



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 03:26 PM UTC

PDB ID : 9NBG / pdb_00009nbg
EMDB ID : EMD-49228
Title : H-1 Parvovirus VLP - Glycan [s(Lex)2]
Authors : Busuttil, K.B.; Bennett, A.B.; McKenna, R.
Deposited on : 2025-02-13
Resolution : 2.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

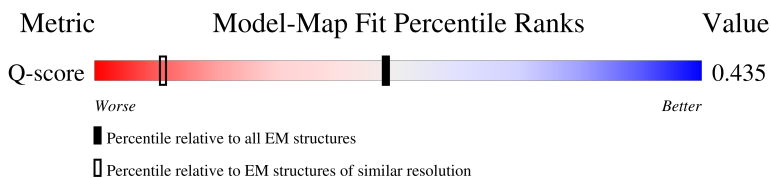
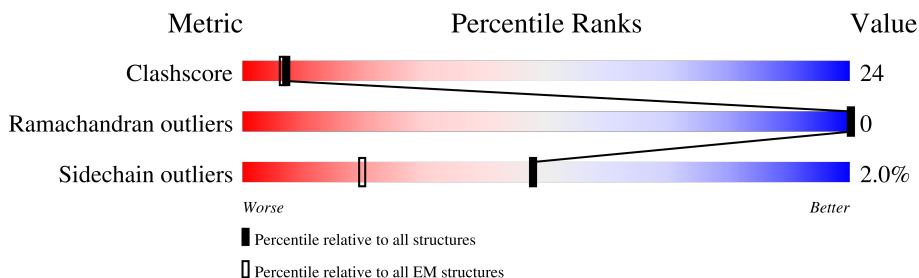
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.57 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7615 (2.07 - 3.07)

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

Mol	Chain	Length	Quality of chain
1	1	559	
1	2	559	
1	3	559	
1	4	559	

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Mol	Chain	Length	Quality of chain
1	5	559	 65% 34% .
1	6	559	 65% 34% .
1	7	559	 65% 34% .
1	8	559	 66% 32% .
1	A	559	 65% 33% .
1	B	559	 65% 33% .
1	C	559	 65% 34% .
1	D	559	 65% 34% .
1	E	559	 65% 33% .
1	F	559	 65% 34% .
1	G	559	 65% 33% .
1	H	559	 65% 34% .
1	I	559	 64% 34% .
1	J	559	 65% 34% .
1	K	559	 65% 33% .
1	L	559	 65% 34% .
1	M	559	 65% 34% .
1	N	559	 65% 34% .
1	O	559	 65% 33% .
1	P	559	 65% 34% .
1	Q	559	 64% 34% .
1	R	559	 64% 35% .
1	S	559	 65% 34% .
1	T	559	 65% 33% .
1	U	559	 65% 33% .

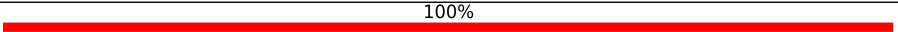
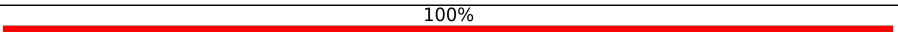
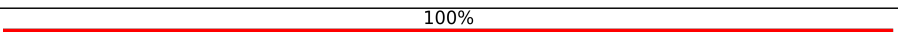
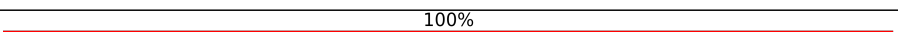
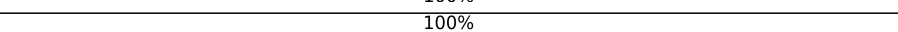
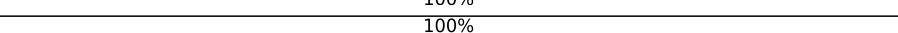
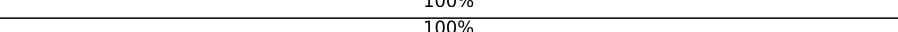
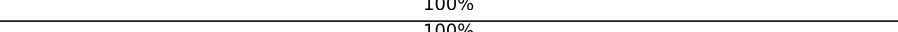
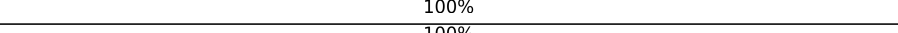
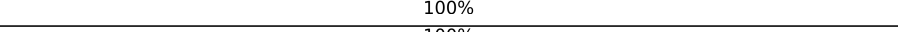
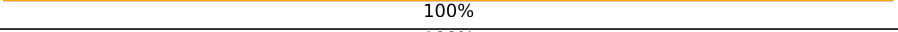
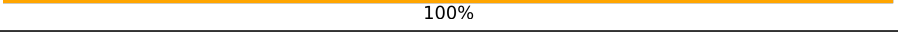
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Mol	Chain	Length	Quality of chain
1	V	559	 65% 33% .
1	W	559	 65% 34% .
1	X	559	 65% 34% .
1	Y	559	 65% 33% .
1	Z	559	 65% 33% .
1	a	559	 65% 33% .
1	b	559	 65% 33% .
1	c	559	 65% 34% .
1	d	559	 65% 33% .
1	e	559	 65% 34% .
1	f	559	 65% 33% .
1	g	559	 65% 34% .
1	h	559	 65% 33% .
1	i	559	 65% 33% .
1	j	559	 65% 34% .
1	k	559	 65% 34% .
1	l	559	 65% 34% .
1	m	559	 65% 33% .
1	n	559	 65% 33% .
1	o	559	 65% 33% .
1	p	559	 65% 34% .
1	q	559	 64% 35% .
1	r	559	 65% 34% .
1	s	559	 65% 34% .
1	t	559	 65% 33% .

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Mol	Chain	Length	Quality of chain
1	u	559	 65% 34% .
1	v	559	 65% 33% .
1	w	559	 65% 34% .
1	x	559	 64% 34% .
1	y	559	 65% 33% .
1	z	559	 65% 34% .
2	1A	3	 100%
2	2A	3	 100%
2	4A	3	 100%
2	5A	3	 100%
2	7A	3	 100%
2	8A	3	 100%
2	9	3	 100%
2	AA	3	 100%
2	AB	3	 100%
2	BB	3	 100%
2	CA	3	 100%
2	DA	3	 100%
2	DB	3	 100%
2	EB	3	 100%
2	FA	3	 100%
2	GA	3	 100%
2	GB	3	 100%
2	HB	3	 100%
2	IA	3	 100%

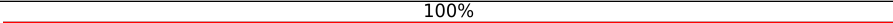
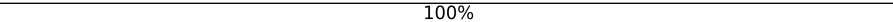
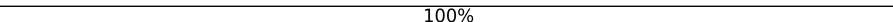
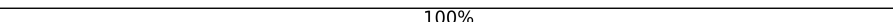
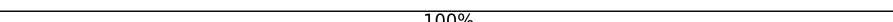
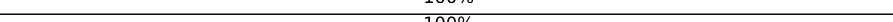
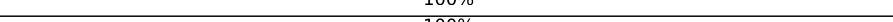
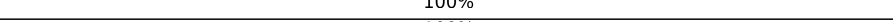
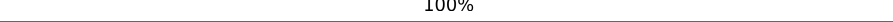
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Mol	Chain	Length	Quality of chain
2	JA	3	100%
2	JB	3	100%
2	KB	3	100%
2	LA	3	100%
2	MA	3	100%
2	MB	3	100%
2	NB	3	100%
2	OA	3	100%
2	PA	3	100%
2	PB	3	100%
2	QB	3	100%
2	RA	3	100%
2	SA	3	100%
2	SB	3	100%
2	TB	3	100%
2	UA	3	100%
2	VA	3	100%
2	VB	3	100%
2	WB	3	100%
2	XA	3	100%
2	YA	3	100%
2	YB	3	100%
2	ZB	3	100%
2	aA	3	100%
2	bA	3	100%

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Mol	Chain	Length	Quality of chain
2	dA	3	100% 
2	eA	3	100% 
2	gA	3	100% 
2	hA	3	100% 
2	jA	3	100% 
2	kA	3	100% 
2	mA	3	100% 
2	nA	3	100% 
2	pA	3	100% 
2	qA	3	100% 
2	sA	3	100% 
2	tA	3	100% 
2	vA	3	100% 
2	wA	3	100% 
2	yA	3	100% 
2	zA	3	100% 

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 267000 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	B	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	C	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	D	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	E	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	F	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	G	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	H	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	I	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	J	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	K	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	L	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	M	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	N	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	O	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	P	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	Q	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	S	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	T	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	U	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	V	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	W	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	X	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	Y	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	Z	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	a	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	b	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	c	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	d	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	e	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	f	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	g	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	h	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	i	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	j	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	k	559	Total 4404	C 2784	N 761	O 842	S 17	0	0
1	l	559	Total 4404	C 2784	N 761	O 842	S 17	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	n	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	o	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	p	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	q	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	r	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	s	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	t	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	u	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	v	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	w	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	x	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	y	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	z	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	1	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	2	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	3	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	4	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	5	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	6	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		
1	7	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	559	Total	C	N	O	S	0	0
			4404	2784	761	842	17		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	9	3	Total	C	N	O	0	0
			46	25	2	19		
2	AA	3	Total	C	N	O	0	0
			46	25	2	19		
2	CA	3	Total	C	N	O	0	0
			46	25	2	19		
2	DA	3	Total	C	N	O	0	0
			46	25	2	19		
2	FA	3	Total	C	N	O	0	0
			46	25	2	19		
2	GA	3	Total	C	N	O	0	0
			46	25	2	19		
2	IA	3	Total	C	N	O	0	0
			46	25	2	19		
2	JA	3	Total	C	N	O	0	0
			46	25	2	19		
2	LA	3	Total	C	N	O	0	0
			46	25	2	19		
2	MA	3	Total	C	N	O	0	0
			46	25	2	19		
2	OA	3	Total	C	N	O	0	0
			46	25	2	19		
2	PA	3	Total	C	N	O	0	0
			46	25	2	19		
2	RA	3	Total	C	N	O	0	0
			46	25	2	19		
2	SA	3	Total	C	N	O	0	0
			46	25	2	19		
2	UA	3	Total	C	N	O	0	0
			46	25	2	19		
2	VA	3	Total	C	N	O	0	0
			46	25	2	19		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	XA	3	Total 46	C 25	N 2	O 19	0	0
2	YA	3	Total 46	C 25	N 2	O 19	0	0
2	aA	3	Total 46	C 25	N 2	O 19	0	0
2	bA	3	Total 46	C 25	N 2	O 19	0	0
2	dA	3	Total 46	C 25	N 2	O 19	0	0
2	eA	3	Total 46	C 25	N 2	O 19	0	0
2	gA	3	Total 46	C 25	N 2	O 19	0	0
2	hA	3	Total 46	C 25	N 2	O 19	0	0
2	jA	3	Total 46	C 25	N 2	O 19	0	0
2	kA	3	Total 46	C 25	N 2	O 19	0	0
2	mA	3	Total 46	C 25	N 2	O 19	0	0
2	nA	3	Total 46	C 25	N 2	O 19	0	0
2	pA	3	Total 46	C 25	N 2	O 19	0	0
2	qA	3	Total 46	C 25	N 2	O 19	0	0
2	sA	3	Total 46	C 25	N 2	O 19	0	0
2	tA	3	Total 46	C 25	N 2	O 19	0	0
2	vA	3	Total 46	C 25	N 2	O 19	0	0
2	wA	3	Total 46	C 25	N 2	O 19	0	0
2	yA	3	Total 46	C 25	N 2	O 19	0	0
2	zA	3	Total 46	C 25	N 2	O 19	0	0
2	1A	3	Total 46	C 25	N 2	O 19	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	2A	3	Total 46	C 25	N 2	O 19	0	0
2	4A	3	Total 46	C 25	N 2	O 19	0	0
2	5A	3	Total 46	C 25	N 2	O 19	0	0
2	7A	3	Total 46	C 25	N 2	O 19	0	0
2	8A	3	Total 46	C 25	N 2	O 19	0	0
2	AB	3	Total 46	C 25	N 2	O 19	0	0
2	BB	3	Total 46	C 25	N 2	O 19	0	0
2	DB	3	Total 46	C 25	N 2	O 19	0	0
2	EB	3	Total 46	C 25	N 2	O 19	0	0
2	GB	3	Total 46	C 25	N 2	O 19	0	0
2	HB	3	Total 46	C 25	N 2	O 19	0	0
2	JB	3	Total 46	C 25	N 2	O 19	0	0
2	KB	3	Total 46	C 25	N 2	O 19	0	0
2	MB	3	Total 46	C 25	N 2	O 19	0	0
2	NB	3	Total 46	C 25	N 2	O 19	0	0
2	PB	3	Total 46	C 25	N 2	O 19	0	0
2	QB	3	Total 46	C 25	N 2	O 19	0	0
2	SB	3	Total 46	C 25	N 2	O 19	0	0
2	TB	3	Total 46	C 25	N 2	O 19	0	0
2	VB	3	Total 46	C 25	N 2	O 19	0	0
2	WB	3	Total 46	C 25	N 2	O 19	0	0

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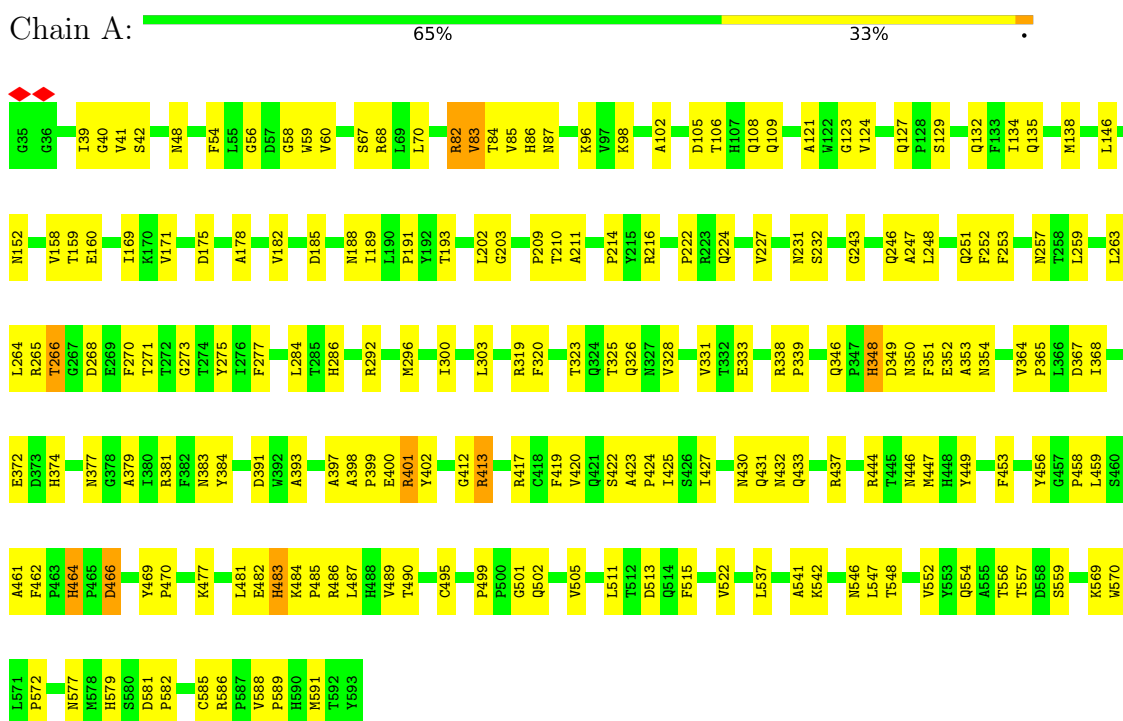
Continued from previous page...

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

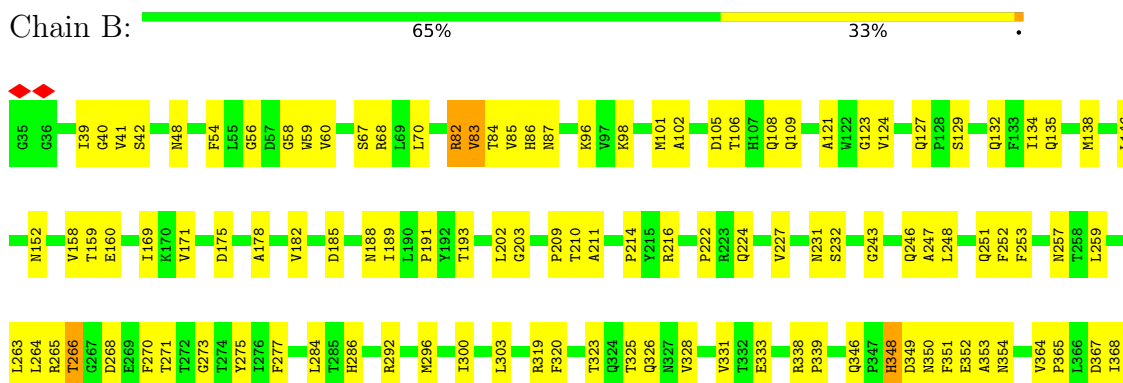
3 Residue-property plots

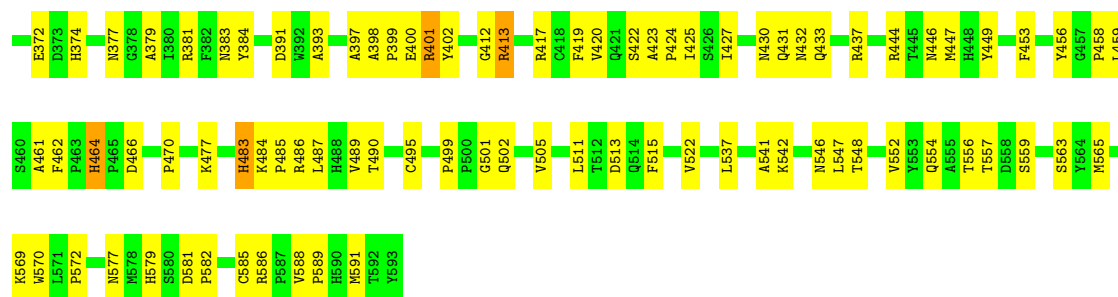
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Major capsid protein



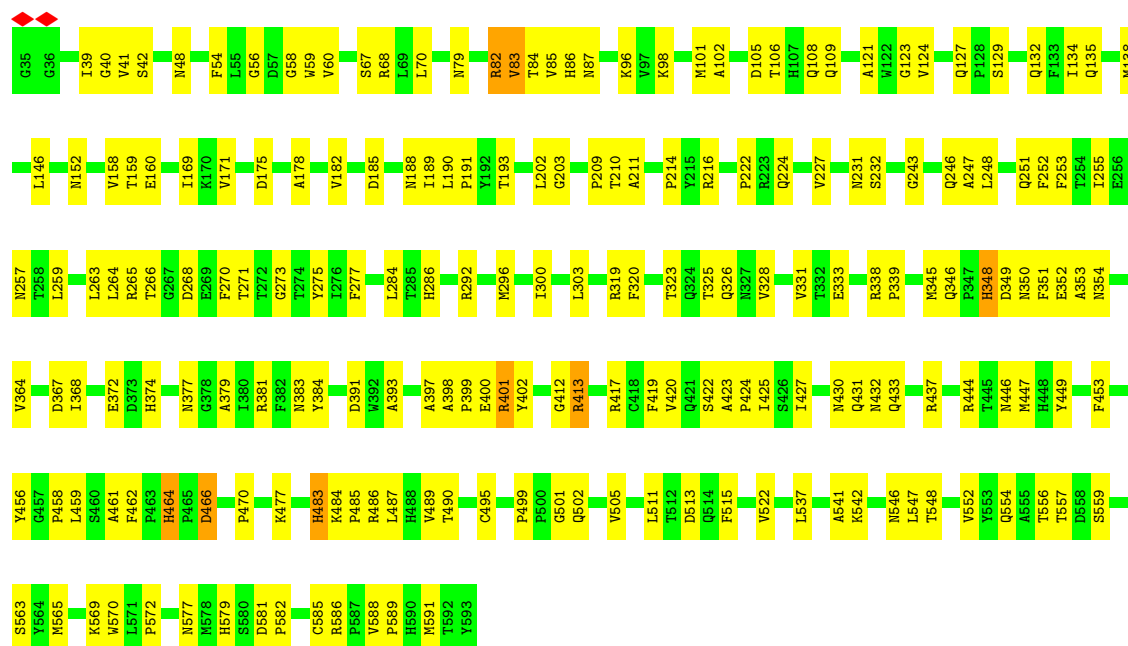
• Molecule 1: Major capsid protein





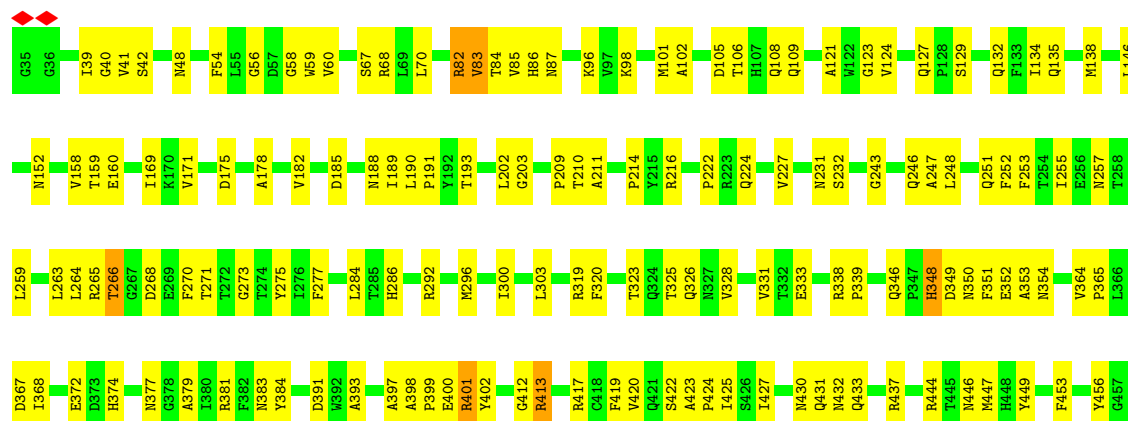
• Molecule 1: Major capsid protein

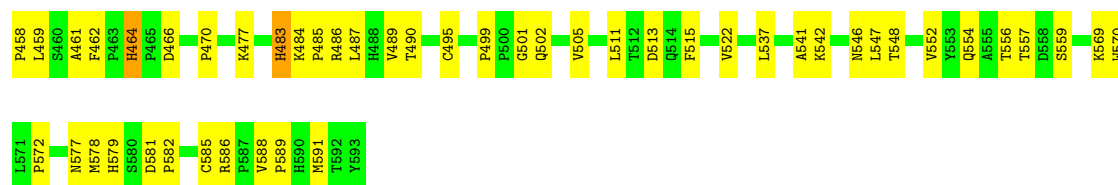
Chain C: 65% 34%



• Molecule 1: Major capsid protein

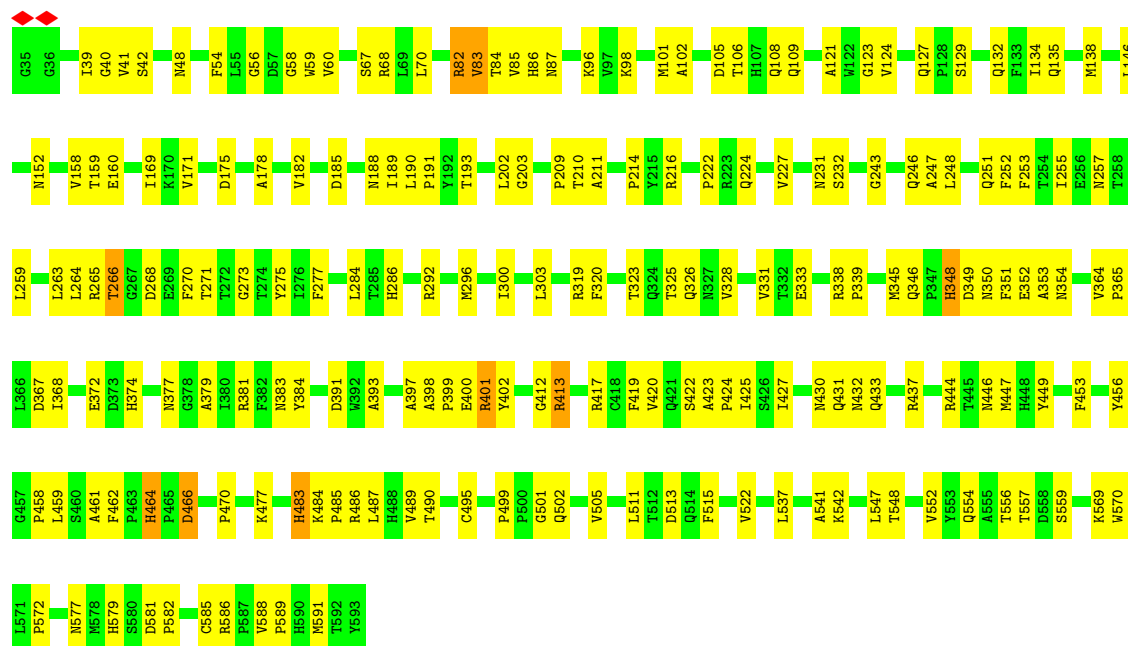
Chain D: 65% 34%





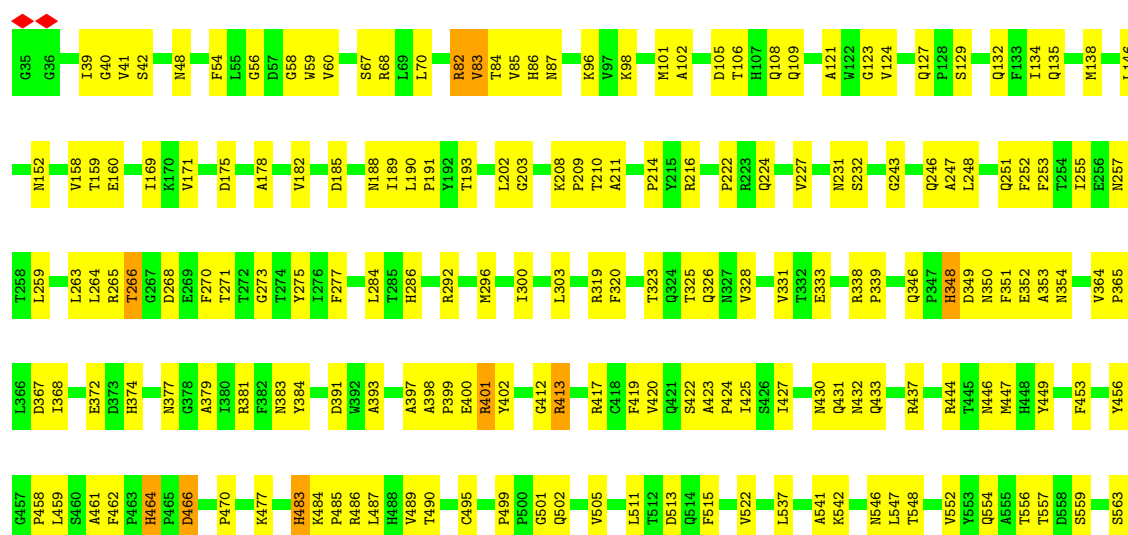
• Molecule 1: Major capsid protein

Chain E: 65% 33% .



• Molecule 1: Major capsid protein

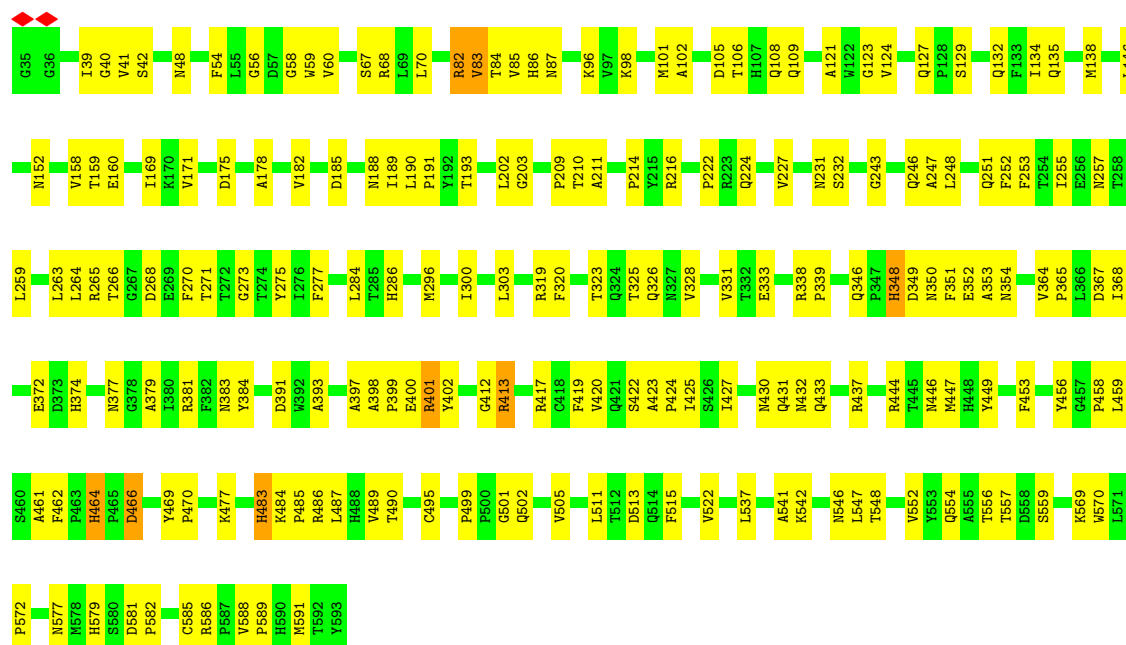
Chain F: 65% 34% .





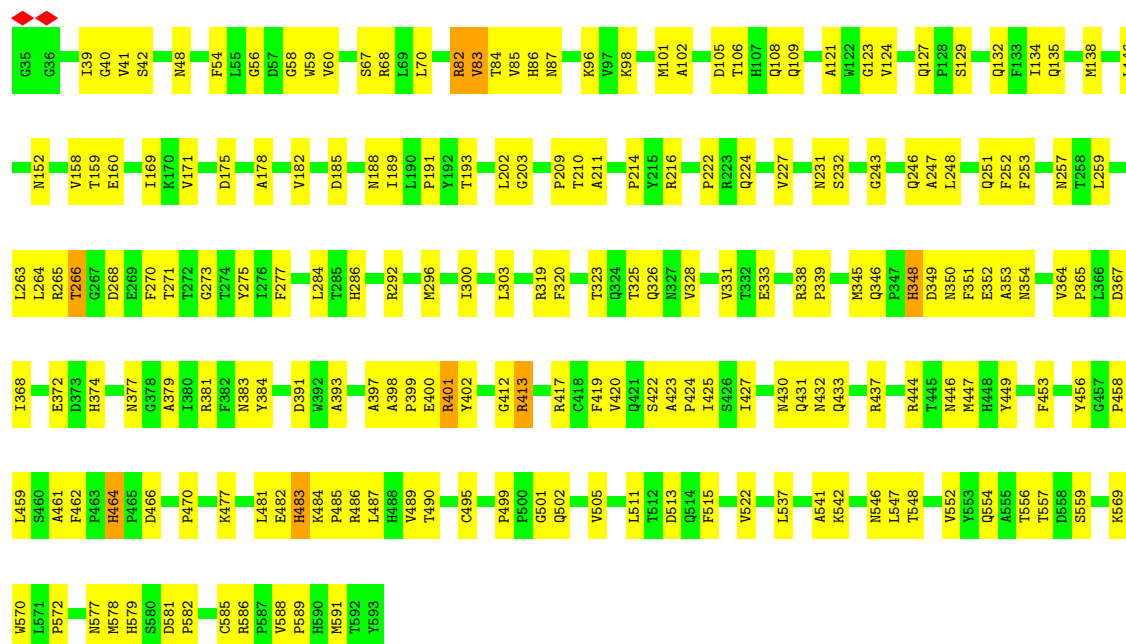
- Molecule 1: Major capsid protein

Chain G: 65% 33%



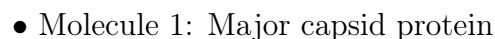
- Molecule 1: Major capsid protein

Chain H: 65% 34%



- Molecule 1: Major capsid protein

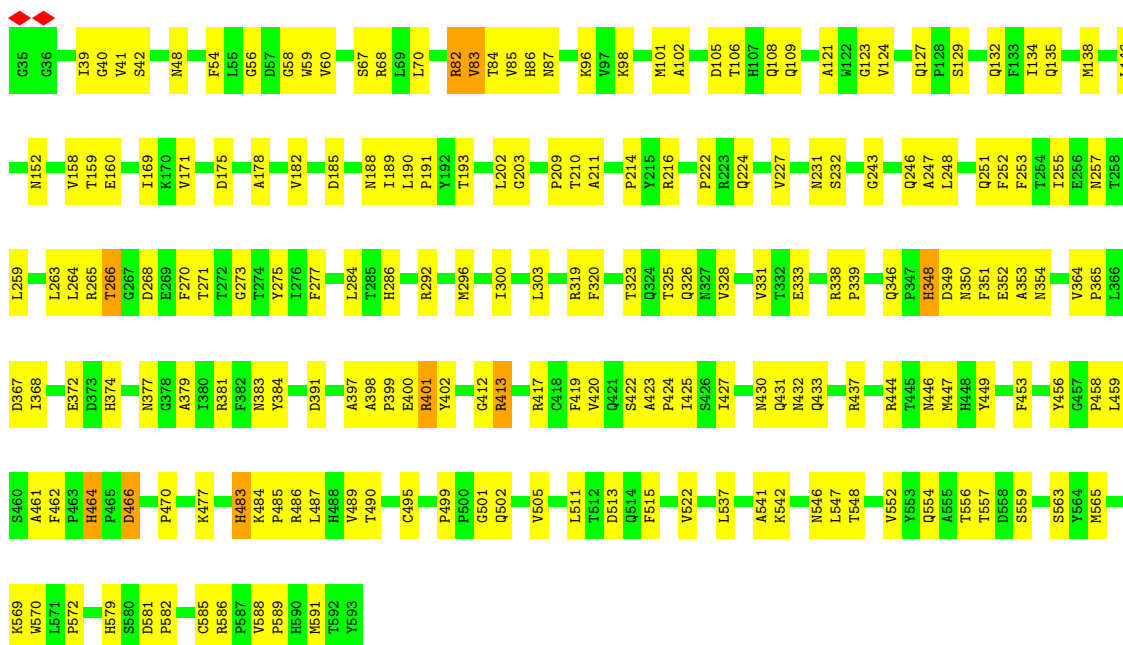
34%



34%

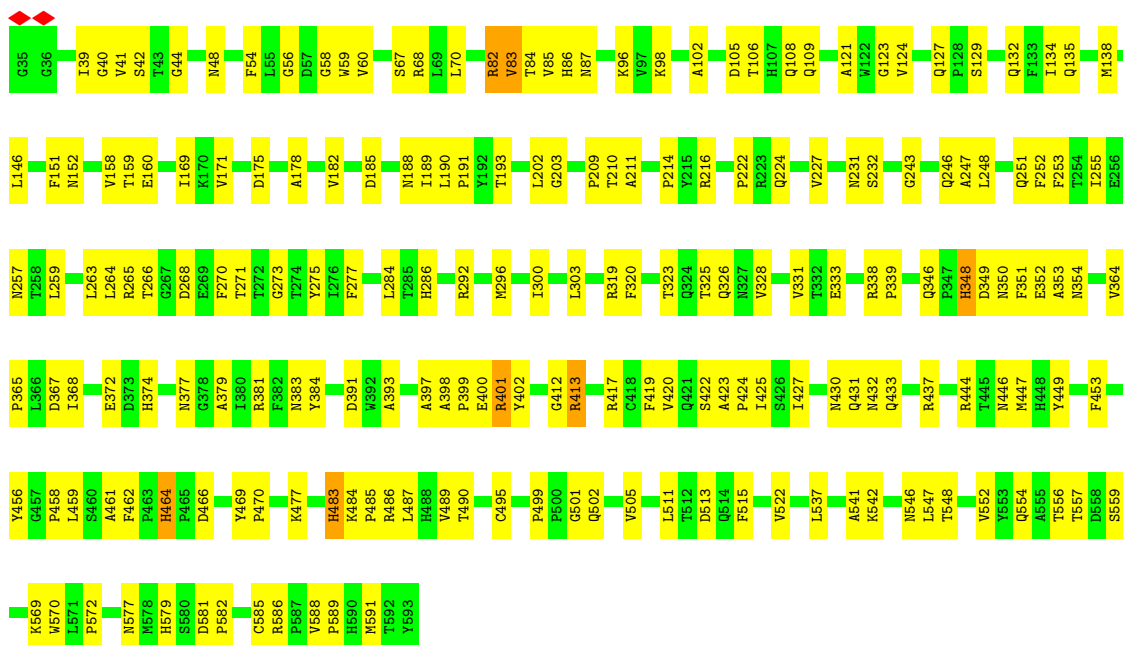


33%



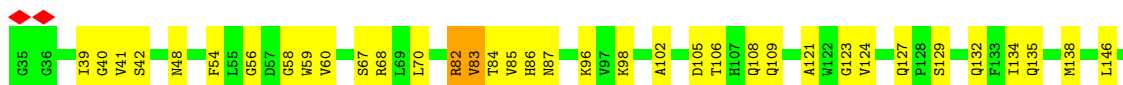
• Molecule 1: Major capsid protein

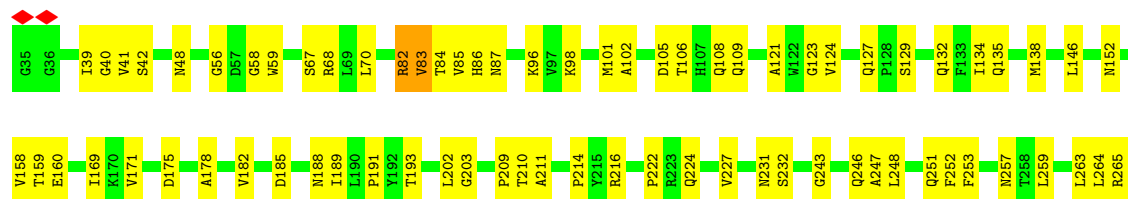
Chain L: 65% 34%

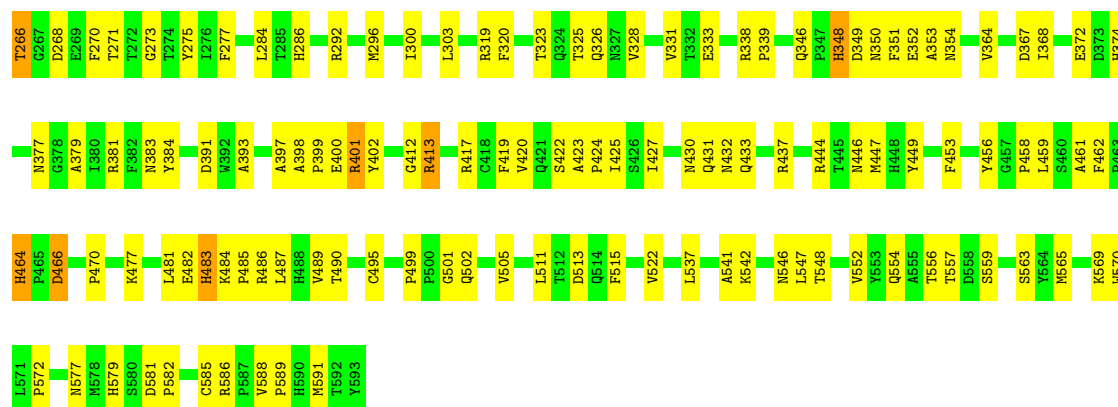


• Molecule 1: Major capsid protein

Chain M: 65% 34%

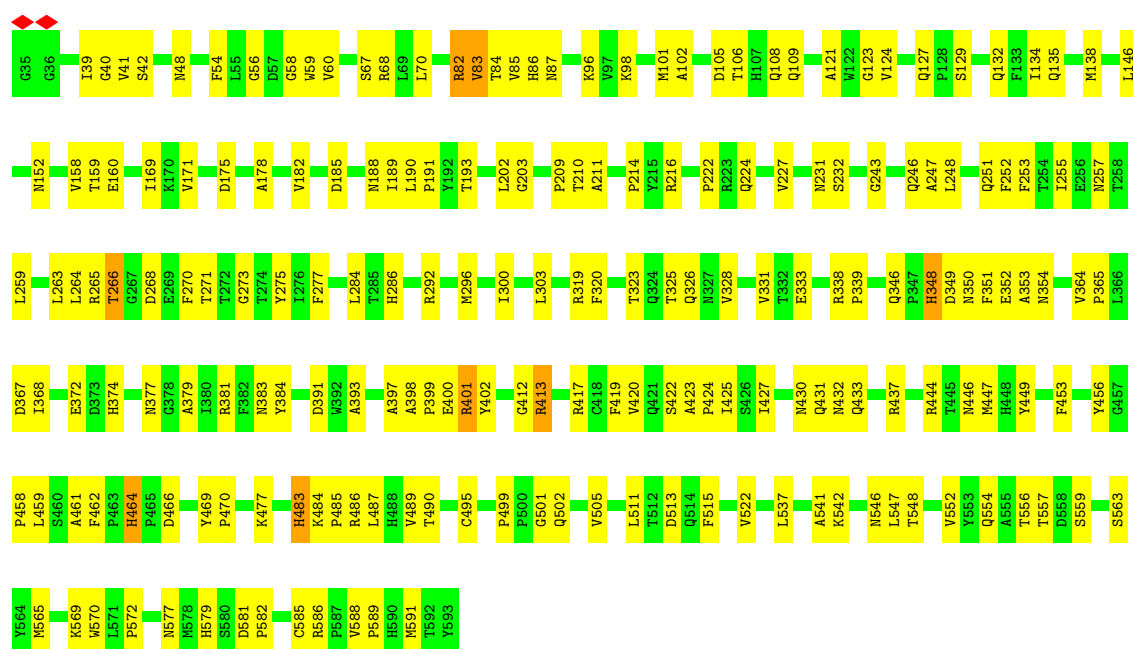






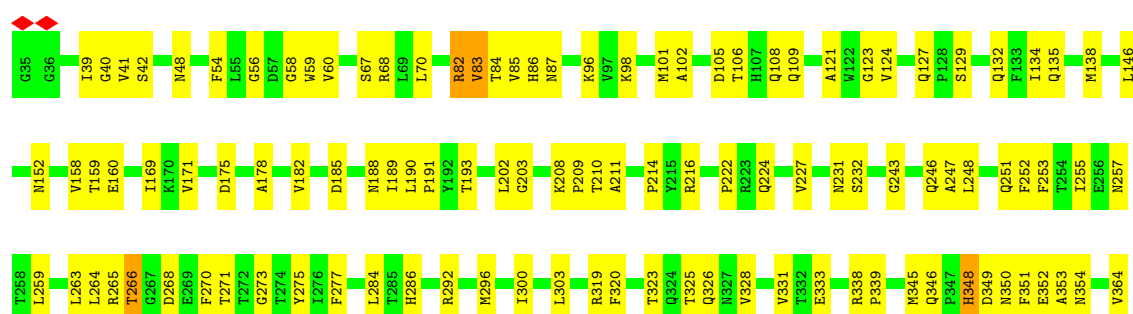
• Molecule 1: Major capsid protein

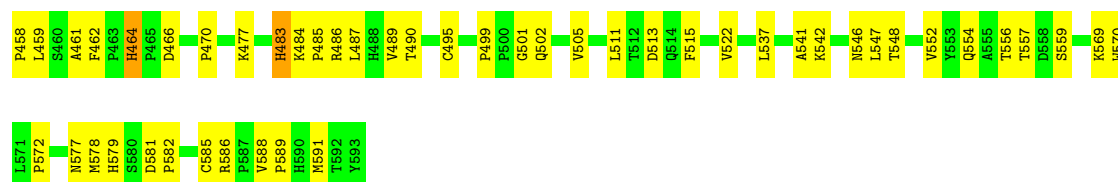
Chain P: 65% 34%



• Molecule 1: Major capsid protein

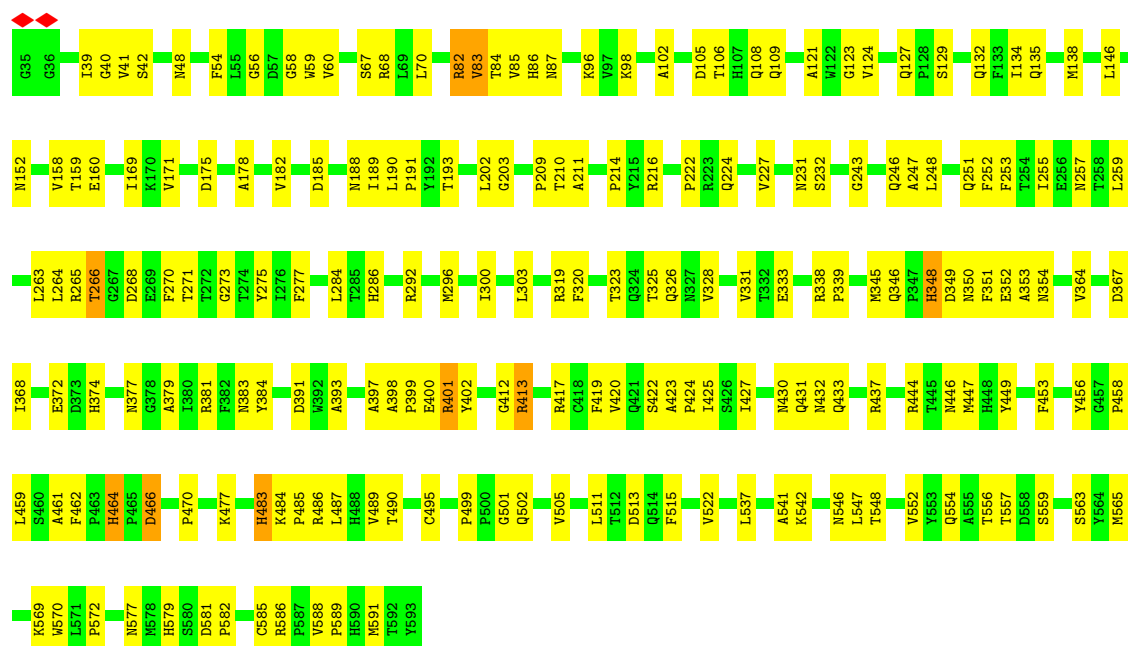
Chain Q: 64% 34%





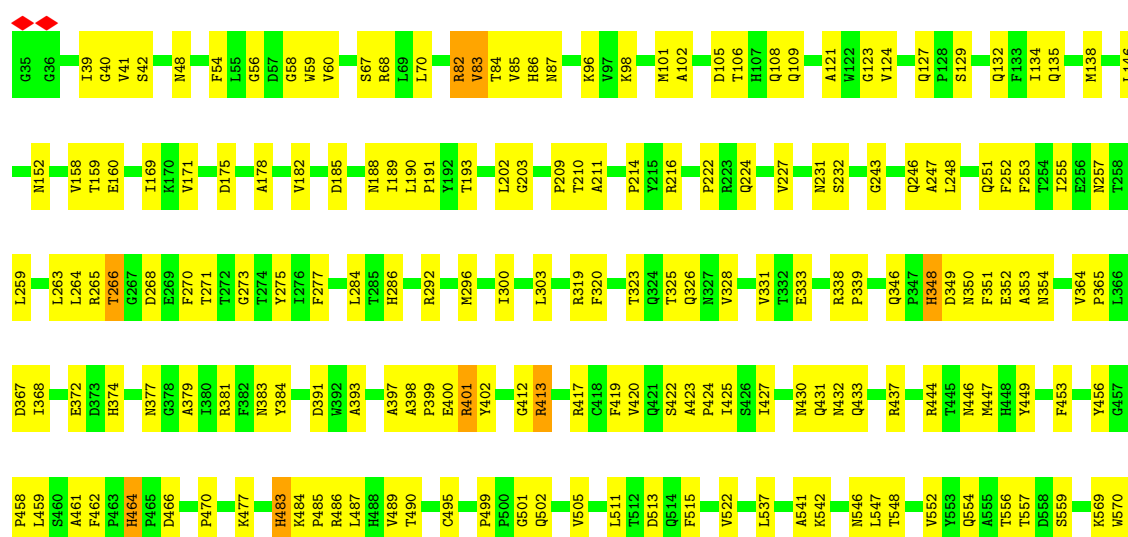
• Molecule 1: Major capsid protein

Chain T: 65% 33%



• Molecule 1: Major capsid protein

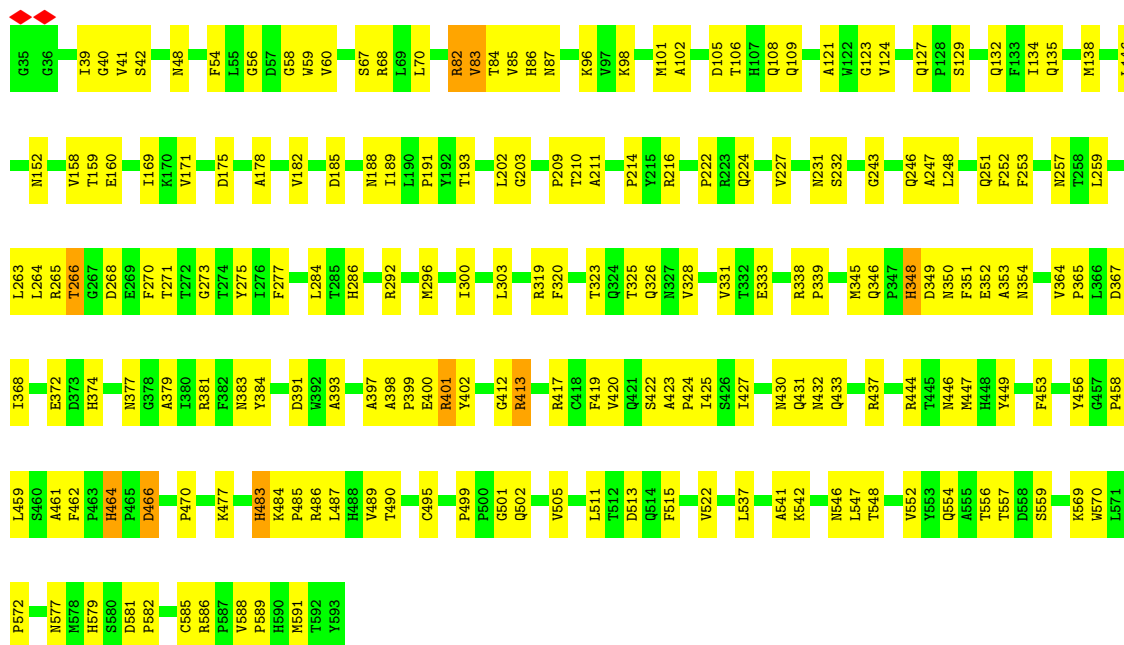
Chain U: 65% 33%





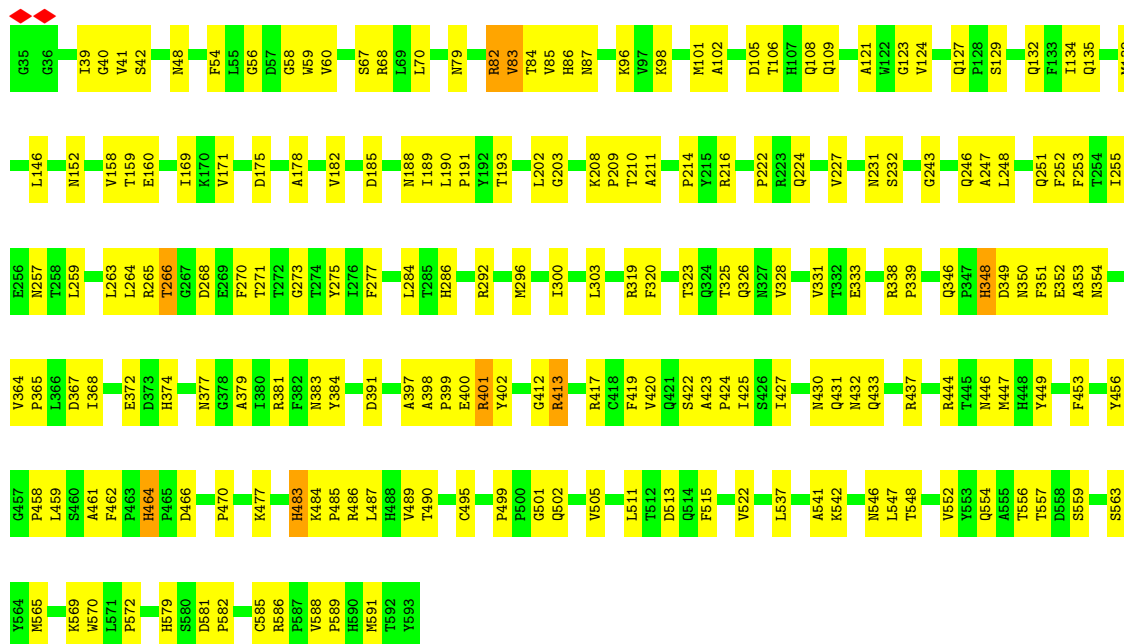
- Molecule 1: Major capsid protein

Chain V: 65% 33%



- Molecule 1: Major capsid protein

Chain W: 65% 34%

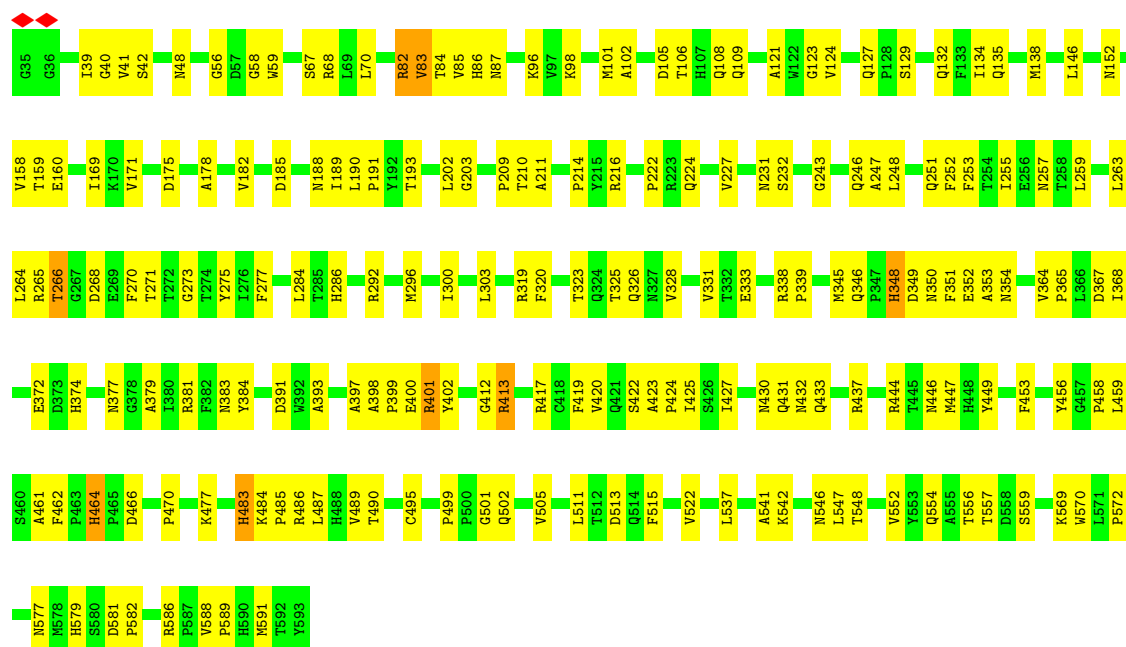


- Molecule 1: Major capsid protein

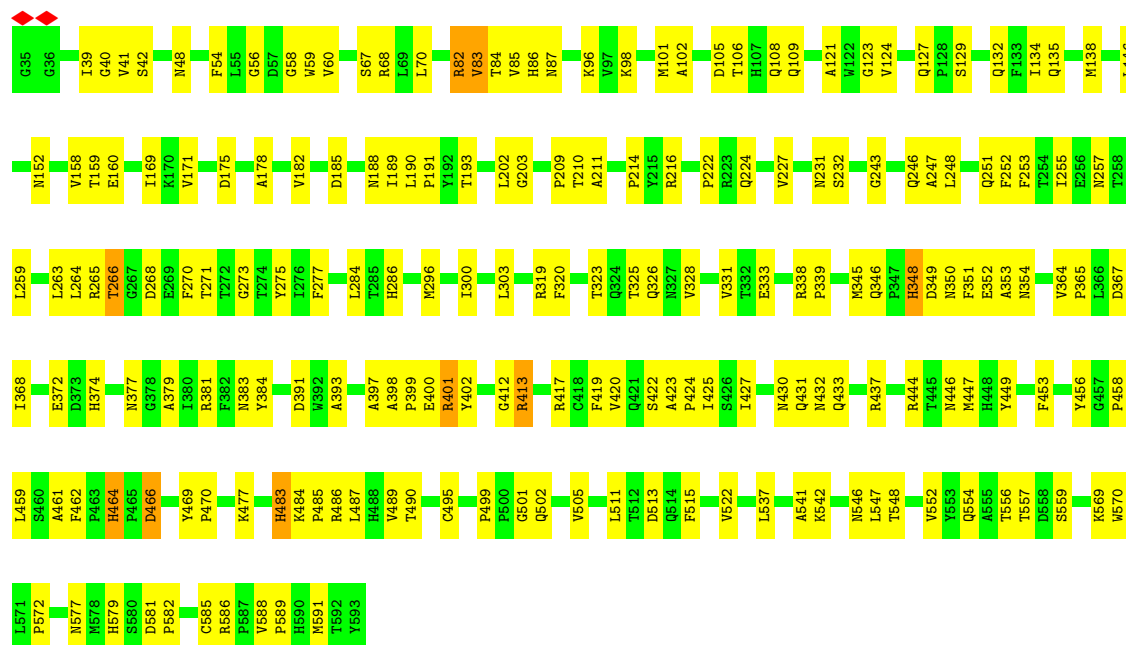
[illegible]

- | |
|------|
| H570 | H571 | H572 | H573 | H574 | H575 | H576 | H577 | H578 | H579 | H580 | H581 | H582 | H583 | H584 | H585 | H586 | H587 | H588 | H589 | H590 | H591 | H592 | H593 | H594 | H595 | H596 | H597 | H598 | H599 | H600 | H601 | H602 | H603 | H604 | H605 | H606 | H607 | H608 | H609 | H610 | H611 | H612 | H613 | H614 | H615 | H616 | H617 | H618 | H619 | H620 | H621 | H622 | H623 | H624 | H625 | H626 | H627 | H628 | H629 | H630 | H631 | H632 | H633 | H634 | H635 | H636 | H637 | H638 | H639 | H640 | H641 | H642 | H643 | H644 | H645 | H646 | H647 | H648 | H649 | H650 | H651 | H652 | H653 | H654 | H655 | H656 | H657 | H658 | H659 | H660 | H661 | H662 | H663 | H664 | H665 | H666 | H667 | H668 | H669 | H670 | H671 | H672 | H673 | H674 | H675 | H676 | H677 | H678 | H679 | H680 | H681 | H682 | H683 | H684 | H685 | H686 | H687 | H688 | H689 | H690 | H691 | H692 | H693 | H694 | H695 | H696 | H697 | H698 | H699 | H700 | H701 | H702 | H703 | H704 | H705 | H706 | H707 | H708 | H709 | H710 | H711 | H712 | H713 | H714 | H715 | H716 | H717 | H718 | H719 | H720 | H721 | H722 | H723 | H724 | H725 | H726 | H727 | H728 | H729 | H730 | H731 | H732 | H733 | H734 | H735 | H736 | H737 | H738 | H739 | H740 | H741 | H742 | H743 | H744 | H745 | H746 | H747 | H748 | H749 | H750 | H751 | H752 | H753 | H754 | H755 | H756 | H757 | H758 | H759 | H760 | H761 | H762 | H763 | H764 | H765 | H766 | H767 | H768 | H769 | H770 | H771 | H772 | H773 | H774 | H775 | H776 | H777 | H778 | H779 | H780 | H781 | H782 | H783 | H784 | H785 | H786 | H787 | H788 | H789 | H790 | H791 | H792 | H793 | H794 | H795 | H796 | H797 | H798 | H799 | H800 | H801 | H802 | H803 | H804 | H805 | H806 | H807 | H808 | H809 | H810 | H811 | H812 | H813 | H814 | H815 | H816 | H817 | H818 | H819 | H820 | H821 | H822 | H823 | H824 | H825 | H826 | H827 | H828 | H829 | H830 | H831 | H832 | H833 | H834 | H835 | H836 | H837 | H838 | H839 | H840 | H841 | H842 | H843 | H844 | H845 | H846 | H847 | H848 | H849 | H850 | H851 | H852 | H853 | H854 | H855 | H856 | H857 | H858 | H859 | H860 | H861 | H862 | H863 | H864 | H865 | H866 | H867 | H868 | H869 | H870 | H871 | H872 | H873 | H874 | H875 | H876 | H877 | H878 | H879 | H880 | H881 | H882 | H883 | H884 |
|------|

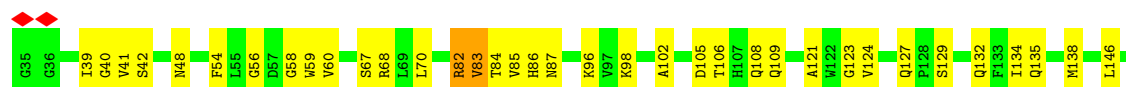
- Chain Z: 65% 33% .

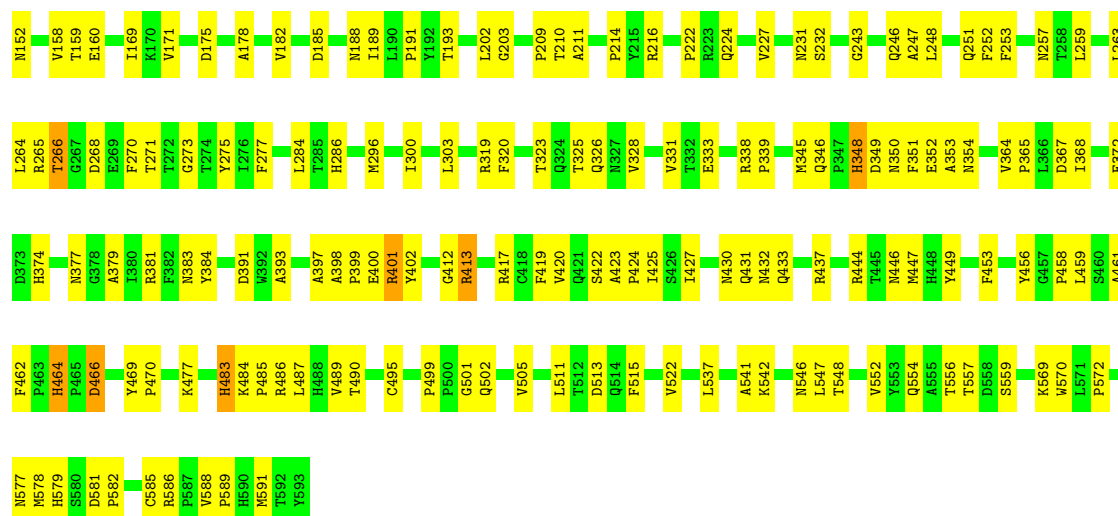


• Molecule 1: Major capsid protein



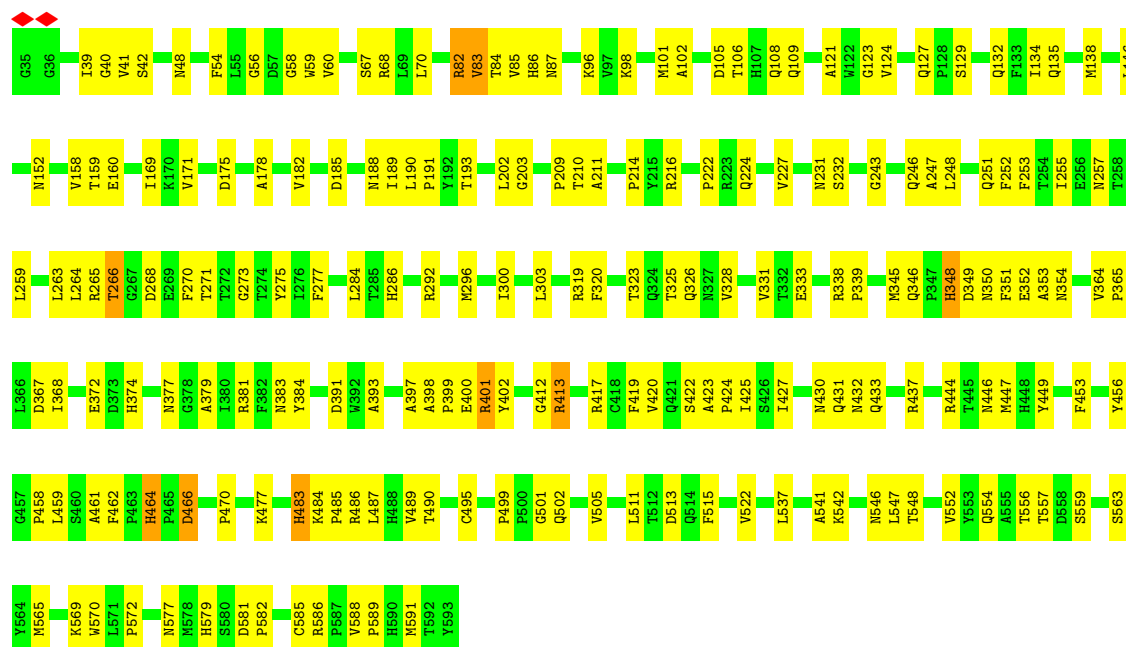
• Molecule 1: Major capsid protein





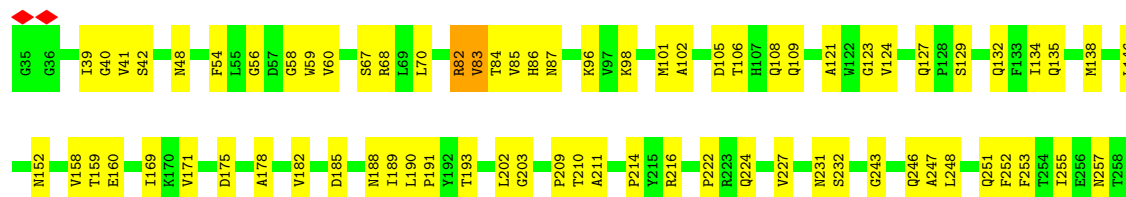
• Molecule 1: Major capsid protein

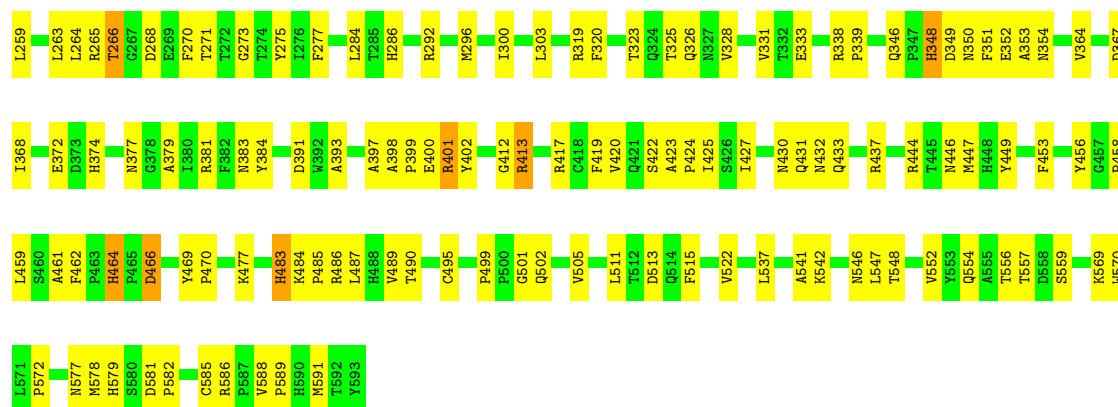
Chain c: 65% 34%



• Molecule 1: Major capsid protein

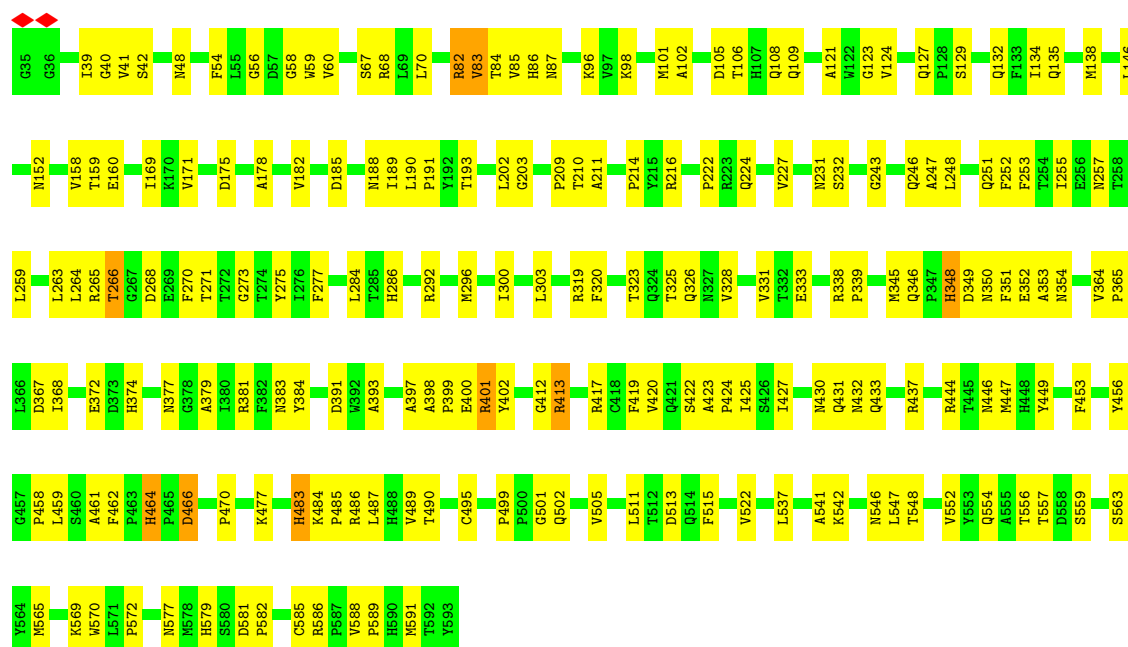
Chain d: 65% 33%





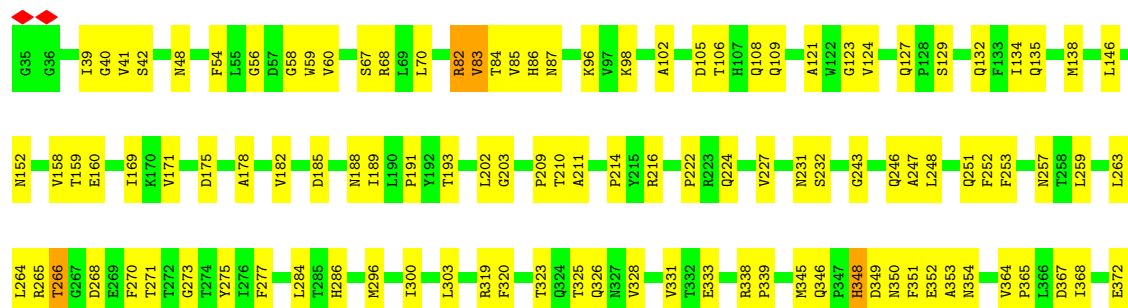
• Molecule 1: Major capsid protein

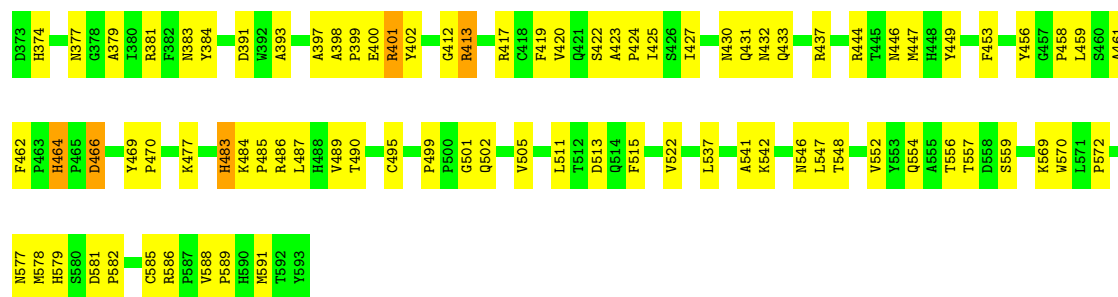
Chain e: 65% 34%



• Molecule 1: Major capsid protein

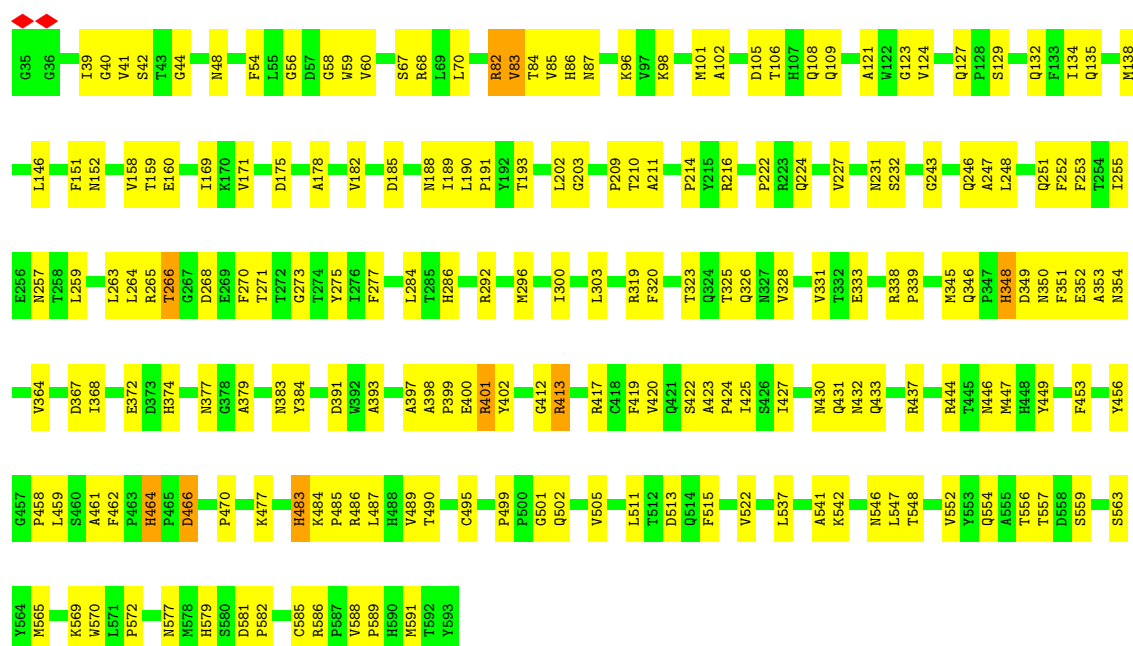
Chain f: 65% 33%





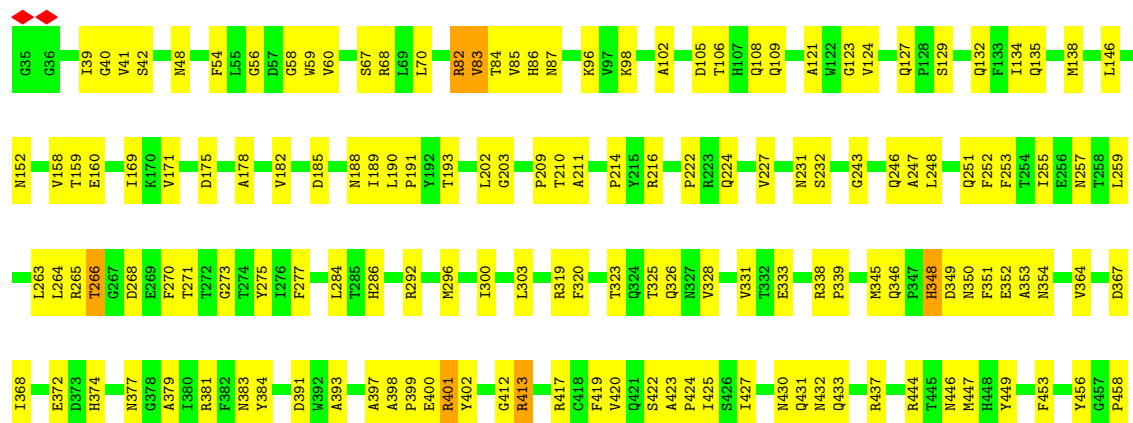
• Molecule 1: Major capsid protein

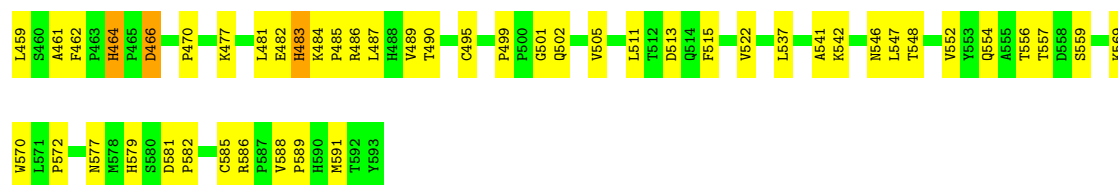
Chain g: 65% 34%



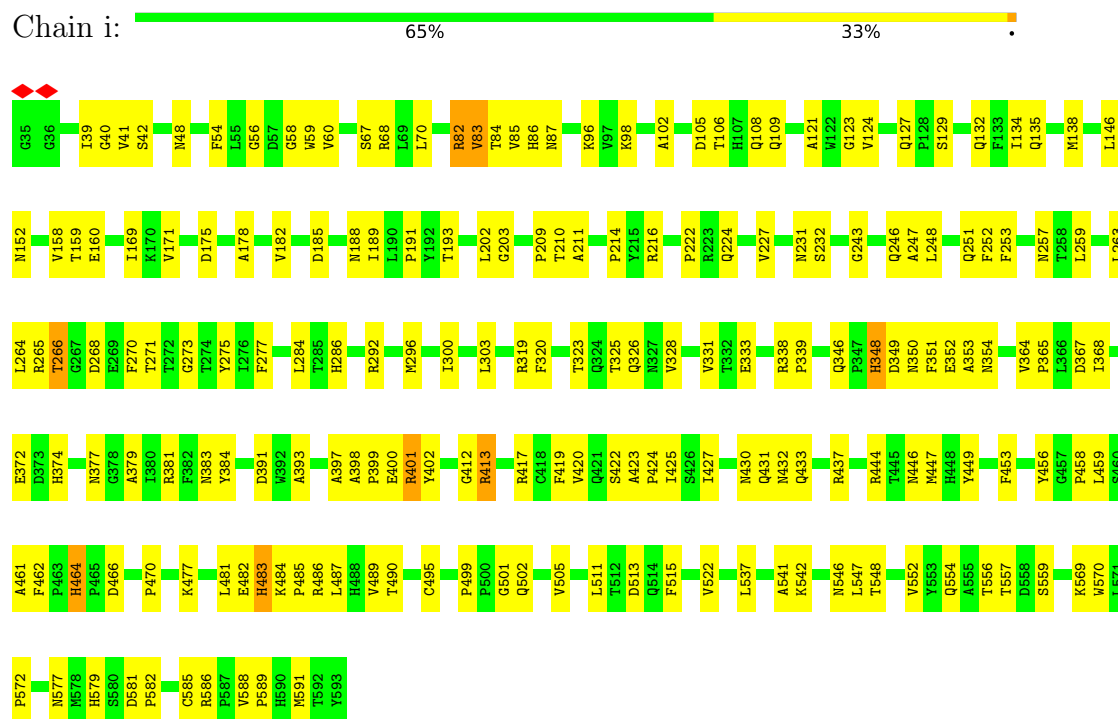
• Molecule 1: Major capsid protein

Chain h: 65% 33%

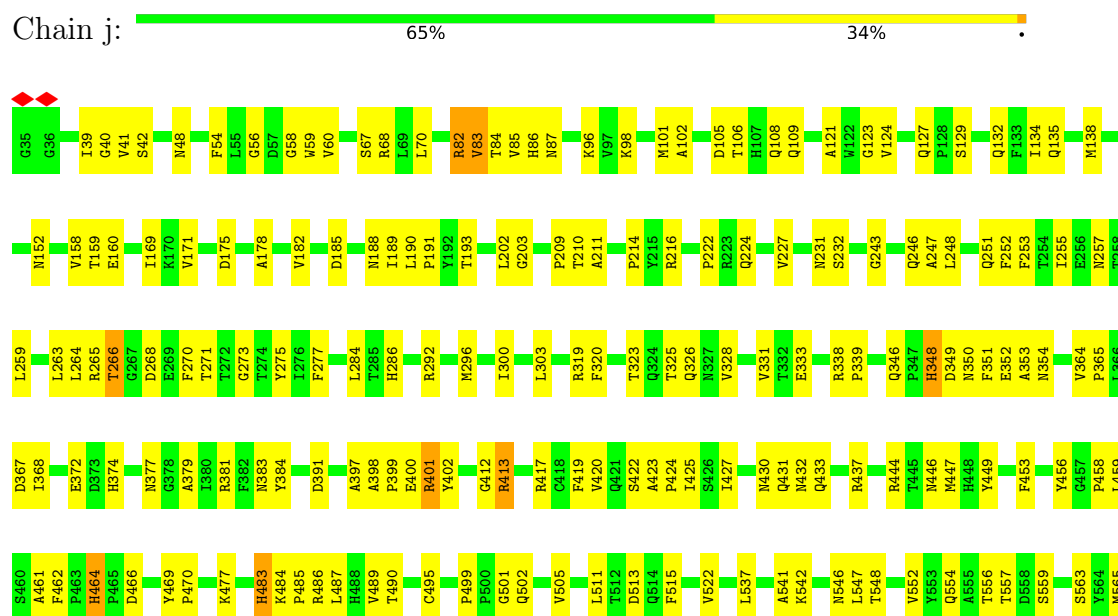




• Molecule 1: Major capsid protein



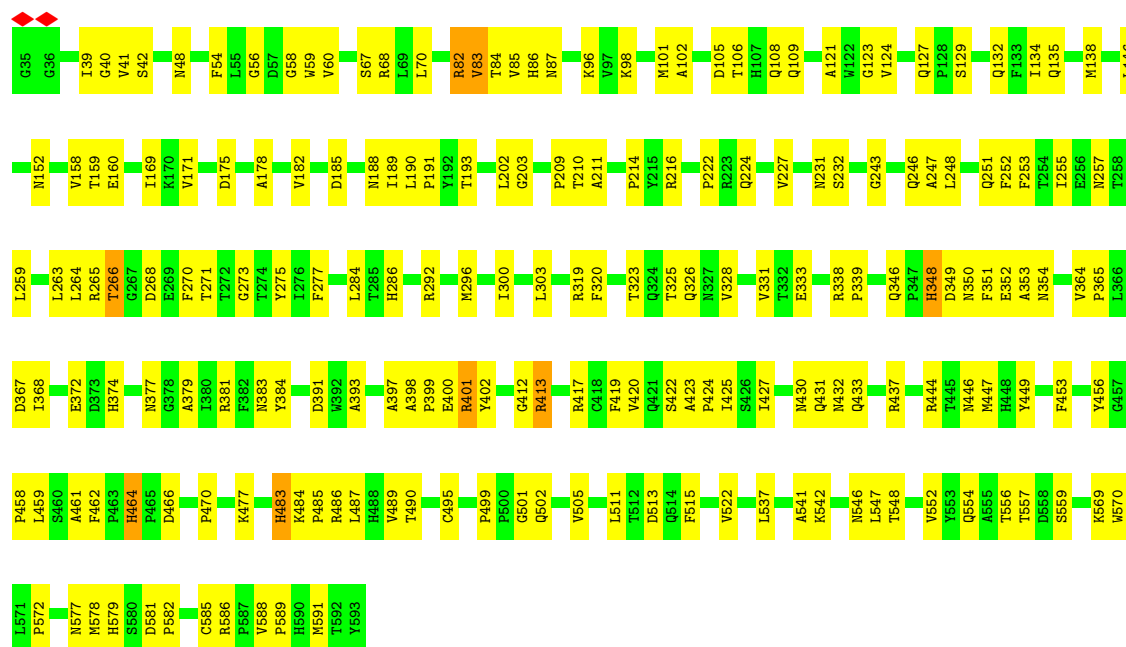
• Molecule 1: Major capsid protein





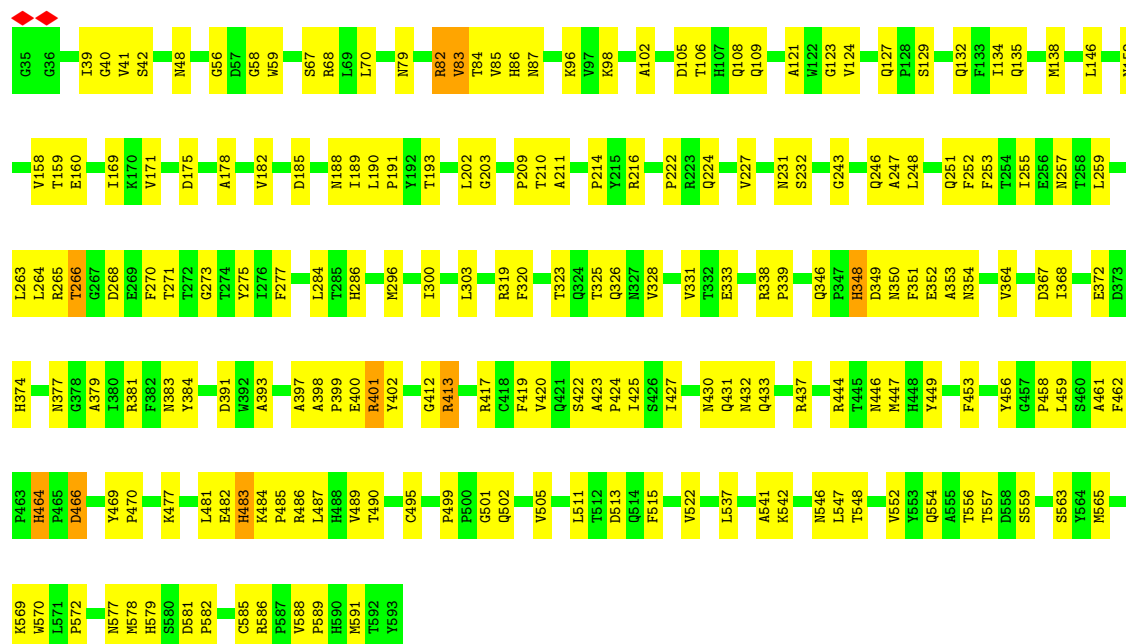
• Molecule 1: Major capsid protein

Chain k: 65% 34%

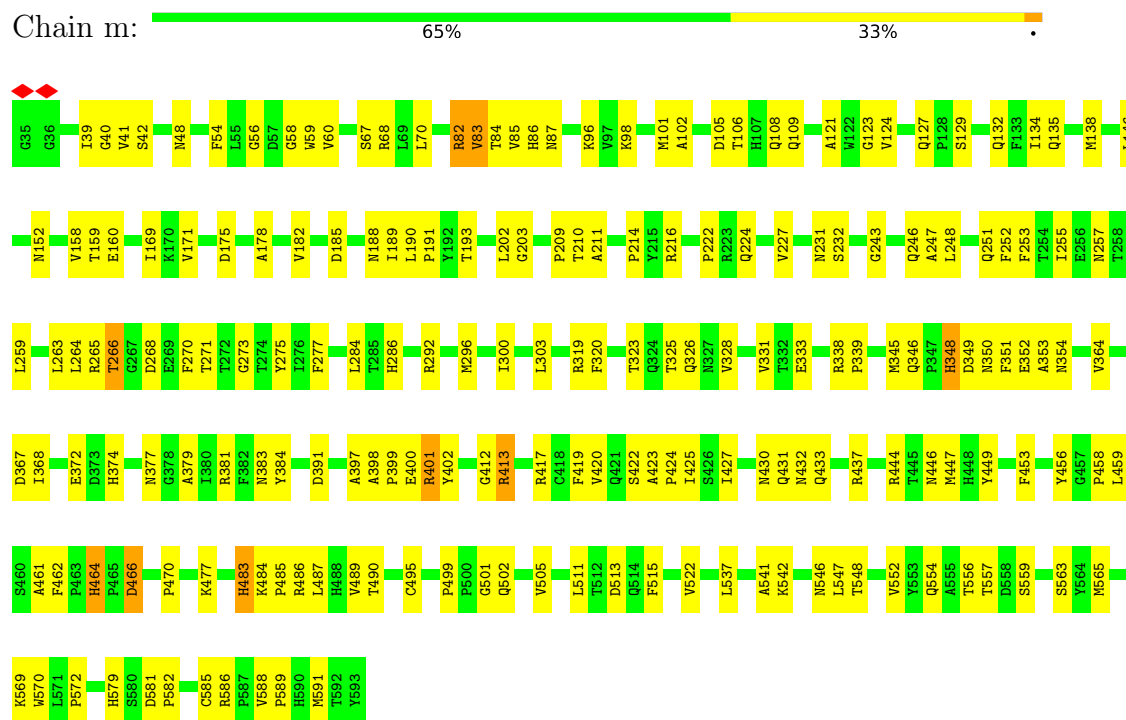


• Molecule 1: Major capsid protein

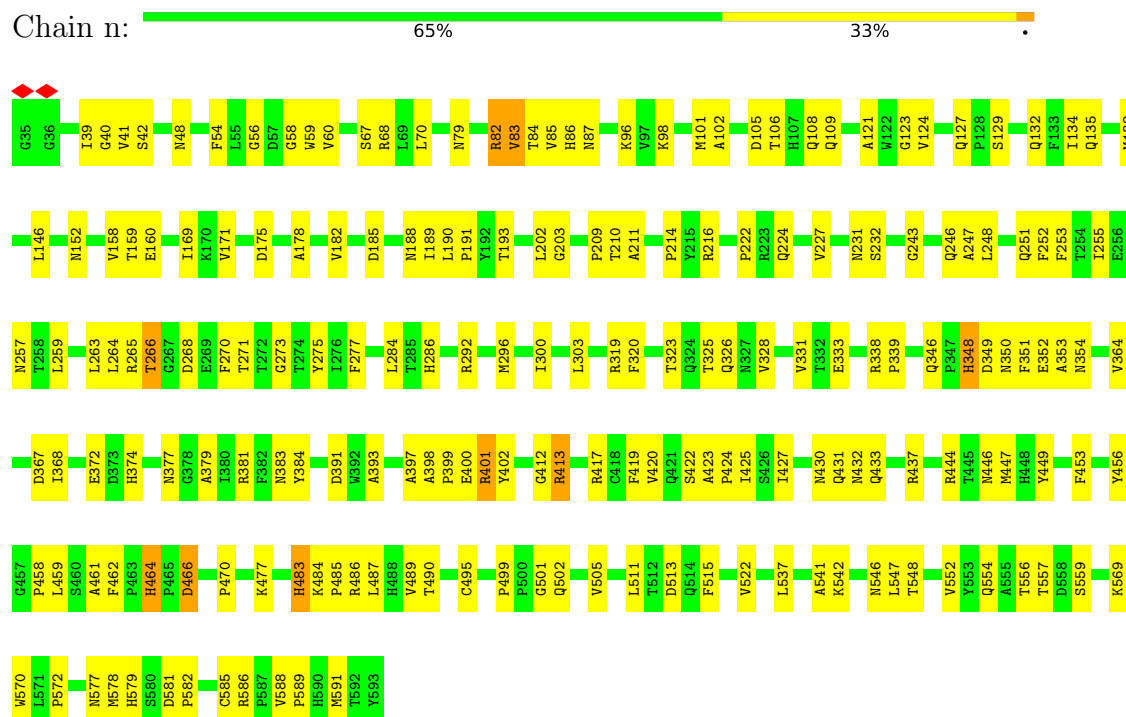
Chain l: 65% 34%



• Molecule 1: Major capsid protein

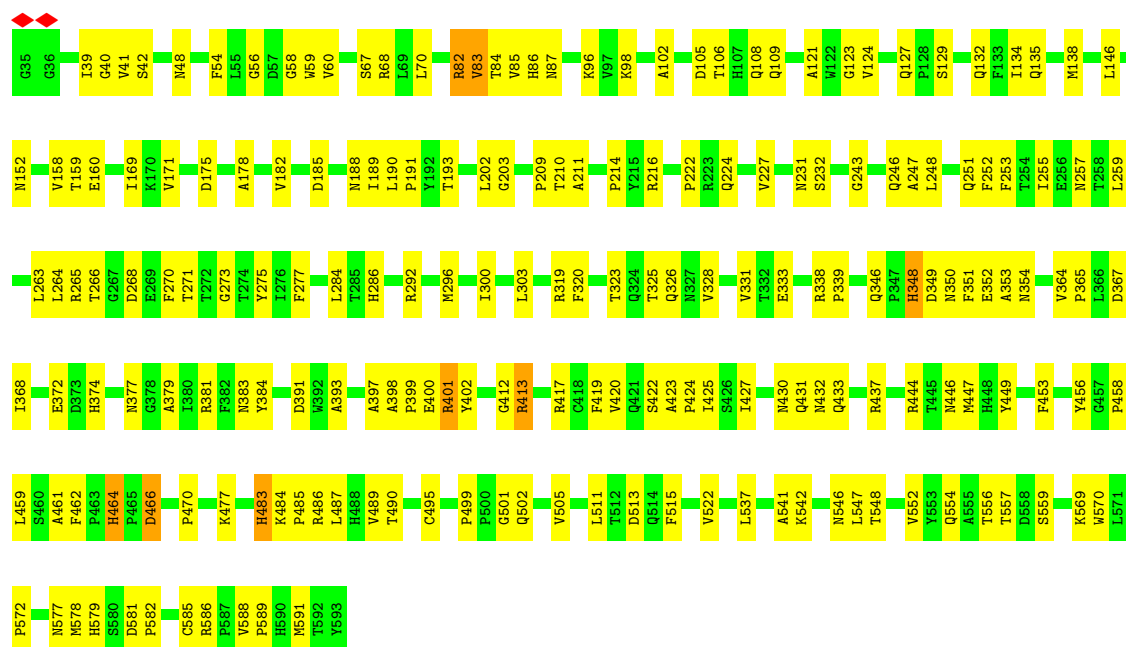


• Molecule 1: Major capsid protein

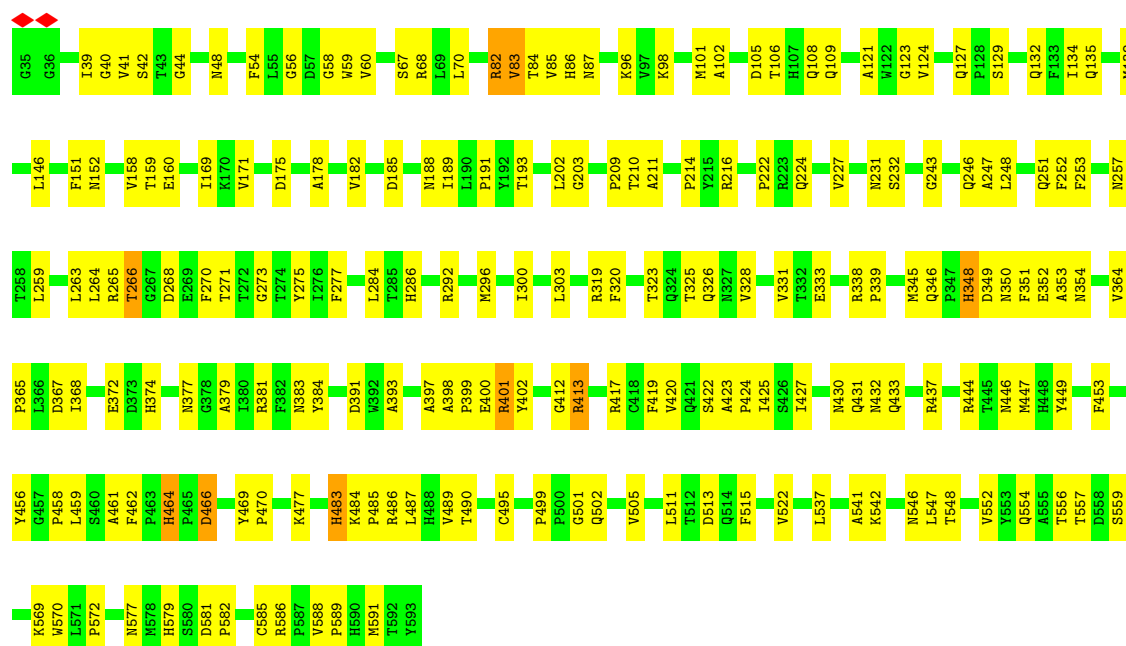


• Molecule 1: Major capsid protein



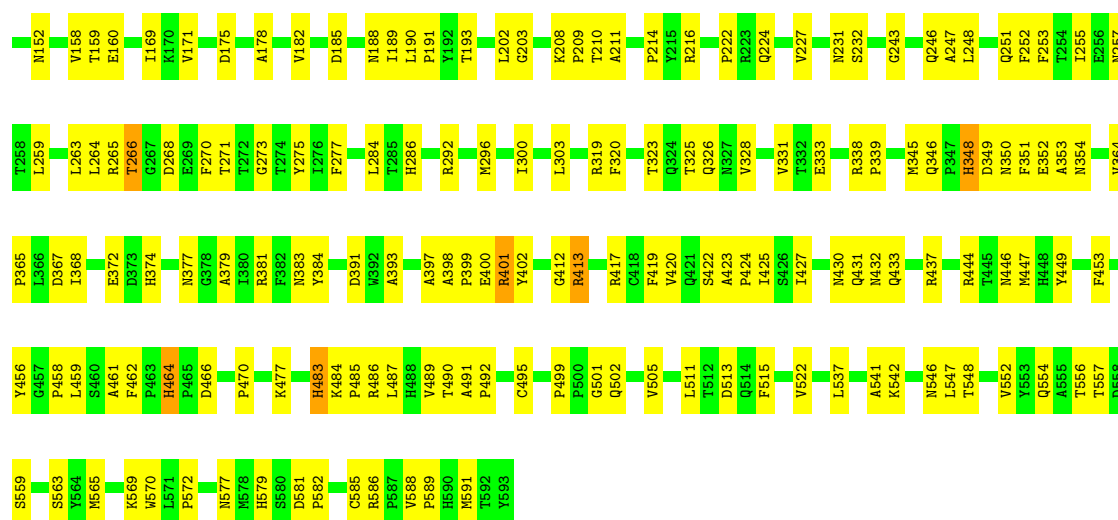


• Molecule 1: Major capsid protein



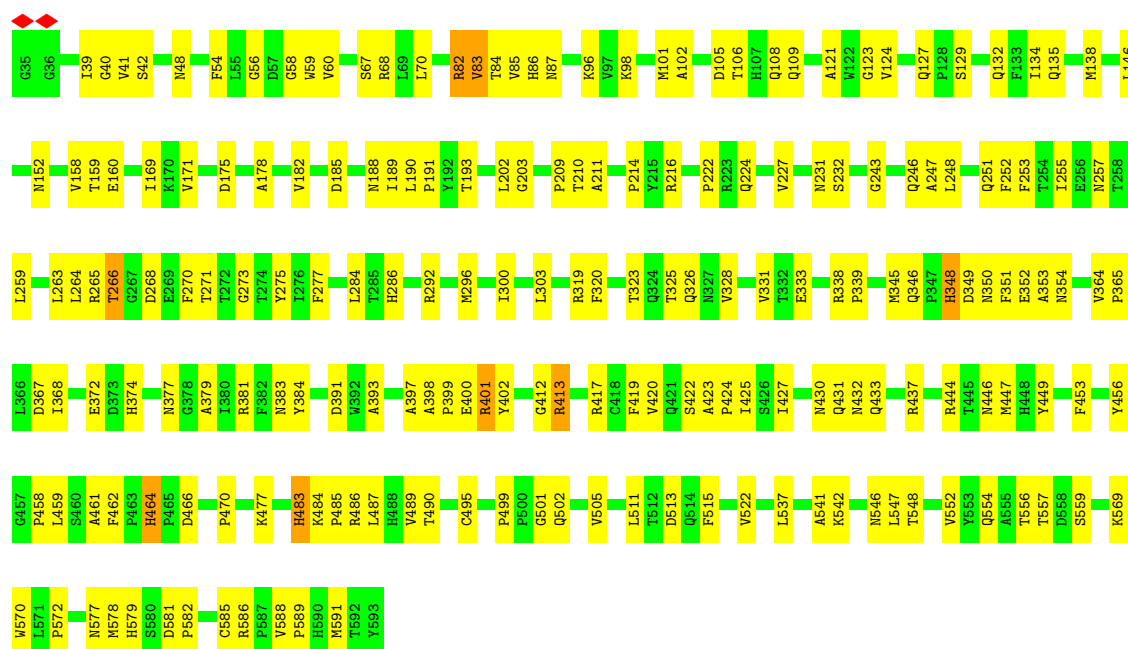
• Molecule 1: Major capsid protein





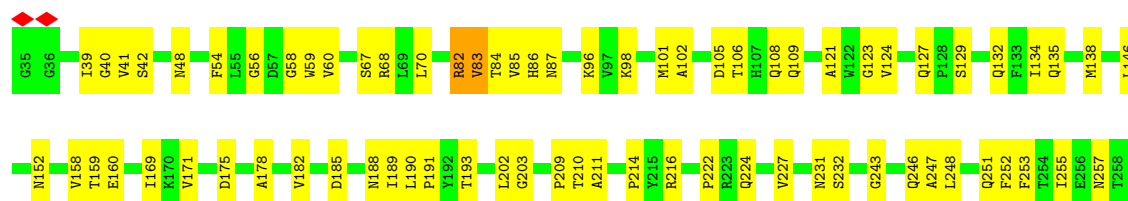
• Molecule 1: Major capsid protein

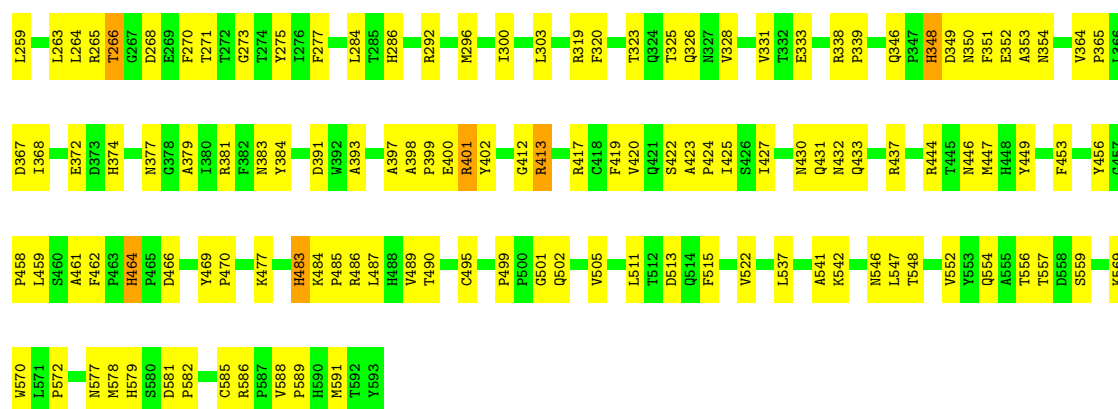
Chain r: 65% 34%



• Molecule 1: Major capsid protein

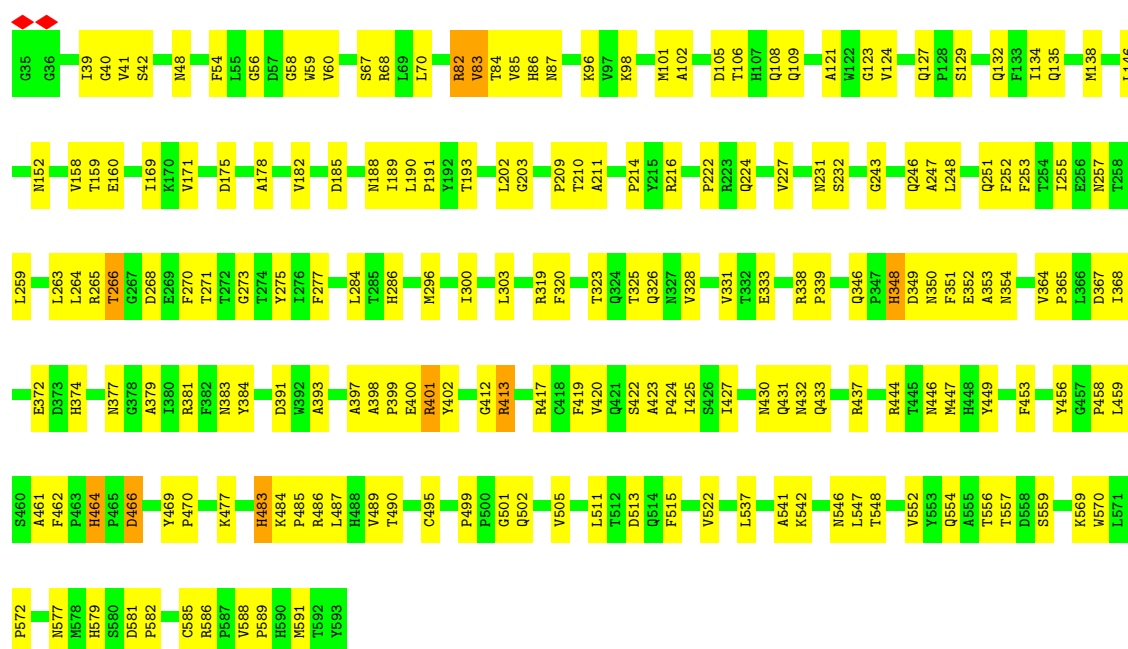
Chain s: 65% 34%





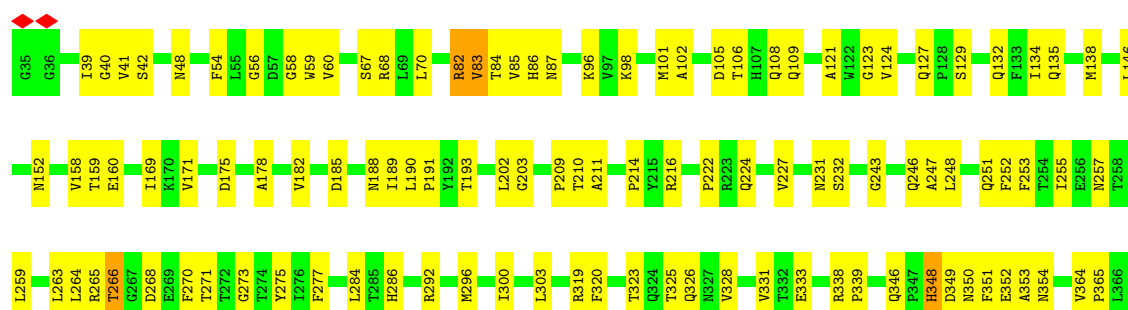
• Molecule 1: Major capsid protein

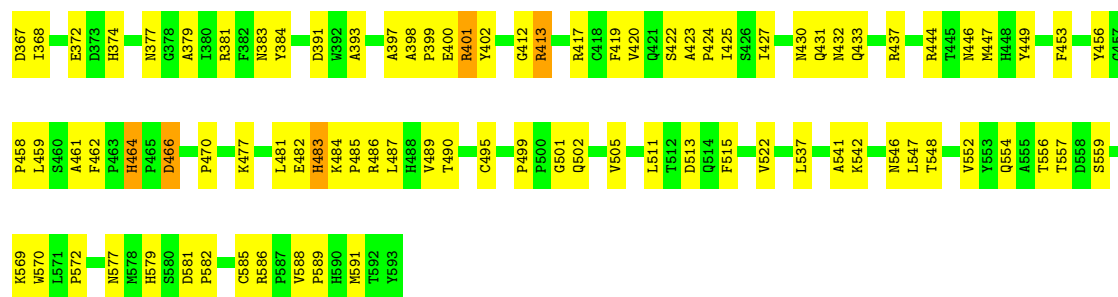
Chain t: 65% 33%



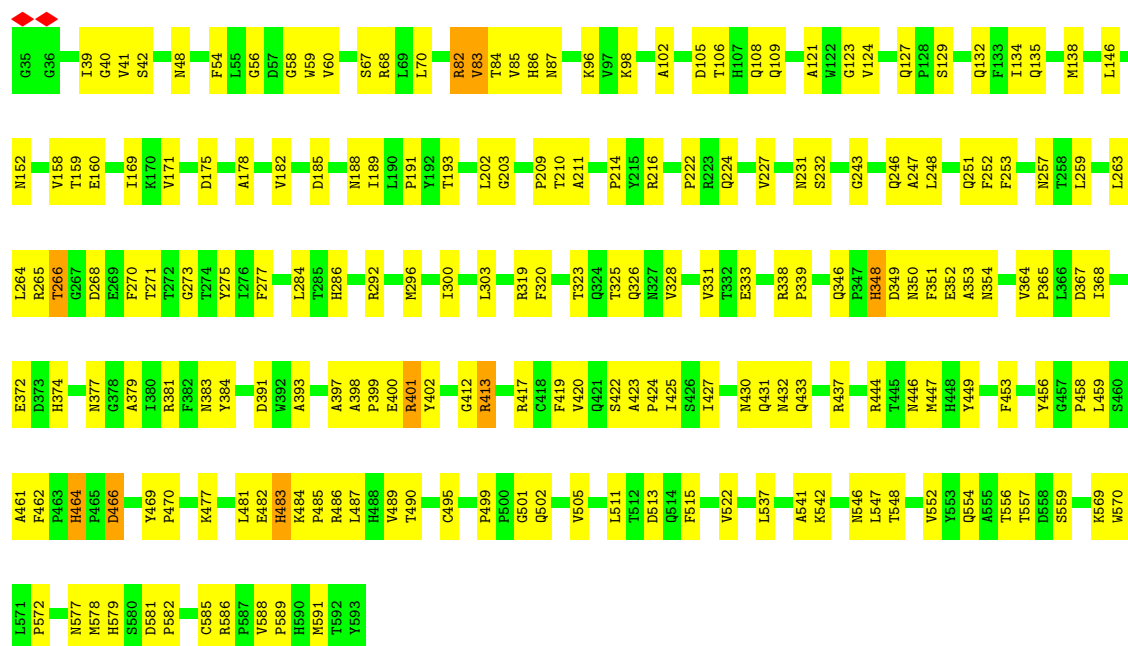
• Molecule 1: Major capsid protein

Chain u: 65% 34%

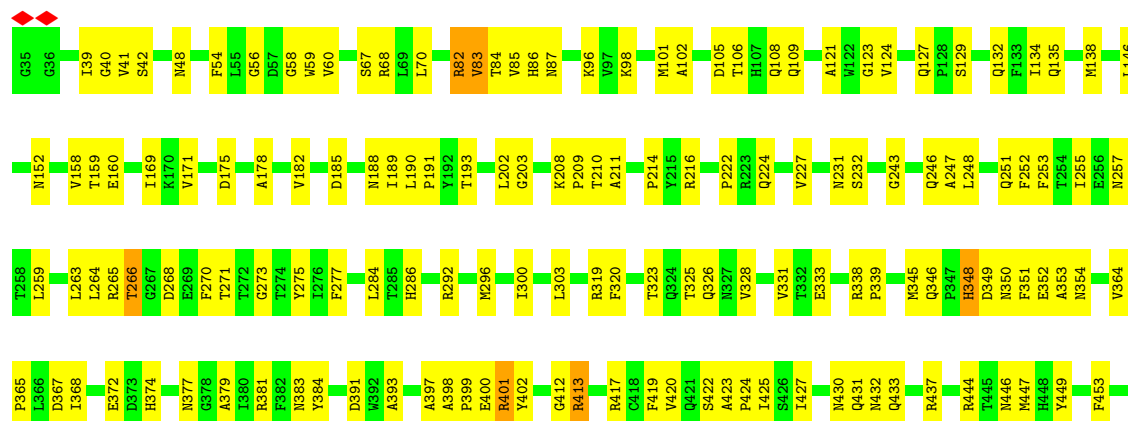


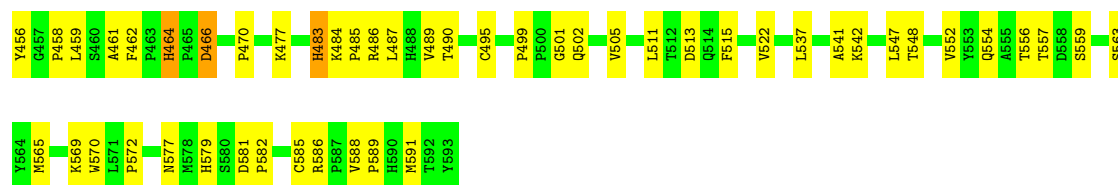


• Molecule 1: Major capsid protein



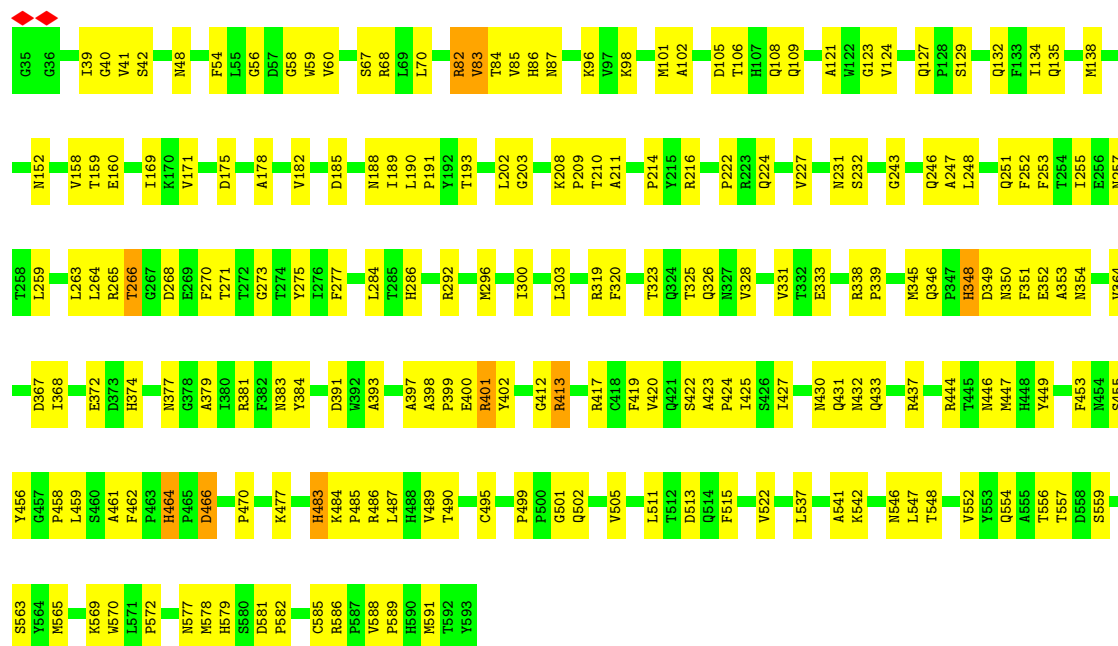
• Molecule 1: Major capsid protein





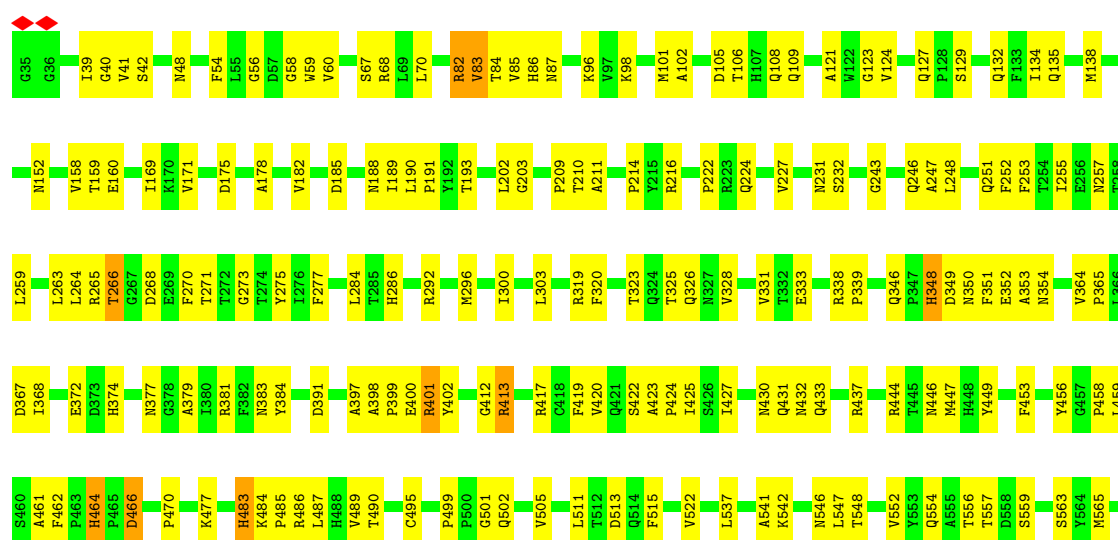
• Molecule 1: Major capsid protein

Chain x: 64% 34%



• Molecule 1: Major capsid protein

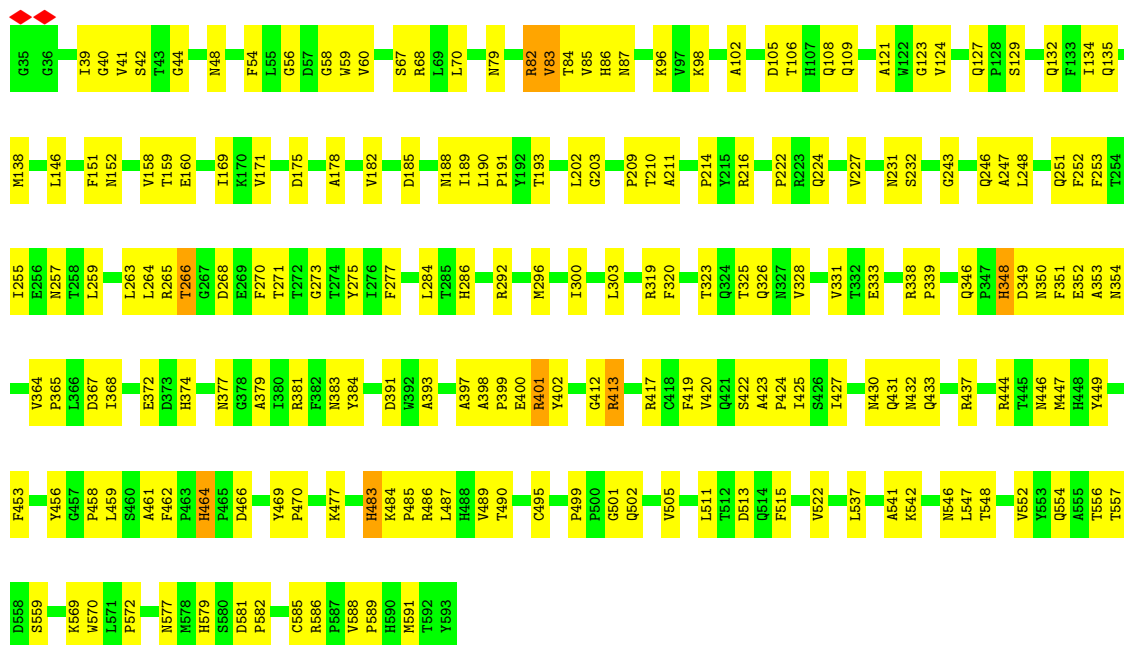
Chain y: 65% 33%





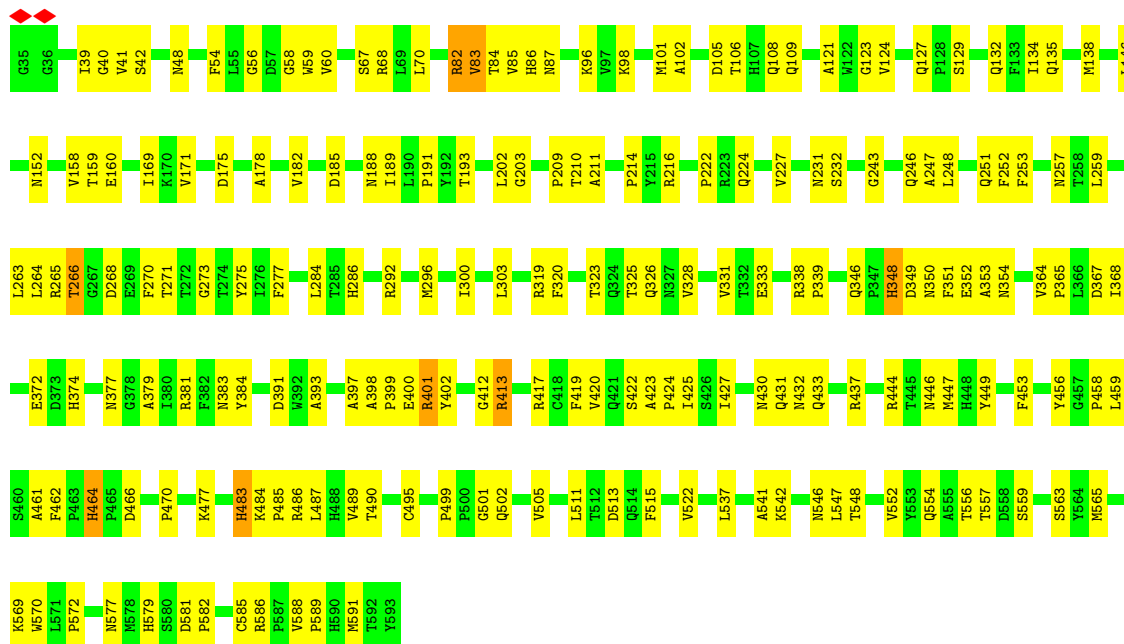
• Molecule 1: Major capsid protein

Chain z: 65% 34%



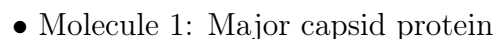
• Molecule 1: Major capsid protein

Chain 1: 65% 33%



• Molecule 1: Major capsid protein

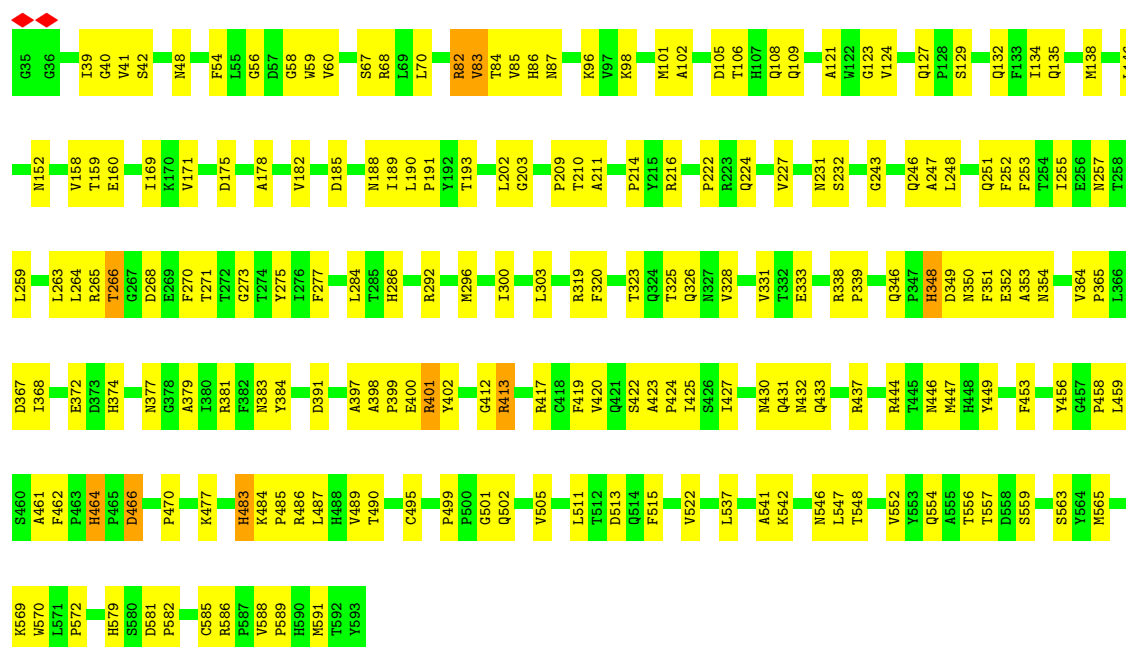
34%



34%

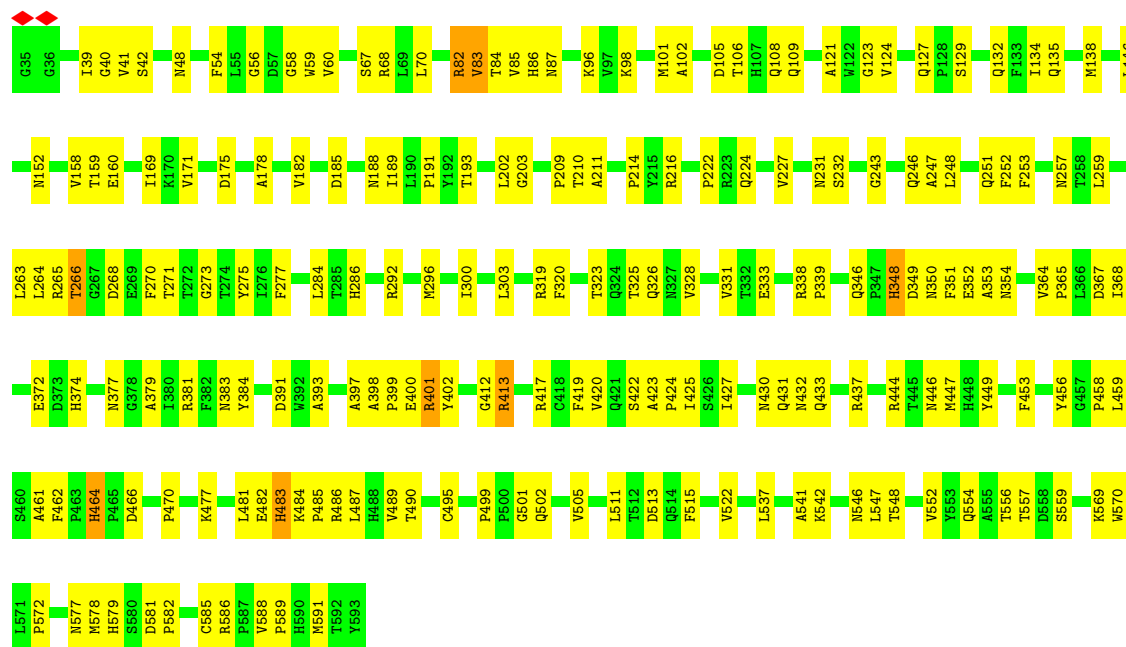


33%



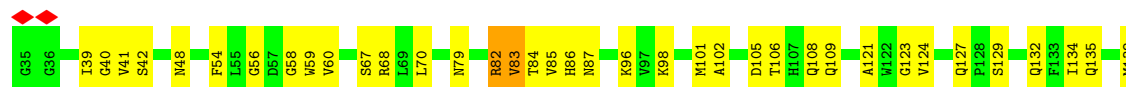
- Molecule 1: Major capsid protein

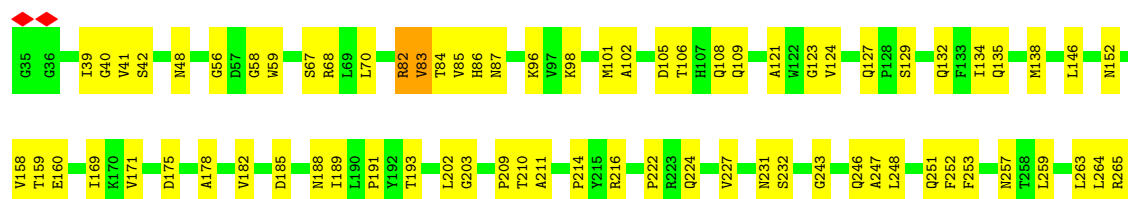
Chain 5: 65% 34%

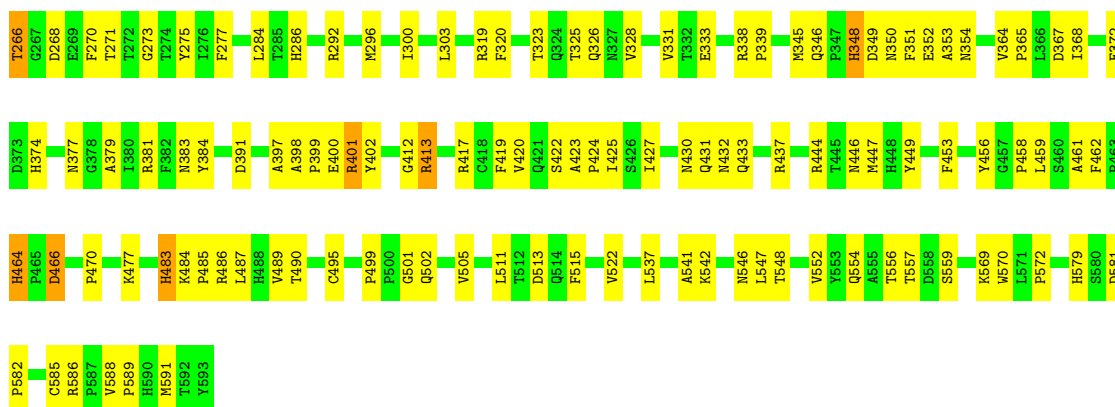


- Molecule 1: Major capsid protein

Chain 6: 65% 34%







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



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



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



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



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



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



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



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



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



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



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

Chain OA:  100%
100%



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

Chain PA:  100%
100%



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

Chain RA:  100%
100%



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

Chain SA:  100%
100%



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

Chain UA:  100%
100%



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

Chain VA:  100%
100%



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



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



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



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



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



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



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



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



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



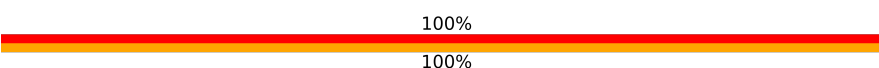
- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

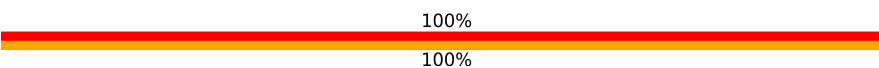


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain nA:  100%
100%

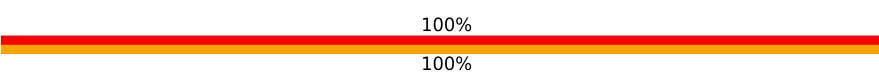


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain pA:  100%
100%

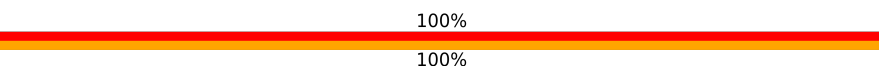


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain qA:  100%
100%

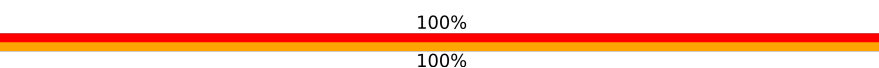


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain sA:  100%
100%

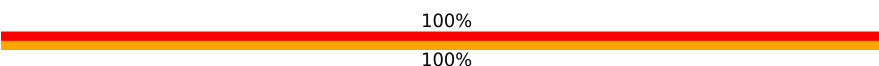


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain tA:  100%
100%



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

Chain vA:  100%
100%



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



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



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



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



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



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



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



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



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



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



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



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

Chain DB:  100%
100%



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

Chain EB:  100%
100%



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

Chain GB:  100%
100%



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

Chain HB:  100%
100%



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

Chain JB:  100%
100%



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

Chain KB:  100%
100%



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



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



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



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



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

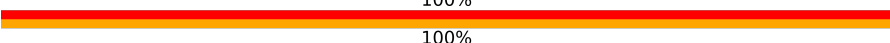


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain TB:  100%
100%



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

Chain VB:  100%
100%



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

Chain WB:  100%
100%



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

Chain YB:  100%
100%



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

Chain ZB:  100%
100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30120	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	1120	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.114	Depositor
Minimum map value	-7.772	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.94	0/4536	1.10	2/6208 (0.0%)
1	2	0.94	0/4536	1.10	2/6208 (0.0%)
1	3	0.94	0/4536	1.10	2/6208 (0.0%)
1	4	0.94	0/4536	1.10	2/6208 (0.0%)
1	5	0.93	0/4536	1.10	2/6208 (0.0%)
1	6	0.93	0/4536	1.10	2/6208 (0.0%)
1	7	0.93	0/4536	1.10	2/6208 (0.0%)
1	8	0.94	0/4536	1.10	2/6208 (0.0%)
1	A	0.93	0/4536	1.10	2/6208 (0.0%)
1	B	0.94	0/4536	1.10	2/6208 (0.0%)
1	C	0.94	0/4536	1.10	2/6208 (0.0%)
1	D	0.93	0/4536	1.10	2/6208 (0.0%)
1	E	0.94	0/4536	1.10	2/6208 (0.0%)
1	F	0.94	0/4536	1.10	2/6208 (0.0%)
1	G	0.94	0/4536	1.10	2/6208 (0.0%)
1	H	0.93	0/4536	1.10	2/6208 (0.0%)
1	I	0.94	0/4536	1.10	2/6208 (0.0%)
1	J	0.94	0/4536	1.10	2/6208 (0.0%)
1	K	0.94	0/4536	1.10	2/6208 (0.0%)
1	L	0.94	0/4536	1.10	2/6208 (0.0%)
1	M	0.94	0/4536	1.10	2/6208 (0.0%)
1	N	0.93	0/4536	1.10	2/6208 (0.0%)
1	O	0.94	0/4536	1.10	2/6208 (0.0%)
1	P	0.94	0/4536	1.10	2/6208 (0.0%)
1	Q	0.94	0/4536	1.10	2/6208 (0.0%)
1	R	0.94	0/4536	1.10	2/6208 (0.0%)
1	S	0.94	0/4536	1.10	2/6208 (0.0%)
1	T	0.94	0/4536	1.10	2/6208 (0.0%)
1	U	0.94	0/4536	1.10	2/6208 (0.0%)
1	V	0.94	0/4536	1.10	2/6208 (0.0%)
1	W	0.93	0/4536	1.10	2/6208 (0.0%)
1	X	0.94	0/4536	1.10	2/6208 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.93	0/4536	1.10	2/6208 (0.0%)
1	Z	0.94	0/4536	1.10	2/6208 (0.0%)
1	a	0.94	0/4536	1.10	2/6208 (0.0%)
1	b	0.94	0/4536	1.10	2/6208 (0.0%)
1	c	0.94	0/4536	1.10	2/6208 (0.0%)
1	d	0.94	0/4536	1.10	2/6208 (0.0%)
1	e	0.94	0/4536	1.10	2/6208 (0.0%)
1	f	0.94	0/4536	1.10	2/6208 (0.0%)
1	g	0.94	0/4536	1.10	2/6208 (0.0%)
1	h	0.94	0/4536	1.10	2/6208 (0.0%)
1	i	0.93	0/4536	1.10	2/6208 (0.0%)
1	j	0.93	0/4536	1.10	2/6208 (0.0%)
1	k	0.93	0/4536	1.10	2/6208 (0.0%)
1	l	0.94	0/4536	1.10	2/6208 (0.0%)
1	m	0.94	0/4536	1.10	2/6208 (0.0%)
1	n	0.94	0/4536	1.10	2/6208 (0.0%)
1	o	0.94	0/4536	1.10	2/6208 (0.0%)
1	p	0.94	0/4536	1.10	2/6208 (0.0%)
1	q	0.94	0/4536	1.10	2/6208 (0.0%)
1	r	0.94	0/4536	1.10	2/6208 (0.0%)
1	s	0.94	0/4536	1.10	2/6208 (0.0%)
1	t	0.94	0/4536	1.10	2/6208 (0.0%)
1	u	0.94	0/4536	1.10	2/6208 (0.0%)
1	v	0.94	0/4536	1.10	2/6208 (0.0%)
1	w	0.94	0/4536	1.10	2/6208 (0.0%)
1	x	0.94	0/4536	1.10	2/6208 (0.0%)
1	y	0.94	0/4536	1.10	2/6208 (0.0%)
1	z	0.94	0/4536	1.10	2/6208 (0.0%)
All	All	0.94	0/272160	1.10	120/372480 (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
1	1	0	3
1	2	0	3
1	3	0	3
1	4	0	3
1	5	0	3
1	6	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	7	0	3
1	8	0	3
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
1	Q	0	3
1	R	0	3
1	S	0	3
1	T	0	3
1	U	0	3
1	V	0	3
1	W	0	3
1	X	0	3
1	Y	0	3
1	Z	0	3
1	a	0	3
1	b	0	3
1	c	0	3
1	d	0	3
1	e	0	3
1	f	0	3
1	g	0	3
1	h	0	3
1	i	0	3
1	j	0	3
1	k	0	3
1	l	0	3
1	m	0	3
1	n	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	o	0	3
1	p	0	3
1	q	0	3
1	r	0	3
1	s	0	3
1	t	0	3
1	u	0	3
1	v	0	3
1	w	0	3
1	x	0	3
1	y	0	3
1	z	0	3
All	All	0	180

There are no bond length outliers.

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	LYS	N-CA-C	-6.09	105.42	112.92
1	J	96	LYS	N-CA-C	-6.09	105.42	112.92
1	L	96	LYS	N-CA-C	-6.09	105.42	112.92
1	R	96	LYS	N-CA-C	-6.09	105.42	112.92
1	S	96	LYS	N-CA-C	-6.09	105.42	112.92

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	ARG	Sidechain
1	A	413	ARG	Sidechain
1	A	82	ARG	Sidechain
1	B	401	ARG	Sidechain
1	B	82	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4404	0	4197	327	0
1	2	4404	0	4197	334	0
1	3	4404	0	4197	329	0
1	4	4404	0	4197	323	0
1	5	4404	0	4197	331	0
1	6	4404	0	4197	323	0
1	7	4404	0	4197	329	0
1	8	4404	0	4197	328	0
1	A	4404	0	4197	330	0
1	B	4404	0	4197	325	0
1	C	4404	0	4197	328	0
1	D	4404	0	4197	328	0
1	E	4404	0	4197	328	0
1	F	4404	0	4197	330	0
1	G	4404	0	4197	330	0
1	H	4404	0	4197	330	0
1	I	4404	0	4197	330	0
1	J	4404	0	4197	333	0
1	K	4404	0	4197	324	0
1	L	4404	0	4197	326	0
1	M	4404	0	4197	331	0
1	N	4404	0	4197	331	0
1	O	4404	0	4197	321	0
1	P	4404	0	4197	325	0
1	Q	4404	0	4197	329	0
1	R	4404	0	4197	333	0
1	S	4404	0	4197	329	0
1	T	4404	0	4197	325	0
1	U	4404	0	4197	328	0
1	V	4404	0	4197	324	0
1	W	4404	0	4197	324	0
1	X	4404	0	4197	328	0
1	Y	4404	0	4197	327	0
1	Z	4404	0	4197	329	0
1	a	4404	0	4197	327	0
1	b	4404	0	4197	324	0
1	c	4404	0	4197	327	0
1	d	4404	0	4197	330	0
1	e	4404	0	4197	328	0
1	f	4404	0	4197	324	0
1	g	4404	0	4197	327	0
1	h	4404	0	4197	330	0
1	i	4404	0	4197	328	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4404	0	4197	328	0
1	k	4404	0	4197	329	0
1	l	4404	0	4197	324	0
1	m	4404	0	4197	326	0
1	n	4404	0	4197	329	0
1	o	4404	0	4197	328	0
1	p	4404	0	4197	326	0
1	q	4404	0	4197	334	0
1	r	4404	0	4197	333	0
1	s	4404	0	4197	330	0
1	t	4404	0	4197	329	0
1	u	4404	0	4197	329	0
1	v	4404	0	4197	334	0
1	w	4404	0	4197	329	0
1	x	4404	0	4197	328	0
1	y	4404	0	4197	329	0
1	z	4404	0	4197	330	0
2	1A	46	0	40	4	0
2	2A	46	0	40	4	0
2	4A	46	0	40	4	0
2	5A	46	0	40	4	0
2	7A	46	0	40	4	0
2	8A	46	0	40	4	0
2	9	46	0	40	4	0
2	AA	46	0	40	4	0
2	AB	46	0	40	4	0
2	BB	46	0	40	4	0
2	CA	46	0	40	4	0
2	DA	46	0	40	4	0
2	DB	46	0	40	4	0
2	EB	46	0	40	4	0
2	FA	46	0	40	4	0
2	GA	46	0	40	4	0
2	GB	46	0	40	4	0
2	HB	46	0	40	4	0
2	IA	46	0	40	4	0
2	JA	46	0	40	4	0
2	JB	46	0	40	4	0
2	KB	46	0	40	4	0
2	LA	46	0	40	4	0
2	MA	46	0	40	4	0
2	MB	46	0	40	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	NB	46	0	40	4	0
2	OA	46	0	40	4	0
2	PA	46	0	40	4	0
2	PB	46	0	40	4	0
2	QB	46	0	40	4	0
2	RA	46	0	40	4	0
2	SA	46	0	40	4	0
2	SB	46	0	40	4	0
2	TB	46	0	40	4	0
2	UA	46	0	40	4	0
2	VA	46	0	40	4	0
2	VB	46	0	40	4	0
2	WB	46	0	40	4	0
2	XA	46	0	40	4	0
2	YA	46	0	40	4	0
2	YB	46	0	40	4	0
2	ZB	46	0	40	4	0
2	aA	46	0	40	4	0
2	bA	46	0	40	4	0
2	dA	46	0	40	4	0
2	eA	46	0	40	4	0
2	gA	46	0	40	4	0
2	hA	46	0	40	4	0
2	jA	46	0	40	4	0
2	kA	46	0	40	4	0
2	mA	46	0	40	4	0
2	nA	46	0	40	4	0
2	pA	46	0	40	4	0
2	qA	46	0	40	4	0
2	sA	46	0	40	4	0
2	tA	46	0	40	4	0
2	vA	46	0	40	4	0
2	wA	46	0	40	4	0
2	yA	46	0	40	4	0
2	zA	46	0	40	4	0
All	All	267000	0	254220	12310	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 12310 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:483:HIS:CE1	1:W:462:PHE:CG	2.19	1.31
1:q:462:PHE:CG	1:v:483:HIS:CE1	2.19	1.31
1:s:483:HIS:CE1	1:6:462:PHE:CG	2.19	1.31
1:A:483:HIS:CE1	1:R:462:PHE:CG	2.19	1.31
1:C:462:PHE:CG	1:I:483:HIS:CE1	2.19	1.31

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	2	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	3	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	4	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	5	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	6	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	7	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	8	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	A	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	B	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	C	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	D	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	E	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	F	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	G	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	H	557/559 (100%)	527 (95%)	30 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	J	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	K	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	L	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	M	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	N	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	O	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	P	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	Q	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	R	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	S	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	T	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	U	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	V	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	W	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	X	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	Y	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	Z	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	a	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	b	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	c	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	d	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	e	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	f	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	g	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	h	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	i	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	j	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	k	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	l	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	m	557/559 (100%)	527 (95%)	30 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	o	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	p	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	q	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	r	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	s	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	t	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	u	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	v	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	w	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
1	x	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	y	557/559 (100%)	527 (95%)	30 (5%)	0	100	100
1	z	557/559 (100%)	528 (95%)	29 (5%)	0	100	100
All	All	33420/33540 (100%)	31644 (95%)	1776 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	2	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	3	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	4	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	5	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	6	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	7	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	8	480/480 (100%)	470 (98%)	10 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	B	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	C	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	D	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	E	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	F	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	G	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	H	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	I	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	J	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	K	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	L	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	M	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	N	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	O	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	P	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	Q	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	R	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	S	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	T	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	U	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	V	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	W	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	X	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	Y	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	Z	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	a	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	b	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	c	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	d	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	e	480/480 (100%)	470 (98%)	10 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	f	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	g	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	h	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	i	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	j	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	k	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	l	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	m	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	n	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	o	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	p	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	q	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	r	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	s	480/480 (100%)	471 (98%)	9 (2%)	50	73
1	t	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	u	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	v	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	w	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	x	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	y	480/480 (100%)	470 (98%)	10 (2%)	47	71
1	z	480/480 (100%)	471 (98%)	9 (2%)	50	73
All	All	28800/28800 (100%)	28224 (98%)	576 (2%)	48	72

5 of 576 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	w	87	ASN
1	8	511	LEU
1	x	384	TYR
1	w	83	VAL
1	3	87	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1238 such sidechains are listed below:

Mol	Chain	Res	Type
1	s	497	ASN
1	4	346	GLN
1	u	135	GLN
1	s	483	HIS
1	y	188	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

180 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	1A	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	1A	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	1A	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	2A	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	2A	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	2A	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	4A	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	4A	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	4A	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	5A	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	5A	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	5A	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	7A	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	7A	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	7A	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	8A	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	8A	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	8A	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	9	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	9	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	9	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	AA	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	AA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	AA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	AB	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	AB	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	AB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	BB	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	BB	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	BB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	CA	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	CA	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	CA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	DA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	DA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	DA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	DB	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	DB	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	DB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	EB	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	EB	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	EB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	FA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	FA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	FA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	GA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	GA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	GA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	GB	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	GB	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	GB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	HB	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	HB	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	HB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	IA	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	IA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	IA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	JA	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	JA	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	JA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	JB	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	JB	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	JB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	KB	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	KB	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	KB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	LA	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	LA	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	LA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	MA	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	MA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	MA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	MB	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	MB	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	MB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	NB	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	NB	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	NB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	OA	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	OA	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	OA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	PA	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLA	PA	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	PA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	PB	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	PB	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	PB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	QB	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	QB	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	QB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	RA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	RA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	RA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	SA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	SA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	SA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	SB	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	SB	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	SB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	TB	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	TB	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	TB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	UA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	UA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	UA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	VA	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	VA	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	VA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	VB	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	VB	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	VB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	WB	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	WB	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	WB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	XA	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	XA	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	XA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	YA	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	YA	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	YA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	YB	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	YB	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	YB	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	ZB	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	ZB	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	ZB	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	aA	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	aA	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	aA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	bA	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	bA	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	bA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	dA	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	dA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	dA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	eA	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	eA	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)
2	SIA	eA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	gA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	gA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	gA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	hA	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	hA	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	hA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	jA	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	jA	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	jA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	kA	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	kA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	kA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	mA	1	2	15,15,15	0.20	0	21,21,21	1.01	1 (4%)
2	GLA	mA	2	2	11,11,12	0.46	0	15,15,17	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	mA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	nA	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	nA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	nA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	pA	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	pA	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	pA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	qA	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	qA	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	qA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	sA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	sA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	sA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	tA	1	2	15,15,15	0.22	0	21,21,21	1.01	1 (4%)
2	GLA	tA	2	2	11,11,12	0.46	0	15,15,17	1.13	1 (6%)
2	SIA	tA	3	2	20,20,21	0.73	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	vA	1	2	15,15,15	0.21	0	21,21,21	1.00	1 (4%)
2	GLA	vA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	vA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	wA	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	wA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	wA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)
2	NAG	yA	1	2	15,15,15	0.21	0	21,21,21	1.02	1 (4%)
2	GLA	yA	2	2	11,11,12	0.45	0	15,15,17	1.13	1 (6%)
2	SIA	yA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.79	1 (4%)
2	NAG	zA	1	2	15,15,15	0.20	0	21,21,21	1.02	1 (4%)
2	GLA	zA	2	2	11,11,12	0.47	0	15,15,17	1.14	1 (6%)
2	SIA	zA	3	2	20,20,21	0.74	1 (5%)	21,28,31	0.80	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	1A	1	2	-	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	1A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	1A	3	2	-	5/18/34/38	0/1/1/1
2	NAG	2A	1	2	-	2/6/26/26	0/1/1/1
2	GLA	2A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	2A	3	2	-	5/18/34/38	0/1/1/1
2	NAG	4A	1	2	-	2/6/26/26	0/1/1/1
2	GLA	4A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	4A	3	2	-	5/18/34/38	0/1/1/1
2	NAG	5A	1	2	-	2/6/26/26	0/1/1/1
2	GLA	5A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	5A	3	2	-	5/18/34/38	0/1/1/1
2	NAG	7A	1	2	-	2/6/26/26	0/1/1/1
2	GLA	7A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	7A	3	2	-	5/18/34/38	0/1/1/1
2	NAG	8A	1	2	-	2/6/26/26	0/1/1/1
2	GLA	8A	2	2	-	1/2/19/22	0/1/1/1
2	SIA	8A	3	2	-	5/18/34/38	0/1/1/1
2	NAG	9	1	2	-	2/6/26/26	0/1/1/1
2	GLA	9	2	2	-	1/2/19/22	0/1/1/1
2	SIA	9	3	2	-	5/18/34/38	0/1/1/1
2	NAG	AA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	AA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	AA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	AB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	AB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	AB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	BB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	BB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	BB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	CA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	CA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	CA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	DA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	DA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	DA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	DB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	DB	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	DB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	EB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	EB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	EB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	FA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	FA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	FA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	GA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	GA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	GA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	GB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	GB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	GB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	HB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	HB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	HB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	IA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	IA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	IA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	JA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	JA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	JA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	JB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	JB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	JB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	KB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	KB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	KB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	LA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	LA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	LA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	MA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	MA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	MA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	MB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	MB	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	MB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	NB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	NB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	NB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	OA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	OA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	OA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	PA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	PA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	PA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	PB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	PB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	PB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	QB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	QB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	QB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	RA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	RA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	RA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	SA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	SA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	SA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	SB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	SB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	SB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	TB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	TB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	TB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	UA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	UA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	UA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	VA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	VA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	VA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	VB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	VB	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	VB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	WB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	WB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	WB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	XA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	XA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	XA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	YA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	YA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	YA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	YB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	YB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	YB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	ZB	1	2	-	2/6/26/26	0/1/1/1
2	GLA	ZB	2	2	-	1/2/19/22	0/1/1/1
2	SIA	ZB	3	2	-	5/18/34/38	0/1/1/1
2	NAG	aA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	aA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	aA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	bA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	bA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	bA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	dA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	dA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	dA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	eA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	eA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	eA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	gA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	gA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	gA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	hA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	hA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	hA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	jA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	jA	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	jA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	kA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	kA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	kA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	mA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	mA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	mA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	nA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	nA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	nA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	pA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	pA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	pA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	qA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	qA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	qA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	sA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	sA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	sA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	tA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	tA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	tA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	vA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	vA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	vA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	wA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	wA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	wA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	yA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	yA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	yA	3	2	-	5/18/34/38	0/1/1/1
2	NAG	zA	1	2	-	2/6/26/26	0/1/1/1
2	GLA	zA	2	2	-	1/2/19/22	0/1/1/1
2	SIA	zA	3	2	-	5/18/34/38	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	3	SIA	O1B-C1	-3.01	1.21	1.30
2	IA	3	SIA	O1B-C1	-3.01	1.21	1.30
2	MA	3	SIA	O1B-C1	-3.01	1.21	1.30
2	dA	3	SIA	O1B-C1	-3.01	1.21	1.30
2	kA	3	SIA	O1B-C1	-3.01	1.21	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AA	1	NAG	O5-C1-C2	4.07	113.60	109.52
2	IA	1	NAG	O5-C1-C2	4.07	113.60	109.52
2	MA	1	NAG	O5-C1-C2	4.07	113.60	109.52
2	dA	1	NAG	O5-C1-C2	4.07	113.60	109.52
2	kA	1	NAG	O5-C1-C2	4.07	113.60	109.52

There are no chirality outliers.

5 of 480 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	9	3	SIA	C11-C10-N5-C5
2	AA	3	SIA	C11-C10-N5-C5
2	CA	3	SIA	C11-C10-N5-C5
2	DA	3	SIA	C11-C10-N5-C5
2	FA	3	SIA	C11-C10-N5-C5

There are no ring outliers.

180 monomers are involved in 240 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	RA	2	GLA	3	0
2	OA	1	NAG	2	0
2	bA	3	SIA	2	0
2	TB	3	SIA	2	0
2	aA	3	SIA	2	0
2	XA	2	GLA	3	0
2	bA	2	GLA	3	0
2	dA	1	NAG	2	0
2	wA	2	GLA	3	0
2	CA	3	SIA	2	0
2	GB	1	NAG	2	0
2	VB	1	NAG	2	0
2	zA	1	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AA	1	NAG	2	0
2	DB	3	SIA	2	0
2	DA	2	GLA	3	0
2	JB	1	NAG	2	0
2	VB	3	SIA	2	0
2	zA	3	SIA	2	0
2	8A	1	NAG	2	0
2	KB	2	GLA	3	0
2	HB	1	NAG	2	0
2	GB	3	SIA	2	0
2	qA	1	NAG	2	0
2	GB	2	GLA	3	0
2	mA	1	NAG	2	0
2	gA	2	GLA	3	0
2	CA	1	NAG	2	0
2	GA	1	NAG	2	0
2	ZB	1	NAG	2	0
2	DB	1	NAG	2	0
2	HB	2	GLA	3	0
2	TB	2	GLA	3	0
2	UA	2	GLA	3	0
2	dA	2	GLA	3	0
2	RA	3	SIA	2	0
2	PB	3	SIA	2	0
2	qA	2	GLA	3	0
2	JA	3	SIA	2	0
2	gA	1	NAG	2	0
2	mA	2	GLA	3	0
2	LA	2	GLA	3	0
2	OA	2	GLA	3	0
2	1A	2	GLA	3	0
2	nA	3	SIA	2	0
2	wA	3	SIA	2	0
2	7A	2	GLA	3	0
2	BB	3	SIA	2	0
2	1A	3	SIA	2	0
2	WB	2	GLA	3	0
2	FA	3	SIA	2	0
2	YA	2	GLA	3	0
2	wA	1	NAG	2	0
2	AA	2	GLA	3	0
2	pA	1	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BB	2	GLA	3	0
2	FA	2	GLA	3	0
2	eA	2	GLA	3	0
2	RA	1	NAG	2	0
2	JA	1	NAG	2	0
2	4A	1	NAG	2	0
2	jA	1	NAG	2	0
2	EB	1	NAG	2	0
2	AB	3	SIA	2	0
2	QB	3	SIA	2	0
2	8A	3	SIA	2	0
2	tA	3	SIA	2	0
2	PA	1	NAG	2	0
2	DA	1	NAG	2	0
2	SA	1	NAG	2	0
2	bA	1	NAG	2	0
2	5A	1	NAG	2	0
2	5A	2	GLA	3	0
2	yA	3	SIA	2	0
2	JB	2	GLA	3	0
2	MB	1	NAG	2	0
2	hA	3	SIA	2	0
2	YB	3	SIA	2	0
2	GA	2	GLA	3	0
2	dA	3	SIA	2	0
2	SA	2	GLA	3	0
2	EB	2	GLA	3	0
2	nA	2	GLA	3	0
2	JB	3	SIA	2	0
2	VB	2	GLA	3	0
2	ZB	3	SIA	2	0
2	HB	3	SIA	2	0
2	GA	3	SIA	2	0
2	LA	1	NAG	2	0
2	qA	3	SIA	2	0
2	PA	3	SIA	2	0
2	vA	3	SIA	2	0
2	mA	3	SIA	2	0
2	LA	3	SIA	2	0
2	SB	1	NAG	2	0
2	VA	1	NAG	2	0
2	SA	3	SIA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	VA	2	GLA	3	0
2	1A	1	NAG	2	0
2	hA	1	NAG	2	0
2	UA	1	NAG	2	0
2	9	2	GLA	3	0
2	9	1	NAG	2	0
2	SB	2	GLA	3	0
2	zA	2	GLA	3	0
2	jA	3	SIA	2	0
2	8A	2	GLA	3	0
2	AB	1	NAG	2	0
2	QB	1	NAG	2	0
2	YA	1	NAG	2	0
2	yA	2	GLA	3	0
2	EB	3	SIA	2	0
2	hA	2	GLA	3	0
2	2A	1	NAG	2	0
2	7A	1	NAG	2	0
2	pA	3	SIA	2	0
2	YB	2	GLA	3	0
2	MB	3	SIA	2	0
2	4A	3	SIA	2	0
2	pA	2	GLA	3	0
2	DB	2	GLA	3	0
2	AB	2	GLA	3	0
2	MB	2	GLA	3	0
2	eA	1	NAG	2	0
2	ZB	2	GLA	3	0
2	KB	1	NAG	2	0
2	4A	2	GLA	3	0
2	DA	3	SIA	2	0
2	IA	1	NAG	2	0
2	5A	3	SIA	2	0
2	PB	1	NAG	2	0
2	PA	2	GLA	3	0
2	MA	1	NAG	2	0
2	NB	1	NAG	2	0
2	kA	3	SIA	2	0
2	aA	1	NAG	2	0
2	MA	3	SIA	2	0
2	IA	2	GLA	3	0
2	nA	1	NAG	2	0

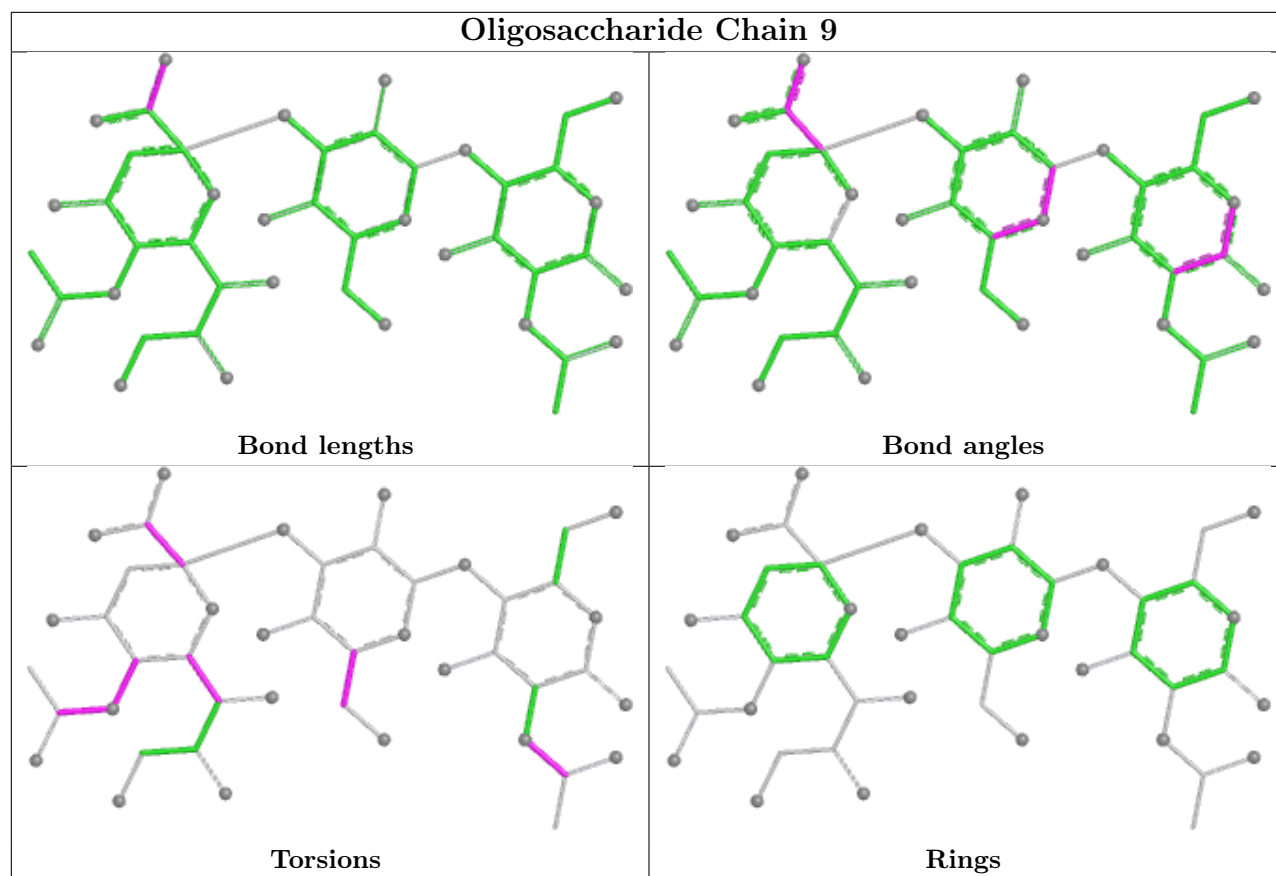
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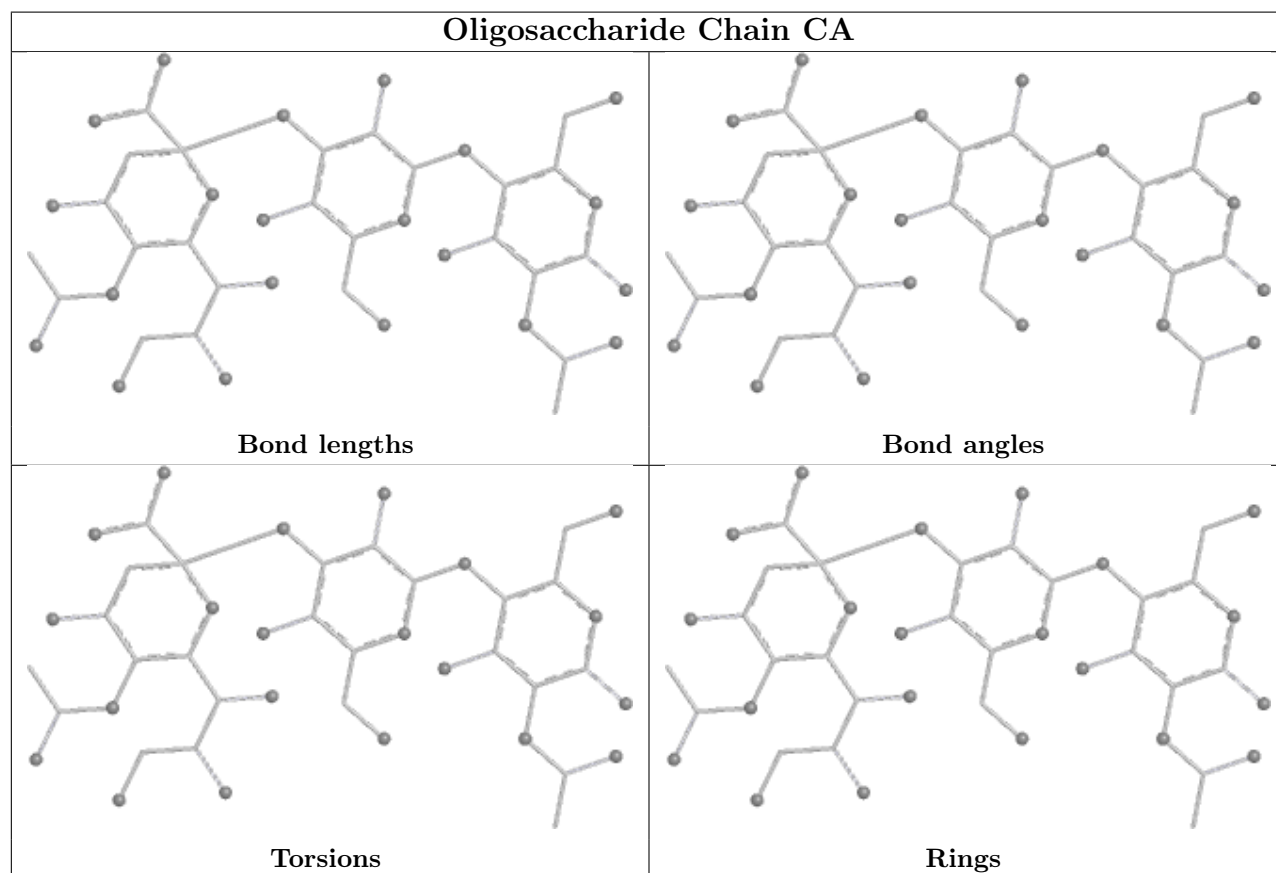
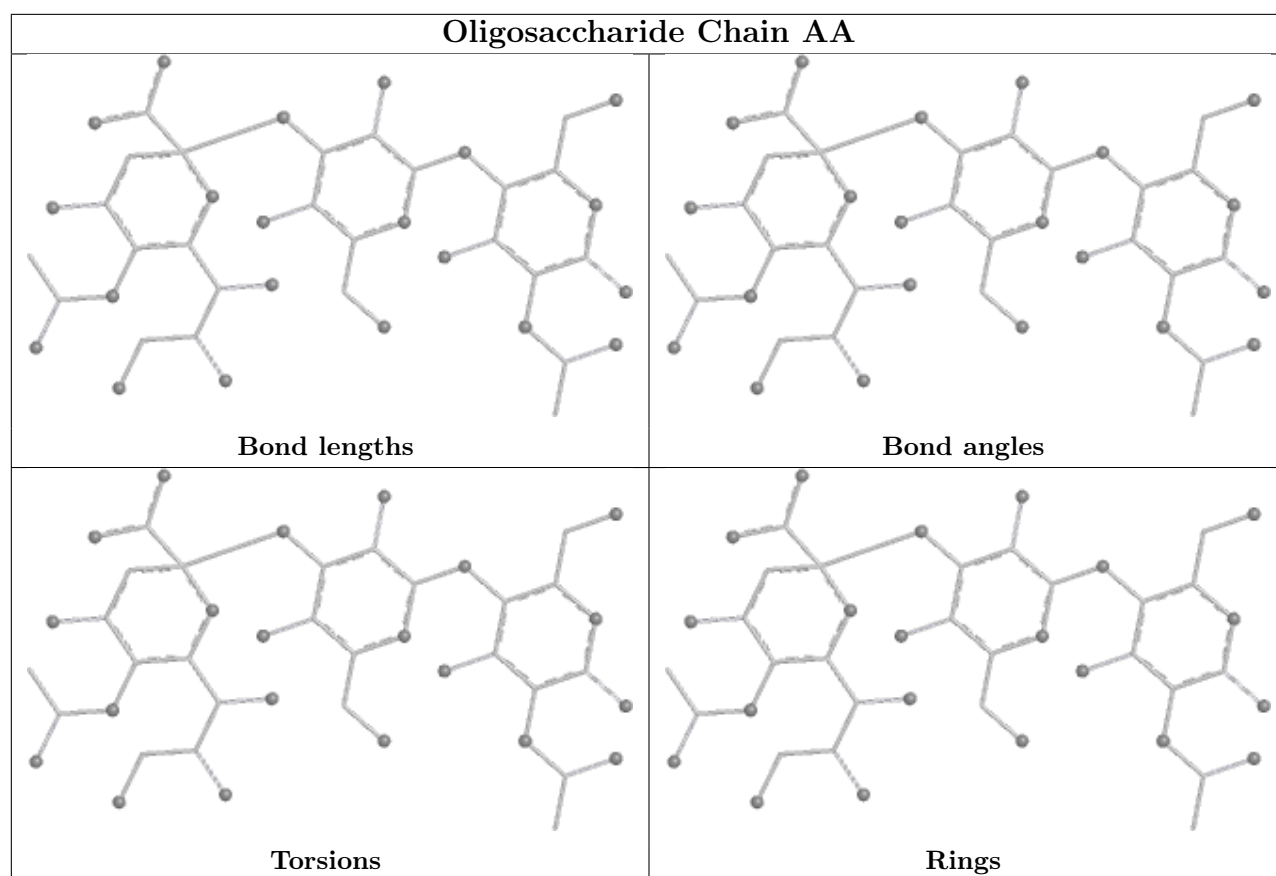
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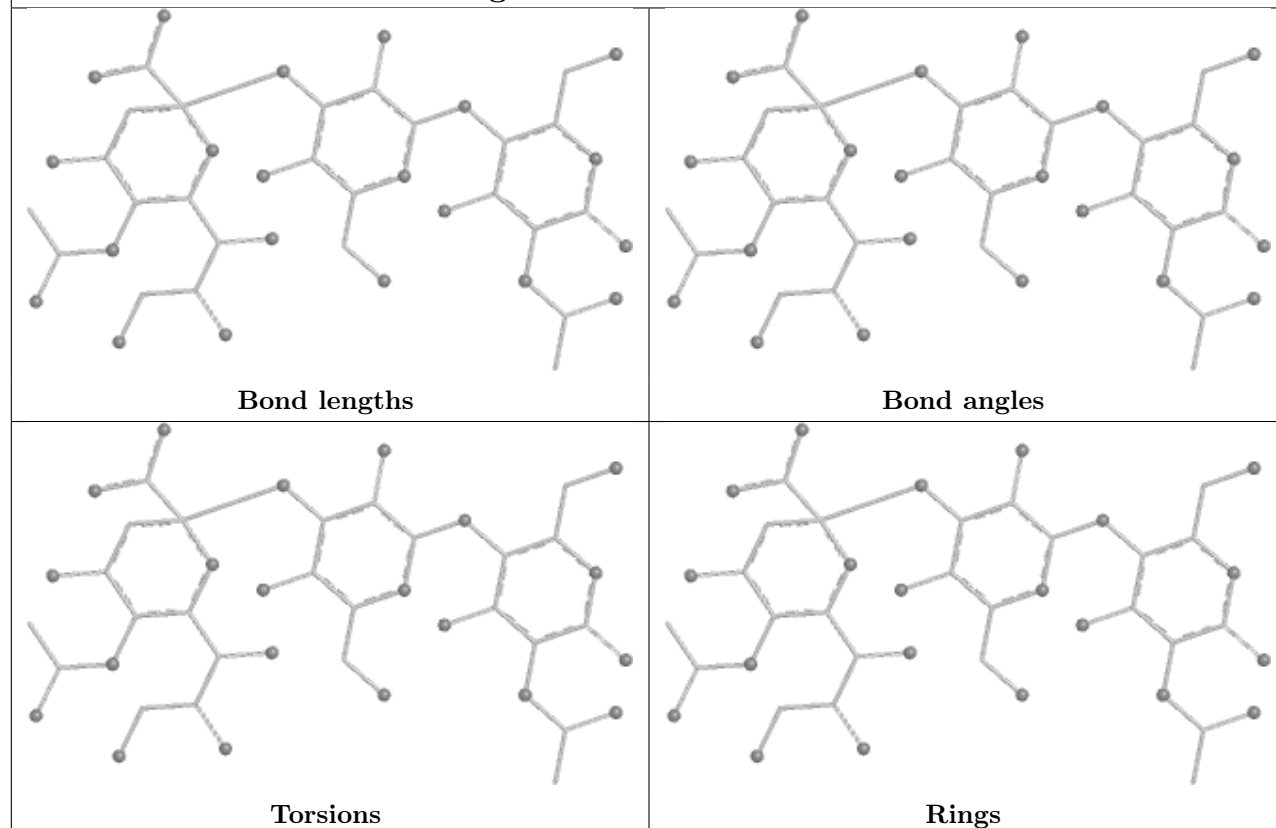
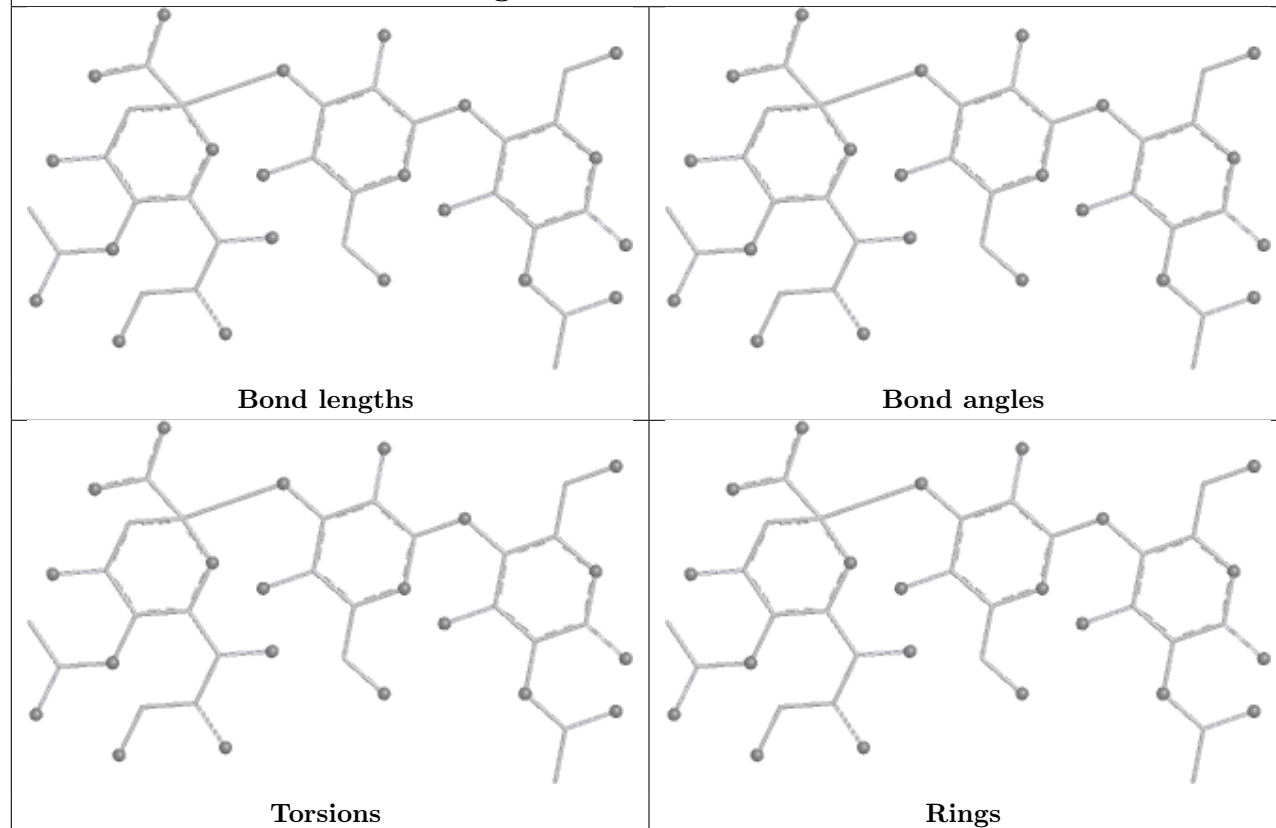
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	NB	3	SIA	2	0
2	sA	1	NAG	2	0
2	UA	3	SIA	2	0
2	MA	2	GLA	3	0
2	NB	2	GLA	3	0
2	XA	1	NAG	2	0
2	sA	3	SIA	2	0
2	QB	2	GLA	3	0
2	SB	3	SIA	2	0
2	jA	2	GLA	3	0
2	XA	3	SIA	2	0
2	KB	3	SIA	2	0
2	2A	2	GLA	3	0
2	WB	1	NAG	2	0
2	tA	1	NAG	2	0
2	YB	1	NAG	2	0
2	7A	3	SIA	2	0
2	vA	1	NAG	2	0
2	yA	1	NAG	2	0
2	WB	3	SIA	2	0
2	CA	2	GLA	3	0
2	IA	3	SIA	2	0
2	VA	3	SIA	2	0
2	9	3	SIA	2	0
2	2A	3	SIA	2	0
2	eA	3	SIA	2	0
2	AA	3	SIA	2	0
2	kA	1	NAG	2	0
2	sA	2	GLA	3	0
2	YA	3	SIA	2	0
2	tA	2	GLA	3	0
2	vA	2	GLA	3	0
2	kA	2	GLA	3	0
2	BB	1	NAG	2	0
2	FA	1	NAG	2	0
2	aA	2	GLA	3	0
2	JA	2	GLA	3	0
2	TB	1	NAG	2	0
2	gA	3	SIA	2	0
2	OA	3	SIA	2	0
2	PB	2	GLA	3	0

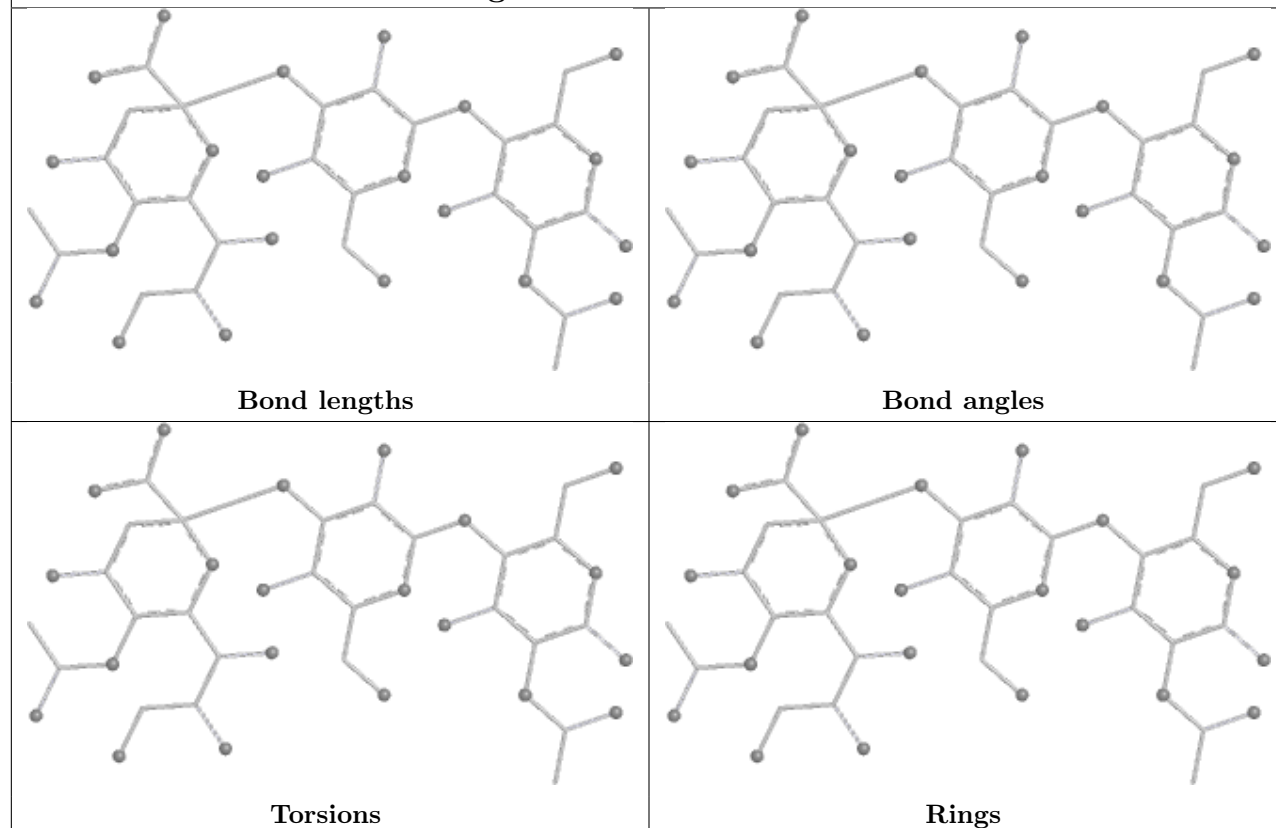
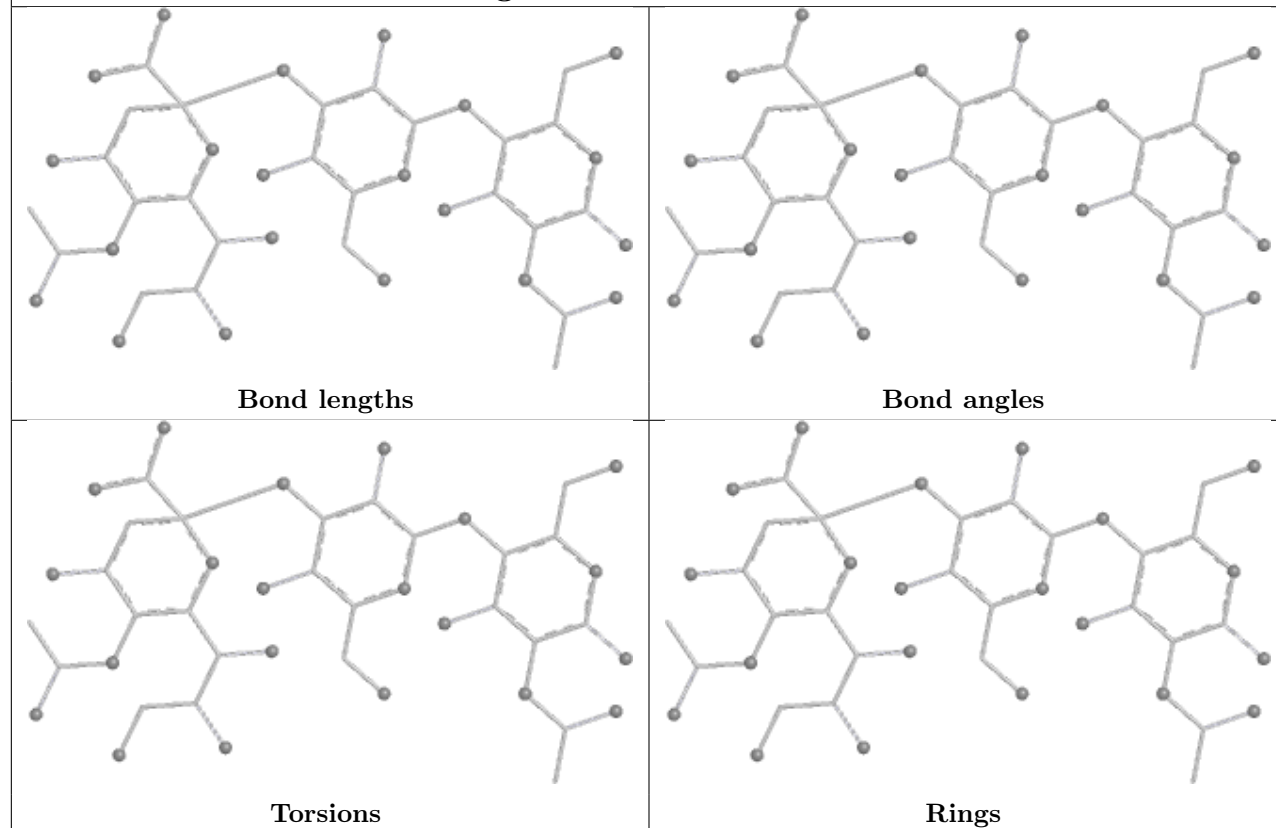
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

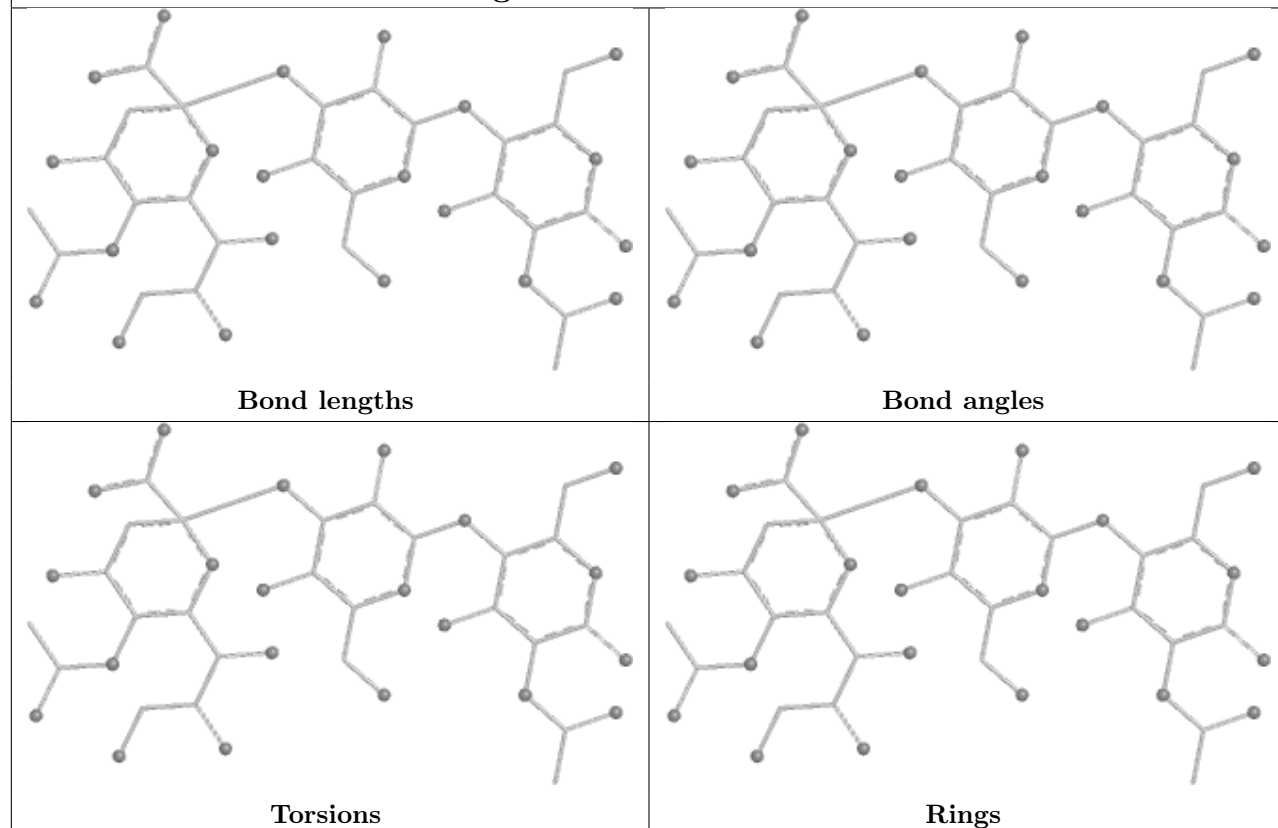
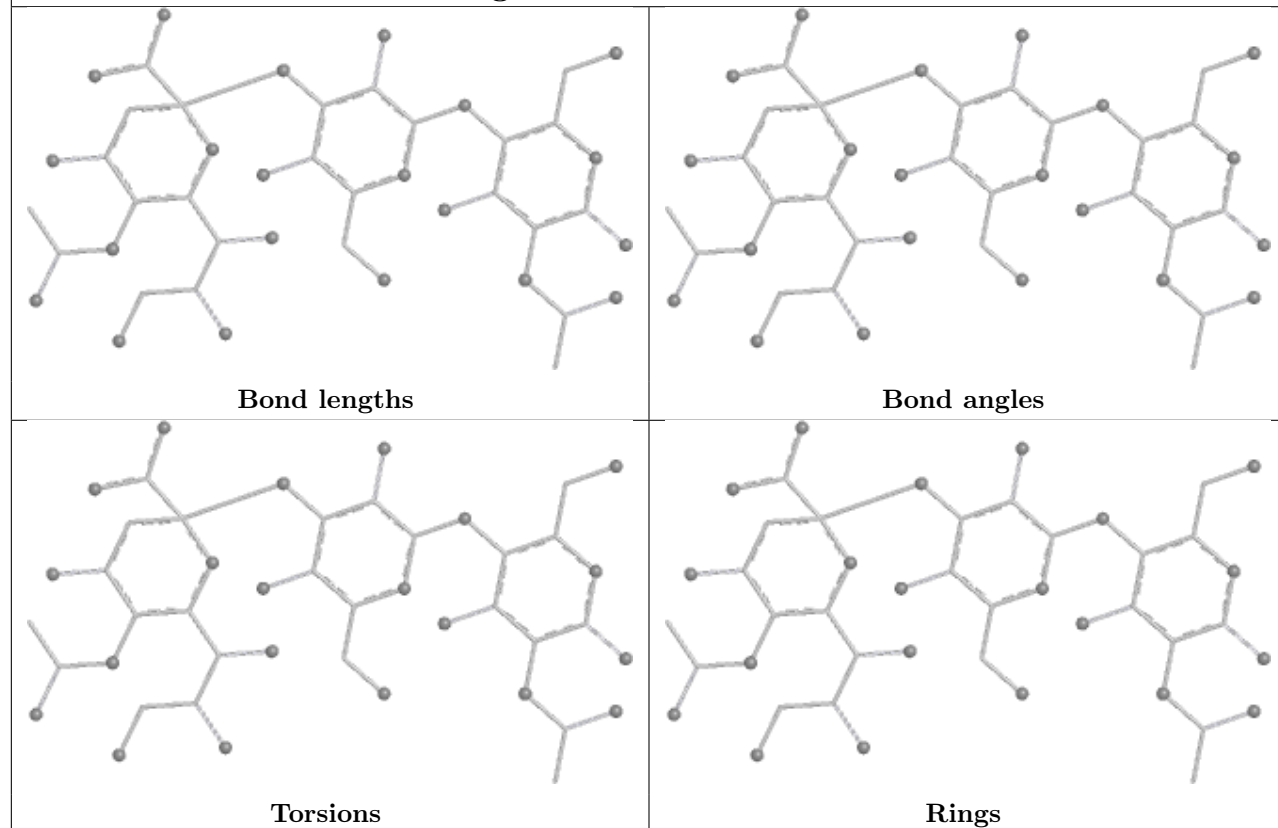
bond angles, torsion angles, and ring geometry for oligosaccharide.

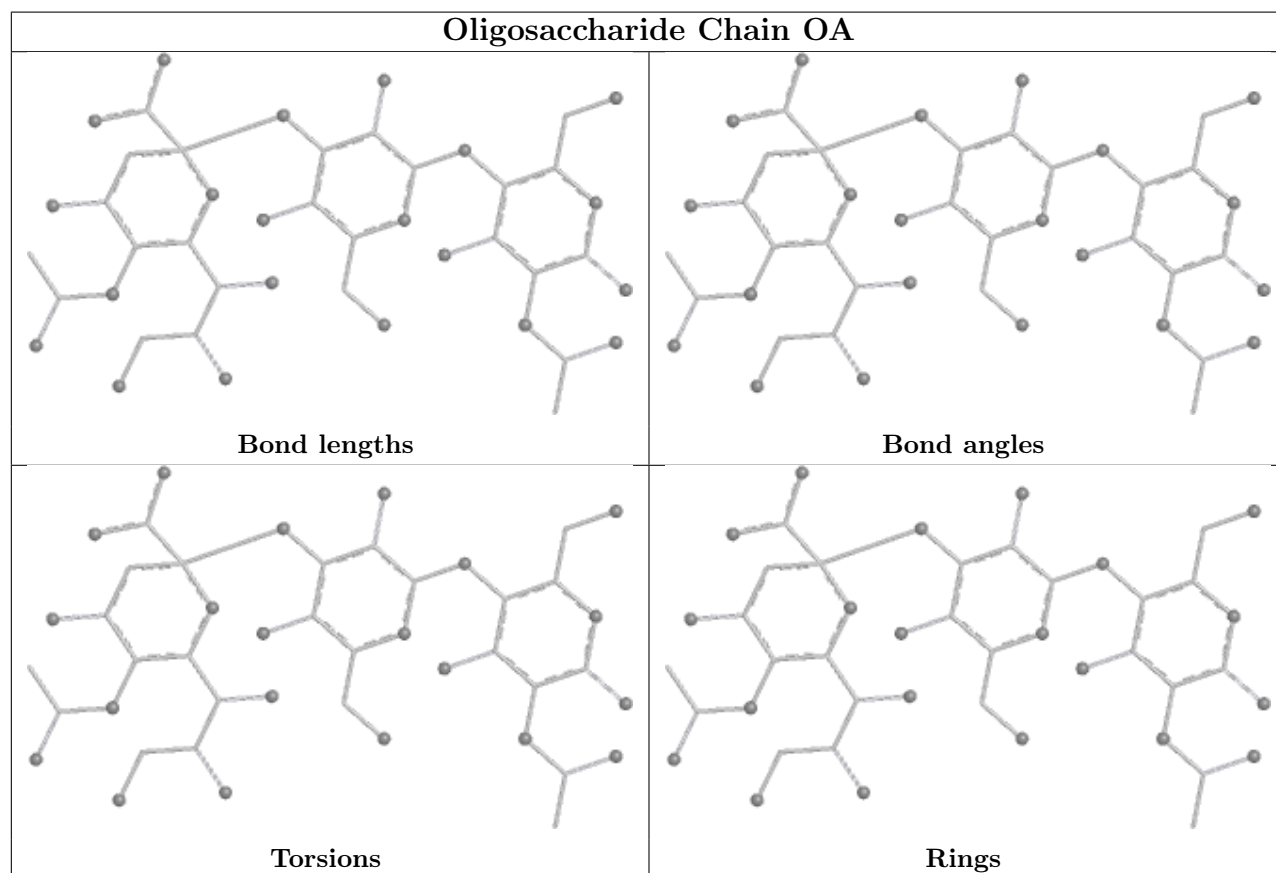
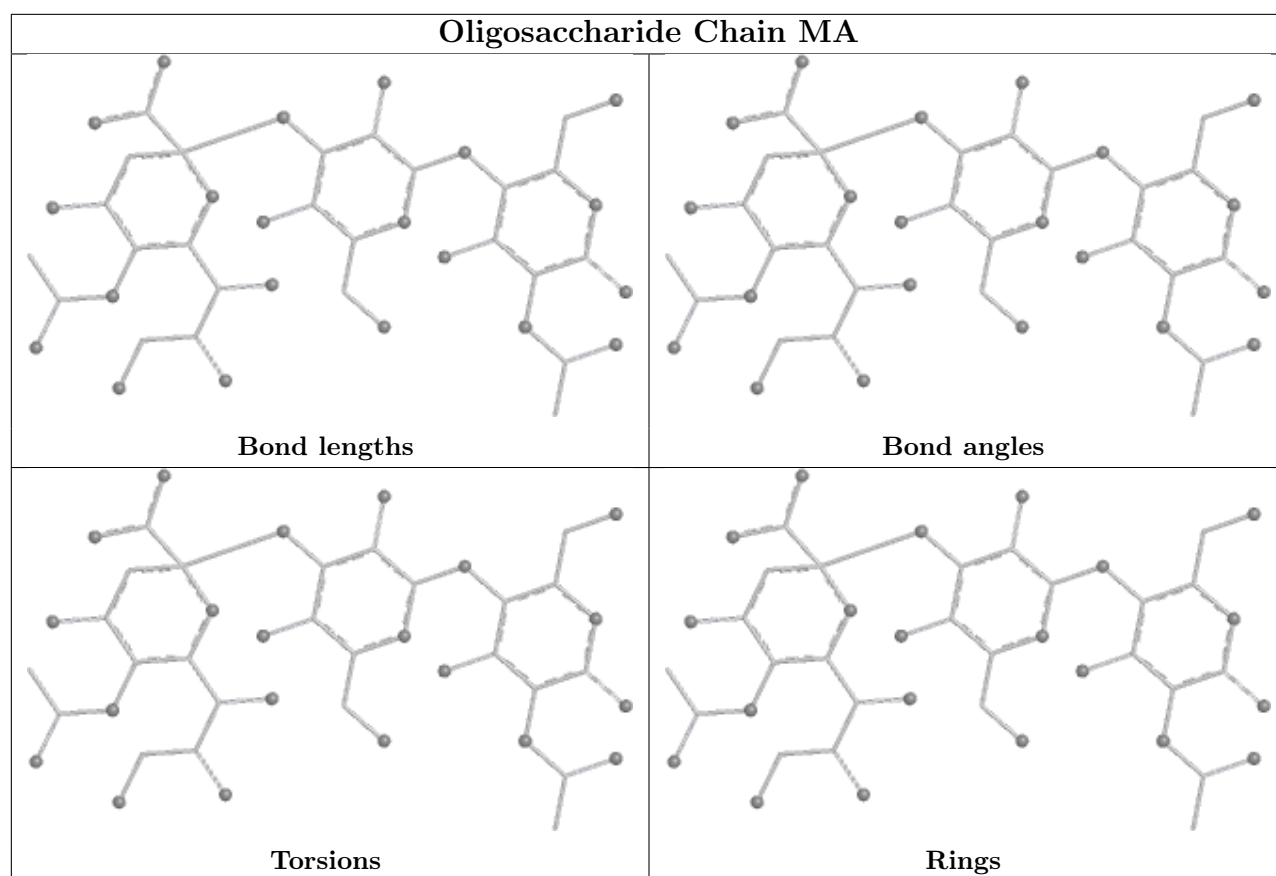


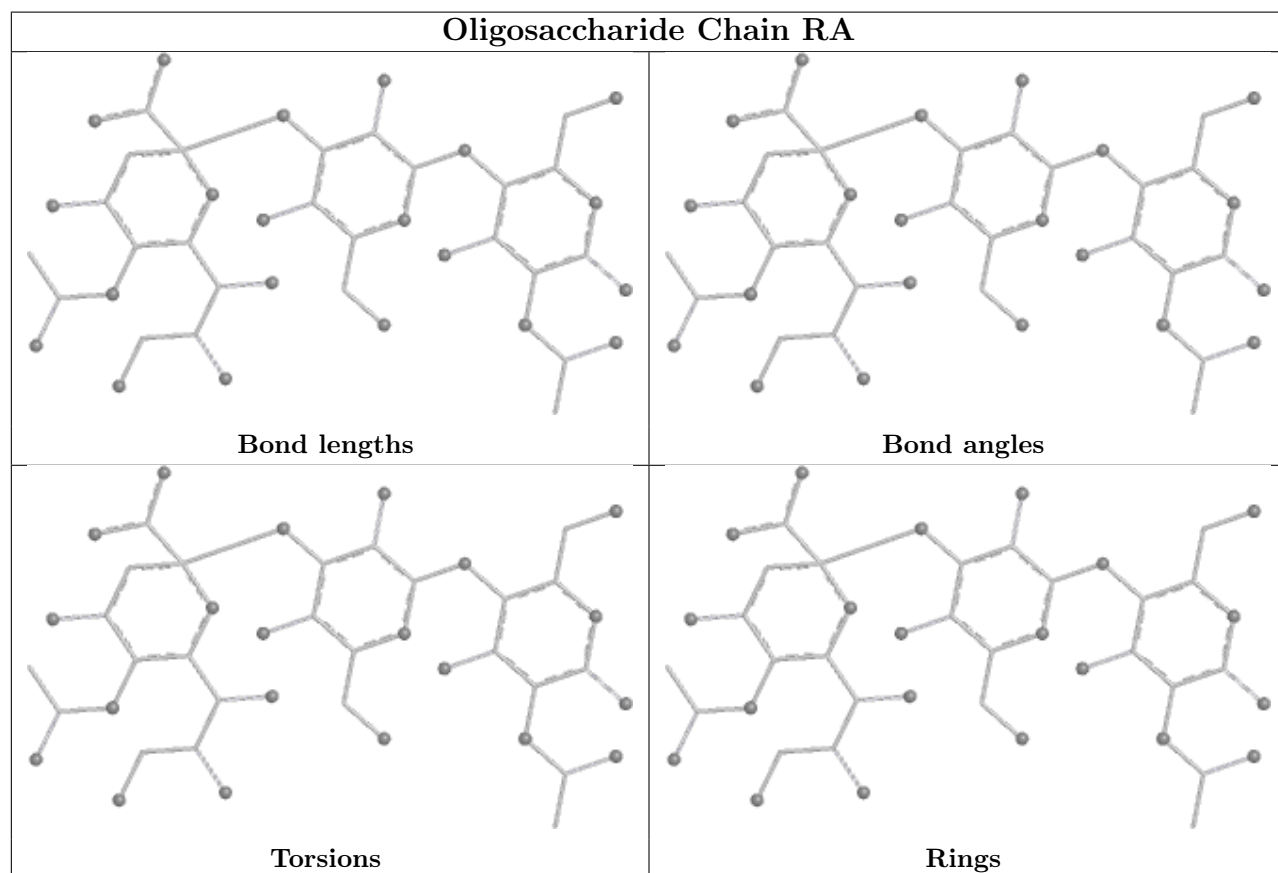
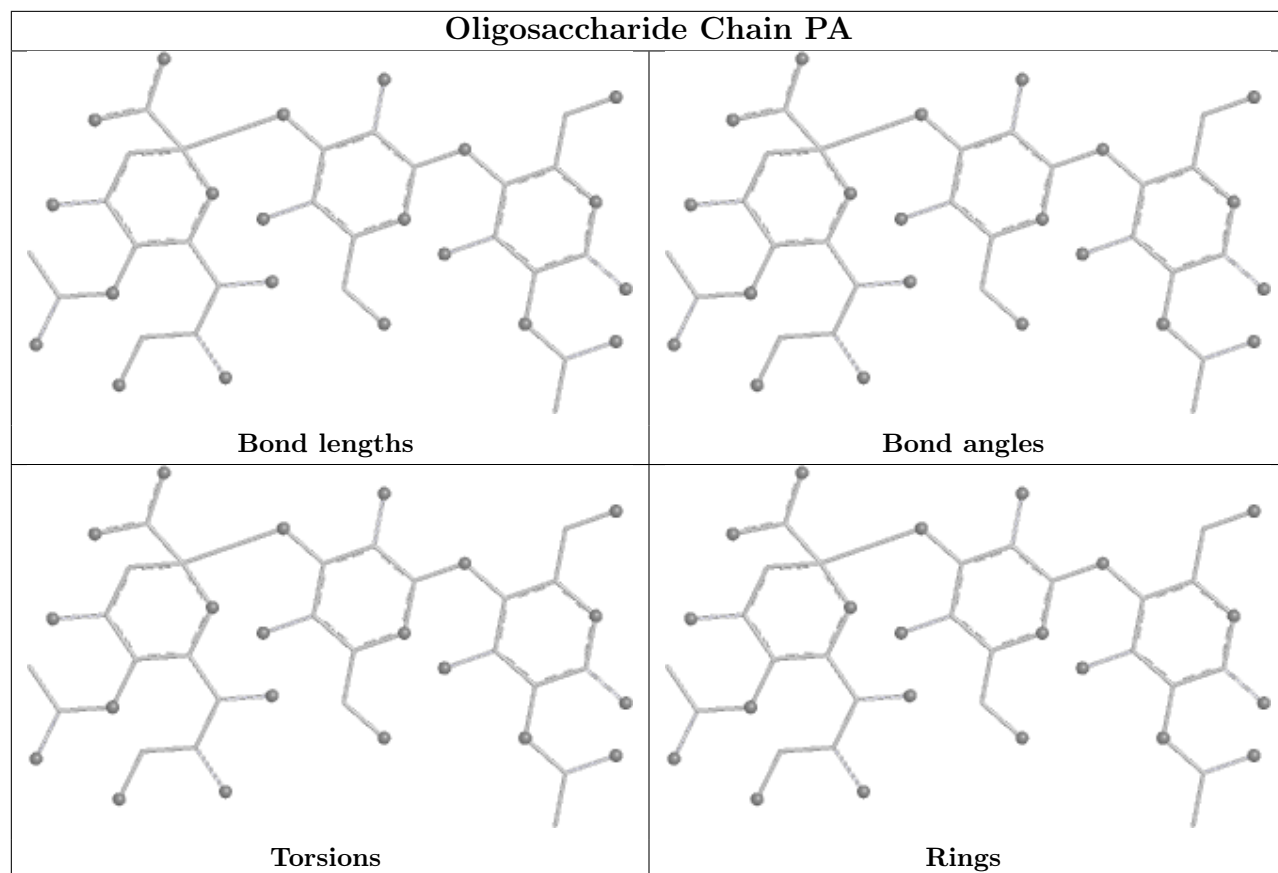


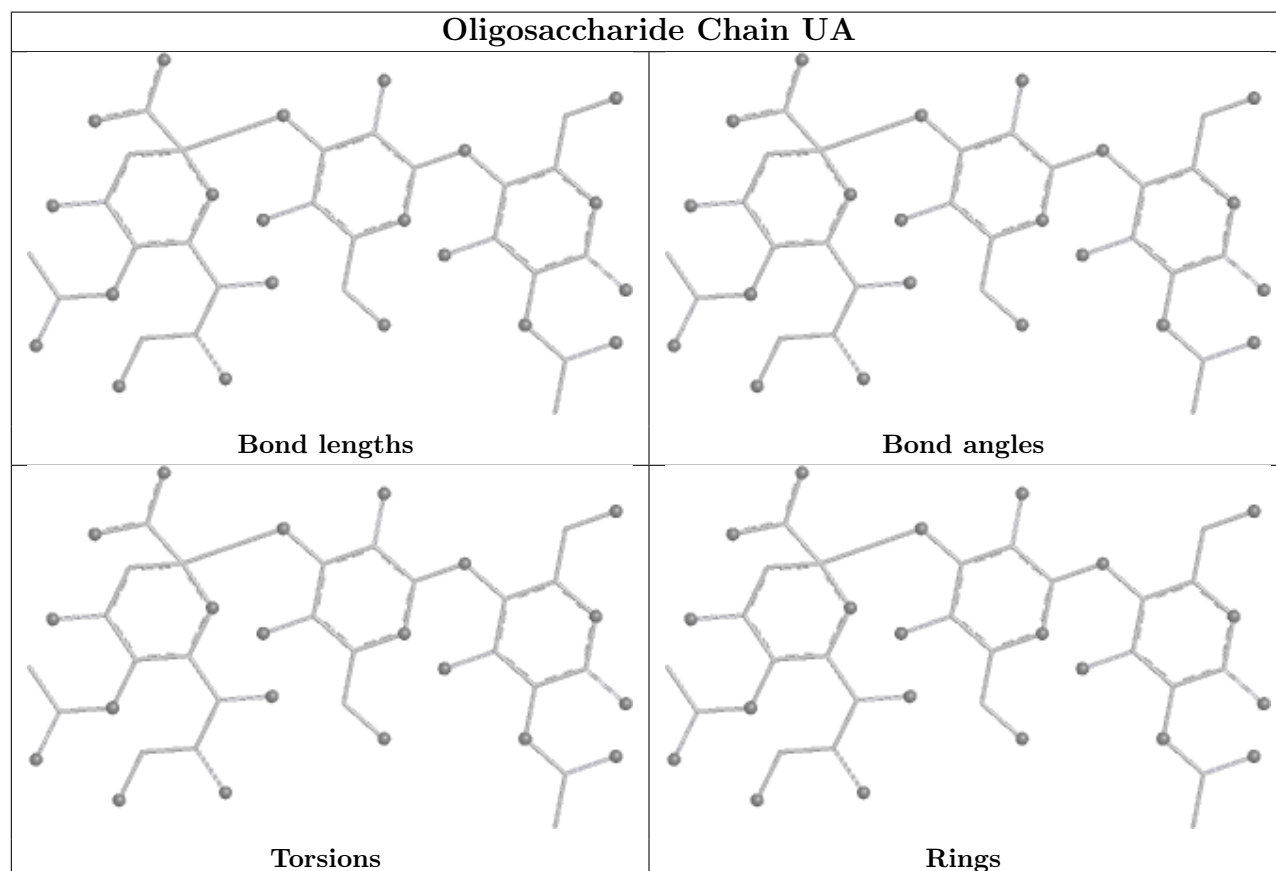
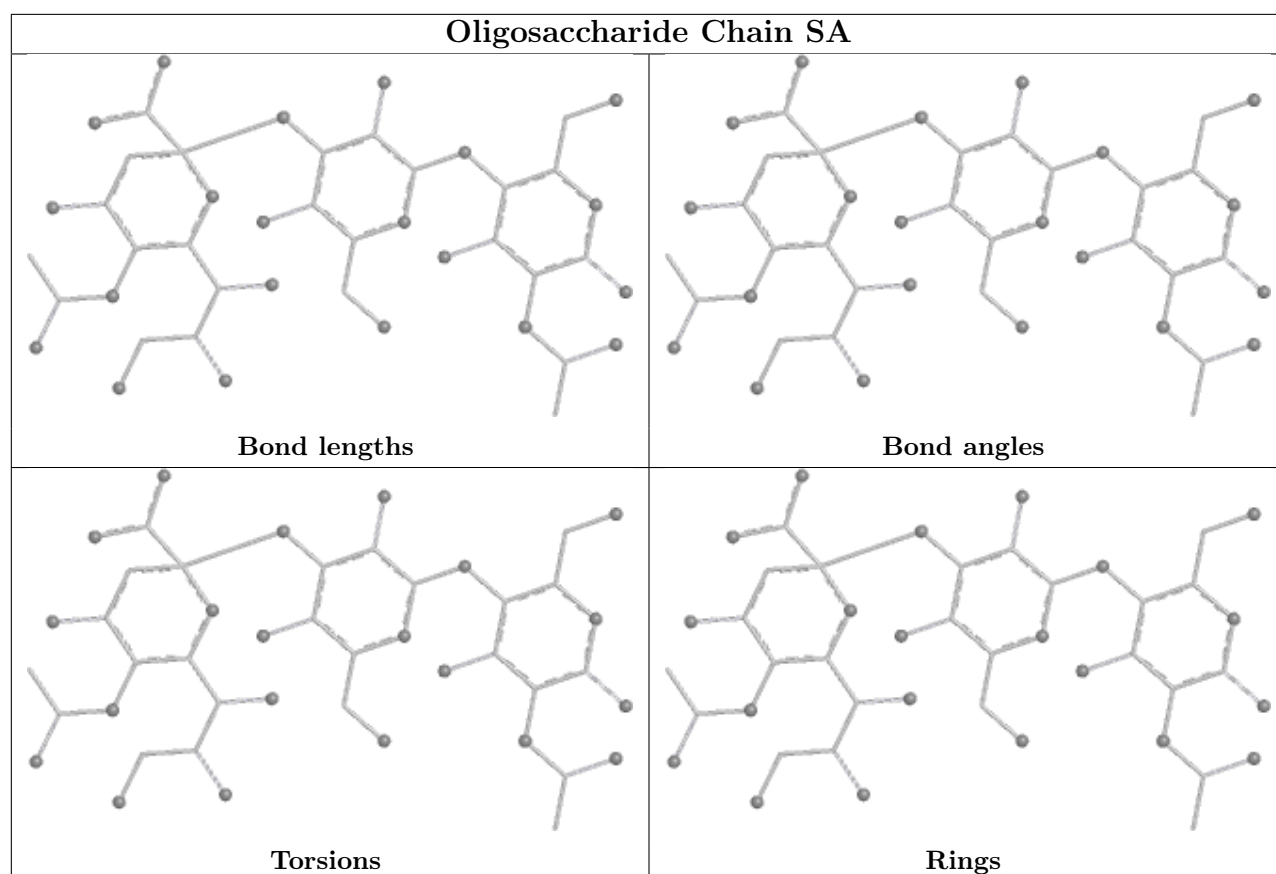
Oligosaccharide Chain DA**Oligosaccharide Chain FA**

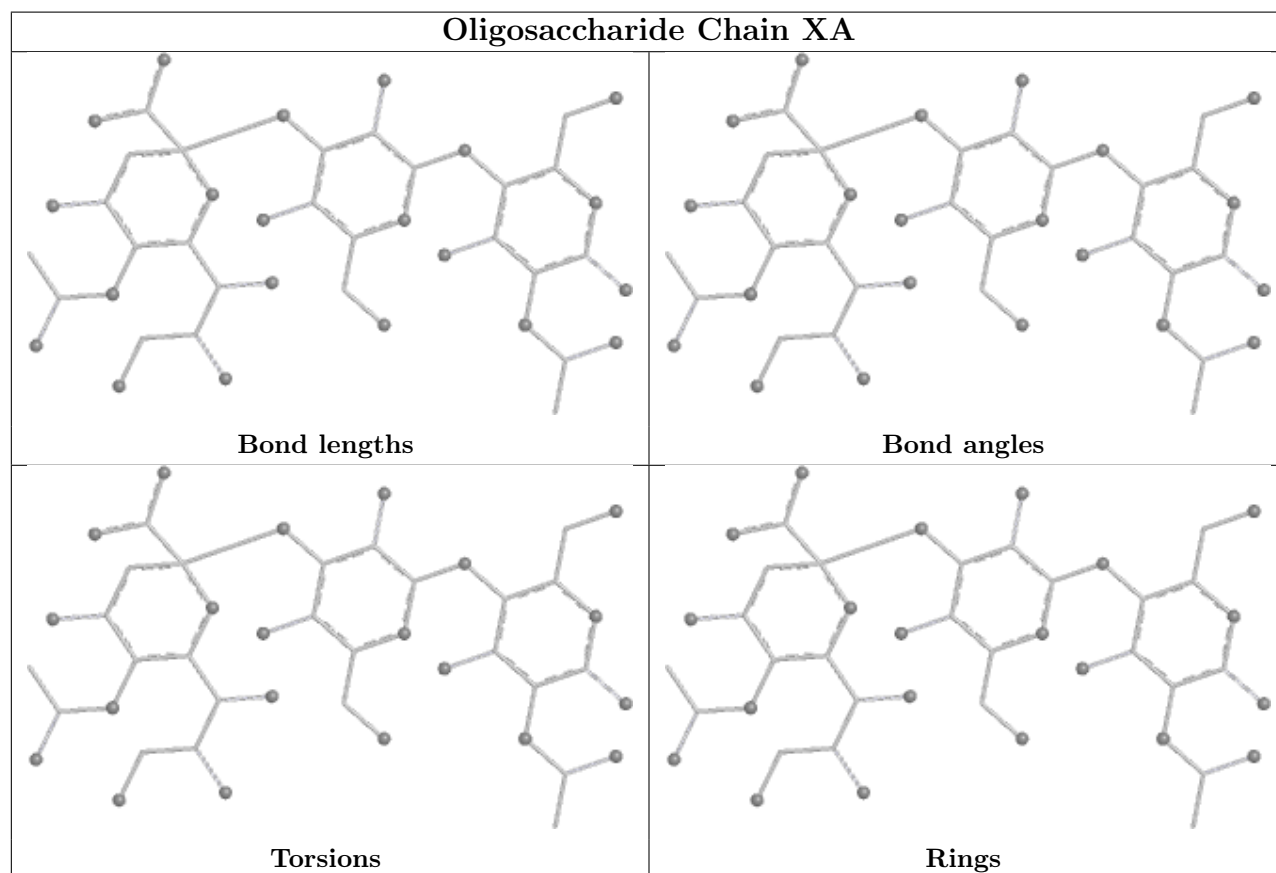
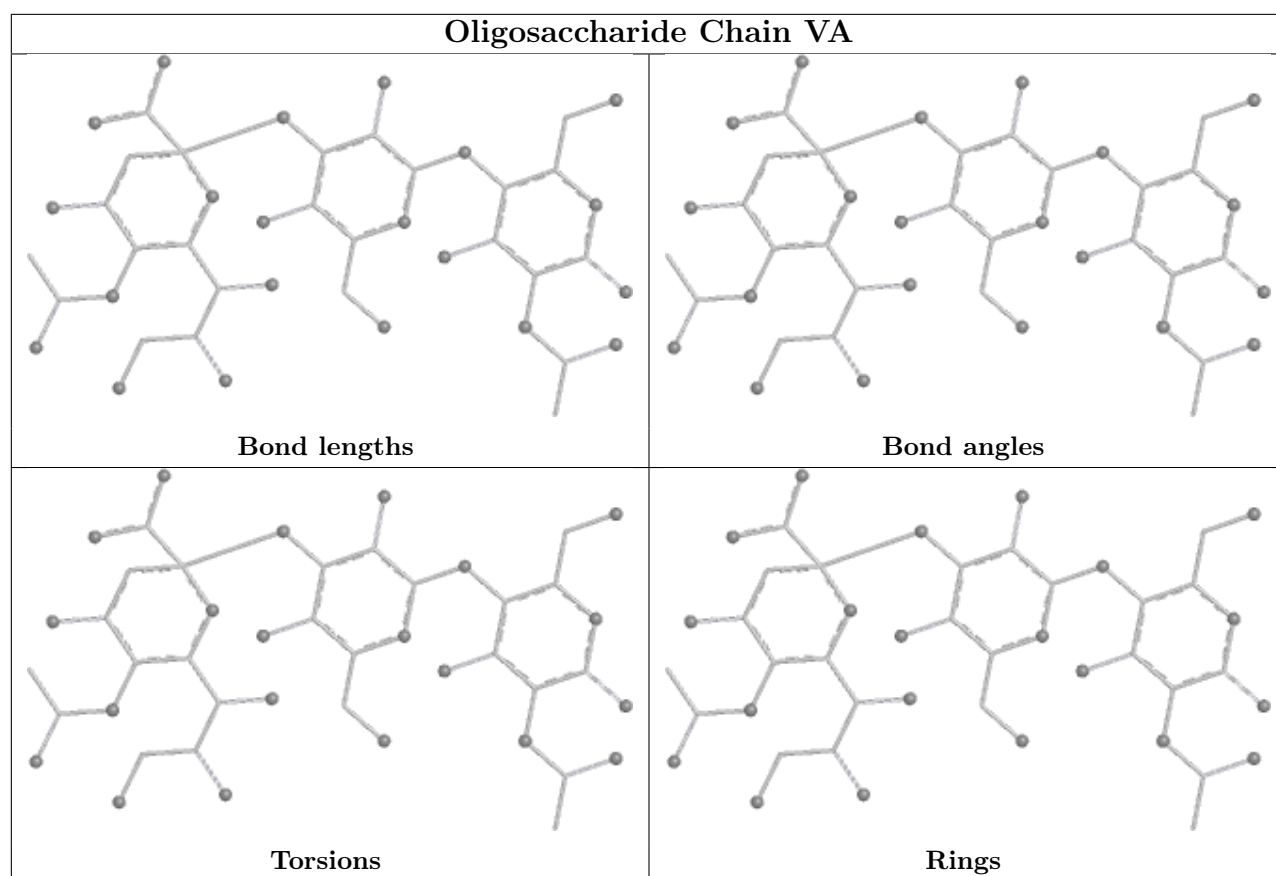
Oligosaccharide Chain GA**Oligosaccharide Chain IA**

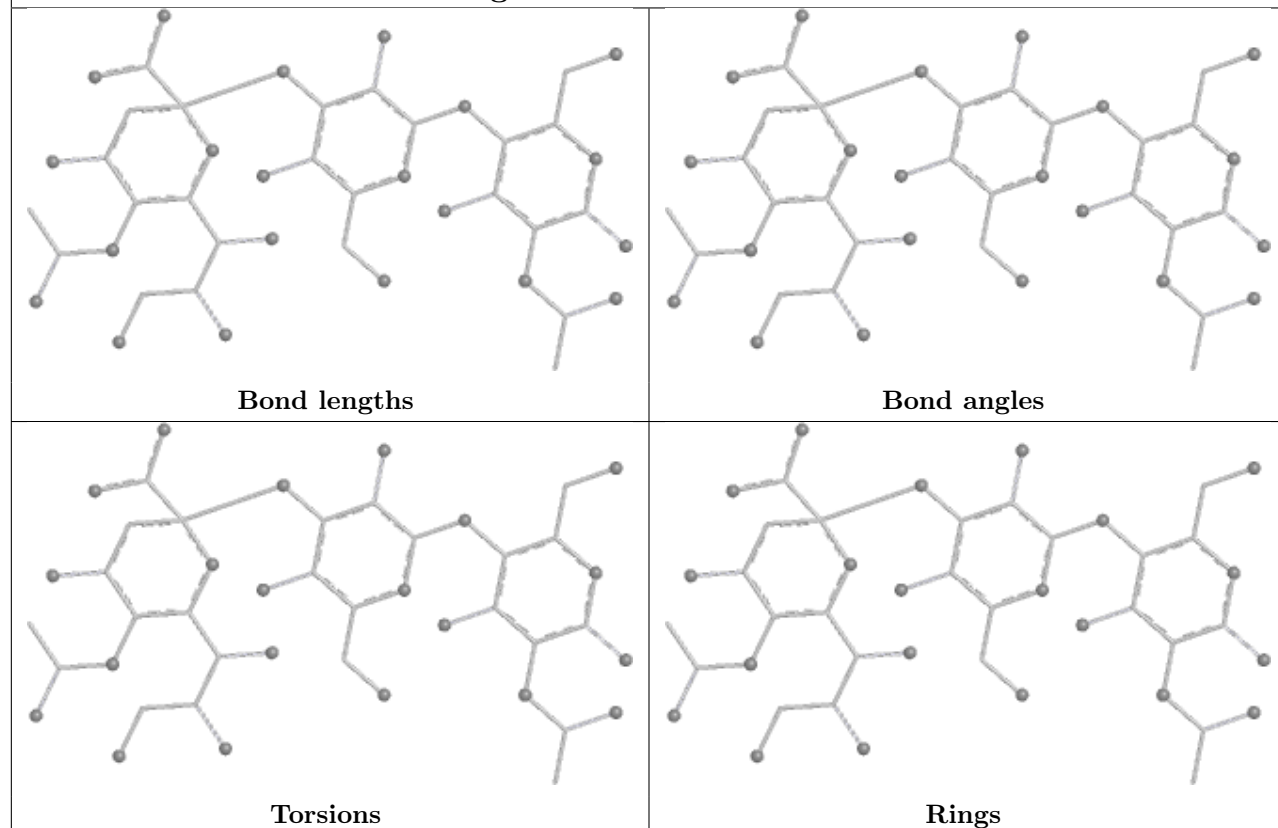
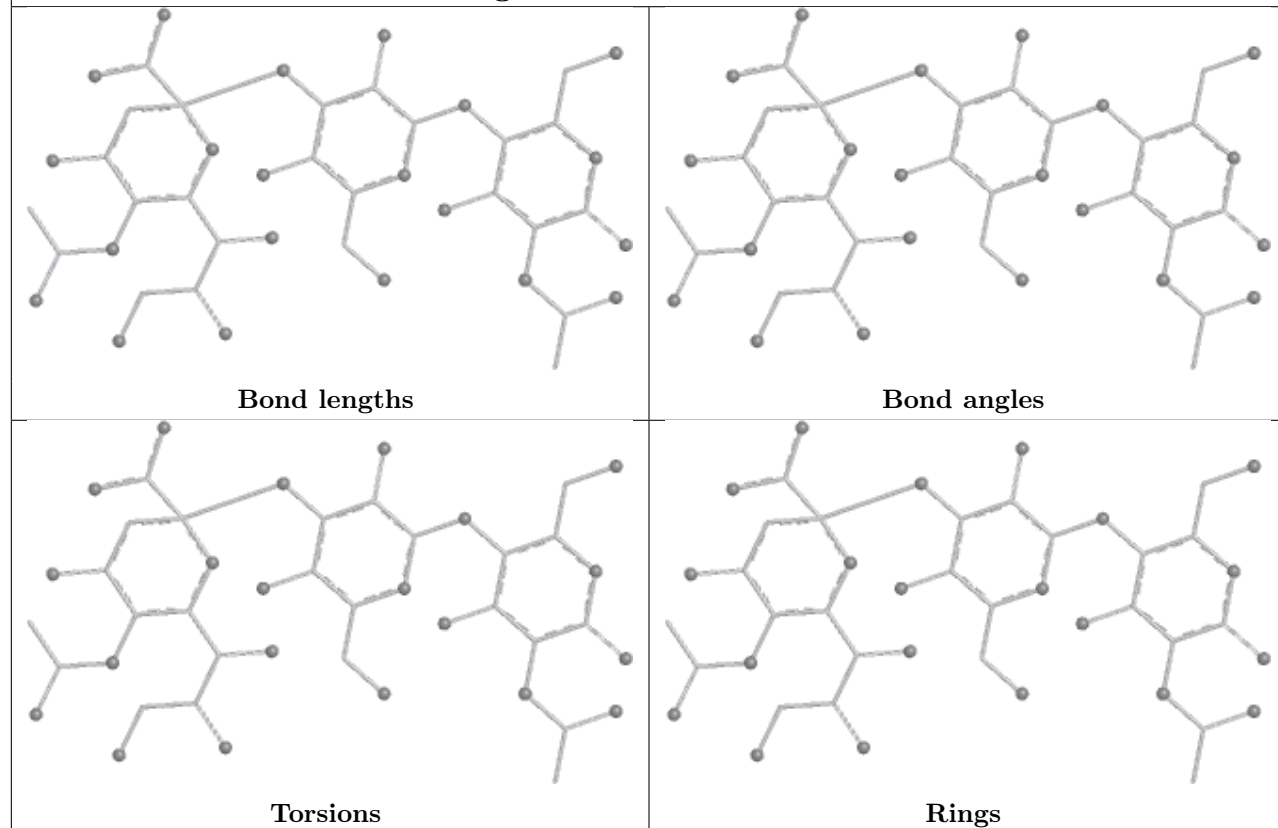
Oligosaccharide Chain JA**Oligosaccharide Chain LA**

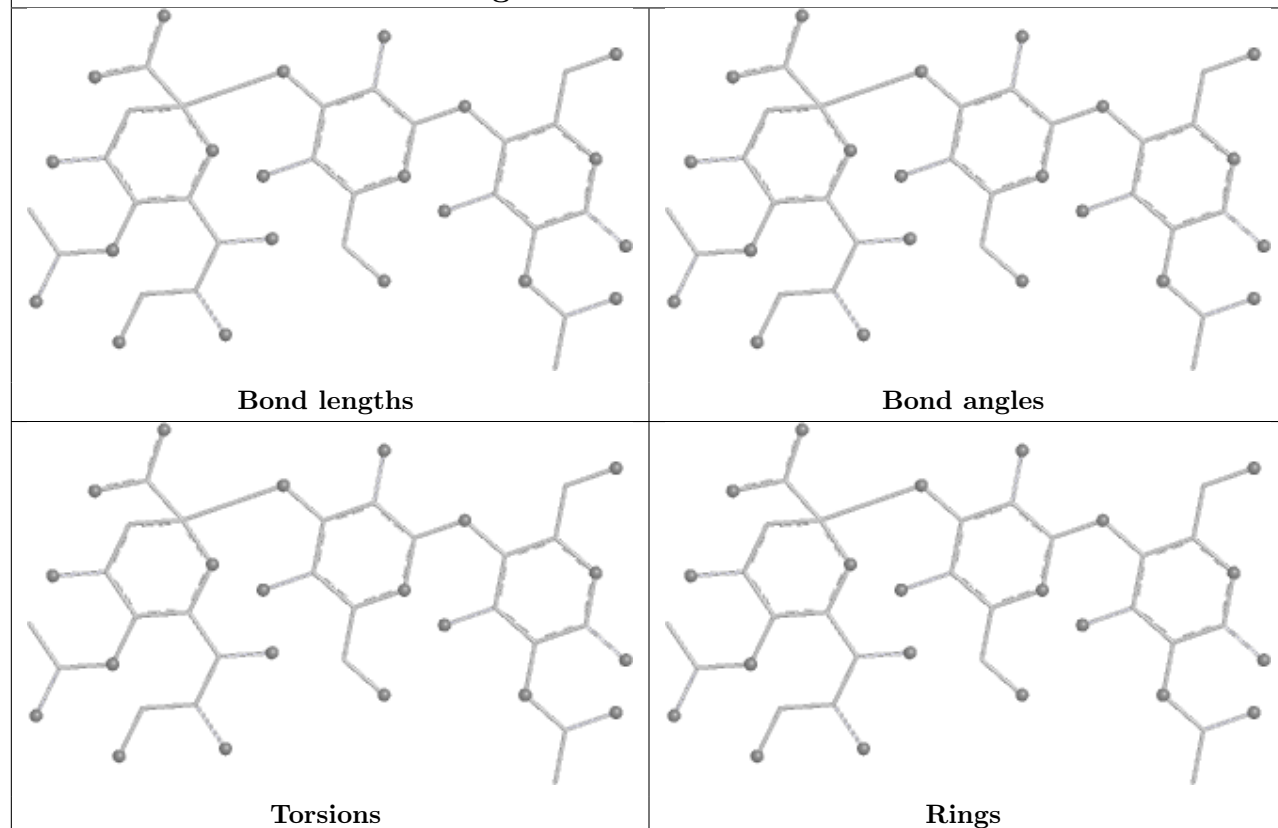
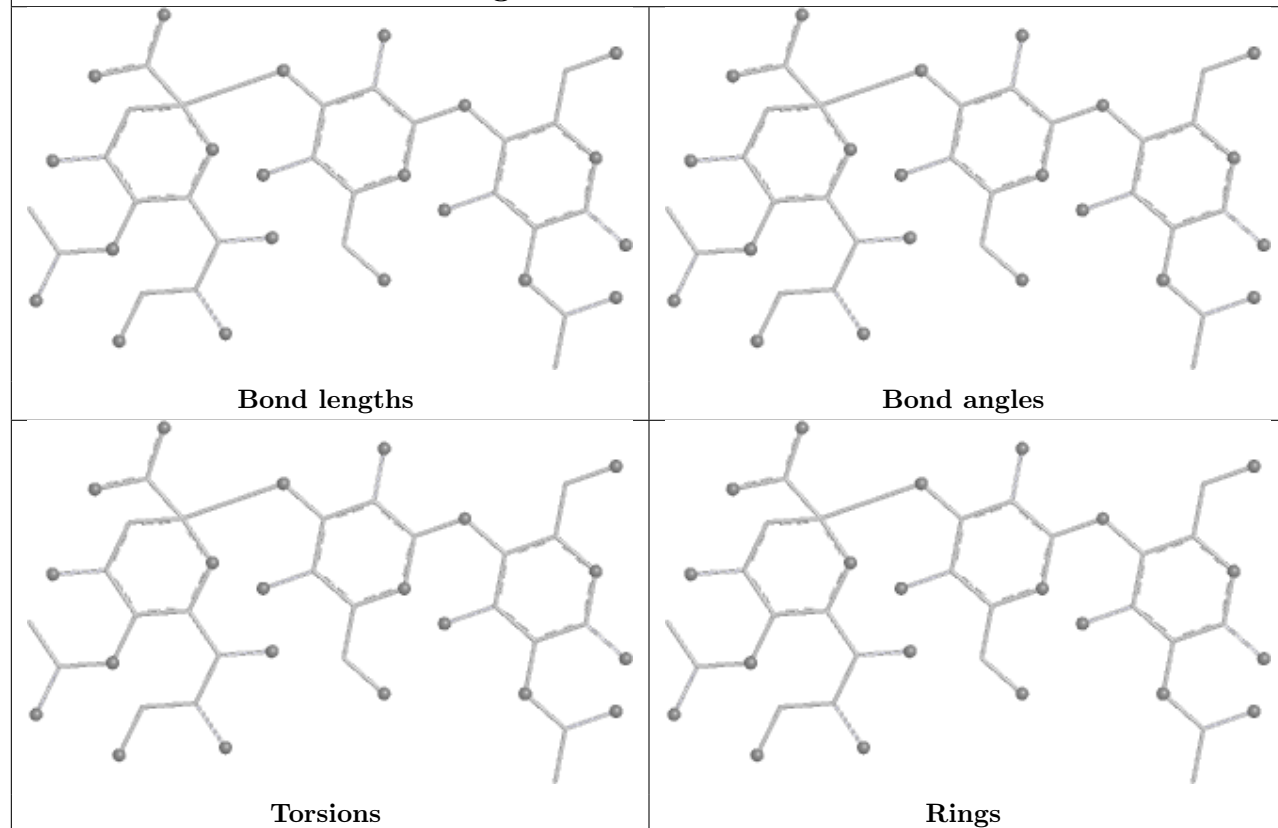


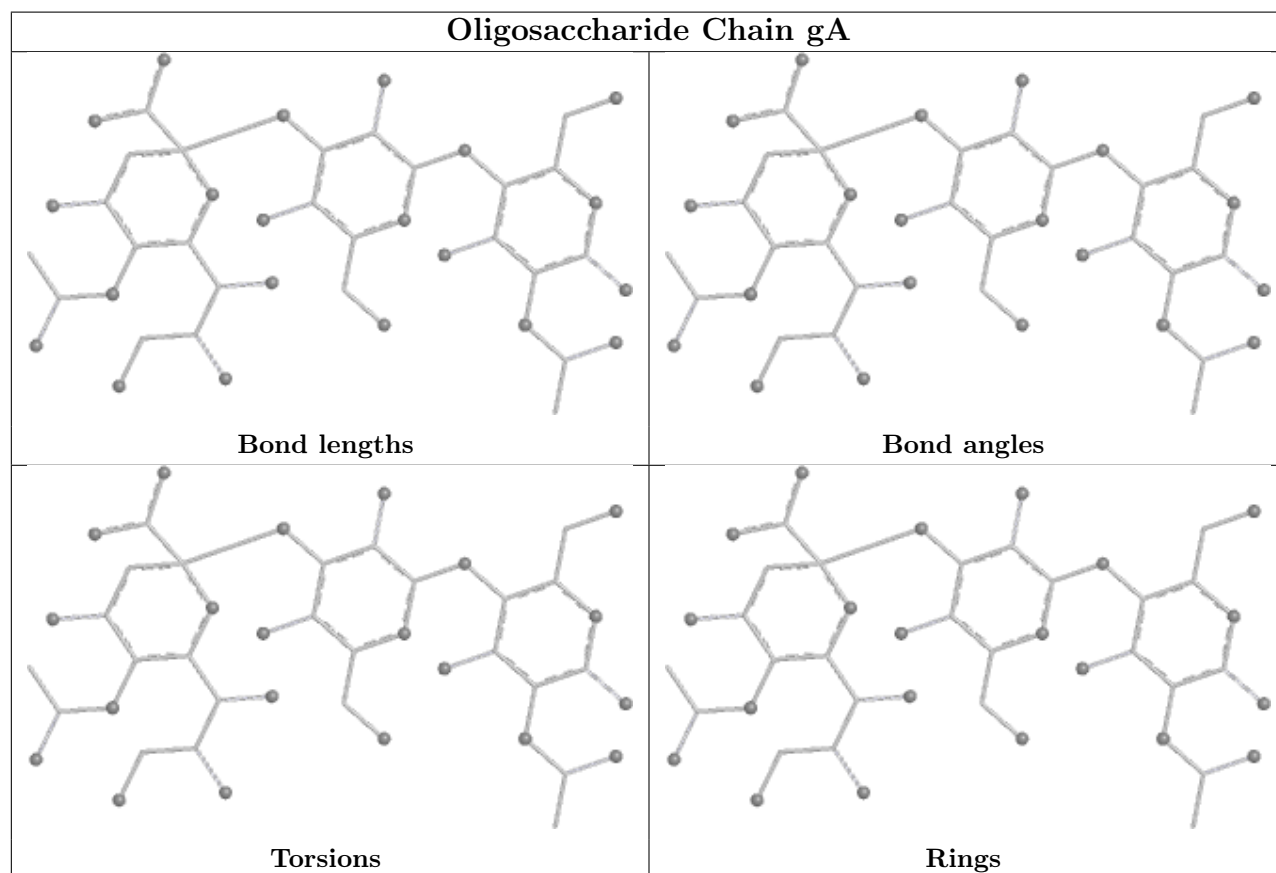
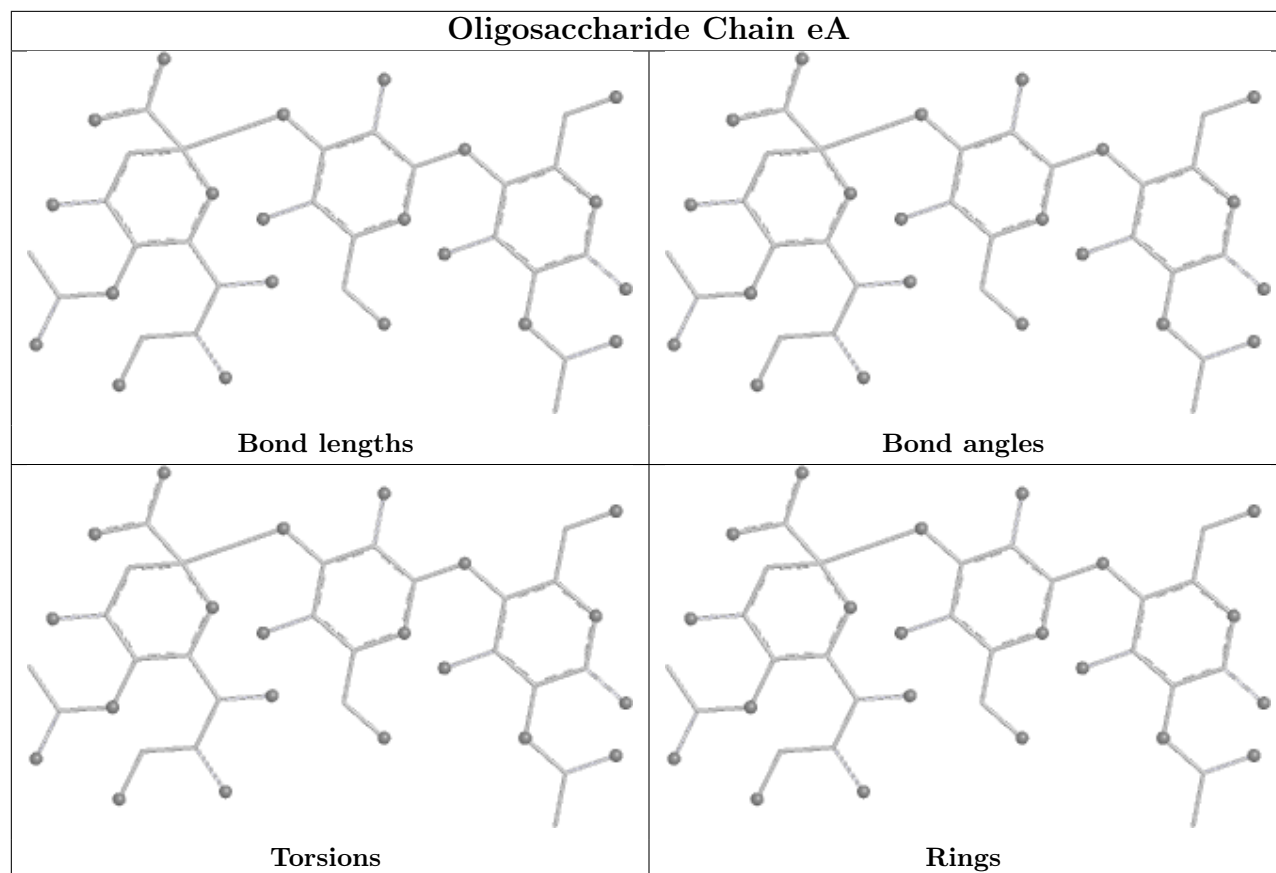


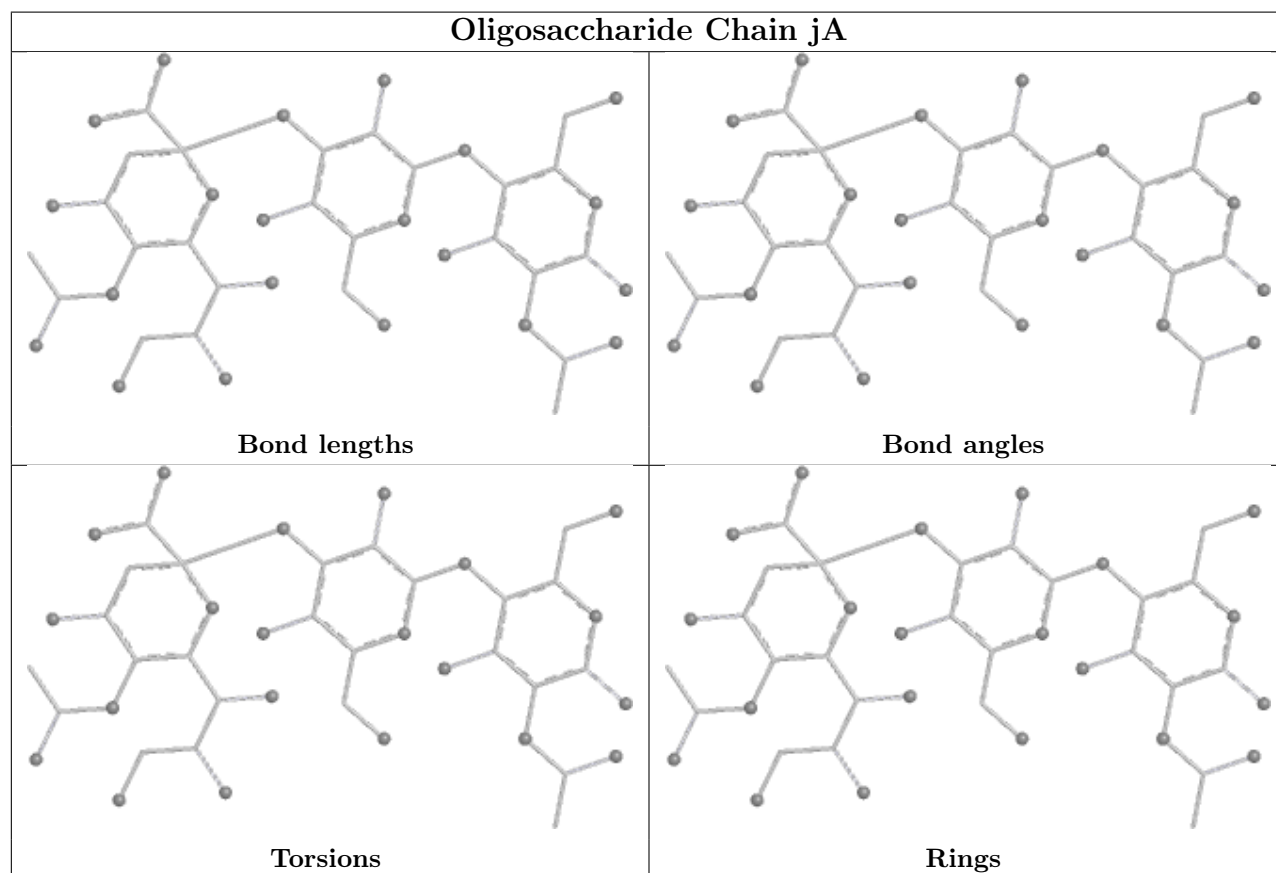
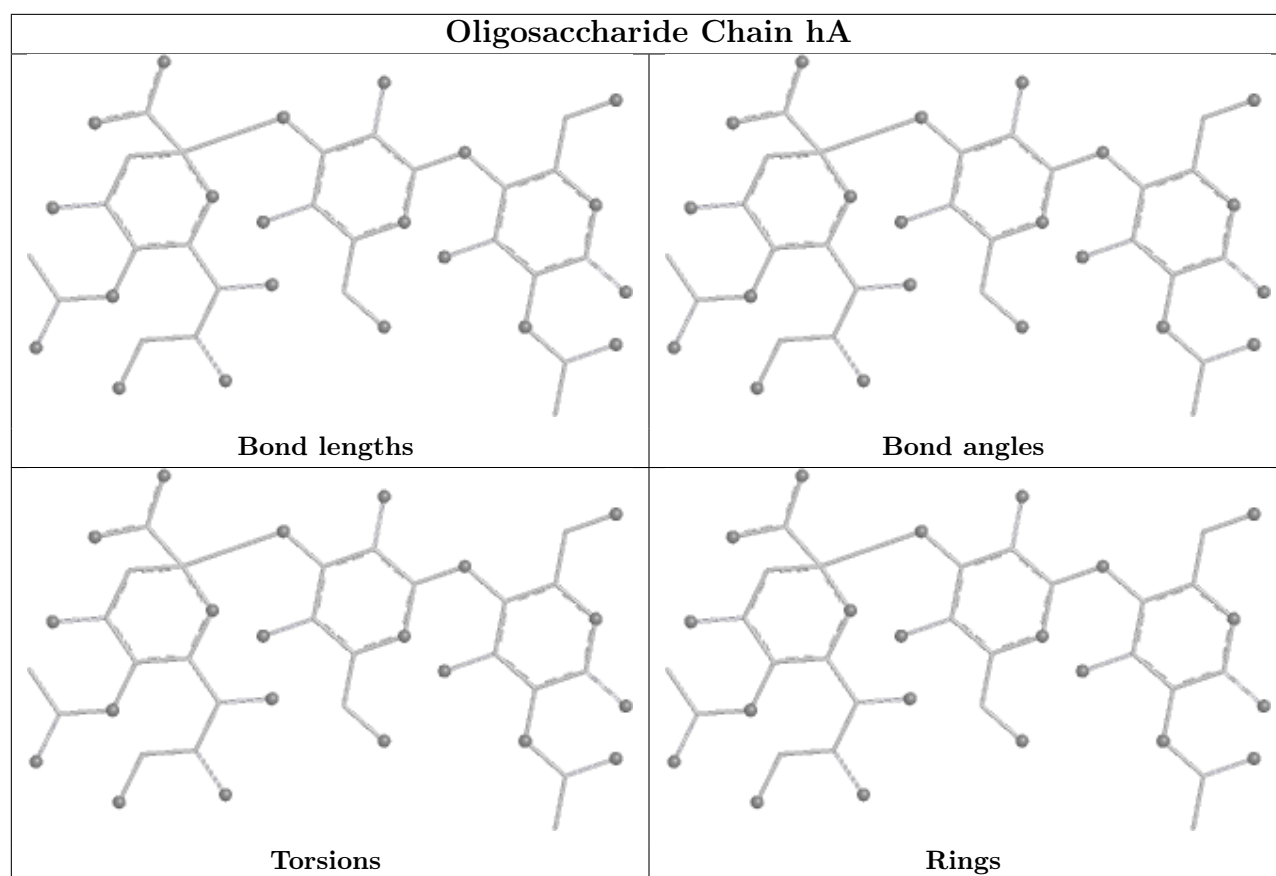


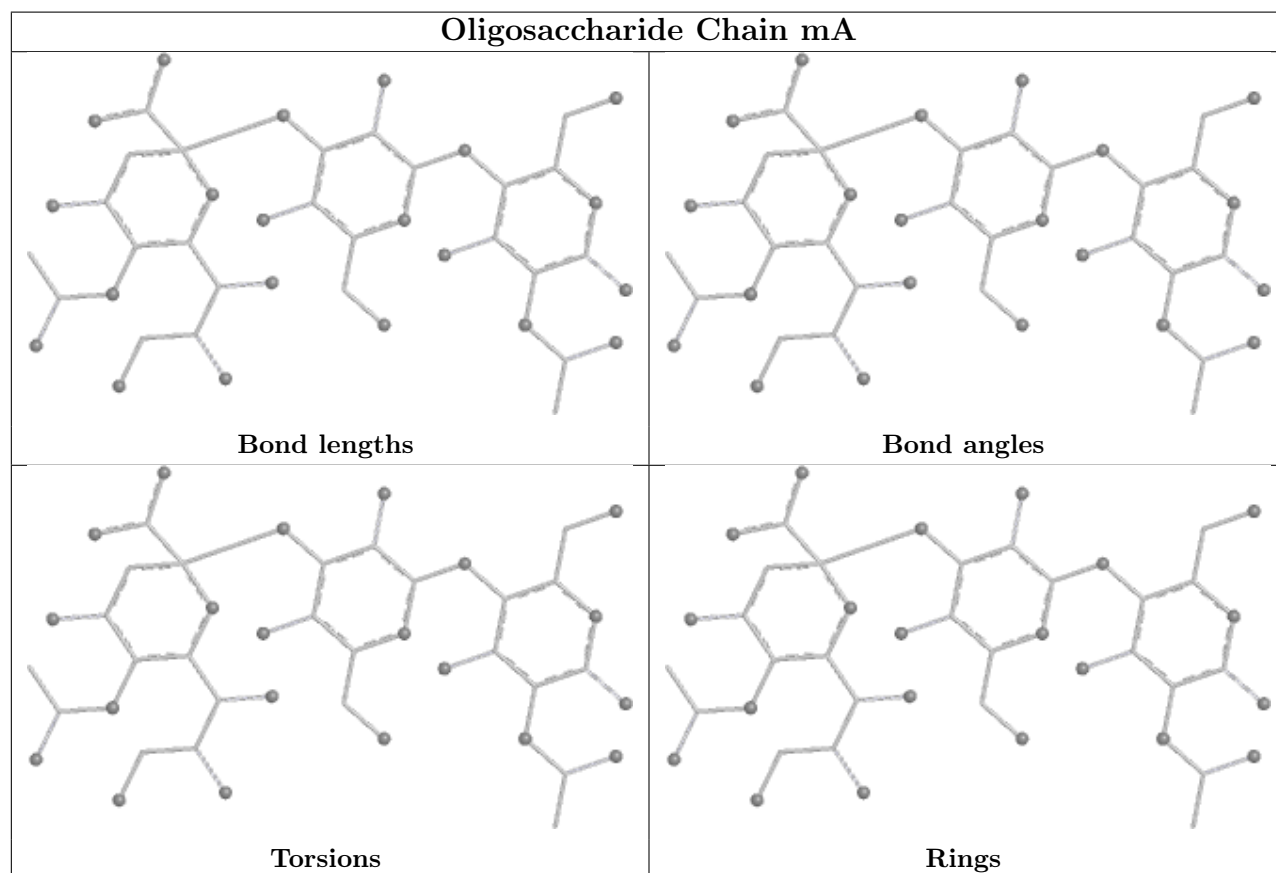
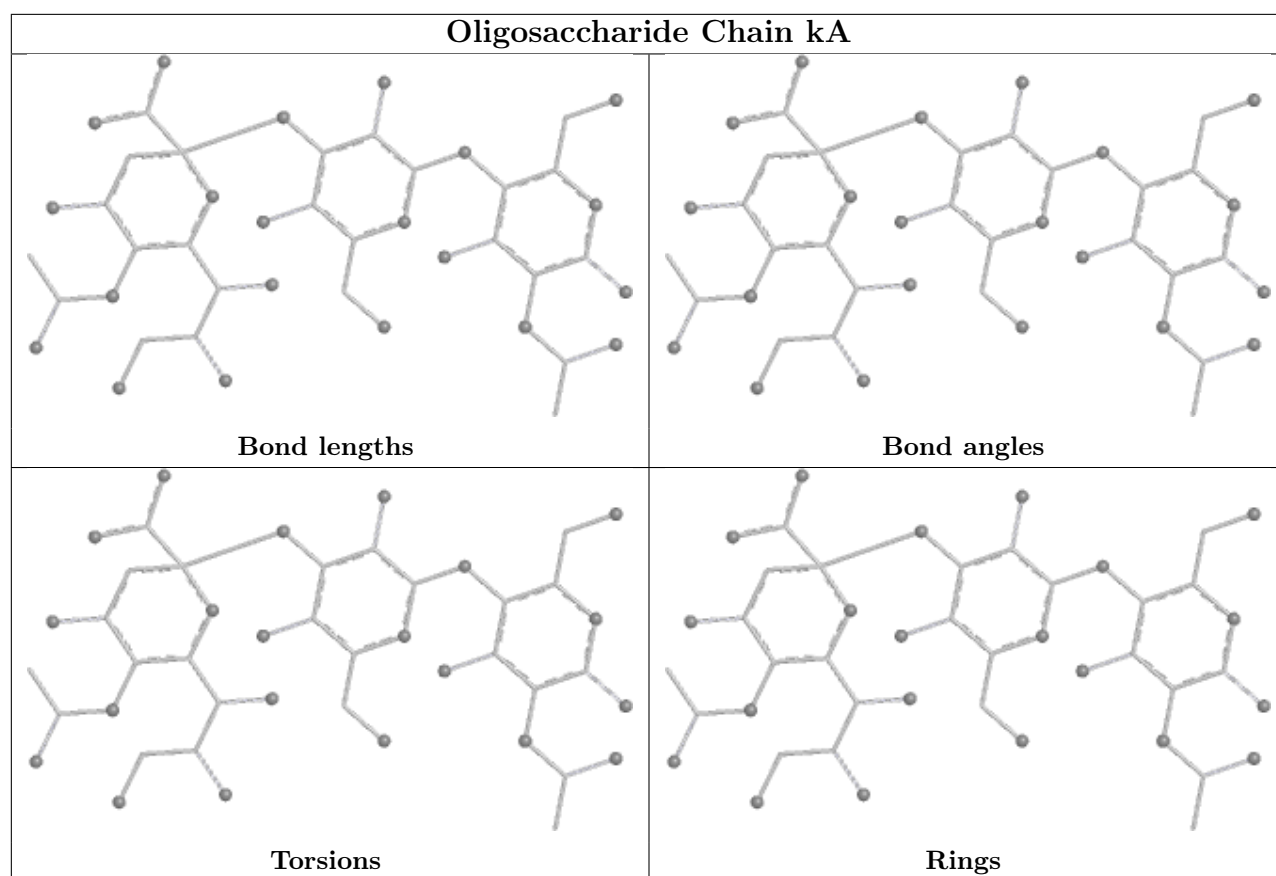


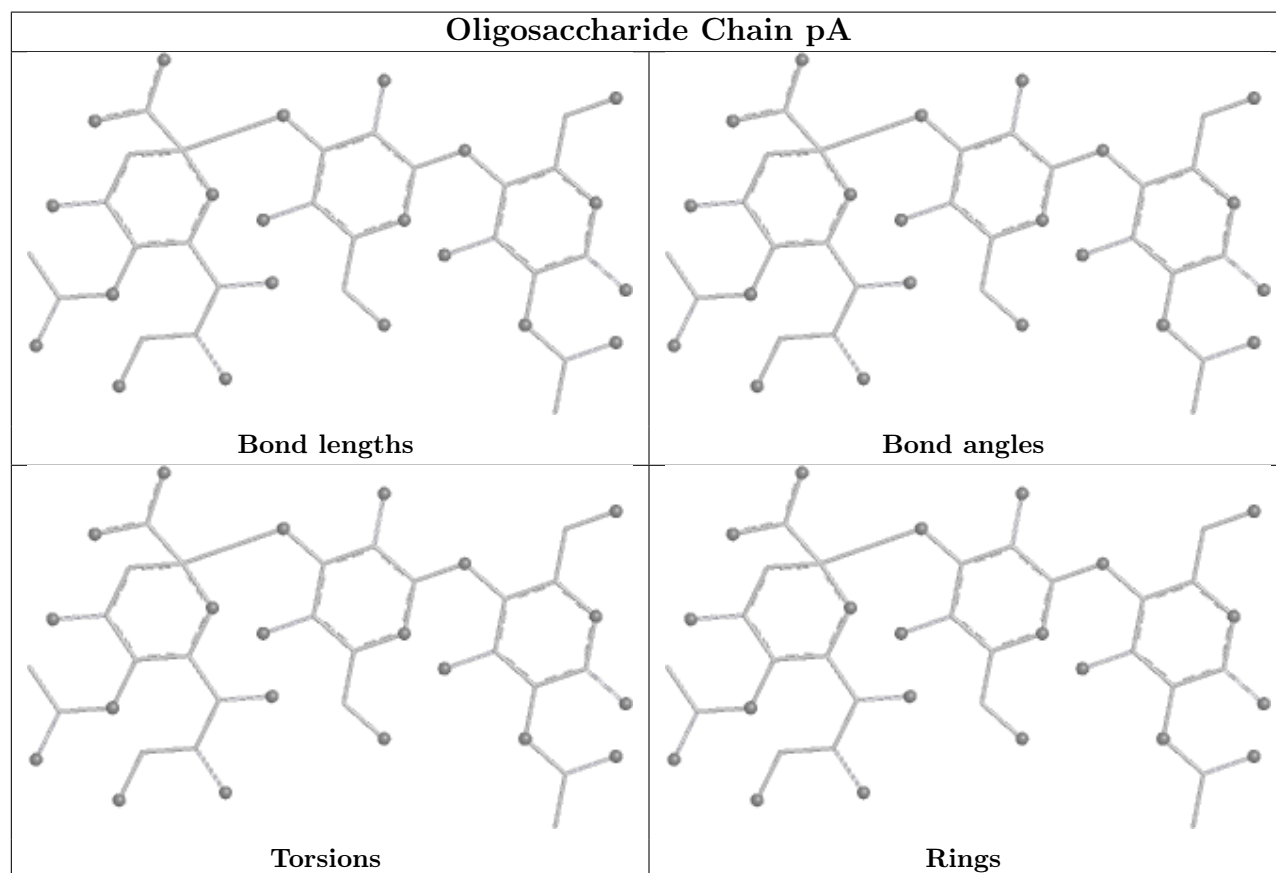
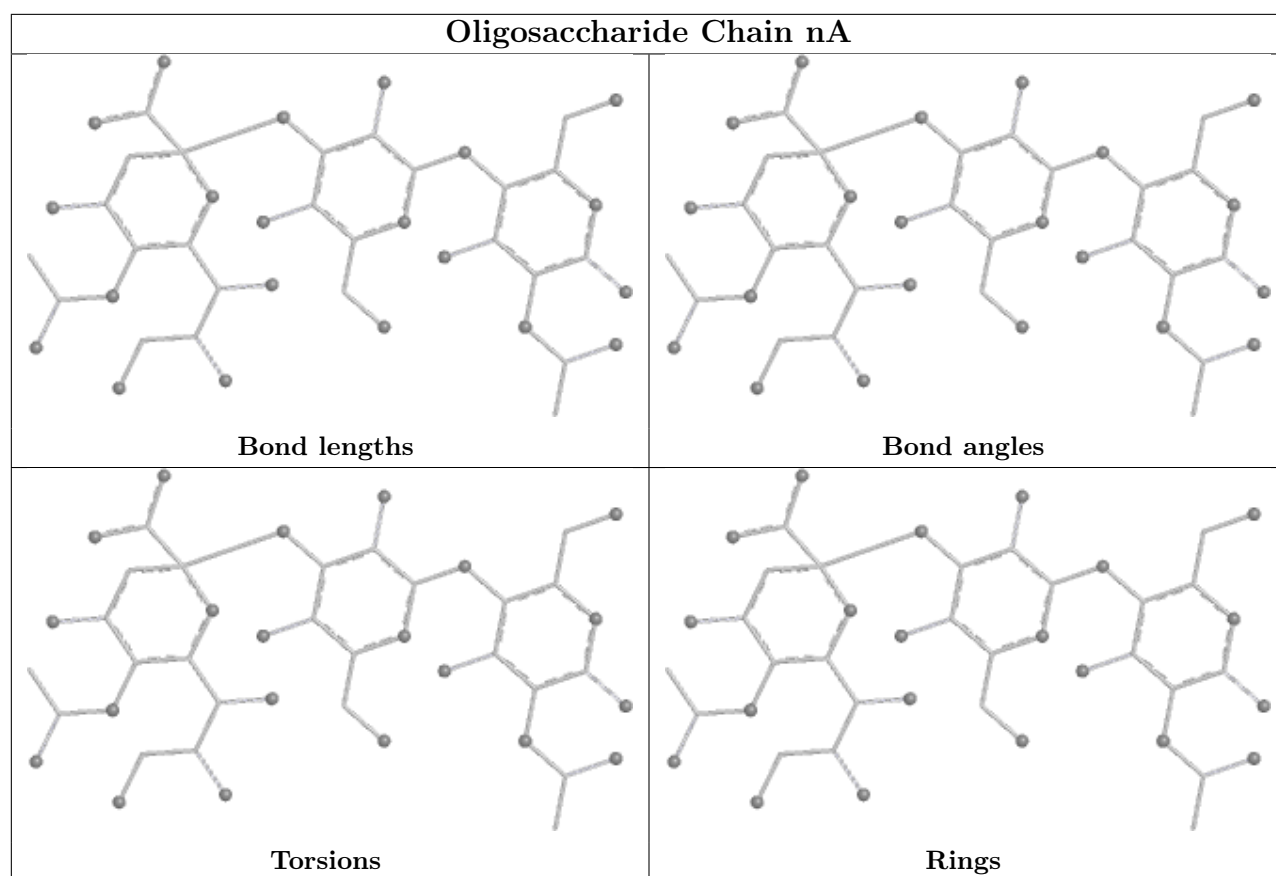
Oligosaccharide Chain YA**Oligosaccharide Chain aA**

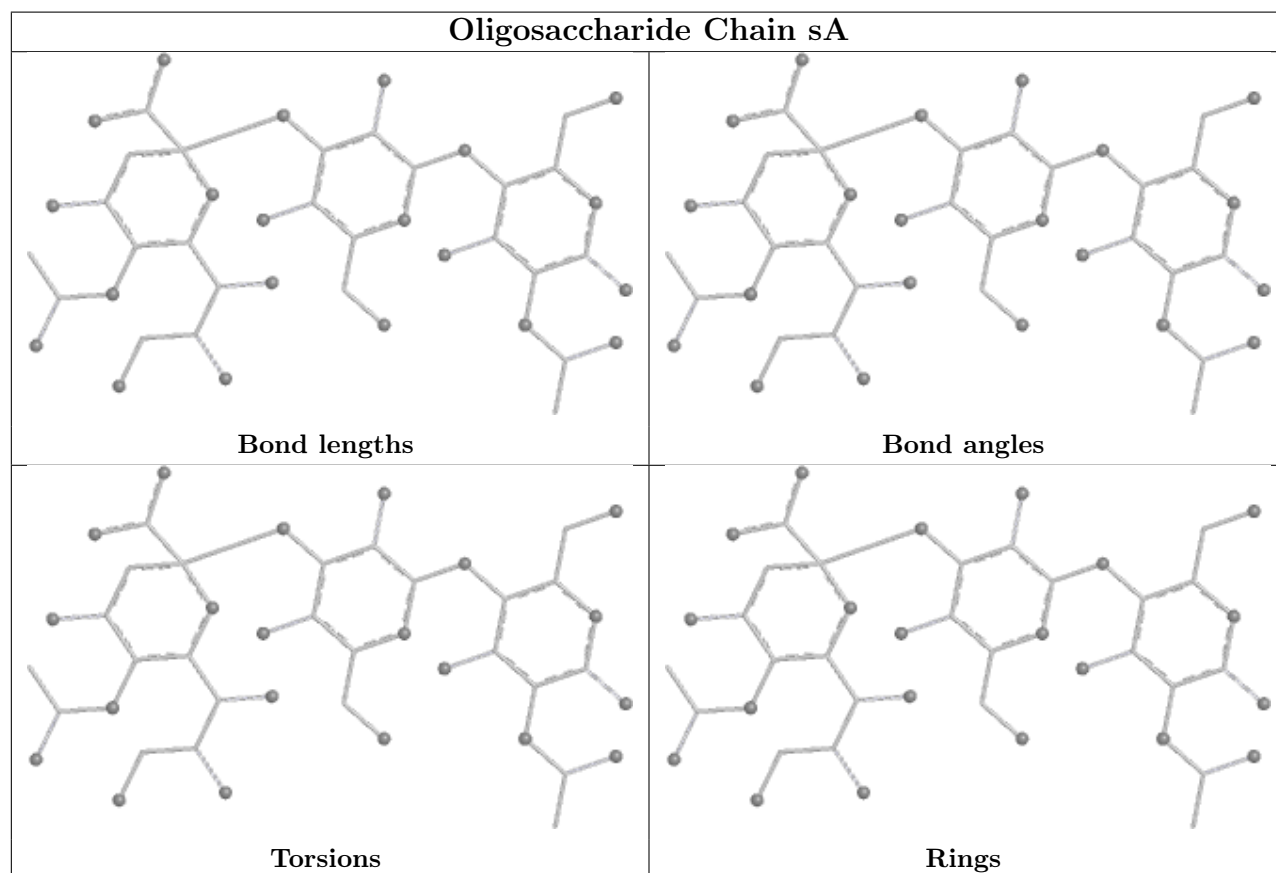
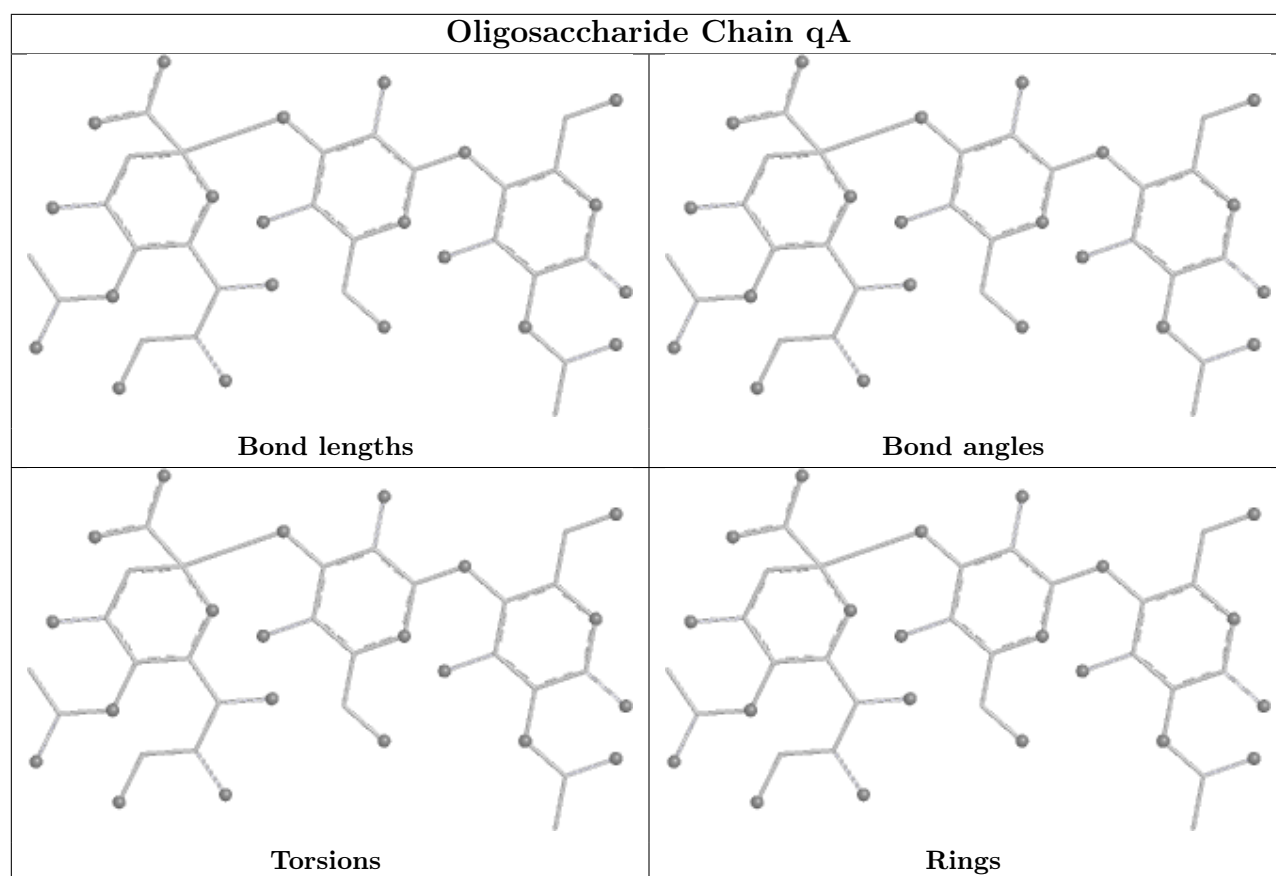
Oligosaccharide Chain bA**Oligosaccharide Chain dA**

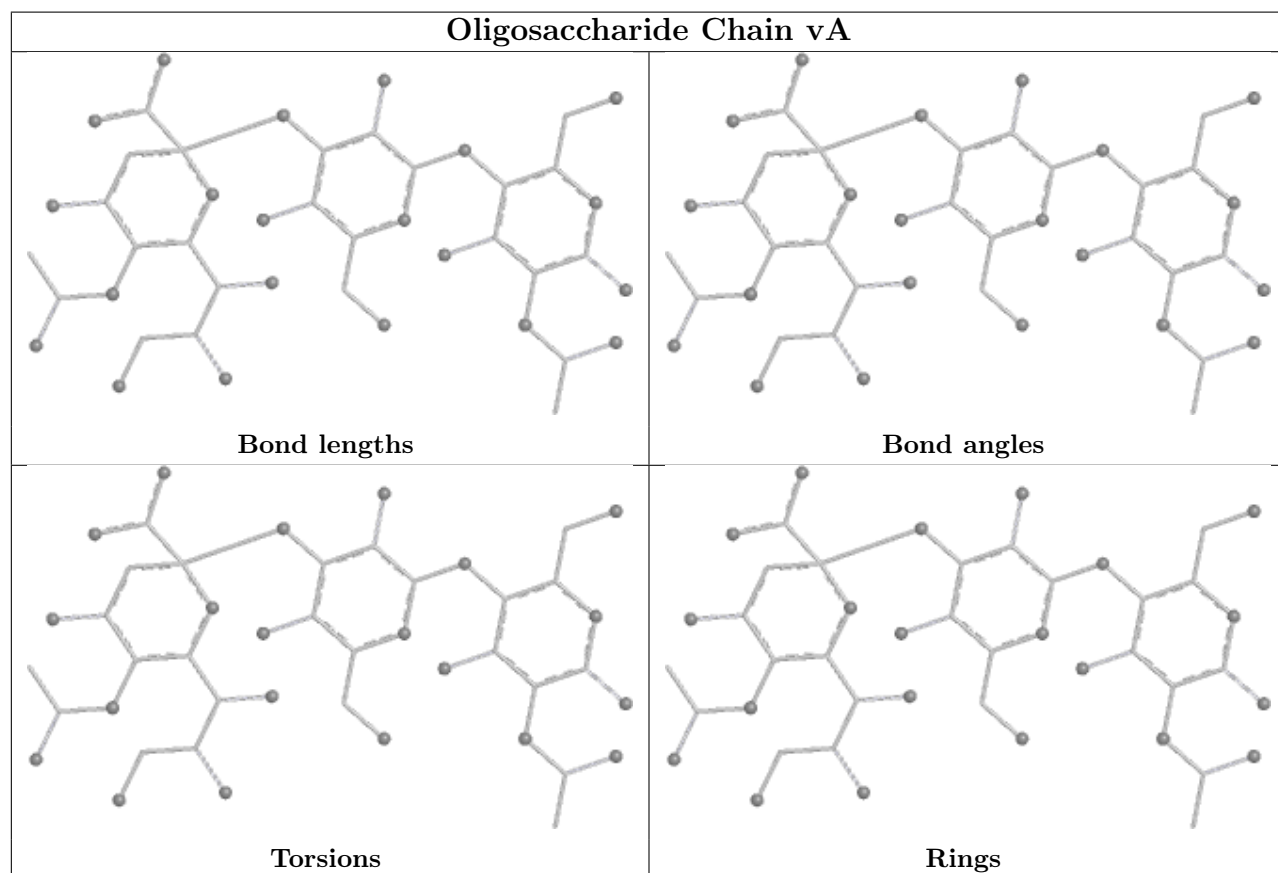
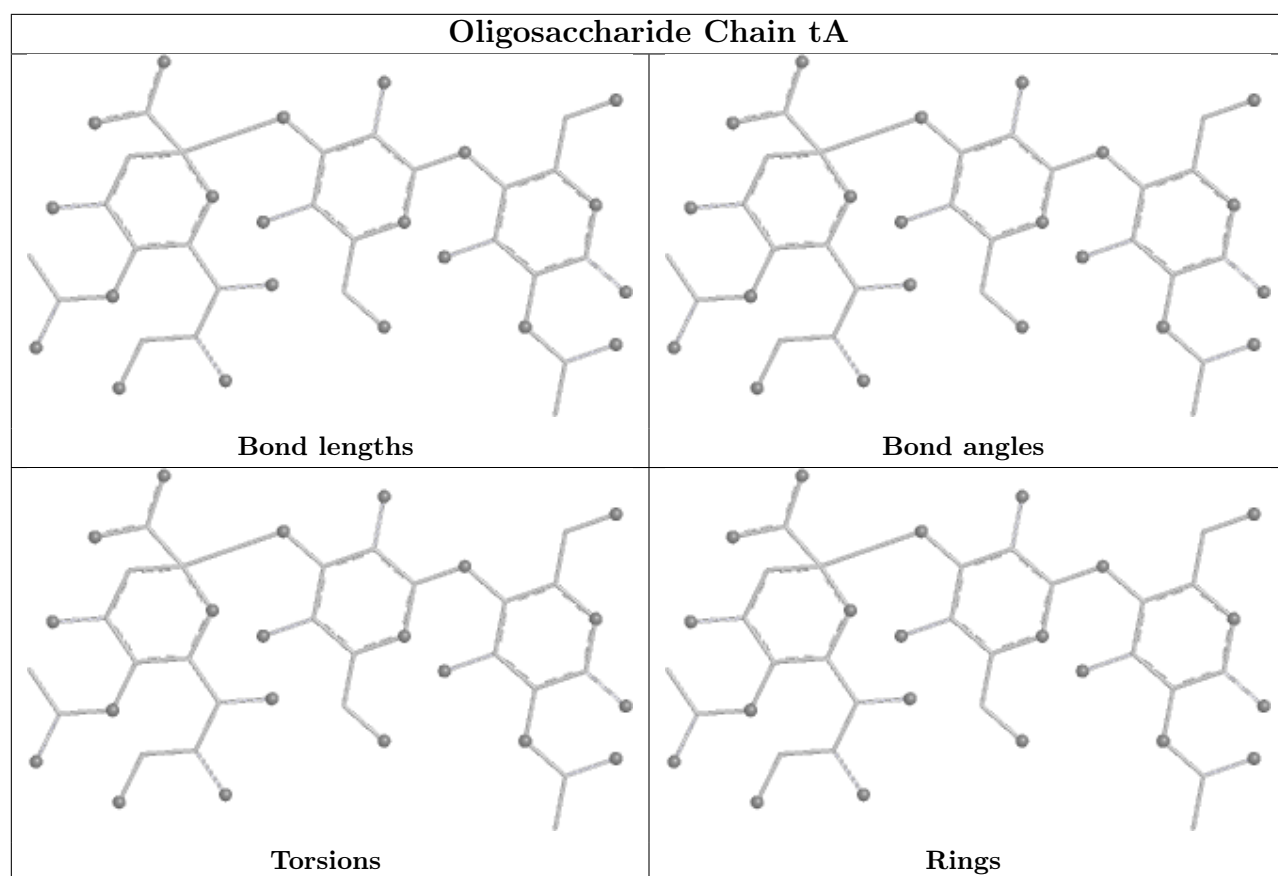




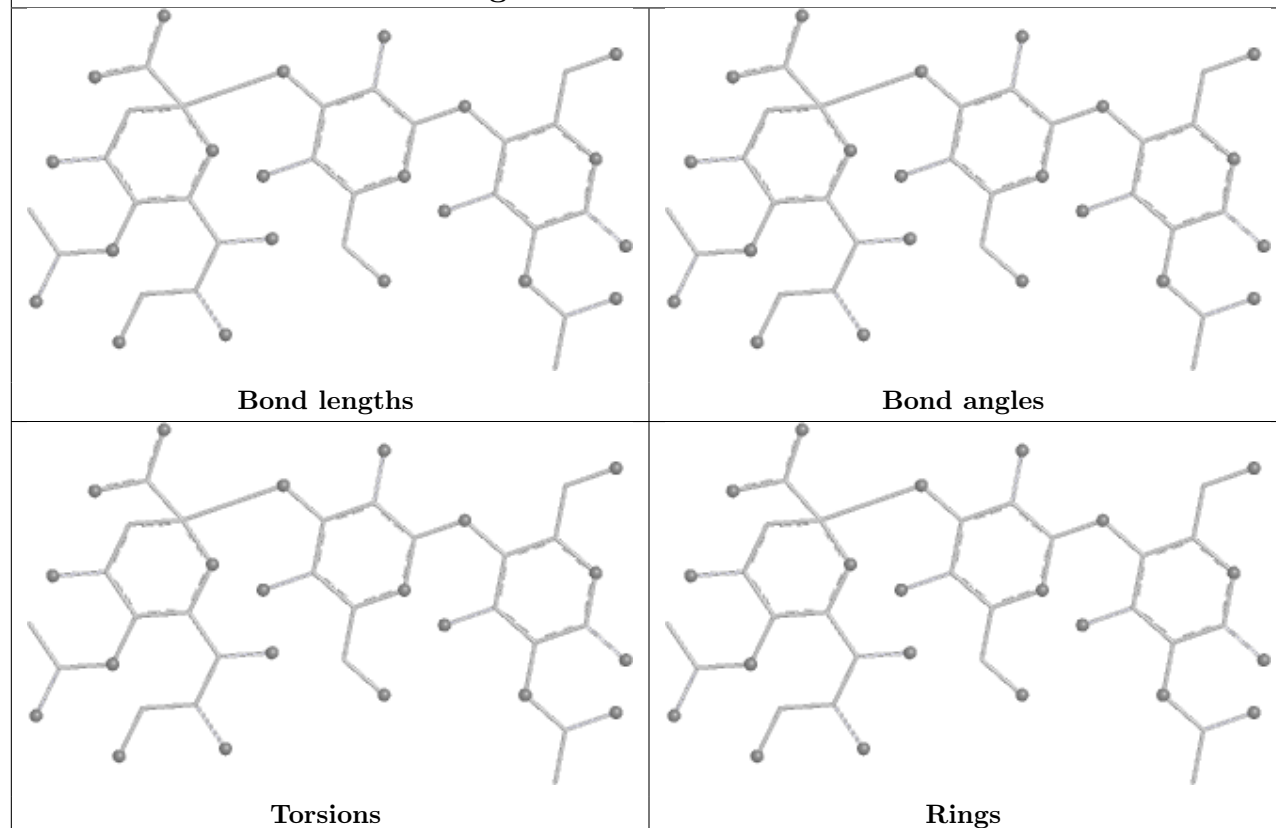




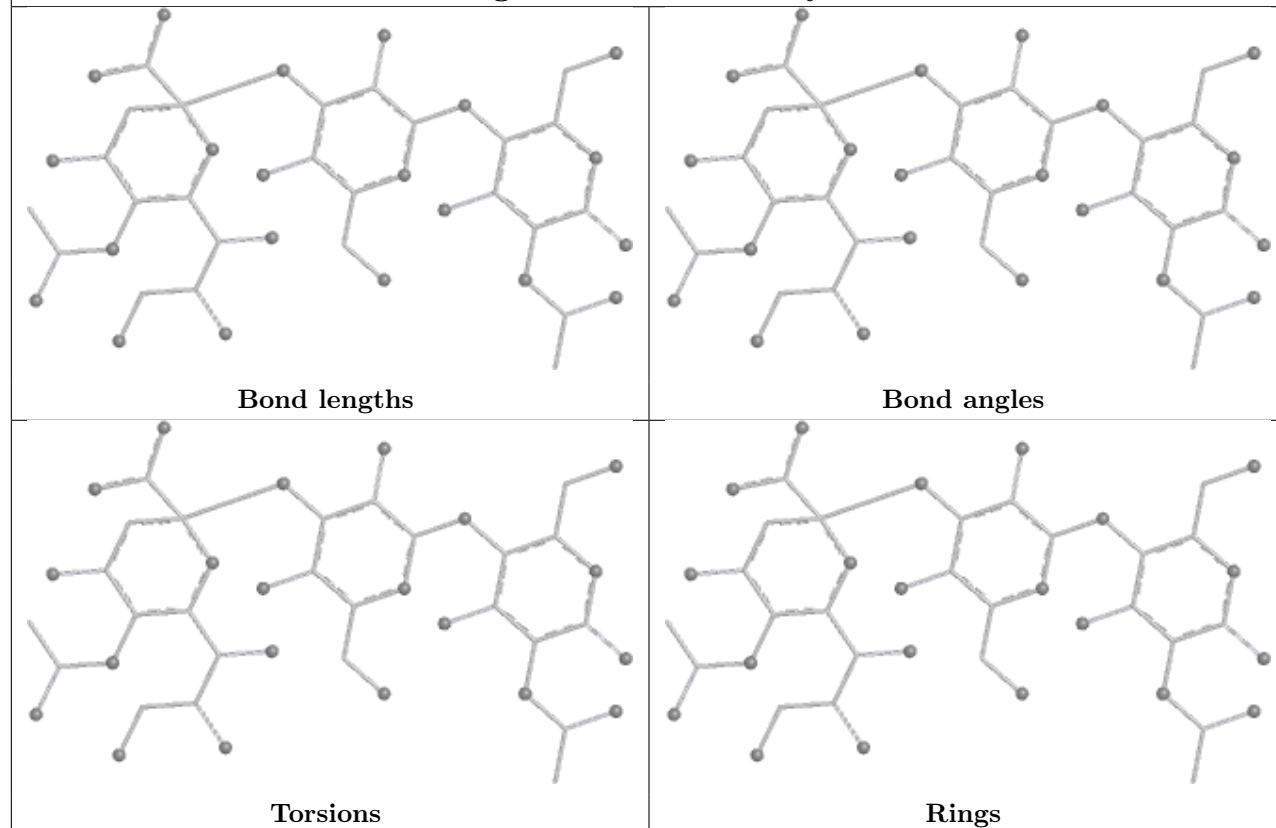


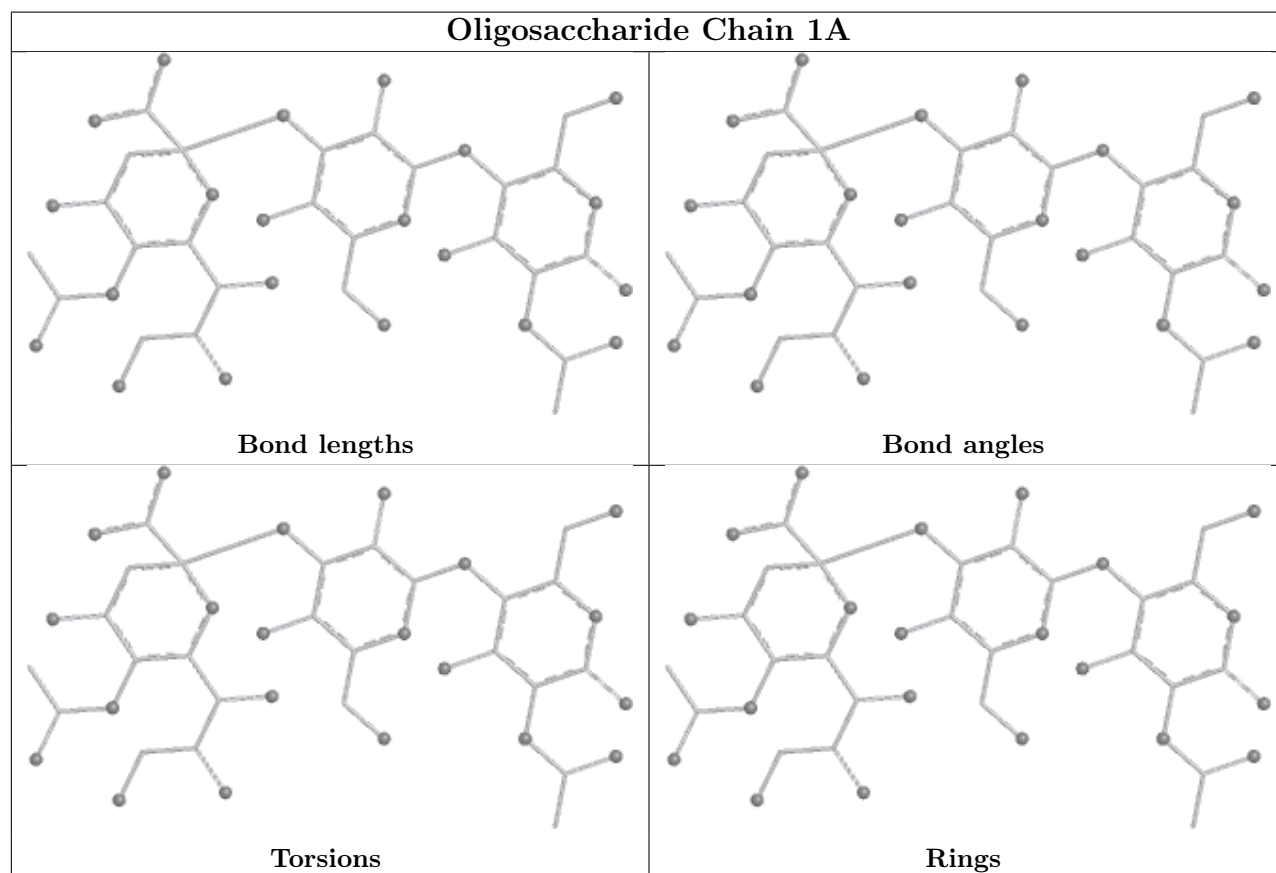
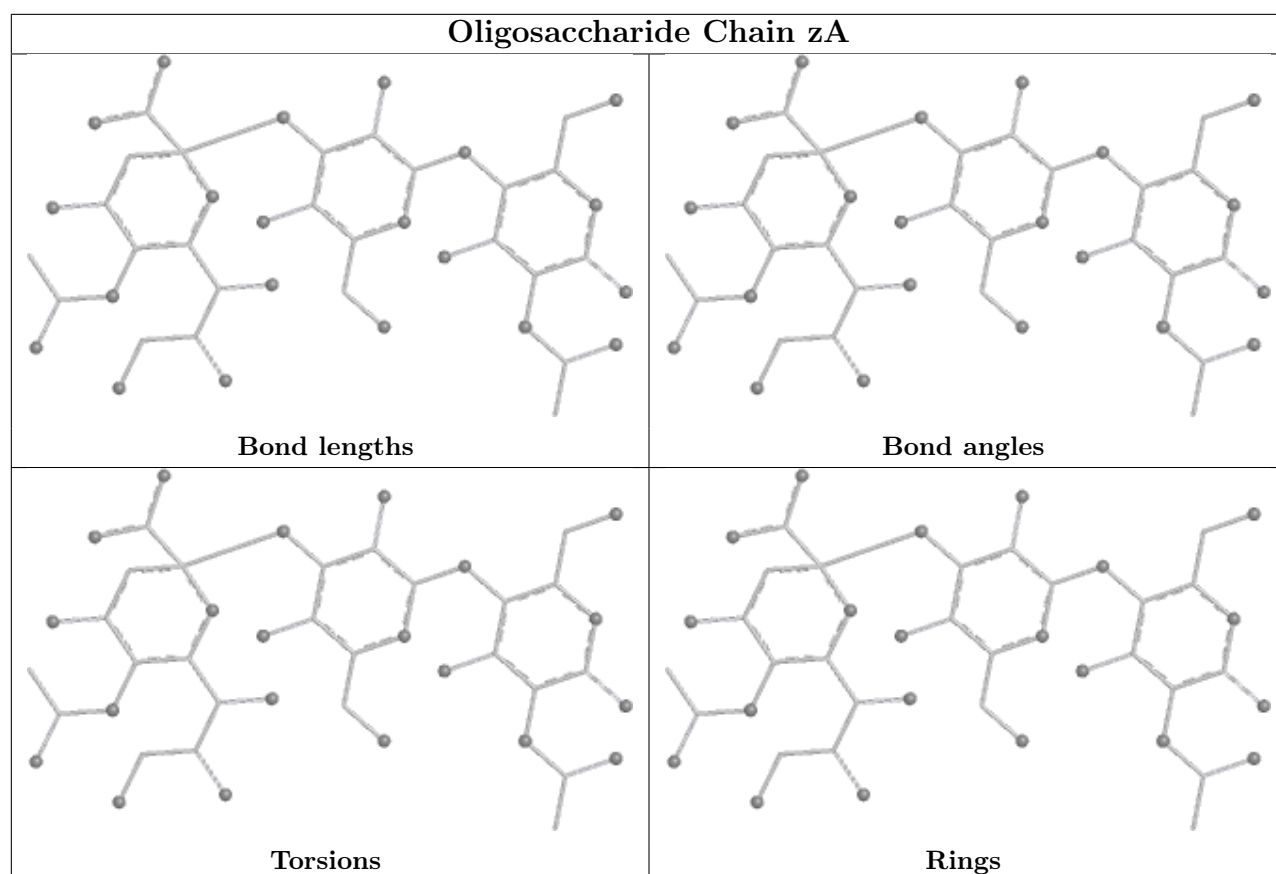


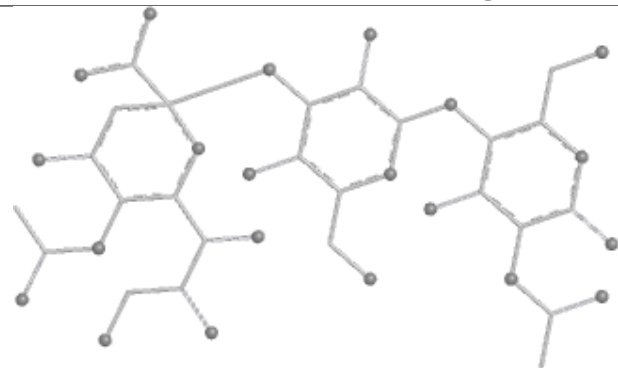
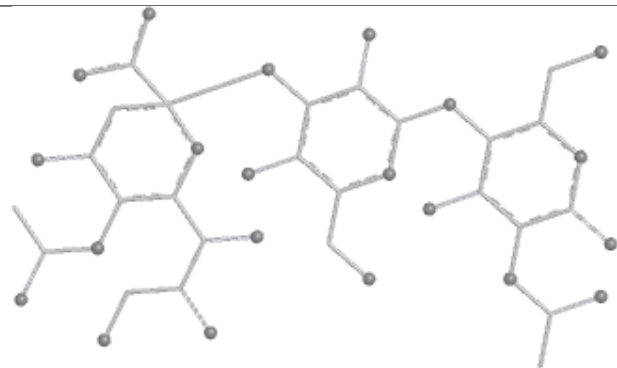
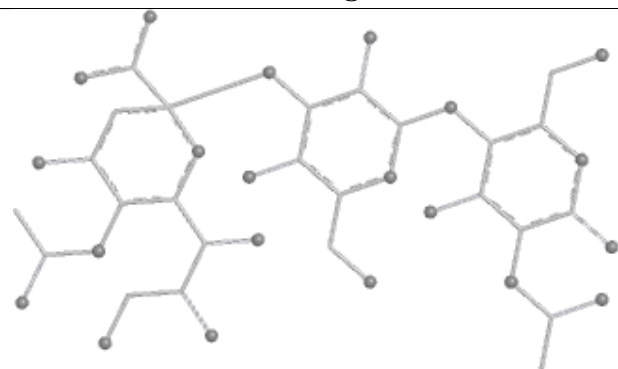
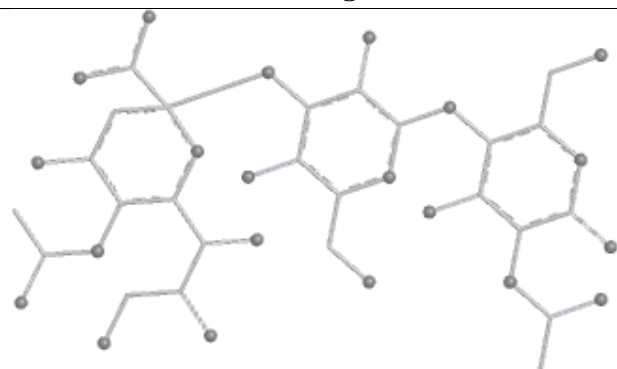
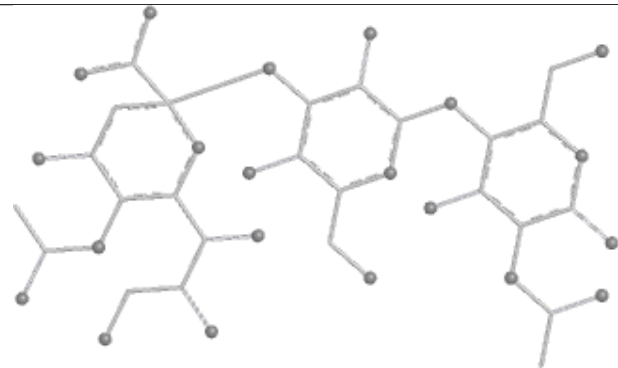
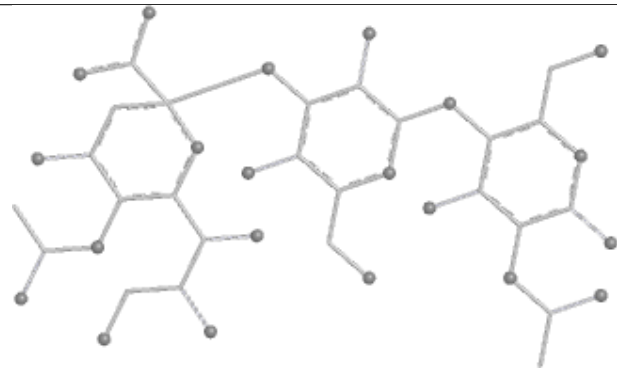
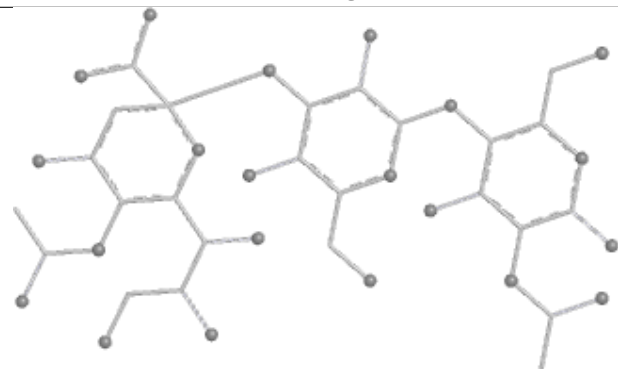
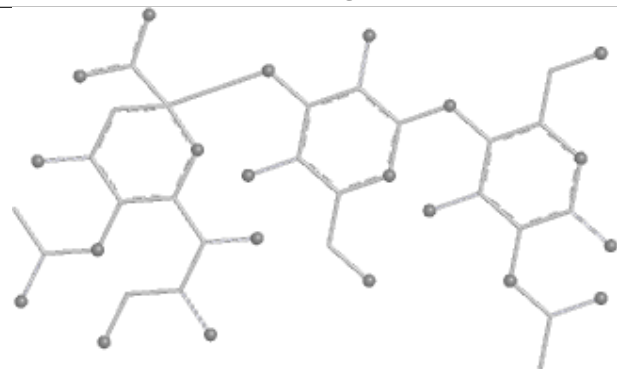
Oligosaccharide Chain wA



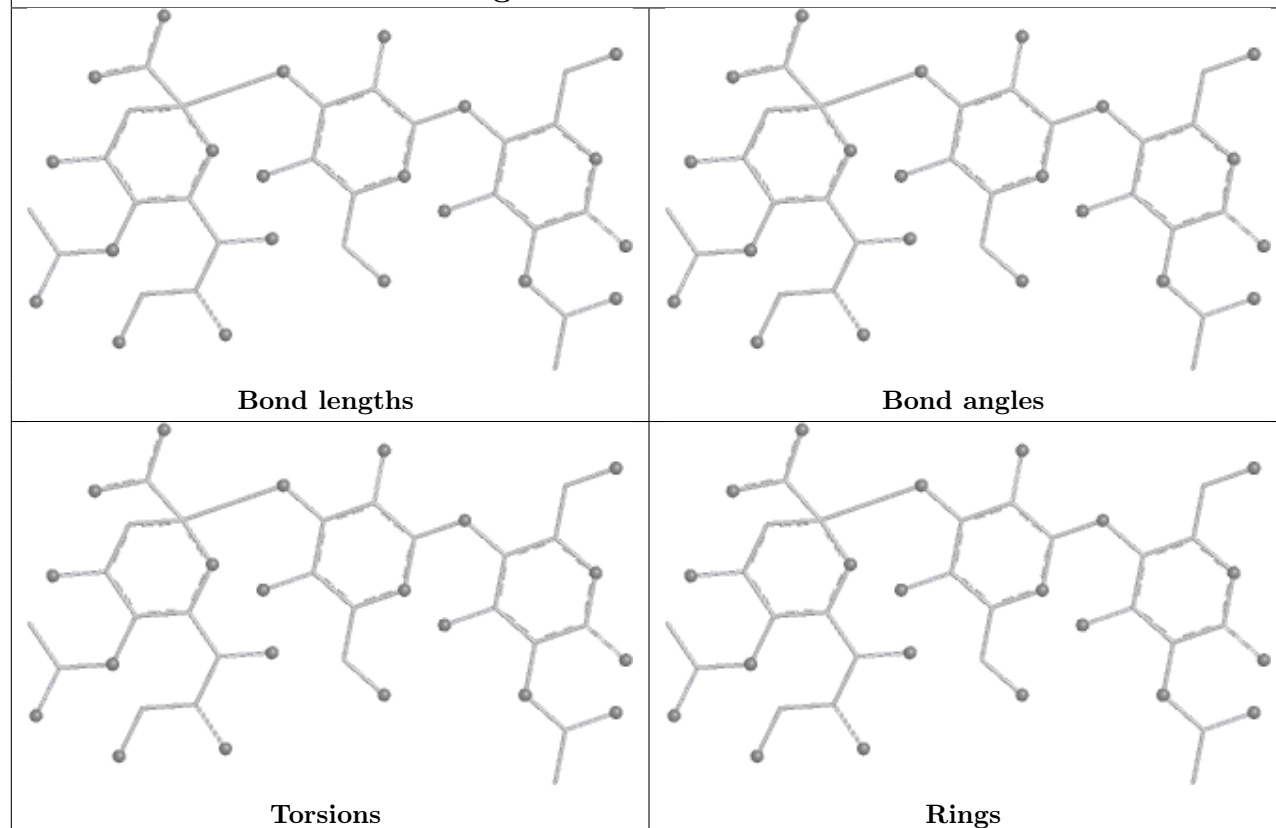
Oligosaccharide Chain yA



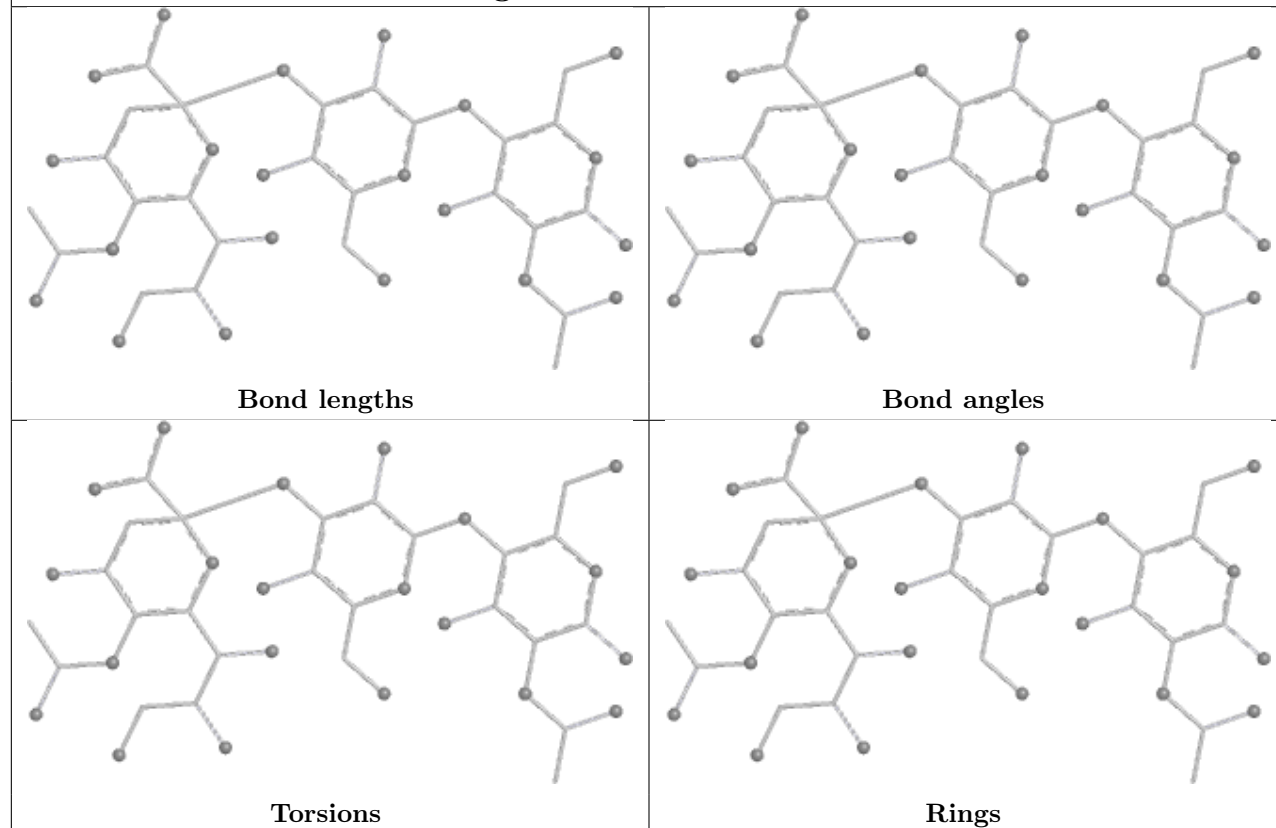


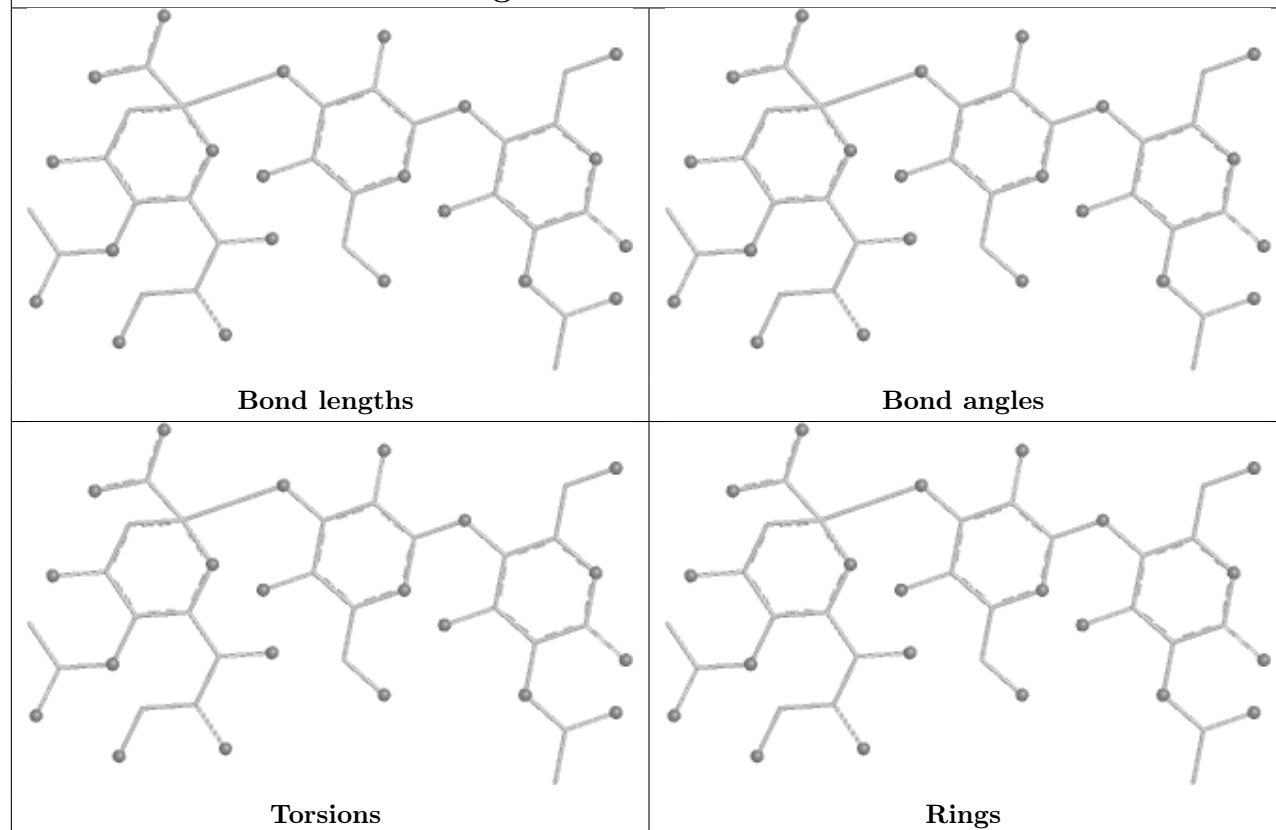
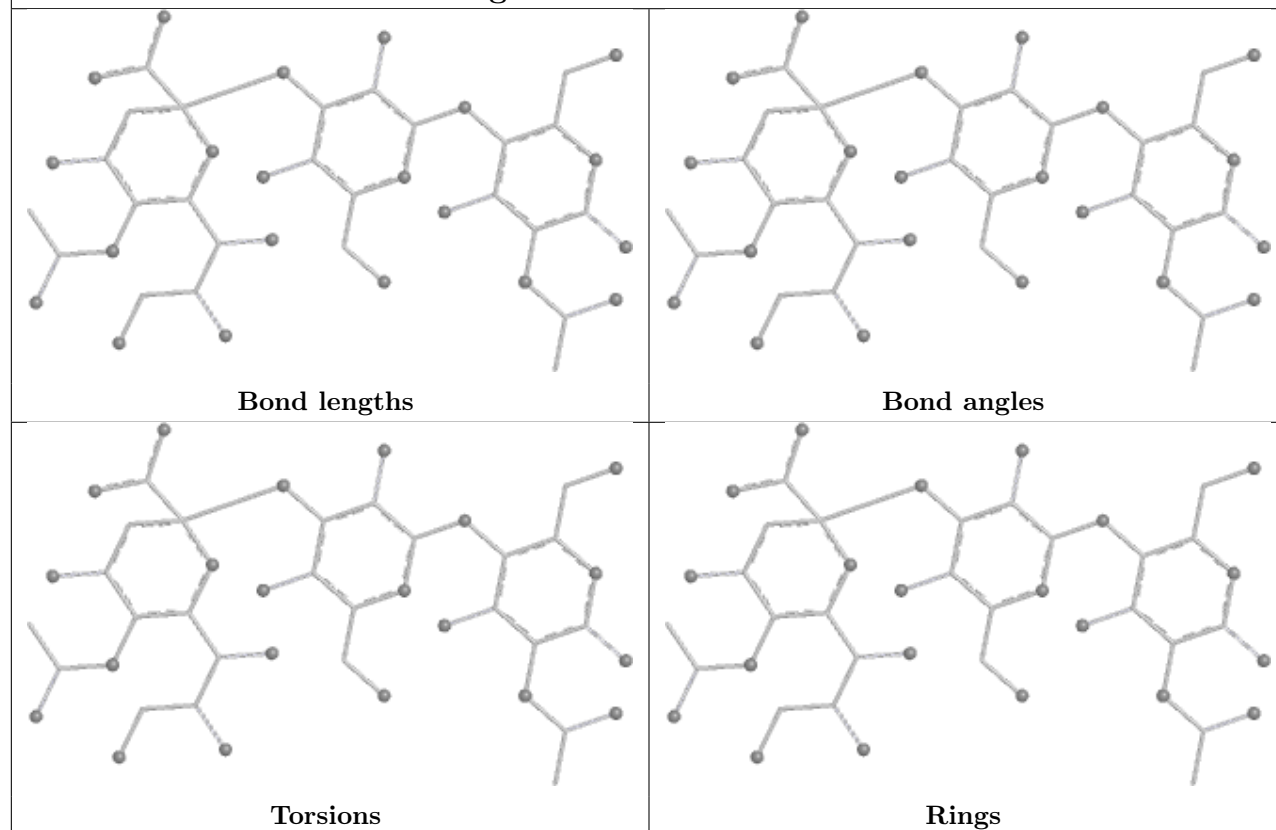
Oligosaccharide Chain 2A**Bond lengths****Bond angles****Torsions****Rings****Oligosaccharide Chain 4A****Bond lengths****Bond angles****Torsions****Rings**

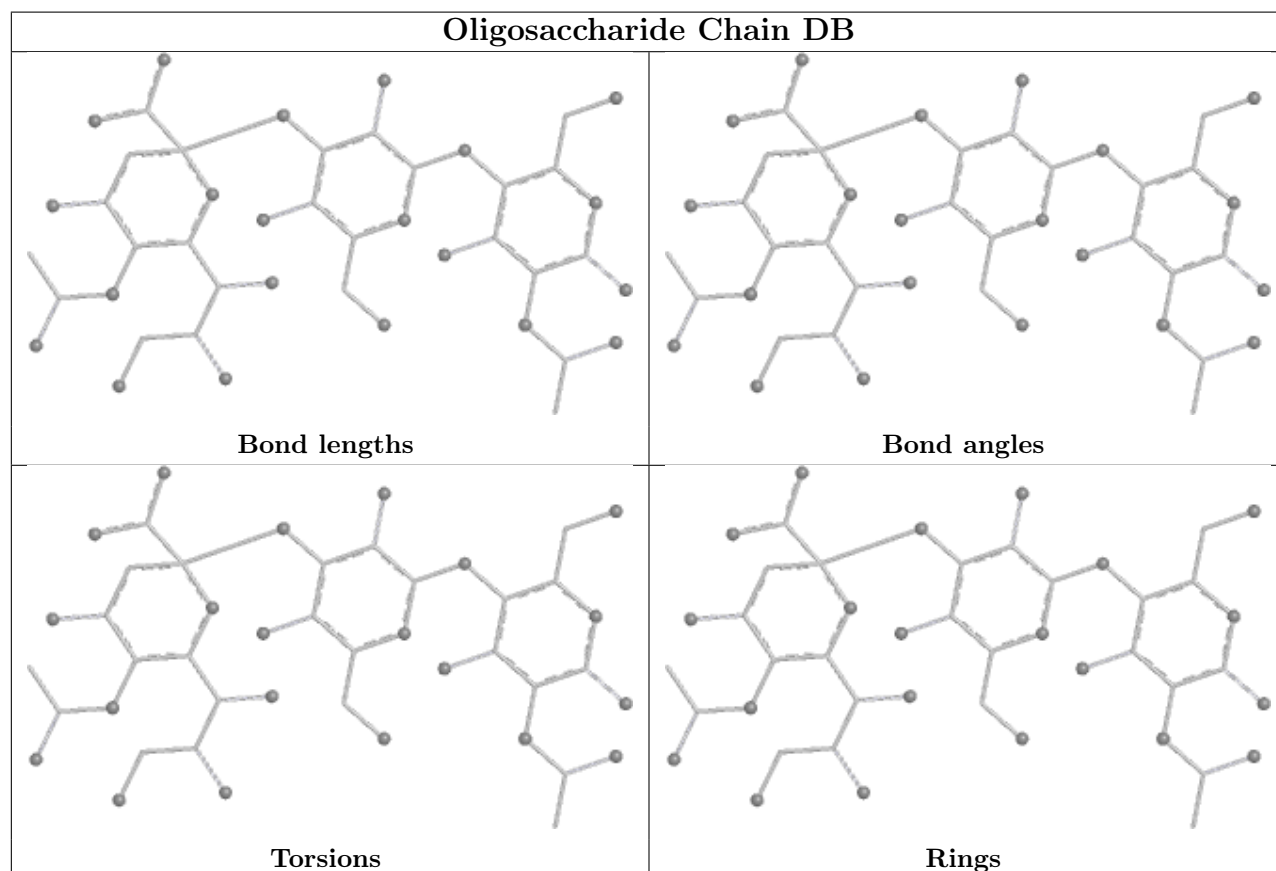
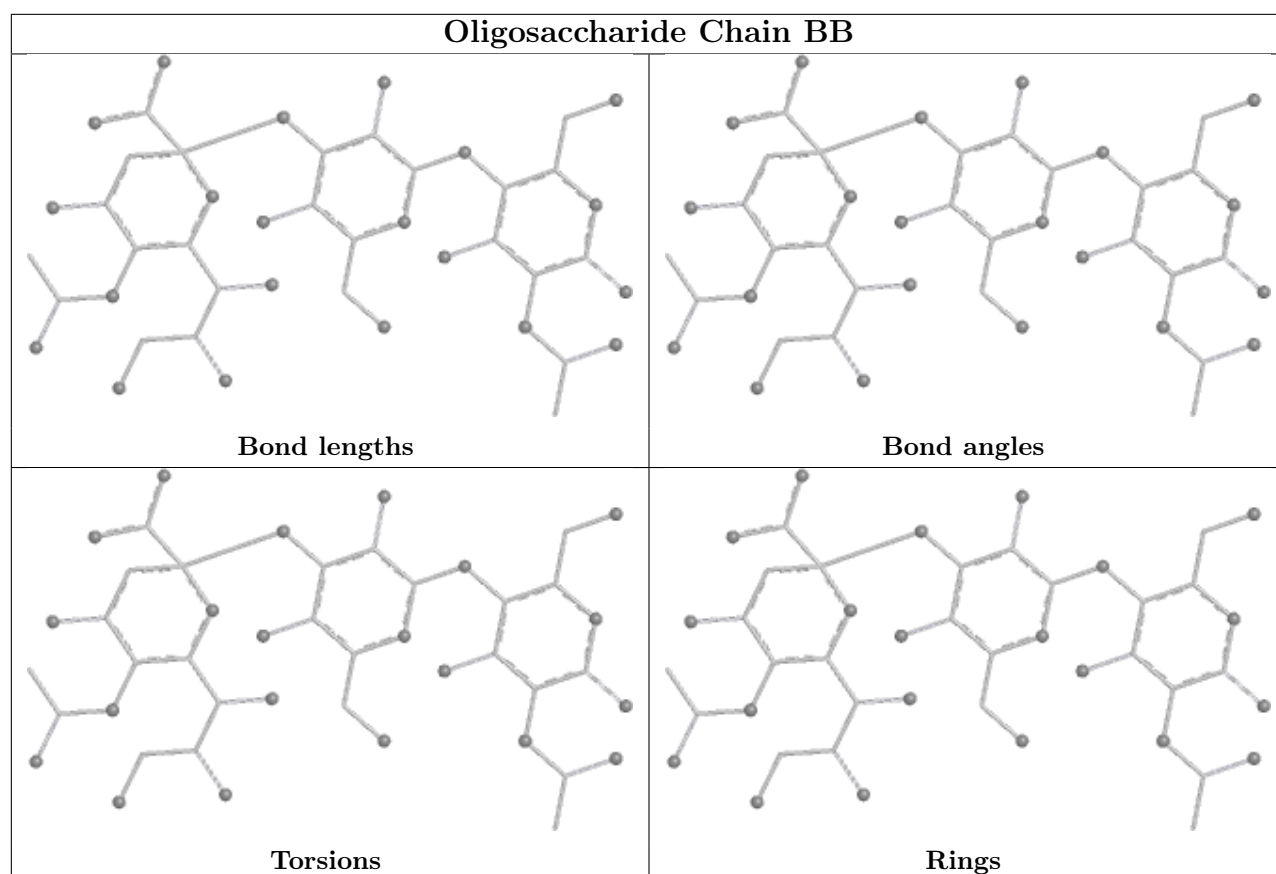
Oligosaccharide Chain 5A

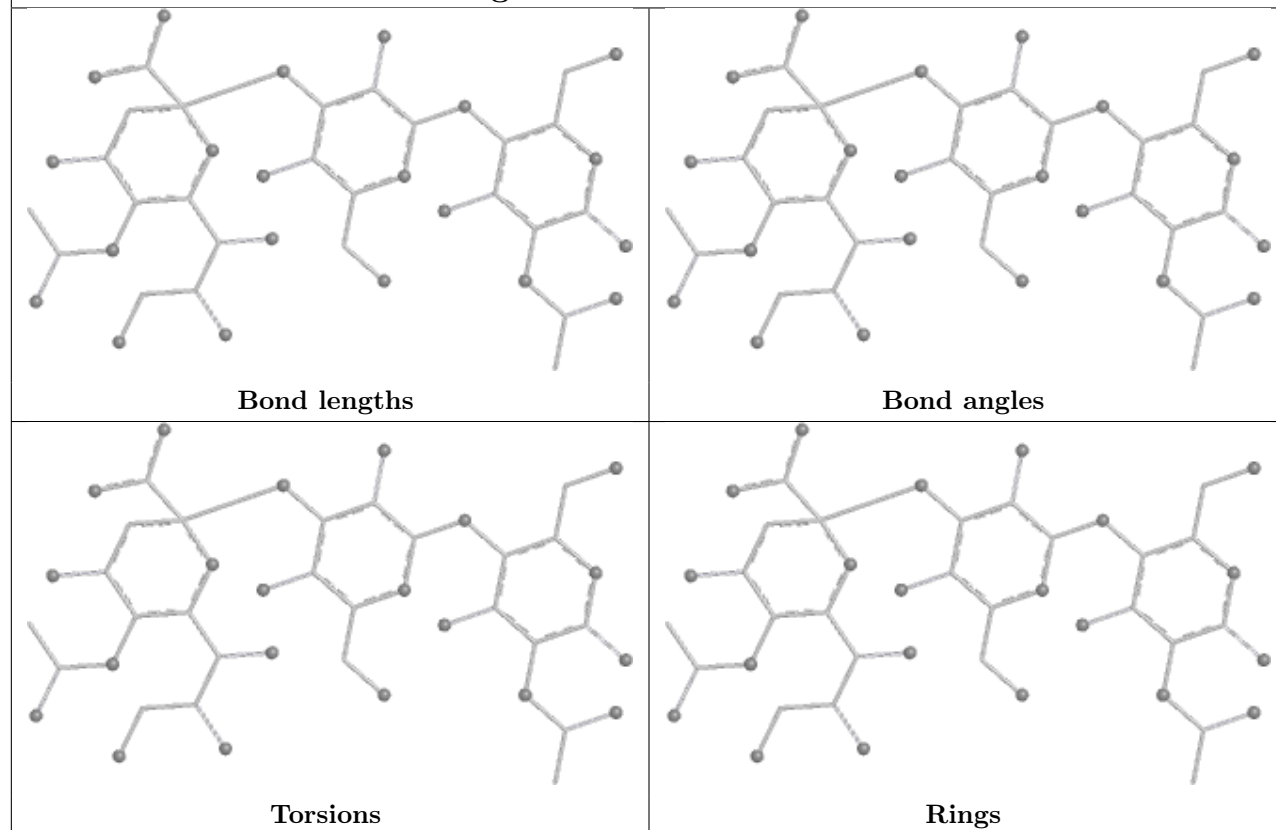
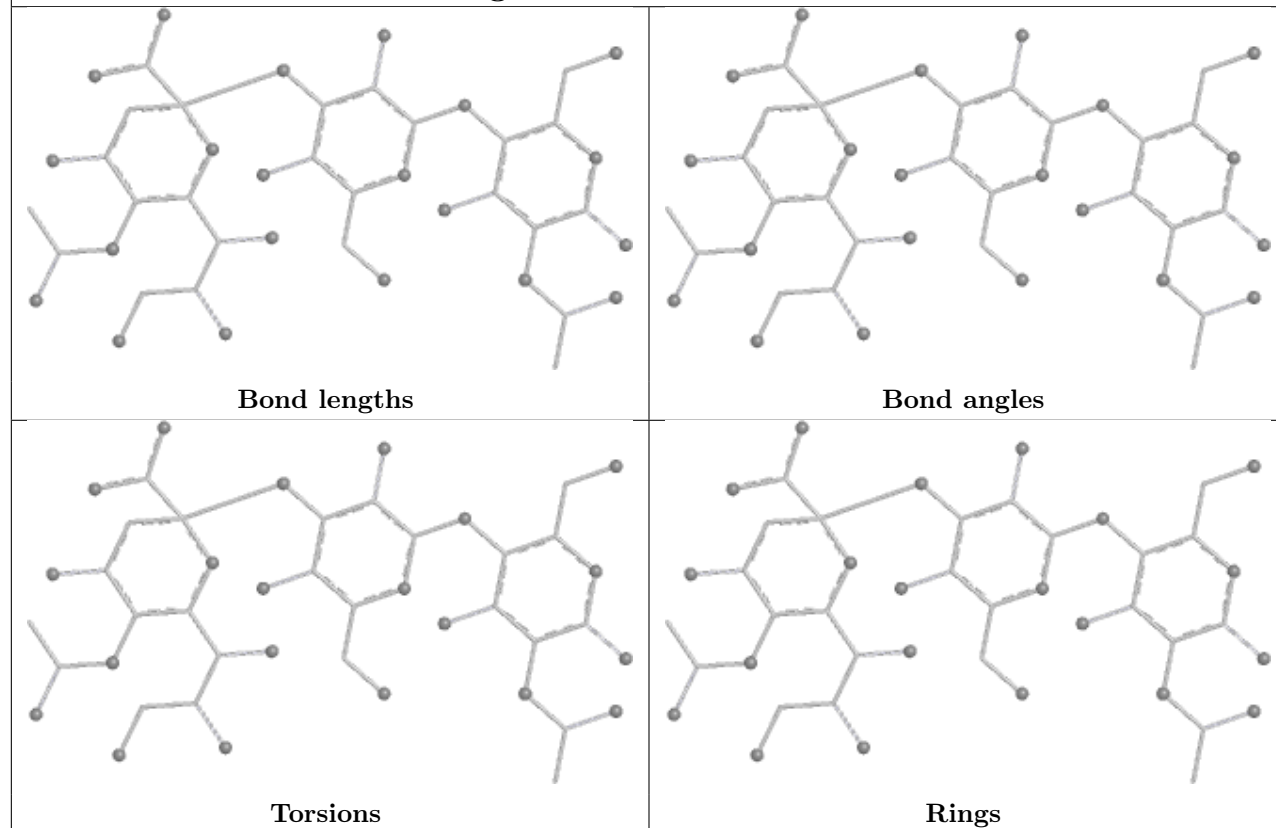


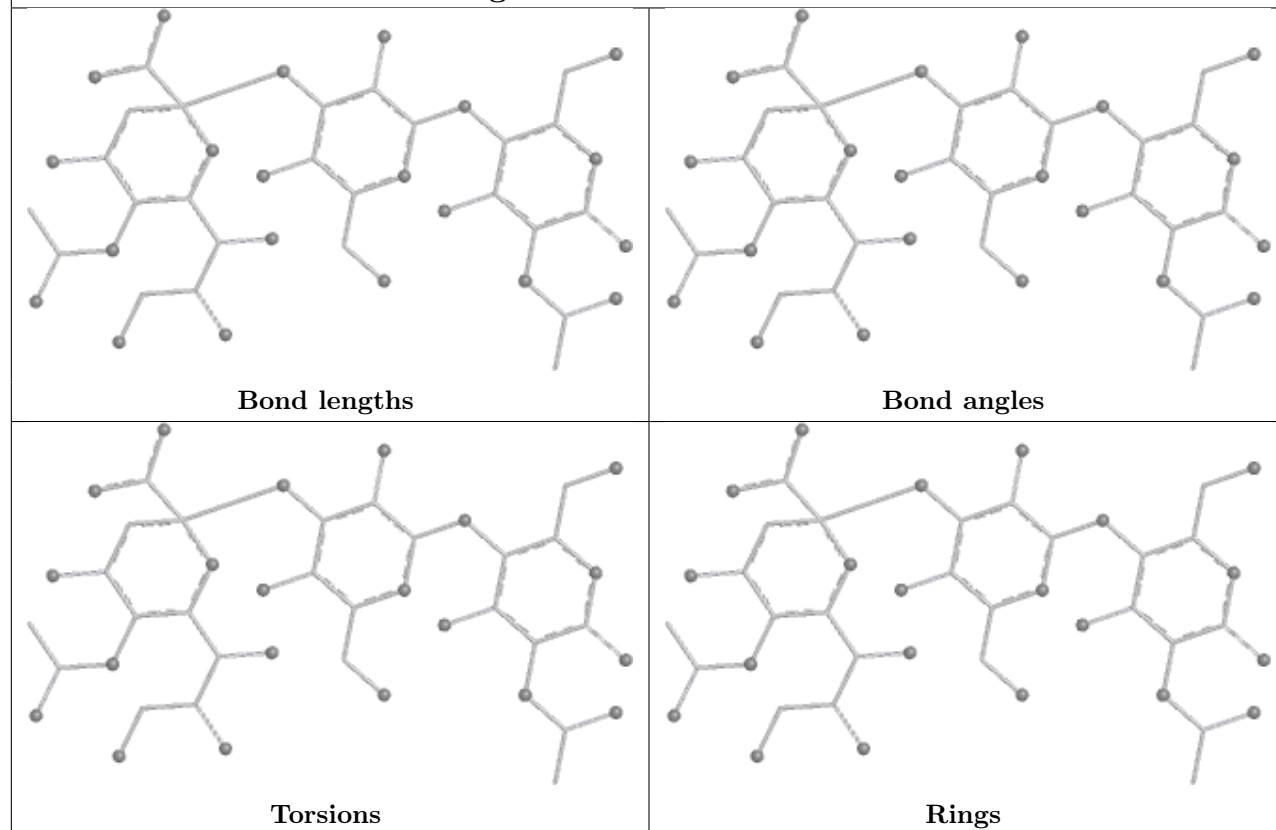
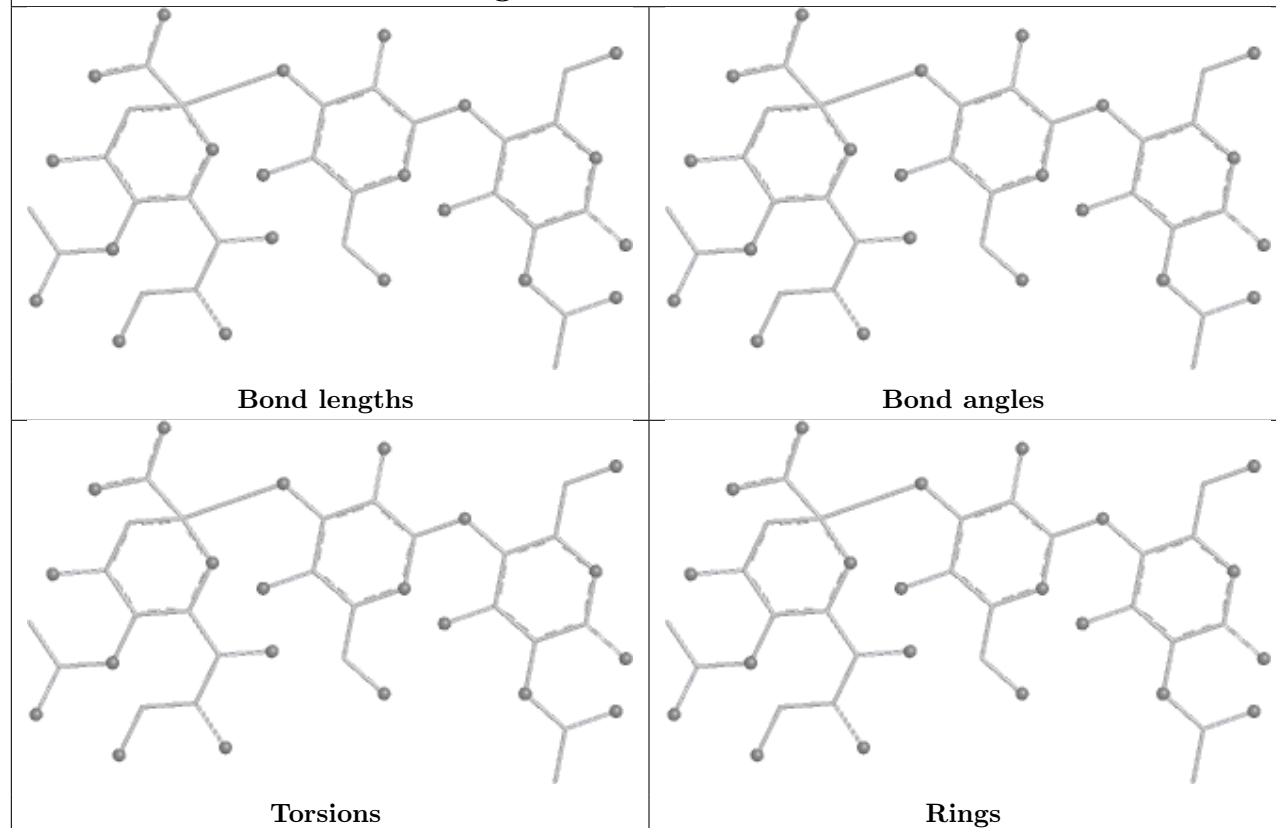
Oligosaccharide Chain 7A

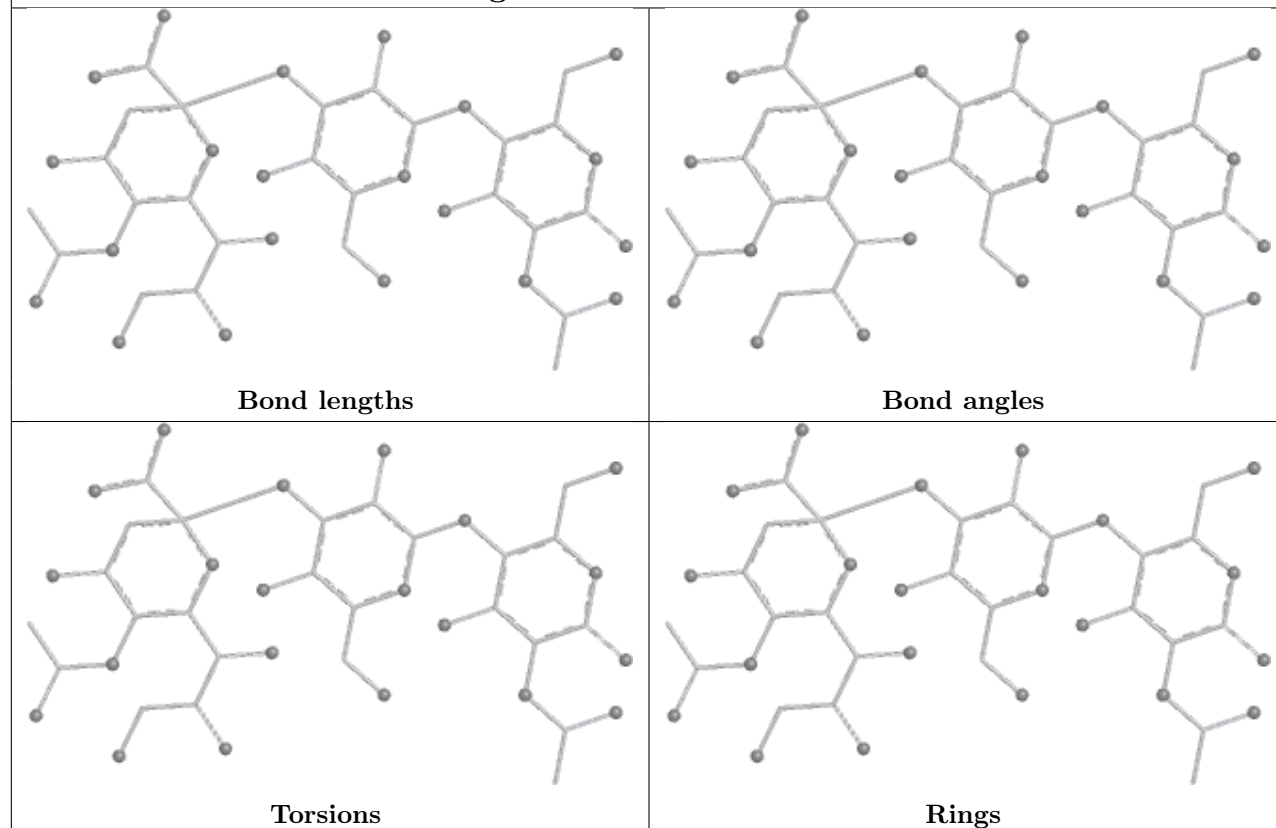
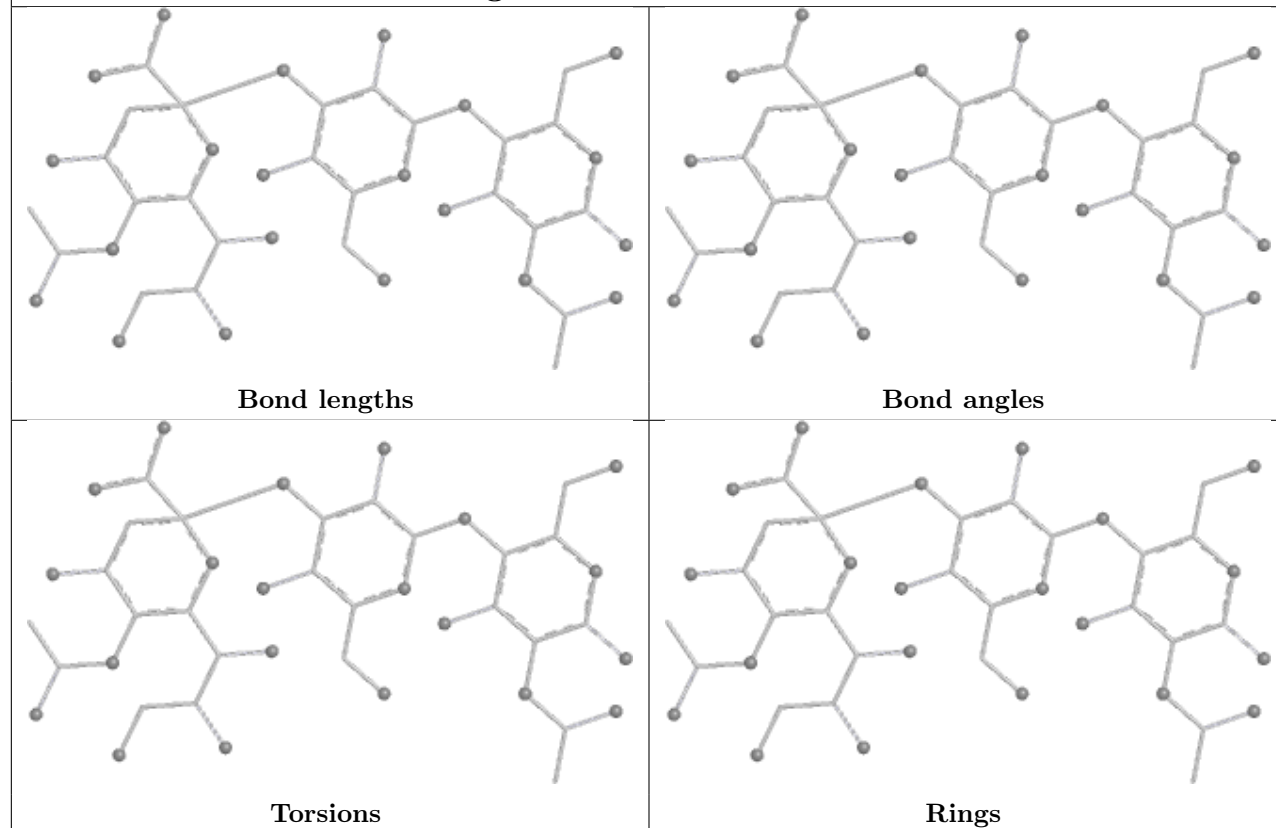


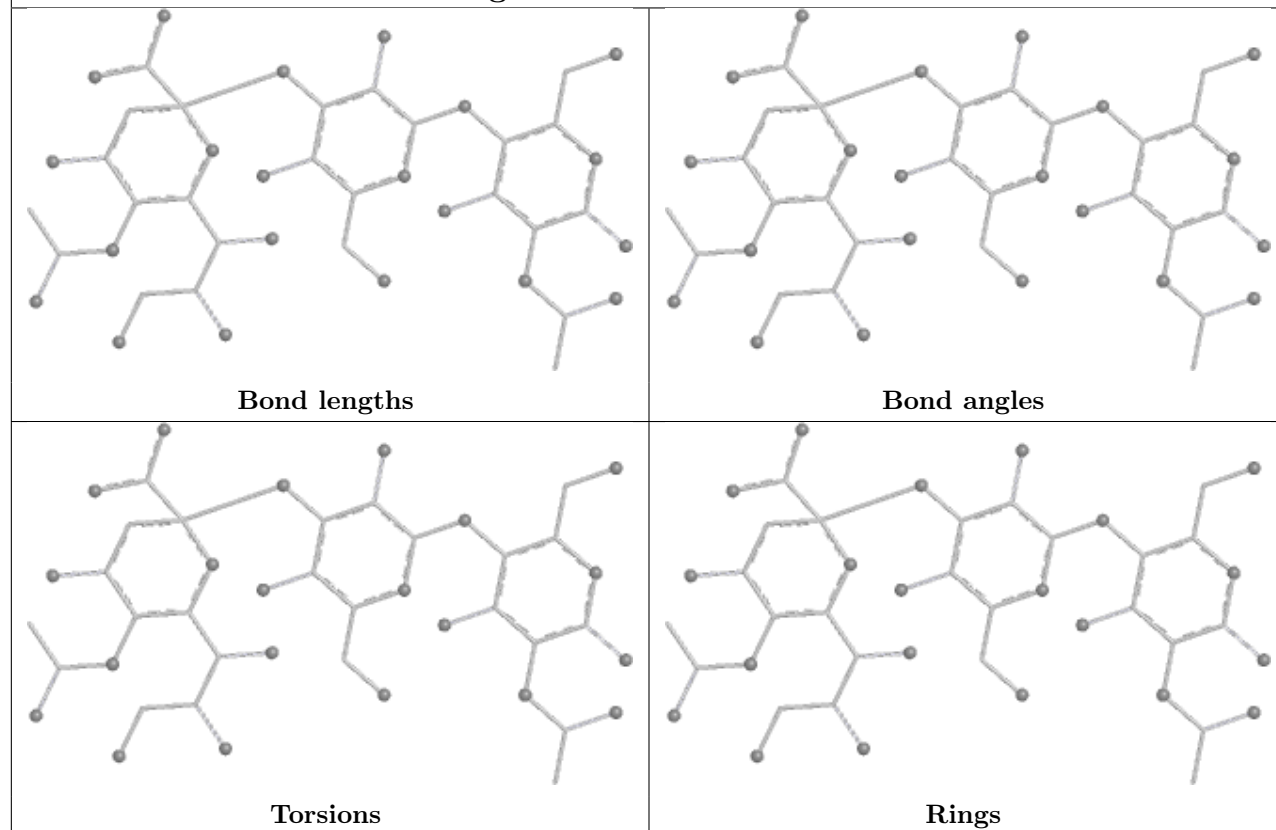
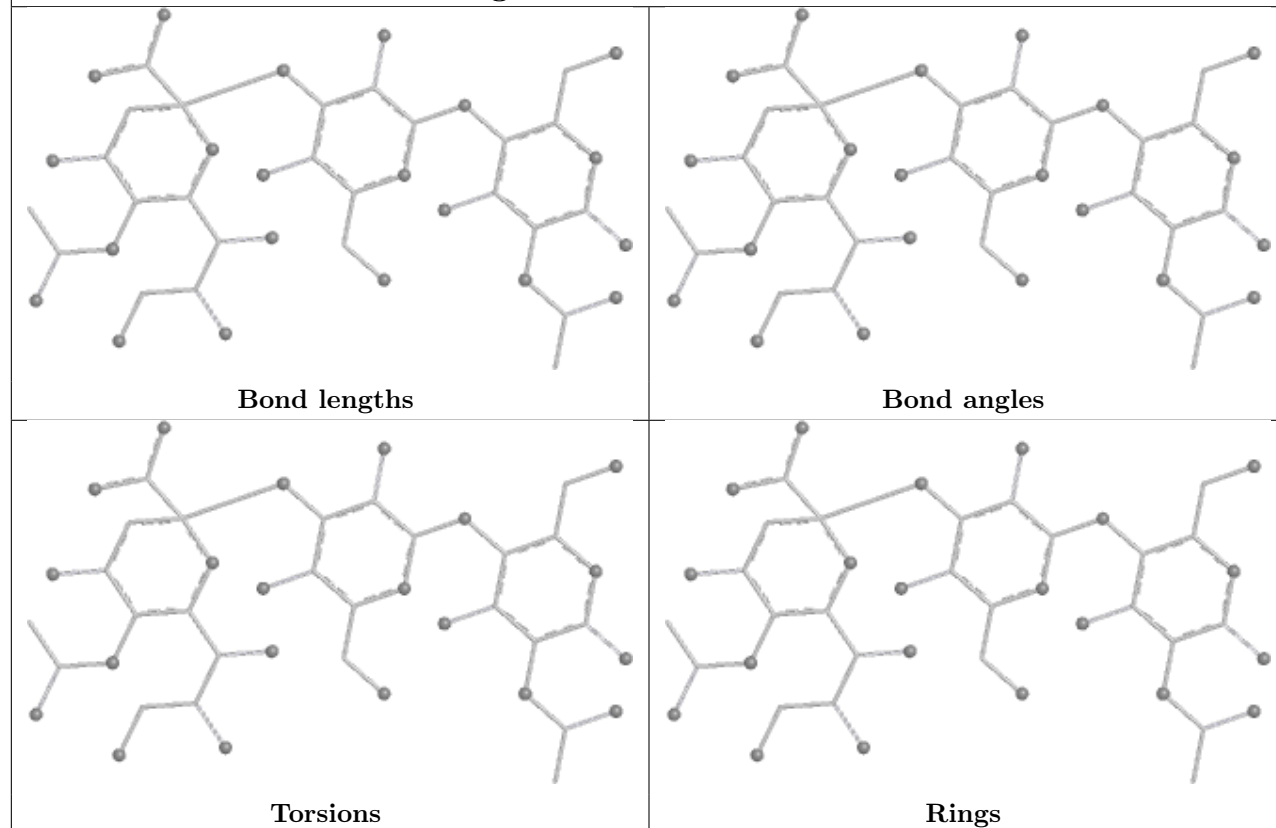
Oligosaccharide Chain 8A**Oligosaccharide Chain AB**

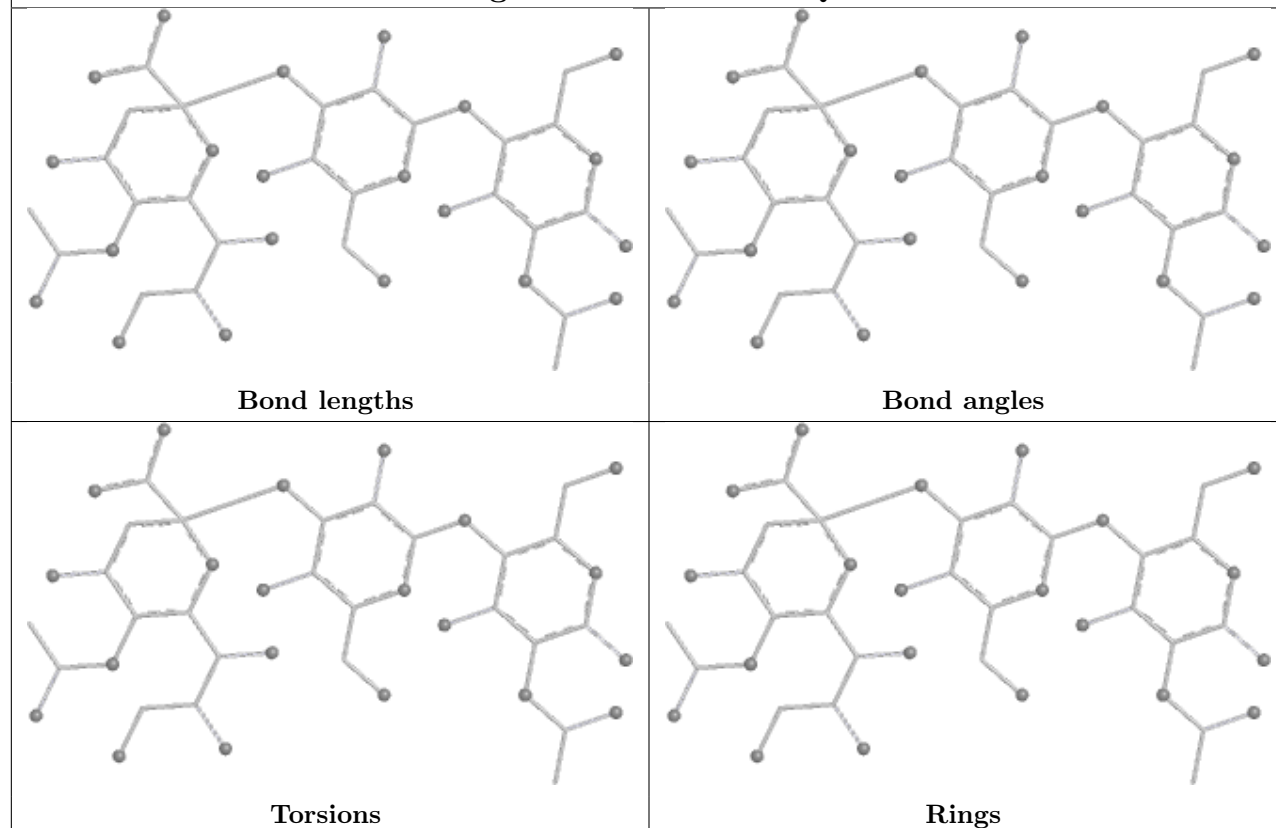
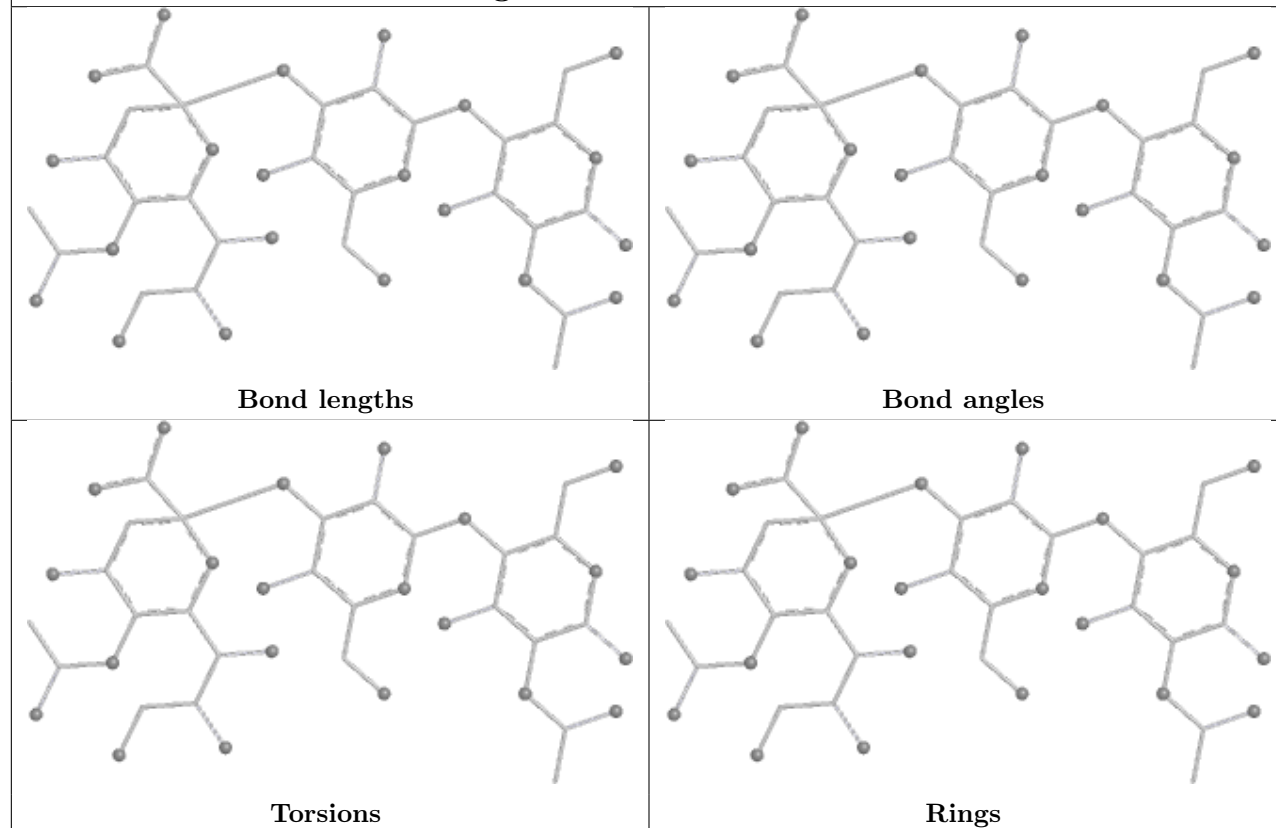


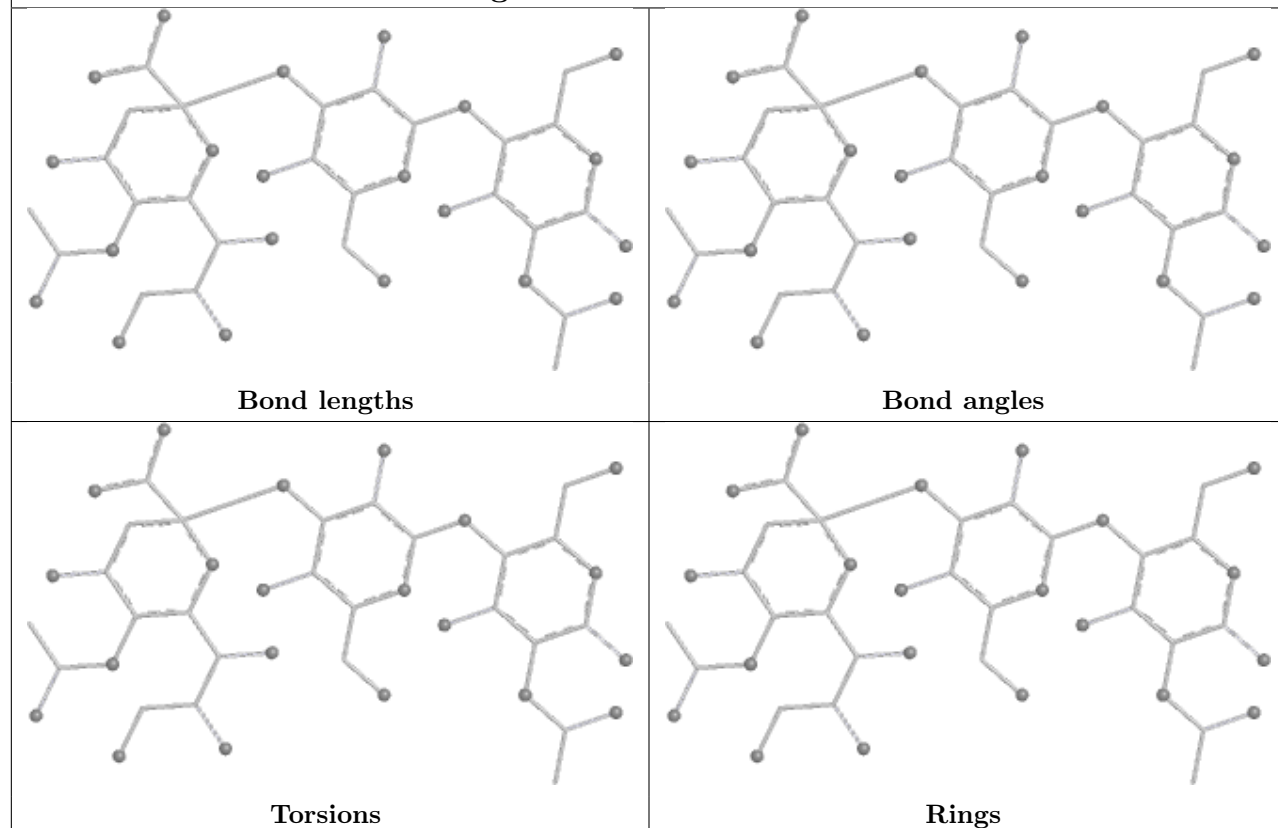
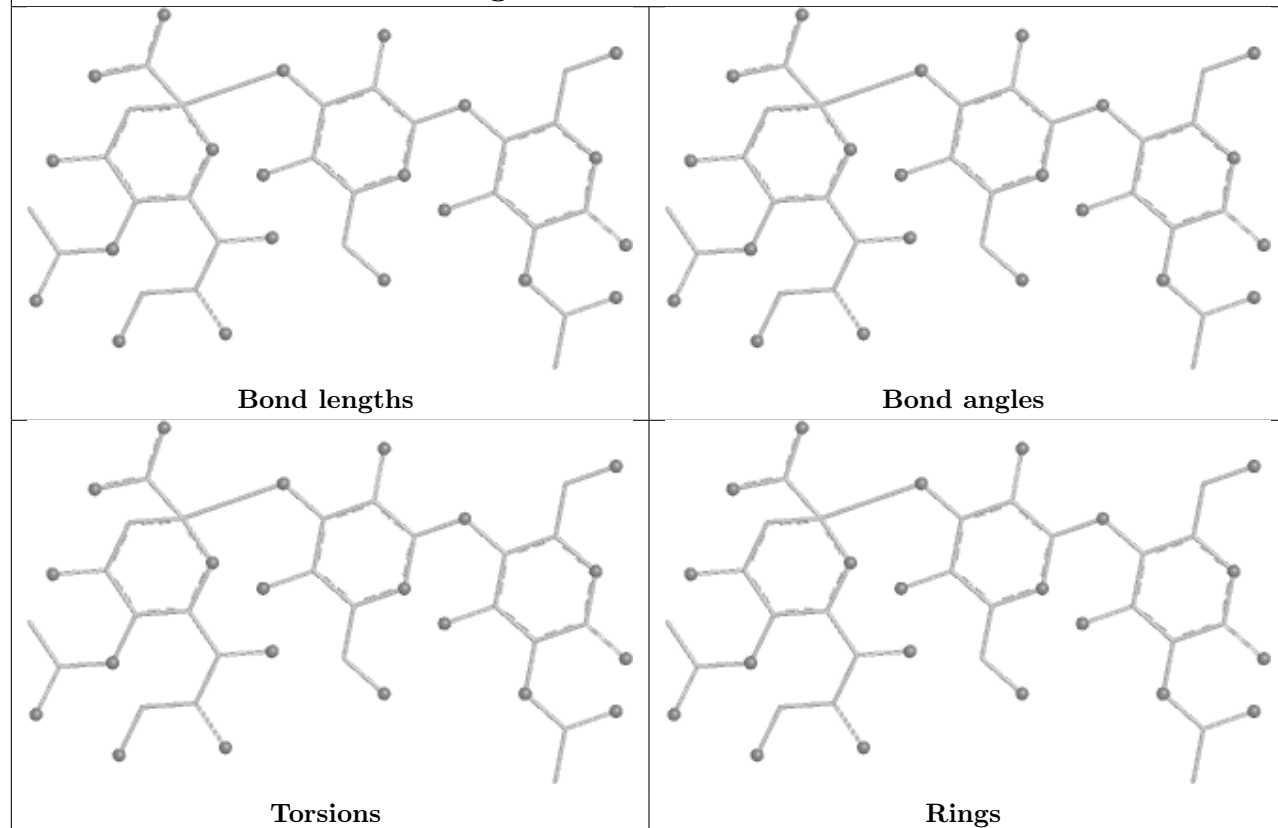
Oligosaccharide Chain EB**Oligosaccharide Chain GB**

Oligosaccharide Chain HB**Oligosaccharide Chain JB**

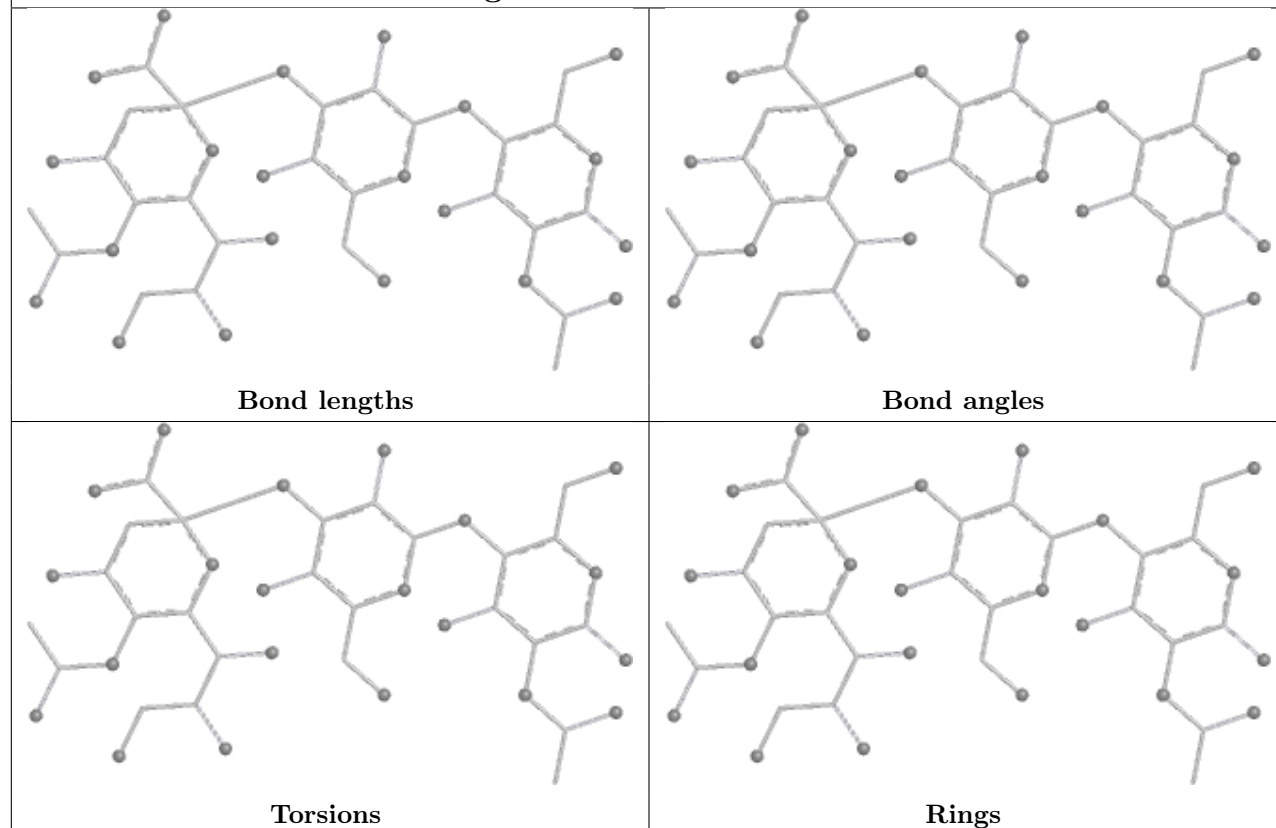
Oligosaccharide Chain KB**Oligosaccharide Chain MB**

Oligosaccharide Chain NB**Oligosaccharide Chain PB**

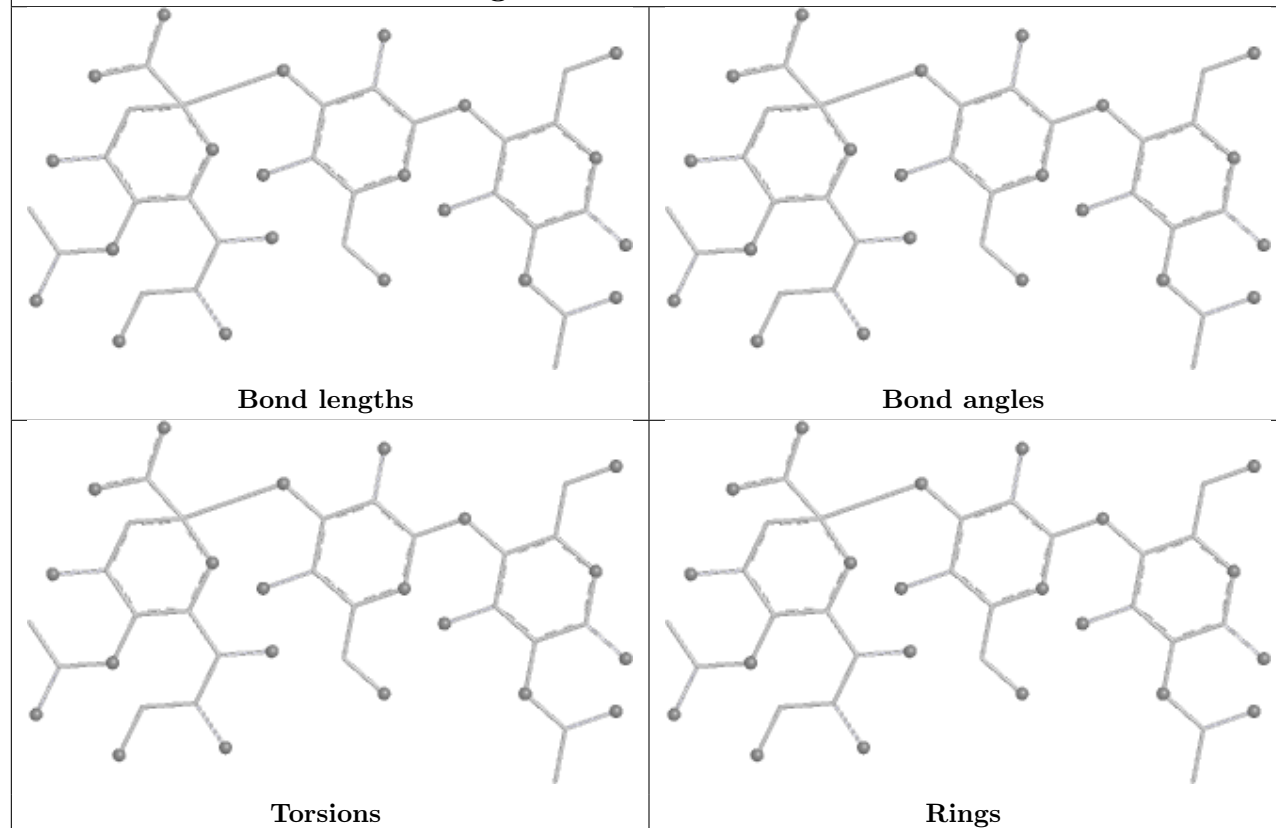
Oligosaccharide Chain QB**Oligosaccharide Chain SB**

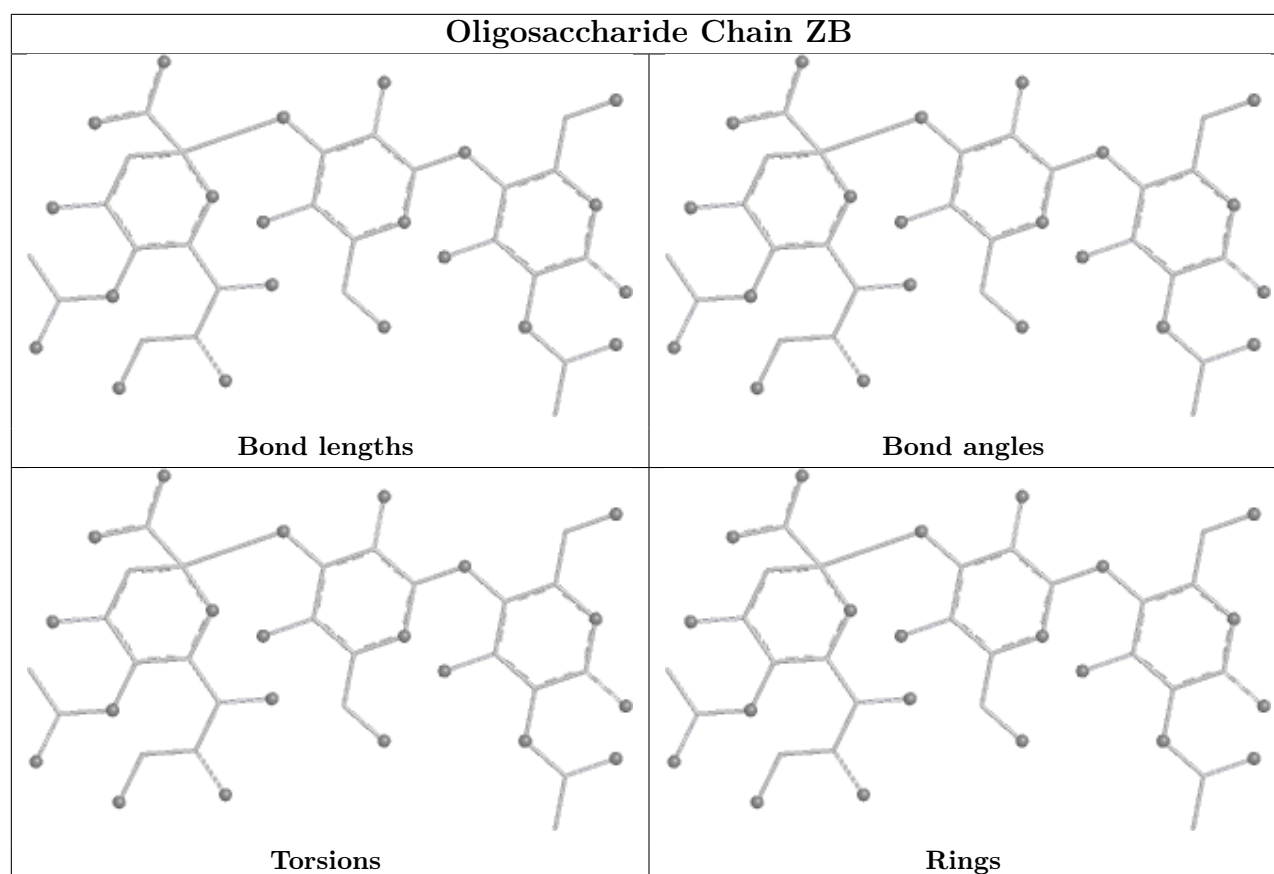
Oligosaccharide Chain TB**Oligosaccharide Chain VB**

Oligosaccharide Chain WB



Oligosaccharide Chain YB





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

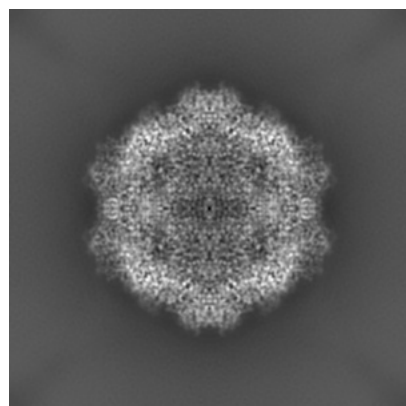
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49228. These allow visual inspection of the internal detail of the map and identification of artifacts.

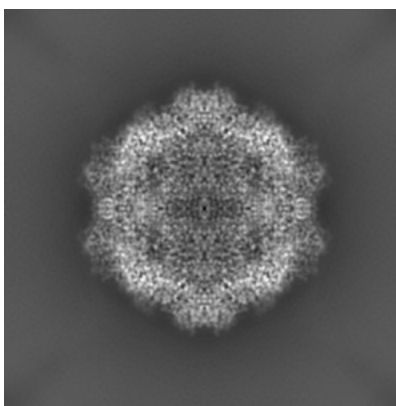
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

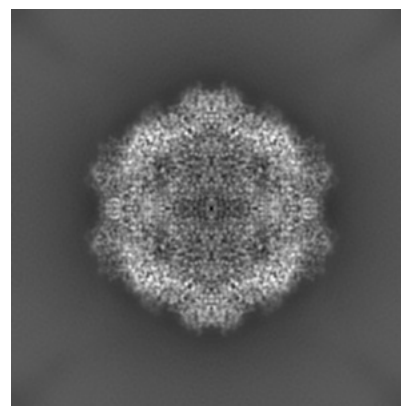
6.1.1 Primary map



X

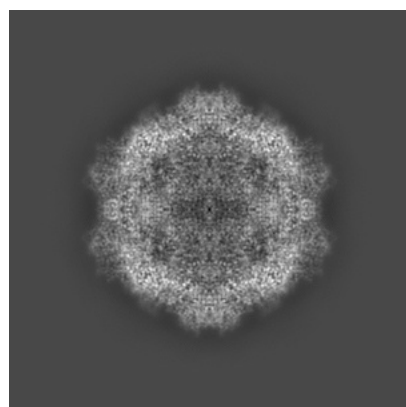


Y

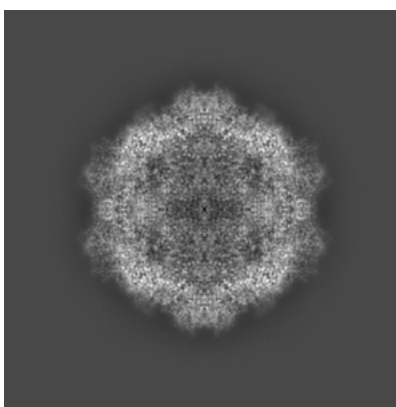


Z

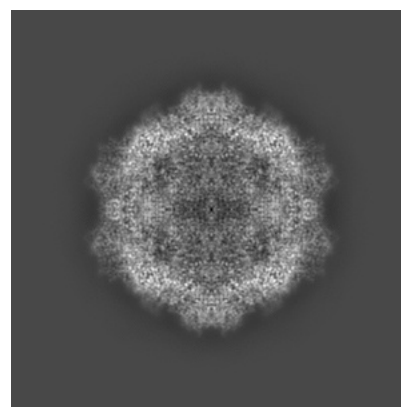
6.1.2 Raw map



X



Y

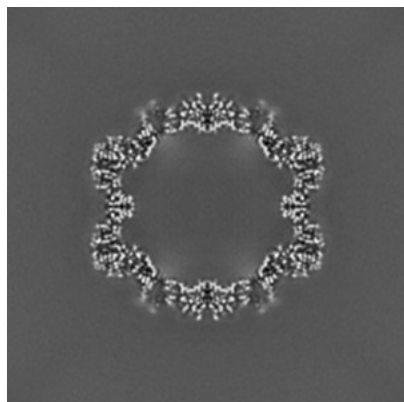


Z

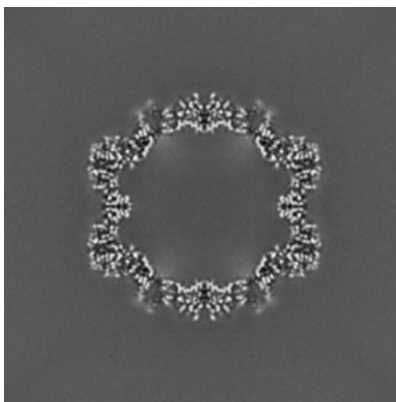
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

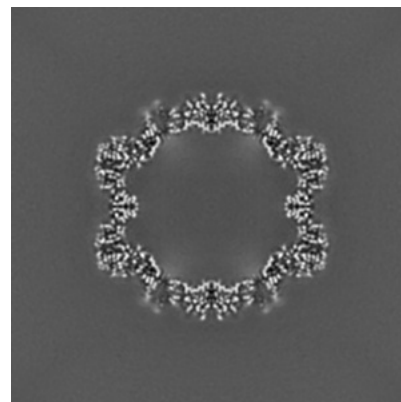
6.2.1 Primary map



X Index: 210

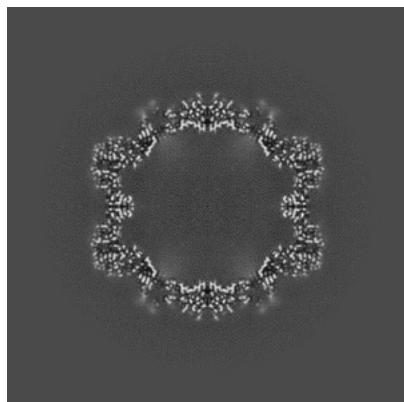


Y Index: 210

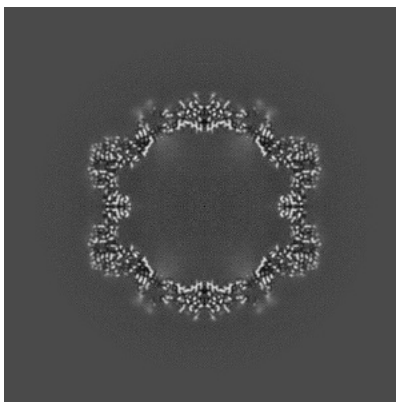


Z Index: 210

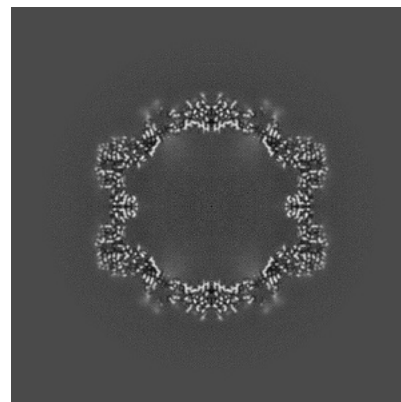
6.2.2 Raw map



X Index: 210



Y Index: 210

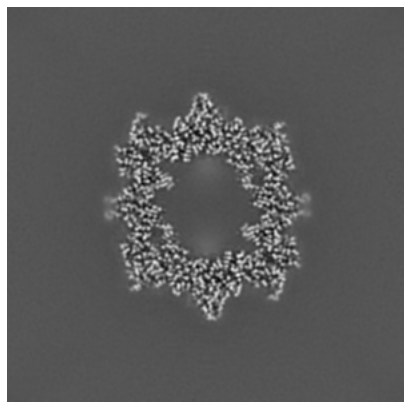


Z Index: 210

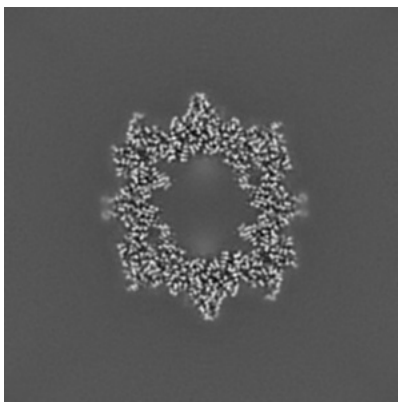
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

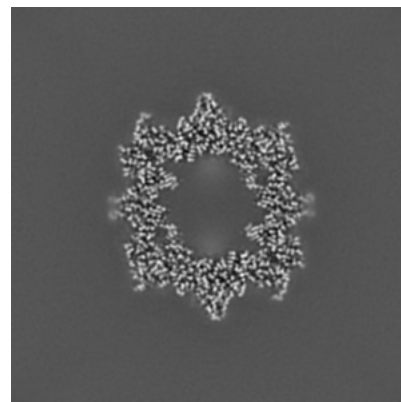
6.3.1 Primary map



X Index: 274

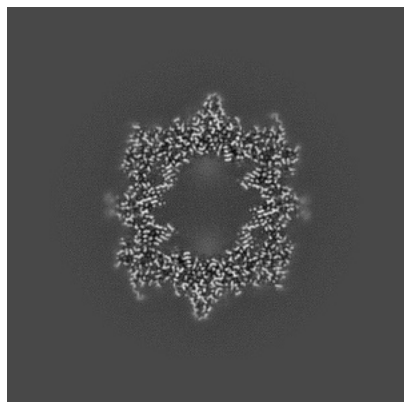


Y Index: 274

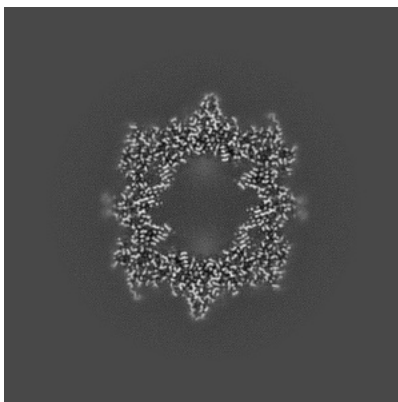


Z Index: 274

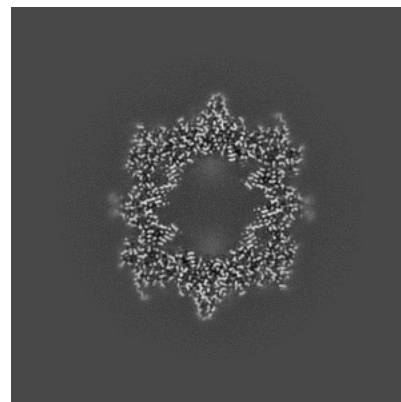
6.3.2 Raw map



X Index: 145



Y Index: 145

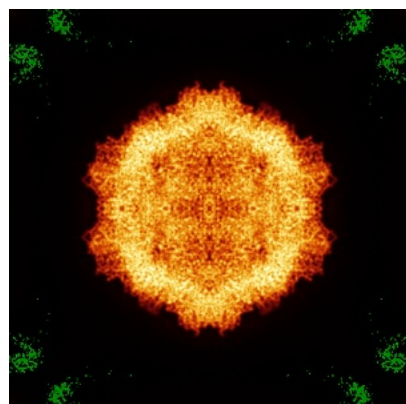


Z Index: 145

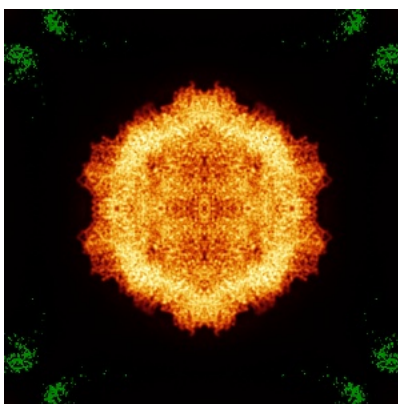
The images above show the largest variance slices of the map in three orthogonal directions.

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

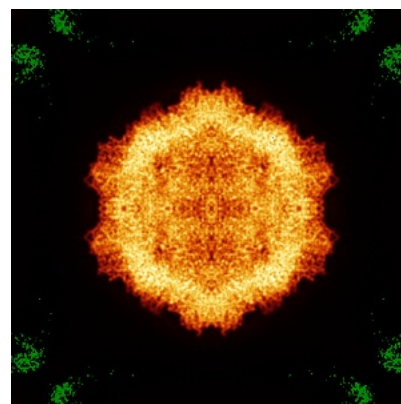
6.4.1 Primary map



X

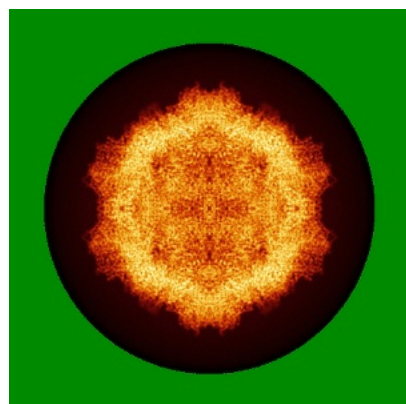


Y

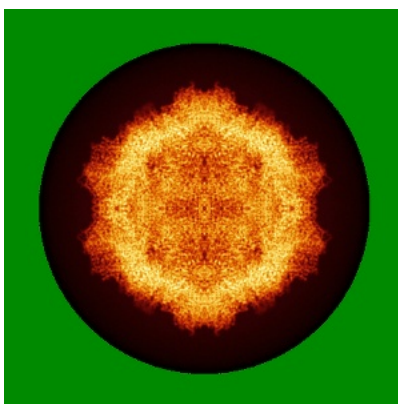


Z

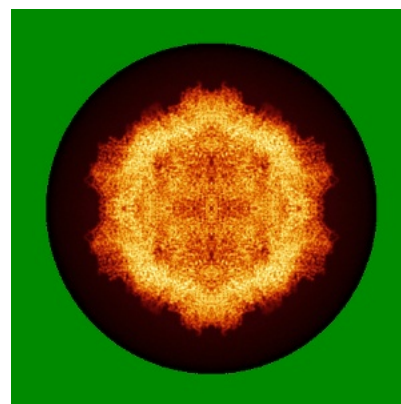
6.4.2 Raw map



X



Y

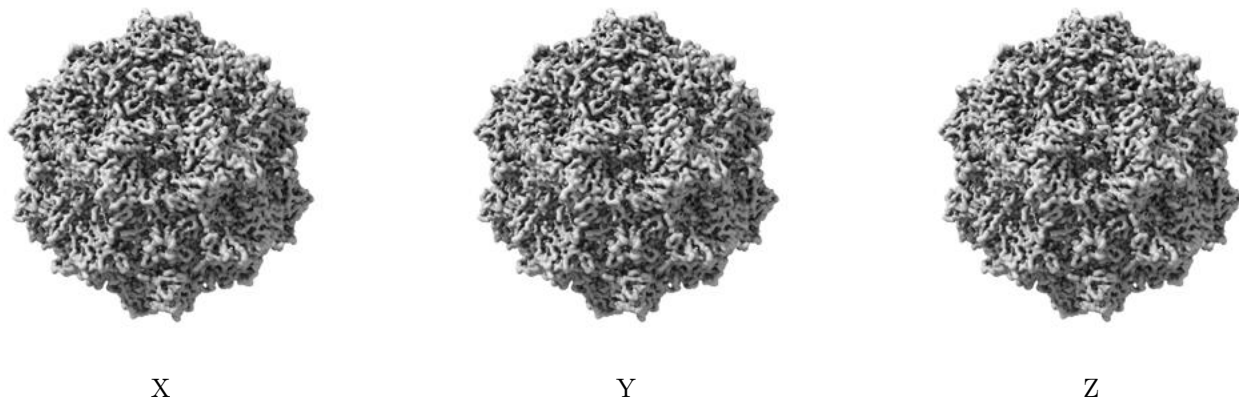


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

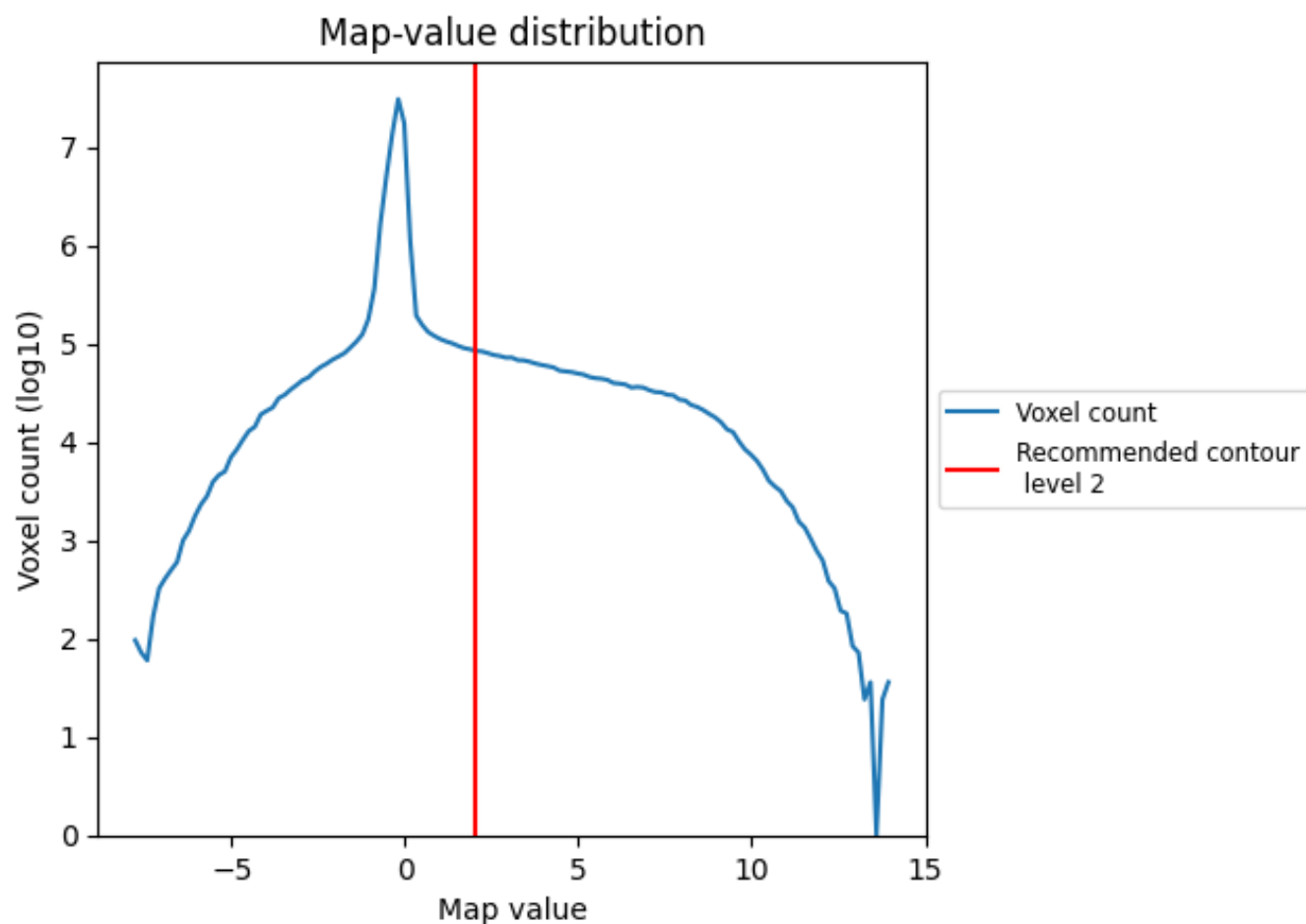
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

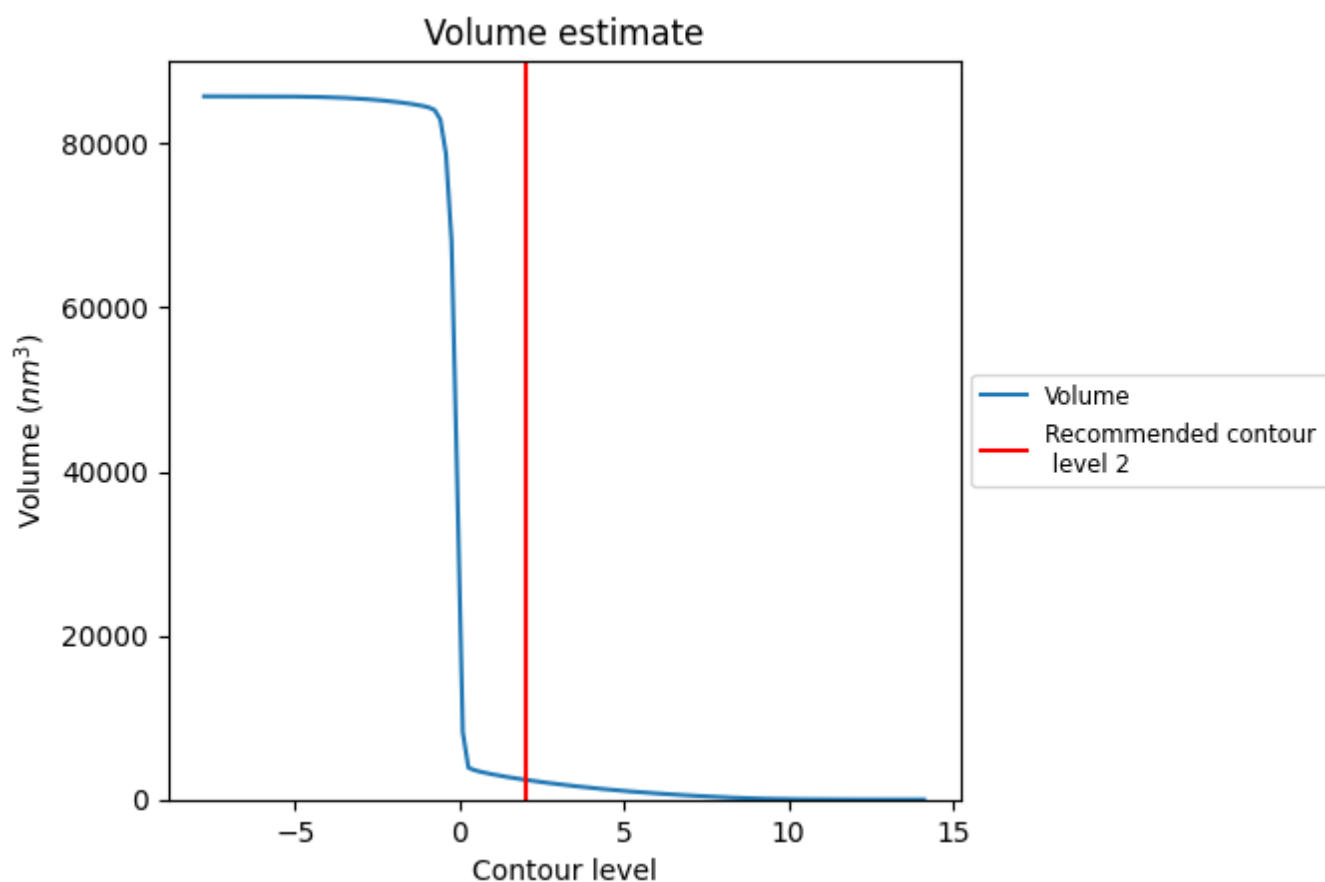
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

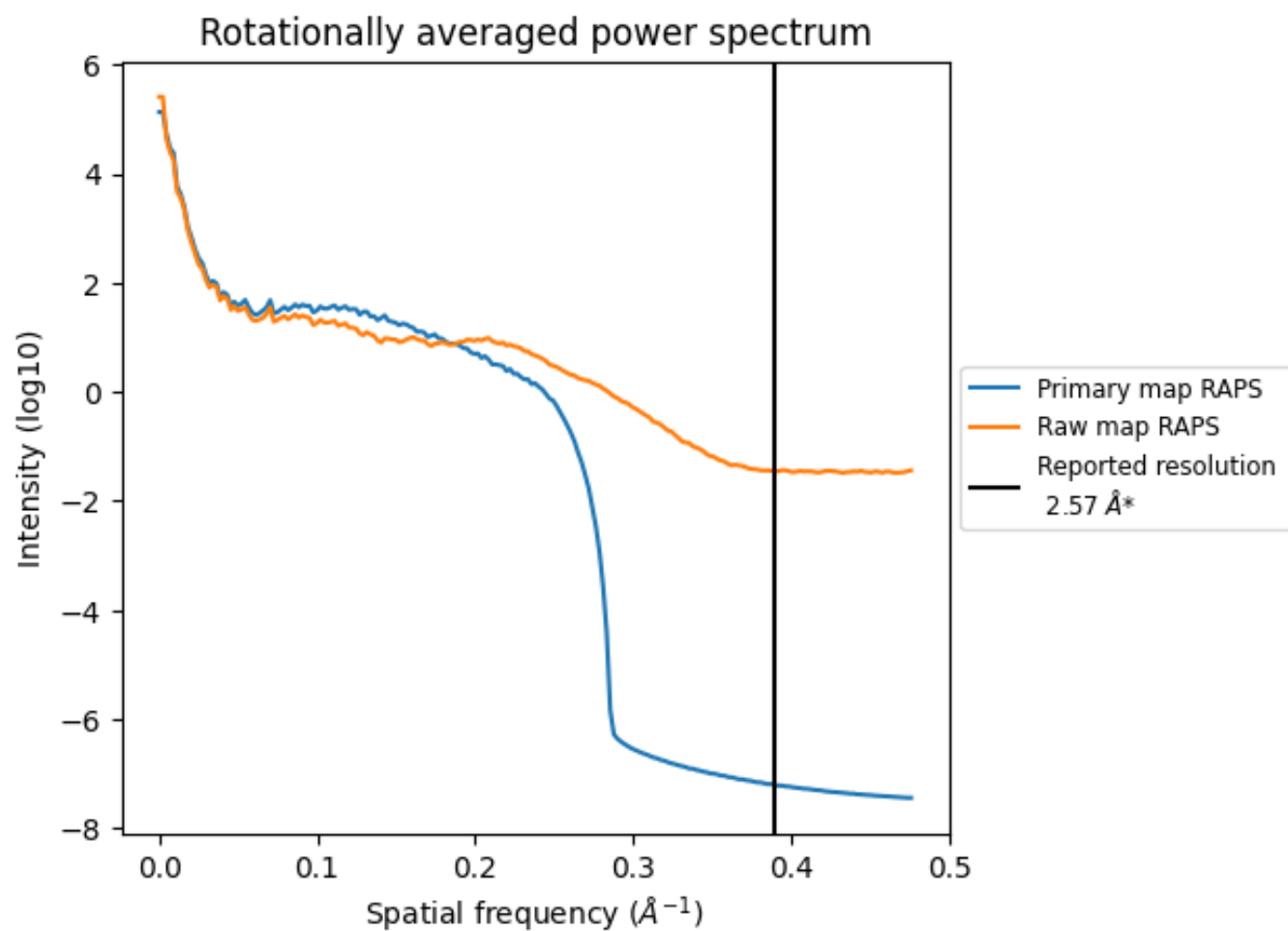
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2407 nm³; this corresponds to an approximate mass of 2174 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 ⓘ

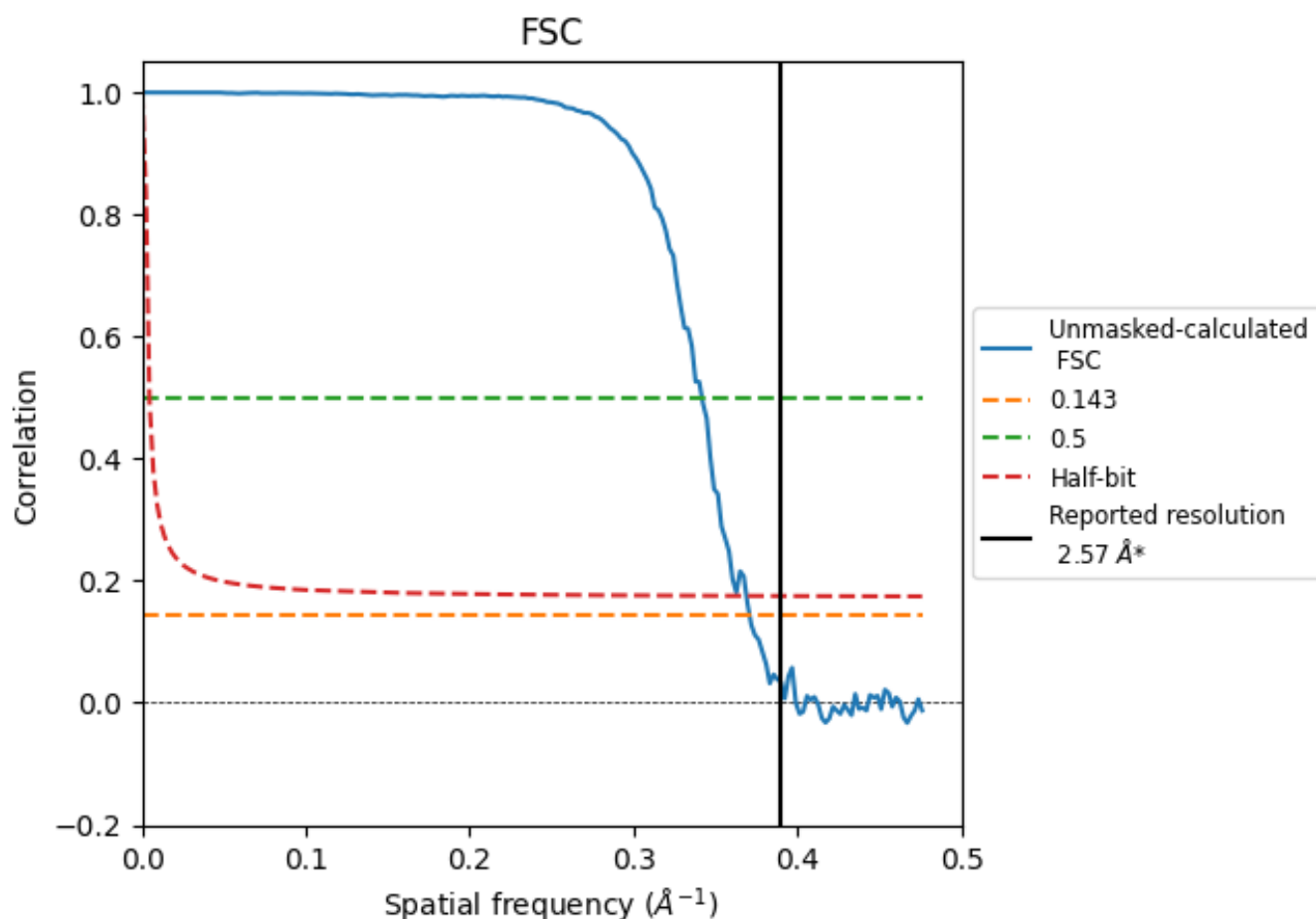


*Reported resolution corresponds to spatial frequency of 0.389 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.389 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

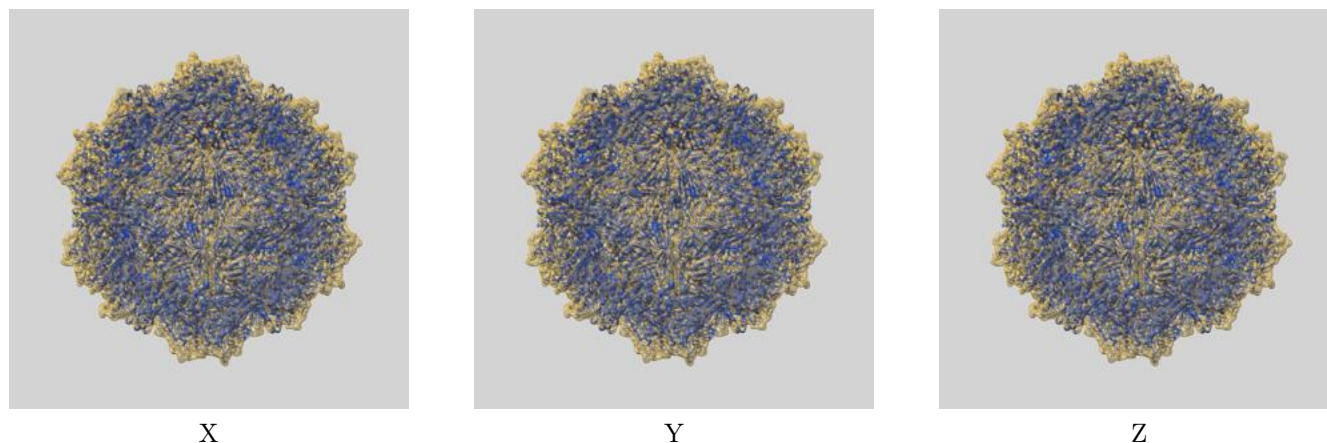
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.70	2.93	2.71

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

9 Map-model fit [i](#)

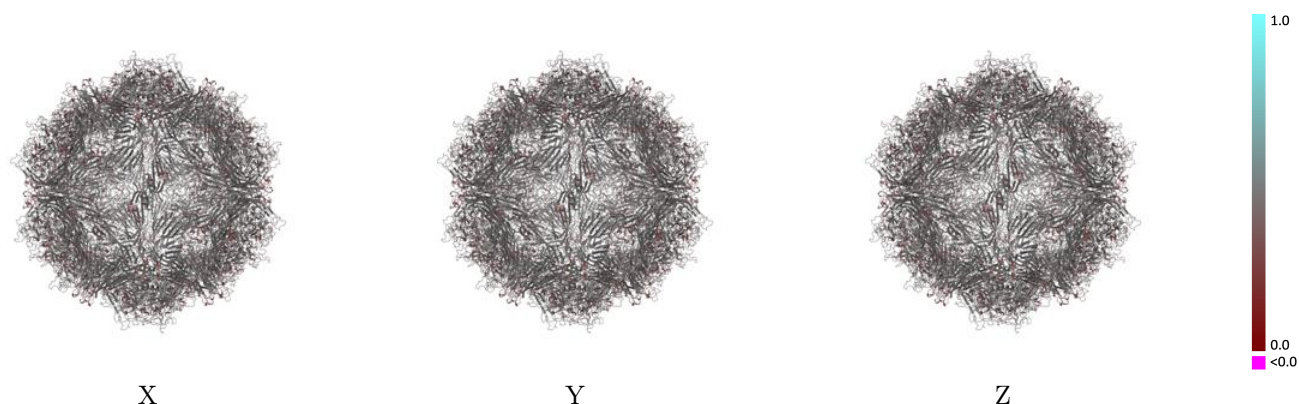
This section contains information regarding the fit between EMDB map EMD-49228 and PDB model 9NBG. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



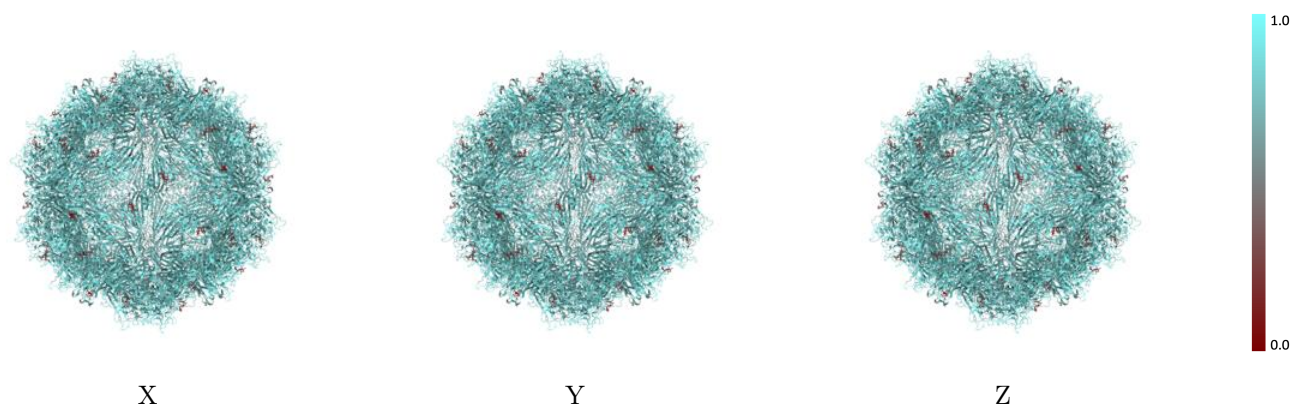
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



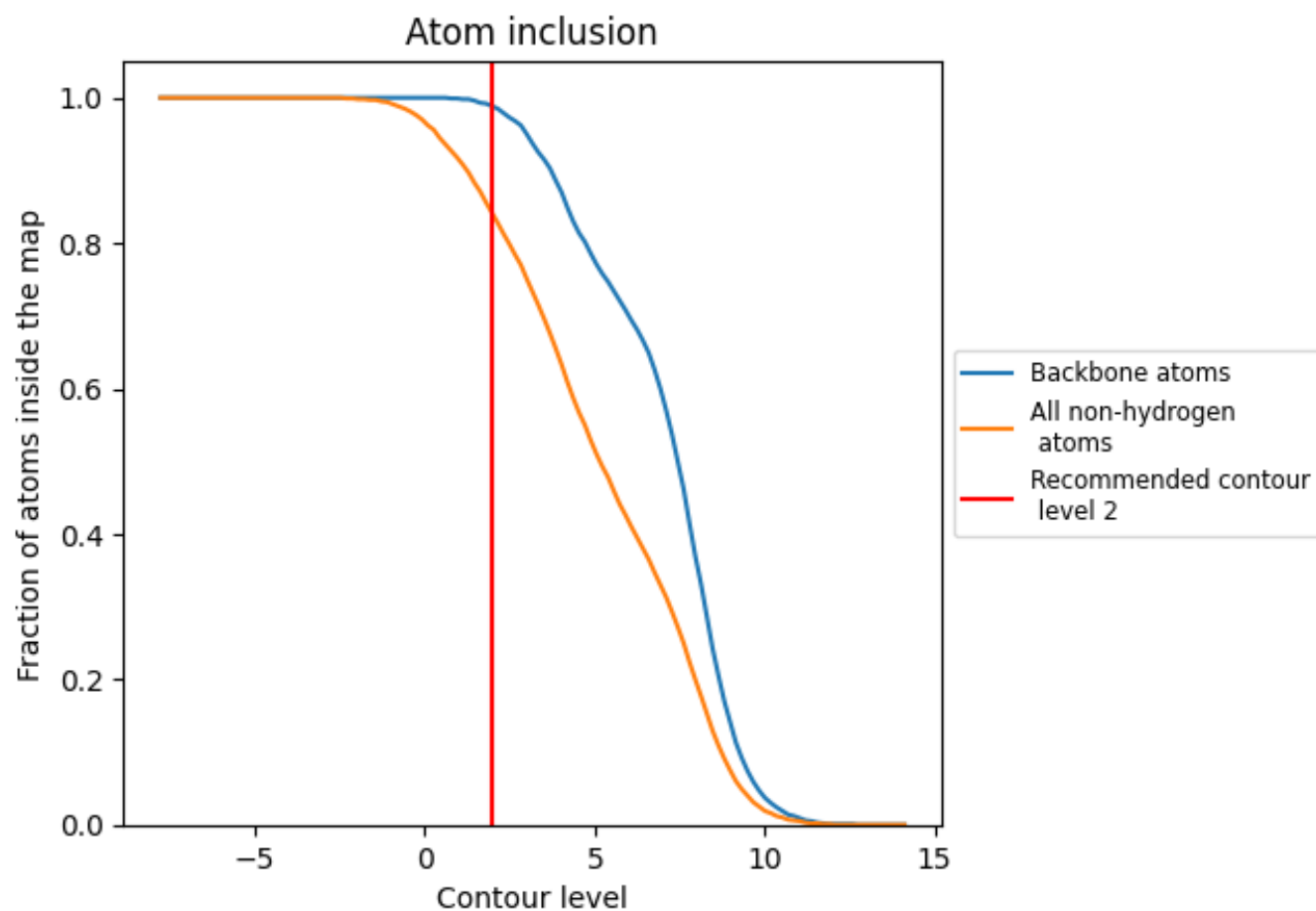
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 84% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.4350
1	 0.8490	 0.4380
1A	 0.0220	 0.2530
2	 0.8490	 0.4380
2A	 0.0220	 0.2530
3	 0.8470	 0.4360
4	 0.8520	 0.4370
4A	 0.0000	 0.2530
5	 0.8480	 0.4370
5A	 0.0000	 0.2470
6	 0.8480	 0.4360
7	 0.8480	 0.4360
7A	 0.0220	 0.2540
8	 0.8500	 0.4380
8A	 0.0000	 0.2490
9	 0.0220	 0.2540
A	 0.8470	 0.4350
AA	 0.0220	 0.2360
AB	 0.0220	 0.2390
B	 0.8490	 0.4360
BB	 0.0220	 0.2430
C	 0.8520	 0.4350
CA	 0.0220	 0.2520
D	 0.8480	 0.4370
DA	 0.0000	 0.2480
DB	 0.0220	 0.2430
E	 0.8500	 0.4370
EB	 0.0220	 0.2410
F	 0.8470	 0.4350
FA	 0.0000	 0.2390
G	 0.8500	 0.4370
GA	 0.0000	 0.2420
GB	 0.0220	 0.2490
H	 0.8480	 0.4350
HB	 0.0220	 0.2460



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
I	 0.8520	 0.4370
IA	 0.0220	 0.2410
J	 0.8490	 0.4380
JA	 0.0220	 0.2380
JB	 0.0220	 0.2360
K	 0.8520	 0.4360
KB	 0.0220	 0.2510
L	 0.8490	 0.4370
LA	 0.0220	 0.2400
M	 0.8500	 0.4360
MA	 0.0220	 0.2410
MB	 0.0220	 0.2390
N	 0.8480	 0.4350
NB	 0.0220	 0.2370
O	 0.8500	 0.4360
OA	 0.0220	 0.2330
P	 0.8480	 0.4340
PA	 0.0220	 0.2340
PB	 0.0220	 0.2550
Q	 0.8520	 0.4350
QB	 0.0220	 0.2390
R	 0.8490	 0.4370
RA	 0.0000	 0.2420
S	 0.8490	 0.4370
SA	 0.0000	 0.2450
SB	 0.0220	 0.2430
T	 0.8520	 0.4360
TB	 0.0220	 0.2470
U	 0.8490	 0.4360
UA	 0.0000	 0.2510
V	 0.8520	 0.4360
VA	 0.0220	 0.2410
VB	 0.0220	 0.2360
W	 0.8480	 0.4360
WB	 0.0220	 0.2490
X	 0.8500	 0.4360
XA	 0.0220	 0.2400
Y	 0.8480	 0.4370
YA	 0.0220	 0.2370
YB	 0.0220	 0.2460
Z	 0.8500	 0.4360
ZB	 0.0220	 0.2400

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Chain	Atom inclusion	Q-score
a	 0.8470	 0.4370
aA	 0.0220	 0.2390
b	 0.8470	 0.4370
bA	 0.0220	 0.2410
c	 0.8470	 0.4360
d	 0.8470	 0.4350
dA	 0.0220	 0.2410
e	 0.8470	 0.4360
eA	 0.0220	 0.2440
f	 0.8470	 0.4350
g	 0.8520	 0.4370
gA	 0.0000	 0.2450
h	 0.8500	 0.4370
hA	 0.0220	 0.2490
i	 0.8480	 0.4350
j	 0.8480	 0.4370
jA	 0.0220	 0.2490
k	 0.8480	 0.4370
kA	 0.0220	 0.2450
l	 0.8500	 0.4370
m	 0.8520	 0.4370
mA	 0.0220	 0.2360
n	 0.8470	 0.4360
nA	 0.0220	 0.2420
o	 0.8500	 0.4380
p	 0.8520	 0.4370
pA	 0.0220	 0.2440
q	 0.8490	 0.4380
qA	 0.0220	 0.2390
r	 0.8490	 0.4360
s	 0.8490	 0.4380
sA	 0.0000	 0.2460
t	 0.8500	 0.4380
tA	 0.0220	 0.2460
u	 0.8520	 0.4370
v	 0.8470	 0.4360
vA	 0.0000	 0.2480
w	 0.8500	 0.4370
wA	 0.0220	 0.2530
x	 0.8520	 0.4360
y	 0.8470	 0.4370
yA	 0.0220	 0.2480

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Chain	Atom inclusion	Q-score
z	 0.8490	 0.4390
zA	 0.0220	 0.2560