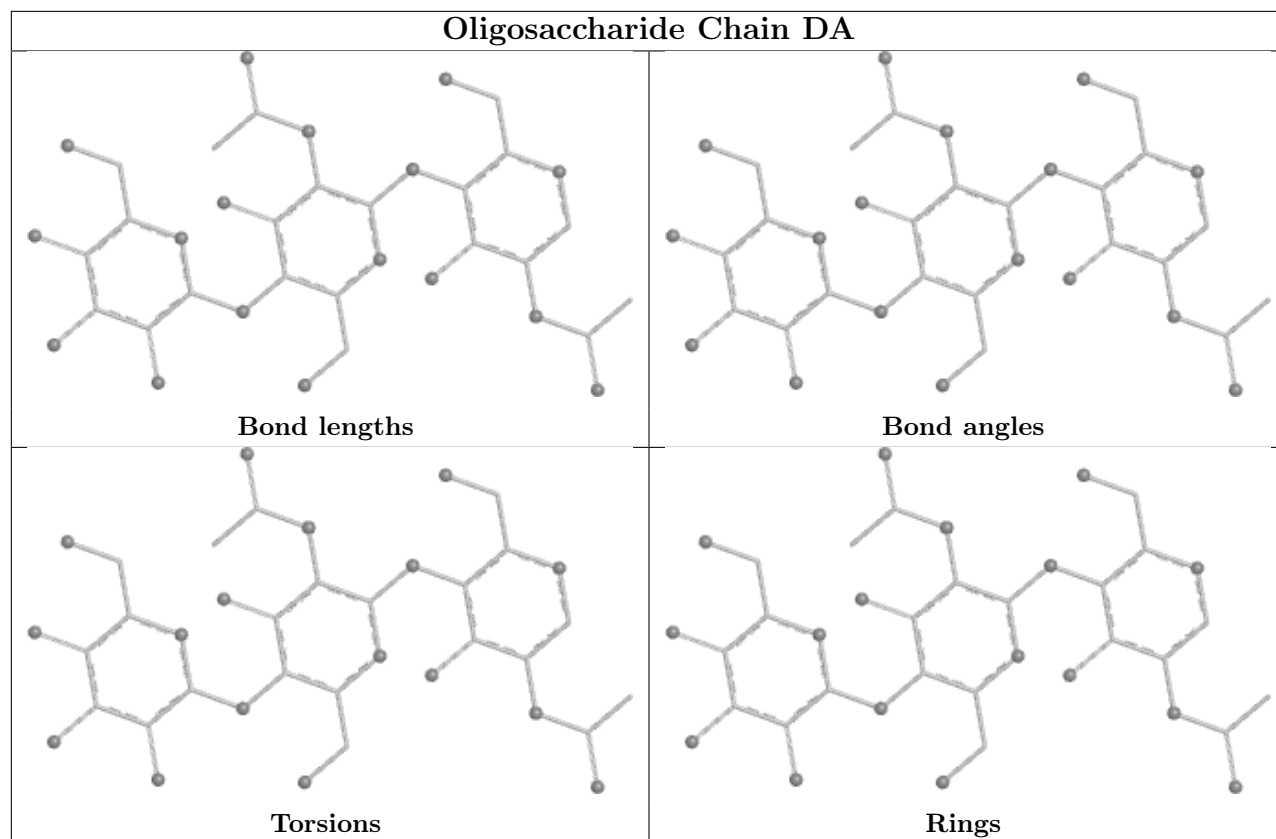


Oligosaccharide Chain 6

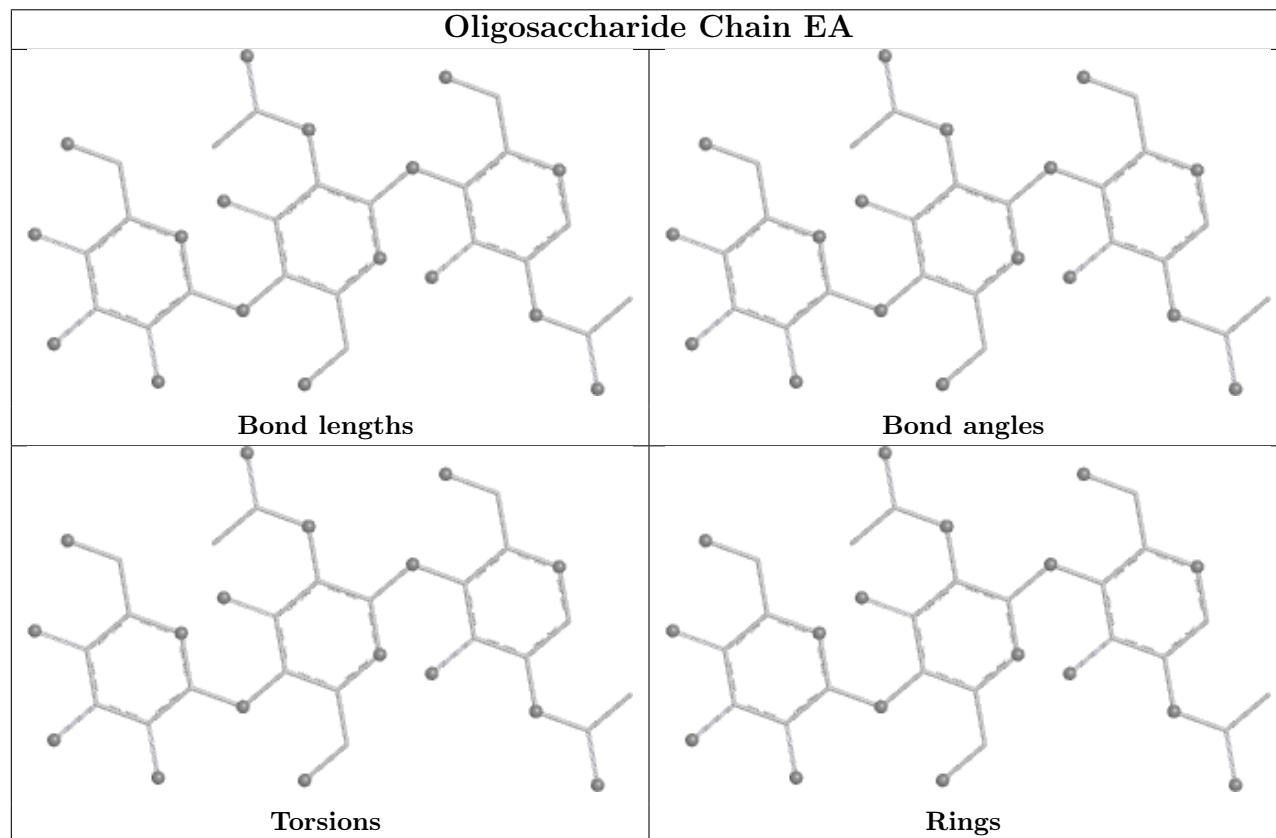


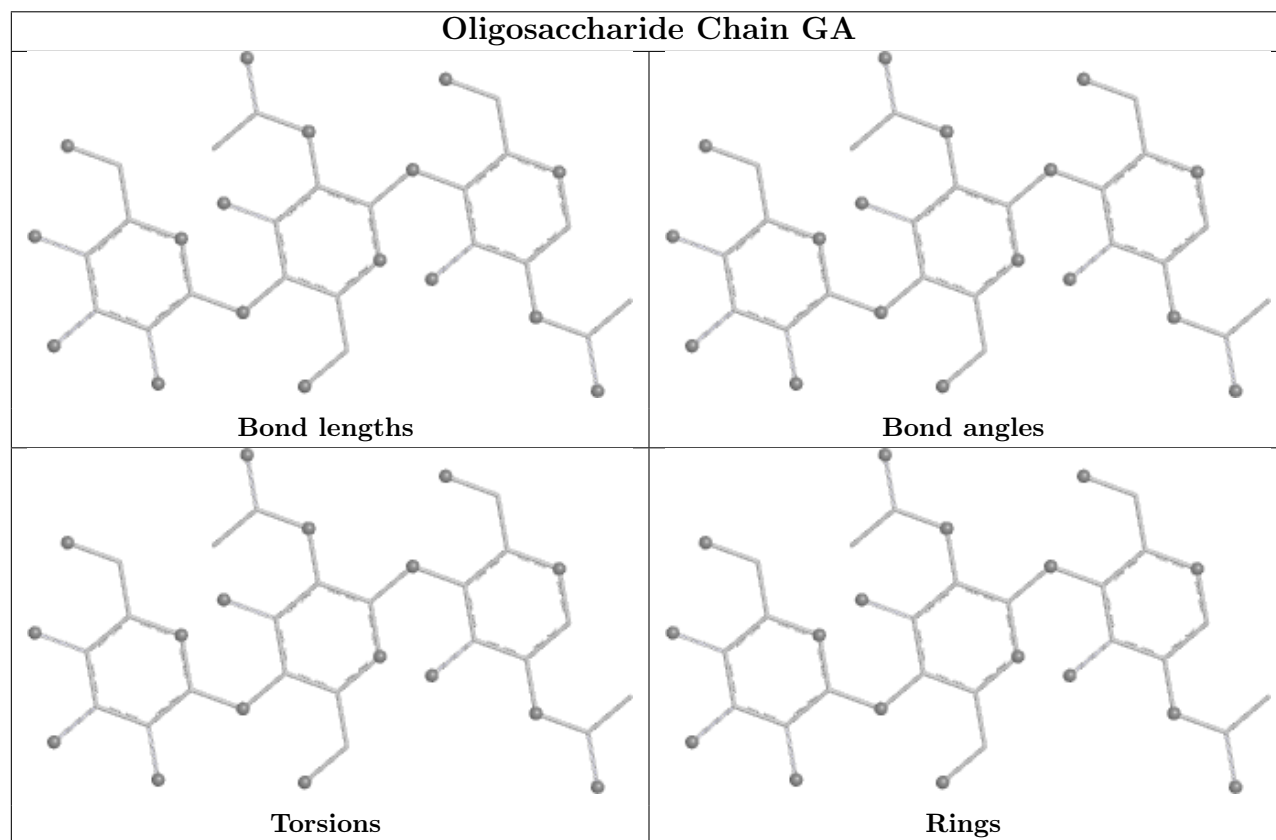
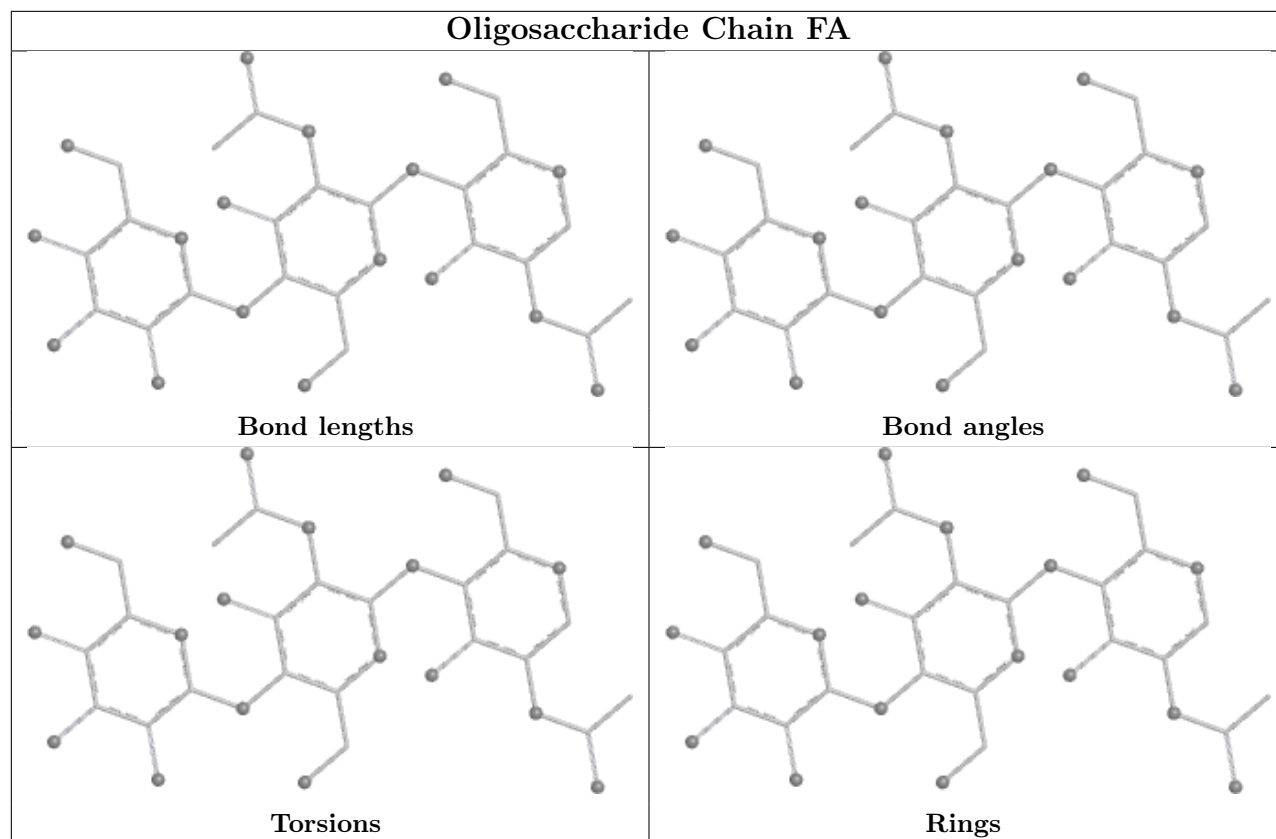


Oligosaccharide Chain DA

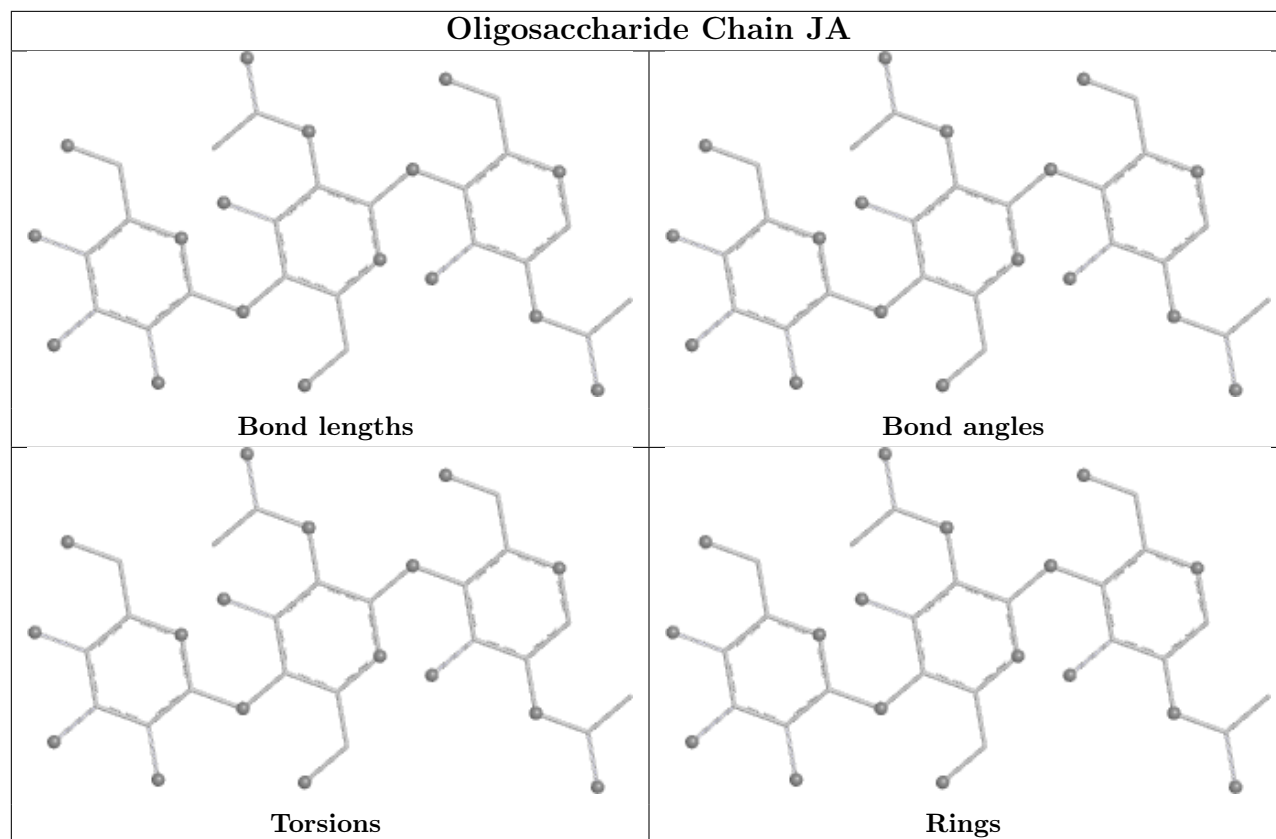


Oligosaccharide Chain EA

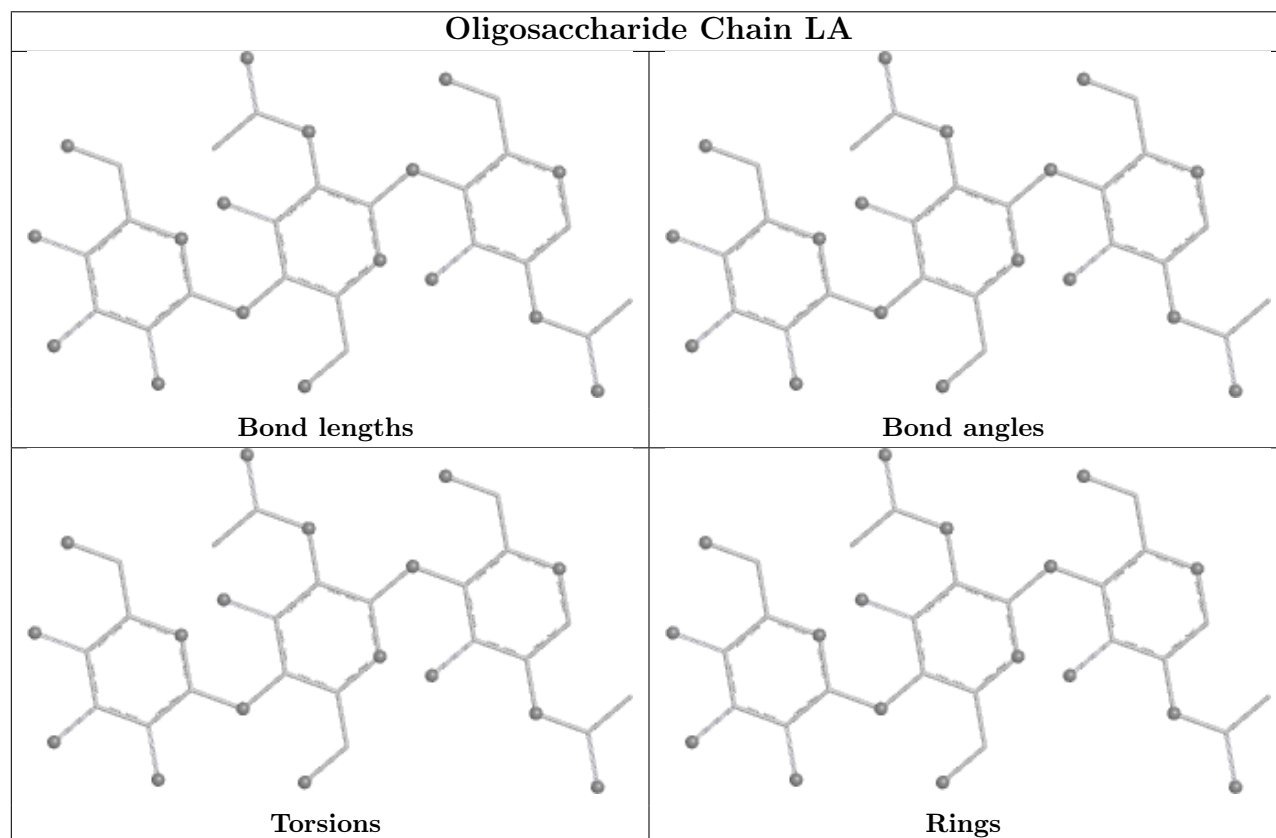


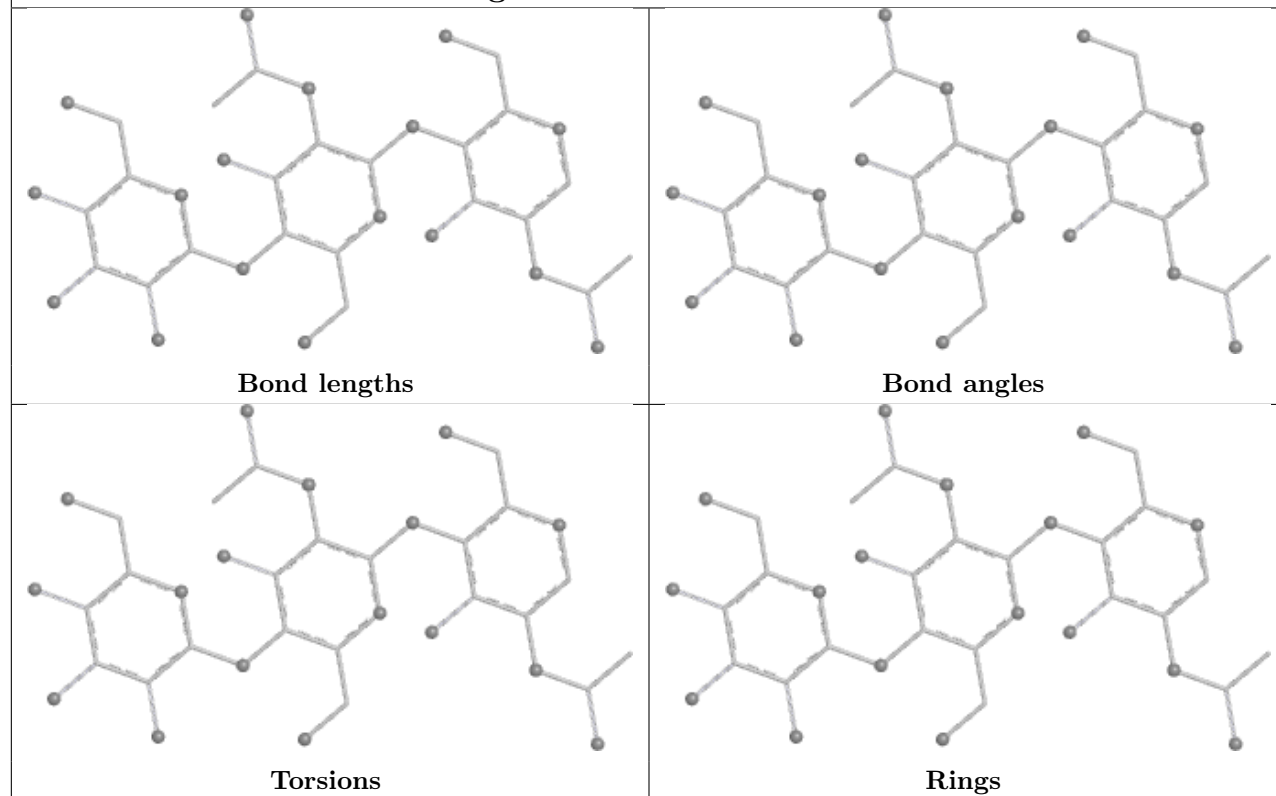
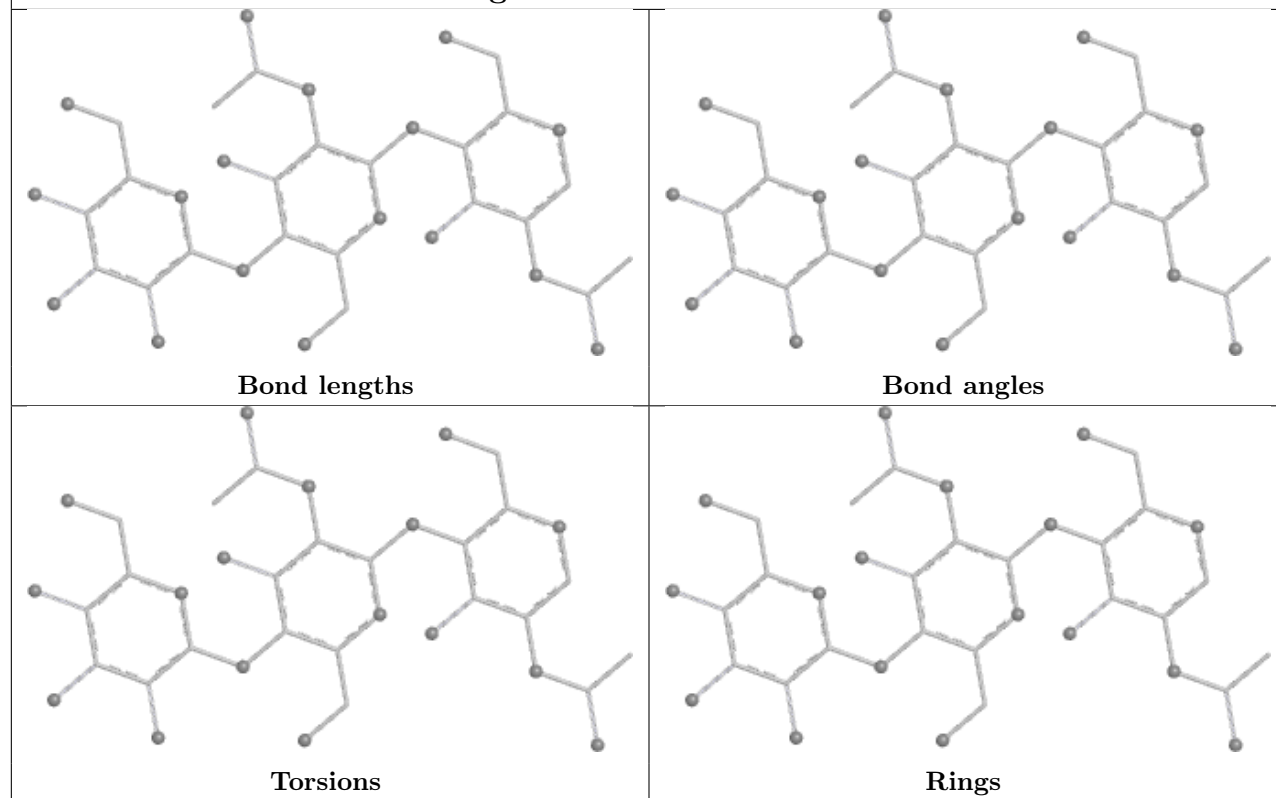


Oligosaccharide Chain JA

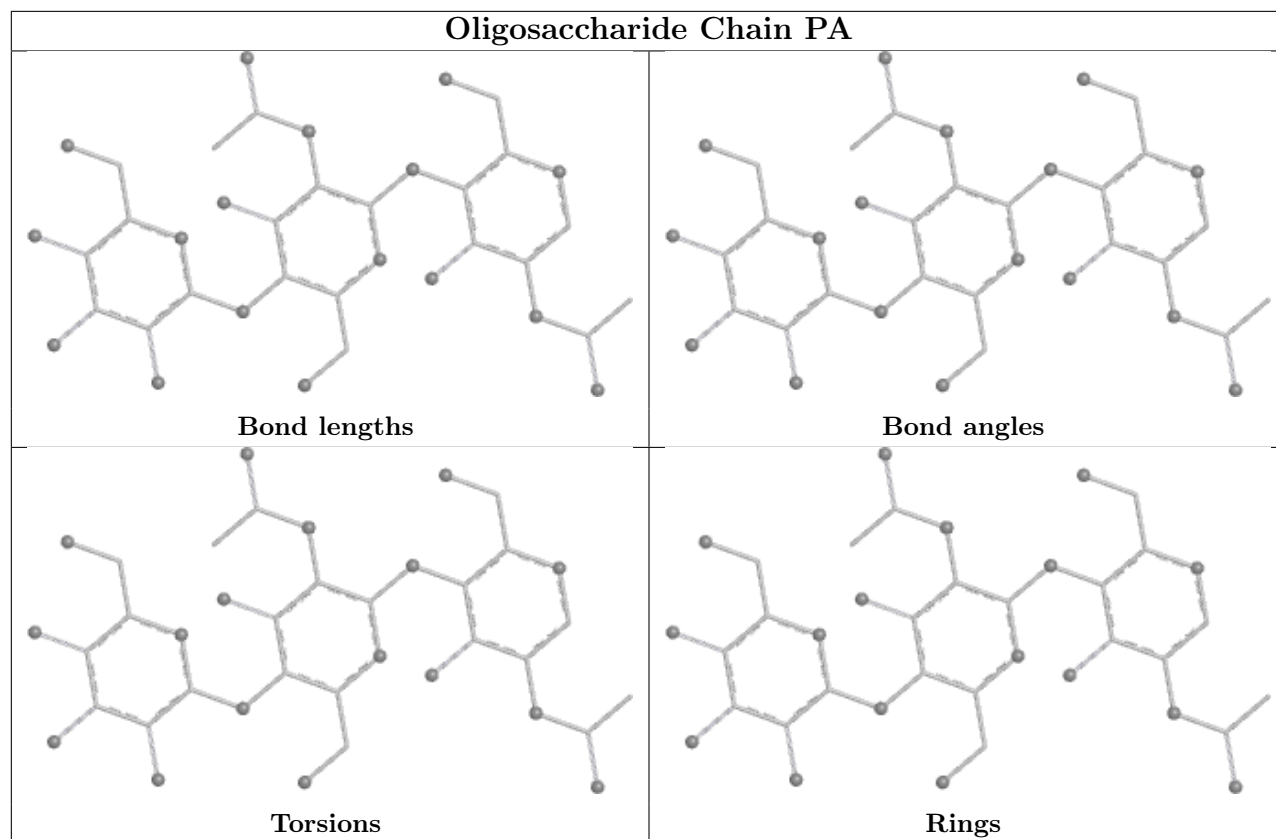


Oligosaccharide Chain LA

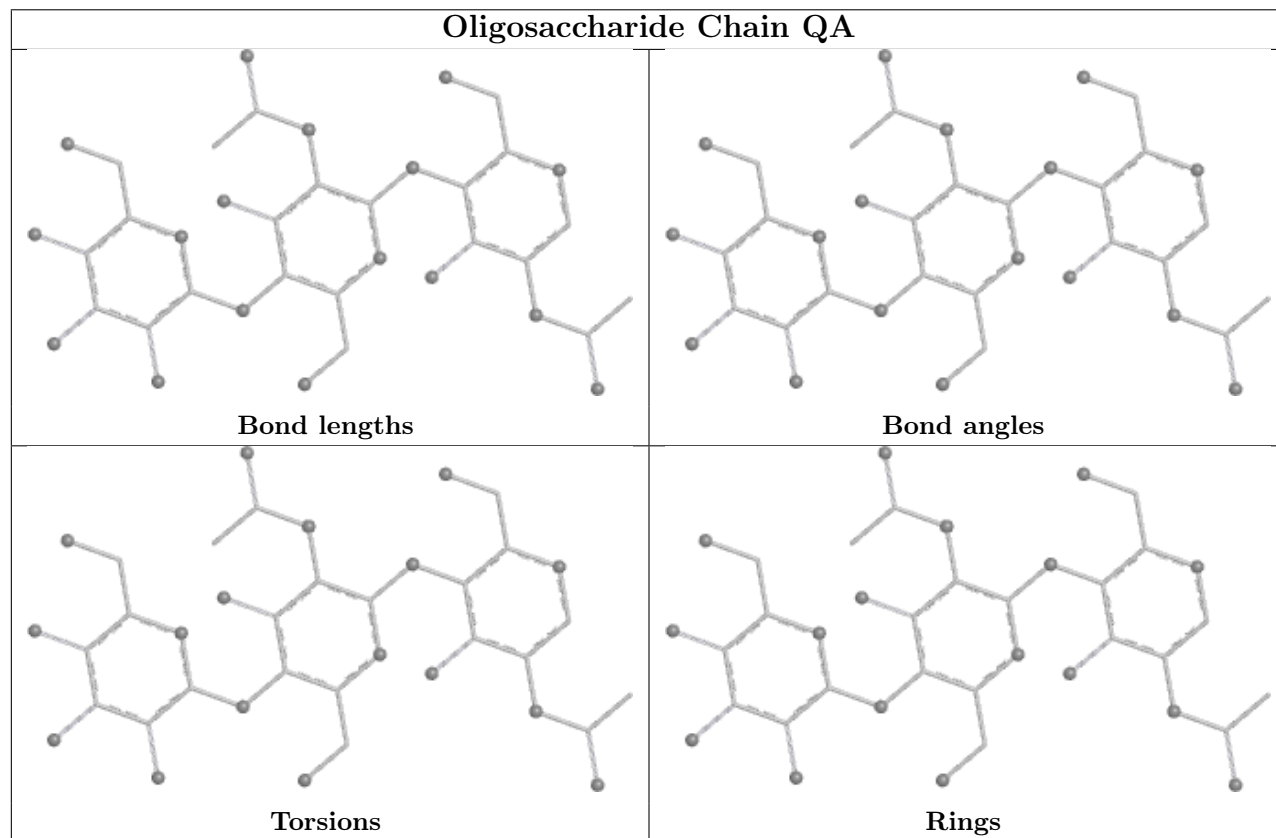


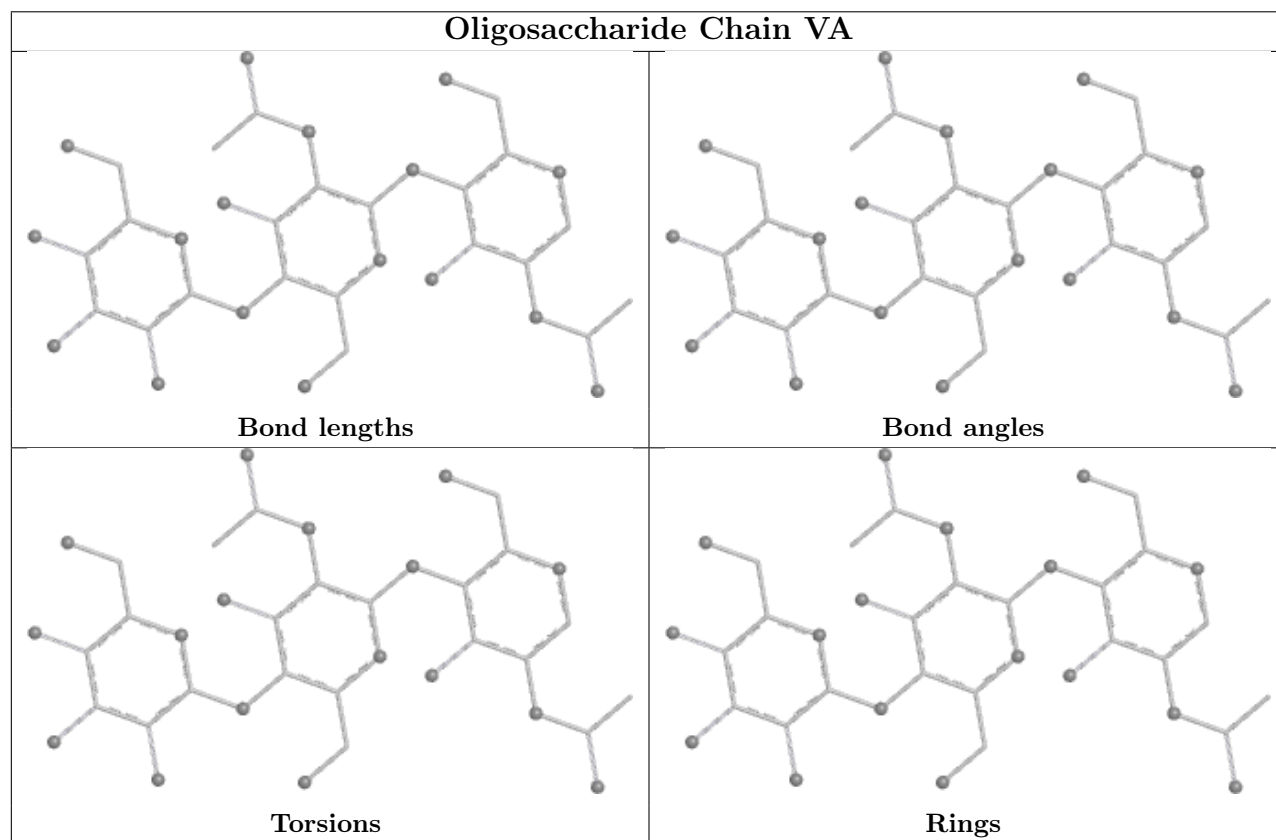
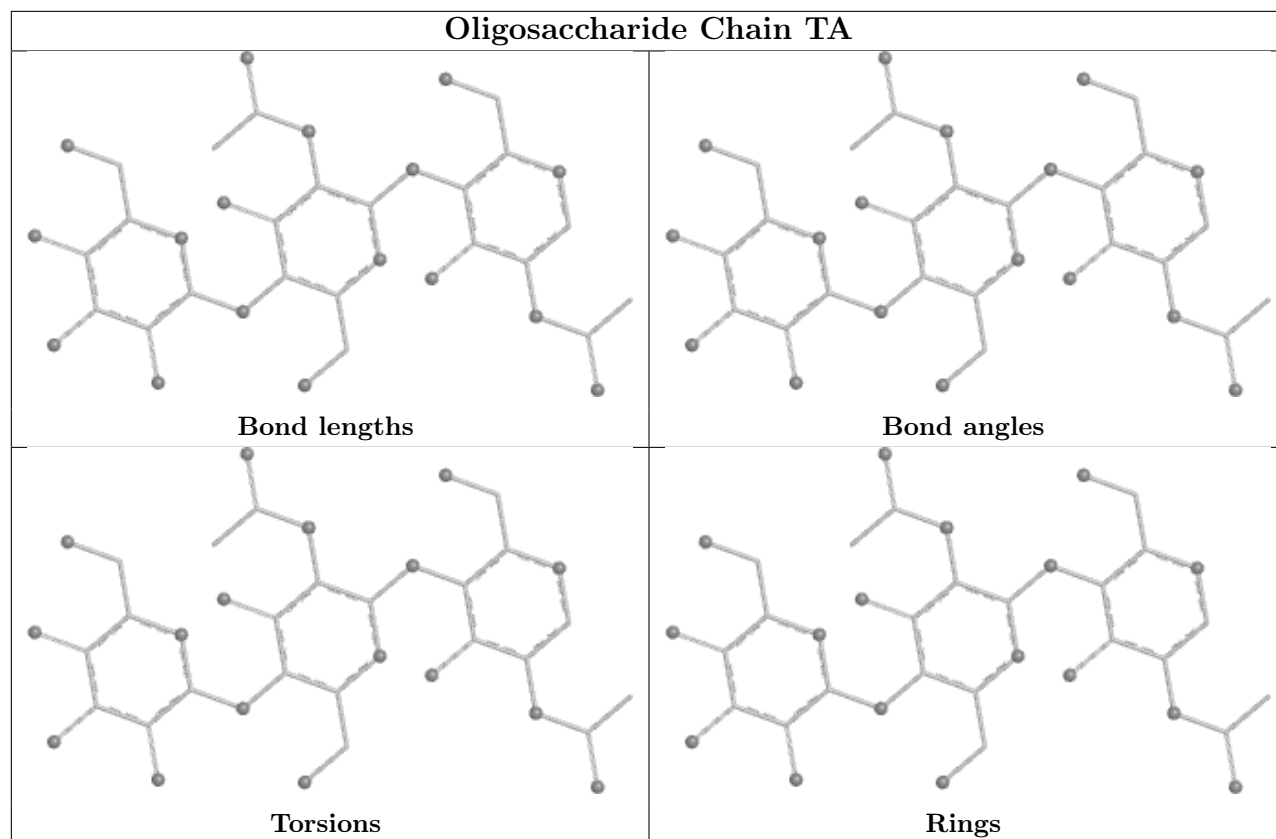
Oligosaccharide Chain NA**Oligosaccharide Chain OA**

Oligosaccharide Chain PA

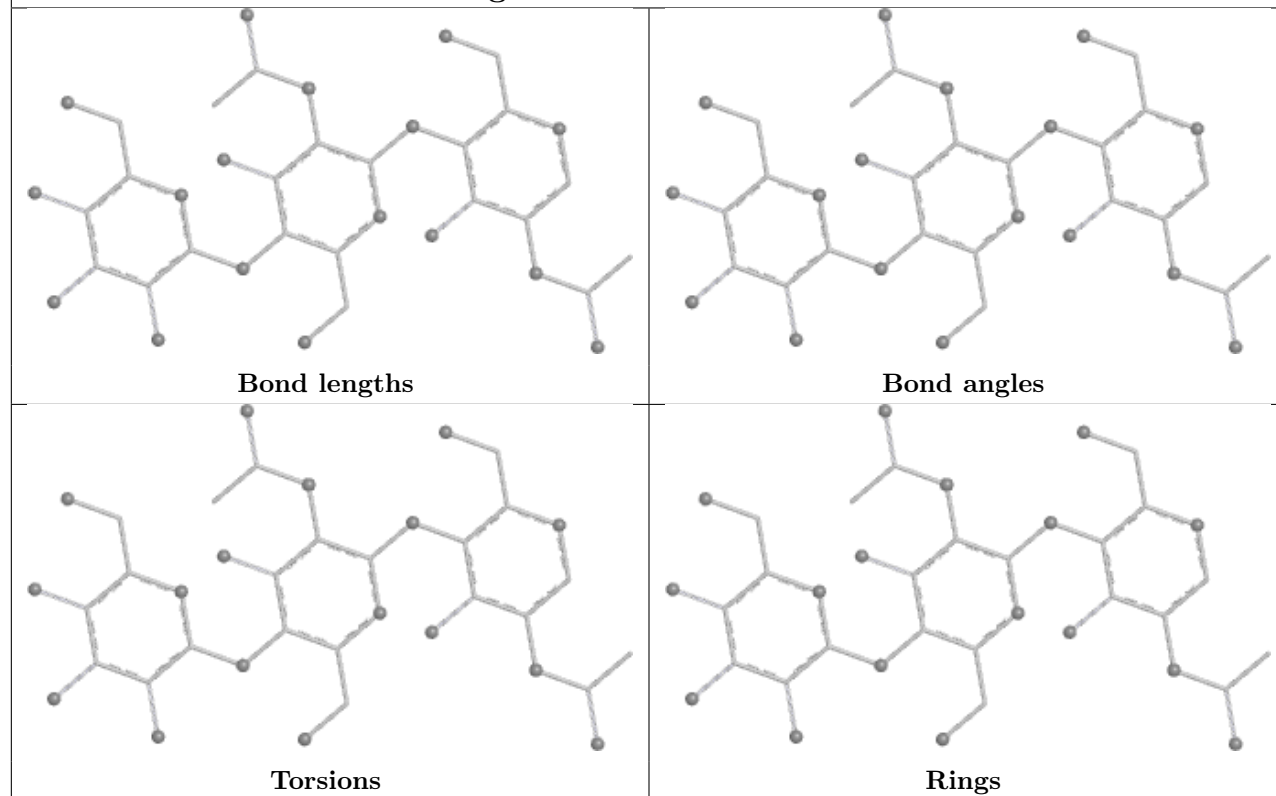


Oligosaccharide Chain QA

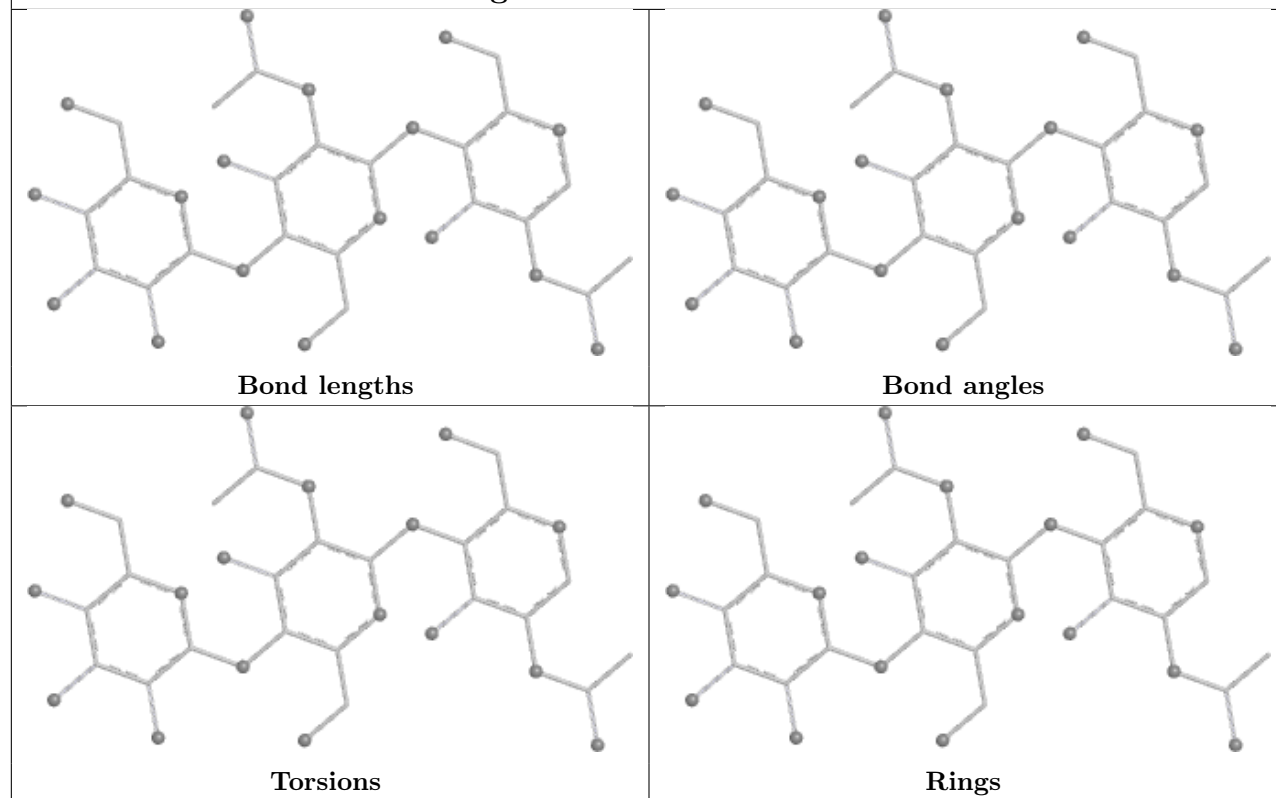




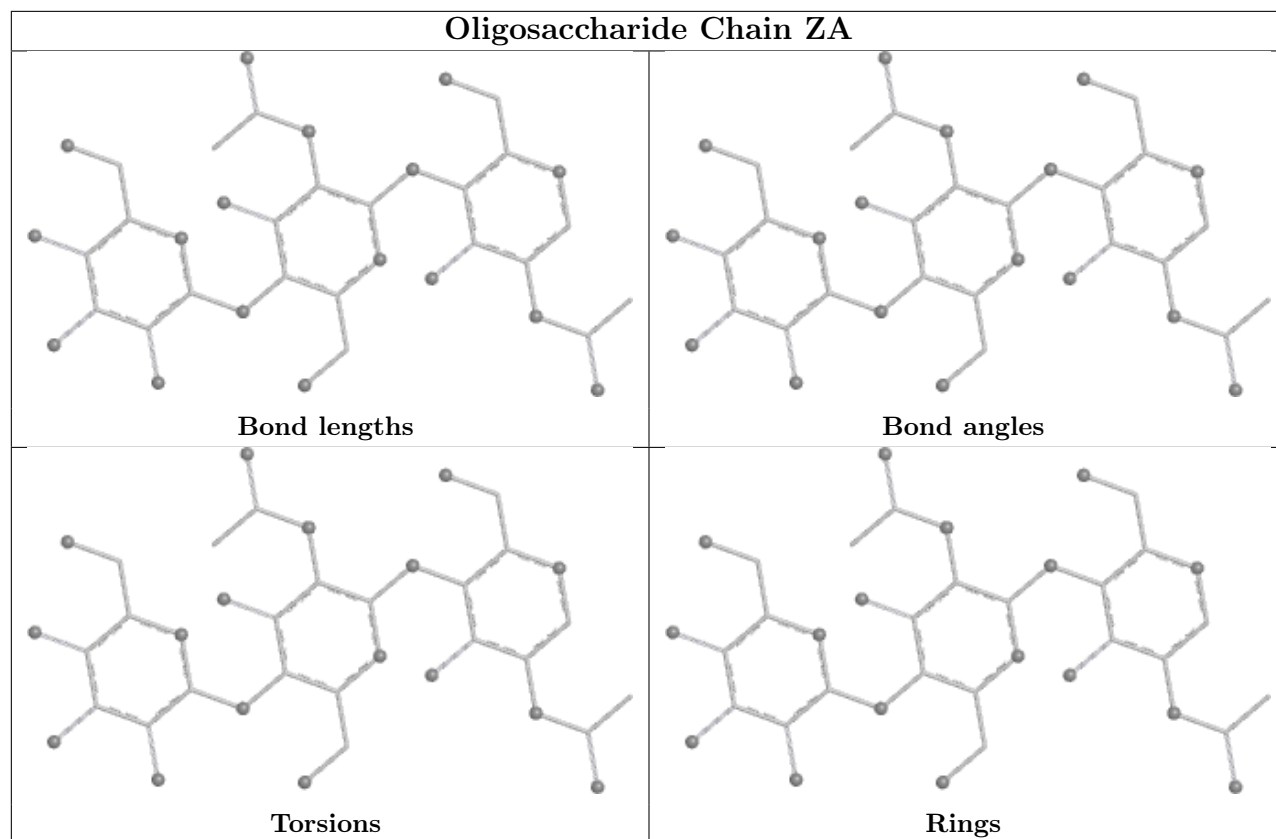
Oligosaccharide Chain XA



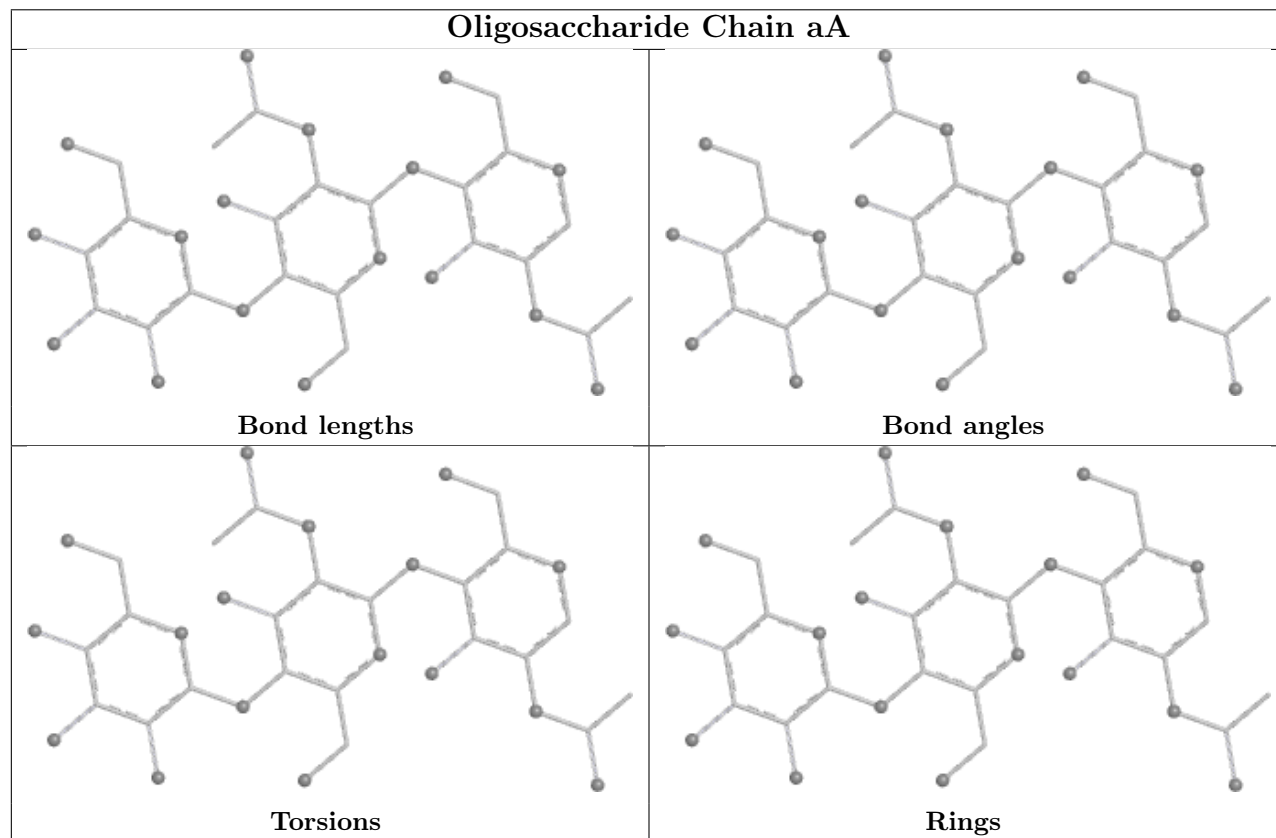
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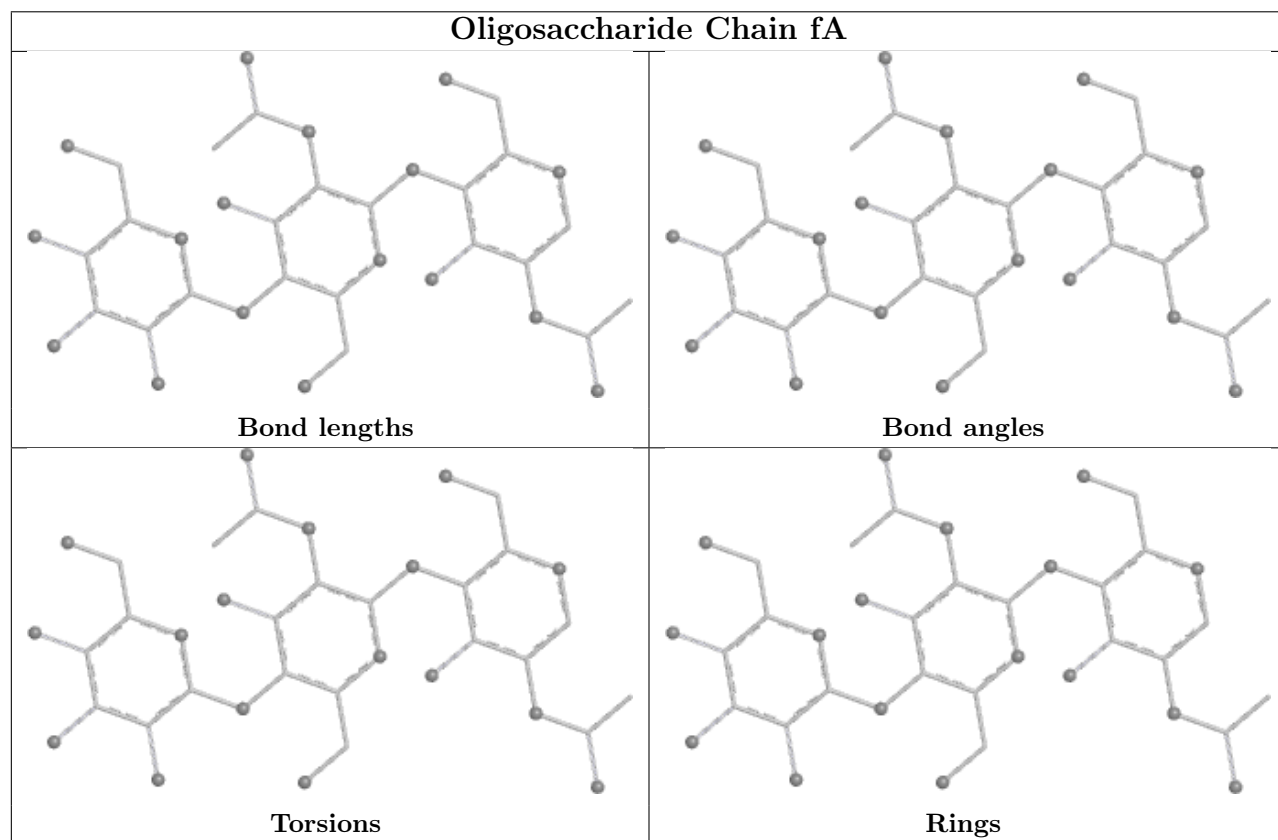
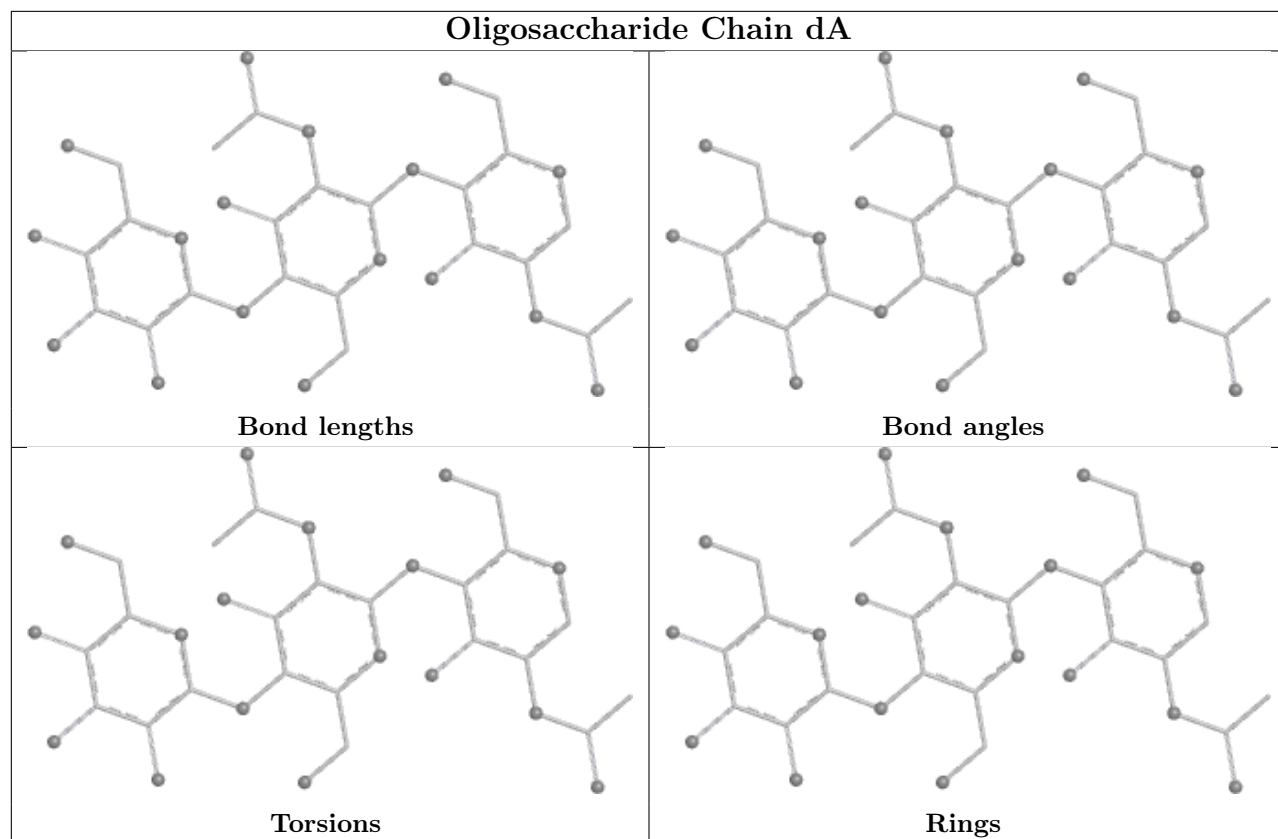


Oligosaccharide Chain ZA

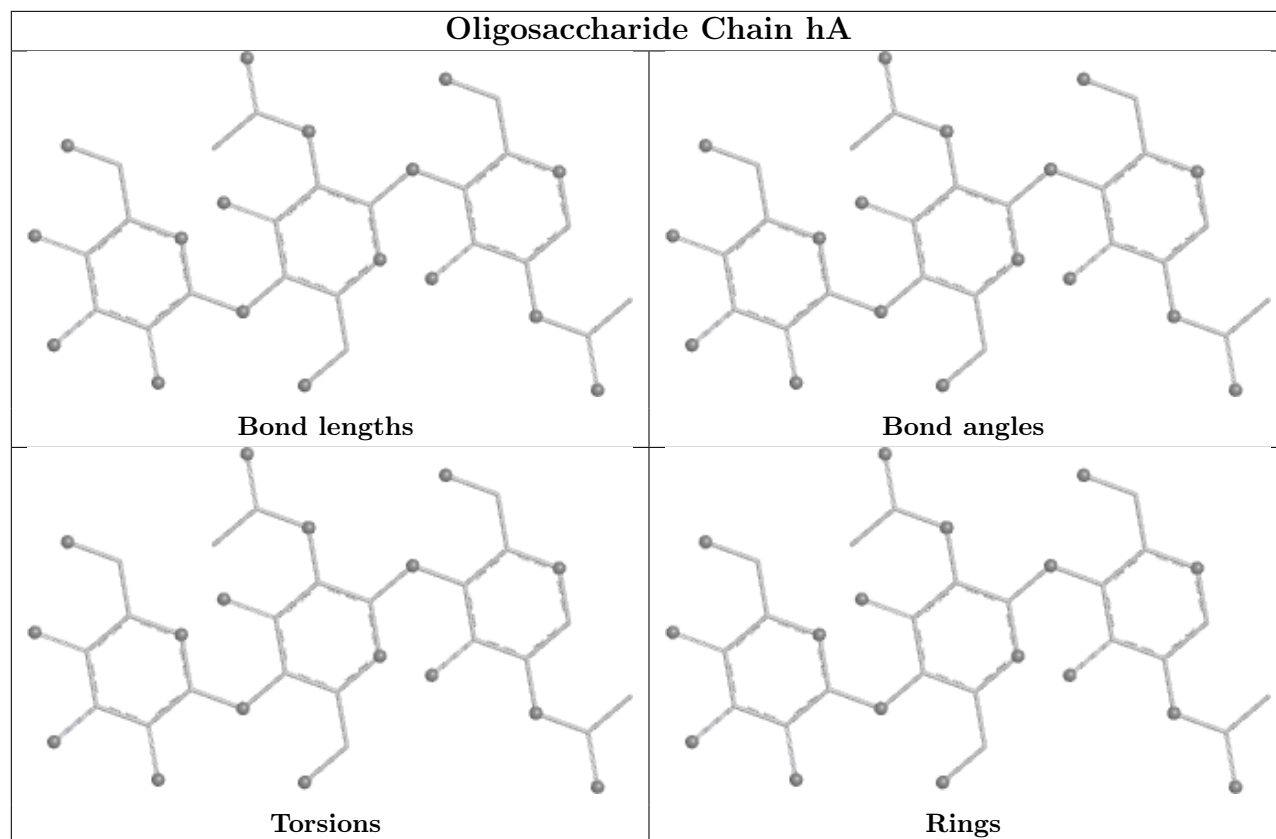


Oligosaccharide Chain aA

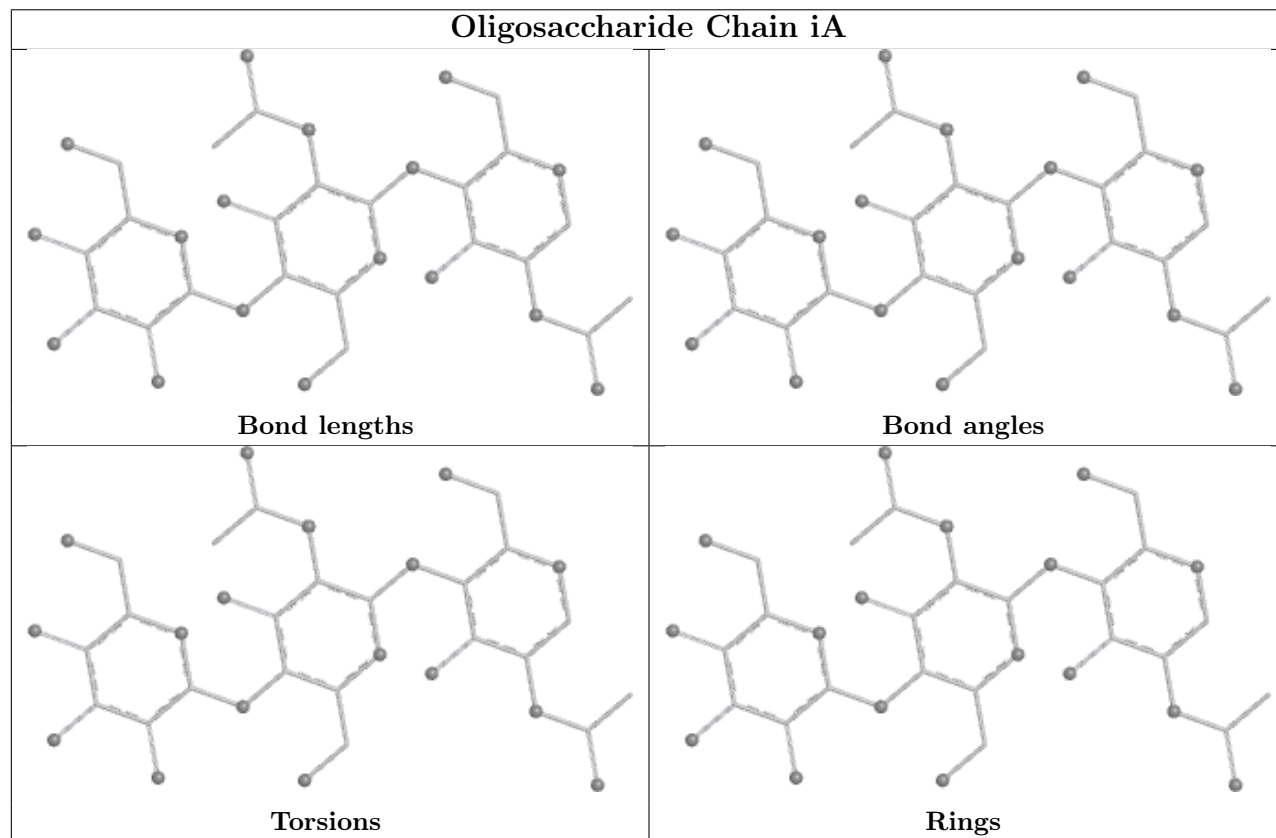




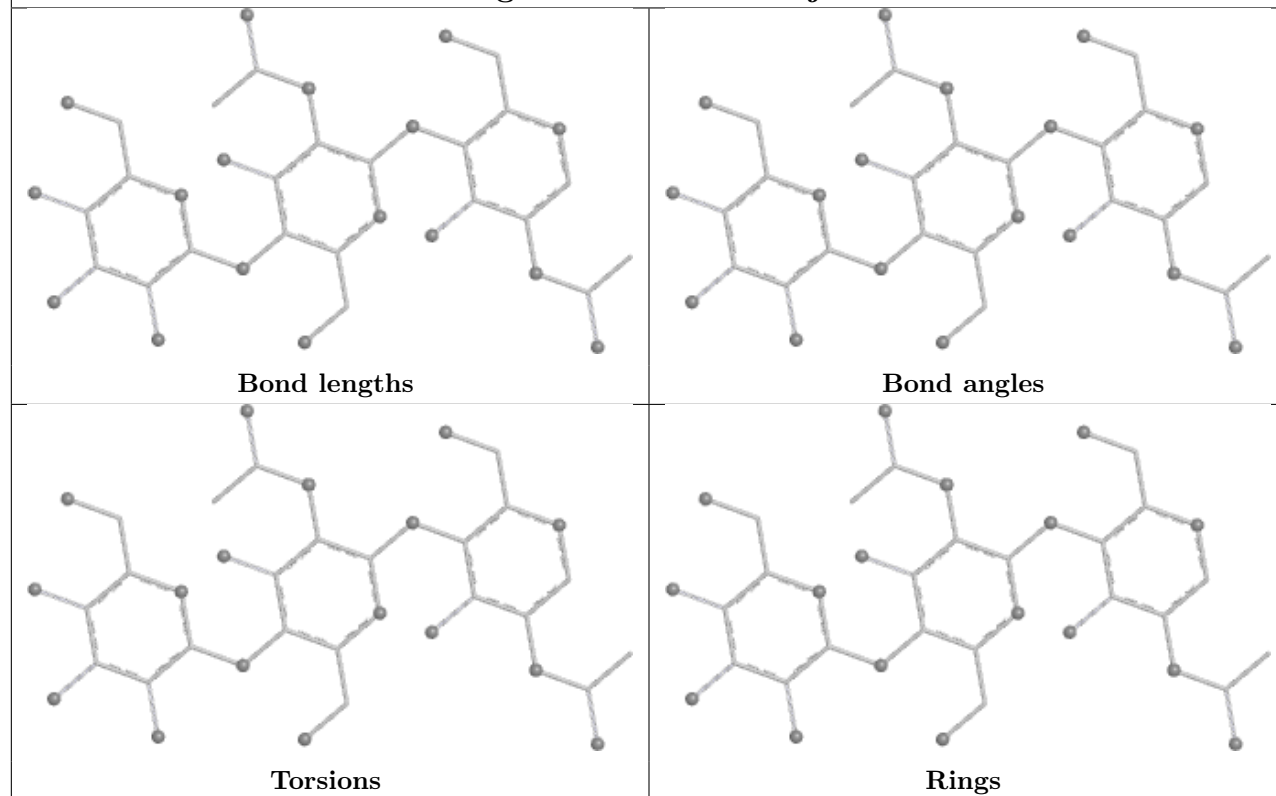
Oligosaccharide Chain hA



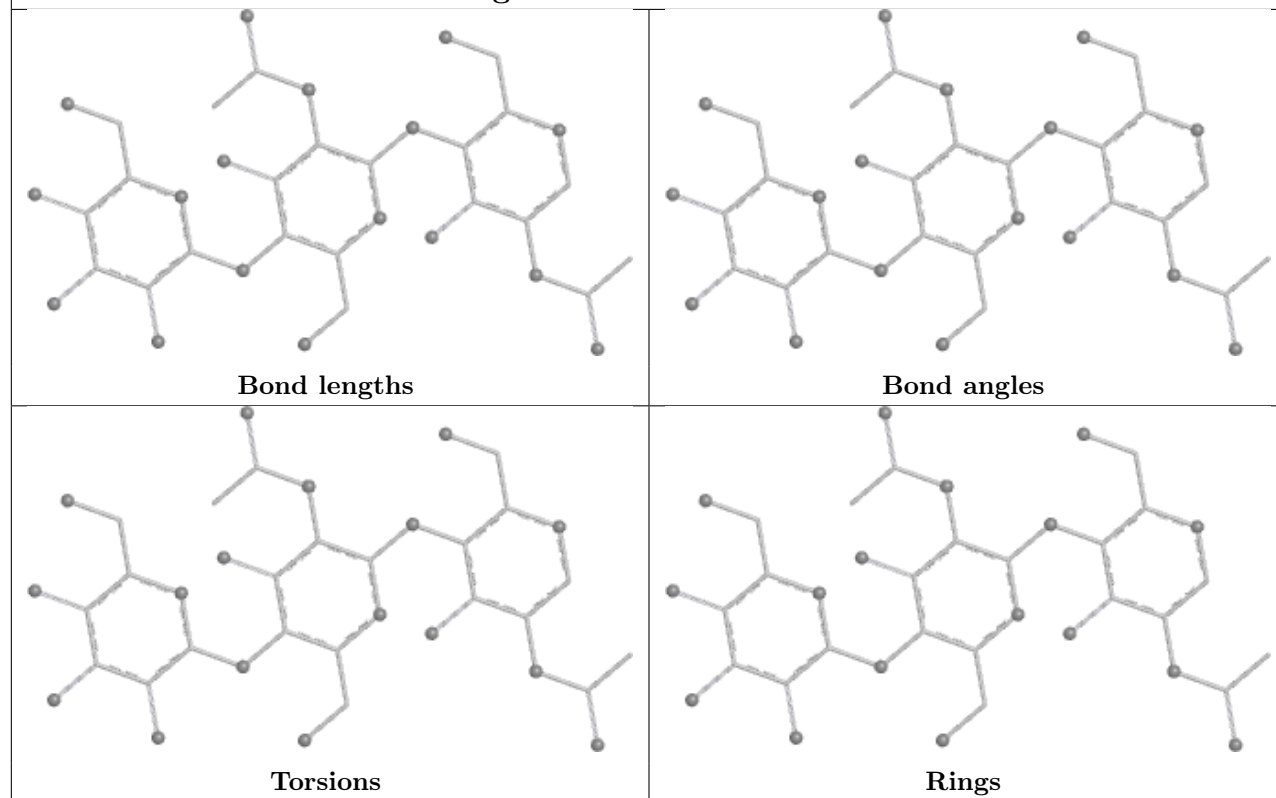
Oligosaccharide Chain iA

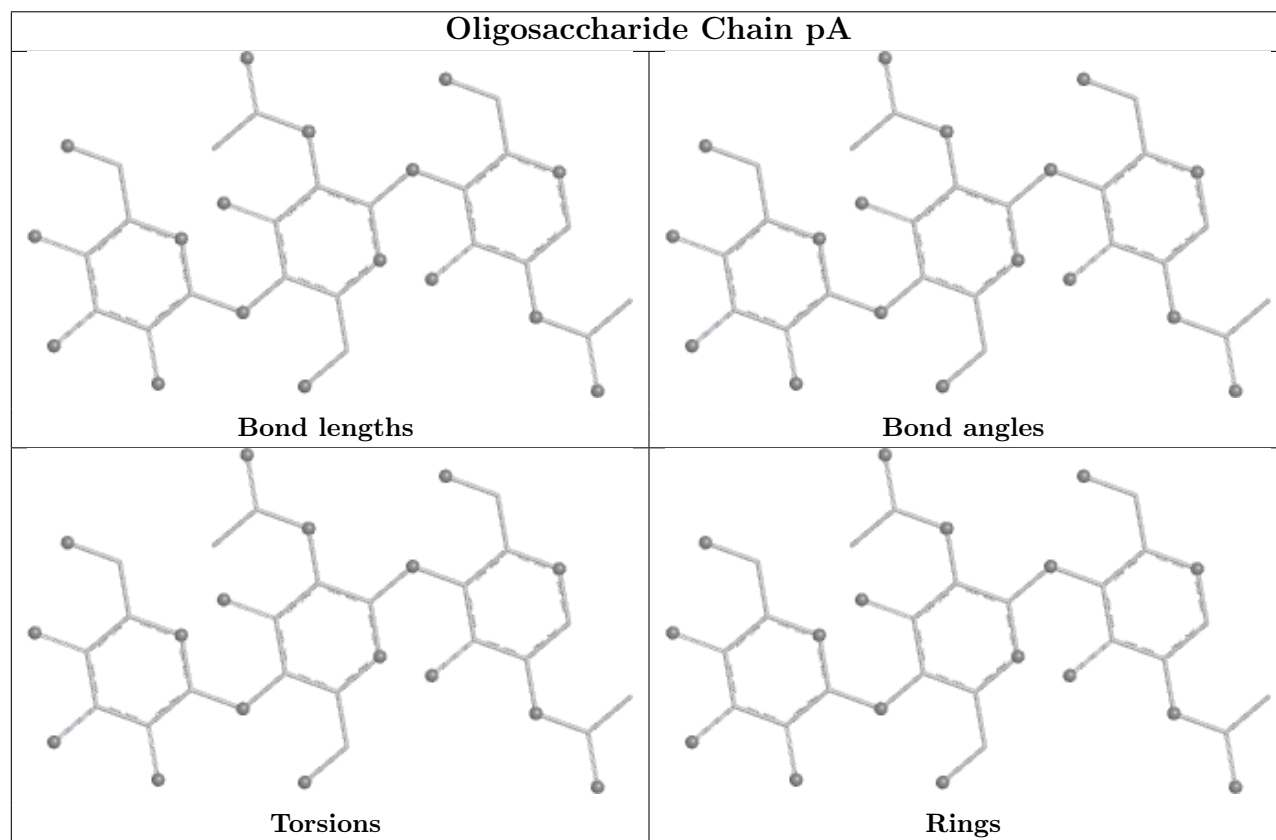
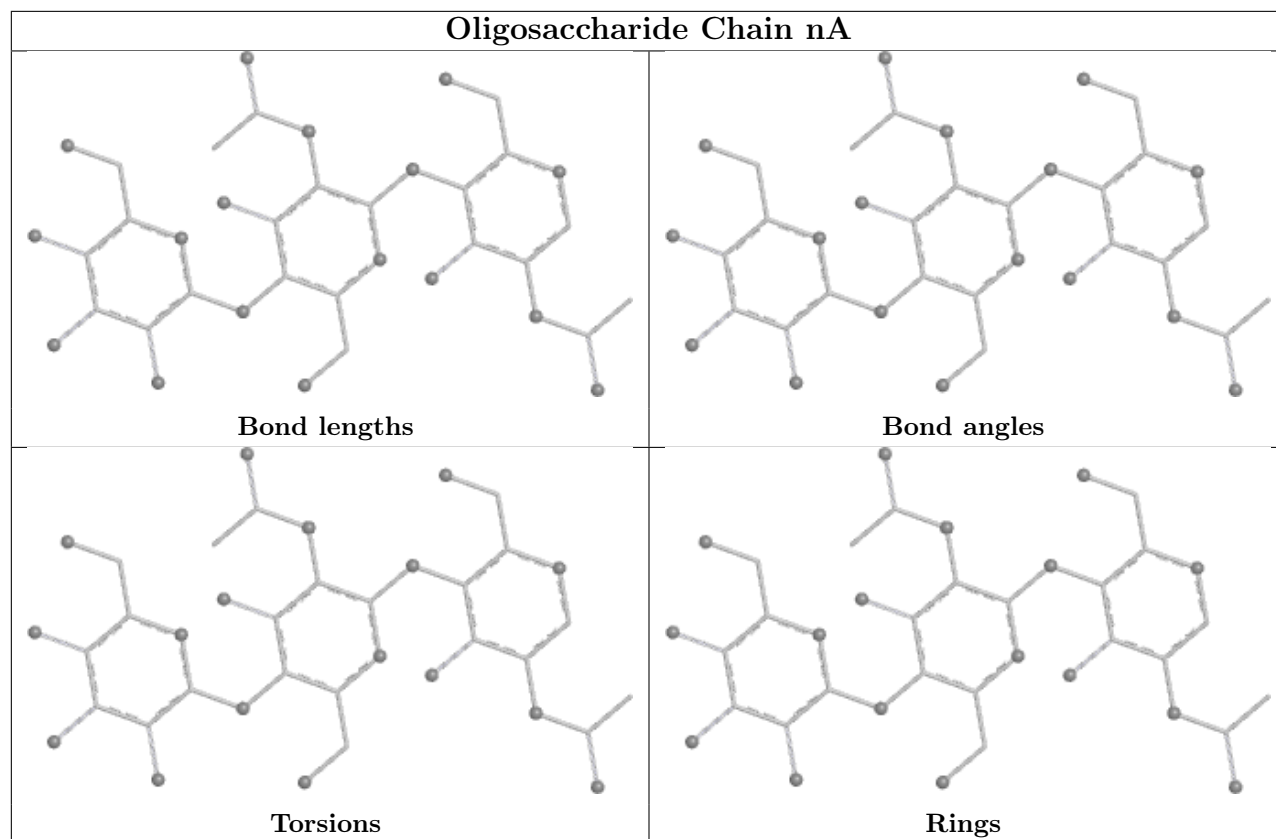


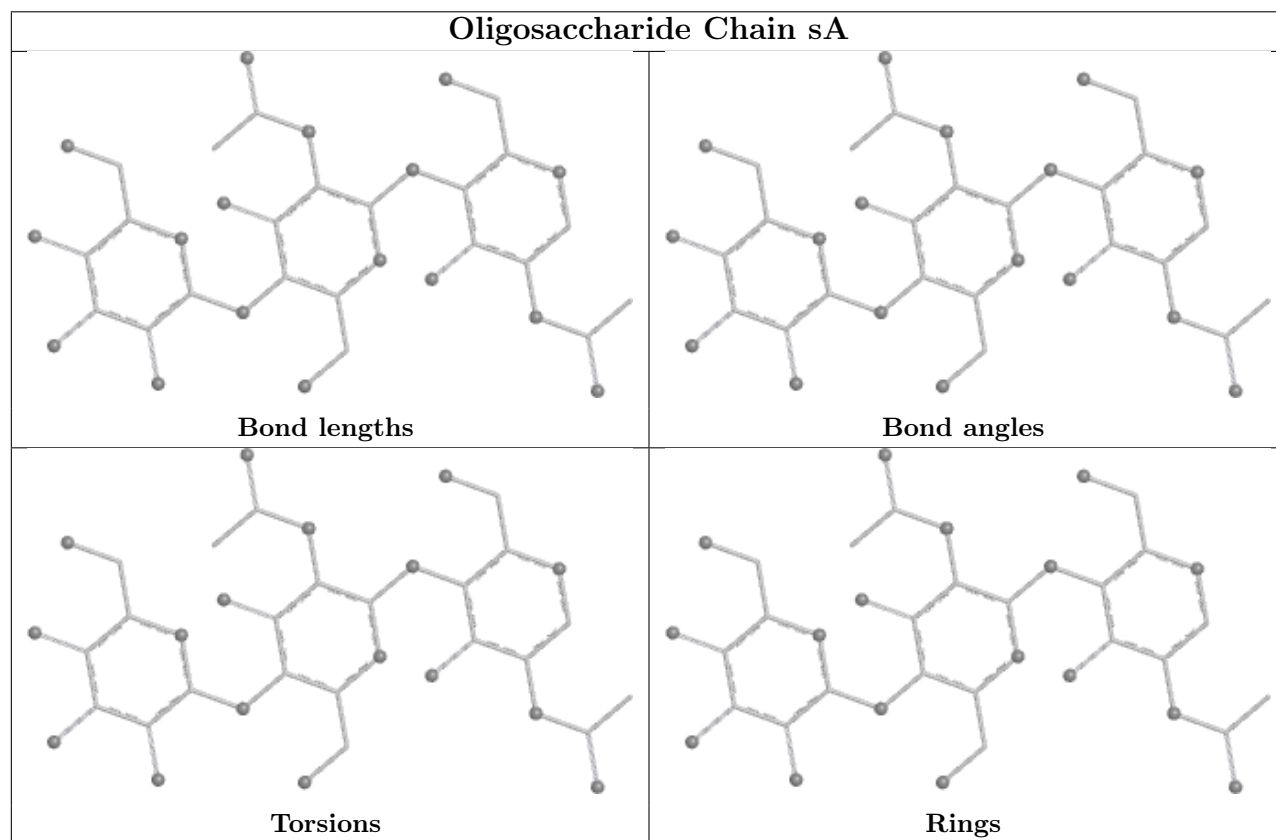
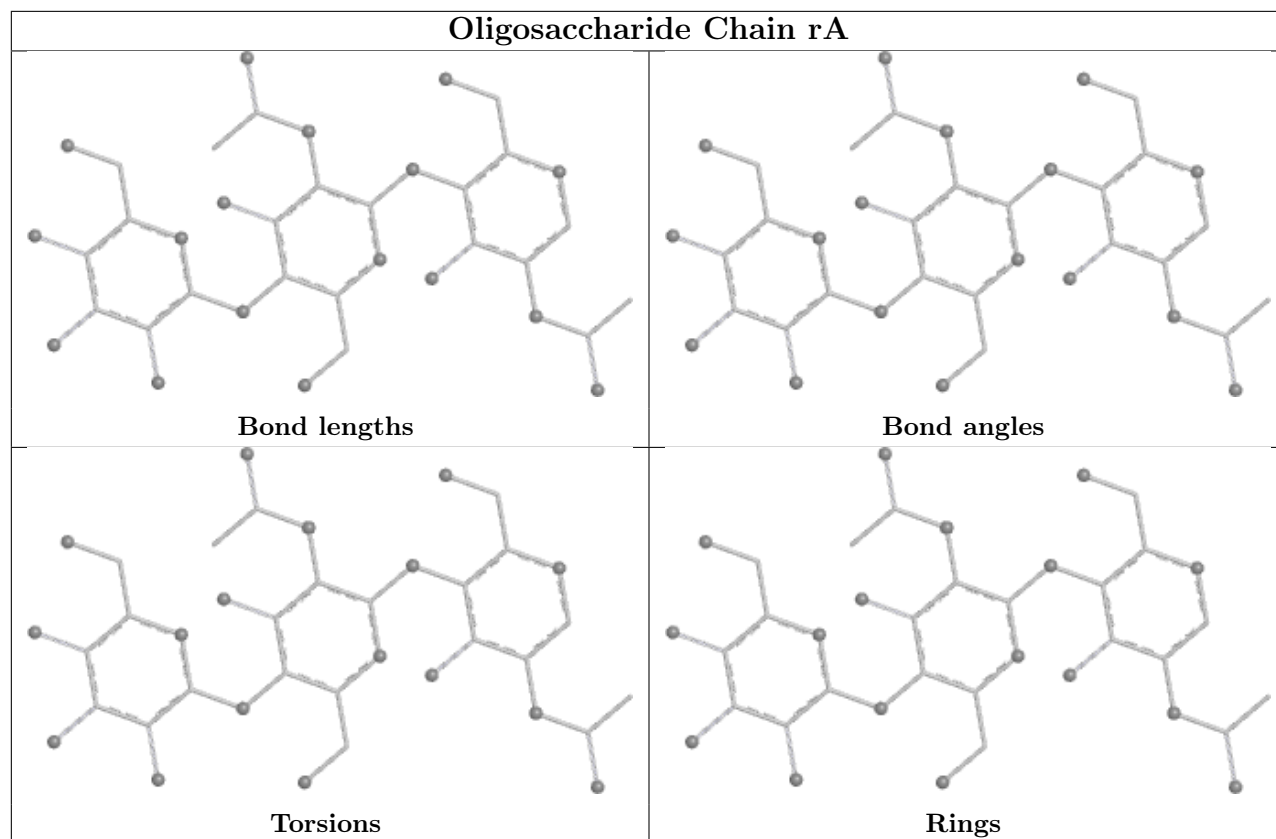
Oligosaccharide Chain jA



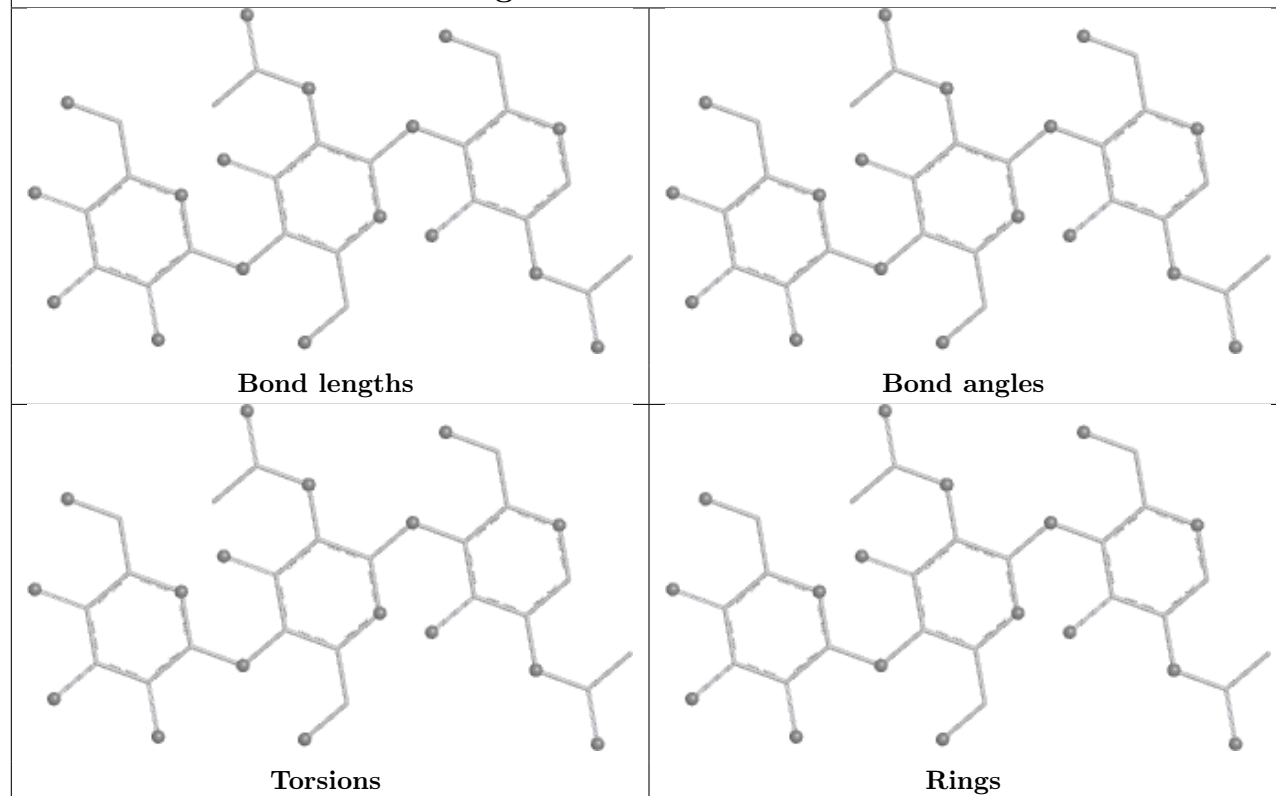
Oligosaccharide Chain kA



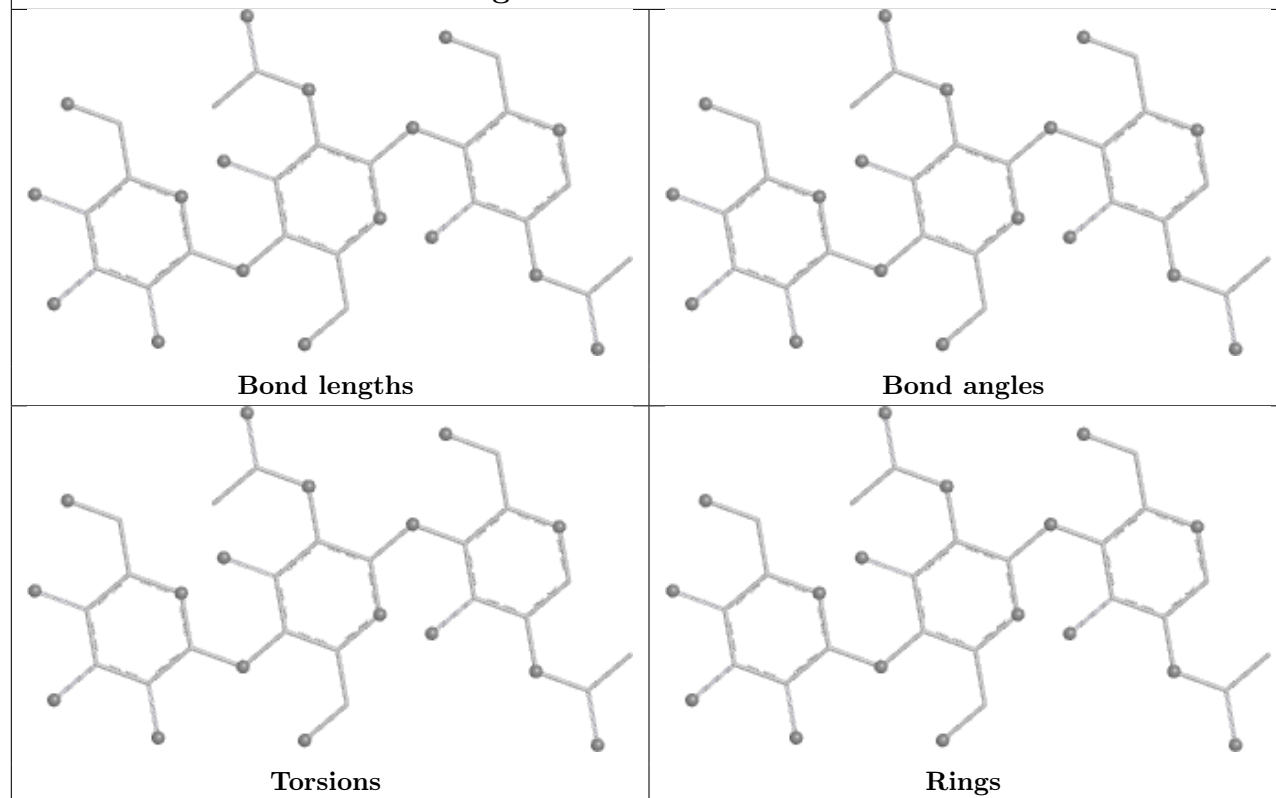


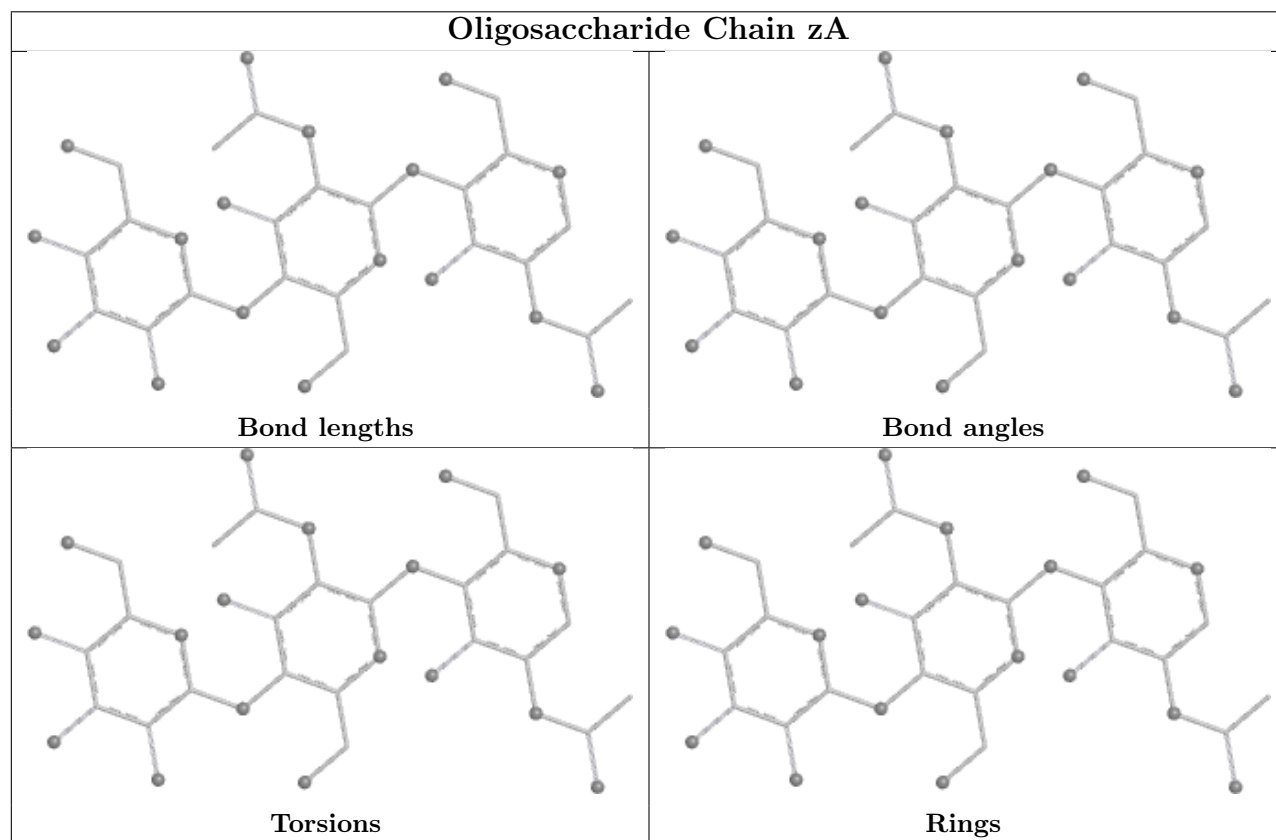
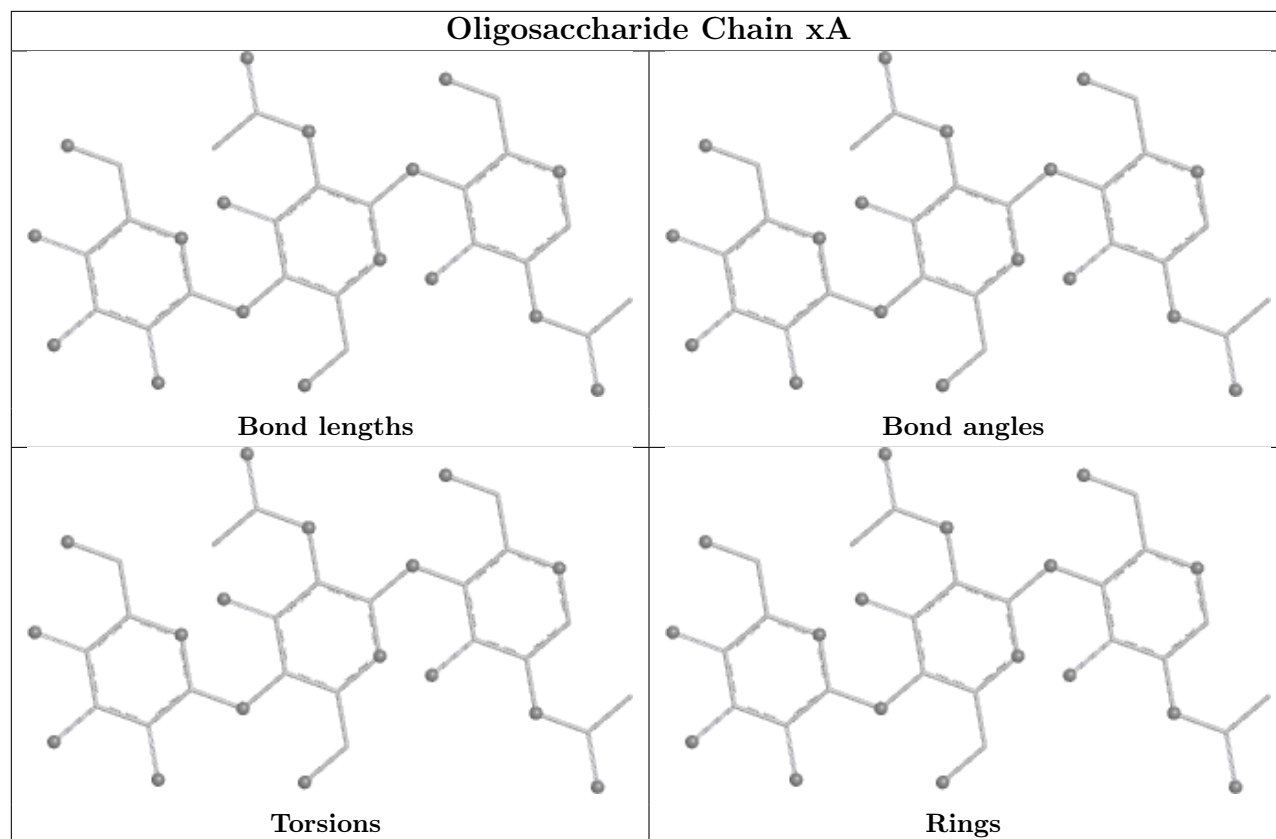


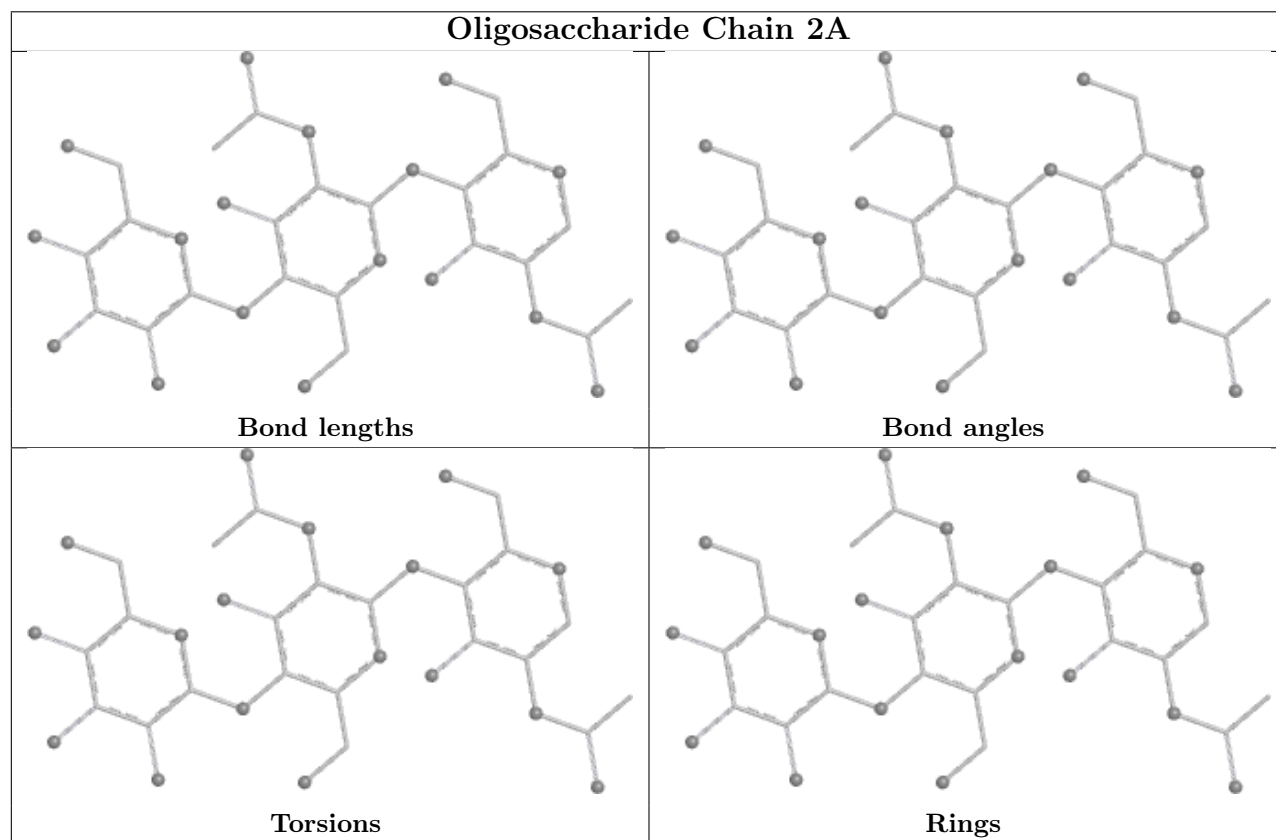
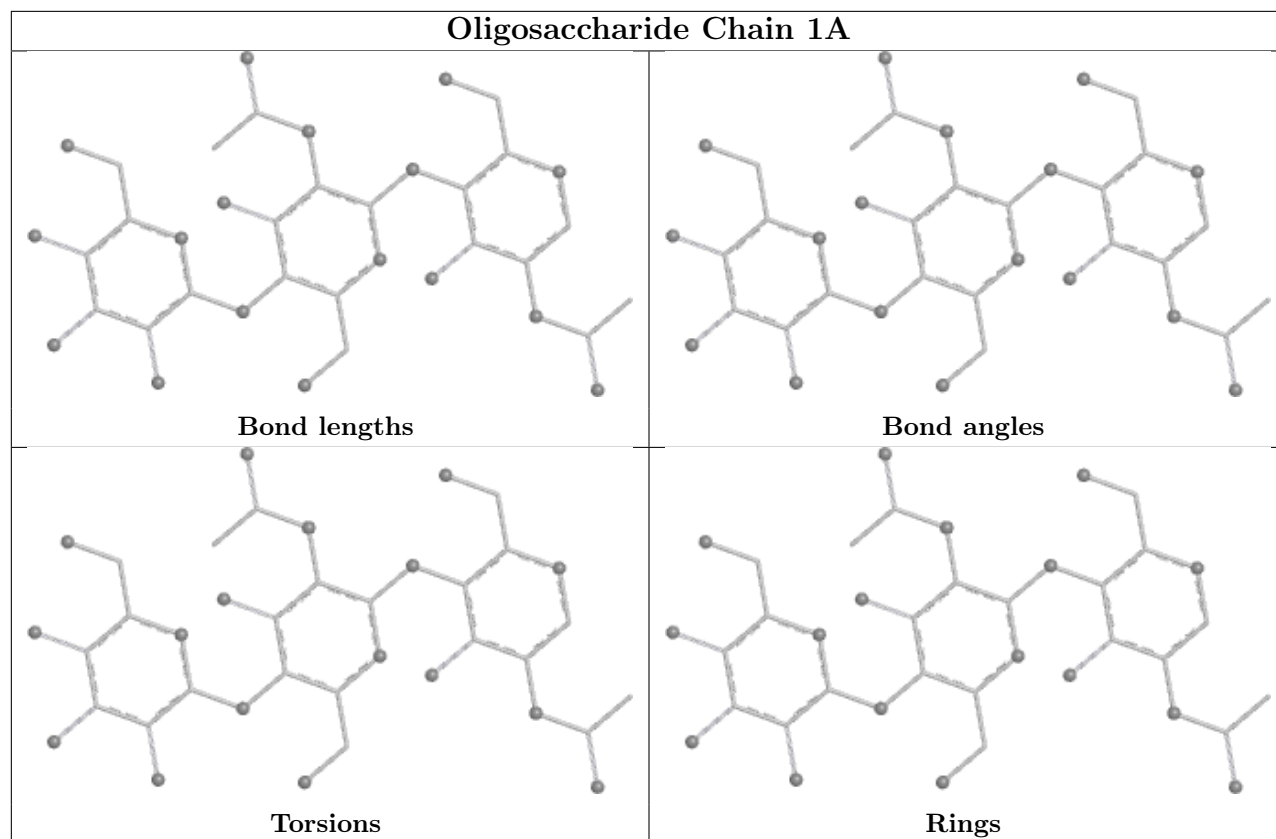
Oligosaccharide Chain tA



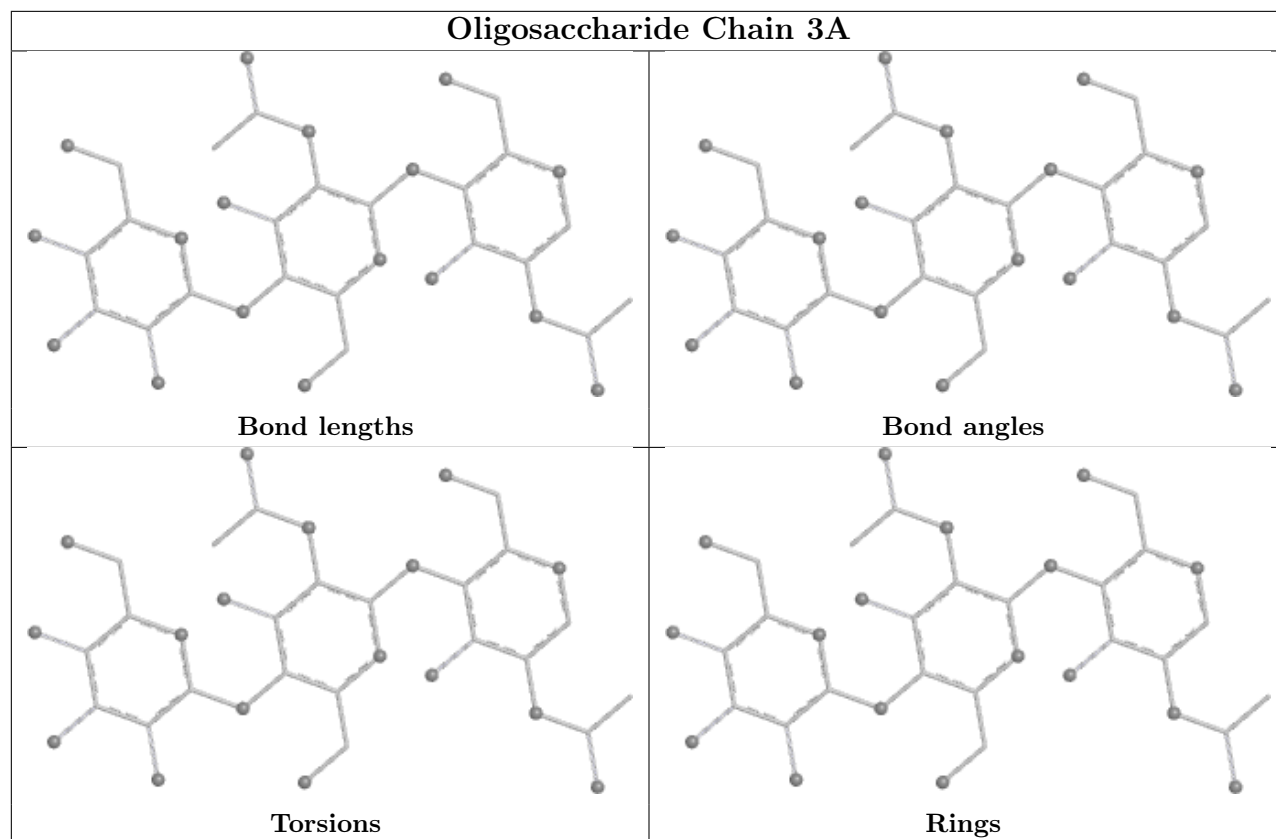
Oligosaccharide Chain uA



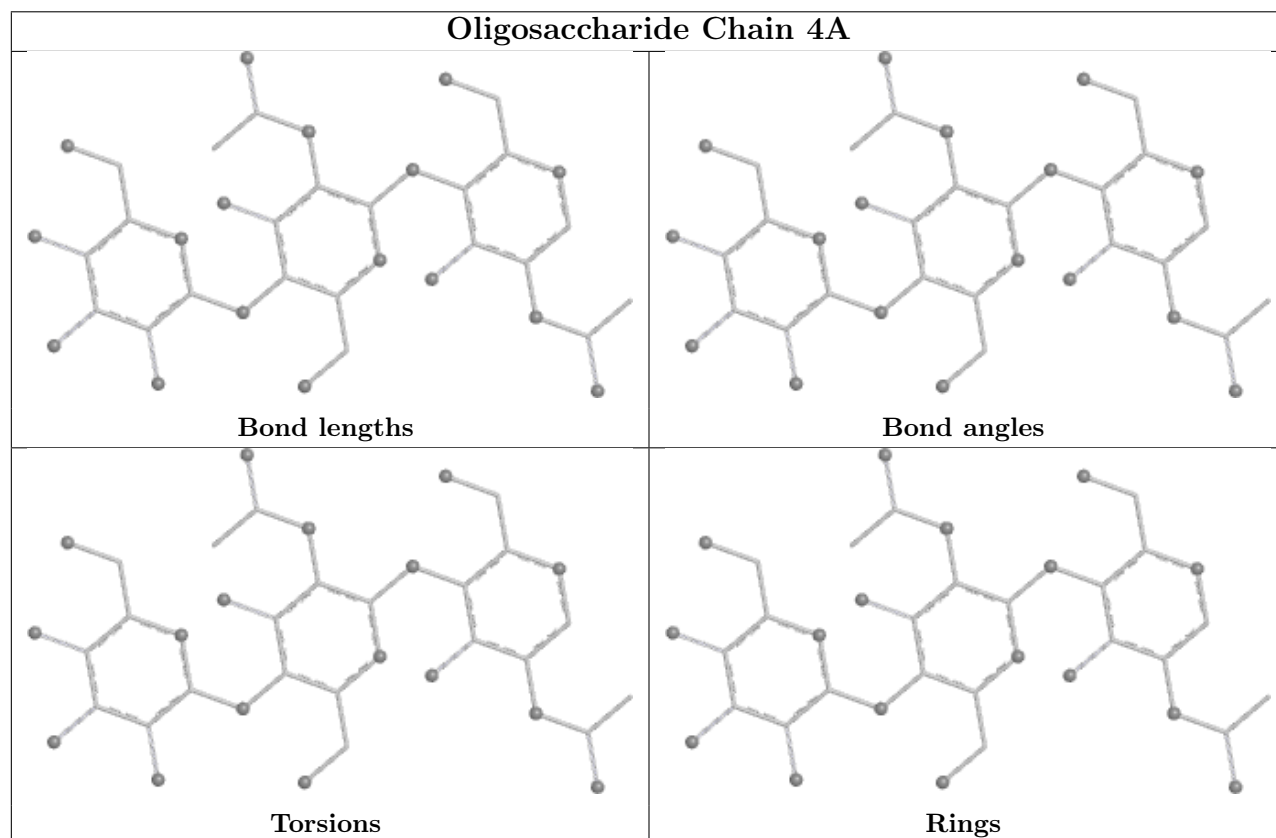




Oligosaccharide Chain 3A



Oligosaccharide Chain 4A



5.6 Ligand geometry

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	3501	1	14,14,15	0.30	0	17,19,21	0.41	0
4	NAG	C	3501	1	14,14,15	0.18	0	17,19,21	0.48	0
4	NAG	P	3501	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	M	3501	1	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	K	3501	1	14,14,15	0.15	0	17,19,21	0.42	0
4	NAG	H	3501	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	R	3501	1	14,14,15	0.21	0	17,19,21	0.35	0
4	NAG	A	3501	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	L	3501	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	I	3501	1	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	S	3501	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	F	3501	1	14,14,15	0.25	0	17,19,21	0.36	0
4	NAG	O	3501	1	14,14,15	0.35	0	17,19,21	0.46	0
4	NAG	D	3501	1	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	E	3501	1	14,14,15	0.16	0	17,19,21	0.44	0
4	NAG	Q	3501	1	14,14,15	0.36	0	17,19,21	0.50	0
4	NAG	N	3501	1	14,14,15	0.21	0	17,19,21	0.36	0
4	NAG	G	3501	1	14,14,15	0.15	0	17,19,21	0.41	0
4	NAG	J	3501	1	14,14,15	0.24	0	17,19,21	0.36	0
4	NAG	T	3501	1	14,14,15	0.24	0	17,19,21	0.65	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	B	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	C	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	P	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	M	3501	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	H	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	R	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	A	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	L	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	I	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	S	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	F	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	O	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	D	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	E	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	Q	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	N	3501	1	-	3/6/23/26	0/1/1/1
4	NAG	G	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	J	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	T	3501	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	3501	NAG	O5-C5-C6-O6
4	K	3501	NAG	C4-C5-C6-O6
4	G	3501	NAG	C4-C5-C6-O6
4	C	3501	NAG	C4-C5-C6-O6
4	E	3501	NAG	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 13 short contacts:

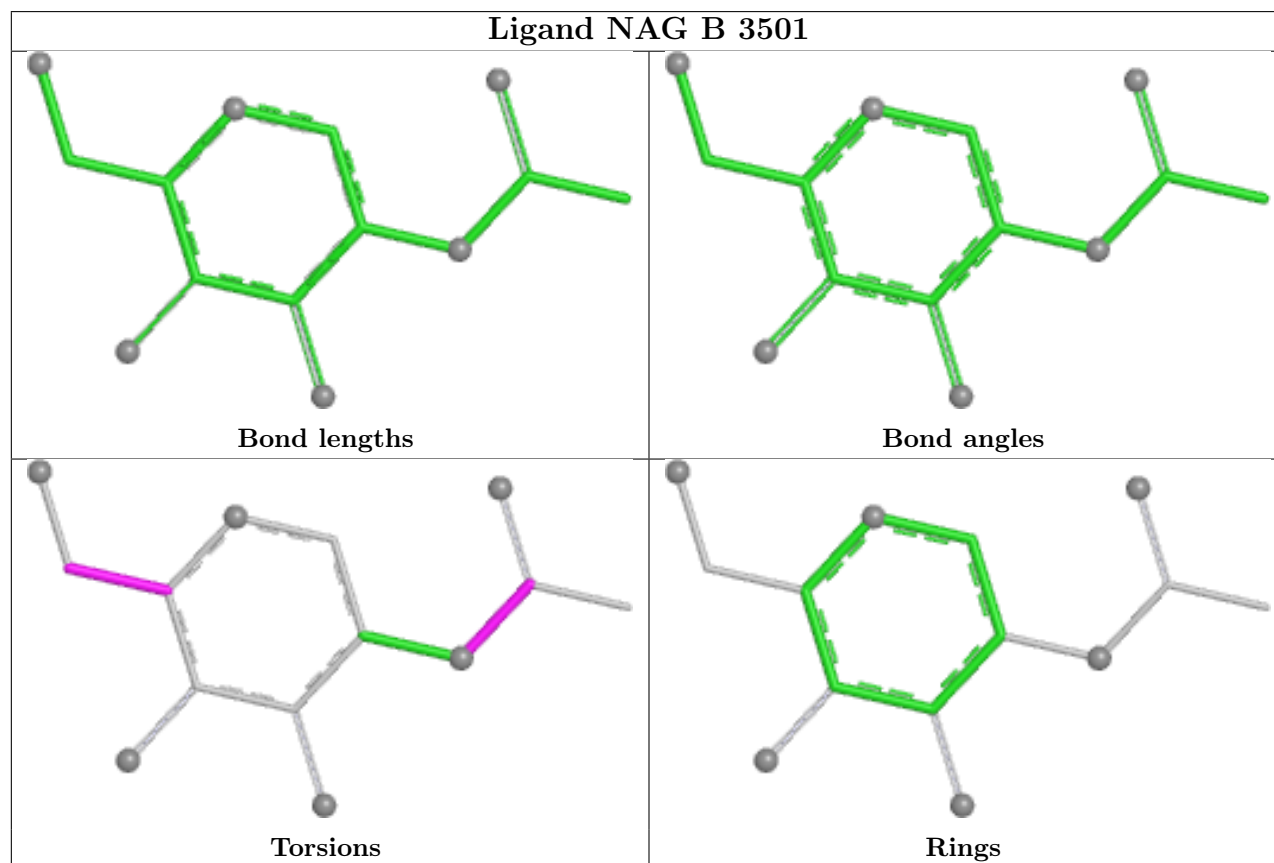
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3501	NAG	1	0
4	K	3501	NAG	1	0
4	H	3501	NAG	1	0
4	R	3501	NAG	1	0
4	I	3501	NAG	1	0

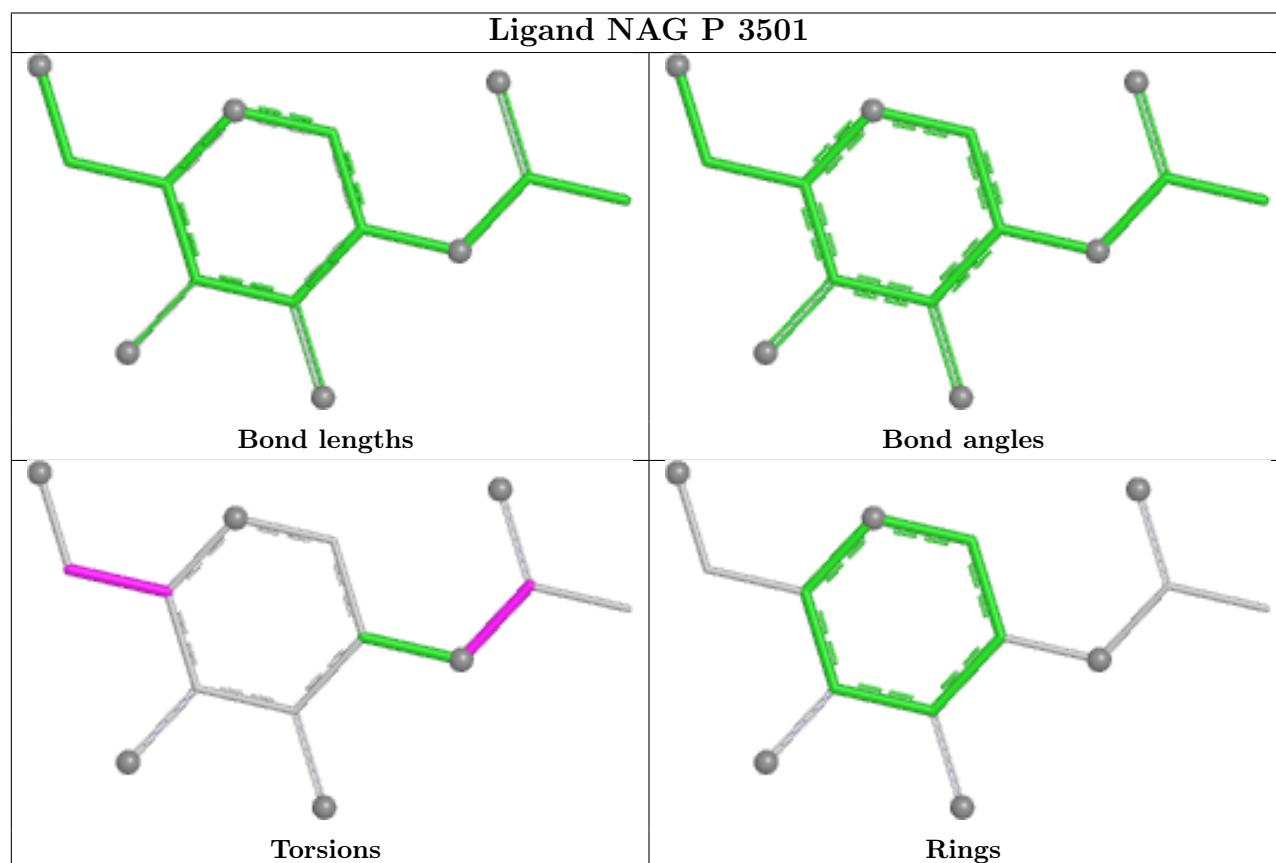
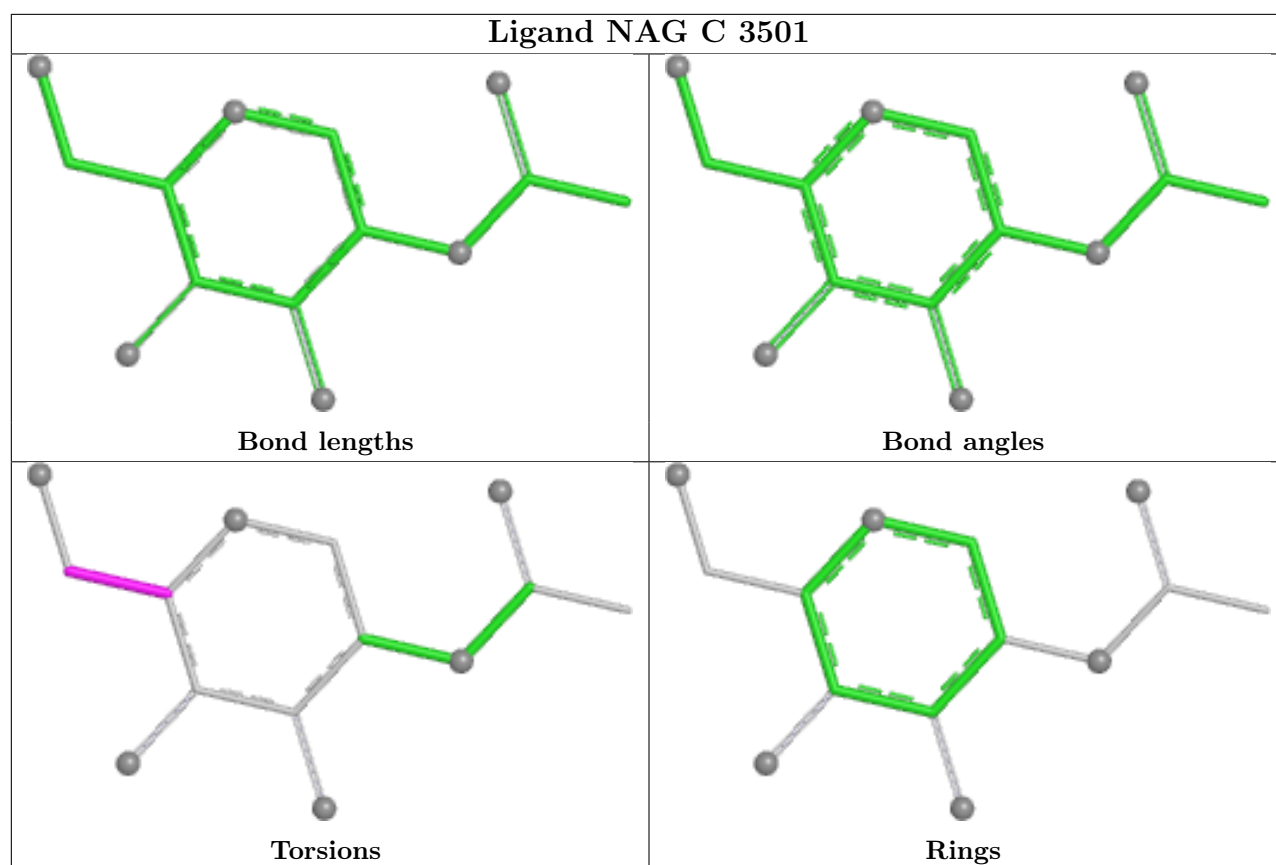
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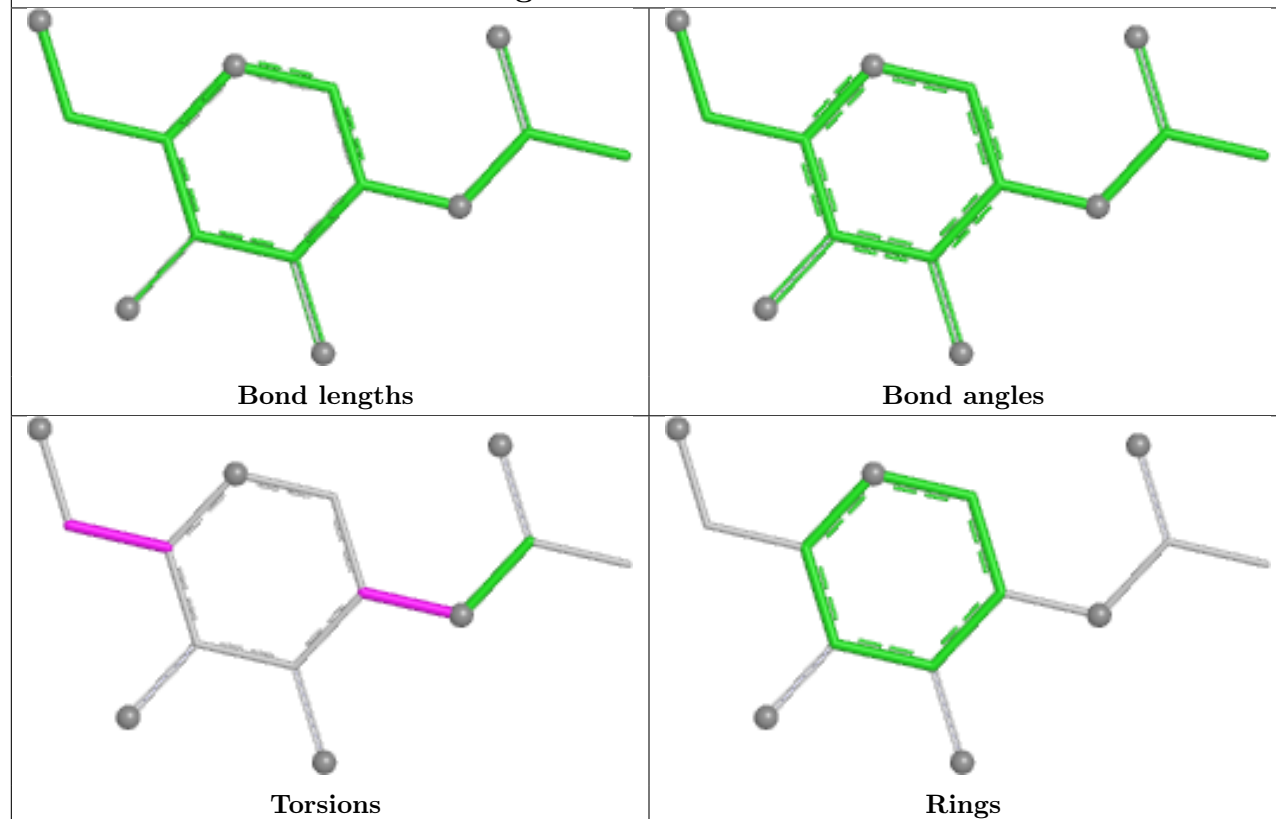
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	3501	NAG	1	0
4	D	3501	NAG	1	0
4	E	3501	NAG	1	0
4	N	3501	NAG	1	0
4	G	3501	NAG	1	0
4	T	3501	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

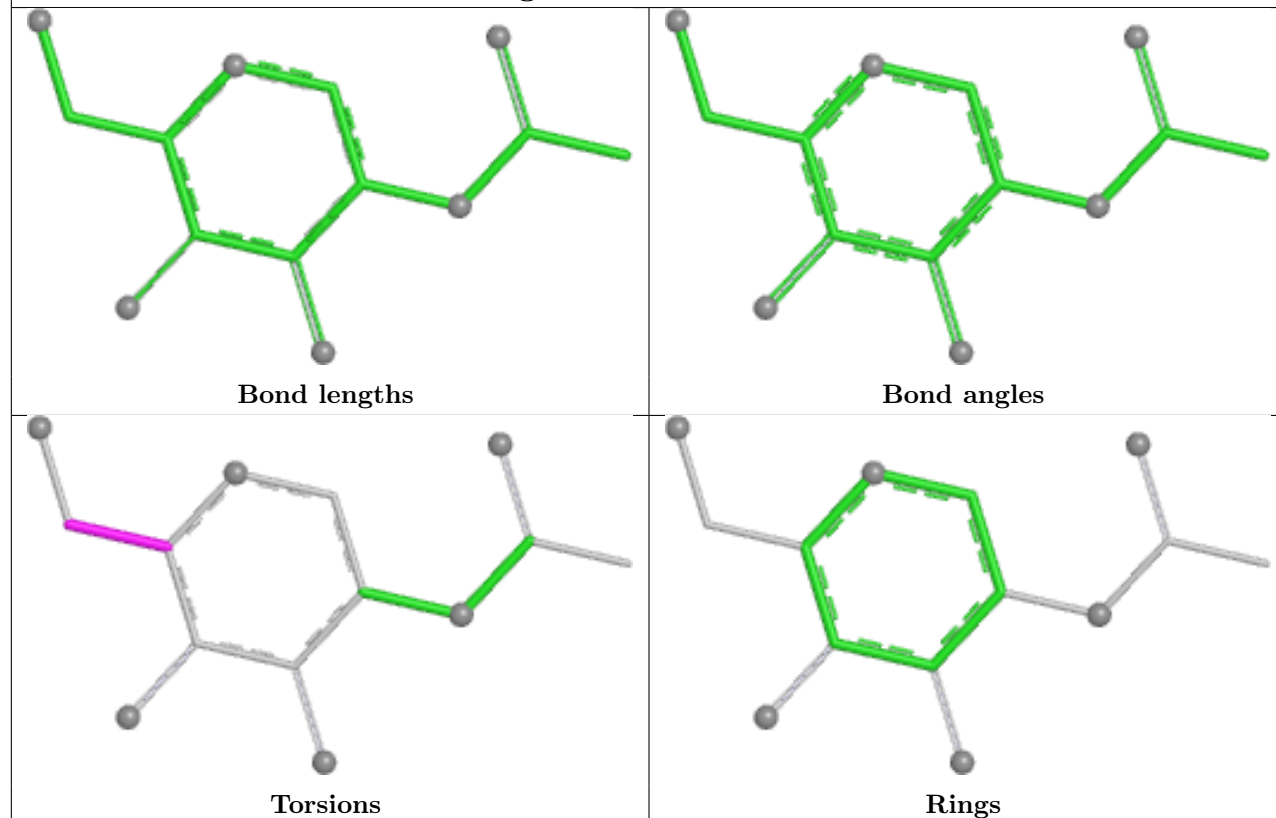




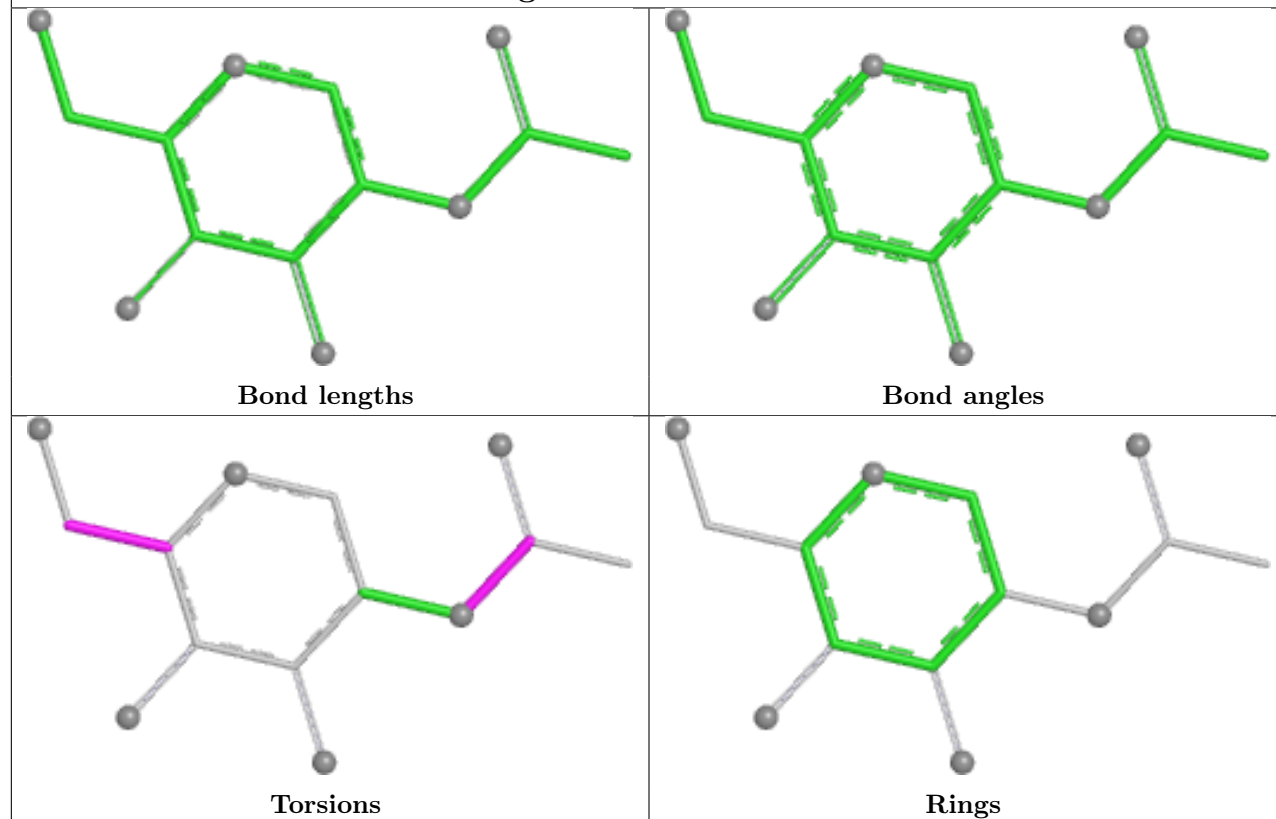
Ligand NAG M 3501



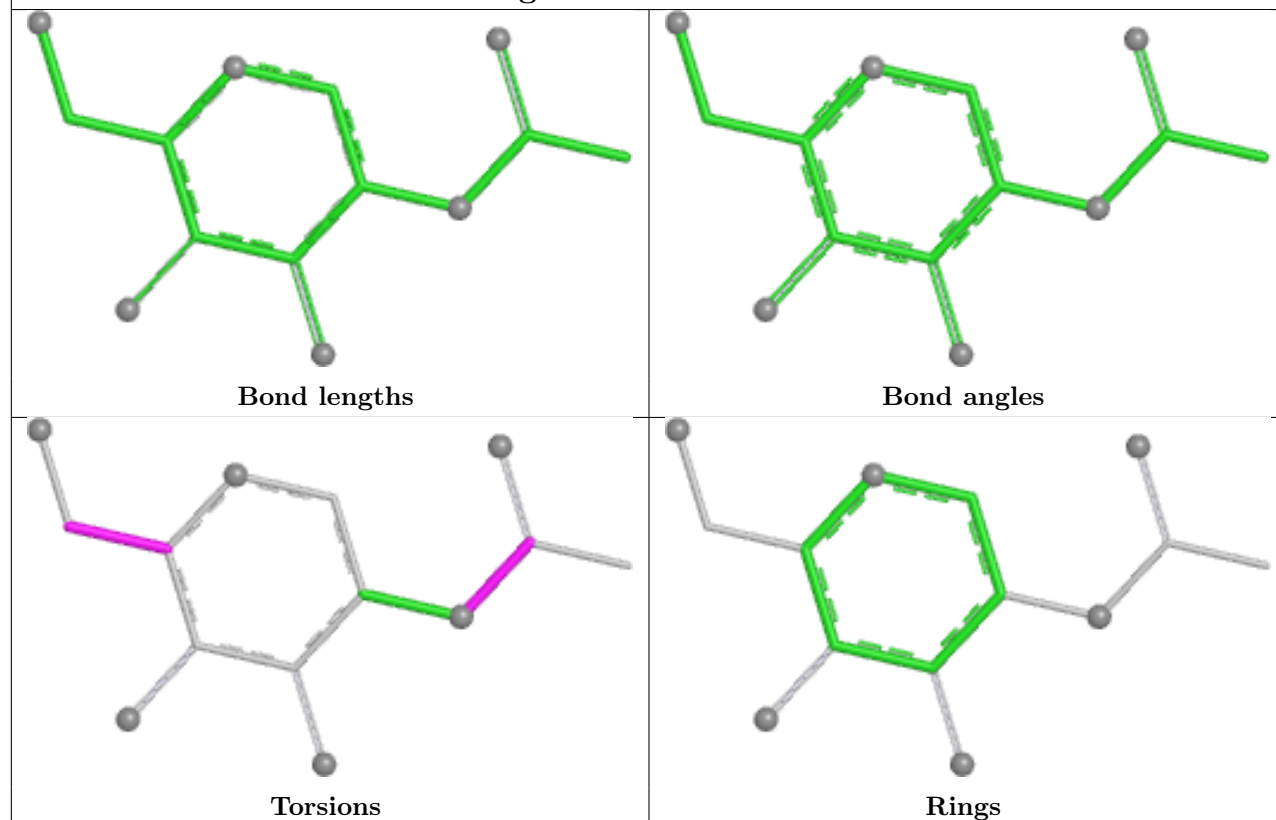
Ligand NAG K 3501



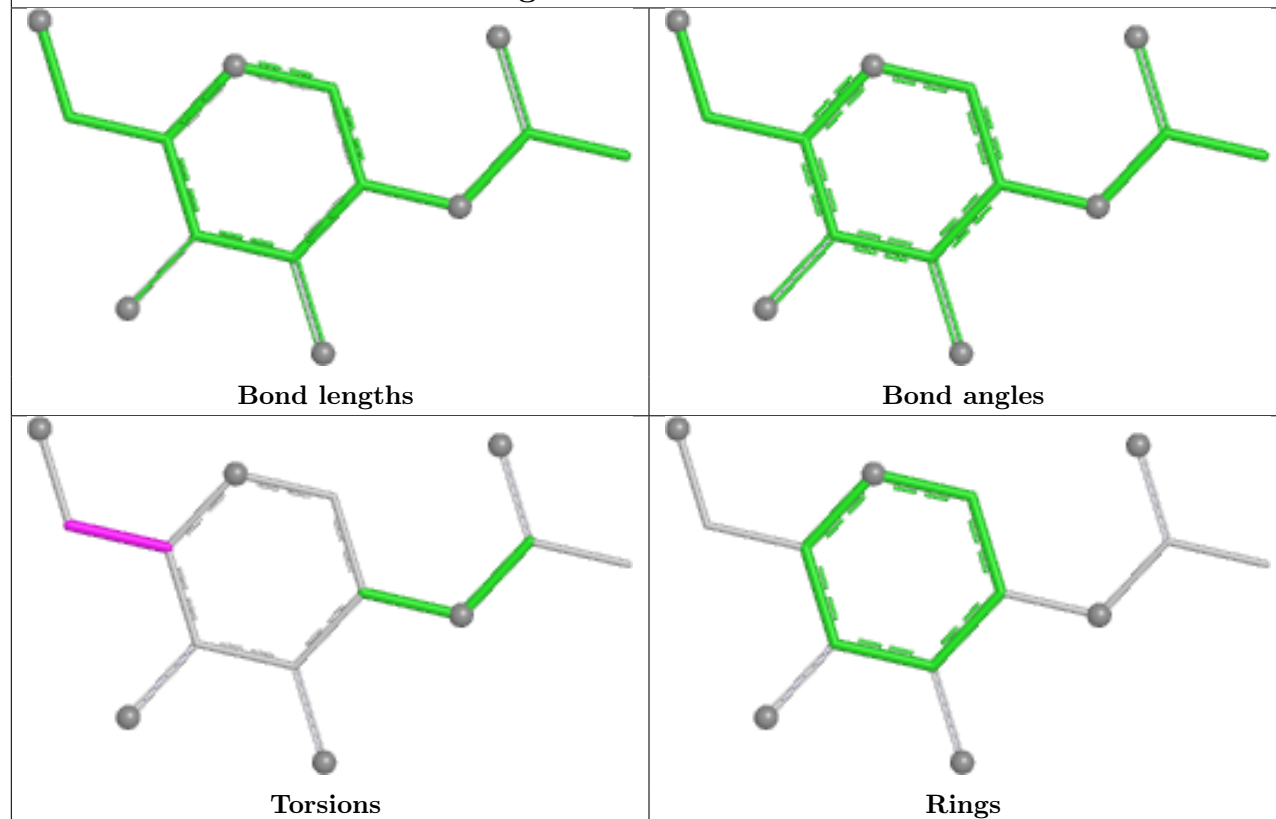
Ligand NAG H 3501



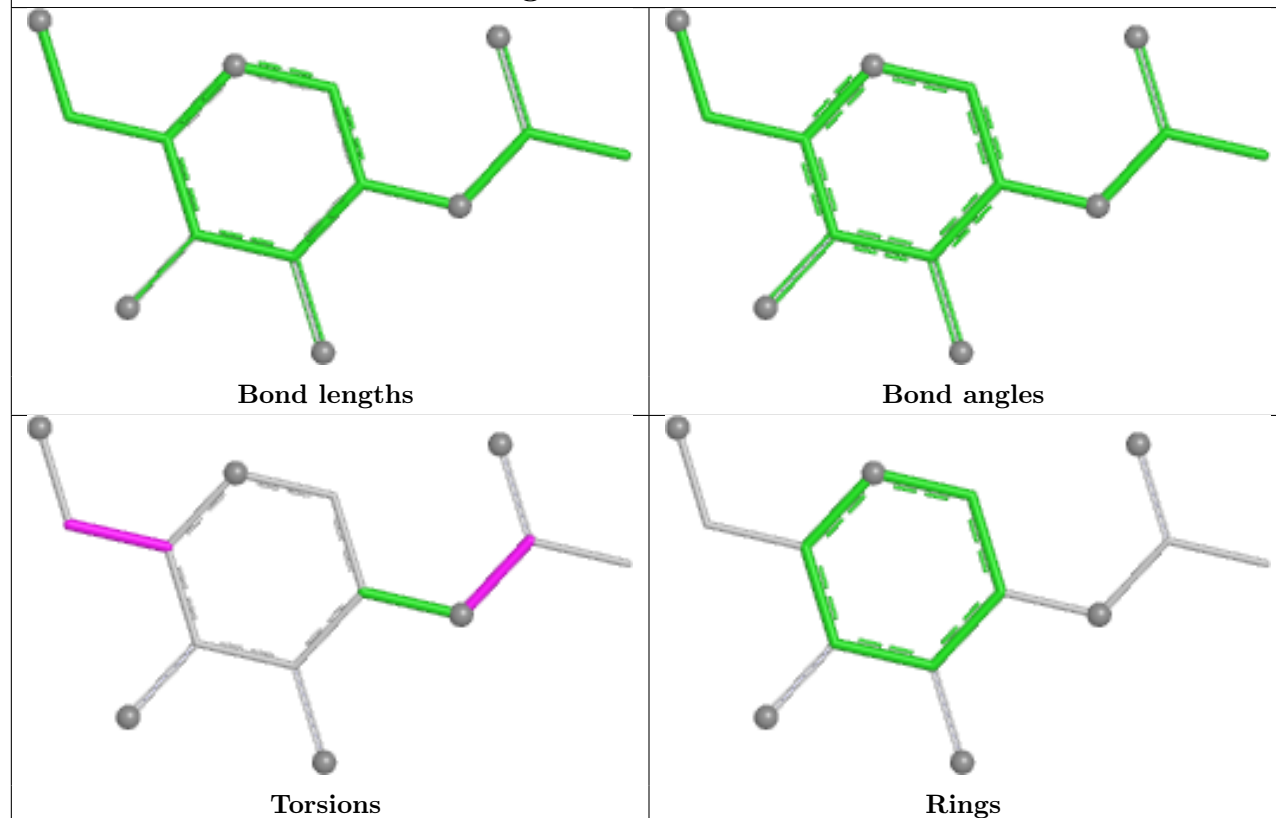
Ligand NAG R 3501

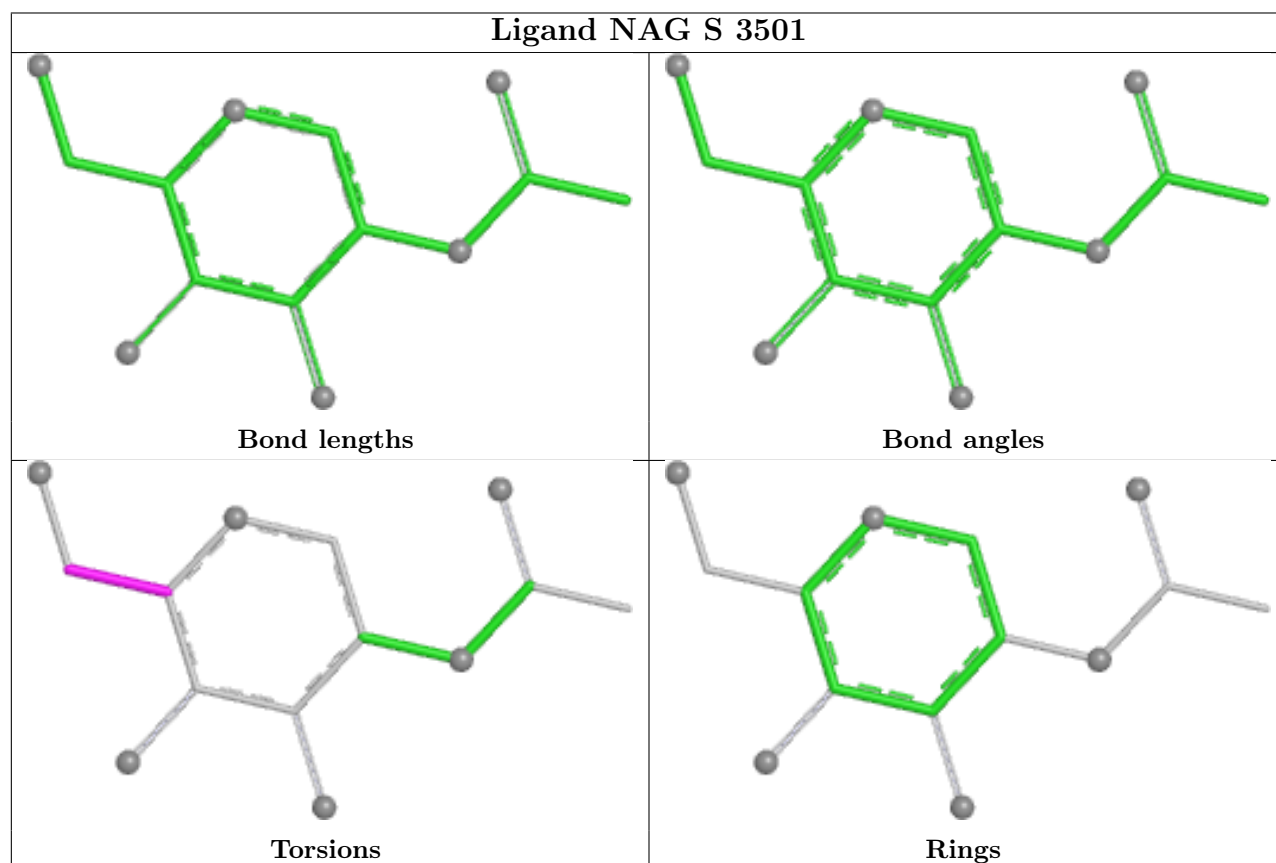
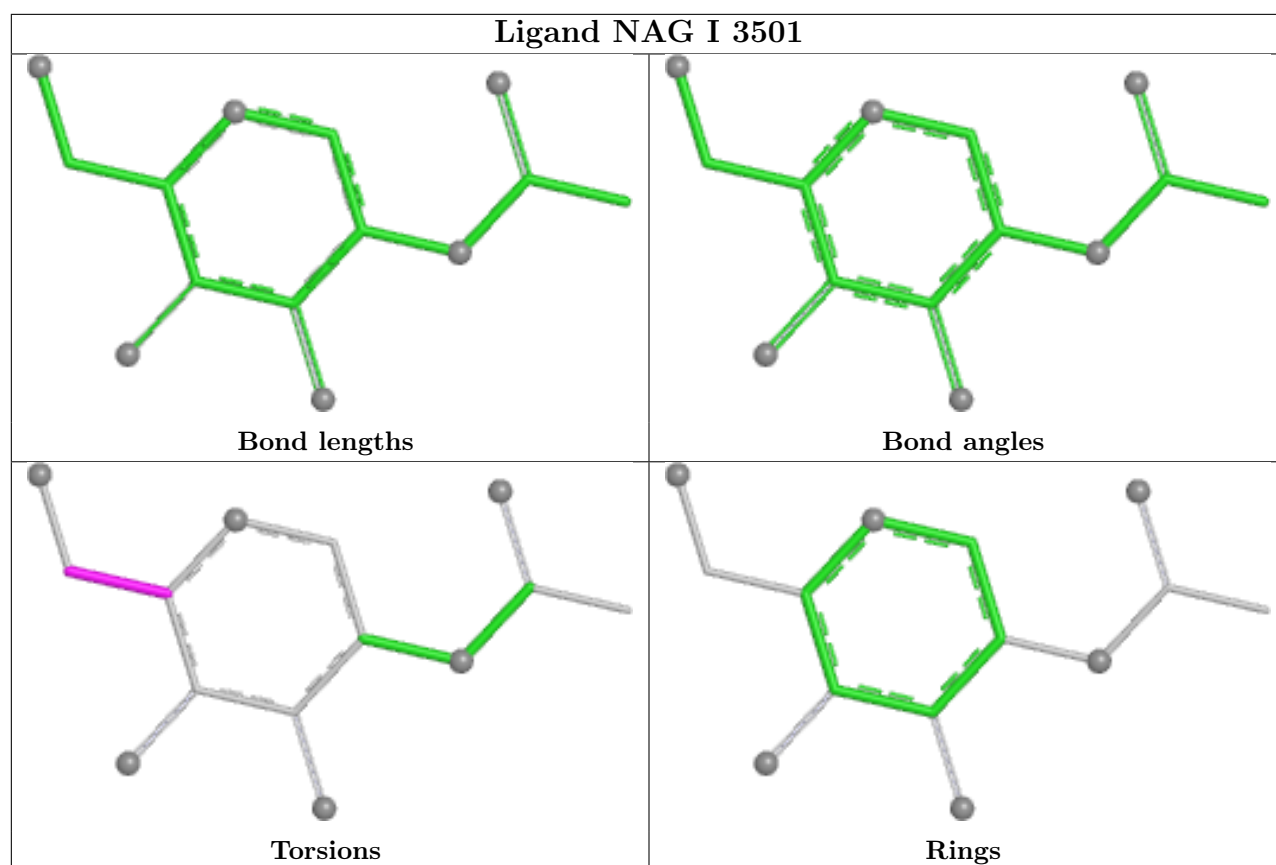


Ligand NAG A 3501

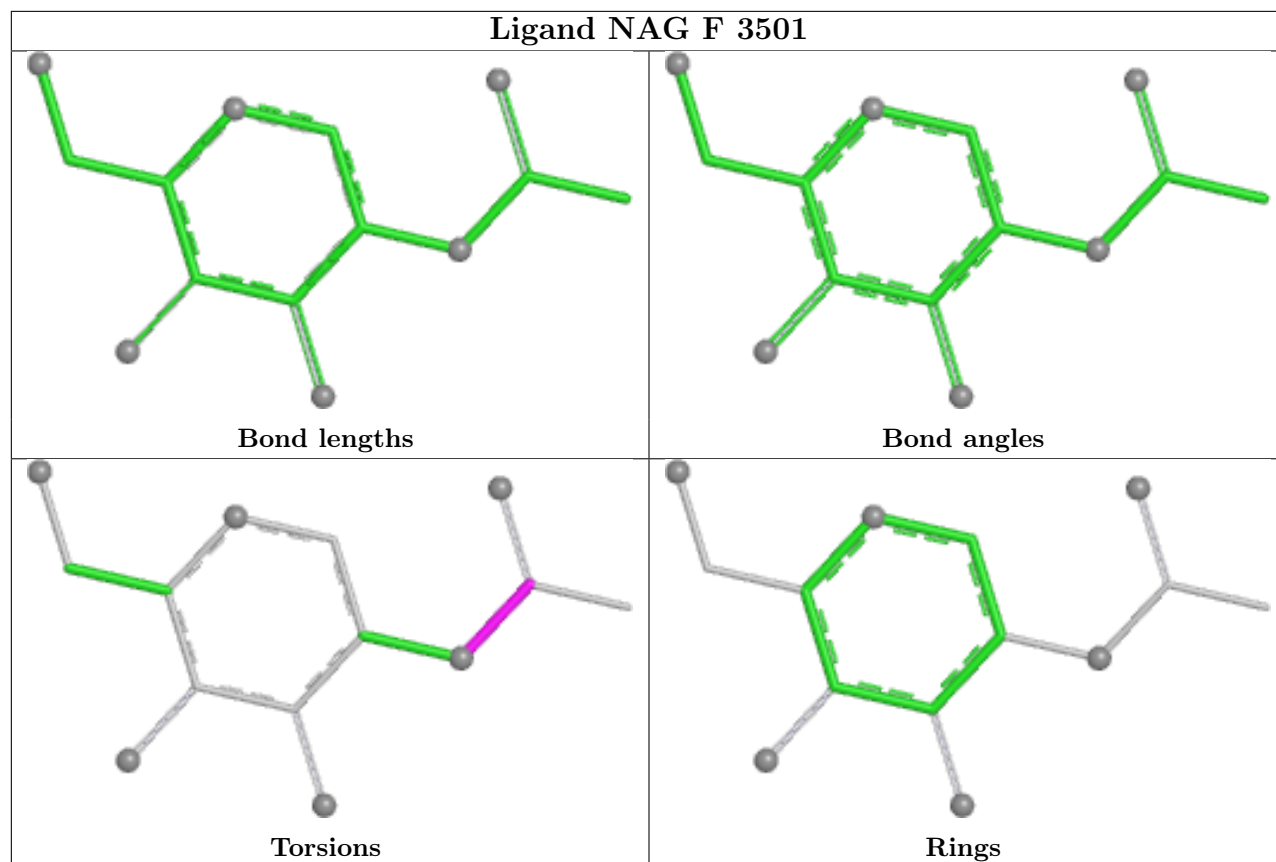


Ligand NAG L 3501

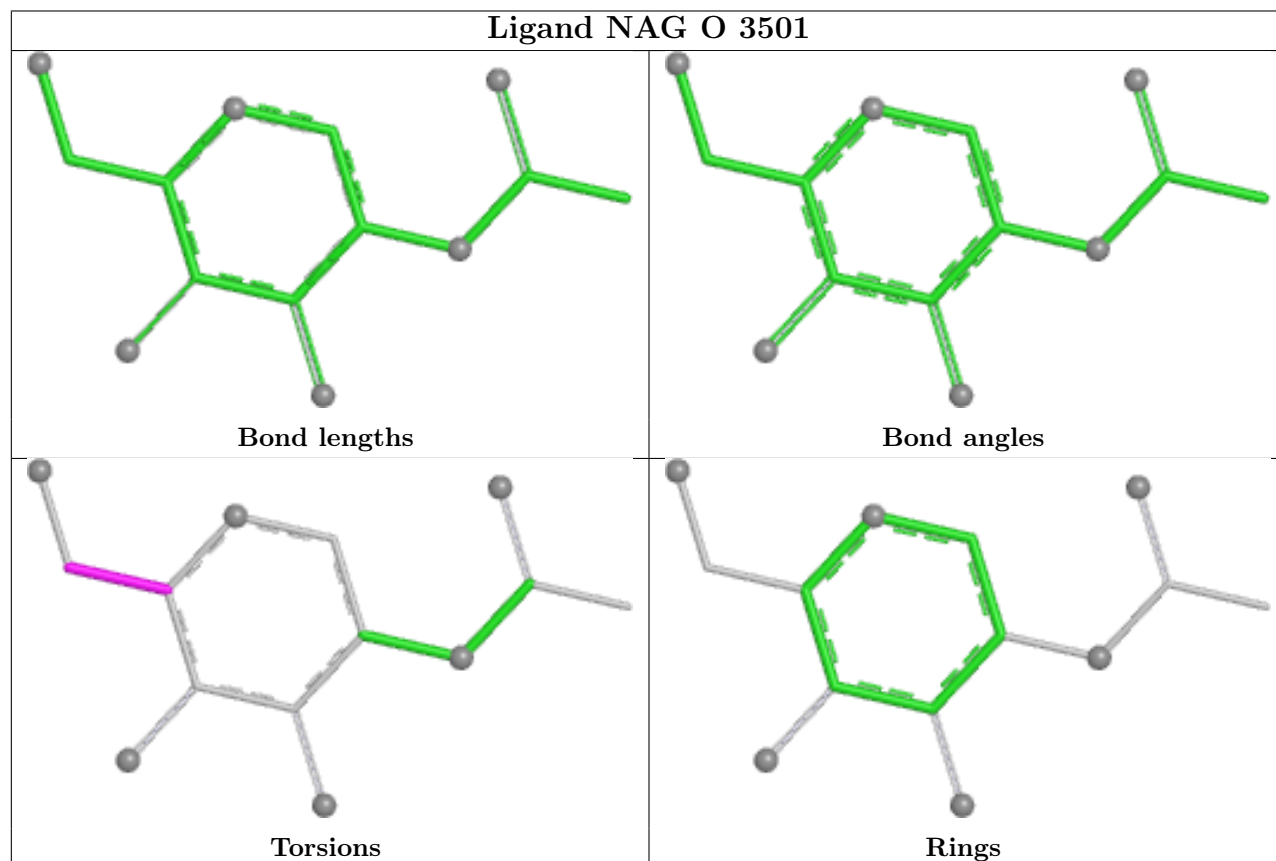




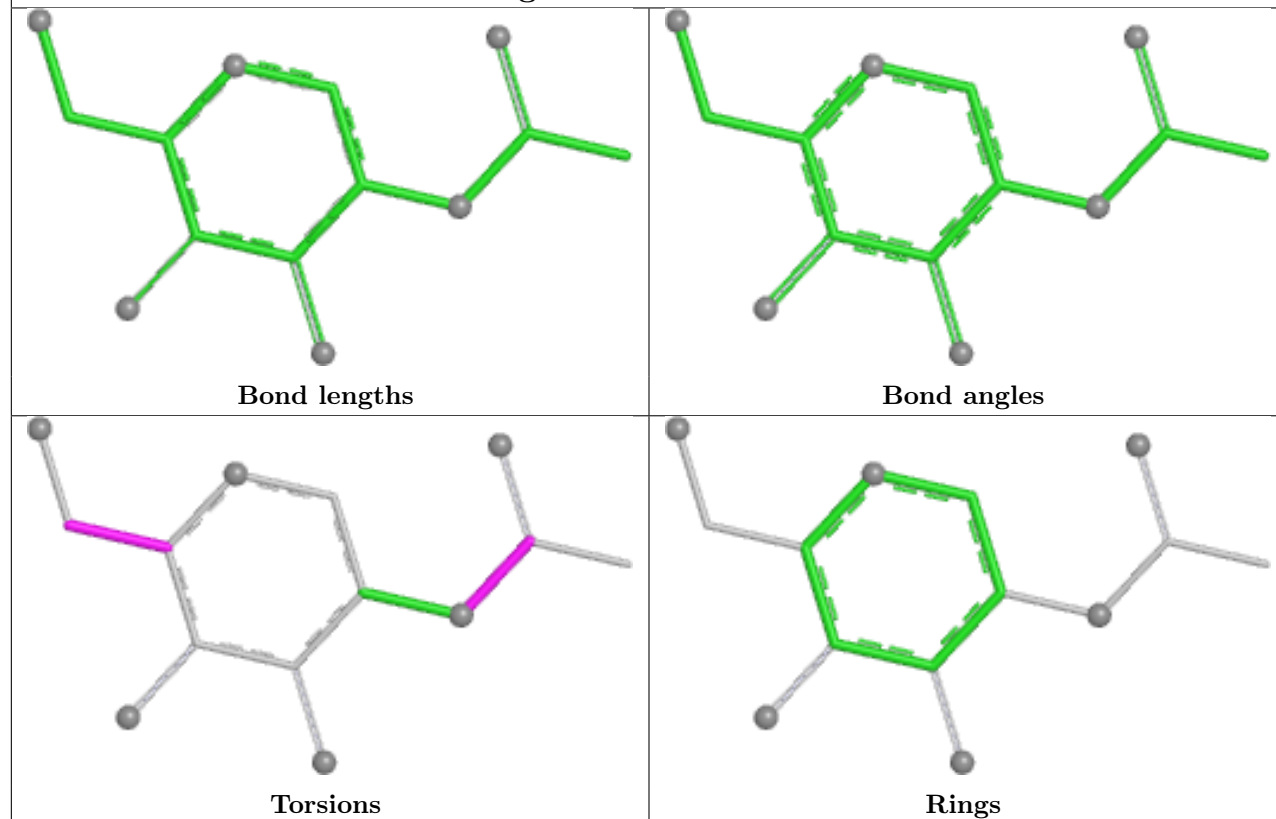
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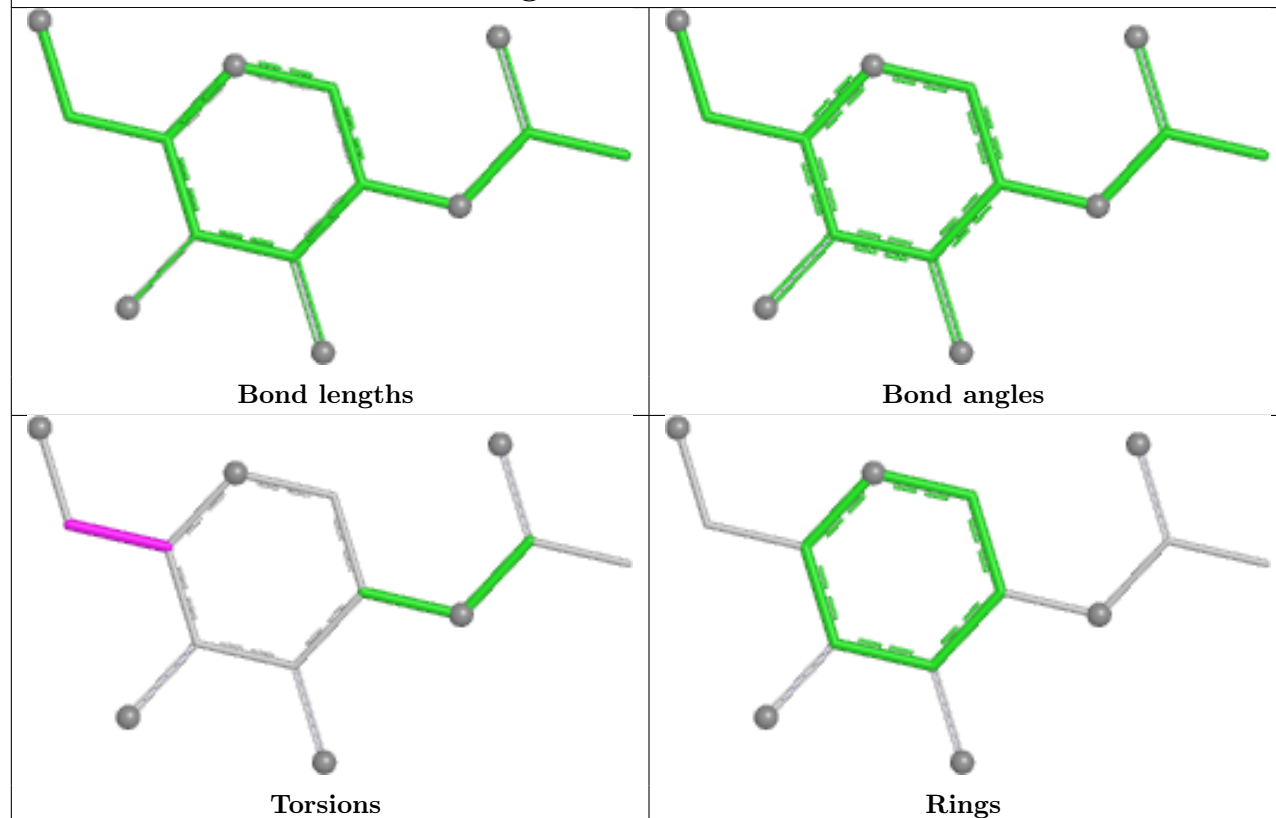
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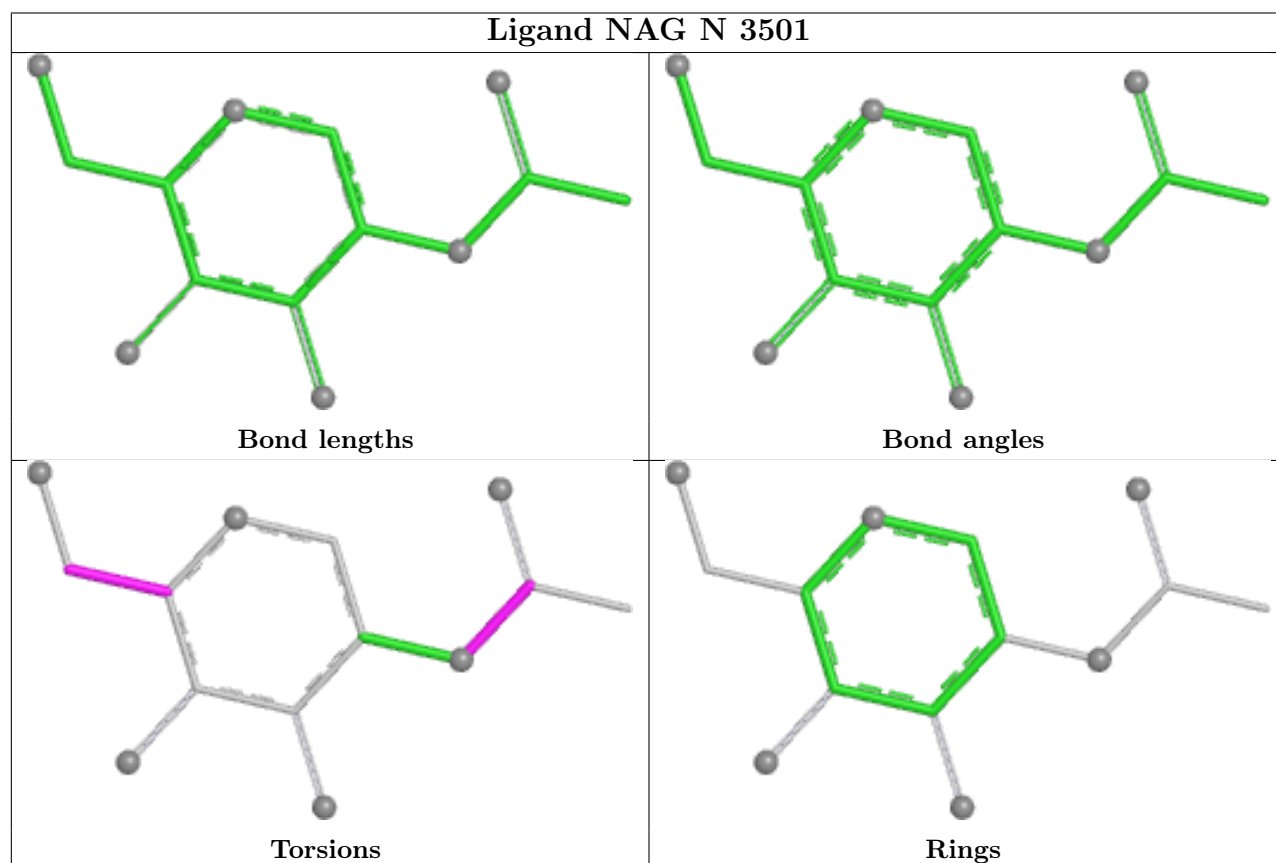
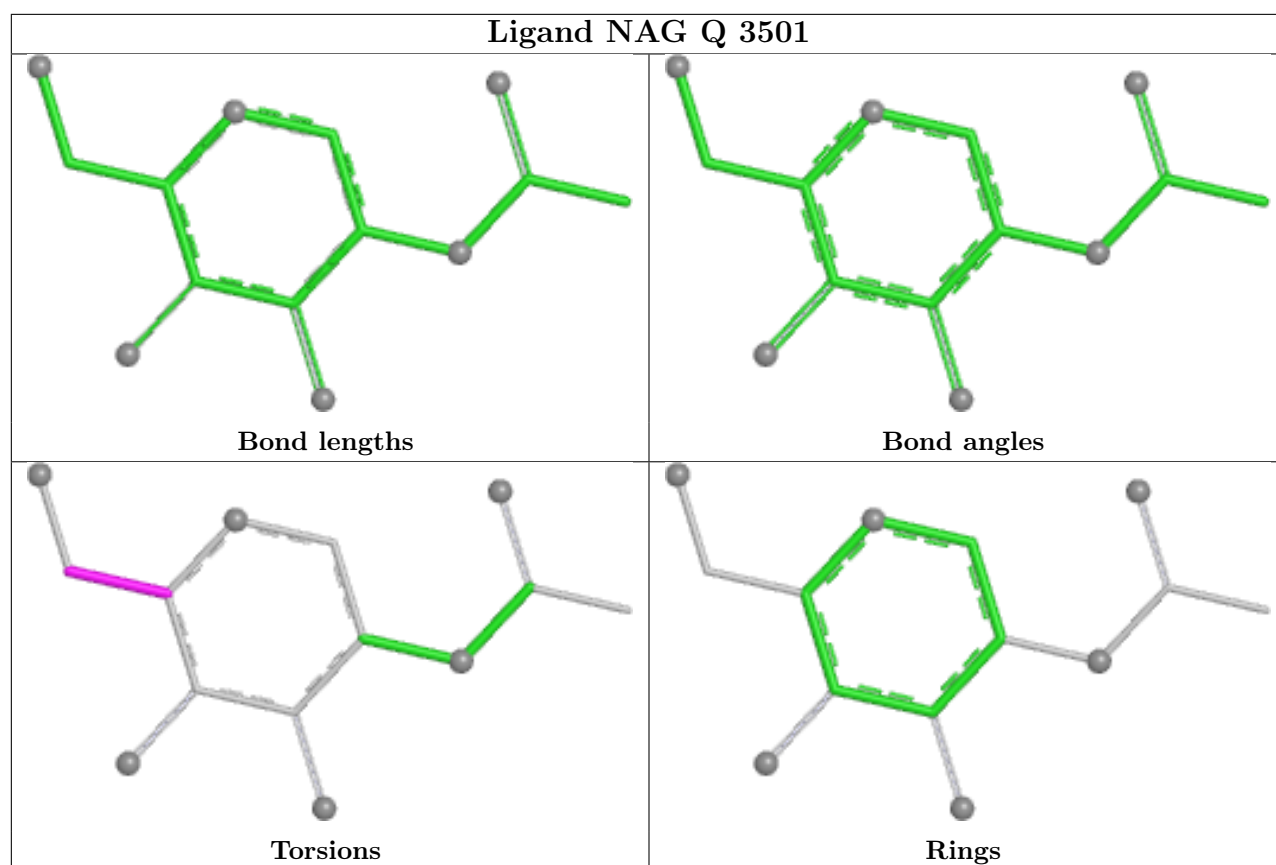


Ligand NAG D 3501

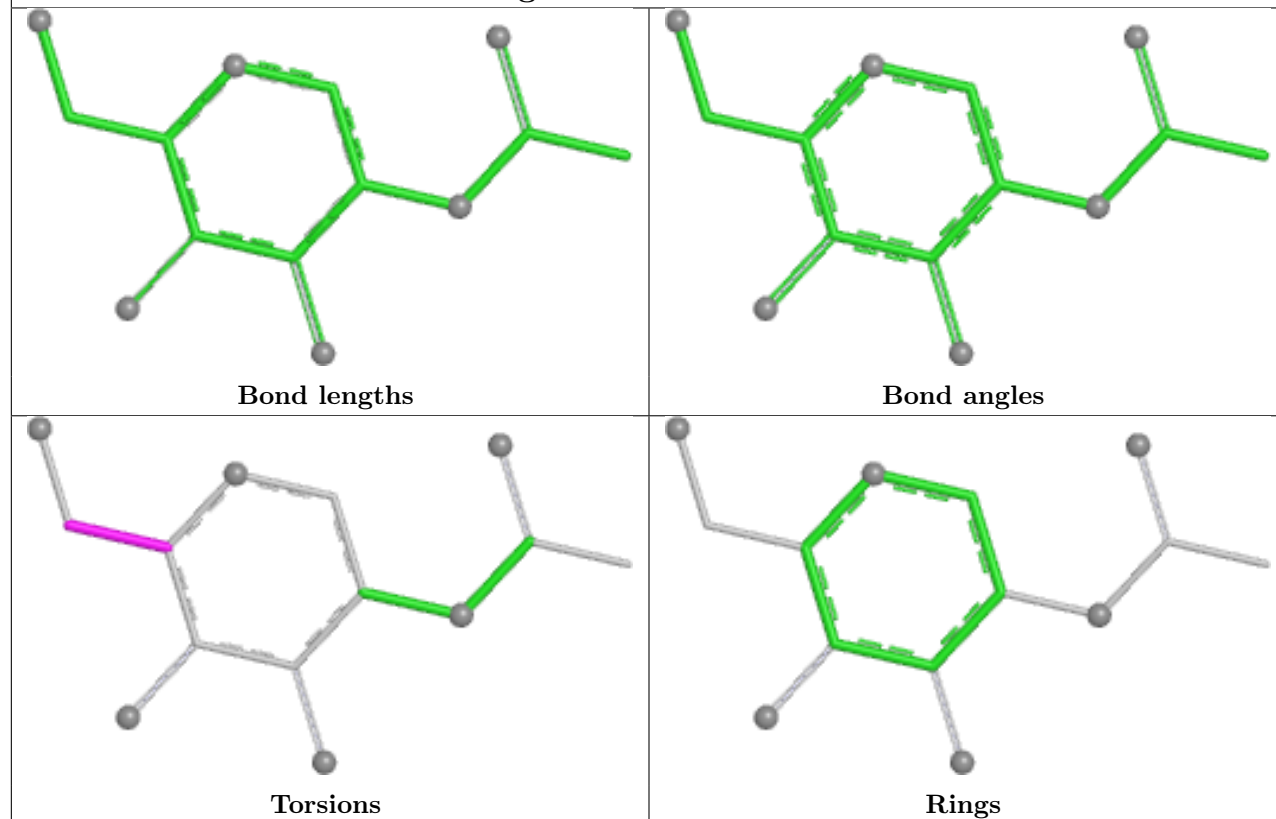


Ligand NAG E 3501

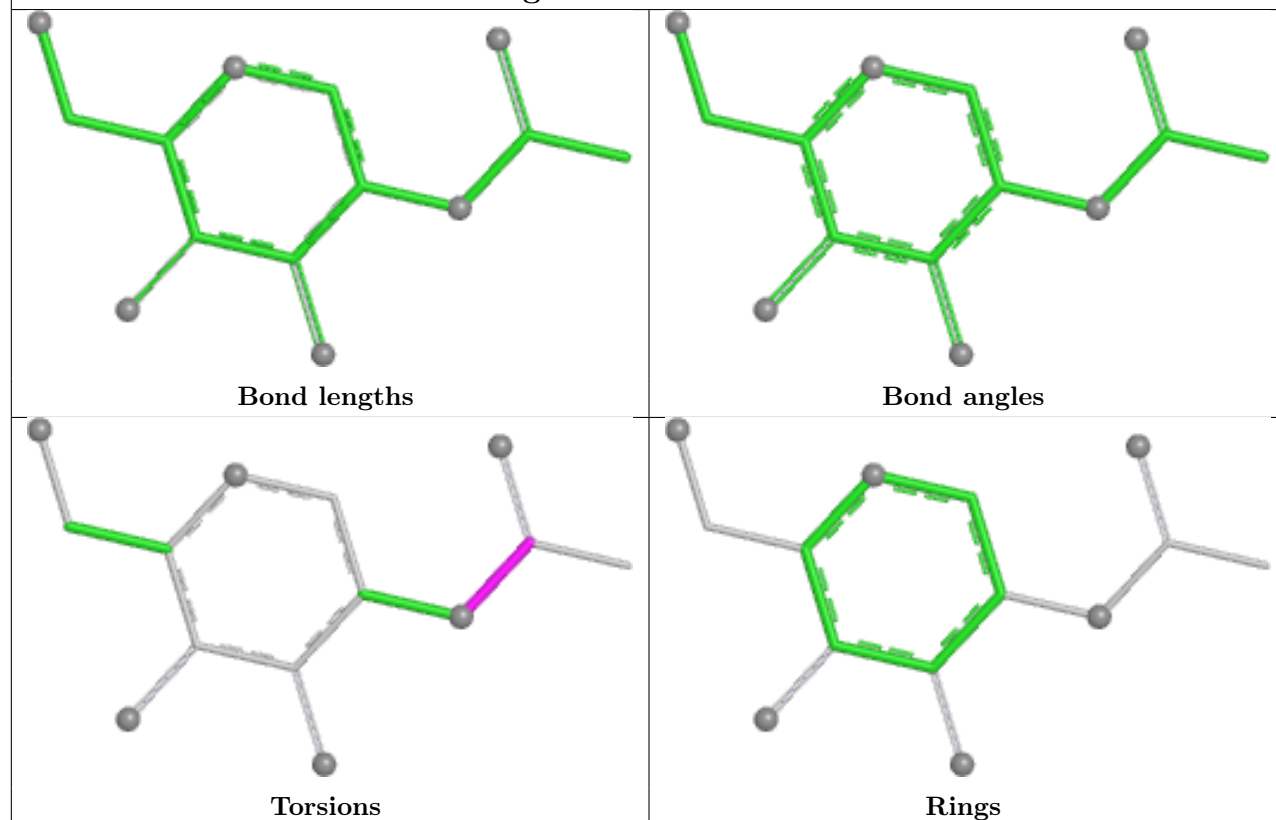


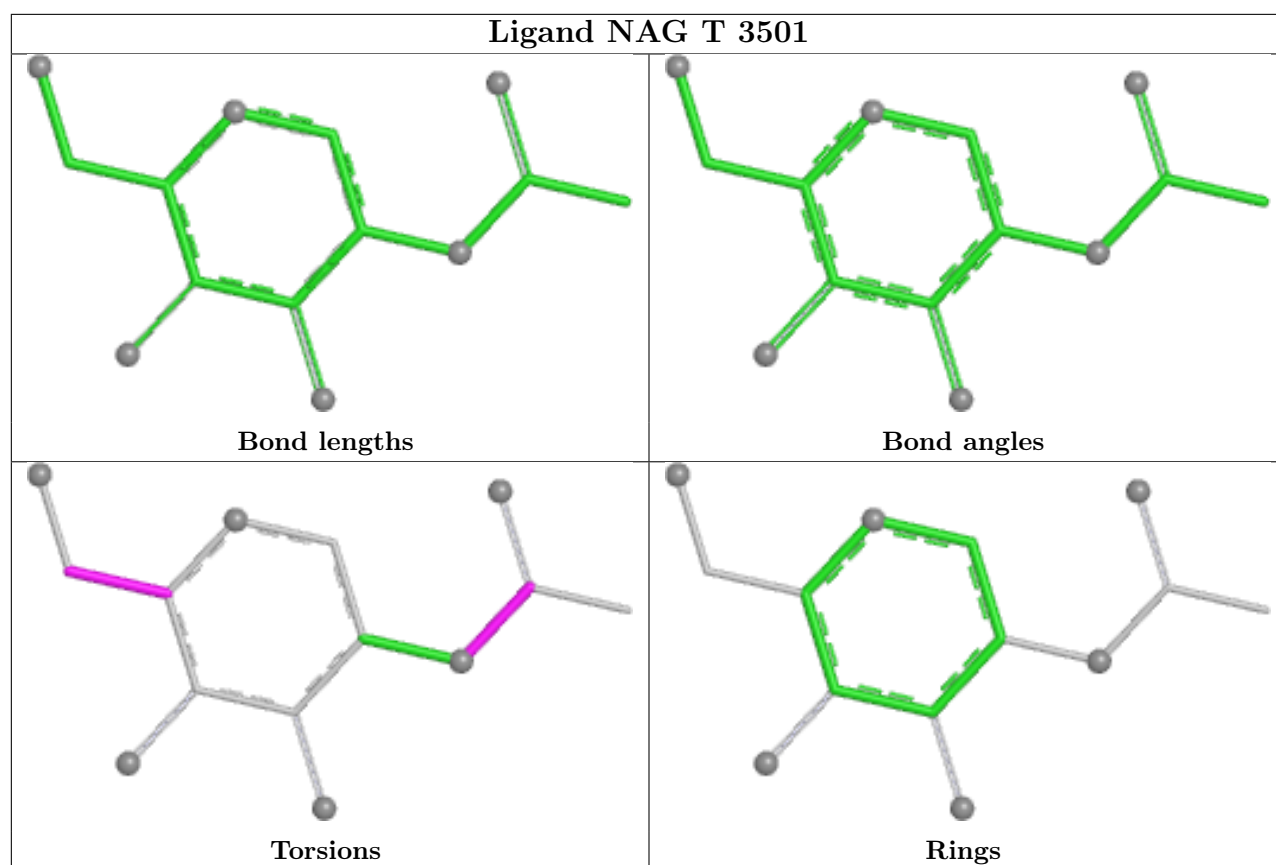


Ligand NAG G 3501



Ligand NAG J 3501





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.

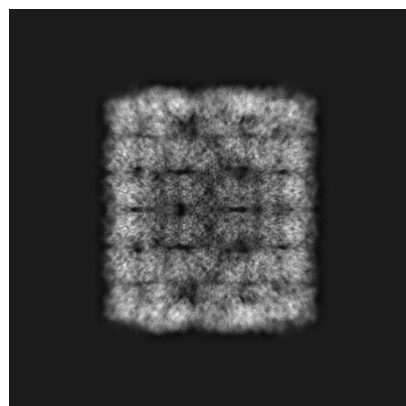
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41586. These allow visual inspection of the internal detail of the map and identification of artifacts.

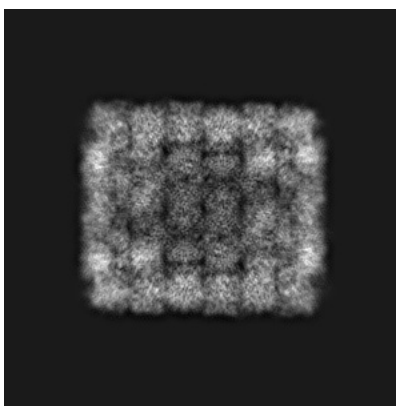
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

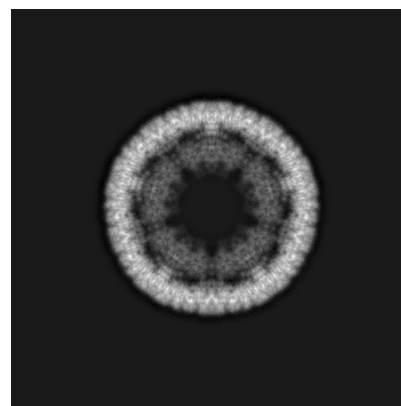
6.1.1 Primary map



X

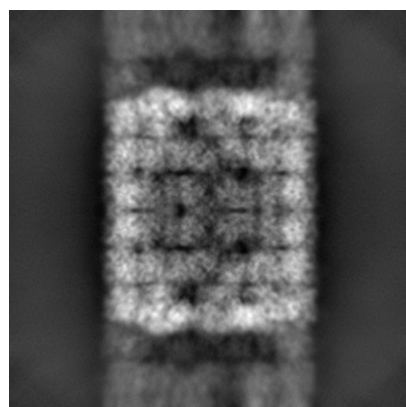


Y

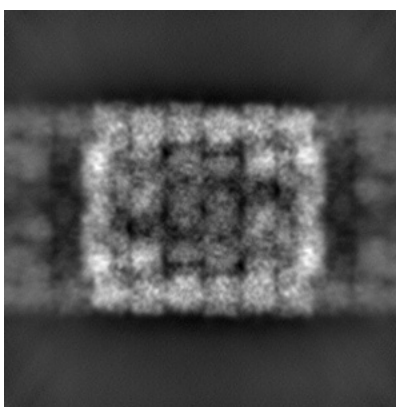


Z

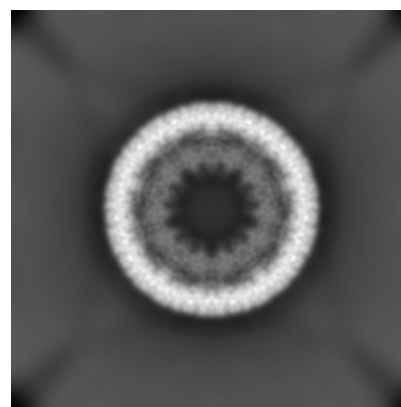
6.1.2 Raw map



X



Y

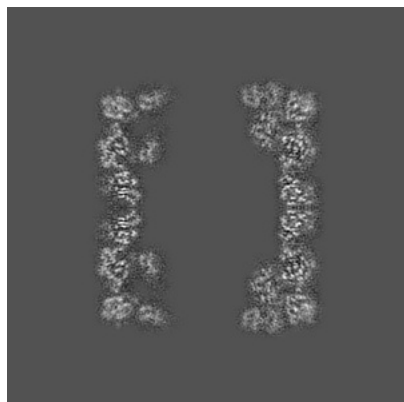


Z

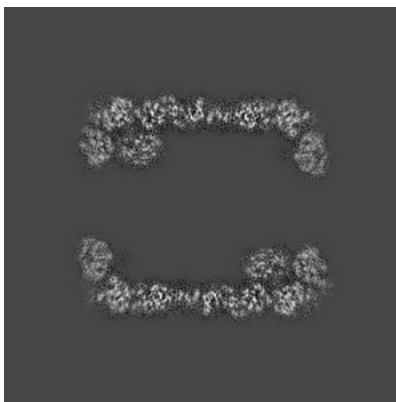
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

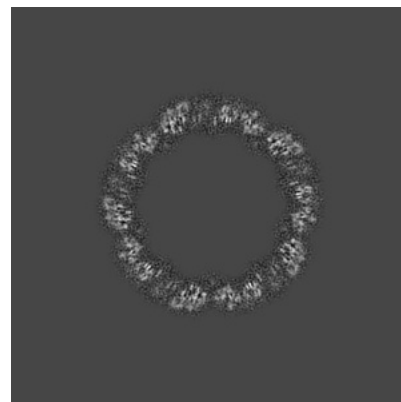
6.2.1 Primary map



X Index: 150

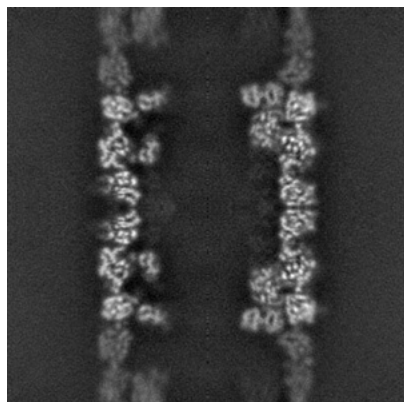


Y Index: 150

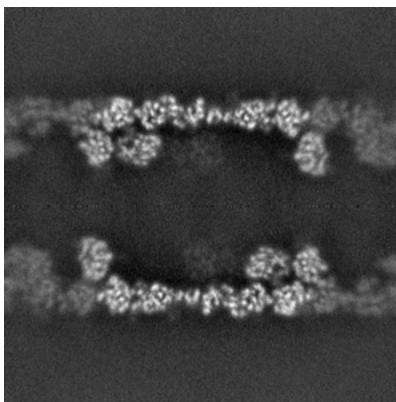


Z Index: 150

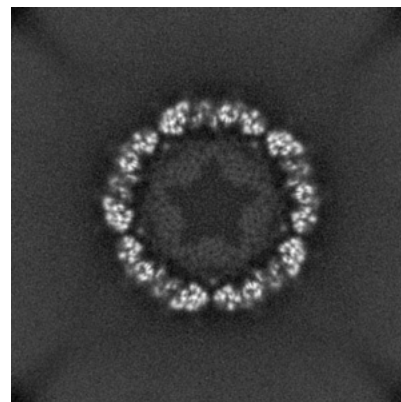
6.2.2 Raw map



X Index: 150



Y Index: 150

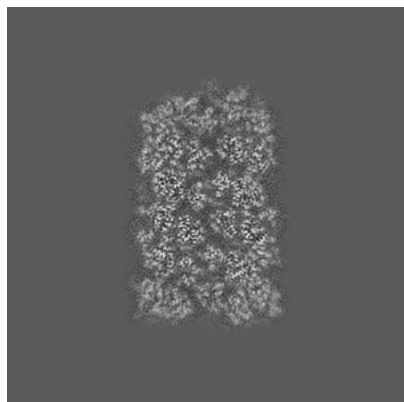


Z Index: 150

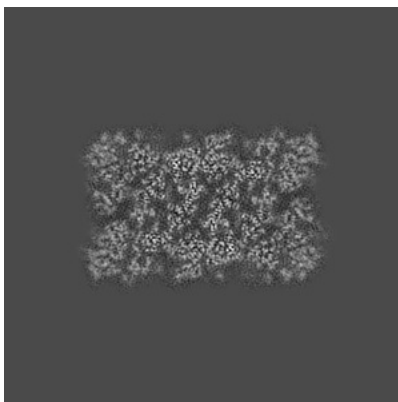
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 89

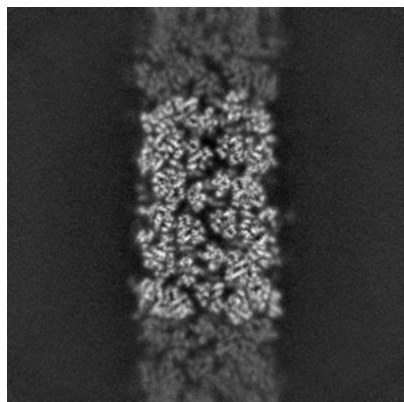


Y Index: 90

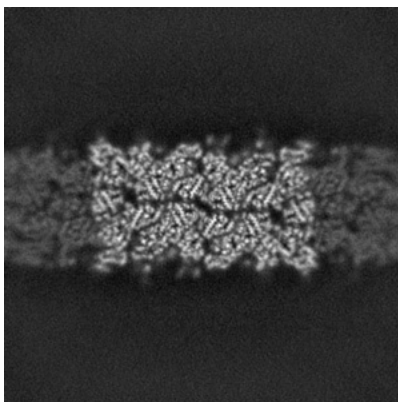


Z Index: 165

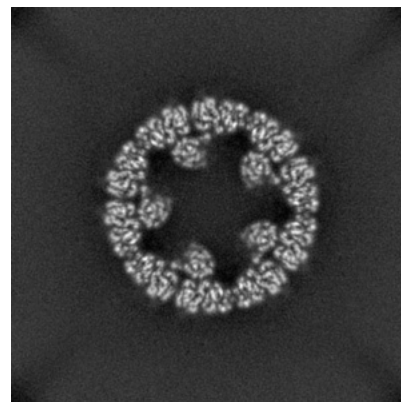
6.3.2 Raw map



X Index: 89



Y Index: 85

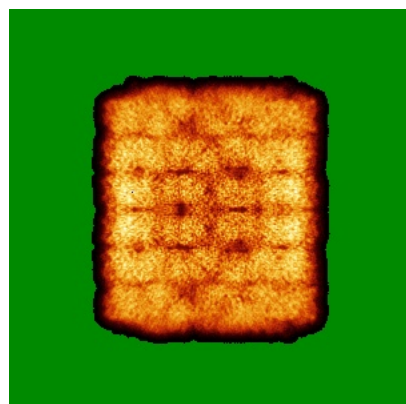


Z Index: 191

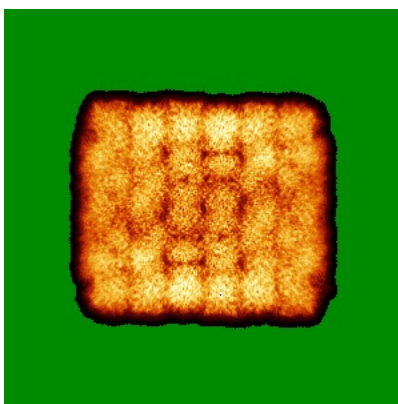
The images above show the largest variance slices of the map in three orthogonal directions.

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

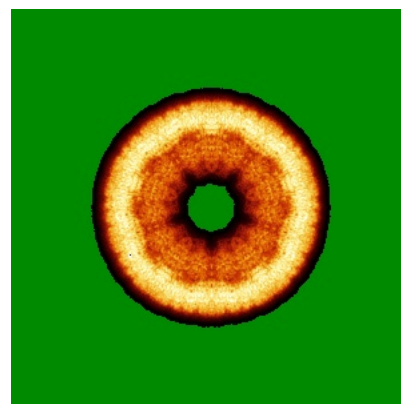
6.4.1 Primary map



X

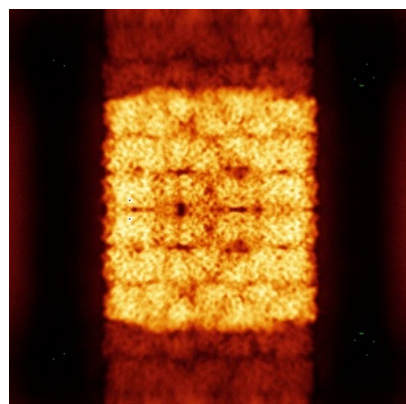


Y

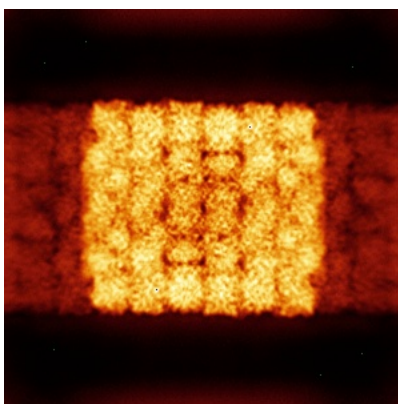


Z

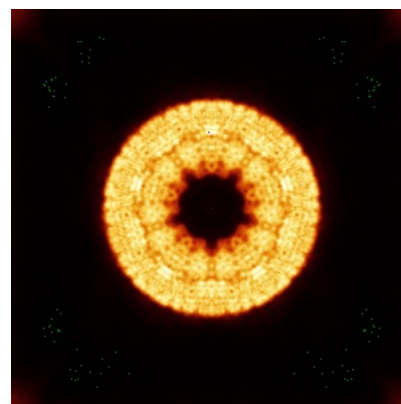
6.4.2 Raw map



X



Y

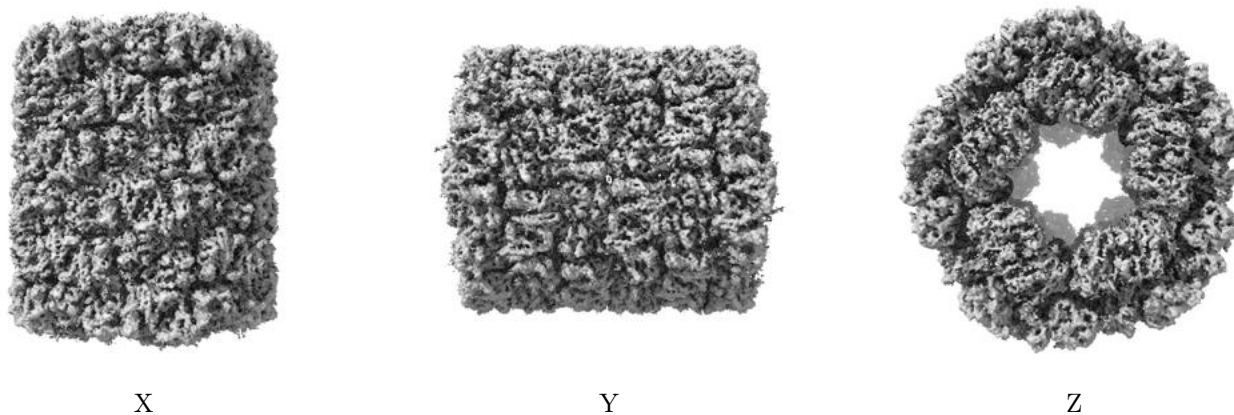


Z

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

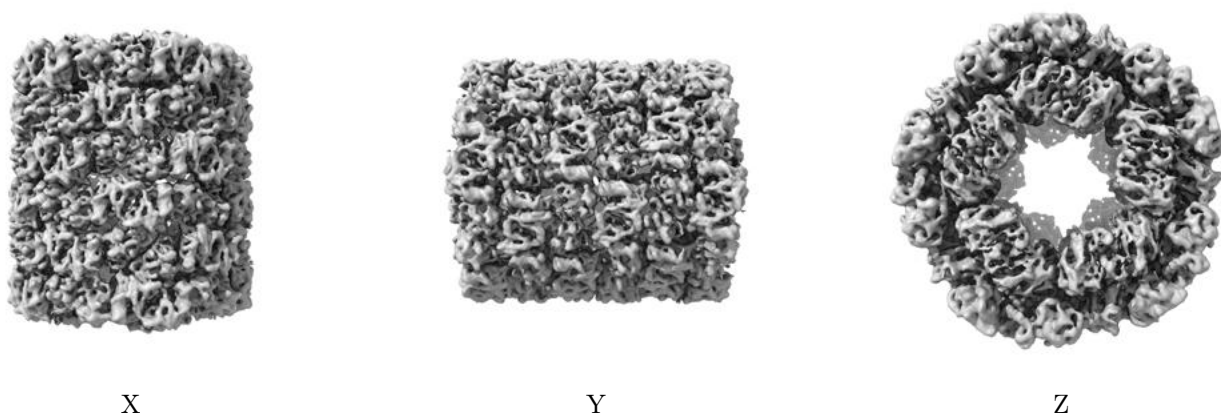
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.637. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

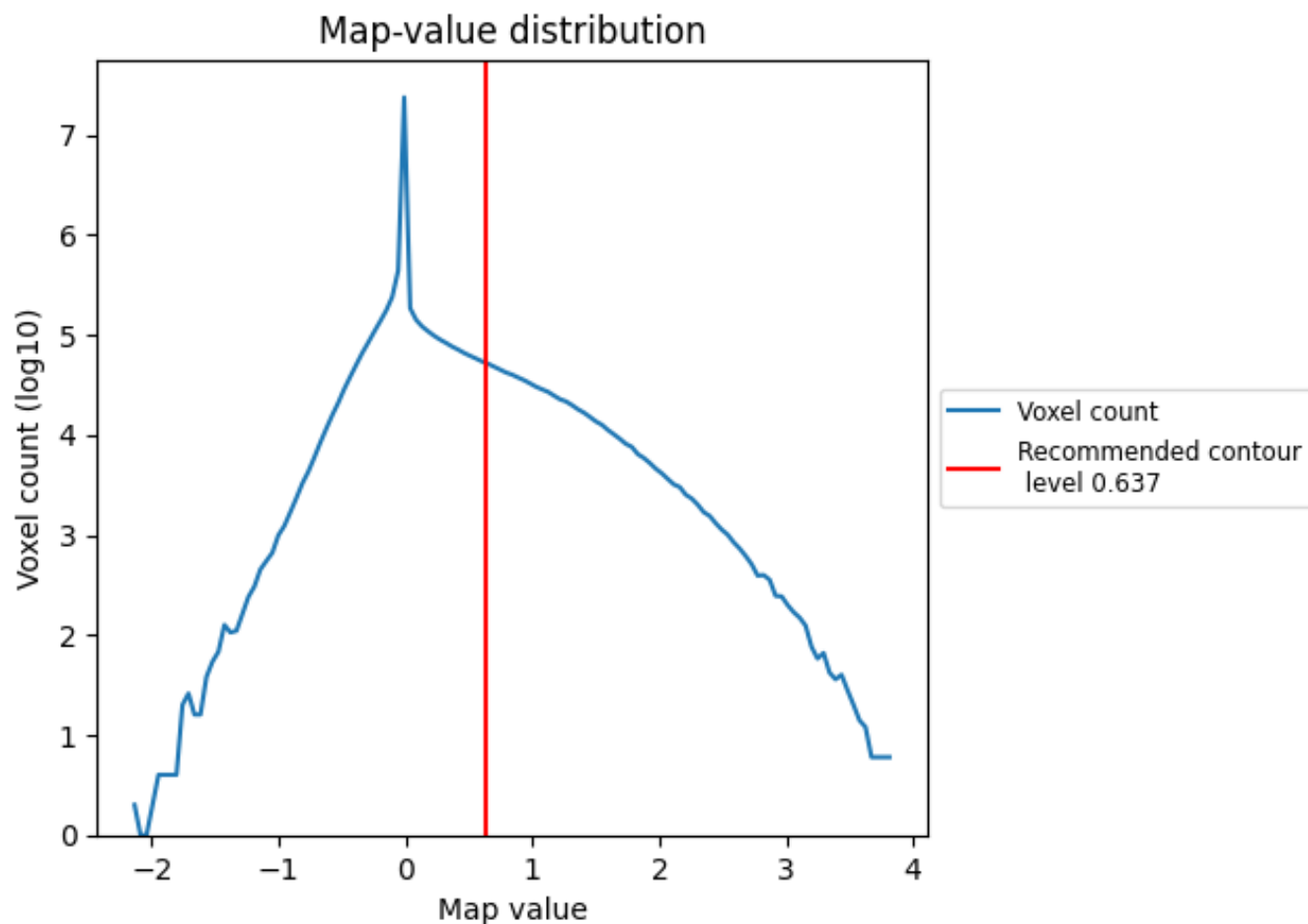
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

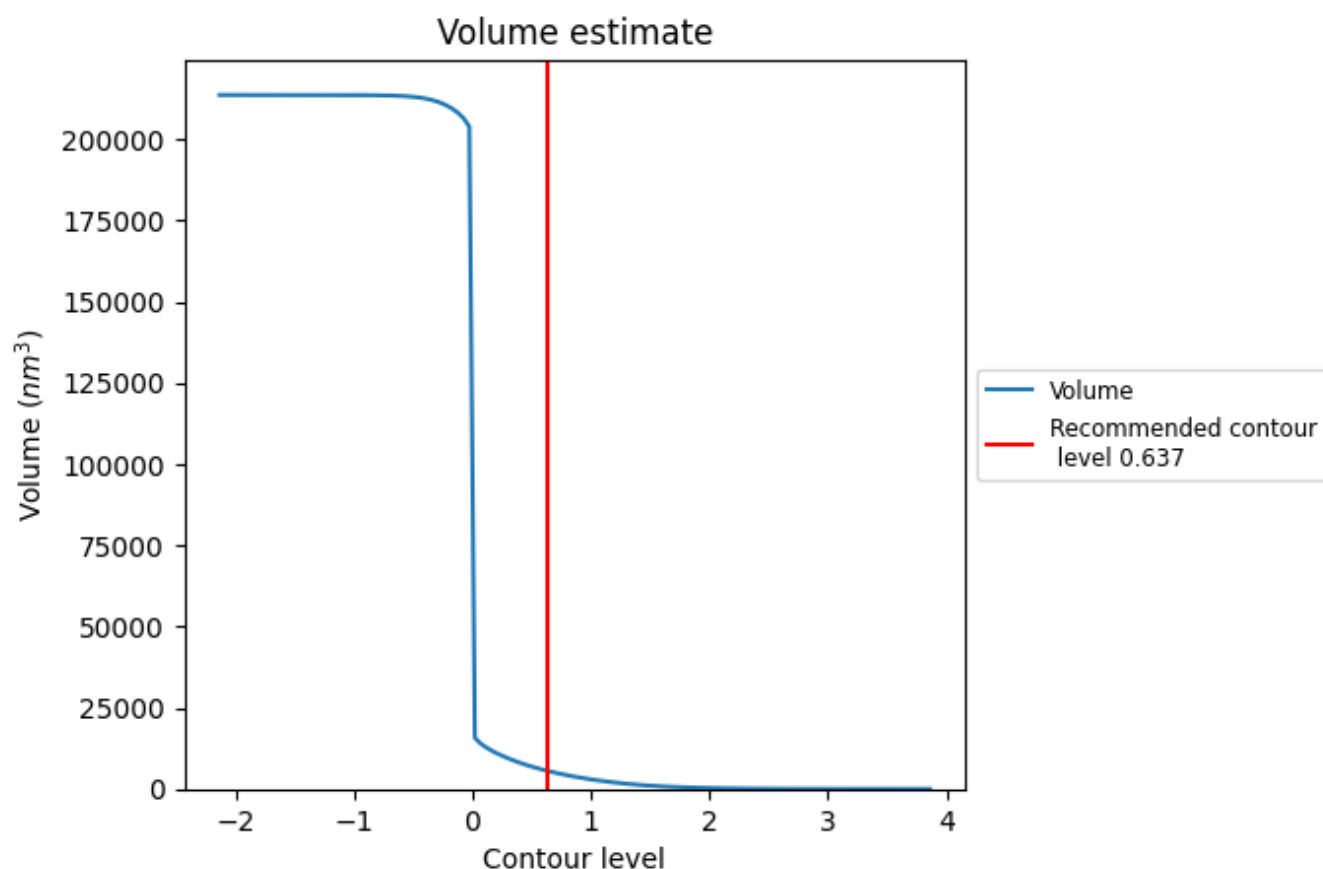
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

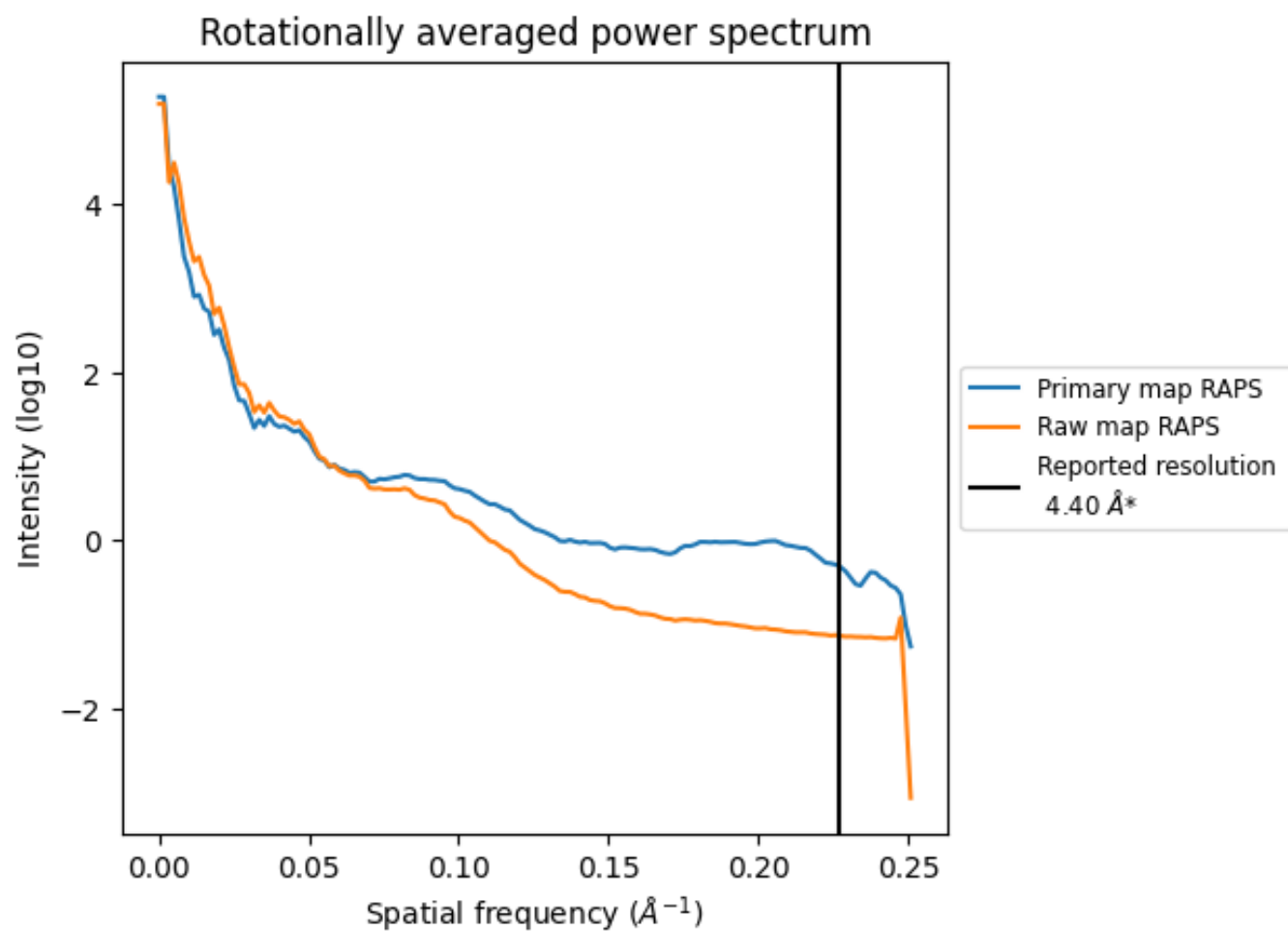
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5531 nm^3 ; this corresponds to an approximate mass of 4996 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

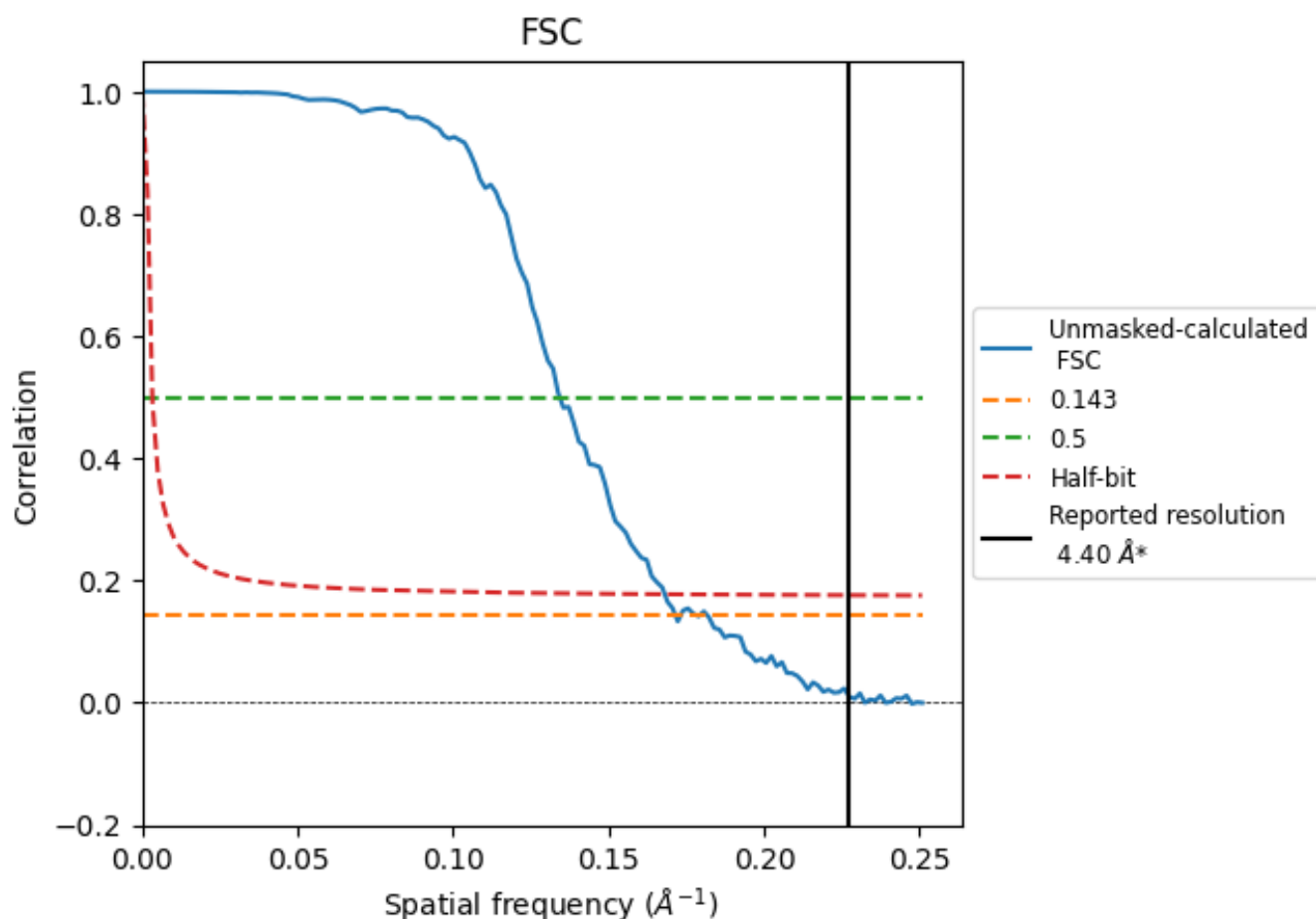


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

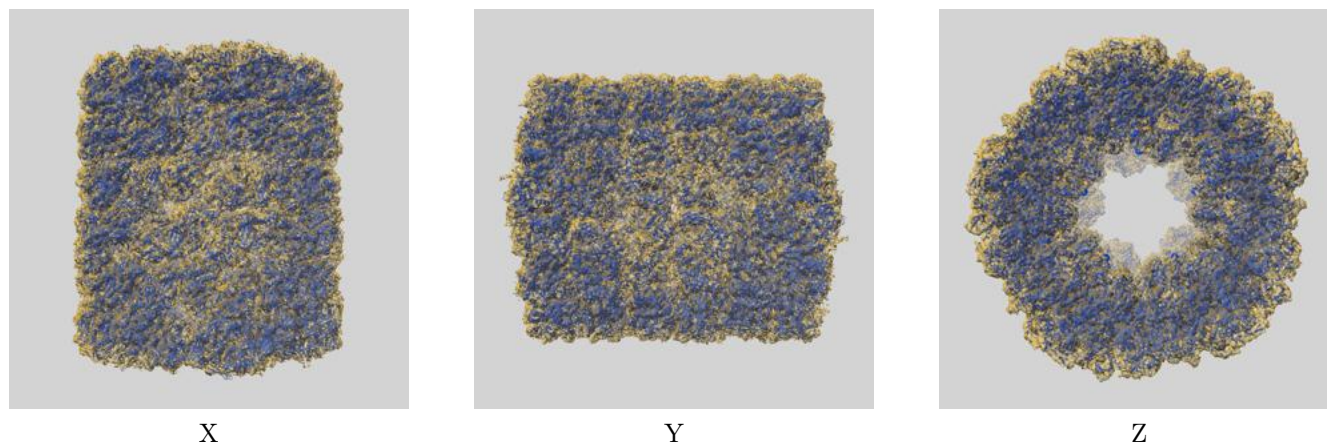
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.83	7.45	5.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.83 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

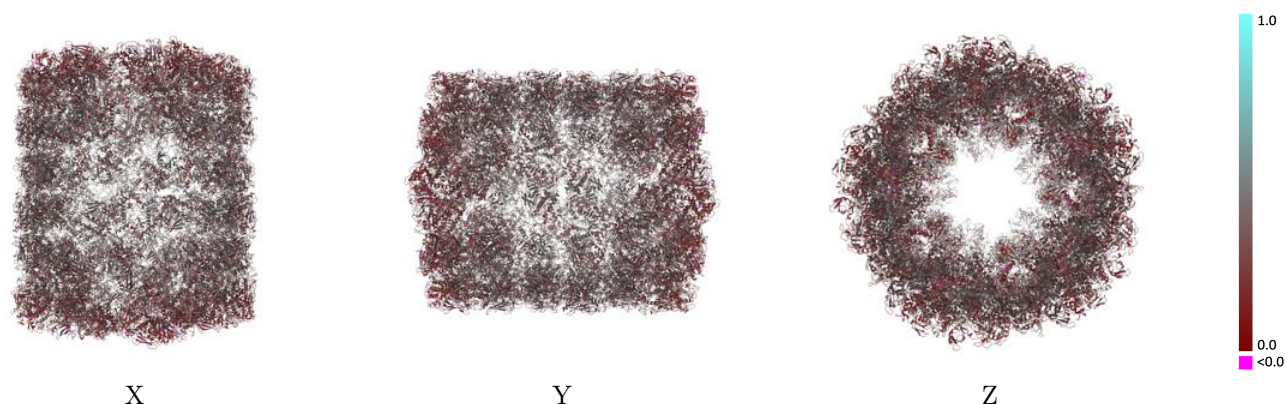
This section contains information regarding the fit between EMDB map EMD-41586 and PDB model 8TRZ. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



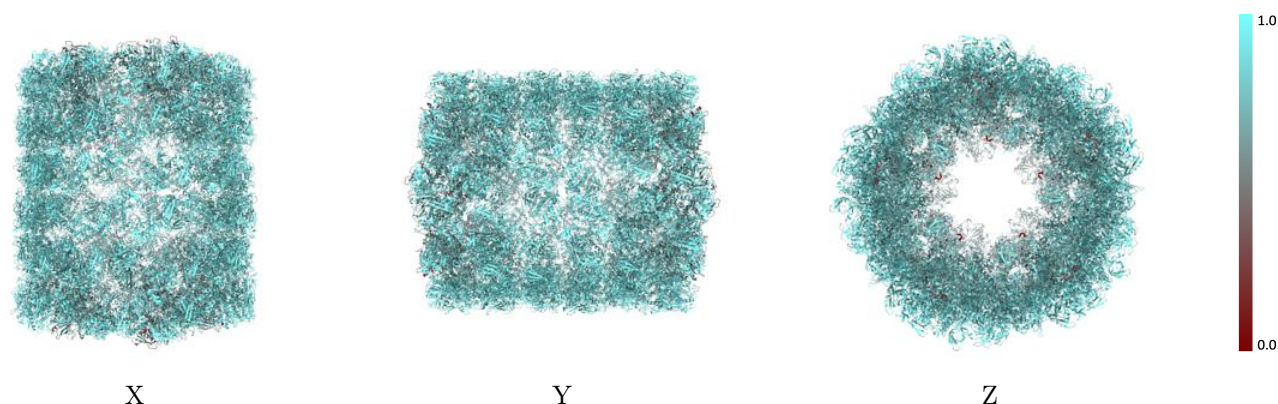
The images above show the 3D surface view of the map at the recommended contour level 0.637 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



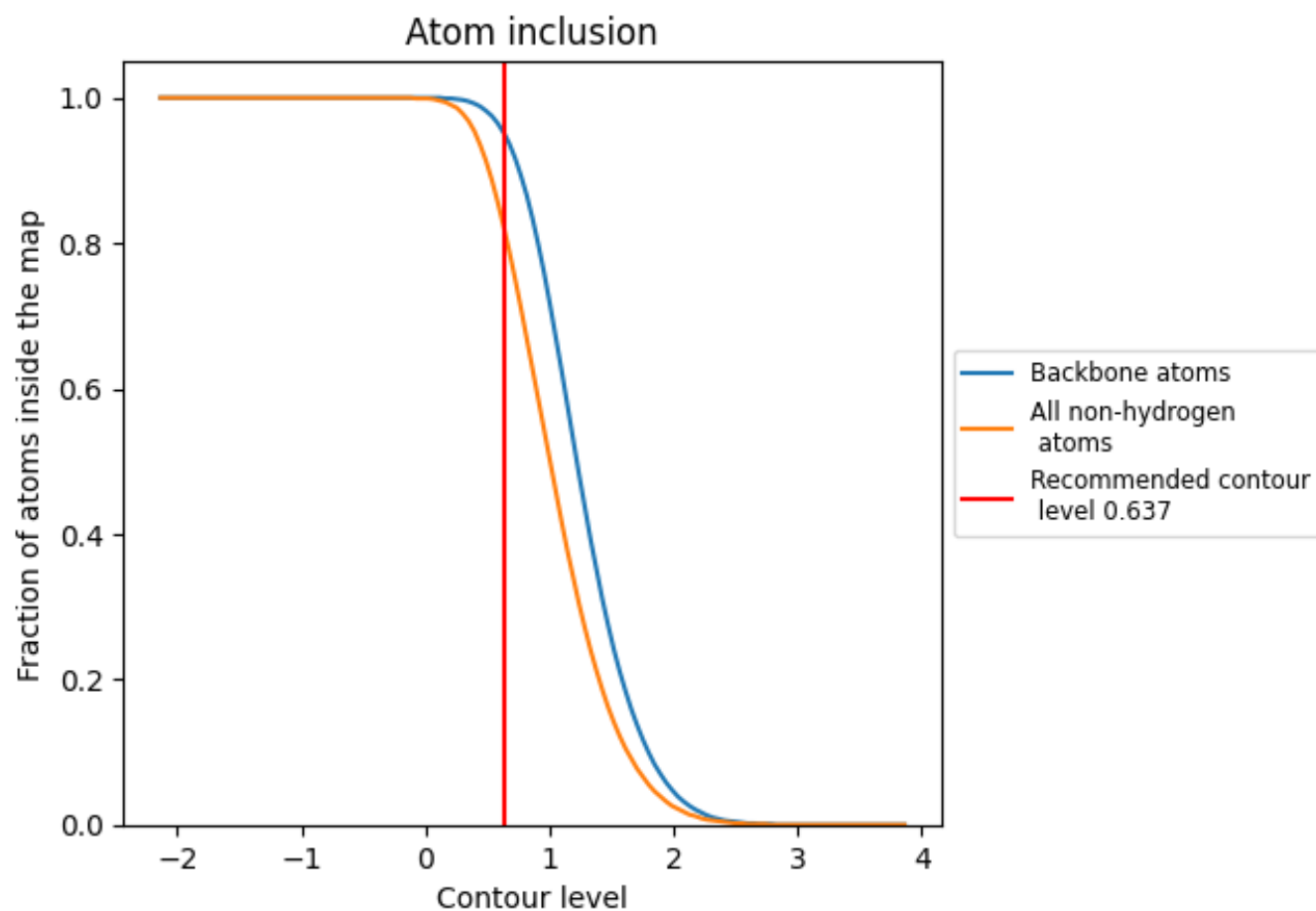
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.637).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 82% 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 (0.637) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.3460
0	 0.8570	 0.4210
0A	 0.6430	 0.2730
1	 0.8460	 0.4420
1A	 0.9490	 0.4190
2	 0.7140	 0.3260
2A	 0.7440	 0.3960
3	 0.9490	 0.4180
3A	 0.8210	 0.4200
4	 0.7440	 0.3860
4A	 0.8460	 0.3690
5	 0.8210	 0.4350
5A	 0.7500	 0.4130
6	 0.8460	 0.4270
7	 0.7500	 0.4250
8	 0.9640	 0.4330
9	 0.9490	 0.4620
A	 0.8210	 0.3590
AA	 0.8570	 0.4470
B	 0.8180	 0.3320
BA	 0.8460	 0.4330
C	 0.8210	 0.3580
CA	 0.6070	 0.2600
D	 0.8160	 0.3330
DA	 0.9490	 0.4330
E	 0.8220	 0.3590
EA	 0.7950	 0.4410
F	 0.8140	 0.3320
FA	 0.8460	 0.4350
G	 0.8200	 0.3580
GA	 0.8210	 0.4590
H	 0.8150	 0.3320
HA	 0.7140	 0.4060
I	 0.8200	 0.3580
IA	 0.9290	 0.4410



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Chain	Atom inclusion	Q-score
J	 0.8190	 0.3320
JA	 0.9490	 0.4600
K	 0.8210	 0.3570
KA	 0.8570	 0.3900
L	 0.8140	 0.3300
LA	 0.8210	 0.4390
M	 0.8190	 0.3580
MA	 0.7500	 0.3090
N	 0.8160	 0.3310
NA	 0.9230	 0.3900
O	 0.8220	 0.3600
OA	 0.7440	 0.3850
P	 0.8180	 0.3320
PA	 0.8210	 0.4320
Q	 0.8210	 0.3580
QA	 0.8210	 0.4470
R	 0.8180	 0.3330
RA	 0.7500	 0.4130
S	 0.8210	 0.3590
SA	 0.8570	 0.4200
T	 0.8120	 0.3320
TA	 0.9490	 0.4490
U	 0.8930	 0.4440
UA	 0.8570	 0.4460
V	 0.9230	 0.4860
VA	 0.8460	 0.4280
W	 0.7860	 0.4330
WA	 0.7140	 0.2600
X	 0.8460	 0.4110
XA	 0.9490	 0.4060
Y	 0.6430	 0.3080
YA	 0.7950	 0.4560
Z	 0.9740	 0.4590
ZA	 0.8460	 0.4390
a	 0.7950	 0.4010
aA	 0.8460	 0.4480
b	 0.8460	 0.4570
bA	 0.7140	 0.4030
c	 0.7440	 0.4650
cA	 0.8930	 0.4500
d	 0.7500	 0.4180
dA	 0.9230	 0.4750

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Chain	Atom inclusion	Q-score
e	 0.8930	 0.4480
eA	 0.8570	 0.4410
f	 0.9490	 0.4660
fA	 0.8970	 0.4330
g	 0.7860	 0.4400
gA	 0.6430	 0.2960
h	 0.8720	 0.4100
hA	 0.9740	 0.4690
i	 0.6790	 0.3330
iA	 0.8210	 0.4000
j	 0.9230	 0.4420
jA	 0.8210	 0.4460
k	 0.7440	 0.3850
kA	 0.6920	 0.4030
l	 0.8210	 0.4490
lA	 0.6430	 0.4200
m	 0.7690	 0.4140
mA	 0.8930	 0.4500
n	 0.2860	 0.3940
nA	 0.9490	 0.4720
o	 0.8210	 0.4050
oA	 0.8570	 0.4370
p	 0.9230	 0.4790
pA	 0.7950	 0.4200
q	 0.8570	 0.4090
qA	 0.7860	 0.3180
r	 0.8720	 0.4200
rA	 0.8970	 0.4090
s	 0.6790	 0.2760
sA	 0.7440	 0.3860
t	 0.9230	 0.4560
tA	 0.8210	 0.4520
u	 0.7440	 0.3950
uA	 0.7690	 0.4040
v	 0.8210	 0.4270
vA	 0.7860	 0.3800
w	 0.7690	 0.4100
wA	 0.7860	 0.4140
x	 0.7140	 0.4100
xA	 0.9230	 0.4420
y	 0.8930	 0.4310
yA	 0.8570	 0.4120

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Chain	Atom inclusion	Q-score
z	 0.9490	 0.4510
zA	 0.7440	 0.4040