Full wwPDB EM Validation Report (i)

Nov 9, 2022 – 07:04 AM EST

PDB ID	:	6OT1
EMDB ID	:	EMD-20191
Title	:	Cryo-EM structure of vaccine-elicited antibody 0PV-b.01 in complex with HIV-1 Env BG505 DS-SOSIP and antibodies VRC03 and PGT122
Authors	:	Gorman, J.; Kwong, P.D.
Deposited on	:	2019-05-02
Resolution	:	3.50 Å(reported)
Based on initial model	:	6CDI

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

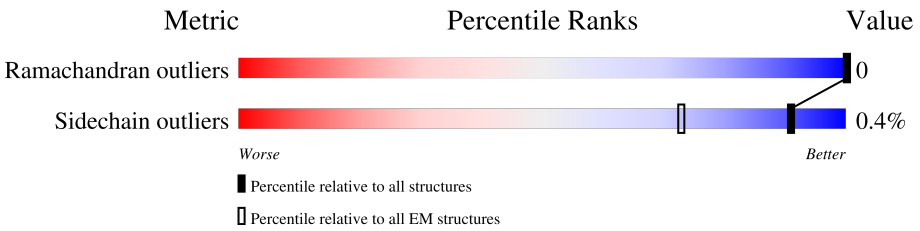
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	B	153	86% 14%
1	D	153	86% 14%
1	O	153	86% 14%
2	E	480	94% • 6%
2	G	480	94% • 6%
2	P	480	94% • 6%
3	A	230	13% 54% 46%
3	H	230	13% 54% 46%
3	M	230	13% 54% 46%

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Mol	Chain	Length	Quality of chain
4	C	219	19% 51% 49%
4	L	219	19% 51% 49%
4	N	219	20% 51% 49%
5	F	235	56% 44%
5	Q	235	56% 44%
5	m	235	56% 44%
6	I	213	49% 51%
6	R	213	49% 51%
6	n	213	49% 51%
7	J	233	53% 45%
7	S	233	53% 45%
7	q	233	53% 45%
8	K	209	49% 51%
8	T	209	49% 51%
8	r	209	49% 51%
9	0	2	50% 50%
9	2	2	100%
9	5	2	50% 50%
9	6	2	50% 50%
9	7	2	50% 50%
9	9	2	100%
9	AA	2	100%
9	FA	2	50% 50%
9	U	2	50% 50%
9	X	2	50% 50%

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Mol	Chain	Length	Quality of chain
9	Y	2	50% 50%
9	Z	2	50% 50%
9	b	2	100%
9	c	2	100%
9	h	2	50% 50%
9	j	2	50% 50%
9	o	2	50% 50%
9	p	2	50% 50%
9	s	2	50% 50%
9	u	2	100%
9	v	2	100%
10	1	5	40% 60%
10	3	5	100%
10	DA	5	40% 60%
10	GA	5	40% 60%
10	V	5	100%
10	f	5	40% 60%
10	i	5	40% 60%
10	k	5	100%
10	y	5	40% 60%
11	4	3	33% 67%
11	CA	3	67% 33%
11	EA	3	67% 33%
11	W	3	33% 67%
11	e	3	67% 33%

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Mol	Chain	Length	Quality of chain
11	g	3	67% 33%
11	l	3	33% 67%
11	x	3	100%
11	z	3	67% 33%
12	8	4	25% 75%
12	a	4	25% 75%
12	t	4	25% 75%
13	BA	6	33% 67%
13	d	6	33% 67%
13	w	6	33% 67%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 32247 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 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	132	1034	654	178	196	6	0	0
1	O	132	1034	654	178	196	6	0	0
1	D	132	1034	654	178	196	6	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
O	559	PRO	ILE	engineered mutation	UNP Q2N0S6
O	605	CYS	THR	engineered mutation	UNP Q2N0S6
D	559	PRO	ILE	engineered mutation	UNP Q2N0S6
D	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called BG505 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	453	3564	2233	630	671	30	0	0
2	E	453	3564	2233	630	671	30	0	0
2	P	453	3564	2233	630	671	30	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	201	CYS	ILE	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	433	CYS	ALA	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	506	GLY	VAL	conflict	UNP Q2N0S6
G	507	ARG	GLY	conflict	UNP Q2N0S6
G	509	ARG	GLU	conflict	UNP Q2N0S6
G	510	ARG	LYS	conflict	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
E	201	CYS	ILE	conflict	UNP Q2N0S6
E	332	ASN	THR	conflict	UNP Q2N0S6
E	433	CYS	ALA	conflict	UNP Q2N0S6
E	501	CYS	ALA	conflict	UNP Q2N0S6
E	506	GLY	VAL	conflict	UNP Q2N0S6
E	507	ARG	GLY	conflict	UNP Q2N0S6
E	509	ARG	GLU	conflict	UNP Q2N0S6
E	510	ARG	LYS	conflict	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
P	201	CYS	ILE	conflict	UNP Q2N0S6
P	332	ASN	THR	conflict	UNP Q2N0S6
P	433	CYS	ALA	conflict	UNP Q2N0S6
P	501	CYS	ALA	conflict	UNP Q2N0S6
P	506	GLY	VAL	conflict	UNP Q2N0S6
P	507	ARG	GLY	conflict	UNP Q2N0S6
P	509	ARG	GLU	conflict	UNP Q2N0S6
P	510	ARG	LYS	conflict	UNP Q2N0S6
P	512	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called 0PV-b.01 heavy.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	125	945	597	160	186	2	0	0
			Total	C	N	O	S		
3	A	125	945	597	160	186	2	0	0
			Total	C	N	O	S		
3	M	125	945	597	160	186	2	0	0

- Molecule 4 is a protein called 0PV-b.01 light.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	112	855	538	144	170	3	0	0
			Total	C	N	O	S		
4	C	112	855	538	144	170	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	112	855	538	144	170	3	0	0

- Molecule 5 is a protein called PGT122 heavy.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	m	132	1047	669	180	195	3	0	0
5	F	132	1047	669	180	195	3	0	0
5	Q	132	1047	669	180	195	3	0	0

- Molecule 6 is a protein called PGT122 light.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	n	105	805	504	139	160	2	0	0
6	I	105	805	504	139	160	2	0	0
6	R	105	805	504	139	160	2	0	0

- Molecule 7 is a protein called VRC03 heavy.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	q	128	1023	657	175	185	6	0	0
7	J	128	1023	657	175	185	6	0	0
7	S	128	1023	657	175	185	6	0	0

- Molecule 8 is a protein called VRC03 light.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	r	102	802	510	137	152	3	0	0
8	K	102	802	510	137	152	3	0	0
8	T	102	802	510	137	152	3	0	0

- Molecule 9 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
			Total	C	N	O		
9	U	2	28	16	2	10	0	0
9	X	2	28	16	2	10	0	0
9	Y	2	28	16	2	10	0	0
9	Z	2	28	16	2	10	0	0
9	b	2	28	16	2	10	0	0
9	c	2	28	16	2	10	0	0
9	h	2	28	16	2	10	0	0
9	j	2	28	16	2	10	0	0
9	o	2	28	16	2	10	0	0
9	p	2	28	16	2	10	0	0
9	s	2	28	16	2	10	0	0
9	u	2	28	16	2	10	0	0
9	v	2	28	16	2	10	0	0
9	0	2	28	16	2	10	0	0
9	2	2	28	16	2	10	0	0
9	5	2	28	16	2	10	0	0
9	6	2	28	16	2	10	0	0
9	7	2	28	16	2	10	0	0

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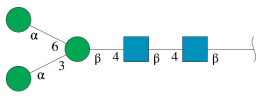
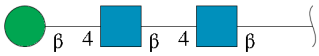
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	9	2	28	16	2	10	0	0
9	AA	2	28	16	2	10	0	0
9	FA	2	28	16	2	10	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
			Total	C	N	O		
10	V	5	61	34	2	25	0	0
10	f	5	61	34	2	25	0	0
10	i	5	61	34	2	25	0	0
10	k	5	61	34	2	25	0	0
10	y	5	61	34	2	25	0	0
10	1	5	61	34	2	25	0	0
10	3	5	61	34	2	25	0	0
10	DA	5	61	34	2	25	0	0
10	GA	5	61	34	2	25	0	0

- Molecule 11 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.

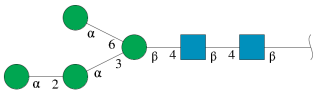


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	W	3	39	22	2	15	0	0
11	e	3	39	22	2	15	0	0
11	g	3	39	22	2	15	0	0
11	l	3	39	22	2	15	0	0
11	x	3	39	22	2	15	0	0
11	z	3	39	22	2	15	0	0
11	4	3	39	22	2	15	0	0
11	CA	3	39	22	2	15	0	0
11	EA	3	39	22	2	15	0	0

- Molecule 12 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.

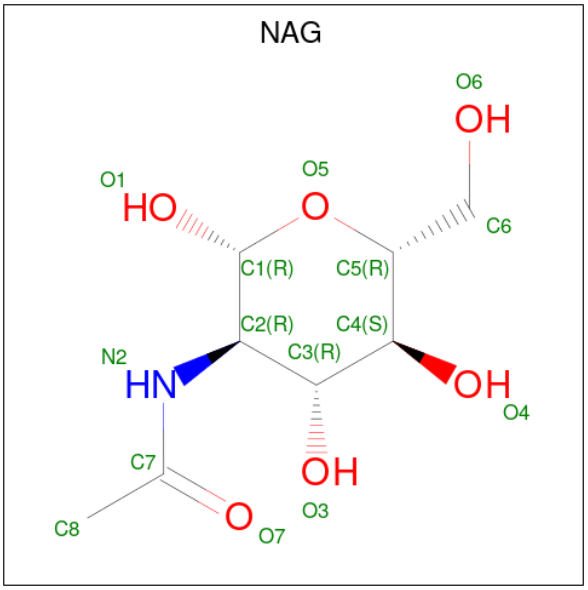
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	a	4	50	28	2	20	0	0
12	t	4	50	28	2	20	0	0
12	8	4	50	28	2	20	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
			Total	C	N	O		
13	d	6	72	40	2	30	0	0
			Total	C	N	O		
13	w	6	72	40	2	30	0	0
			Total	C	N	O		
13	BA	6	72	40	2	30	0	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
14	B	1	14	8	1	5	0
			Total	C	N	O	
14	G	1	42	24	3	15	0
			Total	C	N	O	
14	G	1	42	24	3	15	0
			Total	C	N	O	
14	G	1	42	24	3	15	0
			Total	C	N	O	
14	O	1	14	8	1	5	0
			Total	C	N	O	
14	E	1	42	24	3	15	0
			Total	C	N	O	
14	E	1	42	24	3	15	0
			Total	C	N	O	
14	E	1	42	24	3	15	0

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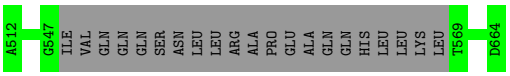
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
14	D	1	14	8	1	5	0
			Total	C	N	O	
14	P	1	42	24	3	15	0
			Total	C	N	O	
14	P	1	42	24	3	15	0
			Total	C	N	O	
14	P	1	42	24	3	15	0

3 Residue-property plots (i)

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

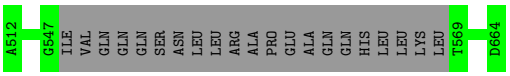
- Molecule 1: Envelope glycoprotein gp41

Chain B:



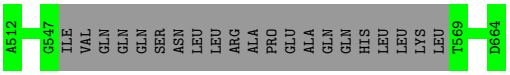
- Molecule 1: Envelope glycoprotein gp41

Chain O:



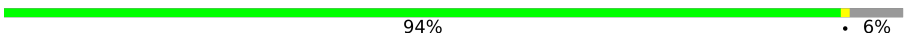
- Molecule 1: Envelope glycoprotein gp41

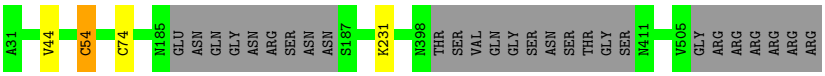
Chain D:



- Molecule 2: BG505 gp120

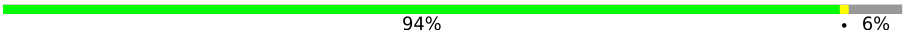
Chain G:

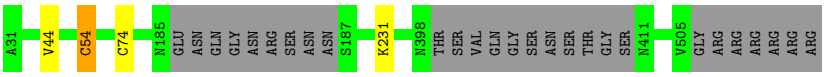




- Molecule 2: BG505 gp120

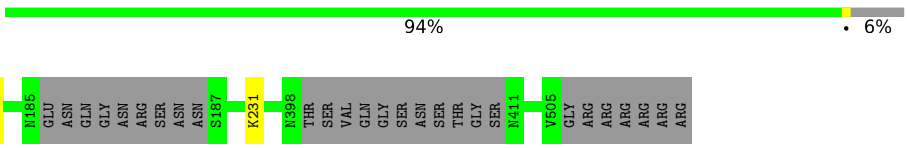
Chain E:





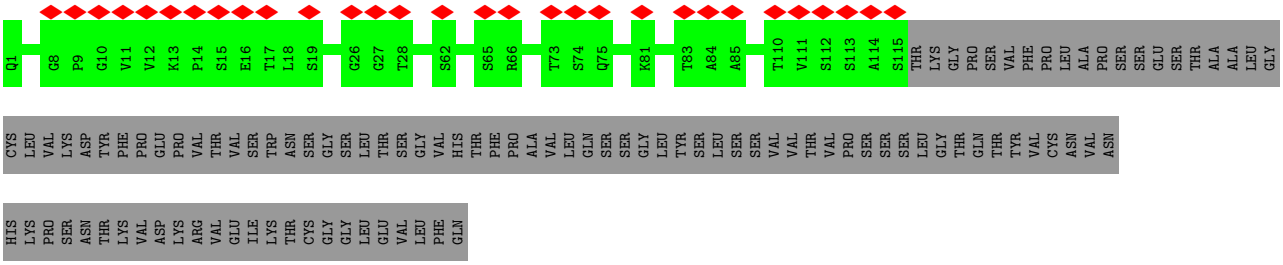
- Molecule 2: BG505 gp120

Chain P:



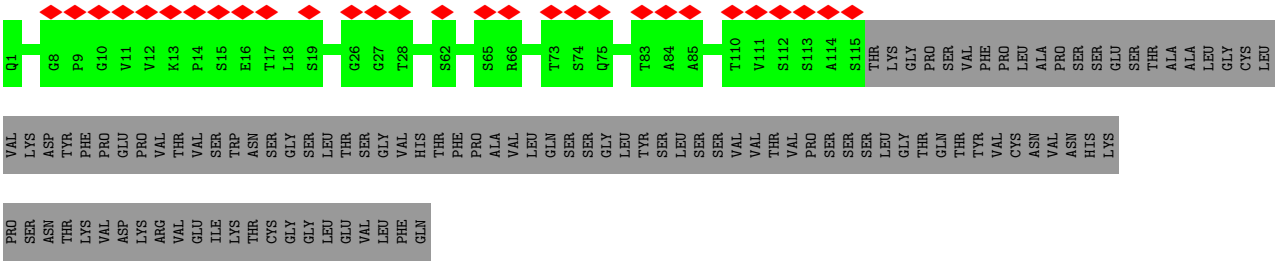
• Molecule 3: 0PV-b.01 heavy

Chain H:



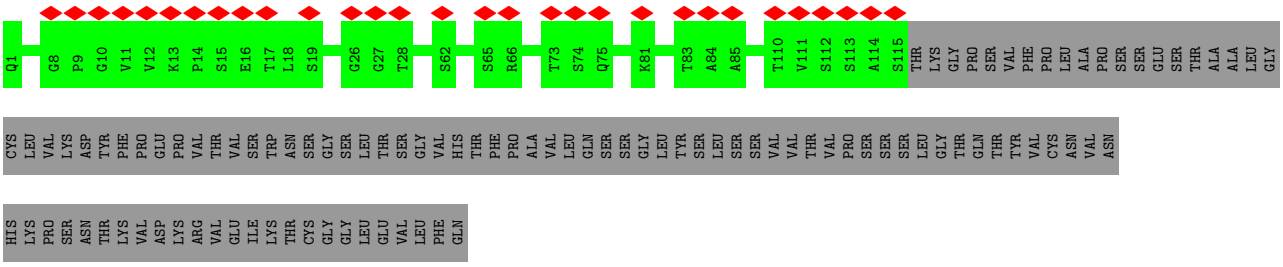
• Molecule 3: 0PV-b.01 heavy

Chain A:



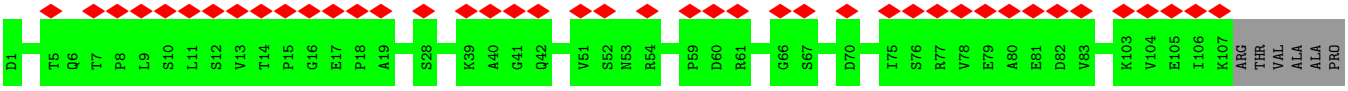
• Molecule 3: 0PV-b.01 heavy

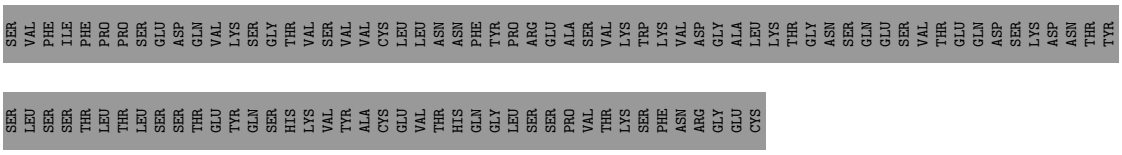
Chain M:



• Molecule 4: 0PV-b.01 light

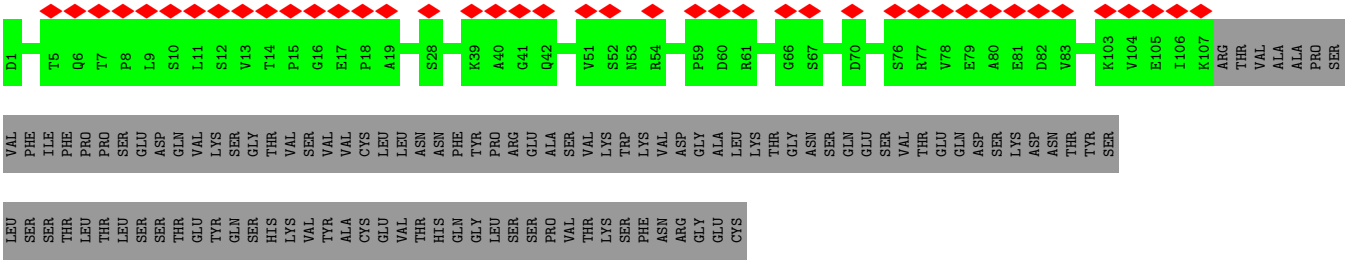
Chain L:





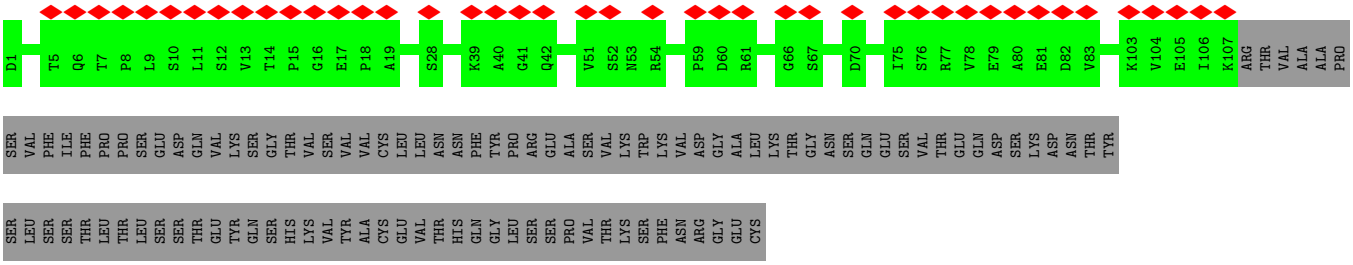
- Molecule 4: 0PV-b.01 light

Chain C:



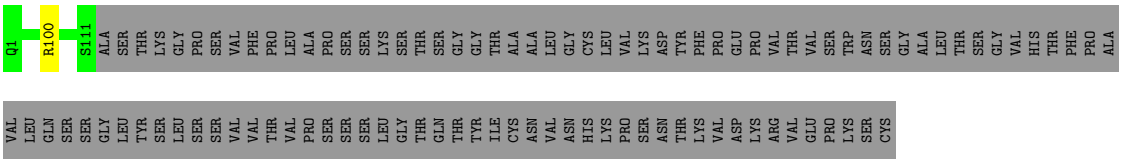
- Molecule 4: 0PV-b.01 light

Chain N:



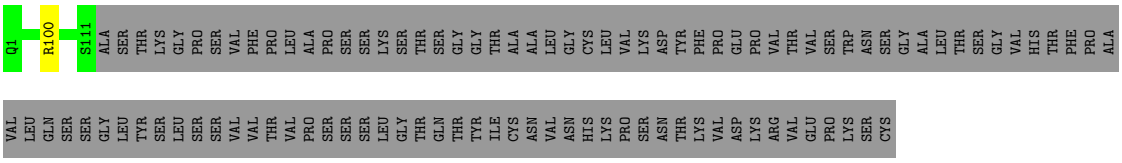
- Molecule 5: PGT122 heavy

Chain m:



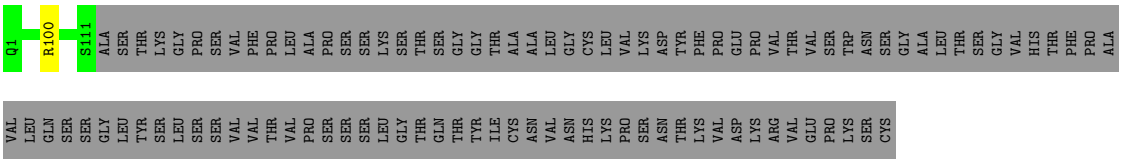
- Molecule 5: PGT122 heavy

Chain F:



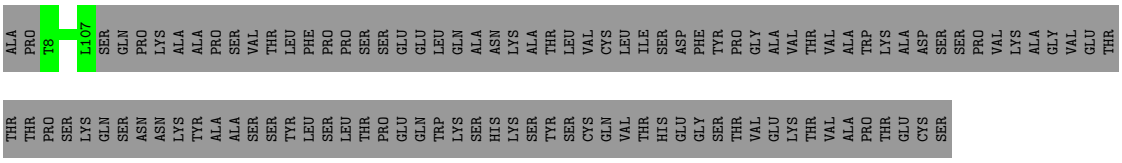
- Molecule 5: PGT122 heavy

Chain Q: 56% 44%



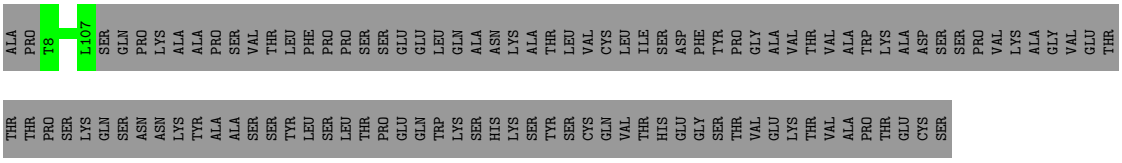
- Molecule 6: PGT122 light

Chain n: 49% 51%



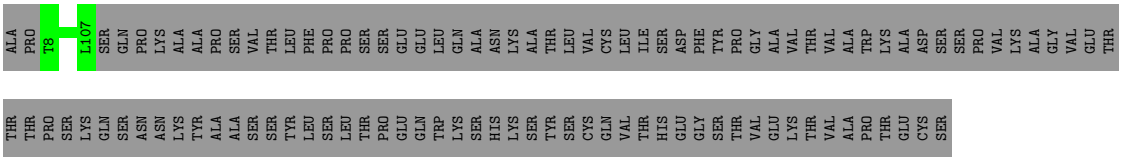
- Molecule 6: PGT122 light

Chain I: 49% 51%



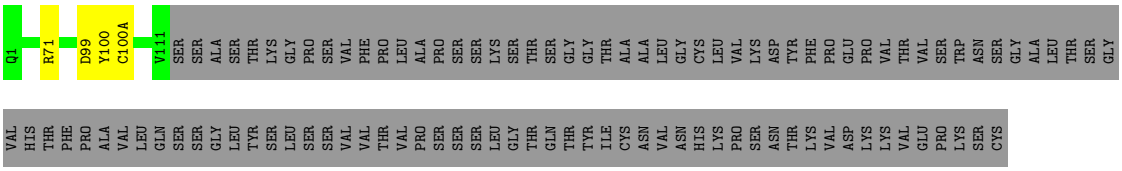
- Molecule 6: PGT122 light

Chain R: 49% 51%



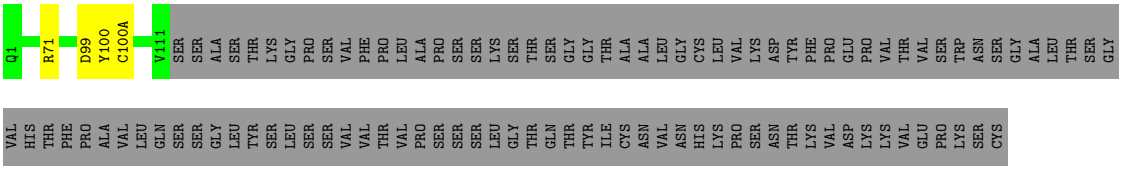
- Molecule 7: VRC03 heavy

Chain q: 53% • 45%



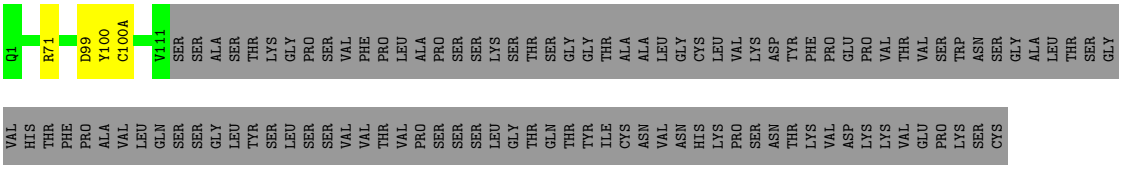
- Molecule 7: VRC03 heavy

Chain J: 53% • 45%



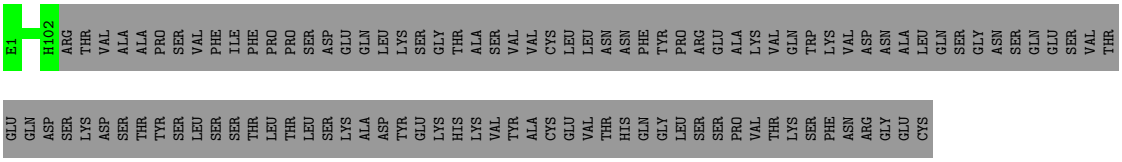
• Molecule 7: VRC03 heavy

Chain S:



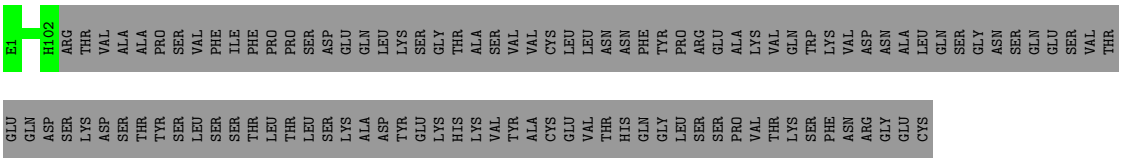
• Molecule 8: VRC03 light

Chain r:



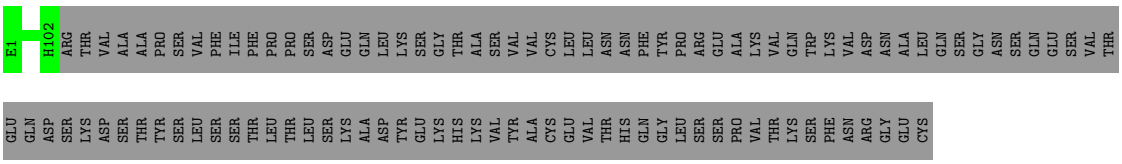
• Molecule 8: VRC03 light

Chain K:



• Molecule 8: VRC03 light

Chain T:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

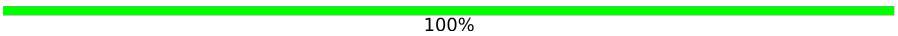
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

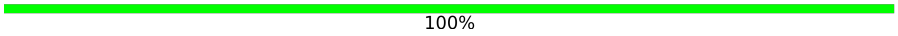
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 50% 50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 50% 50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p: 50% 50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s: 50% 50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u: 100%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v: 100%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0: 50% 50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2: 100%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5: 50% 50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6: 50% 50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7: 50% 50%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9: 100%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA: 100%

NAG1 NAG2

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA: 50% 50%

NAG1 NAG2

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 100%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 40% 60%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 40% 60%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 100%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y: 40% 60%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1: 40% 60%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3: 100%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA: 40% 60%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA: 40% 60%

NAG1 NAG2 BMA3 MAN4 MAN5

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 33% 67%

NAG1 NAG2 BMA3

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 67% 33%

NAG1 NAG2 BMA3

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 67% 33%

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 33% 67%

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x: 100%

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z: 67% 33%

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4: 33% 67%

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA: 67% 33%

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA: 67% 33%

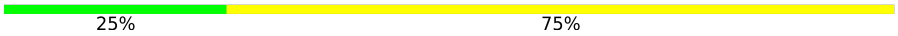
• Molecule 12: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

• Molecule 12: 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 t:

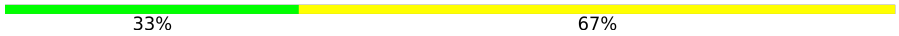
• Molecule 12: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8: 

• Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

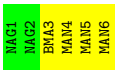
Chain d:

• Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w: 

• Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:


NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	57864	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 ($e^-/Å^2$)	73.46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.746	Depositor
Minimum map value	-1.714	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	377.78403, 377.78403, 377.78403	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07325, 1.07325, 1.07325	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	B	0.34	0/1052	0.54	0/1427
1	D	0.34	0/1052	0.54	0/1427
1	O	0.34	0/1052	0.54	0/1427
2	E	0.42	0/3638	0.59	1/4939 (0.0%)
2	G	0.43	0/3638	0.59	1/4939 (0.0%)
2	P	0.43	0/3638	0.59	1/4939 (0.0%)
3	A	0.26	0/966	0.52	0/1320
3	H	0.26	0/966	0.52	0/1320
3	M	0.26	0/966	0.52	0/1320
4	C	0.27	0/874	0.54	0/1187
4	L	0.27	0/874	0.54	0/1187
4	N	0.27	0/874	0.54	0/1187
5	F	0.32	0/1076	0.51	0/1465
5	Q	0.32	0/1076	0.51	0/1465
5	m	0.32	0/1076	0.51	0/1465
6	I	0.35	0/826	0.51	0/1130
6	R	0.35	0/826	0.51	0/1130
6	n	0.35	0/826	0.52	0/1130
7	J	0.46	0/1056	0.58	1/1439 (0.1%)
7	S	0.46	0/1056	0.58	1/1439 (0.1%)
7	q	0.46	0/1056	0.58	1/1439 (0.1%)
8	K	0.36	0/820	0.52	0/1107
8	T	0.36	0/820	0.52	0/1107
8	r	0.36	0/820	0.52	0/1107
All	All	0.38	0/30924	0.55	6/42042 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	2
2	G	0	2
2	P	0	2
7	J	0	1
7	S	0	1
7	q	0	1
All	All	0	9

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	q	99	ASP	CB-CG-OD1	6.63	124.27	118.30
7	J	99	ASP	CB-CG-OD1	6.50	124.15	118.30
7	S	99	ASP	CB-CG-OD1	6.47	124.12	118.30
2	E	54	CYS	CA-CB-SG	5.39	123.70	114.00
2	G	54	CYS	CA-CB-SG	5.33	123.60	114.00
2	P	54	CYS	CA-CB-SG	5.33	123.60	114.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	54	CYS	Peptide
2	E	74	CYS	Peptide
2	G	54	CYS	Peptide
2	G	74	CYS	Peptide
7	J	100	TYR	Peptide
2	P	54	CYS	Peptide
2	P	74	CYS	Peptide
7	S	100	TYR	Peptide
7	q	100	TYR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	128/153 (84%)	115 (90%)	13 (10%)	0	100	100
1	D	128/153 (84%)	116 (91%)	12 (9%)	0	100	100
1	O	128/153 (84%)	115 (90%)	13 (10%)	0	100	100
2	E	447/480 (93%)	397 (89%)	50 (11%)	0	100	100
2	G	447/480 (93%)	397 (89%)	50 (11%)	0	100	100
2	P	447/480 (93%)	396 (89%)	51 (11%)	0	100	100
3	A	123/230 (54%)	123 (100%)	0	0	100	100
3	H	123/230 (54%)	123 (100%)	0	0	100	100
3	M	123/230 (54%)	123 (100%)	0	0	100	100
4	C	110/219 (50%)	104 (94%)	6 (6%)	0	100	100
4	L	110/219 (50%)	104 (94%)	6 (6%)	0	100	100
4	N	110/219 (50%)	104 (94%)	6 (6%)	0	100	100
5	F	130/235 (55%)	117 (90%)	13 (10%)	0	100	100
5	Q	130/235 (55%)	117 (90%)	13 (10%)	0	100	100
5	m	130/235 (55%)	117 (90%)	13 (10%)	0	100	100
6	I	103/213 (48%)	94 (91%)	9 (9%)	0	100	100
6	R	103/213 (48%)	94 (91%)	9 (9%)	0	100	100
6	n	103/213 (48%)	94 (91%)	9 (9%)	0	100	100
7	J	126/233 (54%)	111 (88%)	15 (12%)	0	100	100
7	S	126/233 (54%)	112 (89%)	14 (11%)	0	100	100
7	q	126/233 (54%)	111 (88%)	15 (12%)	0	100	100
8	K	100/209 (48%)	93 (93%)	7 (7%)	0	100	100
8	T	100/209 (48%)	93 (93%)	7 (7%)	0	100	100
8	r	100/209 (48%)	93 (93%)	7 (7%)	0	100	100
All	All	3801/5916 (64%)	3463 (91%)	338 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	B	110/129 (85%)	110 (100%)	0	100	100
1	D	110/129 (85%)	110 (100%)	0	100	100
1	O	110/129 (85%)	110 (100%)	0	100	100
2	E	405/428 (95%)	403 (100%)	2 (0%)	88	94
2	G	405/428 (95%)	403 (100%)	2 (0%)	88	94
2	P	405/428 (95%)	403 (100%)	2 (0%)	88	94
3	A	105/198 (53%)	105 (100%)	0	100	100
3	H	105/198 (53%)	105 (100%)	0	100	100
3	M	105/198 (53%)	105 (100%)	0	100	100
4	C	97/194 (50%)	97 (100%)	0	100	100
4	L	97/194 (50%)	97 (100%)	0	100	100
4	N	97/194 (50%)	97 (100%)	0	100	100
5	F	116/205 (57%)	115 (99%)	1 (1%)	78	90
5	Q	116/205 (57%)	115 (99%)	1 (1%)	78	90
5	m	116/205 (57%)	115 (99%)	1 (1%)	78	90
6	I	88/181 (49%)	88 (100%)	0	100	100
6	R	88/181 (49%)	88 (100%)	0	100	100
6	n	88/181 (49%)	88 (100%)	0	100	100
7	J	108/199 (54%)	106 (98%)	2 (2%)	57	80
7	S	108/199 (54%)	106 (98%)	2 (2%)	57	80
7	q	108/199 (54%)	106 (98%)	2 (2%)	57	80
8	K	86/182 (47%)	86 (100%)	0	100	100
8	T	86/182 (47%)	86 (100%)	0	100	100
8	r	86/182 (47%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3345/5148 (65%)	3330 (100%)	15 (0%)	91 96

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	44	VAL
2	G	231	LYS
5	m	100	ARG
7	q	71	ARG
7	q	100(A)	CYS
2	E	44	VAL
2	E	231	LYS
5	F	100	ARG
7	J	71	ARG
7	J	100(A)	CYS
2	P	44	VAL
2	P	231	LYS
5	Q	100	ARG
7	S	71	ARG
7	S	100(A)	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	67	ASN
2	G	80	ASN
2	G	82	GLN
2	G	103	GLN
2	G	183	GLN
2	G	203	GLN
2	G	258	GLN
4	L	93	GLN
5	m	1	GLN
5	m	39	GLN
5	m	60	ASN
6	n	37	GLN
6	n	38	GLN
6	n	51	ASN
2	E	67	ASN
2	E	80	ASN
2	E	82	GLN

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Mol	Chain	Res	Type
2	E	103	GLN
2	E	183	GLN
2	E	203	GLN
2	E	258	GLN
4	C	93	GLN
5	F	1	GLN
5	F	39	GLN
5	F	60	ASN
6	I	37	GLN
6	I	38	GLN
6	I	51	ASN
2	P	67	ASN
2	P	80	ASN
2	P	82	GLN
2	P	103	GLN
2	P	183	GLN
2	P	203	GLN
2	P	258	GLN
4	N	93	GLN
5	Q	1	GLN
5	Q	39	GLN
5	Q	60	ASN
6	R	37	GLN
6	R	38	GLN
6	R	51	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

144 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	0	1	9,2	14,14,15	0.28	0	17,19,21	1.17	2 (11%)
9	NAG	0	2	9	14,14,15	0.30	0	17,19,21	0.51	0
10	NAG	1	1	2,10	14,14,15	0.49	0	17,19,21	0.58	0
10	NAG	1	2	10	14,14,15	0.20	0	17,19,21	0.99	1 (5%)
10	BMA	1	3	10	11,11,12	0.64	0	15,15,17	0.77	0
10	MAN	1	4	10	11,11,12	0.73	0	15,15,17	1.12	2 (13%)
10	MAN	1	5	10	11,11,12	0.79	0	15,15,17	1.04	2 (13%)
9	NAG	2	1	9,2	14,14,15	0.73	1 (7%)	17,19,21	1.29	2 (11%)
9	NAG	2	2	9	14,14,15	0.30	0	17,19,21	0.58	1 (5%)
10	NAG	3	1	2,10	14,14,15	0.61	0	17,19,21	2.31	3 (17%)
10	NAG	3	2	10	14,14,15	0.30	0	17,19,21	1.03	1 (5%)
10	BMA	3	3	10	11,11,12	0.59	0	15,15,17	0.97	1 (6%)
10	MAN	3	4	10	11,11,12	0.69	0	15,15,17	1.10	2 (13%)
10	MAN	3	5	10	11,11,12	0.81	1 (9%)	15,15,17	1.20	2 (13%)
11	NAG	4	1	11,2	14,14,15	0.64	1 (7%)	17,19,21	0.66	0
11	NAG	4	2	11	14,14,15	0.29	0	17,19,21	1.02	1 (5%)
11	BMA	4	3	11	11,11,12	0.69	0	15,15,17	0.85	0
9	NAG	5	1	9,2	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
9	NAG	5	2	9	14,14,15	0.30	0	17,19,21	0.51	0
9	NAG	6	1	9,2	14,14,15	0.41	0	17,19,21	0.94	1 (5%)
9	NAG	6	2	9	14,14,15	0.43	0	17,19,21	0.39	0
9	NAG	7	1	9,2	14,14,15	0.22	0	17,19,21	0.40	0
9	NAG	7	2	9	14,14,15	0.45	0	17,19,21	1.01	1 (5%)
12	NAG	8	1	12,2	14,14,15	0.37	0	17,19,21	0.59	0
12	NAG	8	2	12	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
12	BMA	8	3	12	11,11,12	0.64	0	15,15,17	1.02	1 (6%)
12	MAN	8	4	12	11,11,12	0.72	1 (9%)	15,15,17	1.27	2 (13%)
9	NAG	9	1	9,2	14,14,15	0.22	0	17,19,21	0.46	0
9	NAG	9	2	9	14,14,15	0.29	0	17,19,21	0.45	0
9	NAG	AA	1	9,2	14,14,15	0.46	0	17,19,21	0.59	0
9	NAG	AA	2	9	14,14,15	0.35	0	17,19,21	0.47	0
13	NAG	BA	1	2,13	14,14,15	0.37	0	17,19,21	0.58	0
13	NAG	BA	2	13	14,14,15	0.36	0	17,19,21	0.62	0
13	BMA	BA	3	13	11,11,12	1.04	1 (9%)	15,15,17	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	MAN	BA	4	13	11,11,12	0.61	0	15,15,17	1.46	2 (13%)
13	MAN	BA	5	13	11,11,12	0.73	0	15,15,17	1.29	2 (13%)
13	MAN	BA	6	13	11,11,12	0.78	0	15,15,17	1.05	2 (13%)
11	NAG	CA	1	11,2	14,14,15	0.26	0	17,19,21	0.43	0
11	NAG	CA	2	11	14,14,15	0.23	0	17,19,21	0.64	1 (5%)
11	BMA	CA	3	11	11,11,12	0.76	0	15,15,17	0.94	0
10	NAG	DA	1	2,10	14,14,15	0.46	0	17,19,21	0.64	0
10	NAG	DA	2	10	14,14,15	0.26	0	17,19,21	0.57	0
10	BMA	DA	3	10	11,11,12	0.64	0	15,15,17	0.91	1 (6%)
10	MAN	DA	4	10	11,11,12	0.74	0	15,15,17	1.16	2 (13%)
10	MAN	DA	5	10	11,11,12	0.80	0	15,15,17	1.17	2 (13%)
11	NAG	EA	1	11,2	14,14,15	0.37	0	17,19,21	0.50	0
11	NAG	EA	2	11	14,14,15	0.24	0	17,19,21	0.53	0
11	BMA	EA	3	11	11,11,12	0.93	1 (9%)	15,15,17	0.94	0
9	NAG	FA	1	9,2	14,14,15	0.26	0	17,19,21	1.16	2 (11%)
9	NAG	FA	2	9	14,14,15	0.29	0	17,19,21	0.51	0
10	NAG	GA	1	2,10	14,14,15	0.52	0	17,19,21	0.58	0
10	NAG	GA	2	10	14,14,15	0.19	0	17,19,21	0.98	1 (5%)
10	BMA	GA	3	10	11,11,12	0.63	0	15,15,17	0.78	0
10	MAN	GA	4	10	11,11,12	0.70	0	15,15,17	1.11	2 (13%)
10	MAN	GA	5	10	11,11,12	0.80	0	15,15,17	1.04	2 (13%)
9	NAG	U	1	9,2	14,14,15	0.75	1 (7%)	17,19,21	1.28	2 (11%)
9	NAG	U	2	9	14,14,15	0.32	0	17,19,21	0.57	0
10	NAG	V	1	2,10	14,14,15	0.60	0	17,19,21	2.31	3 (17%)
10	NAG	V	2	10	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
10	BMA	V	3	10	11,11,12	0.60	0	15,15,17	0.98	1 (6%)
10	MAN	V	4	10	11,11,12	0.69	0	15,15,17	1.11	2 (13%)
10	MAN	V	5	10	11,11,12	0.80	1 (9%)	15,15,17	1.21	2 (13%)
11	NAG	W	1	11,2	14,14,15	0.63	1 (7%)	17,19,21	0.67	0
11	NAG	W	2	11	14,14,15	0.31	0	17,19,21	1.02	1 (5%)
11	BMA	W	3	11	11,11,12	0.69	0	15,15,17	0.85	0
9	NAG	X	1	9,2	14,14,15	0.32	0	17,19,21	0.99	1 (5%)
9	NAG	X	2	9	14,14,15	0.31	0	17,19,21	0.52	0
9	NAG	Y	1	9,2	14,14,15	0.43	0	17,19,21	0.94	1 (5%)
9	NAG	Y	2	9	14,14,15	0.42	0	17,19,21	0.38	0
9	NAG	Z	1	9,2	14,14,15	0.23	0	17,19,21	0.41	0
9	NAG	Z	2	9	14,14,15	0.46	0	17,19,21	0.99	1 (5%)
12	NAG	a	1	12,2	14,14,15	0.37	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	NAG	a	2	12	14,14,15	0.28	0	17,19,21	1.02	1 (5%)
12	BMA	a	3	12	11,11,12	0.63	0	15,15,17	1.02	1 (6%)
12	MAN	a	4	12	11,11,12	0.74	1 (9%)	15,15,17	1.28	2 (13%)
9	NAG	b	1	9,2	14,14,15	0.22	0	17,19,21	0.46	0
9	NAG	b	2	9	14,14,15	0.29	0	17,19,21	0.45	0
9	NAG	c	1	9,2	14,14,15	0.46	0	17,19,21	0.59	0
9	NAG	c	2	9	14,14,15	0.35	0	17,19,21	0.46	0
13	NAG	d	1	2,13	14,14,15	0.35	0	17,19,21	0.59	0
13	NAG	d	2	13	14,14,15	0.35	0	17,19,21	0.63	0
13	BMA	d	3	13	11,11,12	1.03	1 (9%)	15,15,17	1.13	0
13	MAN	d	4	13	11,11,12	0.61	0	15,15,17	1.47	2 (13%)
13	MAN	d	5	13	11,11,12	0.72	0	15,15,17	1.29	2 (13%)
13	MAN	d	6	13	11,11,12	0.75	0	15,15,17	1.05	2 (13%)
11	NAG	e	1	11,2	14,14,15	0.25	0	17,19,21	0.43	0
11	NAG	e	2	11	14,14,15	0.21	0	17,19,21	0.64	1 (5%)
11	BMA	e	3	11	11,11,12	0.77	0	15,15,17	0.94	0
10	NAG	f	1	2,10	14,14,15	0.46	0	17,19,21	0.64	0
10	NAG	f	2	10	14,14,15	0.23	0	17,19,21	0.56	0
10	BMA	f	3	10	11,11,12	0.62	0	15,15,17	0.91	1 (6%)
10	MAN	f	4	10	11,11,12	0.73	0	15,15,17	1.16	2 (13%)
10	MAN	f	5	10	11,11,12	0.80	0	15,15,17	1.18	2 (13%)
11	NAG	g	1	11,2	14,14,15	0.37	0	17,19,21	0.49	0
11	NAG	g	2	11	14,14,15	0.23	0	17,19,21	0.55	0
11	BMA	g	3	11	11,11,12	0.93	1 (9%)	15,15,17	0.93	0
9	NAG	h	1	9,2	14,14,15	0.28	0	17,19,21	1.16	2 (11%)
9	NAG	h	2	9	14,14,15	0.28	0	17,19,21	0.51	0
10	NAG	i	1	2,10	14,14,15	0.53	0	17,19,21	0.59	0
10	NAG	i	2	10	14,14,15	0.22	0	17,19,21	1.00	1 (5%)
10	BMA	i	3	10	11,11,12	0.65	0	15,15,17	0.78	0
10	MAN	i	4	10	11,11,12	0.72	0	15,15,17	1.12	2 (13%)
10	MAN	i	5	10	11,11,12	0.78	0	15,15,17	1.05	2 (13%)
9	NAG	j	1	9,2	14,14,15	0.74	1 (7%)	17,19,21	1.30	2 (11%)
9	NAG	j	2	9	14,14,15	0.31	0	17,19,21	0.57	0
10	NAG	k	1	2,10	14,14,15	0.63	0	17,19,21	2.31	3 (17%)
10	NAG	k	2	10	14,14,15	0.30	0	17,19,21	1.02	1 (5%)
10	BMA	k	3	10	11,11,12	0.59	0	15,15,17	0.98	1 (6%)
10	MAN	k	4	10	11,11,12	0.69	0	15,15,17	1.10	2 (13%)
10	MAN	k	5	10	11,11,12	0.80	1 (9%)	15,15,17	1.21	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	l	1	11,2	14,14,15	0.64	1 (7%)	17,19,21	0.67	0
11	NAG	l	2	11	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
11	BMA	l	3	11	11,11,12	0.68	0	15,15,17	0.84	0
9	NAG	o	1	9,2	14,14,15	0.31	0	17,19,21	0.98	1 (5%)
9	NAG	o	2	9	14,14,15	0.32	0	17,19,21	0.53	0
9	NAG	p	1	9,2	14,14,15	0.42	0	17,19,21	0.94	1 (5%)
9	NAG	p	2	9	14,14,15	0.44	0	17,19,21	0.39	0
9	NAG	s	1	9,2	14,14,15	0.22	0	17,19,21	0.40	0
9	NAG	s	2	9	14,14,15	0.46	0	17,19,21	1.00	1 (5%)
12	NAG	t	1	12,2	14,14,15	0.38	0	17,19,21	0.61	0
12	NAG	t	2	12	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
12	BMA	t	3	12	11,11,12	0.63	0	15,15,17	1.01	1 (6%)
12	MAN	t	4	12	11,11,12	0.73	1 (9%)	15,15,17	1.29	2 (13%)
9	NAG	u	1	9,2	14,14,15	0.21	0	17,19,21	0.47	0
9	NAG	u	2	9	14,14,15	0.29	0	17,19,21	0.45	0
9	NAG	v	1	9,2	14,14,15	0.46	0	17,19,21	0.60	0
9	NAG	v	2	9	14,14,15	0.36	0	17,19,21	0.46	0
13	NAG	w	1	2,13	14,14,15	0.35	0	17,19,21	0.59	0
13	NAG	w	2	13	14,14,15	0.38	0	17,19,21	0.63	0
13	BMA	w	3	13	11,11,12	1.01	1 (9%)	15,15,17	1.13	0
13	MAN	w	4	13	11,11,12	0.61	0	15,15,17	1.46	2 (13%)
13	MAN	w	5	13	11,11,12	0.73	0	15,15,17	1.30	2 (13%)
13	MAN	w	6	13	11,11,12	0.77	0	15,15,17	1.05	2 (13%)
11	NAG	x	1	11,2	14,14,15	0.24	0	17,19,21	0.43	0
11	NAG	x	2	11	14,14,15	0.22	0	17,19,21	0.64	0
11	BMA	x	3	11	11,11,12	0.76	0	15,15,17	0.94	0
10	NAG	y	1	2,10	14,14,15	0.44	0	17,19,21	0.64	0
10	NAG	y	2	10	14,14,15	0.26	0	17,19,21	0.58	0
10	BMA	y	3	10	11,11,12	0.63	0	15,15,17	0.91	1 (6%)
10	MAN	y	4	10	11,11,12	0.75	0	15,15,17	1.16	2 (13%)
10	MAN	y	5	10	11,11,12	0.80	0	15,15,17	1.17	2 (13%)
11	NAG	z	1	11,2	14,14,15	0.38	0	17,19,21	0.50	0
11	NAG	z	2	11	14,14,15	0.25	0	17,19,21	0.54	0
11	BMA	z	3	11	11,11,12	0.94	1 (9%)	15,15,17	0.94	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
9	NAG	0	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	0	2	9	-	2/6/23/26	0/1/1/1
10	NAG	1	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	1	2	10	-	3/6/23/26	0/1/1/1
10	BMA	1	3	10	-	0/2/19/22	0/1/1/1
10	MAN	1	4	10	-	2/2/19/22	0/1/1/1
10	MAN	1	5	10	-	0/2/19/22	0/1/1/1
9	NAG	2	1	9,2	-	3/6/23/26	0/1/1/1
9	NAG	2	2	9	-	0/6/23/26	0/1/1/1
10	NAG	3	1	2,10	-	3/6/23/26	0/1/1/1
10	NAG	3	2	10	-	3/6/23/26	0/1/1/1
10	BMA	3	3	10	-	2/2/19/22	0/1/1/1
10	MAN	3	4	10	-	1/2/19/22	0/1/1/1
10	MAN	3	5	10	-	1/2/19/22	0/1/1/1
11	NAG	4	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	4	2	11	-	1/6/23/26	0/1/1/1
11	BMA	4	3	11	-	0/2/19/22	0/1/1/1
9	NAG	5	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	5	2	9	-	0/6/23/26	0/1/1/1
9	NAG	6	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	6	2	9	-	2/6/23/26	0/1/1/1
9	NAG	7	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	7	2	9	-	3/6/23/26	0/1/1/1
12	NAG	8	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	8	2	12	-	3/6/23/26	0/1/1/1
12	BMA	8	3	12	-	0/2/19/22	0/1/1/1
12	MAN	8	4	12	-	2/2/19/22	0/1/1/1
9	NAG	9	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	9	2	9	-	1/6/23/26	0/1/1/1
9	NAG	AA	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	AA	2	9	-	2/6/23/26	0/1/1/1
13	NAG	BA	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	BA	2	13	-	1/6/23/26	0/1/1/1
13	BMA	BA	3	13	-	0/2/19/22	0/1/1/1
13	MAN	BA	4	13	-	2/2/19/22	0/1/1/1
13	MAN	BA	5	13	-	2/2/19/22	0/1/1/1
13	MAN	BA	6	13	-	1/2/19/22	0/1/1/1
11	NAG	CA	1	11,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	CA	2	11	-	2/6/23/26	0/1/1/1
11	BMA	CA	3	11	-	0/2/19/22	0/1/1/1
10	NAG	DA	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	DA	2	10	-	2/6/23/26	0/1/1/1
10	BMA	DA	3	10	-	0/2/19/22	0/1/1/1
10	MAN	DA	4	10	-	0/2/19/22	0/1/1/1
10	MAN	DA	5	10	-	0/2/19/22	0/1/1/1
11	NAG	EA	1	11,2	-	0/6/23/26	0/1/1/1
11	NAG	EA	2	11	-	0/6/23/26	0/1/1/1
11	BMA	EA	3	11	-	2/2/19/22	0/1/1/1
9	NAG	FA	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	FA	2	9	-	2/6/23/26	0/1/1/1
10	NAG	GA	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	GA	2	10	-	3/6/23/26	0/1/1/1
10	BMA	GA	3	10	-	0/2/19/22	0/1/1/1
10	MAN	GA	4	10	-	2/2/19/22	0/1/1/1
10	MAN	GA	5	10	-	0/2/19/22	0/1/1/1
9	NAG	U	1	9,2	-	3/6/23/26	0/1/1/1
9	NAG	U	2	9	-	0/6/23/26	0/1/1/1
10	NAG	V	1	2,10	-	3/6/23/26	0/1/1/1
10	NAG	V	2	10	-	3/6/23/26	0/1/1/1
10	BMA	V	3	10	-	2/2/19/22	0/1/1/1
10	MAN	V	4	10	-	1/2/19/22	0/1/1/1
10	MAN	V	5	10	-	1/2/19/22	0/1/1/1
11	NAG	W	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	W	2	11	-	1/6/23/26	0/1/1/1
11	BMA	W	3	11	-	0/2/19/22	0/1/1/1
9	NAG	X	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	X	2	9	-	0/6/23/26	0/1/1/1
9	NAG	Y	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	NAG	Z	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	3/6/23/26	0/1/1/1
12	NAG	a	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	a	2	12	-	3/6/23/26	0/1/1/1
12	BMA	a	3	12	-	0/2/19/22	0/1/1/1
12	MAN	a	4	12	-	2/2/19/22	0/1/1/1
9	NAG	b	1	9,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	b	2	9	-	1/6/23/26	0/1/1/1
9	NAG	c	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	c	2	9	-	2/6/23/26	0/1/1/1
13	NAG	d	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	d	2	13	-	1/6/23/26	0/1/1/1
13	BMA	d	3	13	-	0/2/19/22	0/1/1/1
13	MAN	d	4	13	-	2/2/19/22	0/1/1/1
13	MAN	d	5	13	-	2/2/19/22	0/1/1/1
13	MAN	d	6	13	-	1/2/19/22	0/1/1/1
11	NAG	e	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	e	2	11	-	2/6/23/26	0/1/1/1
11	BMA	e	3	11	-	0/2/19/22	0/1/1/1
10	NAG	f	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	f	2	10	-	2/6/23/26	0/1/1/1
10	BMA	f	3	10	-	0/2/19/22	0/1/1/1
10	MAN	f	4	10	-	0/2/19/22	0/1/1/1
10	MAN	f	5	10	-	0/2/19/22	0/1/1/1
11	NAG	g	1	11,2	-	0/6/23/26	0/1/1/1
11	NAG	g	2	11	-	0/6/23/26	0/1/1/1
11	BMA	g	3	11	-	2/2/19/22	0/1/1/1
9	NAG	h	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	h	2	9	-	2/6/23/26	0/1/1/1
10	NAG	i	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	i	2	10	-	3/6/23/26	0/1/1/1
10	BMA	i	3	10	-	0/2/19/22	0/1/1/1
10	MAN	i	4	10	-	2/2/19/22	0/1/1/1
10	MAN	i	5	10	-	0/2/19/22	0/1/1/1
9	NAG	j	1	9,2	-	3/6/23/26	0/1/1/1
9	NAG	j	2	9	-	0/6/23/26	0/1/1/1
10	NAG	k	1	2,10	-	3/6/23/26	0/1/1/1
10	NAG	k	2	10	-	3/6/23/26	0/1/1/1
10	BMA	k	3	10	-	2/2/19/22	0/1/1/1
10	MAN	k	4	10	-	1/2/19/22	0/1/1/1
10	MAN	k	5	10	-	1/2/19/22	0/1/1/1
11	NAG	l	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	l	2	11	-	1/6/23/26	0/1/1/1
11	BMA	l	3	11	-	0/2/19/22	0/1/1/1
9	NAG	o	1	9,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	o	2	9	-	0/6/23/26	0/1/1/1
9	NAG	p	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	p	2	9	-	2/6/23/26	0/1/1/1
9	NAG	s	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	s	2	9	-	3/6/23/26	0/1/1/1
12	NAG	t	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	t	2	12	-	3/6/23/26	0/1/1/1
12	BMA	t	3	12	-	0/2/19/22	0/1/1/1
12	MAN	t	4	12	-	2/2/19/22	0/1/1/1
9	NAG	u	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	u	2	9	-	0/6/23/26	0/1/1/1
9	NAG	v	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	v	2	9	-	2/6/23/26	0/1/1/1
13	NAG	w	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	w	2	13	-	1/6/23/26	0/1/1/1
13	BMA	w	3	13	-	0/2/19/22	0/1/1/1
13	MAN	w	4	13	-	2/2/19/22	0/1/1/1
13	MAN	w	5	13	-	2/2/19/22	0/1/1/1
13	MAN	w	6	13	-	1/2/19/22	0/1/1/1
11	NAG	x	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	x	2	11	-	2/6/23/26	0/1/1/1
11	BMA	x	3	11	-	0/2/19/22	0/1/1/1
10	NAG	y	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	y	2	10	-	2/6/23/26	0/1/1/1
10	BMA	y	3	10	-	0/2/19/22	0/1/1/1
10	MAN	y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	y	5	10	-	0/2/19/22	0/1/1/1
11	NAG	z	1	11,2	-	0/6/23/26	0/1/1/1
11	NAG	z	2	11	-	0/6/23/26	0/1/1/1
11	BMA	z	3	11	-	2/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	1	NAG	C1-C2	2.32	1.55	1.52
9	j	1	NAG	C1-C2	2.29	1.55	1.52
13	BA	3	BMA	O5-C1	-2.25	1.40	1.43
11	z	3	BMA	C1-C2	2.24	1.57	1.52
11	g	3	BMA	C1-C2	2.22	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	3	BMA	O5-C1	-2.21	1.40	1.43
10	3	5	MAN	C1-C2	2.20	1.57	1.52
11	EA	3	BMA	C1-C2	2.20	1.57	1.52
9	2	1	NAG	C1-C2	2.18	1.55	1.52
10	V	5	MAN	C1-C2	2.17	1.57	1.52
10	k	5	MAN	C1-C2	2.17	1.57	1.52
11	l	1	NAG	O5-C1	-2.16	1.40	1.43
11	4	1	NAG	O5-C1	-2.16	1.40	1.43
13	w	3	BMA	O5-C1	-2.15	1.40	1.43
12	t	4	MAN	C1-C2	2.15	1.57	1.52
11	W	1	NAG	O5-C1	-2.14	1.40	1.43
12	8	4	MAN	C1-C2	2.13	1.57	1.52
12	a	4	MAN	C1-C2	2.12	1.57	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	k	1	NAG	C2-N2-C7	7.97	134.26	122.90
10	V	1	NAG	C2-N2-C7	7.94	134.21	122.90
10	3	1	NAG	C2-N2-C7	7.92	134.19	122.90
13	d	4	MAN	C1-O5-C5	4.83	118.74	112.19
13	BA	4	MAN	C1-O5-C5	4.80	118.70	112.19
13	w	4	MAN	C1-O5-C5	4.80	118.70	112.19
10	V	1	NAG	C1-C2-N2	3.88	117.12	110.49
10	3	1	NAG	C1-C2-N2	3.83	117.03	110.49
10	k	1	NAG	C1-C2-N2	3.80	116.98	110.49
12	t	4	MAN	C1-O5-C5	3.60	117.06	112.19
12	8	4	MAN	C1-O5-C5	3.51	116.95	112.19
12	a	4	MAN	C1-O5-C5	3.50	116.93	112.19
13	w	5	MAN	C1-O5-C5	3.48	116.91	112.19
13	BA	5	MAN	C1-O5-C5	3.47	116.90	112.19
13	d	5	MAN	C1-O5-C5	3.47	116.89	112.19
9	j	1	NAG	C1-O5-C5	3.45	116.87	112.19
9	2	1	NAG	C1-O5-C5	3.45	116.86	112.19
10	f	4	MAN	C1-O5-C5	3.40	116.80	112.19
9	U	1	NAG	C1-O5-C5	3.39	116.79	112.19
10	DA	4	MAN	C1-O5-C5	3.37	116.76	112.19
10	y	4	MAN	C1-O5-C5	3.36	116.75	112.19
10	V	5	MAN	C1-O5-C5	3.25	116.60	112.19
10	k	5	MAN	C1-O5-C5	3.24	116.58	112.19
10	f	5	MAN	C1-O5-C5	3.23	116.57	112.19
10	3	5	MAN	C1-O5-C5	3.21	116.54	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	1	4	MAN	C1-O5-C5	3.20	116.52	112.19
10	DA	5	MAN	C1-O5-C5	3.19	116.52	112.19
10	y	5	MAN	C1-O5-C5	3.18	116.51	112.19
10	i	4	MAN	C1-O5-C5	3.18	116.50	112.19
10	GA	4	MAN	C1-O5-C5	3.14	116.44	112.19
11	l	2	NAG	C2-N2-C7	3.09	127.30	122.90
9	0	1	NAG	C2-N2-C7	3.08	127.29	122.90
12	t	2	NAG	C2-N2-C7	3.08	127.29	122.90
11	W	2	NAG	C2-N2-C7	3.08	127.29	122.90
9	h	1	NAG	C2-N2-C7	3.06	127.26	122.90
10	i	2	NAG	C2-N2-C7	3.06	127.26	122.90
10	3	2	NAG	C2-N2-C7	3.06	127.26	122.90
9	7	2	NAG	C2-N2-C7	3.06	127.26	122.90
12	a	2	NAG	C2-N2-C7	3.06	127.25	122.90
10	V	2	NAG	C2-N2-C7	3.05	127.25	122.90
11	4	2	NAG	C2-N2-C7	3.05	127.25	122.90
10	k	2	NAG	C2-N2-C7	3.04	127.24	122.90
10	1	2	NAG	C2-N2-C7	3.03	127.22	122.90
9	FA	1	NAG	C2-N2-C7	3.02	127.20	122.90
10	GA	2	NAG	C2-N2-C7	3.00	127.18	122.90
9	Y	1	NAG	C2-N2-C7	3.00	127.18	122.90
9	6	1	NAG	C2-N2-C7	2.99	127.17	122.90
9	s	2	NAG	C2-N2-C7	2.98	127.15	122.90
10	V	4	MAN	C1-O5-C5	2.98	116.23	112.19
9	p	1	NAG	C2-N2-C7	2.98	127.15	122.90
9	Z	2	NAG	C2-N2-C7	2.98	127.14	122.90
10	k	4	MAN	C1-O5-C5	2.97	116.22	112.19
9	j	1	NAG	C2-N2-C7	2.97	127.12	122.90
12	8	2	NAG	C2-N2-C7	2.95	127.11	122.90
9	5	1	NAG	C2-N2-C7	2.95	127.11	122.90
9	X	1	NAG	C2-N2-C7	2.94	127.09	122.90
9	o	1	NAG	C2-N2-C7	2.94	127.09	122.90
10	3	4	MAN	C1-O5-C5	2.94	116.17	112.19
9	U	1	NAG	C2-N2-C7	2.93	127.07	122.90
9	2	1	NAG	C2-N2-C7	2.91	127.04	122.90
9	0	1	NAG	C1-O5-C5	2.72	115.88	112.19
9	FA	1	NAG	C1-O5-C5	2.69	115.83	112.19
9	h	1	NAG	C1-O5-C5	2.68	115.82	112.19
13	BA	6	MAN	O2-C2-C3	-2.63	104.87	110.14
13	w	6	MAN	O2-C2-C3	-2.62	104.90	110.14
13	d	6	MAN	O2-C2-C3	-2.61	104.91	110.14
13	d	6	MAN	C1-O5-C5	2.57	115.68	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	w	6	MAN	C1-O5-C5	2.57	115.67	112.19
10	1	5	MAN	C1-O5-C5	2.54	115.64	112.19
13	BA	6	MAN	C1-O5-C5	2.54	115.63	112.19
10	i	5	MAN	C1-O5-C5	2.51	115.60	112.19
12	a	4	MAN	O2-C2-C3	-2.49	105.14	110.14
10	GA	5	MAN	C1-O5-C5	2.48	115.55	112.19
12	8	4	MAN	O2-C2-C3	-2.47	105.19	110.14
12	t	4	MAN	O2-C2-C3	-2.44	105.25	110.14
10	3	3	BMA	C1-O5-C5	2.43	115.49	112.19
10	k	3	BMA	C1-O5-C5	2.41	115.46	112.19
12	8	3	BMA	C1-O5-C5	2.41	115.46	112.19
10	V	3	BMA	C1-O5-C5	2.40	115.45	112.19
12	a	3	BMA	C1-O5-C5	2.38	115.41	112.19
10	f	5	MAN	O2-C2-C3	-2.36	105.40	110.14
10	y	5	MAN	O2-C2-C3	-2.36	105.40	110.14
10	DA	5	MAN	O2-C2-C3	-2.35	105.44	110.14
12	t	3	BMA	C1-O5-C5	2.34	115.36	112.19
10	3	4	MAN	O2-C2-C3	-2.32	105.49	110.14
10	k	4	MAN	O2-C2-C3	-2.32	105.50	110.14
10	V	4	MAN	O2-C2-C3	-2.31	105.50	110.14
10	y	4	MAN	O2-C2-C3	-2.29	105.54	110.14
10	f	4	MAN	O2-C2-C3	-2.28	105.57	110.14
10	V	5	MAN	O2-C2-C3	-2.27	105.58	110.14
10	k	5	MAN	O2-C2-C3	-2.27	105.59	110.14
10	3	5	MAN	O2-C2-C3	-2.26	105.60	110.14
10	DA	4	MAN	O2-C2-C3	-2.26	105.61	110.14
10	i	5	MAN	O2-C2-C3	-2.22	105.69	110.14
10	GA	5	MAN	O2-C2-C3	-2.21	105.71	110.14
13	BA	5	MAN	O2-C2-C3	-2.20	105.73	110.14
13	w	5	MAN	O2-C2-C3	-2.20	105.73	110.14
13	d	5	MAN	O2-C2-C3	-2.19	105.74	110.14
10	1	5	MAN	O2-C2-C3	-2.16	105.80	110.14
10	3	1	NAG	C8-C7-N2	2.16	119.76	116.10
10	1	4	MAN	O2-C2-C3	-2.15	105.83	110.14
10	i	4	MAN	O2-C2-C3	-2.15	105.83	110.14
10	GA	4	MAN	O2-C2-C3	-2.15	105.83	110.14
10	k	1	NAG	C8-C7-N2	2.14	119.72	116.10
10	y	3	BMA	O2-C2-C3	-2.12	105.89	110.14
10	DA	3	BMA	O2-C2-C3	-2.12	105.89	110.14
10	f	3	BMA	O2-C2-C3	-2.12	105.89	110.14
13	d	4	MAN	O2-C2-C3	-2.11	105.90	110.14
10	V	1	NAG	C8-C7-N2	2.09	119.64	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	BA	4	MAN	O2-C2-C3	-2.09	105.96	110.14
13	w	4	MAN	O2-C2-C3	-2.07	105.99	110.14
11	CA	2	NAG	C1-O5-C5	2.05	114.97	112.19
11	e	2	NAG	C1-O5-C5	2.04	114.95	112.19
13	BA	3	BMA	C1-O5-C5	2.02	114.93	112.19
9	2	2	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (182) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	h	2	NAG	C4-C5-C6-O6
9	0	2	NAG	C4-C5-C6-O6
9	FA	2	NAG	C4-C5-C6-O6
12	a	2	NAG	O5-C5-C6-O6
12	t	2	NAG	O5-C5-C6-O6
12	8	2	NAG	O5-C5-C6-O6
9	h	2	NAG	O5-C5-C6-O6
9	0	2	NAG	O5-C5-C6-O6
9	FA	2	NAG	O5-C5-C6-O6
9	Z	2	NAG	C4-C5-C6-O6
9	s	2	NAG	C4-C5-C6-O6
9	7	2	NAG	C4-C5-C6-O6
9	c	2	NAG	O5-C5-C6-O6
9	v	2	NAG	O5-C5-C6-O6
9	6	2	NAG	O5-C5-C6-O6
9	AA	2	NAG	O5-C5-C6-O6
10	i	1	NAG	O5-C5-C6-O6
10	1	1	NAG	O5-C5-C6-O6
10	GA	1	NAG	O5-C5-C6-O6
9	Y	2	NAG	O5-C5-C6-O6
9	p	2	NAG	O5-C5-C6-O6
12	a	2	NAG	C4-C5-C6-O6
12	t	2	NAG	C4-C5-C6-O6
12	8	2	NAG	C4-C5-C6-O6
9	b	1	NAG	O5-C5-C6-O6
9	u	1	NAG	O5-C5-C6-O6
9	9	1	NAG	O5-C5-C6-O6
13	d	5	MAN	O5-C5-C6-O6
13	BA	5	MAN	O5-C5-C6-O6
13	d	1	NAG	C4-C5-C6-O6
13	w	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	BA	1	NAG	C4-C5-C6-O6
13	w	5	MAN	O5-C5-C6-O6
10	i	1	NAG	C4-C5-C6-O6
10	1	1	NAG	C4-C5-C6-O6
10	GA	1	NAG	C4-C5-C6-O6
9	Z	2	NAG	O5-C5-C6-O6
9	s	2	NAG	O5-C5-C6-O6
9	7	2	NAG	O5-C5-C6-O6
11	e	1	NAG	C4-C5-C6-O6
11	x	1	NAG	C4-C5-C6-O6
11	CA	1	NAG	C4-C5-C6-O6
9	c	2	NAG	C4-C5-C6-O6
9	v	2	NAG	C4-C5-C6-O6
9	AA	2	NAG	C4-C5-C6-O6
9	b	1	NAG	C4-C5-C6-O6
9	u	1	NAG	C4-C5-C6-O6
9	9	1	NAG	C4-C5-C6-O6
10	V	1	NAG	C8-C7-N2-C2
10	V	1	NAG	O7-C7-N2-C2
10	f	2	NAG	C8-C7-N2-C2
10	f	2	NAG	O7-C7-N2-C2
10	k	1	NAG	C8-C7-N2-C2
10	k	1	NAG	O7-C7-N2-C2
10	y	2	NAG	C8-C7-N2-C2
10	y	2	NAG	O7-C7-N2-C2
10	3	1	NAG	C8-C7-N2-C2
10	3	1	NAG	O7-C7-N2-C2
10	DA	2	NAG	C8-C7-N2-C2
10	DA	2	NAG	O7-C7-N2-C2
10	V	3	BMA	O5-C5-C6-O6
10	k	3	BMA	O5-C5-C6-O6
10	3	3	BMA	O5-C5-C6-O6
12	8	1	NAG	O5-C5-C6-O6
12	a	1	NAG	O5-C5-C6-O6
12	t	1	NAG	O5-C5-C6-O6
11	x	2	NAG	O5-C5-C6-O6
11	CA	2	NAG	O5-C5-C6-O6
11	e	2	NAG	O5-C5-C6-O6
9	j	1	NAG	C4-C5-C6-O6
13	d	1	NAG	O5-C5-C6-O6
13	w	1	NAG	O5-C5-C6-O6
13	BA	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	U	1	NAG	C4-C5-C6-O6
9	2	1	NAG	C4-C5-C6-O6
10	3	3	BMA	C4-C5-C6-O6
10	V	2	NAG	O5-C5-C6-O6
10	k	2	NAG	O5-C5-C6-O6
10	3	2	NAG	O5-C5-C6-O6
10	V	3	BMA	C4-C5-C6-O6
10	k	3	BMA	C4-C5-C6-O6
11	e	1	NAG	O5-C5-C6-O6
11	x	1	NAG	O5-C5-C6-O6
11	CA	1	NAG	O5-C5-C6-O6
9	Y	2	NAG	C4-C5-C6-O6
9	p	2	NAG	C4-C5-C6-O6
9	6	2	NAG	C4-C5-C6-O6
11	e	2	NAG	C4-C5-C6-O6
11	x	2	NAG	C4-C5-C6-O6
11	CA	2	NAG	C4-C5-C6-O6
10	V	4	MAN	O5-C5-C6-O6
10	k	4	MAN	O5-C5-C6-O6
10	3	4	MAN	O5-C5-C6-O6
13	w	4	MAN	O5-C5-C6-O6
13	d	4	MAN	O5-C5-C6-O6
13	BA	4	MAN	O5-C5-C6-O6
10	1	2	NAG	C4-C5-C6-O6
10	GA	2	NAG	C4-C5-C6-O6
10	i	2	NAG	C4-C5-C6-O6
13	d	4	MAN	C4-C5-C6-O6
13	w	4	MAN	C4-C5-C6-O6
13	BA	4	MAN	C4-C5-C6-O6
10	i	2	NAG	O5-C5-C6-O6
9	j	1	NAG	O5-C5-C6-O6
9	2	1	NAG	O5-C5-C6-O6
10	1	2	NAG	O5-C5-C6-O6
10	GA	2	NAG	O5-C5-C6-O6
9	U	1	NAG	O5-C5-C6-O6
13	d	6	MAN	O5-C5-C6-O6
13	w	6	MAN	O5-C5-C6-O6
13	BA	6	MAN	O5-C5-C6-O6
10	i	4	MAN	C4-C5-C6-O6
10	1	4	MAN	C4-C5-C6-O6
10	GA	4	MAN	C4-C5-C6-O6
10	i	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	1	4	MAN	O5-C5-C6-O6
10	GA	4	MAN	O5-C5-C6-O6
13	BA	2	NAG	O5-C5-C6-O6
13	d	2	NAG	O5-C5-C6-O6
13	w	2	NAG	O5-C5-C6-O6
12	a	1	NAG	C4-C5-C6-O6
12	t	1	NAG	C4-C5-C6-O6
12	8	1	NAG	C4-C5-C6-O6
11	g	3	BMA	C4-C5-C6-O6
11	z	3	BMA	C4-C5-C6-O6
11	EA	3	BMA	C4-C5-C6-O6
11	EA	3	BMA	O5-C5-C6-O6
11	g	3	BMA	O5-C5-C6-O6
11	z	3	BMA	O5-C5-C6-O6
13	BA	5	MAN	C4-C5-C6-O6
13	d	5	MAN	C4-C5-C6-O6
13	w	5	MAN	C4-C5-C6-O6
9	U	1	NAG	C3-C2-N2-C7
9	j	1	NAG	C3-C2-N2-C7
9	2	1	NAG	C3-C2-N2-C7
10	V	2	NAG	C3-C2-N2-C7
10	k	2	NAG	C3-C2-N2-C7
10	3	2	NAG	C3-C2-N2-C7
12	a	4	MAN	O5-C5-C6-O6
12	t	4	MAN	O5-C5-C6-O6
12	8	4	MAN	O5-C5-C6-O6
10	V	5	MAN	O5-C5-C6-O6
10	k	5	MAN	O5-C5-C6-O6
10	3	5	MAN	O5-C5-C6-O6
11	l	1	NAG	C4-C5-C6-O6
11	4	1	NAG	C4-C5-C6-O6
11	W	1	NAG	C4-C5-C6-O6
12	t	4	MAN	C4-C5-C6-O6
12	a	4	MAN	C4-C5-C6-O6
12	8	4	MAN	C4-C5-C6-O6
11	W	1	NAG	C1-C2-N2-C7
11	l	1	NAG	C1-C2-N2-C7
11	4	1	NAG	C1-C2-N2-C7
9	X	1	NAG	C3-C2-N2-C7
9	Y	1	NAG	C3-C2-N2-C7
9	Z	2	NAG	C3-C2-N2-C7
9	h	1	NAG	C3-C2-N2-C7

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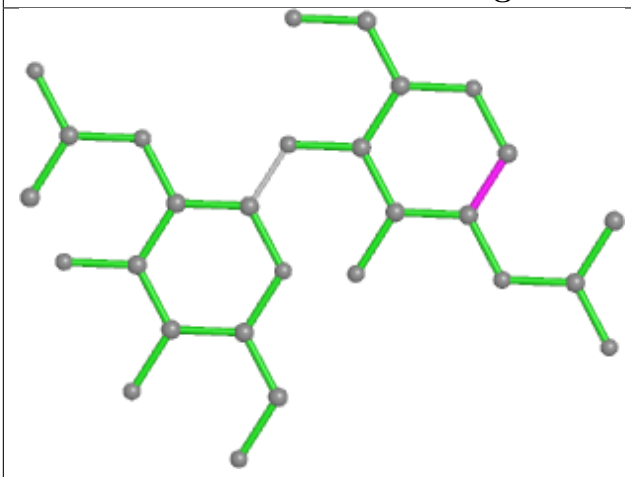
Mol	Chain	Res	Type	Atoms
9	o	1	NAG	C3-C2-N2-C7
9	p	1	NAG	C3-C2-N2-C7
9	s	2	NAG	C3-C2-N2-C7
9	0	1	NAG	C3-C2-N2-C7
9	5	1	NAG	C3-C2-N2-C7
9	6	1	NAG	C3-C2-N2-C7
9	7	2	NAG	C3-C2-N2-C7
9	FA	1	NAG	C3-C2-N2-C7
10	V	1	NAG	C3-C2-N2-C7
10	i	2	NAG	C3-C2-N2-C7
10	k	1	NAG	C3-C2-N2-C7
10	1	2	NAG	C3-C2-N2-C7
10	3	1	NAG	C3-C2-N2-C7
10	GA	2	NAG	C3-C2-N2-C7
11	W	2	NAG	C3-C2-N2-C7
11	l	2	NAG	C3-C2-N2-C7
11	4	2	NAG	C3-C2-N2-C7
12	a	2	NAG	C3-C2-N2-C7
12	t	2	NAG	C3-C2-N2-C7
12	8	2	NAG	C3-C2-N2-C7
10	3	2	NAG	C4-C5-C6-O6
10	V	2	NAG	C4-C5-C6-O6
10	k	2	NAG	C4-C5-C6-O6
9	9	2	NAG	C4-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6

There are no ring outliers.

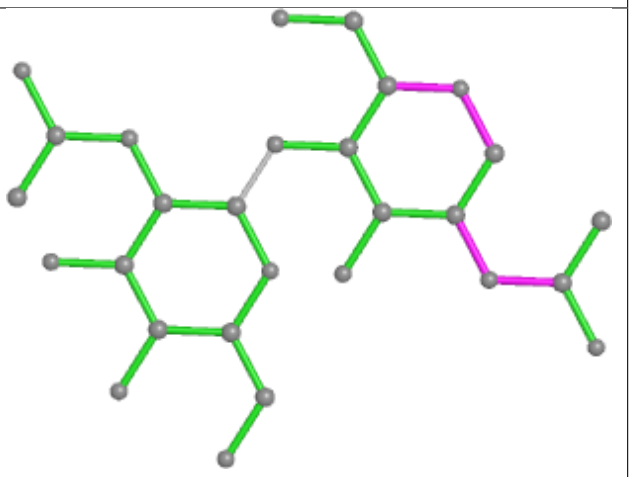
No monomer is involved in short contacts.

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

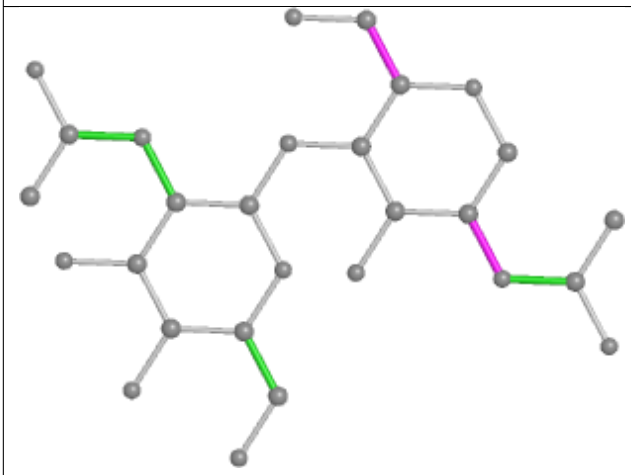
Oligosaccharide Chain U



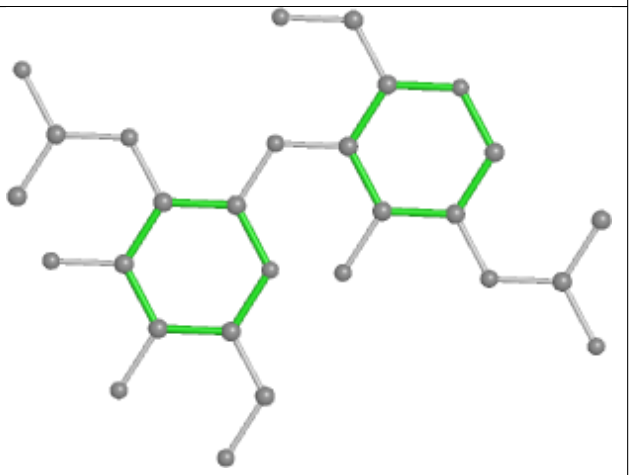
Bond lengths



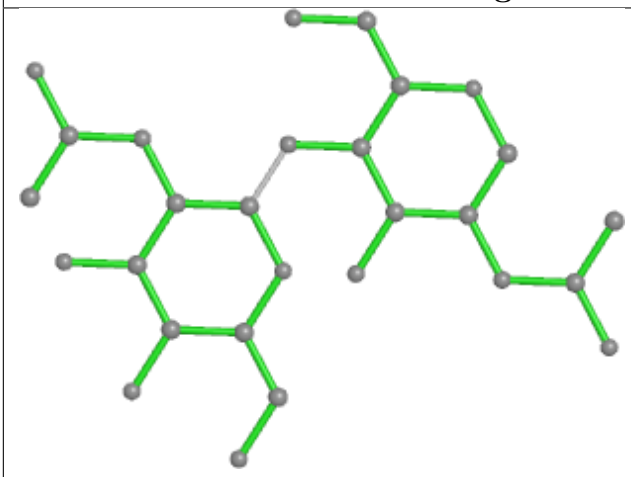
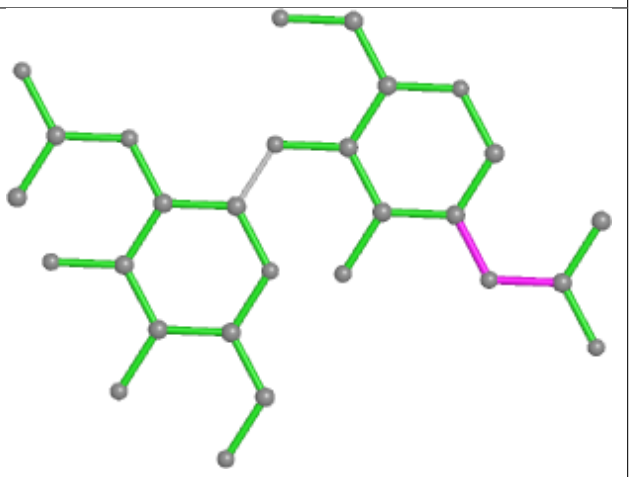
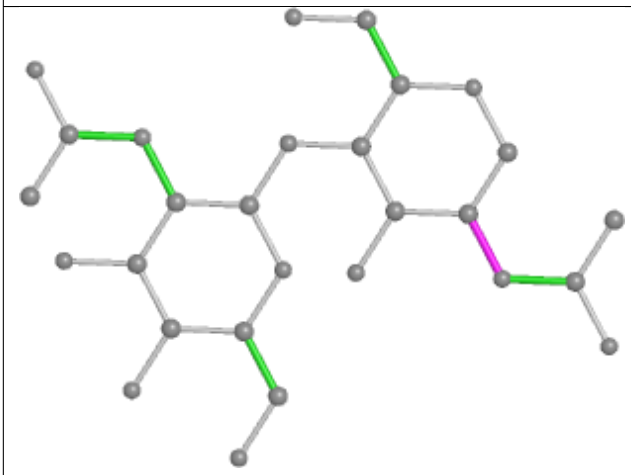
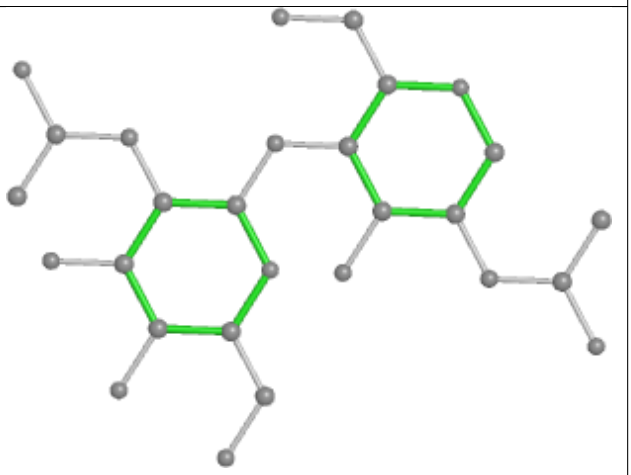
Bond angles



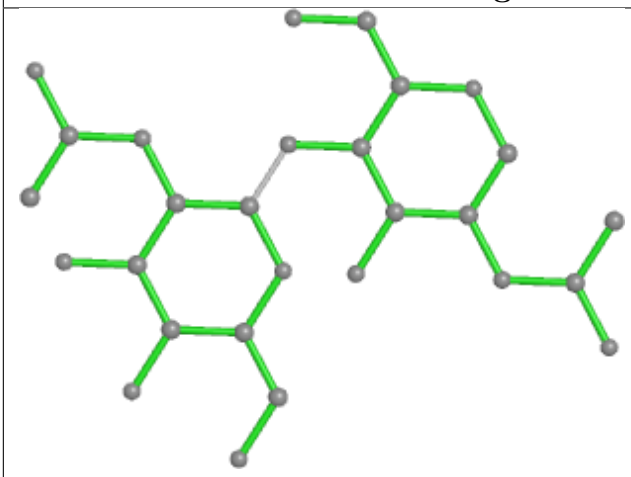
Torsions



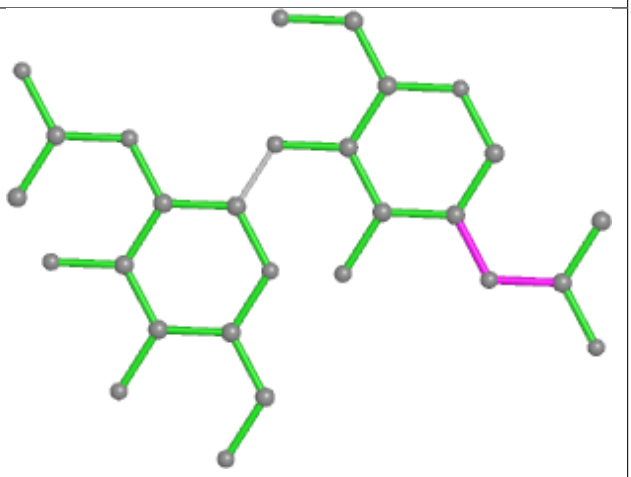
Rings

Oligosaccharide Chain X	
 Bond lengths	 Bond angles
 Torsions	 Rings

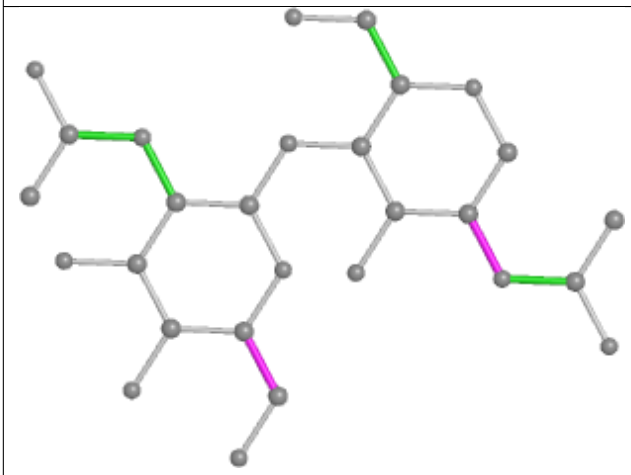
Oligosaccharide Chain Y



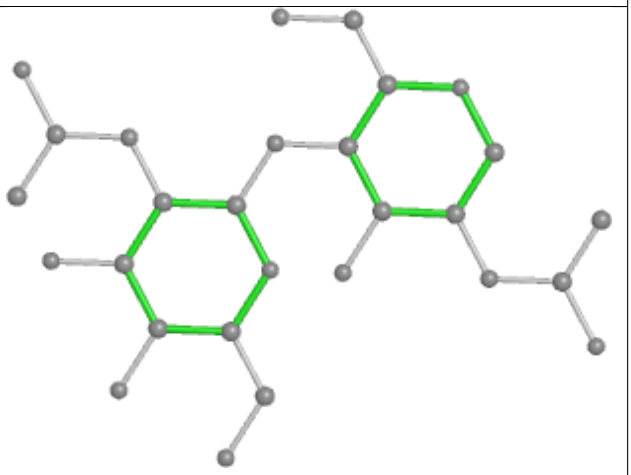
Bond lengths



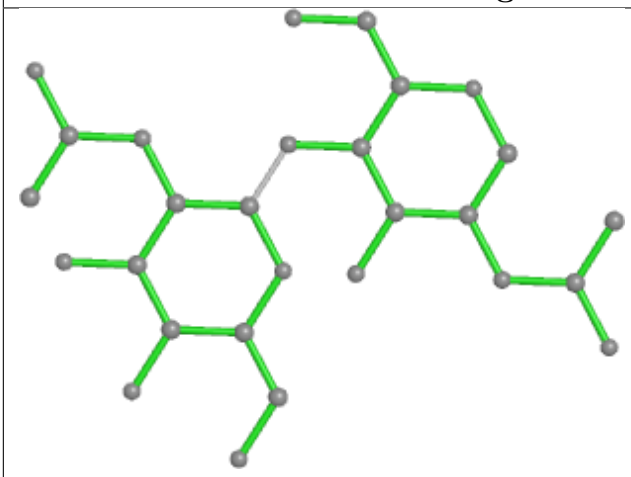
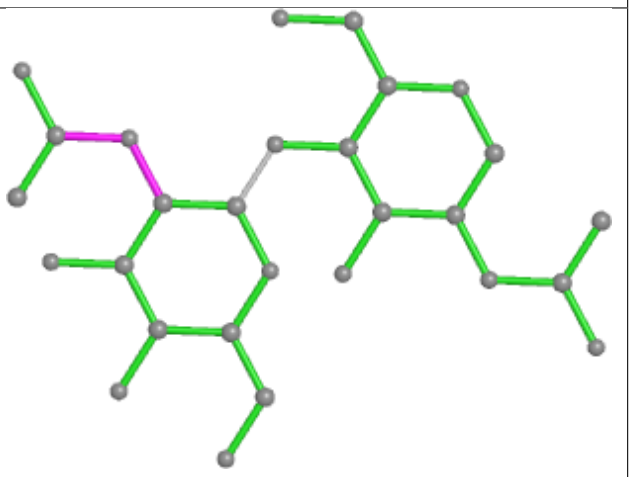
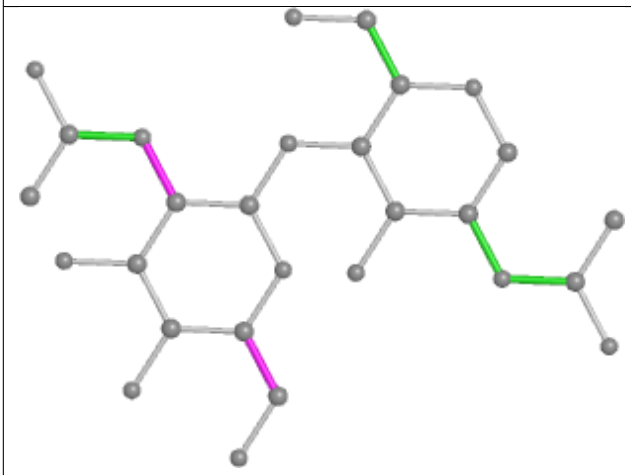
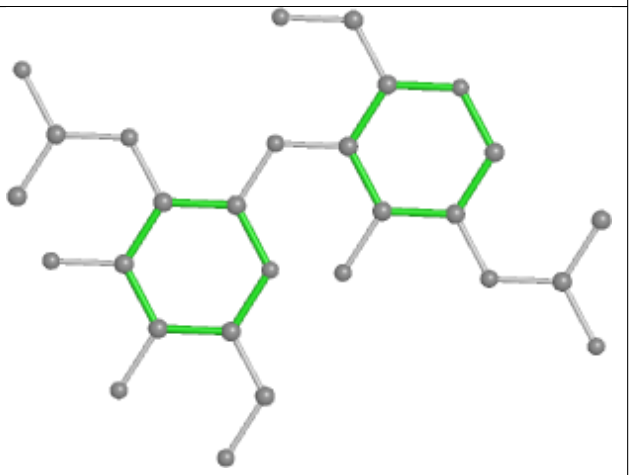
Bond angles

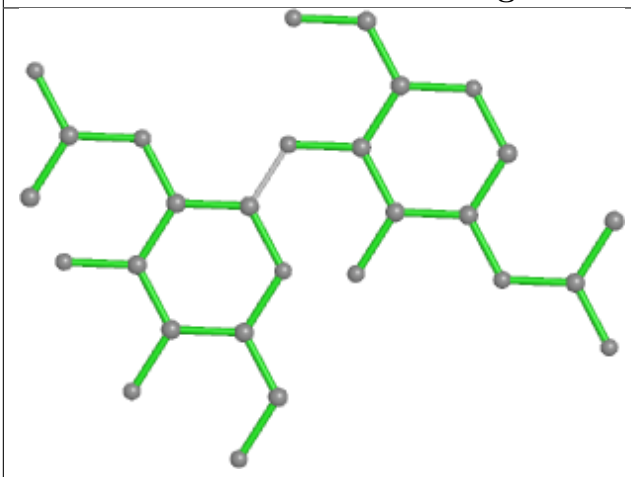
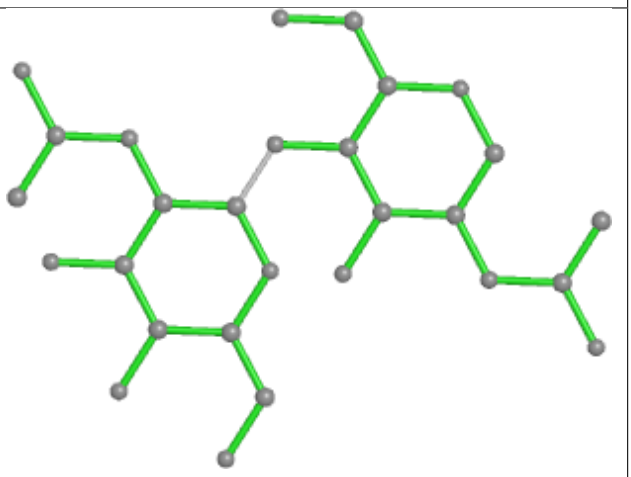
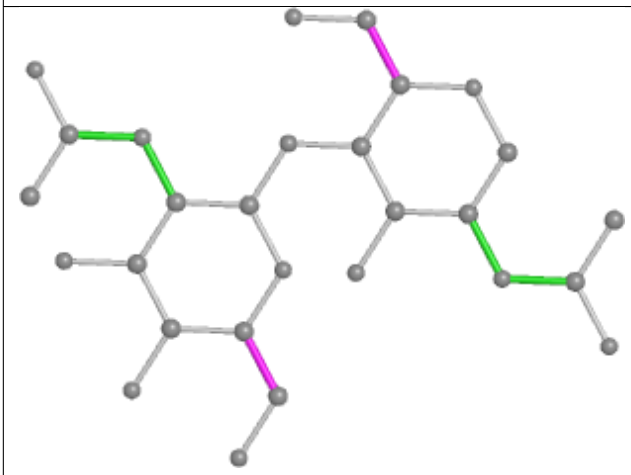
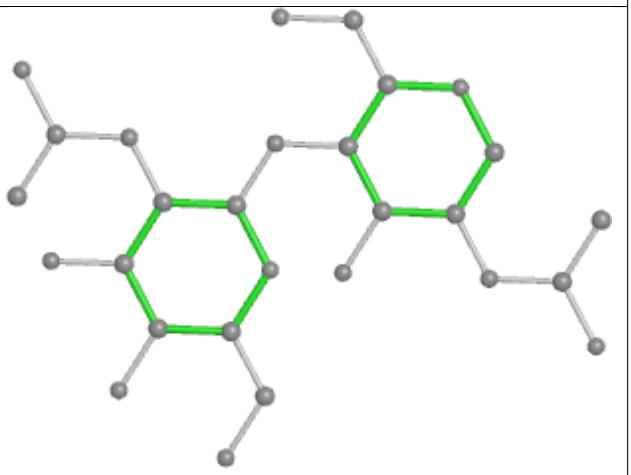


Torsions

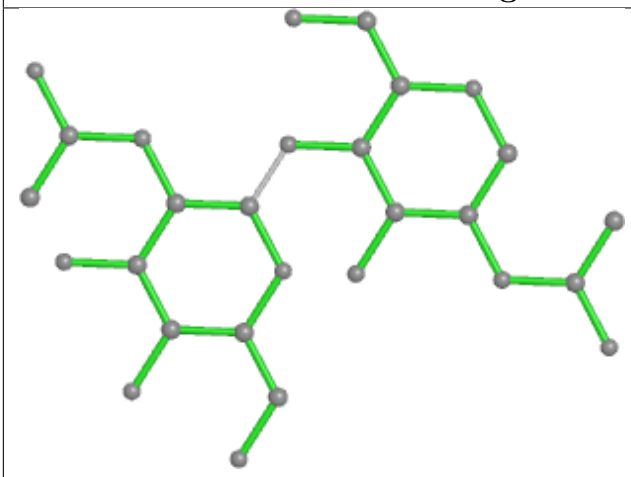


Rings

Oligosaccharide Chain Z	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain b	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain c



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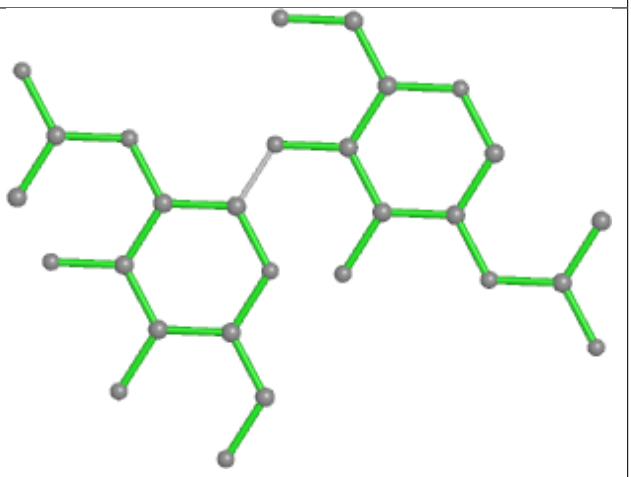

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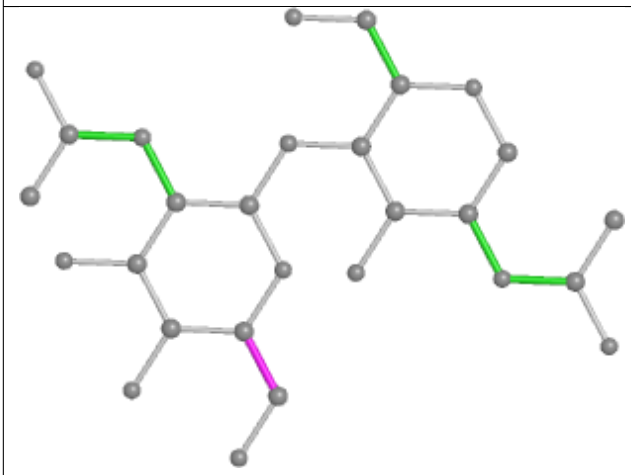

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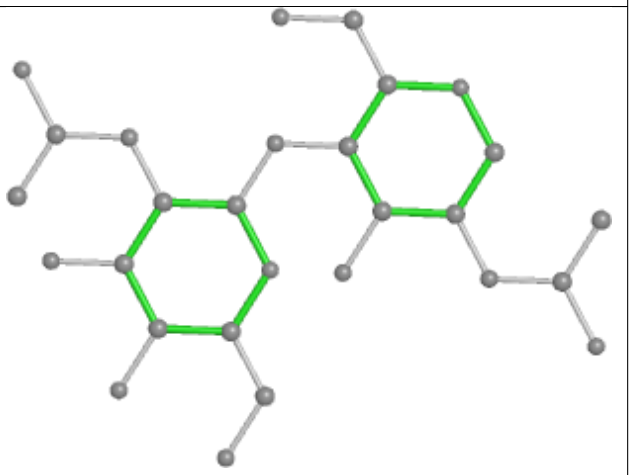
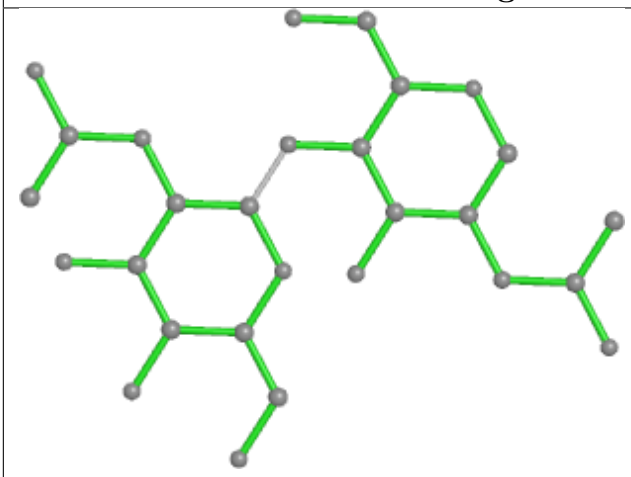


Rings

Oligosaccharide Chain h



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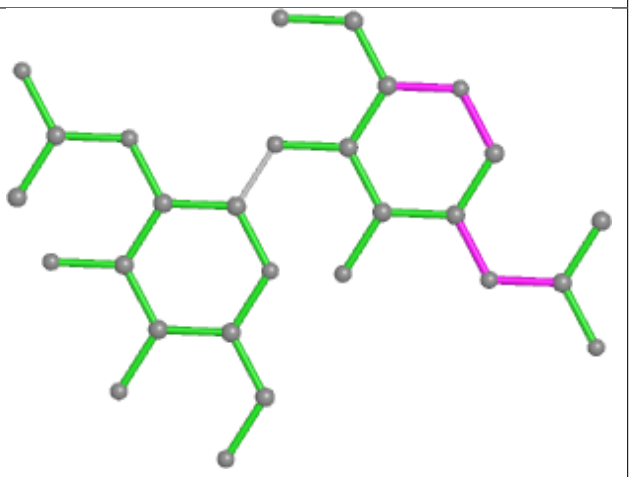

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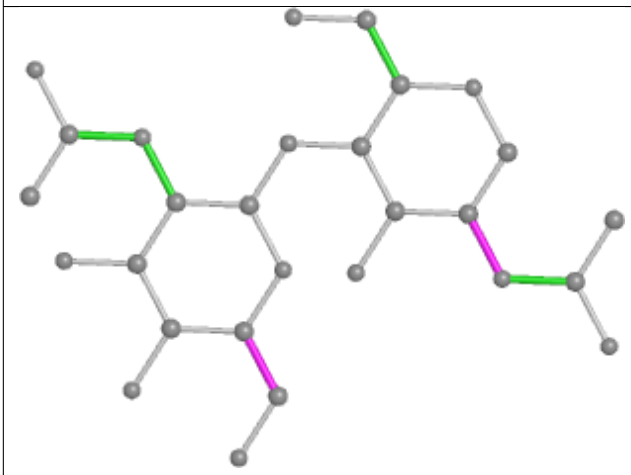

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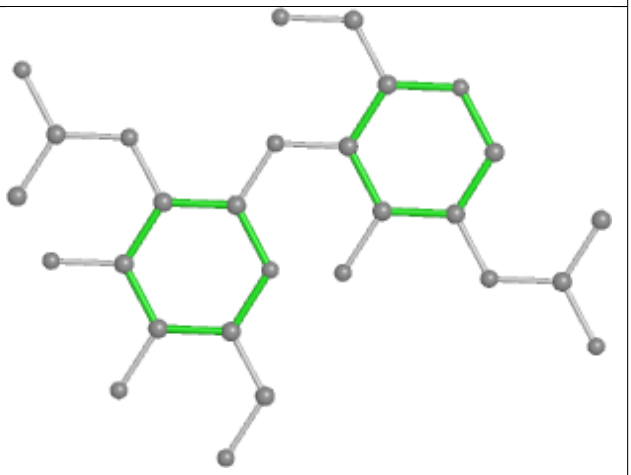
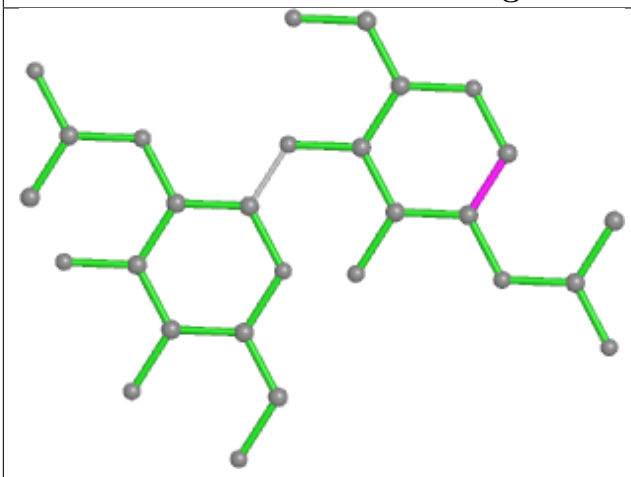


Rings

Oligosaccharide Chain j



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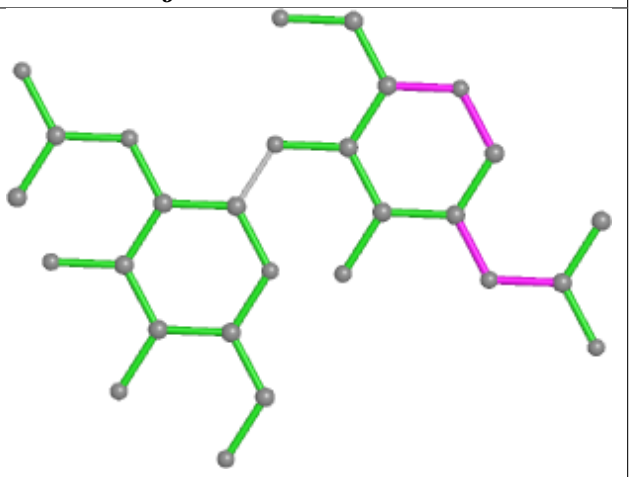

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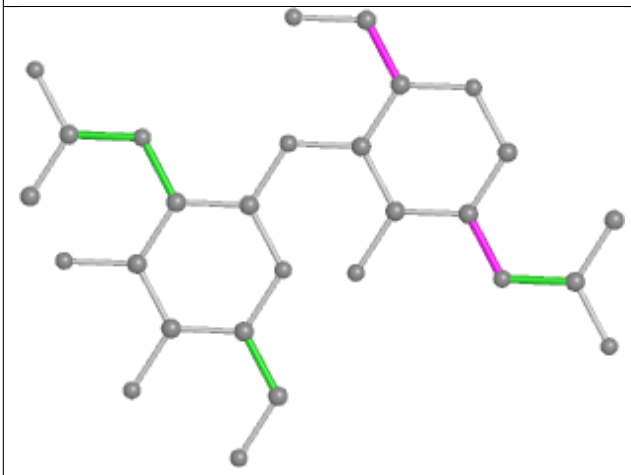

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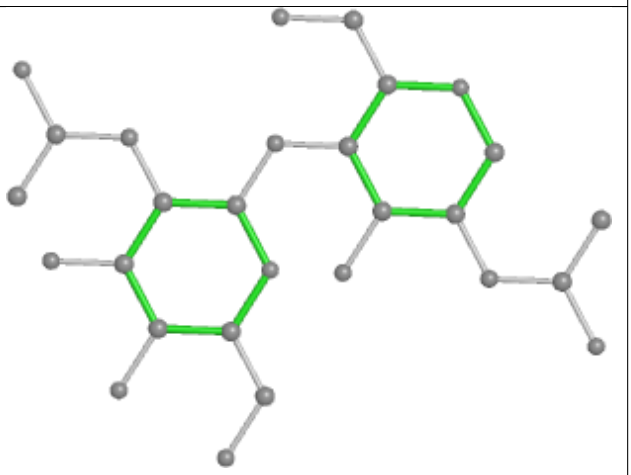
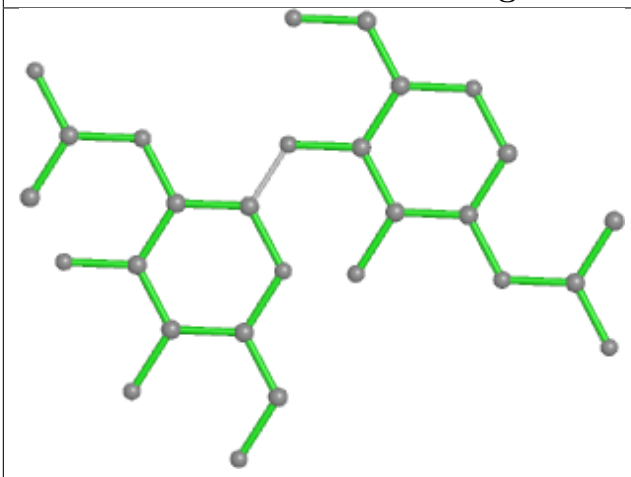


Rings

Oligosaccharide Chain o



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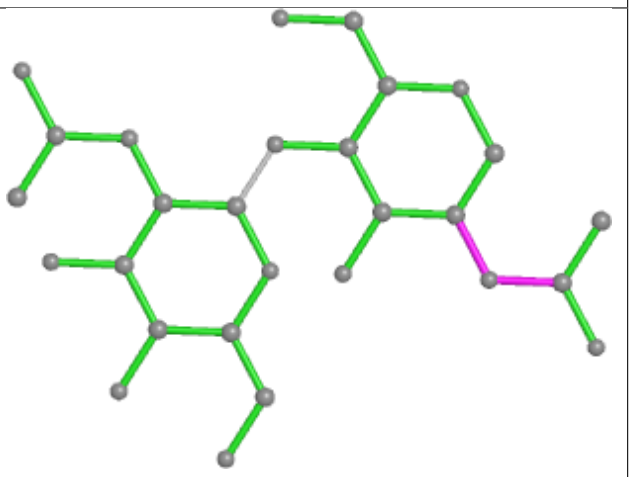

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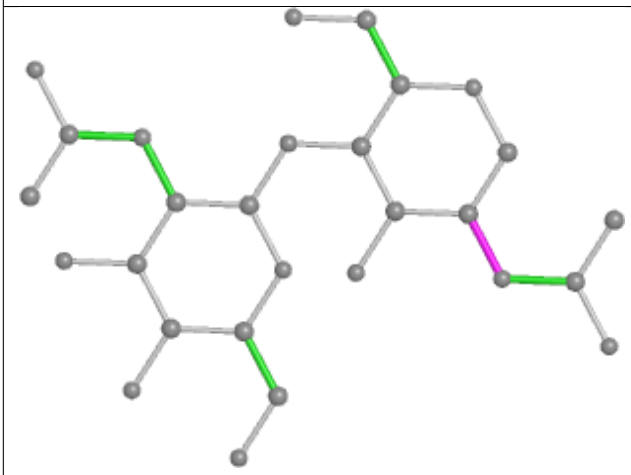

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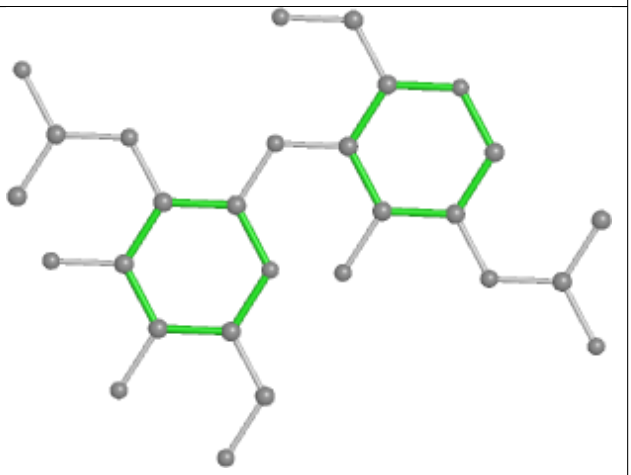
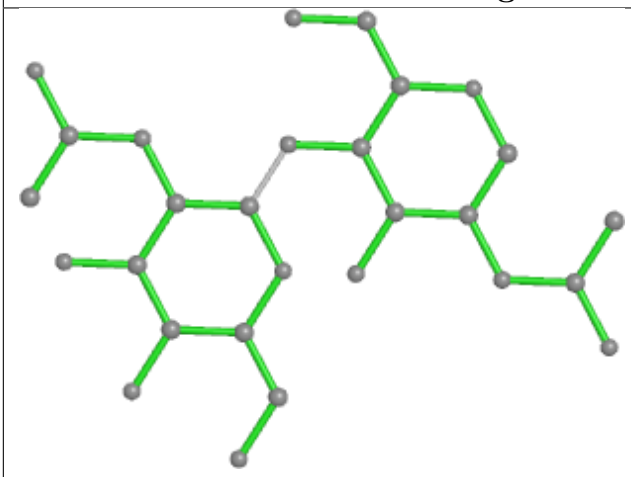


Rings

Oligosaccharide Chain p



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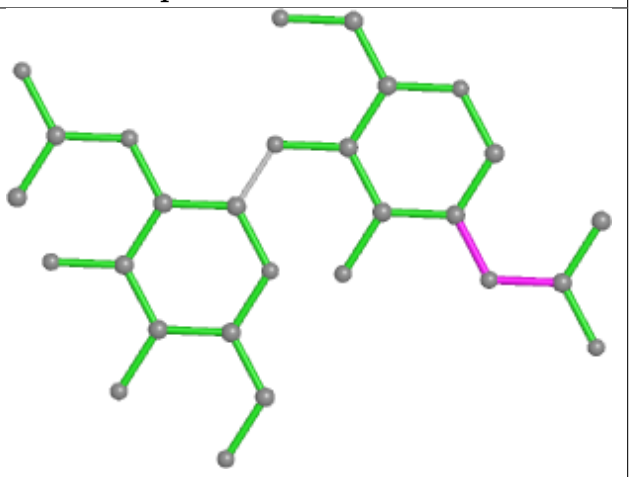

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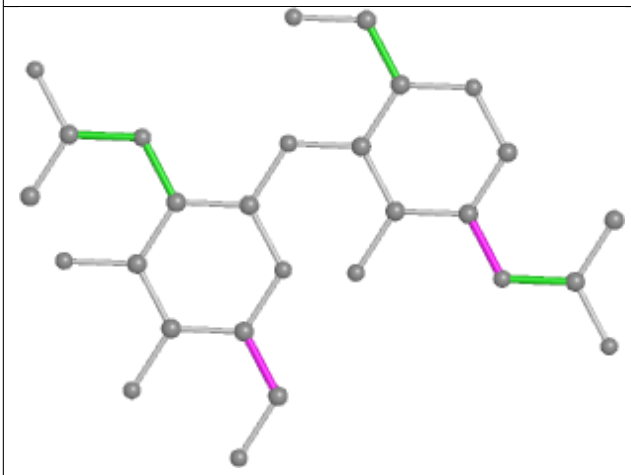

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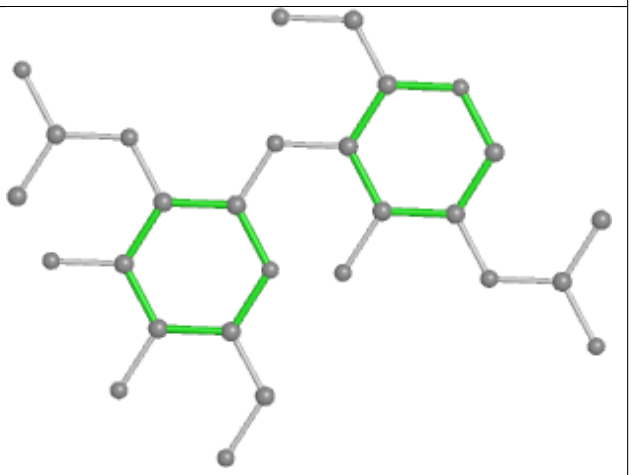
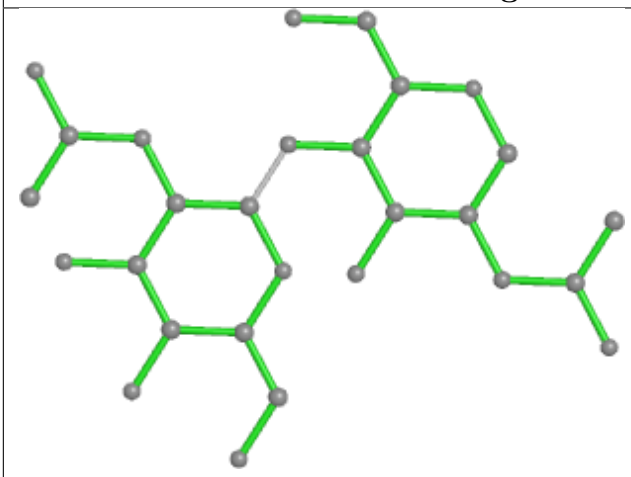


Rings

Oligosaccharide Chain s



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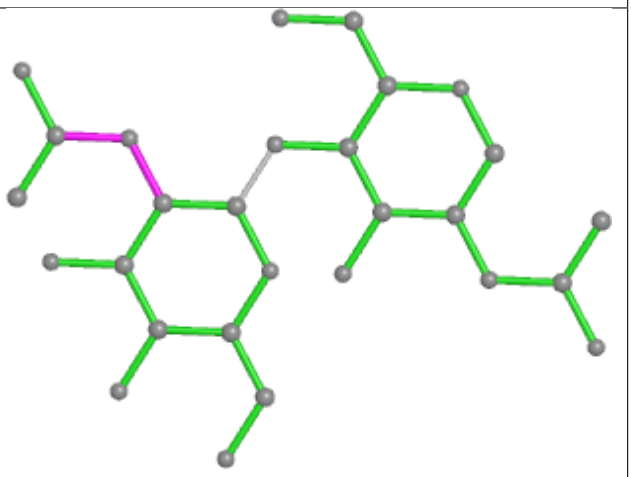

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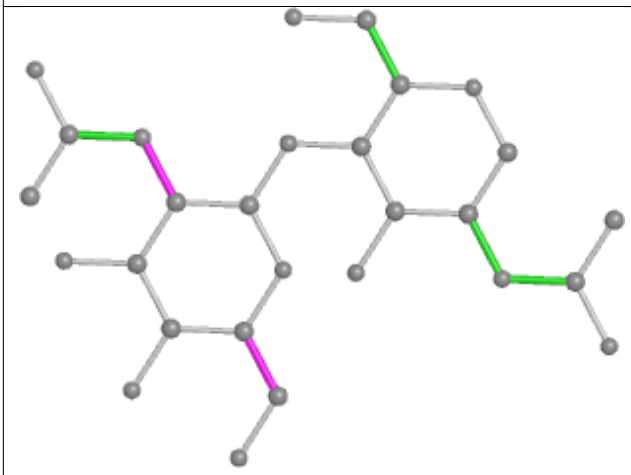

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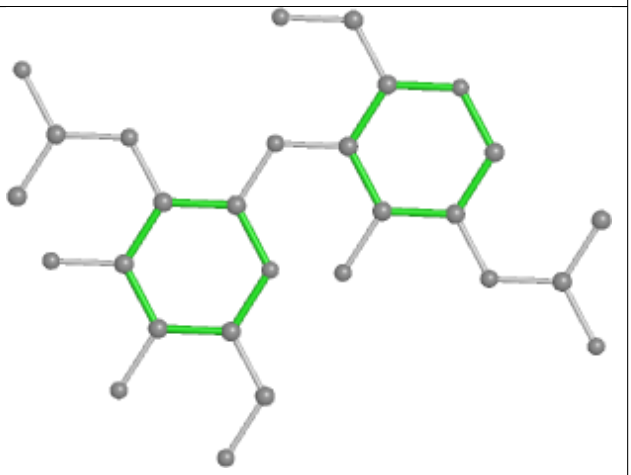
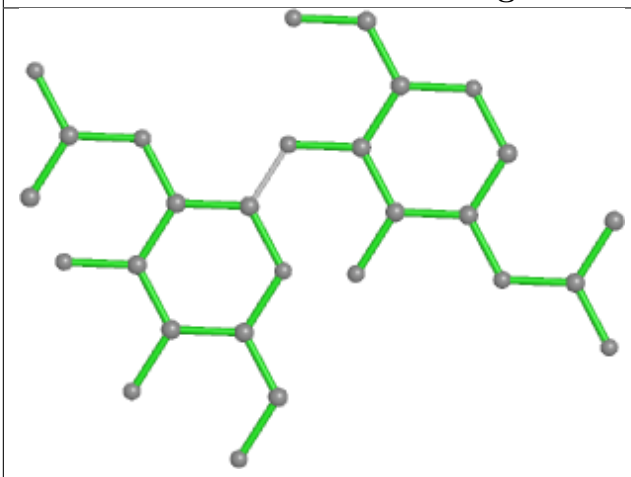
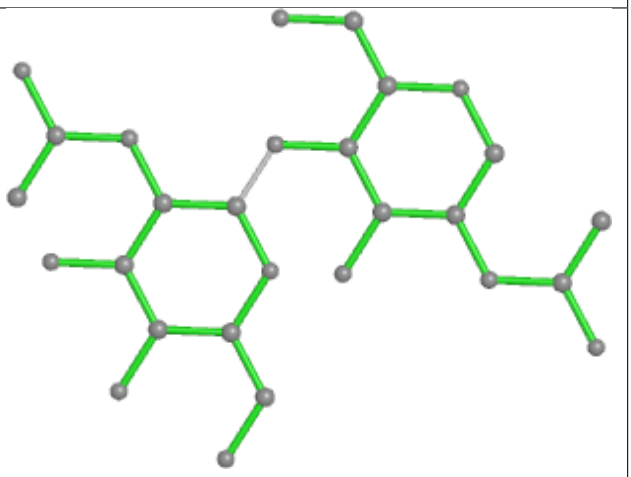
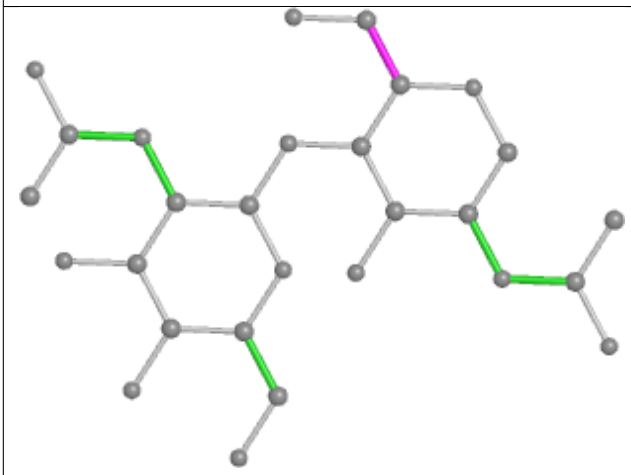
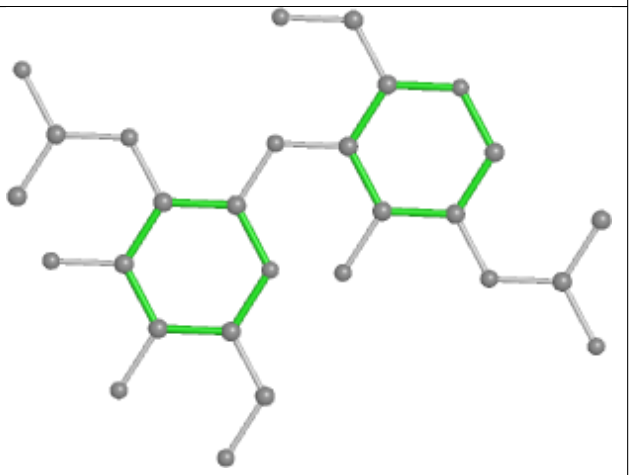
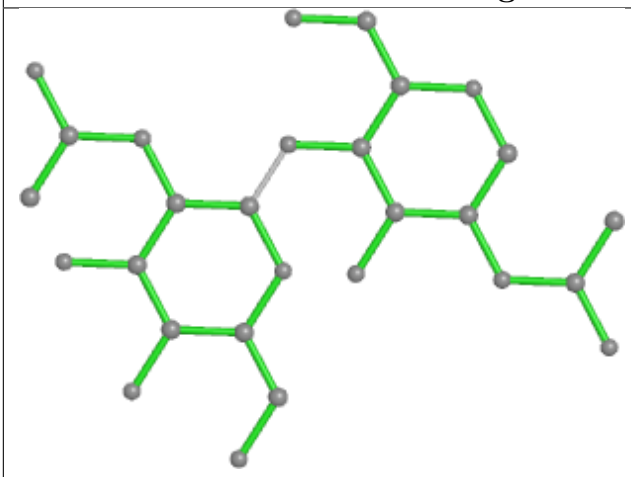


Rings

Oligosaccharide Chain u	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain v



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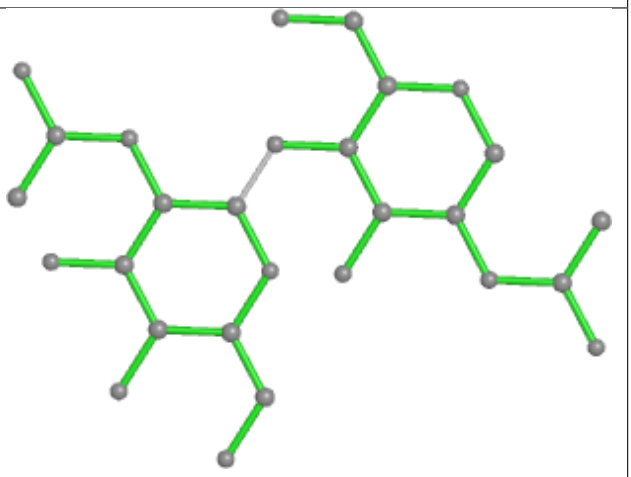
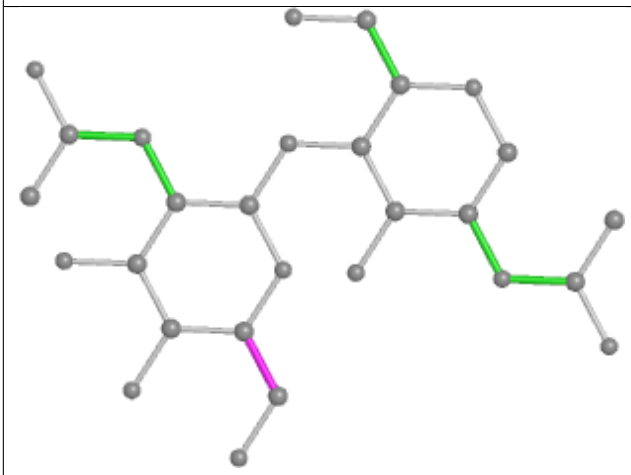


Bond angles



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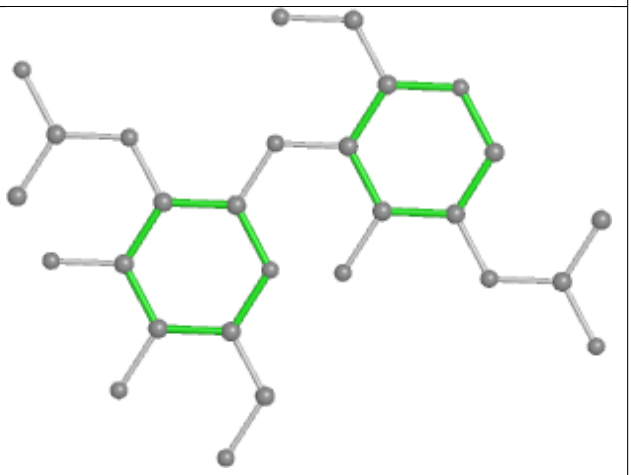
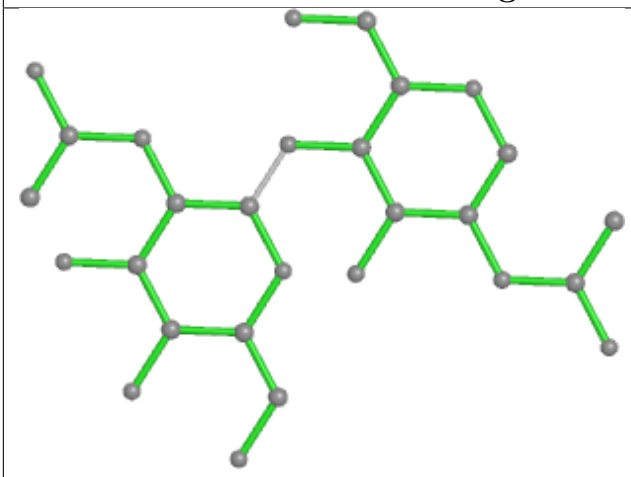


Rings

Oligosaccharide Chain 0



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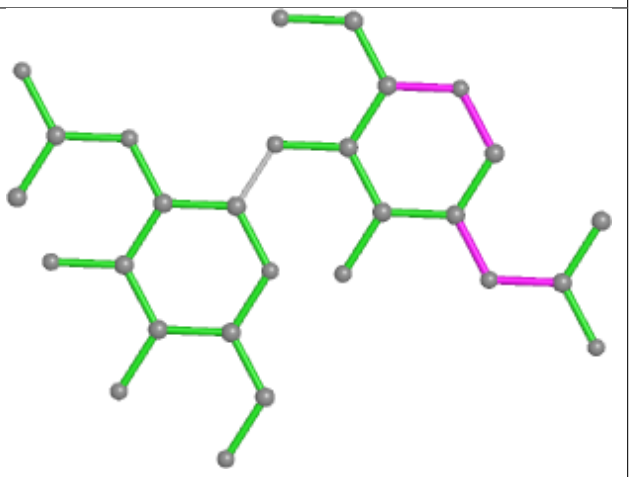

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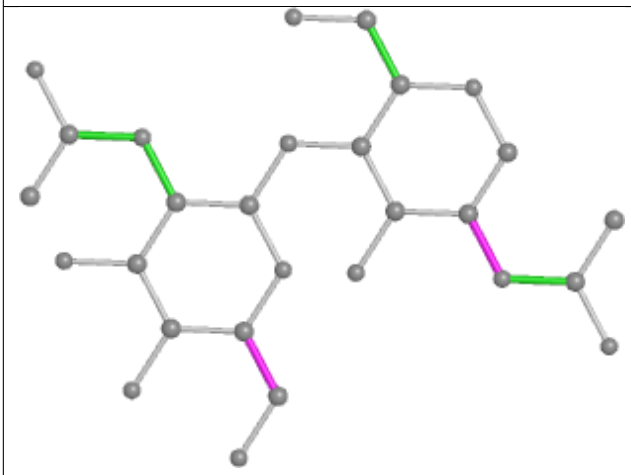

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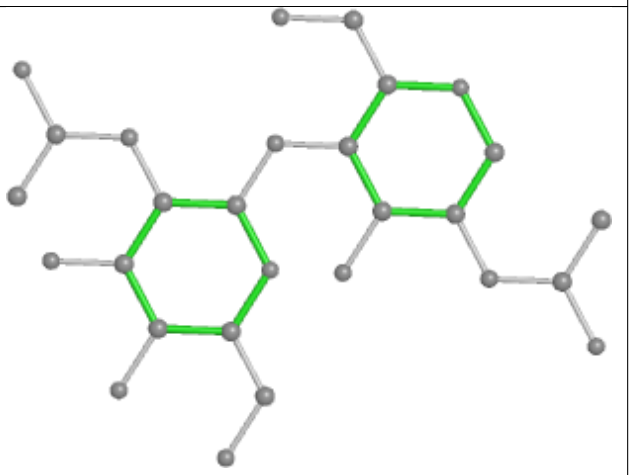
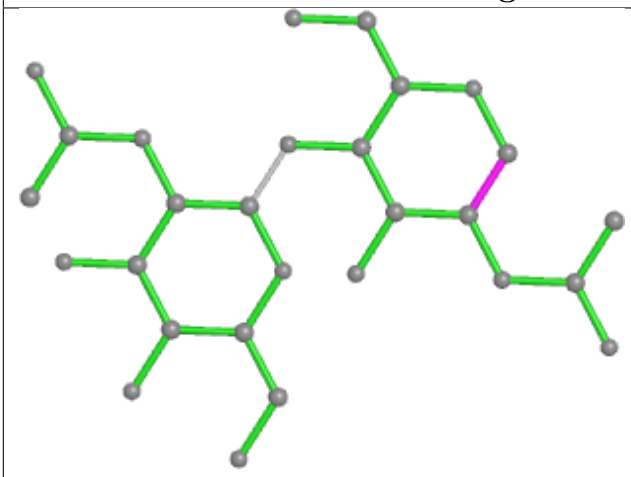


Rings

Oligosaccharide Chain 2



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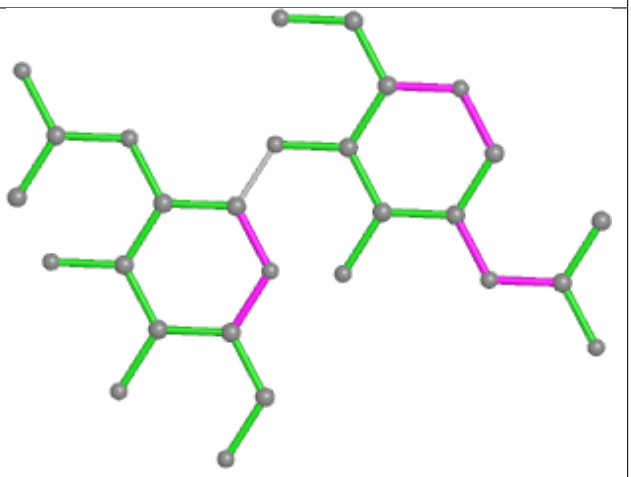

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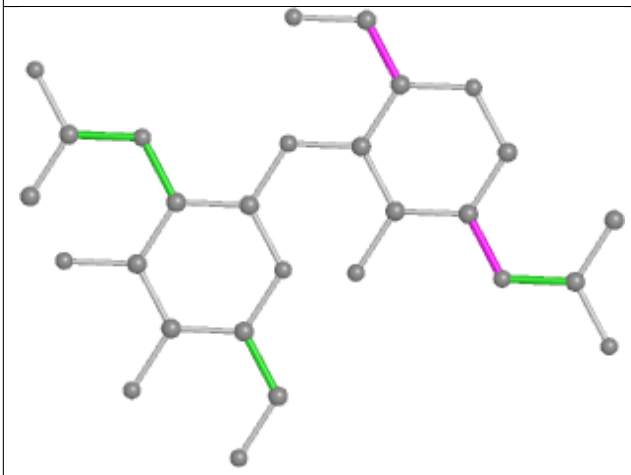

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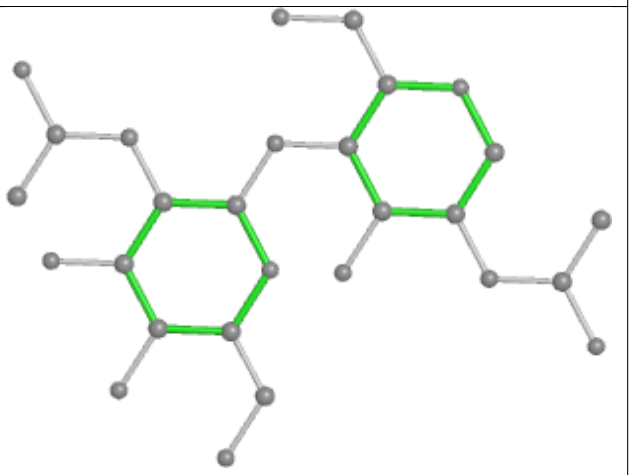
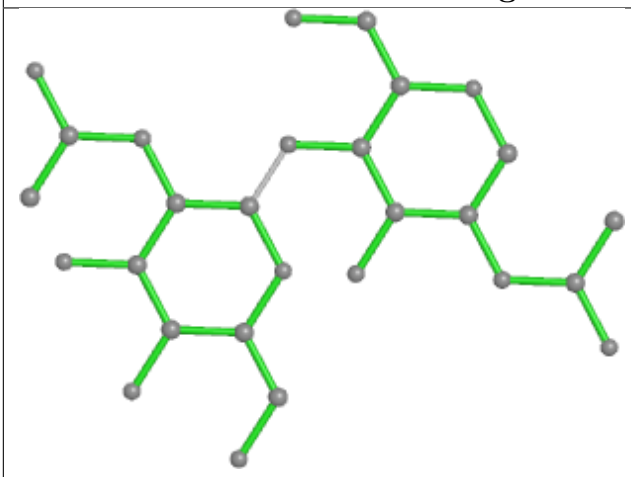


Rings

Oligosaccharide Chain 5



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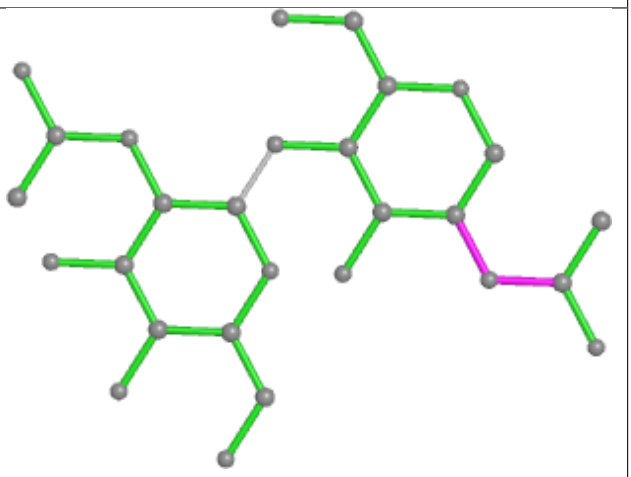

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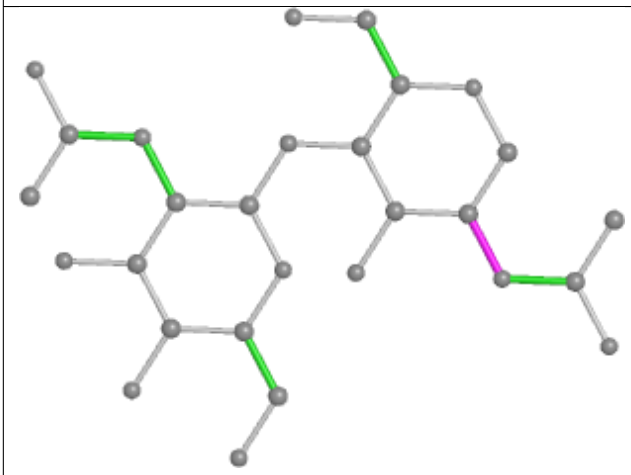

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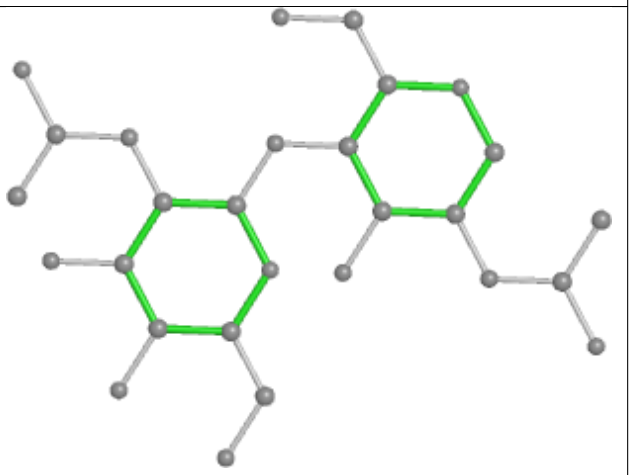
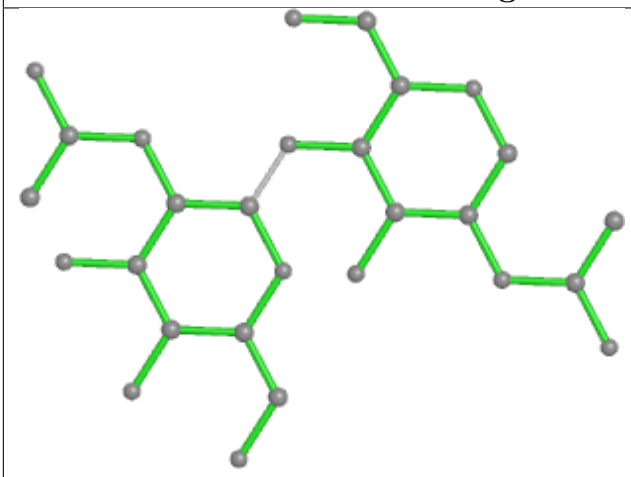
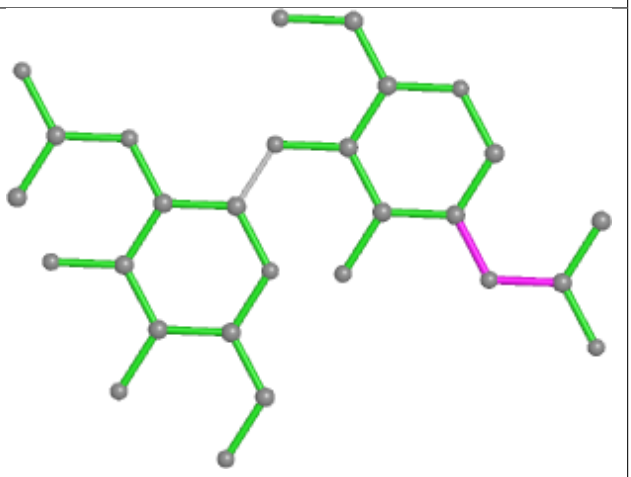


Rings

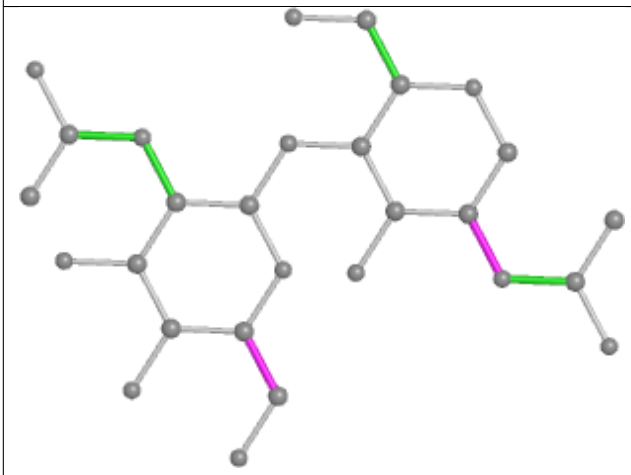
Oligosaccharide Chain 6



Bond lengths



Bond angles



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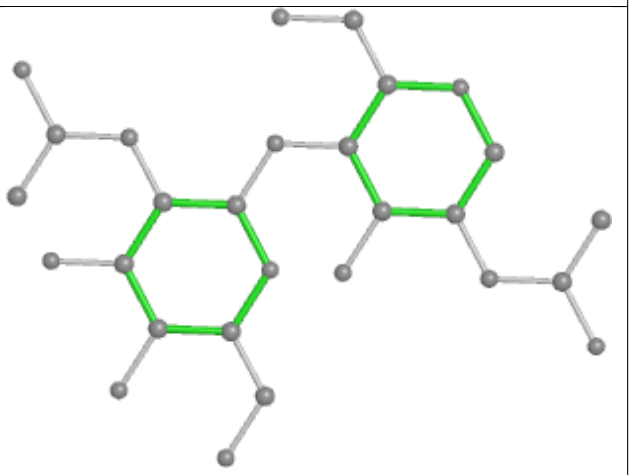
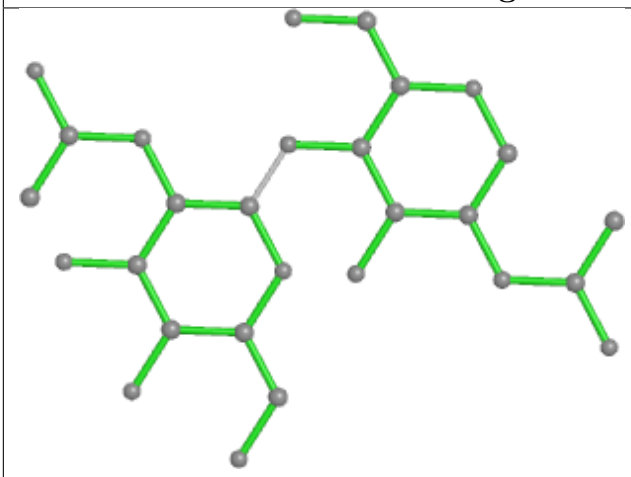


Rings

Oligosaccharide Chain 7



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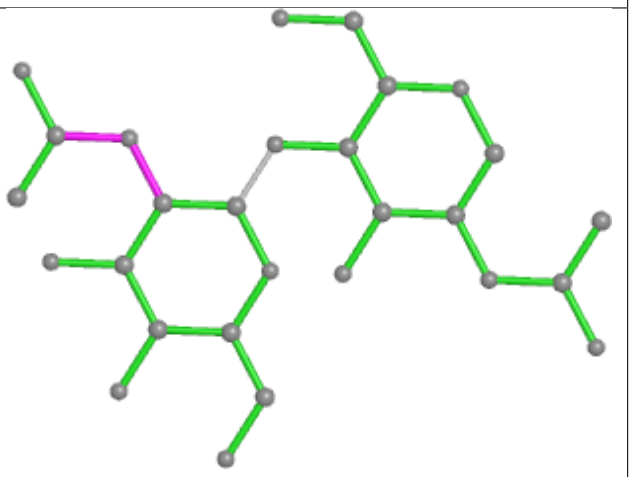
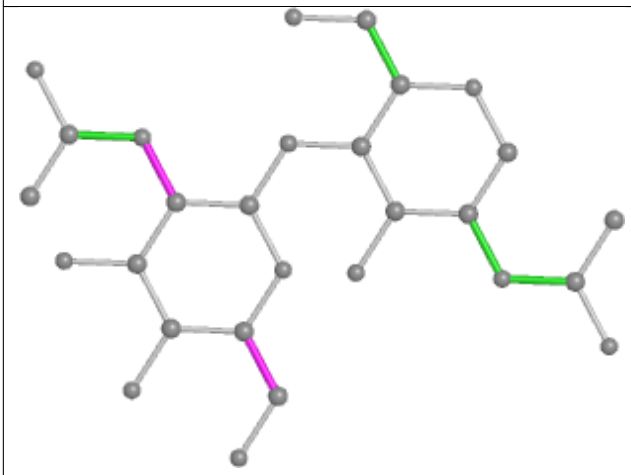
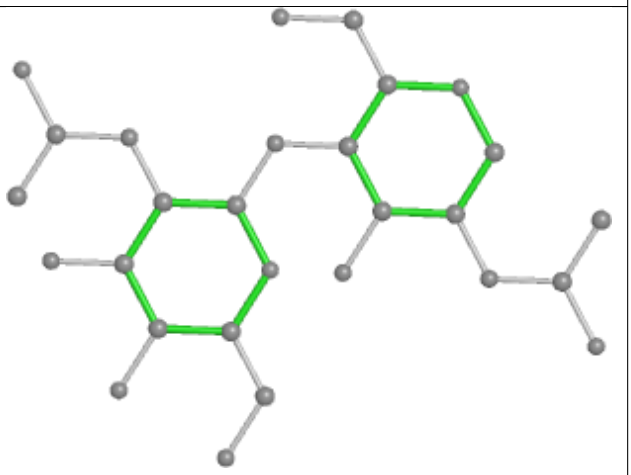


Bond angles

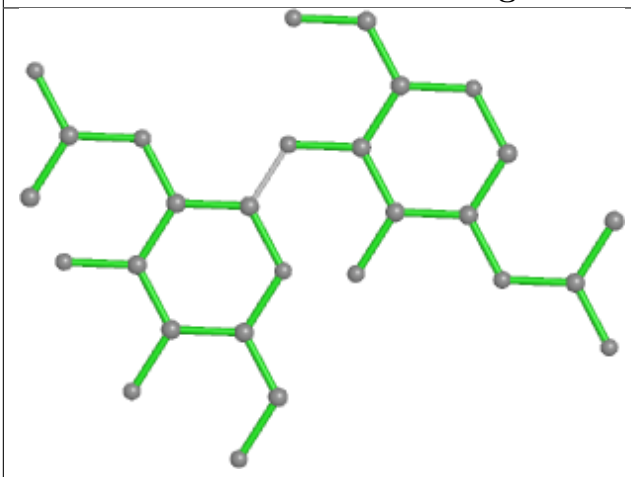


Torsions

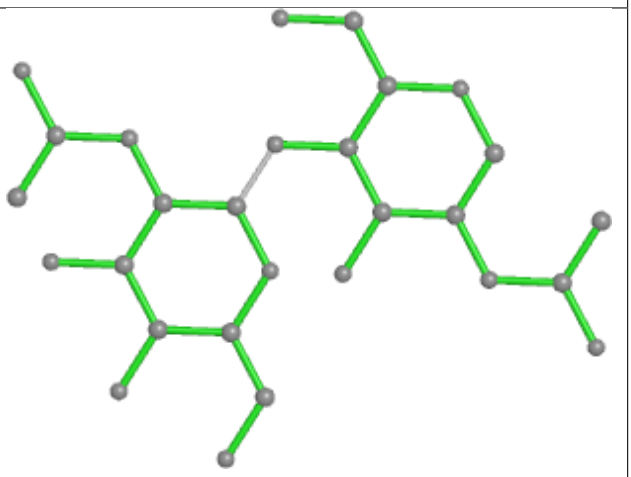


Rings

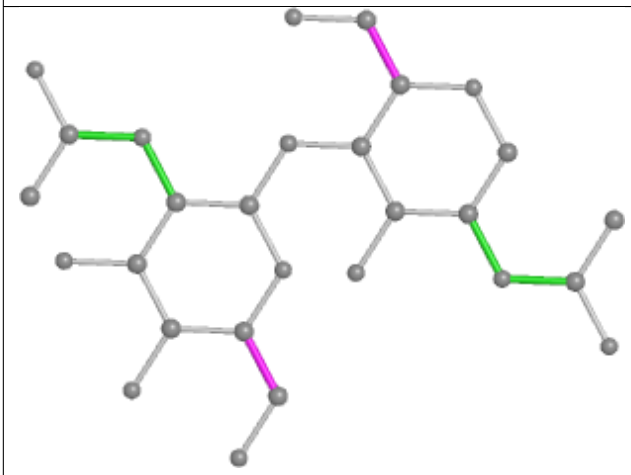
Oligosaccharide Chain 9



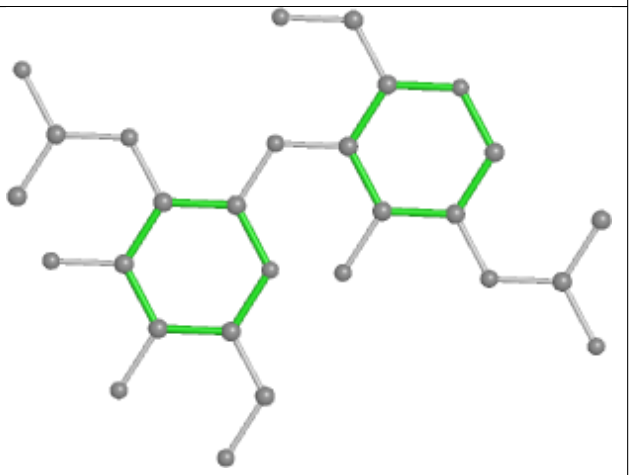
Bond lengths



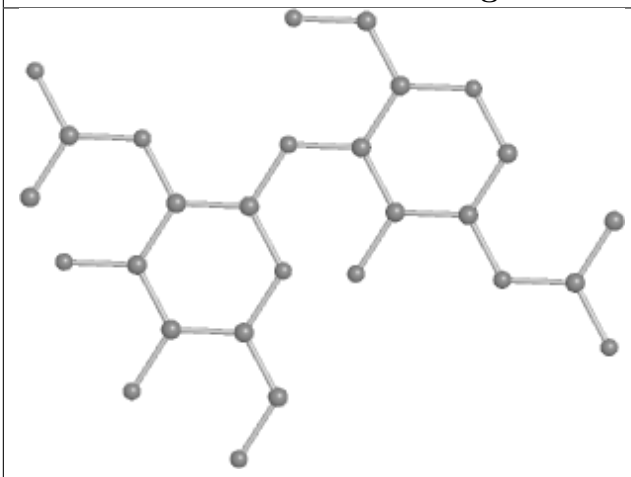
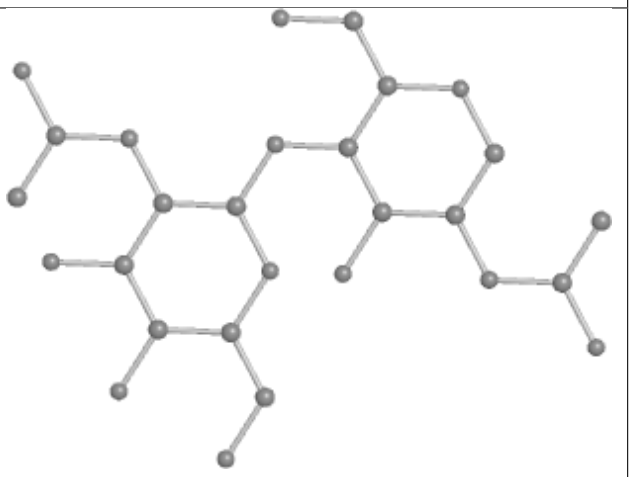
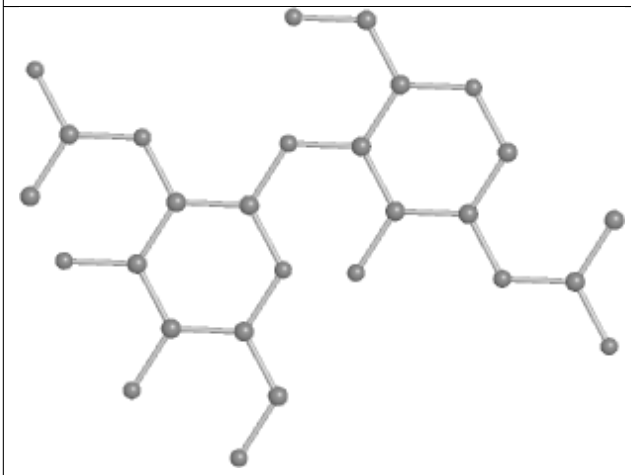
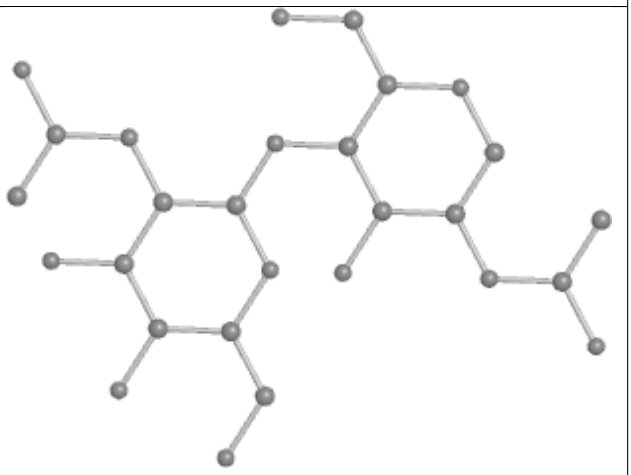
Bond angles

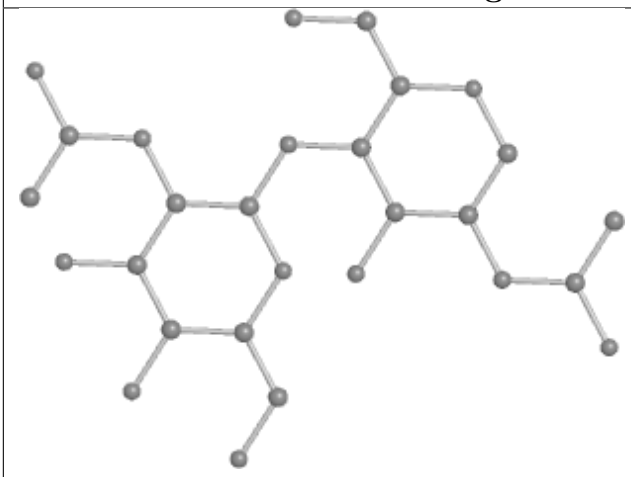
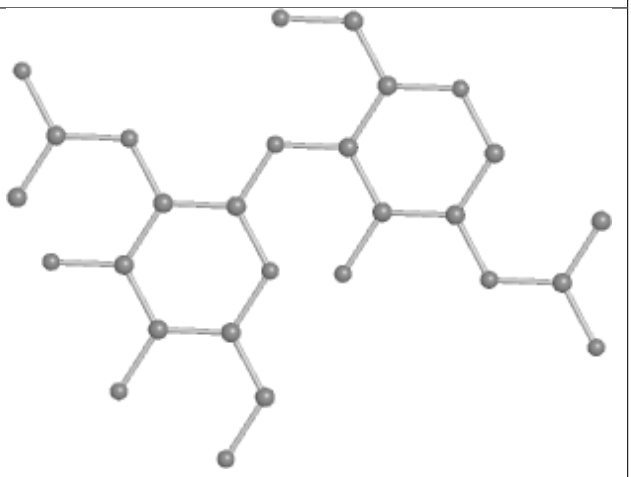
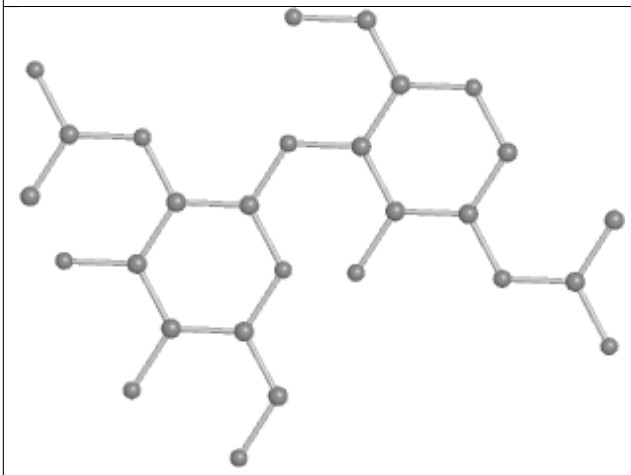
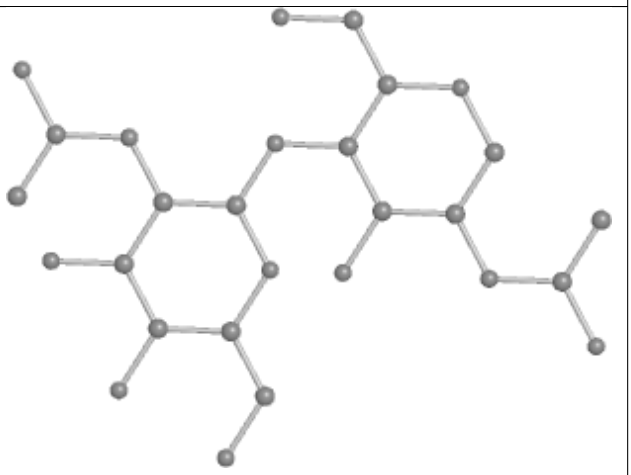


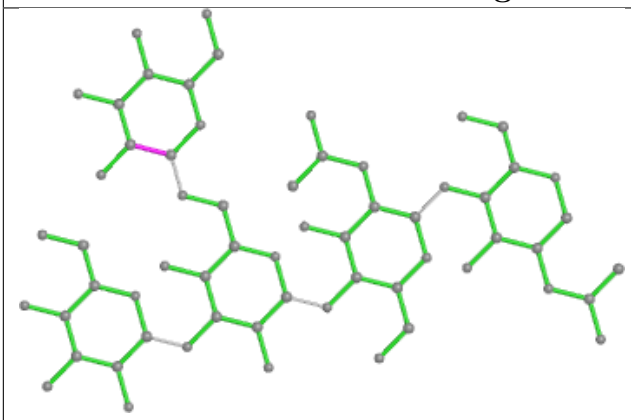
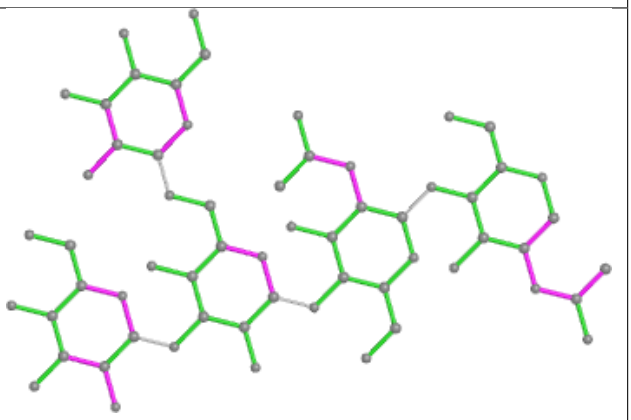
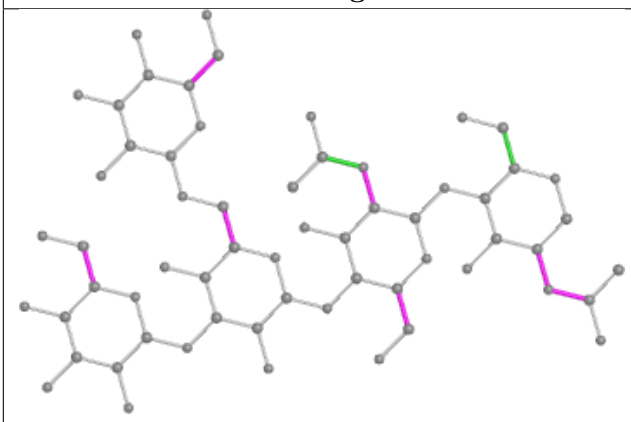
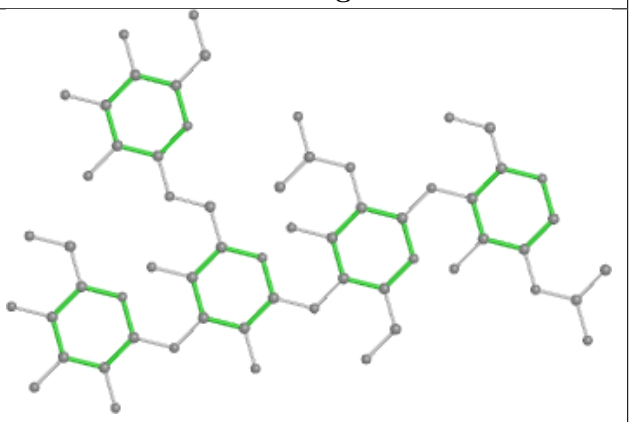
Torsions



Rings

Oligosaccharide Chain AA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain FA	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain V	
 Bond lengths	 Bond angles
 Torsions	 Rings

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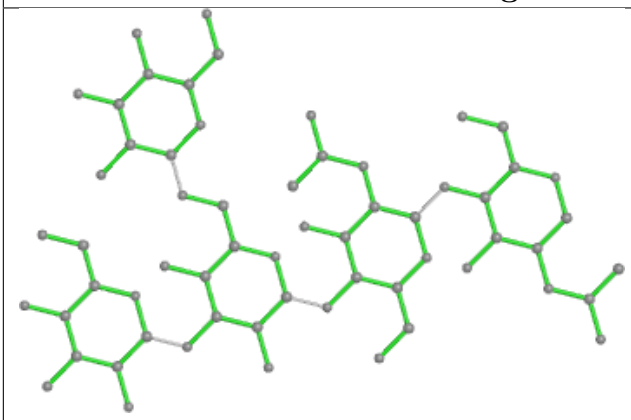
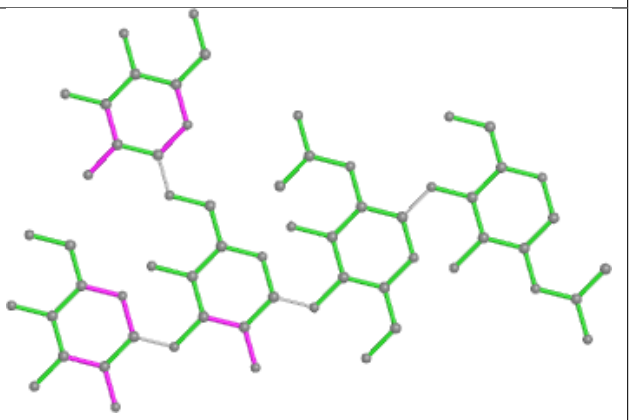
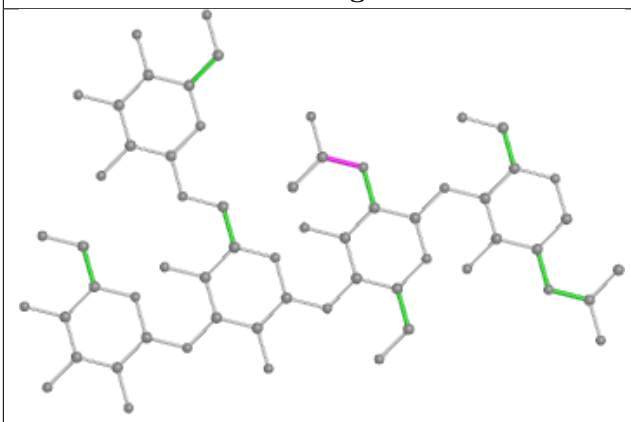
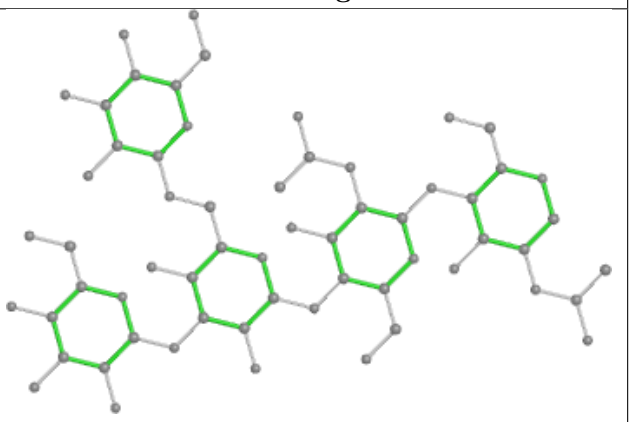
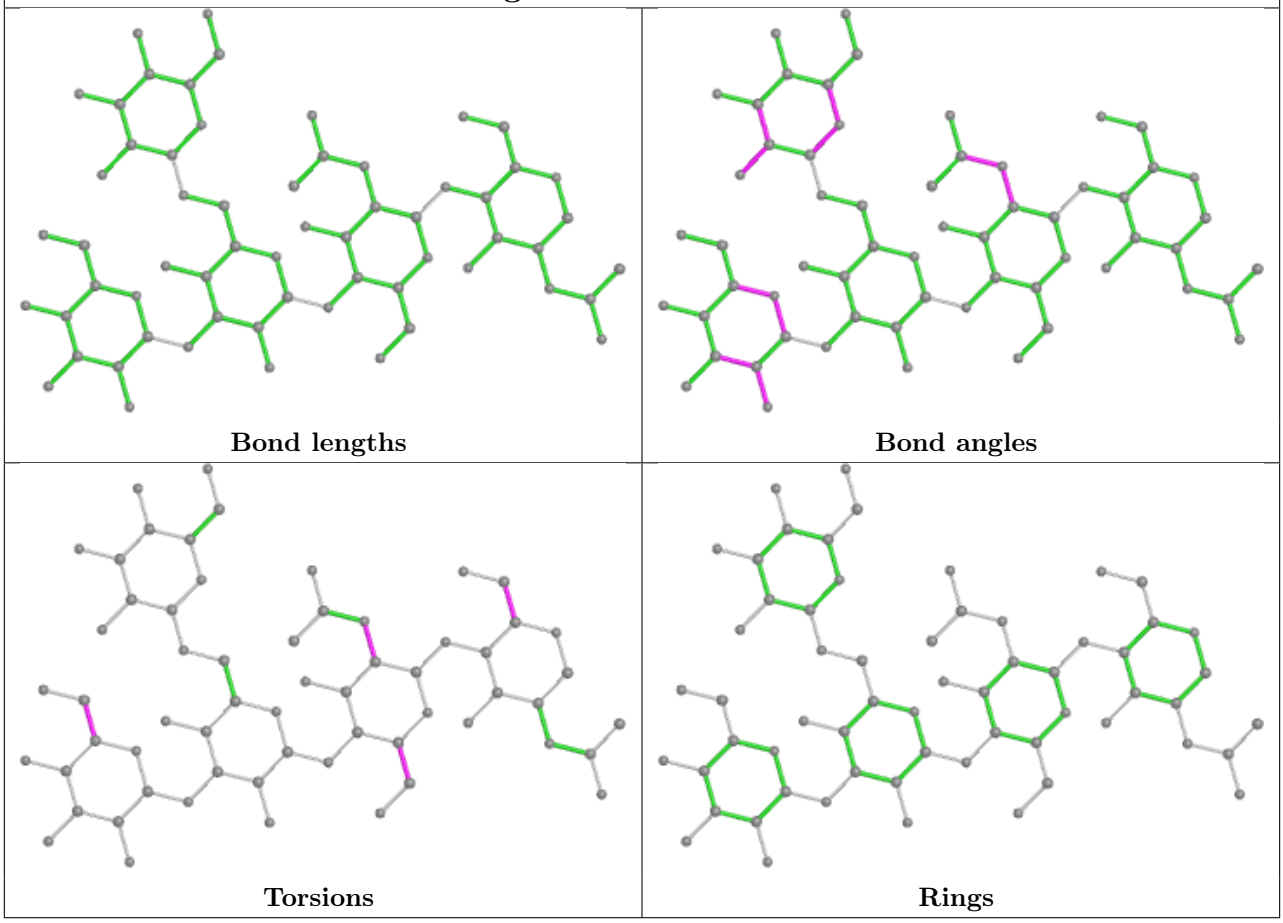
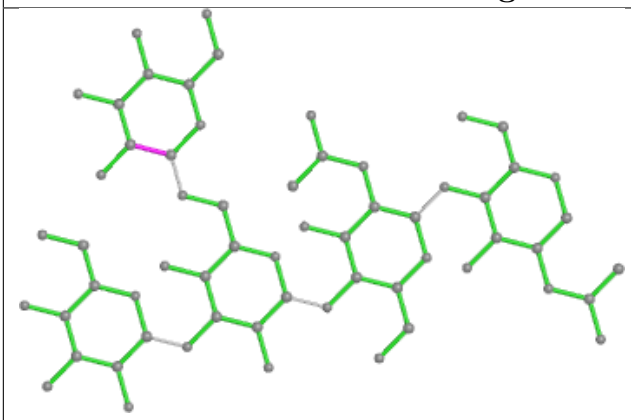
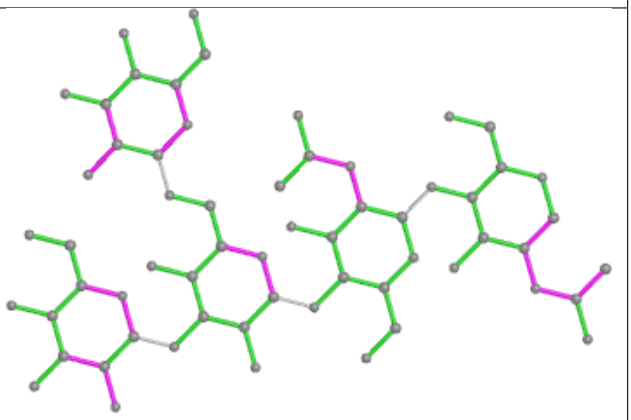
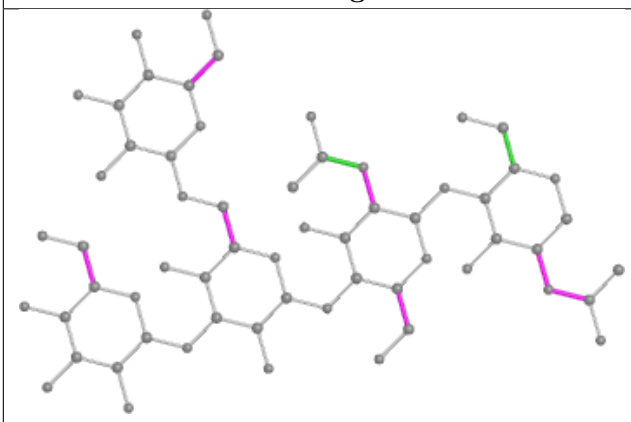
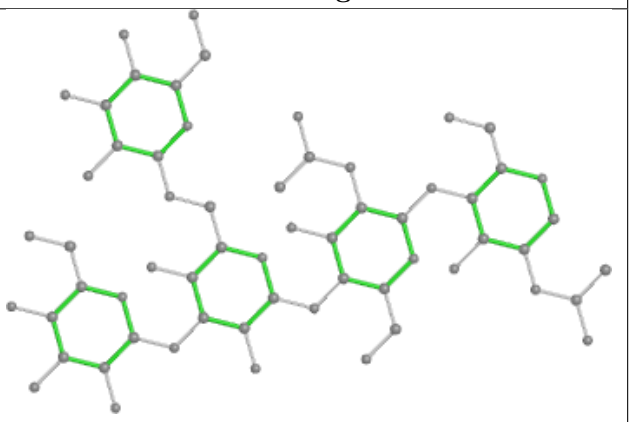
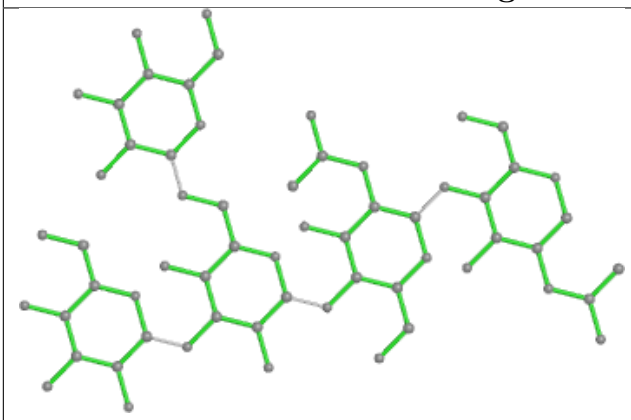
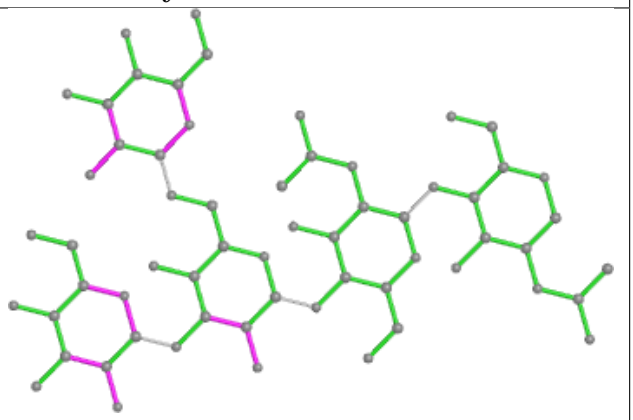
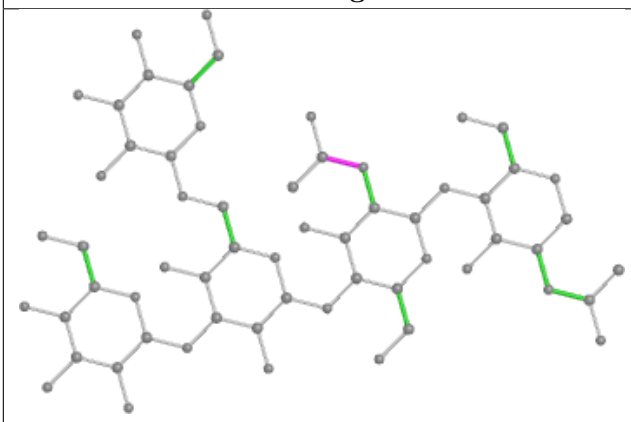
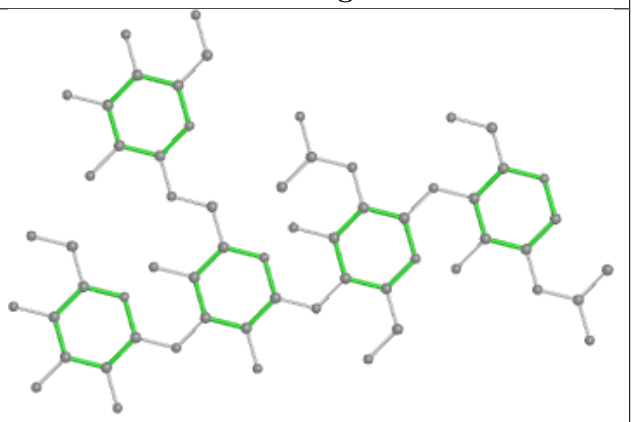
 Bond lengths	 Bond angles
 Torsions	 Rings

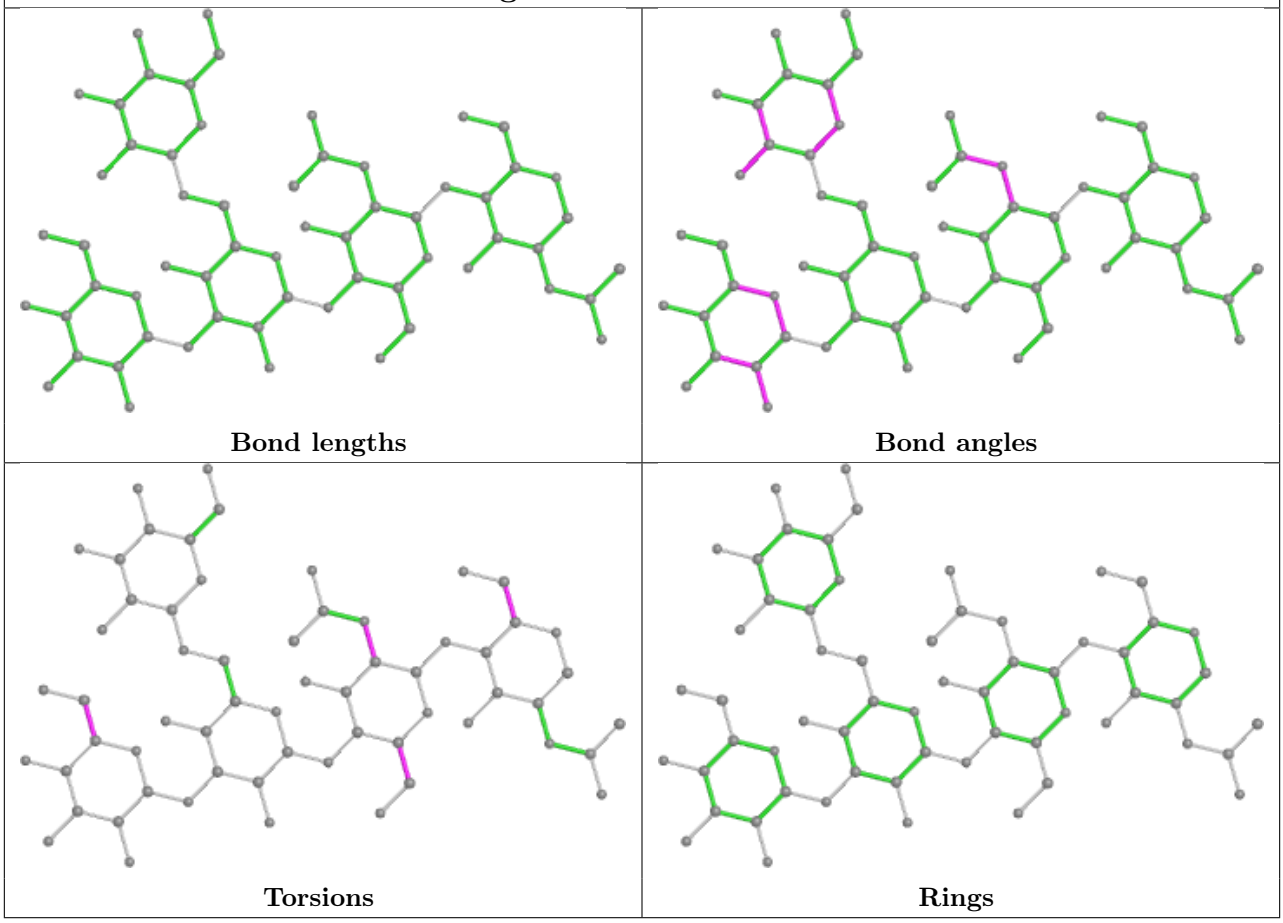
Oligosaccharide Chain i



Oligosaccharide Chain k	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain y	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain 1



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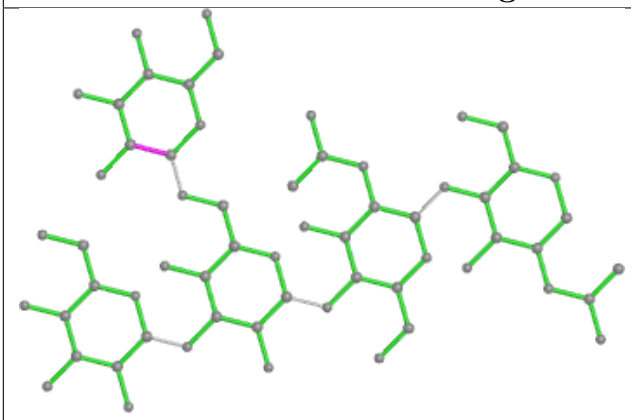
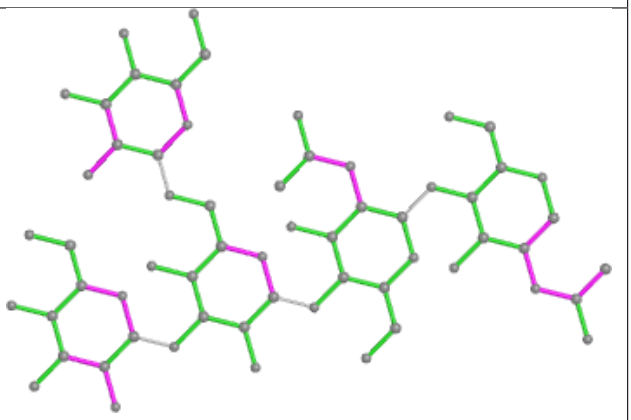
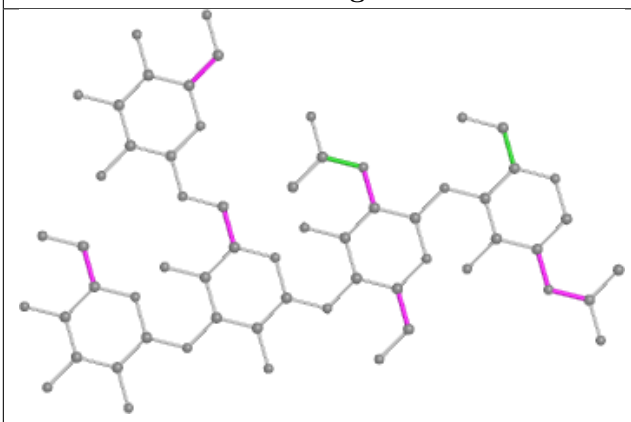
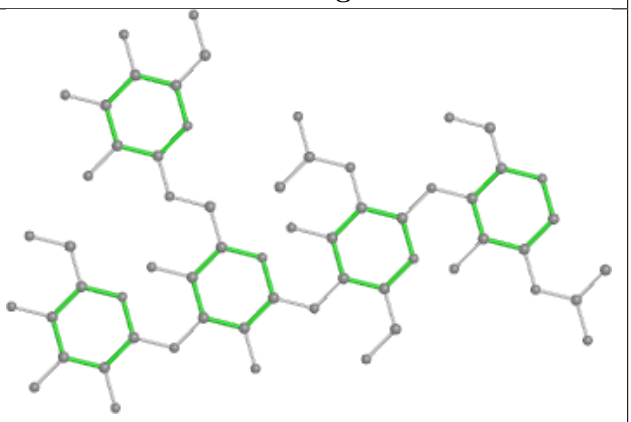
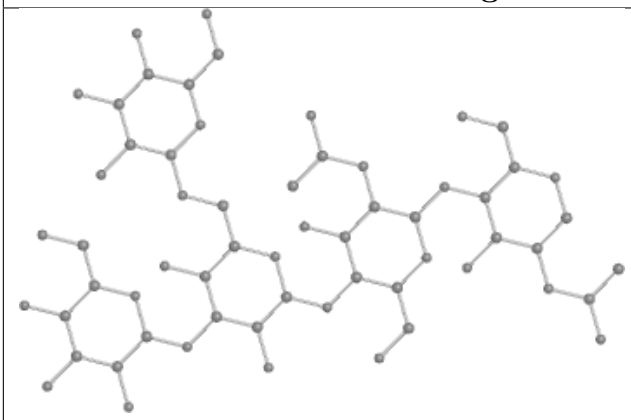
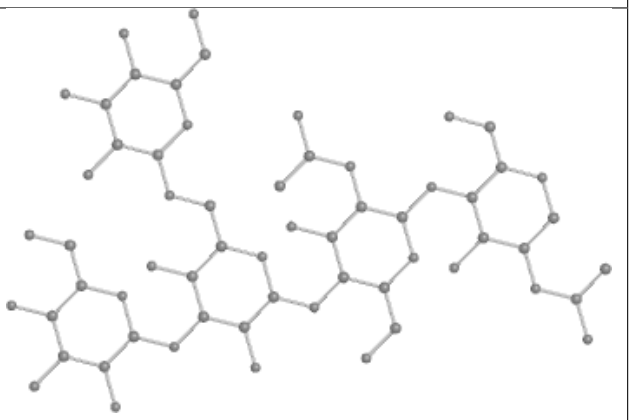
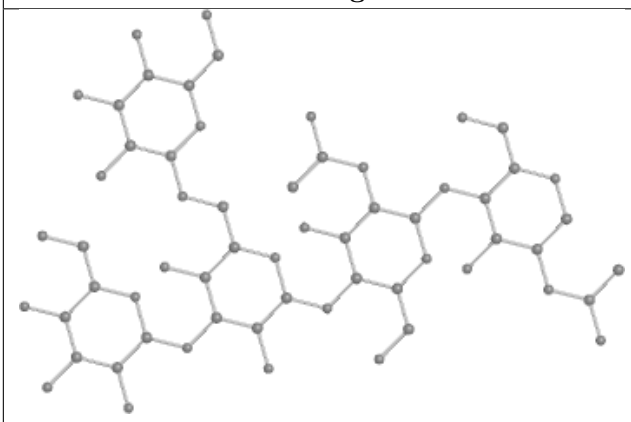
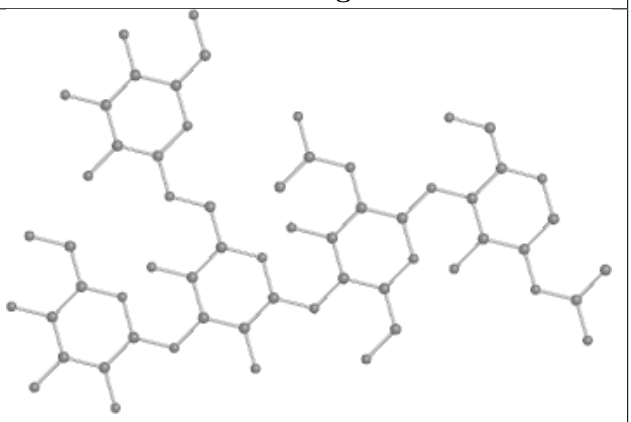
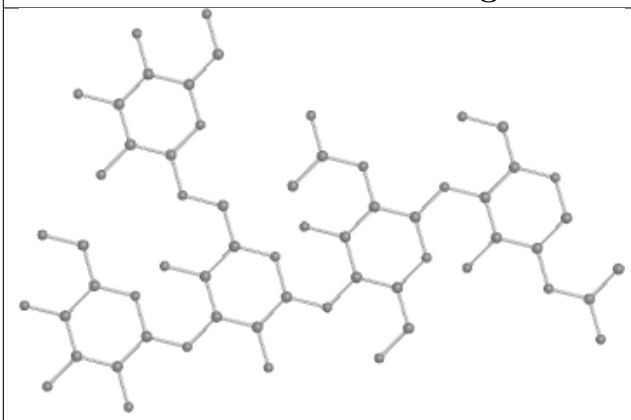
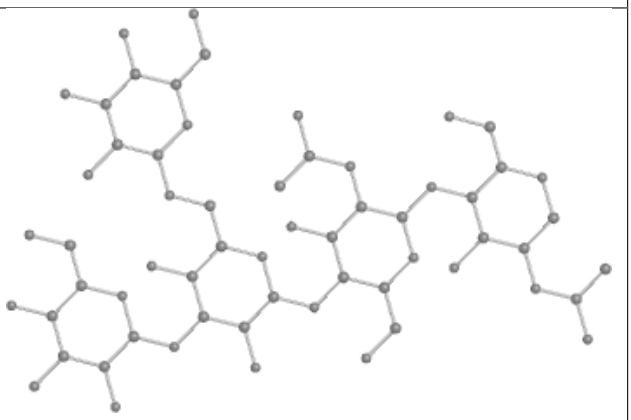
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain DA	
 Bond lengths	 Bond angles
 Torsions	 Rings

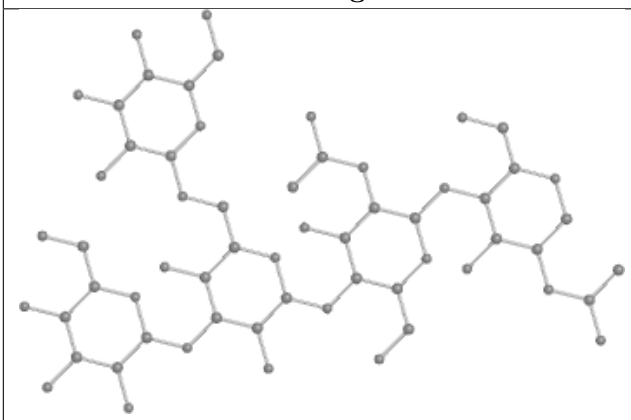
Oligosaccharide Chain GA



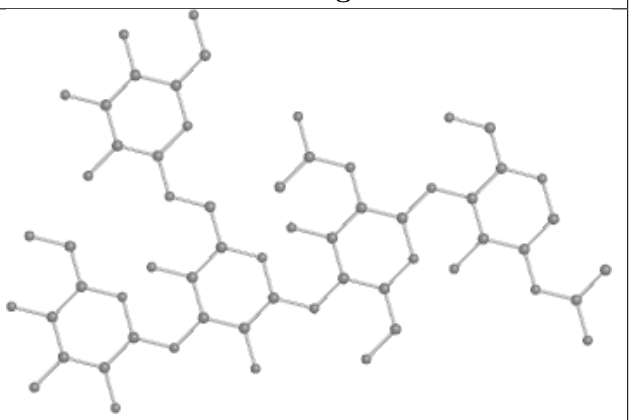
Bond lengths



Bond angles

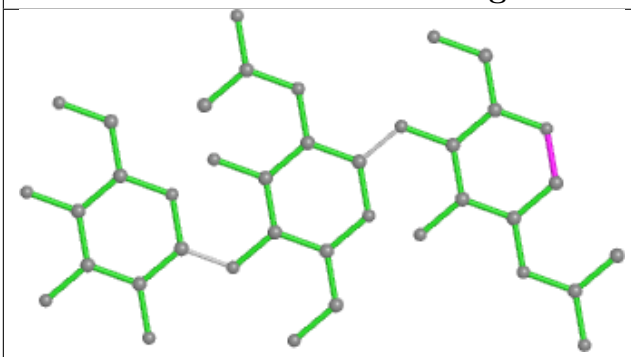


Torsions

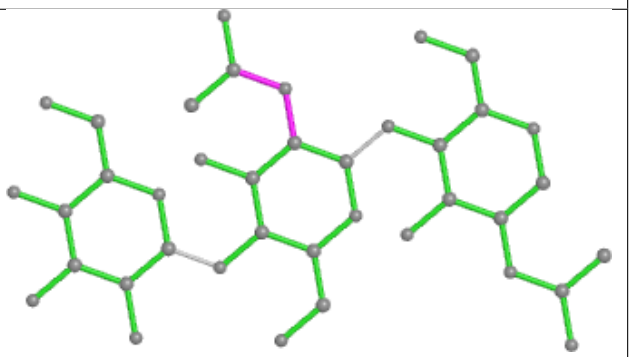


Rings

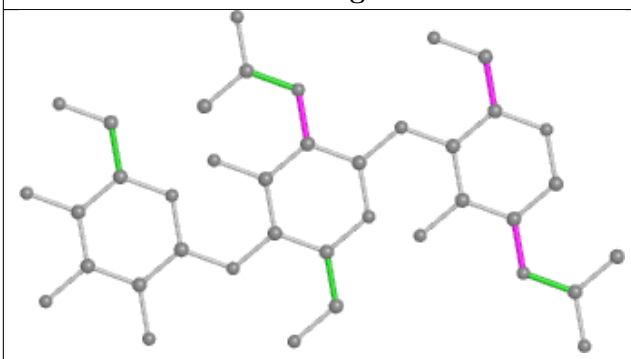
Oligosaccharide Chain W



Bond lengths



Bond angles



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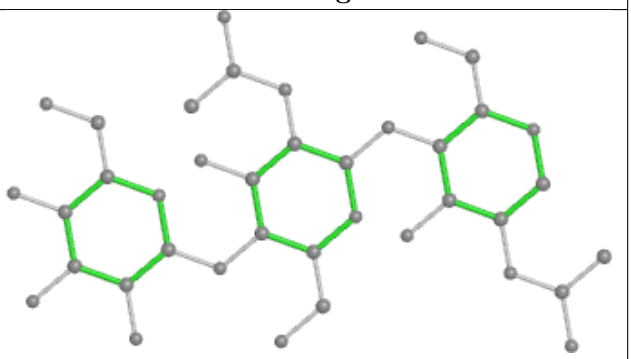
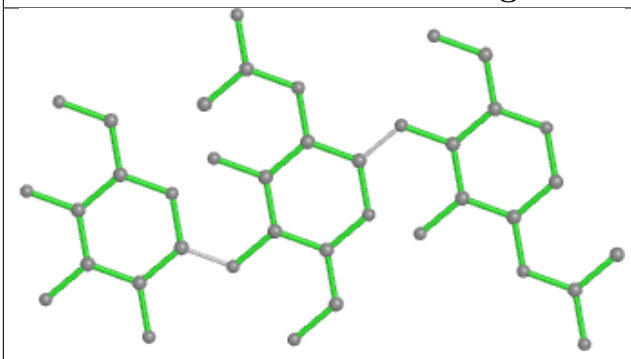
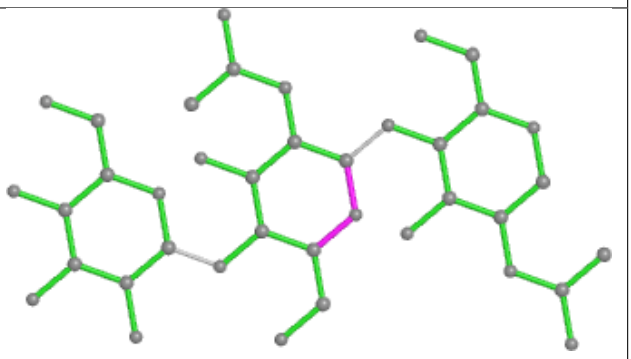


Rings

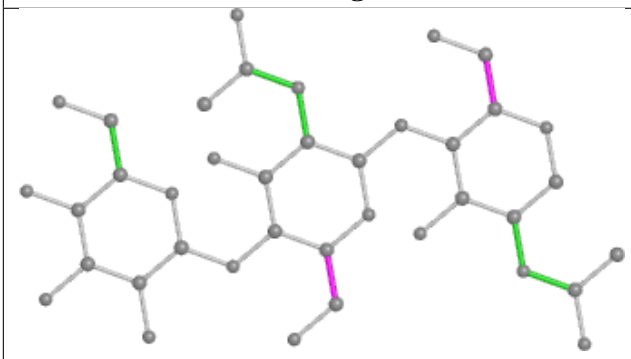
Oligosaccharide Chain e



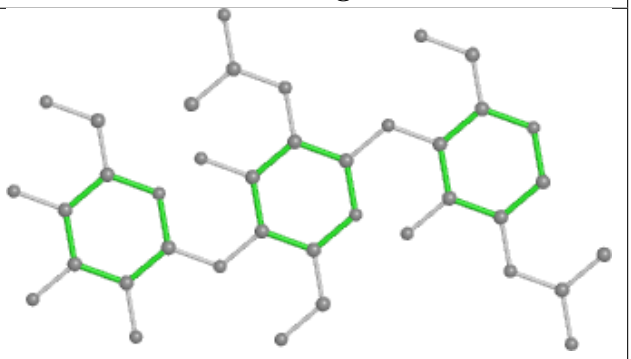
Bond lengths



Bond angles

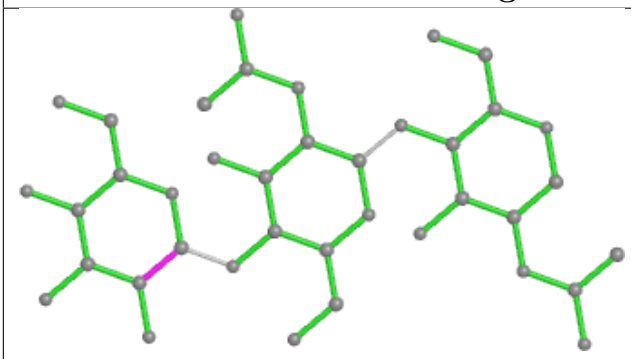


Torsions

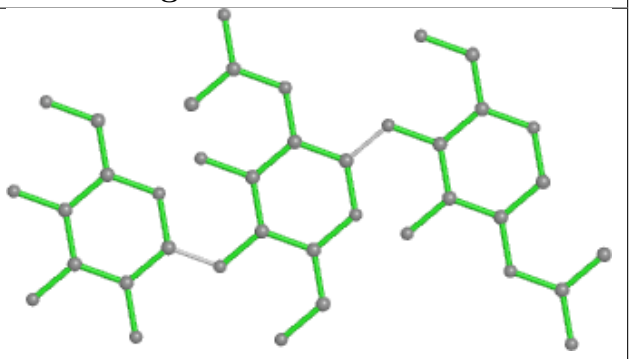


Rings

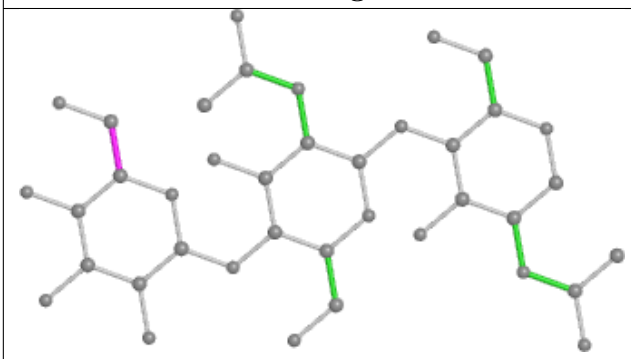
Oligosaccharide Chain g



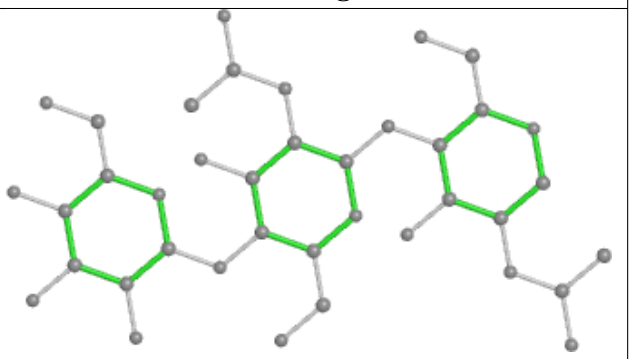
Bond lengths



Bond angles

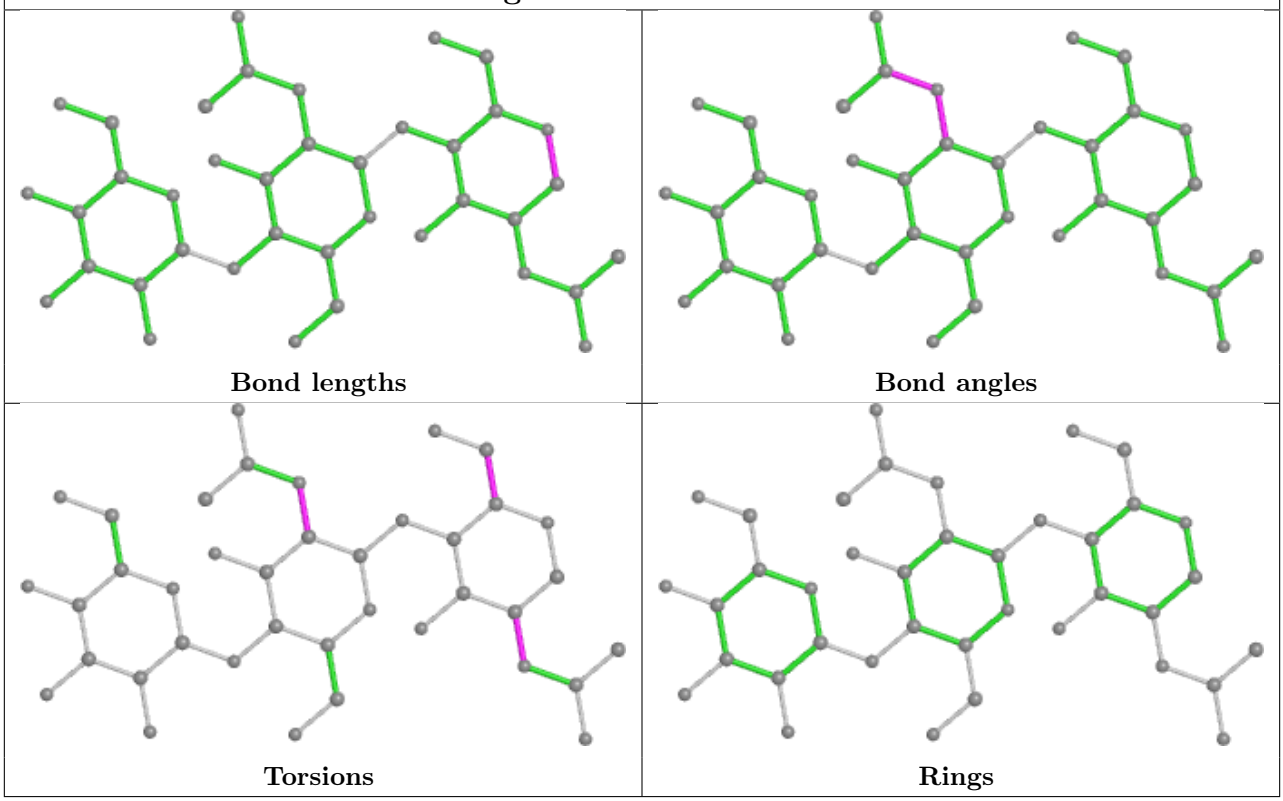


Torsions

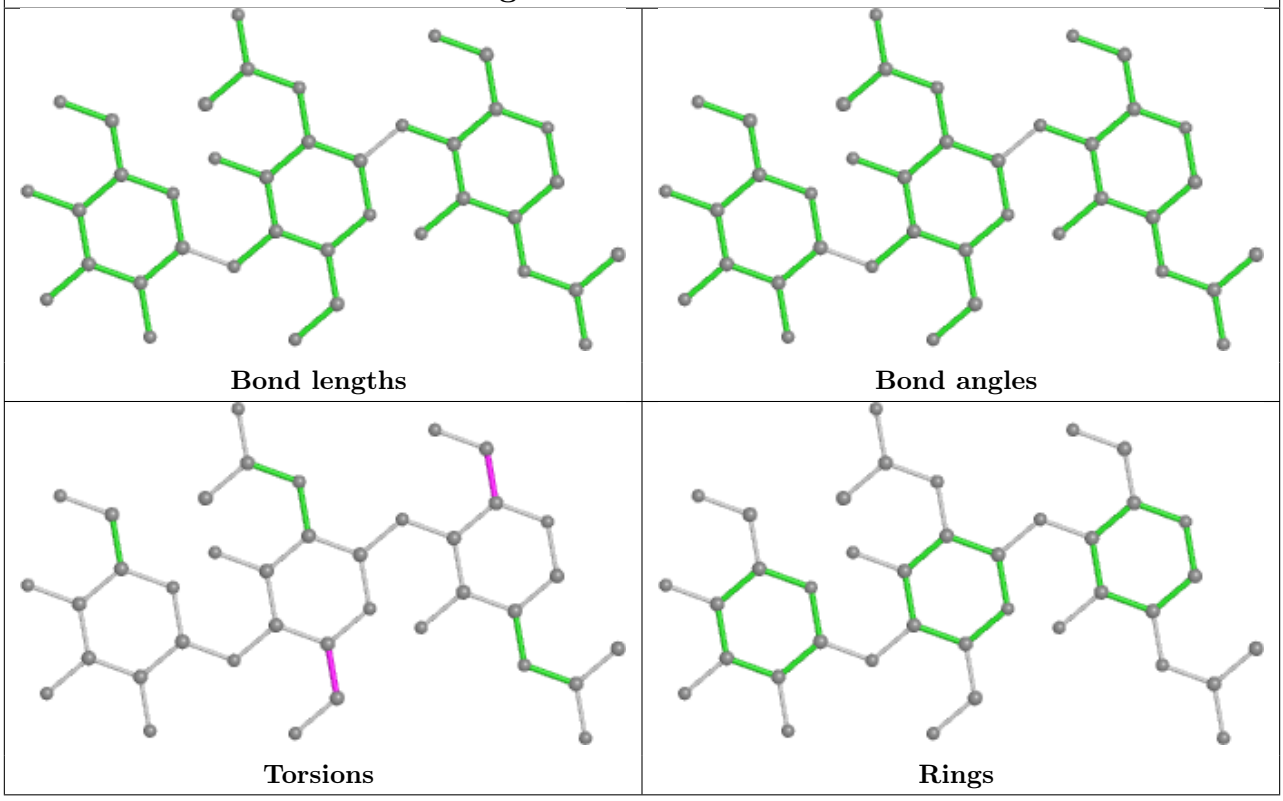


Rings

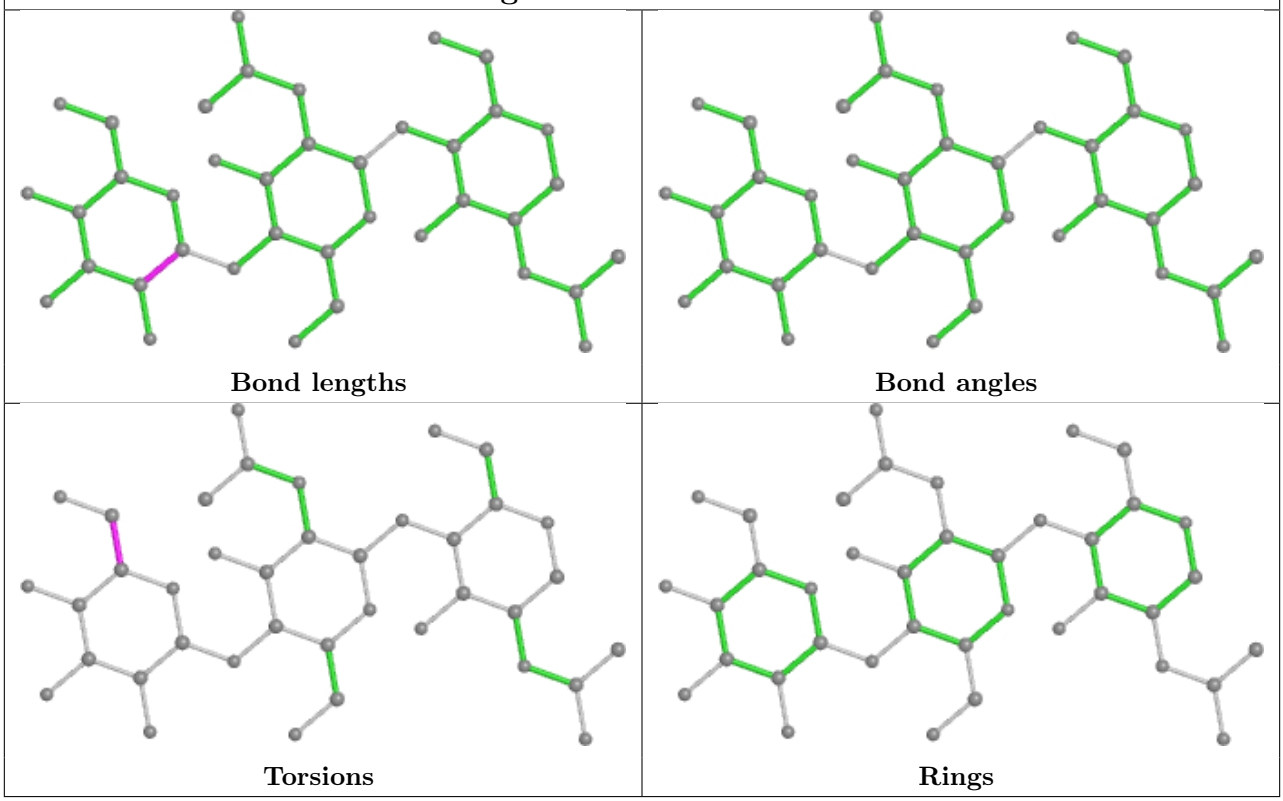
Oligosaccharide Chain l



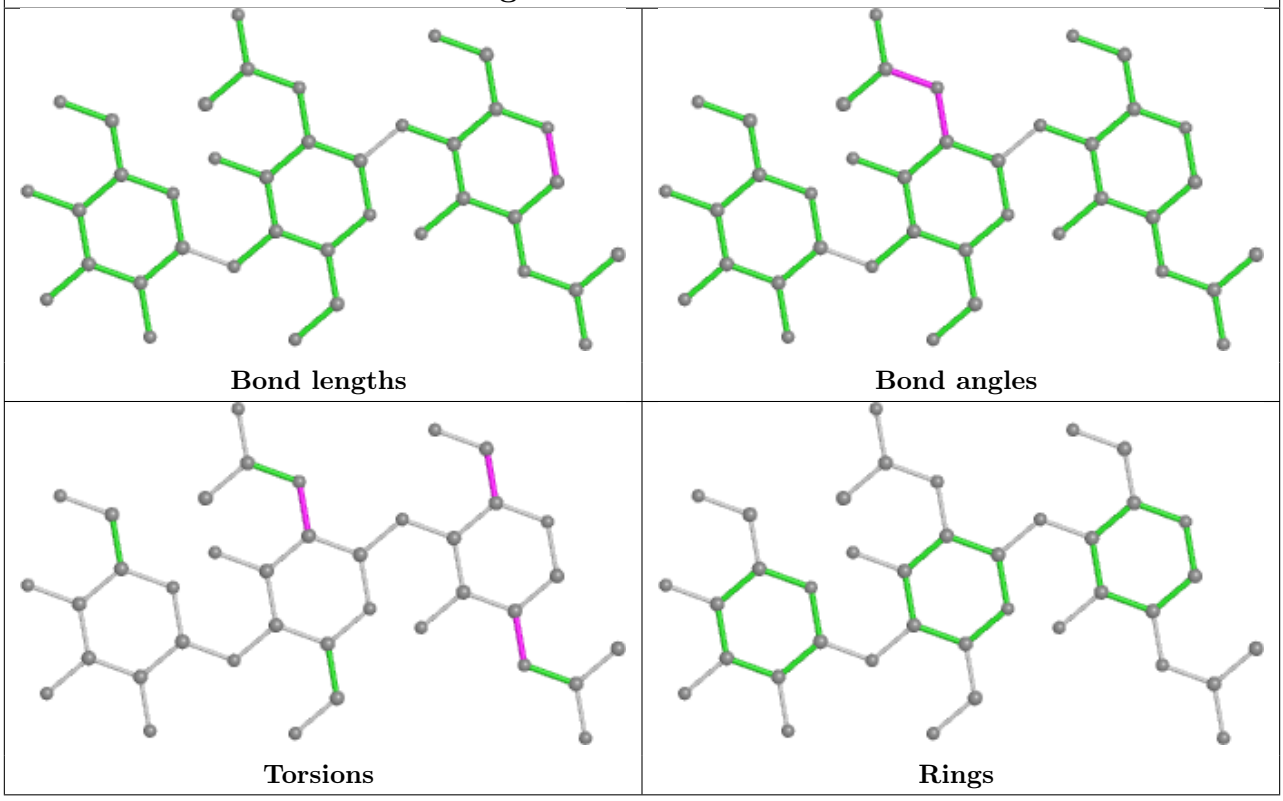
Oligosaccharide Chain x



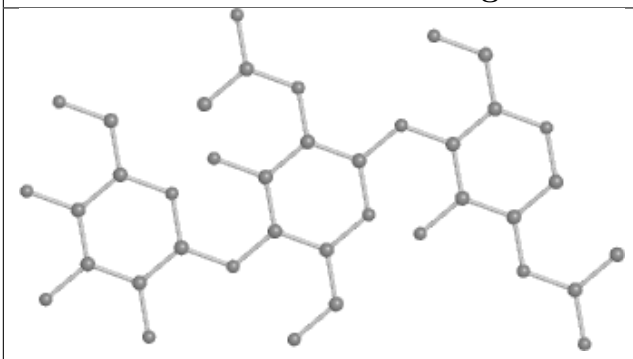
Oligosaccharide Chain z



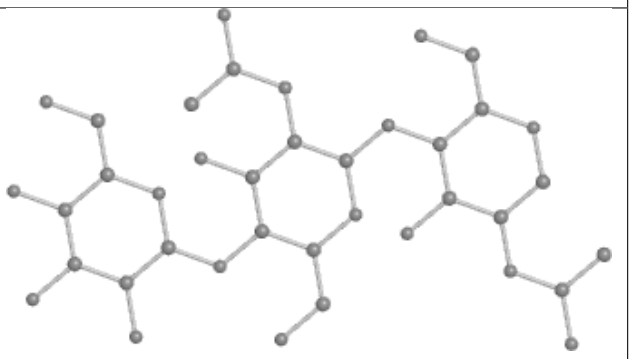
Oligosaccharide Chain 4



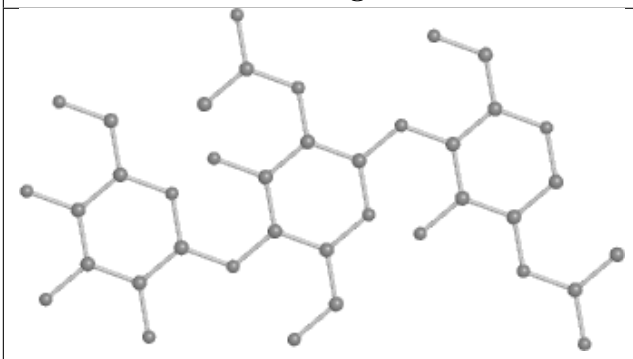
Oligosaccharide Chain CA



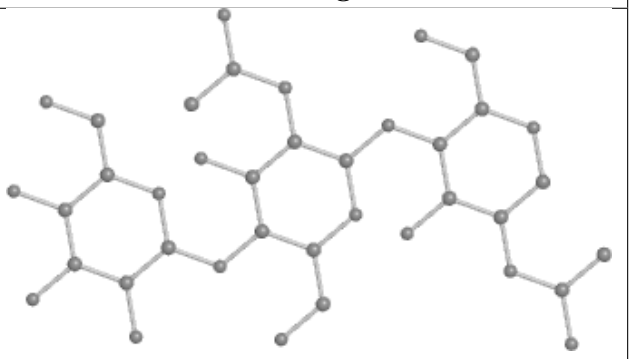
Bond lengths



Bond angles

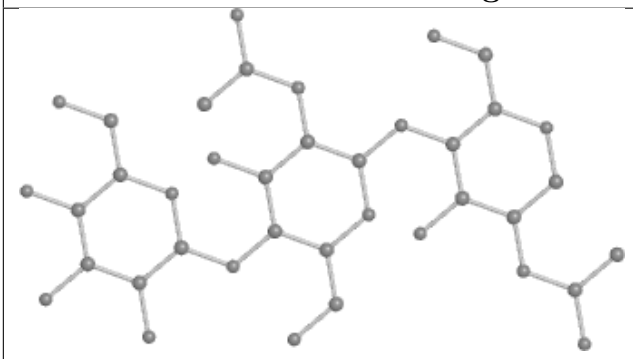


Torsions

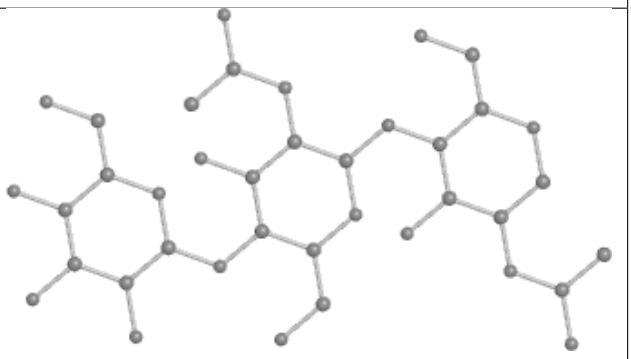


Rings

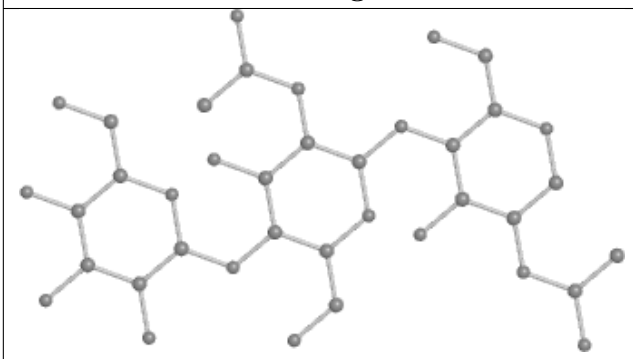
Oligosaccharide Chain EA



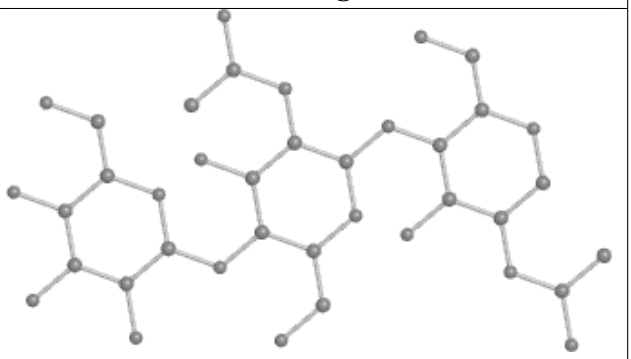
Bond lengths



Bond angles

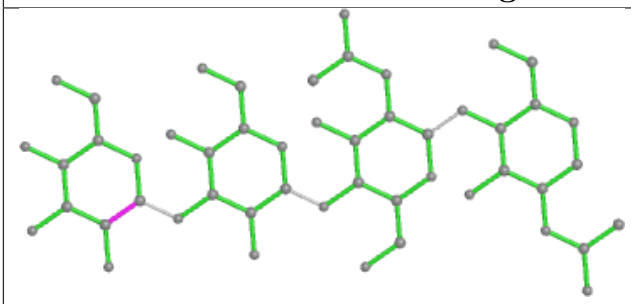


Torsions

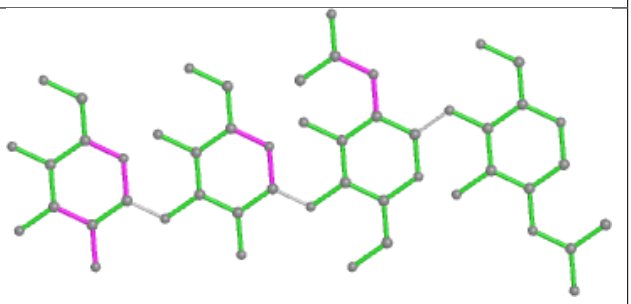


Rings

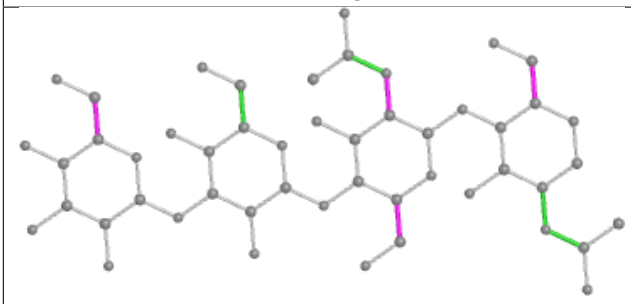
Oligosaccharide Chain a



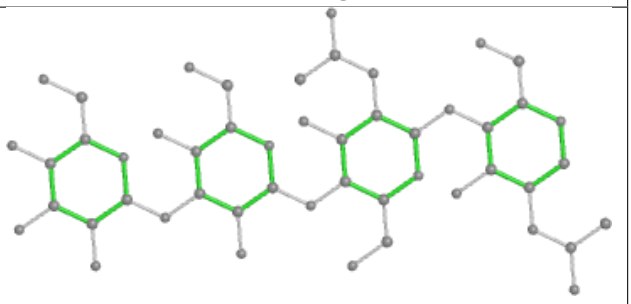
Bond lengths



Bond angles

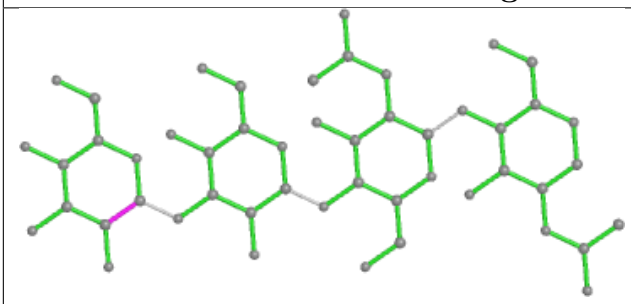


Torsions

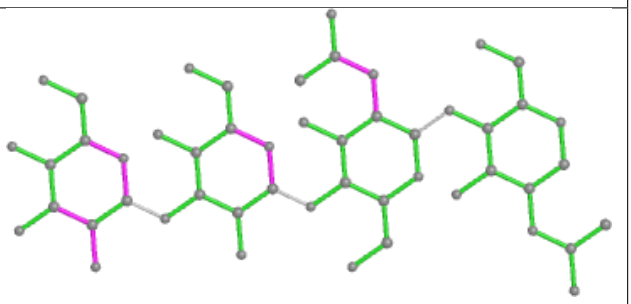


Rings

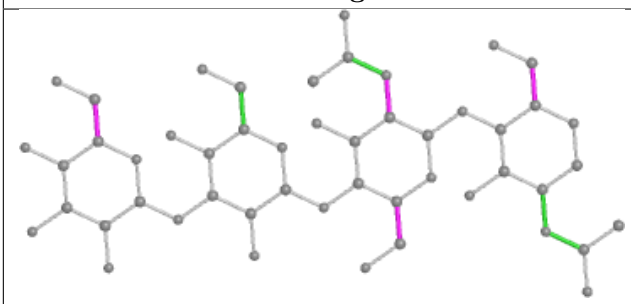
Oligosaccharide Chain t



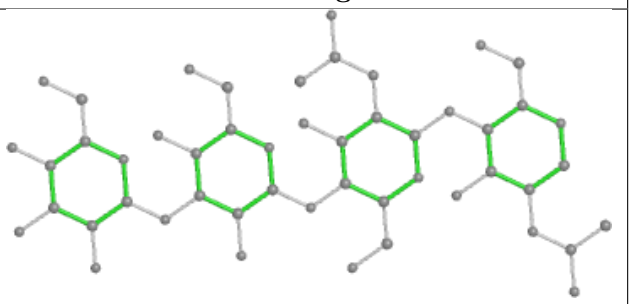
Bond lengths



Bond angles

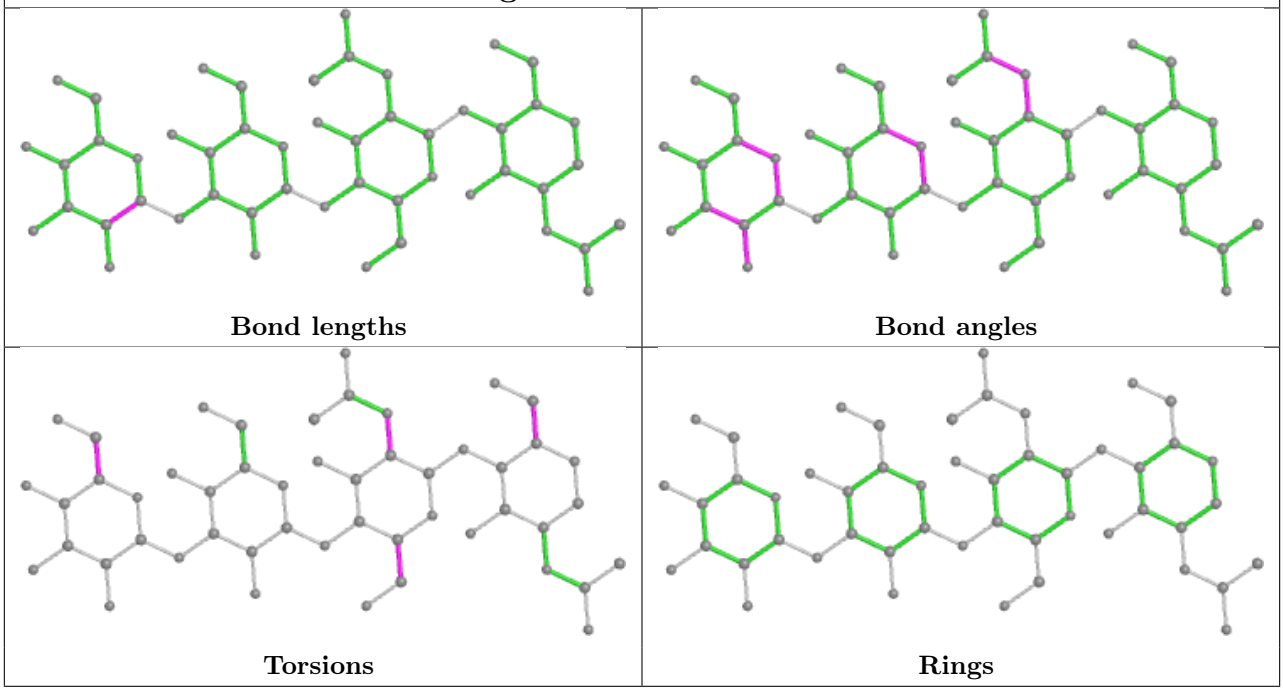


Torsions

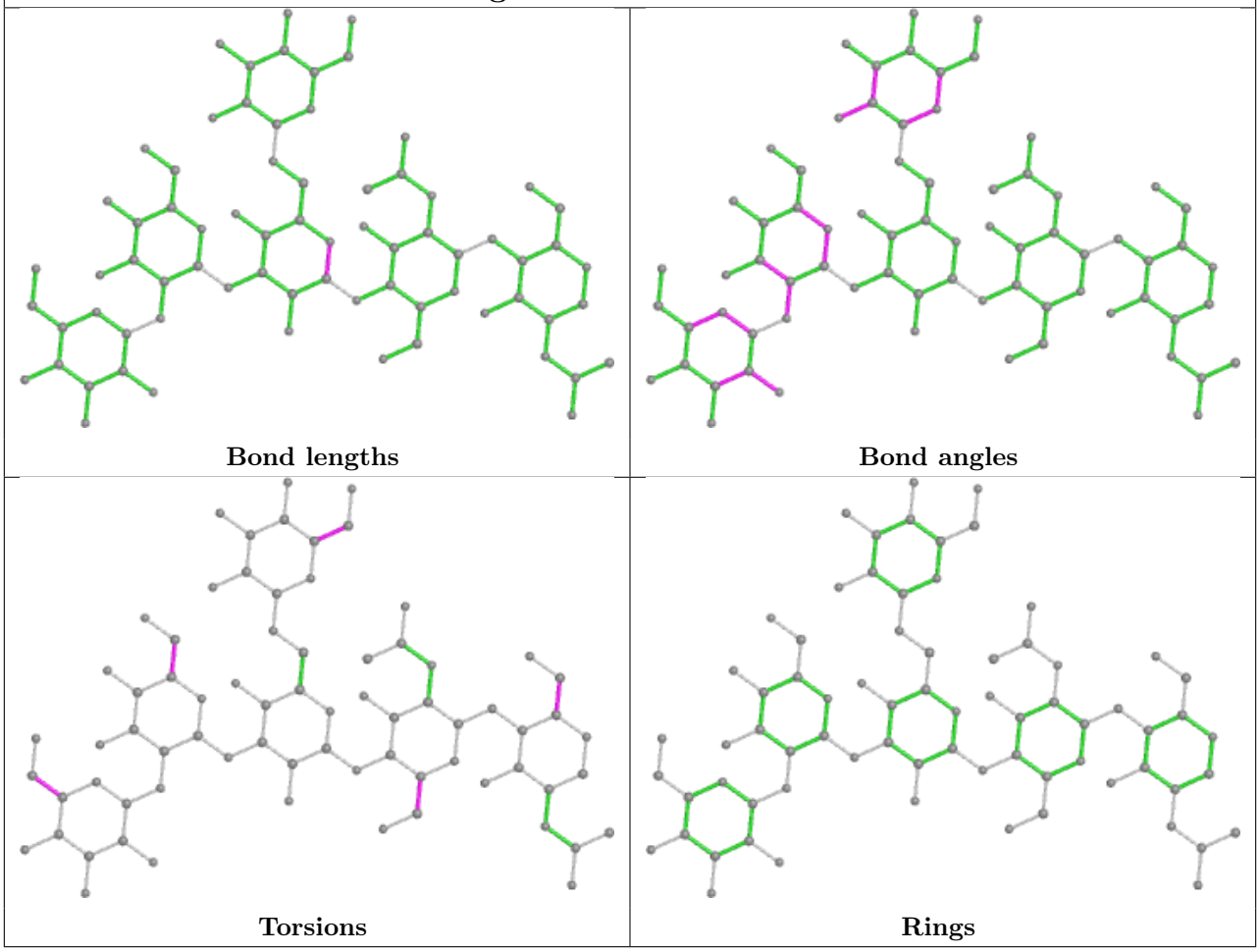


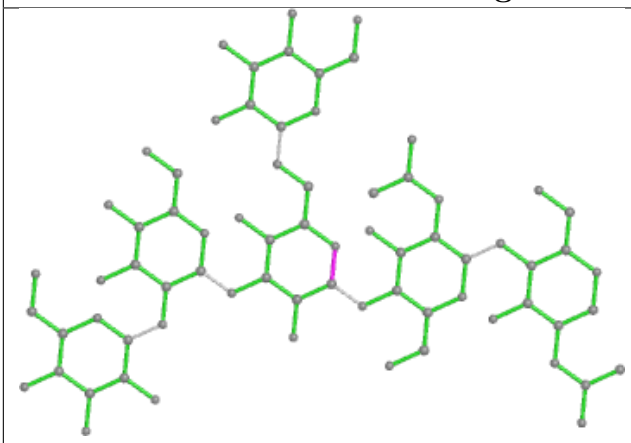
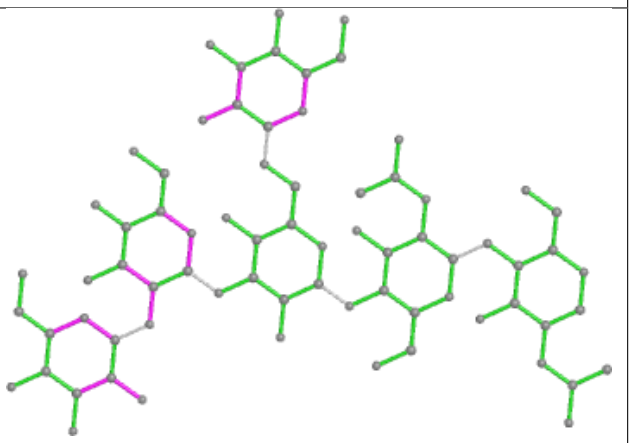
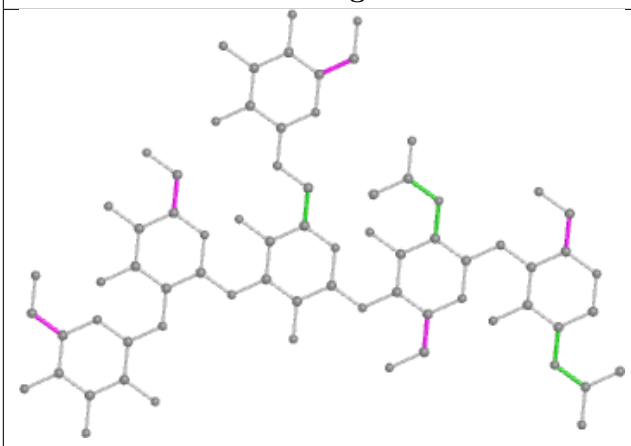
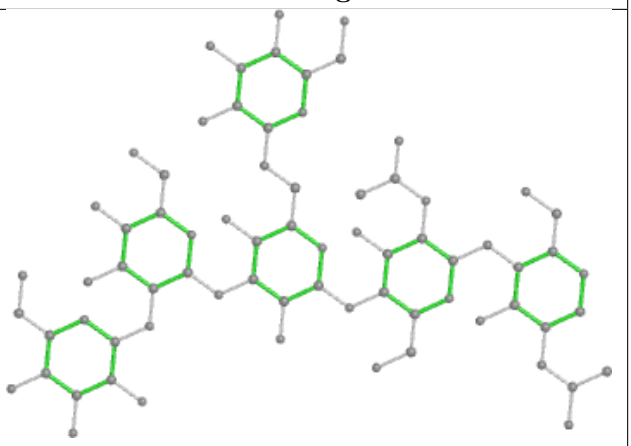
Rings

Oligosaccharide Chain 8

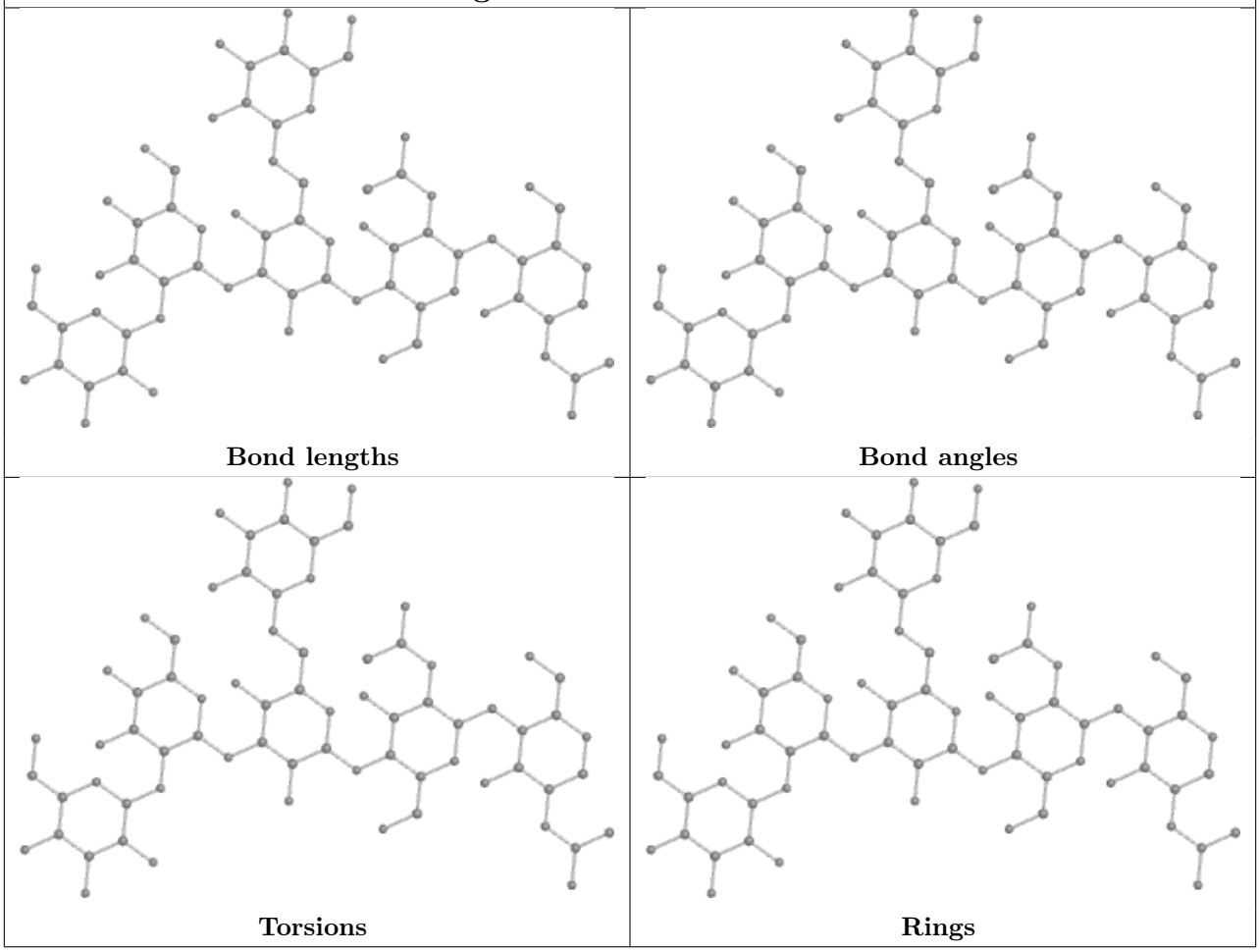


Oligosaccharide Chain d



Oligosaccharide Chain w	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain BA



5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
14	NAG	P	625	2	14,14,15	0.49	0	17,19,21	1.06	2 (11%)
14	NAG	G	625	2	14,14,15	0.49	0	17,19,21	1.05	1 (5%)
14	NAG	P	632	2	14,14,15	0.87	1 (7%)	17,19,21	2.25	3 (17%)
14	NAG	D	701	1	14,14,15	0.30	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	NAG	E	625	2	14,14,15	0.50	0	17,19,21	1.06	1 (5%)
14	NAG	P	633	2	14,14,15	0.35	0	17,19,21	0.46	0
14	NAG	B	701	1	14,14,15	0.29	0	17,19,21	0.51	0
14	NAG	G	632	2	14,14,15	0.85	1 (7%)	17,19,21	2.25	3 (17%)
14	NAG	E	633	2	14,14,15	0.35	0	17,19,21	0.48	0
14	NAG	O	701	1	14,14,15	0.28	0	17,19,21	0.51	0
14	NAG	E	632	2	14,14,15	0.85	1 (7%)	17,19,21	2.25	3 (17%)
14	NAG	G	633	2	14,14,15	0.35	0	17,19,21	0.46	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
14	NAG	P	625	2	-	2/6/23/26	0/1/1/1
14	NAG	G	625	2	-	2/6/23/26	0/1/1/1
14	NAG	P	632	2	-	5/6/23/26	0/1/1/1
14	NAG	D	701	1	-	2/6/23/26	0/1/1/1
14	NAG	E	625	2	-	2/6/23/26	0/1/1/1
14	NAG	P	633	2	-	1/6/23/26	0/1/1/1
14	NAG	B	701	1	-	2/6/23/26	0/1/1/1
14	NAG	G	632	2	-	5/6/23/26	0/1/1/1
14	NAG	E	633	2	-	1/6/23/26	0/1/1/1
14	NAG	O	701	1	-	2/6/23/26	0/1/1/1
14	NAG	E	632	2	-	5/6/23/26	0/1/1/1
14	NAG	G	633	2	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	632	NAG	C1-C2	2.59	1.56	1.52
14	E	632	NAG	C1-C2	2.53	1.56	1.52
14	G	632	NAG	C1-C2	2.50	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	632	NAG	C2-N2-C7	7.88	134.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	632	NAG	C2-N2-C7	7.88	134.12	122.90
14	E	632	NAG	C2-N2-C7	7.86	134.10	122.90
14	E	632	NAG	C1-C2-N2	3.52	116.50	110.49
14	G	632	NAG	C1-C2-N2	3.51	116.49	110.49
14	P	632	NAG	C1-C2-N2	3.51	116.48	110.49
14	E	625	NAG	C2-N2-C7	3.09	127.30	122.90
14	P	625	NAG	C2-N2-C7	3.05	127.24	122.90
14	G	625	NAG	C2-N2-C7	3.02	127.20	122.90
14	E	632	NAG	C8-C7-N2	2.17	119.78	116.10
14	G	632	NAG	C8-C7-N2	2.16	119.76	116.10
14	P	632	NAG	C8-C7-N2	2.16	119.75	116.10
14	P	625	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	701	NAG	O5-C5-C6-O6
14	O	701	NAG	O5-C5-C6-O6
14	D	701	NAG	O5-C5-C6-O6
14	G	632	NAG	C4-C5-C6-O6
14	E	632	NAG	C4-C5-C6-O6
14	P	632	NAG	C4-C5-C6-O6
14	G	632	NAG	O5-C5-C6-O6
14	E	632	NAG	O5-C5-C6-O6
14	P	632	NAG	O5-C5-C6-O6
14	B	701	NAG	C4-C5-C6-O6
14	O	701	NAG	C4-C5-C6-O6
14	D	701	NAG	C4-C5-C6-O6
14	G	632	NAG	C8-C7-N2-C2
14	G	632	NAG	O7-C7-N2-C2
14	E	632	NAG	C8-C7-N2-C2
14	E	632	NAG	O7-C7-N2-C2
14	P	632	NAG	C8-C7-N2-C2
14	P	632	NAG	O7-C7-N2-C2
14	G	633	NAG	O5-C5-C6-O6
14	E	633	NAG	O5-C5-C6-O6
14	P	633	NAG	O5-C5-C6-O6
14	G	625	NAG	O5-C5-C6-O6
14	E	625	NAG	O5-C5-C6-O6
14	P	625	NAG	O5-C5-C6-O6
14	G	625	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
14	E	625	NAG	C3-C2-N2-C7
14	P	625	NAG	C3-C2-N2-C7
14	G	632	NAG	C3-C2-N2-C7
14	E	632	NAG	C3-C2-N2-C7
14	P	632	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

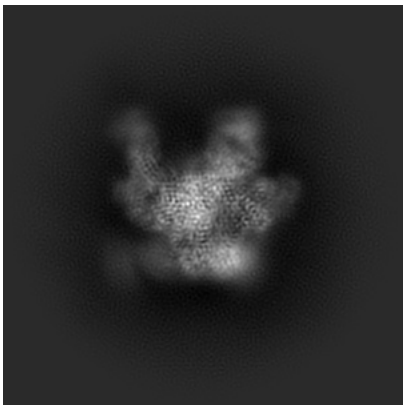
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20191. These allow visual inspection of the internal detail of the map and identification of artifacts.

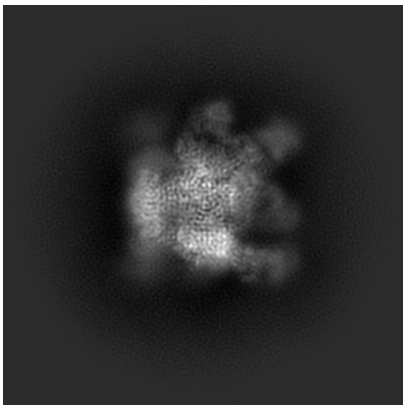
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

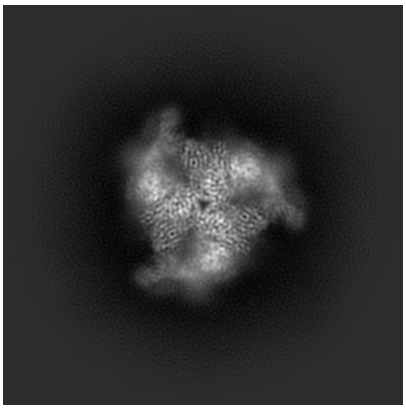
6.1.1 Primary map



X

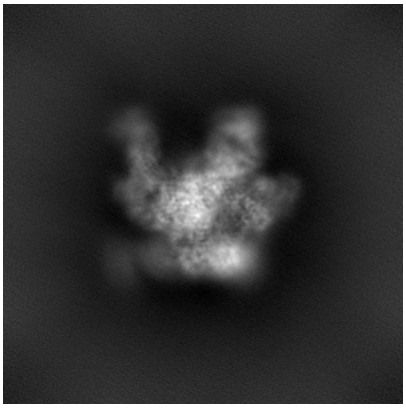


Y

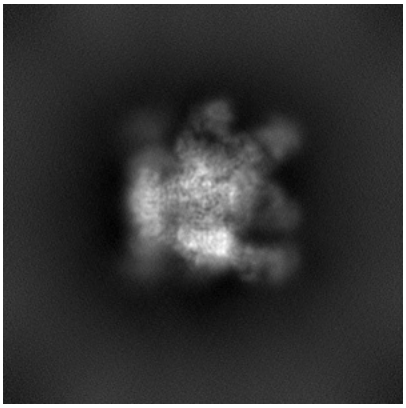


Z

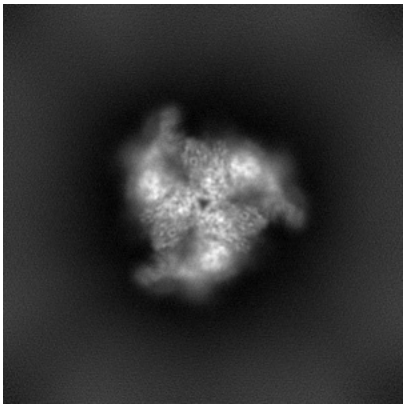
6.1.2 Raw map



X



Y

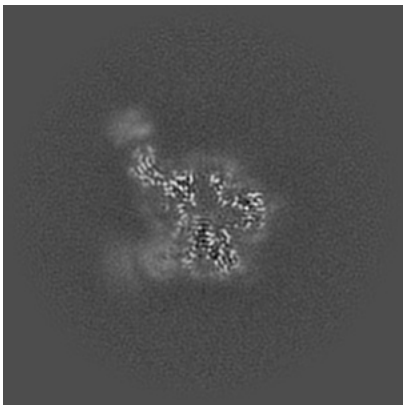


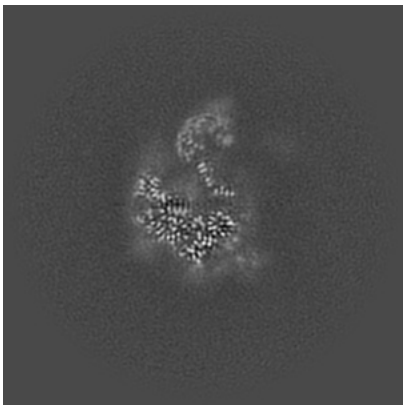
Z

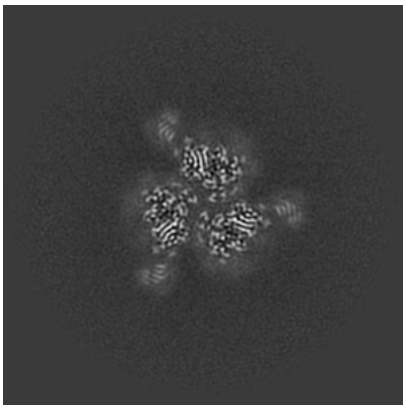
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

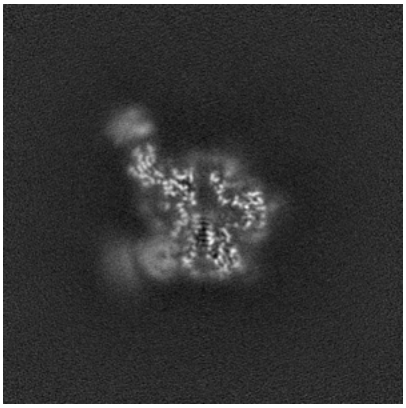
6.2.1 Primary map

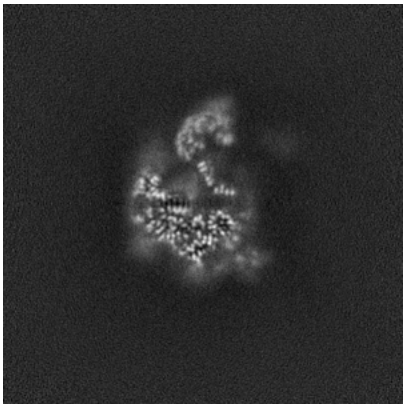

X Index: 176

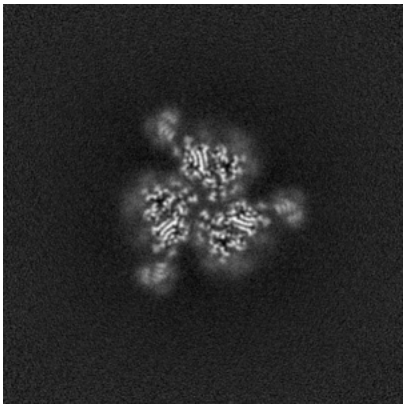

Y Index: 176


Z Index: 176

6.2.2 Raw map


X Index: 176

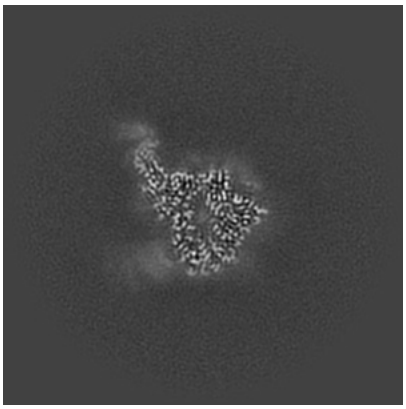

Y Index: 176

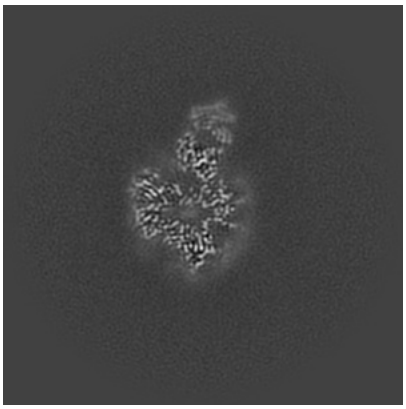

Z Index: 176

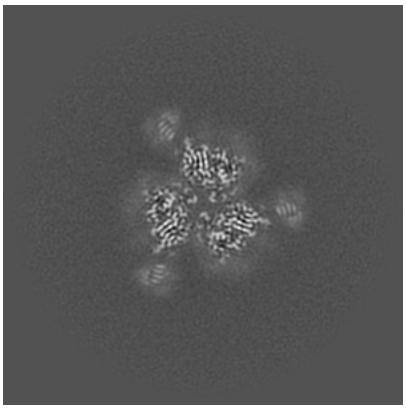
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

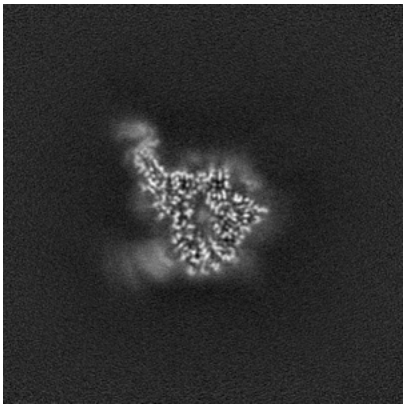
6.3.1 Primary map

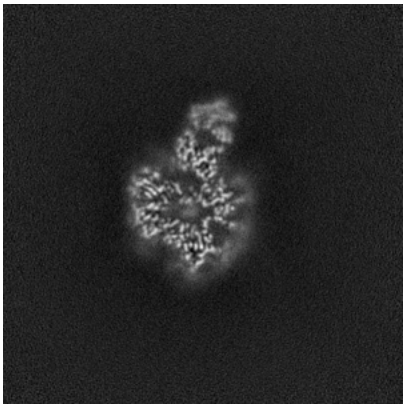

X Index: 185

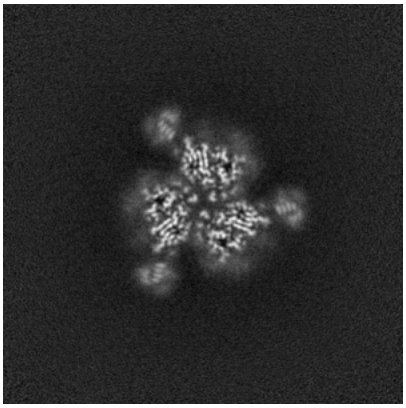

Y Index: 167


Z Index: 177

6.3.2 Raw map


X Index: 185


Y Index: 167


Z Index: 177

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

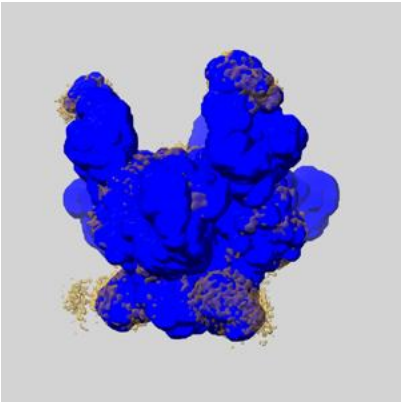
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

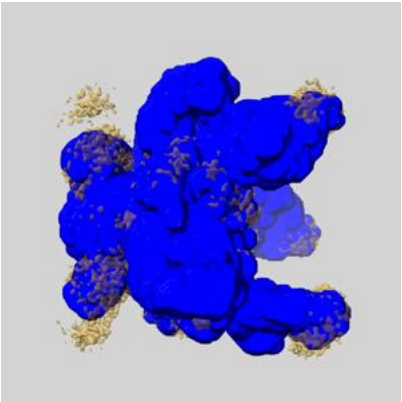
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

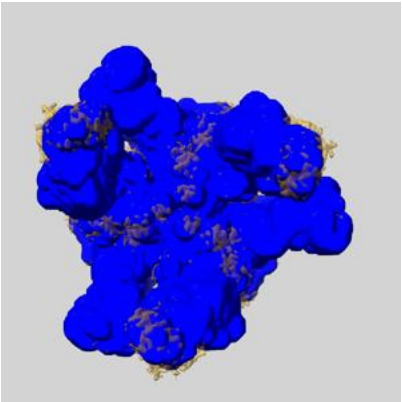
6.5.1 emd_20191_msk_1.map (i)



X



Y

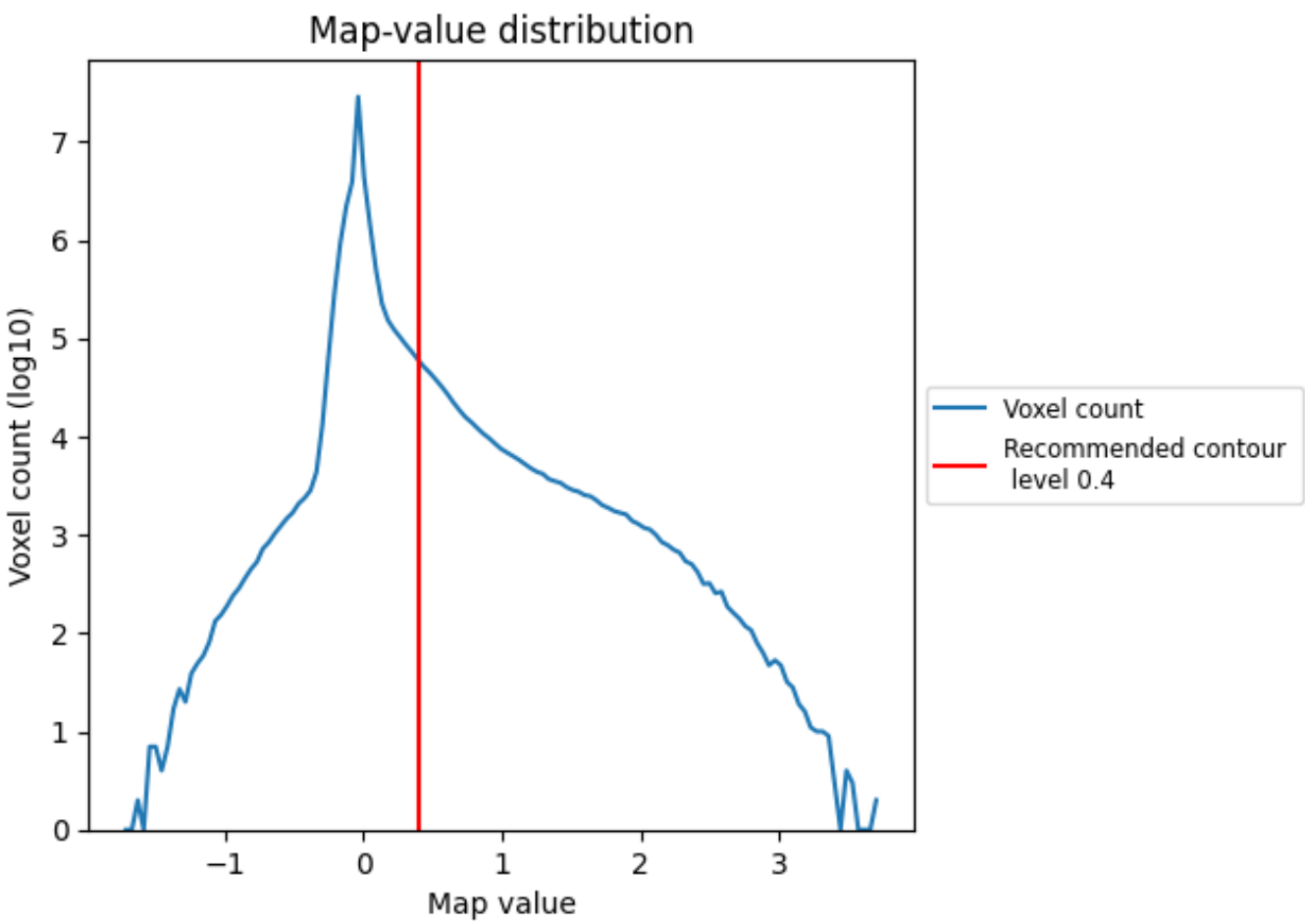


Z

7 Map analysis (i)

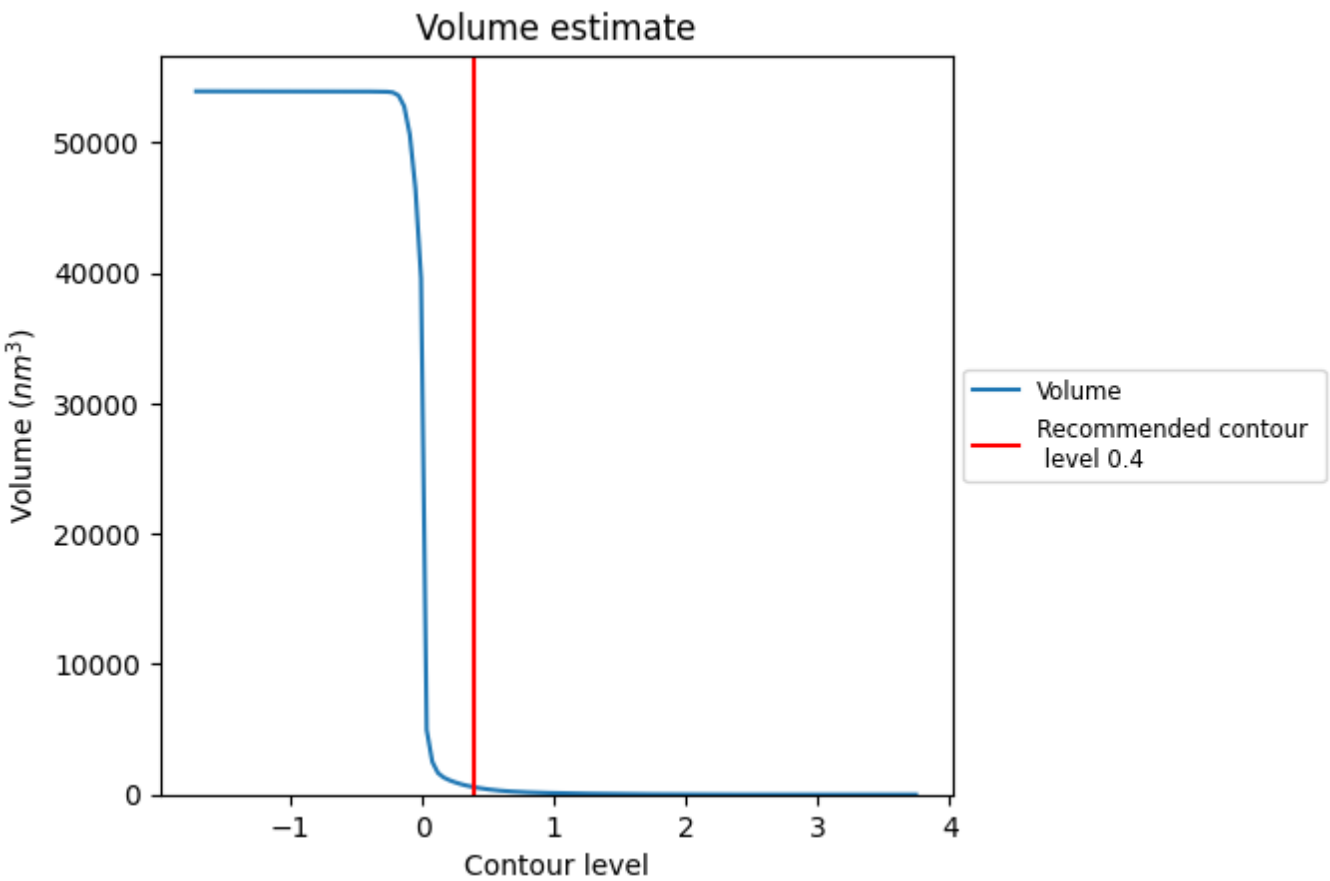
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

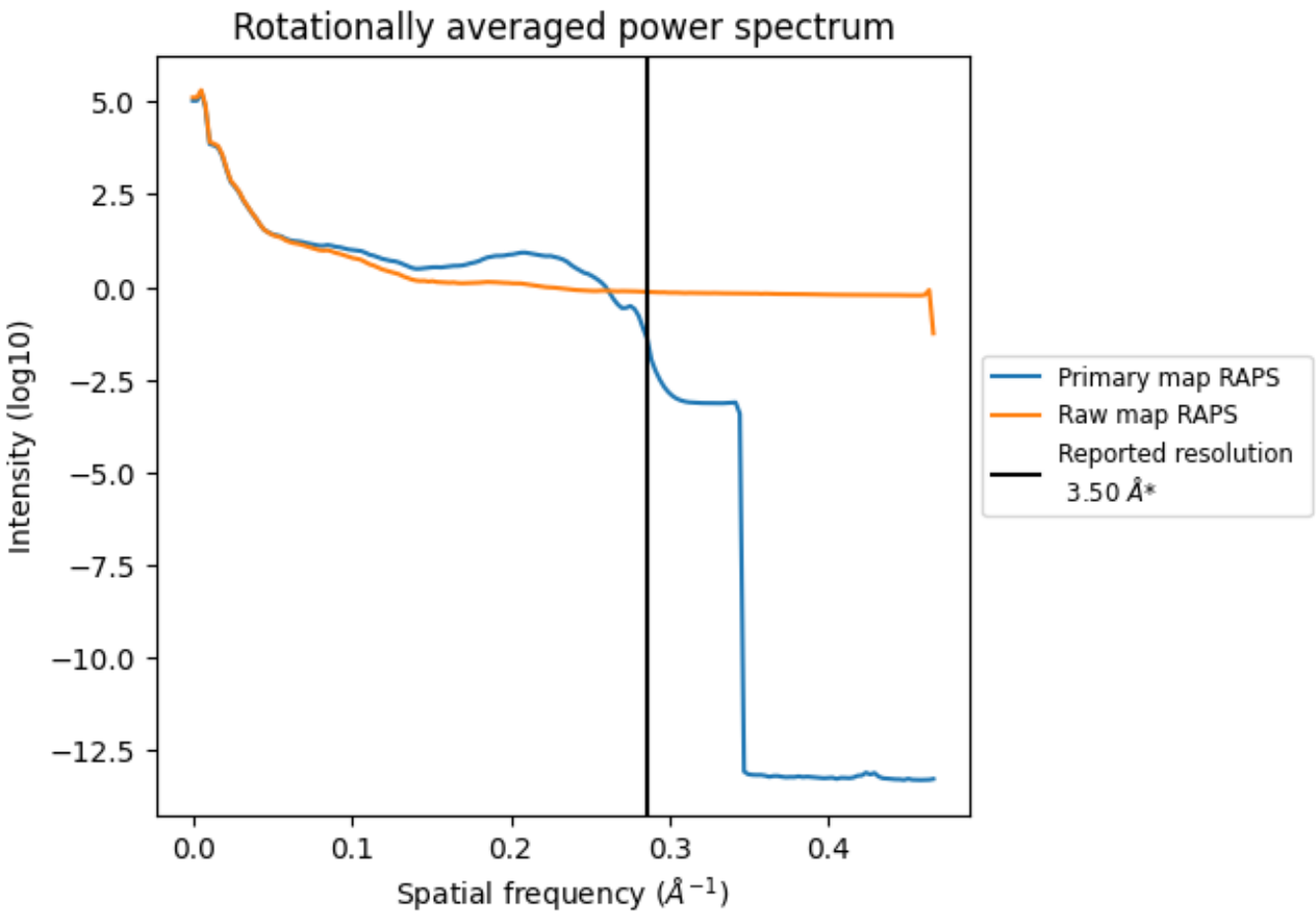
7.2 Volume estimate (i)



The volume at the recommended contour level is 557 nm^3; this corresponds to an approximate mass of 503 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 (i)

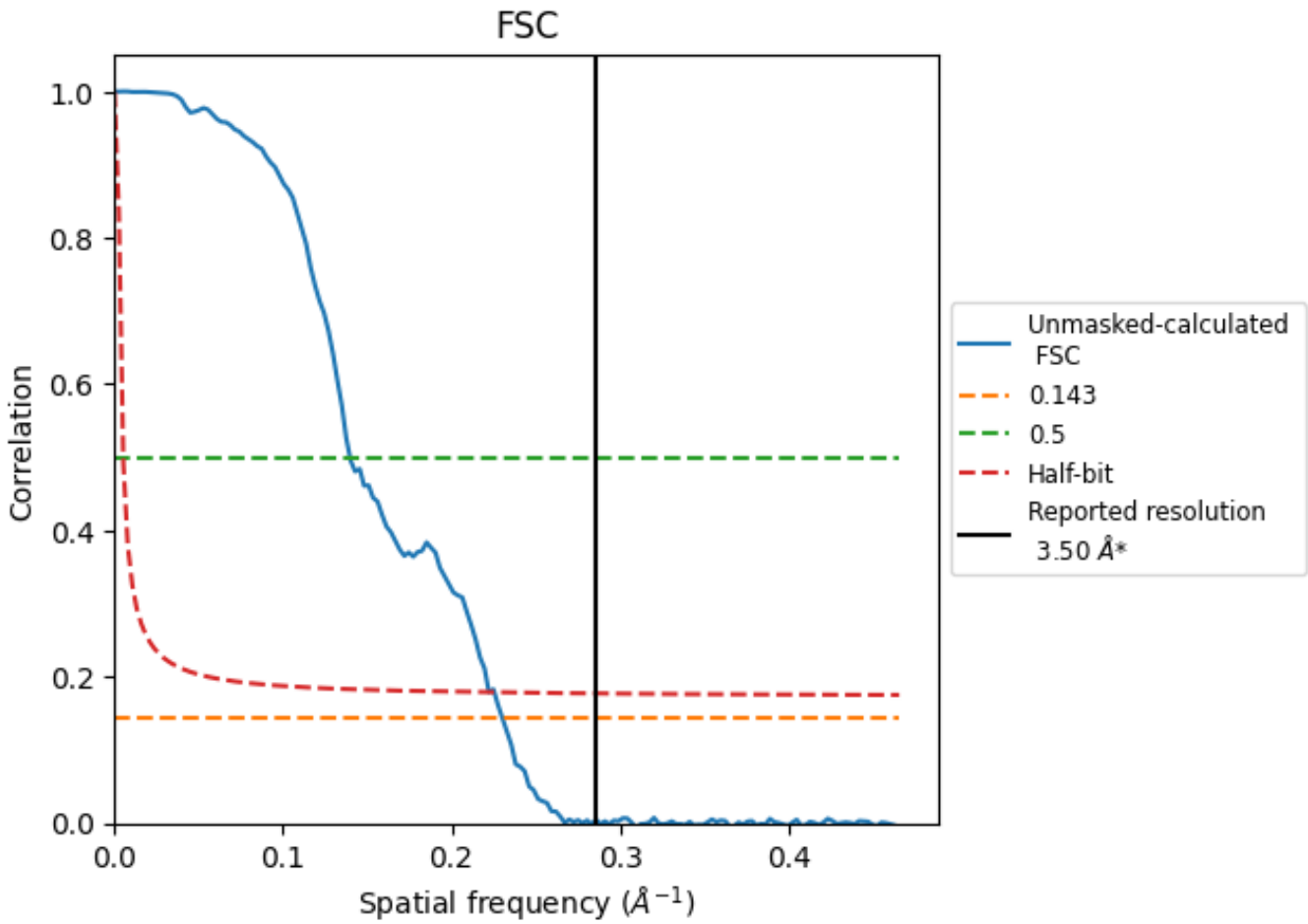


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

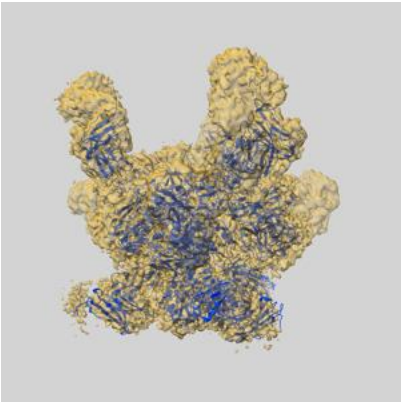
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.34	7.15	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.5 by more than 10 %

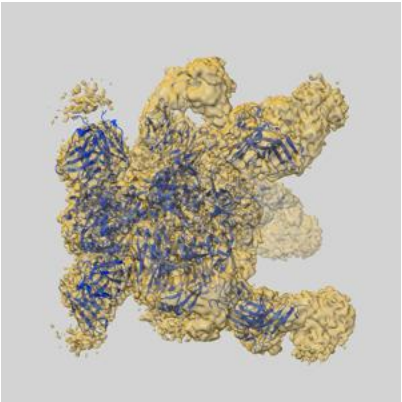
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20191 and PDB model 6OT1. Per-residue inclusion information can be found in section 3 on page 14.

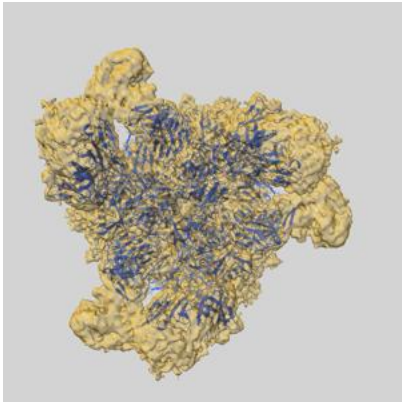
9.1 Map-model overlay (i)



X



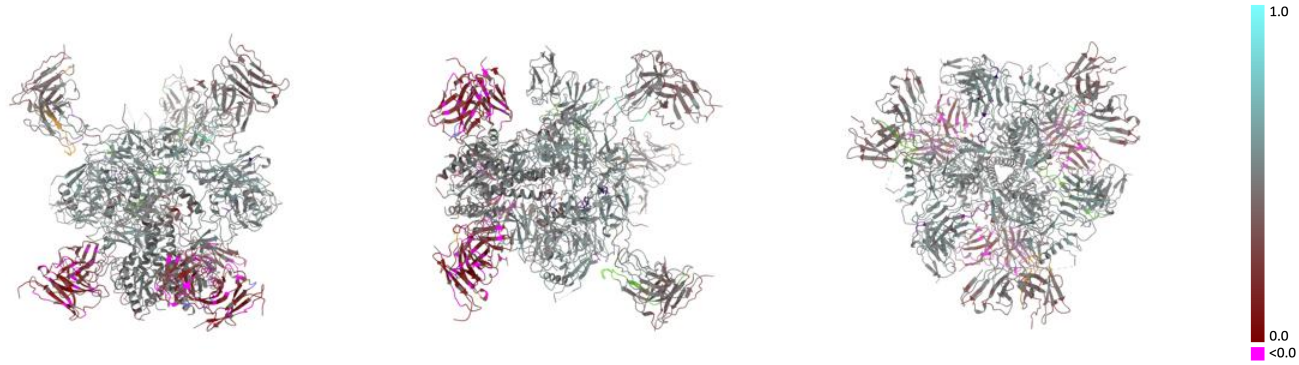
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

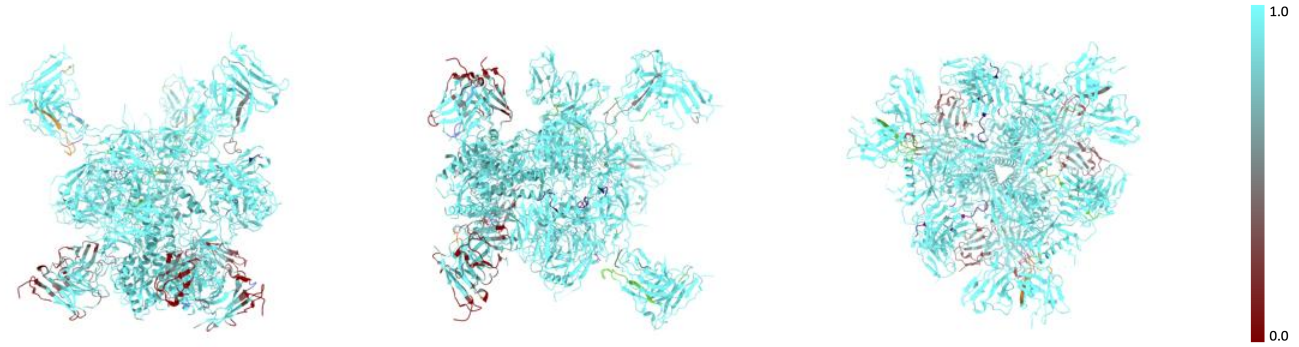
9.2 Q-score mapped to coordinate model (i)



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.

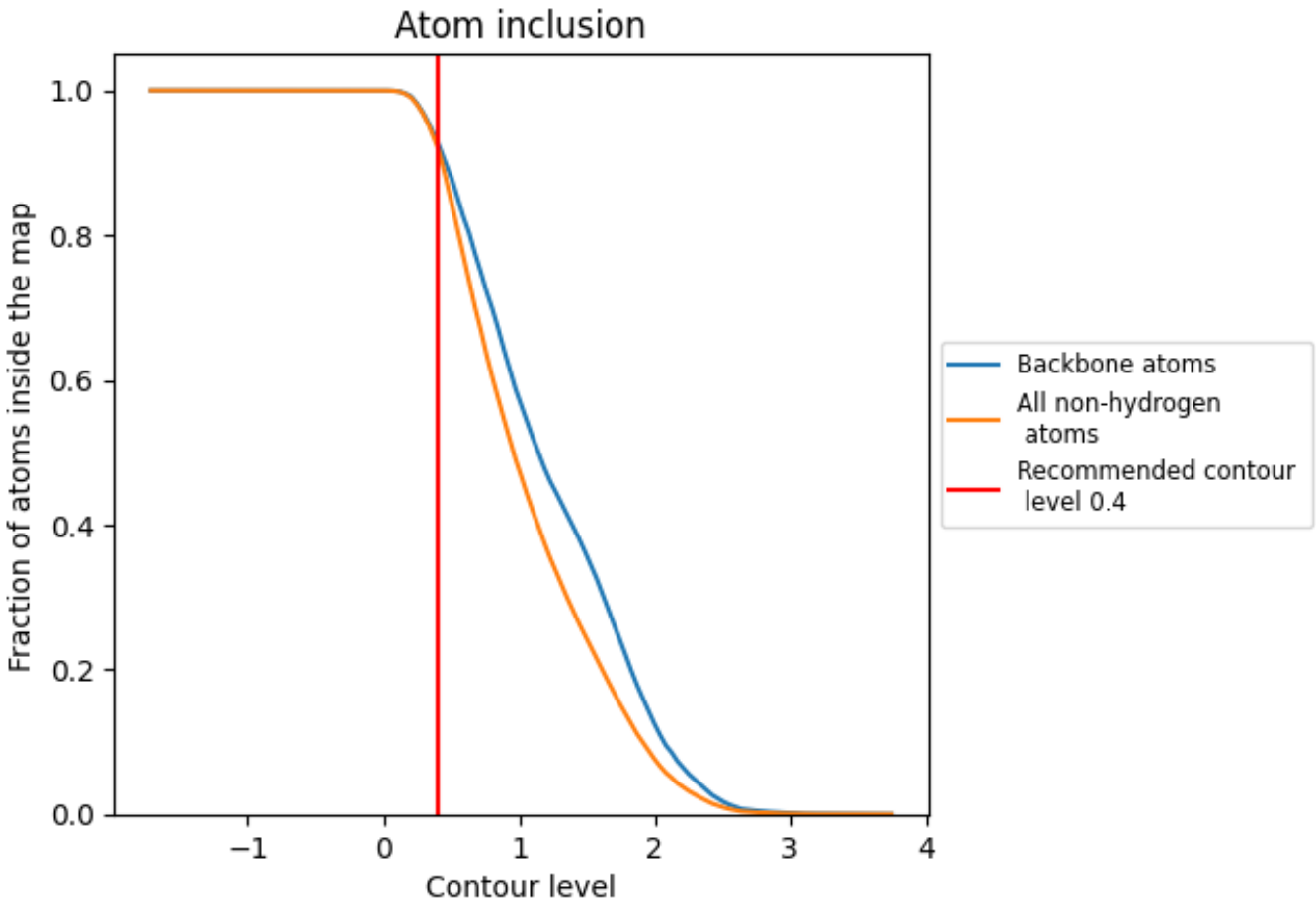
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9208	0.4290
0	0.9643	0.4420
1	0.9344	0.4390
2	0.9643	0.3310
3	0.9836	0.4820
4	1.0000	0.4860
5	0.9643	0.4430
6	0.8571	0.4450
7	0.9286	0.4730
8	1.0000	0.4920
9	0.9643	0.4840
A	0.7138	0.1620
AA	1.0000	0.4740
B	0.9728	0.4680
BA	1.0000	0.5400
C	0.5743	0.1690
CA	0.9744	0.5100
D	0.9718	0.4660
DA	1.0000	0.4690
E	0.9738	0.4990
EA	0.9231	0.4650
F	0.9765	0.4210
FA	0.9643	0.4370
G	0.9740	0.5010
GA	0.9344	0.4350
H	0.7138	0.1590
I	0.9745	0.4570
J	0.9768	0.5150
K	0.9885	0.4970
L	0.5743	0.1680
M	0.7181	0.1610
N	0.5707	0.1670
O	0.9737	0.4650
P	0.9735	0.5000
Q	0.9765	0.4190

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Chain	Atom inclusion	Q-score
R	0.9783	0.4620
S	0.9799	0.5130
T	0.9898	0.4990
U	0.9643	0.3170
V	0.9836	0.4850
W	1.0000	0.4860
X	0.9286	0.4420
Y	0.8571	0.4530
Z	0.9286	0.4550
a	0.9800	0.4880
b	0.9643	0.4930
c	1.0000	0.4860
d	1.0000	0.5350
e	0.9744	0.4930
f	1.0000	0.4800
g	1.0000	0.4640
h	0.9643	0.4400
i	0.9344	0.4360
j	0.9643	0.3350
k	0.9836	0.4850
l	1.0000	0.4750
m	0.9775	0.4210
n	0.9783	0.4590
o	0.9286	0.4500
p	0.8571	0.4370
q	0.9789	0.5170
r	0.9911	0.4990
s	0.9286	0.4660
t	0.9800	0.4960
u	0.9286	0.4920
v	1.0000	0.4720
w	1.0000	0.5280
x	0.9744	0.4910
y	1.0000	0.4780
z	0.9231	0.4560