



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:04 PM UTC

PDB ID : 8RH5 / pdb_00008rh5
EMDB ID : EMD-19168
Title : Oxiplasma meridianum archaellum
Authors : Isupov, M.N.; Gaines, M.; Daum, B.; McLaren, M.
Deposited on : 2023-12-14
Resolution : 2.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

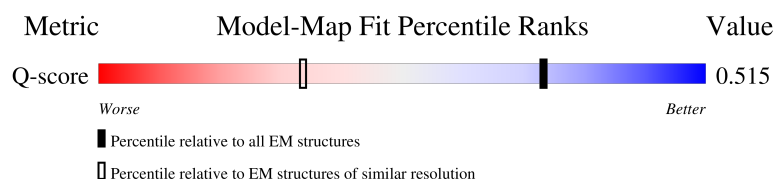
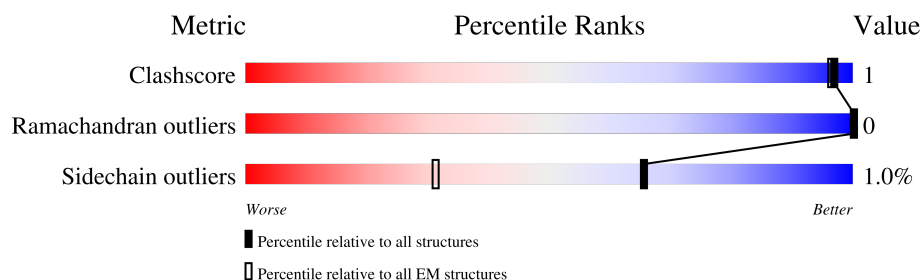
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.54 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.



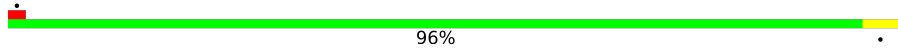
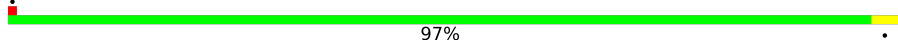
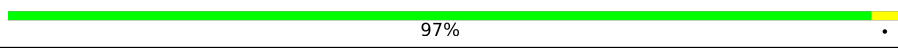
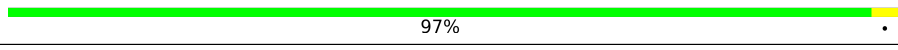
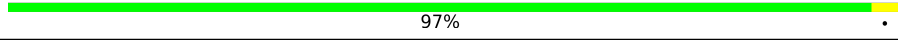
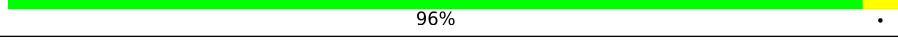
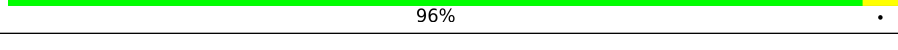
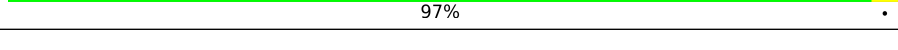
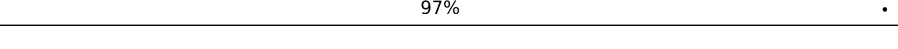
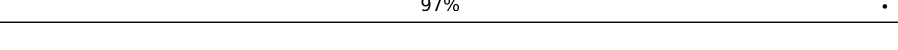
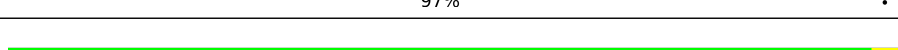
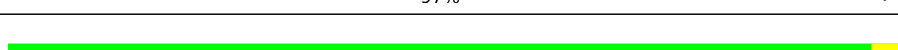
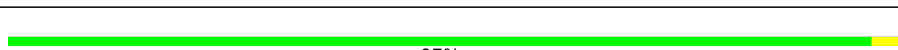
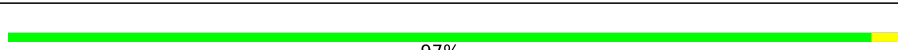
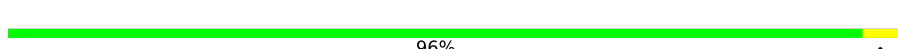
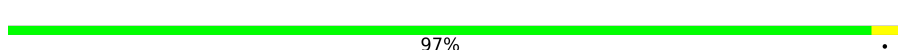
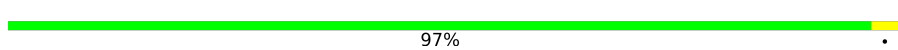
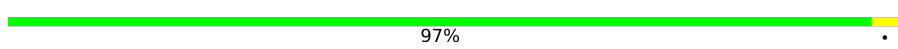
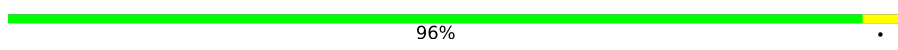
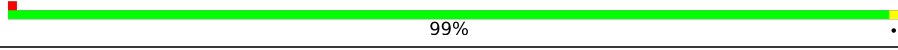
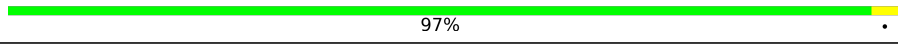
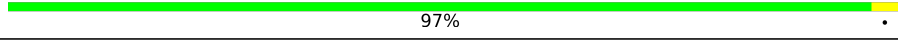
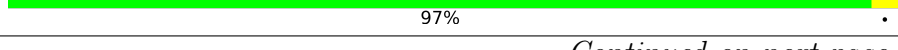
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7403 (2.04 - 3.04)

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	230	9% 96% .
1	B	230	6% 97% .
1	C	230	5% 97% .
1	D	230	. 97% .

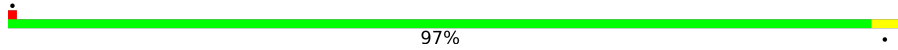
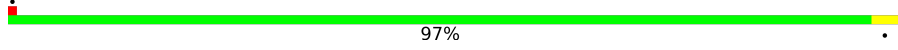
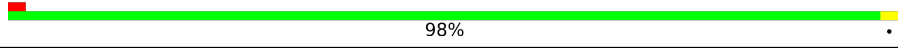
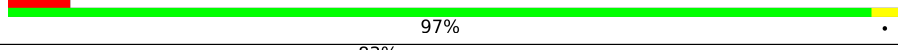
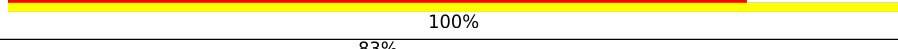
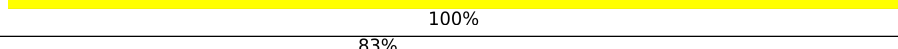
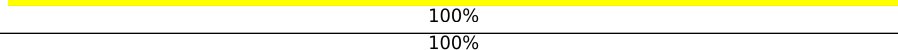
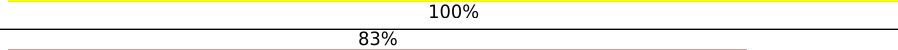
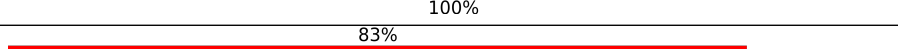
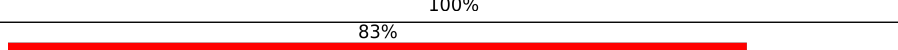
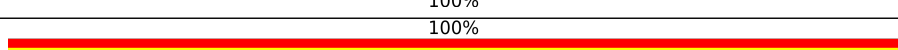
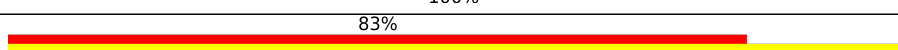
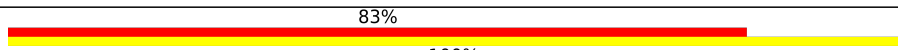
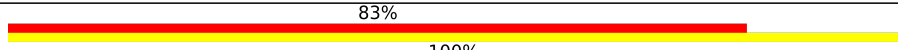
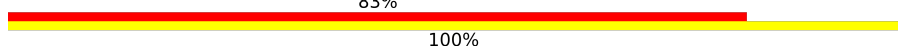
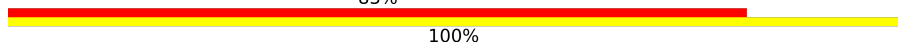
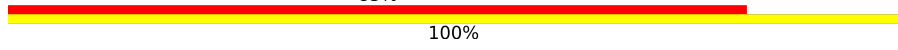
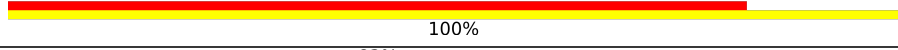
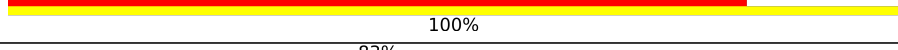
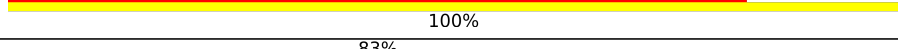
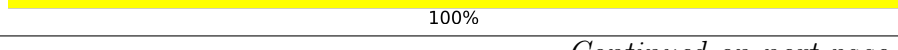
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Mol	Chain	Length	Quality of chain
1	E	230	 96%
1	F	230	 97%
1	G	230	 97%
1	H	230	 97%
1	I	230	 97%
1	J	230	 96%
1	K	230	 96%
1	L	230	 97%
1	M	230	 97%
1	N	230	 97%
1	O	230	 97%
1	P	230	 97%
1	Q	230	 97%
1	R	230	 97%
1	S	230	 97%
1	T	230	 97%
1	U	230	 96%
1	V	230	 97%
1	W	230	 97%
1	X	230	 97%
1	Y	230	 96%
1	Z	230	 99%
1	a	230	 97%
1	b	230	 97%
1	c	230	 97%

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Mol	Chain	Length	Quality of chain
1	d	230	 97%
1	e	230	 97%
1	f	230	 98%
1	g	230	 97%
2	2	6	 83% 100%
2	3A	6	 83% 100%
2	4B	6	 83% 100%
2	5C	6	 100%
2	9	6	 83% 100%
2	AB	6	 83% 100%
2	BC	6	 83% 100%
2	CD	6	 100%
2	GA	6	 83% 100%
2	HB	6	 83% 100%
2	IC	6	 83% 100%
2	NA	6	 83% 100%
2	OB	6	 83% 100%
2	PC	6	 83% 100%
2	UA	6	 83% 100%
2	VB	6	 83% 100%
2	WC	6	 83% 100%
2	bA	6	 83% 100%
2	cB	6	 83% 100%
2	dC	6	 83% 100%
2	h	6	 83% 100%

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Mol	Chain	Length	Quality of chain
2	iA	6	83% 100%
2	jB	6	83% 100%
2	kC	6	83% 100%
2	o	6	83% 100%
2	pA	6	83% 100%
2	qB	6	83% 100%
2	rC	6	83% 100%
2	v	6	83% 100%
2	wA	6	83% 100%
2	xB	6	83% 100%
2	yC	6	100%
3	0	5	60% 100%
3	0B	5	20% 60% 80%
3	0C	5	60% 100%
3	1A	5	60% 100%
3	1C	5	20% 60% 80%
3	2B	5	60% 100%
3	3C	5	60% 100%
3	4	5	60% 100%
3	5	5	20% 60% 80%
3	5A	5	60% 100%
3	6A	5	20% 60% 80%
3	6B	5	60% 100%
3	7	5	60% 100%
3	7B	5	20% 60% 80%

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Mol	Chain	Length	Quality of chain
3	7C	5	
3	8A	5	
3	8C	5	
3	9B	5	
3	AD	5	
3	BA	5	
3	CA	5	
3	CB	5	
3	DB	5	
3	DC	5	
3	EA	5	
3	EC	5	
3	ED	5	
3	FB	5	
3	FD	5	
3	GC	5	
3	HD	5	
3	IA	5	
3	JA	5	
3	JB	5	
3	KB	5	
3	KC	5	
3	LA	5	
3	LC	5	
3	MB	5	

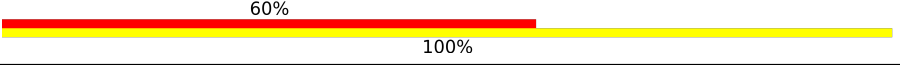
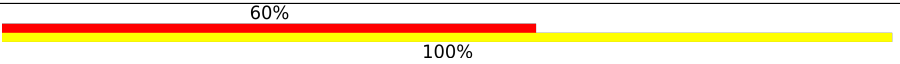
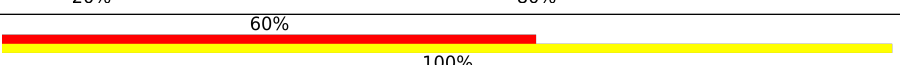
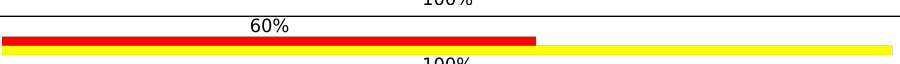
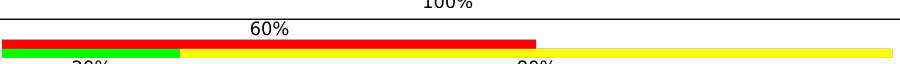
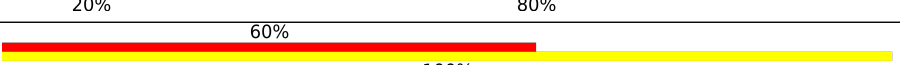
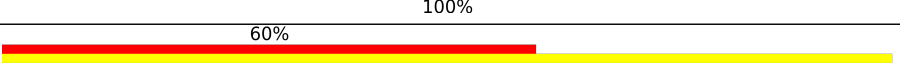
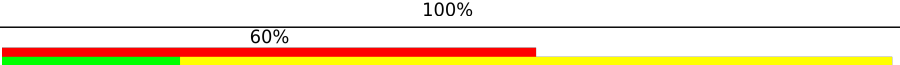
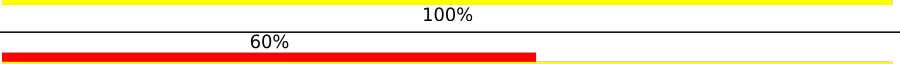
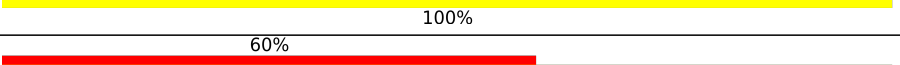
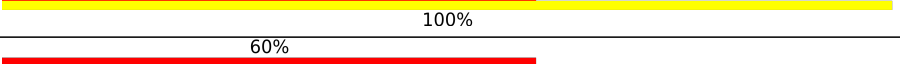
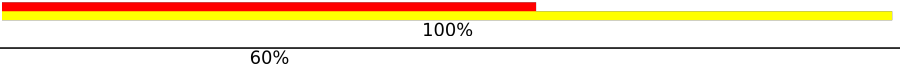
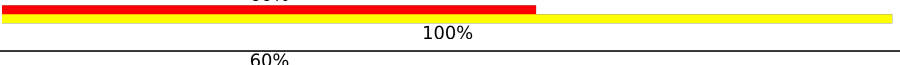
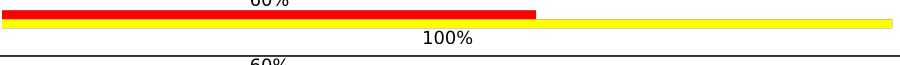
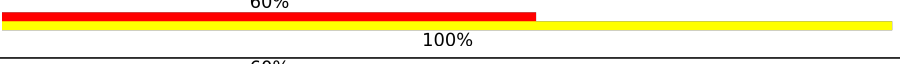
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Mol	Chain	Length	Quality of chain
3	NC	5	
3	PA	5	
3	QA	5	
3	QB	5	
3	RB	5	
3	RC	5	
3	SA	5	
3	SC	5	
3	TB	5	
3	UC	5	
3	WA	5	
3	XA	5	
3	XB	5	
3	YB	5	
3	YC	5	
3	ZA	5	
3	ZC	5	
3	aB	5	
3	bC	5	
3	dA	5	
3	eA	5	
3	eB	5	
3	fB	5	
3	fC	5	
3	gA	5	

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Mol	Chain	Length	Quality of chain
3	gC	5	
3	hB	5	
3	iC	5	
3	j	5	
3	k	5	
3	kA	5	
3	lA	5	
3	lB	5	
3	m	5	
3	mB	5	
3	mC	5	
3	nA	5	
3	nC	5	
3	oB	5	
3	pC	5	
3	q	5	
3	r	5	
3	rA	5	
3	sA	5	
3	sB	5	
3	t	5	
3	tB	5	
3	tC	5	
3	uA	5	
3	uC	5	

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Mol	Chain	Length	Quality of chain
3	vB	5	60% 100%
3	wC	5	60% 100%
3	x	5	60% 100%
3	y	5	20% 60% 80%
3	yA	5	60% 100%
3	zA	5	20% 60% 80%
3	zB	5	60% 100%
4	0A	4	50% 100%
4	1	4	50% 100%
4	1B	4	50% 100%
4	2A	4	50% 100%
4	2C	4	75% 100%
4	3B	4	50% 100%
4	4C	4	50% 100%
4	6	4	50% 100%
4	7A	4	50% 100%
4	8	4	50% 100%
4	8B	4	50% 100%
4	9A	4	50% 100%
4	9C	4	75% 100%
4	AC	4	50% 100%
4	BD	4	50% 100%
4	DA	4	50% 100%
4	EB	4	50% 100%
4	FA	4	50% 100%

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Mol	Chain	Length	Quality of chain
4	FC	4	50% 100%
4	GB	4	50% 100%
4	GD	4	75% 100%
4	HC	4	50% 100%
4	ID	4	75% 100%
4	KA	4	50% 100%
4	LB	4	50% 100%
4	MA	4	50% 100%
4	MC	4	50% 100%
4	NB	4	50% 100%
4	OC	4	50% 100%
4	RA	4	50% 100%
4	SB	4	50% 100%
4	TA	4	50% 100%
4	TC	4	50% 100%
4	UB	4	50% 100%
4	VC	4	50% 100%
4	YA	4	50% 100%
4	ZB	4	50% 100%
4	aA	4	50% 100%
4	aC	4	50% 100%
4	bB	4	50% 100%
4	cC	4	50% 100%
4	fA	4	50% 100%
4	gB	4	50% 100%

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Mol	Chain	Length	Quality of chain	
4	hA	4	50%	100%
4	hC	4	50%	100%
4	iB	4	50%	100%
4	jC	4	50%	100%
4	l	4	50%	100%
4	mA	4	50%	100%
4	n	4	50%	100%
4	nB	4	50%	100%
4	oA	4	50%	100%
4	oC	4	50%	100%
4	pB	4	50%	100%
4	qC	4	50%	100%
4	s	4	50%	100%
4	tA	4	50%	100%
4	u	4	50%	100%
4	uB	4	50%	100%
4	vA	4	50%	100%
4	vC	4	50%	100%
4	wB	4	50%	100%
4	xC	4	50%	100%
4	z	4	50%	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 67118 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 Oxiplasma meridianum archaellum.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	V	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	A	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	B	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	C	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	D	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	E	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	F	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	G	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	H	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	I	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	J	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	K	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	L	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	M	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	N	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	O	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	Q	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	R	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	S	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	T	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	U	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	W	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	X	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	Y	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	a	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	b	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	c	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	d	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	e	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	f	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		
1	g	230	Total	C	N	O	S	0	0
			1678	1048	279	347	4		

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	h	6	Total	C	O	S	0	0
			71	37	33	1		
2	o	6	Total	C	O	S	0	0
			71	37	33	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	v	6	Total 71	C 37	O 33	S 1	0	0
2	2	6	Total 71	C 37	O 33	S 1	0	0
2	9	6	Total 71	C 37	O 33	S 1	0	0
2	GA	6	Total 71	C 37	O 33	S 1	0	0
2	NA	6	Total 71	C 37	O 33	S 1	0	0
2	UA	6	Total 71	C 37	O 33	S 1	0	0
2	bA	6	Total 71	C 37	O 33	S 1	0	0
2	iA	6	Total 71	C 37	O 33	S 1	0	0
2	pA	6	Total 71	C 37	O 33	S 1	0	0
2	wA	6	Total 71	C 37	O 33	S 1	0	0
2	3A	6	Total 71	C 37	O 33	S 1	0	0
2	AB	6	Total 71	C 37	O 33	S 1	0	0
2	HB	6	Total 71	C 37	O 33	S 1	0	0
2	OB	6	Total 71	C 37	O 33	S 1	0	0
2	VB	6	Total 71	C 37	O 33	S 1	0	0
2	cB	6	Total 71	C 37	O 33	S 1	0	0
2	jB	6	Total 71	C 37	O 33	S 1	0	0
2	qB	6	Total 71	C 37	O 33	S 1	0	0
2	xB	6	Total 71	C 37	O 33	S 1	0	0
2	4B	6	Total 71	C 37	O 33	S 1	0	0
2	BC	6	Total 71	C 37	O 33	S 1	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	IC	6	Total 71	C 37	O 33	S 1	0	0
2	PC	6	Total 71	C 37	O 33	S 1	0	0
2	WC	6	Total 71	C 37	O 33	S 1	0	0
2	dC	6	Total 71	C 37	O 33	S 1	0	0
2	kC	6	Total 71	C 37	O 33	S 1	0	0
2	rC	6	Total 71	C 37	O 33	S 1	0	0
2	yC	6	Total 71	C 37	O 33	S 1	0	0
2	5C	6	Total 71	C 37	O 33	S 1	0	0
2	CD	6	Total 71	C 37	O 33	S 1	0	0

- Molecule 3 is an oligosaccharide called L-glycero- α -D-galacto-heptopyranose-(1-2)-[α -D-mannopyranose-(1-3)]6-deoxy-6-sulfo- β -D-galacto-heptopyranose-(1-4)- β -D-glucopyranose-(1-3)- β -D-galactopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	j	5	Total 60	C 31	O 28	S 1	0	0
3	k	5	Total 60	C 31	O 28	S 1	0	0
3	m	5	Total 60	C 31	O 28	S 1	0	0
3	q	5	Total 60	C 31	O 28	S 1	0	0
3	r	5	Total 60	C 31	O 28	S 1	0	0
3	t	5	Total 60	C 31	O 28	S 1	0	0
3	x	5	Total 60	C 31	O 28	S 1	0	0
3	y	5	Total 60	C 31	O 28	S 1	0	0
3	0	5	Total 60	C 31	O 28	S 1	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	4	5	Total 60	C 31	O 28	S 1	0	0
3	5	5	Total 60	C 31	O 28	S 1	0	0
3	7	5	Total 60	C 31	O 28	S 1	0	0
3	BA	5	Total 60	C 31	O 28	S 1	0	0
3	CA	5	Total 60	C 31	O 28	S 1	0	0
3	EA	5	Total 60	C 31	O 28	S 1	0	0
3	IA	5	Total 60	C 31	O 28	S 1	0	0
3	JA	5	Total 60	C 31	O 28	S 1	0	0
3	LA	5	Total 60	C 31	O 28	S 1	0	0
3	PA	5	Total 60	C 31	O 28	S 1	0	0
3	QA	5	Total 60	C 31	O 28	S 1	0	0
3	SA	5	Total 60	C 31	O 28	S 1	0	0
3	WA	5	Total 60	C 31	O 28	S 1	0	0
3	XA	5	Total 60	C 31	O 28	S 1	0	0
3	ZA	5	Total 60	C 31	O 28	S 1	0	0
3	dA	5	Total 60	C 31	O 28	S 1	0	0
3	eA	5	Total 60	C 31	O 28	S 1	0	0
3	gA	5	Total 60	C 31	O 28	S 1	0	0
3	kA	5	Total 60	C 31	O 28	S 1	0	0
3	lA	5	Total 60	C 31	O 28	S 1	0	0
3	nA	5	Total 60	C 31	O 28	S 1	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	rA	5	Total 60	C 31	O 28	S 1	0	0
3	sA	5	Total 60	C 31	O 28	S 1	0	0
3	uA	5	Total 60	C 31	O 28	S 1	0	0
3	yA	5	Total 60	C 31	O 28	S 1	0	0
3	zA	5	Total 60	C 31	O 28	S 1	0	0
3	1A	5	Total 60	C 31	O 28	S 1	0	0
3	5A	5	Total 60	C 31	O 28	S 1	0	0
3	6A	5	Total 60	C 31	O 28	S 1	0	0
3	8A	5	Total 60	C 31	O 28	S 1	0	0
3	CB	5	Total 60	C 31	O 28	S 1	0	0
3	DB	5	Total 60	C 31	O 28	S 1	0	0
3	FB	5	Total 60	C 31	O 28	S 1	0	0
3	JB	5	Total 60	C 31	O 28	S 1	0	0
3	KB	5	Total 60	C 31	O 28	S 1	0	0
3	MB	5	Total 60	C 31	O 28	S 1	0	0
3	QB	5	Total 60	C 31	O 28	S 1	0	0
3	RB	5	Total 60	C 31	O 28	S 1	0	0
3	TB	5	Total 60	C 31	O 28	S 1	0	0
3	XB	5	Total 60	C 31	O 28	S 1	0	0
3	YB	5	Total 60	C 31	O 28	S 1	0	0
3	aB	5	Total 60	C 31	O 28	S 1	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	eB	5	Total 60	C 31	O 28	S 1	0	0
3	fB	5	Total 60	C 31	O 28	S 1	0	0
3	hB	5	Total 60	C 31	O 28	S 1	0	0
3	lB	5	Total 60	C 31	O 28	S 1	0	0
3	mB	5	Total 60	C 31	O 28	S 1	0	0
3	oB	5	Total 60	C 31	O 28	S 1	0	0
3	sB	5	Total 60	C 31	O 28	S 1	0	0
3	tB	5	Total 60	C 31	O 28	S 1	0	0
3	vB	5	Total 60	C 31	O 28	S 1	0	0
3	zB	5	Total 60	C 31	O 28	S 1	0	0
3	0B	5	Total 60	C 31	O 28	S 1	0	0
3	2B	5	Total 60	C 31	O 28	S 1	0	0
3	6B	5	Total 60	C 31	O 28	S 1	0	0
3	7B	5	Total 60	C 31	O 28	S 1	0	0
3	9B	5	Total 60	C 31	O 28	S 1	0	0
3	DC	5	Total 60	C 31	O 28	S 1	0	0
3	EC	5	Total 60	C 31	O 28	S 1	0	0
3	GC	5	Total 60	C 31	O 28	S 1	0	0
3	KC	5	Total 60	C 31	O 28	S 1	0	0
3	LC	5	Total 60	C 31	O 28	S 1	0	0
3	NC	5	Total 60	C 31	O 28	S 1	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	RC	5	Total	C	O	S	0	0
			60	31	28	1		
3	SC	5	Total	C	O	S	0	0
			60	31	28	1		
3	UC	5	Total	C	O	S	0	0
			60	31	28	1		
3	YC	5	Total	C	O	S	0	0
			60	31	28	1		
3	ZC	5	Total	C	O	S	0	0
			60	31	28	1		
3	bC	5	Total	C	O	S	0	0
			60	31	28	1		
3	fC	5	Total	C	O	S	0	0
			60	31	28	1		
3	gC	5	Total	C	O	S	0	0
			60	31	28	1		
3	iC	5	Total	C	O	S	0	0
			60	31	28	1		
3	mC	5	Total	C	O	S	0	0
			60	31	28	1		
3	nC	5	Total	C	O	S	0	0
			60	31	28	1		
3	pC	5	Total	C	O	S	0	0
			60	31	28	1		
3	tC	5	Total	C	O	S	0	0
			60	31	28	1		
3	uC	5	Total	C	O	S	0	0
			60	31	28	1		
3	wC	5	Total	C	O	S	0	0
			60	31	28	1		
3	0C	5	Total	C	O	S	0	0
			60	31	28	1		
3	1C	5	Total	C	O	S	0	0
			60	31	28	1		
3	3C	5	Total	C	O	S	0	0
			60	31	28	1		
3	7C	5	Total	C	O	S	0	0
			60	31	28	1		
3	8C	5	Total	C	O	S	0	0
			60	31	28	1		
3	AD	5	Total	C	O	S	0	0
			60	31	28	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	ED	5	Total	C	O	S	0	0
			60	31	28	1		
3	FD	5	Total	C	O	S	0	0
			60	31	28	1		
3	HD	5	Total	C	O	S	0	0
			60	31	28	1		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	l	4	Total	C	O	S	0	0
			47	24	22	1		
4	n	4	Total	C	O	S	0	0
			47	24	22	1		
4	s	4	Total	C	O	S	0	0
			47	24	22	1		
4	u	4	Total	C	O	S	0	0
			47	24	22	1		
4	z	4	Total	C	O	S	0	0
			47	24	22	1		
4	1	4	Total	C	O	S	0	0
			47	24	22	1		
4	6	4	Total	C	O	S	0	0
			47	24	22	1		
4	8	4	Total	C	O	S	0	0
			47	24	22	1		
4	DA	4	Total	C	O	S	0	0
			47	24	22	1		
4	FA	4	Total	C	O	S	0	0
			47	24	22	1		
4	KA	4	Total	C	O	S	0	0
			47	24	22	1		
4	MA	4	Total	C	O	S	0	0
			47	24	22	1		
4	RA	4	Total	C	O	S	0	0
			47	24	22	1		
4	TA	4	Total	C	O	S	0	0
			47	24	22	1		
4	YA	4	Total	C	O	S	0	0
			47	24	22	1		
4	aA	4	Total	C	O	S	0	0
			47	24	22	1		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	fA	4	Total 47	C 24	O 22	S 1	0	0
4	hA	4	Total 47	C 24	O 22	S 1	0	0
4	mA	4	Total 47	C 24	O 22	S 1	0	0
4	oA	4	Total 47	C 24	O 22	S 1	0	0
4	tA	4	Total 47	C 24	O 22	S 1	0	0
4	vA	4	Total 47	C 24	O 22	S 1	0	0
4	0A	4	Total 47	C 24	O 22	S 1	0	0
4	2A	4	Total 47	C 24	O 22	S 1	0	0
4	7A	4	Total 47	C 24	O 22	S 1	0	0
4	9A	4	Total 47	C 24	O 22	S 1	0	0
4	EB	4	Total 47	C 24	O 22	S 1	0	0
4	GB	4	Total 47	C 24	O 22	S 1	0	0
4	LB	4	Total 47	C 24	O 22	S 1	0	0
4	NB	4	Total 47	C 24	O 22	S 1	0	0
4	SB	4	Total 47	C 24	O 22	S 1	0	0
4	UB	4	Total 47	C 24	O 22	S 1	0	0
4	ZB	4	Total 47	C 24	O 22	S 1	0	0
4	bB	4	Total 47	C 24	O 22	S 1	0	0
4	gB	4	Total 47	C 24	O 22	S 1	0	0
4	iB	4	Total 47	C 24	O 22	S 1	0	0
4	nB	4	Total 47	C 24	O 22	S 1	0	0

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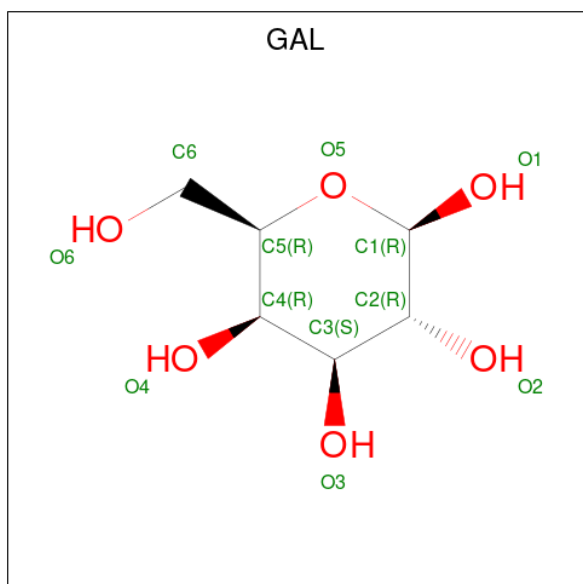
Mol	Chain	Residues	Atoms				AltConf	Trace
4	pB	4	Total 47	C 24	O 22	S 1	0	0
4	uB	4	Total 47	C 24	O 22	S 1	0	0
4	wB	4	Total 47	C 24	O 22	S 1	0	0
4	1B	4	Total 47	C 24	O 22	S 1	0	0
4	3B	4	Total 47	C 24	O 22	S 1	0	0
4	8B	4	Total 47	C 24	O 22	S 1	0	0
4	AC	4	Total 47	C 24	O 22	S 1	0	0
4	FC	4	Total 47	C 24	O 22	S 1	0	0
4	HC	4	Total 47	C 24	O 22	S 1	0	0
4	MC	4	Total 47	C 24	O 22	S 1	0	0
4	OC	4	Total 47	C 24	O 22	S 1	0	0
4	TC	4	Total 47	C 24	O 22	S 1	0	0
4	VC	4	Total 47	C 24	O 22	S 1	0	0
4	aC	4	Total 47	C 24	O 22	S 1	0	0
4	cC	4	Total 47	C 24	O 22	S 1	0	0
4	hC	4	Total 47	C 24	O 22	S 1	0	0
4	jC	4	Total 47	C 24	O 22	S 1	0	0
4	oC	4	Total 47	C 24	O 22	S 1	0	0
4	qC	4	Total 47	C 24	O 22	S 1	0	0
4	vC	4	Total 47	C 24	O 22	S 1	0	0
4	xC	4	Total 47	C 24	O 22	S 1	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	2C	4	Total	C	O	S	0	0
			47	24	22	1		
4	4C	4	Total	C	O	S	0	0
			47	24	22	1		
4	9C	4	Total	C	O	S	0	0
			47	24	22	1		
4	BD	4	Total	C	O	S	0	0
			47	24	22	1		
4	GD	4	Total	C	O	S	0	0
			47	24	22	1		
4	ID	4	Total	C	O	S	0	0
			47	24	22	1		

- Molecule 5 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
5	V	1	Total	C	O	0
			11	6	5	
5	V	1	Total	C	O	0
			11	6	5	
5	A	1	Total	C	O	0
			11	6	5	
5	A	1	Total	C	O	0
			11	6	5	
5	B	1	Total	C	O	0
			11	6	5	

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Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			11	6	5	
5	C	1	Total	C	O	0
			11	6	5	
5	C	1	Total	C	O	0
			11	6	5	
5	D	1	Total	C	O	0
			11	6	5	
5	D	1	Total	C	O	0
			11	6	5	
5	E	1	Total	C	O	0
			11	6	5	
5	E	1	Total	C	O	0
			11	6	5	
5	F	1	Total	C	O	0
			11	6	5	
5	F	1	Total	C	O	0
			11	6	5	
5	G	1	Total	C	O	0
			11	6	5	
5	G	1	Total	C	O	0
			11	6	5	
5	H	1	Total	C	O	0
			11	6	5	
5	H	1	Total	C	O	0
			11	6	5	
5	I	1	Total	C	O	0
			11	6	5	
5	I	1	Total	C	O	0
			11	6	5	
5	J	1	Total	C	O	0
			11	6	5	
5	J	1	Total	C	O	0
			11	6	5	
5	K	1	Total	C	O	0
			11	6	5	
5	K	1	Total	C	O	0
			11	6	5	
5	L	1	Total	C	O	0
			11	6	5	
5	L	1	Total	C	O	0
			11	6	5	

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Mol	Chain	Residues	Atoms			AltConf
5	M	1	Total	C	O	0
			11	6	5	
5	M	1	Total	C	O	0
			11	6	5	
5	N	1	Total	C	O	0
			11	6	5	
5	N	1	Total	C	O	0
			11	6	5	
5	O	1	Total	C	O	0
			11	6	5	
5	O	1	Total	C	O	0
			11	6	5	
5	P	1	Total	C	O	0
			11	6	5	
5	P	1	Total	C	O	0
			11	6	5	
5	Q	1	Total	C	O	0
			11	6	5	
5	Q	1	Total	C	O	0
			11	6	5	
5	R	1	Total	C	O	0
			11	6	5	
5	R	1	Total	C	O	0
			11	6	5	
5	S	1	Total	C	O	0
			11	6	5	
5	S	1	Total	C	O	0
			11	6	5	
5	T	1	Total	C	O	0
			11	6	5	
5	T	1	Total	C	O	0
			11	6	5	
5	U	1	Total	C	O	0
			11	6	5	
5	U	1	Total	C	O	0
			11	6	5	
5	W	1	Total	C	O	0
			11	6	5	
5	W	1	Total	C	O	0
			11	6	5	
5	X	1	Total	C	O	0
			11	6	5	

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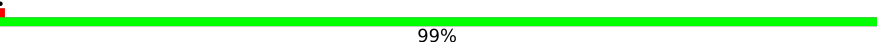
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
5	X	1	Total	C	O	0
			11	6	5	
5	Y	1	Total	C	O	0
			11	6	5	
5	Y	1	Total	C	O	0
			11	6	5	
5	a	1	Total	C	O	0
			11	6	5	
5	a	1	Total	C	O	0
			11	6	5	
5	b	1	Total	C	O	0
			11	6	5	
5	b	1	Total	C	O	0
			11	6	5	
5	c	1	Total	C	O	0
			11	6	5	
5	c	1	Total	C	O	0
			11	6	5	
5	d	1	Total	C	O	0
			11	6	5	
5	d	1	Total	C	O	0
			11	6	5	
5	e	1	Total	C	O	0
			11	6	5	
5	e	1	Total	C	O	0
			11	6	5	
5	f	1	Total	C	O	0
			11	6	5	
5	f	1	Total	C	O	0
			11	6	5	
5	g	1	Total	C	O	0
			11	6	5	
5	g	1	Total	C	O	0
			11	6	5	

3 Residue-property plots [i](#)

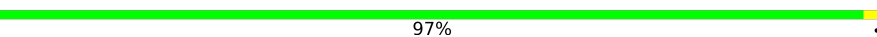
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain Z:  99%

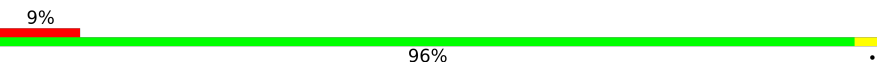


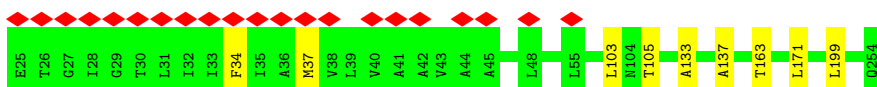
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain V:  97%

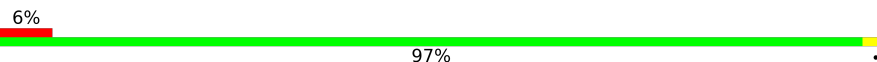


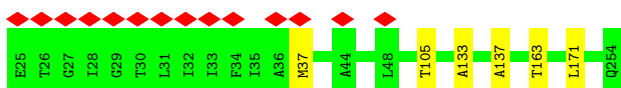
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain A:  96%

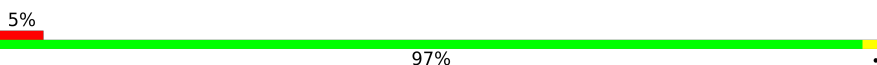


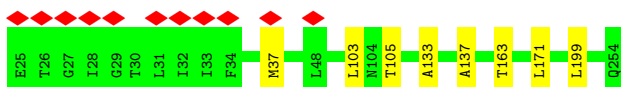
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain B:  97%

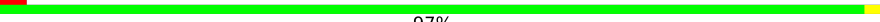


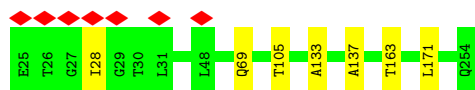
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain C:  97%

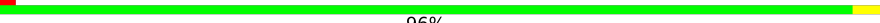


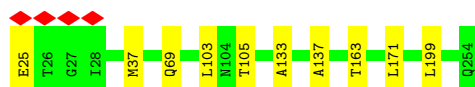
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain D:  97%

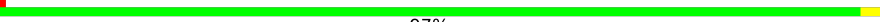


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain E:  96%

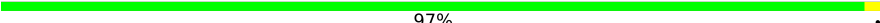


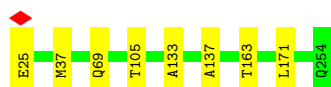
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain F:  97%

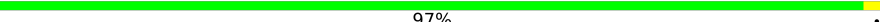


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain G:  97%



- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain H:  97%

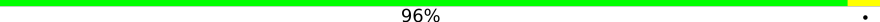


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain I:  97%

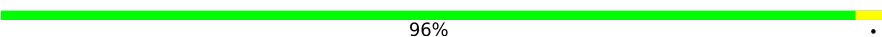


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain J:  96%

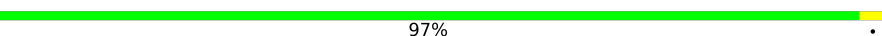


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain K:  96%



- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain L:  97%

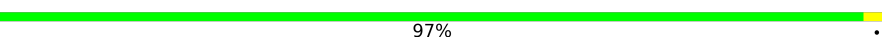


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain M:  97%

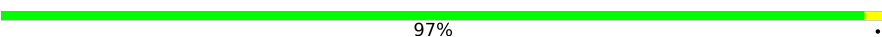


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain N:  97%

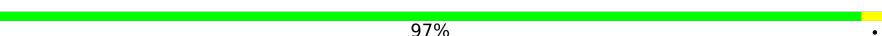


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain O:  97%



- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain P:  97%



- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain Q:  97% .



- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain R:  97% .



- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain S:  97% .



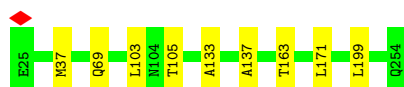
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain T:  97% .



- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain U:  96% .



- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain W:  97% .

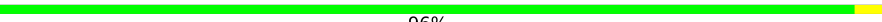


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain X:  97% .

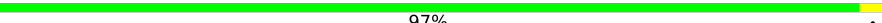


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain Y:  96%

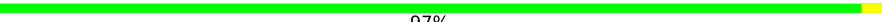


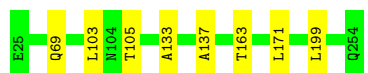
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain a:  97%

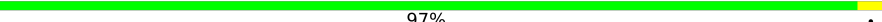


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain b:  97%

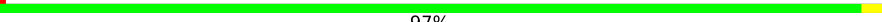


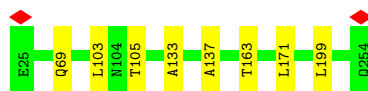
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain c:  97%

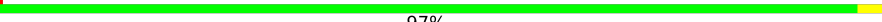


- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain d:  97%

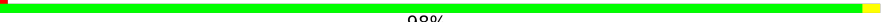


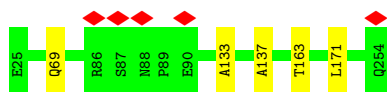
- Molecule 1: *Oxiplasma meridianum* archaeellum

Chain e:  97%



- Molecule 1: *Oxiplasma meridianum* archaeellum

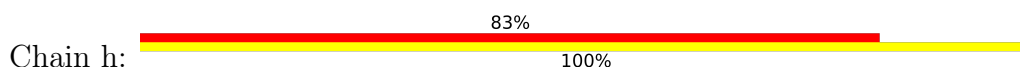
Chain f:  98%



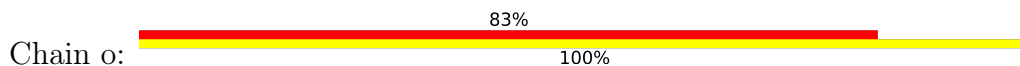
- Molecule 1: *Oxiplasma meridianum* archaeellum



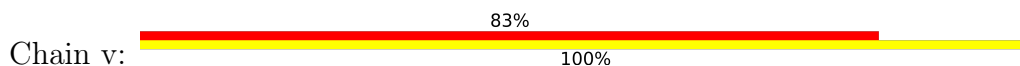
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



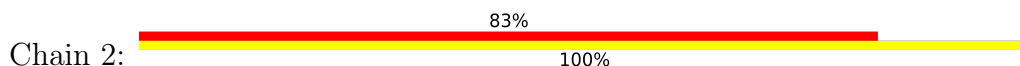
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

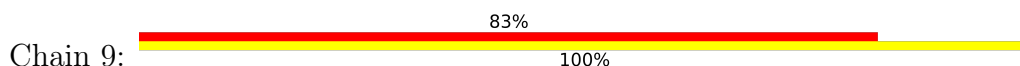


- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

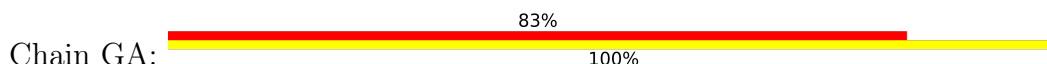




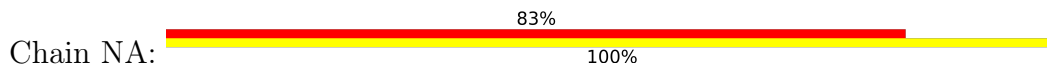
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



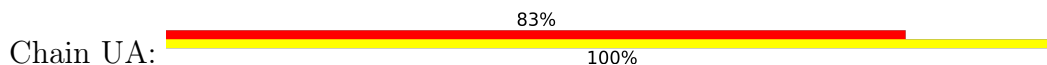
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



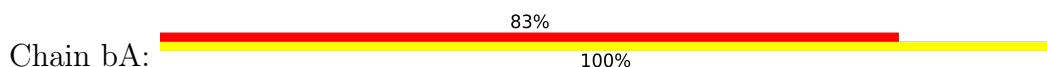
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

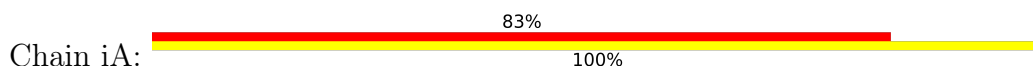


- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

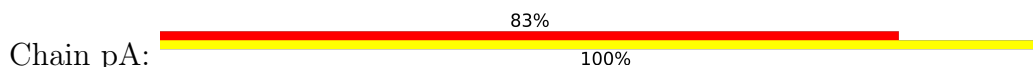




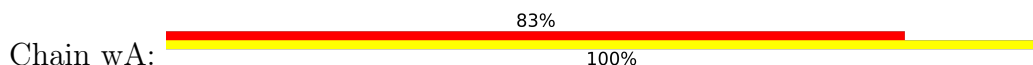
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



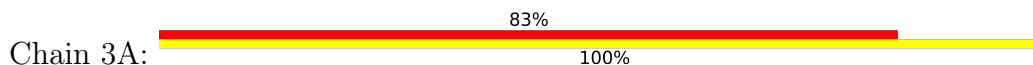
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



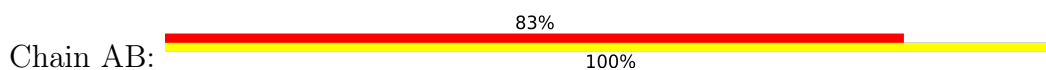
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



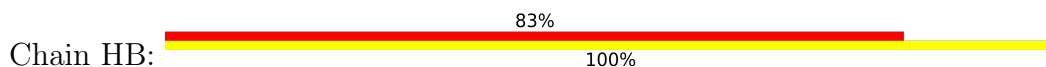
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



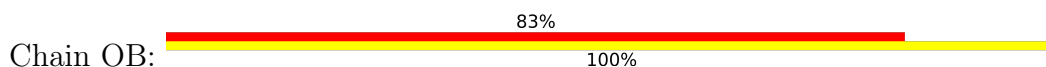
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



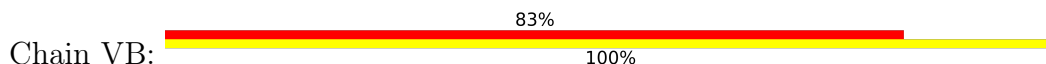
• Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[L-glycero-alpha-D-galacto-heptopyranose-(1-2)]6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



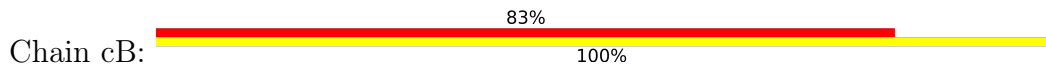
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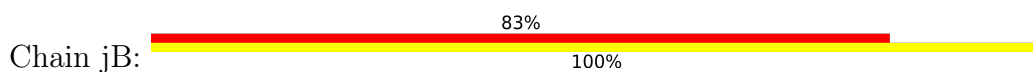
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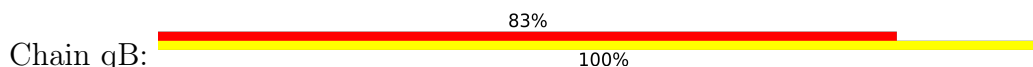
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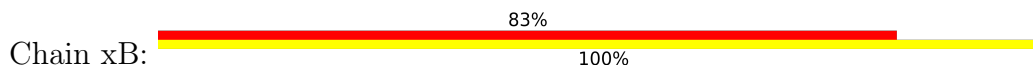
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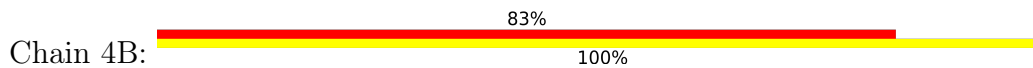
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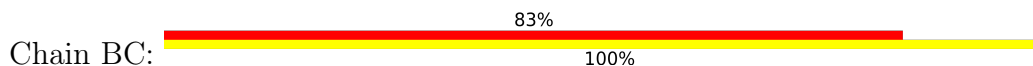
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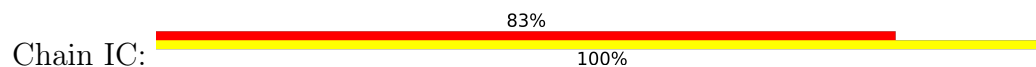


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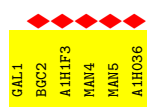
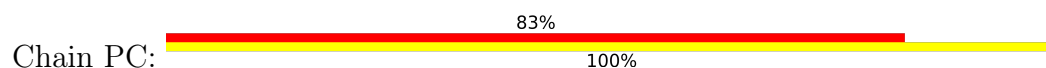


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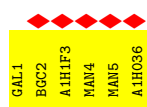
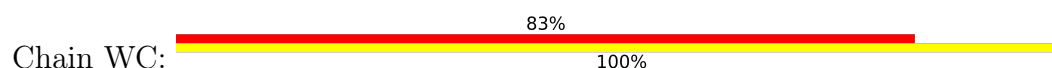
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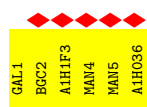
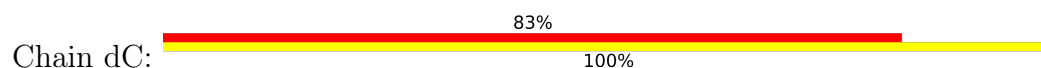
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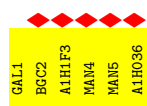
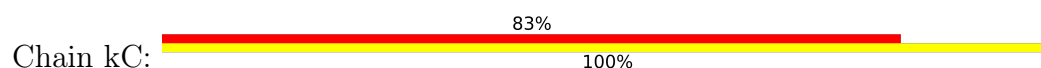
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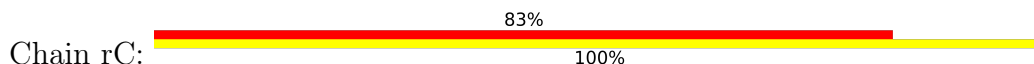
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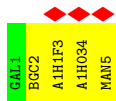
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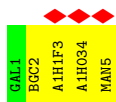
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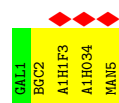
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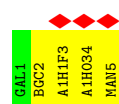
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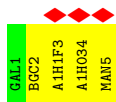
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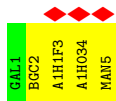
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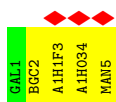
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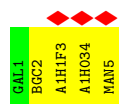
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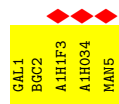
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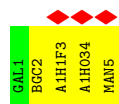
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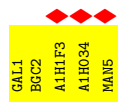
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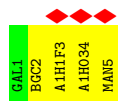
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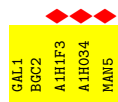
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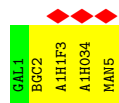
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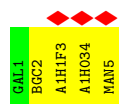
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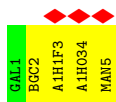
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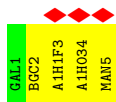
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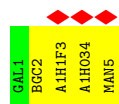
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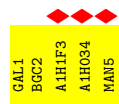
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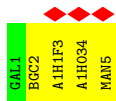
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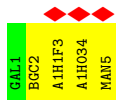
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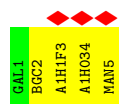
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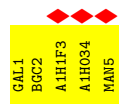
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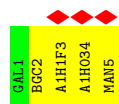
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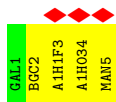
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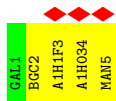
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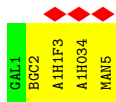
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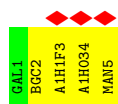
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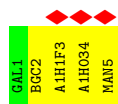
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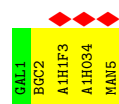
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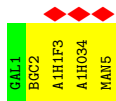
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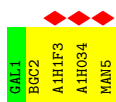
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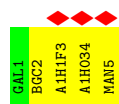
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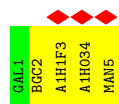
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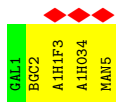
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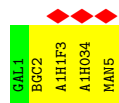
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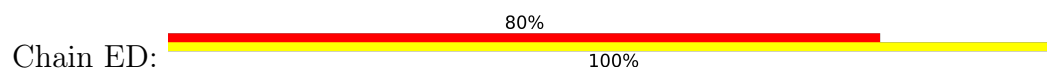
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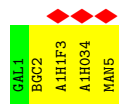
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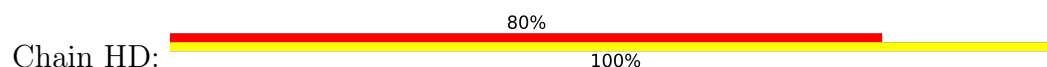
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- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

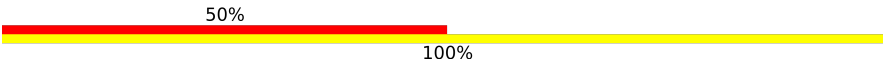


- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain MA: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain RA: 

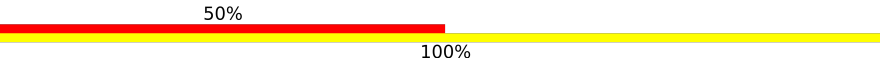


- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain TA: 

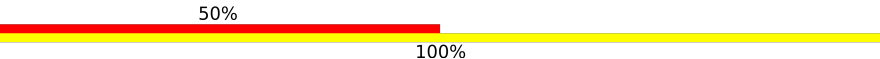


- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain YA: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain aA: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain fA: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose





- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

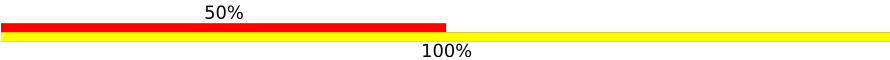


- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain bB: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain gB: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain iB: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain nB: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain pB: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain uB: 



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose





- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



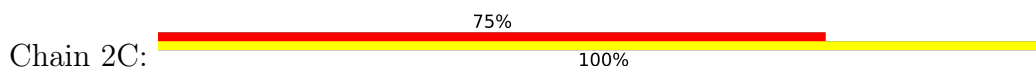
- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



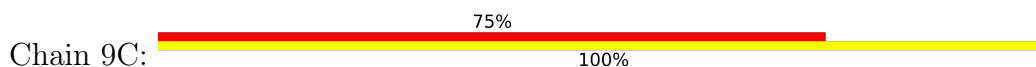
- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

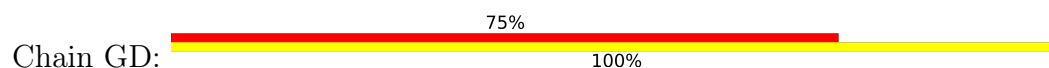




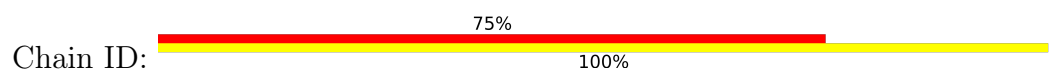
- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 4: alpha-D-mannopyranose-(1-3)-6-deoxy-6-sulfo-beta-D-galacto-heptopyranose-(1-4)-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=107.922°, rise=5.641 Å, axial sym=C1	Depositor
Number of segments used	1374113	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	51.45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.164	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GAL, A1H03, A1H1F, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/1701	1.01	0/2325
1	B	0.48	0/1701	1.00	0/2325
1	C	0.47	0/1701	1.01	0/2325
1	D	0.47	0/1701	1.01	0/2325
1	E	0.47	0/1701	1.01	0/2325
1	F	0.47	0/1701	1.00	0/2325
1	G	0.47	0/1701	1.01	0/2325
1	H	0.48	0/1701	1.01	0/2325
1	I	0.47	0/1701	1.00	0/2325
1	J	0.48	0/1701	1.00	0/2325
1	K	0.48	0/1701	1.00	0/2325
1	L	0.48	0/1701	1.00	0/2325
1	M	0.48	0/1701	1.00	0/2325
1	N	0.48	0/1701	1.00	0/2325
1	O	0.48	0/1701	1.00	0/2325
1	P	0.48	0/1701	1.01	0/2325
1	Q	0.48	0/1701	1.00	0/2325
1	R	0.47	0/1701	1.01	0/2325
1	S	0.47	0/1701	1.01	0/2325
1	T	0.48	0/1701	1.01	0/2325
1	U	0.48	0/1701	1.00	0/2325
1	V	0.47	0/1701	1.00	0/2325
1	W	0.48	0/1701	1.00	0/2325
1	X	0.48	0/1701	1.00	0/2325
1	Y	0.47	0/1701	1.00	0/2325
1	Z	0.48	0/1701	1.01	0/2325
1	a	0.48	0/1701	1.01	0/2325
1	b	0.48	0/1701	1.00	0/2325
1	c	0.47	0/1701	1.01	0/2325
1	d	0.47	0/1701	1.01	0/2325
1	e	0.47	0/1701	1.01	0/2325
1	f	0.47	0/1701	1.00	0/2325

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.48	0/1701	1.01	0/2325
All	All	0.48	0/56133	1.01	0/76725

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1678	0	1676	5	0
1	B	1678	0	1676	3	0
1	C	1678	0	1676	4	0
1	D	1678	0	1676	4	0
1	E	1678	0	1676	6	0
1	F	1678	0	1676	5	0
1	G	1678	0	1676	5	0
1	H	1678	0	1676	4	0
1	I	1678	0	1676	4	0
1	J	1678	0	1676	5	0
1	K	1678	0	1676	5	0
1	L	1678	0	1676	3	0
1	M	1678	0	1676	4	0
1	N	1678	0	1676	3	0
1	O	1678	0	1676	4	0
1	P	1678	0	1676	3	0
1	Q	1678	0	1676	3	0
1	R	1678	0	1676	4	0
1	S	1678	0	1676	3	0
1	T	1678	0	1676	4	0
1	U	1678	0	1676	5	0
1	V	1678	0	1676	3	0
1	W	1678	0	1676	4	0
1	X	1678	0	1676	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1678	0	1676	5	0
1	Z	1678	0	1684	2	0
1	a	1678	0	1676	4	0
1	b	1678	0	1676	4	0
1	c	1678	0	1676	3	0
1	d	1678	0	1676	4	0
1	e	1678	0	1676	3	0
1	f	1678	0	1676	2	0
1	g	1678	0	1676	3	0
2	2	71	0	37	0	0
2	3A	71	0	37	0	0
2	4B	71	0	37	0	0
2	5C	71	0	37	0	0
2	9	71	0	37	0	0
2	AB	71	0	37	0	0
2	BC	71	0	37	0	0
2	CD	71	0	37	0	0
2	GA	71	0	37	0	0
2	HB	71	0	37	0	0
2	IC	71	0	37	0	0
2	NA	71	0	37	0	0
2	OB	71	0	37	0	0
2	PC	71	0	37	0	0
2	UA	71	0	37	0	0
2	VB	71	0	37	0	0
2	WC	71	0	37	0	0
2	bA	71	0	37	0	0
2	cB	71	0	37	0	0
2	dC	71	0	37	0	0
2	h	71	0	37	0	0
2	iA	71	0	37	0	0
2	jB	71	0	37	0	0
2	kC	71	0	37	0	0
2	o	71	0	37	0	0
2	pA	71	0	37	0	0
2	qB	71	0	37	0	0
2	rC	71	0	37	0	0
2	v	71	0	37	0	0
2	wA	71	0	37	0	0
2	xB	71	0	37	0	0
2	yC	71	0	37	0	0
3	0	60	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	0B	60	0	28	0	0
3	0C	60	0	28	0	0
3	1A	60	0	28	0	0
3	1C	60	0	28	0	0
3	2B	60	0	28	0	0
3	3C	60	0	28	0	0
3	4	60	0	28	0	0
3	5	60	0	28	0	0
3	5A	60	0	28	0	0
3	6A	60	0	28	0	0
3	6B	60	0	28	0	0
3	7	60	0	28	0	0
3	7B	60	0	28	0	0
3	7C	60	0	28	0	0
3	8A	60	0	28	0	0
3	8C	60	0	28	0	0
3	9B	60	0	28	0	0
3	AD	60	0	28	0	0
3	BA	60	0	28	0	0
3	CA	60	0	28	0	0
3	CB	60	0	28	0	0
3	DB	60	0	28	0	0
3	DC	60	0	28	0	0
3	EA	60	0	28	0	0
3	EC	60	0	28	0	0
3	ED	60	0	28	0	0
3	FB	60	0	28	0	0
3	FD	60	0	28	0	0
3	GC	60	0	28	0	0
3	HD	60	0	28	0	0
3	IA	60	0	28	0	0
3	JA	60	0	28	0	0
3	JB	60	0	28	0	0
3	KB	60	0	28	0	0
3	KC	60	0	28	0	0
3	LA	60	0	28	0	0
3	LC	60	0	28	0	0
3	MB	60	0	28	0	0
3	NC	60	0	28	0	0
3	PA	60	0	28	0	0
3	QA	60	0	28	0	0
3	QB	60	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	RB	60	0	28	0	0
3	RC	60	0	28	0	0
3	SA	60	0	28	0	0
3	SC	60	0	28	0	0
3	TB	60	0	28	0	0
3	UC	60	0	28	0	0
3	WA	60	0	28	0	0
3	XA	60	0	28	0	0
3	XB	60	0	28	0	0
3	YB	60	0	28	0	0
3	YC	60	0	28	0	0
3	ZA	60	0	28	0	0
3	ZC	60	0	28	0	0
3	aB	60	0	28	0	0
3	bC	60	0	28	0	0
3	dA	60	0	28	0	0
3	eA	60	0	28	0	0
3	eB	60	0	28	0	0
3	fB	60	0	28	0	0
3	fC	60	0	28	0	0
3	gA	60	0	28	0	0
3	gC	60	0	28	0	0
3	hB	60	0	28	0	0
3	iC	60	0	28	0	0
3	j	60	0	28	0	0
3	k	60	0	28	0	0
3	kA	60	0	28	0	0
3	lA	60	0	28	0	0
3	lB	60	0	28	0	0
3	m	60	0	28	0	0
3	mB	60	0	28	0	0
3	mC	60	0	28	0	0
3	nA	60	0	28	0	0
3	nC	60	0	28	0	0
3	oB	60	0	28	0	0
3	pC	60	0	28	0	0
3	q	60	0	28	0	0
3	r	60	0	28	0	0
3	rA	60	0	28	0	0
3	sA	60	0	28	0	0
3	sB	60	0	28	0	0
3	t	60	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	tB	60	0	28	0	0
3	tC	60	0	28	0	0
3	uA	60	0	28	0	0
3	uC	60	0	28	0	0
3	vB	60	0	28	0	0
3	wC	60	0	28	0	0
3	x	60	0	28	0	0
3	y	60	0	28	0	0
3	yA	60	0	28	0	0
3	zA	60	0	28	0	0
3	zB	60	0	28	0	0
4	0A	47	0	28	0	0
4	1	47	0	28	0	0
4	1B	47	0	28	0	0
4	2A	47	0	28	0	0
4	2C	47	0	28	0	0
4	3B	47	0	28	0	0
4	4C	47	0	28	0	0
4	6	47	0	28	0	0
4	7A	47	0	28	0	0
4	8	47	0	28	0	0
4	8B	47	0	28	0	0
4	9A	47	0	28	0	0
4	9C	47	0	28	0	0
4	AC	47	0	28	0	0
4	BD	47	0	28	0	0
4	DA	47	0	28	0	0
4	EB	47	0	28	0	0
4	FA	47	0	28	0	0
4	FC	47	0	28	0	0
4	GB	47	0	28	0	0
4	GD	47	0	28	0	0
4	HC	47	0	28	0	0
4	ID	47	0	28	0	0
4	KA	47	0	28	0	0
4	LB	47	0	28	0	0
4	MA	47	0	28	0	0
4	MC	47	0	28	0	0
4	NB	47	0	28	0	0
4	OC	47	0	28	0	0
4	RA	47	0	28	0	0
4	SB	47	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	TA	47	0	28	0	0
4	TC	47	0	28	0	0
4	UB	47	0	28	0	0
4	VC	47	0	28	0	0
4	YA	47	0	28	0	0
4	ZB	47	0	28	0	0
4	aA	47	0	28	0	0
4	aC	47	0	28	0	0
4	bB	47	0	28	0	0
4	cC	47	0	28	0	0
4	fA	47	0	28	0	0
4	gB	47	0	28	0	0
4	hA	47	0	28	0	0
4	hC	47	0	28	0	0
4	iB	47	0	28	0	0
4	jC	47	0	28	0	0
4	l	47	0	28	0	0
4	mA	47	0	28	0	0
4	n	47	0	28	0	0
4	nB	47	0	28	0	0
4	oA	47	0	28	0	0
4	oC	47	0	28	0	0
4	pB	47	0	28	0	0
4	qC	47	0	28	0	0
4	s	47	0	28	0	0
4	tA	47	0	28	0	0
4	u	47	0	28	0	0
4	uB	47	0	28	0	0
4	vA	47	0	28	0	0
4	vC	47	0	28	0	0
4	wB	47	0	28	0	0
4	xC	47	0	28	0	0
4	z	47	0	28	0	0
5	A	22	0	20	0	0
5	B	22	0	20	0	0
5	C	22	0	20	0	0
5	D	22	0	20	0	0
5	E	22	0	20	0	0
5	F	22	0	20	0	0
5	G	22	0	20	0	0
5	H	22	0	20	0	0
5	I	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	22	0	20	0	0
5	K	22	0	20	0	0
5	L	22	0	20	0	0
5	M	22	0	20	0	0
5	N	22	0	20	0	0
5	O	22	0	20	0	0
5	P	22	0	20	0	0
5	Q	22	0	20	0	0
5	R	22	0	20	0	0
5	S	22	0	20	0	0
5	T	22	0	20	0	0
5	U	22	0	20	0	0
5	V	22	0	20	0	0
5	W	22	0	20	0	0
5	X	22	0	20	0	0
5	Y	22	0	20	0	0
5	a	22	0	20	0	0
5	b	22	0	20	0	0
5	c	22	0	20	0	0
5	d	22	0	20	0	0
5	e	22	0	20	0	0
5	f	22	0	20	0	0
5	g	22	0	20	0	0
All	All	67118	0	61620	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:THR:HG21	1:D:69:GLN:HG3	1.90	0.53
1:A:37:MET:SD	1:E:25:GLU:HB2	2.52	0.50
1:d:105:THR:HG21	1:g:69:GLN:HG3	1.95	0.48
1:E:105:THR:HG21	1:H:69:GLN:HG3	1.97	0.47
1:a:105:THR:HG21	1:d:69:GLN:HG3	1.95	0.47
1:U:105:THR:HG21	1:X:69:GLN:HG3	1.97	0.46
1:b:105:THR:HG21	1:e:69:GLN:HG3	1.96	0.46
1:B:105:THR:HG21	1:E:69:GLN:HG3	1.97	0.46
1:K:105:THR:HG21	1:N:69:GLN:HG3	1.97	0.46
1:B:37:MET:SD	1:F:25:GLU:HB2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:82:THR:HG21	1:c:69:GLN:HG3	1.98	0.46
1:Y:105:THR:HG21	1:b:69:GLN:HG3	1.98	0.46
1:P:105:THR:HG21	1:S:69:GLN:HG3	1.97	0.46
1:X:105:THR:HG21	1:a:69:GLN:HG3	1.97	0.46
1:c:105:THR:HG21	1:f:69:GLN:HG3	1.96	0.46
1:V:105:THR:HG21	1:Y:69:GLN:HG3	1.97	0.46
1:J:105:THR:HG21	1:M:69:GLN:HG3	1.97	0.45
1:D:105:THR:HG21	1:G:69:GLN:HG3	1.98	0.45
1:M:105:THR:HG21	1:P:69:GLN:HG3	1.98	0.45
1:F:133:ALA:HB3	1:F:137:ALA:HB2	1.99	0.45
1:L:105:THR:HG21	1:O:69:GLN:HG3	1.98	0.45
1:I:133:ALA:HB3	1:I:137:ALA:HB2	1.99	0.45
1:P:133:ALA:HB3	1:P:137:ALA:HB2	1.99	0.45
1:W:133:ALA:HB3	1:W:137:ALA:HB2	1.99	0.45
1:g:133:ALA:HB3	1:g:137:ALA:HB2	1.99	0.45
1:V:69:GLN:HG3	1:S:105:THR:HG21	1.98	0.45
1:F:105:THR:HG21	1:I:69:GLN:HG3	1.98	0.45
1:M:133:ALA:HB3	1:M:137:ALA:HB2	1.99	0.45
1:N:105:THR:HG21	1:Q:69:GLN:HG3	1.98	0.45
1:S:133:ALA:HB3	1:S:137:ALA:HB2	1.99	0.45
1:C:133:ALA:HB3	1:C:137:ALA:HB2	1.99	0.45
1:H:105:THR:HG21	1:K:69:GLN:HG3	1.98	0.45
1:Q:105:THR:HG21	1:T:69:GLN:HG3	1.98	0.45
1:R:105:THR:HG21	1:U:69:GLN:HG3	1.98	0.44
1:c:133:ALA:HB3	1:c:137:ALA:HB2	1.99	0.44
1:C:105:THR:HG21	1:F:69:GLN:HG3	1.98	0.44
1:B:133:ALA:HB3	1:B:137:ALA:HB2	1.99	0.44
1:O:105:THR:HG21	1:R:69:GLN:HG3	1.99	0.44
1:d:133:ALA:HB3	1:d:137:ALA:HB2	1.99	0.44
1:J:133:ALA:HB3	1:J:137:ALA:HB2	1.99	0.44
1:T:133:ALA:HB3	1:T:137:ALA:HB2	1.99	0.44
1:f:133:ALA:HB3	1:f:137:ALA:HB2	1.99	0.44
1:V:133:ALA:HB3	1:V:137:ALA:HB2	1.99	0.44
1:T:105:THR:HG21	1:W:69:GLN:HG3	1.99	0.44
1:E:133:ALA:HB3	1:E:137:ALA:HB2	1.99	0.44
1:G:105:THR:HG21	1:J:69:GLN:HG3	1.98	0.44
1:L:133:ALA:HB3	1:L:137:ALA:HB2	1.99	0.44
1:O:133:ALA:HB3	1:O:137:ALA:HB2	1.99	0.44
1:Y:133:ALA:HB3	1:Y:137:ALA:HB2	1.99	0.44
1:G:133:ALA:HB3	1:G:137:ALA:HB2	1.99	0.44
1:Q:133:ALA:HB3	1:Q:137:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:133:ALA:HB3	1:a:137:ALA:HB2	1.99	0.43
1:e:133:ALA:HB3	1:e:137:ALA:HB2	1.99	0.43
1:I:105:THR:HG21	1:L:69:GLN:HG3	1.98	0.43
1:K:133:ALA:HB3	1:K:137:ALA:HB2	1.99	0.43
1:U:133:ALA:HB3	1:U:137:ALA:HB2	1.99	0.43
1:N:133:ALA:HB3	1:N:137:ALA:HB2	1.99	0.43
1:X:133:ALA:HB3	1:X:137:ALA:HB2	1.99	0.43
1:Z:110:ALA:HB3	1:Z:114:ALA:HB2	2.01	0.43
1:A:133:ALA:HB3	1:A:137:ALA:HB2	1.99	0.43
1:D:133:ALA:HB3	1:D:137:ALA:HB2	1.99	0.43
1:E:37:MET:SD	1:I:25:GLU:HB2	2.58	0.43
1:H:133:ALA:HB3	1:H:137:ALA:HB2	1.99	0.43
1:R:133:ALA:HB3	1:R:137:ALA:HB2	1.99	0.43
1:b:133:ALA:HB3	1:b:137:ALA:HB2	1.99	0.43
1:U:37:MET:SD	1:Y:25:GLU:OE2	2.78	0.41
1:A:34:PHE:HE1	1:D:28:ILE:HG13	1.85	0.41
1:G:37:MET:SD	1:K:25:GLU:HB2	2.60	0.41
1:W:37:MET:SD	1:a:25:GLU:OE2	2.79	0.41
1:g:103:LEU:HG	1:g:199:LEU:HD23	2.03	0.41
1:C:37:MET:SD	1:G:25:GLU:HB2	2.61	0.41
1:J:103:LEU:HG	1:J:199:LEU:HD23	2.03	0.41
1:M:103:LEU:HG	1:M:199:LEU:HD23	2.03	0.41
1:T:103:LEU:HG	1:T:199:LEU:HD23	2.03	0.41
1:U:103:LEU:HG	1:U:199:LEU:HD23	2.03	0.41
1:W:103:LEU:HG	1:W:199:LEU:HD23	2.03	0.41
1:d:103:LEU:HG	1:d:199:LEU:HD23	2.03	0.41
1:e:103:LEU:HG	1:e:199:LEU:HD23	2.03	0.41
1:H:103:LEU:HG	1:H:199:LEU:HD23	2.03	0.41
1:R:103:LEU:HG	1:R:199:LEU:HD23	2.03	0.41
1:b:103:LEU:HG	1:b:199:LEU:HD23	2.03	0.41
1:A:103:LEU:HG	1:A:199:LEU:HD23	2.03	0.40
1:K:103:LEU:HG	1:K:199:LEU:HD23	2.03	0.40
1:C:103:LEU:HG	1:C:199:LEU:HD23	2.03	0.40
1:Y:103:LEU:HG	1:Y:199:LEU:HD23	2.03	0.40
1:E:103:LEU:HG	1:E:199:LEU:HD23	2.03	0.40
1:F:37:MET:SD	1:J:25:GLU:HB2	2.61	0.40
1:O:103:LEU:HG	1:O:199:LEU:HD23	2.03	0.40

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	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	B	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	C	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	D	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	E	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	F	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	G	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	H	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	I	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	J	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	K	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	L	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	M	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	N	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	O	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	P	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	Q	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	R	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	S	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	T	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	U	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	V	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	W	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	X	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	Y	228/230 (99%)	220 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	228/230 (99%)	223 (98%)	5 (2%)	0	100	100
1	a	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	b	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	c	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	d	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	e	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	f	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
1	g	228/230 (99%)	220 (96%)	8 (4%)	0	100	100
All	All	7524/7590 (99%)	7263 (96%)	261 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	B	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	C	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	D	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	E	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	F	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	G	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	H	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	I	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	J	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	K	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	L	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	M	193/193 (100%)	191 (99%)	2 (1%)	68	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	O	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	P	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	Q	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	R	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	S	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	T	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	U	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	V	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	W	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	X	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	Y	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	Z	193/193 (100%)	193 (100%)	0	100	100
1	a	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	b	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	c	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	d	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	e	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	f	193/193 (100%)	191 (99%)	2 (1%)	68	80
1	g	193/193 (100%)	191 (99%)	2 (1%)	68	80
All	All	6369/6369 (100%)	6305 (99%)	64 (1%)	65	80

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	163	THR
1	V	171	LEU
1	A	163	THR
1	A	171	LEU
1	B	163	THR
1	B	171	LEU
1	C	163	THR
1	C	171	LEU
1	D	163	THR
1	D	171	LEU

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Mol	Chain	Res	Type
1	E	163	THR
1	E	171	LEU
1	F	163	THR
1	F	171	LEU
1	G	163	THR
1	G	171	LEU
1	H	163	THR
1	H	171	LEU
1	I	163	THR
1	I	171	LEU
1	J	163	THR
1	J	171	LEU
1	K	163	THR
1	K	171	LEU
1	L	163	THR
1	L	171	LEU
1	M	163	THR
1	M	171	LEU
1	N	163	THR
1	N	171	LEU
1	O	163	THR
1	O	171	LEU
1	P	163	THR
1	P	171	LEU
1	Q	163	THR
1	Q	171	LEU
1	R	163	THR
1	R	171	LEU
1	S	163	THR
1	S	171	LEU
1	T	163	THR
1	T	171	LEU
1	U	163	THR
1	U	171	LEU
1	W	163	THR
1	W	171	LEU
1	X	163	THR
1	X	171	LEU
1	Y	163	THR
1	Y	171	LEU
1	a	163	THR
1	a	171	LEU

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Mol	Chain	Res	Type
1	b	163	THR
1	b	171	LEU
1	c	163	THR
1	c	171	LEU
1	d	163	THR
1	d	171	LEU
1	e	163	THR
1	e	171	LEU
1	f	163	THR
1	f	171	LEU
1	g	163	THR
1	g	171	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	34	GLN
1	Z	42	GLN
1	Z	99	GLN
1	Z	131	ASN
1	Z	173	HIS
1	Z	216	GLN
1	Z	231	GLN
1	V	57	GLN
1	V	65	GLN
1	V	122	GLN
1	V	154	ASN
1	V	239	GLN
1	V	254	GLN
1	A	122	GLN
1	A	154	ASN
1	A	239	GLN
1	A	254	GLN
1	B	122	GLN
1	B	154	ASN
1	B	239	GLN
1	B	254	GLN
1	C	122	GLN
1	C	154	ASN
1	C	239	GLN
1	C	254	GLN
1	D	65	GLN

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Mol	Chain	Res	Type
1	D	122	GLN
1	D	154	ASN
1	D	239	GLN
1	D	254	GLN
1	E	65	GLN
1	E	122	GLN
1	E	154	ASN
1	E	239	GLN
1	E	254	GLN
1	F	65	GLN
1	F	122	GLN
1	F	154	ASN
1	F	196	HIS
1	F	239	GLN
1	F	254	GLN
1	G	65	GLN
1	G	122	GLN
1	G	154	ASN
1	G	196	HIS
1	G	239	GLN
1	G	254	GLN
1	H	57	GLN
1	H	65	GLN
1	H	122	GLN
1	H	154	ASN
1	H	239	GLN
1	H	254	GLN
1	I	57	GLN
1	I	65	GLN
1	I	122	GLN
1	I	154	ASN
1	I	239	GLN
1	I	254	GLN
1	J	57	GLN
1	J	65	GLN
1	J	122	GLN
1	J	154	ASN
1	J	239	GLN
1	J	254	GLN
1	K	57	GLN
1	K	65	GLN
1	K	122	GLN

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Mol	Chain	Res	Type
1	K	154	ASN
1	K	239	GLN
1	K	254	GLN
1	L	57	GLN
1	L	65	GLN
1	L	122	GLN
1	L	154	ASN
1	L	239	GLN
1	L	254	GLN
1	M	57	GLN
1	M	65	GLN
1	M	122	GLN
1	M	154	ASN
1	M	239	GLN
1	M	254	GLN
1	N	57	GLN
1	N	65	GLN
1	N	122	GLN
1	N	154	ASN
1	N	239	GLN
1	N	254	GLN
1	O	57	GLN
1	O	65	GLN
1	O	122	GLN
1	O	154	ASN
1	O	239	GLN
1	O	254	GLN
1	P	57	GLN
1	P	65	GLN
1	P	122	GLN
1	P	154	ASN
1	P	239	GLN
1	P	254	GLN
1	Q	57	GLN
1	Q	65	GLN
1	Q	122	GLN
1	Q	154	ASN
1	Q	239	GLN
1	Q	254	GLN
1	R	57	GLN
1	R	65	GLN
1	R	122	GLN

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Mol	Chain	Res	Type
1	R	154	ASN
1	R	239	GLN
1	R	254	GLN
1	S	57	GLN
1	S	65	GLN
1	S	122	GLN
1	S	154	ASN
1	S	239	GLN
1	S	254	GLN
1	T	57	GLN
1	T	65	GLN
1	T	122	GLN
1	T	154	ASN
1	T	239	GLN
1	T	254	GLN
1	U	57	GLN
1	U	65	GLN
1	U	122	GLN
1	U	154	ASN
1	U	239	GLN
1	U	254	GLN
1	W	57	GLN
1	W	65	GLN
1	W	122	GLN
1	W	154	ASN
1	W	239	GLN
1	W	254	GLN
1	X	57	GLN
1	X	65	GLN
1	X	122	GLN
1	X	154	ASN
1	X	239	GLN
1	X	254	GLN
1	Y	57	GLN
1	Y	65	GLN
1	Y	122	GLN
1	Y	154	ASN
1	Y	239	GLN
1	Y	254	GLN
1	a	57	GLN
1	a	65	GLN
1	a	122	GLN

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Mol	Chain	Res	Type
1	a	154	ASN
1	b	57	GLN
1	b	65	GLN
1	b	122	GLN
1	b	154	ASN
1	c	57	GLN
1	c	65	GLN
1	c	122	GLN
1	c	154	ASN
1	d	57	GLN
1	d	65	GLN
1	d	122	GLN
1	d	154	ASN
1	e	57	GLN
1	e	65	GLN
1	e	122	GLN
1	e	154	ASN
1	f	57	GLN
1	f	65	GLN
1	f	122	GLN
1	f	154	ASN
1	g	57	GLN
1	g	65	GLN
1	g	122	GLN
1	g	154	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

928 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
3	GAL	0	1	3,1	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
3	BGC	0	2	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
3	A1H1F	0	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	0	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	0	5	3	11,11,12	0.64	0	15,15,17	1.11	1 (6%)
4	GAL	0A	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	0A	2	4	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	A1H1F	0A	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	0A	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	0B	1	3,1	11,11,12	0.61	0	15,15,17	0.86	0
3	BGC	0B	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	0B	3	3	12,14,15	0.89	0	18,21,23	1.50	3 (16%)
3	A1H03	0B	4	3	13,13,14	0.70	0	16,18,20	0.97	2 (12%)
3	MAN	0B	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	0C	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	0C	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	0C	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	0C	4	3	13,13,14	0.70	0	16,18,20	0.92	1 (6%)
3	MAN	0C	5	3	11,11,12	0.65	0	15,15,17	1.37	2 (13%)
4	GAL	1	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)
4	BGC	1	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	1	3	4	12,14,15	0.77	0	18,21,23	1.26	3 (16%)
4	MAN	1	4	4	11,11,12	0.58	0	15,15,17	1.15	1 (6%)
3	GAL	1A	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	1A	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	1A	3	3	12,14,15	0.87	0	18,21,23	1.23	2 (11%)
3	A1H03	1A	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	1A	5	3	11,11,12	0.63	0	15,15,17	1.13	1 (6%)
4	GAL	1B	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	1B	2	4	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	A1H1F	1B	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	1B	4	4	11,11,12	0.63	0	15,15,17	1.37	3 (20%)
3	GAL	1C	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	1C	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	1C	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	1C	4	3	13,13,14	0.70	0	16,18,20	0.97	2 (12%)
3	MAN	1C	5	3	11,11,12	0.61	0	15,15,17	1.14	1 (6%)
2	GAL	2	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	2	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	2	3	2	12,14,15	0.84	0	18,21,23	1.26	3 (16%)
2	MAN	2	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	2	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	2	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	2A	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)
4	BGC	2A	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	2A	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	2A	4	4	11,11,12	0.59	0	15,15,17	1.16	1 (6%)
3	GAL	2B	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	2B	2	3	11,11,12	0.60	0	15,15,17	1.37	3 (20%)
3	A1H1F	2B	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	2B	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	2B	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
4	GAL	2C	1	1,4	11,11,12	0.68	0	15,15,17	1.15	2 (13%)
4	BGC	2C	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	2C	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	2C	4	4	11,11,12	0.64	0	15,15,17	1.36	2 (13%)
2	GAL	3A	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	3A	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	3A	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	3A	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	3A	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	3A	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	3B	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	3B	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	3B	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	3B	4	4	11,11,12	0.58	0	15,15,17	1.17	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	3C	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	3C	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	3C	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	3C	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	3C	5	3	11,11,12	0.63	0	15,15,17	1.12	1 (6%)
3	GAL	4	1	3,1	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
3	BGC	4	2	3	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
3	A1H1F	4	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	4	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	4	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
2	GAL	4B	1	2,1	11,11,12	0.66	0	15,15,17	0.97	1 (6%)
2	BGC	4B	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	4B	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)
2	MAN	4B	4	2	11,11,12	0.61	0	15,15,17	1.37	1 (6%)
2	MAN	4B	5	2	11,11,12	0.65	0	15,15,17	1.78	2 (13%)
2	A1H03	4B	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	4C	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)
4	BGC	4C	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	4C	3	4	12,14,15	0.76	0	18,21,23	1.26	3 (16%)
4	MAN	4C	4	4	11,11,12	0.58	0	15,15,17	1.15	1 (6%)
3	GAL	5	1	3,1	11,11,12	0.59	0	15,15,17	0.87	0
3	BGC	5	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	5	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	5	4	3	13,13,14	0.71	0	16,18,20	0.98	2 (12%)
3	MAN	5	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	5A	1	3,1	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
3	BGC	5A	2	3	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
3	A1H1F	5A	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	5A	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	5A	5	3	11,11,12	0.64	0	15,15,17	1.38	2 (13%)
2	GAL	5C	1	2,1	11,11,12	0.67	0	15,15,17	0.97	1 (6%)
2	BGC	5C	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	5C	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	5C	4	2	11,11,12	0.61	0	15,15,17	1.38	1 (6%)
2	MAN	5C	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1H03	5C	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	6	1	1,4	11,11,12	0.67	0	15,15,17	1.16	2 (13%)
4	BGC	6	2	4	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	A1H1F	6	3	4	12,14,15	0.87	0	18,21,23	2.17	4 (22%)
4	MAN	6	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	6A	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	6A	2	3	11,11,12	0.60	0	15,15,17	1.37	3 (20%)
3	A1H1F	6A	3	3	12,14,15	0.89	0	18,21,23	1.50	3 (16%)
3	A1H03	6A	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	6A	5	3	11,11,12	0.61	0	15,15,17	1.15	1 (6%)
3	GAL	6B	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	6B	2	3	11,11,12	0.59	0	15,15,17	1.20	2 (13%)
3	A1H1F	6B	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	6B	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	6B	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
3	GAL	7	1	3,1	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
3	BGC	7	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	7	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	7	4	3	13,13,14	0.72	0	16,18,20	0.88	1 (6%)
3	MAN	7	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
4	GAL	7A	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	7A	2	4	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
4	A1H1F	7A	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	7A	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	7B	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	7B	2	3	11,11,12	0.61	0	15,15,17	1.38	3 (20%)
3	A1H1F	7B	3	3	12,14,15	0.89	0	18,21,23	1.51	3 (16%)
3	A1H03	7B	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)
3	MAN	7B	5	3	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
3	GAL	7C	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	7C	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	7C	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	7C	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	7C	5	3	11,11,12	0.63	0	15,15,17	1.38	2 (13%)
4	GAL	8	1	1,4	11,11,12	0.65	0	15,15,17	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BGC	8	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	8	3	4	12,14,15	0.76	0	18,21,23	1.26	3 (16%)
4	MAN	8	4	4	11,11,12	0.58	0	15,15,17	1.15	1 (6%)
3	GAL	8A	1	3,1	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
3	BGC	8A	2	3	11,11,12	0.58	0	15,15,17	1.38	3 (20%)
3	A1H1F	8A	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	8A	4	3	13,13,14	0.70	0	16,18,20	0.89	1 (6%)
3	MAN	8A	5	3	11,11,12	0.65	0	15,15,17	1.12	1 (6%)
4	GAL	8B	1	1,4	11,11,12	0.68	0	15,15,17	1.15	2 (13%)
4	BGC	8B	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	8B	3	4	12,14,15	0.87	0	18,21,23	2.17	4 (22%)
4	MAN	8B	4	4	11,11,12	0.63	0	15,15,17	1.37	3 (20%)
3	GAL	8C	1	3,1	11,11,12	0.59	0	15,15,17	0.87	0
3	BGC	8C	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	8C	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	8C	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	8C	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
2	GAL	9	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	9	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	9	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)
2	MAN	9	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	9	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	9	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	9A	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	9A	2	4	11,11,12	0.57	0	15,15,17	1.01	2 (13%)
4	A1H1F	9A	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	9A	4	4	11,11,12	0.59	0	15,15,17	1.16	1 (6%)
3	GAL	9B	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	9B	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	9B	3	3	12,14,15	0.88	0	18,21,23	1.23	2 (11%)
3	A1H03	9B	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	9B	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
4	GAL	9C	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	9C	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	9C	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	9C	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
2	GAL	AB	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	AB	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	AB	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	AB	4	2	11,11,12	0.62	0	15,15,17	1.39	1 (6%)
2	MAN	AB	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	AB	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	AC	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	AC	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	AC	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	AC	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	AD	1	3,1	11,11,12	0.65	0	15,15,17	1.00	1 (6%)
3	BGC	AD	2	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
3	A1H1F	AD	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	AD	4	3	13,13,14	0.71	0	16,18,20	0.89	1 (6%)
3	MAN	AD	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
3	GAL	BA	1	3,1	11,11,12	0.66	0	15,15,17	1.12	2 (13%)
3	BGC	BA	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	BA	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	BA	4	3	13,13,14	0.72	0	16,18,20	0.91	1 (6%)
3	MAN	BA	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
2	GAL	BC	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	BC	2	2	11,11,12	0.65	0	15,15,17	1.17	2 (13%)
2	A1H1F	BC	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	BC	4	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	BC	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	BC	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	BD	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	BD	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	BD	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	BD	4	4	11,11,12	0.59	0	15,15,17	1.15	1 (6%)
3	GAL	CA	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	CA	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	CA	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	CA	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	CA	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	CB	1	3,1	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
3	BGC	CB	2	3	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
3	A1H1F	CB	3	3	12,14,15	0.96	0	18,21,23	1.66	5 (27%)
3	A1H03	CB	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	CB	5	3	11,11,12	0.64	0	15,15,17	1.38	2 (13%)
2	GAL	CD	1	2,1	11,11,12	0.65	0	15,15,17	0.98	1 (6%)
2	BGC	CD	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	CD	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)
2	MAN	CD	4	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	CD	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	CD	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	DA	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	DA	2	4	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	A1H1F	DA	3	4	12,14,15	0.87	0	18,21,23	2.17	4 (22%)
4	MAN	DA	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	DB	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	DB	2	3	11,11,12	0.62	0	15,15,17	1.37	3 (20%)
3	A1H1F	DB	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	DB	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)
3	MAN	DB	5	3	11,11,12	0.61	0	15,15,17	1.15	1 (6%)
3	GAL	DC	1	3,1	11,11,12	0.66	0	15,15,17	1.12	2 (13%)
3	BGC	DC	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	DC	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	DC	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	DC	5	3	11,11,12	0.64	0	15,15,17	1.38	2 (13%)
3	GAL	EA	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	EA	2	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
3	A1H1F	EA	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	EA	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	EA	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
4	GAL	EB	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	EB	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	EB	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	EB	4	4	11,11,12	0.62	0	15,15,17	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	EC	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	EC	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	EC	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	EC	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	EC	5	3	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
3	GAL	ED	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	ED	2	3	11,11,12	0.59	0	15,15,17	1.20	2 (13%)
3	A1H1F	ED	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	ED	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	ED	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
4	GAL	FA	1	1,4	11,11,12	0.65	0	15,15,17	1.31	2 (13%)
4	BGC	FA	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	FA	3	4	12,14,15	0.77	0	18,21,23	1.26	3 (16%)
4	MAN	FA	4	4	11,11,12	0.58	0	15,15,17	1.17	1 (6%)
3	GAL	FB	1	3,1	11,11,12	0.65	0	15,15,17	1.00	1 (6%)
3	BGC	FB	2	3	11,11,12	0.60	0	15,15,17	1.37	3 (20%)
3	A1H1F	FB	3	3	12,14,15	0.87	0	18,21,23	1.23	2 (11%)
3	A1H03	FB	4	3	13,13,14	0.70	0	16,18,20	0.88	1 (6%)
3	MAN	FB	5	3	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
4	GAL	FC	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	FC	2	4	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
4	A1H1F	FC	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	FC	4	4	11,11,12	0.62	0	15,15,17	1.37	3 (20%)
3	GAL	FD	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	FD	2	3	11,11,12	0.62	0	15,15,17	1.37	3 (20%)
3	A1H1F	FD	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	FD	4	3	13,13,14	0.70	0	16,18,20	0.97	2 (12%)
3	MAN	FD	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
2	GAL	GA	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	GA	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	GA	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	GA	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	GA	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	GA	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	GB	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BGC	GB	2	4	11,11,12	0.57	0	15,15,17	1.03	2 (13%)
4	A1H1F	GB	3	4	12,14,15	0.78	0	18,21,23	1.26	3 (16%)
4	MAN	GB	4	4	11,11,12	0.58	0	15,15,17	1.17	1 (6%)
3	GAL	GC	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	GC	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	GC	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	GC	4	3	13,13,14	0.72	0	16,18,20	0.88	1 (6%)
3	MAN	GC	5	3	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
4	GAL	GD	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	GD	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	GD	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	GD	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
2	GAL	HB	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	HB	2	2	11,11,12	0.64	0	15,15,17	1.16	2 (13%)
2	A1H1F	HB	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	HB	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	HB	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	HB	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	HC	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	HC	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	HC	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	HC	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	HD	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	HD	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	HD	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	HD	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	HD	5	3	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
3	GAL	IA	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	IA	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	IA	3	3	12,14,15	0.96	0	18,21,23	1.65	5 (27%)
3	A1H03	IA	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	IA	5	3	11,11,12	0.65	0	15,15,17	1.37	2 (13%)
2	GAL	IC	1	2,1	11,11,12	0.67	0	15,15,17	0.97	1 (6%)
2	BGC	IC	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	IC	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	IC	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	IC	5	2	11,11,12	0.64	0	15,15,17	1.79	2 (13%)
2	A1H03	IC	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	ID	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	ID	2	4	11,11,12	0.57	0	15,15,17	1.03	2 (13%)
4	A1H1F	ID	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	ID	4	4	11,11,12	0.59	0	15,15,17	1.16	1 (6%)
3	GAL	JA	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	JA	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	JA	3	3	12,14,15	0.87	0	18,21,23	1.50	3 (16%)
3	A1H03	JA	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	JA	5	3	11,11,12	0.61	0	15,15,17	1.14	1 (6%)
3	GAL	JB	1	3,1	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
3	BGC	JB	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	JB	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	JB	4	3	13,13,14	0.73	0	16,18,20	0.91	1 (6%)
3	MAN	JB	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
4	GAL	KA	1	1,4	11,11,12	0.67	0	15,15,17	1.14	2 (13%)
4	BGC	KA	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	KA	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	KA	4	4	11,11,12	0.63	0	15,15,17	1.36	2 (13%)
3	GAL	KB	1	3,1	11,11,12	0.59	0	15,15,17	0.87	0
3	BGC	KB	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	KB	3	3	12,14,15	0.89	0	18,21,23	1.50	3 (16%)
3	A1H03	KB	4	3	13,13,14	0.69	0	16,18,20	0.97	2 (12%)
3	MAN	KB	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	KC	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	KC	2	3	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
3	A1H1F	KC	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	KC	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	KC	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
3	GAL	LA	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	LA	2	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
3	A1H1F	LA	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	LA	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	LA	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
4	GAL	LB	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	LB	2	4	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	A1H1F	LB	3	4	12,14,15	0.87	0	18,21,23	2.15	4 (22%)
4	MAN	LB	4	4	11,11,12	0.63	0	15,15,17	1.38	2 (13%)
3	GAL	LC	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	LC	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	LC	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	LC	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	LC	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
4	GAL	MA	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	MA	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	MA	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	MA	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	MB	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	MB	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	MB	3	3	12,14,15	0.87	0	18,21,23	1.22	2 (11%)
3	A1H03	MB	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	MB	5	3	11,11,12	0.63	0	15,15,17	1.13	1 (6%)
4	GAL	MC	1	1,4	11,11,12	0.67	0	15,15,17	1.14	2 (13%)
4	BGC	MC	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	MC	3	4	12,14,15	0.88	0	18,21,23	2.16	4 (22%)
4	MAN	MC	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
2	GAL	NA	1	2,1	11,11,12	0.66	0	15,15,17	0.97	1 (6%)
2	BGC	NA	2	2	11,11,12	0.64	0	15,15,17	1.16	2 (13%)
2	A1H1F	NA	3	2	12,14,15	0.84	0	18,21,23	1.28	3 (16%)
2	MAN	NA	4	2	11,11,12	0.61	0	15,15,17	1.38	1 (6%)
2	MAN	NA	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	NA	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	NB	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)
4	BGC	NB	2	4	11,11,12	0.57	0	15,15,17	1.01	2 (13%)
4	A1H1F	NB	3	4	12,14,15	0.76	0	18,21,23	1.25	3 (16%)
4	MAN	NB	4	4	11,11,12	0.58	0	15,15,17	1.14	1 (6%)
3	GAL	NC	1	3,1	11,11,12	0.65	0	15,15,17	1.00	1 (6%)
3	BGC	NC	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1H1F	NC	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	NC	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	NC	5	3	11,11,12	0.63	0	15,15,17	1.13	1 (6%)
2	GAL	OB	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	OB	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	OB	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)
2	MAN	OB	4	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	OB	5	2	11,11,12	0.64	0	15,15,17	1.79	2 (13%)
2	A1H03	OB	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	OC	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	OC	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	OC	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	OC	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	PA	1	3,1	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
3	BGC	PA	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	PA	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	PA	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	PA	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
2	GAL	PC	1	2,1	11,11,12	0.67	0	15,15,17	0.97	1 (6%)
2	BGC	PC	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	PC	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	PC	4	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	PC	5	2	11,11,12	0.65	0	15,15,17	1.78	2 (13%)
2	A1H03	PC	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
3	GAL	QA	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	QA	2	3	11,11,12	0.62	0	15,15,17	1.37	3 (20%)
3	A1H1F	QA	3	3	12,14,15	0.89	0	18,21,23	1.51	3 (16%)
3	A1H03	QA	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	QA	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	QB	1	3,1	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
3	BGC	QB	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	QB	3	3	12,14,15	0.96	0	18,21,23	1.66	5 (27%)
3	A1H03	QB	4	3	13,13,14	0.72	0	16,18,20	0.92	1 (6%)
3	MAN	QB	5	3	11,11,12	0.63	0	15,15,17	1.38	2 (13%)
4	GAL	RA	1	1,4	11,11,12	0.68	0	15,15,17	1.15	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BGC	RA	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	RA	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	RA	4	4	11,11,12	0.63	0	15,15,17	1.37	3 (20%)
3	GAL	RB	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	RB	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	RB	3	3	12,14,15	0.89	0	18,21,23	1.51	3 (16%)
3	A1H03	RB	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)
3	MAN	RB	5	3	11,11,12	0.61	0	15,15,17	1.14	1 (6%)
3	GAL	RC	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	RC	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	RC	3	3	12,14,15	0.95	0	18,21,23	1.67	5 (27%)
3	A1H03	RC	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	RC	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
3	GAL	SA	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	SA	2	3	11,11,12	0.60	0	15,15,17	1.38	3 (20%)
3	A1H1F	SA	3	3	12,14,15	0.88	0	18,21,23	1.23	2 (11%)
3	A1H03	SA	4	3	13,13,14	0.72	0	16,18,20	0.88	1 (6%)
3	MAN	SA	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
4	GAL	SB	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	SB	2	4	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
4	A1H1F	SB	3	4	12,14,15	0.86	0	18,21,23	2.16	4 (22%)
4	MAN	SB	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	SC	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	SC	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	SC	3	3	12,14,15	0.87	0	18,21,23	1.50	3 (16%)
3	A1H03	SC	4	3	13,13,14	0.70	0	16,18,20	0.97	2 (12%)
3	MAN	SC	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
4	GAL	TA	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)
4	BGC	TA	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	TA	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	TA	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	TB	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	TB	2	3	11,11,12	0.60	0	15,15,17	1.37	3 (20%)
3	A1H1F	TB	3	3	12,14,15	0.88	0	18,21,23	1.23	2 (11%)
3	A1H03	TB	4	3	13,13,14	0.70	0	16,18,20	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	TB	5	3	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
4	GAL	TC	1	1,4	11,11,12	0.68	0	15,15,17	1.14	2 (13%)
4	BGC	TC	2	4	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	A1H1F	TC	3	4	12,14,15	0.87	0	18,21,23	2.17	4 (22%)
4	MAN	TC	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
2	GAL	UA	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	UA	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	UA	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	UA	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	UA	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	UA	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	UB	1	1,4	11,11,12	0.66	0	15,15,17	1.29	2 (13%)
4	BGC	UB	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	UB	3	4	12,14,15	0.76	0	18,21,23	1.26	3 (16%)
4	MAN	UB	4	4	11,11,12	0.59	0	15,15,17	1.15	1 (6%)
3	GAL	UC	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	UC	2	3	11,11,12	0.58	0	15,15,17	1.38	3 (20%)
3	A1H1F	UC	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	UC	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	UC	5	3	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
2	GAL	VB	1	2,1	11,11,12	0.66	0	15,15,17	0.97	1 (6%)
2	BGC	VB	2	2	11,11,12	0.64	0	15,15,17	1.18	2 (13%)
2	A1H1F	VB	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)
2	MAN	VB	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	VB	5	2	11,11,12	0.64	0	15,15,17	1.77	2 (13%)
2	A1H03	VB	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	VC	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	VC	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	VC	3	4	12,14,15	0.76	0	18,21,23	1.26	3 (16%)
4	MAN	VC	4	4	11,11,12	0.58	0	15,15,17	1.17	1 (6%)
3	GAL	WA	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	WA	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	WA	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	WA	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	WA	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	WC	1	2,1	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
2	BGC	WC	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	WC	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	WC	4	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	WC	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	WC	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
3	GAL	XA	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	XA	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	XA	3	3	12,14,15	0.89	0	18,21,23	1.50	3 (16%)
3	A1H03	XA	4	3	13,13,14	0.69	0	16,18,20	0.99	2 (12%)
3	MAN	XA	5	3	11,11,12	0.61	0	15,15,17	1.15	1 (6%)
3	GAL	XB	1	3,1	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
3	BGC	XB	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	XB	3	3	12,14,15	0.96	0	18,21,23	1.66	5 (27%)
3	A1H03	XB	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	XB	5	3	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
4	GAL	YA	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	YA	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	YA	3	4	12,14,15	0.87	0	18,21,23	2.15	4 (22%)
4	MAN	YA	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	YB	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	YB	2	3	11,11,12	0.62	0	15,15,17	1.37	3 (20%)
3	A1H1F	YB	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	YB	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	YB	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	YC	1	3,1	11,11,12	0.66	0	15,15,17	1.12	2 (13%)
3	BGC	YC	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	YC	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	YC	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	YC	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
3	GAL	ZA	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	ZA	2	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
3	A1H1F	ZA	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	ZA	4	3	13,13,14	0.70	0	16,18,20	0.88	1 (6%)
3	MAN	ZA	5	3	11,11,12	0.63	0	15,15,17	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GAL	ZB	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	ZB	2	4	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
4	A1H1F	ZB	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	ZB	4	4	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
3	GAL	ZC	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	ZC	2	3	11,11,12	0.61	0	15,15,17	1.36	3 (20%)
3	A1H1F	ZC	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	ZC	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)
3	MAN	ZC	5	3	11,11,12	0.61	0	15,15,17	1.15	1 (6%)
4	GAL	aA	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	aA	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	aA	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	aA	4	4	11,11,12	0.59	0	15,15,17	1.15	1 (6%)
3	GAL	aB	1	3,1	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
3	BGC	aB	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	aB	3	3	12,14,15	0.88	0	18,21,23	1.23	2 (11%)
3	A1H03	aB	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	aB	5	3	11,11,12	0.63	0	15,15,17	1.13	1 (6%)
4	GAL	aC	1	1,4	11,11,12	0.68	0	15,15,17	1.15	2 (13%)
4	BGC	aC	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	aC	3	4	12,14,15	0.87	0	18,21,23	2.15	4 (22%)
4	MAN	aC	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
2	GAL	bA	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	bA	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	bA	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	bA	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	bA	5	2	11,11,12	0.65	0	15,15,17	1.78	2 (13%)
2	A1H03	bA	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	bB	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	bB	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	bB	3	4	12,14,15	0.77	0	18,21,23	1.26	3 (16%)
4	MAN	bB	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	bC	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	bC	2	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
3	A1H1F	bC	3	3	12,14,15	0.87	0	18,21,23	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1H03	bC	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	bC	5	3	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
2	GAL	cB	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	cB	2	2	11,11,12	0.65	0	15,15,17	1.17	2 (13%)
2	A1H1F	cB	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)
2	MAN	cB	4	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	cB	5	2	11,11,12	0.65	0	15,15,17	1.78	2 (13%)
2	A1H03	cB	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	cC	1	1,4	11,11,12	0.64	0	15,15,17	1.30	2 (13%)
4	BGC	cC	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	cC	3	4	12,14,15	0.77	0	18,21,23	1.26	3 (16%)
4	MAN	cC	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	dA	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	dA	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	dA	3	3	12,14,15	0.95	0	18,21,23	1.66	4 (22%)
3	A1H03	dA	4	3	13,13,14	0.70	0	16,18,20	0.91	1 (6%)
3	MAN	dA	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
2	GAL	dC	1	2,1	11,11,12	0.66	0	15,15,17	0.97	1 (6%)
2	BGC	dC	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	dC	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)
2	MAN	dC	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	dC	5	2	11,11,12	0.63	0	15,15,17	1.79	2 (13%)
2	A1H03	dC	6	2	13,13,14	0.81	0	16,18,20	1.00	2 (12%)
3	GAL	eA	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	eA	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	eA	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	eA	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	eA	5	3	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
3	GAL	eB	1	3,1	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
3	BGC	eB	2	3	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
3	A1H1F	eB	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	eB	4	3	13,13,14	0.72	0	16,18,20	0.91	1 (6%)
3	MAN	eB	5	3	11,11,12	0.65	0	15,15,17	1.37	2 (13%)
4	GAL	fA	1	1,4	11,11,12	0.68	0	15,15,17	1.14	2 (13%)
4	BGC	fA	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A1H1F	fA	3	4	12,14,15	0.86	0	18,21,23	2.16	4 (22%)
4	MAN	fA	4	4	11,11,12	0.63	0	15,15,17	1.37	3 (20%)
3	GAL	fB	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	fB	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	fB	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	fB	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)
3	MAN	fB	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	fC	1	3,1	11,11,12	0.65	0	15,15,17	1.14	2 (13%)
3	BGC	fC	2	3	11,11,12	0.61	0	15,15,17	1.19	2 (13%)
3	A1H1F	fC	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	fC	4	3	13,13,14	0.72	0	16,18,20	0.92	1 (6%)
3	MAN	fC	5	3	11,11,12	0.64	0	15,15,17	1.36	2 (13%)
3	GAL	gA	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	gA	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	gA	3	3	12,14,15	0.88	0	18,21,23	1.23	2 (11%)
3	A1H03	gA	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	gA	5	3	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
4	GAL	gB	1	1,4	11,11,12	0.67	0	15,15,17	1.16	2 (13%)
4	BGC	gB	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	gB	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	gB	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	gC	1	3,1	11,11,12	0.59	0	15,15,17	0.87	0
3	BGC	gC	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	gC	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	gC	4	3	13,13,14	0.69	0	16,18,20	0.99	2 (12%)
3	MAN	gC	5	3	11,11,12	0.61	0	15,15,17	1.15	1 (6%)
2	GAL	h	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	h	2	2	11,11,12	0.64	0	15,15,17	1.16	2 (13%)
2	A1H1F	h	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	h	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	h	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	h	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	hA	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)
4	BGC	hA	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	hA	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	hA	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	hB	1	3,1	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
3	BGC	hB	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	hB	3	3	12,14,15	0.89	0	18,21,23	1.23	2 (11%)
3	A1H03	hB	4	3	13,13,14	0.70	0	16,18,20	0.89	1 (6%)
3	MAN	hB	5	3	11,11,12	0.63	0	15,15,17	1.14	1 (6%)
4	GAL	hC	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	hC	2	4	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
4	A1H1F	hC	3	4	12,14,15	0.87	0	18,21,23	2.15	4 (22%)
4	MAN	hC	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
2	GAL	iA	1	2,1	11,11,12	0.66	0	15,15,17	0.97	1 (6%)
2	BGC	iA	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	iA	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	iA	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	iA	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	iA	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	iB	1	1,4	11,11,12	0.65	0	15,15,17	1.29	2 (13%)
4	BGC	iB	2	4	11,11,12	0.56	0	15,15,17	1.02	2 (13%)
4	A1H1F	iB	3	4	12,14,15	0.77	0	18,21,23	1.26	3 (16%)
4	MAN	iB	4	4	11,11,12	0.56	0	15,15,17	1.16	1 (6%)
3	GAL	iC	1	3,1	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
3	BGC	iC	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	iC	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	iC	4	3	13,13,14	0.72	0	16,18,20	0.88	1 (6%)
3	MAN	iC	5	3	11,11,12	0.65	0	15,15,17	1.13	1 (6%)
3	GAL	j	1	3,1	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
3	BGC	j	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	j	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	j	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	j	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
2	GAL	jB	1	2,1	11,11,12	0.67	0	15,15,17	0.97	1 (6%)
2	BGC	jB	2	2	11,11,12	0.63	0	15,15,17	1.17	2 (13%)
2	A1H1F	jB	3	2	12,14,15	0.83	0	18,21,23	1.28	3 (16%)
2	MAN	jB	4	2	11,11,12	0.61	0	15,15,17	1.38	1 (6%)
2	MAN	jB	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1H03	jB	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	jC	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	jC	2	4	11,11,12	0.57	0	15,15,17	1.03	2 (13%)
4	A1H1F	jC	3	4	12,14,15	0.77	0	18,21,23	1.26	3 (16%)
4	MAN	jC	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	k	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	k	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	k	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	k	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	k	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	kA	1	3,1	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
3	BGC	kA	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	kA	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	kA	4	3	13,13,14	0.70	0	16,18,20	0.92	1 (6%)
3	MAN	kA	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
2	GAL	kC	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	kC	2	2	11,11,12	0.65	0	15,15,17	1.17	2 (13%)
2	A1H1F	kC	3	2	12,14,15	0.83	0	18,21,23	1.26	3 (16%)
2	MAN	kC	4	2	11,11,12	0.61	0	15,15,17	1.37	1 (6%)
2	MAN	kC	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	kC	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	l	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	l	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	l	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	l	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	lA	1	3,1	11,11,12	0.61	0	15,15,17	0.86	0
3	BGC	lA	2	3	11,11,12	0.63	0	15,15,17	1.37	3 (20%)
3	A1H1F	lA	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	lA	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	lA	5	3	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
3	GAL	lB	1	3,1	11,11,12	0.66	0	15,15,17	1.12	2 (13%)
3	BGC	lB	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	lB	3	3	12,14,15	0.97	0	18,21,23	1.66	5 (27%)
3	A1H03	lB	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	lB	5	3	11,11,12	0.63	0	15,15,17	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	m	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	m	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	m	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	m	4	3	13,13,14	0.71	0	16,18,20	0.88	1 (6%)
3	MAN	m	5	3	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
4	GAL	mA	1	1,4	11,11,12	0.67	0	15,15,17	1.16	2 (13%)
4	BGC	mA	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	mA	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	mA	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	mB	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	mB	2	3	11,11,12	0.60	0	15,15,17	1.37	3 (20%)
3	A1H1F	mB	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	mB	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)
3	MAN	mB	5	3	11,11,12	0.61	0	15,15,17	1.16	1 (6%)
3	GAL	mC	1	3,1	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
3	BGC	mC	2	3	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
3	A1H1F	mC	3	3	12,14,15	0.96	0	18,21,23	1.66	5 (27%)
3	A1H03	mC	4	3	13,13,14	0.70	0	16,18,20	0.92	1 (6%)
3	MAN	mC	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
4	GAL	n	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	n	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	n	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	n	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	nA	1	3,1	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
3	BGC	nA	2	3	11,11,12	0.60	0	15,15,17	1.37	3 (20%)
3	A1H1F	nA	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	nA	4	3	13,13,14	0.70	0	16,18,20	0.88	1 (6%)
3	MAN	nA	5	3	11,11,12	0.63	0	15,15,17	1.12	1 (6%)
4	GAL	nB	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	nB	2	4	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
4	A1H1F	nB	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	nB	4	4	11,11,12	0.62	0	15,15,17	1.37	3 (20%)
3	GAL	nC	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	nC	2	3	11,11,12	0.60	0	15,15,17	1.37	3 (20%)
3	A1H1F	nC	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1H03	nC	4	3	13,13,14	0.70	0	16,18,20	0.97	2 (12%)
3	MAN	nC	5	3	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
2	GAL	o	1	2,1	11,11,12	0.65	0	15,15,17	0.98	1 (6%)
2	BGC	o	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	o	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	o	4	2	11,11,12	0.63	0	15,15,17	1.37	1 (6%)
2	MAN	o	5	2	11,11,12	0.64	0	15,15,17	1.79	2 (13%)
2	A1H03	o	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	oA	1	1,4	11,11,12	0.64	0	15,15,17	1.31	2 (13%)
4	BGC	oA	2	4	11,11,12	0.56	0	15,15,17	1.02	2 (13%)
4	A1H1F	oA	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	oA	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	oB	1	3,1	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
3	BGC	oB	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	oB	3	3	12,14,15	0.88	0	18,21,23	1.23	2 (11%)
3	A1H03	oB	4	3	13,13,14	0.70	0	16,18,20	0.88	1 (6%)
3	MAN	oB	5	3	11,11,12	0.65	0	15,15,17	1.12	1 (6%)
4	GAL	oC	1	1,4	11,11,12	0.68	0	15,15,17	1.14	2 (13%)
4	BGC	oC	2	4	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
4	A1H1F	oC	3	4	12,14,15	0.86	0	18,21,23	2.16	4 (22%)
4	MAN	oC	4	4	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
2	GAL	pA	1	2,1	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
2	BGC	pA	2	2	11,11,12	0.64	0	15,15,17	1.16	2 (13%)
2	A1H1F	pA	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)
2	MAN	pA	4	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	pA	5	2	11,11,12	0.63	0	15,15,17	1.79	2 (13%)
2	A1H03	pA	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	pB	1	1,4	11,11,12	0.64	0	15,15,17	1.30	2 (13%)
4	BGC	pB	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	pB	3	4	12,14,15	0.78	0	18,21,23	1.25	3 (16%)
4	MAN	pB	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	pC	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	pC	2	3	11,11,12	0.60	0	15,15,17	1.38	3 (20%)
3	A1H1F	pC	3	3	12,14,15	0.89	0	18,21,23	1.22	2 (11%)
3	A1H03	pC	4	3	13,13,14	0.71	0	16,18,20	0.89	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	pC	5	3	11,11,12	0.63	0	15,15,17	1.12	1 (6%)
3	GAL	q	1	3,1	11,11,12	0.66	0	15,15,17	1.12	2 (13%)
3	BGC	q	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	q	3	3	12,14,15	0.96	0	18,21,23	1.66	5 (27%)
3	A1H03	q	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	q	5	3	11,11,12	0.64	0	15,15,17	1.38	2 (13%)
2	GAL	qB	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	qB	2	2	11,11,12	0.63	0	15,15,17	1.17	2 (13%)
2	A1H1F	qB	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	qB	4	2	11,11,12	0.63	0	15,15,17	1.38	1 (6%)
2	MAN	qB	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	qB	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	qC	1	1,4	11,11,12	0.65	0	15,15,17	1.30	2 (13%)
4	BGC	qC	2	4	11,11,12	0.57	0	15,15,17	1.03	2 (13%)
4	A1H1F	qC	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	qC	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	r	1	3,1	11,11,12	0.60	0	15,15,17	0.86	0
3	BGC	r	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	r	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	r	4	3	13,13,14	0.69	0	16,18,20	0.97	2 (12%)
3	MAN	r	5	3	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
3	GAL	rA	1	3,1	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
3	BGC	rA	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	rA	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	rA	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	rA	5	3	11,11,12	0.65	0	15,15,17	1.38	2 (13%)
2	GAL	rC	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	rC	2	2	11,11,12	0.65	0	15,15,17	1.17	2 (13%)
2	A1H1F	rC	3	2	12,14,15	0.83	0	18,21,23	1.26	3 (16%)
2	MAN	rC	4	2	11,11,12	0.61	0	15,15,17	1.38	1 (6%)
2	MAN	rC	5	2	11,11,12	0.65	0	15,15,17	1.77	2 (13%)
2	A1H03	rC	6	2	13,13,14	0.80	0	16,18,20	1.00	2 (12%)
4	GAL	s	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	s	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	s	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	s	4	4	11,11,12	0.63	0	15,15,17	1.36	2 (13%)
3	GAL	sA	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	sA	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	sA	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	sA	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)
3	MAN	sA	5	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
3	GAL	sB	1	3,1	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
3	BGC	sB	2	3	11,11,12	0.59	0	15,15,17	1.19	2 (13%)
3	A1H1F	sB	3	3	12,14,15	0.96	0	18,21,23	1.66	5 (27%)
3	A1H03	sB	4	3	13,13,14	0.70	0	16,18,20	0.91	1 (6%)
3	MAN	sB	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
3	GAL	t	1	3,1	11,11,12	0.65	0	15,15,17	1.01	1 (6%)
3	BGC	t	2	3	11,11,12	0.59	0	15,15,17	1.38	3 (20%)
3	A1H1F	t	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	t	4	3	13,13,14	0.70	0	16,18,20	0.89	1 (6%)
3	MAN	t	5	3	11,11,12	0.65	0	15,15,17	1.13	1 (6%)
4	GAL	tA	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	tA	2	4	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
4	A1H1F	tA	3	4	12,14,15	0.87	0	18,21,23	2.17	4 (22%)
4	MAN	tA	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	tB	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	tB	2	3	11,11,12	0.61	0	15,15,17	1.38	3 (20%)
3	A1H1F	tB	3	3	12,14,15	0.88	0	18,21,23	1.50	3 (16%)
3	A1H03	tB	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	tB	5	3	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
3	GAL	tC	1	3,1	11,11,12	0.67	0	15,15,17	1.13	2 (13%)
3	BGC	tC	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	tC	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	tC	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	tC	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
4	GAL	u	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)
4	BGC	u	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	u	3	4	12,14,15	0.76	0	18,21,23	1.26	3 (16%)
4	MAN	u	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	uA	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	uA	2	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
3	A1H1F	uA	3	3	12,14,15	0.88	0	18,21,23	1.22	2 (11%)
3	A1H03	uA	4	3	13,13,14	0.70	0	16,18,20	0.88	1 (6%)
3	MAN	uA	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
4	GAL	uB	1	1,4	11,11,12	0.69	0	15,15,17	1.14	2 (13%)
4	BGC	uB	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	uB	3	4	12,14,15	0.86	0	18,21,23	2.16	4 (22%)
4	MAN	uB	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
3	GAL	uC	1	3,1	11,11,12	0.61	0	15,15,17	0.87	0
3	BGC	uC	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	uC	3	3	12,14,15	0.89	0	18,21,23	1.51	3 (16%)
3	A1H03	uC	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	uC	5	3	11,11,12	0.61	0	15,15,17	1.15	1 (6%)
2	GAL	v	1	2,1	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
2	BGC	v	2	2	11,11,12	0.65	0	15,15,17	1.17	2 (13%)
2	A1H1F	v	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	v	4	2	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
2	MAN	v	5	2	11,11,12	0.64	0	15,15,17	1.79	2 (13%)
2	A1H03	v	6	2	13,13,14	0.81	0	16,18,20	1.00	2 (12%)
4	GAL	vA	1	1,4	11,11,12	0.64	0	15,15,17	1.31	2 (13%)
4	BGC	vA	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	vA	3	4	12,14,15	0.76	0	18,21,23	1.25	3 (16%)
4	MAN	vA	4	4	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
3	GAL	vB	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	vB	2	3	11,11,12	0.59	0	15,15,17	1.37	3 (20%)
3	A1H1F	vB	3	3	12,14,15	0.88	0	18,21,23	1.23	2 (11%)
3	A1H03	vB	4	3	13,13,14	0.70	0	16,18,20	0.89	1 (6%)
3	MAN	vB	5	3	11,11,12	0.64	0	15,15,17	1.12	1 (6%)
4	GAL	vC	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	vC	2	4	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
4	A1H1F	vC	3	4	12,14,15	0.86	0	18,21,23	2.16	4 (22%)
4	MAN	vC	4	4	11,11,12	0.63	0	15,15,17	1.37	2 (13%)
2	GAL	wA	1	2,1	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
2	BGC	wA	2	2	11,11,12	0.64	0	15,15,17	1.17	2 (13%)
2	A1H1F	wA	3	2	12,14,15	0.84	0	18,21,23	1.27	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	wA	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	wA	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	wA	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	wB	1	1,4	11,11,12	0.66	0	15,15,17	1.29	2 (13%)
4	BGC	wB	2	4	11,11,12	0.57	0	15,15,17	1.02	2 (13%)
4	A1H1F	wB	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	wB	4	4	11,11,12	0.58	0	15,15,17	1.15	1 (6%)
3	GAL	wC	1	3,1	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
3	BGC	wC	2	3	11,11,12	0.60	0	15,15,17	1.38	3 (20%)
3	A1H1F	wC	3	3	12,14,15	0.89	0	18,21,23	1.22	2 (11%)
3	A1H03	wC	4	3	13,13,14	0.70	0	16,18,20	0.88	1 (6%)
3	MAN	wC	5	3	11,11,12	0.63	0	15,15,17	1.12	1 (6%)
3	GAL	x	1	3,1	11,11,12	0.65	0	15,15,17	1.14	2 (13%)
3	BGC	x	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	x	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	x	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	x	5	3	11,11,12	0.64	0	15,15,17	1.36	2 (13%)
2	GAL	xB	1	2,1	11,11,12	0.66	0	15,15,17	0.98	1 (6%)
2	BGC	xB	2	2	11,11,12	0.64	0	15,15,17	1.16	2 (13%)
2	A1H1F	xB	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	xB	4	2	11,11,12	0.61	0	15,15,17	1.38	1 (6%)
2	MAN	xB	5	2	11,11,12	0.64	0	15,15,17	1.79	2 (13%)
2	A1H03	xB	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	xC	1	1,4	11,11,12	0.66	0	15,15,17	1.30	2 (13%)
4	BGC	xC	2	4	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
4	A1H1F	xC	3	4	12,14,15	0.77	0	18,21,23	1.25	3 (16%)
4	MAN	xC	4	4	11,11,12	0.58	0	15,15,17	1.15	1 (6%)
3	GAL	y	1	3,1	11,11,12	0.60	0	15,15,17	0.87	0
3	BGC	y	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	y	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	y	4	3	13,13,14	0.69	0	16,18,20	0.98	2 (12%)
3	MAN	y	5	3	11,11,12	0.61	0	15,15,17	1.14	1 (6%)
3	GAL	yA	1	3,1	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
3	BGC	yA	2	3	11,11,12	0.60	0	15,15,17	1.20	2 (13%)
3	A1H1F	yA	3	3	12,14,15	0.96	0	18,21,23	1.65	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1H03	yA	4	3	13,13,14	0.71	0	16,18,20	0.91	1 (6%)
3	MAN	yA	5	3	11,11,12	0.65	0	15,15,17	1.37	2 (13%)
2	GAL	yC	1	2,1	11,11,12	0.66	0	15,15,17	0.97	1 (6%)
2	BGC	yC	2	2	11,11,12	0.65	0	15,15,17	1.16	2 (13%)
2	A1H1F	yC	3	2	12,14,15	0.83	0	18,21,23	1.27	3 (16%)
2	MAN	yC	4	2	11,11,12	0.62	0	15,15,17	1.38	1 (6%)
2	MAN	yC	5	2	11,11,12	0.64	0	15,15,17	1.78	2 (13%)
2	A1H03	yC	6	2	13,13,14	0.79	0	16,18,20	1.00	2 (12%)
4	GAL	z	1	1,4	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
4	BGC	z	2	4	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
4	A1H1F	z	3	4	12,14,15	0.87	0	18,21,23	2.16	4 (22%)
4	MAN	z	4	4	11,11,12	0.63	0	15,15,17	1.36	2 (13%)
3	GAL	zA	1	3,1	11,11,12	0.61	0	15,15,17	0.86	0
3	BGC	zA	2	3	11,11,12	0.61	0	15,15,17	1.37	3 (20%)
3	A1H1F	zA	3	3	12,14,15	0.88	0	18,21,23	1.51	3 (16%)
3	A1H03	zA	4	3	13,13,14	0.70	0	16,18,20	0.98	2 (12%)
3	MAN	zA	5	3	11,11,12	0.60	0	15,15,17	1.14	1 (6%)
3	GAL	zB	1	3,1	11,11,12	0.66	0	15,15,17	1.12	2 (13%)
3	BGC	zB	2	3	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
3	A1H1F	zB	3	3	12,14,15	0.95	0	18,21,23	1.66	5 (27%)
3	A1H03	zB	4	3	13,13,14	0.71	0	16,18,20	0.92	1 (6%)
3	MAN	zB	5	3	11,11,12	0.64	0	15,15,17	1.37	2 (13%)

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
3	GAL	0	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	0	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	0	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	0	4	3	-	3/6/23/26	0/1/1/1
3	MAN	0	5	3	-	1/2/19/22	0/1/1/1
4	GAL	0A	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	0A	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	0A	3	4	-	0/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	0A	4	4	-	2/2/19/22	0/1/1/1
3	GAL	0B	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	0B	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	0B	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	0B	4	3	-	0/6/23/26	0/1/1/1
3	MAN	0B	5	3	-	2/2/19/22	0/1/1/1
3	GAL	0C	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	0C	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	0C	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	0C	4	3	-	3/6/23/26	0/1/1/1
3	MAN	0C	5	3	-	1/2/19/22	0/1/1/1
4	GAL	1	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	1	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	1	3	4	-	1/5/22/25	0/1/1/1
4	MAN	1	4	4	-	2/2/19/22	0/1/1/1
3	GAL	1A	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	1A	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	1A	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	1A	4	3	-	3/6/23/26	0/1/1/1
3	MAN	1A	5	3	-	1/2/19/22	0/1/1/1
4	GAL	1B	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	1B	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	1B	3	4	-	0/5/22/25	0/1/1/1
4	MAN	1B	4	4	-	2/2/19/22	0/1/1/1
3	GAL	1C	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	1C	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	1C	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	1C	4	3	-	0/6/23/26	0/1/1/1
3	MAN	1C	5	3	-	2/2/19/22	0/1/1/1
2	GAL	2	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	2	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	2	3	2	-	2/5/22/25	0/1/1/1
2	MAN	2	4	2	-	0/2/19/22	0/1/1/1
2	MAN	2	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	2	6	2	-	2/6/23/26	0/1/1/1
4	GAL	2A	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	2A	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	2A	3	4	-	1/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	2A	4	4	-	2/2/19/22	0/1/1/1
3	GAL	2B	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	2B	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	2B	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	2B	4	3	-	3/6/23/26	0/1/1/1
3	MAN	2B	5	3	-	1/2/19/22	0/1/1/1
4	GAL	2C	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	2C	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	2C	3	4	-	0/5/22/25	0/1/1/1
4	MAN	2C	4	4	-	2/2/19/22	0/1/1/1
2	GAL	3A	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	3A	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	3A	3	2	-	2/5/22/25	0/1/1/1
2	MAN	3A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	3A	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	3A	6	2	-	2/6/23/26	0/1/1/1
4	GAL	3B	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	3B	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	3B	3	4	-	1/5/22/25	0/1/1/1
4	MAN	3B	4	4	-	2/2/19/22	0/1/1/1
3	GAL	3C	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	3C	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	3C	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	3C	4	3	-	3/6/23/26	0/1/1/1
3	MAN	3C	5	3	-	1/2/19/22	0/1/1/1
3	GAL	4	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	4	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	4	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	4	4	3	-	3/6/23/26	0/1/1/1
3	MAN	4	5	3	-	1/2/19/22	0/1/1/1
2	GAL	4B	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	4B	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	4B	3	2	-	2/5/22/25	0/1/1/1
2	MAN	4B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	4B	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	4B	6	2	-	2/6/23/26	0/1/1/1
4	GAL	4C	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	4C	2	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1H1F	4C	3	4	-	1/5/22/25	0/1/1/1
4	MAN	4C	4	4	-	2/2/19/22	0/1/1/1
3	GAL	5	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	5	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	5	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	5	4	3	-	0/6/23/26	0/1/1/1
3	MAN	5	5	3	-	2/2/19/22	0/1/1/1
3	GAL	5A	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	5A	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	5A	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	5A	4	3	-	2/6/23/26	0/1/1/1
3	MAN	5A	5	3	-	1/2/19/22	0/1/1/1
2	GAL	5C	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	5C	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	5C	3	2	-	2/5/22/25	0/1/1/1
2	MAN	5C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	5C	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	5C	6	2	-	2/6/23/26	0/1/1/1
4	GAL	6	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	6	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	6	3	4	-	0/5/22/25	0/1/1/1
4	MAN	6	4	4	-	2/2/19/22	0/1/1/1
3	GAL	6A	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	6A	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	6A	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	6A	4	3	-	0/6/23/26	0/1/1/1
3	MAN	6A	5	3	-	2/2/19/22	0/1/1/1
3	GAL	6B	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	6B	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	6B	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	6B	4	3	-	3/6/23/26	0/1/1/1
3	MAN	6B	5	3	-	1/2/19/22	0/1/1/1
3	GAL	7	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	7	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	7	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	7	4	3	-	3/6/23/26	0/1/1/1
3	MAN	7	5	3	-	1/2/19/22	0/1/1/1
4	GAL	7A	1	1,4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	7A	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	7A	3	4	-	0/5/22/25	0/1/1/1
4	MAN	7A	4	4	-	2/2/19/22	0/1/1/1
3	GAL	7B	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	7B	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	7B	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	7B	4	3	-	0/6/23/26	0/1/1/1
3	MAN	7B	5	3	-	2/2/19/22	0/1/1/1
3	GAL	7C	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	7C	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	7C	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	7C	4	3	-	3/6/23/26	0/1/1/1
3	MAN	7C	5	3	-	1/2/19/22	0/1/1/1
4	GAL	8	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	8	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	8	3	4	-	1/5/22/25	0/1/1/1
4	MAN	8	4	4	-	2/2/19/22	0/1/1/1
3	GAL	8A	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	8A	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	8A	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	8A	4	3	-	3/6/23/26	0/1/1/1
3	MAN	8A	5	3	-	1/2/19/22	0/1/1/1
4	GAL	8B	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	8B	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	8B	3	4	-	0/5/22/25	0/1/1/1
4	MAN	8B	4	4	-	2/2/19/22	0/1/1/1
3	GAL	8C	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	8C	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	8C	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	8C	4	3	-	0/6/23/26	0/1/1/1
3	MAN	8C	5	3	-	2/2/19/22	0/1/1/1
2	GAL	9	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	9	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	9	3	2	-	2/5/22/25	0/1/1/1
2	MAN	9	4	2	-	0/2/19/22	0/1/1/1
2	MAN	9	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	9	6	2	-	2/6/23/26	0/1/1/1
4	GAL	9A	1	1,4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	9A	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	9A	3	4	-	1/5/22/25	0/1/1/1
4	MAN	9A	4	4	-	2/2/19/22	0/1/1/1
3	GAL	9B	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	9B	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	9B	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	9B	4	3	-	3/6/23/26	0/1/1/1
3	MAN	9B	5	3	-	1/2/19/22	0/1/1/1
4	GAL	9C	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	9C	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	9C	3	4	-	0/5/22/25	0/1/1/1
4	MAN	9C	4	4	-	2/2/19/22	0/1/1/1
2	GAL	AB	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	AB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	AB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	AB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	AB	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	AB	6	2	-	2/6/23/26	0/1/1/1
4	GAL	AC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	AC	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	AC	3	4	-	1/5/22/25	0/1/1/1
4	MAN	AC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	AD	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	AD	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	AD	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	AD	4	3	-	3/6/23/26	0/1/1/1
3	MAN	AD	5	3	-	1/2/19/22	0/1/1/1
3	GAL	BA	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	BA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	BA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	BA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	BA	5	3	-	1/2/19/22	0/1/1/1
2	GAL	BC	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	BC	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	BC	3	2	-	2/5/22/25	0/1/1/1
2	MAN	BC	4	2	-	0/2/19/22	0/1/1/1
2	MAN	BC	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	BC	6	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	BD	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	BD	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	BD	3	4	-	1/5/22/25	0/1/1/1
4	MAN	BD	4	4	-	2/2/19/22	0/1/1/1
3	GAL	CA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	CA	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	CA	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	CA	4	3	-	0/6/23/26	0/1/1/1
3	MAN	CA	5	3	-	2/2/19/22	0/1/1/1
3	GAL	CB	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	CB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	CB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	CB	4	3	-	2/6/23/26	0/1/1/1
3	MAN	CB	5	3	-	1/2/19/22	0/1/1/1
2	GAL	CD	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	CD	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	CD	3	2	-	2/5/22/25	0/1/1/1
2	MAN	CD	4	2	-	0/2/19/22	0/1/1/1
2	MAN	CD	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	CD	6	2	-	2/6/23/26	0/1/1/1
4	GAL	DA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	DA	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	DA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	DA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	DB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	DB	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	DB	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	DB	4	3	-	0/6/23/26	0/1/1/1
3	MAN	DB	5	3	-	2/2/19/22	0/1/1/1
3	GAL	DC	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	DC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	DC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	DC	4	3	-	2/6/23/26	0/1/1/1
3	MAN	DC	5	3	-	1/2/19/22	0/1/1/1
3	GAL	EA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	EA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	EA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	EA	4	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	EA	5	3	-	1/2/19/22	0/1/1/1
4	GAL	EB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	EB	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	EB	3	4	-	0/5/22/25	0/1/1/1
4	MAN	EB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	EC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	EC	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	EC	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	EC	4	3	-	0/6/23/26	0/1/1/1
3	MAN	EC	5	3	-	2/2/19/22	0/1/1/1
3	GAL	ED	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	ED	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	ED	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	ED	4	3	-	3/6/23/26	0/1/1/1
3	MAN	ED	5	3	-	1/2/19/22	0/1/1/1
4	GAL	FA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	FA	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	FA	3	4	-	1/5/22/25	0/1/1/1
4	MAN	FA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	FB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	FB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	FB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	FB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	FB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	FC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	FC	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	FC	3	4	-	0/5/22/25	0/1/1/1
4	MAN	FC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	FD	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	FD	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	FD	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	FD	4	3	-	0/6/23/26	0/1/1/1
3	MAN	FD	5	3	-	2/2/19/22	0/1/1/1
2	GAL	GA	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	GA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	GA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	GA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	GA	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	GA	6	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	GB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	GB	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	GB	3	4	-	1/5/22/25	0/1/1/1
4	MAN	GB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	GC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	GC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	GC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	GC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	GC	5	3	-	1/2/19/22	0/1/1/1
4	GAL	GD	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	GD	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	GD	3	4	-	0/5/22/25	0/1/1/1
4	MAN	GD	4	4	-	2/2/19/22	0/1/1/1
2	GAL	HB	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	HB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	HB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	HB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	HB	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	HB	6	2	-	2/6/23/26	0/1/1/1
4	GAL	HC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	HC	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	HC	3	4	-	1/5/22/25	0/1/1/1
4	MAN	HC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	HD	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	HD	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	HD	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	HD	4	3	-	3/6/23/26	0/1/1/1
3	MAN	HD	5	3	-	1/2/19/22	0/1/1/1
3	GAL	IA	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	IA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	IA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	IA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	IA	5	3	-	1/2/19/22	0/1/1/1
2	GAL	IC	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	IC	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	IC	3	2	-	2/5/22/25	0/1/1/1
2	MAN	IC	4	2	-	0/2/19/22	0/1/1/1
2	MAN	IC	5	2	-	0/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H03	IC	6	2	-	2/6/23/26	0/1/1/1
4	GAL	ID	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	ID	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	ID	3	4	-	1/5/22/25	0/1/1/1
4	MAN	ID	4	4	-	2/2/19/22	0/1/1/1
3	GAL	JA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	JA	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	JA	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	JA	4	3	-	0/6/23/26	0/1/1/1
3	MAN	JA	5	3	-	2/2/19/22	0/1/1/1
3	GAL	JB	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	JB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	JB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	JB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	JB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	KA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	KA	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	KA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	KA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	KB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	KB	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	KB	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	KB	4	3	-	0/6/23/26	0/1/1/1
3	MAN	KB	5	3	-	2/2/19/22	0/1/1/1
3	GAL	KC	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	KC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	KC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	KC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	KC	5	3	-	1/2/19/22	0/1/1/1
3	GAL	LA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	LA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	LA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	LA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	LA	5	3	-	1/2/19/22	0/1/1/1
4	GAL	LB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	LB	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	LB	3	4	-	0/5/22/25	0/1/1/1
4	MAN	LB	4	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	LC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	LC	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	LC	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	LC	4	3	-	0/6/23/26	0/1/1/1
3	MAN	LC	5	3	-	2/2/19/22	0/1/1/1
4	GAL	MA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	MA	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	MA	3	4	-	1/5/22/25	0/1/1/1
4	MAN	MA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	MB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	MB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	MB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	MB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	MB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	MC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	MC	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	MC	3	4	-	0/5/22/25	0/1/1/1
4	MAN	MC	4	4	-	2/2/19/22	0/1/1/1
2	GAL	NA	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	NA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	NA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	NA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	NA	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	NA	6	2	-	2/6/23/26	0/1/1/1
4	GAL	NB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	NB	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	NB	3	4	-	1/5/22/25	0/1/1/1
4	MAN	NB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	NC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	NC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	NC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	NC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	NC	5	3	-	1/2/19/22	0/1/1/1
2	GAL	OB	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	OB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	OB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	OB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	OB	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	OB	6	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	OC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	OC	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	OC	3	4	-	1/5/22/25	0/1/1/1
4	MAN	OC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	PA	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	PA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	PA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	PA	4	3	-	2/6/23/26	0/1/1/1
3	MAN	PA	5	3	-	1/2/19/22	0/1/1/1
2	GAL	PC	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	PC	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	PC	3	2	-	2/5/22/25	0/1/1/1
2	MAN	PC	4	2	-	0/2/19/22	0/1/1/1
2	MAN	PC	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	PC	6	2	-	2/6/23/26	0/1/1/1
3	GAL	QA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	QA	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	QA	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	QA	4	3	-	0/6/23/26	0/1/1/1
3	MAN	QA	5	3	-	2/2/19/22	0/1/1/1
3	GAL	QB	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	QB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	QB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	QB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	QB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	RA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	RA	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	RA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	RA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	RB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	RB	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	RB	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	RB	4	3	-	0/6/23/26	0/1/1/1
3	MAN	RB	5	3	-	2/2/19/22	0/1/1/1
3	GAL	RC	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	RC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	RC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	RC	4	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	RC	5	3	-	1/2/19/22	0/1/1/1
3	GAL	SA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	SA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	SA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	SA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	SA	5	3	-	1/2/19/22	0/1/1/1
4	GAL	SB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	SB	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	SB	3	4	-	0/5/22/25	0/1/1/1
4	MAN	SB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	SC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	SC	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	SC	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	SC	4	3	-	0/6/23/26	0/1/1/1
3	MAN	SC	5	3	-	2/2/19/22	0/1/1/1
4	GAL	TA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	TA	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	TA	3	4	-	1/5/22/25	0/1/1/1
4	MAN	TA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	TB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	TB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	TB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	TB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	TB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	TC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	TC	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	TC	3	4	-	0/5/22/25	0/1/1/1
4	MAN	TC	4	4	-	2/2/19/22	0/1/1/1
2	GAL	UA	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	UA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	UA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	UA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	UA	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	UA	6	2	-	2/6/23/26	0/1/1/1
4	GAL	UB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	UB	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	UB	3	4	-	1/5/22/25	0/1/1/1
4	MAN	UB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	UC	1	3,1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	UC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	UC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	UC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	UC	5	3	-	1/2/19/22	0/1/1/1
2	GAL	VB	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	VB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	VB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	VB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	VB	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	VB	6	2	-	2/6/23/26	0/1/1/1
4	GAL	VC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	VC	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	VC	3	4	-	1/5/22/25	0/1/1/1
4	MAN	VC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	WA	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	WA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	WA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	WA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	WA	5	3	-	1/2/19/22	0/1/1/1
2	GAL	WC	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	WC	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	WC	3	2	-	2/5/22/25	0/1/1/1
2	MAN	WC	4	2	-	0/2/19/22	0/1/1/1
2	MAN	WC	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	WC	6	2	-	2/6/23/26	0/1/1/1
3	GAL	XA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	XA	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	XA	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	XA	4	3	-	0/6/23/26	0/1/1/1
3	MAN	XA	5	3	-	2/2/19/22	0/1/1/1
3	GAL	XB	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	XB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	XB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	XB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	XB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	YA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	YA	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	YA	3	4	-	0/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	YA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	YB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	YB	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	YB	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	YB	4	3	-	0/6/23/26	0/1/1/1
3	MAN	YB	5	3	-	2/2/19/22	0/1/1/1
3	GAL	YC	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	YC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	YC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	YC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	YC	5	3	-	1/2/19/22	0/1/1/1
3	GAL	ZA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	ZA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	ZA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	ZA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	ZA	5	3	-	1/2/19/22	0/1/1/1
4	GAL	ZB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	ZB	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	ZB	3	4	-	0/5/22/25	0/1/1/1
4	MAN	ZB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	ZC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	ZC	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	ZC	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	ZC	4	3	-	0/6/23/26	0/1/1/1
3	MAN	ZC	5	3	-	2/2/19/22	0/1/1/1
4	GAL	aA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	aA	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	aA	3	4	-	1/5/22/25	0/1/1/1
4	MAN	aA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	aB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	aB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	aB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	aB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	aB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	aC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	aC	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	aC	3	4	-	0/5/22/25	0/1/1/1
4	MAN	aC	4	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	bA	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	bA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	bA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	bA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	bA	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	bA	6	2	-	2/6/23/26	0/1/1/1
4	GAL	bB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	bB	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	bB	3	4	-	1/5/22/25	0/1/1/1
4	MAN	bB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	bC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	bC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	bC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	bC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	bC	5	3	-	1/2/19/22	0/1/1/1
2	GAL	cB	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	cB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	cB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	cB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	cB	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	cB	6	2	-	2/6/23/26	0/1/1/1
4	GAL	cC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	cC	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	cC	3	4	-	1/5/22/25	0/1/1/1
4	MAN	cC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	dA	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	dA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	dA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	dA	4	3	-	2/6/23/26	0/1/1/1
3	MAN	dA	5	3	-	1/2/19/22	0/1/1/1
2	GAL	dC	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	dC	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	dC	3	2	-	2/5/22/25	0/1/1/1
2	MAN	dC	4	2	-	0/2/19/22	0/1/1/1
2	MAN	dC	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	dC	6	2	-	2/6/23/26	0/1/1/1
3	GAL	eA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	eA	2	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1H1F	eA	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	eA	4	3	-	0/6/23/26	0/1/1/1
3	MAN	eA	5	3	-	2/2/19/22	0/1/1/1
3	GAL	eB	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	eB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	eB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	eB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	eB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	fA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	fA	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	fA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	fA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	fB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	fB	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	fB	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	fB	4	3	-	0/6/23/26	0/1/1/1
3	MAN	fB	5	3	-	2/2/19/22	0/1/1/1
3	GAL	fC	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	fC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	fC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	fC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	fC	5	3	-	1/2/19/22	0/1/1/1
3	GAL	gA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	gA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	gA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	gA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	gA	5	3	-	1/2/19/22	0/1/1/1
4	GAL	gB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	gB	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	gB	3	4	-	0/5/22/25	0/1/1/1
4	MAN	gB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	gC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	gC	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	gC	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	gC	4	3	-	0/6/23/26	0/1/1/1
3	MAN	gC	5	3	-	2/2/19/22	0/1/1/1
2	GAL	h	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	h	2	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H1F	h	3	2	-	2/5/22/25	0/1/1/1
2	MAN	h	4	2	-	0/2/19/22	0/1/1/1
2	MAN	h	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	h	6	2	-	2/6/23/26	0/1/1/1
4	GAL	hA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	hA	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	hA	3	4	-	1/5/22/25	0/1/1/1
4	MAN	hA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	hB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	hB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	hB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	hB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	hB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	hC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	hC	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	hC	3	4	-	0/5/22/25	0/1/1/1
4	MAN	hC	4	4	-	2/2/19/22	0/1/1/1
2	GAL	iA	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	iA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	iA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	iA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	iA	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	iA	6	2	-	2/6/23/26	0/1/1/1
4	GAL	iB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	iB	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	iB	3	4	-	1/5/22/25	0/1/1/1
4	MAN	iB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	iC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	iC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	iC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	iC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	iC	5	3	-	1/2/19/22	0/1/1/1
3	GAL	j	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	j	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	j	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	j	4	3	-	3/6/23/26	0/1/1/1
3	MAN	j	5	3	-	1/2/19/22	0/1/1/1
2	GAL	jB	1	2,1	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	jB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	jB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	jB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	jB	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	jB	6	2	-	2/6/23/26	0/1/1/1
4	GAL	jC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	jC	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	jC	3	4	-	1/5/22/25	0/1/1/1
4	MAN	jC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	k	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	k	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	k	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	k	4	3	-	0/6/23/26	0/1/1/1
3	MAN	k	5	3	-	2/2/19/22	0/1/1/1
3	GAL	kA	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	kA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	kA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	kA	4	3	-	2/6/23/26	0/1/1/1
3	MAN	kA	5	3	-	1/2/19/22	0/1/1/1
2	GAL	kC	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	kC	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	kC	3	2	-	2/5/22/25	0/1/1/1
2	MAN	kC	4	2	-	0/2/19/22	0/1/1/1
2	MAN	kC	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	kC	6	2	-	2/6/23/26	0/1/1/1
4	GAL	l	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	l	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	l	3	4	-	0/5/22/25	0/1/1/1
4	MAN	l	4	4	-	2/2/19/22	0/1/1/1
3	GAL	lA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	lA	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	lA	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	lA	4	3	-	0/6/23/26	0/1/1/1
3	MAN	lA	5	3	-	2/2/19/22	0/1/1/1
3	GAL	lB	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	lB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	lB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	lB	4	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	lB	5	3	-	1/2/19/22	0/1/1/1
3	GAL	m	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	m	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	m	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	m	4	3	-	3/6/23/26	0/1/1/1
3	MAN	m	5	3	-	1/2/19/22	0/1/1/1
4	GAL	mA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	mA	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	mA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	mA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	mB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	mB	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	mB	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	mB	4	3	-	0/6/23/26	0/1/1/1
3	MAN	mB	5	3	-	2/2/19/22	0/1/1/1
3	GAL	mC	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	mC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	mC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	mC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	mC	5	3	-	1/2/19/22	0/1/1/1
4	GAL	n	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	n	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	n	3	4	-	1/5/22/25	0/1/1/1
4	MAN	n	4	4	-	2/2/19/22	0/1/1/1
3	GAL	nA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	nA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	nA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	nA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	nA	5	3	-	1/2/19/22	0/1/1/1
4	GAL	nB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	nB	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	nB	3	4	-	0/5/22/25	0/1/1/1
4	MAN	nB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	nC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	nC	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	nC	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	nC	4	3	-	0/6/23/26	0/1/1/1
3	MAN	nC	5	3	-	2/2/19/22	0/1/1/1
2	GAL	o	1	2,1	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	o	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	o	3	2	-	2/5/22/25	0/1/1/1
2	MAN	o	4	2	-	0/2/19/22	0/1/1/1
2	MAN	o	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	o	6	2	-	3/6/23/26	0/1/1/1
4	GAL	oA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	oA	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	oA	3	4	-	1/5/22/25	0/1/1/1
4	MAN	oA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	oB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	oB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	oB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	oB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	oB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	oC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	oC	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	oC	3	4	-	0/5/22/25	0/1/1/1
4	MAN	oC	4	4	-	2/2/19/22	0/1/1/1
2	GAL	pA	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	pA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	pA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	pA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	pA	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	pA	6	2	-	2/6/23/26	0/1/1/1
4	GAL	pB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	pB	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	pB	3	4	-	1/5/22/25	0/1/1/1
4	MAN	pB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	pC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	pC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	pC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	pC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	pC	5	3	-	1/2/19/22	0/1/1/1
3	GAL	q	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	q	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	q	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	q	4	3	-	3/6/23/26	0/1/1/1
3	MAN	q	5	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	qB	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	qB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	qB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	qB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	qB	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	qB	6	2	-	2/6/23/26	0/1/1/1
4	GAL	qC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	qC	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	qC	3	4	-	1/5/22/25	0/1/1/1
4	MAN	qC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	r	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	r	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	r	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	r	4	3	-	0/6/23/26	0/1/1/1
3	MAN	r	5	3	-	2/2/19/22	0/1/1/1
3	GAL	rA	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	rA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	rA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	rA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	rA	5	3	-	1/2/19/22	0/1/1/1
2	GAL	rC	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	rC	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	rC	3	2	-	2/5/22/25	0/1/1/1
2	MAN	rC	4	2	-	0/2/19/22	0/1/1/1
2	MAN	rC	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	rC	6	2	-	2/6/23/26	0/1/1/1
4	GAL	s	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	s	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	s	3	4	-	0/5/22/25	0/1/1/1
4	MAN	s	4	4	-	2/2/19/22	0/1/1/1
3	GAL	sA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	sA	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	sA	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	sA	4	3	-	0/6/23/26	0/1/1/1
3	MAN	sA	5	3	-	2/2/19/22	0/1/1/1
3	GAL	sB	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	sB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	sB	3	3	-	2/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1H03	sB	4	3	-	2/6/23/26	0/1/1/1
3	MAN	sB	5	3	-	1/2/19/22	0/1/1/1
3	GAL	t	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	t	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	t	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	t	4	3	-	3/6/23/26	0/1/1/1
3	MAN	t	5	3	-	1/2/19/22	0/1/1/1
4	GAL	tA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	tA	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	tA	3	4	-	0/5/22/25	0/1/1/1
4	MAN	tA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	tB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	tB	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	tB	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	tB	4	3	-	0/6/23/26	0/1/1/1
3	MAN	tB	5	3	-	2/2/19/22	0/1/1/1
3	GAL	tC	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	tC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	tC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	tC	4	3	-	2/6/23/26	0/1/1/1
3	MAN	tC	5	3	-	1/2/19/22	0/1/1/1
4	GAL	u	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	u	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	u	3	4	-	1/5/22/25	0/1/1/1
4	MAN	u	4	4	-	2/2/19/22	0/1/1/1
3	GAL	uA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	uA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	uA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	uA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	uA	5	3	-	1/2/19/22	0/1/1/1
4	GAL	uB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	uB	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	uB	3	4	-	0/5/22/25	0/1/1/1
4	MAN	uB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	uC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	uC	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	uC	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	uC	4	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	uC	5	3	-	2/2/19/22	0/1/1/1
2	GAL	v	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	v	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	v	3	2	-	2/5/22/25	0/1/1/1
2	MAN	v	4	2	-	0/2/19/22	0/1/1/1
2	MAN	v	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	v	6	2	-	2/6/23/26	0/1/1/1
4	GAL	vA	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	vA	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	vA	3	4	-	1/5/22/25	0/1/1/1
4	MAN	vA	4	4	-	2/2/19/22	0/1/1/1
3	GAL	vB	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	vB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	vB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	vB	4	3	-	3/6/23/26	0/1/1/1
3	MAN	vB	5	3	-	1/2/19/22	0/1/1/1
4	GAL	vC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	vC	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	vC	3	4	-	0/5/22/25	0/1/1/1
4	MAN	vC	4	4	-	2/2/19/22	0/1/1/1
2	GAL	wA	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	wA	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	wA	3	2	-	2/5/22/25	0/1/1/1
2	MAN	wA	4	2	-	0/2/19/22	0/1/1/1
2	MAN	wA	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	wA	6	2	-	2/6/23/26	0/1/1/1
4	GAL	wB	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	wB	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	wB	3	4	-	1/5/22/25	0/1/1/1
4	MAN	wB	4	4	-	2/2/19/22	0/1/1/1
3	GAL	wC	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	wC	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	wC	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	wC	4	3	-	3/6/23/26	0/1/1/1
3	MAN	wC	5	3	-	1/2/19/22	0/1/1/1
3	GAL	x	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	x	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	x	3	3	-	2/5/22/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1H03	x	4	3	-	3/6/23/26	0/1/1/1
3	MAN	x	5	3	-	1/2/19/22	0/1/1/1
2	GAL	xB	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	xB	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	xB	3	2	-	2/5/22/25	0/1/1/1
2	MAN	xB	4	2	-	0/2/19/22	0/1/1/1
2	MAN	xB	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	xB	6	2	-	2/6/23/26	0/1/1/1
4	GAL	xC	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	xC	2	4	-	2/2/19/22	0/1/1/1
4	A1H1F	xC	3	4	-	1/5/22/25	0/1/1/1
4	MAN	xC	4	4	-	2/2/19/22	0/1/1/1
3	GAL	y	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	y	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	y	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	y	4	3	-	0/6/23/26	0/1/1/1
3	MAN	y	5	3	-	2/2/19/22	0/1/1/1
3	GAL	yA	1	3,1	-	2/2/19/22	0/1/1/1
3	BGC	yA	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	yA	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	yA	4	3	-	3/6/23/26	0/1/1/1
3	MAN	yA	5	3	-	1/2/19/22	0/1/1/1
2	GAL	yC	1	2,1	-	1/2/19/22	0/1/1/1
2	BGC	yC	2	2	-	0/2/19/22	0/1/1/1
2	A1H1F	yC	3	2	-	2/5/22/25	0/1/1/1
2	MAN	yC	4	2	-	0/2/19/22	0/1/1/1
2	MAN	yC	5	2	-	0/2/19/22	1/1/1/1
2	A1H03	yC	6	2	-	2/6/23/26	0/1/1/1
4	GAL	z	1	1,4	-	1/2/19/22	0/1/1/1
4	BGC	z	2	4	-	0/2/19/22	0/1/1/1
4	A1H1F	z	3	4	-	0/5/22/25	0/1/1/1
4	MAN	z	4	4	-	2/2/19/22	0/1/1/1
3	GAL	zA	1	3,1	-	0/2/19/22	0/1/1/1
3	BGC	zA	2	3	-	2/2/19/22	0/1/1/1
3	A1H1F	zA	3	3	-	0/5/22/25	0/1/1/1
3	A1H03	zA	4	3	-	0/6/23/26	0/1/1/1
3	MAN	zA	5	3	-	2/2/19/22	0/1/1/1
3	GAL	zB	1	3,1	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	zB	2	3	-	0/2/19/22	0/1/1/1
3	A1H1F	zB	3	3	-	2/5/22/25	0/1/1/1
3	A1H03	zB	4	3	-	2/6/23/26	0/1/1/1
3	MAN	zB	5	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1861) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	DA	3	A1H1F	C1-O5-C5	6.65	121.09	112.19
4	6	3	A1H1F	C1-O5-C5	6.63	121.06	112.19
4	8B	3	A1H1F	C1-O5-C5	6.63	121.06	112.19
4	nB	3	A1H1F	C1-O5-C5	6.62	121.06	112.19
4	KA	3	A1H1F	C1-O5-C5	6.62	121.06	112.19
4	TC	3	A1H1F	C1-O5-C5	6.62	121.06	112.19
4	mA	3	A1H1F	C1-O5-C5	6.62	121.05	112.19
4	0A	3	A1H1F	C1-O5-C5	6.61	121.05	112.19
4	9C	3	A1H1F	C1-O5-C5	6.61	121.05	112.19
4	z	3	A1H1F	C1-O5-C5	6.61	121.05	112.19
4	tA	3	A1H1F	C1-O5-C5	6.61	121.05	112.19
4	1B	3	A1H1F	C1-O5-C5	6.61	121.05	112.19
4	EB	3	A1H1F	C1-O5-C5	6.60	121.04	112.19
4	MC	3	A1H1F	C1-O5-C5	6.60	121.03	112.19
4	SB	3	A1H1F	C1-O5-C5	6.60	121.03	112.19
4	vC	3	A1H1F	C1-O5-C5	6.60	121.03	112.19
4	GD	3	A1H1F	C1-O5-C5	6.60	121.03	112.19
4	2C	3	A1H1F	C1-O5-C5	6.59	121.02	112.19
4	l	3	A1H1F	C1-O5-C5	6.59	121.02	112.19
4	s	3	A1H1F	C1-O5-C5	6.59	121.02	112.19
4	gB	3	A1H1F	C1-O5-C5	6.59	121.02	112.19
4	fA	3	A1H1F	C1-O5-C5	6.59	121.01	112.19
4	YA	3	A1H1F	C1-O5-C5	6.59	121.01	112.19
4	7A	3	A1H1F	C1-O5-C5	6.59	121.01	112.19
4	RA	3	A1H1F	C1-O5-C5	6.58	121.01	112.19
4	FC	3	A1H1F	C1-O5-C5	6.58	121.01	112.19
4	ZB	3	A1H1F	C1-O5-C5	6.58	121.01	112.19
4	oC	3	A1H1F	C1-O5-C5	6.58	121.00	112.19
4	uB	3	A1H1F	C1-O5-C5	6.58	121.00	112.19
4	LB	3	A1H1F	C1-O5-C5	6.58	121.00	112.19
4	aC	3	A1H1F	C1-O5-C5	6.57	121.00	112.19
4	hC	3	A1H1F	C1-O5-C5	6.55	120.97	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	OB	5	MAN	C1-O5-C5	5.71	119.83	112.19
2	pA	5	MAN	C1-O5-C5	5.70	119.83	112.19
2	o	5	MAN	C1-O5-C5	5.70	119.82	112.19
2	IC	5	MAN	C1-O5-C5	5.70	119.82	112.19
2	v	5	MAN	C1-O5-C5	5.69	119.81	112.19
2	dC	5	MAN	C1-O5-C5	5.69	119.81	112.19
2	kC	5	MAN	C1-O5-C5	5.69	119.81	112.19
2	3A	5	MAN	C1-O5-C5	5.69	119.81	112.19
2	HB	5	MAN	C1-O5-C5	5.69	119.81	112.19
2	5C	5	MAN	C1-O5-C5	5.69	119.81	112.19
2	iA	5	MAN	C1-O5-C5	5.68	119.81	112.19
2	GA	5	MAN	C1-O5-C5	5.68	119.80	112.19
2	WC	5	MAN	C1-O5-C5	5.68	119.80	112.19
2	xB	5	MAN	C1-O5-C5	5.68	119.80	112.19
2	2	5	MAN	C1-O5-C5	5.67	119.79	112.19
2	BC	5	MAN	C1-O5-C5	5.67	119.79	112.19
2	h	5	MAN	C1-O5-C5	5.67	119.79	112.19
2	PC	5	MAN	C1-O5-C5	5.67	119.78	112.19
2	cB	5	MAN	C1-O5-C5	5.67	119.78	112.19
2	4B	5	MAN	C1-O5-C5	5.67	119.78	112.19
2	CD	5	MAN	C1-O5-C5	5.66	119.78	112.19
2	NA	5	MAN	C1-O5-C5	5.66	119.78	112.19
2	UA	5	MAN	C1-O5-C5	5.66	119.77	112.19
2	AB	5	MAN	C1-O5-C5	5.66	119.77	112.19
2	jB	5	MAN	C1-O5-C5	5.65	119.76	112.19
2	qB	5	MAN	C1-O5-C5	5.65	119.76	112.19
2	VB	5	MAN	C1-O5-C5	5.65	119.75	112.19
2	9	5	MAN	C1-O5-C5	5.64	119.75	112.19
2	wA	5	MAN	C1-O5-C5	5.64	119.75	112.19
2	rC	5	MAN	C1-O5-C5	5.64	119.74	112.19
2	yC	5	MAN	C1-O5-C5	5.64	119.74	112.19
2	bA	5	MAN	C1-O5-C5	5.63	119.73	112.19
2	AB	4	MAN	C1-O5-C5	4.51	118.23	112.19
2	NA	4	MAN	C1-O5-C5	4.50	118.22	112.19
2	IC	4	MAN	C1-O5-C5	4.49	118.20	112.19
2	iA	4	MAN	C1-O5-C5	4.48	118.19	112.19
2	xB	4	MAN	C1-O5-C5	4.48	118.19	112.19
2	dC	4	MAN	C1-O5-C5	4.48	118.19	112.19
2	9	4	MAN	C1-O5-C5	4.48	118.19	112.19
2	GA	4	MAN	C1-O5-C5	4.48	118.19	112.19
2	rC	4	MAN	C1-O5-C5	4.48	118.19	112.19
2	5C	4	MAN	C1-O5-C5	4.48	118.19	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	4	MAN	C1-O5-C5	4.48	118.19	112.19
2	UA	4	MAN	C1-O5-C5	4.48	118.18	112.19
2	3A	4	MAN	C1-O5-C5	4.47	118.18	112.19
2	HB	4	MAN	C1-O5-C5	4.47	118.18	112.19
2	qB	4	MAN	C1-O5-C5	4.47	118.17	112.19
2	wA	4	MAN	C1-O5-C5	4.47	118.17	112.19
2	yC	4	MAN	C1-O5-C5	4.47	118.17	112.19
2	bA	4	MAN	C1-O5-C5	4.46	118.17	112.19
2	pA	4	MAN	C1-O5-C5	4.46	118.17	112.19
2	h	4	MAN	C1-O5-C5	4.46	118.17	112.19
2	VB	4	MAN	C1-O5-C5	4.46	118.17	112.19
2	jB	4	MAN	C1-O5-C5	4.46	118.16	112.19
2	PC	4	MAN	C1-O5-C5	4.45	118.15	112.19
2	CD	4	MAN	C1-O5-C5	4.45	118.15	112.19
2	v	4	MAN	C1-O5-C5	4.45	118.15	112.19
2	o	4	MAN	C1-O5-C5	4.45	118.15	112.19
2	kC	4	MAN	C1-O5-C5	4.45	118.15	112.19
2	cB	4	MAN	C1-O5-C5	4.45	118.15	112.19
2	WC	4	MAN	C1-O5-C5	4.44	118.14	112.19
2	4B	4	MAN	C1-O5-C5	4.44	118.13	112.19
2	BC	4	MAN	C1-O5-C5	4.44	118.13	112.19
2	OB	4	MAN	C1-O5-C5	4.43	118.12	112.19
4	VC	4	MAN	C1-O5-C5	3.68	117.12	112.19
4	GB	4	MAN	C1-O5-C5	3.67	117.11	112.19
4	AC	4	MAN	C1-O5-C5	3.67	117.11	112.19
4	FA	4	MAN	C1-O5-C5	3.67	117.10	112.19
4	oA	4	MAN	C1-O5-C5	3.67	117.10	112.19
4	3B	4	MAN	C1-O5-C5	3.66	117.10	112.19
4	hA	4	MAN	C1-O5-C5	3.66	117.09	112.19
4	ID	4	MAN	C1-O5-C5	3.66	117.09	112.19
4	2A	4	MAN	C1-O5-C5	3.66	117.09	112.19
4	n	4	MAN	C1-O5-C5	3.65	117.07	112.19
4	u	4	MAN	C1-O5-C5	3.65	117.07	112.19
4	bB	4	MAN	C1-O5-C5	3.65	117.07	112.19
4	pB	4	MAN	C1-O5-C5	3.65	117.07	112.19
4	MA	4	MAN	C1-O5-C5	3.64	117.07	112.19
4	TA	4	MAN	C1-O5-C5	3.64	117.07	112.19
4	cC	4	MAN	C1-O5-C5	3.64	117.07	112.19
4	9A	4	MAN	C1-O5-C5	3.64	117.06	112.19
4	xC	4	MAN	C1-O5-C5	3.64	117.06	112.19
4	vA	4	MAN	C1-O5-C5	3.64	117.06	112.19
4	HC	4	MAN	C1-O5-C5	3.64	117.06	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	OC	4	MAN	C1-O5-C5	3.64	117.06	112.19
4	qC	4	MAN	C1-O5-C5	3.63	117.05	112.19
4	iB	4	MAN	C1-O5-C5	3.63	117.05	112.19
4	jC	4	MAN	C1-O5-C5	3.63	117.05	112.19
3	dA	3	A1H1F	C1-C2-C3	3.63	114.93	109.64
4	UB	4	MAN	C1-O5-C5	3.62	117.04	112.19
4	4C	4	MAN	C1-O5-C5	3.62	117.04	112.19
4	8	4	MAN	C1-O5-C5	3.62	117.04	112.19
4	1	4	MAN	C1-O5-C5	3.62	117.04	112.19
4	aA	4	MAN	C1-O5-C5	3.62	117.03	112.19
4	BD	4	MAN	C1-O5-C5	3.62	117.03	112.19
3	x	3	A1H1F	C1-C2-C3	3.62	114.91	109.64
3	eB	3	A1H1F	C1-C2-C3	3.62	114.91	109.64
3	RC	3	A1H1F	C1-C2-C3	3.61	114.90	109.64
3	4	3	A1H1F	C1-C2-C3	3.61	114.90	109.64
3	5A	3	A1H1F	C1-C2-C3	3.60	114.89	109.64
3	JB	3	A1H1F	C1-C2-C3	3.60	114.89	109.64
3	WA	3	A1H1F	C1-C2-C3	3.60	114.89	109.64
3	ED	3	A1H1F	C1-C2-C3	3.60	114.89	109.64
3	zB	3	A1H1F	C1-C2-C3	3.60	114.89	109.64
3	DC	3	A1H1F	C1-C2-C3	3.60	114.89	109.64
3	fC	3	A1H1F	C1-C2-C3	3.60	114.89	109.64
4	wB	4	MAN	C1-O5-C5	3.60	117.01	112.19
3	lB	3	A1H1F	C1-C2-C3	3.60	114.88	109.64
3	tC	3	A1H1F	C1-C2-C3	3.60	114.88	109.64
3	j	3	A1H1F	C1-C2-C3	3.60	114.88	109.64
3	q	3	A1H1F	C1-C2-C3	3.60	114.88	109.64
3	mC	3	A1H1F	C1-C2-C3	3.59	114.88	109.64
3	PA	3	A1H1F	C1-C2-C3	3.59	114.88	109.64
3	BA	3	A1H1F	C1-C2-C3	3.59	114.87	109.64
3	QB	3	A1H1F	C1-C2-C3	3.59	114.87	109.64
3	yA	3	A1H1F	C1-C2-C3	3.59	114.87	109.64
3	kA	3	A1H1F	C1-C2-C3	3.59	114.87	109.64
3	7C	3	A1H1F	C1-C2-C3	3.59	114.87	109.64
3	sB	3	A1H1F	C1-C2-C3	3.59	114.87	109.64
3	6B	3	A1H1F	C1-C2-C3	3.59	114.87	109.64
4	NB	4	MAN	C1-O5-C5	3.59	116.99	112.19
3	rA	3	A1H1F	C1-C2-C3	3.59	114.86	109.64
3	KC	3	A1H1F	C1-C2-C3	3.59	114.86	109.64
3	XB	3	A1H1F	C1-C2-C3	3.58	114.86	109.64
3	CB	3	A1H1F	C1-C2-C3	3.58	114.86	109.64
3	YC	3	A1H1F	C1-C2-C3	3.58	114.86	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	0C	3	A1H1F	C1-C2-C3	3.58	114.86	109.64
3	IA	3	A1H1F	C1-C2-C3	3.56	114.83	109.64
3	mB	5	MAN	C1-O5-C5	3.56	116.95	112.19
4	tA	3	A1H1F	C1-C2-C3	3.55	114.81	109.64
3	SC	5	MAN	C1-O5-C5	3.55	116.94	112.19
3	YB	5	MAN	C1-O5-C5	3.55	116.94	112.19
3	FD	5	MAN	C1-O5-C5	3.53	116.92	112.19
3	5	5	MAN	C1-O5-C5	3.53	116.92	112.19
3	sA	5	MAN	C1-O5-C5	3.53	116.92	112.19
3	fB	5	MAN	C1-O5-C5	3.53	116.92	112.19
3	0B	5	MAN	C1-O5-C5	3.53	116.92	112.19
4	oC	3	A1H1F	C1-C2-C3	3.53	114.78	109.64
3	QA	5	MAN	C1-O5-C5	3.53	116.91	112.19
3	gC	5	MAN	C1-O5-C5	3.53	116.91	112.19
4	gB	3	A1H1F	C1-C2-C3	3.52	114.77	109.64
3	KB	5	MAN	C1-O5-C5	3.52	116.90	112.19
3	CA	5	MAN	C1-O5-C5	3.52	116.90	112.19
3	6A	5	MAN	C1-O5-C5	3.52	116.90	112.19
3	XA	5	MAN	C1-O5-C5	3.51	116.90	112.19
3	DB	5	MAN	C1-O5-C5	3.51	116.90	112.19
3	LC	5	MAN	C1-O5-C5	3.51	116.90	112.19
3	uC	5	MAN	C1-O5-C5	3.51	116.90	112.19
4	MC	3	A1H1F	C1-C2-C3	3.51	114.76	109.64
4	6	3	A1H1F	C1-C2-C3	3.51	114.76	109.64
4	SB	3	A1H1F	C1-C2-C3	3.51	114.76	109.64
4	TC	3	A1H1F	C1-C2-C3	3.51	114.76	109.64
4	mA	3	A1H1F	C1-C2-C3	3.51	114.76	109.64
3	ZC	5	MAN	C1-O5-C5	3.51	116.89	112.19
3	k	5	MAN	C1-O5-C5	3.51	116.89	112.19
3	8C	5	MAN	C1-O5-C5	3.51	116.89	112.19
4	vC	3	A1H1F	C1-C2-C3	3.51	114.75	109.64
4	z	3	A1H1F	C1-C2-C3	3.51	114.75	109.64
4	1B	3	A1H1F	C1-C2-C3	3.51	114.75	109.64
4	ZB	3	A1H1F	C1-C2-C3	3.51	114.75	109.64
4	9C	3	A1H1F	C1-C2-C3	3.50	114.75	109.64
3	eA	5	MAN	C1-O5-C5	3.50	116.88	112.19
3	nC	5	MAN	C1-O5-C5	3.50	116.88	112.19
4	7A	3	A1H1F	C1-C2-C3	3.50	114.74	109.64
4	EB	3	A1H1F	C1-C2-C3	3.50	114.74	109.64
4	FC	3	A1H1F	C1-C2-C3	3.50	114.74	109.64
4	RA	3	A1H1F	C1-C2-C3	3.50	114.74	109.64
3	tB	5	MAN	C1-O5-C5	3.50	116.88	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7B	5	MAN	C1-O5-C5	3.50	116.88	112.19
4	GD	3	A1H1F	C1-C2-C3	3.50	114.74	109.64
4	2C	3	A1H1F	C1-C2-C3	3.50	114.74	109.64
3	1C	5	MAN	C1-O5-C5	3.50	116.87	112.19
4	l	3	A1H1F	C1-C2-C3	3.50	114.73	109.64
4	fA	3	A1H1F	C1-C2-C3	3.50	114.73	109.64
4	nB	3	A1H1F	C1-C2-C3	3.50	114.73	109.64
3	EC	5	MAN	C1-O5-C5	3.49	116.87	112.19
3	y	5	MAN	C1-O5-C5	3.49	116.87	112.19
4	DA	3	A1H1F	C1-C2-C3	3.49	114.73	109.64
4	aC	3	A1H1F	C1-C2-C3	3.49	114.73	109.64
3	r	5	MAN	C1-O5-C5	3.49	116.86	112.19
3	JA	5	MAN	C1-O5-C5	3.49	116.86	112.19
4	uB	3	A1H1F	C1-C2-C3	3.49	114.72	109.64
3	lA	5	MAN	C1-O5-C5	3.49	116.86	112.19
3	RB	5	MAN	C1-O5-C5	3.49	116.86	112.19
4	KA	3	A1H1F	C1-C2-C3	3.48	114.71	109.64
4	8B	3	A1H1F	C1-C2-C3	3.48	114.71	109.64
4	hC	3	A1H1F	C1-C2-C3	3.48	114.71	109.64
3	zA	5	MAN	C1-O5-C5	3.48	116.84	112.19
4	s	3	A1H1F	C1-C2-C3	3.47	114.70	109.64
4	LB	3	A1H1F	C1-C2-C3	3.47	114.70	109.64
4	YA	3	A1H1F	C1-C2-C3	3.47	114.70	109.64
3	uC	3	A1H1F	C1-O5-C5	3.47	116.83	112.19
3	7B	3	A1H1F	C1-O5-C5	3.47	116.83	112.19
3	y	3	A1H1F	C1-O5-C5	3.47	116.83	112.19
3	mB	3	A1H1F	C1-O5-C5	3.46	116.83	112.19
4	0A	3	A1H1F	C1-C2-C3	3.46	114.69	109.64
3	lA	3	A1H1F	C1-O5-C5	3.46	116.83	112.19
3	sA	3	A1H1F	C1-O5-C5	3.46	116.83	112.19
3	QA	3	A1H1F	C1-O5-C5	3.46	116.82	112.19
3	DB	3	A1H1F	C1-O5-C5	3.46	116.82	112.19
3	RB	3	A1H1F	C1-O5-C5	3.46	116.82	112.19
3	ZC	3	A1H1F	C1-O5-C5	3.45	116.82	112.19
3	zA	3	A1H1F	C1-O5-C5	3.45	116.81	112.19
3	YB	3	A1H1F	C1-O5-C5	3.44	116.80	112.19
3	6A	3	A1H1F	C1-O5-C5	3.44	116.80	112.19
3	8C	3	A1H1F	C1-O5-C5	3.44	116.80	112.19
3	fB	3	A1H1F	C1-O5-C5	3.44	116.79	112.19
3	FD	3	A1H1F	C1-O5-C5	3.44	116.79	112.19
3	k	3	A1H1F	C1-O5-C5	3.43	116.78	112.19
3	XA	3	A1H1F	C1-O5-C5	3.43	116.78	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EC	3	A1H1F	C1-O5-C5	3.43	116.78	112.19
3	nC	3	A1H1F	C1-O5-C5	3.43	116.78	112.19
3	5	3	A1H1F	C1-O5-C5	3.43	116.78	112.19
3	LC	3	A1H1F	C1-O5-C5	3.43	116.78	112.19
3	r	3	A1H1F	C1-O5-C5	3.43	116.78	112.19
3	KB	3	A1H1F	C1-O5-C5	3.42	116.77	112.19
3	JA	3	A1H1F	C1-O5-C5	3.42	116.77	112.19
3	CA	3	A1H1F	C1-O5-C5	3.42	116.77	112.19
3	tB	3	A1H1F	C1-O5-C5	3.41	116.76	112.19
3	1C	3	A1H1F	C1-O5-C5	3.41	116.76	112.19
3	eA	3	A1H1F	C1-O5-C5	3.41	116.76	112.19
3	0B	3	A1H1F	C1-O5-C5	3.41	116.75	112.19
3	SC	3	A1H1F	C1-O5-C5	3.41	116.75	112.19
3	gC	3	A1H1F	C1-O5-C5	3.40	116.74	112.19
3	sB	3	A1H1F	C1-O5-C5	3.37	116.70	112.19
3	6B	3	A1H1F	C1-O5-C5	3.36	116.69	112.19
3	RC	3	A1H1F	C1-O5-C5	3.35	116.68	112.19
3	tC	3	A1H1F	C1-O5-C5	3.35	116.68	112.19
3	rA	3	A1H1F	C1-O5-C5	3.35	116.68	112.19
3	KC	3	A1H1F	C1-O5-C5	3.35	116.68	112.19
3	4	3	A1H1F	C1-O5-C5	3.35	116.68	112.19
4	jC	1	GAL	C1-C2-C3	3.35	114.53	109.64
3	kA	3	A1H1F	C1-O5-C5	3.35	116.68	112.19
3	SA	2	BGC	C1-O5-C5	3.35	116.68	112.19
3	fC	3	A1H1F	C1-O5-C5	3.35	116.67	112.19
4	HC	1	GAL	C1-C2-C3	3.35	114.52	109.64
3	JB	3	A1H1F	C1-O5-C5	3.35	116.67	112.19
3	pC	2	BGC	C1-O5-C5	3.35	116.67	112.19
4	AC	1	GAL	C1-C2-C3	3.35	114.52	109.64
4	FA	1	GAL	C1-C2-C3	3.34	114.51	109.64
4	oA	1	GAL	C1-C2-C3	3.34	114.51	109.64
3	BA	3	A1H1F	C1-O5-C5	3.34	116.67	112.19
3	mC	3	A1H1F	C1-O5-C5	3.34	116.66	112.19
3	3C	2	BGC	C1-O5-C5	3.34	116.66	112.19
4	BD	1	GAL	C1-C2-C3	3.34	114.51	109.64
3	WA	3	A1H1F	C1-O5-C5	3.34	116.66	112.19
3	1A	2	BGC	C1-O5-C5	3.34	116.66	112.19
4	pB	1	GAL	C1-C2-C3	3.34	114.50	109.64
3	XB	3	A1H1F	C1-O5-C5	3.34	116.66	112.19
3	GC	2	BGC	C1-O5-C5	3.34	116.66	112.19
3	j	3	A1H1F	C1-O5-C5	3.34	116.66	112.19
4	OC	1	GAL	C1-C2-C3	3.34	114.50	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	YC	3	A1H1F	C1-O5-C5	3.34	116.66	112.19
3	UC	2	BGC	C1-O5-C5	3.34	116.66	112.19
4	1	1	GAL	C1-C2-C3	3.33	114.50	109.64
3	5A	3	A1H1F	C1-O5-C5	3.33	116.66	112.19
3	wC	2	BGC	C1-O5-C5	3.33	116.65	112.19
3	CB	3	A1H1F	C1-O5-C5	3.33	116.65	112.19
3	7C	3	A1H1F	C1-O5-C5	3.33	116.65	112.19
4	MA	1	GAL	C1-C2-C3	3.33	114.49	109.64
4	TA	1	GAL	C1-C2-C3	3.33	114.49	109.64
3	x	3	A1H1F	C1-O5-C5	3.33	116.65	112.19
4	cC	1	GAL	C1-C2-C3	3.33	114.49	109.64
3	HD	2	BGC	C1-O5-C5	3.33	116.65	112.19
3	7	2	BGC	C1-O5-C5	3.33	116.65	112.19
3	DC	3	A1H1F	C1-O5-C5	3.33	116.65	112.19
3	0C	3	A1H1F	C1-O5-C5	3.33	116.65	112.19
4	vA	1	GAL	C1-C2-C3	3.33	114.49	109.64
4	u	1	GAL	C1-C2-C3	3.33	114.49	109.64
3	PA	3	A1H1F	C1-O5-C5	3.33	116.64	112.19
4	VC	1	GAL	C1-C2-C3	3.33	114.49	109.64
4	9A	1	GAL	C1-C2-C3	3.33	114.49	109.64
4	3B	1	GAL	C1-C2-C3	3.33	114.49	109.64
4	xC	1	GAL	C1-C2-C3	3.33	114.49	109.64
4	4C	1	GAL	C1-C2-C3	3.33	114.49	109.64
3	eB	3	A1H1F	C1-O5-C5	3.32	116.64	112.19
3	iC	2	BGC	C1-O5-C5	3.32	116.64	112.19
3	dA	3	A1H1F	C1-O5-C5	3.32	116.64	112.19
3	q	3	A1H1F	C1-O5-C5	3.32	116.64	112.19
3	lB	3	A1H1F	C1-O5-C5	3.32	116.64	112.19
3	ED	3	A1H1F	C1-O5-C5	3.32	116.64	112.19
4	n	1	GAL	C1-C2-C3	3.32	114.48	109.64
4	GB	1	GAL	C1-C2-C3	3.32	114.48	109.64
4	qC	1	GAL	C1-C2-C3	3.32	114.48	109.64
3	QB	3	A1H1F	C1-O5-C5	3.32	116.64	112.19
4	NB	1	GAL	C1-C2-C3	3.32	114.48	109.64
4	ID	1	GAL	C1-C2-C3	3.32	114.47	109.64
3	NC	2	BGC	C1-O5-C5	3.32	116.63	112.19
4	8	1	GAL	C1-C2-C3	3.32	114.47	109.64
3	m	2	BGC	C1-O5-C5	3.32	116.63	112.19
3	FB	2	BGC	C1-O5-C5	3.32	116.63	112.19
3	zB	3	A1H1F	C1-O5-C5	3.32	116.63	112.19
3	gA	2	BGC	C1-O5-C5	3.31	116.63	112.19
3	nA	2	BGC	C1-O5-C5	3.31	116.63	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	oB	2	BGC	C1-O5-C5	3.31	116.63	112.19
3	9B	2	BGC	C1-O5-C5	3.31	116.63	112.19
4	hA	1	GAL	C1-C2-C3	3.31	114.47	109.64
4	bB	1	GAL	C1-C2-C3	3.31	114.47	109.64
3	yA	3	A1H1F	C1-O5-C5	3.31	116.62	112.19
3	8A	2	BGC	C1-O5-C5	3.31	116.62	112.19
3	vB	2	BGC	C1-O5-C5	3.31	116.62	112.19
4	aA	1	GAL	C1-C2-C3	3.31	114.46	109.64
3	t	2	BGC	C1-O5-C5	3.30	116.61	112.19
3	MB	2	BGC	C1-O5-C5	3.30	116.61	112.19
3	hB	2	BGC	C1-O5-C5	3.30	116.61	112.19
4	2A	1	GAL	C1-C2-C3	3.30	114.45	109.64
3	ZA	2	BGC	C1-O5-C5	3.30	116.61	112.19
3	TB	2	BGC	C1-O5-C5	3.30	116.61	112.19
3	AD	2	BGC	C1-O5-C5	3.30	116.61	112.19
3	aB	2	BGC	C1-O5-C5	3.30	116.61	112.19
3	2B	2	BGC	C1-O5-C5	3.30	116.61	112.19
4	UB	1	GAL	C1-C2-C3	3.30	114.44	109.64
3	uA	2	BGC	C1-O5-C5	3.30	116.60	112.19
4	wB	1	GAL	C1-C2-C3	3.29	114.44	109.64
4	iB	1	GAL	C1-C2-C3	3.29	114.44	109.64
3	LA	2	BGC	C1-O5-C5	3.29	116.59	112.19
3	bC	2	BGC	C1-O5-C5	3.29	116.59	112.19
3	0	2	BGC	C1-O5-C5	3.29	116.59	112.19
3	IA	3	A1H1F	C1-O5-C5	3.29	116.59	112.19
3	EA	2	BGC	C1-O5-C5	3.28	116.59	112.19
3	DC	2	BGC	C2-C3-C4	3.23	116.54	110.86
3	rA	2	BGC	C2-C3-C4	3.23	116.53	110.86
3	6B	2	BGC	C2-C3-C4	3.23	116.53	110.86
3	lB	2	BGC	C2-C3-C4	3.22	116.53	110.86
3	ED	2	BGC	C2-C3-C4	3.22	116.52	110.86
3	0C	2	BGC	C2-C3-C4	3.22	116.52	110.86
3	WA	2	BGC	C2-C3-C4	3.22	116.52	110.86
3	YC	2	BGC	C2-C3-C4	3.21	116.51	110.86
3	yA	2	BGC	C2-C3-C4	3.21	116.51	110.86
3	CB	2	BGC	C2-C3-C4	3.21	116.51	110.86
3	tC	2	BGC	C2-C3-C4	3.21	116.51	110.86
3	QB	2	BGC	C2-C3-C4	3.21	116.50	110.86
3	PA	2	BGC	C2-C3-C4	3.21	116.50	110.86
3	j	2	BGC	C2-C3-C4	3.21	116.50	110.86
3	mC	2	BGC	C2-C3-C4	3.21	116.50	110.86
3	dA	2	BGC	C2-C3-C4	3.20	116.50	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BA	2	BGC	C2-C3-C4	3.20	116.50	110.86
3	zB	2	BGC	C2-C3-C4	3.20	116.50	110.86
3	5A	2	BGC	C2-C3-C4	3.20	116.49	110.86
3	IA	2	BGC	C2-C3-C4	3.20	116.49	110.86
3	kA	2	BGC	C2-C3-C4	3.20	116.48	110.86
3	XB	2	BGC	C2-C3-C4	3.20	116.48	110.86
3	KC	2	BGC	C2-C3-C4	3.20	116.48	110.86
3	eB	2	BGC	C2-C3-C4	3.20	116.48	110.86
3	7C	2	BGC	C2-C3-C4	3.20	116.48	110.86
3	sB	2	BGC	C2-C3-C4	3.19	116.48	110.86
3	x	2	BGC	C2-C3-C4	3.19	116.48	110.86
3	fC	2	BGC	C2-C3-C4	3.19	116.47	110.86
3	JB	2	BGC	C2-C3-C4	3.19	116.47	110.86
3	4	2	BGC	C2-C3-C4	3.18	116.46	110.86
3	hB	5	MAN	C1-O5-C5	3.18	116.45	112.19
3	q	2	BGC	C2-C3-C4	3.18	116.45	110.86
3	RC	2	BGC	C2-C3-C4	3.18	116.45	110.86
3	MB	5	MAN	C1-O5-C5	3.17	116.44	112.19
3	gA	5	MAN	C1-O5-C5	3.17	116.43	112.19
3	FB	5	MAN	C1-O5-C5	3.16	116.42	112.19
3	HD	5	MAN	C1-O5-C5	3.15	116.41	112.19
3	UC	5	MAN	C1-O5-C5	3.15	116.41	112.19
3	ZA	5	MAN	C1-O5-C5	3.15	116.41	112.19
3	NC	5	MAN	C1-O5-C5	3.15	116.41	112.19
3	t	5	MAN	C1-O5-C5	3.15	116.41	112.19
3	TB	5	MAN	C1-O5-C5	3.15	116.40	112.19
3	iC	5	MAN	C1-O5-C5	3.15	116.40	112.19
3	aB	5	MAN	C1-O5-C5	3.14	116.40	112.19
3	m	5	MAN	C1-O5-C5	3.14	116.40	112.19
3	bC	5	MAN	C1-O5-C5	3.14	116.40	112.19
3	1A	5	MAN	C1-O5-C5	3.14	116.39	112.19
3	wC	5	MAN	C1-O5-C5	3.14	116.39	112.19
3	8A	5	MAN	C1-O5-C5	3.14	116.39	112.19
3	GC	5	MAN	C1-O5-C5	3.14	116.39	112.19
3	oB	5	MAN	C1-O5-C5	3.14	116.39	112.19
3	vB	5	MAN	C1-O5-C5	3.13	116.39	112.19
3	9B	5	MAN	C1-O5-C5	3.13	116.38	112.19
3	pC	5	MAN	C1-O5-C5	3.13	116.38	112.19
3	2B	5	MAN	C1-O5-C5	3.13	116.38	112.19
3	3C	5	MAN	C1-O5-C5	3.12	116.37	112.19
3	nA	5	MAN	C1-O5-C5	3.12	116.37	112.19
3	LA	5	MAN	C1-O5-C5	3.12	116.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	5	MAN	C1-O5-C5	3.12	116.36	112.19
3	uA	5	MAN	C1-O5-C5	3.12	116.36	112.19
3	SA	5	MAN	C1-O5-C5	3.11	116.36	112.19
3	EA	5	MAN	C1-O5-C5	3.11	116.35	112.19
3	7	5	MAN	C1-O5-C5	3.10	116.34	112.19
3	6A	2	BGC	C2-C3-C4	3.10	116.31	110.86
3	SC	2	BGC	C2-C3-C4	3.10	116.31	110.86
3	gC	2	BGC	C2-C3-C4	3.10	116.31	110.86
3	0	5	MAN	C1-O5-C5	3.10	116.33	112.19
3	q	5	MAN	C1-C2-C3	3.09	114.15	109.64
3	CA	2	BGC	C2-C3-C4	3.09	116.30	110.86
3	fB	2	BGC	C2-C3-C4	3.09	116.29	110.86
3	r	2	BGC	C2-C3-C4	3.09	116.29	110.86
3	RB	2	BGC	C2-C3-C4	3.09	116.29	110.86
3	nC	2	BGC	C2-C3-C4	3.09	116.29	110.86
3	XB	5	MAN	C1-C2-C3	3.09	114.14	109.64
3	5	2	BGC	C2-C3-C4	3.08	116.28	110.86
3	8C	2	BGC	C2-C3-C4	3.08	116.28	110.86
3	y	2	BGC	C2-C3-C4	3.08	116.28	110.86
3	mB	2	BGC	C2-C3-C4	3.08	116.28	110.86
3	DC	5	MAN	C1-C2-C3	3.08	114.13	109.64
3	DB	2	BGC	C2-C3-C4	3.08	116.28	110.86
3	k	2	BGC	C2-C3-C4	3.08	116.27	110.86
3	ZC	2	BGC	C2-C3-C4	3.08	116.27	110.86
3	QB	5	MAN	C1-C2-C3	3.07	114.12	109.64
3	lA	2	BGC	C2-C3-C4	3.07	116.27	110.86
3	1C	2	BGC	C2-C3-C4	3.07	116.26	110.86
3	FD	2	BGC	C2-C3-C4	3.07	116.26	110.86
3	EC	2	BGC	C2-C3-C4	3.07	116.26	110.86
3	QA	2	BGC	C2-C3-C4	3.07	116.26	110.86
3	zA	2	BGC	C2-C3-C4	3.07	116.26	110.86
3	JA	2	BGC	C2-C3-C4	3.07	116.26	110.86
3	dA	5	MAN	C1-C2-C3	3.07	114.11	109.64
3	KB	2	BGC	C2-C3-C4	3.07	116.26	110.86
3	7B	2	BGC	C2-C3-C4	3.07	116.26	110.86
3	sA	2	BGC	C2-C3-C4	3.07	116.25	110.86
3	JB	5	MAN	C1-C2-C3	3.07	114.11	109.64
3	eA	2	BGC	C2-C3-C4	3.07	116.25	110.86
3	PA	5	MAN	C1-C2-C3	3.07	114.11	109.64
3	6B	5	MAN	C1-C2-C3	3.07	114.11	109.64
3	mC	5	MAN	C1-C2-C3	3.07	114.11	109.64
3	XA	2	BGC	C2-C3-C4	3.06	116.25	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	rA	5	MAN	C1-C2-C3	3.06	114.11	109.64
3	7C	5	MAN	C1-C2-C3	3.06	114.11	109.64
3	YB	2	BGC	C2-C3-C4	3.06	116.25	110.86
3	0B	2	BGC	C2-C3-C4	3.06	116.25	110.86
3	WA	5	MAN	C1-C2-C3	3.06	114.10	109.64
3	lB	5	MAN	C1-C2-C3	3.06	114.10	109.64
3	eB	5	MAN	C1-C2-C3	3.06	114.10	109.64
3	0C	5	MAN	C1-C2-C3	3.06	114.10	109.64
3	CB	5	MAN	C1-C2-C3	3.06	114.10	109.64
3	uC	2	BGC	C2-C3-C4	3.06	116.24	110.86
3	j	5	MAN	C1-C2-C3	3.06	114.10	109.64
3	sB	5	MAN	C1-C2-C3	3.06	114.10	109.64
3	tB	2	BGC	C2-C3-C4	3.06	116.24	110.86
3	LC	2	BGC	C2-C3-C4	3.06	116.24	110.86
3	fC	5	MAN	C1-C2-C3	3.06	114.09	109.64
3	BA	5	MAN	C1-C2-C3	3.05	114.09	109.64
3	ED	5	MAN	C1-C2-C3	3.05	114.09	109.64
3	5A	5	MAN	C1-C2-C3	3.05	114.09	109.64
3	RC	5	MAN	C1-C2-C3	3.05	114.09	109.64
3	tC	5	MAN	C1-C2-C3	3.05	114.09	109.64
3	kA	5	MAN	C1-C2-C3	3.05	114.08	109.64
3	KC	5	MAN	C1-C2-C3	3.05	114.08	109.64
3	IA	5	MAN	C1-C2-C3	3.04	114.07	109.64
3	yA	5	MAN	C1-C2-C3	3.04	114.07	109.64
3	YC	5	MAN	C1-C2-C3	3.03	114.06	109.64
3	4	5	MAN	C1-C2-C3	3.03	114.06	109.64
3	zB	5	MAN	C1-C2-C3	3.03	114.06	109.64
3	x	5	MAN	C1-C2-C3	3.02	114.04	109.64
3	tB	2	BGC	C1-C2-C3	3.00	114.01	109.64
3	7B	2	BGC	C1-C2-C3	2.99	114.00	109.64
3	sA	2	BGC	C1-C2-C3	2.99	114.00	109.64
3	1C	2	BGC	C1-C2-C3	2.98	113.99	109.64
3	8C	2	BGC	C1-C2-C3	2.98	113.99	109.64
3	CA	2	BGC	C1-C2-C3	2.98	113.98	109.64
3	mB	2	BGC	C1-C2-C3	2.98	113.98	109.64
3	uC	2	BGC	C1-C2-C3	2.98	113.98	109.64
3	eA	2	BGC	C1-C2-C3	2.97	113.97	109.64
3	0B	2	BGC	C1-C2-C3	2.97	113.97	109.64
3	EC	2	BGC	C1-C2-C3	2.97	113.97	109.64
3	FD	2	BGC	C1-C2-C3	2.97	113.97	109.64
3	5	2	BGC	C1-C2-C3	2.97	113.97	109.64
4	LB	4	MAN	C1-C2-C3	2.97	113.97	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	KB	2	BGC	C1-C2-C3	2.97	113.97	109.64
3	XA	2	BGC	C1-C2-C3	2.97	113.97	109.64
3	LC	2	BGC	C1-C2-C3	2.97	113.97	109.64
3	JA	2	BGC	C1-C2-C3	2.97	113.96	109.64
3	k	2	BGC	C1-C2-C3	2.97	113.96	109.64
4	9C	4	MAN	C1-C2-C3	2.97	113.96	109.64
4	GD	4	MAN	C1-C2-C3	2.97	113.96	109.64
3	y	2	BGC	C1-C2-C3	2.96	113.96	109.64
3	r	2	BGC	C1-C2-C3	2.96	113.96	109.64
3	fB	2	BGC	C1-C2-C3	2.96	113.96	109.64
3	gC	2	BGC	C1-C2-C3	2.96	113.96	109.64
4	ZB	4	MAN	C1-C2-C3	2.96	113.96	109.64
3	zA	2	BGC	C1-C2-C3	2.96	113.96	109.64
3	6A	2	BGC	C1-C2-C3	2.96	113.96	109.64
4	tA	4	MAN	C1-C2-C3	2.96	113.96	109.64
4	1B	4	MAN	C1-C2-C3	2.96	113.96	109.64
3	lA	2	BGC	C1-C2-C3	2.96	113.95	109.64
4	DA	4	MAN	C1-C2-C3	2.96	113.95	109.64
4	SB	4	MAN	C1-C2-C3	2.96	113.95	109.64
4	vC	4	MAN	C1-C2-C3	2.96	113.95	109.64
3	nC	2	BGC	C1-C2-C3	2.96	113.95	109.64
4	EB	4	MAN	C1-C2-C3	2.96	113.95	109.64
4	FA	1	GAL	C1-O5-C5	2.96	116.15	112.19
4	nB	4	MAN	C1-C2-C3	2.96	113.95	109.64
4	aC	4	MAN	C1-C2-C3	2.96	113.95	109.64
3	YB	2	BGC	C1-C2-C3	2.95	113.95	109.64
4	LB	4	MAN	C1-O5-C5	2.95	116.14	112.19
4	l	4	MAN	C1-C2-C3	2.95	113.94	109.64
4	7A	4	MAN	C1-C2-C3	2.95	113.94	109.64
4	MC	4	MAN	C1-C2-C3	2.95	113.94	109.64
4	z	4	MAN	C1-C2-C3	2.95	113.94	109.64
4	RA	4	MAN	C1-C2-C3	2.95	113.94	109.64
4	8B	4	MAN	C1-C2-C3	2.95	113.94	109.64
4	oA	1	GAL	C1-O5-C5	2.95	116.14	112.19
3	DB	2	BGC	C1-C2-C3	2.95	113.94	109.64
3	SC	2	BGC	C1-C2-C3	2.95	113.94	109.64
3	RB	2	BGC	C1-C2-C3	2.95	113.93	109.64
4	gB	4	MAN	C1-O5-C5	2.95	116.13	112.19
4	u	1	GAL	C1-O5-C5	2.95	116.13	112.19
4	TC	4	MAN	C1-O5-C5	2.95	116.13	112.19
3	QA	2	BGC	C1-C2-C3	2.94	113.93	109.64
4	mA	4	MAN	C1-C2-C3	2.94	113.93	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	vA	1	GAL	C1-O5-C5	2.94	116.13	112.19
3	tC	5	MAN	C1-O5-C5	2.94	116.13	112.19
4	ZB	4	MAN	C1-O5-C5	2.94	116.13	112.19
4	TA	1	GAL	C1-O5-C5	2.94	116.13	112.19
4	KA	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	FC	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	0A	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	gB	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	TC	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	2C	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	xC	1	GAL	C1-O5-C5	2.94	116.12	112.19
4	hC	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	6	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	fA	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	uB	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	oC	4	MAN	C1-C2-C3	2.94	113.92	109.64
4	mA	4	MAN	C1-O5-C5	2.94	116.12	112.19
4	HC	1	GAL	C1-O5-C5	2.94	116.12	112.19
4	pB	1	GAL	C1-O5-C5	2.93	116.12	112.19
3	ZC	2	BGC	C1-C2-C3	2.93	113.92	109.64
4	SB	4	MAN	C1-O5-C5	2.93	116.12	112.19
4	AC	1	GAL	C1-O5-C5	2.93	116.11	112.19
4	4C	1	GAL	C1-O5-C5	2.93	116.11	112.19
3	rA	5	MAN	C1-O5-C5	2.93	116.11	112.19
4	0A	4	MAN	C1-O5-C5	2.93	116.11	112.19
4	nB	4	MAN	C1-O5-C5	2.93	116.11	112.19
4	YA	4	MAN	C1-O5-C5	2.93	116.11	112.19
4	1B	1	GAL	C1-C2-C3	2.93	113.90	109.64
4	9A	1	GAL	C1-O5-C5	2.92	116.11	112.19
4	bB	1	GAL	C1-O5-C5	2.92	116.11	112.19
4	s	4	MAN	C1-C2-C3	2.92	113.90	109.64
3	5A	5	MAN	C1-O5-C5	2.92	116.10	112.19
4	uB	4	MAN	C1-O5-C5	2.92	116.10	112.19
4	7A	4	MAN	C1-O5-C5	2.92	116.10	112.19
3	7C	5	MAN	C1-O5-C5	2.92	116.10	112.19
4	n	1	GAL	C1-O5-C5	2.92	116.10	112.19
4	YA	4	MAN	C1-C2-C3	2.92	113.90	109.64
4	2A	1	GAL	C1-O5-C5	2.92	116.10	112.19
4	gB	1	GAL	C1-C2-C3	2.92	113.89	109.64
3	IA	5	MAN	C1-O5-C5	2.92	116.09	112.19
4	hC	4	MAN	C1-O5-C5	2.92	116.09	112.19
4	EB	4	MAN	C1-O5-C5	2.92	116.09	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GB	1	GAL	C1-O5-C5	2.92	116.09	112.19
4	NB	1	GAL	C1-O5-C5	2.92	116.09	112.19
4	MC	4	MAN	C1-O5-C5	2.92	116.09	112.19
3	yA	5	MAN	C1-O5-C5	2.92	116.09	112.19
3	CB	5	MAN	C1-O5-C5	2.92	116.09	112.19
4	l	1	GAL	C1-O5-C5	2.92	116.09	112.19
4	qC	1	GAL	C1-O5-C5	2.92	116.09	112.19
4	DA	1	GAL	C1-C2-C3	2.91	113.89	109.64
4	nB	1	GAL	C1-C2-C3	2.91	113.89	109.64
4	tA	4	MAN	C1-O5-C5	2.91	116.09	112.19
4	FC	4	MAN	C1-O5-C5	2.91	116.09	112.19
4	l	4	MAN	C1-O5-C5	2.91	116.09	112.19
4	RA	4	MAN	C1-O5-C5	2.91	116.09	112.19
4	wB	1	GAL	C1-O5-C5	2.91	116.09	112.19
4	hC	1	GAL	C1-C2-C3	2.91	113.88	109.64
3	JB	5	MAN	C1-O5-C5	2.91	116.09	112.19
3	QB	5	MAN	C1-O5-C5	2.91	116.09	112.19
4	MA	1	GAL	C1-O5-C5	2.91	116.09	112.19
4	jC	1	GAL	C1-O5-C5	2.91	116.09	112.19
4	SB	1	GAL	C1-C2-C3	2.91	113.88	109.64
4	OC	1	GAL	C1-O5-C5	2.91	116.09	112.19
4	cC	1	GAL	C1-O5-C5	2.91	116.09	112.19
4	z	1	GAL	C1-C2-C3	2.91	113.88	109.64
4	vC	1	GAL	C1-C2-C3	2.91	113.88	109.64
4	6	4	MAN	C1-O5-C5	2.91	116.08	112.19
4	DA	4	MAN	C1-O5-C5	2.91	116.08	112.19
4	aA	1	GAL	C1-O5-C5	2.91	116.08	112.19
4	VC	1	GAL	C1-O5-C5	2.91	116.08	112.19
4	vC	4	MAN	C1-O5-C5	2.91	116.08	112.19
3	DC	5	MAN	C1-O5-C5	2.91	116.08	112.19
3	KC	5	MAN	C1-O5-C5	2.91	116.08	112.19
3	6B	5	MAN	C1-O5-C5	2.91	116.08	112.19
4	fA	4	MAN	C1-O5-C5	2.91	116.08	112.19
4	mA	1	GAL	C1-C2-C3	2.91	113.88	109.64
4	ZB	1	GAL	C1-C2-C3	2.91	113.88	109.64
4	hA	1	GAL	C1-O5-C5	2.91	116.08	112.19
4	1B	4	MAN	C1-O5-C5	2.91	116.08	112.19
4	oC	4	MAN	C1-O5-C5	2.91	116.08	112.19
4	9C	4	MAN	C1-O5-C5	2.91	116.08	112.19
4	aC	4	MAN	C1-O5-C5	2.90	116.08	112.19
4	7A	1	GAL	C1-C2-C3	2.90	113.87	109.64
3	dA	5	MAN	C1-O5-C5	2.90	116.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	iB	1	GAL	C1-O5-C5	2.90	116.08	112.19
4	8B	4	MAN	C1-O5-C5	2.90	116.08	112.19
4	6	1	GAL	C1-C2-C3	2.90	113.87	109.64
3	j	5	MAN	C1-O5-C5	2.90	116.07	112.19
3	q	5	MAN	C1-O5-C5	2.90	116.07	112.19
4	3B	1	GAL	C1-O5-C5	2.90	116.07	112.19
4	0A	1	GAL	C1-C2-C3	2.90	113.87	109.64
4	ID	1	GAL	C1-O5-C5	2.90	116.07	112.19
4	s	1	GAL	C1-C2-C3	2.90	113.86	109.64
4	RA	1	GAL	C1-C2-C3	2.90	113.86	109.64
4	EB	1	GAL	C1-C2-C3	2.90	113.86	109.64
4	FC	1	GAL	C1-C2-C3	2.90	113.86	109.64
3	4	5	MAN	C1-O5-C5	2.90	116.07	112.19
4	BD	1	GAL	C1-O5-C5	2.90	116.07	112.19
4	LB	1	GAL	C1-C2-C3	2.89	113.86	109.64
4	8	1	GAL	C1-O5-C5	2.89	116.06	112.19
4	UB	1	GAL	C1-O5-C5	2.89	116.06	112.19
4	l	1	GAL	C1-C2-C3	2.89	113.86	109.64
4	oC	1	GAL	C1-C2-C3	2.89	113.86	109.64
4	z	4	MAN	C1-O5-C5	2.89	116.06	112.19
4	aC	1	GAL	C1-C2-C3	2.89	113.85	109.64
4	9C	1	GAL	C1-C2-C3	2.89	113.85	109.64
4	GD	1	GAL	C1-C2-C3	2.89	113.85	109.64
3	lB	5	MAN	C1-O5-C5	2.89	116.06	112.19
3	zB	5	MAN	C1-O5-C5	2.89	116.06	112.19
4	2C	4	MAN	C1-O5-C5	2.89	116.06	112.19
4	MC	1	GAL	C1-C2-C3	2.89	113.85	109.64
4	KA	4	MAN	C1-O5-C5	2.89	116.06	112.19
3	PA	5	MAN	C1-O5-C5	2.89	116.06	112.19
3	WA	5	MAN	C1-O5-C5	2.89	116.06	112.19
3	RC	5	MAN	C1-O5-C5	2.89	116.05	112.19
3	mC	5	MAN	C1-O5-C5	2.89	116.05	112.19
4	s	4	MAN	C1-O5-C5	2.89	116.05	112.19
4	fA	1	GAL	C1-C2-C3	2.89	113.84	109.64
3	YC	5	MAN	C1-O5-C5	2.88	116.05	112.19
4	8B	1	GAL	C1-C2-C3	2.88	113.84	109.64
3	0C	5	MAN	C1-O5-C5	2.88	116.05	112.19
4	2C	1	GAL	C1-C2-C3	2.88	113.84	109.64
4	YA	1	GAL	C1-C2-C3	2.88	113.84	109.64
3	eB	5	MAN	C1-O5-C5	2.88	116.05	112.19
3	kA	5	MAN	C1-O5-C5	2.88	116.04	112.19
3	XB	5	MAN	C1-O5-C5	2.88	116.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	KA	1	GAL	C1-C2-C3	2.87	113.83	109.64
4	uB	1	GAL	C1-C2-C3	2.87	113.83	109.64
3	ED	5	MAN	C1-O5-C5	2.87	116.03	112.19
4	GD	4	MAN	C1-O5-C5	2.87	116.03	112.19
3	x	5	MAN	C1-O5-C5	2.87	116.03	112.19
4	tA	1	GAL	C1-C2-C3	2.87	113.82	109.64
3	sB	5	MAN	C1-O5-C5	2.87	116.03	112.19
4	TC	1	GAL	C1-C2-C3	2.86	113.81	109.64
3	fC	5	MAN	C1-O5-C5	2.86	116.02	112.19
3	BA	5	MAN	C1-O5-C5	2.86	116.01	112.19
4	hC	3	A1H1F	O3S6-S6-C6	2.76	110.88	106.76
3	YB	3	A1H1F	O3S6-S6-C6	2.76	110.88	106.76
4	vC	3	A1H1F	O3S6-S6-C6	2.76	110.88	106.76
4	FC	3	A1H1F	O3S6-S6-C6	2.76	110.88	106.76
4	uB	3	A1H1F	O3S6-S6-C6	2.76	110.88	106.76
4	z	3	A1H1F	O3S6-S6-C6	2.76	110.87	106.76
4	fA	3	A1H1F	O3S6-S6-C6	2.76	110.87	106.76
4	EB	3	A1H1F	O3S6-S6-C6	2.76	110.87	106.76
4	6	3	A1H1F	O3S6-S6-C6	2.76	110.87	106.76
4	s	3	A1H1F	O3S6-S6-C6	2.76	110.87	106.76
4	gB	3	A1H1F	O3S6-S6-C6	2.76	110.87	106.76
4	DA	3	A1H1F	O3S6-S6-C6	2.75	110.87	106.76
4	KA	3	A1H1F	O3S6-S6-C6	2.75	110.87	106.76
4	TC	3	A1H1F	O3S6-S6-C6	2.75	110.87	106.76
4	tA	3	A1H1F	O3S6-S6-C6	2.75	110.86	106.76
4	1B	3	A1H1F	O3S6-S6-C6	2.75	110.86	106.76
4	aC	3	A1H1F	O3S6-S6-C6	2.75	110.86	106.76
4	l	3	A1H1F	O3S6-S6-C6	2.75	110.86	106.76
4	SB	3	A1H1F	O3S6-S6-C6	2.75	110.86	106.76
4	nB	3	A1H1F	O3S6-S6-C6	2.75	110.86	106.76
4	8B	3	A1H1F	O3S6-S6-C6	2.75	110.86	106.76
4	9C	3	A1H1F	O3S6-S6-C6	2.75	110.86	106.76
3	uC	3	A1H1F	O3S6-S6-C6	2.74	110.85	106.76
3	fB	3	A1H1F	O3S6-S6-C6	2.74	110.84	106.76
3	7B	3	A1H1F	O3S6-S6-C6	2.74	110.84	106.76
4	oC	3	A1H1F	O3S6-S6-C6	2.74	110.84	106.76
3	sA	3	A1H1F	O3S6-S6-C6	2.74	110.84	106.76
3	r	3	A1H1F	O3S6-S6-C6	2.73	110.84	106.76
3	RB	3	A1H1F	O3S6-S6-C6	2.73	110.84	106.76
4	RA	3	A1H1F	O3S6-S6-C6	2.73	110.84	106.76
4	ZB	3	A1H1F	O3S6-S6-C6	2.73	110.84	106.76
3	zA	3	A1H1F	O3S6-S6-C6	2.73	110.84	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2C	3	A1H1F	O3S6-S6-C6	2.73	110.84	106.76
3	1C	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
3	tB	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
4	LB	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
3	y	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
3	ZC	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
3	JA	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
4	YA	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
4	0A	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
4	MC	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
3	lA	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
3	DB	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
3	SC	3	A1H1F	O3S6-S6-C6	2.73	110.83	106.76
3	nC	3	A1H1F	O3S6-S6-C6	2.72	110.82	106.76
3	LC	3	A1H1F	O3S6-S6-C6	2.72	110.82	106.76
3	k	3	A1H1F	O3S6-S6-C6	2.72	110.82	106.76
3	gC	3	A1H1F	O3S6-S6-C6	2.72	110.82	106.76
4	7A	3	A1H1F	O3S6-S6-C6	2.72	110.82	106.76
4	mA	3	A1H1F	O3S6-S6-C6	2.72	110.81	106.76
3	QA	3	A1H1F	O3S6-S6-C6	2.72	110.81	106.76
3	mB	3	A1H1F	O3S6-S6-C6	2.72	110.81	106.76
3	EC	3	A1H1F	O3S6-S6-C6	2.72	110.81	106.76
3	FD	3	A1H1F	O3S6-S6-C6	2.71	110.81	106.76
3	0B	3	A1H1F	O3S6-S6-C6	2.71	110.80	106.76
3	CA	3	A1H1F	O3S6-S6-C6	2.71	110.80	106.76
3	8C	3	A1H1F	O3S6-S6-C6	2.71	110.80	106.76
3	XA	3	A1H1F	O3S6-S6-C6	2.71	110.80	106.76
3	eA	3	A1H1F	O3S6-S6-C6	2.71	110.80	106.76
4	GD	3	A1H1F	O3S6-S6-C6	2.71	110.80	106.76
3	5	3	A1H1F	O3S6-S6-C6	2.70	110.79	106.76
3	vB	1	GAL	C1-C2-C3	2.70	113.57	109.64
3	KB	3	A1H1F	O3S6-S6-C6	2.70	110.78	106.76
3	6A	3	A1H1F	O3S6-S6-C6	2.70	110.78	106.76
3	t	1	GAL	C1-C2-C3	2.69	113.57	109.64
3	HD	1	GAL	C1-C2-C3	2.69	113.56	109.64
3	EA	1	GAL	C1-C2-C3	2.69	113.56	109.64
3	pC	1	GAL	C1-C2-C3	2.69	113.56	109.64
3	UC	1	GAL	C1-C2-C3	2.68	113.55	109.64
3	SA	1	GAL	C1-C2-C3	2.68	113.55	109.64
3	NC	1	GAL	C1-C2-C3	2.68	113.55	109.64
3	bC	1	GAL	C1-C2-C3	2.68	113.54	109.64
3	3C	1	GAL	C1-C2-C3	2.68	113.54	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1A	1	GAL	C1-C2-C3	2.67	113.54	109.64
3	MB	1	GAL	C1-C2-C3	2.67	113.54	109.64
3	ZA	1	GAL	C1-C2-C3	2.67	113.53	109.64
3	m	1	GAL	C1-C2-C3	2.67	113.53	109.64
3	FB	1	GAL	C1-C2-C3	2.67	113.53	109.64
3	GC	1	GAL	C1-C2-C3	2.67	113.53	109.64
3	1A	2	BGC	C1-C2-C3	2.66	113.52	109.64
3	oB	1	GAL	C1-C2-C3	2.66	113.52	109.64
3	iC	1	GAL	C1-C2-C3	2.66	113.52	109.64
3	TB	1	GAL	C1-C2-C3	2.66	113.52	109.64
3	2B	1	GAL	C1-C2-C3	2.66	113.52	109.64
3	uA	1	GAL	C1-C2-C3	2.66	113.52	109.64
3	hB	1	GAL	C1-C2-C3	2.66	113.51	109.64
3	9B	1	GAL	C1-C2-C3	2.66	113.51	109.64
3	7	1	GAL	C1-C2-C3	2.66	113.51	109.64
3	AD	1	GAL	C1-C2-C3	2.66	113.51	109.64
3	LA	1	GAL	C1-C2-C3	2.66	113.51	109.64
3	8A	1	GAL	C1-C2-C3	2.65	113.51	109.64
3	gA	1	GAL	C1-C2-C3	2.65	113.51	109.64
3	wC	1	GAL	C1-C2-C3	2.65	113.51	109.64
3	0	1	GAL	C1-C2-C3	2.65	113.51	109.64
3	aB	1	GAL	C1-C2-C3	2.65	113.50	109.64
3	7	2	BGC	C1-C2-C3	2.64	113.50	109.64
3	MB	2	BGC	C1-C2-C3	2.64	113.50	109.64
3	fB	4	A1H03	C1-C2-C3	2.64	113.50	109.64
3	gA	2	BGC	C1-C2-C3	2.64	113.49	109.64
3	0C	4	A1H03	C1-O5-C5	2.64	115.81	111.48
3	x	1	GAL	C1-O5-C5	2.64	115.73	112.19
3	XA	4	A1H03	C1-C2-C3	2.64	113.49	109.64
3	JA	4	A1H03	C1-C2-C3	2.64	113.49	109.64
3	8A	2	BGC	C1-C2-C3	2.64	113.49	109.64
3	rA	4	A1H03	C1-O5-C5	2.64	115.80	111.48
3	kA	4	A1H03	C1-O5-C5	2.64	115.80	111.48
3	7C	4	A1H03	C1-O5-C5	2.64	115.80	111.48
3	ZA	2	BGC	C1-C2-C3	2.64	113.48	109.64
3	YB	4	A1H03	C1-C2-C3	2.64	113.48	109.64
3	pC	2	BGC	C1-C2-C3	2.64	113.48	109.64
3	tC	4	A1H03	C1-O5-C5	2.63	115.79	111.48
3	gC	4	A1H03	C1-C2-C3	2.63	113.48	109.64
3	nA	1	GAL	C1-C2-C3	2.63	113.48	109.64
3	y	4	A1H03	C1-C2-C3	2.63	113.47	109.64
2	VB	2	BGC	C1-O5-C5	2.63	115.71	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	UC	2	BGC	C1-C2-C3	2.63	113.47	109.64
3	lA	4	A1H03	C1-C2-C3	2.63	113.47	109.64
3	IA	4	A1H03	C1-O5-C5	2.63	115.78	111.48
3	6B	4	A1H03	C1-O5-C5	2.63	115.78	111.48
3	RB	4	A1H03	C1-C2-C3	2.63	113.47	109.64
3	hB	2	BGC	C1-C2-C3	2.63	113.47	109.64
3	7B	4	A1H03	C1-C2-C3	2.63	113.47	109.64
3	LC	4	A1H03	C1-C2-C3	2.63	113.47	109.64
3	RC	4	A1H03	C1-O5-C5	2.63	115.78	111.48
3	aB	2	BGC	C1-C2-C3	2.63	113.47	109.64
3	EA	2	BGC	C1-C2-C3	2.62	113.47	109.64
3	tB	4	A1H03	C1-C2-C3	2.62	113.47	109.64
3	iC	2	BGC	C1-C2-C3	2.62	113.47	109.64
3	QB	4	A1H03	C1-O5-C5	2.62	115.78	111.48
3	GC	2	BGC	C1-C2-C3	2.62	113.46	109.64
3	zB	4	A1H03	C1-O5-C5	2.62	115.78	111.48
3	8C	4	A1H03	C1-C2-C3	2.62	113.46	109.64
3	m	2	BGC	C1-C2-C3	2.62	113.46	109.64
3	j	4	A1H03	C1-O5-C5	2.62	115.77	111.48
3	CB	4	A1H03	C1-O5-C5	2.62	115.77	111.48
3	YC	4	A1H03	C1-O5-C5	2.62	115.77	111.48
3	eA	4	A1H03	C1-C2-C3	2.62	113.46	109.64
3	t	2	BGC	C1-C2-C3	2.62	113.46	109.64
3	AD	2	BGC	C1-C2-C3	2.62	113.46	109.64
3	mC	4	A1H03	C1-O5-C5	2.62	115.77	111.48
3	2B	2	BGC	C1-C2-C3	2.62	113.46	109.64
3	3C	2	BGC	C1-C2-C3	2.62	113.46	109.64
3	sB	4	A1H03	C1-O5-C5	2.62	115.77	111.48
3	fC	1	GAL	C1-O5-C5	2.62	115.69	112.19
3	QA	4	A1H03	C1-C2-C3	2.62	113.46	109.64
3	SA	2	BGC	C1-C2-C3	2.62	113.46	109.64
3	zA	4	A1H03	C1-C2-C3	2.62	113.46	109.64
3	k	4	A1H03	C1-C2-C3	2.62	113.45	109.64
3	CA	4	A1H03	C1-C2-C3	2.62	113.45	109.64
3	9B	2	BGC	C1-C2-C3	2.62	113.45	109.64
3	EC	4	A1H03	C1-C2-C3	2.62	113.45	109.64
3	wC	2	BGC	C1-C2-C3	2.62	113.45	109.64
3	FD	4	A1H03	C1-C2-C3	2.62	113.45	109.64
3	PA	4	A1H03	C1-O5-C5	2.62	115.77	111.48
3	LA	2	BGC	C1-C2-C3	2.62	113.45	109.64
3	1C	4	A1H03	C1-C2-C3	2.62	113.45	109.64
3	ED	4	A1H03	C1-O5-C5	2.62	115.76	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DB	4	A1H03	C1-C2-C3	2.61	113.45	109.64
3	NC	2	BGC	C1-C2-C3	2.61	113.45	109.64
3	JB	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	r	4	A1H03	C1-C2-C3	2.61	113.45	109.64
3	6A	4	A1H03	C1-C2-C3	2.61	113.45	109.64
3	fC	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	mB	4	A1H03	C1-C2-C3	2.61	113.45	109.64
3	4	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	BA	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	dA	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	DC	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	KC	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	CB	1	GAL	C1-O5-C5	2.61	115.69	112.19
3	nC	4	A1H03	C1-C2-C3	2.61	113.45	109.64
3	WA	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	oB	2	BGC	C1-C2-C3	2.61	113.44	109.64
3	yA	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	XB	4	A1H03	C1-O5-C5	2.61	115.76	111.48
3	eB	4	A1H03	C1-O5-C5	2.61	115.75	111.48
3	lB	4	A1H03	C1-O5-C5	2.61	115.75	111.48
2	kC	2	BGC	C1-O5-C5	2.61	115.68	112.19
3	KC	1	GAL	C1-O5-C5	2.61	115.68	112.19
3	ED	1	GAL	C1-O5-C5	2.61	115.68	112.19
3	uA	2	BGC	C1-C2-C3	2.61	113.44	109.64
3	FB	2	BGC	C1-C2-C3	2.61	113.44	109.64
3	uC	4	A1H03	C1-C2-C3	2.61	113.44	109.64
3	JB	1	GAL	C1-O5-C5	2.61	115.68	112.19
3	SC	4	A1H03	C1-C2-C3	2.61	113.44	109.64
3	IA	1	GAL	C1-O5-C5	2.60	115.68	112.19
2	UA	2	BGC	C1-O5-C5	2.60	115.67	112.19
3	yA	1	GAL	C1-O5-C5	2.60	115.67	112.19
3	sB	1	GAL	C1-O5-C5	2.60	115.67	112.19
3	5A	1	GAL	C1-O5-C5	2.60	115.67	112.19
2	qB	2	BGC	C1-O5-C5	2.60	115.67	112.19
3	0B	4	A1H03	C1-C2-C3	2.60	113.43	109.64
3	RC	1	GAL	C1-O5-C5	2.60	115.67	112.19
3	x	4	A1H03	C1-O5-C5	2.60	115.74	111.48
2	cB	2	BGC	C1-O5-C5	2.60	115.67	112.19
2	jB	2	BGC	C1-O5-C5	2.60	115.67	112.19
2	dC	2	BGC	C1-O5-C5	2.60	115.67	112.19
3	5	4	A1H03	C1-C2-C3	2.60	113.43	109.64
3	HD	2	BGC	C1-C2-C3	2.60	113.43	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	nA	2	BGC	C1-C2-C3	2.60	113.43	109.64
3	ZC	4	A1H03	C1-C2-C3	2.60	113.43	109.64
3	TB	2	BGC	C1-C2-C3	2.60	113.42	109.64
3	kA	1	GAL	C1-O5-C5	2.60	115.67	112.19
3	tC	1	GAL	C1-O5-C5	2.60	115.67	112.19
2	rC	2	BGC	C1-O5-C5	2.60	115.66	112.19
3	BA	1	GAL	C1-O5-C5	2.60	115.66	112.19
3	mC	1	GAL	C1-O5-C5	2.60	115.66	112.19
3	bC	2	BGC	C1-C2-C3	2.59	113.42	109.64
3	sA	4	A1H03	C1-C2-C3	2.59	113.42	109.64
3	PA	1	GAL	C1-O5-C5	2.59	115.66	112.19
2	iA	2	BGC	C1-O5-C5	2.59	115.66	112.19
3	0	2	BGC	C1-C2-C3	2.59	113.42	109.64
2	4B	2	BGC	C1-O5-C5	2.59	115.66	112.19
3	j	1	GAL	C1-O5-C5	2.59	115.66	112.19
3	9B	3	A1H1F	O2S6-S6-C6	2.59	110.62	106.76
3	KB	4	A1H03	C1-C2-C3	2.59	113.41	109.64
3	5A	4	A1H03	C1-O5-C5	2.59	115.72	111.48
3	7C	1	GAL	C1-O5-C5	2.59	115.65	112.19
2	v	2	BGC	C1-O5-C5	2.59	115.65	112.19
2	wA	2	BGC	C1-O5-C5	2.59	115.65	112.19
2	AB	2	BGC	C1-O5-C5	2.59	115.65	112.19
3	vB	2	BGC	C1-C2-C3	2.59	113.41	109.64
3	dA	1	GAL	C1-O5-C5	2.59	115.65	112.19
2	bA	2	BGC	C1-O5-C5	2.59	115.65	112.19
2	BC	2	BGC	C1-O5-C5	2.58	115.65	112.19
3	0C	1	GAL	C1-O5-C5	2.58	115.65	112.19
2	o	2	BGC	C1-O5-C5	2.58	115.65	112.19
3	6B	1	GAL	C1-O5-C5	2.58	115.65	112.19
3	eB	1	GAL	C1-O5-C5	2.58	115.64	112.19
2	xB	2	BGC	C1-O5-C5	2.58	115.64	112.19
2	IC	2	BGC	C1-O5-C5	2.58	115.64	112.19
3	WA	1	GAL	C1-O5-C5	2.58	115.64	112.19
3	q	4	A1H03	C1-O5-C5	2.58	115.71	111.48
2	3A	2	BGC	C1-O5-C5	2.58	115.64	112.19
3	YC	1	GAL	C1-O5-C5	2.58	115.64	112.19
2	h	2	BGC	C1-O5-C5	2.58	115.64	112.19
2	2	2	BGC	C1-O5-C5	2.58	115.64	112.19
3	q	1	GAL	C1-O5-C5	2.58	115.64	112.19
3	QB	1	GAL	C1-O5-C5	2.58	115.64	112.19
2	CD	2	BGC	C1-O5-C5	2.57	115.64	112.19
3	SA	3	A1H1F	O2S6-S6-C6	2.57	110.60	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	zB	1	GAL	C1-O5-C5	2.57	115.64	112.19
2	yC	2	BGC	C1-O5-C5	2.57	115.64	112.19
3	4	1	GAL	C1-O5-C5	2.57	115.64	112.19
3	rA	1	GAL	C1-O5-C5	2.57	115.63	112.19
3	lB	1	GAL	C1-O5-C5	2.57	115.63	112.19
2	5C	2	BGC	C1-O5-C5	2.57	115.63	112.19
2	pA	2	BGC	C1-O5-C5	2.57	115.62	112.19
3	nA	3	A1H1F	O2S6-S6-C6	2.57	110.59	106.76
2	OB	2	BGC	C1-O5-C5	2.56	115.62	112.19
3	ZA	3	A1H1F	O2S6-S6-C6	2.56	110.58	106.76
3	vB	3	A1H1F	O2S6-S6-C6	2.56	110.58	106.76
3	DC	1	GAL	C1-O5-C5	2.56	115.61	112.19
3	EA	3	A1H1F	O2S6-S6-C6	2.56	110.57	106.76
3	hB	3	A1H1F	O2S6-S6-C6	2.56	110.57	106.76
3	XB	1	GAL	C1-O5-C5	2.56	115.61	112.19
2	PC	2	BGC	C1-O5-C5	2.55	115.61	112.19
3	pC	3	A1H1F	O2S6-S6-C6	2.55	110.57	106.76
3	HD	3	A1H1F	O2S6-S6-C6	2.55	110.57	106.76
2	WC	2	BGC	C1-O5-C5	2.55	115.61	112.19
3	gA	3	A1H1F	O2S6-S6-C6	2.55	110.57	106.76
2	GA	2	BGC	C1-O5-C5	2.55	115.61	112.19
3	t	3	A1H1F	O2S6-S6-C6	2.55	110.56	106.76
3	NC	3	A1H1F	O2S6-S6-C6	2.55	110.56	106.76
3	0	3	A1H1F	O2S6-S6-C6	2.55	110.56	106.76
3	m	3	A1H1F	O2S6-S6-C6	2.55	110.56	106.76
2	NA	2	BGC	C1-O5-C5	2.55	115.60	112.19
3	UC	3	A1H1F	O2S6-S6-C6	2.55	110.56	106.76
3	1A	3	A1H1F	O2S6-S6-C6	2.55	110.56	106.76
3	FB	3	A1H1F	O2S6-S6-C6	2.55	110.56	106.76
3	bC	3	A1H1F	O2S6-S6-C6	2.55	110.56	106.76
3	LA	3	A1H1F	O2S6-S6-C6	2.54	110.56	106.76
3	aB	3	A1H1F	O2S6-S6-C6	2.54	110.56	106.76
3	oB	3	A1H1F	O2S6-S6-C6	2.54	110.55	106.76
3	wC	3	A1H1F	O2S6-S6-C6	2.54	110.55	106.76
3	GC	3	A1H1F	O2S6-S6-C6	2.54	110.55	106.76
2	HB	2	BGC	C1-O5-C5	2.54	115.59	112.19
3	uA	3	A1H1F	O2S6-S6-C6	2.54	110.54	106.76
2	9	2	BGC	C1-O5-C5	2.54	115.58	112.19
3	RC	1	GAL	C1-C2-C3	2.53	113.33	109.64
3	5A	1	GAL	C1-C2-C3	2.53	113.33	109.64
3	MB	3	A1H1F	O2S6-S6-C6	2.53	110.54	106.76
3	PA	1	GAL	C1-C2-C3	2.53	113.33	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2B	3	A1H1F	O2S6-S6-C6	2.53	110.54	106.76
3	AD	3	A1H1F	O2S6-S6-C6	2.53	110.53	106.76
3	CB	1	GAL	C1-C2-C3	2.53	113.33	109.64
3	7	3	A1H1F	O2S6-S6-C6	2.53	110.53	106.76
3	TB	3	A1H1F	O2S6-S6-C6	2.53	110.53	106.76
3	iC	3	A1H1F	O2S6-S6-C6	2.52	110.53	106.76
3	0C	1	GAL	C1-C2-C3	2.52	113.31	109.64
3	fC	1	GAL	C1-C2-C3	2.52	113.31	109.64
3	eB	1	GAL	C1-C2-C3	2.52	113.31	109.64
3	3C	3	A1H1F	O2S6-S6-C6	2.52	110.51	106.76
3	dA	1	GAL	C1-C2-C3	2.52	113.31	109.64
3	mC	1	GAL	C1-C2-C3	2.52	113.31	109.64
3	WA	1	GAL	C1-C2-C3	2.51	113.30	109.64
3	7C	1	GAL	C1-C2-C3	2.51	113.30	109.64
4	qC	2	BGC	C1-O5-C5	2.51	115.55	112.19
3	q	1	GAL	C1-C2-C3	2.51	113.30	109.64
3	QB	1	GAL	C1-C2-C3	2.51	113.30	109.64
3	XB	1	GAL	C1-C2-C3	2.51	113.30	109.64
3	YC	1	GAL	C1-C2-C3	2.51	113.30	109.64
3	IA	1	GAL	C1-C2-C3	2.51	113.30	109.64
4	jC	2	BGC	C1-O5-C5	2.51	115.55	112.19
4	GB	2	BGC	C1-O5-C5	2.51	115.55	112.19
3	tC	1	GAL	C1-C2-C3	2.51	113.30	109.64
3	x	1	GAL	C1-C2-C3	2.51	113.29	109.64
3	8A	3	A1H1F	O2S6-S6-C6	2.51	110.50	106.76
3	j	1	GAL	C1-C2-C3	2.51	113.29	109.64
3	rA	1	GAL	C1-C2-C3	2.51	113.29	109.64
3	ED	1	GAL	C1-C2-C3	2.50	113.29	109.64
3	kA	1	GAL	C1-C2-C3	2.50	113.29	109.64
3	6B	1	GAL	C1-C2-C3	2.50	113.29	109.64
4	wB	2	BGC	C1-O5-C5	2.50	115.54	112.19
4	6	1	GAL	C1-O5-C5	2.50	115.54	112.19
4	2A	2	BGC	C1-O5-C5	2.50	115.54	112.19
3	KC	1	GAL	C1-C2-C3	2.50	113.28	109.64
3	sB	1	GAL	C1-C2-C3	2.50	113.28	109.64
4	mA	1	GAL	C1-O5-C5	2.50	115.53	112.19
4	gB	1	GAL	C1-O5-C5	2.50	115.53	112.19
4	FA	2	BGC	C1-O5-C5	2.50	115.53	112.19
3	DC	1	GAL	C1-C2-C3	2.50	113.28	109.64
4	VC	2	BGC	C1-O5-C5	2.49	115.53	112.19
2	pA	2	BGC	C2-C3-C4	2.49	115.25	110.86
3	yA	1	GAL	C1-C2-C3	2.49	113.27	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	9C	1	GAL	C1-O5-C5	2.49	115.53	112.19
4	8B	1	GAL	C1-O5-C5	2.49	115.53	112.19
4	OC	2	BGC	C1-O5-C5	2.49	115.53	112.19
4	YA	1	GAL	C1-O5-C5	2.49	115.52	112.19
4	s	1	GAL	C1-O5-C5	2.49	115.52	112.19
4	8	2	BGC	C1-O5-C5	2.49	115.52	112.19
4	ID	2	BGC	C1-O5-C5	2.49	115.52	112.19
4	RA	1	GAL	C1-O5-C5	2.49	115.52	112.19
4	UB	2	BGC	C1-O5-C5	2.49	115.52	112.19
4	u	2	BGC	C1-O5-C5	2.49	115.52	112.19
4	bB	2	BGC	C1-O5-C5	2.49	115.52	112.19
3	4	1	GAL	C1-C2-C3	2.49	113.26	109.64
3	zB	1	GAL	C1-C2-C3	2.49	113.26	109.64
2	AB	2	BGC	C2-C3-C4	2.48	115.23	110.86
2	yC	2	BGC	C2-C3-C4	2.48	115.23	110.86
4	iB	2	BGC	C1-O5-C5	2.48	115.52	112.19
3	BA	1	GAL	C1-C2-C3	2.48	113.26	109.64
4	LB	1	GAL	C1-O5-C5	2.48	115.51	112.19
4	FC	1	GAL	C1-O5-C5	2.48	115.51	112.19
2	4B	2	BGC	C2-C3-C4	2.48	115.22	110.86
4	hC	1	GAL	C1-O5-C5	2.48	115.51	112.19
4	n	2	BGC	C1-O5-C5	2.48	115.51	112.19
4	DA	1	GAL	C1-O5-C5	2.48	115.51	112.19
4	ZB	1	GAL	C1-O5-C5	2.48	115.51	112.19
4	xC	2	BGC	C1-O5-C5	2.48	115.51	112.19
2	IC	2	BGC	C2-C3-C4	2.48	115.22	110.86
2	HB	2	BGC	C2-C3-C4	2.48	115.22	110.86
4	hA	2	BGC	C1-O5-C5	2.47	115.50	112.19
4	pB	2	BGC	C1-O5-C5	2.47	115.50	112.19
4	3B	2	BGC	C1-O5-C5	2.47	115.50	112.19
3	lB	1	GAL	C1-C2-C3	2.47	113.25	109.64
4	TA	2	BGC	C1-O5-C5	2.47	115.50	112.19
4	aA	2	BGC	C1-O5-C5	2.47	115.50	112.19
2	UA	2	BGC	C2-C3-C4	2.47	115.21	110.86
4	1	2	BGC	C1-O5-C5	2.47	115.50	112.19
3	JB	1	GAL	C1-C2-C3	2.47	113.24	109.64
2	5C	2	BGC	C2-C3-C4	2.47	115.21	110.86
4	SB	1	GAL	C1-O5-C5	2.47	115.50	112.19
2	bA	2	BGC	C2-C3-C4	2.47	115.21	110.86
4	vC	1	GAL	C1-O5-C5	2.47	115.50	112.19
2	wA	2	BGC	C2-C3-C4	2.47	115.20	110.86
2	qB	2	BGC	C2-C3-C4	2.47	115.20	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1B	1	GAL	C1-O5-C5	2.47	115.49	112.19
2	BC	2	BGC	C2-C3-C4	2.47	115.20	110.86
4	BD	2	BGC	C1-O5-C5	2.47	115.49	112.19
4	MA	2	BGC	C1-O5-C5	2.47	115.49	112.19
2	NA	2	BGC	C2-C3-C4	2.47	115.20	110.86
2	jB	2	BGC	C2-C3-C4	2.47	115.20	110.86
2	9	2	BGC	C2-C3-C4	2.47	115.20	110.86
2	UA	3	A1H1F	O3S6-S6-C6	2.46	110.44	106.76
4	l	1	GAL	C1-O5-C5	2.46	115.49	112.19
4	z	1	GAL	C1-O5-C5	2.46	115.49	112.19
2	iA	2	BGC	C2-C3-C4	2.46	115.19	110.86
4	oA	2	BGC	C1-O5-C5	2.46	115.49	112.19
4	aC	1	GAL	C1-O5-C5	2.46	115.49	112.19
4	tA	1	GAL	C1-O5-C5	2.46	115.49	112.19
2	PC	2	BGC	C2-C3-C4	2.46	115.19	110.86
4	GD	1	GAL	C1-O5-C5	2.46	115.49	112.19
4	vA	2	BGC	C1-O5-C5	2.46	115.48	112.19
2	3A	2	BGC	C2-C3-C4	2.46	115.19	110.86
2	OB	2	BGC	C2-C3-C4	2.46	115.19	110.86
4	AC	2	BGC	C1-O5-C5	2.46	115.48	112.19
4	cC	3	A1H1F	O2S6-S6-C6	2.46	110.43	106.76
2	2	2	BGC	C2-C3-C4	2.46	115.19	110.86
2	h	2	BGC	C2-C3-C4	2.46	115.19	110.86
4	nB	1	GAL	C1-O5-C5	2.46	115.48	112.19
2	bA	3	A1H1F	O3S6-S6-C6	2.46	110.43	106.76
4	HC	2	BGC	C1-O5-C5	2.46	115.48	112.19
4	7A	1	GAL	C1-O5-C5	2.46	115.48	112.19
4	cC	2	BGC	C1-O5-C5	2.46	115.48	112.19
2	dC	2	BGC	C2-C3-C4	2.46	115.18	110.86
2	v	2	BGC	C2-C3-C4	2.46	115.18	110.86
2	CD	3	A1H1F	O3S6-S6-C6	2.46	110.42	106.76
4	0A	1	GAL	C1-O5-C5	2.46	115.48	112.19
2	rC	2	BGC	C2-C3-C4	2.46	115.18	110.86
2	HB	3	A1H1F	O3S6-S6-C6	2.46	110.42	106.76
4	EB	1	GAL	C1-O5-C5	2.45	115.48	112.19
4	2C	1	GAL	C1-O5-C5	2.45	115.48	112.19
2	kC	2	BGC	C2-C3-C4	2.45	115.18	110.86
4	4C	2	BGC	C1-O5-C5	2.45	115.47	112.19
2	NA	3	A1H1F	O3S6-S6-C6	2.45	110.42	106.76
2	cB	2	BGC	C2-C3-C4	2.45	115.17	110.86
4	oC	1	GAL	C1-O5-C5	2.45	115.47	112.19
2	GA	2	BGC	C2-C3-C4	2.45	115.17	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3	A1H1F	O3S6-S6-C6	2.45	110.42	106.76
2	o	2	BGC	C2-C3-C4	2.45	115.17	110.86
2	WC	2	BGC	C2-C3-C4	2.45	115.17	110.86
2	v	3	A1H1F	O3S6-S6-C6	2.45	110.41	106.76
2	CD	2	BGC	C2-C3-C4	2.45	115.17	110.86
2	jB	3	A1H1F	O3S6-S6-C6	2.45	110.41	106.76
4	FA	3	A1H1F	O2S6-S6-C6	2.45	110.41	106.76
4	fA	1	GAL	C1-O5-C5	2.45	115.47	112.19
4	TC	1	GAL	C1-O5-C5	2.45	115.47	112.19
2	qB	3	A1H1F	O3S6-S6-C6	2.45	110.41	106.76
4	bB	3	A1H1F	O2S6-S6-C6	2.45	110.41	106.76
4	9A	2	BGC	C1-O5-C5	2.45	115.46	112.19
2	VB	2	BGC	C2-C3-C4	2.45	115.16	110.86
2	PC	3	A1H1F	O3S6-S6-C6	2.45	110.41	106.76
4	wB	3	A1H1F	O2S6-S6-C6	2.44	110.41	106.76
2	h	3	A1H1F	O3S6-S6-C6	2.44	110.41	106.76
2	iA	3	A1H1F	O3S6-S6-C6	2.44	110.40	106.76
2	xB	2	BGC	C2-C3-C4	2.44	115.15	110.86
2	o	3	A1H1F	O3S6-S6-C6	2.44	110.40	106.76
2	cB	3	A1H1F	O3S6-S6-C6	2.44	110.40	106.76
4	iB	3	A1H1F	O2S6-S6-C6	2.44	110.40	106.76
2	wA	3	A1H1F	O3S6-S6-C6	2.44	110.39	106.76
2	WC	3	A1H1F	O3S6-S6-C6	2.44	110.39	106.76
2	kC	3	A1H1F	O3S6-S6-C6	2.44	110.39	106.76
2	GA	3	A1H1F	O3S6-S6-C6	2.44	110.39	106.76
2	pA	3	A1H1F	O3S6-S6-C6	2.44	110.39	106.76
2	IC	3	A1H1F	O3S6-S6-C6	2.44	110.39	106.76
4	NB	2	BGC	C1-O5-C5	2.43	115.45	112.19
4	MC	1	GAL	C1-O5-C5	2.43	115.44	112.19
4	KA	1	GAL	C1-O5-C5	2.43	115.44	112.19
4	qC	3	A1H1F	O2S6-S6-C6	2.43	110.38	106.76
4	uB	1	GAL	C1-O5-C5	2.43	115.44	112.19
3	tB	2	BGC	C3-C4-C5	2.43	114.64	110.23
2	4B	3	A1H1F	O3S6-S6-C6	2.43	110.38	106.76
2	3A	3	A1H1F	O3S6-S6-C6	2.43	110.38	106.76
2	OB	3	A1H1F	O3S6-S6-C6	2.43	110.38	106.76
4	BD	3	A1H1F	O2S6-S6-C6	2.43	110.38	106.76
3	uA	2	BGC	C2-C3-C4	2.43	115.13	110.86
2	VB	3	A1H1F	O3S6-S6-C6	2.43	110.38	106.76
4	7A	2	BGC	C1-O5-C5	2.42	115.44	112.19
4	9C	2	BGC	C1-O5-C5	2.42	115.44	112.19
2	xB	3	A1H1F	O3S6-S6-C6	2.42	110.38	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BC	3	A1H1F	O3S6-S6-C6	2.42	110.38	106.76
2	5C	3	A1H1F	O3S6-S6-C6	2.42	110.38	106.76
3	nC	2	BGC	C3-C4-C5	2.42	114.62	110.23
4	NB	3	A1H1F	O2S6-S6-C6	2.42	110.37	106.76
2	xB	6	A1H03	C1-O5-C5	2.42	115.45	111.48
3	XA	3	A1H1F	O2S6-S6-C6	2.42	110.37	106.76
4	8	3	A1H1F	O2S6-S6-C6	2.42	110.37	106.76
4	2A	3	A1H1F	O2S6-S6-C6	2.42	110.37	106.76
3	t	2	BGC	C2-C3-C4	2.42	115.12	110.86
2	dC	3	A1H1F	O3S6-S6-C6	2.42	110.37	106.76
3	UC	2	BGC	C2-C3-C4	2.42	115.12	110.86
3	zA	3	A1H1F	O2S6-S6-C6	2.42	110.37	106.76
3	0B	3	A1H1F	O2S6-S6-C6	2.42	110.37	106.76
3	uC	2	BGC	C3-C4-C5	2.42	114.62	110.23
2	NA	6	A1H03	C1-O5-C5	2.42	115.44	111.48
3	5	3	A1H1F	O2S6-S6-C6	2.42	110.37	106.76
4	3B	3	A1H1F	O2S6-S6-C6	2.42	110.37	106.76
4	n	3	A1H1F	O2S6-S6-C6	2.42	110.36	106.76
3	JA	3	A1H1F	O2S6-S6-C6	2.42	110.36	106.76
4	9A	3	A1H1F	O2S6-S6-C6	2.42	110.36	106.76
4	GB	3	A1H1F	O2S6-S6-C6	2.42	110.36	106.76
4	UB	3	A1H1F	O2S6-S6-C6	2.42	110.36	106.76
4	HC	3	A1H1F	O2S6-S6-C6	2.42	110.36	106.76
4	4C	3	A1H1F	O2S6-S6-C6	2.42	110.36	106.76
2	rC	3	A1H1F	O3S6-S6-C6	2.42	110.36	106.76
2	UA	6	A1H03	C1-O5-C5	2.42	115.44	111.48
2	AB	3	A1H1F	O3S6-S6-C6	2.42	110.36	106.76
4	hA	3	A1H1F	O2S6-S6-C6	2.42	110.36	106.76
3	NC	2	BGC	C2-C3-C4	2.41	115.11	110.86
2	2	3	A1H1F	O3S6-S6-C6	2.41	110.36	106.76
4	1	3	A1H1F	O2S6-S6-C6	2.41	110.36	106.76
3	9B	2	BGC	C2-C3-C4	2.41	115.11	110.86
2	yC	3	A1H1F	O3S6-S6-C6	2.41	110.36	106.76
4	vA	3	A1H1F	O2S6-S6-C6	2.41	110.36	106.76
2	pA	3	A1H1F	O1S6-S6-C6	2.41	110.63	105.97
4	MA	3	A1H1F	O2S6-S6-C6	2.41	110.36	106.76
4	AC	3	A1H1F	O2S6-S6-C6	2.41	110.36	106.76
4	nB	2	BGC	C1-O5-C5	2.41	115.42	112.19
3	HD	2	BGC	C2-C3-C4	2.41	115.10	110.86
4	ZB	2	BGC	C1-O5-C5	2.41	115.42	112.19
3	bC	2	BGC	C2-C3-C4	2.41	115.10	110.86
4	OC	3	A1H1F	O2S6-S6-C6	2.41	110.36	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	LB	2	BGC	C1-O5-C5	2.41	115.42	112.19
4	uB	2	BGC	C1-O5-C5	2.41	115.42	112.19
3	CA	3	A1H1F	O2S6-S6-C6	2.41	110.36	106.76
4	oA	3	A1H1F	O2S6-S6-C6	2.41	110.36	106.76
4	xC	3	A1H1F	O2S6-S6-C6	2.41	110.36	106.76
3	0B	2	BGC	C3-C4-C5	2.41	114.60	110.23
4	jC	3	A1H1F	O2S6-S6-C6	2.41	110.35	106.76
3	zA	2	BGC	C3-C4-C5	2.41	114.60	110.23
2	jB	3	A1H1F	O1S6-S6-C6	2.41	110.62	105.97
3	eA	2	BGC	C3-C4-C5	2.41	114.60	110.23
2	4B	6	A1H03	C1-O5-C5	2.41	115.42	111.48
4	ID	3	A1H1F	O2S6-S6-C6	2.41	110.35	106.76
2	5C	3	A1H1F	O1S6-S6-C6	2.41	110.62	105.97
2	HB	6	A1H03	C1-O5-C5	2.41	115.42	111.48
4	8B	2	BGC	C1-O5-C5	2.41	115.41	112.19
3	gC	3	A1H1F	O2S6-S6-C6	2.41	110.35	106.76
3	KB	2	BGC	C3-C4-C5	2.41	114.60	110.23
2	3A	6	A1H03	C1-O5-C5	2.41	115.42	111.48
3	iC	2	BGC	C2-C3-C4	2.41	115.09	110.86
2	rC	6	A1H03	C1-O5-C5	2.41	115.42	111.48
3	EC	3	A1H1F	O2S6-S6-C6	2.41	110.35	106.76
3	1C	3	A1H1F	O2S6-S6-C6	2.41	110.35	106.76
3	QA	2	BGC	C3-C4-C5	2.41	114.59	110.23
3	aB	2	BGC	C2-C3-C4	2.41	115.09	110.86
3	3C	2	BGC	C2-C3-C4	2.41	115.09	110.86
4	RA	2	BGC	C1-O5-C5	2.41	115.41	112.19
3	8A	2	BGC	C2-C3-C4	2.41	115.09	110.86
4	VC	3	A1H1F	O2S6-S6-C6	2.41	110.35	106.76
4	pB	3	A1H1F	O2S6-S6-C6	2.40	110.35	106.76
2	GA	6	A1H03	C1-O5-C5	2.40	115.42	111.48
2	NA	3	A1H1F	O1S6-S6-C6	2.40	110.61	105.97
3	m	2	BGC	C2-C3-C4	2.40	115.09	110.86
3	LA	2	BGC	C2-C3-C4	2.40	115.09	110.86
3	KB	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	DB	2	BGC	C3-C4-C5	2.40	114.59	110.23
3	YB	2	BGC	C3-C4-C5	2.40	114.59	110.23
3	7B	2	BGC	C3-C4-C5	2.40	114.59	110.23
2	PC	6	A1H03	C1-O5-C5	2.40	115.42	111.48
4	TA	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	5	2	BGC	C3-C4-C5	2.40	114.59	110.23
2	OB	6	A1H03	C1-O5-C5	2.40	115.42	111.48
3	vB	2	BGC	C2-C3-C4	2.40	115.09	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	nC	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	TB	2	BGC	C2-C3-C4	2.40	115.09	110.86
2	4B	3	A1H1F	O1S6-S6-C6	2.40	110.61	105.97
4	z	2	BGC	C1-O5-C5	2.40	115.41	112.19
3	6A	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
2	WC	6	A1H03	C1-O5-C5	2.40	115.41	111.48
2	PC	3	A1H1F	O1S6-S6-C6	2.40	110.61	105.97
3	JA	2	BGC	C3-C4-C5	2.40	114.59	110.23
2	AB	6	A1H03	C1-O5-C5	2.40	115.41	111.48
4	u	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
4	aA	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
2	cB	3	A1H1F	O1S6-S6-C6	2.40	110.61	105.97
3	GC	2	BGC	C2-C3-C4	2.40	115.08	110.86
3	lA	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	LC	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	8C	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	sA	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	SA	2	BGC	C2-C3-C4	2.40	115.08	110.86
3	eA	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	MB	2	BGC	C2-C3-C4	2.40	115.08	110.86
4	YA	2	BGC	C1-O5-C5	2.40	115.40	112.19
4	EB	2	BGC	C1-O5-C5	2.40	115.40	112.19
2	OB	3	A1H1F	O1S6-S6-C6	2.40	110.60	105.97
3	LC	2	BGC	C3-C4-C5	2.40	114.58	110.23
3	RB	3	A1H1F	O2S6-S6-C6	2.40	110.34	106.76
3	lA	2	BGC	C2-C3-C4	2.40	115.08	110.86
2	pA	6	A1H03	C1-O5-C5	2.40	115.41	111.48
3	r	2	BGC	C3-C4-C5	2.40	114.58	110.23
3	fB	2	BGC	C3-C4-C5	2.40	114.58	110.23
2	HB	3	A1H1F	O1S6-S6-C6	2.40	110.60	105.97
4	s	2	BGC	C1-O5-C5	2.40	115.40	112.19
3	EA	2	BGC	C2-C3-C4	2.40	115.08	110.86
3	r	3	A1H1F	O2S6-S6-C6	2.40	110.33	106.76
3	7B	3	A1H1F	O2S6-S6-C6	2.40	110.33	106.76
2	qB	3	A1H1F	O1S6-S6-C6	2.40	110.60	105.97
4	mA	2	BGC	C1-O5-C5	2.40	115.40	112.19
3	k	3	A1H1F	O2S6-S6-C6	2.40	110.33	106.76
2	cB	6	A1H03	C1-O5-C5	2.40	115.40	111.48
2	CD	6	A1H03	C1-O5-C5	2.40	115.40	111.48
4	6	2	BGC	C1-O5-C5	2.40	115.40	112.19
2	9	3	A1H1F	O1S6-S6-C6	2.39	110.60	105.97
2	2	6	A1H03	C1-O5-C5	2.39	115.40	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	ZC	2	BGC	C3-C4-C5	2.39	114.57	110.23
4	DA	2	BGC	C1-O5-C5	2.39	115.39	112.19
4	fA	2	BGC	C1-O5-C5	2.39	115.39	112.19
2	wA	5	MAN	C1-C2-C3	2.39	113.13	109.64
3	0	2	BGC	C2-C3-C4	2.39	115.07	110.86
3	nA	2	BGC	C2-C3-C4	2.39	115.07	110.86
2	yC	3	A1H1F	O1S6-S6-C6	2.39	110.59	105.97
2	h	6	A1H03	C1-O5-C5	2.39	115.40	111.48
2	9	6	A1H03	C1-O5-C5	2.39	115.40	111.48
3	k	2	BGC	C3-C4-C5	2.39	114.57	110.23
3	YB	3	A1H1F	O2S6-S6-C6	2.39	110.33	106.76
3	SC	3	A1H1F	O2S6-S6-C6	2.39	110.33	106.76
2	AB	3	A1H1F	O1S6-S6-C6	2.39	110.59	105.97
3	QA	3	A1H1F	O2S6-S6-C6	2.39	110.33	106.76
3	tB	3	A1H1F	O2S6-S6-C6	2.39	110.33	106.76
3	ZC	3	A1H1F	O2S6-S6-C6	2.39	110.33	106.76
2	dC	3	A1H1F	O1S6-S6-C6	2.39	110.59	105.97
2	rC	3	A1H1F	O1S6-S6-C6	2.39	110.59	105.97
2	CD	3	A1H1F	O1S6-S6-C6	2.39	110.59	105.97
3	lA	2	BGC	C3-C4-C5	2.39	114.57	110.23
3	6A	2	BGC	C3-C4-C5	2.39	114.57	110.23
4	aC	2	BGC	C1-O5-C5	2.39	115.39	112.19
2	o	3	A1H1F	O1S6-S6-C6	2.39	110.59	105.97
3	mB	2	BGC	C3-C4-C5	2.39	114.56	110.23
3	8C	2	BGC	C3-C4-C5	2.39	114.56	110.23
2	iA	3	A1H1F	O1S6-S6-C6	2.39	110.58	105.97
2	3A	3	A1H1F	O1S6-S6-C6	2.39	110.58	105.97
2	qB	6	A1H03	C1-O5-C5	2.39	115.39	111.48
2	IC	6	A1H03	C1-O5-C5	2.39	115.39	111.48
3	RB	2	BGC	C3-C4-C5	2.39	114.56	110.23
3	EC	2	BGC	C3-C4-C5	2.39	114.56	110.23
3	FD	2	BGC	C3-C4-C5	2.39	114.56	110.23
2	VB	3	A1H1F	O1S6-S6-C6	2.39	110.58	105.97
2	bA	5	MAN	C1-C2-C3	2.39	113.12	109.64
4	l	2	BGC	C1-O5-C5	2.39	115.39	112.19
3	sA	2	BGC	C3-C4-C5	2.39	114.56	110.23
3	SC	2	BGC	C3-C4-C5	2.39	114.56	110.23
3	oB	2	BGC	C2-C3-C4	2.39	115.06	110.86
3	pC	2	BGC	C2-C3-C4	2.39	115.06	110.86
2	xB	5	MAN	C1-C2-C3	2.39	113.12	109.64
3	mB	3	A1H1F	O2S6-S6-C6	2.39	110.32	106.76
3	AD	2	BGC	C2-C3-C4	2.39	115.06	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2C	2	BGC	C1-O5-C5	2.39	115.39	112.19
2	h	3	A1H1F	O1S6-S6-C6	2.39	110.58	105.97
2	BC	6	A1H03	C1-O5-C5	2.39	115.39	111.48
3	1C	2	BGC	C3-C4-C5	2.39	114.56	110.23
2	xB	3	A1H1F	O1S6-S6-C6	2.39	110.58	105.97
2	BC	3	A1H1F	O1S6-S6-C6	2.39	110.58	105.97
2	CD	5	MAN	C1-C2-C3	2.39	113.12	109.64
2	v	3	A1H1F	O1S6-S6-C6	2.39	110.58	105.97
3	wC	2	BGC	C2-C3-C4	2.39	115.06	110.86
3	XA	2	BGC	C3-C4-C5	2.38	114.56	110.23
3	gA	2	BGC	C2-C3-C4	2.38	115.06	110.86
2	5C	6	A1H03	C1-O5-C5	2.38	115.39	111.48
4	1B	2	BGC	C1-O5-C5	2.38	115.38	112.19
2	o	6	A1H03	C1-O5-C5	2.38	115.38	111.48
2	wA	6	A1H03	C1-O5-C5	2.38	115.38	111.48
3	gC	2	BGC	C3-C4-C5	2.38	114.55	110.23
3	ZA	2	BGC	C2-C3-C4	2.38	115.05	110.86
2	bA	6	A1H03	C1-O5-C5	2.38	115.38	111.48
2	wA	3	A1H1F	O1S6-S6-C6	2.38	110.57	105.97
2	dC	6	A1H03	C1-O5-C5	2.38	115.38	111.48
3	hB	2	BGC	C2-C3-C4	2.38	115.05	110.86
3	2B	2	BGC	C2-C3-C4	2.38	115.05	110.86
2	bA	3	A1H1F	O1S6-S6-C6	2.38	110.57	105.97
2	yC	5	MAN	C1-C2-C3	2.38	113.11	109.64
3	7	2	BGC	C2-C3-C4	2.38	115.05	110.86
3	FB	2	BGC	C2-C3-C4	2.38	115.05	110.86
2	yC	6	A1H03	C1-O5-C5	2.38	115.38	111.48
2	2	3	A1H1F	O1S6-S6-C6	2.38	110.57	105.97
2	UA	3	A1H1F	O1S6-S6-C6	2.38	110.57	105.97
2	IC	3	A1H1F	O1S6-S6-C6	2.38	110.57	105.97
4	MC	2	BGC	C1-O5-C5	2.38	115.37	112.19
2	IC	5	MAN	C1-C2-C3	2.38	113.11	109.64
2	iA	6	A1H03	C1-O5-C5	2.38	115.38	111.48
2	jB	6	A1H03	C1-O5-C5	2.38	115.38	111.48
3	y	2	BGC	C3-C4-C5	2.38	114.54	110.23
4	TC	2	BGC	C1-O5-C5	2.38	115.37	112.19
2	GA	3	A1H1F	O1S6-S6-C6	2.38	110.56	105.97
2	kC	6	A1H03	C1-O5-C5	2.38	115.37	111.48
3	DB	3	A1H1F	O2S6-S6-C6	2.38	110.30	106.76
2	WC	3	A1H1F	O1S6-S6-C6	2.38	110.56	105.97
2	v	5	MAN	C1-C2-C3	2.37	113.10	109.64
2	WC	5	MAN	C1-C2-C3	2.37	113.10	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	v	6	A1H03	C1-O5-C5	2.37	115.37	111.48
3	y	3	A1H1F	O2S6-S6-C6	2.37	110.30	106.76
4	0A	2	BGC	C1-O5-C5	2.37	115.37	112.19
2	BC	5	MAN	C1-C2-C3	2.37	113.10	109.64
4	oA	3	A1H1F	C1-C2-C3	2.37	113.10	109.64
4	KA	2	BGC	C1-O5-C5	2.37	115.37	112.19
3	CA	2	BGC	C3-C4-C5	2.37	114.53	110.23
4	GD	2	BGC	C1-O5-C5	2.37	115.36	112.19
4	SB	2	BGC	C1-O5-C5	2.37	115.36	112.19
4	vC	2	BGC	C1-O5-C5	2.37	115.36	112.19
3	fB	3	A1H1F	O2S6-S6-C6	2.37	110.29	106.76
3	uC	3	A1H1F	O2S6-S6-C6	2.37	110.29	106.76
2	VB	6	A1H03	C1-O5-C5	2.37	115.36	111.48
2	qB	5	MAN	C1-C2-C3	2.37	113.09	109.64
2	kC	3	A1H1F	O1S6-S6-C6	2.37	110.54	105.97
4	FC	2	BGC	C1-O5-C5	2.37	115.36	112.19
4	u	3	A1H1F	C1-C2-C3	2.37	113.09	109.64
2	AB	5	MAN	C1-C2-C3	2.37	113.09	109.64
2	jB	5	MAN	C1-C2-C3	2.37	113.09	109.64
4	aA	3	A1H1F	C1-C2-C3	2.37	113.09	109.64
3	FD	3	A1H1F	O2S6-S6-C6	2.37	110.29	106.76
2	rC	5	MAN	C1-C2-C3	2.37	113.09	109.64
2	NA	5	MAN	C1-C2-C3	2.36	113.09	109.64
4	OC	3	A1H1F	C1-C2-C3	2.36	113.09	109.64
4	gB	2	BGC	C1-O5-C5	2.36	115.35	112.19
2	h	5	MAN	C1-C2-C3	2.36	113.08	109.64
4	qC	3	A1H1F	C1-C2-C3	2.36	113.08	109.64
2	9	5	MAN	C1-C2-C3	2.36	113.08	109.64
2	iA	5	MAN	C1-C2-C3	2.36	113.08	109.64
4	2A	3	A1H1F	C1-C2-C3	2.36	113.08	109.64
2	kC	5	MAN	C1-C2-C3	2.36	113.08	109.64
4	hC	2	BGC	C1-O5-C5	2.36	115.34	112.19
4	tA	2	BGC	C1-O5-C5	2.36	115.34	112.19
4	oC	2	BGC	C1-O5-C5	2.36	115.34	112.19
2	VB	5	MAN	C1-C2-C3	2.36	113.08	109.64
4	VC	3	A1H1F	C1-C2-C3	2.36	113.07	109.64
2	2	5	MAN	C1-C2-C3	2.35	113.07	109.64
2	dC	5	MAN	C1-C2-C3	2.35	113.07	109.64
4	AC	3	A1H1F	C1-C2-C3	2.35	113.07	109.64
2	3A	5	MAN	C1-C2-C3	2.35	113.07	109.64
4	vA	3	A1H1F	C1-C2-C3	2.35	113.07	109.64
2	UA	5	MAN	C1-C2-C3	2.35	113.07	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4B	5	MAN	C1-C2-C3	2.35	113.07	109.64
2	o	5	MAN	C1-C2-C3	2.35	113.06	109.64
2	pA	5	MAN	C1-C2-C3	2.35	113.06	109.64
4	8	3	A1H1F	C1-C2-C3	2.35	113.06	109.64
4	FA	3	A1H1F	C1-C2-C3	2.35	113.06	109.64
4	9A	3	A1H1F	C1-C2-C3	2.35	113.06	109.64
2	cB	5	MAN	C1-C2-C3	2.35	113.06	109.64
4	jC	3	A1H1F	C1-C2-C3	2.35	113.06	109.64
4	4C	3	A1H1F	C1-C2-C3	2.35	113.06	109.64
2	5C	5	MAN	C1-C2-C3	2.35	113.06	109.64
2	PC	5	MAN	C1-C2-C3	2.35	113.06	109.64
2	GA	5	MAN	C1-C2-C3	2.35	113.06	109.64
4	iB	3	A1H1F	C1-C2-C3	2.35	113.06	109.64
4	MA	3	A1H1F	C1-C2-C3	2.34	113.06	109.64
2	3A	1	GAL	C1-C2-C3	2.34	113.06	109.64
2	HB	5	MAN	C1-C2-C3	2.34	113.06	109.64
4	ID	3	A1H1F	C1-C2-C3	2.34	113.06	109.64
4	3B	3	A1H1F	C1-C2-C3	2.34	113.05	109.64
4	n	3	A1H1F	C1-C2-C3	2.34	113.05	109.64
4	cC	3	A1H1F	C1-C2-C3	2.34	113.05	109.64
4	NB	3	A1H1F	C1-C2-C3	2.34	113.05	109.64
2	2	1	GAL	C1-C2-C3	2.34	113.05	109.64
4	pB	3	A1H1F	C1-C2-C3	2.34	113.05	109.64
4	BD	3	A1H1F	C1-C2-C3	2.34	113.04	109.64
4	VC	3	A1H1F	O3S6-S6-C6	2.33	110.24	106.76
2	OB	5	MAN	C1-C2-C3	2.33	113.04	109.64
4	TA	3	A1H1F	C1-C2-C3	2.33	113.04	109.64
4	UB	3	A1H1F	C1-C2-C3	2.33	113.04	109.64
4	bB	3	A1H1F	C1-C2-C3	2.33	113.03	109.64
4	GB	3	A1H1F	C1-C2-C3	2.33	113.03	109.64
4	1	3	A1H1F	C1-C2-C3	2.33	113.03	109.64
4	u	3	A1H1F	O3S6-S6-C6	2.32	110.23	106.76
4	hA	3	A1H1F	C1-C2-C3	2.32	113.03	109.64
4	bB	3	A1H1F	O3S6-S6-C6	2.32	110.22	106.76
4	pB	3	A1H1F	O3S6-S6-C6	2.32	110.22	106.76
2	WC	1	GAL	C1-C2-C3	2.32	113.03	109.64
2	dC	1	GAL	C1-C2-C3	2.32	113.03	109.64
4	HC	3	A1H1F	C1-C2-C3	2.32	113.02	109.64
4	1	3	A1H1F	O3S6-S6-C6	2.32	110.22	106.76
2	GA	1	GAL	C1-C2-C3	2.32	113.02	109.64
2	BC	1	GAL	C1-C2-C3	2.32	113.02	109.64
4	UB	3	A1H1F	O3S6-S6-C6	2.32	110.22	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	xC	3	A1H1F	C1-C2-C3	2.32	113.02	109.64
4	hA	3	A1H1F	O3S6-S6-C6	2.32	110.21	106.76
4	GB	3	A1H1F	O3S6-S6-C6	2.32	110.21	106.76
2	4B	1	GAL	C1-C2-C3	2.32	113.02	109.64
2	PC	1	GAL	C1-C2-C3	2.32	113.02	109.64
2	o	1	GAL	C1-C2-C3	2.31	113.01	109.64
2	xB	1	GAL	C1-C2-C3	2.31	113.01	109.64
4	9A	3	A1H1F	O3S6-S6-C6	2.31	110.21	106.76
2	HB	1	GAL	C1-C2-C3	2.31	113.01	109.64
2	kC	1	GAL	C1-C2-C3	2.31	113.01	109.64
2	h	1	GAL	C1-C2-C3	2.31	113.01	109.64
2	UA	1	GAL	C1-C2-C3	2.31	113.01	109.64
2	cB	1	GAL	C1-C2-C3	2.31	113.01	109.64
2	pA	1	GAL	C1-C2-C3	2.31	113.01	109.64
2	wA	1	GAL	C1-C2-C3	2.31	113.01	109.64
4	NB	3	A1H1F	O3S6-S6-C6	2.31	110.21	106.76
4	jC	3	A1H1F	O3S6-S6-C6	2.31	110.21	106.76
4	wB	3	A1H1F	C1-C2-C3	2.31	113.01	109.64
4	TA	3	A1H1F	O3S6-S6-C6	2.31	110.20	106.76
4	ID	3	A1H1F	O3S6-S6-C6	2.31	110.20	106.76
3	7	3	A1H1F	O1S6-S6-C6	2.31	110.43	105.97
2	OB	1	GAL	C1-C2-C3	2.31	113.00	109.64
4	4C	3	A1H1F	O3S6-S6-C6	2.31	110.20	106.76
4	wB	3	A1H1F	O3S6-S6-C6	2.30	110.20	106.76
2	5C	1	GAL	C1-C2-C3	2.30	113.00	109.64
4	2A	3	A1H1F	O3S6-S6-C6	2.30	110.19	106.76
2	AB	1	GAL	C1-C2-C3	2.30	113.00	109.64
4	n	3	A1H1F	O3S6-S6-C6	2.30	110.19	106.76
4	aA	3	A1H1F	O3S6-S6-C6	2.30	110.19	106.76
4	AC	3	A1H1F	O3S6-S6-C6	2.30	110.19	106.76
4	cC	3	A1H1F	O3S6-S6-C6	2.30	110.19	106.76
2	VB	1	GAL	C1-C2-C3	2.30	112.99	109.64
4	xC	3	A1H1F	O3S6-S6-C6	2.30	110.19	106.76
3	hB	4	A1H03	C1-O5-C5	2.30	115.25	111.48
2	bA	1	GAL	C1-C2-C3	2.30	112.99	109.64
4	OC	3	A1H1F	O3S6-S6-C6	2.30	110.19	106.76
3	UC	3	A1H1F	O1S6-S6-C6	2.30	110.41	105.97
2	CD	1	GAL	C1-C2-C3	2.30	112.99	109.64
4	MA	3	A1H1F	O3S6-S6-C6	2.30	110.18	106.76
2	v	1	GAL	C1-C2-C3	2.30	112.99	109.64
3	8A	4	A1H03	C1-O5-C5	2.30	115.24	111.48
2	iA	1	GAL	C1-C2-C3	2.30	112.99	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	qB	1	GAL	C1-C2-C3	2.30	112.99	109.64
4	8	3	A1H1F	O3S6-S6-C6	2.29	110.18	106.76
4	3B	3	A1H1F	O3S6-S6-C6	2.29	110.18	106.76
3	t	4	A1H03	C1-O5-C5	2.29	115.24	111.48
4	FA	3	A1H1F	O3S6-S6-C6	2.29	110.18	106.76
3	oB	4	A1H03	C1-O5-C5	2.29	115.24	111.48
3	oB	3	A1H1F	O1S6-S6-C6	2.29	110.40	105.97
2	jB	1	GAL	C1-C2-C3	2.29	112.98	109.64
3	FB	4	A1H03	C1-O5-C5	2.29	115.23	111.48
3	AD	4	A1H03	C1-O5-C5	2.29	115.23	111.48
2	IC	1	GAL	C1-C2-C3	2.29	112.98	109.64
3	gA	3	A1H1F	O1S6-S6-C6	2.29	110.40	105.97
4	BD	3	A1H1F	O3S6-S6-C6	2.29	110.18	106.76
2	NA	1	GAL	C1-C2-C3	2.29	112.98	109.64
3	MB	4	A1H03	C1-O5-C5	2.29	115.23	111.48
3	hB	3	A1H1F	O1S6-S6-C6	2.29	110.40	105.97
3	SA	3	A1H1F	O1S6-S6-C6	2.29	110.39	105.97
2	yC	1	GAL	C1-C2-C3	2.29	112.98	109.64
3	HD	4	A1H03	C1-O5-C5	2.29	115.23	111.48
2	rC	1	GAL	C1-C2-C3	2.29	112.98	109.64
3	1A	3	A1H1F	O1S6-S6-C6	2.29	110.39	105.97
3	MB	3	A1H1F	O1S6-S6-C6	2.29	110.39	105.97
3	TB	3	A1H1F	O1S6-S6-C6	2.29	110.39	105.97
3	2B	4	A1H03	C1-O5-C5	2.29	115.23	111.48
3	NC	4	A1H03	C1-O5-C5	2.29	115.23	111.48
3	uA	3	A1H1F	O1S6-S6-C6	2.29	110.39	105.97
2	9	1	GAL	C1-C2-C3	2.29	112.97	109.64
3	wC	3	A1H1F	O1S6-S6-C6	2.29	110.39	105.97
3	AD	3	A1H1F	O1S6-S6-C6	2.29	110.39	105.97
3	pC	4	A1H03	C1-O5-C5	2.29	115.22	111.48
3	wC	4	A1H03	C1-O5-C5	2.29	115.22	111.48
3	vB	3	A1H1F	O1S6-S6-C6	2.29	110.39	105.97
4	iB	3	A1H1F	O3S6-S6-C6	2.29	110.17	106.76
3	vB	4	A1H03	C1-O5-C5	2.28	115.22	111.48
3	uA	4	A1H03	C1-O5-C5	2.28	115.22	111.48
3	NC	3	A1H1F	O1S6-S6-C6	2.28	110.38	105.97
3	nA	3	A1H1F	O1S6-S6-C6	2.28	110.38	105.97
3	bC	3	A1H1F	O1S6-S6-C6	2.28	110.38	105.97
3	m	3	A1H1F	O1S6-S6-C6	2.28	110.37	105.97
3	2B	3	A1H1F	O1S6-S6-C6	2.28	110.37	105.97
4	HC	3	A1H1F	O3S6-S6-C6	2.28	110.16	106.76
3	GC	3	A1H1F	O1S6-S6-C6	2.28	110.37	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FB	3	A1H1F	O1S6-S6-C6	2.28	110.37	105.97
4	oA	3	A1H1F	O3S6-S6-C6	2.28	110.16	106.76
3	GC	4	A1H03	C1-O5-C5	2.28	115.21	111.48
3	aB	3	A1H1F	O1S6-S6-C6	2.28	110.37	105.97
3	iC	3	A1H1F	O1S6-S6-C6	2.28	110.37	105.97
3	t	3	A1H1F	O1S6-S6-C6	2.28	110.37	105.97
4	vA	3	A1H1F	O3S6-S6-C6	2.28	110.15	106.76
3	9B	3	A1H1F	O1S6-S6-C6	2.27	110.36	105.97
3	ZA	4	A1H03	C1-O5-C5	2.27	115.20	111.48
3	TB	4	A1H03	C1-O5-C5	2.27	115.20	111.48
3	HD	3	A1H1F	O1S6-S6-C6	2.27	110.36	105.97
3	m	4	A1H03	C1-O5-C5	2.27	115.20	111.48
3	dA	3	A1H1F	O2S6-S6-C6	2.27	110.15	106.76
3	LA	3	A1H1F	O1S6-S6-C6	2.27	110.36	105.97
3	pC	3	A1H1F	O1S6-S6-C6	2.27	110.36	105.97
3	8A	3	A1H1F	O1S6-S6-C6	2.27	110.35	105.97
3	1A	4	A1H03	C1-O5-C5	2.27	115.20	111.48
3	3C	3	A1H1F	O1S6-S6-C6	2.27	110.35	105.97
3	SA	4	A1H03	C1-O5-C5	2.27	115.19	111.48
3	nA	4	A1H03	C1-O5-C5	2.27	115.19	111.48
4	qC	3	A1H1F	O3S6-S6-C6	2.27	110.14	106.76
3	mC	3	A1H1F	O2S6-S6-C6	2.27	110.14	106.76
3	0	3	A1H1F	O1S6-S6-C6	2.27	110.35	105.97
3	JB	3	A1H1F	O2S6-S6-C6	2.27	110.14	106.76
3	EA	3	A1H1F	O1S6-S6-C6	2.27	110.35	105.97
3	ZA	3	A1H1F	O1S6-S6-C6	2.27	110.35	105.97
3	bC	4	A1H03	C1-O5-C5	2.27	115.19	111.48
3	DC	3	A1H1F	O2S6-S6-C6	2.27	110.14	106.76
3	gA	4	A1H03	C1-O5-C5	2.27	115.19	111.48
3	PA	3	A1H1F	O2S6-S6-C6	2.26	110.13	106.76
3	iC	4	A1H03	C1-O5-C5	2.26	115.18	111.48
3	RC	3	A1H1F	O2S6-S6-C6	2.26	110.13	106.76
3	7	4	A1H03	C1-O5-C5	2.26	115.18	111.48
3	rA	3	A1H1F	O2S6-S6-C6	2.26	110.13	106.76
3	5A	3	A1H1F	O2S6-S6-C6	2.26	110.13	106.76
3	x	3	A1H1F	O2S6-S6-C6	2.26	110.12	106.76
3	0	4	A1H03	C1-O5-C5	2.26	115.17	111.48
3	WA	3	A1H1F	O2S6-S6-C6	2.26	110.12	106.76
3	9B	4	A1H03	C1-O5-C5	2.26	115.17	111.48
3	3C	4	A1H03	C1-O5-C5	2.26	115.17	111.48
3	EA	4	A1H03	C1-O5-C5	2.25	115.17	111.48
3	UC	4	A1H03	C1-O5-C5	2.25	115.17	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	LA	4	A1H03	C1-O5-C5	2.25	115.17	111.48
3	IA	3	A1H1F	O2S6-S6-C6	2.25	110.12	106.76
3	kA	3	A1H1F	O2S6-S6-C6	2.25	110.12	106.76
3	yA	3	A1H1F	O2S6-S6-C6	2.25	110.12	106.76
3	tC	3	A1H1F	O2S6-S6-C6	2.25	110.12	106.76
3	fC	3	A1H1F	O2S6-S6-C6	2.25	110.11	106.76
3	XB	3	A1H1F	O1S6-S6-C6	2.25	110.31	105.97
3	4	3	A1H1F	O2S6-S6-C6	2.25	110.11	106.76
3	YC	3	A1H1F	O2S6-S6-C6	2.25	110.11	106.76
3	lB	3	A1H1F	O2S6-S6-C6	2.25	110.11	106.76
3	j	3	A1H1F	O2S6-S6-C6	2.25	110.11	106.76
3	sB	3	A1H1F	O2S6-S6-C6	2.24	110.11	106.76
4	gB	2	BGC	C2-C3-C4	2.24	114.81	110.86
3	KC	3	A1H1F	O2S6-S6-C6	2.24	110.10	106.76
3	0C	3	A1H1F	O2S6-S6-C6	2.24	110.10	106.76
3	QB	3	A1H1F	O2S6-S6-C6	2.24	110.10	106.76
3	zB	3	A1H1F	O2S6-S6-C6	2.24	110.10	106.76
3	ED	3	A1H1F	O2S6-S6-C6	2.24	110.10	106.76
3	0C	3	A1H1F	O1S6-S6-C6	2.24	110.30	105.97
3	aB	4	A1H03	C1-O5-C5	2.24	115.15	111.48
3	IA	3	A1H1F	O1S6-S6-C6	2.24	110.29	105.97
3	QB	3	A1H1F	O1S6-S6-C6	2.24	110.29	105.97
3	7C	3	A1H1F	O1S6-S6-C6	2.24	110.29	105.97
4	KA	2	BGC	C2-C3-C4	2.24	114.79	110.86
3	BA	3	A1H1F	O2S6-S6-C6	2.24	110.09	106.76
3	CB	3	A1H1F	O2S6-S6-C6	2.23	110.09	106.76
3	BA	3	A1H1F	O1S6-S6-C6	2.23	110.28	105.97
3	6B	3	A1H1F	O2S6-S6-C6	2.23	110.09	106.76
4	DA	2	BGC	C2-C3-C4	2.23	114.79	110.86
3	7C	3	A1H1F	O2S6-S6-C6	2.23	110.09	106.76
3	6B	3	A1H1F	O1S6-S6-C6	2.23	110.28	105.97
3	rA	3	A1H1F	O1S6-S6-C6	2.23	110.28	105.97
3	DC	3	A1H1F	O1S6-S6-C6	2.23	110.28	105.97
3	lB	3	A1H1F	O1S6-S6-C6	2.23	110.28	105.97
3	XB	3	A1H1F	O2S6-S6-C6	2.23	110.08	106.76
3	q	3	A1H1F	O2S6-S6-C6	2.23	110.08	106.76
3	PA	3	A1H1F	O1S6-S6-C6	2.23	110.27	105.97
4	EB	2	BGC	C2-C3-C4	2.22	114.77	110.86
3	RC	3	A1H1F	O1S6-S6-C6	2.22	110.27	105.97
3	dA	3	A1H1F	O1S6-S6-C6	2.22	110.27	105.97
3	CB	3	A1H1F	O1S6-S6-C6	2.22	110.26	105.97
3	kA	3	A1H1F	O1S6-S6-C6	2.22	110.26	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	eB	3	A1H1F	O2S6-S6-C6	2.22	110.07	106.76
4	nB	2	BGC	C2-C3-C4	2.22	114.77	110.86
4	MC	2	BGC	C2-C3-C4	2.22	114.77	110.86
3	JB	3	A1H1F	O1S6-S6-C6	2.22	110.26	105.97
3	KC	3	A1H1F	O1S6-S6-C6	2.22	110.26	105.97
3	j	3	A1H1F	O1S6-S6-C6	2.22	110.26	105.97
4	fA	2	BGC	C2-C3-C4	2.22	114.76	110.86
3	zB	3	A1H1F	O1S6-S6-C6	2.22	110.26	105.97
4	ZB	2	BGC	C2-C3-C4	2.22	114.76	110.86
3	sB	3	A1H1F	O1S6-S6-C6	2.22	110.25	105.97
4	uB	2	BGC	C2-C3-C4	2.22	114.76	110.86
3	5A	3	A1H1F	O1S6-S6-C6	2.22	110.25	105.97
4	GD	2	BGC	C2-C3-C4	2.21	114.76	110.86
3	fC	3	A1H1F	O1S6-S6-C6	2.21	110.25	105.97
3	tC	3	A1H1F	O1S6-S6-C6	2.21	110.25	105.97
4	mA	2	BGC	C2-C3-C4	2.21	114.75	110.86
3	x	3	A1H1F	O1S6-S6-C6	2.21	110.25	105.97
4	aC	2	BGC	C2-C3-C4	2.21	114.75	110.86
4	l	2	BGC	C2-C3-C4	2.21	114.75	110.86
3	ED	3	A1H1F	O1S6-S6-C6	2.21	110.24	105.97
3	JB	2	BGC	C3-C4-C5	2.21	114.24	110.23
3	YC	3	A1H1F	O1S6-S6-C6	2.21	110.24	105.97
4	0A	2	BGC	C2-C3-C4	2.21	114.75	110.86
4	8B	2	BGC	C2-C3-C4	2.21	114.75	110.86
4	hC	2	BGC	C2-C3-C4	2.21	114.75	110.86
3	x	2	BGC	C3-C4-C5	2.21	114.24	110.23
3	mC	3	A1H1F	O1S6-S6-C6	2.21	110.24	105.97
3	0C	2	BGC	C3-C4-C5	2.21	114.23	110.23
4	RA	2	BGC	C2-C3-C4	2.21	114.74	110.86
3	4	3	A1H1F	O1S6-S6-C6	2.21	110.23	105.97
3	q	2	BGC	C3-C4-C5	2.21	114.23	110.23
3	6B	2	BGC	C3-C4-C5	2.21	114.23	110.23
4	tA	2	BGC	C2-C3-C4	2.21	114.74	110.86
4	LB	2	BGC	C2-C3-C4	2.21	114.74	110.86
3	eB	2	BGC	C3-C4-C5	2.21	114.23	110.23
4	9C	2	BGC	C2-C3-C4	2.20	114.74	110.86
4	vC	2	BGC	C2-C3-C4	2.20	114.74	110.86
3	PA	2	BGC	C3-C4-C5	2.20	114.22	110.23
3	7C	2	BGC	C3-C4-C5	2.20	114.22	110.23
4	YA	2	BGC	C2-C3-C4	2.20	114.73	110.86
3	BA	2	BGC	C3-C4-C5	2.20	114.22	110.23
4	FC	2	BGC	C2-C3-C4	2.20	114.73	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	yA	3	A1H1F	O1S6-S6-C6	2.20	110.22	105.97
3	4	2	BGC	C3-C4-C5	2.20	114.22	110.23
3	QB	2	BGC	C3-C4-C5	2.20	114.22	110.23
4	6	2	BGC	C2-C3-C4	2.20	114.73	110.86
3	CB	2	BGC	C3-C4-C5	2.20	114.22	110.23
4	SB	2	BGC	C2-C3-C4	2.20	114.73	110.86
3	q	3	A1H1F	O1S6-S6-C6	2.20	110.22	105.97
3	KC	2	BGC	C3-C4-C5	2.20	114.22	110.23
3	YC	2	BGC	C3-C4-C5	2.20	114.22	110.23
4	TC	2	BGC	C2-C3-C4	2.20	114.72	110.86
3	WA	3	A1H1F	O1S6-S6-C6	2.20	110.21	105.97
4	s	2	BGC	C2-C3-C4	2.20	114.72	110.86
4	1B	2	BGC	C2-C3-C4	2.20	114.72	110.86
4	2C	2	BGC	C2-C3-C4	2.20	114.72	110.86
3	DC	2	BGC	C3-C4-C5	2.20	114.21	110.23
3	kA	2	BGC	C3-C4-C5	2.19	114.21	110.23
3	sB	2	BGC	C3-C4-C5	2.19	114.21	110.23
3	RC	2	BGC	C3-C4-C5	2.19	114.21	110.23
3	eB	3	A1H1F	O1S6-S6-C6	2.19	110.21	105.97
4	oC	2	BGC	C2-C3-C4	2.19	114.72	110.86
3	tC	2	BGC	C3-C4-C5	2.19	114.21	110.23
4	7A	2	BGC	C2-C3-C4	2.19	114.72	110.86
4	z	2	BGC	C2-C3-C4	2.19	114.72	110.86
3	j	2	BGC	C3-C4-C5	2.19	114.21	110.23
3	5A	2	BGC	C3-C4-C5	2.19	114.21	110.23
3	IA	2	BGC	C3-C4-C5	2.19	114.20	110.23
3	dA	2	BGC	C3-C4-C5	2.19	114.20	110.23
3	WA	2	BGC	C3-C4-C5	2.19	114.20	110.23
3	yA	2	BGC	C3-C4-C5	2.19	114.19	110.23
3	zB	2	BGC	C3-C4-C5	2.19	114.19	110.23
4	8B	3	A1H1F	O2S6-S6-C6	2.19	110.02	106.76
3	lB	2	BGC	C3-C4-C5	2.18	114.19	110.23
3	XB	2	BGC	C3-C4-C5	2.18	114.19	110.23
3	mC	2	BGC	C3-C4-C5	2.18	114.19	110.23
3	rA	2	BGC	C3-C4-C5	2.18	114.18	110.23
4	uB	3	A1H1F	O2S6-S6-C6	2.18	110.01	106.76
3	ED	2	BGC	C3-C4-C5	2.18	114.18	110.23
4	DA	3	A1H1F	O2S6-S6-C6	2.17	110.00	106.76
4	ZB	3	A1H1F	O2S6-S6-C6	2.17	110.00	106.76
4	6	3	A1H1F	O2S6-S6-C6	2.17	110.00	106.76
3	gC	4	A1H03	C1-O5-C5	2.17	115.03	111.48
4	TC	3	A1H1F	O2S6-S6-C6	2.17	110.00	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	fC	2	BGC	C3-C4-C5	2.17	114.16	110.23
3	XA	4	A1H03	C1-O5-C5	2.17	115.03	111.48
4	MC	3	A1H1F	O2S6-S6-C6	2.17	109.99	106.76
4	vC	3	A1H1F	O2S6-S6-C6	2.16	109.98	106.76
3	mB	4	A1H03	C1-O5-C5	2.16	115.02	111.48
4	7A	3	A1H1F	O2S6-S6-C6	2.16	109.98	106.76
3	tB	4	A1H03	C1-O5-C5	2.16	115.02	111.48
3	RB	4	A1H03	C1-O5-C5	2.16	115.01	111.48
4	fA	3	A1H1F	O2S6-S6-C6	2.16	109.97	106.76
4	SB	3	A1H1F	O2S6-S6-C6	2.16	109.97	106.76
4	l	3	A1H1F	O2S6-S6-C6	2.15	109.97	106.76
4	9C	3	A1H1F	O2S6-S6-C6	2.15	109.97	106.76
4	GD	3	A1H1F	O2S6-S6-C6	2.15	109.97	106.76
4	2C	3	A1H1F	O2S6-S6-C6	2.15	109.97	106.76
4	mA	3	A1H1F	O2S6-S6-C6	2.15	109.97	106.76
4	FC	3	A1H1F	O2S6-S6-C6	2.15	109.97	106.76
2	9	3	A1H1F	O2-C2-C3	2.15	114.61	110.15
3	DB	4	A1H03	C1-O5-C5	2.15	115.00	111.48
4	1B	3	A1H1F	O2S6-S6-C6	2.15	109.96	106.76
4	KA	3	A1H1F	O2S6-S6-C6	2.15	109.96	106.76
2	5C	3	A1H1F	O2-C2-C3	2.14	114.59	110.15
4	hC	3	A1H1F	O2S6-S6-C6	2.14	109.96	106.76
3	7B	4	A1H03	C1-O5-C5	2.14	114.99	111.48
3	EC	4	A1H03	C1-O5-C5	2.14	114.99	111.48
3	ZC	4	A1H03	C1-O5-C5	2.14	114.99	111.48
4	YA	3	A1H1F	O2S6-S6-C6	2.14	109.95	106.76
4	LB	3	A1H1F	O2S6-S6-C6	2.14	109.95	106.76
4	gB	3	A1H1F	O2S6-S6-C6	2.14	109.95	106.76
3	zA	4	A1H03	C1-O5-C5	2.14	114.99	111.48
3	y	4	A1H03	C1-O5-C5	2.14	114.99	111.48
4	z	3	A1H1F	O2S6-S6-C6	2.14	109.95	106.76
4	tA	3	A1H1F	O2S6-S6-C6	2.14	109.95	106.76
2	cB	3	A1H1F	O2-C2-C3	2.14	114.58	110.15
3	YB	4	A1H03	C1-O5-C5	2.14	114.98	111.48
2	yC	3	A1H1F	O2-C2-C3	2.14	114.58	110.15
2	pA	3	A1H1F	O2-C2-C3	2.14	114.58	110.15
4	RA	3	A1H1F	O2S6-S6-C6	2.14	109.95	106.76
4	nB	3	A1H1F	O2S6-S6-C6	2.14	109.95	106.76
3	5	4	A1H03	C1-O5-C5	2.14	114.98	111.48
2	WC	3	A1H1F	O2-C2-C3	2.14	114.58	110.15
4	oA	2	BGC	C2-C3-C4	2.14	114.62	110.86
3	k	4	A1H03	C1-O5-C5	2.14	114.98	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	ID	2	BGC	C2-C3-C4	2.14	114.62	110.86
2	GA	3	A1H1F	O2-C2-C3	2.13	114.57	110.15
4	OC	2	BGC	C2-C3-C4	2.13	114.61	110.86
4	EB	3	A1H1F	O2S6-S6-C6	2.13	109.94	106.76
3	eA	4	A1H03	C1-O5-C5	2.13	114.97	111.48
2	jB	3	A1H1F	O2-C2-C3	2.13	114.57	110.15
4	aC	3	A1H1F	O2S6-S6-C6	2.13	109.94	106.76
2	AB	3	A1H1F	O2-C2-C3	2.13	114.57	110.15
2	qB	3	A1H1F	O2-C2-C3	2.13	114.57	110.15
3	nC	4	A1H03	C1-O5-C5	2.13	114.97	111.48
2	OB	3	A1H1F	O2-C2-C3	2.13	114.56	110.15
4	vA	2	BGC	C2-C3-C4	2.13	114.61	110.86
3	JA	4	A1H03	C1-O5-C5	2.13	114.97	111.48
3	QA	4	A1H03	C1-O5-C5	2.13	114.97	111.48
4	0A	3	A1H1F	O2S6-S6-C6	2.13	109.93	106.76
3	sA	4	A1H03	C1-O5-C5	2.13	114.97	111.48
3	uC	4	A1H03	C1-O5-C5	2.13	114.97	111.48
3	fB	4	A1H03	C1-O5-C5	2.13	114.97	111.48
4	s	3	A1H1F	O2S6-S6-C6	2.13	109.93	106.76
4	AC	2	BGC	C2-C3-C4	2.13	114.60	110.86
4	oC	3	A1H1F	O2S6-S6-C6	2.13	109.93	106.76
3	KB	4	A1H03	C1-O5-C5	2.13	114.96	111.48
4	GB	2	BGC	C2-C3-C4	2.13	114.60	110.86
2	o	3	A1H1F	O2-C2-C3	2.13	114.55	110.15
2	v	3	A1H1F	O2-C2-C3	2.12	114.55	110.15
2	PC	3	A1H1F	O2-C2-C3	2.12	114.55	110.15
2	xB	3	A1H1F	O2-C2-C3	2.12	114.55	110.15
2	h	3	A1H1F	O2-C2-C3	2.12	114.55	110.15
2	BC	3	A1H1F	O2-C2-C3	2.12	114.55	110.15
2	VB	3	A1H1F	O2-C2-C3	2.12	114.55	110.15
2	NA	3	A1H1F	O2-C2-C3	2.12	114.54	110.15
4	iB	2	BGC	C2-C3-C4	2.12	114.59	110.86
2	dC	6	A1H03	O2-C2-C1	2.12	114.08	109.22
2	wA	3	A1H1F	O2-C2-C3	2.12	114.54	110.15
2	rC	3	A1H1F	O2-C2-C3	2.12	114.54	110.15
2	4B	3	A1H1F	O2-C2-C3	2.12	114.54	110.15
2	IC	3	A1H1F	O2-C2-C3	2.12	114.54	110.15
4	jC	2	BGC	C2-C3-C4	2.12	114.58	110.86
4	qC	2	BGC	C2-C3-C4	2.12	114.58	110.86
4	aA	2	BGC	C2-C3-C4	2.12	114.58	110.86
2	kC	6	A1H03	O2-C2-C1	2.12	114.07	109.22
4	4C	2	BGC	C2-C3-C4	2.12	114.58	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CA	4	A1H03	C1-O5-C5	2.12	114.95	111.48
3	lA	4	A1H03	C1-O5-C5	2.12	114.95	111.48
2	WC	6	A1H03	O2-C2-C1	2.12	114.07	109.22
2	CD	3	A1H1F	O2-C2-C3	2.12	114.53	110.15
4	cC	2	BGC	C2-C3-C4	2.12	114.58	110.86
3	0B	4	A1H03	C1-O5-C5	2.12	114.94	111.48
2	3A	3	A1H1F	O2-C2-C3	2.11	114.53	110.15
3	SC	4	A1H03	C1-O5-C5	2.11	114.94	111.48
3	8C	4	A1H03	C1-O5-C5	2.11	114.94	111.48
2	GA	6	A1H03	O2-C2-C1	2.11	114.06	109.22
4	2A	2	BGC	C2-C3-C4	2.11	114.58	110.86
4	wB	2	BGC	C2-C3-C4	2.11	114.58	110.86
3	r	4	A1H03	C1-O5-C5	2.11	114.94	111.48
3	6A	4	A1H03	C1-O5-C5	2.11	114.94	111.48
4	VC	2	BGC	C2-C3-C4	2.11	114.58	110.86
2	HB	3	A1H1F	O2-C2-C3	2.11	114.53	110.15
2	kC	3	A1H1F	O2-C2-C3	2.11	114.53	110.15
2	AB	6	A1H03	O2-C2-C1	2.11	114.06	109.22
4	hA	2	BGC	C2-C3-C4	2.11	114.58	110.86
2	2	3	A1H1F	O2-C2-C3	2.11	114.53	110.15
3	LC	4	A1H03	C1-O5-C5	2.11	114.94	111.48
4	n	2	BGC	C2-C3-C4	2.11	114.58	110.86
4	UB	2	BGC	C2-C3-C4	2.11	114.57	110.86
4	BD	2	BGC	C2-C3-C4	2.11	114.57	110.86
2	IC	6	A1H03	O2-C2-C1	2.11	114.05	109.22
2	CD	6	A1H03	O2-C2-C1	2.11	114.05	109.22
4	1	2	BGC	C2-C3-C4	2.11	114.57	110.86
2	VB	6	A1H03	O2-C2-C1	2.11	114.05	109.22
2	dC	3	A1H1F	O2-C2-C3	2.11	114.52	110.15
4	bB	2	BGC	C2-C3-C4	2.11	114.57	110.86
2	bA	6	A1H03	O2-C2-C1	2.11	114.05	109.22
4	FA	2	BGC	C2-C3-C4	2.11	114.57	110.86
4	9A	2	BGC	C2-C3-C4	2.11	114.57	110.86
2	UA	6	A1H03	O2-C2-C1	2.11	114.05	109.22
2	iA	3	A1H1F	O2-C2-C3	2.11	114.52	110.15
2	yC	6	A1H03	O2-C2-C1	2.11	114.05	109.22
3	FD	4	A1H03	C1-O5-C5	2.11	114.93	111.48
3	1C	4	A1H03	C1-O5-C5	2.11	114.93	111.48
2	3A	6	A1H03	O2-C2-C1	2.10	114.04	109.22
2	5C	6	A1H03	O2-C2-C1	2.10	114.04	109.22
2	2	6	A1H03	O2-C2-C1	2.10	114.04	109.22
2	iA	6	A1H03	O2-C2-C1	2.10	114.04	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	HB	6	A1H03	O2-C2-C1	2.10	114.04	109.22
4	pB	2	BGC	C2-C3-C4	2.10	114.56	110.86
2	qB	6	A1H03	O2-C2-C1	2.10	114.04	109.22
2	BC	6	A1H03	O2-C2-C1	2.10	114.04	109.22
2	h	6	A1H03	O2-C2-C1	2.10	114.03	109.22
2	wA	6	A1H03	O2-C2-C1	2.10	114.03	109.22
2	OB	6	A1H03	O2-C2-C1	2.10	114.03	109.22
2	rC	6	A1H03	O2-C2-C1	2.10	114.03	109.22
2	cB	6	A1H03	O2-C2-C1	2.10	114.03	109.22
4	8	2	BGC	C2-C3-C4	2.10	114.55	110.86
4	TA	2	BGC	C2-C3-C4	2.10	114.55	110.86
4	xC	2	BGC	C2-C3-C4	2.10	114.55	110.86
4	u	2	BGC	C2-C3-C4	2.10	114.55	110.86
2	o	6	A1H03	O2-C2-C1	2.10	114.03	109.22
4	NB	2	BGC	C2-C3-C4	2.10	114.55	110.86
2	4B	6	A1H03	O2-C2-C1	2.10	114.02	109.22
4	HC	2	BGC	C2-C3-C4	2.10	114.55	110.86
2	UA	3	A1H1F	O2-C2-C3	2.10	114.49	110.15
2	v	6	A1H03	O2-C2-C1	2.10	114.02	109.22
2	bA	3	A1H1F	O2-C2-C3	2.09	114.49	110.15
2	9	6	A1H03	O2-C2-C1	2.09	114.02	109.22
2	xB	6	A1H03	O2-C2-C1	2.09	114.02	109.22
2	pA	6	A1H03	O2-C2-C1	2.09	114.01	109.22
4	3B	2	BGC	C2-C3-C4	2.09	114.54	110.86
2	jB	6	A1H03	O2-C2-C1	2.09	114.00	109.22
2	PC	6	A1H03	O2-C2-C1	2.09	114.00	109.22
2	NA	6	A1H03	O2-C2-C1	2.08	113.99	109.22
4	MA	2	BGC	C2-C3-C4	2.08	114.52	110.86
3	PA	3	A1H1F	C2-C3-C4	2.05	114.47	110.86
3	fC	3	A1H1F	C2-C3-C4	2.05	114.47	110.86
3	WA	3	A1H1F	C2-C3-C4	2.05	114.46	110.86
3	kA	3	A1H1F	C2-C3-C4	2.04	114.45	110.86
3	XB	3	A1H1F	C2-C3-C4	2.04	114.45	110.86
3	CB	3	A1H1F	C2-C3-C4	2.04	114.45	110.86
3	rA	3	A1H1F	C2-C3-C4	2.04	114.44	110.86
3	q	3	A1H1F	C2-C3-C4	2.04	114.44	110.86
3	QB	3	A1H1F	C2-C3-C4	2.04	114.44	110.86
3	KC	3	A1H1F	C2-C3-C4	2.03	114.44	110.86
3	yA	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	zB	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	tC	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	IA	3	A1H1F	C2-C3-C4	2.03	114.43	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6B	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	j	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	BA	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	DC	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	RC	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	7C	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	0C	3	A1H1F	C2-C3-C4	2.03	114.43	110.86
3	sB	3	A1H1F	C2-C3-C4	2.02	114.42	110.86
3	x	3	A1H1F	C2-C3-C4	2.02	114.41	110.86
3	JB	3	A1H1F	C2-C3-C4	2.02	114.41	110.86
3	4	3	A1H1F	C2-C3-C4	2.02	114.41	110.86
3	YC	3	A1H1F	C2-C3-C4	2.02	114.41	110.86
3	mC	3	A1H1F	C2-C3-C4	2.02	114.41	110.86
3	ED	3	A1H1F	C2-C3-C4	2.02	114.41	110.86
3	eB	3	A1H1F	C2-C3-C4	2.02	114.41	110.86
4	fA	4	MAN	C2-C3-C4	2.01	114.39	110.86
4	nB	4	MAN	C2-C3-C4	2.01	114.39	110.86
4	FC	4	MAN	C2-C3-C4	2.01	114.39	110.86
3	5A	3	A1H1F	C2-C3-C4	2.00	114.39	110.86
4	1B	4	MAN	C2-C3-C4	2.00	114.39	110.86
4	8B	4	MAN	C2-C3-C4	2.00	114.38	110.86
3	lB	3	A1H1F	C2-C3-C4	2.00	114.38	110.86
4	RA	4	MAN	C2-C3-C4	2.00	114.38	110.86

There are no chirality outliers.

All (1015) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	h	3	A1H1F	O5-C5-C6-S6
2	o	3	A1H1F	O5-C5-C6-S6
2	v	3	A1H1F	O5-C5-C6-S6
2	2	3	A1H1F	O5-C5-C6-S6
2	9	3	A1H1F	O5-C5-C6-S6
2	GA	3	A1H1F	O5-C5-C6-S6
2	NA	3	A1H1F	O5-C5-C6-S6
2	UA	3	A1H1F	O5-C5-C6-S6
2	bA	3	A1H1F	O5-C5-C6-S6
2	iA	3	A1H1F	O5-C5-C6-S6
2	pA	3	A1H1F	O5-C5-C6-S6
2	wA	3	A1H1F	O5-C5-C6-S6
2	3A	3	A1H1F	O5-C5-C6-S6
2	AB	3	A1H1F	O5-C5-C6-S6

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Mol	Chain	Res	Type	Atoms
2	HB	3	A1H1F	O5-C5-C6-S6
2	OB	3	A1H1F	O5-C5-C6-S6
2	VB	3	A1H1F	O5-C5-C6-S6
2	cB	3	A1H1F	O5-C5-C6-S6
2	jB	3	A1H1F	O5-C5-C6-S6
2	qB	3	A1H1F	O5-C5-C6-S6
2	xB	3	A1H1F	O5-C5-C6-S6
2	4B	3	A1H1F	O5-C5-C6-S6
2	BC	3	A1H1F	O5-C5-C6-S6
2	IC	3	A1H1F	O5-C5-C6-S6
2	PC	3	A1H1F	O5-C5-C6-S6
2	WC	3	A1H1F	O5-C5-C6-S6
2	dC	3	A1H1F	O5-C5-C6-S6
2	kC	3	A1H1F	O5-C5-C6-S6
2	rC	3	A1H1F	O5-C5-C6-S6
2	yC	3	A1H1F	O5-C5-C6-S6
2	5C	3	A1H1F	O5-C5-C6-S6
2	CD	3	A1H1F	O5-C5-C6-S6
3	j	3	A1H1F	O5-C5-C6-S6
3	m	3	A1H1F	O5-C5-C6-S6
3	q	3	A1H1F	O5-C5-C6-S6
3	t	3	A1H1F	O5-C5-C6-S6
3	x	3	A1H1F	O5-C5-C6-S6
3	0	3	A1H1F	O5-C5-C6-S6
3	4	3	A1H1F	O5-C5-C6-S6
3	7	3	A1H1F	O5-C5-C6-S6
3	BA	3	A1H1F	O5-C5-C6-S6
3	EA	3	A1H1F	O5-C5-C6-S6
3	IA	3	A1H1F	O5-C5-C6-S6
3	LA	3	A1H1F	O5-C5-C6-S6
3	PA	3	A1H1F	O5-C5-C6-S6
3	SA	3	A1H1F	O5-C5-C6-S6
3	WA	3	A1H1F	O5-C5-C6-S6
3	ZA	3	A1H1F	O5-C5-C6-S6
3	dA	3	A1H1F	O5-C5-C6-S6
3	gA	3	A1H1F	O5-C5-C6-S6
3	kA	3	A1H1F	O5-C5-C6-S6
3	nA	3	A1H1F	O5-C5-C6-S6
3	rA	3	A1H1F	O5-C5-C6-S6
3	uA	3	A1H1F	O5-C5-C6-S6
3	yA	3	A1H1F	O5-C5-C6-S6
3	1A	3	A1H1F	O5-C5-C6-S6

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Mol	Chain	Res	Type	Atoms
3	5A	3	A1H1F	O5-C5-C6-S6
3	8A	3	A1H1F	O5-C5-C6-S6
3	CB	3	A1H1F	O5-C5-C6-S6
3	FB	3	A1H1F	O5-C5-C6-S6
3	JB	3	A1H1F	O5-C5-C6-S6
3	MB	3	A1H1F	O5-C5-C6-S6
3	QB	3	A1H1F	O5-C5-C6-S6
3	TB	3	A1H1F	O5-C5-C6-S6
3	XB	3	A1H1F	O5-C5-C6-S6
3	aB	3	A1H1F	O5-C5-C6-S6
3	eB	3	A1H1F	O5-C5-C6-S6
3	hB	3	A1H1F	O5-C5-C6-S6
3	lB	3	A1H1F	O5-C5-C6-S6
3	oB	3	A1H1F	O5-C5-C6-S6
3	sB	3	A1H1F	O5-C5-C6-S6
3	vB	3	A1H1F	O5-C5-C6-S6
3	zB	3	A1H1F	O5-C5-C6-S6
3	2B	3	A1H1F	O5-C5-C6-S6
3	6B	3	A1H1F	O5-C5-C6-S6
3	9B	3	A1H1F	O5-C5-C6-S6
3	DC	3	A1H1F	O5-C5-C6-S6
3	GC	3	A1H1F	O5-C5-C6-S6
3	KC	3	A1H1F	O5-C5-C6-S6
3	NC	3	A1H1F	O5-C5-C6-S6
3	RC	3	A1H1F	O5-C5-C6-S6
3	UC	3	A1H1F	O5-C5-C6-S6
3	YC	3	A1H1F	O5-C5-C6-S6
3	bC	3	A1H1F	O5-C5-C6-S6
3	fC	3	A1H1F	O5-C5-C6-S6
3	iC	3	A1H1F	O5-C5-C6-S6
3	mC	3	A1H1F	O5-C5-C6-S6
3	pC	3	A1H1F	O5-C5-C6-S6
3	tC	3	A1H1F	O5-C5-C6-S6
3	wC	3	A1H1F	O5-C5-C6-S6
3	0C	3	A1H1F	O5-C5-C6-S6
3	3C	3	A1H1F	O5-C5-C6-S6
3	7C	3	A1H1F	O5-C5-C6-S6
3	AD	3	A1H1F	O5-C5-C6-S6
3	ED	3	A1H1F	O5-C5-C6-S6
3	HD	3	A1H1F	O5-C5-C6-S6
4	l	4	MAN	C4-C5-C6-O6
4	s	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	z	4	MAN	C4-C5-C6-O6
4	6	4	MAN	C4-C5-C6-O6
4	DA	4	MAN	C4-C5-C6-O6
4	KA	4	MAN	C4-C5-C6-O6
4	RA	4	MAN	C4-C5-C6-O6
4	YA	4	MAN	C4-C5-C6-O6
4	fA	4	MAN	C4-C5-C6-O6
4	mA	4	MAN	C4-C5-C6-O6
4	tA	4	MAN	C4-C5-C6-O6
4	0A	4	MAN	C4-C5-C6-O6
4	7A	4	MAN	C4-C5-C6-O6
4	EB	4	MAN	C4-C5-C6-O6
4	LB	4	MAN	C4-C5-C6-O6
4	SB	4	MAN	C4-C5-C6-O6
4	ZB	4	MAN	C4-C5-C6-O6
4	gB	4	MAN	C4-C5-C6-O6
4	nB	4	MAN	C4-C5-C6-O6
4	uB	4	MAN	C4-C5-C6-O6
4	1B	4	MAN	C4-C5-C6-O6
4	8B	4	MAN	C4-C5-C6-O6
4	FC	4	MAN	C4-C5-C6-O6
4	MC	4	MAN	C4-C5-C6-O6
4	TC	4	MAN	C4-C5-C6-O6
4	aC	4	MAN	C4-C5-C6-O6
4	hC	4	MAN	C4-C5-C6-O6
4	oC	4	MAN	C4-C5-C6-O6
4	vC	4	MAN	C4-C5-C6-O6
4	2C	4	MAN	C4-C5-C6-O6
4	9C	4	MAN	C4-C5-C6-O6
4	GD	4	MAN	C4-C5-C6-O6
3	j	1	GAL	O5-C5-C6-O6
3	q	1	GAL	O5-C5-C6-O6
3	4	1	GAL	O5-C5-C6-O6
3	BA	1	GAL	O5-C5-C6-O6
3	IA	1	GAL	O5-C5-C6-O6
3	WA	1	GAL	O5-C5-C6-O6
3	dA	1	GAL	O5-C5-C6-O6
3	rA	1	GAL	O5-C5-C6-O6
3	yA	1	GAL	O5-C5-C6-O6
3	5A	1	GAL	O5-C5-C6-O6
3	JB	1	GAL	O5-C5-C6-O6
3	QB	1	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	XB	1	GAL	O5-C5-C6-O6
3	eB	1	GAL	O5-C5-C6-O6
3	sB	1	GAL	O5-C5-C6-O6
3	zB	1	GAL	O5-C5-C6-O6
3	6B	1	GAL	O5-C5-C6-O6
3	DC	1	GAL	O5-C5-C6-O6
3	fC	1	GAL	O5-C5-C6-O6
3	mC	1	GAL	O5-C5-C6-O6
3	tC	1	GAL	O5-C5-C6-O6
3	7C	1	GAL	O5-C5-C6-O6
3	ED	1	GAL	O5-C5-C6-O6
3	PA	1	GAL	O5-C5-C6-O6
3	CB	1	GAL	O5-C5-C6-O6
3	RC	1	GAL	O5-C5-C6-O6
3	YC	1	GAL	O5-C5-C6-O6
3	x	1	GAL	O5-C5-C6-O6
3	kA	1	GAL	O5-C5-C6-O6
3	lB	1	GAL	O5-C5-C6-O6
3	KC	1	GAL	O5-C5-C6-O6
3	0C	1	GAL	O5-C5-C6-O6
3	k	2	BGC	C4-C5-C6-O6
3	r	2	BGC	C4-C5-C6-O6
3	y	2	BGC	C4-C5-C6-O6
3	5	2	BGC	C4-C5-C6-O6
3	CA	2	BGC	C4-C5-C6-O6
3	JA	2	BGC	C4-C5-C6-O6
3	QA	2	BGC	C4-C5-C6-O6
3	XA	2	BGC	C4-C5-C6-O6
3	eA	2	BGC	C4-C5-C6-O6
3	lA	2	BGC	C4-C5-C6-O6
3	sA	2	BGC	C4-C5-C6-O6
3	zA	2	BGC	C4-C5-C6-O6
3	6A	2	BGC	C4-C5-C6-O6
3	DB	2	BGC	C4-C5-C6-O6
3	KB	2	BGC	C4-C5-C6-O6
3	RB	2	BGC	C4-C5-C6-O6
3	YB	2	BGC	C4-C5-C6-O6
3	fB	2	BGC	C4-C5-C6-O6
3	mB	2	BGC	C4-C5-C6-O6
3	tB	2	BGC	C4-C5-C6-O6
3	0B	2	BGC	C4-C5-C6-O6
3	7B	2	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	EC	2	BGC	C4-C5-C6-O6
3	LC	2	BGC	C4-C5-C6-O6
3	SC	2	BGC	C4-C5-C6-O6
3	ZC	2	BGC	C4-C5-C6-O6
3	gC	2	BGC	C4-C5-C6-O6
3	nC	2	BGC	C4-C5-C6-O6
3	uC	2	BGC	C4-C5-C6-O6
3	lC	2	BGC	C4-C5-C6-O6
3	8C	2	BGC	C4-C5-C6-O6
3	FD	2	BGC	C4-C5-C6-O6
3	j	1	GAL	C4-C5-C6-O6
3	q	1	GAL	C4-C5-C6-O6
3	x	1	GAL	C4-C5-C6-O6
3	BA	1	GAL	C4-C5-C6-O6
3	IA	1	GAL	C4-C5-C6-O6
3	PA	1	GAL	C4-C5-C6-O6
3	WA	1	GAL	C4-C5-C6-O6
3	dA	1	GAL	C4-C5-C6-O6
3	rA	1	GAL	C4-C5-C6-O6
3	yA	1	GAL	C4-C5-C6-O6
3	5A	1	GAL	C4-C5-C6-O6
3	CB	1	GAL	C4-C5-C6-O6
3	JB	1	GAL	C4-C5-C6-O6
3	QB	1	GAL	C4-C5-C6-O6
3	XB	1	GAL	C4-C5-C6-O6
3	eB	1	GAL	C4-C5-C6-O6
3	lB	1	GAL	C4-C5-C6-O6
3	sB	1	GAL	C4-C5-C6-O6
3	6B	1	GAL	C4-C5-C6-O6
3	DC	1	GAL	C4-C5-C6-O6
3	KC	1	GAL	C4-C5-C6-O6
3	RC	1	GAL	C4-C5-C6-O6
3	YC	1	GAL	C4-C5-C6-O6
3	fC	1	GAL	C4-C5-C6-O6
3	mC	1	GAL	C4-C5-C6-O6
3	tC	1	GAL	C4-C5-C6-O6
3	0C	1	GAL	C4-C5-C6-O6
3	7C	1	GAL	C4-C5-C6-O6
3	ED	1	GAL	C4-C5-C6-O6
4	l	4	MAN	O5-C5-C6-O6
4	s	4	MAN	O5-C5-C6-O6
4	z	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	6	4	MAN	O5-C5-C6-O6
4	DA	4	MAN	O5-C5-C6-O6
4	KA	4	MAN	O5-C5-C6-O6
4	RA	4	MAN	O5-C5-C6-O6
4	YA	4	MAN	O5-C5-C6-O6
4	fA	4	MAN	O5-C5-C6-O6
4	mA	4	MAN	O5-C5-C6-O6
4	tA	4	MAN	O5-C5-C6-O6
4	0A	4	MAN	O5-C5-C6-O6
4	7A	4	MAN	O5-C5-C6-O6
4	EB	4	MAN	O5-C5-C6-O6
4	LB	4	MAN	O5-C5-C6-O6
4	SB	4	MAN	O5-C5-C6-O6
4	ZB	4	MAN	O5-C5-C6-O6
4	gB	4	MAN	O5-C5-C6-O6
4	nB	4	MAN	O5-C5-C6-O6
4	uB	4	MAN	O5-C5-C6-O6
4	1B	4	MAN	O5-C5-C6-O6
4	8B	4	MAN	O5-C5-C6-O6
4	FC	4	MAN	O5-C5-C6-O6
4	MC	4	MAN	O5-C5-C6-O6
4	TC	4	MAN	O5-C5-C6-O6
4	aC	4	MAN	O5-C5-C6-O6
4	hC	4	MAN	O5-C5-C6-O6
4	oC	4	MAN	O5-C5-C6-O6
4	vC	4	MAN	O5-C5-C6-O6
4	2C	4	MAN	O5-C5-C6-O6
4	9C	4	MAN	O5-C5-C6-O6
4	GD	4	MAN	O5-C5-C6-O6
3	4	1	GAL	C4-C5-C6-O6
3	kA	1	GAL	C4-C5-C6-O6
3	zB	1	GAL	C4-C5-C6-O6
4	MA	4	MAN	C4-C5-C6-O6
4	hA	4	MAN	C4-C5-C6-O6
4	2A	4	MAN	C4-C5-C6-O6
4	GB	4	MAN	C4-C5-C6-O6
4	NB	4	MAN	C4-C5-C6-O6
4	UB	4	MAN	C4-C5-C6-O6
4	iB	4	MAN	C4-C5-C6-O6
4	3B	4	MAN	C4-C5-C6-O6
4	AC	4	MAN	C4-C5-C6-O6
4	qC	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	4C	4	MAN	C4-C5-C6-O6
4	ID	4	MAN	C4-C5-C6-O6
4	n	4	MAN	C4-C5-C6-O6
4	u	4	MAN	C4-C5-C6-O6
4	l	4	MAN	C4-C5-C6-O6
4	8	4	MAN	C4-C5-C6-O6
4	FA	4	MAN	C4-C5-C6-O6
4	TA	4	MAN	C4-C5-C6-O6
4	aA	4	MAN	C4-C5-C6-O6
4	oA	4	MAN	C4-C5-C6-O6
4	vA	4	MAN	C4-C5-C6-O6
4	9A	4	MAN	C4-C5-C6-O6
4	bB	4	MAN	C4-C5-C6-O6
4	pB	4	MAN	C4-C5-C6-O6
4	wB	4	MAN	C4-C5-C6-O6
4	HC	4	MAN	C4-C5-C6-O6
4	OC	4	MAN	C4-C5-C6-O6
4	VC	4	MAN	C4-C5-C6-O6
4	cC	4	MAN	C4-C5-C6-O6
4	jC	4	MAN	C4-C5-C6-O6
4	xC	4	MAN	C4-C5-C6-O6
4	BD	4	MAN	C4-C5-C6-O6
3	DB	2	BGC	O5-C5-C6-O6
3	SC	2	BGC	O5-C5-C6-O6
3	k	2	BGC	O5-C5-C6-O6
3	r	2	BGC	O5-C5-C6-O6
3	y	2	BGC	O5-C5-C6-O6
3	5	2	BGC	O5-C5-C6-O6
3	CA	2	BGC	O5-C5-C6-O6
3	JA	2	BGC	O5-C5-C6-O6
3	QA	2	BGC	O5-C5-C6-O6
3	XA	2	BGC	O5-C5-C6-O6
3	eA	2	BGC	O5-C5-C6-O6
3	lA	2	BGC	O5-C5-C6-O6
3	sA	2	BGC	O5-C5-C6-O6
3	zA	2	BGC	O5-C5-C6-O6
3	6A	2	BGC	O5-C5-C6-O6
3	KB	2	BGC	O5-C5-C6-O6
3	RB	2	BGC	O5-C5-C6-O6
3	YB	2	BGC	O5-C5-C6-O6
3	fB	2	BGC	O5-C5-C6-O6
3	mB	2	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	tB	2	BGC	O5-C5-C6-O6
3	0B	2	BGC	O5-C5-C6-O6
3	7B	2	BGC	O5-C5-C6-O6
3	EC	2	BGC	O5-C5-C6-O6
3	LC	2	BGC	O5-C5-C6-O6
3	ZC	2	BGC	O5-C5-C6-O6
3	gC	2	BGC	O5-C5-C6-O6
3	nC	2	BGC	O5-C5-C6-O6
3	uC	2	BGC	O5-C5-C6-O6
3	1C	2	BGC	O5-C5-C6-O6
3	8C	2	BGC	O5-C5-C6-O6
3	FD	2	BGC	O5-C5-C6-O6
3	k	5	MAN	C4-C5-C6-O6
3	y	5	MAN	C4-C5-C6-O6
3	zA	5	MAN	C4-C5-C6-O6
3	6A	5	MAN	C4-C5-C6-O6
3	KB	5	MAN	C4-C5-C6-O6
3	YB	5	MAN	C4-C5-C6-O6
3	fB	5	MAN	C4-C5-C6-O6
3	mB	5	MAN	C4-C5-C6-O6
3	0B	5	MAN	C4-C5-C6-O6
3	7B	5	MAN	C4-C5-C6-O6
3	uC	5	MAN	C4-C5-C6-O6
3	FD	5	MAN	C4-C5-C6-O6
3	r	5	MAN	C4-C5-C6-O6
3	5	5	MAN	C4-C5-C6-O6
3	CA	5	MAN	C4-C5-C6-O6
3	JA	5	MAN	C4-C5-C6-O6
3	QA	5	MAN	C4-C5-C6-O6
3	XA	5	MAN	C4-C5-C6-O6
3	eA	5	MAN	C4-C5-C6-O6
3	lA	5	MAN	C4-C5-C6-O6
3	sA	5	MAN	C4-C5-C6-O6
3	DB	5	MAN	C4-C5-C6-O6
3	RB	5	MAN	C4-C5-C6-O6
3	tB	5	MAN	C4-C5-C6-O6
3	EC	5	MAN	C4-C5-C6-O6
3	LC	5	MAN	C4-C5-C6-O6
3	SC	5	MAN	C4-C5-C6-O6
3	ZC	5	MAN	C4-C5-C6-O6
3	gC	5	MAN	C4-C5-C6-O6
3	nC	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	1C	5	MAN	C4-C5-C6-O6
3	8C	5	MAN	C4-C5-C6-O6
4	u	4	MAN	O5-C5-C6-O6
4	oA	4	MAN	O5-C5-C6-O6
4	vA	4	MAN	O5-C5-C6-O6
4	9A	4	MAN	O5-C5-C6-O6
4	NB	4	MAN	O5-C5-C6-O6
4	jC	4	MAN	O5-C5-C6-O6
4	qC	4	MAN	O5-C5-C6-O6
4	aA	2	BGC	C4-C5-C6-O6
4	oA	2	BGC	C4-C5-C6-O6
4	vA	2	BGC	C4-C5-C6-O6
4	bB	2	BGC	C4-C5-C6-O6
4	wB	2	BGC	C4-C5-C6-O6
4	3B	2	BGC	C4-C5-C6-O6
4	cC	2	BGC	C4-C5-C6-O6
4	xC	2	BGC	C4-C5-C6-O6
4	ID	2	BGC	C4-C5-C6-O6
4	aA	4	MAN	O5-C5-C6-O6
4	GB	4	MAN	O5-C5-C6-O6
4	xC	4	MAN	O5-C5-C6-O6
4	n	2	BGC	C4-C5-C6-O6
4	u	2	BGC	C4-C5-C6-O6
4	1	2	BGC	C4-C5-C6-O6
4	8	2	BGC	C4-C5-C6-O6
4	FA	2	BGC	C4-C5-C6-O6
4	MA	2	BGC	C4-C5-C6-O6
4	TA	2	BGC	C4-C5-C6-O6
4	hA	2	BGC	C4-C5-C6-O6
4	2A	2	BGC	C4-C5-C6-O6
4	9A	2	BGC	C4-C5-C6-O6
4	GB	2	BGC	C4-C5-C6-O6
4	NB	2	BGC	C4-C5-C6-O6
4	UB	2	BGC	C4-C5-C6-O6
4	iB	2	BGC	C4-C5-C6-O6
4	pB	2	BGC	C4-C5-C6-O6
4	AC	2	BGC	C4-C5-C6-O6
4	HC	2	BGC	C4-C5-C6-O6
4	OC	2	BGC	C4-C5-C6-O6
4	VC	2	BGC	C4-C5-C6-O6
4	jC	2	BGC	C4-C5-C6-O6
4	qC	2	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	4C	2	BGC	C4-C5-C6-O6
4	BD	2	BGC	C4-C5-C6-O6
4	n	4	MAN	O5-C5-C6-O6
4	8	4	MAN	O5-C5-C6-O6
4	MA	4	MAN	O5-C5-C6-O6
4	hA	4	MAN	O5-C5-C6-O6
4	UB	4	MAN	O5-C5-C6-O6
4	iB	4	MAN	O5-C5-C6-O6
4	wB	4	MAN	O5-C5-C6-O6
4	3B	4	MAN	O5-C5-C6-O6
4	AC	4	MAN	O5-C5-C6-O6
4	OC	4	MAN	O5-C5-C6-O6
4	VC	4	MAN	O5-C5-C6-O6
4	4C	4	MAN	O5-C5-C6-O6
4	BD	4	MAN	O5-C5-C6-O6
4	ID	4	MAN	O5-C5-C6-O6
4	1	4	MAN	O5-C5-C6-O6
4	FA	4	MAN	O5-C5-C6-O6
4	TA	4	MAN	O5-C5-C6-O6
4	2A	4	MAN	O5-C5-C6-O6
4	bB	4	MAN	O5-C5-C6-O6
4	pB	4	MAN	O5-C5-C6-O6
4	HC	4	MAN	O5-C5-C6-O6
4	cC	4	MAN	O5-C5-C6-O6
3	k	5	MAN	O5-C5-C6-O6
3	r	5	MAN	O5-C5-C6-O6
3	y	5	MAN	O5-C5-C6-O6
3	5	5	MAN	O5-C5-C6-O6
3	CA	5	MAN	O5-C5-C6-O6
3	JA	5	MAN	O5-C5-C6-O6
3	QA	5	MAN	O5-C5-C6-O6
3	XA	5	MAN	O5-C5-C6-O6
3	eA	5	MAN	O5-C5-C6-O6
3	lA	5	MAN	O5-C5-C6-O6
3	sA	5	MAN	O5-C5-C6-O6
3	zA	5	MAN	O5-C5-C6-O6
3	6A	5	MAN	O5-C5-C6-O6
3	DB	5	MAN	O5-C5-C6-O6
3	KB	5	MAN	O5-C5-C6-O6
3	RB	5	MAN	O5-C5-C6-O6
3	YB	5	MAN	O5-C5-C6-O6
3	fB	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	tB	5	MAN	O5-C5-C6-O6
3	0B	5	MAN	O5-C5-C6-O6
3	7B	5	MAN	O5-C5-C6-O6
3	EC	5	MAN	O5-C5-C6-O6
3	LC	5	MAN	O5-C5-C6-O6
3	SC	5	MAN	O5-C5-C6-O6
3	ZC	5	MAN	O5-C5-C6-O6
3	gC	5	MAN	O5-C5-C6-O6
3	nC	5	MAN	O5-C5-C6-O6
3	uC	5	MAN	O5-C5-C6-O6
3	1C	5	MAN	O5-C5-C6-O6
3	8C	5	MAN	O5-C5-C6-O6
3	FD	5	MAN	O5-C5-C6-O6
3	mB	5	MAN	O5-C5-C6-O6
2	h	6	A1H03	C4-C5-C6-O6
2	o	6	A1H03	C4-C5-C6-O6
2	v	6	A1H03	C4-C5-C6-O6
2	2	6	A1H03	C4-C5-C6-O6
2	9	6	A1H03	C4-C5-C6-O6
2	GA	6	A1H03	C4-C5-C6-O6
2	NA	6	A1H03	C4-C5-C6-O6
2	UA	6	A1H03	C4-C5-C6-O6
2	bA	6	A1H03	C4-C5-C6-O6
2	iA	6	A1H03	C4-C5-C6-O6
2	pA	6	A1H03	C4-C5-C6-O6
2	wA	6	A1H03	C4-C5-C6-O6
2	3A	6	A1H03	C4-C5-C6-O6
2	AB	6	A1H03	C4-C5-C6-O6
2	HB	6	A1H03	C4-C5-C6-O6
2	OB	6	A1H03	C4-C5-C6-O6
2	VB	6	A1H03	C4-C5-C6-O6
2	cB	6	A1H03	C4-C5-C6-O6
2	jB	6	A1H03	C4-C5-C6-O6
2	qB	6	A1H03	C4-C5-C6-O6
2	xB	6	A1H03	C4-C5-C6-O6
2	4B	6	A1H03	C4-C5-C6-O6
2	BC	6	A1H03	C4-C5-C6-O6
2	IC	6	A1H03	C4-C5-C6-O6
2	PC	6	A1H03	C4-C5-C6-O6
2	WC	6	A1H03	C4-C5-C6-O6
2	dC	6	A1H03	C4-C5-C6-O6
2	kC	6	A1H03	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	rC	6	A1H03	C4-C5-C6-O6
2	yC	6	A1H03	C4-C5-C6-O6
2	5C	6	A1H03	C4-C5-C6-O6
2	CD	6	A1H03	C4-C5-C6-O6
3	j	4	A1H03	C4-C5-C6-O6
3	m	4	A1H03	C4-C5-C6-O6
3	q	4	A1H03	C4-C5-C6-O6
3	t	4	A1H03	C4-C5-C6-O6
3	x	4	A1H03	C4-C5-C6-O6
3	0	4	A1H03	C4-C5-C6-O6
3	4	4	A1H03	C4-C5-C6-O6
3	7	4	A1H03	C4-C5-C6-O6
3	BA	4	A1H03	C4-C5-C6-O6
3	EA	4	A1H03	C4-C5-C6-O6
3	IA	4	A1H03	C4-C5-C6-O6
3	LA	4	A1H03	C4-C5-C6-O6
3	PA	4	A1H03	C4-C5-C6-O6
3	SA	4	A1H03	C4-C5-C6-O6
3	WA	4	A1H03	C4-C5-C6-O6
3	ZA	4	A1H03	C4-C5-C6-O6
3	dA	4	A1H03	C4-C5-C6-O6
3	gA	4	A1H03	C4-C5-C6-O6
3	kA	4	A1H03	C4-C5-C6-O6
3	nA	4	A1H03	C4-C5-C6-O6
3	rA	4	A1H03	C4-C5-C6-O6
3	uA	4	A1H03	C4-C5-C6-O6
3	yA	4	A1H03	C4-C5-C6-O6
3	1A	4	A1H03	C4-C5-C6-O6
3	5A	4	A1H03	C4-C5-C6-O6
3	8A	4	A1H03	C4-C5-C6-O6
3	CB	4	A1H03	C4-C5-C6-O6
3	FB	4	A1H03	C4-C5-C6-O6
3	JB	4	A1H03	C4-C5-C6-O6
3	MB	4	A1H03	C4-C5-C6-O6
3	QB	4	A1H03	C4-C5-C6-O6
3	TB	4	A1H03	C4-C5-C6-O6
3	XB	4	A1H03	C4-C5-C6-O6
3	aB	4	A1H03	C4-C5-C6-O6
3	eB	4	A1H03	C4-C5-C6-O6
3	hB	4	A1H03	C4-C5-C6-O6
3	lB	4	A1H03	C4-C5-C6-O6
3	oB	4	A1H03	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	sB	4	A1H03	C4-C5-C6-O6
3	vB	4	A1H03	C4-C5-C6-O6
3	zB	4	A1H03	C4-C5-C6-O6
3	2B	4	A1H03	C4-C5-C6-O6
3	6B	4	A1H03	C4-C5-C6-O6
3	9B	4	A1H03	C4-C5-C6-O6
3	DC	4	A1H03	C4-C5-C6-O6
3	GC	4	A1H03	C4-C5-C6-O6
3	KC	4	A1H03	C4-C5-C6-O6
3	NC	4	A1H03	C4-C5-C6-O6
3	RC	4	A1H03	C4-C5-C6-O6
3	UC	4	A1H03	C4-C5-C6-O6
3	YC	4	A1H03	C4-C5-C6-O6
3	bC	4	A1H03	C4-C5-C6-O6
3	fC	4	A1H03	C4-C5-C6-O6
3	iC	4	A1H03	C4-C5-C6-O6
3	mC	4	A1H03	C4-C5-C6-O6
3	pC	4	A1H03	C4-C5-C6-O6
3	tC	4	A1H03	C4-C5-C6-O6
3	wC	4	A1H03	C4-C5-C6-O6
3	0C	4	A1H03	C4-C5-C6-O6
3	3C	4	A1H03	C4-C5-C6-O6
3	7C	4	A1H03	C4-C5-C6-O6
3	AD	4	A1H03	C4-C5-C6-O6
3	ED	4	A1H03	C4-C5-C6-O6
3	HD	4	A1H03	C4-C5-C6-O6
3	x	5	MAN	C4-C5-C6-O6
3	BA	5	MAN	C4-C5-C6-O6
3	IA	5	MAN	C4-C5-C6-O6
3	PA	5	MAN	C4-C5-C6-O6
3	WA	5	MAN	C4-C5-C6-O6
3	dA	5	MAN	C4-C5-C6-O6
3	kA	5	MAN	C4-C5-C6-O6
3	sB	5	MAN	C4-C5-C6-O6
3	6B	5	MAN	C4-C5-C6-O6
3	fC	5	MAN	C4-C5-C6-O6
3	tC	5	MAN	C4-C5-C6-O6
3	7C	5	MAN	C4-C5-C6-O6
3	5A	5	MAN	C4-C5-C6-O6
3	j	5	MAN	C4-C5-C6-O6
3	q	5	MAN	C4-C5-C6-O6
3	4	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	rA	5	MAN	C4-C5-C6-O6
3	yA	5	MAN	C4-C5-C6-O6
3	CB	5	MAN	C4-C5-C6-O6
3	JB	5	MAN	C4-C5-C6-O6
3	XB	5	MAN	C4-C5-C6-O6
3	lB	5	MAN	C4-C5-C6-O6
3	zB	5	MAN	C4-C5-C6-O6
3	DC	5	MAN	C4-C5-C6-O6
3	KC	5	MAN	C4-C5-C6-O6
3	RC	5	MAN	C4-C5-C6-O6
3	YC	5	MAN	C4-C5-C6-O6
3	mC	5	MAN	C4-C5-C6-O6
3	0C	5	MAN	C4-C5-C6-O6
3	ED	5	MAN	C4-C5-C6-O6
3	QB	5	MAN	C4-C5-C6-O6
3	eB	5	MAN	C4-C5-C6-O6
2	h	3	A1H1F	C4-C5-C6-S6
2	o	3	A1H1F	C4-C5-C6-S6
2	v	3	A1H1F	C4-C5-C6-S6
2	2	3	A1H1F	C4-C5-C6-S6
2	9	3	A1H1F	C4-C5-C6-S6
2	GA	3	A1H1F	C4-C5-C6-S6
2	NA	3	A1H1F	C4-C5-C6-S6
2	UA	3	A1H1F	C4-C5-C6-S6
2	bA	3	A1H1F	C4-C5-C6-S6
2	iA	3	A1H1F	C4-C5-C6-S6
2	pA	3	A1H1F	C4-C5-C6-S6
2	wA	3	A1H1F	C4-C5-C6-S6
2	3A	3	A1H1F	C4-C5-C6-S6
2	AB	3	A1H1F	C4-C5-C6-S6
2	HB	3	A1H1F	C4-C5-C6-S6
2	OB	3	A1H1F	C4-C5-C6-S6
2	VB	3	A1H1F	C4-C5-C6-S6
2	cB	3	A1H1F	C4-C5-C6-S6
2	jB	3	A1H1F	C4-C5-C6-S6
2	qB	3	A1H1F	C4-C5-C6-S6
2	xB	3	A1H1F	C4-C5-C6-S6
2	4B	3	A1H1F	C4-C5-C6-S6
2	BC	3	A1H1F	C4-C5-C6-S6
2	IC	3	A1H1F	C4-C5-C6-S6
2	PC	3	A1H1F	C4-C5-C6-S6
2	WC	3	A1H1F	C4-C5-C6-S6

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Mol	Chain	Res	Type	Atoms
2	dC	3	A1H1F	C4-C5-C6-S6
2	kC	3	A1H1F	C4-C5-C6-S6
2	rC	3	A1H1F	C4-C5-C6-S6
2	yC	3	A1H1F	C4-C5-C6-S6
2	5C	3	A1H1F	C4-C5-C6-S6
2	CD	3	A1H1F	C4-C5-C6-S6
3	j	3	A1H1F	C4-C5-C6-S6
3	m	3	A1H1F	C4-C5-C6-S6
3	q	3	A1H1F	C4-C5-C6-S6
3	t	3	A1H1F	C4-C5-C6-S6
3	x	3	A1H1F	C4-C5-C6-S6
3	0	3	A1H1F	C4-C5-C6-S6
3	4	3	A1H1F	C4-C5-C6-S6
3	7	3	A1H1F	C4-C5-C6-S6
3	BA	3	A1H1F	C4-C5-C6-S6
3	EA	3	A1H1F	C4-C5-C6-S6
3	IA	3	A1H1F	C4-C5-C6-S6
3	LA	3	A1H1F	C4-C5-C6-S6
3	PA	3	A1H1F	C4-C5-C6-S6
3	SA	3	A1H1F	C4-C5-C6-S6
3	WA	3	A1H1F	C4-C5-C6-S6
3	ZA	3	A1H1F	C4-C5-C6-S6
3	dA	3	A1H1F	C4-C5-C6-S6
3	gA	3	A1H1F	C4-C5-C6-S6
3	kA	3	A1H1F	C4-C5-C6-S6
3	nA	3	A1H1F	C4-C5-C6-S6
3	rA	3	A1H1F	C4-C5-C6-S6
3	uA	3	A1H1F	C4-C5-C6-S6
3	yA	3	A1H1F	C4-C5-C6-S6
3	1A	3	A1H1F	C4-C5-C6-S6
3	5A	3	A1H1F	C4-C5-C6-S6
3	8A	3	A1H1F	C4-C5-C6-S6
3	CB	3	A1H1F	C4-C5-C6-S6
3	FB	3	A1H1F	C4-C5-C6-S6
3	JB	3	A1H1F	C4-C5-C6-S6
3	MB	3	A1H1F	C4-C5-C6-S6
3	QB	3	A1H1F	C4-C5-C6-S6
3	TB	3	A1H1F	C4-C5-C6-S6
3	XB	3	A1H1F	C4-C5-C6-S6
3	aB	3	A1H1F	C4-C5-C6-S6
3	eB	3	A1H1F	C4-C5-C6-S6
3	hB	3	A1H1F	C4-C5-C6-S6

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Mol	Chain	Res	Type	Atoms
3	lB	3	A1H1F	C4-C5-C6-S6
3	oB	3	A1H1F	C4-C5-C6-S6
3	sB	3	A1H1F	C4-C5-C6-S6
3	vB	3	A1H1F	C4-C5-C6-S6
3	zB	3	A1H1F	C4-C5-C6-S6
3	2B	3	A1H1F	C4-C5-C6-S6
3	6B	3	A1H1F	C4-C5-C6-S6
3	9B	3	A1H1F	C4-C5-C6-S6
3	DC	3	A1H1F	C4-C5-C6-S6
3	GC	3	A1H1F	C4-C5-C6-S6
3	KC	3	A1H1F	C4-C5-C6-S6
3	NC	3	A1H1F	C4-C5-C6-S6
3	RC	3	A1H1F	C4-C5-C6-S6
3	UC	3	A1H1F	C4-C5-C6-S6
3	YC	3	A1H1F	C4-C5-C6-S6
3	bC	3	A1H1F	C4-C5-C6-S6
3	fC	3	A1H1F	C4-C5-C6-S6
3	iC	3	A1H1F	C4-C5-C6-S6
3	mC	3	A1H1F	C4-C5-C6-S6
3	pC	3	A1H1F	C4-C5-C6-S6
3	tC	3	A1H1F	C4-C5-C6-S6
3	wC	3	A1H1F	C4-C5-C6-S6
3	0C	3	A1H1F	C4-C5-C6-S6
3	3C	3	A1H1F	C4-C5-C6-S6
3	7C	3	A1H1F	C4-C5-C6-S6
3	AD	3	A1H1F	C4-C5-C6-S6
3	ED	3	A1H1F	C4-C5-C6-S6
3	HD	3	A1H1F	C4-C5-C6-S6
4	xC	2	BGC	O5-C5-C6-O6
4	3B	2	BGC	O5-C5-C6-O6
4	TA	2	BGC	O5-C5-C6-O6
4	2A	2	BGC	O5-C5-C6-O6
4	wB	2	BGC	O5-C5-C6-O6
4	vA	2	BGC	O5-C5-C6-O6
4	1	2	BGC	O5-C5-C6-O6
4	8	2	BGC	O5-C5-C6-O6
4	MA	2	BGC	O5-C5-C6-O6
4	oA	2	BGC	O5-C5-C6-O6
4	bB	2	BGC	O5-C5-C6-O6
4	jC	2	BGC	O5-C5-C6-O6
4	n	2	BGC	O5-C5-C6-O6
4	GB	2	BGC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	UB	2	BGC	O5-C5-C6-O6
4	pB	2	BGC	O5-C5-C6-O6
4	AC	2	BGC	O5-C5-C6-O6
4	OC	2	BGC	O5-C5-C6-O6
4	aA	2	BGC	O5-C5-C6-O6
4	hA	2	BGC	O5-C5-C6-O6
4	9A	2	BGC	O5-C5-C6-O6
4	NB	2	BGC	O5-C5-C6-O6
4	iB	2	BGC	O5-C5-C6-O6
4	HC	2	BGC	O5-C5-C6-O6
4	VC	2	BGC	O5-C5-C6-O6
4	cC	2	BGC	O5-C5-C6-O6
4	qC	2	BGC	O5-C5-C6-O6
4	4C	2	BGC	O5-C5-C6-O6
4	BD	2	BGC	O5-C5-C6-O6
4	ID	2	BGC	O5-C5-C6-O6
4	u	2	BGC	O5-C5-C6-O6
4	FA	2	BGC	O5-C5-C6-O6
2	9	1	GAL	C4-C5-C6-O6
2	yC	1	GAL	C4-C5-C6-O6
2	AB	1	GAL	C4-C5-C6-O6
2	cB	1	GAL	C4-C5-C6-O6
2	IC	1	GAL	C4-C5-C6-O6
2	CD	1	GAL	C4-C5-C6-O6
2	iA	1	GAL	C4-C5-C6-O6
2	pA	1	GAL	C4-C5-C6-O6
2	wA	1	GAL	C4-C5-C6-O6
2	3A	1	GAL	C4-C5-C6-O6
2	OB	1	GAL	C4-C5-C6-O6
2	PC	1	GAL	C4-C5-C6-O6
2	h	1	GAL	C4-C5-C6-O6
2	v	1	GAL	C4-C5-C6-O6
2	2	1	GAL	C4-C5-C6-O6
2	GA	1	GAL	C4-C5-C6-O6
2	bA	1	GAL	C4-C5-C6-O6
2	VB	1	GAL	C4-C5-C6-O6
2	xB	1	GAL	C4-C5-C6-O6
2	BC	1	GAL	C4-C5-C6-O6
2	kC	1	GAL	C4-C5-C6-O6
2	rC	1	GAL	C4-C5-C6-O6
2	5C	1	GAL	C4-C5-C6-O6
2	o	1	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	NA	1	GAL	C4-C5-C6-O6
2	jB	1	GAL	C4-C5-C6-O6
2	UA	1	GAL	C4-C5-C6-O6
2	qB	1	GAL	C4-C5-C6-O6
2	4B	1	GAL	C4-C5-C6-O6
3	t	5	MAN	C4-C5-C6-O6
3	ZA	5	MAN	C4-C5-C6-O6
3	nA	5	MAN	C4-C5-C6-O6
2	HB	1	GAL	C4-C5-C6-O6
2	WC	1	GAL	C4-C5-C6-O6
2	dC	1	GAL	C4-C5-C6-O6
3	7	5	MAN	C4-C5-C6-O6
3	gA	5	MAN	C4-C5-C6-O6
3	hB	5	MAN	C4-C5-C6-O6
3	oB	5	MAN	C4-C5-C6-O6
3	2B	5	MAN	C4-C5-C6-O6
3	bC	5	MAN	C4-C5-C6-O6
3	LA	5	MAN	C4-C5-C6-O6
3	1A	5	MAN	C4-C5-C6-O6
3	aB	5	MAN	C4-C5-C6-O6
3	UC	5	MAN	C4-C5-C6-O6
3	iC	5	MAN	C4-C5-C6-O6
3	wC	5	MAN	C4-C5-C6-O6
3	AD	5	MAN	C4-C5-C6-O6
3	HD	5	MAN	C4-C5-C6-O6
3	m	5	MAN	C4-C5-C6-O6
3	SA	5	MAN	C4-C5-C6-O6
3	uA	5	MAN	C4-C5-C6-O6
3	EA	5	MAN	C4-C5-C6-O6
3	FB	5	MAN	C4-C5-C6-O6
3	TB	5	MAN	C4-C5-C6-O6
3	9B	5	MAN	C4-C5-C6-O6
3	GC	5	MAN	C4-C5-C6-O6
3	NC	5	MAN	C4-C5-C6-O6
3	pC	5	MAN	C4-C5-C6-O6
3	3C	5	MAN	C4-C5-C6-O6
3	0	5	MAN	C4-C5-C6-O6
3	8A	5	MAN	C4-C5-C6-O6
3	MB	5	MAN	C4-C5-C6-O6
3	vB	5	MAN	C4-C5-C6-O6
4	LB	1	GAL	C4-C5-C6-O6
4	SB	1	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	l	1	GAL	C4-C5-C6-O6
4	s	1	GAL	C4-C5-C6-O6
4	6	1	GAL	C4-C5-C6-O6
4	RA	1	GAL	C4-C5-C6-O6
4	YA	1	GAL	C4-C5-C6-O6
4	fA	1	GAL	C4-C5-C6-O6
4	mA	1	GAL	C4-C5-C6-O6
4	7A	1	GAL	C4-C5-C6-O6
4	EB	1	GAL	C4-C5-C6-O6
4	ZB	1	GAL	C4-C5-C6-O6
4	1B	1	GAL	C4-C5-C6-O6
4	MC	1	GAL	C4-C5-C6-O6
4	TC	1	GAL	C4-C5-C6-O6
4	hC	1	GAL	C4-C5-C6-O6
4	oC	1	GAL	C4-C5-C6-O6
4	GD	1	GAL	C4-C5-C6-O6
4	z	1	GAL	C4-C5-C6-O6
4	KA	1	GAL	C4-C5-C6-O6
4	0A	1	GAL	C4-C5-C6-O6
4	gB	1	GAL	C4-C5-C6-O6
4	nB	1	GAL	C4-C5-C6-O6
4	uB	1	GAL	C4-C5-C6-O6
4	8B	1	GAL	C4-C5-C6-O6
4	FC	1	GAL	C4-C5-C6-O6
4	aC	1	GAL	C4-C5-C6-O6
4	vC	1	GAL	C4-C5-C6-O6
4	9C	1	GAL	C4-C5-C6-O6
4	DA	1	GAL	C4-C5-C6-O6
4	2C	1	GAL	C4-C5-C6-O6
4	tA	1	GAL	C4-C5-C6-O6
2	h	6	A1H03	C4-C5-C6-C7
2	o	6	A1H03	C4-C5-C6-C7
2	v	6	A1H03	C4-C5-C6-C7
2	2	6	A1H03	C4-C5-C6-C7
2	9	6	A1H03	C4-C5-C6-C7
2	GA	6	A1H03	C4-C5-C6-C7
2	NA	6	A1H03	C4-C5-C6-C7
2	UA	6	A1H03	C4-C5-C6-C7
2	bA	6	A1H03	C4-C5-C6-C7
2	iA	6	A1H03	C4-C5-C6-C7
2	pA	6	A1H03	C4-C5-C6-C7
2	wA	6	A1H03	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	3A	6	A1H03	C4-C5-C6-C7
2	AB	6	A1H03	C4-C5-C6-C7
2	HB	6	A1H03	C4-C5-C6-C7
2	OB	6	A1H03	C4-C5-C6-C7
2	VB	6	A1H03	C4-C5-C6-C7
2	cB	6	A1H03	C4-C5-C6-C7
2	jB	6	A1H03	C4-C5-C6-C7
2	qB	6	A1H03	C4-C5-C6-C7
2	xB	6	A1H03	C4-C5-C6-C7
2	4B	6	A1H03	C4-C5-C6-C7
2	BC	6	A1H03	C4-C5-C6-C7
2	IC	6	A1H03	C4-C5-C6-C7
2	PC	6	A1H03	C4-C5-C6-C7
2	WC	6	A1H03	C4-C5-C6-C7
2	dC	6	A1H03	C4-C5-C6-C7
2	kC	6	A1H03	C4-C5-C6-C7
2	rC	6	A1H03	C4-C5-C6-C7
2	yC	6	A1H03	C4-C5-C6-C7
2	5C	6	A1H03	C4-C5-C6-C7
2	CD	6	A1H03	C4-C5-C6-C7
3	j	4	A1H03	C4-C5-C6-C7
3	m	4	A1H03	C4-C5-C6-C7
3	q	4	A1H03	C4-C5-C6-C7
3	t	4	A1H03	C4-C5-C6-C7
3	x	4	A1H03	C4-C5-C6-C7
3	0	4	A1H03	C4-C5-C6-C7
3	4	4	A1H03	C4-C5-C6-C7
3	7	4	A1H03	C4-C5-C6-C7
3	BA	4	A1H03	C4-C5-C6-C7
3	EA	4	A1H03	C4-C5-C6-C7
3	IA	4	A1H03	C4-C5-C6-C7
3	LA	4	A1H03	C4-C5-C6-C7
3	PA	4	A1H03	C4-C5-C6-C7
3	SA	4	A1H03	C4-C5-C6-C7
3	WA	4	A1H03	C4-C5-C6-C7
3	ZA	4	A1H03	C4-C5-C6-C7
3	dA	4	A1H03	C4-C5-C6-C7
3	gA	4	A1H03	C4-C5-C6-C7
3	kA	4	A1H03	C4-C5-C6-C7
3	nA	4	A1H03	C4-C5-C6-C7
3	rA	4	A1H03	C4-C5-C6-C7
3	uA	4	A1H03	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	yA	4	A1H03	C4-C5-C6-C7
3	1A	4	A1H03	C4-C5-C6-C7
3	5A	4	A1H03	C4-C5-C6-C7
3	8A	4	A1H03	C4-C5-C6-C7
3	CB	4	A1H03	C4-C5-C6-C7
3	FB	4	A1H03	C4-C5-C6-C7
3	JB	4	A1H03	C4-C5-C6-C7
3	MB	4	A1H03	C4-C5-C6-C7
3	QB	4	A1H03	C4-C5-C6-C7
3	TB	4	A1H03	C4-C5-C6-C7
3	XB	4	A1H03	C4-C5-C6-C7
3	aB	4	A1H03	C4-C5-C6-C7
3	eB	4	A1H03	C4-C5-C6-C7
3	hB	4	A1H03	C4-C5-C6-C7
3	lB	4	A1H03	C4-C5-C6-C7
3	oB	4	A1H03	C4-C5-C6-C7
3	sB	4	A1H03	C4-C5-C6-C7
3	vB	4	A1H03	C4-C5-C6-C7
3	zB	4	A1H03	C4-C5-C6-C7
3	2B	4	A1H03	C4-C5-C6-C7
3	6B	4	A1H03	C4-C5-C6-C7
3	9B	4	A1H03	C4-C5-C6-C7
3	DC	4	A1H03	C4-C5-C6-C7
3	GC	4	A1H03	C4-C5-C6-C7
3	KC	4	A1H03	C4-C5-C6-C7
3	NC	4	A1H03	C4-C5-C6-C7
3	RC	4	A1H03	C4-C5-C6-C7
3	UC	4	A1H03	C4-C5-C6-C7
3	YC	4	A1H03	C4-C5-C6-C7
3	bC	4	A1H03	C4-C5-C6-C7
3	fC	4	A1H03	C4-C5-C6-C7
3	iC	4	A1H03	C4-C5-C6-C7
3	mC	4	A1H03	C4-C5-C6-C7
3	pC	4	A1H03	C4-C5-C6-C7
3	tC	4	A1H03	C4-C5-C6-C7
3	wC	4	A1H03	C4-C5-C6-C7
3	0C	4	A1H03	C4-C5-C6-C7
3	3C	4	A1H03	C4-C5-C6-C7
3	7C	4	A1H03	C4-C5-C6-C7
3	AD	4	A1H03	C4-C5-C6-C7
3	ED	4	A1H03	C4-C5-C6-C7
3	HD	4	A1H03	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	FA	1	GAL	C4-C5-C6-O6
4	u	1	GAL	C4-C5-C6-O6
4	hA	1	GAL	C4-C5-C6-O6
4	TA	1	GAL	C4-C5-C6-O6
4	aA	1	GAL	C4-C5-C6-O6
4	vA	1	GAL	C4-C5-C6-O6
4	GB	1	GAL	C4-C5-C6-O6
4	NB	1	GAL	C4-C5-C6-O6
4	pB	1	GAL	C4-C5-C6-O6
4	AC	1	GAL	C4-C5-C6-O6
4	HC	1	GAL	C4-C5-C6-O6
4	VC	1	GAL	C4-C5-C6-O6
4	cC	1	GAL	C4-C5-C6-O6
4	jC	1	GAL	C4-C5-C6-O6
4	ID	1	GAL	C4-C5-C6-O6
4	n	1	GAL	C4-C5-C6-O6
4	8	1	GAL	C4-C5-C6-O6
4	bB	1	GAL	C4-C5-C6-O6
4	4C	1	GAL	C4-C5-C6-O6
2	o	6	A1H03	O5-C5-C6-O6
3	j	4	A1H03	O5-C5-C6-O6
3	m	4	A1H03	O5-C5-C6-O6
3	q	4	A1H03	O5-C5-C6-O6
3	t	4	A1H03	O5-C5-C6-O6
3	x	4	A1H03	O5-C5-C6-O6
3	0	4	A1H03	O5-C5-C6-O6
3	4	4	A1H03	O5-C5-C6-O6
3	7	4	A1H03	O5-C5-C6-O6
3	BA	4	A1H03	O5-C5-C6-O6
3	EA	4	A1H03	O5-C5-C6-O6
3	IA	4	A1H03	O5-C5-C6-O6
3	LA	4	A1H03	O5-C5-C6-O6
3	SA	4	A1H03	O5-C5-C6-O6
3	WA	4	A1H03	O5-C5-C6-O6
3	ZA	4	A1H03	O5-C5-C6-O6
3	gA	4	A1H03	O5-C5-C6-O6
3	nA	4	A1H03	O5-C5-C6-O6
3	rA	4	A1H03	O5-C5-C6-O6
3	uA	4	A1H03	O5-C5-C6-O6
3	yA	4	A1H03	O5-C5-C6-O6
3	1A	4	A1H03	O5-C5-C6-O6
3	8A	4	A1H03	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	FB	4	A1H03	O5-C5-C6-O6
3	JB	4	A1H03	O5-C5-C6-O6
3	MB	4	A1H03	O5-C5-C6-O6
3	QB	4	A1H03	O5-C5-C6-O6
3	TB	4	A1H03	O5-C5-C6-O6
3	XB	4	A1H03	O5-C5-C6-O6
3	aB	4	A1H03	O5-C5-C6-O6
3	eB	4	A1H03	O5-C5-C6-O6
3	hB	4	A1H03	O5-C5-C6-O6
3	lB	4	A1H03	O5-C5-C6-O6
3	oB	4	A1H03	O5-C5-C6-O6
3	vB	4	A1H03	O5-C5-C6-O6
3	2B	4	A1H03	O5-C5-C6-O6
3	6B	4	A1H03	O5-C5-C6-O6
3	9B	4	A1H03	O5-C5-C6-O6
3	GC	4	A1H03	O5-C5-C6-O6
3	KC	4	A1H03	O5-C5-C6-O6
3	NC	4	A1H03	O5-C5-C6-O6
3	UC	4	A1H03	O5-C5-C6-O6
3	YC	4	A1H03	O5-C5-C6-O6
3	bC	4	A1H03	O5-C5-C6-O6
3	fC	4	A1H03	O5-C5-C6-O6
3	iC	4	A1H03	O5-C5-C6-O6
3	mC	4	A1H03	O5-C5-C6-O6
3	pC	4	A1H03	O5-C5-C6-O6
3	wC	4	A1H03	O5-C5-C6-O6
3	0C	4	A1H03	O5-C5-C6-O6
3	3C	4	A1H03	O5-C5-C6-O6
3	7C	4	A1H03	O5-C5-C6-O6
3	AD	4	A1H03	O5-C5-C6-O6
3	ED	4	A1H03	O5-C5-C6-O6
3	HD	4	A1H03	O5-C5-C6-O6
4	oA	1	GAL	C4-C5-C6-O6
4	OC	1	GAL	C4-C5-C6-O6
4	2A	1	GAL	C4-C5-C6-O6
4	9A	1	GAL	C4-C5-C6-O6
4	wB	1	GAL	C4-C5-C6-O6
4	3B	1	GAL	C4-C5-C6-O6
4	xC	1	GAL	C4-C5-C6-O6
4	BD	1	GAL	C4-C5-C6-O6
4	MA	1	GAL	C4-C5-C6-O6
4	UB	1	GAL	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	iB	1	GAL	C4-C5-C6-O6
4	l	1	GAL	C4-C5-C6-O6
4	qC	1	GAL	C4-C5-C6-O6
4	n	3	A1H1F	O5-C5-C6-S6
4	u	3	A1H1F	O5-C5-C6-S6
4	l	3	A1H1F	O5-C5-C6-S6
4	8	3	A1H1F	O5-C5-C6-S6
4	FA	3	A1H1F	O5-C5-C6-S6
4	MA	3	A1H1F	O5-C5-C6-S6
4	TA	3	A1H1F	O5-C5-C6-S6
4	aA	3	A1H1F	O5-C5-C6-S6
4	hA	3	A1H1F	O5-C5-C6-S6
4	oA	3	A1H1F	O5-C5-C6-S6
4	vA	3	A1H1F	O5-C5-C6-S6
4	2A	3	A1H1F	O5-C5-C6-S6
4	9A	3	A1H1F	O5-C5-C6-S6
4	GB	3	A1H1F	O5-C5-C6-S6
4	NB	3	A1H1F	O5-C5-C6-S6
4	UB	3	A1H1F	O5-C5-C6-S6
4	bB	3	A1H1F	O5-C5-C6-S6
4	iB	3	A1H1F	O5-C5-C6-S6
4	pB	3	A1H1F	O5-C5-C6-S6
4	wB	3	A1H1F	O5-C5-C6-S6
4	3B	3	A1H1F	O5-C5-C6-S6
4	AC	3	A1H1F	O5-C5-C6-S6
4	HC	3	A1H1F	O5-C5-C6-S6
4	OC	3	A1H1F	O5-C5-C6-S6
4	VC	3	A1H1F	O5-C5-C6-S6
4	cC	3	A1H1F	O5-C5-C6-S6
4	jC	3	A1H1F	O5-C5-C6-S6
4	qC	3	A1H1F	O5-C5-C6-S6
4	xC	3	A1H1F	O5-C5-C6-S6
4	4C	3	A1H1F	O5-C5-C6-S6
4	BD	3	A1H1F	O5-C5-C6-S6
4	ID	3	A1H1F	O5-C5-C6-S6

All (32) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BC	5	MAN	C1-C2-C3-C4-C5-O5
2	UA	5	MAN	C1-C2-C3-C4-C5-O5
2	HB	5	MAN	C1-C2-C3-C4-C5-O5

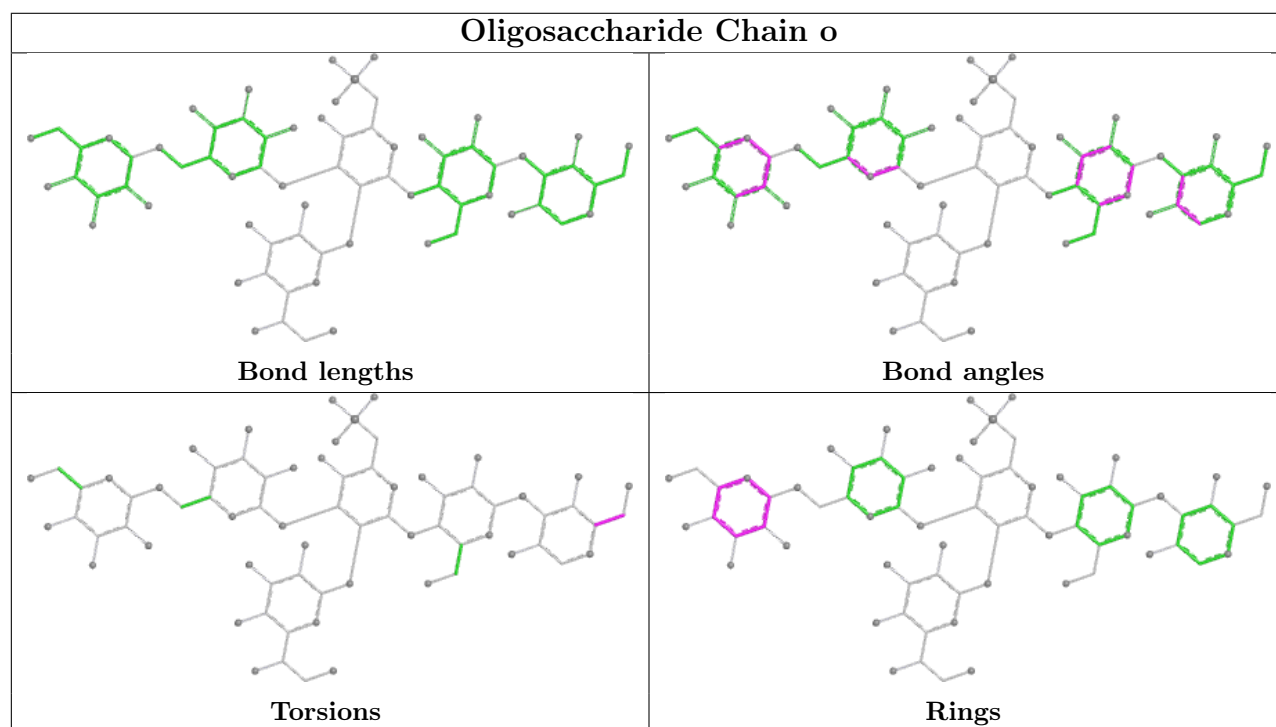
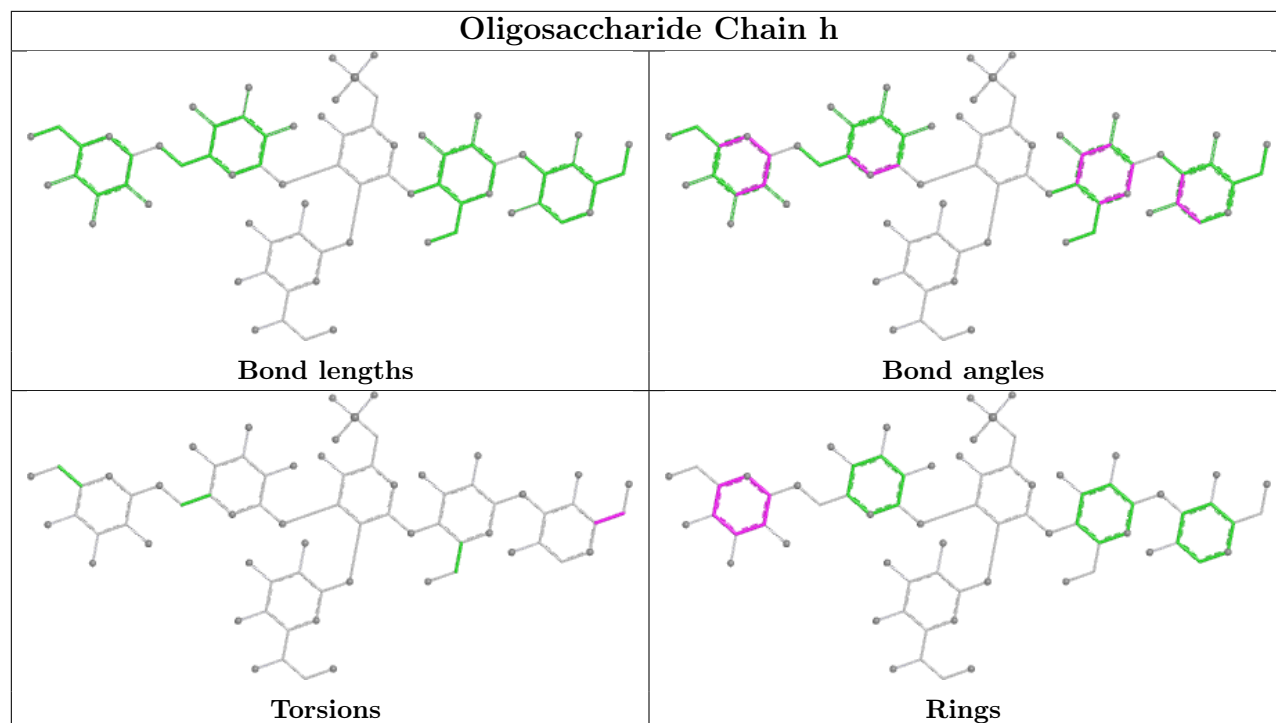
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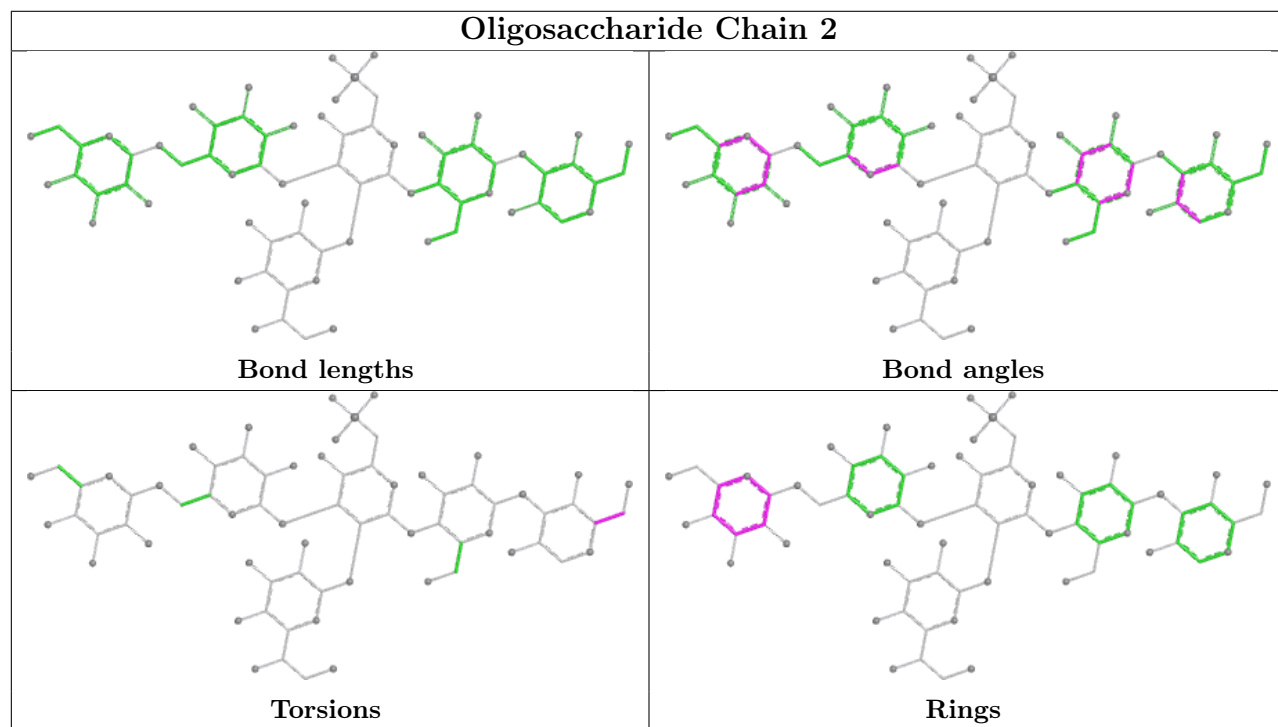
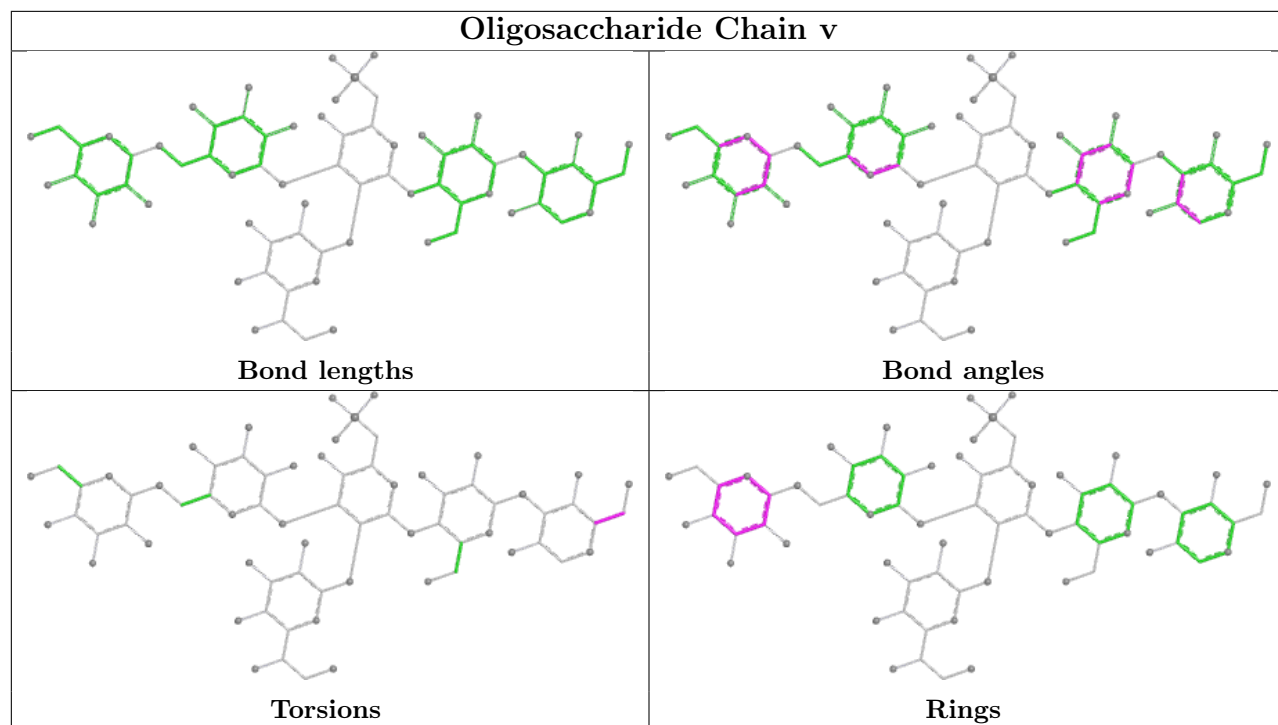
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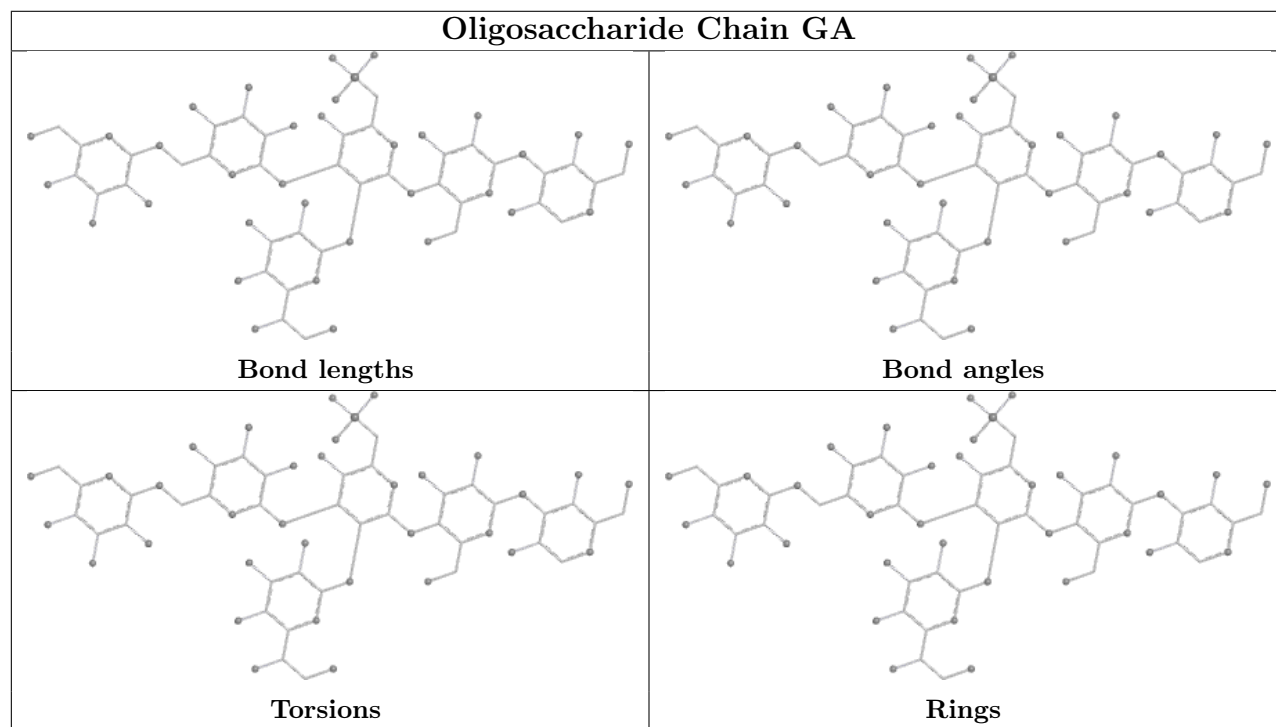
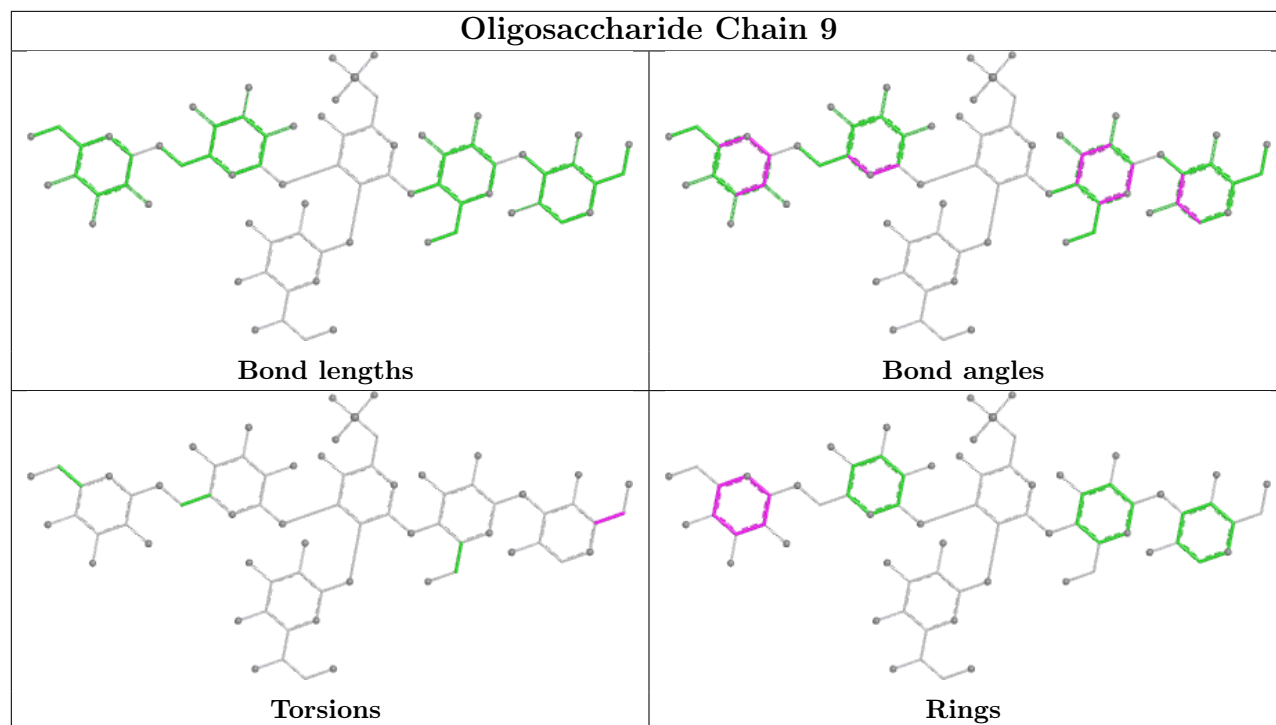
Mol	Chain	Res	Type	Atoms
2	pA	5	MAN	C1-C2-C3-C4-C5-O5
2	rC	5	MAN	C1-C2-C3-C4-C5-O5
2	IC	5	MAN	C1-C2-C3-C4-C5-O5
2	o	5	MAN	C1-C2-C3-C4-C5-O5
2	AB	5	MAN	C1-C2-C3-C4-C5-O5
2	qB	5	MAN	C1-C2-C3-C4-C5-O5
2	yC	5	MAN	C1-C2-C3-C4-C5-O5
2	4B	5	MAN	C1-C2-C3-C4-C5-O5
2	VB	5	MAN	C1-C2-C3-C4-C5-O5
2	bA	5	MAN	C1-C2-C3-C4-C5-O5
2	iA	5	MAN	C1-C2-C3-C4-C5-O5
2	h	5	MAN	C1-C2-C3-C4-C5-O5
2	9	5	MAN	C1-C2-C3-C4-C5-O5
2	5C	5	MAN	C1-C2-C3-C4-C5-O5
2	kC	5	MAN	C1-C2-C3-C4-C5-O5
2	NA	5	MAN	C1-C2-C3-C4-C5-O5
2	dC	5	MAN	C1-C2-C3-C4-C5-O5
2	CD	5	MAN	C1-C2-C3-C4-C5-O5
2	v	5	MAN	C1-C2-C3-C4-C5-O5
2	jB	5	MAN	C1-C2-C3-C4-C5-O5
2	3A	5	MAN	C1-C2-C3-C4-C5-O5
2	xB	5	MAN	C1-C2-C3-C4-C5-O5
2	wA	5	MAN	C1-C2-C3-C4-C5-O5
2	2	5	MAN	C1-C2-C3-C4-C5-O5
2	GA	5	MAN	C1-C2-C3-C4-C5-O5
2	PC	5	MAN	C1-C2-C3-C4-C5-O5
2	cB	5	MAN	C1-C2-C3-C4-C5-O5
2	WC	5	MAN	C1-C2-C3-C4-C5-O5
2	OB	5	MAN	C1-C2-C3-C4-C5-O5

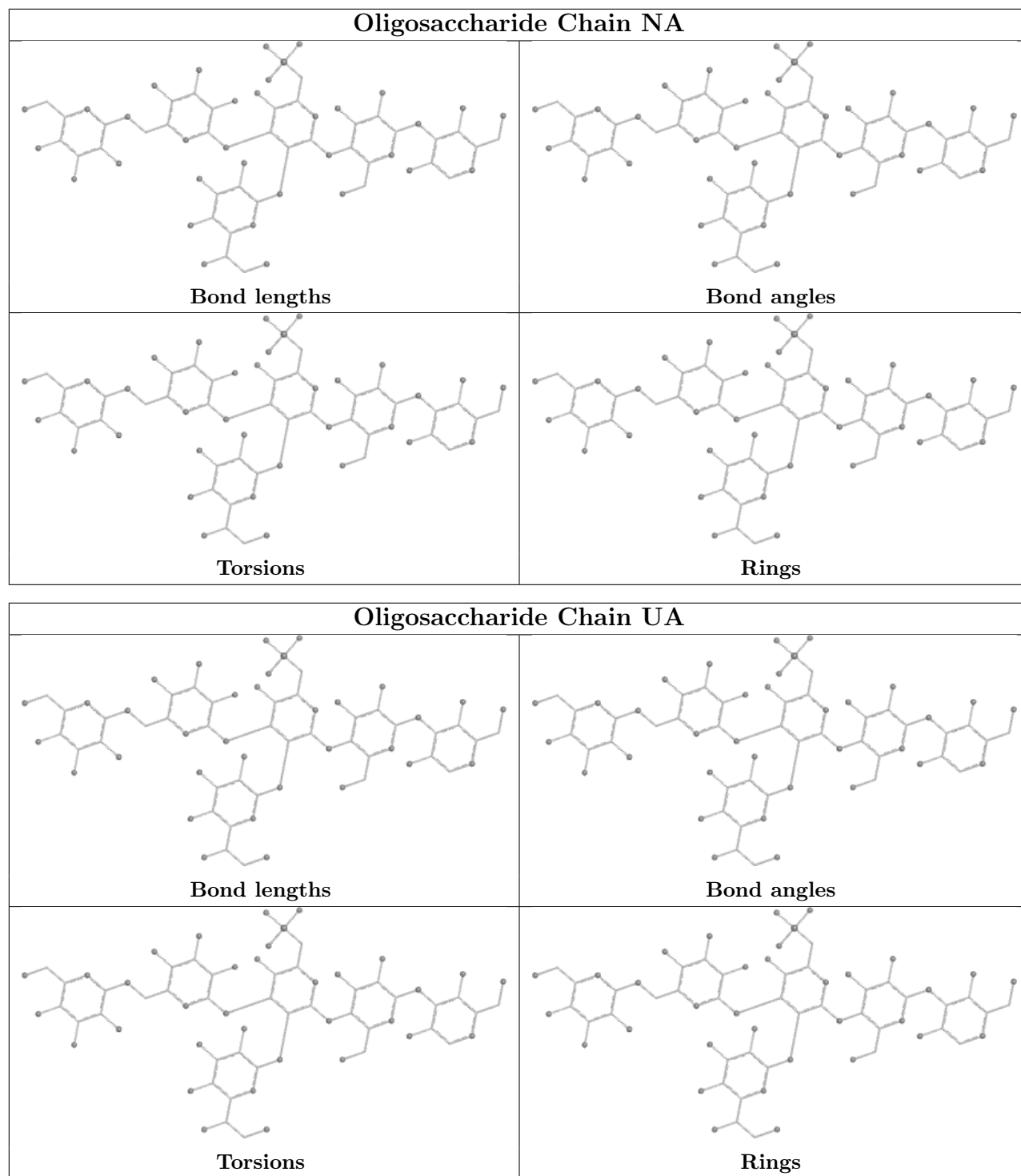
No monomer is involved in short contacts.

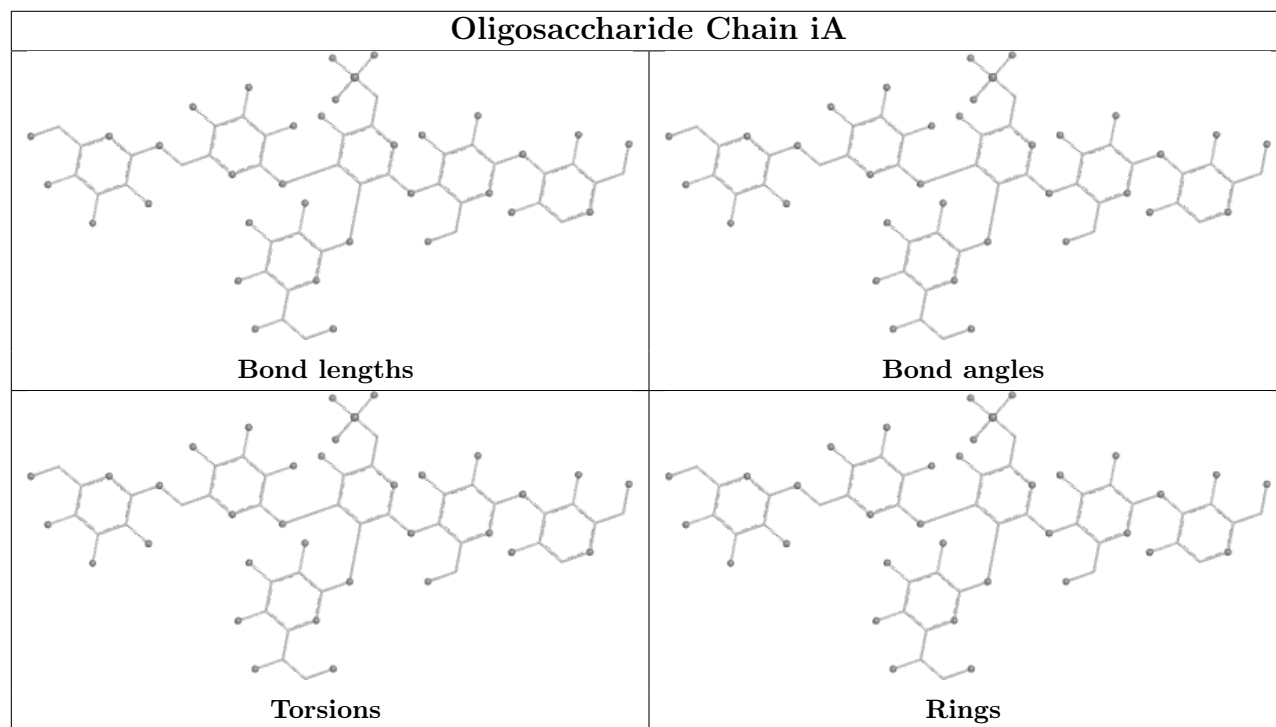
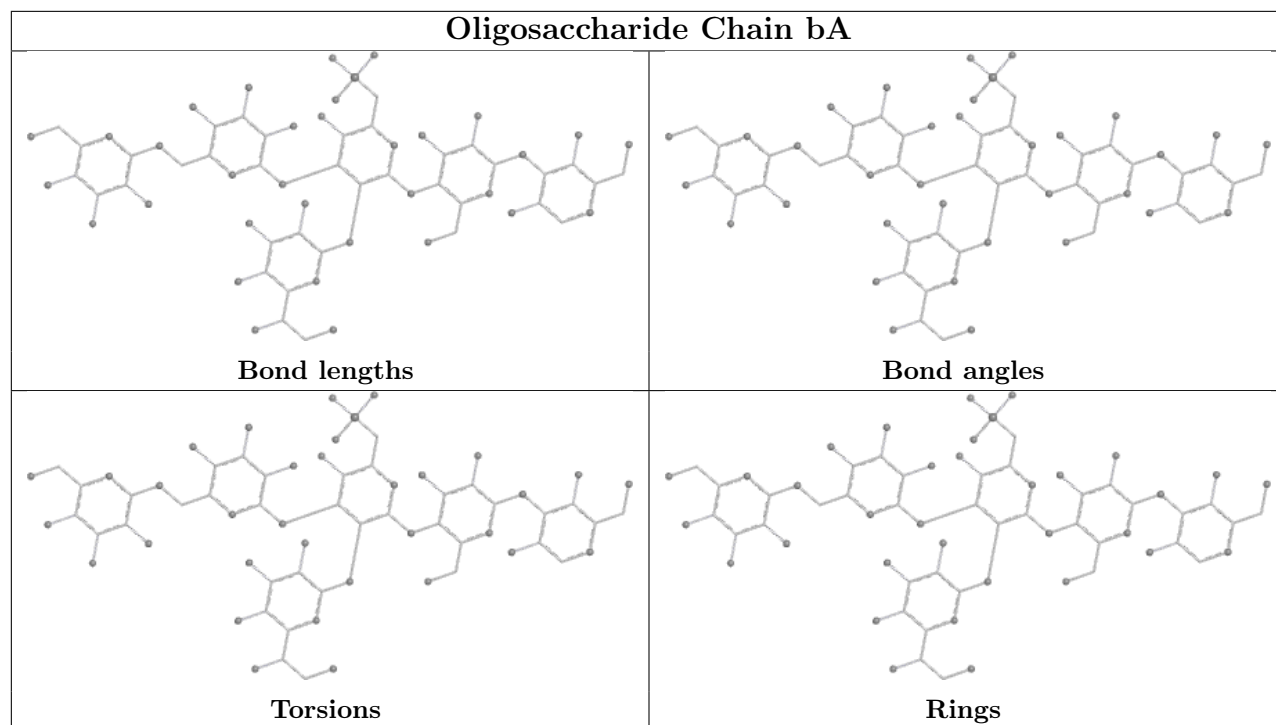
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

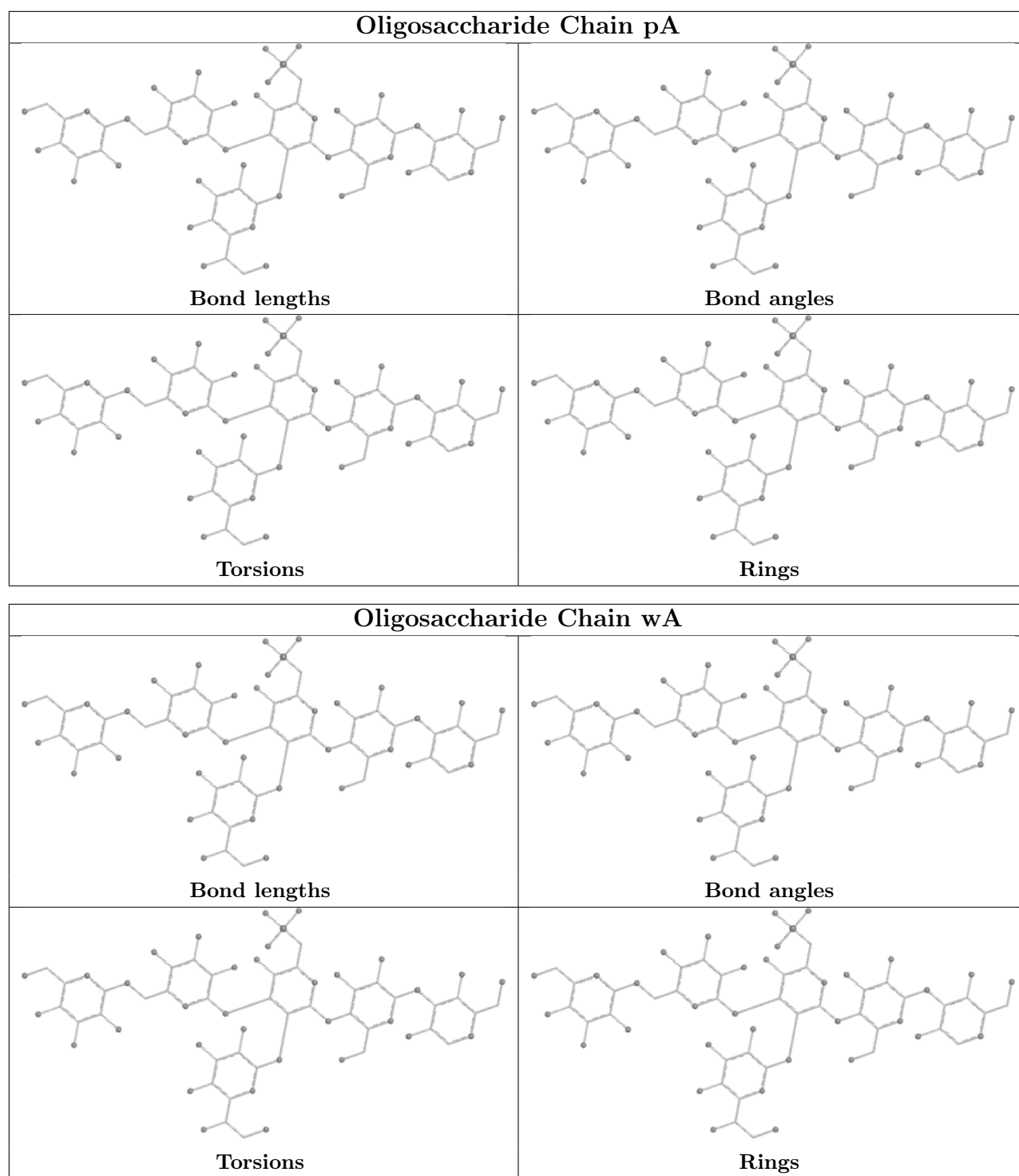


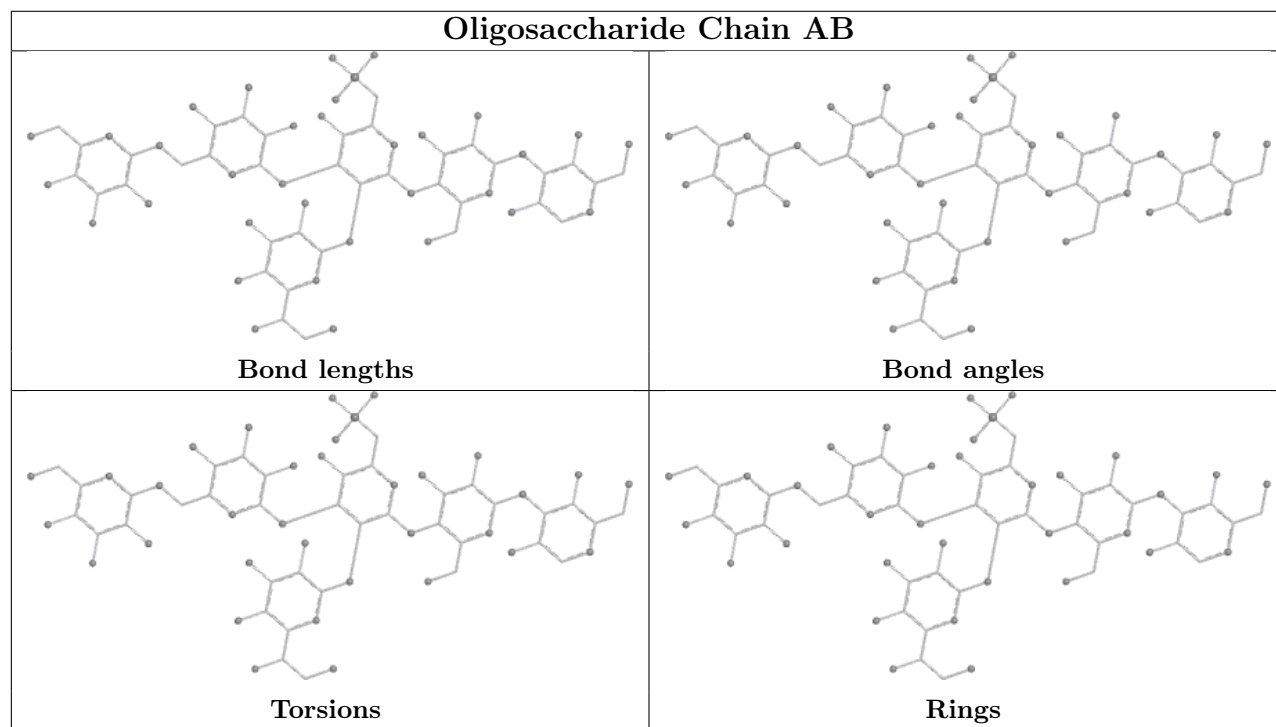
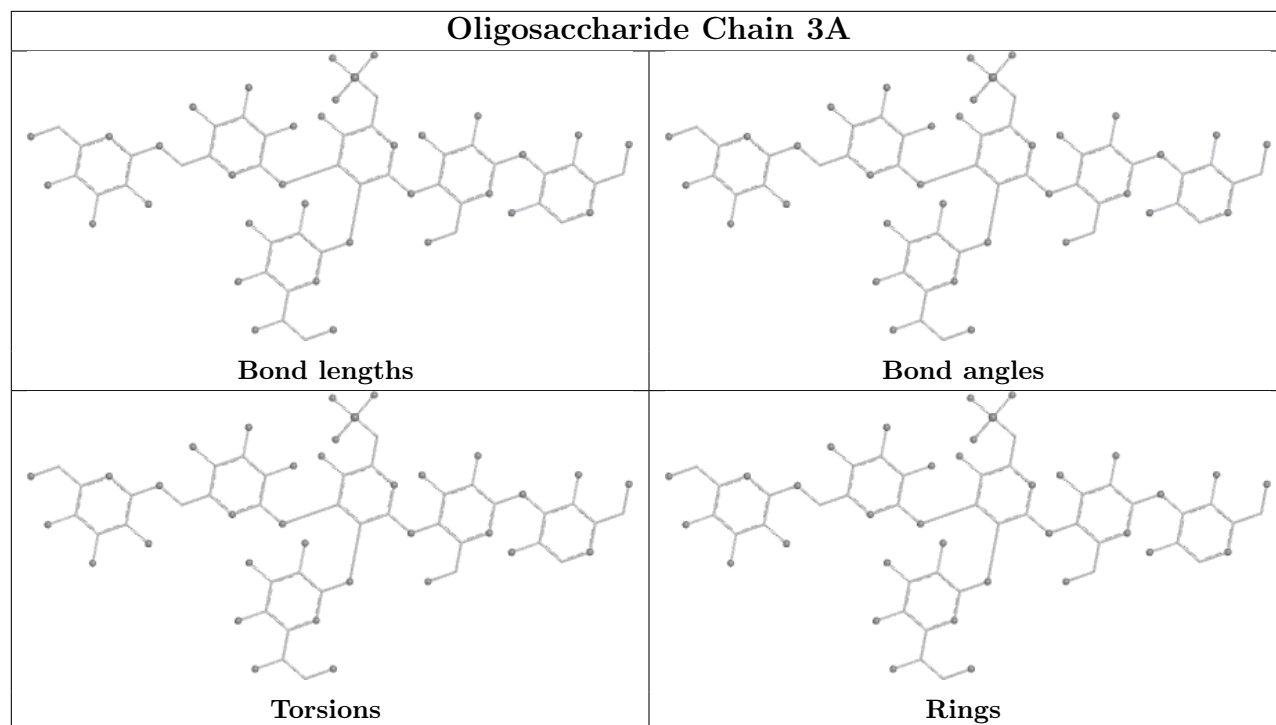


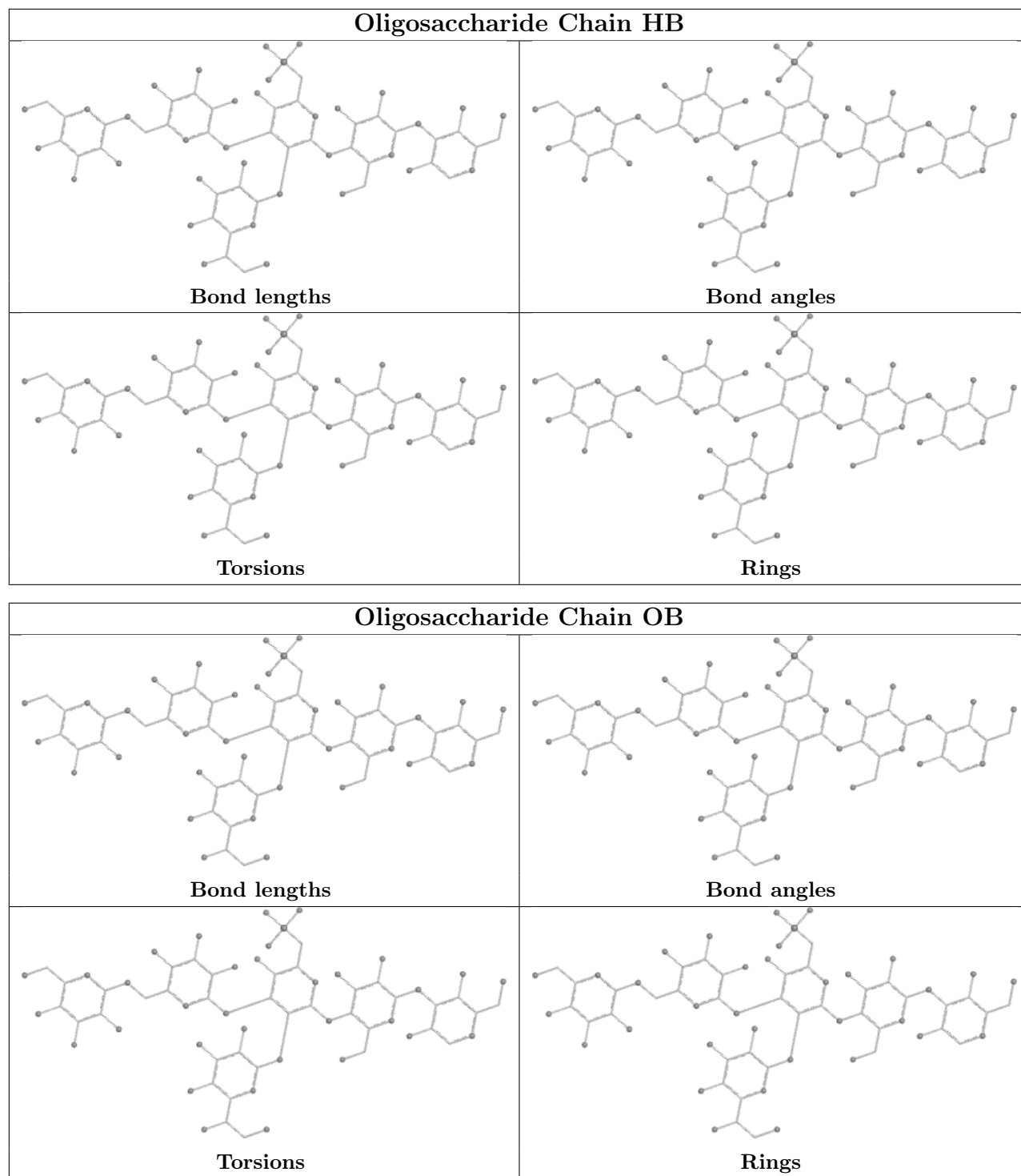


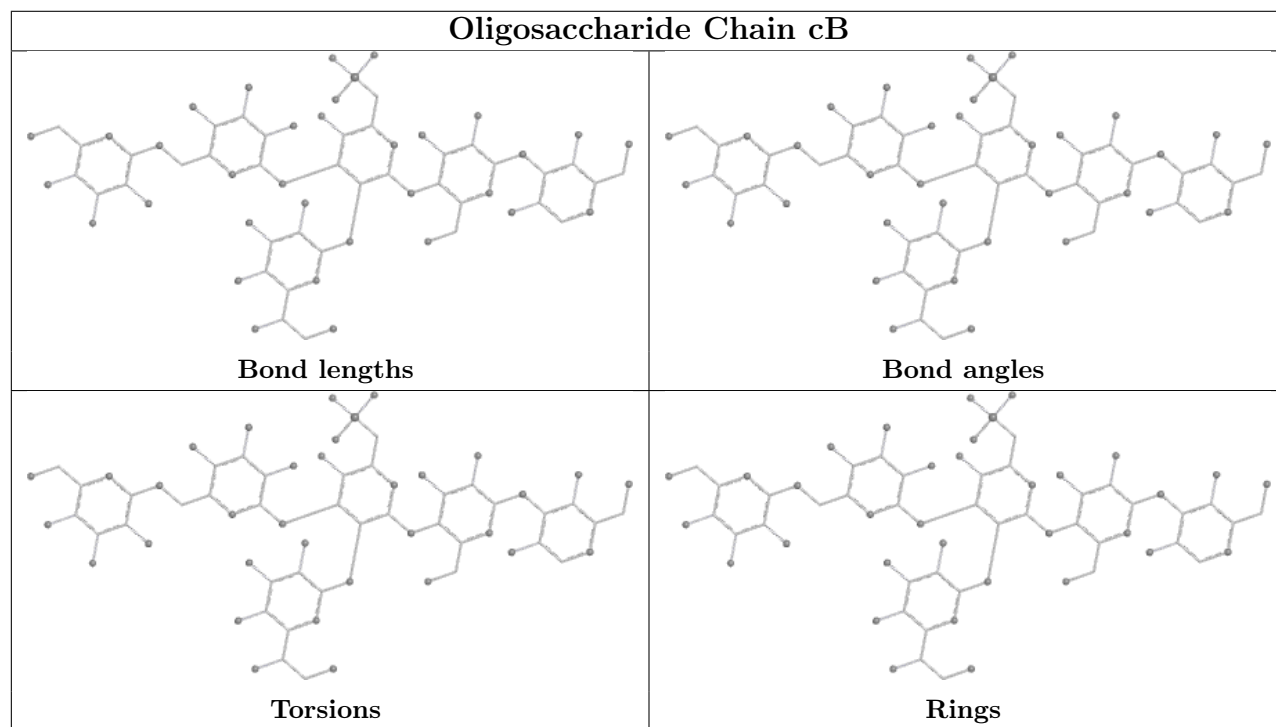
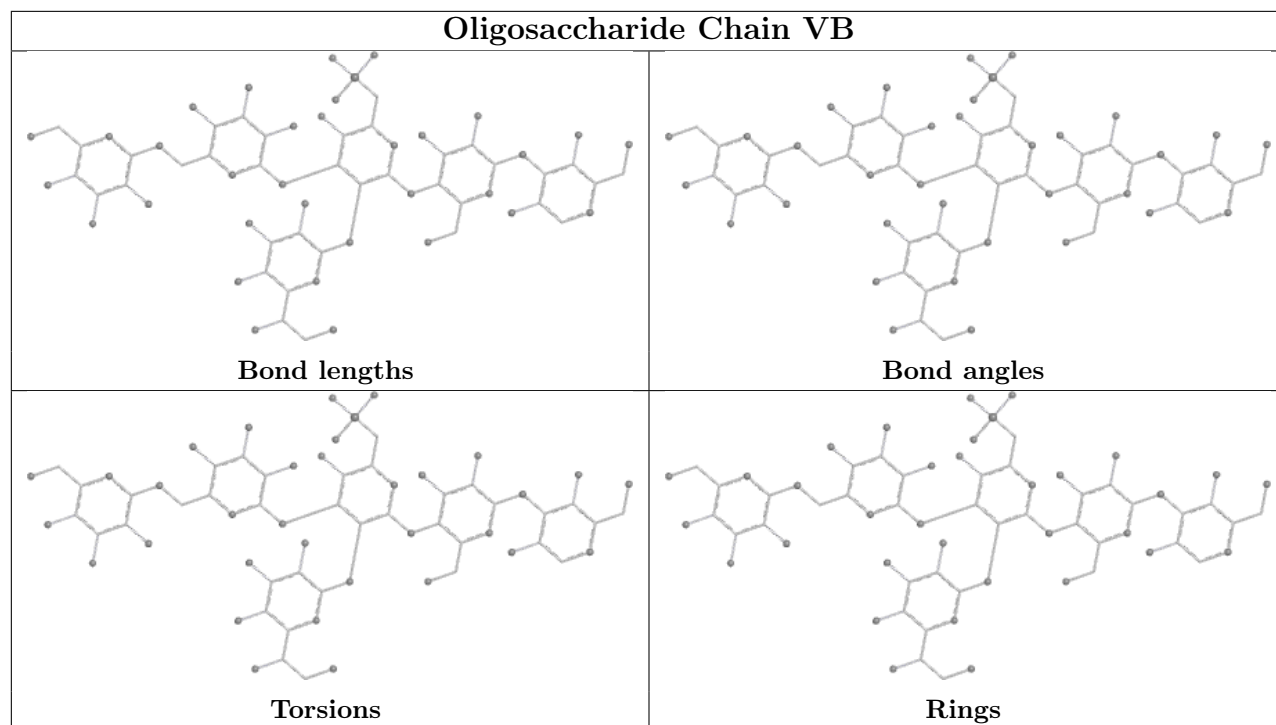


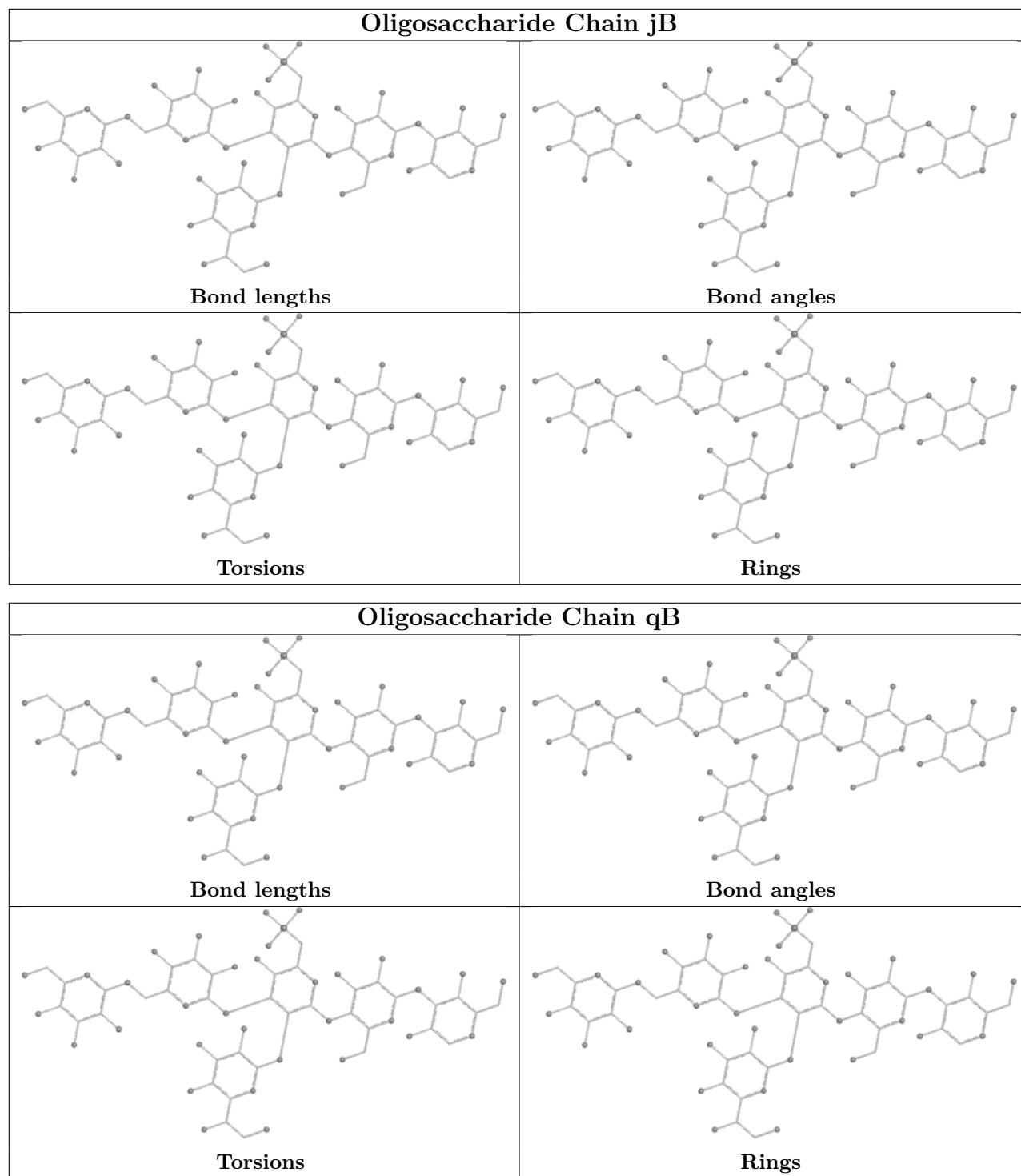


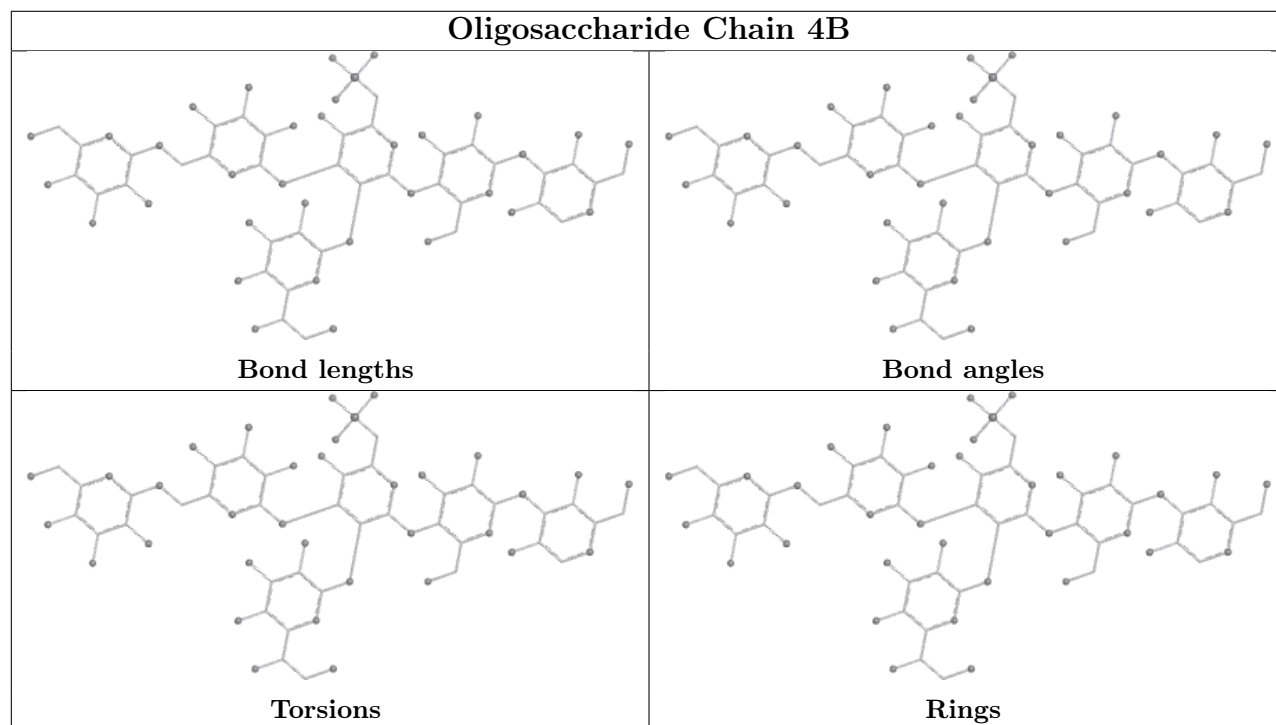
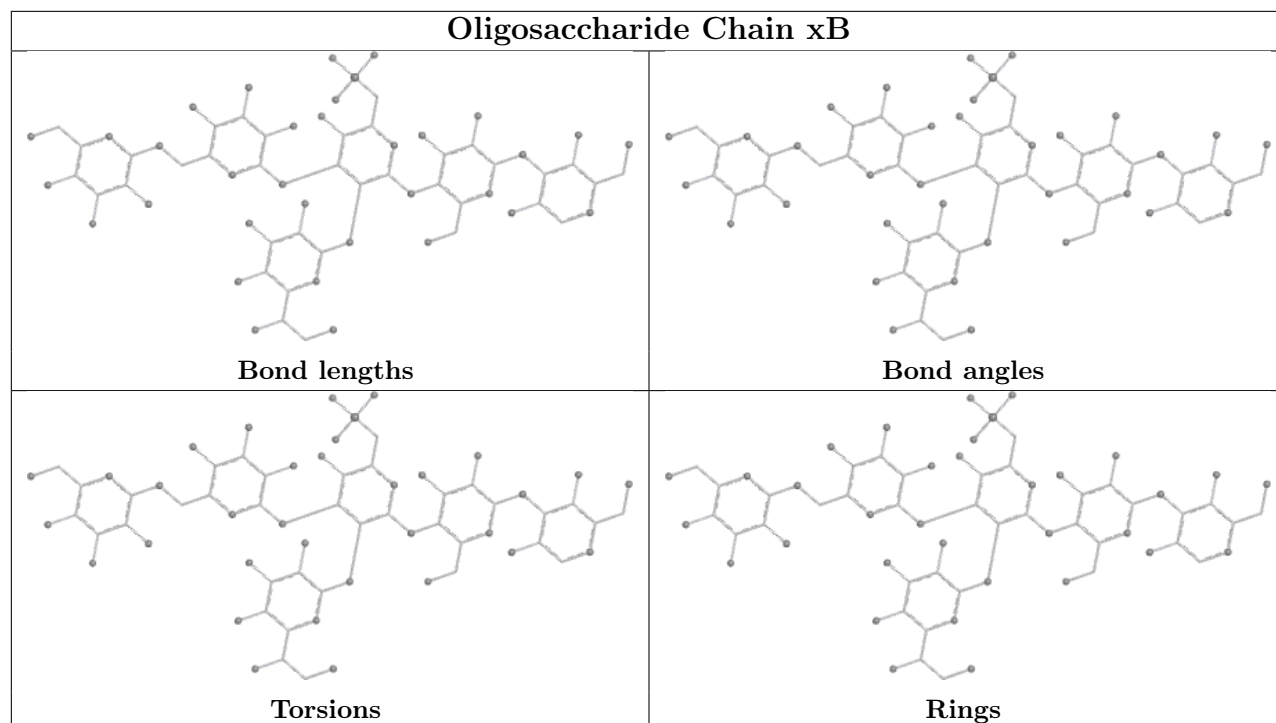


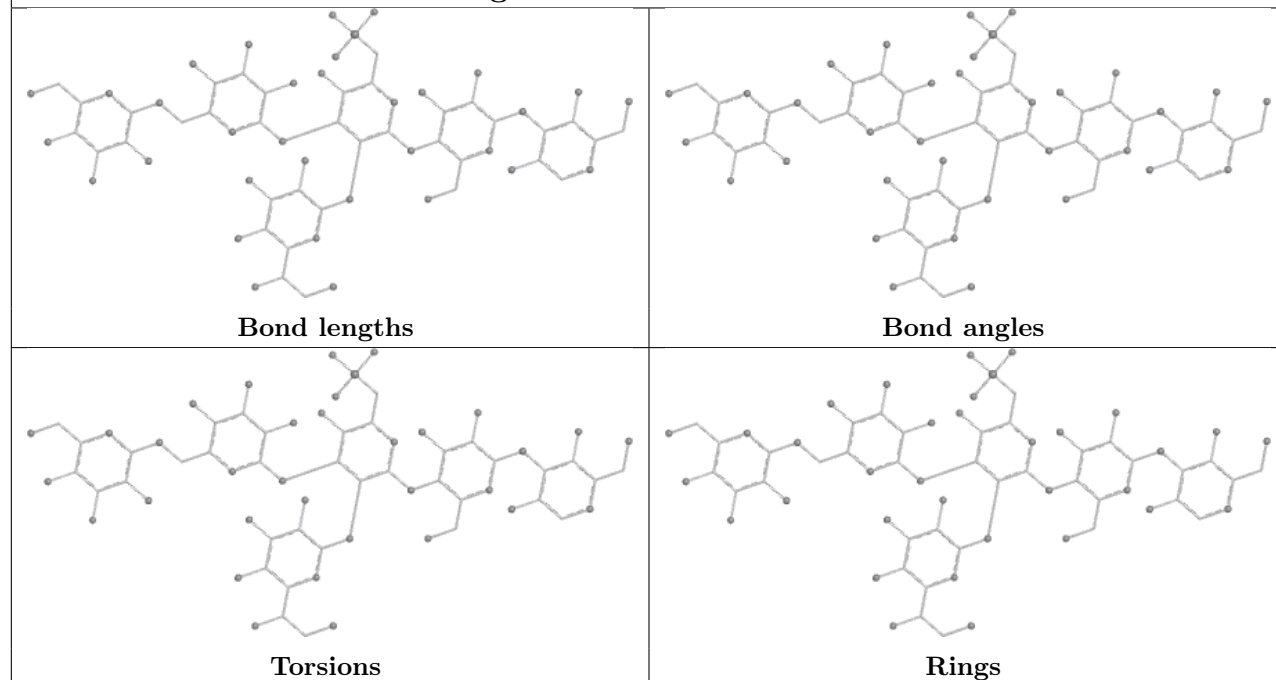
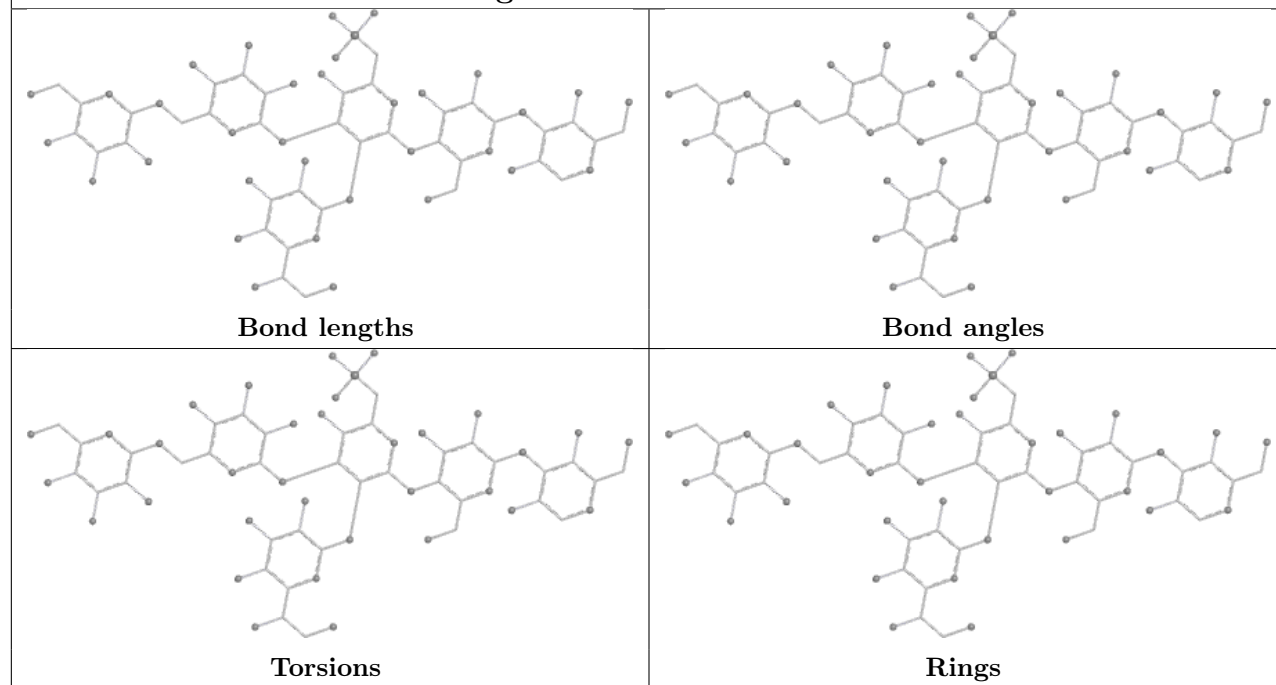


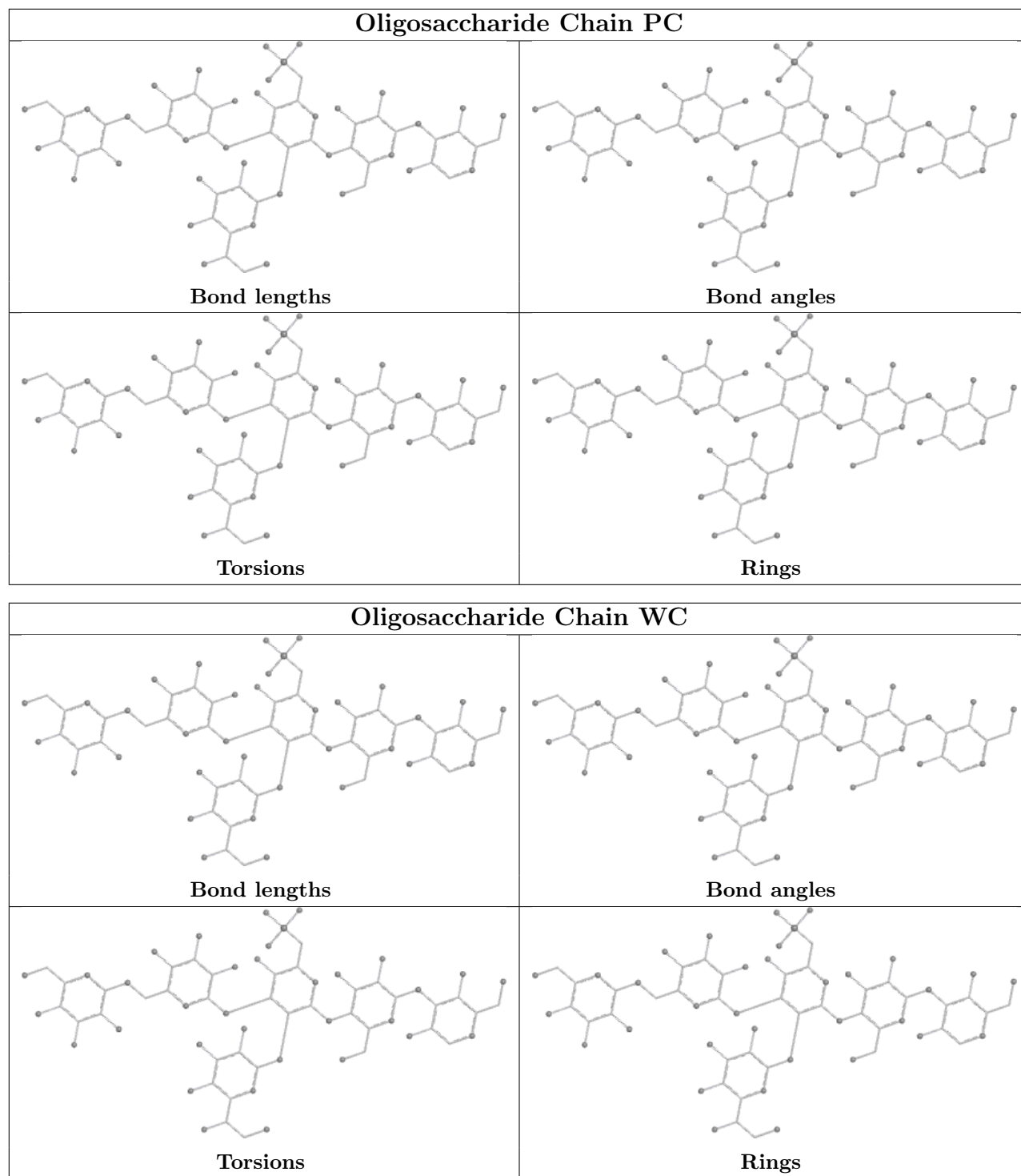


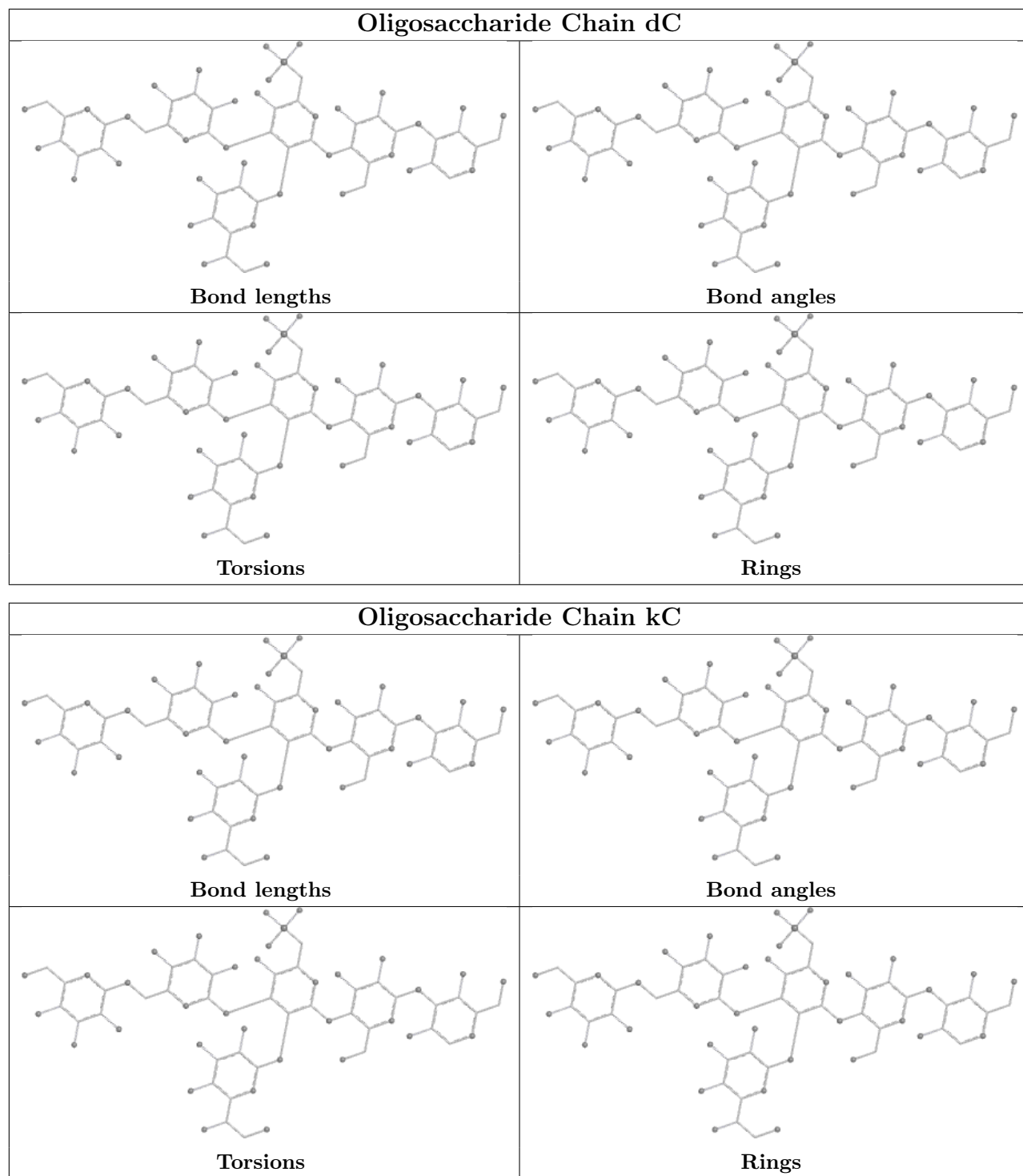


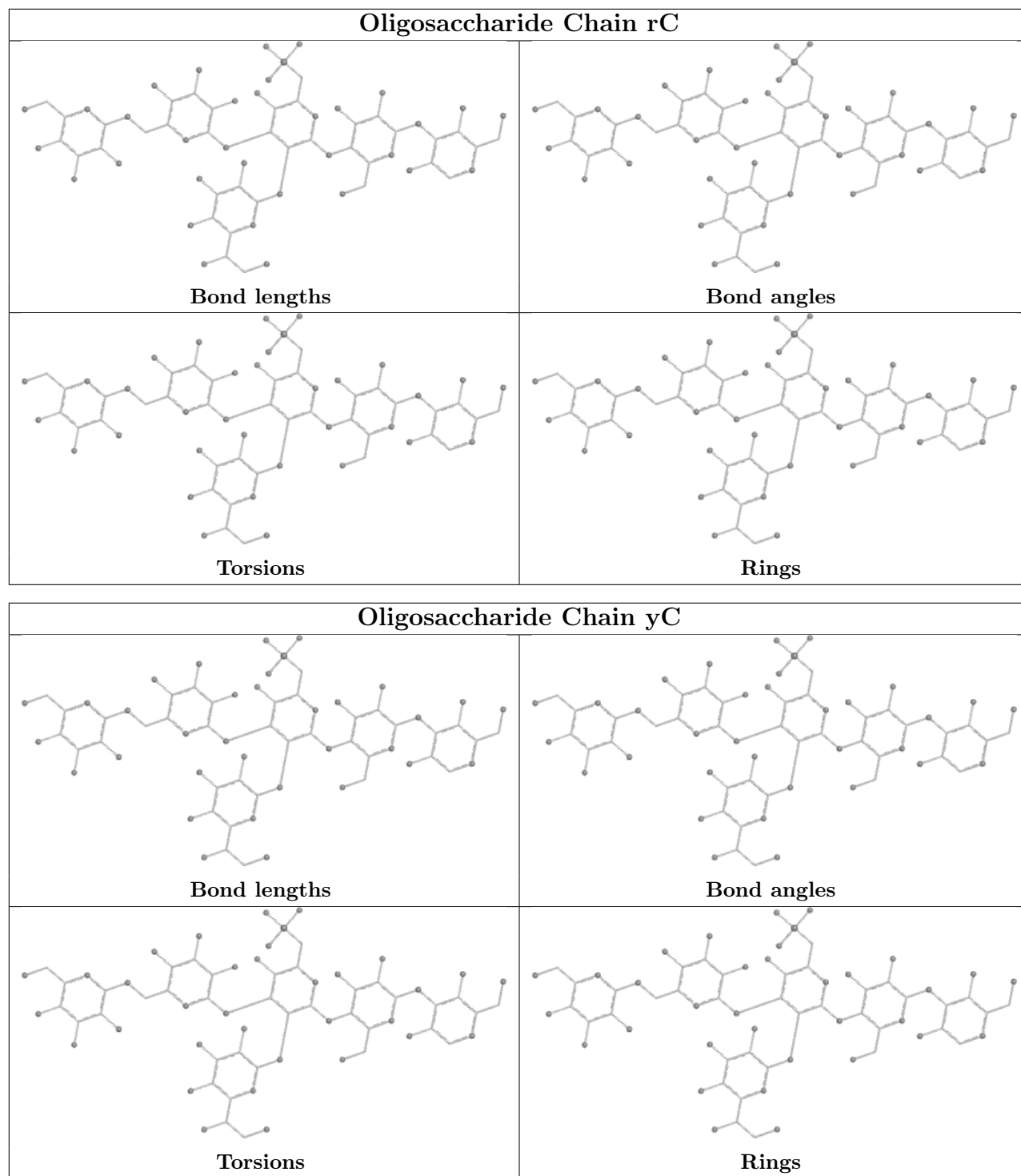


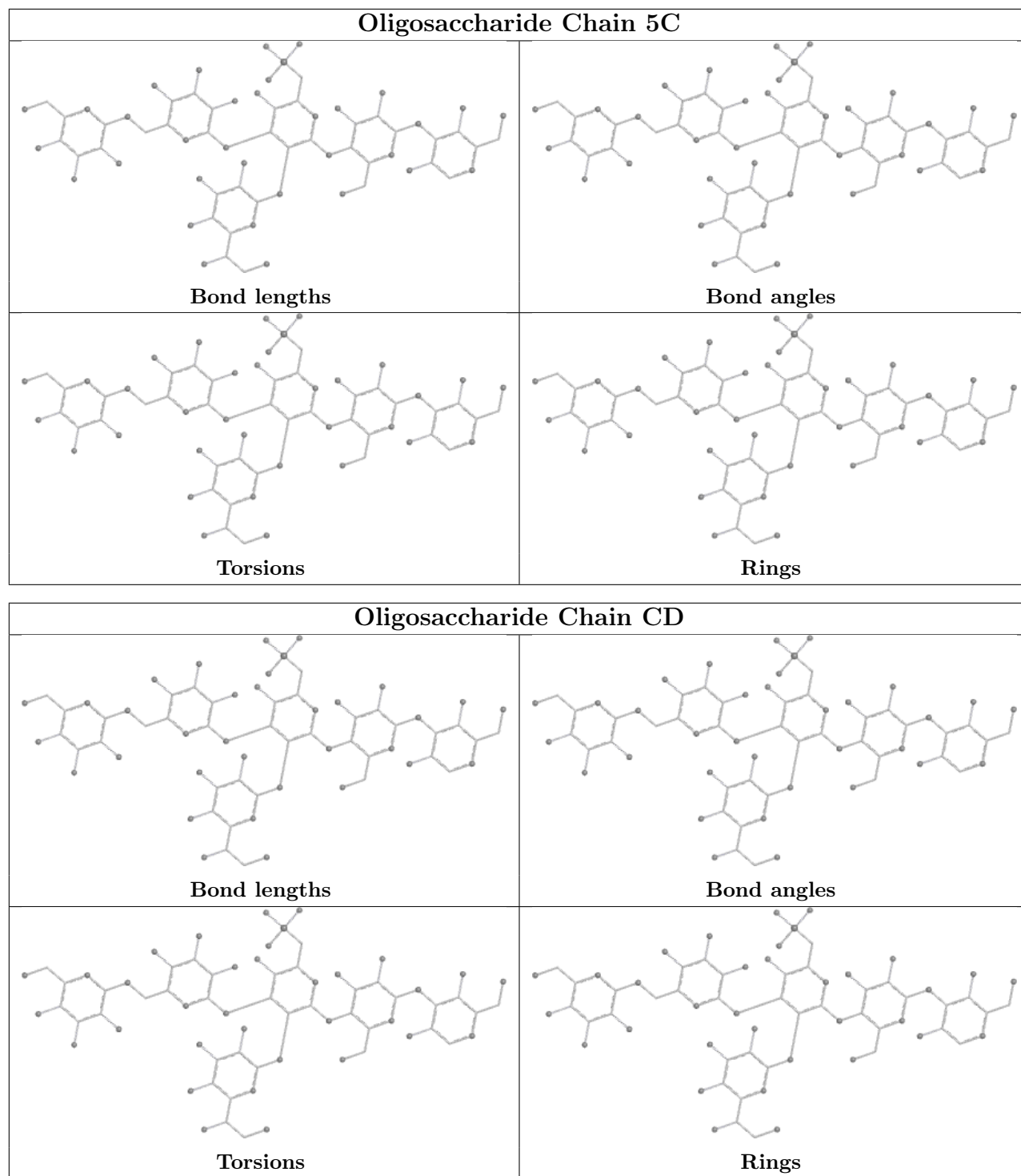


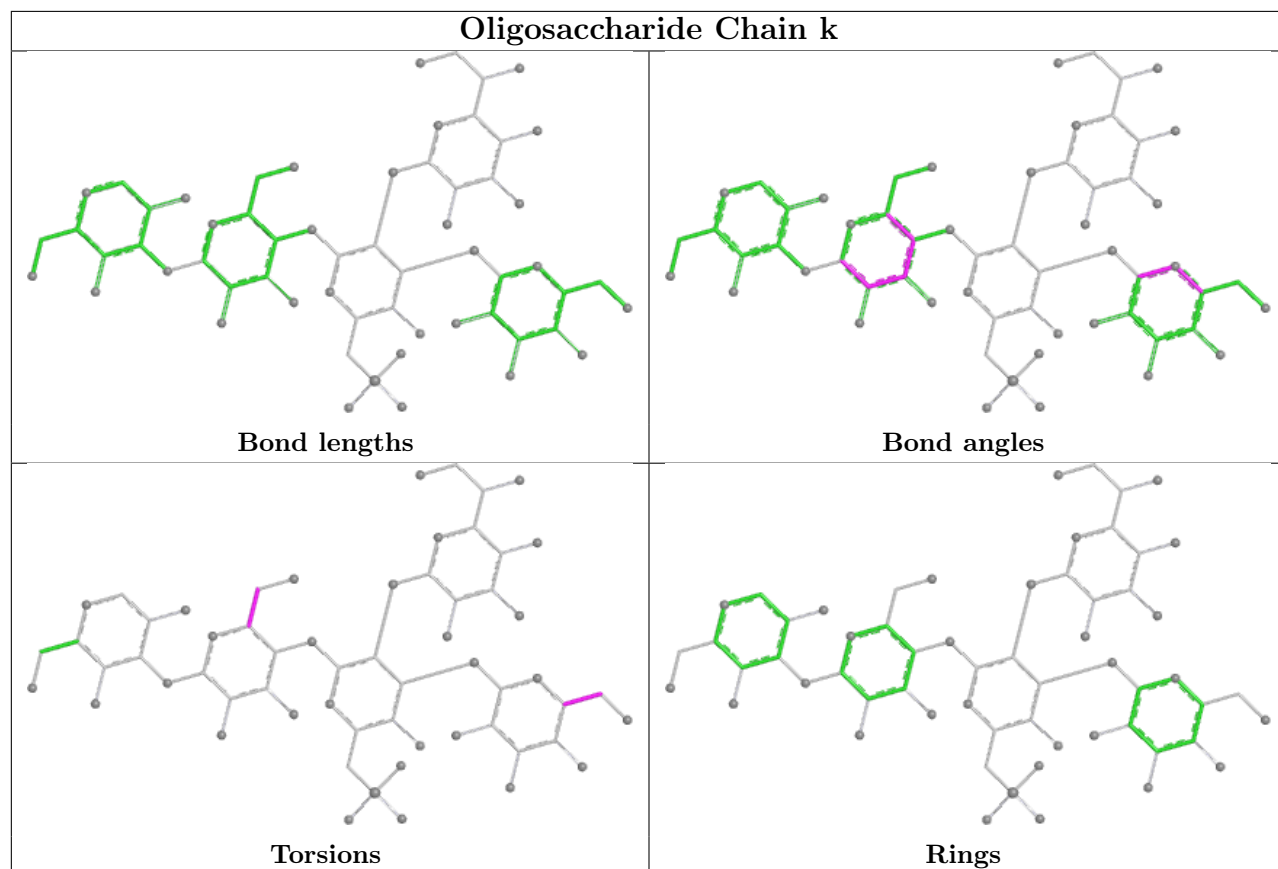
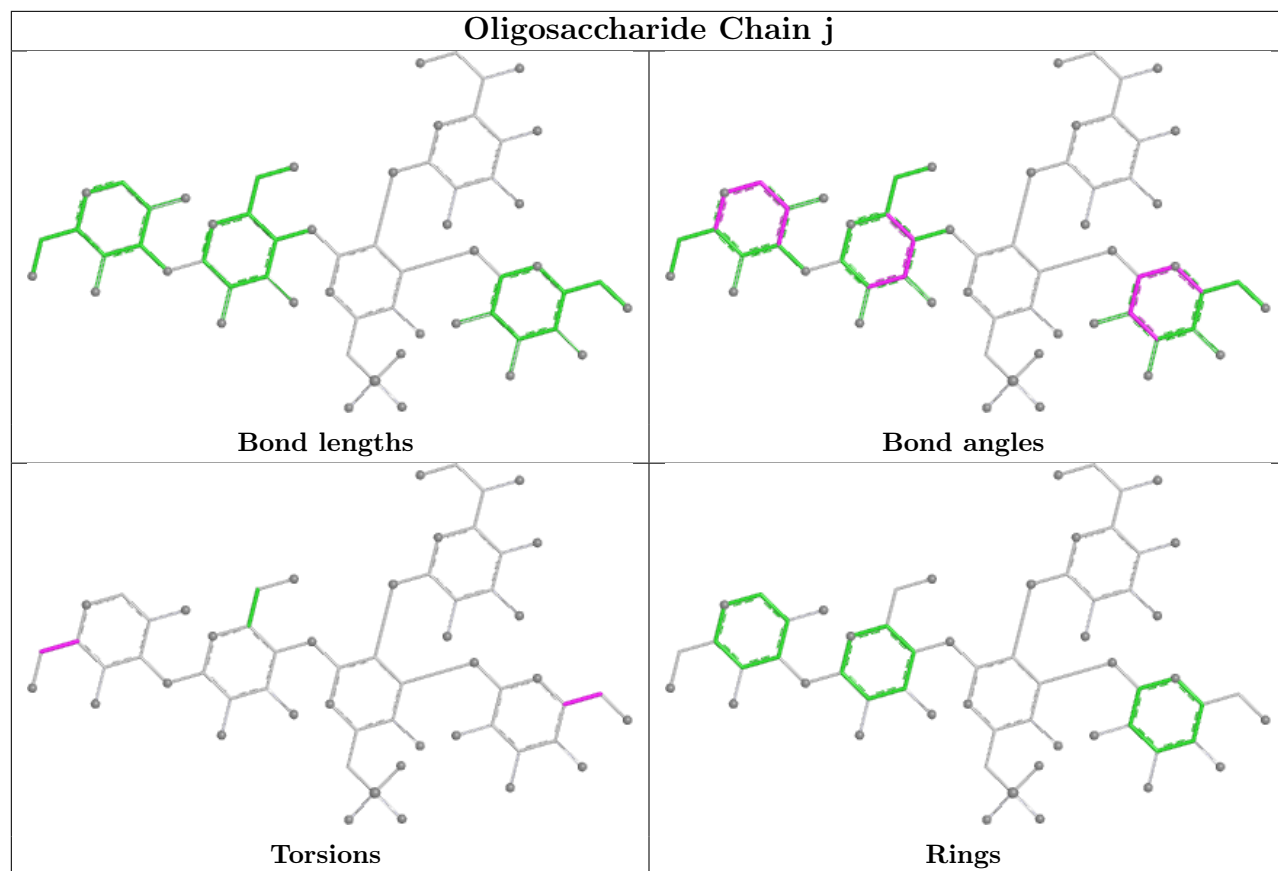
Oligosaccharide Chain BC**Oligosaccharide Chain IC**

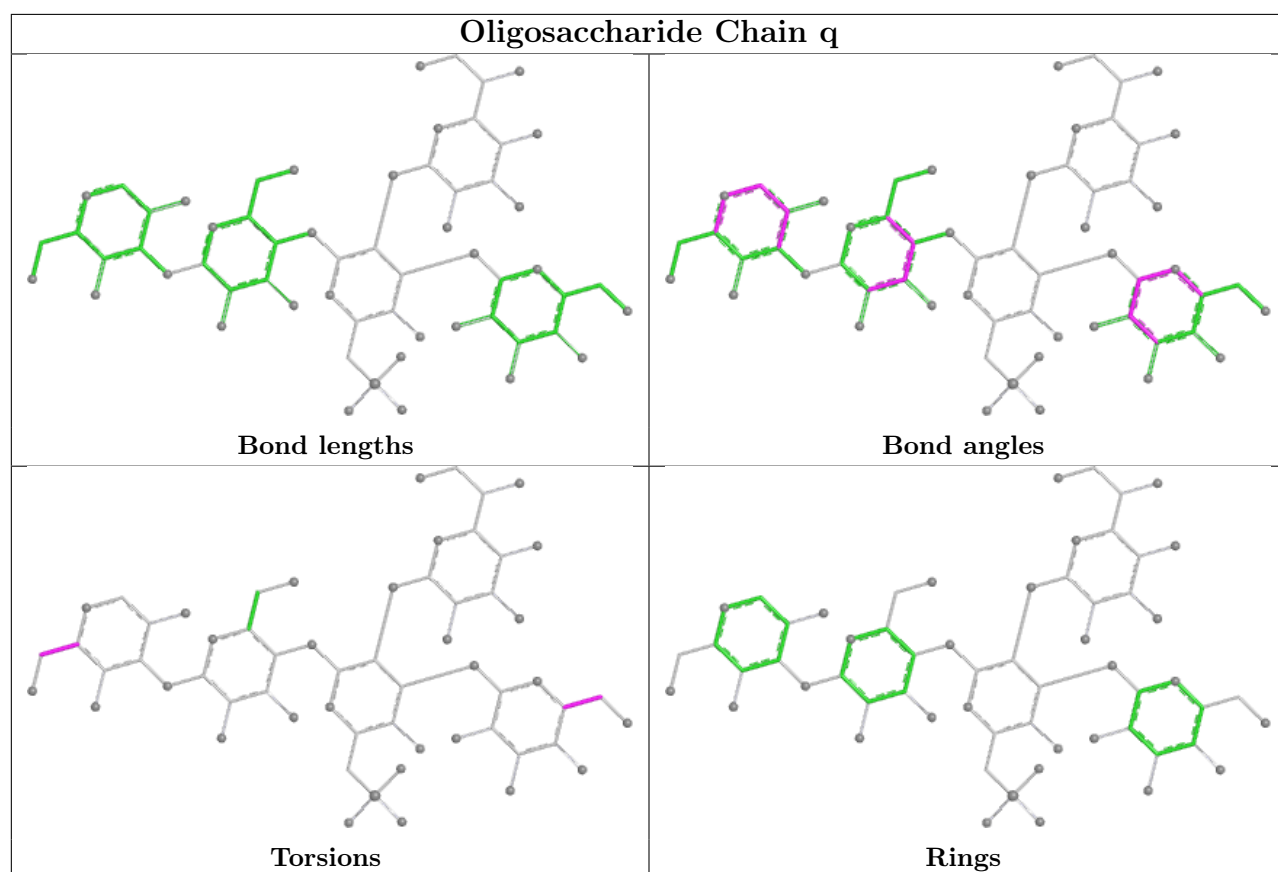
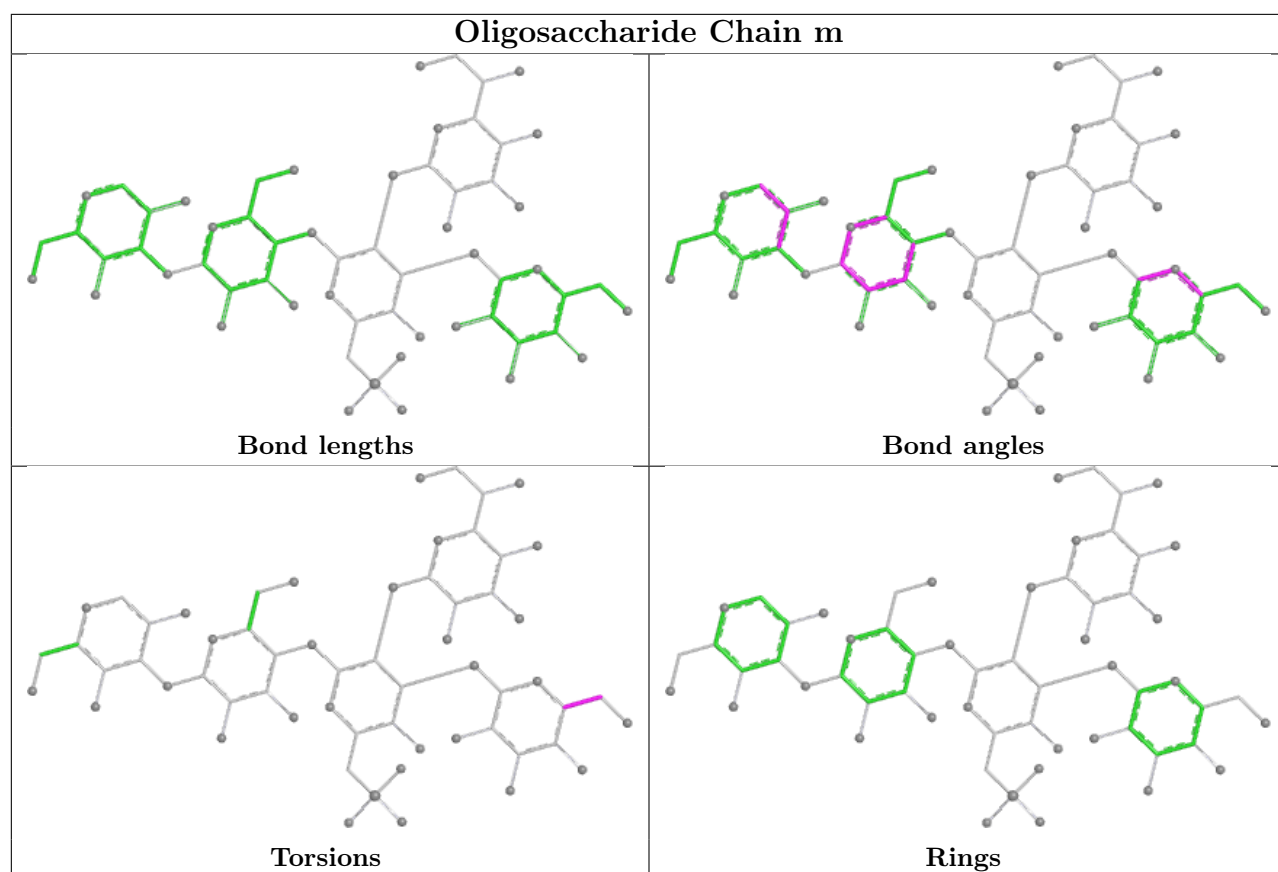


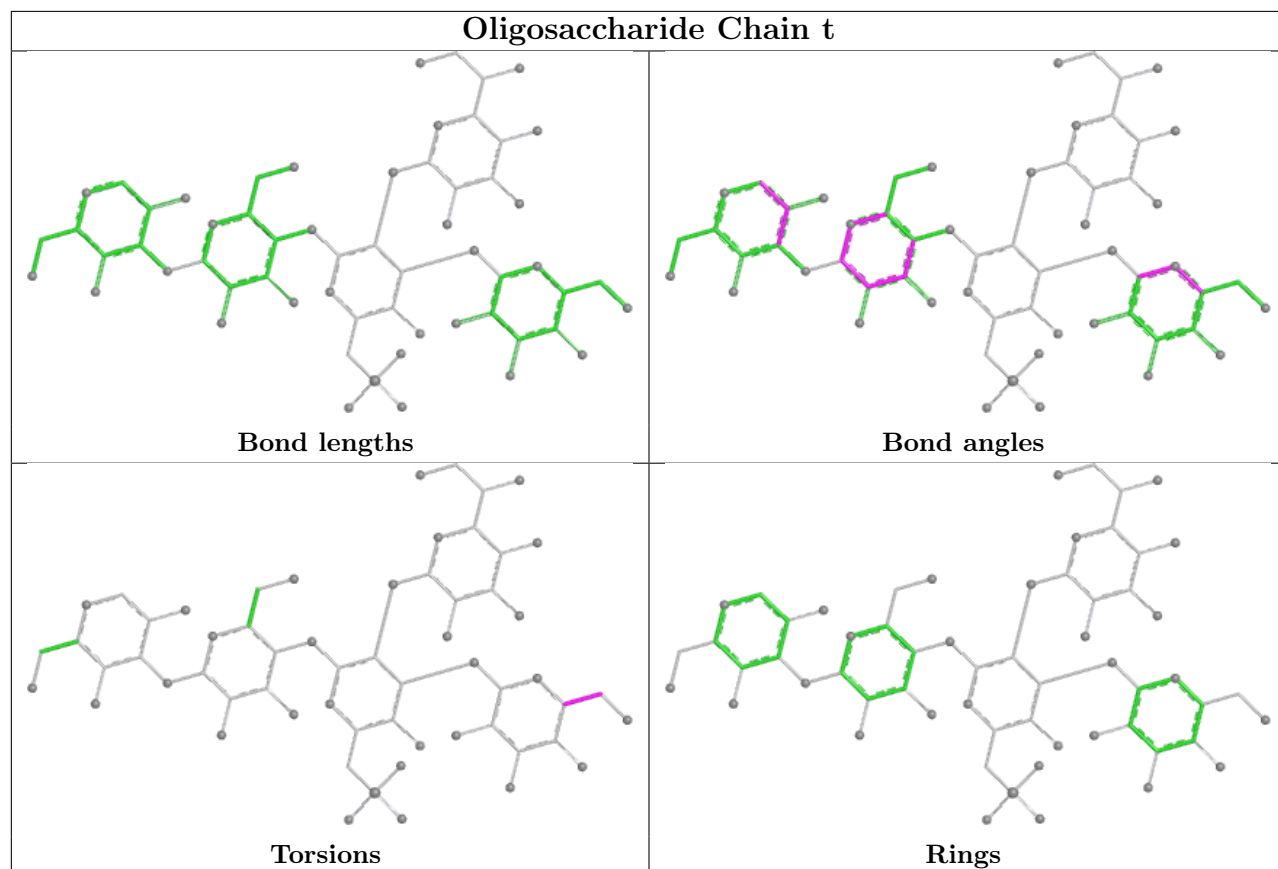
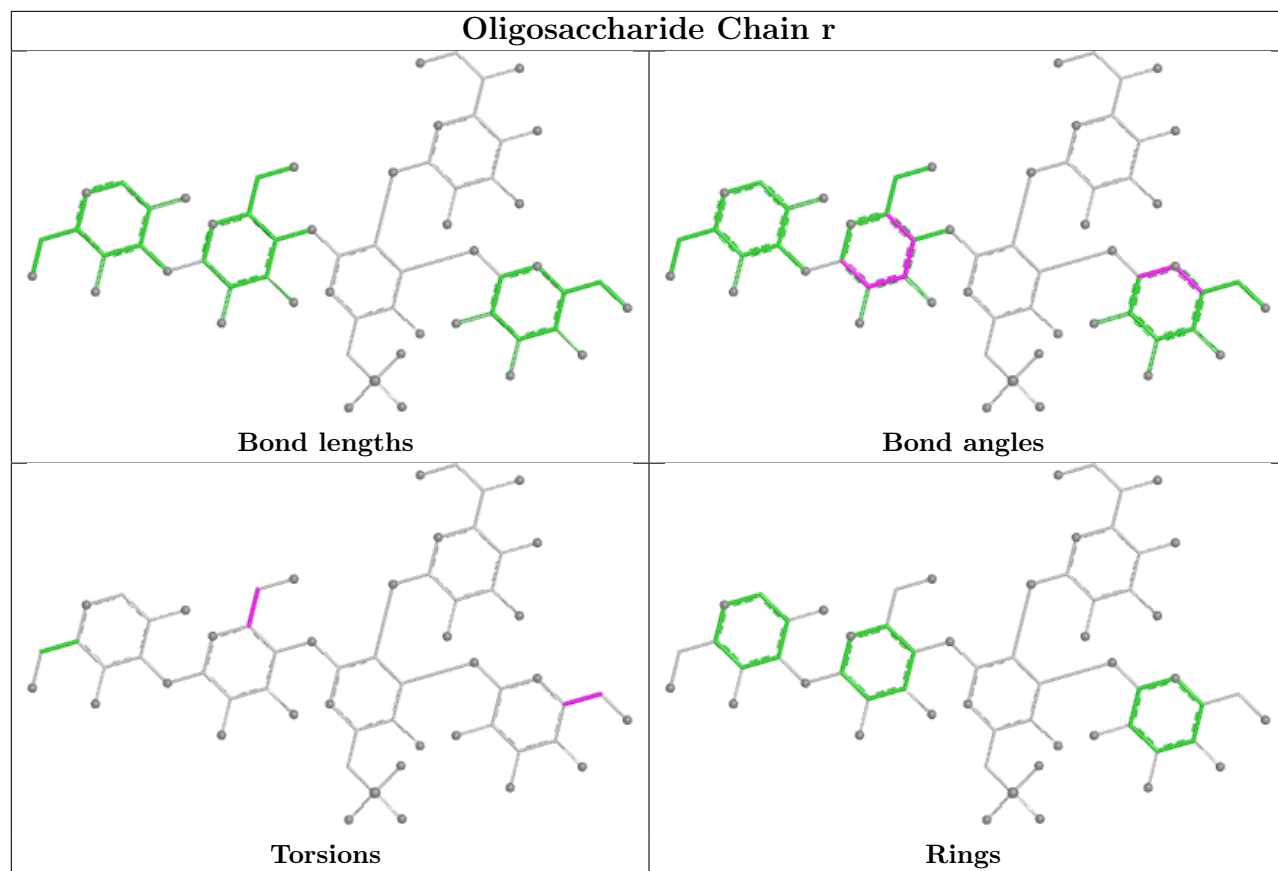


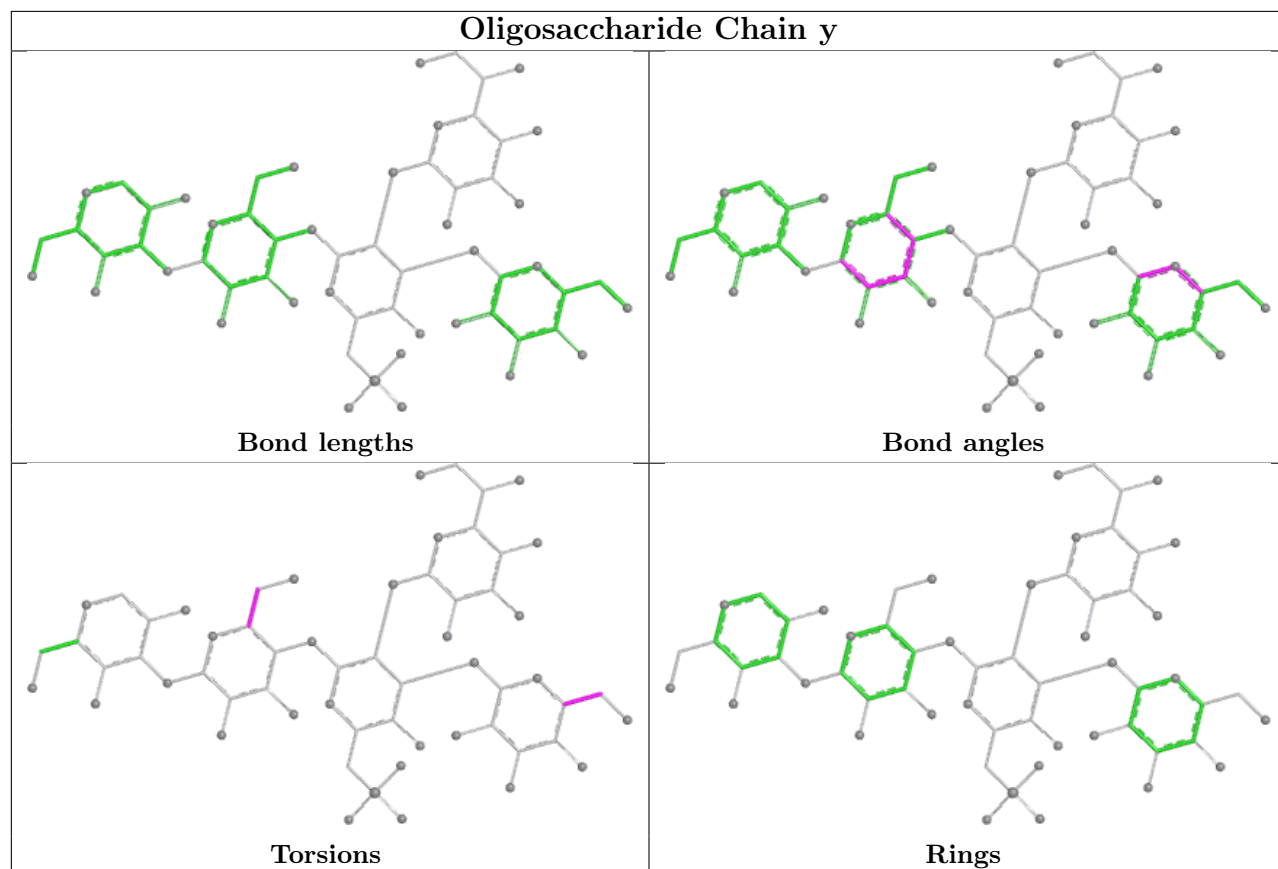
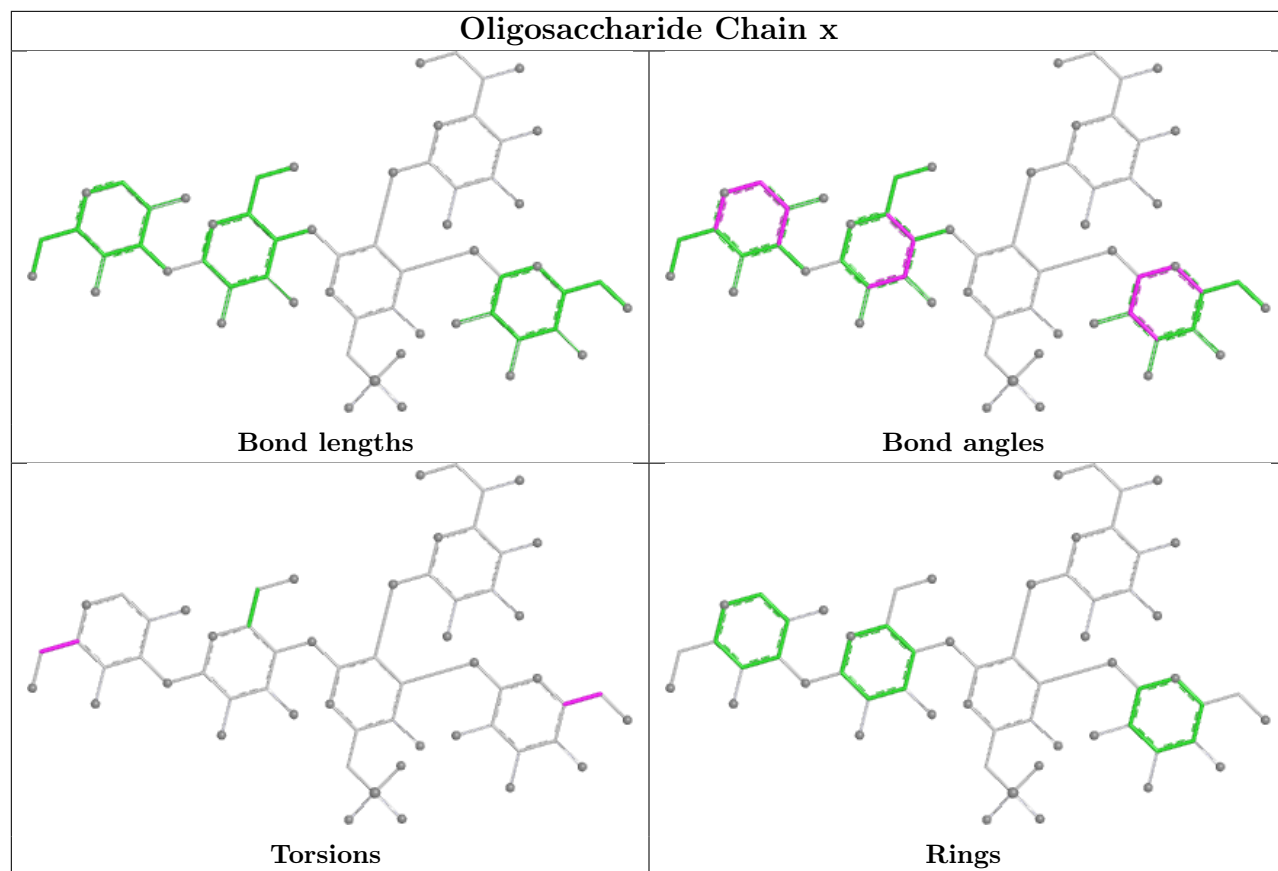


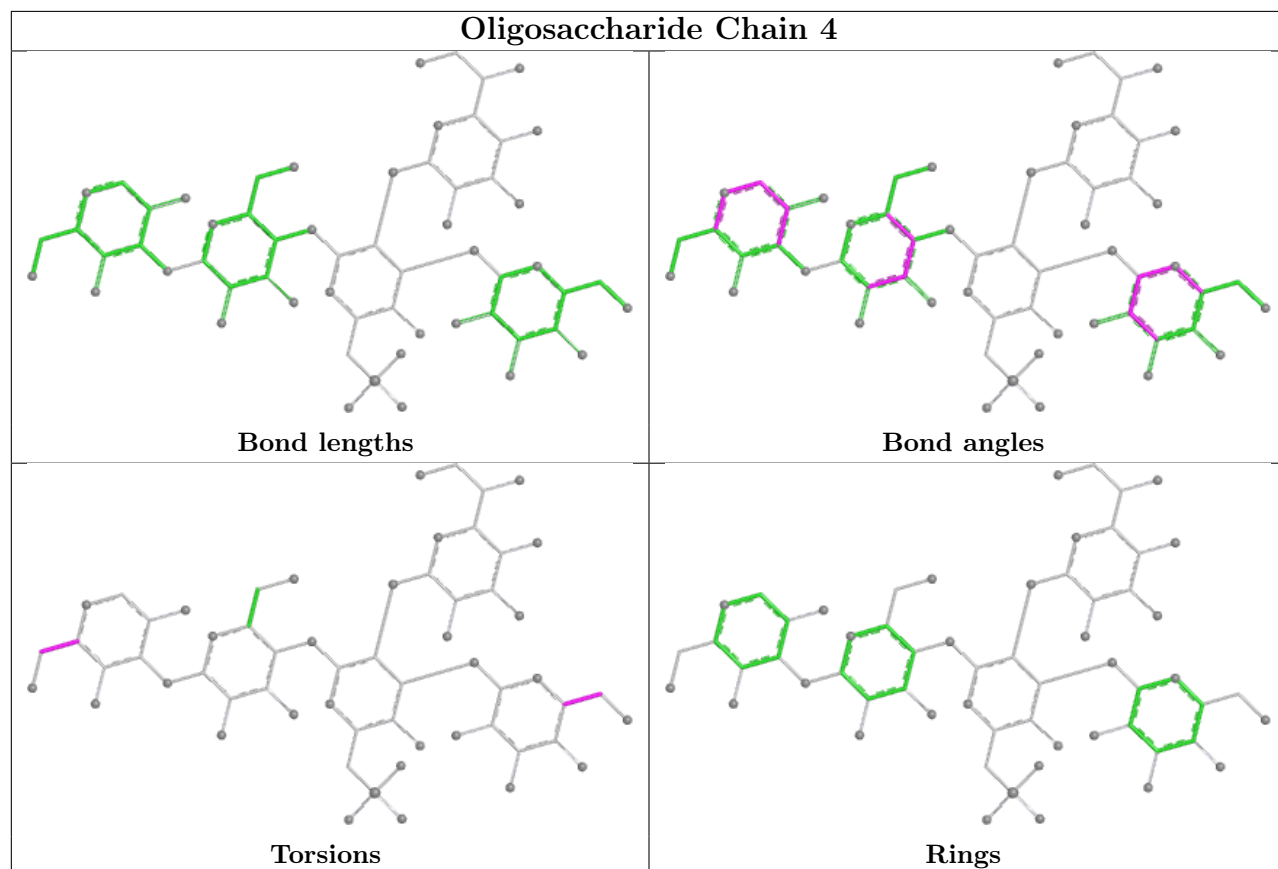
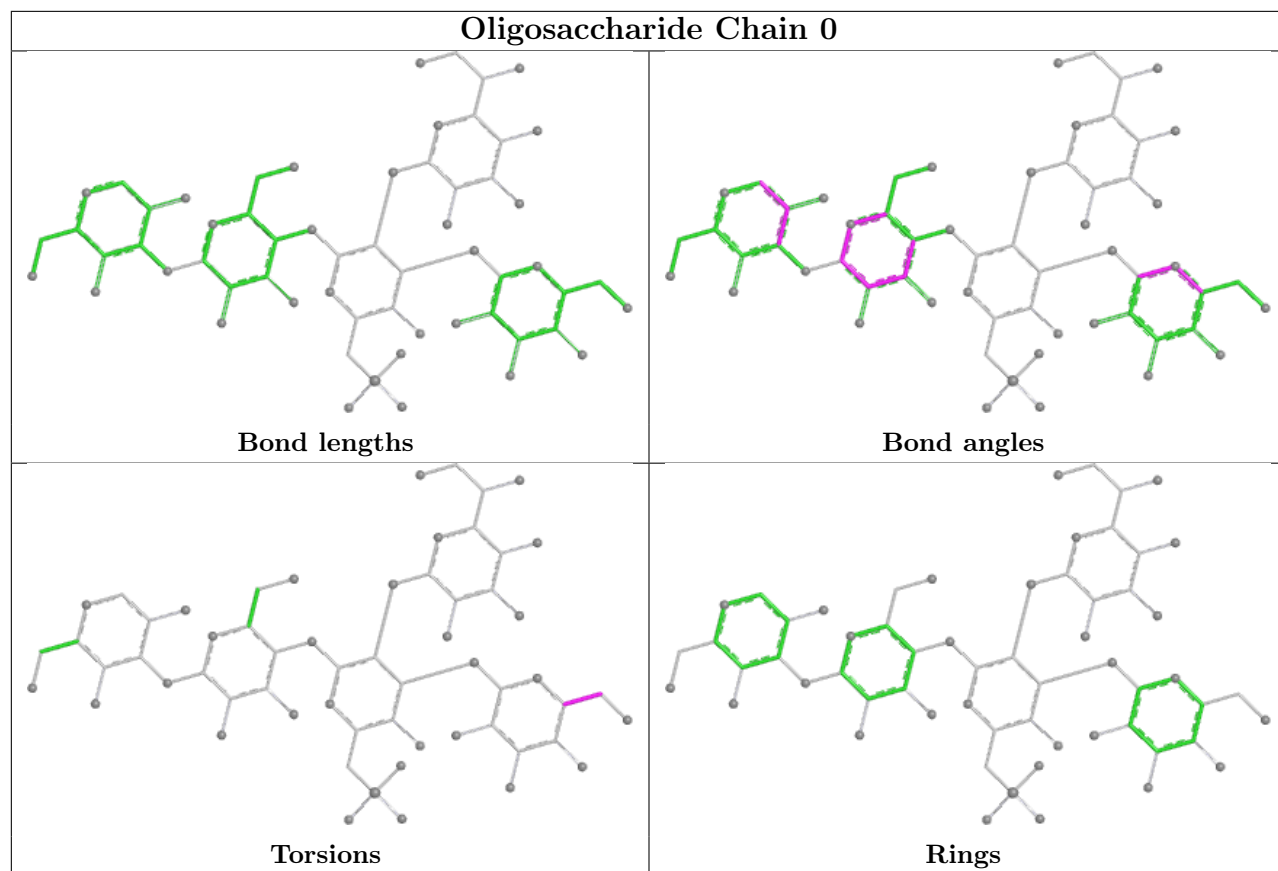




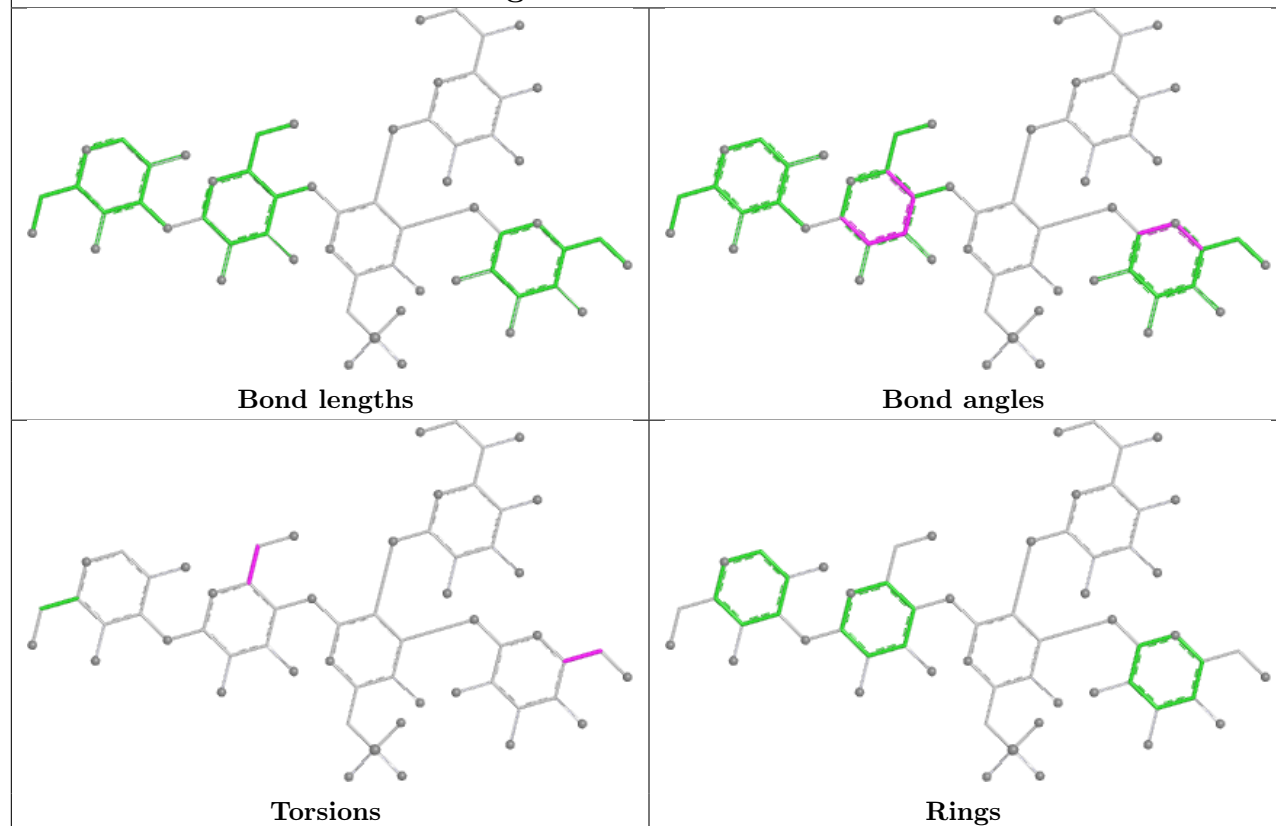




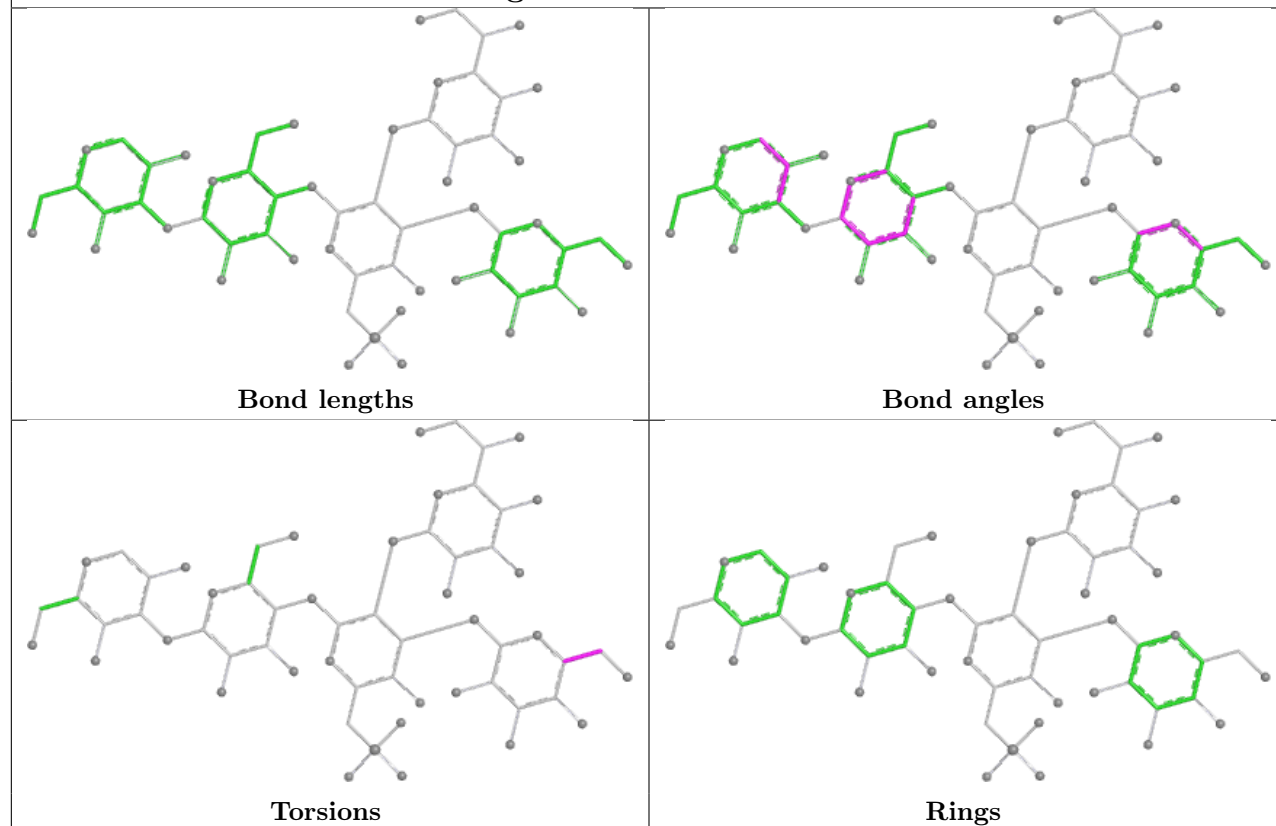


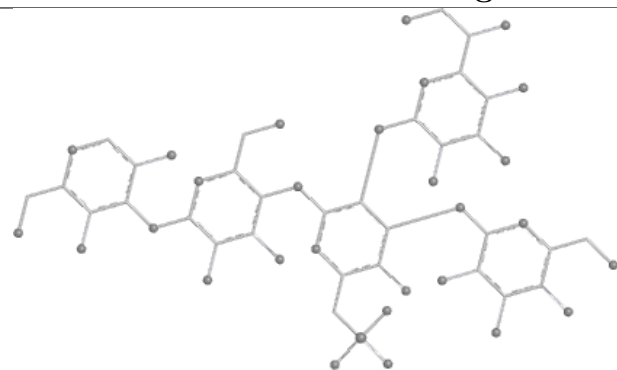
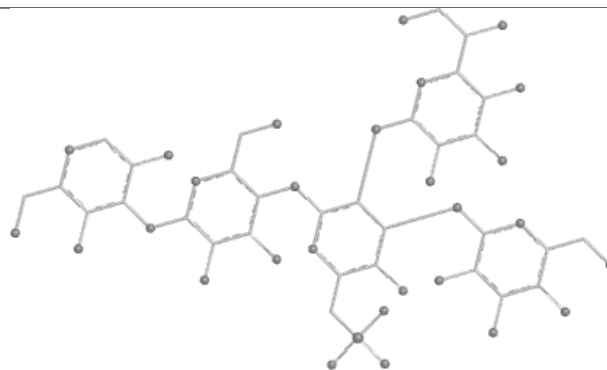
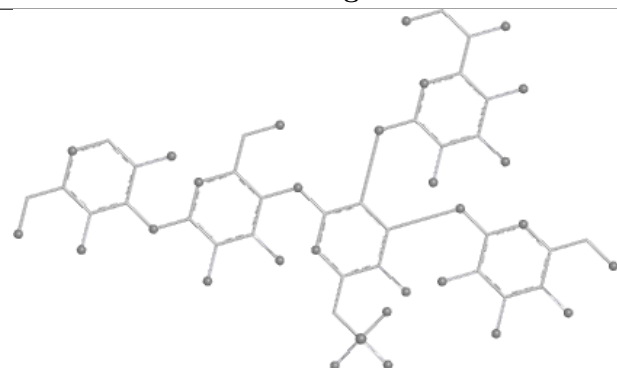
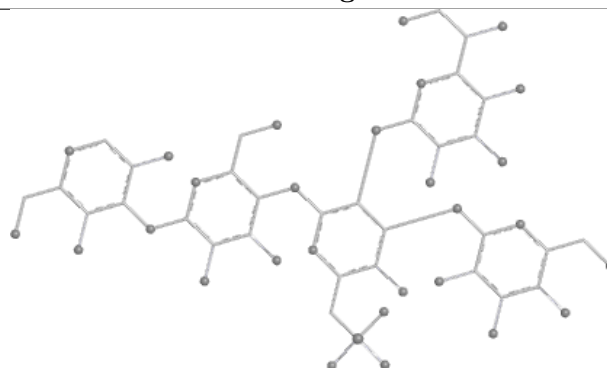
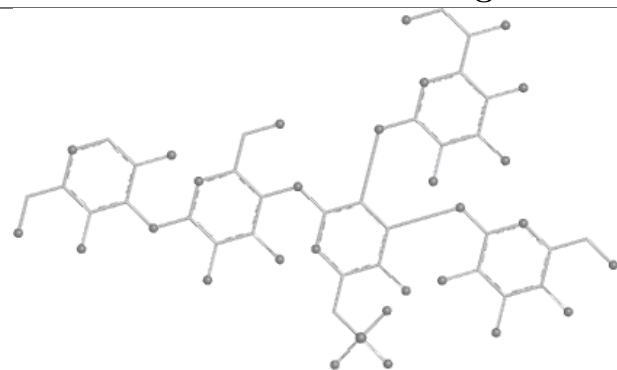
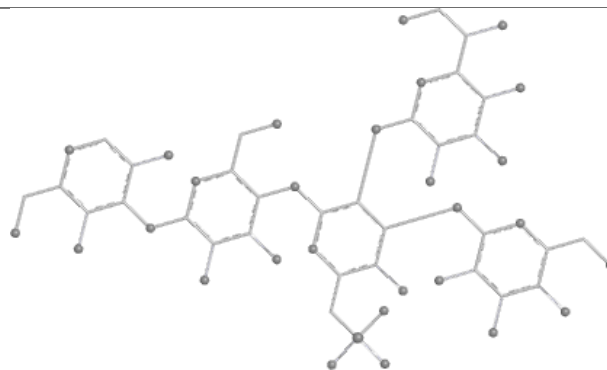
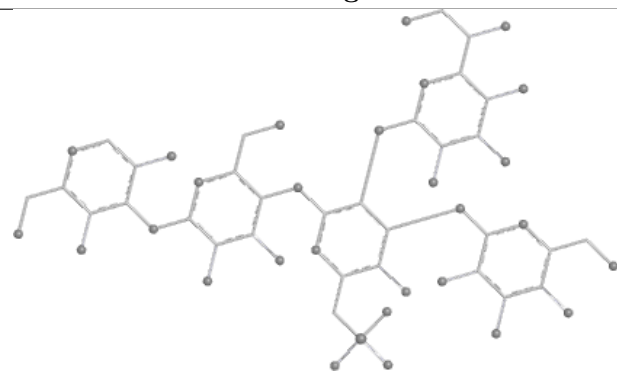
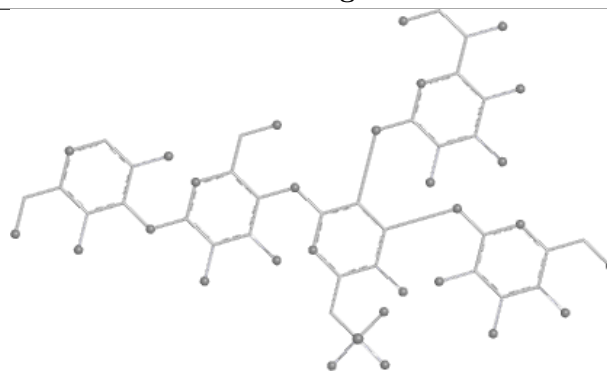


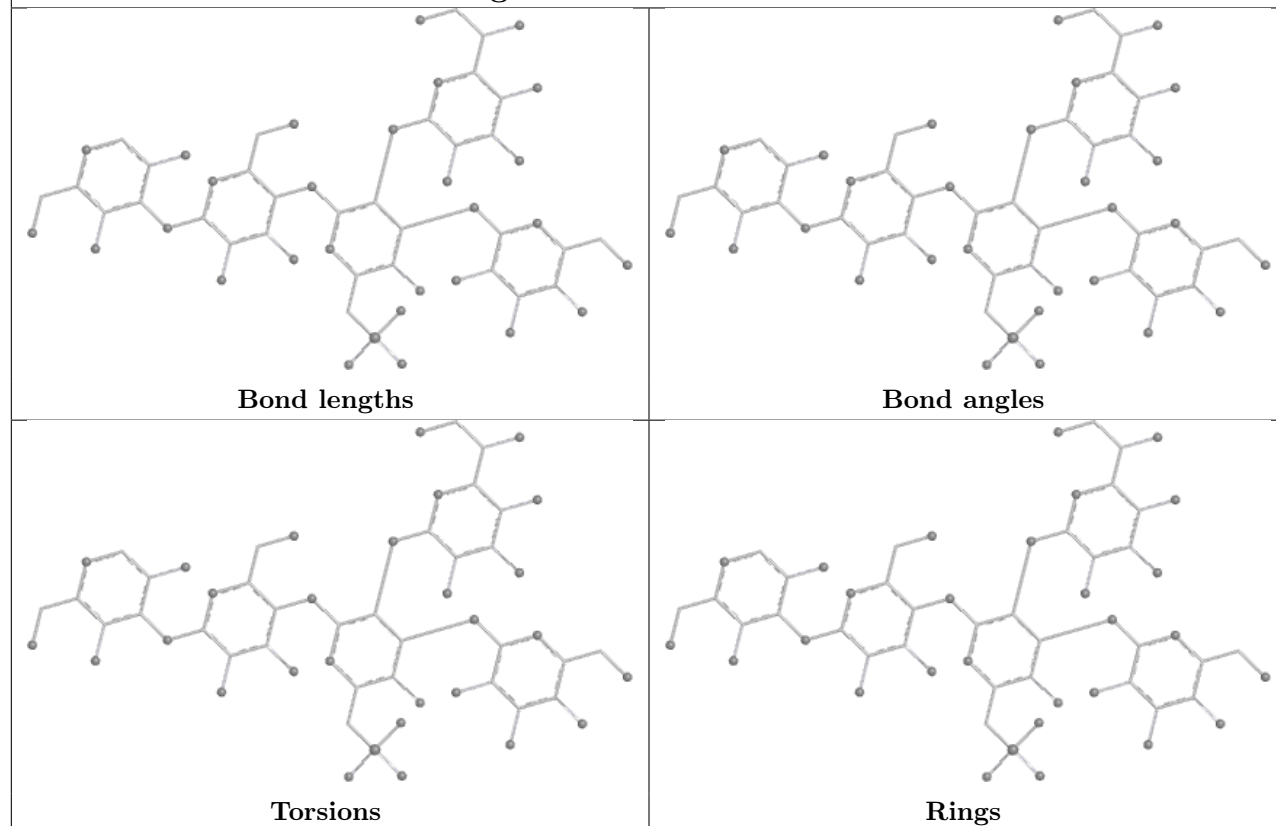
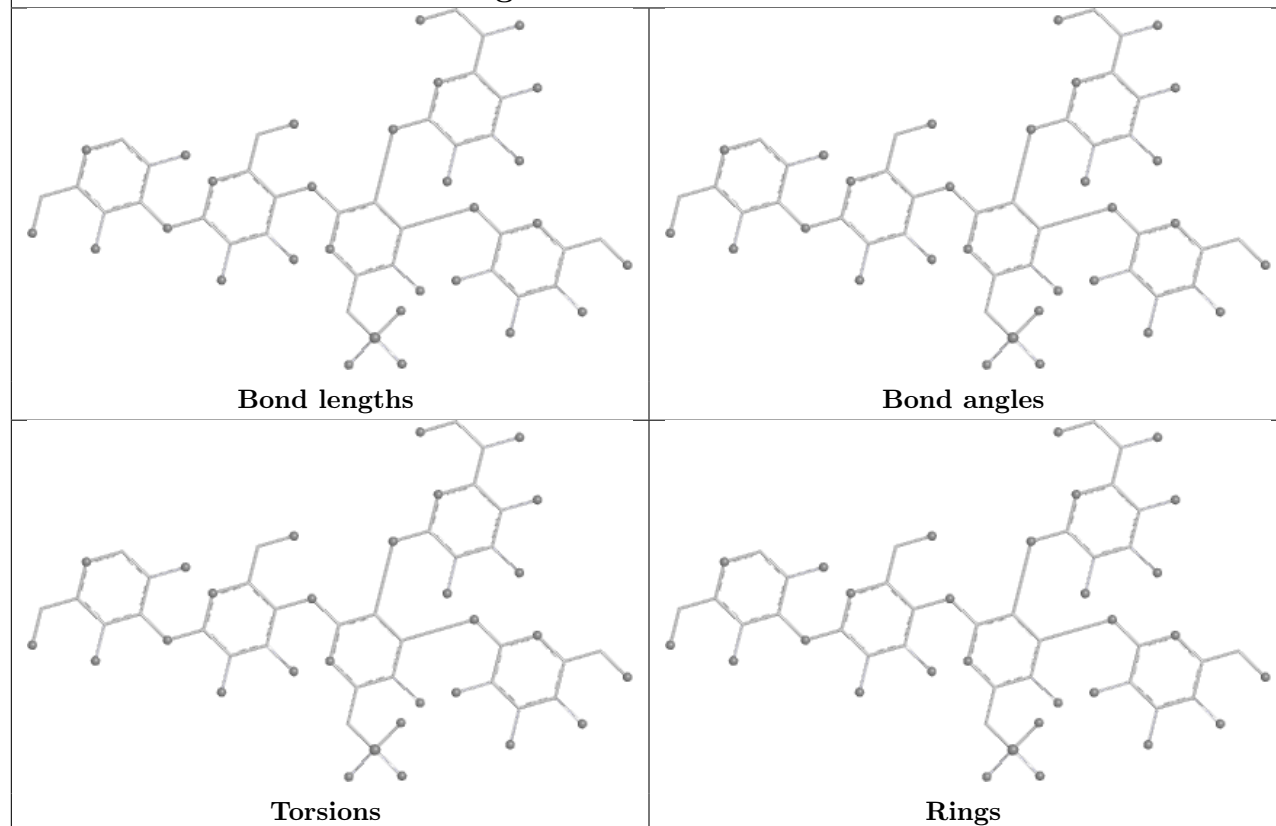
Oligosaccharide Chain 5

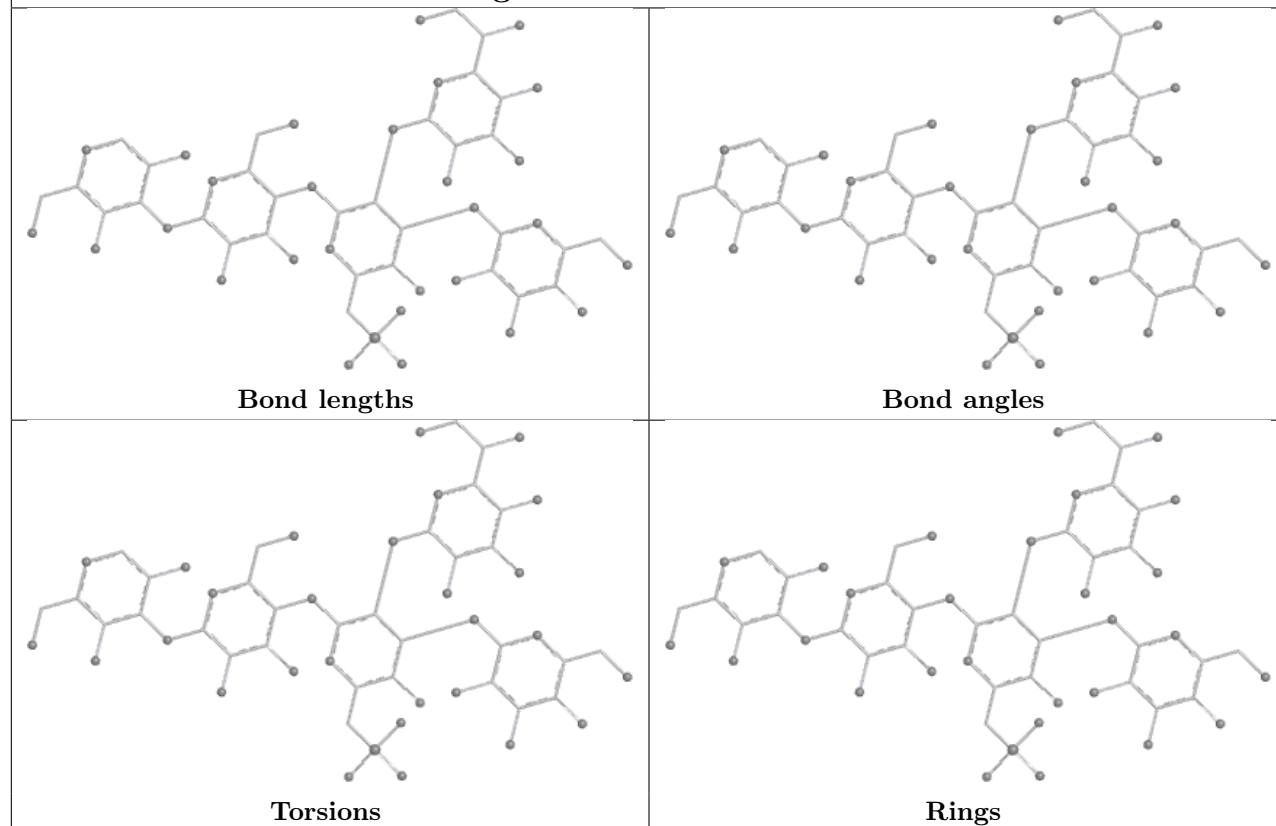
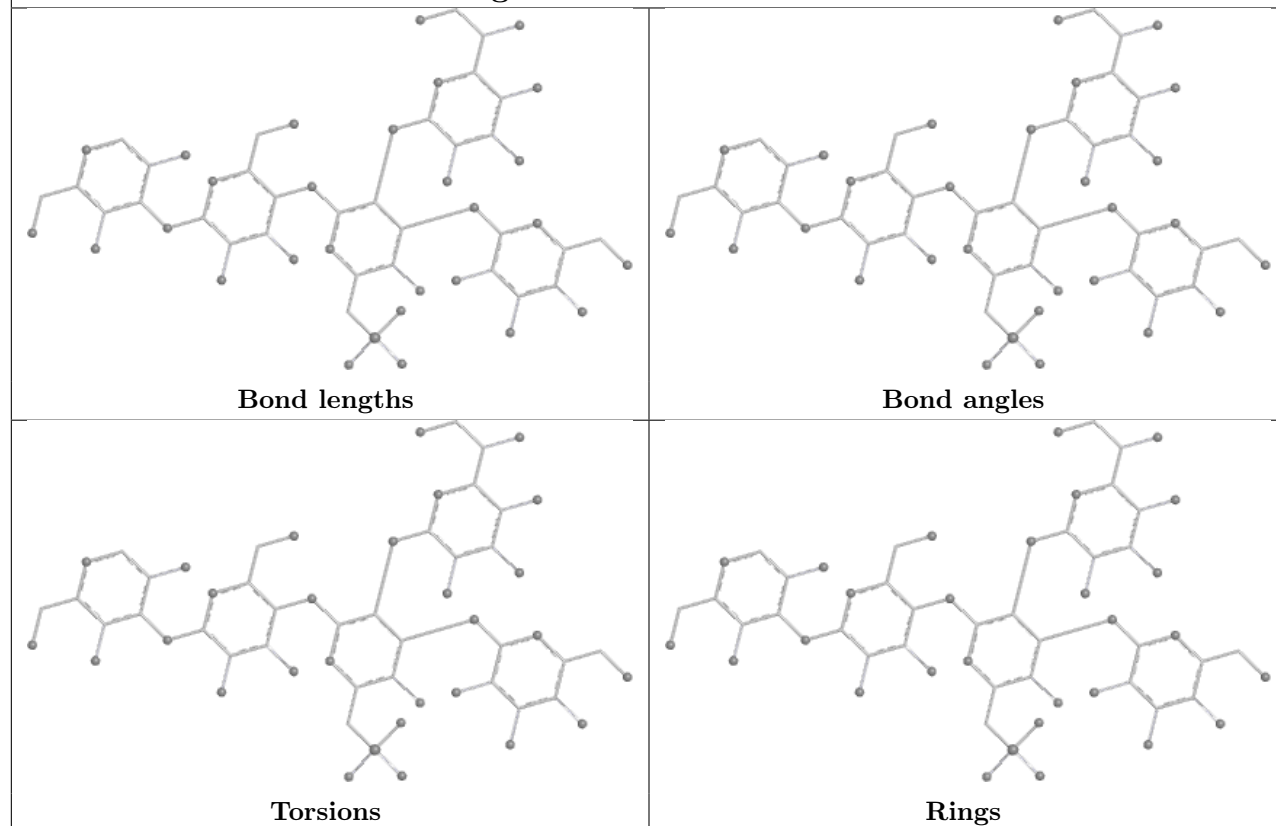


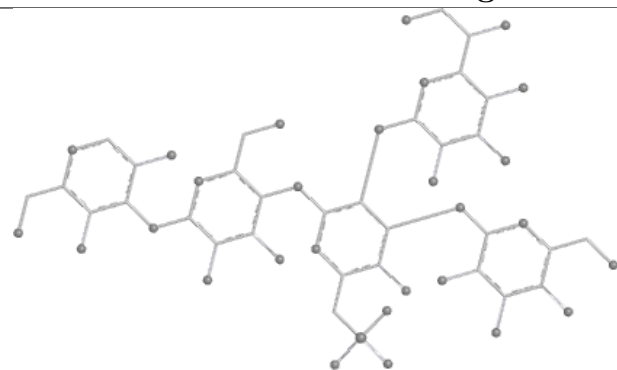
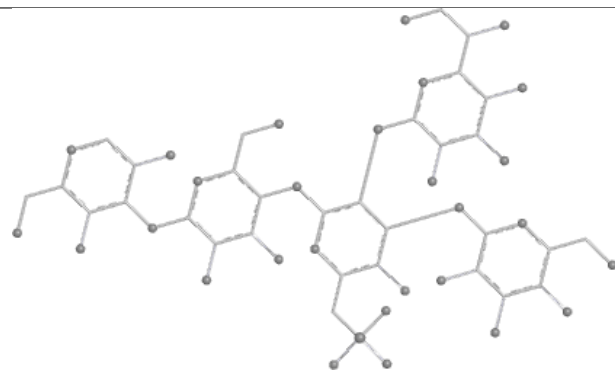
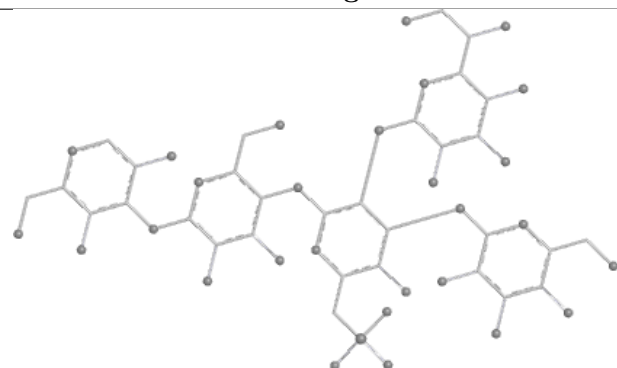
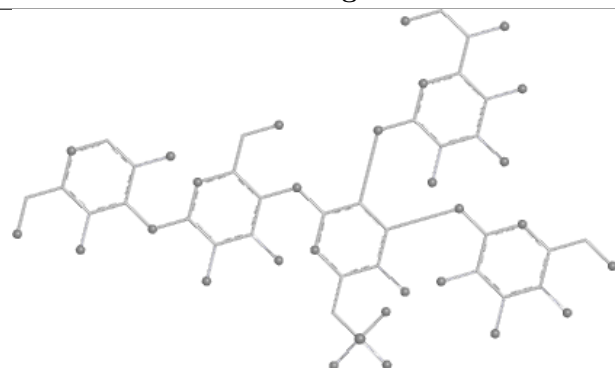
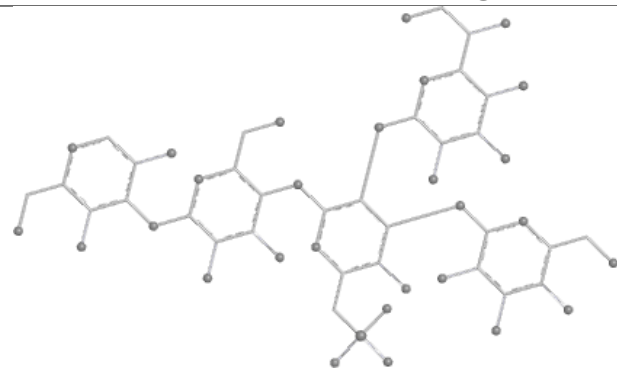
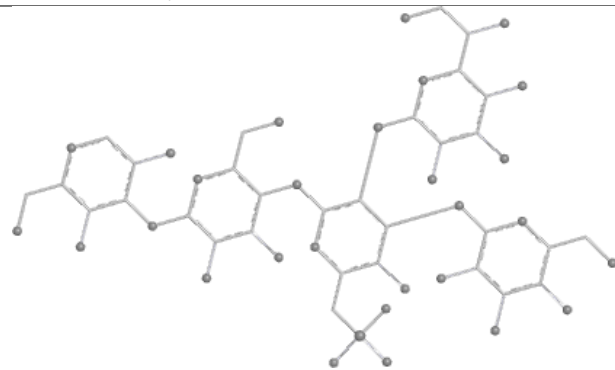
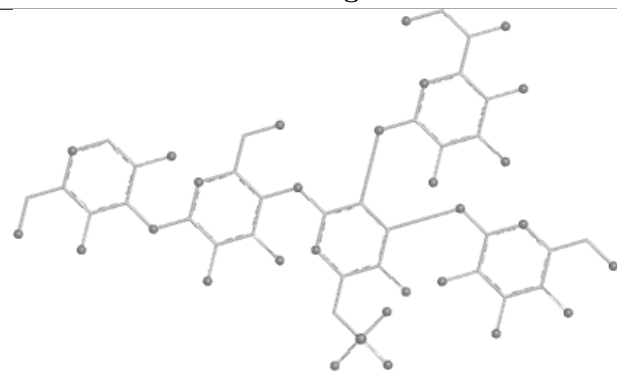
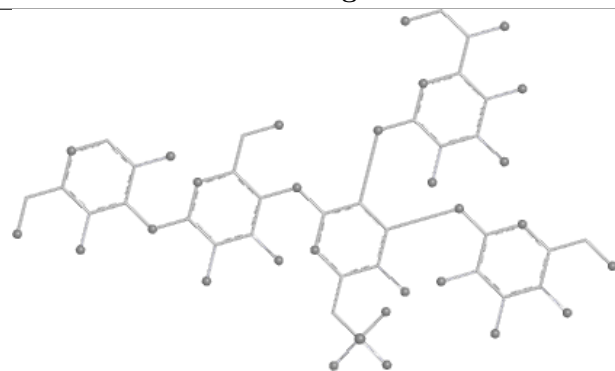
Oligosaccharide Chain 7

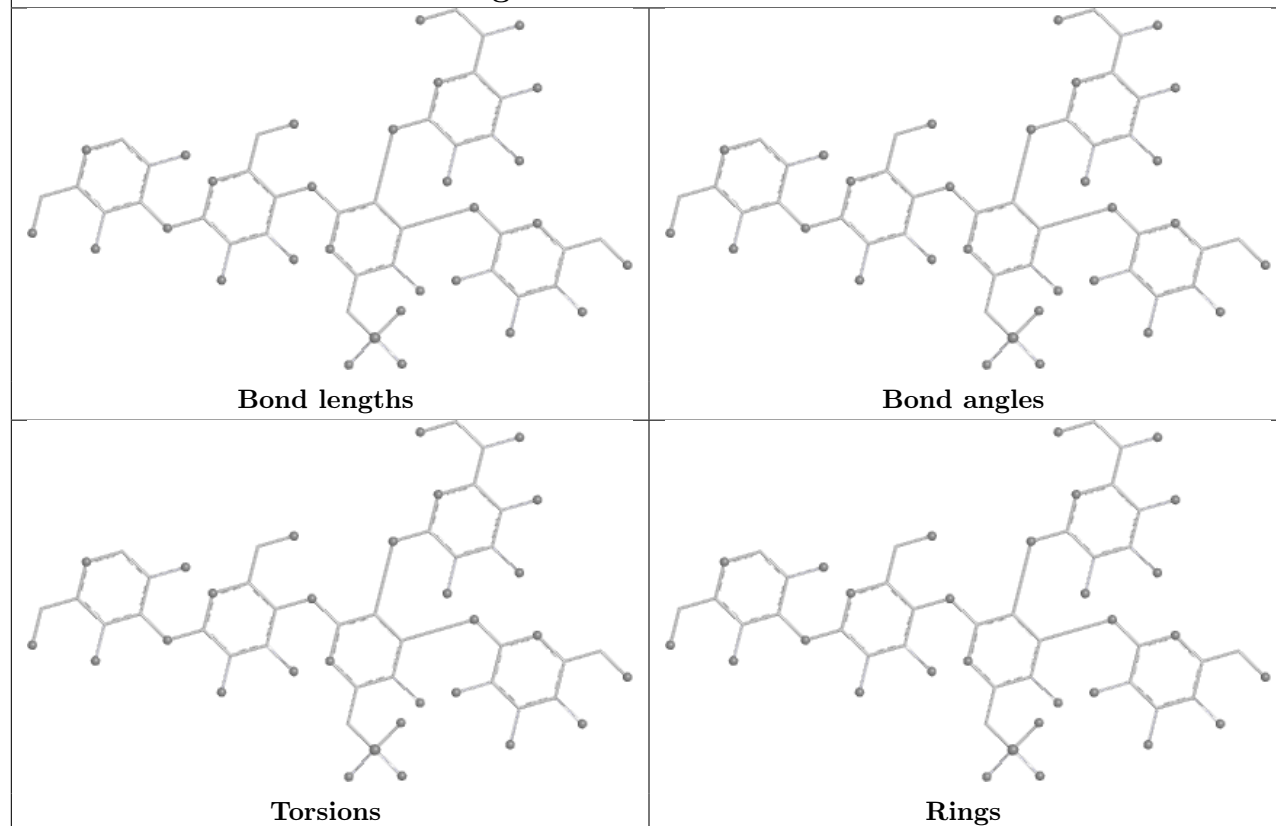
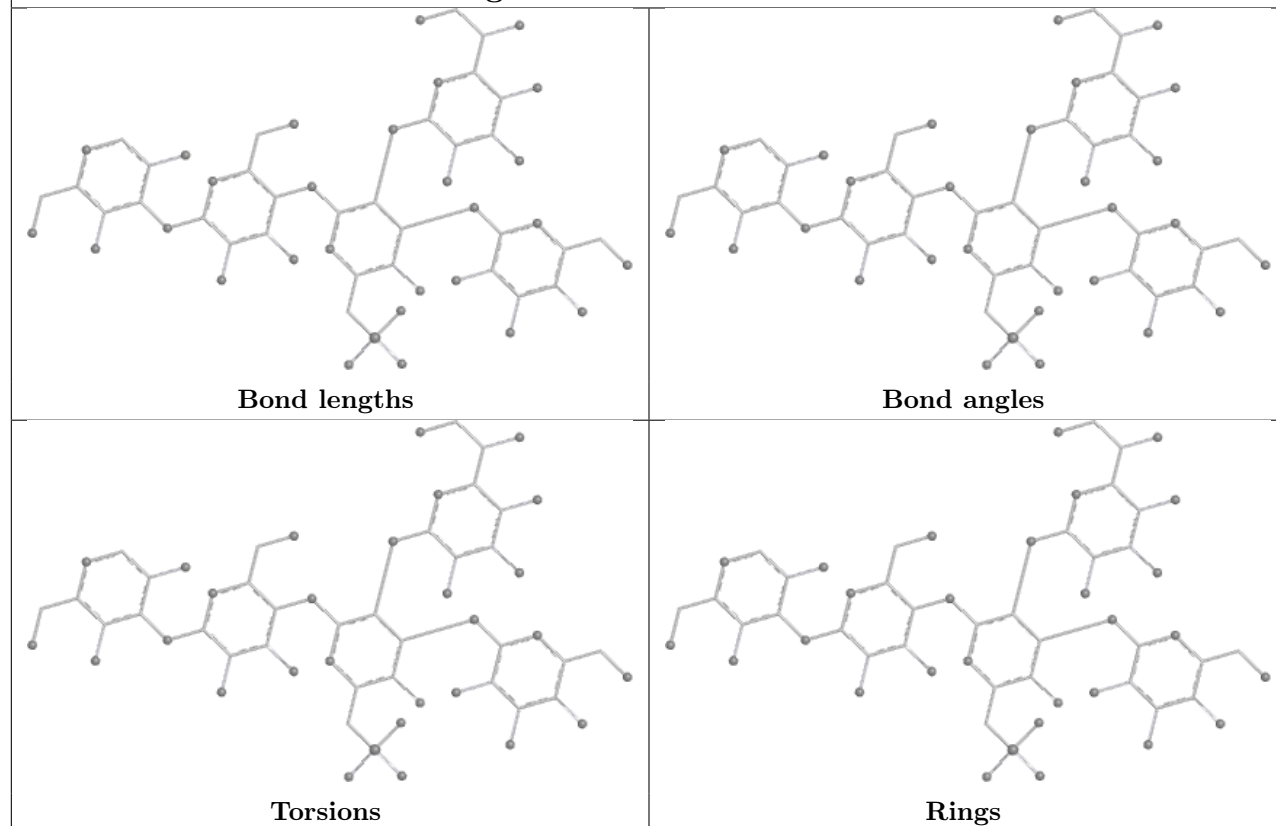


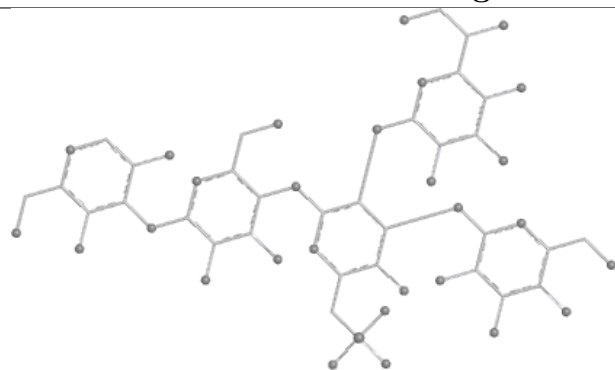
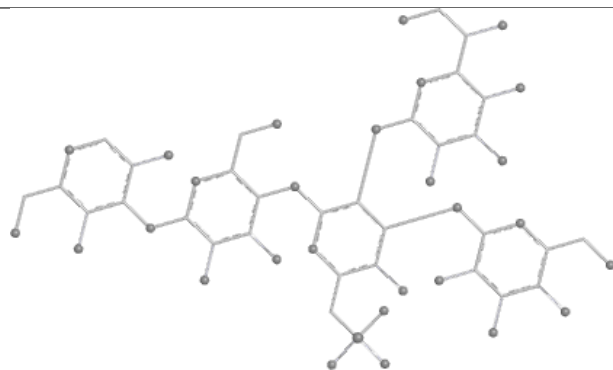
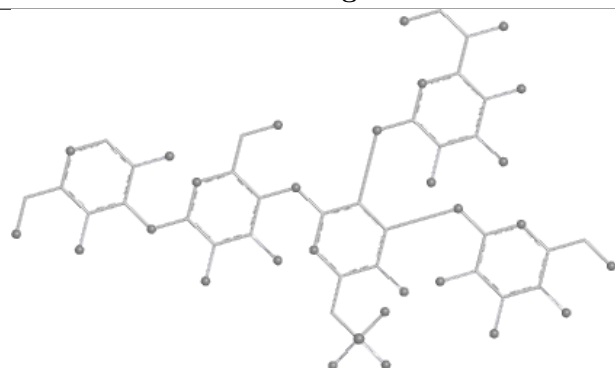
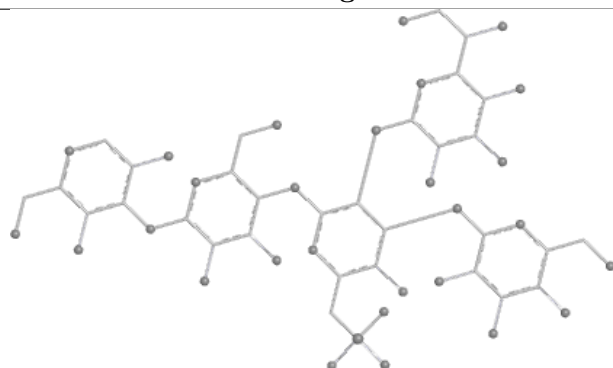
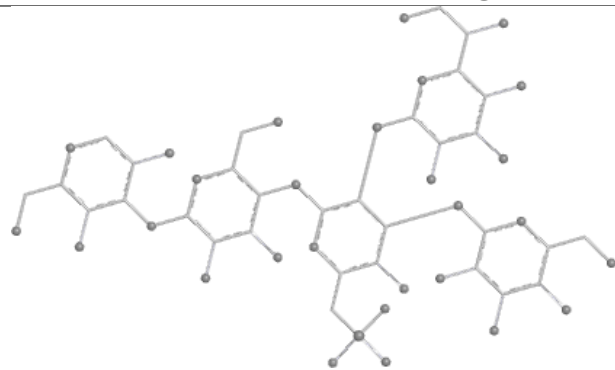
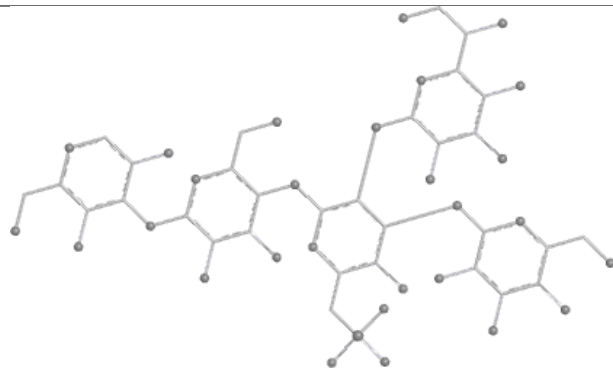
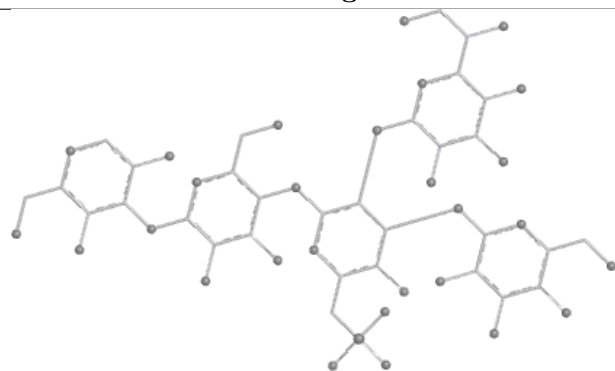
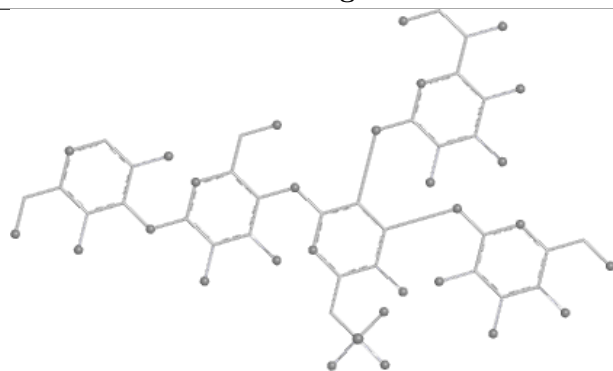
Oligosaccharide Chain BA**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain CA****Bond lengths****Bond angles****Torsions****Rings**

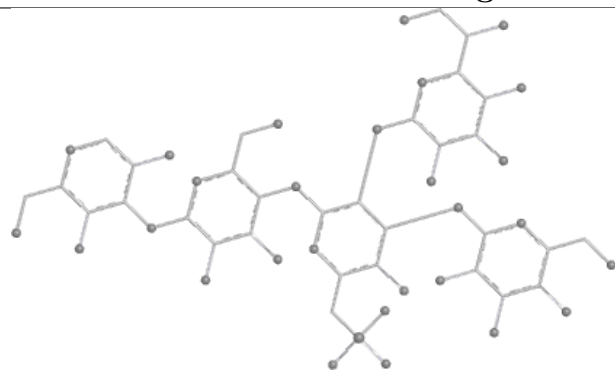
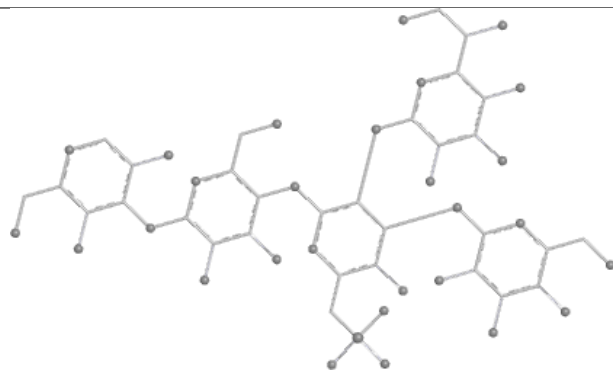
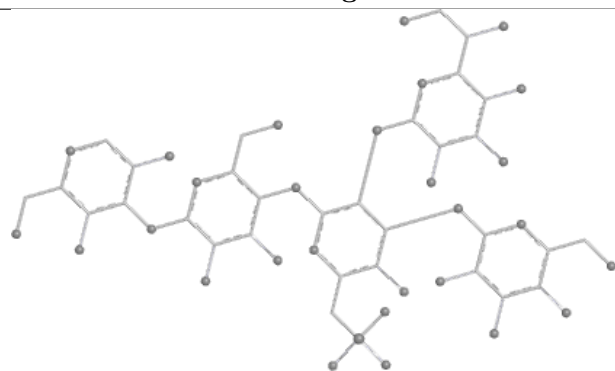
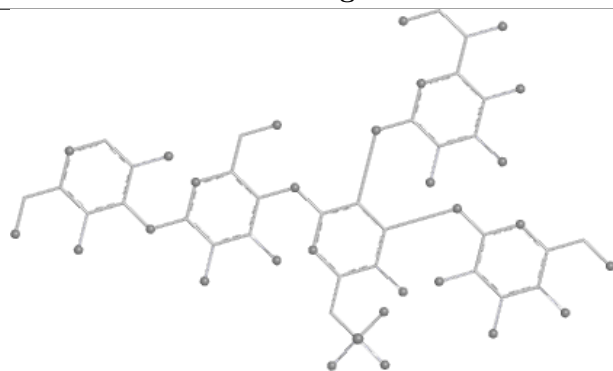
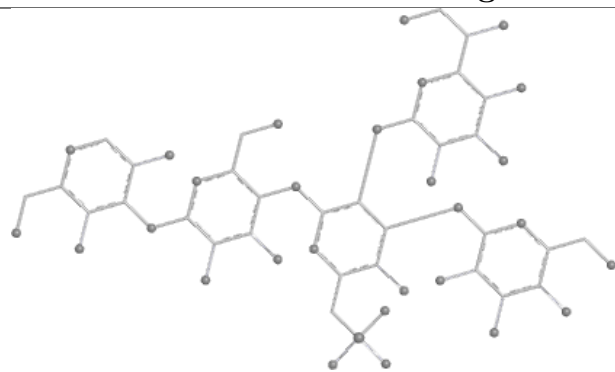
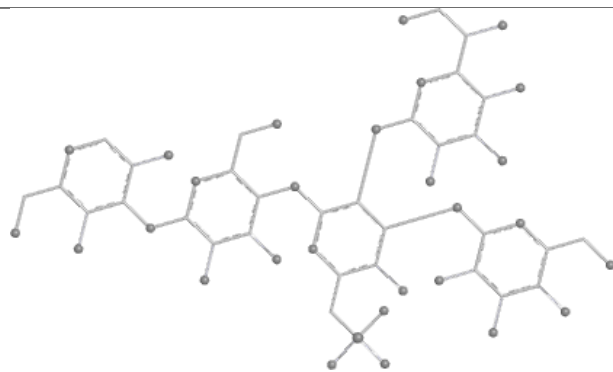
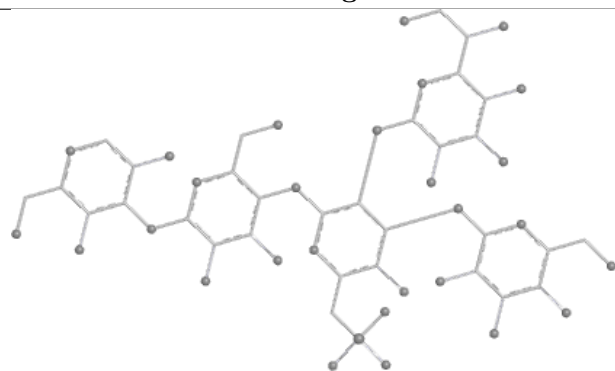
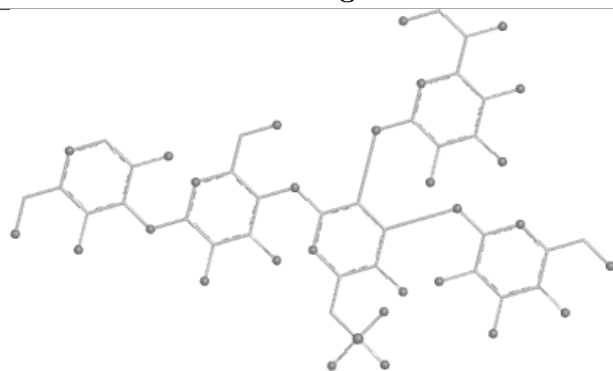
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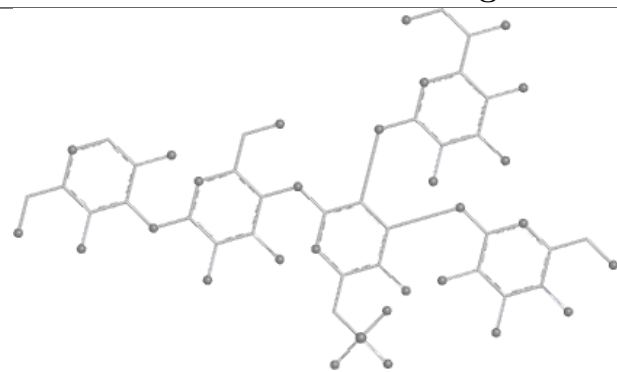
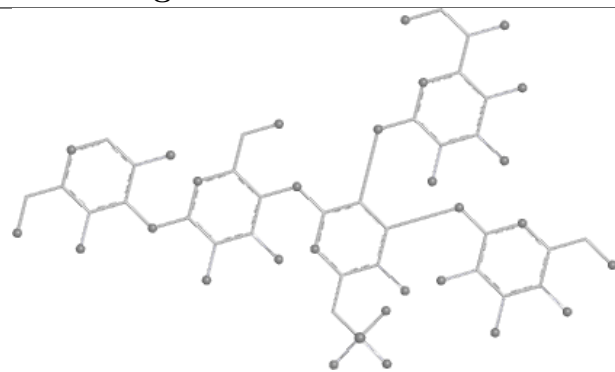
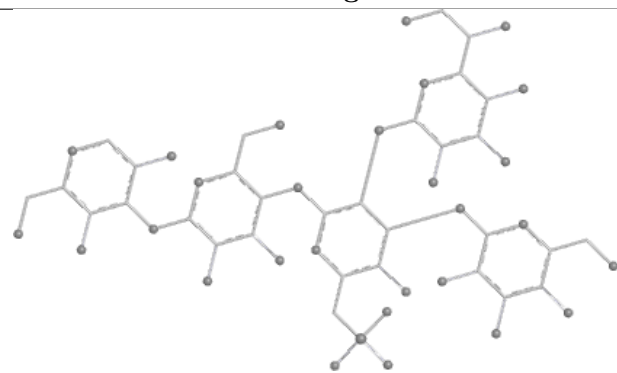
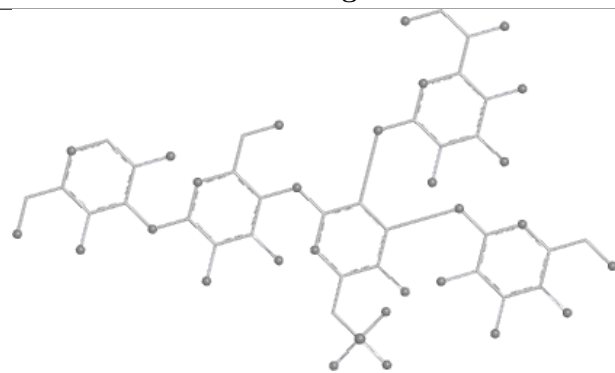
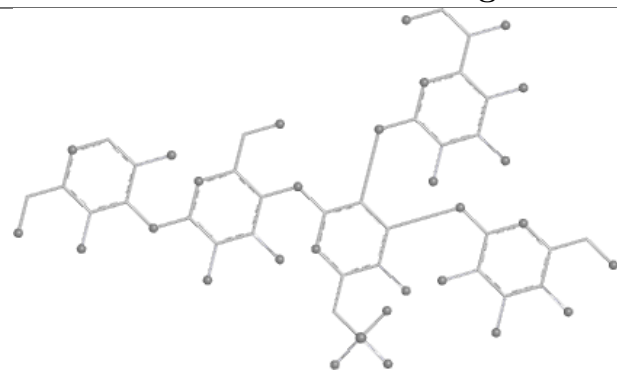
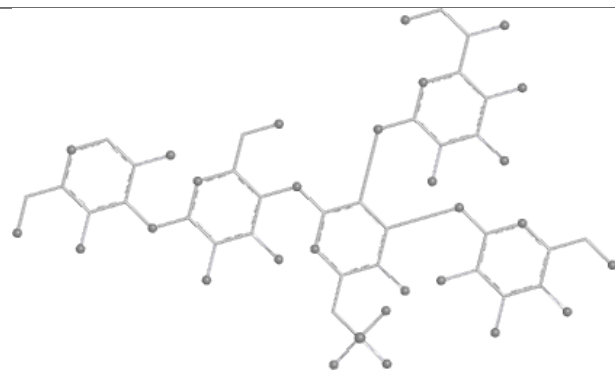
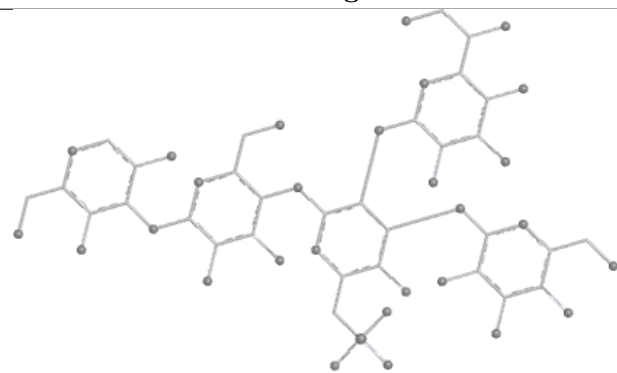
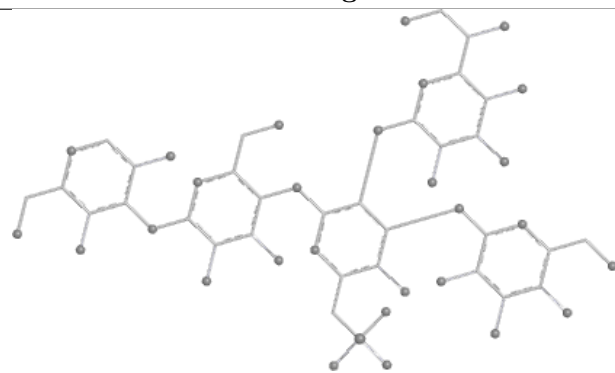
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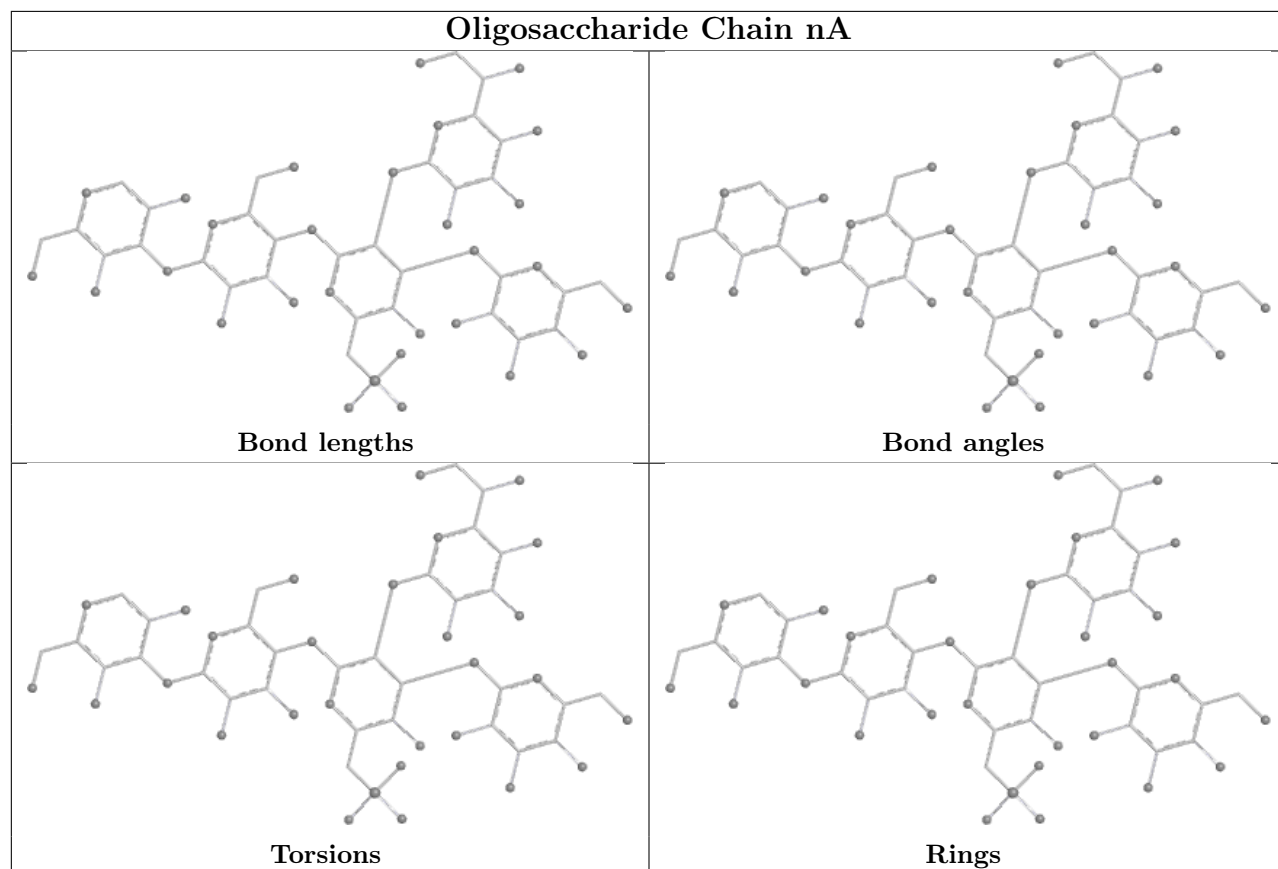
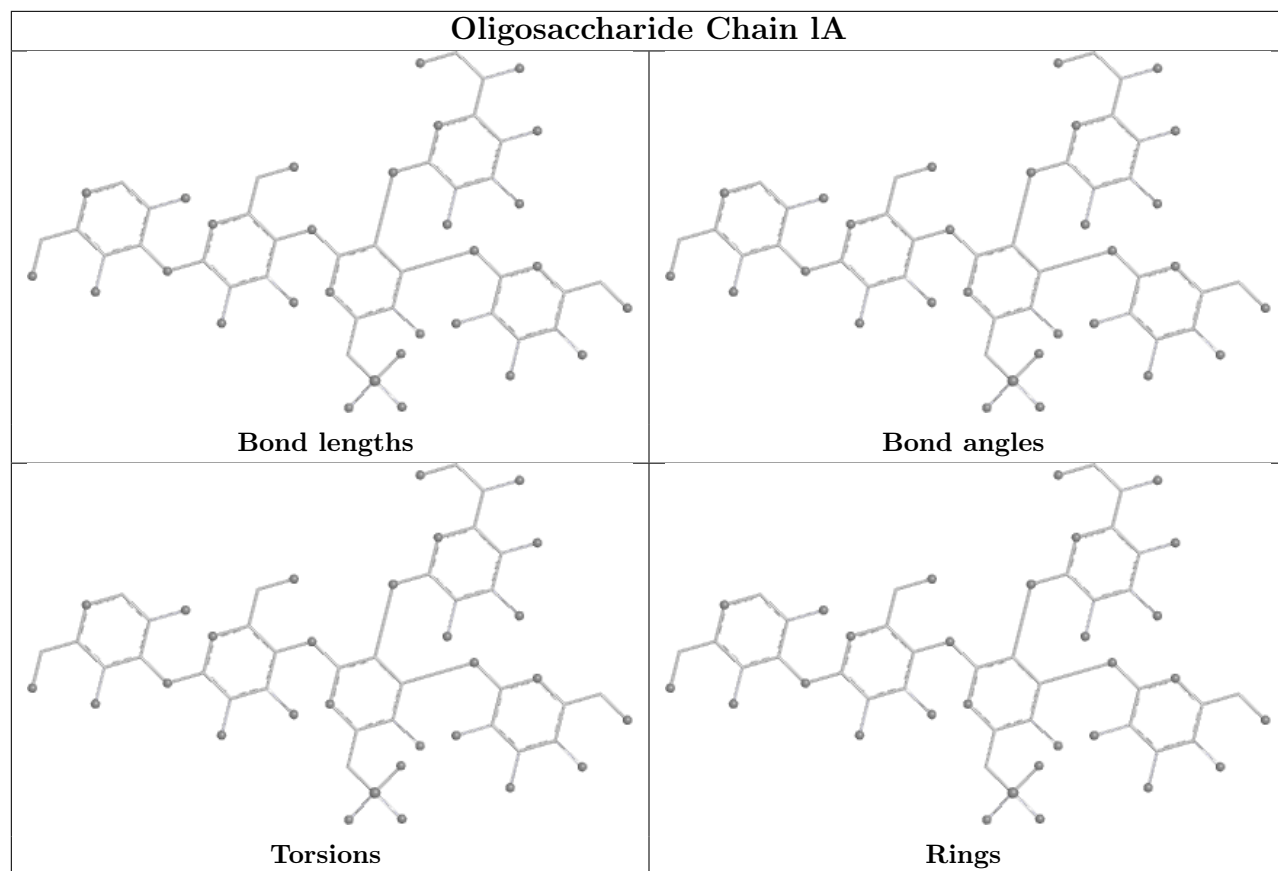
Oligosaccharide Chain PA**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain QA****Bond lengths****Bond angles****Torsions****Rings**

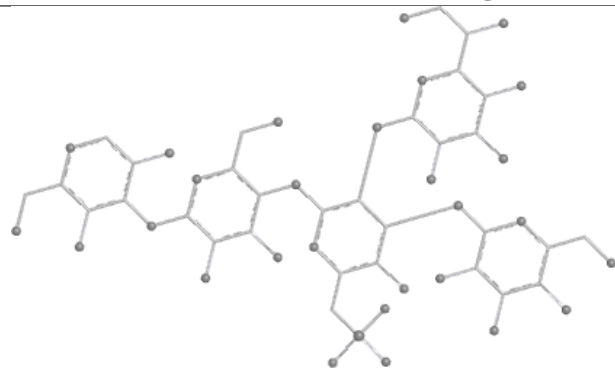
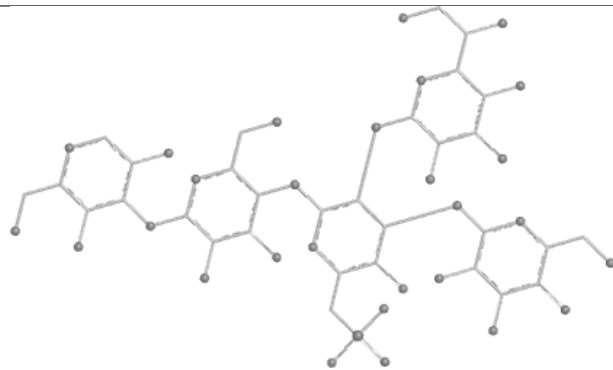
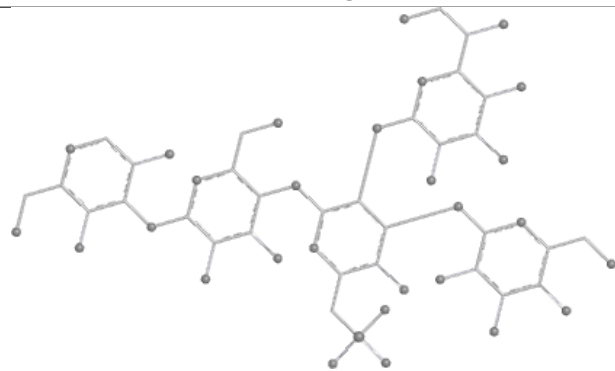
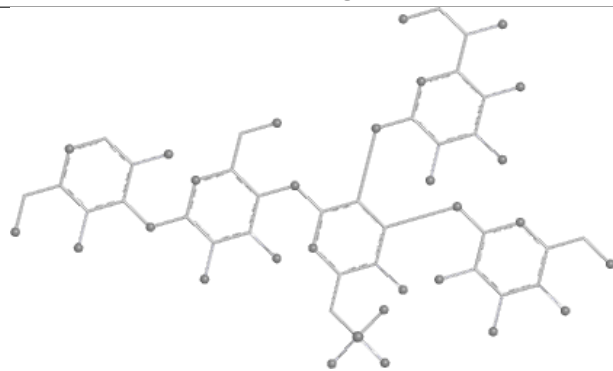
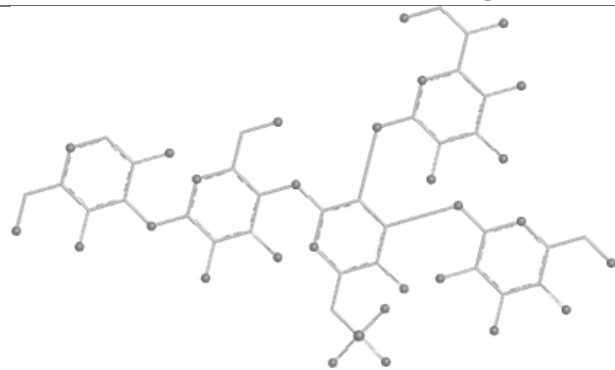
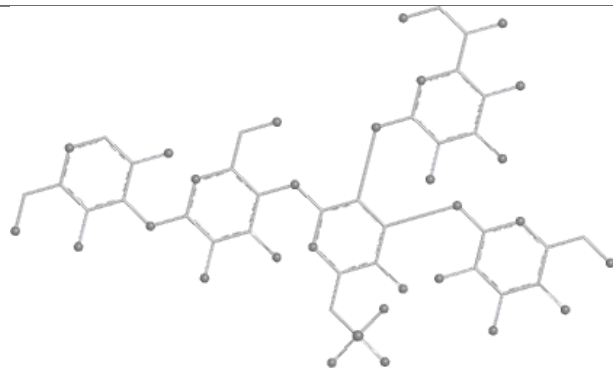
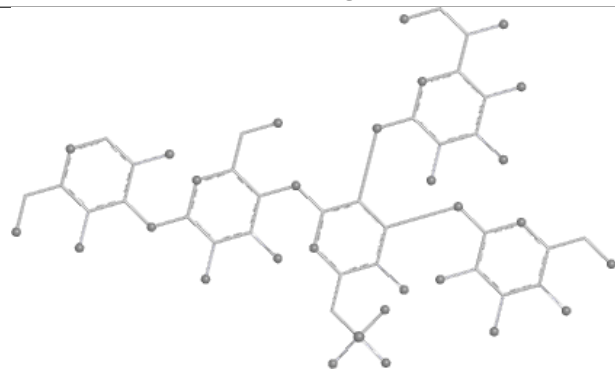
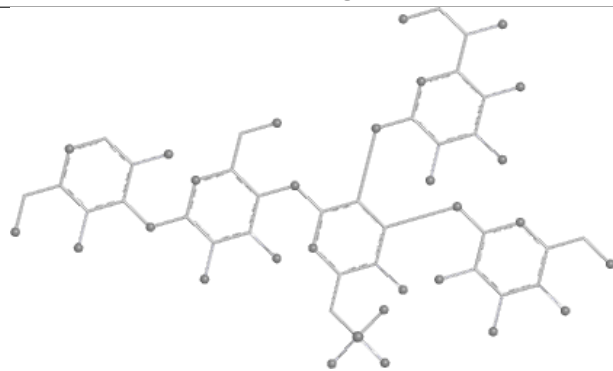
Oligosaccharide Chain SA**Oligosaccharide Chain WA**

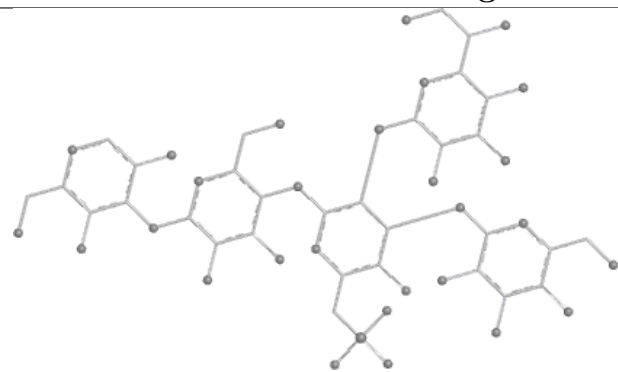
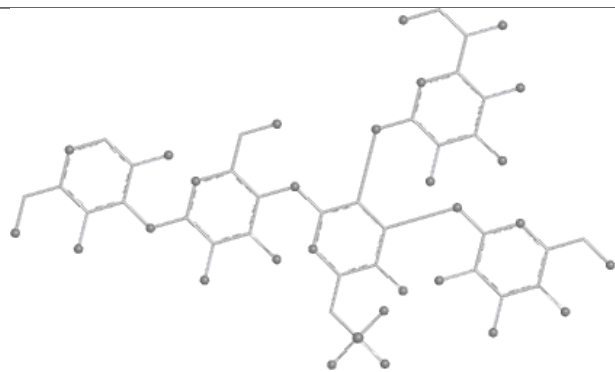
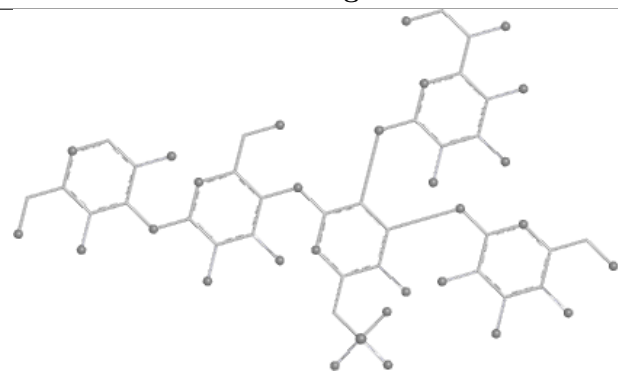
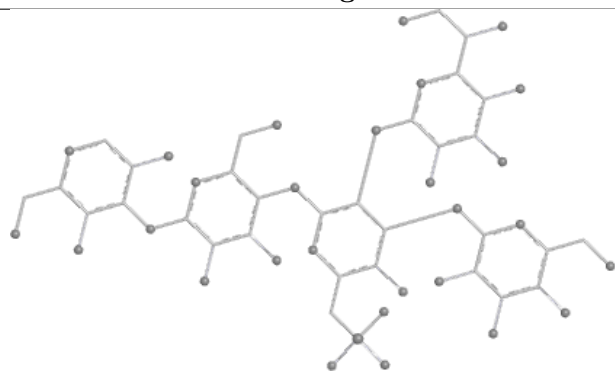
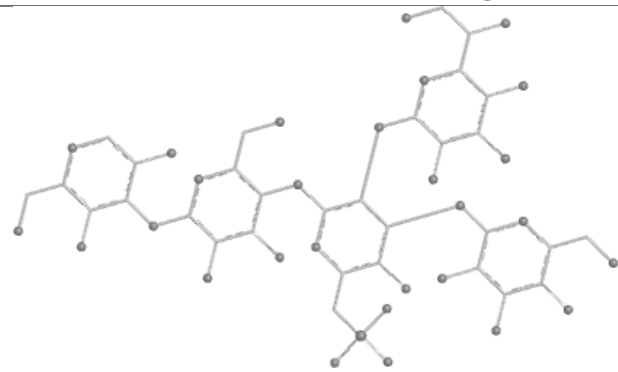
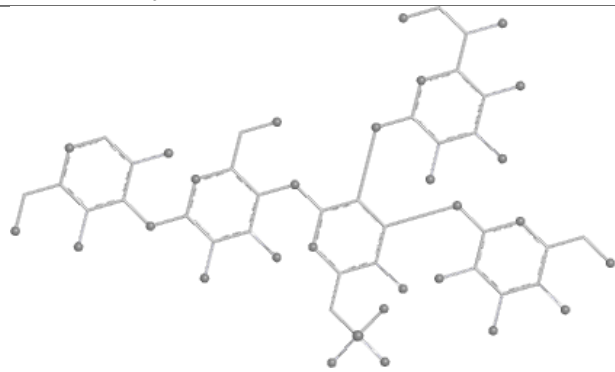
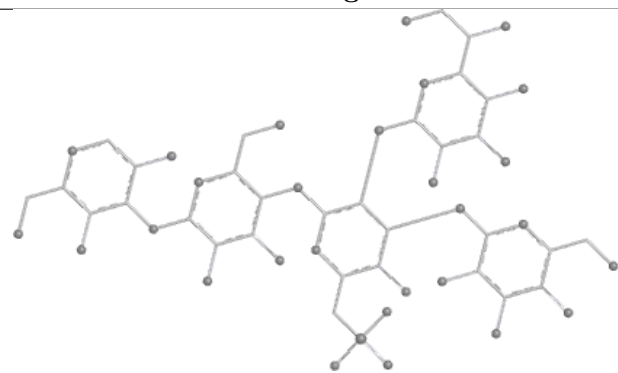
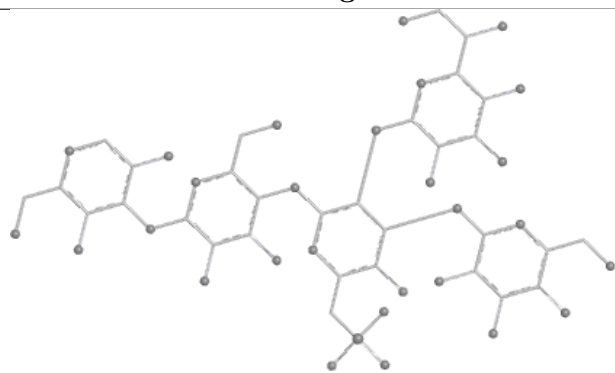
Oligosaccharide Chain XA**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain ZA****Bond lengths****Bond angles****Torsions****Rings**

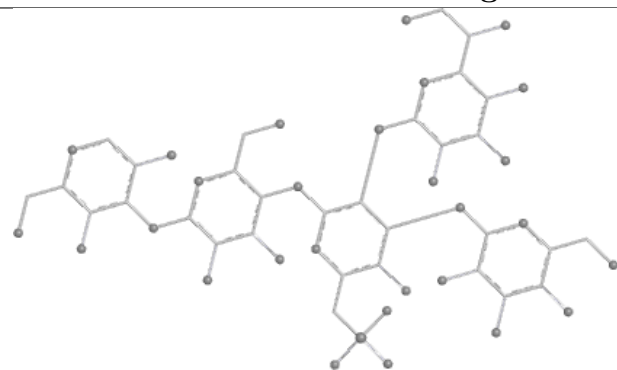
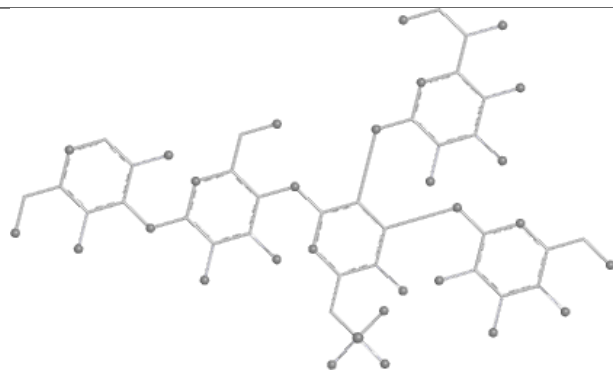
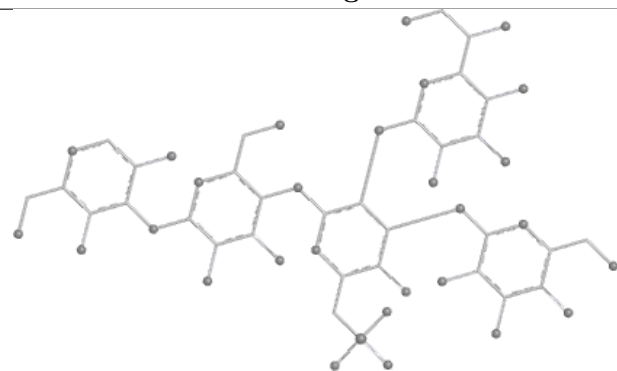
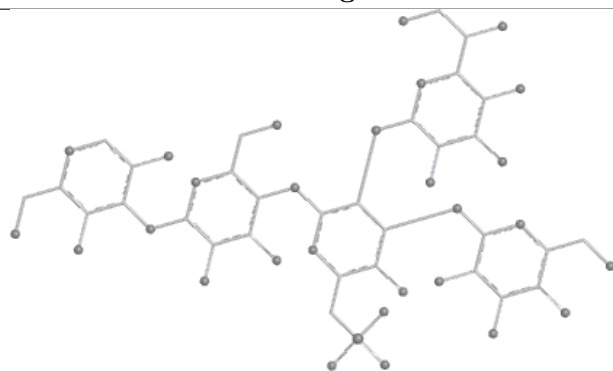
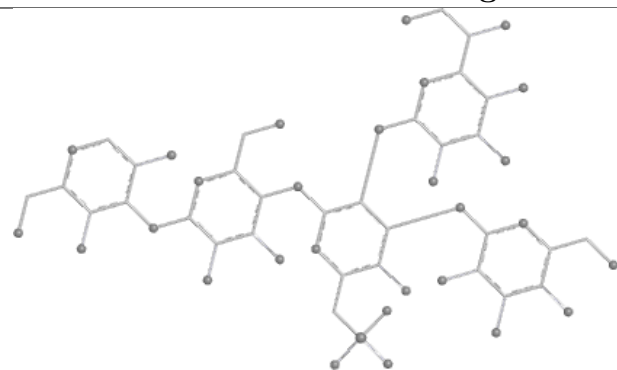
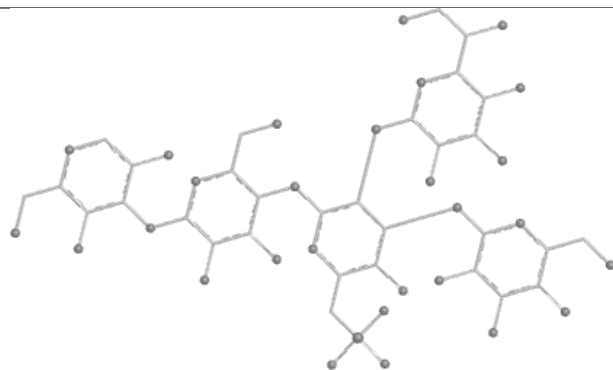
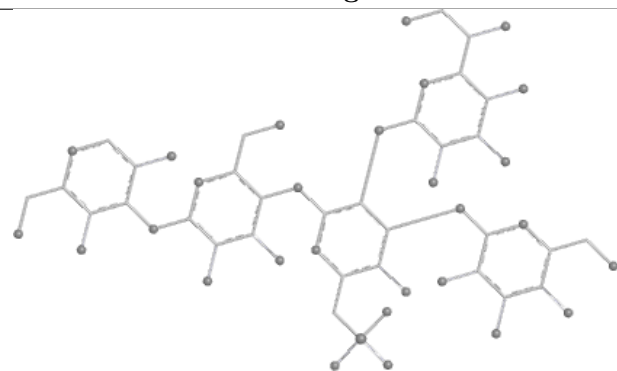
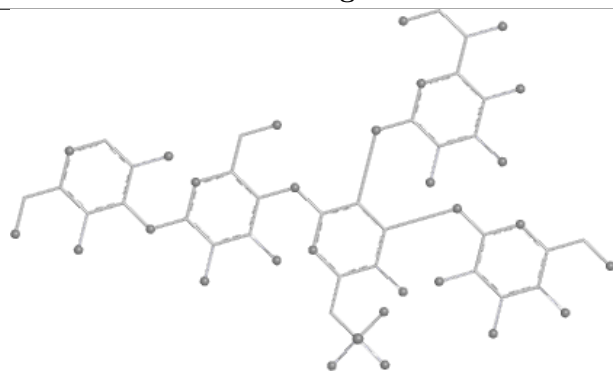
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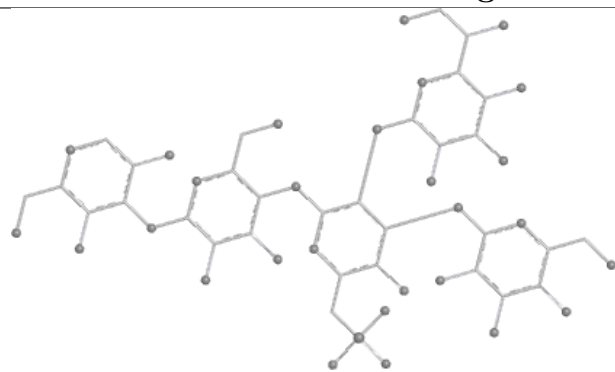
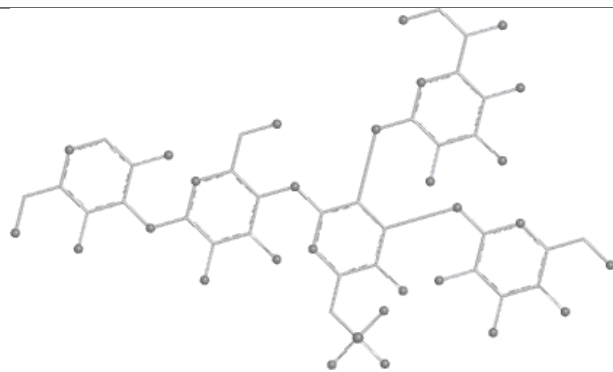
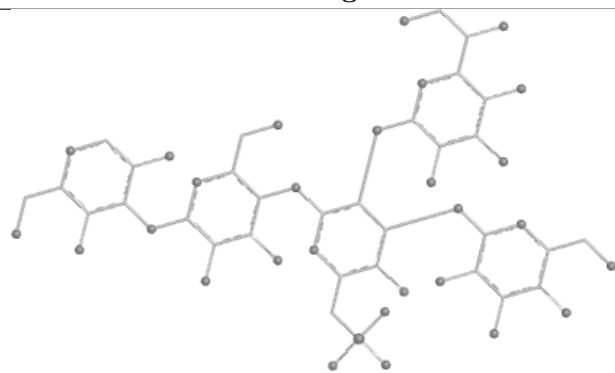
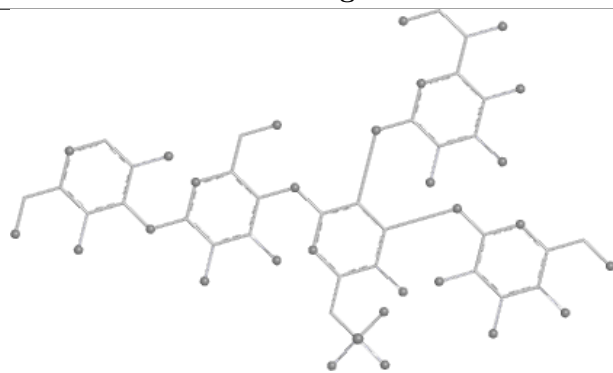
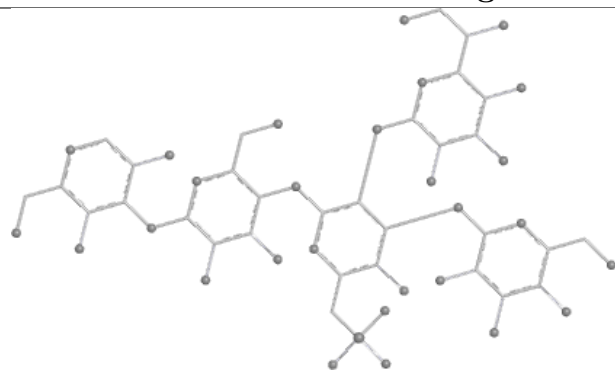
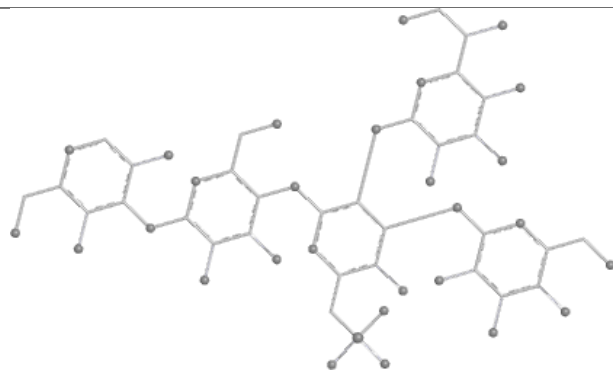
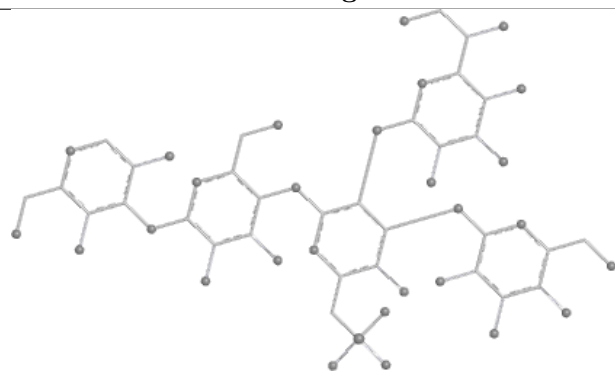
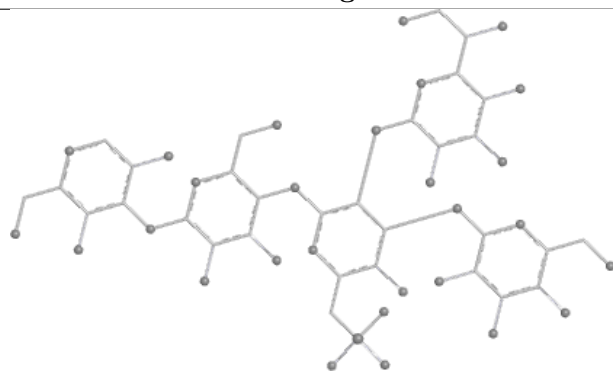
Oligosaccharide Chain gA**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain kA****Bond lengths****Bond angles****Torsions****Rings**

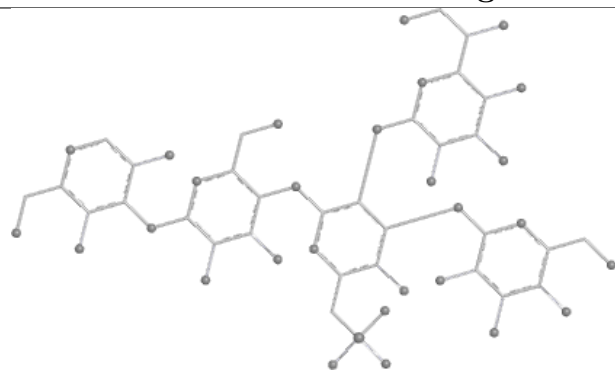
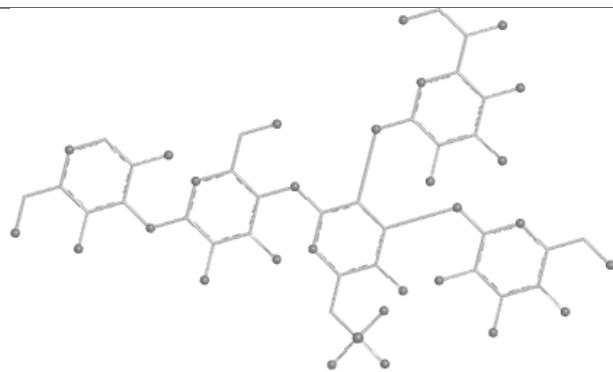
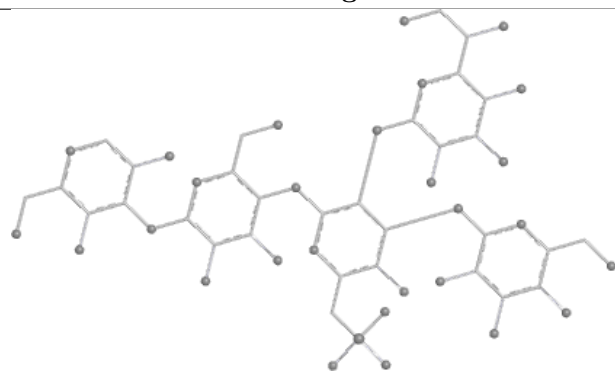
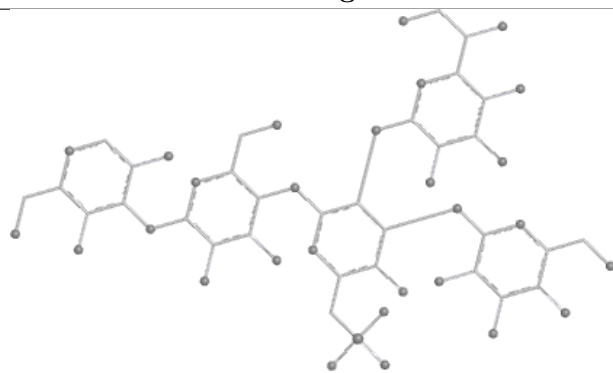
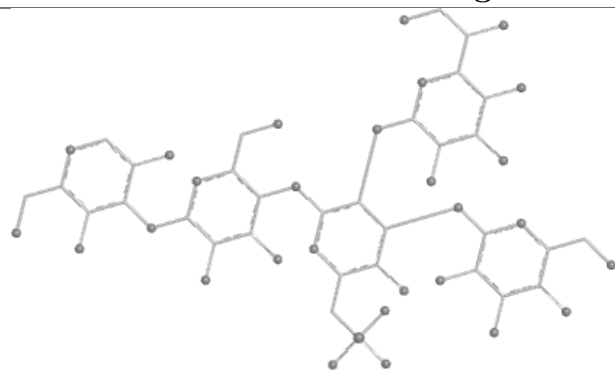
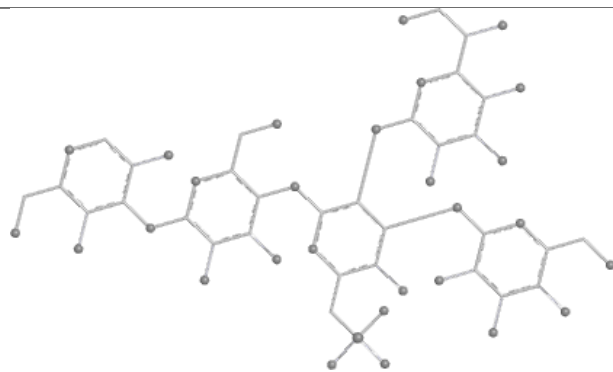
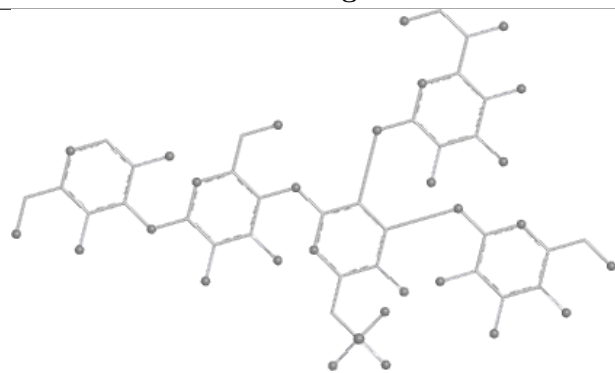
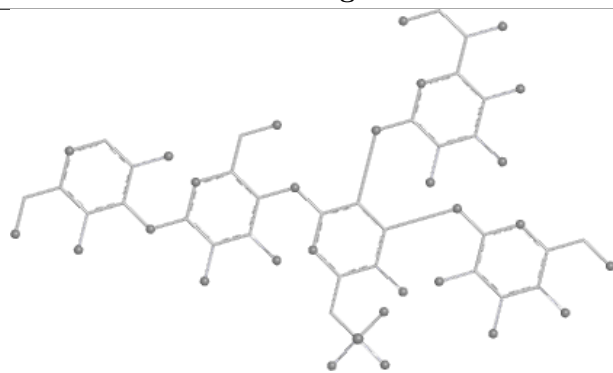


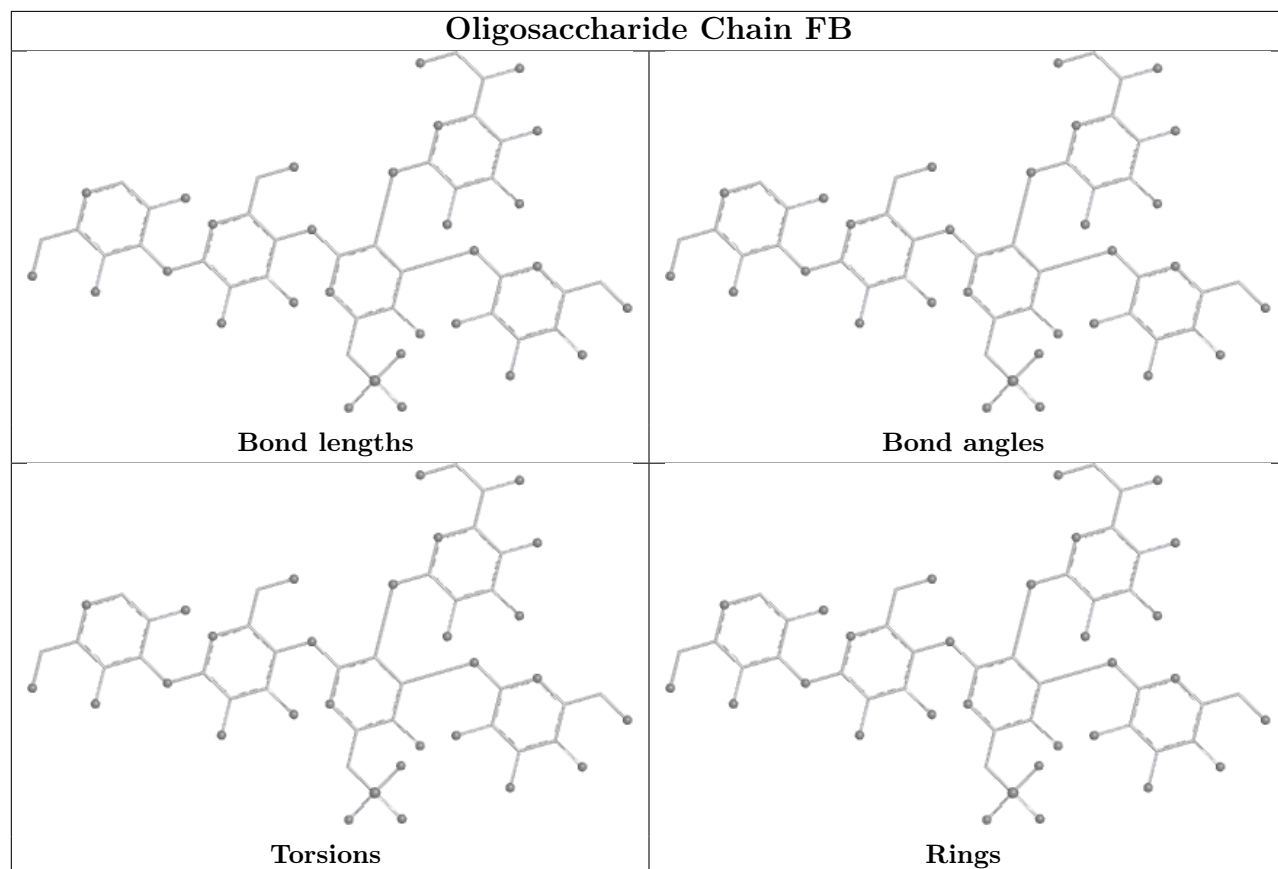
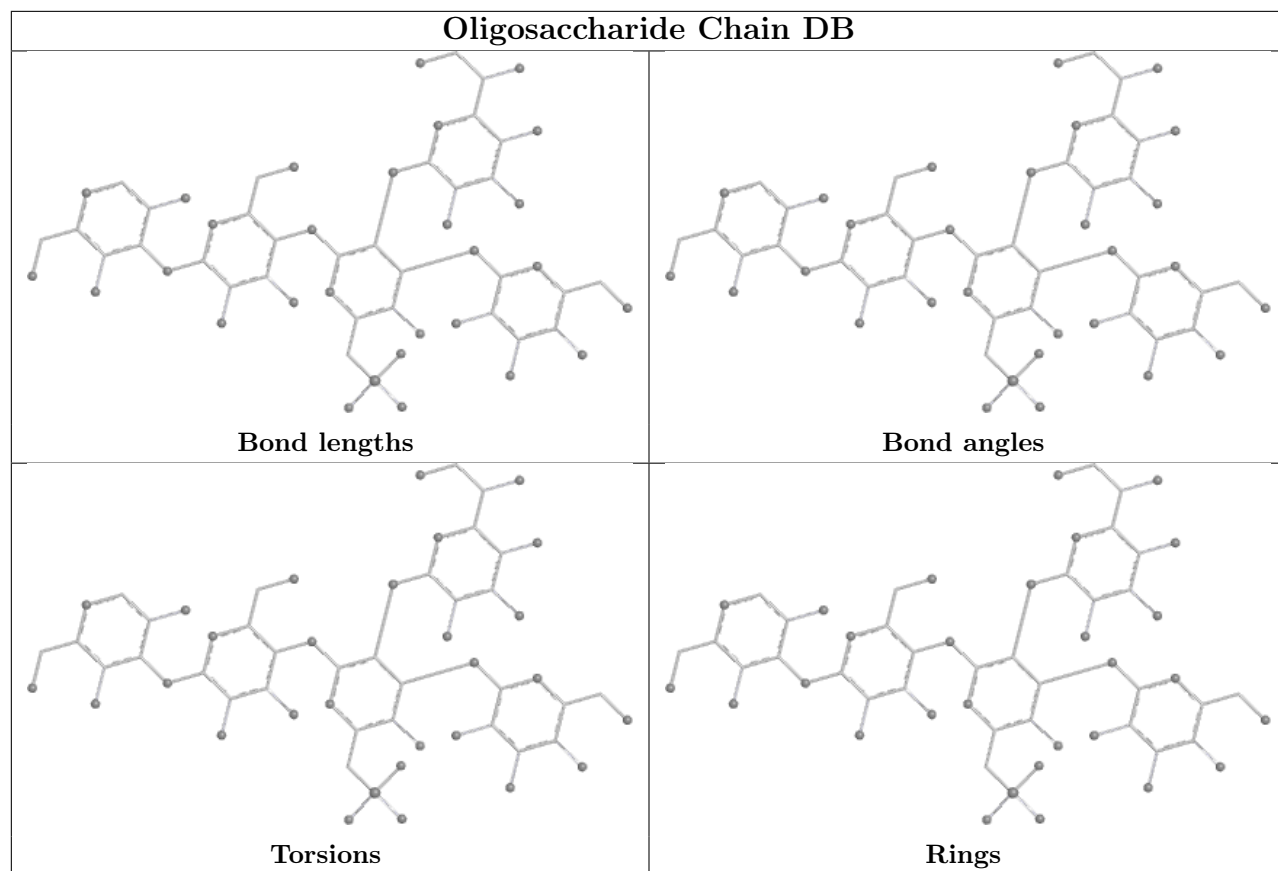
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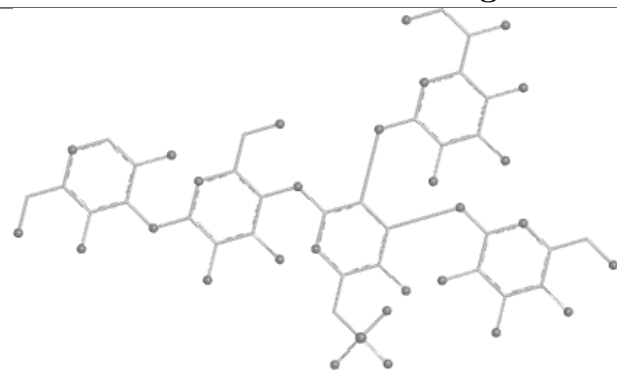
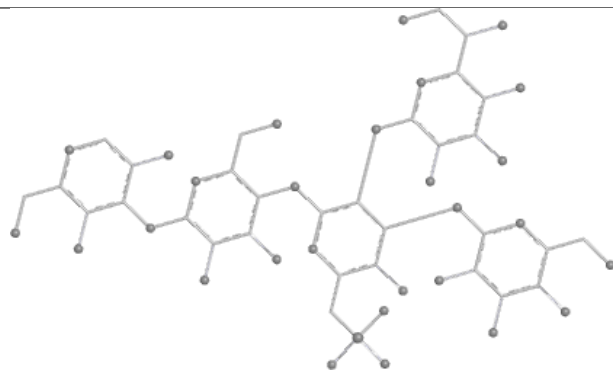
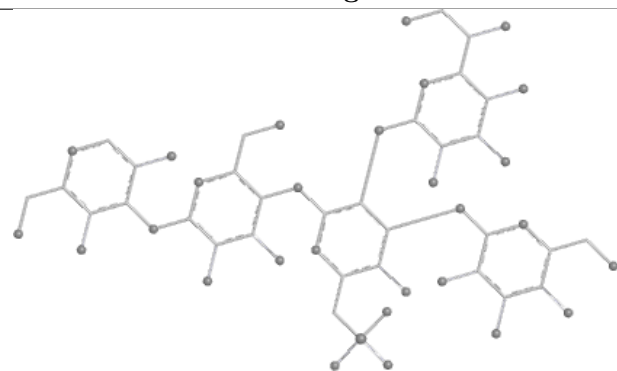
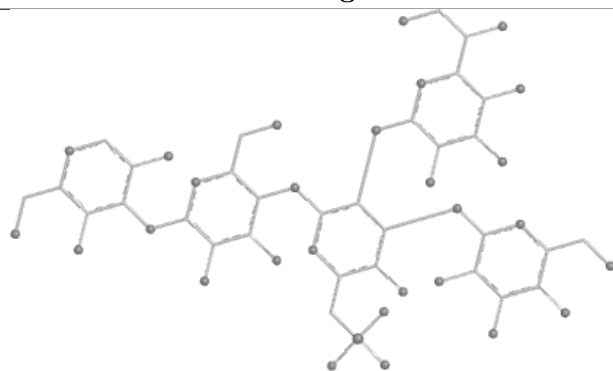
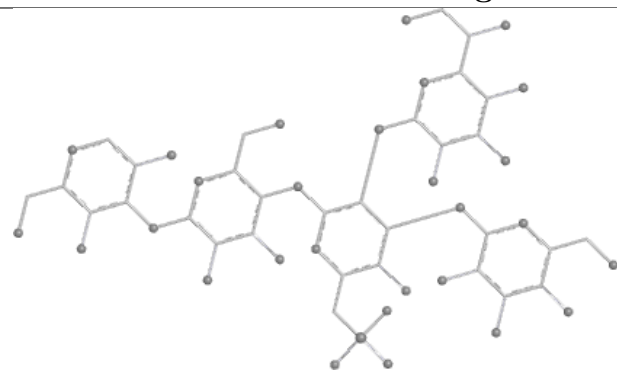
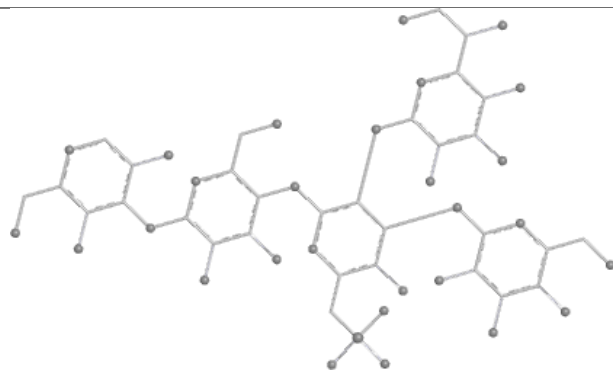
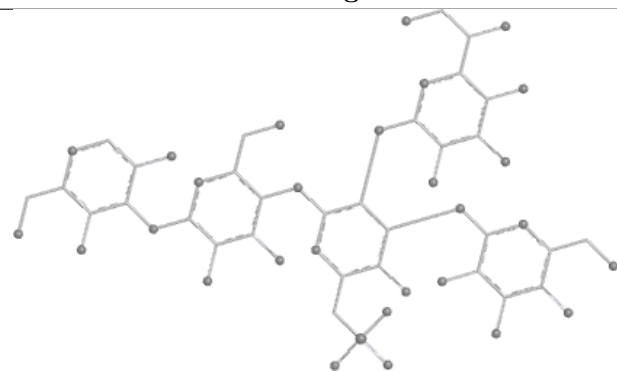
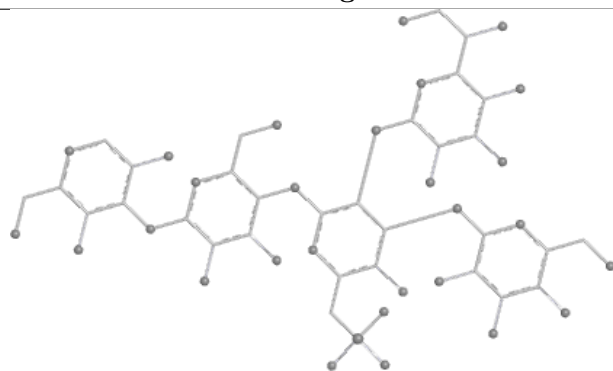
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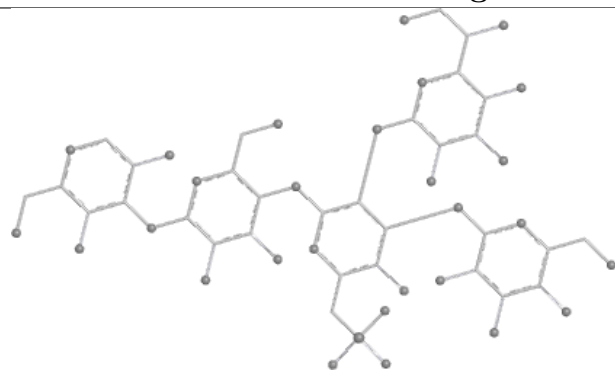
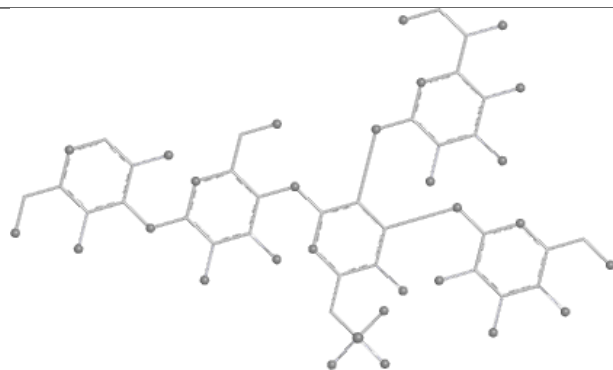
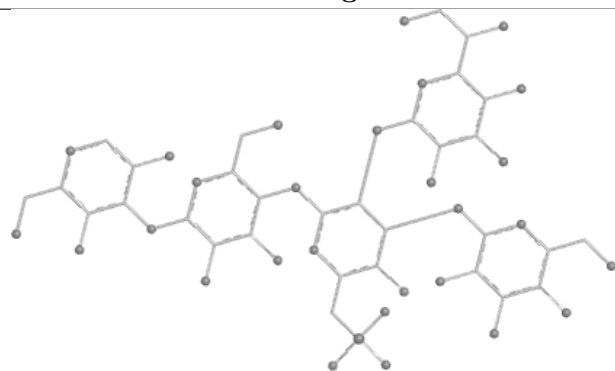
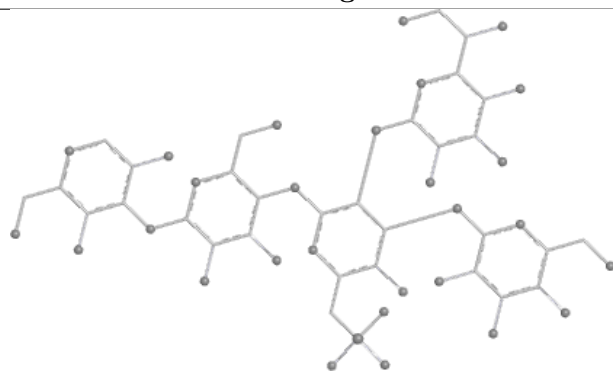
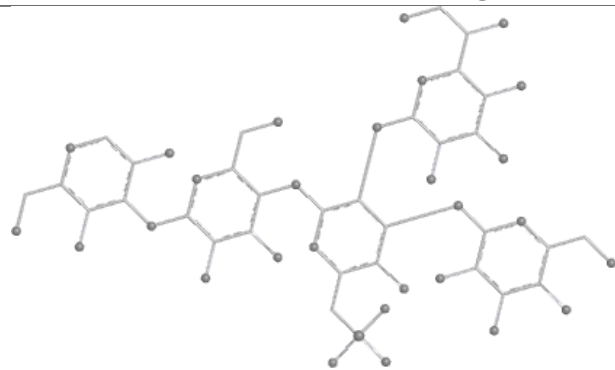
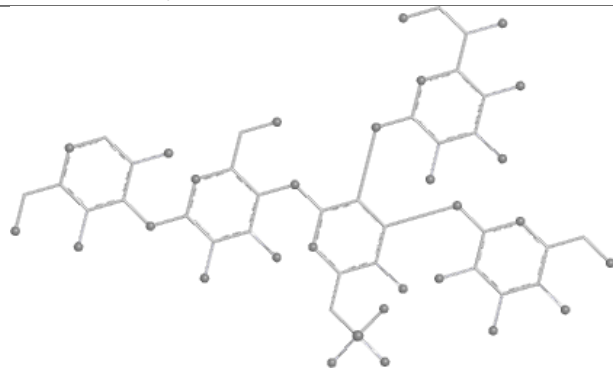
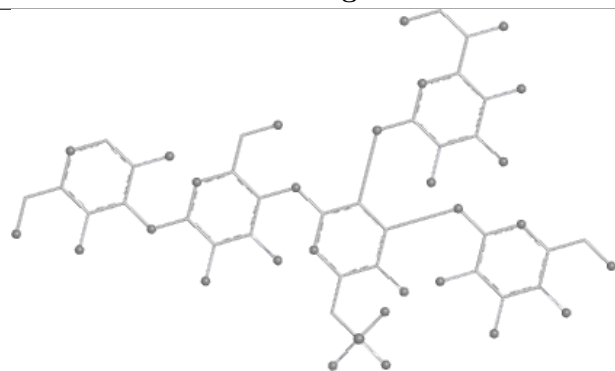
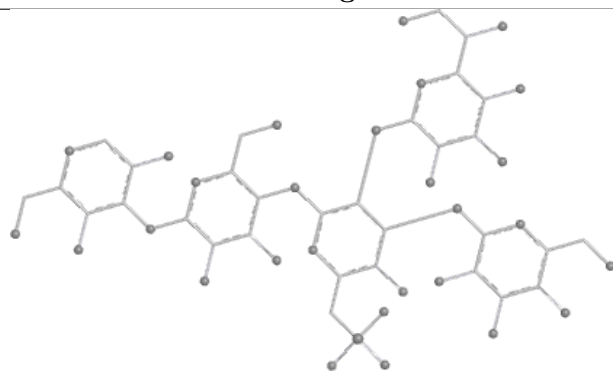
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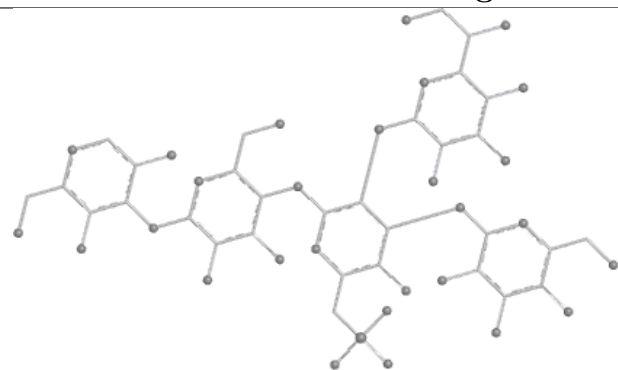
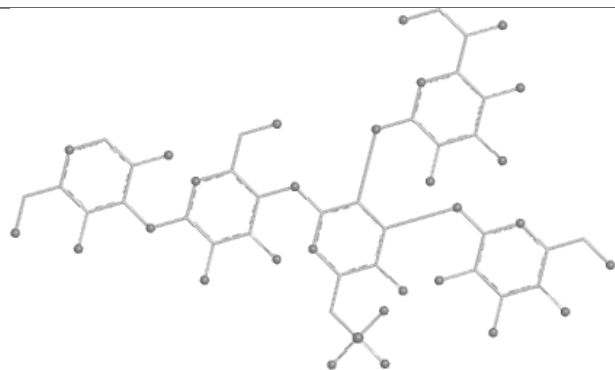
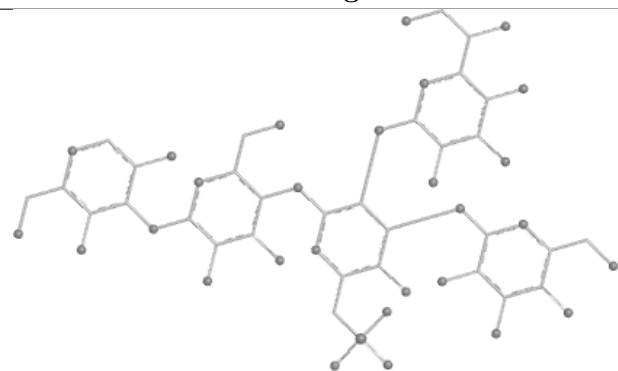
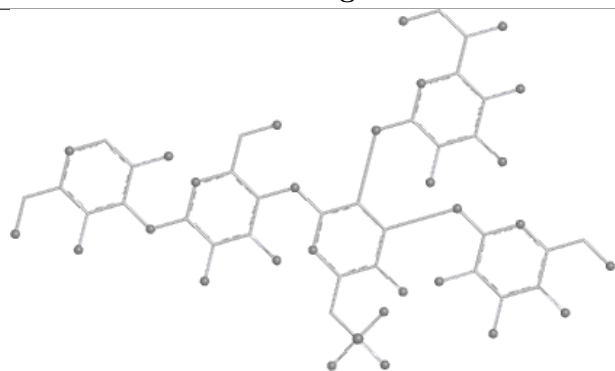
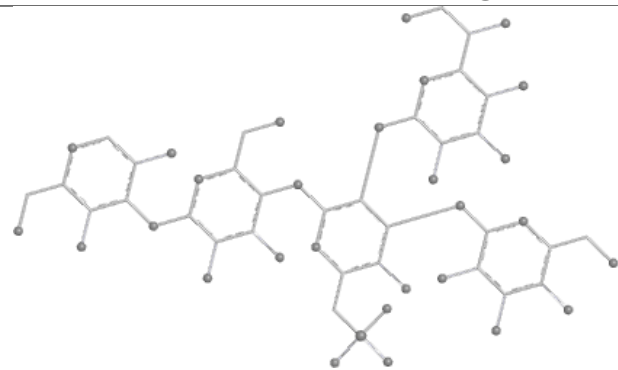
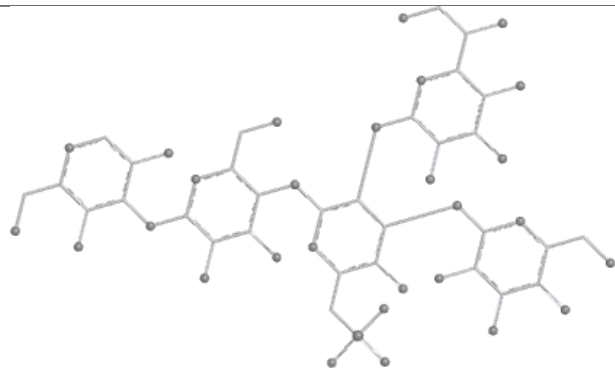
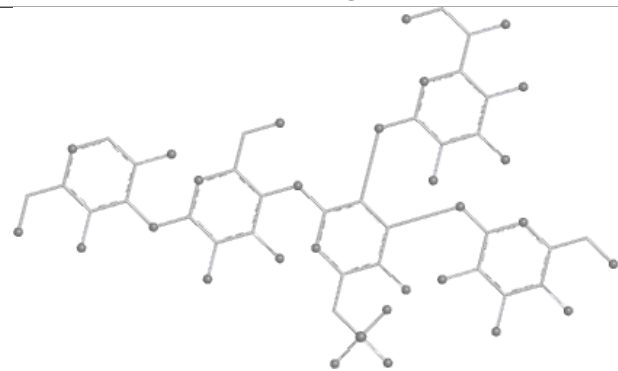
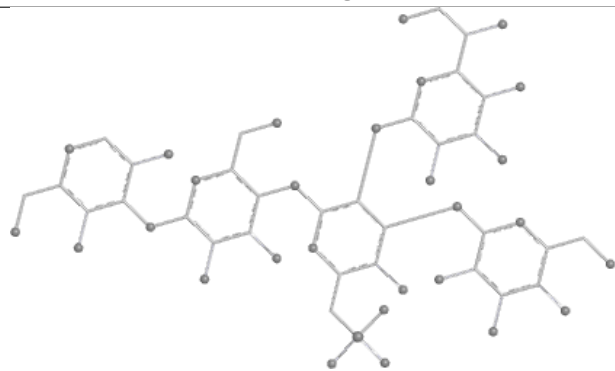
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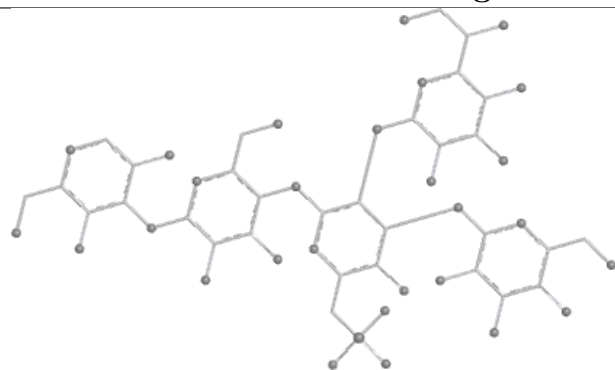
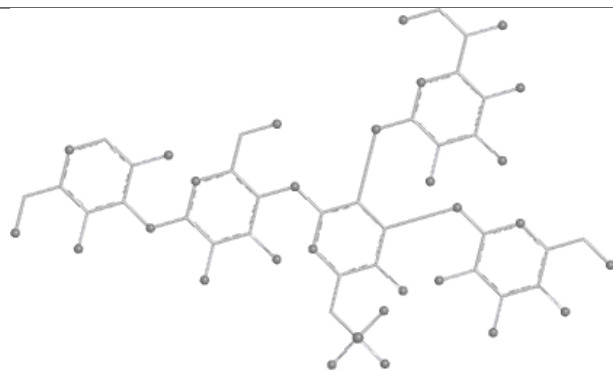
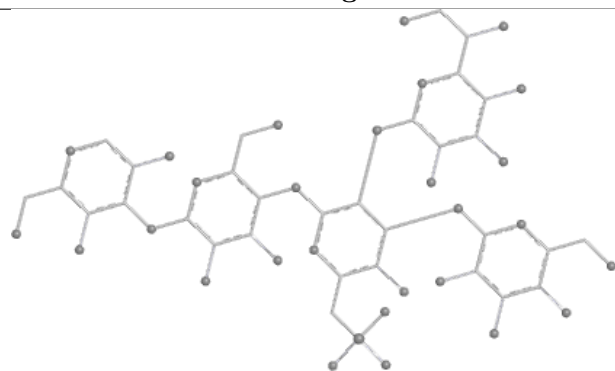
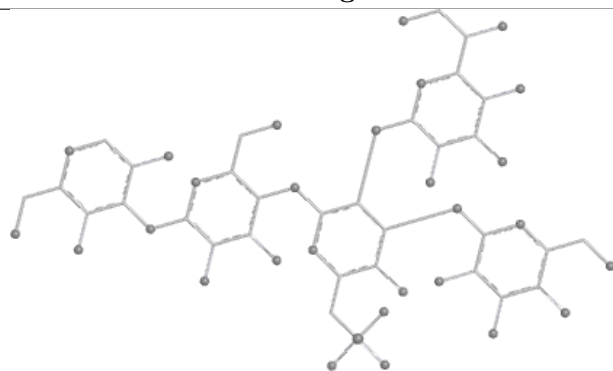
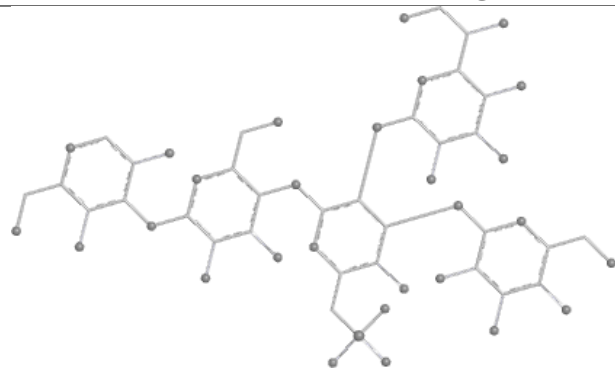
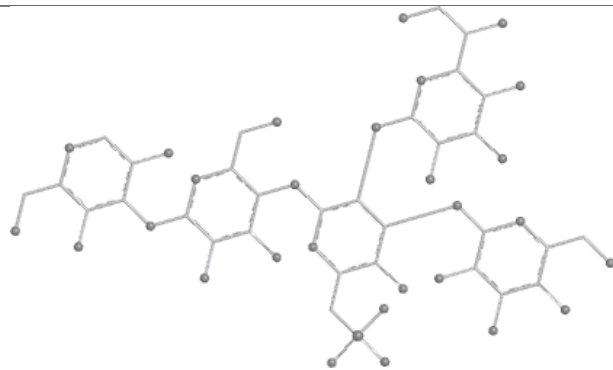
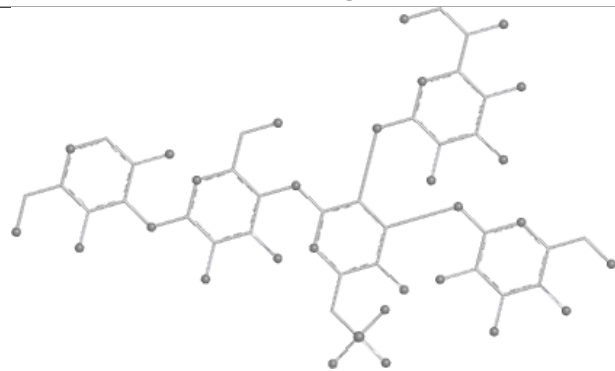
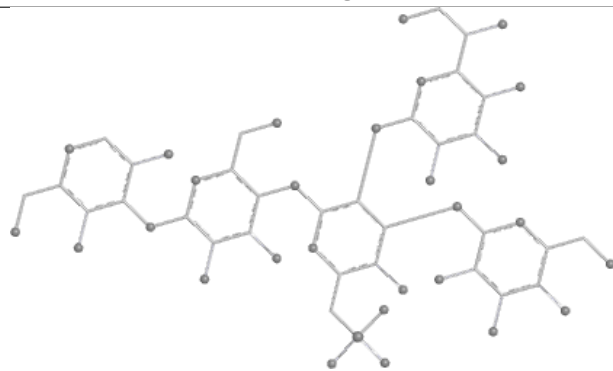
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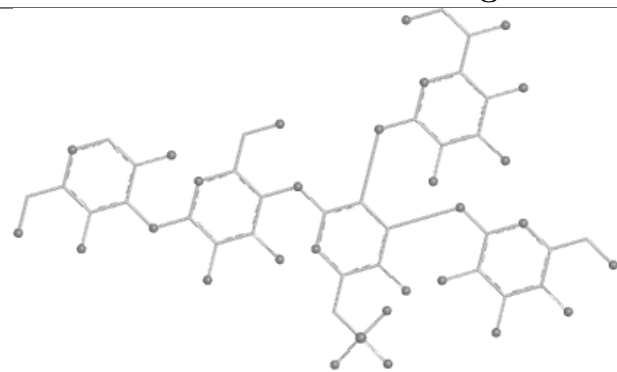
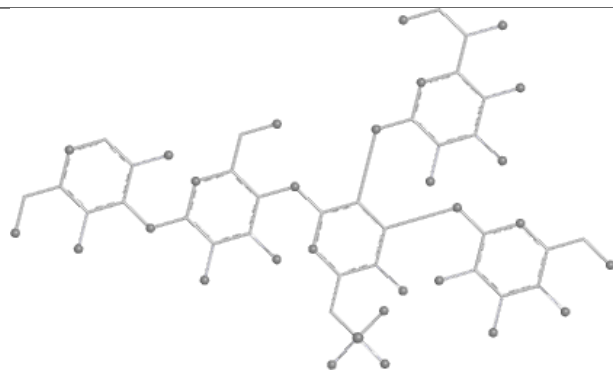
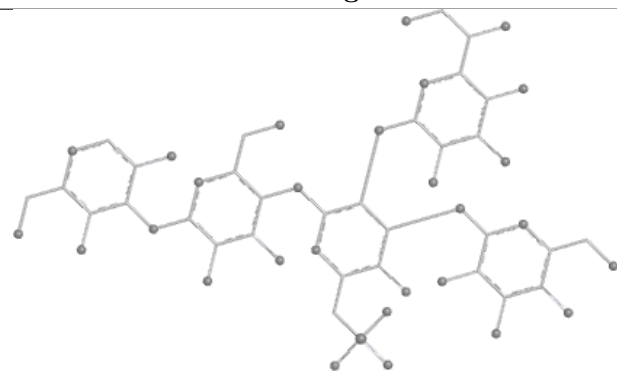
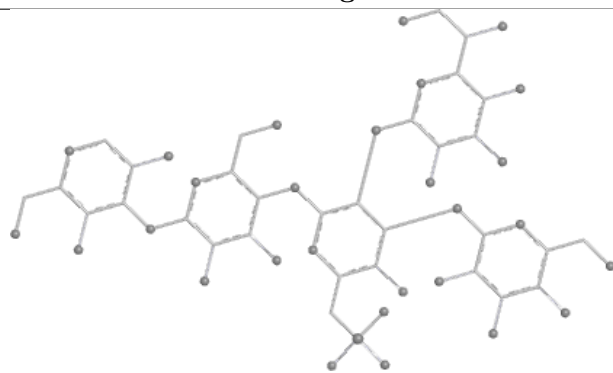
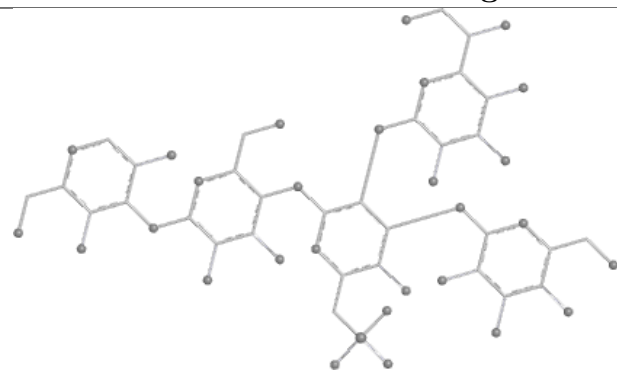
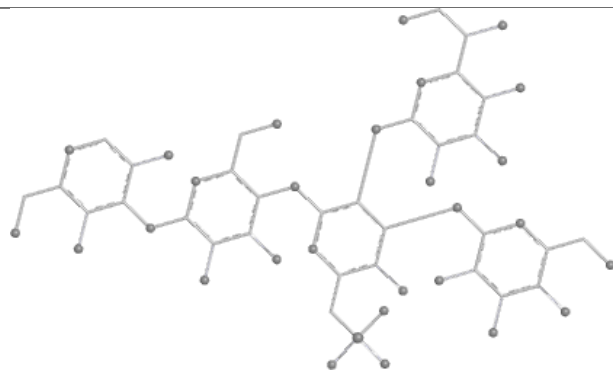
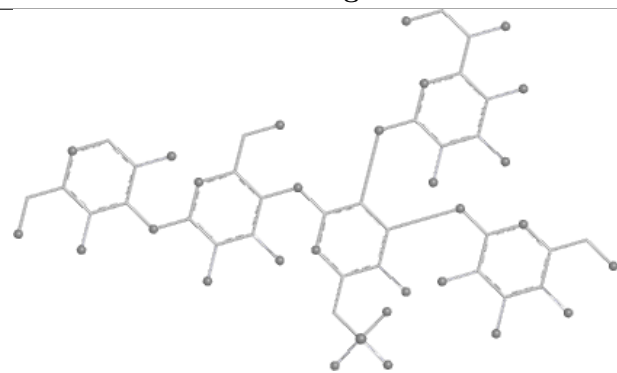
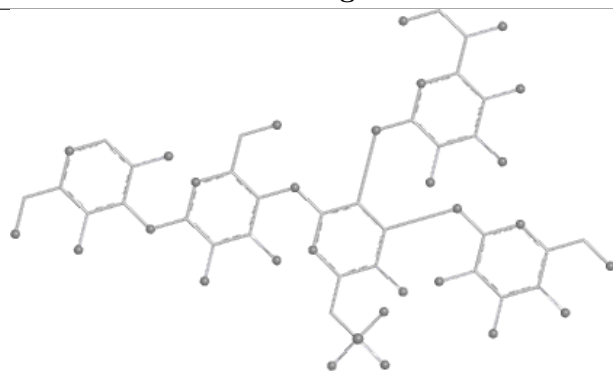


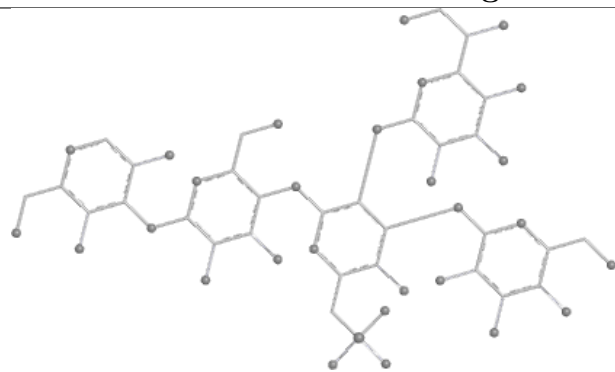
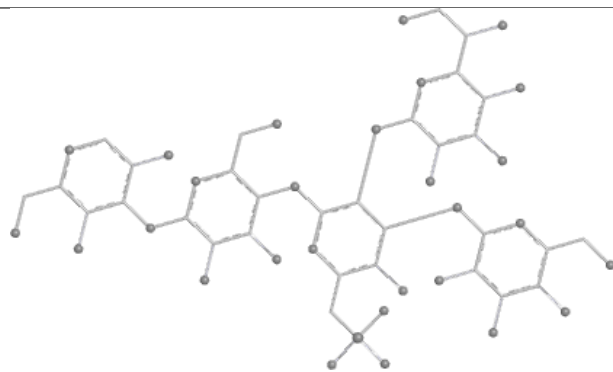
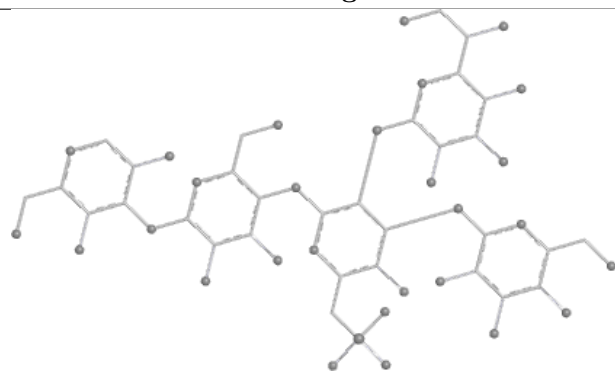
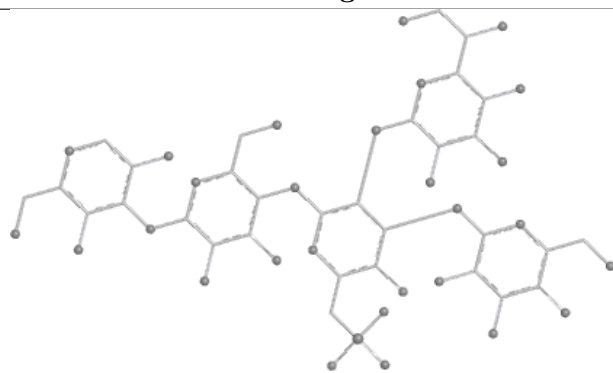
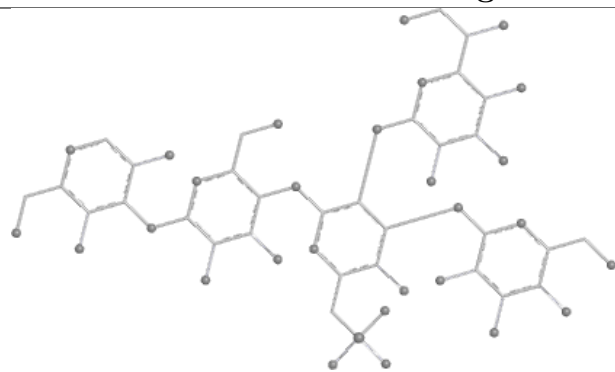
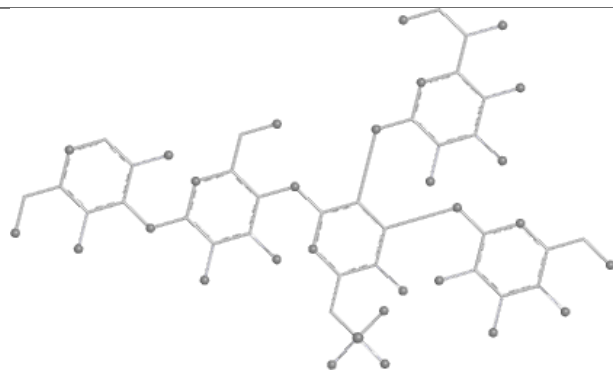
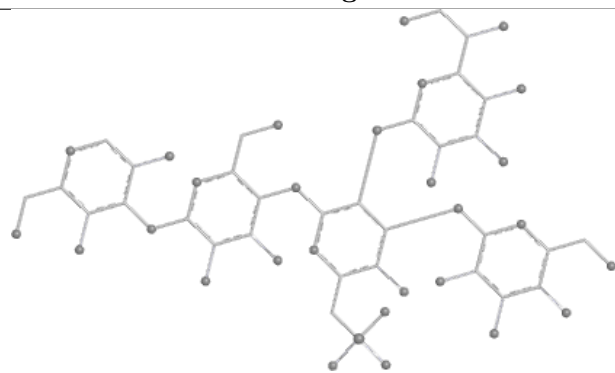
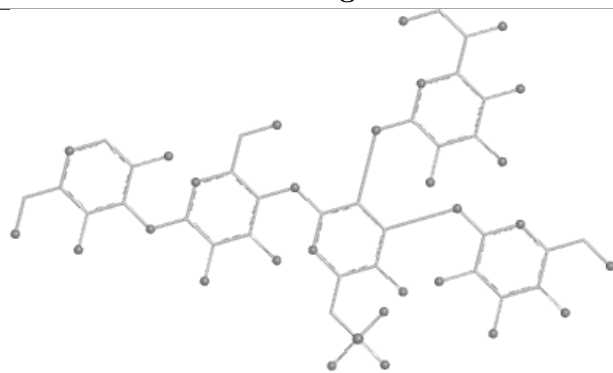
Oligosaccharide Chain JB**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain KB****Bond lengths****Bond angles****Torsions****Rings**

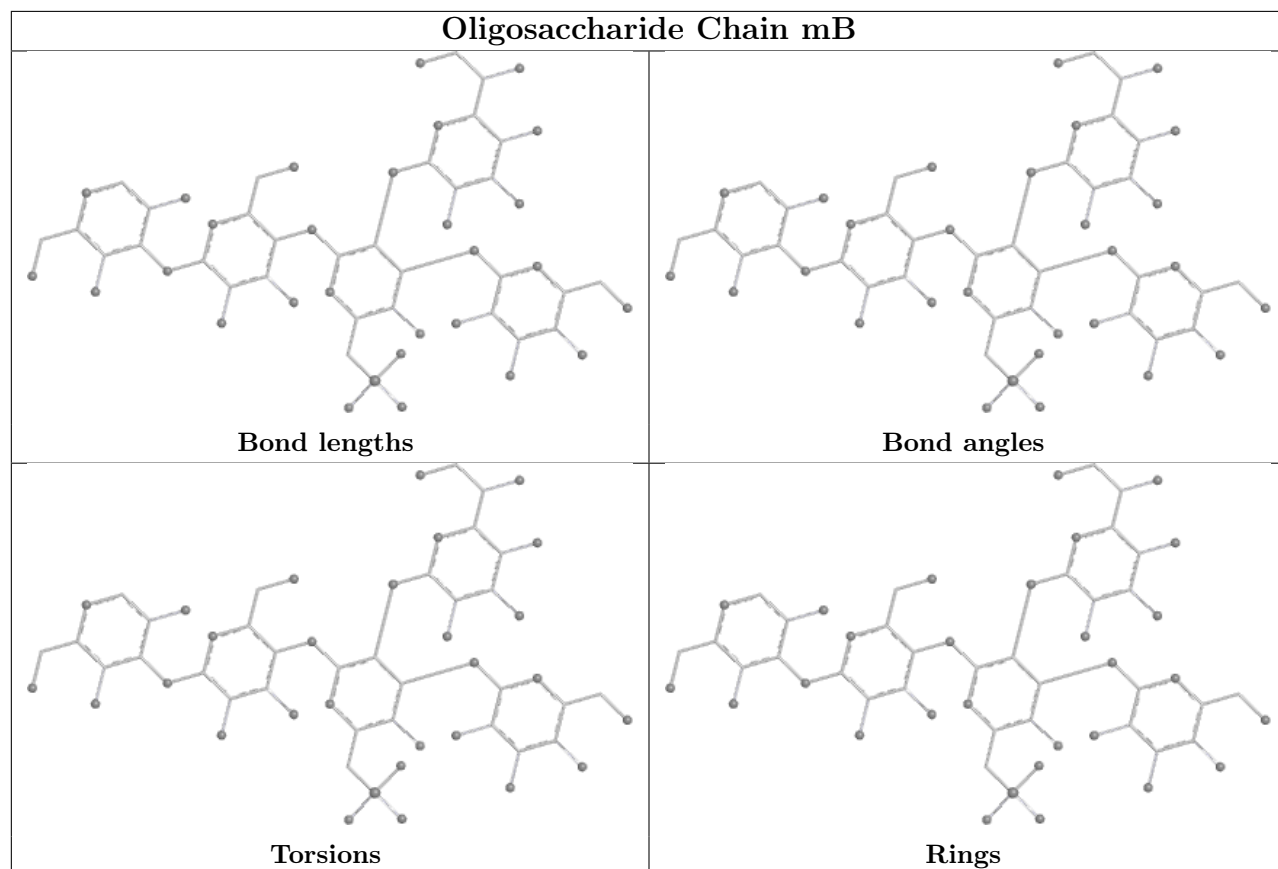
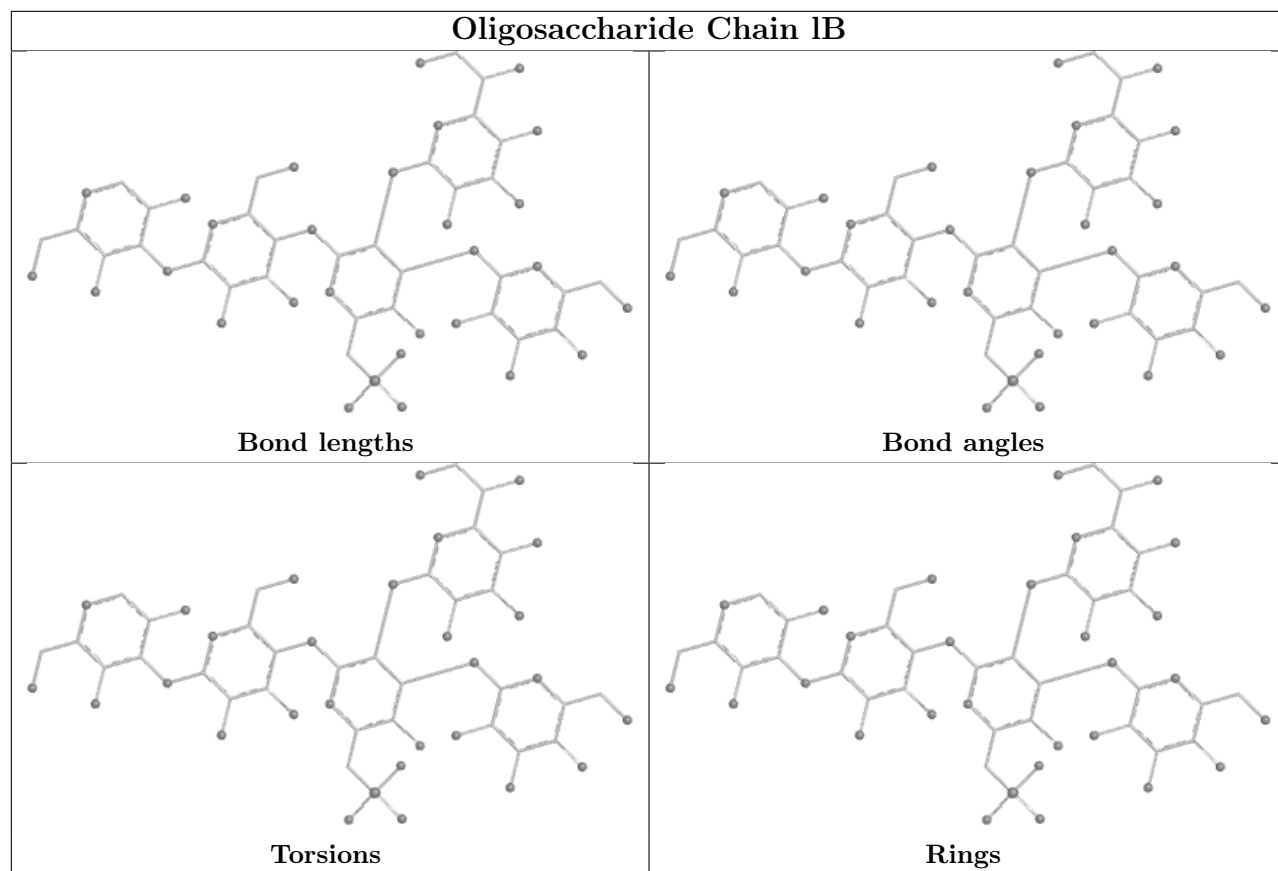
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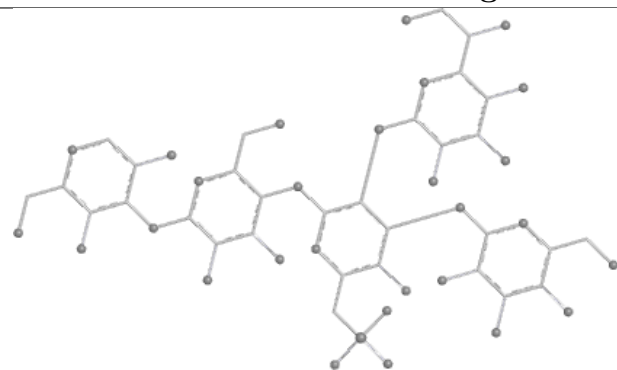
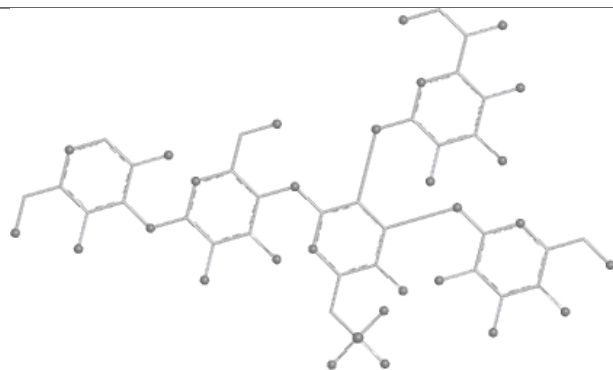
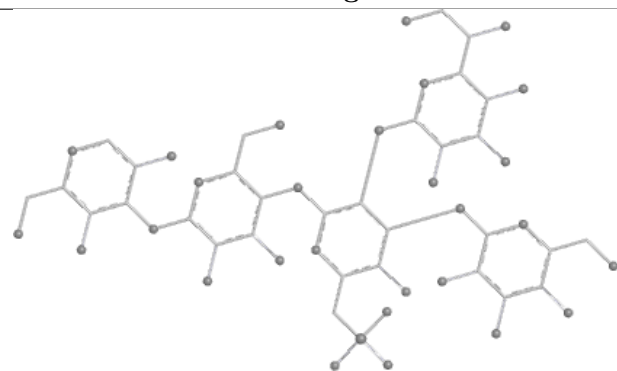
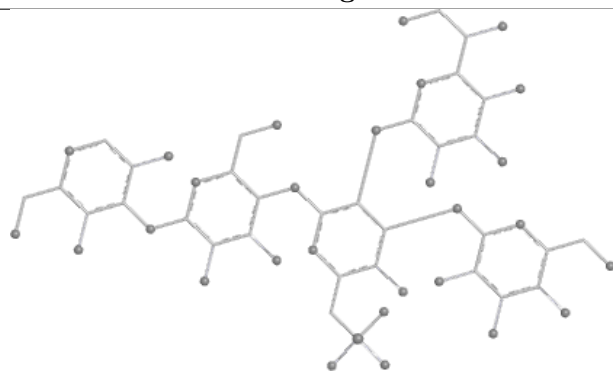
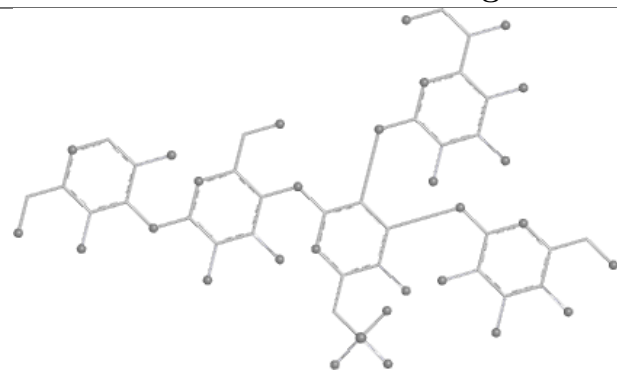
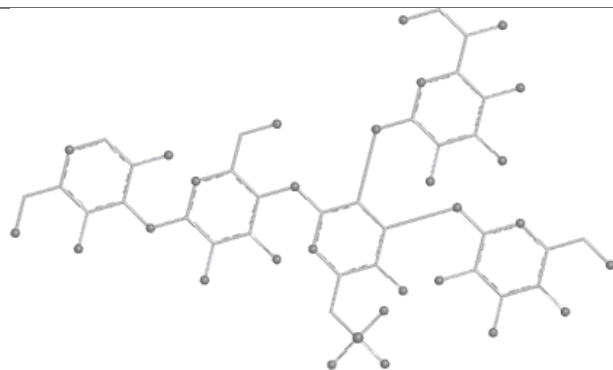
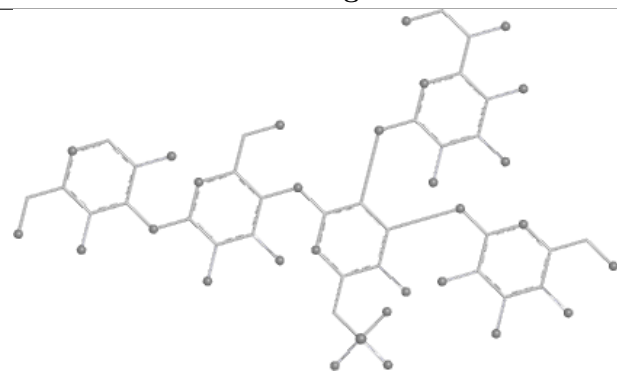
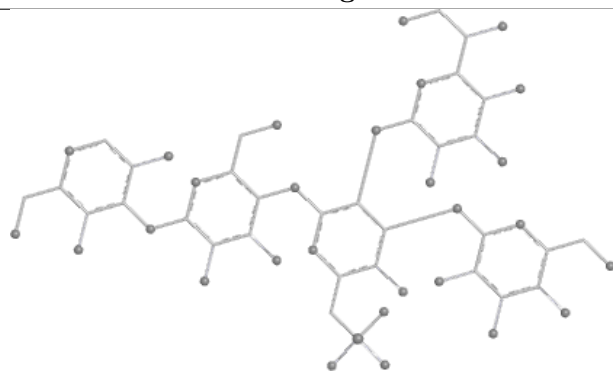
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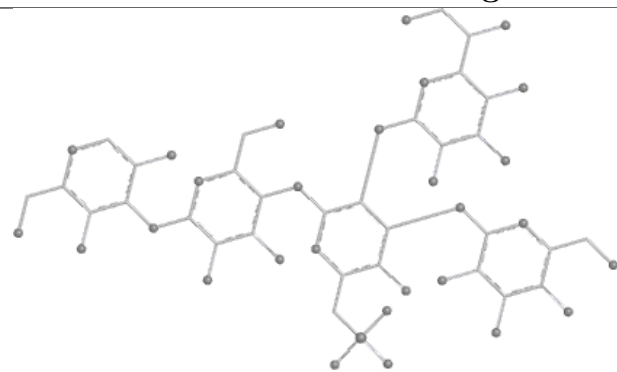
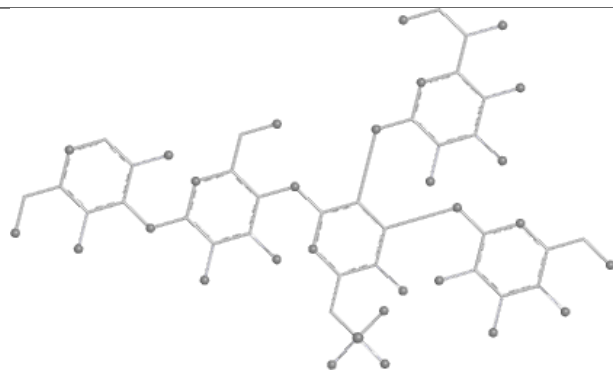
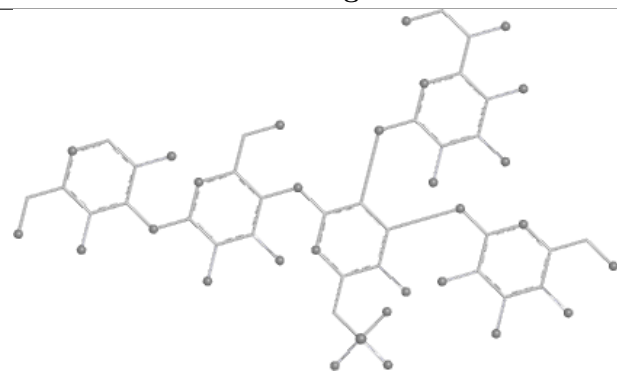
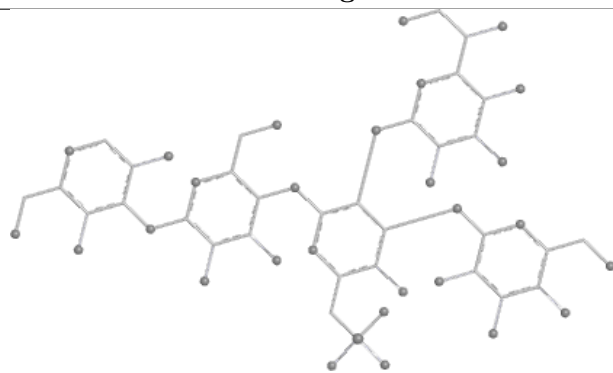
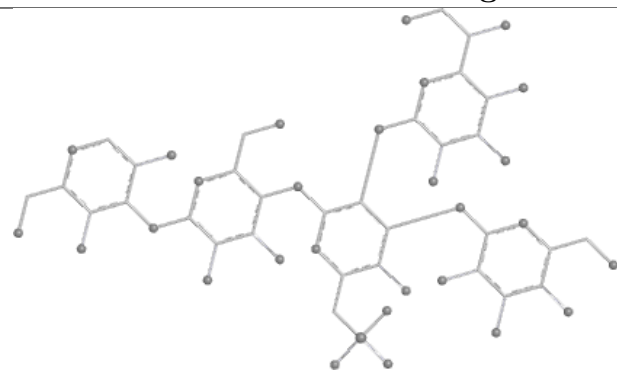
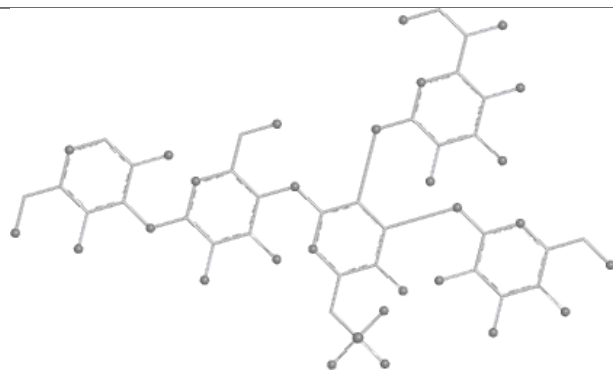
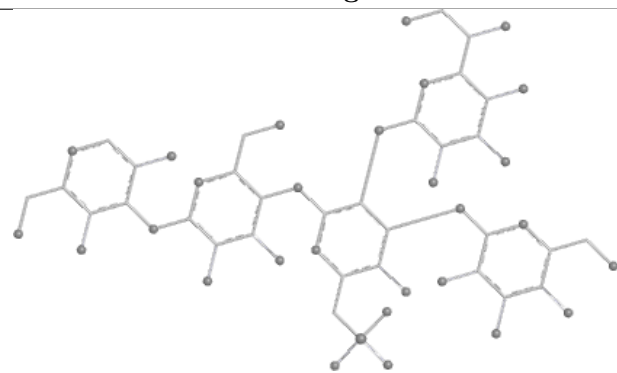
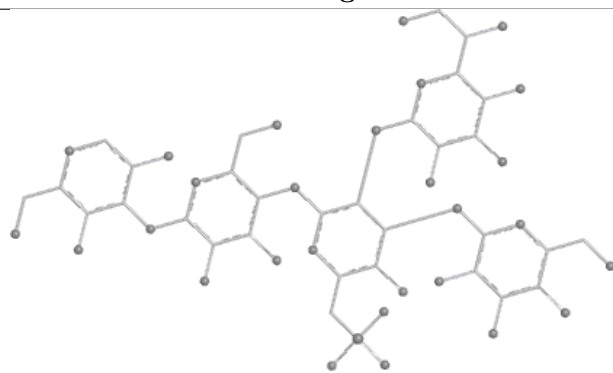
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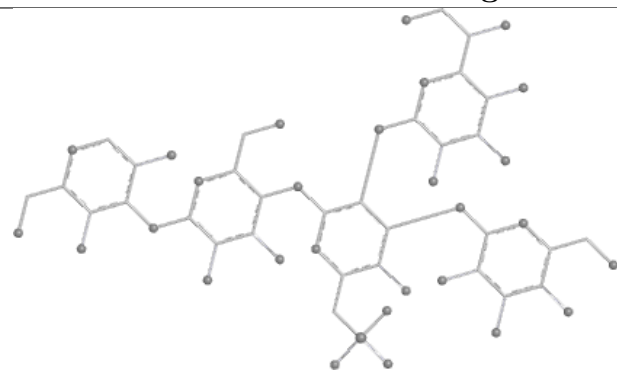
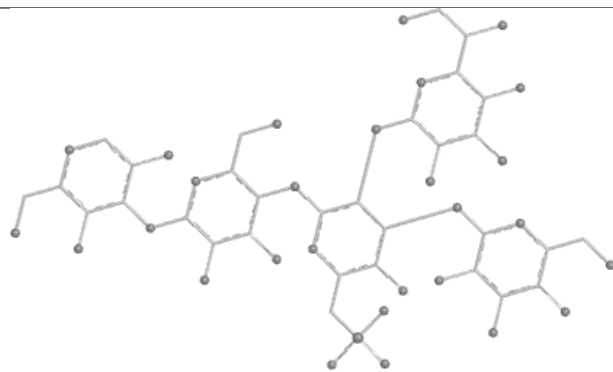
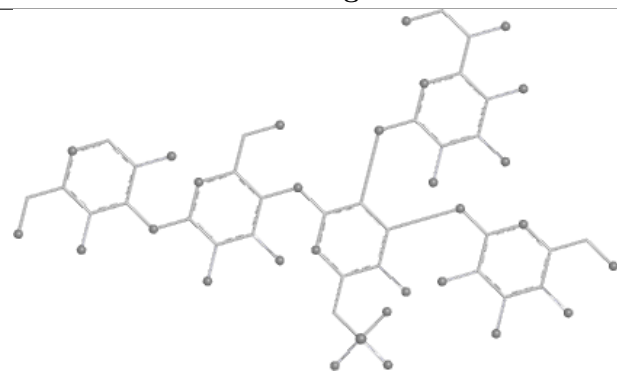
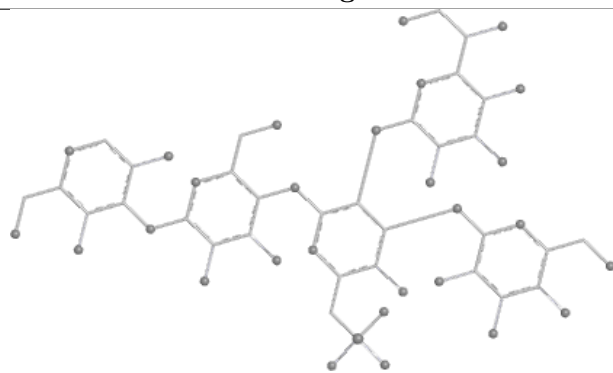
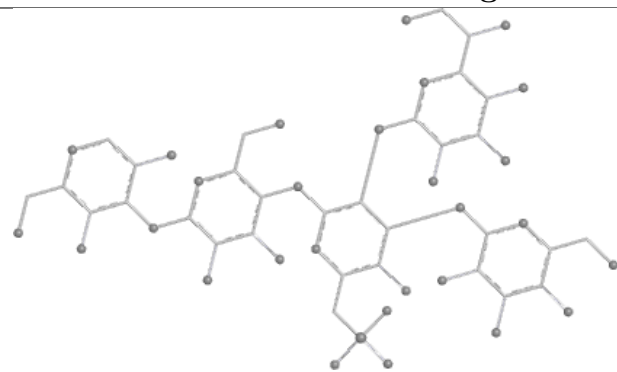
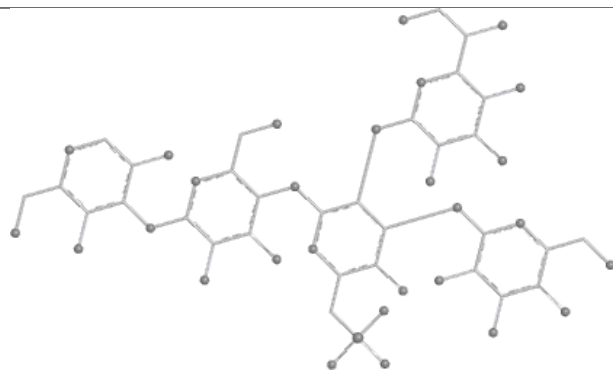
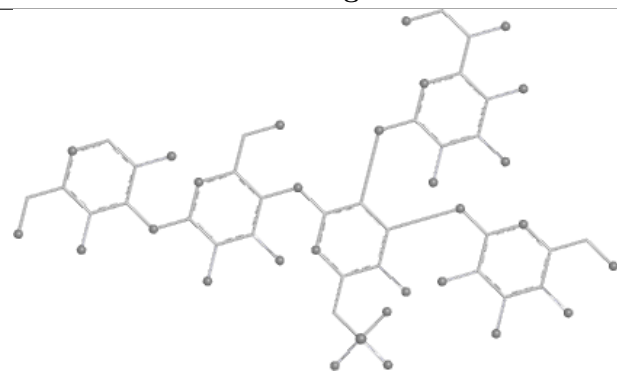
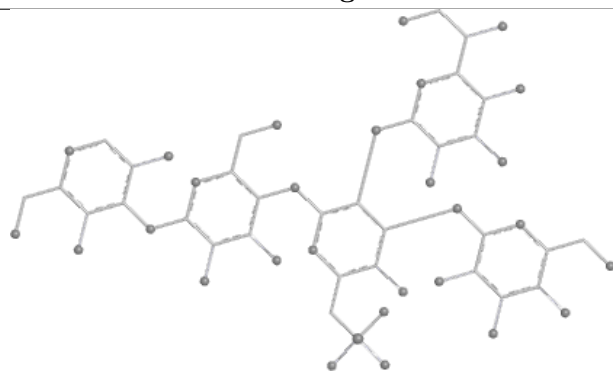
Oligosaccharide Chain aB**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain eB****Bond lengths****Bond angles****Torsions****Rings**

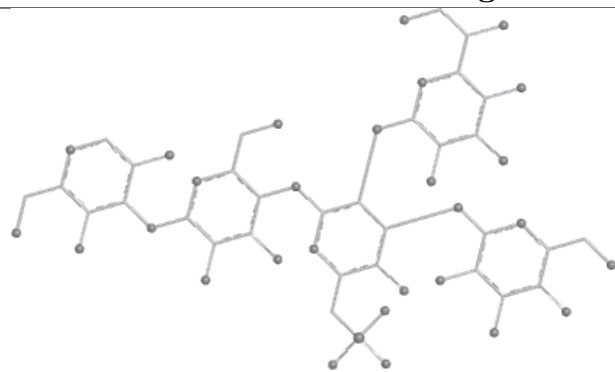
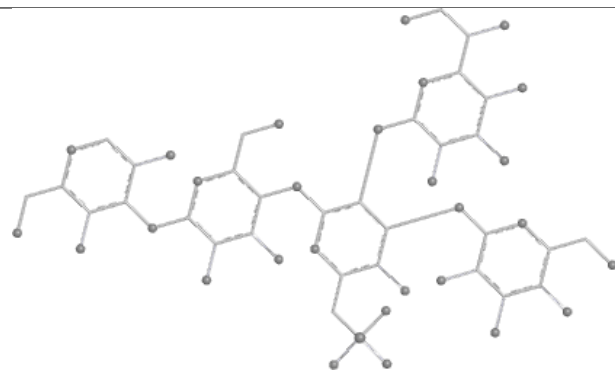
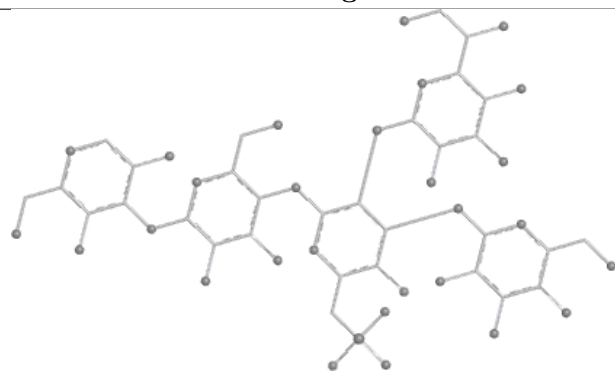
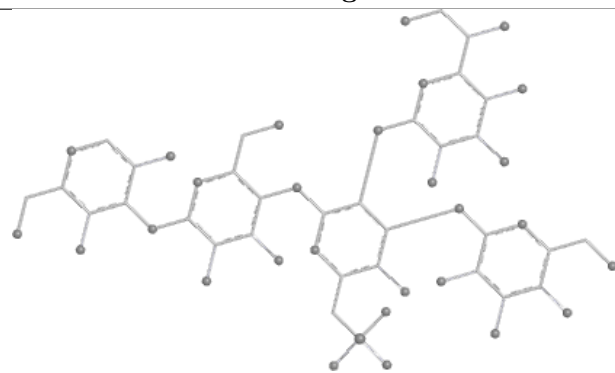
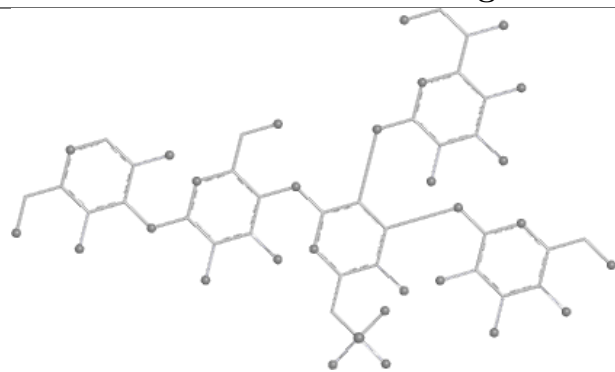
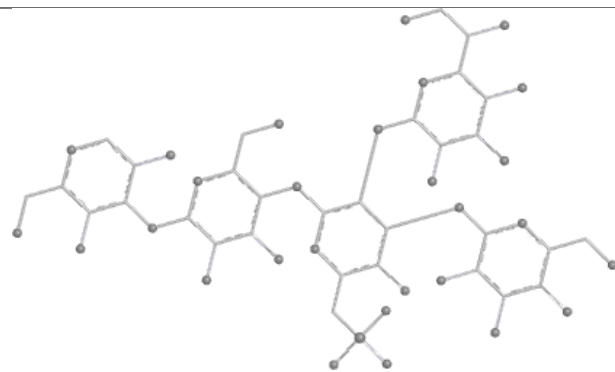
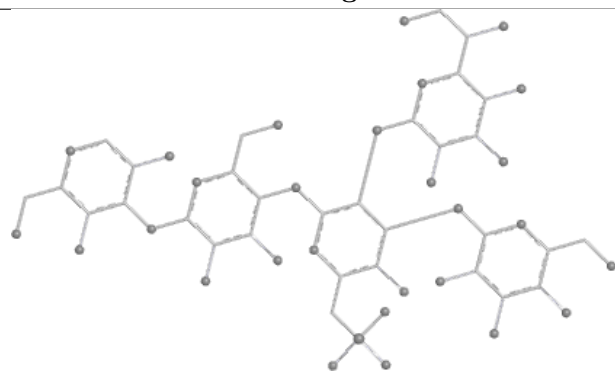
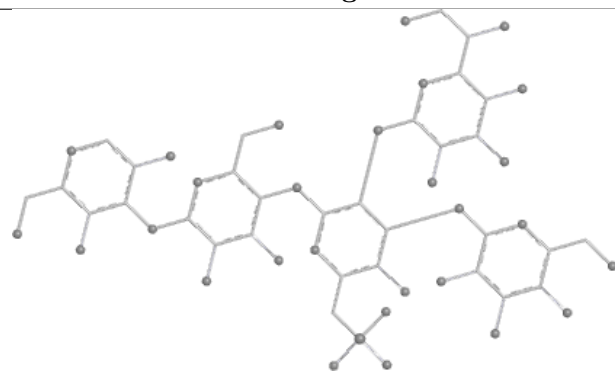
Oligosaccharide Chain fB**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain hB****Bond lengths****Bond angles****Torsions****Rings**

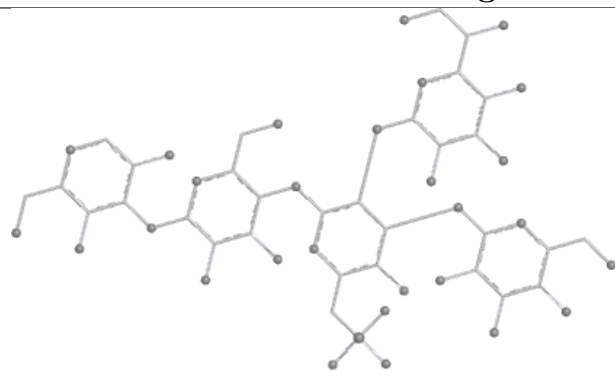
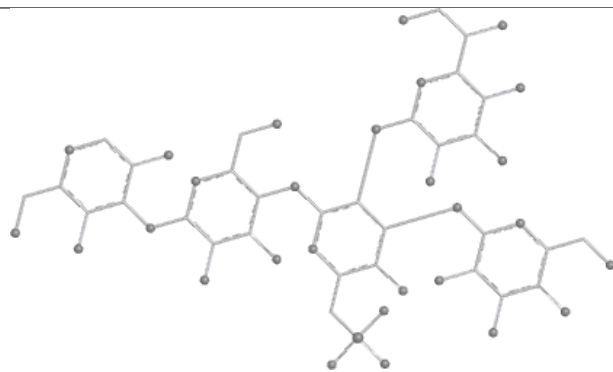
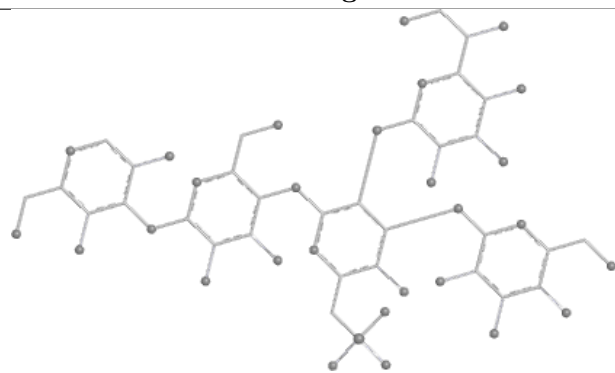
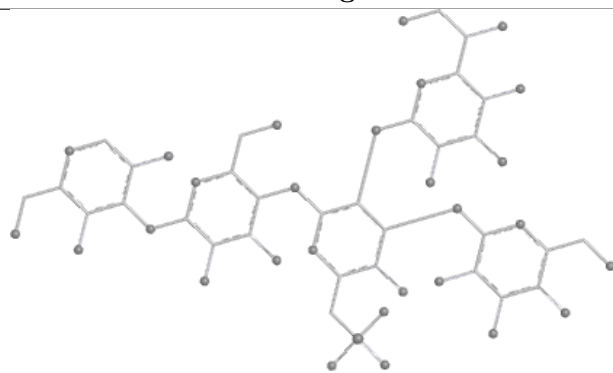
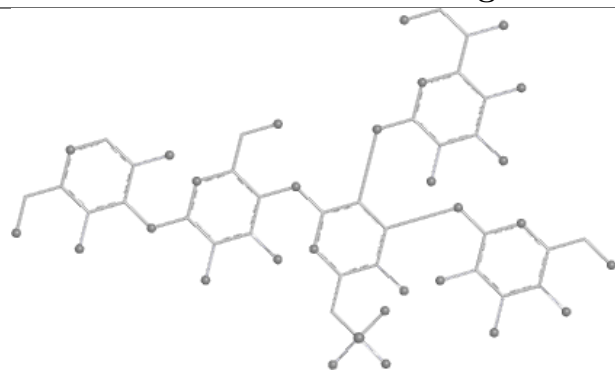
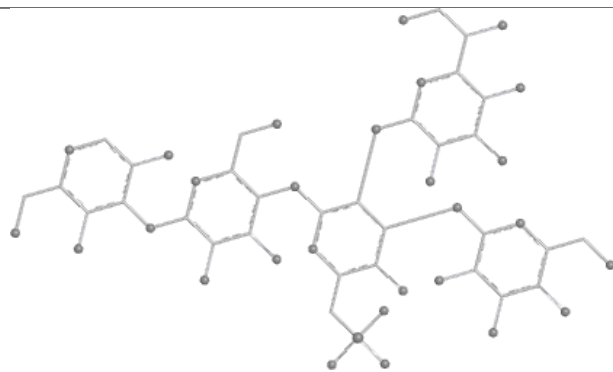
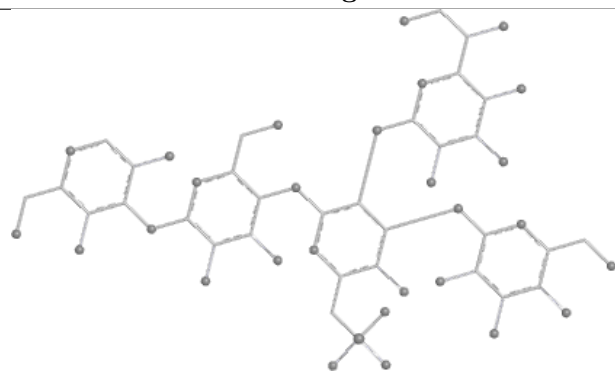
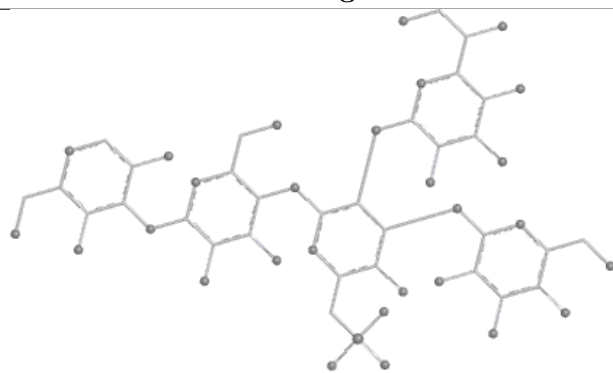


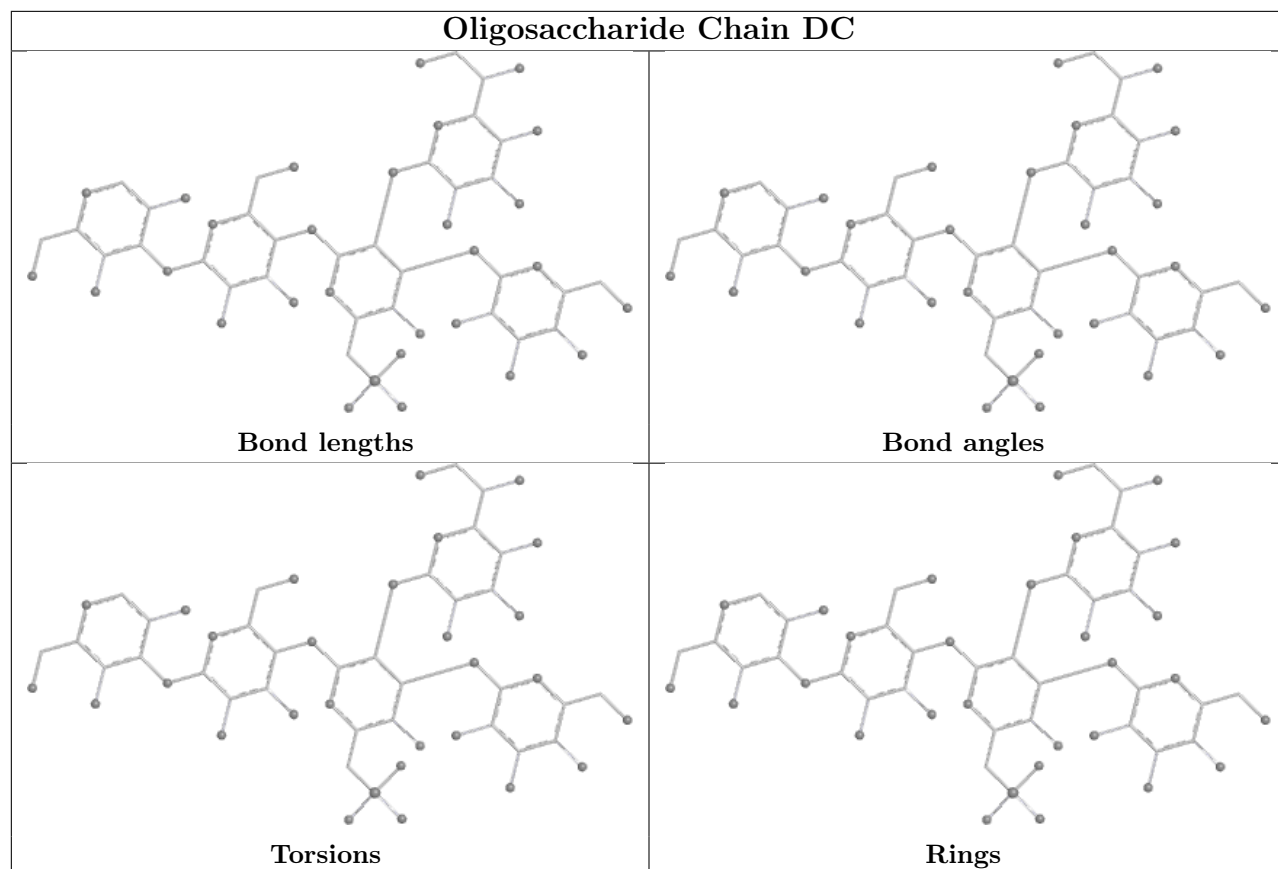
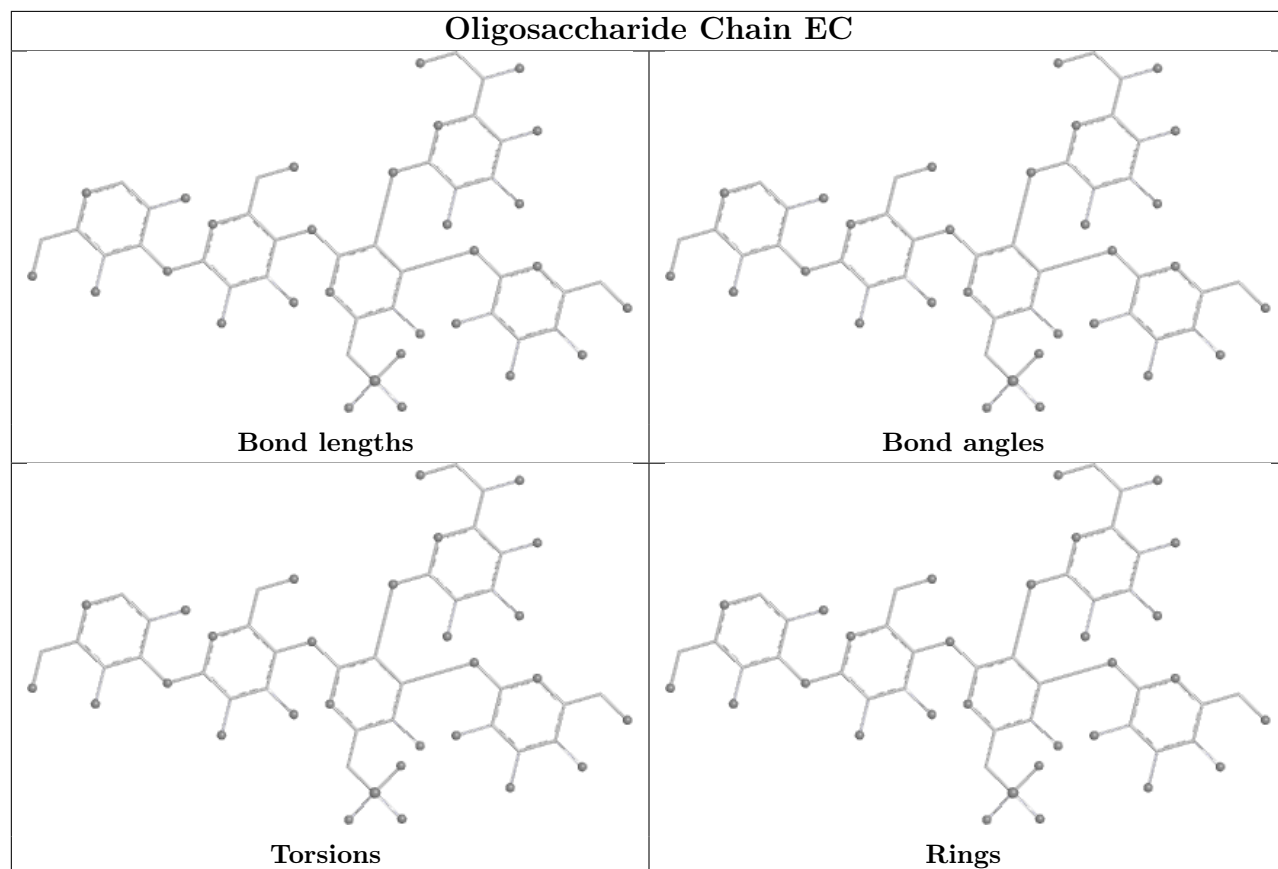
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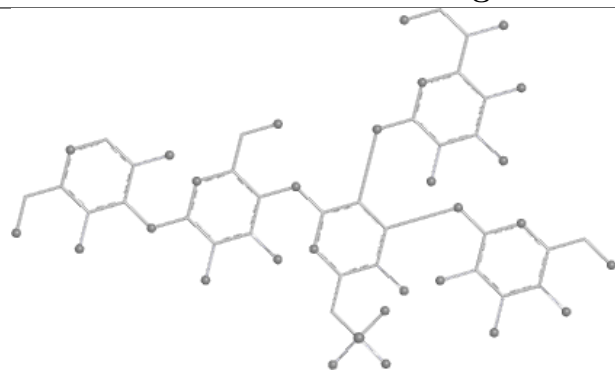
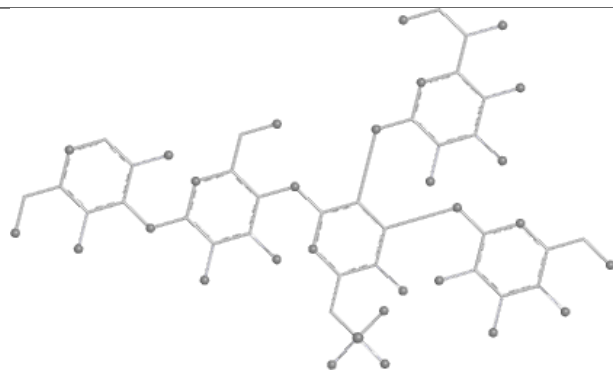
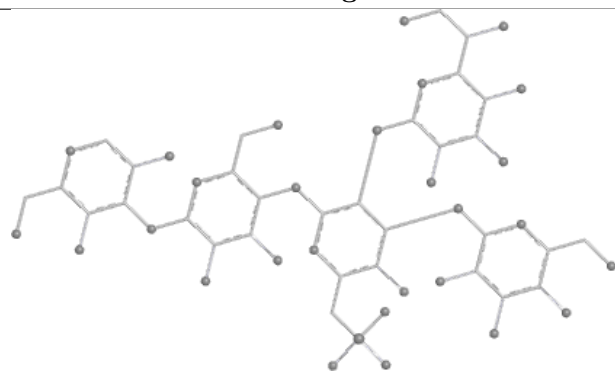
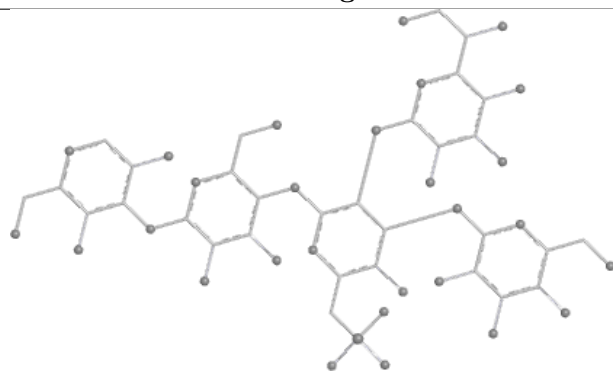
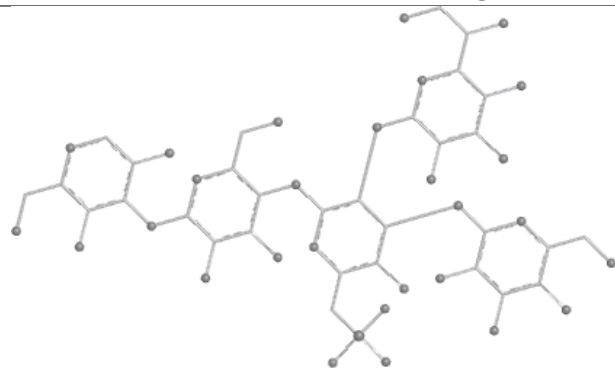
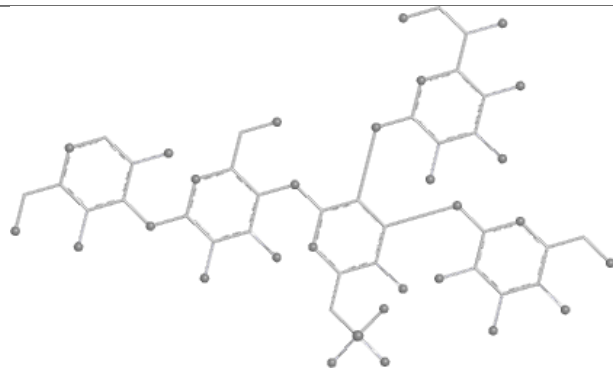
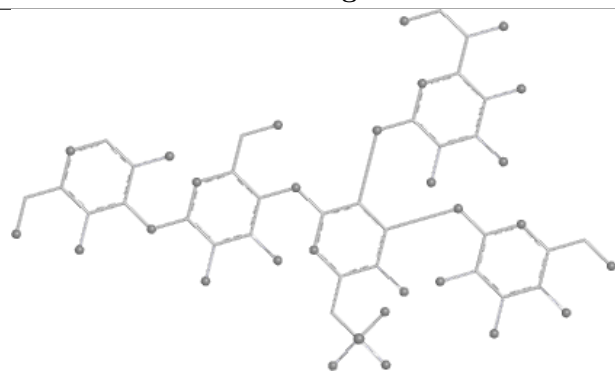
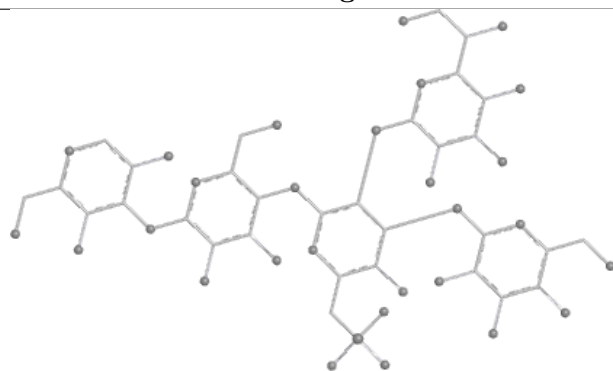
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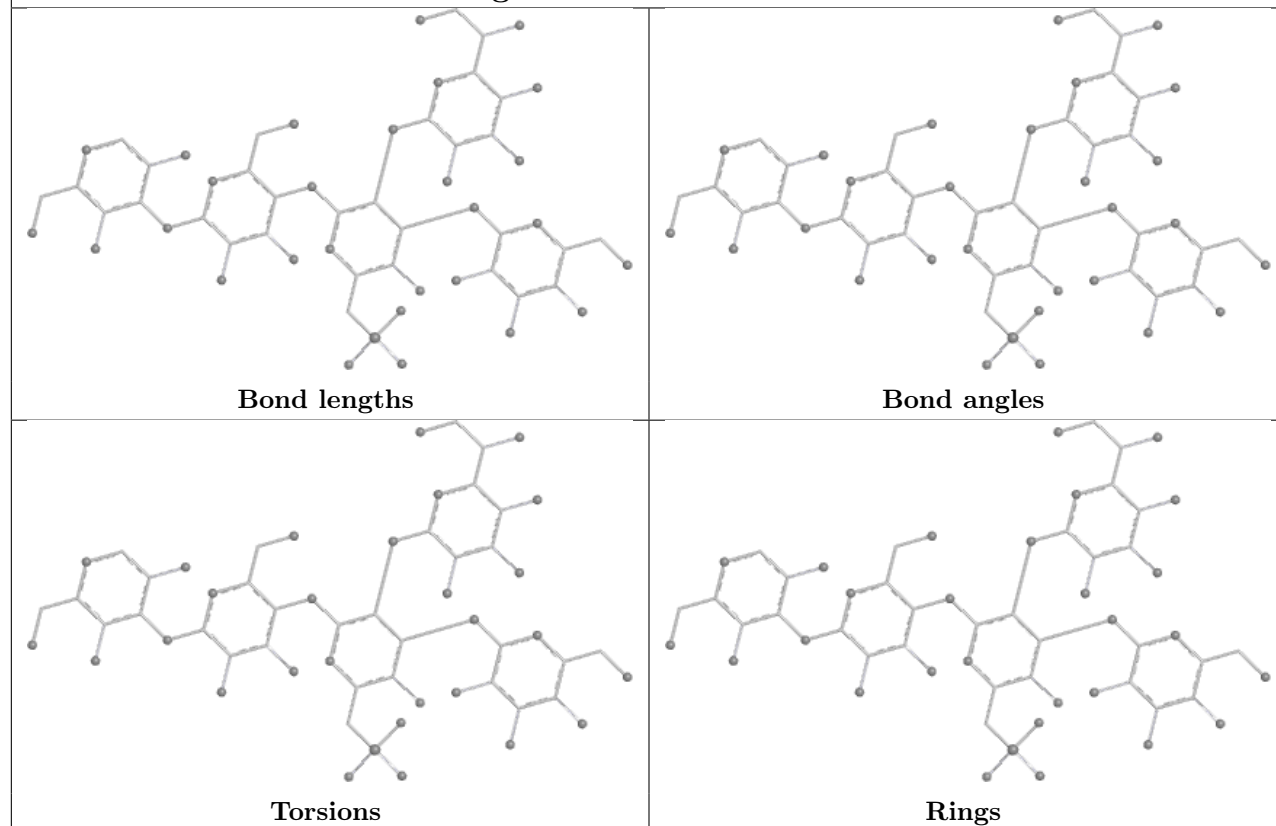
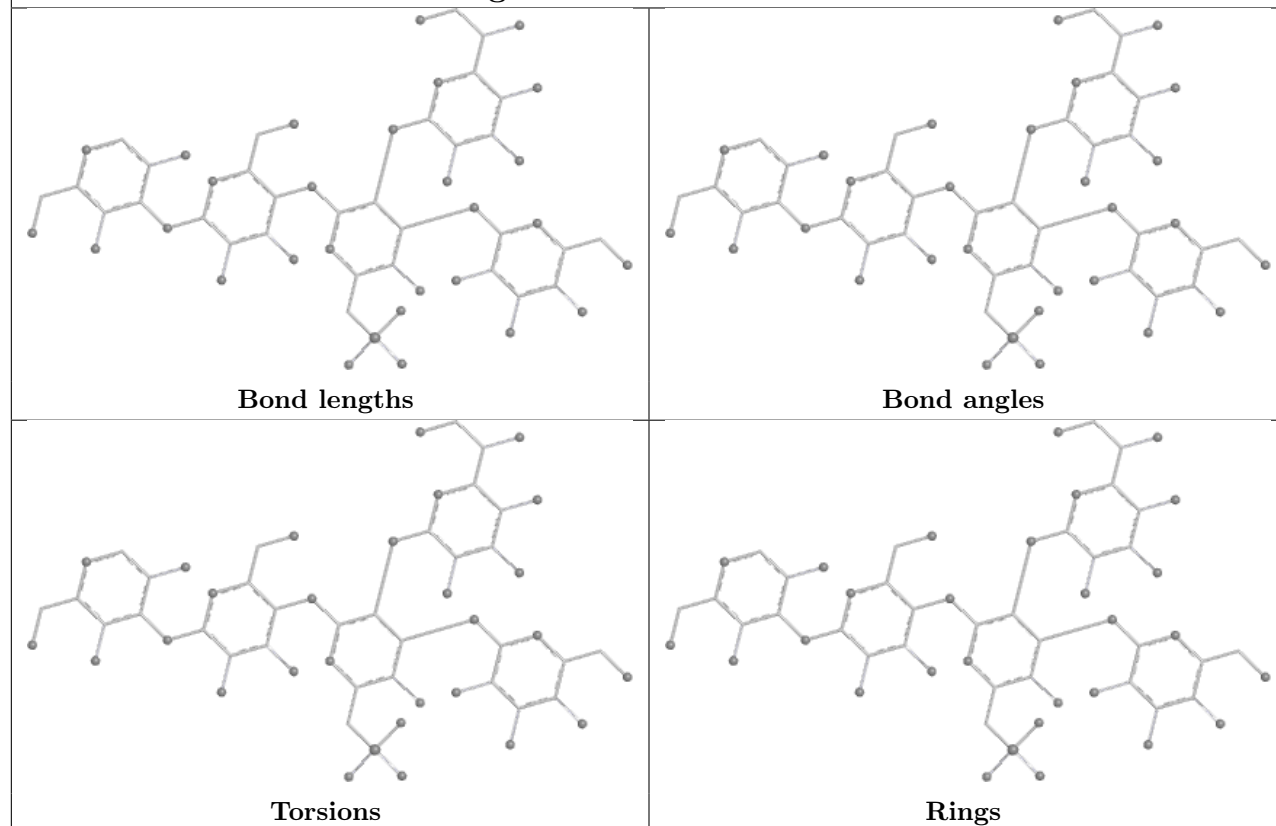
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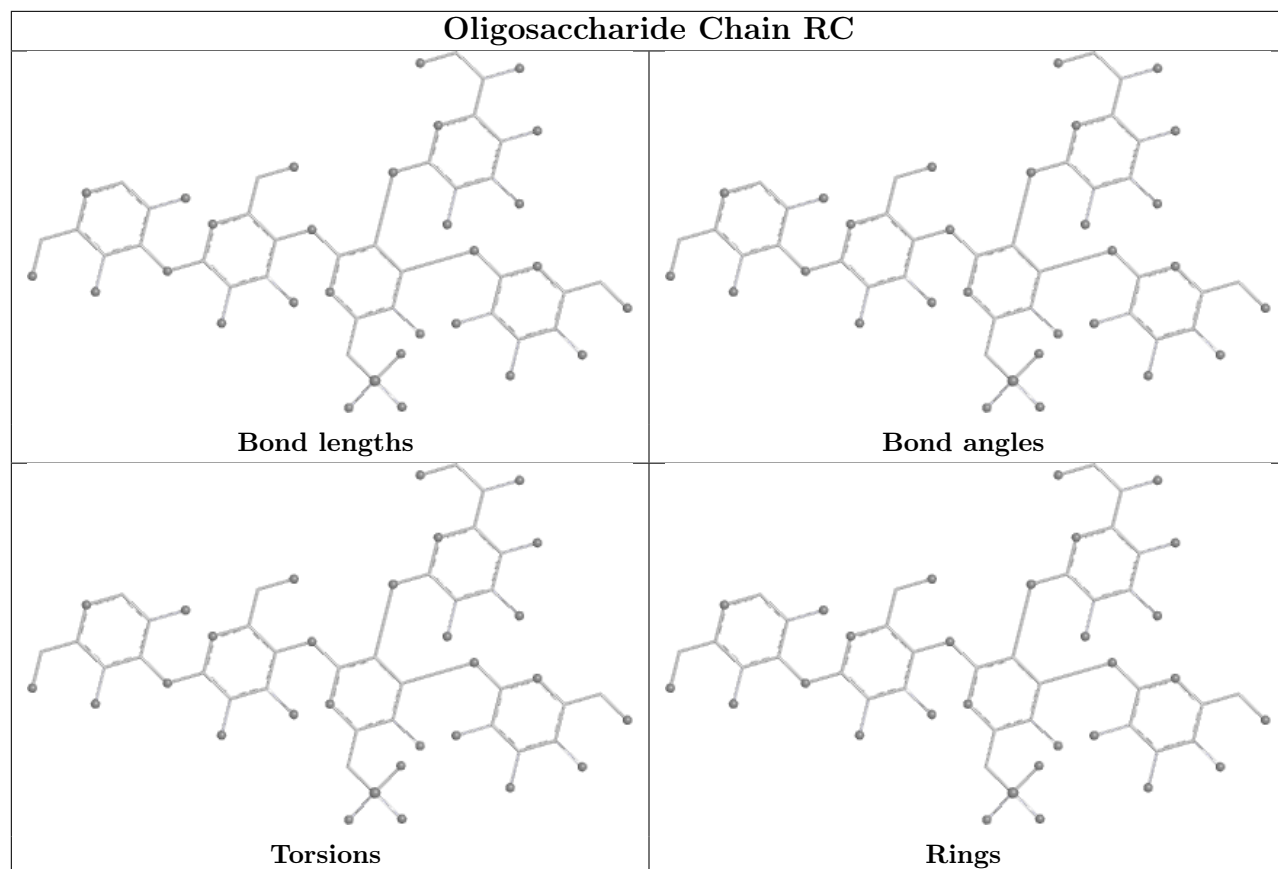
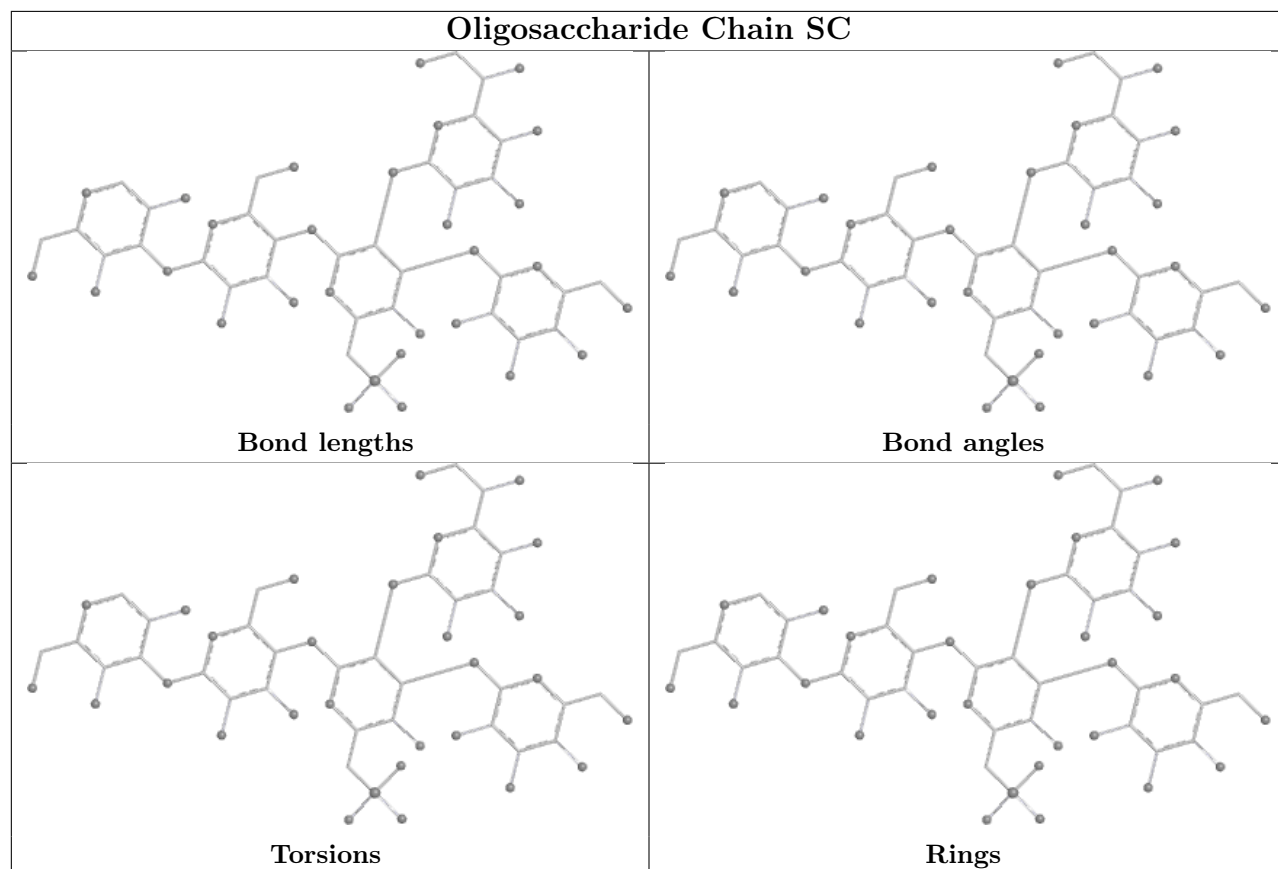
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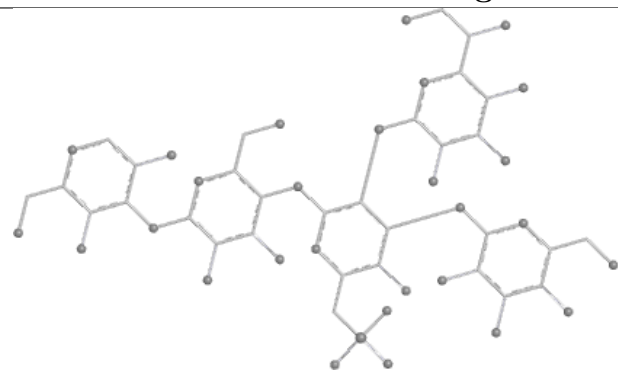
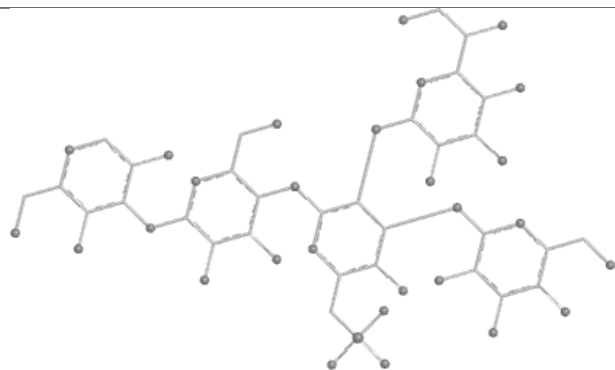
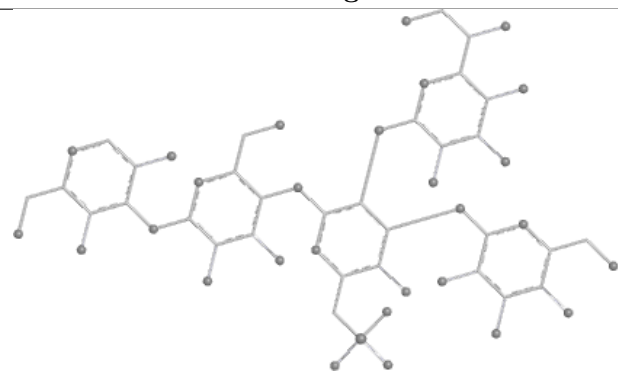
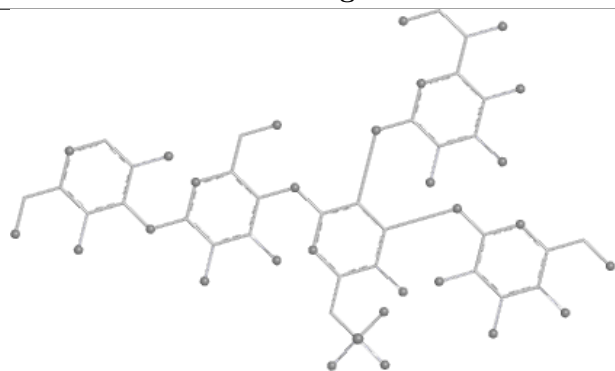
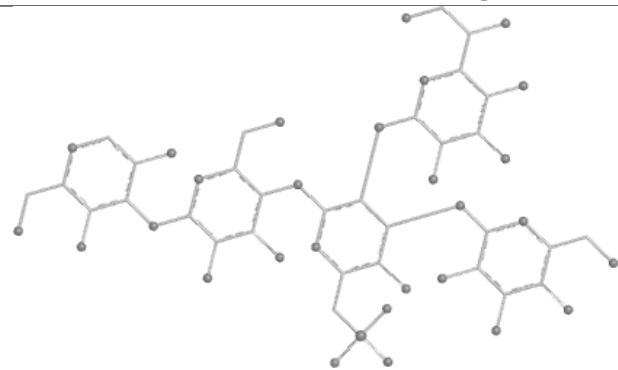
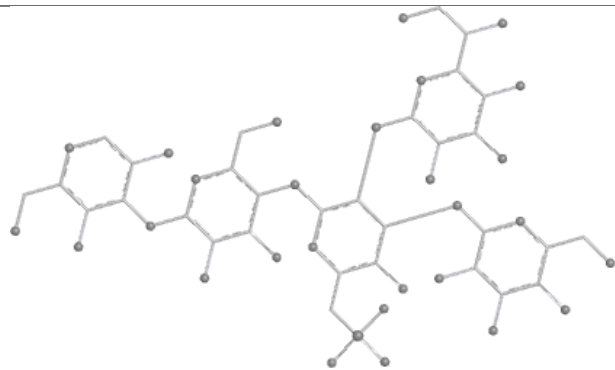
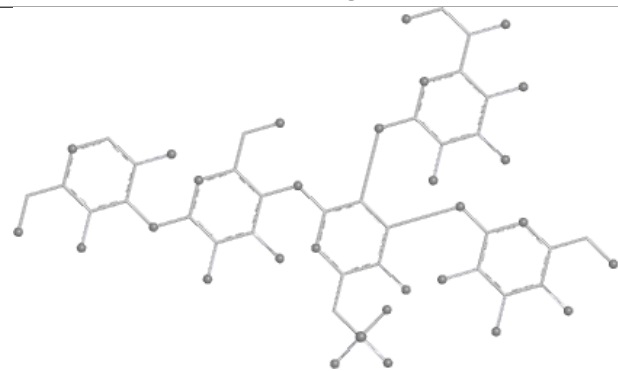
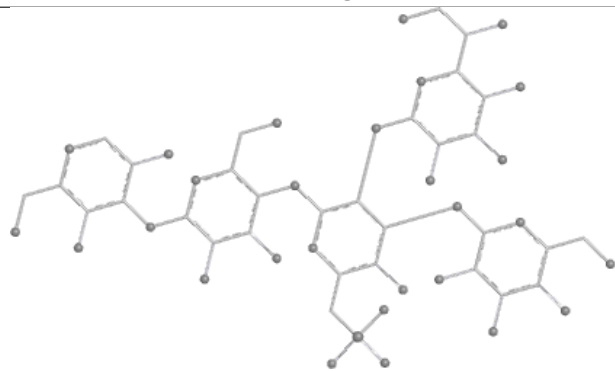
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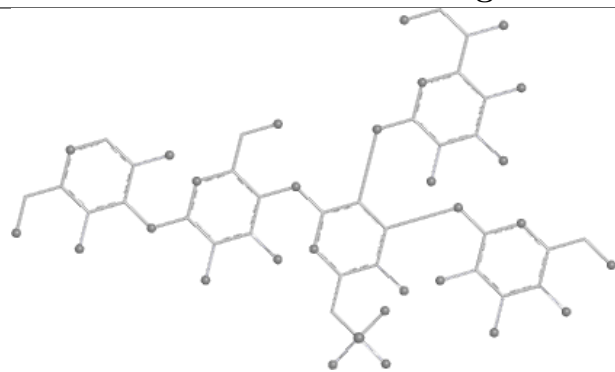
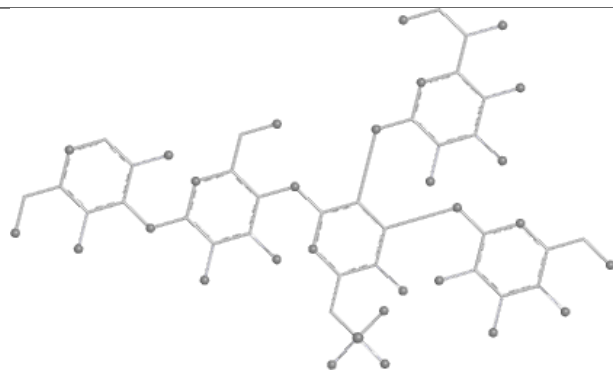
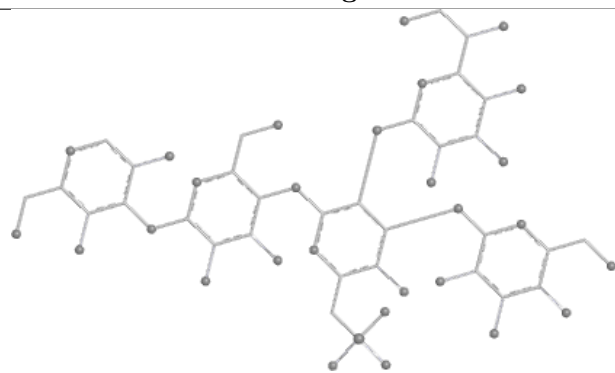
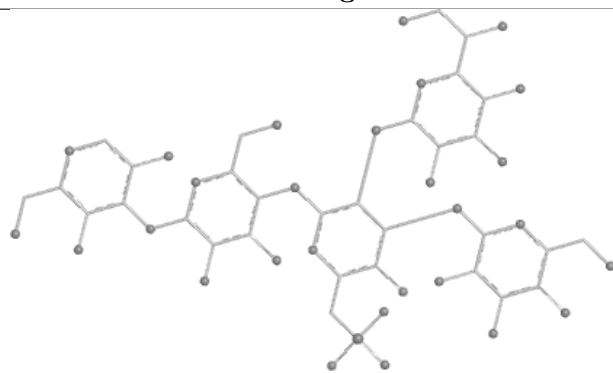
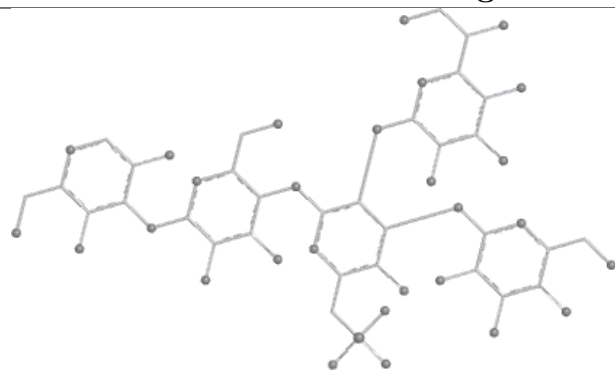
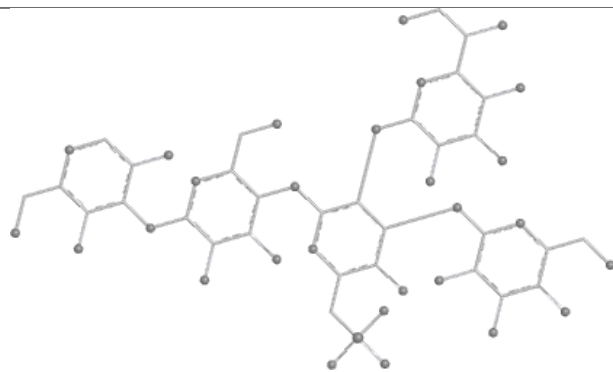
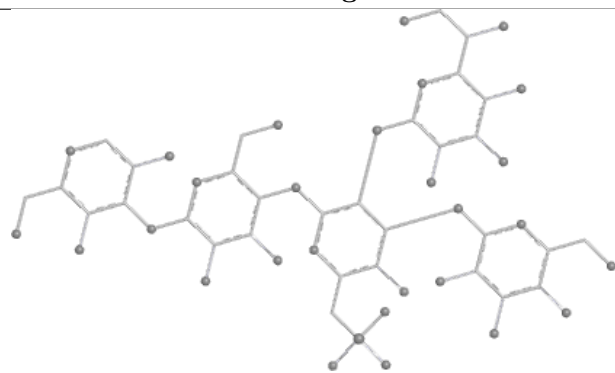
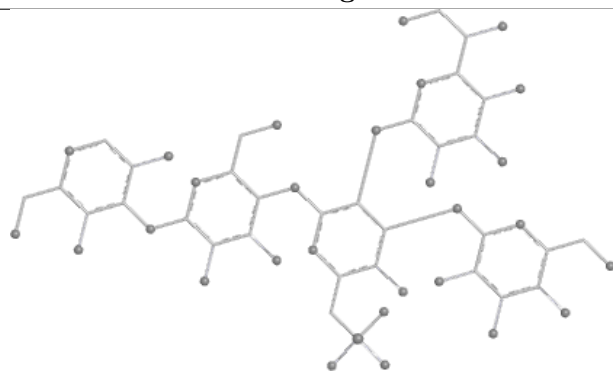
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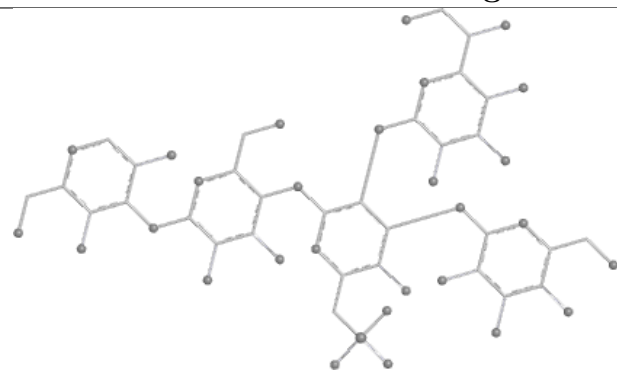
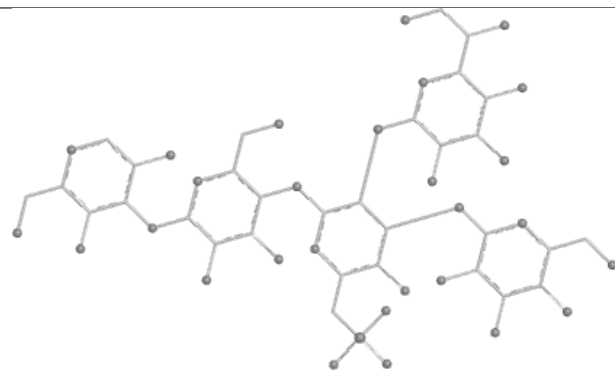
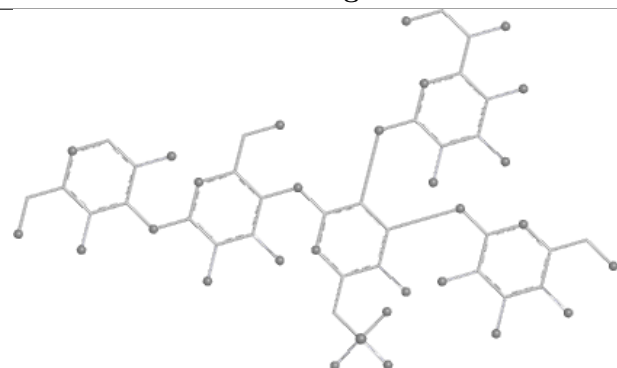
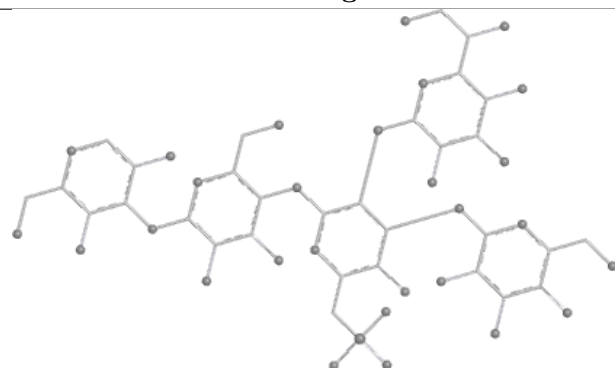
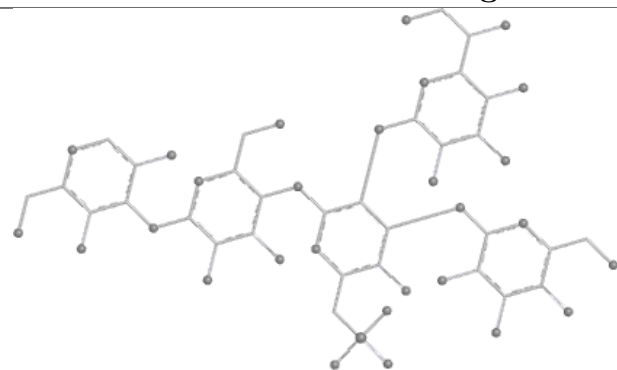
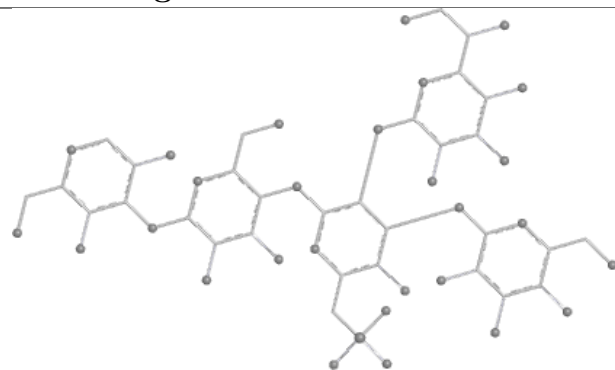
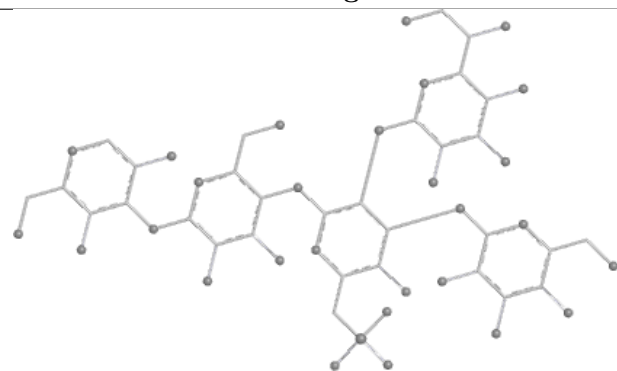
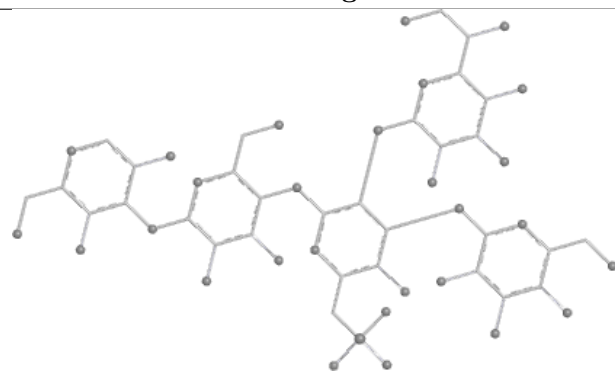
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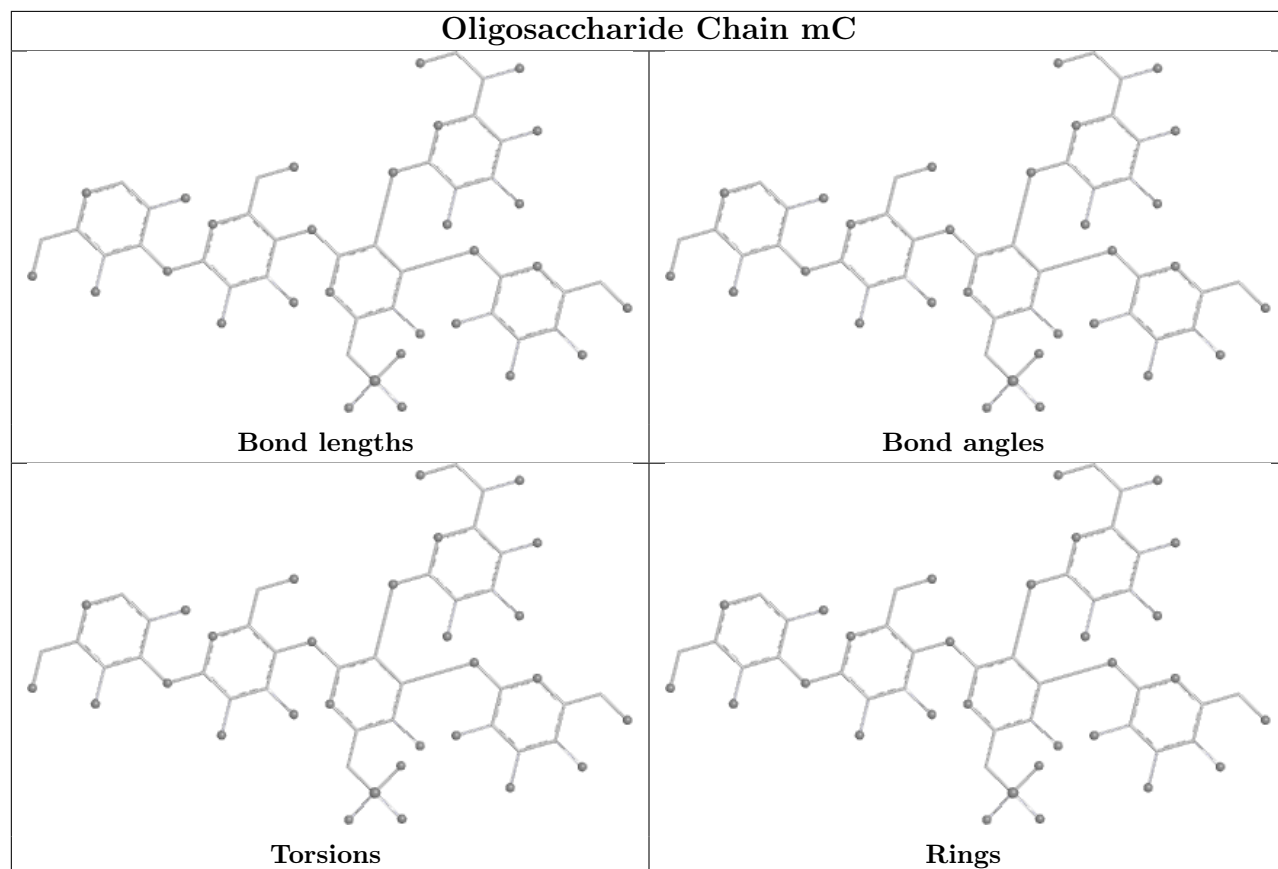
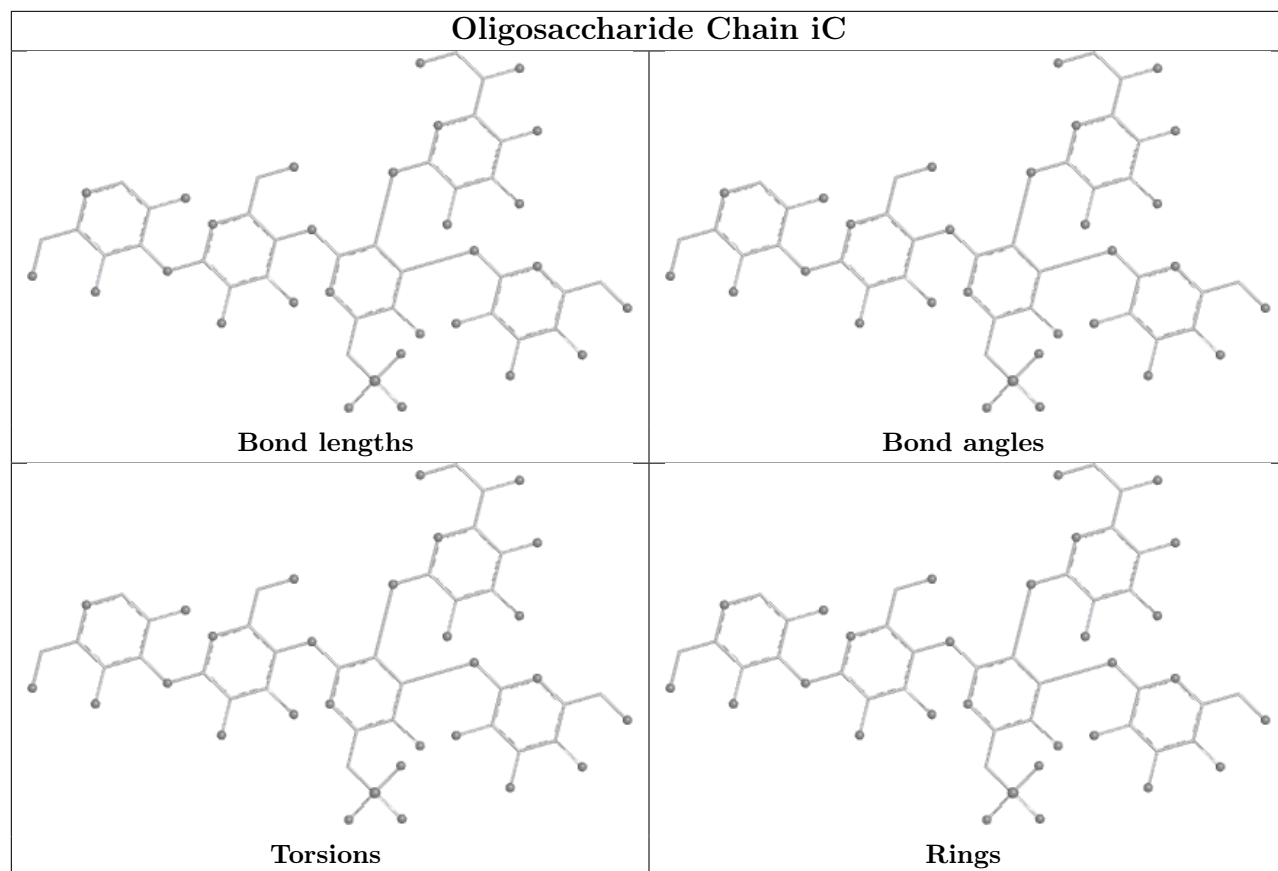
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Oligosaccharide Chain RC**Oligosaccharide Chain SC**

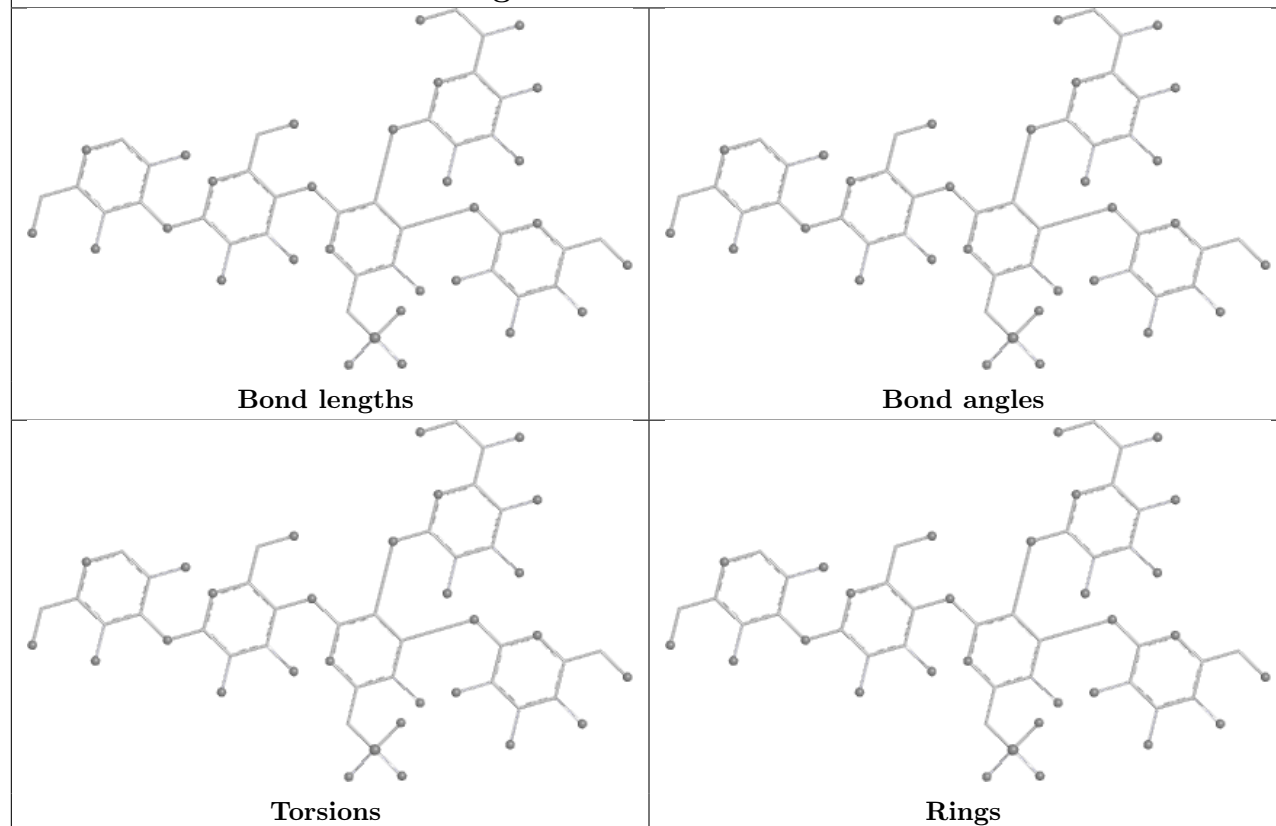
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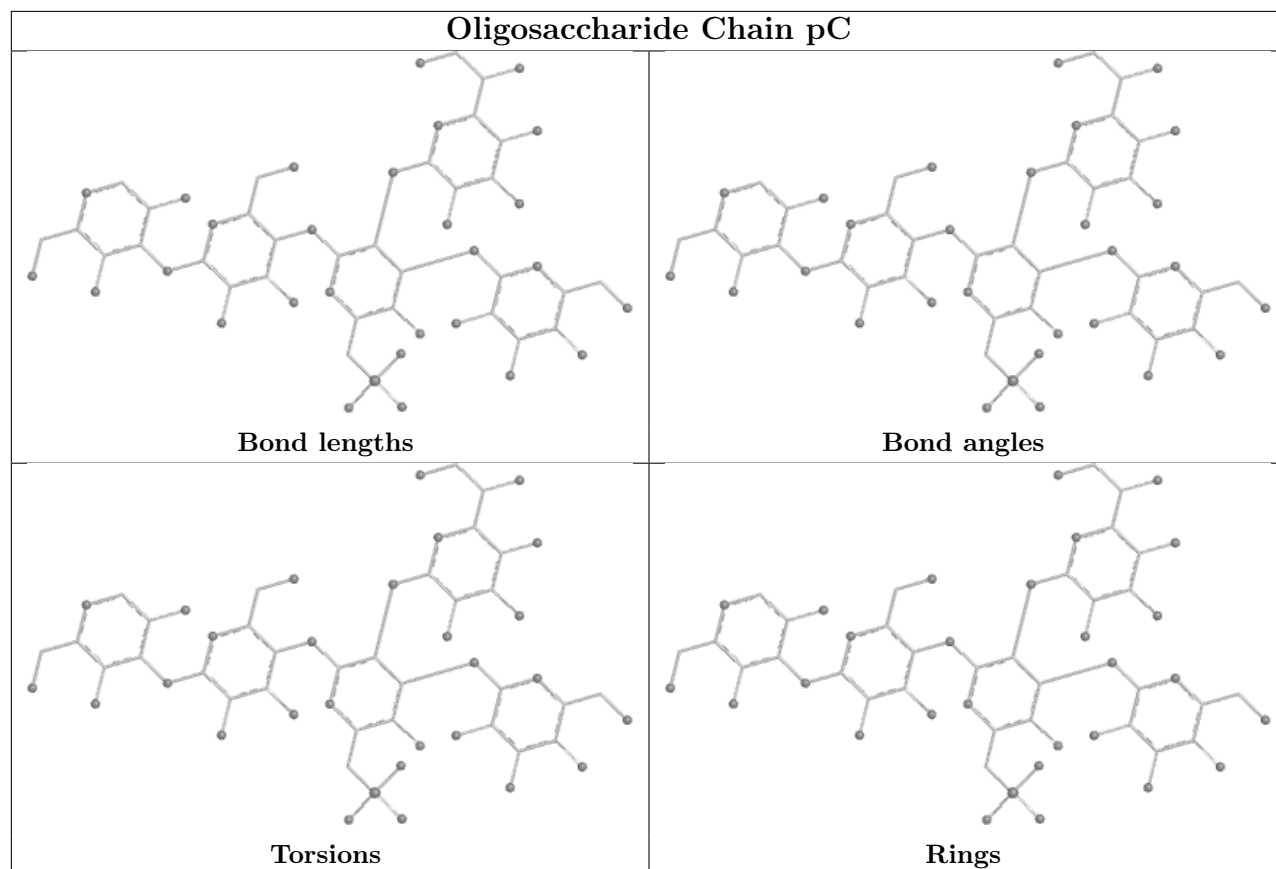
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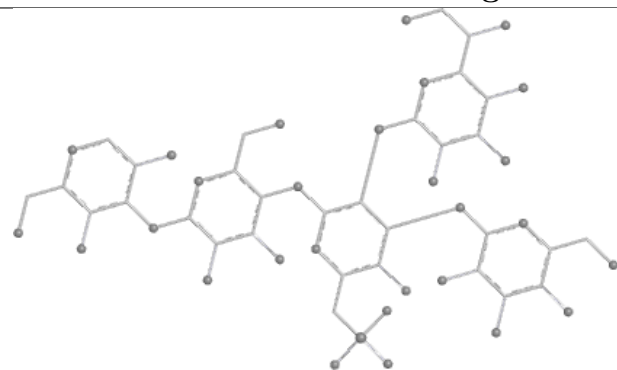
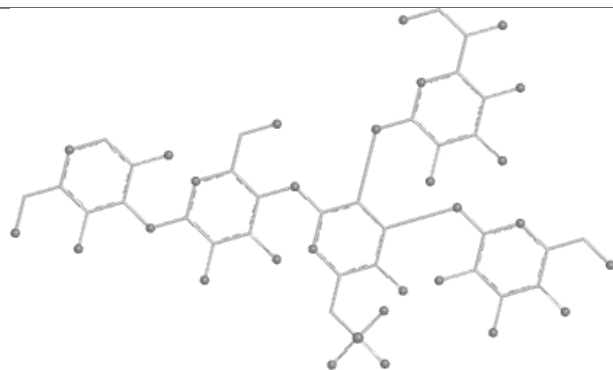
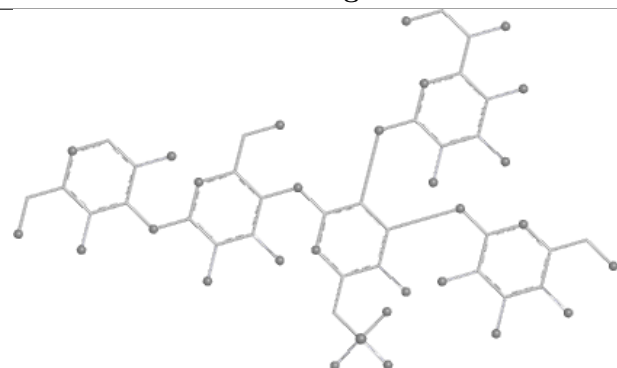
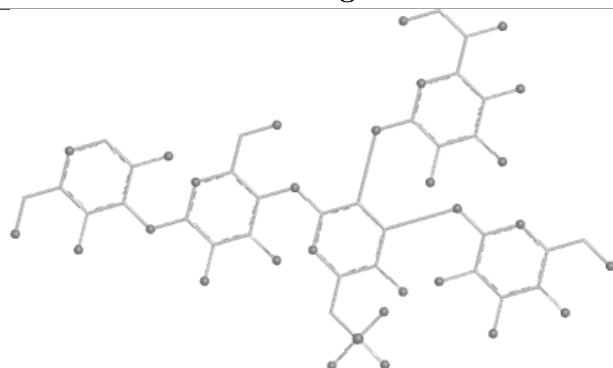
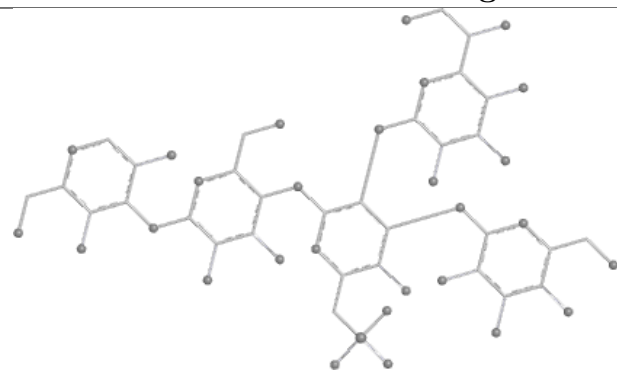
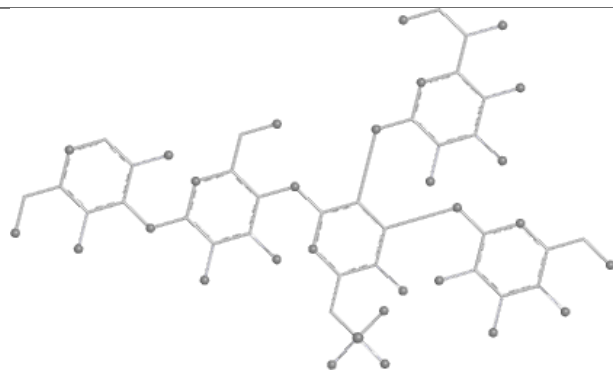
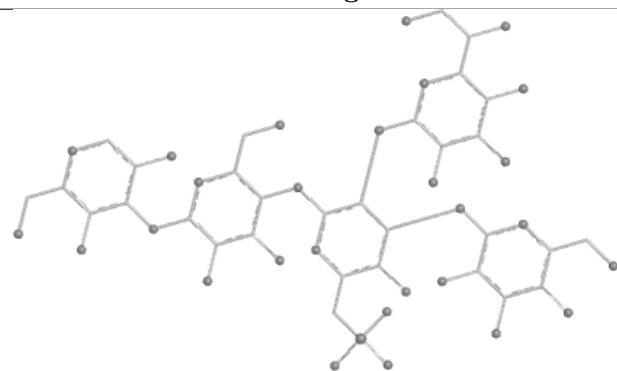
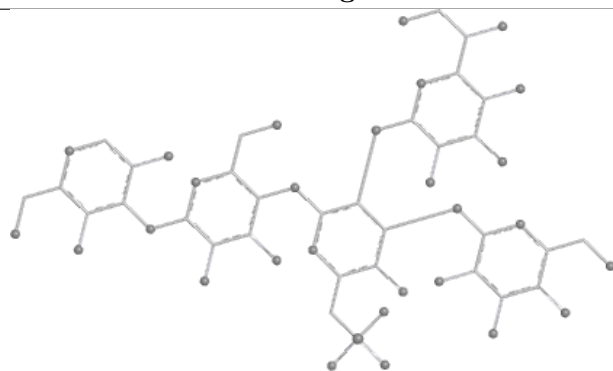


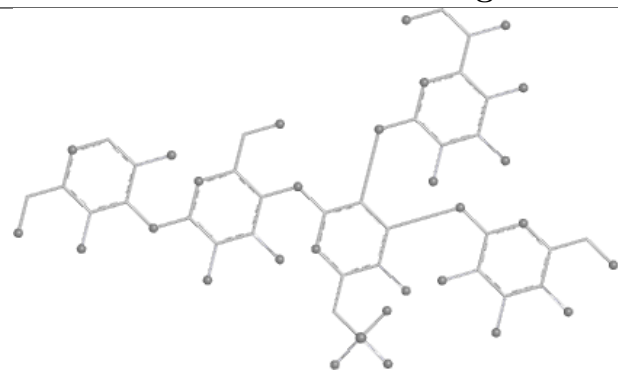
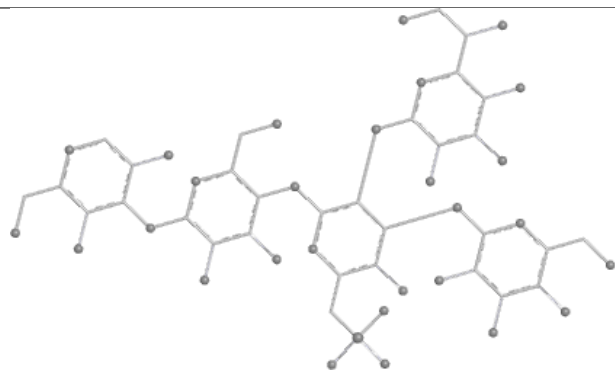
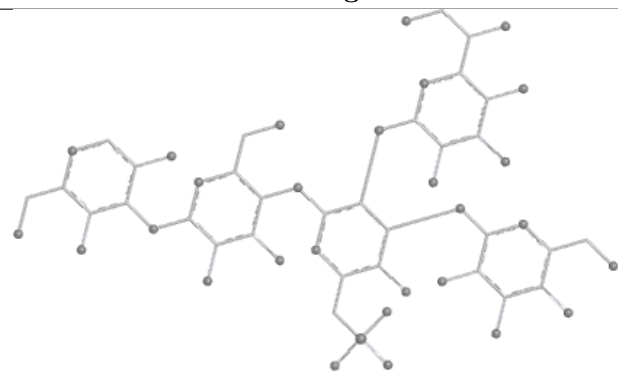
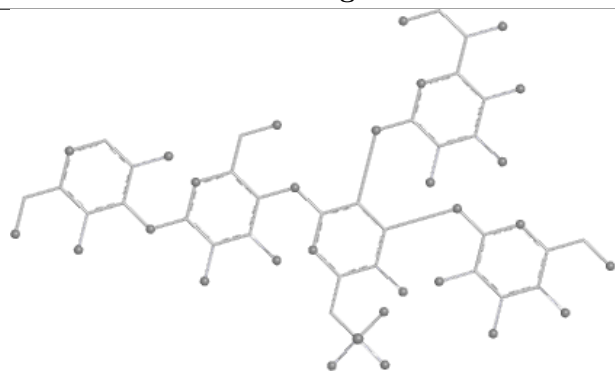
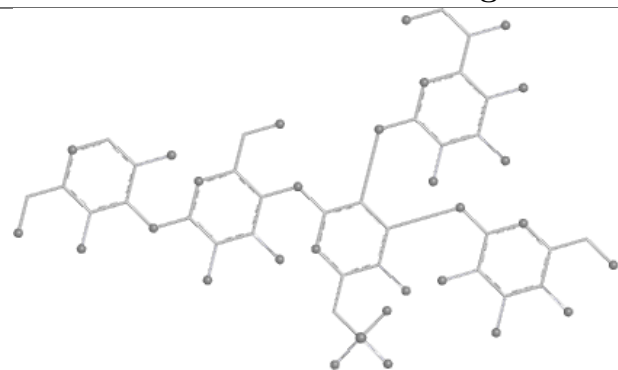
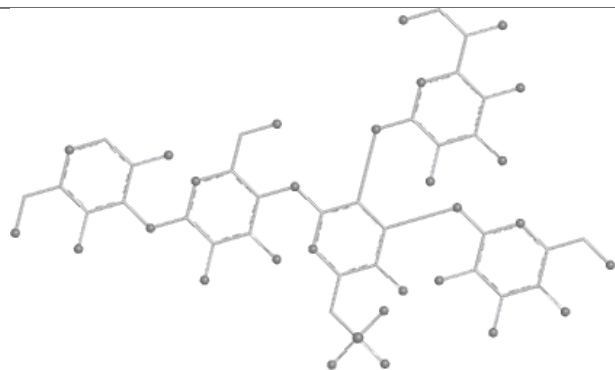
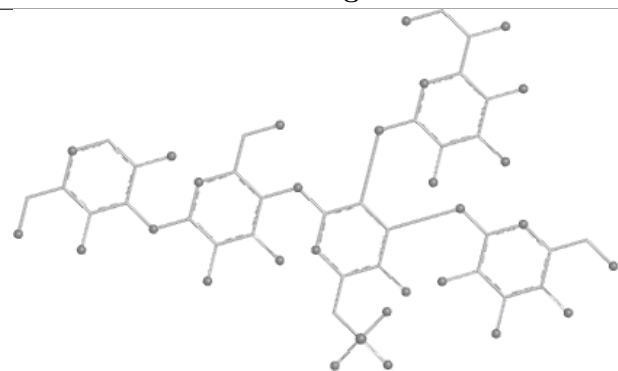
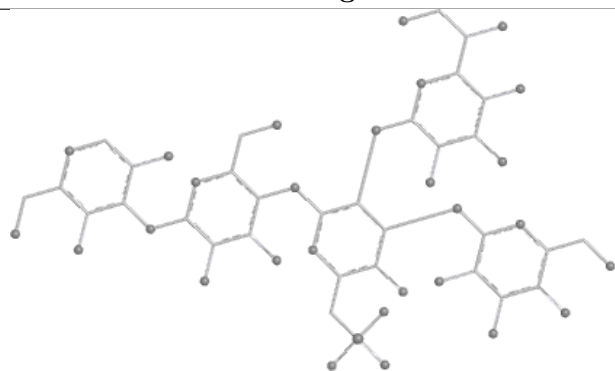
Oligosaccharide Chain nC

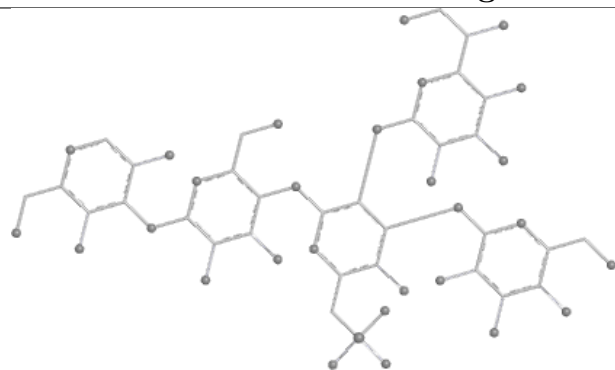
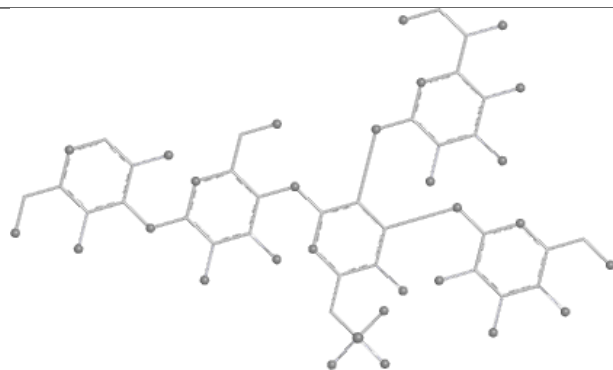
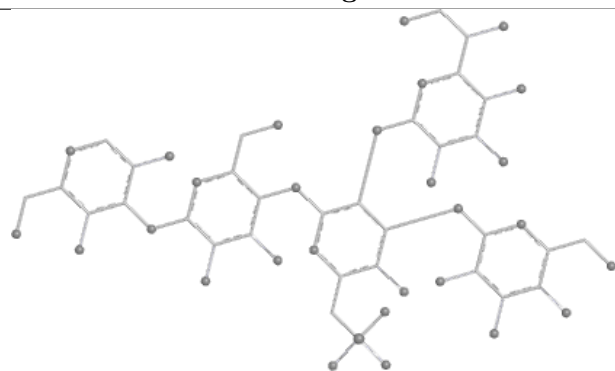
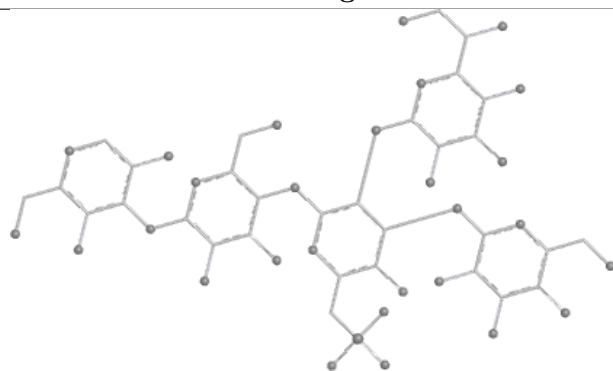
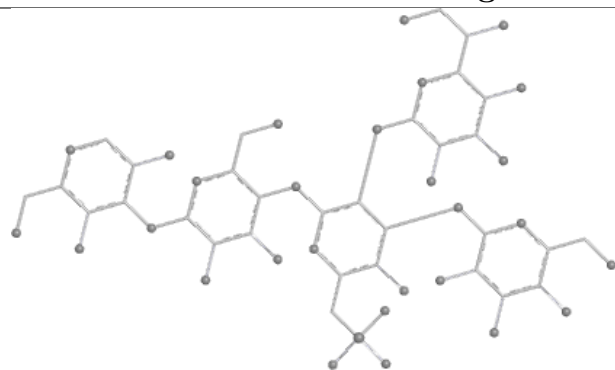
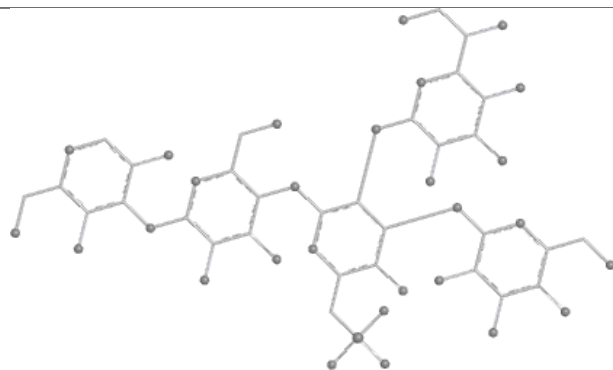
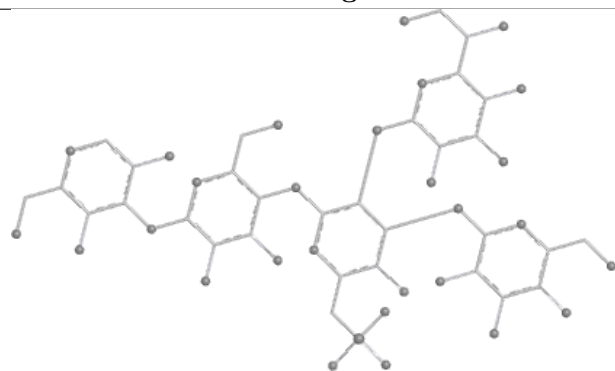
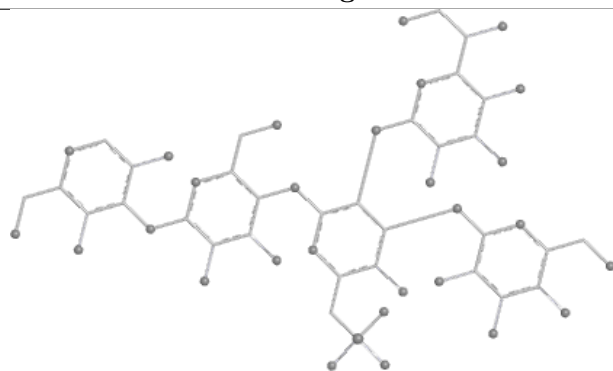


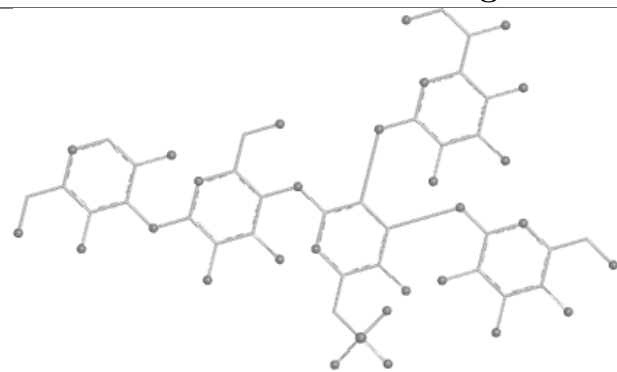
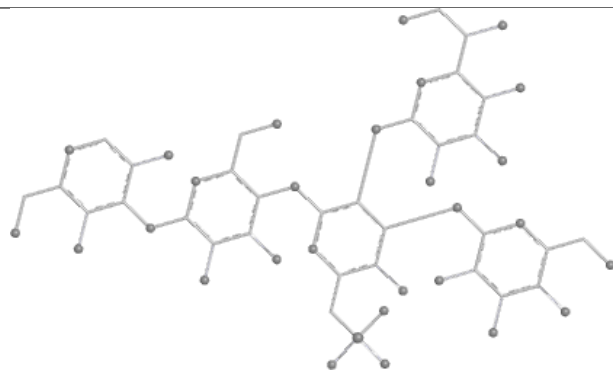
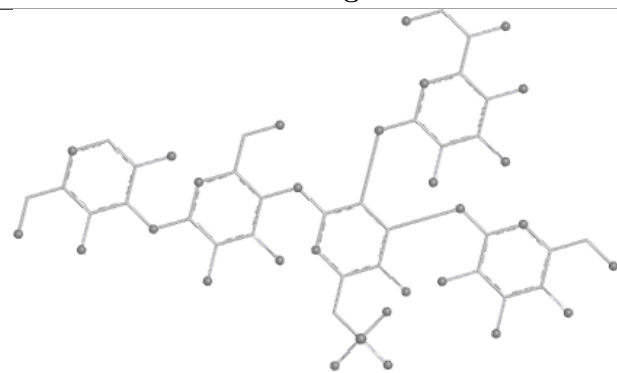
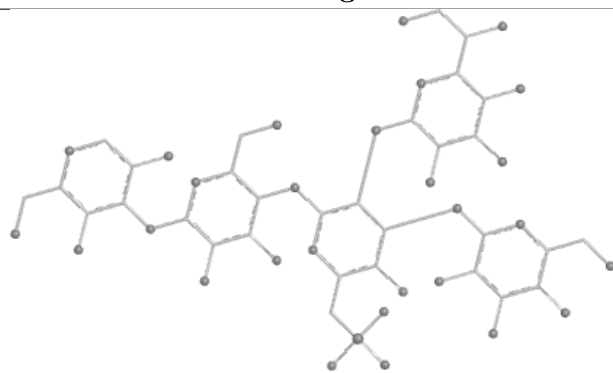
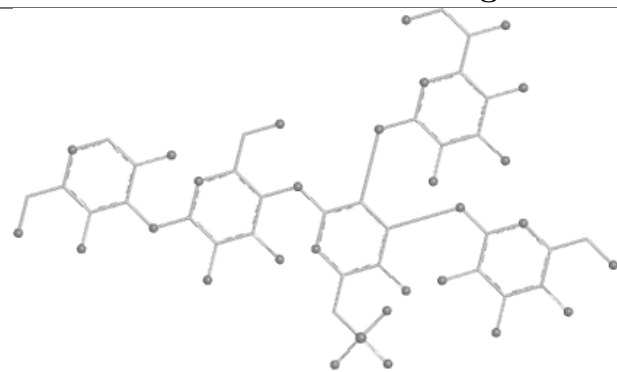
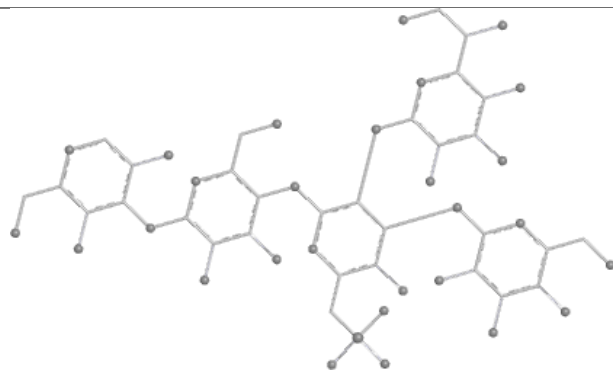
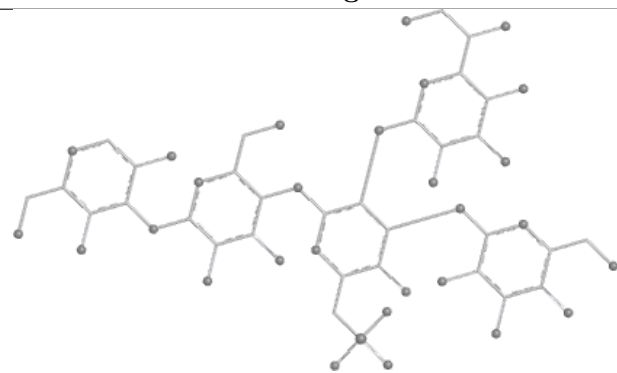
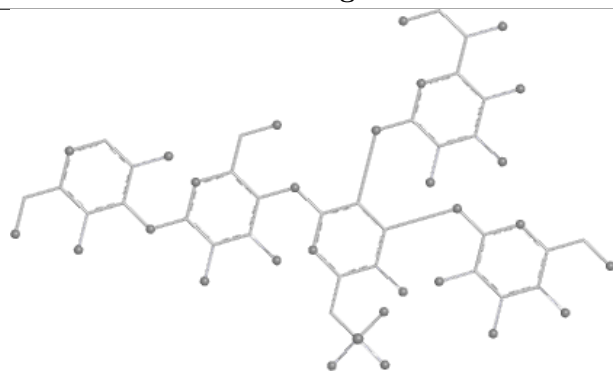
Oligosaccharide Chain pC

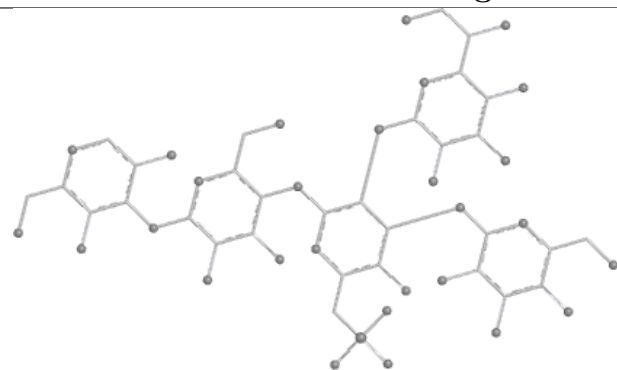
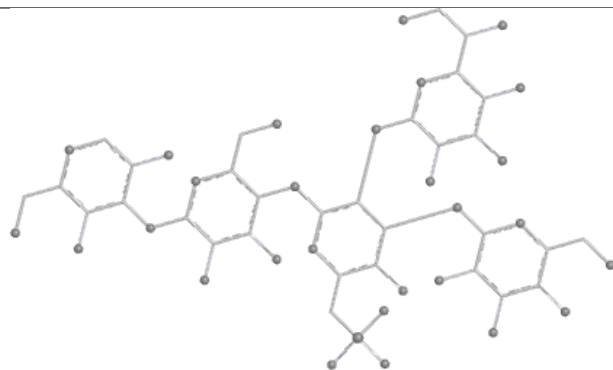
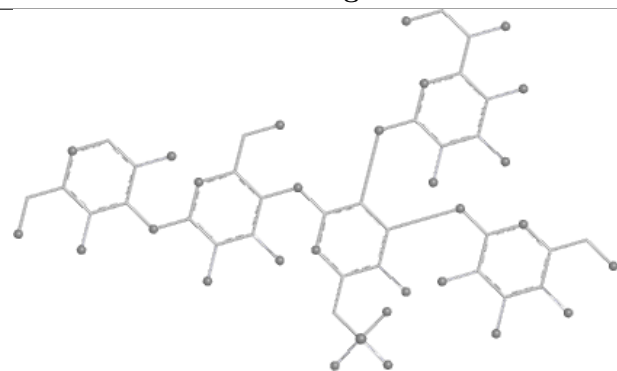
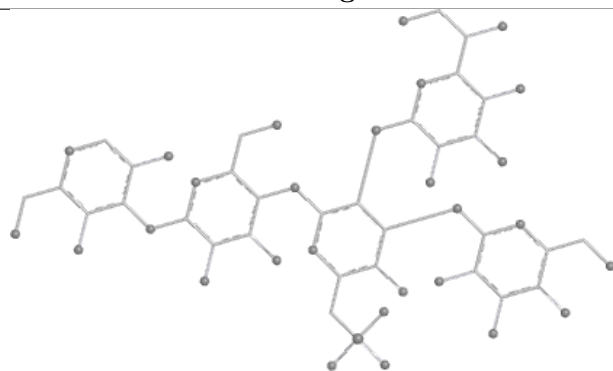
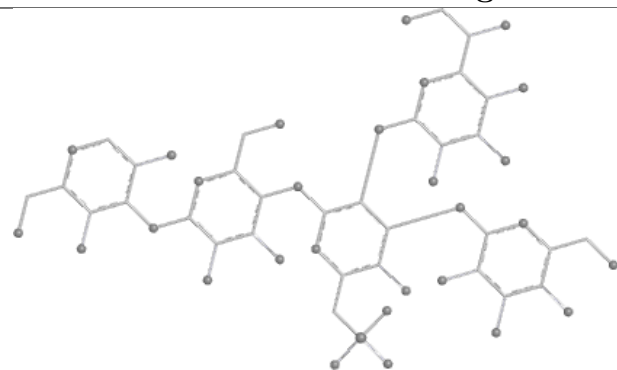
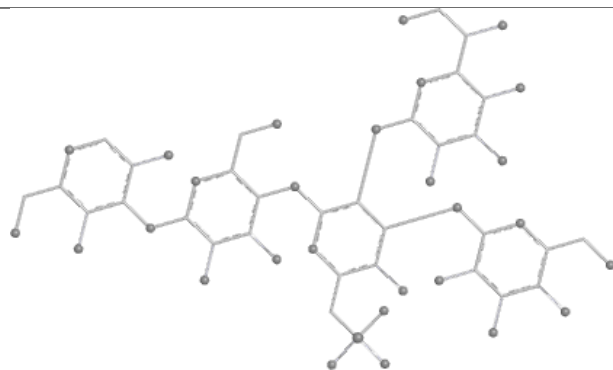
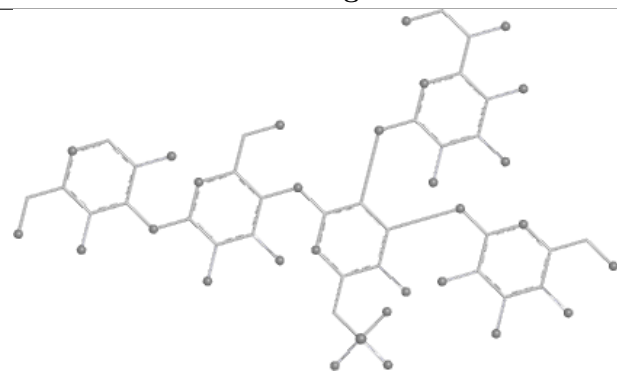
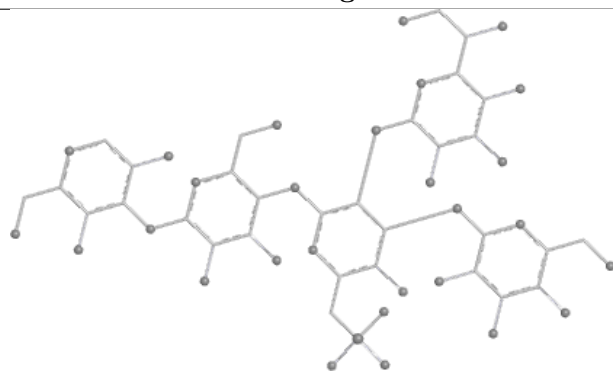


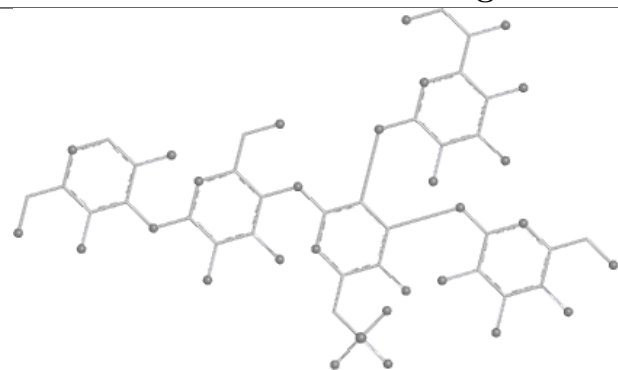
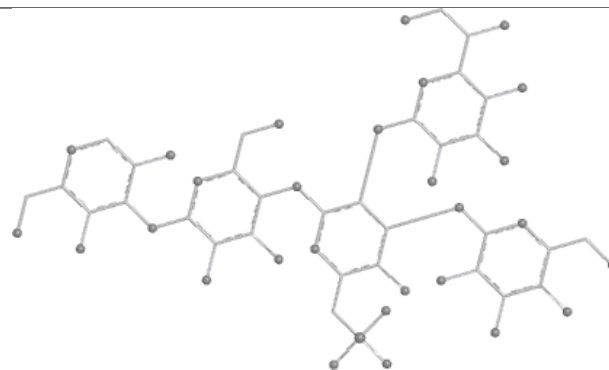
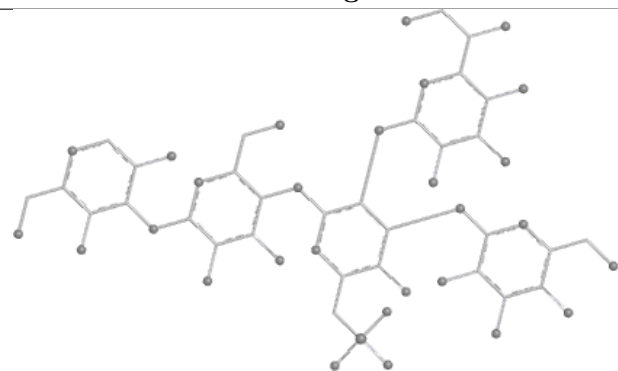
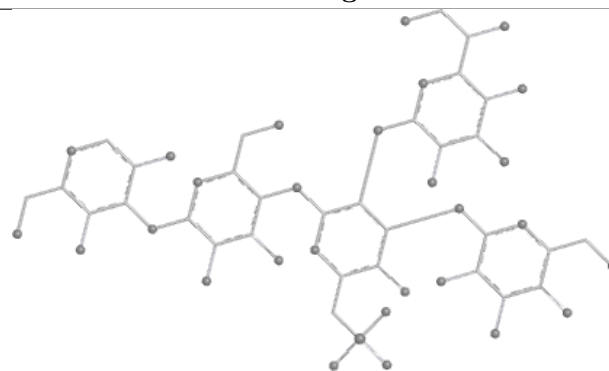
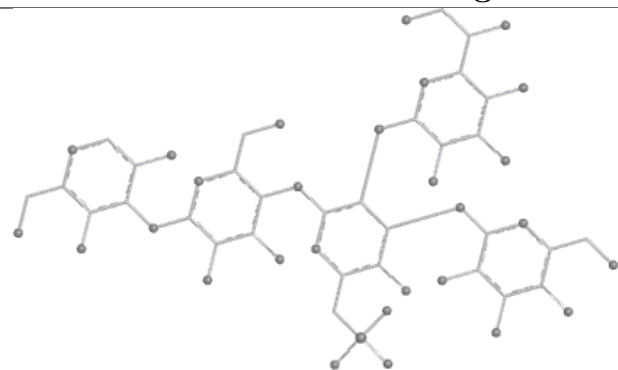
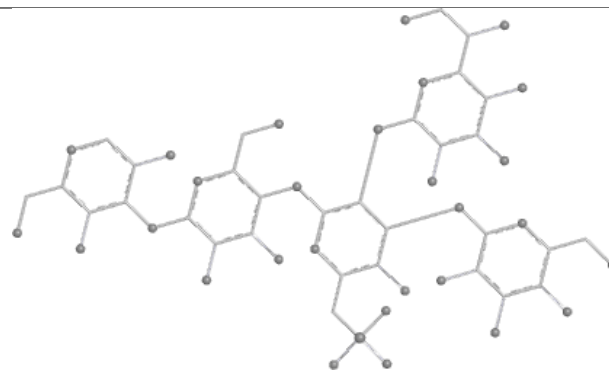
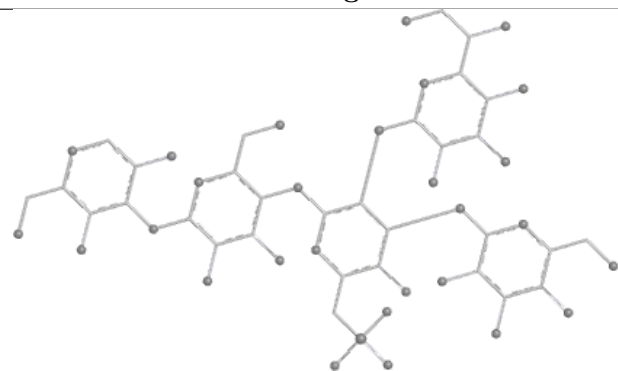
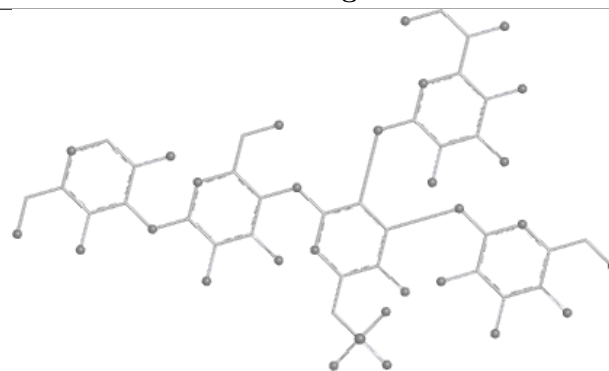
Oligosaccharide Chain tC**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain uC****Bond lengths****Bond angles****Torsions****Rings**

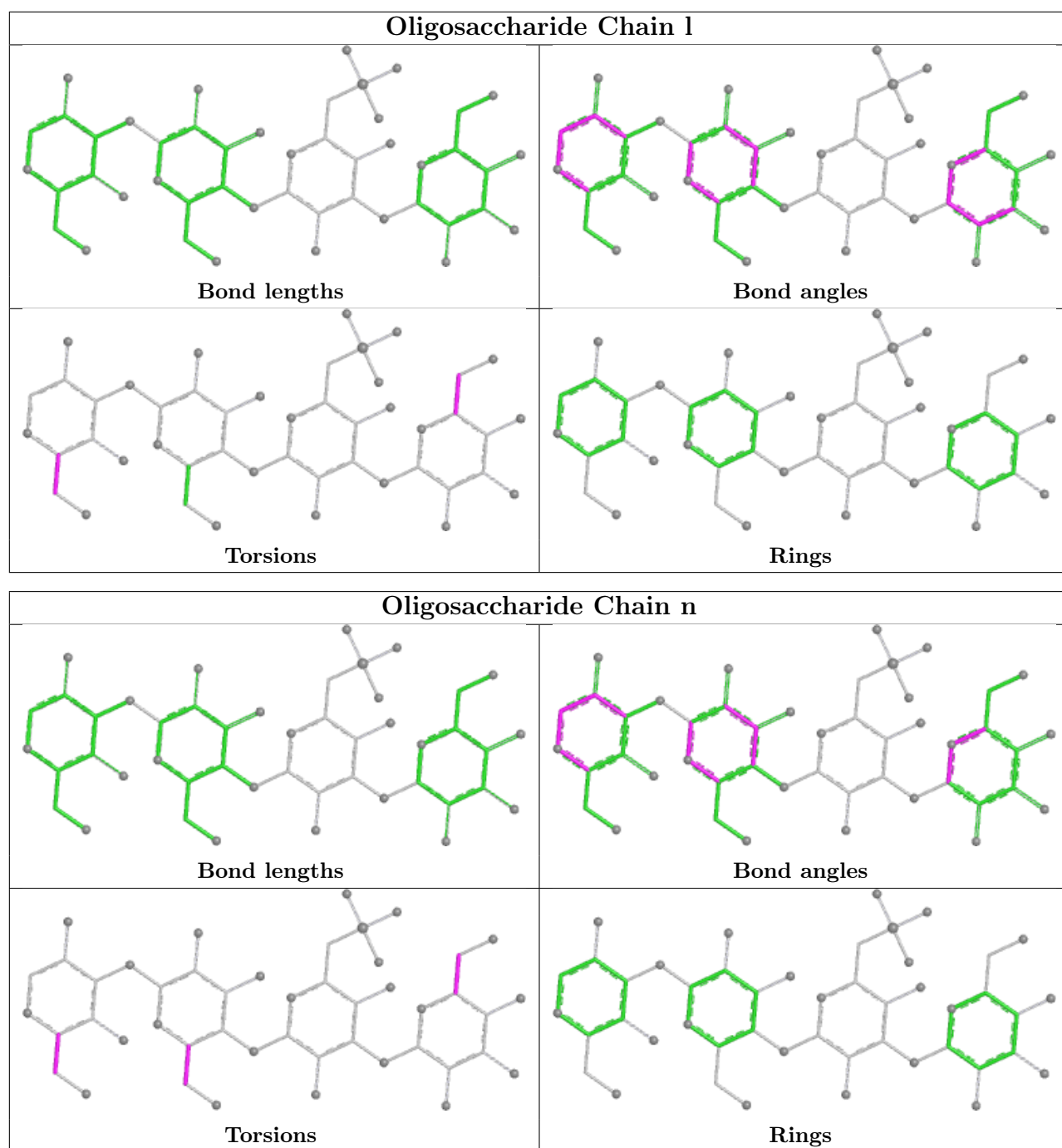
Oligosaccharide Chain wC**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain 0C****Bond lengths****Bond angles****Torsions****Rings**

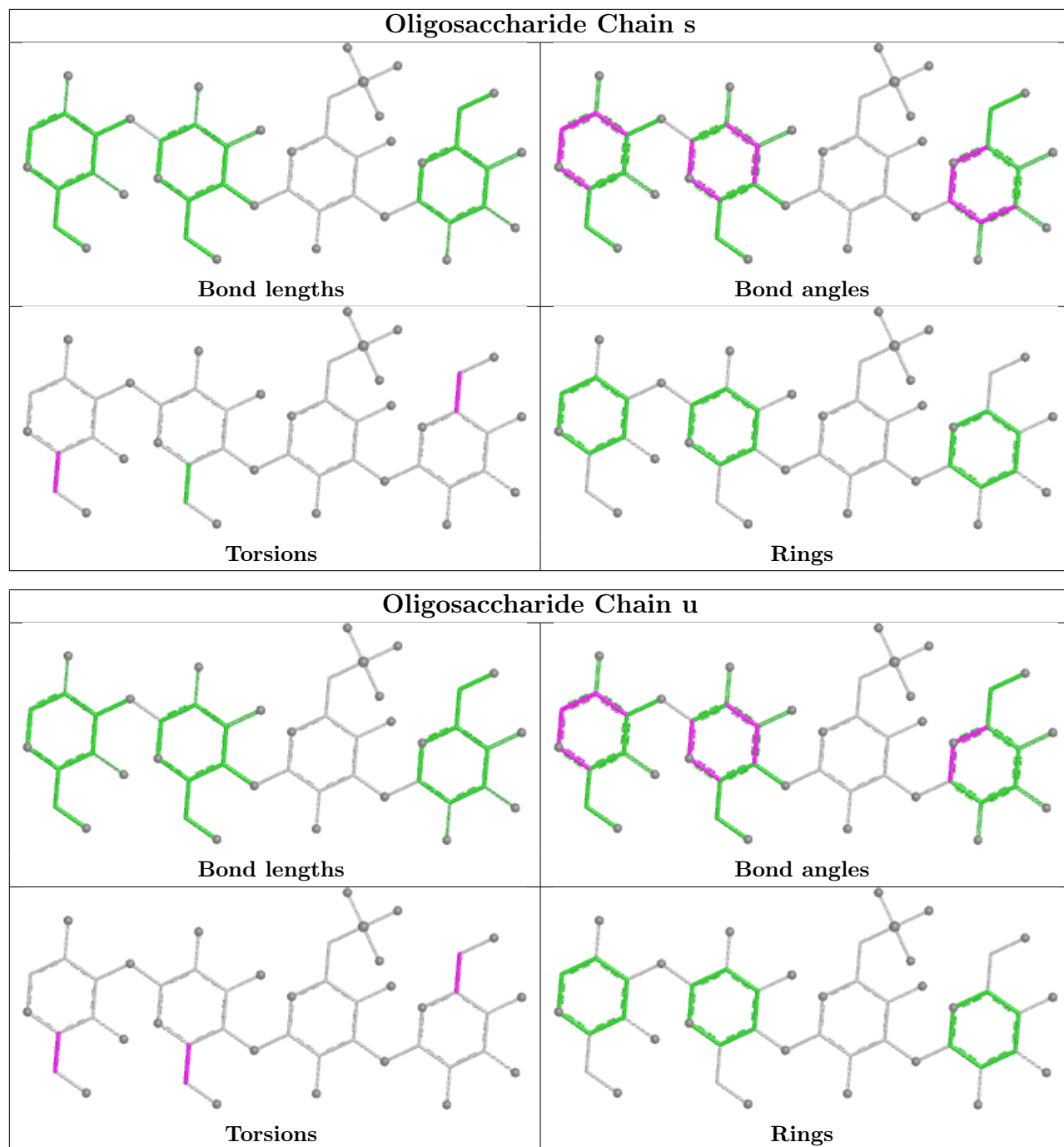
Oligosaccharide Chain 1C**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain 3C****Bond lengths****Bond angles****Torsions****Rings**

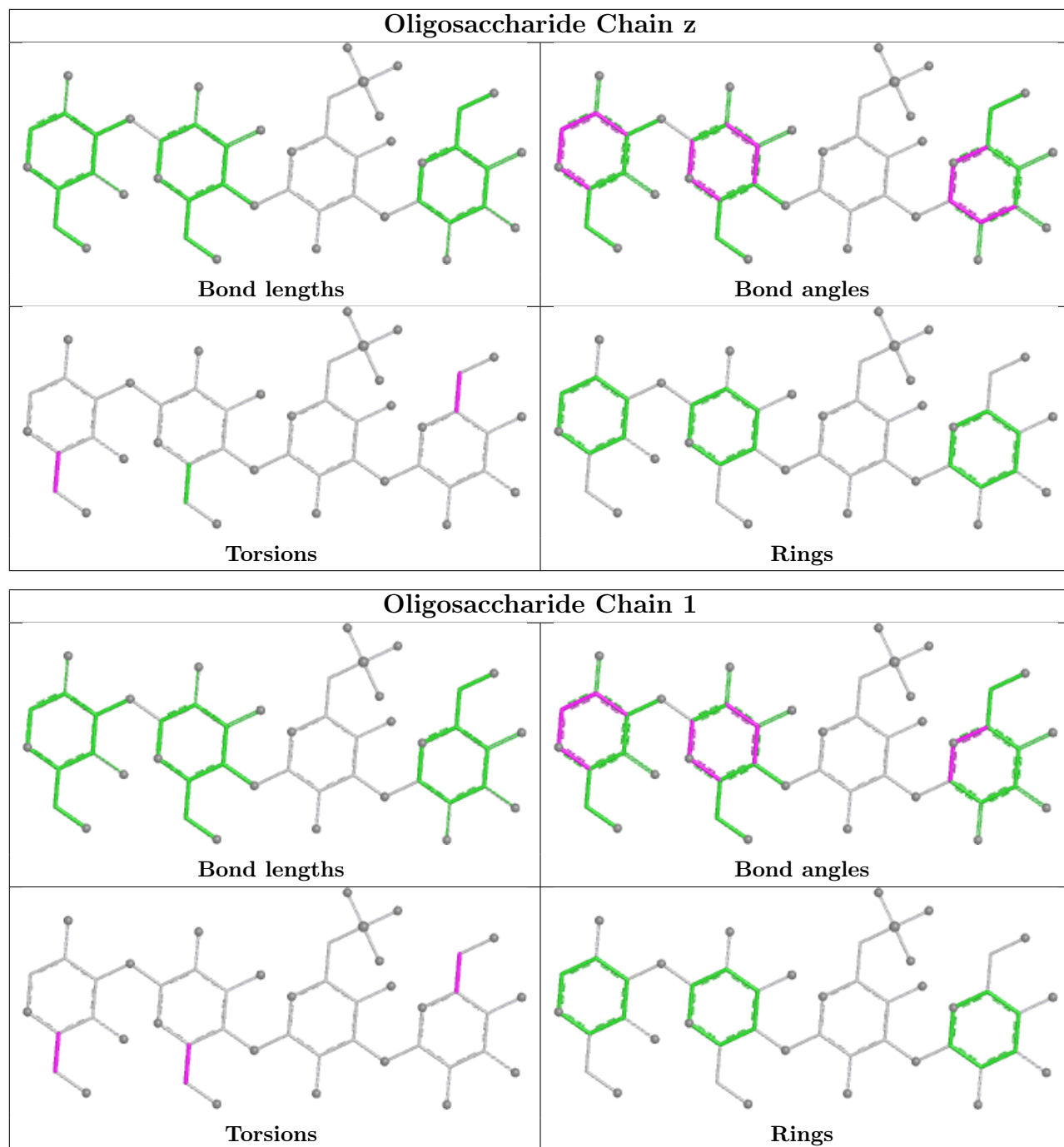
Oligosaccharide Chain 7C**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain 8C****Bond lengths****Bond angles****Torsions****Rings**

Oligosaccharide Chain AD**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain ED****Bond lengths****Bond angles****Torsions****Rings**

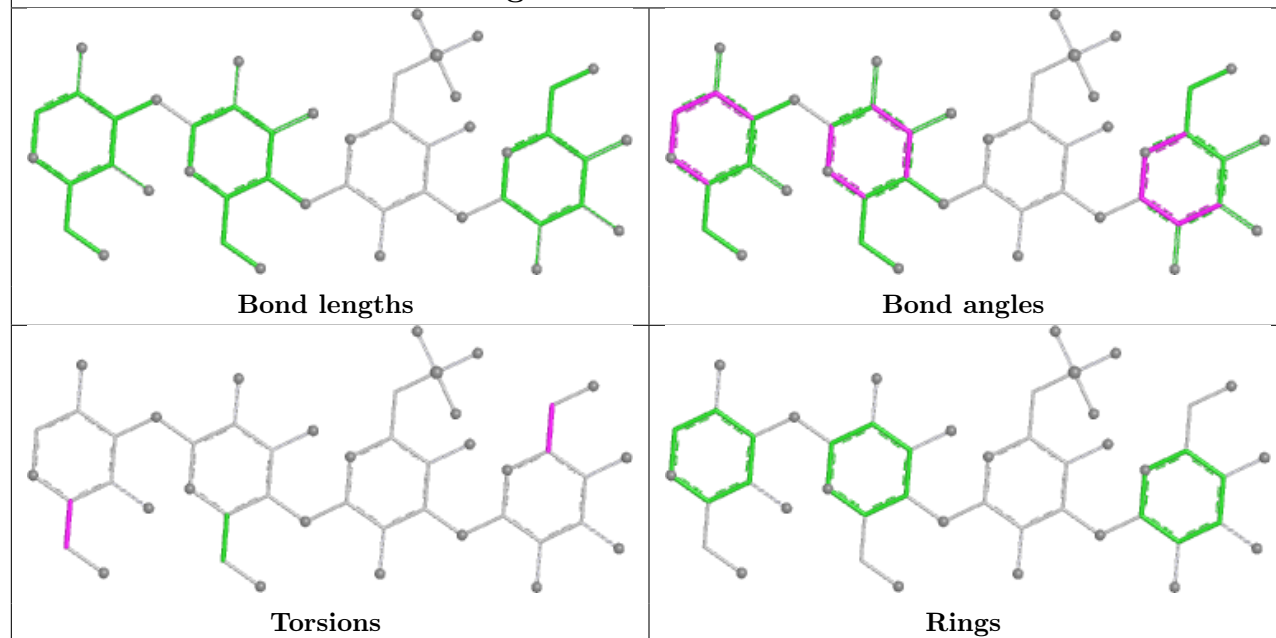
Oligosaccharide Chain FD**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain HD****Bond lengths****Bond angles****Torsions****Rings**



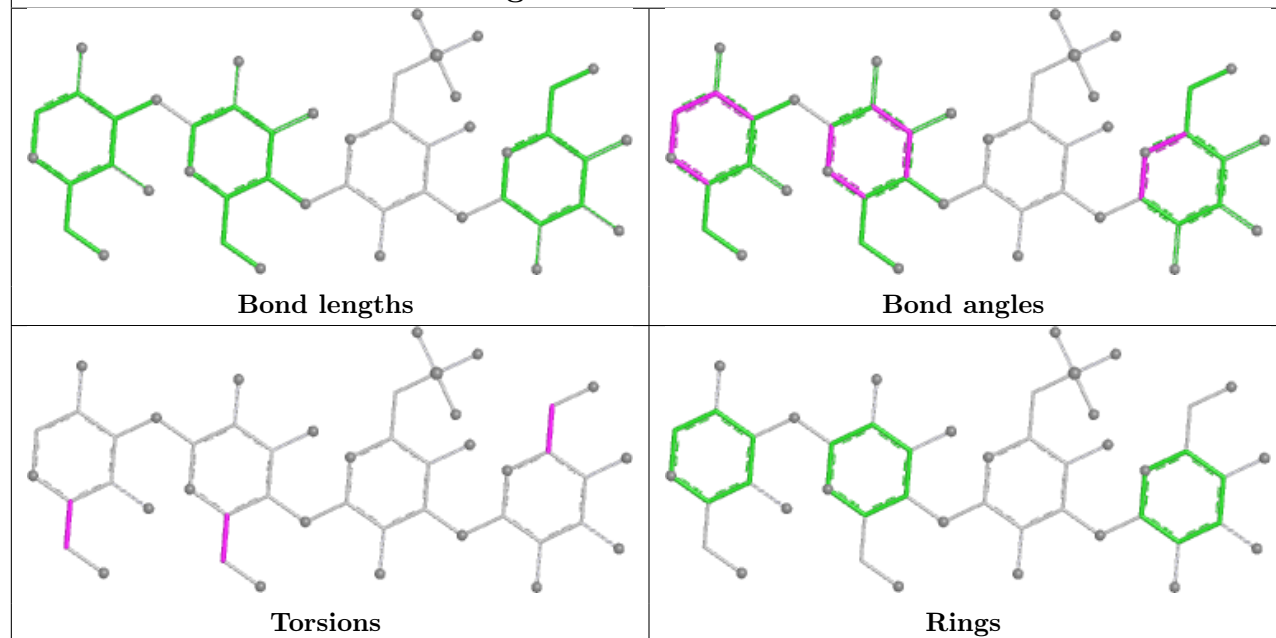


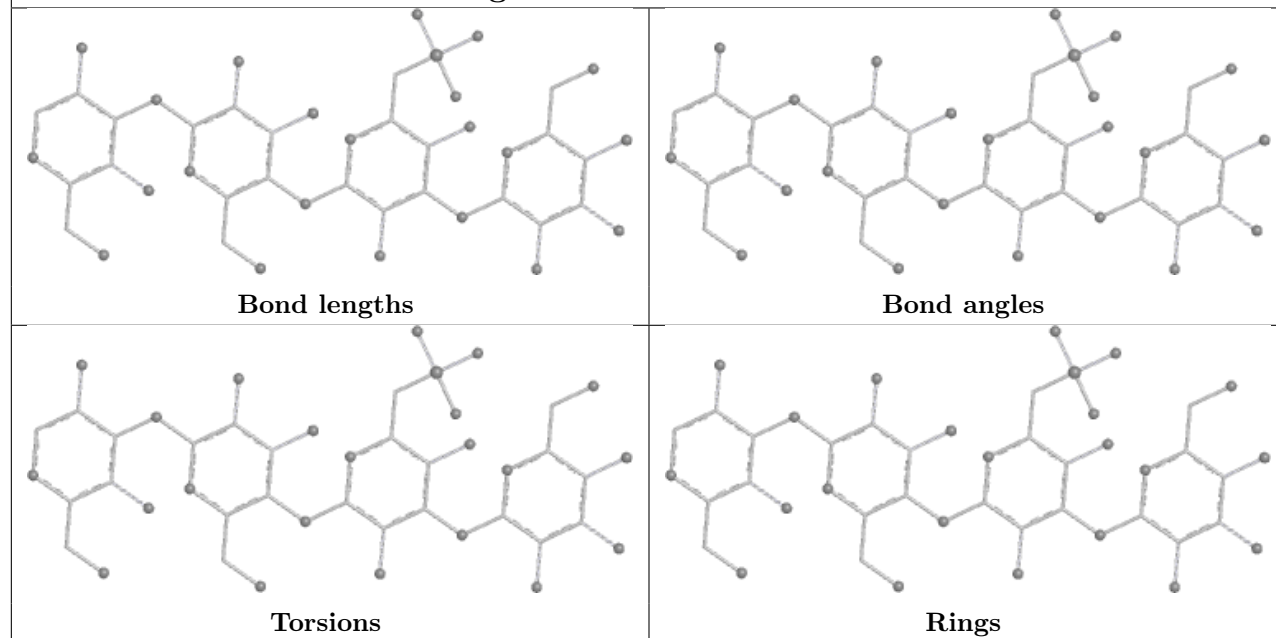
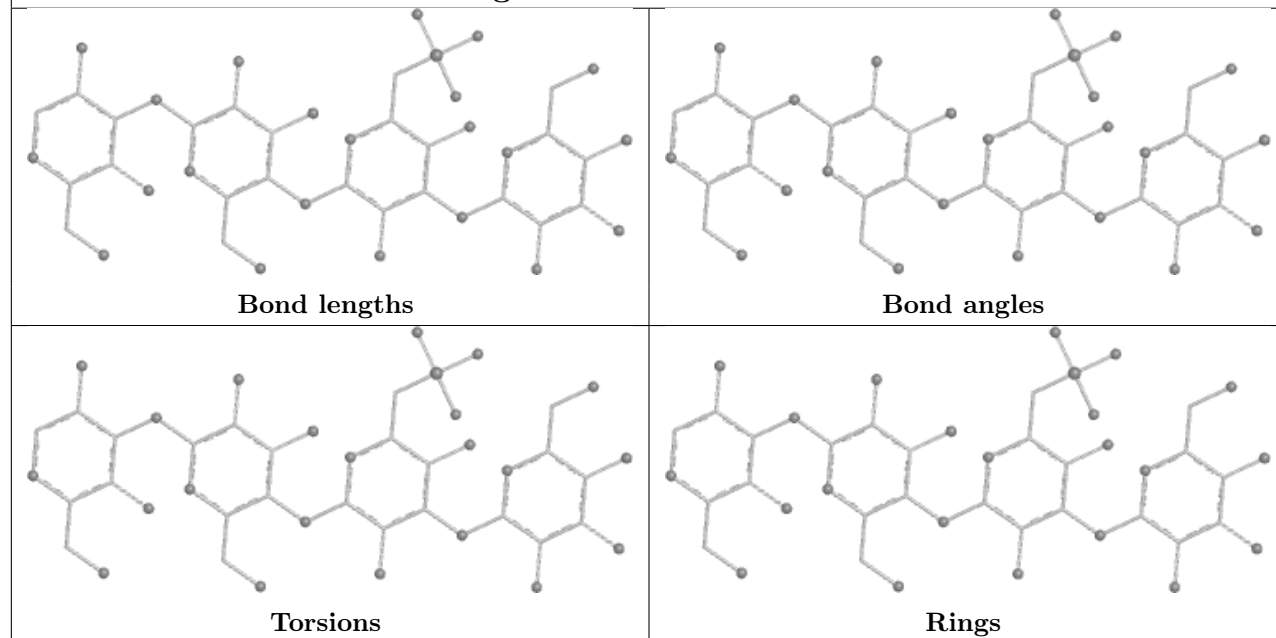


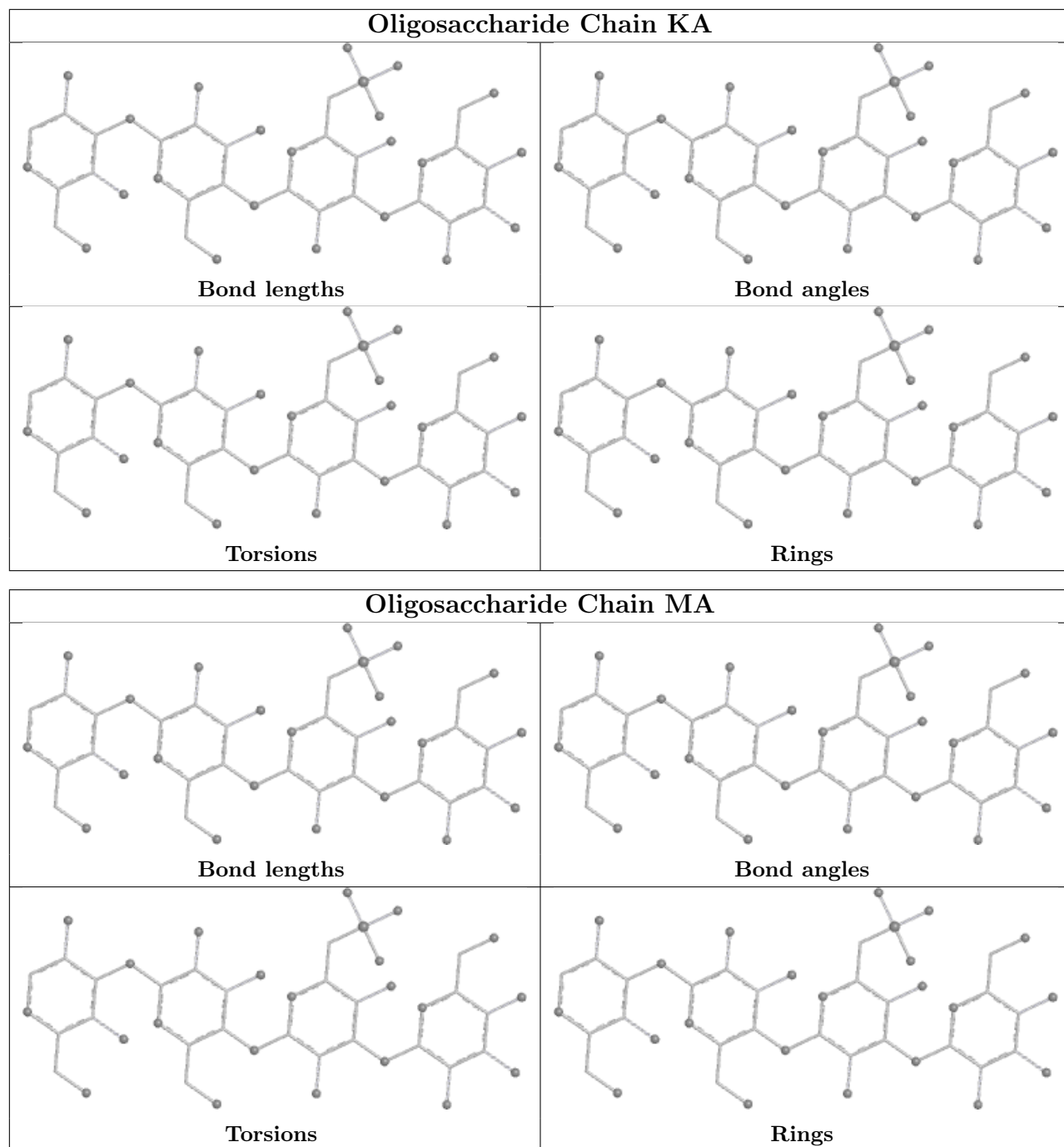
Oligosaccharide Chain 6

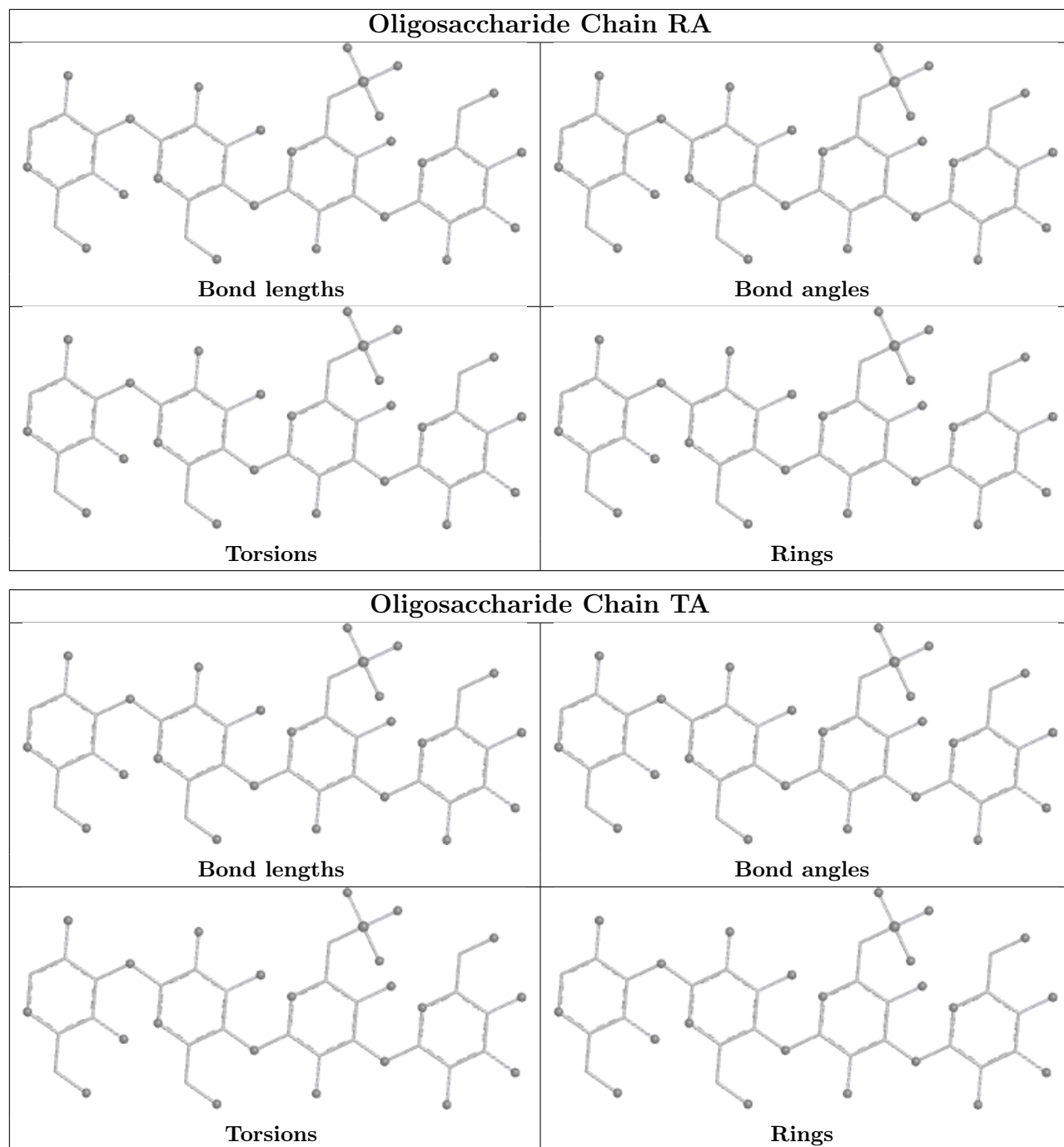


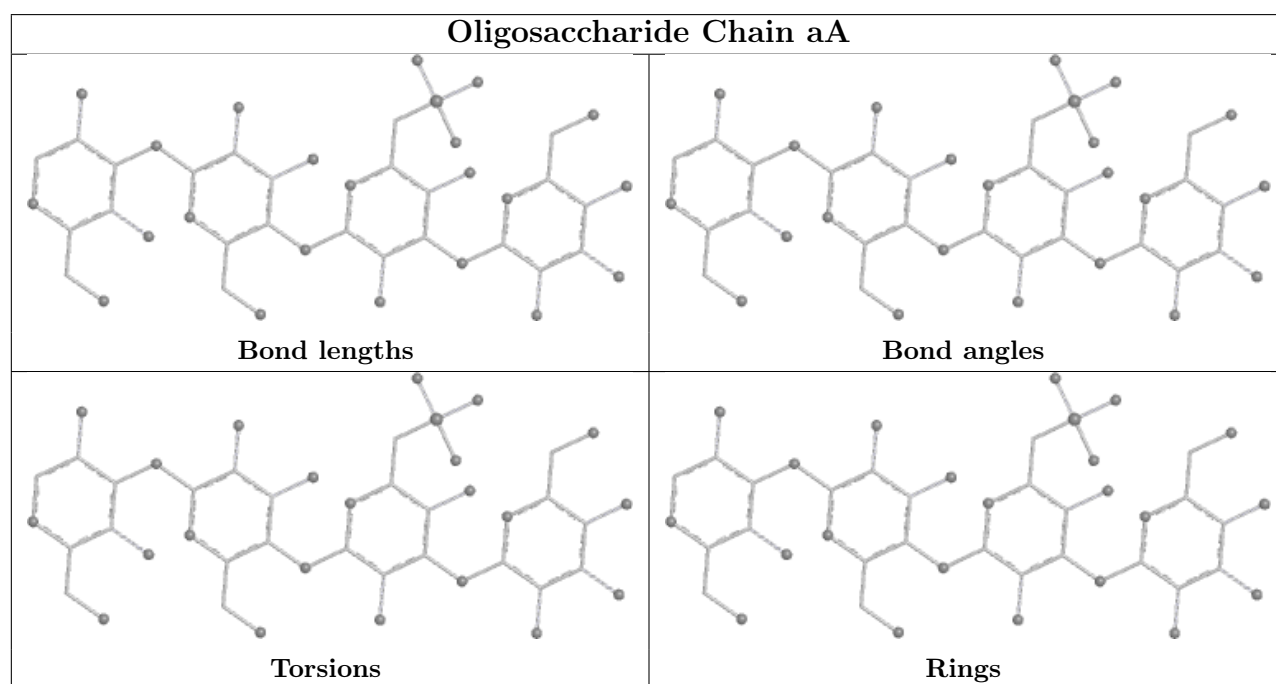
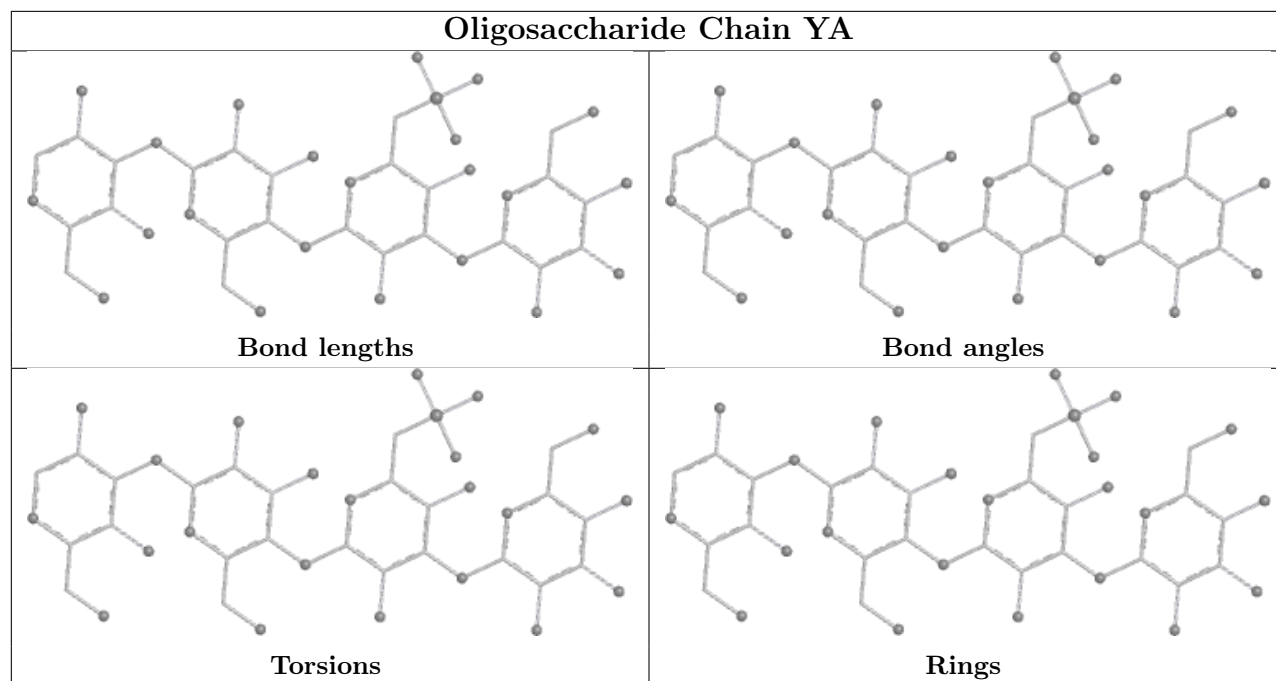
Oligosaccharide Chain 8

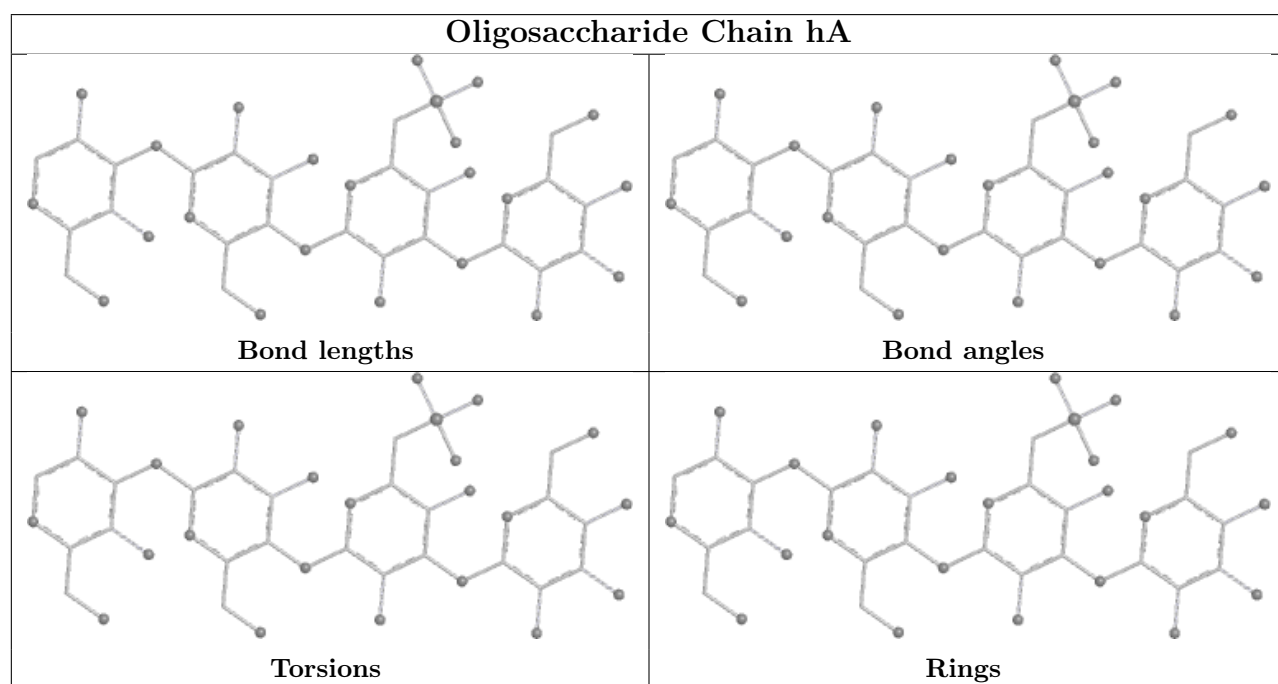
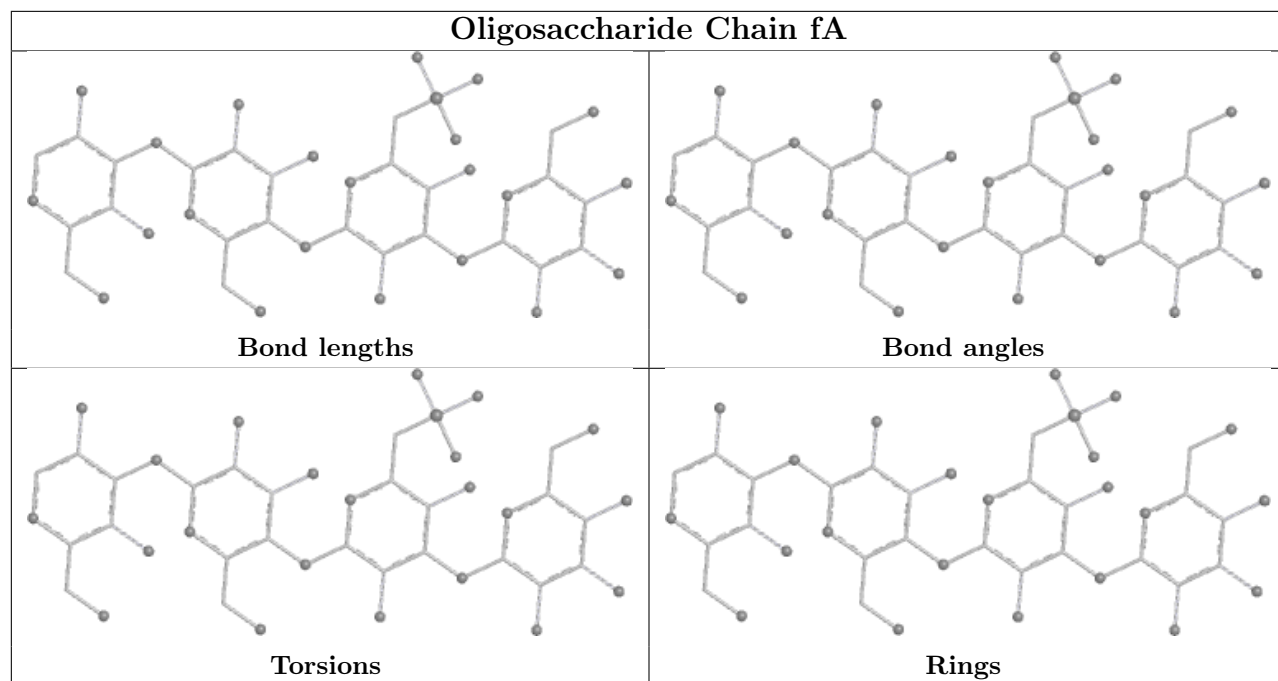


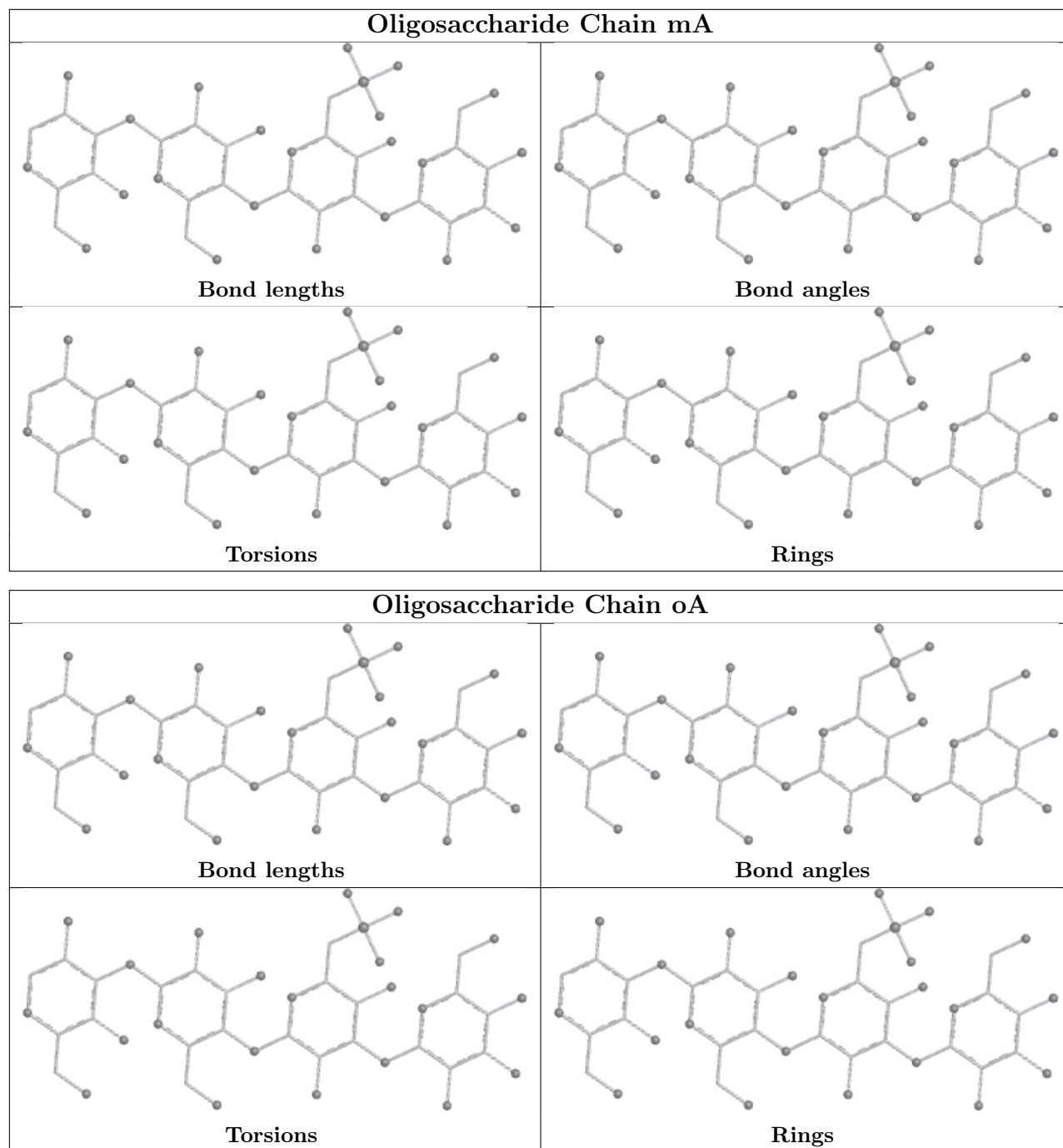
Oligosaccharide Chain DA**Oligosaccharide Chain FA**



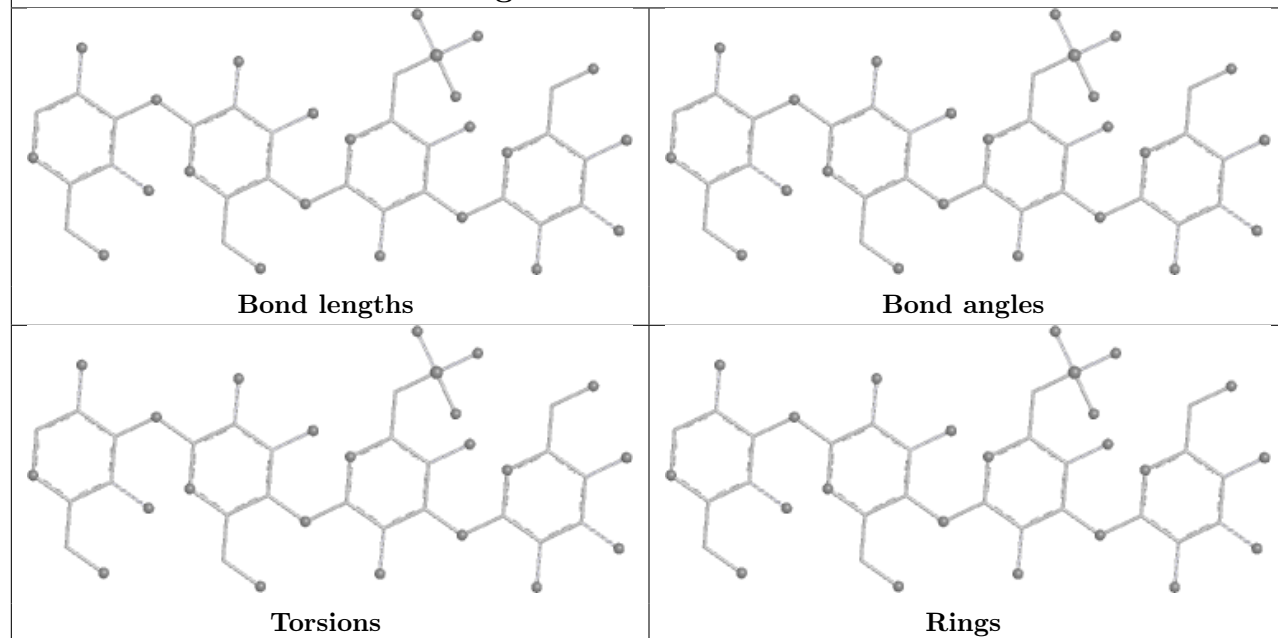




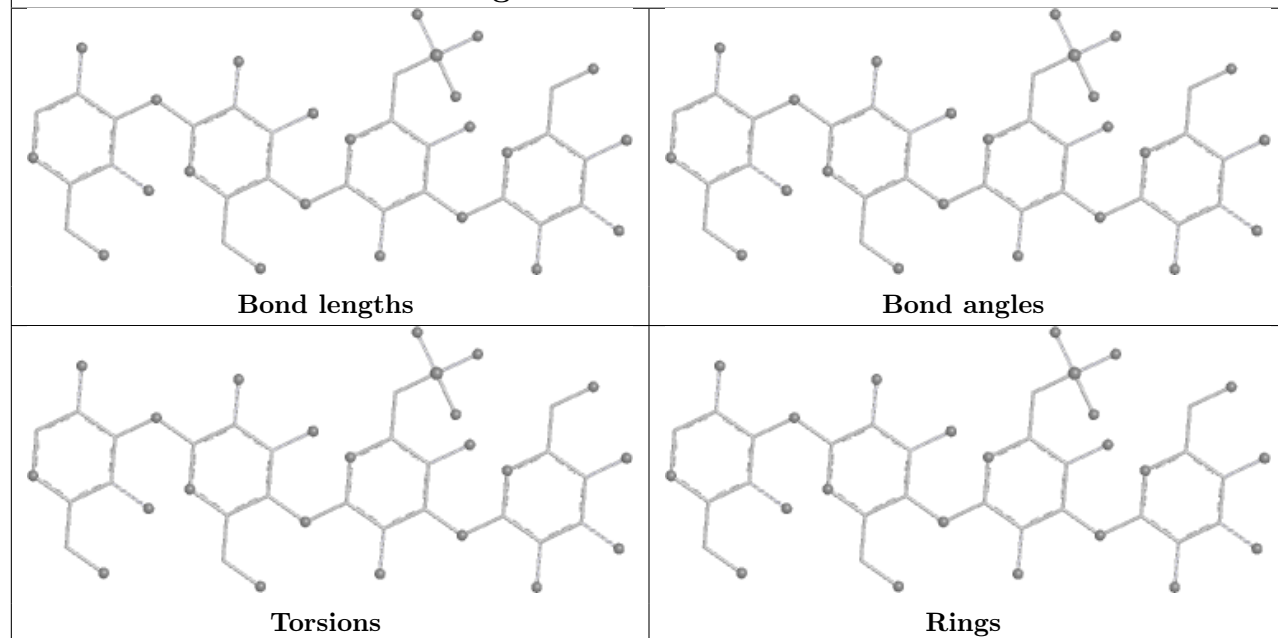


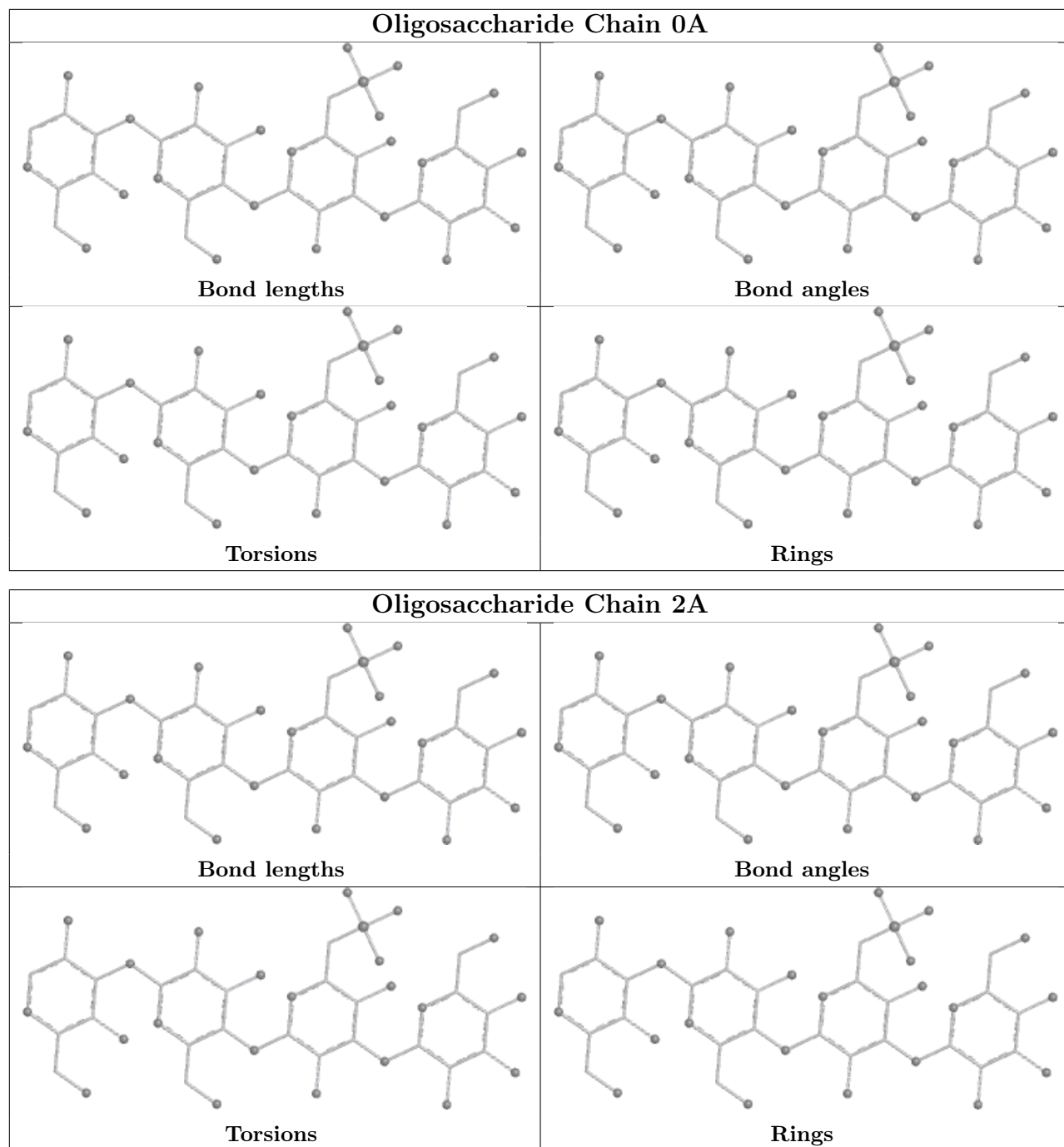


Oligosaccharide Chain tA

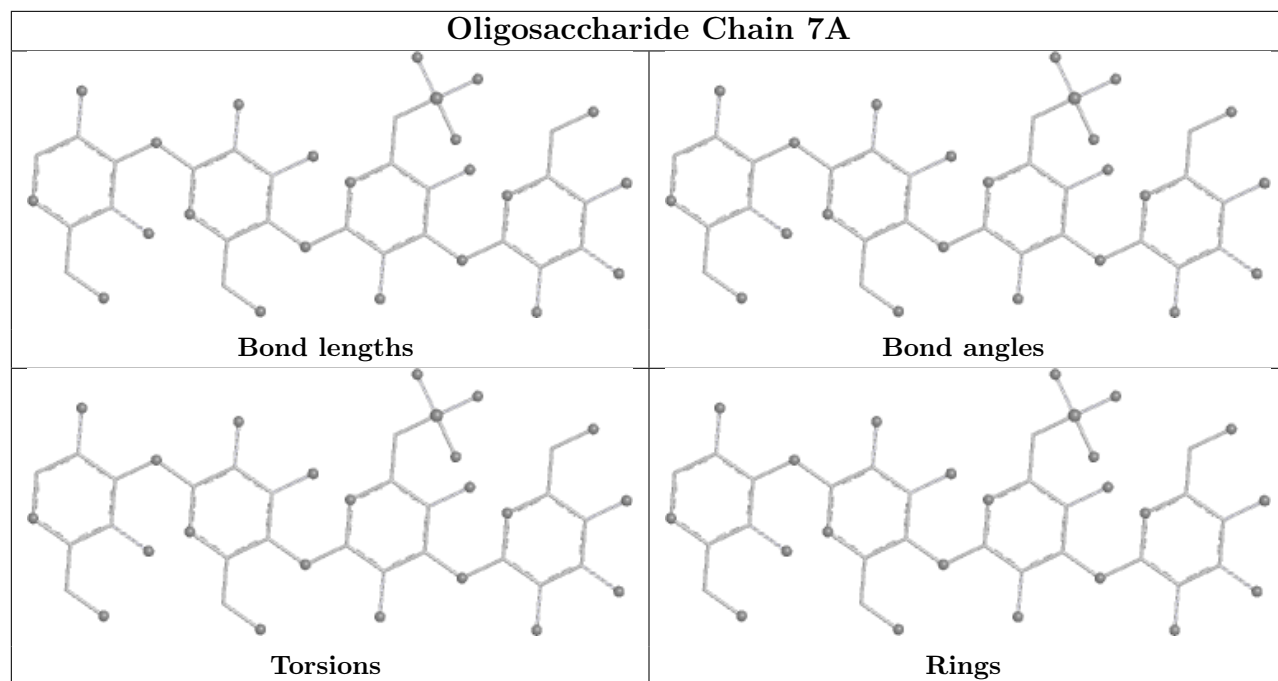


Oligosaccharide Chain vA

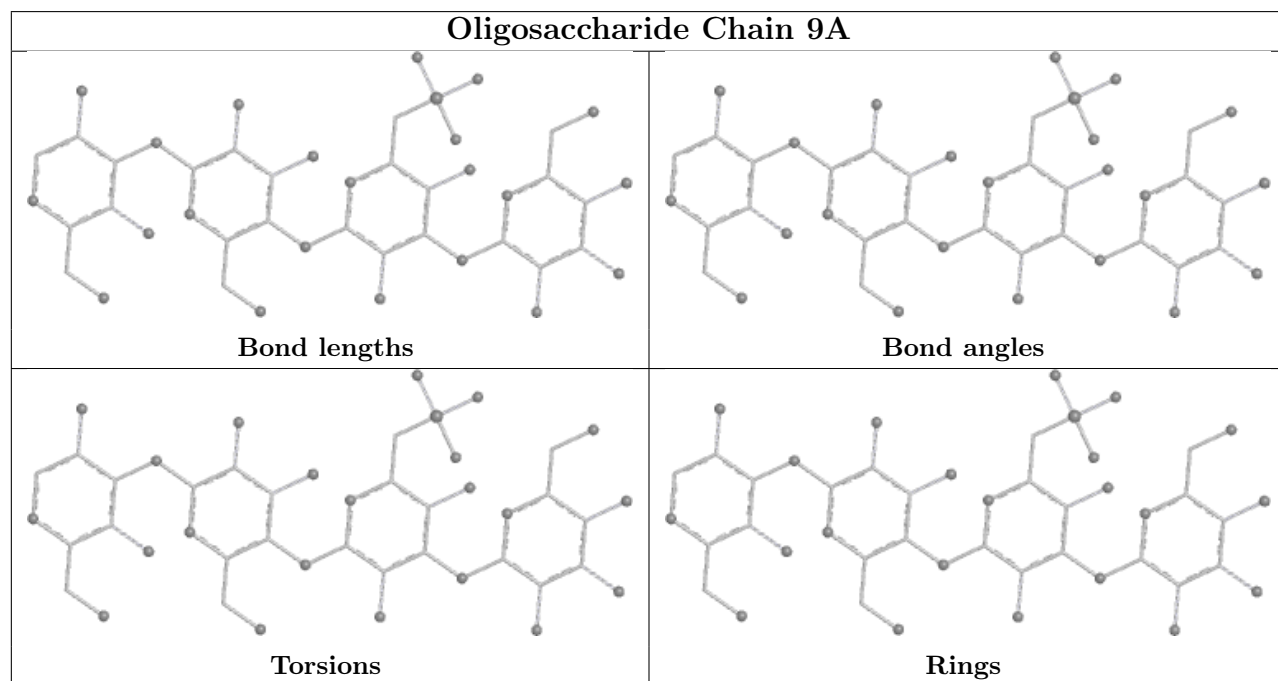


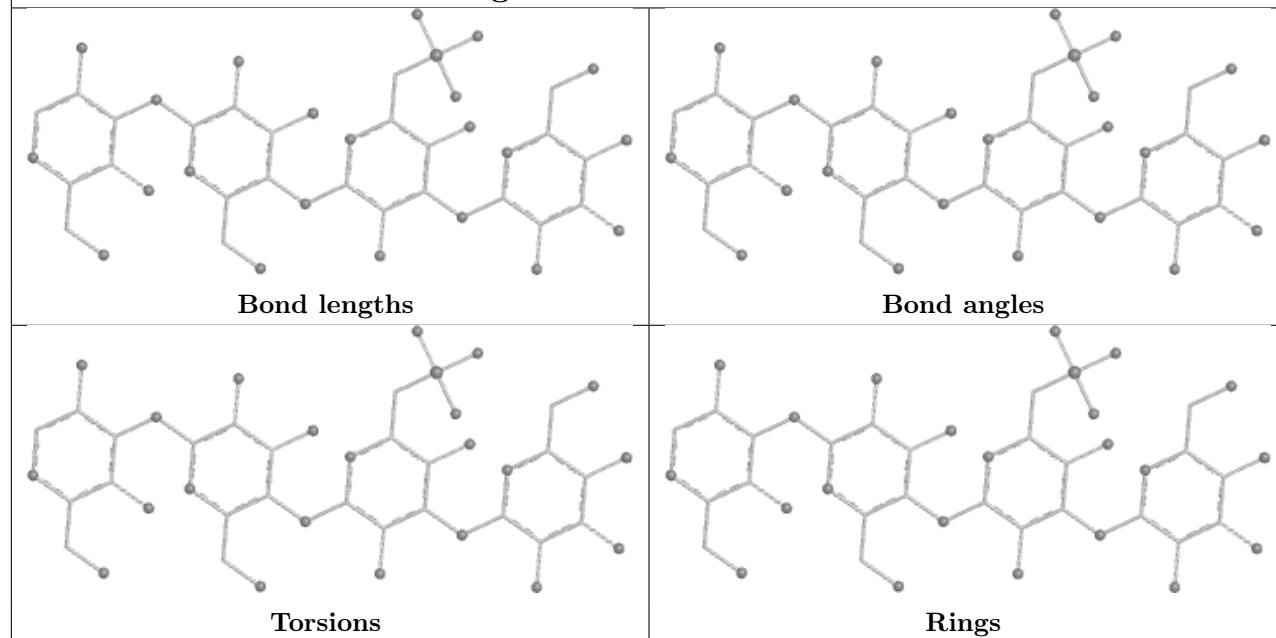
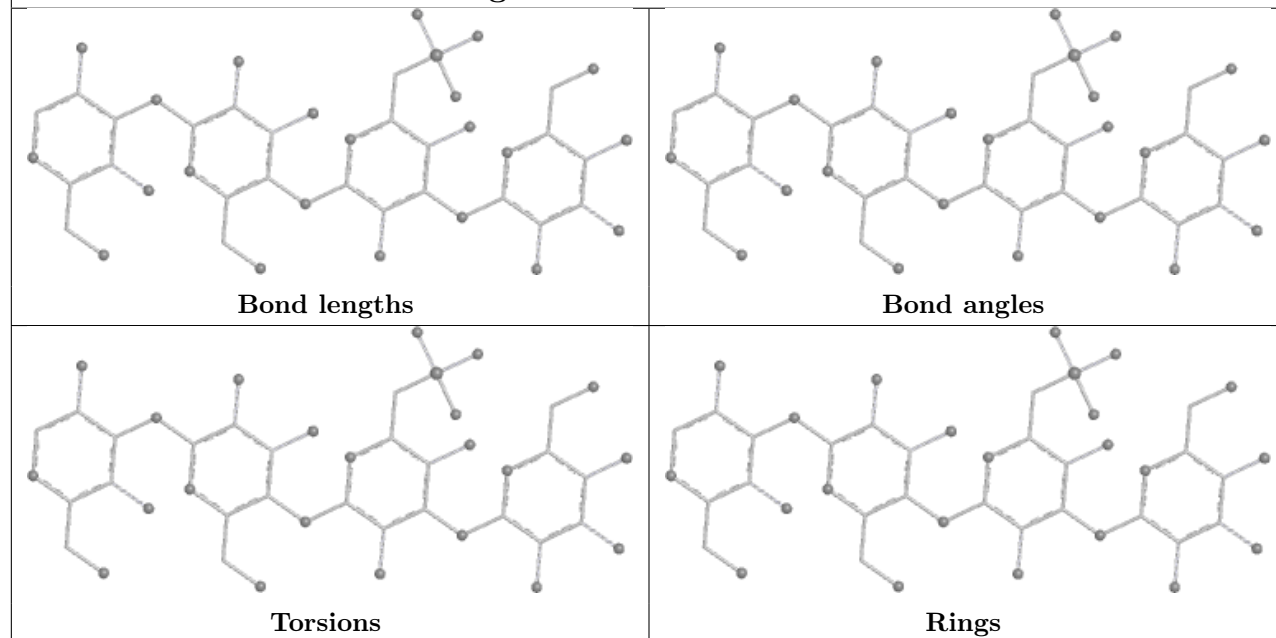


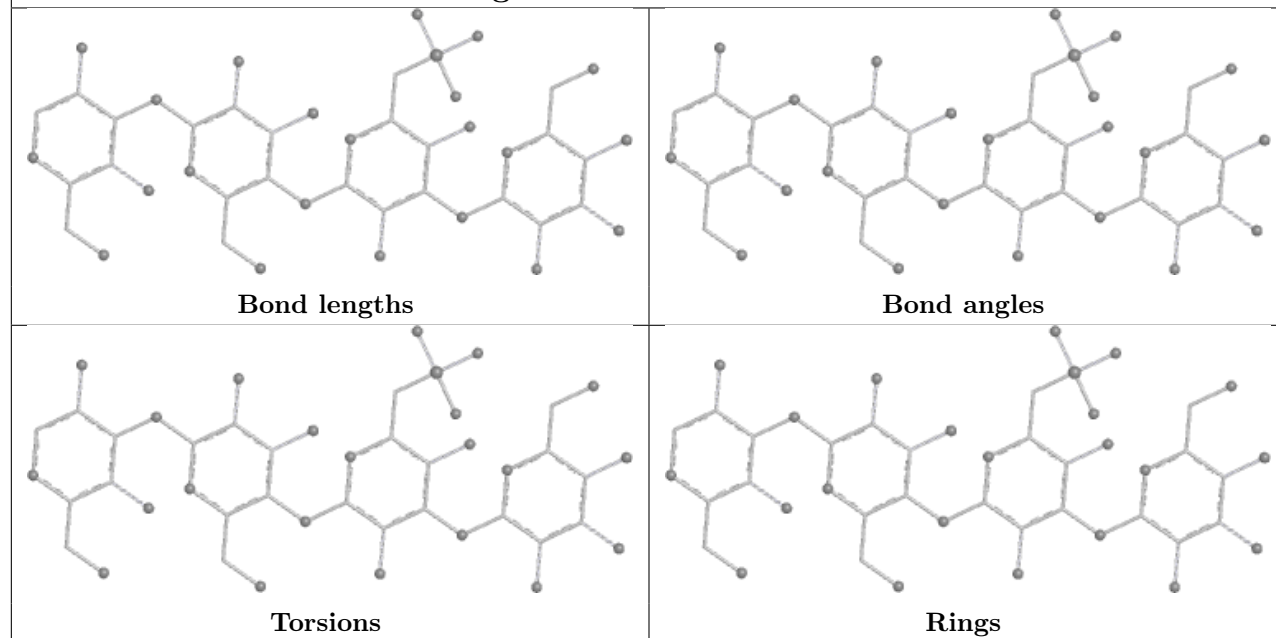
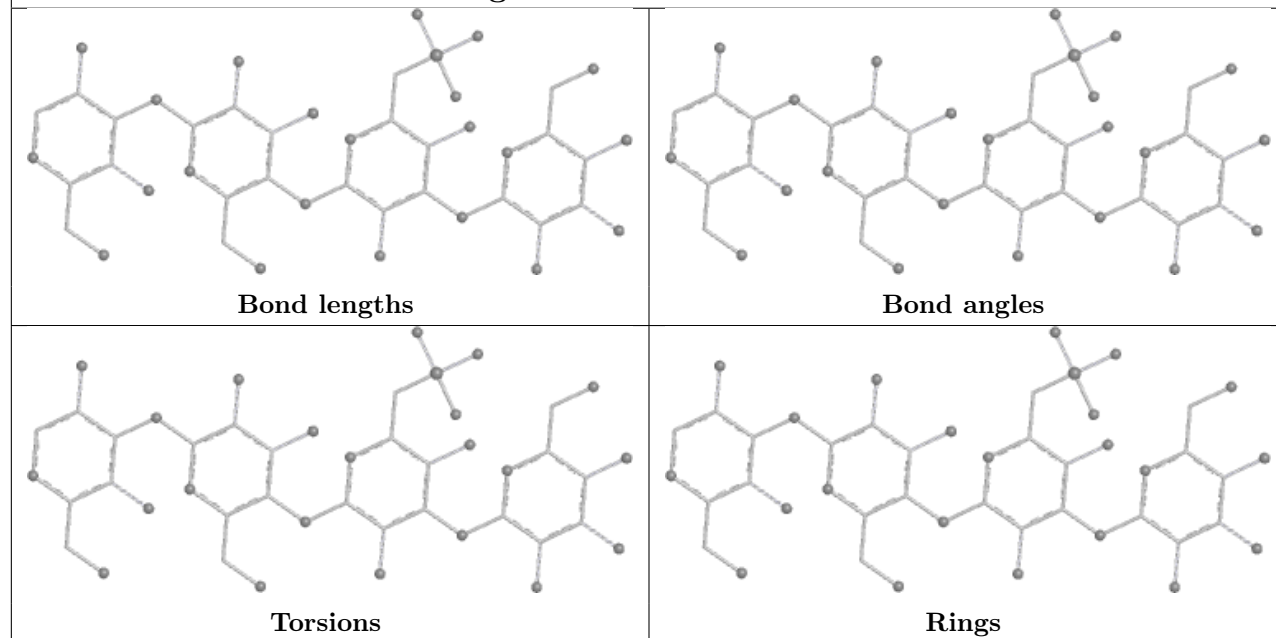
Oligosaccharide Chain 7A

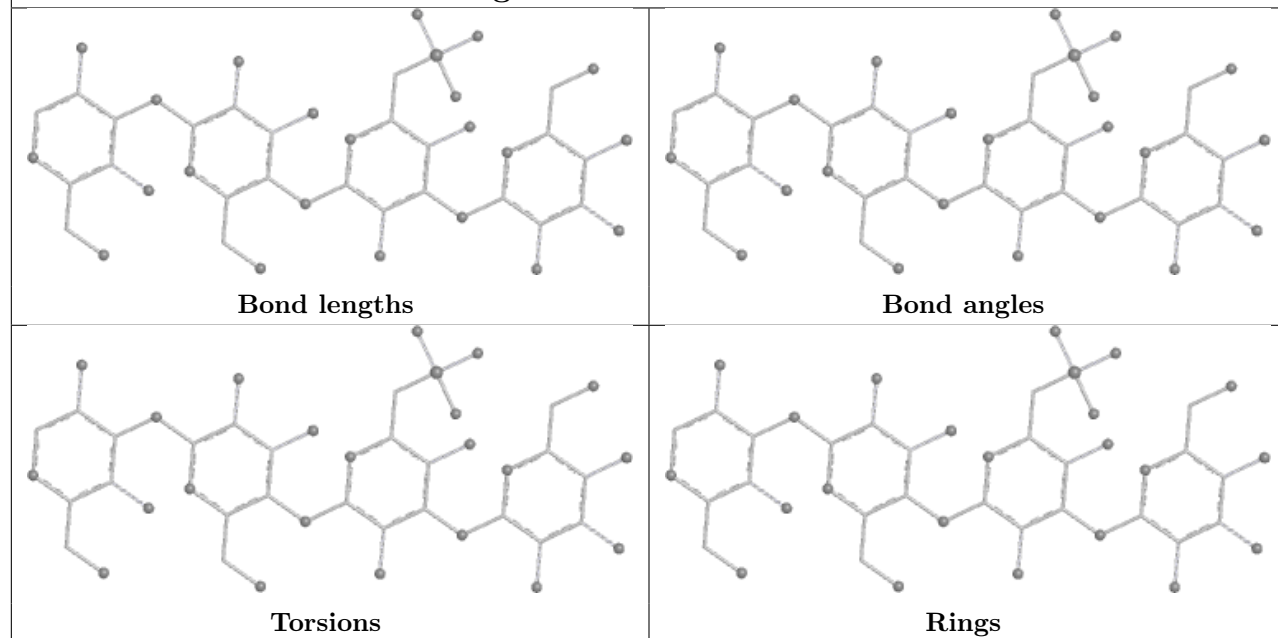
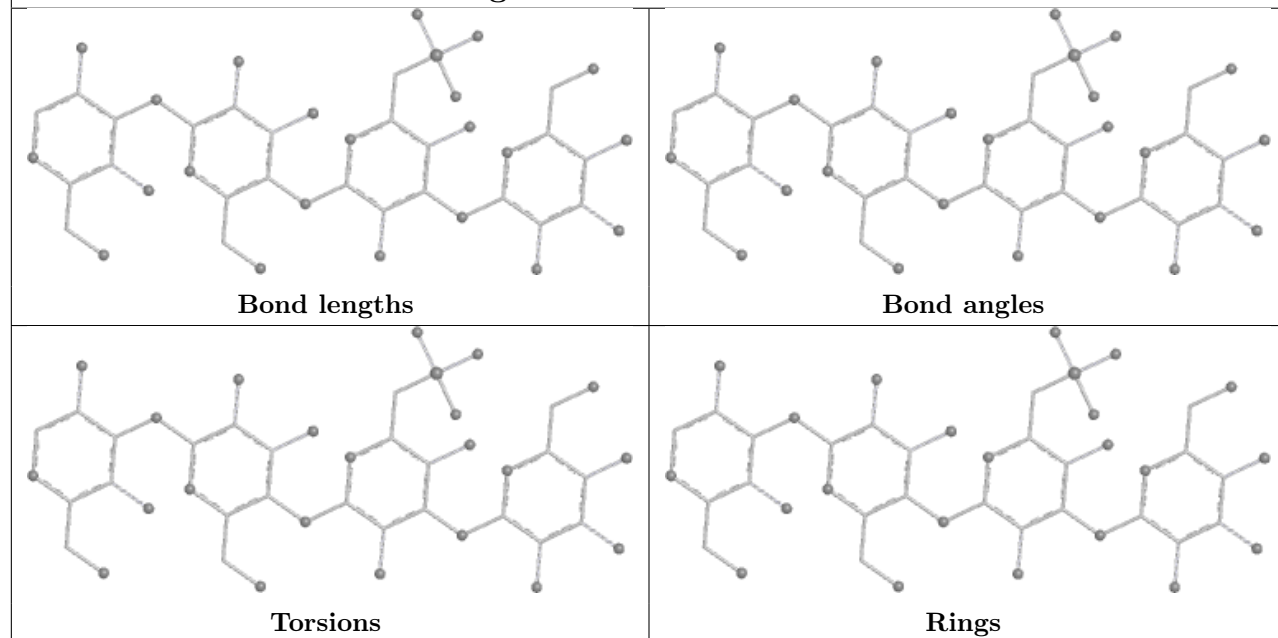


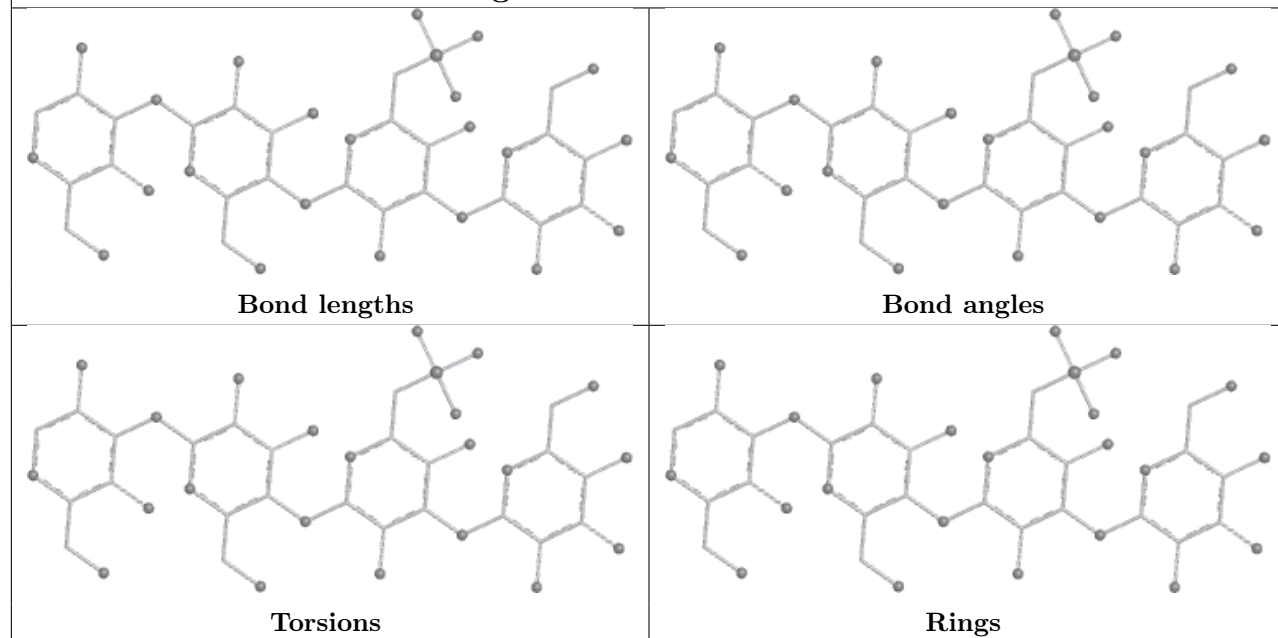
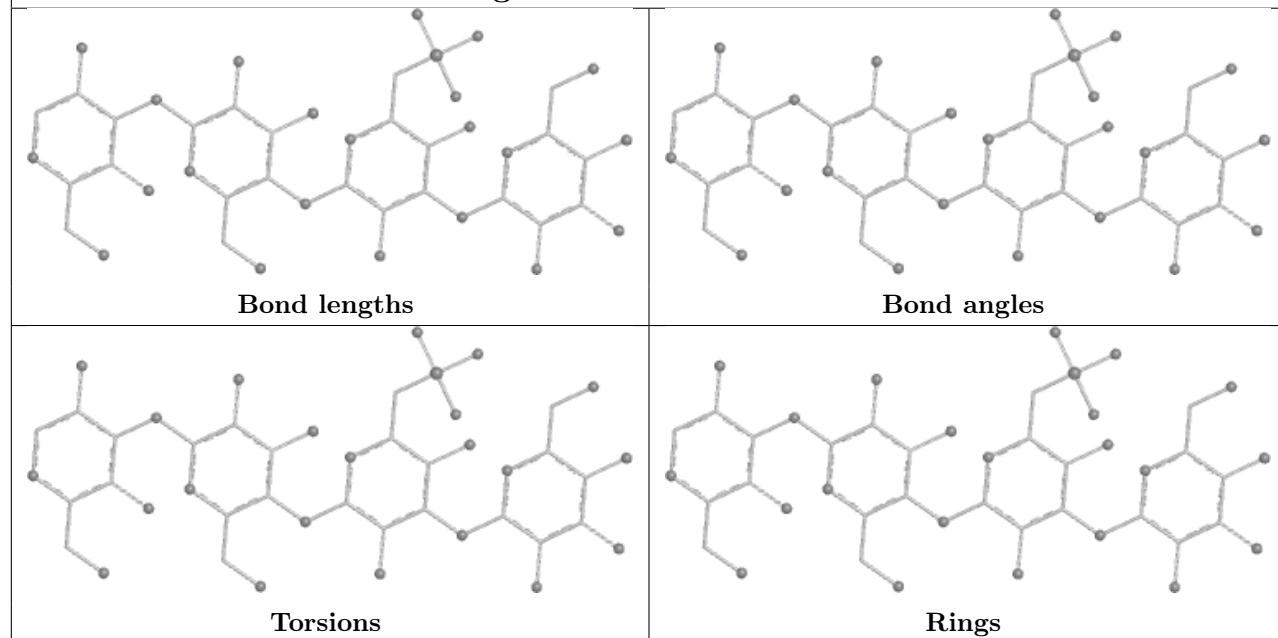
Oligosaccharide Chain 9A

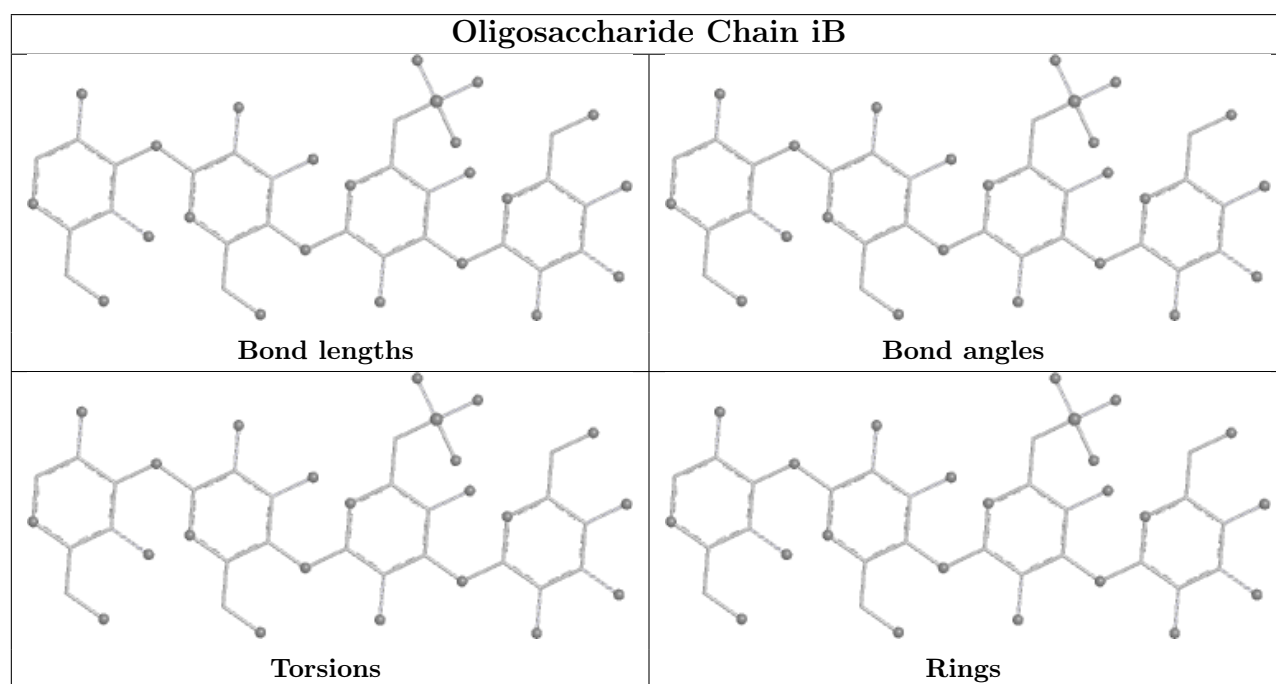
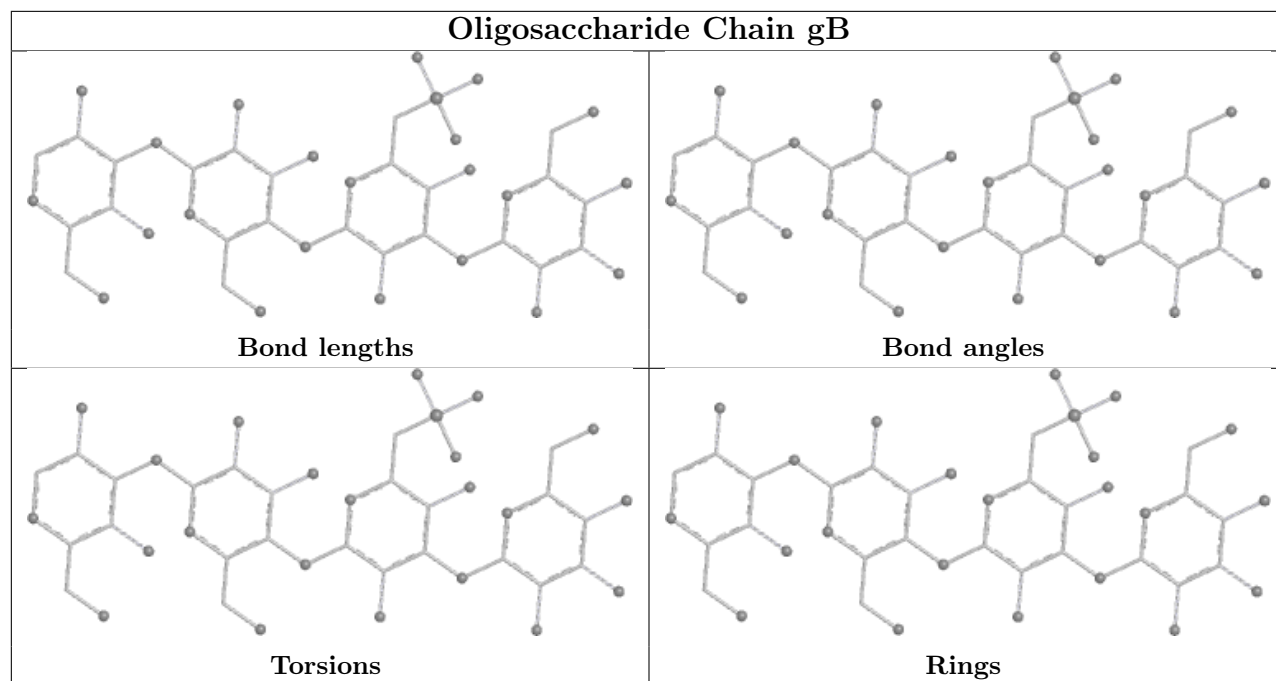


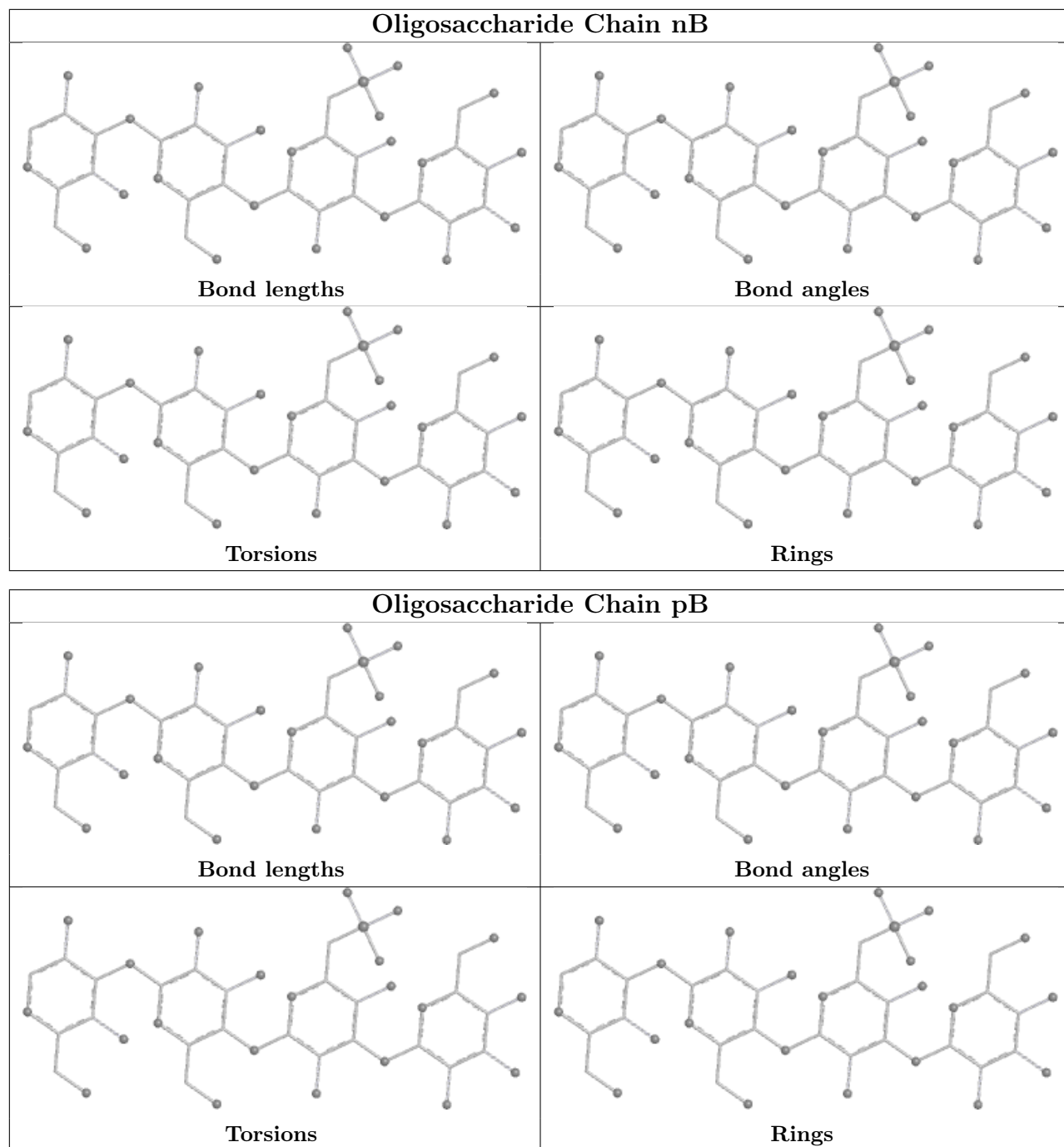
Oligosaccharide Chain EB**Oligosaccharide Chain GB**

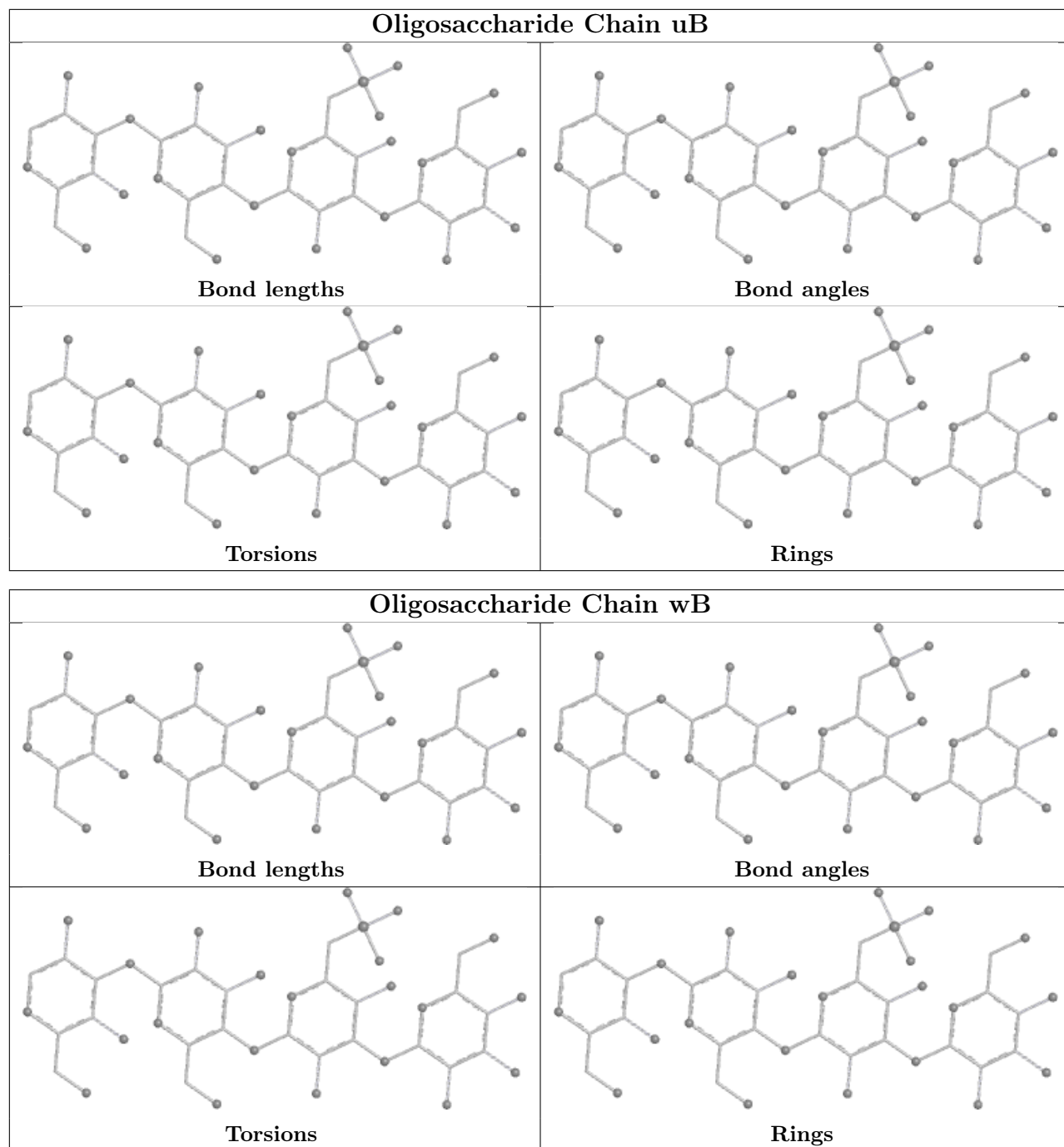
Oligosaccharide Chain LB**Oligosaccharide Chain NB**

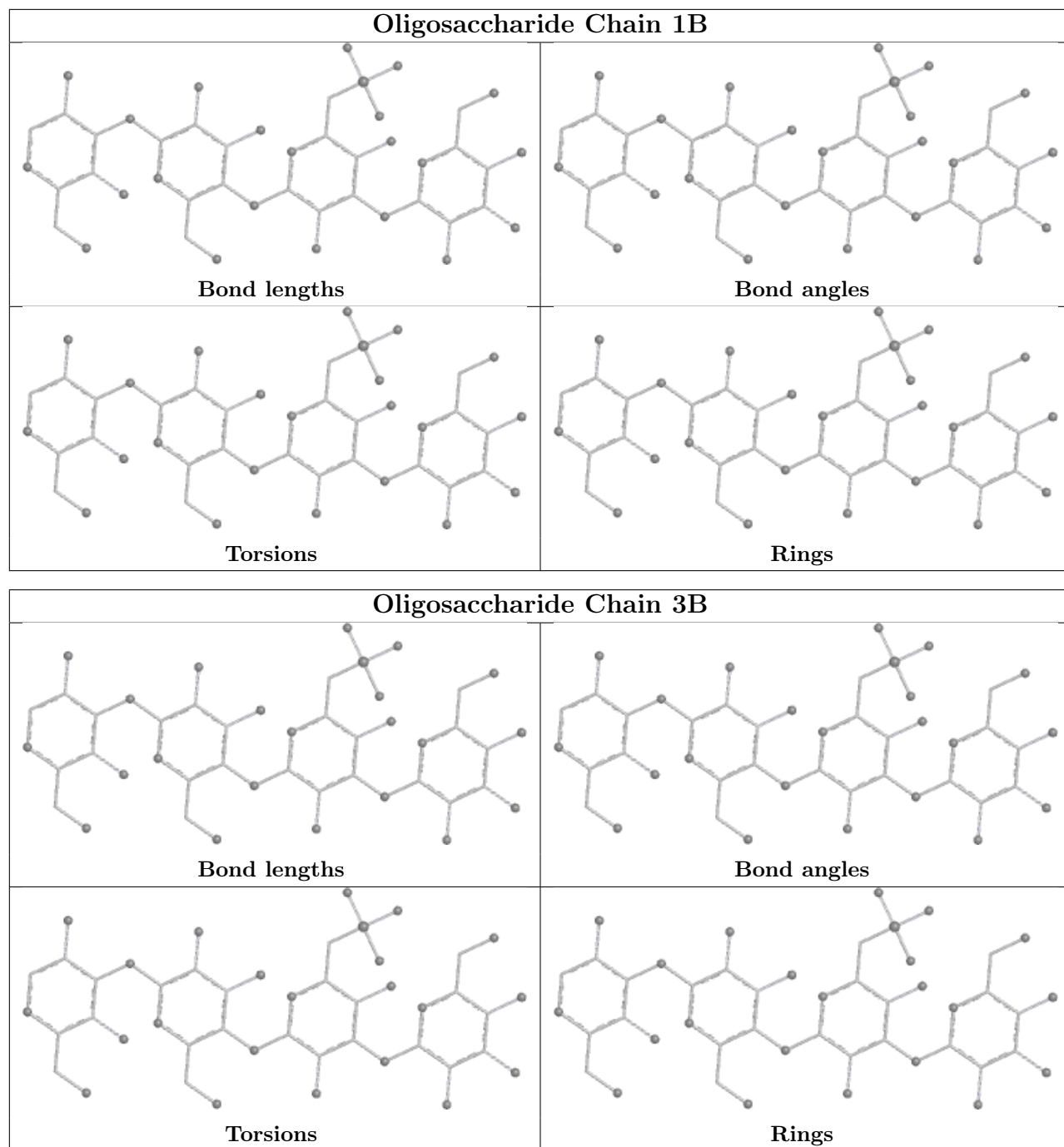
Oligosaccharide Chain SB**Oligosaccharide Chain UB**

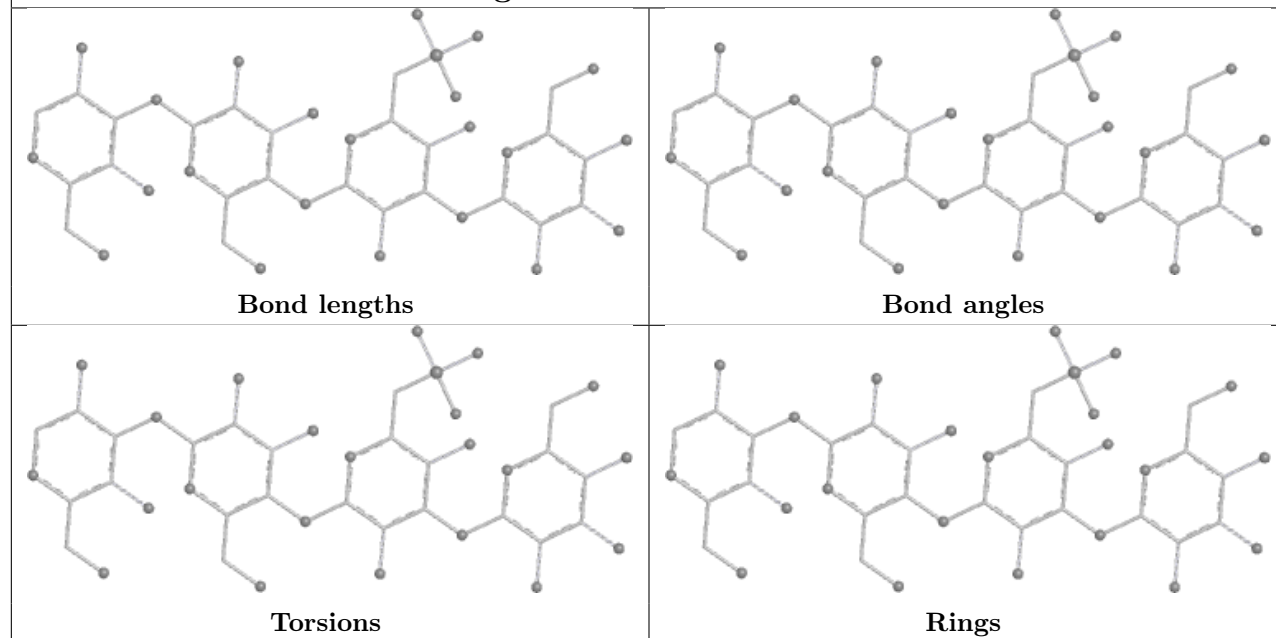
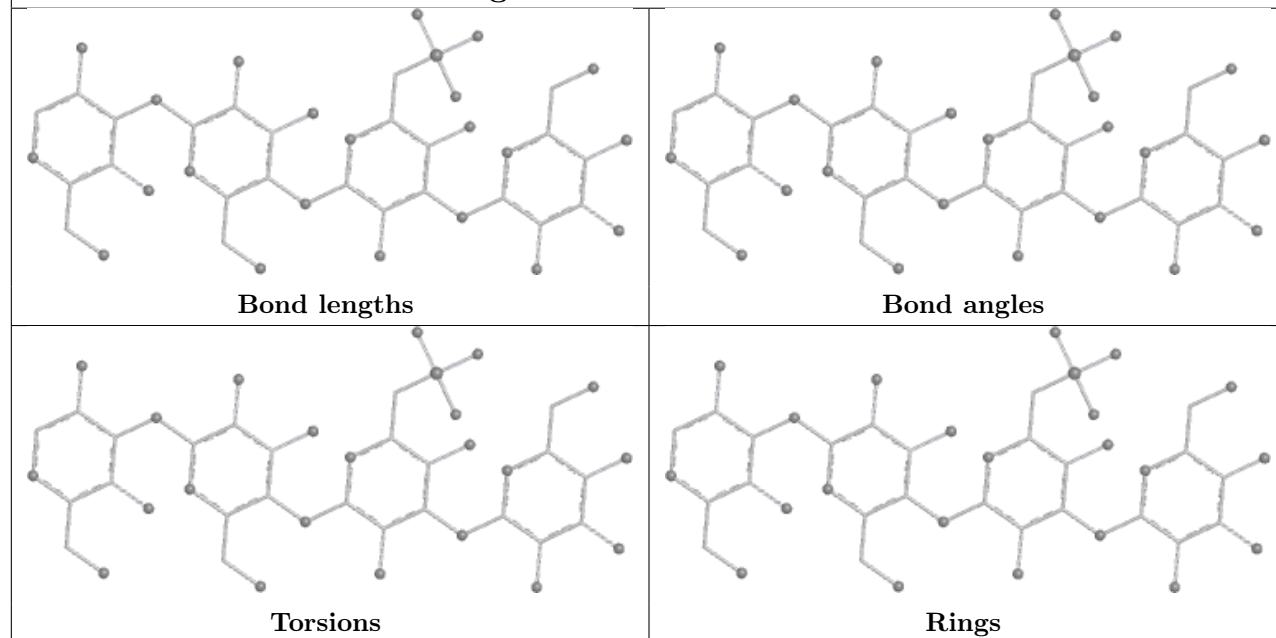
Oligosaccharide Chain ZB**Oligosaccharide Chain bB**

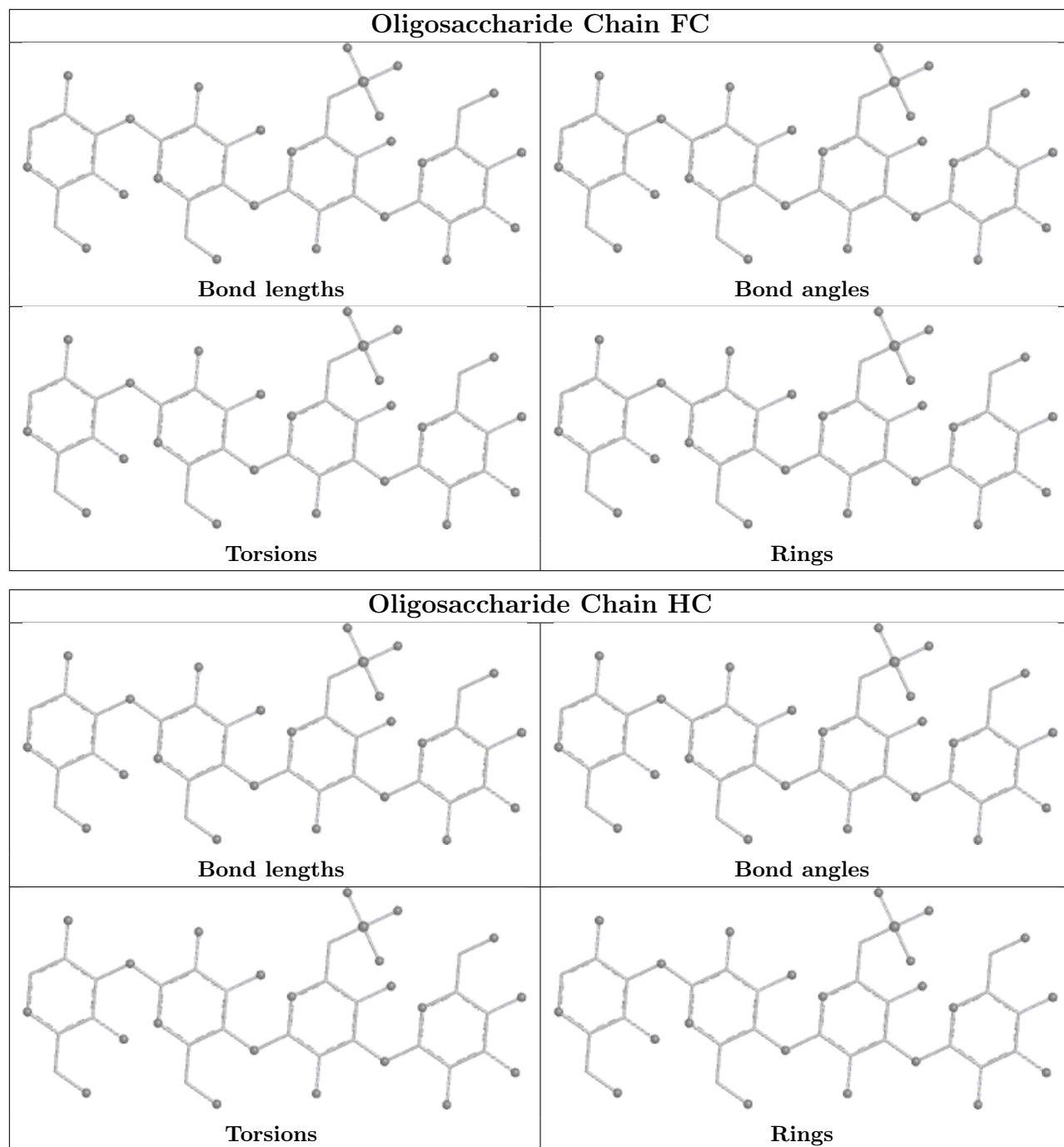


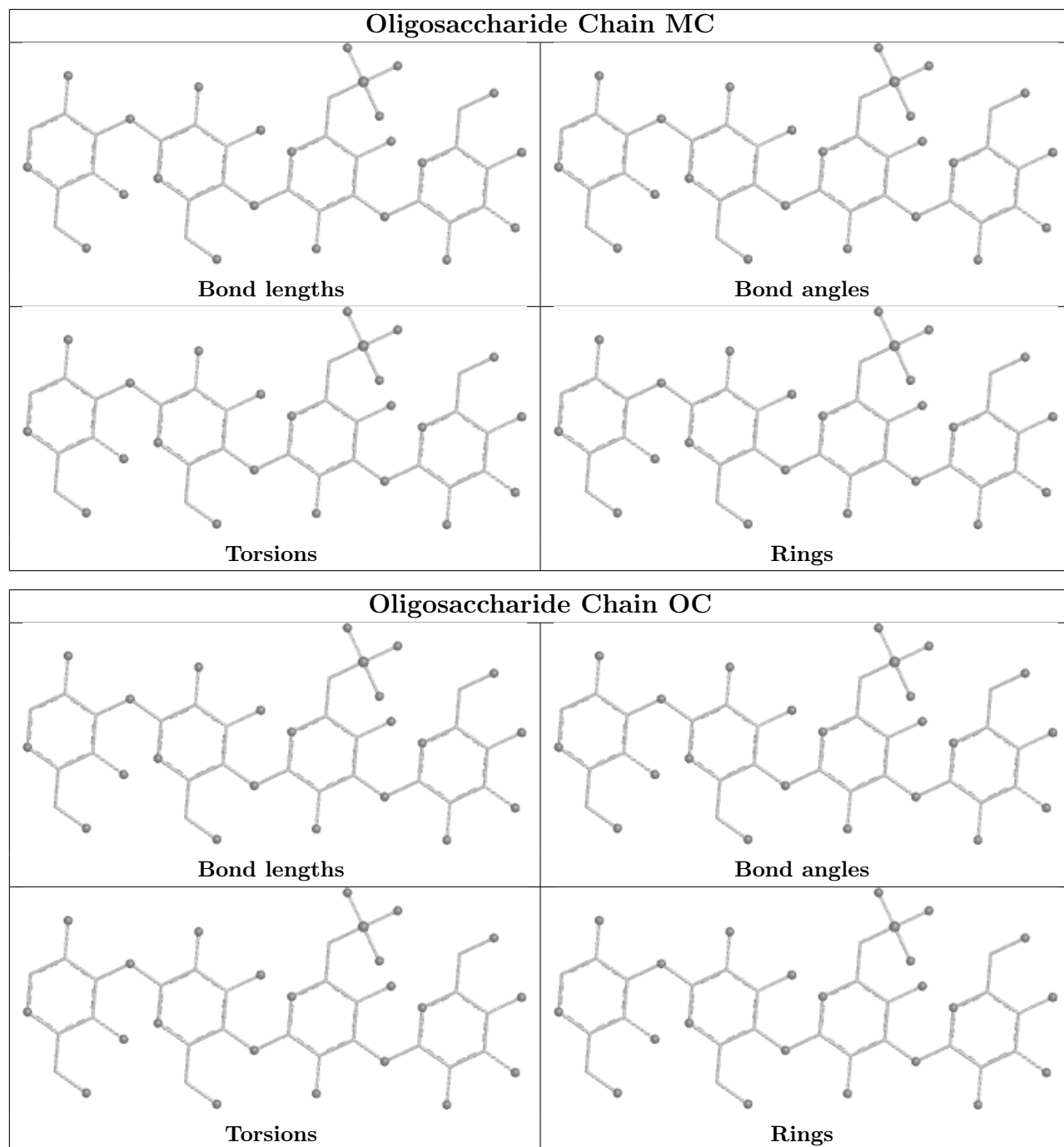




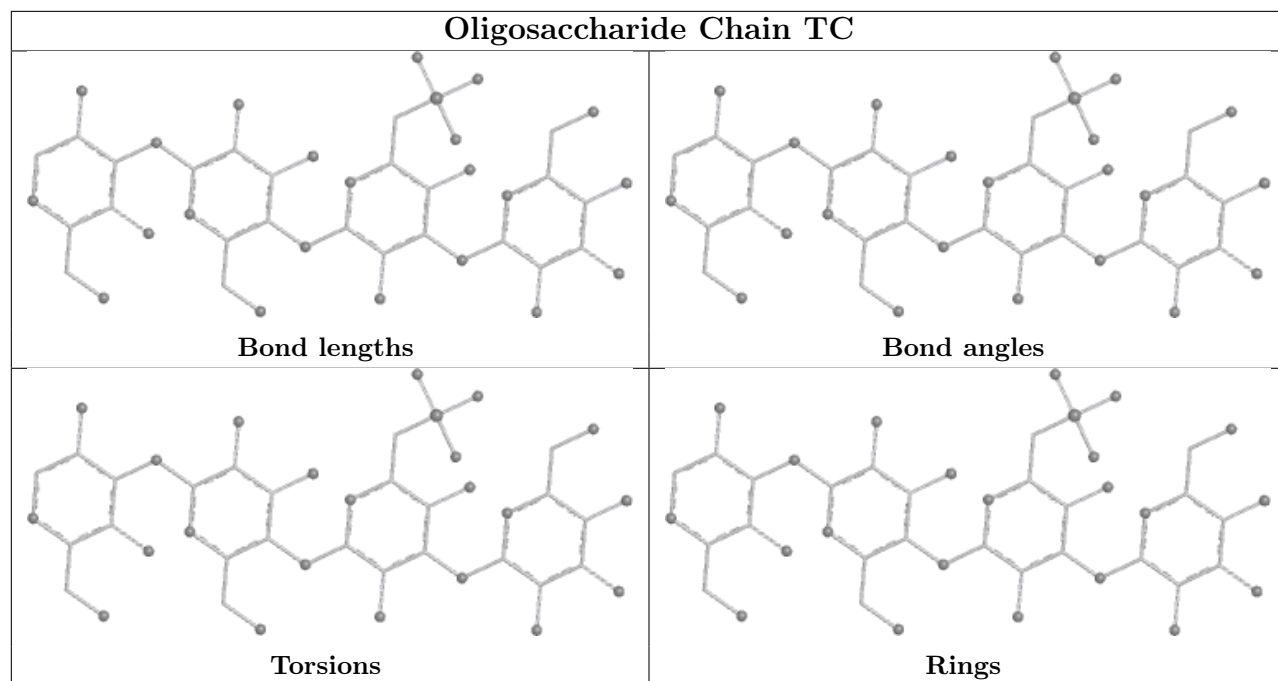


Oligosaccharide Chain 8B**Oligosaccharide Chain AC**

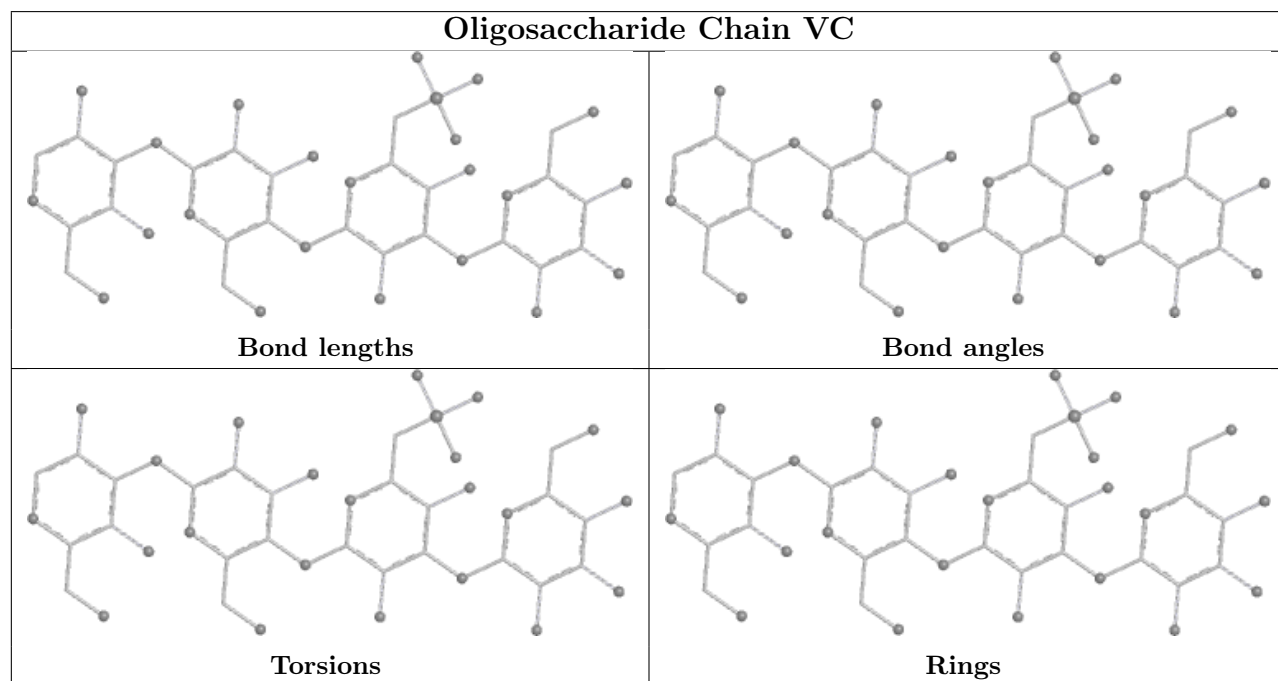




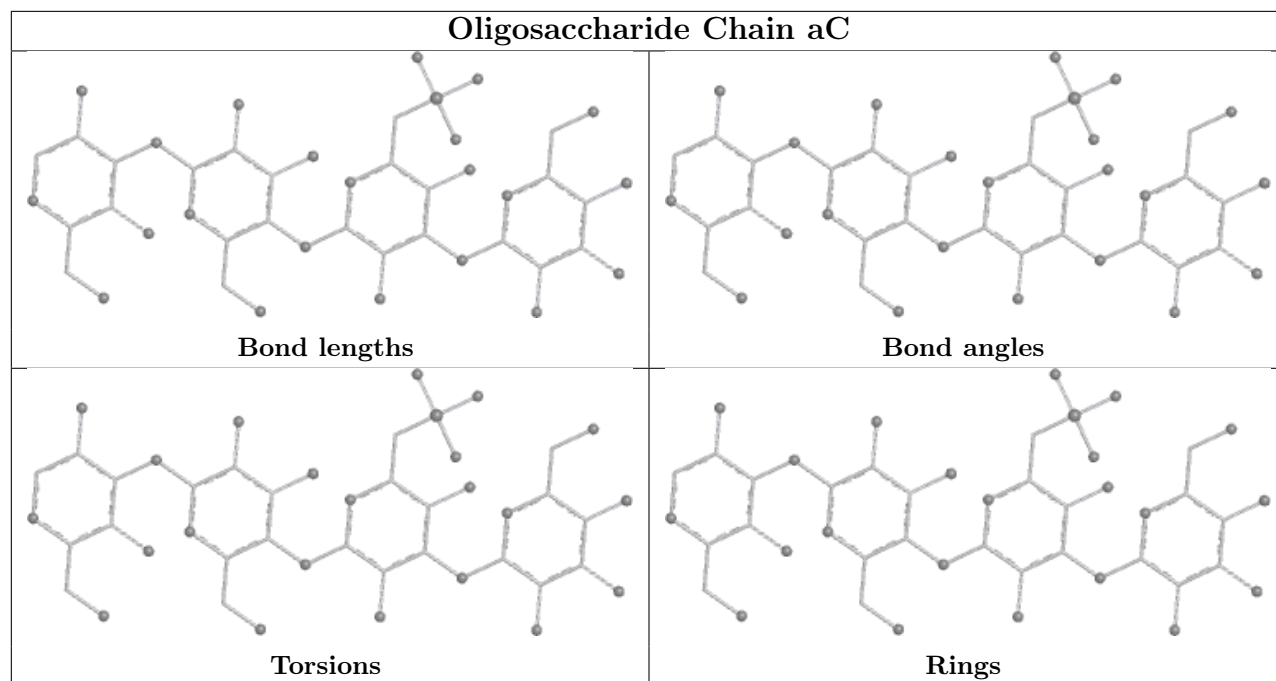
Oligosaccharide Chain TC



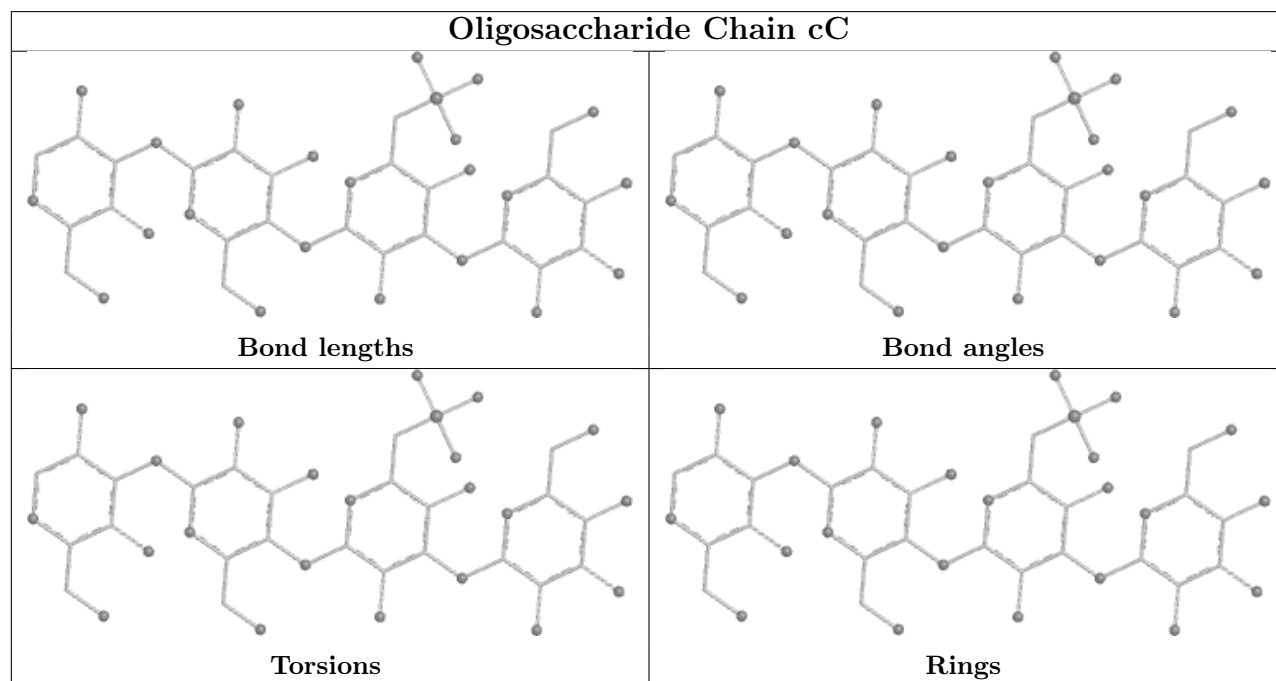
Oligosaccharide Chain VC

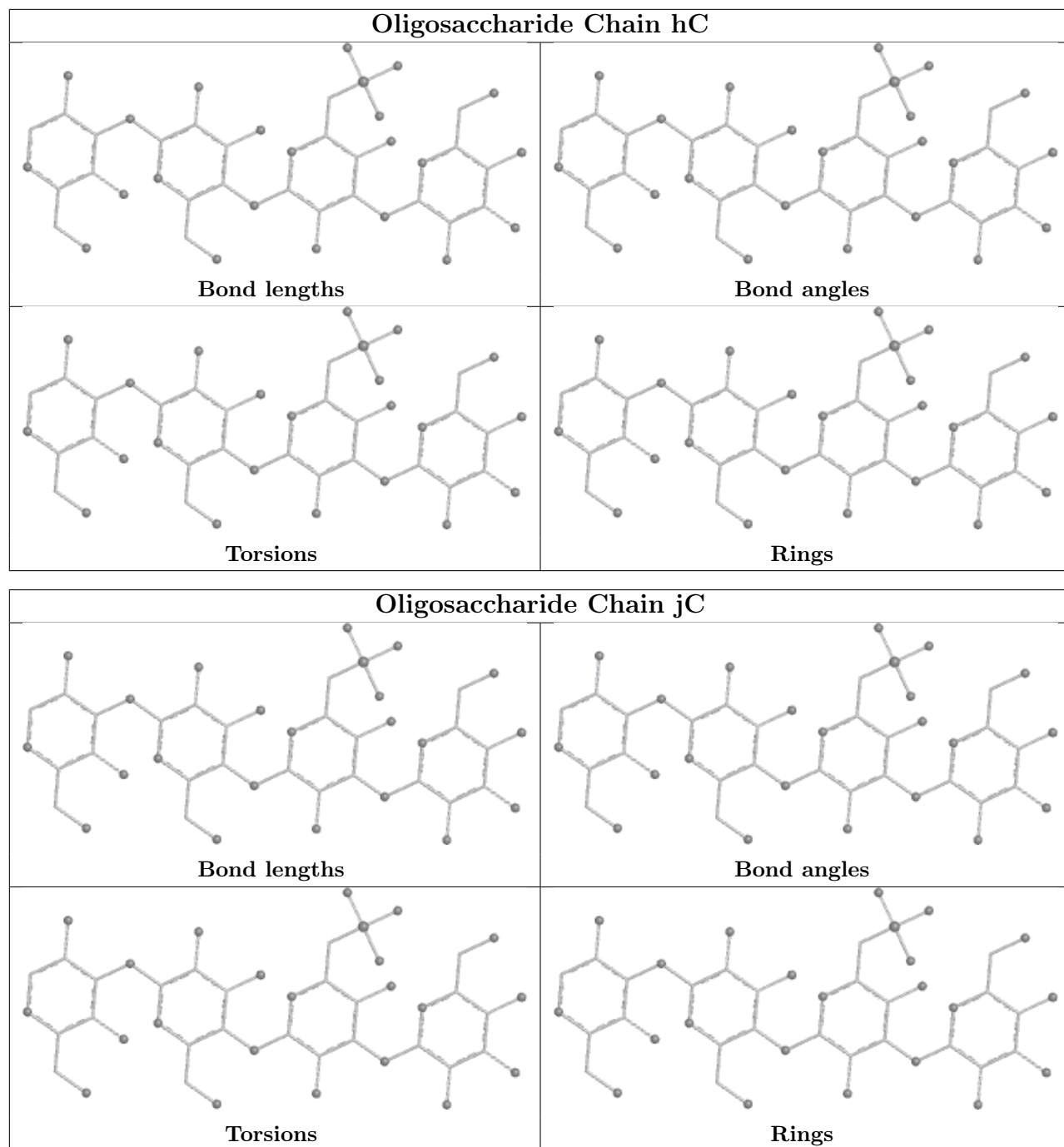


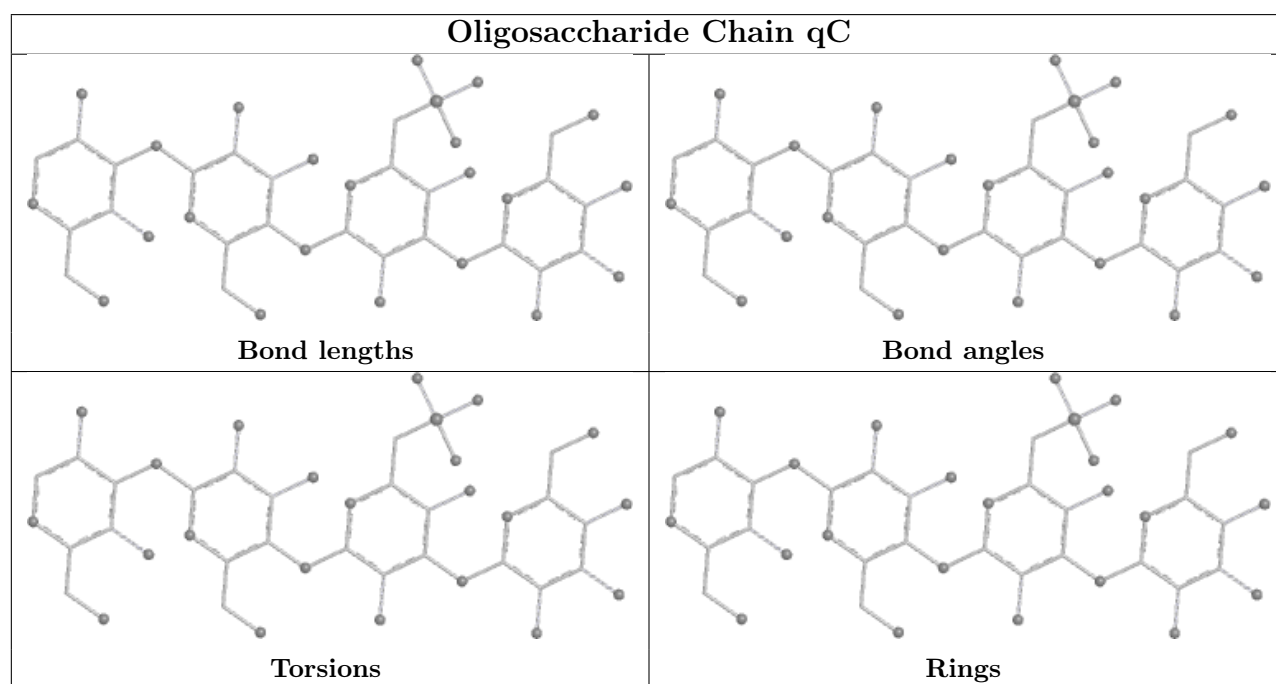
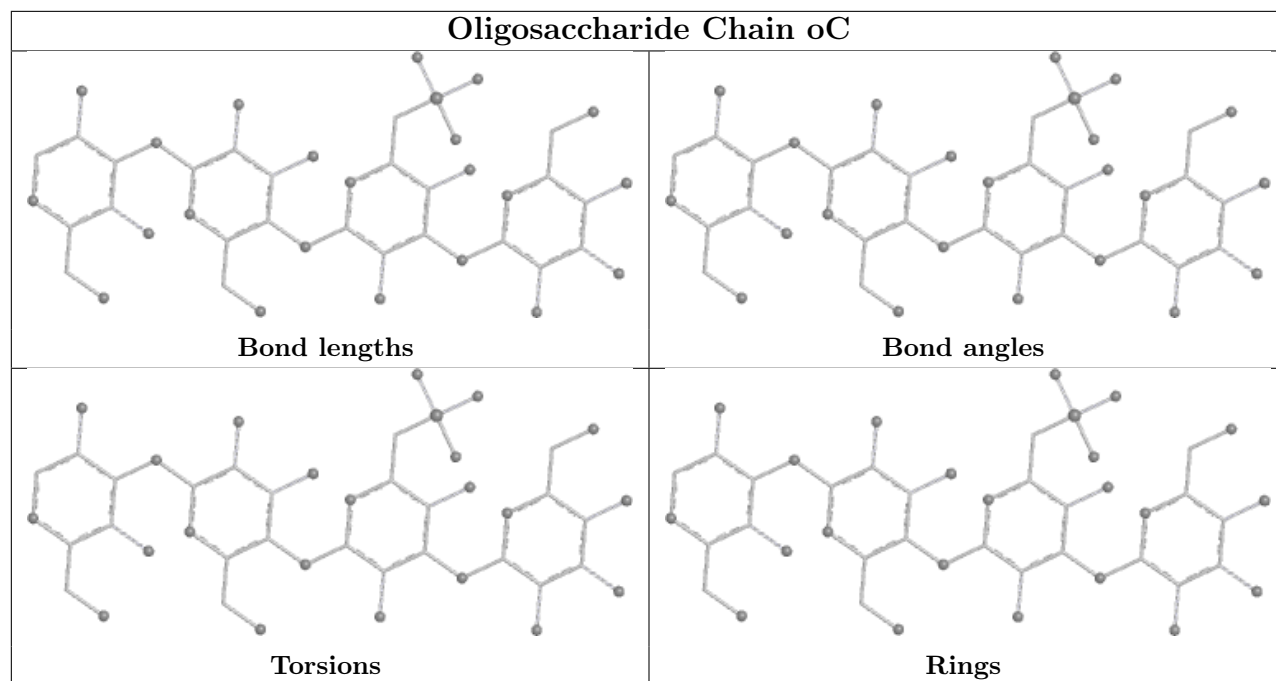
Oligosaccharide Chain aC

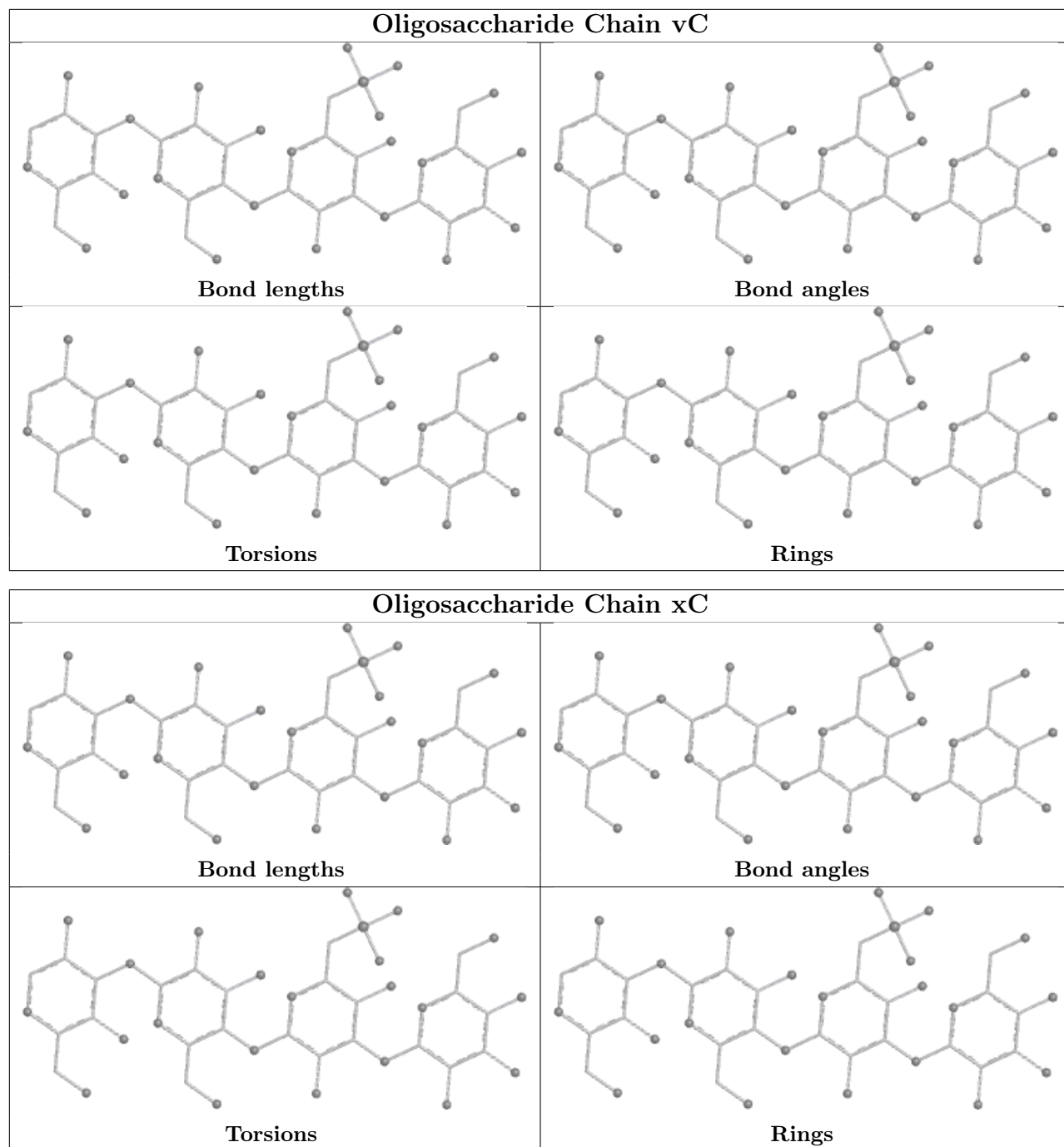


Oligosaccharide Chain cC

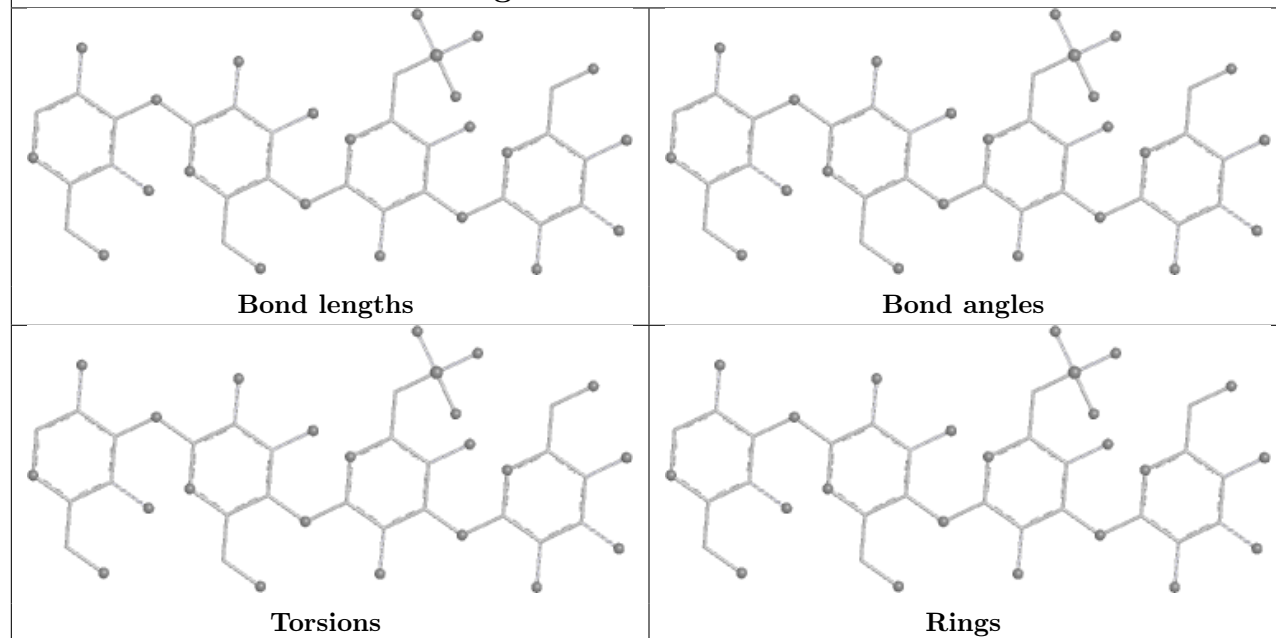




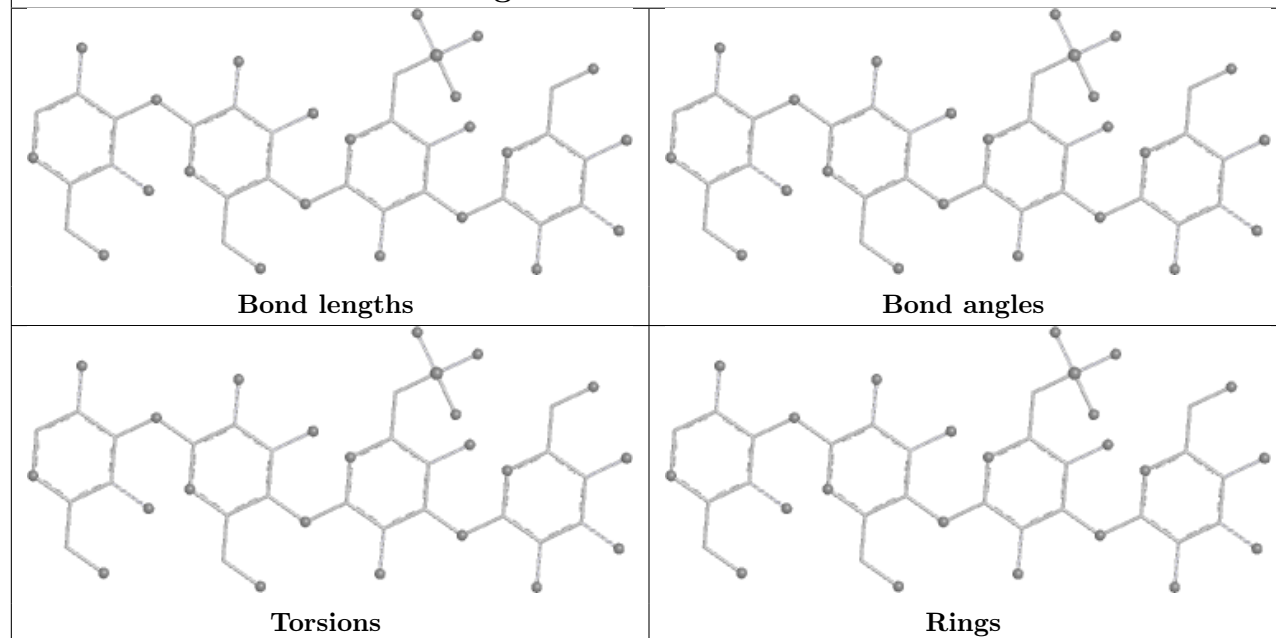




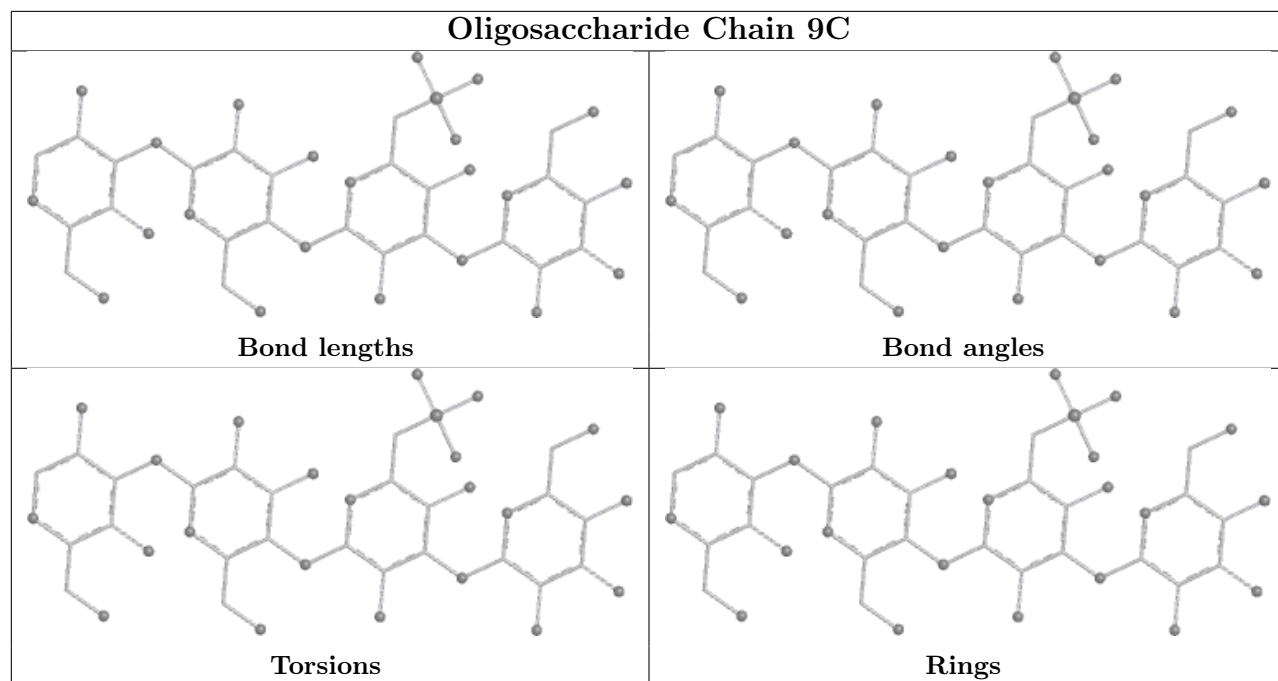
Oligosaccharide Chain 2C



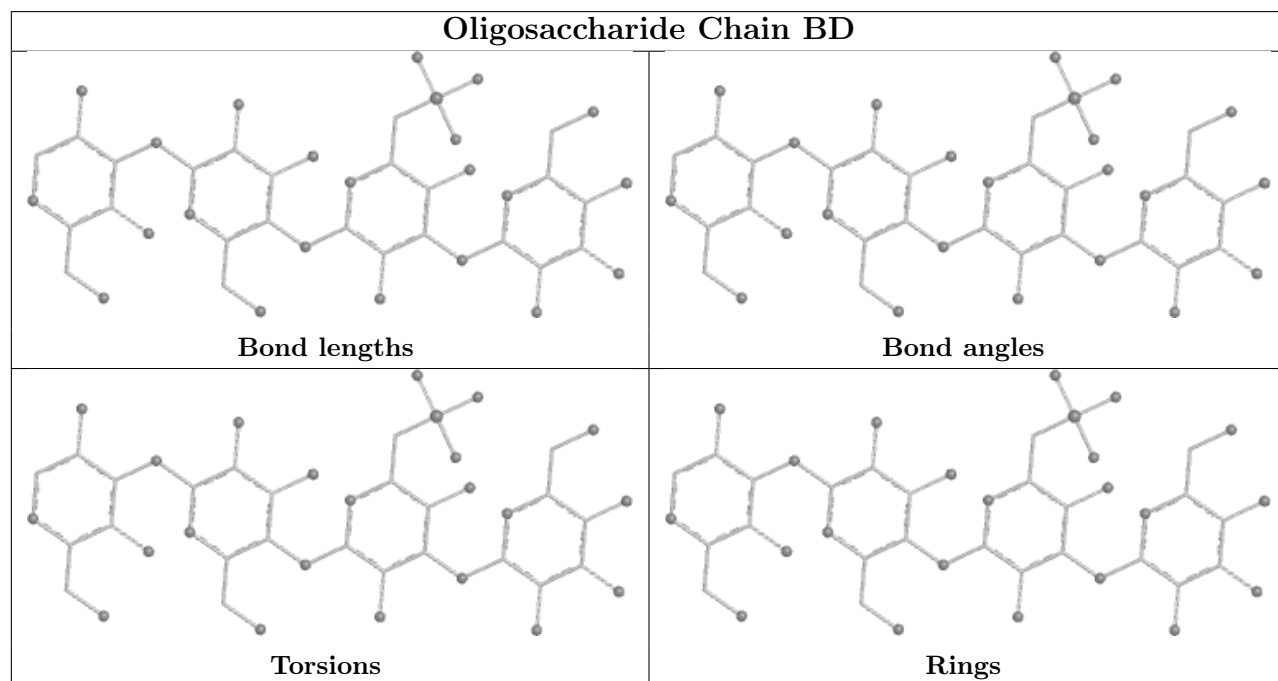
Oligosaccharide Chain 4C

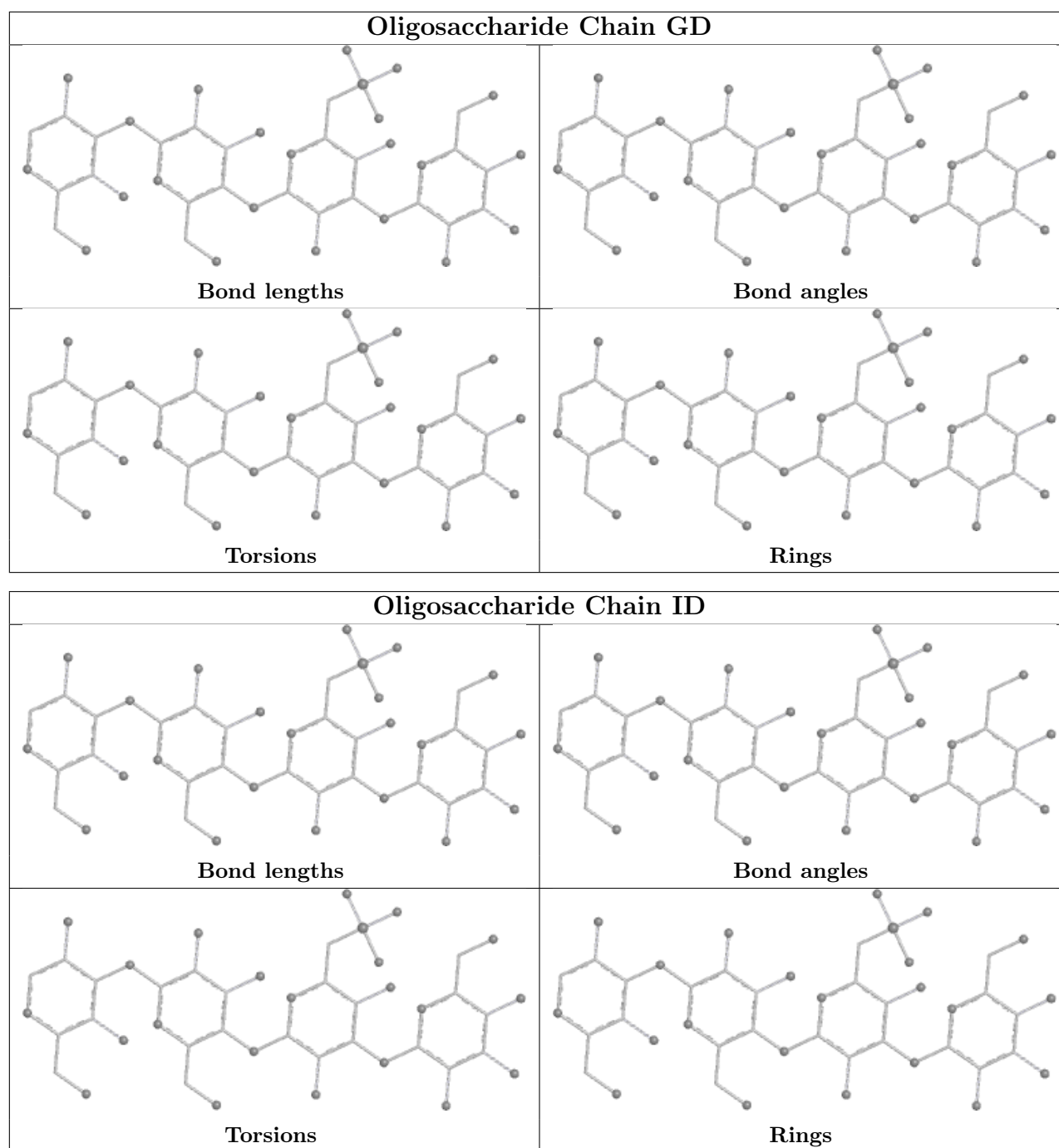


Oligosaccharide Chain 9C



Oligosaccharide Chain BD





5.6 Ligand geometry [i](#)

64 ligands are modelled in this entry.

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GAL	c	310	1	11,11,12	0.60	0	15,15,17	0.73	0
5	GAL	g	310	1	11,11,12	0.58	0	15,15,17	0.79	0
5	GAL	A	311	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	L	310	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	R	310	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	d	311	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	L	309	1	11,11,12	0.59	0	15,15,17	0.74	0
5	GAL	G	309	1	11,11,12	0.59	0	15,15,17	0.74	0
5	GAL	P	309	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	N	309	1	11,11,12	0.58	0	15,15,17	0.74	0
5	GAL	C	311	1	11,11,12	0.57	0	15,15,17	0.77	0
5	GAL	Q	309	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	X	310	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	K	309	1	11,11,12	0.58	0	15,15,17	0.74	0
5	GAL	a	310	1	11,11,12	0.58	0	15,15,17	0.74	0
5	GAL	A	310	1	11,11,12	0.58	0	15,15,17	0.74	0
5	GAL	U	310	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	V	308	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	W	310	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	E	309	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	H	309	1	11,11,12	0.58	0	15,15,17	0.74	0
5	GAL	I	309	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	O	312	1	11,11,12	0.57	0	15,15,17	0.79	0
5	GAL	S	309	1	11,11,12	0.59	0	15,15,17	0.74	0
5	GAL	C	310	1	11,11,12	0.60	0	15,15,17	0.74	0
5	GAL	T	310	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	Y	309	1	11,11,12	0.58	0	15,15,17	0.73	0
5	GAL	W	309	1	11,11,12	0.58	0	15,15,17	0.73	0
5	GAL	H	310	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	D	310	1	11,11,12	0.57	0	15,15,17	0.79	0
5	GAL	M	310	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	O	311	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	J	309	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	F	310	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	E	310	1	11,11,12	0.57	0	15,15,17	0.79	0
5	GAL	F	309	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	T	309	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	S	310	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	b	311	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	B	311	1	11,11,12	0.56	0	15,15,17	0.79	0
5	GAL	I	310	1	11,11,12	0.57	0	15,15,17	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GAL	M	309	1	11,11,12	0.59	0	15,15,17	0.74	0
5	GAL	e	310	1	11,11,12	0.58	0	15,15,17	0.73	0
5	GAL	D	309	1	11,11,12	0.59	0	15,15,17	0.74	0
5	GAL	X	309	1	11,11,12	0.59	0	15,15,17	0.74	0
5	GAL	Y	310	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	b	310	1	11,11,12	0.59	0	15,15,17	0.74	0
5	GAL	f	311	1	11,11,12	0.57	0	15,15,17	0.77	0
5	GAL	Q	310	1	11,11,12	0.56	0	15,15,17	0.78	0
5	GAL	U	309	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	R	309	1	11,11,12	0.60	0	15,15,17	0.74	0
5	GAL	a	311	1	11,11,12	0.58	0	15,15,17	0.77	0
5	GAL	B	310	1	11,11,12	0.58	0	15,15,17	0.74	0
5	GAL	c	311	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	g	309	1	11,11,12	0.58	0	15,15,17	0.73	0
5	GAL	e	311	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	d	310	1	11,11,12	0.59	0	15,15,17	0.73	0
5	GAL	V	309	1	11,11,12	0.57	0	15,15,17	0.78	0
5	GAL	J	310	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	P	310	1	11,11,12	0.58	0	15,15,17	0.77	0
5	GAL	G	310	1	11,11,12	0.57	0	15,15,17	0.79	0
5	GAL	f	310	1	11,11,12	0.59	0	15,15,17	0.74	0
5	GAL	K	310	1	11,11,12	0.58	0	15,15,17	0.78	0
5	GAL	N	310	1	11,11,12	0.58	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
5	GAL	c	310	1	-	0/2/19/22	0/1/1/1
5	GAL	g	310	1	-	0/2/19/22	0/1/1/1
5	GAL	A	311	1	-	0/2/19/22	0/1/1/1
5	GAL	L	310	1	-	0/2/19/22	0/1/1/1
5	GAL	R	310	1	-	0/2/19/22	0/1/1/1
5	GAL	d	311	1	-	0/2/19/22	0/1/1/1
5	GAL	L	309	1	-	0/2/19/22	0/1/1/1
5	GAL	G	309	1	-	0/2/19/22	0/1/1/1
5	GAL	P	309	1	-	0/2/19/22	0/1/1/1
5	GAL	N	309	1	-	0/2/19/22	0/1/1/1
5	GAL	C	311	1	-	0/2/19/22	0/1/1/1
5	GAL	Q	309	1	-	0/2/19/22	0/1/1/1
5	GAL	X	310	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GAL	K	309	1	-	0/2/19/22	0/1/1/1
5	GAL	a	310	1	-	0/2/19/22	0/1/1/1
5	GAL	A	310	1	-	0/2/19/22	0/1/1/1
5	GAL	U	310	1	-	0/2/19/22	0/1/1/1
5	GAL	V	308	1	-	0/2/19/22	0/1/1/1
5	GAL	W	310	1	-	0/2/19/22	0/1/1/1
5	GAL	E	309	1	-	0/2/19/22	0/1/1/1
5	GAL	H	309	1	-	0/2/19/22	0/1/1/1
5	GAL	I	309	1	-	0/2/19/22	0/1/1/1
5	GAL	O	312	1	-	0/2/19/22	0/1/1/1
5	GAL	S	309	1	-	0/2/19/22	0/1/1/1
5	GAL	C	310	1	-	0/2/19/22	0/1/1/1
5	GAL	T	310	1	-	0/2/19/22	0/1/1/1
5	GAL	Y	309	1	-	0/2/19/22	0/1/1/1
5	GAL	W	309	1	-	0/2/19/22	0/1/1/1
5	GAL	H	310	1	-	0/2/19/22	0/1/1/1
5	GAL	D	310	1	-	0/2/19/22	0/1/1/1
5	GAL	M	310	1	-	0/2/19/22	0/1/1/1
5	GAL	O	311	1	-	0/2/19/22	0/1/1/1
5	GAL	J	309	1	-	0/2/19/22	0/1/1/1
5	GAL	F	310	1	-	0/2/19/22	0/1/1/1
5	GAL	E	310	1	-	0/2/19/22	0/1/1/1
5	GAL	F	309	1	-	0/2/19/22	0/1/1/1
5	GAL	T	309	1	-	0/2/19/22	0/1/1/1
5	GAL	S	310	1	-	0/2/19/22	0/1/1/1
5	GAL	b	311	1	-	0/2/19/22	0/1/1/1
5	GAL	B	311	1	-	0/2/19/22	0/1/1/1
5	GAL	I	310	1	-	0/2/19/22	0/1/1/1
5	GAL	M	309	1	-	0/2/19/22	0/1/1/1
5	GAL	e	310	1	-	0/2/19/22	0/1/1/1
5	GAL	D	309	1	-	0/2/19/22	0/1/1/1
5	GAL	X	309	1	-	0/2/19/22	0/1/1/1
5	GAL	Y	310	1	-	0/2/19/22	0/1/1/1
5	GAL	b	310	1	-	0/2/19/22	0/1/1/1
5	GAL	f	311	1	-	0/2/19/22	0/1/1/1
5	GAL	Q	310	1	-	0/2/19/22	0/1/1/1
5	GAL	U	309	1	-	0/2/19/22	0/1/1/1
5	GAL	R	309	1	-	0/2/19/22	0/1/1/1
5	GAL	a	311	1	-	0/2/19/22	0/1/1/1
5	GAL	B	310	1	-	0/2/19/22	0/1/1/1
5	GAL	c	311	1	-	0/2/19/22	0/1/1/1
5	GAL	g	309	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GAL	e	311	1	-	0/2/19/22	0/1/1/1
5	GAL	d	310	1	-	0/2/19/22	0/1/1/1
5	GAL	V	309	1	-	0/2/19/22	0/1/1/1
5	GAL	J	310	1	-	0/2/19/22	0/1/1/1
5	GAL	P	310	1	-	0/2/19/22	0/1/1/1
5	GAL	G	310	1	-	0/2/19/22	0/1/1/1
5	GAL	f	310	1	-	0/2/19/22	0/1/1/1
5	GAL	K	310	1	-	0/2/19/22	0/1/1/1
5	GAL	N	310	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

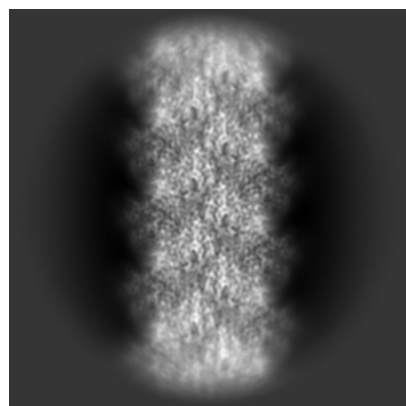
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19168. These allow visual inspection of the internal detail of the map and identification of artifacts.

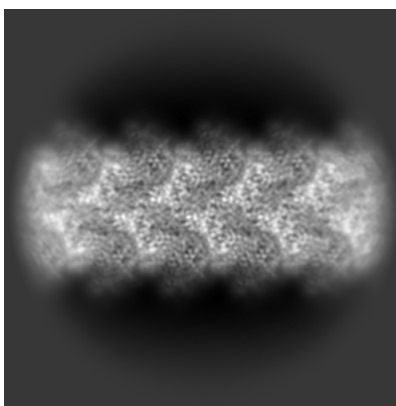
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

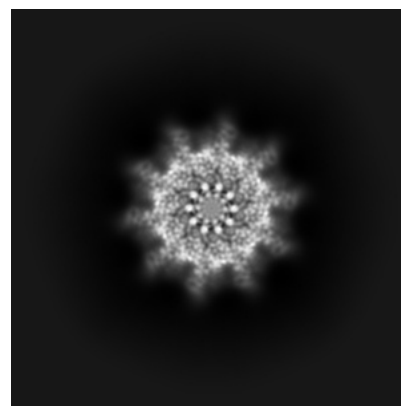
6.1.1 Primary map



X

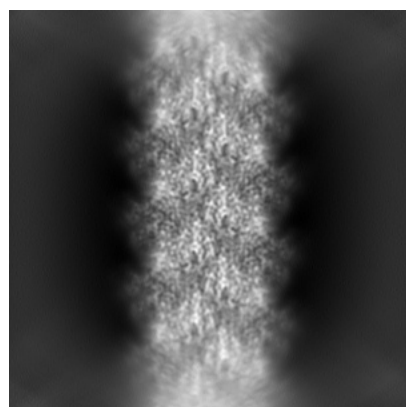


Y

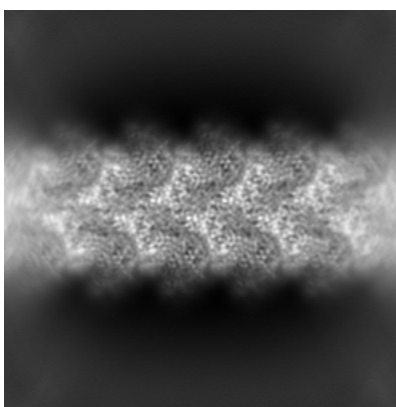


Z

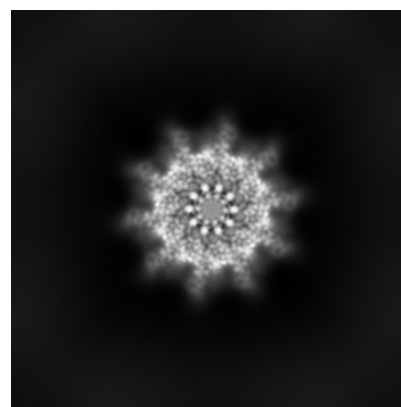
6.1.2 Raw map



X



Y

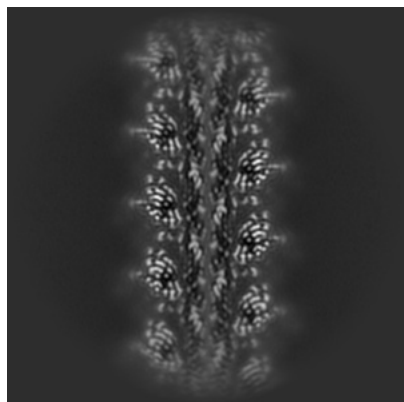


Z

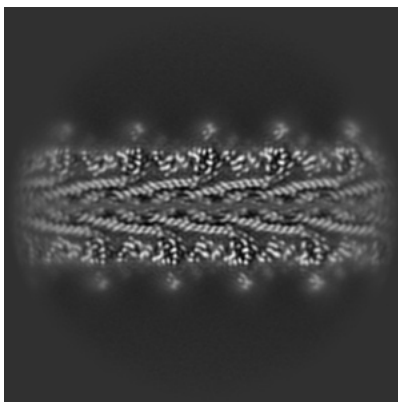
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

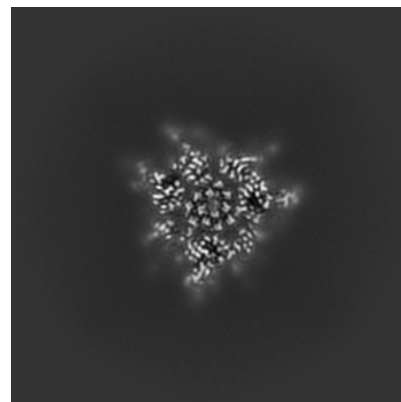
6.2.1 Primary map



X Index: 150

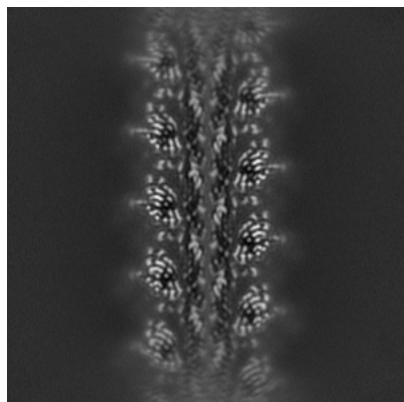


Y Index: 150

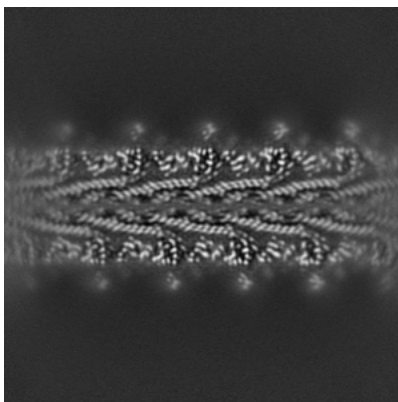


Z Index: 150

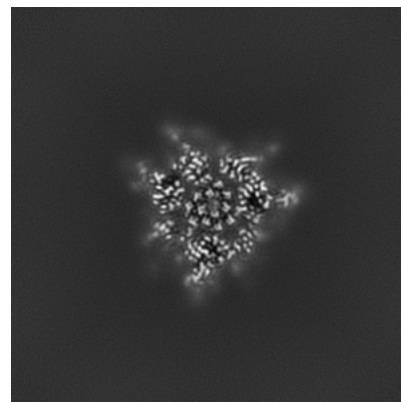
6.2.2 Raw map



X Index: 150



Y Index: 150

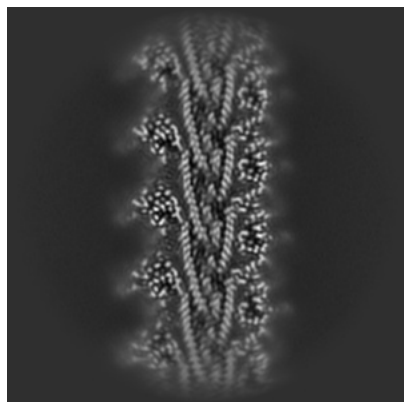


Z Index: 150

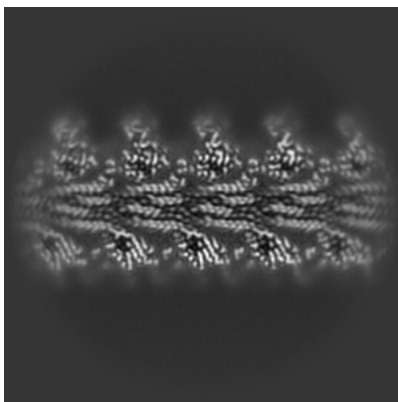
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

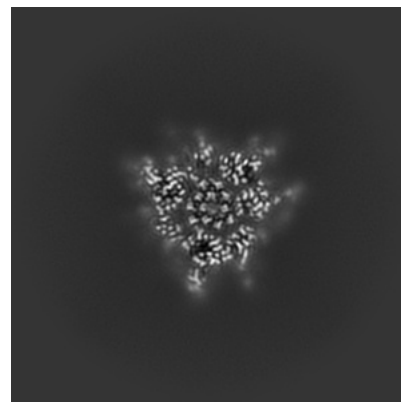
6.3.1 Primary map



X Index: 145

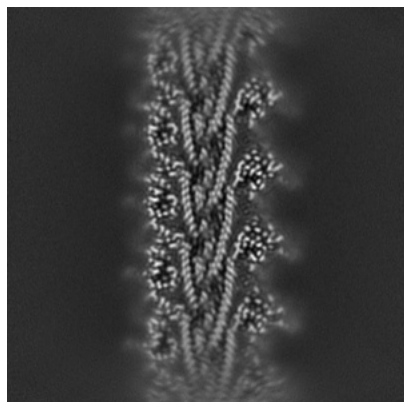


Y Index: 161

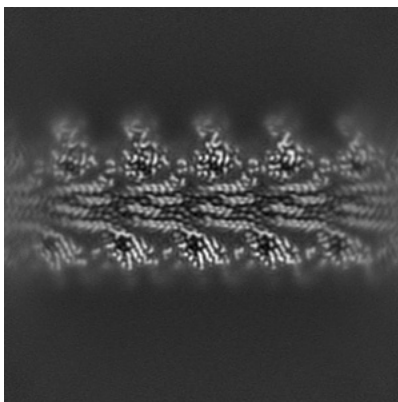


Z Index: 145

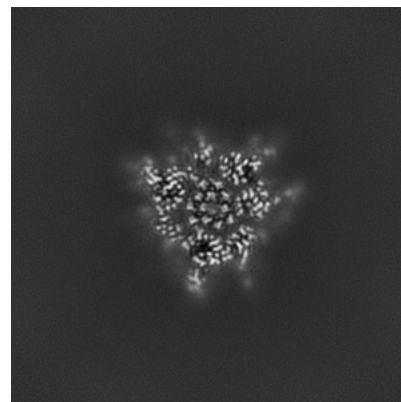
6.3.2 Raw map



X Index: 155



Y Index: 161

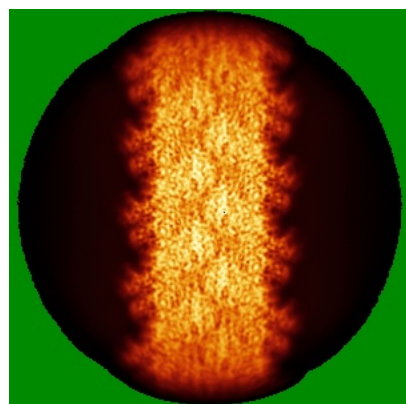


Z Index: 145

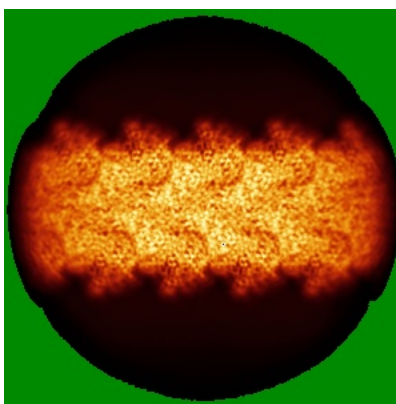
The images above show the largest variance slices of the map in three orthogonal directions.

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

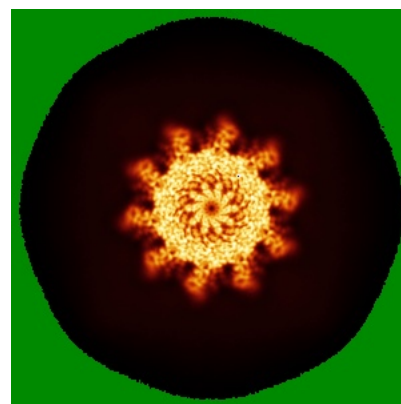
6.4.1 Primary map



X

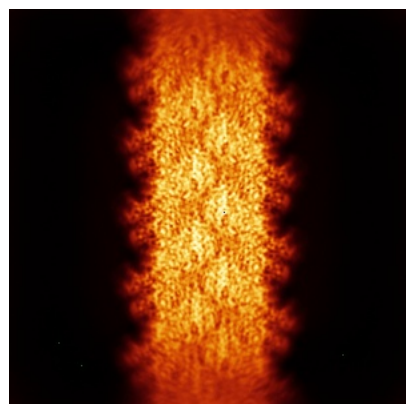


Y

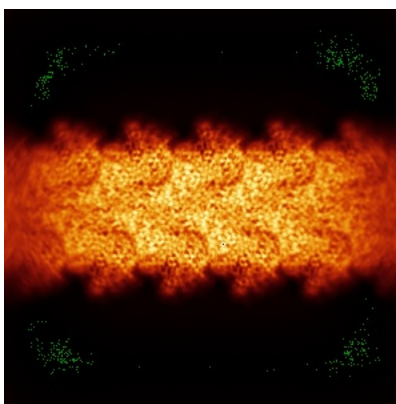


Z

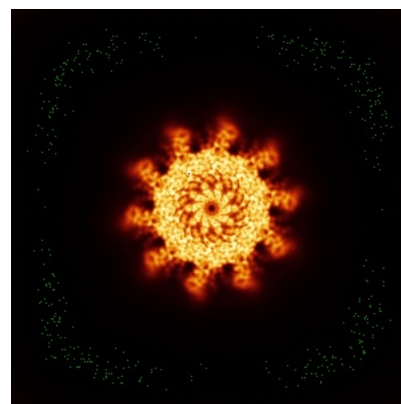
6.4.2 Raw map



X



Y

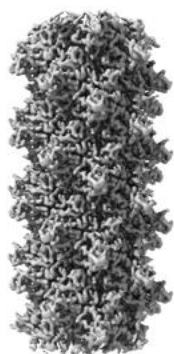


Z

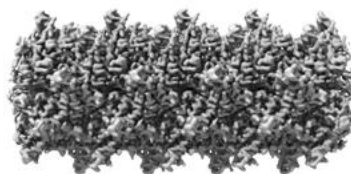
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

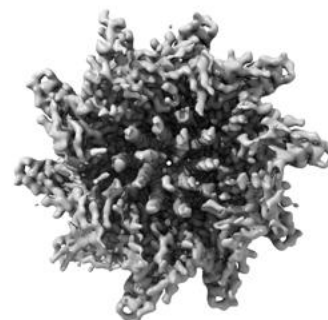
6.5.1 Primary map



X



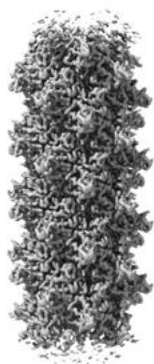
Y



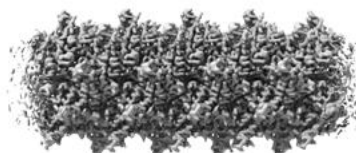
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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



X



Y



Z

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.

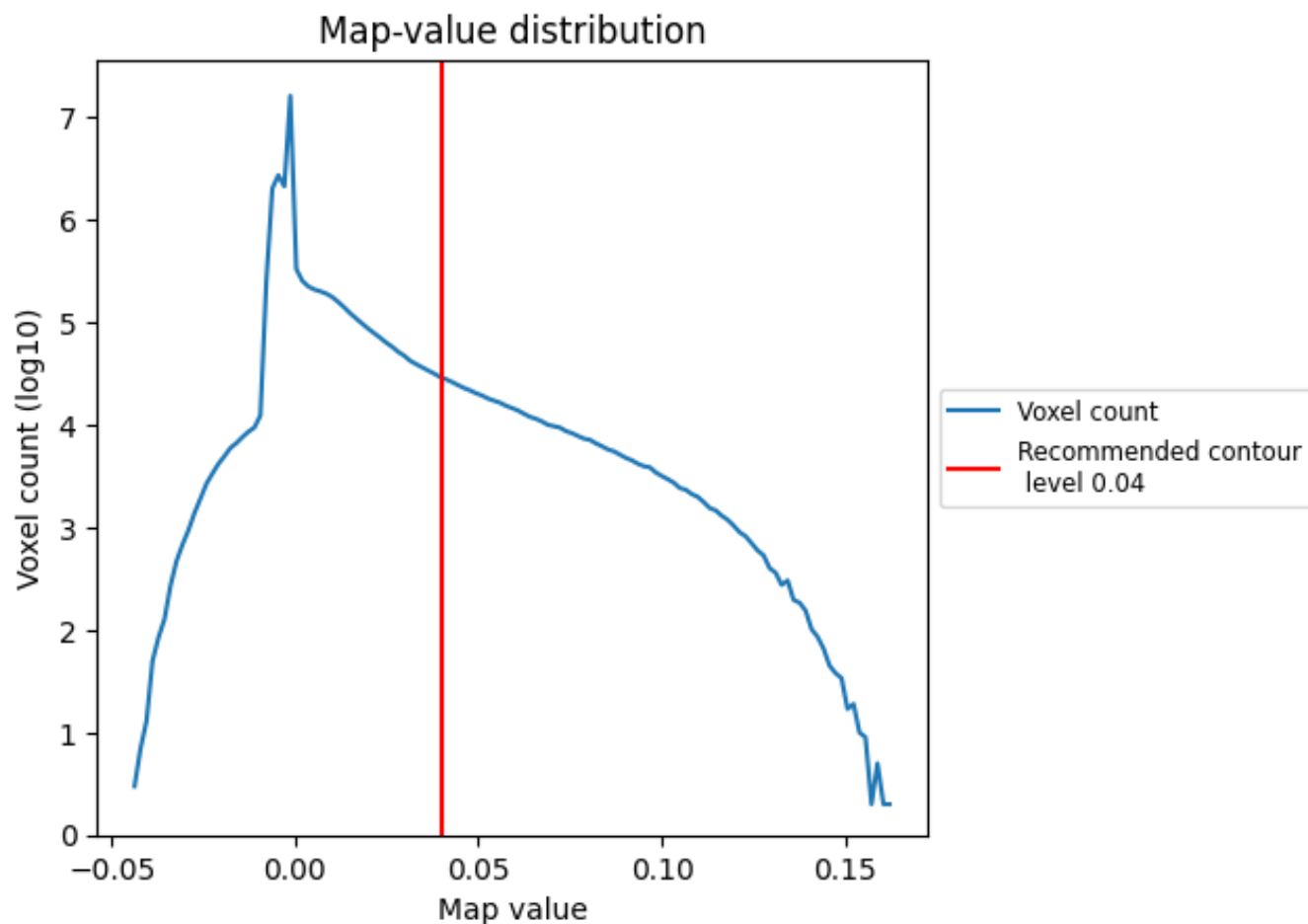
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

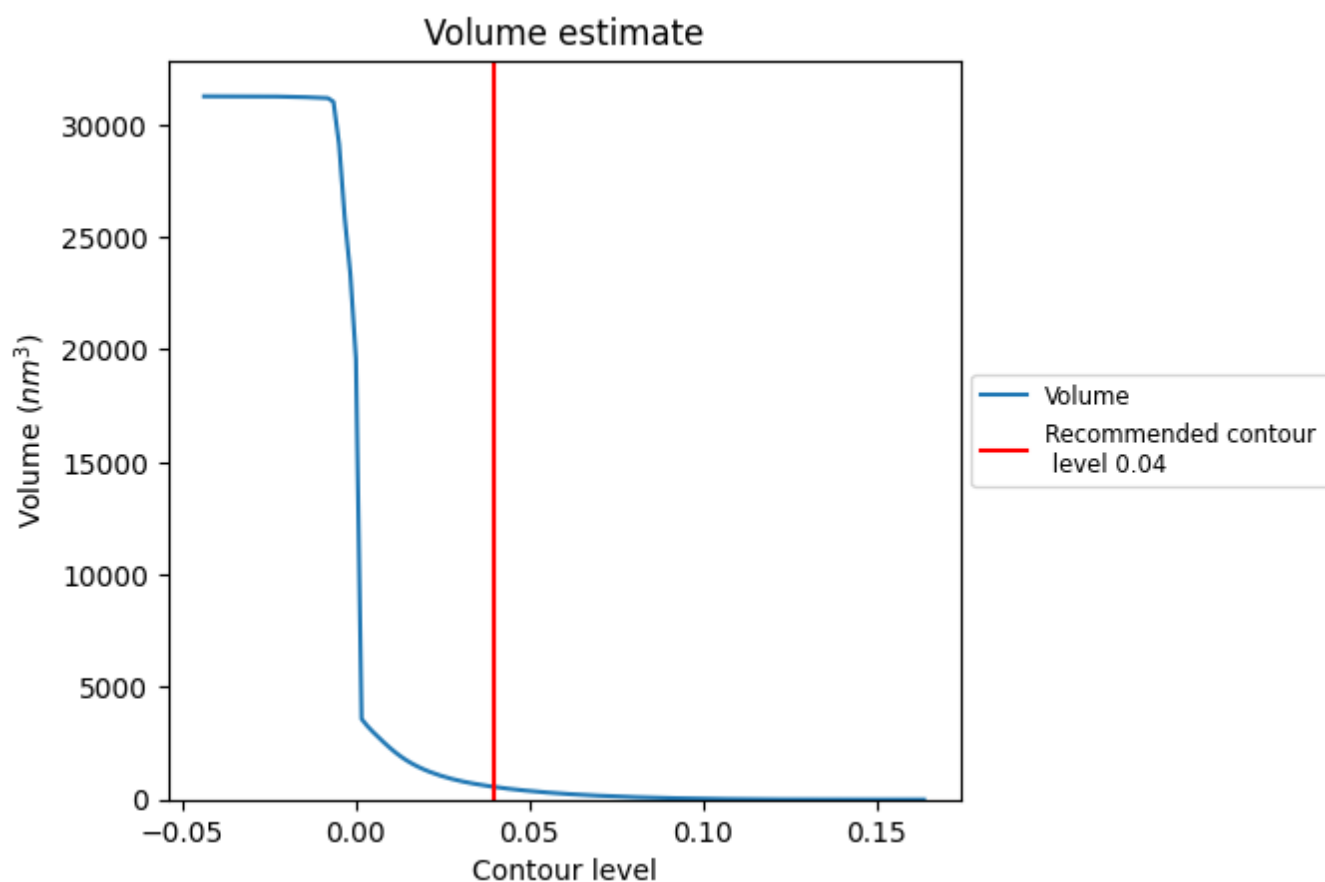
This section contains the results of statistical analysis of the map.

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.

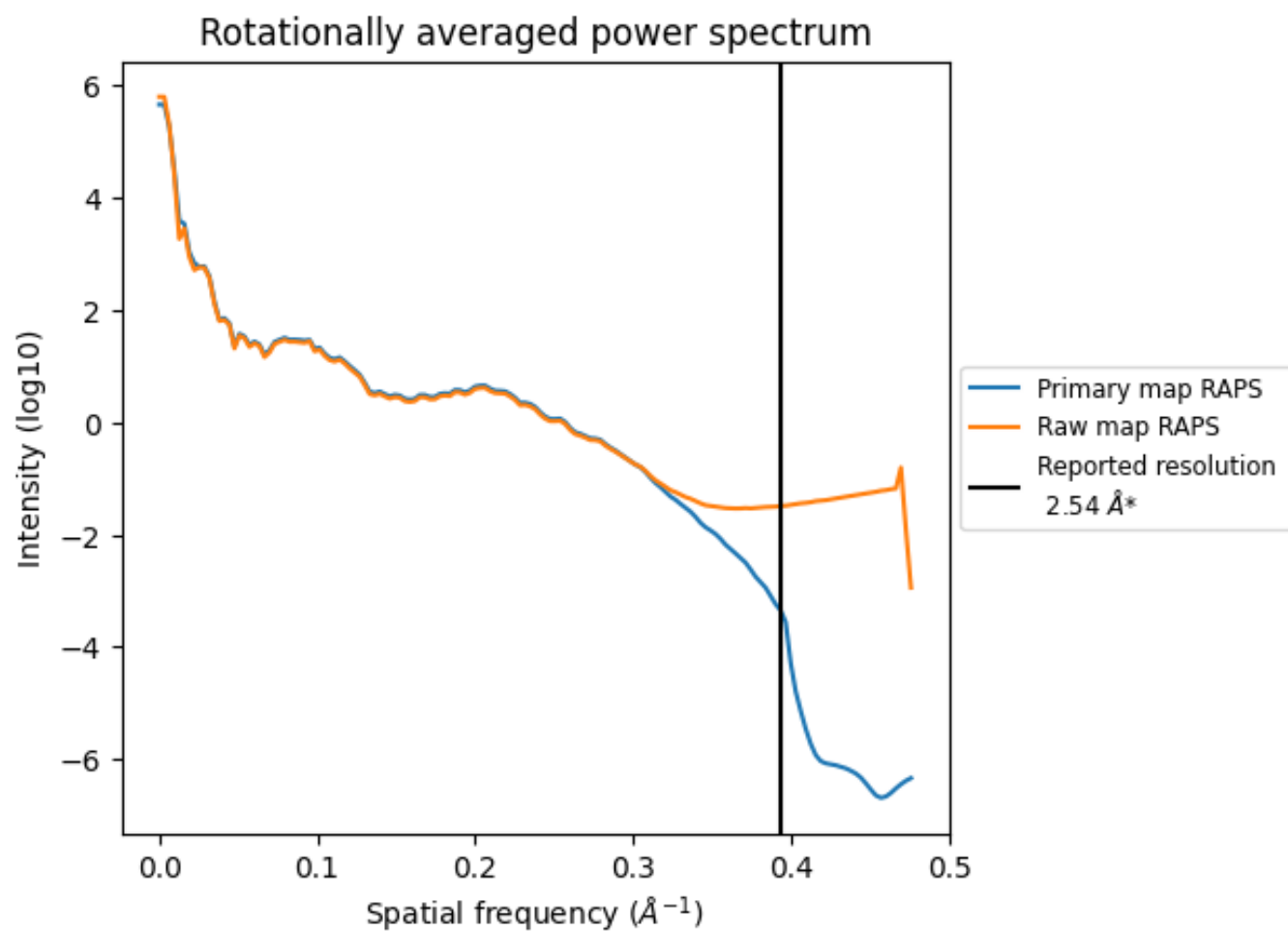
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 560 nm³; this corresponds to an approximate mass of 506 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 ⓘ

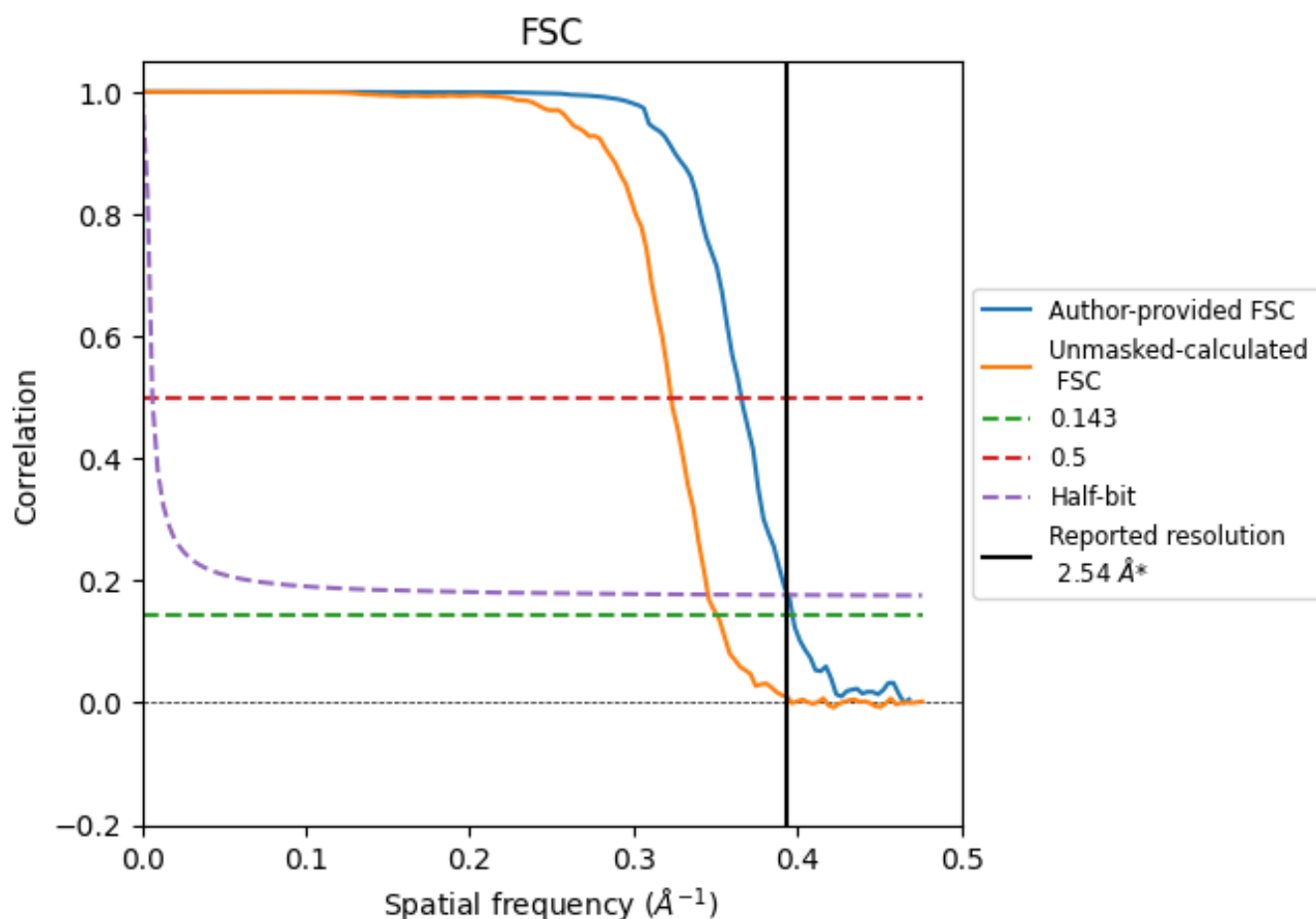


*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

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 0.394 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

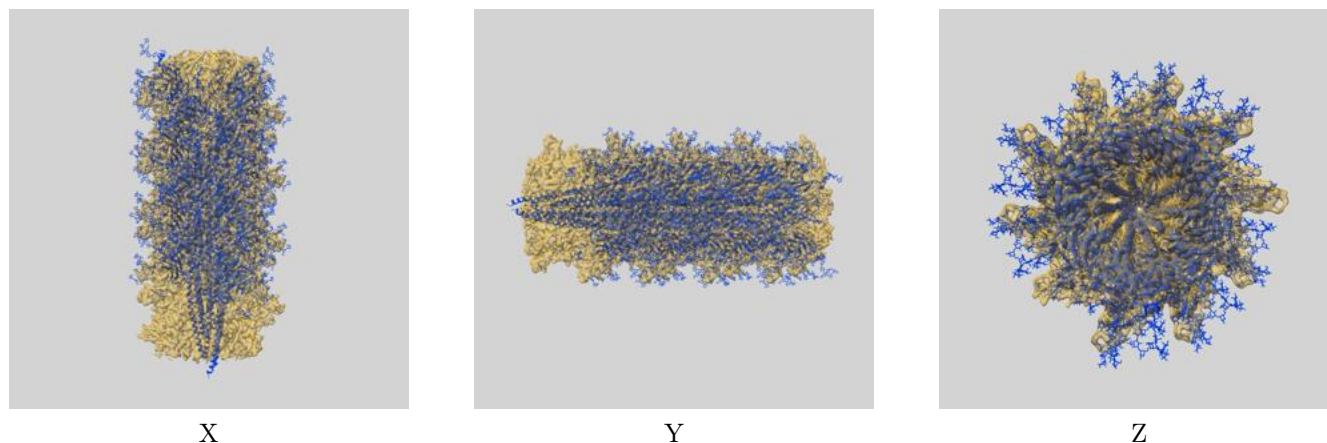
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.52	2.73	2.54
Unmasked-calculated*	2.85	3.10	2.89

*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 2.85 differs from the reported value 2.54 by more than 10 %

9 Map-model fit [i](#)

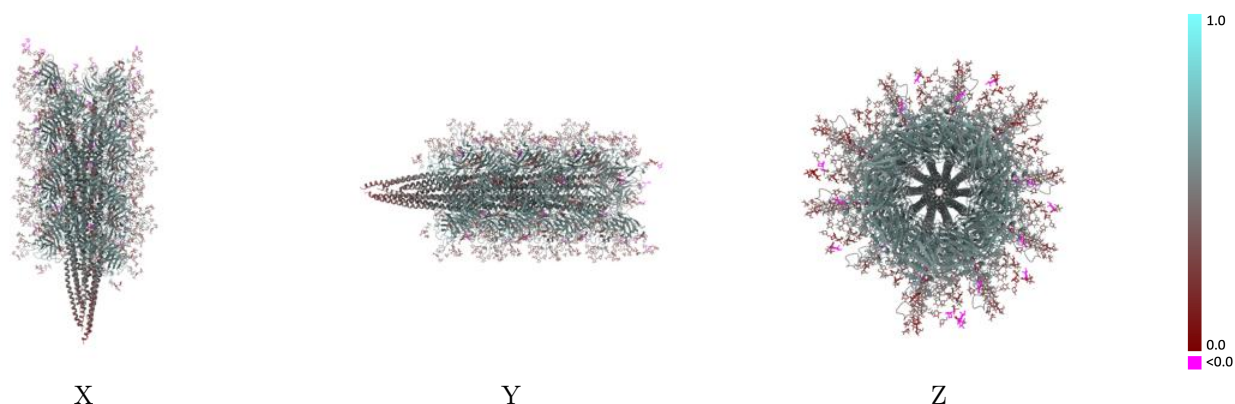
This section contains information regarding the fit between EMDB map EMD-19168 and PDB model 8RH5. Per-residue inclusion information can be found in [section 3](#) on page [27](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)

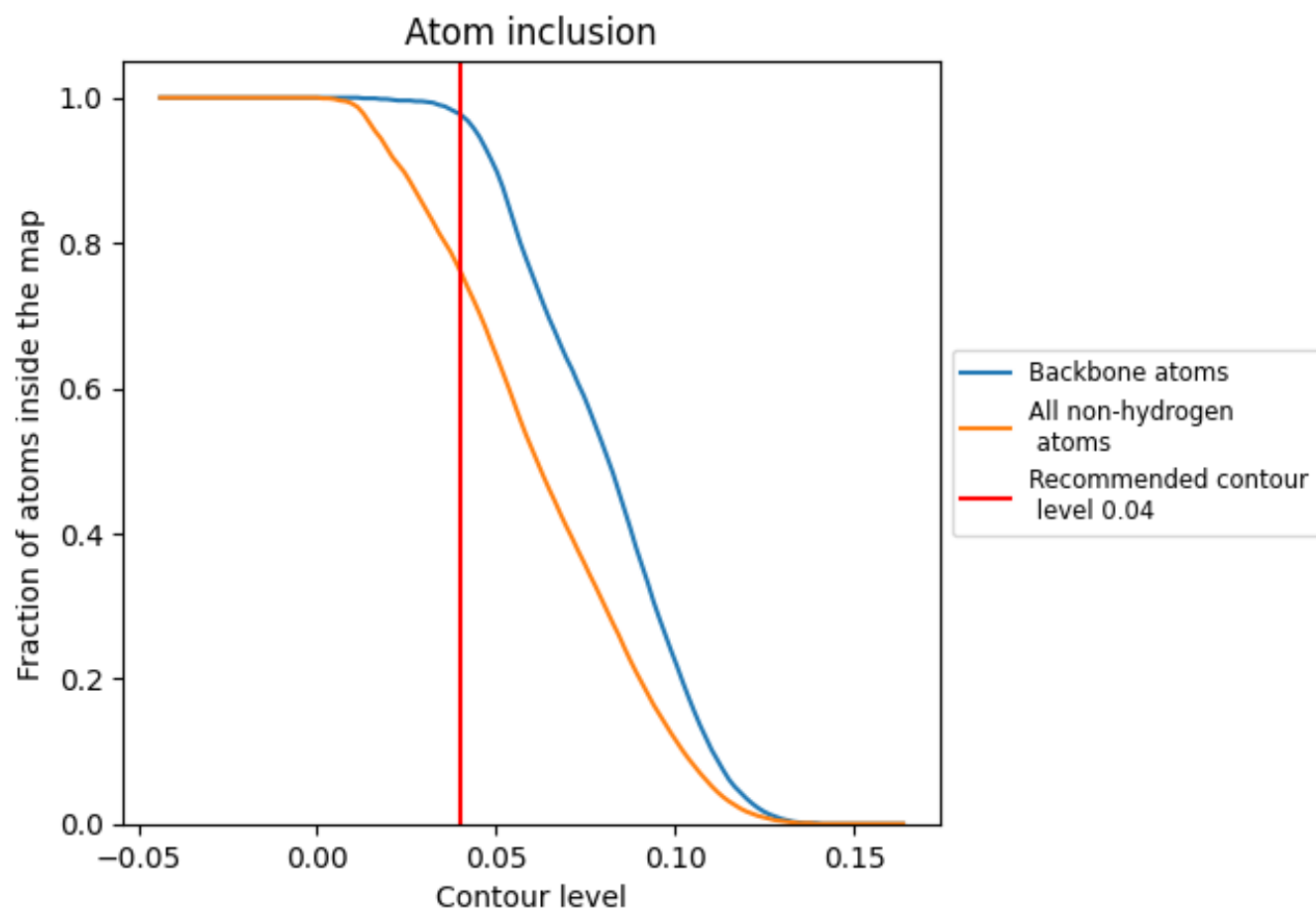


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 76% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7610	 0.5150
0	 0.3170	 0.3410
0A	 0.3400	 0.3680
0B	 0.3170	 0.3230
0C	 0.3330	 0.2700
1	 0.3620	 0.4000
1A	 0.3500	 0.3350
1B	 0.3400	 0.3510
1C	 0.3170	 0.3010
2	 0.1270	 0.2820
2A	 0.4470	 0.4220
2B	 0.3330	 0.3320
2C	 0.2340	 0.3230
3A	 0.1270	 0.2540
3B	 0.3830	 0.4200
3C	 0.2500	 0.3090
4	 0.3830	 0.2650
4B	 0.0990	 0.2730
4C	 0.3190	 0.3840
5	 0.3330	 0.3090
5A	 0.4170	 0.2680
5C	 0.0000	 0.1600
6	 0.3400	 0.3450
6A	 0.3170	 0.3180
6B	 0.4170	 0.2720
7	 0.3000	 0.3440
7A	 0.3400	 0.3660
7B	 0.3170	 0.3040
7C	 0.3000	 0.2680
8	 0.3620	 0.4010
8A	 0.3330	 0.3410
8B	 0.3400	 0.3660
8C	 0.3000	 0.3100
9	 0.1270	 0.2710
9A	 0.4250	 0.4160



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Chain	Atom inclusion	Q-score
9B	 0.3330	 0.3290
9C	 0.1920	 0.3140
A	 0.7910	 0.5260
AB	 0.1270	 0.2460
AC	 0.4040	 0.4180
AD	 0.2500	 0.3090
B	 0.8110	 0.5310
BA	 0.4000	 0.2690
BC	 0.0850	 0.2820
BD	 0.3190	 0.3800
C	 0.8260	 0.5400
CA	 0.3170	 0.3030
CB	 0.4170	 0.2660
CD	 0.0000	 0.0960
D	 0.8380	 0.5430
DA	 0.3400	 0.3460
DB	 0.3170	 0.3130
DC	 0.4000	 0.2650
E	 0.8510	 0.5500
EA	 0.3330	 0.3410
EB	 0.3400	 0.3660
EC	 0.3170	 0.3170
ED	 0.2000	 0.2590
F	 0.8600	 0.5530
FA	 0.4040	 0.4180
FB	 0.3330	 0.3470
FC	 0.3400	 0.3490
FD	 0.3000	 0.3100
G	 0.8670	 0.5550
GA	 0.1270	 0.2850
GB	 0.4890	 0.4160
GC	 0.3170	 0.3270
GD	 0.1920	 0.3030
H	 0.8700	 0.5600
HB	 0.1270	 0.2400
HC	 0.3830	 0.4150
HD	 0.1830	 0.2810
I	 0.8740	 0.5610
IA	 0.4000	 0.2690
IC	 0.0850	 0.2720
ID	 0.2340	 0.3700
J	 0.8770	 0.5650

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Chain	Atom inclusion	Q-score
JA	 0.3330	 0.3030
JB	 0.4000	 0.2670
K	 0.8810	 0.5670
KA	 0.3400	 0.3620
KB	 0.3170	 0.3020
KC	 0.4000	 0.2660
L	 0.8830	 0.5650
LA	 0.3330	 0.3440
LB	 0.3400	 0.3640
LC	 0.3330	 0.3040
M	 0.8860	 0.5690
MA	 0.3830	 0.4140
MB	 0.3330	 0.3380
MC	 0.3400	 0.3570
N	 0.8870	 0.5680
NA	 0.1270	 0.2790
NB	 0.4040	 0.4200
NC	 0.3000	 0.3250
O	 0.8840	 0.5690
OB	 0.1270	 0.2420
OC	 0.4040	 0.4220
P	 0.8840	 0.5710
PA	 0.4000	 0.2710
PC	 0.0850	 0.2680
Q	 0.8860	 0.5700
QA	 0.3330	 0.3110
QB	 0.4000	 0.2760
R	 0.8870	 0.5690
RA	 0.3400	 0.3590
RB	 0.3170	 0.3270
RC	 0.4000	 0.2760
S	 0.8840	 0.5700
SA	 0.3330	 0.3440
SB	 0.3400	 0.3710
SC	 0.3330	 0.3140
T	 0.8820	 0.5670
TA	 0.4250	 0.4120
TB	 0.3330	 0.3380
TC	 0.3400	 0.3610
U	 0.8800	 0.5670
UA	 0.1270	 0.2840
UB	 0.4250	 0.4200

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Chain	Atom inclusion	Q-score
UC	 0.2830	 0.3210
V	 0.8800	 0.5660
VB	 0.1130	 0.2420
VC	 0.3830	 0.4050
W	 0.8740	 0.5640
WA	 0.4000	 0.2670
WC	 0.0850	 0.2600
X	 0.8710	 0.5620
XA	 0.3330	 0.3100
XB	 0.4000	 0.2640
Y	 0.8650	 0.5600
YA	 0.3400	 0.3560
YB	 0.3170	 0.3150
YC	 0.4000	 0.2700
Z	 0.8640	 0.5580
ZA	 0.3170	 0.3400
ZB	 0.3400	 0.3630
ZC	 0.3170	 0.3110
a	 0.8540	 0.5530
aA	 0.4470	 0.4150
aB	 0.3330	 0.3400
aC	 0.3190	 0.3530
b	 0.8440	 0.5490
bA	 0.1270	 0.2840
bB	 0.4250	 0.4170
bC	 0.2830	 0.3240
c	 0.8290	 0.5450
cB	 0.1270	 0.2550
cC	 0.3620	 0.3930
d	 0.8130	 0.5410
dA	 0.4000	 0.2720
dC	 0.0850	 0.2390
e	 0.7970	 0.5340
eA	 0.3170	 0.2960
eB	 0.4170	 0.2700
f	 0.7730	 0.5260
fA	 0.3400	 0.3610
fB	 0.3170	 0.3160
fC	 0.3830	 0.2700
g	 0.7170	 0.5180
gA	 0.3500	 0.3470
gB	 0.3400	 0.3620

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Chain	Atom inclusion	Q-score
gC	 0.3170	 0.3010
h	 0.0990	 0.2790
hA	 0.4250	 0.4230
hB	 0.3330	 0.3270
hC	 0.2980	 0.3420
iA	 0.1270	 0.2660
iB	 0.3830	 0.4140
iC	 0.2670	 0.3170
j	 0.4000	 0.2670
jB	 0.1270	 0.2590
jC	 0.3400	 0.4020
k	 0.3170	 0.3070
kA	 0.4000	 0.2650
kC	 0.0850	 0.2230
l	 0.3400	 0.3510
lA	 0.3170	 0.3110
lB	 0.4170	 0.2710
m	 0.3170	 0.3290
mA	 0.3400	 0.3720
mB	 0.3170	 0.3040
mC	 0.3670	 0.2730
n	 0.4040	 0.4130
nA	 0.3330	 0.3570
nB	 0.3400	 0.3550
nC	 0.3170	 0.3080
o	 0.1130	 0.2630
oA	 0.4040	 0.4210
oB	 0.3330	 0.3220
oC	 0.2980	 0.3500
pA	 0.1270	 0.2630
pB	 0.4250	 0.4310
pC	 0.2670	 0.3300
q	 0.3830	 0.2690
qB	 0.1130	 0.2630
qC	 0.3400	 0.3960
r	 0.3000	 0.2950
rA	 0.4170	 0.2600
rC	 0.0850	 0.1990
s	 0.3400	 0.3510
sA	 0.3170	 0.3190
sB	 0.4170	 0.2670
t	 0.3170	 0.3300

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Chain	Atom inclusion	Q-score
tA	 0.3400	 0.3600
tB	 0.3170	 0.3060
tC	 0.3500	 0.2650
u	 0.3620	 0.4000
uA	 0.3330	 0.3460
uB	 0.3400	 0.3660
uC	 0.3170	 0.3180
v	 0.1270	 0.2810
vA	 0.4680	 0.4240
vB	 0.3330	 0.3390
vC	 0.2770	 0.3270
wA	 0.1270	 0.2510
wB	 0.4250	 0.4190
wC	 0.2670	 0.3100
x	 0.4000	 0.2640
xB	 0.1130	 0.2650
xC	 0.3190	 0.3790
y	 0.3000	 0.3060
yA	 0.3830	 0.2630
yC	 0.0280	 0.1730
z	 0.3400	 0.3490
zA	 0.3330	 0.3050
zB	 0.4000	 0.2660