Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 01:11 AM EST

PDB ID	:	6V8X
EMDB ID	:	EMD-21111
Title	:	VRC01 Bound BG505 F14 HIV-1 SOSIP Envelope Trimer Structure
Authors	:	Henderson, R.; Acharya, P.
Deposited on	:	2019-12-12
Resolution	:	3.00 Å(reported)

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

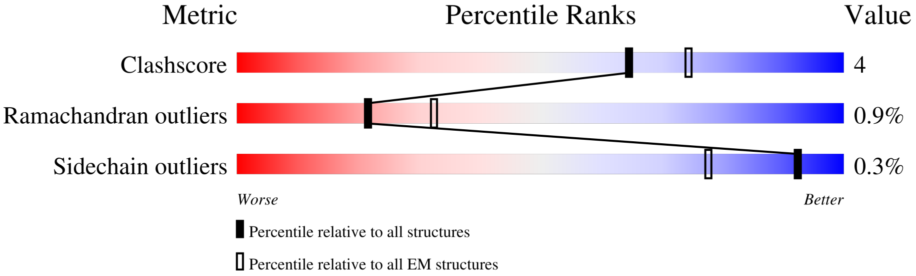
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

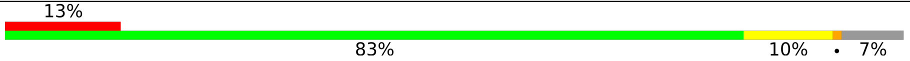
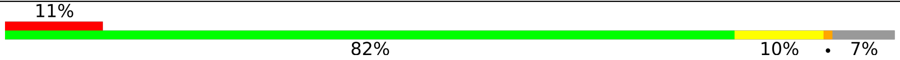
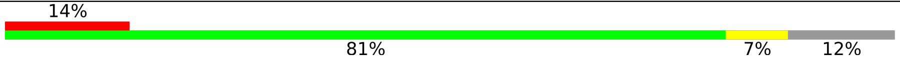
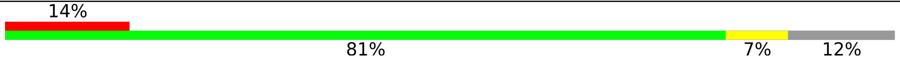
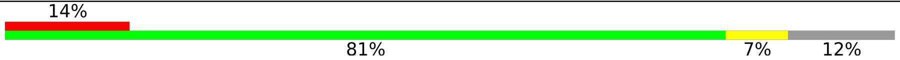
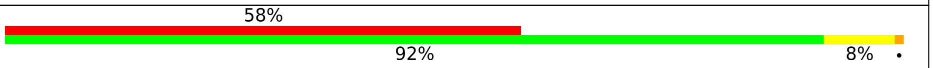
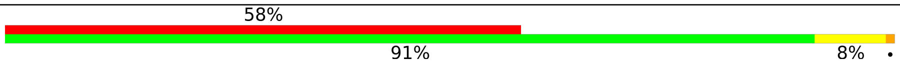
The reported resolution of this entry is 3.00 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	
1	E	471	
1	I	471	
2	B	145	
2	F	145	
2	J	145	
3	C	224	
3	G	224	

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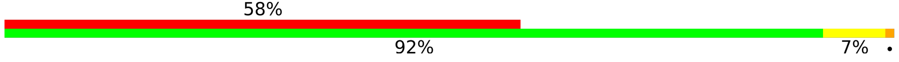
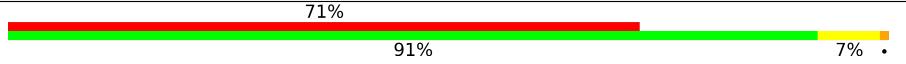
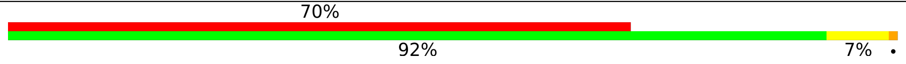
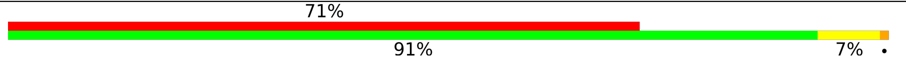
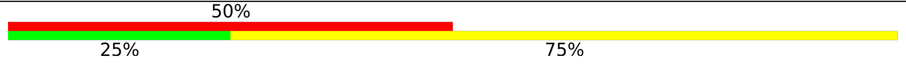
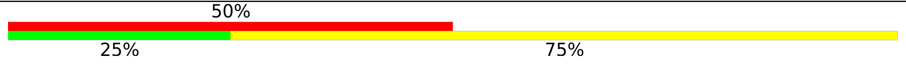
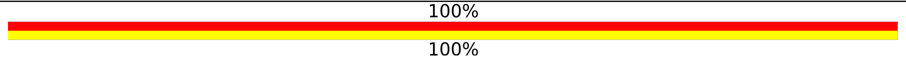
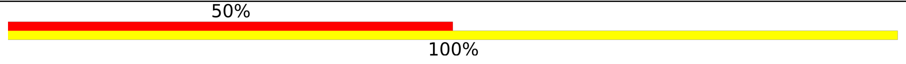
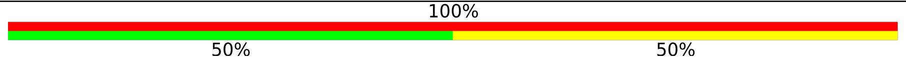
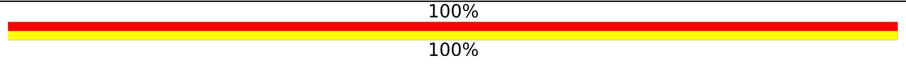
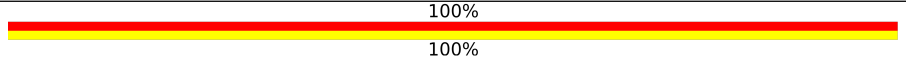
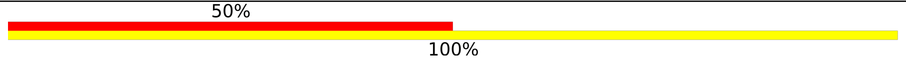
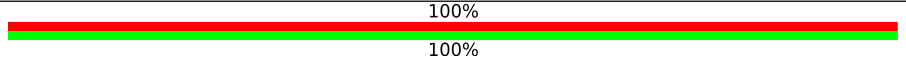
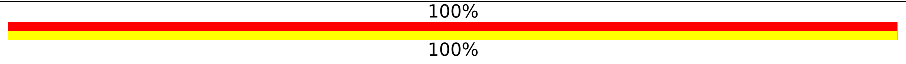
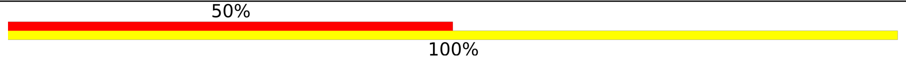
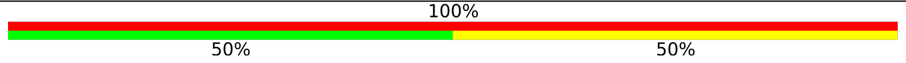
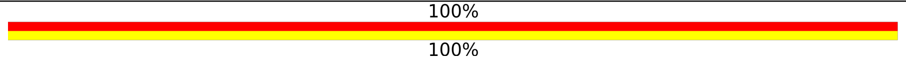
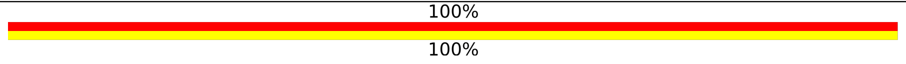
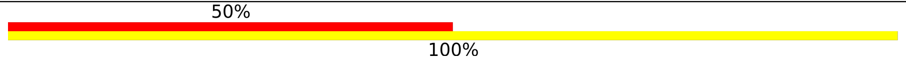
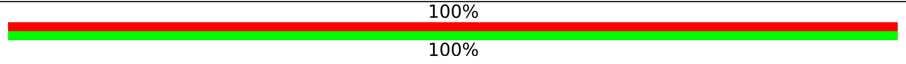
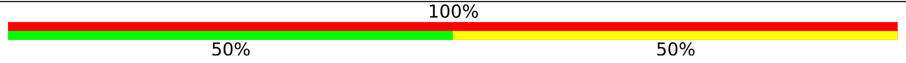
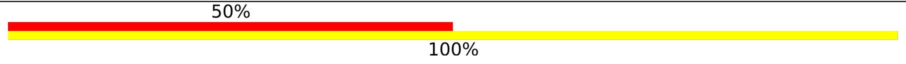
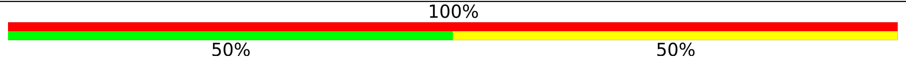
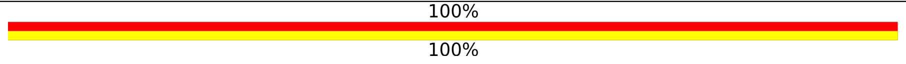
Mol	Chain	Length	Quality of chain
3	K	224	
4	D	208	
4	H	208	
4	L	208	
5	M	4	
5	Y	4	
5	k	4	
6	N	2	
6	R	2	
6	S	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	Z	2	
6	d	2	
6	e	2	
6	g	2	
6	h	2	
6	i	2	
6	j	2	
6	l	2	
6	p	2	
6	q	2	
6	s	2	

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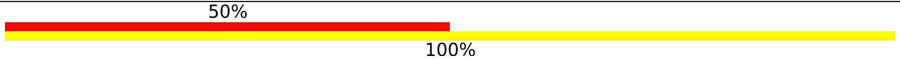
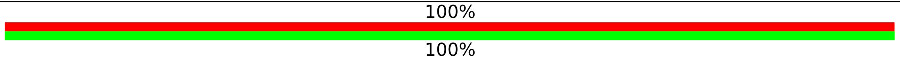
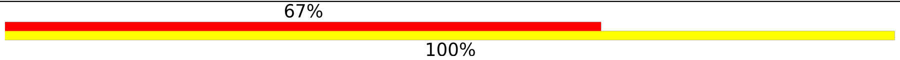
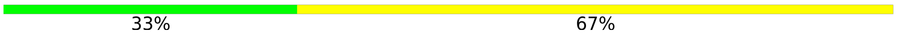
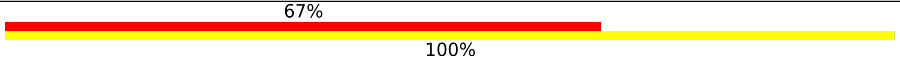
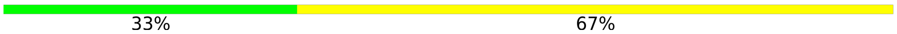
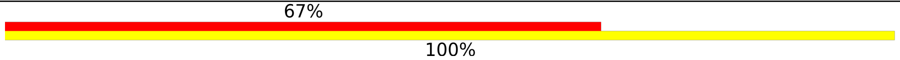
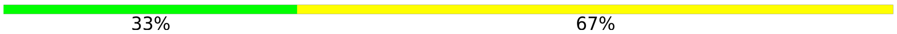
Mol	Chain	Length	Quality of chain
6	t	2	
6	u	2	
6	v	2	
7	O	3	
7	P	3	
7	Q	3	
7	T	3	
7	a	3	
7	b	3	
7	c	3	
7	f	3	
7	m	3	
7	n	3	
7	o	3	
7	r	3	

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 24825 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total 3453	C 2172	N 609	O 645	S 27	0	0
1	E	439	Total 3453	C 2172	N 609	O 645	S 27	0	0
1	I	439	Total 3453	C 2172	N 609	O 645	S 27	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ILE	VAL	conflict	UNP Q2N0S6
A	148	ALA	ASN	conflict	UNP Q2N0S6
A	204	VAL	ALA	conflict	UNP Q2N0S6
A	208	LEU	VAL	conflict	UNP Q2N0S6
A	255	LEU	VAL	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
E	68	ILE	VAL	conflict	UNP Q2N0S6
E	148	ALA	ASN	conflict	UNP Q2N0S6
E	204	VAL	ALA	conflict	UNP Q2N0S6
E	208	LEU	VAL	conflict	UNP Q2N0S6
E	255	LEU	VAL	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
I	68	ILE	VAL	conflict	UNP Q2N0S6
I	148	ALA	ASN	conflict	UNP Q2N0S6
I	204	VAL	ALA	conflict	UNP Q2N0S6
I	208	LEU	VAL	conflict	UNP Q2N0S6
I	255	LEU	VAL	conflict	UNP Q2N0S6
I	332	ASN	THR	conflict	UNP Q2N0S6
I	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	128	1025	649	178	192	6	0	0
2	F	128	1025	649	178	192	6	0	0
2	J	128	1025	649	178	192	6	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S9
F	605	CYS	THR	conflict	UNP Q2N0S9
J	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 3 is a protein called VRC01 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	224	1710	1077	297	325	11	0	0
3	G	224	1710	1077	297	325	11	0	0
3	K	224	1710	1077	297	325	11	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	211	ALA	VAL	conflict	UNP Q6N095
G	211	ALA	VAL	conflict	UNP Q6N095
K	211	ALA	VAL	conflict	UNP Q6N095

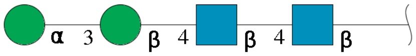
- Molecule 4 is a protein called VRC01 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	208	1615	1011	277	322	5	0	0
4	H	208	1615	1011	277	322	5	0	0
4	L	208	1615	1011	277	322	5	0	0

There are 3 discrepancies between the modelled and reference sequences:

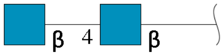
Chain	Residue	Modelled	Actual	Comment	Reference
D	204	ARG	SER	conflict	UNP Q6PIL8
H	204	ARG	SER	conflict	UNP Q6PIL8
L	204	ARG	SER	conflict	UNP Q6PIL8

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
5	M	4	Total C N O 50 28 2 20	0	0
5	Y	4	Total C N O 50 28 2 20	0	0
5	k	4	Total C N O 50 28 2 20	0	0

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



Mol	Chain	Residues	Atoms	AltConf	Trace
6	N	2	Total C N O 28 16 2 10	0	0
6	R	2	Total C N O 28 16 2 10	0	0
6	S	2	Total C N O 28 16 2 10	0	0
6	U	2	Total C N O 28 16 2 10	0	0
6	V	2	Total C N O 28 16 2 10	0	0
6	W	2	Total C N O 28 16 2 10	0	0
6	X	2	Total C N O 28 16 2 10	0	0

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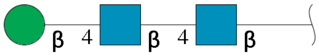
Mol	Chain	Residues	Atoms	AltConf	Trace
6	Z	2	Total C N O 28 16 2 10	0	0
6	d	2	Total C N O 28 16 2 10	0	0
6	e	2	Total C N O 28 16 2 10	0	0
6	g	2	Total C N O 28 16 2 10	0	0
6	h	2	Total C N O 28 16 2 10	0	0
6	i	2	Total C N O 28 16 2 10	0	0
6	j	2	Total C N O 28 16 2 10	0	0
6	l	2	Total C N O 28 16 2 10	0	0
6	p	2	Total C N O 28 16 2 10	0	0
6	q	2	Total C N O 28 16 2 10	0	0
6	s	2	Total C N O 28 16 2 10	0	0
6	t	2	Total C N O 28 16 2 10	0	0
6	u	2	Total C N O 28 16 2 10	0	0
6	v	2	Total C N O 28 16 2 10	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
7	O	3	Total C N O 39 22 2 15	0	0
7	P	3	Total C N O 39 22 2 15	0	0
7	Q	3	Total C N O 39 22 2 15	0	0

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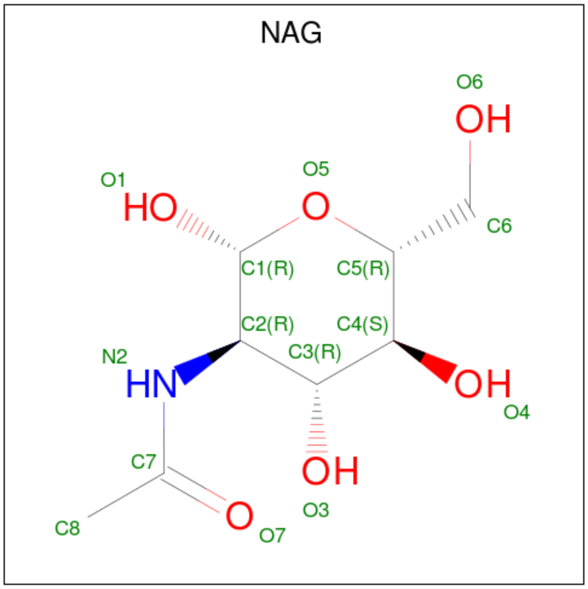
Mol	Chain	Residues	Atoms	AltConf	Trace
7	T	3	Total C N O 39 22 2 15	0	0
7	a	3	Total C N O 39 22 2 15	0	0
7	b	3	Total C N O 39 22 2 15	0	0
7	c	3	Total C N O 39 22 2 15	0	0
7	f	3	Total C N O 39 22 2 15	0	0
7	m	3	Total C N O 39 22 2 15	0	0
7	n	3	Total C N O 39 22 2 15	0	0
7	o	3	Total C N O 39 22 2 15	0	0
7	r	3	Total C N O 39 22 2 15	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O 56 32 4 20	0
8	A	1	Total C N O 56 32 4 20	0

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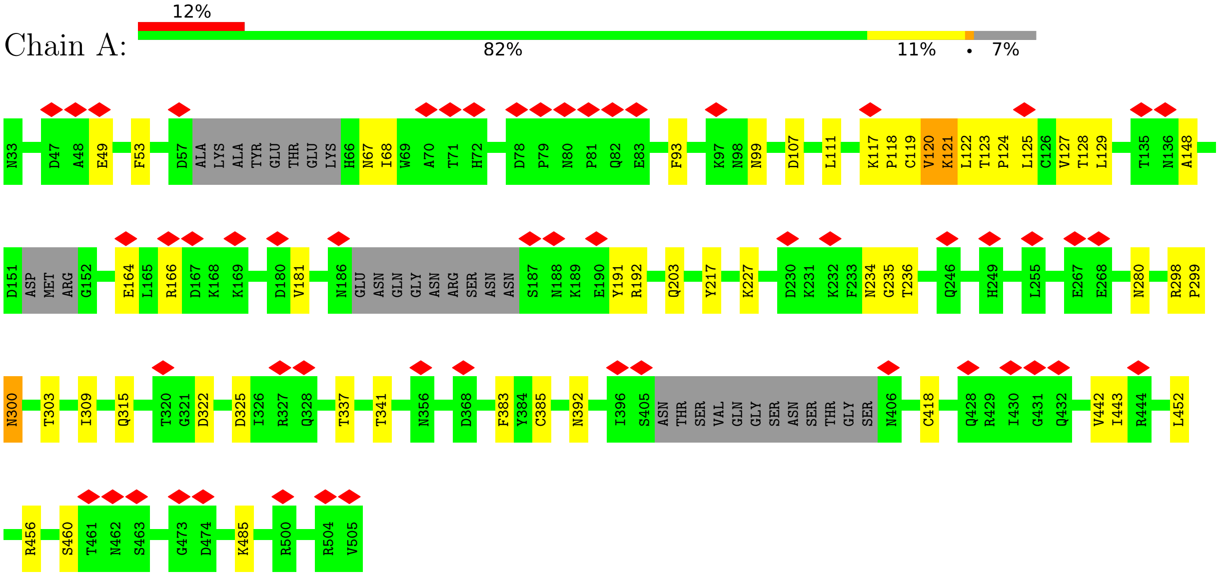
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O 56 32 4 20	0
8	A	1	Total C N O 56 32 4 20	0
8	B	1	Total C N O 14 8 1 5	0
8	E	1	Total C N O 56 32 4 20	0
8	E	1	Total C N O 56 32 4 20	0
8	E	1	Total C N O 56 32 4 20	0
8	E	1	Total C N O 56 32 4 20	0
8	F	1	Total C N O 14 8 1 5	0
8	I	1	Total C N O 56 32 4 20	0
8	I	1	Total C N O 56 32 4 20	0
8	I	1	Total C N O 56 32 4 20	0
8	I	1	Total C N O 56 32 4 20	0
8	J	1	Total C N O 14 8 1 5	0

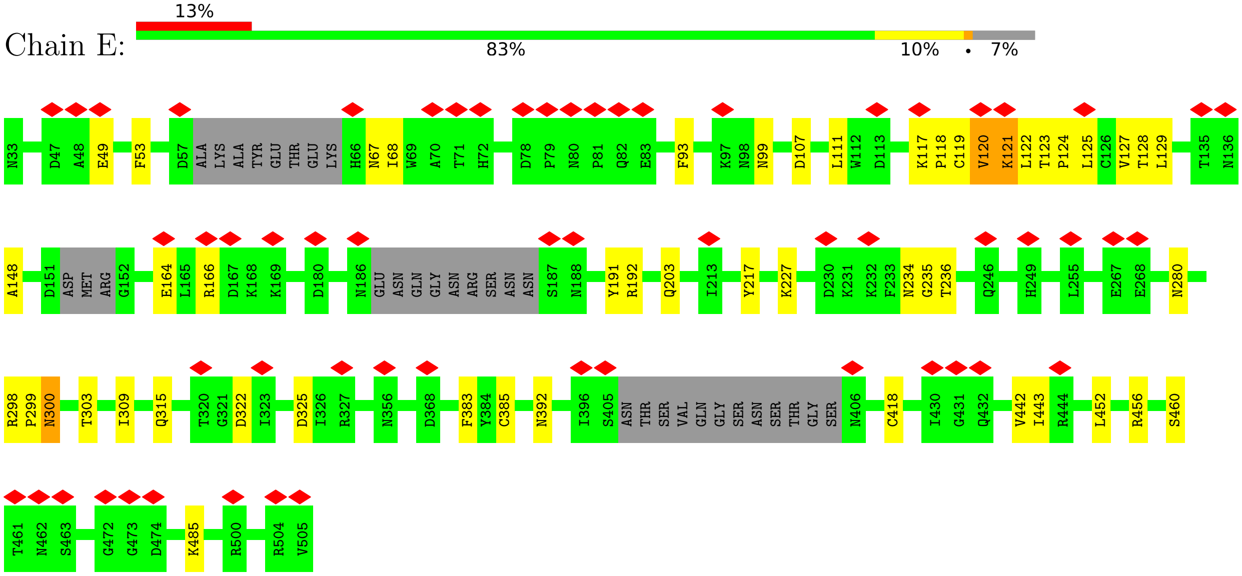
3 Residue-property plots

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.

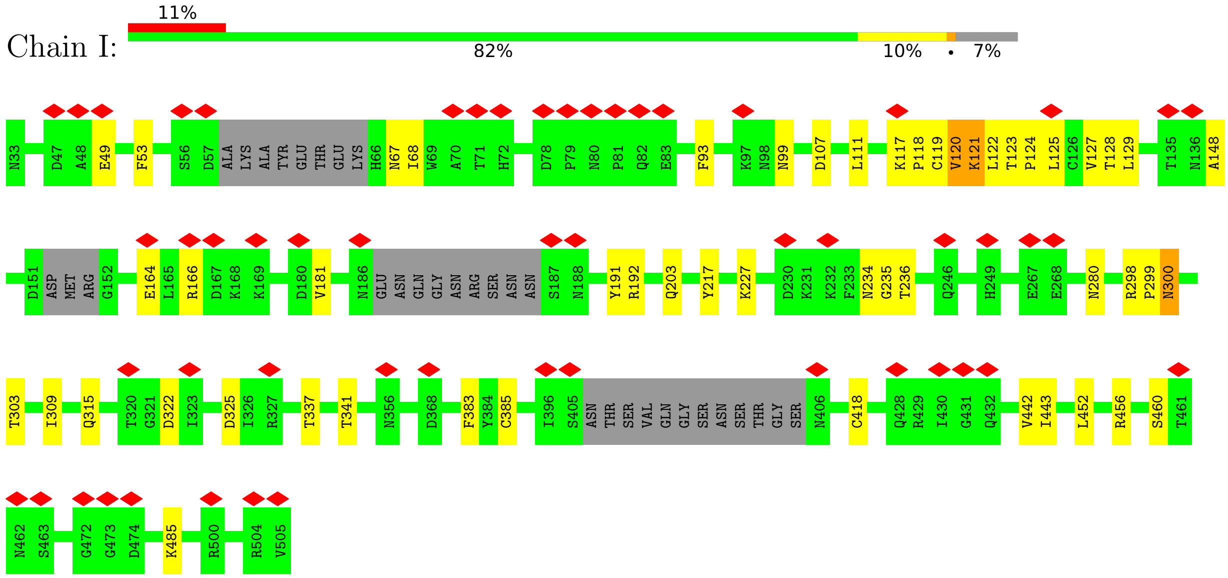
- Molecule 1: Envelope glycoprotein gp120



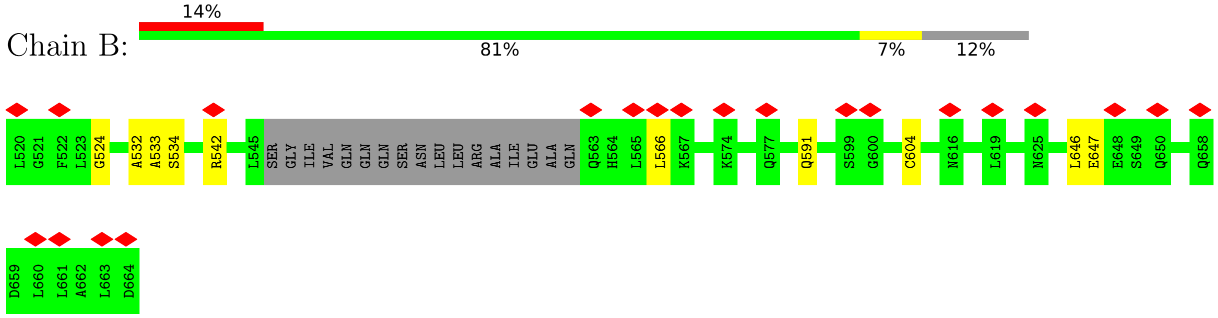
- Molecule 1: Envelope glycoprotein gp120



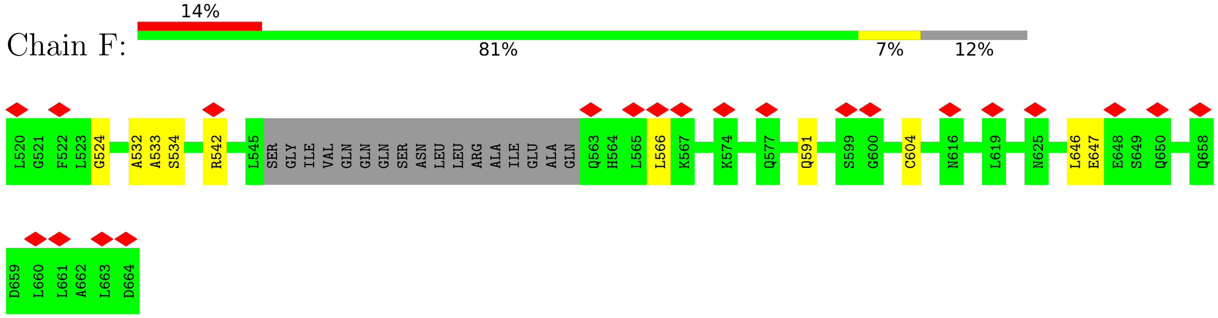
- Molecule 1: Envelope glycoprotein gp120



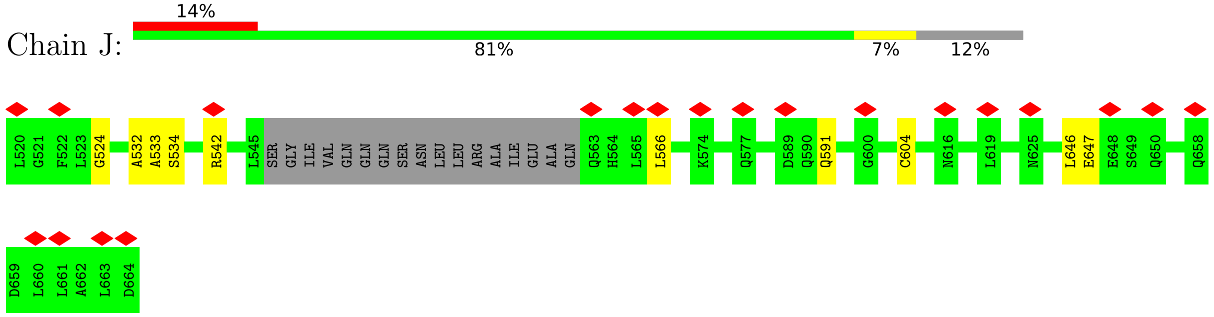
- Molecule 2: Envelope glycoprotein gp41



- Molecule 2: Envelope glycoprotein gp41

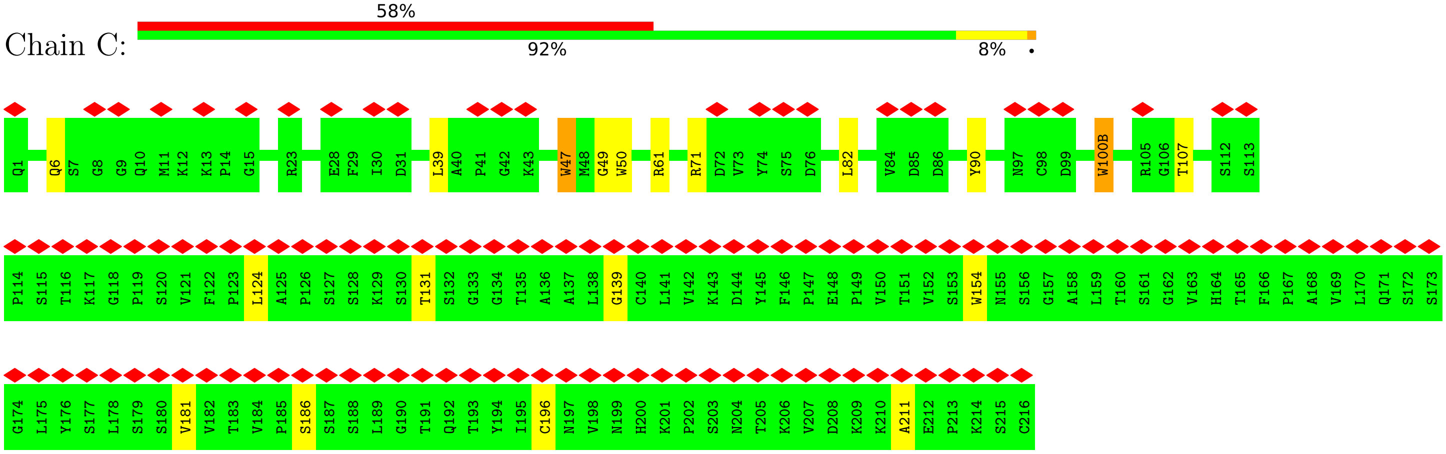


- Molecule 2: Envelope glycoprotein gp41



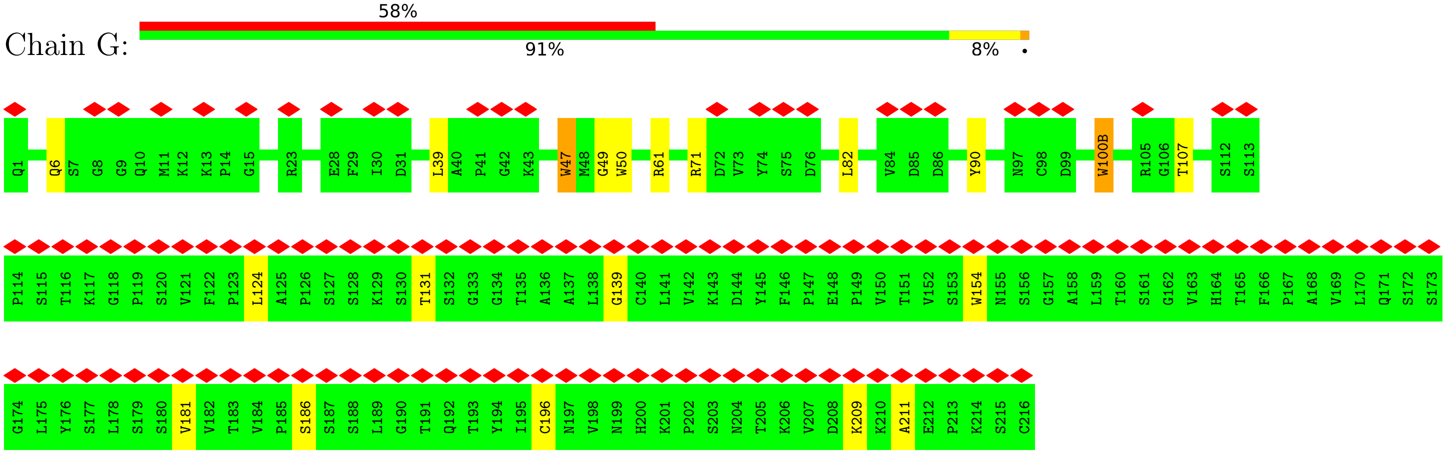
- Molecule 3: VRC01 Fab Heavy Chain

Chain C:



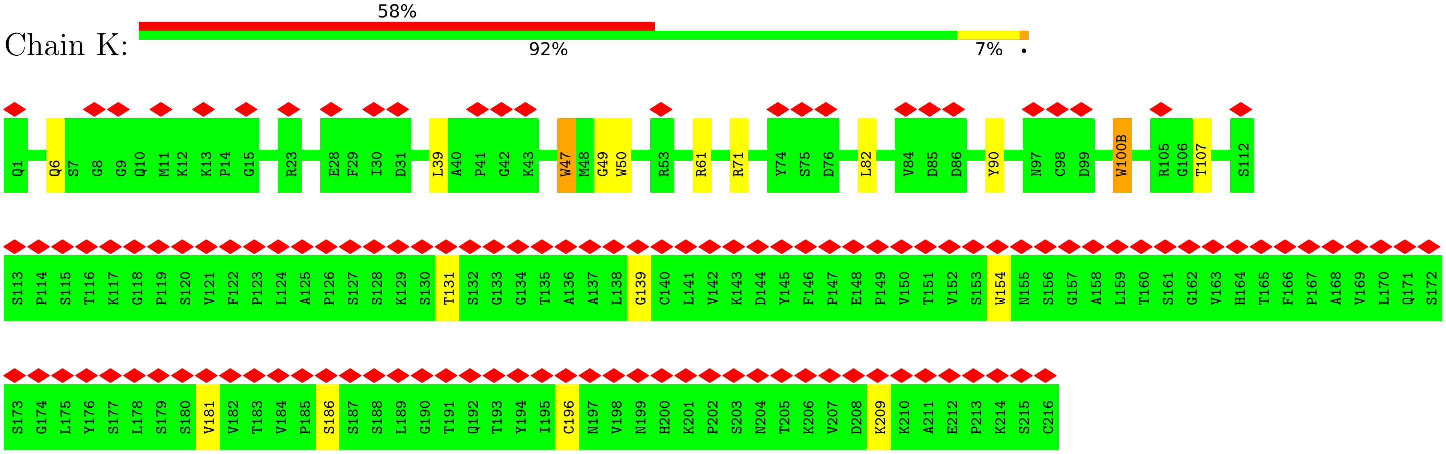
- Molecule 3: VRC01 Fab Heavy Chain

Chain G:



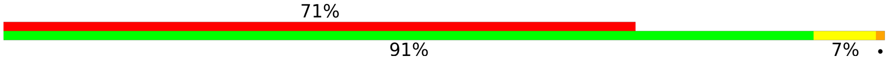
- Molecule 3: VRC01 Fab Heavy Chain

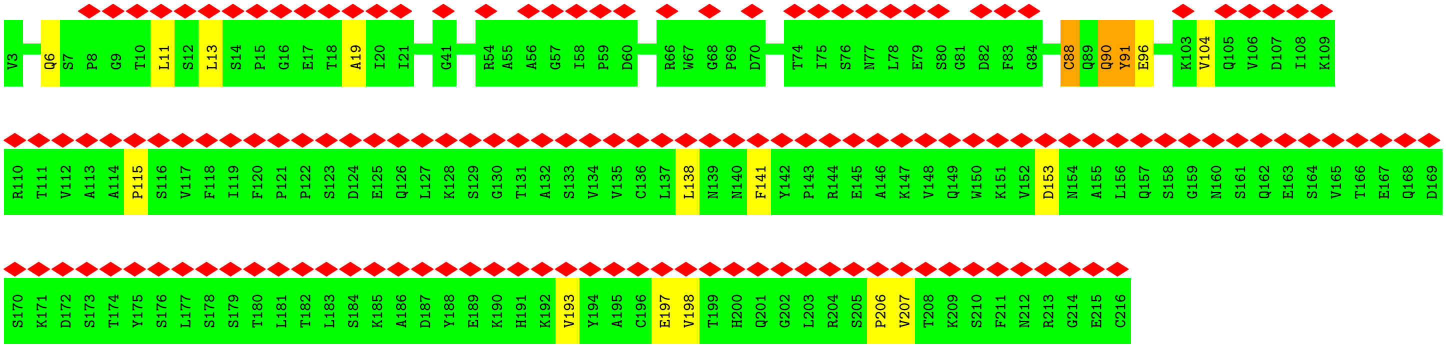
Chain K:



- Molecule 4: VRC01 Fab Light Chain

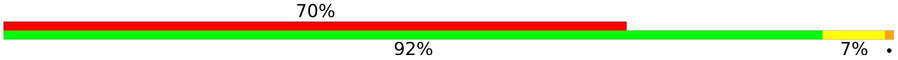
Chain D:

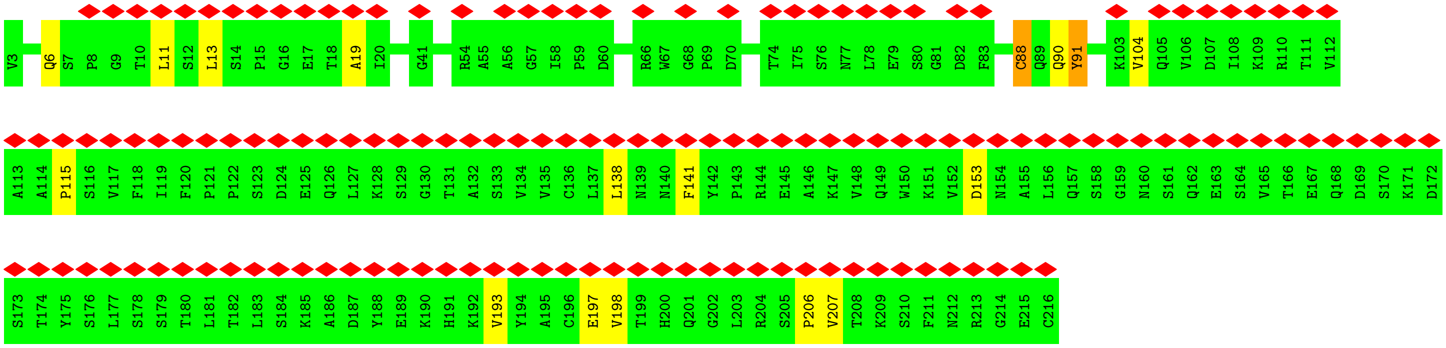




- Molecule 4: VRC01 Fab Light Chain

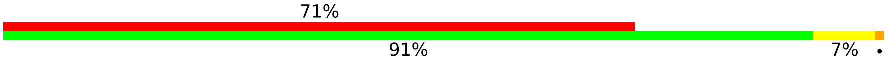
Chain H:

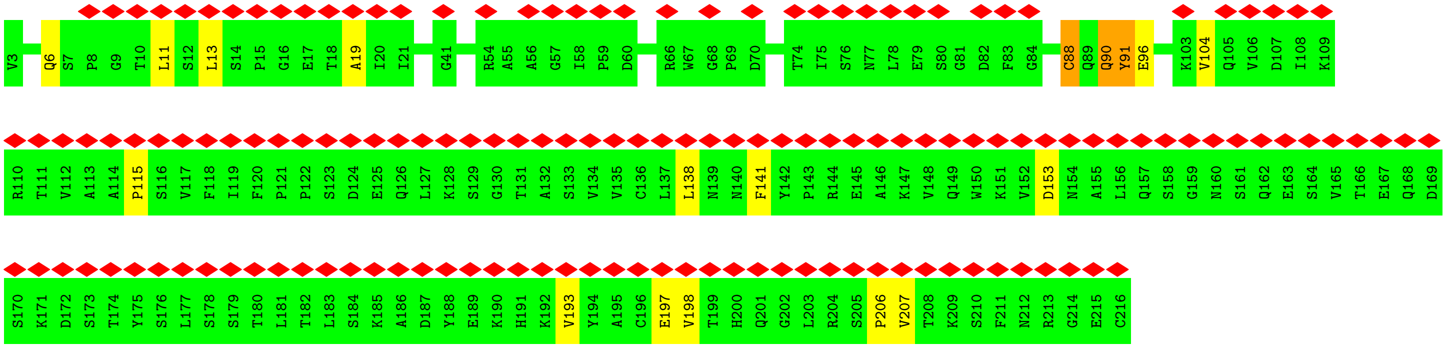




- Molecule 4: VRC01 Fab Light Chain

Chain L:





- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

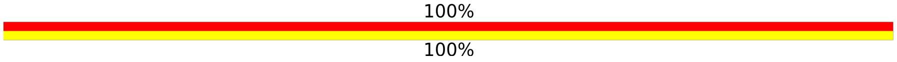
Chain Y:

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

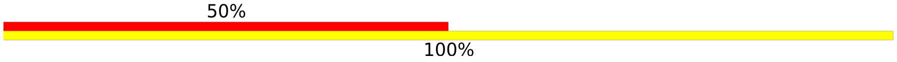
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain R:

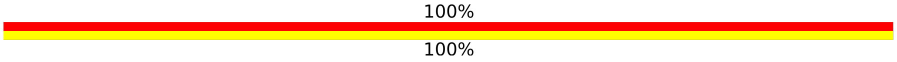


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

Chain U:

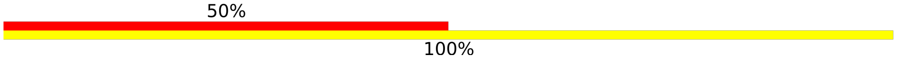


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

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

Chain W:



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

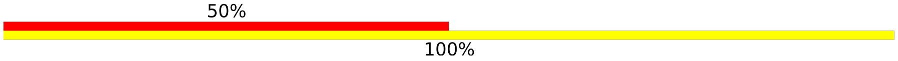
Chain X:

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

Chain Z:

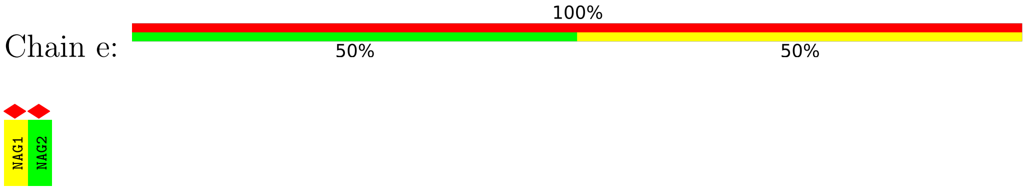
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



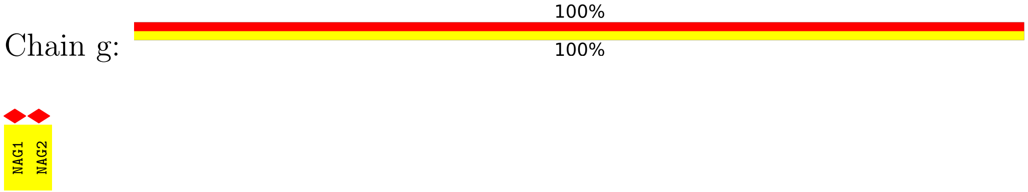
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



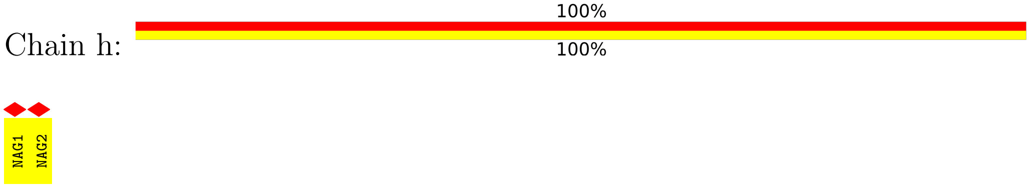
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



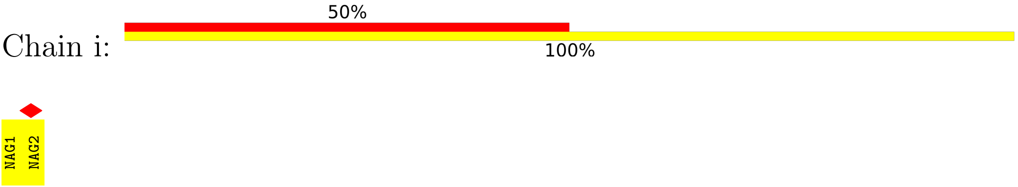
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



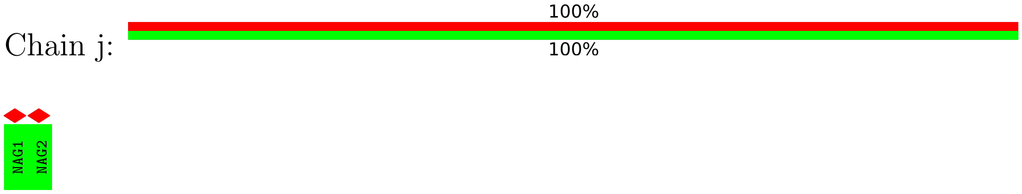
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



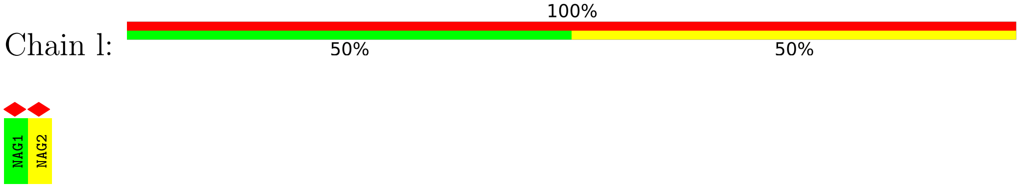
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



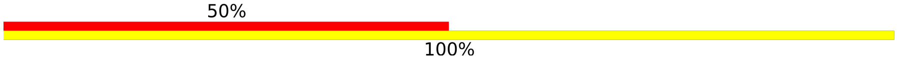
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



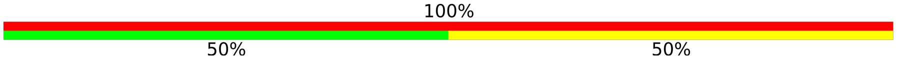
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



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

Chain q:

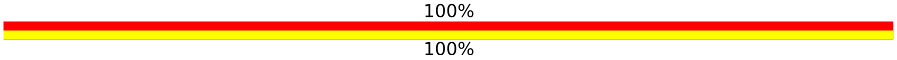


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

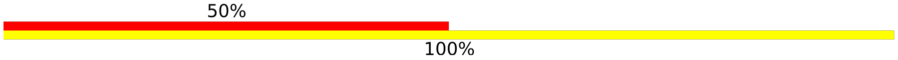
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



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

Chain u:

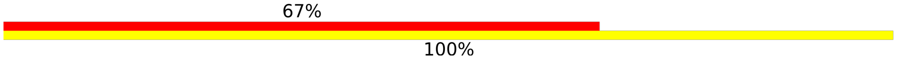


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:

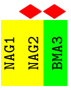
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



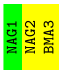
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



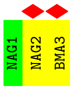
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



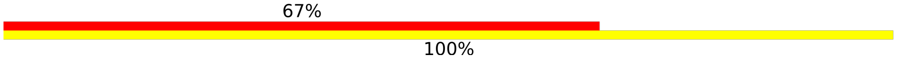
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



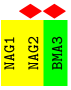
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



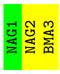
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

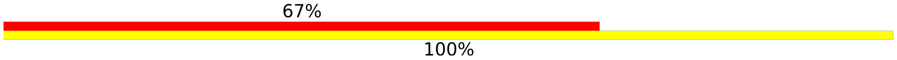


- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

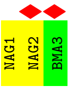
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:



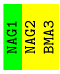
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:


NAG1
NAG2
BMA3

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	77632	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	54.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	10.300	Depositor
Minimum map value	-4.695	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	415.9181, 415.9181, 415.9181	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08312, 1.08312, 1.08312	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
1	E	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
1	I	0.90	1/3524 (0.0%)	0.81	4/4784 (0.1%)
2	B	0.80	1/1043 (0.1%)	0.81	0/1414
2	F	0.80	1/1043 (0.1%)	0.81	0/1414
2	J	0.81	1/1043 (0.1%)	0.81	0/1414
3	C	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
3	G	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
3	K	0.87	5/1755 (0.3%)	0.75	4/2387 (0.2%)
4	D	0.61	0/1652	0.70	1/2242 (0.0%)
4	H	0.61	0/1652	0.70	1/2242 (0.0%)
4	L	0.61	0/1652	0.70	1/2242 (0.0%)
All	All	0.83	21/23922 (0.1%)	0.78	27/32481 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
4	H	0	1
4	L	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	50	TRP	CB-CG	-11.02	1.30	1.50
3	K	50	TRP	CB-CG	-11.02	1.30	1.50
3	C	50	TRP	CB-CG	-11.01	1.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	299	PRO	N-CD	7.37	1.58	1.47
1	A	299	PRO	N-CD	7.30	1.58	1.47
1	E	299	PRO	N-CD	7.29	1.58	1.47
3	G	100(B)	TRP	CB-CG	-6.52	1.38	1.50
3	C	100(B)	TRP	CB-CG	-6.52	1.38	1.50
3	K	100(B)	TRP	CB-CG	-6.52	1.38	1.50
3	K	100(B)	TRP	CE3-CZ3	-6.19	1.27	1.38
3	G	100(B)	TRP	CE3-CZ3	-6.17	1.27	1.38
3	C	100(B)	TRP	CE3-CZ3	-6.16	1.27	1.38
3	K	90	TYR	CD1-CE1	-5.57	1.30	1.39
3	G	90	TYR	CD1-CE1	-5.55	1.31	1.39
3	C	90	TYR	CD1-CE1	-5.55	1.31	1.39
3	K	47	TRP	CB-CG	-5.32	1.40	1.50
3	C	47	TRP	CB-CG	-5.29	1.40	1.50
3	G	47	TRP	CB-CG	-5.28	1.40	1.50
2	J	604	CYS	CB-SG	-5.04	1.73	1.81
2	F	604	CYS	CB-SG	-5.04	1.73	1.81
2	B	604	CYS	CB-SG	-5.04	1.73	1.81

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	88	CYS	CA-CB-SG	6.31	125.35	114.00
4	L	88	CYS	CA-CB-SG	6.31	125.35	114.00
4	H	88	CYS	CA-CB-SG	6.30	125.35	114.00
1	A	129	LEU	CA-CB-CG	6.19	129.54	115.30
1	E	129	LEU	CA-CB-CG	6.19	129.53	115.30
1	I	129	LEU	CA-CB-CG	6.18	129.50	115.30
3	C	50	TRP	CB-CA-C	-6.13	98.15	110.40
3	K	50	TRP	CB-CA-C	-6.12	98.16	110.40
3	G	50	TRP	CB-CA-C	-6.12	98.17	110.40
1	I	299	PRO	N-CD-CG	-5.95	94.27	103.20
1	A	299	PRO	N-CD-CG	-5.95	94.28	103.20
1	E	299	PRO	N-CD-CG	-5.94	94.29	103.20
1	A	452	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	E	452	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	I	452	LEU	CB-CG-CD2	-5.72	101.28	111.00
3	K	50	TRP	CA-CB-CG	5.69	124.51	113.70
3	G	50	TRP	CA-CB-CG	5.69	124.50	113.70
3	C	50	TRP	CA-CB-CG	5.68	124.49	113.70
3	C	82	LEU	CB-CG-CD2	-5.45	101.74	111.00
3	G	82	LEU	CB-CG-CD2	-5.45	101.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	82	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	I	93	PHE	CB-CG-CD1	5.22	124.45	120.80
1	A	93	PHE	CB-CG-CD1	5.16	124.41	120.80
1	E	93	PHE	CB-CG-CD1	5.12	124.39	120.80
3	C	39	LEU	CB-CG-CD2	-5.03	102.45	111.00
3	G	39	LEU	CB-CG-CD2	-5.01	102.47	111.00
3	K	39	LEU	CB-CG-CD2	-5.00	102.50	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	90	GLN	Peptide
4	H	90	GLN	Peptide
4	L	90	GLN	Peptide

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	A	3453	0	3397	48	0
1	E	3453	0	3397	46	0
1	I	3453	0	3397	48	0
2	B	1025	0	1012	4	0
2	F	1025	0	1012	4	0
2	J	1025	0	1012	4	0
3	C	1710	0	1680	8	0
3	G	1710	0	1680	9	0
3	K	1710	0	1680	8	0
4	D	1615	0	1554	12	0
4	H	1615	0	1554	11	0
4	L	1615	0	1554	12	0
5	M	50	0	43	0	0
5	Y	50	0	43	0	0
5	k	50	0	43	0	0
6	N	28	0	25	1	0
6	R	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	28	0	25	0	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
6	W	28	0	25	0	0
6	X	28	0	25	0	0
6	Z	28	0	25	1	0
6	d	28	0	25	0	0
6	e	28	0	25	0	0
6	g	28	0	25	0	0
6	h	28	0	25	0	0
6	i	28	0	25	0	0
6	j	28	0	25	0	0
6	l	28	0	25	0	0
6	p	28	0	25	0	0
6	q	28	0	25	0	0
6	s	28	0	25	0	0
6	t	28	0	25	0	0
6	u	28	0	25	0	0
6	v	28	0	25	0	0
7	O	39	0	34	0	0
7	P	39	0	34	0	0
7	Q	39	0	34	0	0
7	T	39	0	34	0	0
7	a	39	0	34	0	0
7	b	39	0	34	0	0
7	c	39	0	34	0	0
7	f	39	0	34	0	0
7	m	39	0	34	0	0
7	n	39	0	34	0	0
7	o	39	0	34	0	0
7	r	39	0	34	0	0
8	A	56	0	52	0	0
8	B	14	0	13	0	0
8	E	56	0	52	0	0
8	F	14	0	13	0	0
8	I	56	0	52	0	0
8	J	14	0	13	0	0
All	All	24825	0	24186	199	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 4.

All (199) 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:I:120:VAL:CG1	1:I:121:LYS:H	1.56	1.17
1:E:120:VAL:HG12	1:E:121:LYS:N	1.54	1.17
1:A:120:VAL:HG12	1:A:121:LYS:N	1.54	1.15
1:I:120:VAL:HG12	1:I:121:LYS:N	1.54	1.15
1:A:120:VAL:CG1	1:A:121:LYS:H	1.56	1.09
1:E:120:VAL:CG1	1:E:121:LYS:H	1.56	1.08
1:E:124:PRO:HG2	1:E:309:ILE:HD11	1.33	1.08
1:A:124:PRO:HG2	1:A:309:ILE:HD11	1.33	1.07
1:I:124:PRO:HG2	1:I:309:ILE:HD11	1.33	1.04
1:I:124:PRO:CG	1:I:309:ILE:HD11	1.93	0.98
1:E:124:PRO:CG	1:E:309:ILE:HD11	1.93	0.98
1:A:124:PRO:CG	1:A:309:ILE:HD11	1.93	0.97
1:A:120:VAL:HG12	1:A:121:LYS:H	0.72	0.86
1:E:120:VAL:HG12	1:E:121:LYS:H	0.72	0.86
1:I:120:VAL:HG12	1:I:121:LYS:H	0.72	0.85
1:I:120:VAL:CG1	1:I:121:LYS:N	2.28	0.80
1:A:124:PRO:HG2	1:A:309:ILE:CD1	2.13	0.79
1:E:124:PRO:HG2	1:E:309:ILE:CD1	2.13	0.79
1:E:122:LEU:HD13	1:E:125:LEU:HD22	1.65	0.79
1:A:120:VAL:CG1	1:A:121:LYS:N	2.28	0.78
1:I:122:LEU:HD13	1:I:125:LEU:HD22	1.65	0.78
1:I:124:PRO:HG2	1:I:309:ILE:CD1	2.13	0.77
1:A:122:LEU:HD13	1:A:125:LEU:HD22	1.65	0.76
1:I:121:LYS:O	1:I:122:LEU:HD23	1.86	0.76
1:E:120:VAL:CG1	1:E:121:LYS:N	2.28	0.76
1:A:121:LYS:O	1:A:122:LEU:HD23	1.86	0.75
1:E:121:LYS:O	1:E:122:LEU:HD23	1.86	0.75
1:E:303:THR:OG1	1:E:322:ASP:N	2.26	0.69
1:I:303:THR:OG1	1:I:322:ASP:N	2.26	0.69
1:A:303:THR:OG1	1:A:322:ASP:N	2.26	0.68
1:I:123:THR:N	1:I:124:PRO:HD2	2.10	0.67
1:A:123:THR:N	1:A:124:PRO:HD2	2.10	0.67
1:E:123:THR:N	1:E:124:PRO:HD2	2.10	0.65
1:E:123:THR:N	1:E:124:PRO:CD	2.60	0.65
4:H:153:ASP:OD1	4:H:193:VAL:HB	1.97	0.65
4:L:153:ASP:OD1	4:L:193:VAL:HB	1.97	0.64
1:A:123:THR:N	1:A:124:PRO:CD	2.60	0.64
1:I:123:THR:N	1:I:124:PRO:CD	2.60	0.64
1:A:121:LYS:O	1:A:122:LEU:CD2	2.46	0.64
1:I:121:LYS:O	1:I:122:LEU:CD2	2.46	0.64
4:D:153:ASP:OD1	4:D:193:VAL:HB	1.97	0.63
1:E:121:LYS:O	1:E:122:LEU:CD2	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:PRO:CG	1:E:309:ILE:CD1	2.76	0.61
1:I:234:ASN:O	1:I:236:THR:N	2.34	0.61
1:E:234:ASN:O	1:E:236:THR:N	2.34	0.61
1:A:234:ASN:O	1:A:236:THR:N	2.34	0.60
1:A:120:VAL:HG12	1:A:121:LYS:O	2.01	0.60
2:B:532:ALA:O	2:B:534:SER:N	2.30	0.60
1:E:120:VAL:HG12	1:E:121:LYS:O	2.01	0.59
2:J:532:ALA:O	2:J:534:SER:N	2.30	0.59
1:I:120:VAL:HG12	1:I:121:LYS:O	2.01	0.59
1:E:303:THR:HG1	1:E:322:ASP:N	2.00	0.58
2:F:542:ARG:HA	2:J:591:GLN:HE22	1.67	0.58
2:B:591:GLN:HE22	2:J:542:ARG:HA	1.67	0.58
2:B:542:ARG:HA	2:F:591:GLN:HE22	1.67	0.58
1:I:303:THR:HG1	1:I:322:ASP:N	2.01	0.58
3:K:6:GLN:OE1	3:K:107:THR:OG1	2.18	0.57
3:G:6:GLN:OE1	3:G:107:THR:OG1	2.18	0.57
1:E:164:GLU:OE1	1:I:192:ARG:NH1	2.38	0.56
1:A:124:PRO:CG	1:A:309:ILE:CD1	2.76	0.56
2:F:532:ALA:O	2:F:534:SER:N	2.30	0.56
1:A:164:GLU:OE1	1:E:192:ARG:NH1	2.39	0.56
1:A:192:ARG:NH1	1:I:164:GLU:OE1	2.38	0.56
1:I:117:LYS:HB2	1:I:118:PRO:HD3	1.88	0.56
1:I:124:PRO:CG	1:I:309:ILE:CD1	2.76	0.56
1:A:122:LEU:C	1:A:124:PRO:HD2	2.27	0.55
1:E:300:ASN:OD1	1:E:442:VAL:HA	2.06	0.55
1:E:122:LEU:C	1:E:124:PRO:HD2	2.27	0.55
1:I:300:ASN:OD1	1:I:442:VAL:HA	2.06	0.55
1:A:117:LYS:HB2	1:A:118:PRO:HD3	1.88	0.55
1:I:122:LEU:C	1:I:124:PRO:HD2	2.27	0.55
1:A:300:ASN:OD1	1:A:442:VAL:HA	2.06	0.54
1:A:383:PHE:HB3	1:A:418:CYS:SG	2.48	0.54
1:E:117:LYS:HB2	1:E:118:PRO:HD3	1.88	0.54
1:I:383:PHE:HB3	1:I:418:CYS:SG	2.48	0.53
1:E:383:PHE:HB3	1:E:418:CYS:SG	2.48	0.53
3:C:6:GLN:OE1	3:C:107:THR:OG1	2.18	0.53
4:D:6:GLN:HE21	4:D:88:CYS:HB3	1.74	0.53
4:H:6:GLN:HE21	4:H:88:CYS:HB3	1.74	0.53
4:L:6:GLN:HE21	4:L:88:CYS:HB3	1.74	0.53
3:K:100(B):TRP:CD1	4:L:91:TYR:O	2.63	0.52
1:A:303:THR:HG1	1:A:322:ASP:N	2.07	0.52
3:C:100(B):TRP:CD1	4:D:91:TYR:O	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:100(B):TRP:CD1	4:H:91:TYR:O	2.63	0.52
1:A:49:GLU:HG3	1:A:99:ASN:HD22	1.75	0.51
4:H:13:LEU:CD1	4:H:19:ALA:HB2	2.40	0.51
1:I:49:GLU:HG3	1:I:99:ASN:HD22	1.75	0.51
1:A:122:LEU:HD13	1:A:125:LEU:CD2	2.39	0.51
4:D:13:LEU:CD1	4:D:19:ALA:HB2	2.40	0.51
4:L:13:LEU:CD1	4:L:19:ALA:HB2	2.40	0.50
1:E:49:GLU:HG3	1:E:99:ASN:HD22	1.75	0.50
3:K:154:TRP:CH2	3:K:196:CYS:HB2	2.47	0.49
1:A:121:LYS:C	1:A:122:LEU:HG	2.33	0.48
3:G:154:TRP:CH2	3:G:196:CYS:HB2	2.47	0.48
3:C:154:TRP:CH2	3:C:196:CYS:HB2	2.47	0.48
1:I:121:LYS:C	1:I:122:LEU:HG	2.33	0.48
1:E:122:LEU:HD13	1:E:125:LEU:CD2	2.39	0.48
1:I:122:LEU:HD13	1:I:125:LEU:CD2	2.39	0.48
1:A:120:VAL:HG22	1:A:315:GLN:OE1	2.14	0.48
1:I:280:ASN:OD1	1:I:456:ARG:NH2	2.47	0.47
1:E:121:LYS:C	1:E:122:LEU:HG	2.33	0.47
1:E:120:VAL:HG22	1:E:315:GLN:OE1	2.14	0.47
4:H:11:LEU:HB2	4:H:104:VAL:HA	1.97	0.47
1:A:280:ASN:OD1	1:A:456:ARG:NH2	2.47	0.47
1:E:67:ASN:OD1	1:E:68:ILE:N	2.48	0.47
1:E:280:ASN:OD1	1:E:456:ARG:NH2	2.47	0.47
1:I:67:ASN:OD1	1:I:68:ILE:N	2.48	0.47
1:E:122:LEU:HB3	1:E:125:LEU:HB2	1.97	0.47
4:L:6:GLN:HE21	4:L:88:CYS:CB	2.27	0.47
4:D:6:GLN:HE21	4:D:88:CYS:CB	2.27	0.47
1:I:120:VAL:HG22	1:I:315:GLN:OE1	2.14	0.47
4:L:11:LEU:HB2	4:L:104:VAL:HA	1.96	0.47
1:I:117:LYS:N	1:I:118:PRO:CD	2.78	0.46
1:E:117:LYS:N	1:E:118:PRO:CD	2.78	0.46
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.51	0.46
3:K:196:CYS:N	3:K:209:LYS:O	2.46	0.46
1:A:122:LEU:HB3	1:A:125:LEU:HB2	1.97	0.46
1:A:67:ASN:OD1	1:A:68:ILE:N	2.48	0.46
4:D:11:LEU:HB2	4:D:104:VAL:HA	1.97	0.46
3:G:196:CYS:N	3:G:209:LYS:O	2.46	0.46
4:H:6:GLN:HE21	4:H:88:CYS:CB	2.27	0.46
1:A:117:LYS:N	1:A:118:PRO:CD	2.78	0.46
1:I:122:LEU:HB3	1:I:125:LEU:HB2	1.97	0.46
3:G:47:TRP:CZ2	3:G:49:GLY:HA2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LYS:HG3	2:F:566:LEU:HD21	1.98	0.46
4:H:141:PHE:CE2	4:H:198:VAL:HG11	2.51	0.46
1:I:117:LYS:HG3	2:J:566:LEU:HD21	1.98	0.46
3:K:47:TRP:CZ2	3:K:49:GLY:HA2	2.51	0.46
4:L:141:PHE:CE2	4:L:198:VAL:HG11	2.51	0.46
1:A:117:LYS:HG3	2:B:566:LEU:HD21	1.98	0.45
4:D:141:PHE:CE2	4:D:198:VAL:HG11	2.51	0.45
1:E:385:CYS:HA	1:E:418:CYS:HA	1.99	0.44
4:L:197:GLU:HA	4:L:207:VAL:O	2.17	0.44
4:D:197:GLU:HA	4:D:207:VAL:O	2.17	0.44
1:I:119:CYS:HB3	1:I:203:GLN:O	2.18	0.44
1:A:121:LYS:O	1:A:122:LEU:HG	2.17	0.44
1:A:121:LYS:O	1:A:122:LEU:CG	2.66	0.44
1:A:128:THR:O	1:A:191:TYR:O	2.35	0.44
1:E:121:LYS:O	1:E:122:LEU:CG	2.66	0.44
1:E:128:THR:O	1:E:191:TYR:O	2.35	0.44
1:I:128:THR:O	1:I:191:TYR:O	2.35	0.44
1:A:119:CYS:HB3	1:A:203:GLN:O	2.18	0.44
1:A:385:CYS:HA	1:A:418:CYS:HA	1.99	0.44
4:D:197:GLU:HB3	4:D:206:PRO:HB2	2.00	0.44
1:E:119:CYS:HB3	1:E:203:GLN:O	2.18	0.44
1:I:385:CYS:HA	1:I:418:CYS:HA	1.99	0.44
1:E:121:LYS:O	1:E:122:LEU:HG	2.17	0.44
4:H:197:GLU:HA	4:H:207:VAL:O	2.17	0.44
4:L:197:GLU:HB3	4:L:206:PRO:HB2	2.00	0.43
1:I:121:LYS:O	1:I:122:LEU:CG	2.66	0.43
1:E:298:ARG:CZ	1:E:300:ASN:HB3	2.48	0.43
1:I:303:THR:HG23	1:I:322:ASP:O	2.19	0.43
1:E:303:THR:HG23	1:E:322:ASP:O	2.19	0.43
3:G:131:THR:O	3:G:186:SER:HB3	2.19	0.43
1:A:303:THR:HG23	1:A:322:ASP:O	2.19	0.43
3:C:139:GLY:HA3	3:C:181:VAL:HA	2.01	0.43
3:C:131:THR:O	3:C:186:SER:HB3	2.19	0.43
1:A:53:PHE:O	1:A:217:TYR:CD1	2.72	0.43
1:I:121:LYS:O	1:I:122:LEU:HG	2.17	0.43
3:K:131:THR:O	3:K:186:SER:HB3	2.19	0.43
4:L:115:PRO:HB2	4:L:207:VAL:HG11	2.01	0.43
1:A:298:ARG:CZ	1:A:300:ASN:HB3	2.48	0.43
3:G:139:GLY:HA3	3:G:181:VAL:HA	2.01	0.42
1:A:148:ALA:HB3	1:A:325:ASP:OD1	2.19	0.42
1:A:392:ASN:HD22	6:N:1:NAG:C7	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:115:PRO:HB2	4:D:207:VAL:HG11	2.01	0.42
1:E:148:ALA:HB3	1:E:325:ASP:OD1	2.19	0.42
1:I:298:ARG:CZ	1:I:300:ASN:HB3	2.48	0.42
1:I:53:PHE:O	1:I:217:TYR:CD1	2.72	0.42
1:I:148:ALA:HB3	1:I:325:ASP:OD1	2.19	0.42
3:K:139:GLY:HA3	3:K:181:VAL:HA	2.00	0.42
1:E:53:PHE:O	1:E:217:TYR:CD1	2.72	0.42
4:H:197:GLU:HB3	4:H:206:PRO:HB2	2.00	0.42
1:I:125:LEU:HD12	1:I:125:LEU:HA	1.81	0.42
4:H:115:PRO:HB2	4:H:207:VAL:HG11	2.01	0.41
1:E:443:ILE:N	1:E:443:ILE:CD1	2.83	0.41
1:I:227:LYS:HA	1:I:485:LYS:O	2.21	0.41
1:A:227:LYS:HA	1:A:485:LYS:O	2.20	0.41
1:E:227:LYS:HA	1:E:485:LYS:O	2.20	0.41
1:E:460:SER:O	3:G:61:ARG:NH2	2.54	0.41
1:A:460:SER:O	3:C:61:ARG:NH2	2.54	0.41
4:D:90:GLN:O	4:D:96:GLU:N	2.54	0.41
1:E:392:ASN:HD22	6:Z:1:NAG:C7	2.32	0.41
4:L:138:LEU:HB3	4:L:141:PHE:CZ	2.56	0.41
1:I:107:ASP:O	1:I:111:LEU:HG	2.21	0.41
3:G:124:LEU:O	3:G:211:ALA:HB1	2.21	0.41
1:I:181:VAL:CG1	1:I:191:TYR:CD2	3.04	0.41
1:I:443:ILE:CD1	1:I:443:ILE:N	2.83	0.41
3:C:124:LEU:O	3:C:211:ALA:HB1	2.21	0.41
1:A:107:ASP:O	1:A:111:LEU:HG	2.21	0.41
4:H:138:LEU:HB3	4:H:141:PHE:CZ	2.56	0.40
1:I:337:THR:O	1:I:341:THR:OG1	2.30	0.40
1:A:181:VAL:CG1	1:A:191:TYR:CD2	3.04	0.40
1:A:337:THR:O	1:A:341:THR:OG1	2.30	0.40
1:A:443:ILE:N	1:A:443:ILE:CD1	2.83	0.40
1:E:107:ASP:O	1:E:111:LEU:HG	2.21	0.40
4:D:138:LEU:HB3	4:D:141:PHE:CZ	2.56	0.40
4:L:90:GLN:O	4:L:96:GLU:N	2.54	0.40
1:I:460:SER:O	3:K:61:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	17	55
1	E	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	17	55
1	I	429/471 (91%)	387 (90%)	38 (9%)	4 (1%)	17	55
2	B	124/145 (86%)	114 (92%)	6 (5%)	4 (3%)	4	22
2	F	124/145 (86%)	113 (91%)	7 (6%)	4 (3%)	4	22
2	J	124/145 (86%)	114 (92%)	6 (5%)	4 (3%)	4	22
3	C	222/224 (99%)	195 (88%)	27 (12%)	0	100	100
3	G	222/224 (99%)	195 (88%)	27 (12%)	0	100	100
3	K	222/224 (99%)	195 (88%)	27 (12%)	0	100	100
4	D	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	29	68
4	H	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	29	68
4	L	206/208 (99%)	193 (94%)	12 (6%)	1 (0%)	29	68
All	All	2943/3144 (94%)	2666 (91%)	250 (8%)	27 (1%)	21	55

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	533	ALA
2	B	646	LEU
2	F	533	ALA
2	F	646	LEU
2	J	533	ALA
2	J	646	LEU
1	A	235	GLY
2	B	647	GLU
4	D	91	TYR
1	E	235	GLY
2	F	647	GLU
4	H	91	TYR

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Mol	Chain	Res	Type
1	I	235	GLY
2	J	647	GLU
4	L	91	TYR
1	A	121	LYS
1	E	121	LYS
1	I	121	LYS
1	A	120	VAL
2	B	524	GLY
1	E	120	VAL
2	F	524	GLY
1	I	120	VAL
2	J	524	GLY
1	A	300	ASN
1	E	300	ASN
1	I	300	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/420 (94%)	391 (100%)	2 (0%)	88	96
1	E	393/420 (94%)	391 (100%)	2 (0%)	88	96
1	I	393/420 (94%)	391 (100%)	2 (0%)	88	96
2	B	111/125 (89%)	111 (100%)	0	100	100
2	F	111/125 (89%)	111 (100%)	0	100	100
2	J	111/125 (89%)	111 (100%)	0	100	100
3	C	192/192 (100%)	191 (100%)	1 (0%)	88	96
3	G	192/192 (100%)	191 (100%)	1 (0%)	88	96
3	K	192/192 (100%)	191 (100%)	1 (0%)	88	96
4	D	180/180 (100%)	180 (100%)	0	100	100
4	H	180/180 (100%)	180 (100%)	0	100	100
4	L	180/180 (100%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2628/2751 (96%)	2619 (100%)	9 (0%)	92	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	A	166	ARG
3	C	71	ARG
1	E	127	VAL
1	E	166	ARG
3	G	71	ARG
1	I	127	VAL
1	I	166	ARG
3	K	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	130	GLN
1	A	234	ASN
2	B	591	GLN
4	D	6	GLN
1	E	99	ASN
1	E	130	GLN
1	E	234	ASN
2	F	591	GLN
4	H	6	GLN
1	I	99	ASN
1	I	130	GLN
1	I	234	ASN
2	J	591	GLN
4	L	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

90 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	$\#\|Z\| > 2$
5	NAG	M	1	5,1	14,14,15	0.69	0	17,19,21	0.50	0
5	NAG	M	2	5	14,14,15	0.75	1 (7%)	17,19,21	1.12	1 (5%)
5	BMA	M	3	5	11,11,12	1.07	0	15,15,17	1.19	2 (13%)
5	MAN	M	4	5	11,11,12	0.90	0	15,15,17	1.14	2 (13%)
6	NAG	N	1	6,1	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	N	2	6	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
7	NAG	O	1	7,1	14,14,15	0.78	0	17,19,21	0.82	1 (5%)
7	NAG	O	2	7	14,14,15	0.44	0	17,19,21	2.42	3 (17%)
7	BMA	O	3	7	11,11,12	0.67	0	15,15,17	1.10	1 (6%)
7	NAG	P	1	7,1	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
7	NAG	P	2	7	14,14,15	0.68	0	17,19,21	2.26	3 (17%)
7	BMA	P	3	7	11,11,12	0.74	0	15,15,17	0.88	0
7	NAG	Q	1	7,1	14,14,15	0.30	0	17,19,21	0.65	0
7	NAG	Q	2	7	14,14,15	0.68	1 (7%)	17,19,21	0.74	0
7	BMA	Q	3	7	11,11,12	0.92	0	15,15,17	1.29	3 (20%)
6	NAG	R	1	6,1	14,14,15	0.61	1 (7%)	17,19,21	0.65	0
6	NAG	R	2	6	14,14,15	0.31	0	17,19,21	0.96	1 (5%)
6	NAG	S	1	6,1	14,14,15	0.47	0	17,19,21	1.22	2 (11%)
6	NAG	S	2	6	14,14,15	0.23	0	17,19,21	0.53	0
7	NAG	T	1	7,1	14,14,15	0.53	0	17,19,21	0.60	0
7	NAG	T	2	7	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
7	BMA	T	3	7	11,11,12	0.50	0	15,15,17	1.36	1 (6%)
6	NAG	U	1	6,1	14,14,15	0.28	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	NAG	U	2	6	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
6	NAG	V	1	6,1	14,14,15	0.71	1 (7%)	17,19,21	0.98	1 (5%)
6	NAG	V	2	6	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
6	NAG	W	1	6,1	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
6	NAG	W	2	6	14,14,15	0.75	1 (7%)	17,19,21	0.55	0
6	NAG	X	1	6,1	14,14,15	0.29	0	17,19,21	0.65	0
6	NAG	X	2	6	14,14,15	0.29	0	17,19,21	0.72	0
5	NAG	Y	1	5,1	14,14,15	0.69	0	17,19,21	0.50	0
5	NAG	Y	2	5	14,14,15	0.76	1 (7%)	17,19,21	1.12	1 (5%)
5	BMA	Y	3	5	11,11,12	1.06	0	15,15,17	1.19	2 (13%)
5	MAN	Y	4	5	11,11,12	0.92	0	15,15,17	1.14	2 (13%)
6	NAG	Z	1	6,1	14,14,15	0.26	0	17,19,21	0.53	0
6	NAG	Z	2	6	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
7	NAG	a	1	7,1	14,14,15	0.79	0	17,19,21	0.82	1 (5%)
7	NAG	a	2	7	14,14,15	0.44	0	17,19,21	2.42	3 (17%)
7	BMA	a	3	7	11,11,12	0.67	0	15,15,17	1.10	1 (6%)
7	NAG	b	1	7,1	14,14,15	0.63	0	17,19,21	1.06	1 (5%)
7	NAG	b	2	7	14,14,15	0.69	0	17,19,21	2.26	3 (17%)
7	BMA	b	3	7	11,11,12	0.74	0	15,15,17	0.88	0
7	NAG	c	1	7,1	14,14,15	0.31	0	17,19,21	0.65	0
7	NAG	c	2	7	14,14,15	0.68	1 (7%)	17,19,21	0.73	0
7	BMA	c	3	7	11,11,12	0.93	0	15,15,17	1.29	3 (20%)
6	NAG	d	1	6,1	14,14,15	0.61	1 (7%)	17,19,21	0.65	0
6	NAG	d	2	6	14,14,15	0.30	0	17,19,21	0.96	1 (5%)
6	NAG	e	1	6,1	14,14,15	0.47	0	17,19,21	1.22	2 (11%)
6	NAG	e	2	6	14,14,15	0.23	0	17,19,21	0.53	0
7	NAG	f	1	7,1	14,14,15	0.54	0	17,19,21	0.60	0
7	NAG	f	2	7	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
7	BMA	f	3	7	11,11,12	0.49	0	15,15,17	1.35	1 (6%)
6	NAG	g	1	6,1	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
6	NAG	g	2	6	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
6	NAG	h	1	6,1	14,14,15	0.71	1 (7%)	17,19,21	0.98	1 (5%)
6	NAG	h	2	6	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
6	NAG	i	1	6,1	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
6	NAG	i	2	6	14,14,15	0.75	1 (7%)	17,19,21	0.55	0
6	NAG	j	1	6,1	14,14,15	0.29	0	17,19,21	0.65	0
6	NAG	j	2	6	14,14,15	0.29	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	k	1	5,1	14,14,15	0.69	0	17,19,21	0.50	0
5	NAG	k	2	5	14,14,15	0.76	1 (7%)	17,19,21	1.13	1 (5%)
5	BMA	k	3	5	11,11,12	1.08	0	15,15,17	1.18	2 (13%)
5	MAN	k	4	5	11,11,12	0.90	0	15,15,17	1.14	2 (13%)
6	NAG	l	1	6,1	14,14,15	0.26	0	17,19,21	0.53	0
6	NAG	l	2	6	14,14,15	0.46	0	17,19,21	0.83	1 (5%)
7	NAG	m	1	7,1	14,14,15	0.79	0	17,19,21	0.82	1 (5%)
7	NAG	m	2	7	14,14,15	0.44	0	17,19,21	2.42	3 (17%)
7	BMA	m	3	7	11,11,12	0.67	0	15,15,17	1.10	1 (6%)
7	NAG	n	1	7,1	14,14,15	0.64	0	17,19,21	1.05	1 (5%)
7	NAG	n	2	7	14,14,15	0.67	0	17,19,21	2.26	3 (17%)
7	BMA	n	3	7	11,11,12	0.73	0	15,15,17	0.88	0
7	NAG	o	1	7,1	14,14,15	0.30	0	17,19,21	0.65	0
7	NAG	o	2	7	14,14,15	0.67	1 (7%)	17,19,21	0.73	0
7	BMA	o	3	7	11,11,12	0.92	0	15,15,17	1.30	3 (20%)
6	NAG	p	1	6,1	14,14,15	0.62	1 (7%)	17,19,21	0.65	0
6	NAG	p	2	6	14,14,15	0.31	0	17,19,21	0.96	1 (5%)
6	NAG	q	1	6,1	14,14,15	0.47	0	17,19,21	1.22	2 (11%)
6	NAG	q	2	6	14,14,15	0.23	0	17,19,21	0.53	0
7	NAG	r	1	7,1	14,14,15	0.52	0	17,19,21	0.60	0
7	NAG	r	2	7	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
7	BMA	r	3	7	11,11,12	0.51	0	15,15,17	1.36	1 (6%)
6	NAG	s	1	6,1	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
6	NAG	s	2	6	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
6	NAG	t	1	6,1	14,14,15	0.70	1 (7%)	17,19,21	0.98	1 (5%)
6	NAG	t	2	6	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
6	NAG	u	1	6,1	14,14,15	0.58	0	17,19,21	1.19	1 (5%)
6	NAG	u	2	6	14,14,15	0.74	1 (7%)	17,19,21	0.55	0
6	NAG	v	1	6,1	14,14,15	0.29	0	17,19,21	0.65	0
6	NAG	v	2	6	14,14,15	0.29	0	17,19,21	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	1	5,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
7	NAG	O	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	5/6/23/26	0/1/1/1
7	BMA	O	3	7	-	1/2/19/22	0/1/1/1
7	NAG	P	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	P	2	7	-	4/6/23/26	0/1/1/1
7	BMA	P	3	7	-	2/2/19/22	0/1/1/1
7	NAG	Q	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	0/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	1/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	3/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
7	NAG	T	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	3/6/23/26	0/1/1/1
7	BMA	T	3	7	-	2/2/19/22	0/1/1/1
6	NAG	U	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	U	2	6	-	1/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	V	2	6	-	3/6/23/26	0/1/1/1
6	NAG	W	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	0/6/23/26	0/1/1/1
6	NAG	X	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	X	2	6	-	0/6/23/26	0/1/1/1
5	NAG	Y	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	0/2/19/22	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
7	NAG	a	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	a	3	7	-	1/2/19/22	0/1/1/1
7	NAG	b	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	b	2	7	-	4/6/23/26	0/1/1/1
7	BMA	b	3	7	-	2/2/19/22	0/1/1/1
7	NAG	c	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	BMA	c	3	7	-	1/2/19/22	0/1/1/1
6	NAG	d	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	-	3/6/23/26	0/1/1/1
6	NAG	e	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
7	NAG	f	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	f	2	7	-	3/6/23/26	0/1/1/1
7	BMA	f	3	7	-	2/2/19/22	0/1/1/1
6	NAG	g	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	g	2	6	-	1/6/23/26	0/1/1/1
6	NAG	h	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	h	2	6	-	3/6/23/26	0/1/1/1
6	NAG	i	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	i	2	6	-	0/6/23/26	0/1/1/1
6	NAG	j	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	j	2	6	-	0/6/23/26	0/1/1/1
5	NAG	k	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	k	2	5	-	2/6/23/26	0/1/1/1
5	BMA	k	3	5	-	2/2/19/22	0/1/1/1
5	MAN	k	4	5	-	0/2/19/22	0/1/1/1
6	NAG	l	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	l	2	6	-	2/6/23/26	0/1/1/1
7	NAG	m	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	m	2	7	-	5/6/23/26	0/1/1/1
7	BMA	m	3	7	-	1/2/19/22	0/1/1/1
7	NAG	n	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	n	2	7	-	4/6/23/26	0/1/1/1
7	BMA	n	3	7	-	2/2/19/22	0/1/1/1
7	NAG	o	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	o	2	7	-	0/6/23/26	0/1/1/1
7	BMA	o	3	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	p	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	p	2	6	-	3/6/23/26	0/1/1/1
6	NAG	q	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	q	2	6	-	2/6/23/26	0/1/1/1
7	NAG	r	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	r	2	7	-	3/6/23/26	0/1/1/1
7	BMA	r	3	7	-	2/2/19/22	0/1/1/1
6	NAG	s	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	s	2	6	-	1/6/23/26	0/1/1/1
6	NAG	t	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	t	2	6	-	3/6/23/26	0/1/1/1
6	NAG	u	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	u	2	6	-	0/6/23/26	0/1/1/1
6	NAG	v	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	v	2	6	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	k	2	NAG	O5-C1	-2.75	1.39	1.43
5	Y	2	NAG	O5-C1	-2.73	1.39	1.43
5	M	2	NAG	O5-C1	-2.73	1.39	1.43
6	V	1	NAG	O5-C1	-2.46	1.39	1.43
6	h	1	NAG	O5-C1	-2.45	1.39	1.43
6	t	1	NAG	O5-C1	-2.43	1.39	1.43
6	i	2	NAG	O5-C1	2.35	1.47	1.43
6	W	2	NAG	O5-C1	2.35	1.47	1.43
7	Q	2	NAG	O5-C1	-2.33	1.40	1.43
6	u	2	NAG	O5-C1	2.32	1.47	1.43
7	c	2	NAG	O5-C1	-2.31	1.40	1.43
7	o	2	NAG	O5-C1	-2.29	1.40	1.43
6	p	1	NAG	O5-C1	-2.15	1.40	1.43
6	R	1	NAG	O5-C1	-2.12	1.40	1.43
6	d	1	NAG	O5-C1	-2.11	1.40	1.43

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	b	2	NAG	C2-N2-C7	7.93	134.20	122.90
7	n	2	NAG	C2-N2-C7	7.92	134.19	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	2	NAG	C2-N2-C7	7.91	134.17	122.90
7	a	2	NAG	C2-N2-C7	7.77	133.97	122.90
7	O	2	NAG	C2-N2-C7	7.77	133.96	122.90
7	m	2	NAG	C2-N2-C7	7.76	133.96	122.90
7	m	2	NAG	C1-C2-N2	4.77	118.63	110.49
7	a	2	NAG	C1-C2-N2	4.76	118.62	110.49
7	O	2	NAG	C1-C2-N2	4.76	118.62	110.49
7	r	3	BMA	C1-O5-C5	4.42	118.18	112.19
7	T	3	BMA	C1-O5-C5	4.40	118.16	112.19
7	f	3	BMA	C1-O5-C5	4.39	118.14	112.19
7	n	2	NAG	C1-C2-N2	3.69	116.79	110.49
7	P	2	NAG	C1-C2-N2	3.68	116.78	110.49
7	b	2	NAG	C1-C2-N2	3.67	116.76	110.49
7	b	1	NAG	C1-O5-C5	3.54	116.98	112.19
7	P	1	NAG	C1-O5-C5	3.54	116.98	112.19
7	n	1	NAG	C1-O5-C5	3.50	116.94	112.19
6	S	1	NAG	C2-N2-C7	3.36	127.69	122.90
6	e	1	NAG	C2-N2-C7	3.36	127.68	122.90
6	q	1	NAG	C2-N2-C7	3.35	127.67	122.90
6	d	2	NAG	C2-N2-C7	3.12	127.34	122.90
6	p	2	NAG	C2-N2-C7	3.11	127.34	122.90
6	R	2	NAG	C2-N2-C7	3.10	127.31	122.90
7	f	2	NAG	C2-N2-C7	3.07	127.28	122.90
7	T	2	NAG	C2-N2-C7	3.07	127.28	122.90
7	r	2	NAG	C2-N2-C7	3.06	127.27	122.90
6	h	2	NAG	C2-N2-C7	3.00	127.17	122.90
6	V	2	NAG	C2-N2-C7	2.99	127.16	122.90
6	t	1	NAG	C2-N2-C7	2.97	127.14	122.90
6	h	1	NAG	C2-N2-C7	2.97	127.13	122.90
6	t	2	NAG	C2-N2-C7	2.97	127.13	122.90
6	V	1	NAG	C2-N2-C7	2.97	127.13	122.90
6	W	1	NAG	O4-C4-C5	-2.96	101.94	109.30
6	l	2	NAG	C1-O5-C5	2.96	116.21	112.19
6	i	1	NAG	O4-C4-C5	-2.96	101.95	109.30
6	u	1	NAG	O4-C4-C5	-2.96	101.95	109.30
5	M	4	MAN	C1-O5-C5	2.96	116.20	112.19
5	Y	4	MAN	C1-O5-C5	2.96	116.20	112.19
5	k	4	MAN	C1-O5-C5	2.95	116.19	112.19
6	g	2	NAG	C2-N2-C7	2.95	127.10	122.90
6	U	2	NAG	C2-N2-C7	2.94	127.09	122.90
6	N	2	NAG	C1-O5-C5	2.94	116.17	112.19
6	s	2	NAG	C2-N2-C7	2.93	127.08	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	2	NAG	C1-O5-C5	2.93	116.17	112.19
5	k	2	NAG	C2-N2-C7	2.92	127.06	122.90
5	M	2	NAG	C2-N2-C7	2.91	127.05	122.90
5	Y	2	NAG	C2-N2-C7	2.90	127.03	122.90
7	O	3	BMA	C1-O5-C5	2.87	116.08	112.19
7	a	3	BMA	C1-O5-C5	2.86	116.06	112.19
7	m	3	BMA	C1-O5-C5	2.86	116.06	112.19
6	e	1	NAG	C1-O5-C5	2.75	115.92	112.19
6	q	1	NAG	C1-O5-C5	2.74	115.91	112.19
6	S	1	NAG	C1-O5-C5	2.74	115.91	112.19
7	c	3	BMA	O5-C1-C2	-2.58	106.79	110.77
7	Q	3	BMA	O5-C1-C2	-2.58	106.80	110.77
7	o	3	BMA	O5-C1-C2	-2.56	106.82	110.77
5	k	3	BMA	C3-C4-C5	-2.43	105.90	110.24
5	M	3	BMA	C3-C4-C5	-2.43	105.90	110.24
5	Y	3	BMA	C3-C4-C5	-2.43	105.90	110.24
6	g	1	NAG	C1-O5-C5	2.33	115.35	112.19
6	U	1	NAG	C1-O5-C5	2.32	115.33	112.19
6	s	1	NAG	C1-O5-C5	2.29	115.29	112.19
5	Y	3	BMA	O5-C5-C4	-2.27	105.31	110.83
7	m	1	NAG	C3-C4-C5	-2.26	106.21	110.24
5	M	3	BMA	O5-C5-C4	-2.25	105.34	110.83
7	a	1	NAG	C3-C4-C5	-2.25	106.22	110.24
7	O	1	NAG	C3-C4-C5	-2.25	106.22	110.24
5	k	3	BMA	O5-C5-C4	-2.24	105.37	110.83
5	M	4	MAN	O2-C2-C3	-2.22	105.70	110.14
5	k	4	MAN	O2-C2-C3	-2.21	105.70	110.14
6	s	2	NAG	C1-O5-C5	2.20	115.18	112.19
5	Y	4	MAN	O2-C2-C3	-2.20	105.73	110.14
6	U	2	NAG	C1-O5-C5	2.18	115.15	112.19
7	P	2	NAG	C8-C7-N2	2.18	119.79	116.10
6	g	2	NAG	C1-O5-C5	2.17	115.14	112.19
7	n	2	NAG	C8-C7-N2	2.17	119.77	116.10
7	b	2	NAG	C8-C7-N2	2.16	119.76	116.10
7	o	3	BMA	C1-C2-C3	-2.14	107.03	109.67
7	c	3	BMA	C1-C2-C3	-2.14	107.03	109.67
7	Q	3	BMA	C1-C2-C3	-2.13	107.05	109.67
7	o	3	BMA	O2-C2-C3	-2.06	106.01	110.14
7	Q	3	BMA	O2-C2-C3	-2.05	106.04	110.14
7	O	2	NAG	C8-C7-N2	2.04	119.56	116.10
7	m	2	NAG	C8-C7-N2	2.04	119.56	116.10
7	c	3	BMA	O2-C2-C3	-2.04	106.05	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	a	2	NAG	C8-C7-N2	2.04	119.55	116.10

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
6	j	1	NAG	C8-C7-N2-C2
6	j	1	NAG	O7-C7-N2-C2
6	v	1	NAG	C8-C7-N2-C2
6	v	1	NAG	O7-C7-N2-C2
6	W	1	NAG	C4-C5-C6-O6
6	i	1	NAG	C4-C5-C6-O6
6	u	1	NAG	C4-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
6	i	1	NAG	O5-C5-C6-O6
6	u	1	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	l	2	NAG	O5-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
7	b	3	BMA	O5-C5-C6-O6
7	n	3	BMA	O5-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
7	r	1	NAG	O5-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
6	e	2	NAG	C4-C5-C6-O6
6	q	2	NAG	C4-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	d	2	NAG	O5-C5-C6-O6
6	p	2	NAG	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
6	q	2	NAG	O5-C5-C6-O6
7	Q	1	NAG	C4-C5-C6-O6
7	c	1	NAG	C4-C5-C6-O6
7	o	1	NAG	C4-C5-C6-O6
7	T	2	NAG	O5-C5-C6-O6
7	f	2	NAG	O5-C5-C6-O6
7	r	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	h	1	NAG	O5-C5-C6-O6
6	t	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
7	T	1	NAG	C4-C5-C6-O6
7	f	1	NAG	C4-C5-C6-O6
7	r	1	NAG	C4-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	d	2	NAG	C4-C5-C6-O6
6	l	2	NAG	C4-C5-C6-O6
6	p	2	NAG	C4-C5-C6-O6
7	P	3	BMA	C4-C5-C6-O6
7	b	3	BMA	C4-C5-C6-O6
7	n	3	BMA	C4-C5-C6-O6
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
6	d	1	NAG	C8-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
6	p	1	NAG	C8-C7-N2-C2
6	p	1	NAG	O7-C7-N2-C2
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
7	a	2	NAG	C8-C7-N2-C2
7	a	2	NAG	O7-C7-N2-C2
7	b	2	NAG	C8-C7-N2-C2
7	b	2	NAG	O7-C7-N2-C2
7	m	2	NAG	C8-C7-N2-C2
7	m	2	NAG	O7-C7-N2-C2
7	n	2	NAG	C8-C7-N2-C2
7	n	2	NAG	O7-C7-N2-C2
6	V	2	NAG	O5-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
6	t	2	NAG	O5-C5-C6-O6
7	T	2	NAG	C4-C5-C6-O6
7	f	2	NAG	C4-C5-C6-O6
7	r	2	NAG	C4-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
7	m	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	O	2	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
7	m	2	NAG	C4-C5-C6-O6
7	T	3	BMA	O5-C5-C6-O6
7	f	3	BMA	O5-C5-C6-O6
7	r	3	BMA	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	h	2	NAG	C4-C5-C6-O6
6	t	2	NAG	C4-C5-C6-O6
5	M	3	BMA	C4-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
5	k	3	BMA	C4-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	k	3	BMA	O5-C5-C6-O6
7	r	3	BMA	C4-C5-C6-O6
7	T	3	BMA	C4-C5-C6-O6
7	f	3	BMA	C4-C5-C6-O6
7	c	1	NAG	O5-C5-C6-O6
7	Q	1	NAG	O5-C5-C6-O6
7	o	1	NAG	O5-C5-C6-O6
7	O	3	BMA	O5-C5-C6-O6
7	a	3	BMA	O5-C5-C6-O6
7	m	3	BMA	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
7	c	3	BMA	O5-C5-C6-O6
7	o	3	BMA	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	n	2	NAG	O5-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
6	s	1	NAG	O5-C5-C6-O6
6	t	1	NAG	C4-C5-C6-O6
6	h	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	k	2	NAG	O5-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
7	n	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	M	2	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7
5	k	2	NAG	C3-C2-N2-C7
6	S	1	NAG	C3-C2-N2-C7
6	V	1	NAG	C3-C2-N2-C7
6	e	1	NAG	C3-C2-N2-C7
6	h	1	NAG	C3-C2-N2-C7
6	q	1	NAG	C3-C2-N2-C7
6	t	1	NAG	C3-C2-N2-C7
6	R	2	NAG	C3-C2-N2-C7
6	U	2	NAG	C3-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
6	d	2	NAG	C3-C2-N2-C7
6	g	2	NAG	C3-C2-N2-C7
6	h	2	NAG	C3-C2-N2-C7
6	p	2	NAG	C3-C2-N2-C7
6	s	2	NAG	C3-C2-N2-C7
6	t	2	NAG	C3-C2-N2-C7
7	O	2	NAG	C3-C2-N2-C7
7	P	2	NAG	C3-C2-N2-C7
7	T	2	NAG	C3-C2-N2-C7
7	a	2	NAG	C3-C2-N2-C7
7	b	2	NAG	C3-C2-N2-C7
7	f	2	NAG	C3-C2-N2-C7
7	m	2	NAG	C3-C2-N2-C7
7	n	2	NAG	C3-C2-N2-C7
7	r	2	NAG	C3-C2-N2-C7

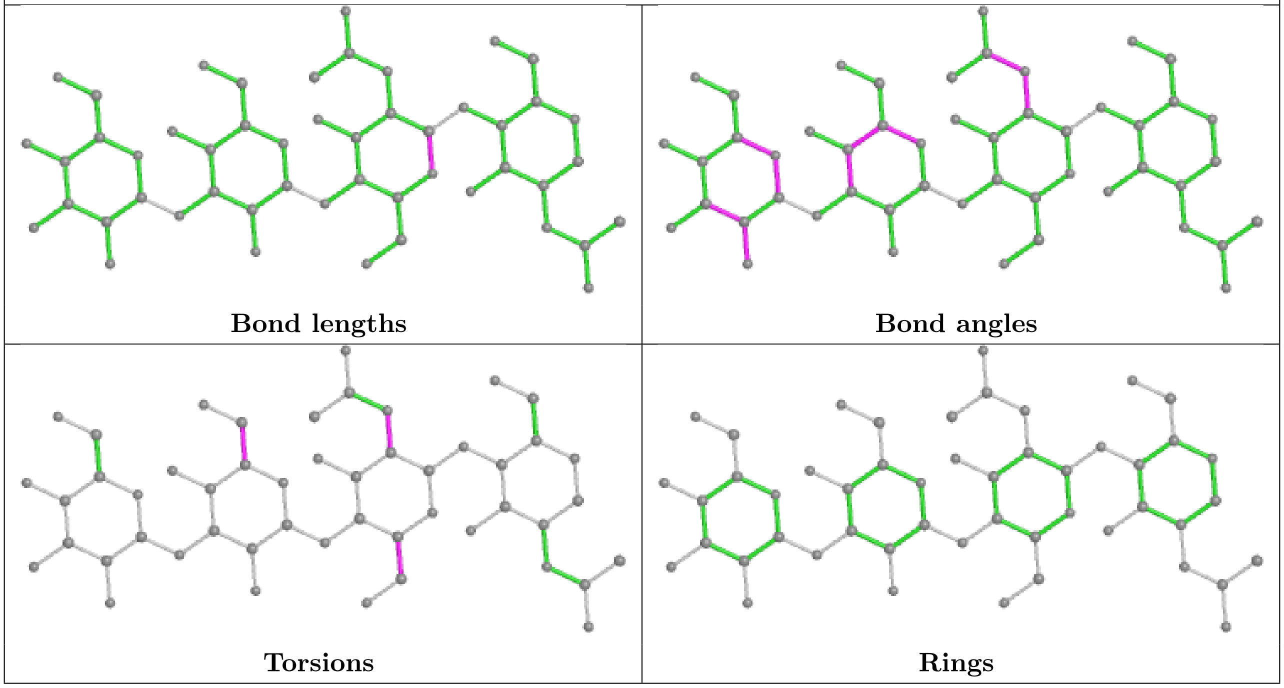
There are no ring outliers.

2 monomers are involved in 2 short contacts:

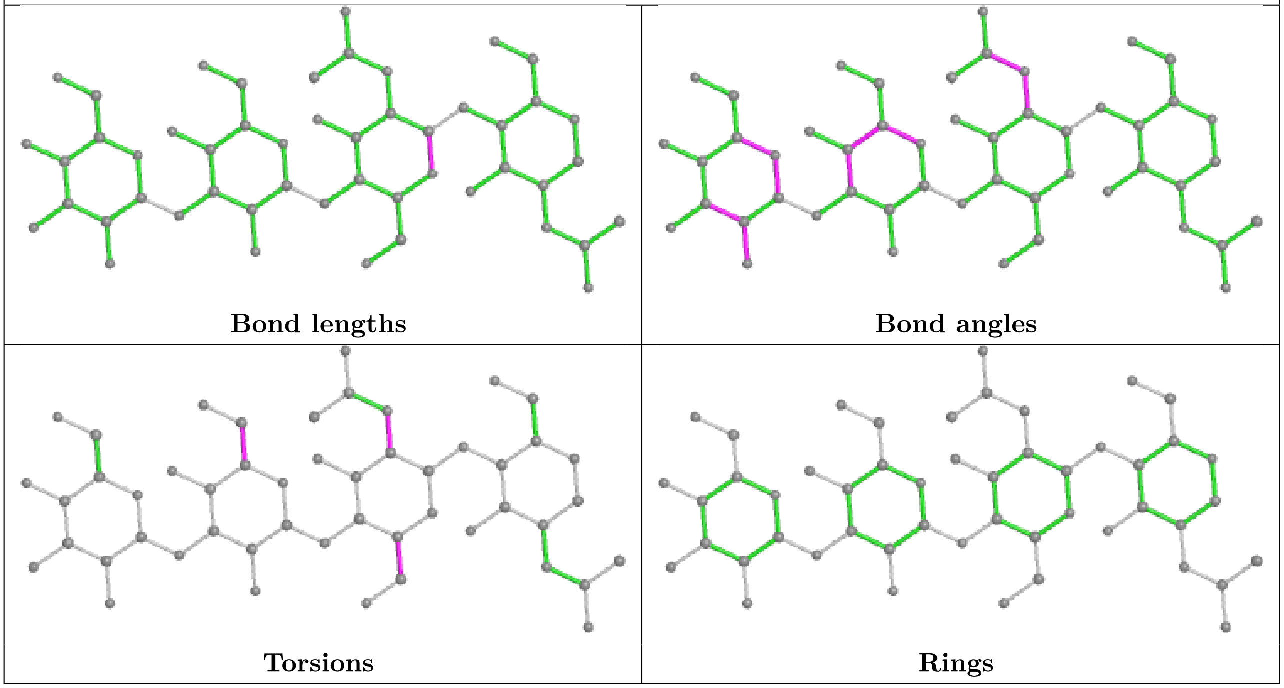
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	1	NAG	1	0
6	N	1	NAG	1	0

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

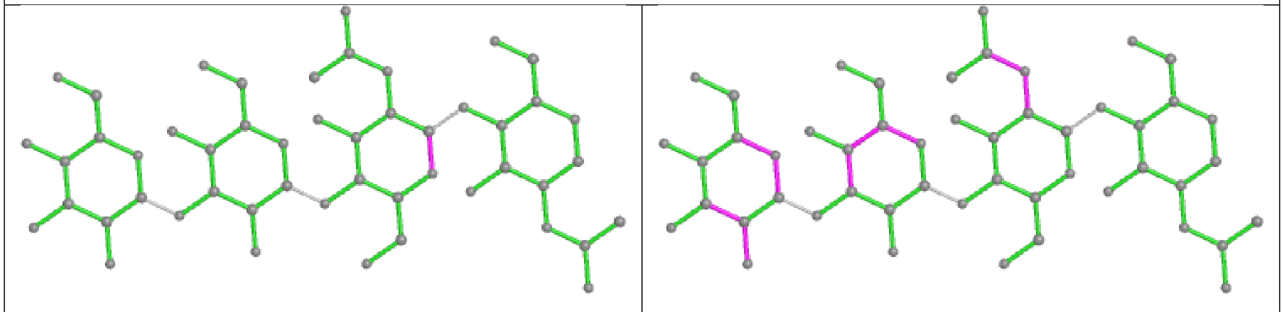
Oligosaccharide Chain M



Oligosaccharide Chain Y

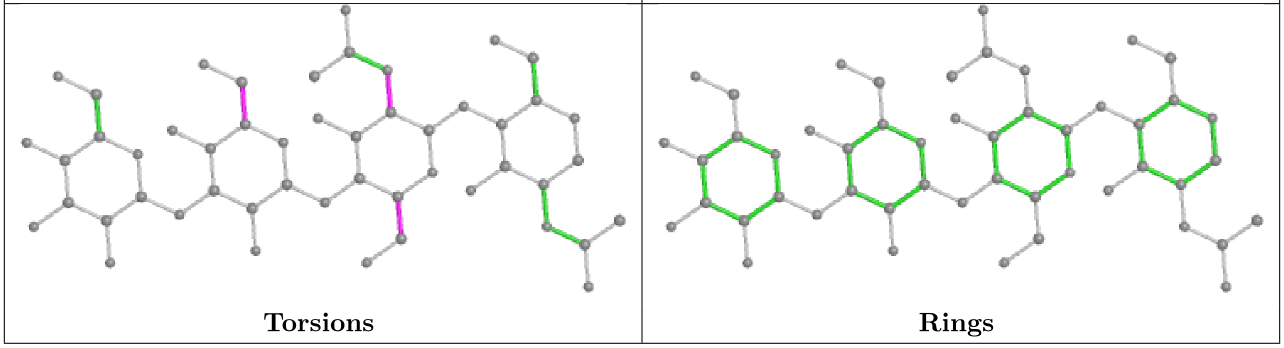


Oligosaccharide Chain k



Bond lengths

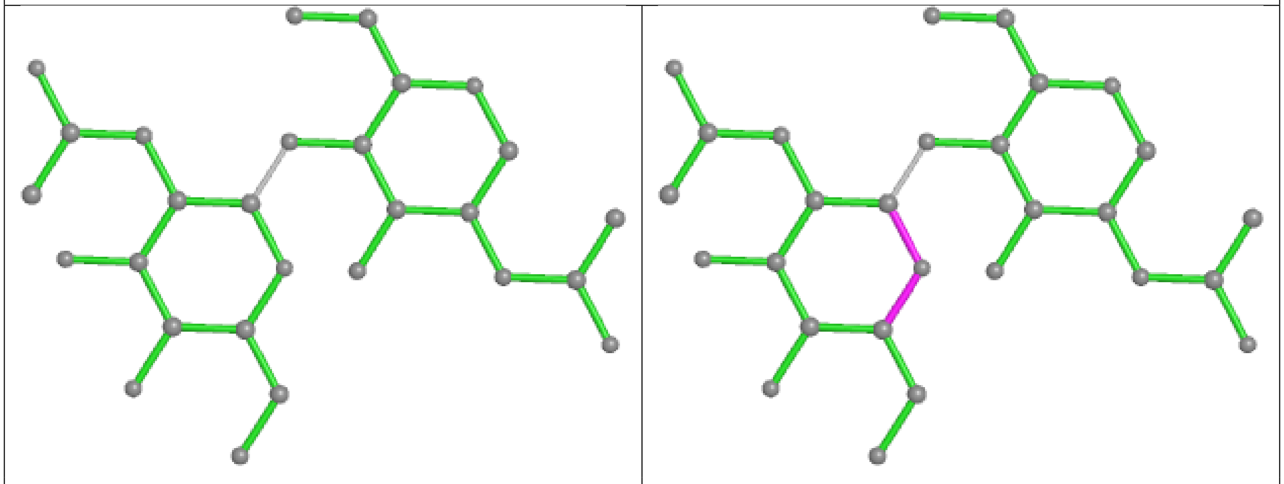
Bond angles



Torsions

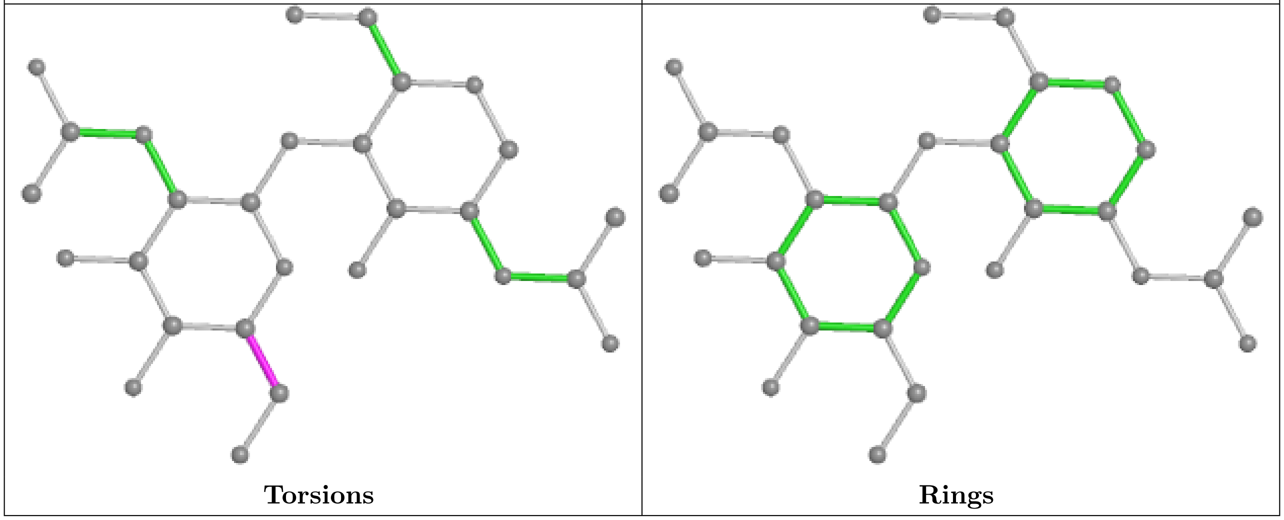
Rings

Oligosaccharide Chain N



Bond lengths

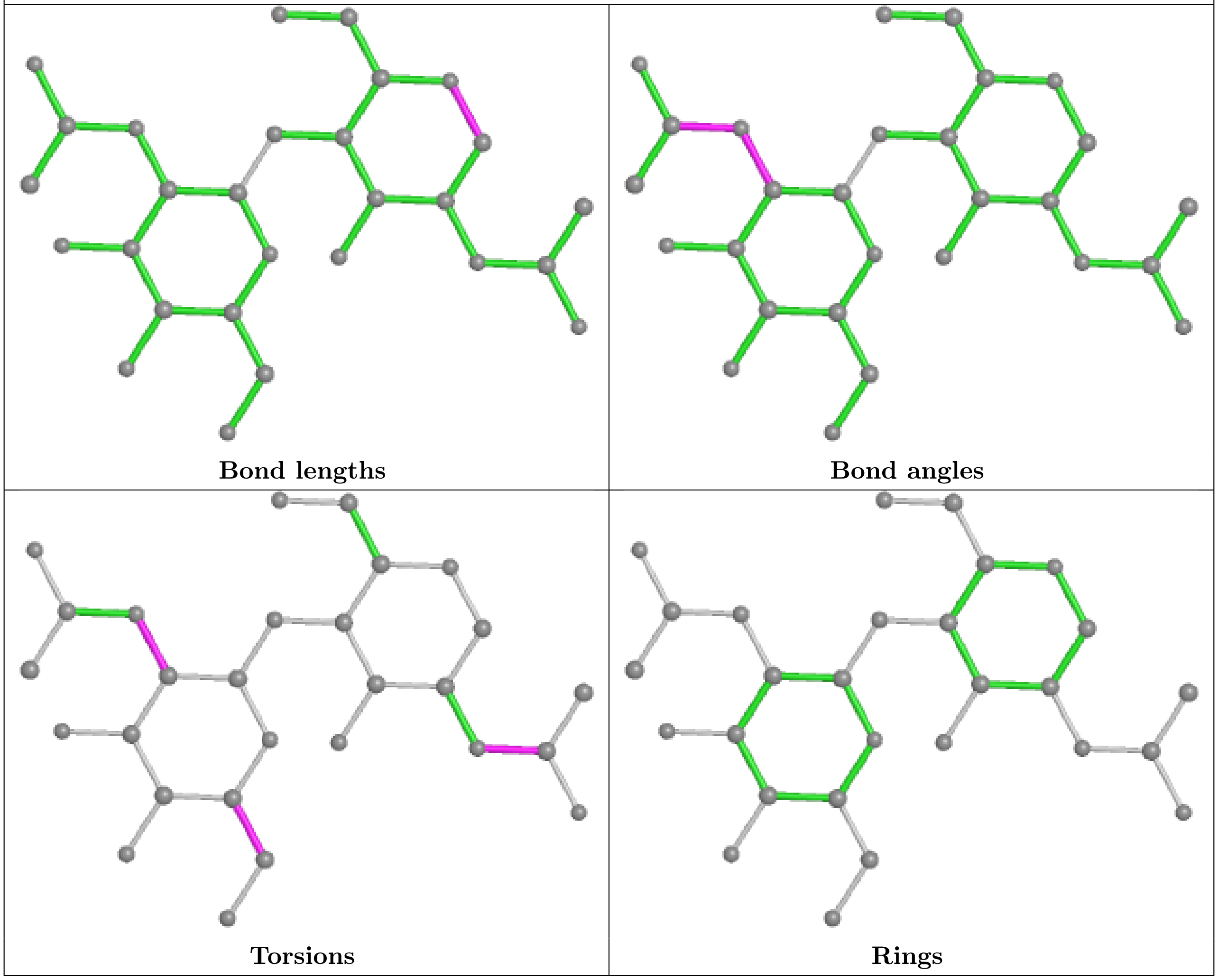
Bond angles



Torsions

Rings

Oligosaccharide Chain R



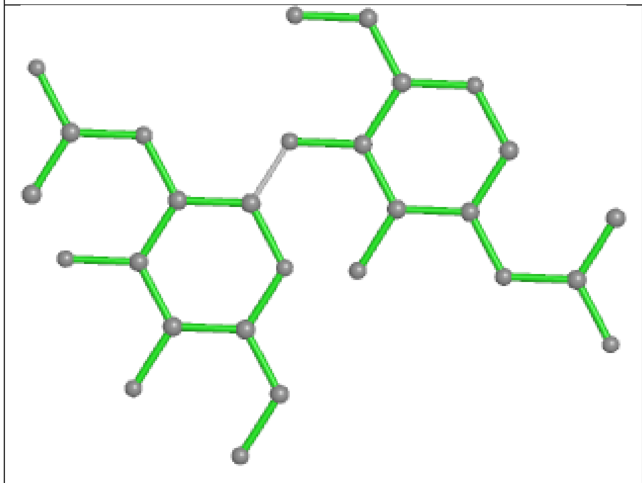
Bond lengths

Bond angles

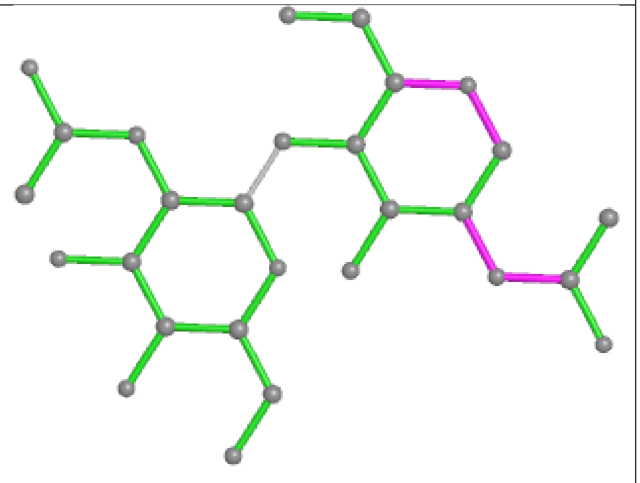
Torsions

Rings

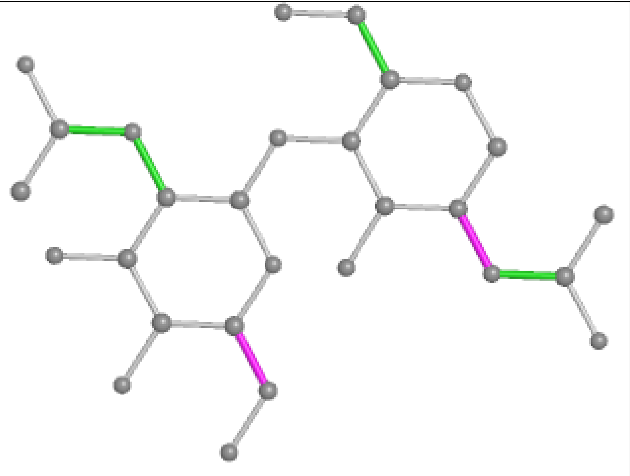
Oligosaccharide Chain S



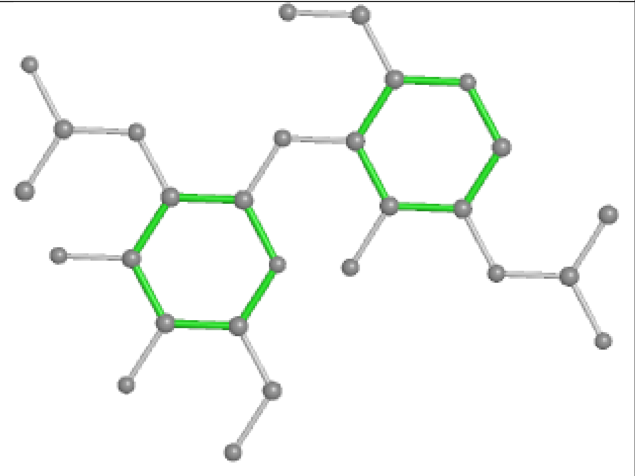
Bond lengths



Bond angles

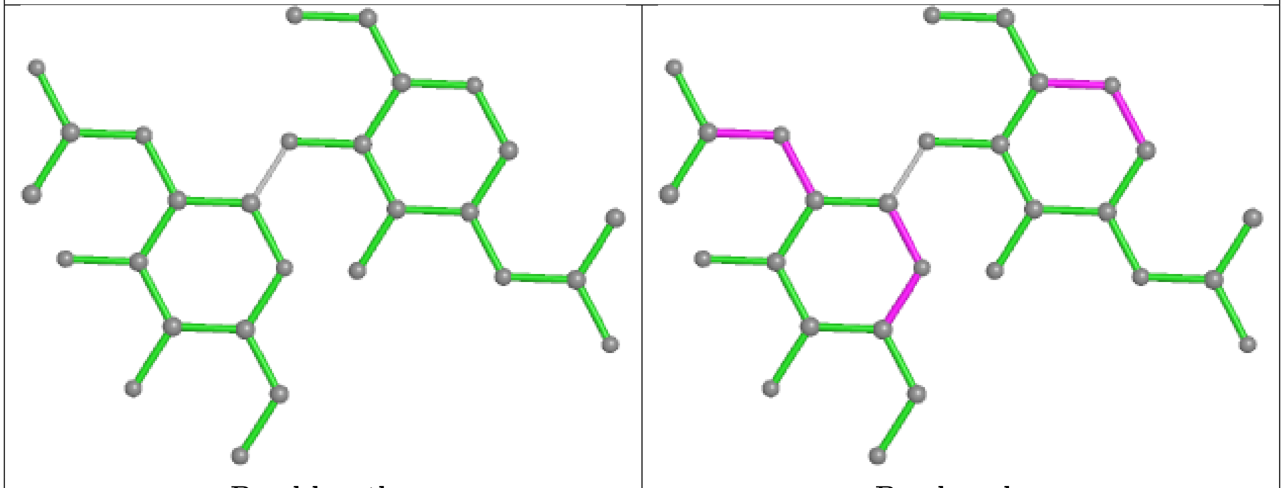


Torsions



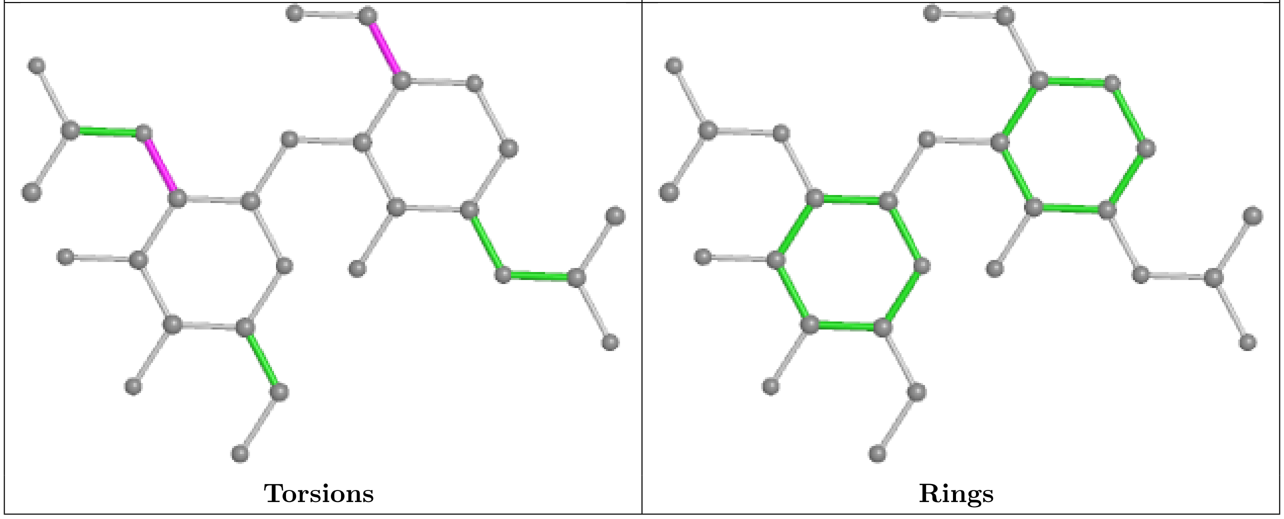
Rings

Oligosaccharide Chain U



Bond lengths

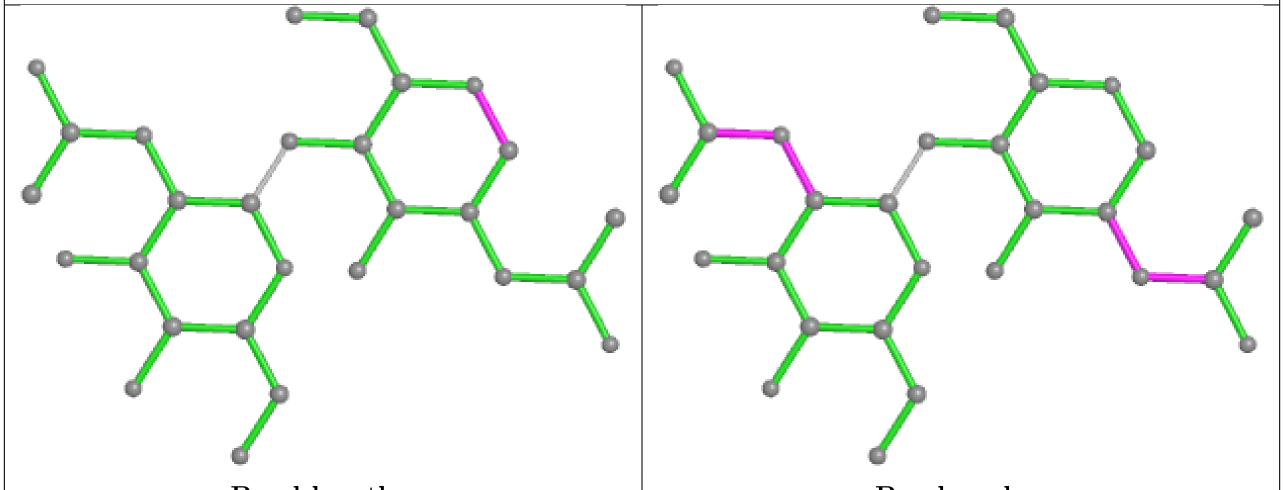
Bond angles



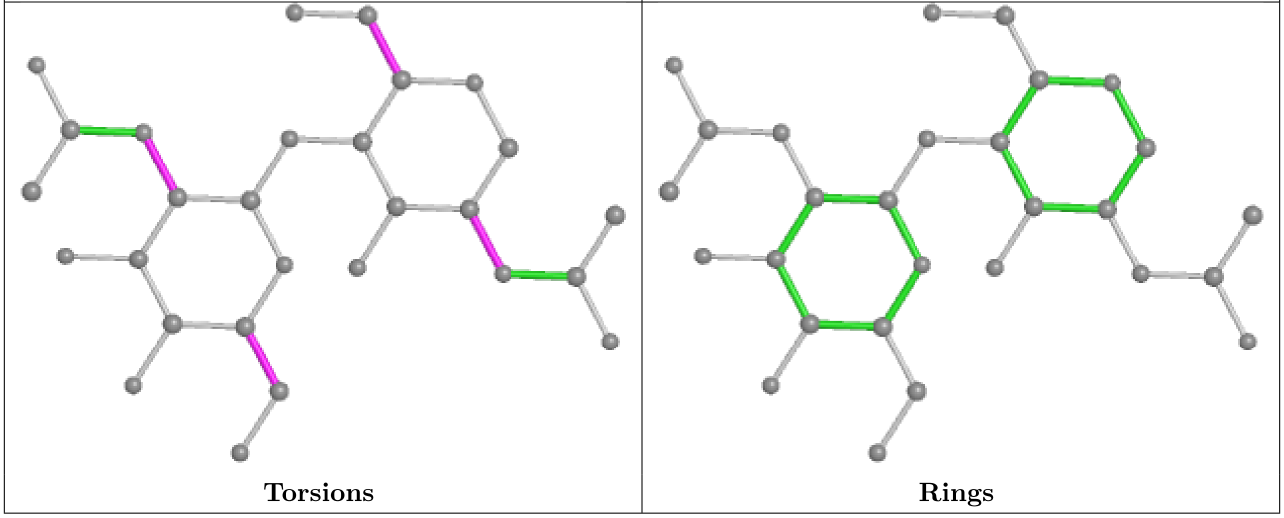
Torsions

Rings

Oligosaccharide Chain V

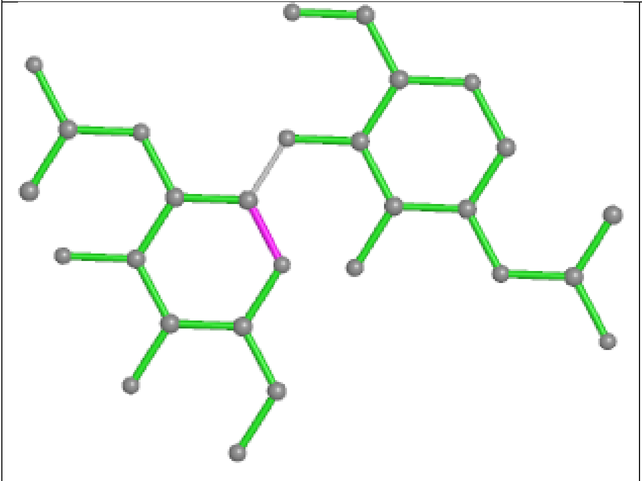


Bond lengths **Bond angles**

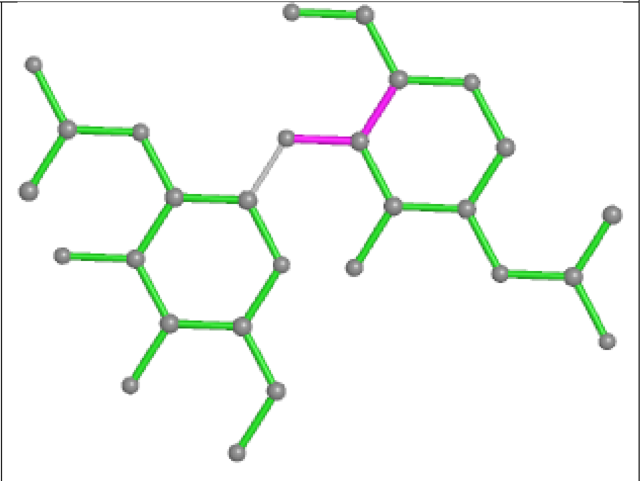


Torsions **Rings**

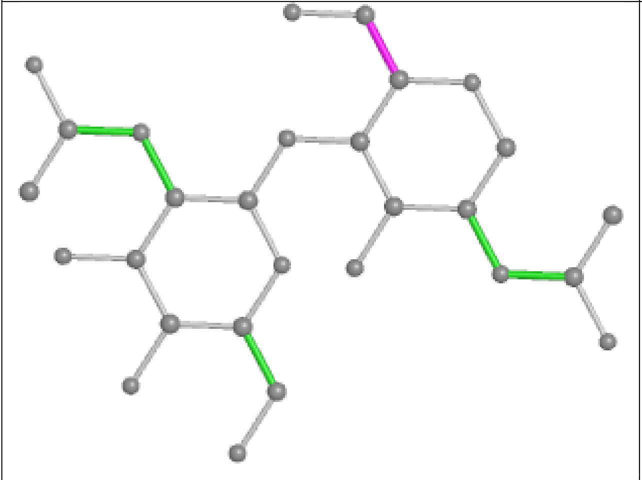
Oligosaccharide Chain W



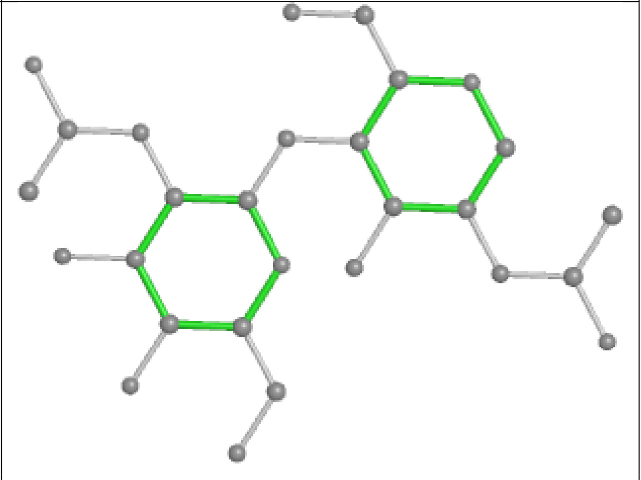
Bond lengths



Bond angles

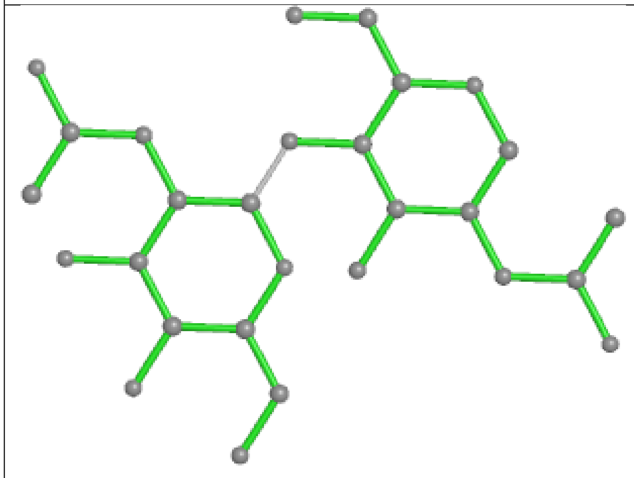


Torsions

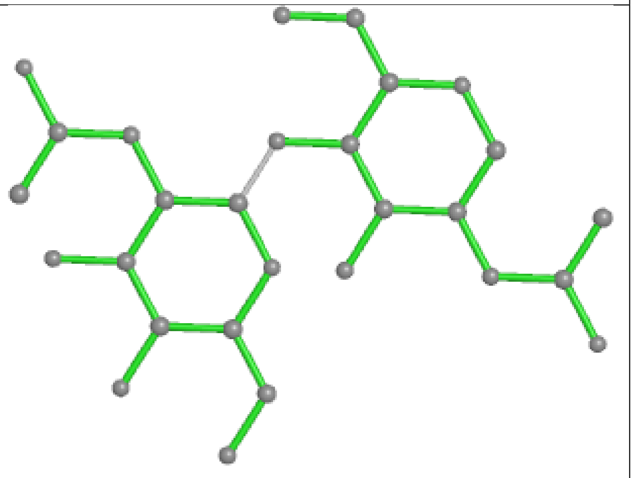


Rings

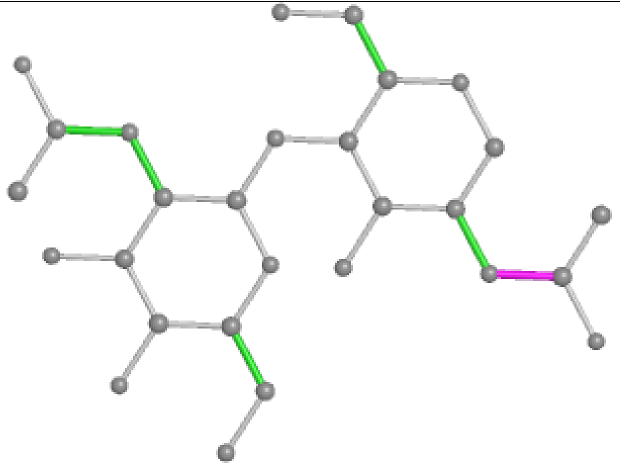
Oligosaccharide Chain X



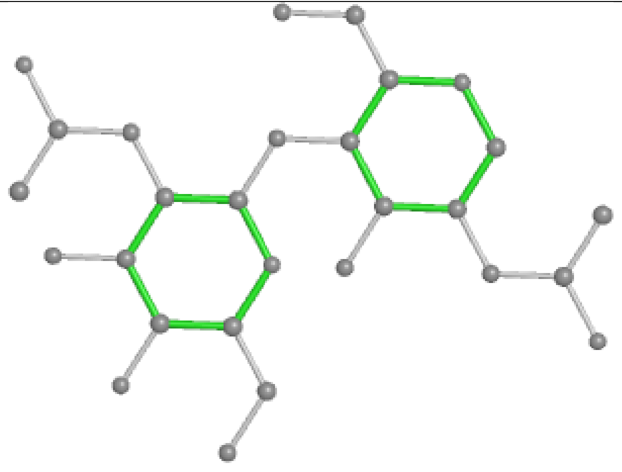
Bond lengths



Bond angles

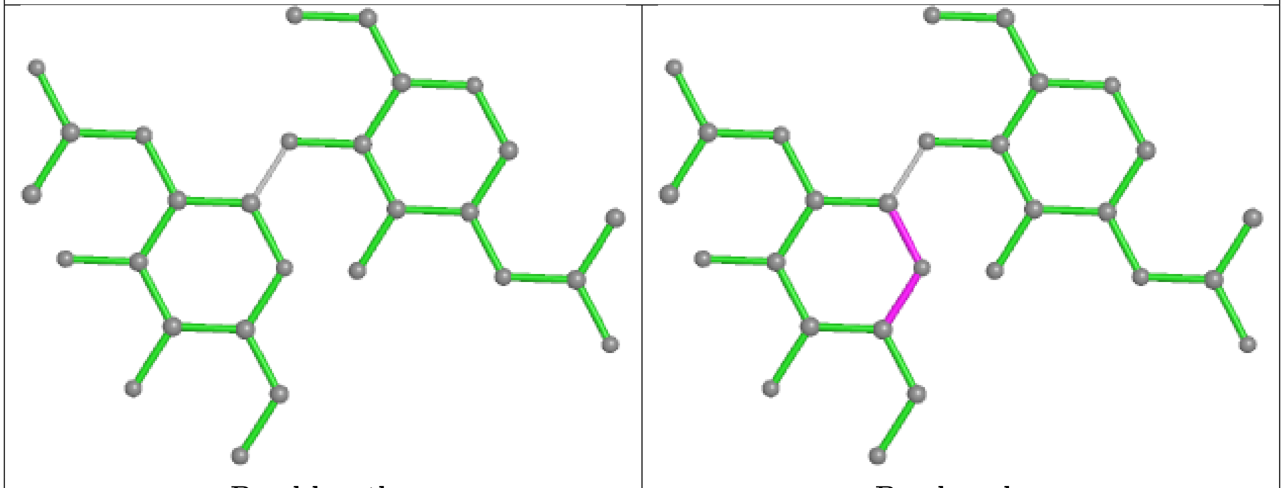


Torsions

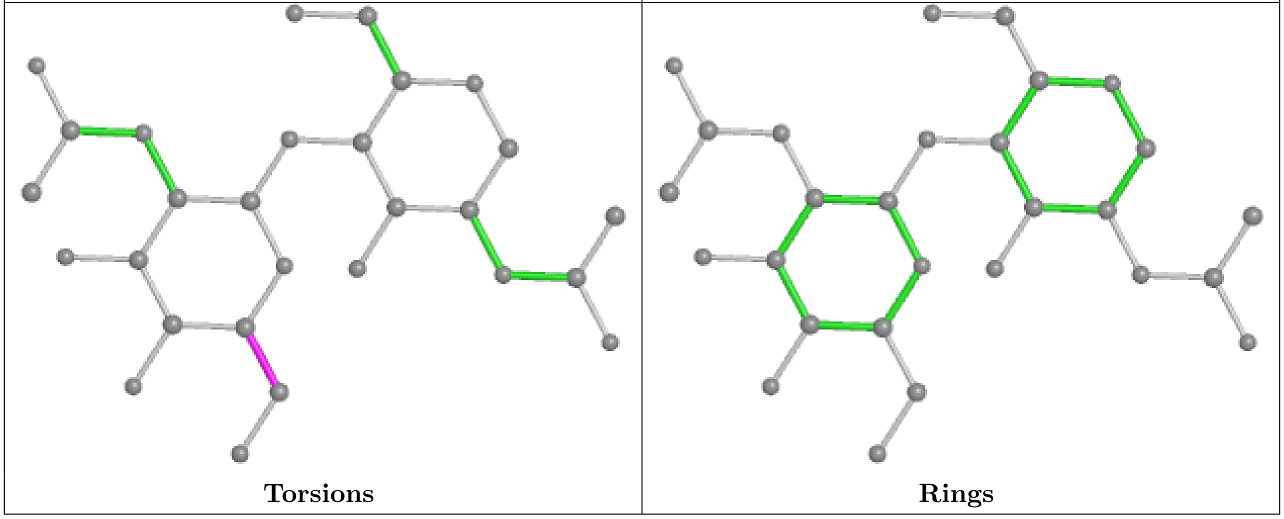


Rings

Oligosaccharide Chain Z

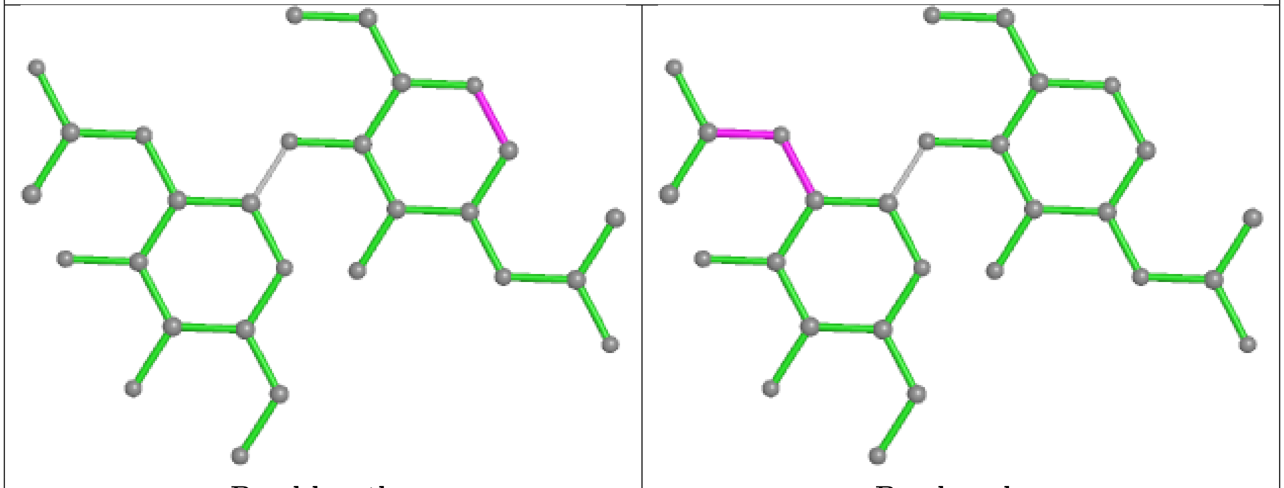


Bond lengths **Bond angles**



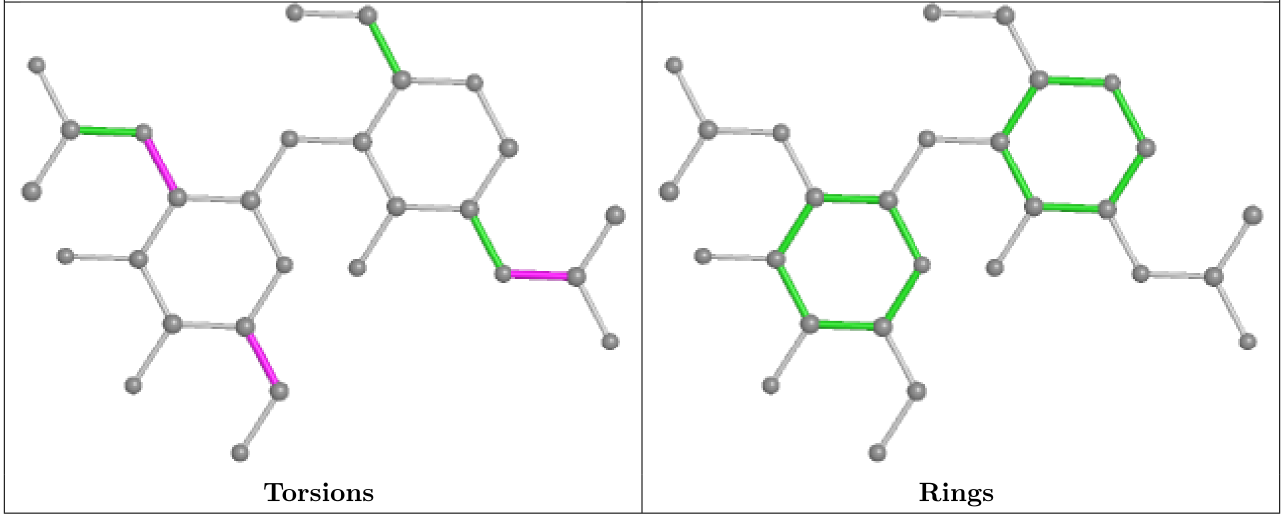
Torsions **Rings**

Oligosaccharide Chain d



Bond lengths

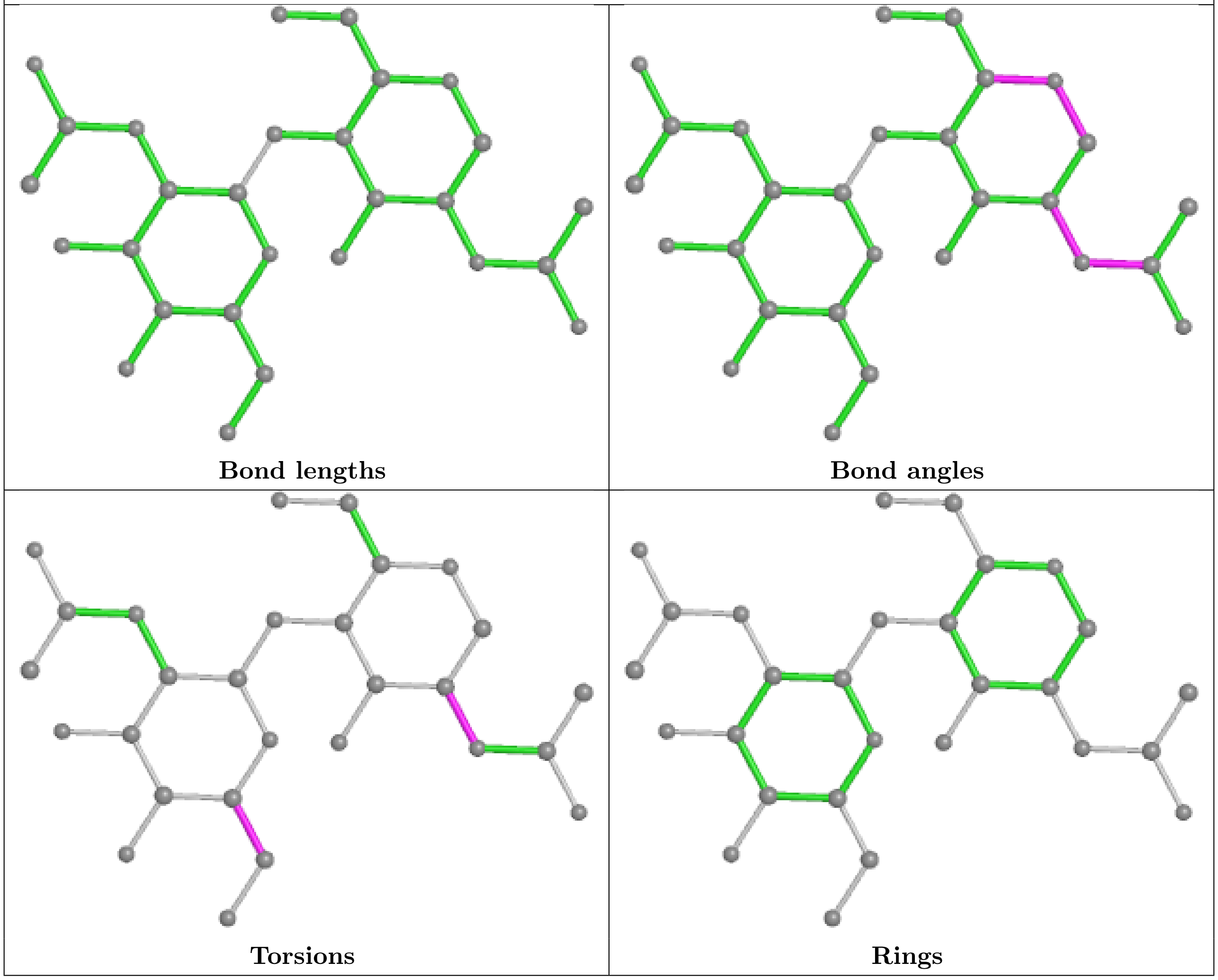
Bond angles



Torsions

Rings

Oligosaccharide Chain e



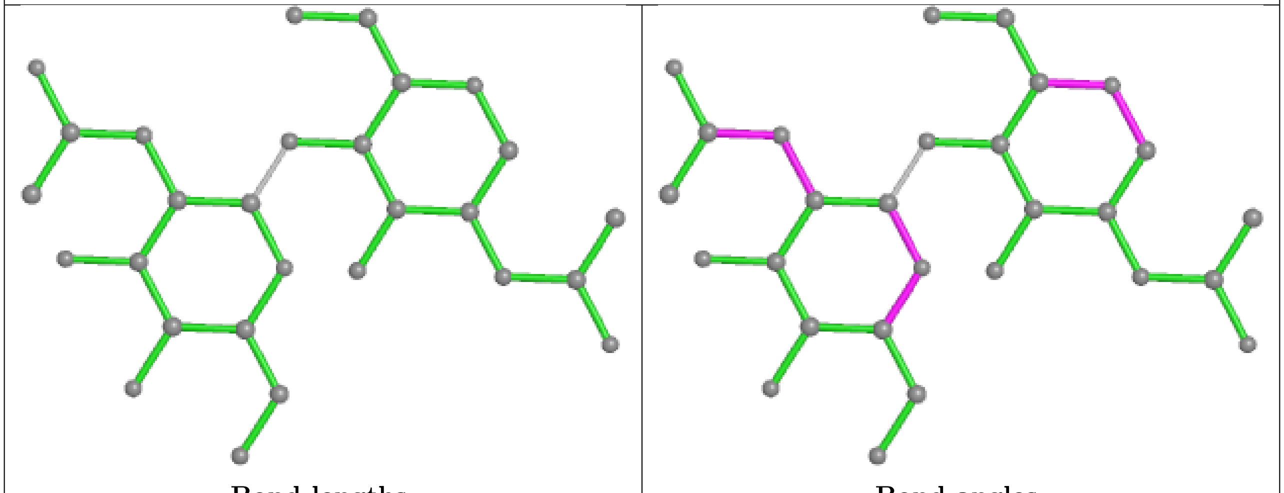
Bond lengths

Bond angles

Torsions

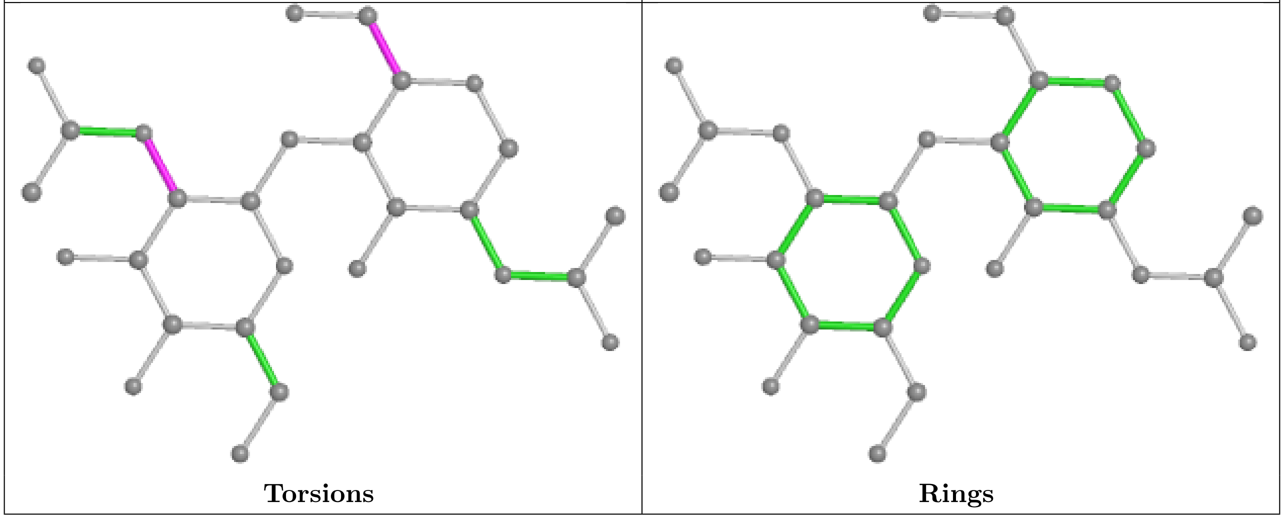
Rings

Oligosaccharide Chain g



Bond lengths

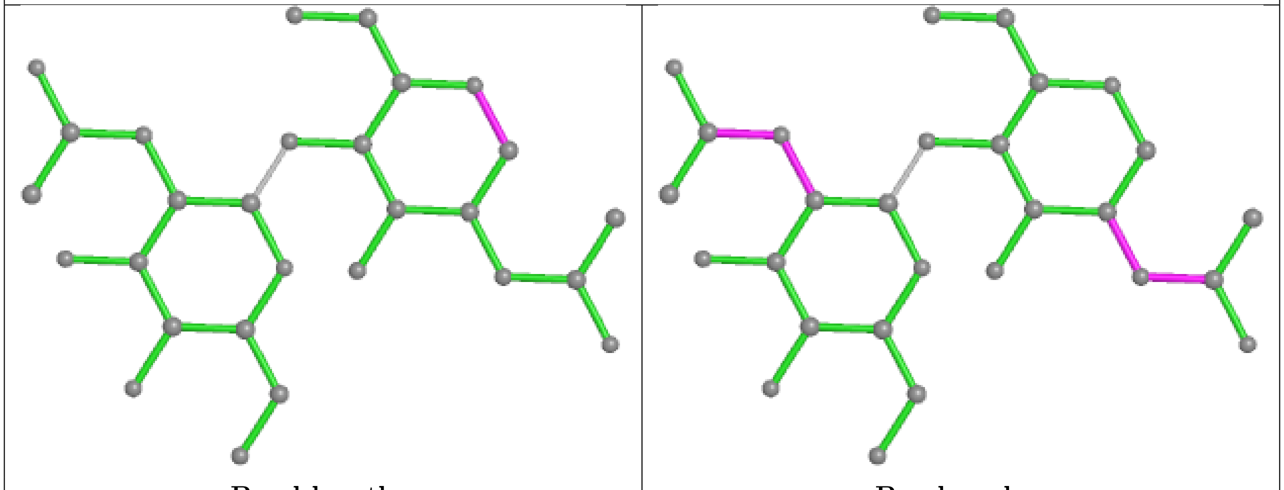
Bond angles



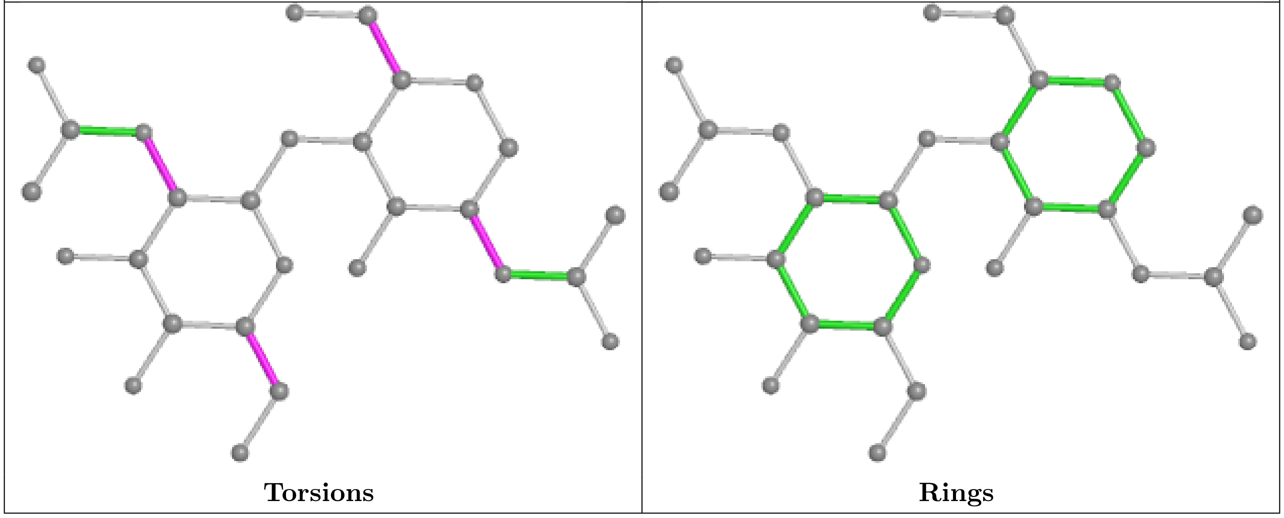
Torsions

Rings

Oligosaccharide Chain h

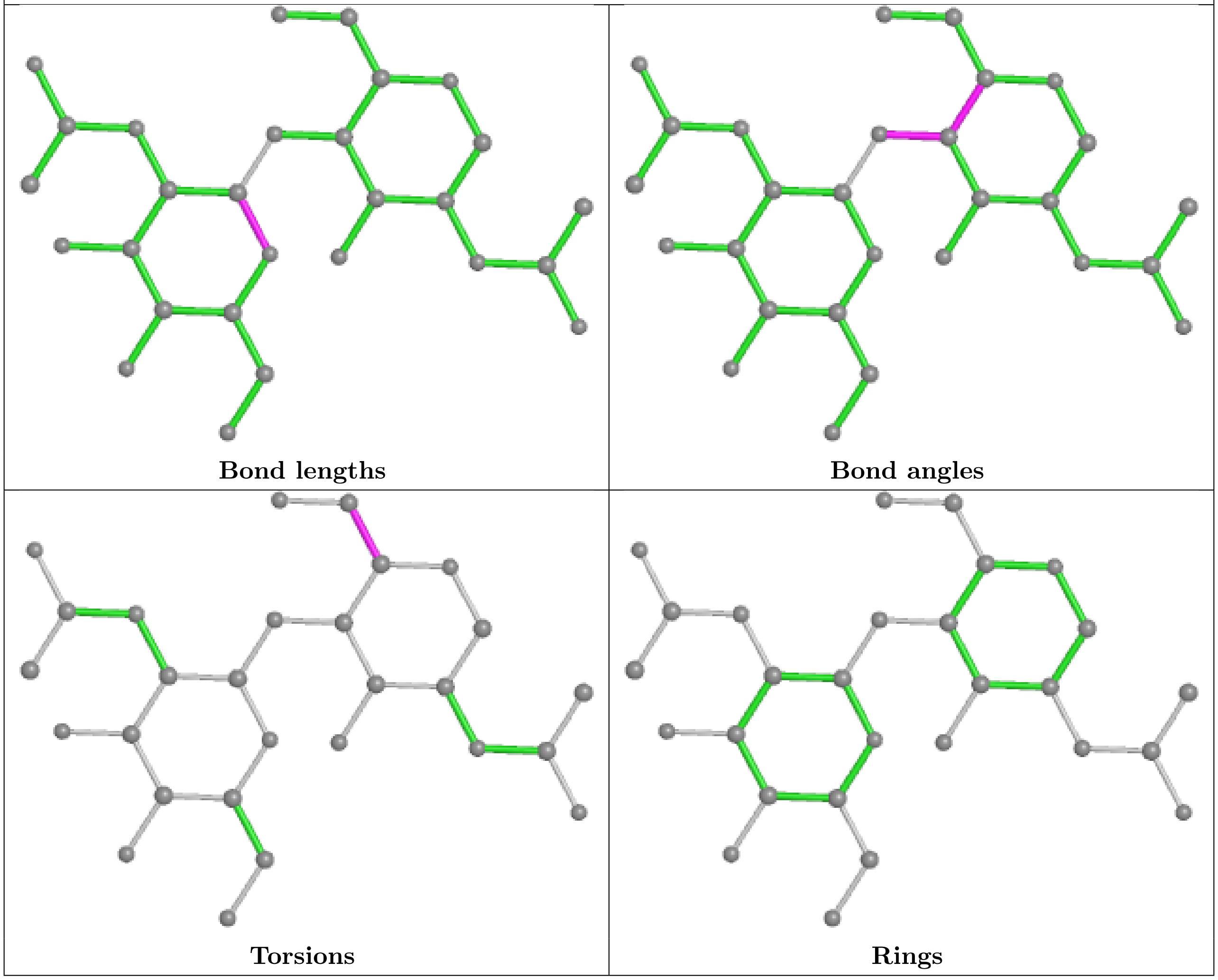


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain i



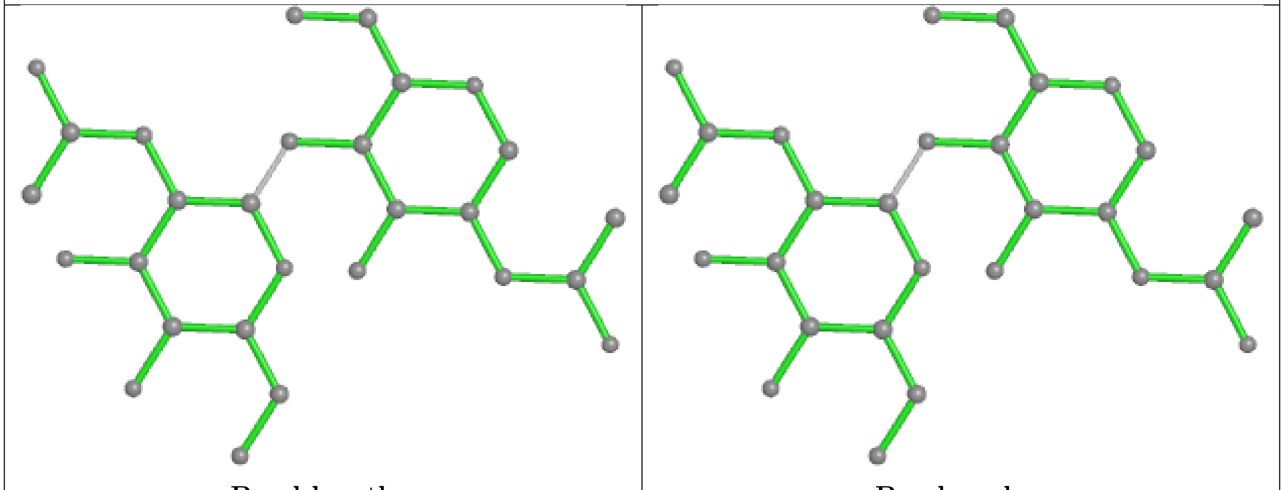
Bond lengths

Bond angles

Torsions

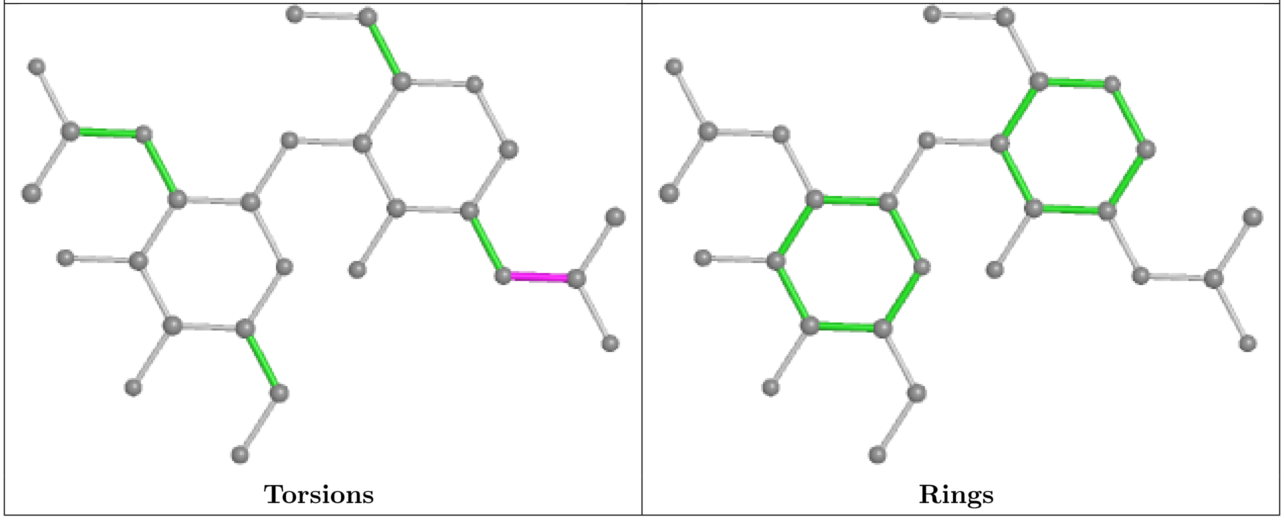
Rings

Oligosaccharide Chain j



Bond lengths

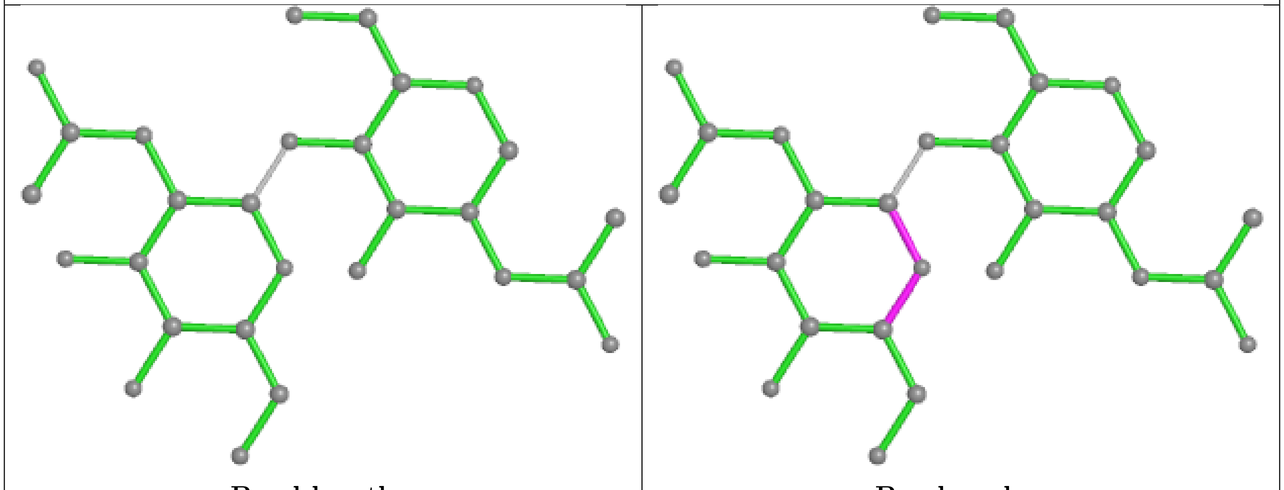
Bond angles



Torsions

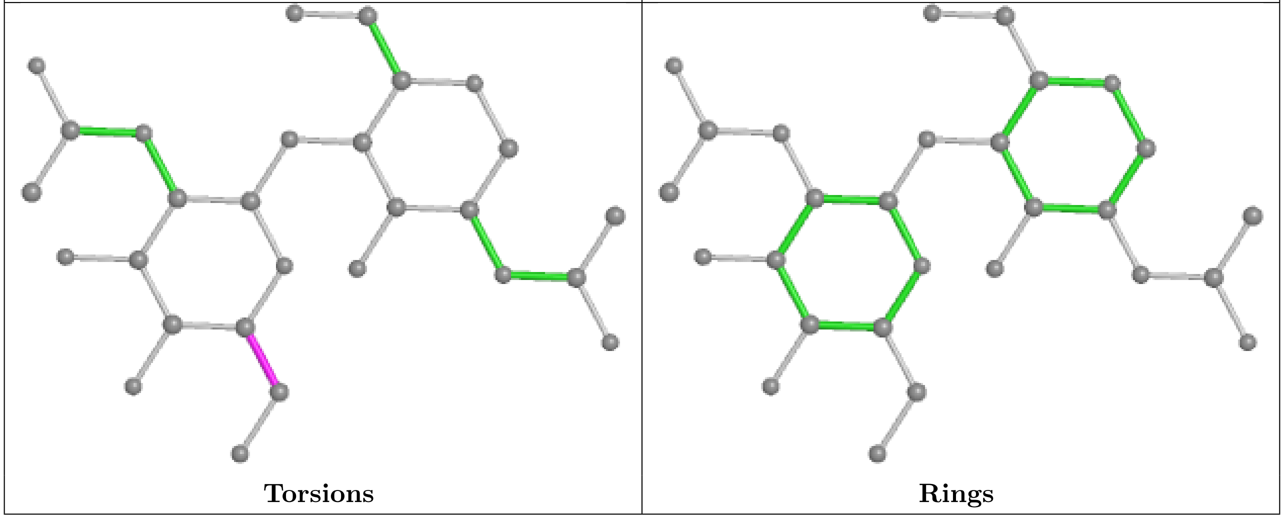
Rings

Oligosaccharide Chain l



Bond lengths

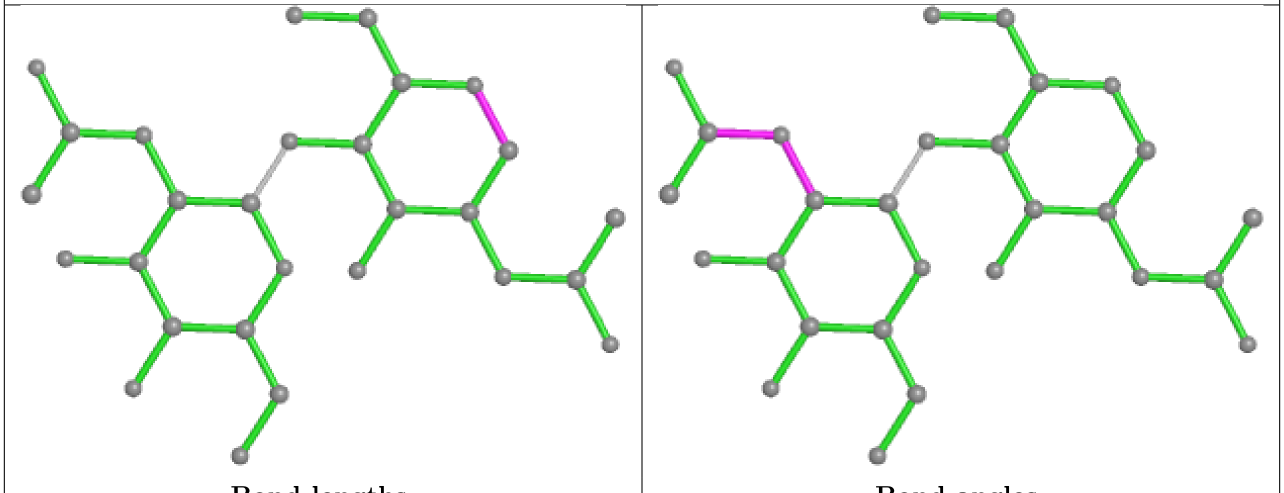
Bond angles



Torsions

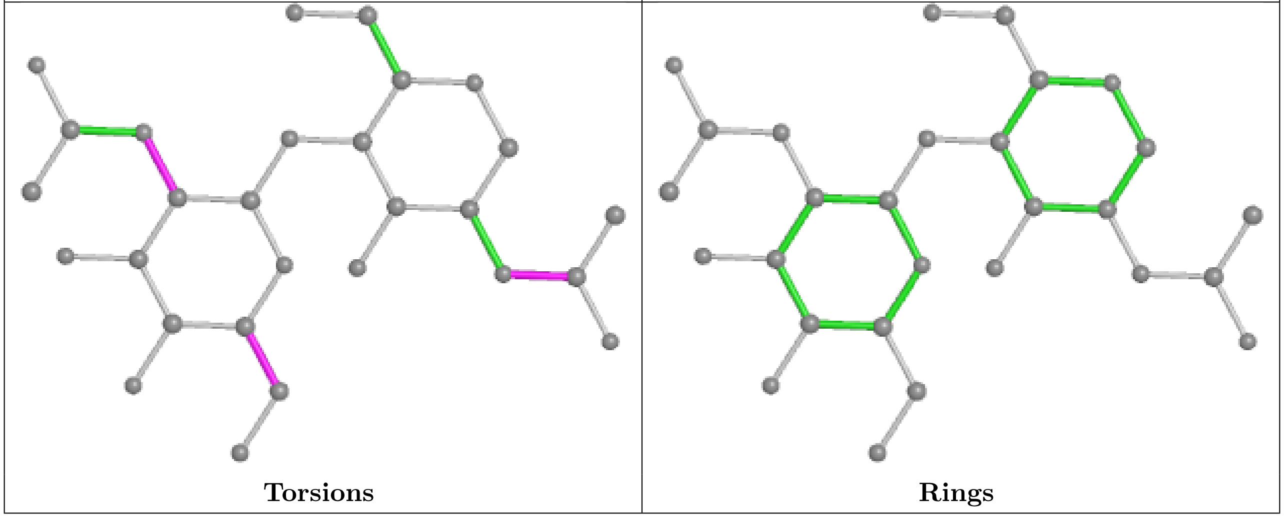
Rings

Oligosaccharide Chain p



Bond lengths

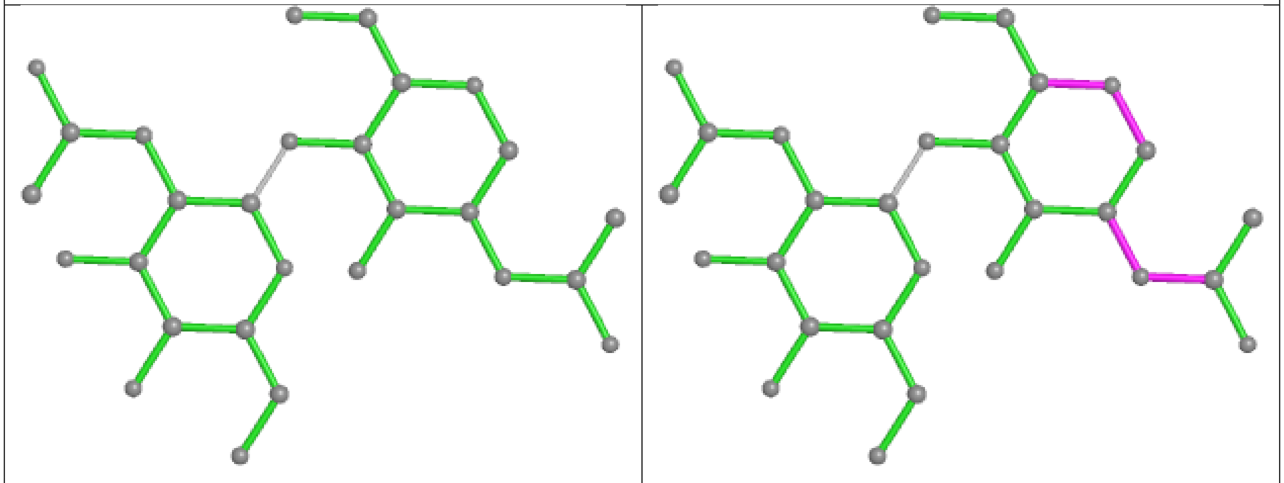
Bond angles



Torsions

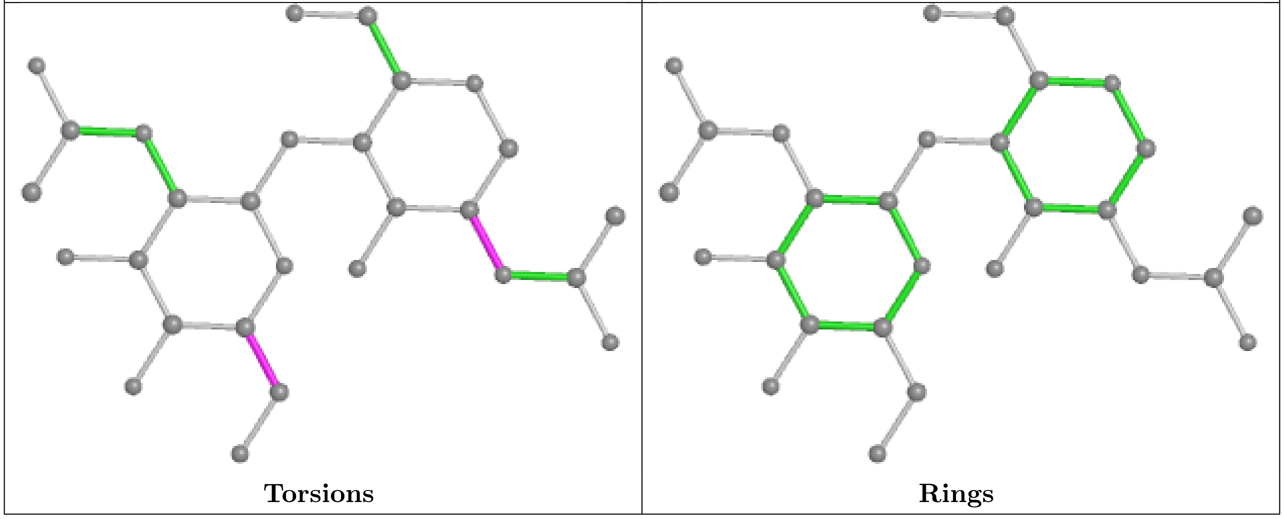
Rings

Oligosaccharide Chain q



Bond lengths

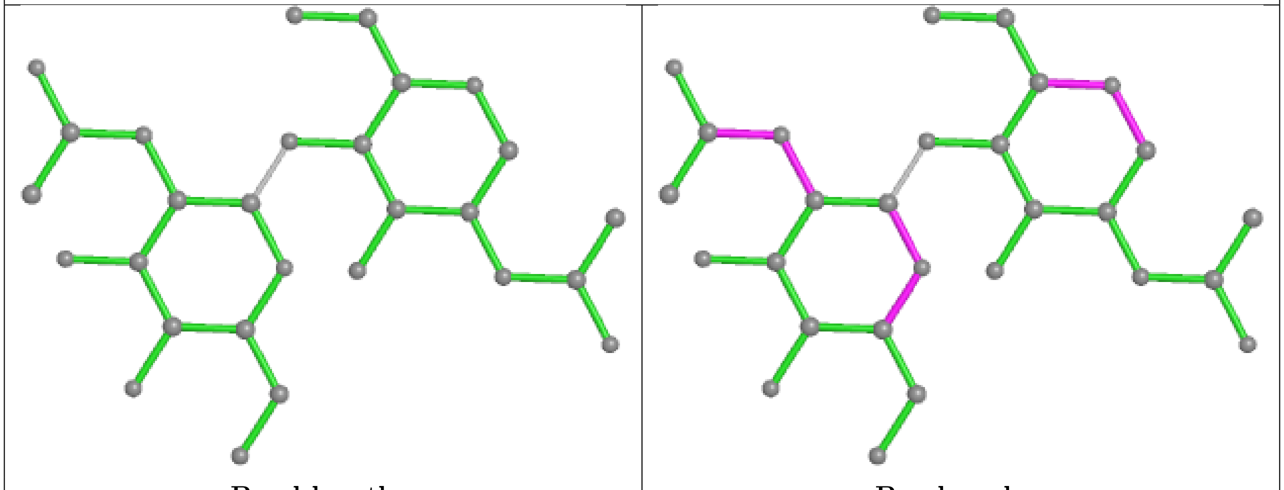
Bond angles



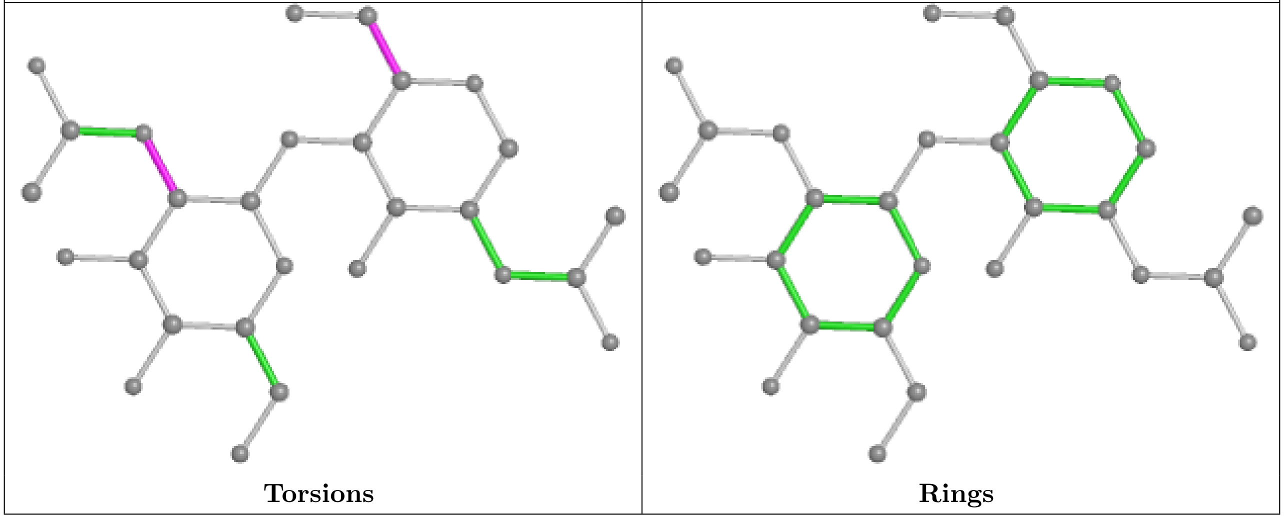
Torsions

Rings

Oligosaccharide Chain s

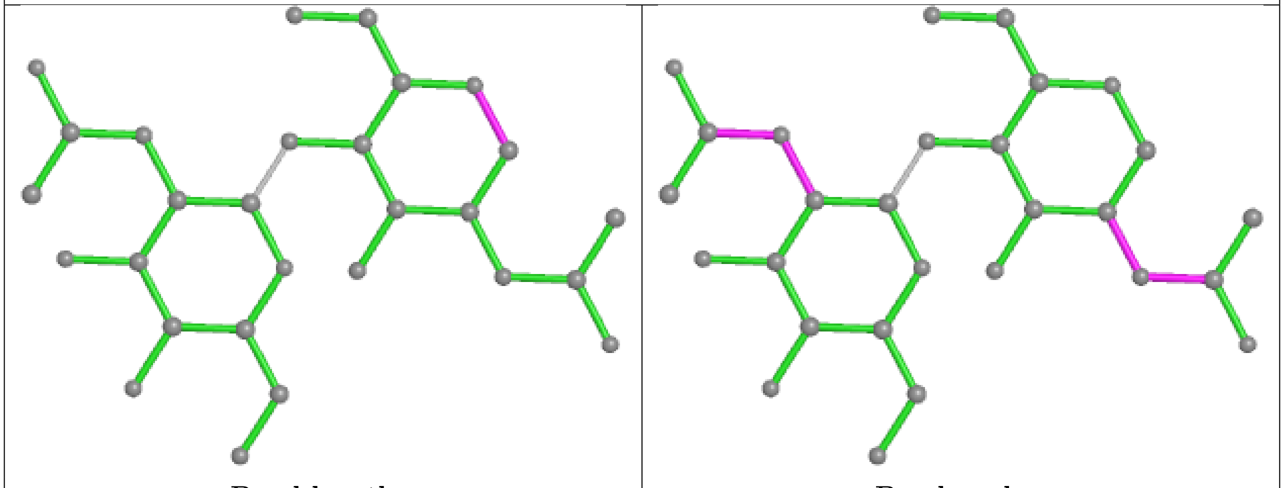


Bond lengths **Bond angles**



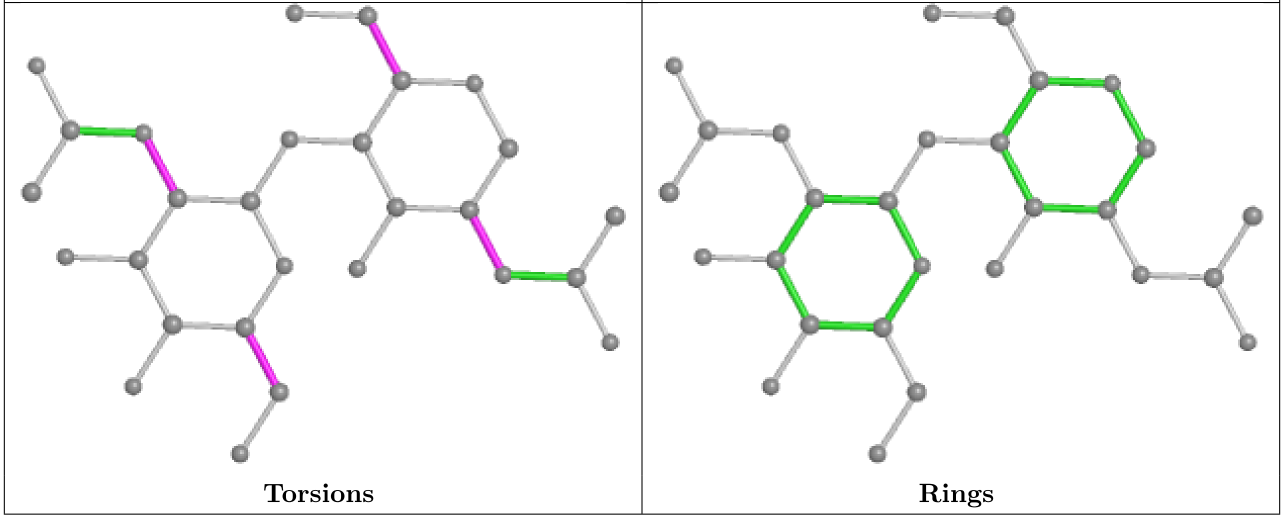
Torsions **Rings**

Oligosaccharide Chain t



Bond lengths

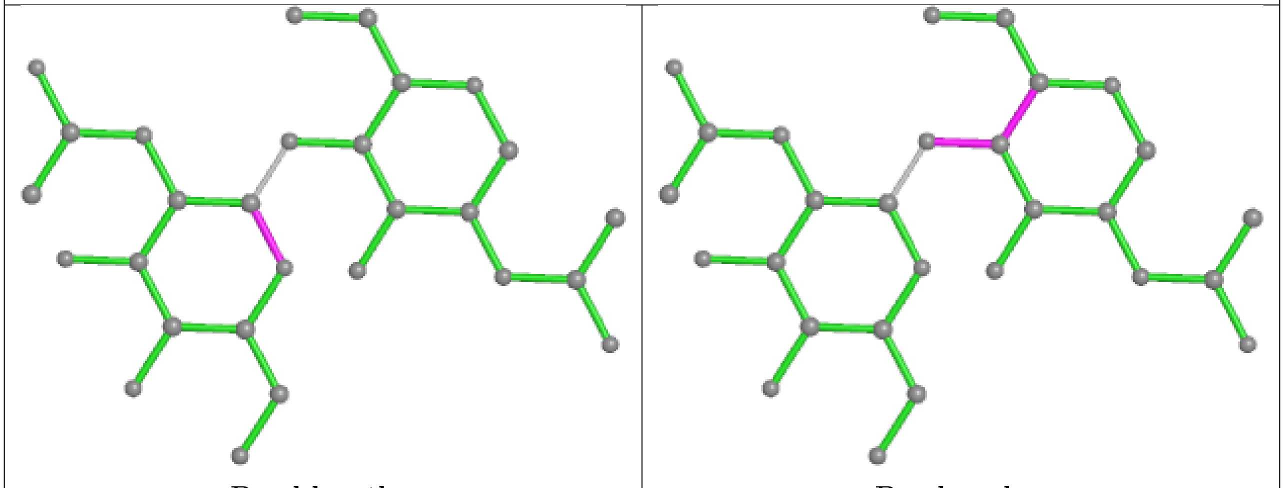
Bond angles



Torsions

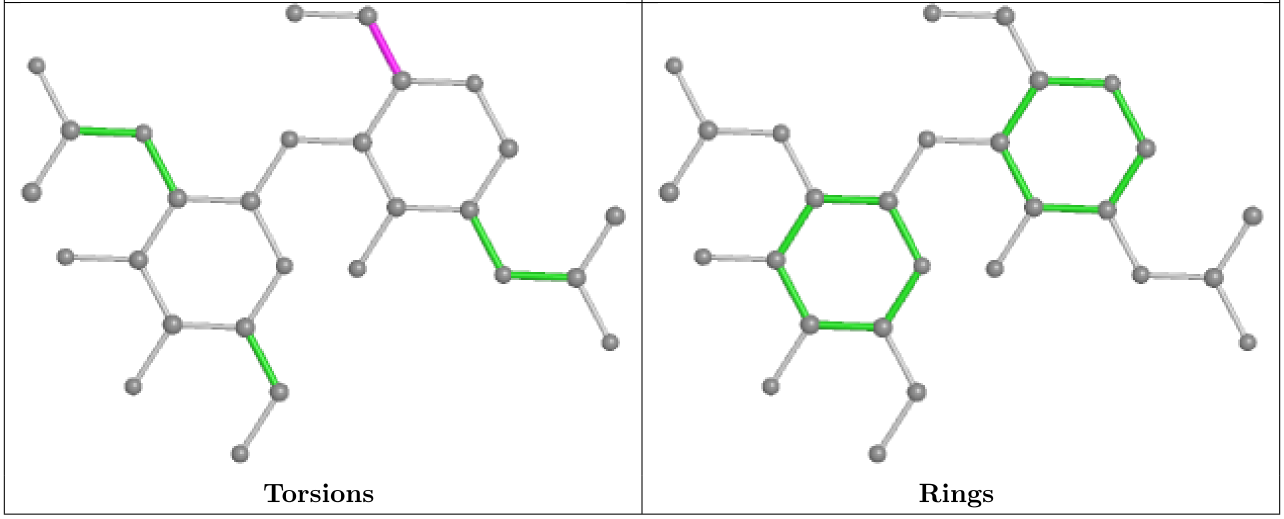
Rings

Oligosaccharide Chain u



Bond lengths

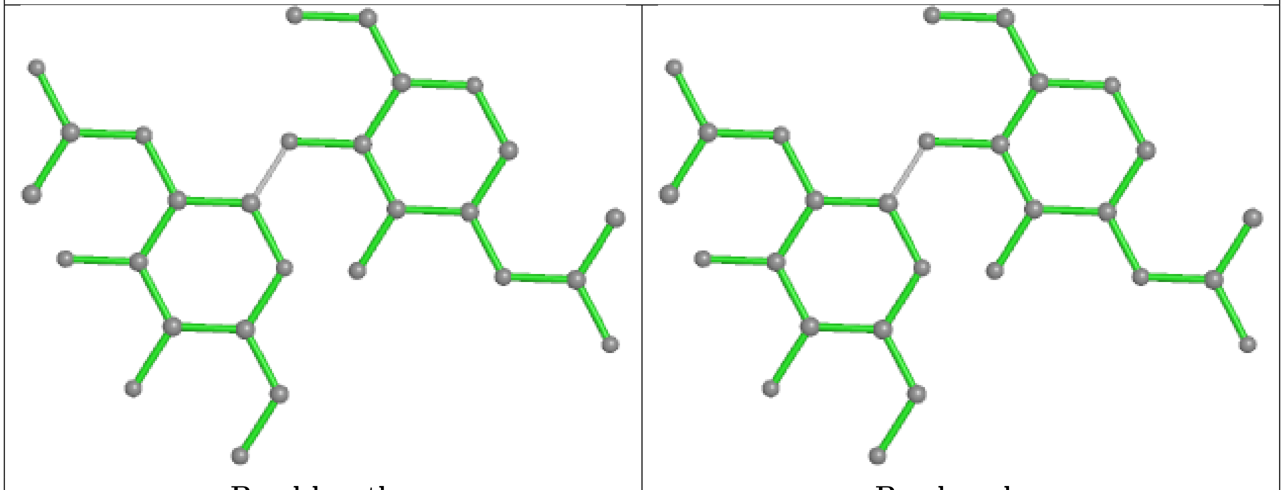
Bond angles



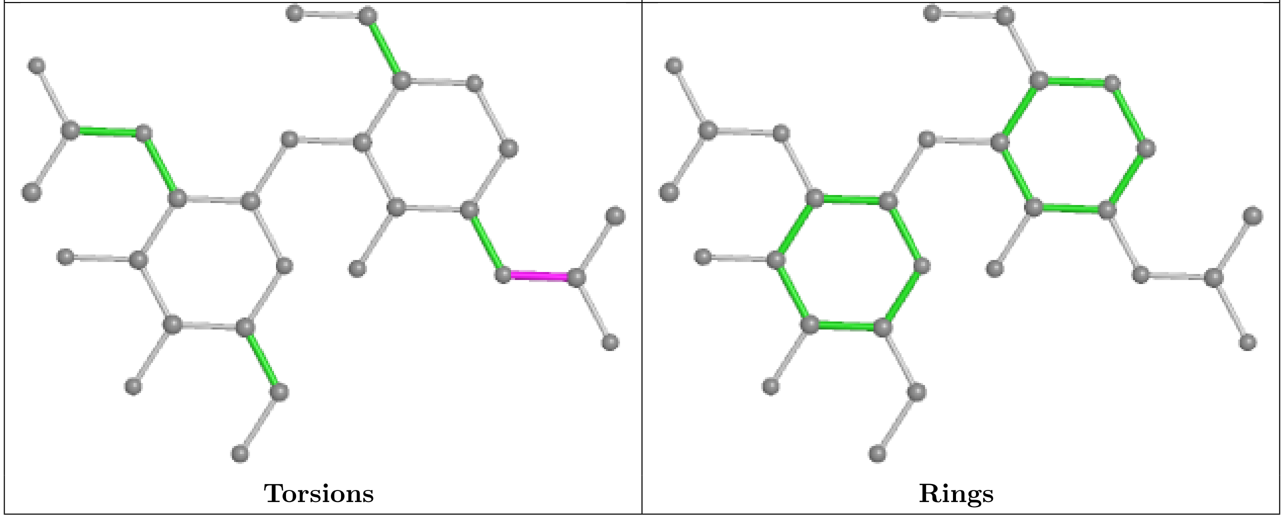
Torsions

Rings

Oligosaccharide Chain v

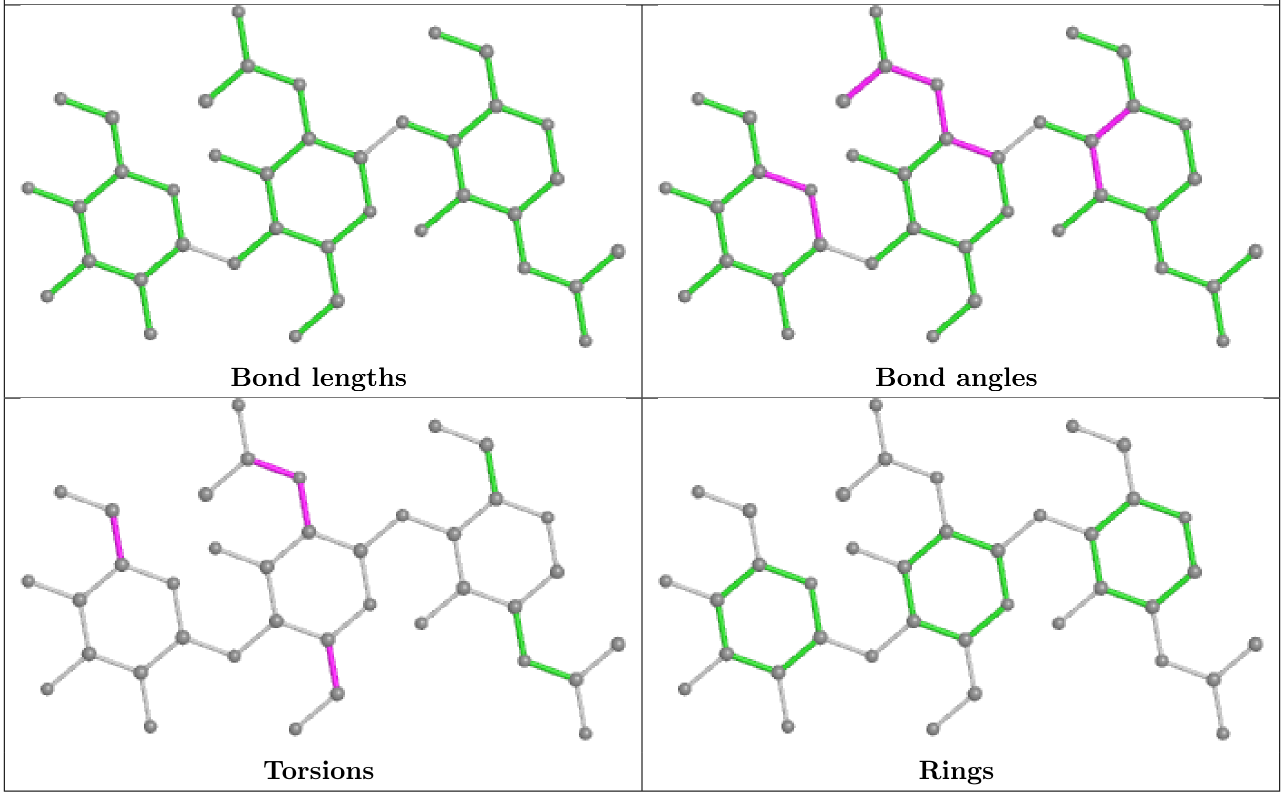


Bond lengths **Bond angles**

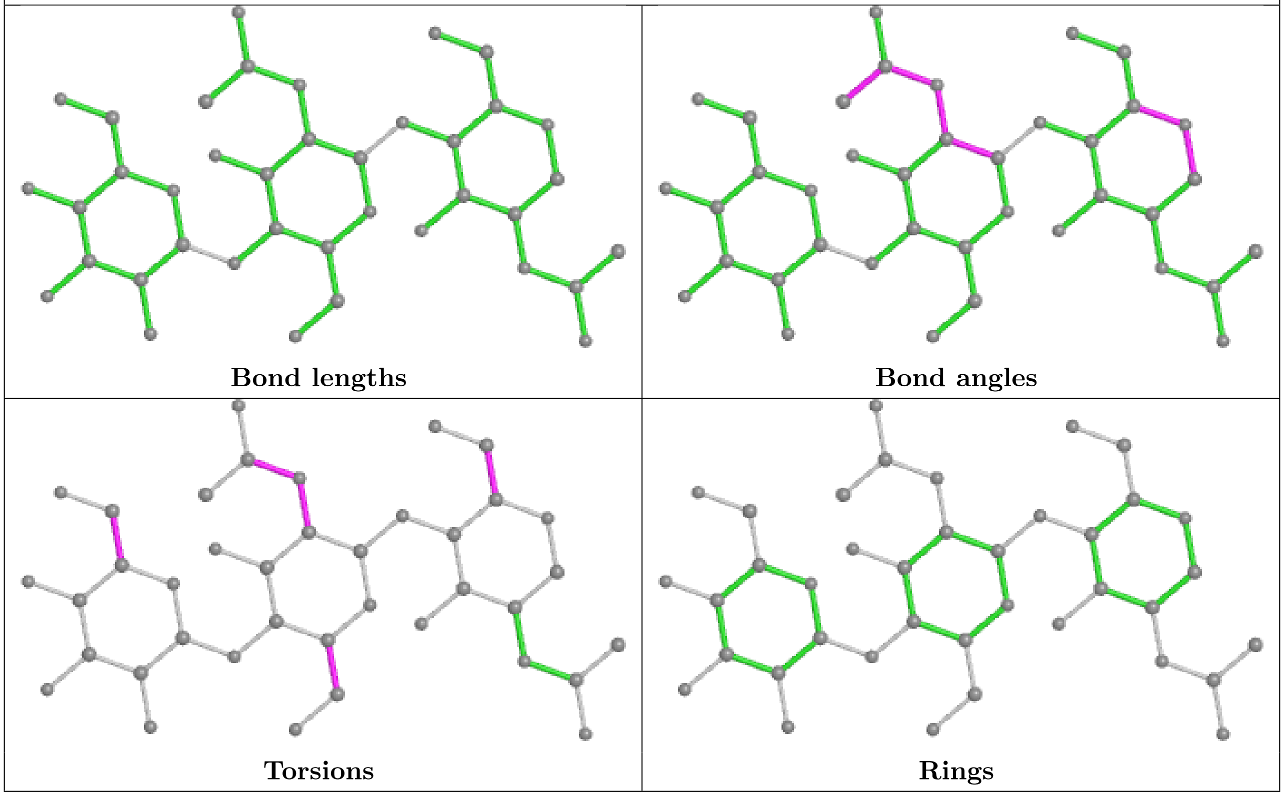


Torsions **Rings**

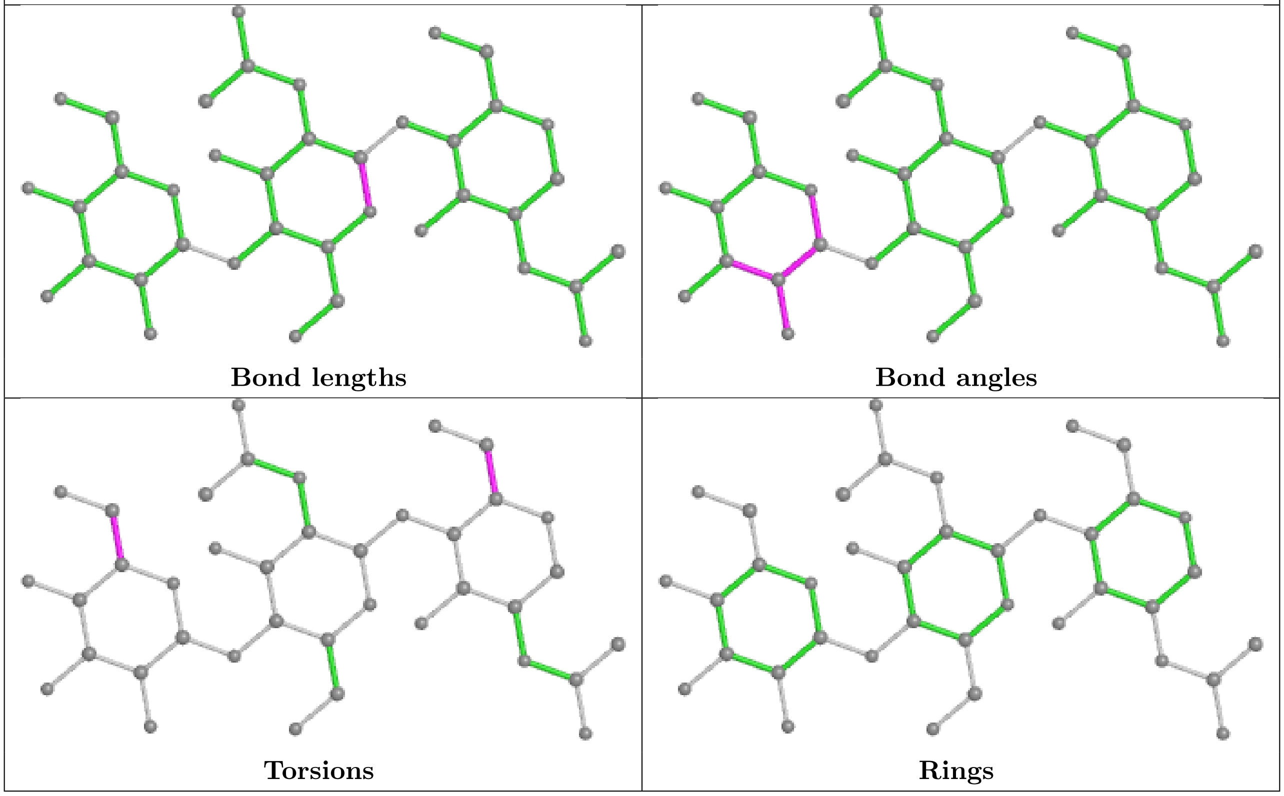
Oligosaccharide Chain O



Oligosaccharide Chain P



Oligosaccharide Chain Q

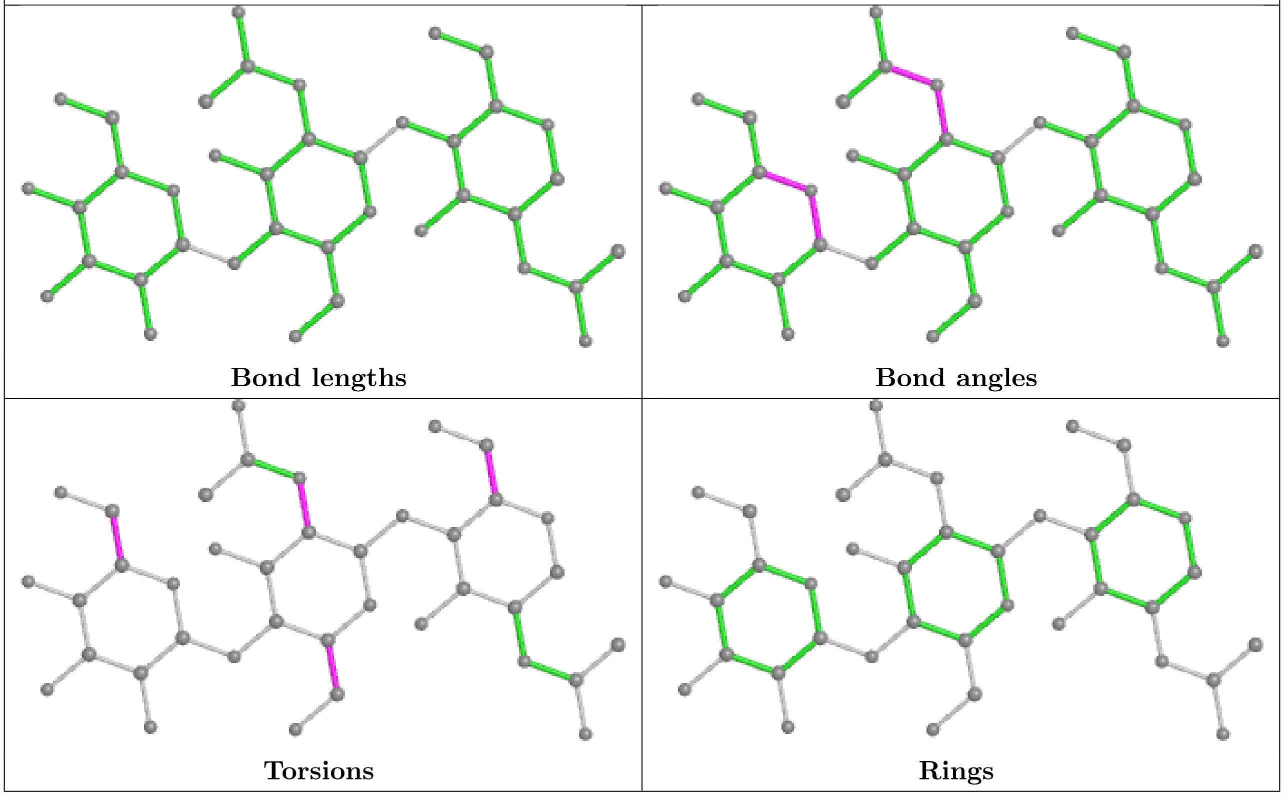

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain T

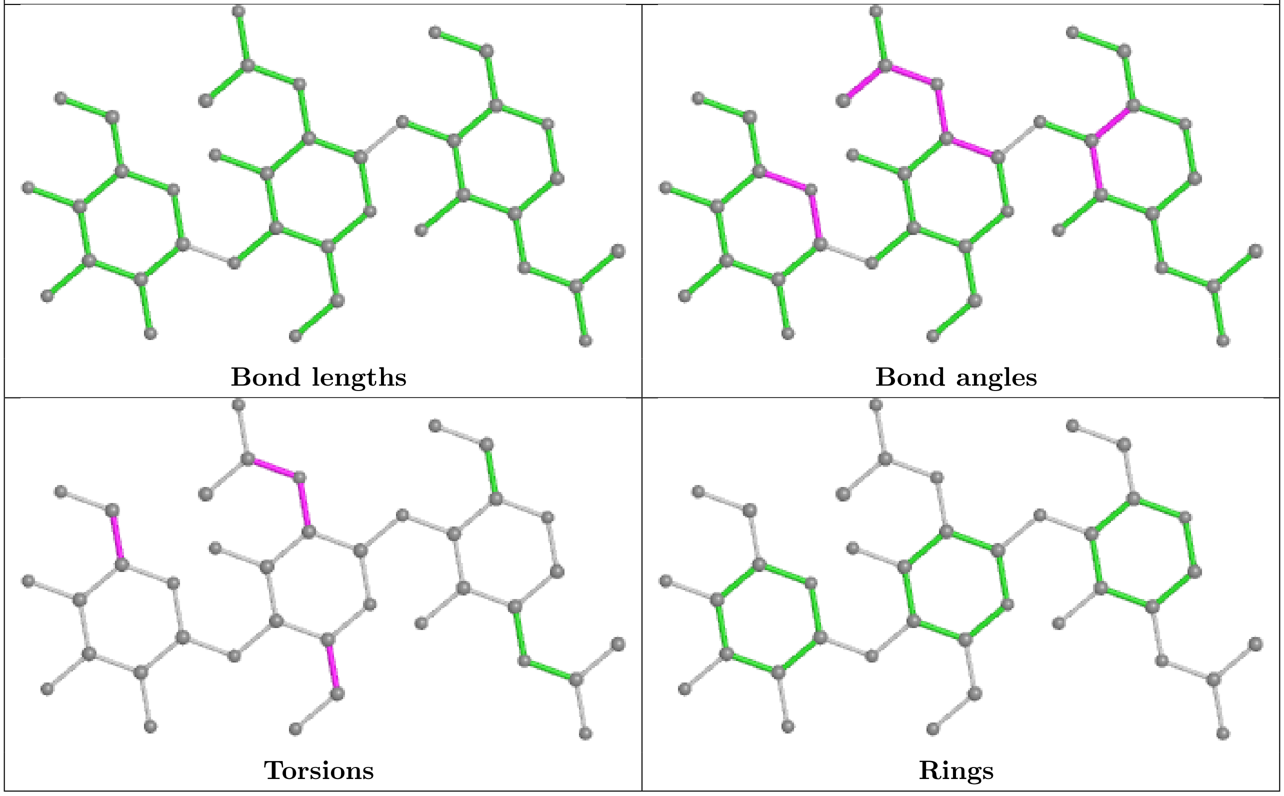

Bond lengths

Bond angles

Torsions

Rings

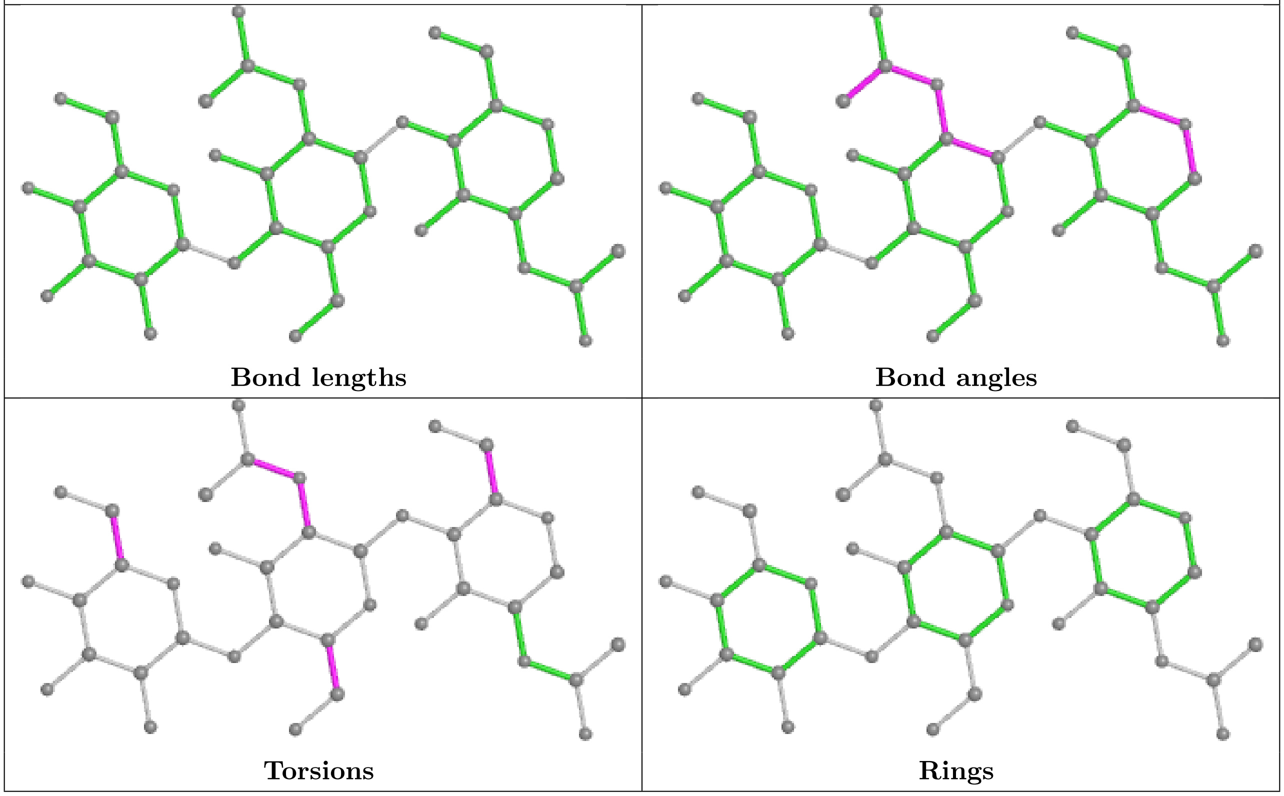
Oligosaccharide Chain a



Bond lengths Bond angles

Torsions Rings

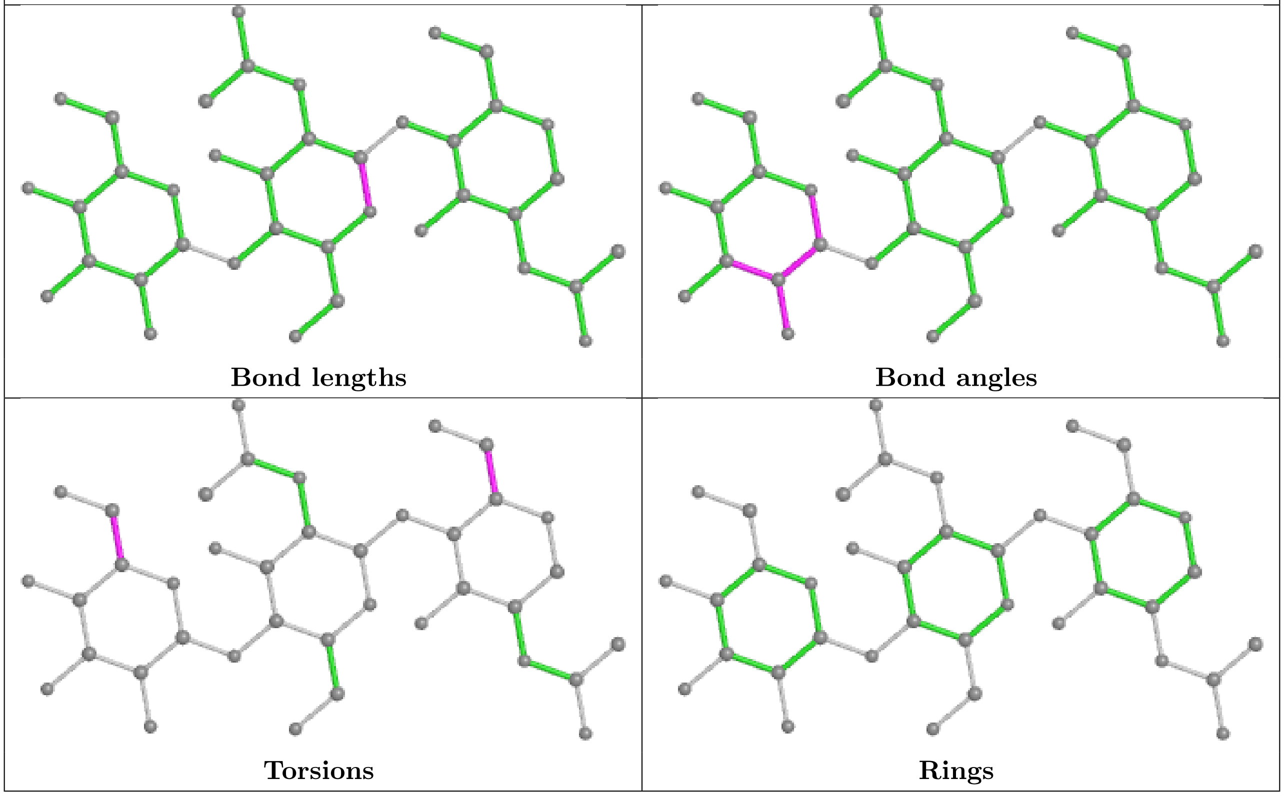
Oligosaccharide Chain b



Bond lengths Bond angles

Torsions Rings

Oligosaccharide Chain c



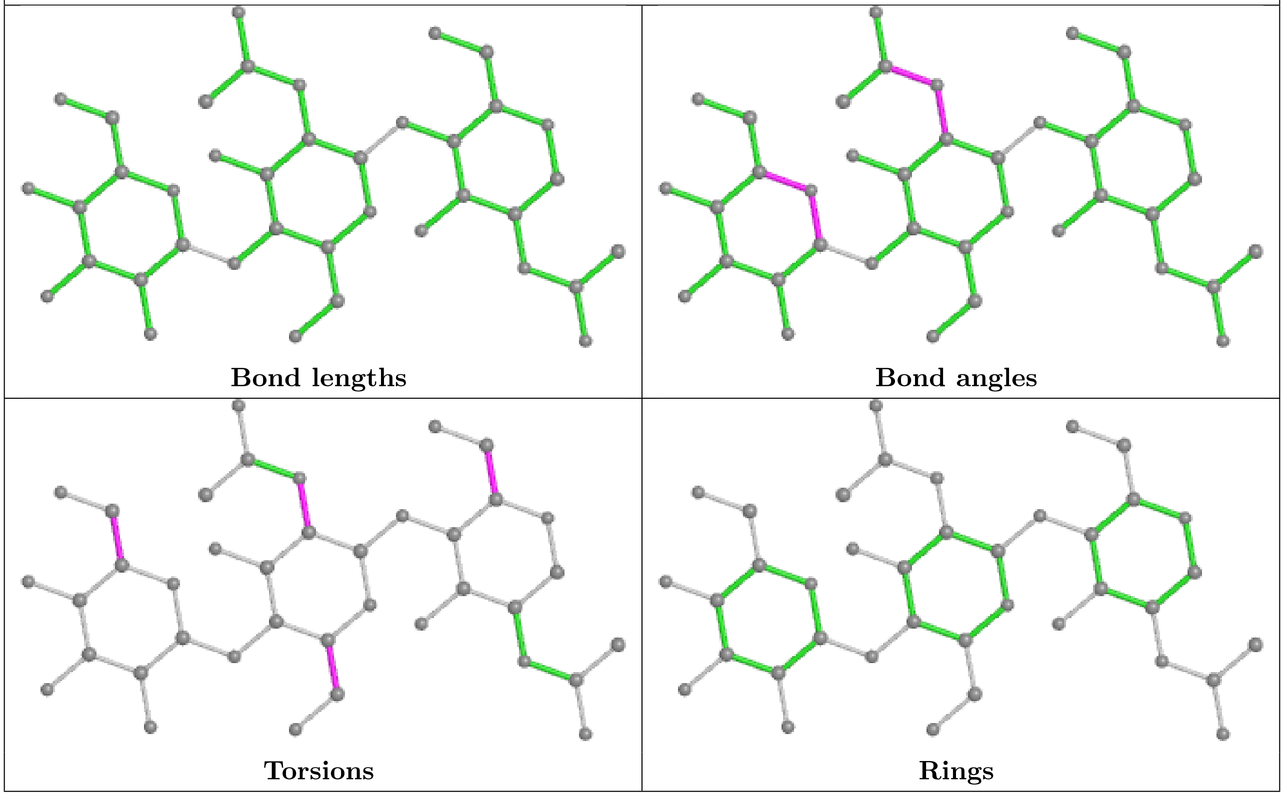
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain f



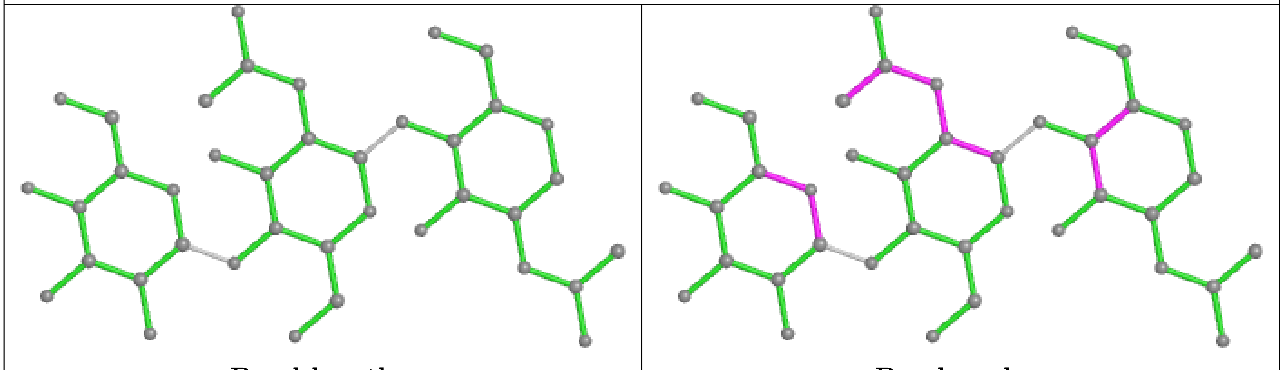
Bond lengths

Bond angles

Torsions

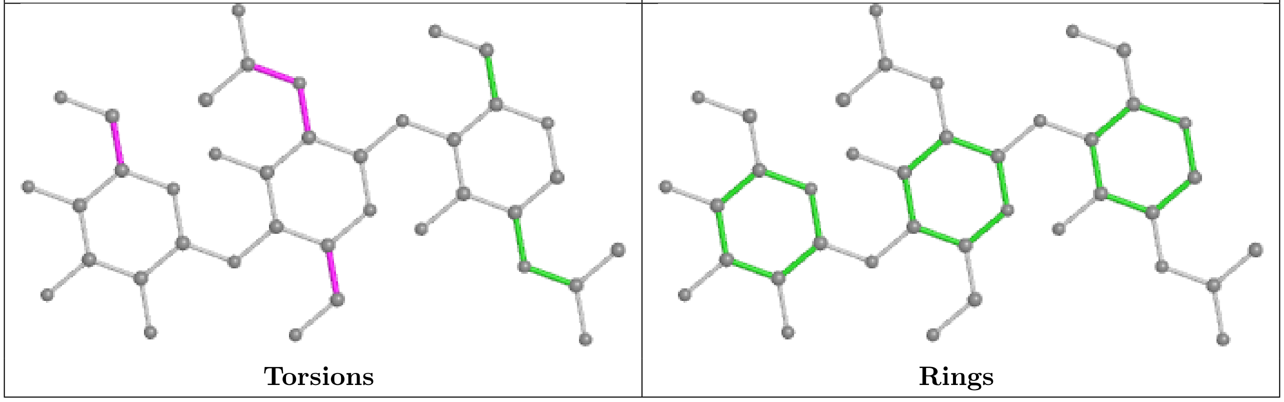
Rings

Oligosaccharide Chain m



Bond lengths

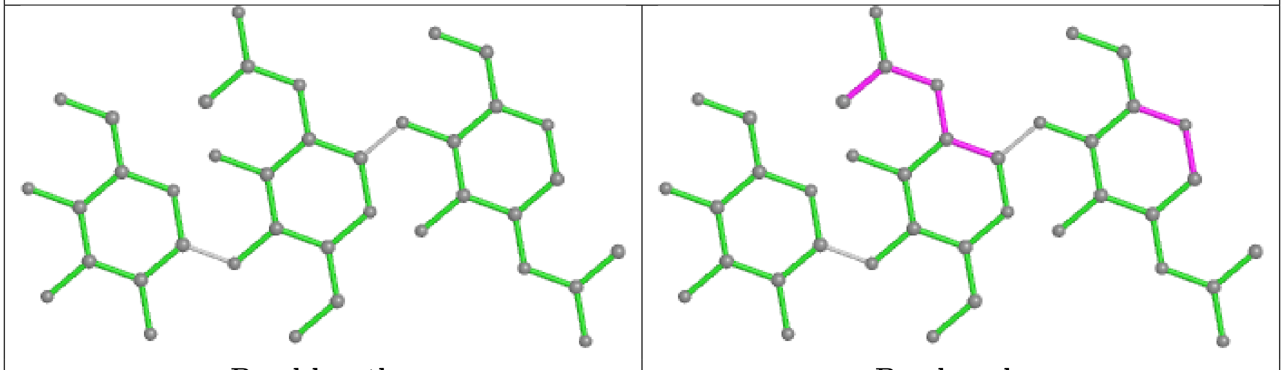
Bond angles



Torsions

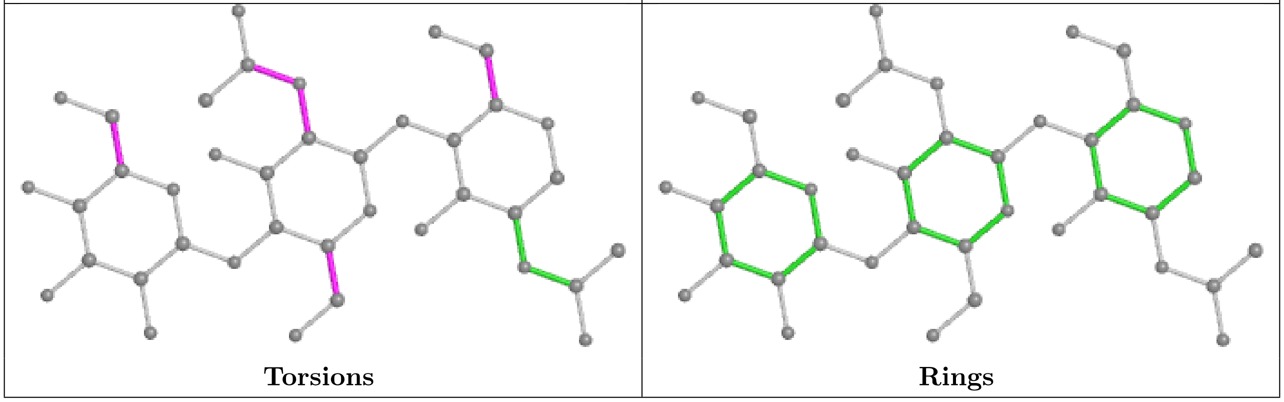
Rings

Oligosaccharide Chain n



Bond lengths

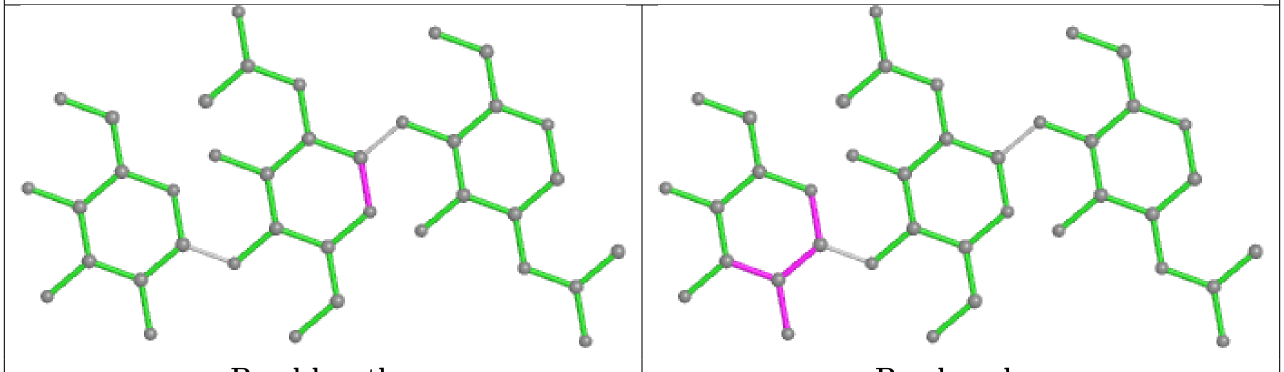
Bond angles



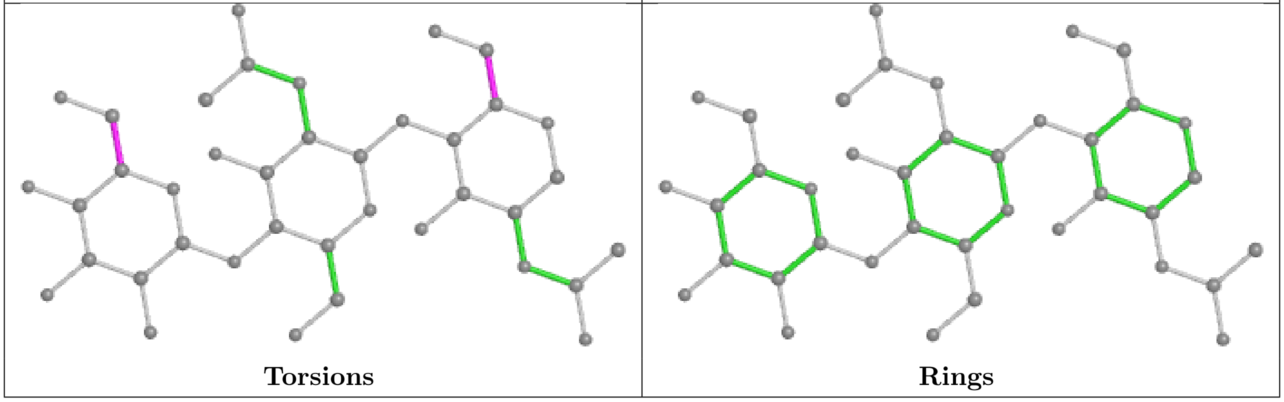
Torsions

Rings

Oligosaccharide Chain o

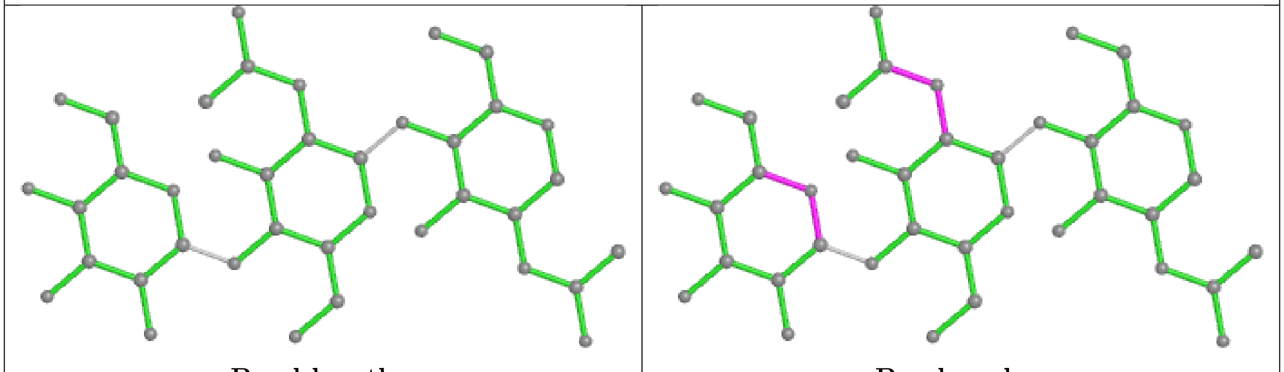


Bond lengths Bond angles

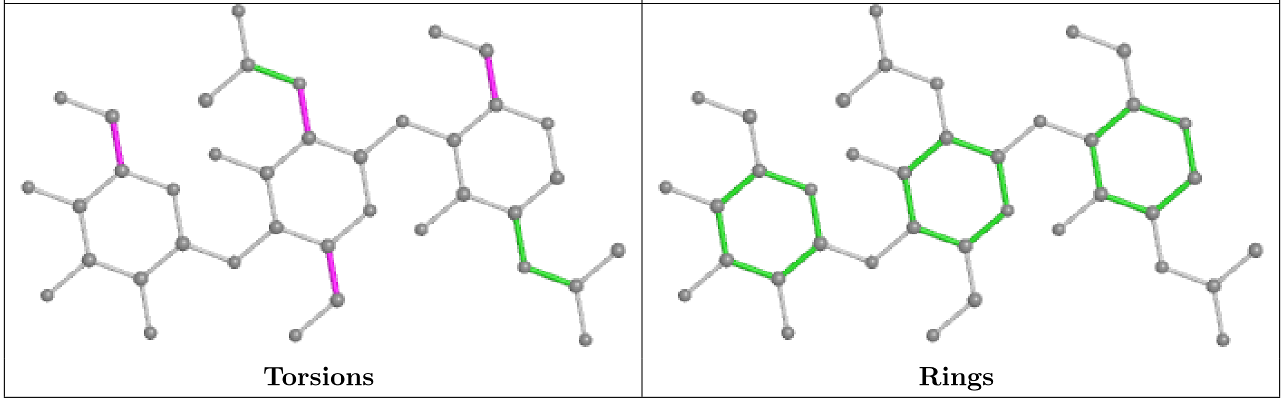


Torsions Rings

Oligosaccharide Chain r



Bond lengths Bond angles



Torsions Rings

5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	E	632	1	14,14,15	0.27	0	17,19,21	1.42	1 (5%)
8	NAG	I	613	1	14,14,15	0.79	1 (7%)	17,19,21	2.33	4 (23%)
8	NAG	E	613	1	14,14,15	0.79	1 (7%)	17,19,21	2.34	4 (23%)
8	NAG	J	701	2	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
8	NAG	F	701	2	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
8	NAG	I	632	1	14,14,15	0.27	0	17,19,21	1.42	1 (5%)
8	NAG	A	617	1	14,14,15	0.41	0	17,19,21	0.51	0
8	NAG	I	627	1	14,14,15	0.30	0	17,19,21	0.51	0
8	NAG	A	613	1	14,14,15	0.79	1 (7%)	17,19,21	2.33	4 (23%)
8	NAG	I	617	1	14,14,15	0.41	0	17,19,21	0.51	0
8	NAG	A	632	1	14,14,15	0.27	0	17,19,21	1.42	1 (5%)
8	NAG	E	617	1	14,14,15	0.41	0	17,19,21	0.51	0
8	NAG	B	701	2	14,14,15	0.25	0	17,19,21	0.67	1 (5%)
8	NAG	A	627	1	14,14,15	0.31	0	17,19,21	0.52	0
8	NAG	E	627	1	14,14,15	0.31	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	E	632	1	-	0/6/23/26	0/1/1/1
8	NAG	I	613	1	-	5/6/23/26	0/1/1/1
8	NAG	E	613	1	-	5/6/23/26	0/1/1/1
8	NAG	J	701	2	-	2/6/23/26	0/1/1/1
8	NAG	F	701	2	-	2/6/23/26	0/1/1/1
8	NAG	I	632	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	617	1	-	1/6/23/26	0/1/1/1
8	NAG	I	627	1	-	2/6/23/26	0/1/1/1
8	NAG	A	613	1	-	5/6/23/26	0/1/1/1
8	NAG	I	617	1	-	1/6/23/26	0/1/1/1
8	NAG	A	632	1	-	0/6/23/26	0/1/1/1
8	NAG	E	617	1	-	1/6/23/26	0/1/1/1
8	NAG	B	701	2	-	2/6/23/26	0/1/1/1
8	NAG	A	627	1	-	2/6/23/26	0/1/1/1
8	NAG	E	627	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	613	NAG	C1-C2	2.50	1.56	1.52
8	A	613	NAG	C1-C2	2.48	1.56	1.52
8	I	613	NAG	C1-C2	2.46	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	613	NAG	C2-N2-C7	7.82	134.04	122.90
8	I	613	NAG	C2-N2-C7	7.80	134.00	122.90
8	A	613	NAG	C2-N2-C7	7.79	133.99	122.90
8	E	632	NAG	C1-O5-C5	5.51	119.66	112.19
8	I	632	NAG	C1-O5-C5	5.51	119.65	112.19
8	A	632	NAG	C1-O5-C5	5.49	119.63	112.19
8	E	613	NAG	C1-C2-N2	3.68	116.77	110.49
8	A	613	NAG	C1-C2-N2	3.67	116.76	110.49
8	I	613	NAG	C1-C2-N2	3.66	116.74	110.49
8	E	613	NAG	C1-O5-C5	3.09	116.38	112.19
8	I	613	NAG	C1-O5-C5	3.09	116.38	112.19
8	A	613	NAG	C1-O5-C5	3.08	116.37	112.19
8	F	701	NAG	C1-O5-C5	2.33	115.34	112.19
8	B	701	NAG	C1-O5-C5	2.31	115.32	112.19
8	J	701	NAG	C1-O5-C5	2.30	115.31	112.19
8	A	613	NAG	C8-C7-N2	2.06	119.59	116.10
8	E	613	NAG	C8-C7-N2	2.04	119.56	116.10
8	I	613	NAG	C8-C7-N2	2.04	119.56	116.10

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	701	NAG	O5-C5-C6-O6
8	F	701	NAG	O5-C5-C6-O6
8	J	701	NAG	O5-C5-C6-O6
8	A	627	NAG	O5-C5-C6-O6
8	E	627	NAG	O5-C5-C6-O6
8	I	627	NAG	O5-C5-C6-O6
8	B	701	NAG	C4-C5-C6-O6
8	F	701	NAG	C4-C5-C6-O6
8	J	701	NAG	C4-C5-C6-O6
8	A	627	NAG	C4-C5-C6-O6
8	E	627	NAG	C4-C5-C6-O6
8	I	627	NAG	C4-C5-C6-O6
8	A	613	NAG	C8-C7-N2-C2
8	A	613	NAG	O7-C7-N2-C2
8	E	613	NAG	C8-C7-N2-C2
8	E	613	NAG	O7-C7-N2-C2
8	I	613	NAG	C8-C7-N2-C2
8	I	613	NAG	O7-C7-N2-C2
8	A	613	NAG	O5-C5-C6-O6
8	E	613	NAG	O5-C5-C6-O6
8	I	613	NAG	O5-C5-C6-O6
8	I	613	NAG	C4-C5-C6-O6
8	A	613	NAG	C4-C5-C6-O6
8	E	613	NAG	C4-C5-C6-O6
8	A	617	NAG	O5-C5-C6-O6
8	E	617	NAG	O5-C5-C6-O6
8	I	617	NAG	O5-C5-C6-O6
8	A	613	NAG	C3-C2-N2-C7
8	E	613	NAG	C3-C2-N2-C7
8	I	613	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

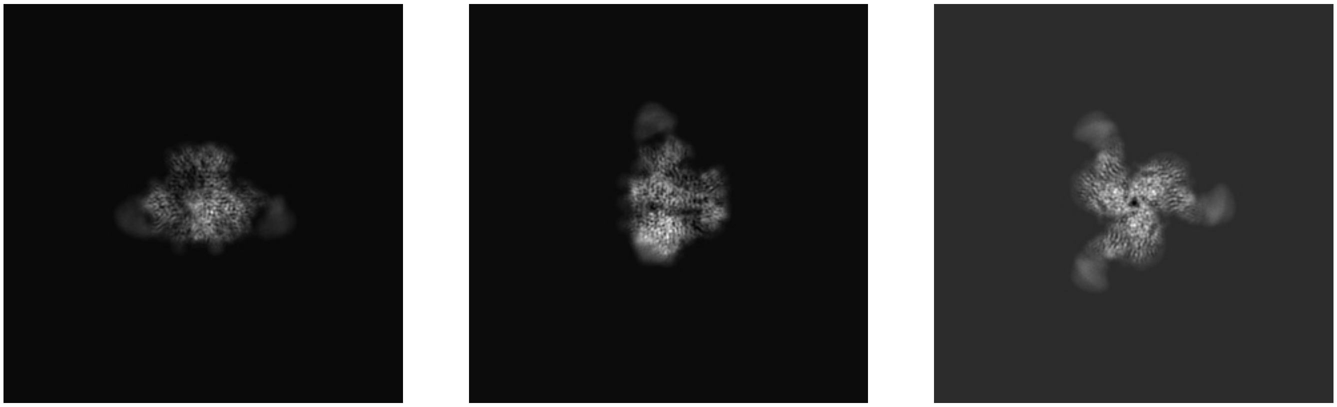
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21111. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

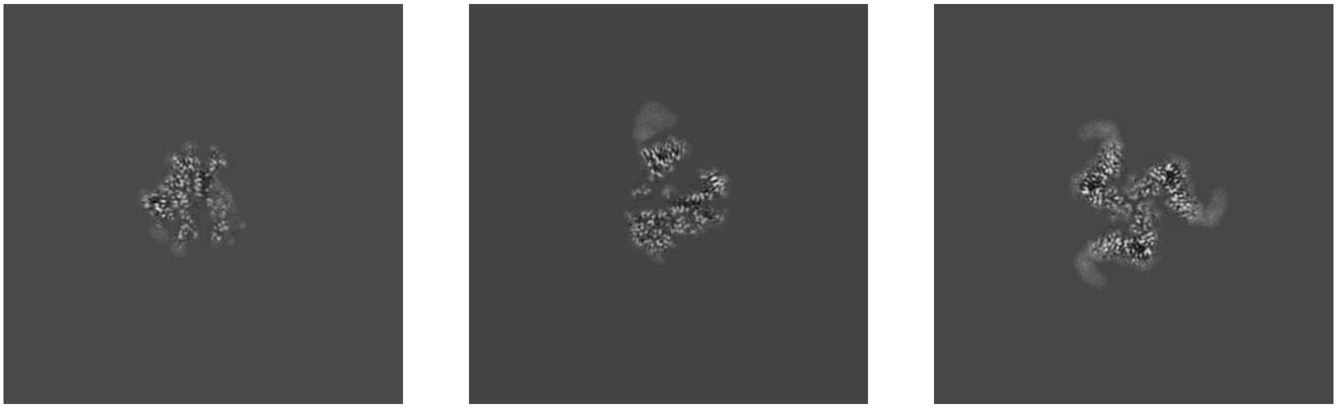


X Y Z

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

6.2 Central slices

6.2.1 Primary map

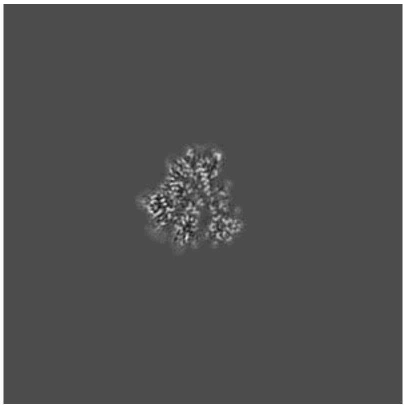


X Index: 192 Y Index: 192 Z Index: 192

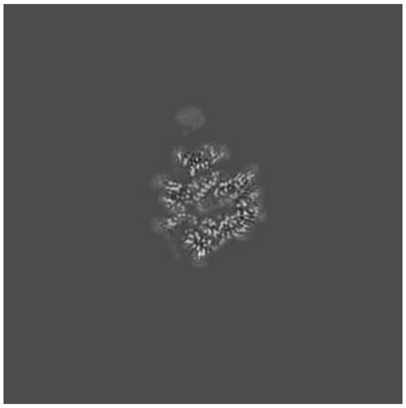
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

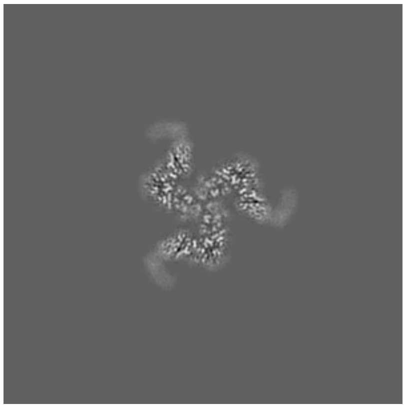
6.3.1 Primary map



X Index: 198



Y Index: 203

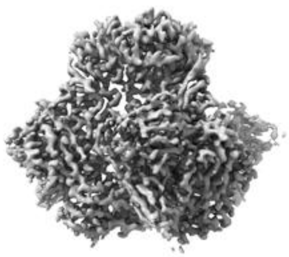


Z Index: 191

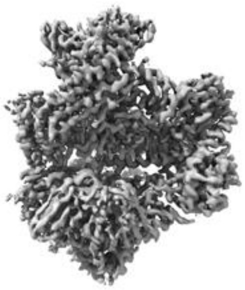
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

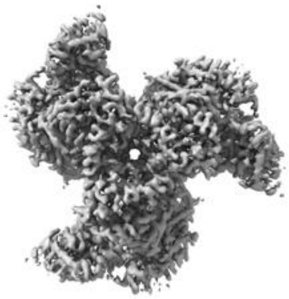
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

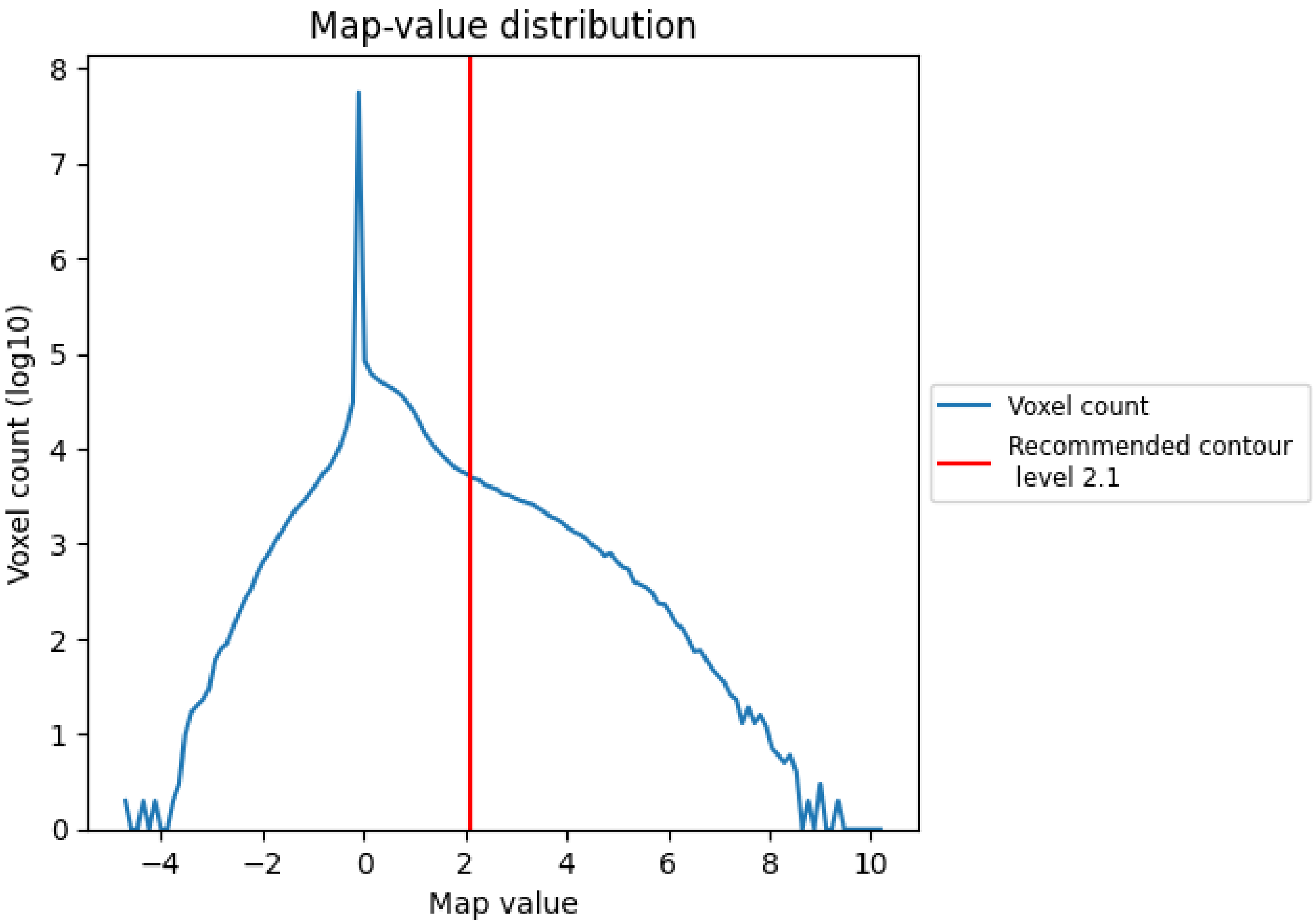
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

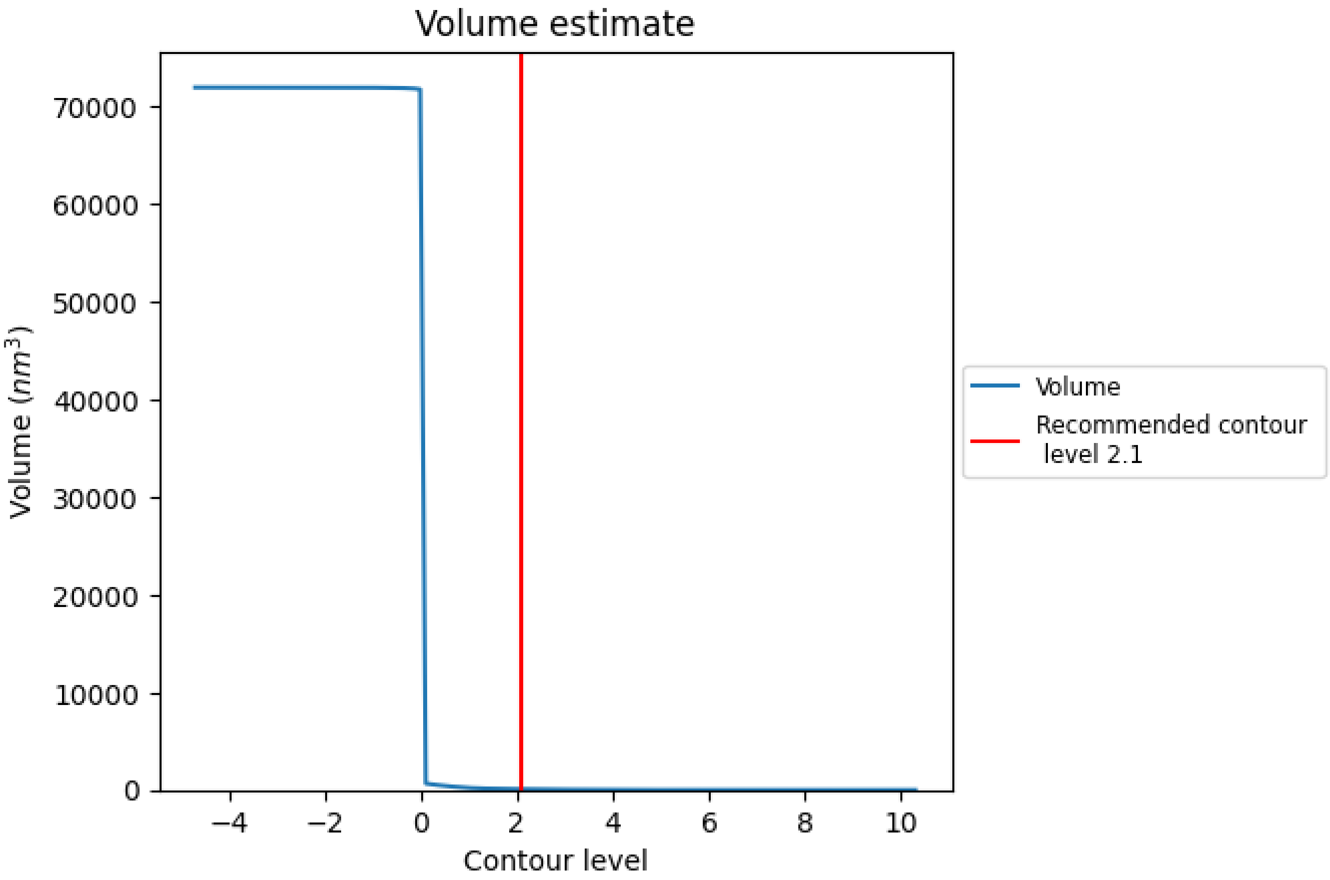
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

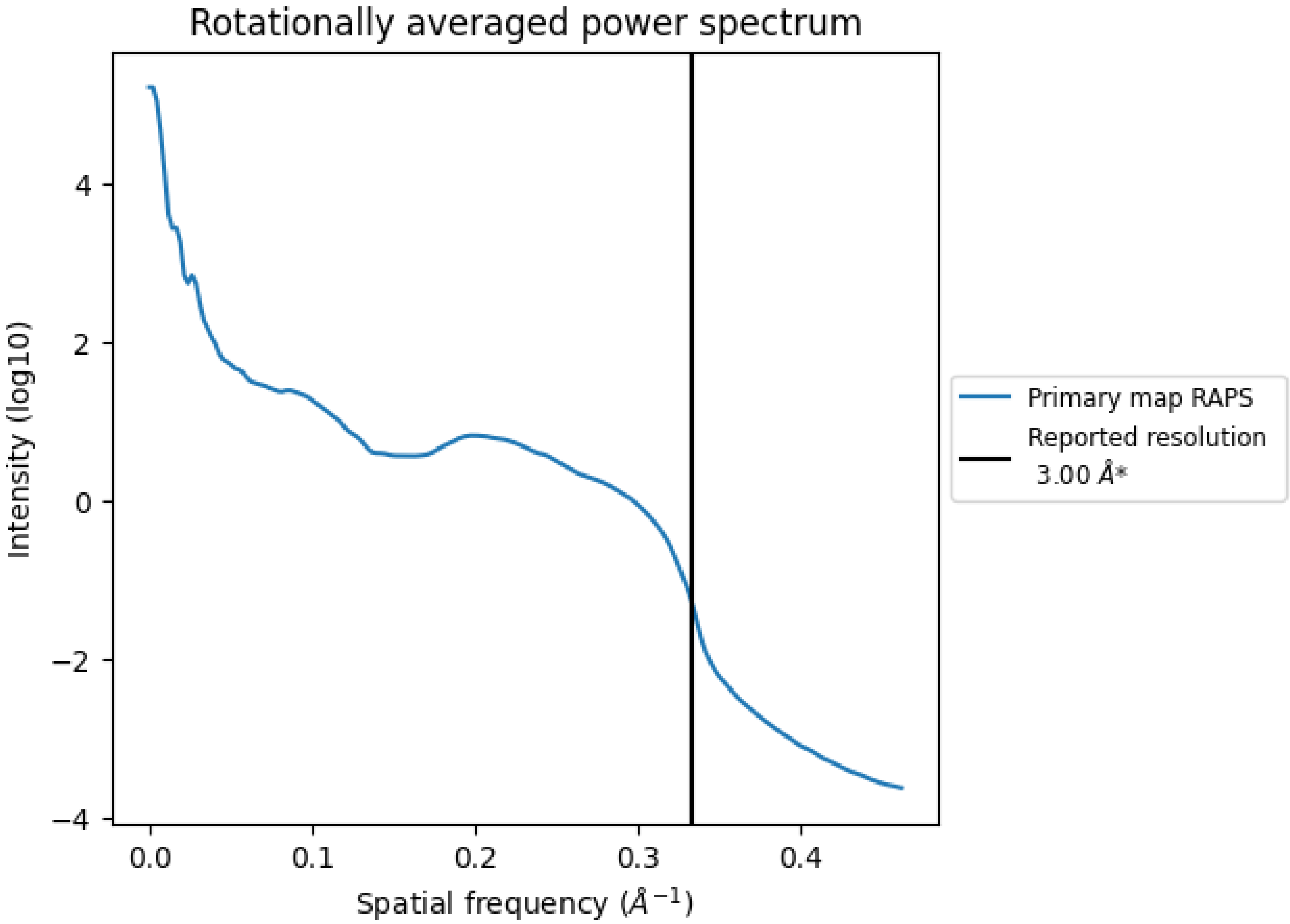
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 82 nm^3; this corresponds to an approximate mass of 75 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 0.333 $Å^{-1}$

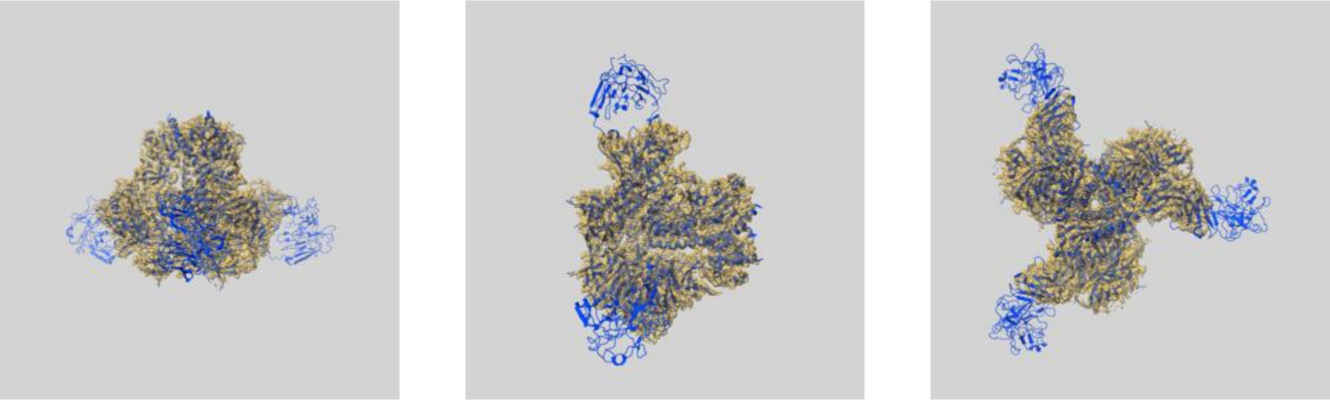
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21111 and PDB model 6V8X. Per-residue inclusion information can be found in section 3 on page 11.

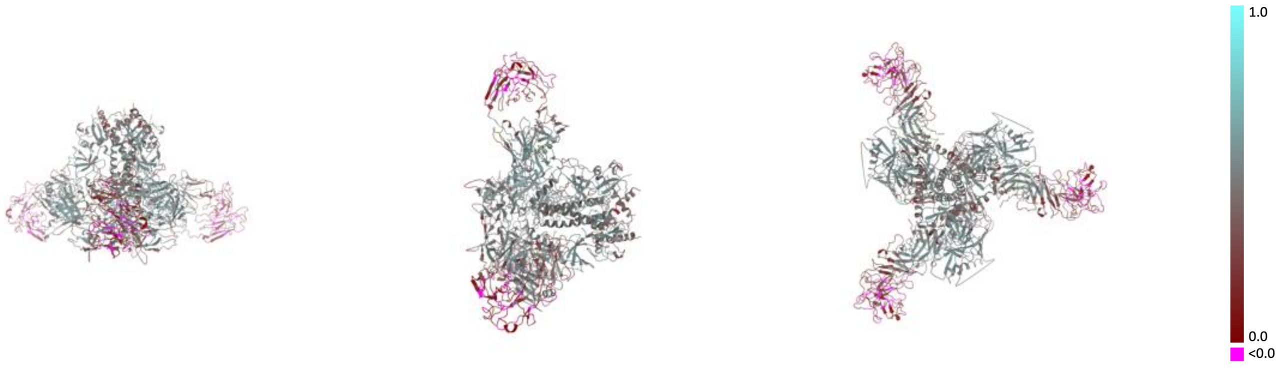
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.1 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.

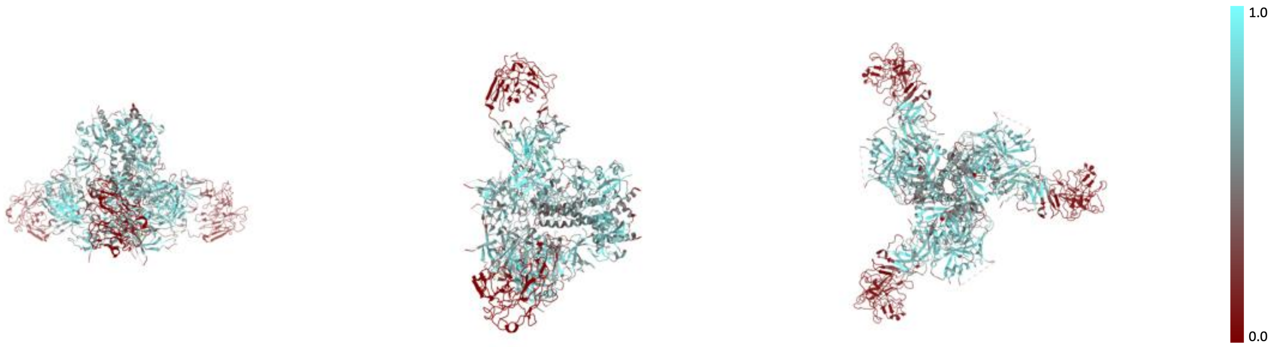
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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.

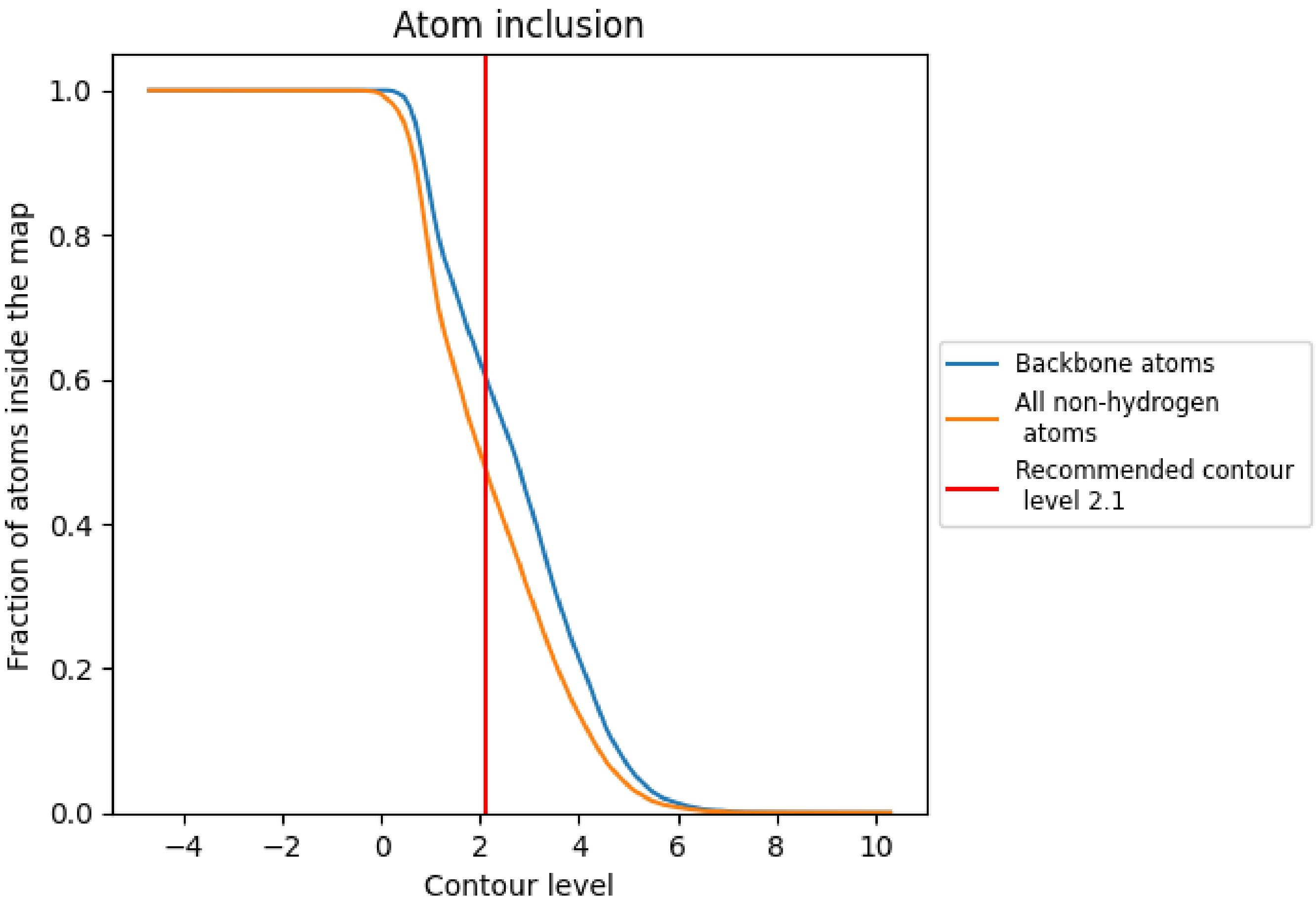
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 (2.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 61% of all backbone atoms, 48% 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 (2.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4770	0.4010
A	0.6364	0.4880
B	0.6143	0.4600
C	0.3584	0.3260
D	0.2359	0.2680
E	0.6312	0.4860
F	0.6114	0.4590
G	0.3554	0.3240
H	0.2372	0.2660
I	0.6335	0.4850
J	0.6114	0.4600
K	0.3548	0.3250
L	0.2347	0.2700
M	0.3200	0.4270
N	0.0000	0.2170
O	0.2821	0.3500
P	0.3590	0.4210
Q	0.5641	0.4900
R	0.2143	0.3580
S	0.1071	0.3280
T	0.2051	0.2980
U	0.1429	0.4270
V	0.0714	0.3520
W	0.3214	0.3180
X	0.0357	0.3260
Y	0.3400	0.4340
Z	0.0000	0.2100
a	0.2821	0.3440
b	0.3590	0.4060
c	0.5641	0.4780
d	0.2143	0.3770
e	0.0714	0.3070
f	0.2051	0.2820
g	0.1429	0.4120
h	0.0714	0.3340

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Chain	Atom inclusion	Q-score
i	0.3214	0.3060
j	0.0357	0.3500
k	0.3400	0.4400
l	0.0357	0.1850
m	0.2821	0.3690
n	0.3590	0.4220
o	0.5897	0.4980
p	0.2143	0.4130
q	0.0714	0.3090
r	0.2051	0.2830
s	0.1071	0.4120
t	0.1071	0.3650
u	0.2857	0.3080
v	0.0357	0.3220