



Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 01:05 PM EDT

PDB ID : 9NAI
EMDB ID : EMD-49195
Title : LuIII VLP - Glycan [s(Lex)2]
Authors : Busuttil, K.B.; Bennett, A.B.
Deposited on : 2025-02-12
Resolution : 2.88 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

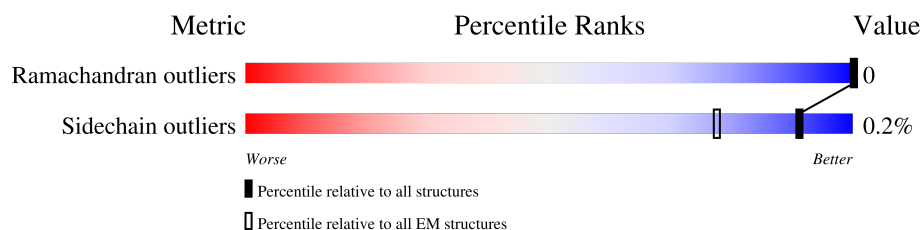
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



The reported resolution of this entry is 2.88 Å.

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



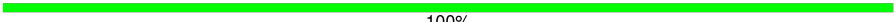
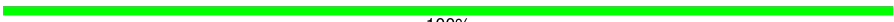













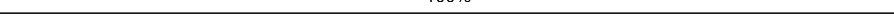
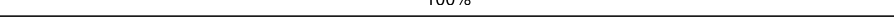
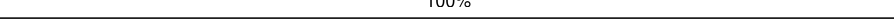
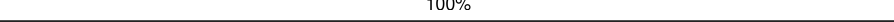
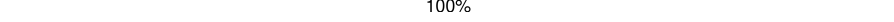
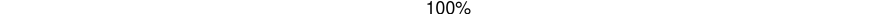
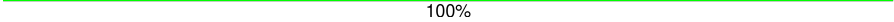
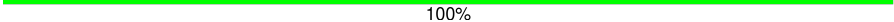

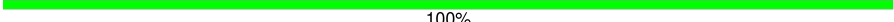
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	551	 100%
1	2	551	 100%
1	3	551	 100%
1	4	551	 100%
1	5	551	 100%
1	6	551	 100%
1	7	551	 100%
1	8	551	 100%
1	A	551	 100%

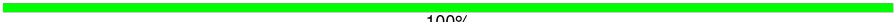
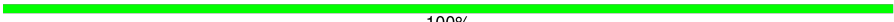
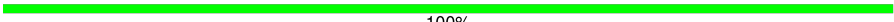
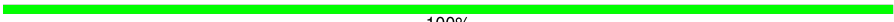
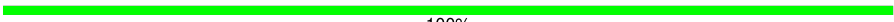
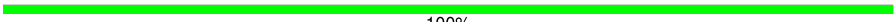
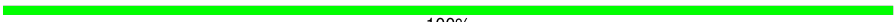
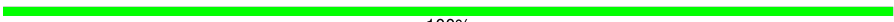
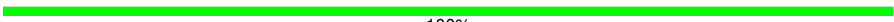
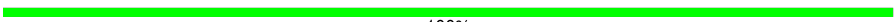















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Mol	Chain	Length	Quality of chain
1	B	551	 100%
1	C	551	 100%
1	D	551	 100%
1	E	551	 100%
1	F	551	 100%
1	G	551	 100%
1	H	551	 100%
1	I	551	 100%
1	J	551	 100%
1	K	551	 100%
1	L	551	 100%
1	M	551	 100%
1	N	551	 100%
1	O	551	 100%
1	P	551	 100%
1	Q	551	 100%
1	R	551	 100%
1	S	551	 100%
1	T	551	 100%
1	U	551	 100%
1	V	551	 100%
1	W	551	 100%
1	X	551	 100%
1	Y	551	 100%
1	Z	551	 100%

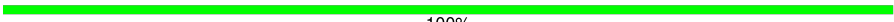


























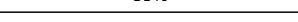

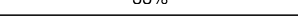
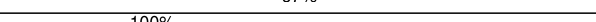
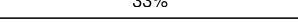
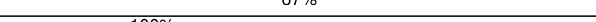
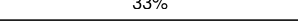
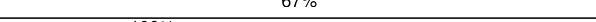
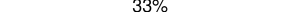
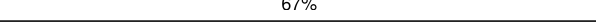
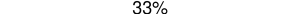
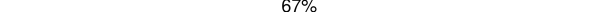
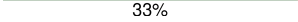
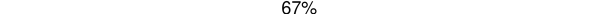

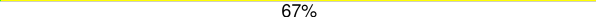

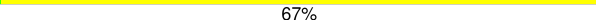
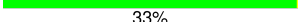
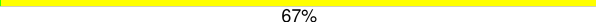

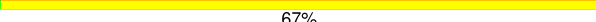
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Mol	Chain	Length	Quality of chain
1	a	551	 100%
1	b	551	 100%
1	c	551	 100%
1	d	551	 100%
1	e	551	 100%
1	f	551	 100%
1	g	551	 100%
1	h	551	 100%
1	i	551	 100%
1	j	551	 100%
1	k	551	 100%
1	l	551	 100%
1	m	551	 100%
1	n	551	 100%
1	o	551	 100%
1	p	551	 100%
1	q	551	 100%
1	r	551	 100%
1	s	551	 100%
1	t	551	 100%
1	u	551	 100%
1	v	551	 100%
1	w	551	 100%
1	x	551	 100%
1	y	551	 100%

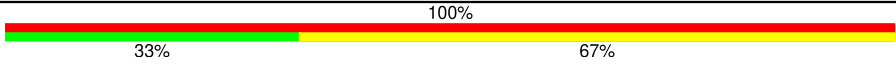

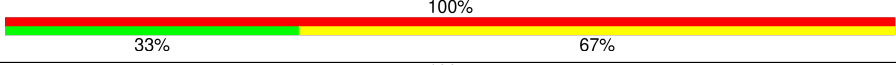
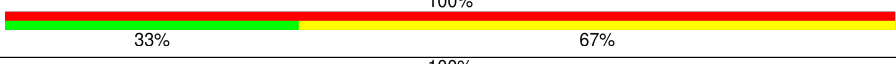
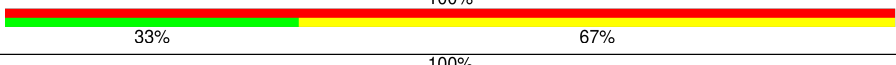
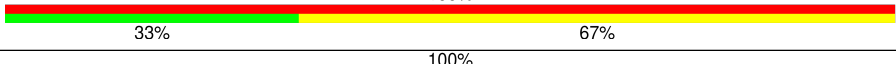
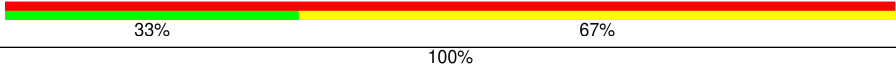
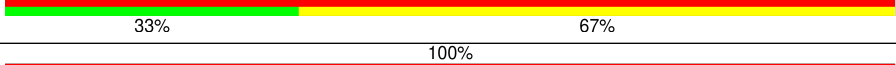

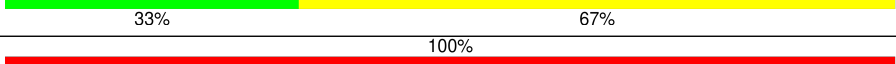


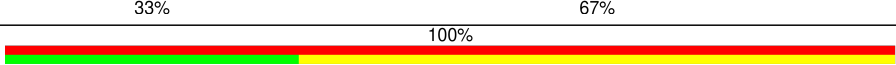
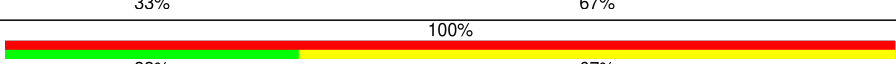
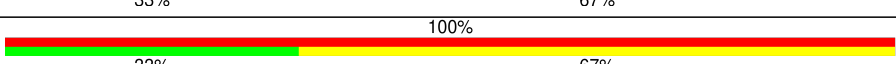
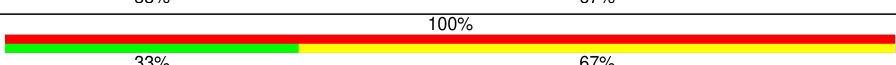
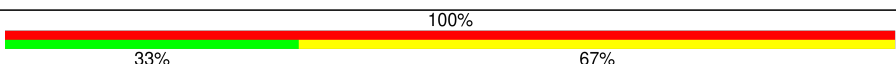
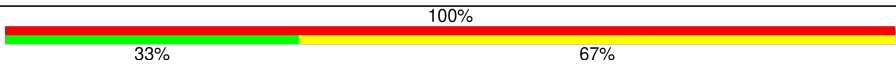


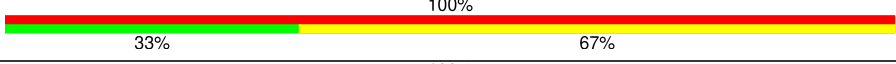
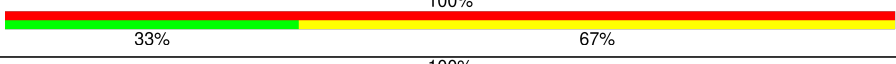
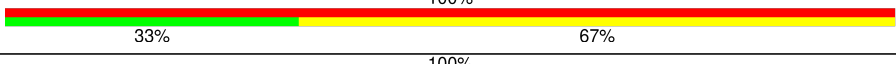


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Mol	Chain	Length	Quality of chain	
1	z	551	 100%	
2	0	3	 33%  67%	
2	0A	3	 33%  67%	
2	1B	3	 33%  67%	
2	3A	3	 33%  67%	
2	4B	3	 33%  67%	
2	6A	3	 33%  67%	
2	7B	3	 33%  67%	
2	9A	3	 33%  67%	
2	AC	3	 33%  67%	
2	BA	3	 33%  67%	
2	CB	3	 33%  67%	
2	DC	3	 33%  67%	
2	EA	3	 33%  67%	
2	FB	3	 33%  67%	
2	GC	3	 33%  67%	
2	HA	3	 33%  67%	
2	IB	3	 33%  67%	
2	JC	3	 33%  67%	
2	KA	3	 33%  67%	
2	LB	3	 33%  67%	
2	MC	3	 33%  67%	
2	NA	3	 33%  67%	
2	OB	3	 33%  67%	
2	PC	3	 33%  67%	

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Mol	Chain	Length	Quality of chain	
2	QA	3		100%
2	RB	3		100%
2	SC	3		100%
2	TA	3		100%
2	UB	3		100%
2	VC	3		100%
2	WA	3		100%
2	XB	3		100%
2	YC	3		100%
2	ZA	3		100%
2	aB	3		100%
2	bC	3		100%
2	cA	3		100%
2	dB	3		100%
2	eC	3		100%
2	fA	3		100%
2	gB	3		100%
2	hC	3		100%
2	iA	3		100%
2	jB	3		100%
2	kC	3		100%
2	lA	3		100%
2	mB	3		100%
2	nC	3		100%
2	oA	3		100%

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Mol	Chain	Length	Quality of chain	
2	pB	3		
2	qC	3		
2	rA	3		
2	sB	3		
2	tC	3		
2	uA	3		
2	vB	3		
2	wC	3		
2	xA	3		
2	yB	3		
2	zC	3		

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 266820 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	B	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	C	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	D	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	E	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	F	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	G	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	H	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	I	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	J	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	K	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	L	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	M	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	N	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	O	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	P	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		
1	Q	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	S	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	T	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	U	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	V	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	W	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	X	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	Y	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	Z	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	a	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	b	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	c	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	d	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	e	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	f	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	g	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	h	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	i	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	j	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	k	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	l	551	Total 4401	C 2767	N 773	O 846	S 15	1	0

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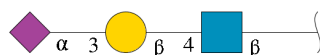
Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	n	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	o	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	p	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	q	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	r	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	s	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	t	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	u	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	v	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	w	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	x	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	y	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	z	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	1	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	2	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	3	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	4	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	5	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	6	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	7	551	Total 4401	C 2767	N 773	O 846	S 15	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	551	Total	C	N	O	S	1	0
			4401	2767	773	846	15		

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	0	3	Total	C	N	O	0	0
			46	25	2	19		
2	BA	3	Total	C	N	O	0	0
			46	25	2	19		
2	EA	3	Total	C	N	O	0	0
			46	25	2	19		
2	HA	3	Total	C	N	O	0	0
			46	25	2	19		
2	KA	3	Total	C	N	O	0	0
			46	25	2	19		
2	NA	3	Total	C	N	O	0	0
			46	25	2	19		
2	QA	3	Total	C	N	O	0	0
			46	25	2	19		
2	TA	3	Total	C	N	O	0	0
			46	25	2	19		
2	WA	3	Total	C	N	O	0	0
			46	25	2	19		
2	ZA	3	Total	C	N	O	0	0
			46	25	2	19		
2	cA	3	Total	C	N	O	0	0
			46	25	2	19		
2	fA	3	Total	C	N	O	0	0
			46	25	2	19		
2	iA	3	Total	C	N	O	0	0
			46	25	2	19		
2	lA	3	Total	C	N	O	0	0
			46	25	2	19		
2	oA	3	Total	C	N	O	0	0
			46	25	2	19		
2	rA	3	Total	C	N	O	0	0
			46	25	2	19		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	uA	3	Total 46	C 25	N 2	O 19	0	0
2	xA	3	Total 46	C 25	N 2	O 19	0	0
2	0A	3	Total 46	C 25	N 2	O 19	0	0
2	3A	3	Total 46	C 25	N 2	O 19	0	0
2	6A	3	Total 46	C 25	N 2	O 19	0	0
2	9A	3	Total 46	C 25	N 2	O 19	0	0
2	CB	3	Total 46	C 25	N 2	O 19	0	0
2	FB	3	Total 46	C 25	N 2	O 19	0	0
2	IB	3	Total 46	C 25	N 2	O 19	0	0
2	LB	3	Total 46	C 25	N 2	O 19	0	0
2	OB	3	Total 46	C 25	N 2	O 19	0	0
2	RB	3	Total 46	C 25	N 2	O 19	0	0
2	UB	3	Total 46	C 25	N 2	O 19	0	0
2	XB	3	Total 46	C 25	N 2	O 19	0	0
2	aB	3	Total 46	C 25	N 2	O 19	0	0
2	dB	3	Total 46	C 25	N 2	O 19	0	0
2	gB	3	Total 46	C 25	N 2	O 19	0	0
2	jB	3	Total 46	C 25	N 2	O 19	0	0
2	mB	3	Total 46	C 25	N 2	O 19	0	0
2	pB	3	Total 46	C 25	N 2	O 19	0	0
2	sB	3	Total 46	C 25	N 2	O 19	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	vB	3	Total 46	C 25	N 2	O 19	0	0
2	yB	3	Total 46	C 25	N 2	O 19	0	0
2	1B	3	Total 46	C 25	N 2	O 19	0	0
2	4B	3	Total 46	C 25	N 2	O 19	0	0
2	7B	3	Total 46	C 25	N 2	O 19	0	0
2	AC	3	Total 46	C 25	N 2	O 19	0	0
2	DC	3	Total 46	C 25	N 2	O 19	0	0
2	GC	3	Total 46	C 25	N 2	O 19	0	0
2	JC	3	Total 46	C 25	N 2	O 19	0	0
2	MC	3	Total 46	C 25	N 2	O 19	0	0
2	PC	3	Total 46	C 25	N 2	O 19	0	0
2	SC	3	Total 46	C 25	N 2	O 19	0	0
2	VC	3	Total 46	C 25	N 2	O 19	0	0
2	YC	3	Total 46	C 25	N 2	O 19	0	0
2	bC	3	Total 46	C 25	N 2	O 19	0	0
2	eC	3	Total 46	C 25	N 2	O 19	0	0
2	hC	3	Total 46	C 25	N 2	O 19	0	0
2	kC	3	Total 46	C 25	N 2	O 19	0	0
2	nC	3	Total 46	C 25	N 2	O 19	0	0
2	qC	3	Total 46	C 25	N 2	O 19	0	0
2	tC	3	Total 46	C 25	N 2	O 19	0	0

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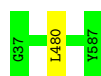
Mol	Chain	Residues	Atoms				AltConf	Trace
2	wC	3	Total	C	N	O	0	0
			46	25	2	19		
2	zC	3	Total	C	N	O	0	0
			46	25	2	19		

3 Residue-property plots

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

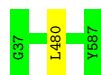
- Molecule 1: Capsid protein VP1

Chain A:  100%



- Molecule 1: Capsid protein VP1

Chain B:  100%



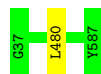
- Molecule 1: Capsid protein VP1

Chain C:  100%



- Molecule 1: Capsid protein VP1

Chain D:  100%



- Molecule 1: Capsid protein VP1

Chain E:  100%



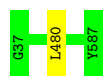
- Molecule 1: Capsid protein VP1

Chain F:  100%



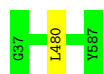
- Molecule 1: Capsid protein VP1

Chain G:  100%



- Molecule 1: Capsid protein VP1

Chain H:  100%



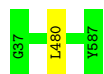
- Molecule 1: Capsid protein VP1

Chain I:  100%



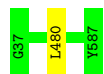
- Molecule 1: Capsid protein VP1

Chain J:  100%



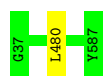
- Molecule 1: Capsid protein VP1

Chain K:  100%



- Molecule 1: Capsid protein VP1

Chain L:  100%



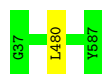
- Molecule 1: Capsid protein VP1

Chain M:  100%



- Molecule 1: Capsid protein VP1

Chain N:  100%



- Molecule 1: Capsid protein VP1

Chain O:  100%



- Molecule 1: Capsid protein VP1

Chain P:  100%



- Molecule 1: Capsid protein VP1

Chain Q:  100%



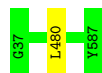
- Molecule 1: Capsid protein VP1

Chain R:  100%



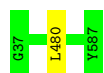
- Molecule 1: Capsid protein VP1

Chain S:  100%



- Molecule 1: Capsid protein VP1

Chain T:  100%



- Molecule 1: Capsid protein VP1

Chain U:  100%



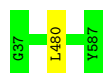
- Molecule 1: Capsid protein VP1

Chain V:  100%



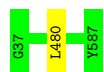
- Molecule 1: Capsid protein VP1

Chain W:  100%



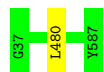
- Molecule 1: Capsid protein VP1

Chain X:  100%



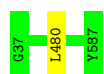
- Molecule 1: Capsid protein VP1

Chain Y:  100%



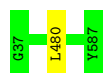
- Molecule 1: Capsid protein VP1

Chain Z:  100%



- Molecule 1: Capsid protein VP1

Chain a:  100%



- Molecule 1: Capsid protein VP1

Chain b:  100%



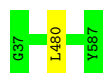
- Molecule 1: Capsid protein VP1

Chain c:  100%



- Molecule 1: Capsid protein VP1

Chain d:  100%



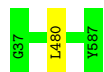
- Molecule 1: Capsid protein VP1

Chain e:  100%



- Molecule 1: Capsid protein VP1

Chain f:  100%




- Molecule 1: Capsid protein VP1

Chain g:  100%



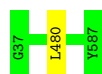
- Molecule 1: Capsid protein VP1

Chain h:  100%



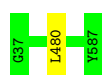
- Molecule 1: Capsid protein VP1

Chain i:  100%



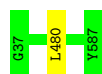
- Molecule 1: Capsid protein VP1

Chain j:  100%



- Molecule 1: Capsid protein VP1

Chain k:  100%



- Molecule 1: Capsid protein VP1

Chain l:  100%



- Molecule 1: Capsid protein VP1

Chain m:  100%



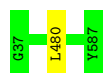
- Molecule 1: Capsid protein VP1

Chain n:  100%



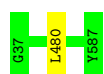
- Molecule 1: Capsid protein VP1

Chain o:  100%



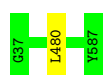
- Molecule 1: Capsid protein VP1

Chain p:  100%



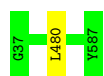
- Molecule 1: Capsid protein VP1

Chain q:  100%



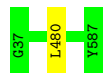
- Molecule 1: Capsid protein VP1

Chain r:  100%



- Molecule 1: Capsid protein VP1

Chain s:  100%



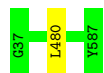
- Molecule 1: Capsid protein VP1

Chain t:  100%



- Molecule 1: Capsid protein VP1

Chain u:  100%



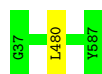
- Molecule 1: Capsid protein VP1

Chain v:  100%



- Molecule 1: Capsid protein VP1

Chain w:  100%



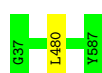
- Molecule 1: Capsid protein VP1

Chain x:  100%



- Molecule 1: Capsid protein VP1

Chain y:  100%



- Molecule 1: Capsid protein VP1

Chain z:  100%



- Molecule 1: Capsid protein VP1

Chain 1:  100%



- Molecule 1: Capsid protein VP1

Chain 2:  100%



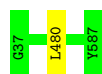
- Molecule 1: Capsid protein VP1

Chain 3:  100%



- Molecule 1: Capsid protein VP1

Chain 4:  100%



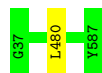
- Molecule 1: Capsid protein VP1

Chain 5:  100%



- Molecule 1: Capsid protein VP1

Chain 6:  100%



- Molecule 1: Capsid protein VP1

Chain 7:  100%



- Molecule 1: Capsid protein VP1

Chain 8:  100%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  100%
33% 67%



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	890	Depositor
Maximum defocus (nm)	3110	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	16.629	Depositor
Minimum map value	-9.923	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	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: GAL, SIA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.54	0/4530	0.53	0/6196
1	2	0.54	0/4530	0.53	0/6196
1	3	0.54	0/4530	0.53	0/6196
1	4	0.54	0/4530	0.53	0/6196
1	5	0.54	0/4530	0.53	0/6196
1	6	0.54	0/4530	0.53	0/6196
1	7	0.54	0/4530	0.53	0/6196
1	8	0.54	0/4530	0.53	0/6196
1	A	0.54	0/4530	0.53	0/6196
1	B	0.54	0/4530	0.53	0/6196
1	C	0.54	0/4530	0.53	0/6196
1	D	0.54	0/4530	0.53	0/6196
1	E	0.54	0/4530	0.53	0/6196
1	F	0.54	0/4530	0.53	0/6196
1	G	0.54	0/4530	0.53	0/6196
1	H	0.54	0/4530	0.53	0/6196
1	I	0.54	0/4530	0.53	0/6196
1	J	0.54	0/4530	0.53	0/6196
1	K	0.54	0/4530	0.53	0/6196
1	L	0.54	0/4530	0.53	0/6196
1	M	0.54	0/4530	0.53	0/6196
1	N	0.54	0/4530	0.53	0/6196
1	O	0.54	0/4530	0.53	0/6196
1	P	0.54	0/4530	0.53	0/6196
1	Q	0.54	0/4530	0.53	0/6196
1	R	0.54	0/4530	0.53	0/6196
1	S	0.54	0/4530	0.53	0/6196
1	T	0.54	0/4530	0.53	0/6196
1	U	0.54	0/4530	0.53	0/6196
1	V	0.54	0/4530	0.53	0/6196
1	W	0.54	0/4530	0.53	0/6196
1	X	0.54	0/4530	0.53	0/6196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.54	0/4530	0.53	0/6196
1	Z	0.54	0/4530	0.53	0/6196
1	a	0.54	0/4530	0.53	0/6196
1	b	0.54	0/4530	0.53	0/6196
1	c	0.54	0/4530	0.53	0/6196
1	d	0.54	0/4530	0.53	0/6196
1	e	0.54	0/4530	0.53	0/6196
1	f	0.54	0/4530	0.53	0/6196
1	g	0.54	0/4530	0.53	0/6196
1	h	0.54	0/4530	0.53	0/6196
1	i	0.54	0/4530	0.53	0/6196
1	j	0.54	0/4530	0.53	0/6196
1	k	0.54	0/4530	0.53	0/6196
1	l	0.54	0/4530	0.53	0/6196
1	m	0.54	0/4530	0.53	0/6196
1	n	0.54	0/4530	0.53	0/6196
1	o	0.54	0/4530	0.53	0/6196
1	p	0.54	0/4530	0.53	0/6196
1	q	0.54	0/4530	0.53	0/6196
1	r	0.54	0/4530	0.53	0/6196
1	s	0.54	0/4530	0.53	0/6196
1	t	0.54	0/4530	0.53	0/6196
1	u	0.54	0/4530	0.53	0/6196
1	v	0.54	0/4530	0.53	0/6196
1	w	0.54	0/4530	0.53	0/6196
1	x	0.54	0/4530	0.53	0/6196
1	y	0.54	0/4530	0.53	0/6196
1	z	0.54	0/4530	0.53	0/6196
All	All	0.54	0/271800	0.53	0/371760

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 ⓘ

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

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	1	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	2	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	3	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	4	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	5	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	6	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	7	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	8	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	A	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	B	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	C	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	D	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	E	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	F	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	G	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	H	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	I	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	J	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	K	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	L	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	M	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	N	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	O	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	P	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	Q	550/551 (100%)	542 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	S	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	T	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	U	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	V	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	W	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	X	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	Y	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	Z	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	a	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	b	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	c	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	d	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	e	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	f	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	g	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	h	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	i	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	j	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	k	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	l	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	m	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	n	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	o	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	p	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	q	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	r	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	s	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	t	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	u	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	v	550/551 (100%)	542 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	x	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	y	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
1	z	550/551 (100%)	542 (98%)	8 (2%)	0	100	100
All	All	33000/33060 (100%)	32520 (98%)	480 (2%)	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	1	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	2	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	3	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	4	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	5	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	6	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	7	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	8	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	A	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	B	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	C	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	D	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	E	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	F	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	G	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	H	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	I	480/479 (100%)	479 (100%)	1 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	K	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	L	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	M	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	N	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	O	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	P	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	Q	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	R	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	S	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	T	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	U	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	V	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	W	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	X	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	Y	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	Z	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	a	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	b	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	c	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	d	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	e	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	f	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	g	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	h	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	i	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	j	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	k	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	l	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	m	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	n	480/479 (100%)	479 (100%)	1 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	p	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	q	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	r	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	s	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	t	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	u	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	v	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	w	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	x	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	y	480/479 (100%)	479 (100%)	1 (0%)	92	98
1	z	480/479 (100%)	479 (100%)	1 (0%)	92	98
All	All	28800/28740 (100%)	28740 (100%)	60 (0%)	91	98

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	LEU
1	B	480	LEU
1	C	480	LEU
1	D	480	LEU
1	E	480	LEU
1	F	480	LEU
1	G	480	LEU
1	H	480	LEU
1	I	480	LEU
1	J	480	LEU
1	K	480	LEU
1	L	480	LEU
1	M	480	LEU
1	N	480	LEU
1	O	480	LEU
1	P	480	LEU
1	Q	480	LEU
1	R	480	LEU
1	S	480	LEU
1	T	480	LEU
1	U	480	LEU

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Mol	Chain	Res	Type
1	V	480	LEU
1	W	480	LEU
1	X	480	LEU
1	Y	480	LEU
1	Z	480	LEU
1	a	480	LEU
1	b	480	LEU
1	c	480	LEU
1	d	480	LEU
1	e	480	LEU
1	f	480	LEU
1	g	480	LEU
1	h	480	LEU
1	i	480	LEU
1	j	480	LEU
1	k	480	LEU
1	l	480	LEU
1	m	480	LEU
1	n	480	LEU
1	o	480	LEU
1	p	480	LEU
1	q	480	LEU
1	r	480	LEU
1	s	480	LEU
1	t	480	LEU
1	u	480	LEU
1	v	480	LEU
1	w	480	LEU
1	x	480	LEU
1	y	480	LEU
1	z	480	LEU
1	1	480	LEU
1	2	480	LEU
1	3	480	LEU
1	4	480	LEU
1	5	480	LEU
1	6	480	LEU
1	7	480	LEU
1	8	480	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (958) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	74	ASN
1	A	80	ASN
1	A	251	ASN
1	A	287	HIS
1	A	342	HIS
1	A	381	GLN
1	A	391	ASN
1	A	409	ASN
1	A	430	ASN
1	A	457	HIS
1	A	495	GLN
1	A	511	ASN
1	A	547	GLN
1	A	552	ASN
1	B	49	ASN
1	B	74	ASN
1	B	80	ASN
1	B	195	GLN
1	B	251	ASN
1	B	287	HIS
1	B	342	HIS
1	B	381	GLN
1	B	391	ASN
1	B	409	ASN
1	B	430	ASN
1	B	457	HIS
1	B	495	GLN
1	B	511	ASN
1	B	547	GLN
1	B	552	ASN
1	B	585	ASN
1	C	49	ASN
1	C	74	ASN
1	C	80	ASN
1	C	251	ASN
1	C	287	HIS
1	C	342	HIS
1	C	381	GLN
1	C	391	ASN
1	C	409	ASN
1	C	430	ASN
1	C	457	HIS

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Mol	Chain	Res	Type
1	C	495	GLN
1	C	511	ASN
1	C	547	GLN
1	C	552	ASN
1	C	585	ASN
1	D	49	ASN
1	D	74	ASN
1	D	80	ASN
1	D	251	ASN
1	D	287	HIS
1	D	342	HIS
1	D	381	GLN
1	D	391	ASN
1	D	409	ASN
1	D	430	ASN
1	D	457	HIS
1	D	495	GLN
1	D	511	ASN
1	D	547	GLN
1	D	552	ASN
1	D	585	ASN
1	E	49	ASN
1	E	74	ASN
1	E	80	ASN
1	E	251	ASN
1	E	287	HIS
1	E	342	HIS
1	E	381	GLN
1	E	391	ASN
1	E	409	ASN
1	E	430	ASN
1	E	457	HIS
1	E	495	GLN
1	E	511	ASN
1	E	547	GLN
1	E	552	ASN
1	E	585	ASN
1	F	49	ASN
1	F	74	ASN
1	F	80	ASN
1	F	251	ASN
1	F	287	HIS

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Mol	Chain	Res	Type
1	F	342	HIS
1	F	381	GLN
1	F	391	ASN
1	F	409	ASN
1	F	430	ASN
1	F	457	HIS
1	F	495	GLN
1	F	511	ASN
1	F	547	GLN
1	F	552	ASN
1	F	585	ASN
1	G	49	ASN
1	G	74	ASN
1	G	80	ASN
1	G	251	ASN
1	G	287	HIS
1	G	342	HIS
1	G	381	GLN
1	G	391	ASN
1	G	409	ASN
1	G	430	ASN
1	G	457	HIS
1	G	495	GLN
1	G	511	ASN
1	G	547	GLN
1	G	552	ASN
1	G	585	ASN
1	H	49	ASN
1	H	74	ASN
1	H	80	ASN
1	H	251	ASN
1	H	287	HIS
1	H	342	HIS
1	H	381	GLN
1	H	391	ASN
1	H	409	ASN
1	H	430	ASN
1	H	457	HIS
1	H	495	GLN
1	H	511	ASN
1	H	547	GLN
1	H	552	ASN

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Mol	Chain	Res	Type
1	H	585	ASN
1	I	49	ASN
1	I	74	ASN
1	I	80	ASN
1	I	251	ASN
1	I	287	HIS
1	I	342	HIS
1	I	381	GLN
1	I	391	ASN
1	I	409	ASN
1	I	430	ASN
1	I	457	HIS
1	I	495	GLN
1	I	511	ASN
1	I	547	GLN
1	I	552	ASN
1	I	585	ASN
1	J	49	ASN
1	J	74	ASN
1	J	80	ASN
1	J	195	GLN
1	J	251	ASN
1	J	287	HIS
1	J	342	HIS
1	J	381	GLN
1	J	391	ASN
1	J	409	ASN
1	J	430	ASN
1	J	457	HIS
1	J	495	GLN
1	J	511	ASN
1	J	547	GLN
1	J	552	ASN
1	J	585	ASN
1	K	49	ASN
1	K	74	ASN
1	K	80	ASN
1	K	251	ASN
1	K	287	HIS
1	K	342	HIS
1	K	381	GLN
1	K	391	ASN

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Mol	Chain	Res	Type
1	K	409	ASN
1	K	430	ASN
1	K	457	HIS
1	K	495	GLN
1	K	511	ASN
1	K	547	GLN
1	K	552	ASN
1	K	585	ASN
1	L	49	ASN
1	L	74	ASN
1	L	80	ASN
1	L	251	ASN
1	L	287	HIS
1	L	342	HIS
1	L	381	GLN
1	L	391	ASN
1	L	409	ASN
1	L	430	ASN
1	L	457	HIS
1	L	495	GLN
1	L	511	ASN
1	L	547	GLN
1	L	552	ASN
1	L	585	ASN
1	M	49	ASN
1	M	74	ASN
1	M	80	ASN
1	M	251	ASN
1	M	287	HIS
1	M	342	HIS
1	M	381	GLN
1	M	391	ASN
1	M	409	ASN
1	M	430	ASN
1	M	457	HIS
1	M	495	GLN
1	M	511	ASN
1	M	547	GLN
1	M	552	ASN
1	M	585	ASN
1	N	49	ASN
1	N	74	ASN

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Mol	Chain	Res	Type
1	N	80	ASN
1	N	251	ASN
1	N	287	HIS
1	N	342	HIS
1	N	381	GLN
1	N	391	ASN
1	N	409	ASN
1	N	430	ASN
1	N	457	HIS
1	N	495	GLN
1	N	511	ASN
1	N	547	GLN
1	N	552	ASN
1	N	585	ASN
1	O	49	ASN
1	O	74	ASN
1	O	80	ASN
1	O	251	ASN
1	O	287	HIS
1	O	342	HIS
1	O	381	GLN
1	O	391	ASN
1	O	409	ASN
1	O	430	ASN
1	O	457	HIS
1	O	495	GLN
1	O	511	ASN
1	O	547	GLN
1	O	552	ASN
1	O	585	ASN
1	P	49	ASN
1	P	74	ASN
1	P	80	ASN
1	P	251	ASN
1	P	287	HIS
1	P	342	HIS
1	P	381	GLN
1	P	391	ASN
1	P	409	ASN
1	P	430	ASN
1	P	457	HIS
1	P	495	GLN

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Mol	Chain	Res	Type
1	P	511	ASN
1	P	547	GLN
1	P	552	ASN
1	P	585	ASN
1	Q	49	ASN
1	Q	74	ASN
1	Q	80	ASN
1	Q	251	ASN
1	Q	287	HIS
1	Q	342	HIS
1	Q	381	GLN
1	Q	391	ASN
1	Q	409	ASN
1	Q	430	ASN
1	Q	457	HIS
1	Q	495	GLN
1	Q	511	ASN
1	Q	547	GLN
1	Q	552	ASN
1	Q	585	ASN
1	R	49	ASN
1	R	74	ASN
1	R	80	ASN
1	R	251	ASN
1	R	287	HIS
1	R	342	HIS
1	R	381	GLN
1	R	391	ASN
1	R	409	ASN
1	R	430	ASN
1	R	457	HIS
1	R	495	GLN
1	R	511	ASN
1	R	547	GLN
1	R	552	ASN
1	R	585	ASN
1	S	49	ASN
1	S	74	ASN
1	S	80	ASN
1	S	251	ASN
1	S	287	HIS
1	S	342	HIS

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Mol	Chain	Res	Type
1	S	381	GLN
1	S	391	ASN
1	S	409	ASN
1	S	430	ASN
1	S	457	HIS
1	S	495	GLN
1	S	511	ASN
1	S	547	GLN
1	S	552	ASN
1	S	585	ASN
1	T	49	ASN
1	T	74	ASN
1	T	80	ASN
1	T	251	ASN
1	T	287	HIS
1	T	342	HIS
1	T	381	GLN
1	T	391	ASN
1	T	409	ASN
1	T	430	ASN
1	T	457	HIS
1	T	495	GLN
1	T	511	ASN
1	T	547	GLN
1	T	552	ASN
1	T	585	ASN
1	U	49	ASN
1	U	74	ASN
1	U	80	ASN
1	U	251	ASN
1	U	287	HIS
1	U	342	HIS
1	U	381	GLN
1	U	391	ASN
1	U	409	ASN
1	U	430	ASN
1	U	457	HIS
1	U	495	GLN
1	U	511	ASN
1	U	547	GLN
1	U	552	ASN
1	V	49	ASN

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Mol	Chain	Res	Type
1	V	74	ASN
1	V	80	ASN
1	V	195	GLN
1	V	251	ASN
1	V	287	HIS
1	V	342	HIS
1	V	381	GLN
1	V	391	ASN
1	V	409	ASN
1	V	430	ASN
1	V	457	HIS
1	V	495	GLN
1	V	511	ASN
1	V	547	GLN
1	V	552	ASN
1	V	585	ASN
1	W	49	ASN
1	W	74	ASN
1	W	80	ASN
1	W	251	ASN
1	W	287	HIS
1	W	342	HIS
1	W	381	GLN
1	W	391	ASN
1	W	409	ASN
1	W	430	ASN
1	W	457	HIS
1	W	495	GLN
1	W	511	ASN
1	W	547	GLN
1	W	552	ASN
1	W	585	ASN
1	X	49	ASN
1	X	74	ASN
1	X	80	ASN
1	X	251	ASN
1	X	287	HIS
1	X	342	HIS
1	X	381	GLN
1	X	391	ASN
1	X	409	ASN
1	X	430	ASN

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Mol	Chain	Res	Type
1	X	457	HIS
1	X	495	GLN
1	X	511	ASN
1	X	547	GLN
1	X	552	ASN
1	X	585	ASN
1	Y	49	ASN
1	Y	74	ASN
1	Y	80	ASN
1	Y	251	ASN
1	Y	287	HIS
1	Y	342	HIS
1	Y	381	GLN
1	Y	391	ASN
1	Y	409	ASN
1	Y	430	ASN
1	Y	457	HIS
1	Y	495	GLN
1	Y	511	ASN
1	Y	547	GLN
1	Y	552	ASN
1	Z	49	ASN
1	Z	74	ASN
1	Z	80	ASN
1	Z	251	ASN
1	Z	287	HIS
1	Z	342	HIS
1	Z	381	GLN
1	Z	391	ASN
1	Z	409	ASN
1	Z	430	ASN
1	Z	457	HIS
1	Z	495	GLN
1	Z	511	ASN
1	Z	547	GLN
1	Z	552	ASN
1	Z	585	ASN
1	a	49	ASN
1	a	74	ASN
1	a	80	ASN
1	a	251	ASN
1	a	287	HIS

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Mol	Chain	Res	Type
1	a	342	HIS
1	a	381	GLN
1	a	391	ASN
1	a	409	ASN
1	a	430	ASN
1	a	457	HIS
1	a	495	GLN
1	a	511	ASN
1	a	547	GLN
1	a	552	ASN
1	b	49	ASN
1	b	74	ASN
1	b	80	ASN
1	b	195	GLN
1	b	251	ASN
1	b	287	HIS
1	b	342	HIS
1	b	381	GLN
1	b	391	ASN
1	b	409	ASN
1	b	430	ASN
1	b	457	HIS
1	b	495	GLN
1	b	511	ASN
1	b	547	GLN
1	b	552	ASN
1	c	49	ASN
1	c	74	ASN
1	c	80	ASN
1	c	251	ASN
1	c	287	HIS
1	c	342	HIS
1	c	381	GLN
1	c	391	ASN
1	c	409	ASN
1	c	430	ASN
1	c	457	HIS
1	c	495	GLN
1	c	511	ASN
1	c	547	GLN
1	c	552	ASN
1	c	585	ASN

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Mol	Chain	Res	Type
1	d	49	ASN
1	d	74	ASN
1	d	80	ASN
1	d	195	GLN
1	d	251	ASN
1	d	287	HIS
1	d	342	HIS
1	d	381	GLN
1	d	391	ASN
1	d	409	ASN
1	d	430	ASN
1	d	457	HIS
1	d	495	GLN
1	d	511	ASN
1	d	547	GLN
1	d	552	ASN
1	d	585	ASN
1	e	49	ASN
1	e	74	ASN
1	e	80	ASN
1	e	251	ASN
1	e	287	HIS
1	e	342	HIS
1	e	381	GLN
1	e	391	ASN
1	e	409	ASN
1	e	430	ASN
1	e	457	HIS
1	e	495	GLN
1	e	511	ASN
1	e	547	GLN
1	e	552	ASN
1	e	585	ASN
1	f	49	ASN
1	f	74	ASN
1	f	80	ASN
1	f	251	ASN
1	f	287	HIS
1	f	342	HIS
1	f	381	GLN
1	f	391	ASN
1	f	409	ASN

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Mol	Chain	Res	Type
1	f	430	ASN
1	f	457	HIS
1	f	495	GLN
1	f	511	ASN
1	f	547	GLN
1	f	552	ASN
1	g	49	ASN
1	g	74	ASN
1	g	80	ASN
1	g	251	ASN
1	g	287	HIS
1	g	342	HIS
1	g	381	GLN
1	g	391	ASN
1	g	409	ASN
1	g	430	ASN
1	g	457	HIS
1	g	495	GLN
1	g	511	ASN
1	g	547	GLN
1	g	552	ASN
1	g	585	ASN
1	h	49	ASN
1	h	74	ASN
1	h	80	ASN
1	h	251	ASN
1	h	287	HIS
1	h	342	HIS
1	h	381	GLN
1	h	391	ASN
1	h	409	ASN
1	h	430	ASN
1	h	457	HIS
1	h	495	GLN
1	h	511	ASN
1	h	547	GLN
1	h	552	ASN
1	i	49	ASN
1	i	74	ASN
1	i	80	ASN
1	i	251	ASN
1	i	287	HIS

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Mol	Chain	Res	Type
1	i	342	HIS
1	i	381	GLN
1	i	391	ASN
1	i	409	ASN
1	i	430	ASN
1	i	457	HIS
1	i	495	GLN
1	i	511	ASN
1	i	547	GLN
1	i	552	ASN
1	i	585	ASN
1	j	49	ASN
1	j	74	ASN
1	j	80	ASN
1	j	195	GLN
1	j	251	ASN
1	j	287	HIS
1	j	342	HIS
1	j	381	GLN
1	j	391	ASN
1	j	409	ASN
1	j	430	ASN
1	j	457	HIS
1	j	495	GLN
1	j	511	ASN
1	j	547	GLN
1	j	552	ASN
1	j	585	ASN
1	k	49	ASN
1	k	74	ASN
1	k	80	ASN
1	k	251	ASN
1	k	287	HIS
1	k	342	HIS
1	k	381	GLN
1	k	391	ASN
1	k	409	ASN
1	k	430	ASN
1	k	457	HIS
1	k	495	GLN
1	k	511	ASN
1	k	547	GLN

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Mol	Chain	Res	Type
1	k	552	ASN
1	k	585	ASN
1	l	49	ASN
1	l	74	ASN
1	l	80	ASN
1	l	251	ASN
1	l	287	HIS
1	l	342	HIS
1	l	381	GLN
1	l	391	ASN
1	l	409	ASN
1	l	430	ASN
1	l	457	HIS
1	l	495	GLN
1	l	511	ASN
1	l	547	GLN
1	l	552	ASN
1	m	49	ASN
1	m	74	ASN
1	m	80	ASN
1	m	195	GLN
1	m	251	ASN
1	m	287	HIS
1	m	342	HIS
1	m	381	GLN
1	m	391	ASN
1	m	409	ASN
1	m	430	ASN
1	m	457	HIS
1	m	495	GLN
1	m	511	ASN
1	m	547	GLN
1	m	552	ASN
1	n	49	ASN
1	n	74	ASN
1	n	80	ASN
1	n	195	GLN
1	n	251	ASN
1	n	287	HIS
1	n	342	HIS
1	n	381	GLN
1	n	391	ASN

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Mol	Chain	Res	Type
1	n	409	ASN
1	n	430	ASN
1	n	457	HIS
1	n	495	GLN
1	n	511	ASN
1	n	547	GLN
1	n	552	ASN
1	n	585	ASN
1	o	49	ASN
1	o	74	ASN
1	o	80	ASN
1	o	251	ASN
1	o	287	HIS
1	o	342	HIS
1	o	381	GLN
1	o	391	ASN
1	o	409	ASN
1	o	430	ASN
1	o	457	HIS
1	o	495	GLN
1	o	511	ASN
1	o	547	GLN
1	o	552	ASN
1	o	585	ASN
1	p	49	ASN
1	p	74	ASN
1	p	80	ASN
1	p	195	GLN
1	p	251	ASN
1	p	287	HIS
1	p	342	HIS
1	p	381	GLN
1	p	391	ASN
1	p	409	ASN
1	p	430	ASN
1	p	457	HIS
1	p	495	GLN
1	p	511	ASN
1	p	547	GLN
1	p	552	ASN
1	p	585	ASN
1	q	49	ASN

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Mol	Chain	Res	Type
1	q	74	ASN
1	q	80	ASN
1	q	251	ASN
1	q	287	HIS
1	q	342	HIS
1	q	381	GLN
1	q	391	ASN
1	q	409	ASN
1	q	430	ASN
1	q	457	HIS
1	q	495	GLN
1	q	511	ASN
1	q	547	GLN
1	q	552	ASN
1	q	585	ASN
1	r	49	ASN
1	r	74	ASN
1	r	80	ASN
1	r	251	ASN
1	r	287	HIS
1	r	342	HIS
1	r	381	GLN
1	r	391	ASN
1	r	409	ASN
1	r	430	ASN
1	r	457	HIS
1	r	495	GLN
1	r	511	ASN
1	r	547	GLN
1	r	552	ASN
1	r	585	ASN
1	s	49	ASN
1	s	74	ASN
1	s	80	ASN
1	s	251	ASN
1	s	287	HIS
1	s	342	HIS
1	s	381	GLN
1	s	391	ASN
1	s	409	ASN
1	s	430	ASN
1	s	457	HIS

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Mol	Chain	Res	Type
1	s	495	GLN
1	s	511	ASN
1	s	547	GLN
1	s	552	ASN
1	t	49	ASN
1	t	74	ASN
1	t	80	ASN
1	t	251	ASN
1	t	287	HIS
1	t	342	HIS
1	t	381	GLN
1	t	391	ASN
1	t	409	ASN
1	t	430	ASN
1	t	457	HIS
1	t	495	GLN
1	t	511	ASN
1	t	547	GLN
1	t	552	ASN
1	t	585	ASN
1	u	49	ASN
1	u	74	ASN
1	u	80	ASN
1	u	195	GLN
1	u	251	ASN
1	u	287	HIS
1	u	342	HIS
1	u	381	GLN
1	u	391	ASN
1	u	409	ASN
1	u	430	ASN
1	u	457	HIS
1	u	495	GLN
1	u	511	ASN
1	u	547	GLN
1	u	552	ASN
1	u	585	ASN
1	v	49	ASN
1	v	74	ASN
1	v	80	ASN
1	v	251	ASN
1	v	287	HIS

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Mol	Chain	Res	Type
1	v	342	HIS
1	v	381	GLN
1	v	391	ASN
1	v	409	ASN
1	v	430	ASN
1	v	457	HIS
1	v	495	GLN
1	v	511	ASN
1	v	547	GLN
1	v	552	ASN
1	w	49	ASN
1	w	74	ASN
1	w	80	ASN
1	w	251	ASN
1	w	287	HIS
1	w	342	HIS
1	w	381	GLN
1	w	391	ASN
1	w	409	ASN
1	w	430	ASN
1	w	457	HIS
1	w	495	GLN
1	w	511	ASN
1	w	547	GLN
1	w	552	ASN
1	w	585	ASN
1	x	49	ASN
1	x	74	ASN
1	x	80	ASN
1	x	251	ASN
1	x	287	HIS
1	x	342	HIS
1	x	381	GLN
1	x	391	ASN
1	x	409	ASN
1	x	430	ASN
1	x	457	HIS
1	x	495	GLN
1	x	511	ASN
1	x	547	GLN
1	x	552	ASN
1	x	585	ASN

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Mol	Chain	Res	Type
1	y	49	ASN
1	y	74	ASN
1	y	80	ASN
1	y	251	ASN
1	y	287	HIS
1	y	342	HIS
1	y	381	GLN
1	y	391	ASN
1	y	409	ASN
1	y	430	ASN
1	y	457	HIS
1	y	495	GLN
1	y	511	ASN
1	y	547	GLN
1	y	552	ASN
1	y	585	ASN
1	z	49	ASN
1	z	74	ASN
1	z	80	ASN
1	z	251	ASN
1	z	287	HIS
1	z	342	HIS
1	z	381	GLN
1	z	391	ASN
1	z	409	ASN
1	z	430	ASN
1	z	457	HIS
1	z	495	GLN
1	z	511	ASN
1	z	547	GLN
1	z	552	ASN
1	1	49	ASN
1	1	74	ASN
1	1	80	ASN
1	1	195	GLN
1	1	251	ASN
1	1	287	HIS
1	1	342	HIS
1	1	381	GLN
1	1	391	ASN
1	1	409	ASN
1	1	430	ASN

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Mol	Chain	Res	Type
1	1	457	HIS
1	1	495	GLN
1	1	511	ASN
1	1	547	GLN
1	1	552	ASN
1	2	49	ASN
1	2	74	ASN
1	2	80	ASN
1	2	195	GLN
1	2	251	ASN
1	2	287	HIS
1	2	342	HIS
1	2	381	GLN
1	2	391	ASN
1	2	409	ASN
1	2	430	ASN
1	2	457	HIS
1	2	495	GLN
1	2	511	ASN
1	2	547	GLN
1	2	552	ASN
1	2	585	ASN
1	3	49	ASN
1	3	74	ASN
1	3	80	ASN
1	3	251	ASN
1	3	287	HIS
1	3	342	HIS
1	3	381	GLN
1	3	391	ASN
1	3	409	ASN
1	3	430	ASN
1	3	457	HIS
1	3	495	GLN
1	3	511	ASN
1	3	547	GLN
1	3	552	ASN
1	4	49	ASN
1	4	74	ASN
1	4	80	ASN
1	4	251	ASN
1	4	287	HIS

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Mol	Chain	Res	Type
1	4	342	HIS
1	4	381	GLN
1	4	391	ASN
1	4	409	ASN
1	4	430	ASN
1	4	457	HIS
1	4	495	GLN
1	4	511	ASN
1	4	547	GLN
1	4	552	ASN
1	4	585	ASN
1	5	49	ASN
1	5	74	ASN
1	5	80	ASN
1	5	195	GLN
1	5	251	ASN
1	5	287	HIS
1	5	342	HIS
1	5	381	GLN
1	5	391	ASN
1	5	409	ASN
1	5	430	ASN
1	5	457	HIS
1	5	495	GLN
1	5	511	ASN
1	5	547	GLN
1	5	552	ASN
1	5	585	ASN
1	6	49	ASN
1	6	74	ASN
1	6	80	ASN
1	6	251	ASN
1	6	287	HIS
1	6	342	HIS
1	6	381	GLN
1	6	391	ASN
1	6	409	ASN
1	6	430	ASN
1	6	457	HIS
1	6	495	GLN
1	6	511	ASN
1	6	547	GLN

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Mol	Chain	Res	Type
1	6	552	ASN
1	6	585	ASN
1	7	49	ASN
1	7	74	ASN
1	7	80	ASN
1	7	251	ASN
1	7	287	HIS
1	7	342	HIS
1	7	381	GLN
1	7	391	ASN
1	7	409	ASN
1	7	430	ASN
1	7	457	HIS
1	7	495	GLN
1	7	511	ASN
1	7	547	GLN
1	7	552	ASN
1	8	49	ASN
1	8	74	ASN
1	8	80	ASN
1	8	251	ASN
1	8	287	HIS
1	8	342	HIS
1	8	381	GLN
1	8	391	ASN
1	8	409	ASN
1	8	430	ASN
1	8	457	HIS
1	8	495	GLN
1	8	511	ASN
1	8	547	GLN
1	8	552	ASN
1	8	585	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

180 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	0	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	0	2	2	11,11,12	1.02	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	0	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	0A	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	0A	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	0A	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	1B	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	1B	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	1B	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	3A	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	3A	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	3A	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	4B	1	2	15,15,15	0.33	0	21,21,21	0.37	0
2	GAL	4B	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	4B	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	5 (23%)
2	NAG	6A	1	2	15,15,15	0.35	0	21,21,21	0.36	0
2	GAL	6A	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	6A	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	7B	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	7B	2	2	11,11,12	1.05	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	7B	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	9A	1	2	15,15,15	0.35	0	21,21,21	0.36	0
2	GAL	9A	2	2	11,11,12	1.05	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	9A	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	AC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	AC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	AC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	BA	1	2	15,15,15	0.33	0	21,21,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	BA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	BA	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	CB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	CB	2	2	11,11,12	1.02	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	CB	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	DC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	DC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	DC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	EA	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	EA	2	2	11,11,12	1.05	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	EA	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	FB	1	2	15,15,15	0.33	0	21,21,21	0.37	0
2	GAL	FB	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	FB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	GC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	GC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	GC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	HA	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	HA	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	HA	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	IB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	IB	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	IB	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	JC	1	2	15,15,15	0.32	0	21,21,21	0.37	0
2	GAL	JC	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	JC	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	KA	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	KA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	KA	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	LB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	LB	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	LB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	MC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	MC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	MC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	NA	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	NA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	NA	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	OB	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	OB	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	OB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	PC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	PC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	PC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	QA	1	2	15,15,15	0.32	0	21,21,21	0.36	0
2	GAL	QA	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	QA	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	RB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	RB	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	RB	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.62	4 (19%)
2	NAG	SC	1	2	15,15,15	0.35	0	21,21,21	0.36	0
2	GAL	SC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	SC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	TA	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	TA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	TA	3	2	20,20,21	1.55	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	UB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	UB	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	UB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.62	4 (19%)
2	NAG	VC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	VC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	VC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	WA	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	WA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	WA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	XB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	XB	2	2	11,11,12	1.02	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	XB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	YC	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	YC	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	YC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.62	4 (19%)
2	NAG	ZA	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	ZA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	ZA	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	aB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	aB	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	aB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	bC	1	2	15,15,15	0.35	0	21,21,21	0.36	0
2	GAL	bC	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	bC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	cA	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	cA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	cA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	dB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	dB	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	dB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.62	4 (19%)
2	NAG	eC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	eC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	eC	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	fA	1	2	15,15,15	0.35	0	21,21,21	0.36	0
2	GAL	fA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	fA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	gB	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	gB	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	gB	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	hC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	hC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	hC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	iA	1	2	15,15,15	0.33	0	21,21,21	0.37	0
2	GAL	iA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	iA	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	5 (23%)
2	NAG	jB	1	2	15,15,15	0.33	0	21,21,21	0.37	0
2	GAL	jB	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	jB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	kC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	kC	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	kC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	lA	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	lA	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	lA	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	mB	1	2	15,15,15	0.34	0	21,21,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	mB	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	mB	3	2	20,20,21	1.55	2 (10%)	21,28,31	1.62	4 (19%)
2	NAG	nC	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	nC	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	nC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	oA	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	oA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	oA	3	2	20,20,21	1.55	2 (10%)	21,28,31	1.62	4 (19%)
2	NAG	pB	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	pB	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	pB	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	qC	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	qC	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	qC	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	rA	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	rA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	rA	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	sB	1	2	15,15,15	0.32	0	21,21,21	0.36	0
2	GAL	sB	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	sB	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	tC	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	tC	2	2	11,11,12	1.02	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	tC	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	uA	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	uA	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	uA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.62	4 (19%)
2	NAG	vB	1	2	15,15,15	0.35	0	21,21,21	0.36	0
2	GAL	vB	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.07	1 (6%)
2	SIA	vB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	wC	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	wC	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	wC	3	2	20,20,21	1.56	2 (10%)	21,28,31	1.63	4 (19%)
2	NAG	xA	1	2	15,15,15	0.33	0	21,21,21	0.36	0
2	GAL	xA	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	xA	3	2	20,20,21	1.57	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	yB	1	2	15,15,15	0.32	0	21,21,21	0.36	0
2	GAL	yB	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	yB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.63	4 (19%)
2	NAG	zC	1	2	15,15,15	0.34	0	21,21,21	0.36	0
2	GAL	zC	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.06	1 (6%)
2	SIA	zC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.63	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	0	1	2	-	2/6/26/26	0/1/1/1
2	GAL	0	2	2	-	1/2/19/22	0/1/1/1
2	SIA	0	3	2	-	10/18/34/38	0/1/1/1
2	NAG	0A	1	2	-	2/6/26/26	0/1/1/1
2	GAL	0A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	0A	3	2	-	10/18/34/38	0/1/1/1
2	NAG	1B	1	2	-	2/6/26/26	0/1/1/1
2	GAL	1B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	1B	3	2	-	10/18/34/38	0/1/1/1
2	NAG	3A	1	2	-	2/6/26/26	0/1/1/1
2	GAL	3A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	3A	3	2	-	10/18/34/38	0/1/1/1
2	NAG	4B	1	2	-	2/6/26/26	0/1/1/1
2	GAL	4B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	4B	3	2	-	10/18/34/38	0/1/1/1
2	NAG	6A	1	2	-	2/6/26/26	0/1/1/1
2	GAL	6A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	6A	3	2	-	10/18/34/38	0/1/1/1
2	NAG	7B	1	2	-	2/6/26/26	0/1/1/1
2	GAL	7B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	7B	3	2	-	10/18/34/38	0/1/1/1
2	NAG	9A	1	2	-	2/6/26/26	0/1/1/1
2	GAL	9A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	9A	3	2	-	10/18/34/38	0/1/1/1
2	NAG	AC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	AC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	AC	3	2	-	10/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	BA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	BA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	BA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	CB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	CB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	CB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	DC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	DC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	DC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	EA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	EA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	EA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	FB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	FB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	FB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	GC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	GC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	GC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	HA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	HA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	HA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	IB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	IB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	IB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	JC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	JC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	JC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	KA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	KA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	KA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	LB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	LB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	LB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	MC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	MC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	MC	3	2	-	10/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	NA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	NA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	NA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	OB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	OB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	OB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	PC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	PC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	PC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	QA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	QA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	QA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	RB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	RB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	RB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	SC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	SC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	SC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	TA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	TA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	TA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	UB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	UB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	UB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	VC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	VC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	VC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	WA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	WA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	WA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	XB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	XB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	XB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	YC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	YC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	YC	3	2	-	10/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	ZA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	ZA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	ZA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	aB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	aB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	aB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	bC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	bC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	bC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	cA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	cA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	cA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	dB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	dB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	dB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	eC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	eC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	eC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	fA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	fA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	fA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	gB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	gB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	gB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	hC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	hC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	hC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	iA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	iA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	iA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	jB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	jB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	jB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	kC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	kC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	kC	3	2	-	10/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	lA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	lA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	lA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	mB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	mB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	mB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	nC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	nC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	nC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	oA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	oA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	oA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	pB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	pB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	pB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	qC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	qC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	qC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	rA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	rA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	rA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	sB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	sB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	sB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	tC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	tC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	tC	3	2	-	10/18/34/38	0/1/1/1
2	NAG	uA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	uA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	uA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	vB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	vB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	vB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	wC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	wC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	wC	3	2	-	10/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	xA	1	2	-	2/6/26/26	0/1/1/1
2	GAL	xA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	xA	3	2	-	10/18/34/38	0/1/1/1
2	NAG	yB	1	2	-	2/6/26/26	0/1/1/1
2	GAL	yB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	yB	3	2	-	10/18/34/38	0/1/1/1
2	NAG	zC	1	2	-	2/6/26/26	0/1/1/1
2	GAL	zC	2	2	-	1/2/19/22	0/1/1/1
2	SIA	zC	3	2	-	10/18/34/38	0/1/1/1

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	sB	3	SIA	C2-C1	5.54	1.59	1.52
2	BA	3	SIA	C2-C1	5.53	1.59	1.52
2	ZA	3	SIA	C2-C1	5.53	1.59	1.52
2	xA	3	SIA	C2-C1	5.53	1.59	1.52
2	0A	3	SIA	C2-C1	5.53	1.59	1.52
2	DC	3	SIA	C2-C1	5.53	1.59	1.52
2	EA	3	SIA	C2-C1	5.53	1.59	1.52
2	9A	3	SIA	C2-C1	5.53	1.59	1.52
2	gB	3	SIA	C2-C1	5.53	1.59	1.52
2	7B	3	SIA	C2-C1	5.53	1.59	1.52
2	0	3	SIA	C2-C1	5.52	1.59	1.52
2	hC	3	SIA	C2-C1	5.51	1.59	1.52
2	pB	3	SIA	C2-C1	5.50	1.58	1.52
2	KA	3	SIA	C2-C1	5.49	1.58	1.52
2	QA	3	SIA	C2-C1	5.49	1.58	1.52
2	JC	3	SIA	C2-C1	5.49	1.58	1.52
2	SC	3	SIA	C2-C1	5.49	1.58	1.52
2	NA	3	SIA	C2-C1	5.49	1.58	1.52
2	PC	3	SIA	C2-C1	5.49	1.58	1.52
2	YC	3	SIA	C2-C1	5.49	1.58	1.52
2	RB	3	SIA	C2-C1	5.47	1.58	1.52
2	UB	3	SIA	C2-C1	5.47	1.58	1.52
2	dB	3	SIA	C2-C1	5.47	1.58	1.52
2	fA	3	SIA	C2-C1	5.46	1.58	1.52
2	6A	3	SIA	C2-C1	5.46	1.58	1.52
2	AC	3	SIA	C2-C1	5.46	1.58	1.52
2	bC	3	SIA	C2-C1	5.46	1.58	1.52
2	eC	3	SIA	C2-C1	5.46	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	uA	3	SIA	C2-C1	5.46	1.58	1.52
2	yB	3	SIA	C2-C1	5.46	1.58	1.52
2	MC	3	SIA	C2-C1	5.46	1.58	1.52
2	oA	3	SIA	C2-C1	5.45	1.58	1.52
2	LB	3	SIA	C2-C1	5.45	1.58	1.52
2	vB	3	SIA	C2-C1	5.45	1.58	1.52
2	zC	3	SIA	C2-C1	5.45	1.58	1.52
2	WA	3	SIA	C2-C1	5.44	1.58	1.52
2	cA	3	SIA	C2-C1	5.44	1.58	1.52
2	3A	3	SIA	C2-C1	5.44	1.58	1.52
2	VC	3	SIA	C2-C1	5.44	1.58	1.52
2	nC	3	SIA	C2-C1	5.44	1.58	1.52
2	GC	3	SIA	C2-C1	5.44	1.58	1.52
2	HA	3	SIA	C2-C1	5.44	1.58	1.52
2	TA	3	SIA	C2-C1	5.44	1.58	1.52
2	iA	3	SIA	C2-C1	5.44	1.58	1.52
2	lA	3	SIA	C2-C1	5.44	1.58	1.52
2	rA	3	SIA	C2-C1	5.44	1.58	1.52
2	CB	3	SIA	C2-C1	5.44	1.58	1.52
2	IB	3	SIA	C2-C1	5.44	1.58	1.52
2	mB	3	SIA	C2-C1	5.44	1.58	1.52
2	4B	3	SIA	C2-C1	5.44	1.58	1.52
2	qC	3	SIA	C2-C1	5.44	1.58	1.52
2	tC	3	SIA	C2-C1	5.44	1.58	1.52
2	wC	3	SIA	C2-C1	5.44	1.58	1.52
2	XB	3	SIA	C2-C1	5.43	1.58	1.52
2	FB	3	SIA	C2-C1	5.41	1.58	1.52
2	jB	3	SIA	C2-C1	5.41	1.58	1.52
2	OB	3	SIA	C2-C1	5.40	1.58	1.52
2	aB	3	SIA	C2-C1	5.40	1.58	1.52
2	lB	3	SIA	C2-C1	5.40	1.58	1.52
2	kC	3	SIA	C2-C1	5.40	1.58	1.52
2	iA	2	GAL	C4-C3	2.15	1.57	1.52
2	FB	2	GAL	C4-C3	2.15	1.57	1.52
2	vB	2	GAL	C4-C3	2.15	1.57	1.52
2	4B	2	GAL	C4-C3	2.15	1.57	1.52
2	GC	2	GAL	C4-C3	2.15	1.57	1.52
2	QA	2	GAL	C4-C3	2.14	1.57	1.52
2	oA	2	GAL	C4-C3	2.14	1.57	1.52
2	LB	2	GAL	C4-C3	2.14	1.57	1.52
2	JC	2	GAL	C4-C3	2.14	1.57	1.52
2	zC	2	GAL	C4-C3	2.14	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BA	2	GAL	C4-C3	2.14	1.57	1.52
2	fA	2	GAL	C4-C3	2.14	1.57	1.52
2	xA	2	GAL	C4-C3	2.14	1.57	1.52
2	6A	2	GAL	C4-C3	2.14	1.57	1.52
2	AC	2	GAL	C4-C3	2.14	1.57	1.52
2	bC	2	GAL	C4-C3	2.14	1.57	1.52
2	eC	2	GAL	C4-C3	2.14	1.57	1.52
2	hC	2	GAL	C4-C3	2.14	1.57	1.52
2	EA	2	GAL	C4-C3	2.13	1.57	1.52
2	cA	2	GAL	C4-C3	2.13	1.57	1.52
2	9A	2	GAL	C4-C3	2.13	1.57	1.52
2	7B	2	GAL	C4-C3	2.13	1.57	1.52
2	VC	2	GAL	C4-C3	2.13	1.57	1.52
2	nC	2	GAL	C4-C3	2.13	1.57	1.52
2	3A	2	GAL	C4-C3	2.13	1.57	1.52
2	HA	2	GAL	C4-C3	2.13	1.57	1.52
2	TA	2	GAL	C4-C3	2.13	1.57	1.52
2	rA	2	GAL	C4-C3	2.13	1.57	1.52
2	CB	2	GAL	C4-C3	2.13	1.57	1.52
2	mB	2	GAL	C4-C3	2.13	1.57	1.52
2	pB	2	GAL	C4-C3	2.13	1.57	1.52
2	sB	2	GAL	C4-C3	2.13	1.57	1.52
2	DC	2	GAL	C4-C3	2.13	1.57	1.52
2	qC	2	GAL	C4-C3	2.13	1.57	1.52
2	tC	2	GAL	C4-C3	2.13	1.57	1.52
2	0	2	GAL	C4-C3	2.13	1.57	1.52
2	NA	2	GAL	C4-C3	2.13	1.57	1.52
2	OB	2	GAL	C4-C3	2.13	1.57	1.52
2	XB	2	GAL	C4-C3	2.13	1.57	1.52
2	aB	2	GAL	C4-C3	2.13	1.57	1.52
2	1B	2	GAL	C4-C3	2.13	1.57	1.52
2	PC	2	GAL	C4-C3	2.13	1.57	1.52
2	YC	2	GAL	C4-C3	2.13	1.57	1.52
2	kC	2	GAL	C4-C3	2.13	1.57	1.52
2	WA	2	GAL	C4-C3	2.12	1.57	1.52
2	uA	2	GAL	C4-C3	2.12	1.57	1.52
2	gB	2	GAL	C4-C3	2.12	1.57	1.52
2	yB	2	GAL	C4-C3	2.12	1.57	1.52
2	MC	2	GAL	C4-C3	2.12	1.57	1.52
2	RB	2	GAL	C4-C3	2.12	1.57	1.52
2	UB	2	GAL	C4-C3	2.12	1.57	1.52
2	ZA	2	GAL	C4-C3	2.12	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0A	2	GAL	C4-C3	2.12	1.57	1.52
2	jB	2	GAL	C4-C3	2.12	1.57	1.52
2	KA	2	GAL	C4-C3	2.12	1.57	1.52
2	SC	2	GAL	C4-C3	2.12	1.57	1.52
2	lA	2	GAL	C4-C3	2.11	1.57	1.52
2	IB	2	GAL	C4-C3	2.11	1.57	1.52
2	wC	2	GAL	C4-C3	2.11	1.57	1.52
2	dB	2	GAL	C4-C3	2.09	1.57	1.52
2	NA	3	SIA	O6-C2	2.02	1.47	1.43
2	HA	3	SIA	O6-C2	2.01	1.47	1.43
2	TA	3	SIA	O6-C2	2.01	1.47	1.43
2	lA	3	SIA	O6-C2	2.01	1.47	1.43
2	rA	3	SIA	O6-C2	2.01	1.47	1.43
2	CB	3	SIA	O6-C2	2.01	1.47	1.43
2	IB	3	SIA	O6-C2	2.01	1.47	1.43
2	mB	3	SIA	O6-C2	2.01	1.47	1.43
2	pB	3	SIA	O6-C2	2.01	1.47	1.43
2	qC	3	SIA	O6-C2	2.01	1.47	1.43
2	tC	3	SIA	O6-C2	2.01	1.47	1.43
2	wC	3	SIA	O6-C2	2.01	1.47	1.43
2	RB	3	SIA	O6-C2	2.01	1.47	1.43
2	eC	3	SIA	O6-C2	2.00	1.47	1.43
2	oA	3	SIA	O6-C2	2.00	1.47	1.43
2	JC	3	SIA	O6-C2	2.00	1.47	1.43

All (302) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	XB	3	SIA	O1A-C1-C2	-4.83	112.41	122.85
2	sB	3	SIA	O1A-C1-C2	-4.83	112.41	122.85
2	iA	3	SIA	O1A-C1-C2	-4.83	112.41	122.85
2	4B	3	SIA	O1A-C1-C2	-4.83	112.41	122.85
2	BA	3	SIA	O1A-C1-C2	-4.83	112.42	122.85
2	ZA	3	SIA	O1A-C1-C2	-4.83	112.42	122.85
2	xA	3	SIA	O1A-C1-C2	-4.83	112.42	122.85
2	0A	3	SIA	O1A-C1-C2	-4.83	112.42	122.85
2	DC	3	SIA	O1A-C1-C2	-4.83	112.42	122.85
2	JC	3	SIA	O1A-C1-C2	-4.82	112.43	122.85
2	fA	3	SIA	O1A-C1-C2	-4.82	112.43	122.85
2	6A	3	SIA	O1A-C1-C2	-4.82	112.43	122.85
2	AC	3	SIA	O1A-C1-C2	-4.82	112.43	122.85
2	bC	3	SIA	O1A-C1-C2	-4.82	112.43	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	eC	3	SIA	O1A-C1-C2	-4.82	112.43	122.85
2	0	3	SIA	O1A-C1-C2	-4.82	112.44	122.85
2	9A	3	SIA	O1A-C1-C2	-4.82	112.44	122.85
2	gB	3	SIA	O1A-C1-C2	-4.82	112.44	122.85
2	7B	3	SIA	O1A-C1-C2	-4.82	112.44	122.85
2	WA	3	SIA	O1A-C1-C2	-4.82	112.44	122.85
2	HA	3	SIA	O1A-C1-C2	-4.81	112.45	122.85
2	CB	3	SIA	O1A-C1-C2	-4.81	112.45	122.85
2	tC	3	SIA	O1A-C1-C2	-4.81	112.45	122.85
2	hC	3	SIA	O1A-C1-C2	-4.81	112.45	122.85
2	KA	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	SC	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	uA	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	yB	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	MC	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	EA	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	FB	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	jB	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	cA	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	3A	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	VC	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	nC	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	QA	3	SIA	O1A-C1-C2	-4.81	112.46	122.85
2	NA	3	SIA	O1A-C1-C2	-4.81	112.47	122.85
2	GC	3	SIA	O1A-C1-C2	-4.80	112.47	122.85
2	OB	3	SIA	O1A-C1-C2	-4.80	112.47	122.85
2	aB	3	SIA	O1A-C1-C2	-4.80	112.47	122.85
2	1B	3	SIA	O1A-C1-C2	-4.80	112.47	122.85
2	kC	3	SIA	O1A-C1-C2	-4.80	112.47	122.85
2	pB	3	SIA	O1A-C1-C2	-4.80	112.47	122.85
2	oA	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	LB	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	zC	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	lA	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	rA	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	IB	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	wC	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	RB	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	UB	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	dB	3	SIA	O1A-C1-C2	-4.80	112.48	122.85
2	TA	3	SIA	O1A-C1-C2	-4.80	112.49	122.85
2	mB	3	SIA	O1A-C1-C2	-4.80	112.49	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	qC	3	SIA	O1A-C1-C2	-4.80	112.49	122.85
2	PC	3	SIA	O1A-C1-C2	-4.79	112.50	122.85
2	YC	3	SIA	O1A-C1-C2	-4.79	112.50	122.85
2	vB	3	SIA	O1A-C1-C2	-4.79	112.51	122.85
2	sB	3	SIA	O1B-C1-O1A	2.49	129.73	124.08
2	pB	3	SIA	O1B-C1-O1A	2.49	129.72	124.08
2	JC	3	SIA	O1B-C1-O1A	2.49	129.72	124.08
2	xA	3	SIA	O1B-C1-O1A	2.48	129.72	124.08
2	eC	3	SIA	O1B-C1-O1A	2.48	129.72	124.08
2	BA	3	SIA	O1B-C1-O1A	2.48	129.71	124.08
2	ZA	3	SIA	O1B-C1-O1A	2.48	129.71	124.08
2	0A	3	SIA	O1B-C1-O1A	2.48	129.71	124.08
2	AC	3	SIA	O1B-C1-O1A	2.48	129.71	124.08
2	DC	3	SIA	O1B-C1-O1A	2.48	129.71	124.08
2	hC	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	0	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	NA	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	XB	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	KA	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	LB	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	SC	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	zC	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	3A	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	fA	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	6A	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	bC	3	SIA	O1B-C1-O1A	2.47	129.69	124.08
2	cA	3	SIA	O1B-C1-O1A	2.47	129.68	124.08
2	nC	3	SIA	O1B-C1-O1A	2.47	129.68	124.08
2	9A	3	SIA	O1B-C1-O1A	2.47	129.68	124.08
2	gB	3	SIA	O1B-C1-O1A	2.47	129.68	124.08
2	7B	3	SIA	O1B-C1-O1A	2.47	129.68	124.08
2	WA	3	SIA	O1B-C1-O1A	2.47	129.68	124.08
2	lA	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	rA	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	IB	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	wC	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	iA	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	4B	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	HA	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	CB	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	GC	3	SIA	O1B-C1-O1A	2.46	129.67	124.08
2	tC	3	SIA	O1B-C1-O1A	2.46	129.67	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EA	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	uA	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	yB	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	MC	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	VC	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	OB	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	aB	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	lB	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	PC	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	YC	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	kC	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	TA	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	qC	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	QA	3	SIA	O1B-C1-O1A	2.46	129.66	124.08
2	oA	3	SIA	O1B-C1-O1A	2.45	129.65	124.08
2	RB	3	SIA	O1B-C1-O1A	2.45	129.64	124.08
2	UB	3	SIA	O1B-C1-O1A	2.45	129.64	124.08
2	dB	3	SIA	O1B-C1-O1A	2.45	129.64	124.08
2	FB	3	SIA	O1B-C1-O1A	2.45	129.64	124.08
2	jB	3	SIA	O1B-C1-O1A	2.45	129.64	124.08
2	mB	3	SIA	O1B-C1-O1A	2.45	129.63	124.08
2	vB	3	SIA	O1B-C1-O1A	2.45	129.63	124.08
2	OB	3	SIA	C5-N5-C10	2.39	128.71	123.11
2	kC	3	SIA	C5-N5-C10	2.39	128.71	123.11
2	KA	3	SIA	C5-N5-C10	2.39	128.71	123.11
2	XB	3	SIA	C5-N5-C10	2.38	128.68	123.11
2	iA	3	SIA	C5-N5-C10	2.38	128.68	123.11
2	FB	3	SIA	C5-N5-C10	2.38	128.68	123.11
2	jB	3	SIA	C5-N5-C10	2.38	128.68	123.11
2	4B	3	SIA	C5-N5-C10	2.38	128.68	123.11
2	AC	3	SIA	C5-N5-C10	2.38	128.68	123.11
2	ZA	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	fA	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	0A	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	bC	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	eC	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	GC	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	cA	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	3A	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	nC	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	VC	3	SIA	C5-N5-C10	2.38	128.67	123.11
2	mB	3	SIA	C5-N5-C10	2.37	128.67	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	3	SIA	C5-N5-C10	2.37	128.65	123.11
2	PC	3	SIA	C5-N5-C10	2.37	128.65	123.11
2	YC	3	SIA	C5-N5-C10	2.37	128.65	123.11
2	SC	3	SIA	C5-N5-C10	2.37	128.65	123.11
2	yB	3	SIA	C5-N5-C10	2.36	128.64	123.11
2	6A	3	SIA	C5-N5-C10	2.36	128.64	123.11
2	QA	3	SIA	C5-N5-C10	2.36	128.64	123.11
2	uA	3	SIA	C5-N5-C10	2.36	128.64	123.11
2	MC	3	SIA	C5-N5-C10	2.36	128.64	123.11
2	JC	3	SIA	C5-N5-C10	2.36	128.64	123.11
2	EA	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	9A	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	gB	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	7B	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	HA	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	CB	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	sB	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	tC	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	NA	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	aB	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	dB	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	1B	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	TA	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	lA	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	IB	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	wC	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	pB	3	SIA	C5-N5-C10	2.36	128.63	123.11
2	RB	3	SIA	C5-N5-C10	2.36	128.62	123.11
2	UB	3	SIA	C5-N5-C10	2.36	128.62	123.11
2	oA	3	SIA	C5-N5-C10	2.35	128.62	123.11
2	oA	2	GAL	O5-C1-C2	-2.35	105.18	110.79
2	SC	2	GAL	O5-C1-C2	-2.35	105.18	110.79
2	rA	3	SIA	C5-N5-C10	2.35	128.61	123.11
2	qC	3	SIA	C5-N5-C10	2.35	128.61	123.11
2	BA	3	SIA	C5-N5-C10	2.35	128.60	123.11
2	xA	3	SIA	C5-N5-C10	2.35	128.60	123.11
2	DC	3	SIA	C5-N5-C10	2.35	128.60	123.11
2	3A	2	GAL	O5-C1-C2	-2.35	105.19	110.79
2	WA	3	SIA	C5-N5-C10	2.34	128.60	123.11
2	mB	2	GAL	O5-C1-C2	-2.34	105.20	110.79
2	sB	2	GAL	O5-C1-C2	-2.34	105.20	110.79
2	LB	3	SIA	C5-N5-C10	2.34	128.59	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	vB	3	SIA	C5-N5-C10	2.34	128.59	123.11
2	zC	3	SIA	C5-N5-C10	2.34	128.59	123.11
2	tC	2	GAL	O5-C1-C2	-2.34	105.20	110.79
2	gB	2	GAL	O5-C1-C2	-2.34	105.21	110.79
2	hC	3	SIA	C5-N5-C10	2.34	128.58	123.11
2	vB	2	GAL	O5-C1-C2	-2.34	105.22	110.79
2	ZA	2	GAL	O5-C1-C2	-2.34	105.22	110.79
2	0A	2	GAL	O5-C1-C2	-2.34	105.22	110.79
2	0	2	GAL	O5-C1-C2	-2.33	105.22	110.79
2	OB	2	GAL	O5-C1-C2	-2.33	105.22	110.79
2	XB	2	GAL	O5-C1-C2	-2.33	105.22	110.79
2	kC	2	GAL	O5-C1-C2	-2.33	105.22	110.79
2	WA	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	uA	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	yB	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	MC	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	CB	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	RB	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	UB	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	dB	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	PC	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	YC	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	fA	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	6A	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	bC	2	GAL	O5-C1-C2	-2.33	105.23	110.79
2	NA	2	GAL	O5-C1-C2	-2.33	105.24	110.79
2	rA	2	GAL	O5-C1-C2	-2.33	105.24	110.79
2	qC	2	GAL	O5-C1-C2	-2.33	105.24	110.79
2	DC	2	GAL	O5-C1-C2	-2.33	105.24	110.79
2	GC	2	GAL	O5-C1-C2	-2.33	105.24	110.79
2	EA	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	9A	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	7B	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	cA	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	VC	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	nC	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	iA	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	FB	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	jB	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	4B	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	lA	2	GAL	O5-C1-C2	-2.32	105.25	110.79
2	1B	2	GAL	O5-C1-C2	-2.32	105.26	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BA	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	KA	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	xA	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	AC	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	JC	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	TA	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	pB	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	HA	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	hC	2	GAL	O5-C1-C2	-2.32	105.26	110.79
2	LB	2	GAL	O5-C1-C2	-2.31	105.27	110.79
2	zC	2	GAL	O5-C1-C2	-2.31	105.27	110.79
2	IB	2	GAL	O5-C1-C2	-2.31	105.28	110.79
2	wC	2	GAL	O5-C1-C2	-2.31	105.28	110.79
2	QA	2	GAL	O5-C1-C2	-2.31	105.28	110.79
2	eC	2	GAL	O5-C1-C2	-2.31	105.28	110.79
2	aB	2	GAL	O5-C1-C2	-2.31	105.28	110.79
2	LB	3	SIA	O10-C10-N5	2.21	125.88	121.98
2	vB	3	SIA	O10-C10-N5	2.21	125.88	121.98
2	zC	3	SIA	O10-C10-N5	2.21	125.88	121.98
2	pB	3	SIA	O10-C10-N5	2.21	125.88	121.98
2	hC	3	SIA	O10-C10-N5	2.21	125.88	121.98
2	WA	3	SIA	O10-C10-N5	2.20	125.88	121.98
2	0	3	SIA	O10-C10-N5	2.20	125.86	121.98
2	NA	3	SIA	O10-C10-N5	2.20	125.86	121.98
2	PC	3	SIA	O10-C10-N5	2.20	125.86	121.98
2	HA	3	SIA	O10-C10-N5	2.20	125.86	121.98
2	CB	3	SIA	O10-C10-N5	2.20	125.86	121.98
2	tC	3	SIA	O10-C10-N5	2.20	125.86	121.98
2	TA	3	SIA	O10-C10-N5	2.19	125.86	121.98
2	lA	3	SIA	O10-C10-N5	2.19	125.86	121.98
2	rA	3	SIA	O10-C10-N5	2.19	125.86	121.98
2	IB	3	SIA	O10-C10-N5	2.19	125.86	121.98
2	sB	3	SIA	O10-C10-N5	2.19	125.86	121.98
2	qC	3	SIA	O10-C10-N5	2.19	125.86	121.98
2	wC	3	SIA	O10-C10-N5	2.19	125.86	121.98
2	aB	3	SIA	O10-C10-N5	2.19	125.85	121.98
2	lB	3	SIA	O10-C10-N5	2.19	125.85	121.98
2	SC	3	SIA	O10-C10-N5	2.18	125.84	121.98
2	QA	3	SIA	O10-C10-N5	2.18	125.84	121.98
2	oA	3	SIA	O10-C10-N5	2.18	125.84	121.98
2	uA	3	SIA	O10-C10-N5	2.18	125.84	121.98
2	MC	3	SIA	O10-C10-N5	2.18	125.84	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	RB	3	SIA	O10-C10-N5	2.18	125.83	121.98
2	UB	3	SIA	O10-C10-N5	2.18	125.83	121.98
2	dB	3	SIA	O10-C10-N5	2.18	125.83	121.98
2	yB	3	SIA	O10-C10-N5	2.18	125.83	121.98
2	GC	3	SIA	O10-C10-N5	2.18	125.83	121.98
2	fA	3	SIA	O10-C10-N5	2.17	125.82	121.98
2	6A	3	SIA	O10-C10-N5	2.17	125.82	121.98
2	bC	3	SIA	O10-C10-N5	2.17	125.82	121.98
2	BA	3	SIA	O10-C10-N5	2.17	125.81	121.98
2	xA	3	SIA	O10-C10-N5	2.17	125.81	121.98
2	DC	3	SIA	O10-C10-N5	2.17	125.81	121.98
2	EA	3	SIA	O10-C10-N5	2.17	125.81	121.98
2	9A	3	SIA	O10-C10-N5	2.17	125.81	121.98
2	gB	3	SIA	O10-C10-N5	2.17	125.81	121.98
2	7B	3	SIA	O10-C10-N5	2.17	125.81	121.98
2	JC	3	SIA	O10-C10-N5	2.16	125.81	121.98
2	iA	3	SIA	O10-C10-N5	2.16	125.80	121.98
2	FB	3	SIA	O10-C10-N5	2.16	125.80	121.98
2	jB	3	SIA	O10-C10-N5	2.16	125.80	121.98
2	4B	3	SIA	O10-C10-N5	2.16	125.80	121.98
2	YC	3	SIA	O10-C10-N5	2.16	125.80	121.98
2	VC	3	SIA	O10-C10-N5	2.16	125.80	121.98
2	mB	3	SIA	O10-C10-N5	2.15	125.79	121.98
2	cA	3	SIA	O10-C10-N5	2.15	125.79	121.98
2	3A	3	SIA	O10-C10-N5	2.15	125.79	121.98
2	nC	3	SIA	O10-C10-N5	2.15	125.79	121.98
2	OB	3	SIA	O10-C10-N5	2.15	125.78	121.98
2	XB	3	SIA	O10-C10-N5	2.15	125.78	121.98
2	KA	3	SIA	O10-C10-N5	2.15	125.78	121.98
2	ZA	3	SIA	O10-C10-N5	2.15	125.78	121.98
2	0A	3	SIA	O10-C10-N5	2.15	125.78	121.98
2	eC	3	SIA	O10-C10-N5	2.15	125.78	121.98
2	AC	3	SIA	O10-C10-N5	2.15	125.77	121.98
2	kC	3	SIA	O10-C10-N5	2.13	125.75	121.98
2	iA	3	SIA	O1B-C1-C2	2.00	117.92	112.71
2	4B	3	SIA	O1B-C1-C2	2.00	117.92	112.71

There are no chirality outliers.

All (780) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	0	3	SIA	O6-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	BA	3	SIA	O6-C6-C7-O7
2	EA	3	SIA	O6-C6-C7-O7
2	HA	3	SIA	O6-C6-C7-O7
2	KA	3	SIA	O6-C6-C7-O7
2	NA	3	SIA	O6-C6-C7-O7
2	QA	3	SIA	O6-C6-C7-O7
2	TA	3	SIA	O6-C6-C7-O7
2	WA	3	SIA	O6-C6-C7-O7
2	ZA	3	SIA	O6-C6-C7-O7
2	cA	3	SIA	O6-C6-C7-O7
2	fA	3	SIA	O6-C6-C7-O7
2	iA	3	SIA	O6-C6-C7-O7
2	lA	3	SIA	O6-C6-C7-O7
2	oA	3	SIA	O6-C6-C7-O7
2	rA	3	SIA	O6-C6-C7-O7
2	uA	3	SIA	O6-C6-C7-O7
2	xA	3	SIA	O6-C6-C7-O7
2	0A	3	SIA	O6-C6-C7-O7
2	3A	3	SIA	O6-C6-C7-O7
2	6A	3	SIA	O6-C6-C7-O7
2	9A	3	SIA	O6-C6-C7-O7
2	CB	3	SIA	O6-C6-C7-O7
2	FB	3	SIA	O6-C6-C7-O7
2	IB	3	SIA	O6-C6-C7-O7
2	LB	3	SIA	O6-C6-C7-O7
2	OB	3	SIA	O6-C6-C7-O7
2	RB	3	SIA	O6-C6-C7-O7
2	UB	3	SIA	O6-C6-C7-O7
2	XB	3	SIA	O6-C6-C7-O7
2	aB	3	SIA	O6-C6-C7-O7
2	dB	3	SIA	O6-C6-C7-O7
2	gB	3	SIA	O6-C6-C7-O7
2	jB	3	SIA	O6-C6-C7-O7
2	mB	3	SIA	O6-C6-C7-O7
2	pB	3	SIA	O6-C6-C7-O7
2	sB	3	SIA	O6-C6-C7-O7
2	vB	3	SIA	O6-C6-C7-O7
2	yB	3	SIA	O6-C6-C7-O7
2	1B	3	SIA	O6-C6-C7-O7
2	4B	3	SIA	O6-C6-C7-O7
2	7B	3	SIA	O6-C6-C7-O7
2	AC	3	SIA	O6-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	DC	3	SIA	O6-C6-C7-O7
2	GC	3	SIA	O6-C6-C7-O7
2	JC	3	SIA	O6-C6-C7-O7
2	MC	3	SIA	O6-C6-C7-O7
2	PC	3	SIA	O6-C6-C7-O7
2	SC	3	SIA	O6-C6-C7-O7
2	VC	3	SIA	O6-C6-C7-O7
2	YC	3	SIA	O6-C6-C7-O7
2	bC	3	SIA	O6-C6-C7-O7
2	eC	3	SIA	O6-C6-C7-O7
2	hC	3	SIA	O6-C6-C7-O7
2	kC	3	SIA	O6-C6-C7-O7
2	nC	3	SIA	O6-C6-C7-O7
2	qC	3	SIA	O6-C6-C7-O7
2	tC	3	SIA	O6-C6-C7-O7
2	wC	3	SIA	O6-C6-C7-O7
2	zC	3	SIA	O6-C6-C7-O7
2	0	1	NAG	O5-C5-C6-O6
2	BA	1	NAG	O5-C5-C6-O6
2	EA	1	NAG	O5-C5-C6-O6
2	HA	1	NAG	O5-C5-C6-O6
2	KA	1	NAG	O5-C5-C6-O6
2	NA	1	NAG	O5-C5-C6-O6
2	QA	1	NAG	O5-C5-C6-O6
2	TA	1	NAG	O5-C5-C6-O6
2	WA	1	NAG	O5-C5-C6-O6
2	ZA	1	NAG	O5-C5-C6-O6
2	cA	1	NAG	O5-C5-C6-O6
2	fA	1	NAG	O5-C5-C6-O6
2	iA	1	NAG	O5-C5-C6-O6
2	lA	1	NAG	O5-C5-C6-O6
2	oA	1	NAG	O5-C5-C6-O6
2	rA	1	NAG	O5-C5-C6-O6
2	uA	1	NAG	O5-C5-C6-O6
2	xA	1	NAG	O5-C5-C6-O6
2	0A	1	NAG	O5-C5-C6-O6
2	3A	1	NAG	O5-C5-C6-O6
2	6A	1	NAG	O5-C5-C6-O6
2	9A	1	NAG	O5-C5-C6-O6
2	CB	1	NAG	O5-C5-C6-O6
2	FB	1	NAG	O5-C5-C6-O6
2	IB	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	LB	1	NAG	O5-C5-C6-O6
2	OB	1	NAG	O5-C5-C6-O6
2	RB	1	NAG	O5-C5-C6-O6
2	UB	1	NAG	O5-C5-C6-O6
2	XB	1	NAG	O5-C5-C6-O6
2	aB	1	NAG	O5-C5-C6-O6
2	dB	1	NAG	O5-C5-C6-O6
2	gB	1	NAG	O5-C5-C6-O6
2	jB	1	NAG	O5-C5-C6-O6
2	mB	1	NAG	O5-C5-C6-O6
2	pB	1	NAG	O5-C5-C6-O6
2	sB	1	NAG	O5-C5-C6-O6
2	vB	1	NAG	O5-C5-C6-O6
2	yB	1	NAG	O5-C5-C6-O6
2	1B	1	NAG	O5-C5-C6-O6
2	4B	1	NAG	O5-C5-C6-O6
2	7B	1	NAG	O5-C5-C6-O6
2	AC	1	NAG	O5-C5-C6-O6
2	DC	1	NAG	O5-C5-C6-O6
2	GC	1	NAG	O5-C5-C6-O6
2	JC	1	NAG	O5-C5-C6-O6
2	MC	1	NAG	O5-C5-C6-O6
2	PC	1	NAG	O5-C5-C6-O6
2	SC	1	NAG	O5-C5-C6-O6
2	VC	1	NAG	O5-C5-C6-O6
2	YC	1	NAG	O5-C5-C6-O6
2	bC	1	NAG	O5-C5-C6-O6
2	eC	1	NAG	O5-C5-C6-O6
2	hC	1	NAG	O5-C5-C6-O6
2	kC	1	NAG	O5-C5-C6-O6
2	nC	1	NAG	O5-C5-C6-O6
2	qC	1	NAG	O5-C5-C6-O6
2	tC	1	NAG	O5-C5-C6-O6
2	wC	1	NAG	O5-C5-C6-O6
2	zC	1	NAG	O5-C5-C6-O6
2	0	1	NAG	C4-C5-C6-O6
2	BA	1	NAG	C4-C5-C6-O6
2	EA	1	NAG	C4-C5-C6-O6
2	HA	1	NAG	C4-C5-C6-O6
2	KA	1	NAG	C4-C5-C6-O6
2	NA	1	NAG	C4-C5-C6-O6
2	QA	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	TA	1	NAG	C4-C5-C6-O6
2	WA	1	NAG	C4-C5-C6-O6
2	ZA	1	NAG	C4-C5-C6-O6
2	cA	1	NAG	C4-C5-C6-O6
2	fA	1	NAG	C4-C5-C6-O6
2	iA	1	NAG	C4-C5-C6-O6
2	lA	1	NAG	C4-C5-C6-O6
2	oA	1	NAG	C4-C5-C6-O6
2	rA	1	NAG	C4-C5-C6-O6
2	uA	1	NAG	C4-C5-C6-O6
2	xA	1	NAG	C4-C5-C6-O6
2	0A	1	NAG	C4-C5-C6-O6
2	3A	1	NAG	C4-C5-C6-O6
2	6A	1	NAG	C4-C5-C6-O6
2	9A	1	NAG	C4-C5-C6-O6
2	CB	1	NAG	C4-C5-C6-O6
2	FB	1	NAG	C4-C5-C6-O6
2	IB	1	NAG	C4-C5-C6-O6
2	LB	1	NAG	C4-C5-C6-O6
2	OB	1	NAG	C4-C5-C6-O6
2	RB	1	NAG	C4-C5-C6-O6
2	UB	1	NAG	C4-C5-C6-O6
2	XB	1	NAG	C4-C5-C6-O6
2	aB	1	NAG	C4-C5-C6-O6
2	dB	1	NAG	C4-C5-C6-O6
2	gB	1	NAG	C4-C5-C6-O6
2	jB	1	NAG	C4-C5-C6-O6
2	mB	1	NAG	C4-C5-C6-O6
2	pB	1	NAG	C4-C5-C6-O6
2	sB	1	NAG	C4-C5-C6-O6
2	vB	1	NAG	C4-C5-C6-O6
2	yB	1	NAG	C4-C5-C6-O6
2	1B	1	NAG	C4-C5-C6-O6
2	4B	1	NAG	C4-C5-C6-O6
2	7B	1	NAG	C4-C5-C6-O6
2	AC	1	NAG	C4-C5-C6-O6
2	DC	1	NAG	C4-C5-C6-O6
2	GC	1	NAG	C4-C5-C6-O6
2	JC	1	NAG	C4-C5-C6-O6
2	MC	1	NAG	C4-C5-C6-O6
2	PC	1	NAG	C4-C5-C6-O6
2	SC	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	VC	1	NAG	C4-C5-C6-O6
2	YC	1	NAG	C4-C5-C6-O6
2	bC	1	NAG	C4-C5-C6-O6
2	eC	1	NAG	C4-C5-C6-O6
2	hC	1	NAG	C4-C5-C6-O6
2	kC	1	NAG	C4-C5-C6-O6
2	nC	1	NAG	C4-C5-C6-O6
2	qC	1	NAG	C4-C5-C6-O6
2	tC	1	NAG	C4-C5-C6-O6
2	wC	1	NAG	C4-C5-C6-O6
2	zC	1	NAG	C4-C5-C6-O6
2	0	3	SIA	O7-C7-C8-C9
2	BA	3	SIA	O7-C7-C8-C9
2	EA	3	SIA	O7-C7-C8-C9
2	HA	3	SIA	O7-C7-C8-C9
2	KA	3	SIA	O7-C7-C8-C9
2	NA	3	SIA	O7-C7-C8-C9
2	QA	3	SIA	O7-C7-C8-C9
2	TA	3	SIA	O7-C7-C8-C9
2	WA	3	SIA	O7-C7-C8-C9
2	ZA	3	SIA	O7-C7-C8-C9
2	cA	3	SIA	O7-C7-C8-C9
2	fA	3	SIA	O7-C7-C8-C9
2	iA	3	SIA	O7-C7-C8-C9
2	lA	3	SIA	O7-C7-C8-C9
2	oA	3	SIA	O7-C7-C8-C9
2	rA	3	SIA	O7-C7-C8-C9
2	uA	3	SIA	O7-C7-C8-C9
2	xA	3	SIA	O7-C7-C8-C9
2	0A	3	SIA	O7-C7-C8-C9
2	3A	3	SIA	O7-C7-C8-C9
2	6A	3	SIA	O7-C7-C8-C9
2	9A	3	SIA	O7-C7-C8-C9
2	CB	3	SIA	O7-C7-C8-C9
2	FB	3	SIA	O7-C7-C8-C9
2	IB	3	SIA	O7-C7-C8-C9
2	LB	3	SIA	O7-C7-C8-C9
2	OB	3	SIA	O7-C7-C8-C9
2	RB	3	SIA	O7-C7-C8-C9
2	UB	3	SIA	O7-C7-C8-C9
2	XB	3	SIA	O7-C7-C8-C9
2	aB	3	SIA	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	dB	3	SIA	O7-C7-C8-C9
2	gB	3	SIA	O7-C7-C8-C9
2	jB	3	SIA	O7-C7-C8-C9
2	mB	3	SIA	O7-C7-C8-C9
2	pB	3	SIA	O7-C7-C8-C9
2	sB	3	SIA	O7-C7-C8-C9
2	vB	3	SIA	O7-C7-C8-C9
2	yB	3	SIA	O7-C7-C8-C9
2	1B	3	SIA	O7-C7-C8-C9
2	4B	3	SIA	O7-C7-C8-C9
2	7B	3	SIA	O7-C7-C8-C9
2	AC	3	SIA	O7-C7-C8-C9
2	DC	3	SIA	O7-C7-C8-C9
2	GC	3	SIA	O7-C7-C8-C9
2	JC	3	SIA	O7-C7-C8-C9
2	MC	3	SIA	O7-C7-C8-C9
2	PC	3	SIA	O7-C7-C8-C9
2	SC	3	SIA	O7-C7-C8-C9
2	VC	3	SIA	O7-C7-C8-C9
2	YC	3	SIA	O7-C7-C8-C9
2	bC	3	SIA	O7-C7-C8-C9
2	eC	3	SIA	O7-C7-C8-C9
2	hC	3	SIA	O7-C7-C8-C9
2	kC	3	SIA	O7-C7-C8-C9
2	nC	3	SIA	O7-C7-C8-C9
2	qC	3	SIA	O7-C7-C8-C9
2	tC	3	SIA	O7-C7-C8-C9
2	wC	3	SIA	O7-C7-C8-C9
2	zC	3	SIA	O7-C7-C8-C9
2	0	3	SIA	C4-C5-N5-C10
2	BA	3	SIA	C4-C5-N5-C10
2	EA	3	SIA	C4-C5-N5-C10
2	HA	3	SIA	C4-C5-N5-C10
2	KA	3	SIA	C4-C5-N5-C10
2	NA	3	SIA	C4-C5-N5-C10
2	QA	3	SIA	C4-C5-N5-C10
2	TA	3	SIA	C4-C5-N5-C10
2	WA	3	SIA	C4-C5-N5-C10
2	ZA	3	SIA	C4-C5-N5-C10
2	cA	3	SIA	C4-C5-N5-C10
2	fA	3	SIA	C4-C5-N5-C10
2	iA	3	SIA	C4-C5-N5-C10

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Mol	Chain	Res	Type	Atoms
2	lA	3	SIA	C4-C5-N5-C10
2	oA	3	SIA	C4-C5-N5-C10
2	rA	3	SIA	C4-C5-N5-C10
2	uA	3	SIA	C4-C5-N5-C10
2	xA	3	SIA	C4-C5-N5-C10
2	0A	3	SIA	C4-C5-N5-C10
2	3A	3	SIA	C4-C5-N5-C10
2	6A	3	SIA	C4-C5-N5-C10
2	9A	3	SIA	C4-C5-N5-C10
2	CB	3	SIA	C4-C5-N5-C10
2	FB	3	SIA	C4-C5-N5-C10
2	IB	3	SIA	C4-C5-N5-C10
2	LB	3	SIA	C4-C5-N5-C10
2	OB	3	SIA	C4-C5-N5-C10
2	RB	3	SIA	C4-C5-N5-C10
2	UB	3	SIA	C4-C5-N5-C10
2	XB	3	SIA	C4-C5-N5-C10
2	aB	3	SIA	C4-C5-N5-C10
2	dB	3	SIA	C4-C5-N5-C10
2	gB	3	SIA	C4-C5-N5-C10
2	jB	3	SIA	C4-C5-N5-C10
2	mB	3	SIA	C4-C5-N5-C10
2	pB	3	SIA	C4-C5-N5-C10
2	sB	3	SIA	C4-C5-N5-C10
2	vB	3	SIA	C4-C5-N5-C10
2	yB	3	SIA	C4-C5-N5-C10
2	1B	3	SIA	C4-C5-N5-C10
2	4B	3	SIA	C4-C5-N5-C10
2	7B	3	SIA	C4-C5-N5-C10
2	AC	3	SIA	C4-C5-N5-C10
2	DC	3	SIA	C4-C5-N5-C10
2	GC	3	SIA	C4-C5-N5-C10
2	JC	3	SIA	C4-C5-N5-C10
2	MC	3	SIA	C4-C5-N5-C10
2	PC	3	SIA	C4-C5-N5-C10
2	SC	3	SIA	C4-C5-N5-C10
2	VC	3	SIA	C4-C5-N5-C10
2	YC	3	SIA	C4-C5-N5-C10
2	bC	3	SIA	C4-C5-N5-C10
2	eC	3	SIA	C4-C5-N5-C10
2	hC	3	SIA	C4-C5-N5-C10
2	kC	3	SIA	C4-C5-N5-C10

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Mol	Chain	Res	Type	Atoms
2	nC	3	SIA	C4-C5-N5-C10
2	qC	3	SIA	C4-C5-N5-C10
2	tC	3	SIA	C4-C5-N5-C10
2	wC	3	SIA	C4-C5-N5-C10
2	zC	3	SIA	C4-C5-N5-C10
2	0	3	SIA	C6-C7-C8-C9
2	BA	3	SIA	C6-C7-C8-C9
2	EA	3	SIA	C6-C7-C8-C9
2	HA	3	SIA	C6-C7-C8-C9
2	KA	3	SIA	C6-C7-C8-C9
2	NA	3	SIA	C6-C7-C8-C9
2	QA	3	SIA	C6-C7-C8-C9
2	TA	3	SIA	C6-C7-C8-C9
2	WA	3	SIA	C6-C7-C8-C9
2	ZA	3	SIA	C6-C7-C8-C9
2	cA	3	SIA	C6-C7-C8-C9
2	fA	3	SIA	C6-C7-C8-C9
2	iA	3	SIA	C6-C7-C8-C9
2	lA	3	SIA	C6-C7-C8-C9
2	oA	3	SIA	C6-C7-C8-C9
2	rA	3	SIA	C6-C7-C8-C9
2	uA	3	SIA	C6-C7-C8-C9
2	xA	3	SIA	C6-C7-C8-C9
2	0A	3	SIA	C6-C7-C8-C9
2	3A	3	SIA	C6-C7-C8-C9
2	6A	3	SIA	C6-C7-C8-C9
2	9A	3	SIA	C6-C7-C8-C9
2	CB	3	SIA	C6-C7-C8-C9
2	FB	3	SIA	C6-C7-C8-C9
2	IB	3	SIA	C6-C7-C8-C9
2	LB	3	SIA	C6-C7-C8-C9
2	OB	3	SIA	C6-C7-C8-C9
2	RB	3	SIA	C6-C7-C8-C9
2	UB	3	SIA	C6-C7-C8-C9
2	XB	3	SIA	C6-C7-C8-C9
2	aB	3	SIA	C6-C7-C8-C9
2	dB	3	SIA	C6-C7-C8-C9
2	gB	3	SIA	C6-C7-C8-C9
2	jB	3	SIA	C6-C7-C8-C9
2	mB	3	SIA	C6-C7-C8-C9
2	pB	3	SIA	C6-C7-C8-C9
2	sB	3	SIA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	vB	3	SIA	C6-C7-C8-C9
2	yB	3	SIA	C6-C7-C8-C9
2	1B	3	SIA	C6-C7-C8-C9
2	4B	3	SIA	C6-C7-C8-C9
2	7B	3	SIA	C6-C7-C8-C9
2	AC	3	SIA	C6-C7-C8-C9
2	DC	3	SIA	C6-C7-C8-C9
2	GC	3	SIA	C6-C7-C8-C9
2	JC	3	SIA	C6-C7-C8-C9
2	MC	3	SIA	C6-C7-C8-C9
2	PC	3	SIA	C6-C7-C8-C9
2	SC	3	SIA	C6-C7-C8-C9
2	VC	3	SIA	C6-C7-C8-C9
2	YC	3	SIA	C6-C7-C8-C9
2	bC	3	SIA	C6-C7-C8-C9
2	eC	3	SIA	C6-C7-C8-C9
2	hC	3	SIA	C6-C7-C8-C9
2	kC	3	SIA	C6-C7-C8-C9
2	nC	3	SIA	C6-C7-C8-C9
2	qC	3	SIA	C6-C7-C8-C9
2	tC	3	SIA	C6-C7-C8-C9
2	wC	3	SIA	C6-C7-C8-C9
2	zC	3	SIA	C6-C7-C8-C9
2	0	3	SIA	O7-C7-C8-O8
2	BA	3	SIA	O7-C7-C8-O8
2	EA	3	SIA	O7-C7-C8-O8
2	HA	3	SIA	O7-C7-C8-O8
2	KA	3	SIA	O7-C7-C8-O8
2	NA	3	SIA	O7-C7-C8-O8
2	QA	3	SIA	O7-C7-C8-O8
2	TA	3	SIA	O7-C7-C8-O8
2	WA	3	SIA	O7-C7-C8-O8
2	ZA	3	SIA	O7-C7-C8-O8
2	cA	3	SIA	O7-C7-C8-O8
2	fA	3	SIA	O7-C7-C8-O8
2	iA	3	SIA	O7-C7-C8-O8
2	lA	3	SIA	O7-C7-C8-O8
2	oA	3	SIA	O7-C7-C8-O8
2	rA	3	SIA	O7-C7-C8-O8
2	uA	3	SIA	O7-C7-C8-O8
2	xA	3	SIA	O7-C7-C8-O8
2	0A	3	SIA	O7-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	3A	3	SIA	O7-C7-C8-O8
2	6A	3	SIA	O7-C7-C8-O8
2	9A	3	SIA	O7-C7-C8-O8
2	CB	3	SIA	O7-C7-C8-O8
2	FB	3	SIA	O7-C7-C8-O8
2	IB	3	SIA	O7-C7-C8-O8
2	LB	3	SIA	O7-C7-C8-O8
2	OB	3	SIA	O7-C7-C8-O8
2	RB	3	SIA	O7-C7-C8-O8
2	UB	3	SIA	O7-C7-C8-O8
2	XB	3	SIA	O7-C7-C8-O8
2	aB	3	SIA	O7-C7-C8-O8
2	dB	3	SIA	O7-C7-C8-O8
2	gB	3	SIA	O7-C7-C8-O8
2	jB	3	SIA	O7-C7-C8-O8
2	mB	3	SIA	O7-C7-C8-O8
2	pB	3	SIA	O7-C7-C8-O8
2	sB	3	SIA	O7-C7-C8-O8
2	vB	3	SIA	O7-C7-C8-O8
2	yB	3	SIA	O7-C7-C8-O8
2	1B	3	SIA	O7-C7-C8-O8
2	4B	3	SIA	O7-C7-C8-O8
2	7B	3	SIA	O7-C7-C8-O8
2	AC	3	SIA	O7-C7-C8-O8
2	DC	3	SIA	O7-C7-C8-O8
2	GC	3	SIA	O7-C7-C8-O8
2	JC	3	SIA	O7-C7-C8-O8
2	MC	3	SIA	O7-C7-C8-O8
2	PC	3	SIA	O7-C7-C8-O8
2	SC	3	SIA	O7-C7-C8-O8
2	VC	3	SIA	O7-C7-C8-O8
2	YC	3	SIA	O7-C7-C8-O8
2	bC	3	SIA	O7-C7-C8-O8
2	eC	3	SIA	O7-C7-C8-O8
2	hC	3	SIA	O7-C7-C8-O8
2	kC	3	SIA	O7-C7-C8-O8
2	nC	3	SIA	O7-C7-C8-O8
2	qC	3	SIA	O7-C7-C8-O8
2	tC	3	SIA	O7-C7-C8-O8
2	wC	3	SIA	O7-C7-C8-O8
2	zC	3	SIA	O7-C7-C8-O8
2	0	3	SIA	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	BA	3	SIA	C5-C6-C7-O7
2	EA	3	SIA	C5-C6-C7-O7
2	HA	3	SIA	C5-C6-C7-O7
2	KA	3	SIA	C5-C6-C7-O7
2	NA	3	SIA	C5-C6-C7-O7
2	QA	3	SIA	C5-C6-C7-O7
2	TA	3	SIA	C5-C6-C7-O7
2	WA	3	SIA	C5-C6-C7-O7
2	ZA	3	SIA	C5-C6-C7-O7
2	cA	3	SIA	C5-C6-C7-O7
2	fA	3	SIA	C5-C6-C7-O7
2	iA	3	SIA	C5-C6-C7-O7
2	lA	3	SIA	C5-C6-C7-O7
2	oA	3	SIA	C5-C6-C7-O7
2	rA	3	SIA	C5-C6-C7-O7
2	uA	3	SIA	C5-C6-C7-O7
2	xA	3	SIA	C5-C6-C7-O7
2	0A	3	SIA	C5-C6-C7-O7
2	3A	3	SIA	C5-C6-C7-O7
2	6A	3	SIA	C5-C6-C7-O7
2	9A	3	SIA	C5-C6-C7-O7
2	CB	3	SIA	C5-C6-C7-O7
2	FB	3	SIA	C5-C6-C7-O7
2	IB	3	SIA	C5-C6-C7-O7
2	LB	3	SIA	C5-C6-C7-O7
2	OB	3	SIA	C5-C6-C7-O7
2	RB	3	SIA	C5-C6-C7-O7
2	UB	3	SIA	C5-C6-C7-O7
2	XB	3	SIA	C5-C6-C7-O7
2	aB	3	SIA	C5-C6-C7-O7
2	dB	3	SIA	C5-C6-C7-O7
2	gB	3	SIA	C5-C6-C7-O7
2	jB	3	SIA	C5-C6-C7-O7
2	mB	3	SIA	C5-C6-C7-O7
2	pB	3	SIA	C5-C6-C7-O7
2	sB	3	SIA	C5-C6-C7-O7
2	vB	3	SIA	C5-C6-C7-O7
2	yB	3	SIA	C5-C6-C7-O7
2	1B	3	SIA	C5-C6-C7-O7
2	4B	3	SIA	C5-C6-C7-O7
2	7B	3	SIA	C5-C6-C7-O7
2	AC	3	SIA	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	DC	3	SIA	C5-C6-C7-O7
2	GC	3	SIA	C5-C6-C7-O7
2	JC	3	SIA	C5-C6-C7-O7
2	MC	3	SIA	C5-C6-C7-O7
2	PC	3	SIA	C5-C6-C7-O7
2	SC	3	SIA	C5-C6-C7-O7
2	VC	3	SIA	C5-C6-C7-O7
2	YC	3	SIA	C5-C6-C7-O7
2	bC	3	SIA	C5-C6-C7-O7
2	eC	3	SIA	C5-C6-C7-O7
2	hC	3	SIA	C5-C6-C7-O7
2	kC	3	SIA	C5-C6-C7-O7
2	nC	3	SIA	C5-C6-C7-O7
2	qC	3	SIA	C5-C6-C7-O7
2	tC	3	SIA	C5-C6-C7-O7
2	wC	3	SIA	C5-C6-C7-O7
2	zC	3	SIA	C5-C6-C7-O7
2	EA	2	GAL	O5-C5-C6-O6
2	HA	2	GAL	O5-C5-C6-O6
2	cA	2	GAL	O5-C5-C6-O6
2	9A	2	GAL	O5-C5-C6-O6
2	CB	2	GAL	O5-C5-C6-O6
2	OB	2	GAL	O5-C5-C6-O6
2	vB	2	GAL	O5-C5-C6-O6
2	yB	2	GAL	O5-C5-C6-O6
2	7B	2	GAL	O5-C5-C6-O6
2	VC	2	GAL	O5-C5-C6-O6
2	kC	2	GAL	O5-C5-C6-O6
2	nC	2	GAL	O5-C5-C6-O6
2	tC	2	GAL	O5-C5-C6-O6
2	QA	2	GAL	O5-C5-C6-O6
2	iA	2	GAL	O5-C5-C6-O6
2	LB	2	GAL	O5-C5-C6-O6
2	RB	2	GAL	O5-C5-C6-O6
2	UB	2	GAL	O5-C5-C6-O6
2	dB	2	GAL	O5-C5-C6-O6
2	zC	2	GAL	O5-C5-C6-O6
2	0	2	GAL	O5-C5-C6-O6
2	ZA	2	GAL	O5-C5-C6-O6
2	fA	2	GAL	O5-C5-C6-O6
2	0A	2	GAL	O5-C5-C6-O6
2	3A	2	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	6A	2	GAL	O5-C5-C6-O6
2	gB	2	GAL	O5-C5-C6-O6
2	AC	2	GAL	O5-C5-C6-O6
2	GC	2	GAL	O5-C5-C6-O6
2	PC	2	GAL	O5-C5-C6-O6
2	bC	2	GAL	O5-C5-C6-O6
2	KA	2	GAL	O5-C5-C6-O6
2	lA	2	GAL	O5-C5-C6-O6
2	IB	2	GAL	O5-C5-C6-O6
2	aB	2	GAL	O5-C5-C6-O6
2	mB	2	GAL	O5-C5-C6-O6
2	pB	2	GAL	O5-C5-C6-O6
2	lB	2	GAL	O5-C5-C6-O6
2	wC	2	GAL	O5-C5-C6-O6
2	BA	2	GAL	O5-C5-C6-O6
2	NA	2	GAL	O5-C5-C6-O6
2	xA	2	GAL	O5-C5-C6-O6
2	XB	2	GAL	O5-C5-C6-O6
2	DC	2	GAL	O5-C5-C6-O6
2	eC	2	GAL	O5-C5-C6-O6
2	TA	2	GAL	O5-C5-C6-O6
2	oA	2	GAL	O5-C5-C6-O6
2	rA	2	GAL	O5-C5-C6-O6
2	uA	2	GAL	O5-C5-C6-O6
2	FB	2	GAL	O5-C5-C6-O6
2	jB	2	GAL	O5-C5-C6-O6
2	sB	2	GAL	O5-C5-C6-O6
2	4B	2	GAL	O5-C5-C6-O6
2	JC	2	GAL	O5-C5-C6-O6
2	MC	2	GAL	O5-C5-C6-O6
2	SC	2	GAL	O5-C5-C6-O6
2	YC	2	GAL	O5-C5-C6-O6
2	qC	2	GAL	O5-C5-C6-O6
2	WA	2	GAL	O5-C5-C6-O6
2	hC	2	GAL	O5-C5-C6-O6
2	0	3	SIA	O6-C6-C7-C8
2	BA	3	SIA	O6-C6-C7-C8
2	EA	3	SIA	O6-C6-C7-C8
2	HA	3	SIA	O6-C6-C7-C8
2	KA	3	SIA	O6-C6-C7-C8
2	NA	3	SIA	O6-C6-C7-C8
2	QA	3	SIA	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	TA	3	SIA	O6-C6-C7-C8
2	WA	3	SIA	O6-C6-C7-C8
2	ZA	3	SIA	O6-C6-C7-C8
2	cA	3	SIA	O6-C6-C7-C8
2	fA	3	SIA	O6-C6-C7-C8
2	iA	3	SIA	O6-C6-C7-C8
2	lA	3	SIA	O6-C6-C7-C8
2	oA	3	SIA	O6-C6-C7-C8
2	rA	3	SIA	O6-C6-C7-C8
2	uA	3	SIA	O6-C6-C7-C8
2	xA	3	SIA	O6-C6-C7-C8
2	0A	3	SIA	O6-C6-C7-C8
2	3A	3	SIA	O6-C6-C7-C8
2	6A	3	SIA	O6-C6-C7-C8
2	9A	3	SIA	O6-C6-C7-C8
2	CB	3	SIA	O6-C6-C7-C8
2	FB	3	SIA	O6-C6-C7-C8
2	IB	3	SIA	O6-C6-C7-C8
2	LB	3	SIA	O6-C6-C7-C8
2	OB	3	SIA	O6-C6-C7-C8
2	RB	3	SIA	O6-C6-C7-C8
2	UB	3	SIA	O6-C6-C7-C8
2	XB	3	SIA	O6-C6-C7-C8
2	aB	3	SIA	O6-C6-C7-C8
2	dB	3	SIA	O6-C6-C7-C8
2	gB	3	SIA	O6-C6-C7-C8
2	jB	3	SIA	O6-C6-C7-C8
2	mB	3	SIA	O6-C6-C7-C8
2	pB	3	SIA	O6-C6-C7-C8
2	sB	3	SIA	O6-C6-C7-C8
2	vB	3	SIA	O6-C6-C7-C8
2	yB	3	SIA	O6-C6-C7-C8
2	1B	3	SIA	O6-C6-C7-C8
2	4B	3	SIA	O6-C6-C7-C8
2	7B	3	SIA	O6-C6-C7-C8
2	AC	3	SIA	O6-C6-C7-C8
2	DC	3	SIA	O6-C6-C7-C8
2	GC	3	SIA	O6-C6-C7-C8
2	JC	3	SIA	O6-C6-C7-C8
2	MC	3	SIA	O6-C6-C7-C8
2	PC	3	SIA	O6-C6-C7-C8
2	SC	3	SIA	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	VC	3	SIA	O6-C6-C7-C8
2	YC	3	SIA	O6-C6-C7-C8
2	bC	3	SIA	O6-C6-C7-C8
2	eC	3	SIA	O6-C6-C7-C8
2	hC	3	SIA	O6-C6-C7-C8
2	kC	3	SIA	O6-C6-C7-C8
2	nC	3	SIA	O6-C6-C7-C8
2	qC	3	SIA	O6-C6-C7-C8
2	tC	3	SIA	O6-C6-C7-C8
2	wC	3	SIA	O6-C6-C7-C8
2	zC	3	SIA	O6-C6-C7-C8
2	0	3	SIA	C5-C6-C7-C8
2	BA	3	SIA	C5-C6-C7-C8
2	EA	3	SIA	C5-C6-C7-C8
2	HA	3	SIA	C5-C6-C7-C8
2	KA	3	SIA	C5-C6-C7-C8
2	NA	3	SIA	C5-C6-C7-C8
2	QA	3	SIA	C5-C6-C7-C8
2	TA	3	SIA	C5-C6-C7-C8
2	WA	3	SIA	C5-C6-C7-C8
2	ZA	3	SIA	C5-C6-C7-C8
2	cA	3	SIA	C5-C6-C7-C8
2	fA	3	SIA	C5-C6-C7-C8
2	iA	3	SIA	C5-C6-C7-C8
2	lA	3	SIA	C5-C6-C7-C8
2	oA	3	SIA	C5-C6-C7-C8
2	rA	3	SIA	C5-C6-C7-C8
2	uA	3	SIA	C5-C6-C7-C8
2	xA	3	SIA	C5-C6-C7-C8
2	0A	3	SIA	C5-C6-C7-C8
2	3A	3	SIA	C5-C6-C7-C8
2	6A	3	SIA	C5-C6-C7-C8
2	9A	3	SIA	C5-C6-C7-C8
2	CB	3	SIA	C5-C6-C7-C8
2	FB	3	SIA	C5-C6-C7-C8
2	IB	3	SIA	C5-C6-C7-C8
2	LB	3	SIA	C5-C6-C7-C8
2	OB	3	SIA	C5-C6-C7-C8
2	RB	3	SIA	C5-C6-C7-C8
2	UB	3	SIA	C5-C6-C7-C8
2	XB	3	SIA	C5-C6-C7-C8
2	aB	3	SIA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	dB	3	SIA	C5-C6-C7-C8
2	gB	3	SIA	C5-C6-C7-C8
2	jB	3	SIA	C5-C6-C7-C8
2	mB	3	SIA	C5-C6-C7-C8
2	pB	3	SIA	C5-C6-C7-C8
2	sB	3	SIA	C5-C6-C7-C8
2	vB	3	SIA	C5-C6-C7-C8
2	yB	3	SIA	C5-C6-C7-C8
2	1B	3	SIA	C5-C6-C7-C8
2	4B	3	SIA	C5-C6-C7-C8
2	7B	3	SIA	C5-C6-C7-C8
2	AC	3	SIA	C5-C6-C7-C8
2	DC	3	SIA	C5-C6-C7-C8
2	GC	3	SIA	C5-C6-C7-C8
2	JC	3	SIA	C5-C6-C7-C8
2	MC	3	SIA	C5-C6-C7-C8
2	PC	3	SIA	C5-C6-C7-C8
2	SC	3	SIA	C5-C6-C7-C8
2	VC	3	SIA	C5-C6-C7-C8
2	YC	3	SIA	C5-C6-C7-C8
2	bC	3	SIA	C5-C6-C7-C8
2	eC	3	SIA	C5-C6-C7-C8
2	hC	3	SIA	C5-C6-C7-C8
2	kC	3	SIA	C5-C6-C7-C8
2	nC	3	SIA	C5-C6-C7-C8
2	qC	3	SIA	C5-C6-C7-C8
2	tC	3	SIA	C5-C6-C7-C8
2	wC	3	SIA	C5-C6-C7-C8
2	zC	3	SIA	C5-C6-C7-C8
2	0	3	SIA	C6-C7-C8-O8
2	EA	3	SIA	C6-C7-C8-O8
2	uA	3	SIA	C6-C7-C8-O8
2	9A	3	SIA	C6-C7-C8-O8
2	gB	3	SIA	C6-C7-C8-O8
2	sB	3	SIA	C6-C7-C8-O8
2	7B	3	SIA	C6-C7-C8-O8
2	YC	3	SIA	C6-C7-C8-O8
2	HA	3	SIA	C6-C7-C8-O8
2	NA	3	SIA	C6-C7-C8-O8
2	WA	3	SIA	C6-C7-C8-O8
2	iA	3	SIA	C6-C7-C8-O8
2	lA	3	SIA	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	CB	3	SIA	C6-C7-C8-O8
2	FB	3	SIA	C6-C7-C8-O8
2	IB	3	SIA	C6-C7-C8-O8
2	yB	3	SIA	C6-C7-C8-O8
2	4B	3	SIA	C6-C7-C8-O8
2	AC	3	SIA	C6-C7-C8-O8
2	MC	3	SIA	C6-C7-C8-O8
2	PC	3	SIA	C6-C7-C8-O8
2	SC	3	SIA	C6-C7-C8-O8
2	VC	3	SIA	C6-C7-C8-O8
2	tC	3	SIA	C6-C7-C8-O8
2	wC	3	SIA	C6-C7-C8-O8
2	BA	3	SIA	C6-C7-C8-O8
2	KA	3	SIA	C6-C7-C8-O8
2	QA	3	SIA	C6-C7-C8-O8
2	TA	3	SIA	C6-C7-C8-O8
2	ZA	3	SIA	C6-C7-C8-O8
2	cA	3	SIA	C6-C7-C8-O8
2	fA	3	SIA	C6-C7-C8-O8
2	oA	3	SIA	C6-C7-C8-O8
2	rA	3	SIA	C6-C7-C8-O8
2	xA	3	SIA	C6-C7-C8-O8
2	0A	3	SIA	C6-C7-C8-O8
2	3A	3	SIA	C6-C7-C8-O8
2	6A	3	SIA	C6-C7-C8-O8
2	LB	3	SIA	C6-C7-C8-O8
2	OB	3	SIA	C6-C7-C8-O8
2	RB	3	SIA	C6-C7-C8-O8
2	UB	3	SIA	C6-C7-C8-O8
2	XB	3	SIA	C6-C7-C8-O8
2	aB	3	SIA	C6-C7-C8-O8
2	dB	3	SIA	C6-C7-C8-O8
2	jB	3	SIA	C6-C7-C8-O8
2	mB	3	SIA	C6-C7-C8-O8
2	pB	3	SIA	C6-C7-C8-O8
2	vB	3	SIA	C6-C7-C8-O8
2	1B	3	SIA	C6-C7-C8-O8
2	DC	3	SIA	C6-C7-C8-O8
2	GC	3	SIA	C6-C7-C8-O8
2	JC	3	SIA	C6-C7-C8-O8
2	bC	3	SIA	C6-C7-C8-O8
2	eC	3	SIA	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	hC	3	SIA	C6-C7-C8-O8
2	kC	3	SIA	C6-C7-C8-O8
2	nC	3	SIA	C6-C7-C8-O8
2	qC	3	SIA	C6-C7-C8-O8
2	zC	3	SIA	C6-C7-C8-O8
2	0	3	SIA	C6-C5-N5-C10
2	BA	3	SIA	C6-C5-N5-C10
2	EA	3	SIA	C6-C5-N5-C10
2	HA	3	SIA	C6-C5-N5-C10
2	KA	3	SIA	C6-C5-N5-C10
2	NA	3	SIA	C6-C5-N5-C10
2	QA	3	SIA	C6-C5-N5-C10
2	TA	3	SIA	C6-C5-N5-C10
2	WA	3	SIA	C6-C5-N5-C10
2	ZA	3	SIA	C6-C5-N5-C10
2	cA	3	SIA	C6-C5-N5-C10
2	fA	3	SIA	C6-C5-N5-C10
2	iA	3	SIA	C6-C5-N5-C10
2	lA	3	SIA	C6-C5-N5-C10
2	oA	3	SIA	C6-C5-N5-C10
2	rA	3	SIA	C6-C5-N5-C10
2	uA	3	SIA	C6-C5-N5-C10
2	xA	3	SIA	C6-C5-N5-C10
2	0A	3	SIA	C6-C5-N5-C10
2	3A	3	SIA	C6-C5-N5-C10
2	6A	3	SIA	C6-C5-N5-C10
2	9A	3	SIA	C6-C5-N5-C10
2	CB	3	SIA	C6-C5-N5-C10
2	FB	3	SIA	C6-C5-N5-C10
2	IB	3	SIA	C6-C5-N5-C10
2	LB	3	SIA	C6-C5-N5-C10
2	OB	3	SIA	C6-C5-N5-C10
2	RB	3	SIA	C6-C5-N5-C10
2	UB	3	SIA	C6-C5-N5-C10
2	XB	3	SIA	C6-C5-N5-C10
2	aB	3	SIA	C6-C5-N5-C10
2	dB	3	SIA	C6-C5-N5-C10
2	gB	3	SIA	C6-C5-N5-C10
2	jB	3	SIA	C6-C5-N5-C10
2	mB	3	SIA	C6-C5-N5-C10
2	pB	3	SIA	C6-C5-N5-C10
2	sB	3	SIA	C6-C5-N5-C10

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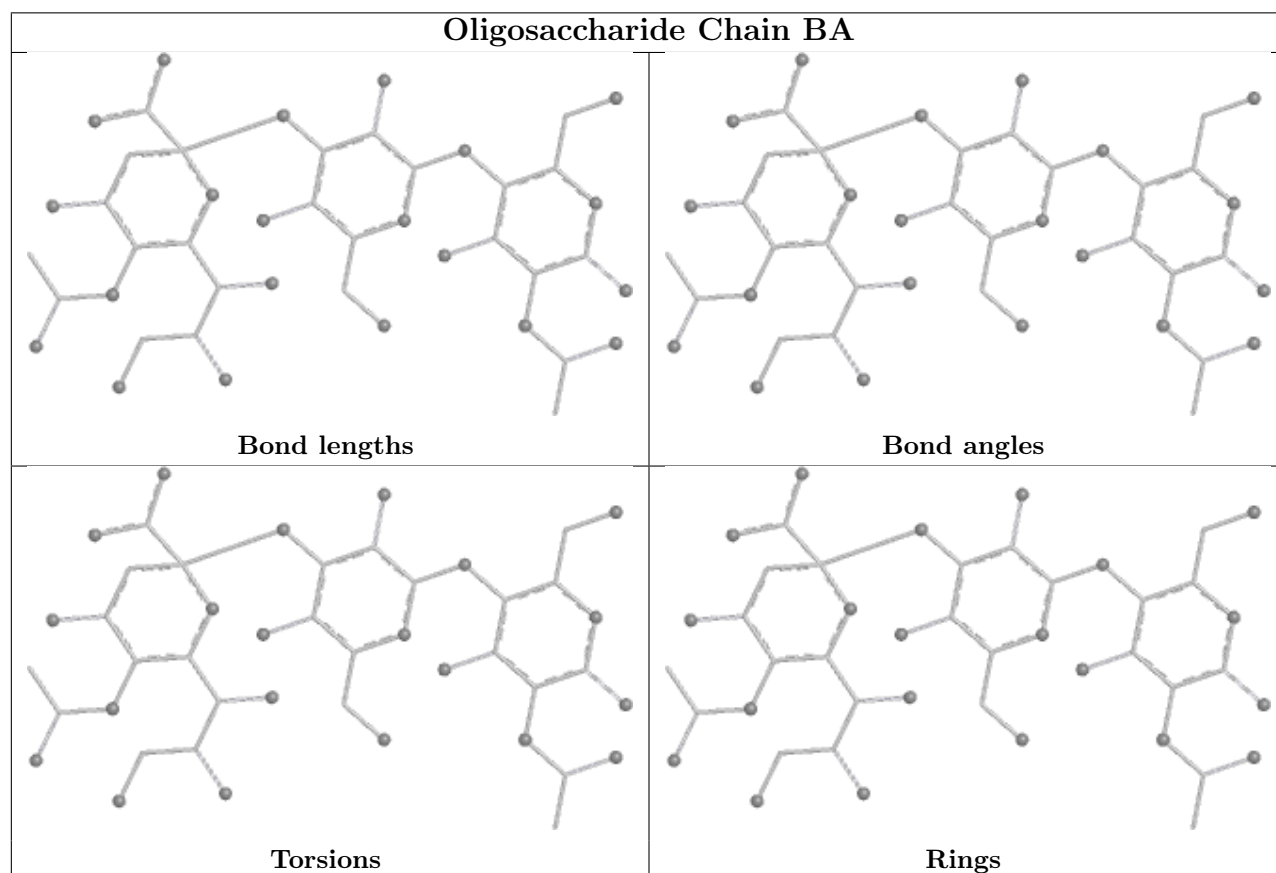
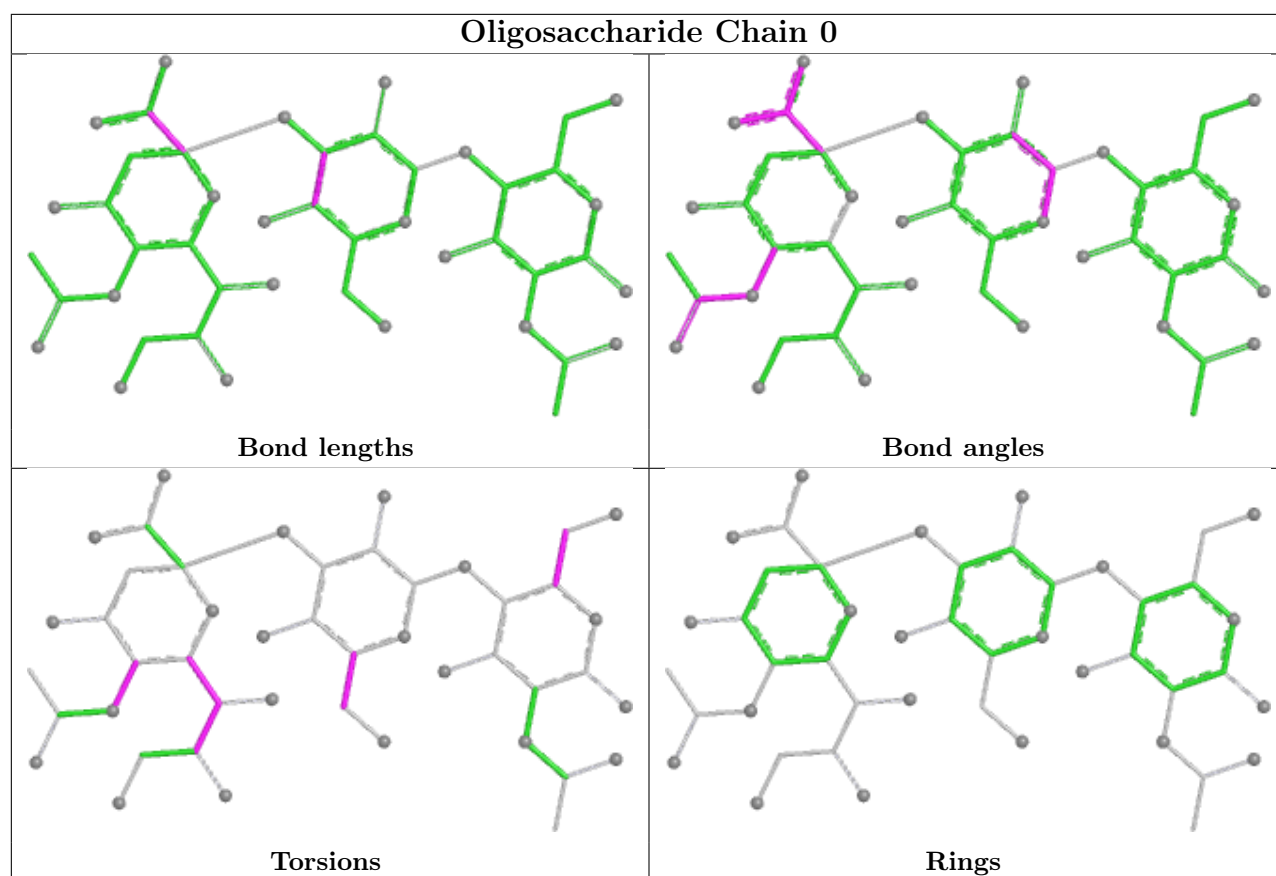
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Mol	Chain	Res	Type	Atoms
2	vB	3	SIA	C6-C5-N5-C10
2	yB	3	SIA	C6-C5-N5-C10
2	1B	3	SIA	C6-C5-N5-C10
2	4B	3	SIA	C6-C5-N5-C10
2	7B	3	SIA	C6-C5-N5-C10
2	AC	3	SIA	C6-C5-N5-C10
2	DC	3	SIA	C6-C5-N5-C10
2	GC	3	SIA	C6-C5-N5-C10
2	JC	3	SIA	C6-C5-N5-C10
2	MC	3	SIA	C6-C5-N5-C10
2	PC	3	SIA	C6-C5-N5-C10
2	SC	3	SIA	C6-C5-N5-C10
2	VC	3	SIA	C6-C5-N5-C10
2	YC	3	SIA	C6-C5-N5-C10
2	bC	3	SIA	C6-C5-N5-C10
2	eC	3	SIA	C6-C5-N5-C10
2	hC	3	SIA	C6-C5-N5-C10
2	kC	3	SIA	C6-C5-N5-C10
2	nC	3	SIA	C6-C5-N5-C10
2	qC	3	SIA	C6-C5-N5-C10
2	tC	3	SIA	C6-C5-N5-C10
2	wC	3	SIA	C6-C5-N5-C10
2	zC	3	SIA	C6-C5-N5-C10

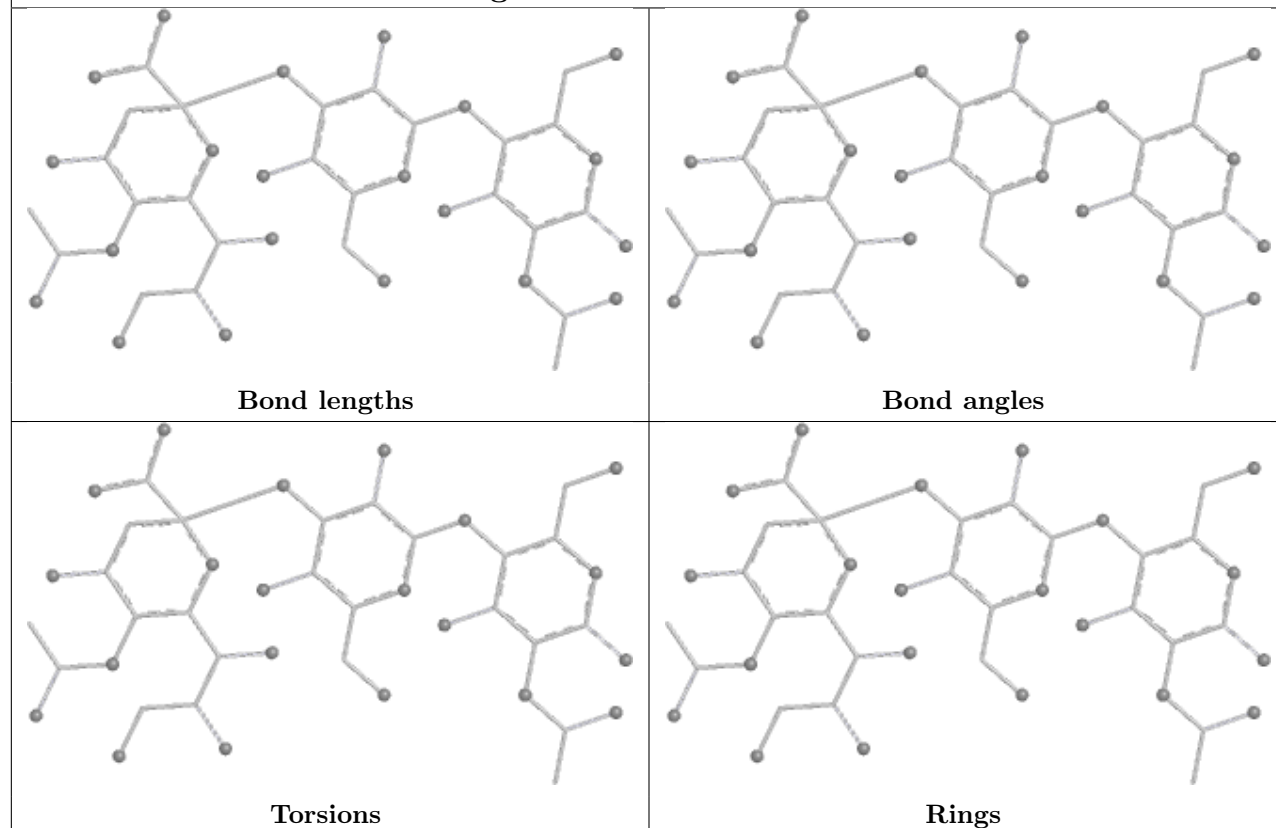
There are no ring outliers.

No monomer is involved in short contacts.

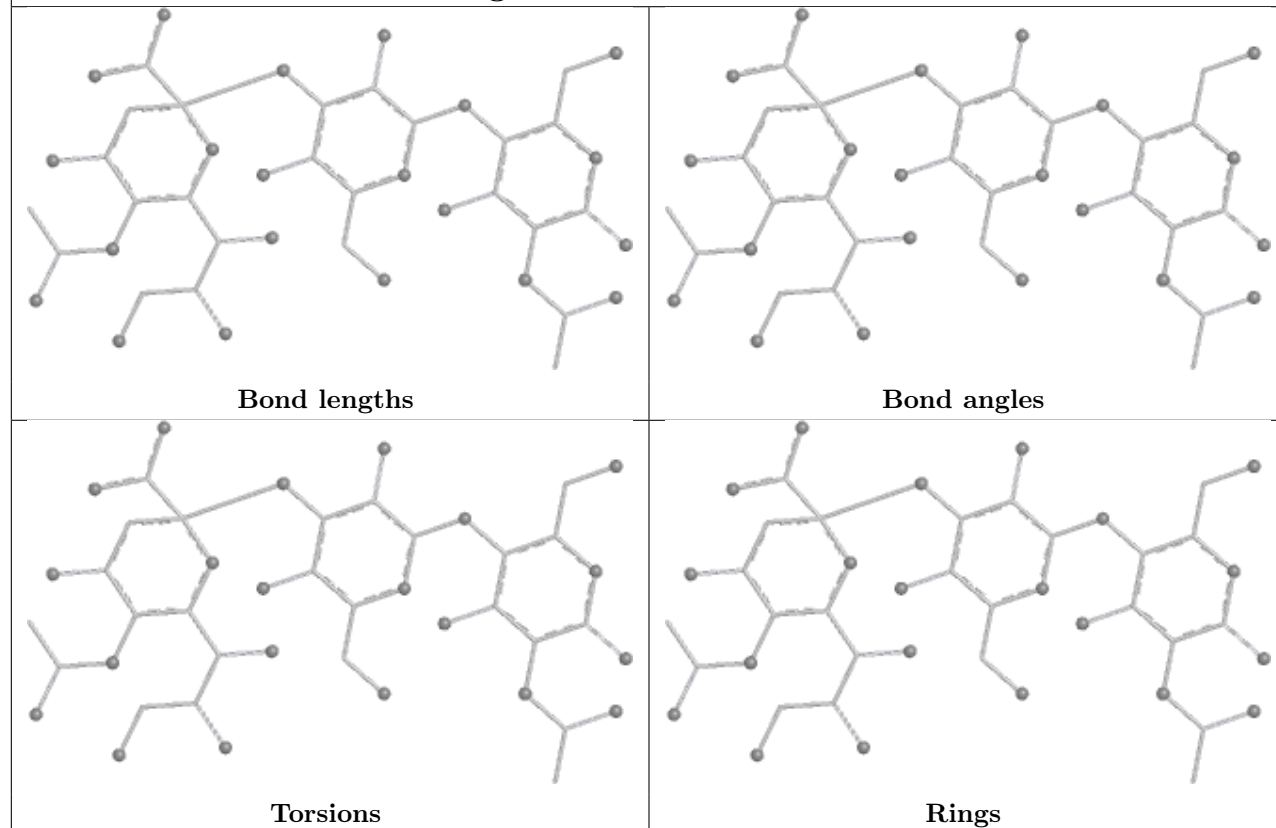
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



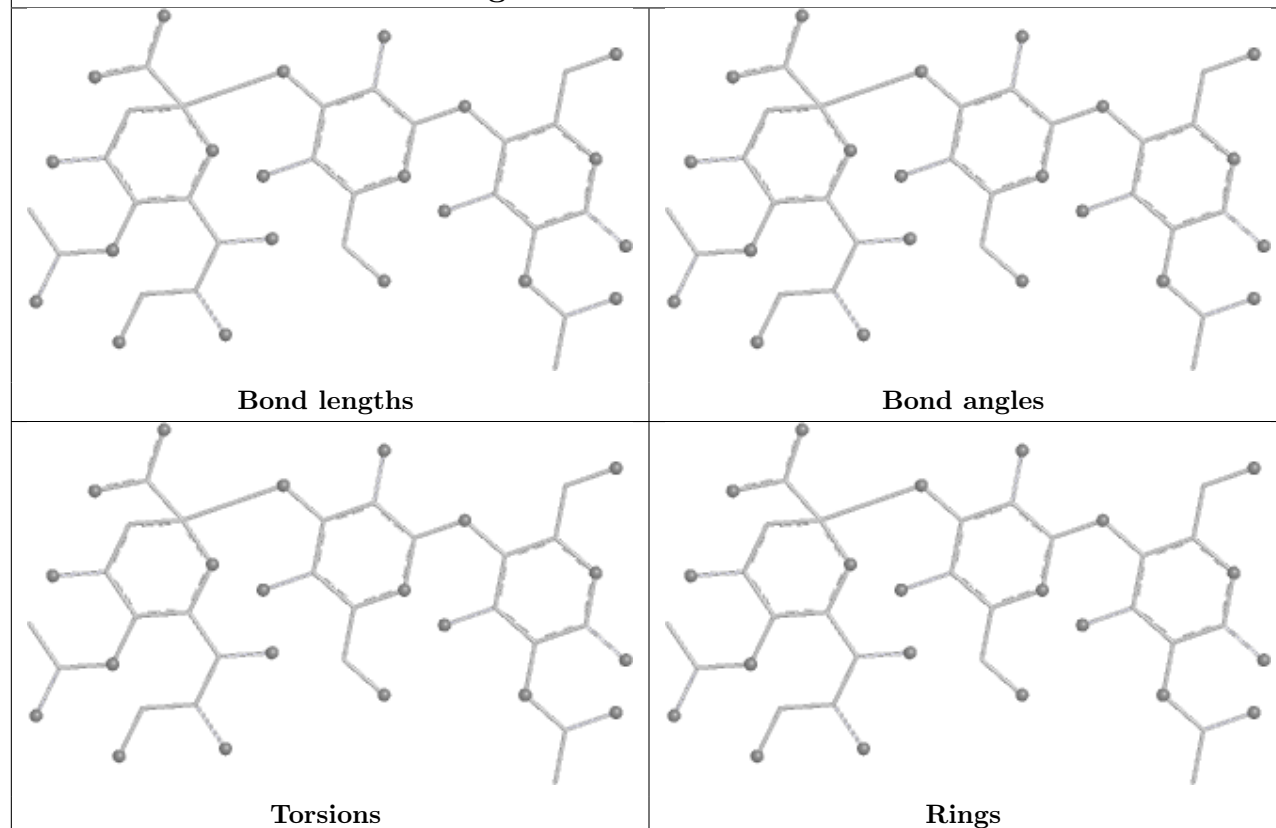
Oligosaccharide Chain EA



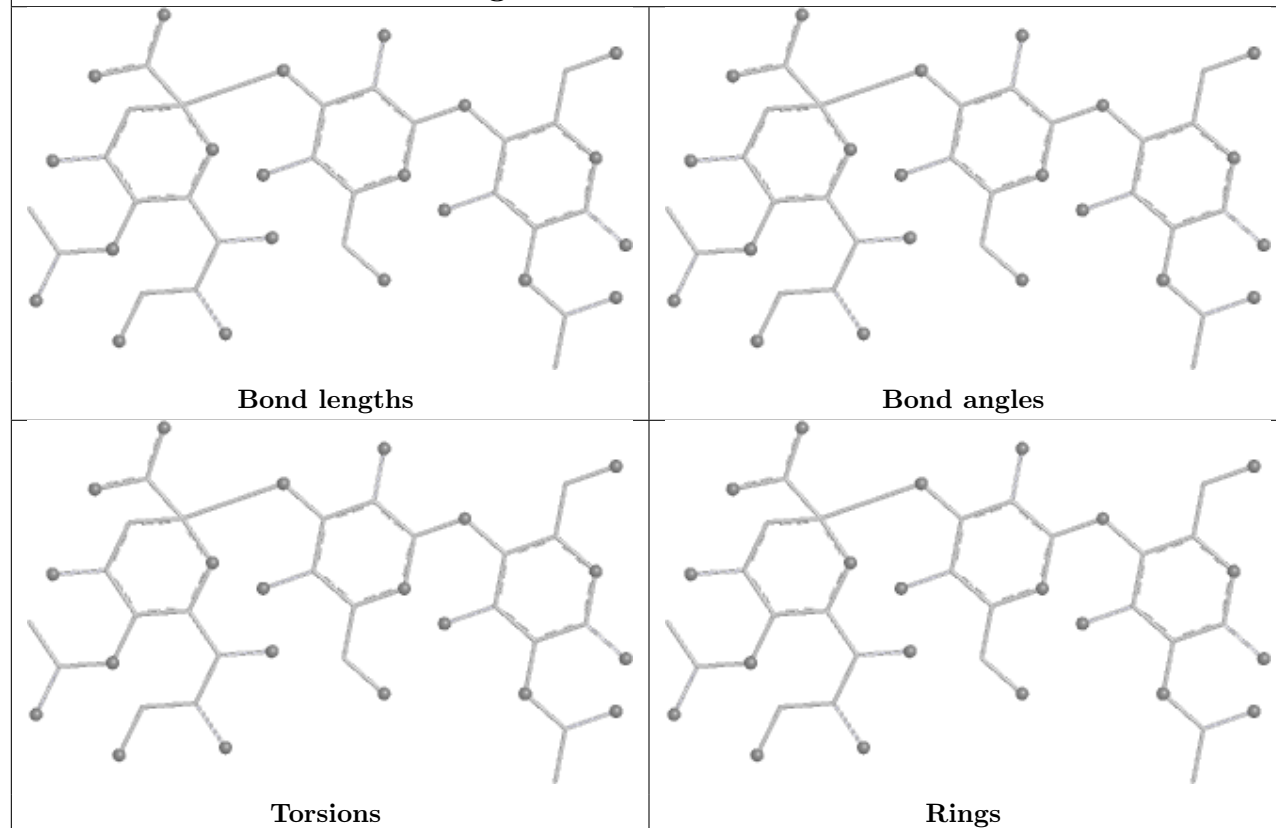
Oligosaccharide Chain HA

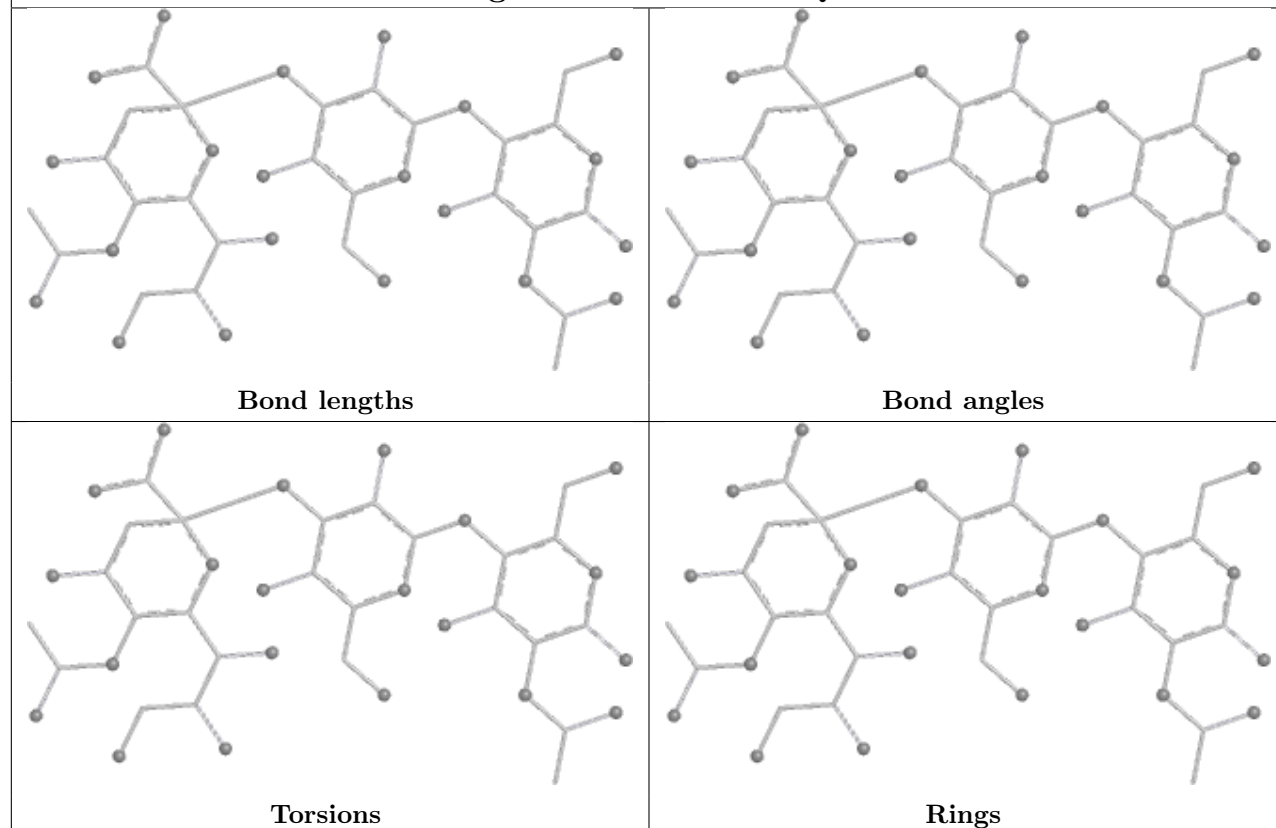
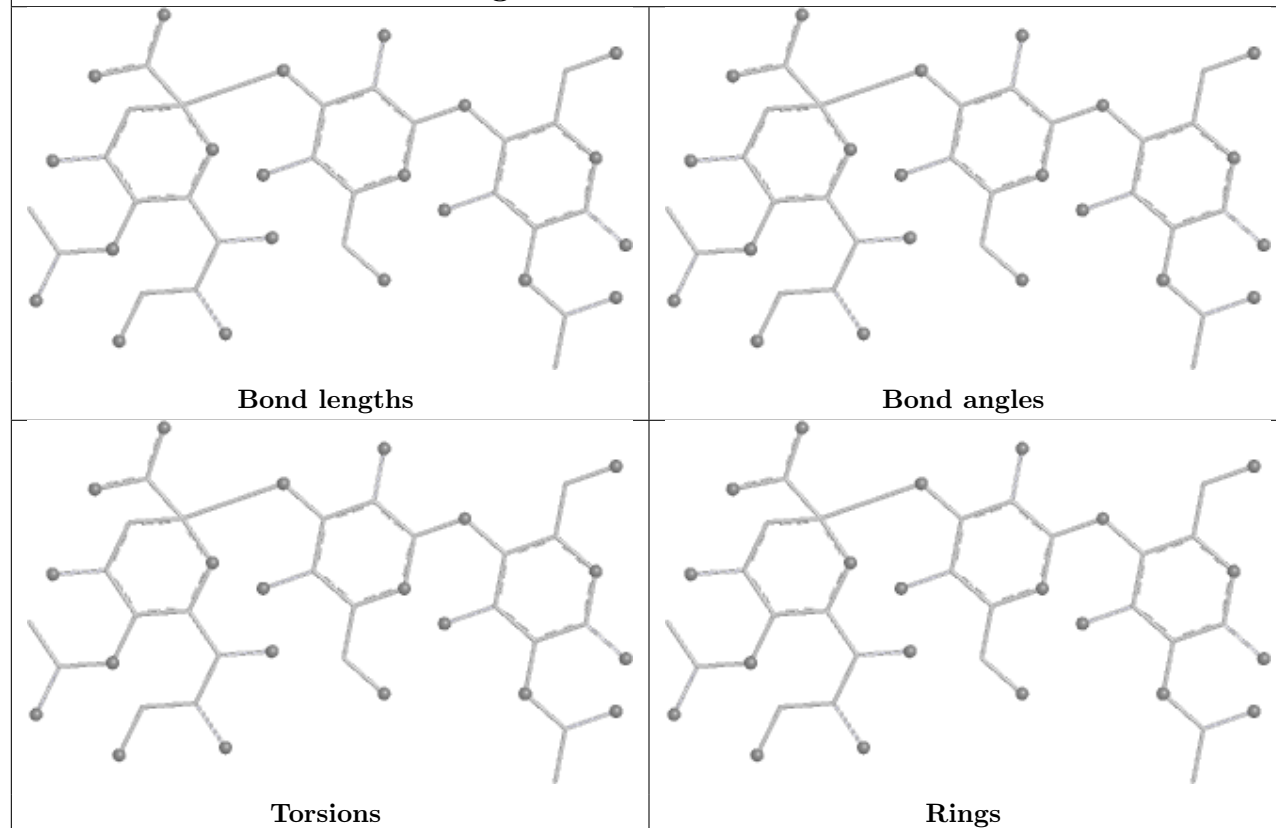


Oligosaccharide Chain KA

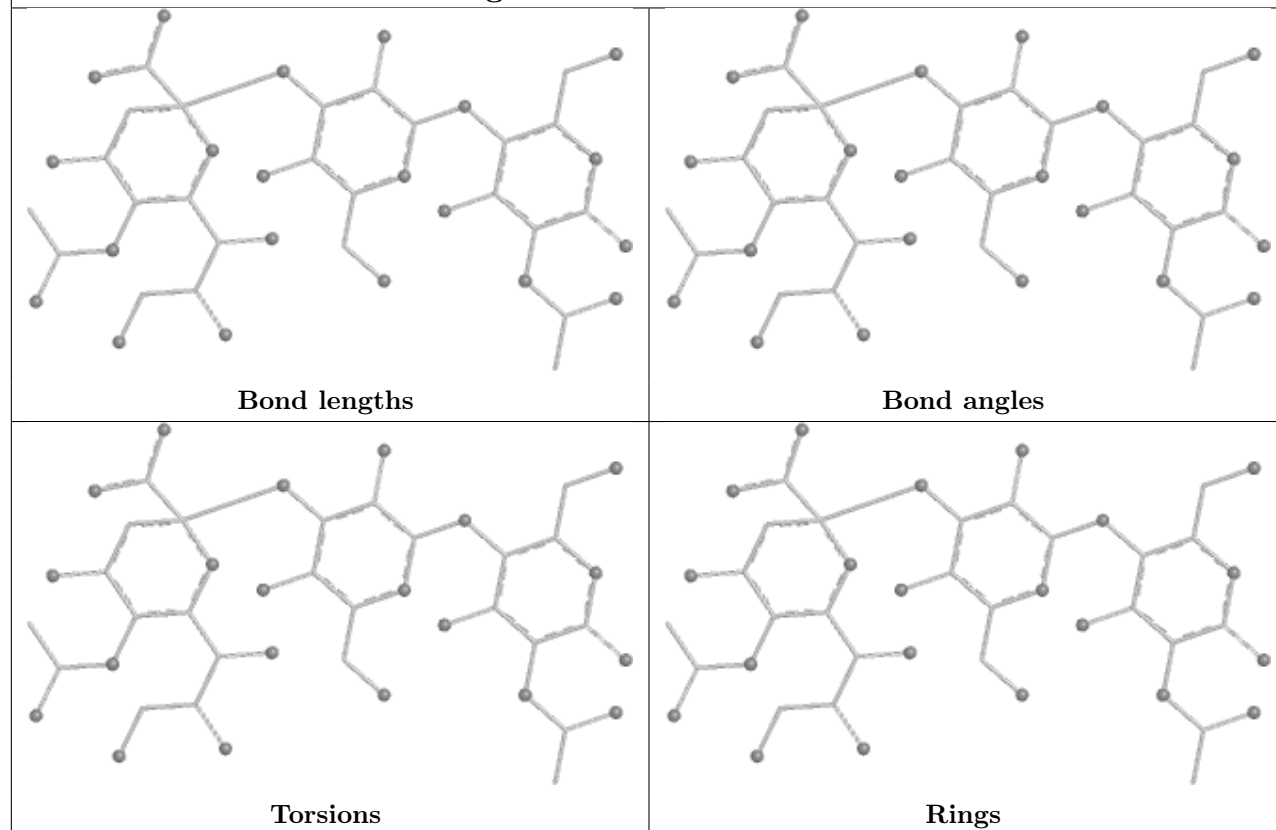


Oligosaccharide Chain NA

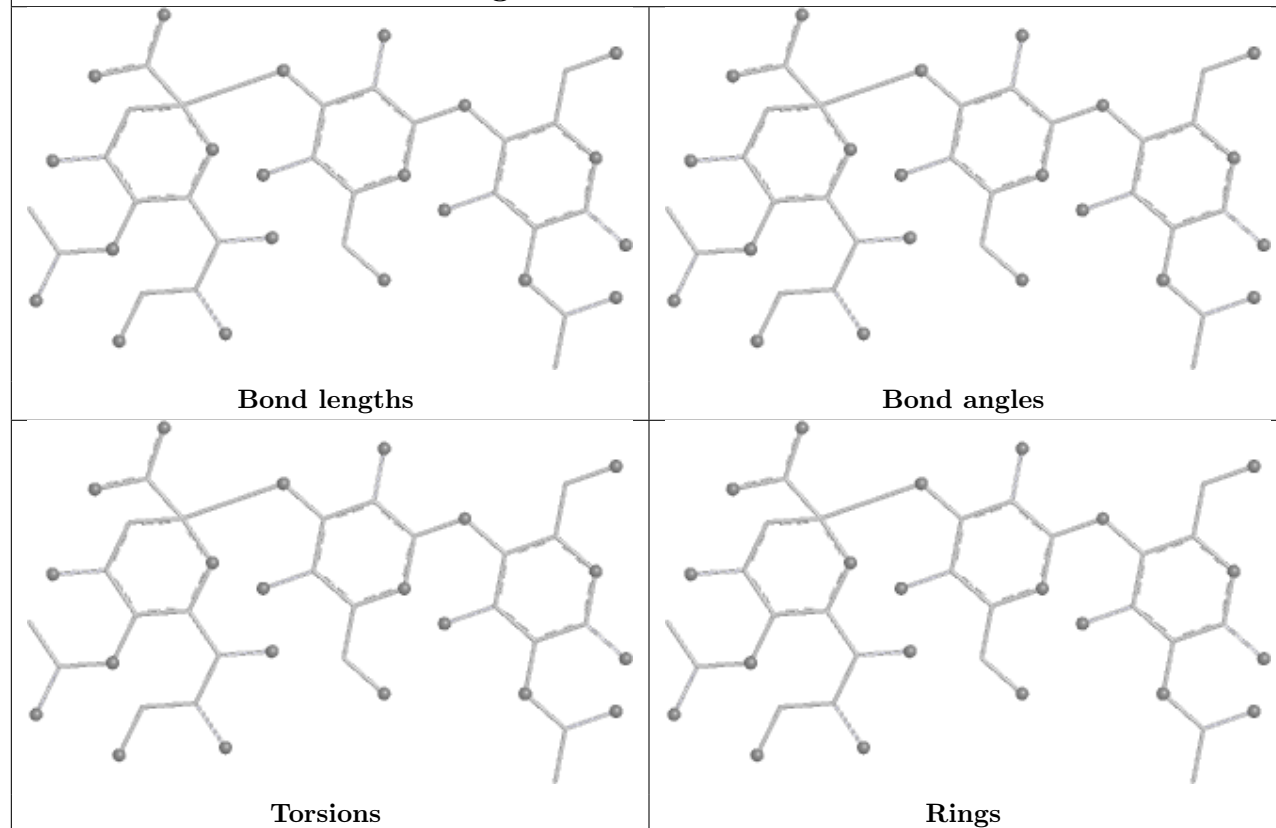


Oligosaccharide Chain QA**Oligosaccharide Chain TA**

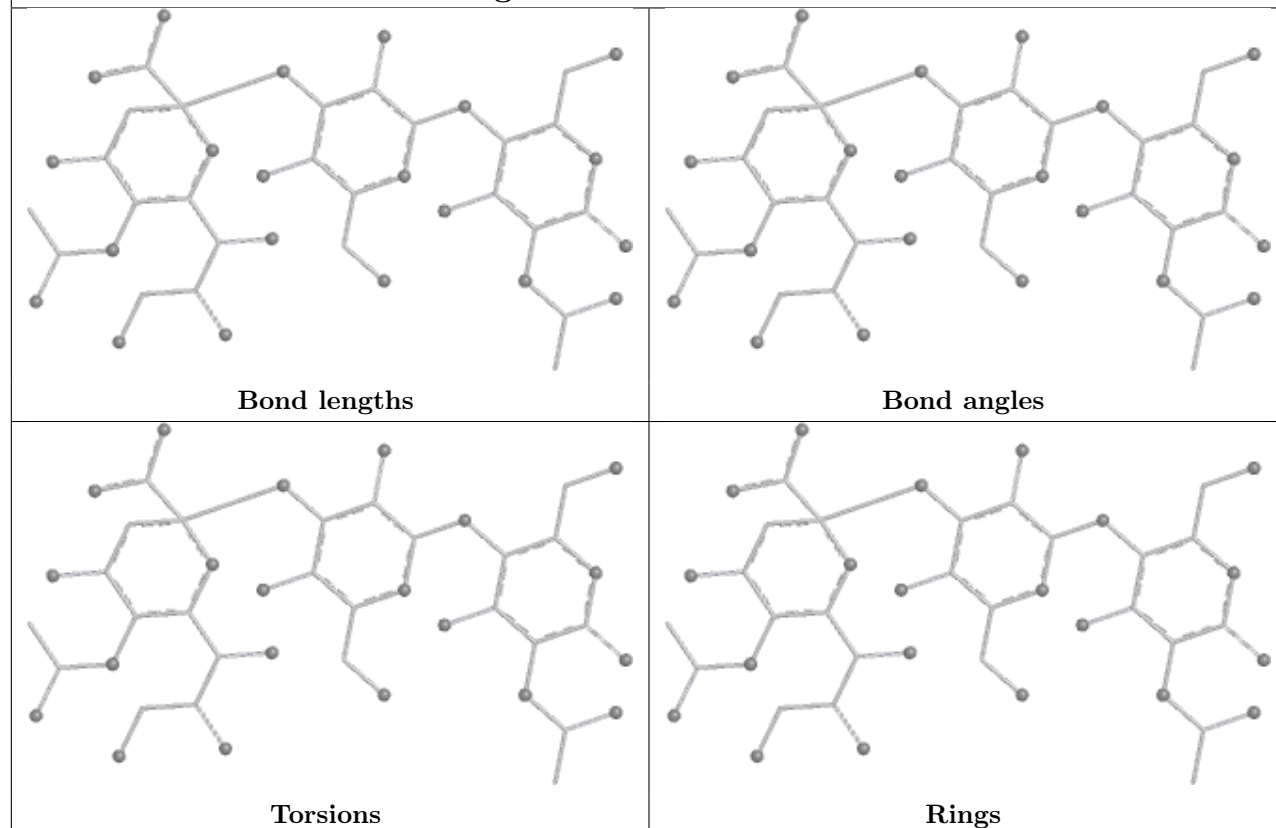
Oligosaccharide Chain WA



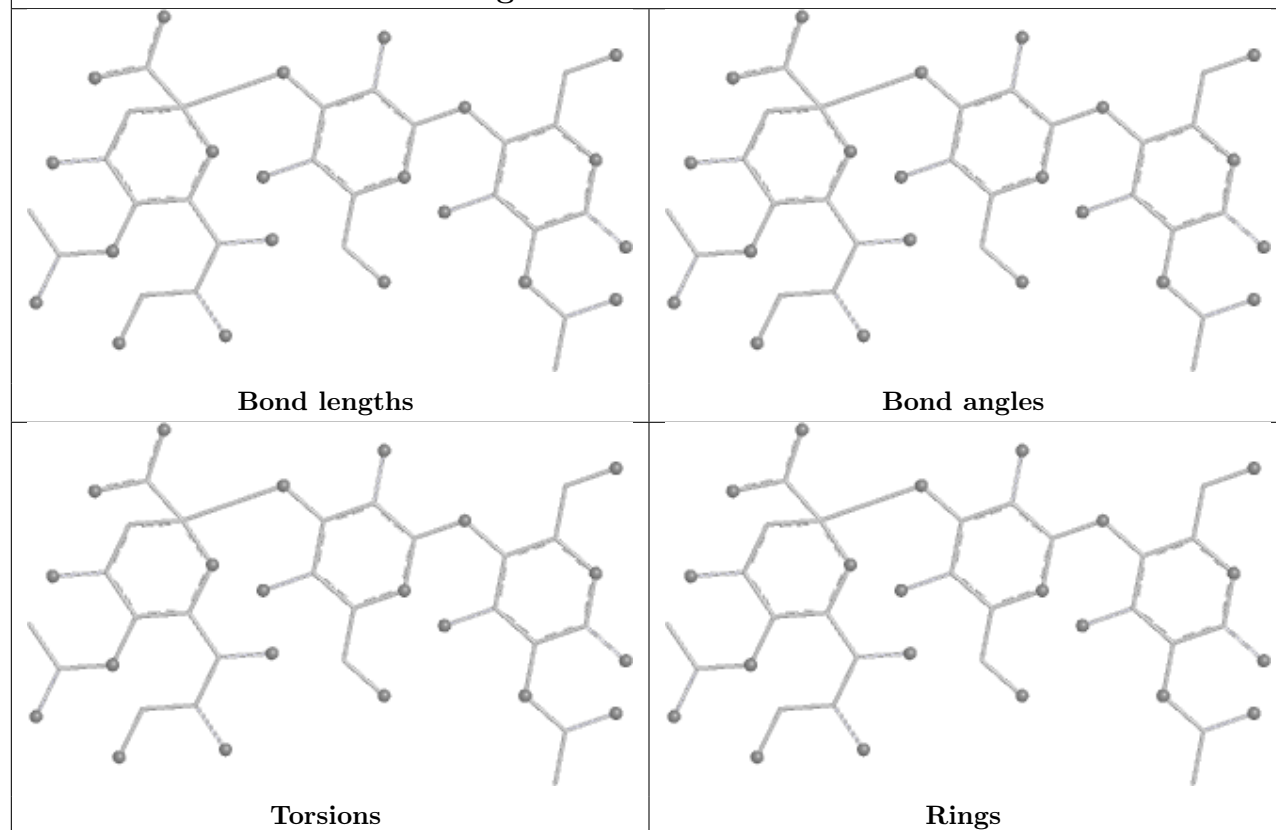
Oligosaccharide Chain ZA

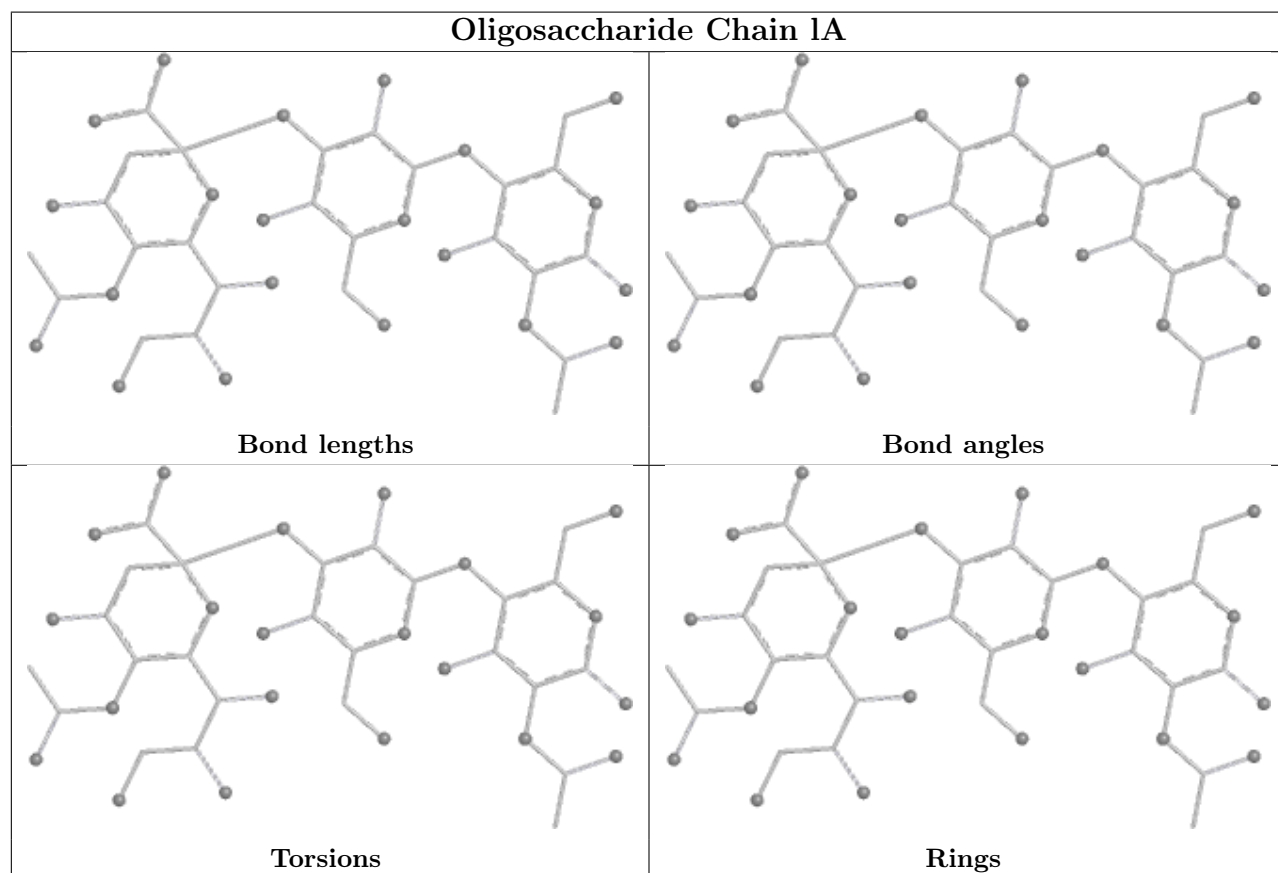
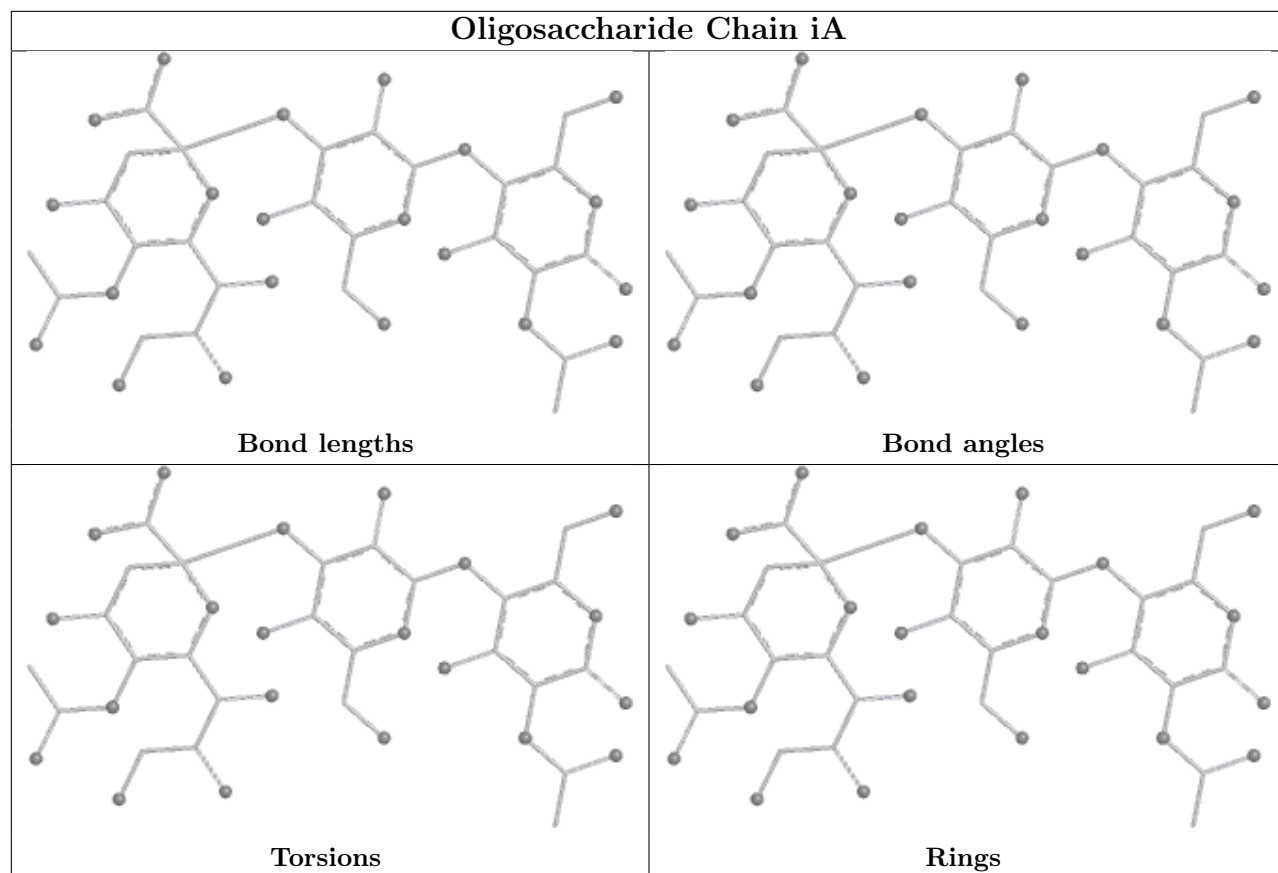


Oligosaccharide Chain cA

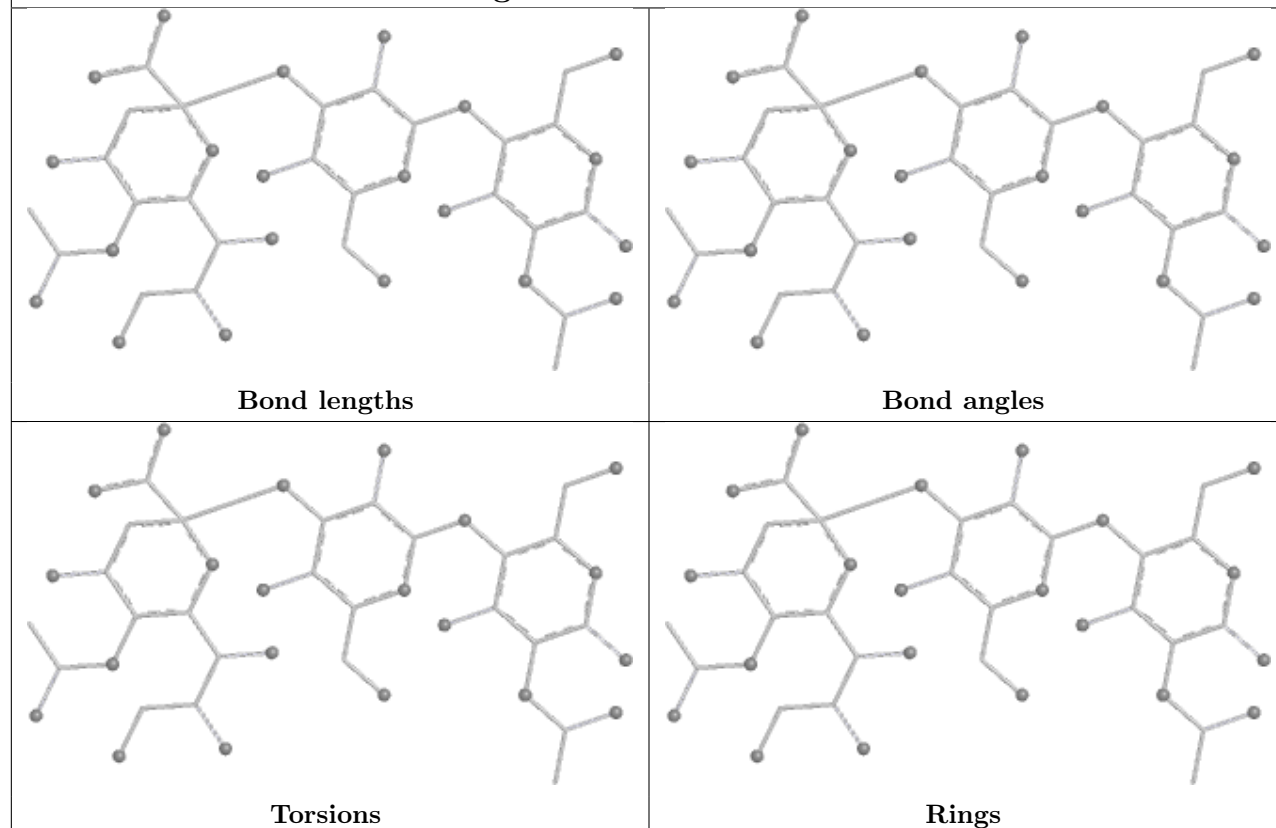


Oligosaccharide Chain fA

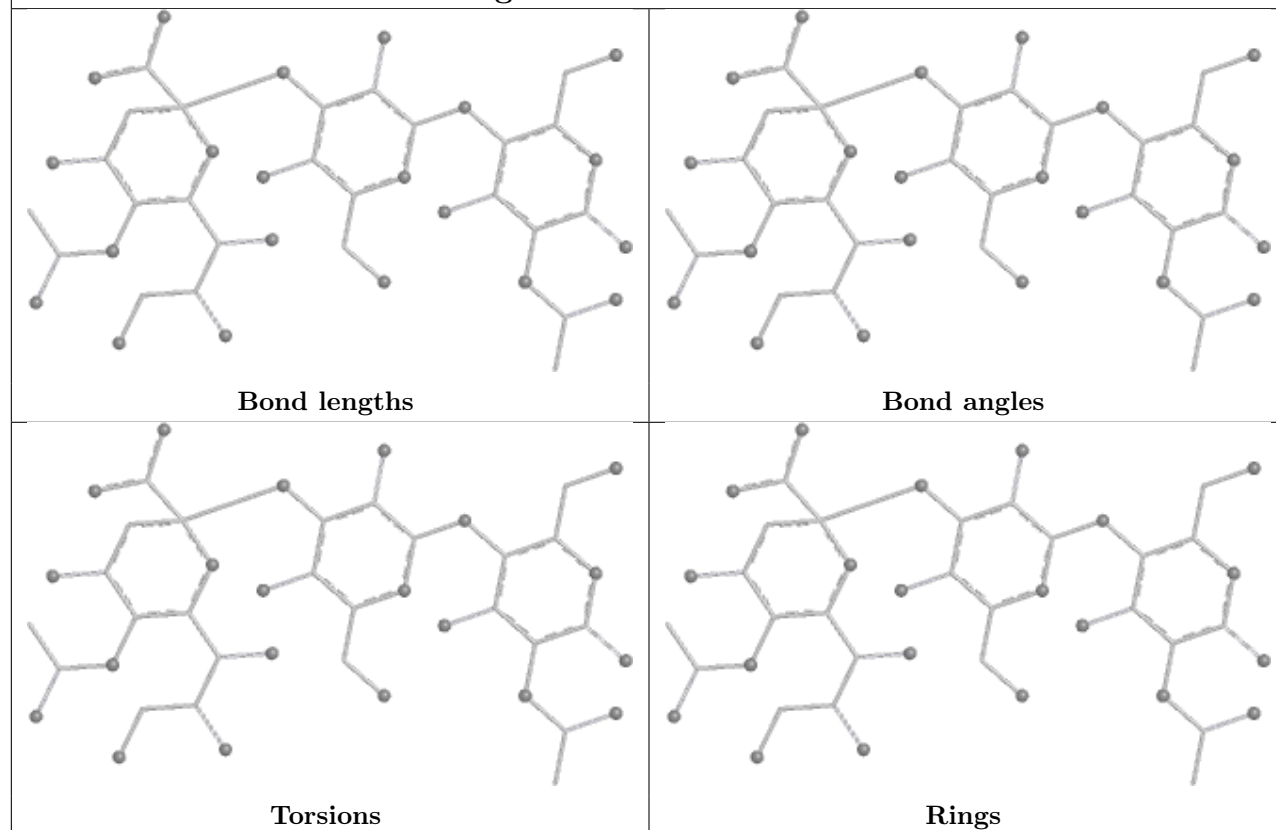




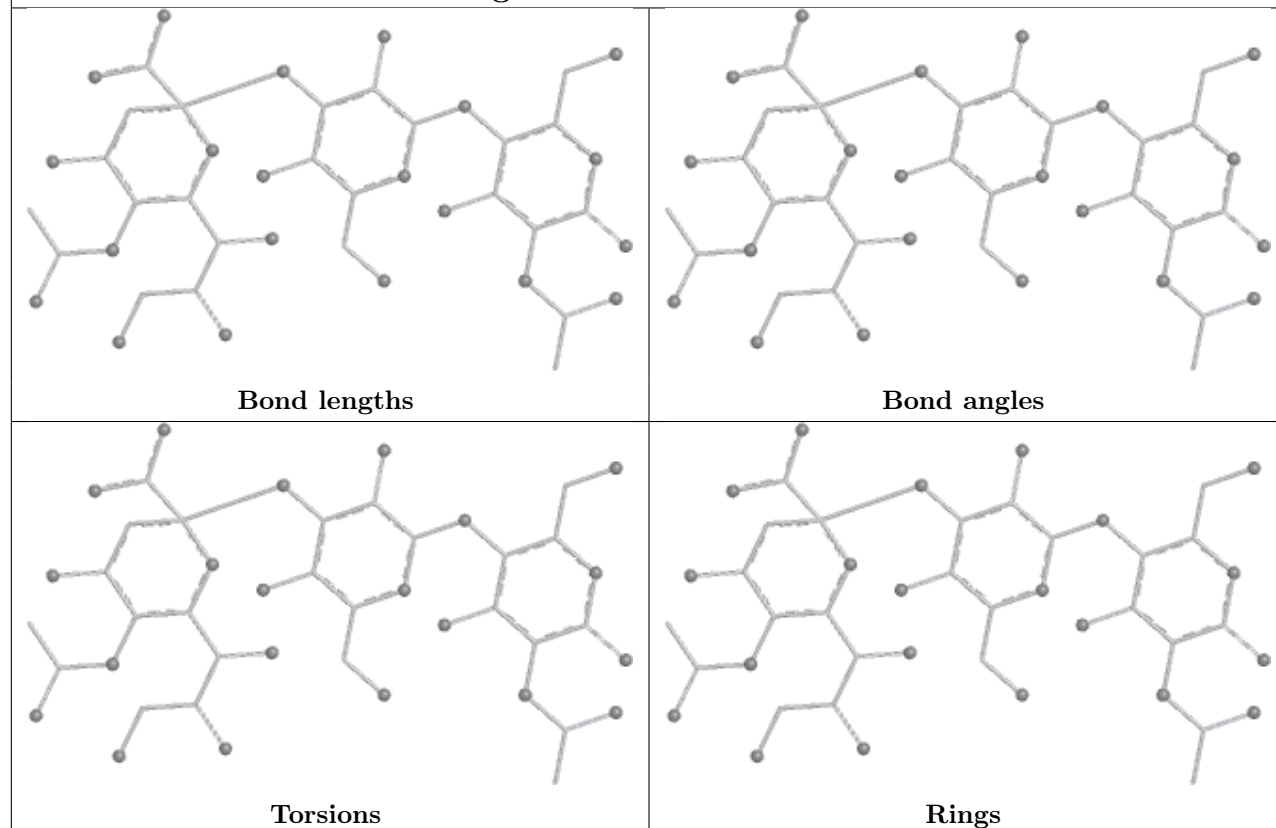
Oligosaccharide Chain oA



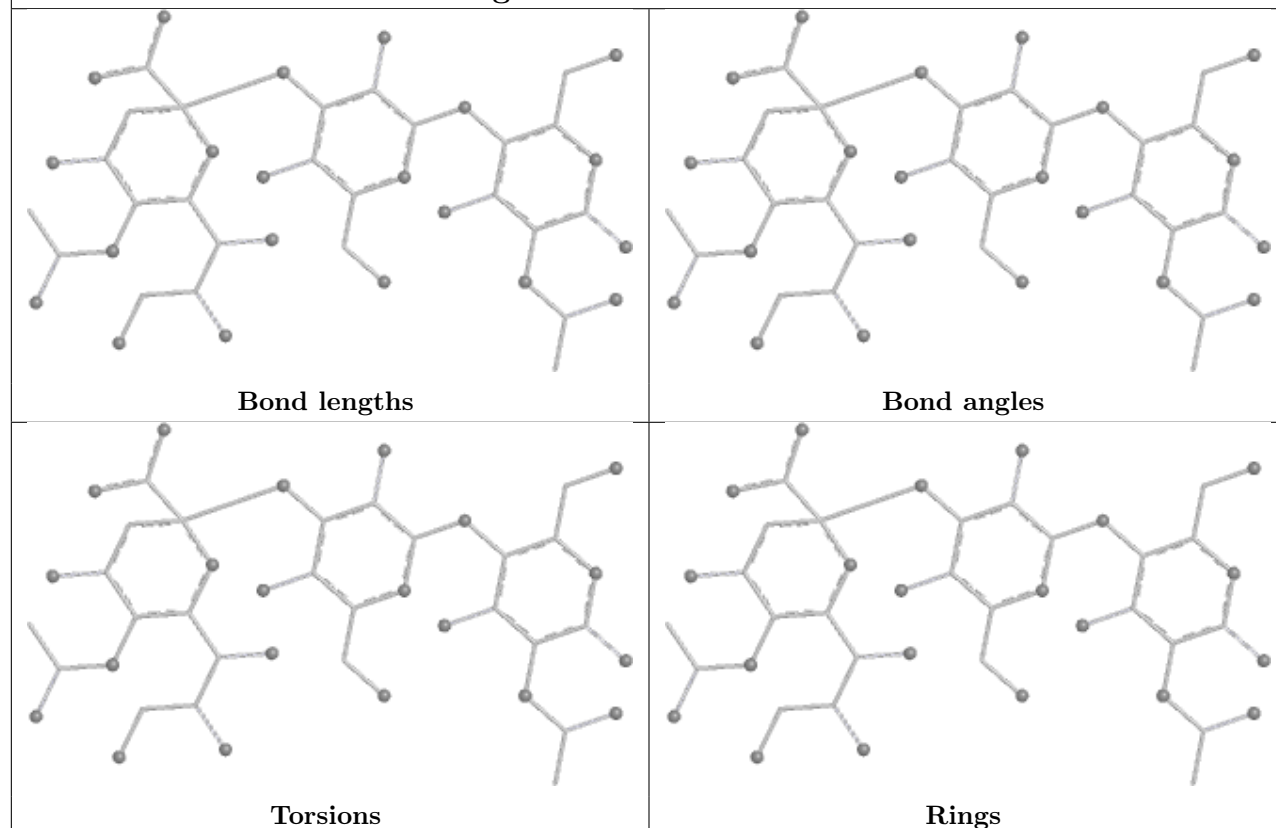
Oligosaccharide Chain rA



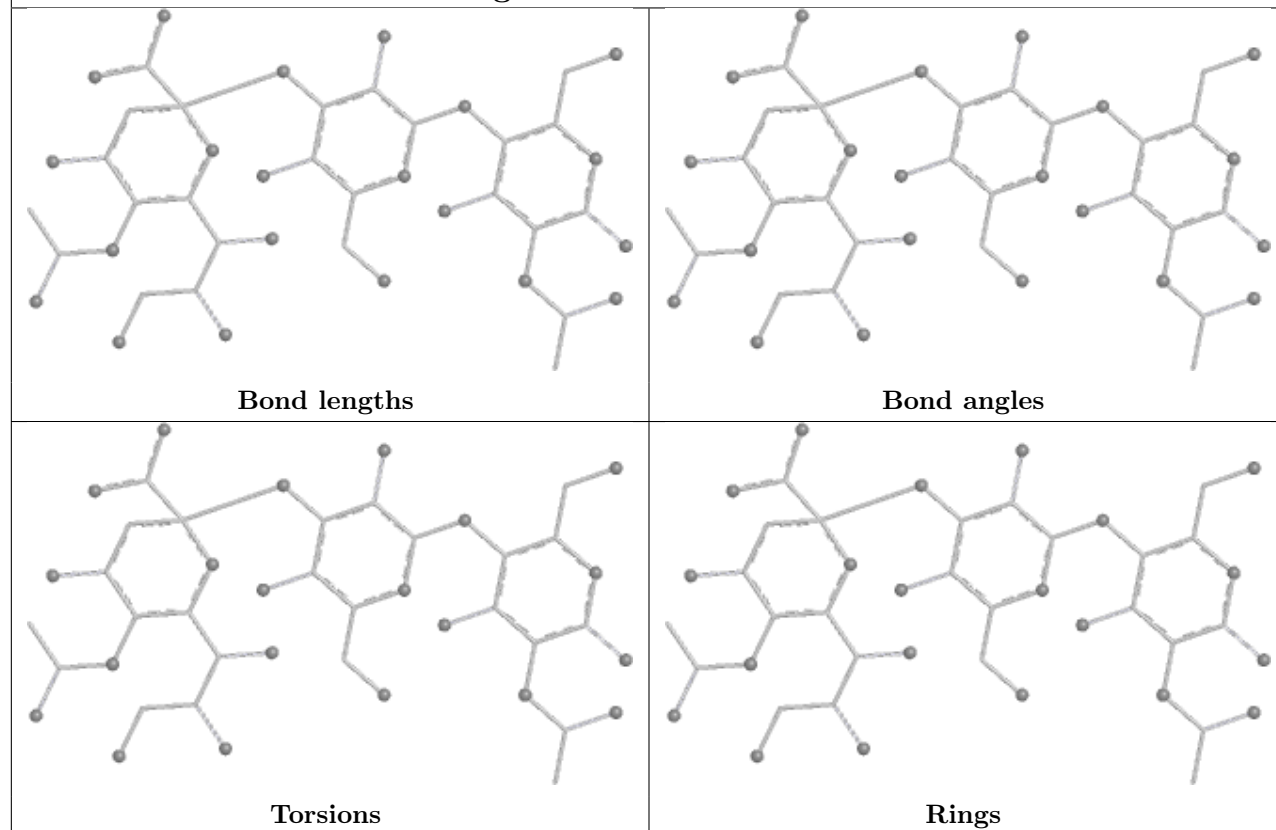
Oligosaccharide Chain uA



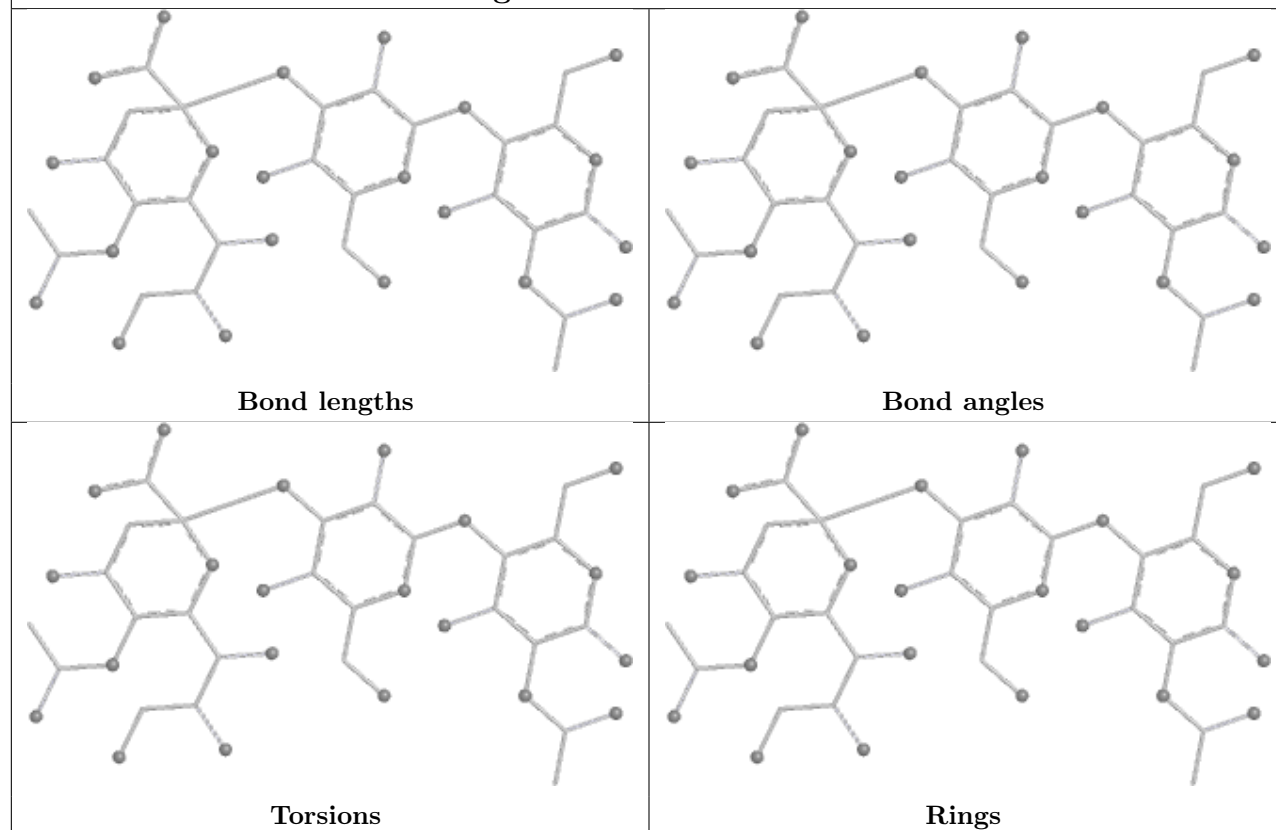
Oligosaccharide Chain xA



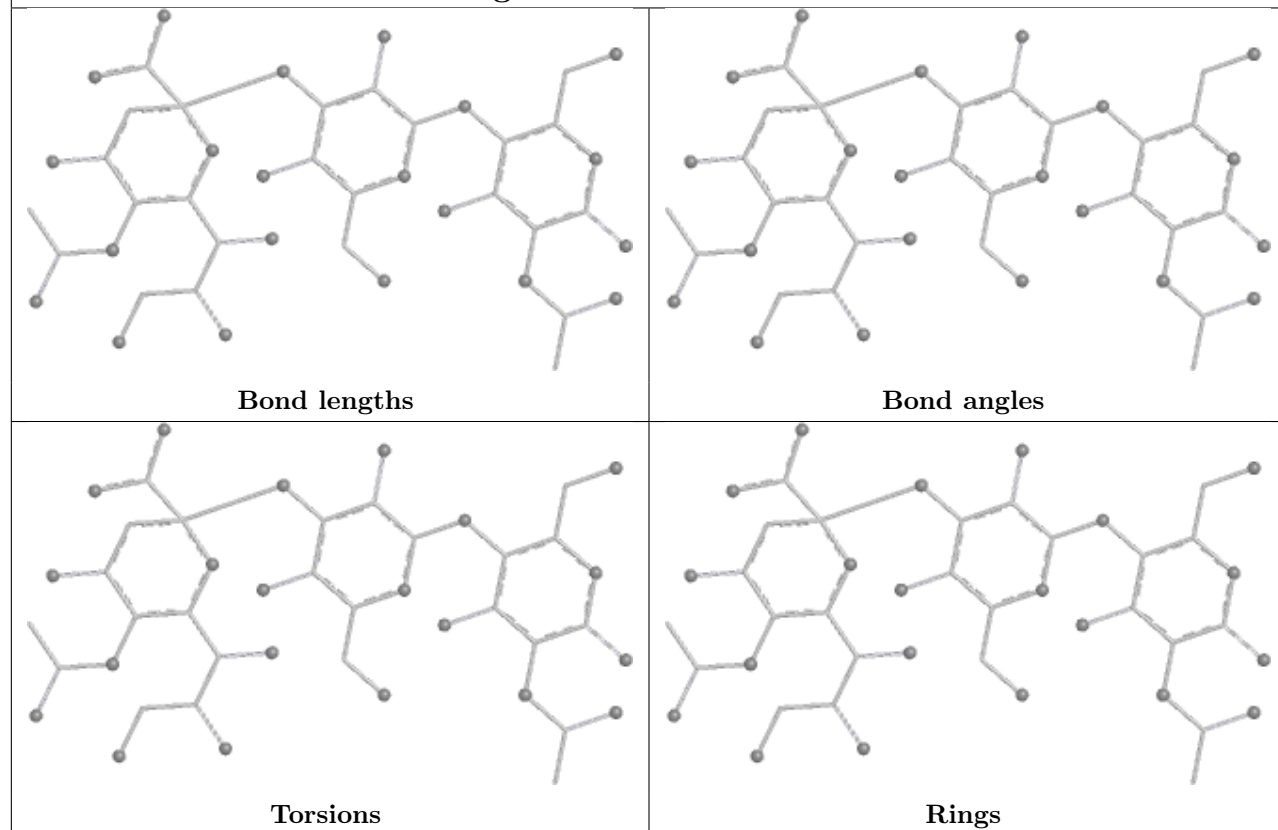
Oligosaccharide Chain 0A



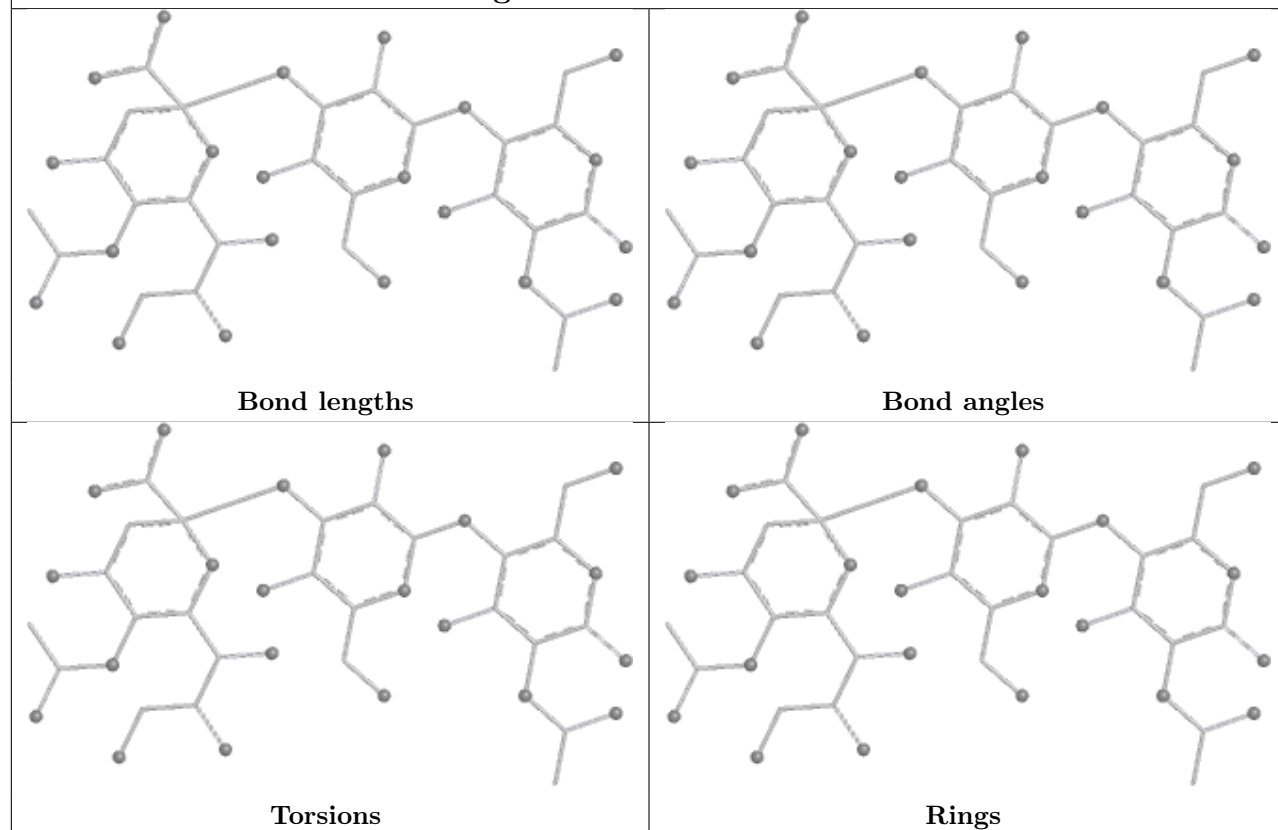
Oligosaccharide Chain 3A

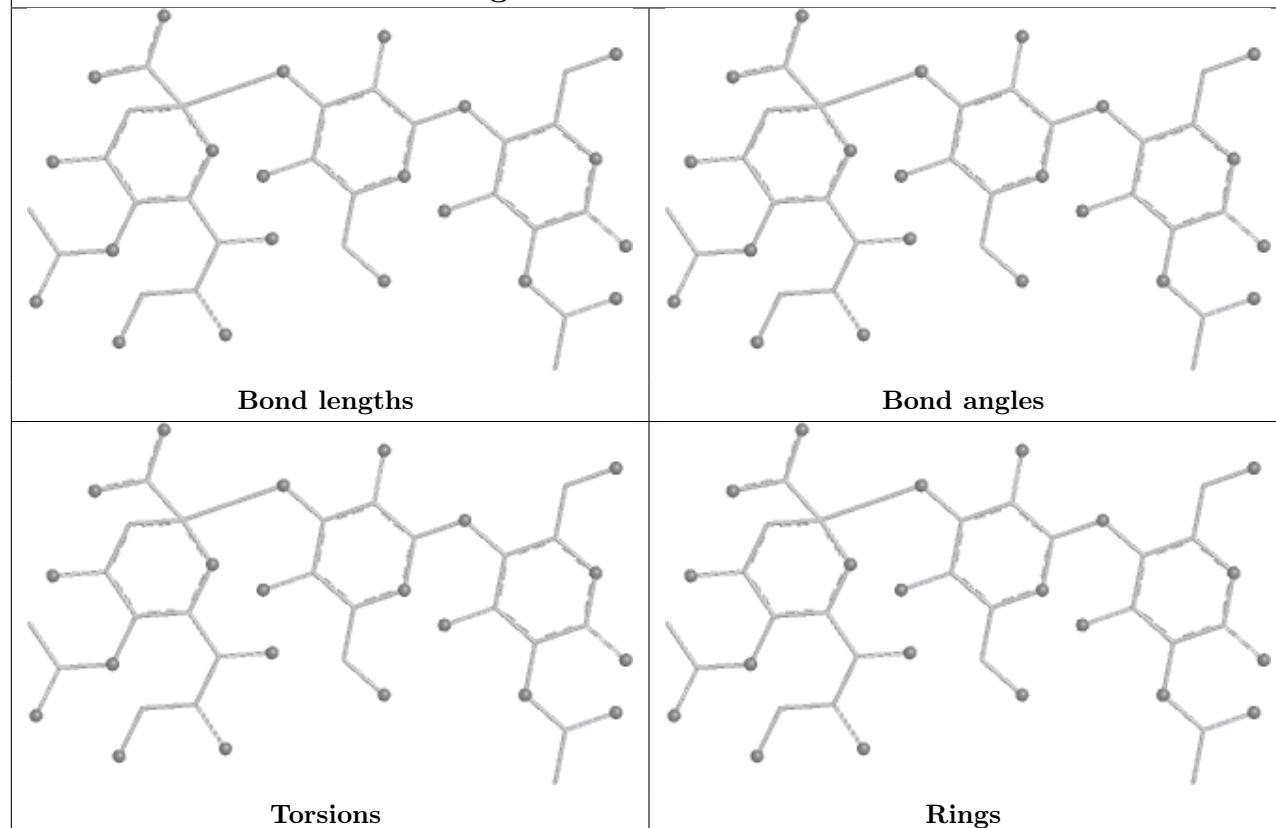
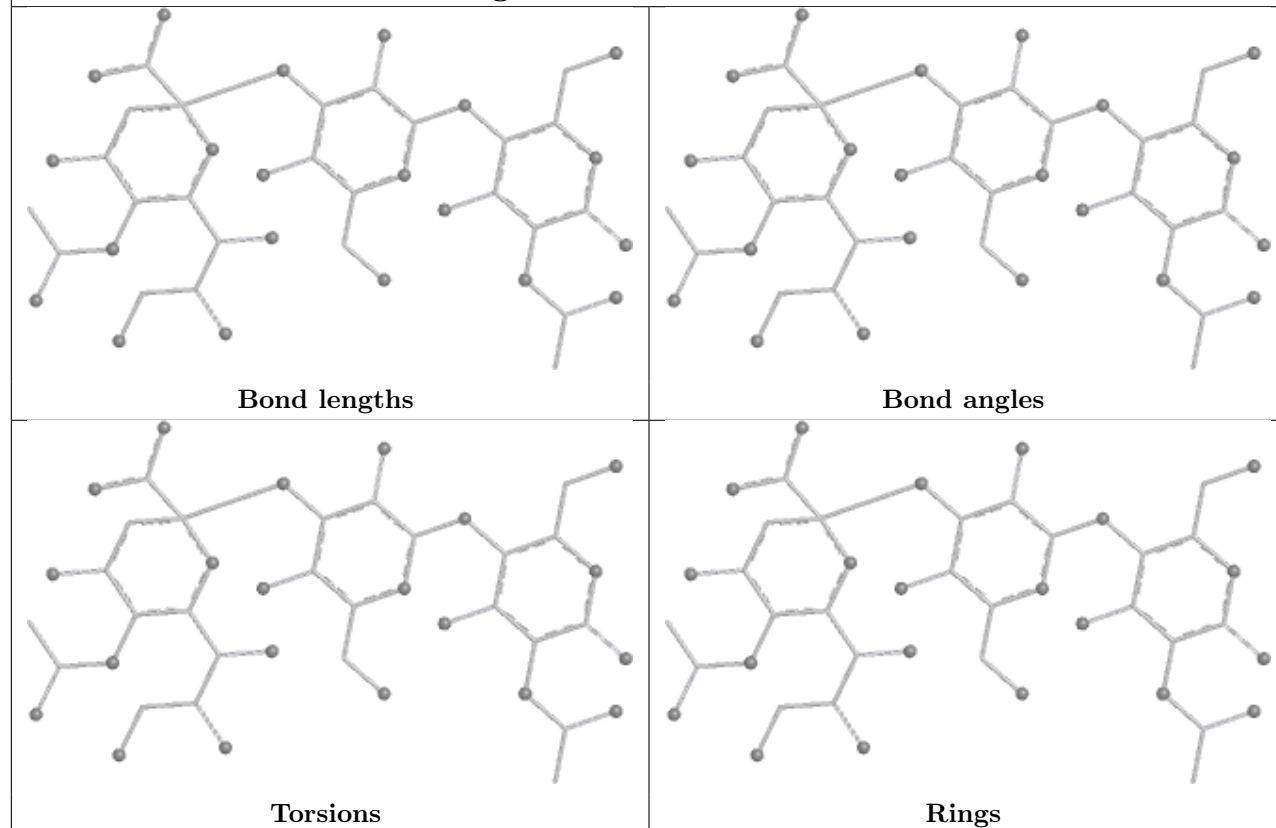


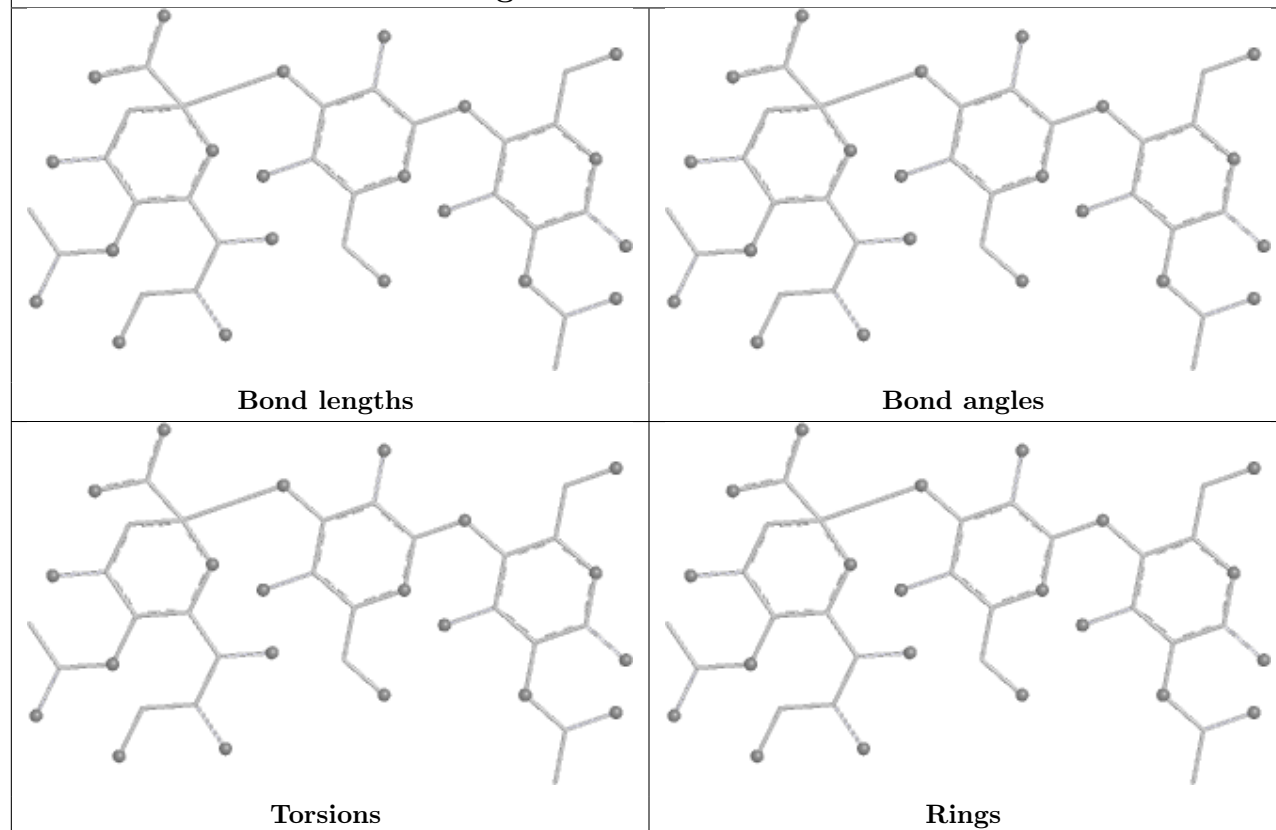
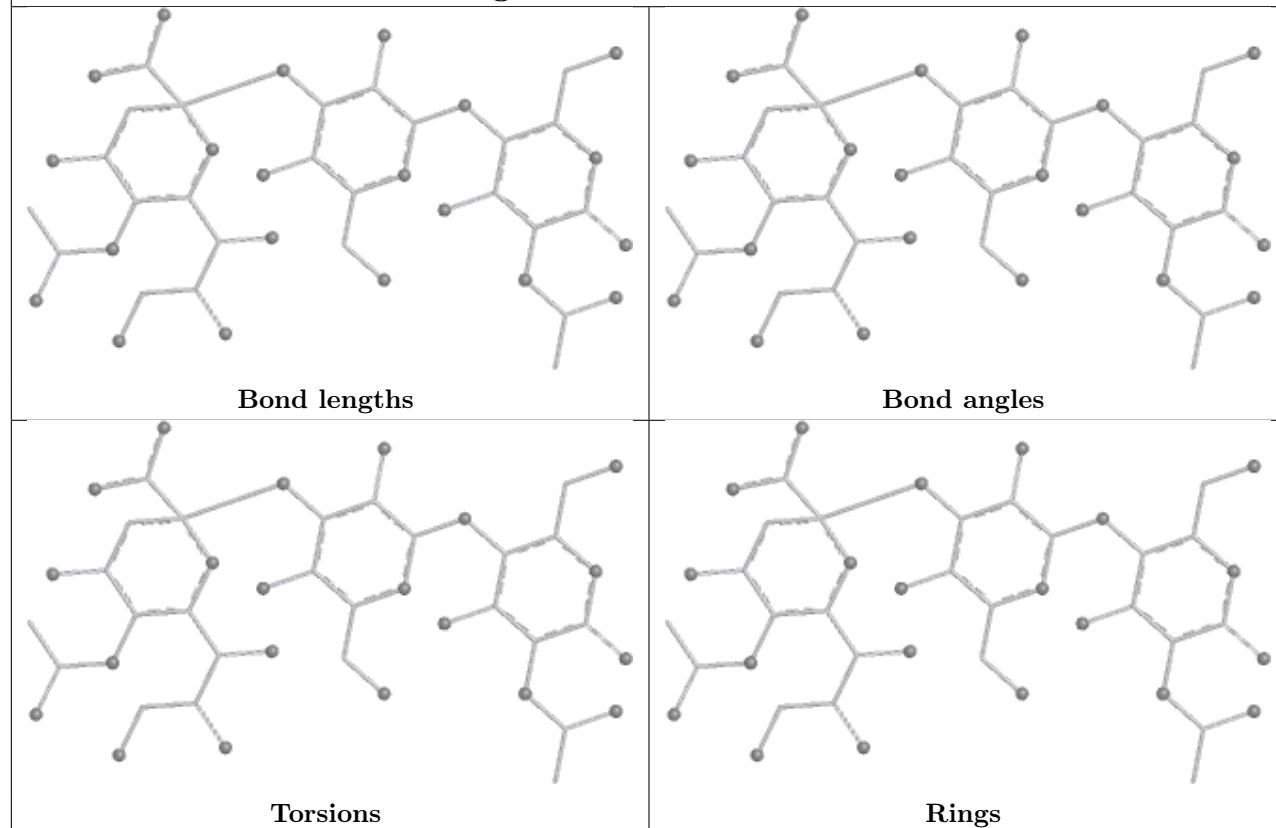
Oligosaccharide Chain 6A



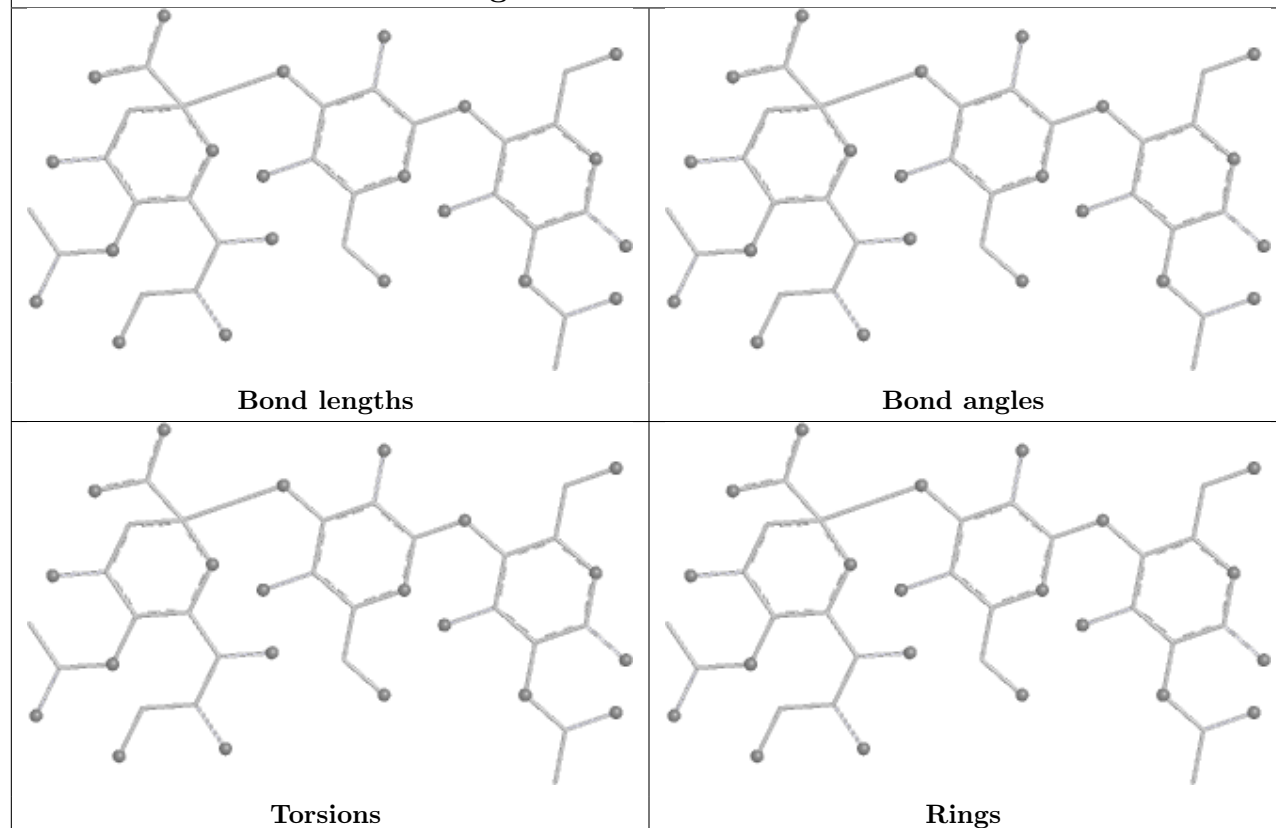
Oligosaccharide Chain 9A



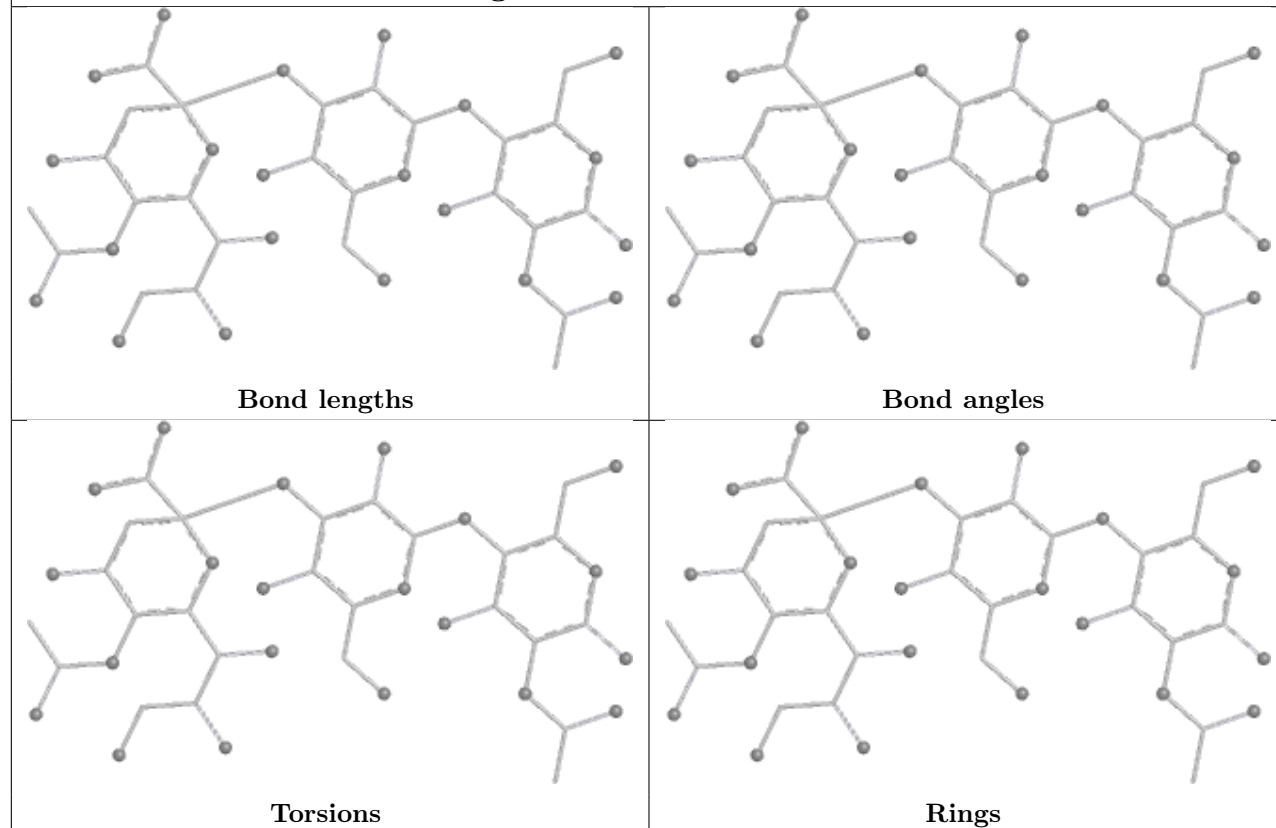
Oligosaccharide Chain CB**Oligosaccharide Chain FB**

Oligosaccharide Chain IB**Oligosaccharide Chain LB**

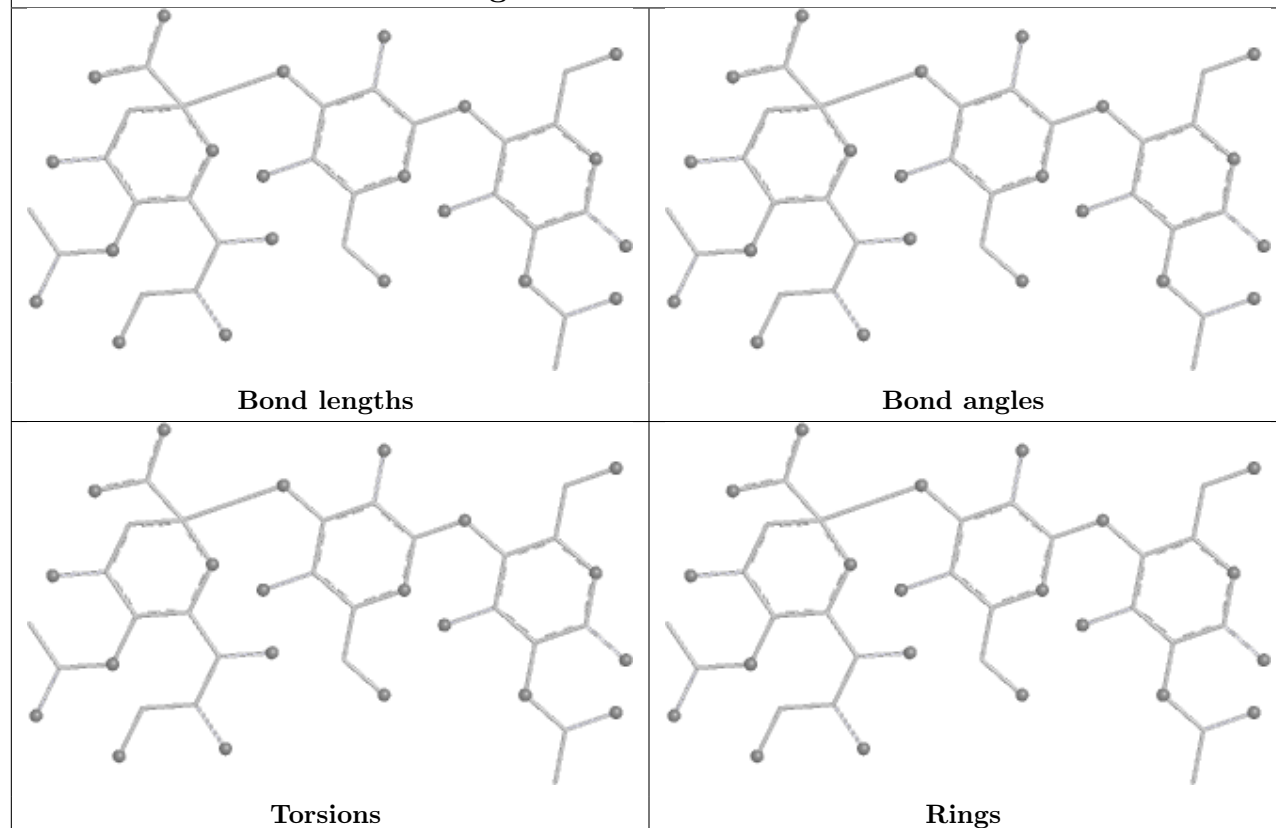
Oligosaccharide Chain OB



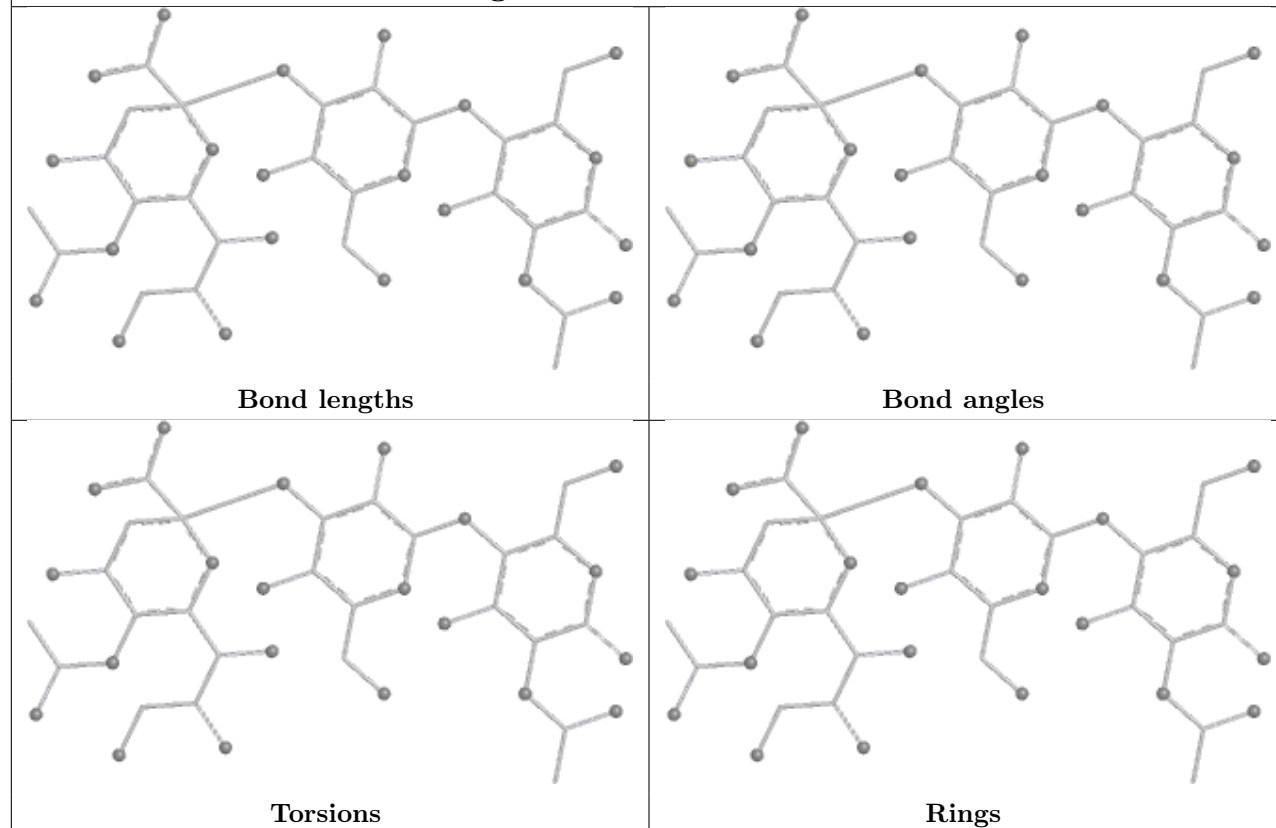
Oligosaccharide Chain RB



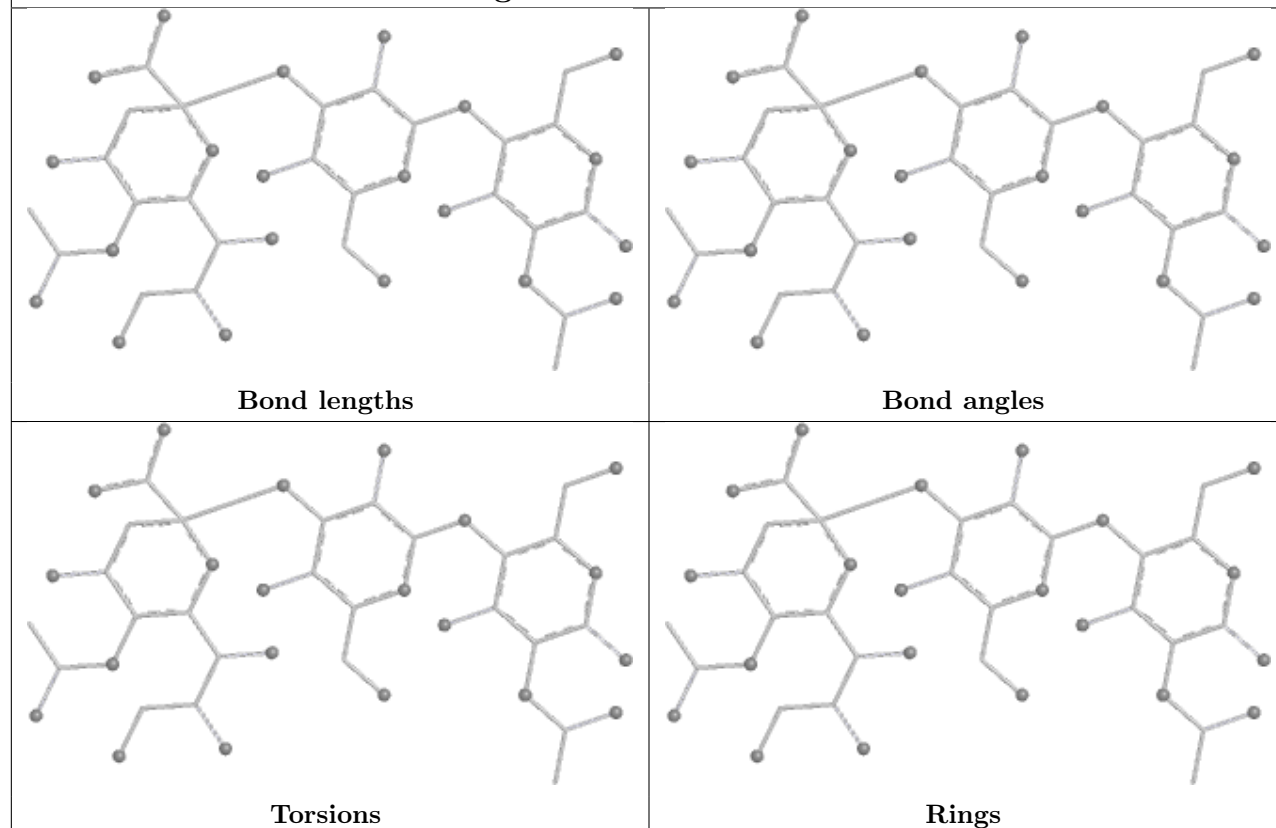
Oligosaccharide Chain UB



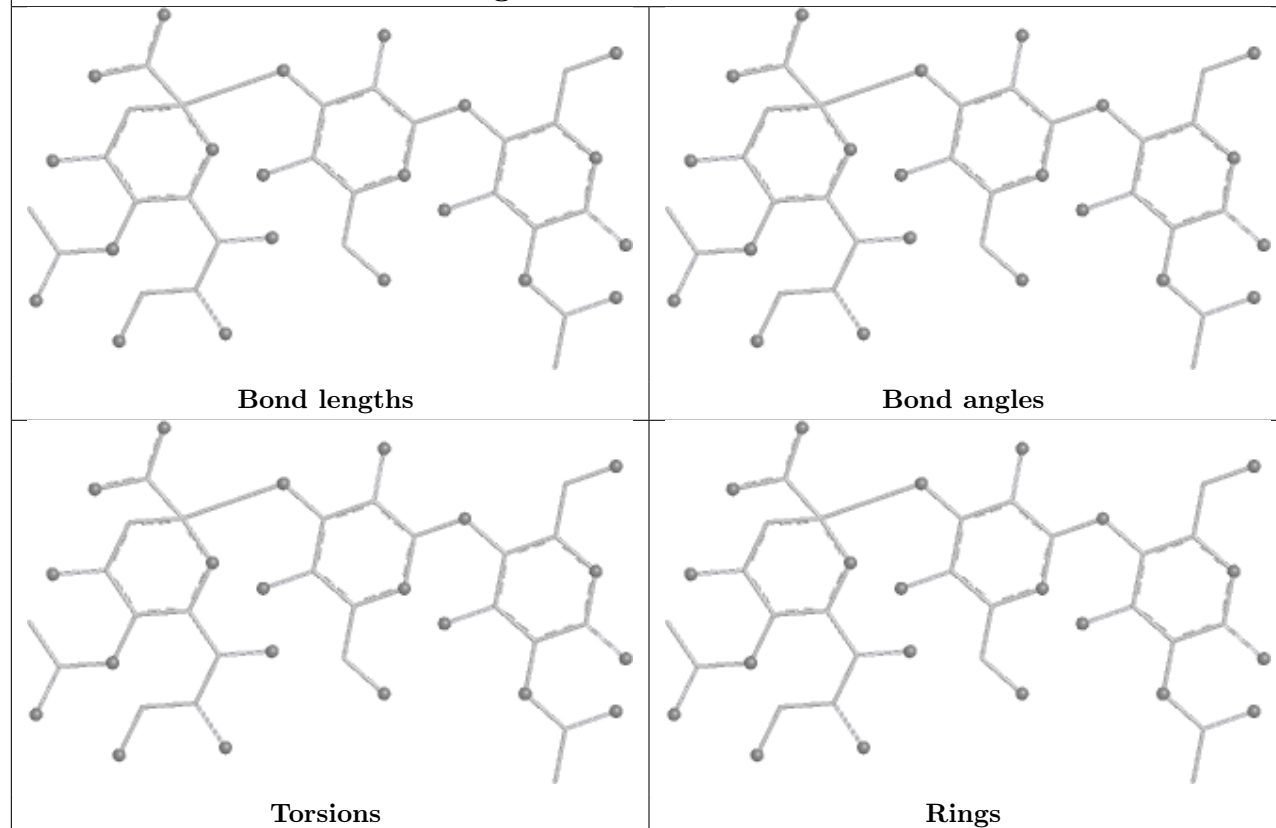
Oligosaccharide Chain XB



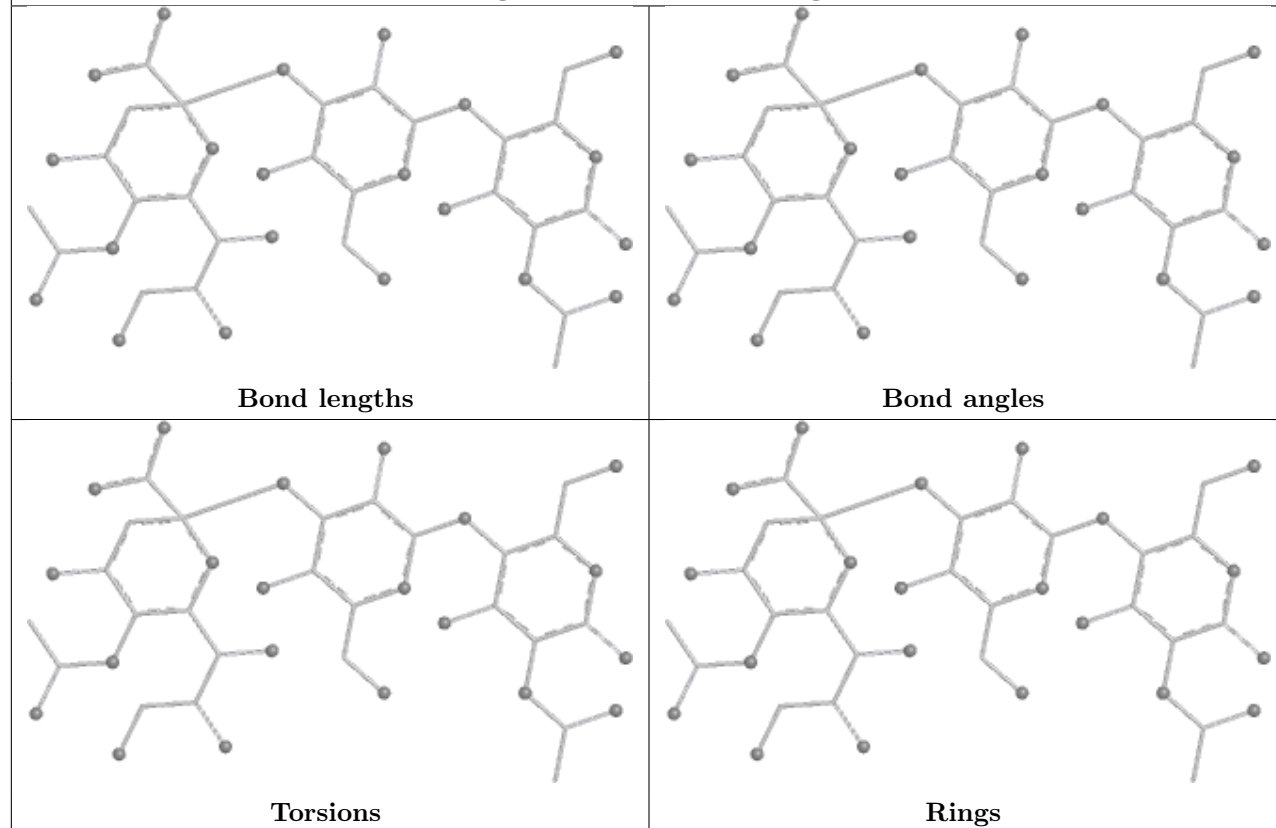
Oligosaccharide Chain aB



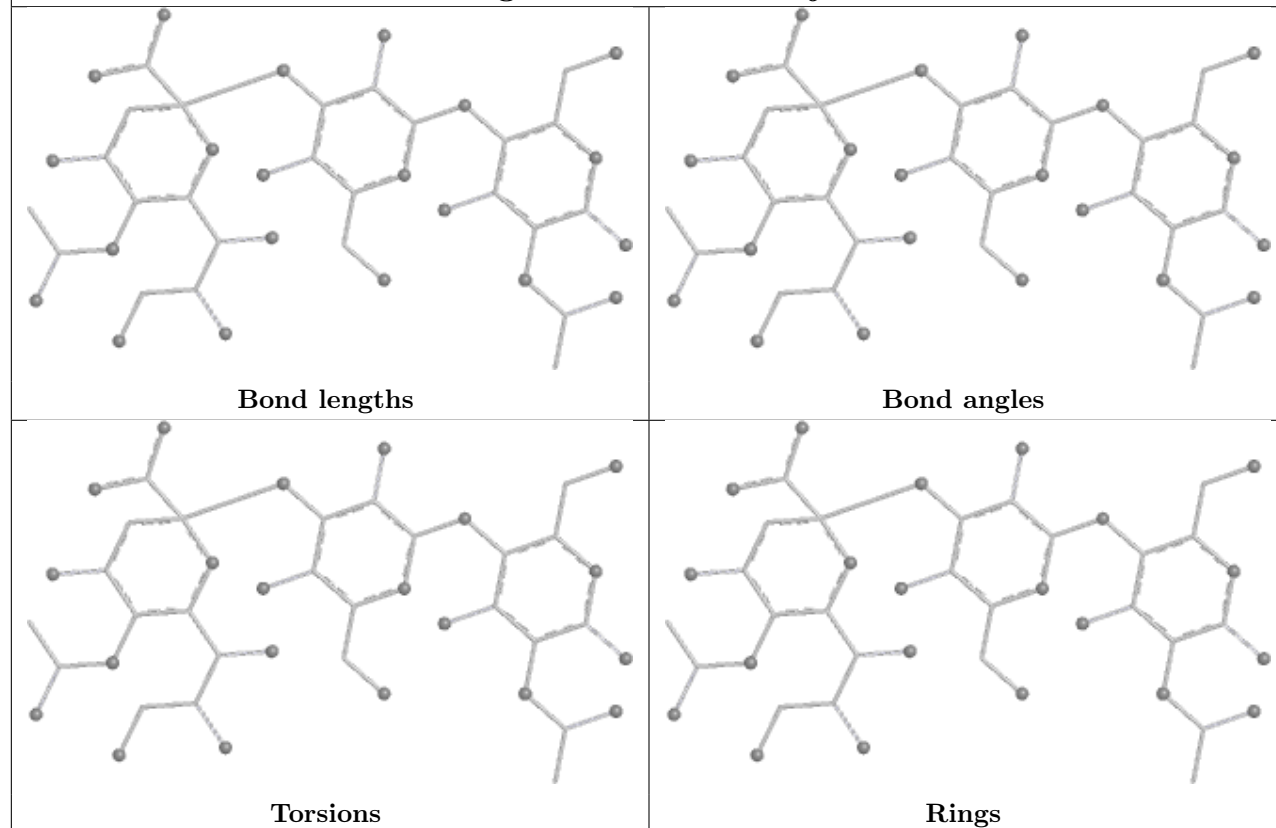
Oligosaccharide Chain dB

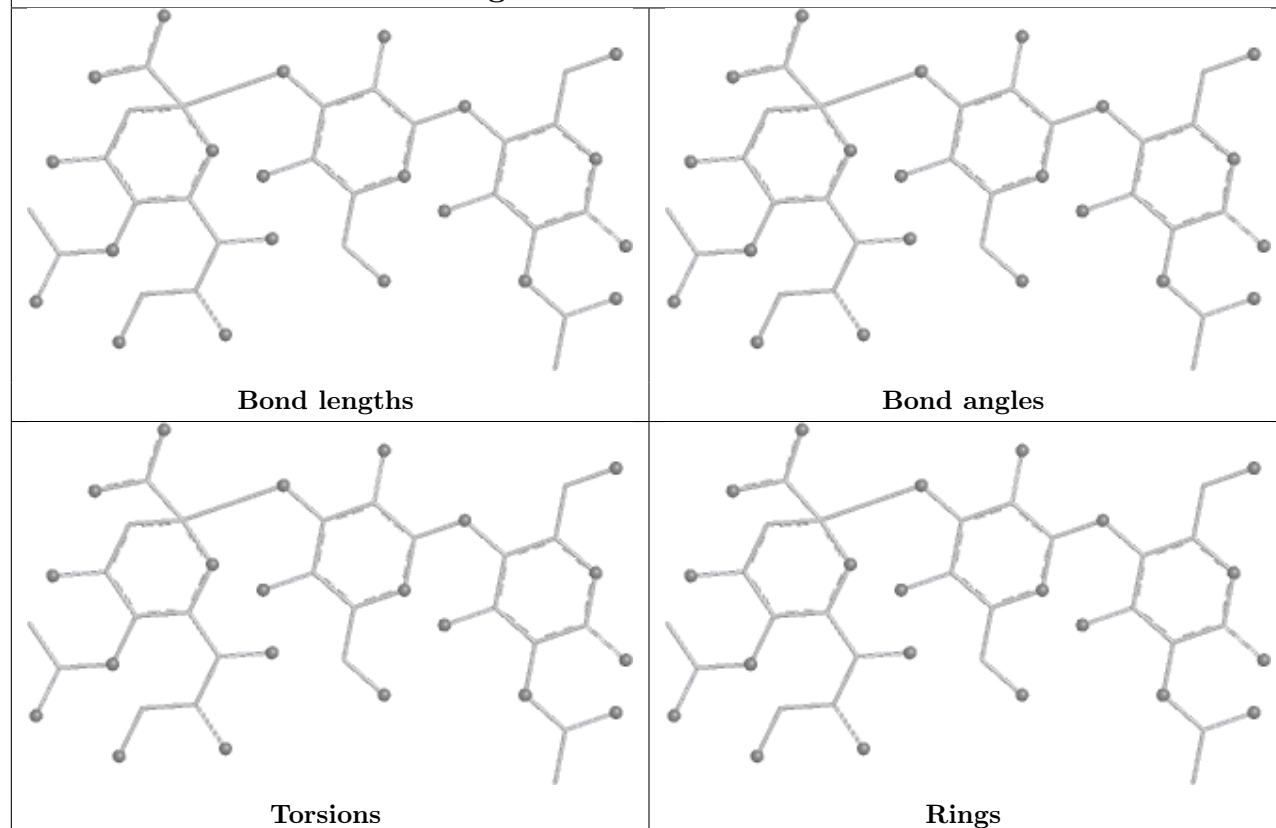
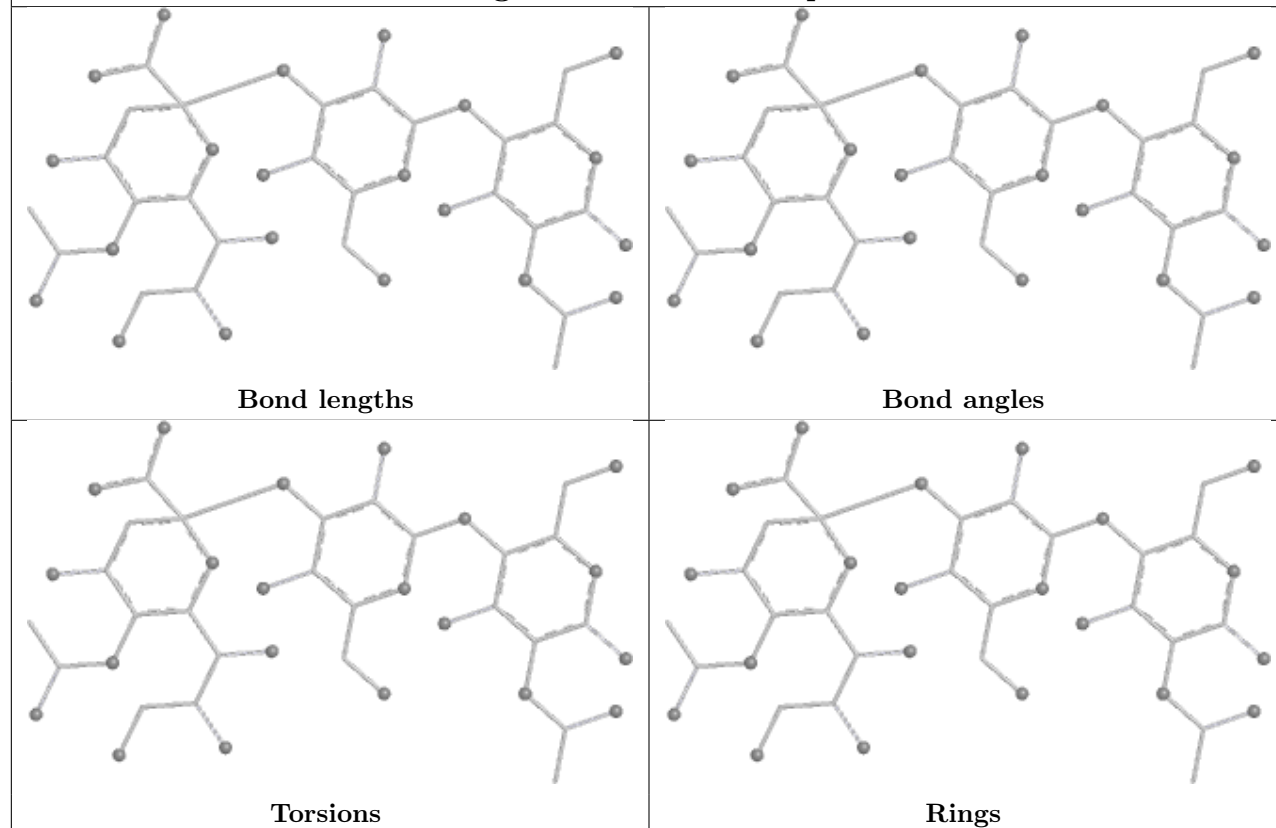


Oligosaccharide Chain gB

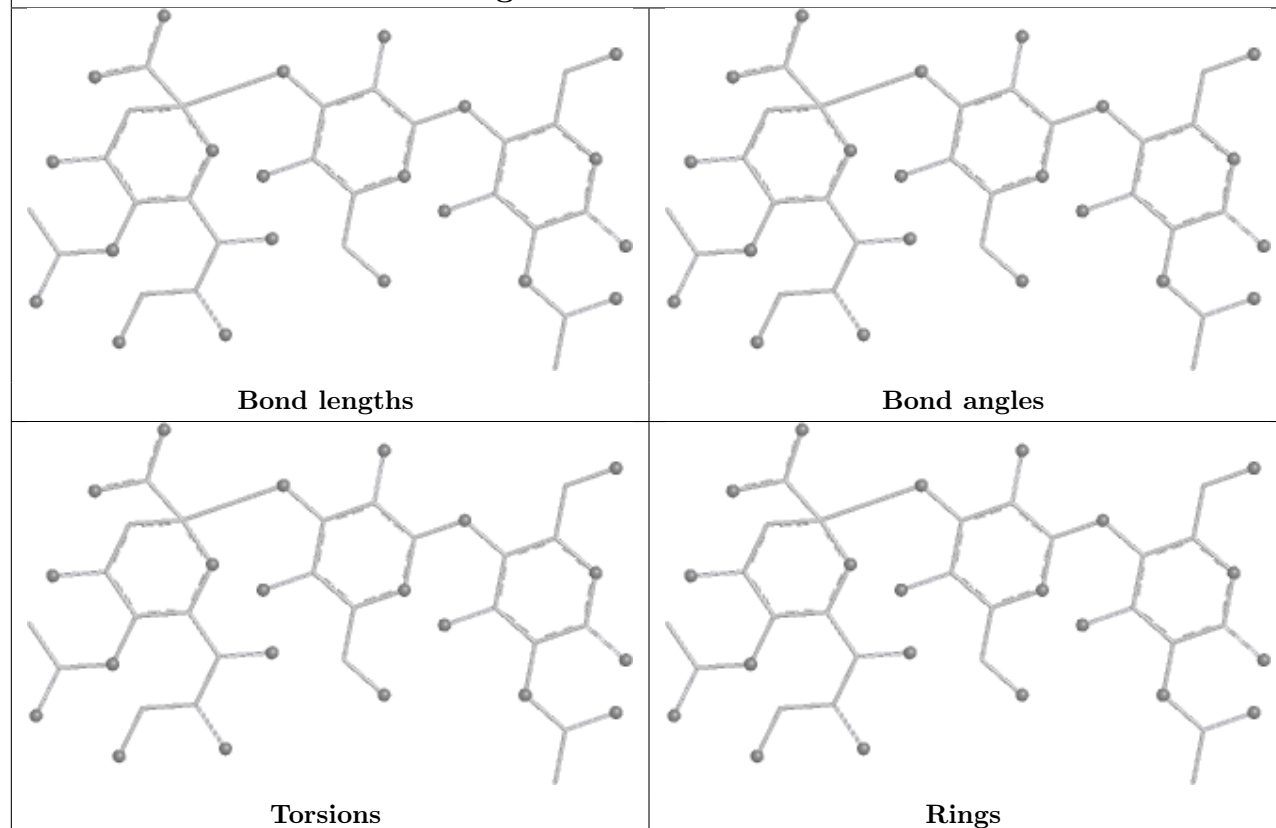


Oligosaccharide Chain jB

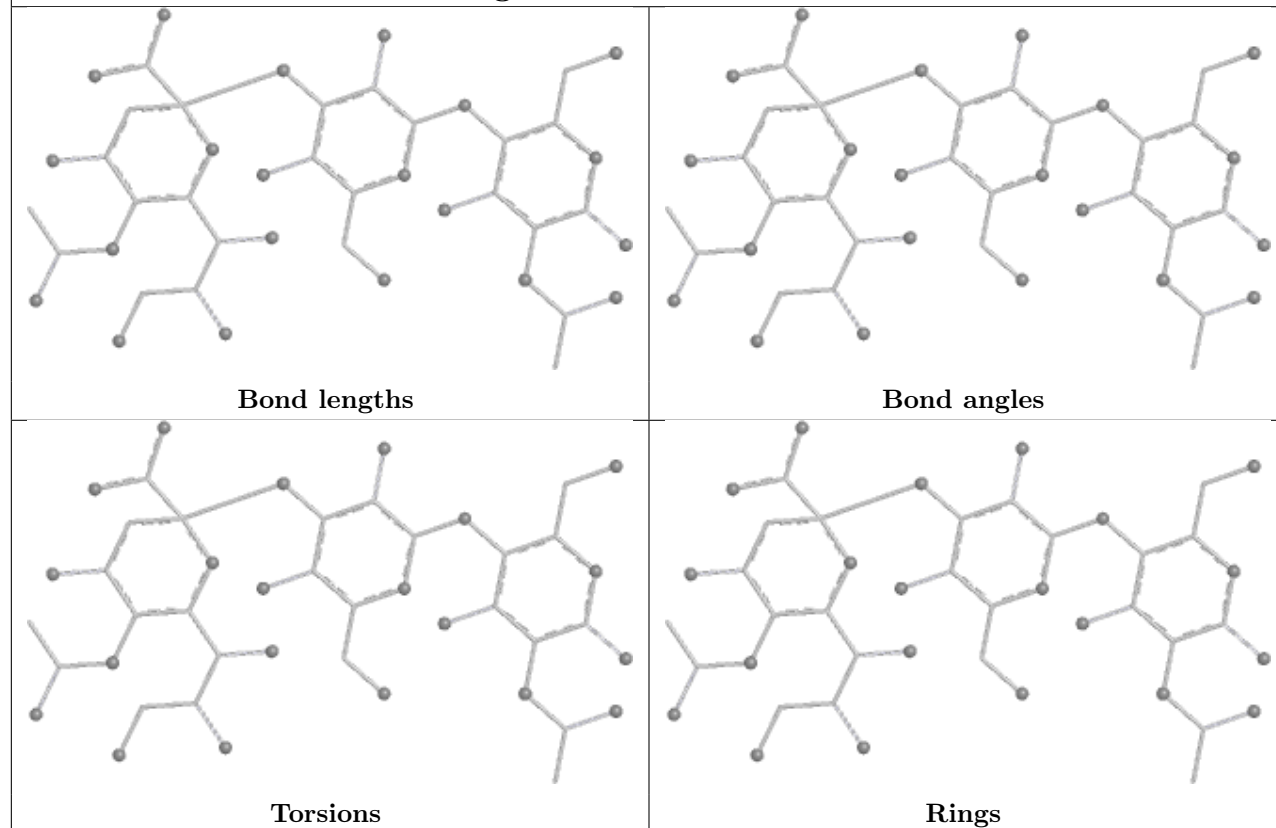


Oligosaccharide Chain mB**Oligosaccharide Chain pB**

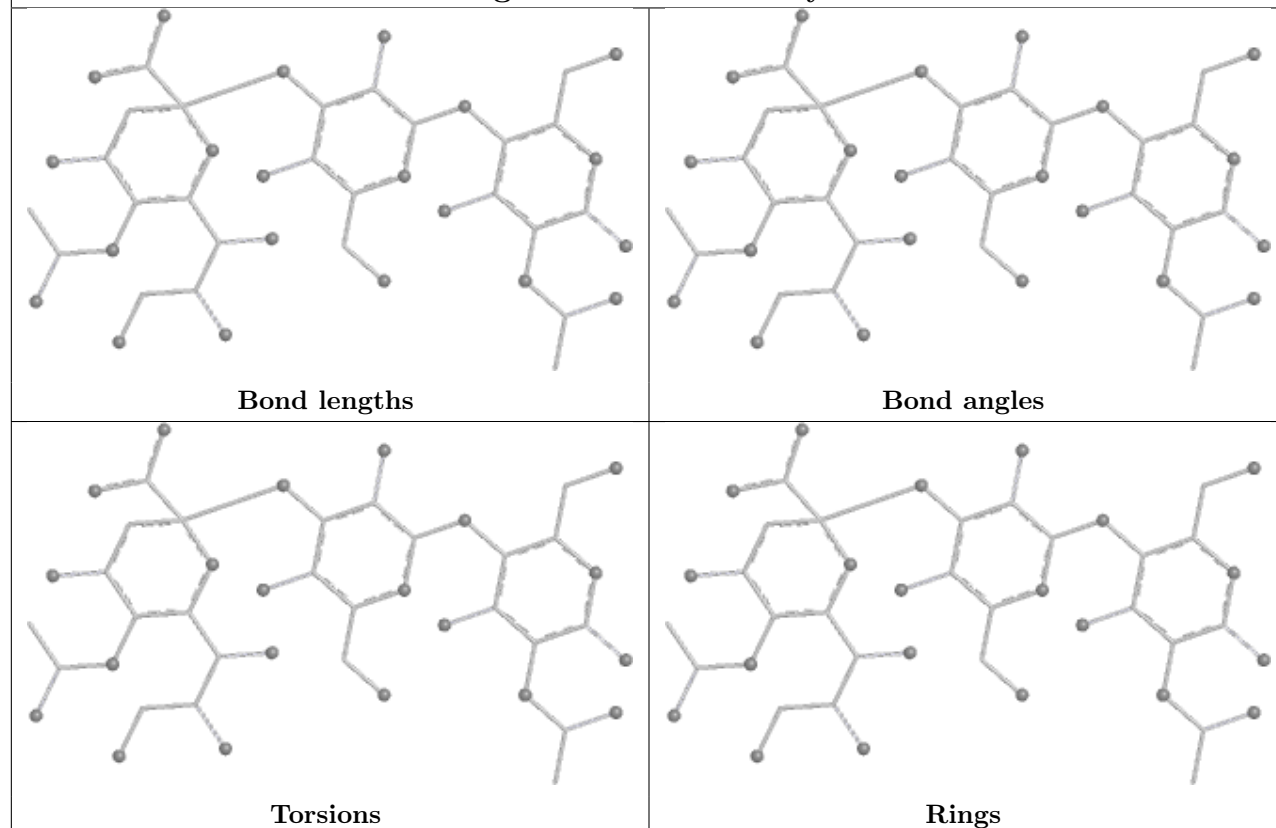
Oligosaccharide Chain sB



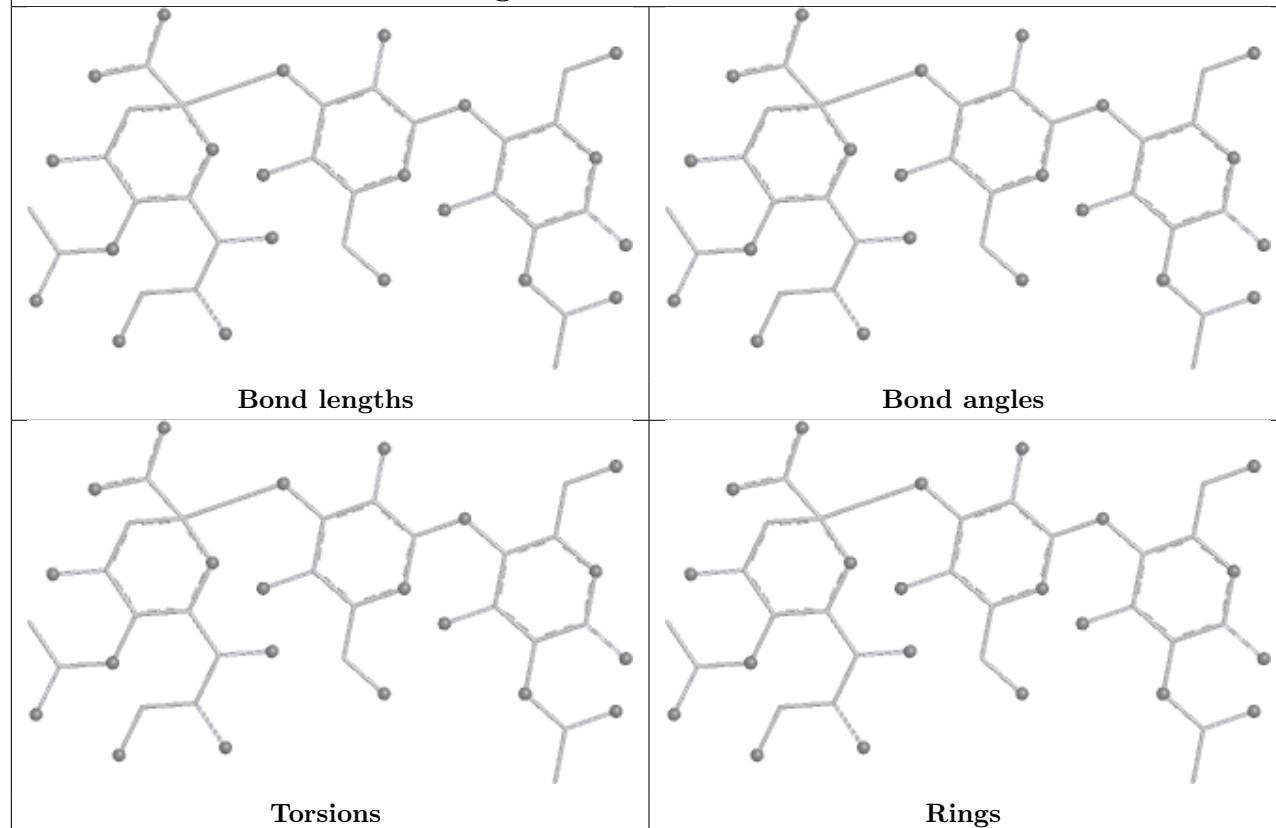
Oligosaccharide Chain vB



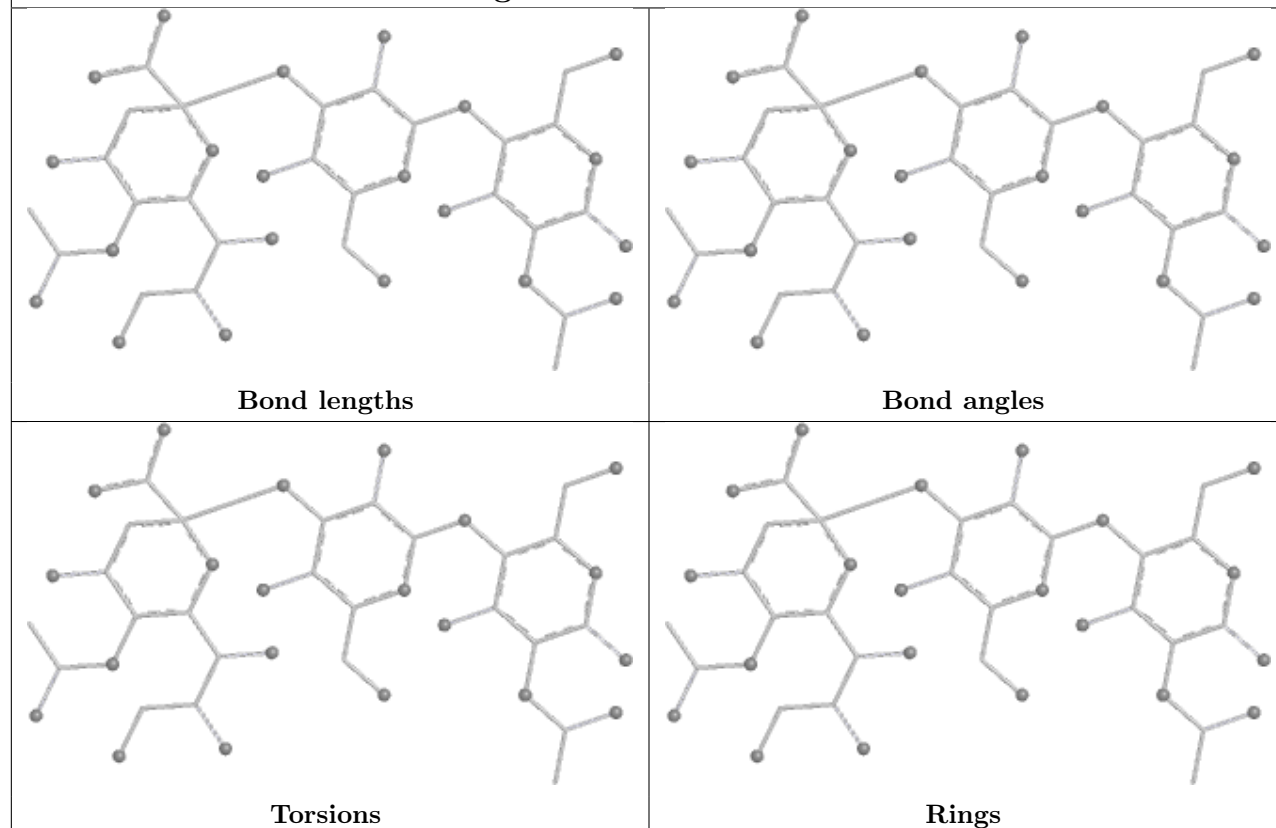
Oligosaccharide Chain yB



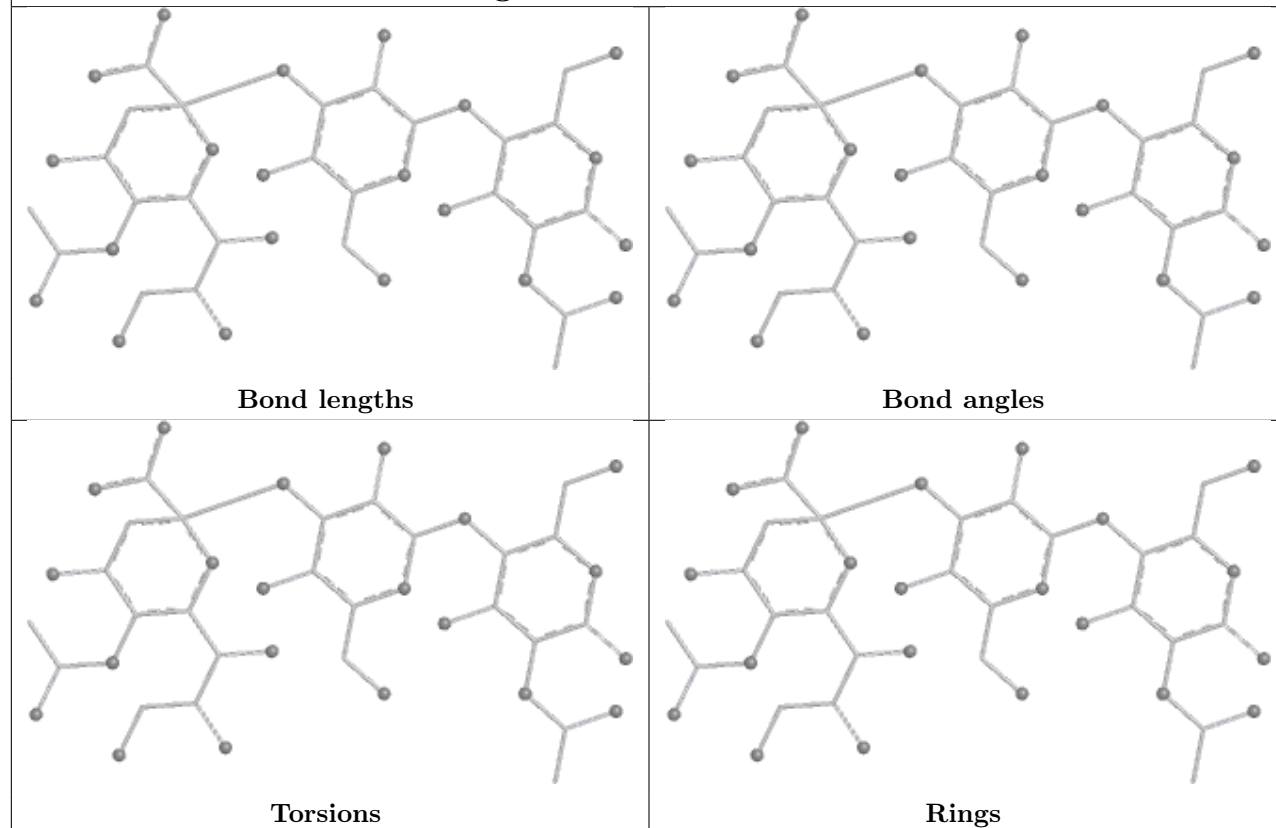
Oligosaccharide Chain 1B



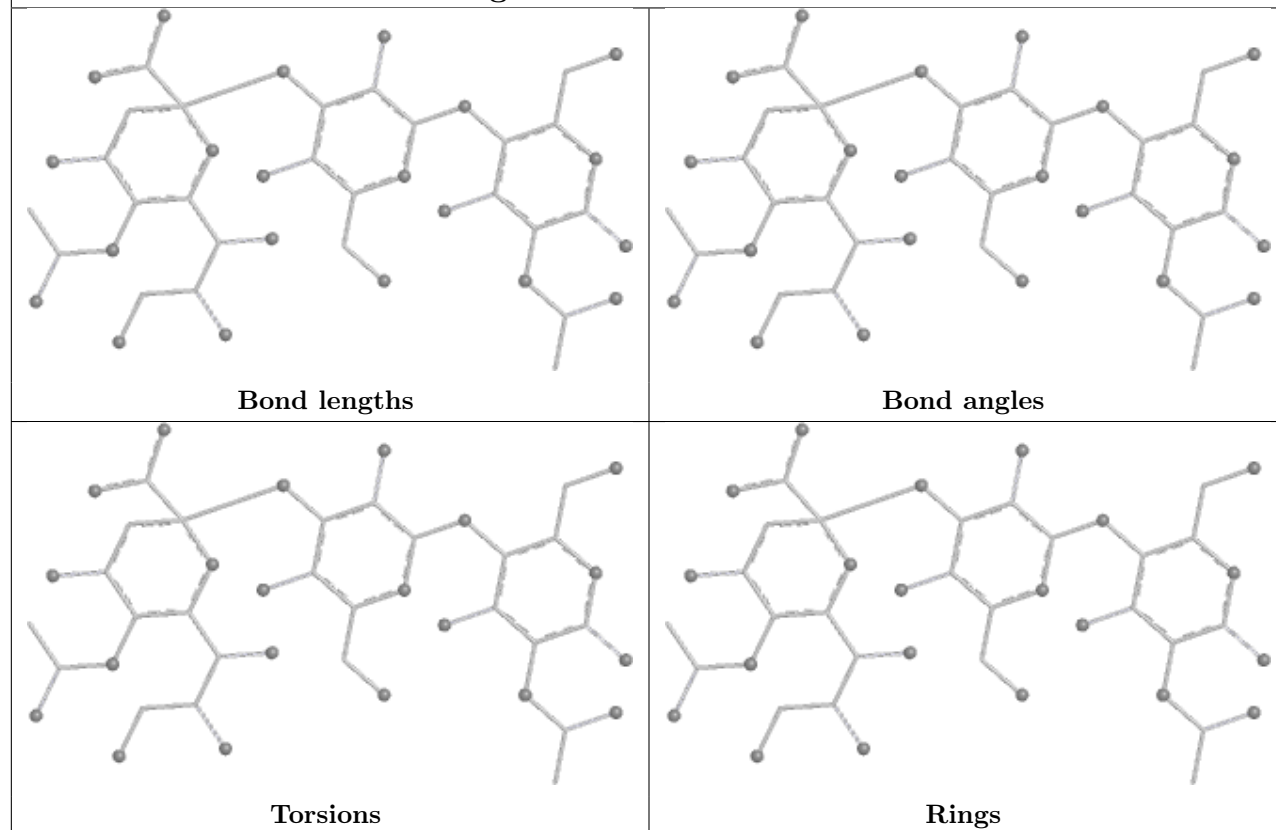
Oligosaccharide Chain 4B



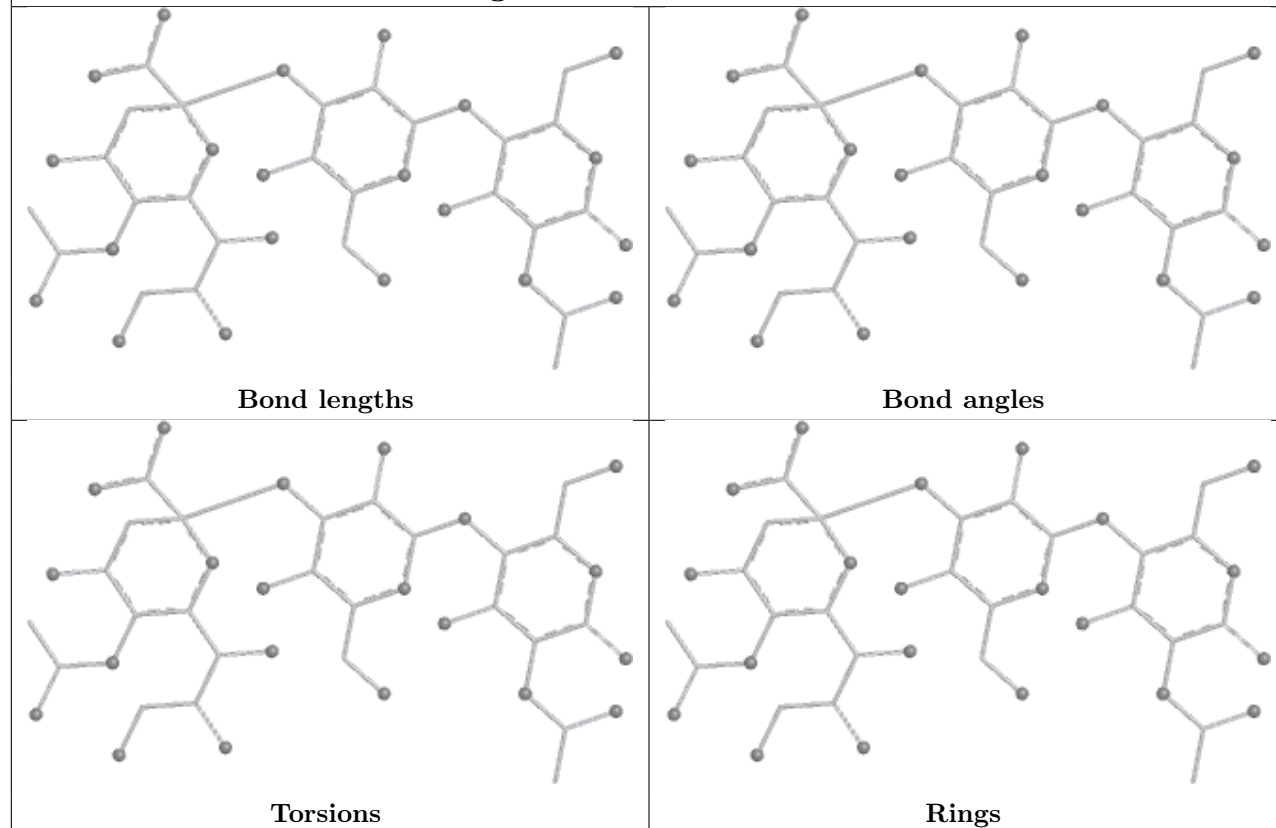
Oligosaccharide Chain 7B



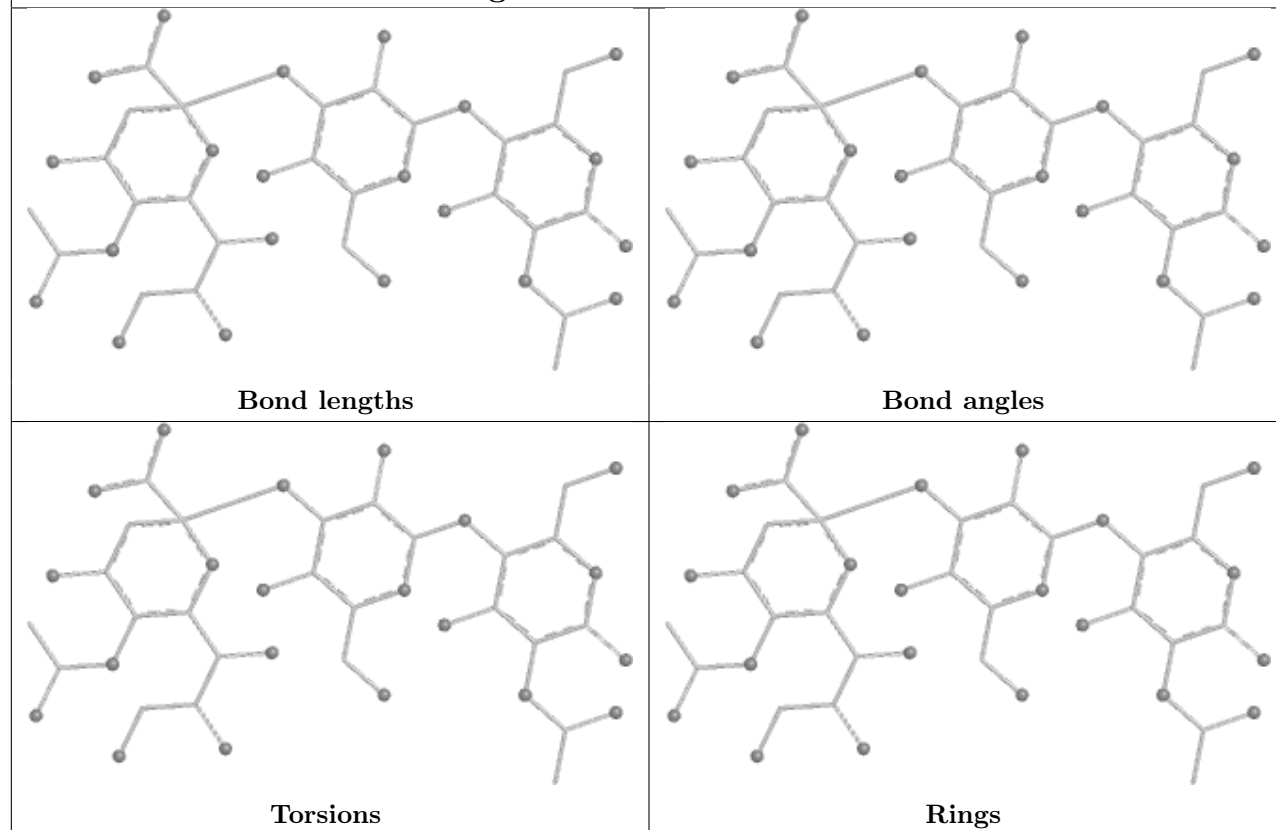
Oligosaccharide Chain AC



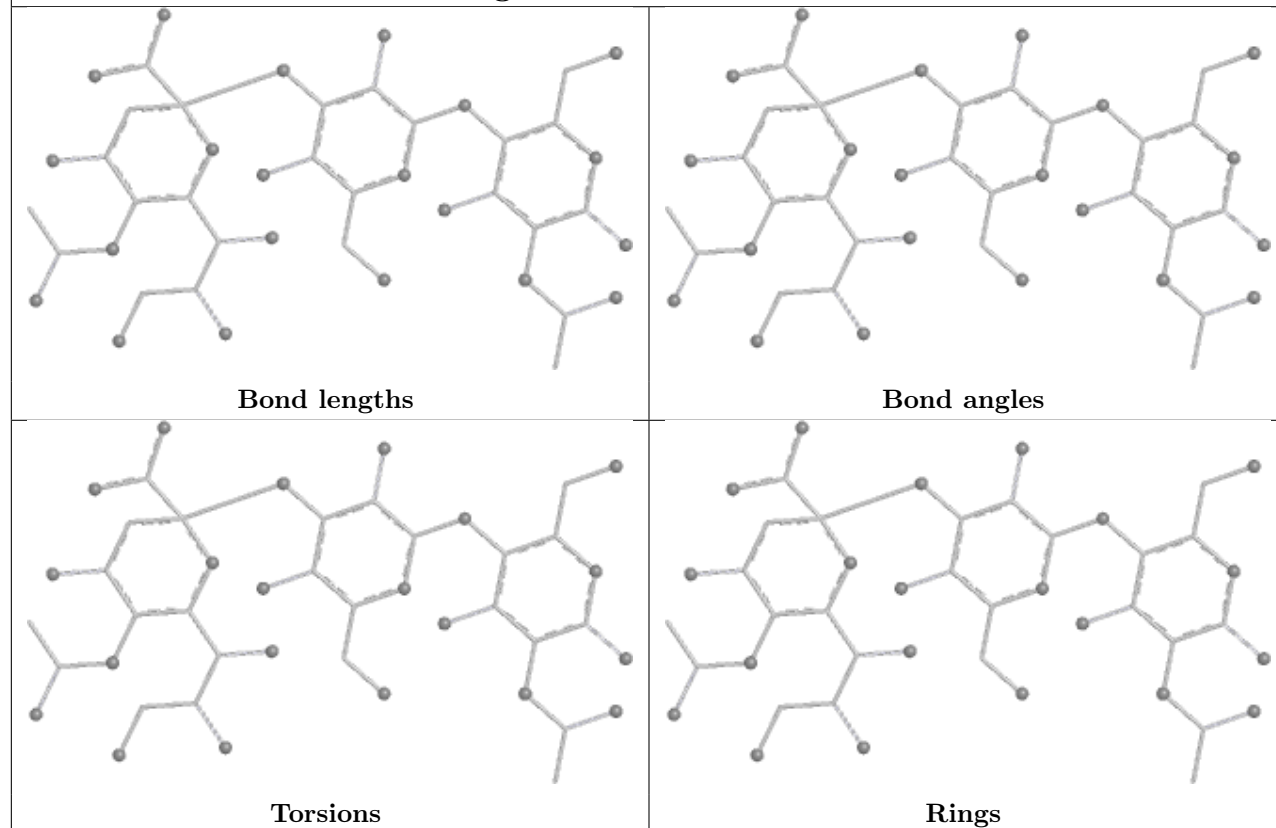
Oligosaccharide Chain DC



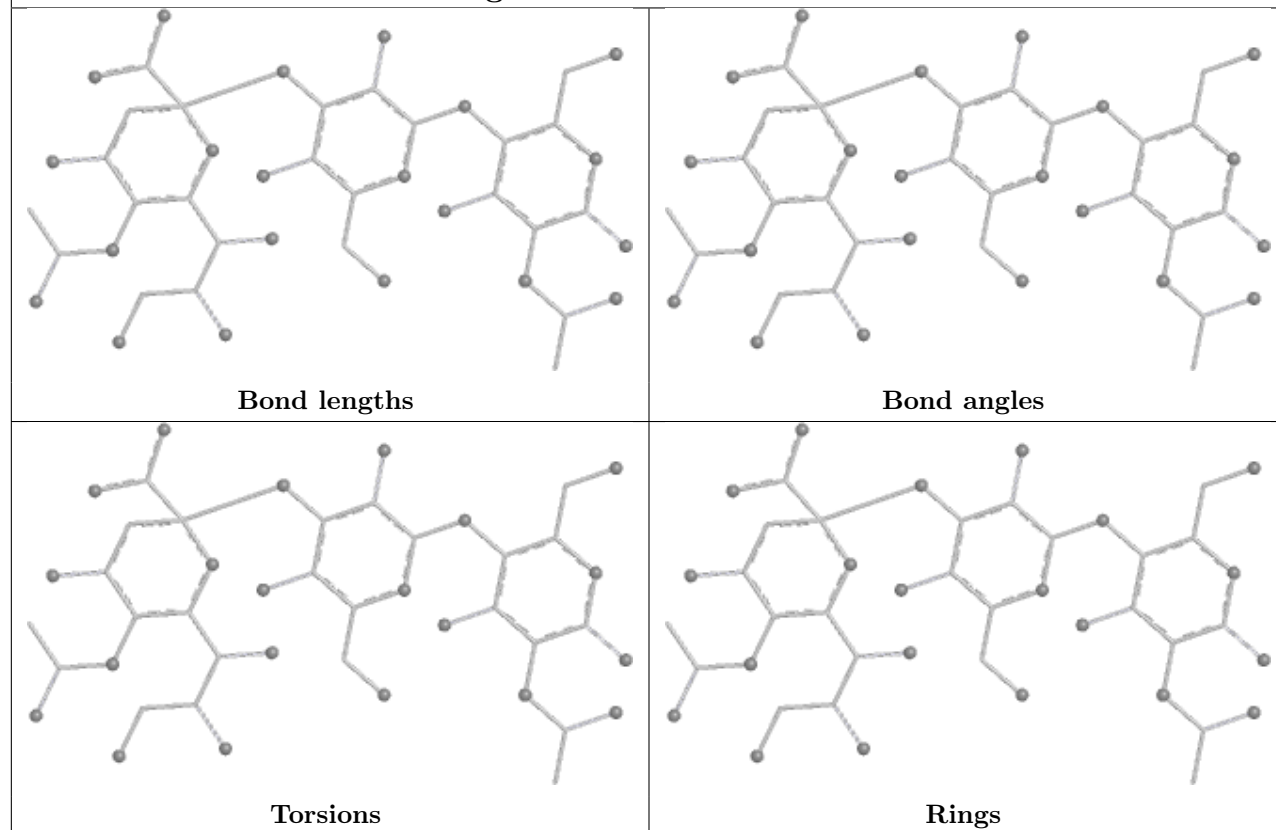
Oligosaccharide Chain GC



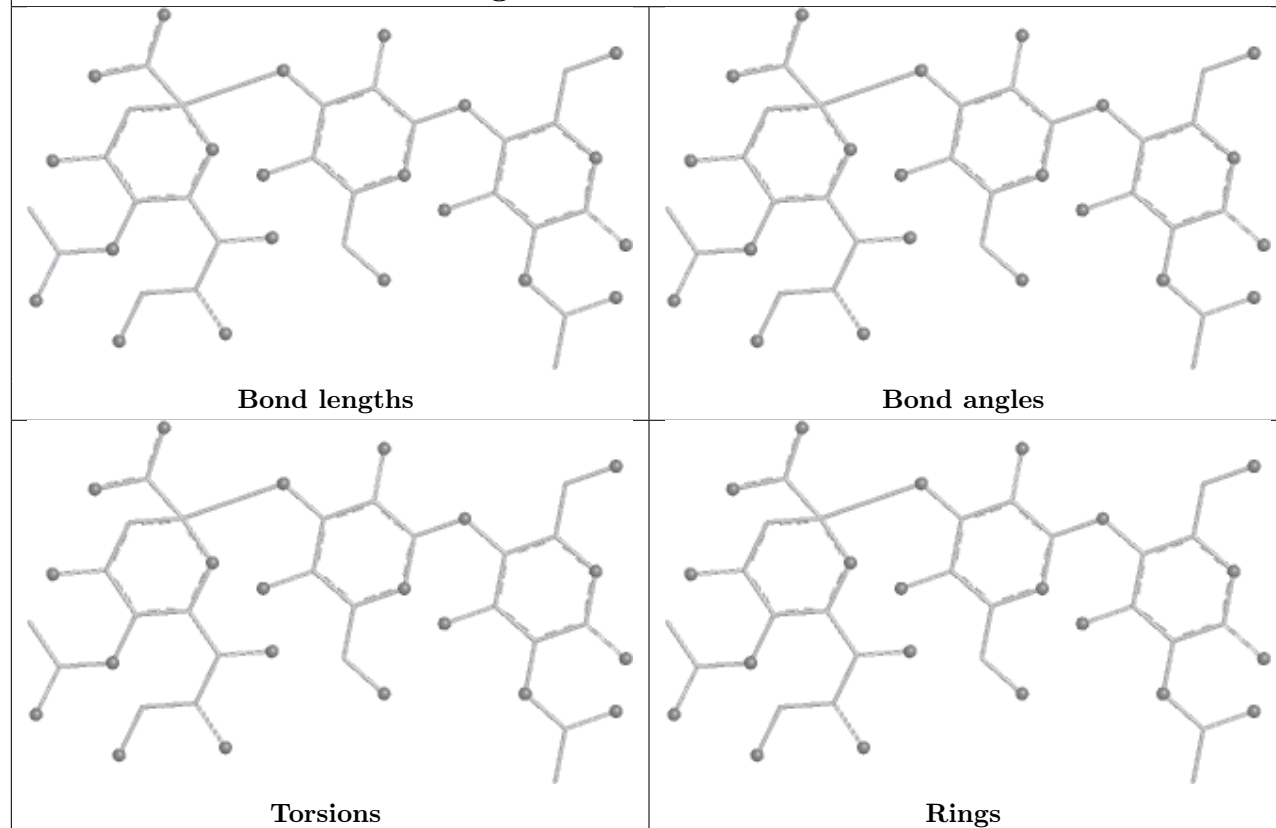
Oligosaccharide Chain JC



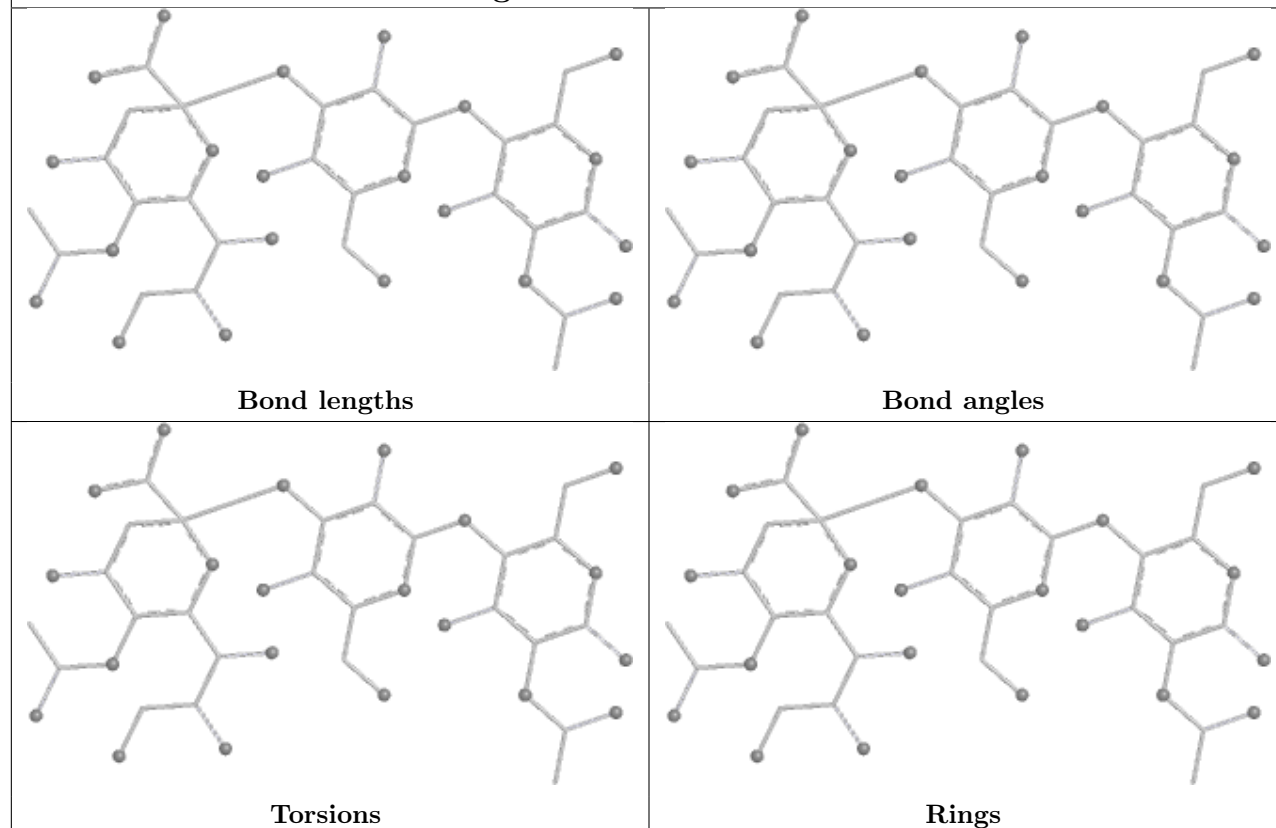
Oligosaccharide Chain MC



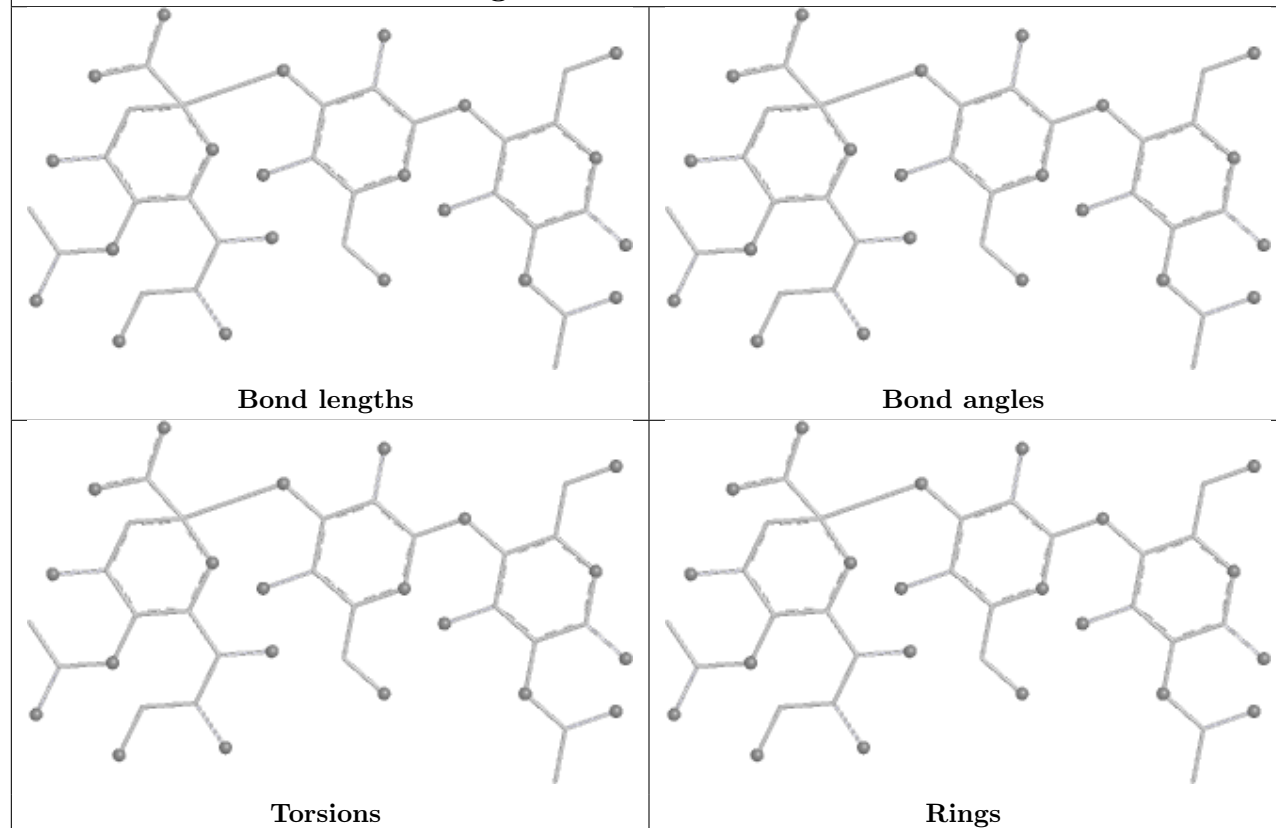
Oligosaccharide Chain PC



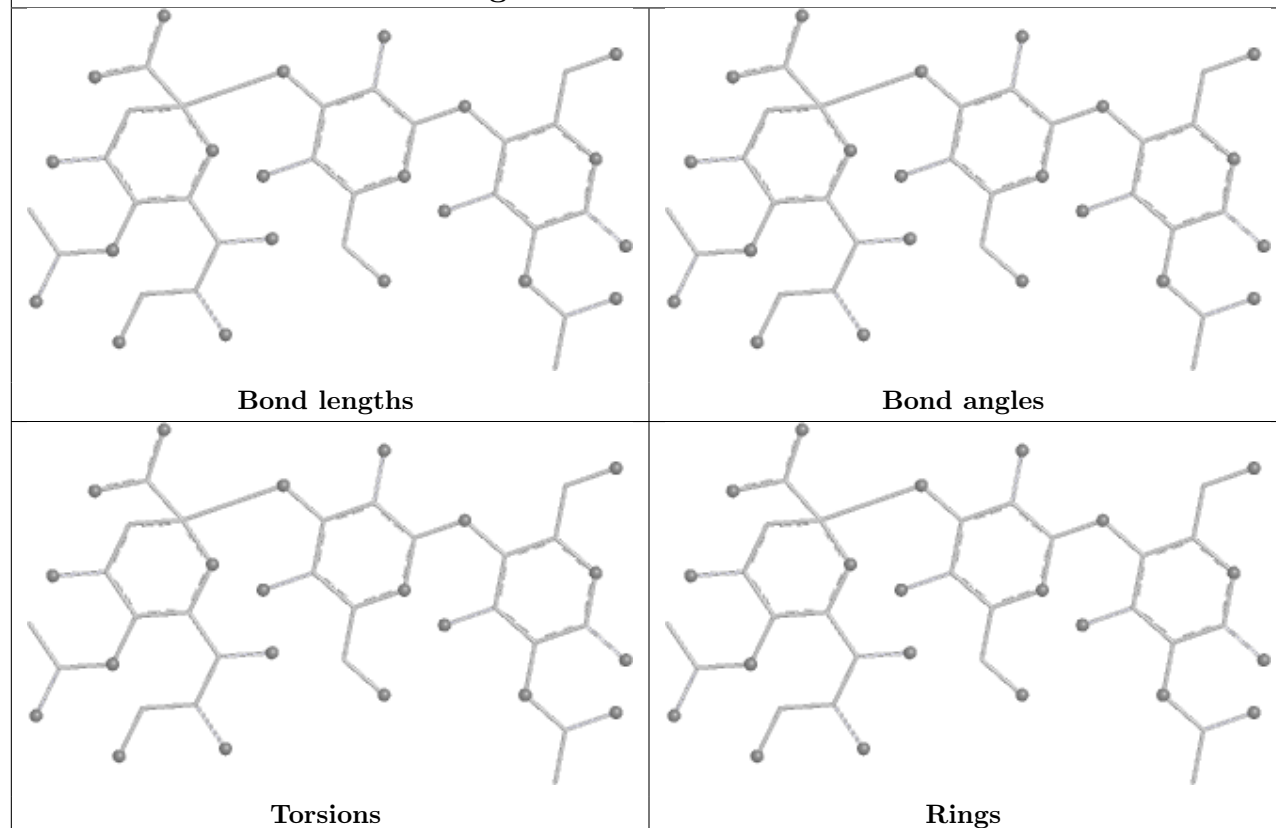
Oligosaccharide Chain SC



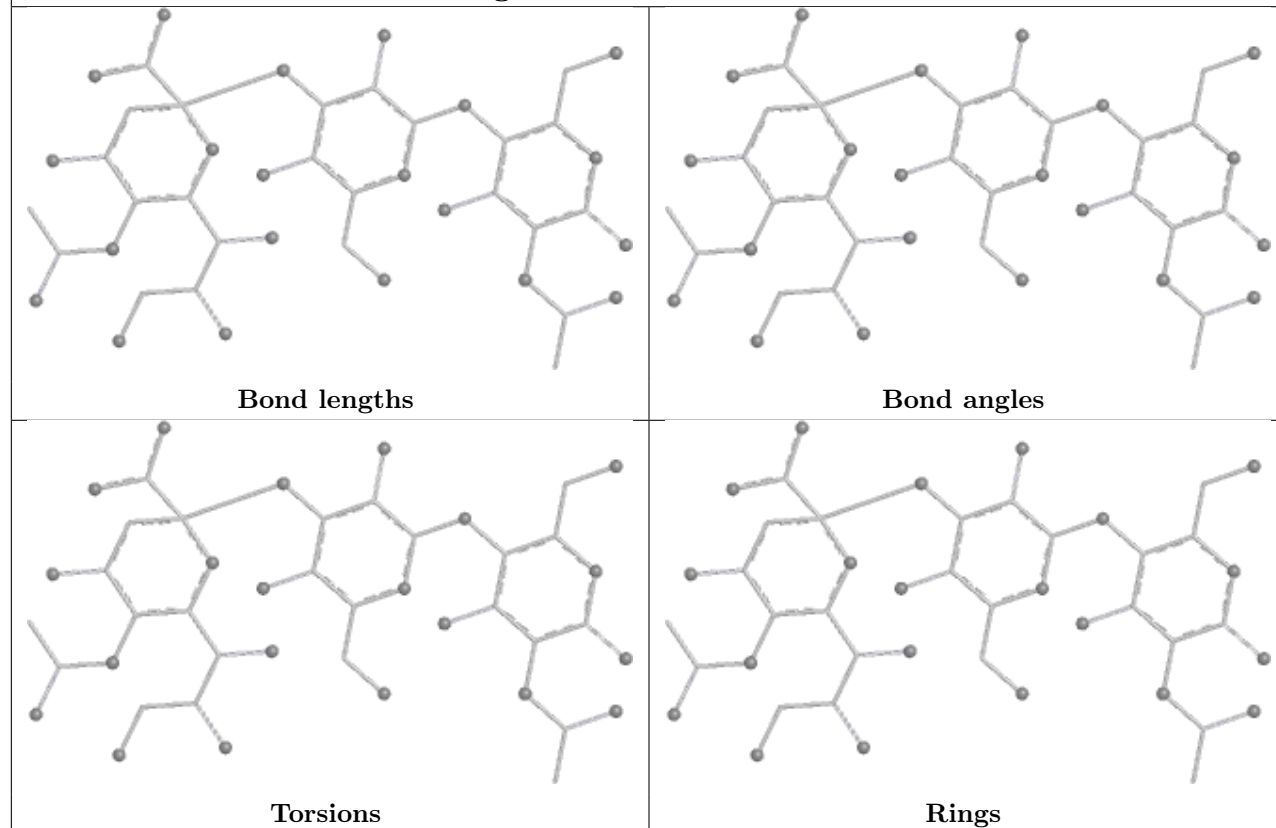
Oligosaccharide Chain VC



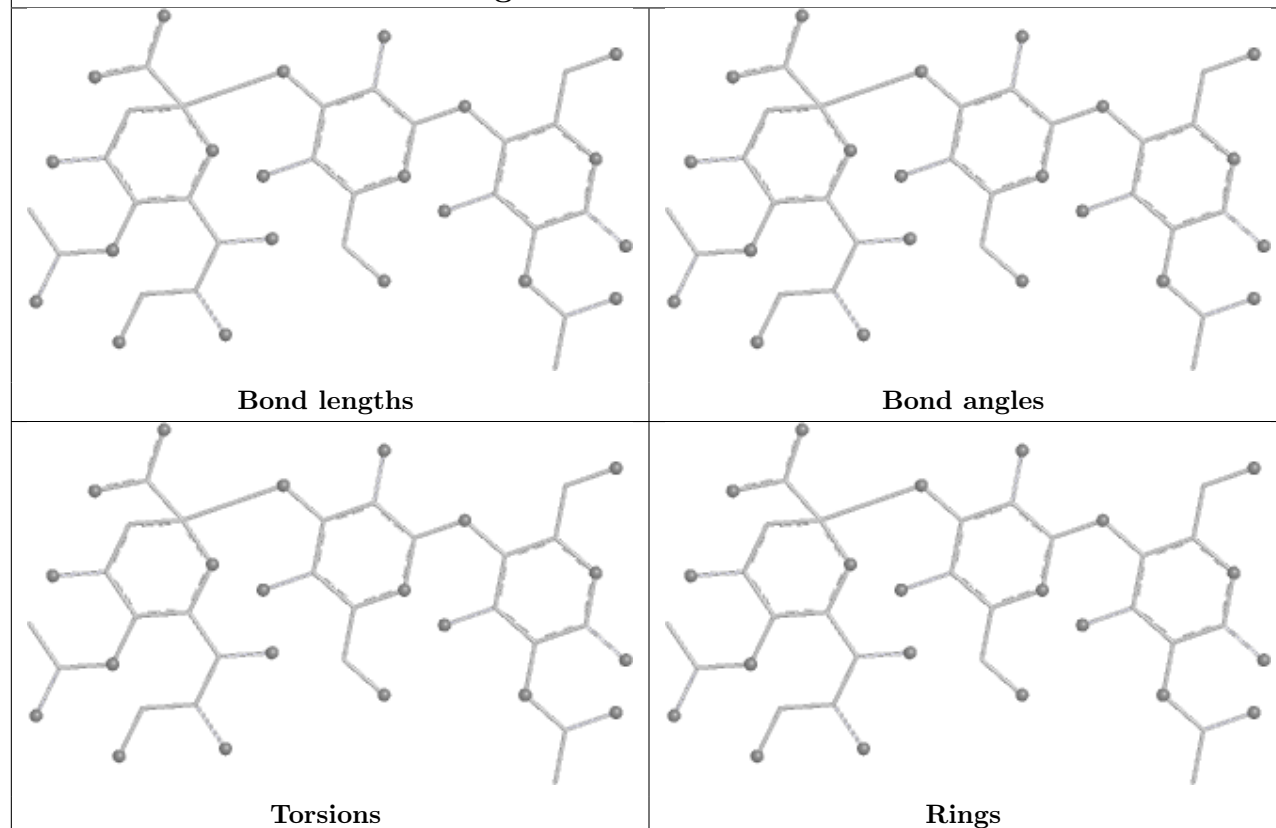
Oligosaccharide Chain YC



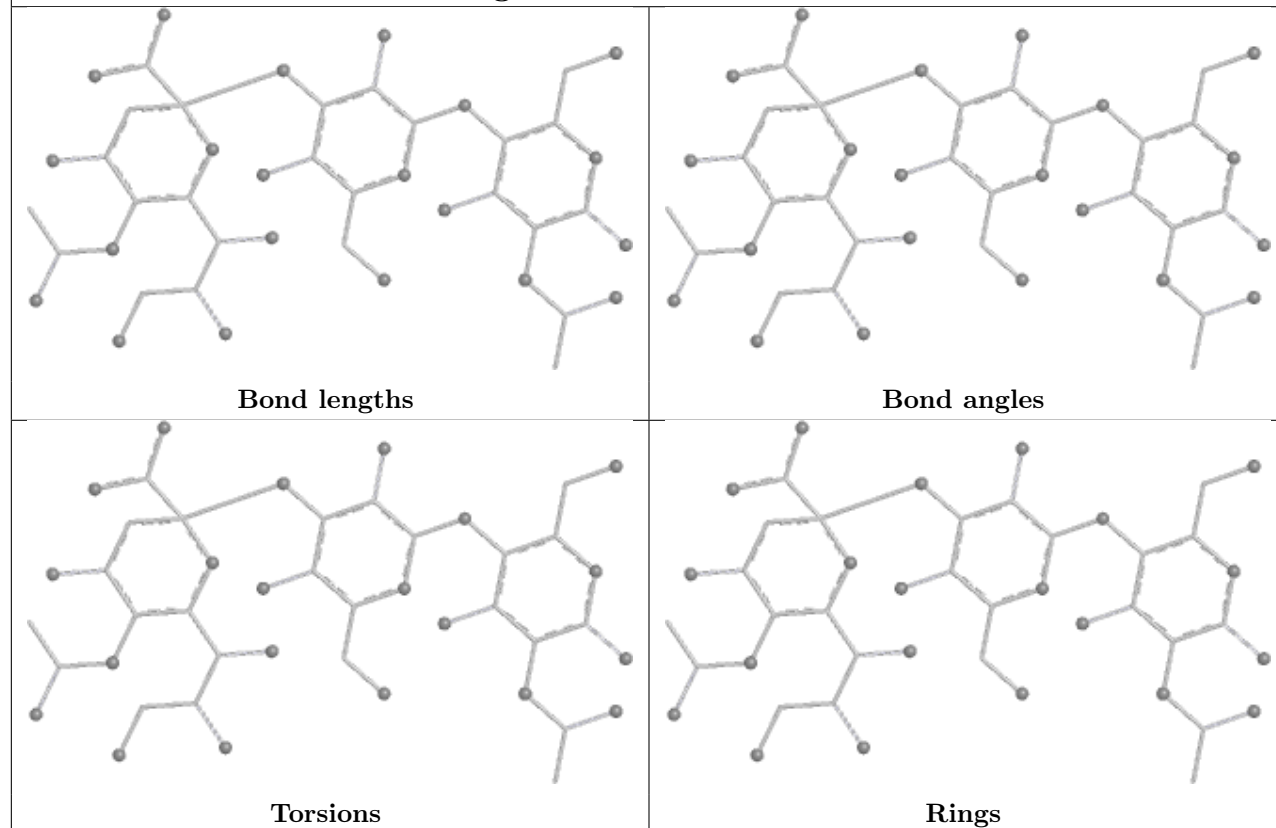
Oligosaccharide Chain bC



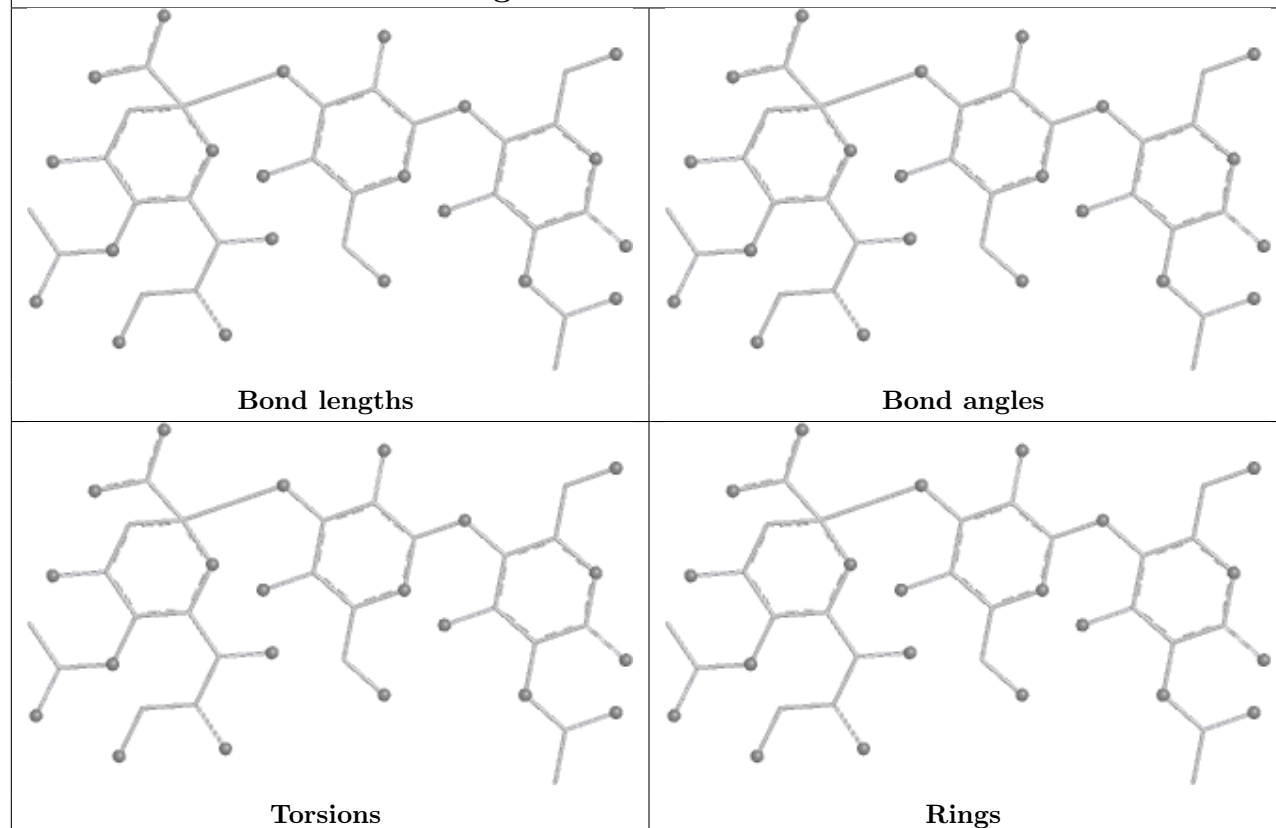
Oligosaccharide Chain eC



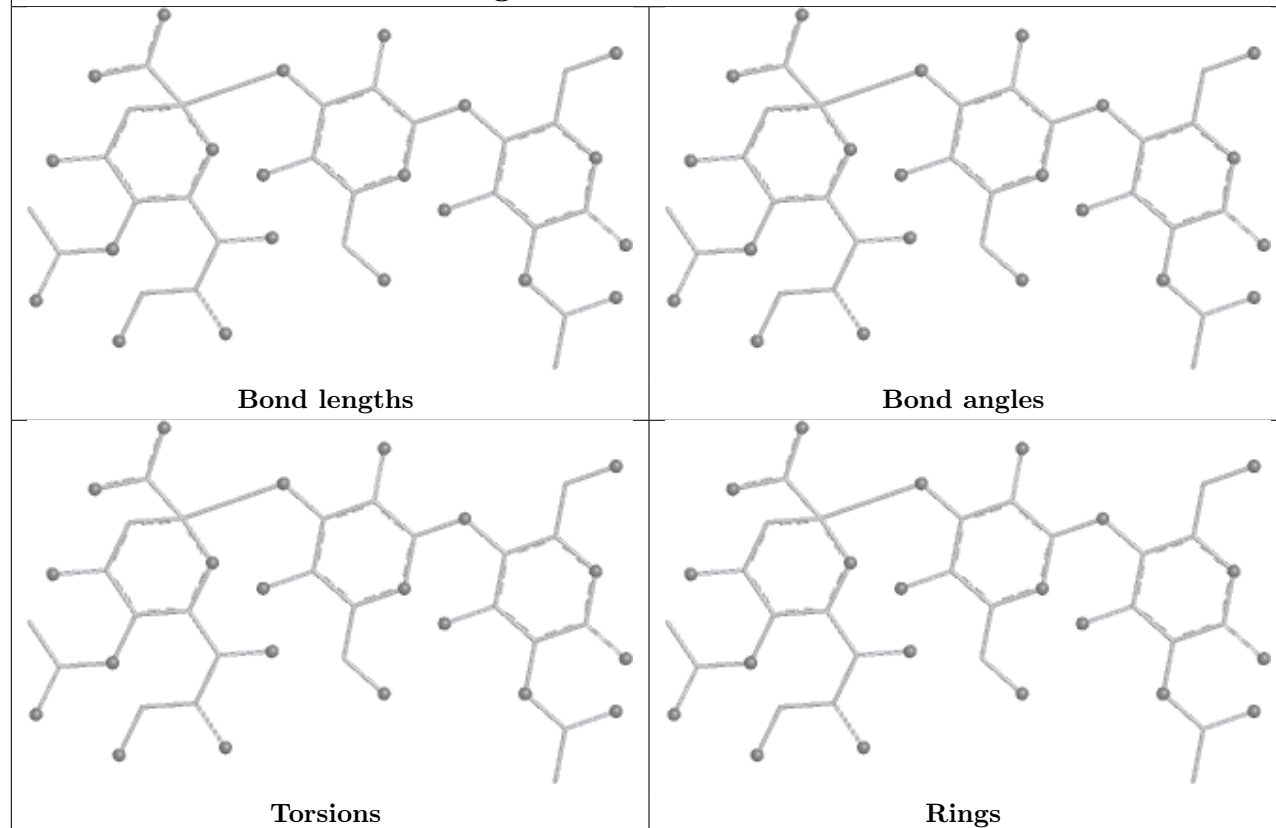
Oligosaccharide Chain hC



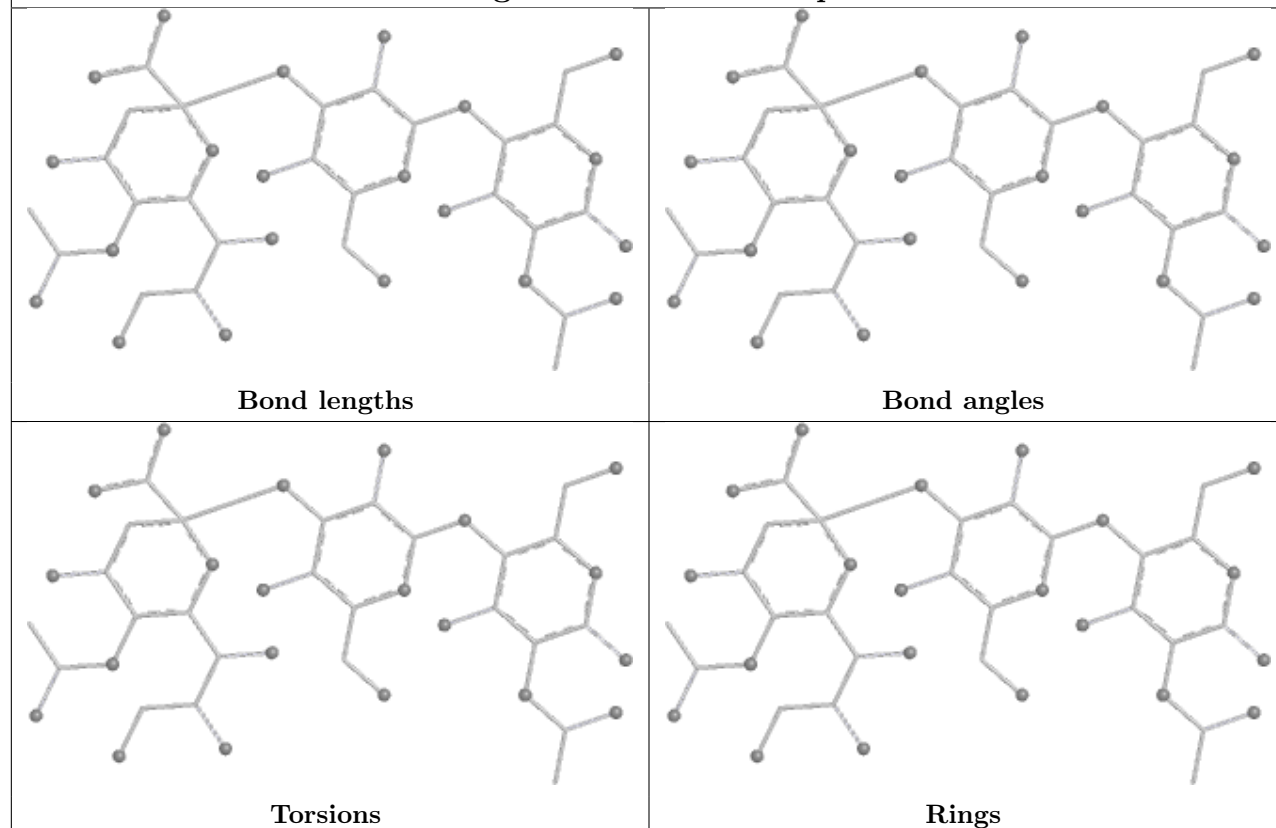
Oligosaccharide Chain kC



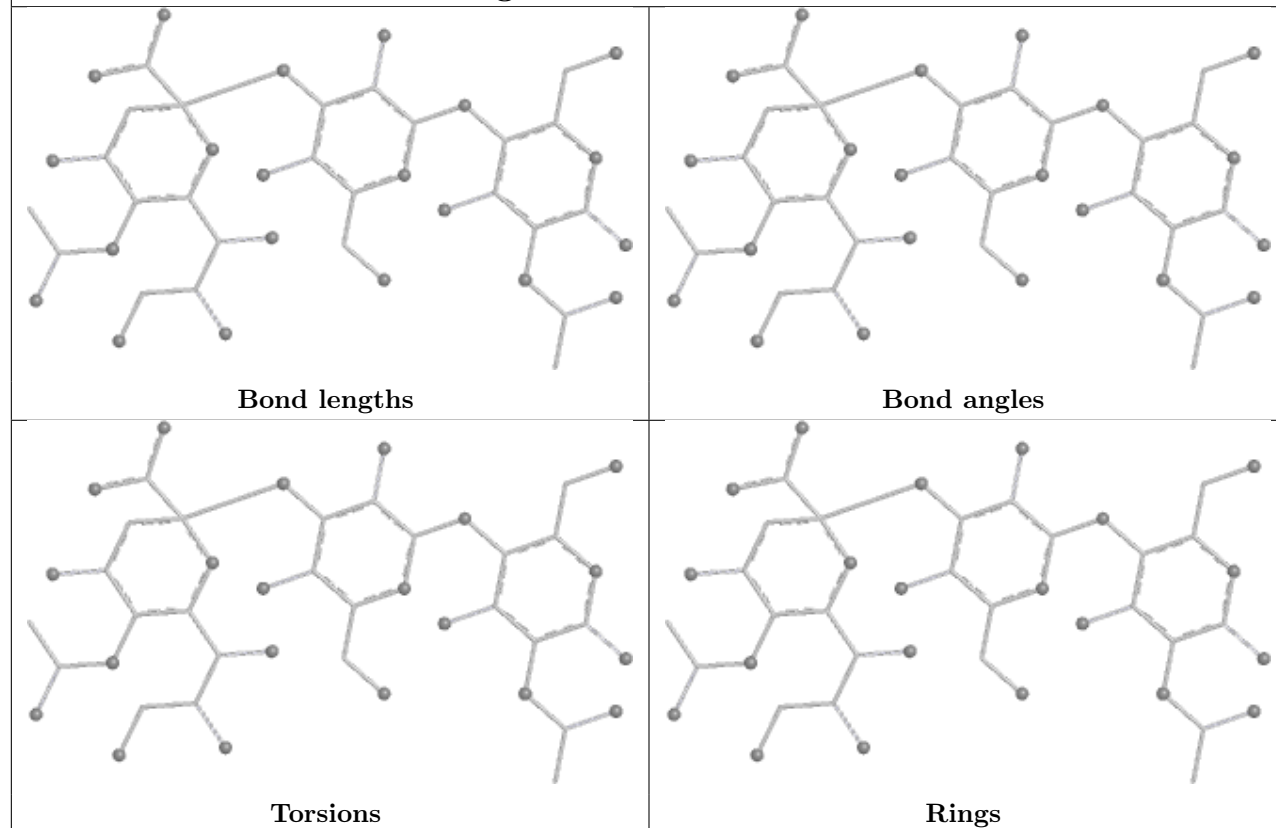
Oligosaccharide Chain nC



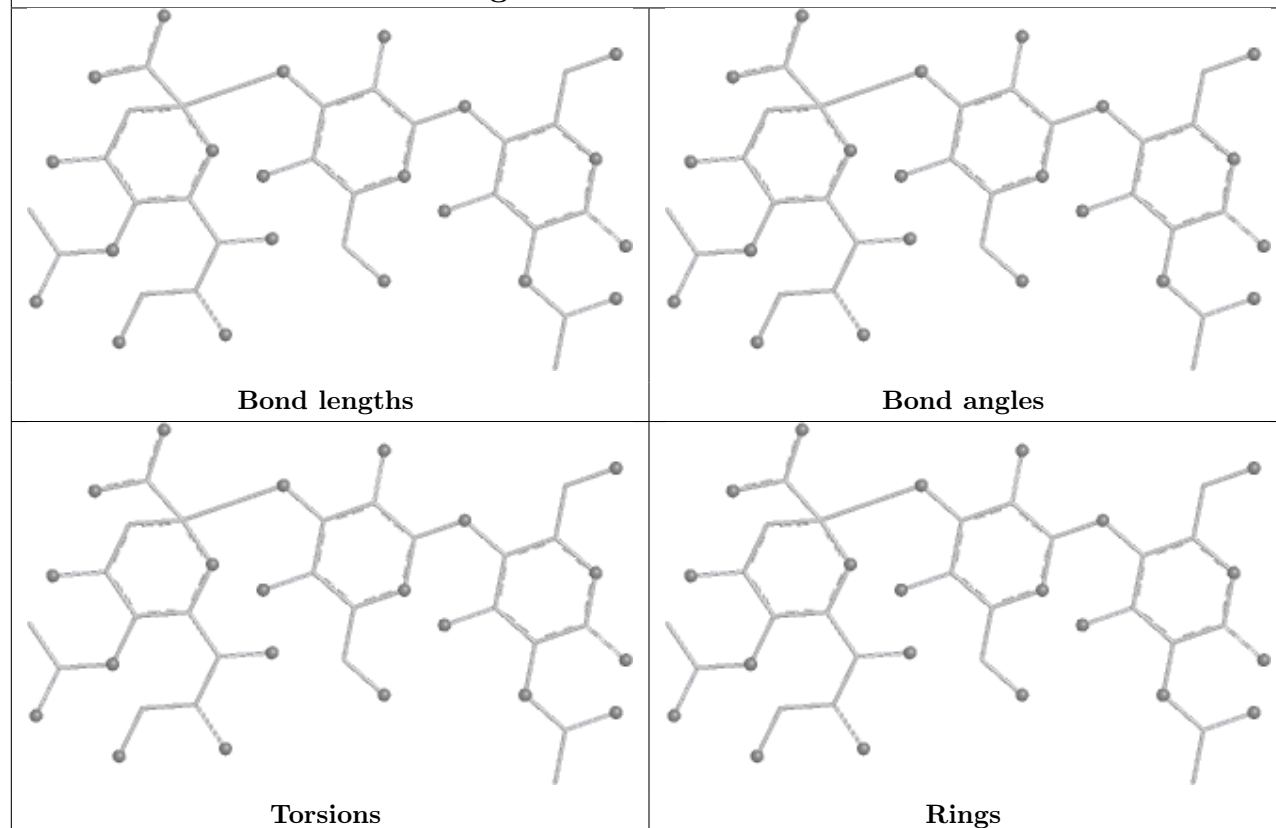
Oligosaccharide Chain qC



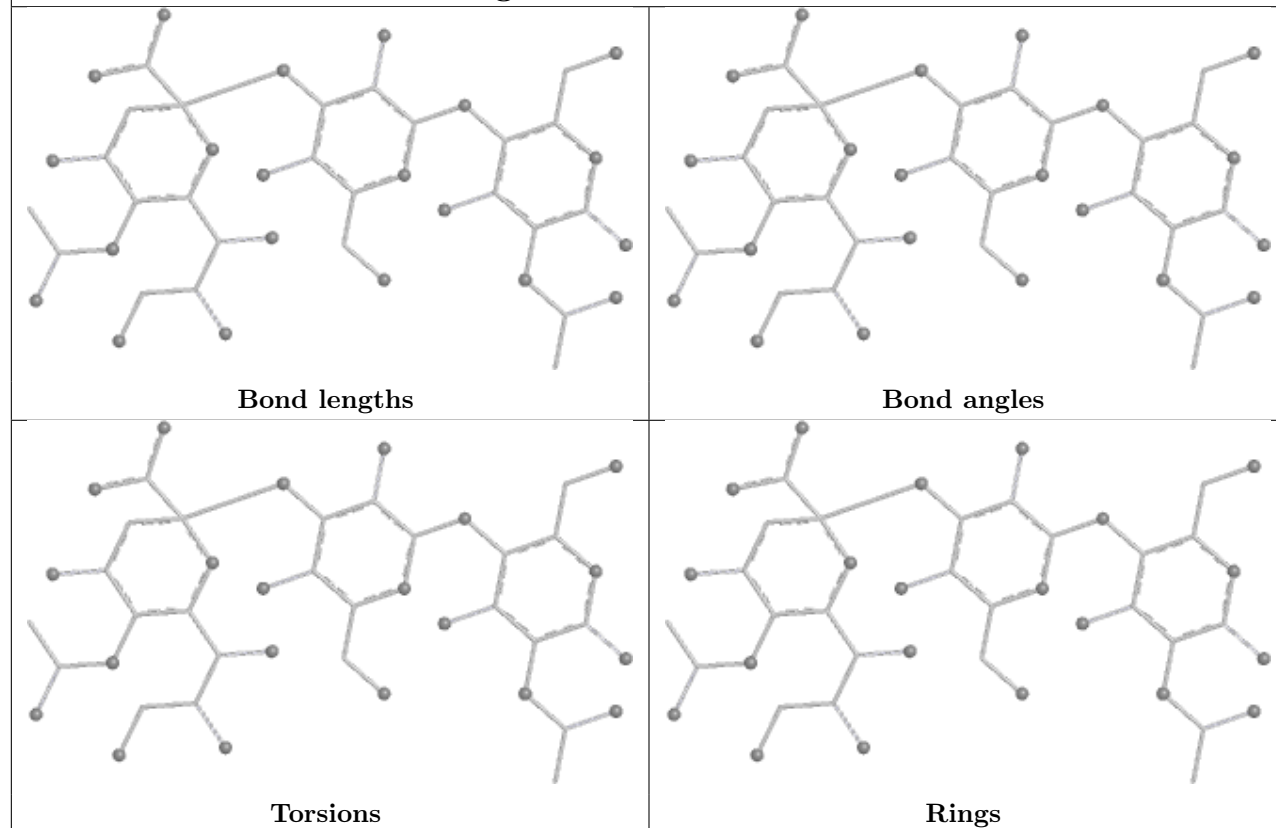
Oligosaccharide Chain tC



Oligosaccharide Chain wC



Oligosaccharide Chain zC



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

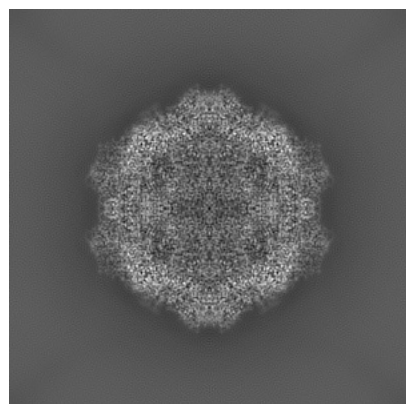
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49195. These allow visual inspection of the internal detail of the map and identification of artifacts.

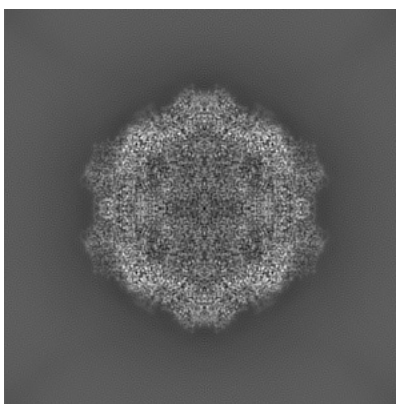
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

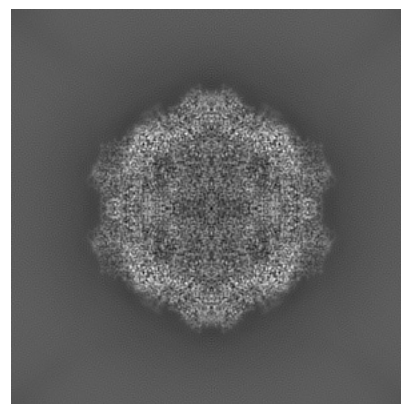
6.1.1 Primary map



X

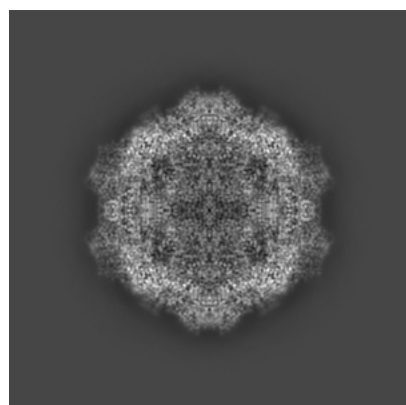


Y

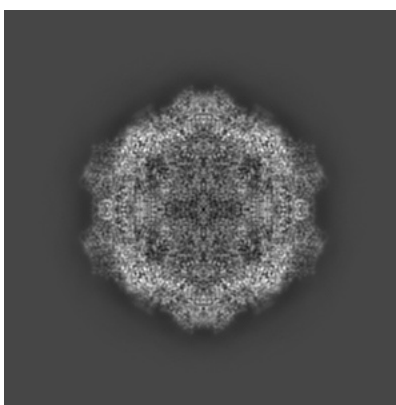


Z

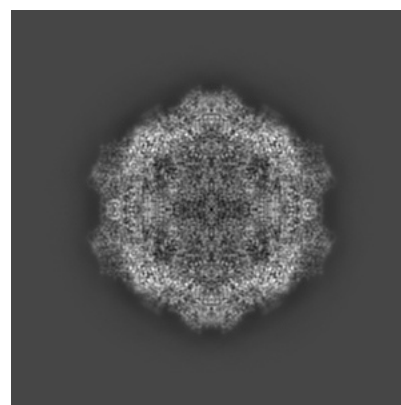
6.1.2 Raw map



X



Y

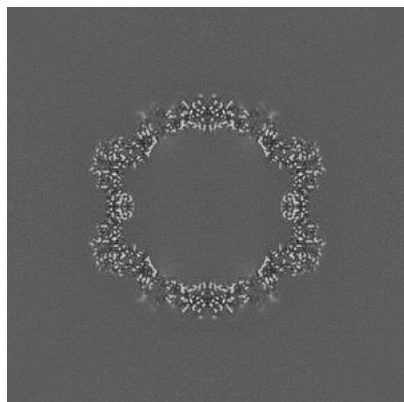


Z

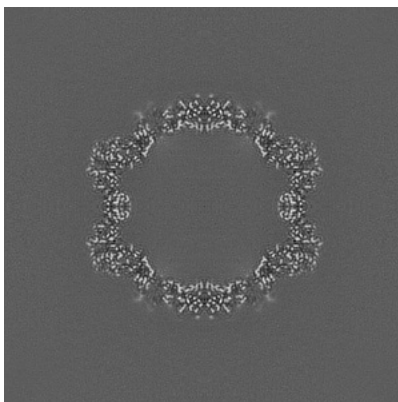
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

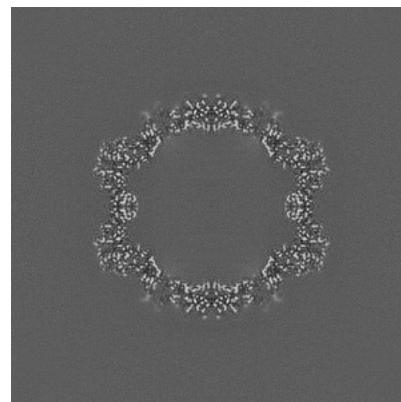
6.2.1 Primary map



X Index: 210

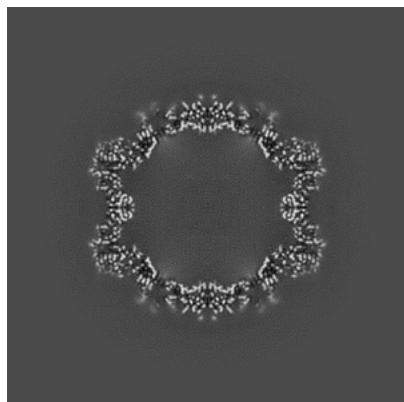


Y Index: 210

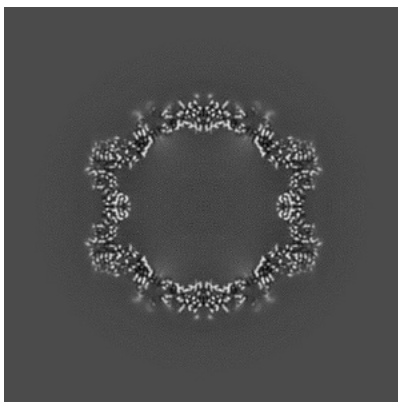


Z Index: 210

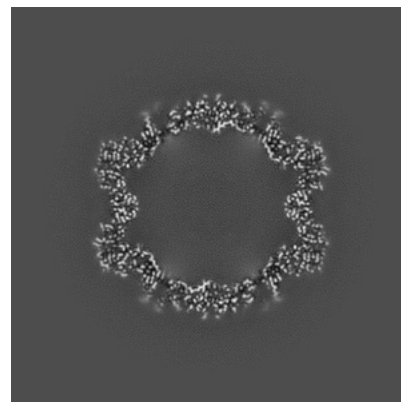
6.2.2 Raw map



X Index: 210



Y Index: 210

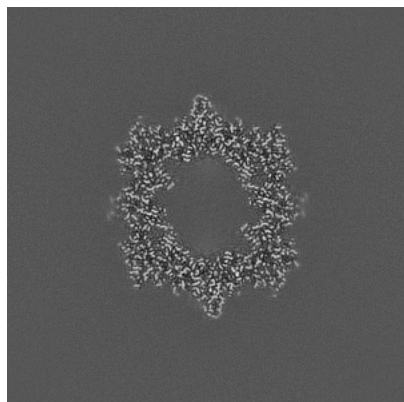


Z Index: 210

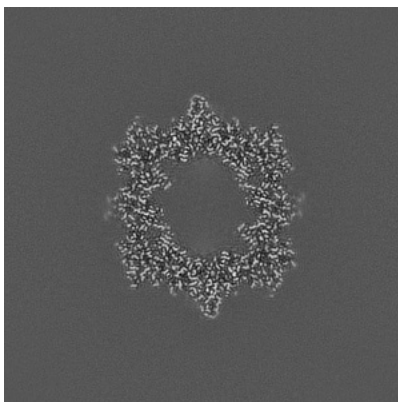
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

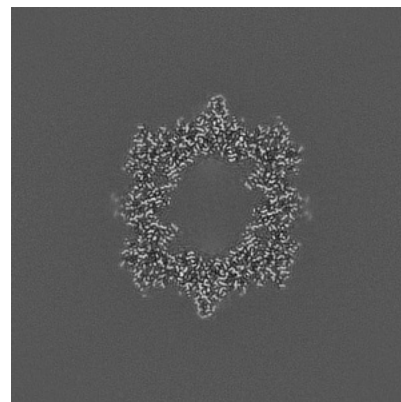
6.3.1 Primary map



X Index: 275

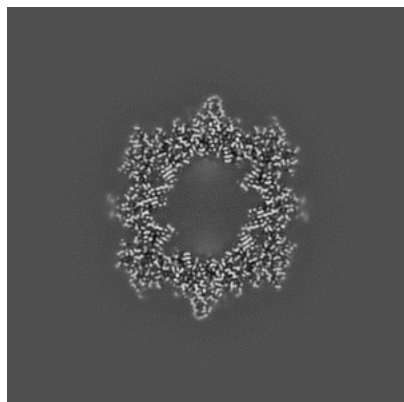


Y Index: 275

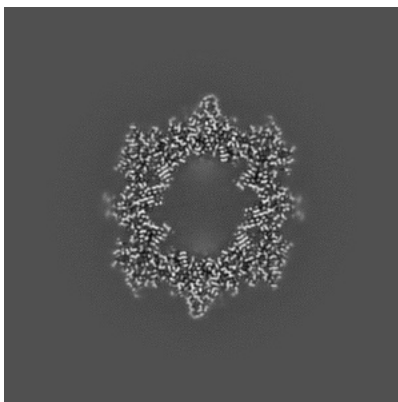


Z Index: 145

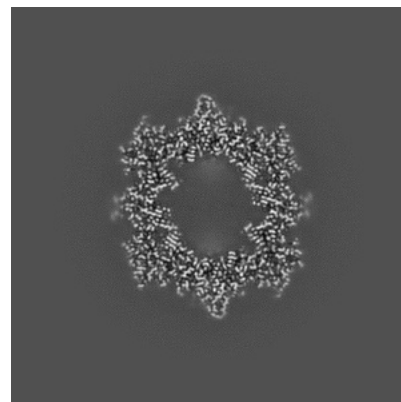
6.3.2 Raw map



X Index: 145



Y Index: 145

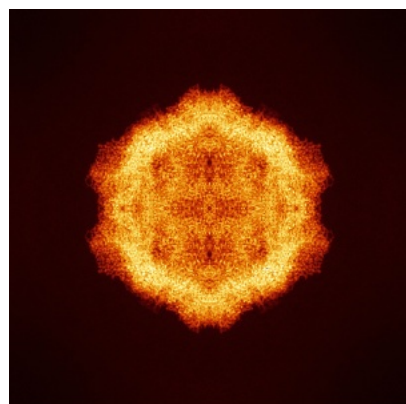


Z Index: 274

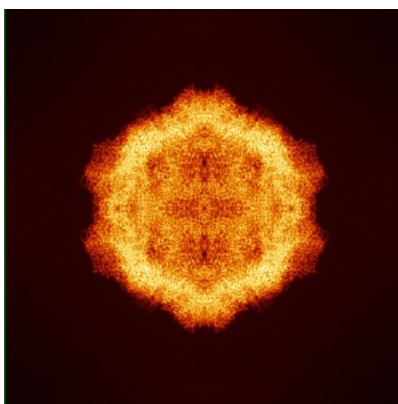
The images above show the largest variance slices of the map in three orthogonal directions.

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

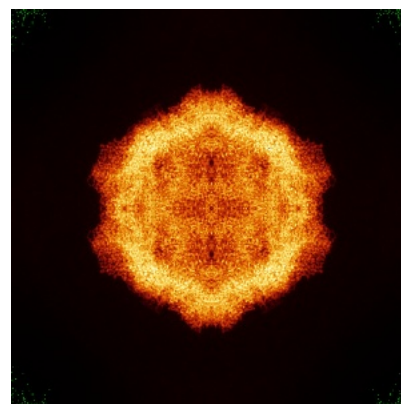
6.4.1 Primary map



X

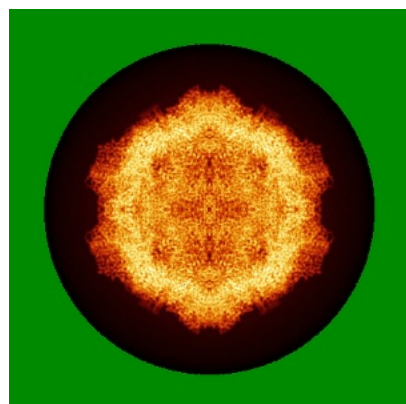


Y

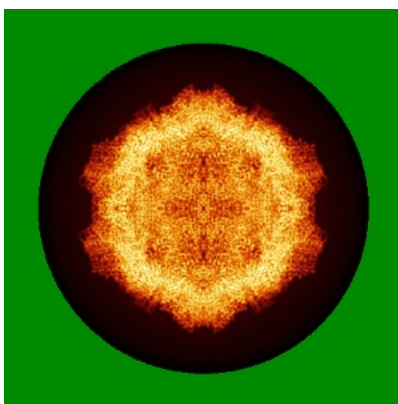


Z

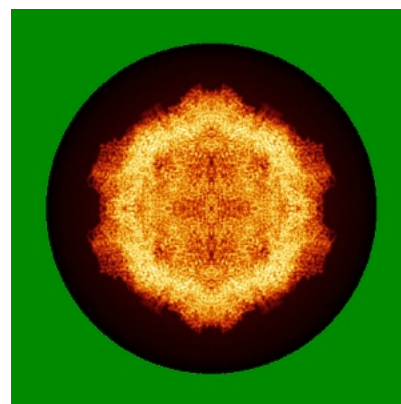
6.4.2 Raw map



X



Y

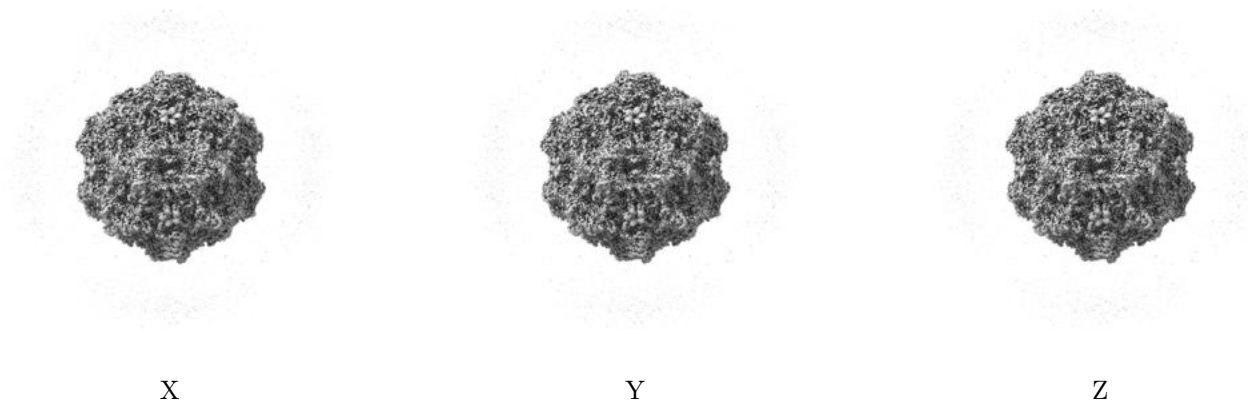


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

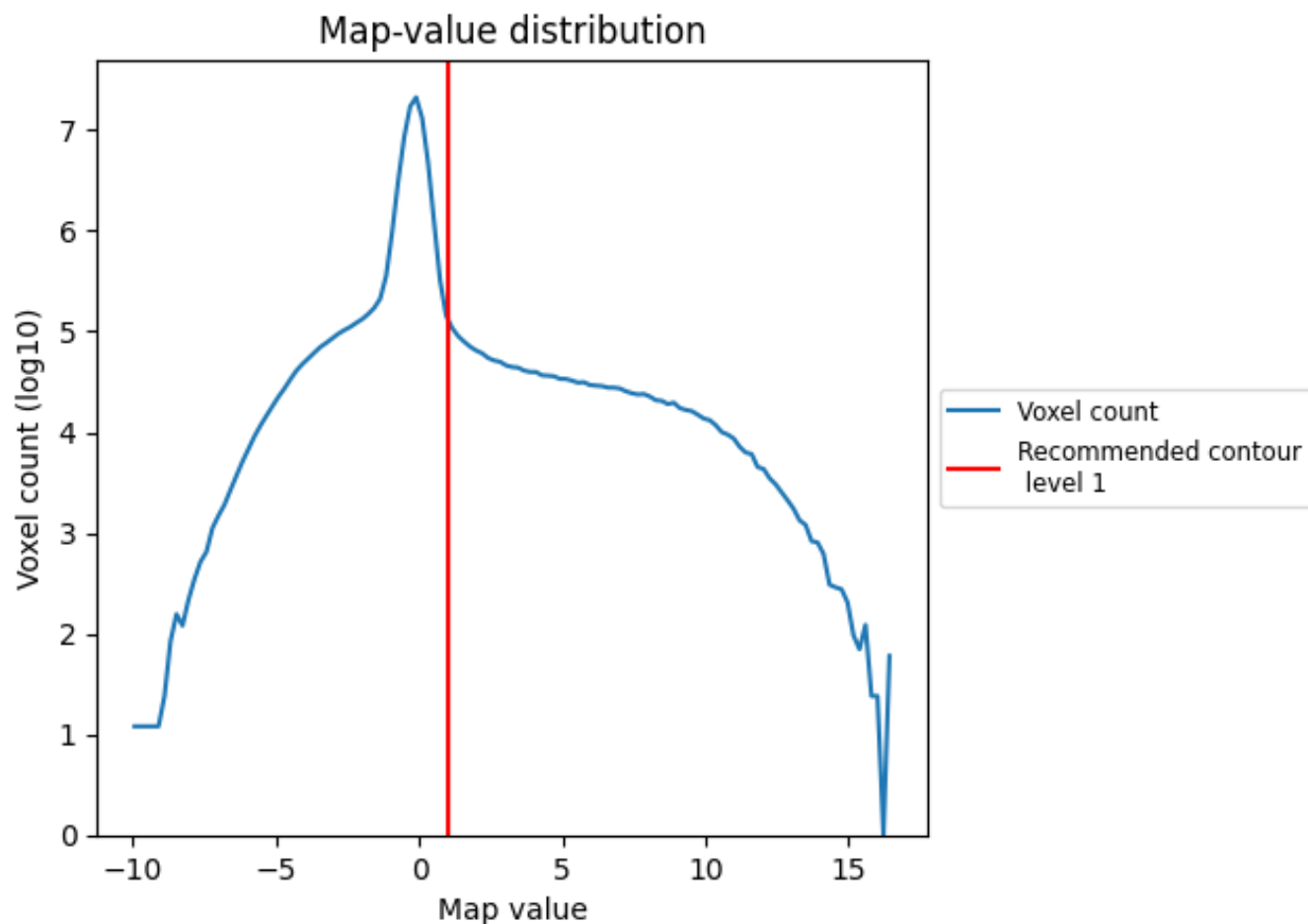
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

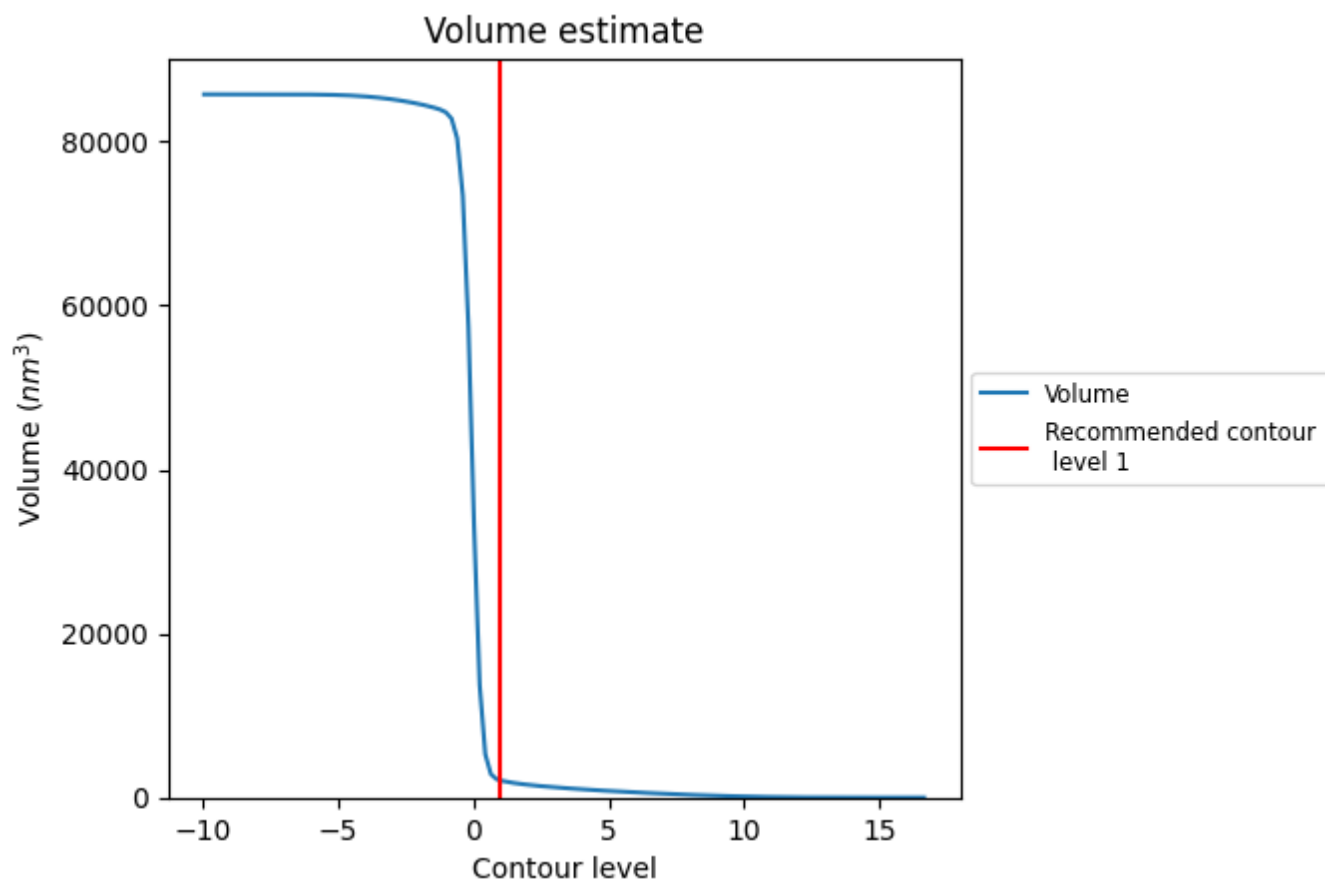
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

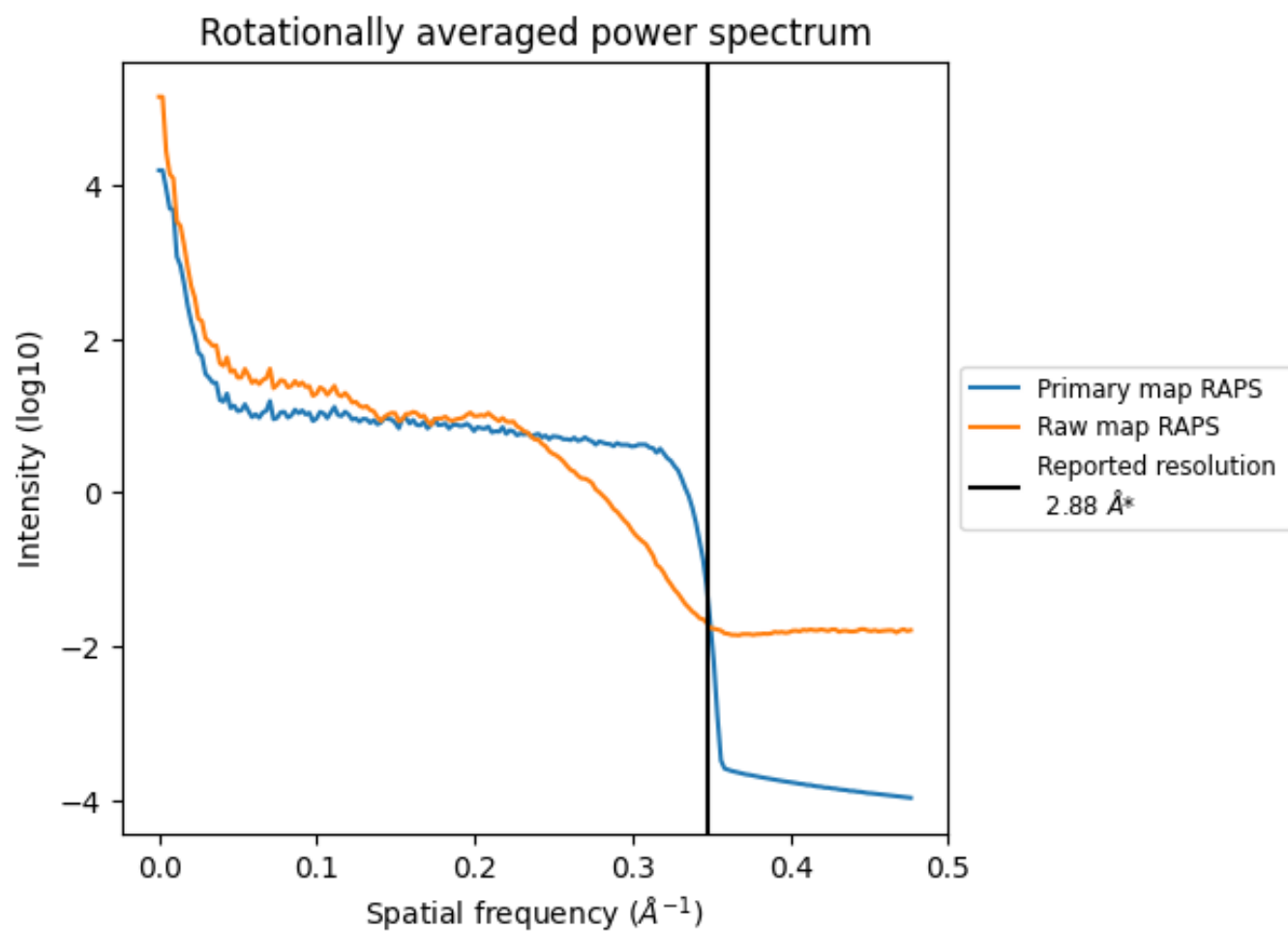
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2107 nm³; this corresponds to an approximate mass of 1903 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 ⓘ

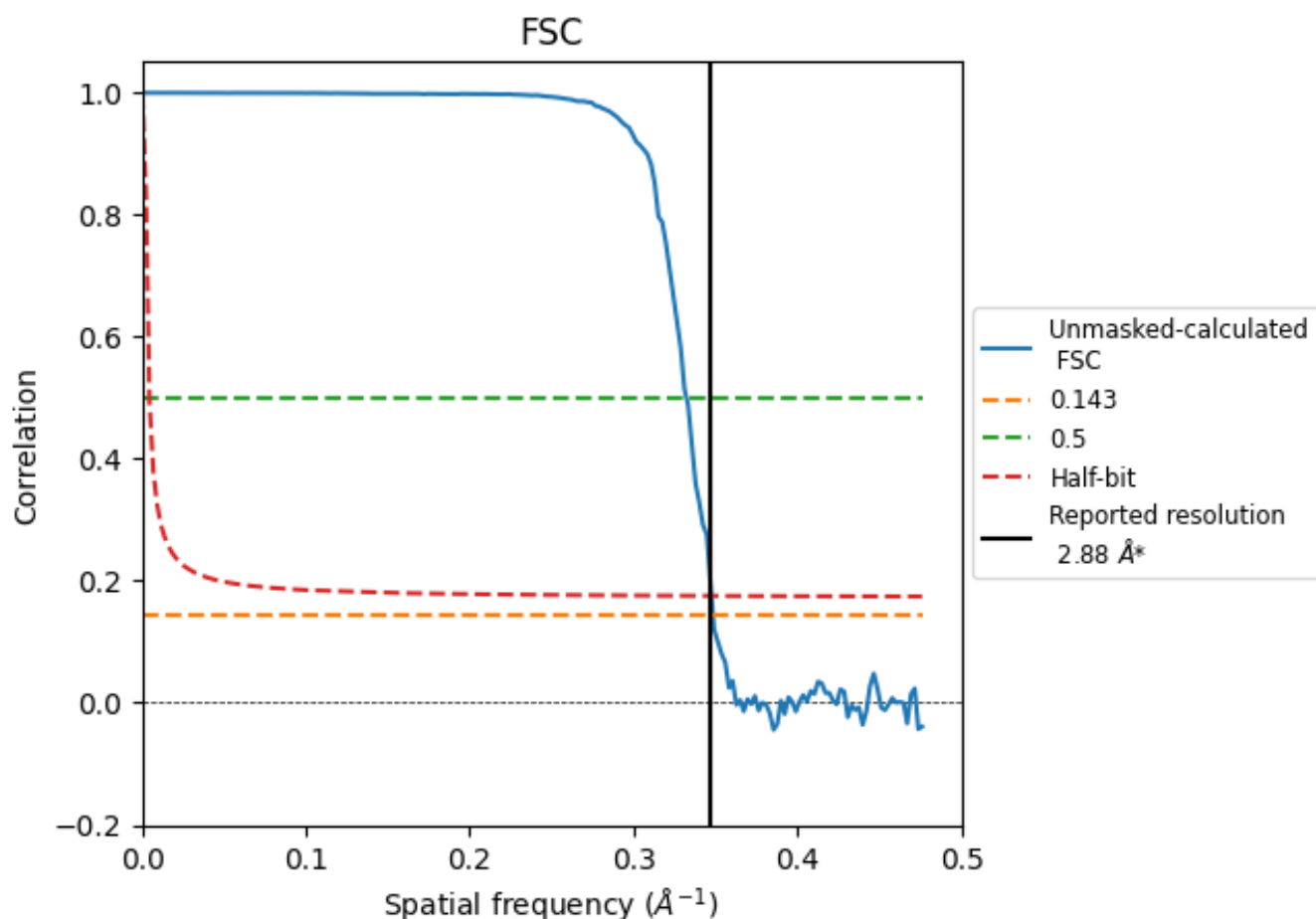


*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

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 0.347 \AA^{-1}

8.2 Resolution estimates [i](#)

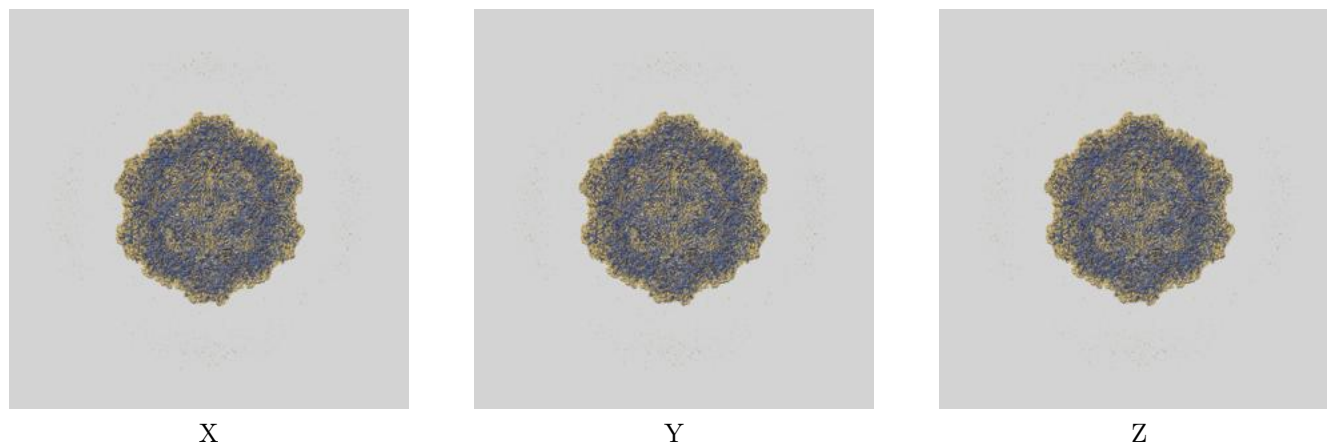
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.87	3.01	2.88

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

9 Map-model fit [i](#)

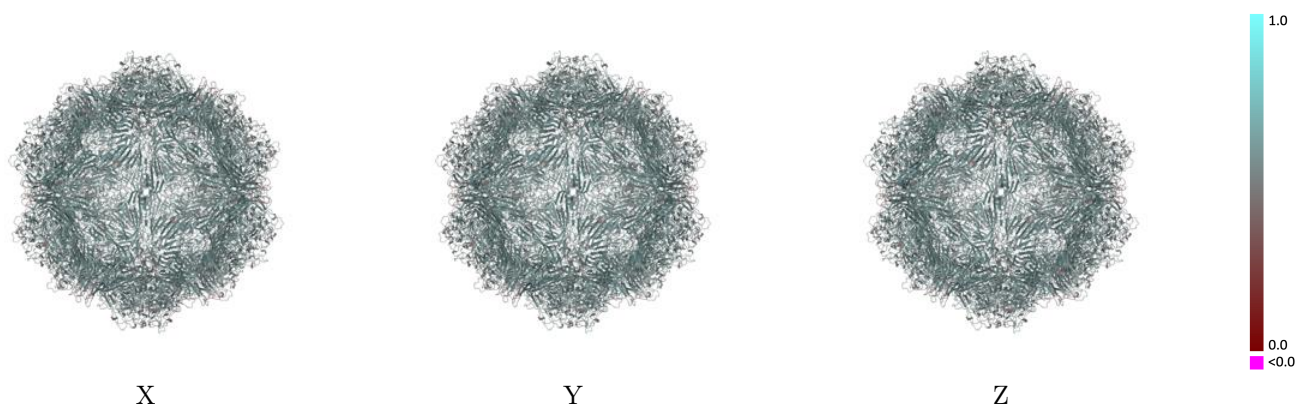
This section contains information regarding the fit between EMDB map EMD-49195 and PDB model 9NAI. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



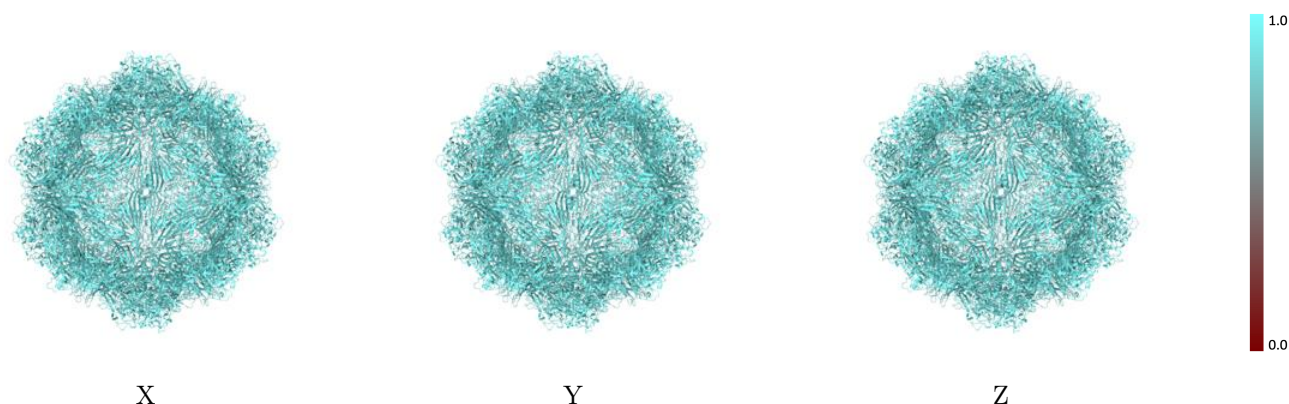
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



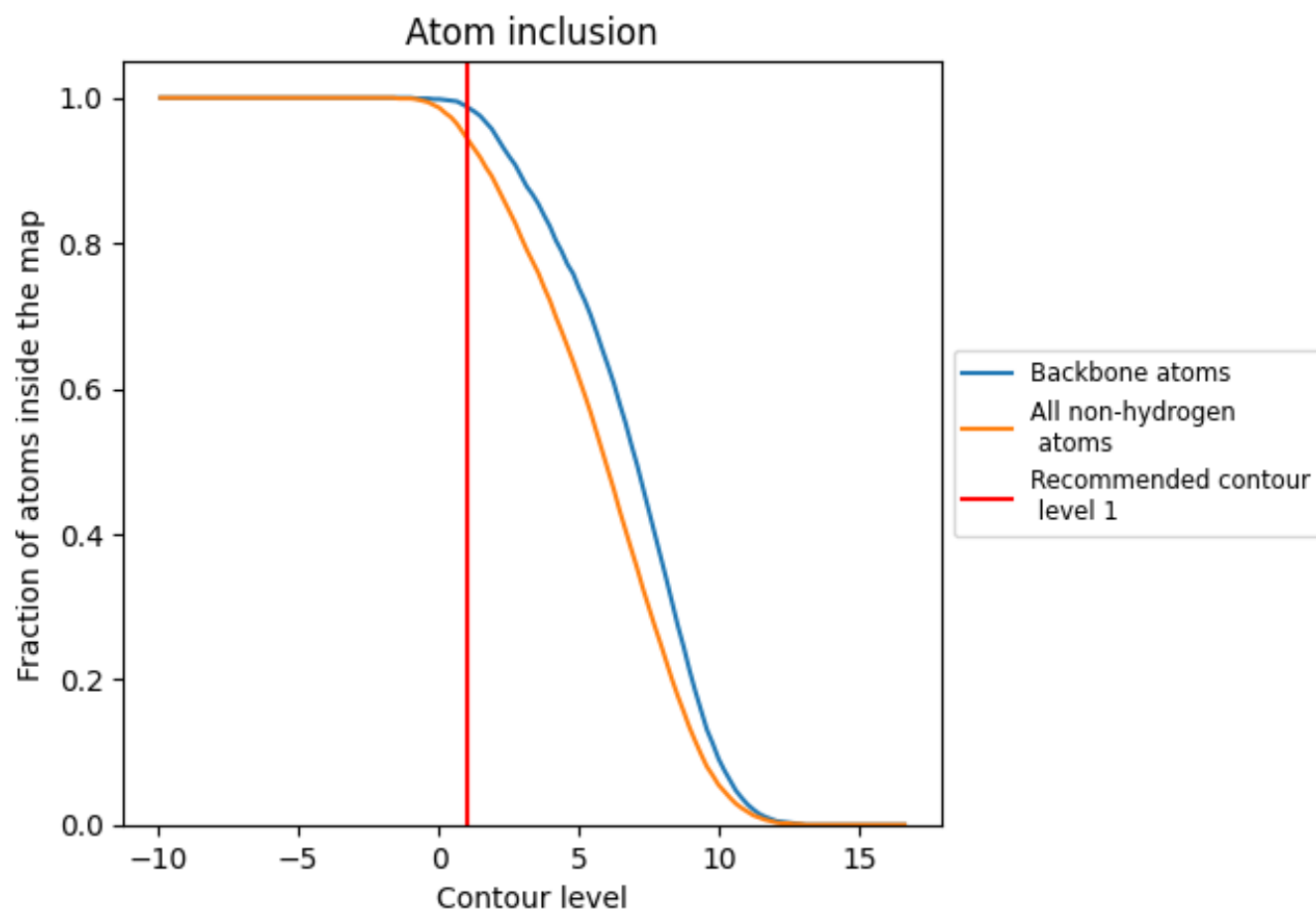
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.5570
0	 0.0870	 0.1470
0A	 0.0870	 0.1220
1	 0.9570	 0.5590
1B	 0.0870	 0.1420
2	 0.9570	 0.5600
3	 0.9540	 0.5610
3A	 0.0870	 0.1290
4	 0.9530	 0.5620
4B	 0.0870	 0.1220
5	 0.9540	 0.5580
6	 0.9540	 0.5590
6A	 0.0870	 0.1310
7	 0.9540	 0.5600
7B	 0.0870	 0.1340
8	 0.9530	 0.5620
9A	 0.0870	 0.1260
A	 0.9540	 0.5610
AC	 0.0870	 0.1270
B	 0.9570	 0.5600
BA	 0.0870	 0.1330
C	 0.9530	 0.5620
CB	 0.0870	 0.1400
D	 0.9540	 0.5640
DC	 0.0870	 0.1150
E	 0.9530	 0.5660
EA	 0.0870	 0.1320
F	 0.9540	 0.5630
FB	 0.0870	 0.1300
G	 0.9530	 0.5610
GC	 0.0870	 0.1230
H	 0.9540	 0.5590
HA	 0.0870	 0.1270
I	 0.9530	 0.5600
IB	 0.0870	 0.1290























































































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Chain	Atom inclusion	Q-score
J	 0.9570	 0.5590
JC	 0.0870	 0.1310
K	 0.9530	 0.5610
KA	 0.0870	 0.1290
L	 0.9570	 0.5610
LB	 0.0870	 0.1330
M	 0.9530	 0.5630
MC	 0.0870	 0.1250
N	 0.9540	 0.5660
NA	 0.0870	 0.1440
O	 0.9530	 0.5670
OB	 0.0870	 0.1420
P	 0.9540	 0.5660
PC	 0.0870	 0.1400
Q	 0.9530	 0.5660
QA	 0.0870	 0.1380
R	 0.9570	 0.5650
RB	 0.0870	 0.1380
S	 0.9570	 0.5670
SC	 0.0870	 0.1180
T	 0.9530	 0.5670
TA	 0.0870	 0.1260
U	 0.9570	 0.5660
UB	 0.0870	 0.1430
V	 0.9530	 0.5630
VC	 0.0870	 0.1210
W	 0.9540	 0.5620
WA	 0.0870	 0.1260
X	 0.9530	 0.5630
XB	 0.0870	 0.1390
Y	 0.9540	 0.5620
YC	 0.0870	 0.1410
Z	 0.9530	 0.5620
ZA	 0.0870	 0.1320
a	 0.9540	 0.5600
aB	 0.0870	 0.1480
b	 0.9530	 0.5630
bC	 0.0870	 0.1260
c	 0.9530	 0.5620
cA	 0.0870	 0.1250
d	 0.9540	 0.5670
dB	 0.0870	 0.1370

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Chain	Atom inclusion	Q-score
e	 0.9530	 0.5650
eC	 0.0870	 0.1230
f	 0.9530	 0.5640
fA	 0.0870	 0.1340
g	 0.9530	 0.5610
gB	 0.0870	 0.1130
h	 0.9530	 0.5630
hC	 0.0870	 0.1250
i	 0.9540	 0.5630
iA	 0.0870	 0.1260
j	 0.9540	 0.5610
jB	 0.0870	 0.1160
k	 0.9540	 0.5600
kC	 0.0870	 0.1380
l	 0.9530	 0.5650
lA	 0.0870	 0.1280
m	 0.9530	 0.5650
mB	 0.0870	 0.1300
n	 0.9540	 0.5630
nC	 0.0870	 0.1150
o	 0.9530	 0.5610
oA	 0.0870	 0.1310
p	 0.9530	 0.5600
pB	 0.0870	 0.1200
q	 0.9570	 0.5590
qC	 0.0870	 0.1210
r	 0.9570	 0.5600
rA	 0.0870	 0.1340
s	 0.9570	 0.5620
sB	 0.0870	 0.1290
t	 0.9530	 0.5570
tC	 0.0870	 0.1300
u	 0.9530	 0.5580
uA	 0.0870	 0.1310
v	 0.9540	 0.5570
vB	 0.0870	 0.1320
w	 0.9530	 0.5590
wC	 0.0870	 0.1280
x	 0.9530	 0.5580
xA	 0.0870	 0.1380
y	 0.9540	 0.5570
yB	 0.0870	 0.1230

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Chain	Atom inclusion	Q-score
z	 0.9570	 0.5600
zC	 0.0870	 0.1240