



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:54 PM UTC

PDB ID : 9NAJ / pdb_00009naj
EMDB ID : EMD-49196
Title : LuIII VLP - Glycan [3's(LN)3]
Authors : Busuttil, K.B.; Bennett, A.B.
Deposited on : 2025-02-12
Resolution : 2.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

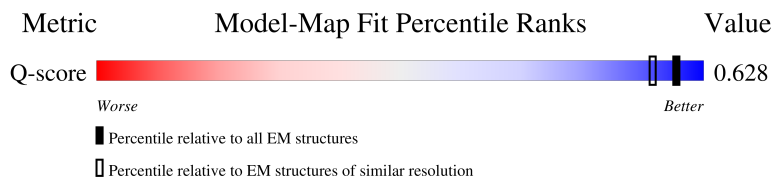
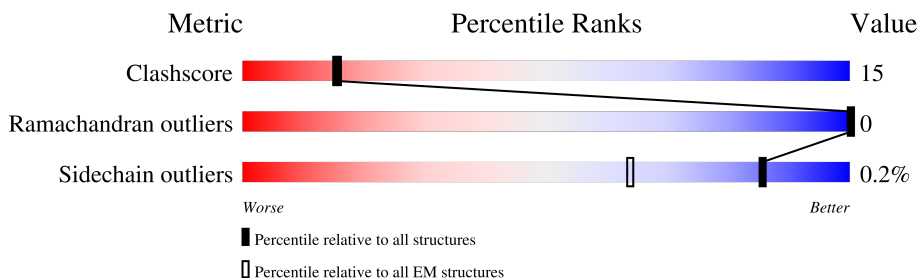
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.66 Å.

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



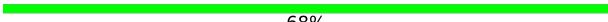
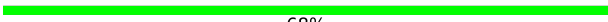
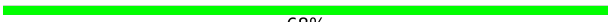
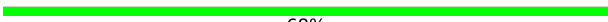
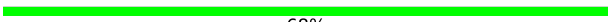
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9119 (2.16 - 3.16)

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	 68% 32%
1	2	551	 68% 32%
1	3	551	 69% 31%
1	4	551	 68% 32%

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Mol	Chain	Length	Quality of chain	
1	5	551		32%
1	6	551		32%
1	7	551		32%
1	8	551		32%
1	A	551		31%
1	B	551		32%
1	C	551		32%
1	D	551		32%
1	E	551		32%
1	F	551		32%
1	G	551		32%
1	H	551		31%
1	I	551		31%
1	J	551		32%
1	K	551		32%
1	L	551		32%
1	M	551		31%
1	N	551		32%
1	O	551		33%
1	P	551		33%
1	Q	551		31%
1	R	551		32%
1	S	551		32%
1	T	551		32%
1	U	551		32%

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Mol	Chain	Length	Quality of chain	
1	V	551		68% 32%
1	W	551		68% 32%
1	X	551		69% 31%
1	Y	551		68% 32%
1	Z	551		67% 33%
1	a	551		69% 31%
1	b	551		68% 32%
1	c	551		68% 32%
1	d	551		68% 32%
1	e	551		68% 32%
1	f	551		68% 32%
1	g	551		68% 32%
1	h	551		69% 31%
1	i	551		68% 32%
1	j	551		68% 32%
1	k	551		67% 32%
1	l	551		68% 32%
1	m	551		68% 32%
1	n	551		68% 32%
1	o	551		68% 32%
1	p	551		68% 32%
1	q	551		68% 32%
1	r	551		68% 32%
1	s	551		68% 32%
1	t	551		68% 32%

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Mol	Chain	Length	Quality of chain		
1	u	551			
1	v	551			
1	w	551			
1	x	551			
1	y	551			
1	z	551			
2	0	3			
2	0A	3			
2	1B	3			
2	3A	3			
2	4B	3			
2	6A	3			
2	7B	3			
2	9A	3			
2	AC	3			
2	BA	3			
2	CB	3			
2	DC	3			
2	EA	3			
2	FB	3			
2	GC	3			
2	HA	3			
2	IB	3			
2	JC	3			
2	KA	3			

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Mol	Chain	Length	Quality of chain
2	LB	3	
2	MC	3	
2	NA	3	
2	OB	3	
2	PC	3	
2	QA	3	
2	RB	3	
2	SC	3	
2	TA	3	
2	UB	3	
2	VC	3	
2	WA	3	
2	XB	3	
2	YC	3	
2	ZA	3	
2	aB	3	
2	bC	3	
2	cA	3	
2	dB	3	
2	eC	3	
2	fA	3	
2	gB	3	
2	hC	3	
2	iA	3	
2	jB	3	

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Mol	Chain	Length	Quality of chain
2	kC	3	
2	lA	3	
2	mB	3	
2	nC	3	
2	oA	3	
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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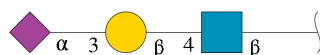
Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	n	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	o	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	p	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	q	551	Total 4401	C 2767	N 773	O 846	S 15	1	0
1	r	551	Total 4401	C 2767	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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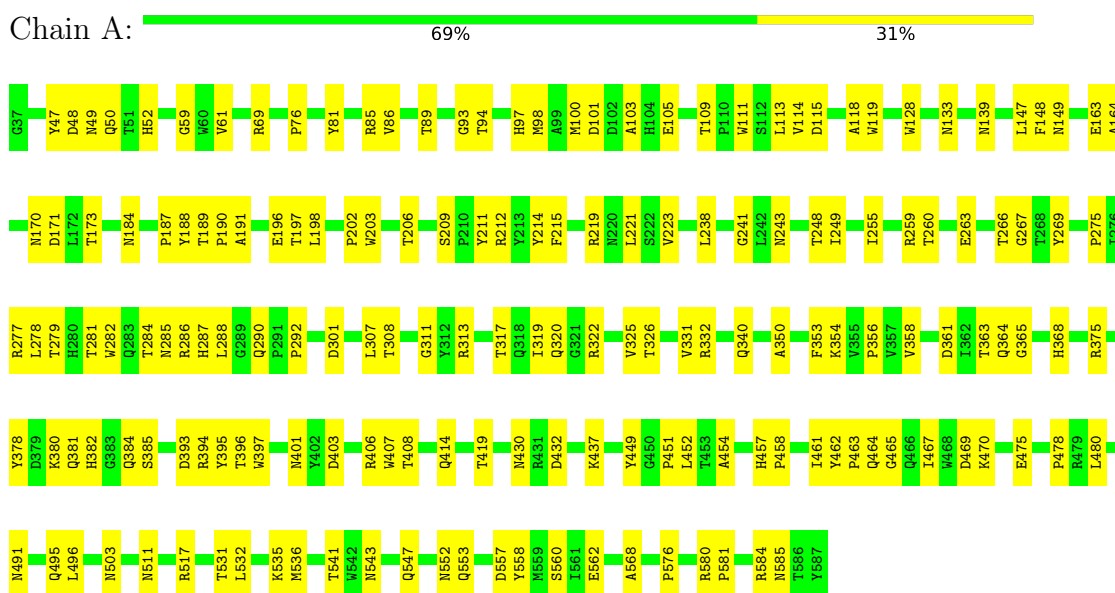
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Mol	Chain	Residues	Atoms				AltConf	Trace
2	wC	3	Total	C	N	O	0	0
			46	25	2	19		
2	zC	3	Total	C	N	O	0	0
			46	25	2	19		

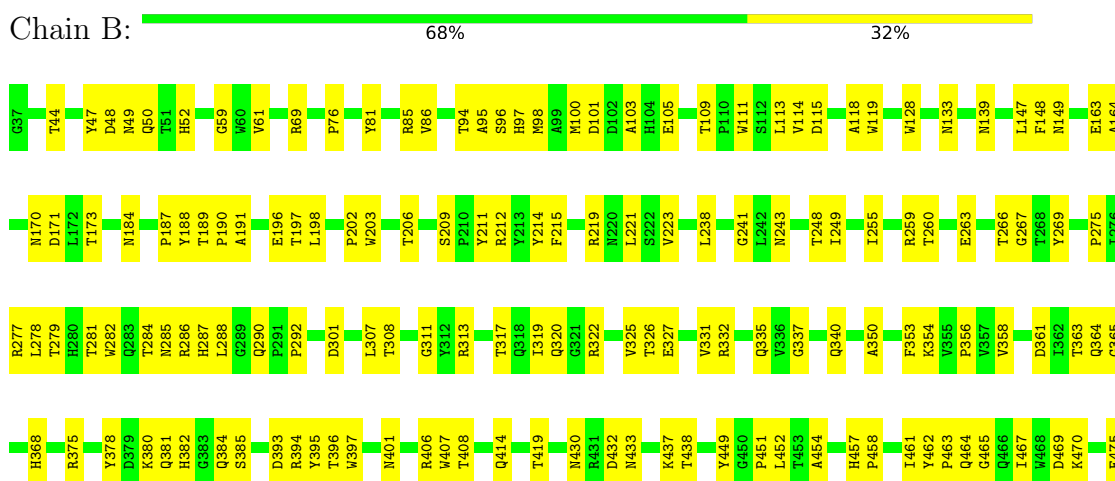
3 Residue-property plots

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

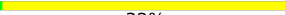


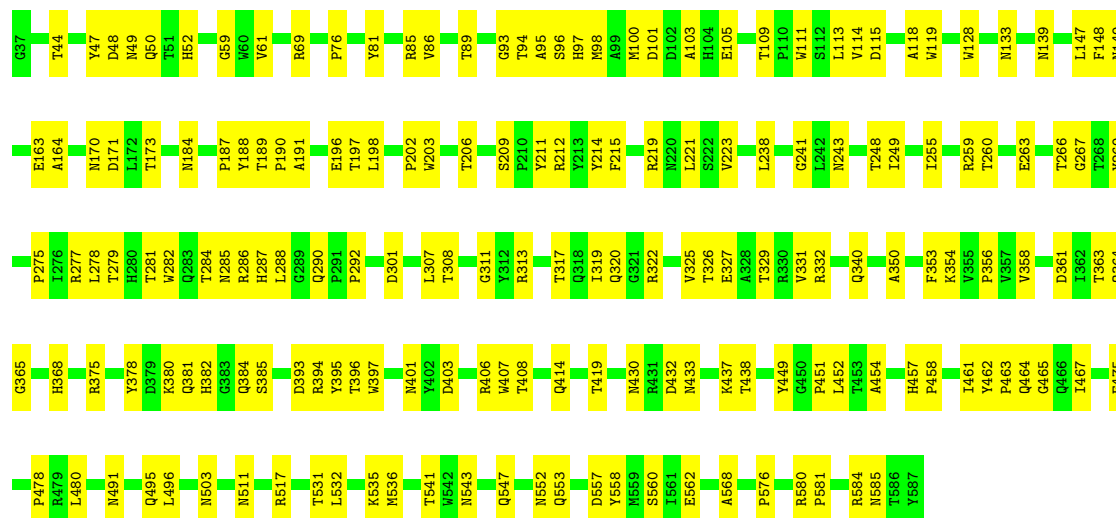
- Molecule 1: Capsid protein VP1





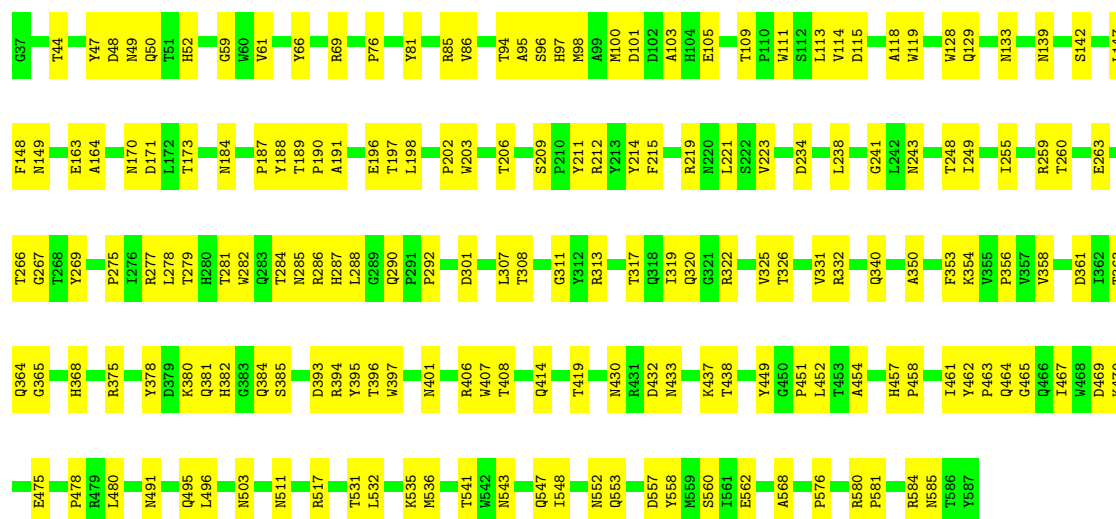
• Molecule 1: Capsid protein VP1

Chain C:  68%  32%



• Molecule 1: Capsid protein VP1

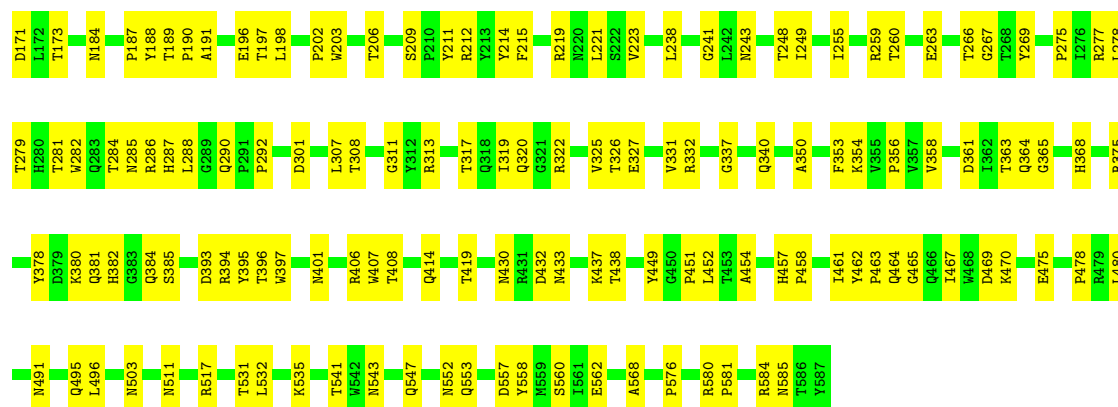
Chain D:  68%  32%



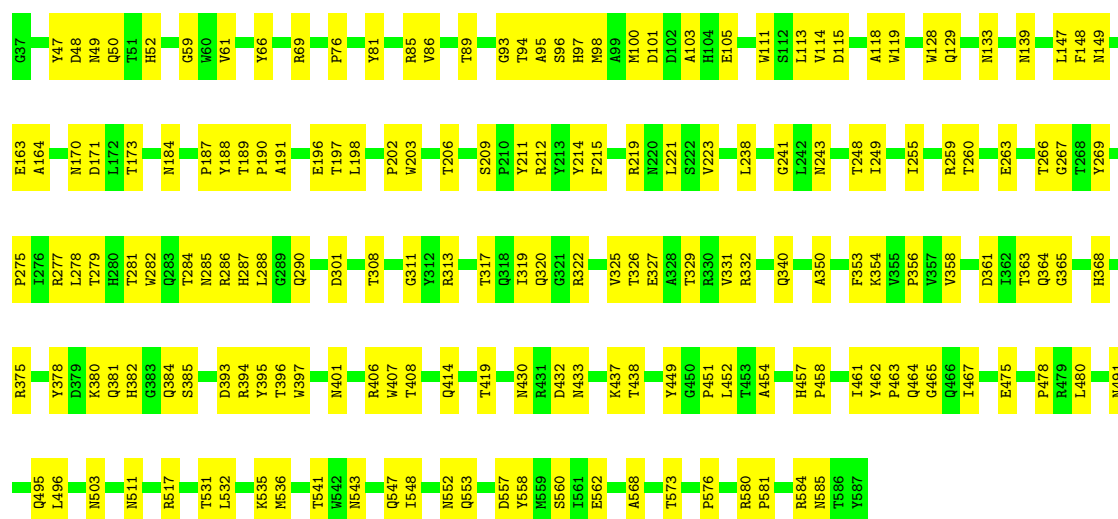
• Molecule 1: Capsid protein VP1

Chain E:  68%  32%

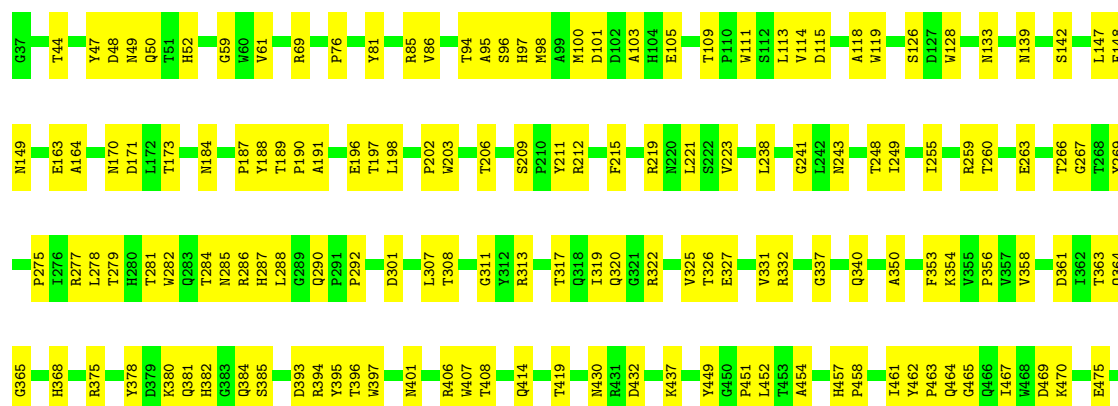


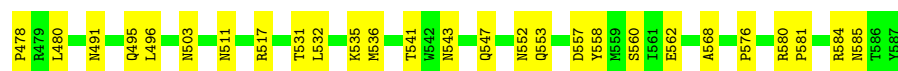


• Molecule 1: Capsid protein VP1

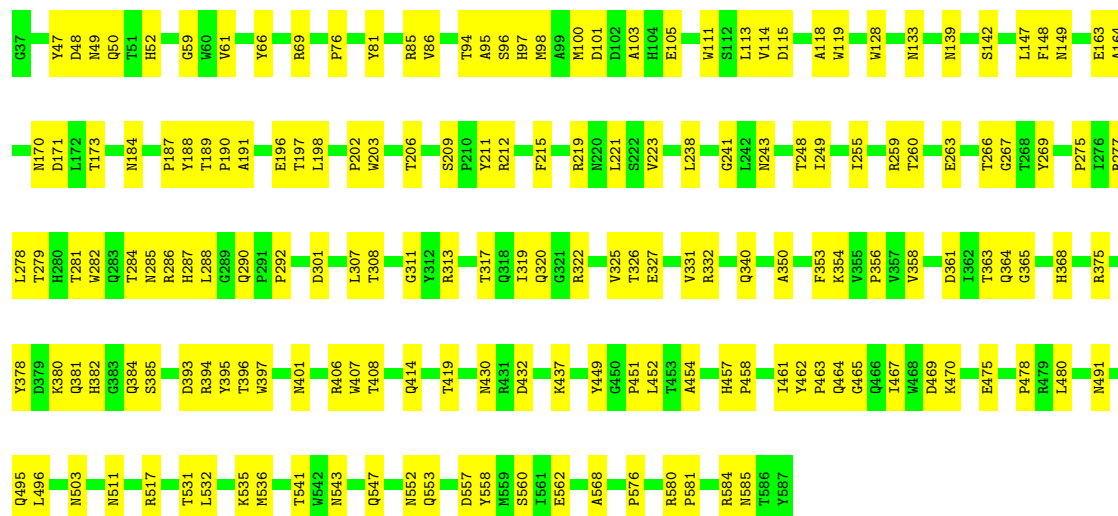


• Molecule 1: Capsid protein VP1

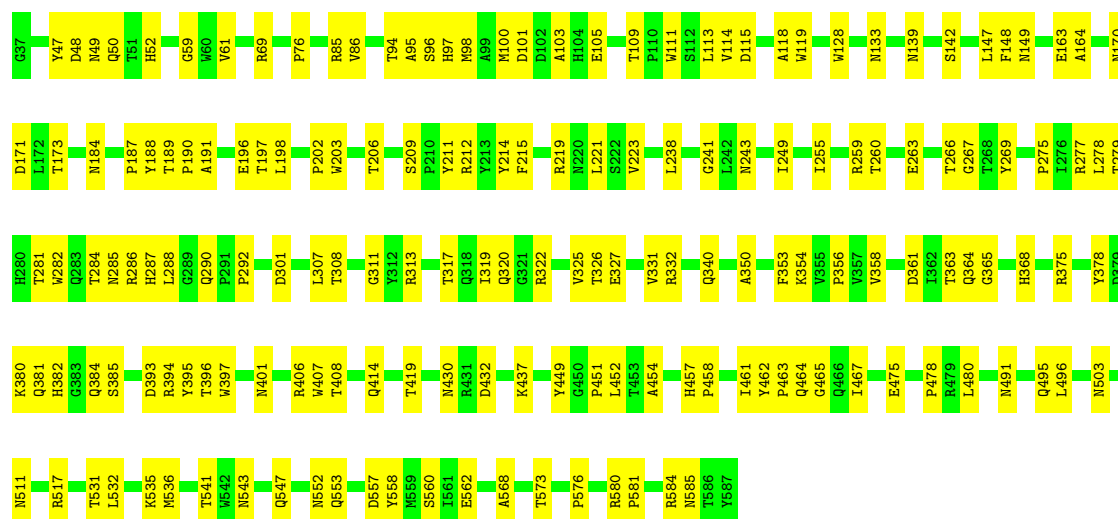




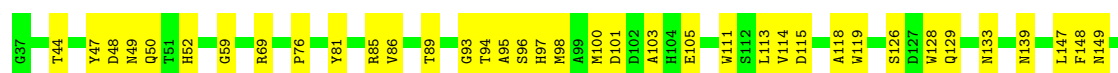
• Molecule 1: Capsid protein VP1

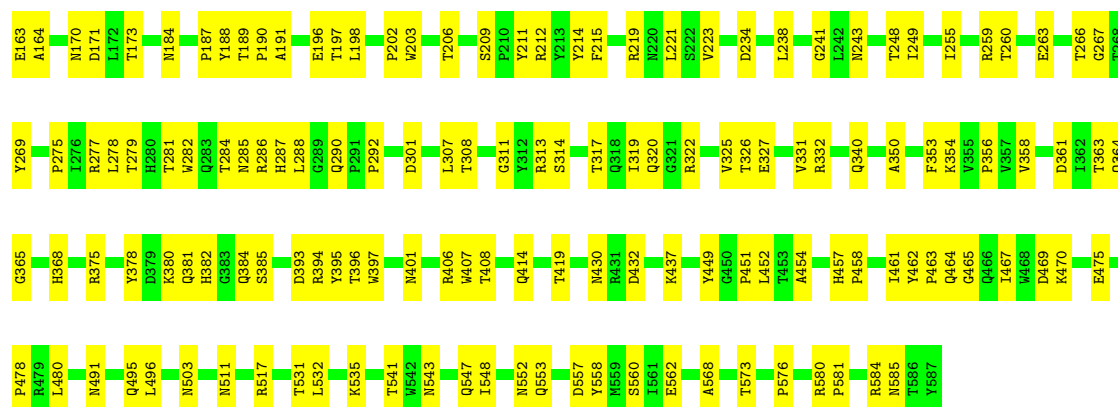


• Molecule 1: Capsid protein VP1



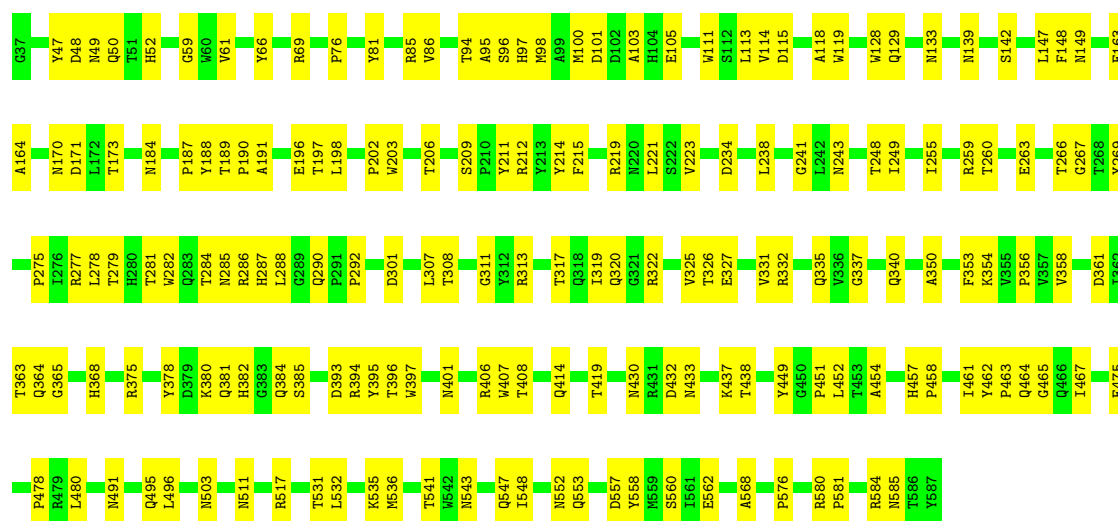
• Molecule 1: Capsid protein VP1





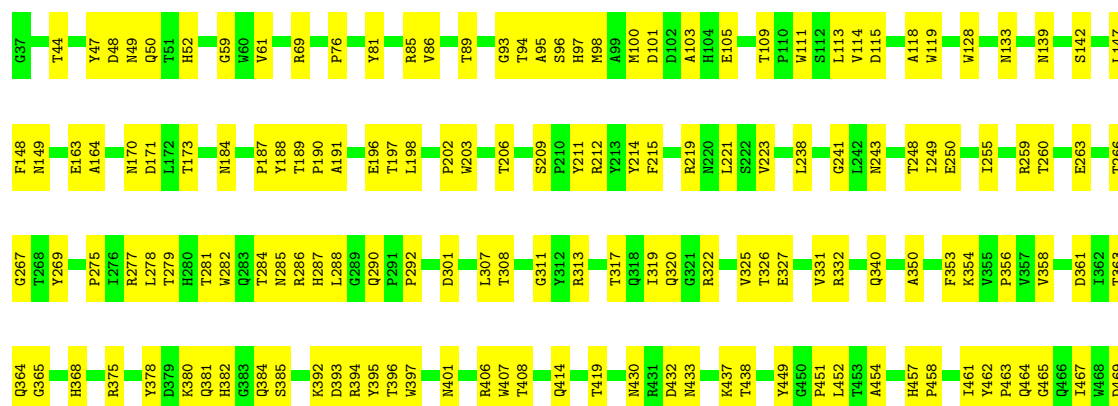
● Molecule 1: Capsid protein VP1

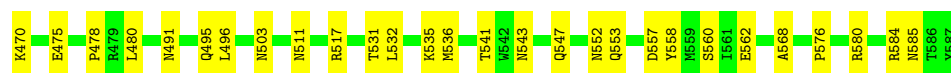
Chain K: 68% 32%



● Molecule 1: Capsid protein VP1

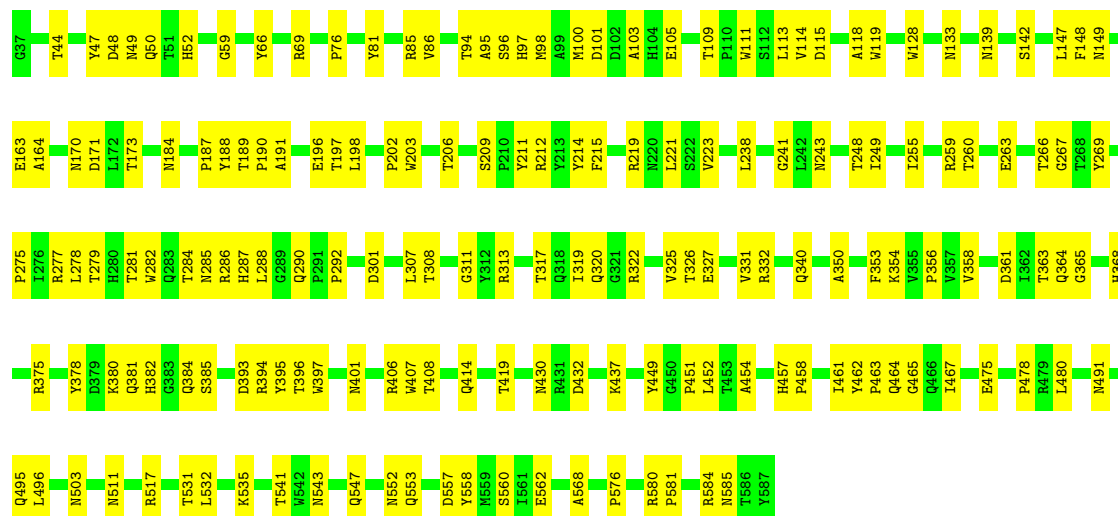
Chain L: 68% 32%





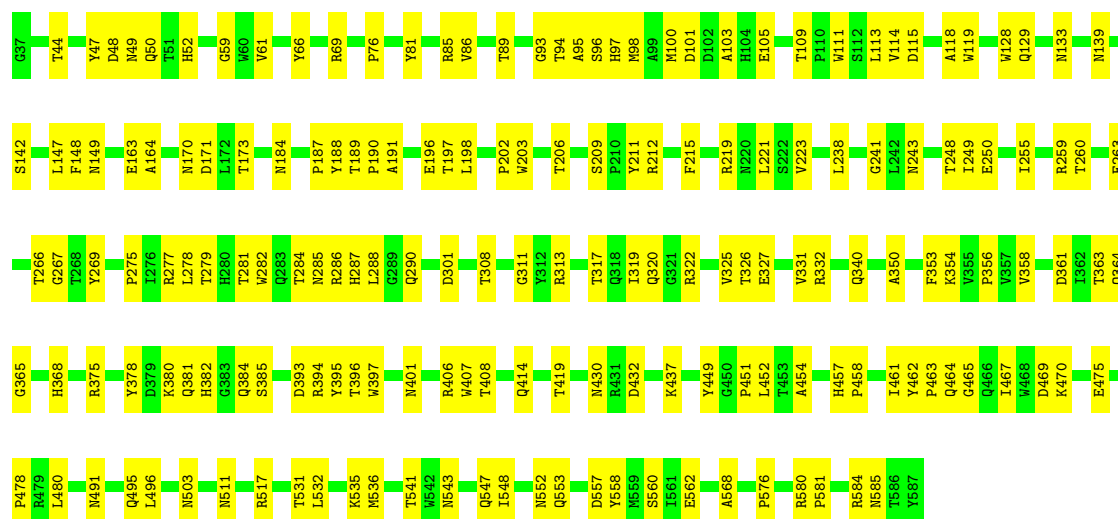
• Molecule 1: Capsid protein VP1

Chain M: 69% 31%



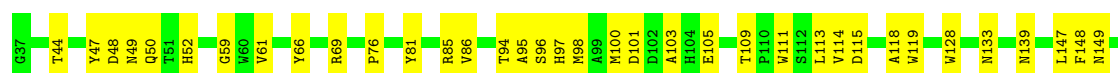
• Molecule 1: Capsid protein VP1

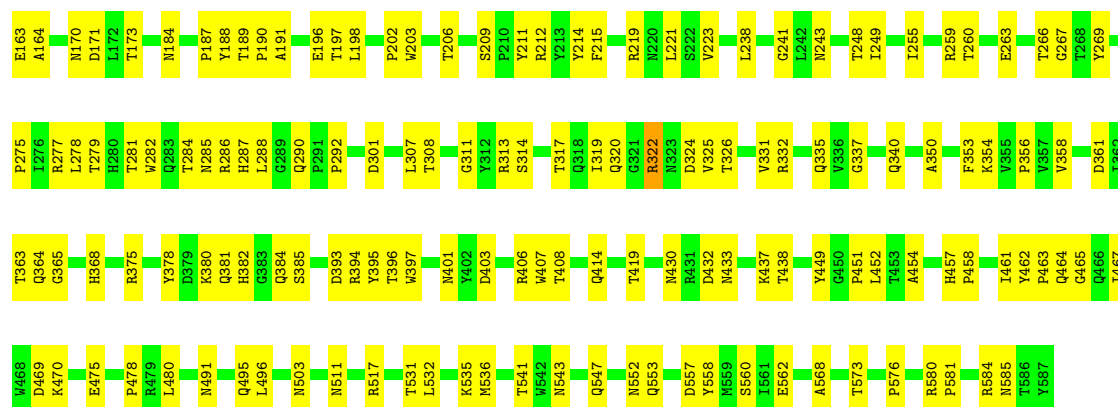
Chain N: 68% 32%



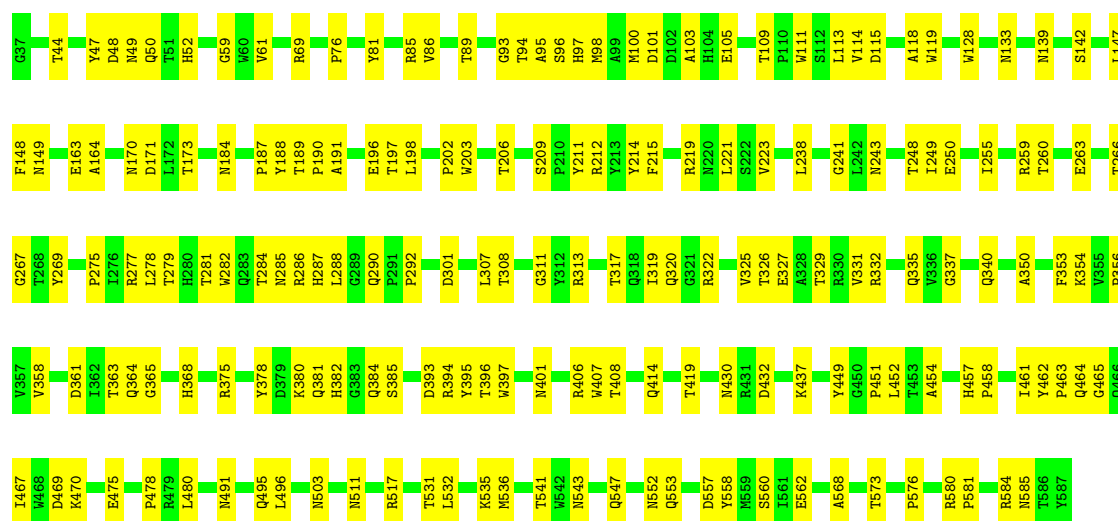
• Molecule 1: Capsid protein VP1

Chain O: 67% 33%

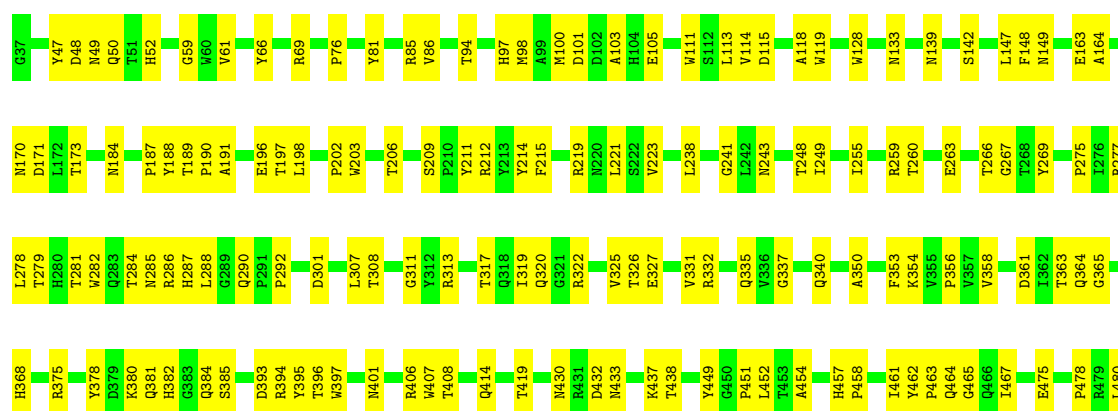




• Molecule 1: Capsid protein VP1



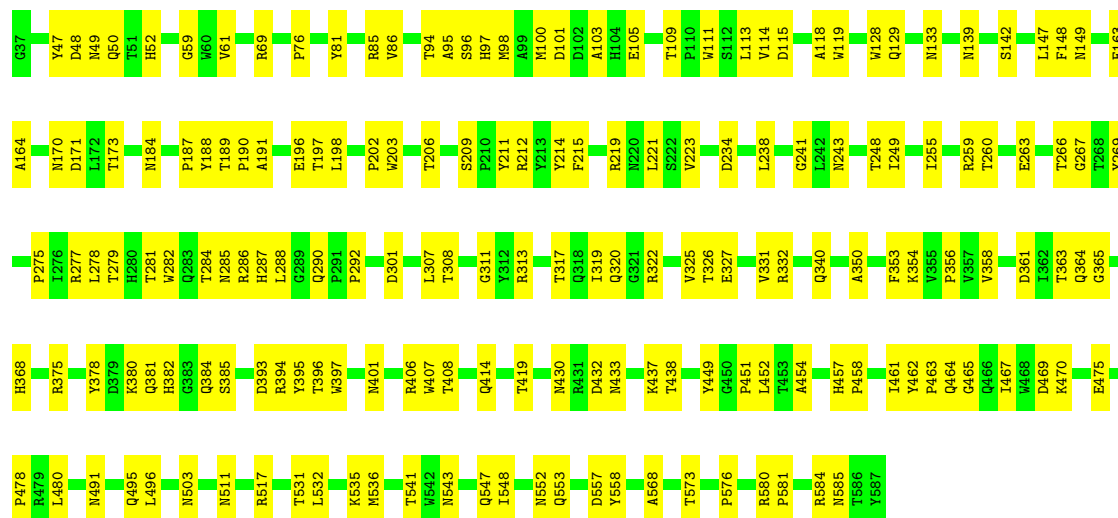
• Molecule 1: Capsid protein VP1





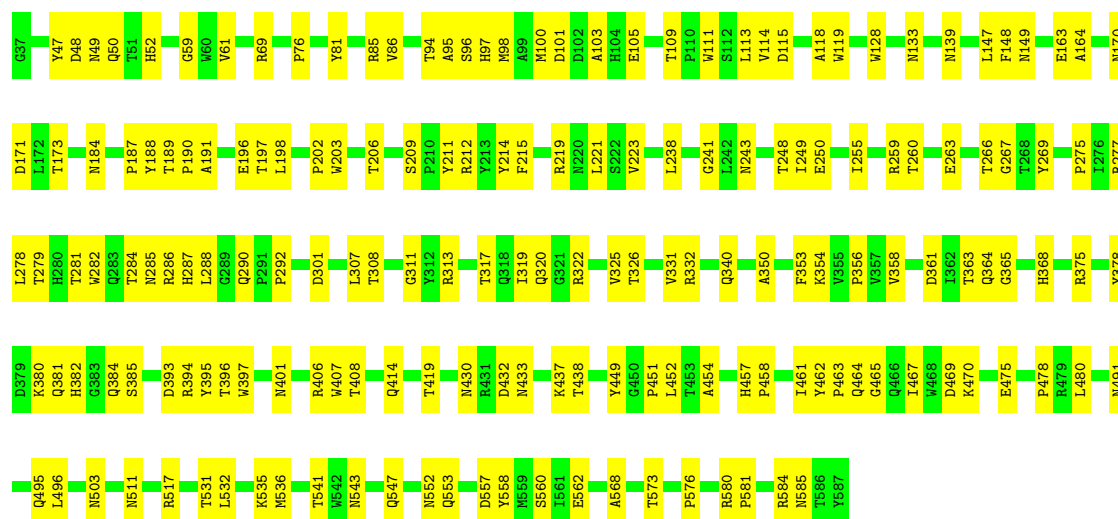
• Molecule 1: Capsid protein VP1

Chain R: 68% 32%



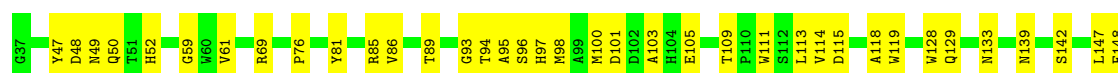
• Molecule 1: Capsid protein VP1

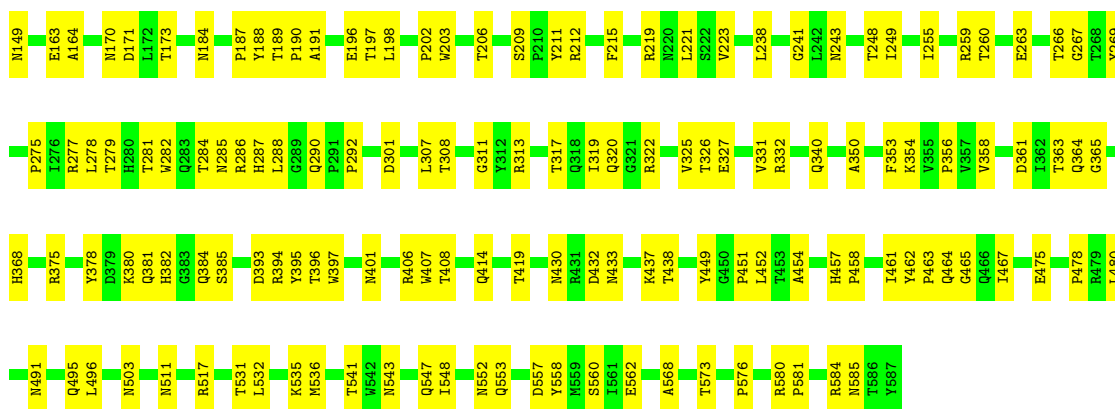
Chain S: 68% 32%



• Molecule 1: Capsid protein VP1

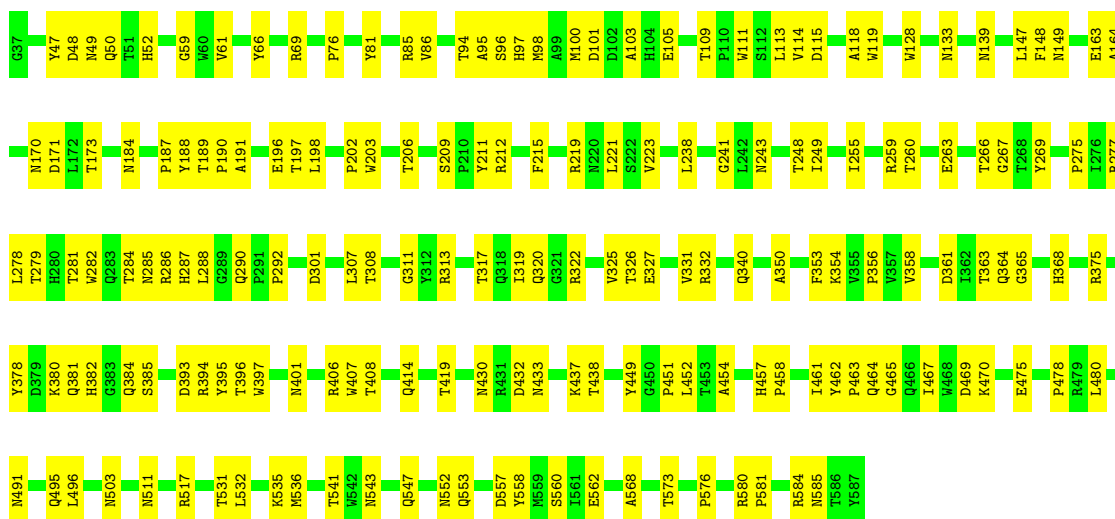
Chain T: 68% 32%





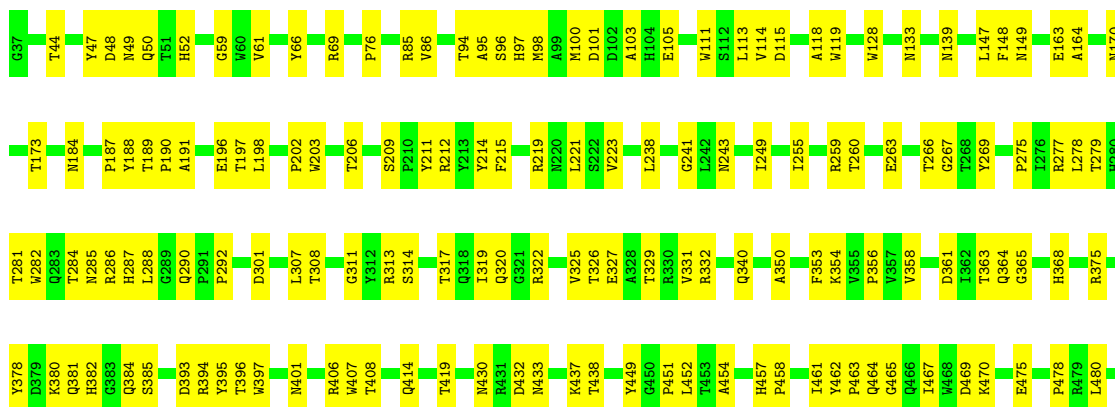
• Molecule 1: Capsid protein VP1

Chain U: 68% 32%



• Molecule 1: Capsid protein VP1

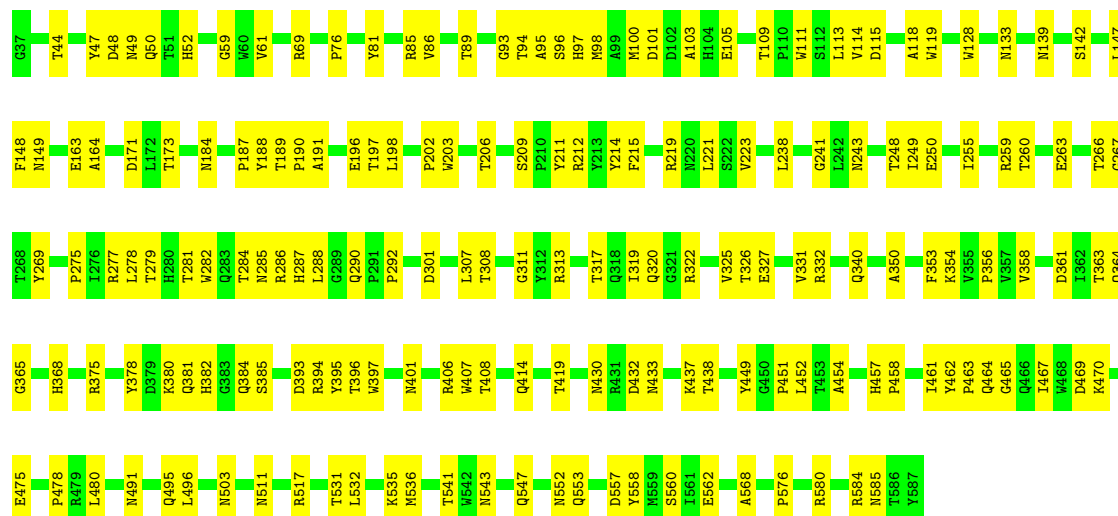
Chain V: 68% 32%





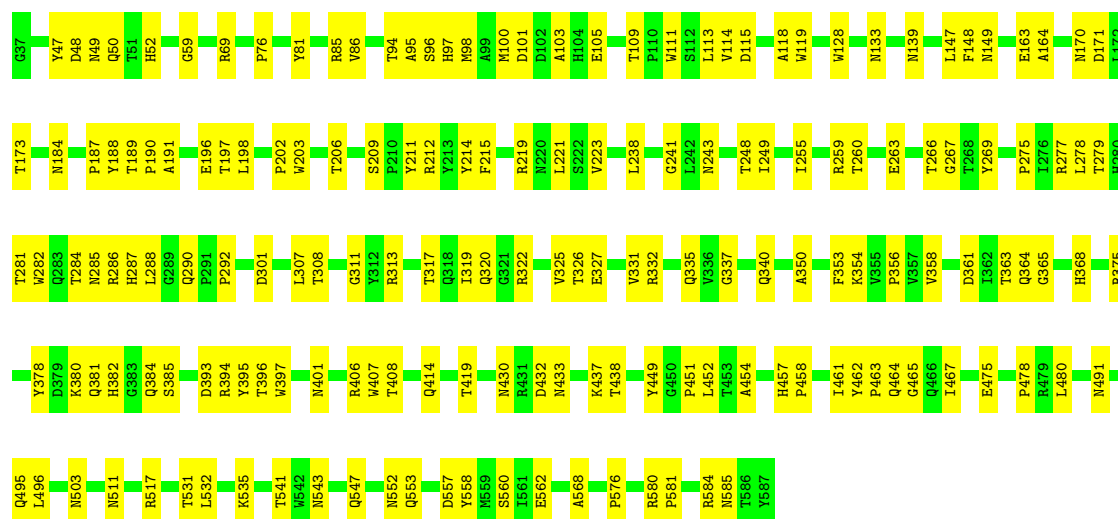
• Molecule 1: Capsid protein VP1

Chain W: 68% 32%



• Molecule 1: Capsid protein VP1

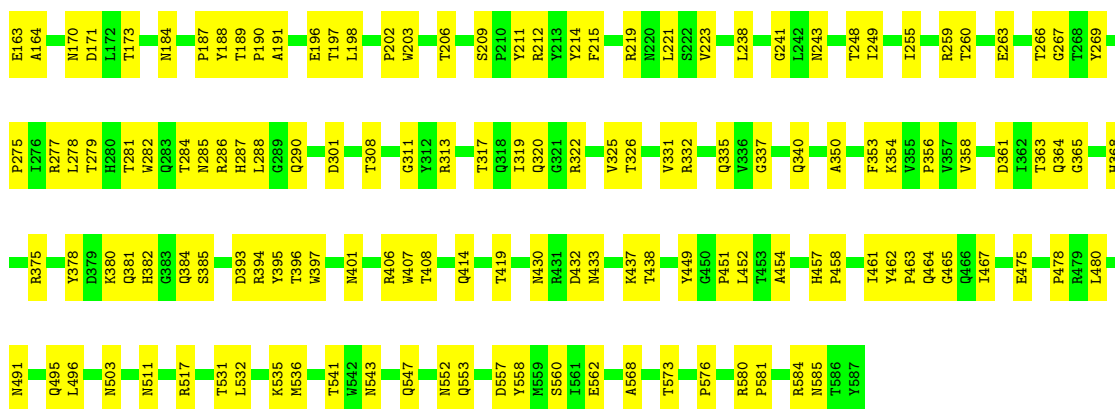
Chain X: 69% 31%



• Molecule 1: Capsid protein VP1

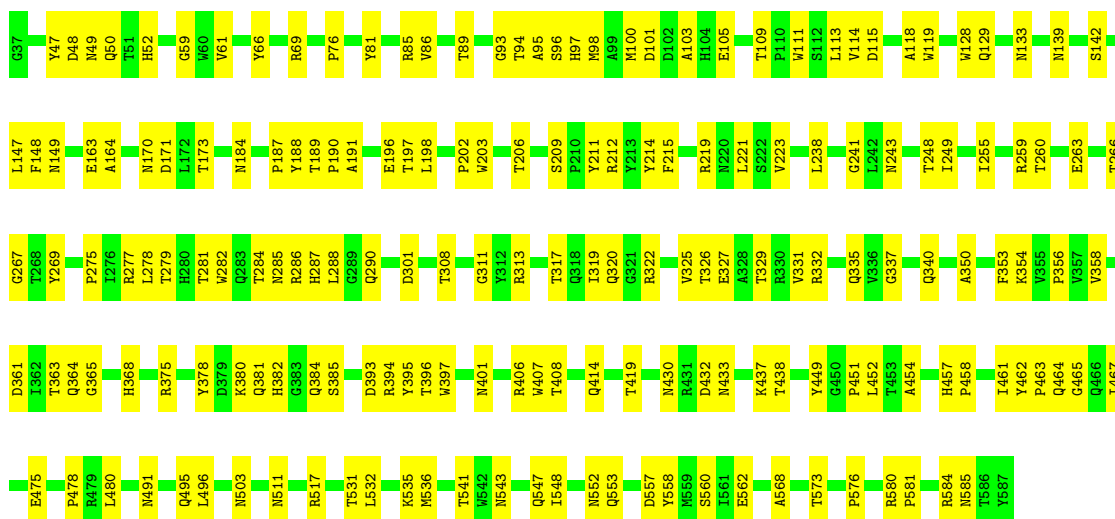
Chain Y: 68% 32%





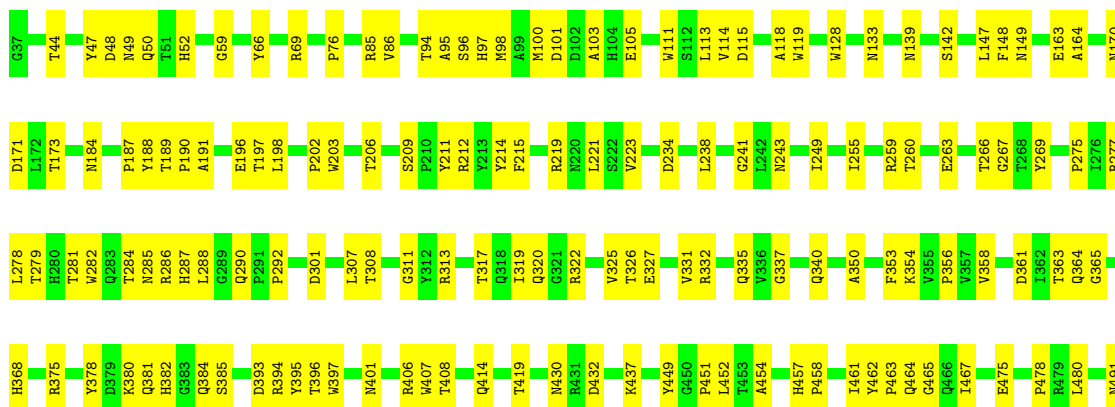
• Molecule 1: Capsid protein VP1

Chain Z: 67% 33%



• Molecule 1: Capsid protein VP1

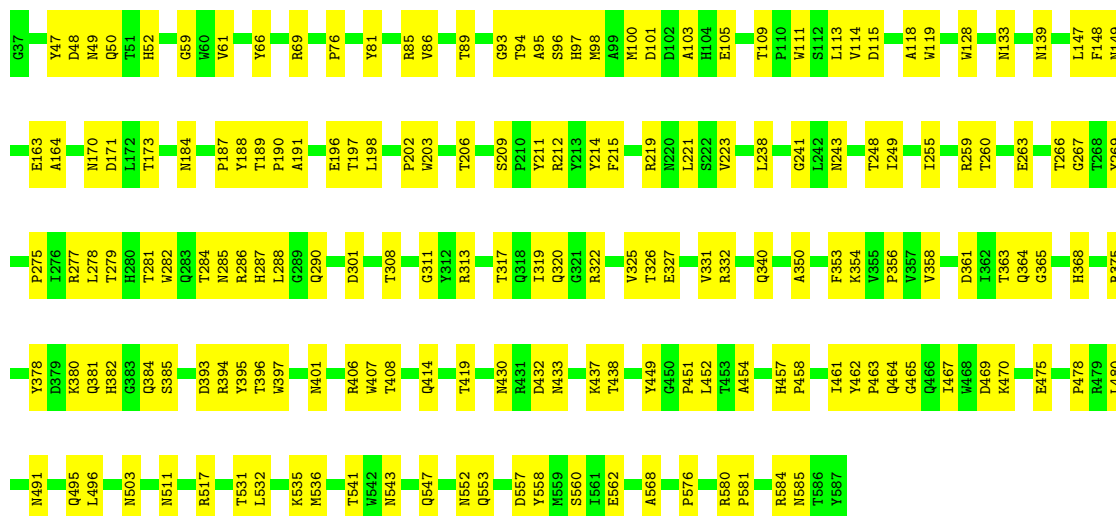
Chain a: 69% 31%





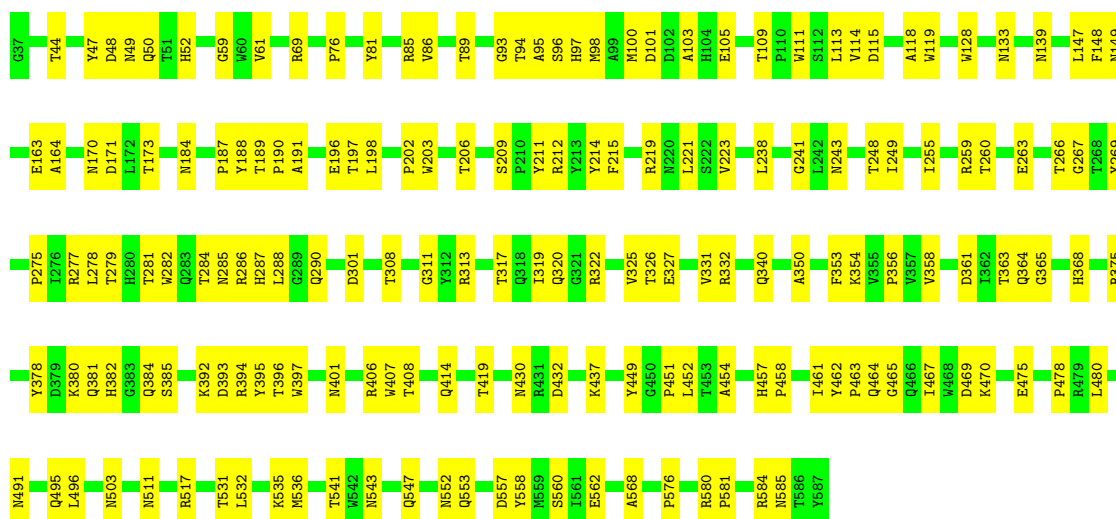
• Molecule 1: Capsid protein VP1

Chain b: 68% 32%



• Molecule 1: Capsid protein VP1

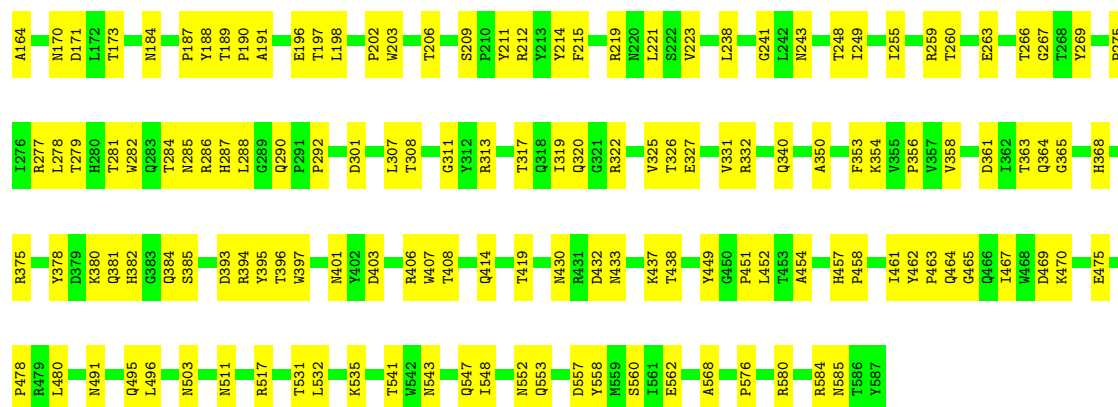
Chain c: 68% 32%



• Molecule 1: Capsid protein VP1

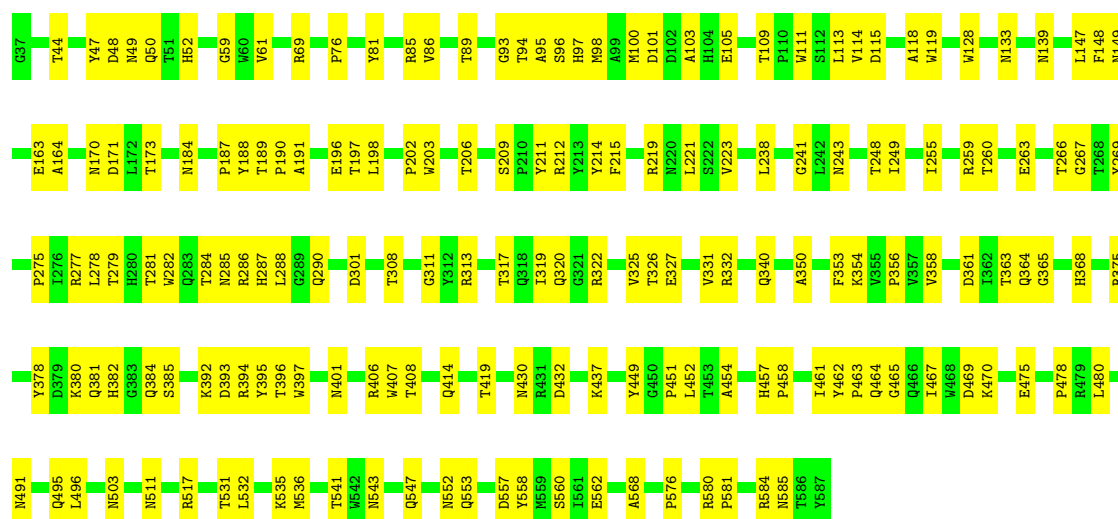
Chain d: 68% 32%





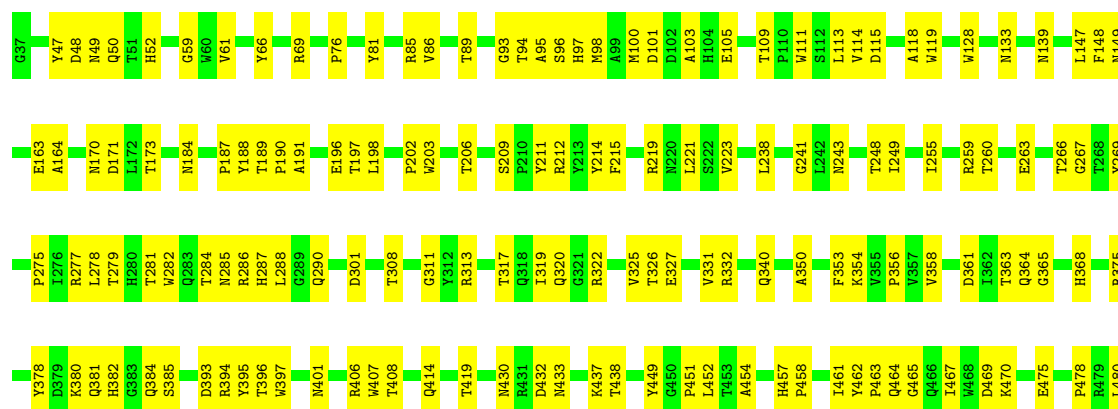
• Molecule 1: Capsid protein VP1

Chain e: 68% 32%



• Molecule 1: Capsid protein VP1

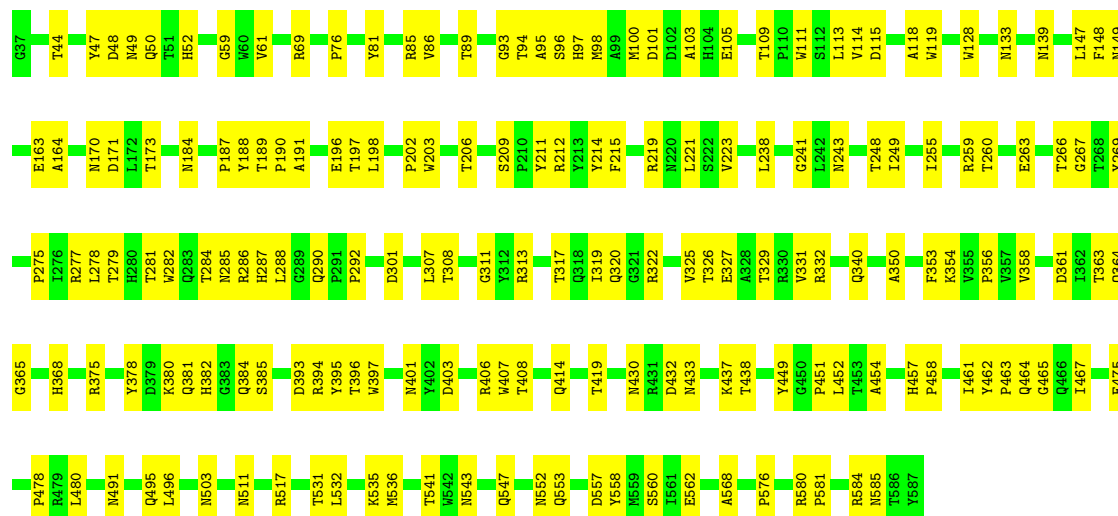
Chain f: 68% 32%





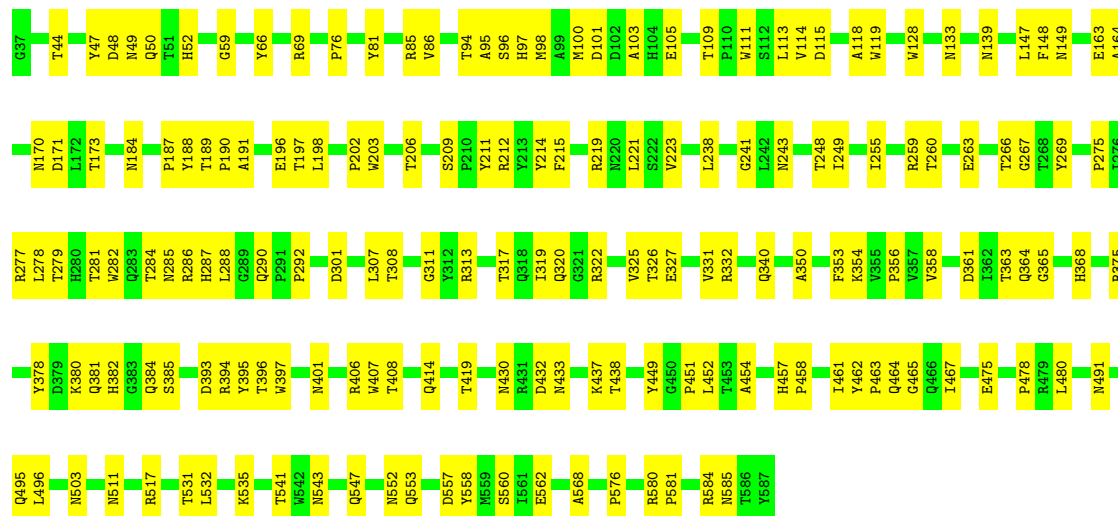
• Molecule 1: Capsid protein VP1

Chain g: 68% 32%



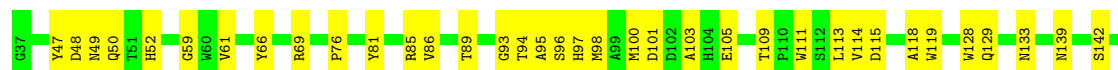
• Molecule 1: Capsid protein VP1

Chain h: 69% 31%



• Molecule 1: Capsid protein VP1

Chain i: 68% 32%

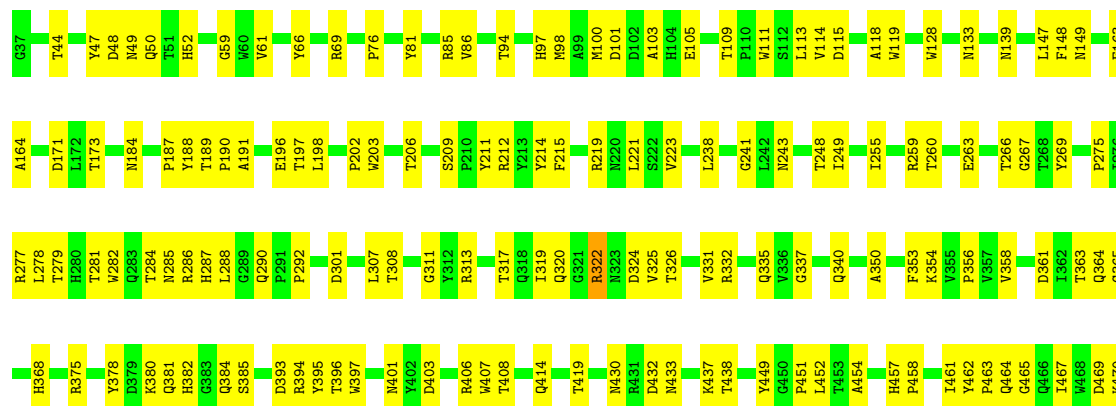






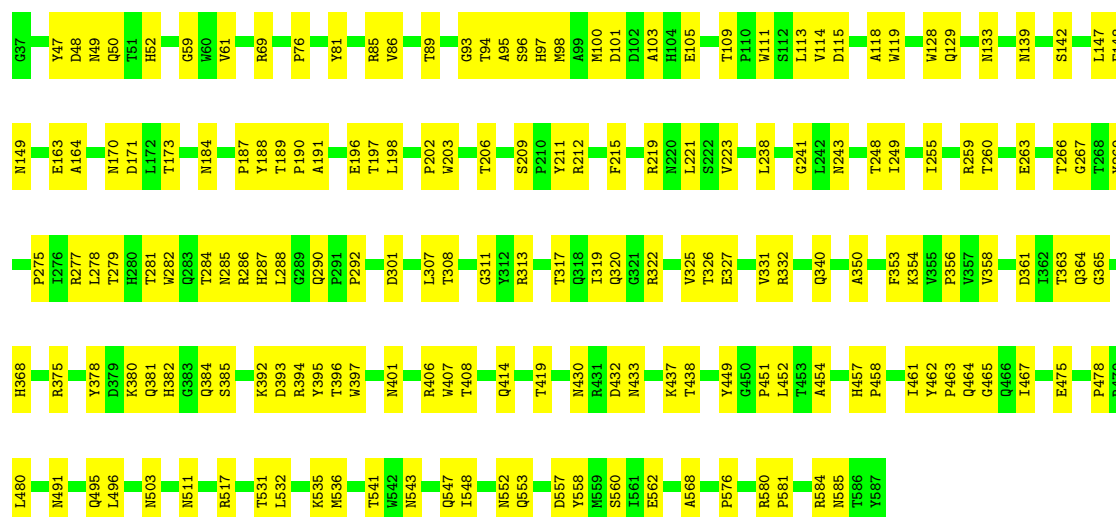
• Molecule 1: Capsid protein VP1

Chain l: 68% 32%



• Molecule 1: Capsid protein VP1

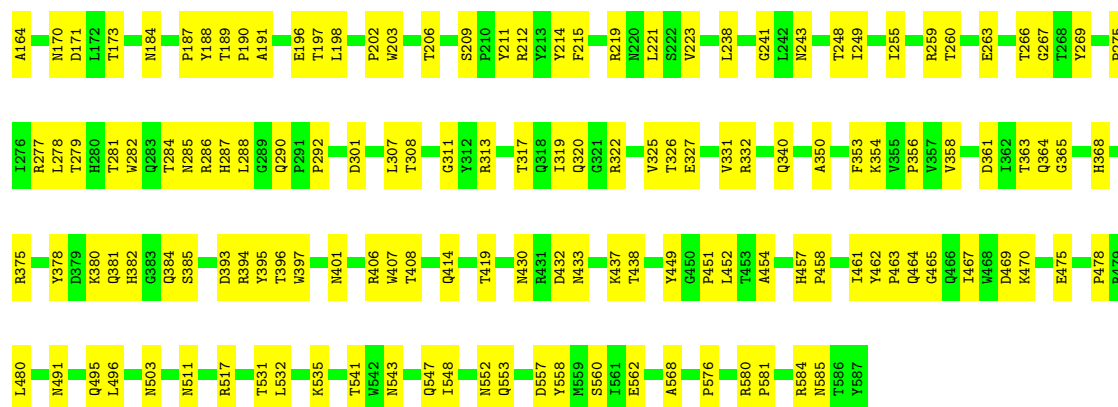
Chain m: 68% 32%



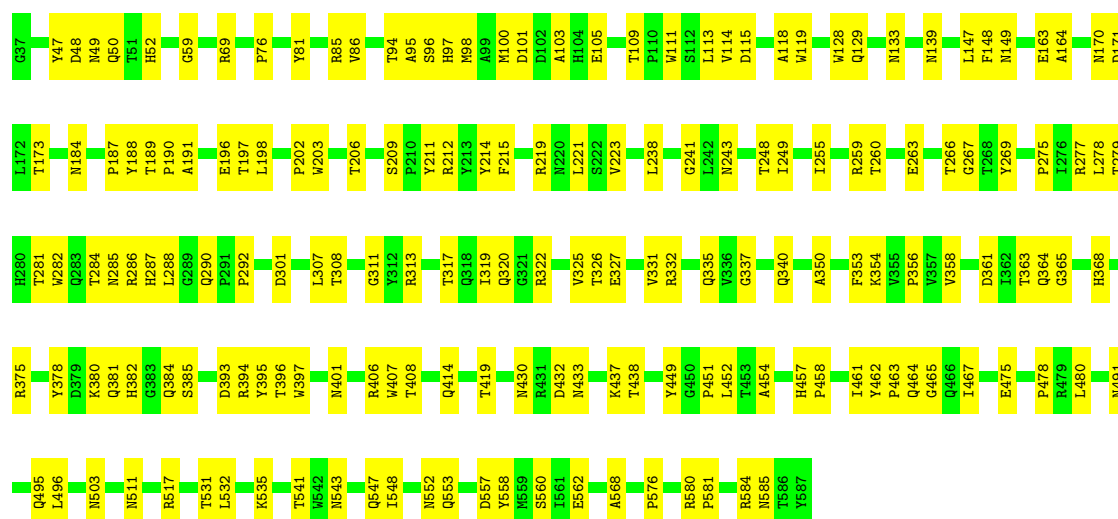
• Molecule 1: Capsid protein VP1

Chain n: 68% 32%

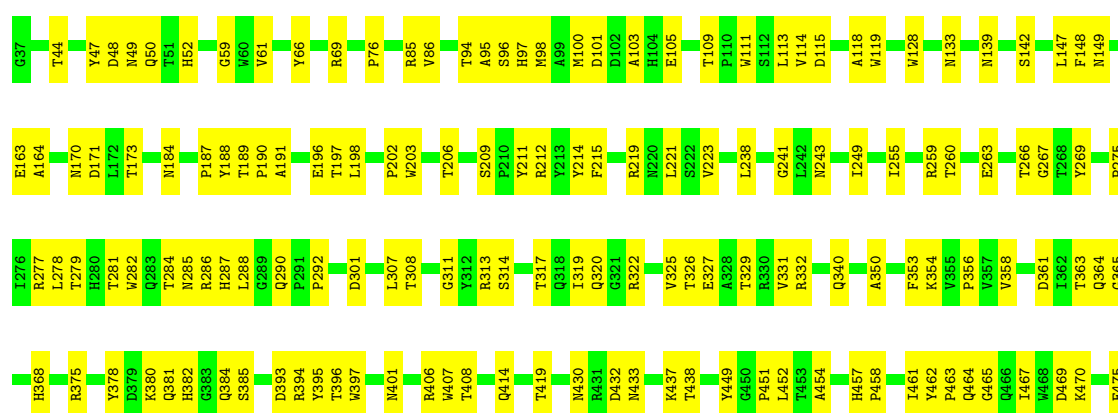




• Molecule 1: Capsid protein VP1

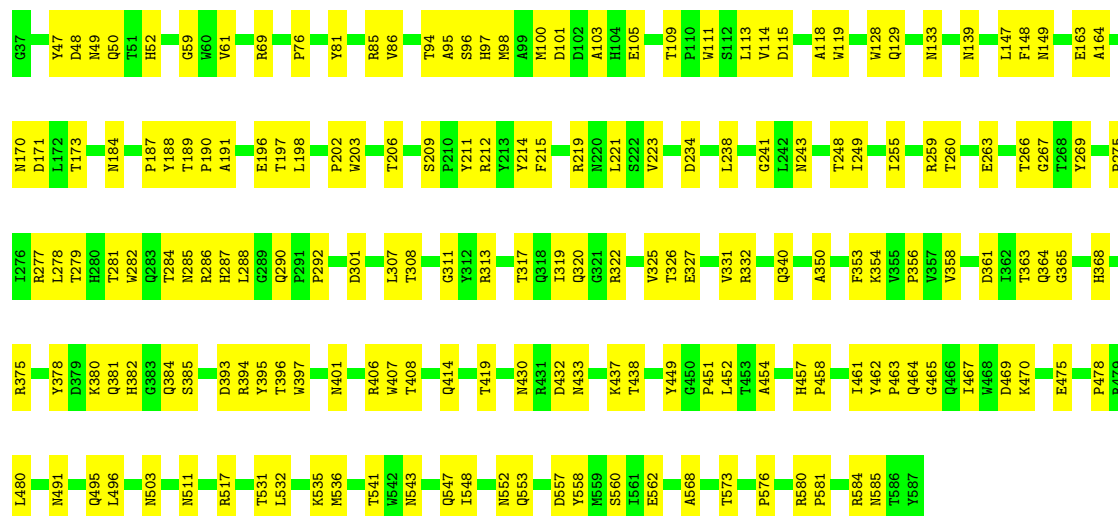


• Molecule 1: Capsid protein VP1

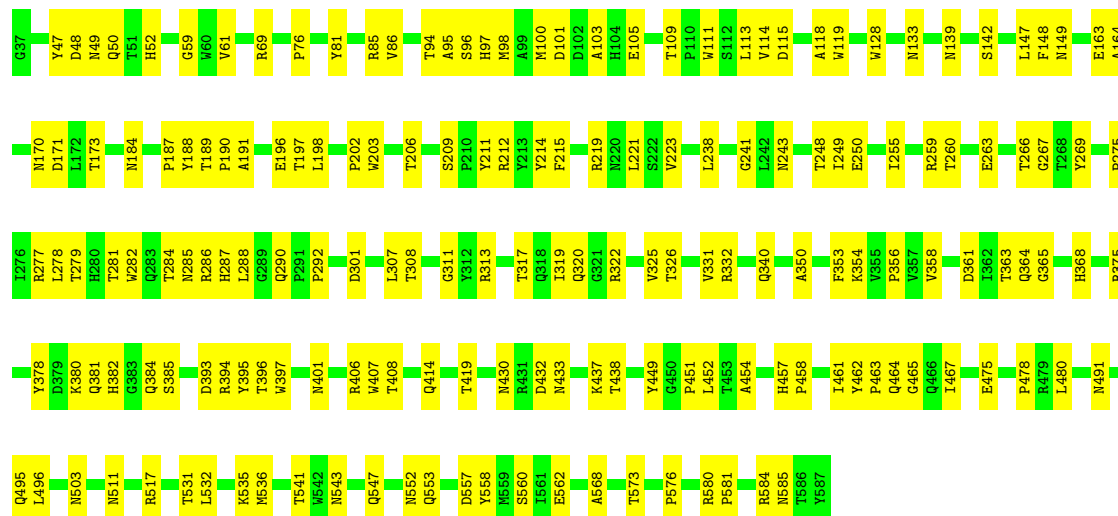




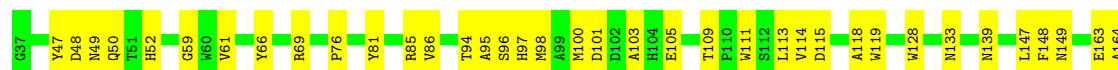
• Molecule 1: Capsid protein VP1

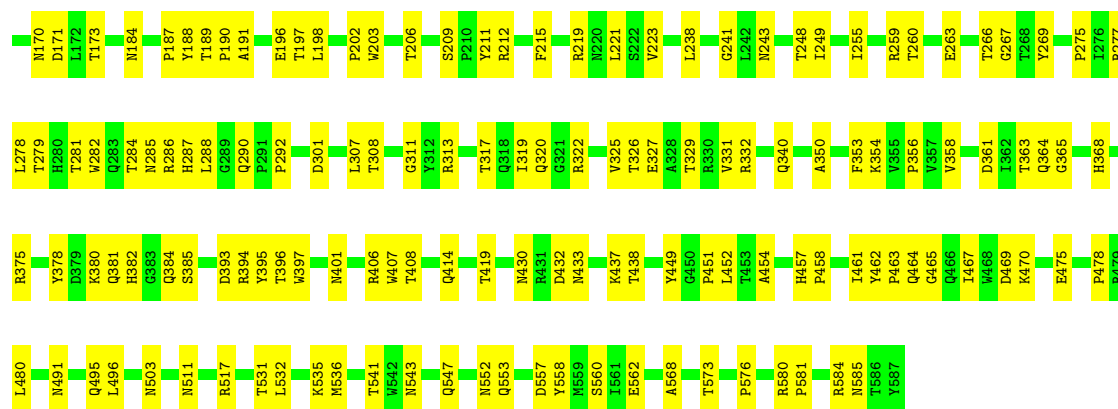


• Molecule 1: Capsid protein VP1



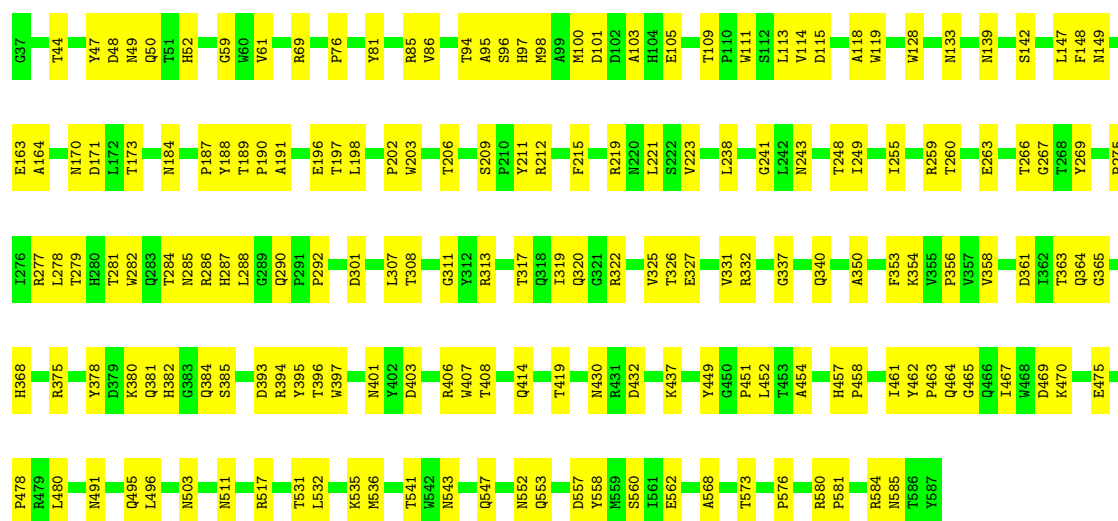
• Molecule 1: Capsid protein VP1





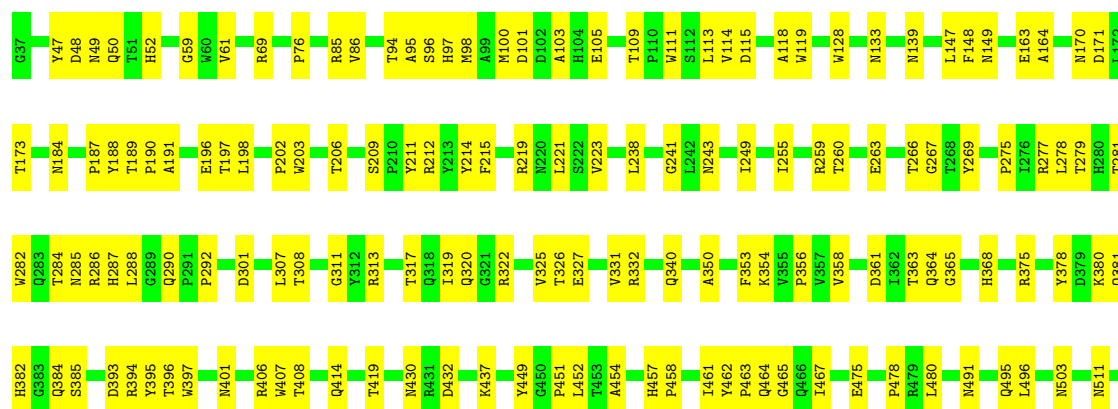
• Molecule 1: Capsid protein VP1

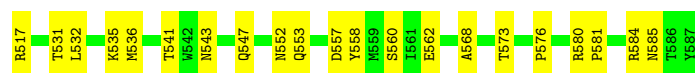
Chain t: 68% 32%



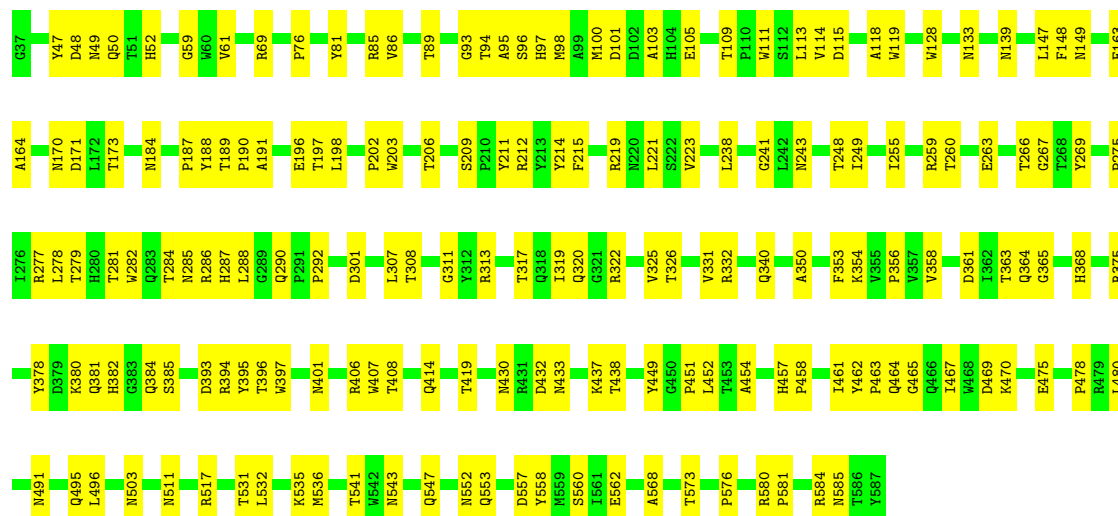
• Molecule 1: Capsid protein VP1

Chain u: 69% 31%

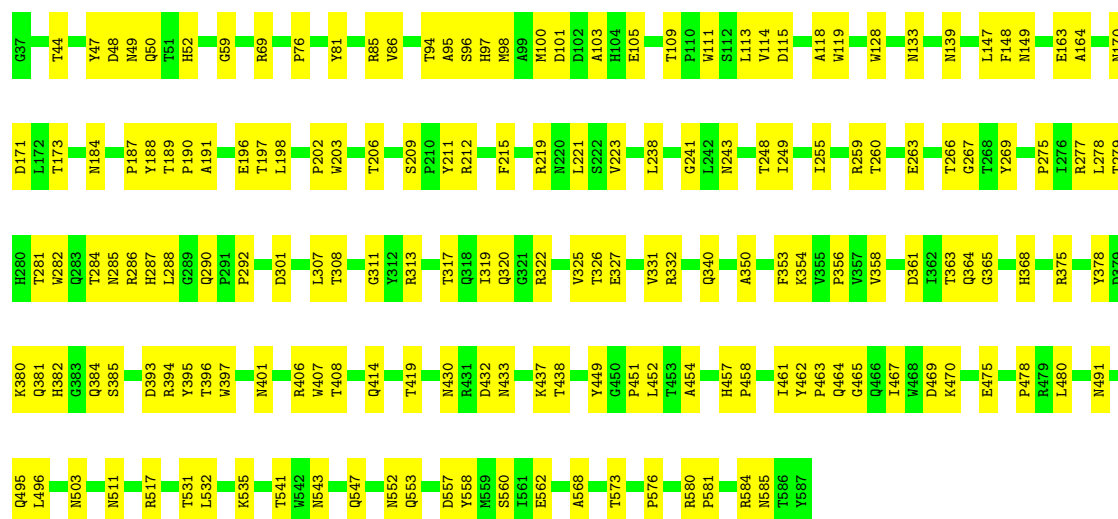




• Molecule 1: Capsid protein VP1

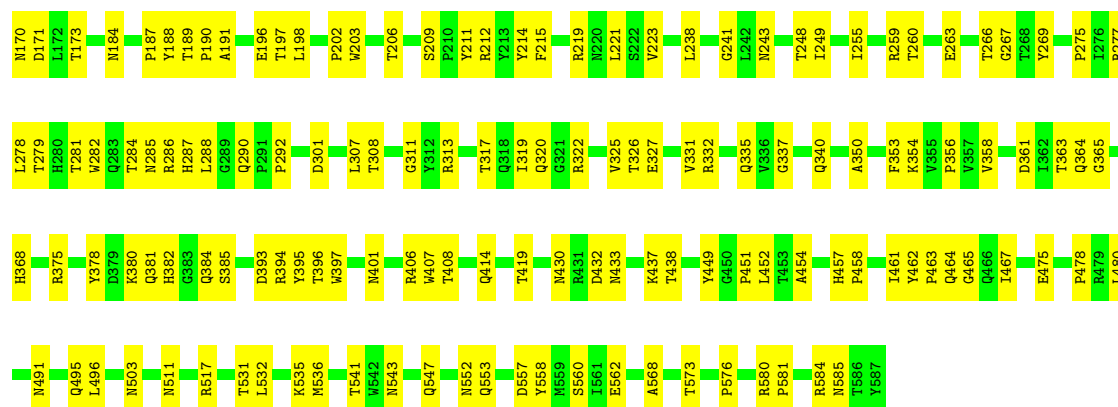


• Molecule 1: Capsid protein VP1

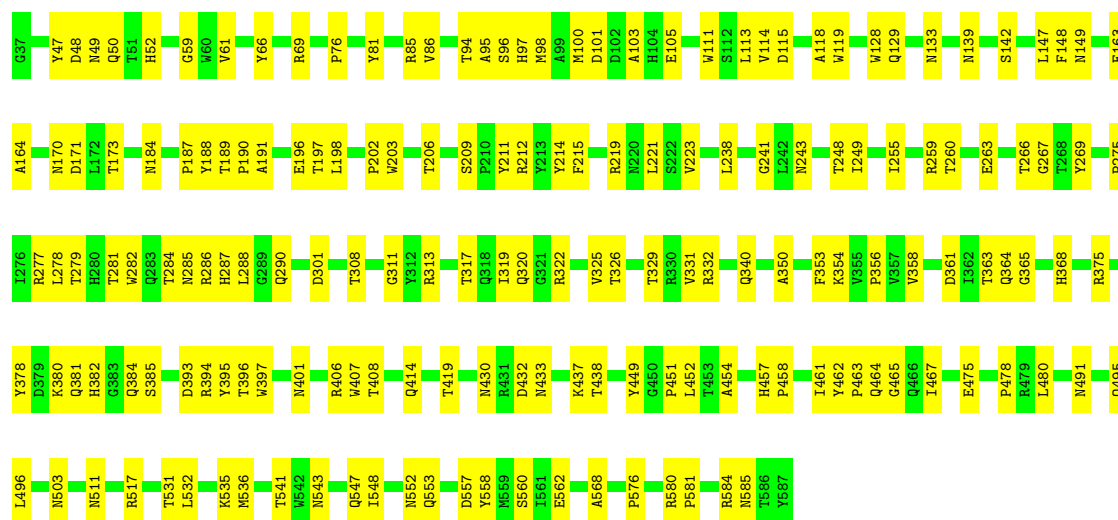


• Molecule 1: Capsid protein VP1

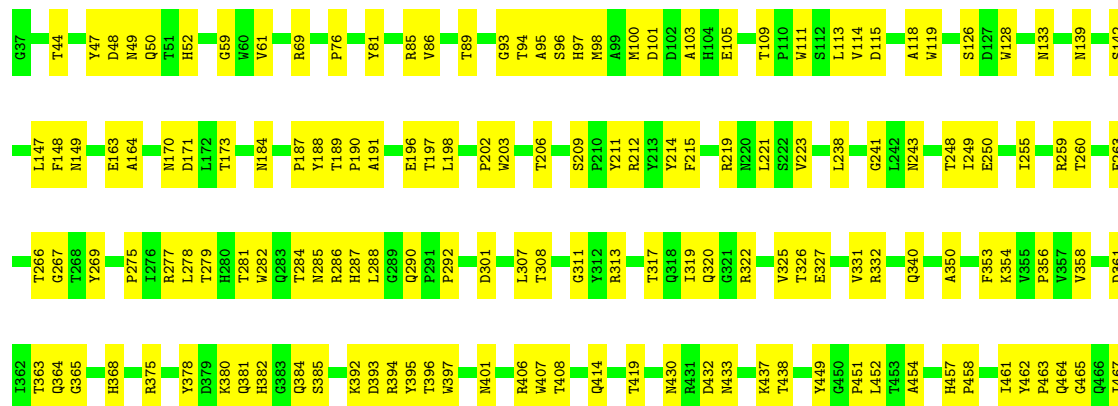




• Molecule 1: Capsid protein VP1



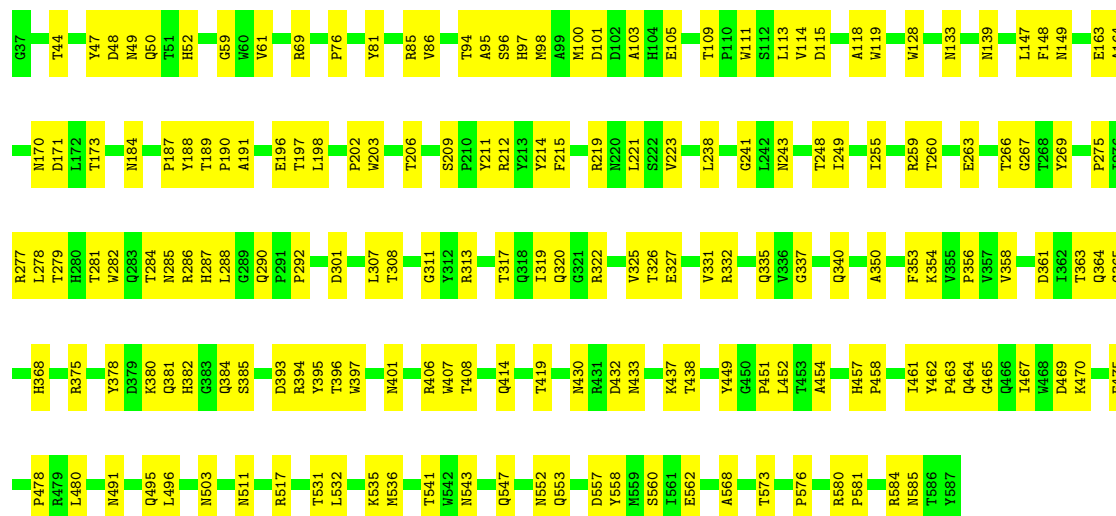
• Molecule 1: Capsid protein VP1





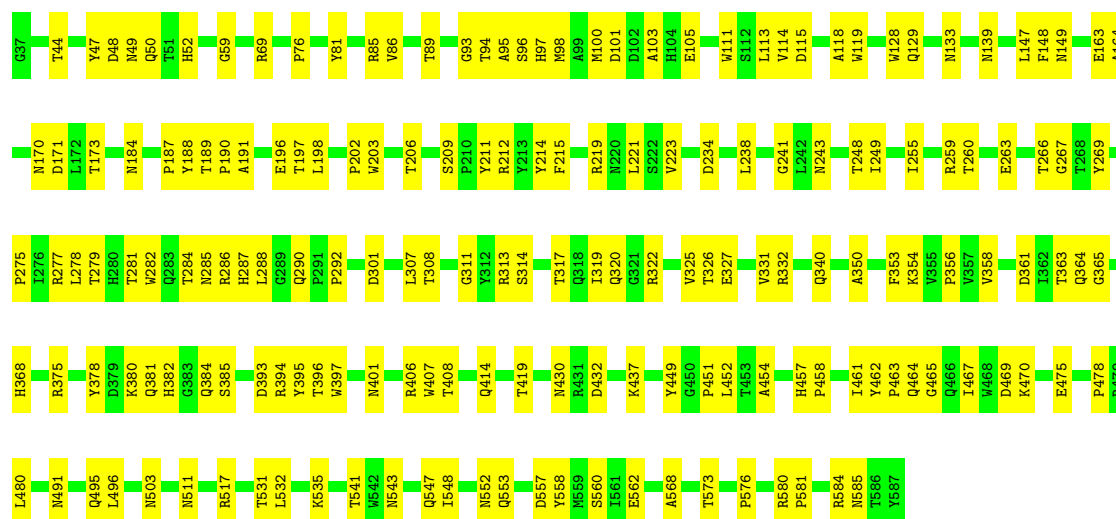
• Molecule 1: Capsid protein VP1

Chain 1: 68% 32%



• Molecule 1: Capsid protein VP1

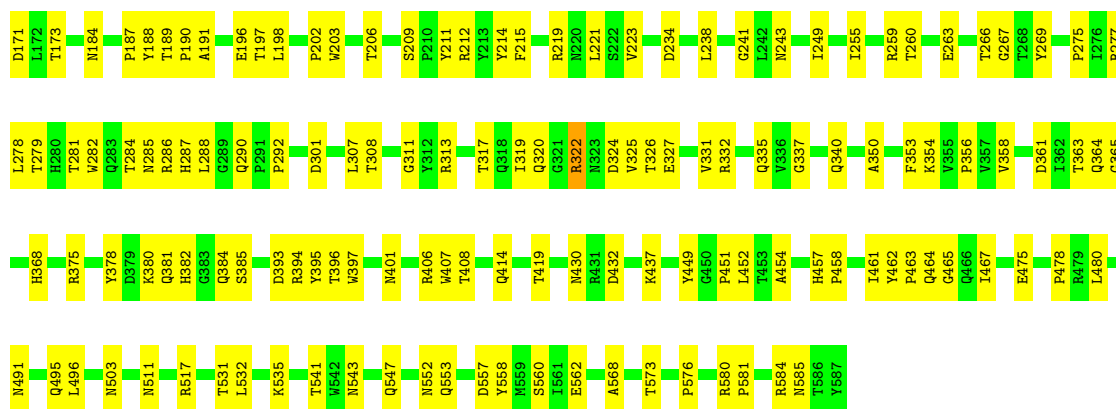
Chain 2: 68% 32%



• Molecule 1: Capsid protein VP1

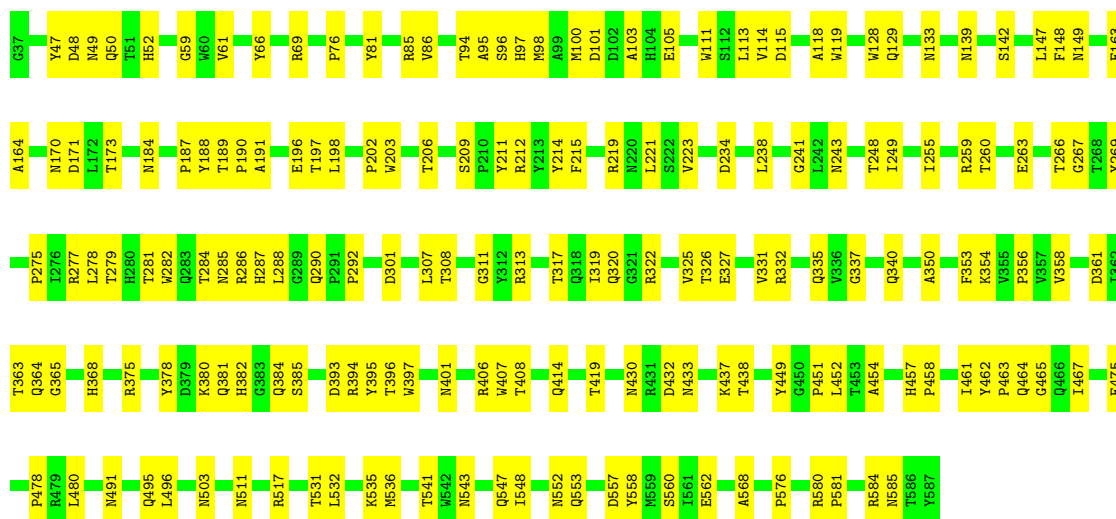
Chain 3: 69% 31%





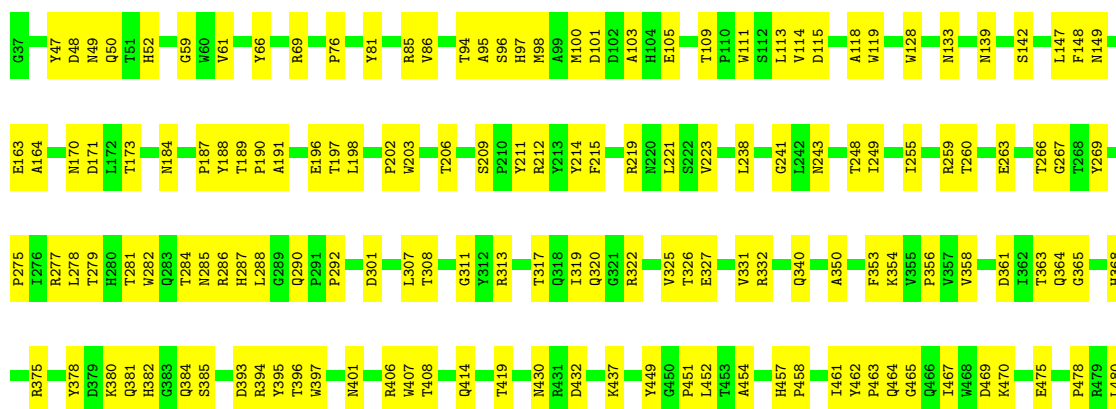
• Molecule 1: Capsid protein VP1

Chain 4: 68% 32%



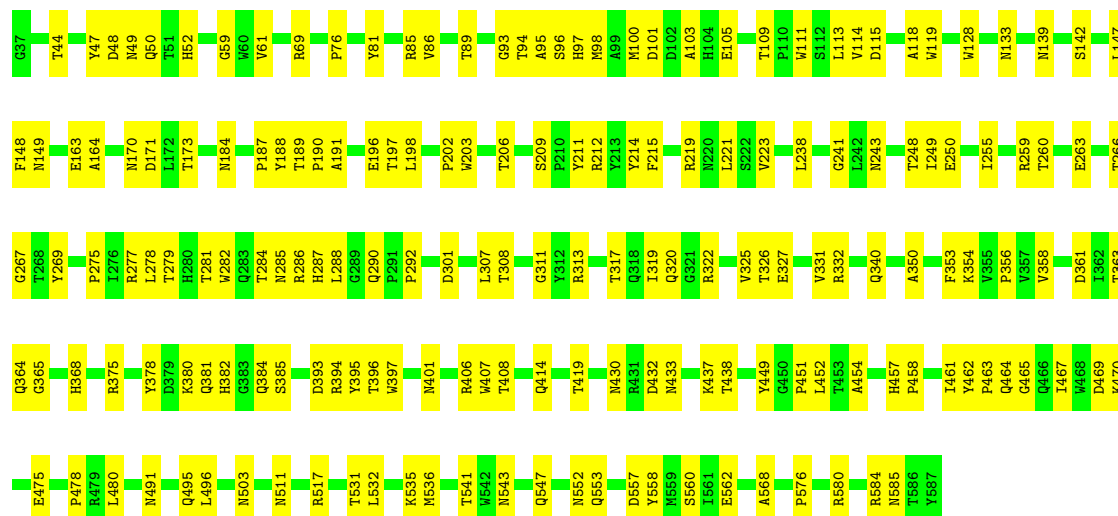
• Molecule 1: Capsid protein VP1

Chain 5: 68% 32%



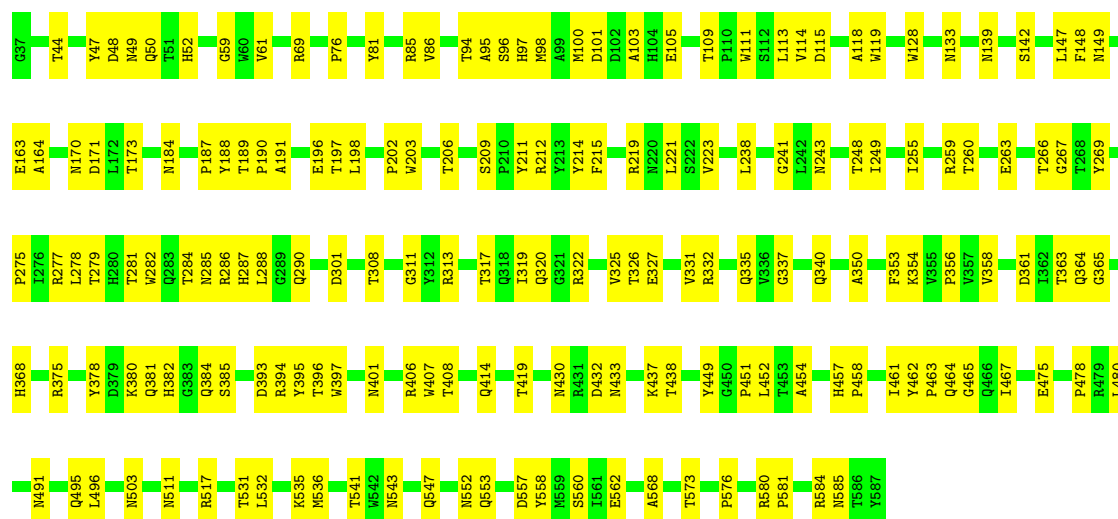
- Molecule 1: Capsid protein VP1

Chain 6:  68% 32%



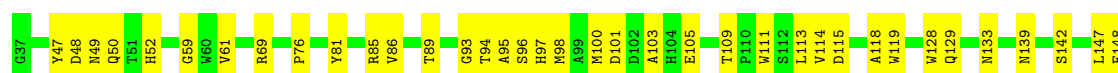
- Molecule 1: Capsid protein VP1

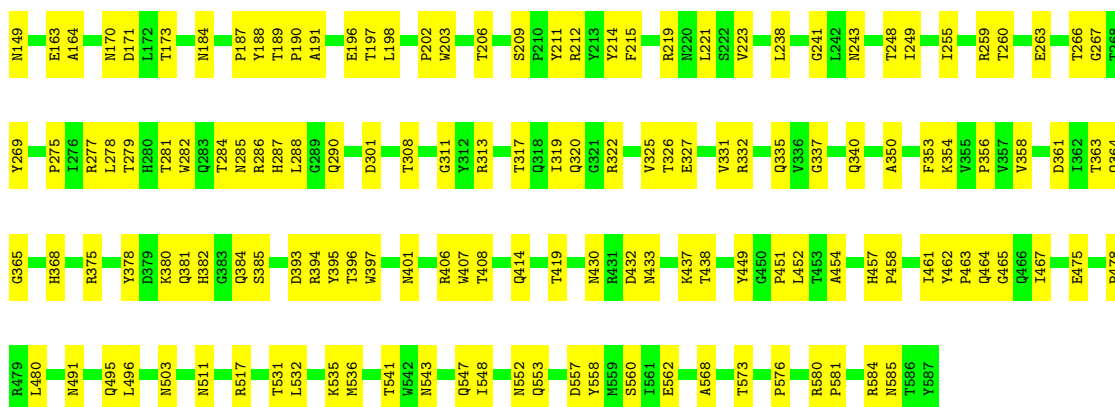
Chain 7: 68% 32%



- Molecule 1: Capsid protein VP1

Chain 8:  68% 32%





- 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



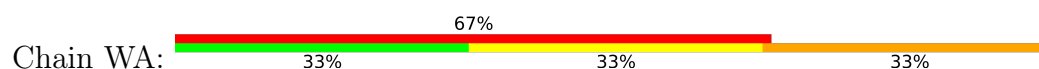
- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



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- 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	38079	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	17.398	Depositor
Minimum map value	-9.306	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	441.84003, 441.84003, 441.84003	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	2	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	3	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	4	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	5	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	6	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	7	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	8	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	A	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	B	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	C	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	D	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	E	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	F	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	G	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	H	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	I	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	J	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	K	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	L	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	M	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	N	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	O	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	P	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	Q	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	R	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	S	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	T	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	U	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	V	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	W	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	X	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	Z	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	a	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	b	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	c	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	d	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	e	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	f	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	g	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	h	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	i	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	j	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	k	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	l	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	m	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	n	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	o	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	p	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	q	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	r	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	s	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	t	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	u	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	v	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	w	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	x	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	y	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
1	z	0.47	1/4530 (0.0%)	0.53	4/6196 (0.1%)
All	All	0.47	60/271800 (0.0%)	0.53	240/371760 (0.1%)

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	203	TRP	C-N	-5.46	1.23	1.33
1	X	203	TRP	C-N	-5.46	1.23	1.33
1	o	203	TRP	C-N	-5.46	1.23	1.33
1	g	203	TRP	C-N	-5.46	1.23	1.33
1	x	203	TRP	C-N	-5.45	1.23	1.33

The worst 5 of 240 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	322[A]	ARG	CA-C-N	-5.82	114.75	122.85
1	O	322[A]	ARG	C-N-CA	-5.82	114.75	122.85
1	O	322[B]	ARG	CA-C-N	-5.82	114.75	122.85
1	O	322[B]	ARG	C-N-CA	-5.82	114.75	122.85
1	R	322[A]	ARG	CA-C-N	-5.82	114.77	122.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4401	0	4174	154	0
1	2	4401	0	4174	151	0
1	3	4401	0	4174	152	0
1	4	4401	0	4174	154	0
1	5	4401	0	4174	152	0
1	6	4401	0	4174	155	0
1	7	4401	0	4174	154	0
1	8	4401	0	4174	155	0
1	A	4401	0	4174	152	0
1	B	4401	0	4174	155	0
1	C	4401	0	4174	156	0
1	D	4401	0	4174	155	0
1	E	4401	0	4174	152	0
1	F	4401	0	4174	153	0
1	G	4401	0	4174	155	0
1	H	4401	0	4174	153	0
1	I	4401	0	4174	150	0
1	J	4401	0	4174	153	0
1	K	4401	0	4174	157	0
1	L	4401	0	4174	156	0
1	M	4401	0	4174	152	0
1	N	4401	0	4174	154	0
1	O	4401	0	4174	159	0
1	P	4401	0	4174	158	0
1	Q	4401	0	4174	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	4401	0	4174	153	0
1	S	4401	0	4174	153	0
1	T	4401	0	4174	154	0
1	U	4401	0	4174	151	0
1	V	4401	0	4174	153	0
1	W	4401	0	4174	154	0
1	X	4401	0	4174	152	0
1	Y	4401	0	4174	154	0
1	Z	4401	0	4174	154	0
1	a	4401	0	4174	152	0
1	b	4401	0	4174	155	0
1	c	4401	0	4174	153	0
1	d	4401	0	4174	154	0
1	e	4401	0	4174	151	0
1	f	4401	0	4174	154	0
1	g	4401	0	4174	157	0
1	h	4401	0	4174	152	0
1	i	4401	0	4174	154	0
1	j	4401	0	4174	154	0
1	k	4401	0	4174	159	0
1	l	4401	0	4174	155	0
1	m	4401	0	4174	155	0
1	n	4401	0	4174	153	0
1	o	4401	0	4174	153	0
1	p	4401	0	4174	155	0
1	q	4401	0	4174	154	0
1	r	4401	0	4174	153	0
1	s	4401	0	4174	154	0
1	t	4401	0	4174	156	0
1	u	4401	0	4174	149	0
1	v	4401	0	4174	154	0
1	w	4401	0	4174	152	0
1	x	4401	0	4174	154	0
1	y	4401	0	4174	152	0
1	z	4401	0	4174	157	0
2	0	46	0	40	2	0
2	0A	46	0	40	2	0
2	1B	46	0	40	2	0
2	3A	46	0	40	2	0
2	4B	46	0	40	2	0
2	6A	46	0	40	2	0
2	7B	46	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9A	46	0	40	2	0
2	AC	46	0	40	2	0
2	BA	46	0	40	2	0
2	CB	46	0	40	2	0
2	DC	46	0	40	2	0
2	EA	46	0	40	2	0
2	FB	46	0	40	2	0
2	GC	46	0	40	2	0
2	HA	46	0	40	2	0
2	IB	46	0	40	2	0
2	JC	46	0	40	2	0
2	KA	46	0	40	2	0
2	LB	46	0	40	2	0
2	MC	46	0	40	2	0
2	NA	46	0	40	2	0
2	OB	46	0	40	2	0
2	PC	46	0	40	2	0
2	QA	46	0	40	2	0
2	RB	46	0	40	2	0
2	SC	46	0	40	2	0
2	TA	46	0	40	2	0
2	UB	46	0	40	2	0
2	VC	46	0	40	2	0
2	WA	46	0	40	2	0
2	XB	46	0	40	2	0
2	YC	46	0	40	2	0
2	ZA	46	0	40	2	0
2	aB	46	0	40	2	0
2	bC	46	0	40	1	0
2	cA	46	0	40	2	0
2	dB	46	0	40	2	0
2	eC	46	0	40	2	0
2	fA	46	0	40	2	0
2	gB	46	0	40	2	0
2	hC	46	0	40	2	0
2	iA	46	0	40	2	0
2	jB	46	0	40	2	0
2	kC	46	0	40	2	0
2	lA	46	0	40	2	0
2	mB	46	0	40	1	0
2	nC	46	0	40	2	0
2	oA	46	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	pB	46	0	40	2	0
2	qC	46	0	40	2	0
2	rA	46	0	40	2	0
2	sB	46	0	40	2	0
2	tC	46	0	40	2	0
2	uA	46	0	40	2	0
2	vB	46	0	40	2	0
2	wC	46	0	40	2	0
2	xA	46	0	40	2	0
2	yB	46	0	40	2	0
2	zC	46	0	40	2	0
All	All	266820	0	252840	7597	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7597 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:148:PHE:HD1	1:q:149:ASN:HD22	1.33	0.77
1:B:148:PHE:HD1	1:B:149:ASN:HD22	1.33	0.77
1:R:148:PHE:HD1	1:R:149:ASN:HD22	1.33	0.77
1:1:148:PHE:HD1	1:1:149:ASN:HD22	1.33	0.77
1:P:148:PHE:HD1	1:P:149:ASN:HD22	1.33	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	550/551 (100%)	540 (98%)	10 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	3	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	4	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	5	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	6	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	7	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	8	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	A	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	B	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	C	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	D	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	E	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	F	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	G	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	H	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	I	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	J	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	K	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	L	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	M	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	N	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	O	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	P	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	Q	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	R	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	S	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	T	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	U	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	V	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	W	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	X	550/551 (100%)	539 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	Z	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	a	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	b	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	c	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	d	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	e	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	f	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	g	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	h	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	i	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	j	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	k	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	l	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	m	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	n	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	o	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	p	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	q	550/551 (100%)	539 (98%)	11 (2%)	0	100	100
1	r	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	s	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	t	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	u	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	v	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	w	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	x	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	y	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
1	z	550/551 (100%)	540 (98%)	10 (2%)	0	100	100
All	All	33000/33060 (100%)	32391 (98%)	609 (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%)	87	95
1	2	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	3	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	4	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	5	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	6	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	7	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	8	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	A	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	B	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	C	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	D	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	E	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	F	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	G	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	H	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	I	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	J	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	K	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	L	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	M	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	N	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	O	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	P	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	Q	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	R	480/479 (100%)	479 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	T	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	U	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	V	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	W	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	X	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	Y	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	Z	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	a	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	b	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	c	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	d	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	e	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	f	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	g	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	h	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	i	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	j	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	k	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	l	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	m	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	n	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	o	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	p	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	q	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	r	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	s	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	t	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	u	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	v	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	w	480/479 (100%)	479 (100%)	1 (0%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	y	480/479 (100%)	479 (100%)	1 (0%)	87	95
1	z	480/479 (100%)	479 (100%)	1 (0%)	87	95
All	All	28800/28740 (100%)	28740 (100%)	60 (0%)	85	95

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	480	LEU
1	4	480	LEU
1	j	480	LEU
1	3	480	LEU
1	8	480	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1548 such sidechains are listed below:

Mol	Chain	Res	Type
1	j	511	ASN
1	s	159	ASN
1	k	511	ASN
1	j	495	GLN
1	o	149	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	0.13	0	21,21,21	0.18	0
2	GAL	0	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	0	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	0A	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	0A	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	0A	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	1B	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	1B	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	1B	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	3A	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	3A	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	3A	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	4B	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	4B	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	4B	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	6A	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	6A	2	2	11,11,12	1.13	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	6A	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	7B	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	7B	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	7B	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	9A	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	9A	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	9A	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	AC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	AC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	AC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	BA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	BA	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	BA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	CB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	CB	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	CB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	DC	1	2	15,15,15	0.13	0	21,21,21	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	DC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	DC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	EA	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	EA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	EA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	FB	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	FB	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	FB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	GC	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	GC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	GC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	HA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	HA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	HA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	IB	1	2	15,15,15	0.14	0	21,21,21	0.17	0
2	GAL	IB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	IB	3	2	20,20,21	1.53	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	JC	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	JC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	JC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	KA	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	KA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	KA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	LB	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	LB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	LB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	MC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	MC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	MC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	NA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	NA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	NA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	OB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	OB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	OB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	PC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	PC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	PC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	QA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	QA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	QA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	RB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	RB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	RB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	SC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	SC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	SC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	TA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	TA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	TA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	UB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	UB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	UB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	VC	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	VC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	VC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	WA	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	WA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	WA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	XB	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	XB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	XB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	YC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	YC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	YC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	ZA	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	ZA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	ZA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	aB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	aB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	aB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	bC	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	bC	2	2	11,11,12	1.13	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	bC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	cA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	cA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	cA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	dB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	dB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	dB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	eC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	eC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	eC	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	fA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	fA	2	2	11,11,12	1.13	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	fA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	gB	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	gB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	gB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	hC	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	hC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	hC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	iA	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	iA	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	iA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	jB	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	jB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	jB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	kC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	kC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	kC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	lA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	lA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	lA	3	2	20,20,21	1.53	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	mB	1	2	15,15,15	0.13	0	21,21,21	0.17	0
2	GAL	mB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	mB	3	2	20,20,21	1.53	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	nC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	nC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	nC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	oA	1	2	15,15,15	0.12	0	21,21,21	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	oA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	oA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	pB	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	pB	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	pB	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	qC	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	qC	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	qC	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	rA	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	rA	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	rA	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	sB	1	2	15,15,15	0.12	0	21,21,21	0.17	0
2	GAL	sB	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	sB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	tC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	tC	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.64	2 (13%)
2	SIA	tC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	uA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	uA	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	uA	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	vB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	vB	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	vB	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	wC	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	wC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	wC	3	2	20,20,21	1.53	1 (5%)	21,28,31	1.65	4 (19%)
2	NAG	xA	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	xA	2	2	11,11,12	1.10	2 (18%)	15,15,17	1.63	2 (13%)
2	SIA	xA	3	2	20,20,21	1.56	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	yB	1	2	15,15,15	0.13	0	21,21,21	0.18	0
2	GAL	yB	2	2	11,11,12	1.12	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	yB	3	2	20,20,21	1.55	1 (5%)	21,28,31	1.66	4 (19%)
2	NAG	zC	1	2	15,15,15	0.12	0	21,21,21	0.18	0
2	GAL	zC	2	2	11,11,12	1.11	2 (18%)	15,15,17	1.62	2 (13%)
2	SIA	zC	3	2	20,20,21	1.54	1 (5%)	21,28,31	1.66	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	0/1/1/1
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	-	3/18/34/38	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	-	3/18/34/38	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	DC	3	2	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	0/1/1/1
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	-	3/18/34/38	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	-	3/18/34/38	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	PC	3	2	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	0/1/1/1
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	-	3/18/34/38	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	-	3/18/34/38	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	bC	3	2	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	0/1/1/1
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	-	3/18/34/38	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	-	3/18/34/38	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	nC	3	2	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	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	-	3/18/34/38	0/1/1/1
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	-	3/18/34/38	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	-	3/18/34/38	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	zC	3	2	-	3/18/34/38	0/1/1/1

The worst 5 of 180 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	RB	3	SIA	C2-C1	5.68	1.59	1.52
2	UB	3	SIA	C2-C1	5.68	1.59	1.52
2	xA	3	SIA	C2-C1	5.67	1.59	1.52
2	eC	3	SIA	C2-C1	5.67	1.59	1.52
2	pB	3	SIA	C2-C1	5.66	1.59	1.52

The worst 5 of 360 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BA	3	SIA	O1A-C1-C2	-5.04	111.96	122.85
2	xA	3	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	eC	3	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	cA	3	SIA	O1A-C1-C2	-5.03	111.98	122.85
2	3A	3	SIA	O1A-C1-C2	-5.03	111.98	122.85

There are no chirality outliers.

5 of 360 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	0	3	SIA	O8-C8-C9-O9
2	BA	3	SIA	O8-C8-C9-O9
2	EA	3	SIA	O8-C8-C9-O9
2	HA	3	SIA	O8-C8-C9-O9
2	KA	3	SIA	O8-C8-C9-O9

There are no ring outliers.

60 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	bC	3	SIA	1	0
2	FB	3	SIA	2	0
2	YC	3	SIA	2	0
2	tC	3	SIA	2	0
2	dB	3	SIA	2	0
2	IB	3	SIA	2	0
2	gB	3	SIA	2	0

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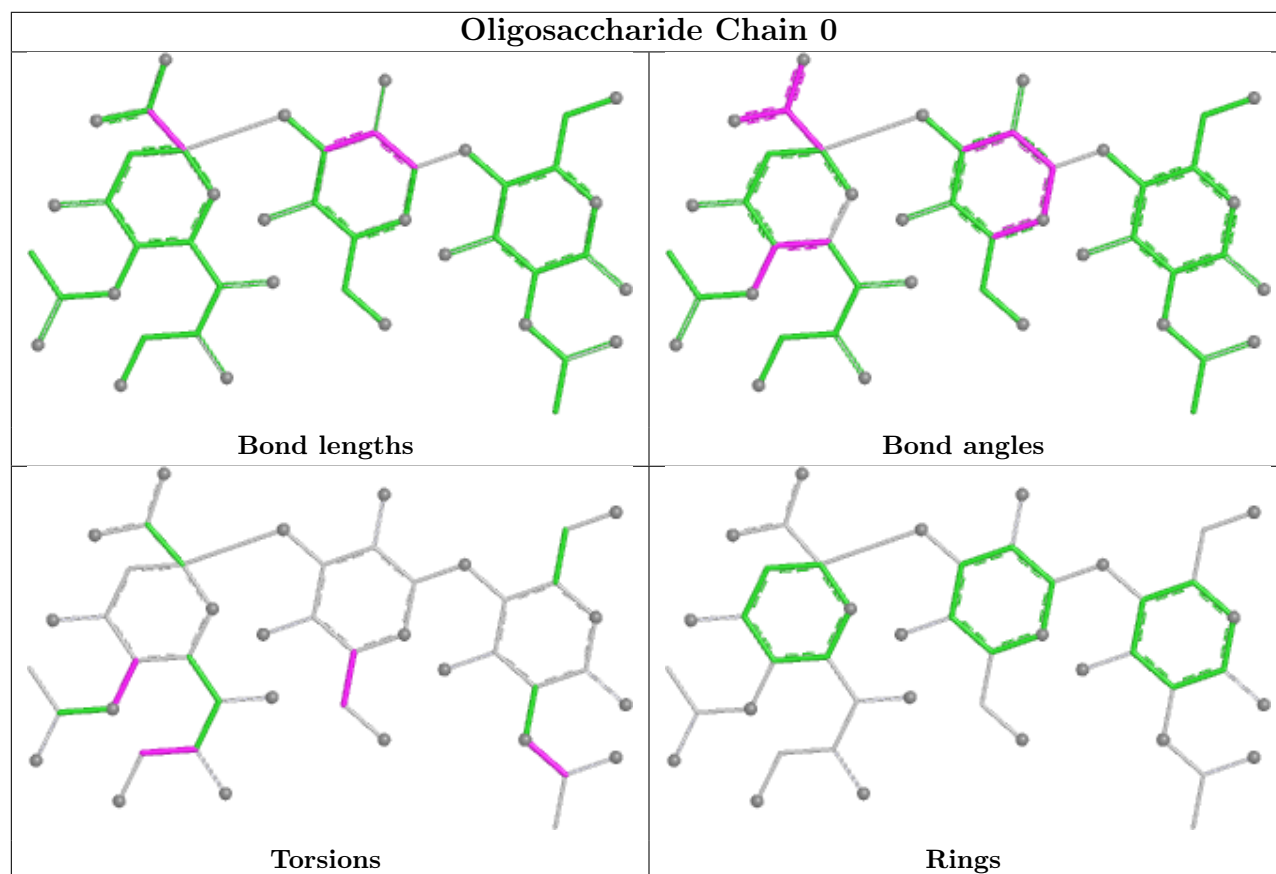
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	JC	3	SIA	2	0
2	eC	3	SIA	2	0
2	sB	3	SIA	2	0
2	MC	3	SIA	2	0
2	EA	3	SIA	2	0
2	6A	3	SIA	2	0
2	NA	3	SIA	2	0
2	RB	3	SIA	2	0
2	0A	3	SIA	2	0
2	QA	3	SIA	2	0
2	OB	3	SIA	2	0
2	4B	3	SIA	2	0
2	GC	3	SIA	2	0
2	SC	3	SIA	2	0
2	cA	3	SIA	2	0
2	hC	3	SIA	2	0
2	nC	3	SIA	2	0
2	wC	3	SIA	2	0
2	lA	3	SIA	2	0
2	HA	3	SIA	2	0
2	7B	3	SIA	2	0
2	9A	3	SIA	2	0
2	uA	3	SIA	2	0
2	mB	3	SIA	1	0
2	KA	3	SIA	2	0
2	kC	3	SIA	2	0
2	BA	3	SIA	2	0
2	AC	3	SIA	2	0
2	iA	3	SIA	2	0
2	1B	3	SIA	2	0
2	LB	3	SIA	2	0
2	pB	3	SIA	2	0
2	VC	3	SIA	2	0
2	jB	3	SIA	2	0
2	aB	3	SIA	2	0
2	DC	3	SIA	2	0
2	UB	3	SIA	2	0
2	oA	3	SIA	2	0
2	qC	3	SIA	2	0
2	yB	3	SIA	2	0
2	3A	3	SIA	2	0
2	TA	3	SIA	2	0

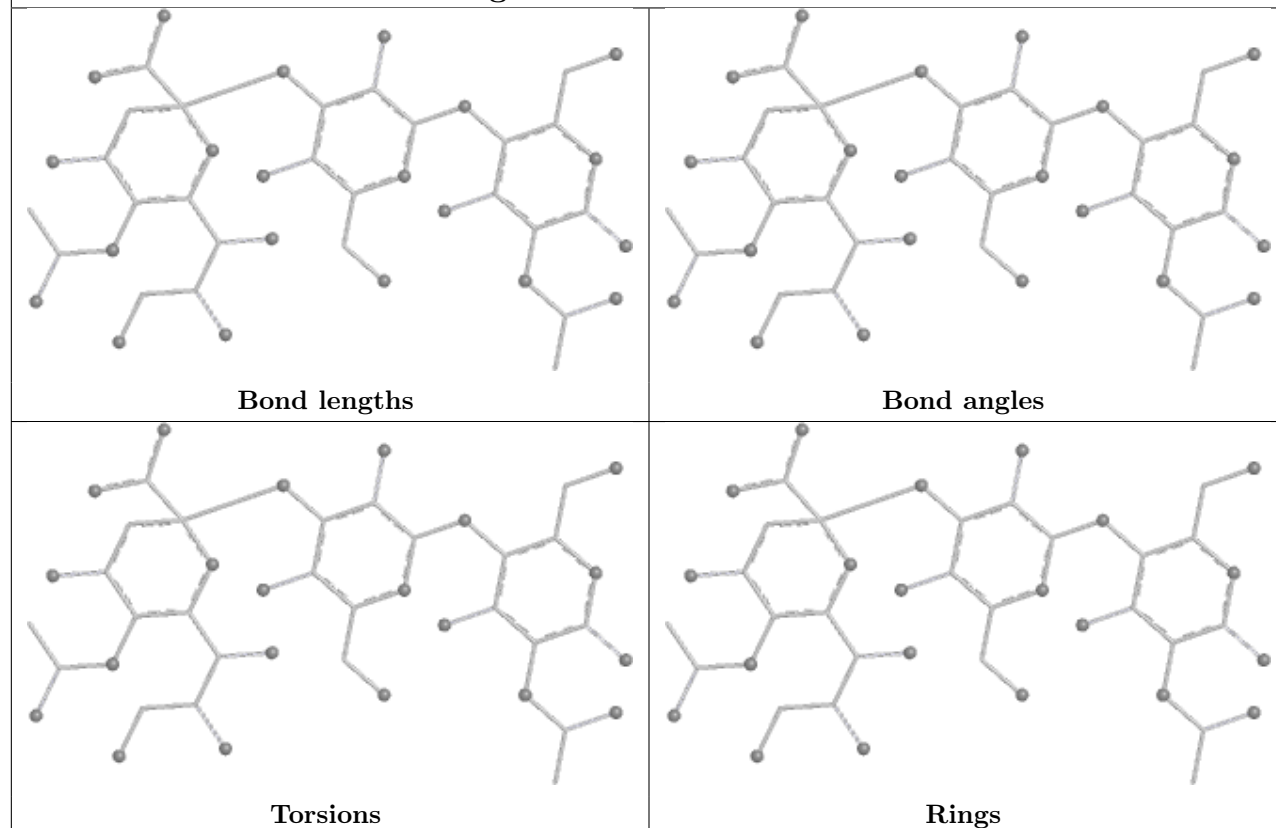
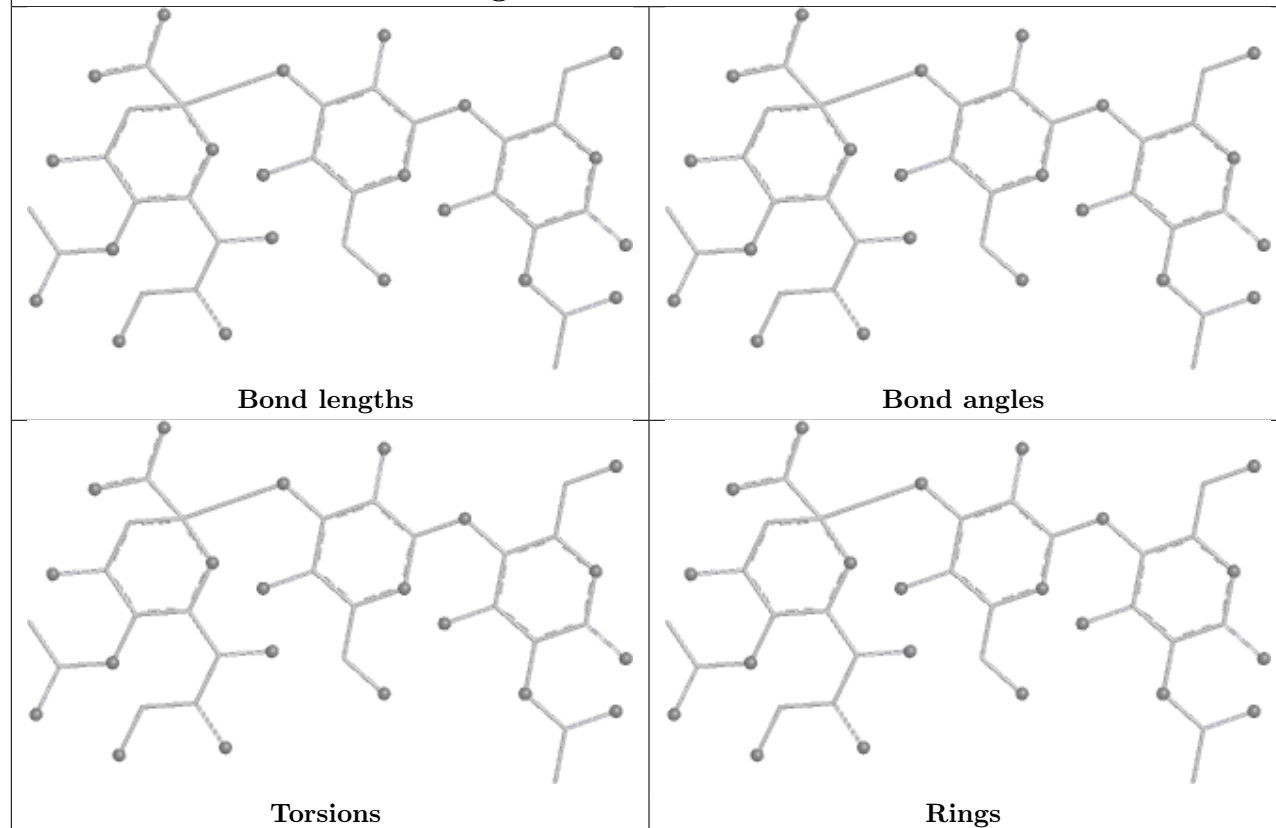
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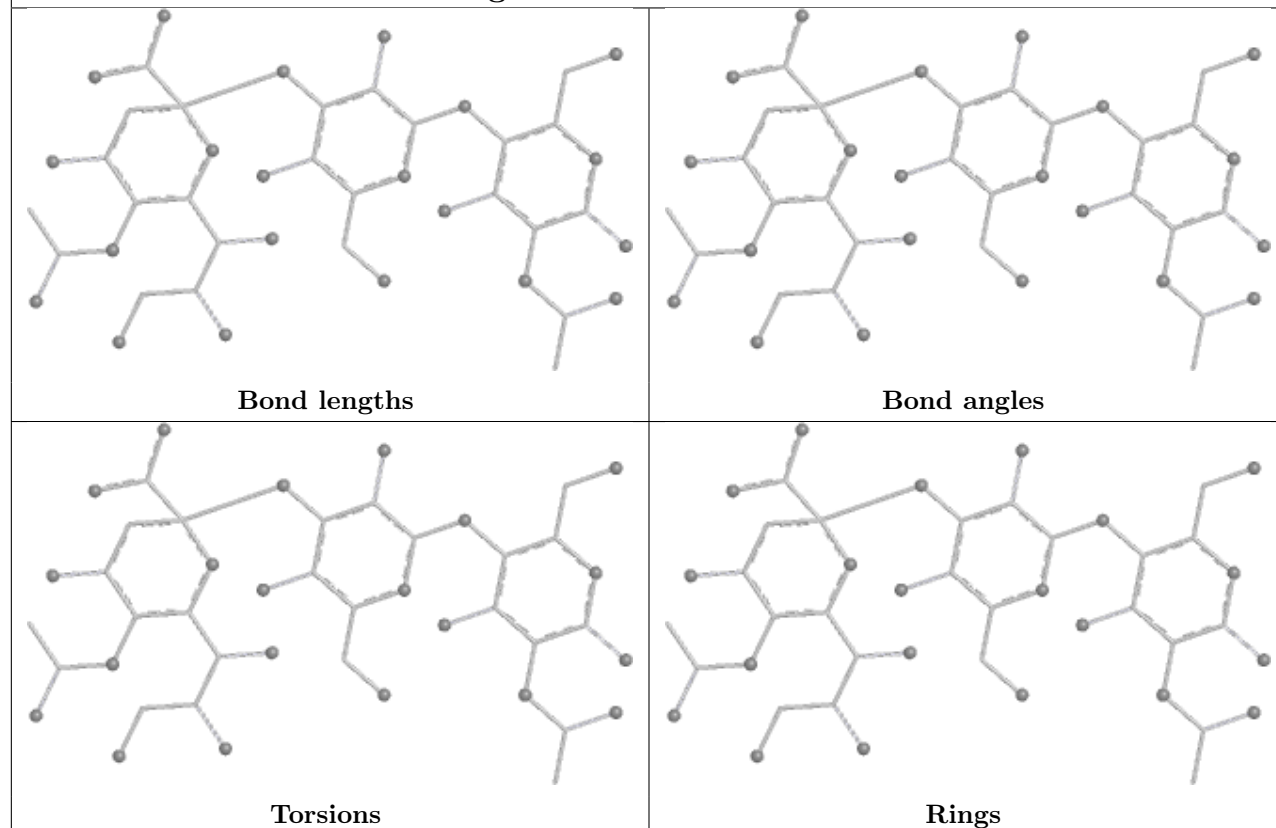
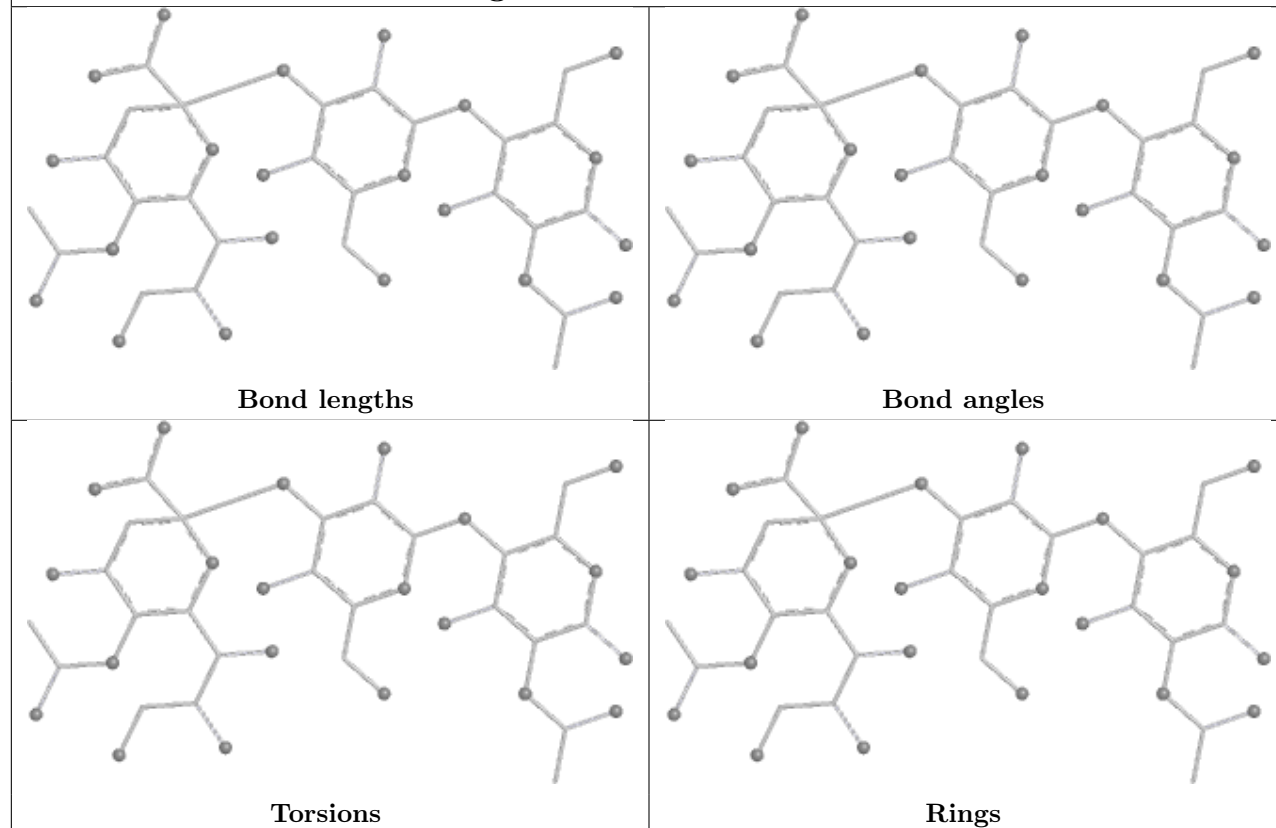
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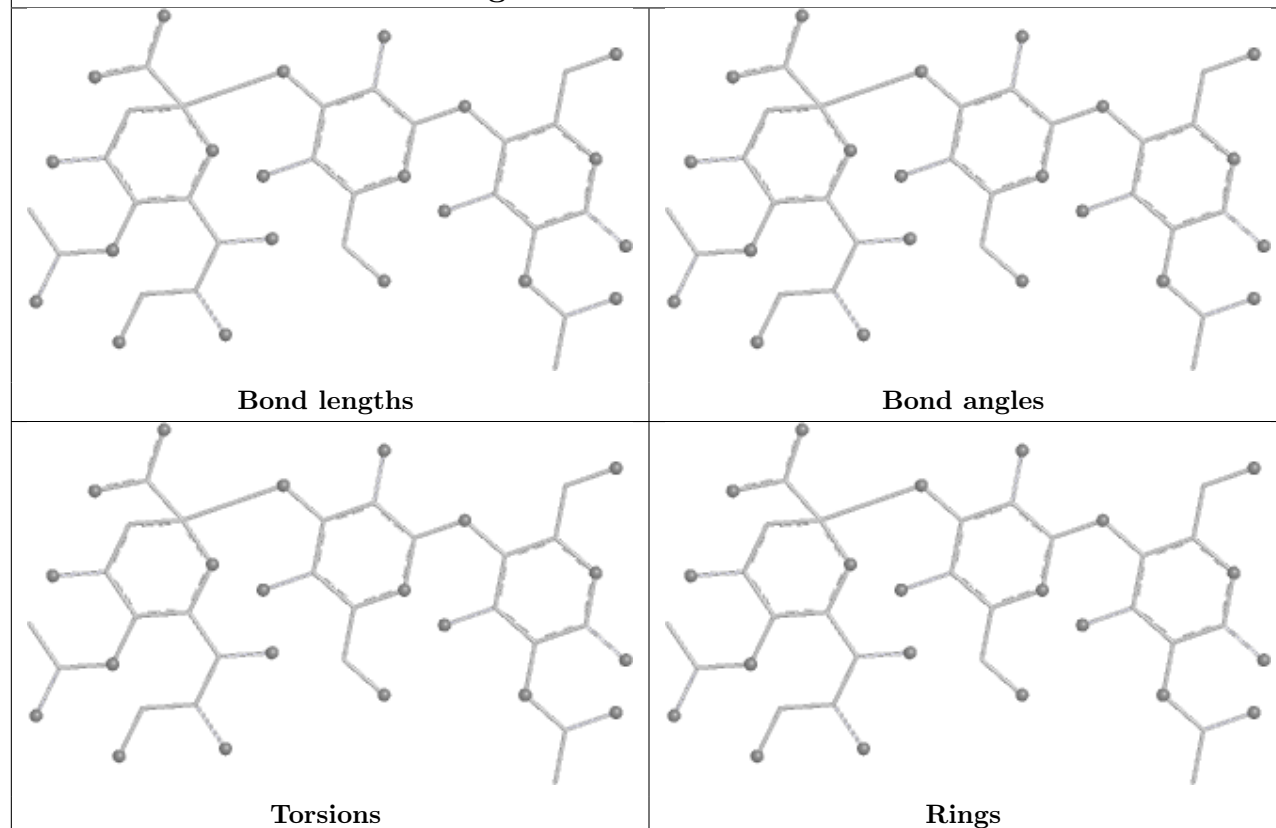
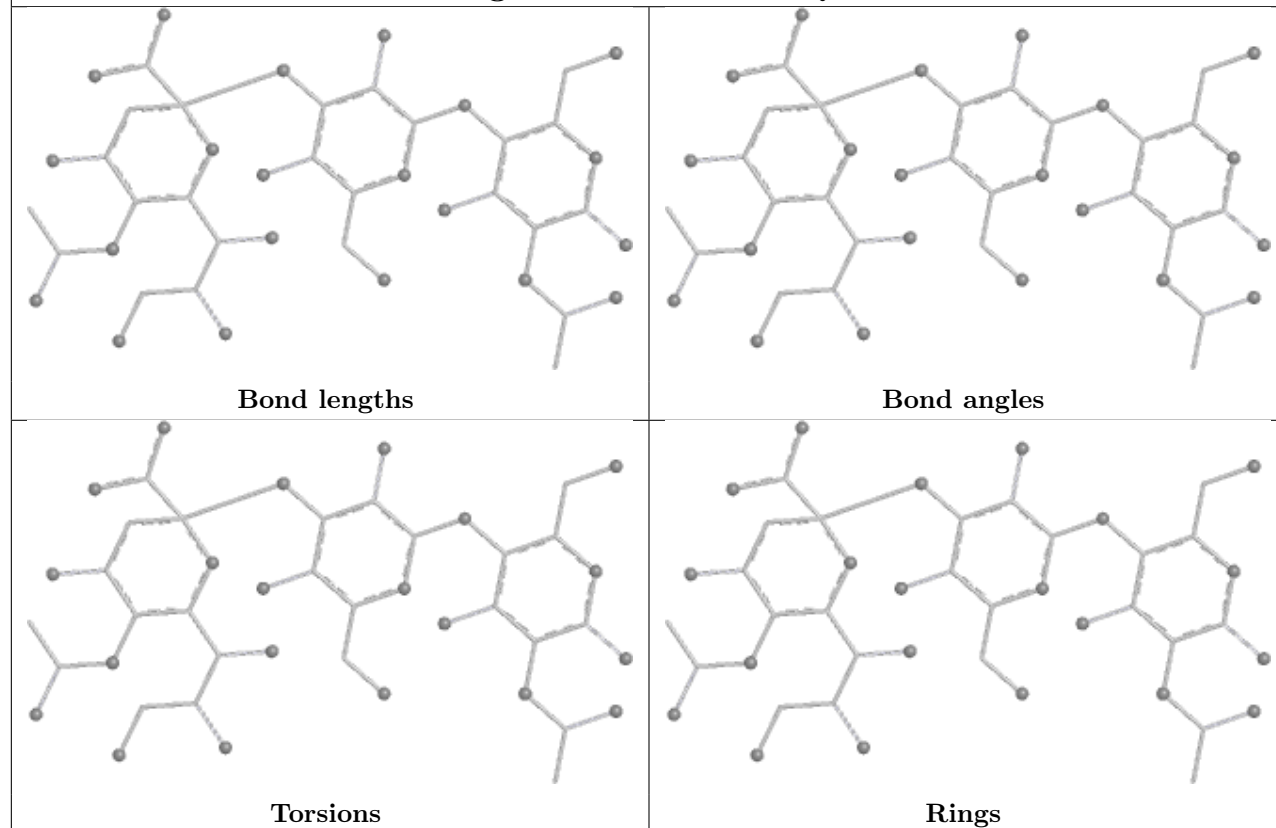
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	ZA	3	SIA	2	0
2	PC	3	SIA	2	0
2	vB	3	SIA	2	0
2	rA	3	SIA	2	0
2	fA	3	SIA	2	0
2	XB	3	SIA	2	0
2	WA	3	SIA	2	0
2	zC	3	SIA	2	0
2	CB	3	SIA	2	0
2	xA	3	SIA	2	0
2	0	3	SIA	2	0

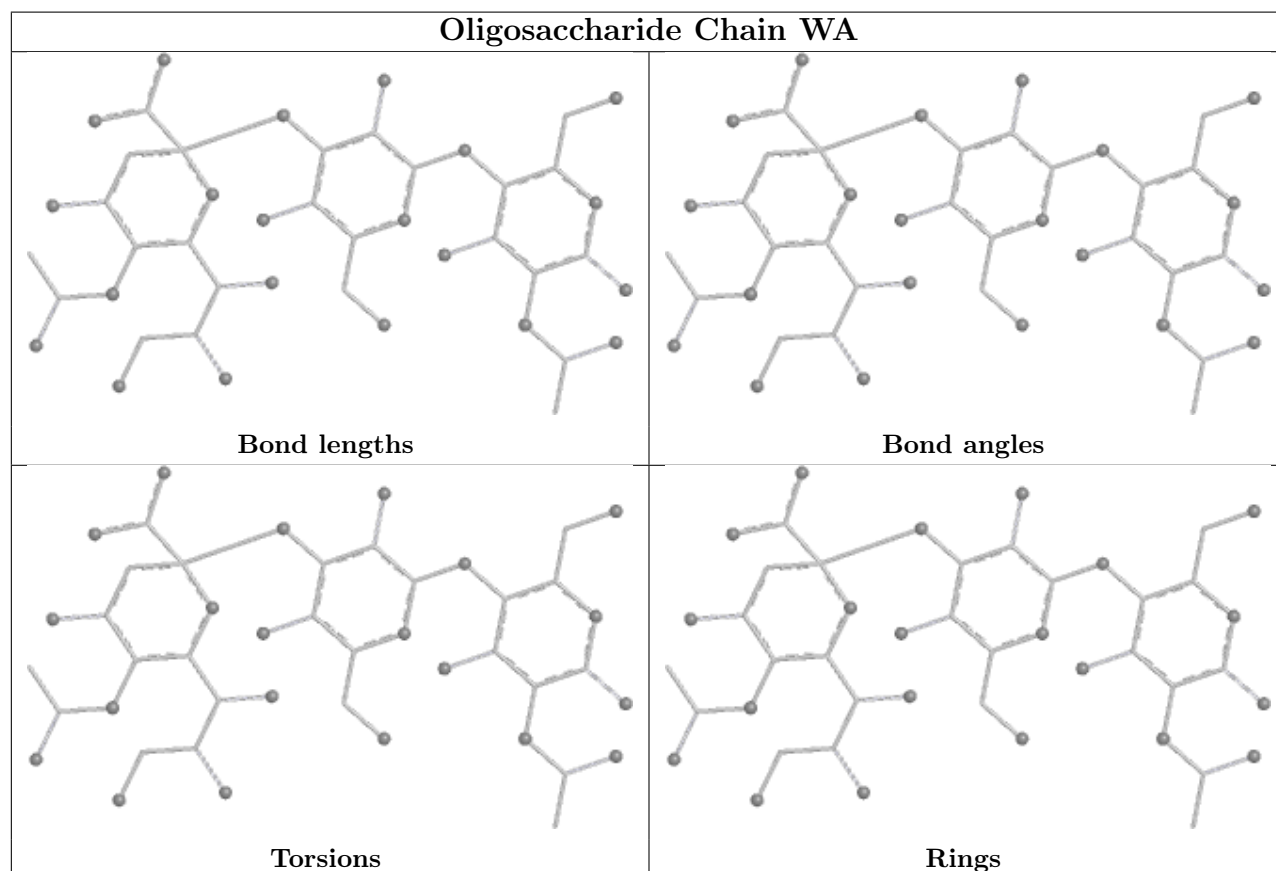
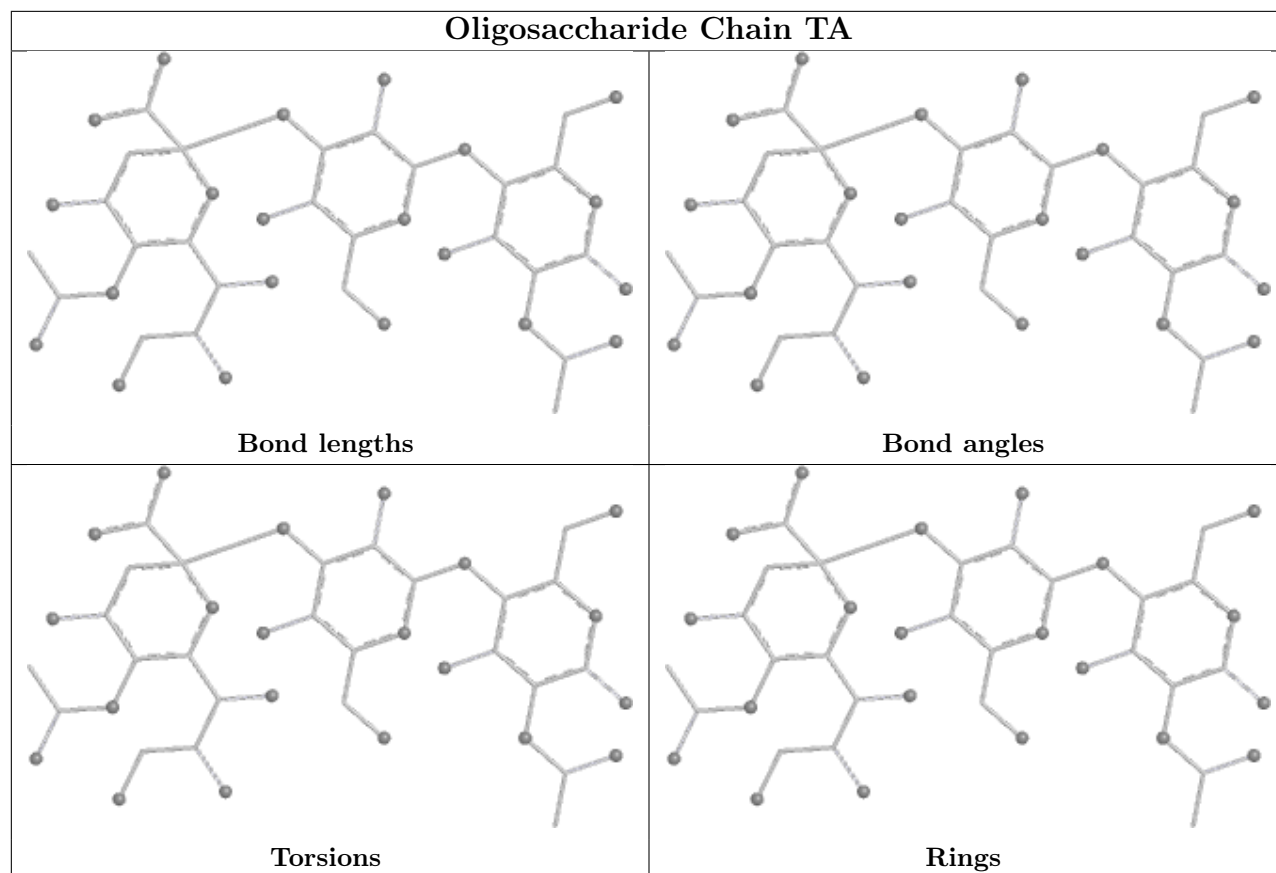
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

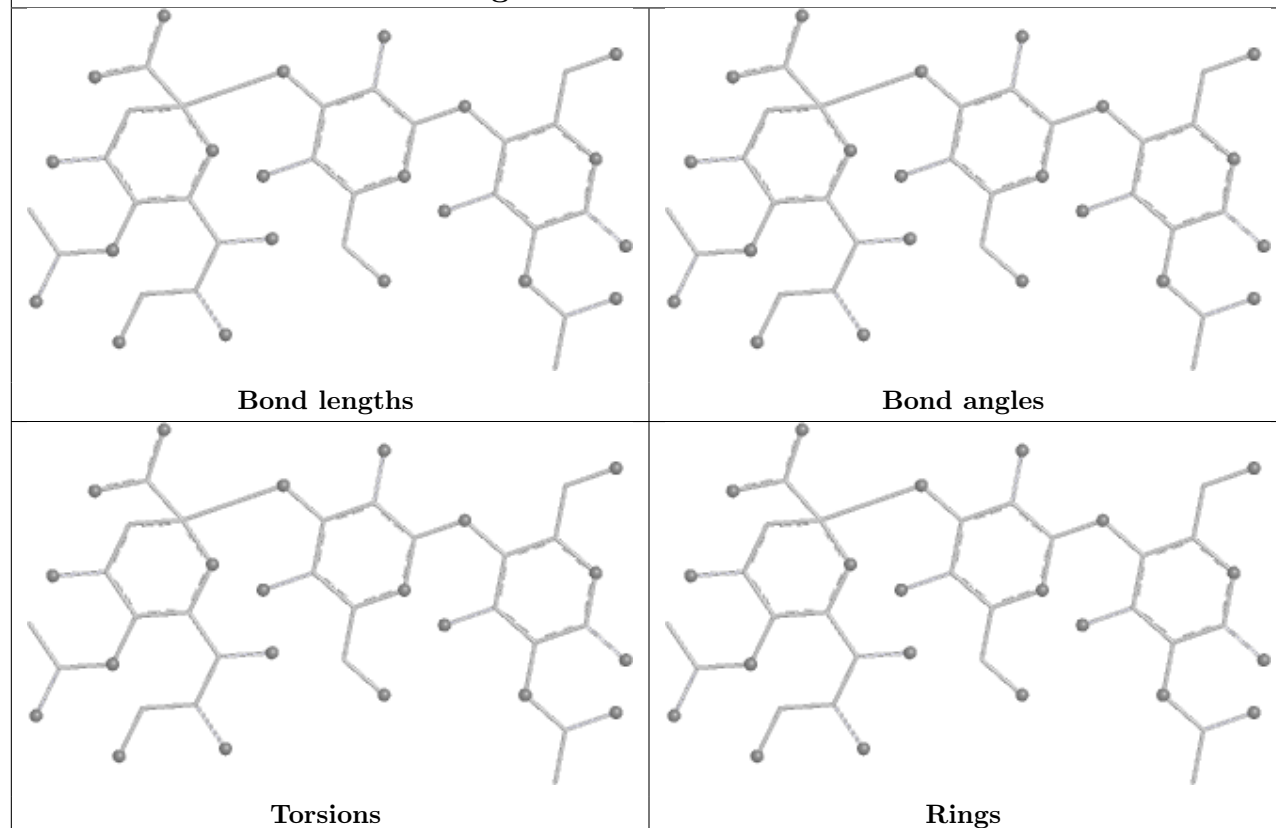
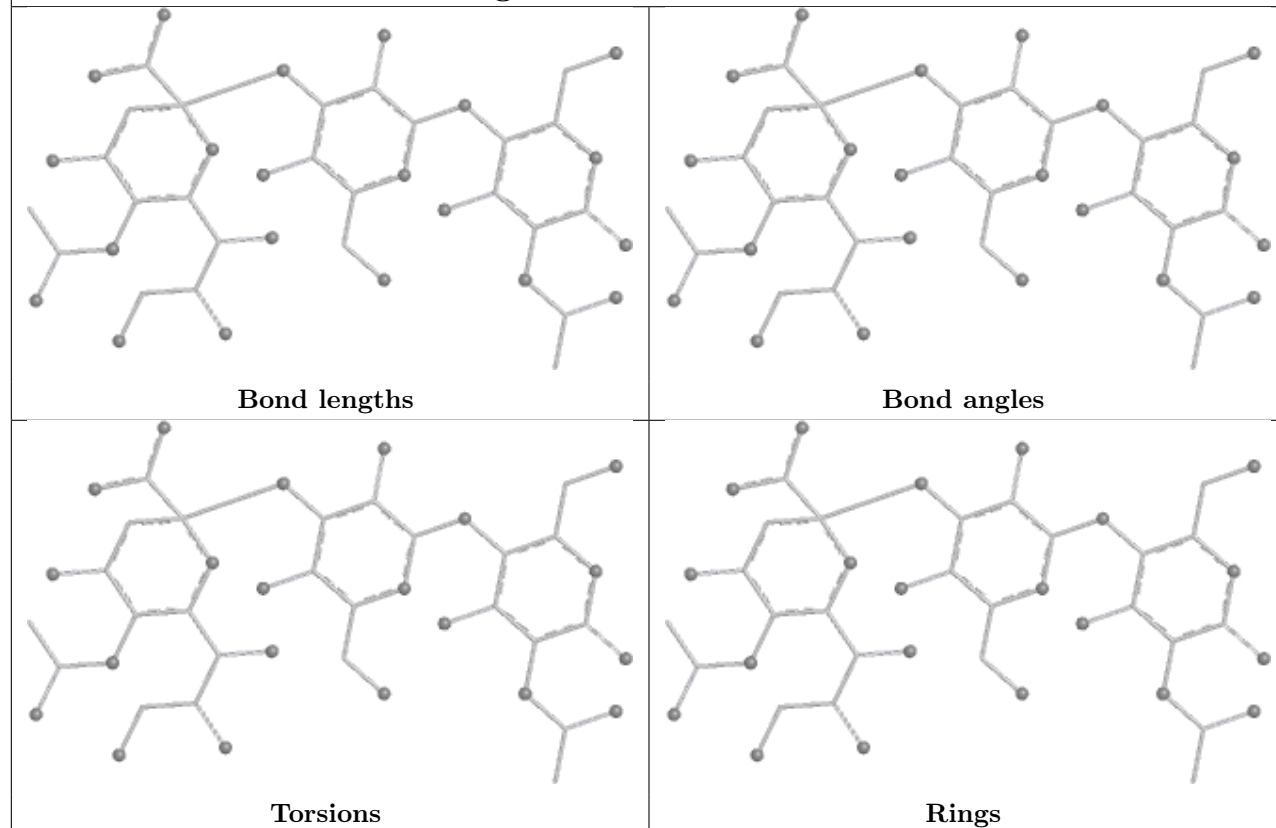


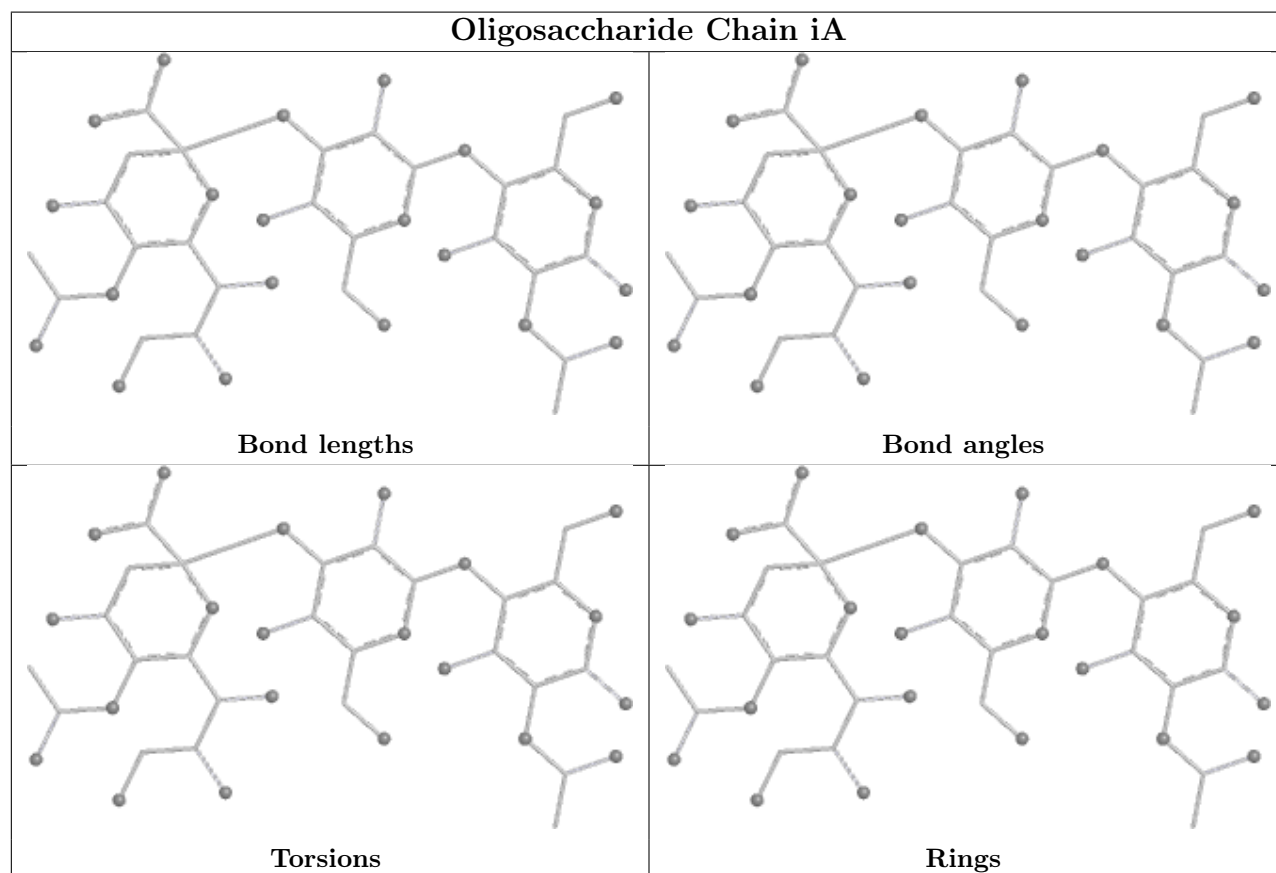
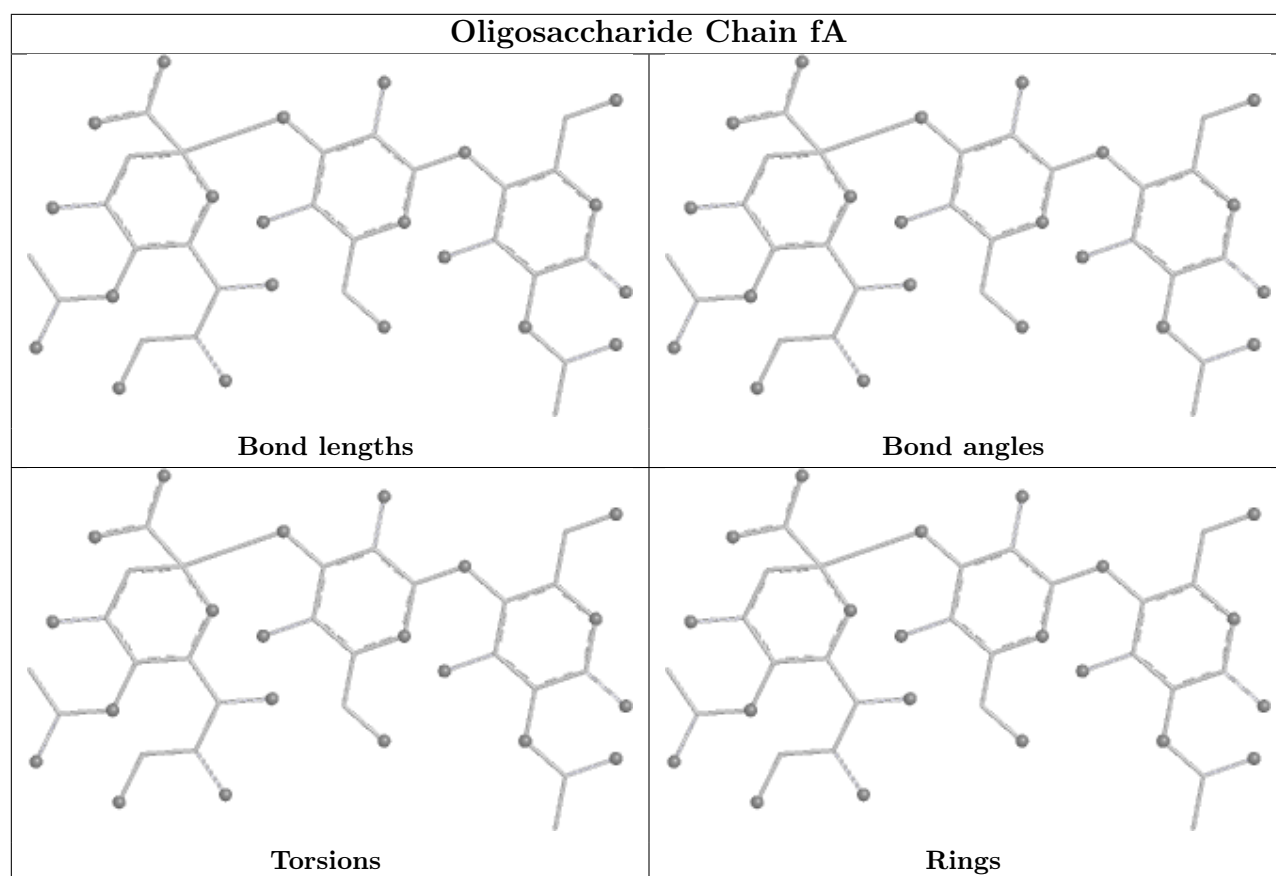
Oligosaccharide Chain BA**Oligosaccharide Chain EA**

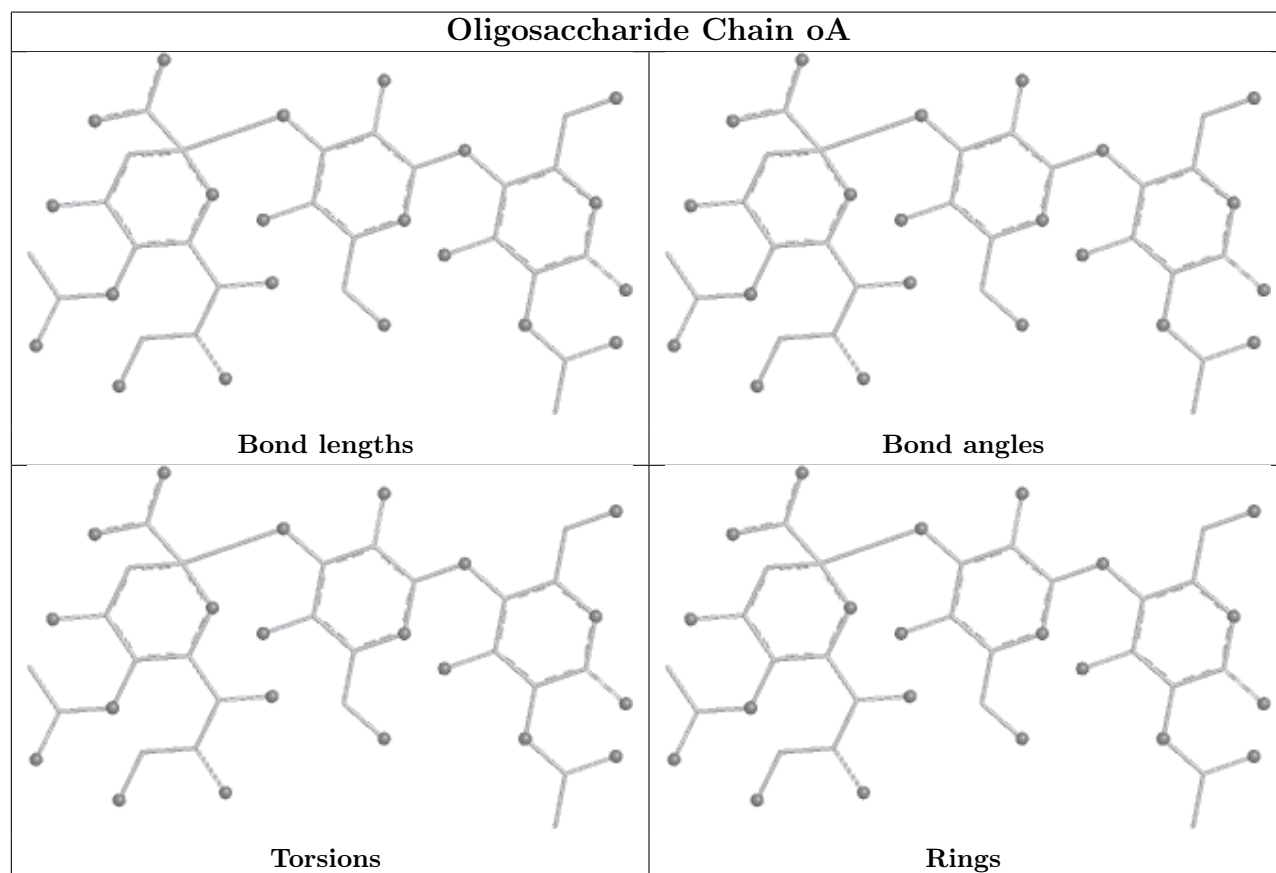
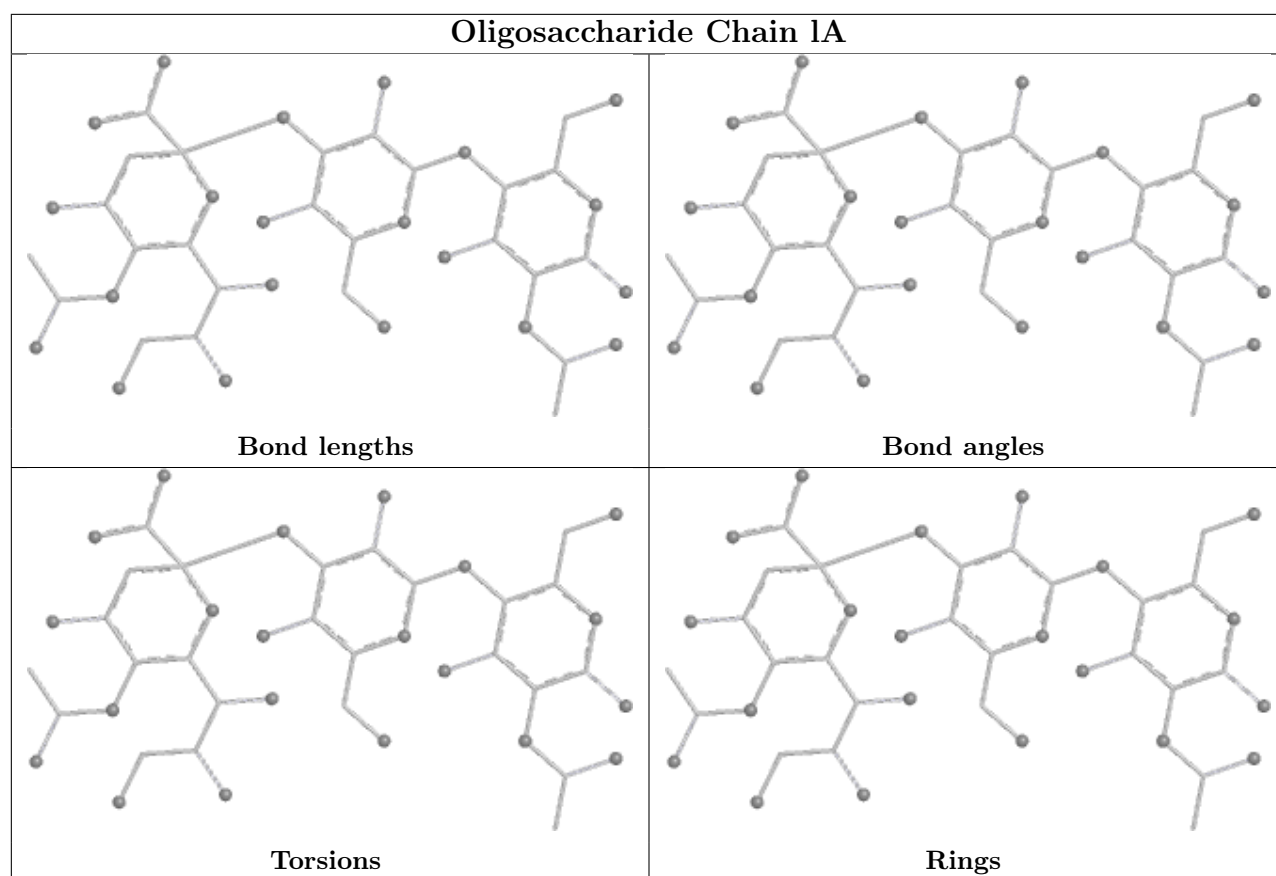
Oligosaccharide Chain HA**Oligosaccharide Chain KA**

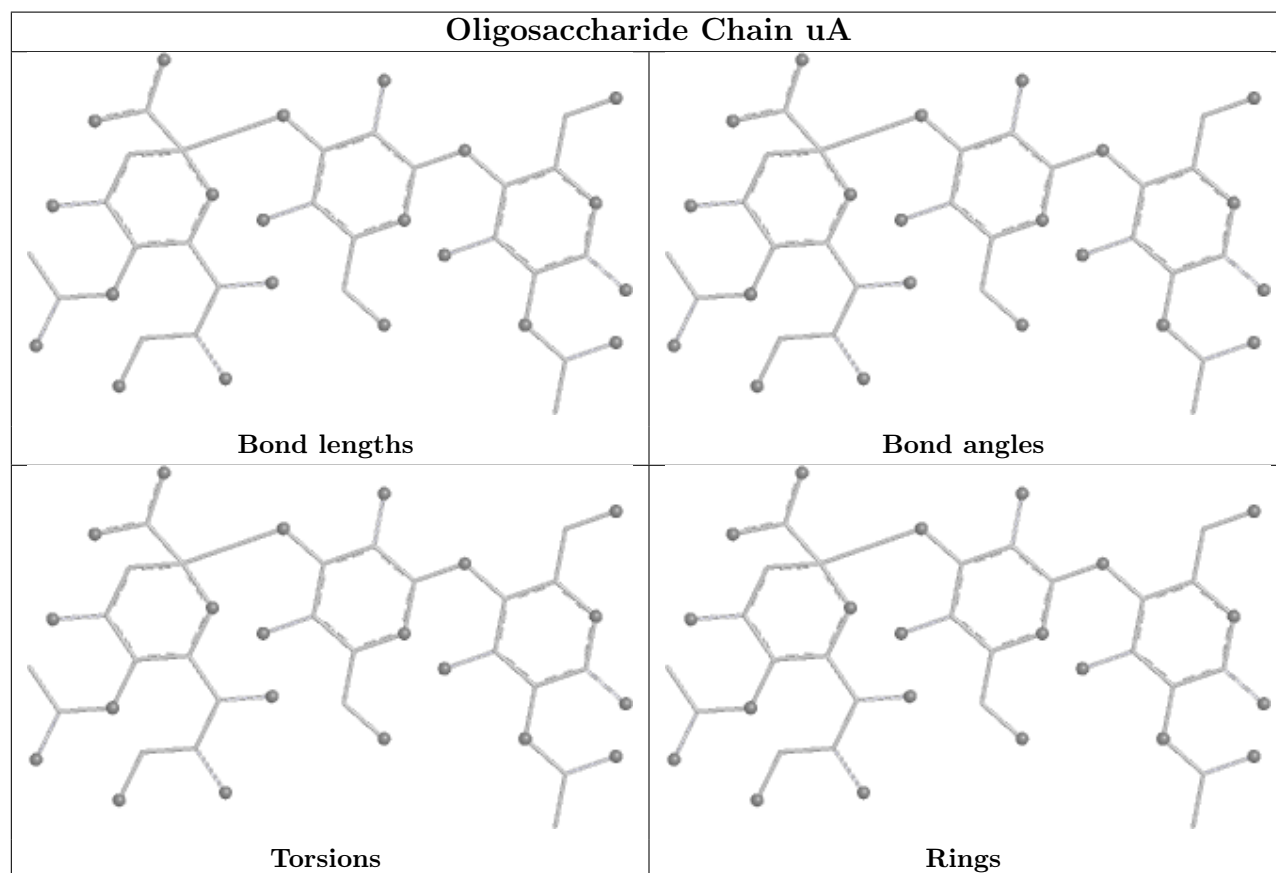
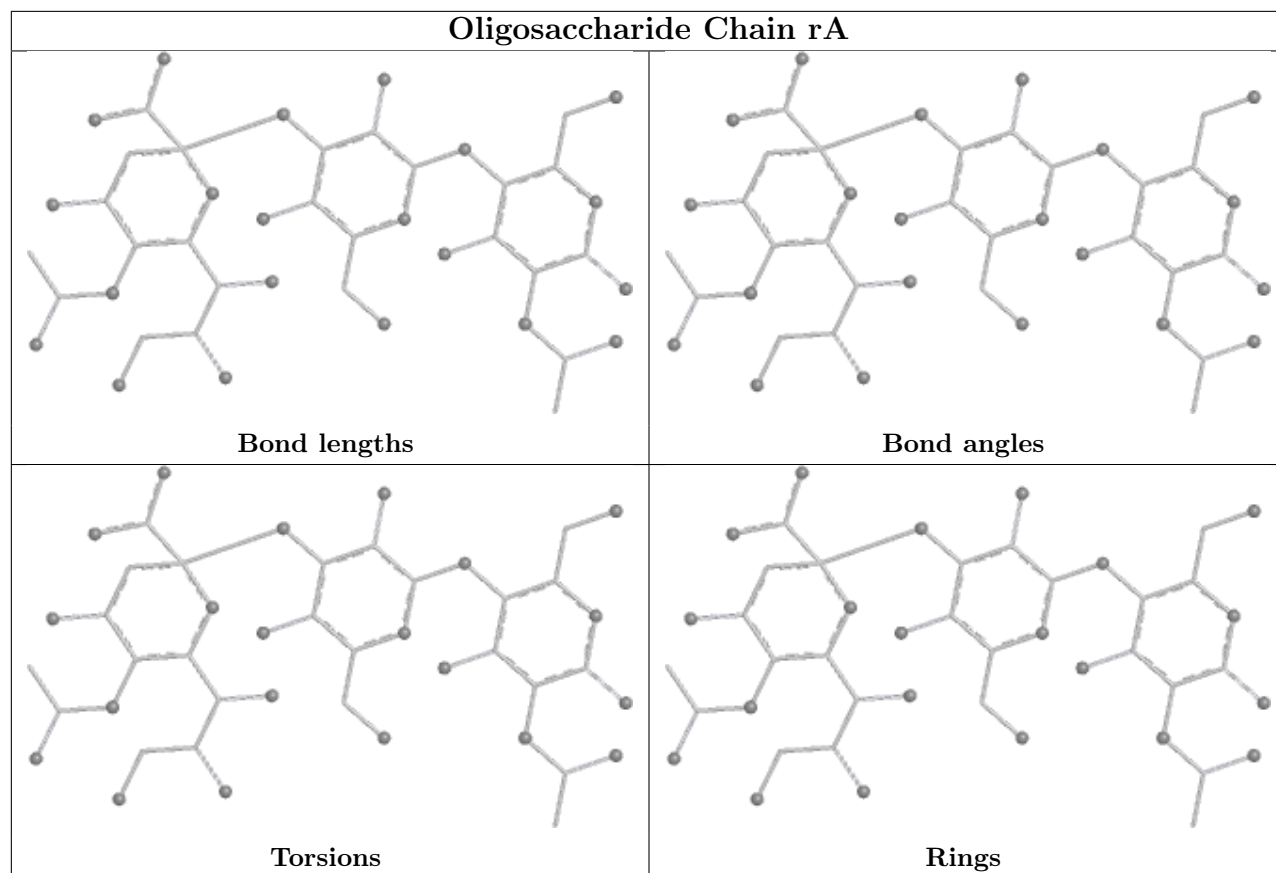
Oligosaccharide Chain NA**Oligosaccharide Chain QA**

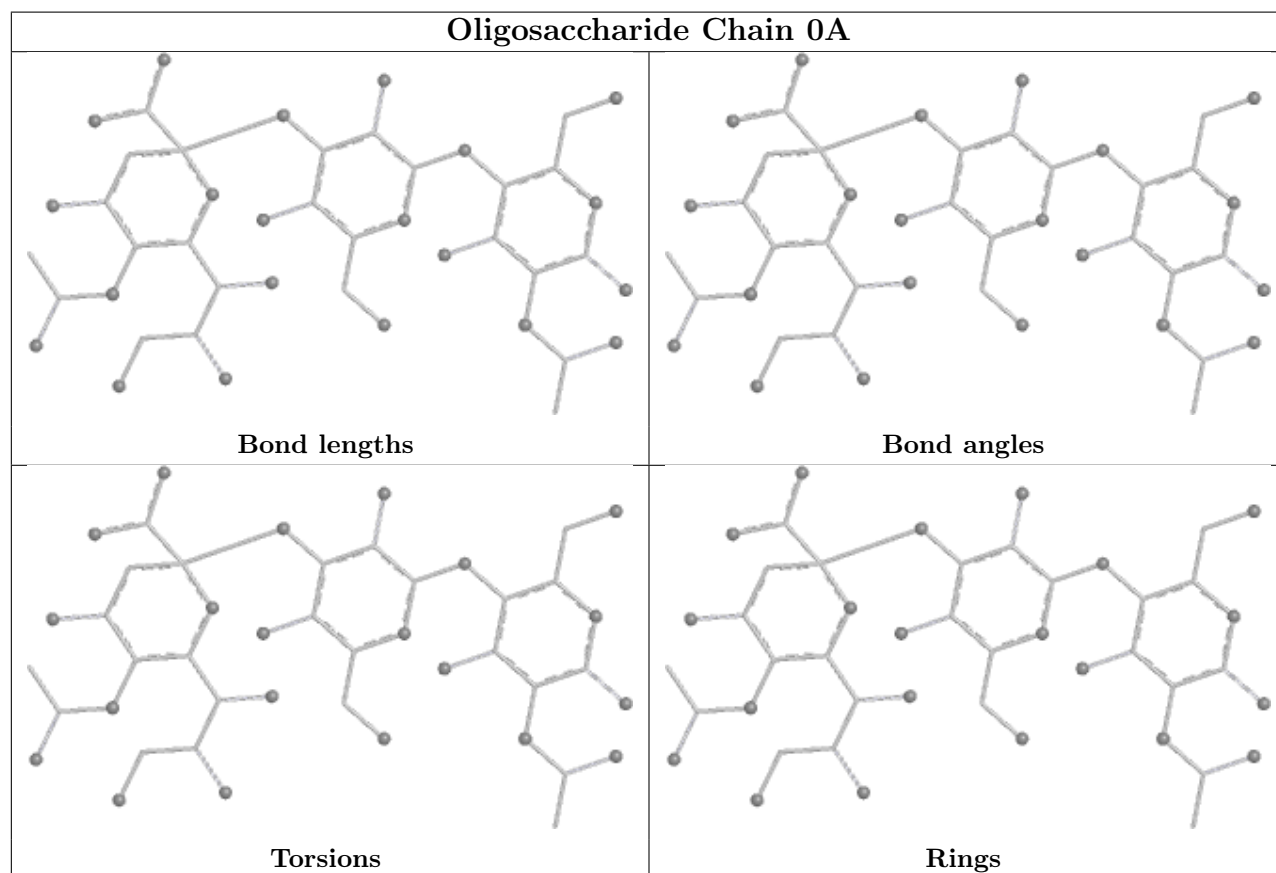
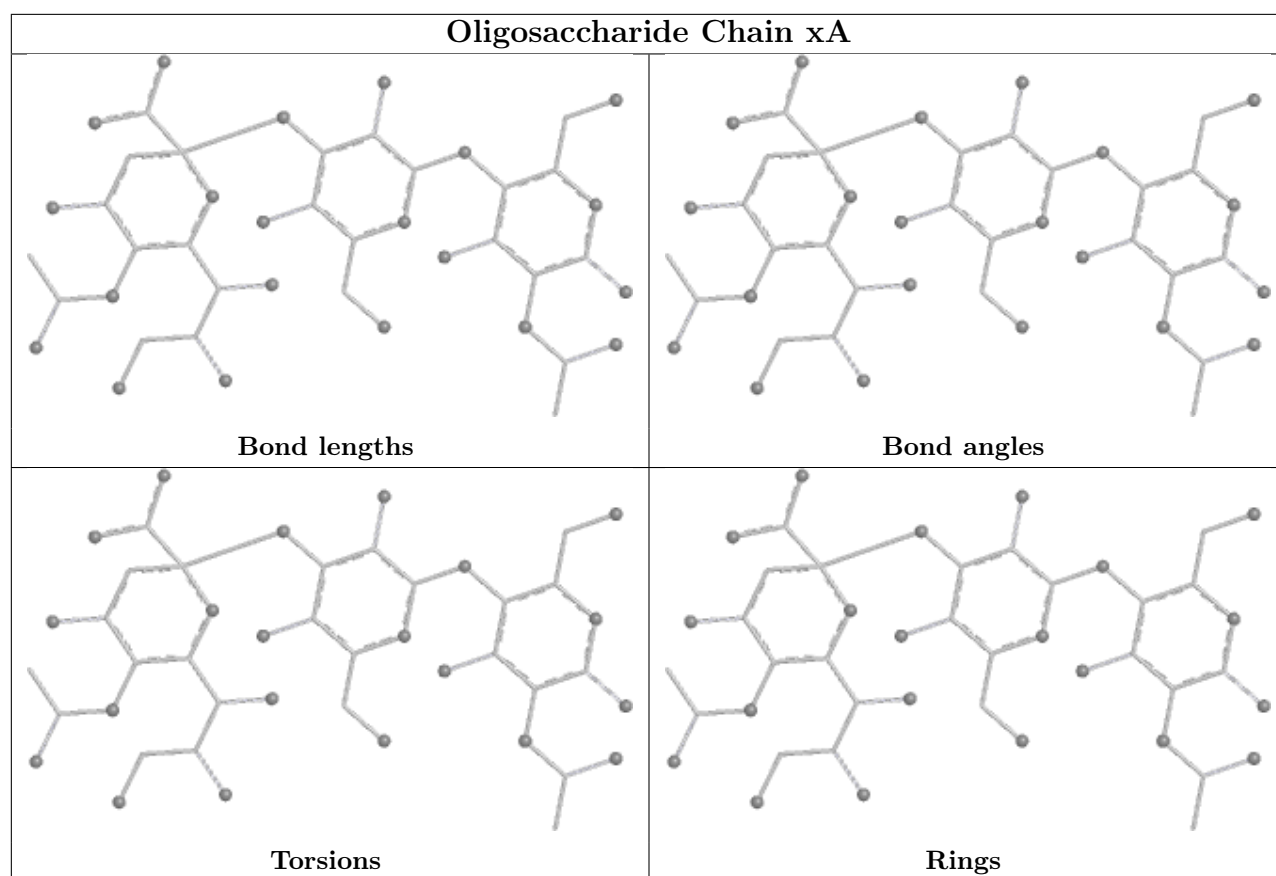


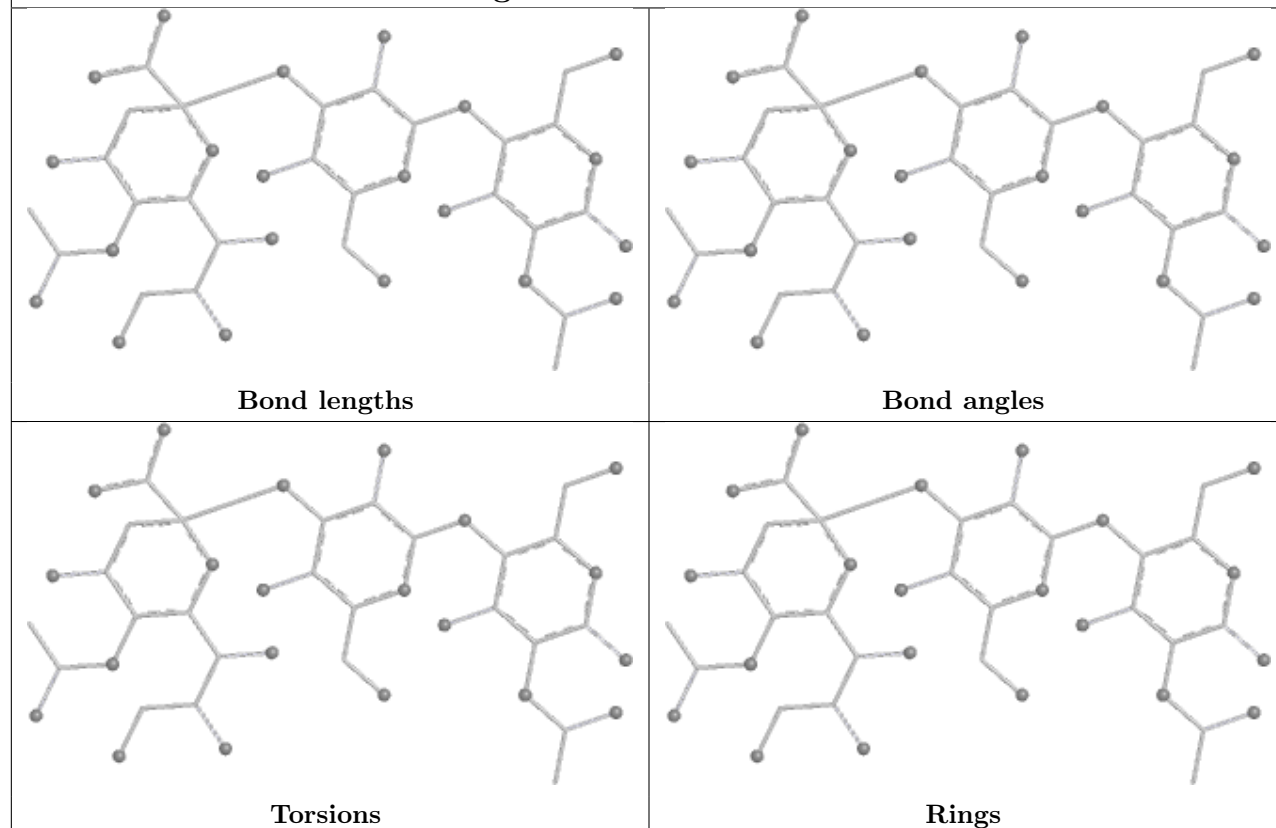
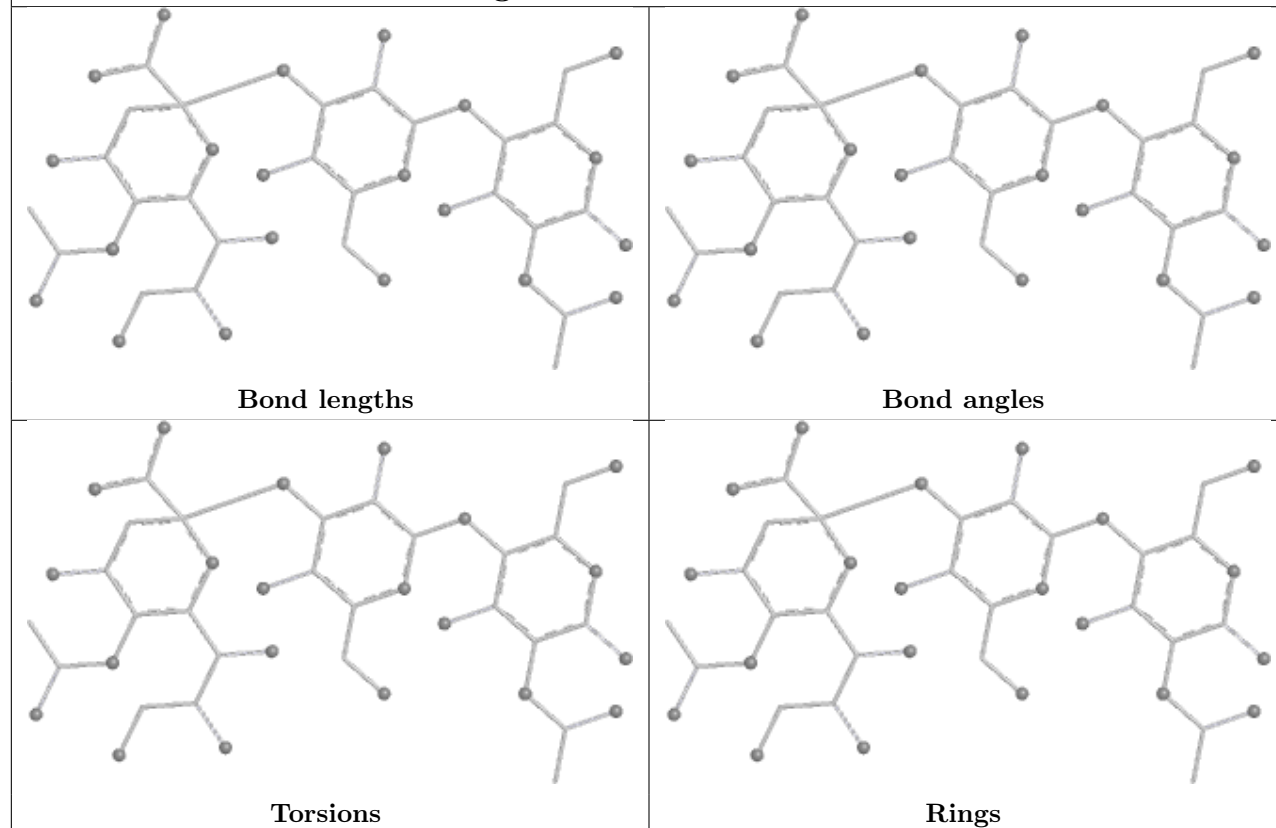
Oligosaccharide Chain ZA**Oligosaccharide Chain cA**

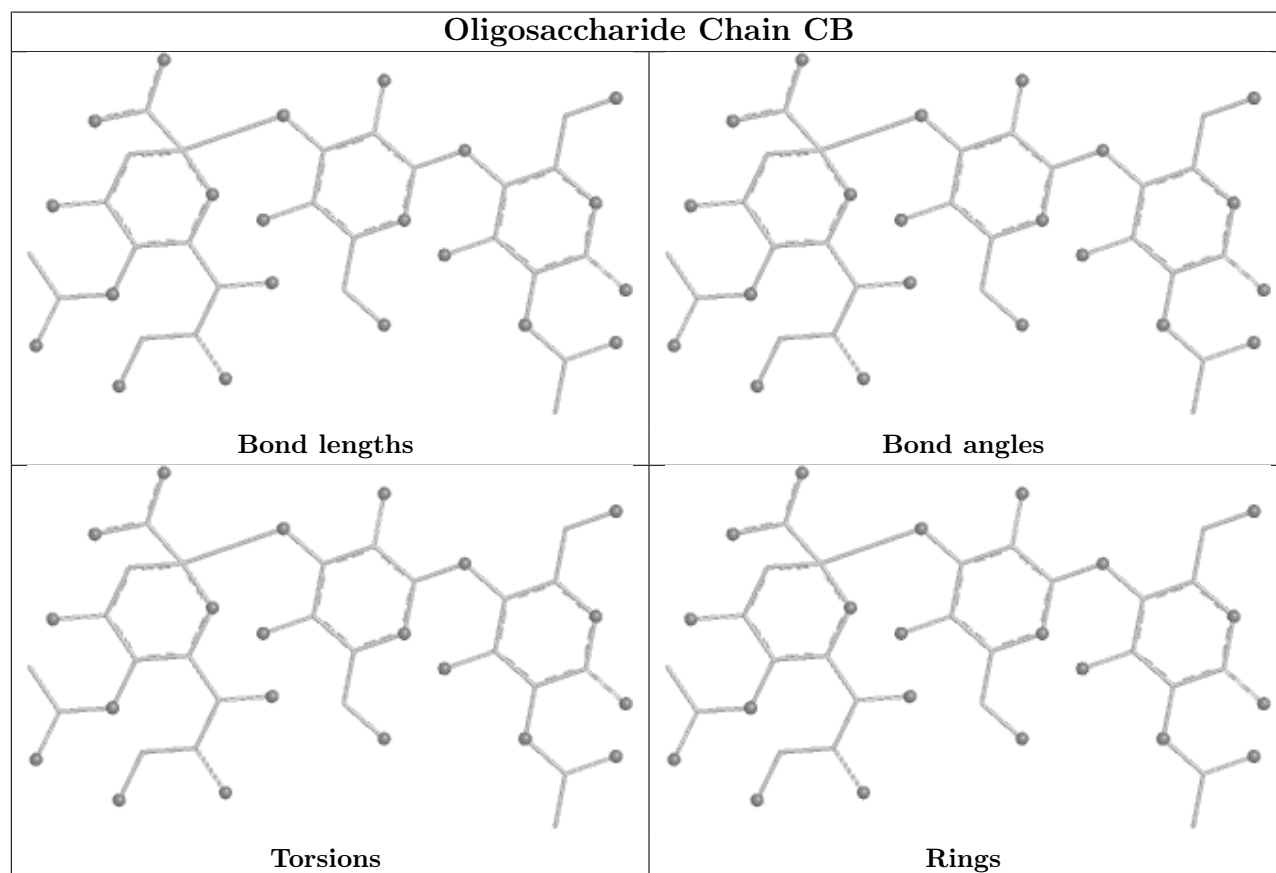
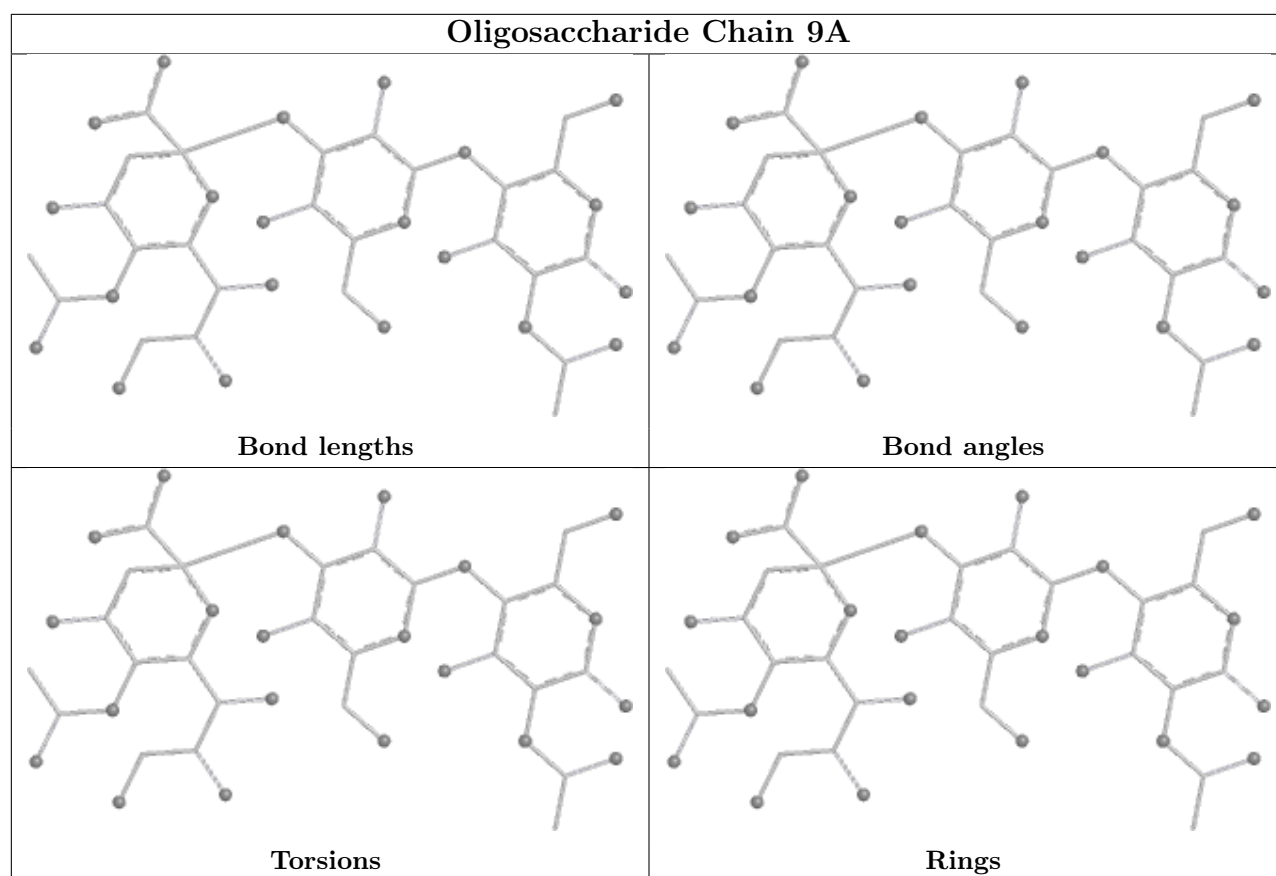


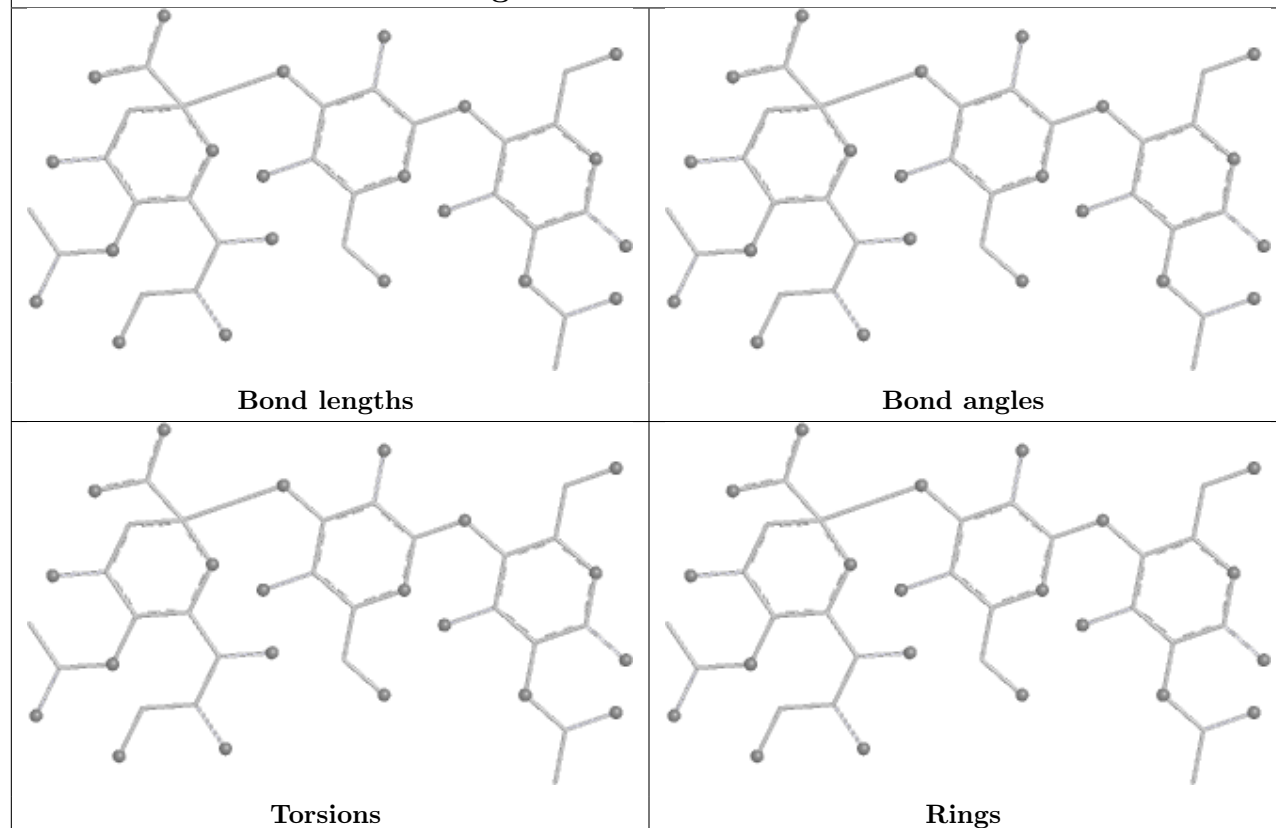
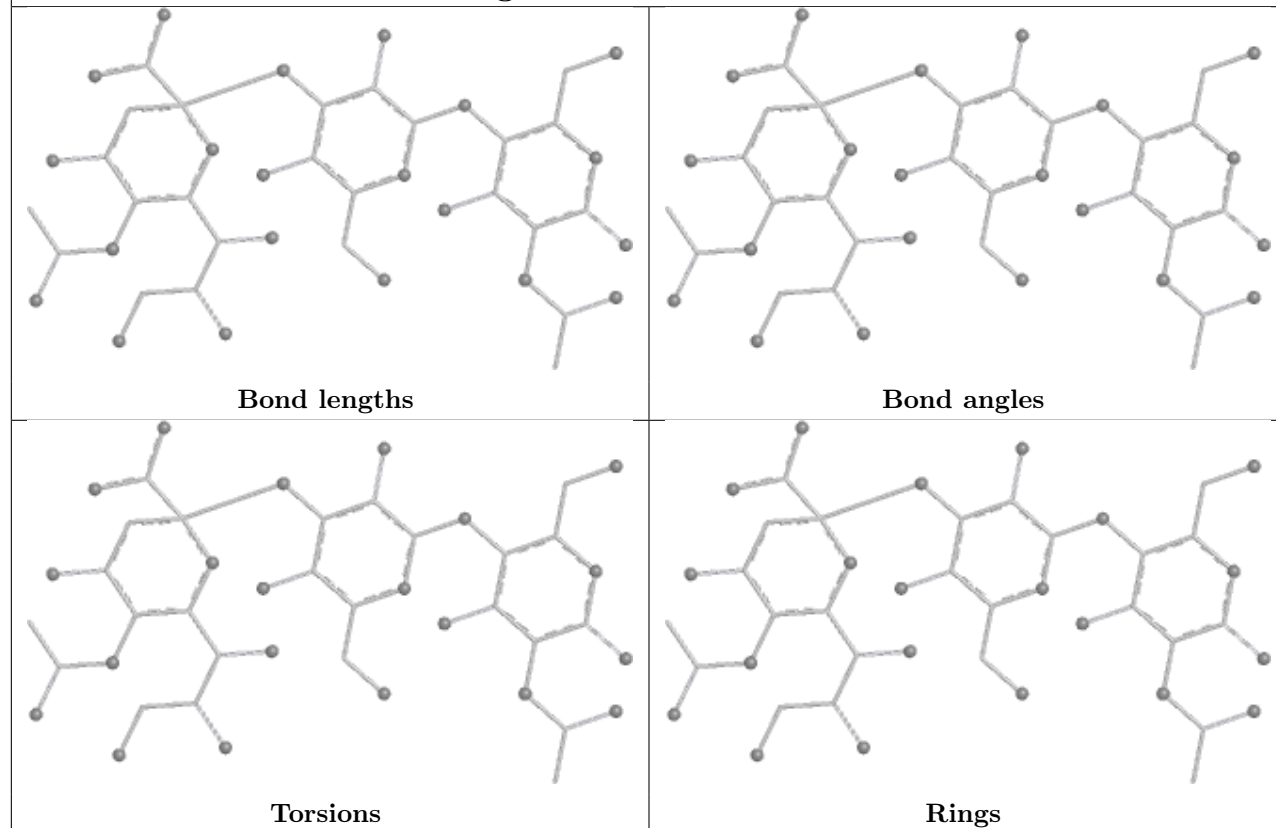


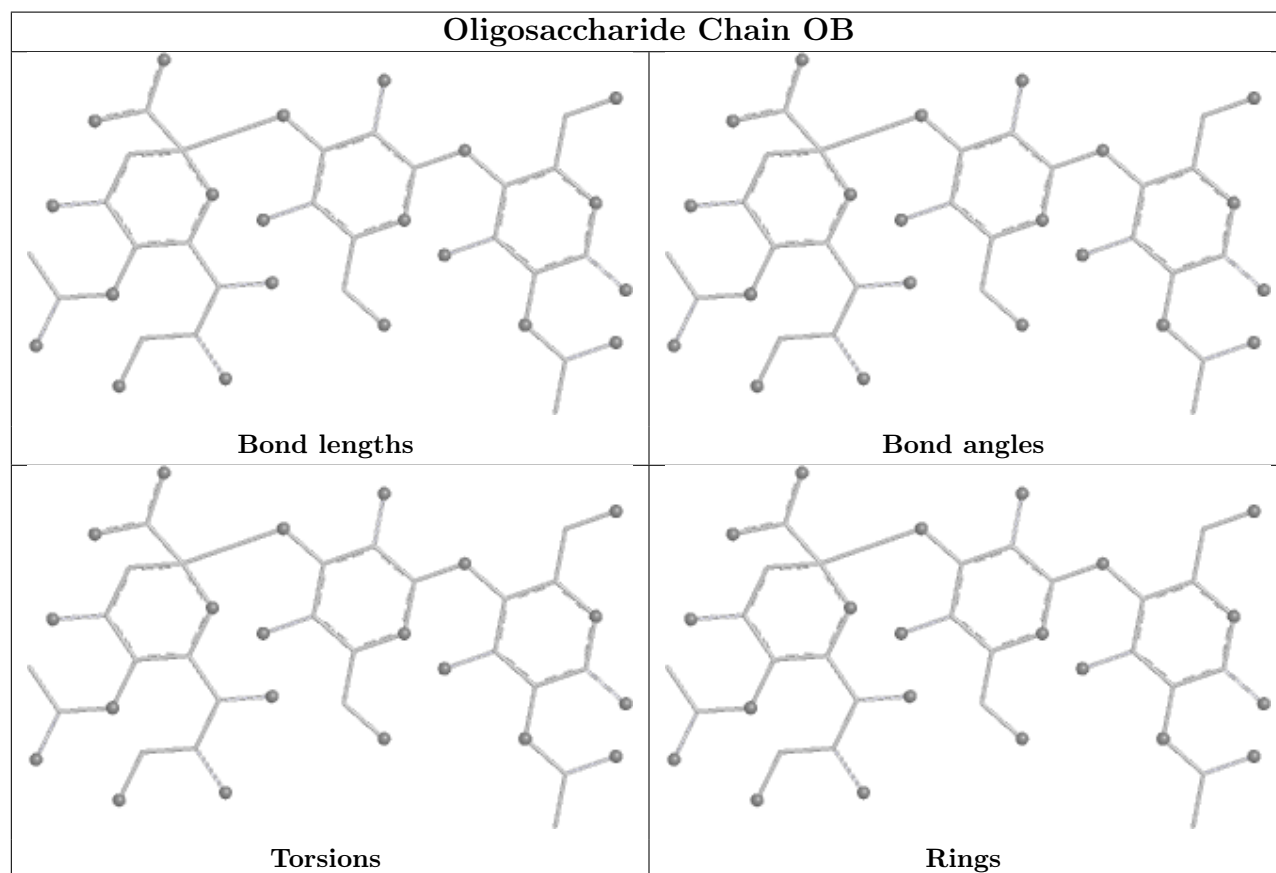
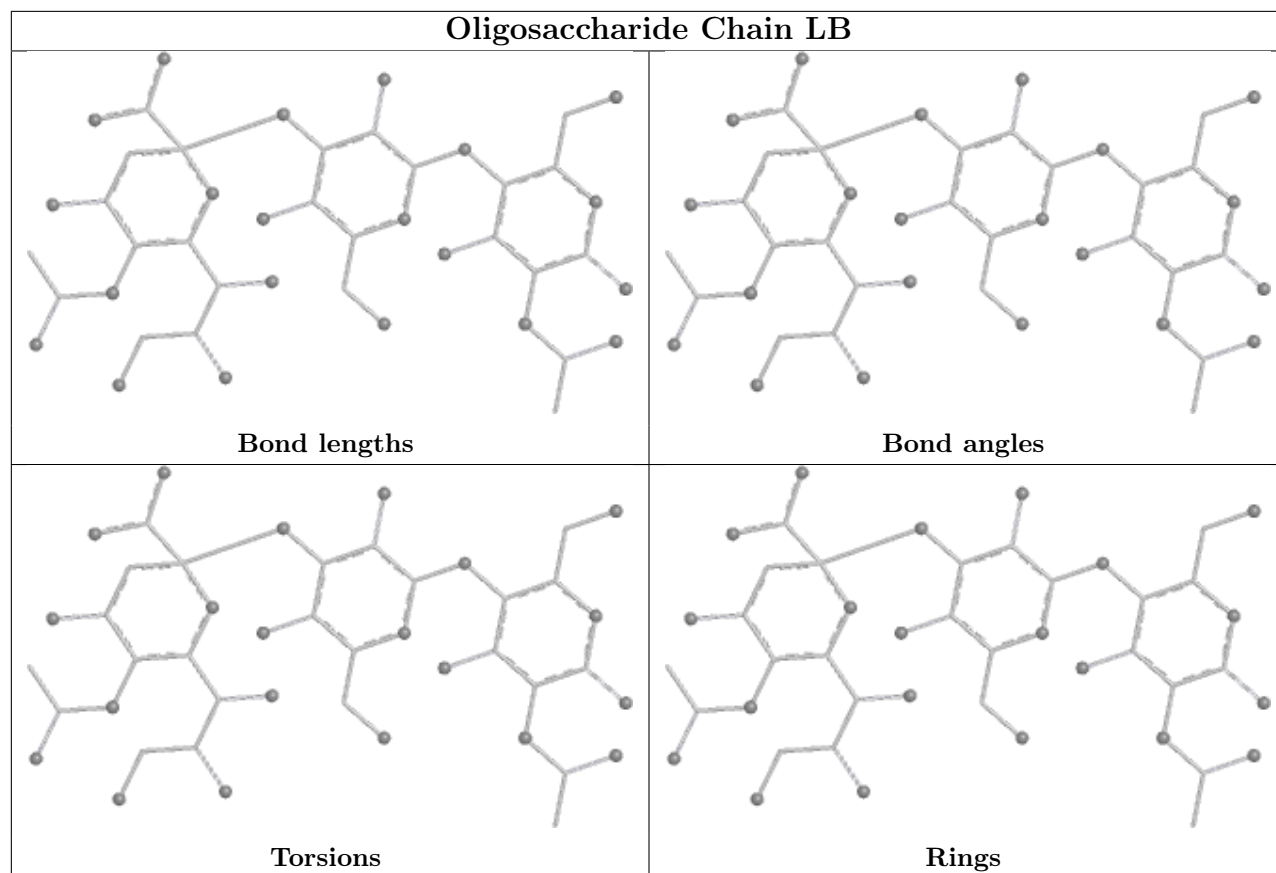


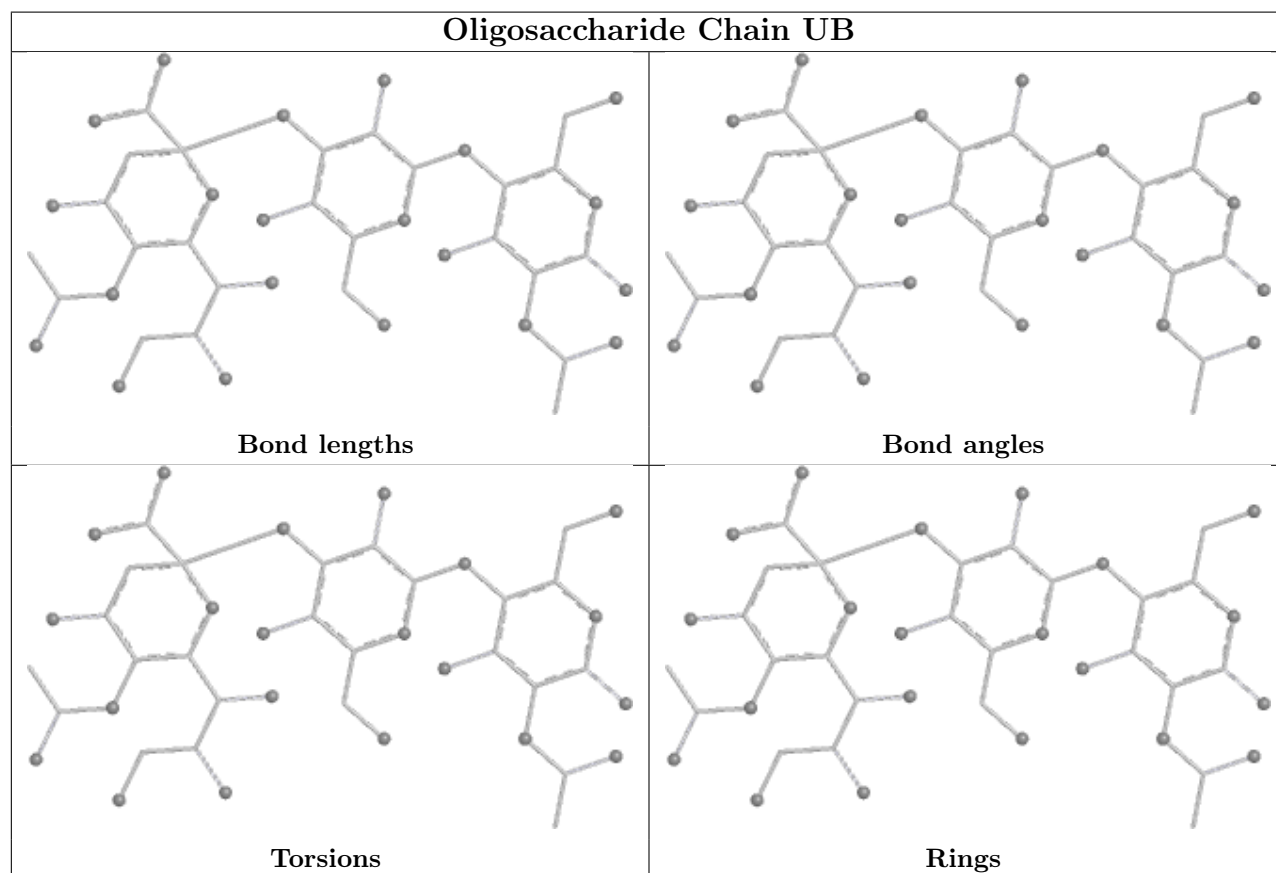
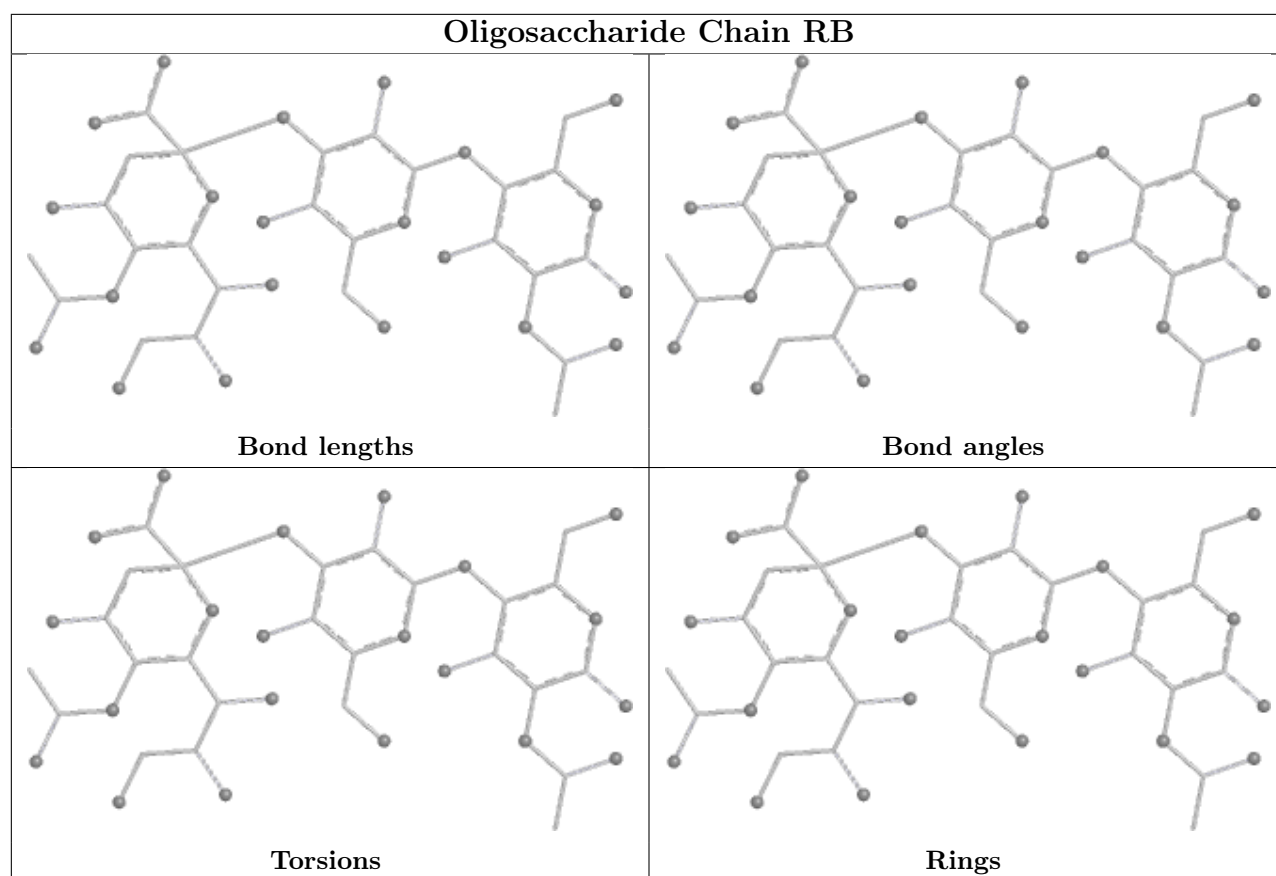


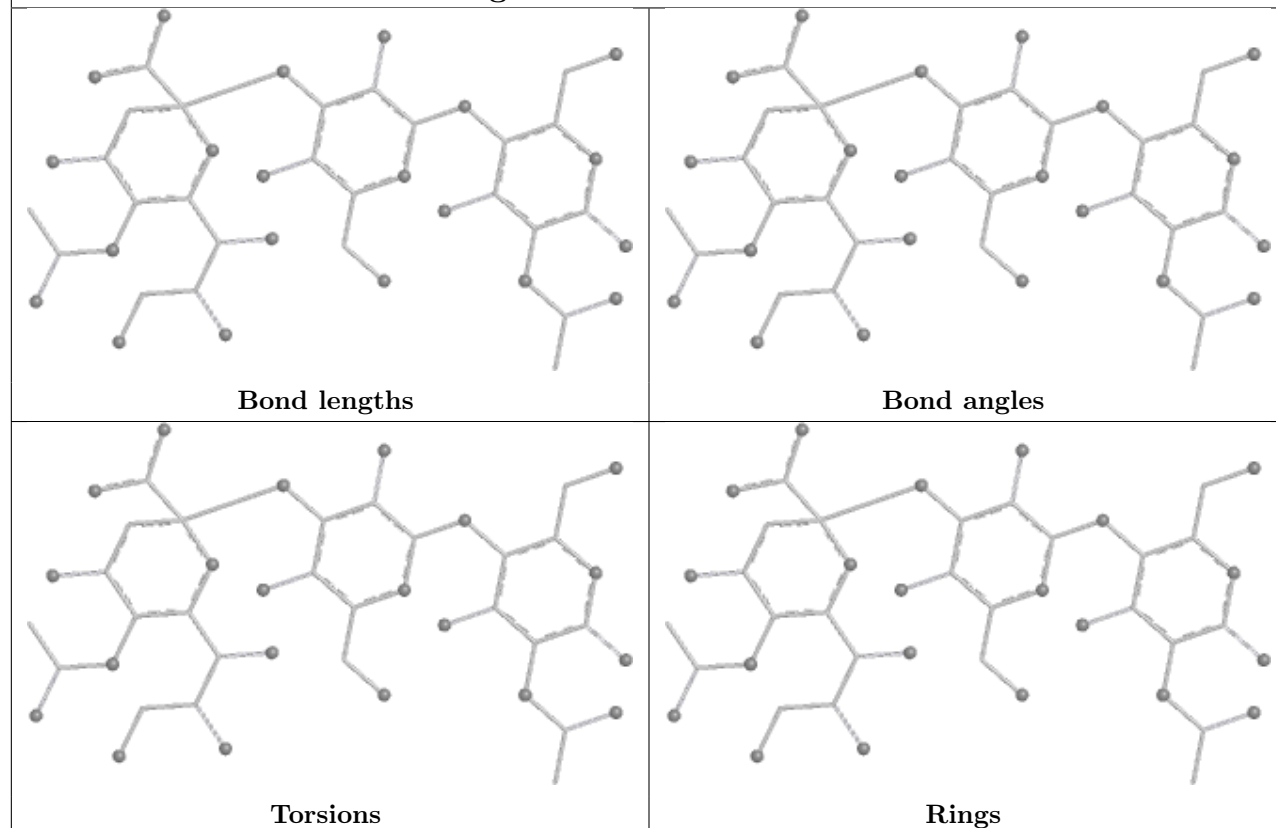
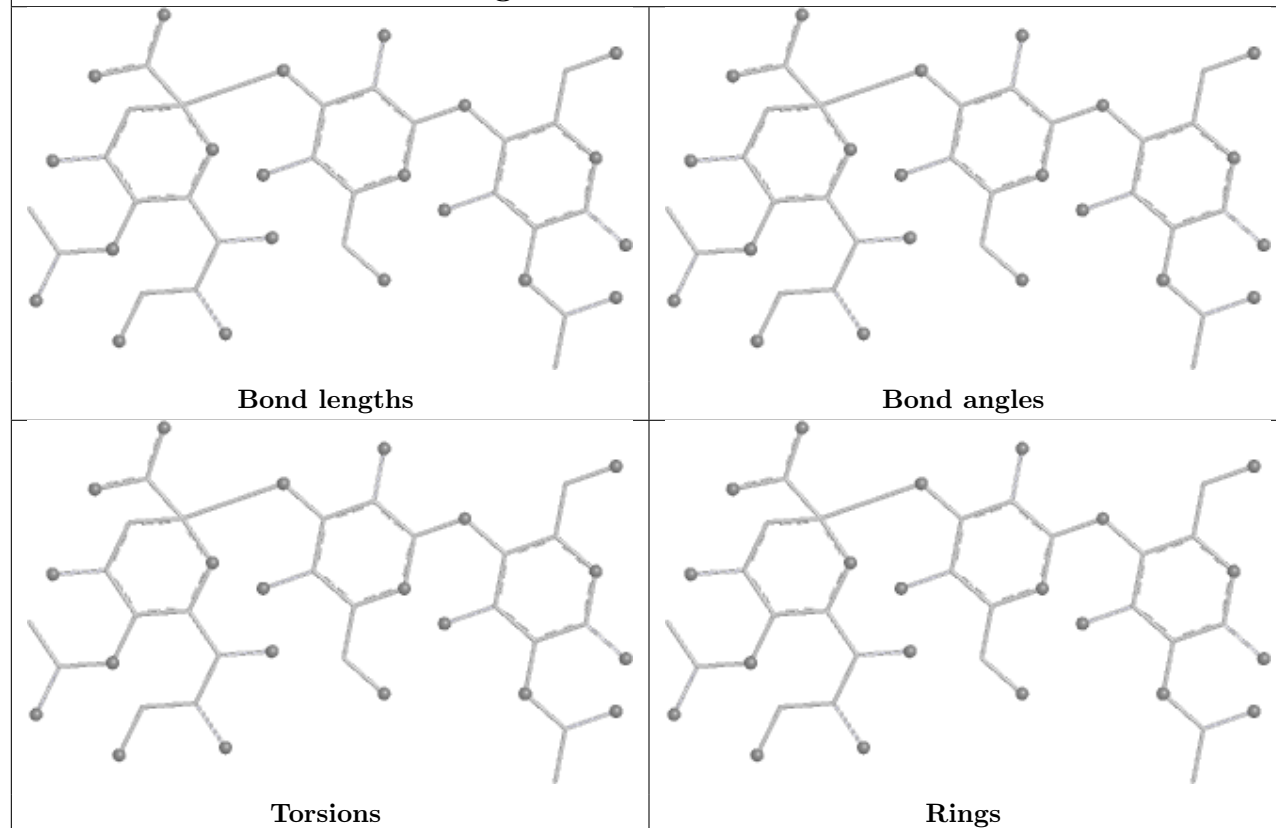
Oligosaccharide Chain 3A**Oligosaccharide Chain 6A**

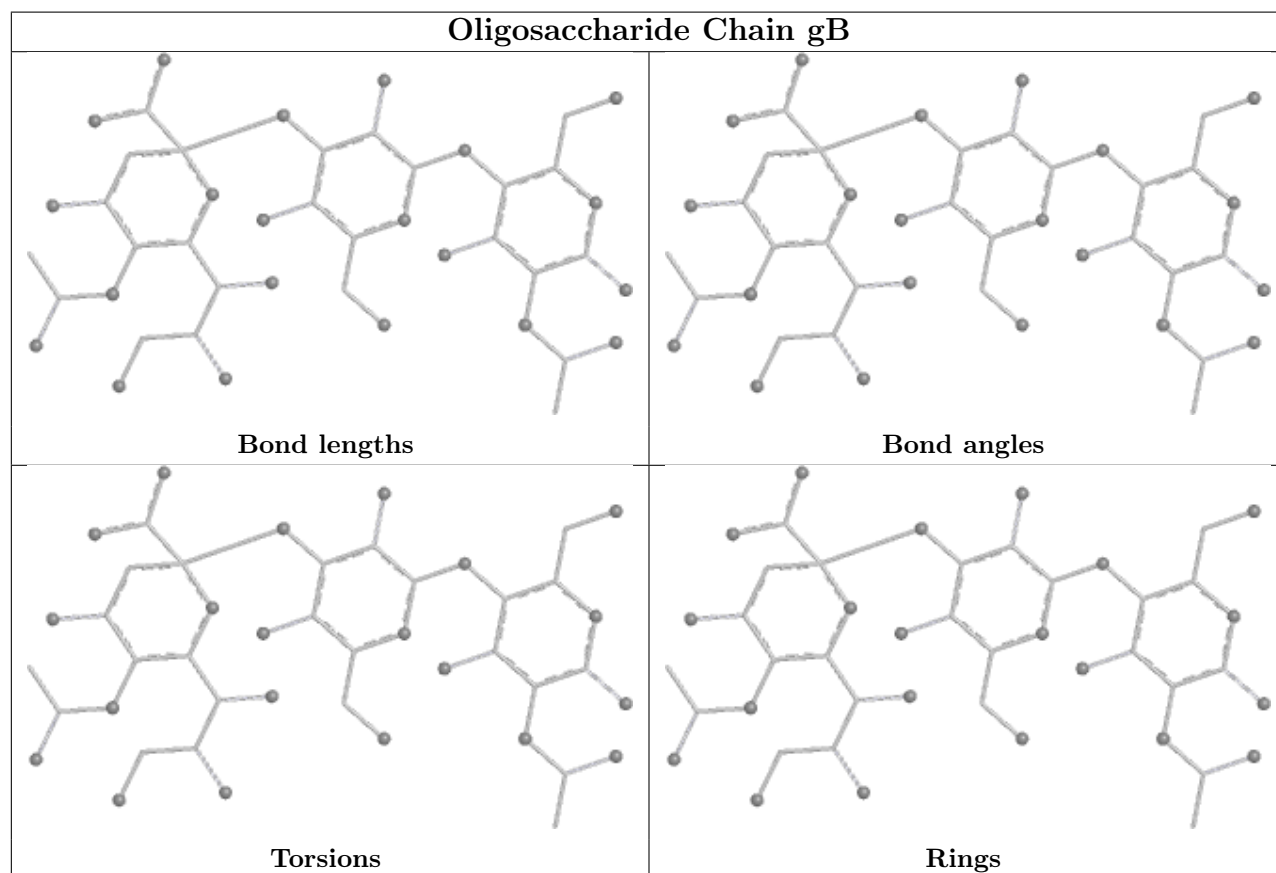
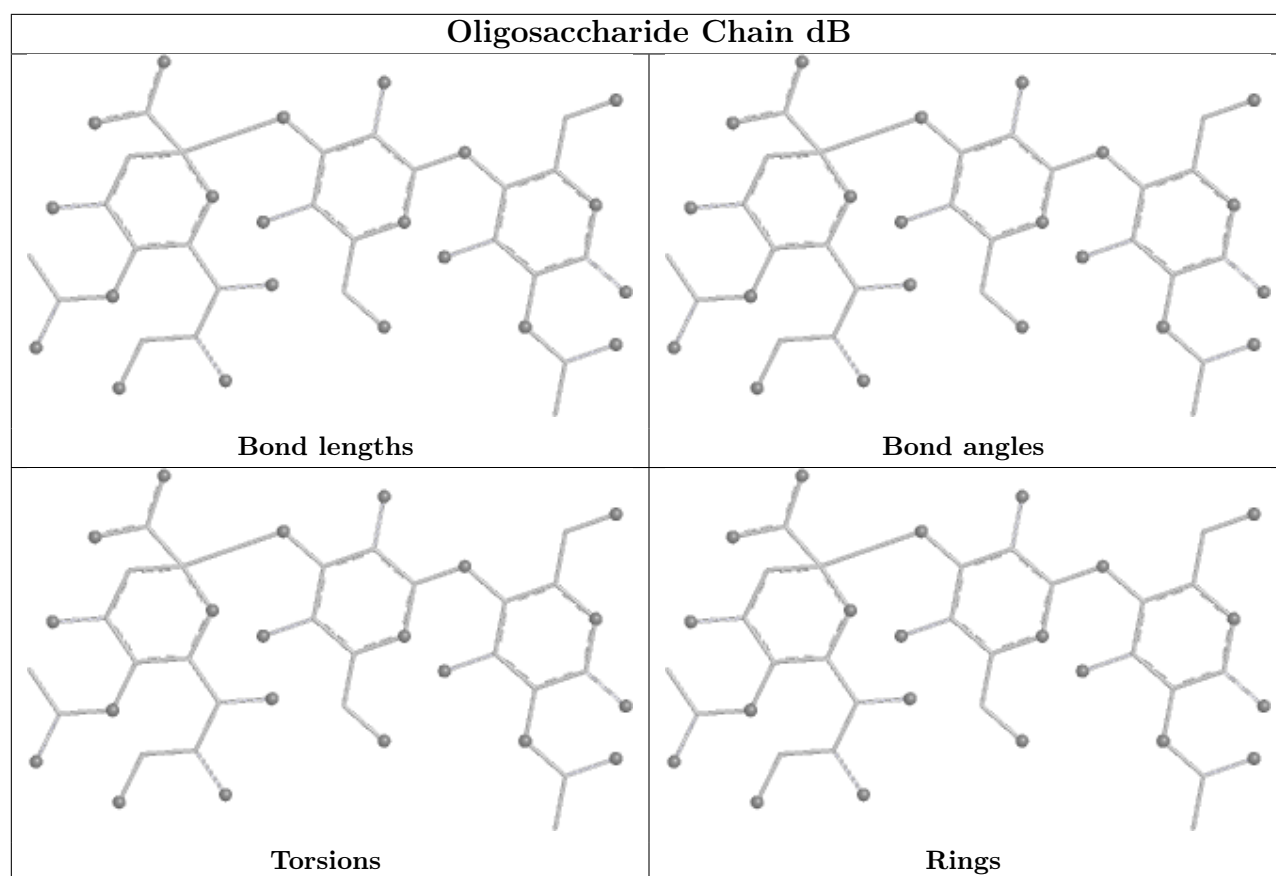


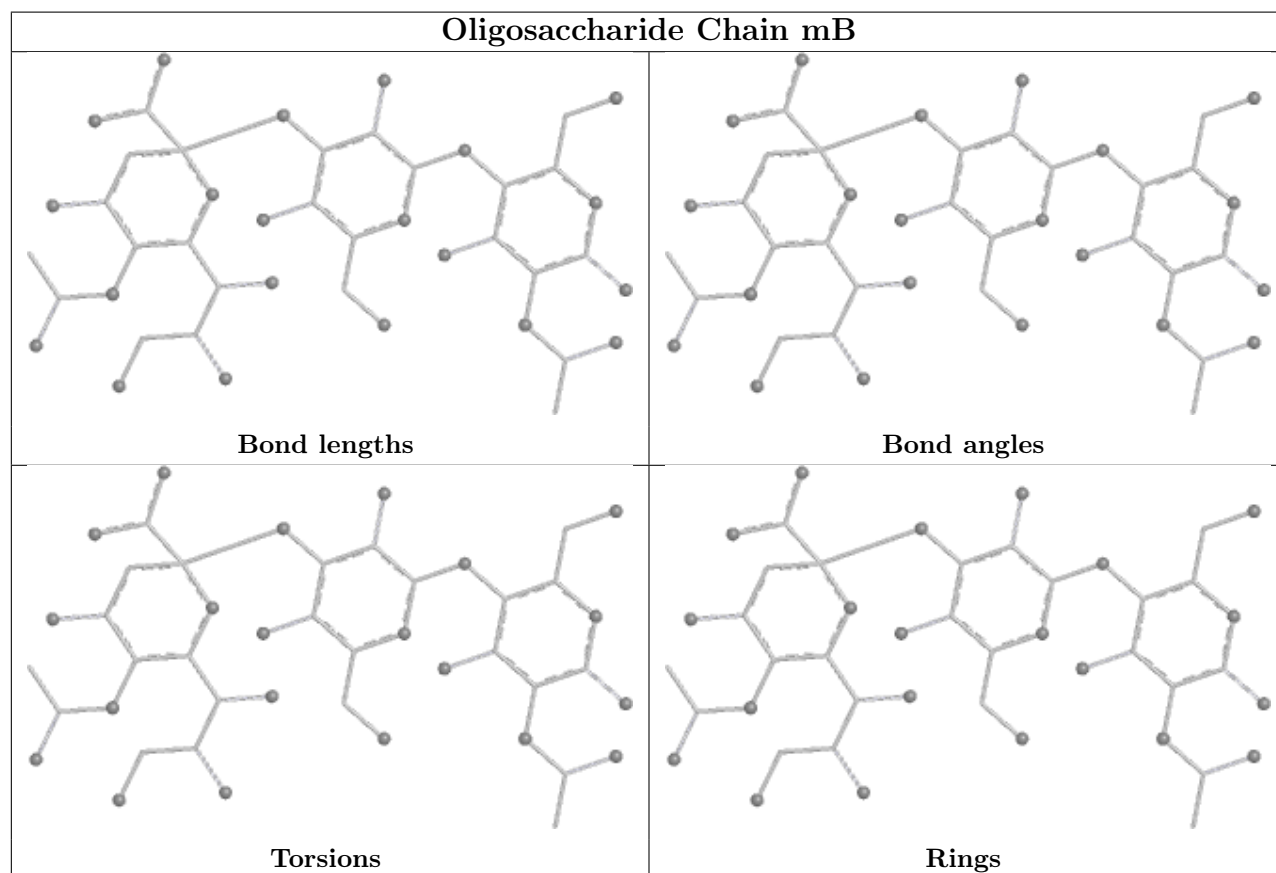
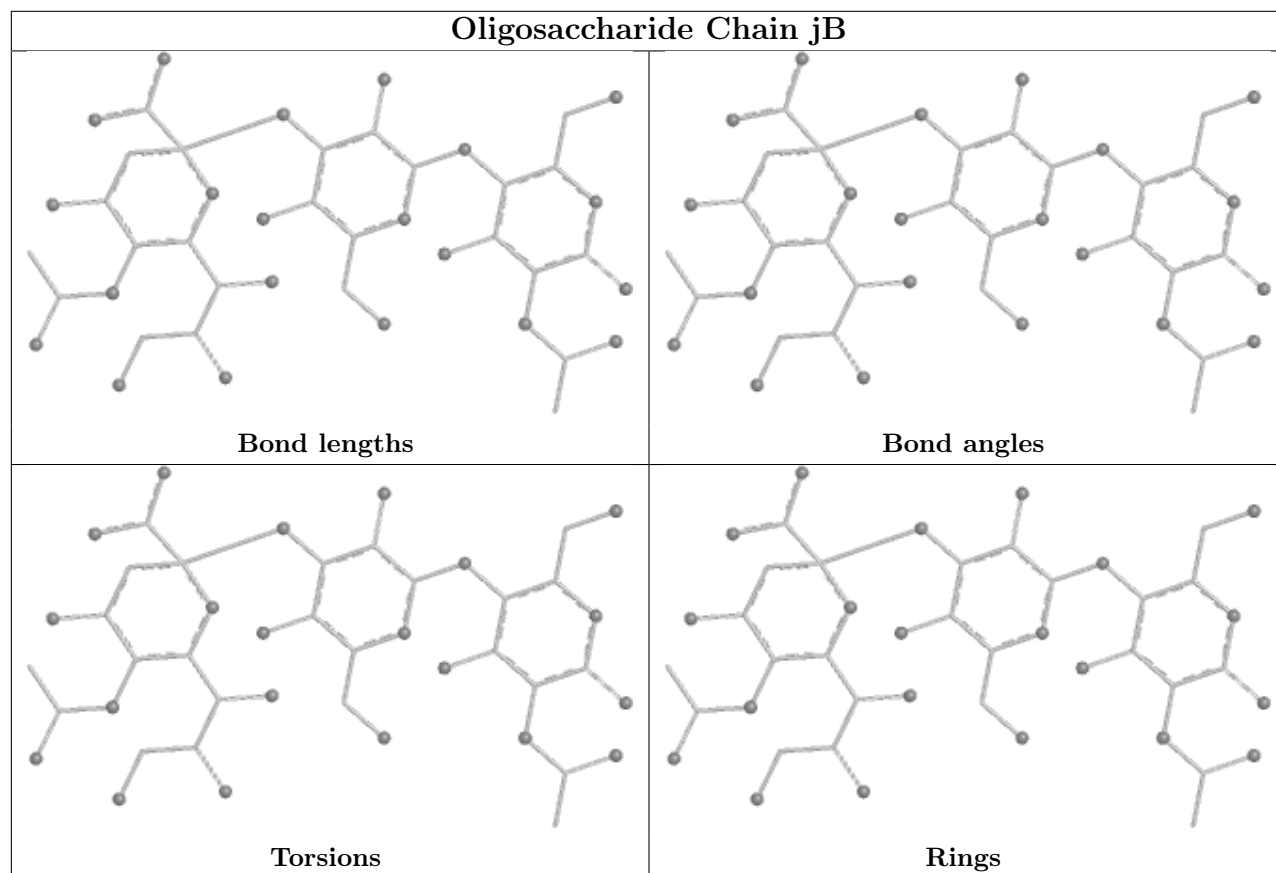
Oligosaccharide Chain FB**Oligosaccharide Chain IB**

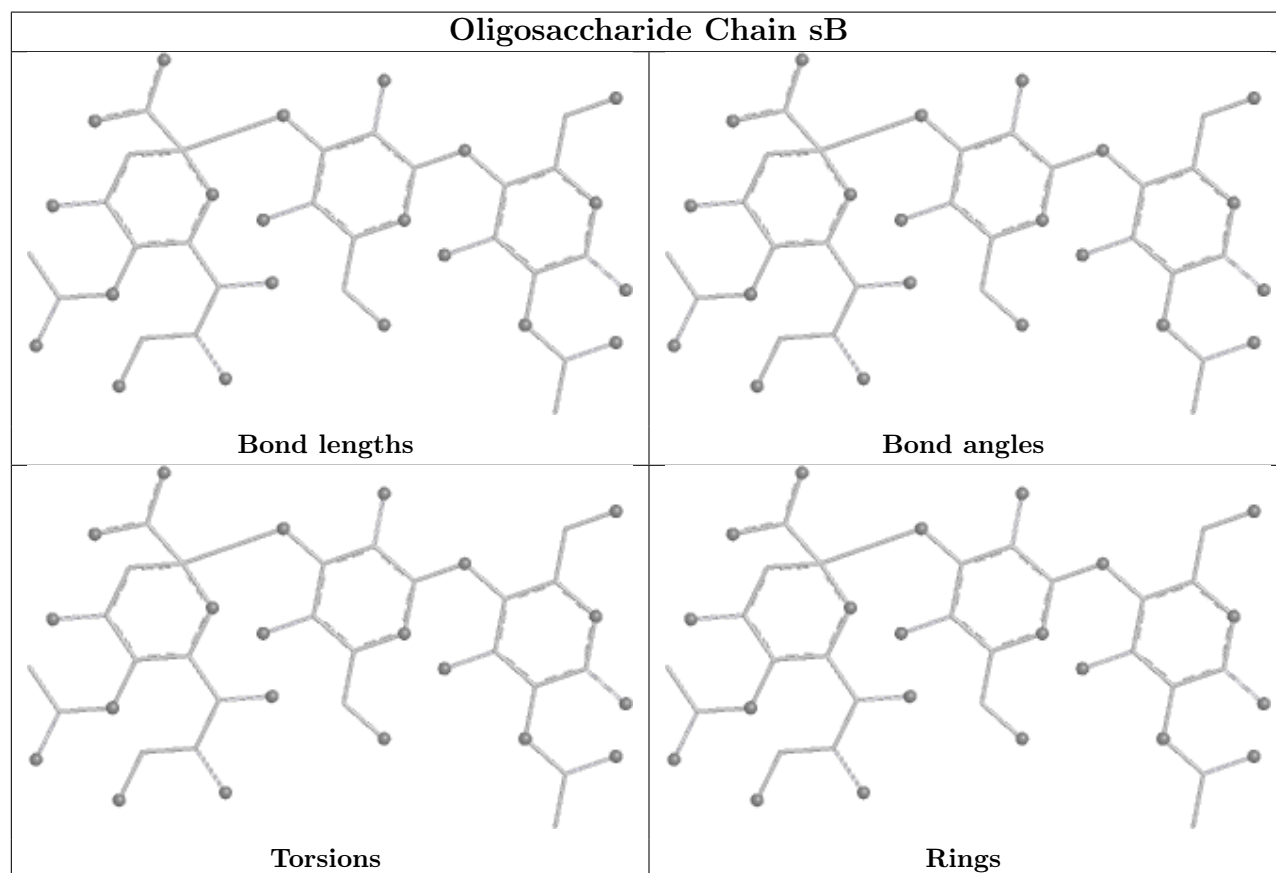
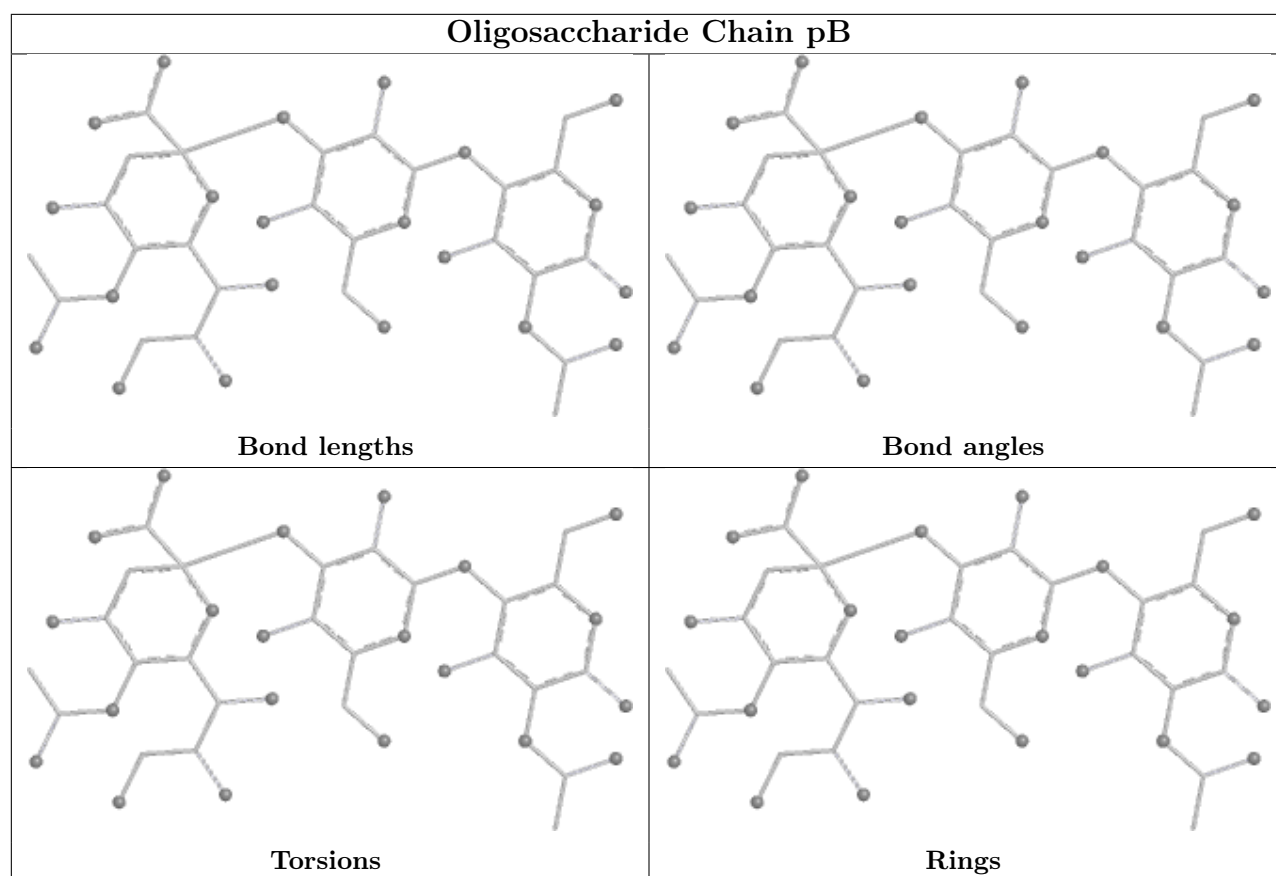


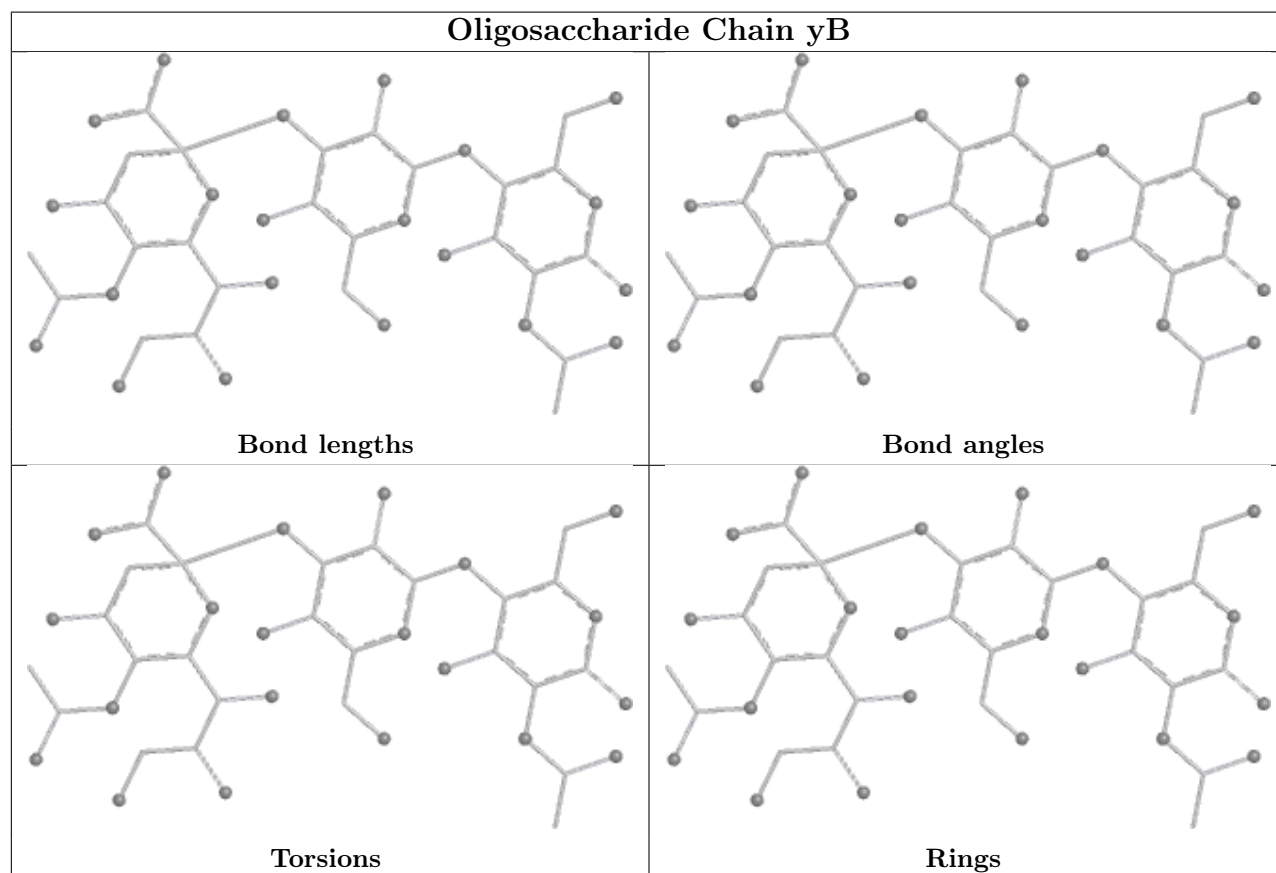
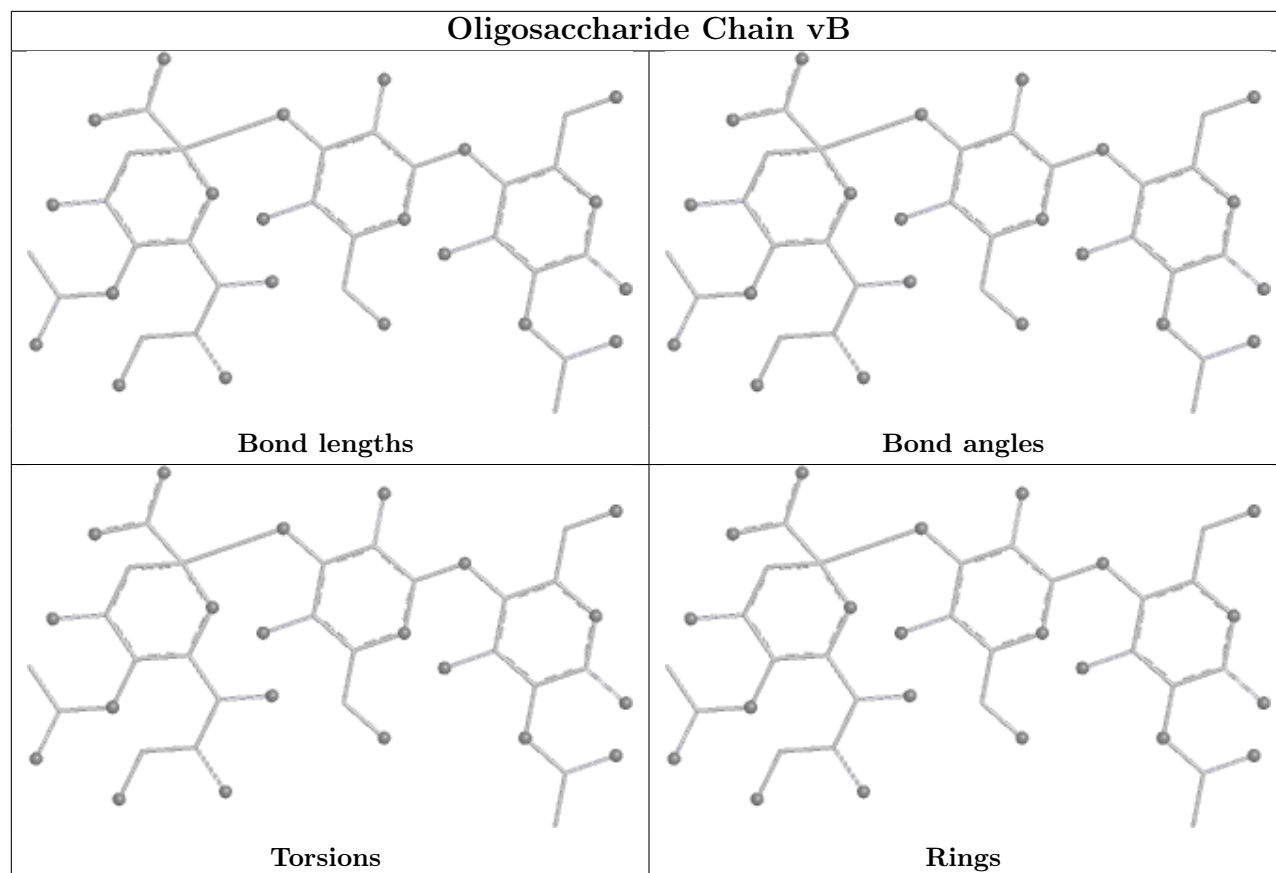


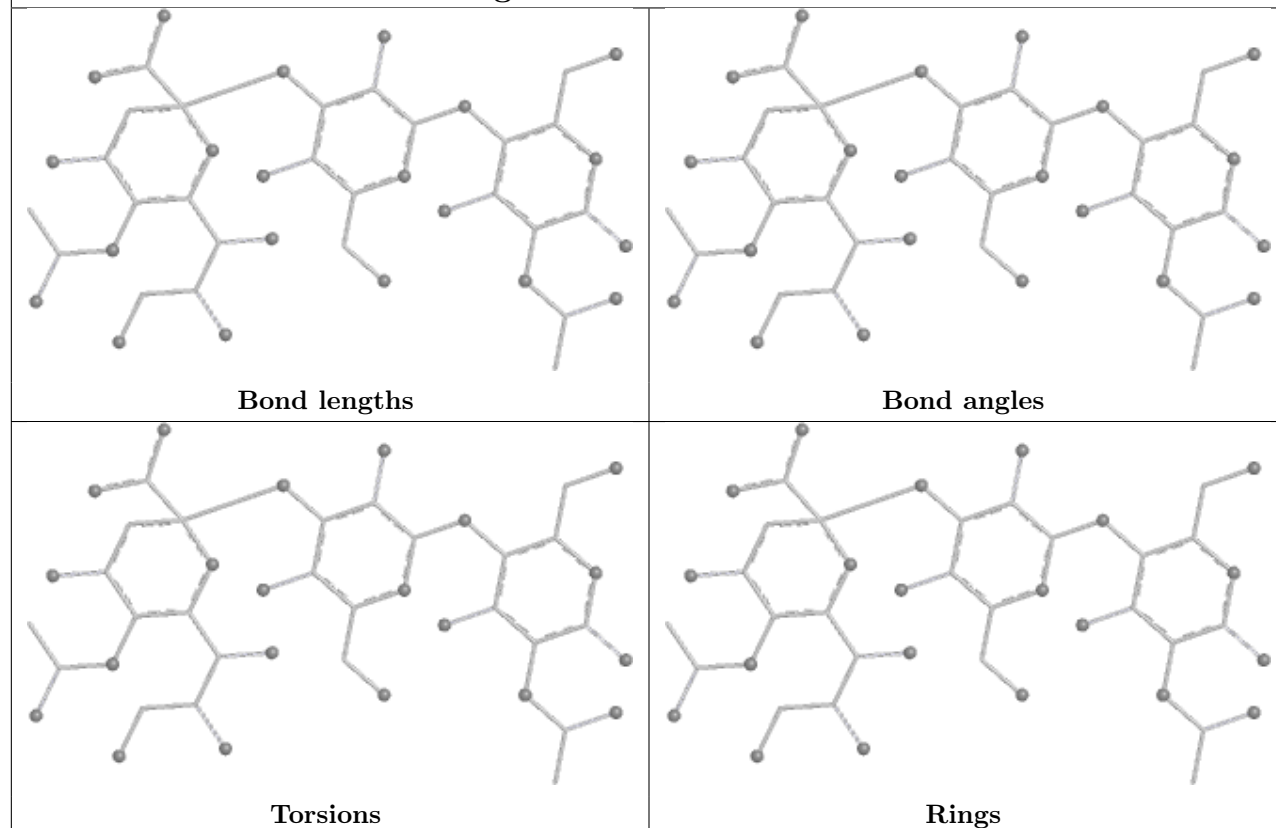
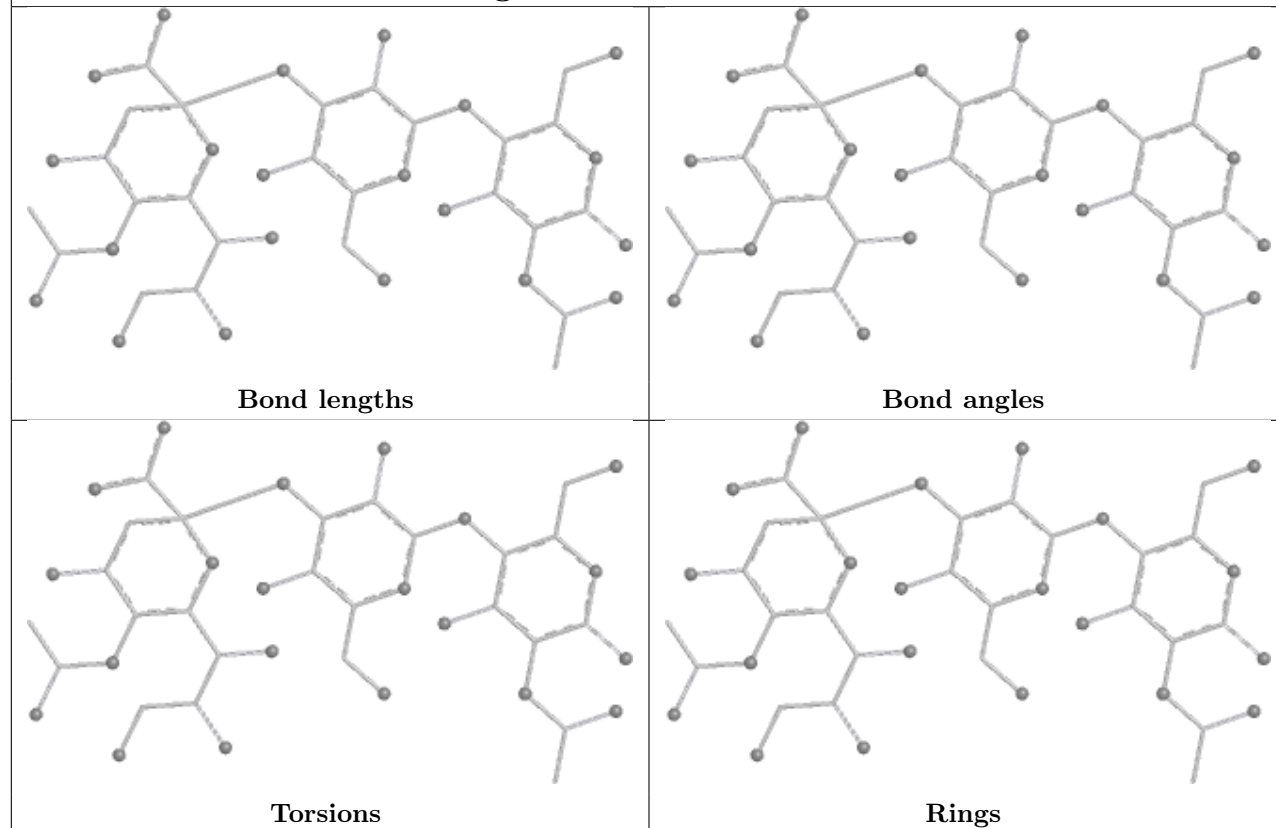
Oligosaccharide Chain XB**Oligosaccharide Chain aB**

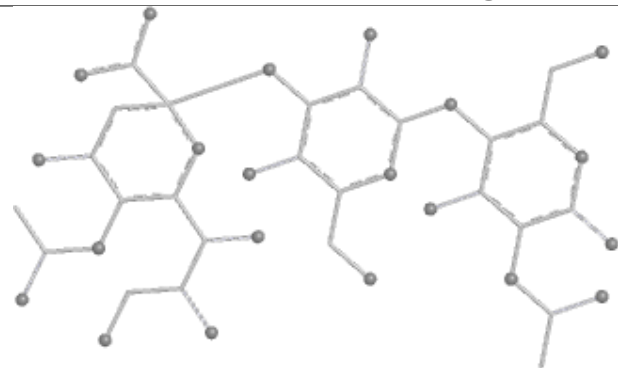
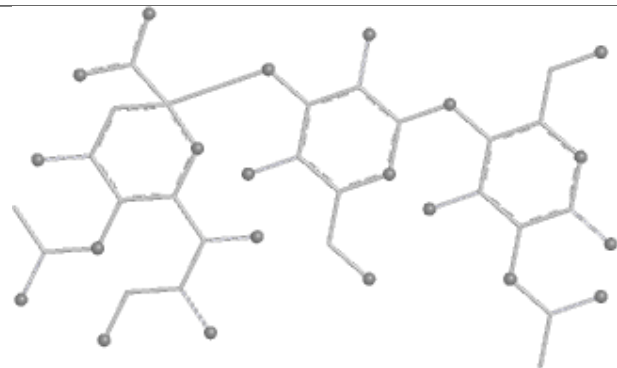
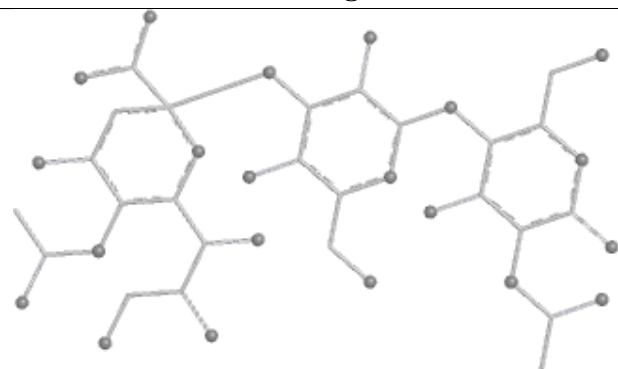
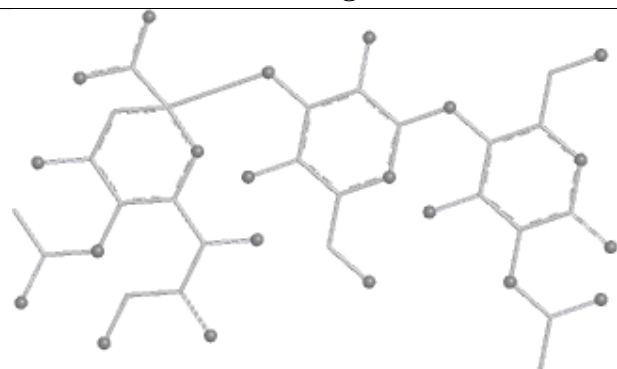
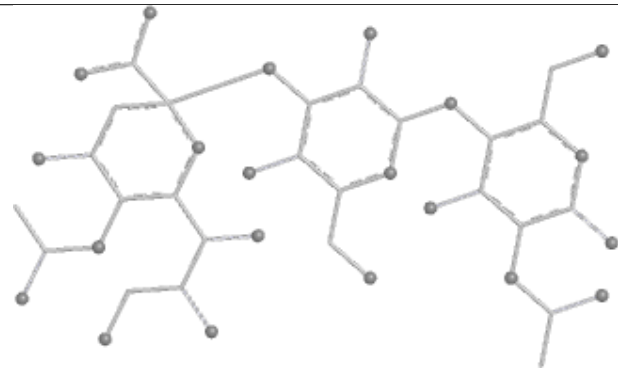
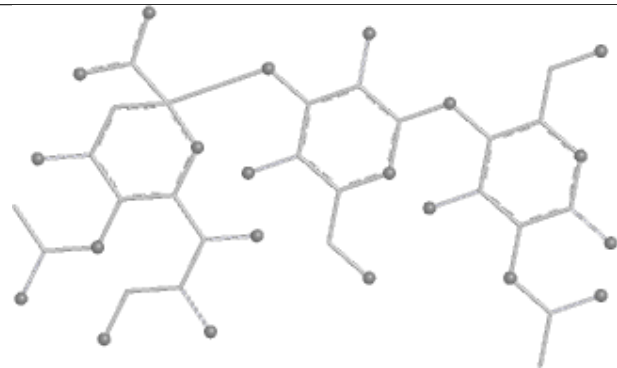
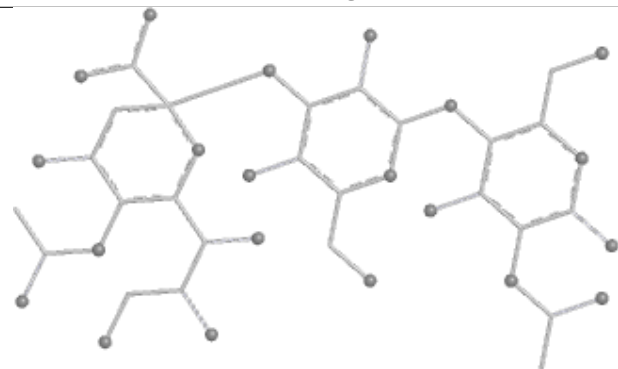
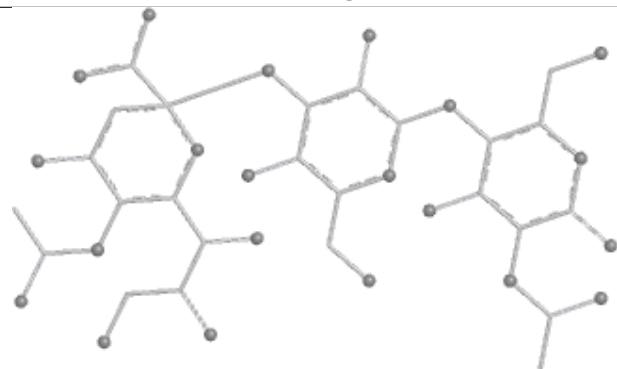




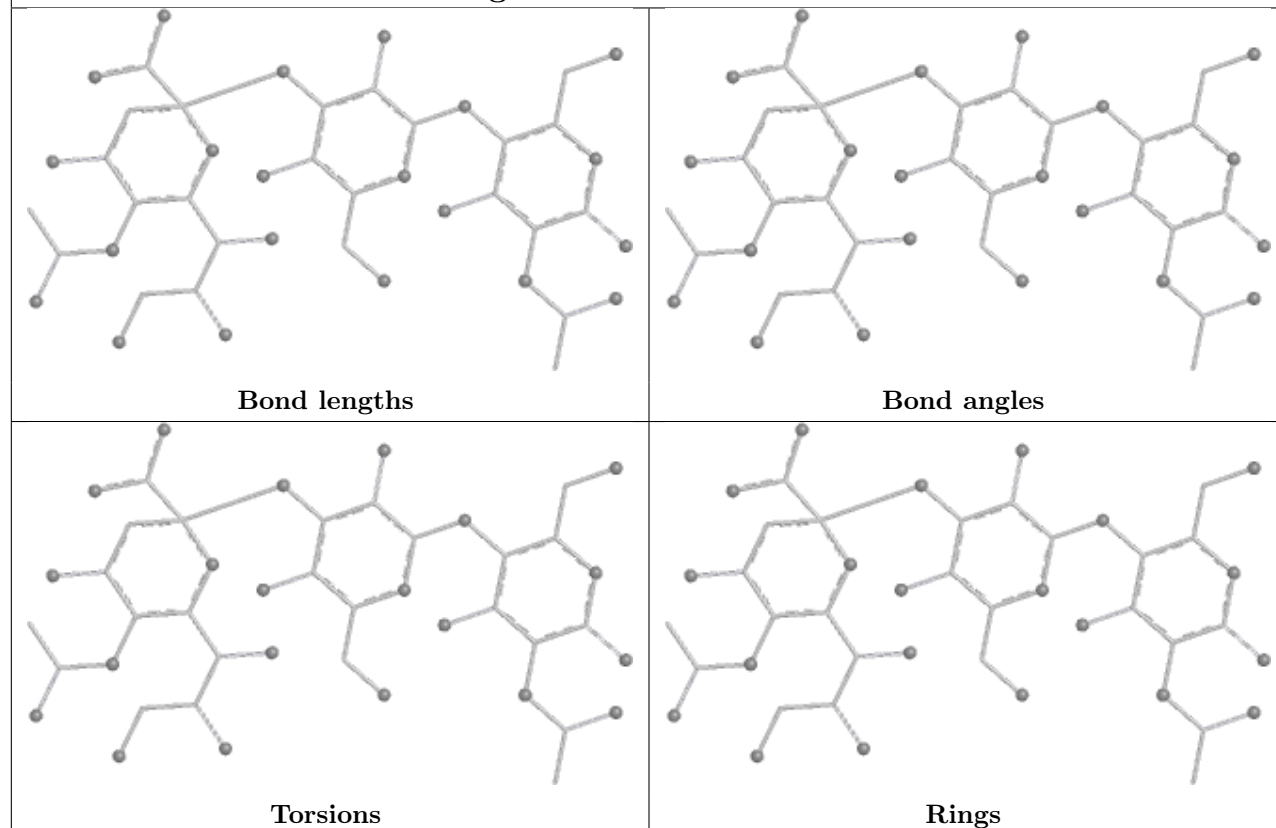




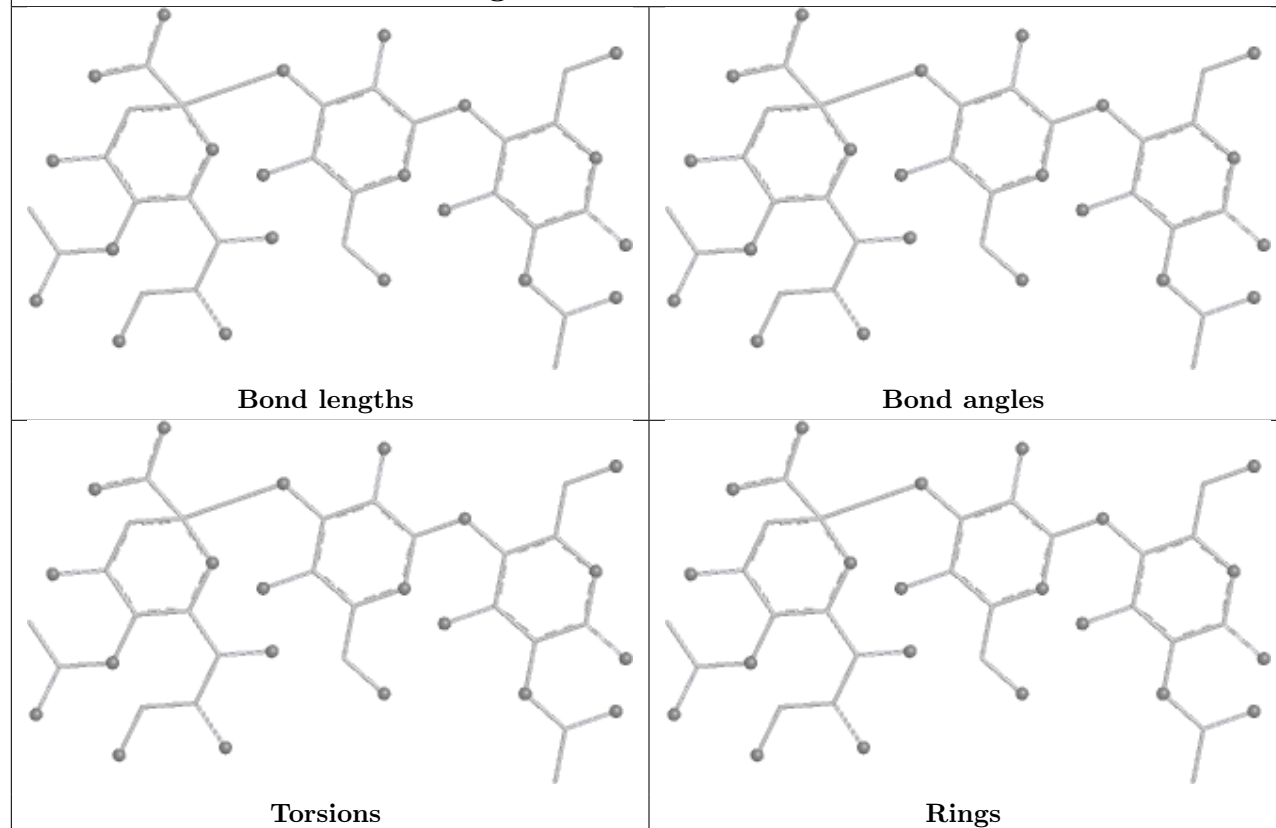
Oligosaccharide Chain 1B**Oligosaccharide Chain 4B**

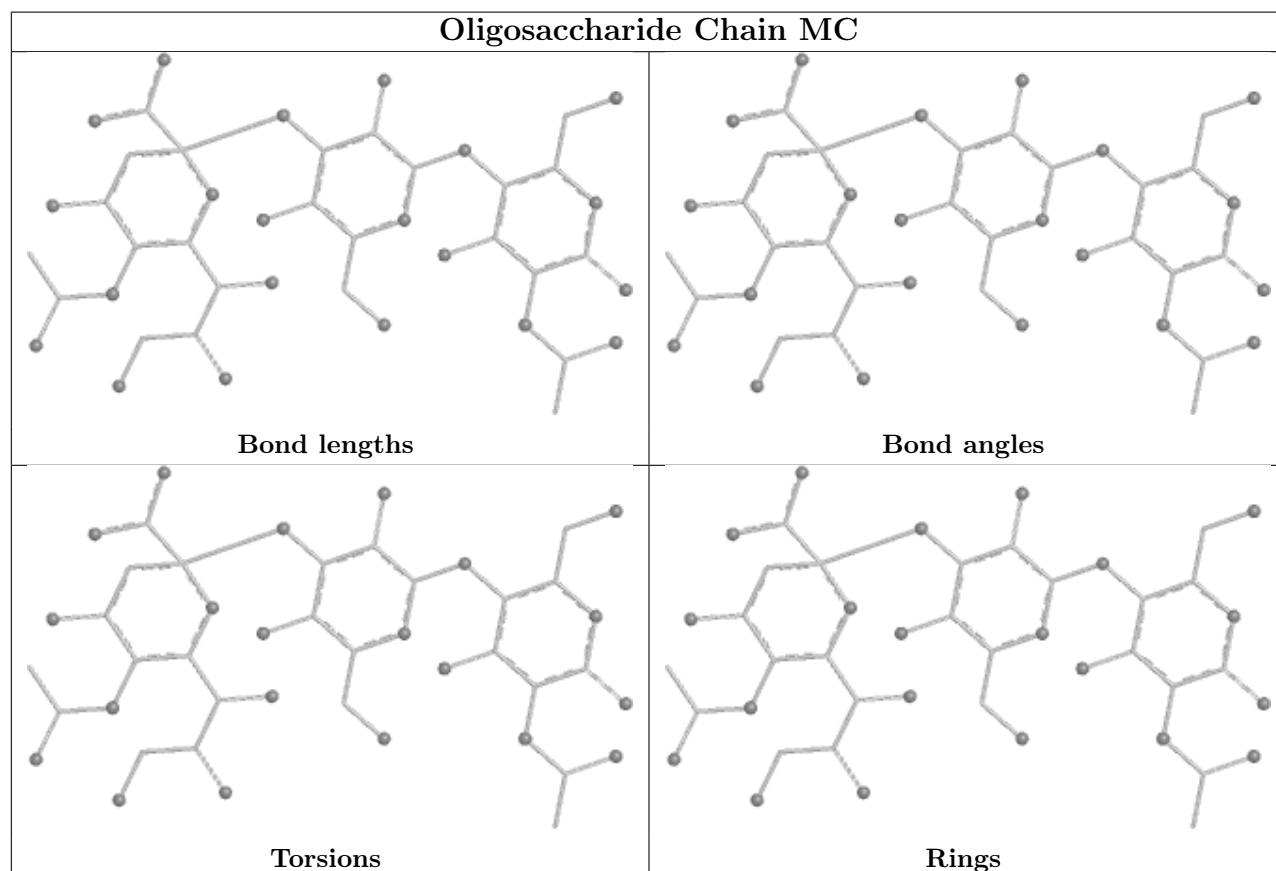
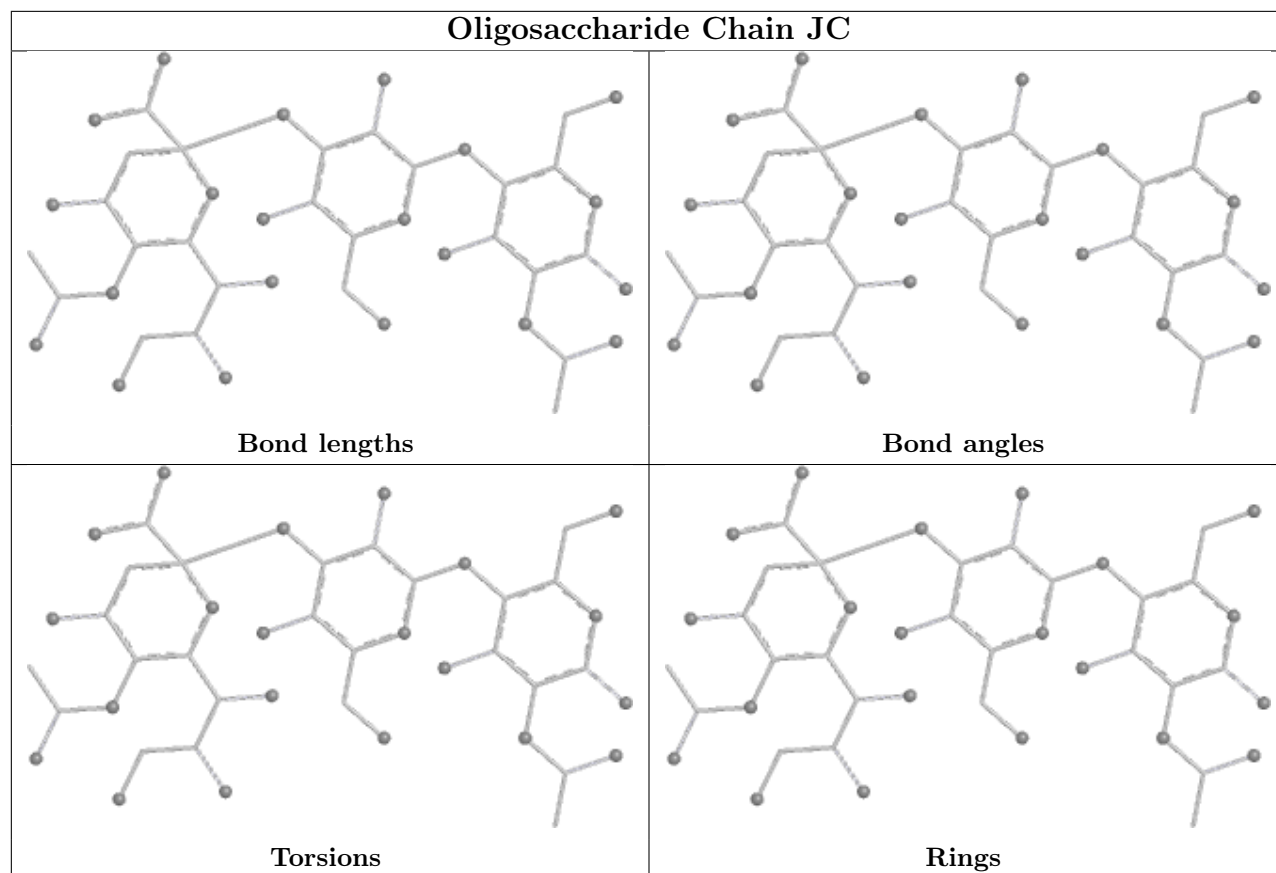
Oligosaccharide Chain 7B**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain AC****Bond lengths****Bond angles****Torsions****Rings**

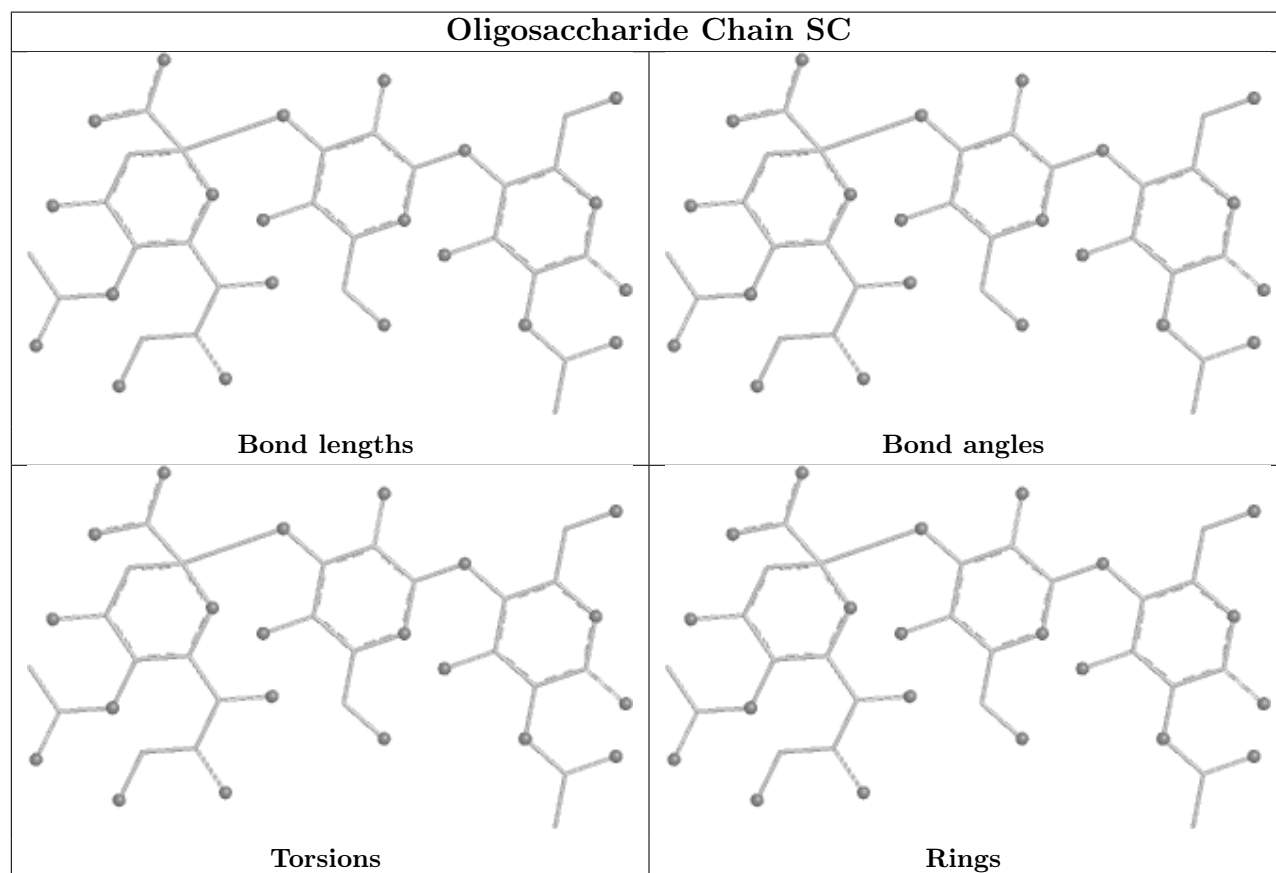
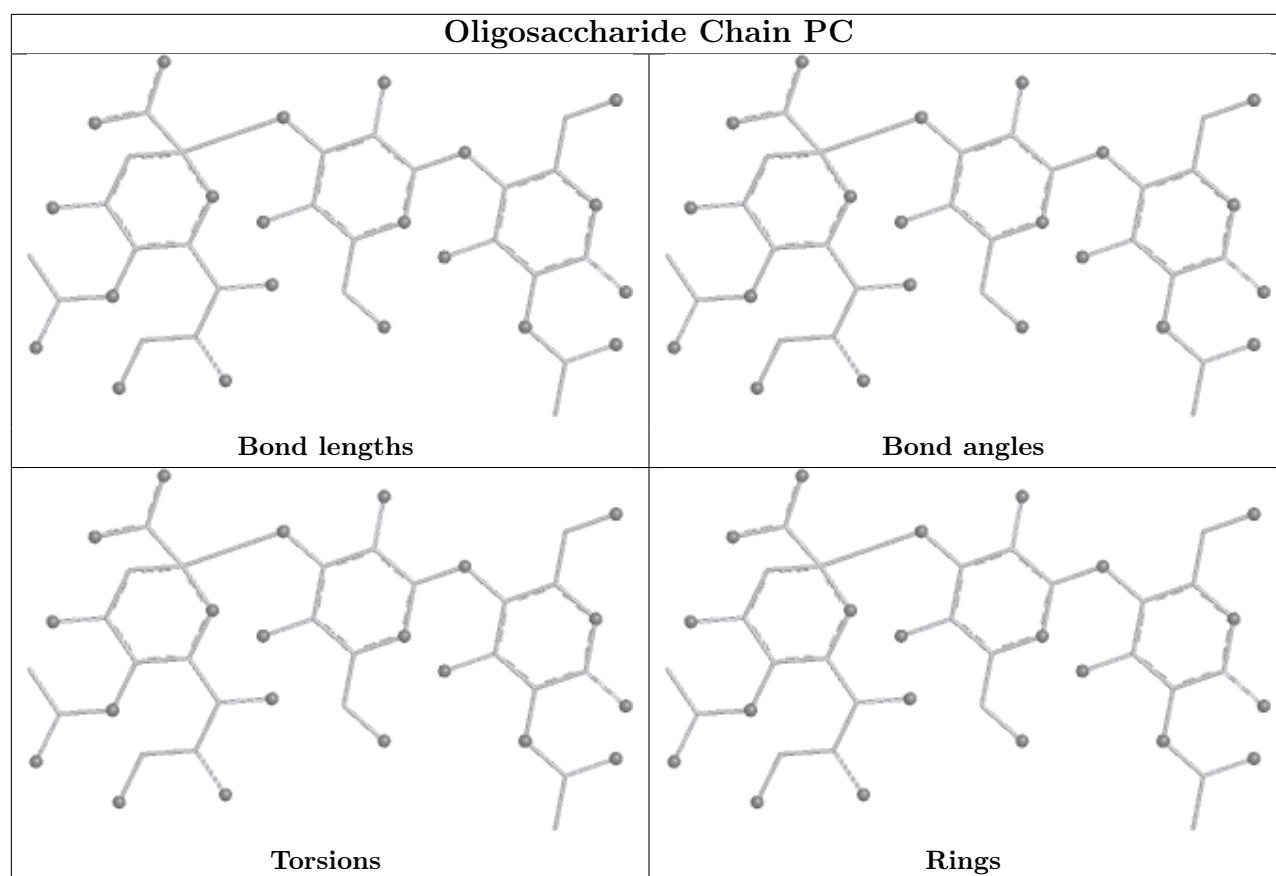
Oligosaccharide Chain DC



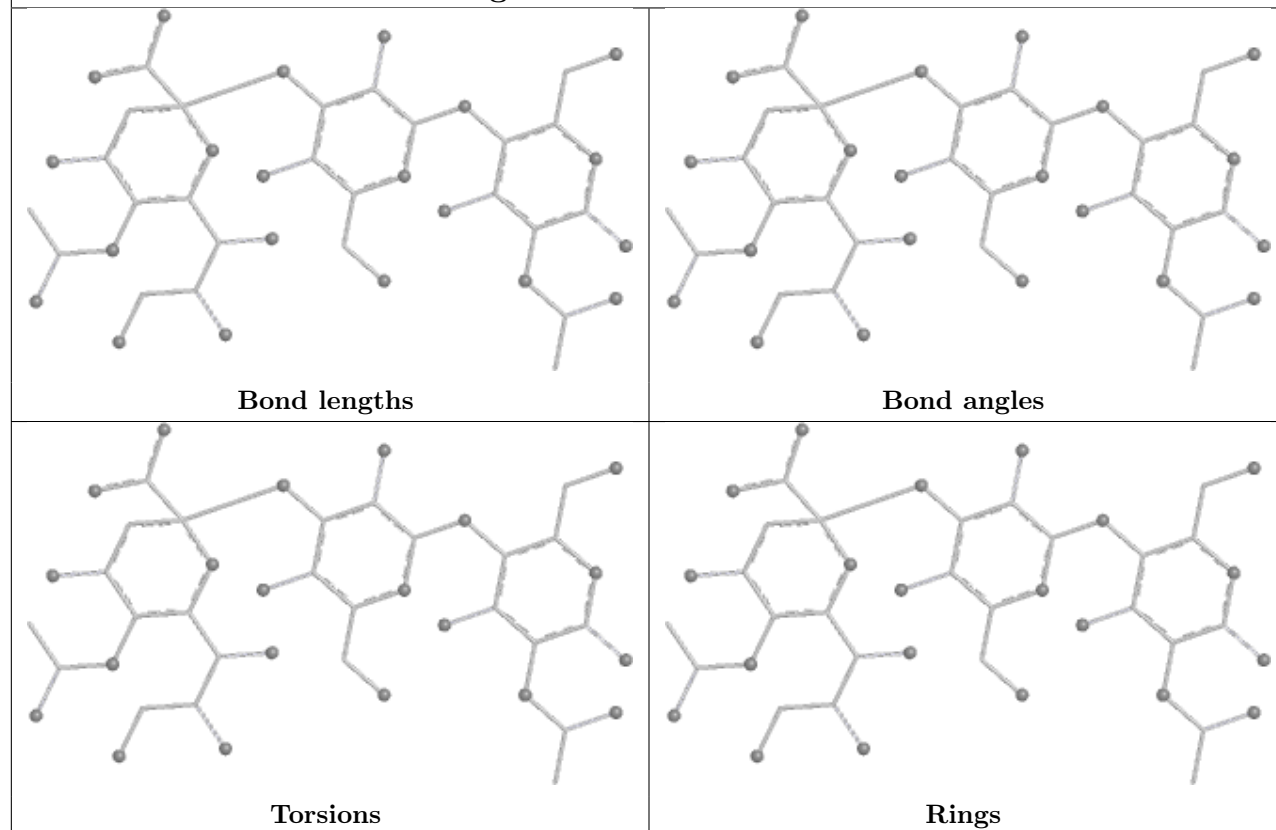
Oligosaccharide Chain GC



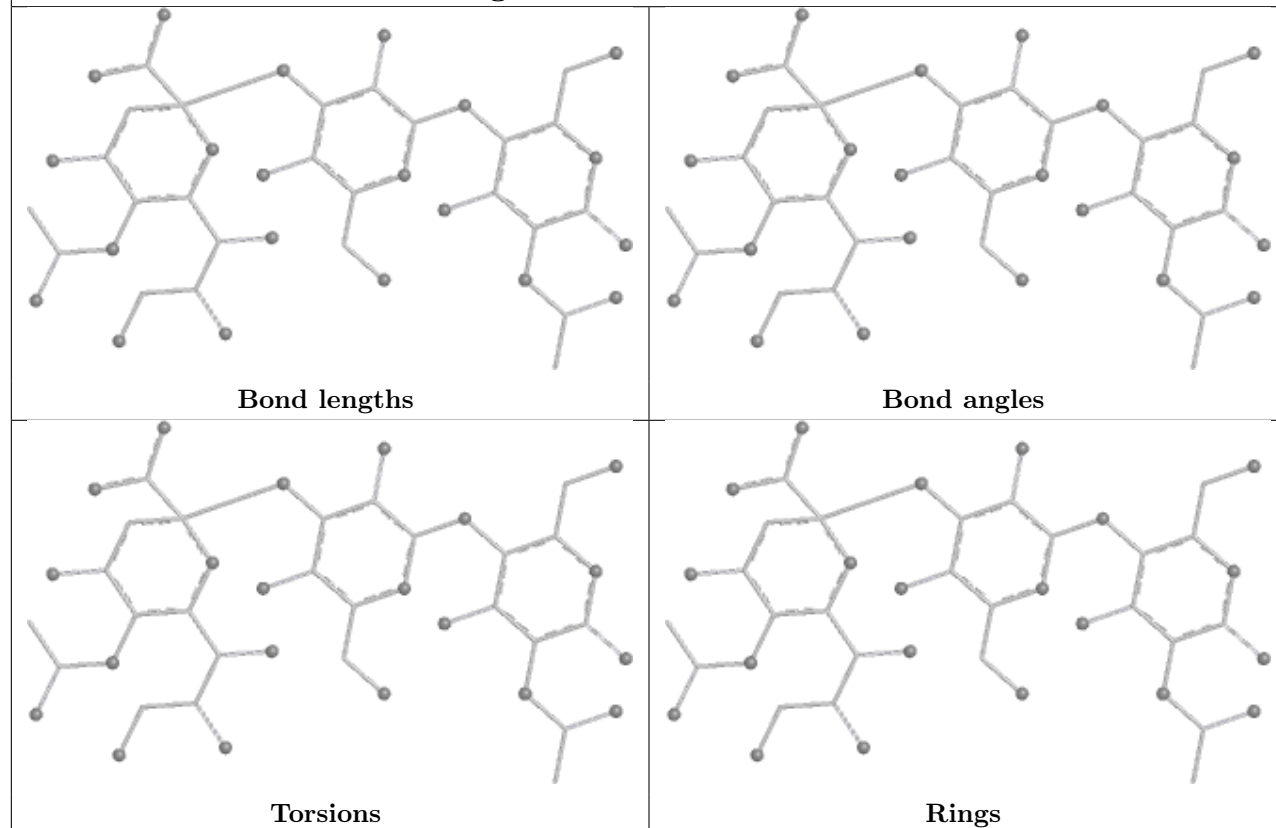




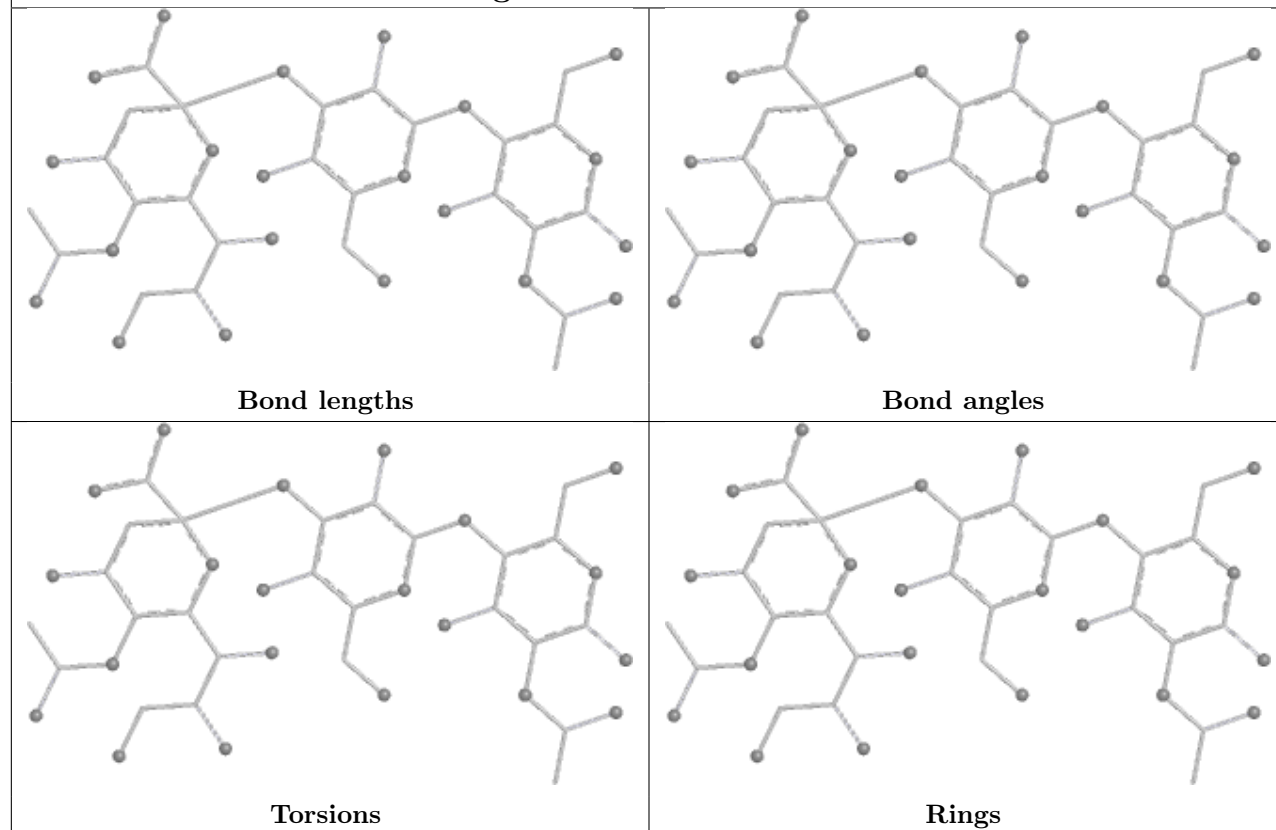
Oligosaccharide Chain VC



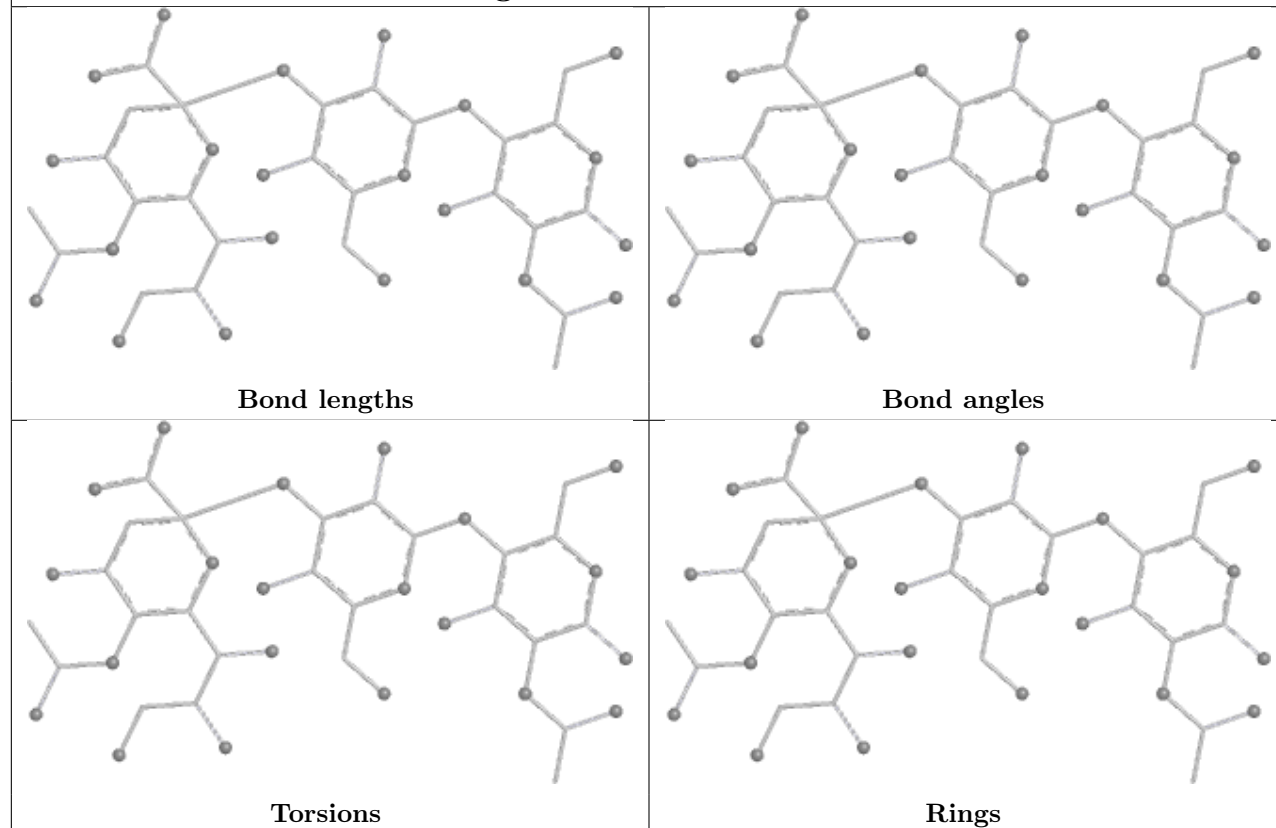
Oligosaccharide Chain YC



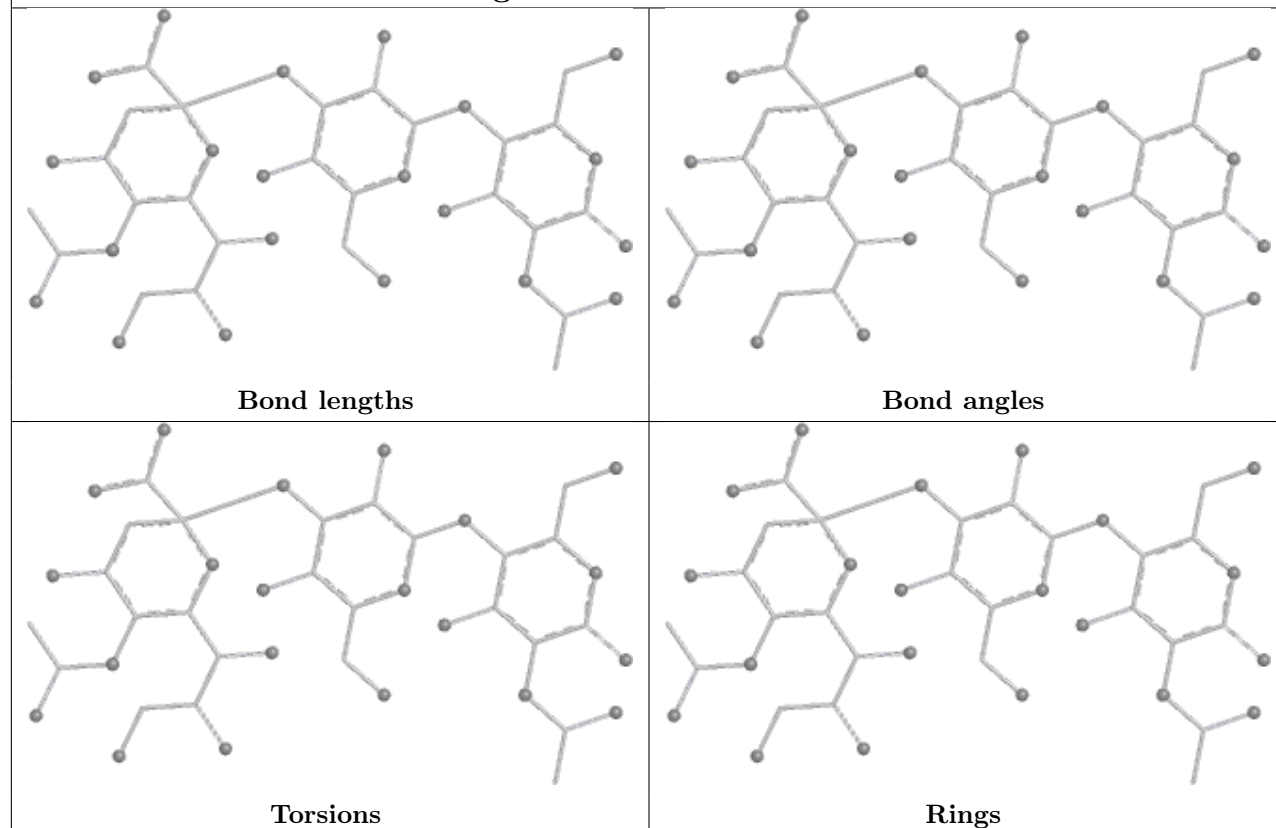
Oligosaccharide Chain bC



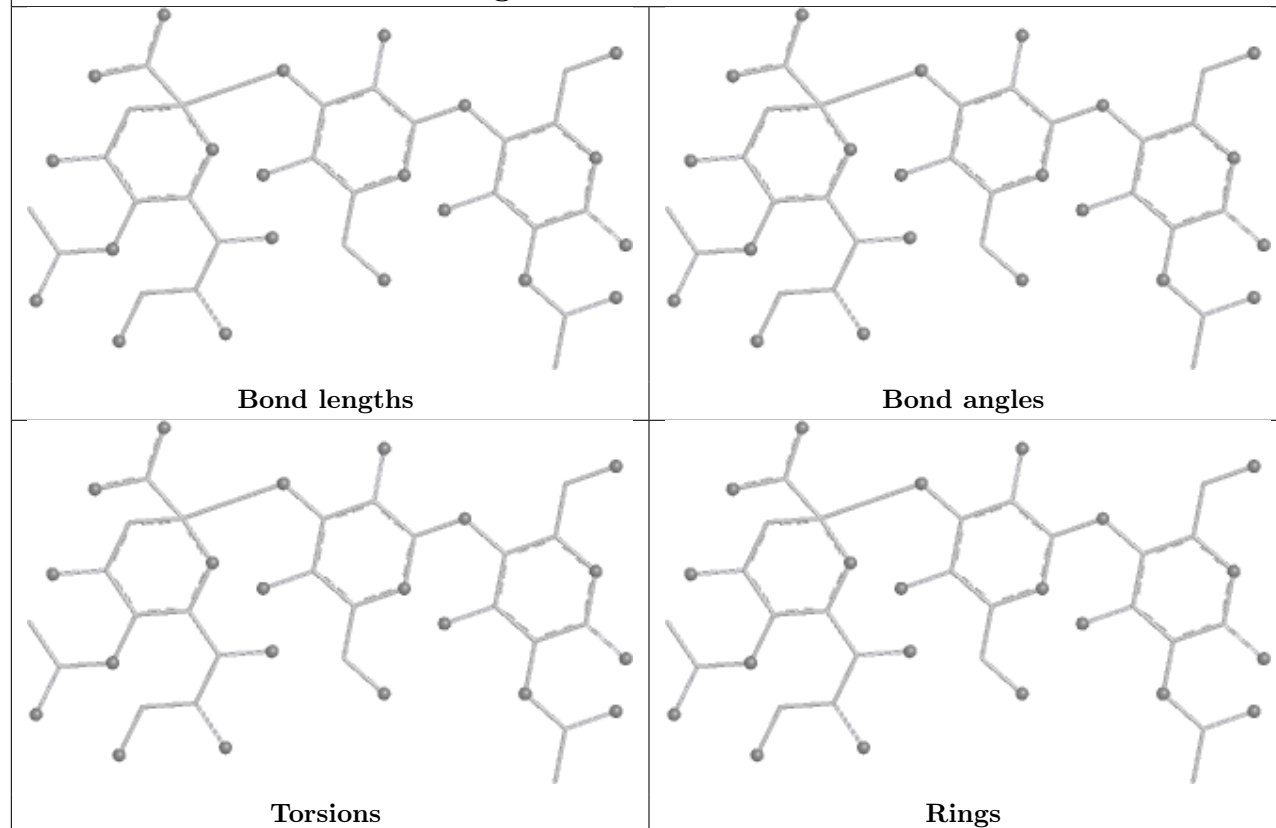
Oligosaccharide Chain eC

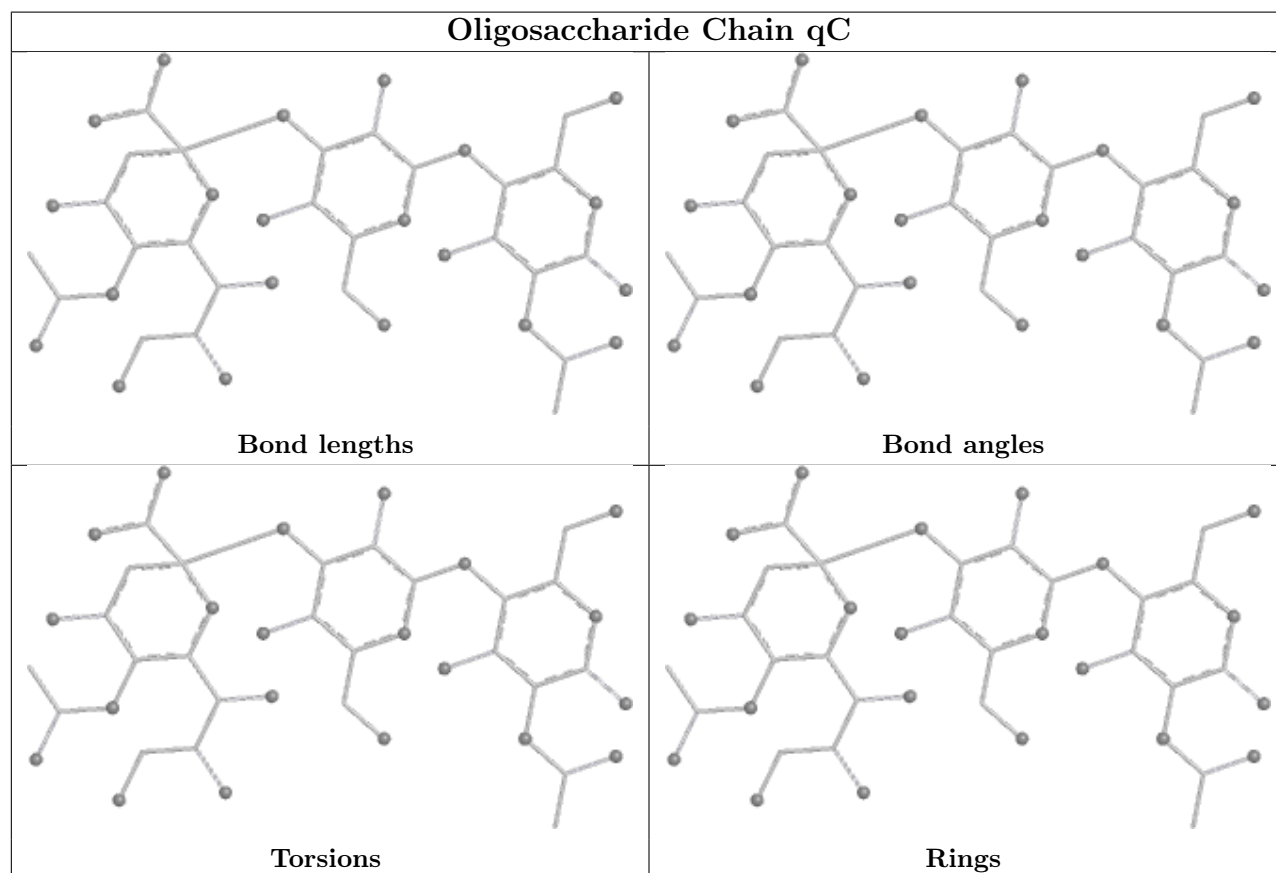
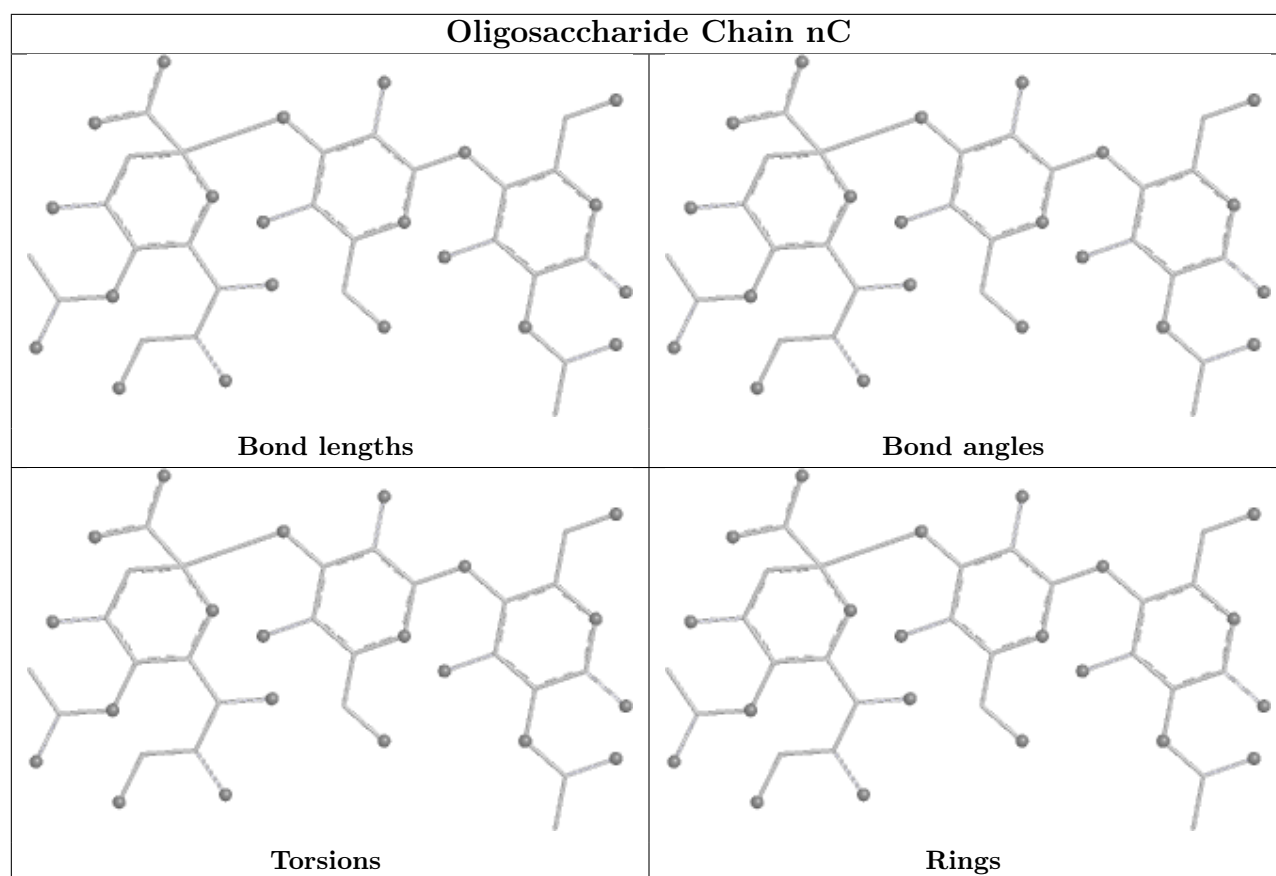


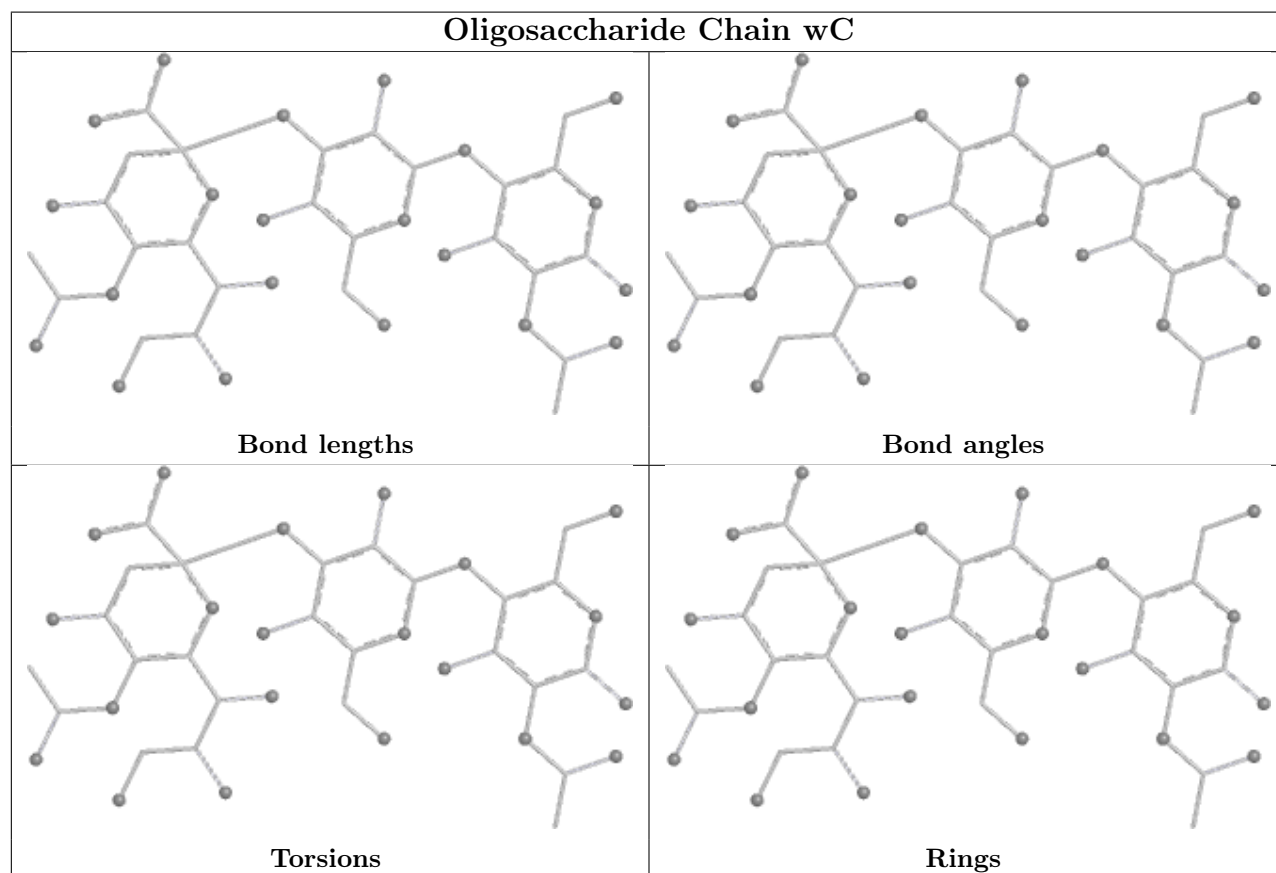
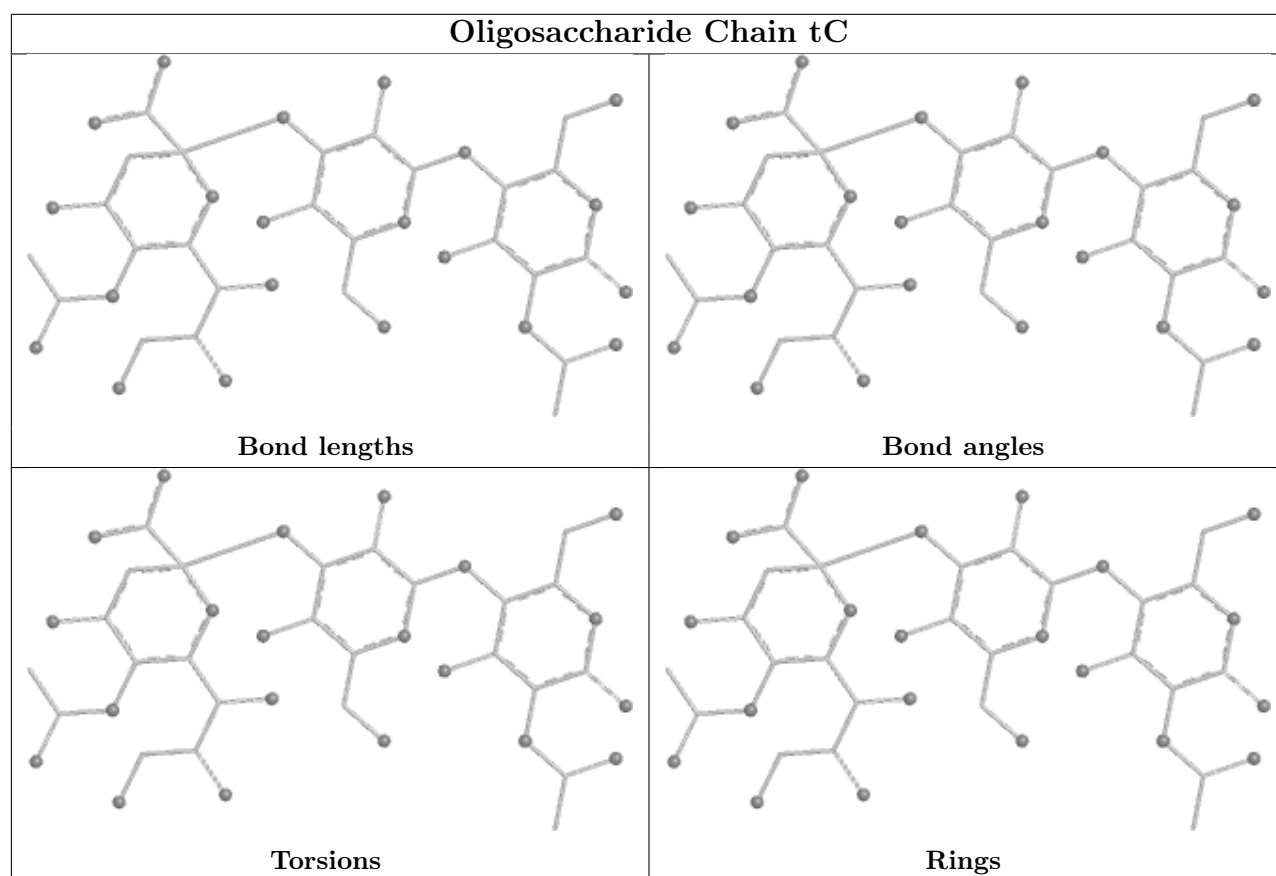
Oligosaccharide Chain hC

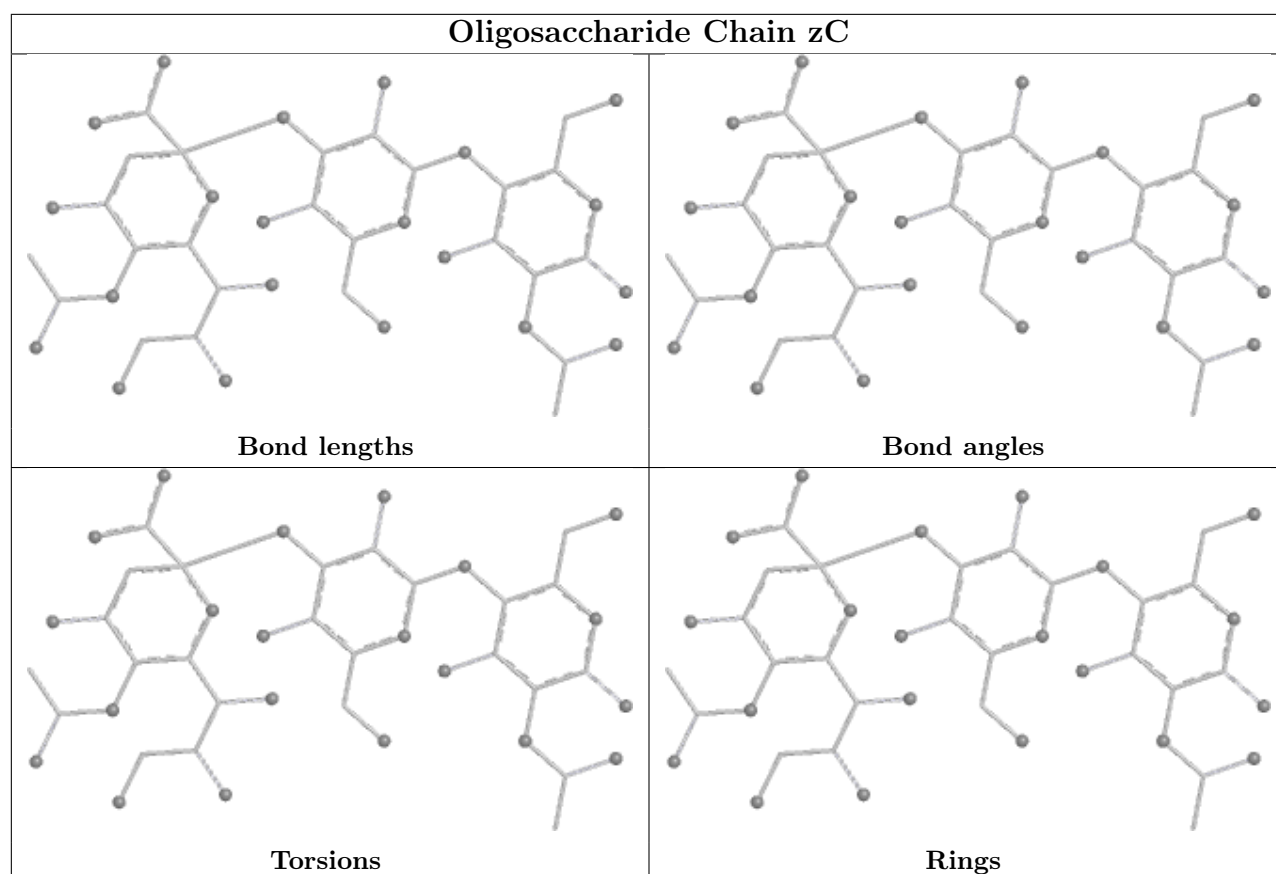


Oligosaccharide Chain kC









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

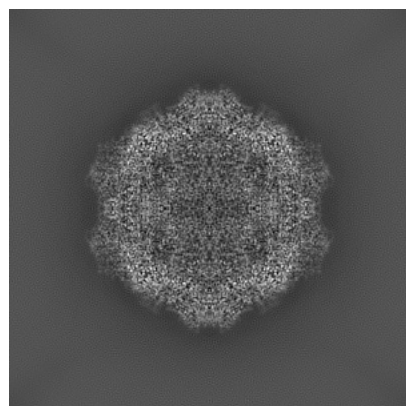
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49196. These allow visual inspection of the internal detail of the map and identification of artifacts.

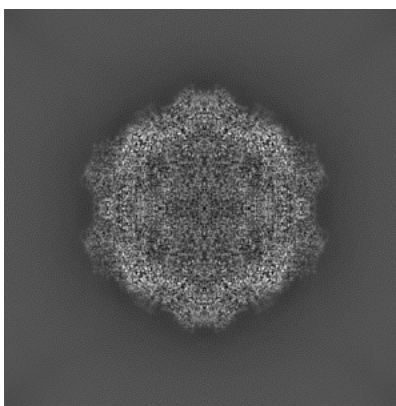
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

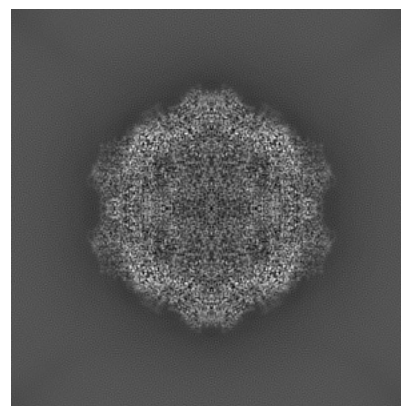
6.1.1 Primary map



X

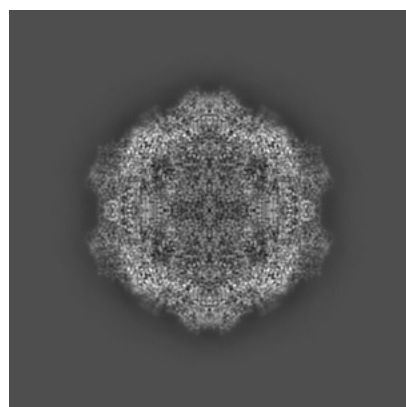


Y

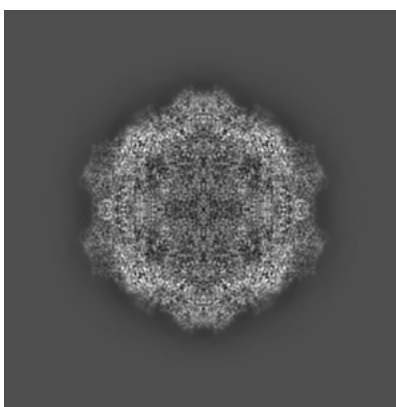


Z

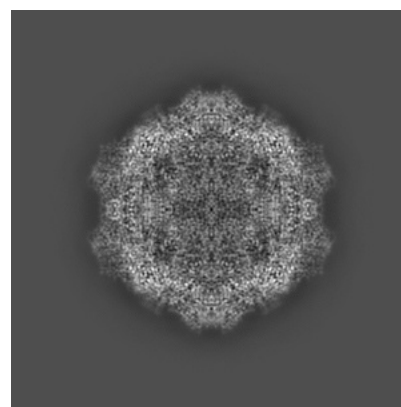
6.1.2 Raw map



X



Y

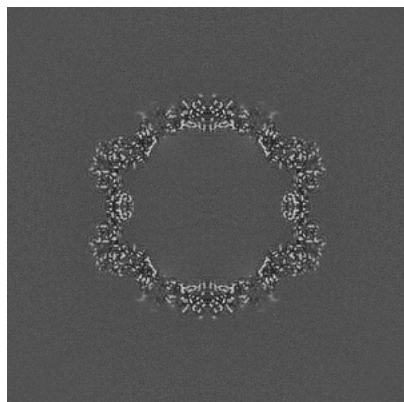


Z

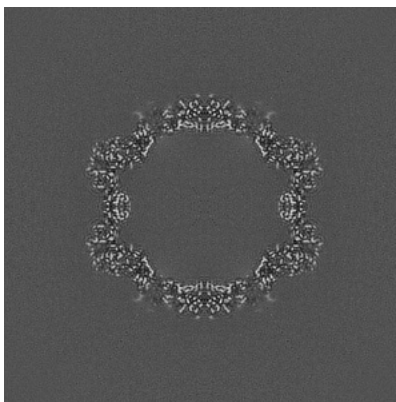
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

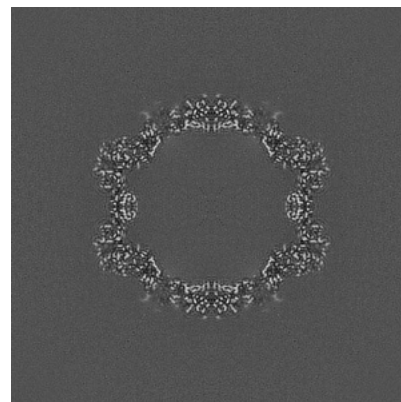
6.2.1 Primary map



X Index: 210

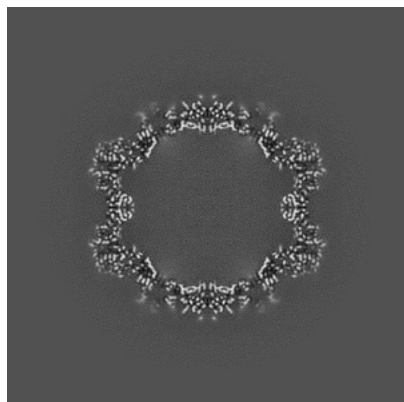


Y Index: 210

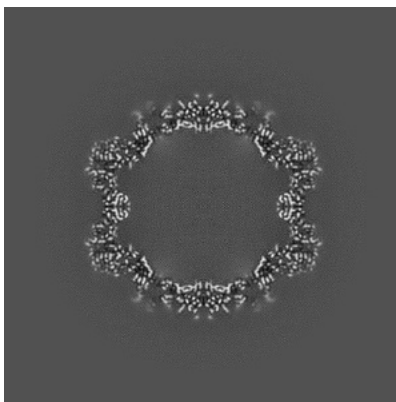


Z Index: 210

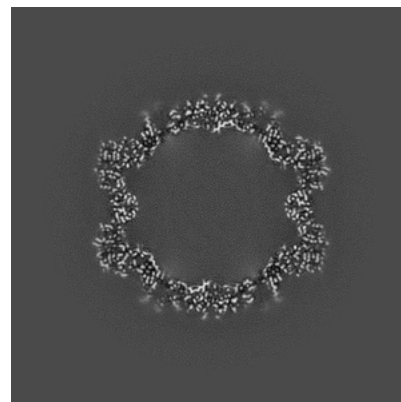
6.2.2 Raw map



X Index: 210



Y Index: 210

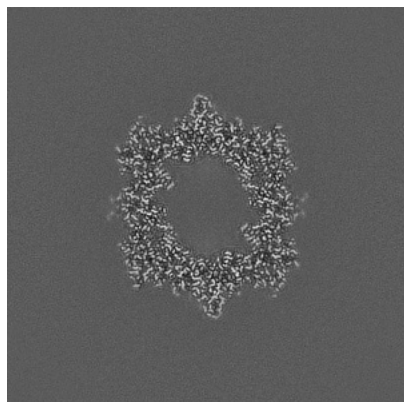


Z Index: 210

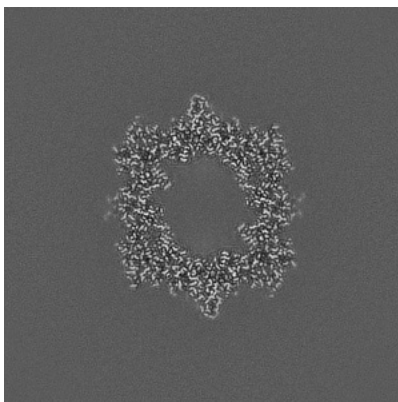
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

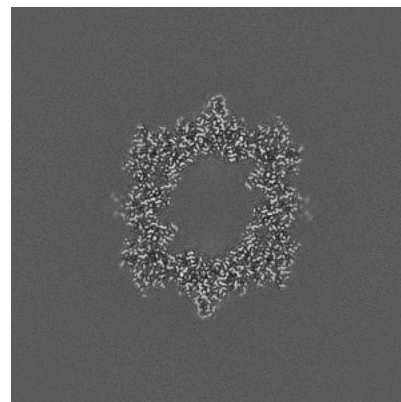
6.3.1 Primary map



X Index: 275

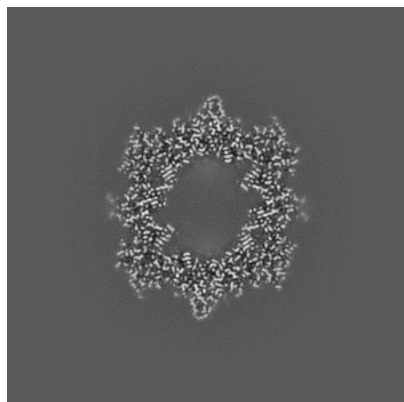


Y Index: 275

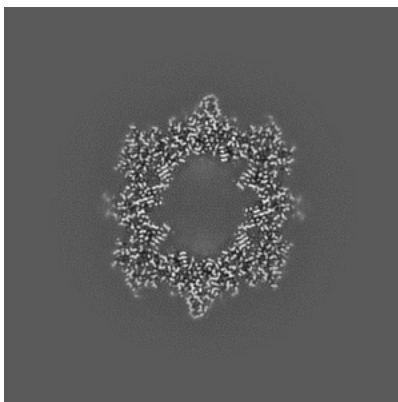


Z Index: 145

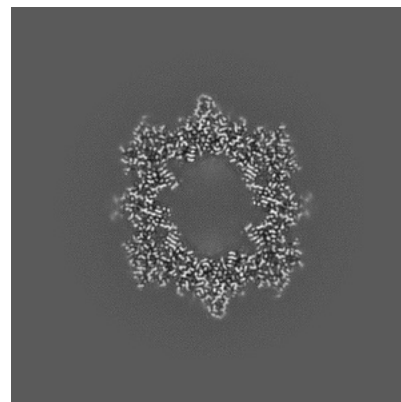
6.3.2 Raw map



X Index: 145



Y Index: 145

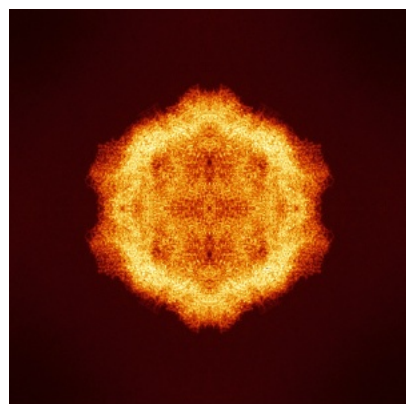


Z Index: 274

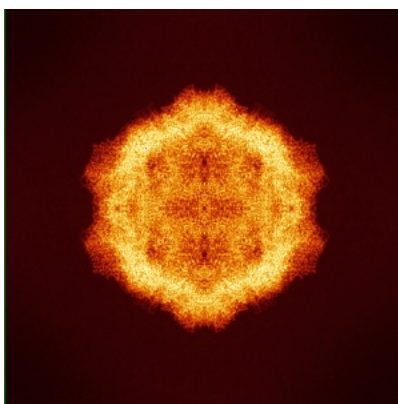
The images above show the largest variance slices of the map in three orthogonal directions.

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

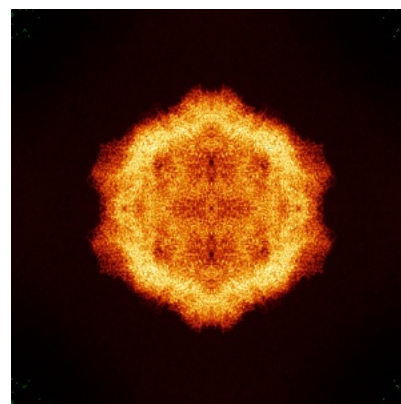
6.4.1 Primary map



X

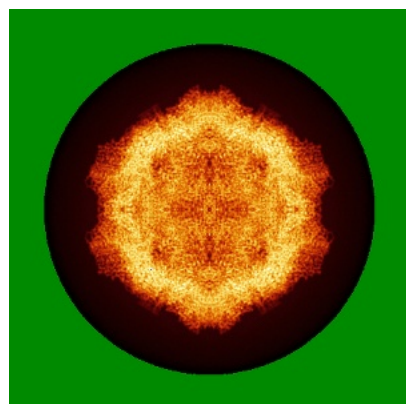


Y

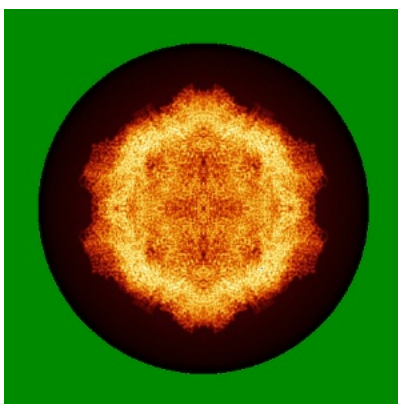


Z

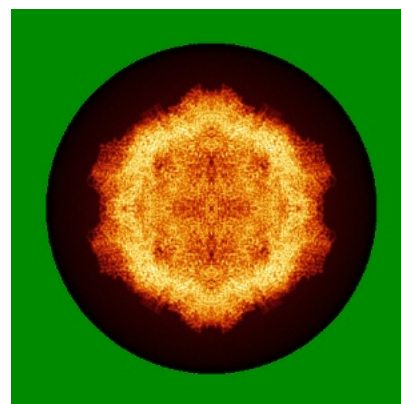
6.4.2 Raw map



X



Y

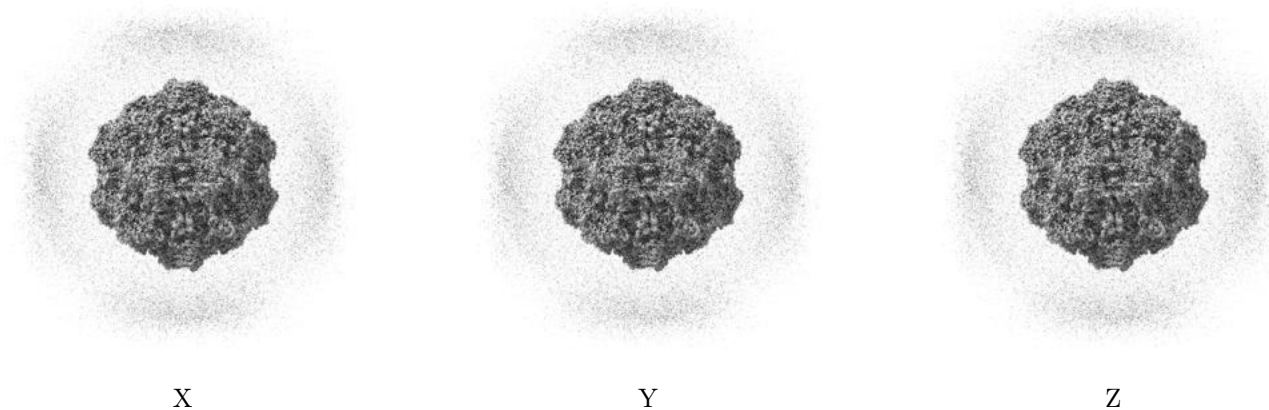


Z

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.

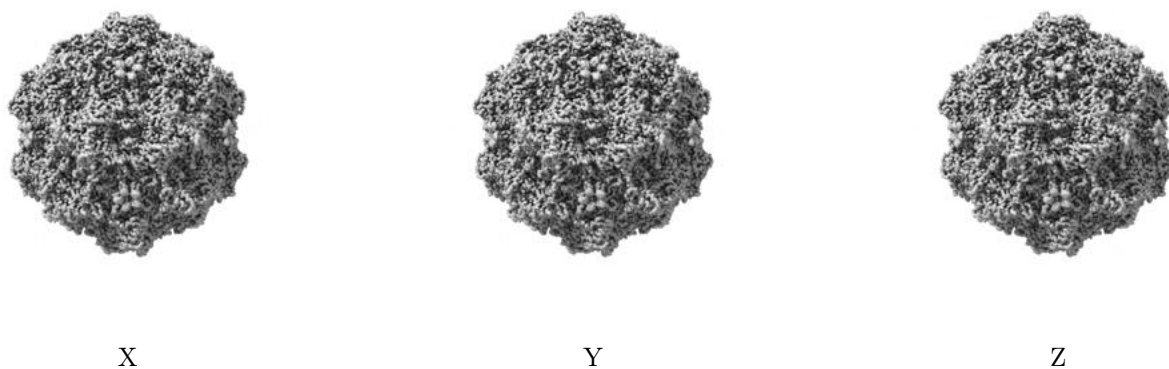
6.5 Orthogonal surface views [i](#)

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.

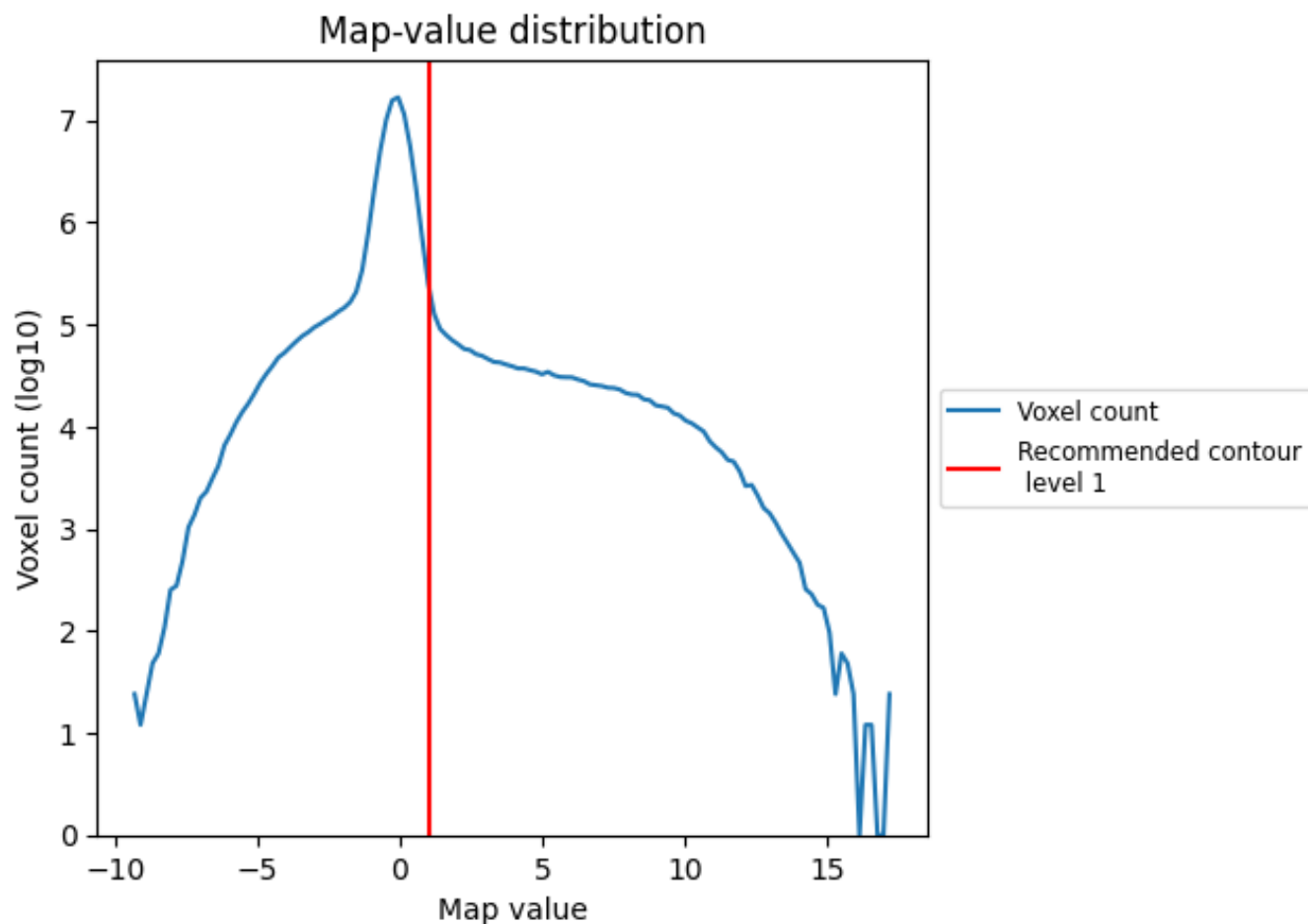
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

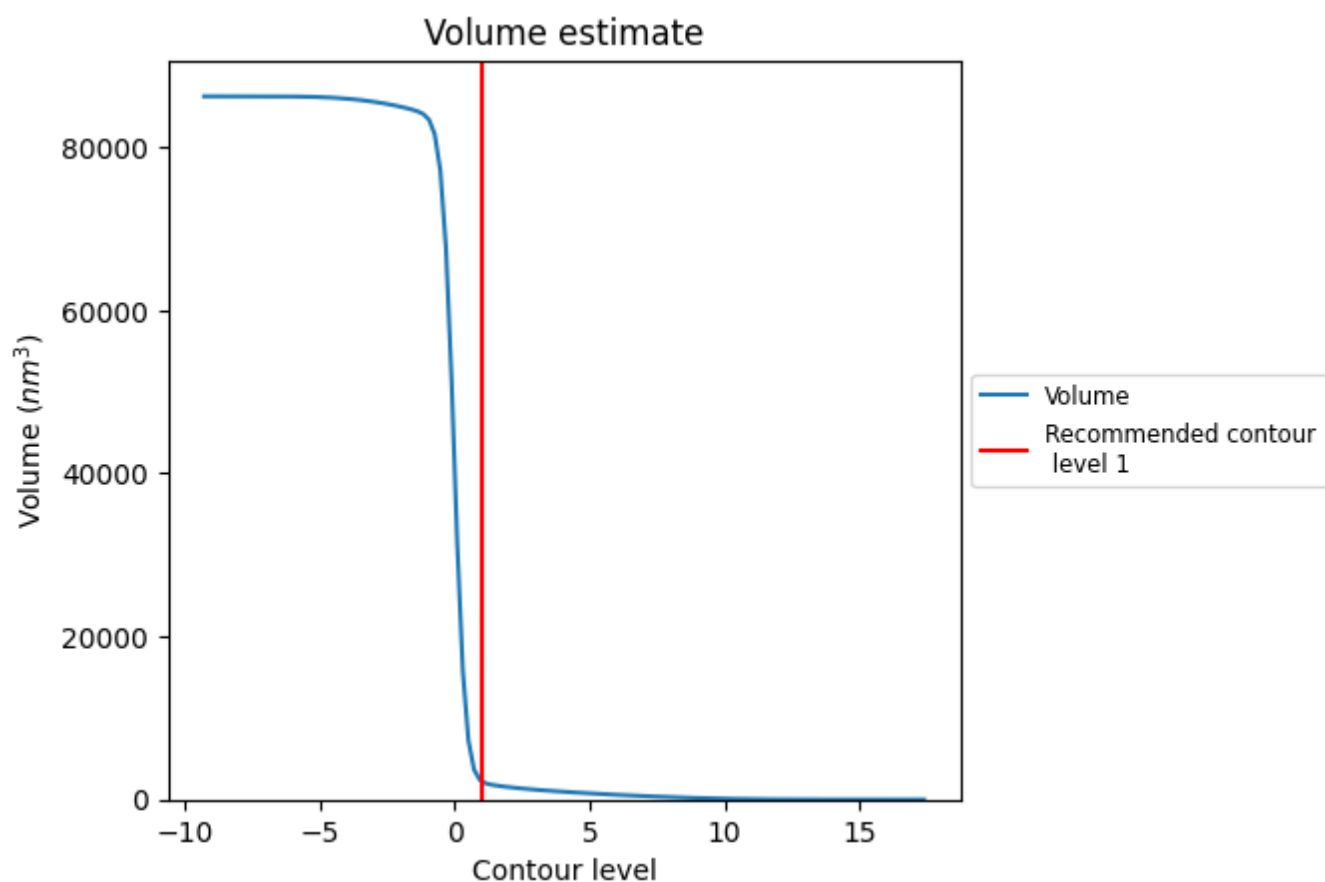
This section contains the results of statistical analysis of the map.

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.

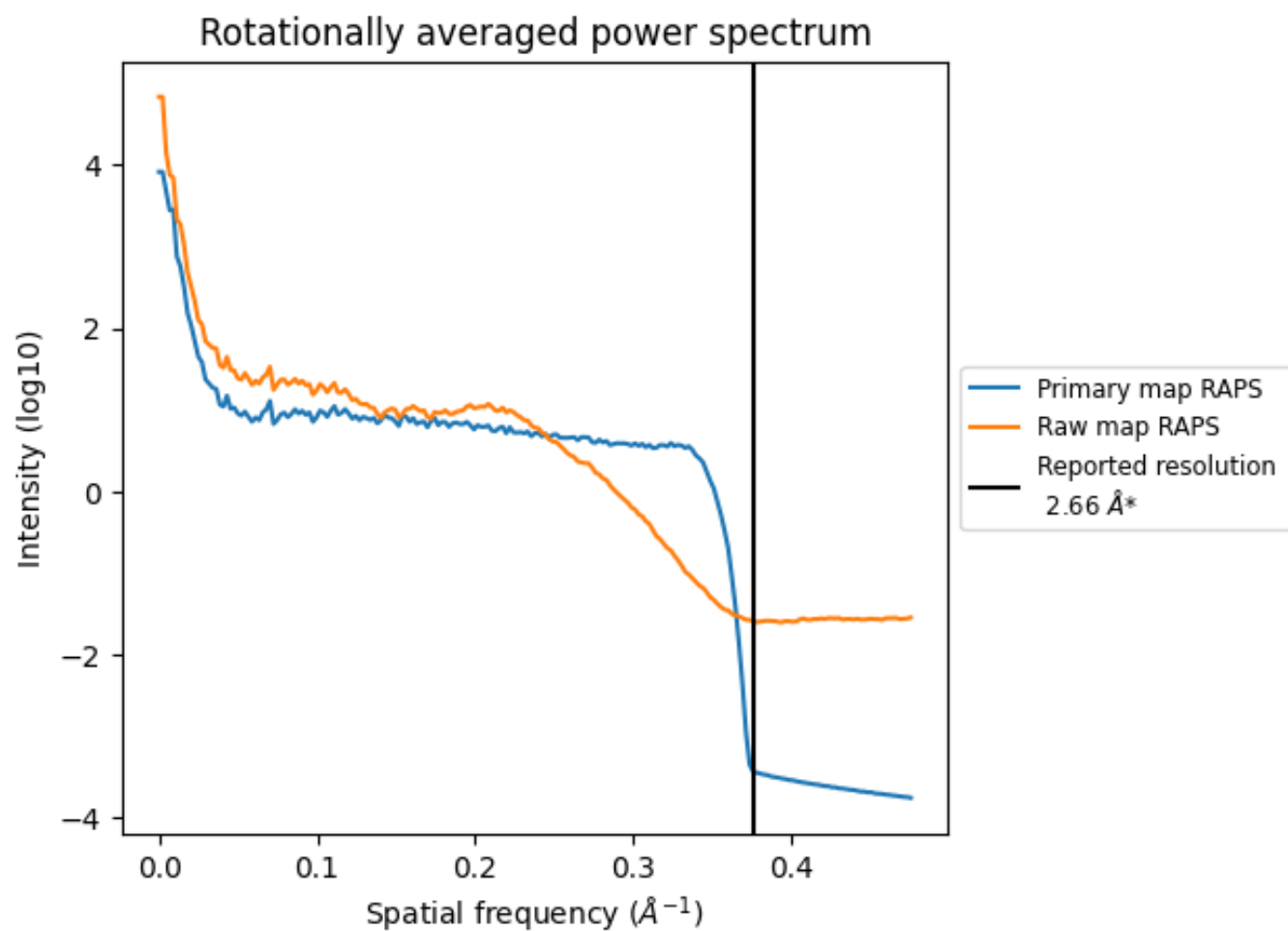
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2263 nm³; this corresponds to an approximate mass of 2045 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 ⓘ

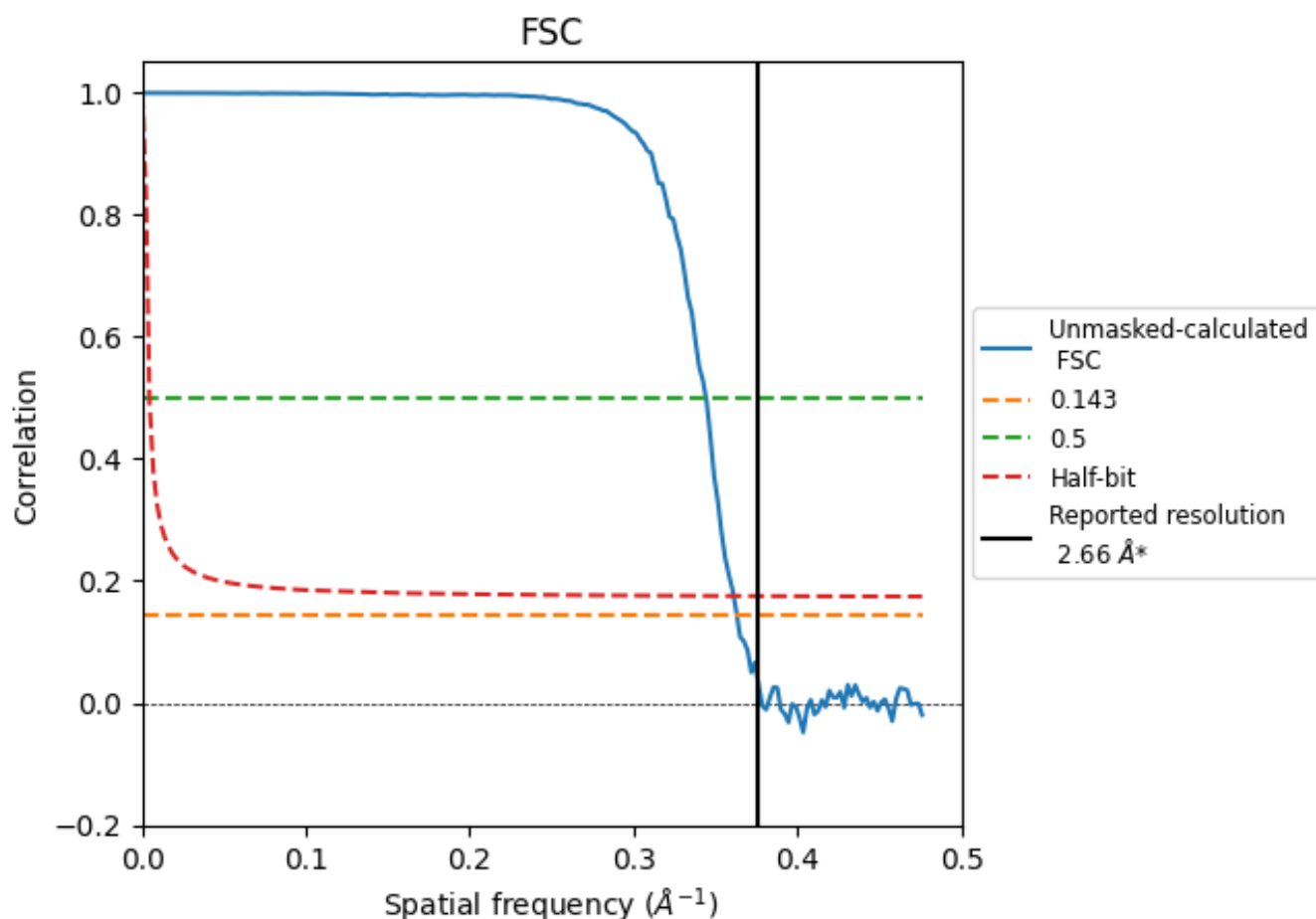


*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

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 0.376 Å⁻¹

8.2 Resolution estimates [i](#)

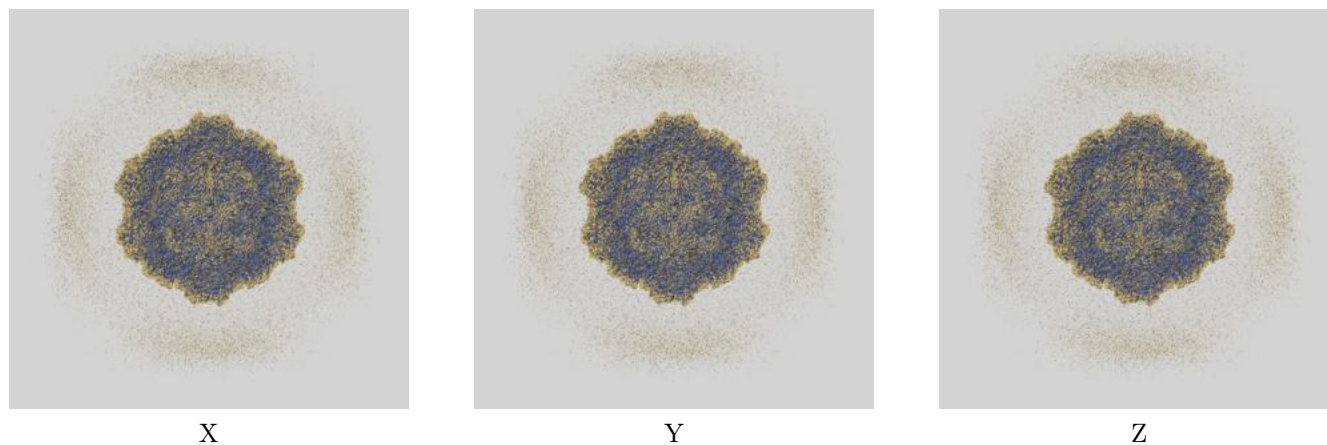
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.75	2.91	2.77

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

9 Map-model fit [i](#)

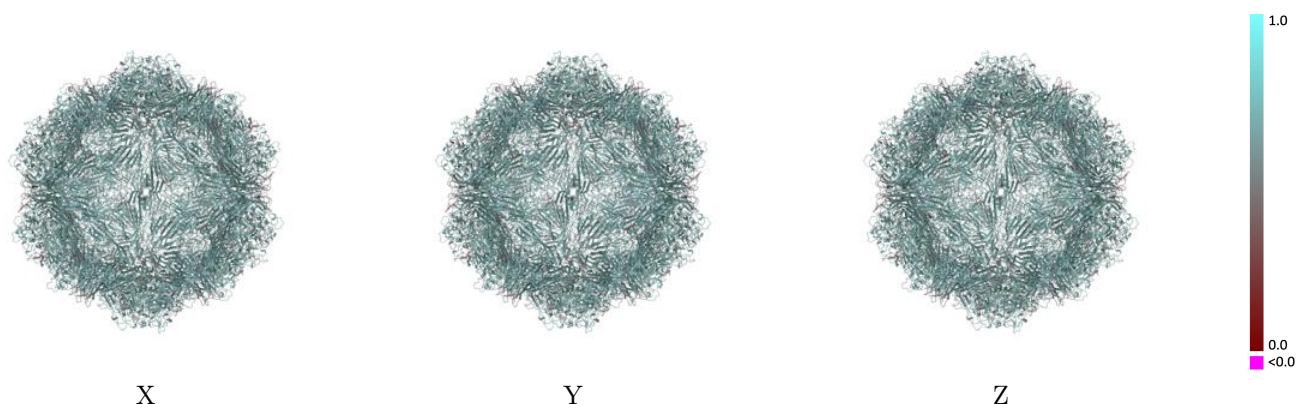
This section contains information regarding the fit between EMDB map EMD-49196 and PDB model 9NAJ. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



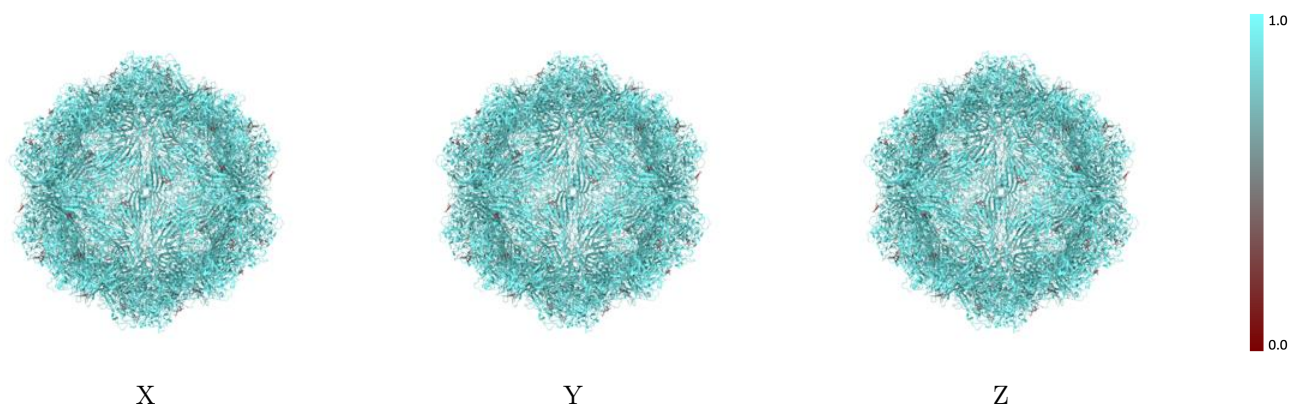
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



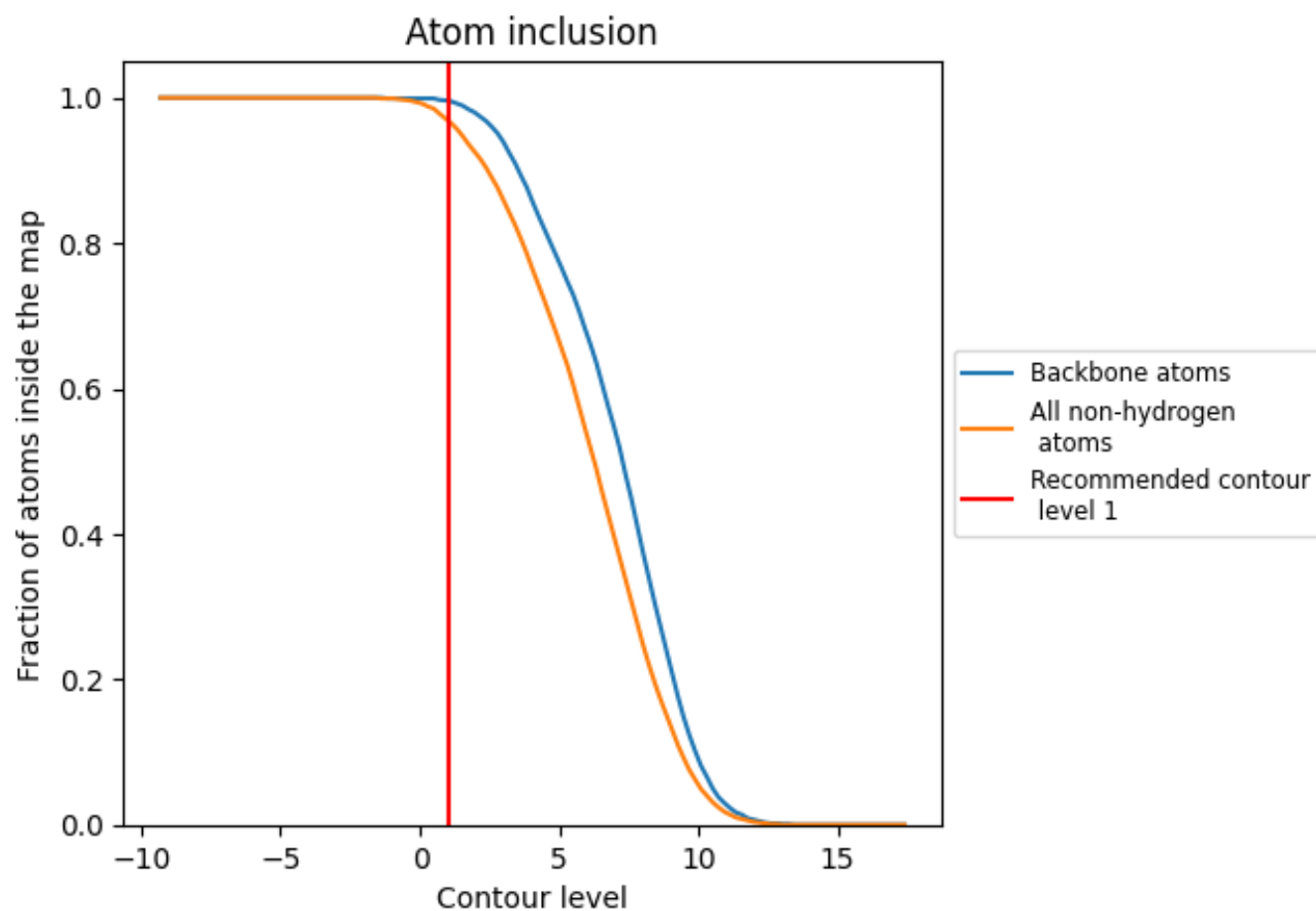
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 100% of all backbone atoms, 97% 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	 0.9690	 0.6280
0	 0.3700	 0.3930
0A	 0.3700	 0.3870
1	 0.9740	 0.6300
1B	 0.3700	 0.4030
2	 0.9740	 0.6300
3	 0.9740	 0.6300
3A	 0.3480	 0.3730
4	 0.9770	 0.6300
4B	 0.3700	 0.3880
5	 0.9760	 0.6290
6	 0.9760	 0.6300
6A	 0.3700	 0.3970
7	 0.9760	 0.6300
7B	 0.3480	 0.3820
8	 0.9740	 0.6300
9A	 0.3480	 0.3830
A	 0.9740	 0.6300
AC	 0.3700	 0.3860
B	 0.9740	 0.6300
BA	 0.3700	 0.3910
C	 0.9770	 0.6300
CB	 0.3480	 0.3820
D	 0.9760	 0.6300
DC	 0.3700	 0.3800
E	 0.9740	 0.6320
EA	 0.3480	 0.3770
F	 0.9740	 0.6300
FB	 0.3700	 0.3810
G	 0.9740	 0.6300
GC	 0.3700	 0.3840
H	 0.9760	 0.6300
HA	 0.3480	 0.3760
I	 0.9770	 0.6300
IB	 0.3480	 0.3770



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Chain	Atom inclusion	Q-score
J	 0.9740	 0.6300
JC	 0.3700	 0.3860
K	 0.9770	 0.6290
KA	 0.3700	 0.3830
L	 0.9740	 0.6300
LB	 0.3700	 0.3920
M	 0.9740	 0.6310
MC	 0.3480	 0.3670
N	 0.9760	 0.6310
NA	 0.3700	 0.3890
O	 0.9740	 0.6310
OB	 0.3700	 0.3950
P	 0.9760	 0.6310
PC	 0.3700	 0.3950
Q	 0.9770	 0.6300
QA	 0.3700	 0.3850
R	 0.9740	 0.6310
RB	 0.3700	 0.3940
S	 0.9740	 0.6310
SC	 0.3700	 0.3800
T	 0.9770	 0.6310
TA	 0.3480	 0.3810
U	 0.9740	 0.6300
UB	 0.3700	 0.3780
V	 0.9770	 0.6300
VC	 0.3480	 0.3770
W	 0.9760	 0.6300
WA	 0.3480	 0.3780
X	 0.9740	 0.6300
XB	 0.3700	 0.3830
Y	 0.9760	 0.6310
YC	 0.3700	 0.3910
Z	 0.9740	 0.6300
ZA	 0.3700	 0.3950
a	 0.9740	 0.6300
aB	 0.3700	 0.3940
b	 0.9740	 0.6300
bC	 0.3700	 0.3850
c	 0.9740	 0.6300
cA	 0.3480	 0.3710
d	 0.9740	 0.6300
dB	 0.3700	 0.3910

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Chain	Atom inclusion	Q-score
e	 0.9740	 0.6300
eC	 0.3700	 0.3870
f	 0.9740	 0.6310
fA	 0.3700	 0.3890
g	 0.9770	 0.6300
gB	 0.3480	 0.3720
h	 0.9740	 0.6300
hC	 0.3700	 0.3950
i	 0.9760	 0.6310
iA	 0.3700	 0.3860
j	 0.9760	 0.6300
jB	 0.3700	 0.3940
k	 0.9760	 0.6300
kC	 0.3700	 0.3910
l	 0.9740	 0.6300
lA	 0.3480	 0.3790
m	 0.9770	 0.6300
mB	 0.3480	 0.3730
n	 0.9740	 0.6290
nC	 0.3480	 0.3710
o	 0.9740	 0.6300
oA	 0.3700	 0.3800
p	 0.9770	 0.6290
pB	 0.3480	 0.3750
q	 0.9740	 0.6300
qC	 0.3480	 0.3650
r	 0.9740	 0.6300
rA	 0.3480	 0.3670
s	 0.9740	 0.6310
sB	 0.3480	 0.3790
t	 0.9740	 0.6300
tC	 0.3480	 0.3770
u	 0.9770	 0.6300
uA	 0.3480	 0.3780
v	 0.9740	 0.6300
vB	 0.3700	 0.3870
w	 0.9740	 0.6310
wC	 0.3480	 0.3700
x	 0.9770	 0.6290
xA	 0.3700	 0.3920
y	 0.9740	 0.6300
yB	 0.3480	 0.3640

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Chain	Atom inclusion	Q-score
z	 0.9740	 0.6300
zC	 0.3700	 0.3870