



## Full wwPDB EM Validation Report ⓘ

Dec 2, 2024 – 01:01 PM JST

PDB ID : 8YW2  
EMDB ID : EMD-39620  
Title : Semliki Forest virus viron in complex with VLDLR  
Authors : Wang, J.; Zheng, T.; Yang, D.  
Deposited on : 2024-03-29  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

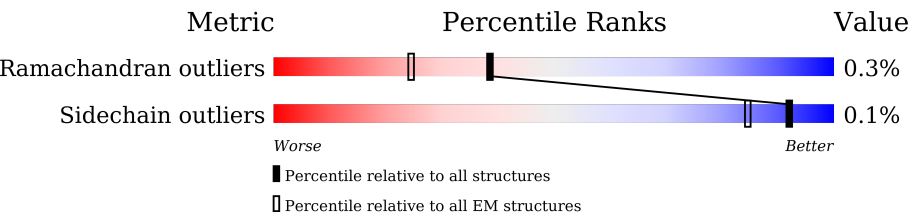
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



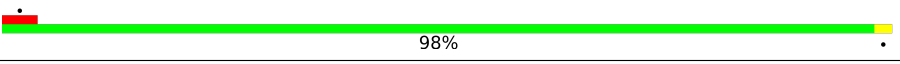
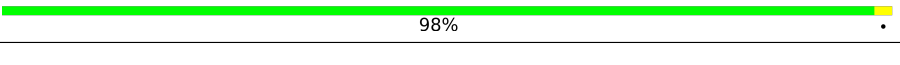
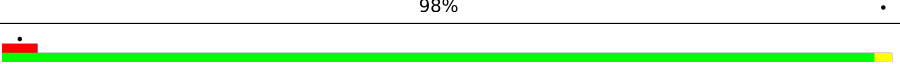
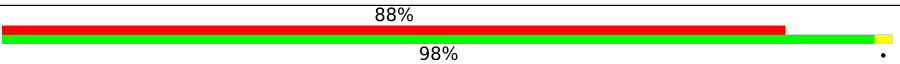
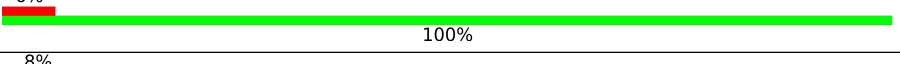
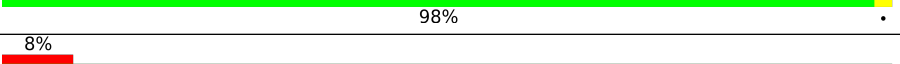
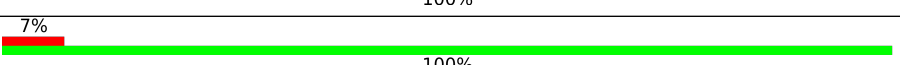
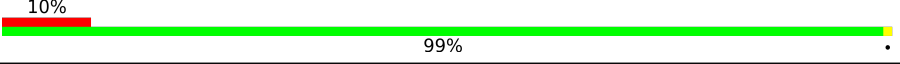
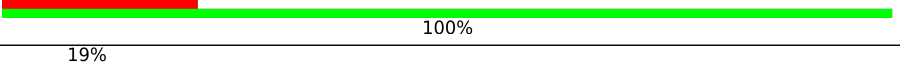
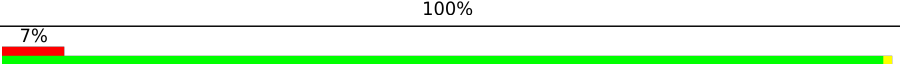
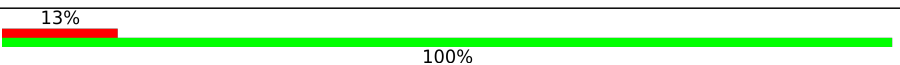
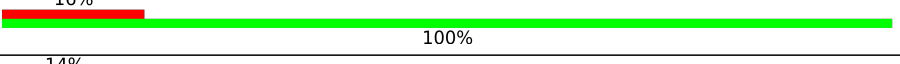
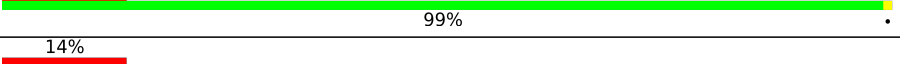
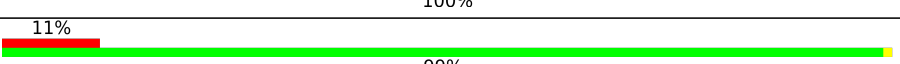
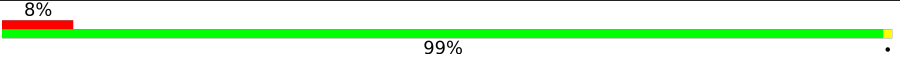
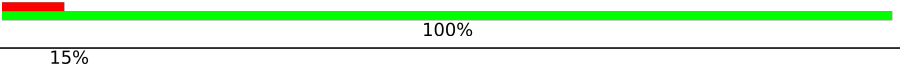
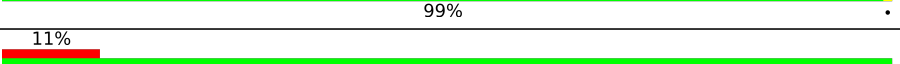
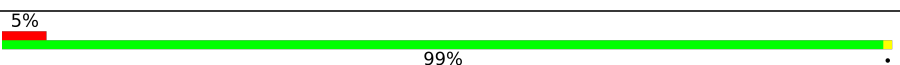
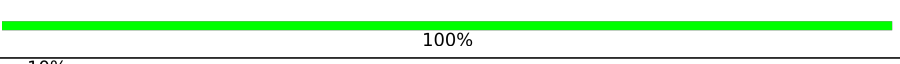
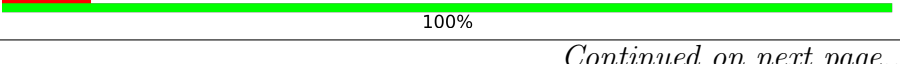



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	0	52	
1	2	52	
1	AA	52	
1	AB	52	
1	L	52	
1	M	52	
1	N	52	
1	S	52	
1	a	52	

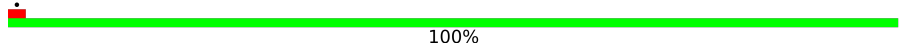
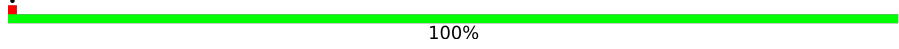
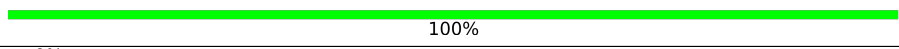
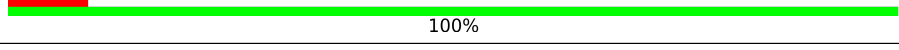
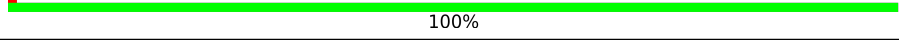
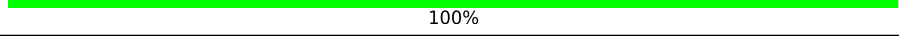
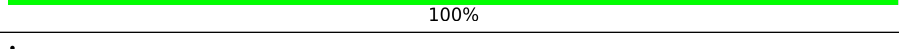
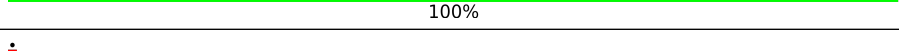
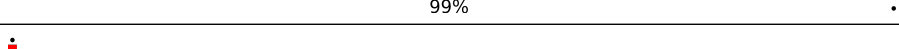
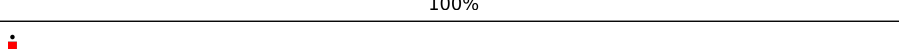
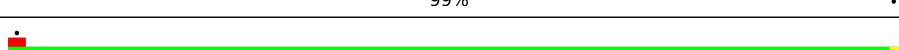
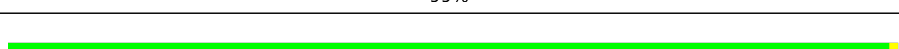
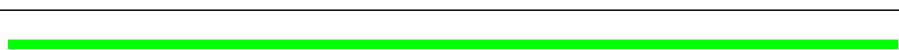
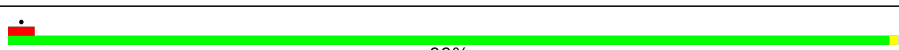
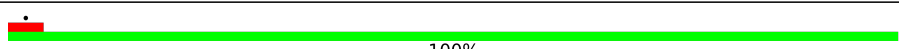
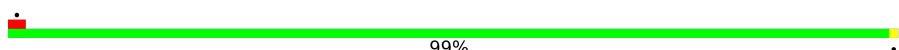
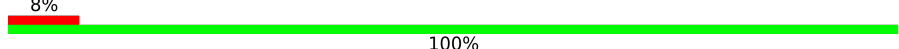
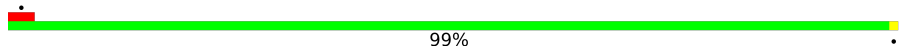
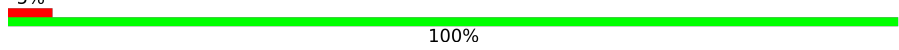
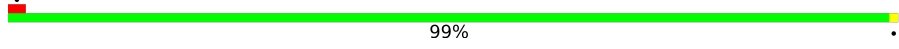
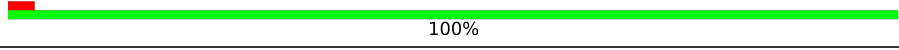
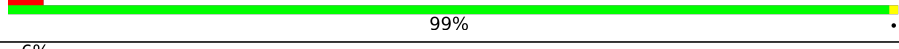
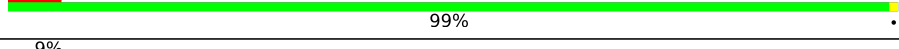
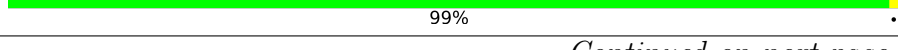

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Mol	Chain	Length	Quality of chain
1	b	52	 98%
1	c	52	 98%
1	g	52	 98%
1	l	52	 98%
1	u	52	 88% 98%
1	v	52	 6% 100%
1	w	52	 8% 98%
2	1	161	 8% 100%
2	3	161	 7% 100%
2	AC	161	 10% 99%
2	AD	161	 22% 100%
2	AE	161	 19% 100%
2	D	161	 7% 99%
2	O	161	 13% 100%
2	P	161	 16% 100%
2	Q	161	 14% 99%
2	T	161	 14% 100%
2	d	161	 11% 99%
2	e	161	 8% 99%
2	f	161	 7% 100%
2	n	161	 15% 99%
2	x	161	 11% 100%
2	y	161	 5% 99%
3	4	438	100%
3	5	438	10% 100%

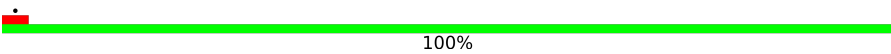
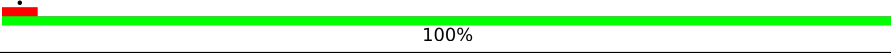
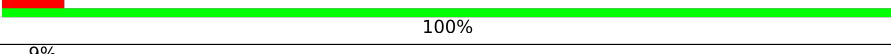
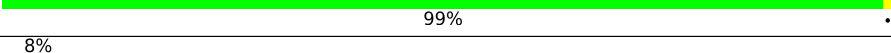
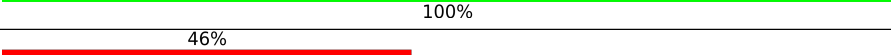
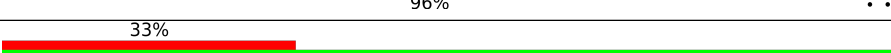
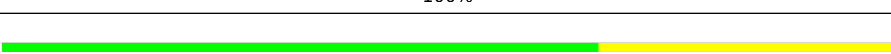
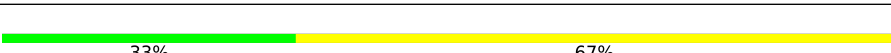


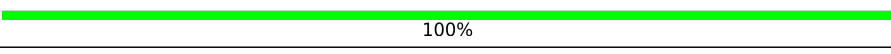
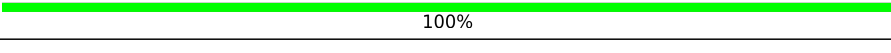
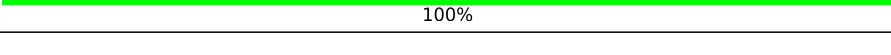
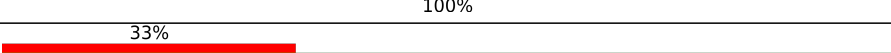
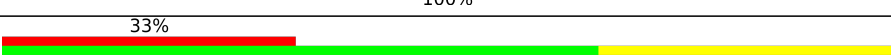
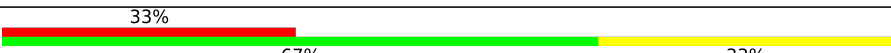

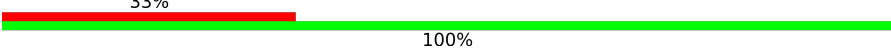
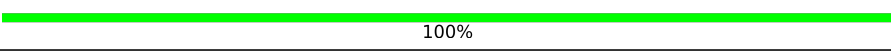

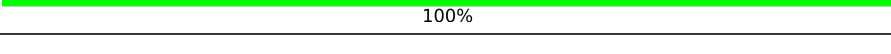
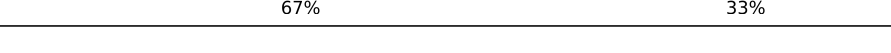



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Mol	Chain	Length	Quality of chain
3	6	438	 100%
3	E	438	 100%
3	F	438	 100%
3	G	438	 9%100%
3	H	438	 100%
3	U	438	 100%
3	V	438	 100%
3	W	438	 100%
3	h	438	 99%.
3	i	438	 100%
3	m	438	 99%.
3	o	438	 99%.
3	p	438	 99%.
3	q	438	 100%
4	7	418	 99%.
4	8	418	 100%
4	9	418	 99%.
4	B	418	 8%100%
4	I	418	 99%.
4	J	418	 5%100%
4	K	418	 99%.
4	R	418	 100%
4	X	418	 99%.
4	Y	418	 6%99%.
4	Z	418	 9%99%.

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Mol	Chain	Length	Quality of chain
4	j	418	 100%
4	r	418	 100%
4	s	418	 7%100%
4	t	418	 9%99%
4	z	418	 8%100%
5	A	162	 46%96%
6	BA	3	 33%100%
6	C	3	 67%33%
6	CA	3	 33%67%
6	DA	3	 100%
6	EA	3	 33%67%
6	FA	3	 100%
6	GA	3	 100%
6	HA	3	 100%
6	IA	3	 100%
6	JA	3	 33%100%
6	KA	3	 33%67%33%
6	LA	3	 33%67%33%
6	MA	3	 33%67%33%
6	NA	3	 33%100%
6	OA	3	 100%
6	PA	3	 33%67%
6	QA	3	 100%
6	RA	3	 67%33%
6	SA	3	 67%33%

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Mol	Chain	Length	Quality of chain
6	TA	3	100%
6	UA	3	67%
6	VA	3	100%
6	WA	3	33%
6	XA	3	67%
6	YA	3	100%
6	ZA	3	67%
6	aA	3	100%
6	bA	3	33%
6	cA	3	100%
6	dA	3	100%
6	eA	3	100%
6	fA	3	67%
6	gA	3	67%
6	hA	3	67%
6	iA	3	100%
6	jA	3	100%
6	k	3	33%
6	kA	3	67%
6	lA	3	67%
6	mA	3	100%
6	nA	3	67%
6	oA	3	67%
6	pA	3	67%
6	qA	3	67%

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Mol	Chain	Length	Quality of chain
6	rA	3	<div><div></div><div>67%</div><div>33%</div></div>
6	sA	3	<div><div>33%</div><div></div><div>100%</div></div>
6	tA	3	<div><div></div><div>33%</div><div>67%</div></div>
6	uA	3	<div><div>33%</div><div></div><div>100%</div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 134901 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein E3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	2	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	AA	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	AB	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	L	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	M	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	N	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	S	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	a	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	b	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	c	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	g	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	l	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	u	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	v	52	Total 404	C 252	N 67	O 77	S 8	0	0
1	w	52	Total 404	C 252	N 67	O 77	S 8	0	0

- Molecule 2 is a protein called capsid protein, partial.



Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	3	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	AC	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	AD	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	AE	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	D	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	O	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	P	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	Q	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	T	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	d	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	e	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	f	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	n	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	x	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		
2	y	161	Total	C	N	O	S	0	0
			1245	779	226	231	9		

- Molecule 3 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	5	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	6	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	E	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	G	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	H	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	U	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	V	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	W	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	h	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	i	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	m	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	o	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	p	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		
3	q	438	Total	C	N	O	S	0	0
			3330	2109	559	637	25		

- Molecule 4 is a protein called Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	8	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	9	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	B	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	I	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	J	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	K	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	X	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	Y	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	Z	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	j	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	r	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	s	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	t	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		
4	z	418	Total	C	N	O	S	0	0
			3260	2058	579	598	25		

- Molecule 5 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	162	Total	C	N	O	S	0	0
			1205	694	210	276	25		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	3	Total	C	N	O		0	0
			39	22	2	15			
6	k	3	Total	C	N	O		0	0
			39	22	2	15			
6	BA	3	Total	C	N	O		0	0
			39	22	2	15			
6	CA	3	Total	C	N	O		0	0
			39	22	2	15			

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	DA	3	Total	C	N	O	0	0
			39	22	2	15		
6	EA	3	Total	C	N	O	0	0
			39	22	2	15		
6	FA	3	Total	C	N	O	0	0
			39	22	2	15		
6	GA	3	Total	C	N	O	0	0
			39	22	2	15		
6	HA	3	Total	C	N	O	0	0
			39	22	2	15		
6	IA	3	Total	C	N	O	0	0
			39	22	2	15		
6	JA	3	Total	C	N	O	0	0
			39	22	2	15		
6	KA	3	Total	C	N	O	0	0
			39	22	2	15		
6	LA	3	Total	C	N	O	0	0
			39	22	2	15		
6	MA	3	Total	C	N	O	0	0
			39	22	2	15		
6	NA	3	Total	C	N	O	0	0
			39	22	2	15		
6	OA	3	Total	C	N	O	0	0
			39	22	2	15		
6	PA	3	Total	C	N	O	0	0
			39	22	2	15		
6	QA	3	Total	C	N	O	0	0
			39	22	2	15		
6	RA	3	Total	C	N	O	0	0
			39	22	2	15		
6	SA	3	Total	C	N	O	0	0
			39	22	2	15		
6	TA	3	Total	C	N	O	0	0
			39	22	2	15		
6	UA	3	Total	C	N	O	0	0
			39	22	2	15		
6	VA	3	Total	C	N	O	0	0
			39	22	2	15		
6	WA	3	Total	C	N	O	0	0
			39	22	2	15		
6	XA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	YA	3	Total	C	N	O	0	0
			39	22	2	15		
6	ZA	3	Total	C	N	O	0	0
			39	22	2	15		
6	aA	3	Total	C	N	O	0	0
			39	22	2	15		
6	bA	3	Total	C	N	O	0	0
			39	22	2	15		
6	cA	3	Total	C	N	O	0	0
			39	22	2	15		
6	dA	3	Total	C	N	O	0	0
			39	22	2	15		
6	eA	3	Total	C	N	O	0	0
			39	22	2	15		
6	fA	3	Total	C	N	O	0	0
			39	22	2	15		
6	gA	3	Total	C	N	O	0	0
			39	22	2	15		
6	hA	3	Total	C	N	O	0	0
			39	22	2	15		
6	iA	3	Total	C	N	O	0	0
			39	22	2	15		
6	jA	3	Total	C	N	O	0	0
			39	22	2	15		
6	kA	3	Total	C	N	O	0	0
			39	22	2	15		
6	lA	3	Total	C	N	O	0	0
			39	22	2	15		
6	mA	3	Total	C	N	O	0	0
			39	22	2	15		
6	nA	3	Total	C	N	O	0	0
			39	22	2	15		
6	oA	3	Total	C	N	O	0	0
			39	22	2	15		
6	pA	3	Total	C	N	O	0	0
			39	22	2	15		
6	qA	3	Total	C	N	O	0	0
			39	22	2	15		
6	rA	3	Total	C	N	O	0	0
			39	22	2	15		
6	sA	3	Total	C	N	O	0	0
			39	22	2	15		

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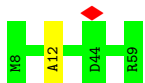
Mol	Chain	Residues	Atoms				AltConf	Trace
6	tA	3	Total	C	N	O	0	0
			39	22	2	15		
6	uA	3	Total	C	N	O	0	0
			39	22	2	15		

### 3 Residue-property plots [i](#)

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

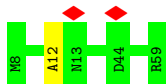
- Molecule 1: Spike glycoprotein E3

Chain 0:  98%



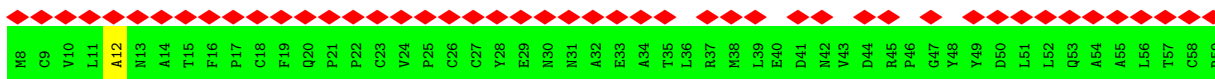
- Molecule 1: Spike glycoprotein E3

Chain 2:  98%



- Molecule 1: Spike glycoprotein E3

Chain AA:  90% 98%



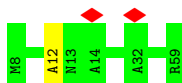
- Molecule 1: Spike glycoprotein E3

Chain AB:  98%

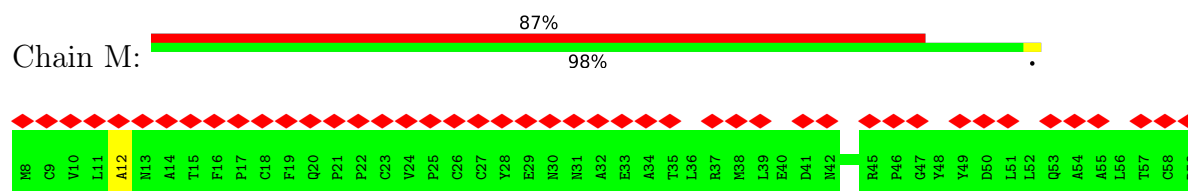


- Molecule 1: Spike glycoprotein E3

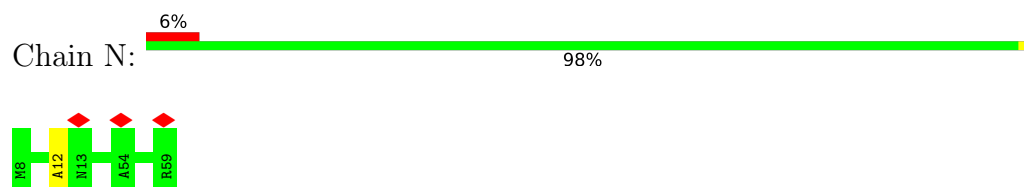
Chain L:  98%



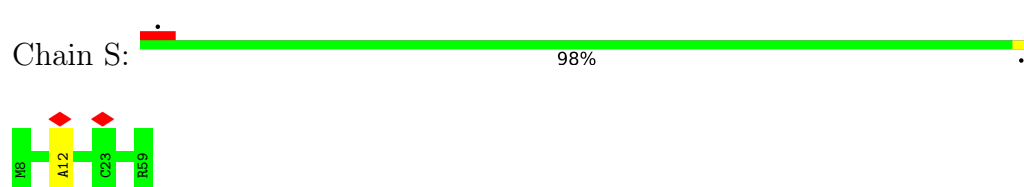
- Molecule 1: Spike glycoprotein E3



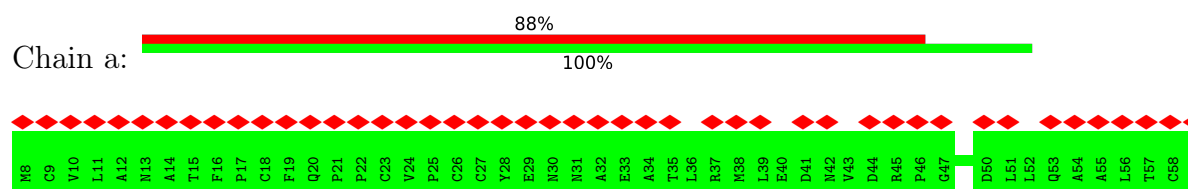
- Molecule 1: Spike glycoprotein E3



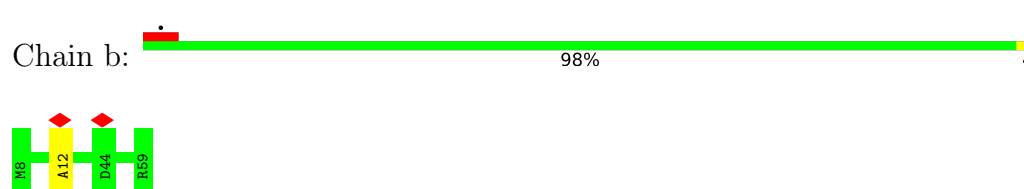
- Molecule 1: Spike glycoprotein E3



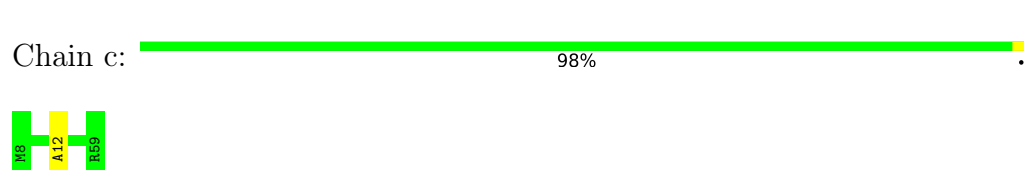
- Molecule 1: Spike glycoprotein E3



- Molecule 1: Spike glycoprotein E3



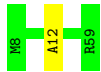
- Molecule 1: Spike glycoprotein E3



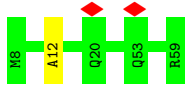
- Molecule 1: Spike glycoprotein E3



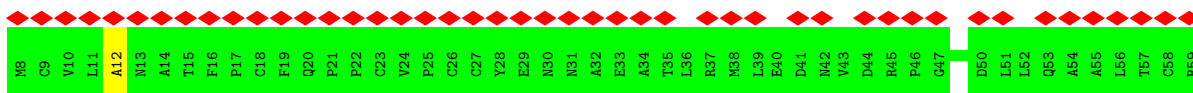
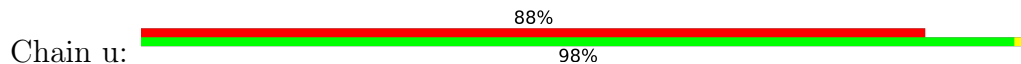




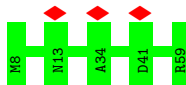
- Molecule 1: Spike glycoprotein E3



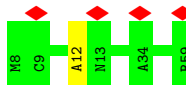
- Molecule 1: Spike glycoprotein E3



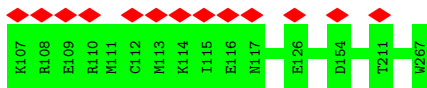
- Molecule 1: Spike glycoprotein E3



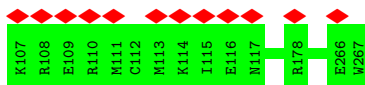
- Molecule 1: Spike glycoprotein E3



- Molecule 2: capsid protein, partial

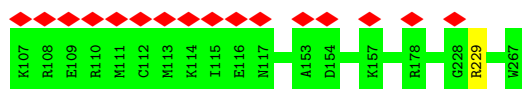


- Molecule 2: capsid protein, partial



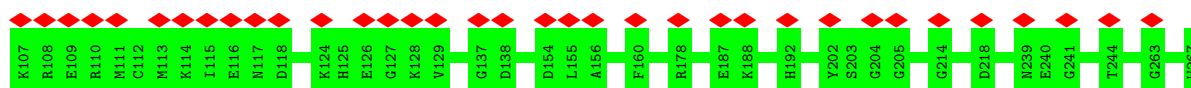
- Molecule 2: capsid protein, partial

Chain AC:  10% 99%



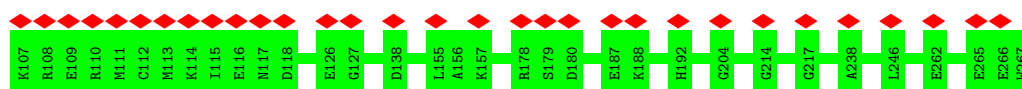
- Molecule 2: capsid protein, partial

Chain AD:  22% 100%



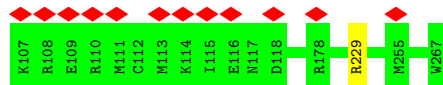
- Molecule 2: capsid protein, partial

Chain AE:  19% 100%



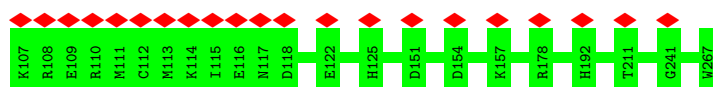
- Molecule 2: capsid protein, partial

Chain D:  7% 99%



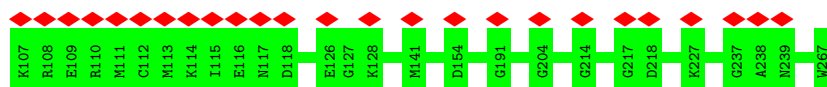
- Molecule 2: capsid protein, partial

Chain O:  13% 100%



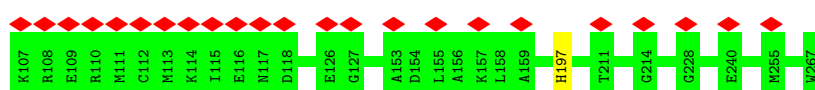
- Molecule 2: capsid protein, partial

Chain P:  16% 100%

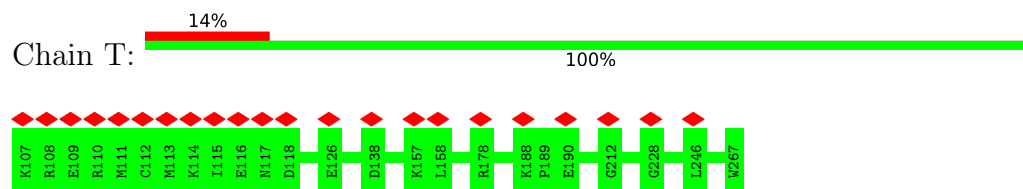


- Molecule 2: capsid protein, partial

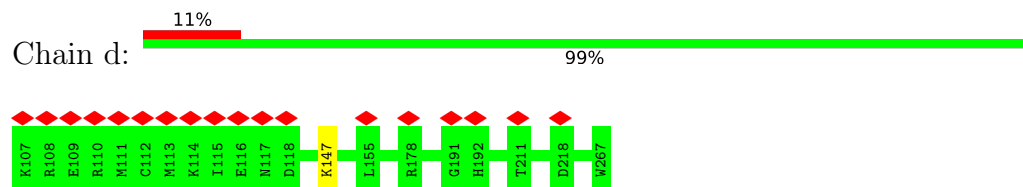
Chain Q:  14% 99%



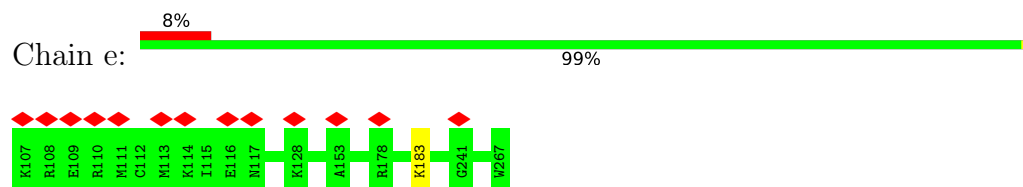
- Molecule 2: capsid protein, partial



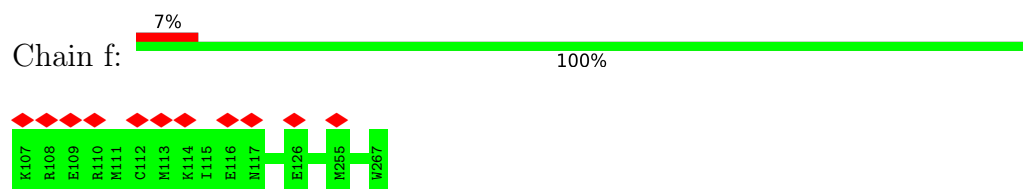
- Molecule 2: capsid protein, partial



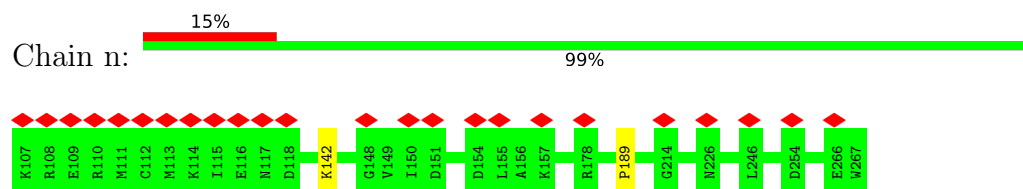
- Molecule 2: capsid protein, partial



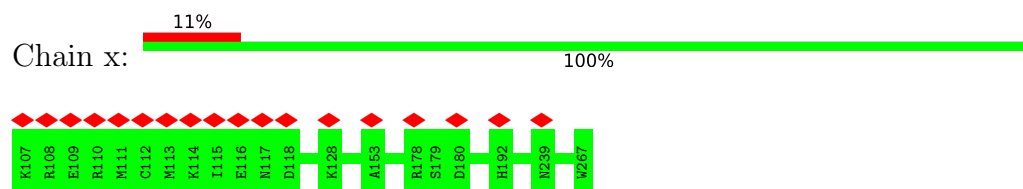
- Molecule 2: capsid protein, partial



- Molecule 2: capsid protein, partial

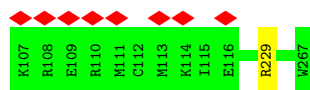


- Molecule 2: capsid protein, partial



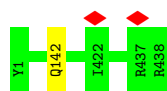
- Molecule 2: capsid protein, partial





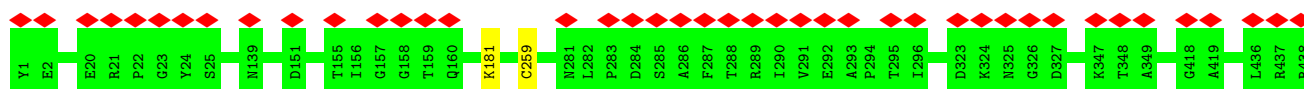
- Molecule 3: Spike glycoprotein E1

Chain 4:  100%



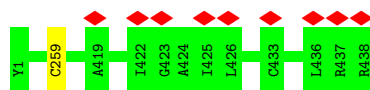
- Molecule 3: Spike glycoprotein E1

Chain 5:  10%  100%



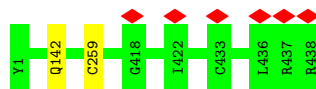
- Molecule 3: Spike glycoprotein E1

Chain 6:  100%



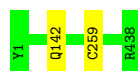
- Molecule 3: Spike glycoprotein E1

Chain E:  100%



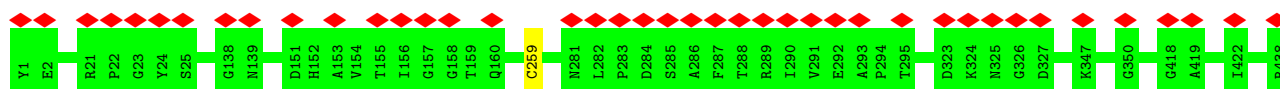
- Molecule 3: Spike glycoprotein E1

Chain F:  100%



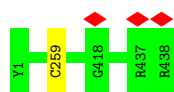
- Molecule 3: Spike glycoprotein E1

Chain G:  9%  100%



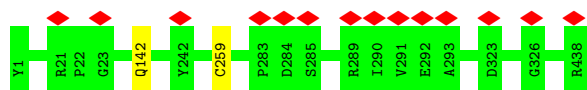
- Molecule 3: Spike glycoprotein E1

Chain H:  100%



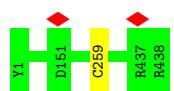
- Molecule 3: Spike glycoprotein E1

Chain U:  100%



- Molecule 3: Spike glycoprotein E1

Chain V:  100%



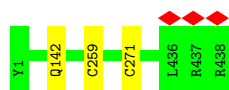
- Molecule 3: Spike glycoprotein E1

Chain W:  100%



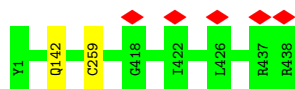
- Molecule 3: Spike glycoprotein E1

Chain h:  99%



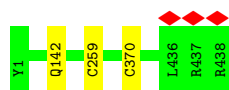
- Molecule 3: Spike glycoprotein E1

Chain i:  100%



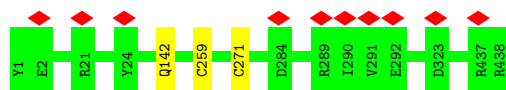
- Molecule 3: Spike glycoprotein E1

Chain m:  99%



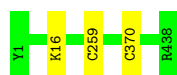
- Molecule 3: Spike glycoprotein E1

Chain o:  99%



- Molecule 3: Spike glycoprotein E1

Chain p:  99%



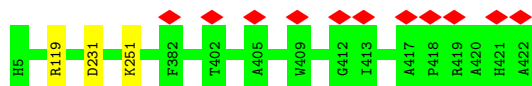
- Molecule 3: Spike glycoprotein E1

Chain q:  100%

There are no outlier residues recorded for this chain.

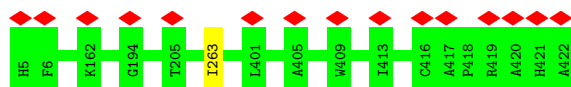
- Molecule 4: Spike glycoprotein E2

Chain 7:  99%



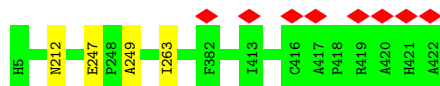
- Molecule 4: Spike glycoprotein E2

Chain 8:  100%



- Molecule 4: Spike glycoprotein E2

Chain 9:  99%

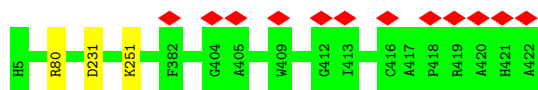


- Molecule 4: Spike glycoprotein E2

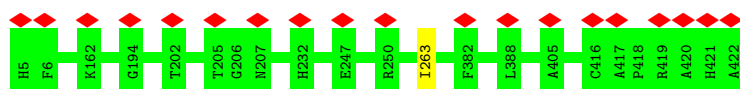
Chain B:  8% 100%



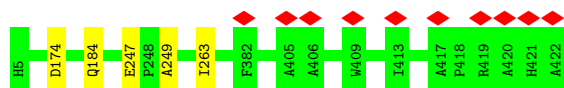
## • Molecule 4: Spike glycoprotein E2

Chain I:  99%

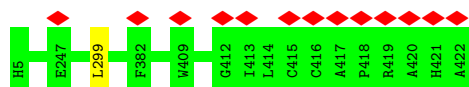
## • Molecule 4: Spike glycoprotein E2

Chain J:  100%

## • Molecule 4: Spike glycoprotein E2

Chain K:  99%

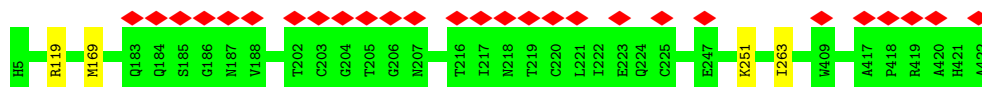
## • Molecule 4: Spike glycoprotein E2

Chain R:  100%

## • Molecule 4: Spike glycoprotein E2

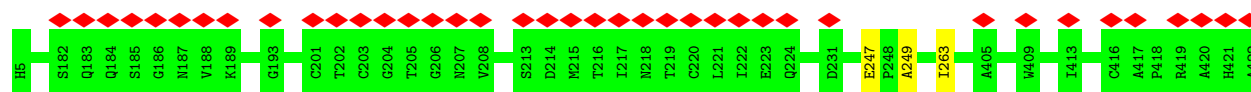
Chain X:  99%

## • Molecule 4: Spike glycoprotein E2

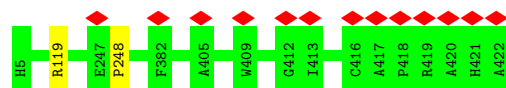
Chain Y:  99%

## • Molecule 4: Spike glycoprotein E2

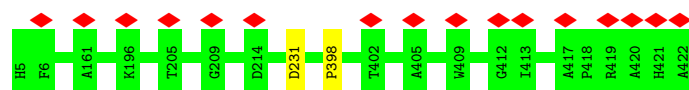
Chain Z:  99%



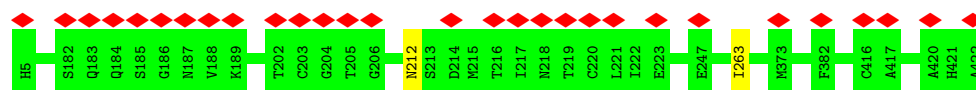
- Molecule 4: Spike glycoprotein E2



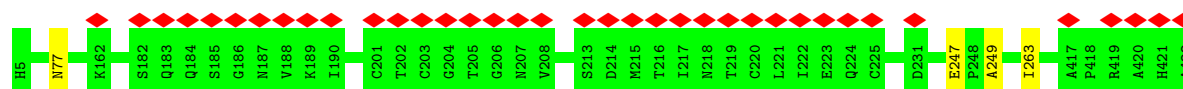
- Molecule 4: Spike glycoprotein E2



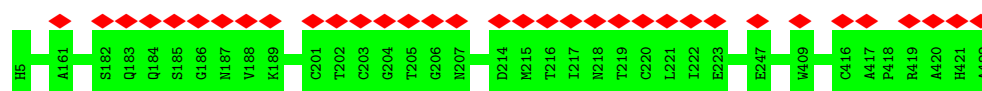
- Molecule 4: Spike glycoprotein E2



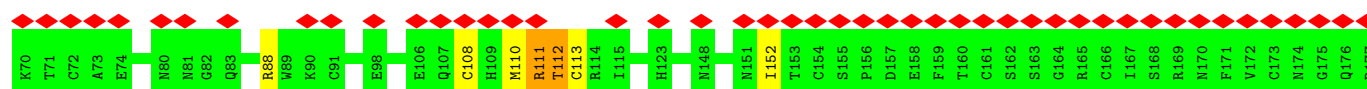
- Molecule 4: Spike glycoprotein E2



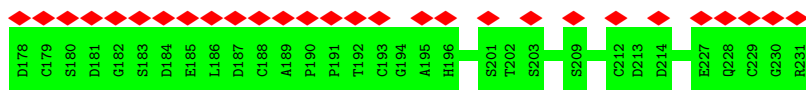
- Molecule 4: Spike glycoprotein E2



- Molecule 5: Very low-density lipoprotein receptor







- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 33% 33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA: 33% 33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA: 33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA: 33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA: 33% 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA: 33% 67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MA: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OA: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PA: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain QA: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain RA:  67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain SA:  67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain TA:  100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain UA:  67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain VA:  100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain WA:  33% 67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain kA:  67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain lA:  33% 33% 67%

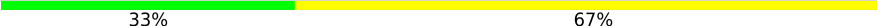


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain mA:  33% 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain nA:  33% 67%

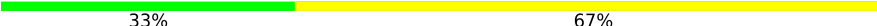


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain oA:  67% 33%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain pA:  33% 67%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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	33471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.827	Depositor
Minimum map value	-1.282	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.33	0/413	0.49	0/563
1	2	0.29	0/413	0.52	0/563
1	AA	0.26	0/413	0.48	0/563
1	AB	0.33	0/413	0.55	0/563
1	L	0.35	0/413	0.51	0/563
1	M	0.25	0/413	0.46	0/563
1	N	0.32	0/413	0.53	0/563
1	S	0.29	0/413	0.50	0/563
1	a	0.26	0/413	0.46	0/563
1	b	0.28	0/413	0.49	0/563
1	c	0.31	0/413	0.50	0/563
1	g	0.31	0/413	0.52	0/563
1	l	0.32	0/413	0.52	0/563
1	u	0.26	0/413	0.47	0/563
1	v	0.29	0/413	0.55	0/563
1	w	0.30	0/413	0.53	0/563
2	1	0.35	0/1273	0.53	0/1714
2	3	0.35	0/1273	0.55	0/1714
2	AC	0.32	0/1273	0.53	0/1714
2	AD	0.29	0/1273	0.52	0/1714
2	AE	0.31	0/1273	0.54	0/1714
2	D	0.34	0/1273	0.54	0/1714
2	O	0.32	0/1273	0.53	0/1714
2	P	0.31	0/1273	0.55	0/1714
2	Q	0.30	0/1273	0.53	0/1714
2	T	0.29	0/1273	0.54	0/1714
2	d	0.31	0/1273	0.55	0/1714
2	e	0.35	0/1273	0.55	0/1714
2	f	0.35	0/1273	0.54	0/1714
2	n	0.34	1/1273 (0.1%)	0.65	2/1714 (0.1%)
2	x	0.31	0/1273	0.53	0/1714
2	y	0.35	0/1273	0.54	0/1714

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	4	0.45	0/3416	0.55	0/4660
3	5	0.37	0/3416	0.54	1/4660 (0.0%)
3	6	0.45	0/3416	0.56	1/4660 (0.0%)
3	E	0.45	0/3416	0.55	1/4660 (0.0%)
3	F	0.45	0/3416	0.57	1/4660 (0.0%)
3	G	0.37	0/3416	0.53	1/4660 (0.0%)
3	H	0.44	0/3416	0.55	1/4660 (0.0%)
3	U	0.37	0/3416	0.54	1/4660 (0.0%)
3	V	0.42	0/3416	0.54	1/4660 (0.0%)
3	W	0.44	0/3416	0.56	0/4660
3	h	0.45	0/3416	0.57	2/4660 (0.0%)
3	i	0.45	0/3416	0.56	1/4660 (0.0%)
3	m	0.46	0/3416	0.56	1/4660 (0.0%)
3	o	0.39	0/3416	0.55	2/4660 (0.0%)
3	p	0.42	0/3416	0.56	1/4660 (0.0%)
3	q	0.45	0/3416	0.54	0/4660
4	7	0.41	0/3354	0.56	0/4574
4	8	0.38	0/3354	0.57	0/4574
4	9	0.41	0/3354	0.56	0/4574
4	B	0.40	0/3354	0.57	0/4574
4	I	0.40	0/3354	0.57	0/4574
4	J	0.38	0/3354	0.56	0/4574
4	K	0.40	0/3354	0.58	1/4574 (0.0%)
4	R	0.42	0/3354	0.58	1/4574 (0.0%)
4	X	0.39	0/3354	0.55	0/4574
4	Y	0.41	0/3354	0.57	1/4574 (0.0%)
4	Z	0.41	0/3354	0.57	0/4574
4	j	0.43	0/3354	0.58	1/4574 (0.0%)
4	r	0.39	0/3354	0.55	1/4574 (0.0%)
4	s	0.41	0/3354	0.57	0/4574
4	t	0.41	0/3354	0.57	0/4574
4	z	0.41	0/3354	0.57	0/4574
5	A	0.29	0/1226	0.50	0/1661
All	All	0.40	1/136522 (0.0%)	0.55	22/185837 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	9	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
4	K	0	1
4	Z	0	1
4	t	0	1
5	A	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	189	PRO	CG-CD	-5.05	1.33	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	189	PRO	CA-N-CD	-12.03	94.66	111.50
4	K	174	ASP	CB-CG-OD1	7.68	125.22	118.30
3	i	259	CYS	CA-CB-SG	6.97	126.54	114.00
2	n	189	PRO	N-CD-CG	-6.63	93.26	103.20
3	H	259	CYS	CA-CB-SG	6.39	125.51	114.00
3	F	259	CYS	CA-CB-SG	6.38	125.47	114.00
3	p	259	CYS	CA-CB-SG	6.17	125.11	114.00
3	o	259	CYS	CA-CB-SG	6.11	125.00	114.00
3	6	259	CYS	CA-CB-SG	6.10	124.99	114.00
3	h	271	CYS	CA-CB-SG	6.07	124.92	114.00
3	E	259	CYS	CA-CB-SG	6.05	124.89	114.00
3	h	259	CYS	CA-CB-SG	5.96	124.73	114.00
3	V	259	CYS	CA-CB-SG	5.96	124.72	114.00
3	U	259	CYS	CA-CB-SG	5.93	124.68	114.00
4	r	398	PRO	CA-N-CD	-5.92	103.22	111.50
3	m	259	CYS	CA-CB-SG	5.79	124.42	114.00
4	j	248	PRO	N-CD-CG	-5.65	94.72	103.20
4	Y	169	MET	CA-CB-CG	5.27	122.27	113.30
3	o	271	CYS	CA-CB-SG	5.25	123.46	114.00
3	G	259	CYS	CA-CB-SG	5.25	123.46	114.00
3	5	259	CYS	CA-CB-SG	5.20	123.35	114.00
4	R	299	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	9	247	GLU	Peptide
5	A	111	ARG	Sidechain
4	K	247	GLU	Peptide
4	Z	247	GLU	Peptide
4	t	247	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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

## 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	0	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	34
1	2	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	34
1	AA	50/52 (96%)	49 (98%)	0	1 (2%)	6	34
1	AB	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	34
1	L	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	34
1	M	50/52 (96%)	49 (98%)	0	1 (2%)	6	34
1	N	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	34
1	S	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	34
1	a	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
1	b	50/52 (96%)	49 (98%)	0	1 (2%)	6	34
1	c	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	34
1	g	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	34
1	l	50/52 (96%)	48 (96%)	1 (2%)	1 (2%)	6	34
1	u	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	6	34
1	v	50/52 (96%)	48 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	50/52 (96%)	49 (98%)	0	1 (2%)	6	34
2	1	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	3	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	AC	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	AD	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	AE	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	D	159/161 (99%)	150 (94%)	9 (6%)	0	100	100
2	O	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	P	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	Q	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	T	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	d	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	e	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
2	f	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	n	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	x	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	y	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
3	4	436/438 (100%)	403 (92%)	32 (7%)	1 (0%)	44	72
3	5	436/438 (100%)	408 (94%)	27 (6%)	1 (0%)	44	72
3	6	436/438 (100%)	402 (92%)	34 (8%)	0	100	100
3	E	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	44	72
3	F	436/438 (100%)	399 (92%)	36 (8%)	1 (0%)	44	72
3	G	436/438 (100%)	411 (94%)	25 (6%)	0	100	100
3	H	436/438 (100%)	404 (93%)	32 (7%)	0	100	100
3	U	436/438 (100%)	404 (93%)	31 (7%)	1 (0%)	44	72
3	V	436/438 (100%)	407 (93%)	29 (7%)	0	100	100
3	W	436/438 (100%)	403 (92%)	33 (8%)	0	100	100
3	h	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	44	72
3	i	436/438 (100%)	405 (93%)	30 (7%)	1 (0%)	44	72
3	m	436/438 (100%)	410 (94%)	24 (6%)	2 (0%)	25	57
3	o	436/438 (100%)	406 (93%)	29 (7%)	1 (0%)	44	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	p	436/438 (100%)	411 (94%)	24 (6%)	1 (0%)	44	72
3	q	436/438 (100%)	406 (93%)	30 (7%)	0	100	100
4	7	416/418 (100%)	363 (87%)	51 (12%)	2 (0%)	25	57
4	8	416/418 (100%)	371 (89%)	44 (11%)	1 (0%)	44	72
4	9	416/418 (100%)	359 (86%)	55 (13%)	2 (0%)	25	57
4	B	416/418 (100%)	373 (90%)	43 (10%)	0	100	100
4	I	416/418 (100%)	362 (87%)	52 (12%)	2 (0%)	25	57
4	J	416/418 (100%)	373 (90%)	42 (10%)	1 (0%)	44	72
4	K	416/418 (100%)	364 (88%)	50 (12%)	2 (0%)	25	57
4	R	416/418 (100%)	370 (89%)	46 (11%)	0	100	100
4	X	416/418 (100%)	365 (88%)	48 (12%)	3 (1%)	19	51
4	Y	416/418 (100%)	367 (88%)	48 (12%)	1 (0%)	44	72
4	Z	416/418 (100%)	364 (88%)	50 (12%)	2 (0%)	25	57
4	j	416/418 (100%)	371 (89%)	45 (11%)	0	100	100
4	r	416/418 (100%)	365 (88%)	50 (12%)	1 (0%)	44	72
4	s	416/418 (100%)	364 (88%)	51 (12%)	1 (0%)	44	72
4	t	416/418 (100%)	364 (88%)	50 (12%)	2 (0%)	25	57
4	z	416/418 (100%)	375 (90%)	41 (10%)	0	100	100
5	A	160/162 (99%)	145 (91%)	11 (7%)	4 (2%)	4	30
All	All	17136/17266 (99%)	15724 (92%)	1363 (8%)	49 (0%)	38	67

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	142	GLN
4	8	263	ILE
4	9	263	ILE
5	A	113	CYS
3	E	142	GLN
3	F	142	GLN
4	J	263	ILE
4	K	263	ILE
3	U	142	GLN
4	Y	263	ILE
4	Z	263	ILE

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Mol	Chain	Res	Type
3	h	142	GLN
3	i	142	GLN
3	m	142	GLN
3	o	142	GLN
4	s	263	ILE
4	t	263	ILE
1	2	12	ALA
5	A	112	THR
5	A	152	ILE
1	S	12	ALA
1	b	12	ALA
1	l	12	ALA
4	7	231	ASP
4	9	249	ALA
5	A	108	CYS
1	AA	12	ALA
1	AB	12	ALA
4	I	231	ASP
1	L	12	ALA
1	M	12	ALA
1	N	12	ALA
4	Z	249	ALA
1	c	12	ALA
1	g	12	ALA
4	r	231	ASP
4	t	249	ALA
4	I	251	LYS
4	K	249	ALA
4	X	231	ASP
4	7	251	LYS
3	m	370	CYS
1	0	12	ALA
3	5	181	LYS
4	X	251	LYS
3	p	370	CYS
1	u	12	ALA
1	w	12	ALA
4	X	164	VAL



### 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	0	45/45 (100%)	45 (100%)	0	100	100
1	2	45/45 (100%)	45 (100%)	0	100	100
1	AA	45/45 (100%)	45 (100%)	0	100	100
1	AB	45/45 (100%)	45 (100%)	0	100	100
1	L	45/45 (100%)	45 (100%)	0	100	100
1	M	45/45 (100%)	45 (100%)	0	100	100
1	N	45/45 (100%)	45 (100%)	0	100	100
1	S	45/45 (100%)	45 (100%)	0	100	100
1	a	45/45 (100%)	45 (100%)	0	100	100
1	b	45/45 (100%)	45 (100%)	0	100	100
1	c	45/45 (100%)	45 (100%)	0	100	100
1	g	45/45 (100%)	45 (100%)	0	100	100
1	l	45/45 (100%)	45 (100%)	0	100	100
1	u	45/45 (100%)	45 (100%)	0	100	100
1	v	45/45 (100%)	45 (100%)	0	100	100
1	w	45/45 (100%)	45 (100%)	0	100	100
2	1	132/132 (100%)	132 (100%)	0	100	100
2	3	132/132 (100%)	132 (100%)	0	100	100
2	AC	132/132 (100%)	131 (99%)	1 (1%)	79	85
2	AD	132/132 (100%)	132 (100%)	0	100	100
2	AE	132/132 (100%)	132 (100%)	0	100	100
2	D	132/132 (100%)	131 (99%)	1 (1%)	79	85
2	O	132/132 (100%)	132 (100%)	0	100	100
2	P	132/132 (100%)	132 (100%)	0	100	100
2	Q	132/132 (100%)	131 (99%)	1 (1%)	79	85
2	T	132/132 (100%)	132 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	132/132 (100%)	131 (99%)	1 (1%)	79	85
2	e	132/132 (100%)	131 (99%)	1 (1%)	79	85
2	f	132/132 (100%)	132 (100%)	0	100	100
2	n	132/132 (100%)	131 (99%)	1 (1%)	79	85
2	x	132/132 (100%)	132 (100%)	0	100	100
2	y	132/132 (100%)	131 (99%)	1 (1%)	79	85
3	4	372/372 (100%)	372 (100%)	0	100	100
3	5	372/372 (100%)	372 (100%)	0	100	100
3	6	372/372 (100%)	372 (100%)	0	100	100
3	E	372/372 (100%)	372 (100%)	0	100	100
3	F	372/372 (100%)	372 (100%)	0	100	100
3	G	372/372 (100%)	372 (100%)	0	100	100
3	H	372/372 (100%)	372 (100%)	0	100	100
3	U	372/372 (100%)	372 (100%)	0	100	100
3	V	372/372 (100%)	372 (100%)	0	100	100
3	W	372/372 (100%)	372 (100%)	0	100	100
3	h	372/372 (100%)	372 (100%)	0	100	100
3	i	372/372 (100%)	372 (100%)	0	100	100
3	m	372/372 (100%)	372 (100%)	0	100	100
3	o	372/372 (100%)	372 (100%)	0	100	100
3	p	372/372 (100%)	371 (100%)	1 (0%)	91	94
3	q	372/372 (100%)	372 (100%)	0	100	100
4	7	356/356 (100%)	355 (100%)	1 (0%)	91	94
4	8	356/356 (100%)	356 (100%)	0	100	100
4	9	356/356 (100%)	355 (100%)	1 (0%)	91	94
4	B	356/356 (100%)	356 (100%)	0	100	100
4	I	356/356 (100%)	355 (100%)	1 (0%)	91	94
4	J	356/356 (100%)	356 (100%)	0	100	100
4	K	356/356 (100%)	355 (100%)	1 (0%)	91	94
4	R	356/356 (100%)	356 (100%)	0	100	100
4	X	356/356 (100%)	356 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Y	356/356 (100%)	354 (99%)	2 (1%)	84	90
4	Z	356/356 (100%)	356 (100%)	0	100	100
4	j	356/356 (100%)	355 (100%)	1 (0%)	91	94
4	r	356/356 (100%)	356 (100%)	0	100	100
4	s	356/356 (100%)	355 (100%)	1 (0%)	91	94
4	t	356/356 (100%)	355 (100%)	1 (0%)	91	94
4	z	356/356 (100%)	356 (100%)	0	100	100
5	A	145/145 (100%)	141 (97%)	4 (3%)	38	60
All	All	14625/14625 (100%)	14604 (100%)	21 (0%)	92	96

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	7	119	ARG
4	9	212	ASN
5	A	88	ARG
5	A	110	MET
5	A	111	ARG
5	A	112	THR
2	AC	229	ARG
2	D	229	ARG
4	I	80	ARG
4	K	184	GLN
2	Q	197	HIS
4	Y	119	ARG
4	Y	251	LYS
2	d	147	LYS
2	e	183	LYS
4	j	119	ARG
2	n	142	LYS
3	p	16	LYS
4	s	212	ASN
4	t	77	ASN
2	y	229	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	196	HIS
3	6	230	HIS
4	7	157	GLN
2	AC	197	HIS
3	E	230	HIS
3	F	230	HIS
3	F	331	HIS
3	H	116	HIS
3	H	230	HIS
4	K	238	ASN
4	K	348	HIS
3	W	230	HIS
4	Y	236	GLN
2	d	145	HIS
2	d	197	HIS
2	e	196	HIS
2	e	197	HIS
2	f	125	HIS
3	h	18	HIS
3	i	32	GLN
3	o	32	GLN
3	o	331	HIS
3	p	102	GLN
3	q	230	HIS
4	s	5	HIS
4	s	53	GLN
4	s	340	GLN
4	t	232	HIS
2	x	201	GLN
2	y	196	HIS
4	z	236	GLN
4	z	340	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

144 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
6	NAG	BA	1	3,6	14,14,15	0.45	0	17,19,21	0.60	0
6	NAG	BA	2	6	14,14,15	0.19	0	17,19,21	0.44	0
6	BMA	BA	3	6	11,11,12	0.54	0	15,15,17	0.69	0
6	NAG	C	1	3,6	14,14,15	0.20	0	17,19,21	0.61	1 (5%)
6	NAG	C	2	6	14,14,15	0.19	0	17,19,21	0.44	0
6	BMA	C	3	6	11,11,12	0.57	0	15,15,17	0.75	0
6	NAG	CA	1	4,6	14,14,15	0.48	0	17,19,21	1.28	1 (5%)
6	NAG	CA	2	6	14,14,15	0.22	0	17,19,21	0.43	0
6	BMA	CA	3	6	11,11,12	0.55	0	15,15,17	0.92	1 (6%)
6	NAG	DA	1	4,6	14,14,15	0.40	0	17,19,21	0.38	0
6	NAG	DA	2	6	14,14,15	0.30	0	17,19,21	0.50	0
6	BMA	DA	3	6	11,11,12	0.70	0	15,15,17	0.74	0
6	NAG	EA	1	4,6	14,14,15	0.62	1 (7%)	17,19,21	0.81	0
6	NAG	EA	2	6	14,14,15	0.32	0	17,19,21	0.80	0
6	BMA	EA	3	6	11,11,12	0.43	0	15,15,17	0.93	1 (6%)
6	NAG	FA	1	4,6	14,14,15	0.33	0	17,19,21	0.61	0
6	NAG	FA	2	6	14,14,15	0.21	0	17,19,21	0.59	0
6	BMA	FA	3	6	11,11,12	0.70	0	15,15,17	0.68	0
6	NAG	GA	1	4,6	14,14,15	0.19	0	17,19,21	0.52	0
6	NAG	GA	2	6	14,14,15	0.18	0	17,19,21	0.41	0
6	BMA	GA	3	6	11,11,12	0.53	0	15,15,17	0.85	0
6	NAG	HA	1	4,6	14,14,15	0.33	0	17,19,21	0.35	0
6	NAG	HA	2	6	14,14,15	0.23	0	17,19,21	0.51	0
6	BMA	HA	3	6	11,11,12	0.60	0	15,15,17	0.79	0
6	NAG	IA	1	4,6	14,14,15	0.35	0	17,19,21	0.92	1 (5%)
6	NAG	IA	2	6	14,14,15	0.35	0	17,19,21	1.30	2 (11%)
6	BMA	IA	3	6	11,11,12	0.90	1 (9%)	15,15,17	1.06	0
6	NAG	JA	1	4,6	14,14,15	0.27	0	17,19,21	0.41	0
6	NAG	JA	2	6	14,14,15	0.22	0	17,19,21	0.43	0
6	BMA	JA	3	6	11,11,12	0.56	0	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	KA	1	3,6	14,14,15	0.19	0	17,19,21	0.48	0
6	NAG	KA	2	6	14,14,15	0.20	0	17,19,21	0.42	0
6	BMA	KA	3	6	11,11,12	0.51	0	15,15,17	0.95	1 (6%)
6	NAG	LA	1	3,6	14,14,15	0.16	0	17,19,21	0.64	1 (5%)
6	NAG	LA	2	6	14,14,15	0.19	0	17,19,21	0.49	0
6	BMA	LA	3	6	11,11,12	0.59	0	15,15,17	0.75	0
6	NAG	MA	1	3,6	14,14,15	0.35	0	17,19,21	0.59	0
6	NAG	MA	2	6	14,14,15	0.71	1 (7%)	17,19,21	1.21	1 (5%)
6	BMA	MA	3	6	11,11,12	0.75	0	15,15,17	1.03	0
6	NAG	NA	1	3,6	14,14,15	0.21	0	17,19,21	0.54	0
6	NAG	NA	2	6	14,14,15	0.34	0	17,19,21	0.41	0
6	BMA	NA	3	6	11,11,12	0.58	0	15,15,17	0.75	0
6	NAG	OA	1	4,6	14,14,15	0.38	0	17,19,21	0.43	0
6	NAG	OA	2	6	14,14,15	0.27	0	17,19,21	0.47	0
6	BMA	OA	3	6	11,11,12	0.71	0	15,15,17	0.77	0
6	NAG	PA	1	4,6	14,14,15	0.25	0	17,19,21	1.28	2 (11%)
6	NAG	PA	2	6	14,14,15	0.21	0	17,19,21	0.40	0
6	BMA	PA	3	6	11,11,12	0.47	0	15,15,17	0.86	1 (6%)
6	NAG	QA	1	4,6	14,14,15	0.21	0	17,19,21	0.63	0
6	NAG	QA	2	6	14,14,15	0.23	0	17,19,21	0.46	0
6	BMA	QA	3	6	11,11,12	0.66	0	15,15,17	0.71	0
6	NAG	RA	1	4,6	14,14,15	0.58	1 (7%)	17,19,21	0.70	0
6	NAG	RA	2	6	14,14,15	0.25	0	17,19,21	0.73	0
6	BMA	RA	3	6	11,11,12	0.50	0	15,15,17	0.85	0
6	NAG	SA	1	4,6	14,14,15	0.18	0	17,19,21	0.51	0
6	NAG	SA	2	6	14,14,15	0.20	0	17,19,21	0.36	0
6	BMA	SA	3	6	11,11,12	0.85	1 (9%)	15,15,17	1.16	1 (6%)
6	NAG	TA	1	4,6	14,14,15	0.27	0	17,19,21	0.42	0
6	NAG	TA	2	6	14,14,15	0.17	0	17,19,21	0.47	0
6	BMA	TA	3	6	11,11,12	0.57	0	15,15,17	0.80	0
6	NAG	UA	1	4,6	14,14,15	0.39	0	17,19,21	0.49	0
6	NAG	UA	2	6	14,14,15	0.38	0	17,19,21	1.26	2 (11%)
6	BMA	UA	3	6	11,11,12	0.56	0	15,15,17	0.87	0
6	NAG	VA	1	4,6	14,14,15	0.25	0	17,19,21	0.42	0
6	NAG	VA	2	6	14,14,15	0.22	0	17,19,21	0.44	0
6	BMA	VA	3	6	11,11,12	0.46	0	15,15,17	0.77	0
6	NAG	WA	1	3,6	14,14,15	0.17	0	17,19,21	0.67	1 (5%)
6	NAG	WA	2	6	14,14,15	0.19	0	17,19,21	0.35	0
6	BMA	WA	3	6	11,11,12	0.57	0	15,15,17	0.80	0
6	NAG	XA	1	3,6	14,14,15	0.51	0	17,19,21	0.76	0
6	NAG	XA	2	6	14,14,15	0.62	0	17,19,21	1.23	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	XA	3	6	11,11,12	0.88	0	15,15,17	0.80	0
6	NAG	YA	1	3,6	14,14,15	0.46	0	17,19,21	0.41	0
6	NAG	YA	2	6	14,14,15	0.29	0	17,19,21	0.45	0
6	BMA	YA	3	6	11,11,12	0.68	0	15,15,17	0.74	0
6	NAG	ZA	1	4,6	14,14,15	0.37	0	17,19,21	1.28	1 (5%)
6	NAG	ZA	2	6	14,14,15	0.23	0	17,19,21	0.58	0
6	BMA	ZA	3	6	11,11,12	0.56	0	15,15,17	0.76	0
6	NAG	aA	1	4,6	14,14,15	0.40	0	17,19,21	0.35	0
6	NAG	aA	2	6	14,14,15	0.20	0	17,19,21	0.43	0
6	BMA	aA	3	6	11,11,12	0.53	0	15,15,17	0.69	0
6	NAG	bA	1	4,6	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
6	NAG	bA	2	6	14,14,15	0.32	0	17,19,21	0.59	0
6	BMA	bA	3	6	11,11,12	0.52	0	15,15,17	1.16	2 (13%)
6	NAG	cA	1	4,6	14,14,15	0.20	0	17,19,21	0.50	0
6	NAG	cA	2	6	14,14,15	0.23	0	17,19,21	0.46	0
6	BMA	cA	3	6	11,11,12	0.53	0	15,15,17	0.71	0
6	NAG	dA	1	4,6	14,14,15	0.19	0	17,19,21	0.56	0
6	NAG	dA	2	6	14,14,15	0.17	0	17,19,21	0.48	0
6	BMA	dA	3	6	11,11,12	0.64	0	15,15,17	0.86	0
6	NAG	eA	1	4,6	14,14,15	0.23	0	17,19,21	0.41	0
6	NAG	eA	2	6	14,14,15	0.19	0	17,19,21	0.43	0
6	BMA	eA	3	6	11,11,12	0.52	0	15,15,17	0.76	0
6	NAG	fA	1	3,6	14,14,15	0.18	0	17,19,21	0.66	1 (5%)
6	NAG	fA	2	6	14,14,15	0.30	0	17,19,21	0.46	0
6	BMA	fA	3	6	11,11,12	0.67	0	15,15,17	0.93	0
6	NAG	gA	1	3,6	14,14,15	0.19	0	17,19,21	0.65	1 (5%)
6	NAG	gA	2	6	14,14,15	0.21	0	17,19,21	0.45	0
6	BMA	gA	3	6	11,11,12	0.55	0	15,15,17	0.82	0
6	NAG	hA	1	4,6	14,14,15	0.38	0	17,19,21	0.57	0
6	NAG	hA	2	6	14,14,15	0.36	0	17,19,21	1.27	2 (11%)
6	BMA	hA	3	6	11,11,12	0.72	0	15,15,17	0.99	0
6	NAG	iA	1	4,6	14,14,15	0.52	0	17,19,21	0.38	0
6	NAG	iA	2	6	14,14,15	0.20	0	17,19,21	0.48	0
6	BMA	iA	3	6	11,11,12	0.70	0	15,15,17	0.74	0
6	NAG	jA	1	3,6	14,14,15	0.20	0	17,19,21	0.63	0
6	NAG	jA	2	6	14,14,15	0.21	0	17,19,21	0.45	0
6	BMA	jA	3	6	11,11,12	0.58	0	15,15,17	0.76	0
6	NAG	k	1	3,6	14,14,15	0.35	0	17,19,21	0.65	0
6	NAG	k	2	6	14,14,15	0.62	1 (7%)	17,19,21	1.26	1 (5%)
6	BMA	k	3	6	11,11,12	0.92	1 (9%)	15,15,17	0.98	0
6	NAG	kA	1	3,6	14,14,15	0.16	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	kA	2	6	14,14,15	0.18	0	17,19,21	0.45	0
6	BMA	kA	3	6	11,11,12	0.58	0	15,15,17	0.86	0
6	NAG	lA	1	3,6	14,14,15	1.05	1 (7%)	17,19,21	1.02	1 (5%)
6	NAG	lA	2	6	14,14,15	1.06	1 (7%)	17,19,21	1.60	2 (11%)
6	BMA	lA	3	6	11,11,12	0.62	0	15,15,17	0.91	0
6	NAG	mA	1	3,6	14,14,15	0.30	0	17,19,21	0.73	0
6	NAG	mA	2	6	14,14,15	0.23	0	17,19,21	0.40	0
6	BMA	mA	3	6	11,11,12	0.61	0	15,15,17	0.70	0
6	NAG	nA	1	4,6	14,14,15	0.39	0	17,19,21	1.28	1 (5%)
6	NAG	nA	2	6	14,14,15	0.26	0	17,19,21	0.44	0
6	BMA	nA	3	6	11,11,12	0.53	0	15,15,17	0.76	1 (6%)
6	NAG	oA	1	4,6	14,14,15	0.26	0	17,19,21	0.41	0
6	NAG	oA	2	6	14,14,15	0.18	0	17,19,21	0.49	0
6	BMA	oA	3	6	11,11,12	0.70	1 (9%)	15,15,17	0.85	0
6	NAG	pA	1	4,6	14,14,15	0.93	1 (7%)	17,19,21	0.91	0
6	NAG	pA	2	6	14,14,15	0.29	0	17,19,21	0.72	0
6	BMA	pA	3	6	11,11,12	0.65	0	15,15,17	1.32	3 (20%)
6	NAG	qA	1	4,6	14,14,15	0.25	0	17,19,21	0.49	0
6	NAG	qA	2	6	14,14,15	0.19	0	17,19,21	0.44	0
6	BMA	qA	3	6	11,11,12	0.78	1 (9%)	15,15,17	0.81	0
6	NAG	rA	1	4,6	14,14,15	0.20	0	17,19,21	0.56	0
6	NAG	rA	2	6	14,14,15	0.22	0	17,19,21	0.46	0
6	BMA	rA	3	6	11,11,12	0.63	0	15,15,17	0.80	1 (6%)
6	NAG	sA	1	4,6	14,14,15	0.18	0	17,19,21	0.43	0
6	NAG	sA	2	6	14,14,15	0.16	0	17,19,21	0.48	0
6	BMA	sA	3	6	11,11,12	0.62	0	15,15,17	0.92	0
6	NAG	tA	1	4,6	14,14,15	0.32	0	17,19,21	0.98	1 (5%)
6	NAG	tA	2	6	14,14,15	0.49	0	17,19,21	1.26	2 (11%)
6	BMA	tA	3	6	11,11,12	0.70	0	15,15,17	1.05	0
6	NAG	uA	1	4,6	14,14,15	0.22	0	17,19,21	0.46	0
6	NAG	uA	2	6	14,14,15	0.23	0	17,19,21	0.48	0
6	BMA	uA	3	6	11,11,12	0.63	0	15,15,17	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	BA	1	3,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	BA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	BA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	C	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	2/6/23/26	0/1/1/1
6	BMA	C	3	6	-	1/2/19/22	0/1/1/1
6	NAG	CA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	CA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	CA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	DA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	DA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	DA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	EA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	EA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	EA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	FA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	FA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	FA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	GA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	GA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	GA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	HA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	HA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	HA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	IA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	IA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	IA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	JA	1	4,6	-	1/6/23/26	0/1/1/1
6	NAG	JA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	JA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	KA	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	KA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	KA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	LA	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	LA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	LA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	MA	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	MA	2	6	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	MA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	NA	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	NA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	NA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	OA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	OA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	OA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	PA	1	4,6	-	5/6/23/26	0/1/1/1
6	NAG	PA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	PA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	QA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	QA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	QA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	RA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	RA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	RA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	SA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	SA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	SA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	TA	1	4,6	-	4/6/23/26	0/1/1/1
6	NAG	TA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	TA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	UA	1	4,6	-	4/6/23/26	0/1/1/1
6	NAG	UA	2	6	-	5/6/23/26	0/1/1/1
6	BMA	UA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	VA	1	4,6	-	1/6/23/26	0/1/1/1
6	NAG	VA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	VA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	WA	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	WA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	WA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	XA	1	3,6	-	1/6/23/26	0/1/1/1
6	NAG	XA	2	6	-	5/6/23/26	0/1/1/1
6	BMA	XA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	YA	1	3,6	-	1/6/23/26	0/1/1/1
6	NAG	YA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	YA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	ZA	1	4,6	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	ZA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	ZA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	aA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	aA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	aA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	bA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	bA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	bA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	cA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	cA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	cA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	dA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	dA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	dA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	eA	1	4,6	-	4/6/23/26	0/1/1/1
6	NAG	eA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	eA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	fA	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	fA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	fA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	gA	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	gA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	gA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	hA	1	4,6	-	4/6/23/26	0/1/1/1
6	NAG	hA	2	6	-	5/6/23/26	0/1/1/1
6	BMA	hA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	iA	1	4,6	-	1/6/23/26	0/1/1/1
6	NAG	iA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	iA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	jA	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	jA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	jA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	k	1	3,6	-	1/6/23/26	0/1/1/1
6	NAG	k	2	6	-	4/6/23/26	0/1/1/1
6	BMA	k	3	6	-	1/2/19/22	0/1/1/1
6	NAG	kA	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	kA	2	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	kA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	lA	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	lA	2	6	-	5/6/23/26	0/1/1/1
6	BMA	lA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	mA	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	mA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	mA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	nA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	nA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	nA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	oA	1	4,6	-	1/6/23/26	0/1/1/1
6	NAG	oA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	oA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	pA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	pA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	pA	3	6	-	1/2/19/22	0/1/1/1
6	NAG	qA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	qA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	qA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	rA	1	4,6	-	3/6/23/26	0/1/1/1
6	NAG	rA	2	6	-	1/6/23/26	0/1/1/1
6	BMA	rA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	sA	1	4,6	-	4/6/23/26	0/1/1/1
6	NAG	sA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	sA	3	6	-	0/2/19/22	0/1/1/1
6	NAG	tA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	tA	2	6	-	4/6/23/26	0/1/1/1
6	BMA	tA	3	6	-	2/2/19/22	0/1/1/1
6	NAG	uA	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	uA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	uA	3	6	-	0/2/19/22	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	lA	1	NAG	O5-C1	-3.36	1.38	1.43
6	pA	1	NAG	O5-C1	-3.32	1.38	1.43
6	lA	2	NAG	C1-C2	3.14	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	IA	3	BMA	C1-C2	2.45	1.57	1.52
6	bA	1	NAG	O5-C1	-2.42	1.39	1.43
6	k	3	BMA	C1-C2	2.36	1.57	1.52
6	SA	3	BMA	C1-C2	2.35	1.57	1.52
6	MA	2	NAG	C1-C2	2.25	1.55	1.52
6	EA	1	NAG	O5-C1	-2.15	1.40	1.43
6	k	2	NAG	C1-C2	2.12	1.55	1.52
6	RA	1	NAG	O5-C1	-2.09	1.40	1.43
6	qA	3	BMA	C1-C2	2.07	1.56	1.52
6	oA	3	BMA	C1-C2	2.07	1.56	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	k	2	NAG	C2-N2-C7	4.30	129.02	122.90
6	IA	2	NAG	C2-N2-C7	4.27	128.99	122.90
6	UA	2	NAG	C2-N2-C7	4.25	128.96	122.90
6	nA	1	NAG	C2-N2-C7	4.22	128.92	122.90
6	PA	1	NAG	C2-N2-C7	4.22	128.91	122.90
6	CA	1	NAG	C2-N2-C7	4.21	128.90	122.90
6	tA	2	NAG	C2-N2-C7	4.20	128.89	122.90
6	hA	2	NAG	C2-N2-C7	4.20	128.88	122.90
6	ZA	1	NAG	C2-N2-C7	4.19	128.87	122.90
6	lA	2	NAG	C1-O5-C5	4.19	117.86	112.19
6	XA	2	NAG	C2-N2-C7	4.18	128.86	122.90
6	MA	2	NAG	C2-N2-C7	4.18	128.85	122.90
6	lA	2	NAG	C2-N2-C7	3.88	128.43	122.90
6	tA	1	NAG	C1-O5-C5	3.31	116.68	112.19
6	IA	1	NAG	C1-O5-C5	3.02	116.29	112.19
6	bA	3	BMA	C1-O5-C5	2.85	116.05	112.19
6	lA	1	NAG	C3-C4-C5	2.63	114.94	110.24
6	pA	3	BMA	C1-O5-C5	2.60	115.71	112.19
6	IA	2	NAG	C1-C2-N2	2.34	114.48	110.49
6	CA	3	BMA	O2-C2-C3	-2.30	105.54	110.14
6	KA	3	BMA	C1-O5-C5	2.24	115.23	112.19
6	gA	1	NAG	C1-O5-C5	2.24	115.22	112.19
6	rA	3	BMA	O2-C2-C3	-2.23	105.66	110.14
6	EA	3	BMA	O2-C2-C3	-2.20	105.72	110.14
6	tA	2	NAG	C1-C2-N2	2.18	114.21	110.49
6	WA	1	NAG	C1-O5-C5	2.16	115.11	112.19
6	hA	2	NAG	C1-C2-N2	2.15	114.17	110.49
6	PA	3	BMA	O2-C2-C3	-2.15	105.83	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	fA	1	NAG	C1-O5-C5	2.14	115.09	112.19
6	SA	3	BMA	C1-C2-C3	2.13	112.29	109.67
6	LA	1	NAG	C1-O5-C5	2.13	115.08	112.19
6	kA	1	NAG	C1-O5-C5	2.12	115.06	112.19
6	PA	1	NAG	C1-C2-N2	2.09	114.05	110.49
6	nA	3	BMA	O2-C2-C3	-2.06	106.02	110.14
6	C	1	NAG	C1-O5-C5	2.06	114.98	112.19
6	bA	3	BMA	O2-C2-C3	-2.05	106.03	110.14
6	UA	2	NAG	C1-C2-N2	2.04	113.98	110.49
6	pA	3	BMA	O2-C2-C3	-2.02	106.10	110.14
6	pA	3	BMA	O5-C1-C2	2.00	113.86	110.77

There are no chirality outliers.

All (267) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	mA	2	NAG	O5-C5-C6-O6
6	oA	2	NAG	O5-C5-C6-O6
6	NA	2	NAG	O5-C5-C6-O6
6	VA	2	NAG	O5-C5-C6-O6
6	aA	2	NAG	O5-C5-C6-O6
6	fA	2	NAG	O5-C5-C6-O6
6	DA	1	NAG	O5-C5-C6-O6
6	DA	2	NAG	O5-C5-C6-O6
6	TA	1	NAG	O5-C5-C6-O6
6	cA	1	NAG	O5-C5-C6-O6
6	gA	2	NAG	O5-C5-C6-O6
6	NA	1	NAG	O5-C5-C6-O6
6	OA	1	NAG	O5-C5-C6-O6
6	eA	2	NAG	O5-C5-C6-O6
6	kA	3	BMA	O5-C5-C6-O6
6	NA	2	NAG	C4-C5-C6-O6
6	VA	2	NAG	C4-C5-C6-O6
6	gA	2	NAG	C4-C5-C6-O6
6	tA	3	BMA	C4-C5-C6-O6
6	KA	2	NAG	O5-C5-C6-O6
6	KA	3	BMA	O5-C5-C6-O6
6	lA	3	BMA	O5-C5-C6-O6
6	fA	2	NAG	C4-C5-C6-O6
6	FA	2	NAG	O5-C5-C6-O6
6	MA	3	BMA	O5-C5-C6-O6
6	nA	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	aA	2	NAG	C4-C5-C6-O6
6	nA	2	NAG	C4-C5-C6-O6
6	oA	2	NAG	C4-C5-C6-O6
6	eA	1	NAG	O5-C5-C6-O6
6	hA	2	NAG	O5-C5-C6-O6
6	jA	2	NAG	O5-C5-C6-O6
6	lA	1	NAG	O5-C5-C6-O6
6	cA	1	NAG	C4-C5-C6-O6
6	mA	2	NAG	C4-C5-C6-O6
6	UA	2	NAG	O5-C5-C6-O6
6	ZA	2	NAG	O5-C5-C6-O6
6	PA	2	NAG	O5-C5-C6-O6
6	sA	1	NAG	O5-C5-C6-O6
6	tA	3	BMA	O5-C5-C6-O6
6	LA	1	NAG	O5-C5-C6-O6
6	WA	3	BMA	O5-C5-C6-O6
6	DA	1	NAG	C4-C5-C6-O6
6	KA	2	NAG	C4-C5-C6-O6
6	OA	1	NAG	C4-C5-C6-O6
6	qA	2	NAG	C4-C5-C6-O6
6	NA	1	NAG	C4-C5-C6-O6
6	uA	1	NAG	O5-C5-C6-O6
6	jA	3	BMA	O5-C5-C6-O6
6	PA	2	NAG	C4-C5-C6-O6
6	lA	1	NAG	C4-C5-C6-O6
6	sA	1	NAG	C4-C5-C6-O6
6	k	2	NAG	C8-C7-N2-C2
6	k	2	NAG	O7-C7-N2-C2
6	BA	2	NAG	C8-C7-N2-C2
6	BA	2	NAG	O7-C7-N2-C2
6	CA	1	NAG	C8-C7-N2-C2
6	CA	1	NAG	O7-C7-N2-C2
6	DA	2	NAG	C8-C7-N2-C2
6	DA	2	NAG	O7-C7-N2-C2
6	GA	1	NAG	C8-C7-N2-C2
6	GA	1	NAG	O7-C7-N2-C2
6	HA	1	NAG	C8-C7-N2-C2
6	HA	1	NAG	O7-C7-N2-C2
6	HA	2	NAG	C8-C7-N2-C2
6	HA	2	NAG	O7-C7-N2-C2
6	IA	1	NAG	C8-C7-N2-C2
6	IA	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	IA	2	NAG	C8-C7-N2-C2
6	IA	2	NAG	O7-C7-N2-C2
6	MA	2	NAG	C8-C7-N2-C2
6	MA	2	NAG	O7-C7-N2-C2
6	NA	2	NAG	C8-C7-N2-C2
6	NA	2	NAG	O7-C7-N2-C2
6	OA	2	NAG	C8-C7-N2-C2
6	OA	2	NAG	O7-C7-N2-C2
6	PA	1	NAG	C8-C7-N2-C2
6	PA	1	NAG	O7-C7-N2-C2
6	SA	1	NAG	C8-C7-N2-C2
6	SA	1	NAG	O7-C7-N2-C2
6	TA	1	NAG	C8-C7-N2-C2
6	TA	1	NAG	O7-C7-N2-C2
6	TA	2	NAG	C8-C7-N2-C2
6	TA	2	NAG	O7-C7-N2-C2
6	UA	1	NAG	C8-C7-N2-C2
6	UA	1	NAG	O7-C7-N2-C2
6	UA	2	NAG	C8-C7-N2-C2
6	UA	2	NAG	O7-C7-N2-C2
6	XA	2	NAG	C8-C7-N2-C2
6	XA	2	NAG	O7-C7-N2-C2
6	YA	2	NAG	C8-C7-N2-C2
6	YA	2	NAG	O7-C7-N2-C2
6	ZA	1	NAG	C8-C7-N2-C2
6	ZA	1	NAG	O7-C7-N2-C2
6	aA	2	NAG	C8-C7-N2-C2
6	aA	2	NAG	O7-C7-N2-C2
6	dA	1	NAG	C8-C7-N2-C2
6	dA	1	NAG	O7-C7-N2-C2
6	eA	1	NAG	C8-C7-N2-C2
6	eA	1	NAG	O7-C7-N2-C2
6	eA	2	NAG	C8-C7-N2-C2
6	eA	2	NAG	O7-C7-N2-C2
6	hA	1	NAG	C8-C7-N2-C2
6	hA	1	NAG	O7-C7-N2-C2
6	hA	2	NAG	C8-C7-N2-C2
6	hA	2	NAG	O7-C7-N2-C2
6	lA	2	NAG	C8-C7-N2-C2
6	lA	2	NAG	O7-C7-N2-C2
6	mA	2	NAG	C8-C7-N2-C2
6	mA	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	nA	1	NAG	C8-C7-N2-C2
6	nA	1	NAG	O7-C7-N2-C2
6	oA	2	NAG	C8-C7-N2-C2
6	oA	2	NAG	O7-C7-N2-C2
6	rA	1	NAG	C8-C7-N2-C2
6	rA	1	NAG	O7-C7-N2-C2
6	sA	1	NAG	C8-C7-N2-C2
6	sA	1	NAG	O7-C7-N2-C2
6	sA	2	NAG	C8-C7-N2-C2
6	sA	2	NAG	O7-C7-N2-C2
6	tA	1	NAG	C8-C7-N2-C2
6	tA	1	NAG	O7-C7-N2-C2
6	tA	2	NAG	C8-C7-N2-C2
6	tA	2	NAG	O7-C7-N2-C2
6	LA	1	NAG	C4-C5-C6-O6
6	UA	2	NAG	C4-C5-C6-O6
6	eA	1	NAG	C4-C5-C6-O6
6	DA	2	NAG	C4-C5-C6-O6
6	jA	2	NAG	C4-C5-C6-O6
6	C	1	NAG	O5-C5-C6-O6
6	UA	1	NAG	O5-C5-C6-O6
6	ZA	2	NAG	C4-C5-C6-O6
6	hA	2	NAG	C4-C5-C6-O6
6	UA	3	BMA	O5-C5-C6-O6
6	kA	3	BMA	C4-C5-C6-O6
6	BA	3	BMA	O5-C5-C6-O6
6	TA	1	NAG	C4-C5-C6-O6
6	oA	3	BMA	O5-C5-C6-O6
6	qA	2	NAG	O5-C5-C6-O6
6	C	1	NAG	C4-C5-C6-O6
6	UA	1	NAG	C4-C5-C6-O6
6	PA	1	NAG	O5-C5-C6-O6
6	QA	1	NAG	C4-C5-C6-O6
6	QA	1	NAG	O5-C5-C6-O6
6	PA	1	NAG	C4-C5-C6-O6
6	eA	2	NAG	C4-C5-C6-O6
6	RA	1	NAG	O5-C5-C6-O6
6	fA	1	NAG	O5-C5-C6-O6
6	lA	3	BMA	C4-C5-C6-O6
6	hA	1	NAG	O5-C5-C6-O6
6	KA	1	NAG	O5-C5-C6-O6
6	fA	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	NA	3	BMA	O5-C5-C6-O6
6	jA	1	NAG	O5-C5-C6-O6
6	rA	2	NAG	O5-C5-C6-O6
6	mA	3	BMA	O5-C5-C6-O6
6	fA	1	NAG	C1-C2-N2-C7
6	iA	2	NAG	C4-C5-C6-O6
6	hA	1	NAG	C4-C5-C6-O6
6	jA	1	NAG	C4-C5-C6-O6
6	rA	3	BMA	O5-C5-C6-O6
6	KA	1	NAG	C4-C5-C6-O6
6	FA	2	NAG	C4-C5-C6-O6
6	oA	1	NAG	O5-C5-C6-O6
6	tA	2	NAG	O5-C5-C6-O6
6	gA	3	BMA	O5-C5-C6-O6
6	VA	1	NAG	O5-C5-C6-O6
6	rA	1	NAG	O5-C5-C6-O6
6	C	3	BMA	O5-C5-C6-O6
6	TA	2	NAG	O5-C5-C6-O6
6	HA	2	NAG	O5-C5-C6-O6
6	bA	1	NAG	O5-C5-C6-O6
6	fA	3	BMA	O5-C5-C6-O6
6	iA	1	NAG	O5-C5-C6-O6
6	rA	3	BMA	C4-C5-C6-O6
6	uA	2	NAG	C4-C5-C6-O6
6	IA	3	BMA	O5-C5-C6-O6
6	LA	3	BMA	O5-C5-C6-O6
6	SA	2	NAG	O5-C5-C6-O6
6	YA	3	BMA	O5-C5-C6-O6
6	aA	3	BMA	O5-C5-C6-O6
6	dA	1	NAG	O5-C5-C6-O6
6	XA	3	BMA	O5-C5-C6-O6
6	sA	2	NAG	O5-C5-C6-O6
6	GA	2	NAG	O5-C5-C6-O6
6	QA	2	NAG	O5-C5-C6-O6
6	YA	1	NAG	O5-C5-C6-O6
6	uA	2	NAG	O5-C5-C6-O6
6	EA	1	NAG	O5-C5-C6-O6
6	EA	3	BMA	O5-C5-C6-O6
6	RA	3	BMA	O5-C5-C6-O6
6	HA	3	BMA	O5-C5-C6-O6
6	IA	2	NAG	O5-C5-C6-O6
6	dA	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	DA	3	BMA	O5-C5-C6-O6
6	k	3	BMA	O5-C5-C6-O6
6	OA	3	BMA	O5-C5-C6-O6
6	SA	1	NAG	O5-C5-C6-O6
6	cA	2	NAG	O5-C5-C6-O6
6	pA	1	NAG	O5-C5-C6-O6
6	pA	3	BMA	O5-C5-C6-O6
6	JA	1	NAG	O5-C5-C6-O6
6	bA	3	BMA	O5-C5-C6-O6
6	hA	3	BMA	O5-C5-C6-O6
6	GA	1	NAG	O5-C5-C6-O6
6	HA	1	NAG	O5-C5-C6-O6
6	cA	3	BMA	O5-C5-C6-O6
6	uA	1	NAG	C4-C5-C6-O6
6	HA	3	BMA	C4-C5-C6-O6
6	aA	1	NAG	C1-C2-N2-C7
6	RA	2	NAG	C4-C5-C6-O6
6	lA	2	NAG	O5-C5-C6-O6
6	ZA	1	NAG	C4-C5-C6-O6
6	cA	3	BMA	C4-C5-C6-O6
6	FA	1	NAG	C4-C5-C6-O6
6	ZA	1	NAG	O5-C5-C6-O6
6	iA	2	NAG	O5-C5-C6-O6
6	C	2	NAG	C4-C5-C6-O6
6	jA	1	NAG	C1-C2-N2-C7
6	OA	2	NAG	O5-C5-C6-O6
6	KA	3	BMA	C4-C5-C6-O6
6	lA	2	NAG	C4-C5-C6-O6
6	C	2	NAG	O5-C5-C6-O6
6	CA	1	NAG	C3-C2-N2-C7
6	EA	1	NAG	C3-C2-N2-C7
6	FA	1	NAG	C3-C2-N2-C7
6	QA	1	NAG	C3-C2-N2-C7
6	RA	1	NAG	C3-C2-N2-C7
6	ZA	1	NAG	C3-C2-N2-C7
6	bA	1	NAG	C3-C2-N2-C7
6	cA	1	NAG	C3-C2-N2-C7
6	nA	1	NAG	C3-C2-N2-C7
6	pA	1	NAG	C3-C2-N2-C7
6	qA	1	NAG	C3-C2-N2-C7
6	MA	2	NAG	C4-C5-C6-O6
6	aA	1	NAG	O5-C5-C6-O6

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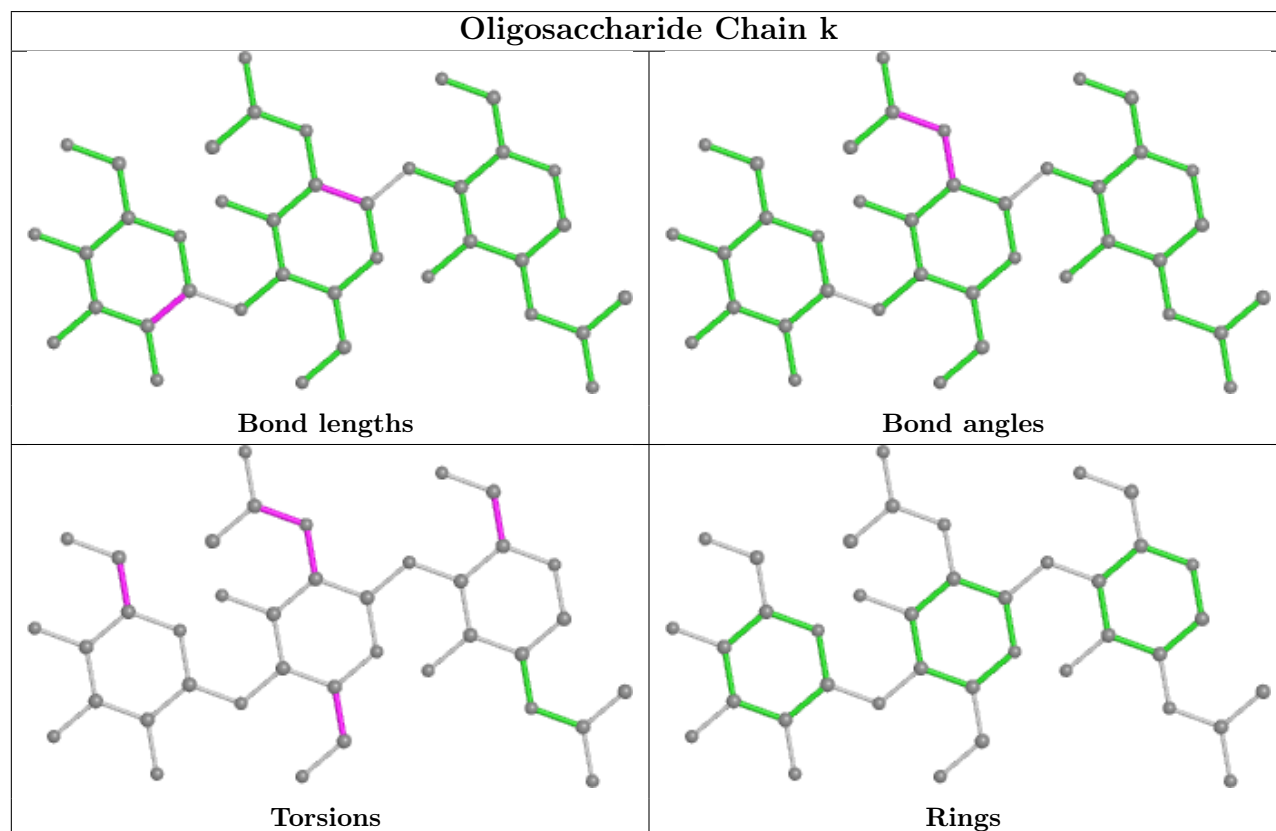
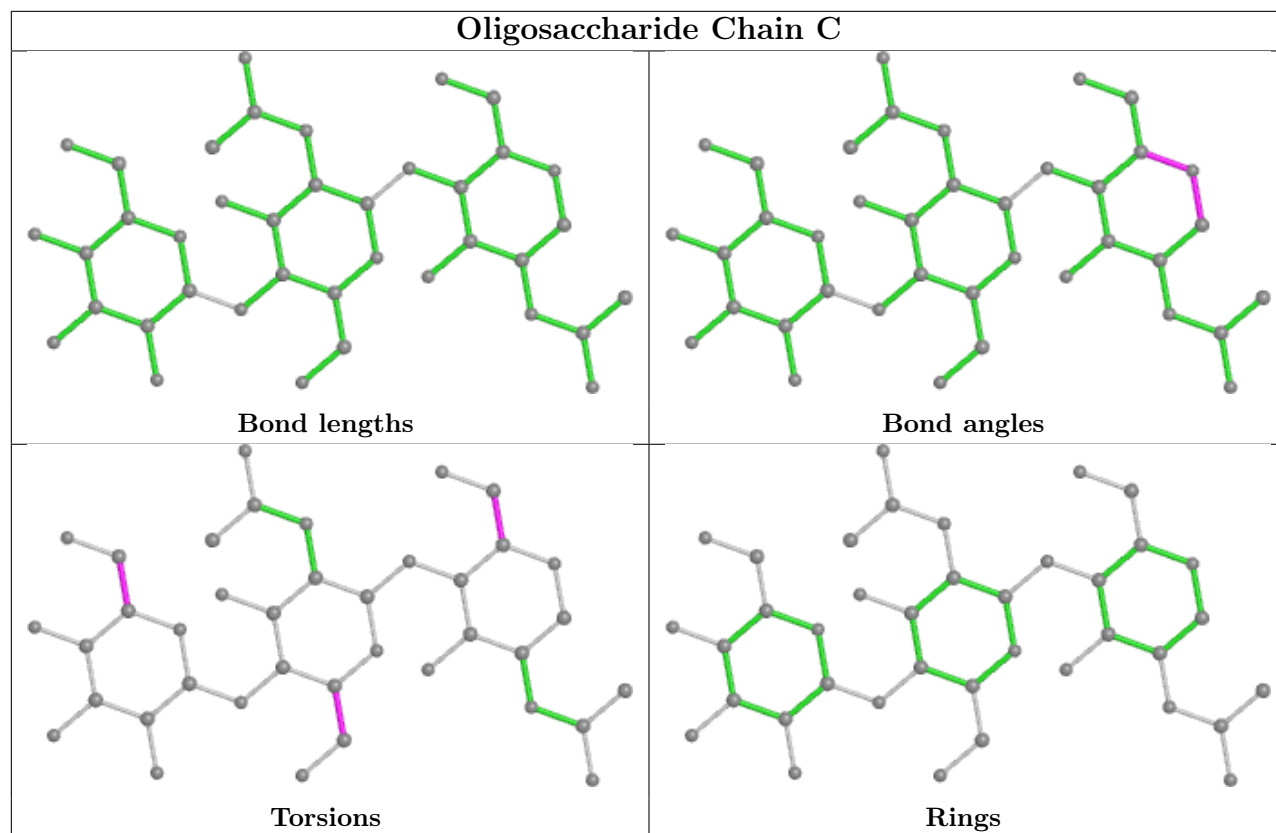
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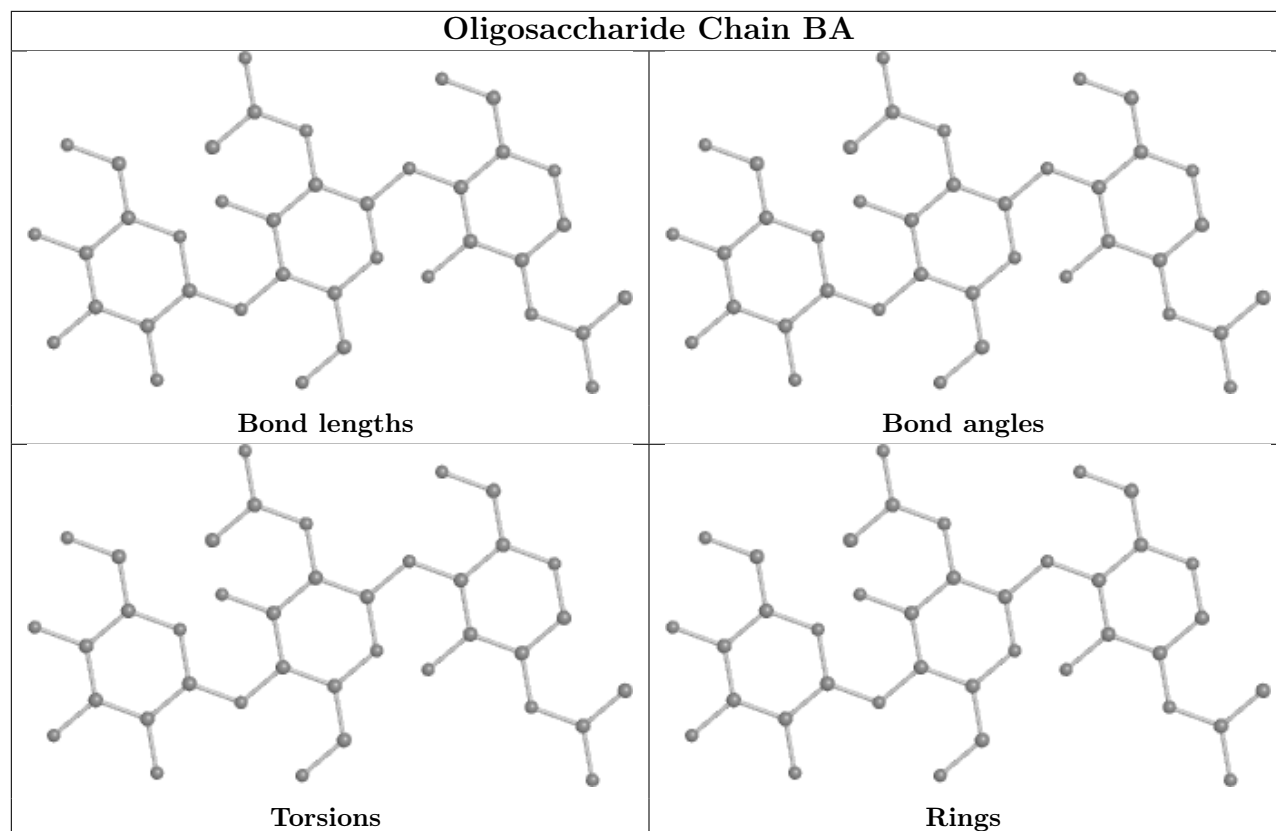
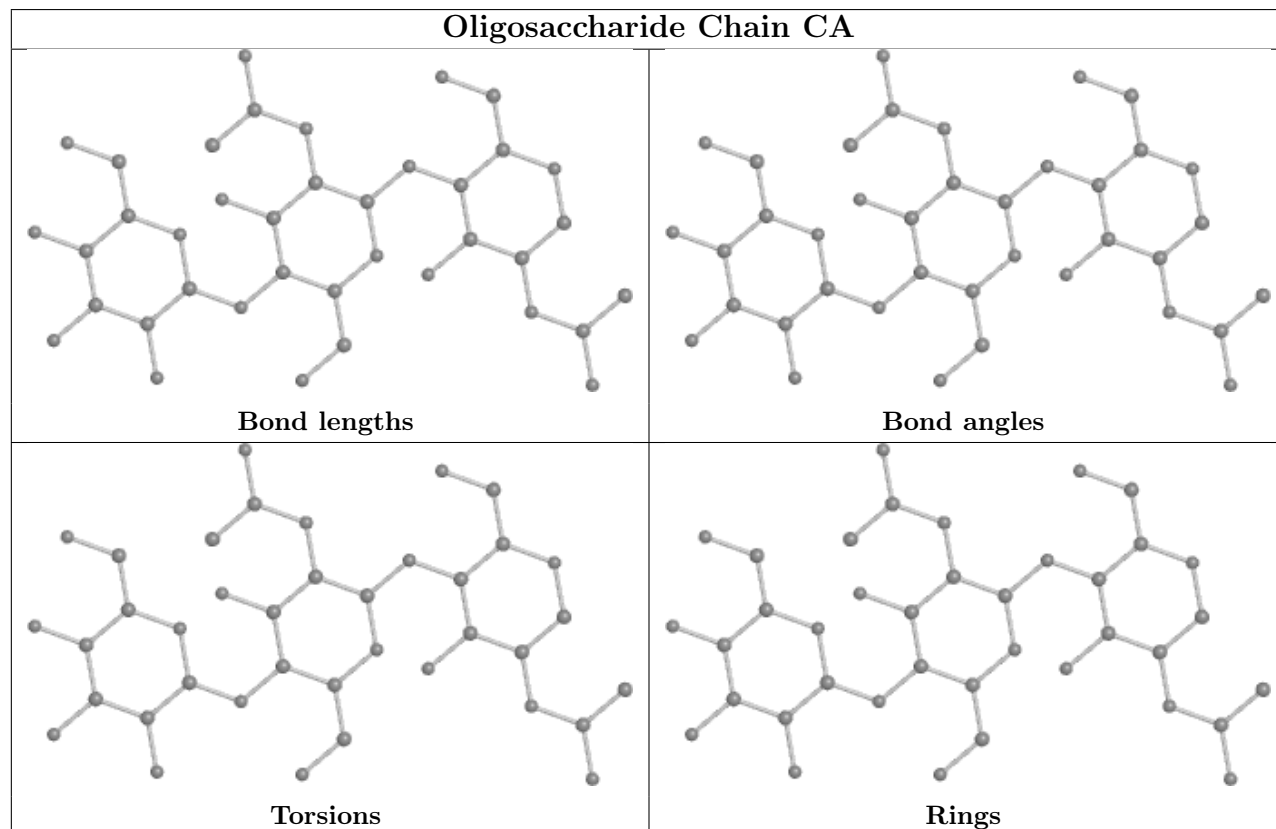
Mol	Chain	Res	Type	Atoms
6	gA	1	NAG	C4-C5-C6-O6
6	MA	2	NAG	O5-C5-C6-O6
6	VA	2	NAG	C1-C2-N2-C7
6	k	2	NAG	C4-C5-C6-O6
6	jA	3	BMA	C4-C5-C6-O6
6	XA	2	NAG	C4-C5-C6-O6
6	XA	2	NAG	O5-C5-C6-O6
6	gA	1	NAG	O5-C5-C6-O6
6	LA	2	NAG	C4-C5-C6-O6
6	MA	3	BMA	C4-C5-C6-O6
6	BA	2	NAG	C4-C5-C6-O6
6	XA	1	NAG	C4-C5-C6-O6
6	WA	3	BMA	C4-C5-C6-O6
6	k	2	NAG	C3-C2-N2-C7
6	IA	2	NAG	C3-C2-N2-C7
6	MA	2	NAG	C3-C2-N2-C7
6	PA	1	NAG	C3-C2-N2-C7
6	UA	2	NAG	C3-C2-N2-C7
6	XA	2	NAG	C3-C2-N2-C7
6	aA	1	NAG	C3-C2-N2-C7
6	fA	1	NAG	C3-C2-N2-C7
6	hA	2	NAG	C3-C2-N2-C7
6	jA	1	NAG	C3-C2-N2-C7
6	lA	2	NAG	C3-C2-N2-C7
6	tA	2	NAG	C3-C2-N2-C7
6	qA	1	NAG	O5-C5-C6-O6
6	k	1	NAG	C4-C5-C6-O6
6	CA	2	NAG	C4-C5-C6-O6
6	BA	2	NAG	O5-C5-C6-O6
6	QA	3	BMA	O5-C5-C6-O6
6	FA	1	NAG	O5-C5-C6-O6

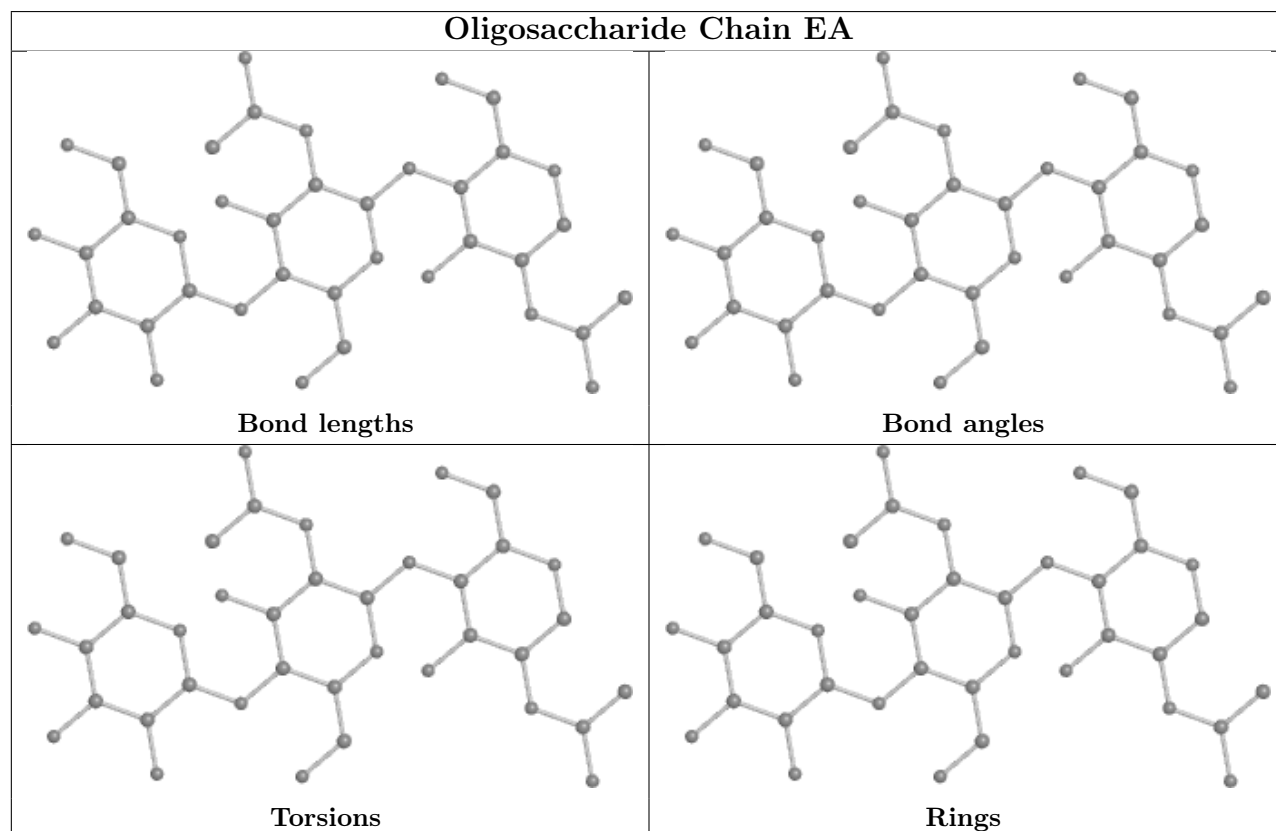
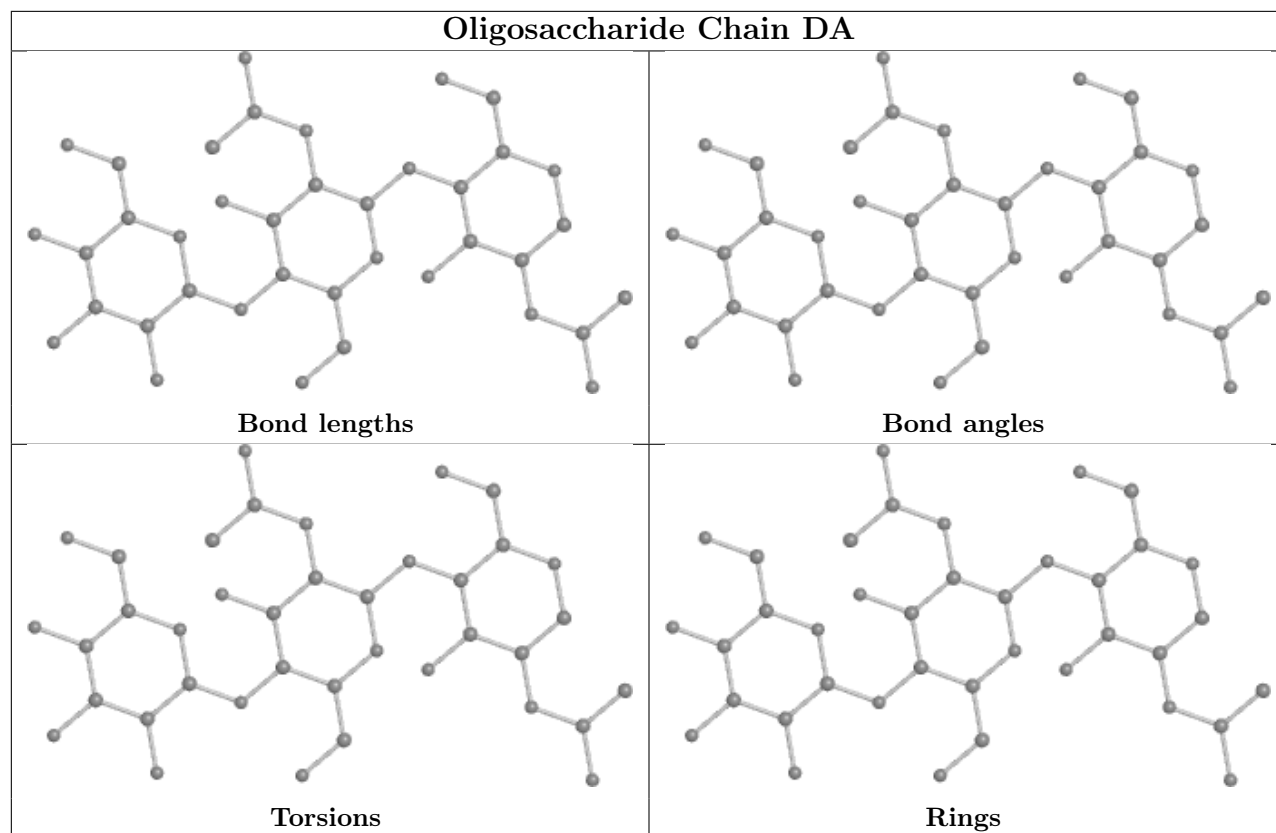
There are no ring outliers.

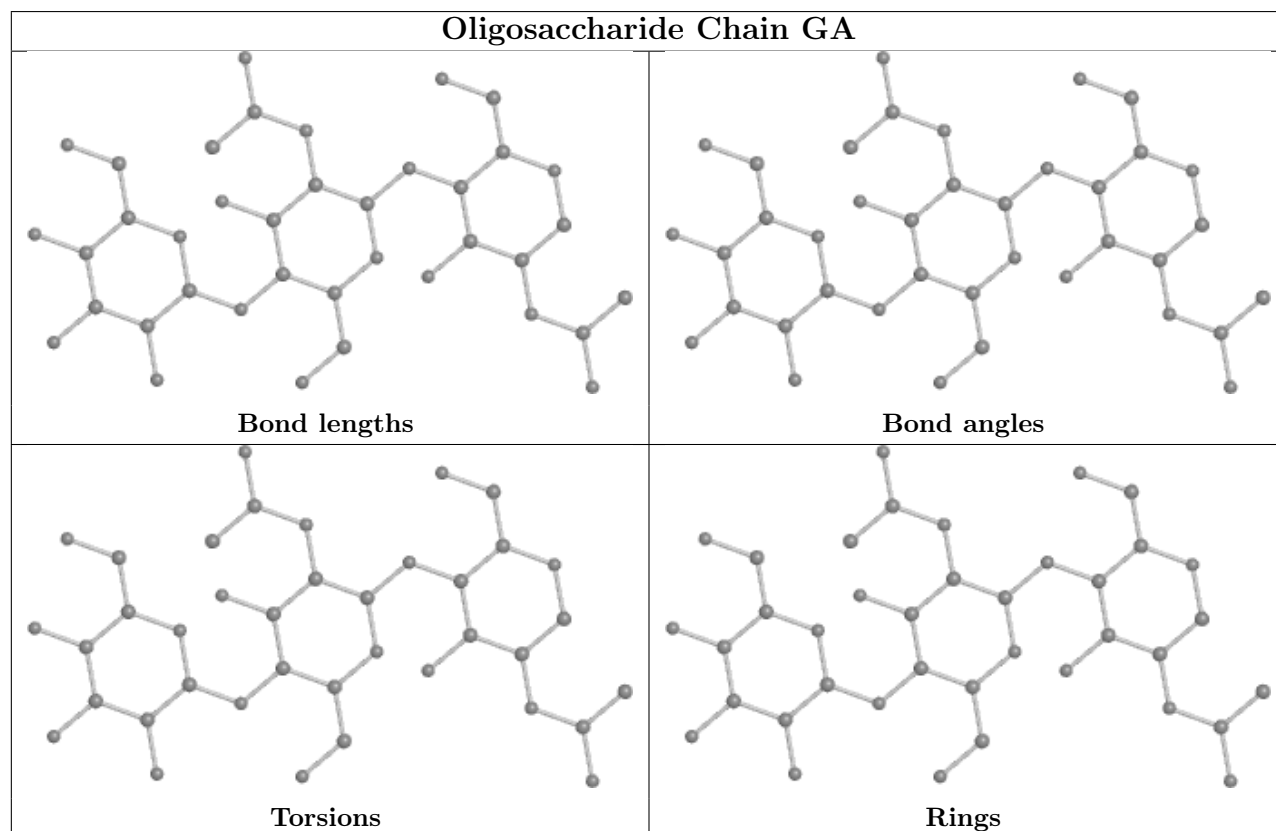
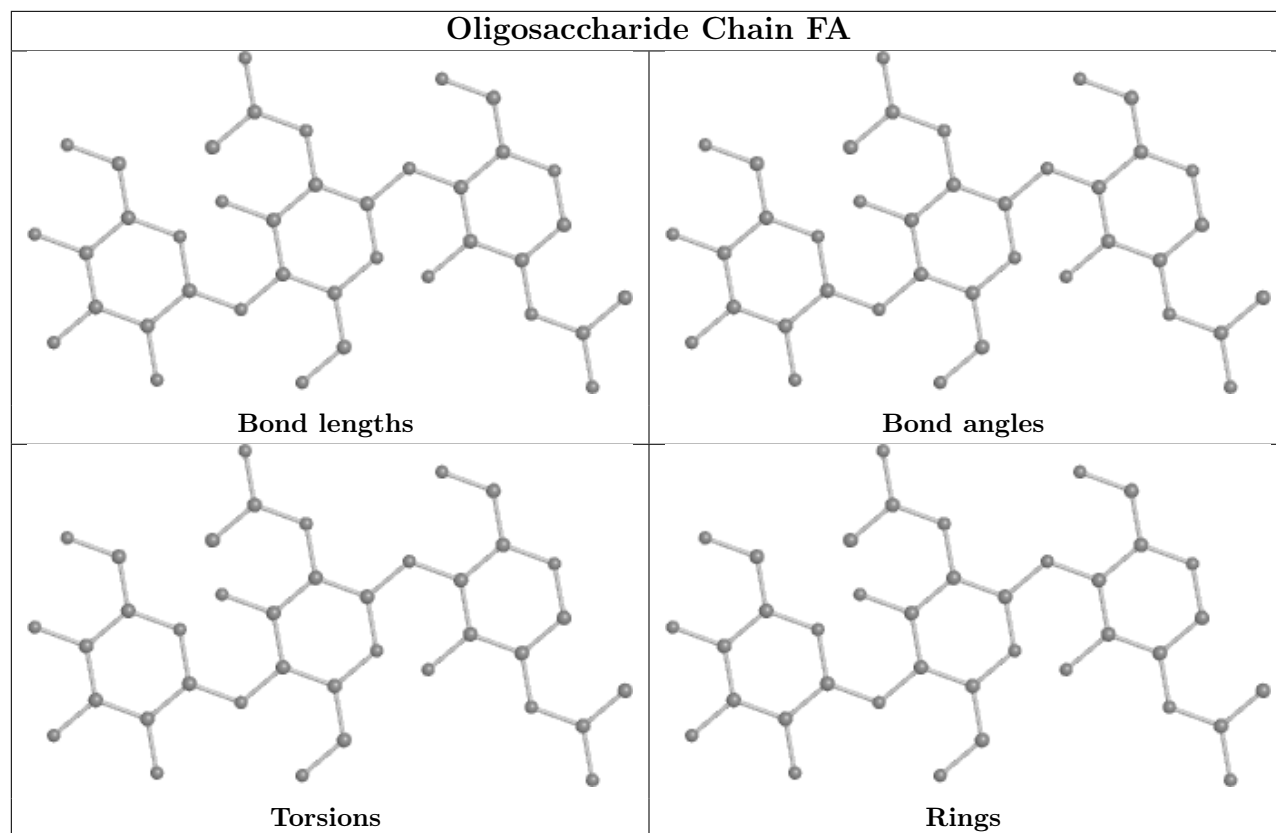
No monomer is involved in short contacts.

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

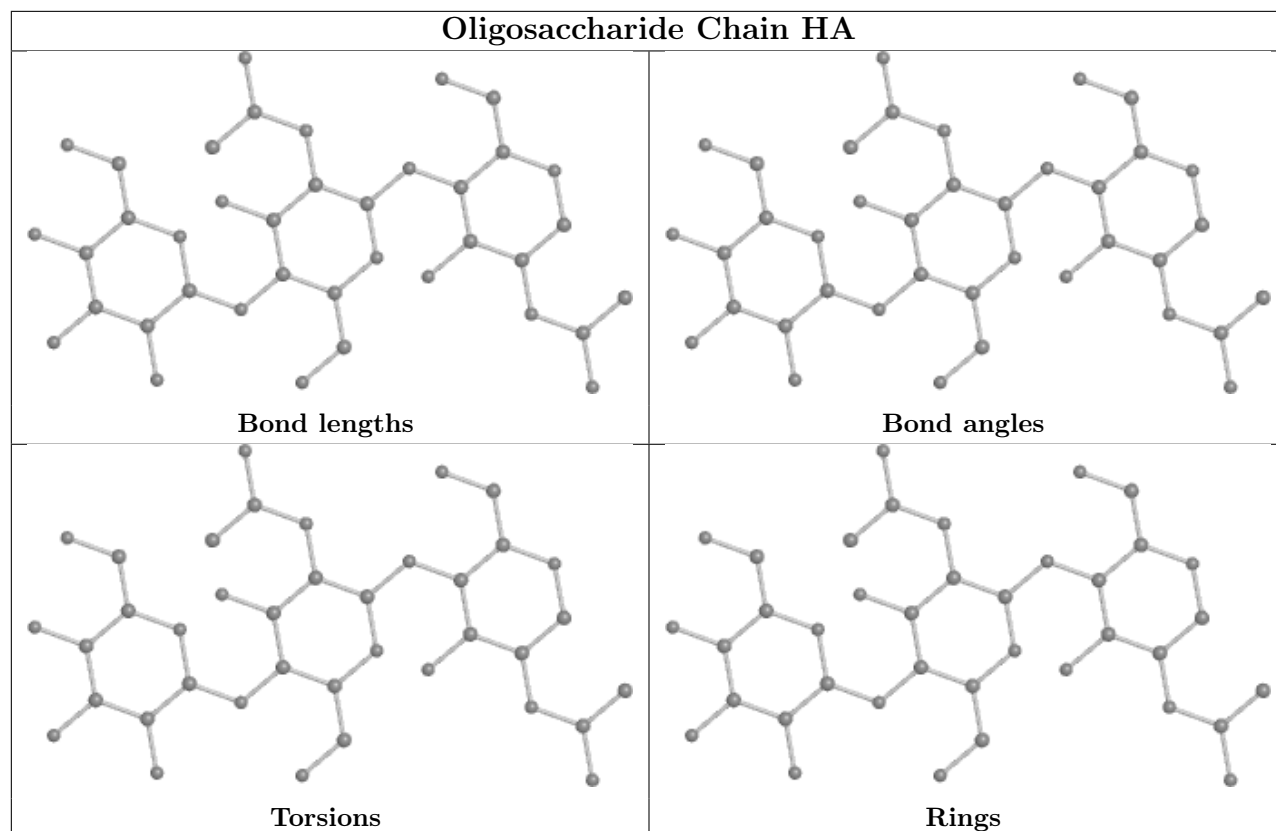
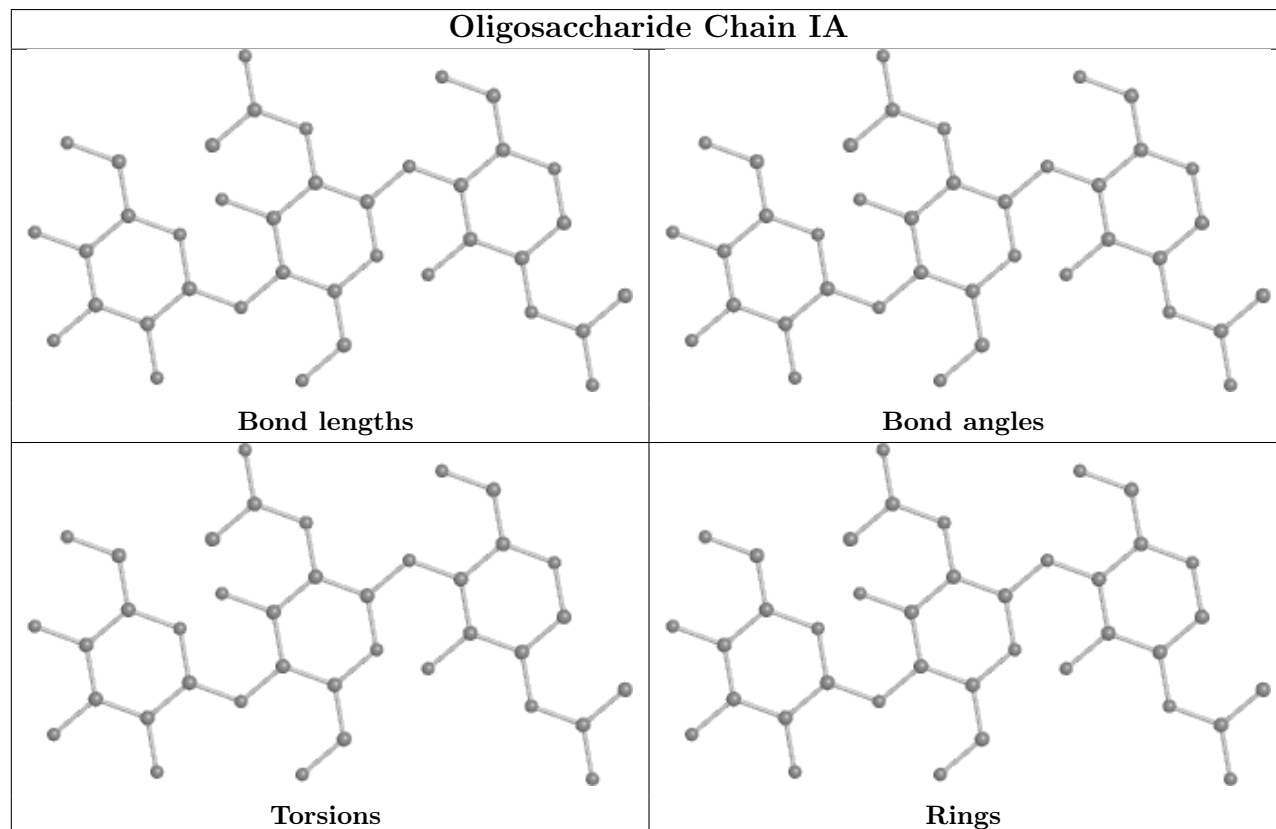


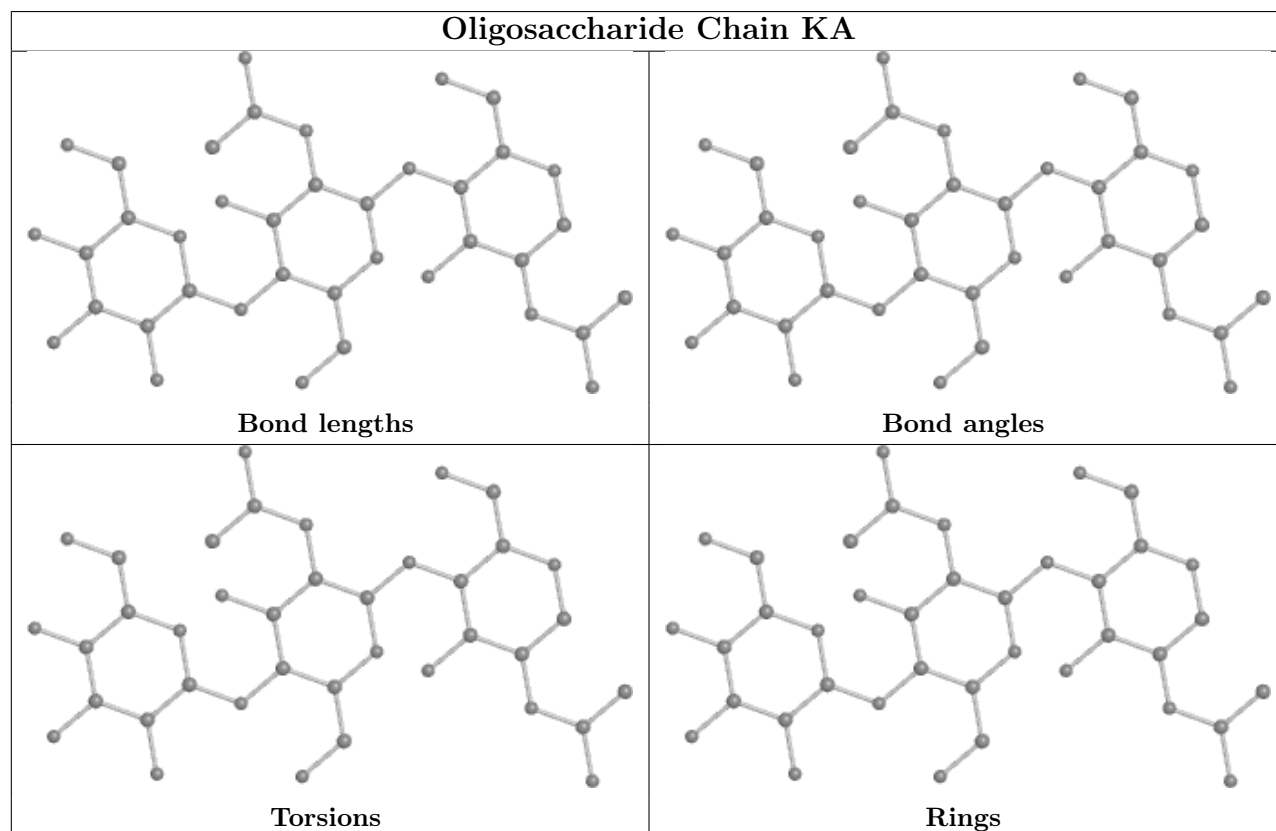
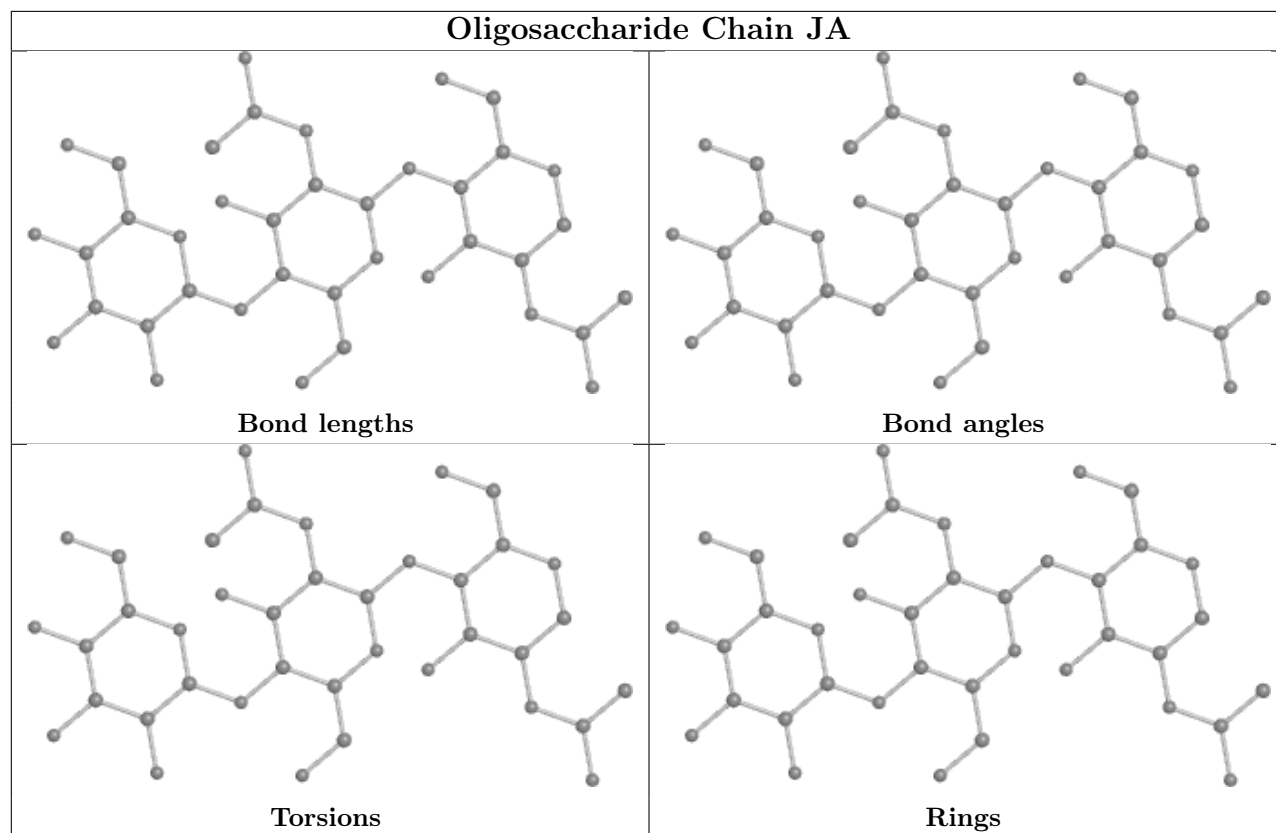
**Oligosaccharide Chain BA****Oligosaccharide Chain CA**

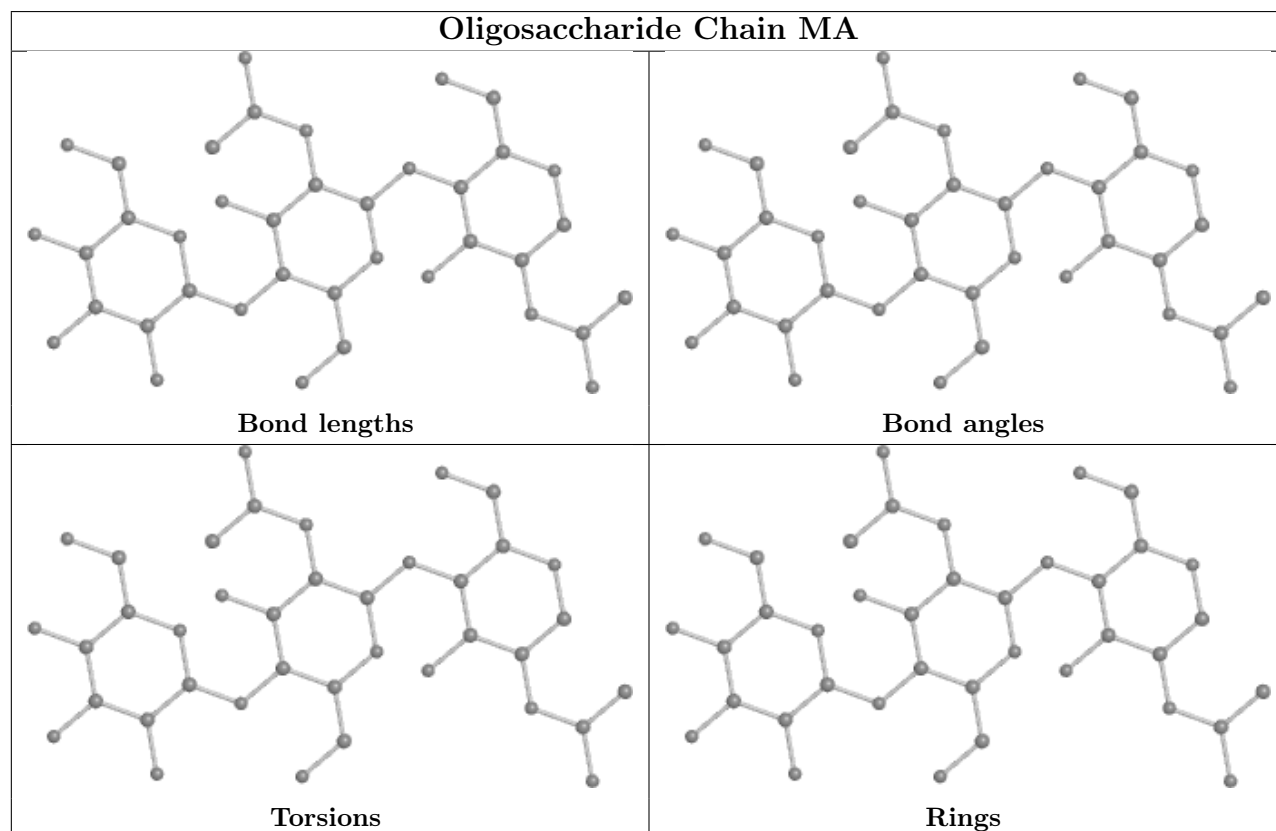
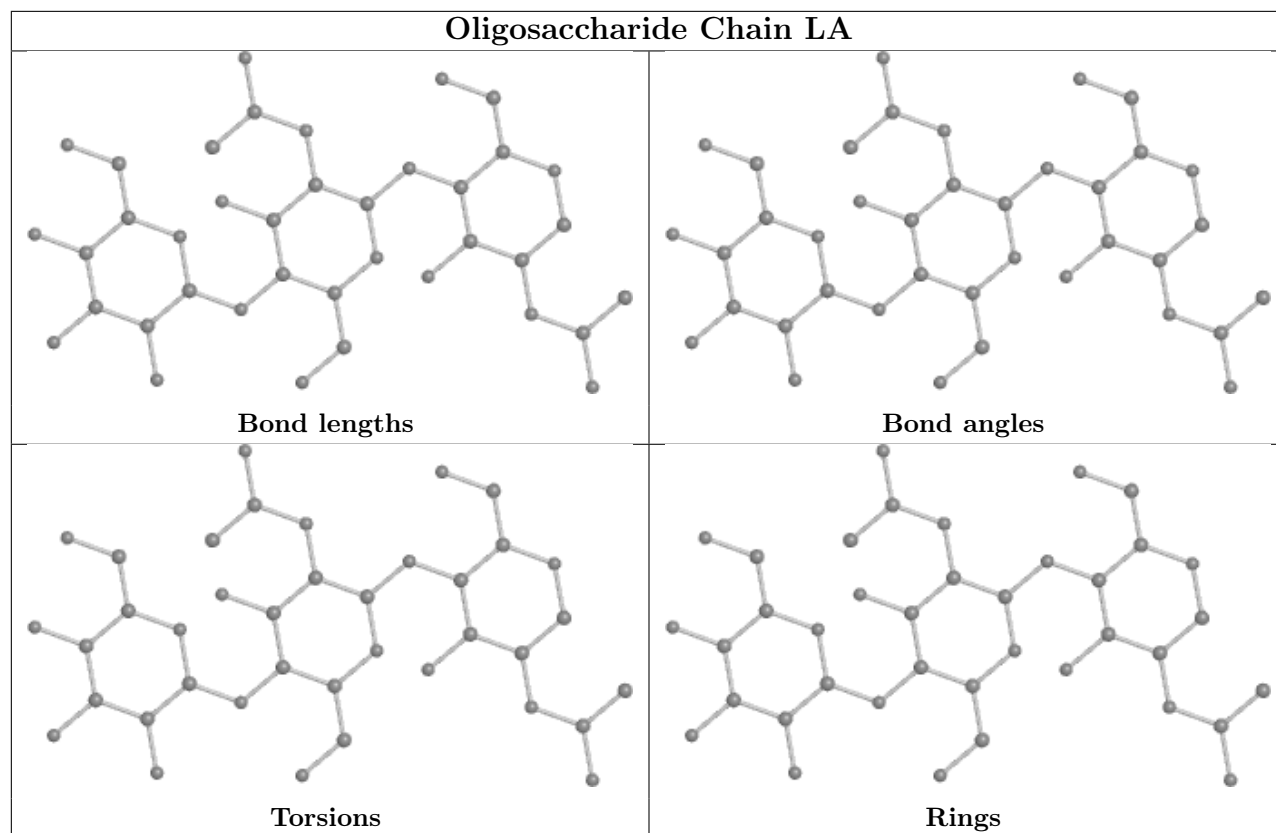


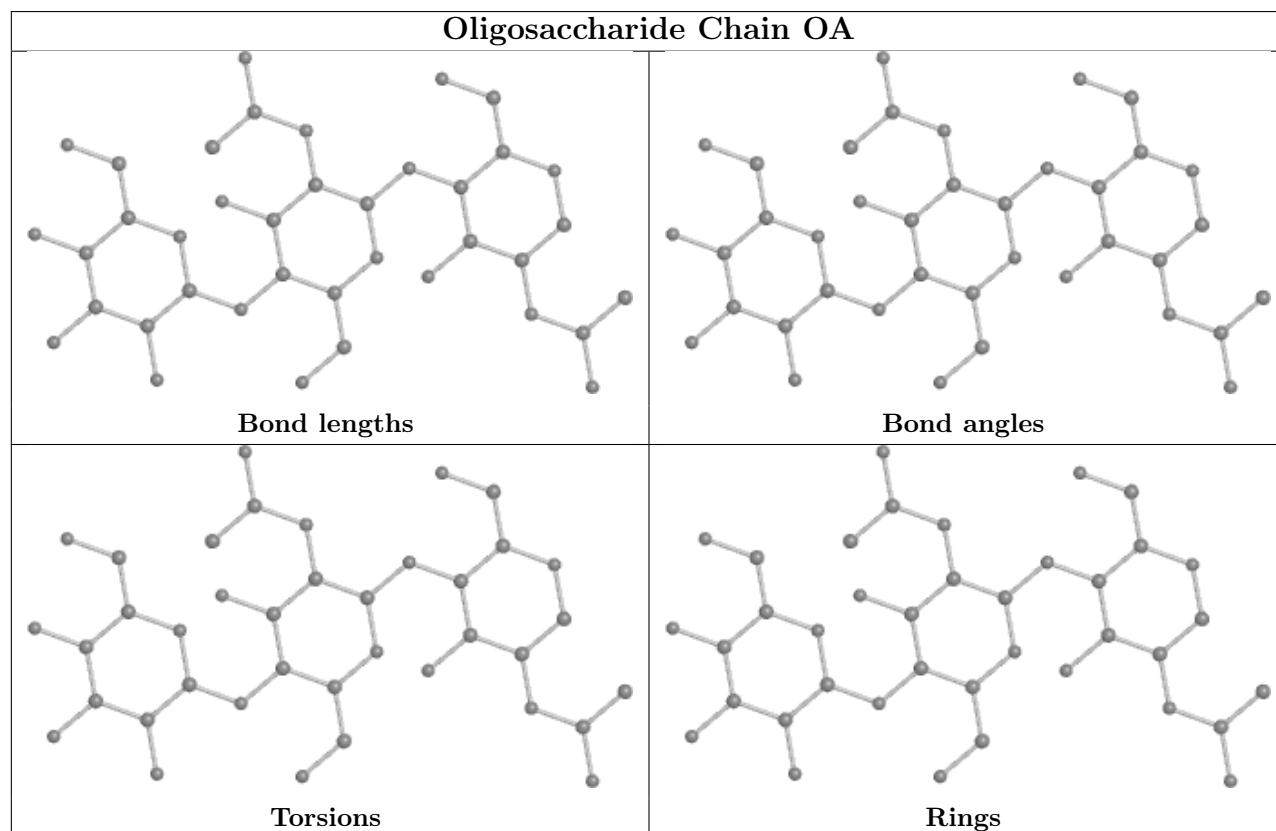
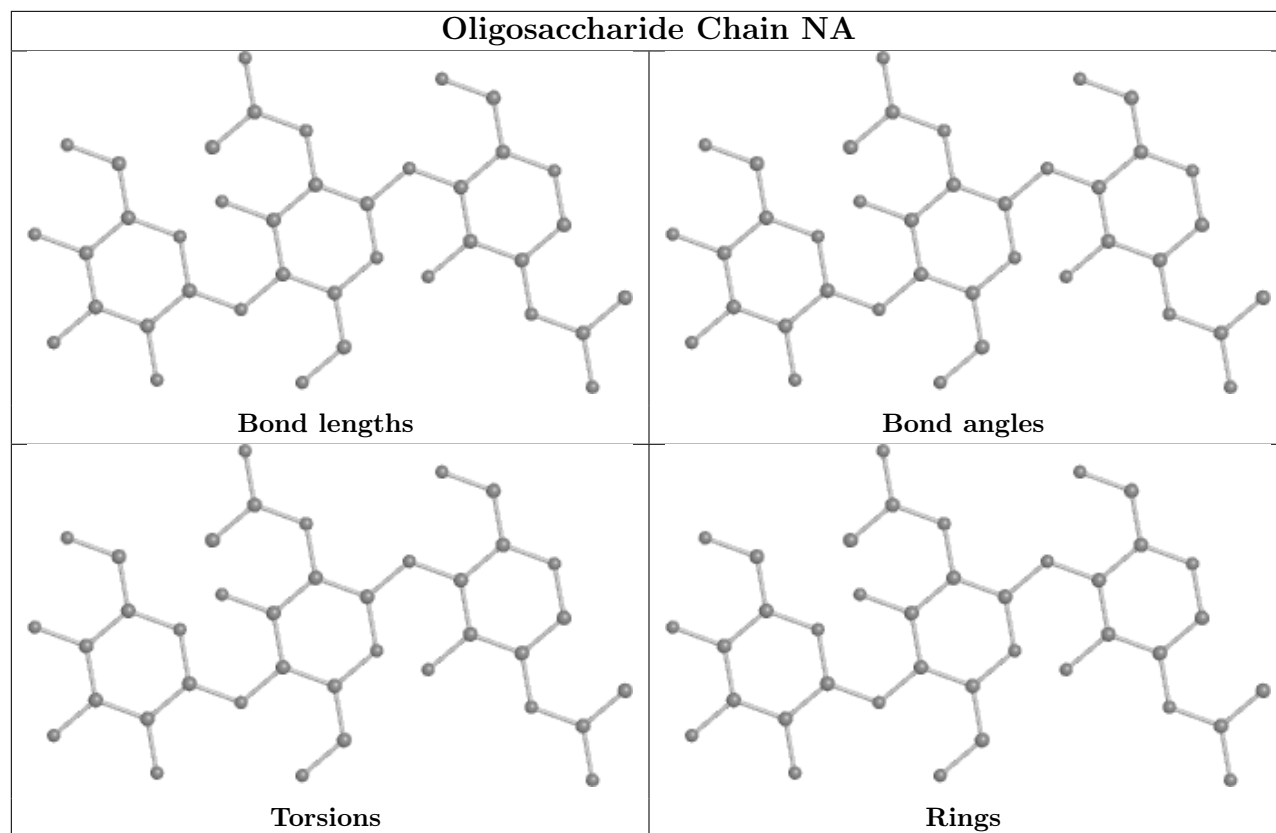


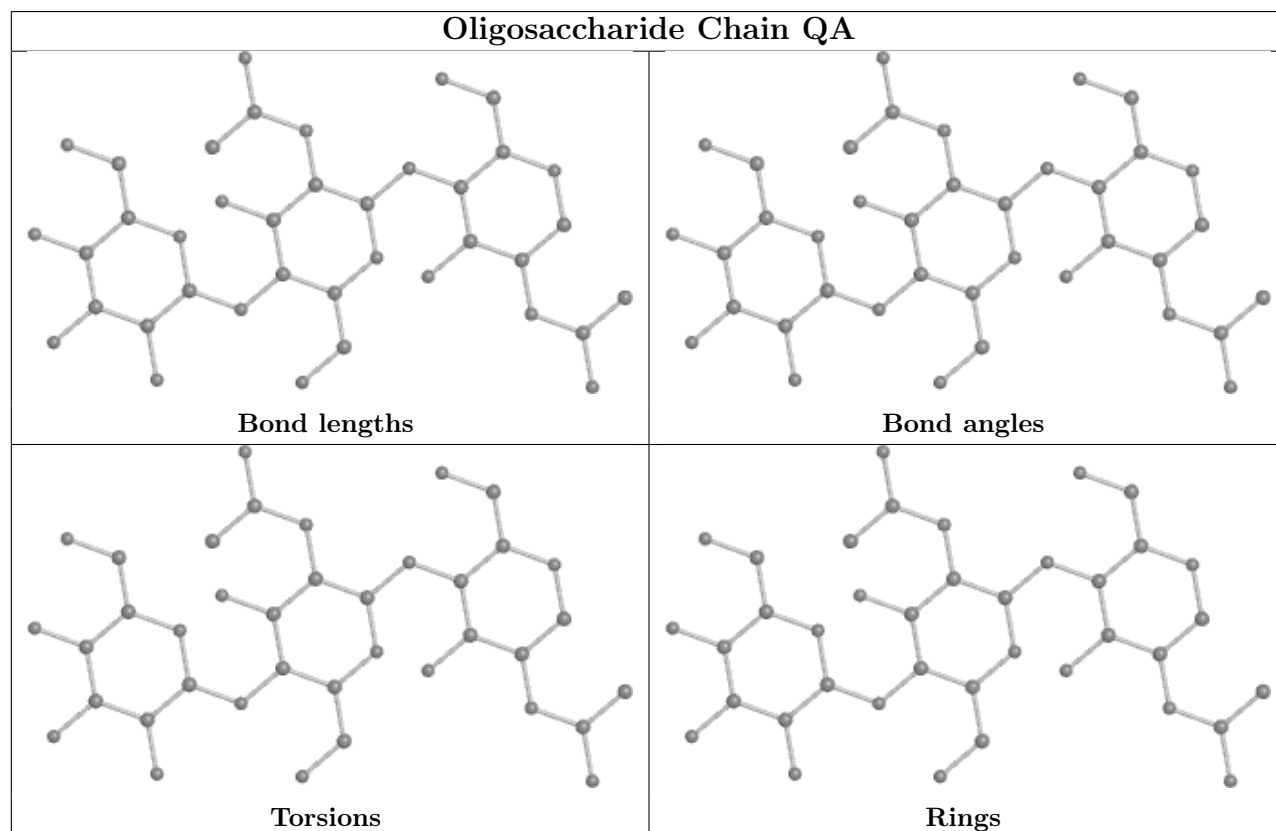
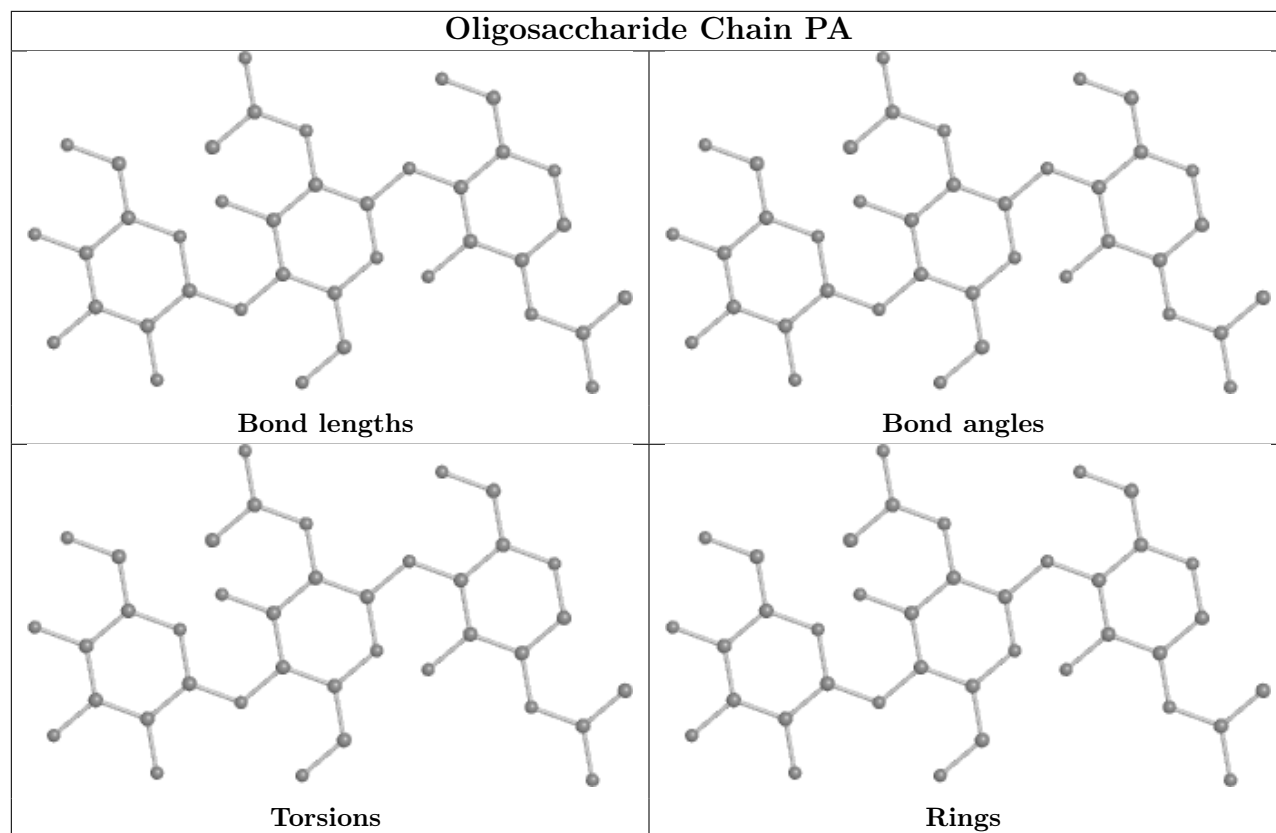


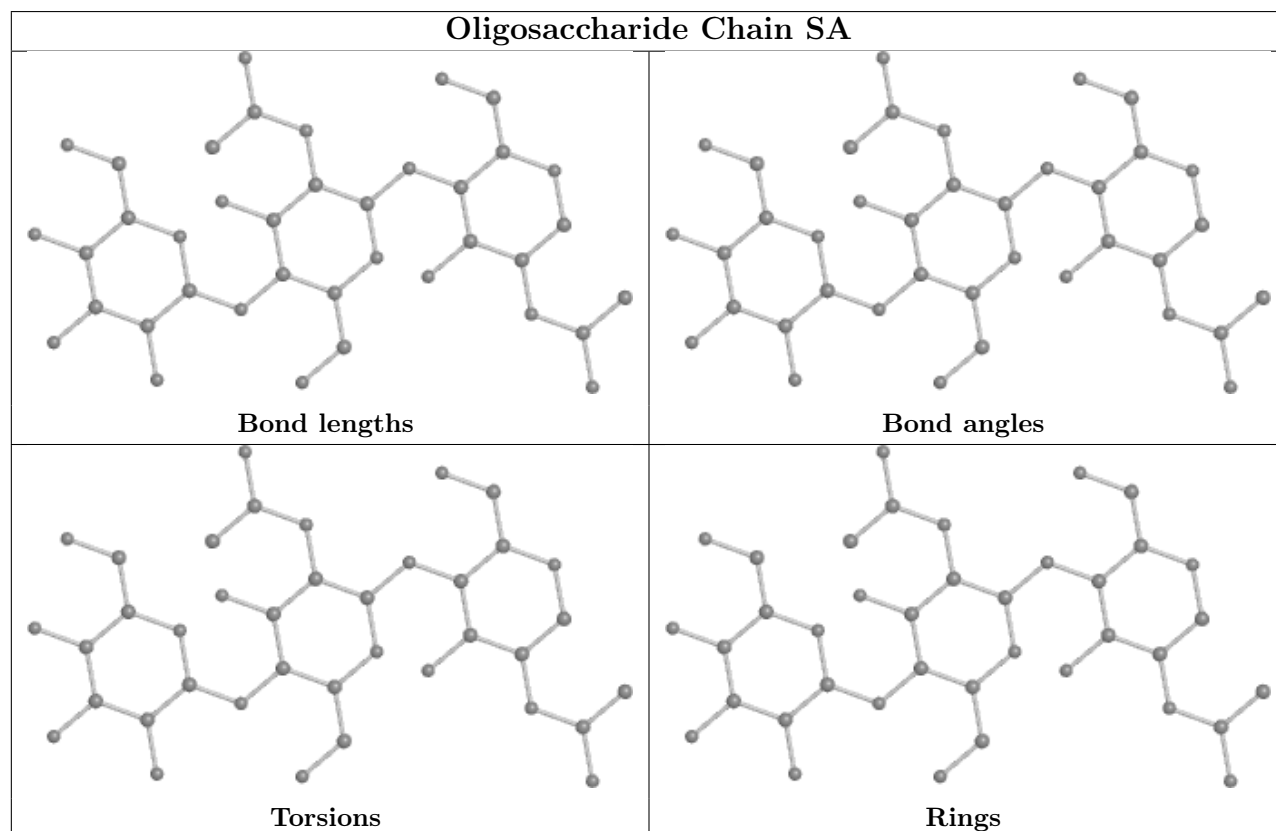
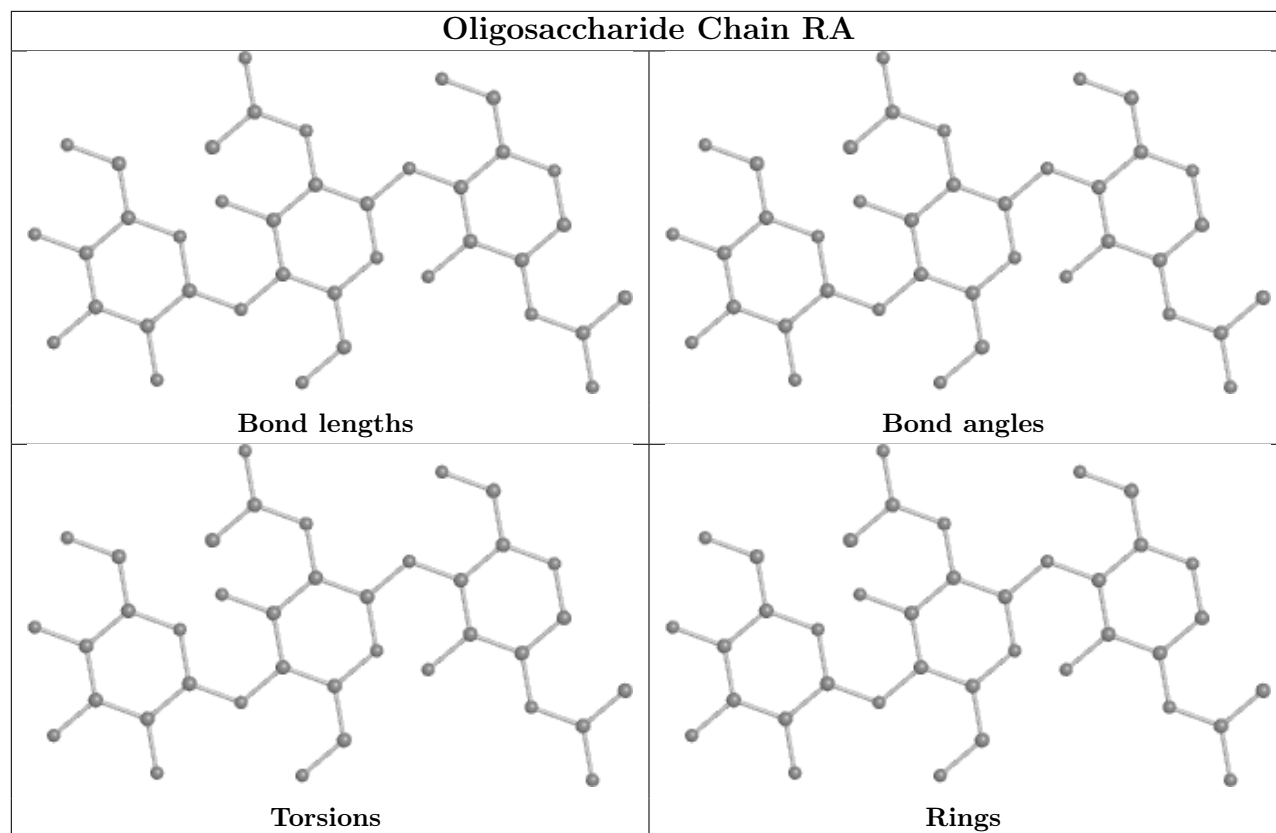
**Oligosaccharide Chain HA****Oligosaccharide Chain IA**

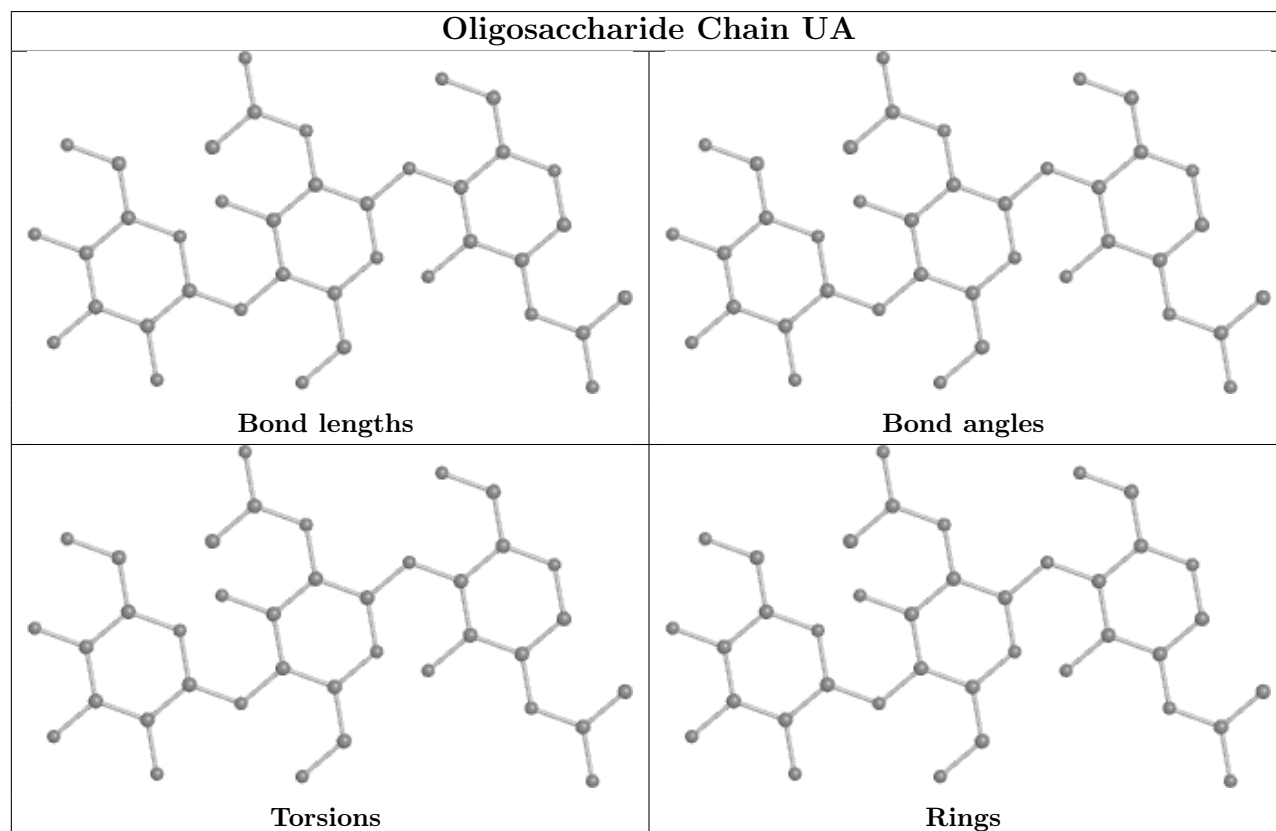
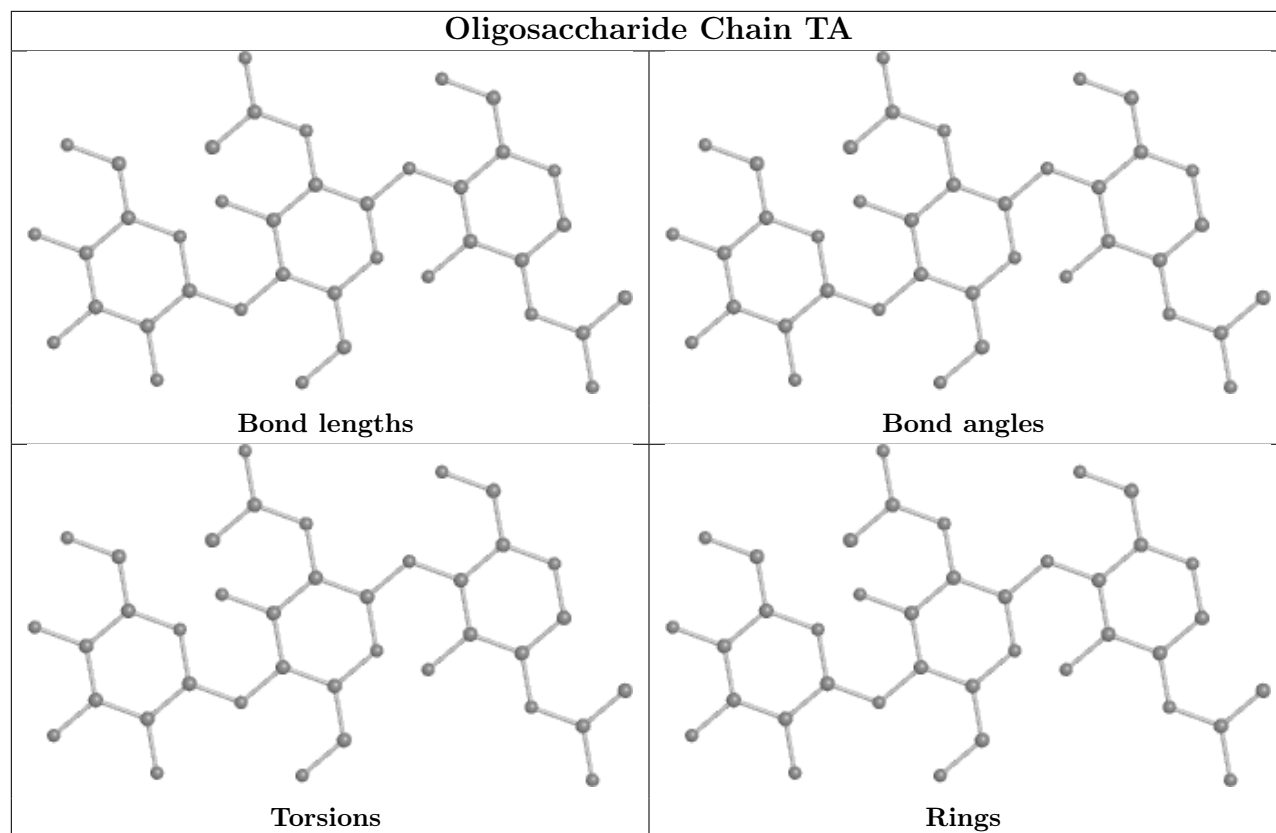




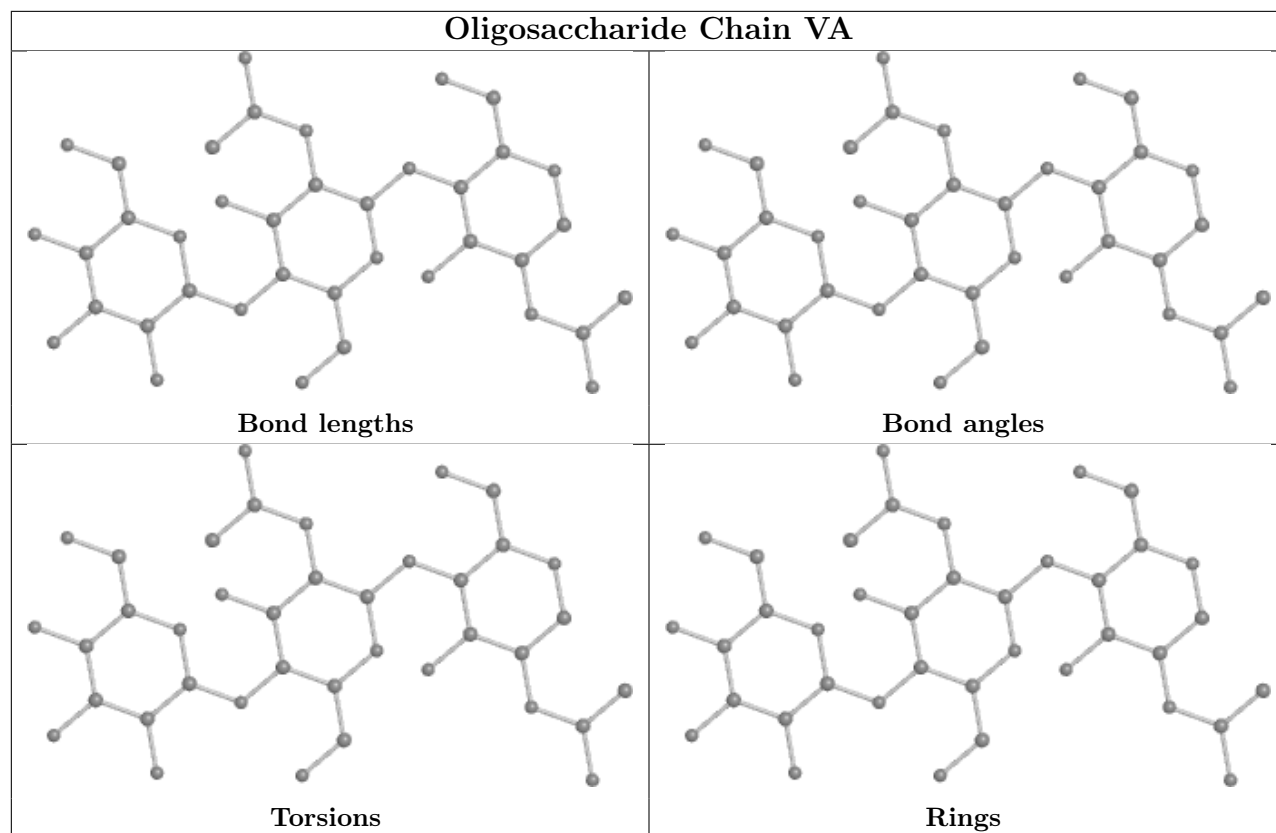




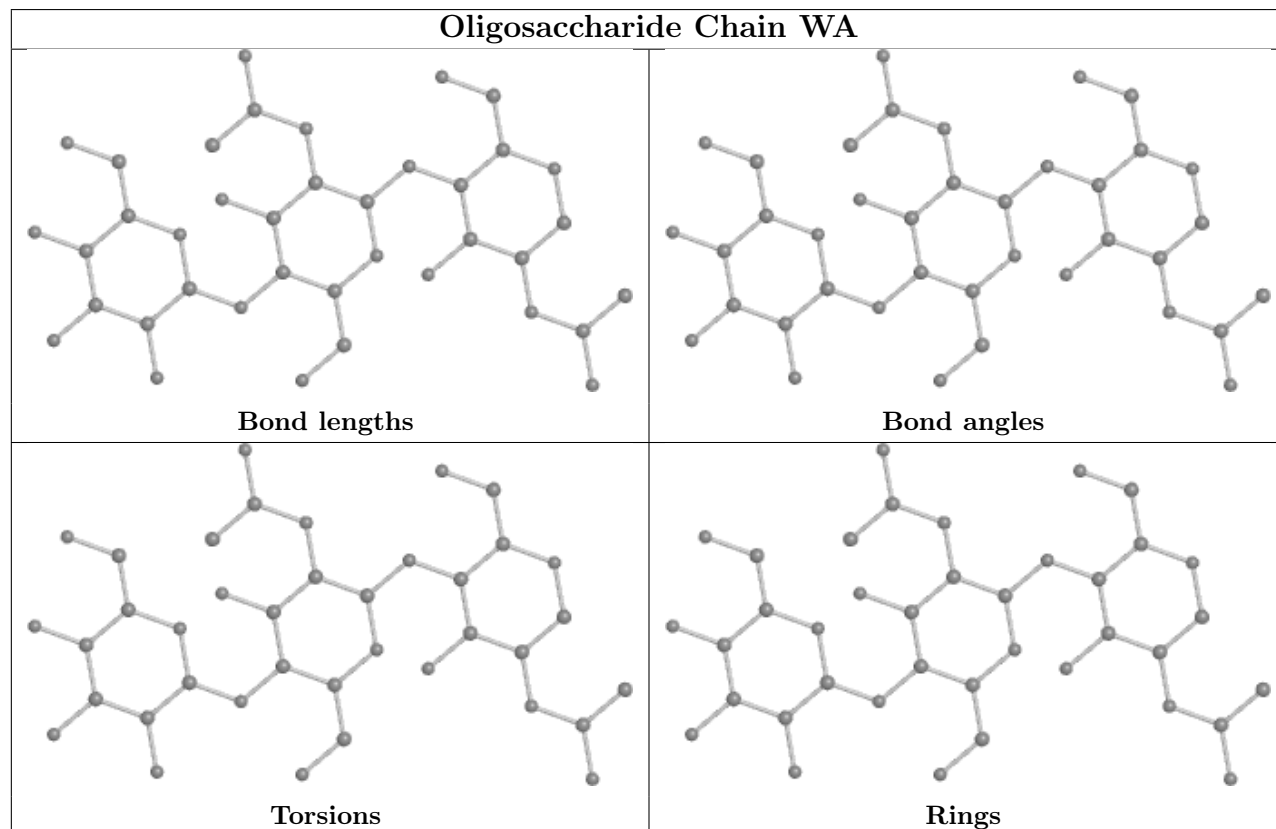




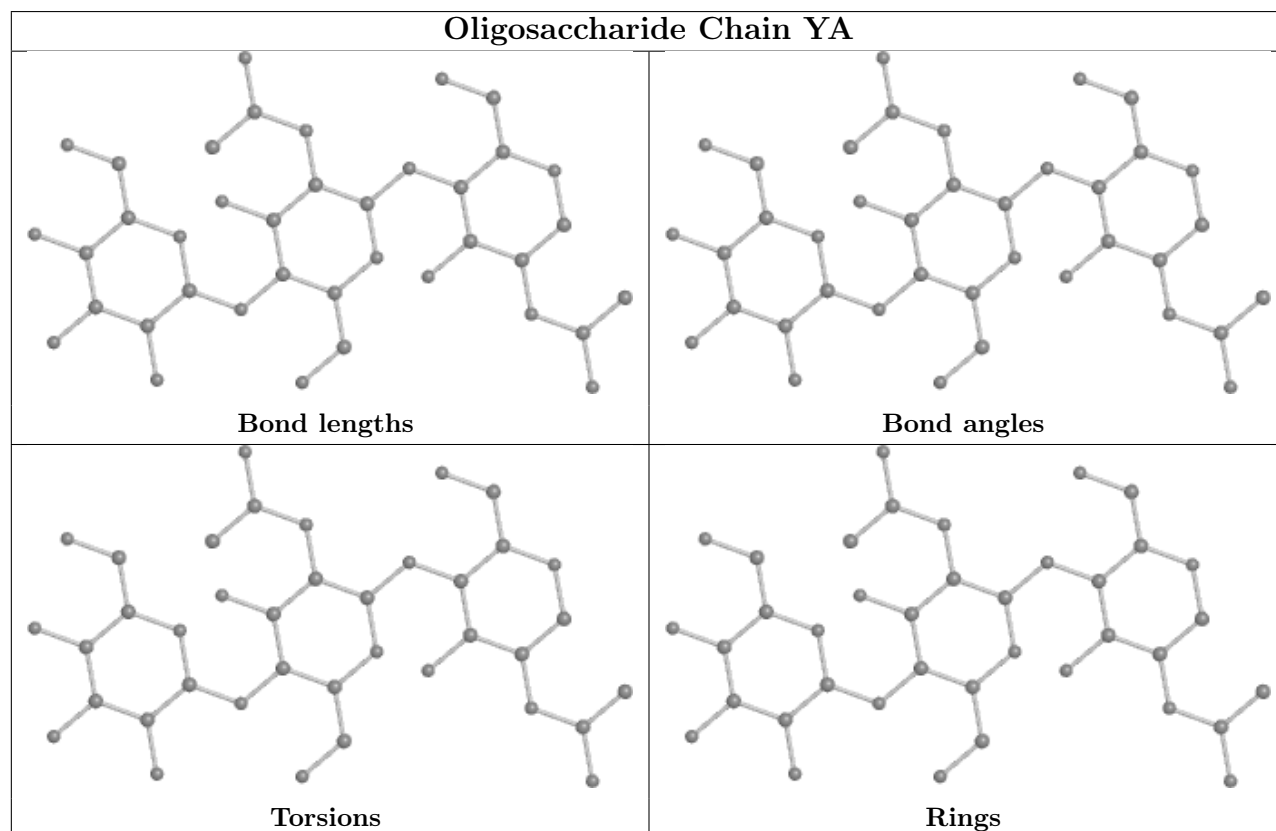
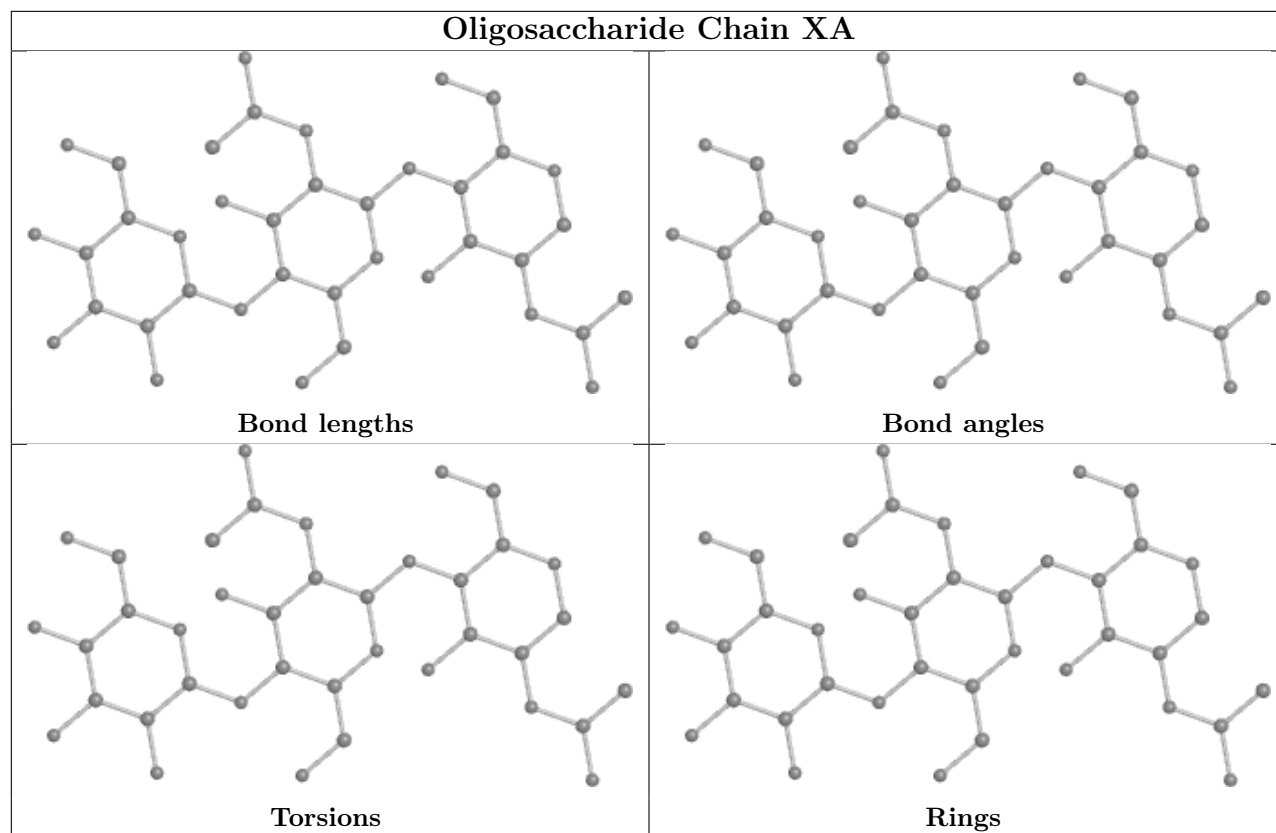
## Oligosaccharide Chain VA

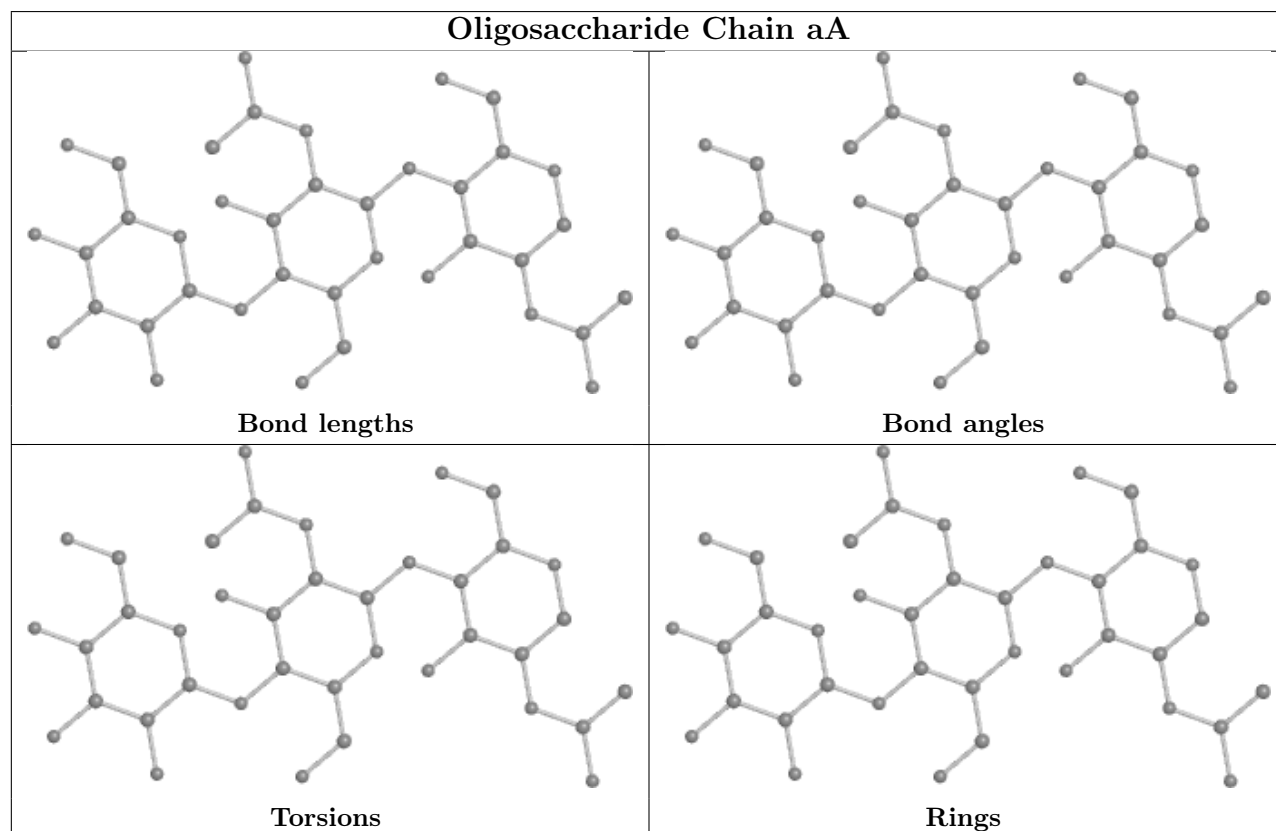
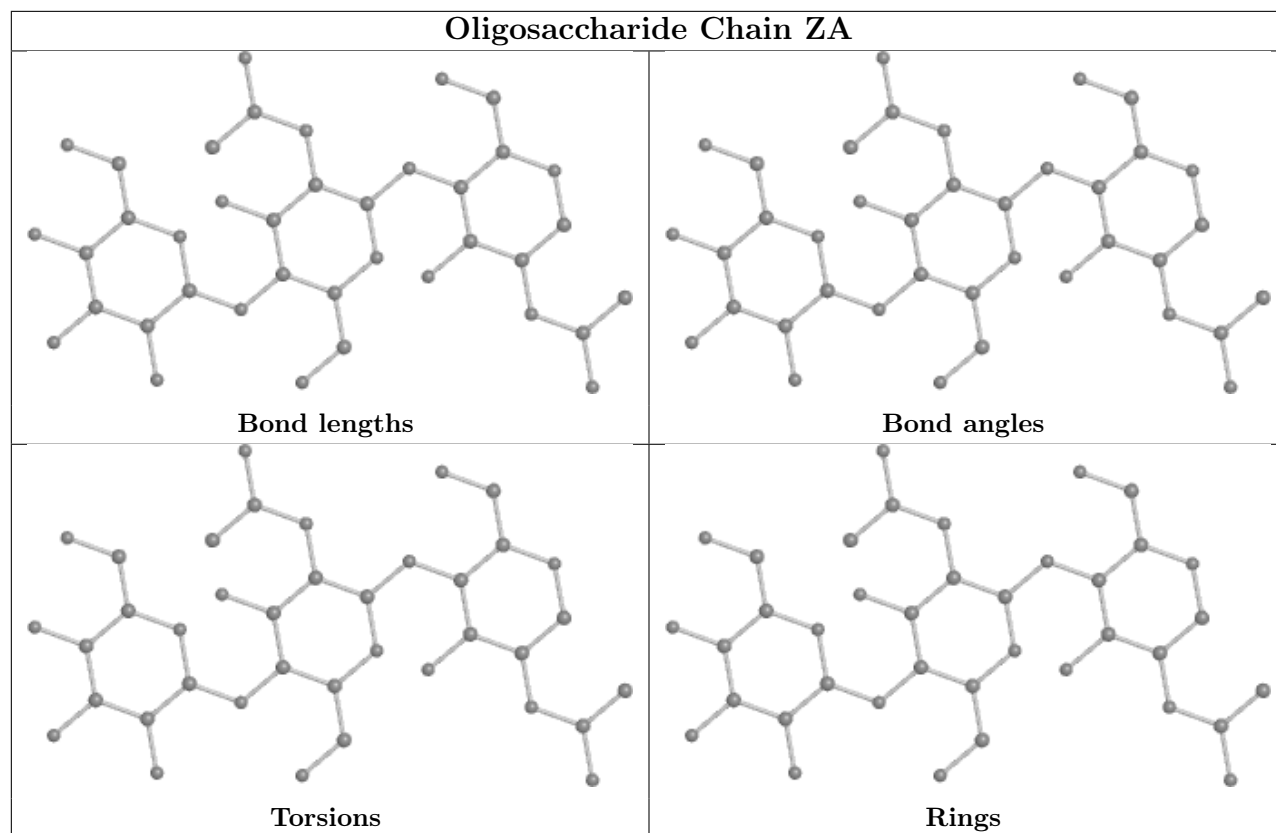


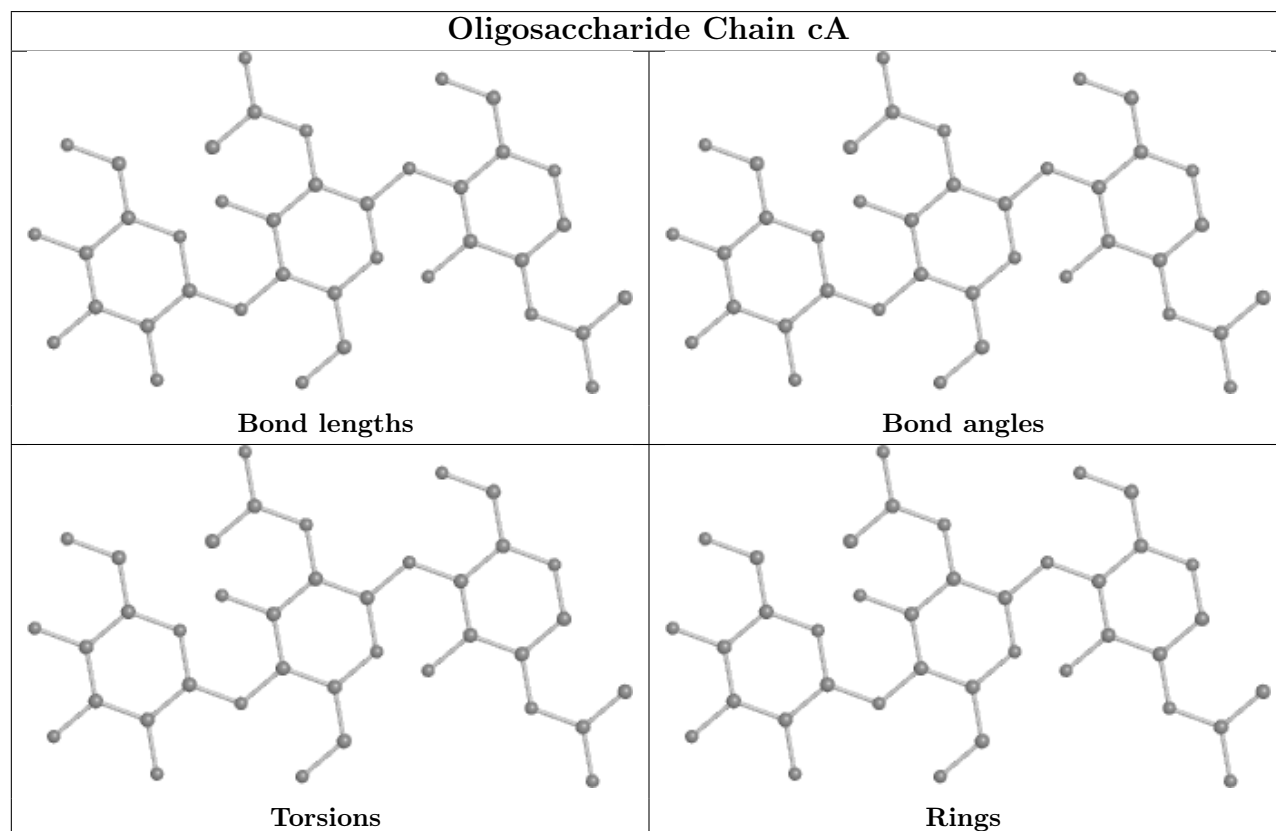
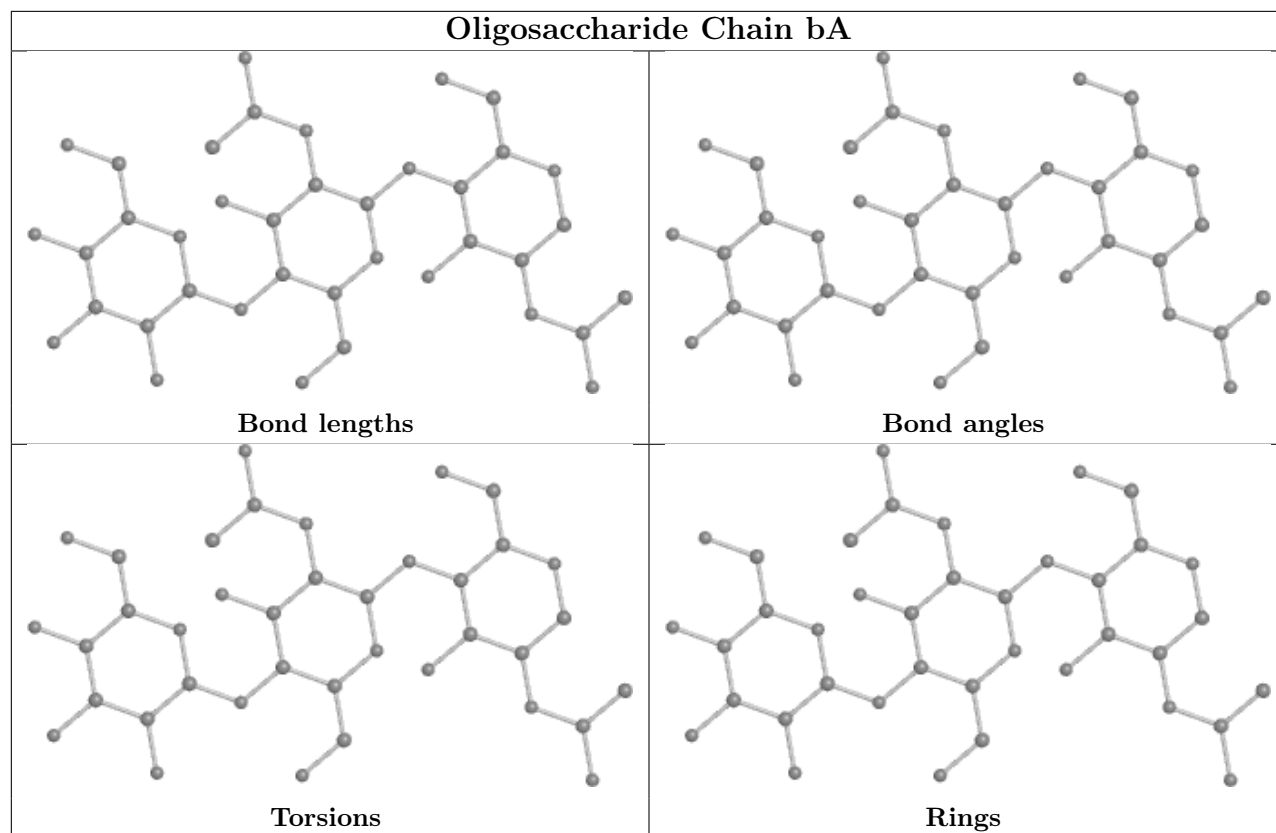
## Oligosaccharide Chain WA

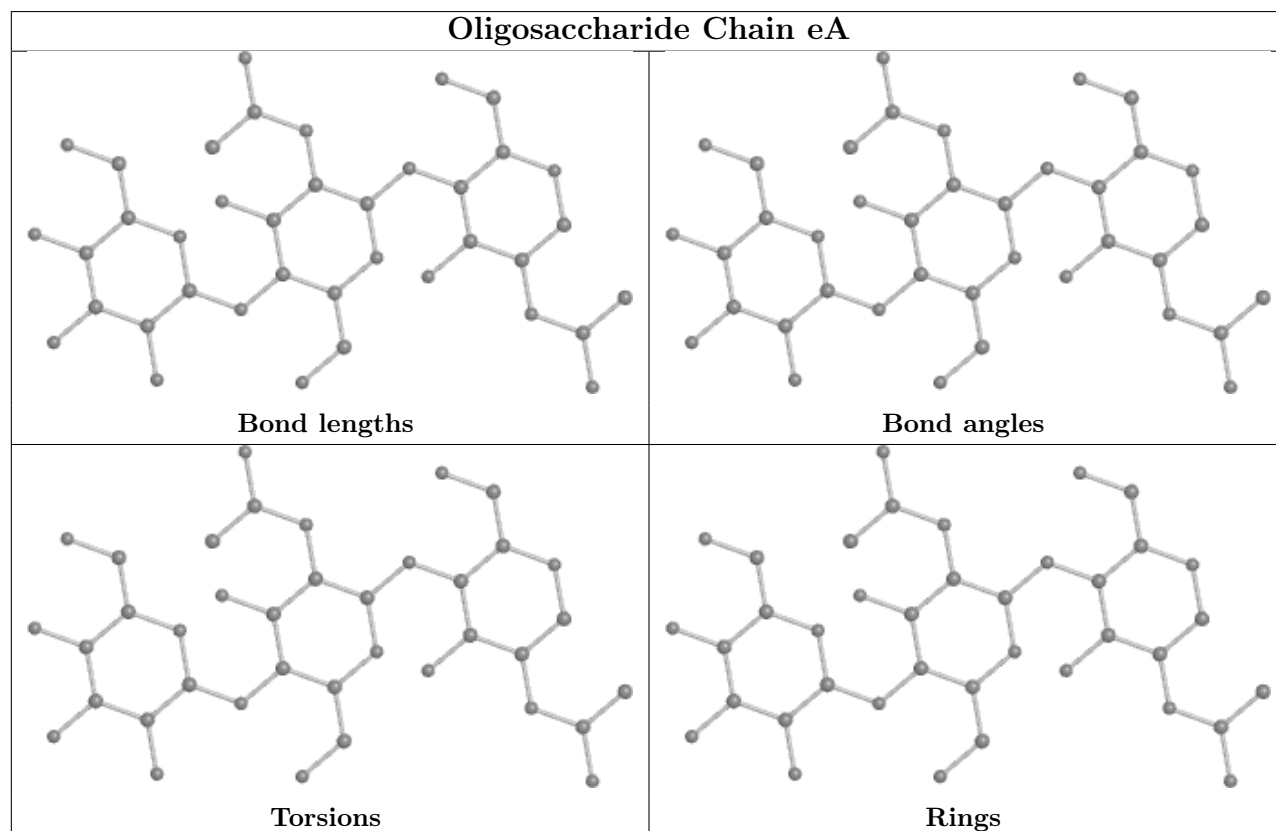
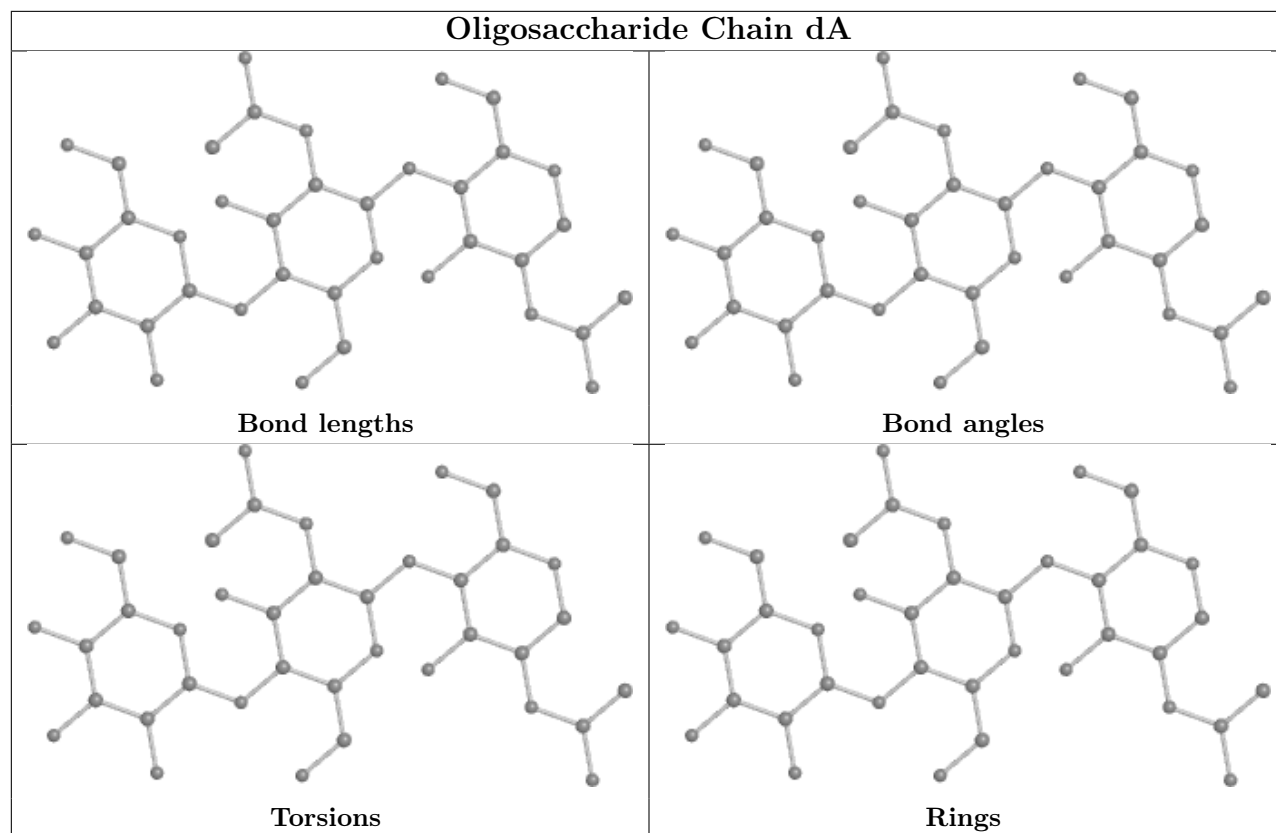


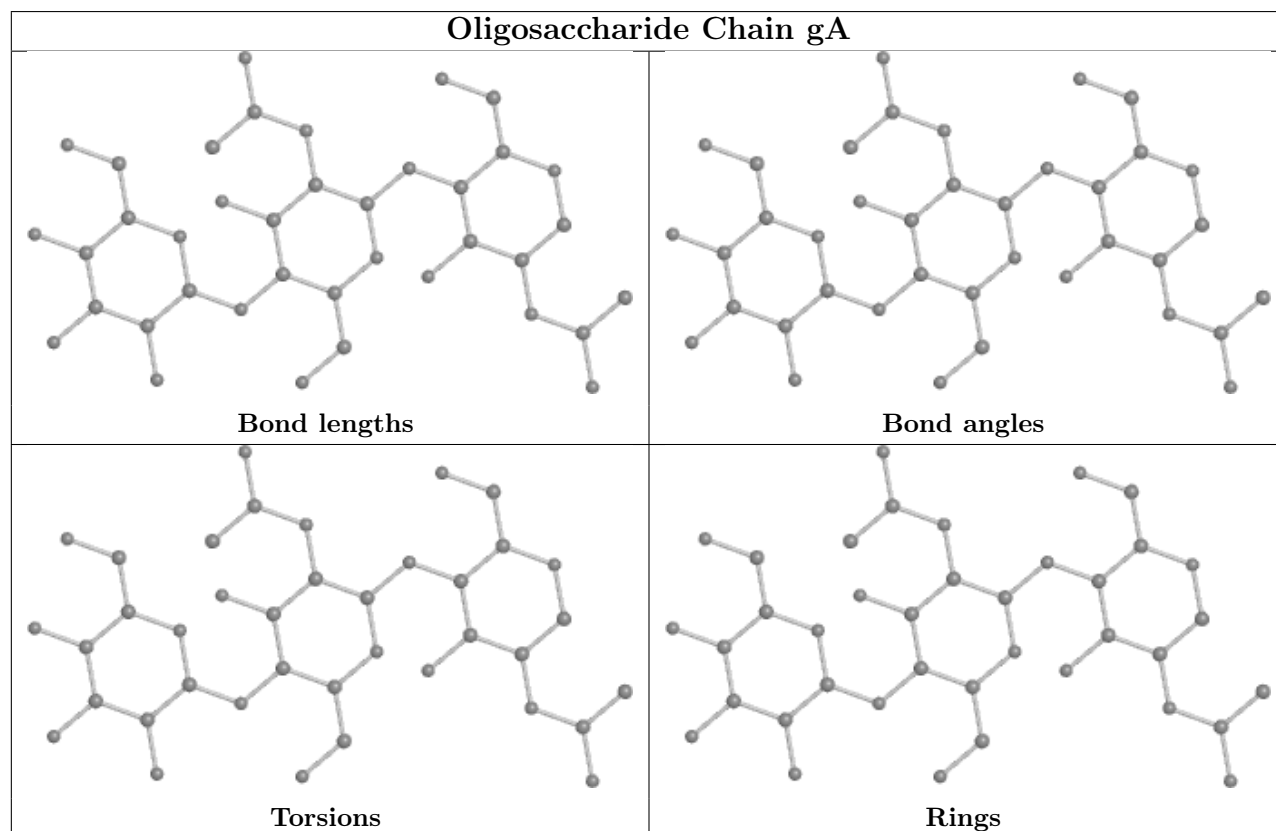
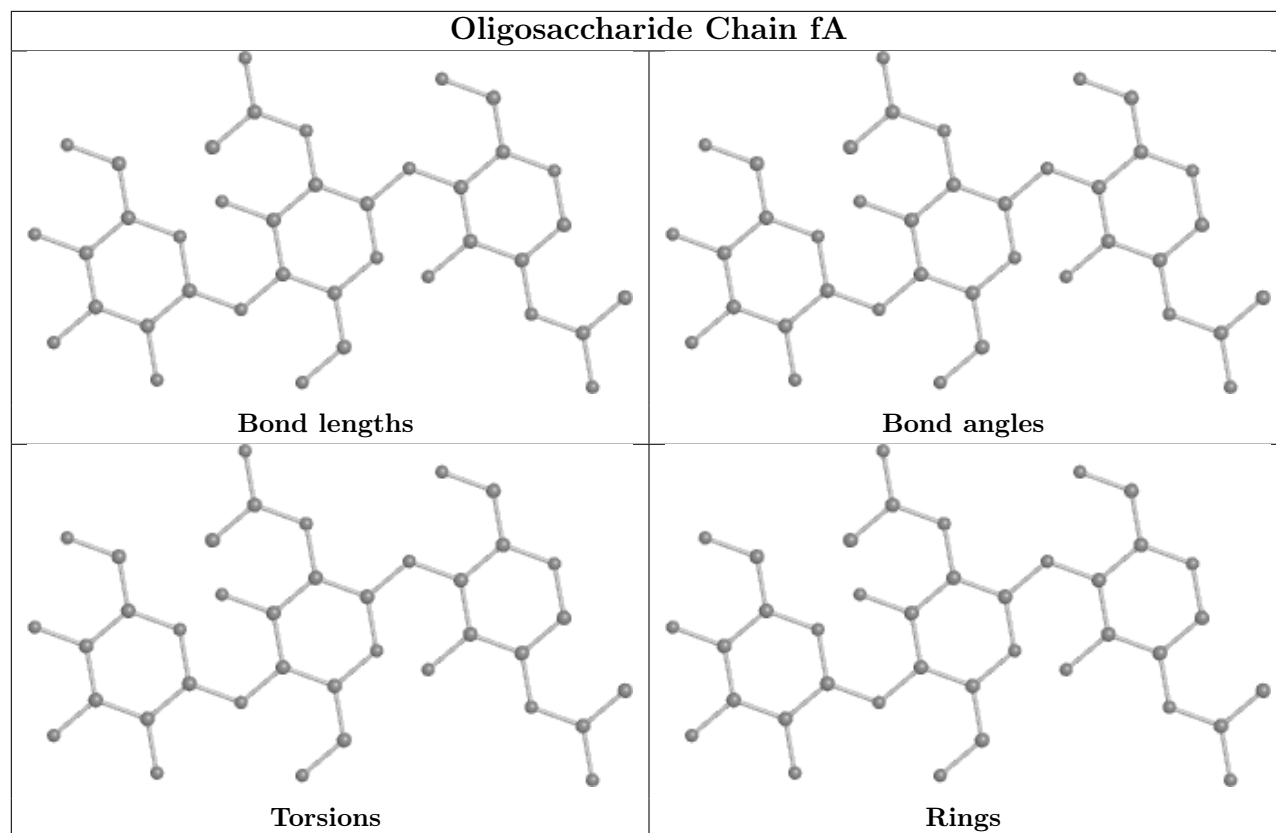


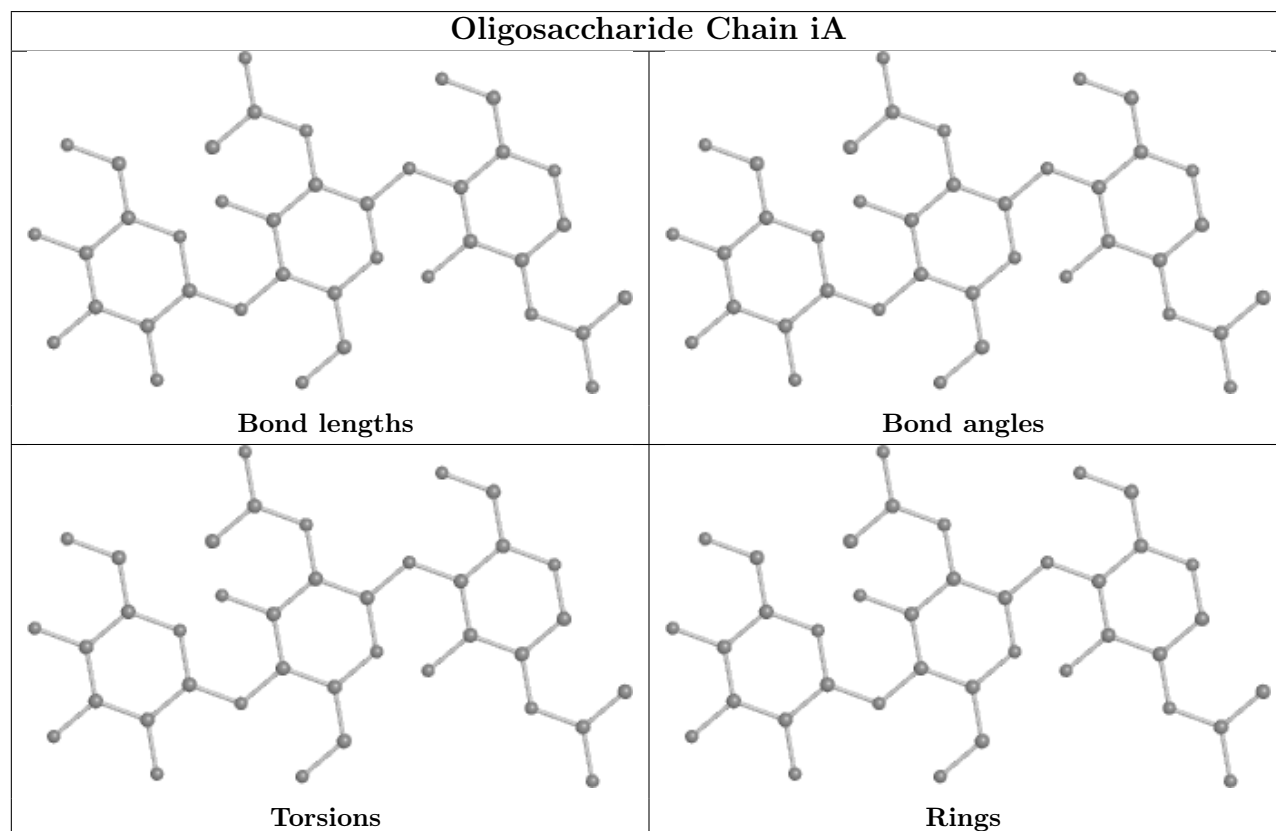
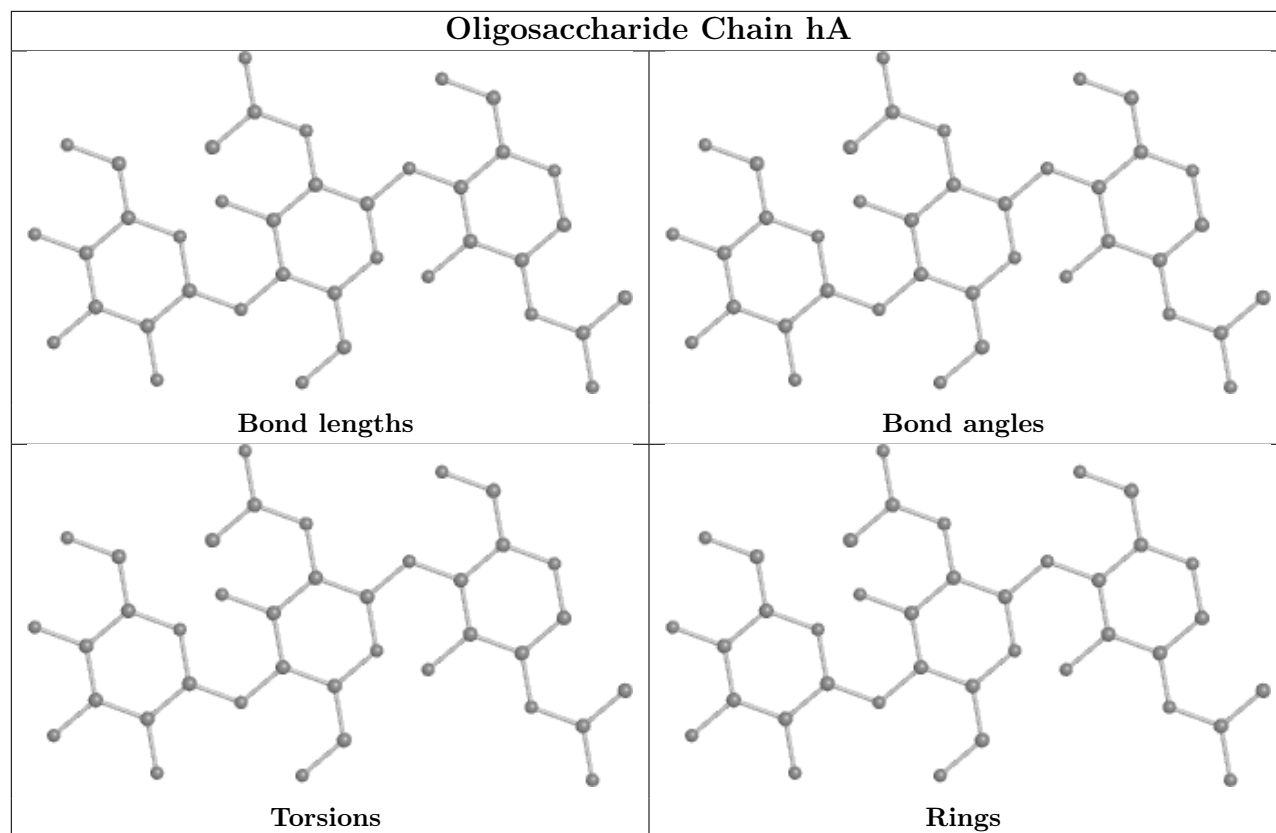


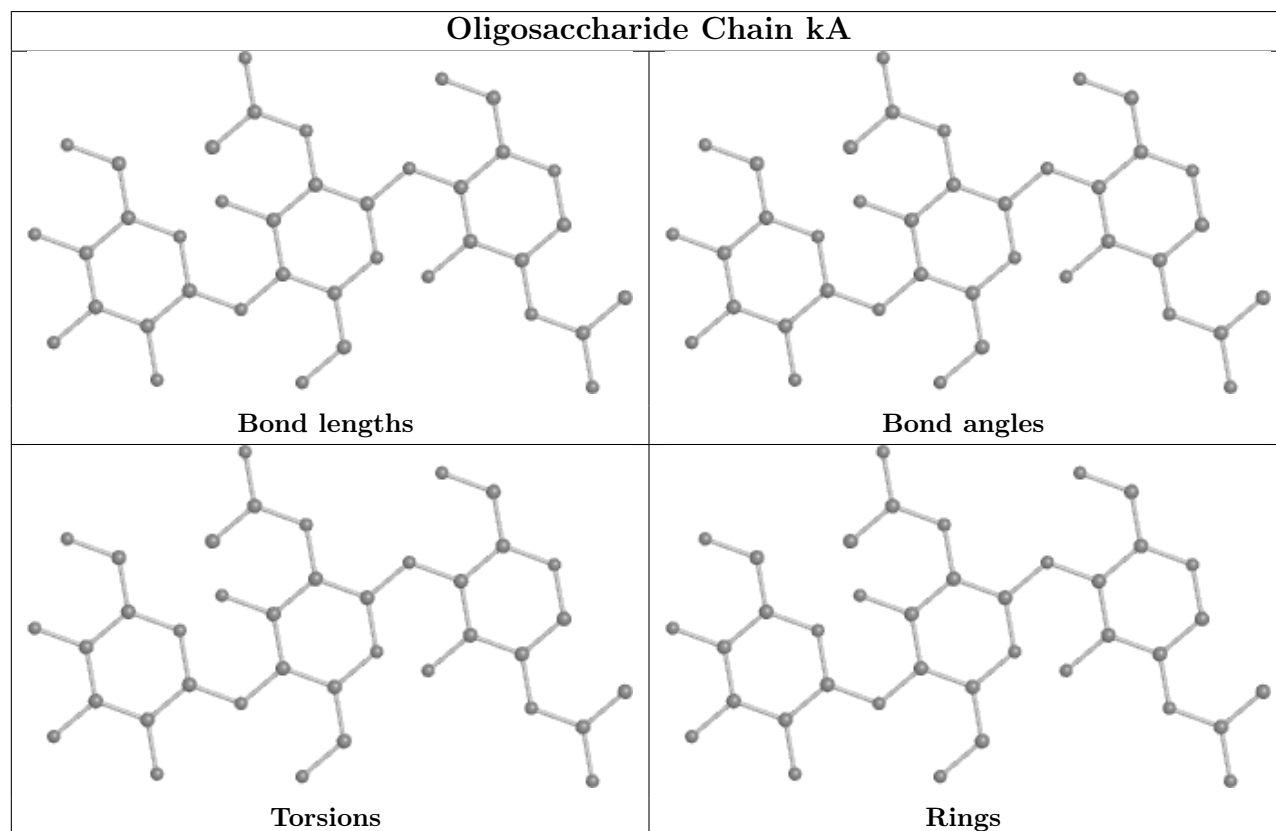
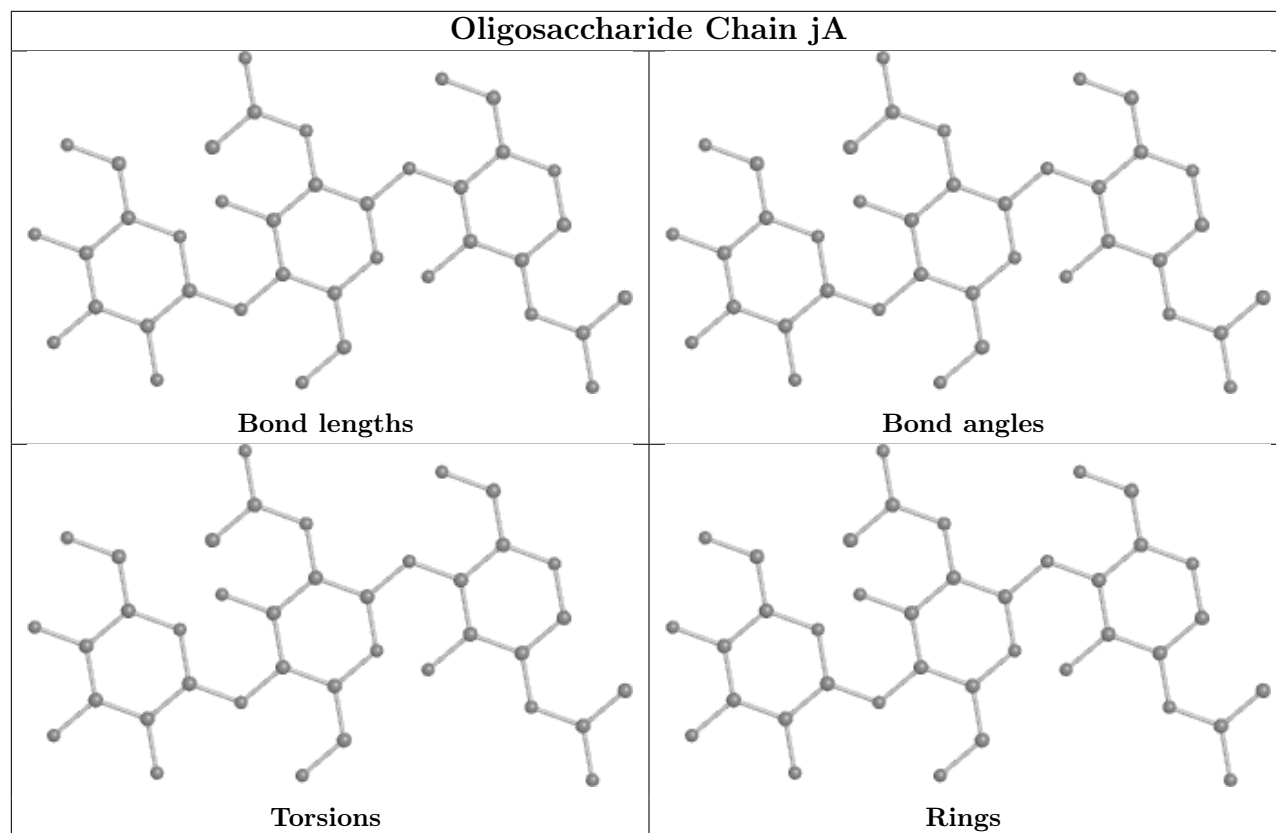


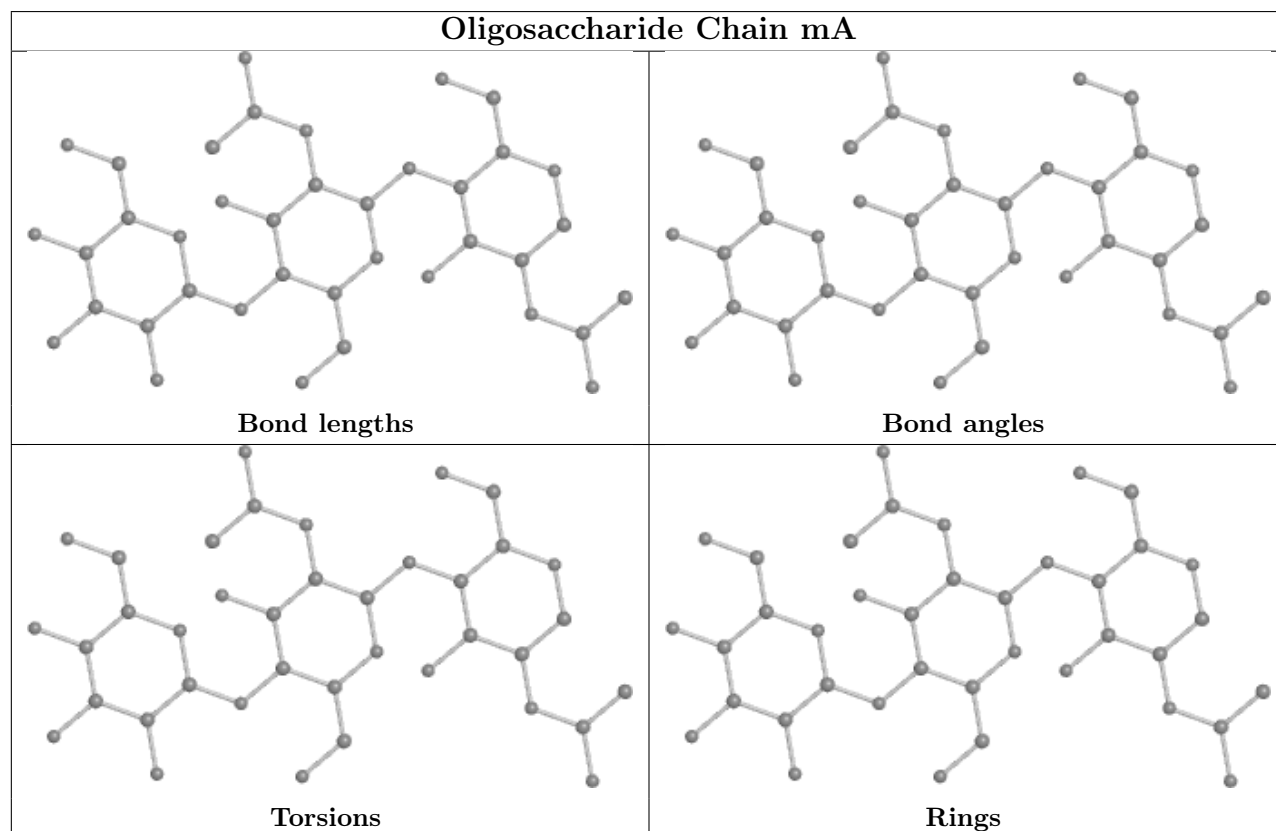
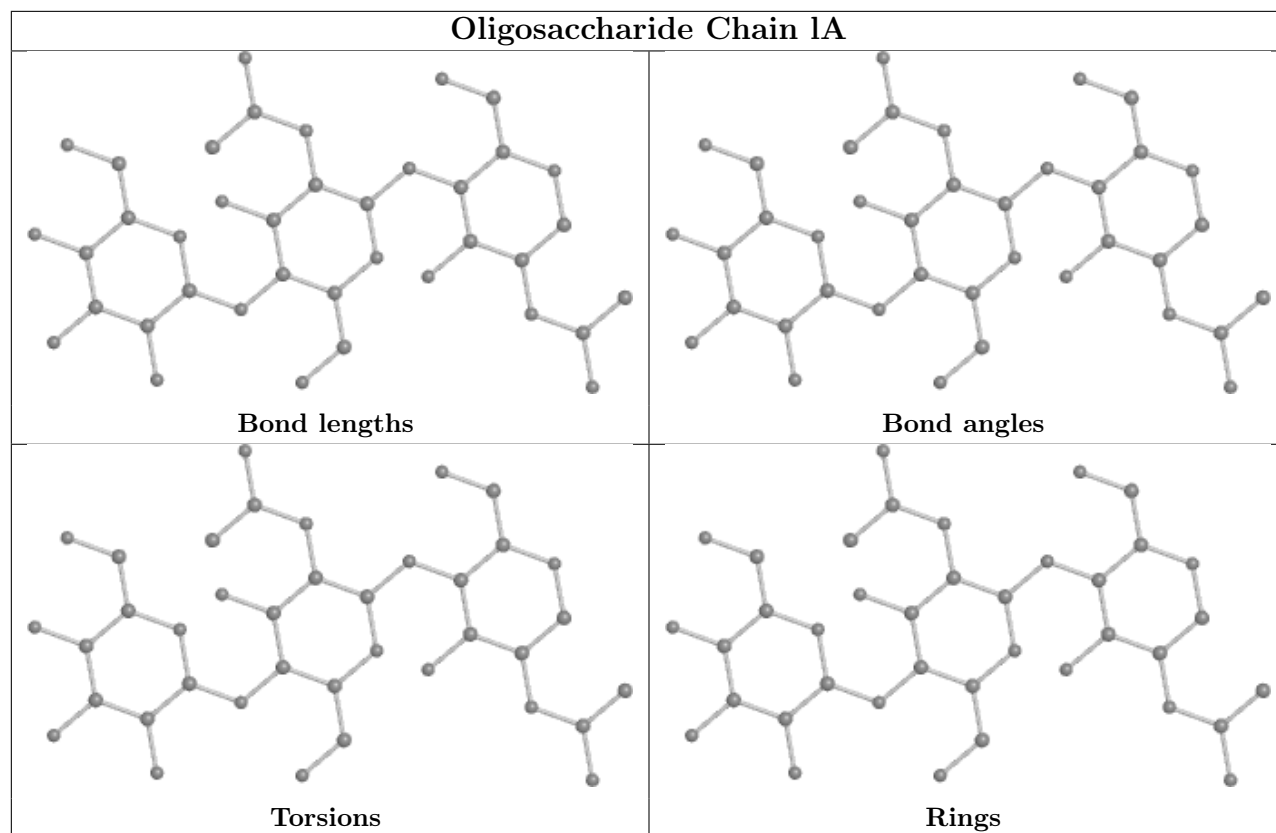




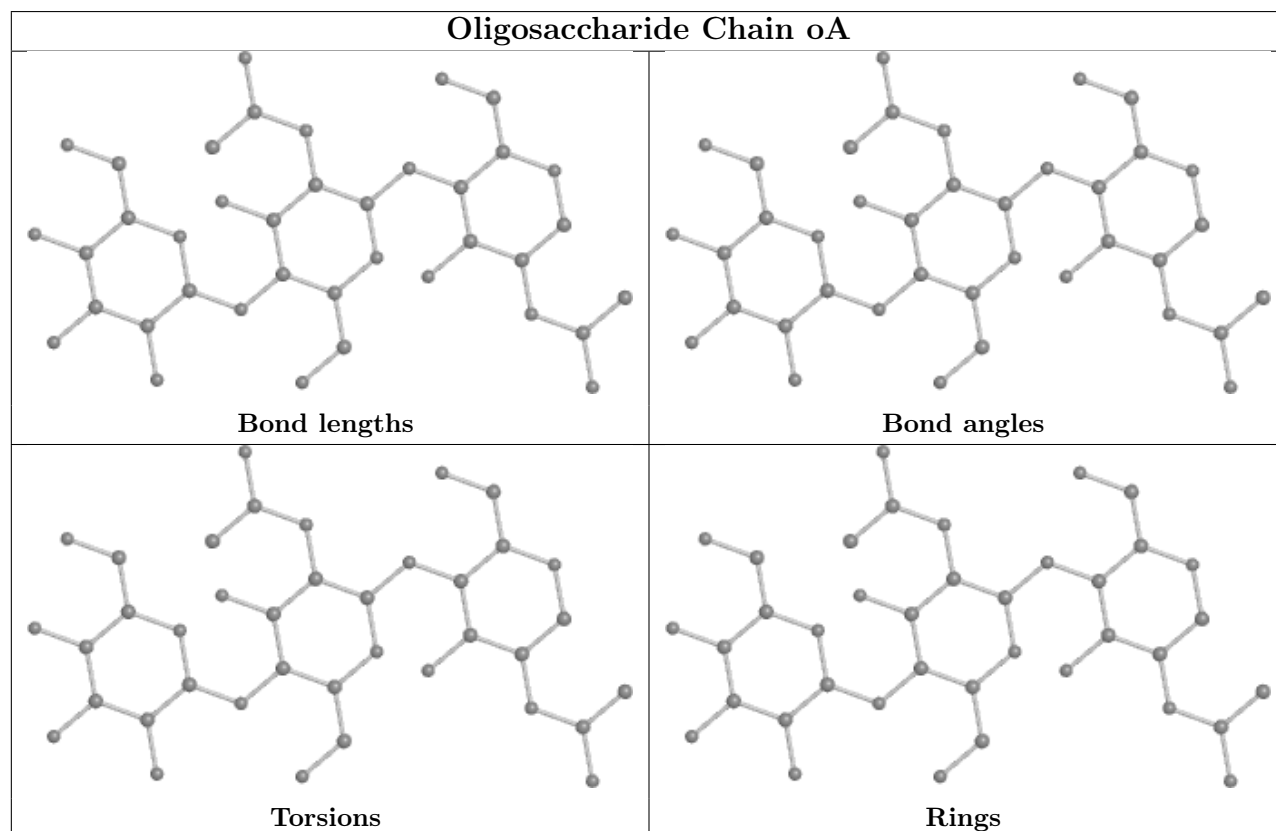
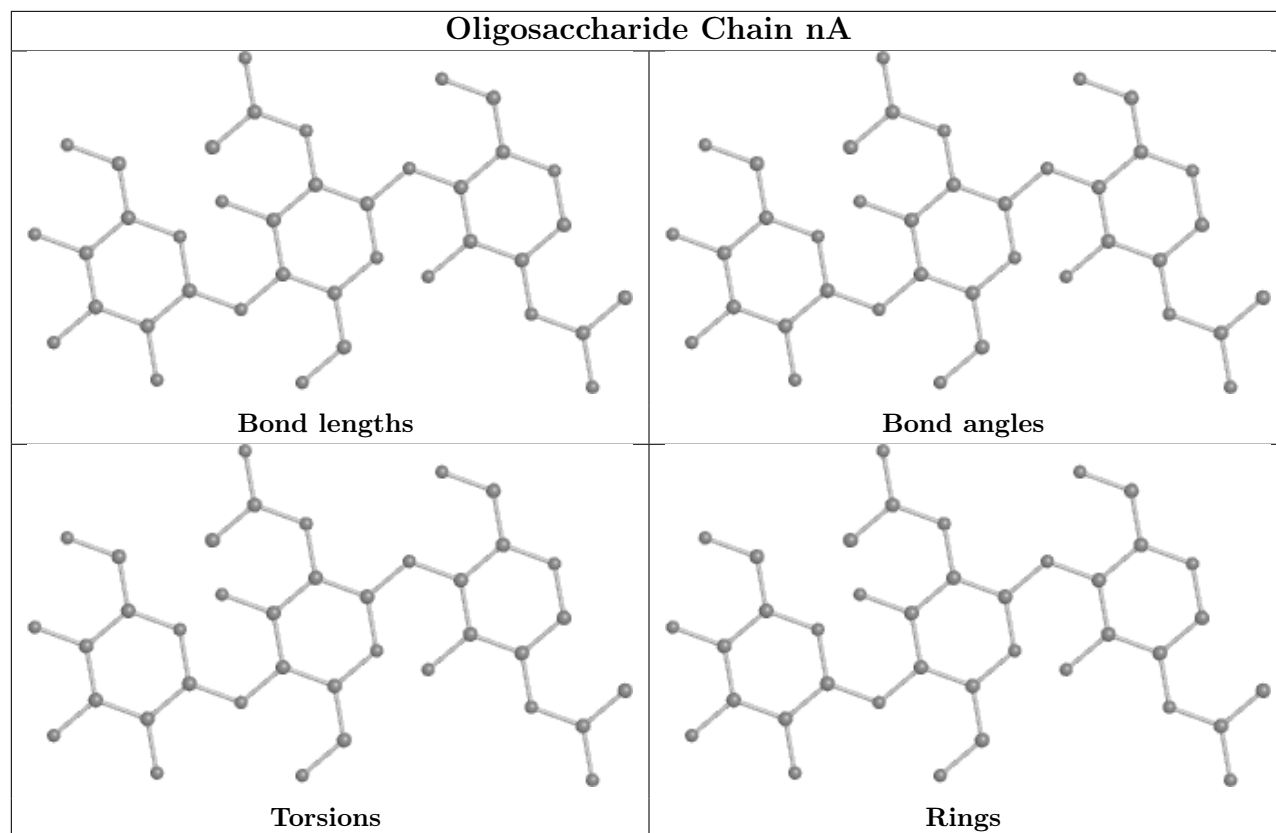


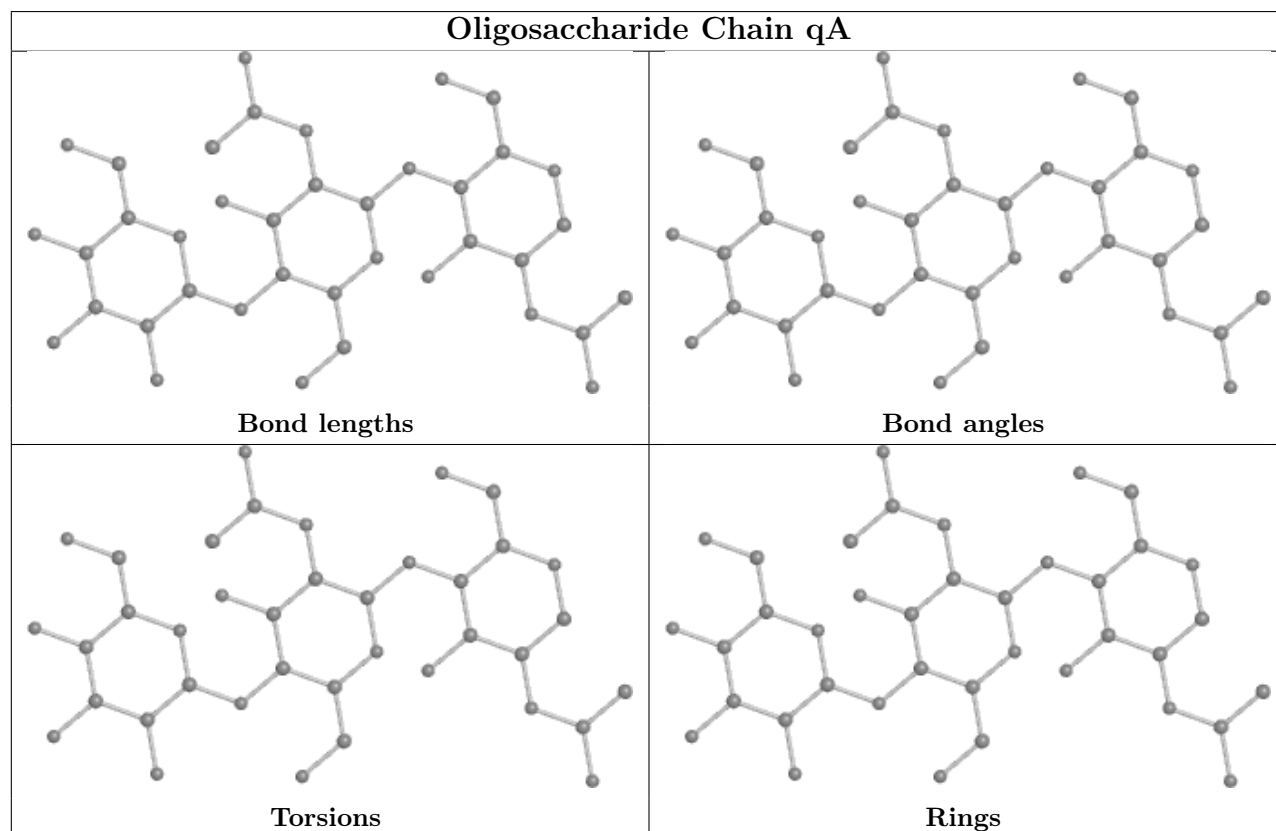
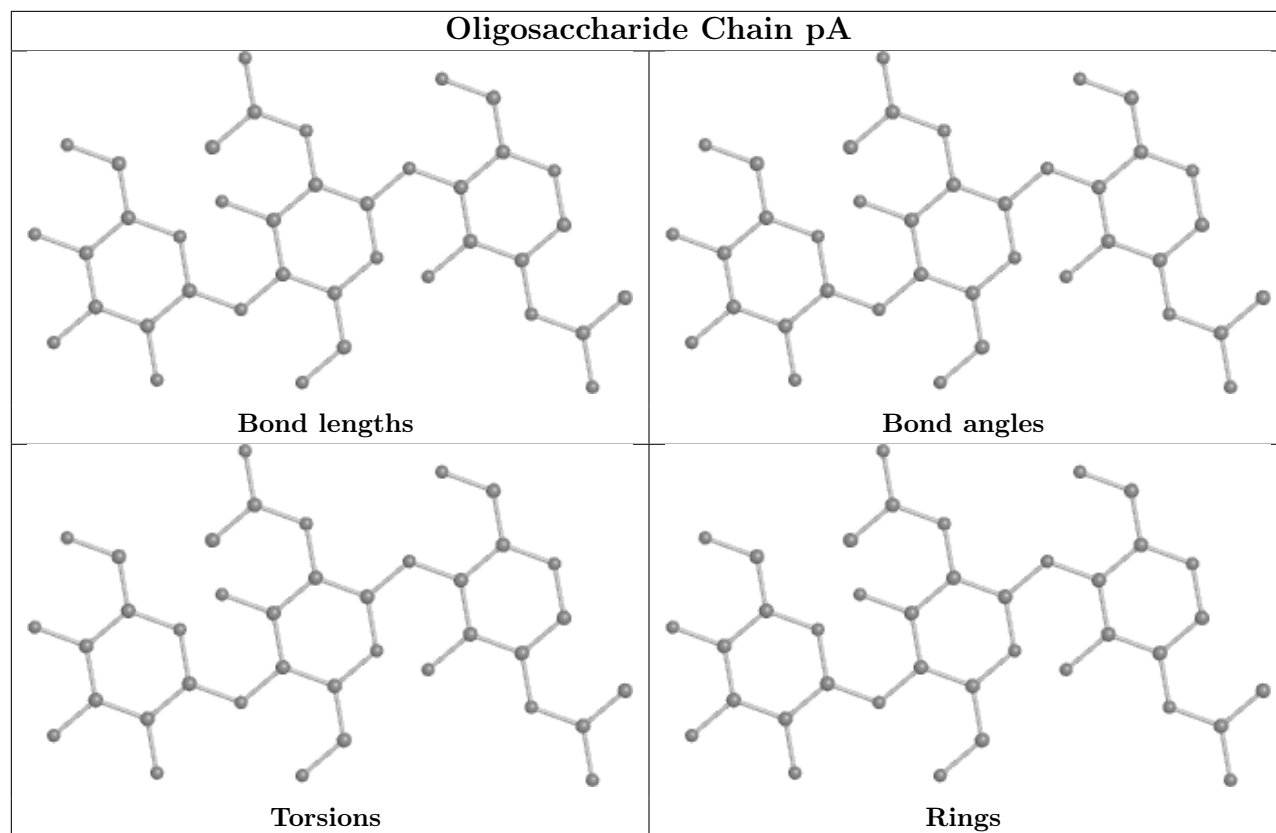


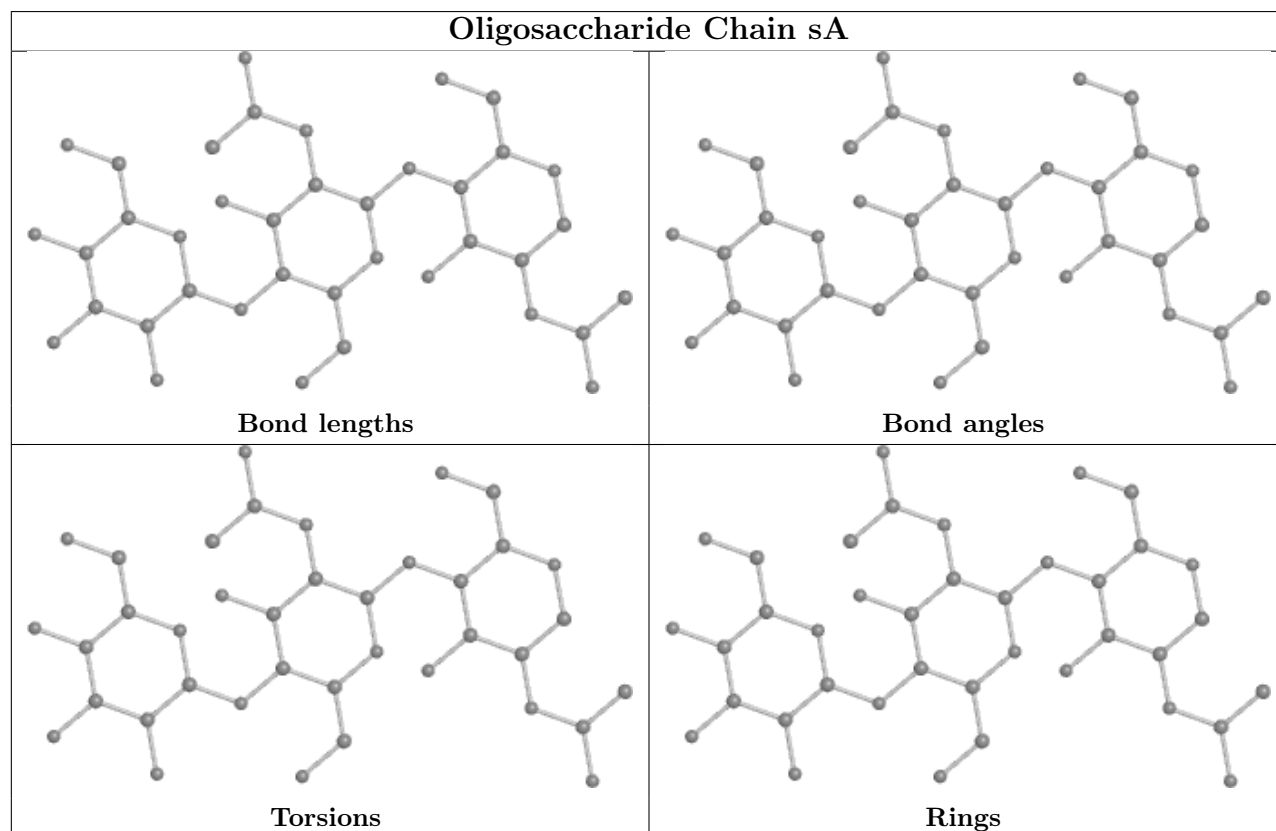
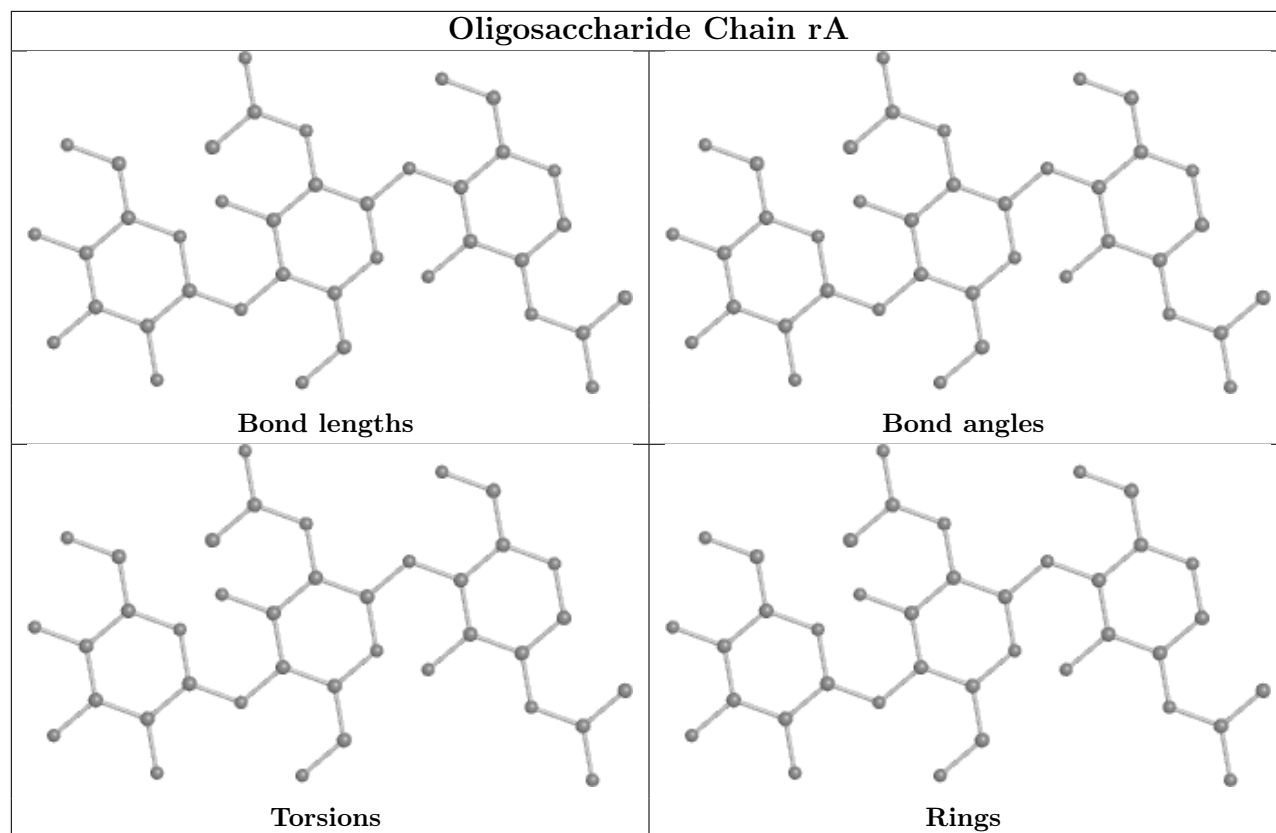


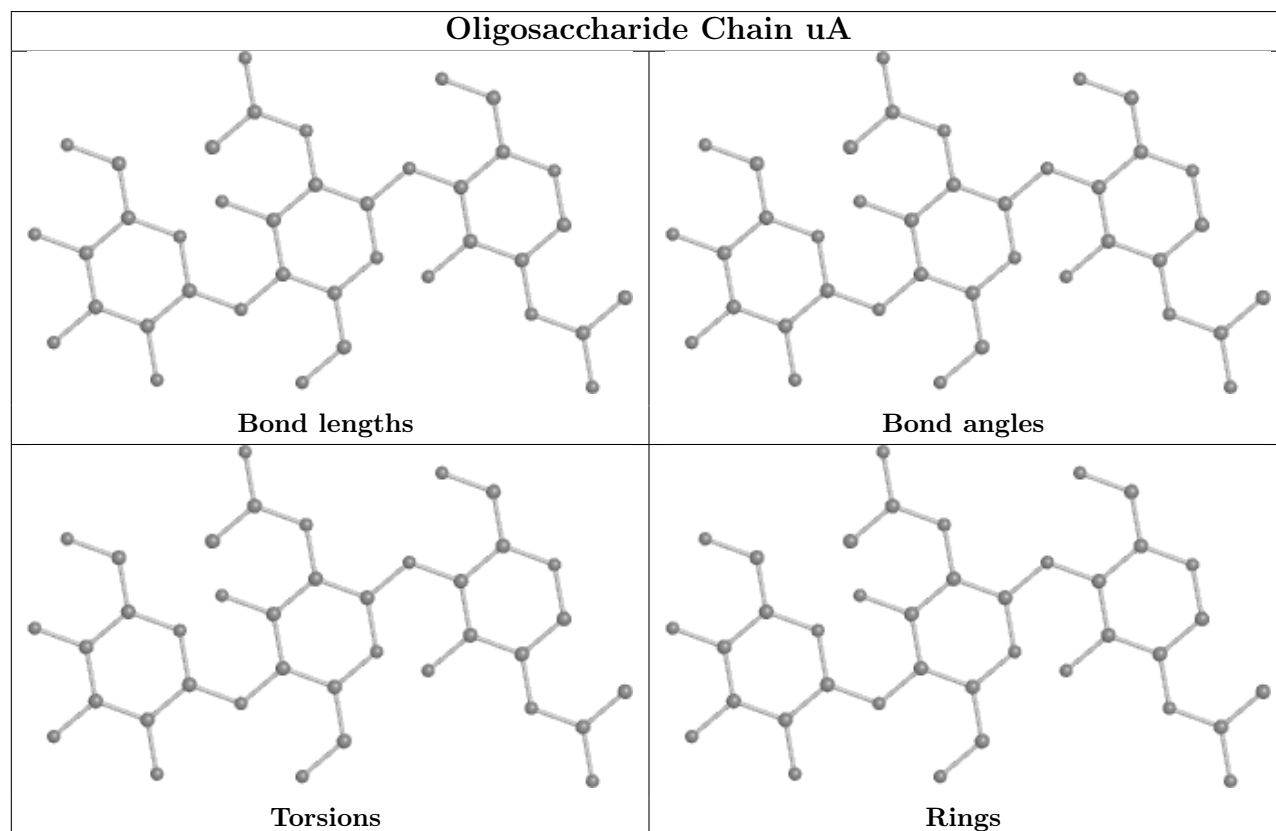
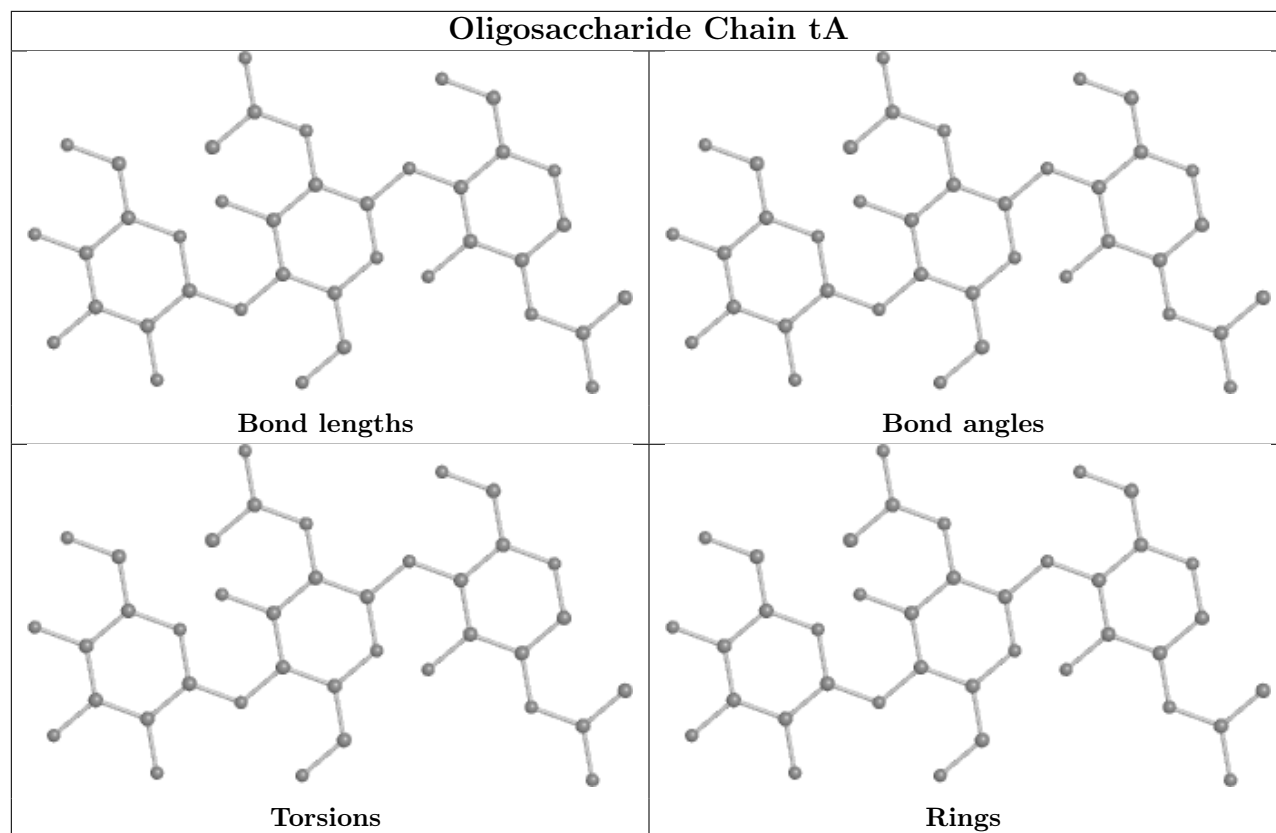












## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

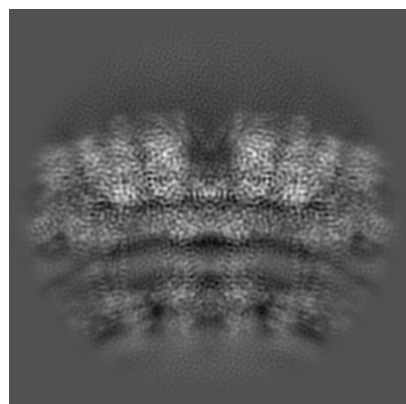
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39620. These allow visual inspection of the internal detail of the map and identification of artifacts.

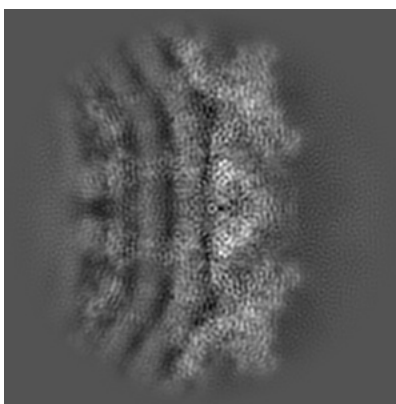
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

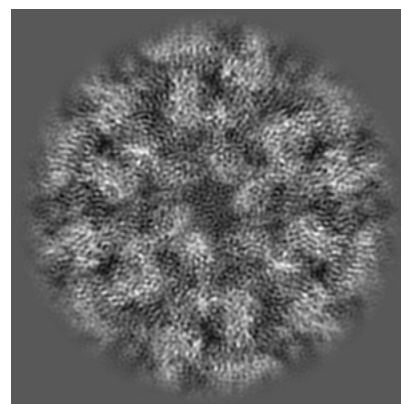
#### 6.1.1 Primary map



X

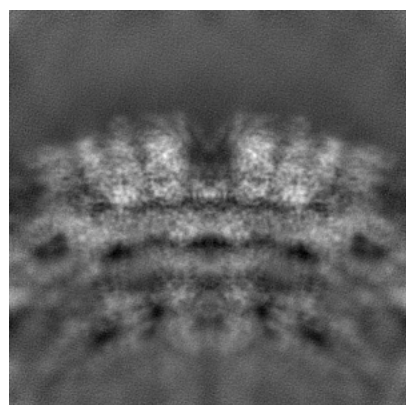


Y

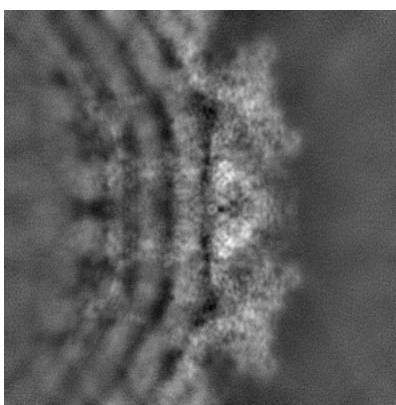


Z

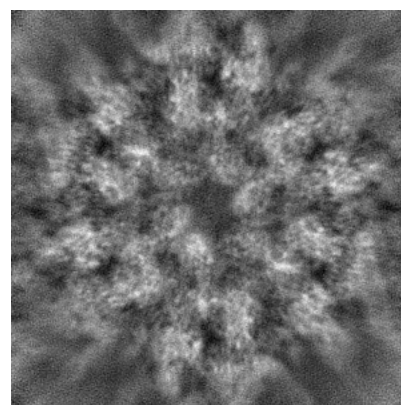
#### 6.1.2 Raw map



X



Y

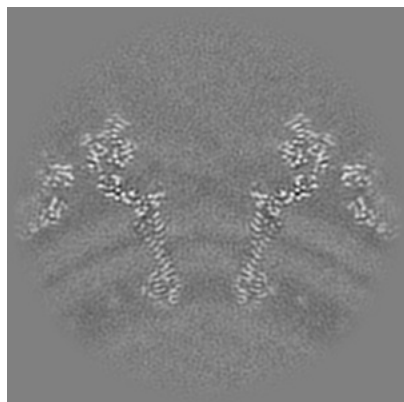


Z

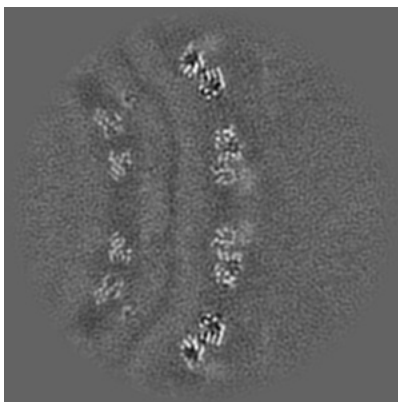
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

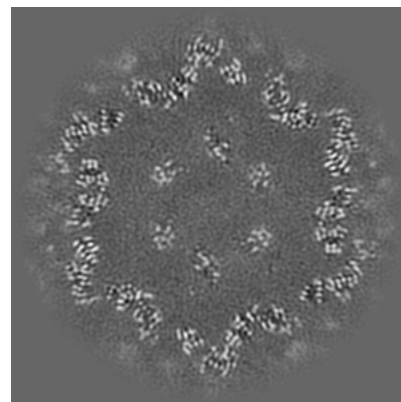
### 6.2.1 Primary map



X Index: 160

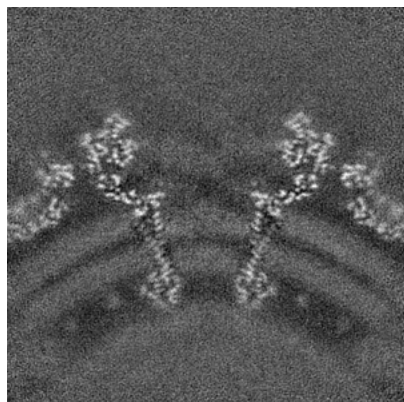


Y Index: 160

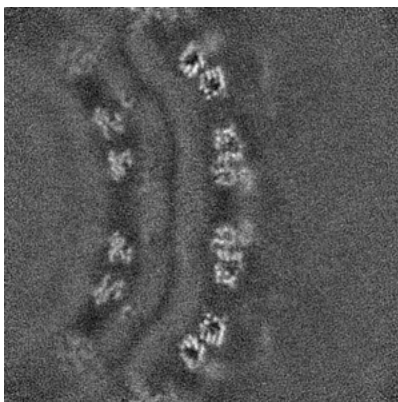


Z Index: 160

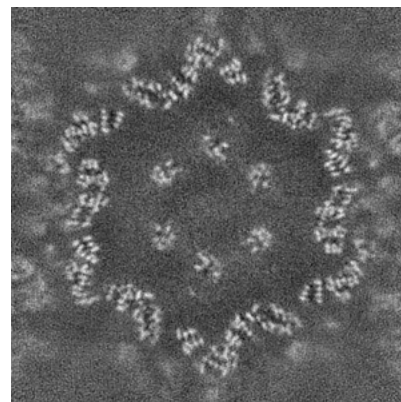
### 6.2.2 Raw map



X Index: 160



Y Index: 160



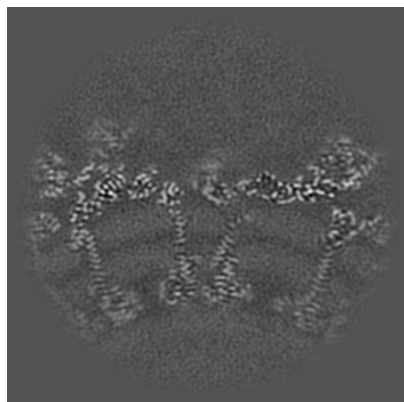
Z Index: 160

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

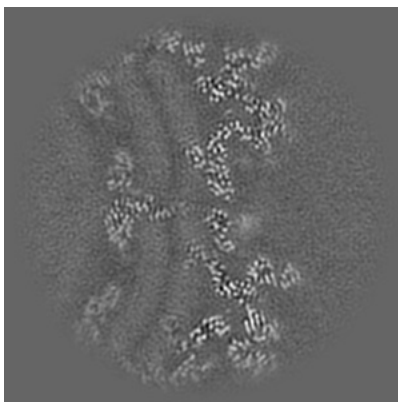


## 6.3 Largest variance slices [i](#)

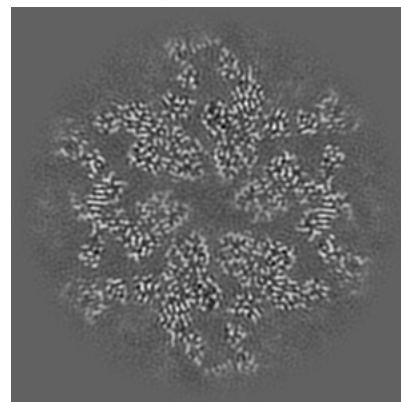
### 6.3.1 Primary map



X Index: 188

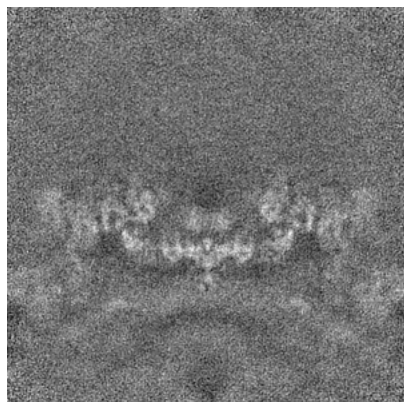


Y Index: 127

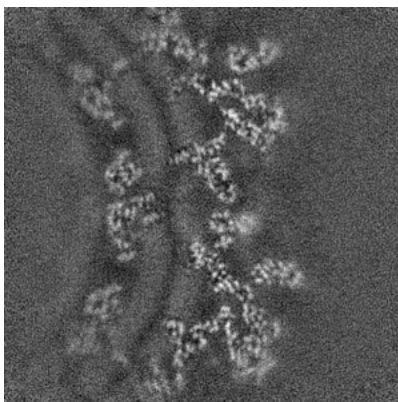


Z Index: 172

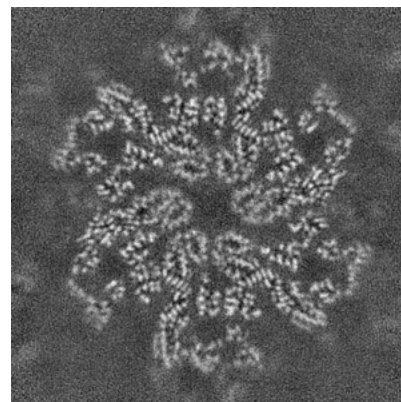
### 6.3.2 Raw map



X Index: 0



Y Index: 131



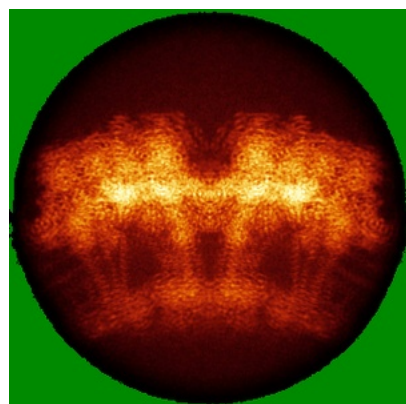
Z Index: 177

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

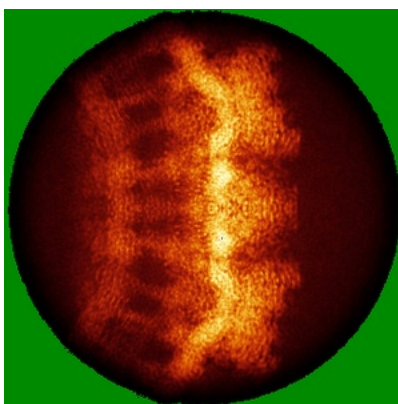


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

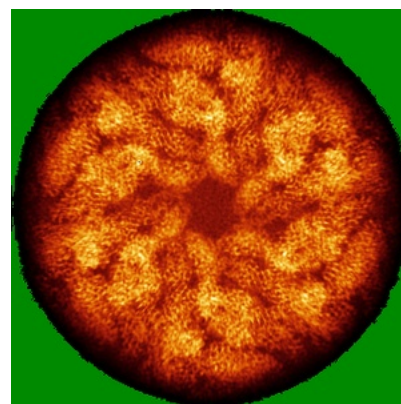
### 6.4.1 Primary map



X

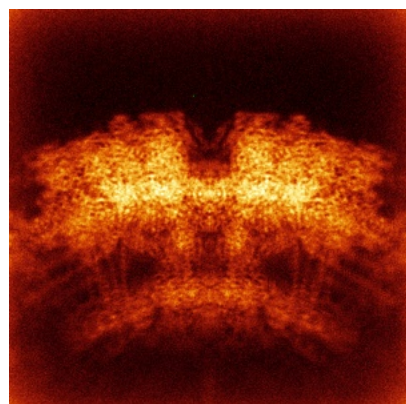


Y

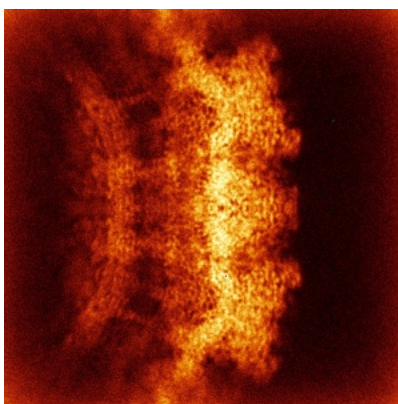


Z

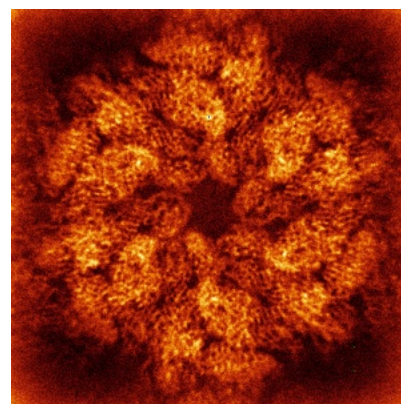
### 6.4.2 Raw map



X



Y

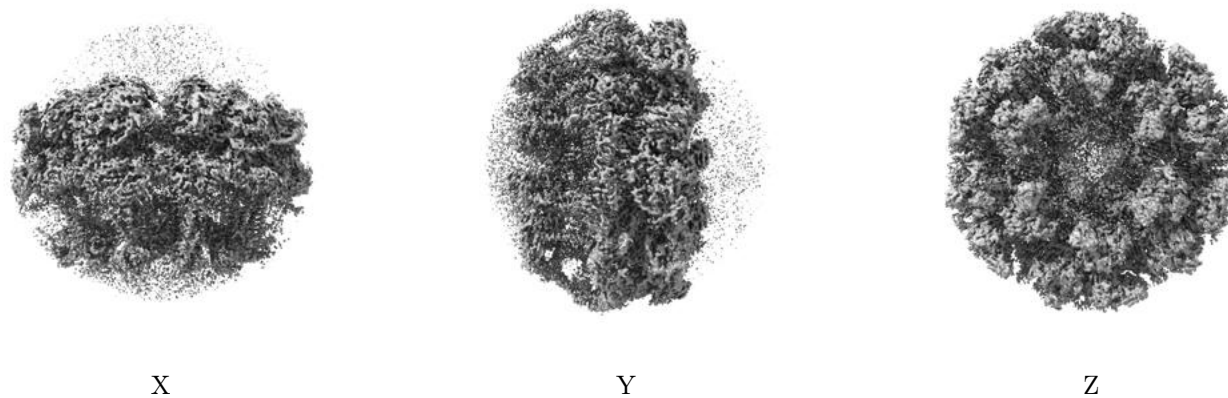


Z

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

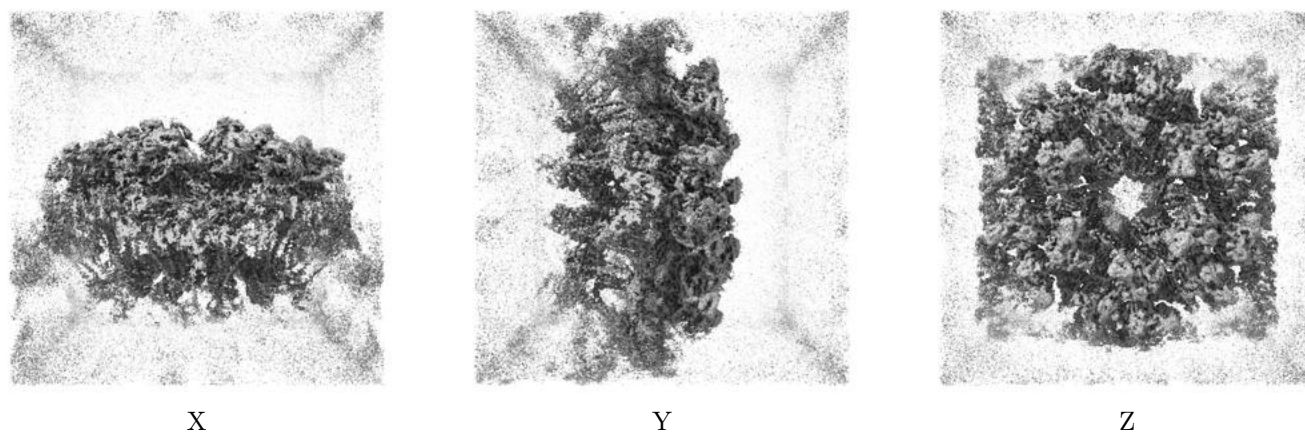
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

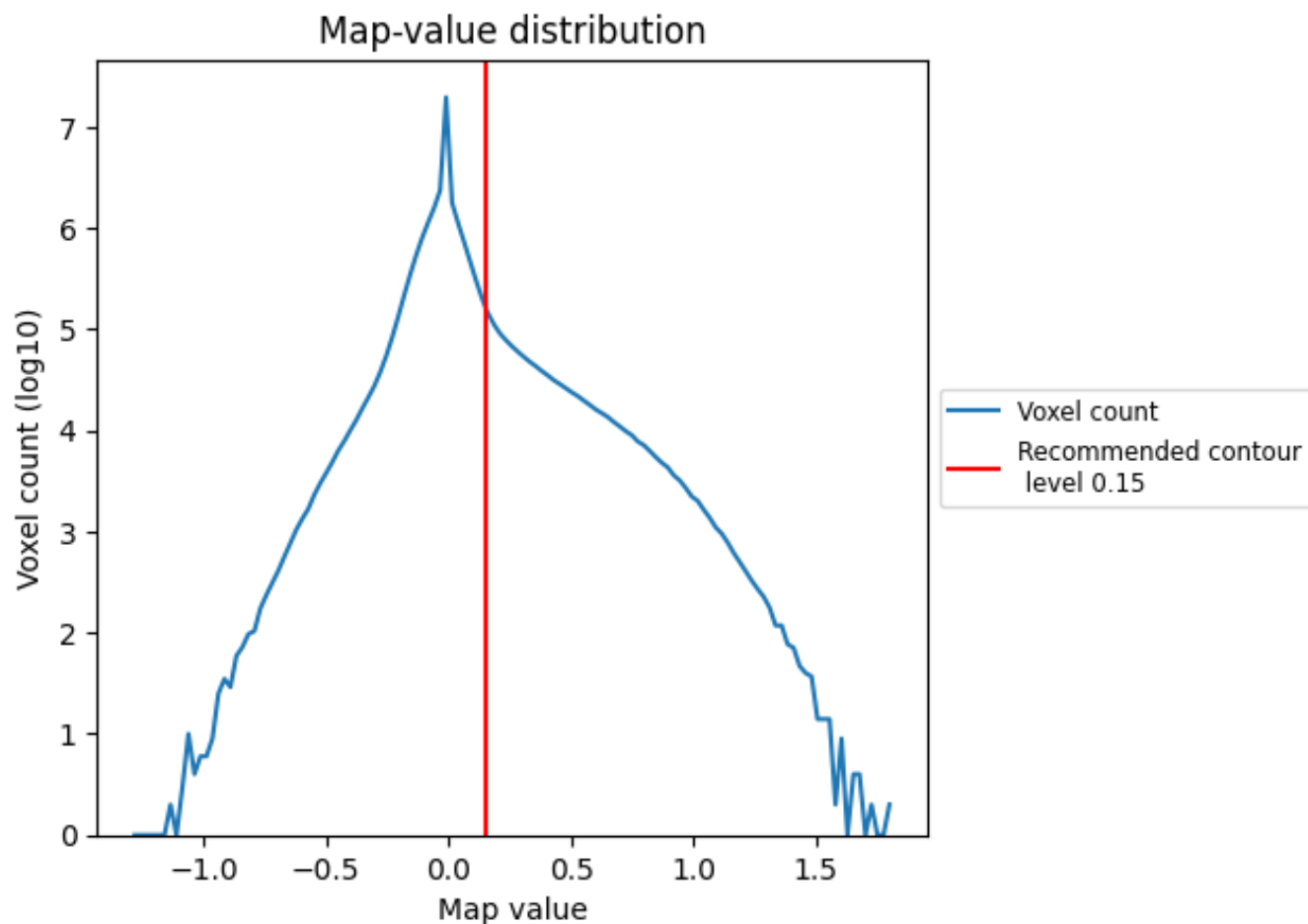
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

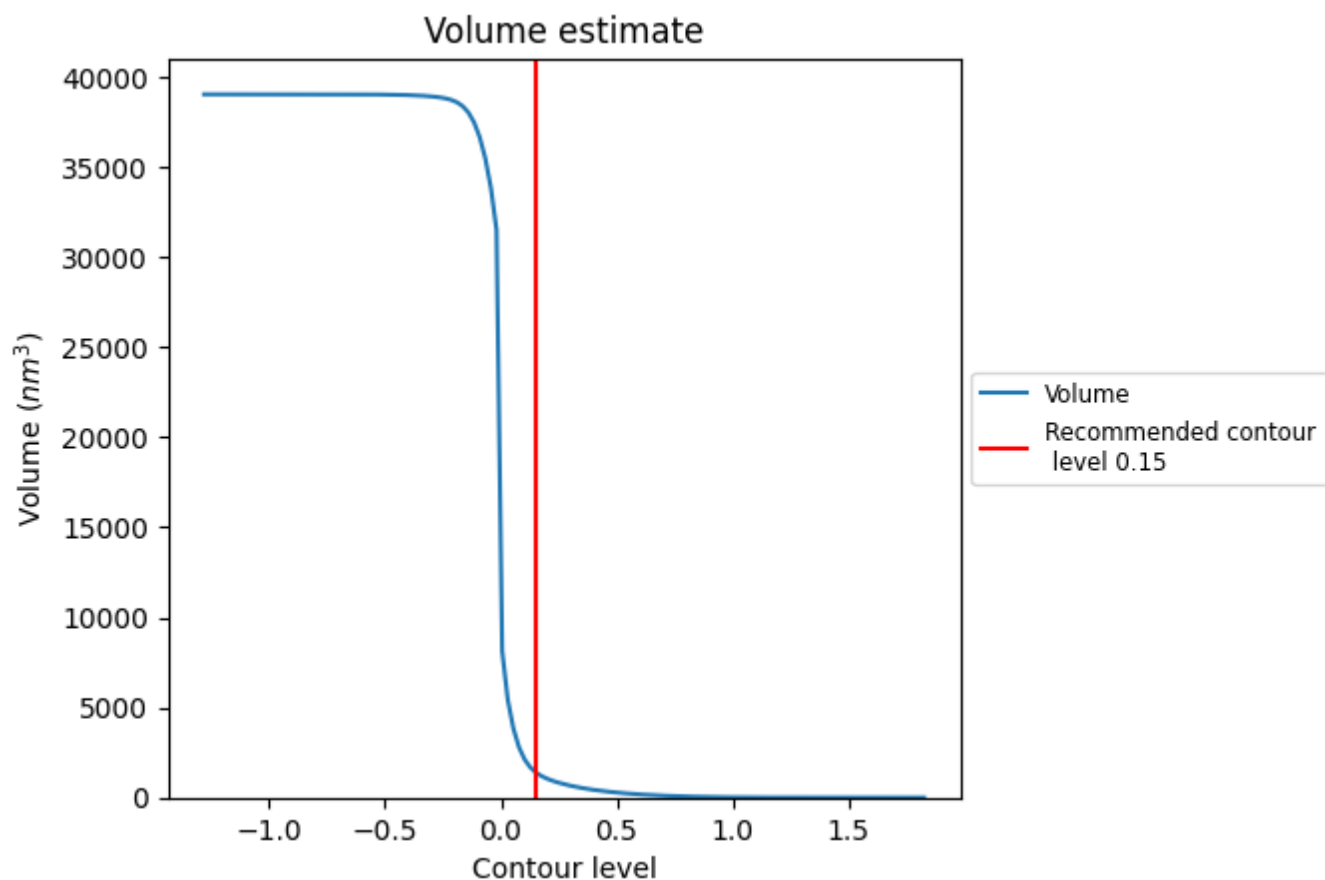
This section contains the results of statistical analysis of the map.

### 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.

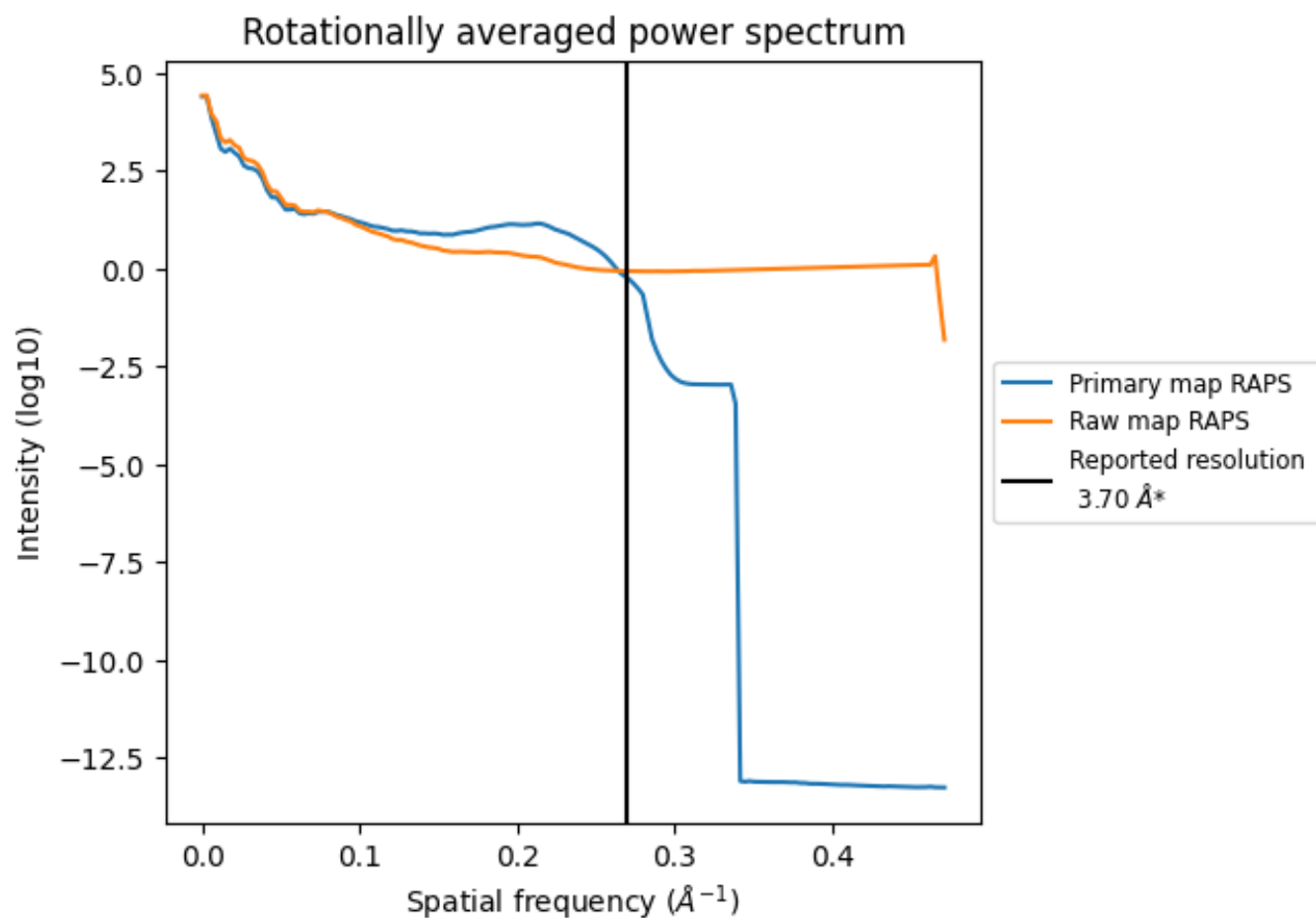
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1404  $\text{nm}^3$ ; this corresponds to an approximate mass of 1268 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 ⓘ

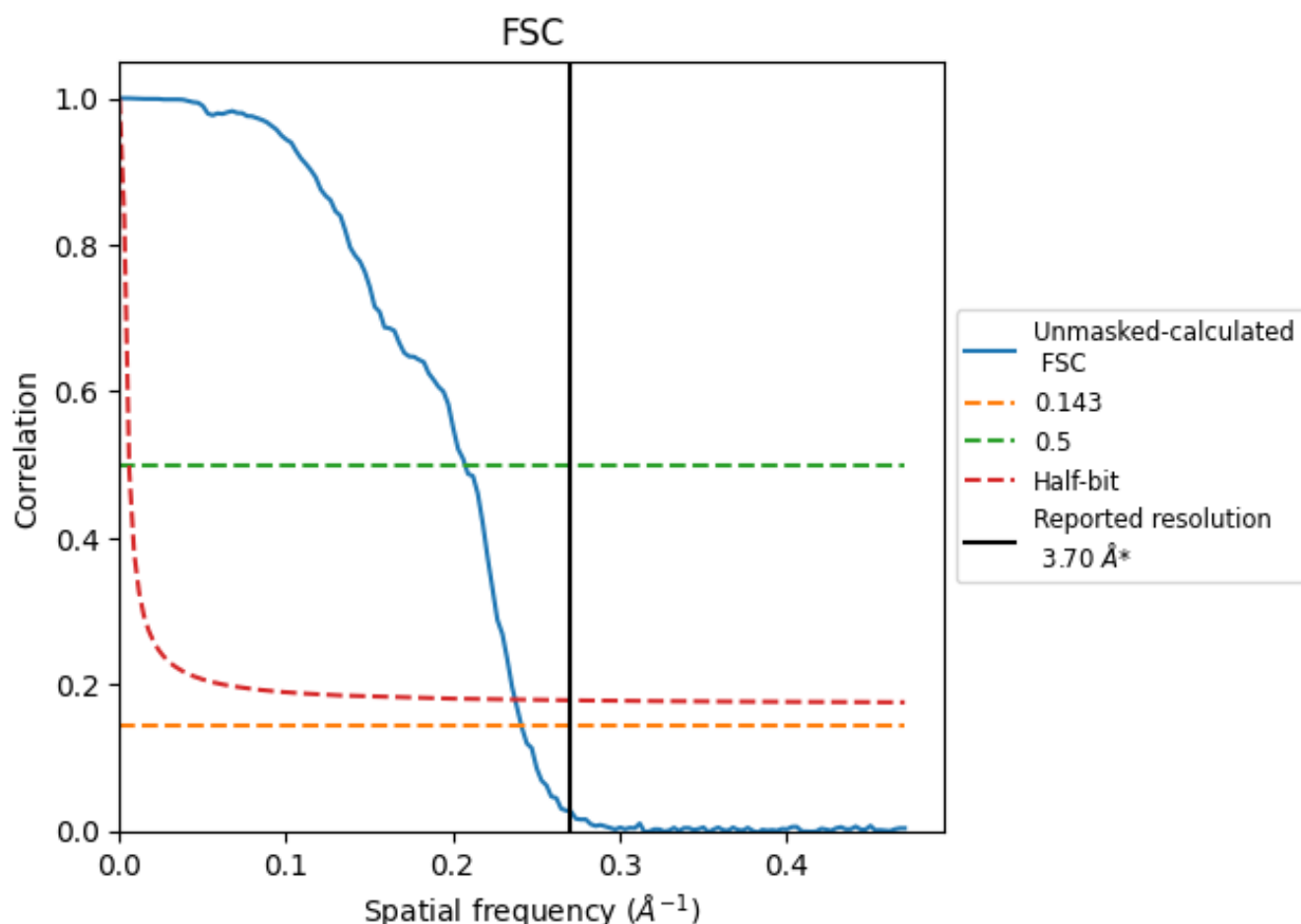


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	4.82	4.21

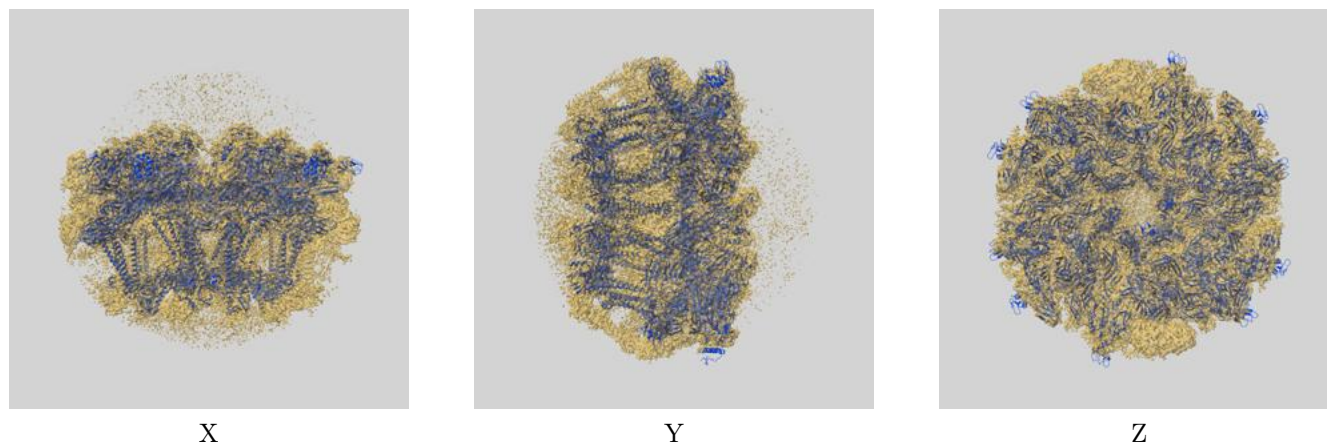
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.7 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39620 and PDB model 8YW2. Per-residue inclusion information can be found in section [3](#) on page [15](#).

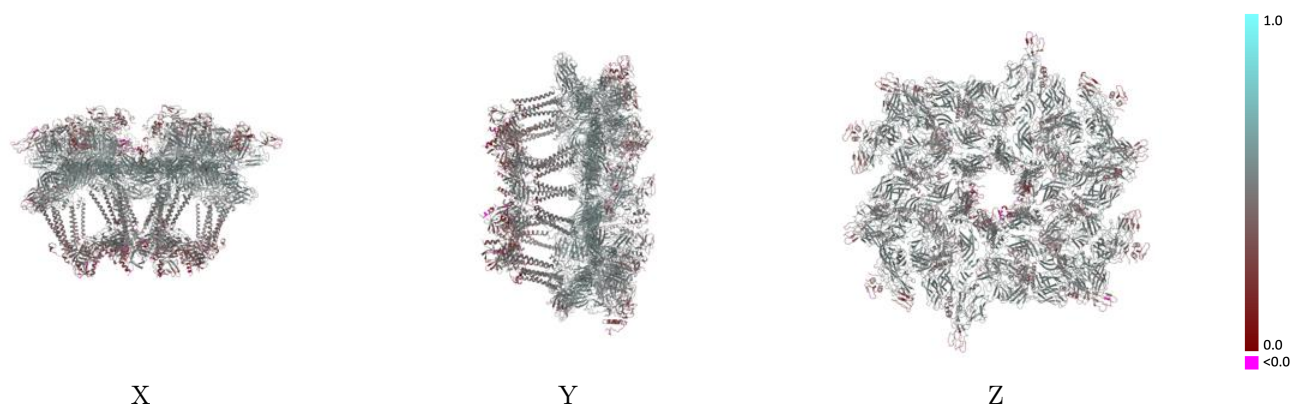
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

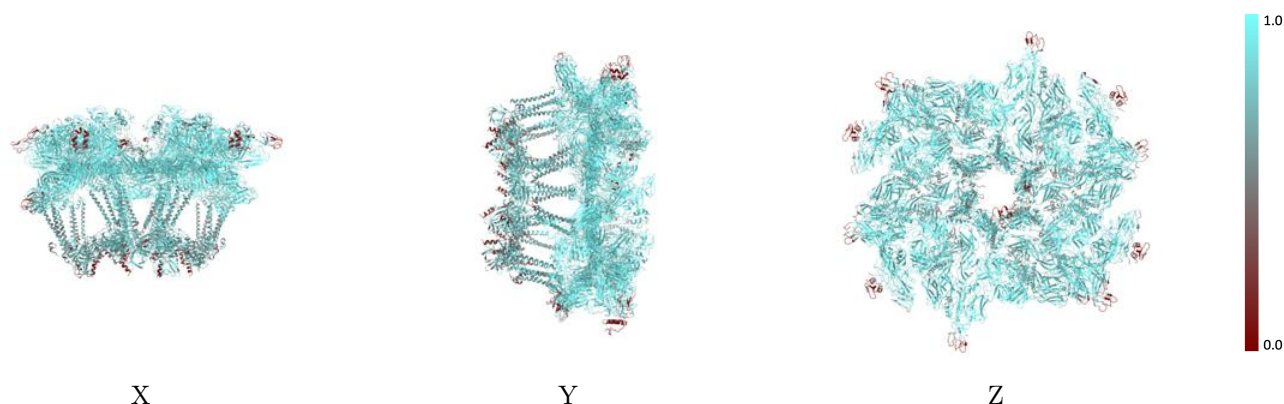


## 9.2 Q-score mapped to coordinate model [i](#)



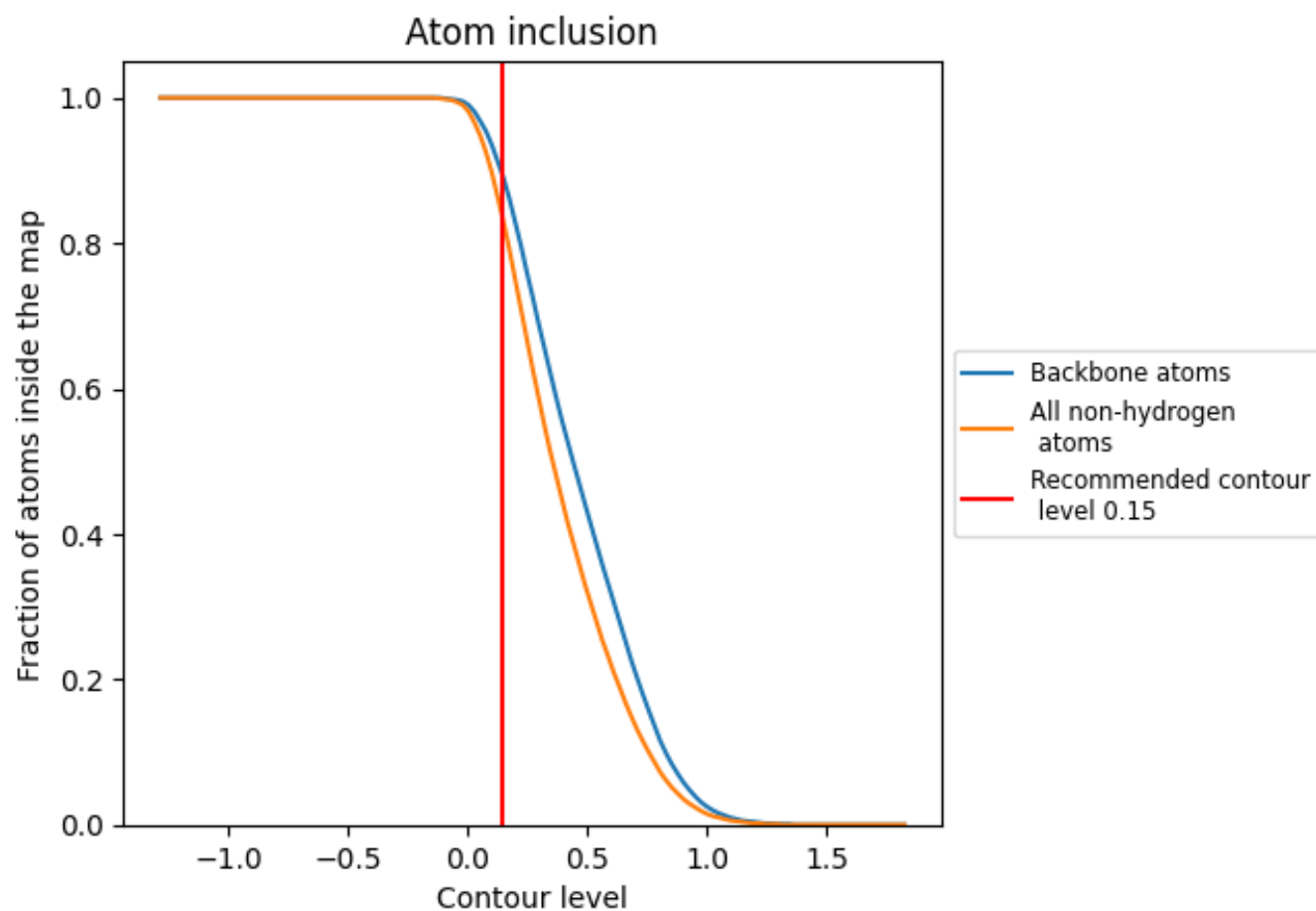
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.4670
0	 0.8230	 0.4150
1	 0.7890	 0.4550
2	 0.7320	 0.4030
3	 0.7460	 0.4480
4	 0.9230	 0.5120
5	 0.8010	 0.4780
6	 0.9100	 0.5070
7	 0.8960	 0.4780
8	 0.8530	 0.4600
9	 0.8950	 0.4760
A	 0.4770	 0.1720
AA	 0.1290	 0.2760
AB	 0.7950	 0.4150
AC	 0.7150	 0.4170
AD	 0.5910	 0.3640
AE	 0.5920	 0.3640
B	 0.8450	 0.4710
BA	 0.6150	 0.3090
C	 0.6920	 0.3730
CA	 0.7950	 0.4230
D	 0.7710	 0.4400
DA	 0.8460	 0.4480
E	 0.9060	 0.5060
EA	 0.6670	 0.3430
F	 0.9210	 0.5130
FA	 0.6920	 0.3490
G	 0.8010	 0.4700
GA	 0.8460	 0.3790
H	 0.9040	 0.5080
HA	 0.8970	 0.4570
I	 0.8990	 0.4760
IA	 0.7690	 0.4030
J	 0.8490	 0.4610
JA	 0.5380	 0.4160













































































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Chain	Atom inclusion	Q-score
K	 0.8860	 0.4770
KA	 0.6670	 0.4200
L	 0.7670	 0.3680
LA	 0.6150	 0.3970
M	 0.1390	 0.2730
MA	 0.5900	 0.3100
N	 0.7340	 0.3580
NA	 0.6410	 0.3380
O	 0.6900	 0.4170
OA	 0.8720	 0.4030
P	 0.6010	 0.3680
PA	 0.9230	 0.4480
Q	 0.6450	 0.3750
QA	 0.6920	 0.3350
R	 0.8920	 0.4800
RA	 0.5900	 0.3420
S	 0.7520	 0.4070
SA	 0.8210	 0.3880
T	 0.6310	 0.3800
TA	 0.8210	 0.4420
U	 0.8520	 0.4970
UA	 0.7690	 0.4020
V	 0.9140	 0.5050
VA	 0.8720	 0.4850
W	 0.9220	 0.5140
WA	 0.6670	 0.3890
X	 0.8620	 0.4650
XA	 0.5380	 0.2470
Y	 0.8590	 0.4770
YA	 0.7180	 0.3670
Z	 0.8290	 0.4660
ZA	 0.7690	 0.3530
a	 0.1440	 0.2800
aA	 0.7180	 0.4010
b	 0.7470	 0.4070
bA	 0.6920	 0.3460
c	 0.7670	 0.4080
cA	 0.6670	 0.3310
d	 0.6680	 0.4020
dA	 0.8720	 0.4580
e	 0.7360	 0.4370
eA	 0.3850	 0.4240

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Chain	Atom inclusion	Q-score
f	 0.7620	 0.4460
fA	 0.7180	 0.4060
g	 0.7870	 0.4150
gA	 0.5900	 0.3420
h	 0.9150	 0.5140
hA	 0.8210	 0.4180
i	 0.9030	 0.5080
iA	 1.0000	 0.4840
j	 0.8920	 0.4780
jA	 0.7690	 0.4140
k	 0.5900	 0.2680
kA	 0.7180	 0.4020
l	 0.7670	 0.4030
lA	 0.6150	 0.2790
m	 0.9140	 0.5140
mA	 0.6150	 0.3140
n	 0.6400	 0.3570
nA	 0.8460	 0.4450
o	 0.8580	 0.4990
oA	 0.8460	 0.4500
p	 0.9040	 0.5020
pA	 0.7440	 0.3710
q	 0.9230	 0.5190
qA	 0.6410	 0.4120
r	 0.8700	 0.4750
rA	 0.7950	 0.4140
s	 0.8590	 0.4770
sA	 0.4100	 0.4420
t	 0.8340	 0.4700
tA	 0.8460	 0.3930
u	 0.1420	 0.2710
uA	 0.5380	 0.4020
v	 0.7420	 0.3710
w	 0.7170	 0.3870
x	 0.6770	 0.4070
y	 0.7540	 0.4430
z	 0.8460	 0.4770