wwPDB EM Validation Summary Report

Oct 30, 2023 – 02:29 PM EDT

PDB ID	:	8G6U
EMDB ID	:	EMD-29783
Title	:	Cryo-EM structure of T/F100 SOSIP.664 HIV-1 Env trimer with LMHS mutations in complex with 8ANC195 and 10-1074
Authors	:	Chen, Y.; Zhou, F.; Huang, R.; Tolbert, W.; Pazgier, M.
Deposited on	:	2023-02-16
Resolution	:	3.16 Å(reported)
Based on initial model	:	8DOK

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

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

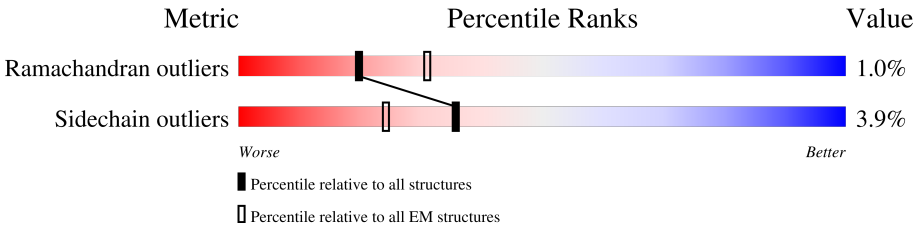
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.16 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	A	485	89% · 9%
1	E	485	89% · 9%
1	I	485	89% · 9%
2	B	155	70% 6% · 23%
2	F	155	70% 6% · 23%
2	J	155	70% 6% · 23%
3	C	238	53% · 45%
3	G	238	53% · 45%
3	K	238	53% · 45%

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Mol	Chain	Length	Quality of chain
4	D	215	47% 50%
4	H	215	47% 50%
4	L	215	47% 50%
5	M	238	10% 53% 45%
5	O	238	11% 53% 45%
5	Q	238	11% 53% 45%
6	N	214	47% 50%
6	P	214	47% 50%
6	R	214	5% 47% 50%
7	S	11	18% 82%
7	a	11	18% 82%
7	j	11	18% 82%
8	T	6	50% 50%
8	Y	6	50% 50%
8	b	6	50% 50%
8	h	6	50% 50%
8	k	6	50% 50%
8	r	6	50% 50%
9	U	10	40% 60%
9	d	10	40% 60%
9	n	10	40% 60%
10	0	2	50% 50%
10	1	2	50% 50%
10	2	2	50% 50%
10	V	2	100%

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Mol	Chain	Length	Quality of chain
10	X	2	100%
10	c	2	100%
10	e	2	100%
10	f	2	100%
10	g	2	100%
10	l	2	100%
10	m	2	50% 50%
10	o	2	100%
10	p	2	100%
10	q	2	100%
10	t	2	100%
10	u	2	100%
10	v	2	50% 50%
10	w	2	50% 50%
10	x	2	100%
10	y	2	100%
10	z	2	100%
11	Z	5	60% 40%
11	i	5	60% 40%
11	s	5	60% 40%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 26871 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 CRF01_AE T/F100 HIV-1 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	443	Total	C	N	O	S	0	0
			3510	2212	620	650	28		
1	E	443	Total	C	N	O	S	0	0
			3510	2212	620	650	28		
1	I	443	Total	C	N	O	S	0	0
			3510	2212	620	650	28		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	TYR	HIS	engineered mutation	UNP A0A6C0ZY47
A	105	HIS	GLN	engineered mutation	UNP A0A6C0ZY47
A	108	ILE	VAL	engineered mutation	UNP A0A6C0ZY47
A	375	SER	HIS	conflict	UNP A0A6C0ZY47
A	?	-	SER	deletion	UNP A0A6C0ZY47
A	474	ASP	ASN	engineered mutation	UNP A0A6C0ZY47
A	475	MET	ILE	engineered mutation	UNP A0A6C0ZY47
A	476	ARG	LYS	engineered mutation	UNP A0A6C0ZY47
A	501	CYS	ALA	conflict	UNP A0A6C0ZY47
A	508	ARG	-	expression tag	UNP A0A6C0ZY47
A	509	ARG	-	expression tag	UNP A0A6C0ZY47
A	510	ARG	-	expression tag	UNP A0A6C0ZY47
A	511	ARG	-	expression tag	UNP A0A6C0ZY47
A	512	ARG	-	expression tag	UNP A0A6C0ZY47
A	513	ARG	-	expression tag	UNP A0A6C0ZY47
E	61	TYR	HIS	engineered mutation	UNP A0A6C0ZY47
E	105	HIS	GLN	engineered mutation	UNP A0A6C0ZY47
E	108	ILE	VAL	engineered mutation	UNP A0A6C0ZY47
E	375	SER	HIS	conflict	UNP A0A6C0ZY47
E	?	-	SER	deletion	UNP A0A6C0ZY47
E	474	ASP	ASN	engineered mutation	UNP A0A6C0ZY47
E	475	MET	ILE	engineered mutation	UNP A0A6C0ZY47
E	476	ARG	LYS	engineered mutation	UNP A0A6C0ZY47
E	501	CYS	ALA	conflict	UNP A0A6C0ZY47

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Chain	Residue	Modelled	Actual	Comment	Reference
E	508	ARG	-	expression tag	UNP A0A6C0ZY47
E	509	ARG	-	expression tag	UNP A0A6C0ZY47
E	510	ARG	-	expression tag	UNP A0A6C0ZY47
E	511	ARG	-	expression tag	UNP A0A6C0ZY47
E	512	ARG	-	expression tag	UNP A0A6C0ZY47
E	513	ARG	-	expression tag	UNP A0A6C0ZY47
I	61	TYR	HIS	engineered mutation	UNP A0A6C0ZY47
I	105	HIS	GLN	engineered mutation	UNP A0A6C0ZY47
I	108	ILE	VAL	engineered mutation	UNP A0A6C0ZY47
I	375	SER	HIS	conflict	UNP A0A6C0ZY47
I	?	-	SER	deletion	UNP A0A6C0ZY47
I	474	ASP	ASN	engineered mutation	UNP A0A6C0ZY47
I	475	MET	ILE	engineered mutation	UNP A0A6C0ZY47
I	476	ARG	LYS	engineered mutation	UNP A0A6C0ZY47
I	501	CYS	ALA	conflict	UNP A0A6C0ZY47
I	508	ARG	-	expression tag	UNP A0A6C0ZY47
I	509	ARG	-	expression tag	UNP A0A6C0ZY47
I	510	ARG	-	expression tag	UNP A0A6C0ZY47
I	511	ARG	-	expression tag	UNP A0A6C0ZY47
I	512	ARG	-	expression tag	UNP A0A6C0ZY47
I	513	ARG	-	expression tag	UNP A0A6C0ZY47

- Molecule 2 is a protein called CRF-1_AE T/F100 HIV-1 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			964	616	161	182	5		
2	F	120	Total	C	N	O	S	0	0
			964	616	161	182	5		
2	J	120	Total	C	N	O	S	0	0
			964	616	161	182	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP A0A6C0ZY47
B	605	CYS	THR	conflict	UNP A0A6C0ZY47
B	665	ALA	-	expression tag	UNP A0A6C0ZY47
B	666	ALA	-	expression tag	UNP A0A6C0ZY47
F	559	PRO	ILE	conflict	UNP A0A6C0ZY47
F	605	CYS	THR	conflict	UNP A0A6C0ZY47
F	665	ALA	-	expression tag	UNP A0A6C0ZY47

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Chain	Residue	Modelled	Actual	Comment	Reference
F	666	ALA	-	expression tag	UNP A0A6C0ZY47
J	559	PRO	ILE	conflict	UNP A0A6C0ZY47
J	605	CYS	THR	conflict	UNP A0A6C0ZY47
J	665	ALA	-	expression tag	UNP A0A6C0ZY47
J	666	ALA	-	expression tag	UNP A0A6C0ZY47

- Molecule 3 is a protein called Heavy chain of 8ANC195.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		
3	G	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		
3	K	130	Total	C	N	O	S	0	0
			1003	636	174	190	3		

- Molecule 4 is a protein called Light chain of 8ANC195.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	107	Total	C	N	O	S	0	0
			814	510	143	158	3		
4	H	107	Total	C	N	O	S	0	0
			814	510	143	158	3		
4	L	107	Total	C	N	O	S	0	0
			814	510	143	158	3		

- Molecule 5 is a protein called Heavy chain of 10-1074.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		
5	O	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		
5	Q	131	Total	C	N	O	S	0	0
			1030	651	173	202	4		

- Molecule 6 is a protein called Light chain of 10-1074.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

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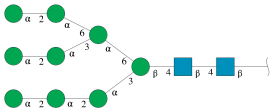
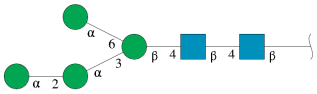
Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	107	Total 824	C 515	N 152	O 154	S 3	0	0
6	R	107	Total 824	C 515	N 152	O 154	S 3	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
7	S	11	Total 127	C 70	N 2	O 55	0	0
7	a	11	Total 127	C 70	N 2	O 55	0	0
7	j	11	Total 127	C 70	N 2	O 55	0	0

- Molecule 8 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
8	T	6	Total 72	C 40	N 2	O 30	0	0
8	Y	6	Total 72	C 40	N 2	O 30	0	0
8	b	6	Total 72	C 40	N 2	O 30	0	0
8	h	6	Total 72	C 40	N 2	O 30	0	0
8	k	6	Total 72	C 40	N 2	O 30	0	0

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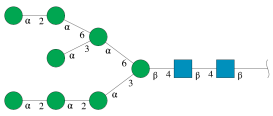
Mol	Chain	Residues	Atoms				AltConf	Trace
8	r	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
9	U	10	Total	C	N	O	0	0
			116	64	2	50		
9	d	10	Total	C	N	O	0	0
			116	64	2	50		
9	n	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 10 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
10	V	2	Total	C	N	O	0	0
			28	16	2	10		
10	X	2	Total	C	N	O	0	0
			28	16	2	10		
10	c	2	Total	C	N	O	0	0
			28	16	2	10		
10	f	2	Total	C	N	O	0	0
			28	16	2	10		
10	e	2	Total	C	N	O	0	0
			28	16	2	10		
10	g	2	Total	C	N	O	0	0
			28	16	2	10		

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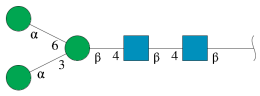
Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	2	Total	C	N	O	0	0
			28	16	2	10		
10	m	2	Total	C	N	O	0	0
			28	16	2	10		
10	o	2	Total	C	N	O	0	0
			28	16	2	10		
10	p	2	Total	C	N	O	0	0
			28	16	2	10		
10	q	2	Total	C	N	O	0	0
			28	16	2	10		
10	t	2	Total	C	N	O	0	0
			28	16	2	10		
10	u	2	Total	C	N	O	0	0
			28	16	2	10		
10	v	2	Total	C	N	O	0	0
			28	16	2	10		
10	w	2	Total	C	N	O	0	0
			28	16	2	10		
10	x	2	Total	C	N	O	0	0
			28	16	2	10		
10	y	2	Total	C	N	O	0	0
			28	16	2	10		
10	z	2	Total	C	N	O	0	0
			28	16	2	10		
10	0	2	Total	C	N	O	0	0
			28	16	2	10		
10	1	2	Total	C	N	O	0	0
			28	16	2	10		
10	2	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 11 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
11	Z	5	Total	C	N	O	0	0
			61	34	2	25		

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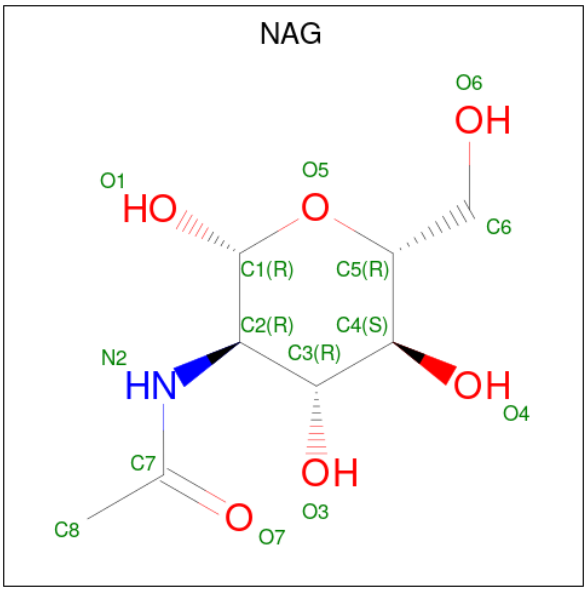
Mol	Chain	Residues	Atoms	AltConf	Trace
11	i	5	Total C N O 61 34 2 25	0	0
11	s	5	Total C N O 61 34 2 25	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C N O 14 8 1 5	0
12	A	1	Total C N O 14 8 1 5	0
12	A	1	Total C N O 14 8 1 5	0
12	A	1	Total C N O 14 8 1 5	0
12	A	1	Total C N O 14 8 1 5	0
12	A	1	Total C N O 14 8 1 5	0
12	A	1	Total C N O 14 8 1 5	0
12	A	1	Total C N O 14 8 1 5	0
12	A	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
12	B	1	Total C N O 14 8 1 5	0
12	B	1	Total C N O 14 8 1 5	0
12	B	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	E	1	Total C N O 14 8 1 5	0
12	F	1	Total C N O 14 8 1 5	0
12	F	1	Total C N O 14 8 1 5	0
12	F	1	Total C N O 14 8 1 5	0
12	I	1	Total C N O 14 8 1 5	0
12	I	1	Total C N O 14 8 1 5	0
12	I	1	Total C N O 14 8 1 5	0
12	I	1	Total C N O 14 8 1 5	0
12	I	1	Total C N O 14 8 1 5	0
12	I	1	Total C N O 14 8 1 5	0

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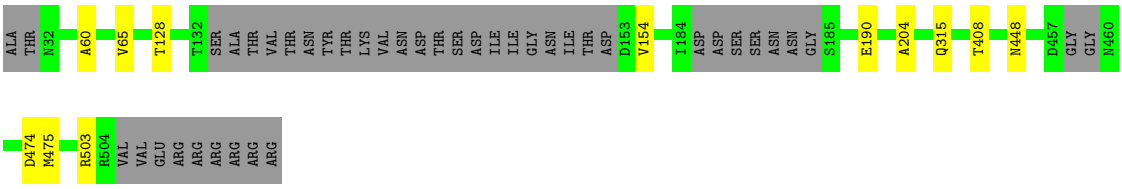
Mol	Chain	Residues	Atoms				AltConf
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	I	1	Total	C	N	O	0
			14	8	1	5	
12	J	1	Total	C	N	O	0
			14	8	1	5	
12	J	1	Total	C	N	O	0
			14	8	1	5	
12	J	1	Total	C	N	O	0
			14	8	1	5	

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.

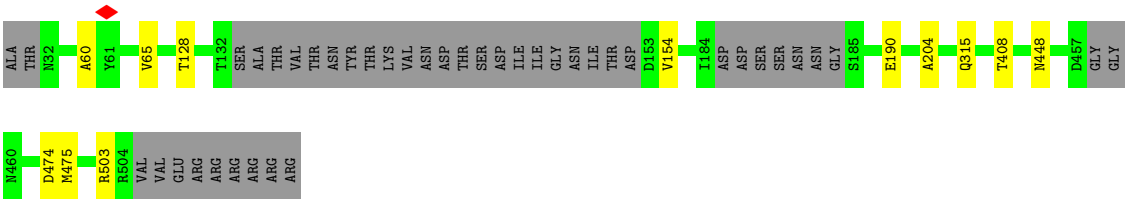
• Molecule 1: CRF01_AE T/F100 HIV-1 gp120

Chain A:



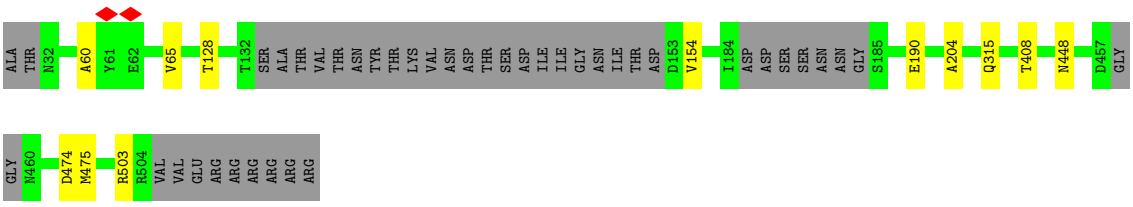
• Molecule 1: CRF01_AE T/F100 HIV-1 gp120

Chain E:



• Molecule 1: CRF01_AE T/F100 HIV-1 gp120

Chain I:



• Molecule 2: CRF-1_AE T/F100 HIV-1 gp41

Chain B:

• Molecule 2: CRF-1_AE T/F100 HIV-1 gp41

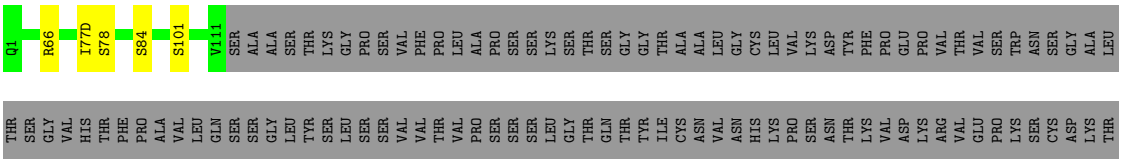
Chain F:

• Molecule 2: CRF-1_AE T/F100 HIV-1 gp41

Chain J:

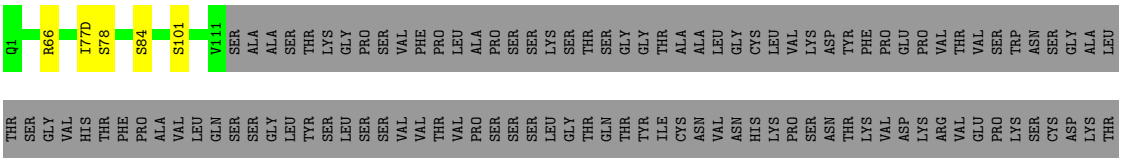
• Molecule 3: Heavy chain of 8ANC195

Chain C:



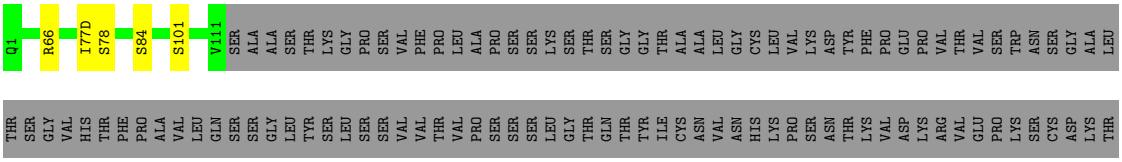
• Molecule 3: Heavy chain of 8ANC195

Chain G:



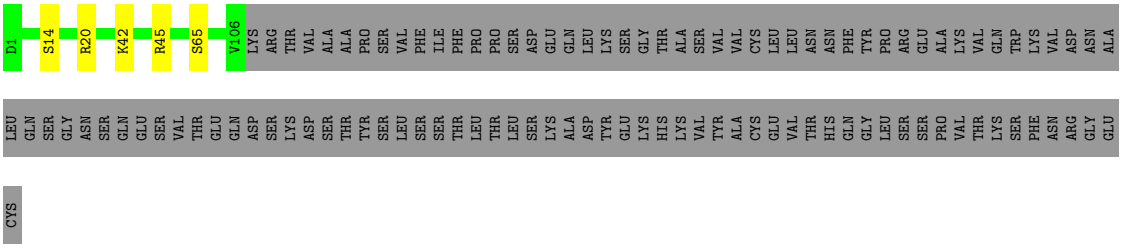
• Molecule 3: Heavy chain of 8ANC195

Chain K:



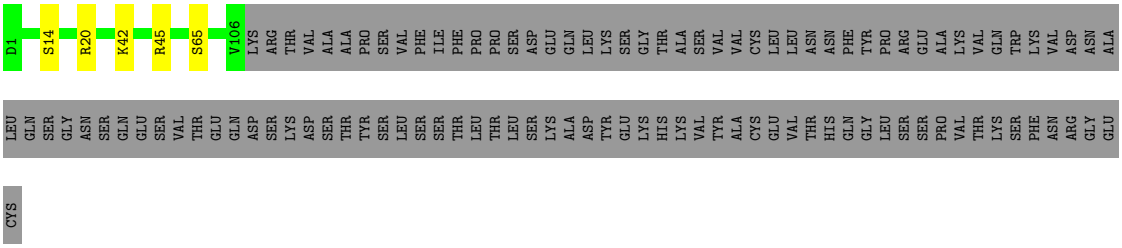
• Molecule 4: Light chain of 8ANC195

Chain D:



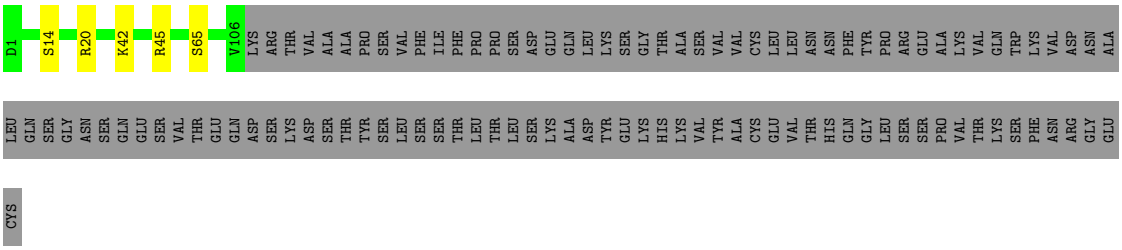
• Molecule 4: Light chain of 8ANC195

Chain H:



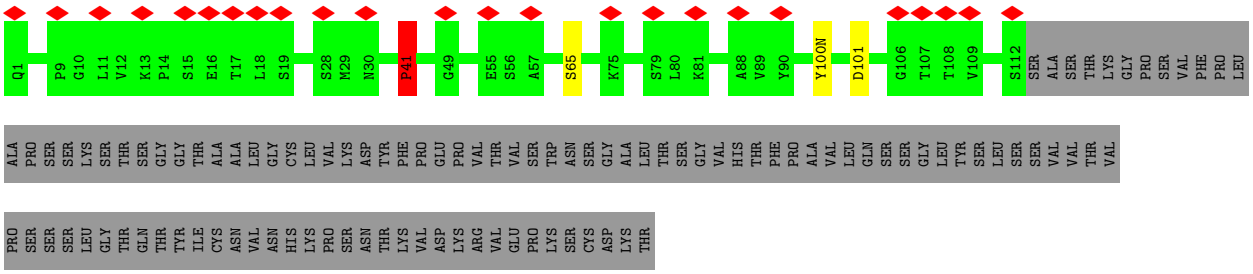
• Molecule 4: Light chain of 8ANC195

Chain L:



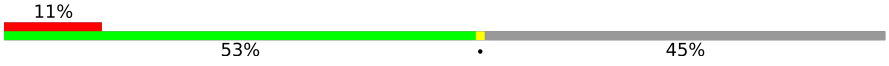
• Molecule 5: Heavy chain of 10-1074

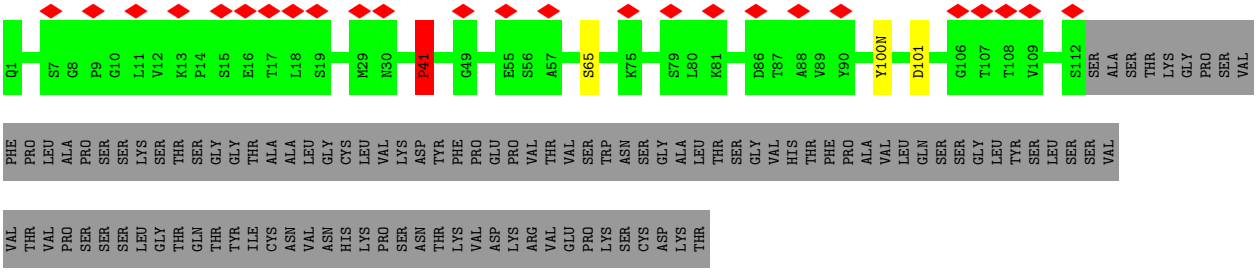
Chain M:



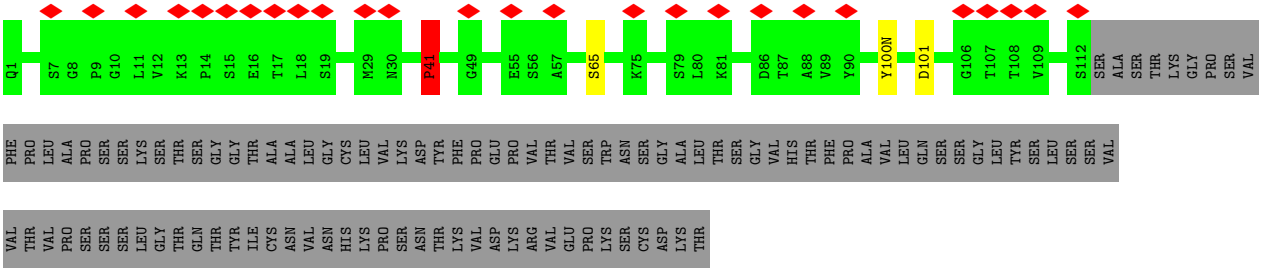
• Molecule 5: Heavy chain of 10-1074

Chain O:

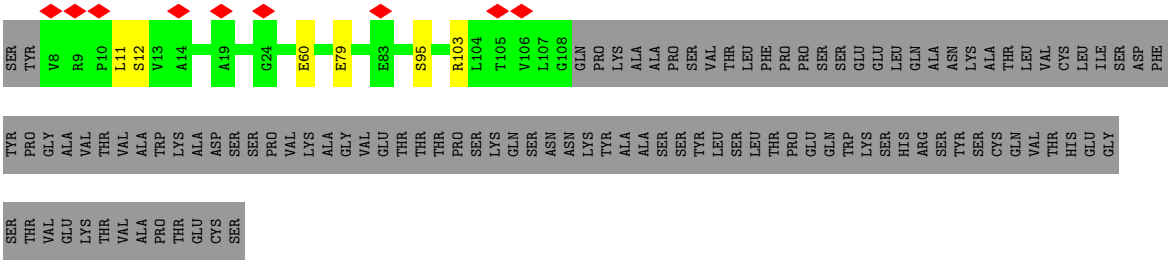




• Molecule 5: Heavy chain of 10-1074

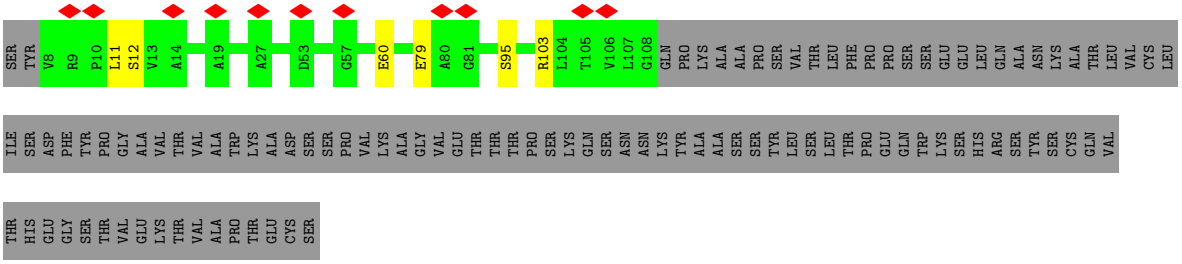


• Molecule 6: Light chain of 10-1074



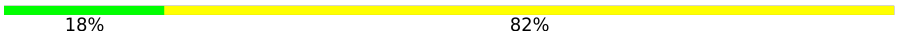
• Molecule 6: Light chain of 10-1074

• Molecule 6: Light chain of 10-1074



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 S:

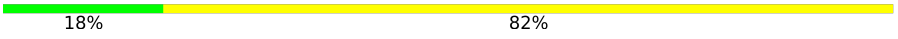


• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

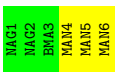
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



• Molecule 8: 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 T:



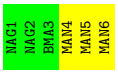
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam

ido-2-deoxy-beta-D-glucopyranose

Chain Y:

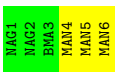
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



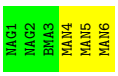
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



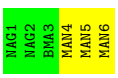
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



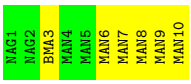
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



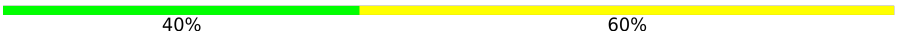
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

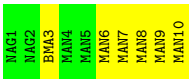
Chain U:



• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

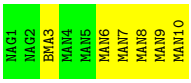
Chain d:





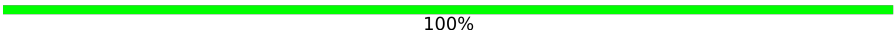
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:



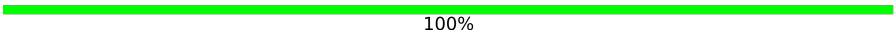
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



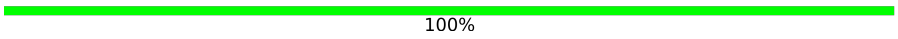
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



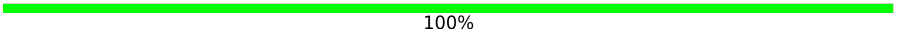
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



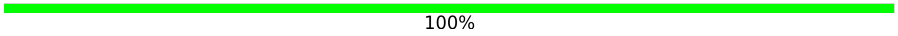
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

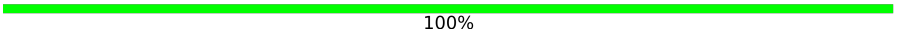


• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

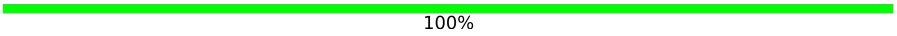


• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

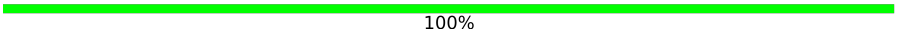
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



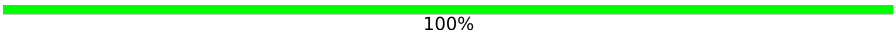
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



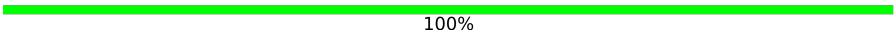
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:



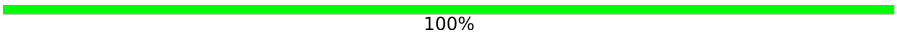
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

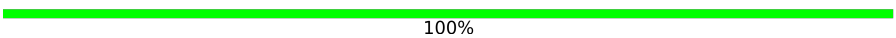
Chain v:

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:

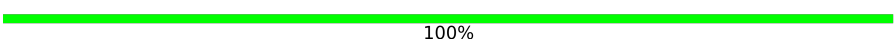
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:



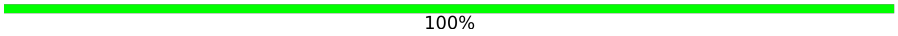
• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:



• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:



• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:

• Molecule 11: 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 Z:

• Molecule 11: 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:

• Molecule 11: 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 s:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	549061	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 ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	60241	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	25.188	Depositor
Minimum map value	-13.205	Depositor
Average map value	-0.014	Depositor
Map value standard deviation	0.602	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	403.38, 403.38, 403.38	wwPDB
Map dimensions	486, 486, 486	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	0/3588	0.53	0/4867
1	E	0.28	0/3588	0.54	0/4867
1	I	0.28	0/3588	0.53	0/4867
2	B	0.35	0/983	0.60	1/1333 (0.1%)
2	F	0.35	0/983	0.60	1/1333 (0.1%)
2	J	0.35	0/983	0.60	1/1333 (0.1%)
3	C	0.26	0/1030	0.51	0/1403
3	G	0.26	0/1030	0.51	0/1403
3	K	0.26	0/1030	0.51	0/1403
4	D	0.26	0/832	0.55	0/1130
4	H	0.26	0/832	0.55	0/1130
4	L	0.26	0/832	0.55	0/1130
5	M	0.28	0/1055	0.59	3/1436 (0.2%)
5	O	0.27	0/1055	0.59	3/1436 (0.2%)
5	Q	0.28	0/1055	0.59	3/1436 (0.2%)
6	N	0.27	0/845	0.62	0/1148
6	P	0.27	0/845	0.62	0/1148
6	R	0.27	0/845	0.62	0/1148
All	All	0.28	0/24999	0.56	12/33951 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	41	PRO	CA-N-CD	-5.60	103.66	111.50
5	M	41	PRO	CA-N-CD	-5.59	103.67	111.50
5	O	41	PRO	CA-N-CD	-5.59	103.68	111.50
2	F	620	GLU	CA-CB-CG	5.55	125.62	113.40
2	J	620	GLU	CA-CB-CG	5.55	125.61	113.40

There are no chirality outliers.

There are no planarity outliers.

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	A	435/485 (90%)	390 (90%)	40 (9%)	5 (1%)	14	48
1	E	435/485 (90%)	390 (90%)	40 (9%)	5 (1%)	14	48
1	I	435/485 (90%)	390 (90%)	40 (9%)	5 (1%)	14	48
2	B	116/155 (75%)	103 (89%)	10 (9%)	3 (3%)	5	28
2	F	116/155 (75%)	103 (89%)	10 (9%)	3 (3%)	5	28
2	J	116/155 (75%)	103 (89%)	10 (9%)	3 (3%)	5	28
3	C	128/238 (54%)	124 (97%)	4 (3%)	0	100	100
3	G	128/238 (54%)	124 (97%)	4 (3%)	0	100	100
3	K	128/238 (54%)	124 (97%)	4 (3%)	0	100	100
4	D	105/215 (49%)	101 (96%)	4 (4%)	0	100	100
4	H	105/215 (49%)	101 (96%)	4 (4%)	0	100	100
4	L	105/215 (49%)	101 (96%)	4 (4%)	0	100	100
5	M	129/238 (54%)	116 (90%)	12 (9%)	1 (1%)	19	55
5	O	129/238 (54%)	116 (90%)	12 (9%)	1 (1%)	19	55
5	Q	129/238 (54%)	116 (90%)	12 (9%)	1 (1%)	19	55
6	N	105/214 (49%)	97 (92%)	7 (7%)	1 (1%)	15	51
6	P	105/214 (49%)	97 (92%)	7 (7%)	1 (1%)	15	51
6	R	105/214 (49%)	97 (92%)	7 (7%)	1 (1%)	15	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3054/4635 (66%)	2793 (92%)	231 (8%)	30 (1%)	20 51

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	A	204	ALA
1	A	408	THR
2	B	544	LEU
2	B	619	PHE

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	A	397/433 (92%)	390 (98%)	7 (2%)	59 81
1	E	397/433 (92%)	390 (98%)	7 (2%)	59 81
1	I	397/433 (92%)	390 (98%)	7 (2%)	59 81
2	B	104/130 (80%)	95 (91%)	9 (9%)	10 34
2	F	104/130 (80%)	95 (91%)	9 (9%)	10 34
2	J	104/130 (80%)	95 (91%)	9 (9%)	10 34
3	C	111/204 (54%)	106 (96%)	5 (4%)	27 61
3	G	111/204 (54%)	106 (96%)	5 (4%)	27 61
3	K	111/204 (54%)	106 (96%)	5 (4%)	27 61
4	D	85/182 (47%)	80 (94%)	5 (6%)	19 51
4	H	85/182 (47%)	80 (94%)	5 (6%)	19 51
4	L	85/182 (47%)	80 (94%)	5 (6%)	19 51
5	M	115/208 (55%)	111 (96%)	4 (4%)	36 67
5	O	115/208 (55%)	111 (96%)	4 (4%)	36 67
5	Q	115/208 (55%)	111 (96%)	4 (4%)	36 67
6	N	85/178 (48%)	80 (94%)	5 (6%)	19 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	P	85/178 (48%)	80 (94%)	5 (6%)	19 51
6	R	85/178 (48%)	80 (94%)	5 (6%)	19 51
All	All	2691/4005 (67%)	2586 (96%)	105 (4%)	36 64

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	20	ARG
1	I	190	GLU
5	Q	101	ASP
4	H	45	ARG
6	P	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	540	GLN
2	J	575	GLN
2	F	575	GLN
3	K	6	GLN
1	I	72	HIS

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)

156 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	$\#\|Z\| > 2$
10	NAG	0	1	1,10	14,14,15	0.66	1 (7%)	17,19,21	0.70	0
10	NAG	0	2	10	14,14,15	0.29	0	17,19,21	0.44	0
10	NAG	1	1	1,10	14,14,15	0.66	1 (7%)	17,19,21	0.71	0
10	NAG	1	2	10	14,14,15	0.29	0	17,19,21	0.44	0
10	NAG	2	1	1,10	14,14,15	0.67	1 (7%)	17,19,21	0.71	0
10	NAG	2	2	10	14,14,15	0.28	0	17,19,21	0.44	0
7	NAG	S	1	1,7	14,14,15	0.37	0	17,19,21	0.73	1 (5%)
7	MAN	S	10	7	11,11,12	0.58	0	15,15,17	1.12	2 (13%)
7	MAN	S	11	7	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
7	NAG	S	2	7	14,14,15	0.32	0	17,19,21	0.43	0
7	BMA	S	3	7	11,11,12	0.60	0	15,15,17	0.81	0
7	MAN	S	4	7	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
7	MAN	S	5	7	11,11,12	0.58	0	15,15,17	1.02	2 (13%)
7	MAN	S	6	7	11,11,12	0.60	0	15,15,17	1.07	2 (13%)
7	MAN	S	7	7	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
7	MAN	S	8	7	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
7	MAN	S	9	7	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
8	NAG	T	1	1,8	14,14,15	0.31	0	17,19,21	0.39	0
8	NAG	T	2	8	14,14,15	0.31	0	17,19,21	0.46	0
8	BMA	T	3	8	11,11,12	0.50	0	15,15,17	0.70	0
8	MAN	T	4	8	11,11,12	0.82	0	15,15,17	1.04	2 (13%)
8	MAN	T	5	8	11,11,12	0.81	1 (9%)	15,15,17	1.29	2 (13%)
8	MAN	T	6	8	11,11,12	0.63	0	15,15,17	0.97	2 (13%)
9	NAG	U	1	1,9	14,14,15	0.27	0	17,19,21	0.45	0
9	MAN	U	10	9	11,11,12	0.65	0	15,15,17	0.93	2 (13%)
9	NAG	U	2	9	14,14,15	0.22	0	17,19,21	0.47	0
9	BMA	U	3	9	11,11,12	0.95	1 (9%)	15,15,17	1.12	0
9	MAN	U	4	9	11,11,12	0.72	0	15,15,17	0.90	0
9	MAN	U	5	9	11,11,12	0.85	0	15,15,17	1.00	0
9	MAN	U	6	9	11,11,12	0.64	0	15,15,17	1.20	2 (13%)
9	MAN	U	7	9	11,11,12	0.61	0	15,15,17	1.18	2 (13%)
9	MAN	U	8	9	11,11,12	0.77	1 (9%)	15,15,17	0.83	1 (6%)
9	MAN	U	9	9	11,11,12	0.61	0	15,15,17	1.00	2 (13%)
10	NAG	V	1	1,10	14,14,15	0.42	0	17,19,21	0.52	0
10	NAG	V	2	10	14,14,15	0.45	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	X	1	1,10	14,14,15	0.21	0	17,19,21	0.41	0
10	NAG	X	2	10	14,14,15	0.22	0	17,19,21	0.41	0
8	NAG	Y	1	1,8	14,14,15	0.22	0	17,19,21	0.55	0
8	NAG	Y	2	8	14,14,15	0.20	0	17,19,21	0.39	0
8	BMA	Y	3	8	11,11,12	0.45	0	15,15,17	0.72	0
8	MAN	Y	4	8	11,11,12	0.71	0	15,15,17	1.01	2 (13%)
8	MAN	Y	5	8	11,11,12	0.81	0	15,15,17	1.32	2 (13%)
8	MAN	Y	6	8	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
11	NAG	Z	1	11,2	14,14,15	0.18	0	17,19,21	0.47	0
11	NAG	Z	2	11	14,14,15	0.24	0	17,19,21	0.44	0
11	BMA	Z	3	11	11,11,12	0.60	0	15,15,17	0.79	0
11	MAN	Z	4	11	11,11,12	0.81	0	15,15,17	1.07	2 (13%)
11	MAN	Z	5	11	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
7	NAG	a	1	1,7	14,14,15	0.37	0	17,19,21	0.74	1 (5%)
7	MAN	a	10	7	11,11,12	0.58	0	15,15,17	1.11	2 (13%)
7	MAN	a	11	7	11,11,12	0.60	0	15,15,17	0.99	2 (13%)
7	NAG	a	2	7	14,14,15	0.30	0	17,19,21	0.43	0
7	BMA	a	3	7	11,11,12	0.59	0	15,15,17	0.80	0
7	MAN	a	4	7	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
7	MAN	a	5	7	11,11,12	0.59	0	15,15,17	1.02	2 (13%)
7	MAN	a	6	7	11,11,12	0.62	0	15,15,17	1.06	2 (13%)
7	MAN	a	7	7	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
7	MAN	a	8	7	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
7	MAN	a	9	7	11,11,12	0.66	0	15,15,17	1.00	2 (13%)
8	NAG	b	1	1,8	14,14,15	0.29	0	17,19,21	0.38	0
8	NAG	b	2	8	14,14,15	0.31	0	17,19,21	0.44	0
8	BMA	b	3	8	11,11,12	0.50	0	15,15,17	0.71	0
8	MAN	b	4	8	11,11,12	0.81	0	15,15,17	1.05	2 (13%)
8	MAN	b	5	8	11,11,12	0.82	0	15,15,17	1.29	2 (13%)
8	MAN	b	6	8	11,11,12	0.64	0	15,15,17	0.98	2 (13%)
10	NAG	c	1	1,10	14,14,15	0.20	0	17,19,21	0.44	0
10	NAG	c	2	10	14,14,15	0.22	0	17,19,21	0.42	0
9	NAG	d	1	1,9	14,14,15	0.28	0	17,19,21	0.45	0
9	MAN	d	10	9	11,11,12	0.67	0	15,15,17	0.93	1 (6%)
9	NAG	d	2	9	14,14,15	0.21	0	17,19,21	0.46	0
9	BMA	d	3	9	11,11,12	0.93	1 (9%)	15,15,17	1.14	2 (13%)
9	MAN	d	4	9	11,11,12	0.70	0	15,15,17	0.90	0
9	MAN	d	5	9	11,11,12	0.81	0	15,15,17	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	d	6	9	11,11,12	0.64	0	15,15,17	1.18	2 (13%)
9	MAN	d	7	9	11,11,12	0.65	0	15,15,17	1.19	2 (13%)
9	MAN	d	8	9	11,11,12	0.79	1 (9%)	15,15,17	0.84	1 (6%)
9	MAN	d	9	9	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
10	NAG	e	1	1,10	14,14,15	0.41	0	17,19,21	0.53	0
10	NAG	e	2	10	14,14,15	0.46	0	17,19,21	0.43	0
10	NAG	f	1	1,10	14,14,15	0.20	0	17,19,21	0.45	0
10	NAG	f	2	10	14,14,15	0.22	0	17,19,21	0.41	0
10	NAG	g	1	1,10	14,14,15	0.22	0	17,19,21	0.42	0
10	NAG	g	2	10	14,14,15	0.22	0	17,19,21	0.41	0
8	NAG	h	1	1,8	14,14,15	0.22	0	17,19,21	0.54	0
8	NAG	h	2	8	14,14,15	0.22	0	17,19,21	0.38	0
8	BMA	h	3	8	11,11,12	0.43	0	15,15,17	0.72	0
8	MAN	h	4	8	11,11,12	0.66	0	15,15,17	1.00	2 (13%)
8	MAN	h	5	8	11,11,12	0.80	0	15,15,17	1.30	2 (13%)
8	MAN	h	6	8	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
11	NAG	i	1	11,2	14,14,15	0.18	0	17,19,21	0.45	0
11	NAG	i	2	11	14,14,15	0.25	0	17,19,21	0.42	0
11	BMA	i	3	11	11,11,12	0.59	0	15,15,17	0.81	0
11	MAN	i	4	11	11,11,12	0.80	0	15,15,17	1.06	2 (13%)
11	MAN	i	5	11	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
7	NAG	j	1	1,7	14,14,15	0.37	0	17,19,21	0.73	1 (5%)
7	MAN	j	10	7	11,11,12	0.57	0	15,15,17	1.09	2 (13%)
7	MAN	j	11	7	11,11,12	0.61	0	15,15,17	0.98	2 (13%)
7	NAG	j	2	7	14,14,15	0.31	0	17,19,21	0.43	0
7	BMA	j	3	7	11,11,12	0.58	0	15,15,17	0.78	0
7	MAN	j	4	7	11,11,12	0.62	0	15,15,17	0.94	2 (13%)
7	MAN	j	5	7	11,11,12	0.58	0	15,15,17	1.03	2 (13%)
7	MAN	j	6	7	11,11,12	0.62	0	15,15,17	1.07	2 (13%)
7	MAN	j	7	7	11,11,12	0.62	0	15,15,17	1.05	2 (13%)
7	MAN	j	8	7	11,11,12	0.64	0	15,15,17	0.95	2 (13%)
7	MAN	j	9	7	11,11,12	0.65	0	15,15,17	1.00	2 (13%)
8	NAG	k	1	1,8	14,14,15	0.29	0	17,19,21	0.38	0
8	NAG	k	2	8	14,14,15	0.31	0	17,19,21	0.43	0
8	BMA	k	3	8	11,11,12	0.51	0	15,15,17	0.70	0
8	MAN	k	4	8	11,11,12	0.82	0	15,15,17	1.05	2 (13%)
8	MAN	k	5	8	11,11,12	0.81	0	15,15,17	1.28	2 (13%)
8	MAN	k	6	8	11,11,12	0.64	0	15,15,17	0.97	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	l	1	1,10	14,14,15	0.19	0	17,19,21	0.44	0
10	NAG	l	2	10	14,14,15	0.22	0	17,19,21	0.41	0
10	NAG	m	1	1,10	14,14,15	0.66	1 (7%)	17,19,21	0.56	0
10	NAG	m	2	10	14,14,15	0.24	0	17,19,21	0.44	0
9	NAG	n	1	1,9	14,14,15	0.26	0	17,19,21	0.45	0
9	MAN	n	10	9	11,11,12	0.66	0	15,15,17	0.93	2 (13%)
9	NAG	n	2	9	14,14,15	0.21	0	17,19,21	0.46	0
9	BMA	n	3	9	11,11,12	0.93	1 (9%)	15,15,17	1.14	2 (13%)
9	MAN	n	4	9	11,11,12	0.71	0	15,15,17	0.89	0
9	MAN	n	5	9	11,11,12	0.81	0	15,15,17	1.01	0
9	MAN	n	6	9	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
9	MAN	n	7	9	11,11,12	0.63	0	15,15,17	1.19	2 (13%)
9	MAN	n	8	9	11,11,12	0.79	1 (9%)	15,15,17	0.84	1 (6%)
9	MAN	n	9	9	11,11,12	0.62	0	15,15,17	0.99	2 (13%)
10	NAG	o	1	1,10	14,14,15	0.42	0	17,19,21	0.52	0
10	NAG	o	2	10	14,14,15	0.46	0	17,19,21	0.43	0
10	NAG	p	1	1,10	14,14,15	0.23	0	17,19,21	0.42	0
10	NAG	p	2	10	14,14,15	0.21	0	17,19,21	0.42	0
10	NAG	q	1	1,10	14,14,15	0.22	0	17,19,21	0.43	0
10	NAG	q	2	10	14,14,15	0.22	0	17,19,21	0.41	0
8	NAG	r	1	1,8	14,14,15	0.23	0	17,19,21	0.52	0
8	NAG	r	2	8	14,14,15	0.20	0	17,19,21	0.39	0
8	BMA	r	3	8	11,11,12	0.44	0	15,15,17	0.72	0
8	MAN	r	4	8	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
8	MAN	r	5	8	11,11,12	0.81	0	15,15,17	1.31	2 (13%)
8	MAN	r	6	8	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
11	NAG	s	1	11,2	14,14,15	0.18	0	17,19,21	0.45	0
11	NAG	s	2	11	14,14,15	0.26	0	17,19,21	0.41	0
11	BMA	s	3	11	11,11,12	0.58	0	15,15,17	0.81	0
11	MAN	s	4	11	11,11,12	0.80	0	15,15,17	1.05	2 (13%)
11	MAN	s	5	11	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
10	NAG	t	1	1,10	14,14,15	0.20	0	17,19,21	0.44	0
10	NAG	t	2	10	14,14,15	0.23	0	17,19,21	0.42	0
10	NAG	u	1	1,10	14,14,15	0.20	0	17,19,21	0.43	0
10	NAG	u	2	10	14,14,15	0.22	0	17,19,21	0.41	0
10	NAG	v	1	1,10	14,14,15	0.66	1 (7%)	17,19,21	0.55	0
10	NAG	v	2	10	14,14,15	0.24	0	17,19,21	0.44	0
10	NAG	w	1	1,10	14,14,15	0.66	1 (7%)	17,19,21	0.55	0
10	NAG	w	2	10	14,14,15	0.23	0	17,19,21	0.44	0
10	NAG	x	1	1,10	14,14,15	0.54	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	x	2	10	14,14,15	0.24	0	17,19,21	0.48	0
10	NAG	y	1	1,10	14,14,15	0.54	0	17,19,21	0.63	0
10	NAG	y	2	10	14,14,15	0.23	0	17,19,21	0.46	0
10	NAG	z	1	1,10	14,14,15	0.54	0	17,19,21	0.62	0
10	NAG	z	2	10	14,14,15	0.22	0	17,19,21	0.47	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
10	NAG	0	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	0	2	10	-	2/6/23/26	0/1/1/1
10	NAG	1	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	1	2	10	-	2/6/23/26	0/1/1/1
10	NAG	2	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	2	2	10	-	2/6/23/26	0/1/1/1
7	NAG	S	1	1,7	-	2/6/23/26	0/1/1/1
7	MAN	S	10	7	-	2/2/19/22	0/1/1/1
7	MAN	S	11	7	-	0/2/19/22	0/1/1/1
7	NAG	S	2	7	-	1/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
7	MAN	S	5	7	-	2/2/19/22	0/1/1/1
7	MAN	S	6	7	-	1/2/19/22	0/1/1/1
7	MAN	S	7	7	-	0/2/19/22	0/1/1/1
7	MAN	S	8	7	-	0/2/19/22	0/1/1/1
7	MAN	S	9	7	-	1/2/19/22	0/1/1/1
8	NAG	T	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	2/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
8	MAN	T	4	8	-	0/2/19/22	0/1/1/1
8	MAN	T	5	8	-	0/2/19/22	0/1/1/1
8	MAN	T	6	8	-	0/2/19/22	0/1/1/1
9	NAG	U	1	1,9	-	2/6/23/26	0/1/1/1
9	MAN	U	10	9	-	0/2/19/22	0/1/1/1
9	NAG	U	2	9	-	0/6/23/26	0/1/1/1
9	BMA	U	3	9	-	0/2/19/22	0/1/1/1
9	MAN	U	4	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	U	5	9	-	2/2/19/22	0/1/1/1
9	MAN	U	6	9	-	2/2/19/22	0/1/1/1
9	MAN	U	7	9	-	0/2/19/22	0/1/1/1
9	MAN	U	8	9	-	0/2/19/22	0/1/1/1
9	MAN	U	9	9	-	0/2/19/22	0/1/1/1
10	NAG	V	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	V	2	10	-	2/6/23/26	0/1/1/1
10	NAG	X	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	X	2	10	-	2/6/23/26	0/1/1/1
8	NAG	Y	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	5	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	6	8	-	0/2/19/22	0/1/1/1
11	NAG	Z	1	11,2	-	1/6/23/26	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
11	MAN	Z	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Z	5	11	-	0/2/19/22	0/1/1/1
7	NAG	a	1	1,7	-	2/6/23/26	0/1/1/1
7	MAN	a	10	7	-	2/2/19/22	0/1/1/1
7	MAN	a	11	7	-	0/2/19/22	0/1/1/1
7	NAG	a	2	7	-	1/6/23/26	0/1/1/1
7	BMA	a	3	7	-	0/2/19/22	0/1/1/1
7	MAN	a	4	7	-	0/2/19/22	0/1/1/1
7	MAN	a	5	7	-	2/2/19/22	0/1/1/1
7	MAN	a	6	7	-	1/2/19/22	0/1/1/1
7	MAN	a	7	7	-	0/2/19/22	0/1/1/1
7	MAN	a	8	7	-	0/2/19/22	0/1/1/1
7	MAN	a	9	7	-	1/2/19/22	0/1/1/1
8	NAG	b	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
8	BMA	b	3	8	-	0/2/19/22	0/1/1/1
8	MAN	b	4	8	-	0/2/19/22	0/1/1/1
8	MAN	b	5	8	-	0/2/19/22	0/1/1/1
8	MAN	b	6	8	-	0/2/19/22	0/1/1/1
10	NAG	c	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	c	2	10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	d	1	1,9	-	2/6/23/26	0/1/1/1
9	MAN	d	10	9	-	0/2/19/22	0/1/1/1
9	NAG	d	2	9	-	0/6/23/26	0/1/1/1
9	BMA	d	3	9	-	0/2/19/22	0/1/1/1
9	MAN	d	4	9	-	0/2/19/22	0/1/1/1
9	MAN	d	5	9	-	2/2/19/22	0/1/1/1
9	MAN	d	6	9	-	2/2/19/22	0/1/1/1
9	MAN	d	7	9	-	0/2/19/22	0/1/1/1
9	MAN	d	8	9	-	0/2/19/22	0/1/1/1
9	MAN	d	9	9	-	0/2/19/22	0/1/1/1
10	NAG	e	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	e	2	10	-	2/6/23/26	0/1/1/1
10	NAG	f	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	f	2	10	-	2/6/23/26	0/1/1/1
10	NAG	g	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	g	2	10	-	2/6/23/26	0/1/1/1
8	NAG	h	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1
8	BMA	h	3	8	-	0/2/19/22	0/1/1/1
8	MAN	h	4	8	-	0/2/19/22	0/1/1/1
8	MAN	h	5	8	-	0/2/19/22	0/1/1/1
8	MAN	h	6	8	-	0/2/19/22	0/1/1/1
11	NAG	i	1	11,2	-	1/6/23/26	0/1/1/1
11	NAG	i	2	11	-	0/6/23/26	0/1/1/1
11	BMA	i	3	11	-	2/2/19/22	0/1/1/1
11	MAN	i	4	11	-	0/2/19/22	0/1/1/1
11	MAN	i	5	11	-	0/2/19/22	0/1/1/1
7	NAG	j	1	1,7	-	2/6/23/26	0/1/1/1
7	MAN	j	10	7	-	0/2/19/22	0/1/1/1
7	MAN	j	11	7	-	0/2/19/22	0/1/1/1
7	NAG	j	2	7	-	0/6/23/26	0/1/1/1
7	BMA	j	3	7	-	0/2/19/22	0/1/1/1
7	MAN	j	4	7	-	0/2/19/22	0/1/1/1
7	MAN	j	5	7	-	2/2/19/22	0/1/1/1
7	MAN	j	6	7	-	1/2/19/22	0/1/1/1
7	MAN	j	7	7	-	0/2/19/22	0/1/1/1
7	MAN	j	8	7	-	0/2/19/22	0/1/1/1
7	MAN	j	9	7	-	1/2/19/22	0/1/1/1
8	NAG	k	1	1,8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	k	2	8	-	2/6/23/26	0/1/1/1
8	BMA	k	3	8	-	0/2/19/22	0/1/1/1
8	MAN	k	4	8	-	0/2/19/22	0/1/1/1
8	MAN	k	5	8	-	0/2/19/22	0/1/1/1
8	MAN	k	6	8	-	0/2/19/22	0/1/1/1
10	NAG	l	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	l	2	10	-	2/6/23/26	0/1/1/1
10	NAG	m	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	m	2	10	-	2/6/23/26	0/1/1/1
9	NAG	n	1	1,9	-	2/6/23/26	0/1/1/1
9	MAN	n	10	9	-	0/2/19/22	0/1/1/1
9	NAG	n	2	9	-	0/6/23/26	0/1/1/1
9	BMA	n	3	9	-	0/2/19/22	0/1/1/1
9	MAN	n	4	9	-	0/2/19/22	0/1/1/1
9	MAN	n	5	9	-	2/2/19/22	0/1/1/1
9	MAN	n	6	9	-	2/2/19/22	0/1/1/1
9	MAN	n	7	9	-	0/2/19/22	0/1/1/1
9	MAN	n	8	9	-	0/2/19/22	0/1/1/1
9	MAN	n	9	9	-	0/2/19/22	0/1/1/1
10	NAG	o	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	o	2	10	-	2/6/23/26	0/1/1/1
10	NAG	p	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	p	2	10	-	2/6/23/26	0/1/1/1
10	NAG	q	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	q	2	10	-	2/6/23/26	0/1/1/1
8	NAG	r	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	r	2	8	-	0/6/23/26	0/1/1/1
8	BMA	r	3	8	-	0/2/19/22	0/1/1/1
8	MAN	r	4	8	-	0/2/19/22	0/1/1/1
8	MAN	r	5	8	-	0/2/19/22	0/1/1/1
8	MAN	r	6	8	-	0/2/19/22	0/1/1/1
11	NAG	s	1	11,2	-	1/6/23/26	0/1/1/1
11	NAG	s	2	11	-	0/6/23/26	0/1/1/1
11	BMA	s	3	11	-	2/2/19/22	0/1/1/1
11	MAN	s	4	11	-	0/2/19/22	0/1/1/1
11	MAN	s	5	11	-	0/2/19/22	0/1/1/1
10	NAG	t	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	t	2	10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	u	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	u	2	10	-	2/6/23/26	0/1/1/1
10	NAG	v	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	v	2	10	-	2/6/23/26	0/1/1/1
10	NAG	w	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	w	2	10	-	2/6/23/26	0/1/1/1
10	NAG	x	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	x	2	10	-	2/6/23/26	0/1/1/1
10	NAG	y	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	y	2	10	-	2/6/23/26	0/1/1/1
10	NAG	z	1	1,10	-	2/6/23/26	0/1/1/1
10	NAG	z	2	10	-	2/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	m	1	NAG	O5-C1	-2.33	1.40	1.43
9	U	3	BMA	O5-C1	-2.33	1.40	1.43
10	v	1	NAG	O5-C1	-2.33	1.40	1.43
10	w	1	NAG	O5-C1	-2.32	1.40	1.43
9	d	3	BMA	O5-C1	-2.30	1.40	1.43

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Y	5	MAN	C1-O5-C5	3.47	116.90	112.19
9	U	6	MAN	C1-O5-C5	3.44	116.85	112.19
8	h	5	MAN	C1-O5-C5	3.43	116.83	112.19
8	T	5	MAN	C1-O5-C5	3.42	116.83	112.19
8	r	5	MAN	C1-O5-C5	3.42	116.83	112.19

There are no chirality outliers.

5 of 143 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	V	1	NAG	C4-C5-C6-O6
10	e	1	NAG	C4-C5-C6-O6
10	o	1	NAG	C4-C5-C6-O6
10	x	2	NAG	O5-C5-C6-O6

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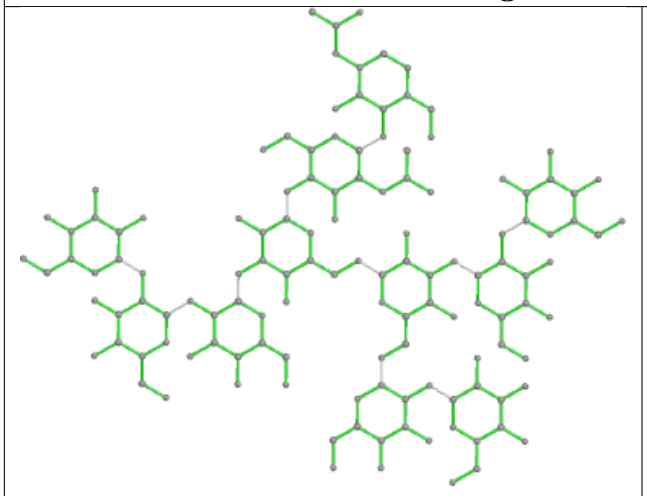
Mol	Chain	Res	Type	Atoms
10	y	2	NAG	O5-C5-C6-O6

There are no ring outliers.

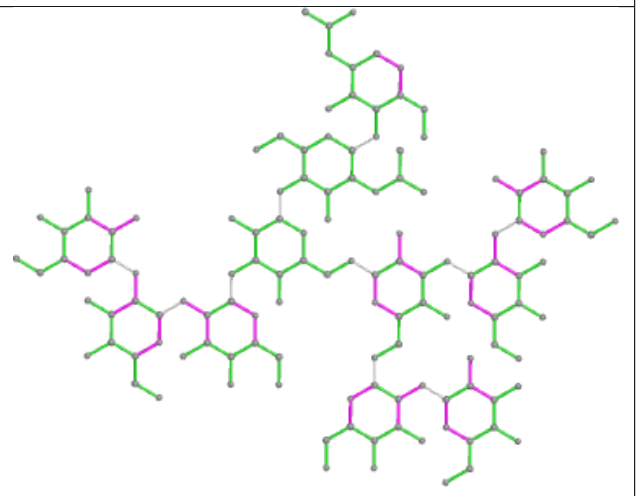
No monomer is involved in short contacts.

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

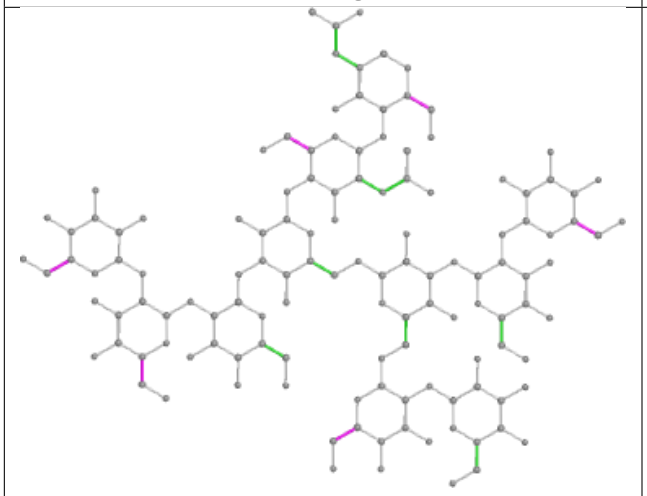
Oligosaccharide Chain S



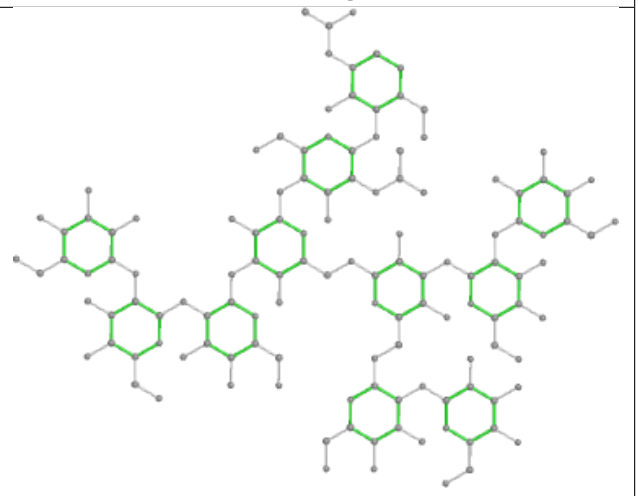
Bond lengths



Bond angles

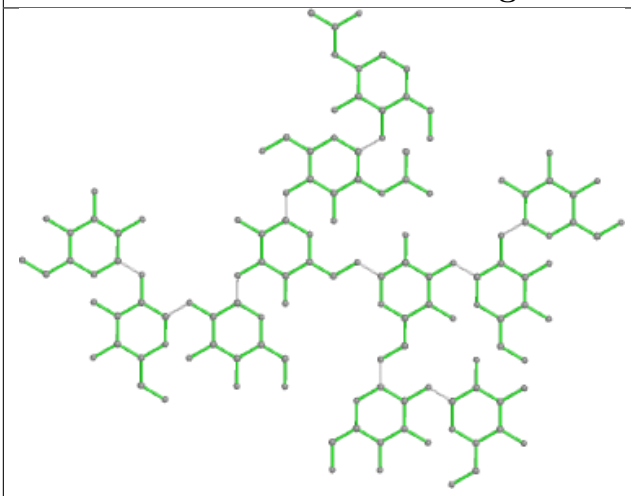


Torsions

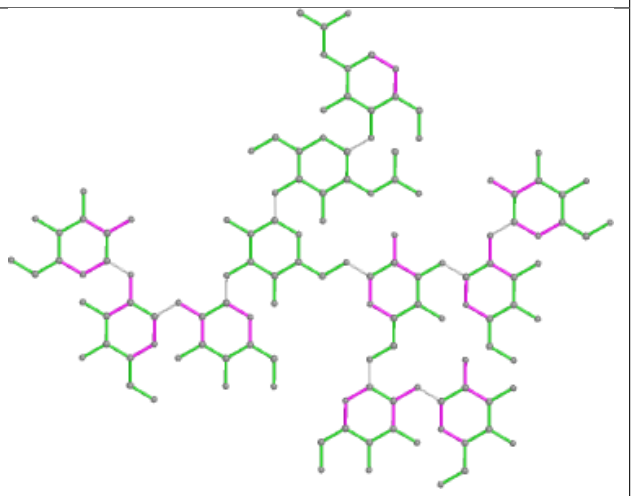


Rings

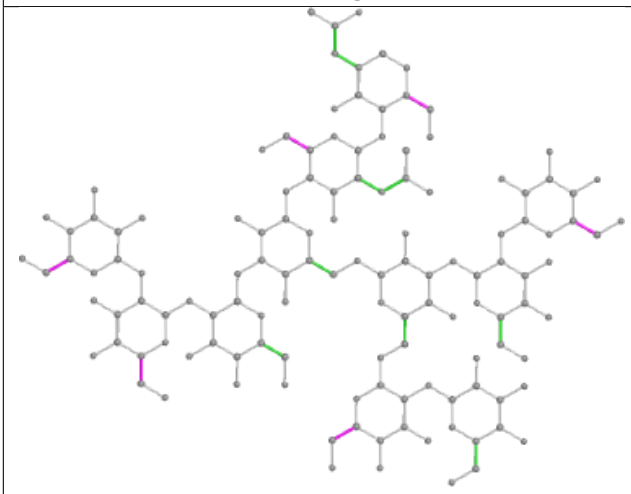
Oligosaccharide Chain a



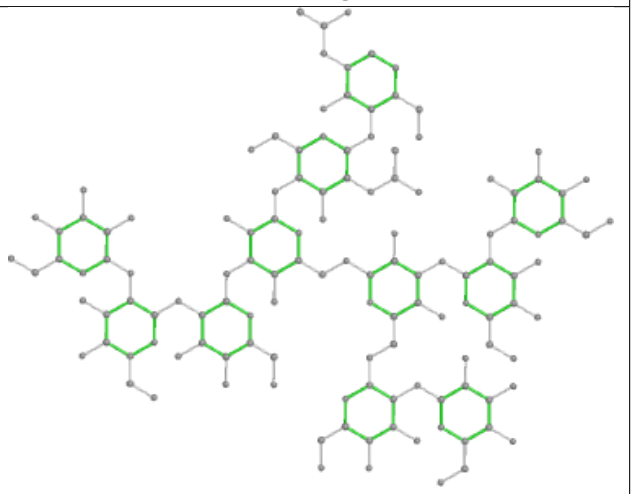
Bond lengths



Bond angles

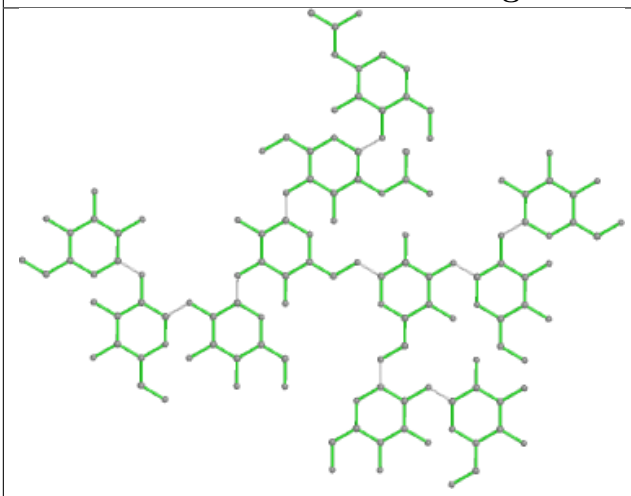


Torsions

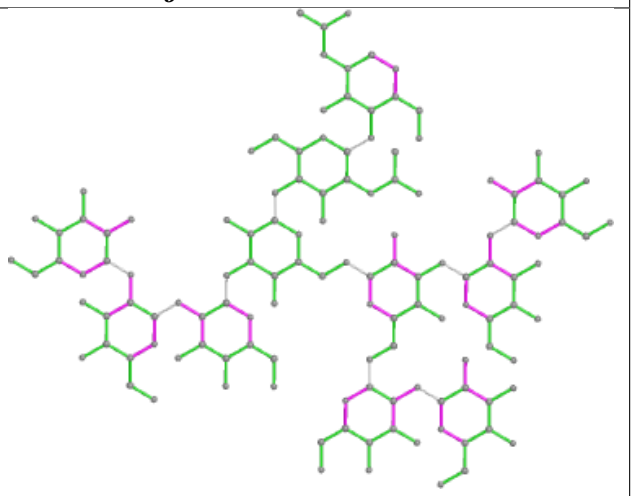


Rings

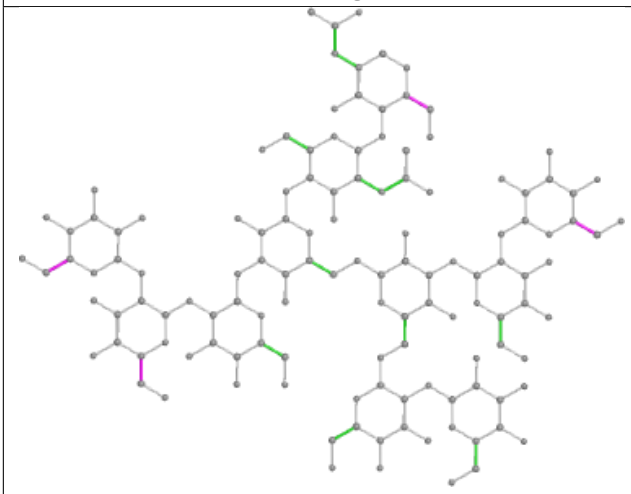
Oligosaccharide Chain j



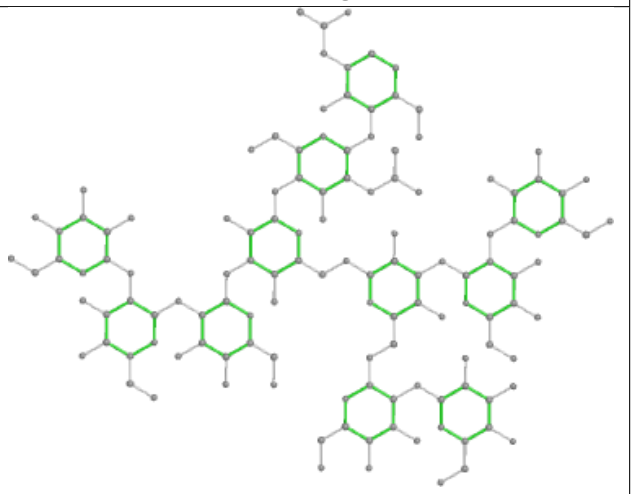
Bond lengths



Bond angles

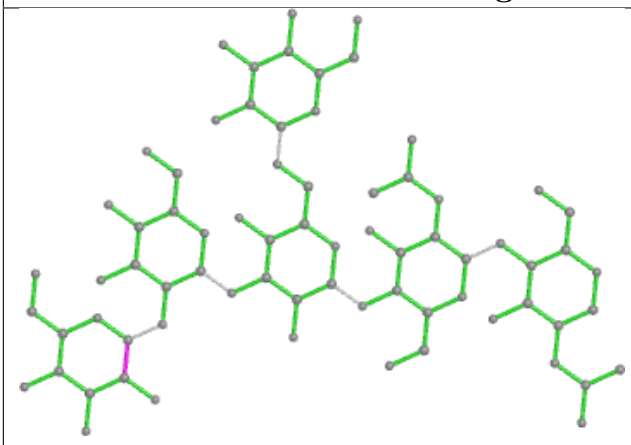


Torsions



Rings

Oligosaccharide Chain T



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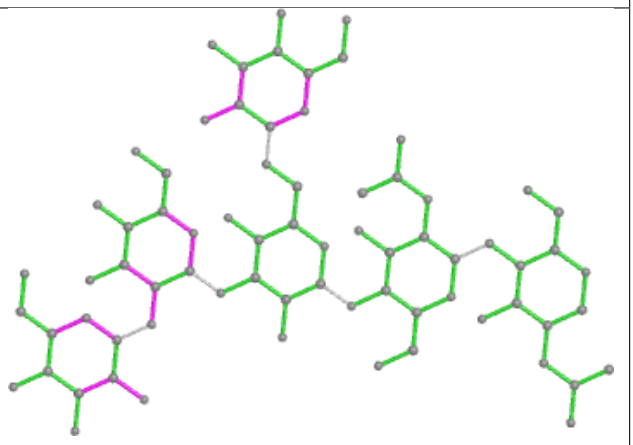
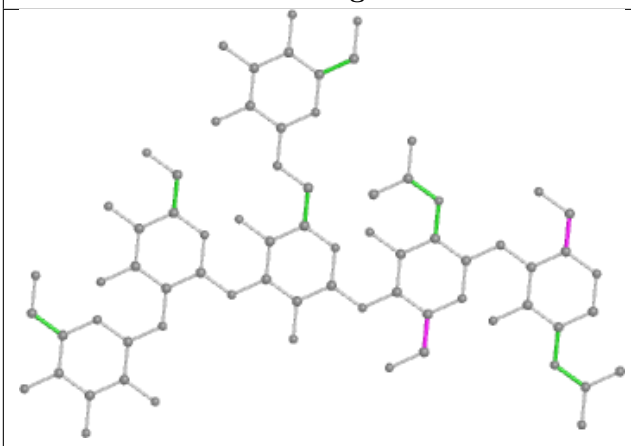


Bond angles



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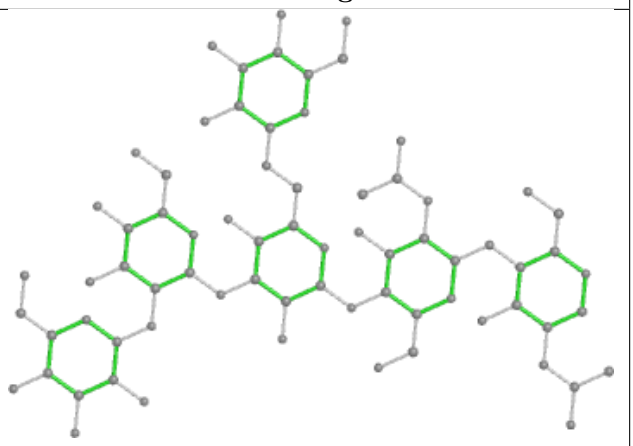
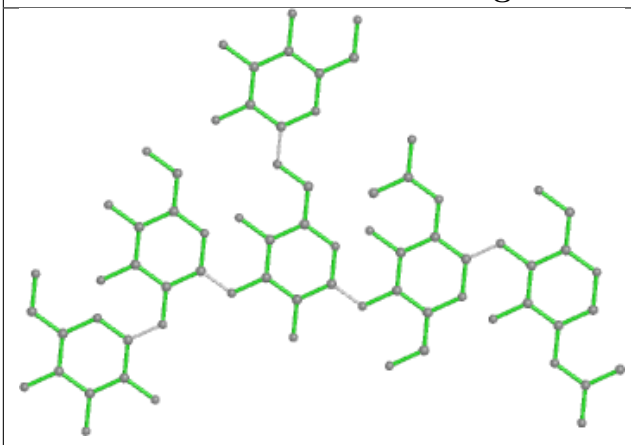


Rings

Oligosaccharide Chain Y



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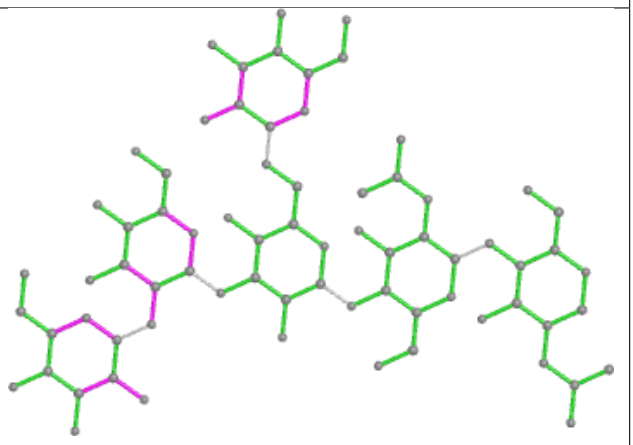

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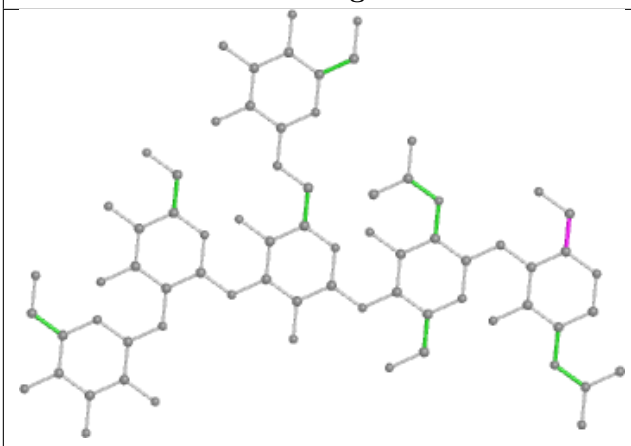

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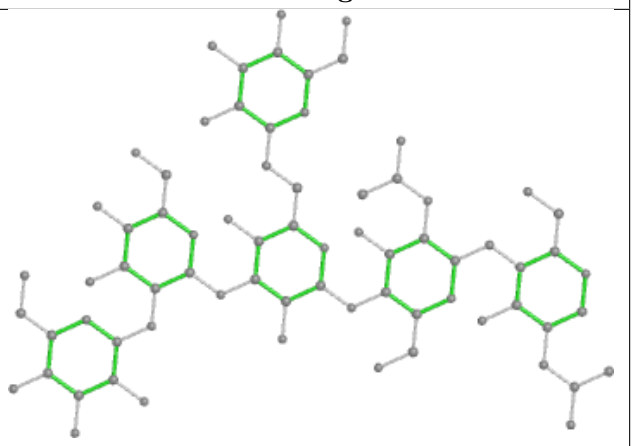
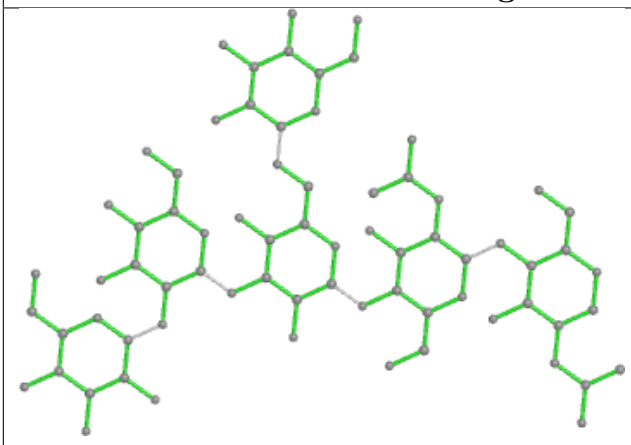


Rings

Oligosaccharide Chain b



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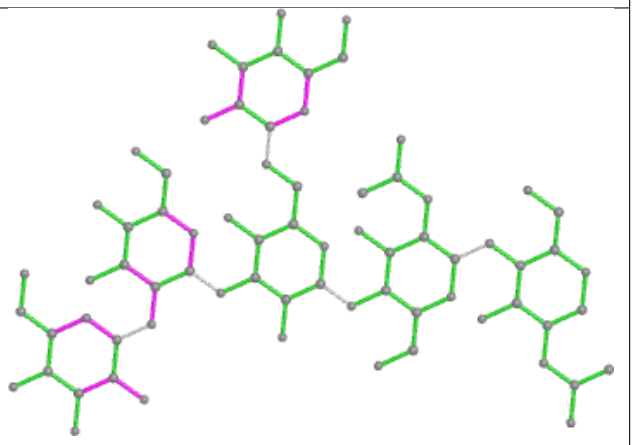

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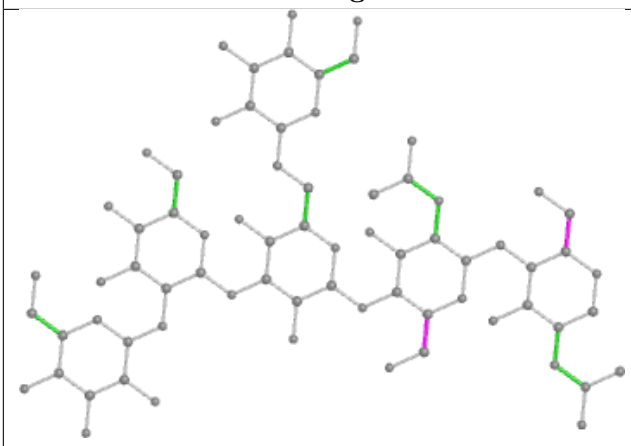

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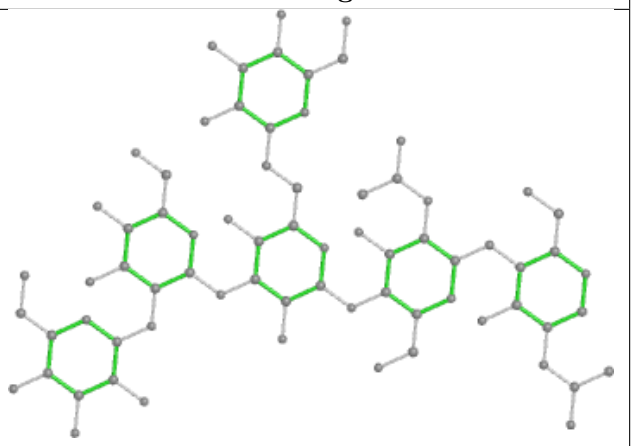
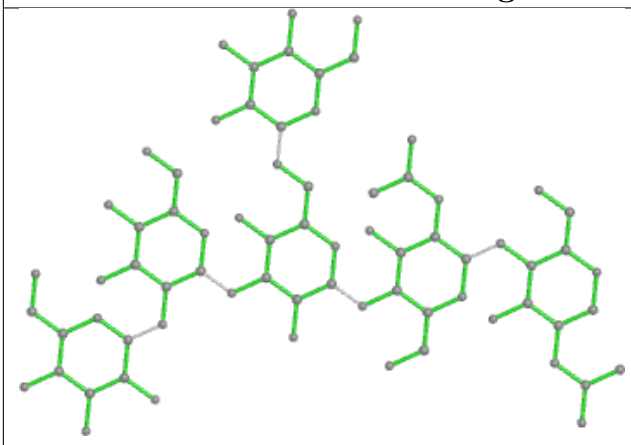


Rings

Oligosaccharide Chain h



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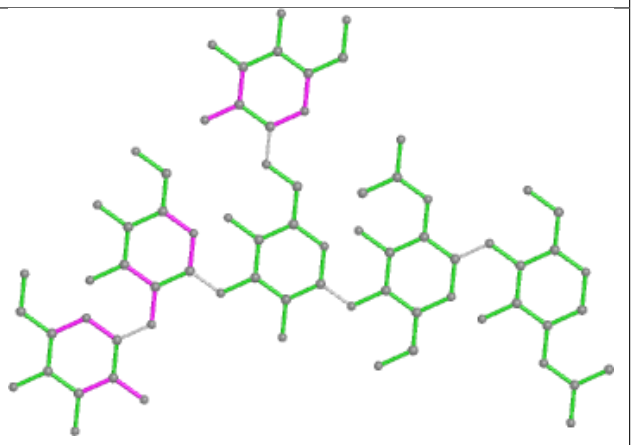

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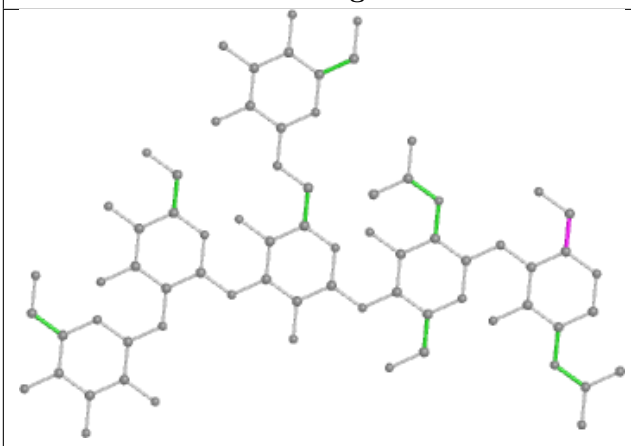

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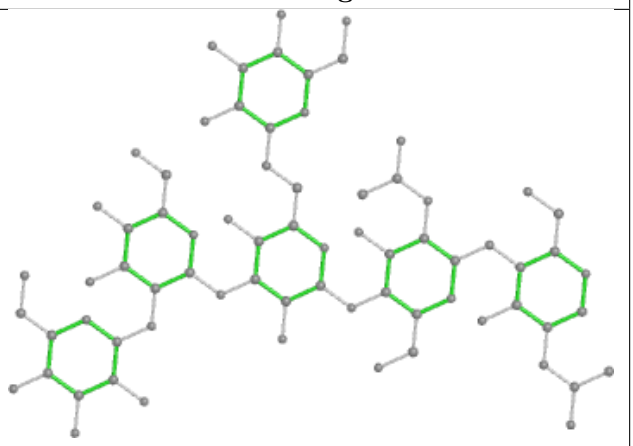
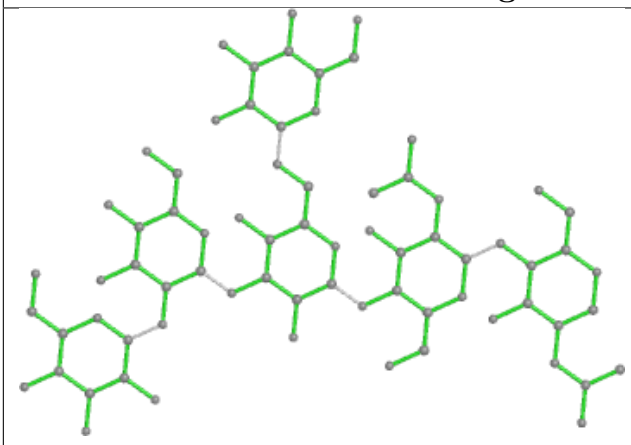


Rings

Oligosaccharide Chain k



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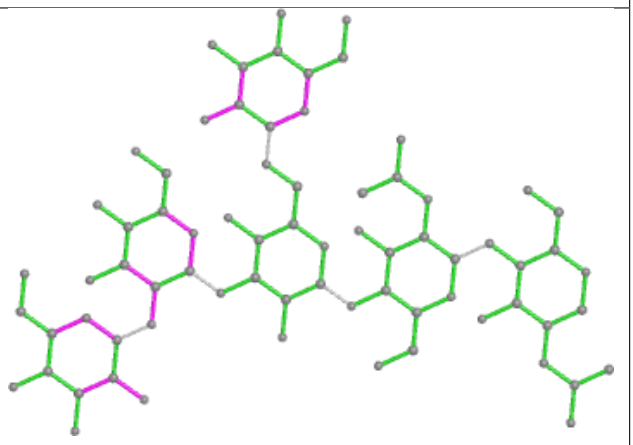

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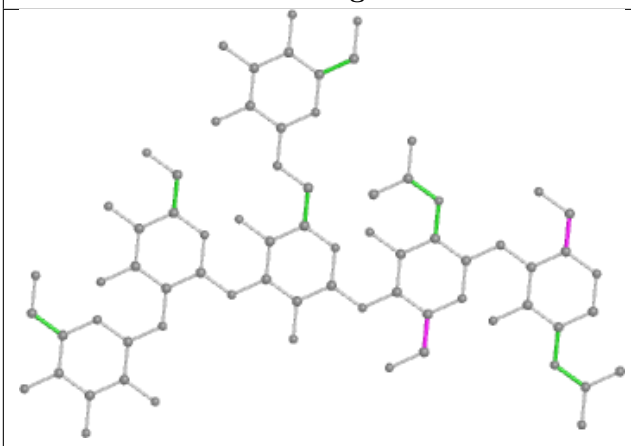

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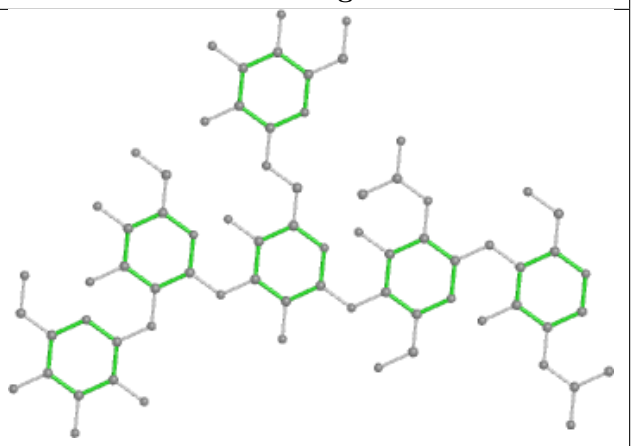
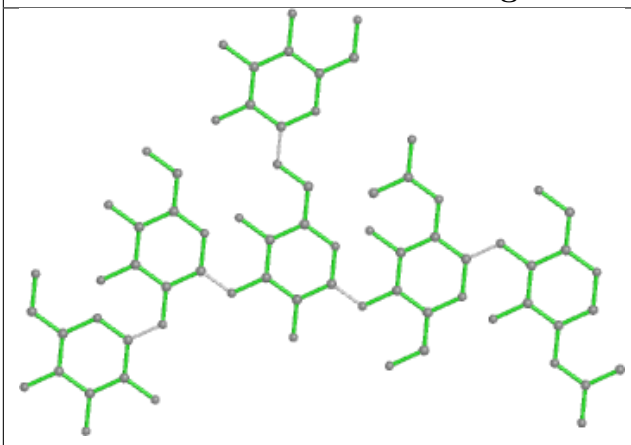


Rings

Oligosaccharide Chain r



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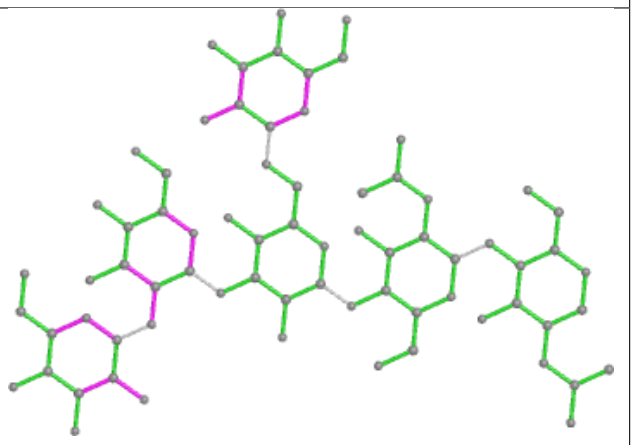
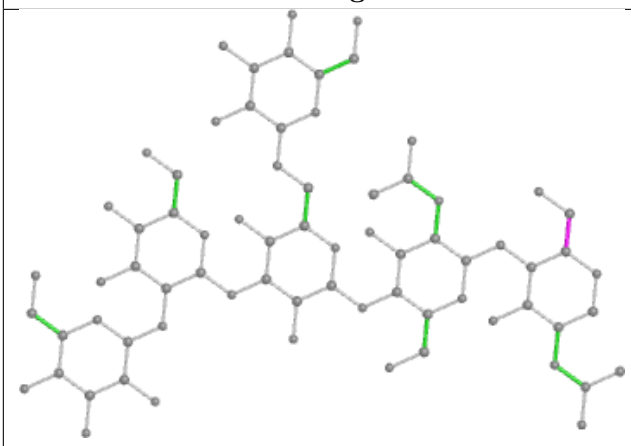


Bond angles



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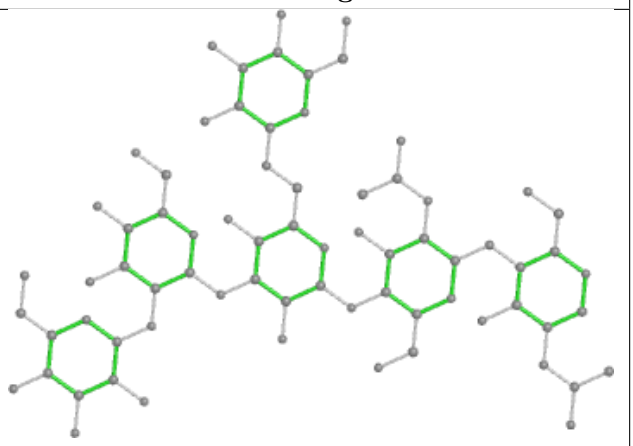
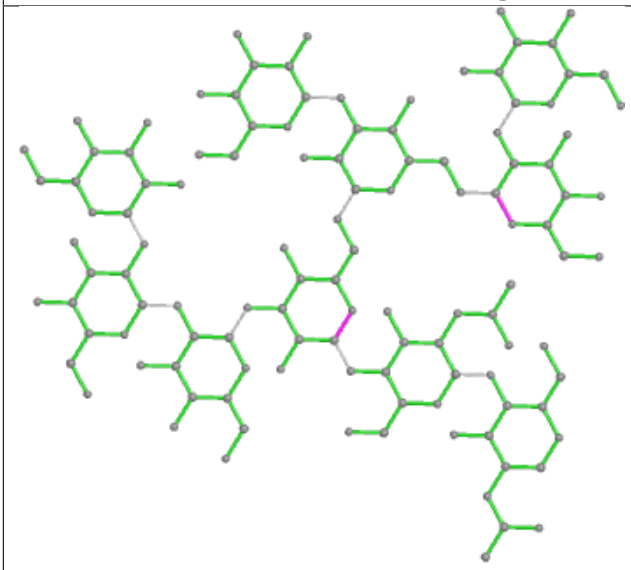


Rings

Oligosaccharide Chain U



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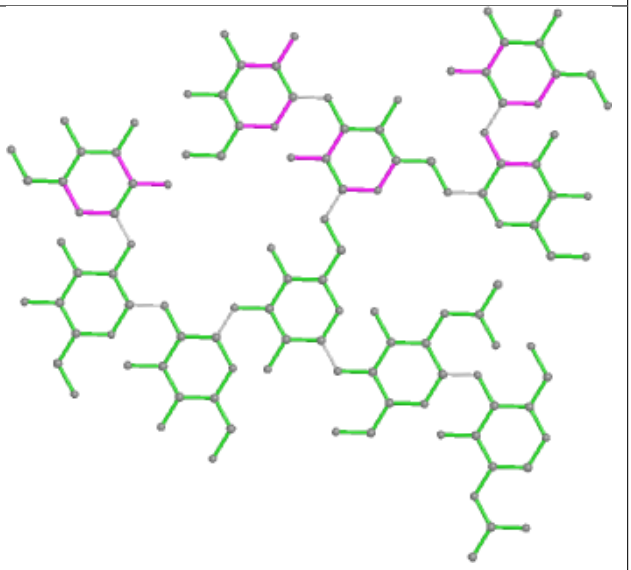
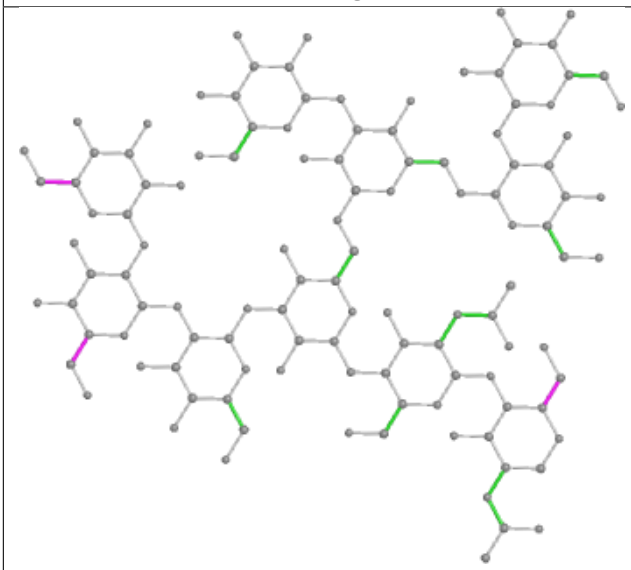


Bond angles



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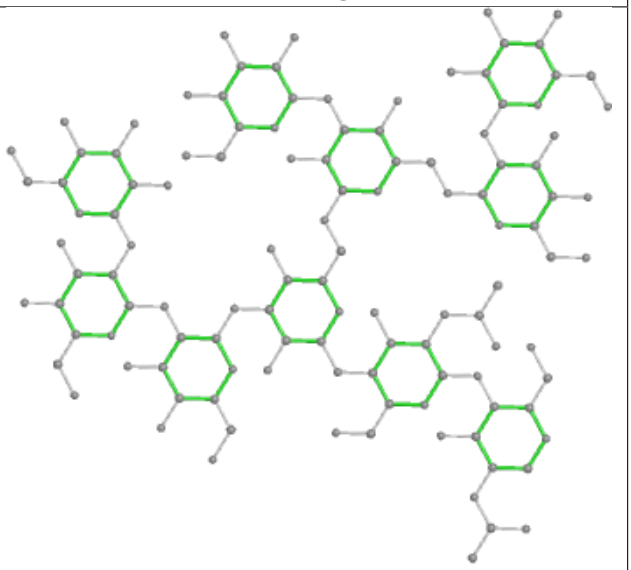
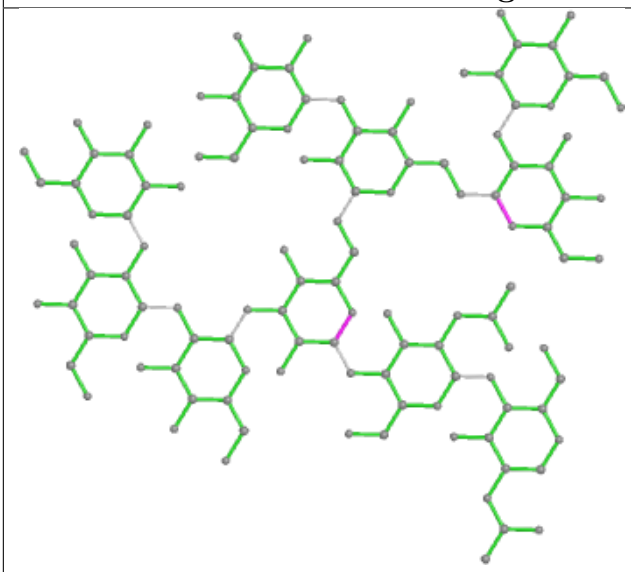


Rings

Oligosaccharide Chain d



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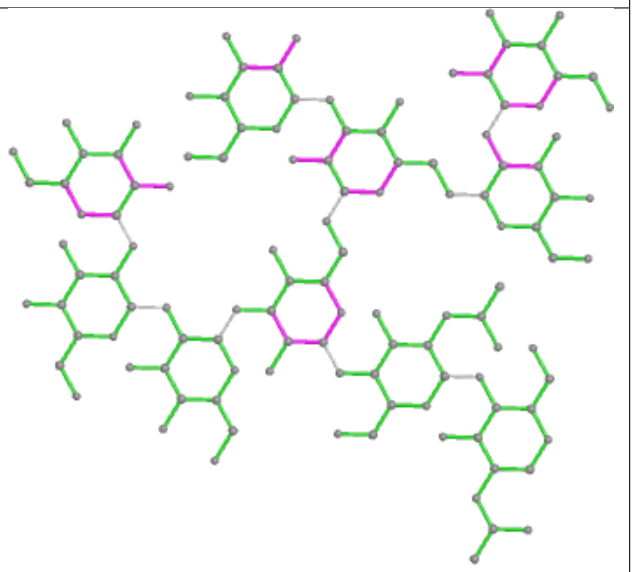
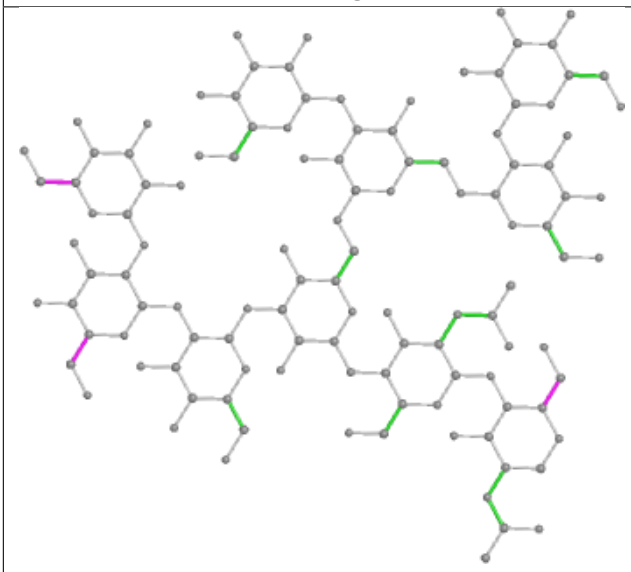


Bond angles



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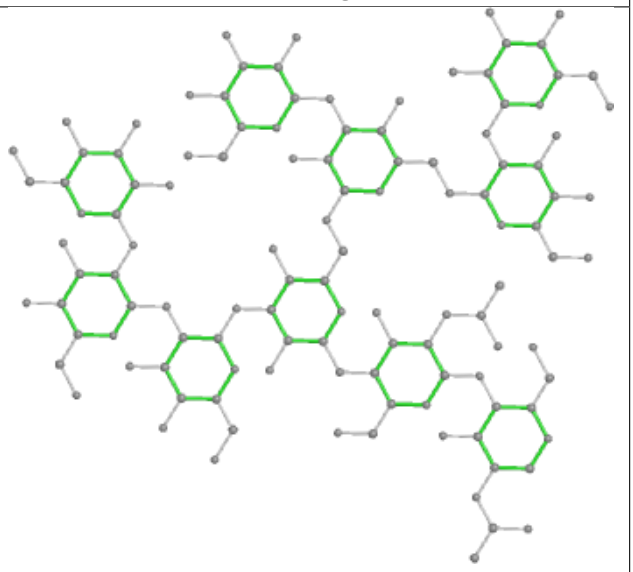
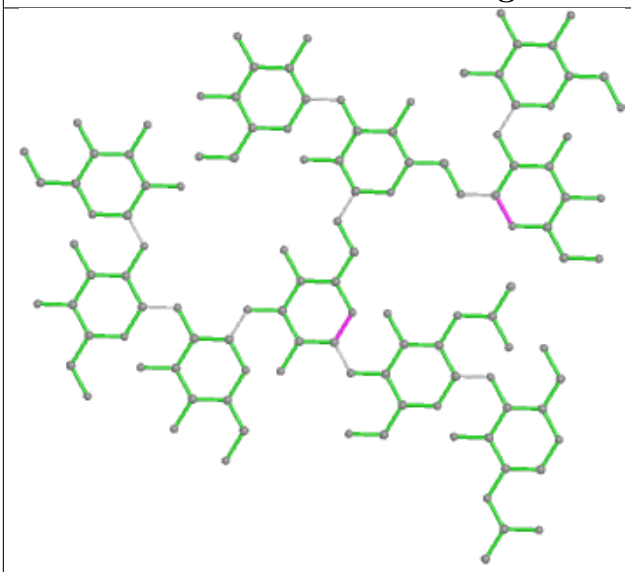


Rings

Oligosaccharide Chain n



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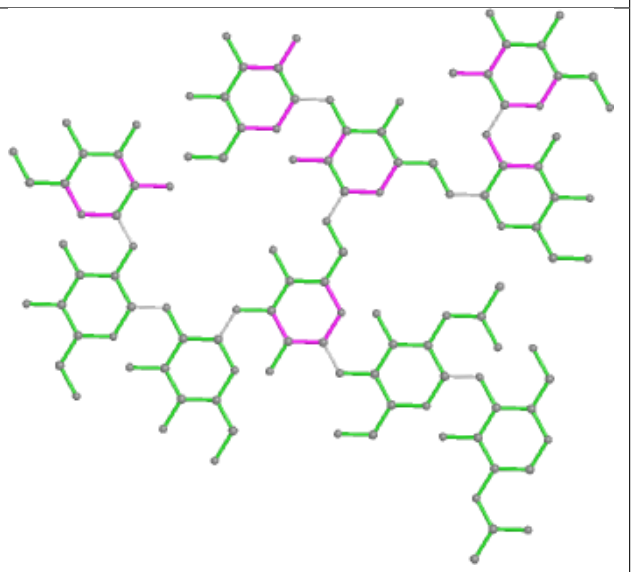

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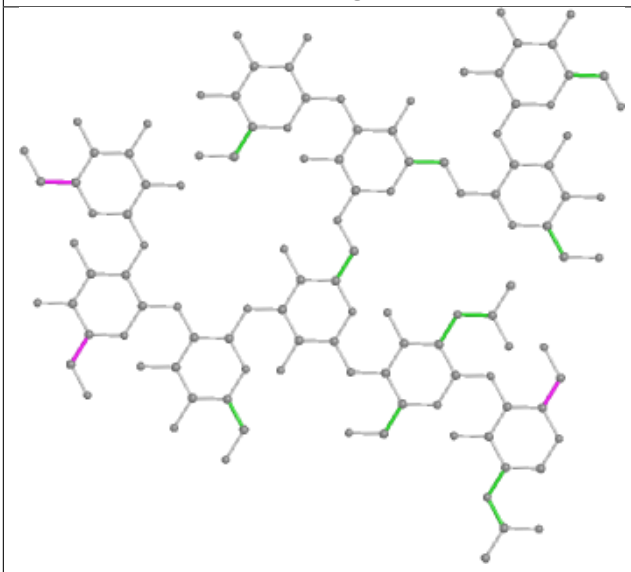

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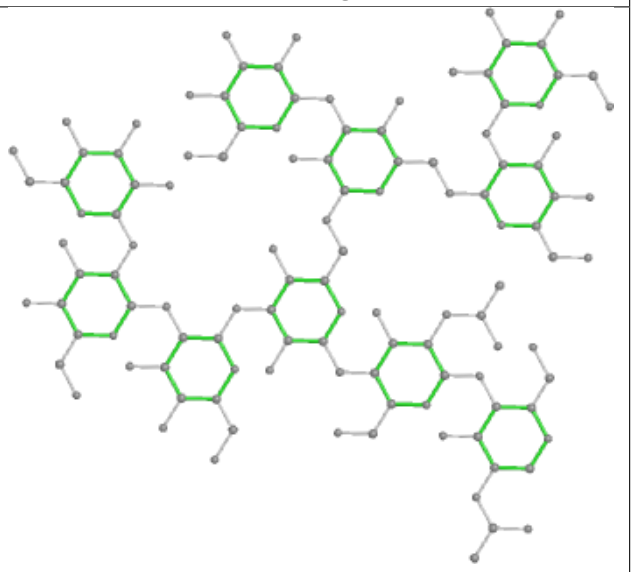
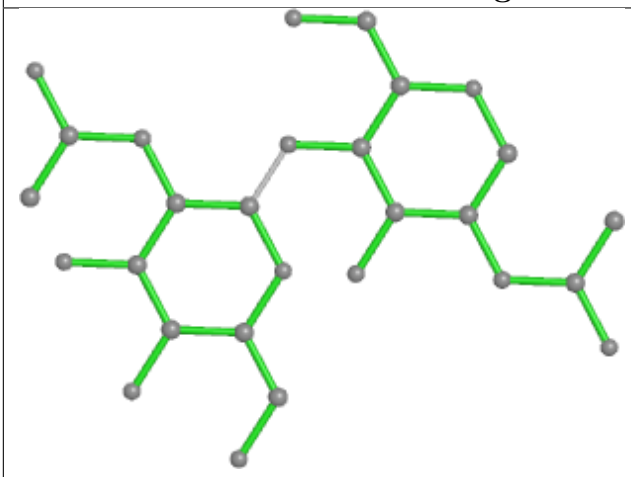


Rings

Oligosaccharide Chain V



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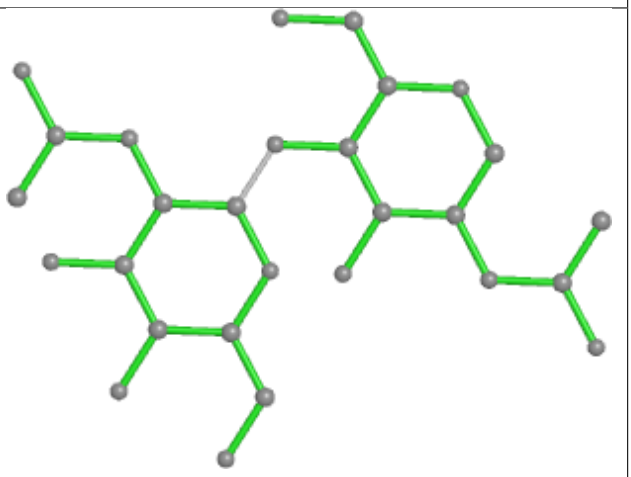
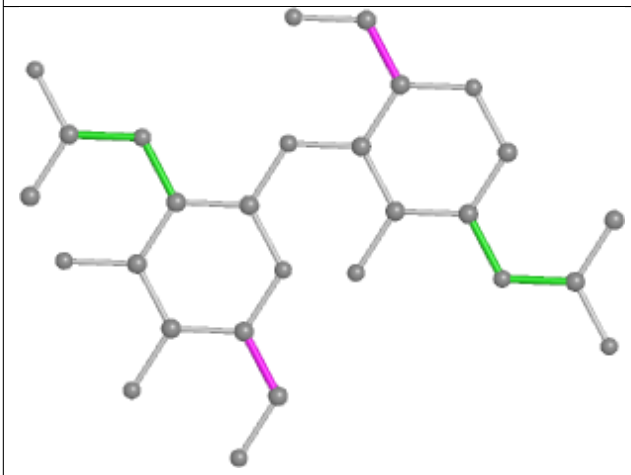


Bond angles



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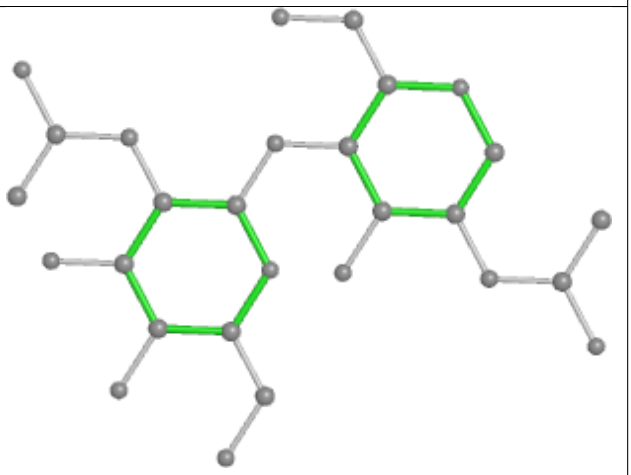
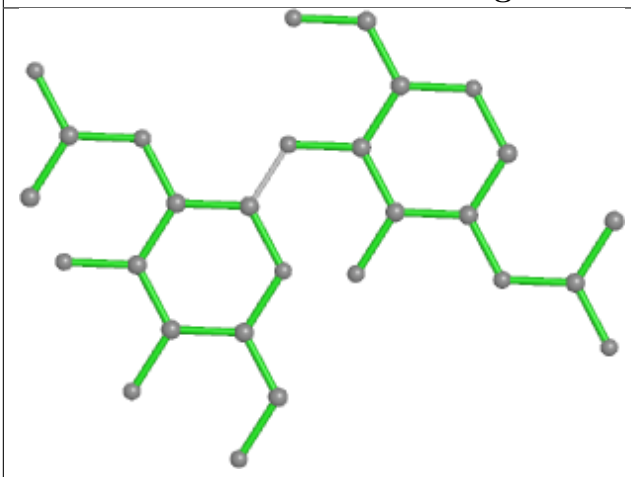


Rings

Oligosaccharide Chain X



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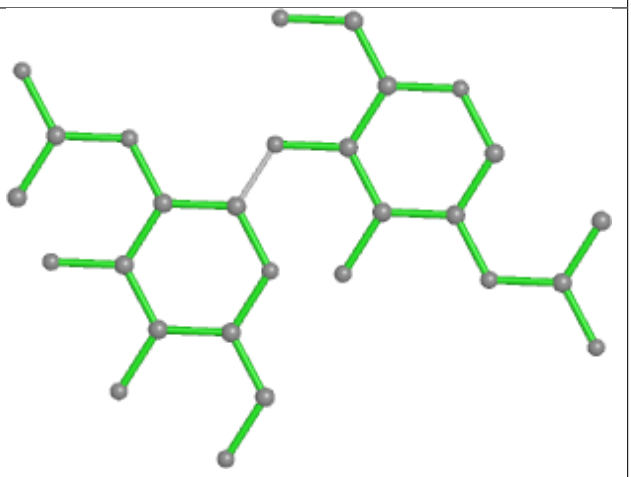

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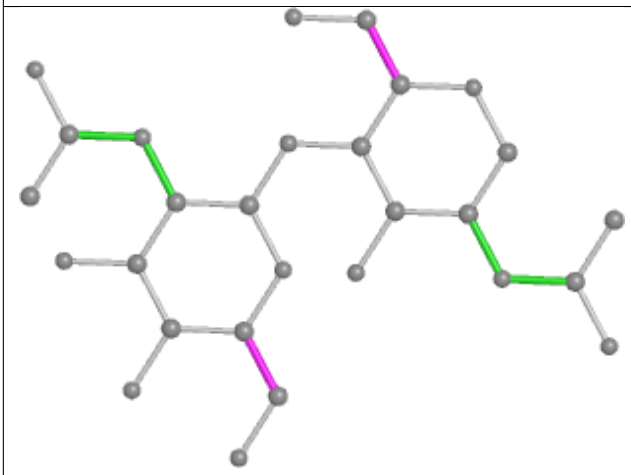

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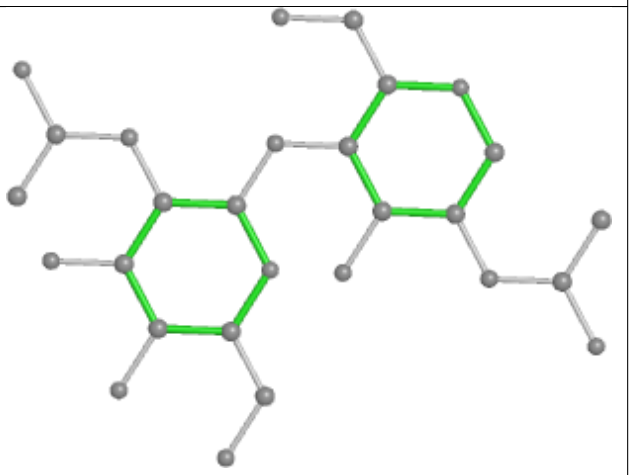
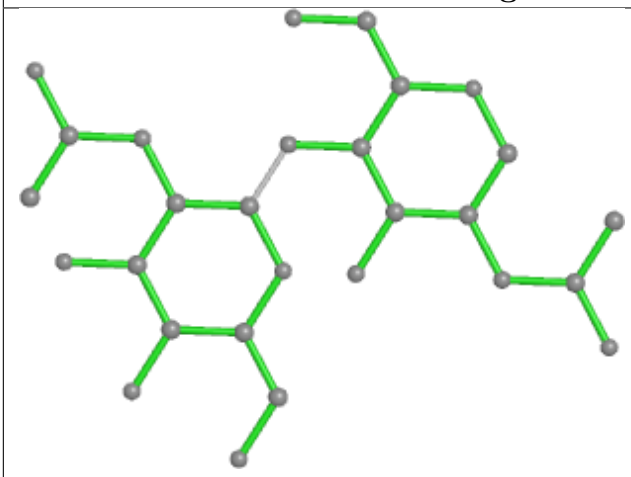


Rings

Oligosaccharide Chain c



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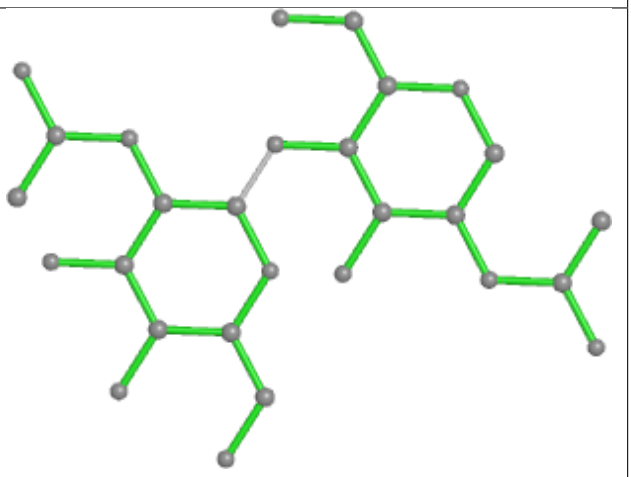

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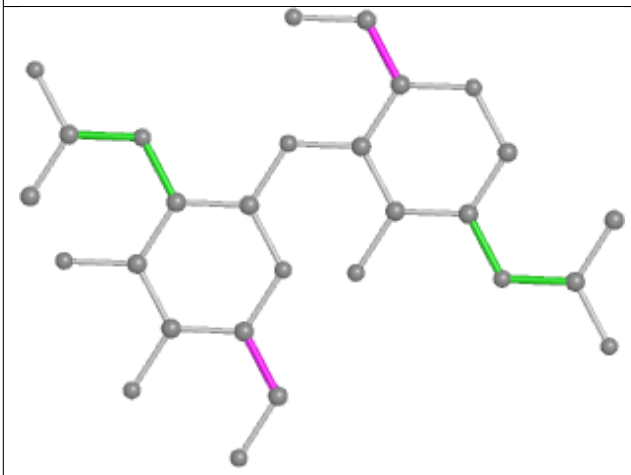

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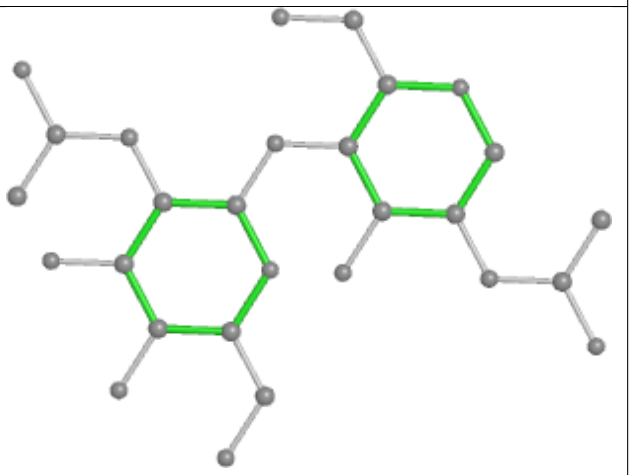
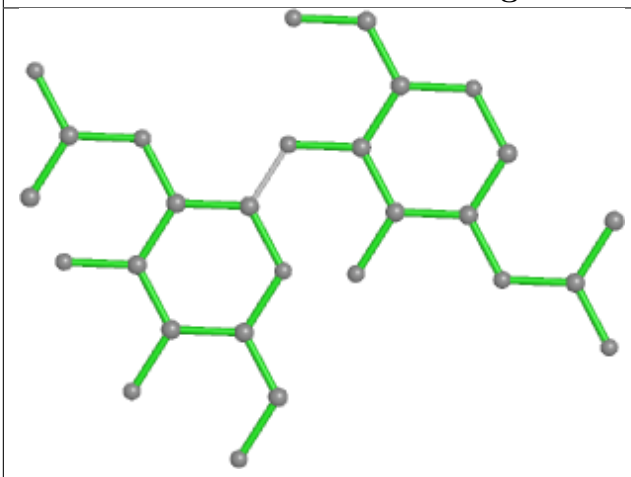


Rings

Oligosaccharide Chain f



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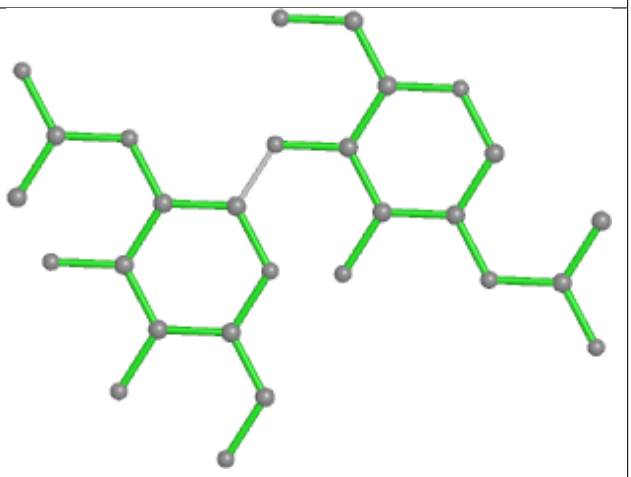
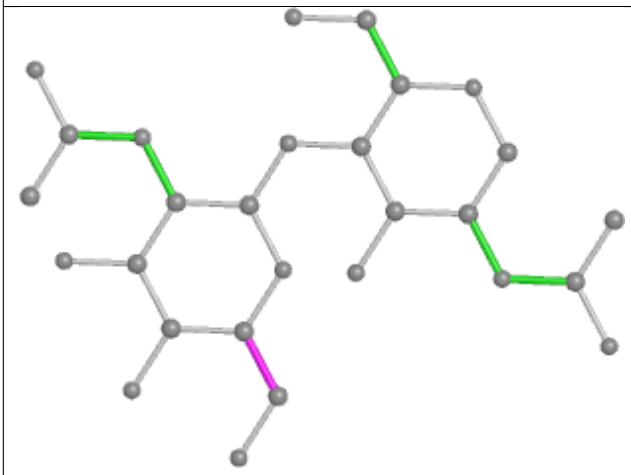
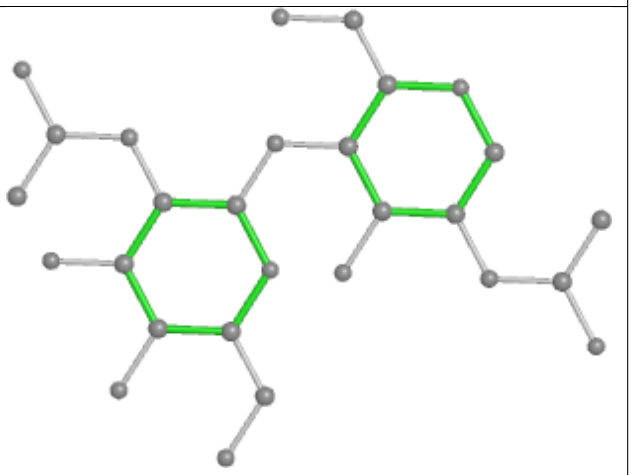


Bond angles

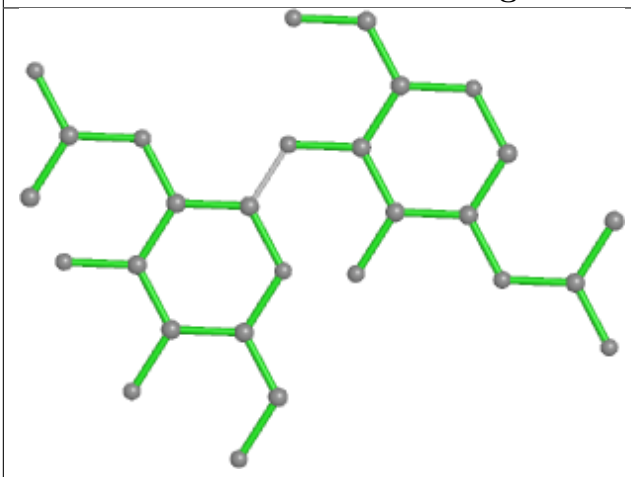


Torsions



Rings

Oligosaccharide Chain e



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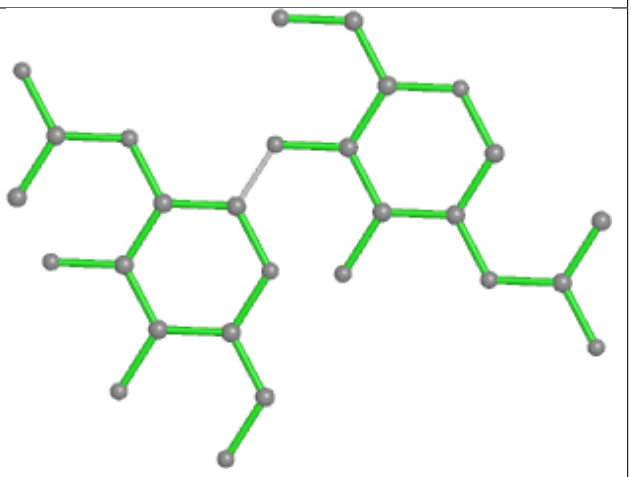
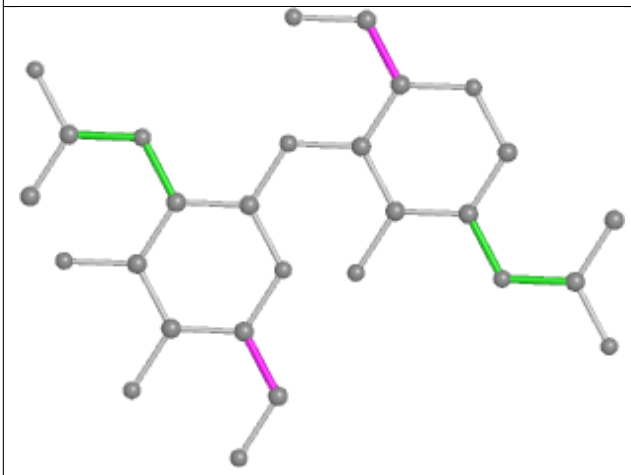


Bond angles



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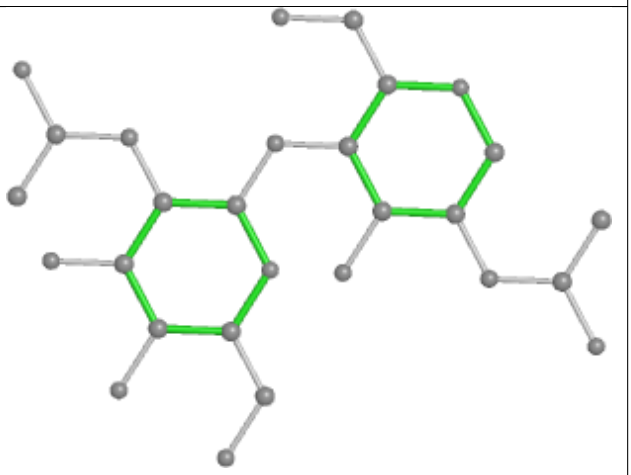
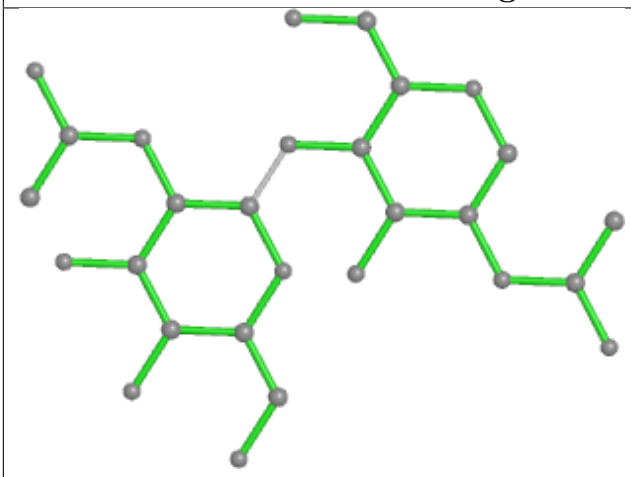
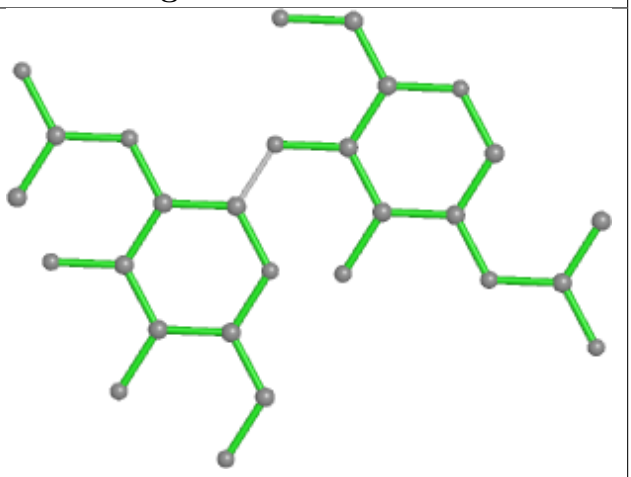


Rings

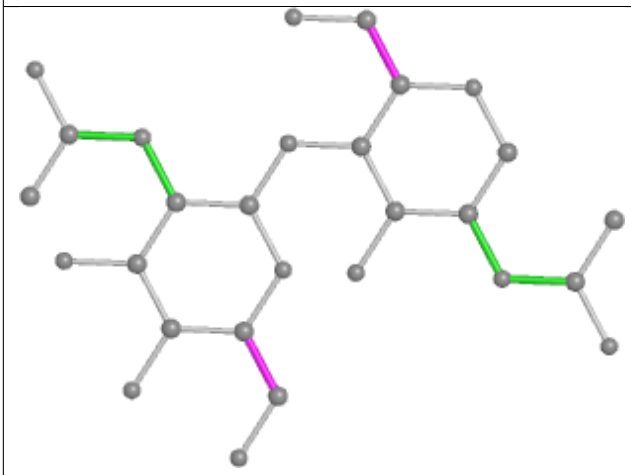
Oligosaccharide Chain g



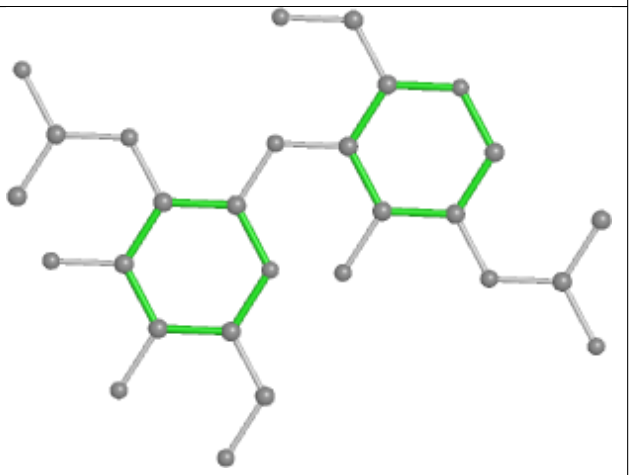
Bond lengths



Bond angles

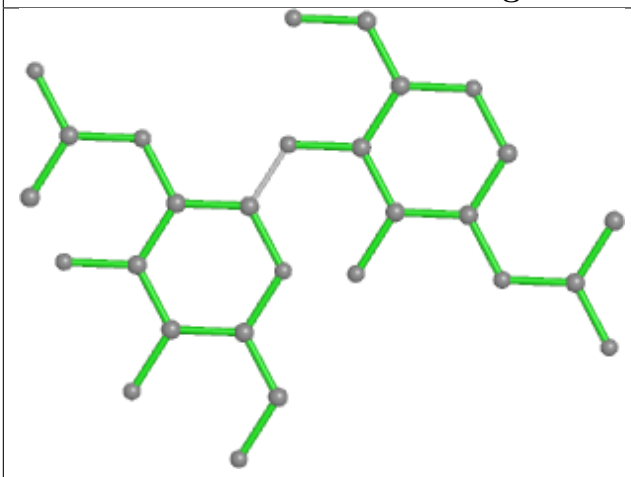


Torsions



Rings

Oligosaccharide Chain l



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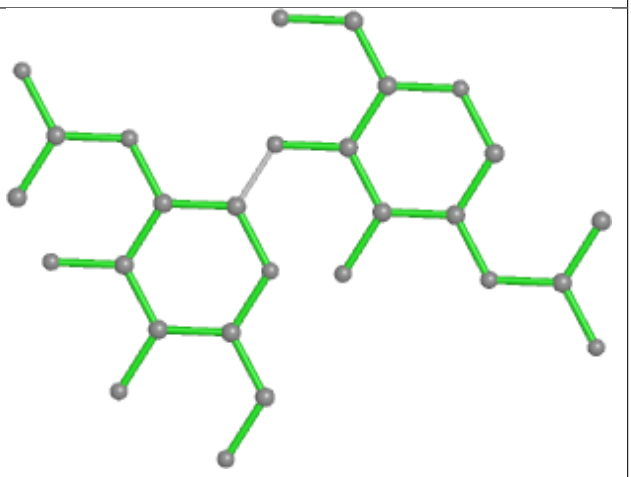
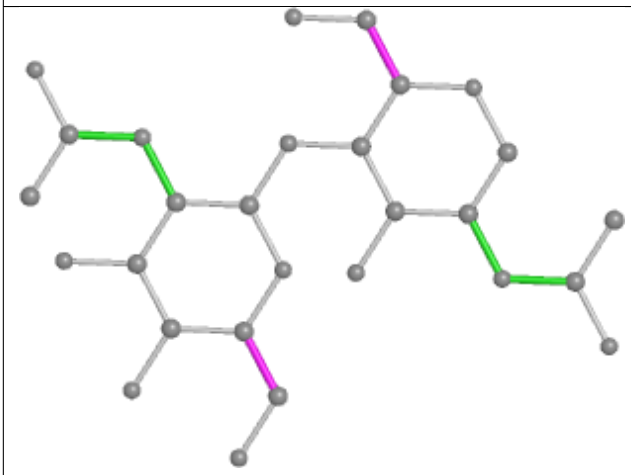


Bond angles



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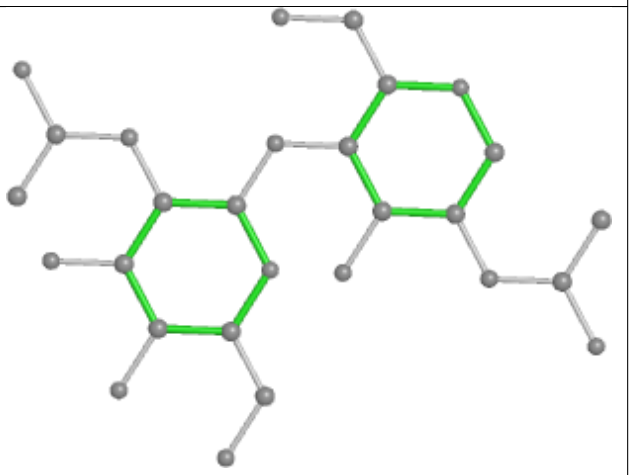
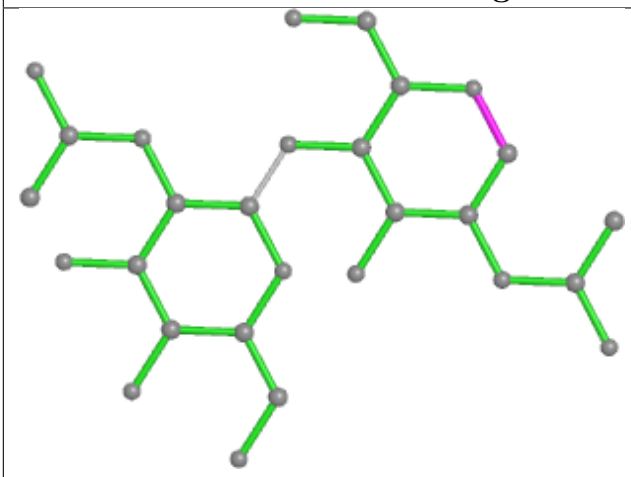
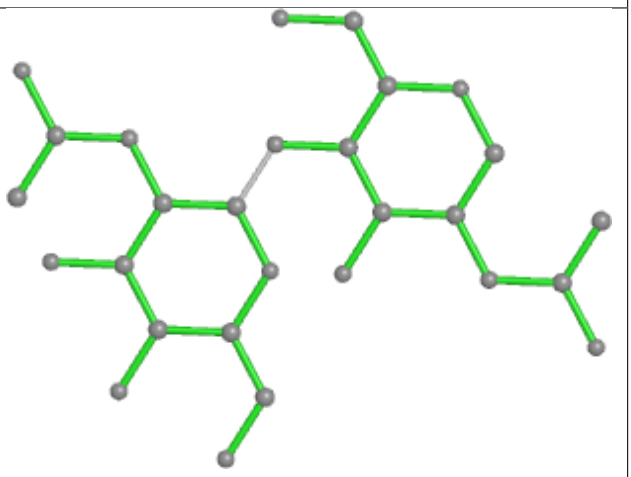
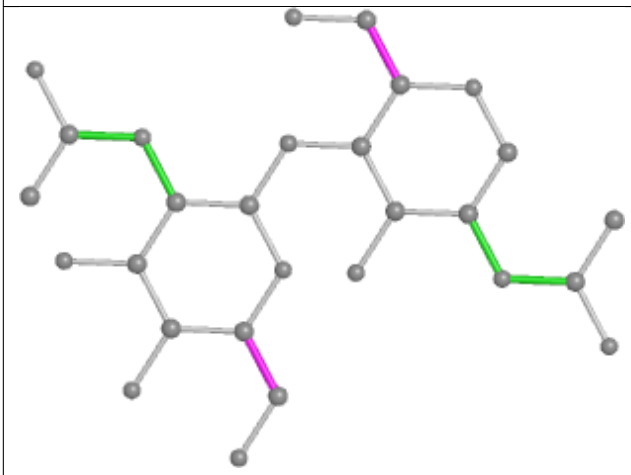
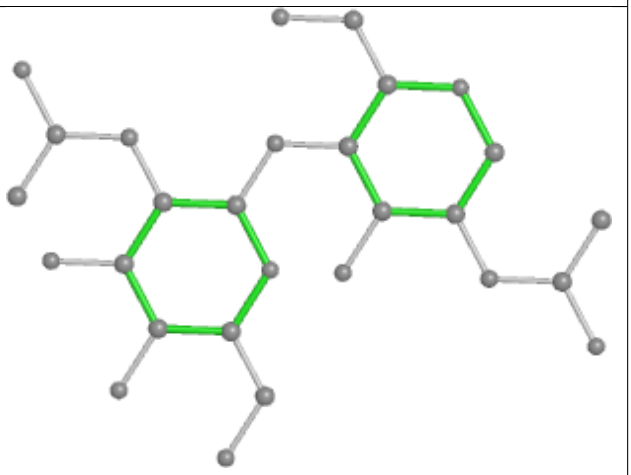
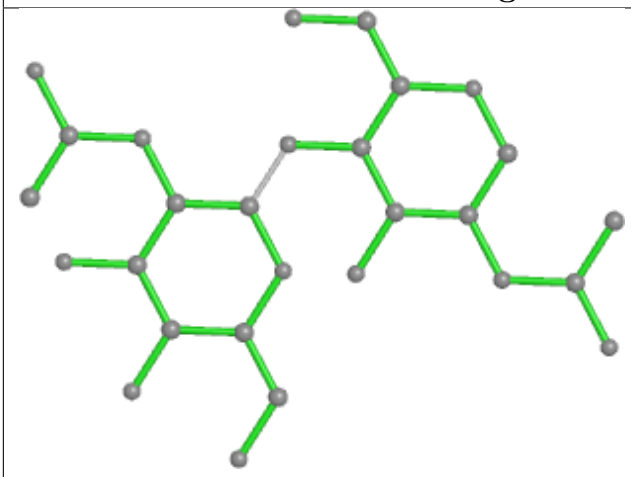


Rings

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

Oligosaccharide Chain o



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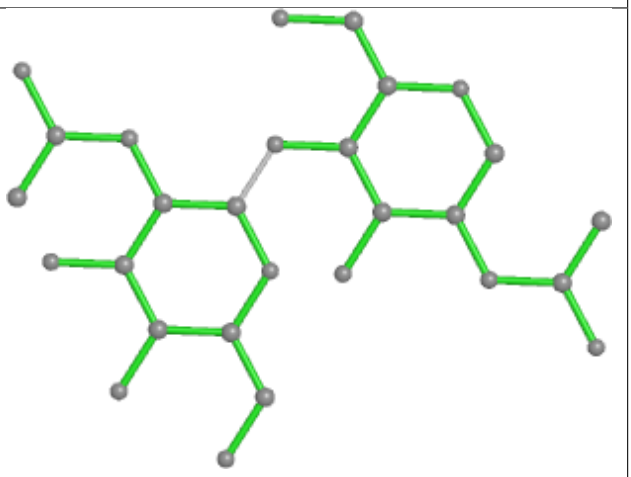
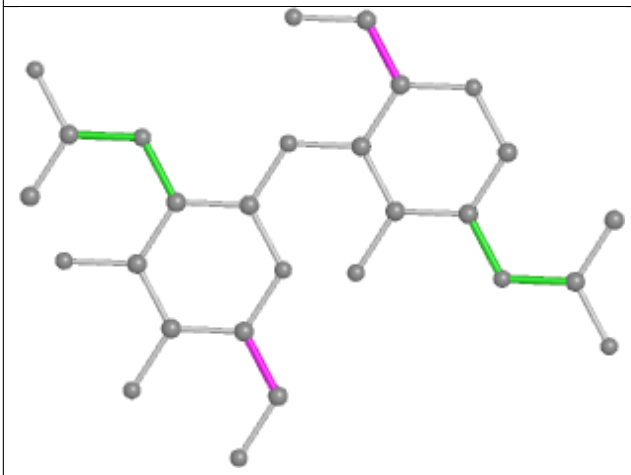


Bond angles



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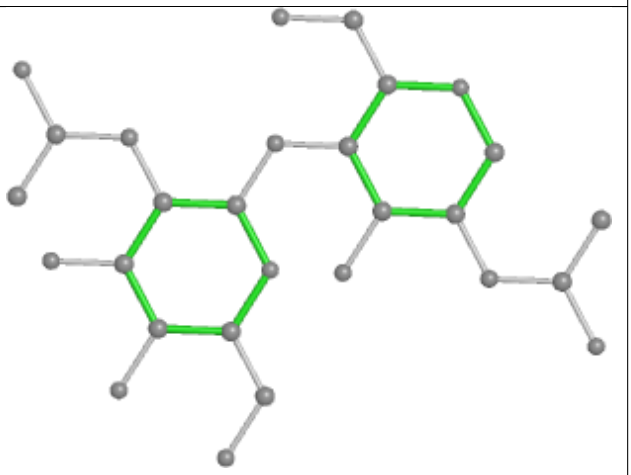
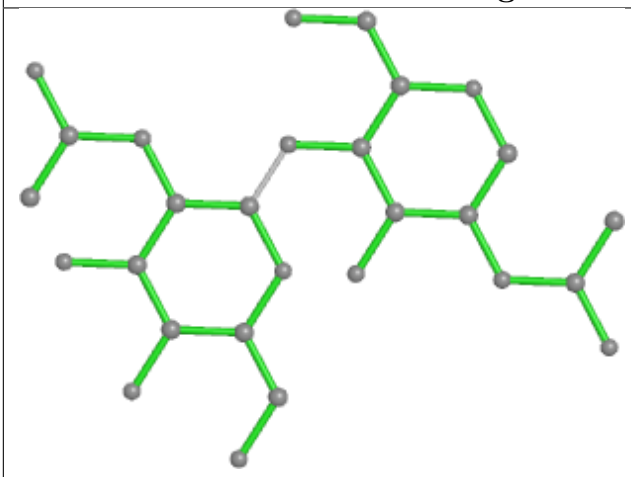


Rings

Oligosaccharide Chain p



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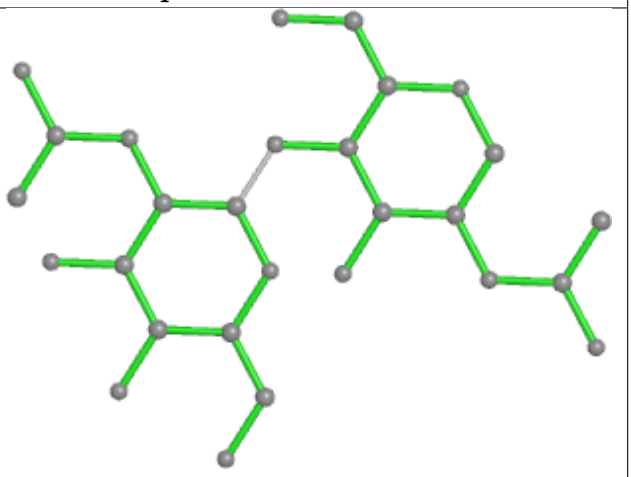

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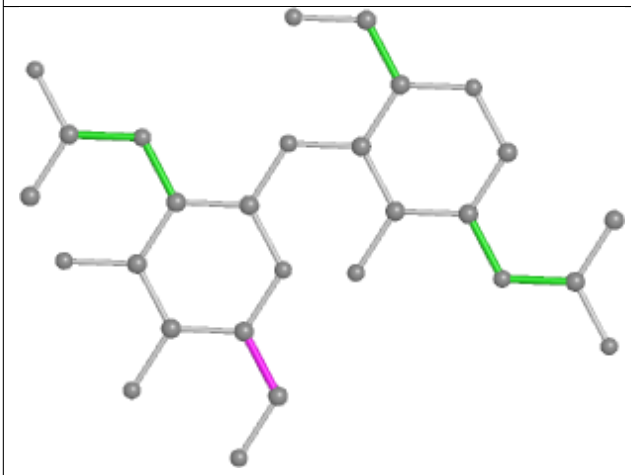

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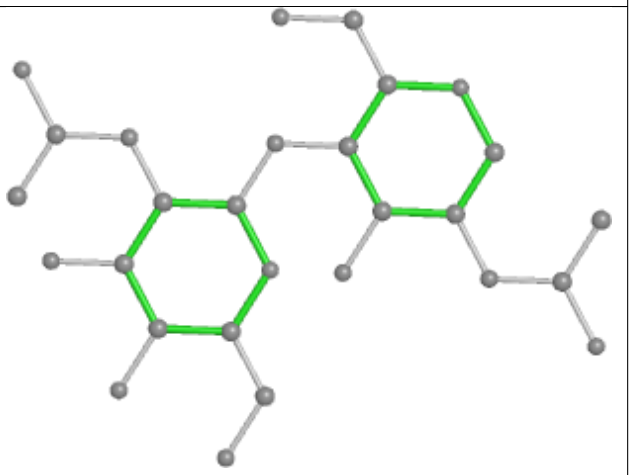
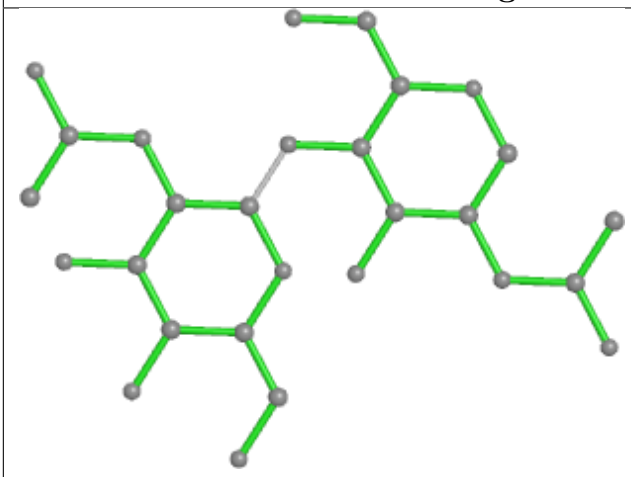


Rings

Oligosaccharide Chain q



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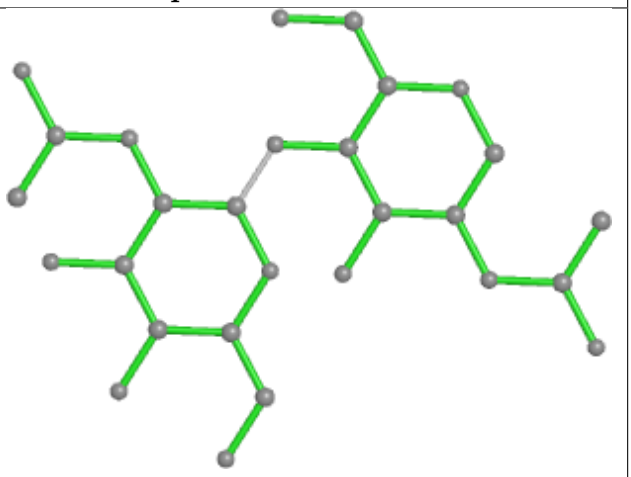

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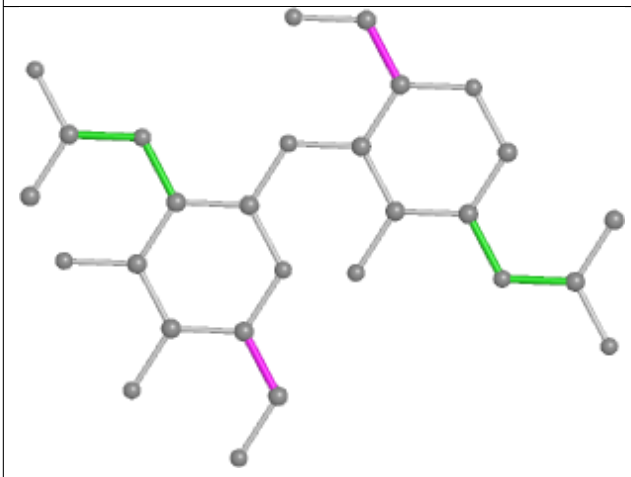

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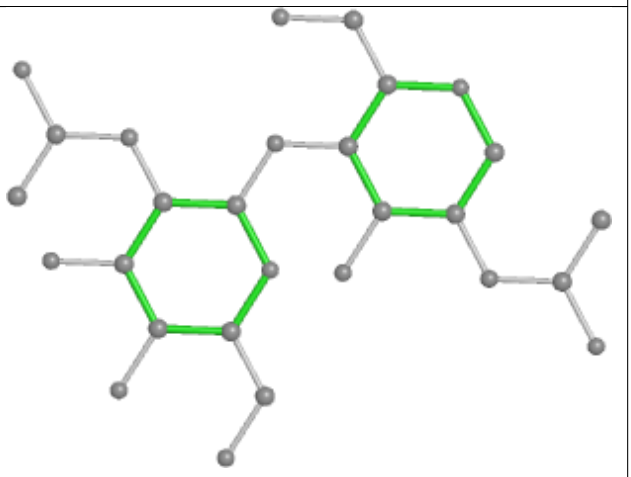
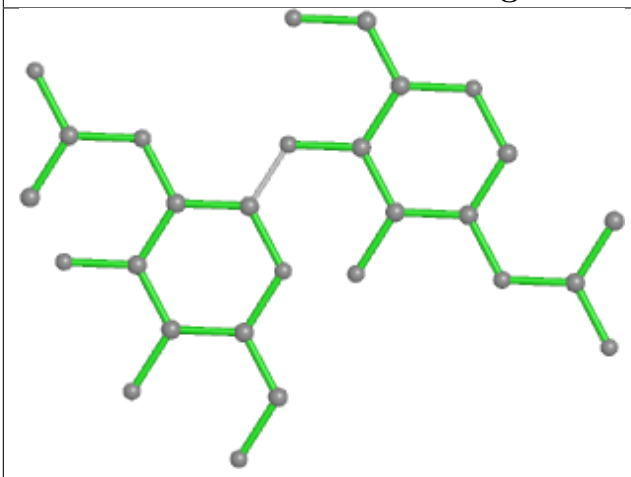


Rings

Oligosaccharide Chain t



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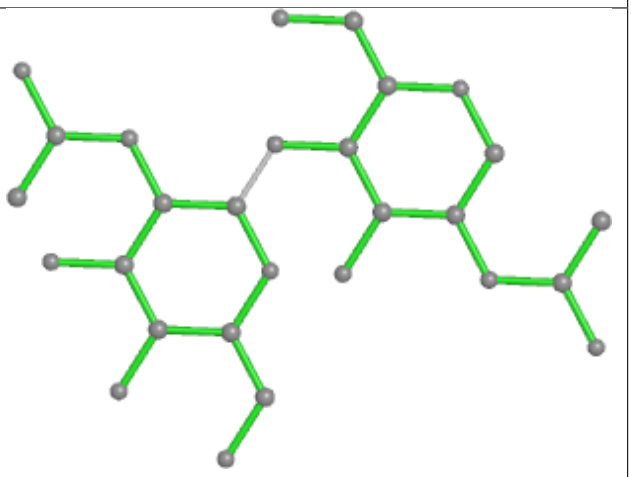
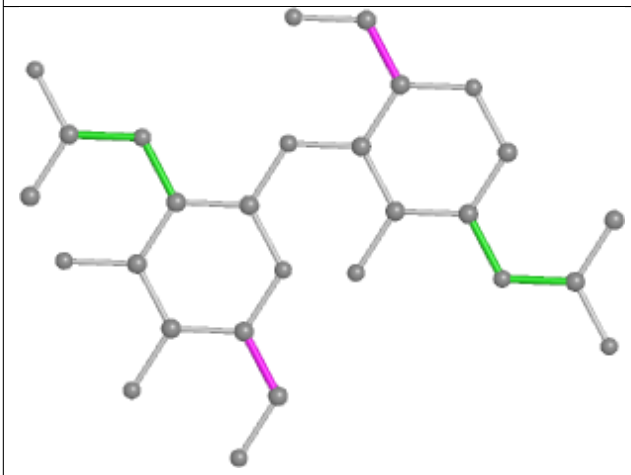


Bond angles



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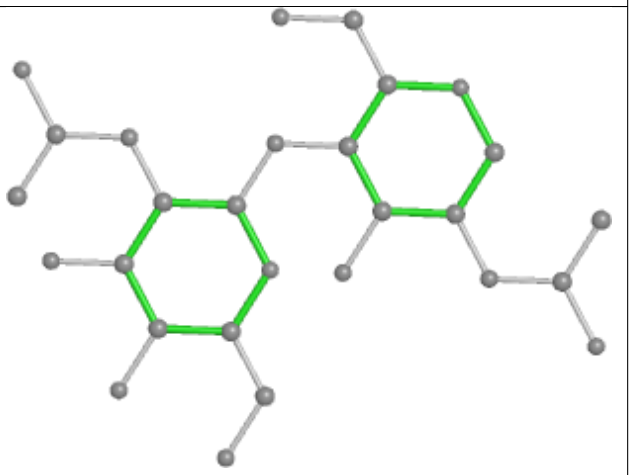
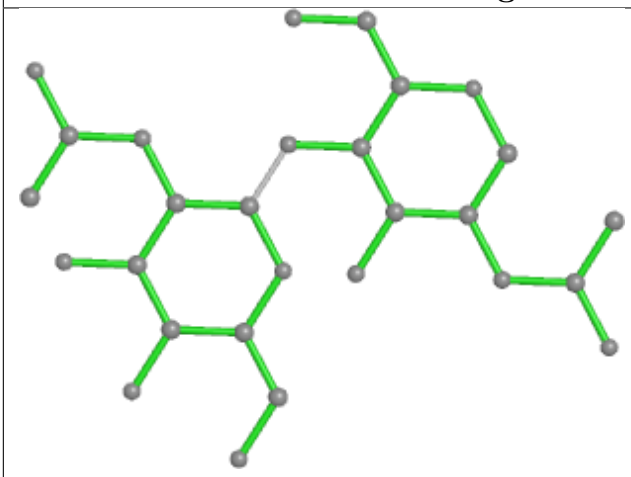


Rings

Oligosaccharide Chain u



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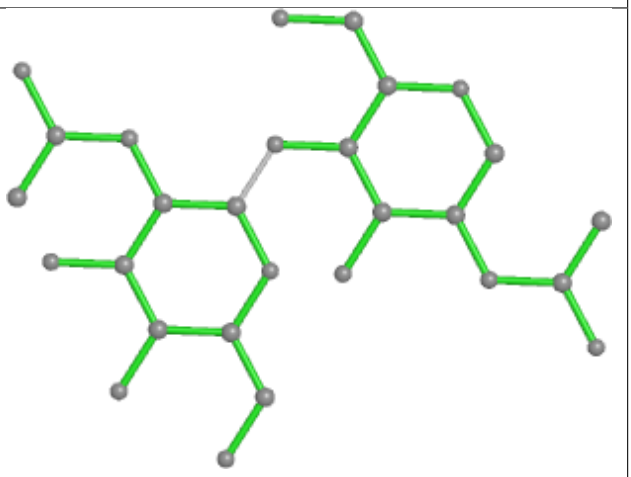
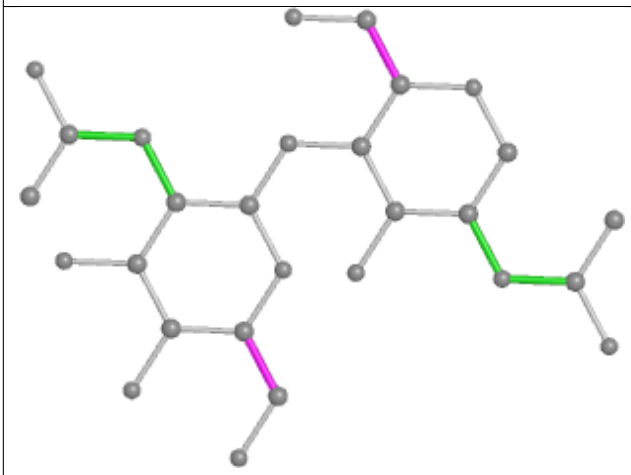


Bond angles



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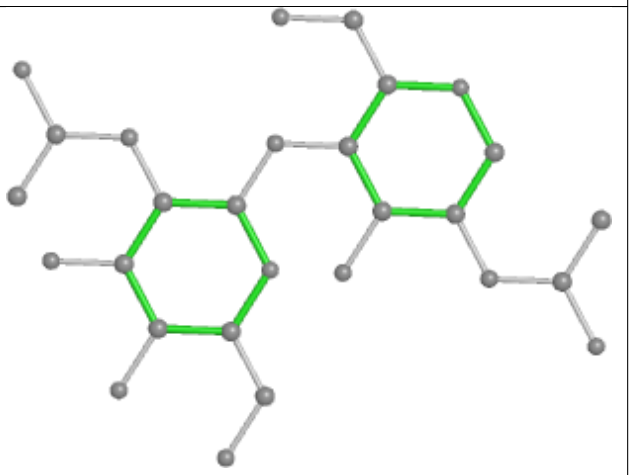
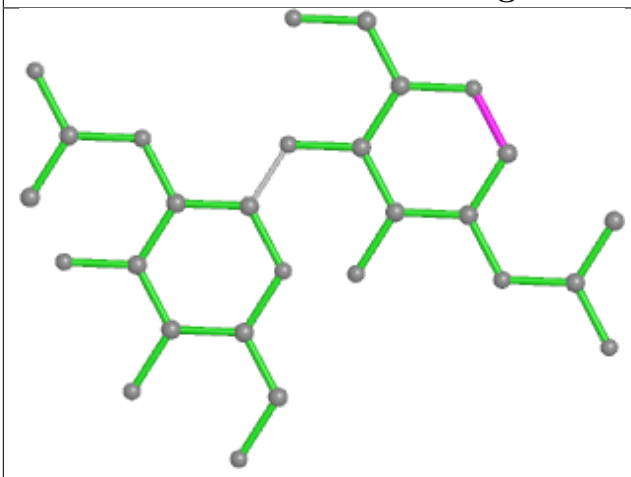


Rings

Oligosaccharide Chain v



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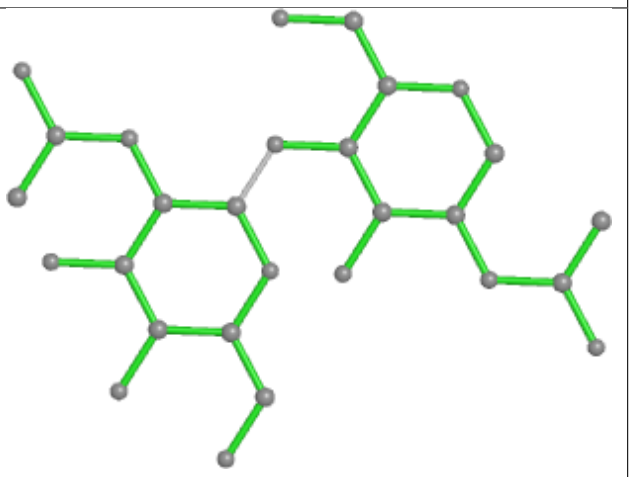

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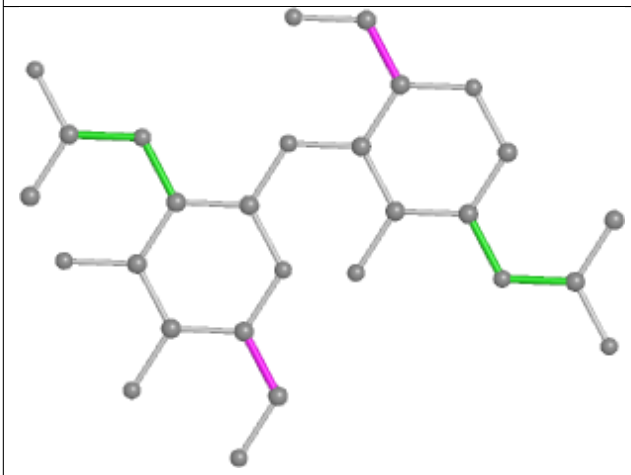

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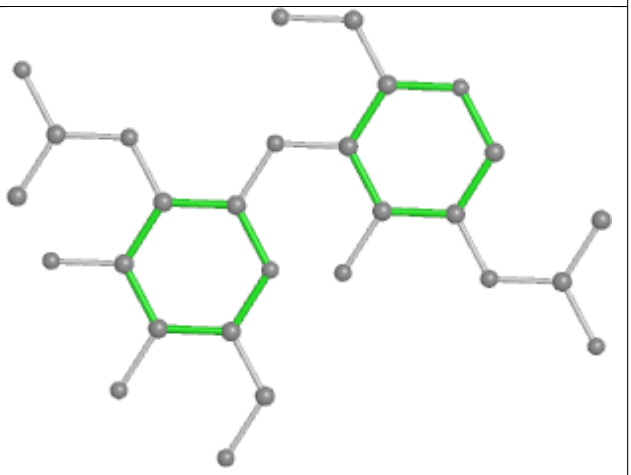
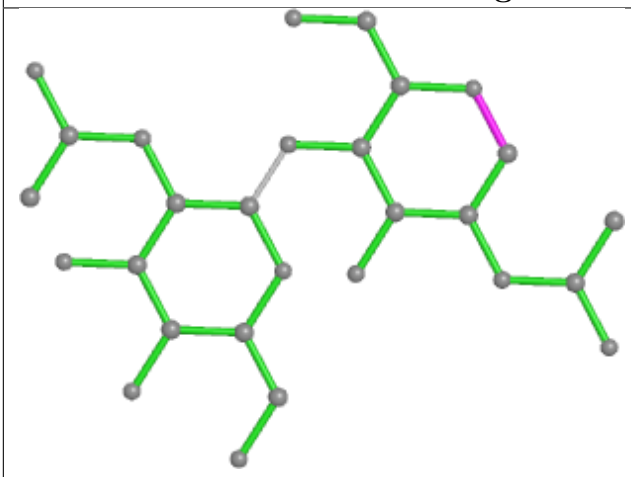
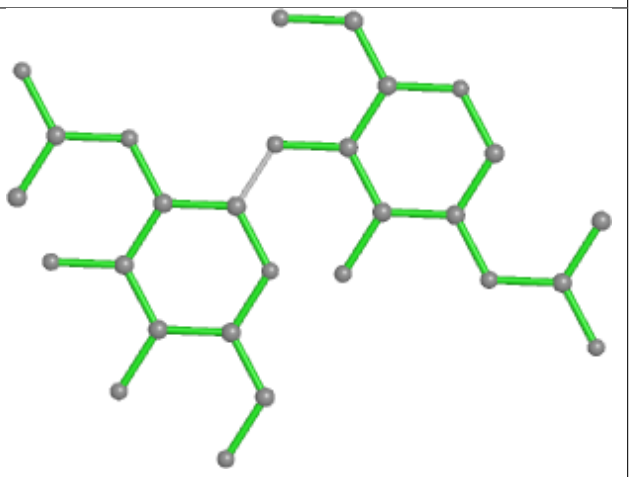
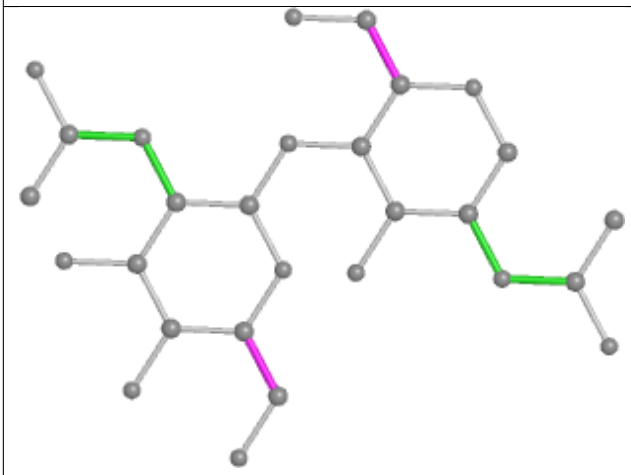
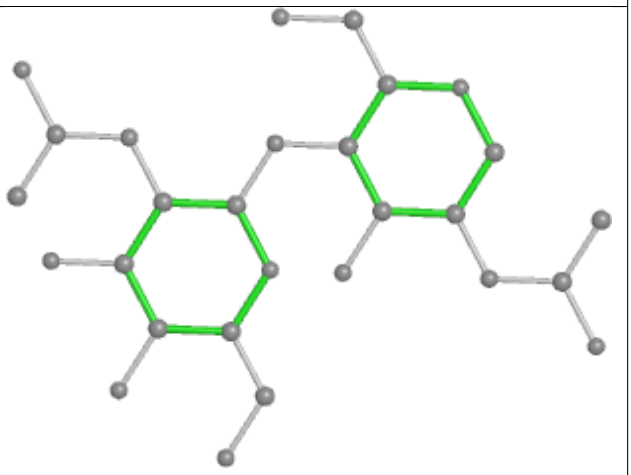
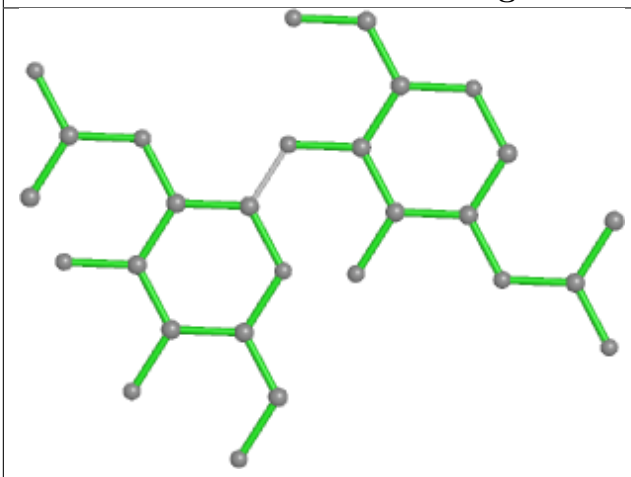


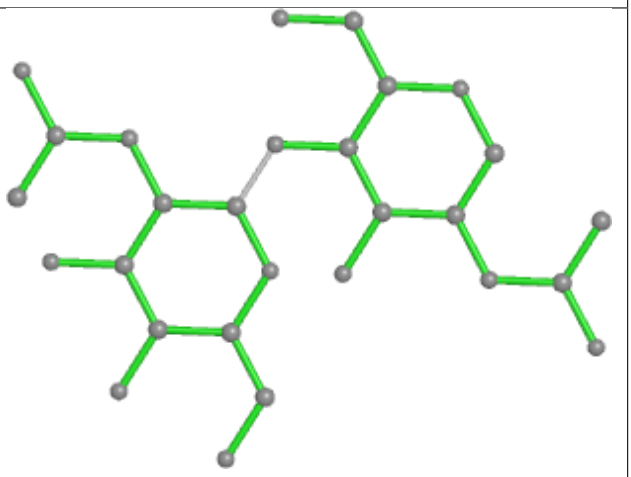
Rings

Oligosaccharide Chain w	
 Bond lengths	 Bond angles
 Torsions	 Rings

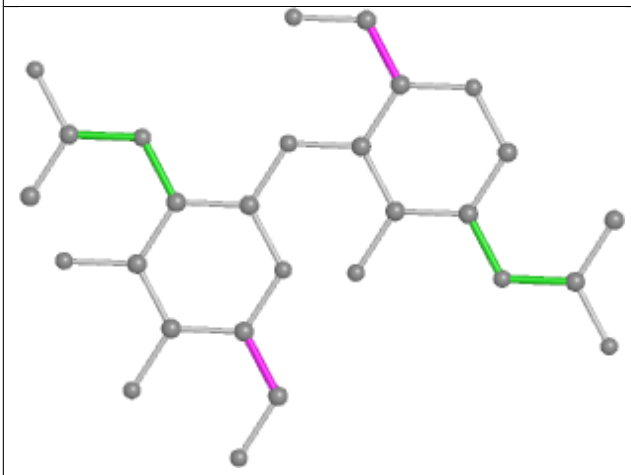
Oligosaccharide Chain x



Bond lengths



Bond angles



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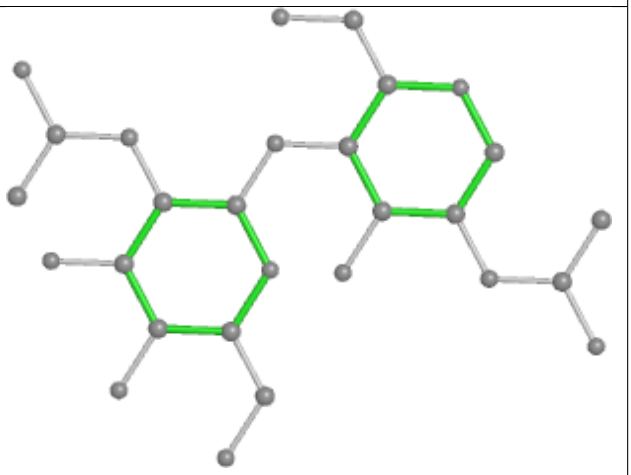
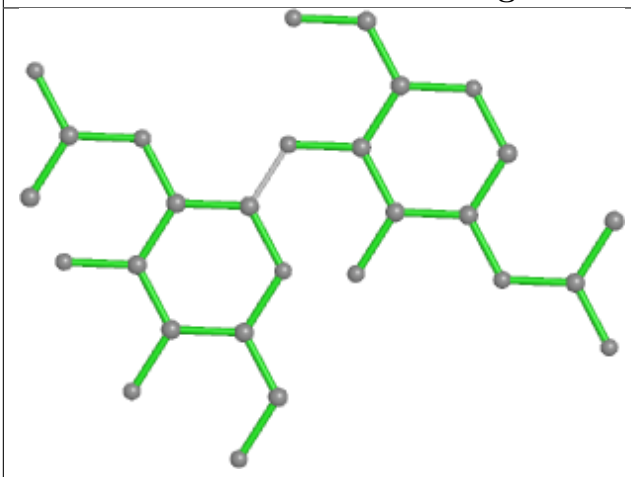


Rings

Oligosaccharide Chain y



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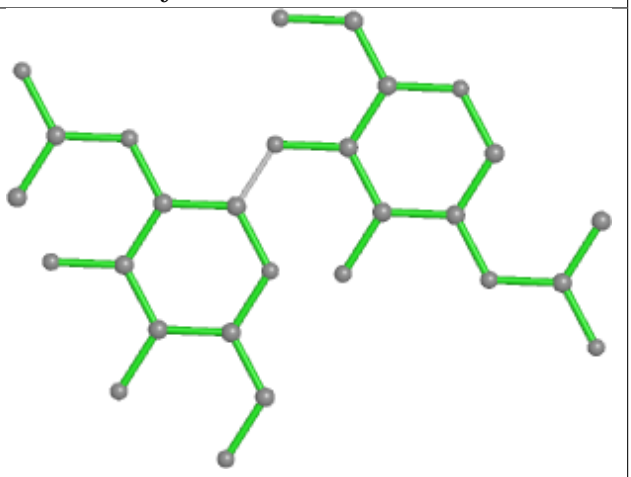
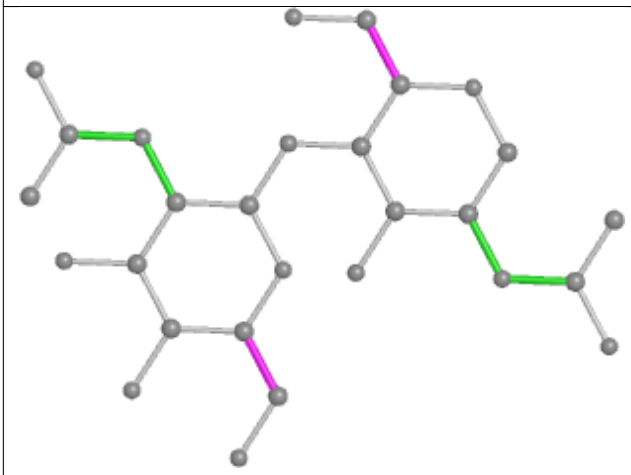


Bond angles



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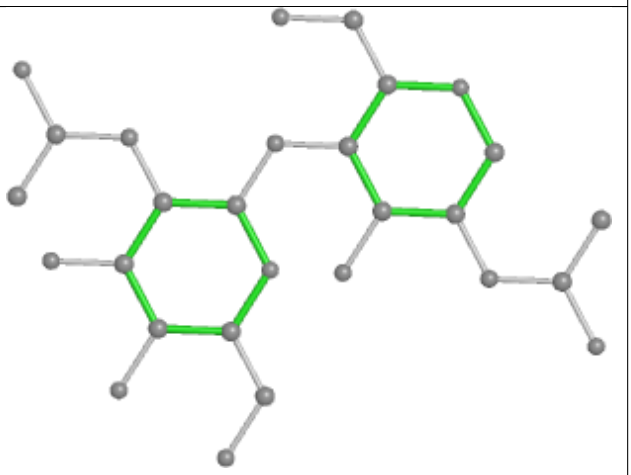
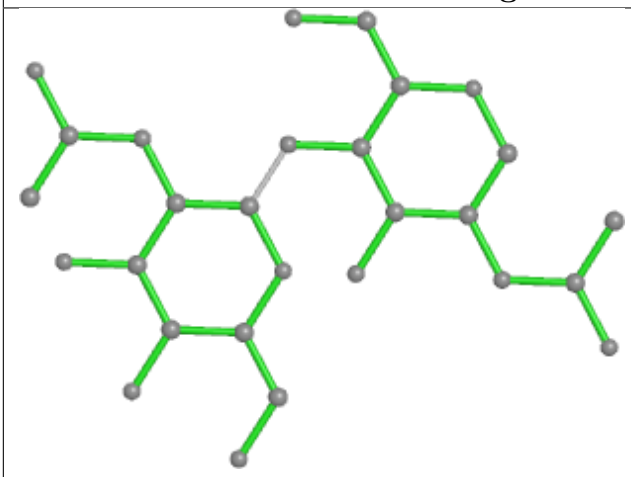


Rings

Oligosaccharide Chain z



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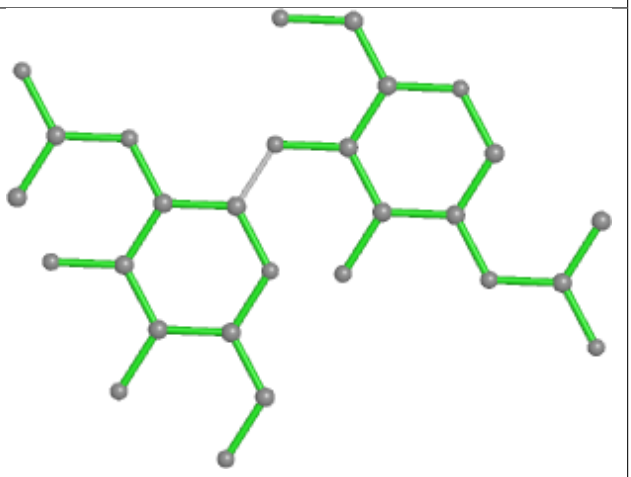
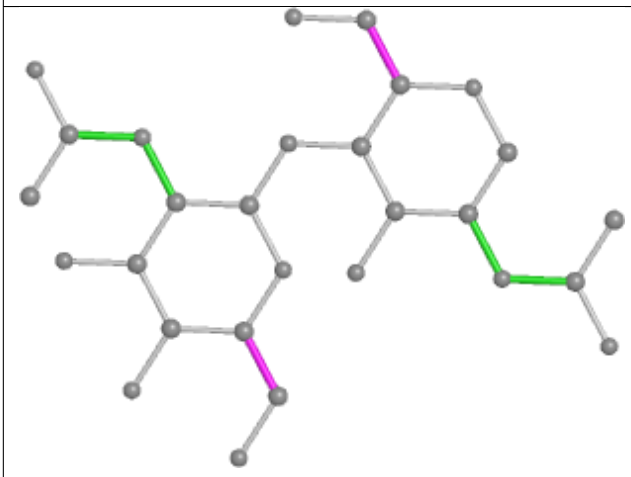
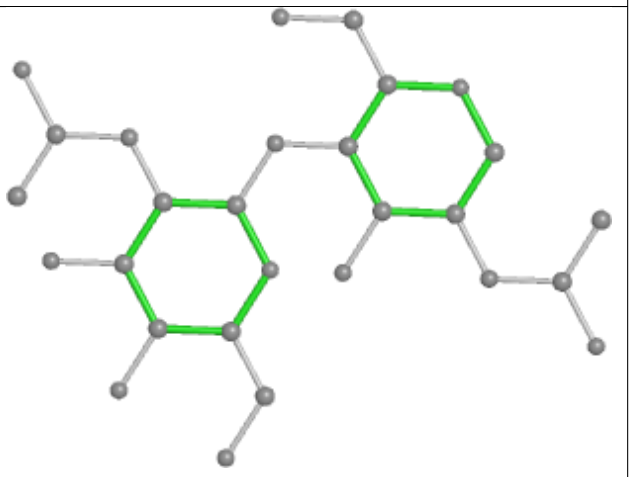


Bond angles

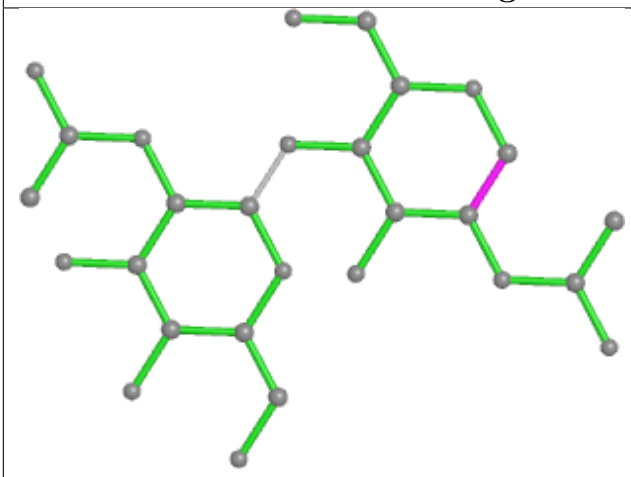


Torsions

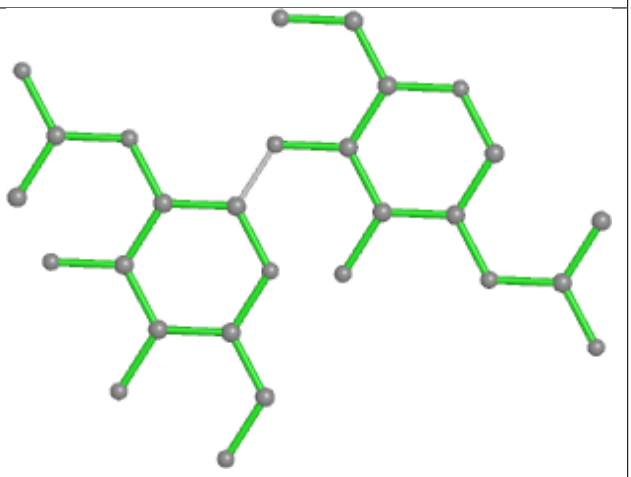


Rings

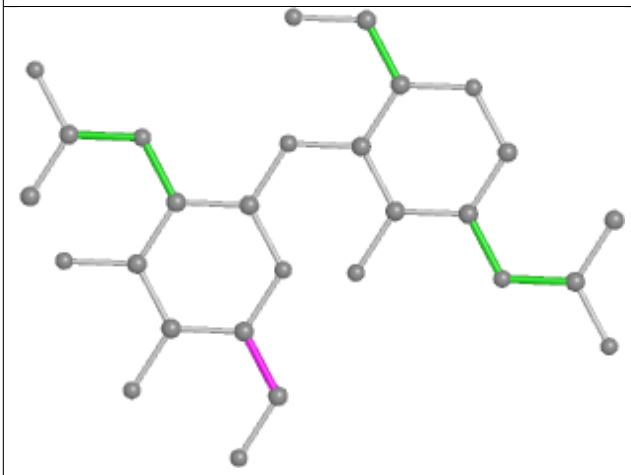
Oligosaccharide Chain 0



Bond lengths



Bond angles



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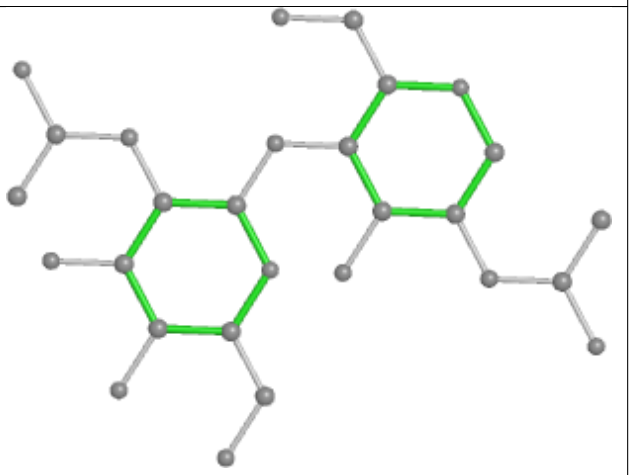
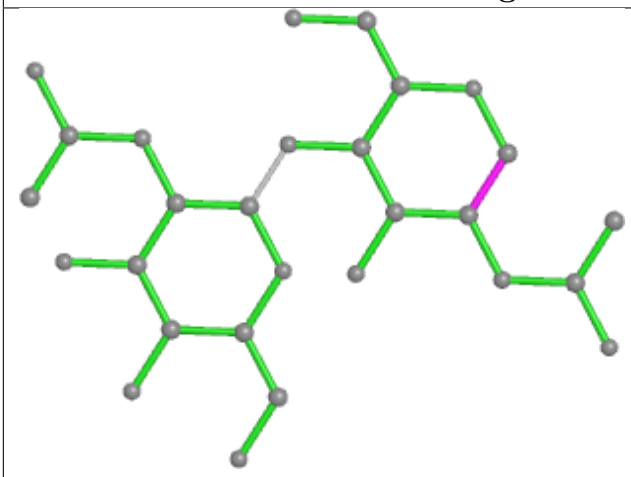
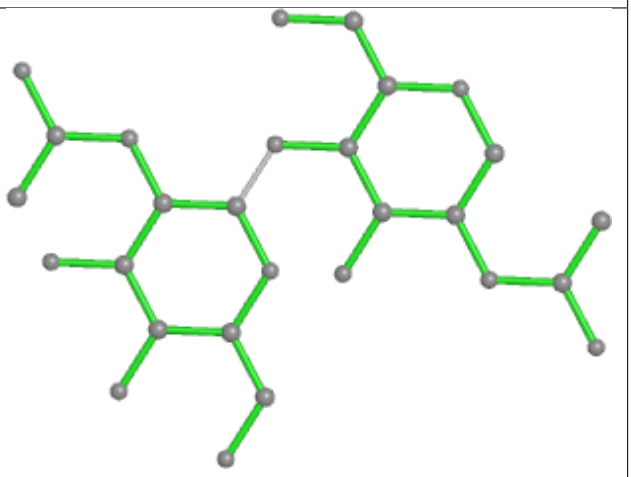


Rings

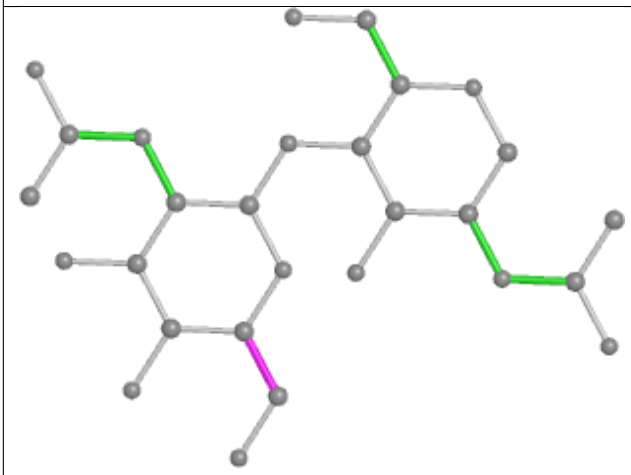
Oligosaccharide Chain 1



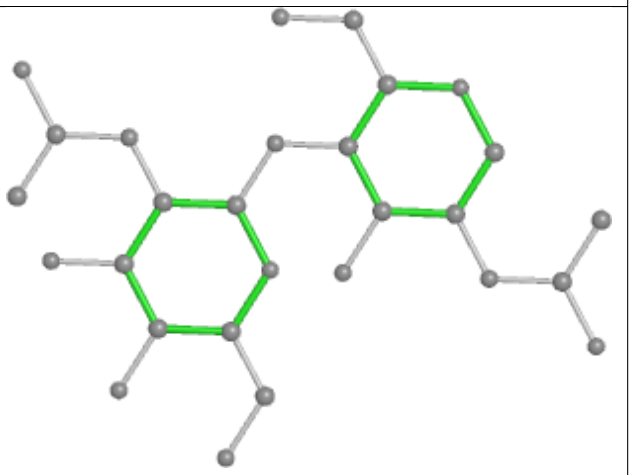
Bond lengths



Bond angles

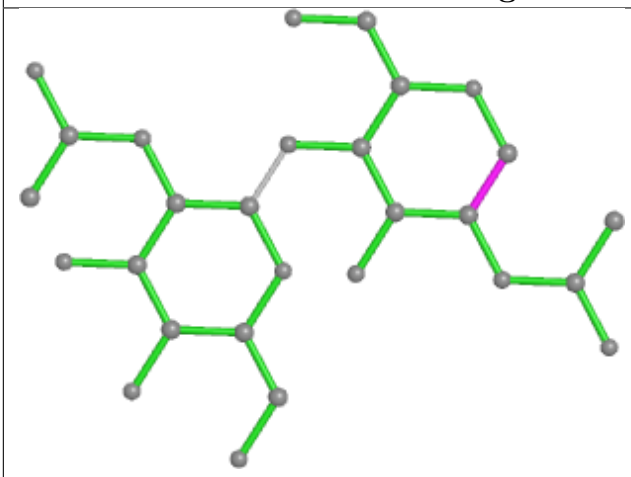


Torsions

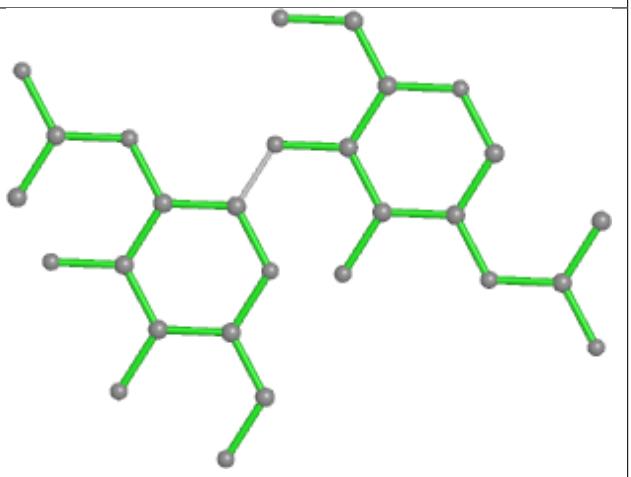


Rings

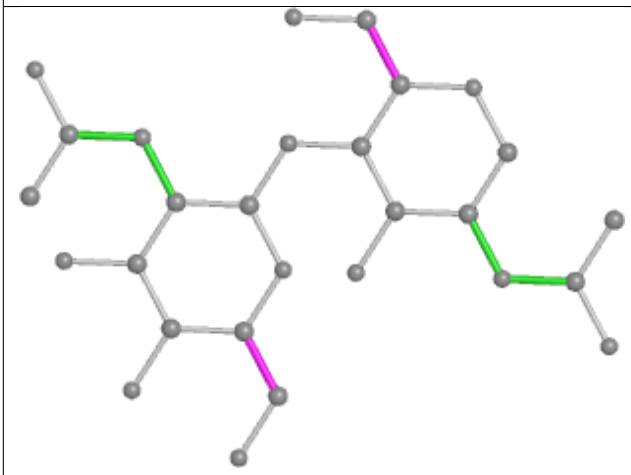
Oligosaccharide Chain 2



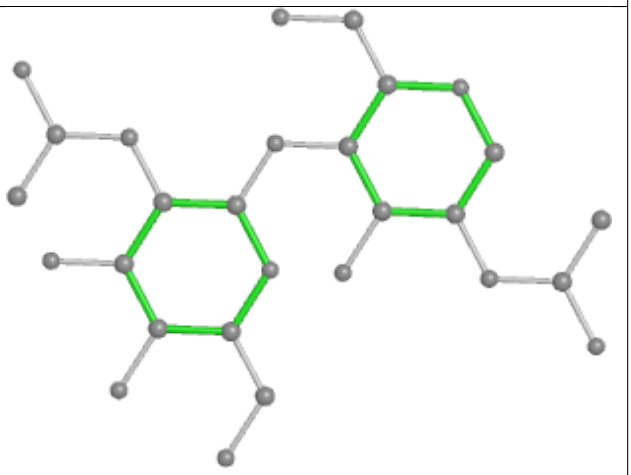
Bond lengths



Bond angles

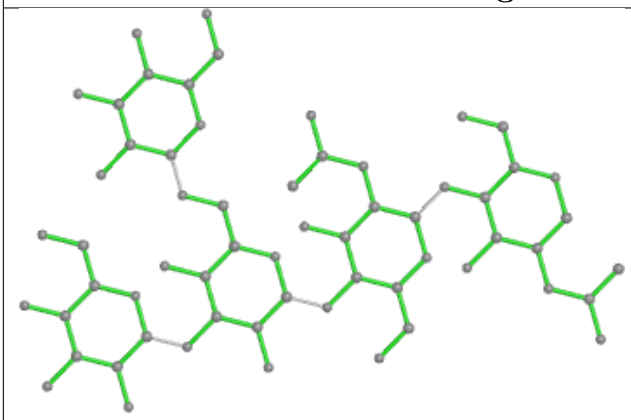


Torsions

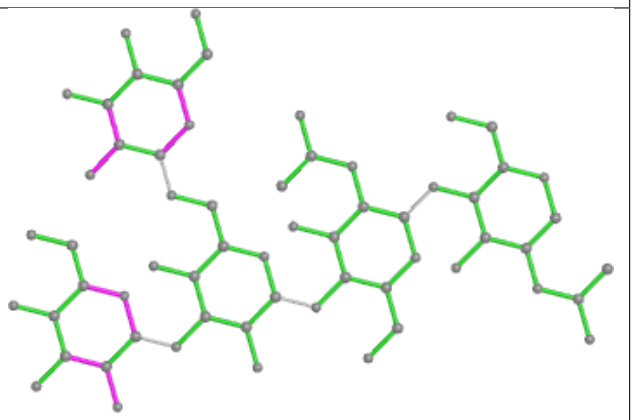


Rings

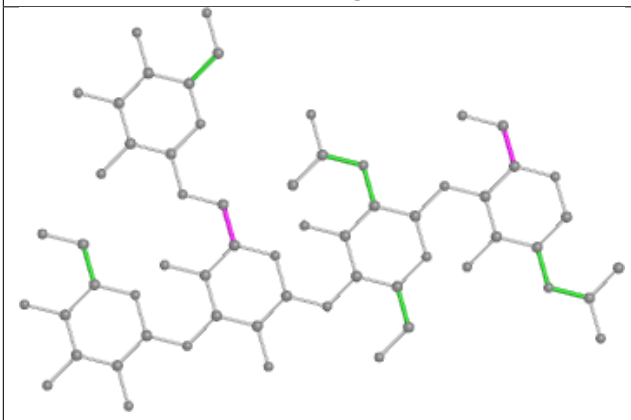
Oligosaccharide Chain Z



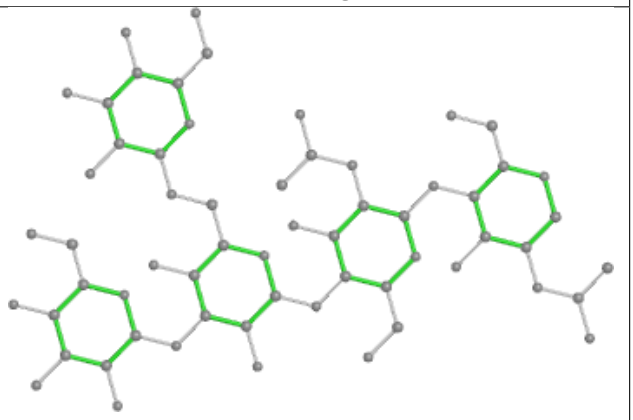
Bond lengths



Bond angles

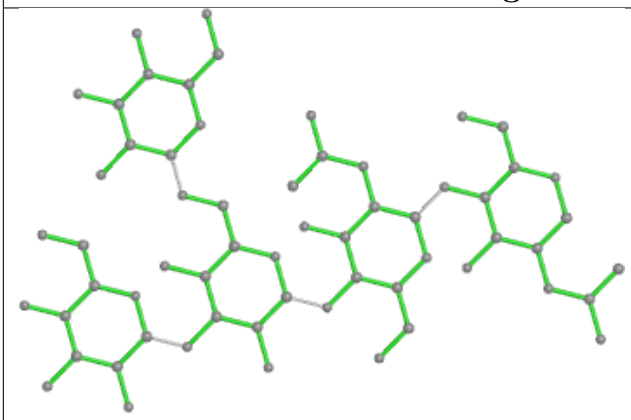


Torsions

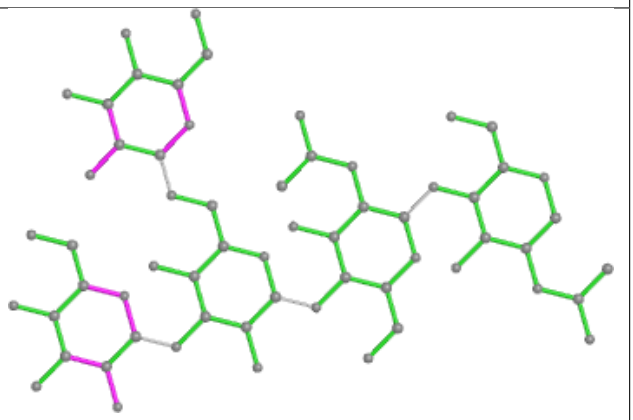


Rings

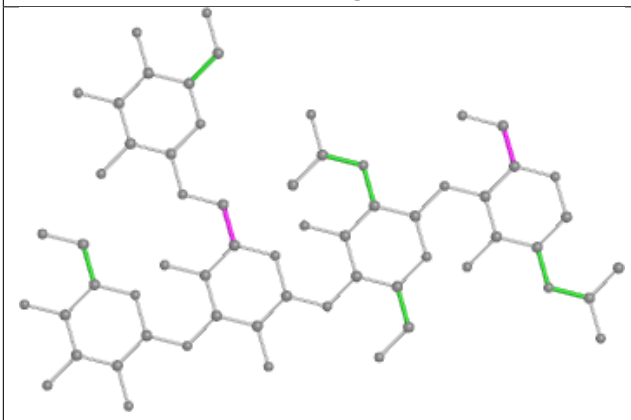
Oligosaccharide Chain i



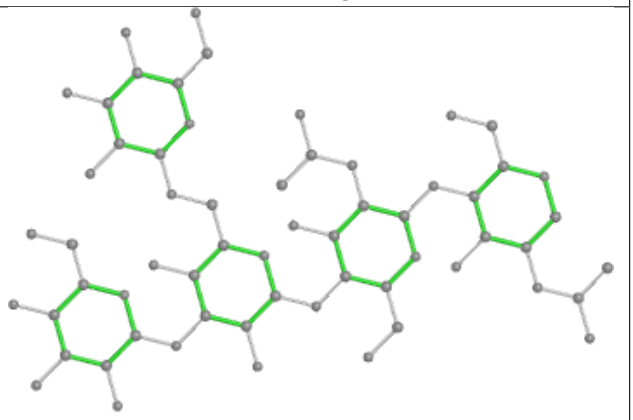
Bond lengths



Bond angles

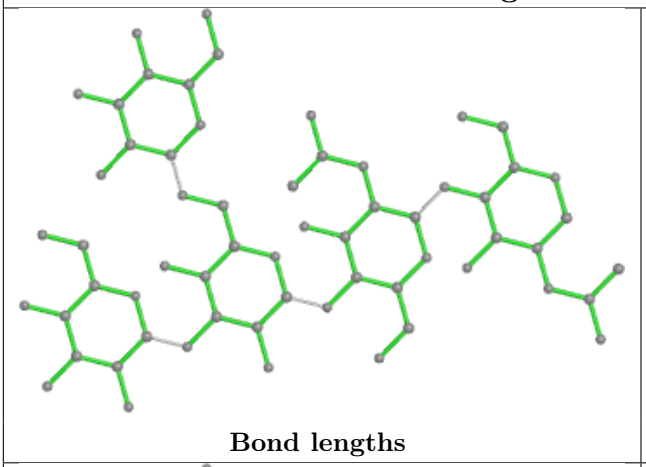


Torsions

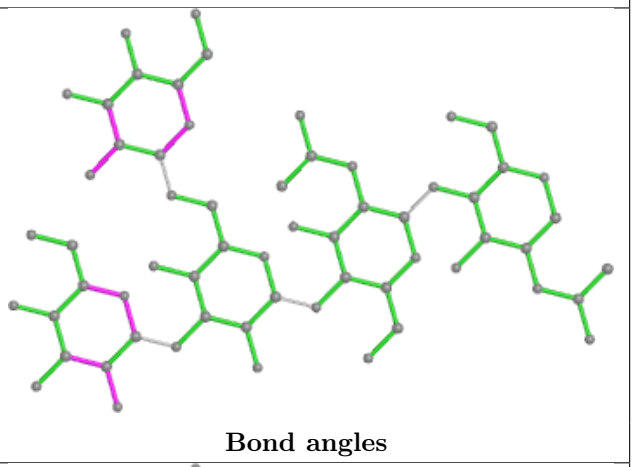


Rings

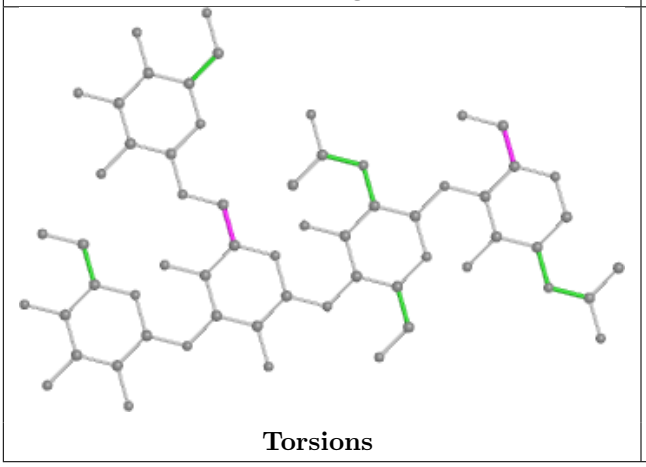
Oligosaccharide Chain s



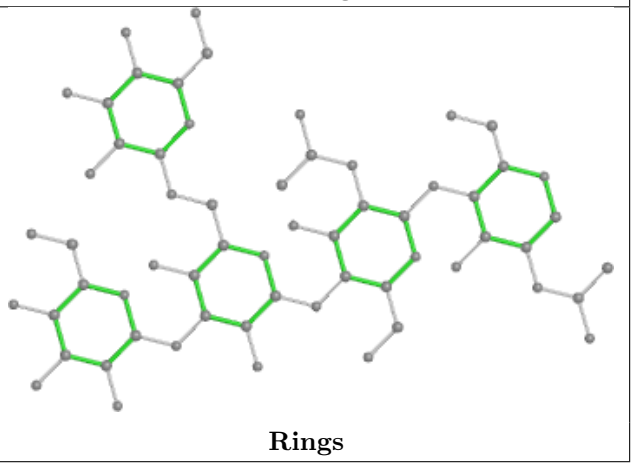
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

36 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	$\#\|Z\| > 2$
12	NAG	A	604	1	14,14,15	0.19	0	17,19,21	0.38	0
12	NAG	I	603	1	14,14,15	0.89	1 (7%)	17,19,21	1.06	1 (5%)
12	NAG	A	606	1	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
12	NAG	A	607	1	14,14,15	0.24	0	17,19,21	0.43	0
12	NAG	I	604	1	14,14,15	0.19	0	17,19,21	0.39	0
12	NAG	I	605	1	14,14,15	0.23	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	NAG	F	701	2	14,14,15	0.22	0	17,19,21	0.42	0
12	NAG	E	605	1	14,14,15	0.24	0	17,19,21	0.43	0
12	NAG	A	601	1	14,14,15	0.24	0	17,19,21	0.40	0
12	NAG	B	700	2	14,14,15	0.44	0	17,19,21	0.56	0
12	NAG	I	607	1	14,14,15	0.23	0	17,19,21	0.44	0
12	NAG	A	608	1	14,14,15	0.37	0	17,19,21	0.55	0
12	NAG	I	601	1	14,14,15	0.24	0	17,19,21	0.41	0
12	NAG	E	609	1	14,14,15	0.22	0	17,19,21	0.41	0
12	NAG	F	700	2	14,14,15	0.44	0	17,19,21	0.56	0
12	NAG	E	603	1	14,14,15	0.89	1 (7%)	17,19,21	1.08	1 (5%)
12	NAG	J	701	2	14,14,15	0.21	0	17,19,21	0.42	0
12	NAG	I	608	1	14,14,15	0.37	0	17,19,21	0.55	0
12	NAG	A	605	1	14,14,15	0.23	0	17,19,21	0.44	0
12	NAG	E	604	1	14,14,15	0.20	0	17,19,21	0.39	0
12	NAG	F	702	2	14,14,15	0.21	0	17,19,21	0.35	0
12	NAG	I	609	1	14,14,15	0.21	0	17,19,21	0.40	0
12	NAG	A	602	1	14,14,15	0.23	0	17,19,21	0.40	0
12	NAG	E	601	1	14,14,15	0.23	0	17,19,21	0.41	0
12	NAG	E	606	1	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
12	NAG	E	602	1	14,14,15	0.23	0	17,19,21	0.40	0
12	NAG	E	608	1	14,14,15	0.36	0	17,19,21	0.56	0
12	NAG	J	702	2	14,14,15	0.20	0	17,19,21	0.36	0
12	NAG	B	702	2	14,14,15	0.20	0	17,19,21	0.35	0
12	NAG	J	700	2	14,14,15	0.44	0	17,19,21	0.56	0
12	NAG	E	607	1	14,14,15	0.24	0	17,19,21	0.43	0
12	NAG	A	609	1	14,14,15	0.21	0	17,19,21	0.41	0
12	NAG	A	603	1	14,14,15	0.88	1 (7%)	17,19,21	1.07	1 (5%)
12	NAG	I	606	1	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
12	NAG	I	602	1	14,14,15	0.23	0	17,19,21	0.40	0
12	NAG	B	701	2	14,14,15	0.21	0	17,19,21	0.41	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
12	NAG	A	604	1	-	2/6/23/26	0/1/1/1
12	NAG	I	603	1	-	3/6/23/26	0/1/1/1
12	NAG	A	606	1	-	0/6/23/26	0/1/1/1
12	NAG	A	607	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	I	604	1	-	2/6/23/26	0/1/1/1
12	NAG	I	605	1	-	2/6/23/26	0/1/1/1
12	NAG	F	701	2	-	2/6/23/26	0/1/1/1
12	NAG	E	605	1	-	2/6/23/26	0/1/1/1
12	NAG	A	601	1	-	0/6/23/26	0/1/1/1
12	NAG	B	700	2	-	4/6/23/26	0/1/1/1
12	NAG	I	607	1	-	2/6/23/26	0/1/1/1
12	NAG	A	608	1	-	3/6/23/26	0/1/1/1
12	NAG	I	601	1	-	0/6/23/26	0/1/1/1
12	NAG	E	609	1	-	2/6/23/26	0/1/1/1
12	NAG	F	700	2	-	4/6/23/26	0/1/1/1
12	NAG	E	603	1	-	3/6/23/26	0/1/1/1
12	NAG	J	701	2	-	2/6/23/26	0/1/1/1
12	NAG	I	608	1	-	3/6/23/26	0/1/1/1
12	NAG	A	605	1	-	2/6/23/26	0/1/1/1
12	NAG	E	604	1	-	2/6/23/26	0/1/1/1
12	NAG	F	702	2	-	0/6/23/26	0/1/1/1
12	NAG	I	609	1	-	2/6/23/26	0/1/1/1
12	NAG	A	602	1	-	2/6/23/26	0/1/1/1
12	NAG	E	601	1	-	0/6/23/26	0/1/1/1
12	NAG	E	606	1	-	0/6/23/26	0/1/1/1
12	NAG	E	602	1	-	2/6/23/26	0/1/1/1
12	NAG	E	608	1	-	3/6/23/26	0/1/1/1
12	NAG	J	702	2	-	0/6/23/26	0/1/1/1
12	NAG	B	702	2	-	0/6/23/26	0/1/1/1
12	NAG	J	700	2	-	4/6/23/26	0/1/1/1
12	NAG	E	607	1	-	2/6/23/26	0/1/1/1
12	NAG	A	609	1	-	2/6/23/26	0/1/1/1
12	NAG	A	603	1	-	3/6/23/26	0/1/1/1
12	NAG	I	606	1	-	0/6/23/26	0/1/1/1
12	NAG	I	602	1	-	2/6/23/26	0/1/1/1
12	NAG	B	701	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	603	NAG	O5-C1	2.99	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	I	603	NAG	O5-C1	2.97	1.48	1.43
12	A	603	NAG	O5-C1	2.93	1.48	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	E	603	NAG	C1-O5-C5	4.02	117.64	112.19
12	A	603	NAG	C1-O5-C5	4.01	117.63	112.19
12	I	603	NAG	C1-O5-C5	3.98	117.59	112.19
12	I	606	NAG	C1-O5-C5	2.41	115.46	112.19
12	A	606	NAG	C1-O5-C5	2.40	115.44	112.19

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	604	NAG	O5-C5-C6-O6
12	E	604	NAG	O5-C5-C6-O6
12	I	604	NAG	O5-C5-C6-O6
12	A	609	NAG	O5-C5-C6-O6
12	E	609	NAG	O5-C5-C6-O6

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.

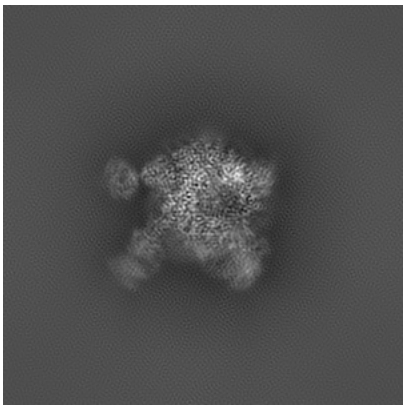
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29783. These allow visual inspection of the internal detail of the map and identification of artifacts.

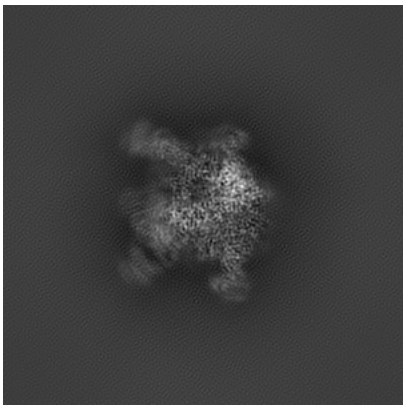
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

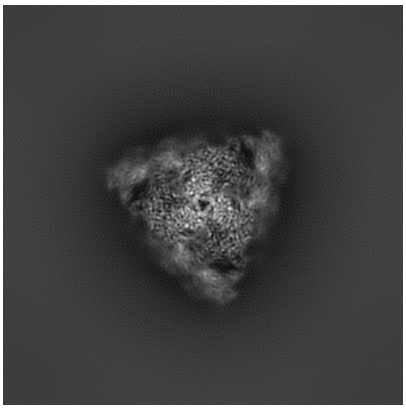
6.1.1 Primary map



X

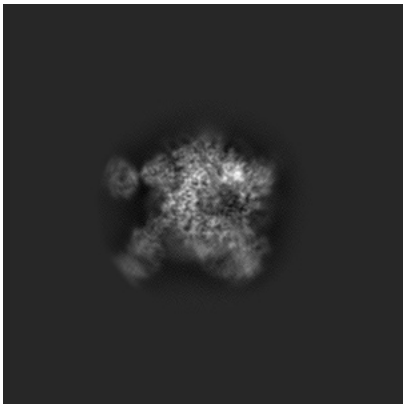


Y

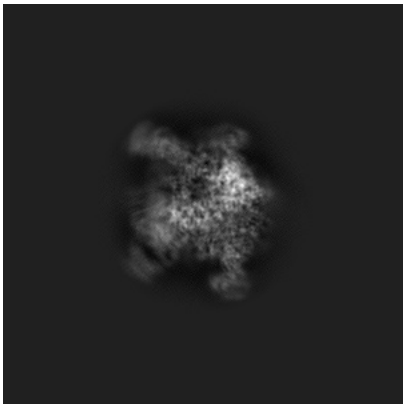


Z

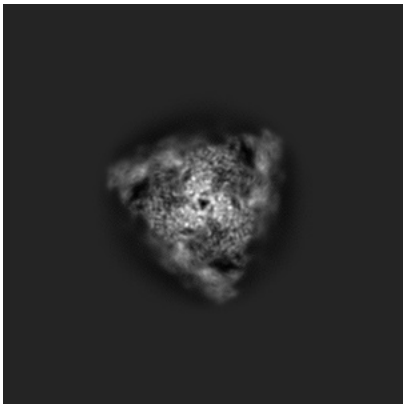
6.1.2 Raw map



X



Y

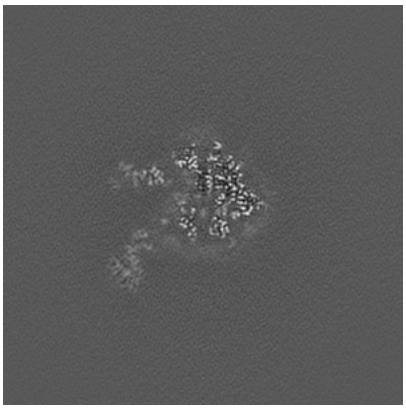


Z

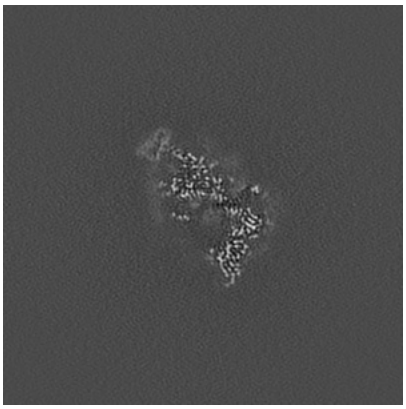
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

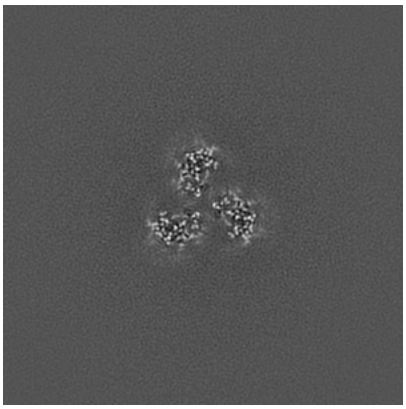
6.2.1 Primary map



X Index: 243

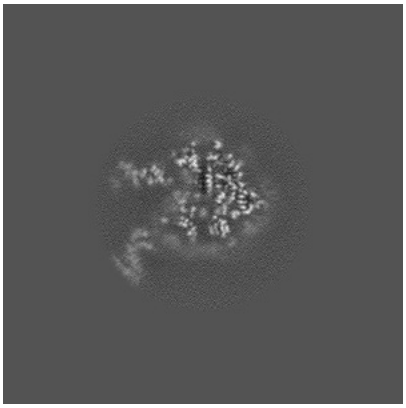


Y Index: 243

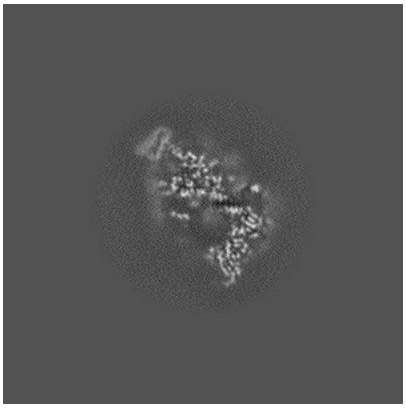


Z Index: 243

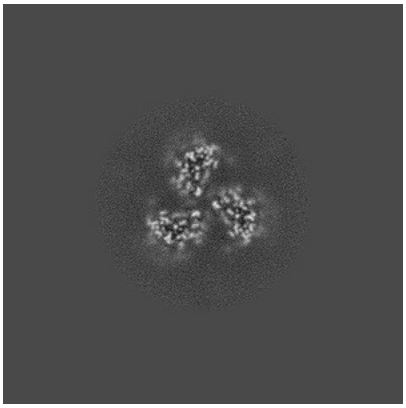
6.2.2 Raw map



X Index: 243



Y Index: 243

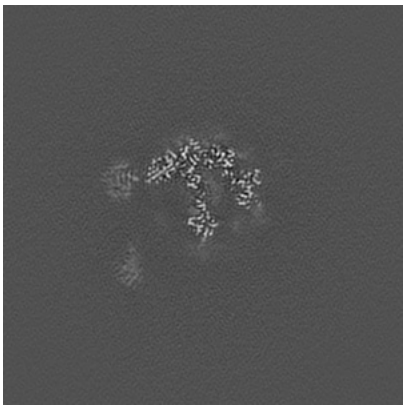


Z Index: 243

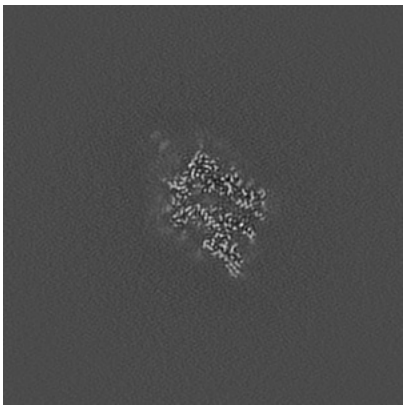
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

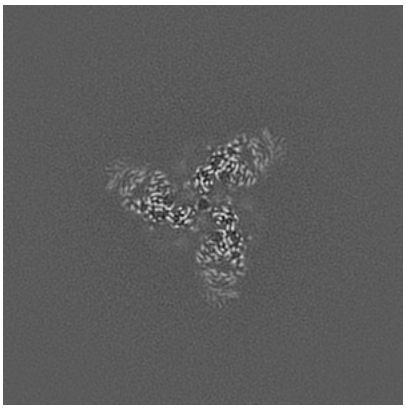
6.3.1 Primary map



X Index: 257

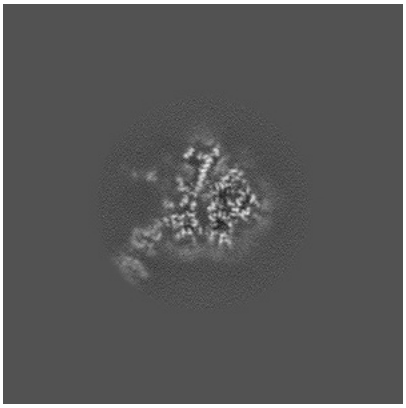


Y Index: 232

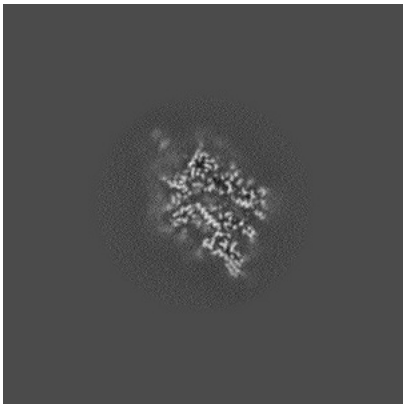


Z Index: 274

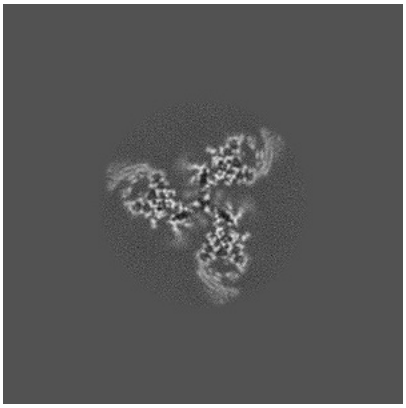
6.3.2 Raw map



X Index: 235



Y Index: 232

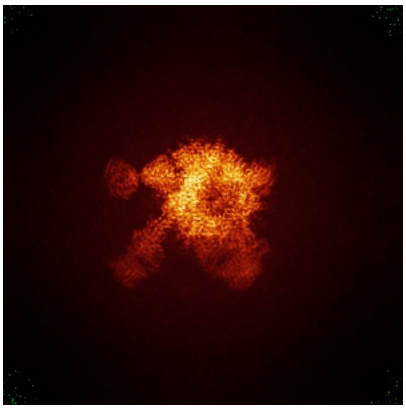


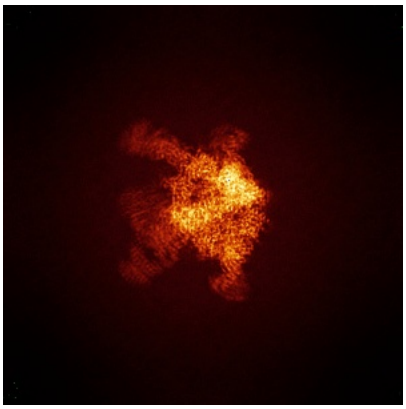
Z Index: 279

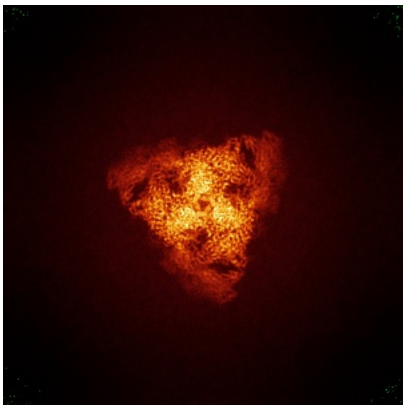
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

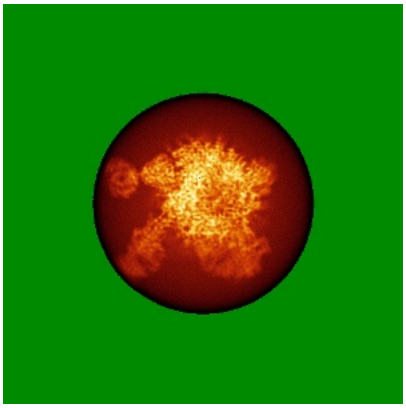
6.4.1 Primary map

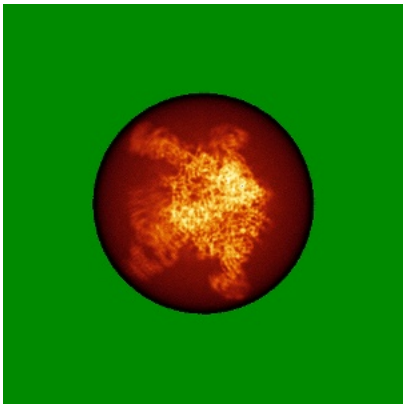

X

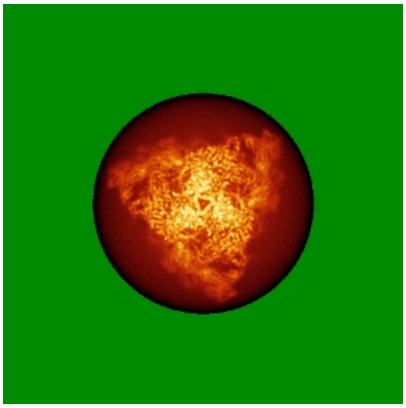

Y


Z

6.4.2 Raw map


X

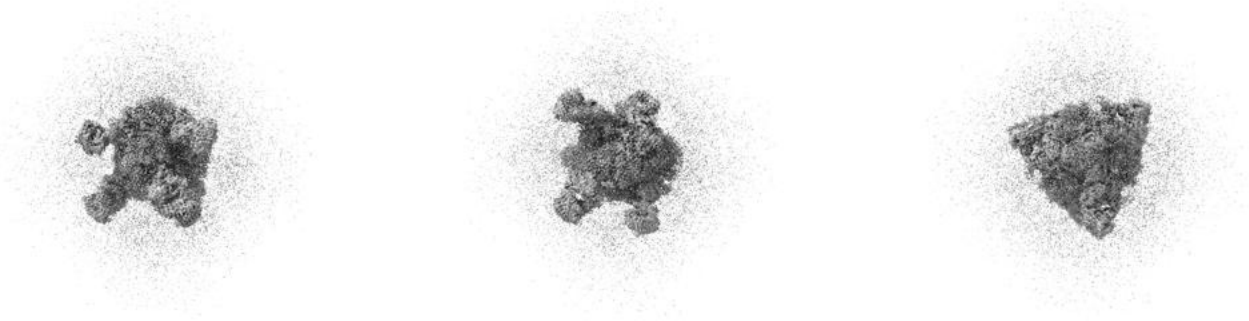

Y


Z

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

6.5 Orthogonal surface views (i)

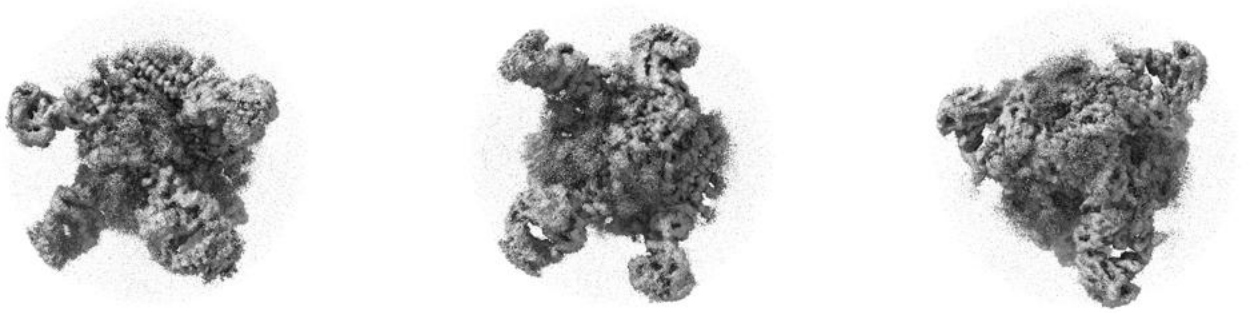
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

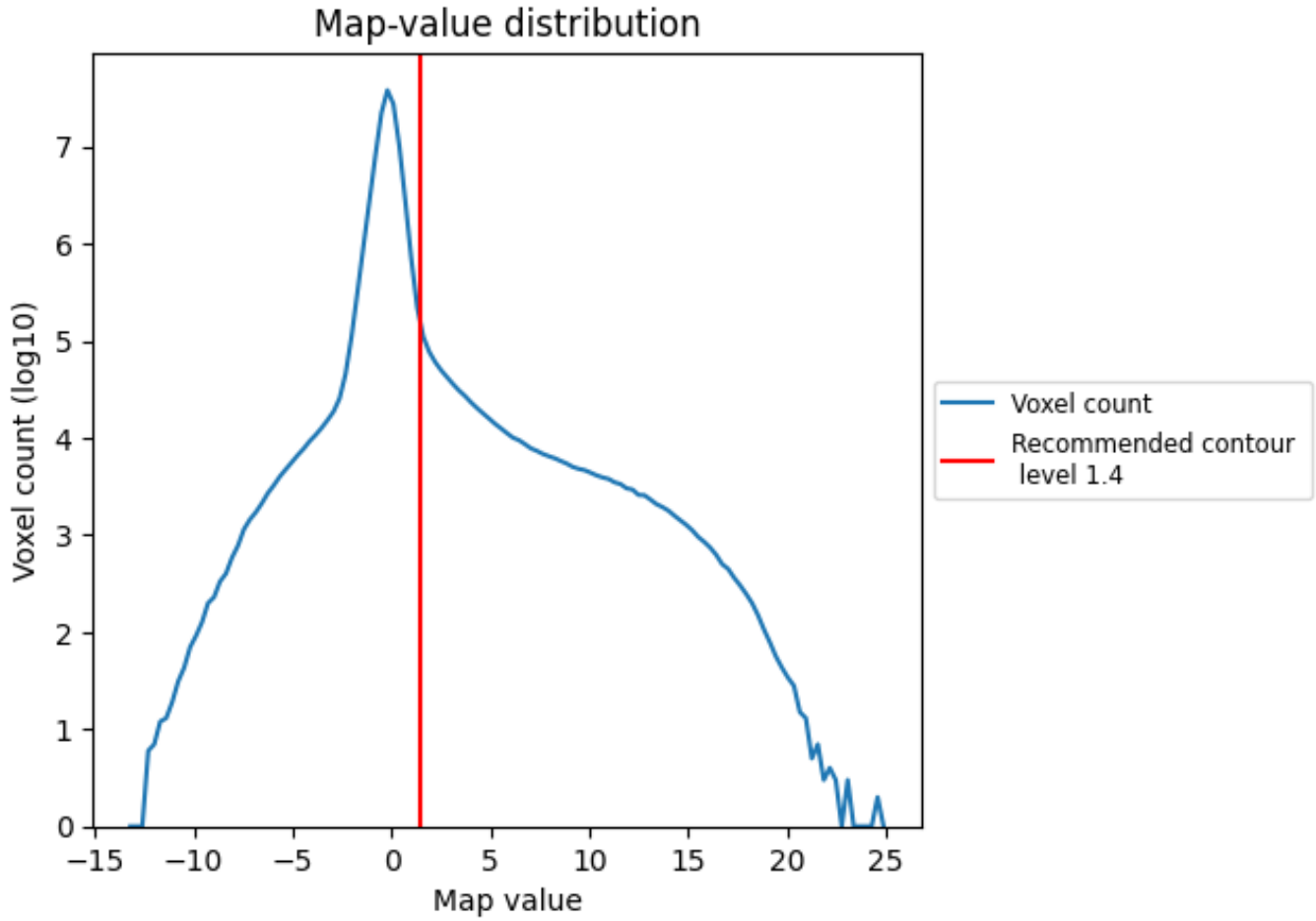
6.6 Mask visualisation (i)

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

7 Map analysis

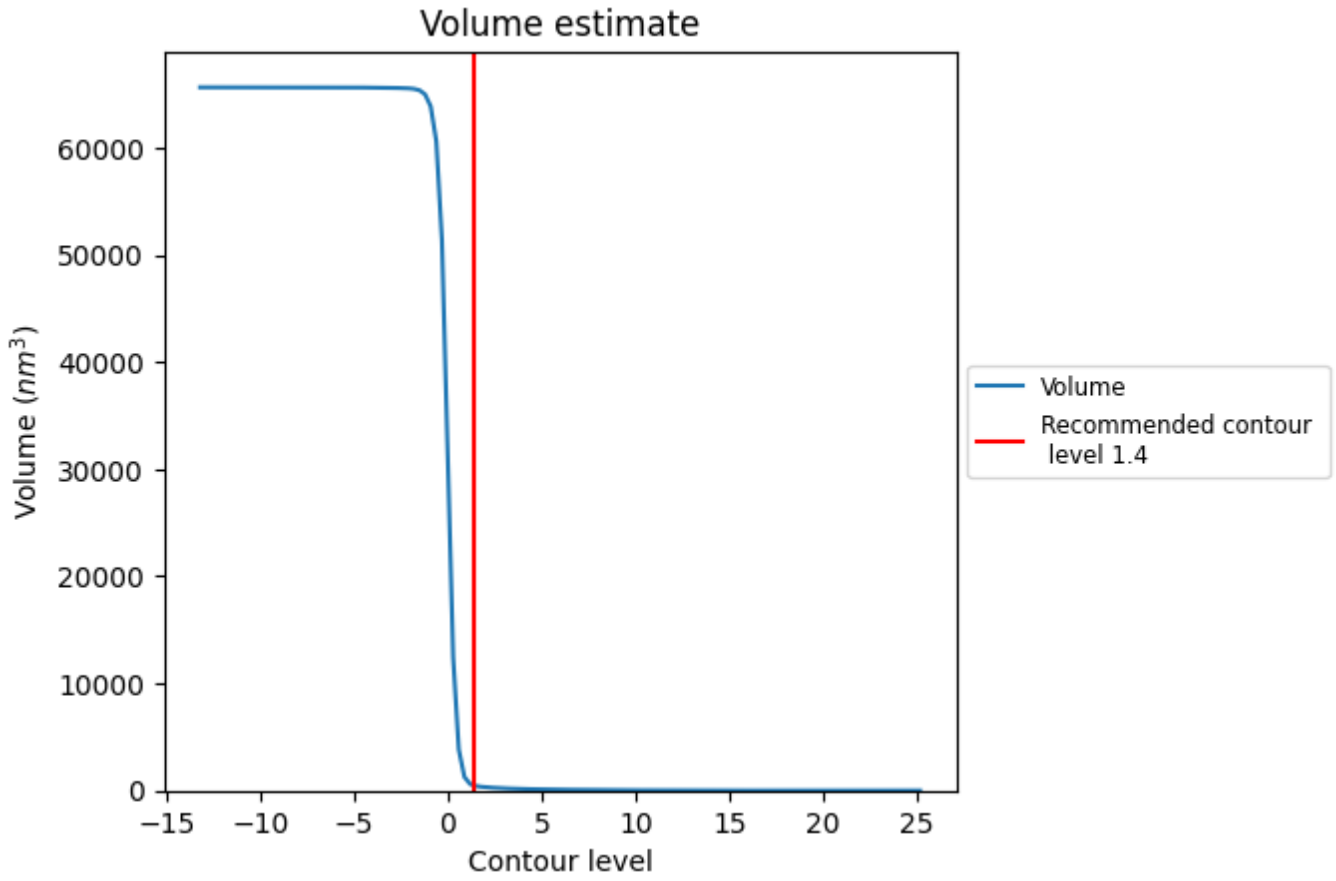
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

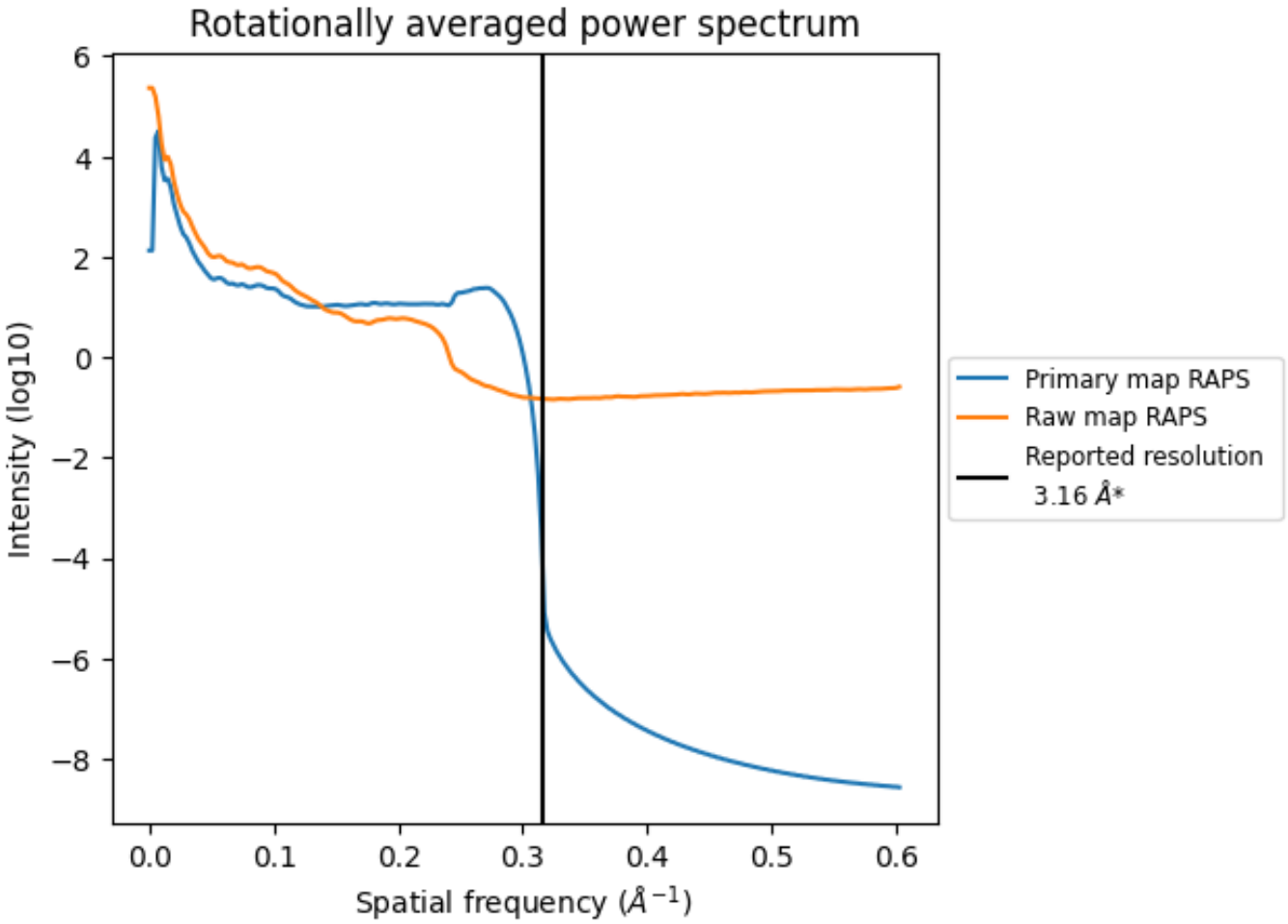
7.2 Volume estimate (i)



The volume at the recommended contour level is 487 nm^3; this corresponds to an approximate mass of 440 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)

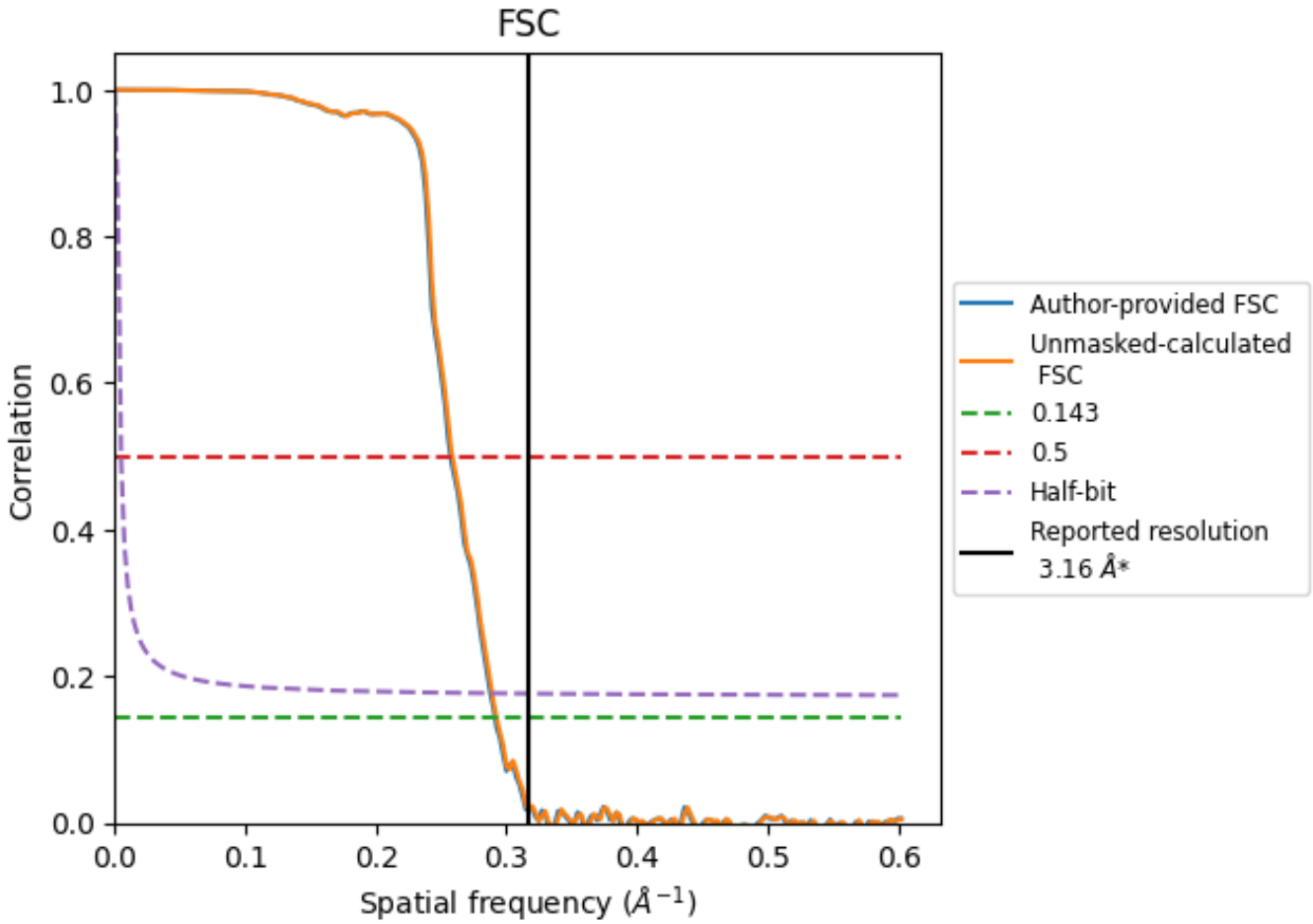


*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8.2 Resolution estimates (i)

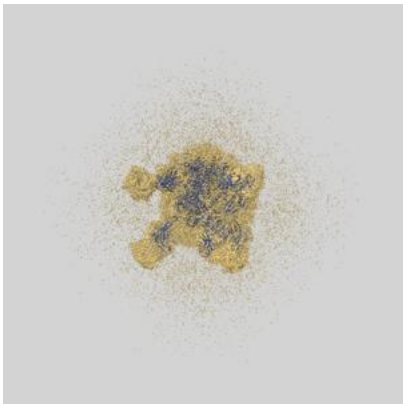
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.43	3.89	3.48
Unmasked-calculated*	3.42	3.87	3.46

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

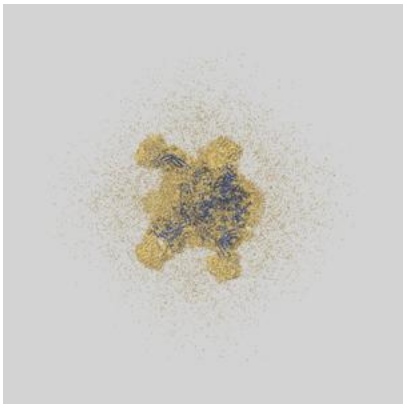
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29783 and PDB model 8G6U. Per-residue inclusion information can be found in section 3 on page 14.

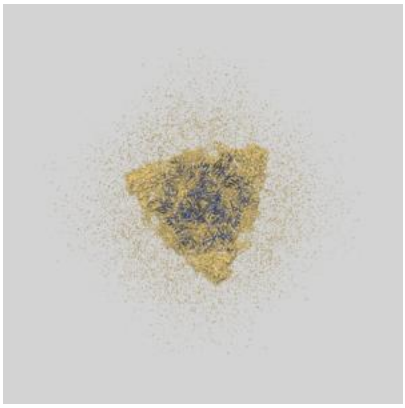
9.1 Map-model overlay



X



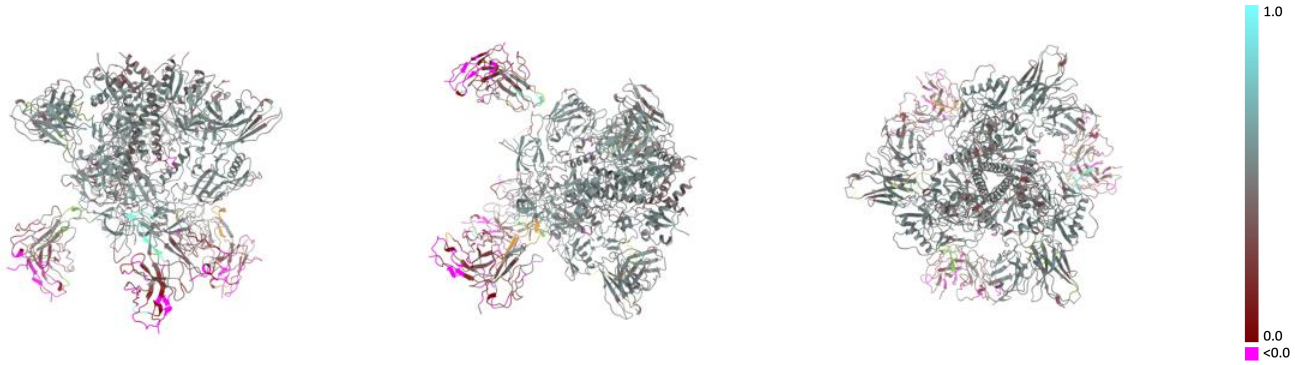
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.4 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.

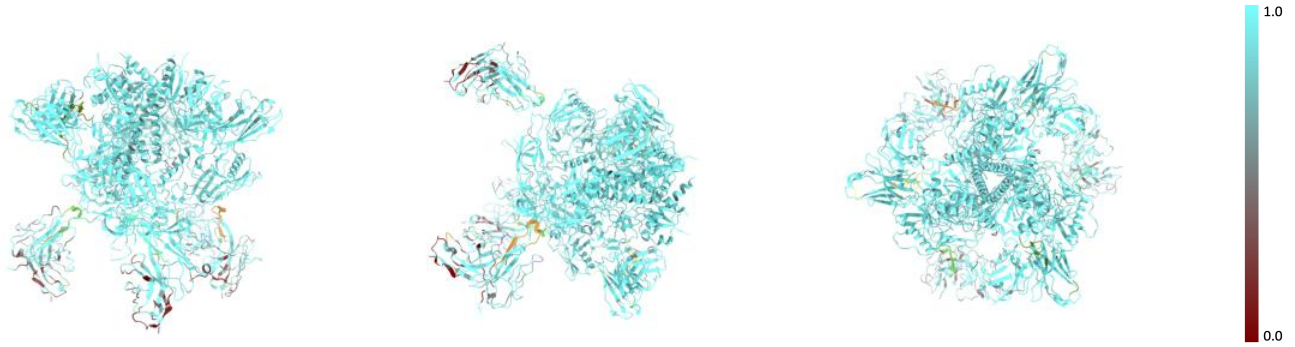
9.2 Q-score mapped to coordinate model



X Y Z

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

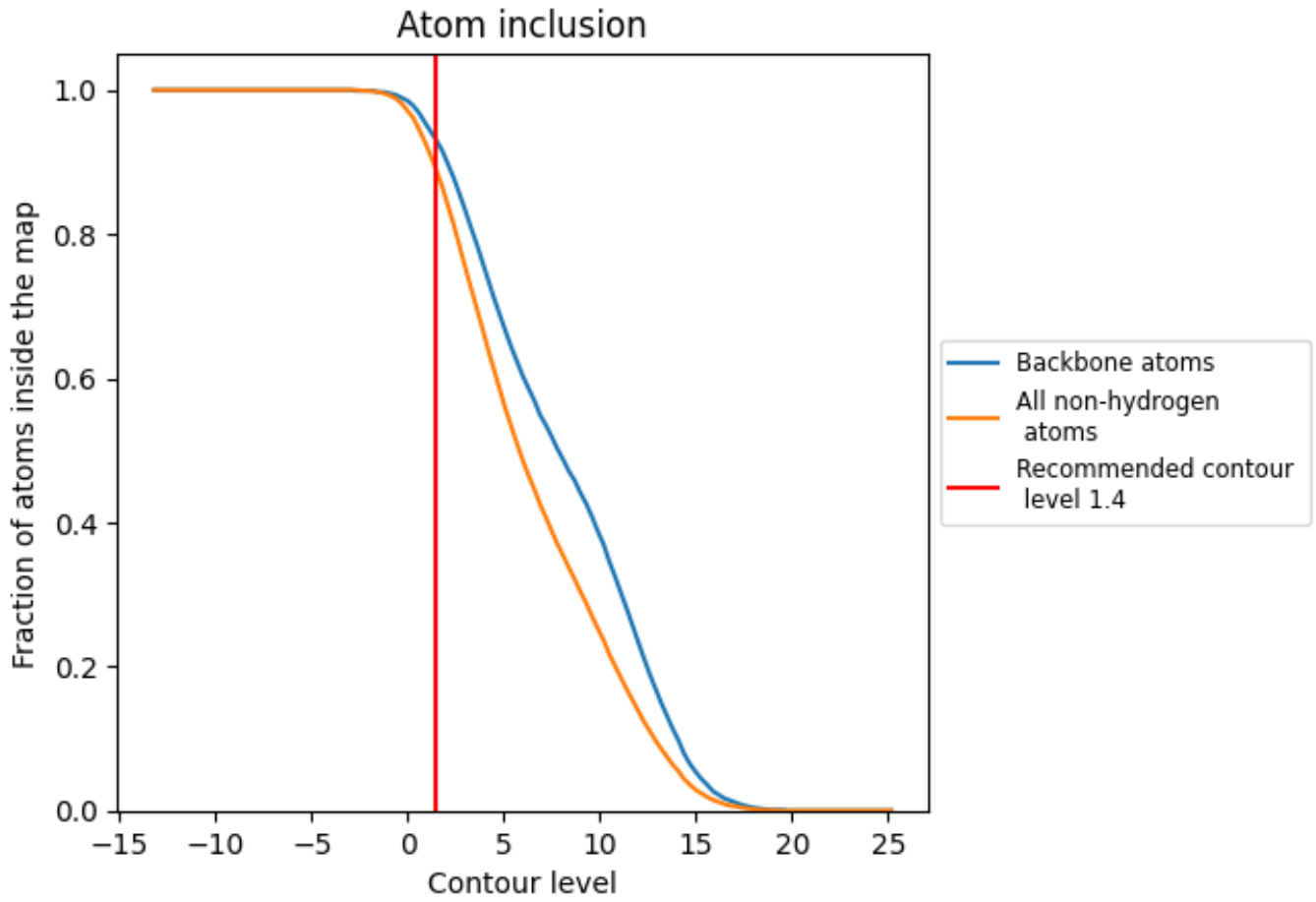
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.4).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.4330
0	0.8210	0.3450
1	0.7860	0.3280
2	0.8210	0.3170
A	0.9370	0.4990
B	0.9220	0.4660
C	0.9400	0.5010
D	0.9400	0.4890
E	0.9370	0.4970
F	0.9230	0.4710
G	0.9500	0.5070
H	0.9470	0.5010
I	0.9280	0.4910
J	0.9170	0.4680
K	0.9480	0.5030
L	0.9430	0.4920
M	0.7470	0.2110
N	0.7990	0.2960
O	0.7360	0.1970
P	0.8070	0.2890
Q	0.7110	0.1720
R	0.8000	0.2740
S	0.8980	0.4230
T	0.8890	0.4170
U	0.8620	0.4040
V	0.8570	0.4000
X	0.8210	0.3400
Y	0.9170	0.3930
Z	0.8850	0.4180
a	0.8900	0.4300
b	0.9030	0.4190
c	0.8930	0.3990
d	0.8530	0.3960
e	0.8570	0.3740
f	0.8930	0.4150

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Chain	Atom inclusion	Q-score
g	0.8210	0.3320
h	0.9170	0.3970
i	0.8850	0.4220
j	0.9050	0.4580
k	0.8750	0.4180
l	0.8930	0.4250
m	0.6790	0.2440
n	0.8360	0.4050
o	0.8570	0.4210
p	0.8210	0.3320
q	0.9640	0.4730
r	0.8890	0.4020
s	0.9020	0.4210
t	0.9640	0.4660
u	1.0000	0.4690
v	0.6790	0.2460
w	0.6790	0.2400
x	0.8930	0.4570
y	0.8930	0.4600
z	0.8930	0.4380