Full wwPDB EM Validation Report (i)

Nov 13, 2022 – 04:07 AM EST

PDB ID	:	6VN0
EMDB ID	:	EMD-21246
Title	:	BG505 SOSIP.v4.1 in complex with rhesus macaque Fab RM20F
Authors	:	Cottrell, C.A.; Shin, M.; Ward, A.B.
Deposited on	:	2020-01-29
Resolution	:	4.25 Å(reported)

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

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

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

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

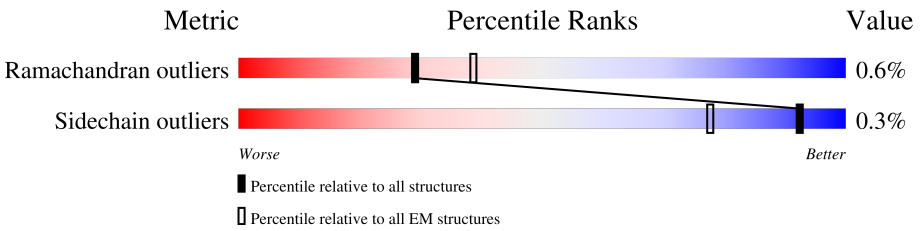
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.25 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	475	87% · 10%
1	C	475	87% · 10%
1	D	475	87% · 10%
2	B	153	5% 82% · 16%
2	E	153	6% 82% · 16%
2	F	153	7% 82% · 16%
3	G	126	6% 96% · ·
3	H	126	96% · ·
3	I	126	6% 96% · ·

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Mol	Chain	Length	Quality of chain
4	J	107	6% 99%
4	K	107	7% 99%
4	L	107	7% 99%
5	M	5	100%
5	Q	5	20% 100%
5	X	5	100%
5	b	5	20% 100%
5	i	5	100%
5	m	5	20% 100%
6	N	2	100%
6	O	2	50% 100%
6	P	2	50% 50% 50%
6	R	2	50% 50% 50%
6	S	2	100%
6	T	2	100%
6	U	2	100%
6	V	2	100%
6	W	2	100%
6	Y	2	100%
6	Z	2	50% 100%
6	a	2	50% 50% 50%
6	c	2	50% 50% 50%
6	d	2	100%
6	e	2	100%
6	f	2	100%

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Mol	Chain	Length	Quality of chain
6	g	2	100%
6	h	2	100%
6	j	2	100%
6	k	2	50% 100%
6	l	2	50% 50% 50%
6	n	2	50% 50% 50%
6	o	2	100%
6	p	2	100%
6	q	2	100%
6	r	2	100%
6	s	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	427	3378	2133	596	621	28	0	0
1	C	427	3378	2133	596	621	28	0	0
1	D	427	3378	2133	596	621	28	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LYS	GLU	conflict	UNP Q2N0S6
A	316	TRP	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
C	64	LYS	GLU	conflict	UNP Q2N0S6
C	316	TRP	ALA	conflict	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
D	64	LYS	GLU	conflict	UNP Q2N0S6
D	316	TRP	ALA	conflict	UNP Q2N0S6
D	332	ASN	THR	conflict	UNP Q2N0S6
D	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	129	1030	652	178	194	6	0	0
2	E	129	1030	652	178	194	6	0	0
2	F	129	1030	652	178	194	6	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6
E	559	PRO	ILE	conflict	UNP Q2N0S6
E	605	CYS	THR	conflict	UNP Q2N0S6
F	559	PRO	ILE	conflict	UNP Q2N0S6
F	605	CYS	THR	conflict	UNP Q2N0S6

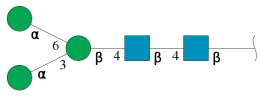
- Molecule 3 is a protein called RM20F Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	125	961	613	164	180	4	0	0
3	G	125	961	613	164	180	4	0	0
3	I	125	961	613	164	180	4	0	0

- Molecule 4 is a protein called RM20F Kappa Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	107	813	509	135	165	4	0	0
4	J	107	813	509	135	165	4	0	0
4	K	107	813	509	135	165	4	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	M	5	61	34	2	25	0	0
5	Q	5	61	34	2	25	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	X	5	61	34	2	25	0	0
5	b	5	61	34	2	25	0	0
5	i	5	61	34	2	25	0	0
5	m	5	61	34	2	25	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	N	2	28	16	2	10	0	0
6	O	2	28	16	2	10	0	0
6	P	2	28	16	2	10	0	0
6	R	2	28	16	2	10	0	0
6	S	2	28	16	2	10	0	0
6	T	2	28	16	2	10	0	0
6	U	2	28	16	2	10	0	0
6	V	2	28	16	2	10	0	0
6	W	2	28	16	2	10	0	0
6	Y	2	28	16	2	10	0	0
6	Z	2	28	16	2	10	0	0
6	a	2	28	16	2	10	0	0
6	c	2	28	16	2	10	0	0

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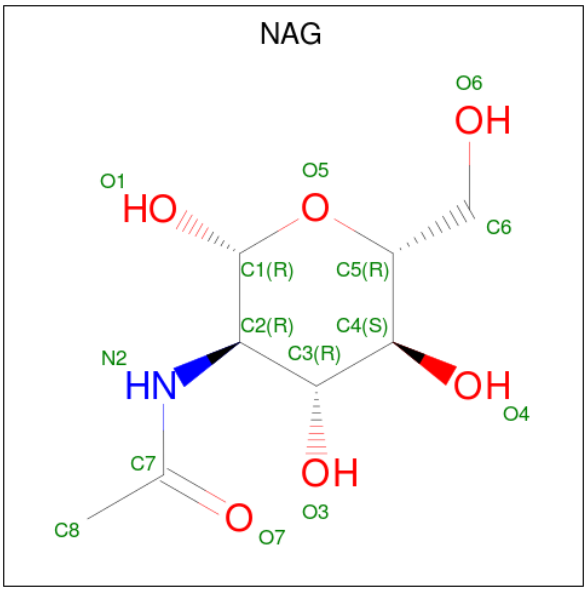
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	d	2	28	16	2	10	0	0
6	e	2	28	16	2	10	0	0
6	f	2	28	16	2	10	0	0
6	g	2	28	16	2	10	0	0
6	h	2	28	16	2	10	0	0
6	j	2	28	16	2	10	0	0
6	k	2	28	16	2	10	0	0
6	l	2	28	16	2	10	0	0
6	n	2	28	16	2	10	0	0
6	o	2	28	16	2	10	0	0
6	p	2	28	16	2	10	0	0
6	q	2	28	16	2	10	0	0
6	r	2	28	16	2	10	0	0
6	s	2	28	16	2	10	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	56	32	4	20	0
			Total	C	N	O	
7	A	1	56	32	4	20	0
			Total	C	N	O	
7	A	1	56	32	4	20	0
			Total	C	N	O	
7	A	1	56	32	4	20	0
			Total	C	N	O	
7	B	1	42	24	3	15	0
			Total	C	N	O	
7	B	1	42	24	3	15	0
			Total	C	N	O	
7	B	1	42	24	3	15	0
			Total	C	N	O	
7	C	1	56	32	4	20	0
			Total	C	N	O	
7	C	1	56	32	4	20	0
			Total	C	N	O	
7	C	1	56	32	4	20	0
			Total	C	N	O	
7	C	1	56	32	4	20	0
			Total	C	N	O	
7	E	1	42	24	3	15	0
			Total	C	N	O	
7	E	1	42	24	3	15	0
			Total	C	N	O	
7	E	1	42	24	3	15	0

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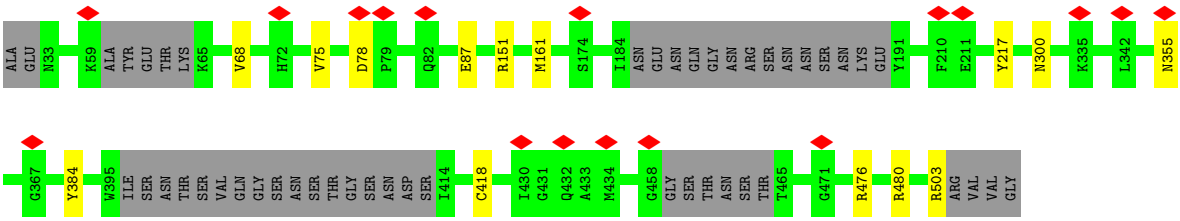
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	D	1	56	32	4	20	0
7	D	1	56	32	4	20	0
7	D	1	56	32	4	20	0
7	D	1	56	32	4	20	0
7	F	1	42	24	3	15	0
7	F	1	42	24	3	15	0
7	F	1	42	24	3	15	0

3 Residue-property plots (i)

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

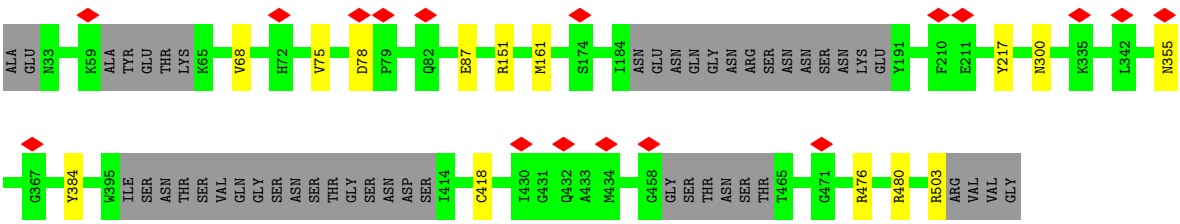
- Molecule 1: Envelope glycoprotein gp160

Chain A:



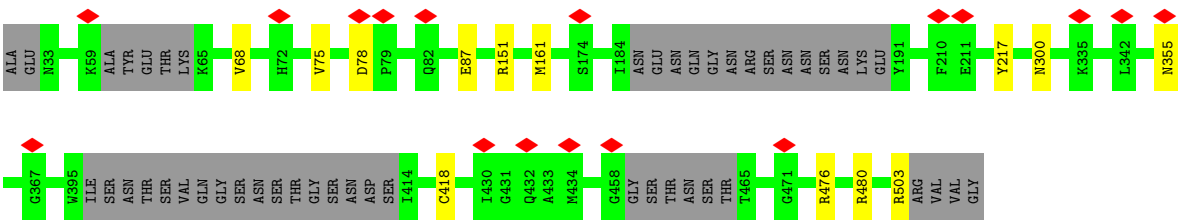
- Molecule 1: Envelope glycoprotein gp160

Chain C:



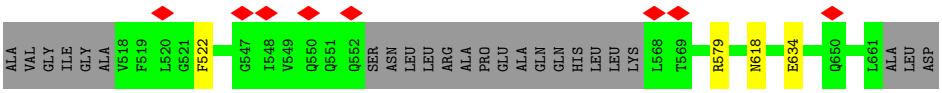
- Molecule 1: Envelope glycoprotein gp160

Chain D:



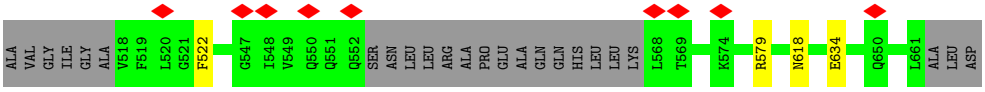
- Molecule 2: Envelope glycoprotein gp41

Chain B:



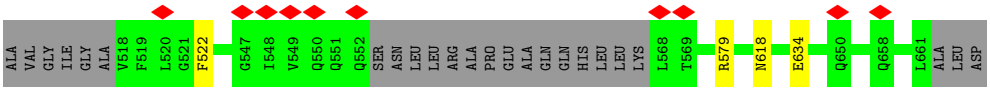
• Molecule 2: Envelope glycoprotein gp41

Chain E:



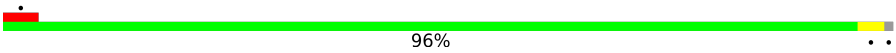
• Molecule 2: Envelope glycoprotein gp41

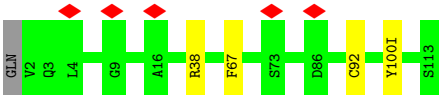
Chain F:



• Molecule 3: RM20F Fab Heavy Chain

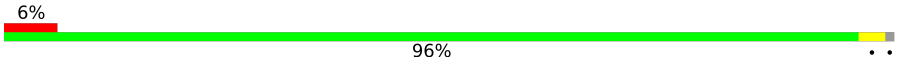
Chain H:

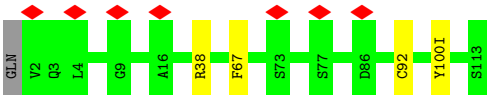




• Molecule 3: RM20F Fab Heavy Chain

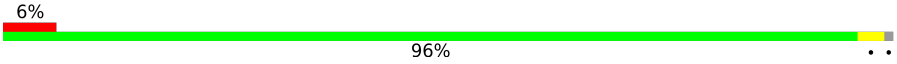
Chain G:

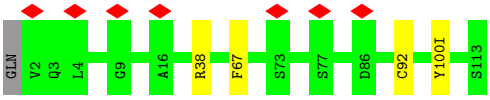




• Molecule 3: RM20F Fab Heavy Chain

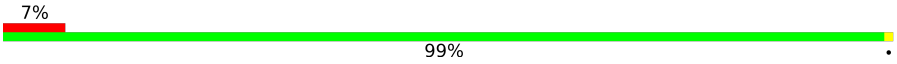
Chain I:

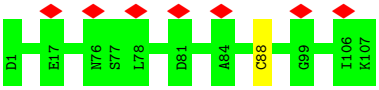




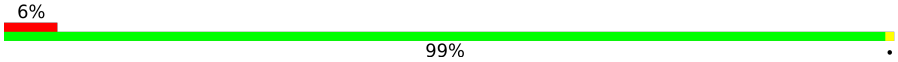
• Molecule 4: RM20F Kappa Chain

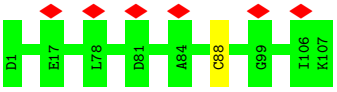
Chain L:



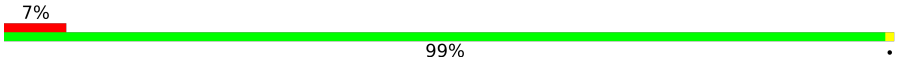


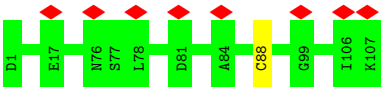
• Molecule 4: RM20F Kappa Chain

Chain J: 

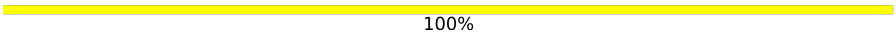


• Molecule 4: RM20F Kappa Chain

Chain K: 



• Molecule 5: 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 M: 

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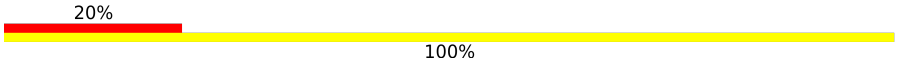
Chain Q: 

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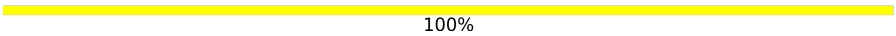
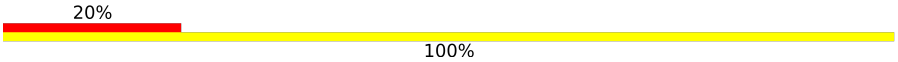
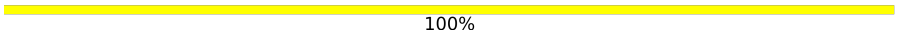
Chain X: 

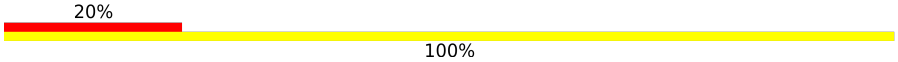
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

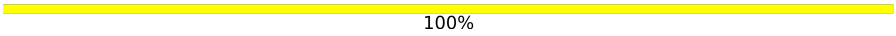
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 

• Molecule 5: 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 m: 

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

Chain N: 

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

Chain O:

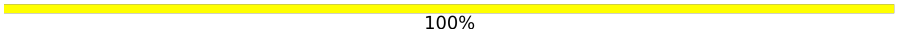
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

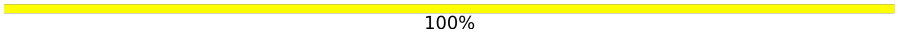
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

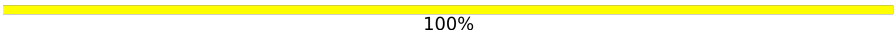
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

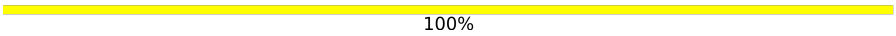
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

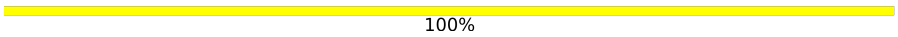
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 

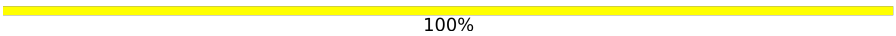
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 

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

Chain W: 

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

Chain Y: 

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

Chain Z:

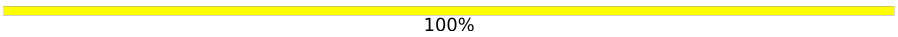
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

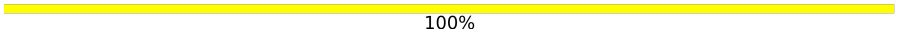
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

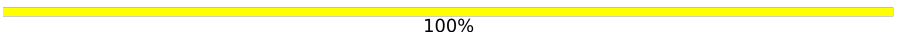
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 

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

Chain e: 

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

Chain f: 

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

Chain g: 100%

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

Chain h: 100%

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

Chain j: 100%

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

Chain k: 50% 100%

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

Chain l: 50% 50% 50%

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

Chain n: 50% 50% 50%

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

Chain o: 100%

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

Chain p: 100%

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

Chain q: 100%

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

Chain r: 100%

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

Chain s: 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	91212	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.168	Depositor
Minimum map value	-0.543	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.31	Depositor
Map size (Å)	309.0, 309.0, 309.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: NAG, BMA, 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	0.91	2/3451 (0.1%)	0.90	9/4684 (0.2%)
1	C	0.91	2/3451 (0.1%)	0.90	9/4684 (0.2%)
1	D	0.91	2/3451 (0.1%)	0.90	8/4684 (0.2%)
2	B	1.00	1/1048 (0.1%)	0.82	1/1421 (0.1%)
2	E	1.00	1/1048 (0.1%)	0.82	1/1421 (0.1%)
2	F	1.00	1/1048 (0.1%)	0.82	1/1421 (0.1%)
3	G	1.00	1/991 (0.1%)	0.99	3/1345 (0.2%)
3	H	1.01	1/991 (0.1%)	0.99	3/1345 (0.2%)
3	I	1.01	1/991 (0.1%)	0.99	3/1345 (0.2%)
4	J	0.91	1/830 (0.1%)	0.86	0/1124
4	K	0.91	1/830 (0.1%)	0.86	0/1124
4	L	0.91	1/830 (0.1%)	0.86	0/1124
All	All	0.94	15/18960 (0.1%)	0.90	38/25722 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	88	CYS	CB-SG	-6.78	1.70	1.82
4	J	88	CYS	CB-SG	-6.77	1.70	1.82
4	L	88	CYS	CB-SG	-6.76	1.70	1.82
1	C	418	CYS	CB-SG	-5.90	1.72	1.81
1	D	418	CYS	CB-SG	-5.89	1.72	1.81
1	A	418	CYS	CB-SG	-5.88	1.72	1.81
1	C	87	GLU	CD-OE2	-5.36	1.19	1.25
1	A	87	GLU	CD-OE2	-5.33	1.19	1.25
1	D	87	GLU	CD-OE2	-5.31	1.19	1.25
3	I	92	CYS	CB-SG	-5.19	1.73	1.81
3	H	92	CYS	CB-SG	-5.17	1.73	1.81
3	G	92	CYS	CB-SG	-5.13	1.73	1.81
2	B	634	GLU	CD-OE1	-5.12	1.20	1.25
2	E	634	GLU	CD-OE1	-5.10	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	634	GLU	CD-OE1	-5.08	1.20	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	C	476	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	D	476	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	476	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	C	476	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	D	476	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	D	480	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	480	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	C	480	ARG	NE-CZ-NH2	-9.11	115.75	120.30
3	H	100(I)	TYR	CB-CG-CD2	-8.56	115.86	121.00
3	I	100(I)	TYR	CB-CG-CD2	-8.55	115.87	121.00
3	G	100(I)	TYR	CB-CG-CD2	-8.54	115.88	121.00
1	A	151	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	151	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	C	151	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	503	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	503	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	C	503	ARG	NE-CZ-NH2	-7.42	116.59	120.30
3	I	67	PHE	CB-CG-CD1	7.09	125.76	120.80
3	G	67	PHE	CB-CG-CD1	7.05	125.73	120.80
3	H	67	PHE	CB-CG-CD1	7.03	125.72	120.80
2	E	579	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	F	579	ARG	NE-CZ-NH2	-6.93	116.83	120.30
2	B	579	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	C	480	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	480	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	D	480	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	161	MET	CG-SD-CE	6.42	110.48	100.20
1	D	161	MET	CG-SD-CE	6.41	110.46	100.20
1	A	161	MET	CG-SD-CE	6.40	110.44	100.20
3	I	38	ARG	NE-CZ-NH2	-5.61	117.50	120.30
3	G	38	ARG	NE-CZ-NH2	-5.57	117.52	120.30
3	H	38	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	217	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	217	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	D	217	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	384	TYR	CB-CG-CD2	-5.06	117.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	384	TYR	CB-CG-CD2	-5.05	117.97	121.00

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	417/475 (88%)	396 (95%)	17 (4%)	4 (1%)	15	54
1	C	417/475 (88%)	396 (95%)	17 (4%)	4 (1%)	15	54
1	D	417/475 (88%)	396 (95%)	17 (4%)	4 (1%)	15	54
2	B	125/153 (82%)	120 (96%)	4 (3%)	1 (1%)	19	60
2	E	125/153 (82%)	120 (96%)	4 (3%)	1 (1%)	19	60
2	F	125/153 (82%)	120 (96%)	4 (3%)	1 (1%)	19	60
3	G	123/126 (98%)	123 (100%)	0	0	100	100
3	H	123/126 (98%)	123 (100%)	0	0	100	100
3	I	123/126 (98%)	123 (100%)	0	0	100	100
4	J	105/107 (98%)	104 (99%)	1 (1%)	0	100	100
4	K	105/107 (98%)	104 (99%)	1 (1%)	0	100	100
4	L	105/107 (98%)	104 (99%)	1 (1%)	0	100	100
All	All	2310/2583 (89%)	2229 (96%)	66 (3%)	15 (1%)	29	65

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	C	78	ASP
1	D	78	ASP
2	B	522	PHE
2	E	522	PHE
2	F	522	PHE
1	A	75	VAL
1	C	75	VAL
1	D	75	VAL
1	A	300	ASN
1	C	300	ASN
1	D	300	ASN
1	A	68	VAL
1	C	68	VAL
1	D	68	VAL

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	382/423 (90%)	381 (100%)	1 (0%)	92 95
1	C	382/423 (90%)	381 (100%)	1 (0%)	92 95
1	D	382/423 (90%)	381 (100%)	1 (0%)	92 95
2	B	112/129 (87%)	111 (99%)	1 (1%)	78 88
2	E	112/129 (87%)	111 (99%)	1 (1%)	78 88
2	F	112/129 (87%)	111 (99%)	1 (1%)	78 88
3	G	101/102 (99%)	101 (100%)	0	100 100
3	H	101/102 (99%)	101 (100%)	0	100 100
3	I	101/102 (99%)	101 (100%)	0	100 100
4	J	94/94 (100%)	94 (100%)	0	100 100
4	K	94/94 (100%)	94 (100%)	0	100 100
4	L	94/94 (100%)	94 (100%)	0	100 100
All	All	2067/2244 (92%)	2061 (100%)	6 (0%)	92 95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ASN
2	B	618	ASN
1	C	355	ASN
2	E	618	ASN
1	D	355	ASN
2	F	618	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	543	ASN
2	E	543	ASN
2	F	543	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

84 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	M	1	5,1	14,14,15	0.76	0	17,19,21	1.35	3 (17%)
5	NAG	M	2	5	14,14,15	0.74	0	17,19,21	1.64	3 (17%)
5	BMA	M	3	5	11,11,12	1.82	2 (18%)	15,15,17	1.08	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MAN	M	4	5	11,11,12	1.85	3 (27%)	15,15,17	1.28	3 (20%)
5	MAN	M	5	5	11,11,12	1.84	2 (18%)	15,15,17	1.10	2 (13%)
6	NAG	N	1	6,1	14,14,15	0.79	0	17,19,21	1.11	1 (5%)
6	NAG	N	2	6	14,14,15	0.82	0	17,19,21	0.91	1 (5%)
6	NAG	O	1	6,1	14,14,15	0.80	0	17,19,21	1.54	3 (17%)
6	NAG	O	2	6	14,14,15	0.88	1 (7%)	17,19,21	1.01	1 (5%)
6	NAG	P	1	6,1	14,14,15	0.92	0	17,19,21	0.95	0
6	NAG	P	2	6	14,14,15	0.77	0	17,19,21	1.12	1 (5%)
5	NAG	Q	1	5,1	14,14,15	0.94	1 (7%)	17,19,21	1.44	5 (29%)
5	NAG	Q	2	5	14,14,15	0.71	0	17,19,21	1.47	3 (17%)
5	BMA	Q	3	5	11,11,12	1.82	2 (18%)	15,15,17	1.47	2 (13%)
5	MAN	Q	4	5	11,11,12	1.61	2 (18%)	15,15,17	0.91	0
5	MAN	Q	5	5	11,11,12	1.83	2 (18%)	15,15,17	1.12	2 (13%)
6	NAG	R	1	6,1	14,14,15	0.77	0	17,19,21	0.98	0
6	NAG	R	2	6	14,14,15	0.82	0	17,19,21	0.94	1 (5%)
6	NAG	S	1	6,1	14,14,15	0.86	1 (7%)	17,19,21	1.44	3 (17%)
6	NAG	S	2	6	14,14,15	0.82	0	17,19,21	0.94	1 (5%)
6	NAG	T	1	6,1	14,14,15	0.80	0	17,19,21	1.28	2 (11%)
6	NAG	T	2	6	14,14,15	0.85	1 (7%)	17,19,21	1.13	2 (11%)
6	NAG	U	1	6,1	14,14,15	0.75	0	17,19,21	1.04	1 (5%)
6	NAG	U	2	6	14,14,15	0.82	0	17,19,21	1.01	1 (5%)
6	NAG	V	1	6,1	14,14,15	0.78	0	17,19,21	1.36	2 (11%)
6	NAG	V	2	6	14,14,15	0.82	0	17,19,21	0.89	1 (5%)
6	NAG	W	1	6,1	14,14,15	0.84	1 (7%)	17,19,21	1.15	2 (11%)
6	NAG	W	2	6	14,14,15	0.84	0	17,19,21	1.03	1 (5%)
5	NAG	X	1	5,1	14,14,15	0.76	0	17,19,21	1.36	3 (17%)
5	NAG	X	2	5	14,14,15	0.73	0	17,19,21	1.64	3 (17%)
5	BMA	X	3	5	11,11,12	1.81	2 (18%)	15,15,17	1.08	1 (6%)
5	MAN	X	4	5	11,11,12	1.85	3 (27%)	15,15,17	1.28	3 (20%)
5	MAN	X	5	5	11,11,12	1.85	2 (18%)	15,15,17	1.10	2 (13%)
6	NAG	Y	1	6,1	14,14,15	0.79	0	17,19,21	1.11	1 (5%)
6	NAG	Y	2	6	14,14,15	0.83	0	17,19,21	0.91	1 (5%)
6	NAG	Z	1	6,1	14,14,15	0.80	0	17,19,21	1.54	3 (17%)
6	NAG	Z	2	6	14,14,15	0.88	1 (7%)	17,19,21	1.01	1 (5%)
6	NAG	a	1	6,1	14,14,15	0.91	0	17,19,21	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	a	2	6	14,14,15	0.77	0	17,19,21	1.12	1 (5%)
5	NAG	b	1	5,1	14,14,15	0.93	1 (7%)	17,19,21	1.43	5 (29%)
5	NAG	b	2	5	14,14,15	0.72	0	17,19,21	1.47	3 (17%)
5	BMA	b	3	5	11,11,12	1.82	2 (18%)	15,15,17	1.47	2 (13%)
5	MAN	b	4	5	11,11,12	1.61	2 (18%)	15,15,17	0.90	0
5	MAN	b	5	5	11,11,12	1.83	2 (18%)	15,15,17	1.11	2 (13%)
6	NAG	c	1	6,1	14,14,15	0.77	0	17,19,21	0.98	0
6	NAG	c	2	6	14,14,15	0.81	0	17,19,21	0.94	1 (5%)
6	NAG	d	1	6,1	14,14,15	0.85	1 (7%)	17,19,21	1.44	3 (17%)
6	NAG	d	2	6	14,14,15	0.81	0	17,19,21	0.94	1 (5%)
6	NAG	e	1	6,1	14,14,15	0.79	0	17,19,21	1.28	2 (11%)
6	NAG	e	2	6	14,14,15	0.85	1 (7%)	17,19,21	1.12	2 (11%)
6	NAG	f	1	6,1	14,14,15	0.76	0	17,19,21	1.04	1 (5%)
6	NAG	f	2	6	14,14,15	0.81	0	17,19,21	1.01	1 (5%)
6	NAG	g	1	6,1	14,14,15	0.78	0	17,19,21	1.36	2 (11%)
6	NAG	g	2	6	14,14,15	0.83	0	17,19,21	0.89	1 (5%)
6	NAG	h	1	6,1	14,14,15	0.84	1 (7%)	17,19,21	1.16	2 (11%)
6	NAG	h	2	6	14,14,15	0.84	0	17,19,21	1.04	1 (5%)
5	NAG	i	1	5,1	14,14,15	0.76	0	17,19,21	1.35	3 (17%)
5	NAG	i	2	5	14,14,15	0.74	0	17,19,21	1.64	3 (17%)
5	BMA	i	3	5	11,11,12	1.81	2 (18%)	15,15,17	1.08	1 (6%)
5	MAN	i	4	5	11,11,12	1.85	3 (27%)	15,15,17	1.28	3 (20%)
5	MAN	i	5	5	11,11,12	1.84	2 (18%)	15,15,17	1.10	2 (13%)
6	NAG	j	1	6,1	14,14,15	0.79	0	17,19,21	1.11	1 (5%)
6	NAG	j	2	6	14,14,15	0.83	0	17,19,21	0.91	1 (5%)
6	NAG	k	1	6,1	14,14,15	0.80	0	17,19,21	1.54	3 (17%)
6	NAG	k	2	6	14,14,15	0.88	1 (7%)	17,19,21	1.01	1 (5%)
6	NAG	l	1	6,1	14,14,15	0.92	0	17,19,21	0.95	0
6	NAG	l	2	6	14,14,15	0.77	0	17,19,21	1.12	1 (5%)
5	NAG	m	1	5,1	14,14,15	0.94	1 (7%)	17,19,21	1.43	5 (29%)
5	NAG	m	2	5	14,14,15	0.71	0	17,19,21	1.47	3 (17%)
5	BMA	m	3	5	11,11,12	1.82	2 (18%)	15,15,17	1.47	2 (13%)
5	MAN	m	4	5	11,11,12	1.62	2 (18%)	15,15,17	0.90	0
5	MAN	m	5	5	11,11,12	1.83	2 (18%)	15,15,17	1.11	2 (13%)
6	NAG	n	1	6,1	14,14,15	0.78	0	17,19,21	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	n	2	6	14,14,15	0.81	0	17,19,21	0.94	1 (5%)
6	NAG	o	1	6,1	14,14,15	0.85	1 (7%)	17,19,21	1.44	3 (17%)
6	NAG	o	2	6	14,14,15	0.82	0	17,19,21	0.93	1 (5%)
6	NAG	p	1	6,1	14,14,15	0.79	0	17,19,21	1.28	2 (11%)
6	NAG	p	2	6	14,14,15	0.85	1 (7%)	17,19,21	1.13	2 (11%)
6	NAG	q	1	6,1	14,14,15	0.76	0	17,19,21	1.04	1 (5%)
6	NAG	q	2	6	14,14,15	0.82	0	17,19,21	1.01	1 (5%)
6	NAG	r	1	6,1	14,14,15	0.78	0	17,19,21	1.36	2 (11%)
6	NAG	r	2	6	14,14,15	0.82	0	17,19,21	0.89	1 (5%)
6	NAG	s	1	6,1	14,14,15	0.83	1 (7%)	17,19,21	1.15	2 (11%)
6	NAG	s	2	6	14,14,15	0.84	0	17,19,21	1.03	1 (5%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	1/6/23/26	0/1/1/1
6	NAG	W	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	W	2	6	-	1/6/23/26	0/1/1/1
5	NAG	X	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	BMA	X	3	5	-	2/2/19/22	0/1/1/1
5	MAN	X	4	5	-	1/2/19/22	0/1/1/1
5	MAN	X	5	5	-	1/2/19/22	0/1/1/1
6	NAG	Y	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	1/6/23/26	0/1/1/1
6	NAG	a	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	1/6/23/26	0/1/1/1
5	NAG	b	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	BMA	b	3	5	-	1/2/19/22	0/1/1/1
5	MAN	b	4	5	-	1/2/19/22	0/1/1/1
5	MAN	b	5	5	-	1/2/19/22	0/1/1/1
6	NAG	c	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	c	2	6	-	1/6/23/26	0/1/1/1
6	NAG	d	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1
6	NAG	e	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
6	NAG	f	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	NAG	g	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	g	2	6	-	1/6/23/26	0/1/1/1
6	NAG	h	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	h	2	6	-	1/6/23/26	0/1/1/1
5	NAG	i	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	i	2	5	-	0/6/23/26	0/1/1/1
5	BMA	i	3	5	-	2/2/19/22	0/1/1/1
5	MAN	i	4	5	-	1/2/19/22	0/1/1/1
5	MAN	i	5	5	-	1/2/19/22	0/1/1/1
6	NAG	j	1	6,1	-	0/6/23/26	0/1/1/1

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

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	m	3	BMA	O2-C2	-4.18	1.34	1.43
5	b	3	BMA	O2-C2	-4.17	1.34	1.43
5	X	5	MAN	O2-C2	-4.17	1.34	1.43
5	Q	3	BMA	O2-C2	-4.15	1.34	1.43
5	i	5	MAN	O2-C2	-4.15	1.34	1.43
5	M	5	MAN	O2-C2	-4.14	1.34	1.43
5	b	5	MAN	O2-C2	-4.12	1.34	1.43
5	m	5	MAN	O2-C2	-4.12	1.34	1.43
5	Q	5	MAN	O2-C2	-4.10	1.34	1.43
5	i	4	MAN	O2-C2	-4.09	1.34	1.43
5	M	3	BMA	O2-C2	-4.08	1.34	1.43
5	X	4	MAN	O2-C2	-4.08	1.34	1.43
5	X	3	BMA	O2-C2	-4.08	1.34	1.43
5	M	4	MAN	O2-C2	-4.06	1.34	1.43
5	i	3	BMA	O2-C2	-4.06	1.34	1.43
5	m	4	MAN	O2-C2	-3.19	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	4	MAN	O2-C2	-3.18	1.36	1.43
5	b	4	MAN	O2-C2	-3.18	1.36	1.43
5	X	5	MAN	C2-C3	-2.50	1.48	1.52
5	M	5	MAN	C2-C3	-2.49	1.48	1.52
5	i	5	MAN	C2-C3	-2.48	1.48	1.52
5	Q	5	MAN	C2-C3	-2.37	1.49	1.52
5	m	5	MAN	C2-C3	-2.36	1.49	1.52
5	b	5	MAN	C2-C3	-2.35	1.49	1.52
5	m	3	BMA	C2-C3	-2.32	1.49	1.52
5	Q	3	BMA	C2-C3	-2.31	1.49	1.52
5	b	3	BMA	C2-C3	-2.31	1.49	1.52
5	M	4	MAN	C2-C3	-2.28	1.49	1.52
5	i	4	MAN	C2-C3	-2.26	1.49	1.52
5	X	3	BMA	C2-C3	-2.25	1.49	1.52
5	i	3	BMA	C2-C3	-2.24	1.49	1.52
5	X	4	MAN	C2-C3	-2.24	1.49	1.52
5	Q	1	NAG	C3-C2	-2.24	1.47	1.52
5	b	4	MAN	O5-C1	2.23	1.47	1.43
5	M	3	BMA	C2-C3	-2.22	1.49	1.52
5	m	1	NAG	C3-C2	-2.22	1.47	1.52
5	m	4	MAN	O5-C1	2.21	1.47	1.43
5	b	1	NAG	C3-C2	-2.20	1.47	1.52
5	Q	4	MAN	O5-C1	2.18	1.47	1.43
6	e	2	NAG	O5-C1	2.17	1.47	1.43
6	T	2	NAG	O5-C1	2.17	1.47	1.43
6	p	2	NAG	O5-C1	2.16	1.47	1.43
6	h	1	NAG	C3-C2	-2.13	1.48	1.52
6	W	1	NAG	C3-C2	-2.13	1.48	1.52
6	o	1	NAG	C3-C2	-2.12	1.48	1.52
6	d	1	NAG	C3-C2	-2.12	1.48	1.52
6	s	1	NAG	C3-C2	-2.11	1.48	1.52
6	S	1	NAG	C3-C2	-2.11	1.48	1.52
5	i	4	MAN	O5-C1	2.06	1.47	1.43
5	M	4	MAN	O5-C1	2.05	1.47	1.43
5	X	4	MAN	O5-C1	2.05	1.47	1.43
6	k	2	NAG	O5-C1	2.01	1.46	1.43
6	Z	2	NAG	O5-C1	2.01	1.46	1.43
6	O	2	NAG	O5-C1	2.00	1.46	1.43

All (144) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	2	NAG	O5-C1-C2	-3.72	105.42	111.29
5	X	2	NAG	O5-C1-C2	-3.72	105.42	111.29
5	i	2	NAG	O5-C1-C2	-3.71	105.43	111.29
6	S	1	NAG	O5-C5-C6	-3.63	101.51	107.20
6	o	1	NAG	O5-C5-C6	-3.63	101.52	107.20
6	d	1	NAG	O5-C5-C6	-3.62	101.53	107.20
5	m	3	BMA	C2-C3-C4	-3.53	104.78	110.89
5	b	3	BMA	C2-C3-C4	-3.53	104.79	110.89
5	Q	3	BMA	C2-C3-C4	-3.52	104.81	110.89
5	X	2	NAG	C4-C3-C2	-3.51	105.87	111.02
5	i	2	NAG	C4-C3-C2	-3.50	105.89	111.02
5	M	2	NAG	C4-C3-C2	-3.50	105.89	111.02
6	r	1	NAG	O5-C5-C6	-3.41	101.86	107.20
6	V	1	NAG	O5-C5-C6	-3.40	101.87	107.20
6	g	1	NAG	O5-C5-C6	-3.40	101.87	107.20
6	O	1	NAG	O5-C5-C6	-3.37	101.92	107.20
6	Z	1	NAG	O5-C5-C6	-3.36	101.94	107.20
6	O	1	NAG	C3-C4-C5	-3.35	104.26	110.24
6	k	1	NAG	O5-C5-C6	-3.35	101.95	107.20
6	Z	1	NAG	C3-C4-C5	-3.35	104.27	110.24
6	k	1	NAG	C3-C4-C5	-3.33	104.29	110.24
6	T	2	NAG	C4-C3-C2	-3.29	106.19	111.02
6	e	2	NAG	C4-C3-C2	-3.29	106.20	111.02
6	p	2	NAG	C4-C3-C2	-3.29	106.20	111.02
6	l	2	NAG	C4-C3-C2	-3.14	106.41	111.02
5	m	2	NAG	C4-C3-C2	-3.13	106.43	111.02
6	P	2	NAG	C4-C3-C2	-3.13	106.43	111.02
5	b	2	NAG	C4-C3-C2	-3.13	106.43	111.02
5	Q	2	NAG	C4-C3-C2	-3.13	106.43	111.02
6	a	2	NAG	C4-C3-C2	-3.13	106.44	111.02
5	X	1	NAG	C2-N2-C7	3.09	127.31	122.90
5	i	1	NAG	C2-N2-C7	3.09	127.30	122.90
5	M	1	NAG	C2-N2-C7	3.09	127.30	122.90
6	h	2	NAG	C4-C3-C2	-2.98	106.64	111.02
6	W	2	NAG	C4-C3-C2	-2.98	106.65	111.02
6	s	2	NAG	C4-C3-C2	-2.98	106.65	111.02
6	f	2	NAG	C4-C3-C2	-2.92	106.73	111.02
6	U	2	NAG	C4-C3-C2	-2.92	106.75	111.02
6	q	2	NAG	C4-C3-C2	-2.90	106.77	111.02
6	p	1	NAG	C3-C4-C5	-2.89	105.08	110.24
6	T	1	NAG	C3-C4-C5	-2.89	105.08	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	e	1	NAG	C3-C4-C5	-2.89	105.09	110.24
6	O	2	NAG	C4-C3-C2	-2.84	106.86	111.02
6	Z	2	NAG	C4-C3-C2	-2.84	106.86	111.02
5	i	4	MAN	C1-C2-C3	2.84	113.16	109.67
5	M	4	MAN	C1-C2-C3	2.83	113.14	109.67
6	k	2	NAG	C4-C3-C2	-2.82	106.88	111.02
5	X	4	MAN	C1-C2-C3	2.82	113.13	109.67
5	X	3	BMA	C2-C3-C4	-2.80	106.06	110.89
6	S	2	NAG	C4-C3-C2	-2.79	106.93	111.02
5	M	3	BMA	C2-C3-C4	-2.79	106.08	110.89
6	d	2	NAG	C4-C3-C2	-2.78	106.94	111.02
5	i	3	BMA	C2-C3-C4	-2.78	106.09	110.89
5	b	3	BMA	C1-C2-C3	2.77	113.06	109.67
6	o	2	NAG	C4-C3-C2	-2.76	106.97	111.02
5	m	3	BMA	C1-C2-C3	2.76	113.06	109.67
5	Q	3	BMA	C1-C2-C3	2.76	113.05	109.67
5	Q	2	NAG	O5-C5-C6	-2.75	102.89	107.20
5	m	2	NAG	O5-C5-C6	-2.75	102.90	107.20
5	b	2	NAG	O5-C5-C6	-2.75	102.90	107.20
6	n	2	NAG	C4-C3-C2	-2.74	107.00	111.02
6	c	2	NAG	C4-C3-C2	-2.72	107.04	111.02
6	R	2	NAG	C4-C3-C2	-2.71	107.04	111.02
6	T	1	NAG	C1-O5-C5	-2.68	108.56	112.19
6	p	1	NAG	C1-O5-C5	-2.68	108.56	112.19
6	s	1	NAG	O4-C4-C3	-2.66	104.19	110.35
6	e	1	NAG	C1-O5-C5	-2.65	108.60	112.19
6	h	1	NAG	O4-C4-C3	-2.65	104.22	110.35
5	b	1	NAG	O4-C4-C3	-2.65	104.23	110.35
6	W	1	NAG	O4-C4-C3	-2.65	104.23	110.35
5	Q	1	NAG	O4-C4-C3	-2.65	104.23	110.35
5	m	1	NAG	O4-C4-C3	-2.64	104.24	110.35
5	m	2	NAG	O5-C1-C2	-2.61	107.16	111.29
5	b	2	NAG	O5-C1-C2	-2.60	107.18	111.29
5	Q	2	NAG	O5-C1-C2	-2.60	107.19	111.29
6	h	1	NAG	C3-C4-C5	-2.50	105.78	110.24
6	W	1	NAG	C3-C4-C5	-2.49	105.80	110.24
5	X	2	NAG	C2-N2-C7	-2.48	119.37	122.90
5	i	2	NAG	C2-N2-C7	-2.48	119.38	122.90
6	s	1	NAG	C3-C4-C5	-2.48	105.82	110.24
5	b	5	MAN	C2-C3-C4	-2.47	106.61	110.89
5	Q	5	MAN	C2-C3-C4	-2.47	106.62	110.89
5	M	2	NAG	C2-N2-C7	-2.47	119.39	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	1	NAG	O4-C4-C3	-2.46	104.65	110.35
6	k	1	NAG	O4-C4-C3	-2.46	104.66	110.35
5	m	5	MAN	C2-C3-C4	-2.46	106.63	110.89
6	Z	1	NAG	O4-C4-C3	-2.45	104.68	110.35
6	S	1	NAG	C3-C4-C5	-2.44	105.88	110.24
6	d	1	NAG	C3-C4-C5	-2.43	105.90	110.24
6	o	1	NAG	C3-C4-C5	-2.43	105.90	110.24
6	S	1	NAG	O4-C4-C3	-2.43	104.73	110.35
6	d	1	NAG	O4-C4-C3	-2.43	104.74	110.35
6	o	1	NAG	O4-C4-C3	-2.43	104.74	110.35
6	V	2	NAG	C4-C3-C2	-2.37	107.55	111.02
6	g	2	NAG	C4-C3-C2	-2.36	107.55	111.02
6	r	2	NAG	C4-C3-C2	-2.36	107.56	111.02
5	i	4	MAN	C2-C3-C4	-2.36	106.82	110.89
5	X	4	MAN	C2-C3-C4	-2.33	106.86	110.89
5	M	4	MAN	C2-C3-C4	-2.33	106.86	110.89
5	i	4	MAN	O5-C1-C2	-2.31	107.21	110.77
5	X	4	MAN	O5-C1-C2	-2.30	107.22	110.77
5	M	4	MAN	O5-C1-C2	-2.29	107.23	110.77
5	M	5	MAN	C2-C3-C4	-2.26	106.99	110.89
5	i	5	MAN	C2-C3-C4	-2.25	107.00	110.89
5	X	5	MAN	C2-C3-C4	-2.24	107.03	110.89
6	p	2	NAG	O5-C1-C2	-2.22	107.78	111.29
6	T	2	NAG	O5-C1-C2	-2.22	107.78	111.29
5	Q	1	NAG	O5-C5-C6	-2.22	103.73	107.20
5	m	1	NAG	O5-C5-C6	-2.22	103.73	107.20
6	e	2	NAG	O5-C1-C2	-2.21	107.80	111.29
5	b	1	NAG	O5-C5-C6	-2.20	103.75	107.20
6	N	2	NAG	C4-C3-C2	-2.18	107.83	111.02
6	Y	2	NAG	C4-C3-C2	-2.17	107.84	111.02
6	j	2	NAG	C4-C3-C2	-2.16	107.85	111.02
6	N	1	NAG	O5-C5-C6	-2.14	103.85	107.20
6	j	1	NAG	O5-C5-C6	-2.13	103.87	107.20
6	g	1	NAG	O4-C4-C3	-2.13	105.44	110.35
6	Y	1	NAG	O5-C5-C6	-2.12	103.88	107.20
6	r	1	NAG	O4-C4-C3	-2.12	105.45	110.35
6	V	1	NAG	O4-C4-C3	-2.12	105.46	110.35
5	b	1	NAG	C3-C4-C5	-2.11	106.48	110.24
5	m	1	NAG	C3-C4-C5	-2.09	106.50	110.24
5	Q	1	NAG	C3-C4-C5	-2.09	106.51	110.24
5	M	1	NAG	C3-C4-C5	-2.09	106.51	110.24
5	X	1	NAG	C3-C4-C5	-2.09	106.51	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	i	1	NAG	C3-C4-C5	-2.08	106.53	110.24
5	Q	1	NAG	O5-C1-C2	-2.08	108.00	111.29
5	X	1	NAG	O5-C1-C2	-2.08	108.01	111.29
5	M	1	NAG	O5-C1-C2	-2.07	108.01	111.29
5	i	1	NAG	O5-C1-C2	-2.07	108.02	111.29
5	m	1	NAG	O5-C1-C2	-2.07	108.03	111.29
5	Q	1	NAG	O4-C4-C5	2.07	114.42	109.30
5	Q	5	MAN	C1-C2-C3	2.06	112.20	109.67
5	m	1	NAG	O4-C4-C5	2.06	114.42	109.30
5	b	1	NAG	O4-C4-C5	2.06	114.42	109.30
6	f	1	NAG	C3-C4-C5	-2.06	106.57	110.24
5	b	1	NAG	O5-C1-C2	-2.06	108.04	111.29
5	b	5	MAN	C1-C2-C3	2.05	112.19	109.67
6	U	1	NAG	C3-C4-C5	-2.05	106.58	110.24
6	q	1	NAG	C3-C4-C5	-2.04	106.59	110.24
5	M	5	MAN	C1-C2-C3	2.04	112.17	109.67
5	i	5	MAN	C1-C2-C3	2.04	112.17	109.67
5	m	5	MAN	C1-C2-C3	2.03	112.17	109.67
5	X	5	MAN	C1-C2-C3	2.02	112.15	109.67

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	C3-C2-N2-C7
5	X	1	NAG	C3-C2-N2-C7
5	i	1	NAG	C3-C2-N2-C7
5	X	3	BMA	C4-C5-C6-O6
5	i	3	BMA	C4-C5-C6-O6
5	M	3	BMA	C4-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	d	2	NAG	O5-C5-C6-O6
6	o	2	NAG	O5-C5-C6-O6
6	T	2	NAG	O5-C5-C6-O6
6	e	2	NAG	O5-C5-C6-O6
6	p	2	NAG	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
5	i	3	BMA	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	f	2	NAG	O5-C5-C6-O6
6	q	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	P	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	l	2	NAG	O5-C5-C6-O6
5	Q	3	BMA	O5-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	m	3	BMA	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	k	2	NAG	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	n	2	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
6	h	2	NAG	O5-C5-C6-O6
6	s	2	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	Y	2	NAG	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
6	r	2	NAG	O5-C5-C6-O6
5	M	5	MAN	O5-C5-C6-O6
5	X	5	MAN	O5-C5-C6-O6
5	i	5	MAN	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
5	X	4	MAN	O5-C5-C6-O6
5	i	4	MAN	O5-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
6	d	2	NAG	C4-C5-C6-O6
6	o	2	NAG	C4-C5-C6-O6
5	Q	4	MAN	O5-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
5	m	4	MAN	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
6	e	1	NAG	O5-C5-C6-O6
6	p	1	NAG	O5-C5-C6-O6
5	Q	5	MAN	O5-C5-C6-O6
5	b	5	MAN	O5-C5-C6-O6
5	m	5	MAN	O5-C5-C6-O6
6	e	2	NAG	C4-C5-C6-O6
6	T	2	NAG	C4-C5-C6-O6
6	p	2	NAG	C4-C5-C6-O6

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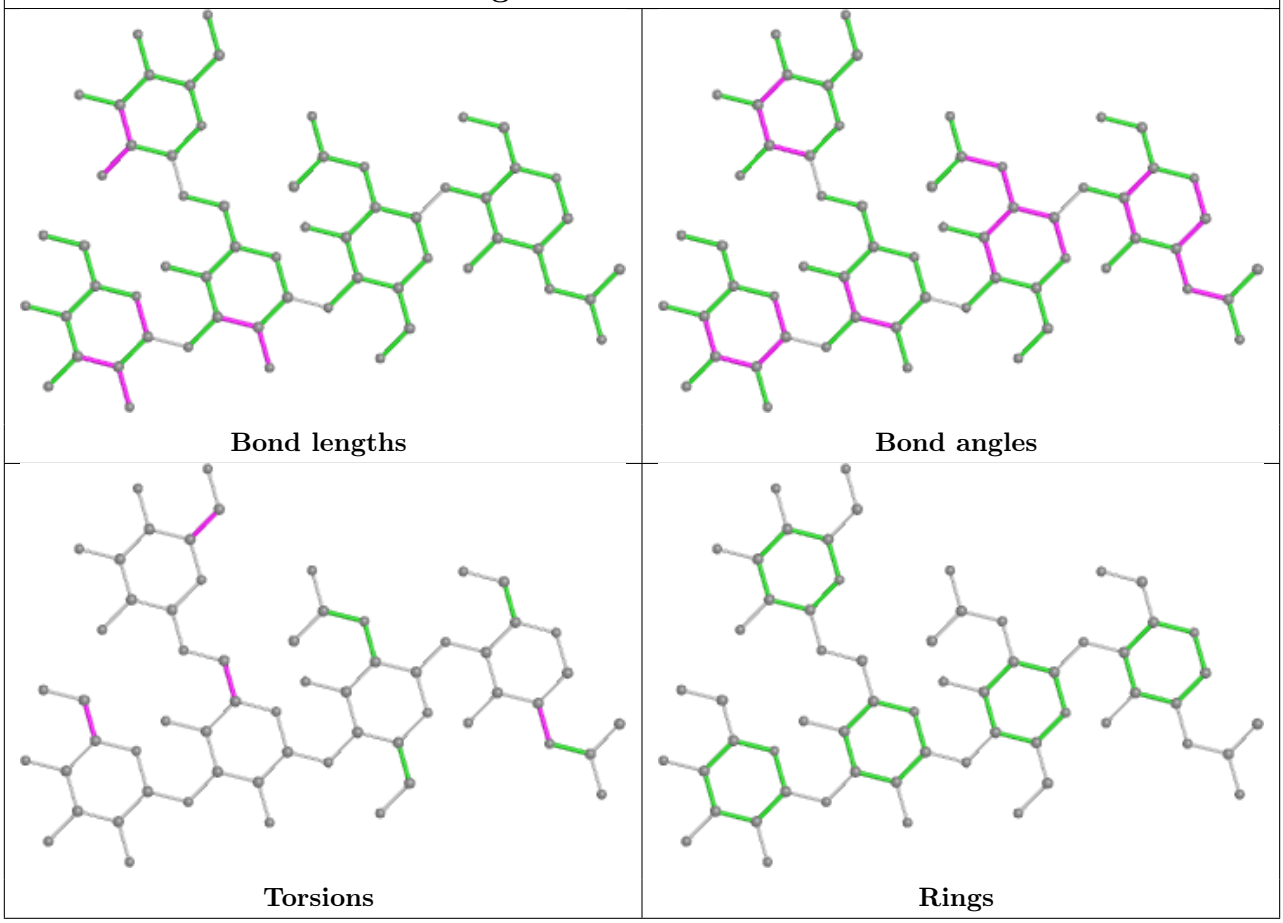
Mol	Chain	Res	Type	Atoms
6	q	2	NAG	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	f	2	NAG	C4-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6

There are no ring outliers.

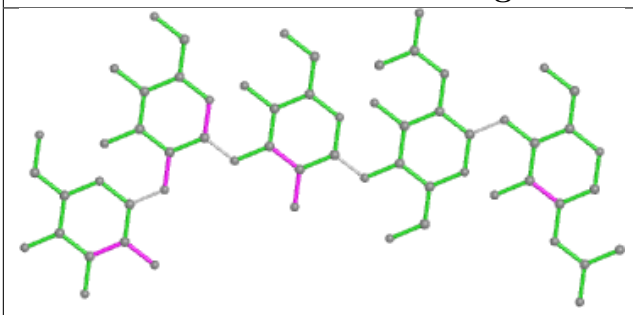
No monomer is involved in short contacts.

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

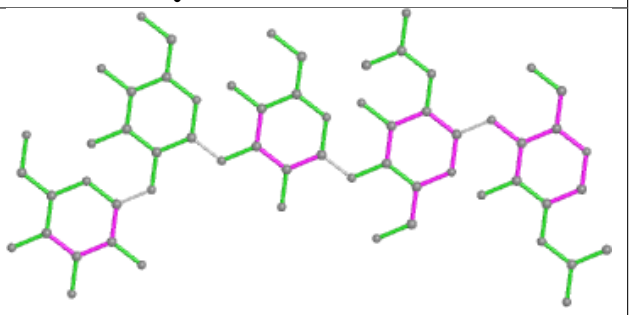
Oligosaccharide Chain M



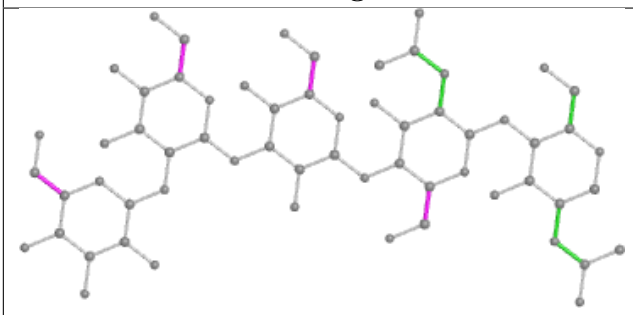
Oligosaccharide Chain Q



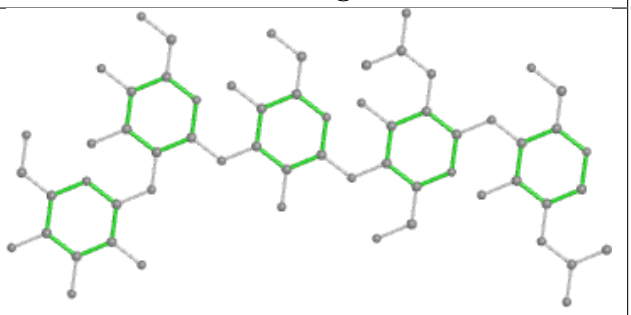
Bond lengths



Bond angles

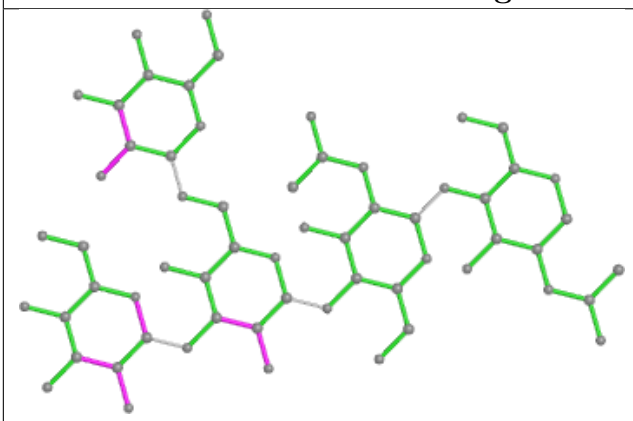


Torsions

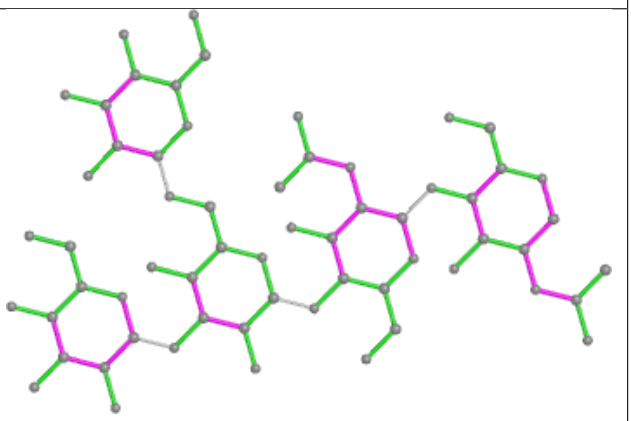


Rings

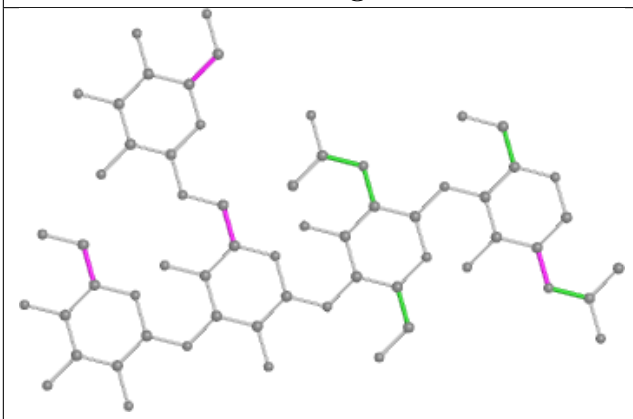
Oligosaccharide Chain X



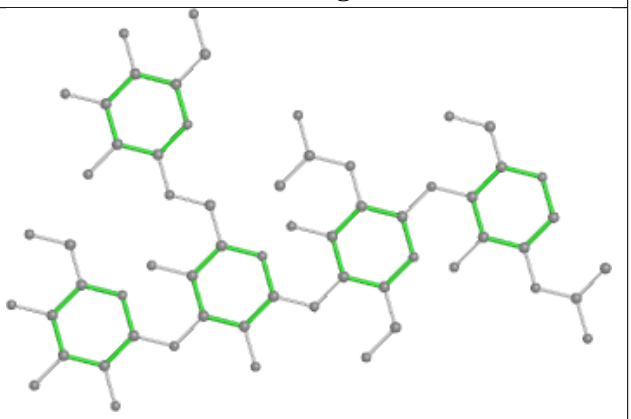
Bond lengths



Bond angles

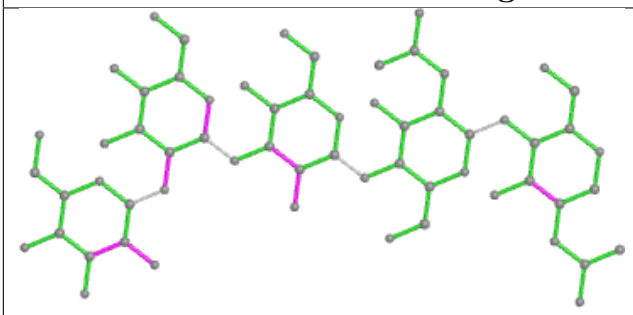


Torsions

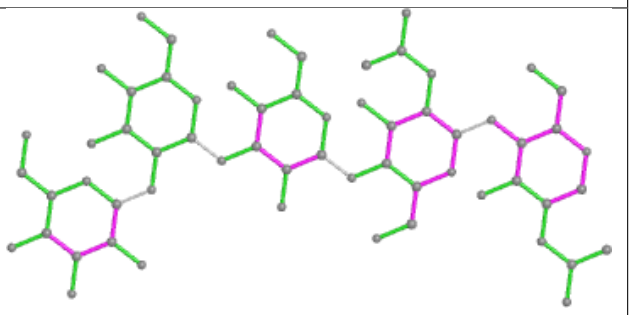


Rings

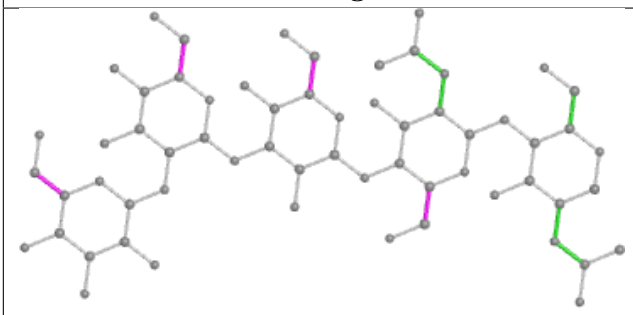
Oligosaccharide Chain b



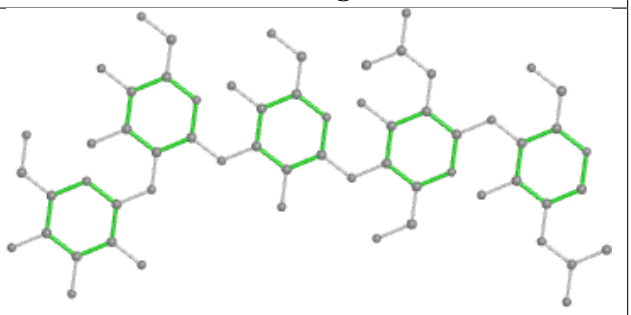
Bond lengths



Bond angles

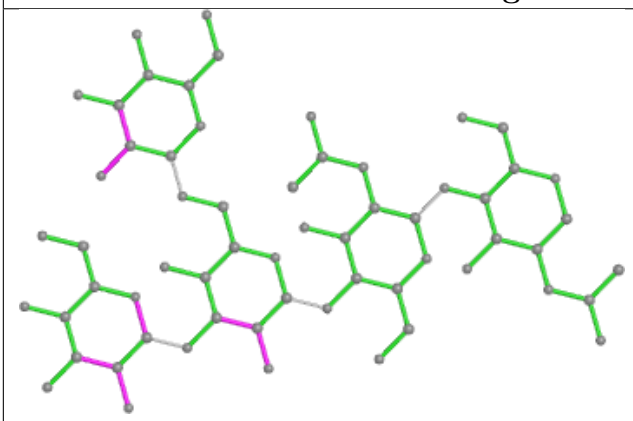


Torsions

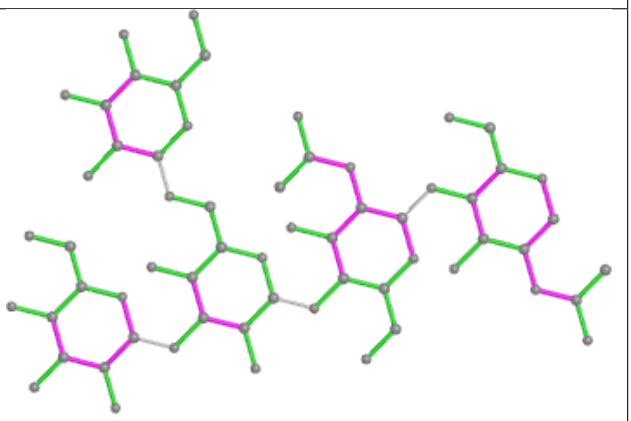


Rings

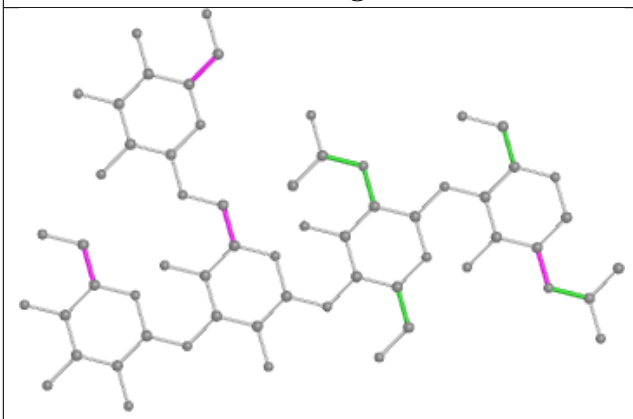
Oligosaccharide Chain i



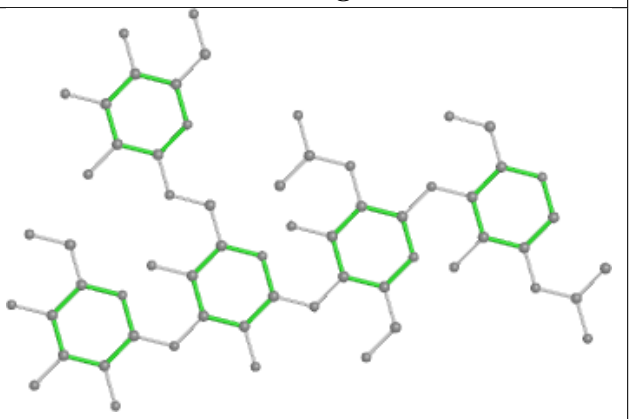
Bond lengths



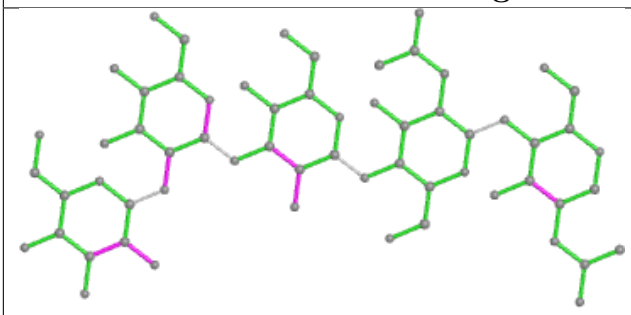
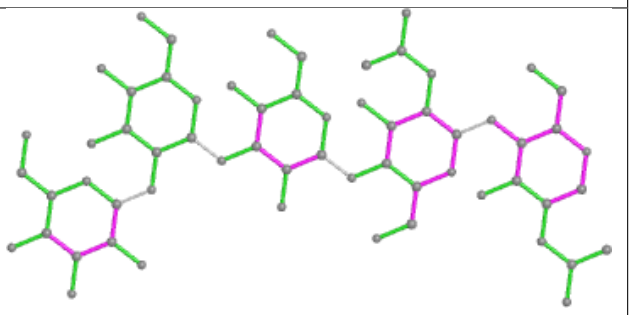
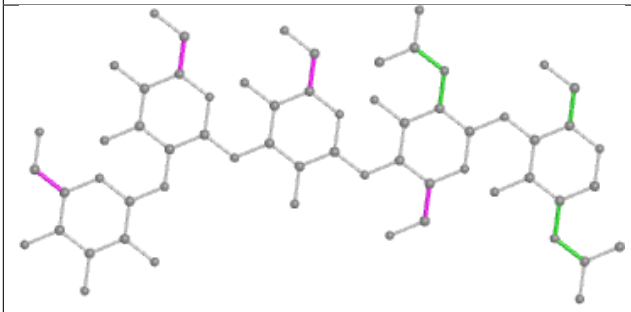
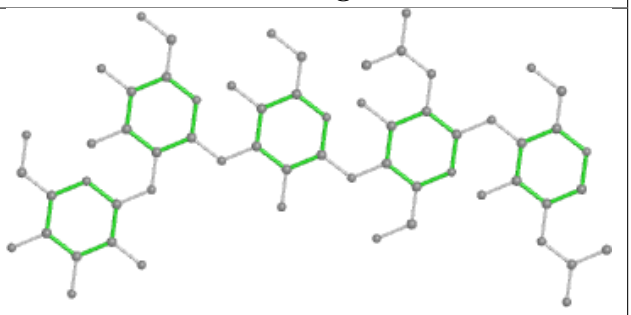
Bond angles



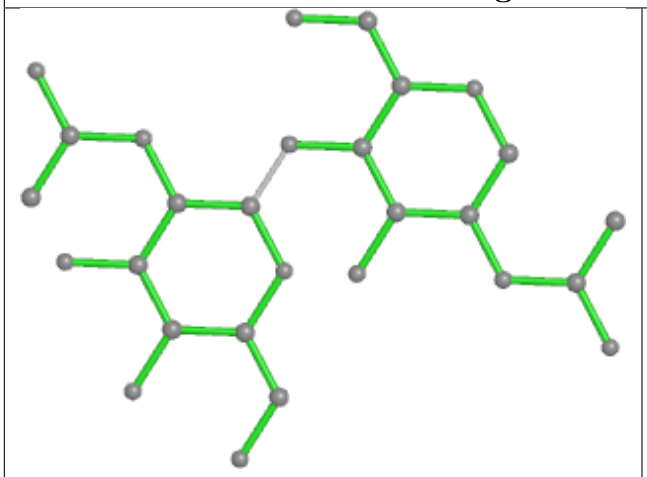
Torsions



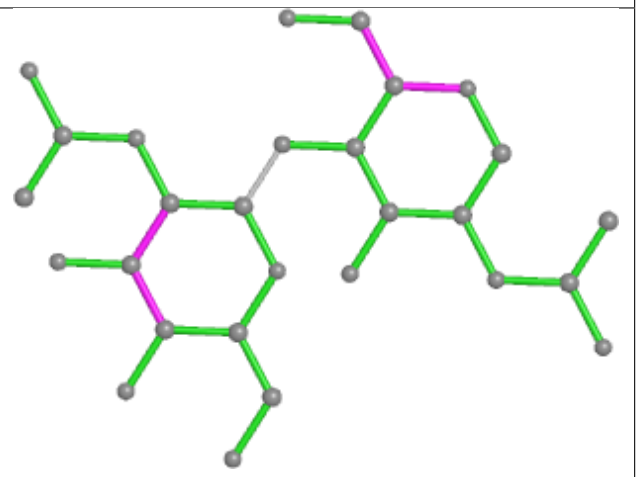
Rings

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

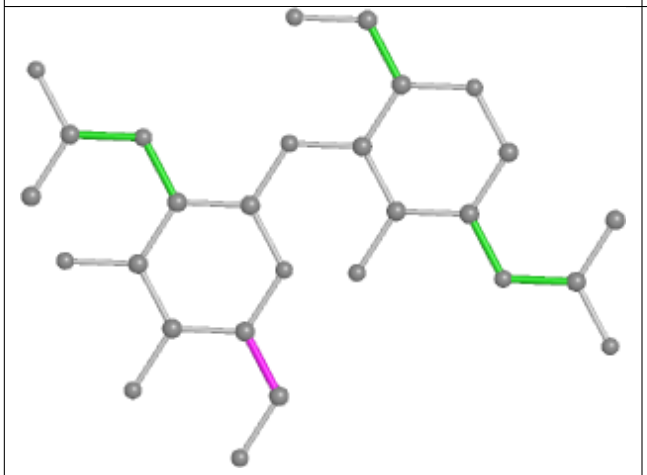
Oligosaccharide Chain N



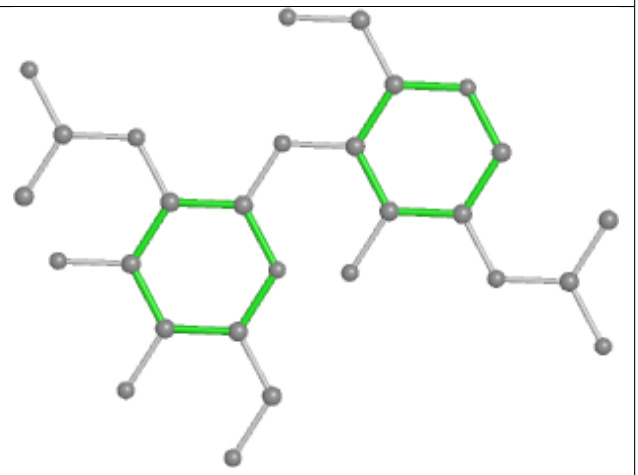
Bond lengths



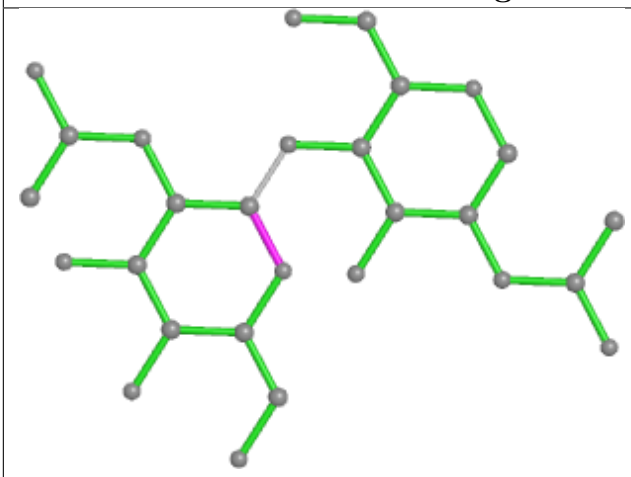
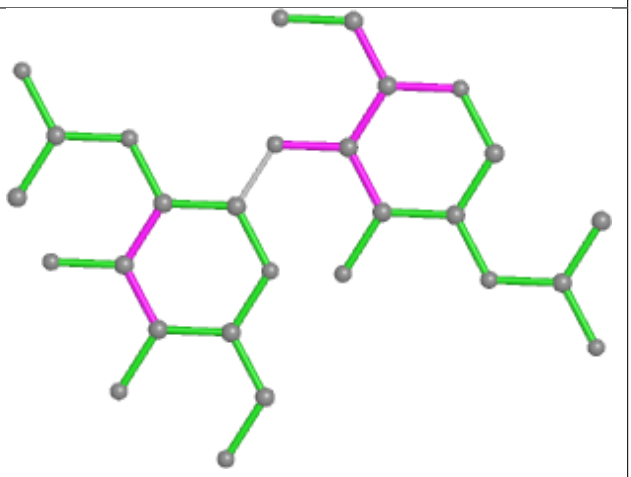
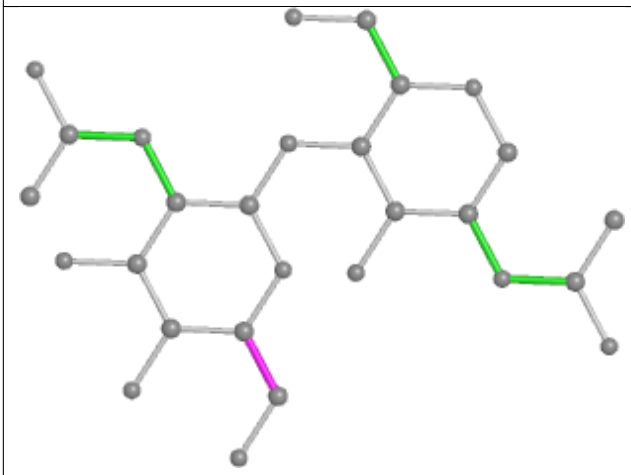
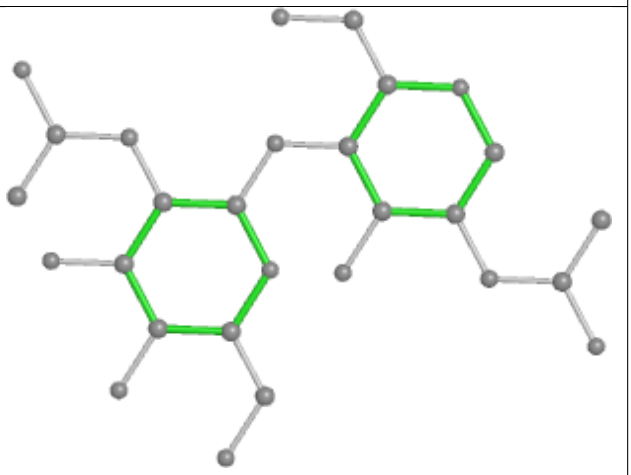
Bond angles

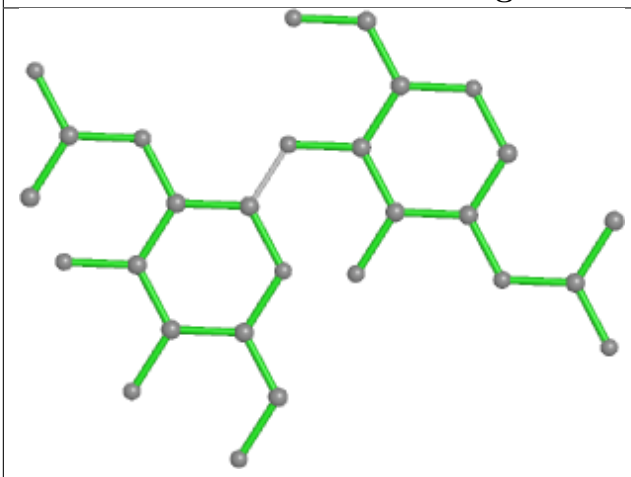
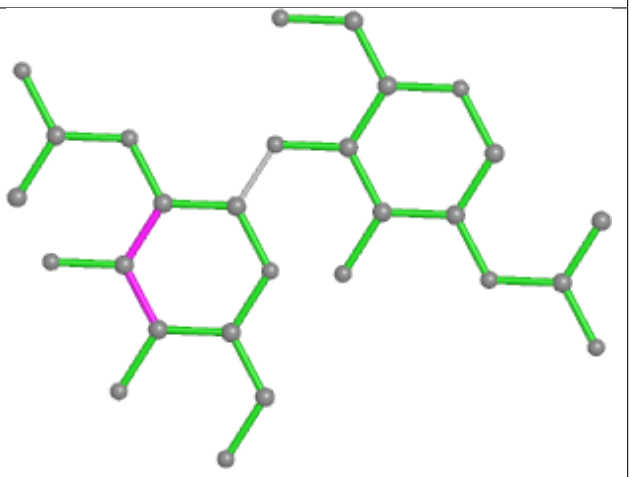
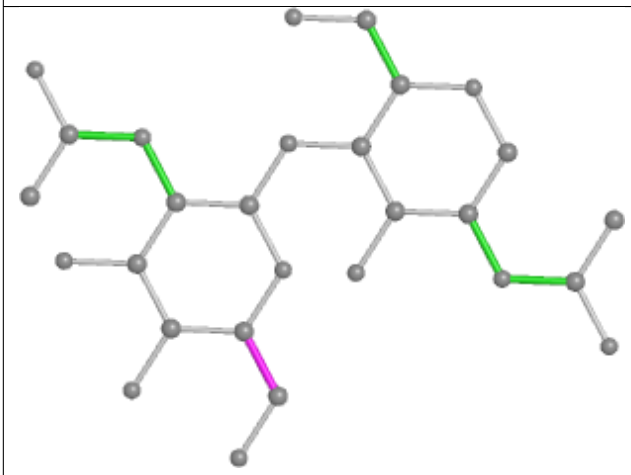
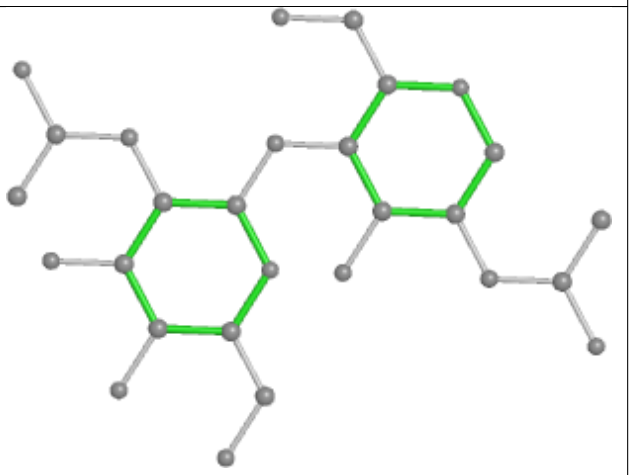


Torsions



Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

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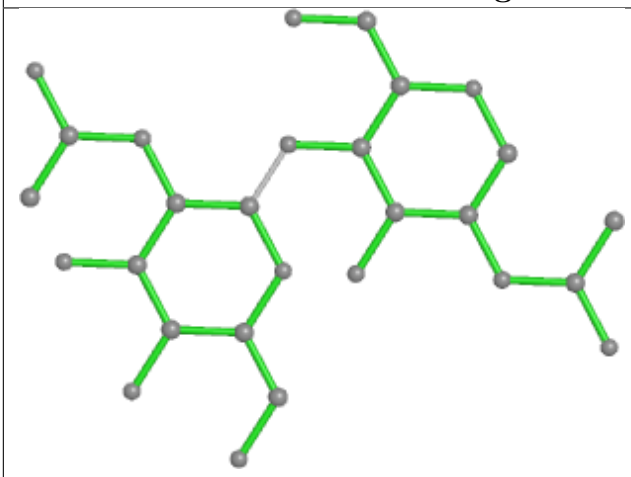
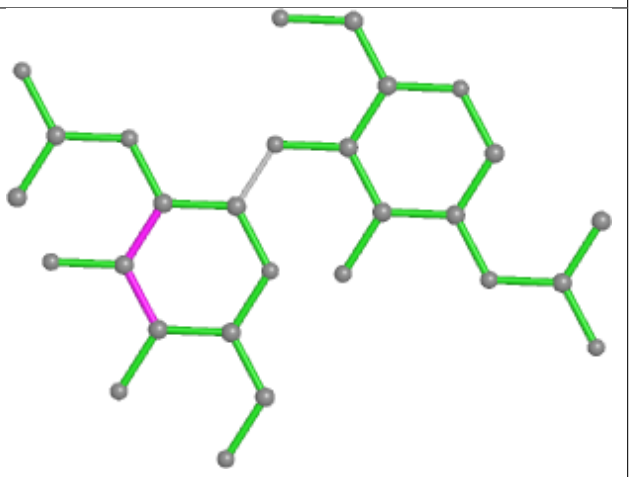
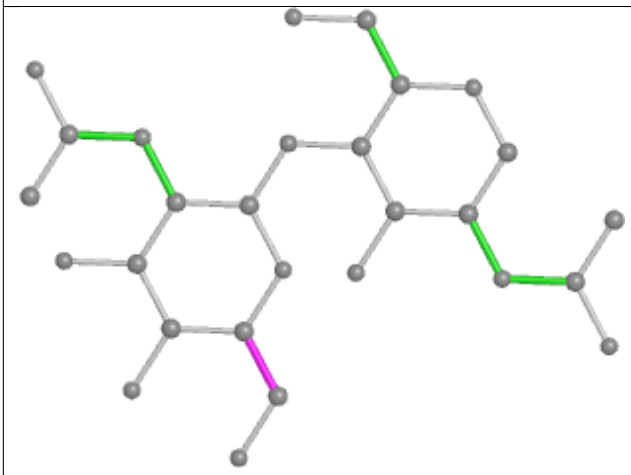
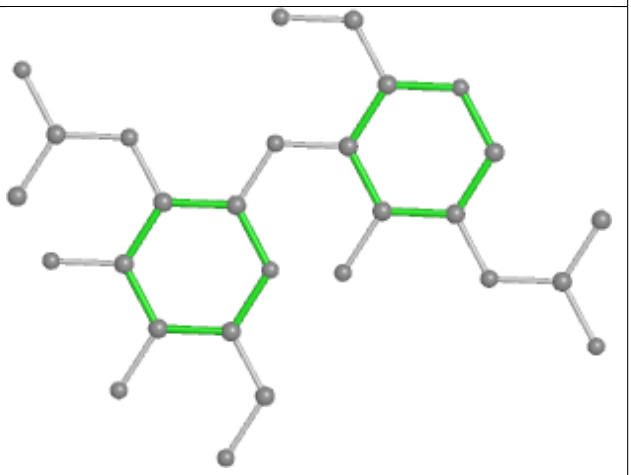
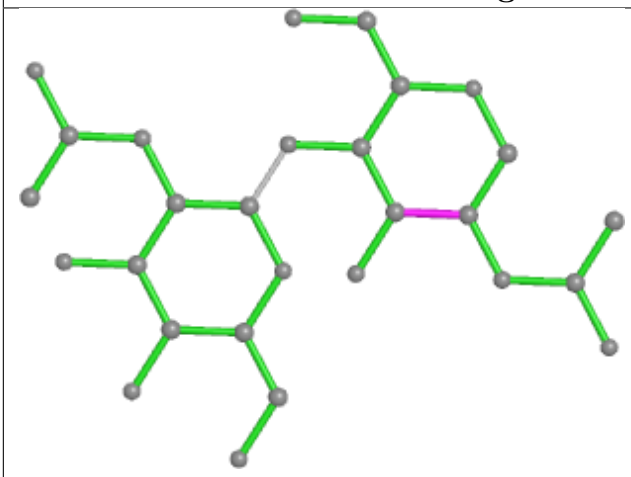
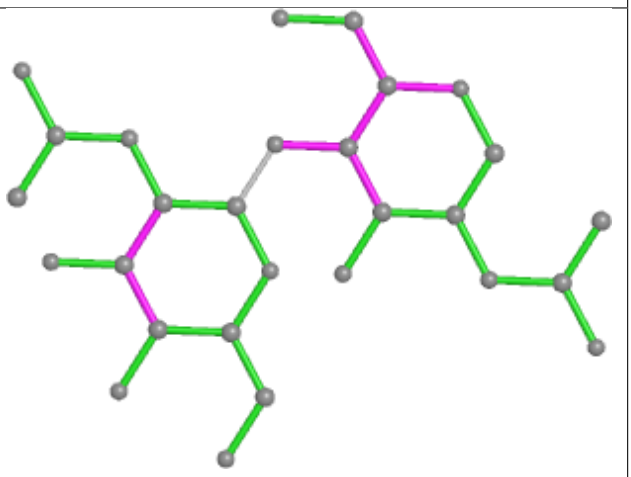
 Bond lengths	 Bond angles
 Torsions	 Rings

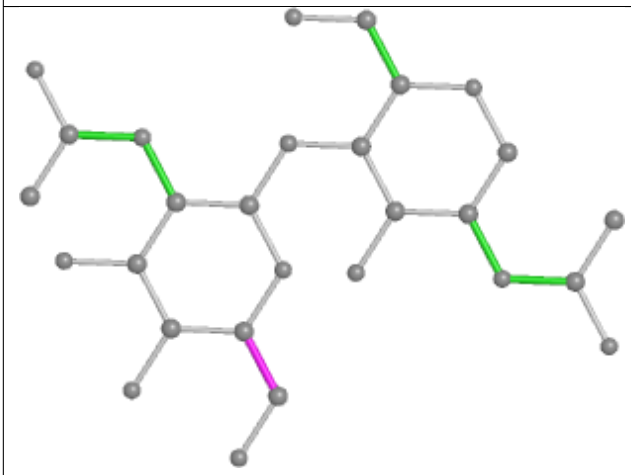
Oligosaccharide Chain S



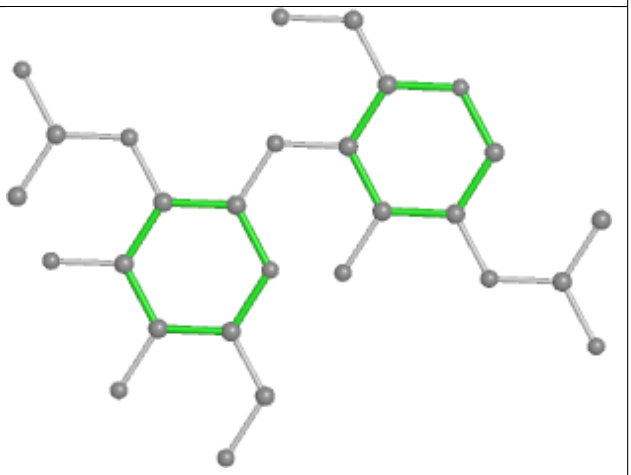
Bond lengths



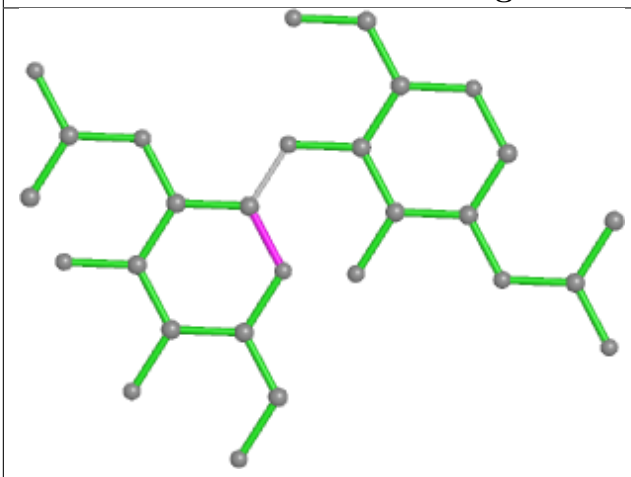
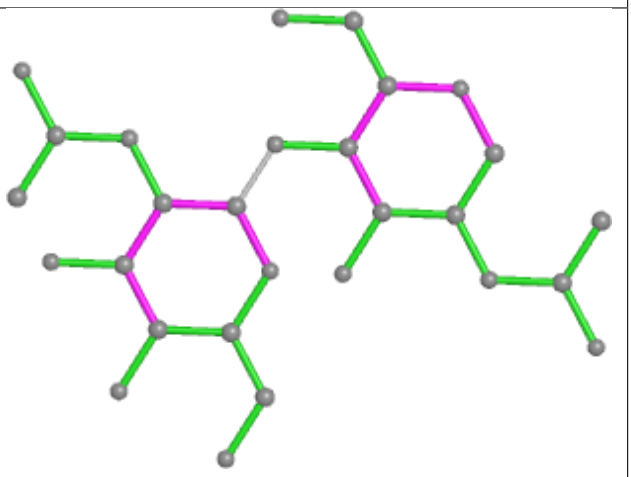
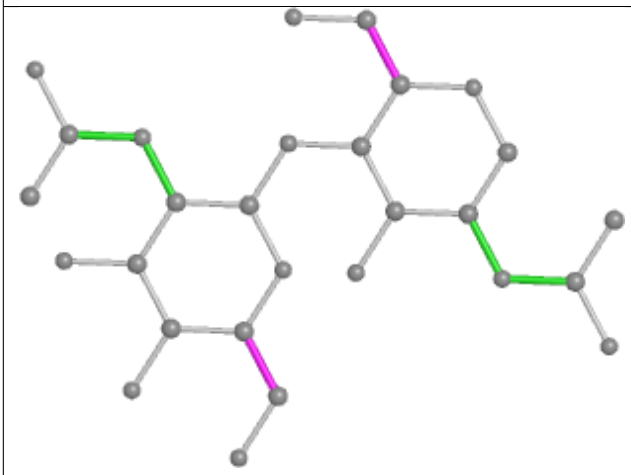
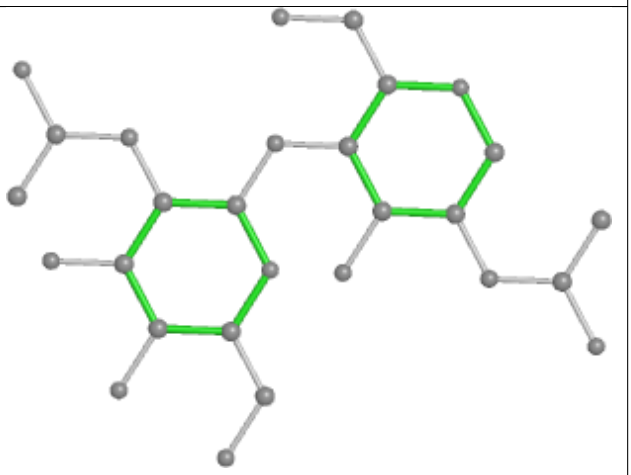
Bond angles



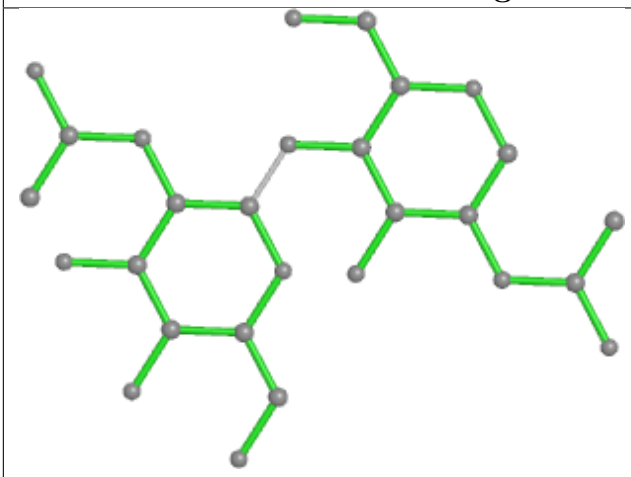
Torsions



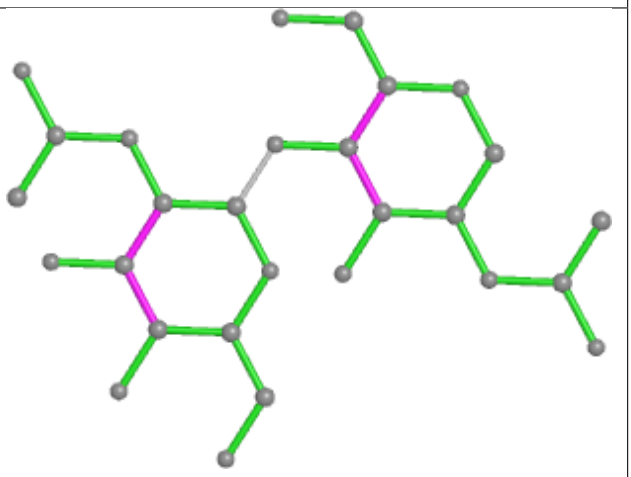
Rings

Oligosaccharide Chain T	
 Bond lengths	 Bond angles
 Torsions	 Rings

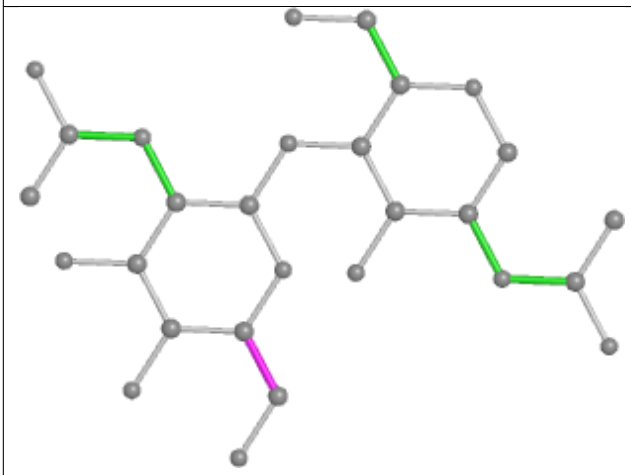
Oligosaccharide Chain U



Bond lengths



Bond angles



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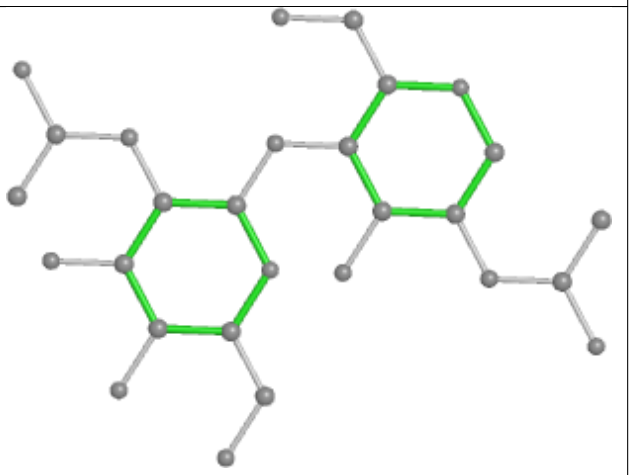
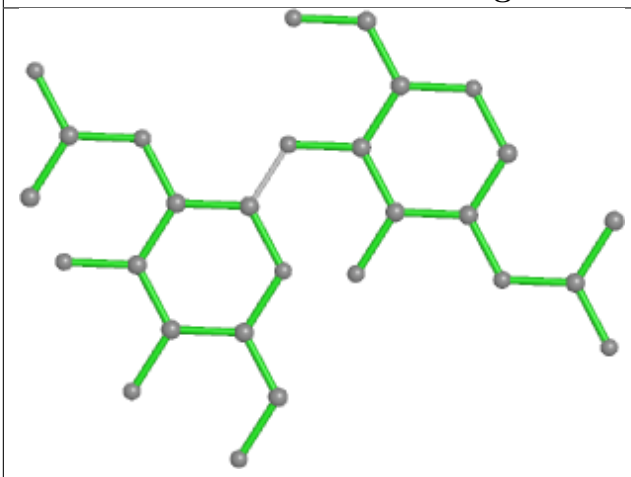


Rings

Oligosaccharide Chain V



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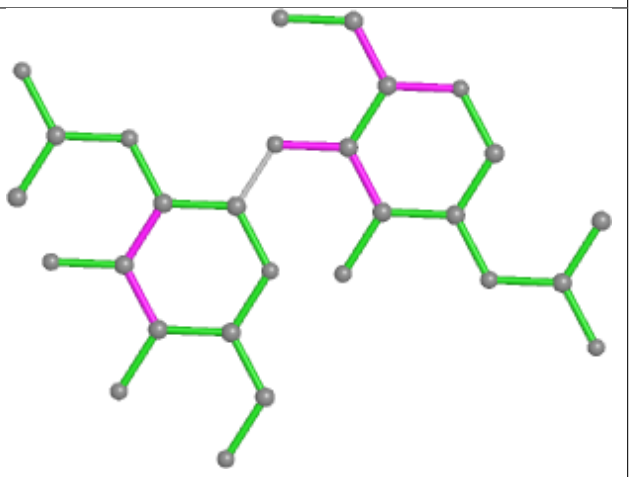
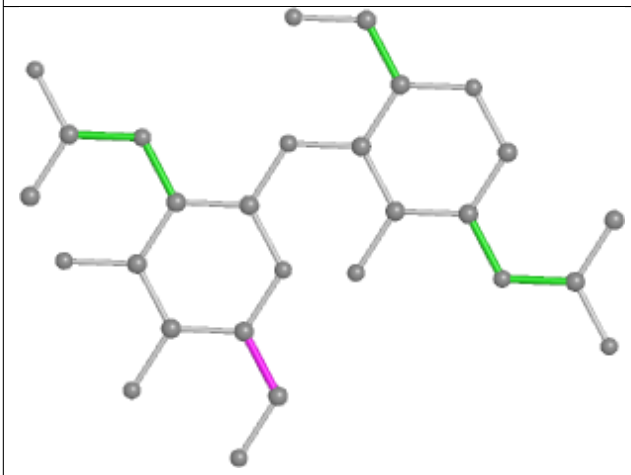


Bond angles



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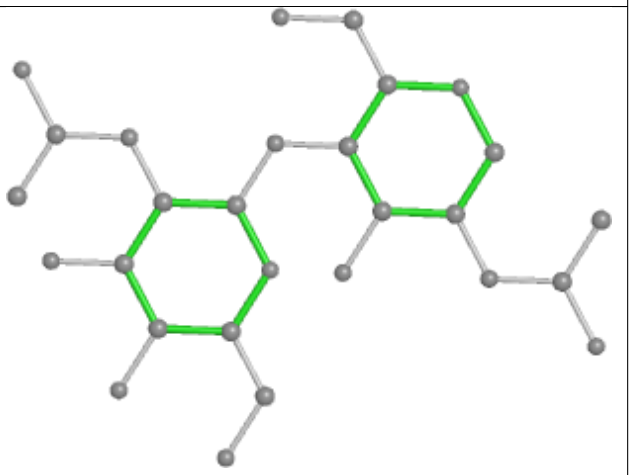
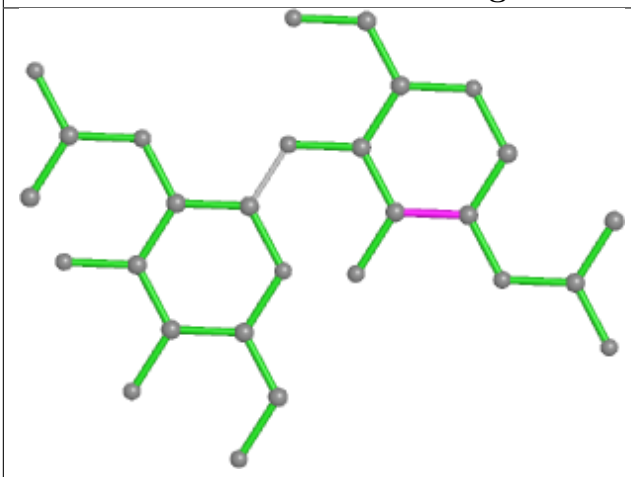
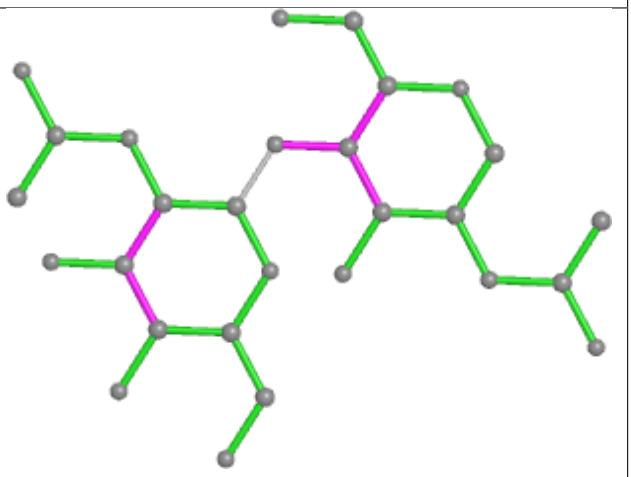
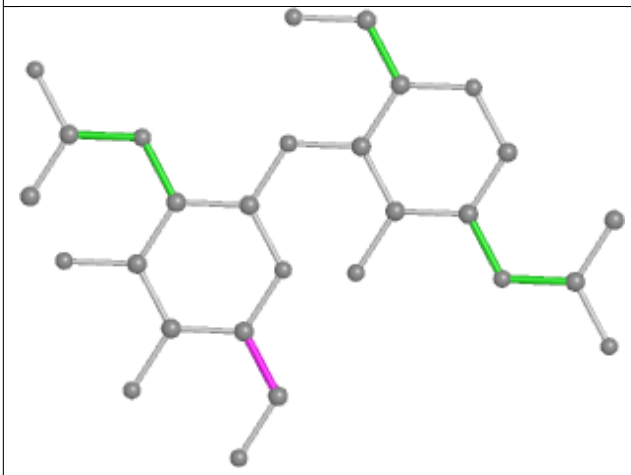
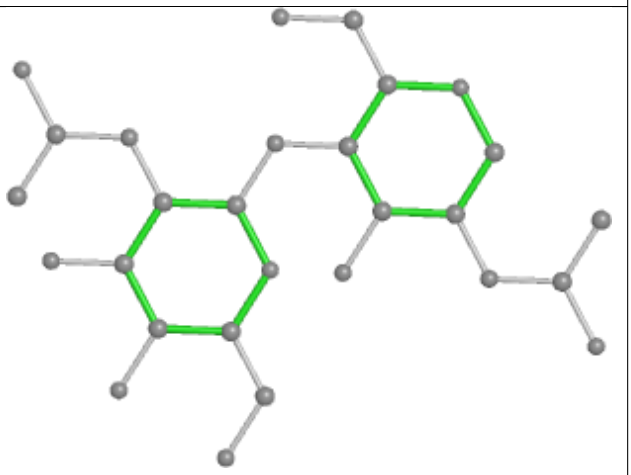
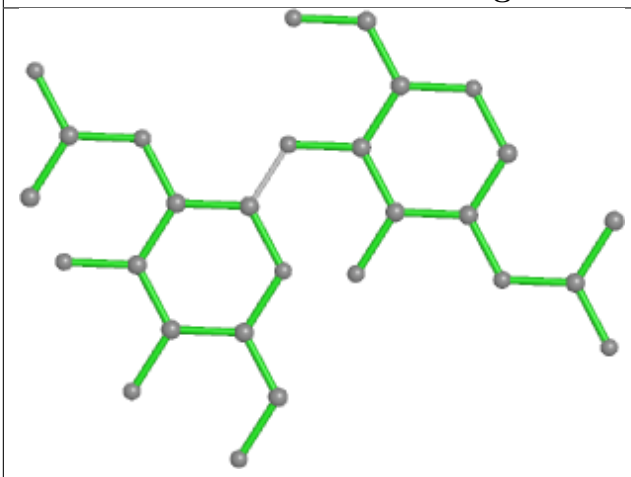


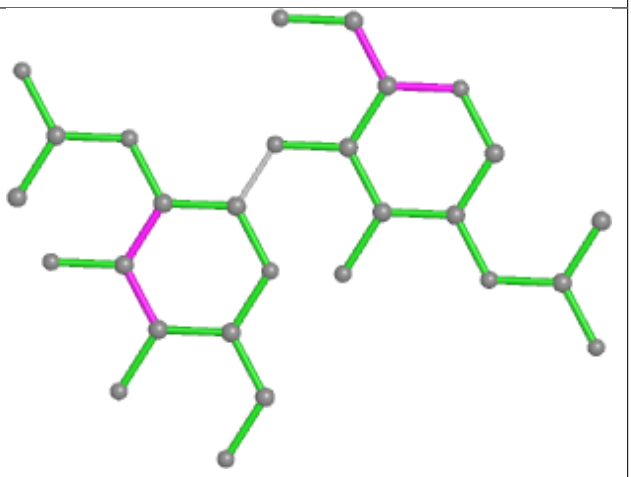
Rings

Oligosaccharide Chain W	
 Bond lengths	 Bond angles
 Torsions	 Rings

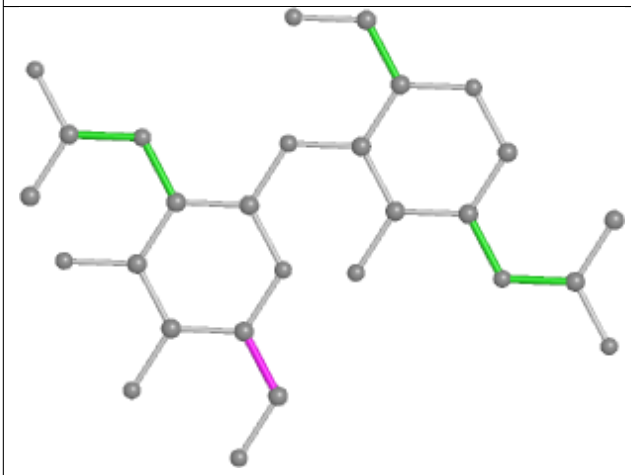
Oligosaccharide Chain Y



Bond lengths



Bond angles



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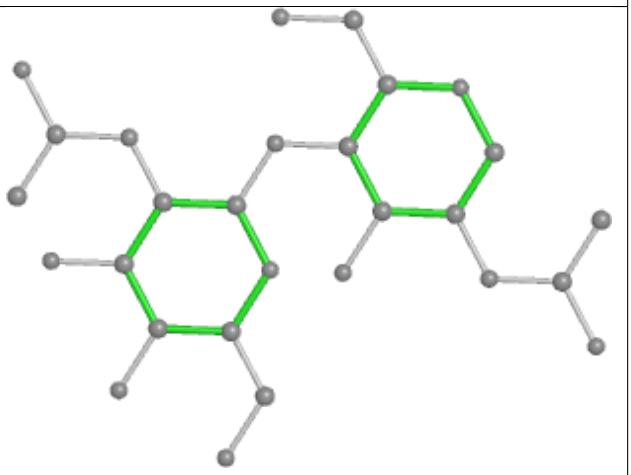
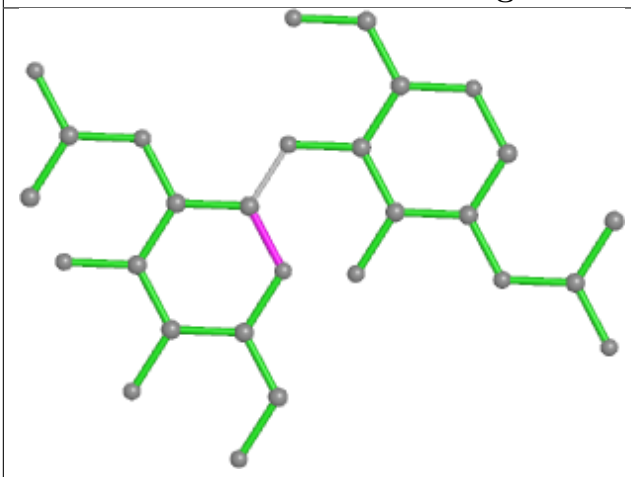


Rings

Oligosaccharide Chain Z



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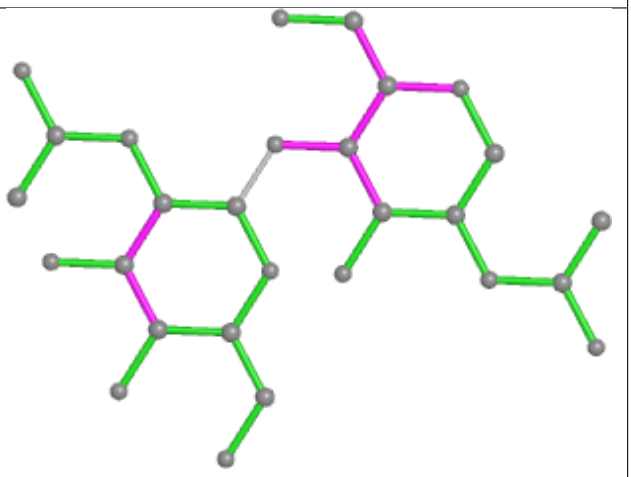
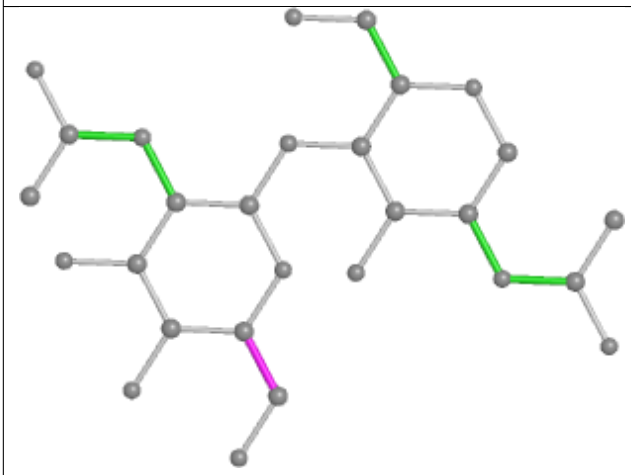


Bond angles



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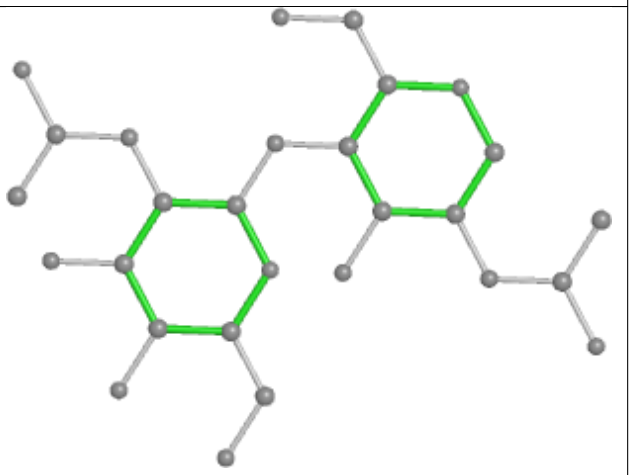
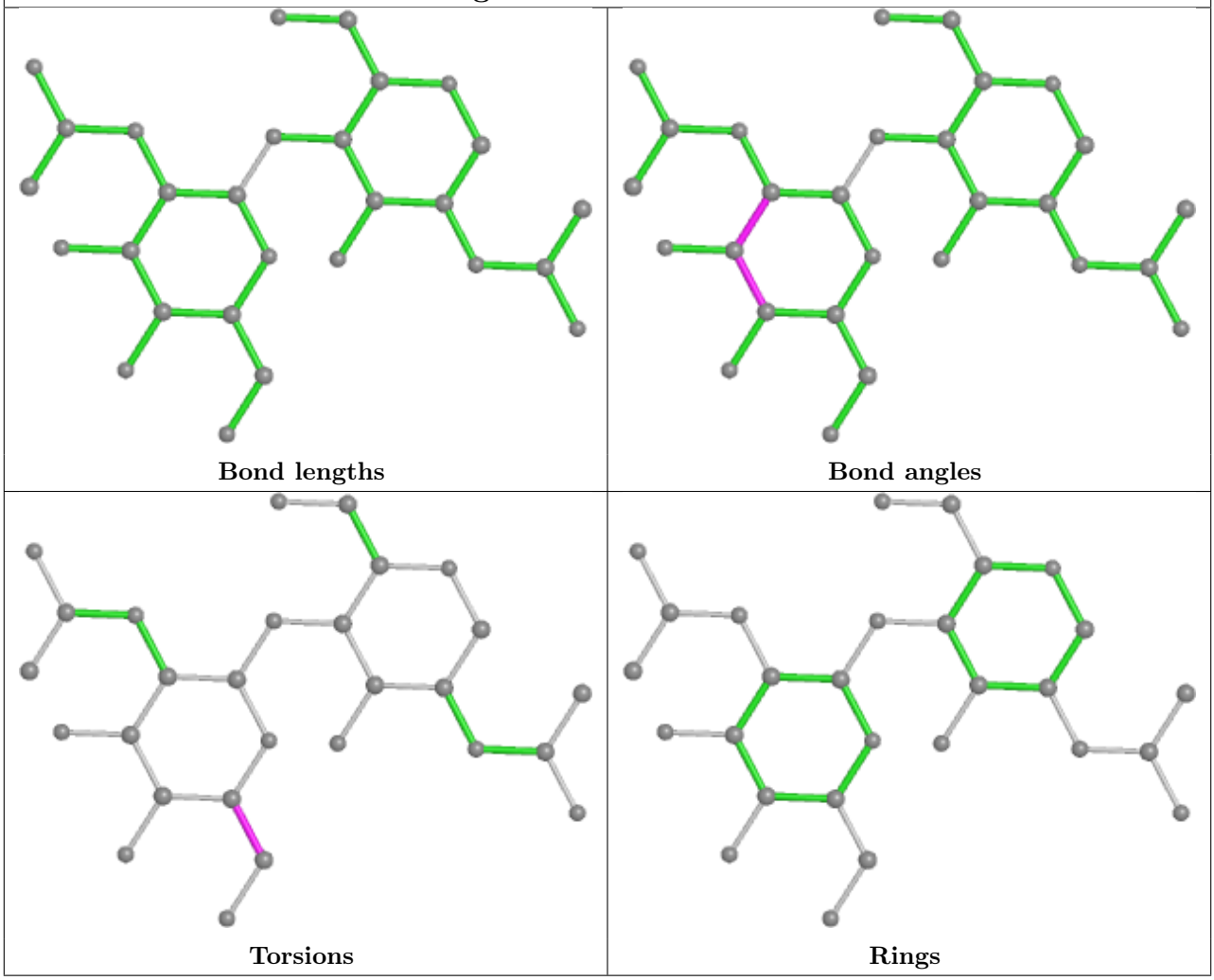
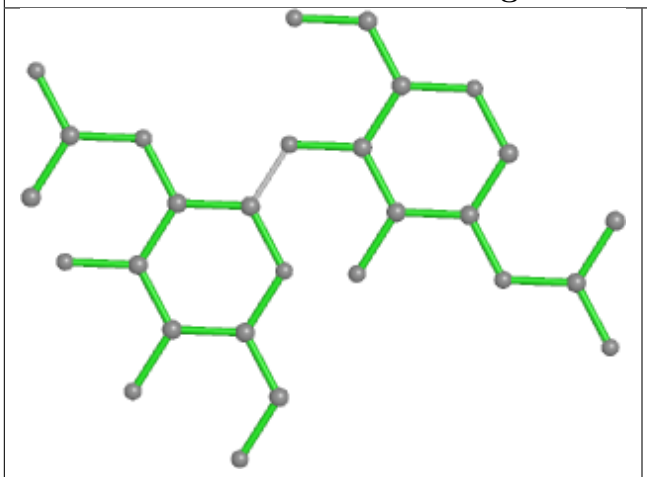


Rings

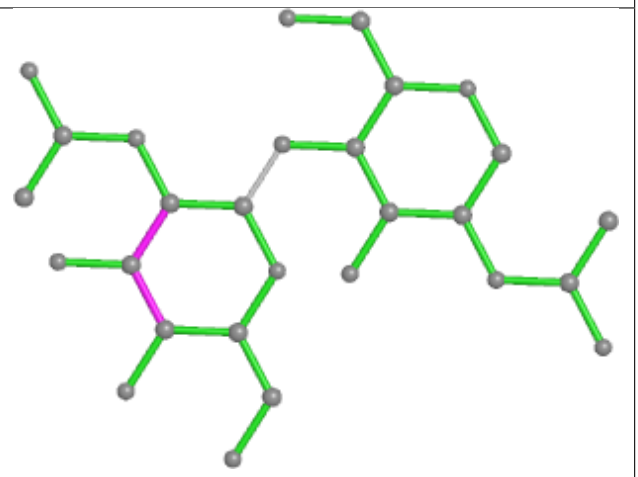
Oligosaccharide Chain a



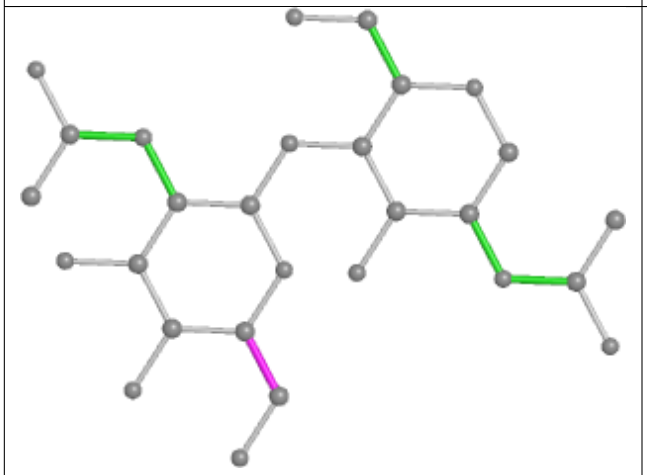
Oligosaccharide Chain c



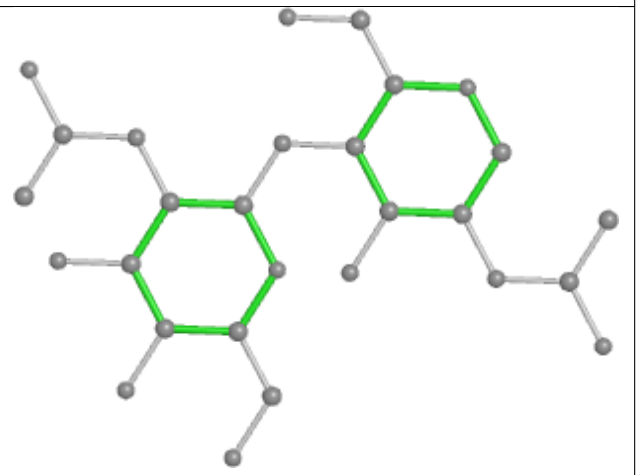
Bond lengths



Bond angles

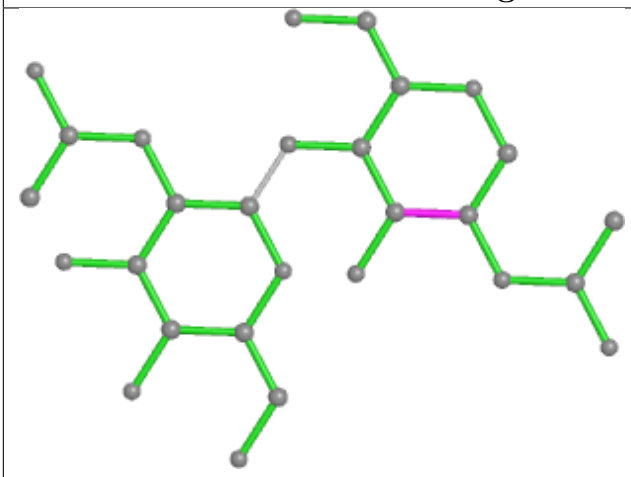


Torsions



Rings

Oligosaccharide Chain d



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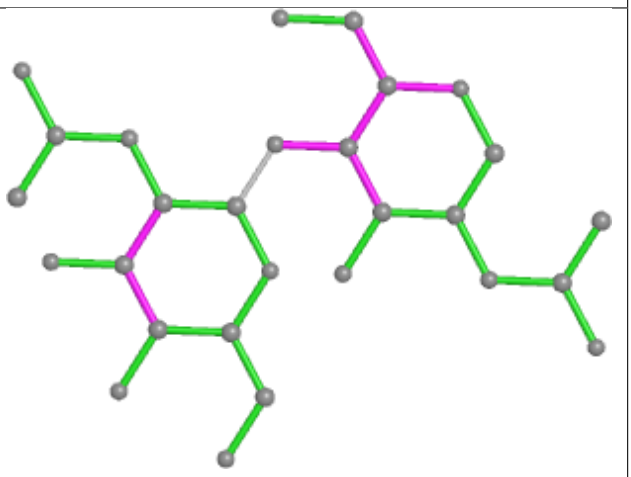

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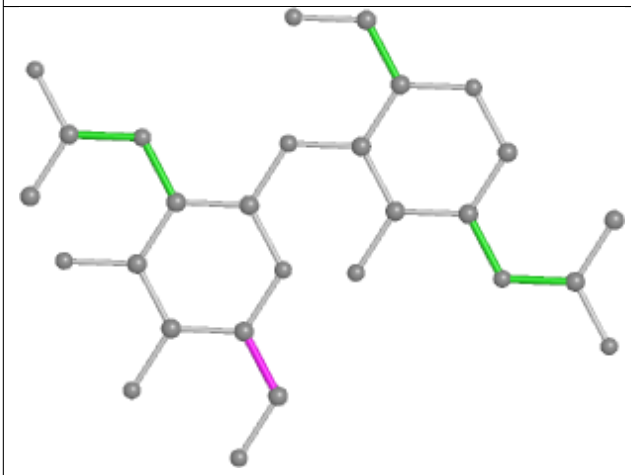

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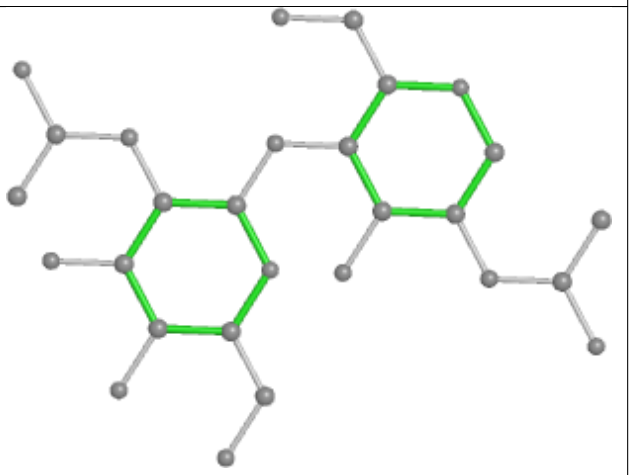
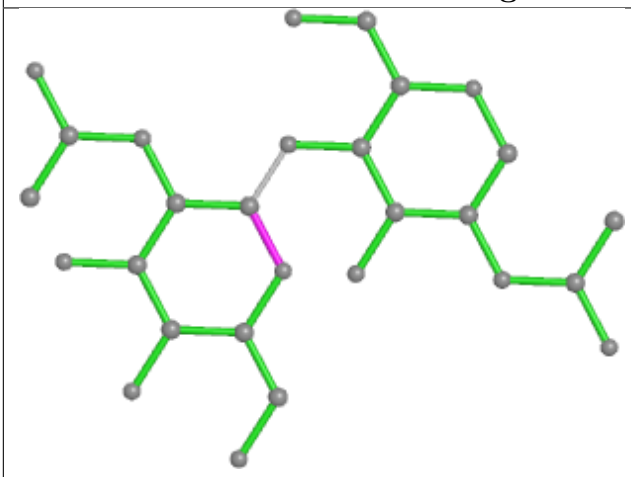


Rings

Oligosaccharide Chain e



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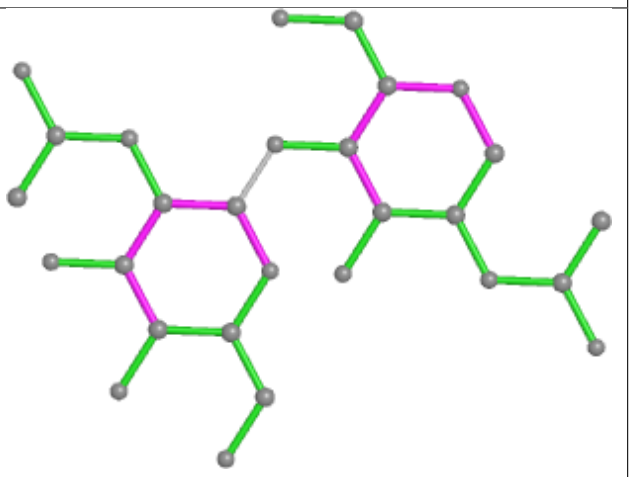

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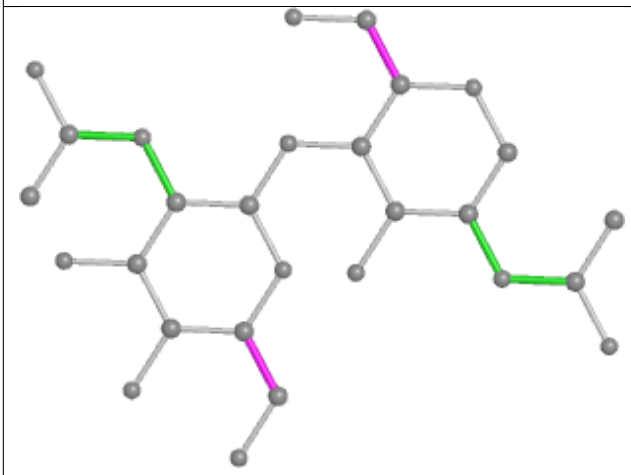

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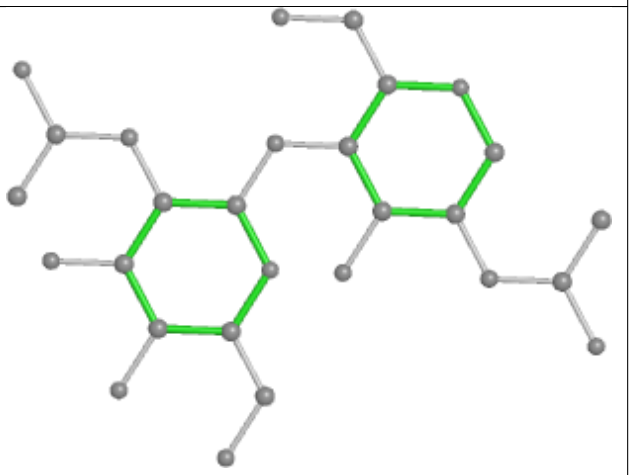

Rings

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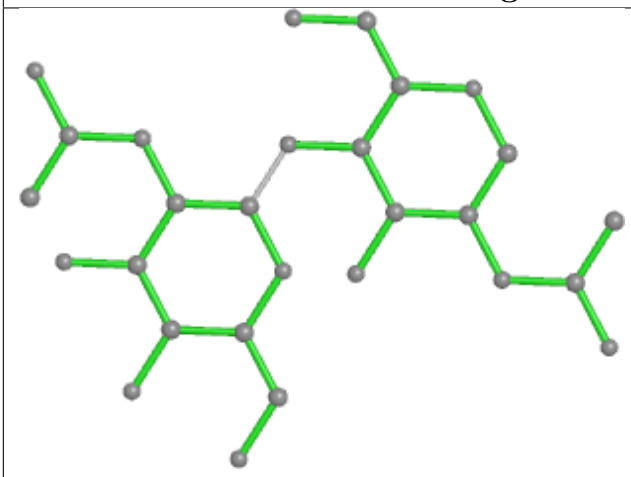
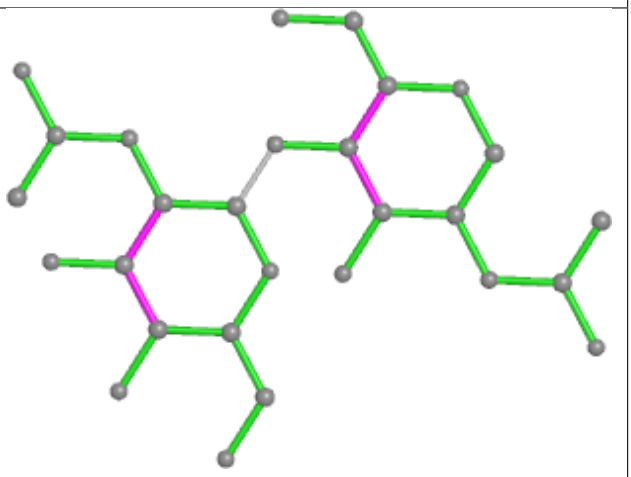
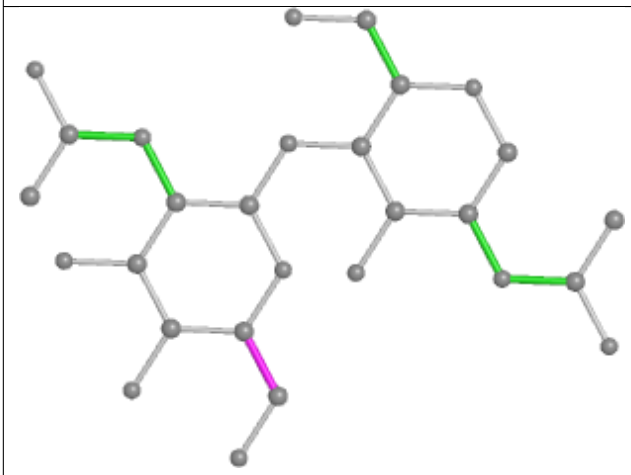
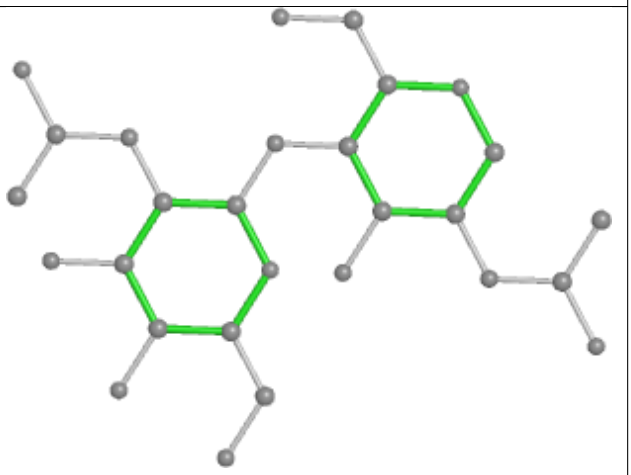
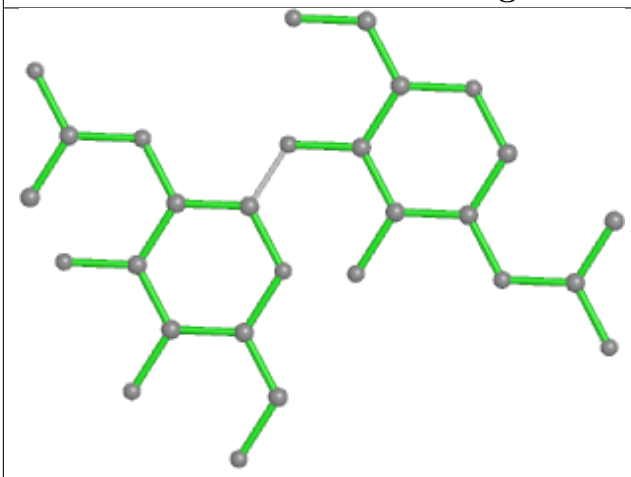
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain g



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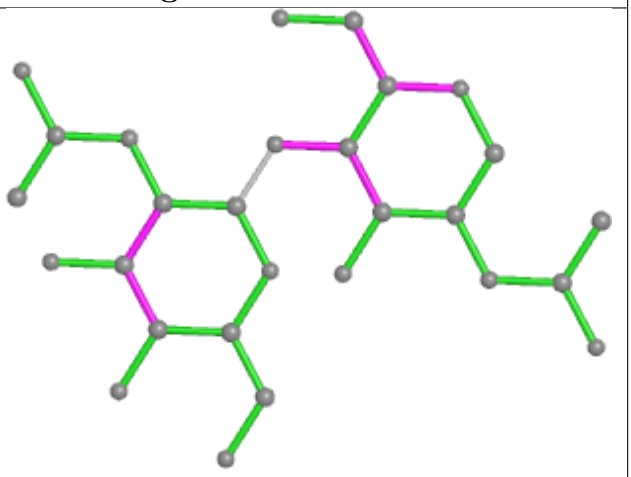

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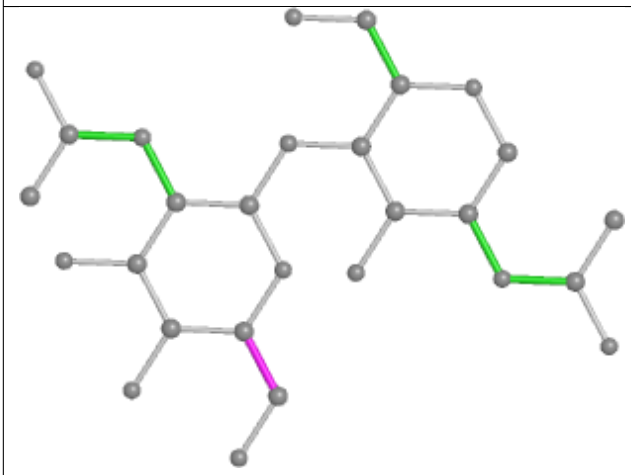
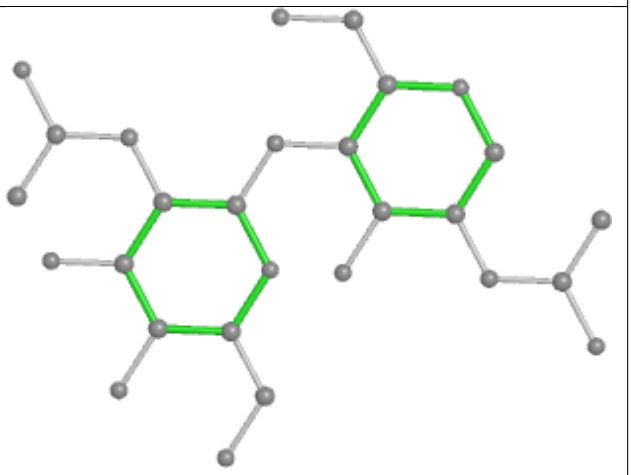
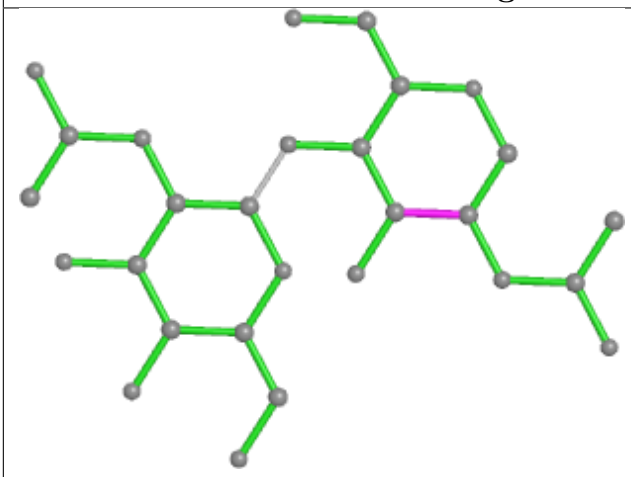
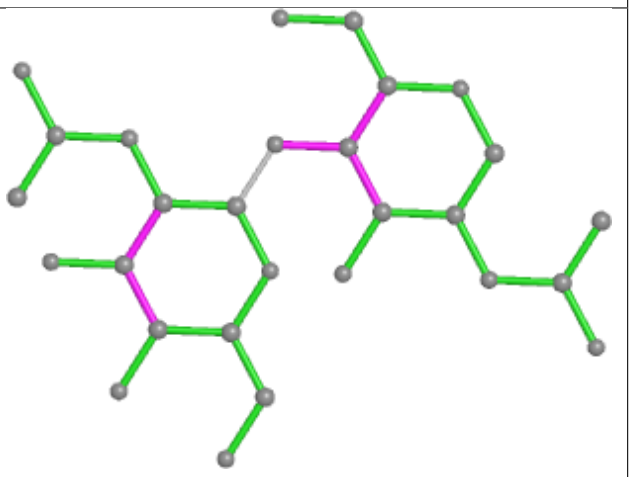
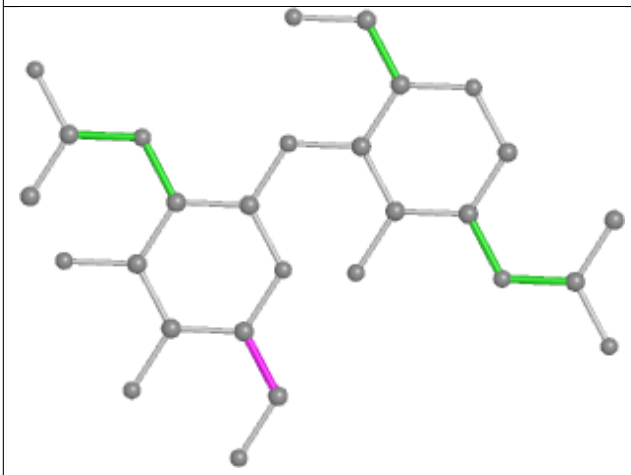
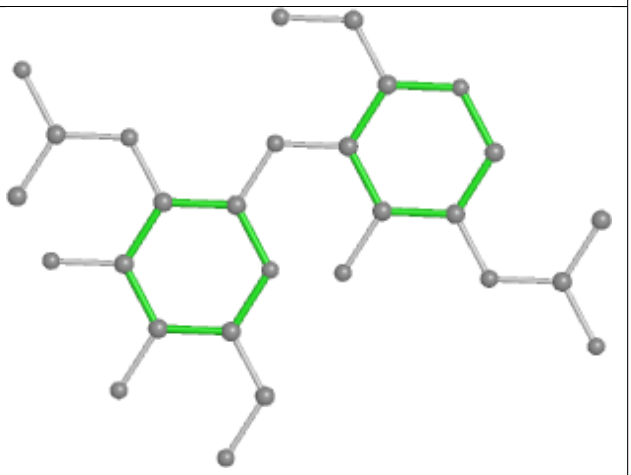


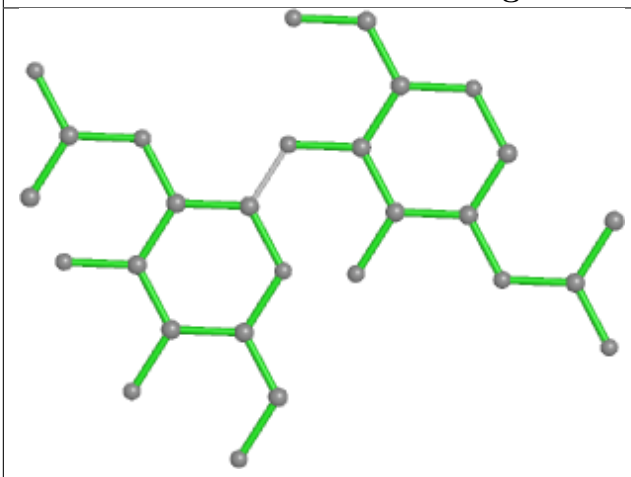
Torsions



Rings

Oligosaccharide Chain h	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain j



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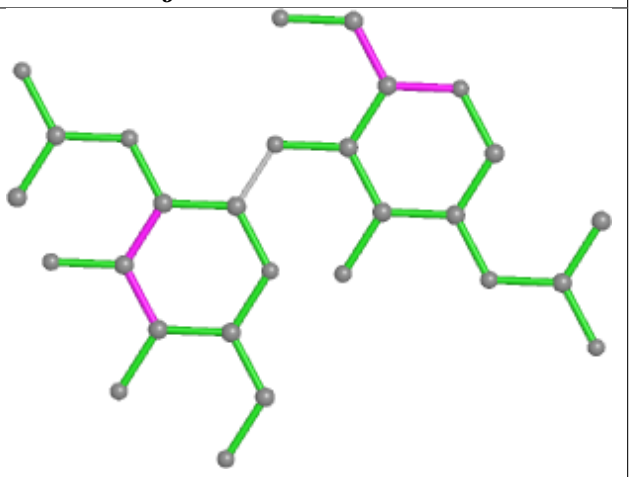
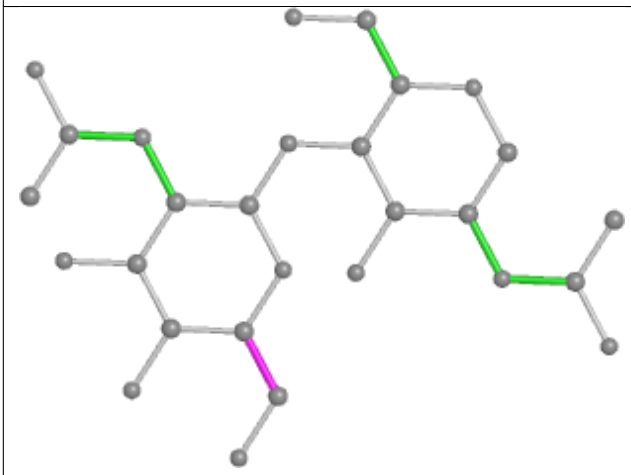


Bond angles



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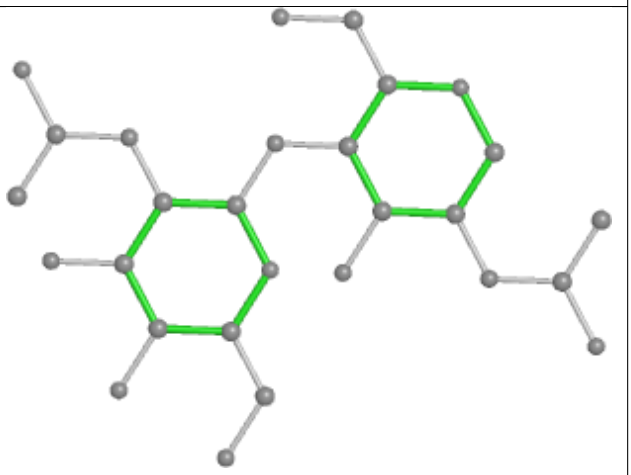
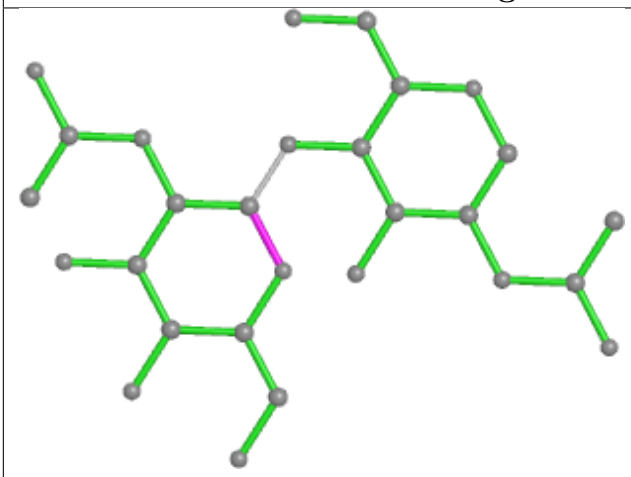


Rings

Oligosaccharide Chain k



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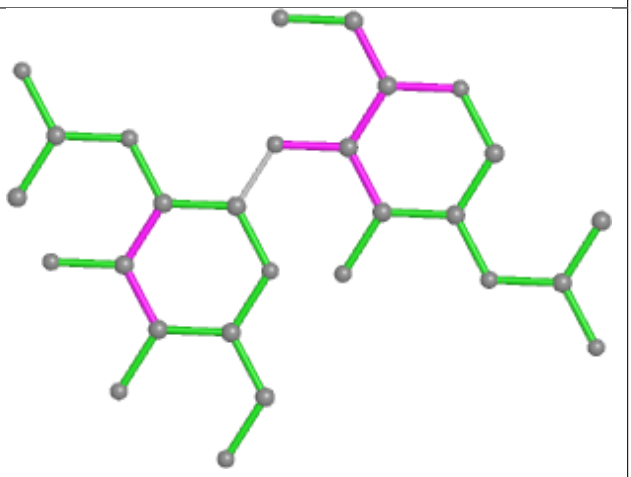

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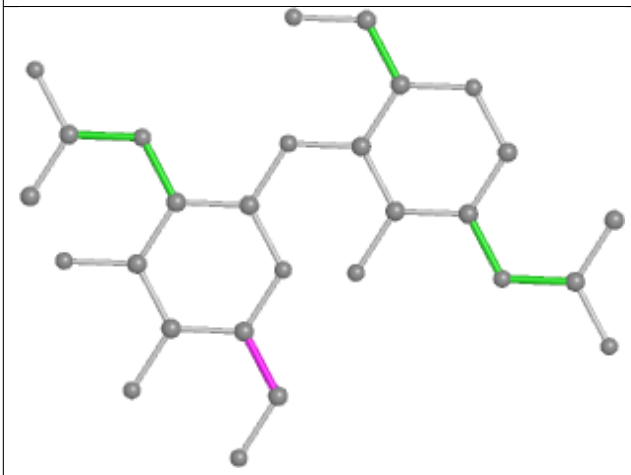

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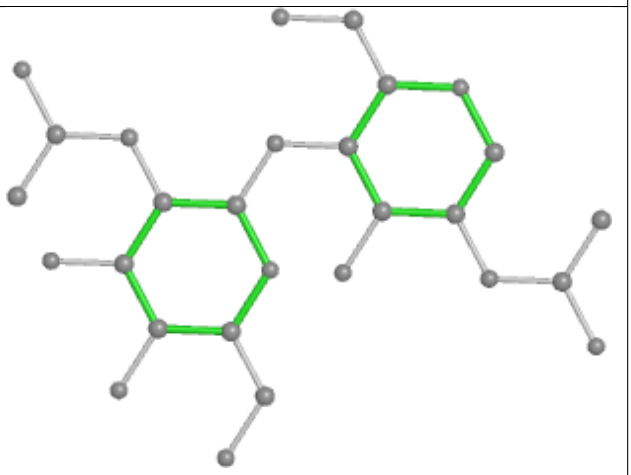
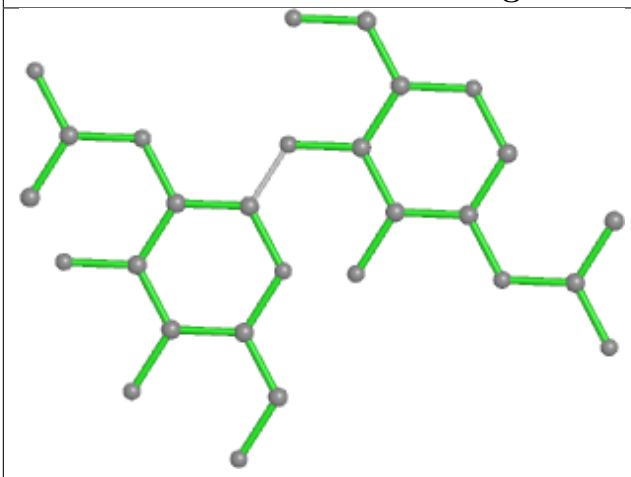


Rings

Oligosaccharide Chain l



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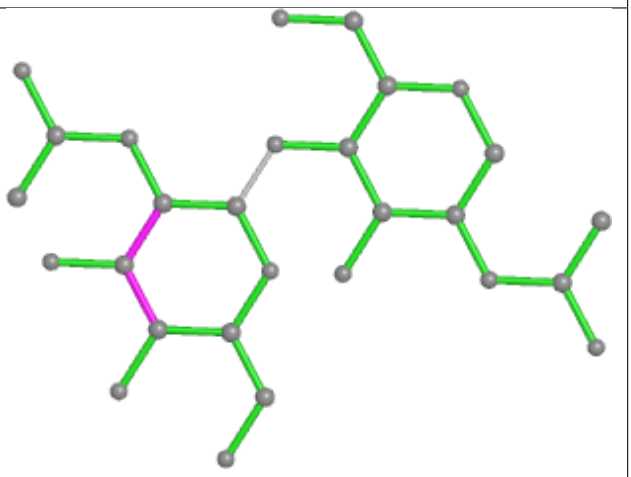
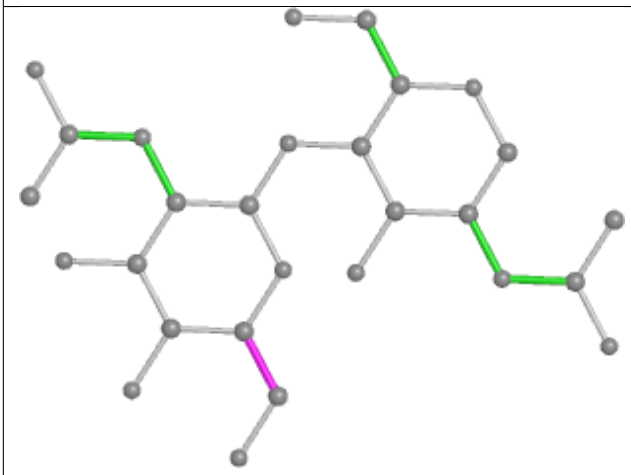


Bond angles



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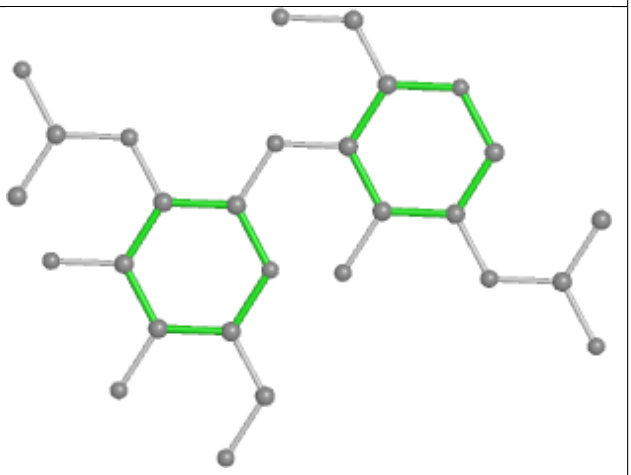

Rings

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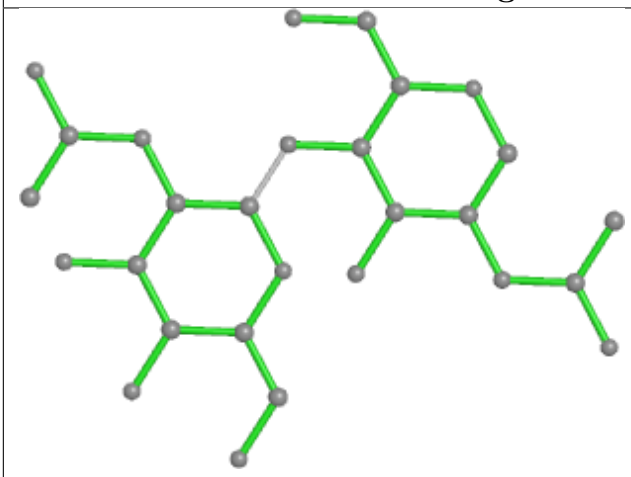
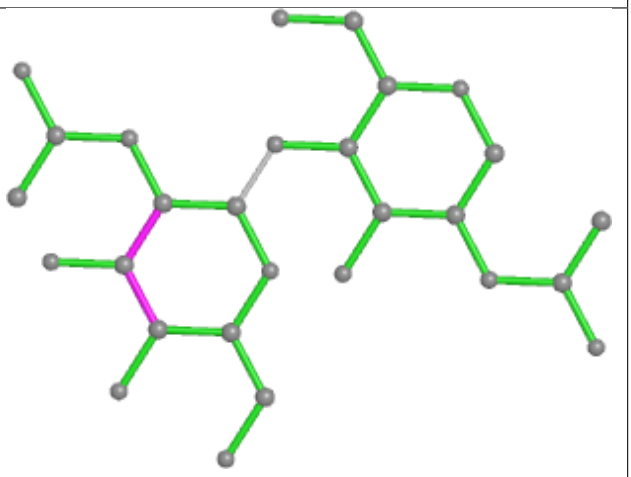
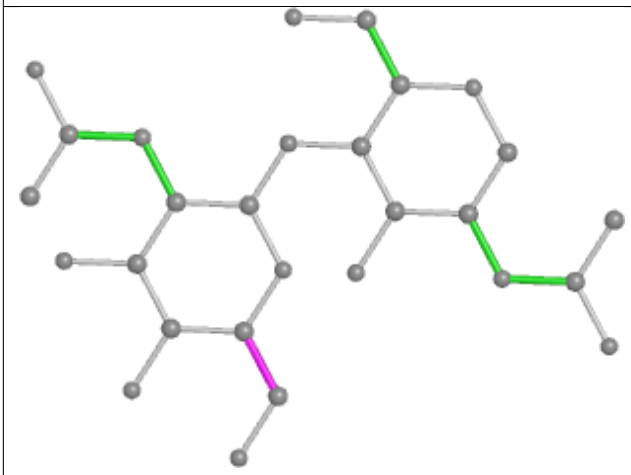
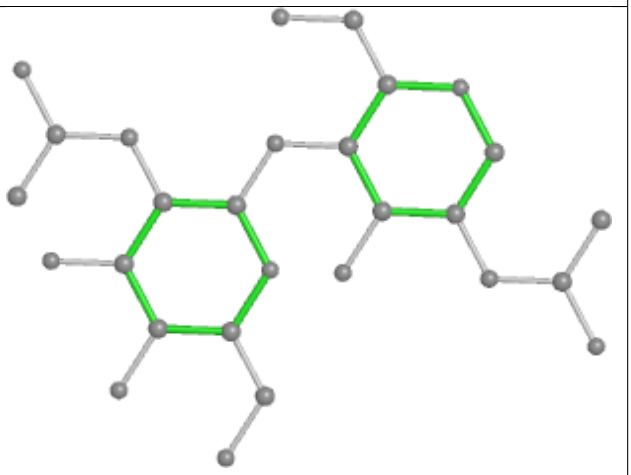
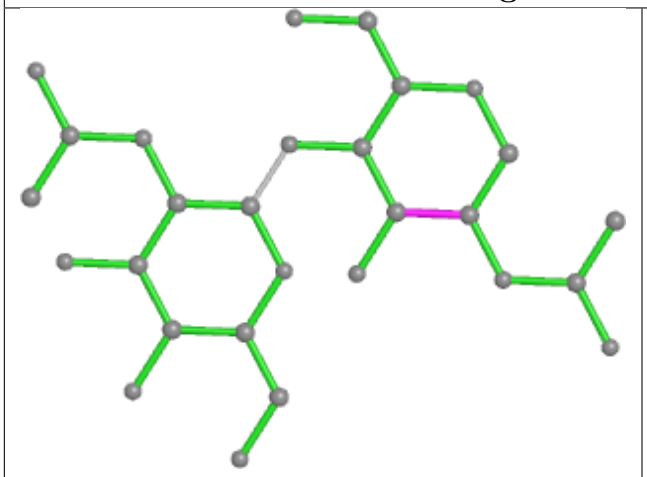
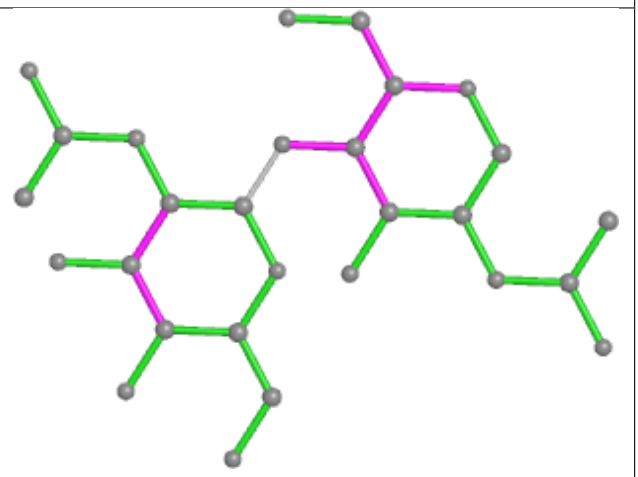
 Bond lengths	 Bond angles
 Torsions	 Rings

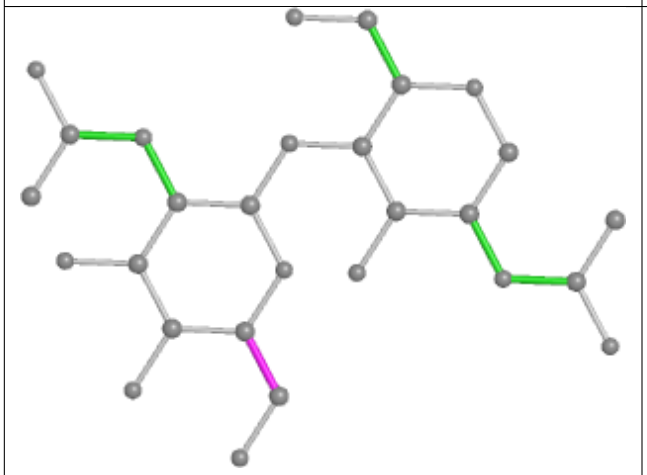
Oligosaccharide Chain o



Bond lengths



Bond angles



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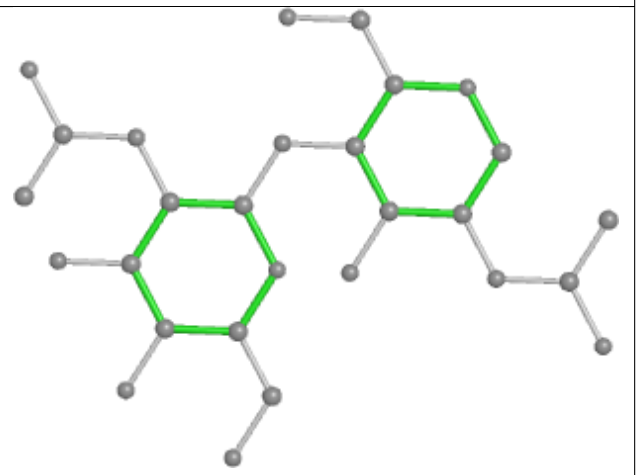
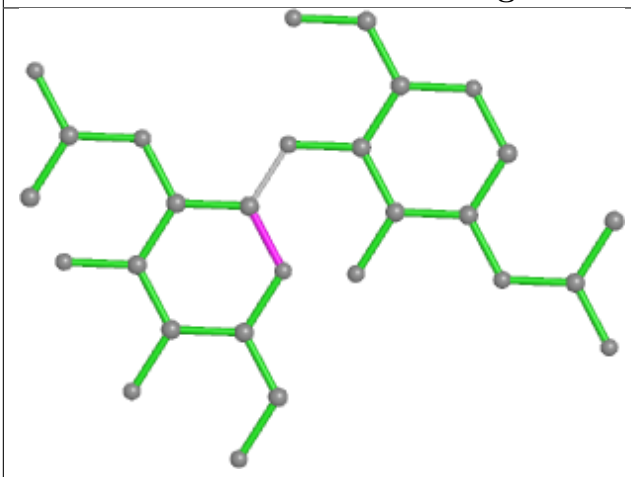


Rings

Oligosaccharide Chain p



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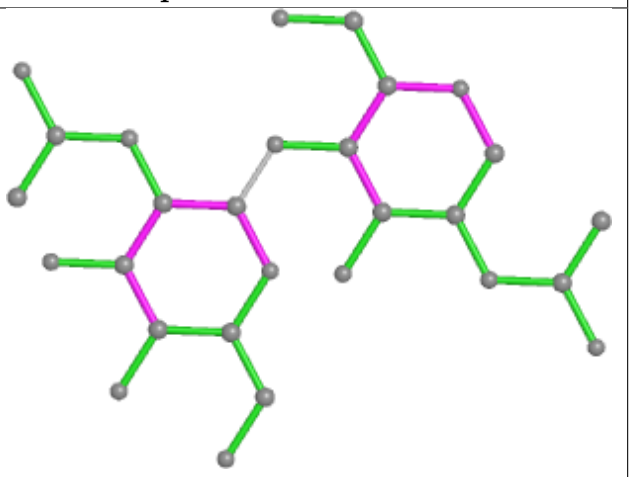

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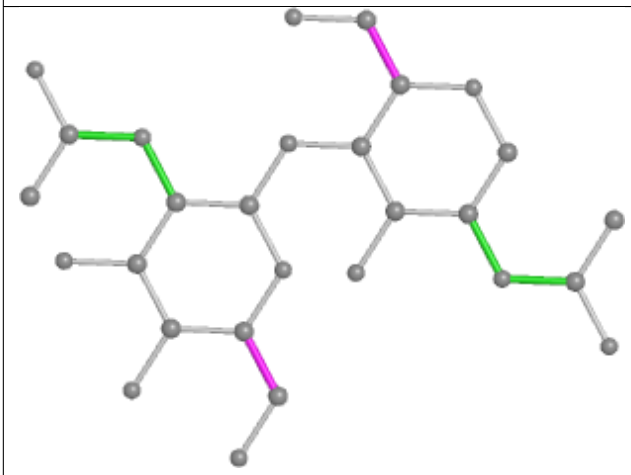

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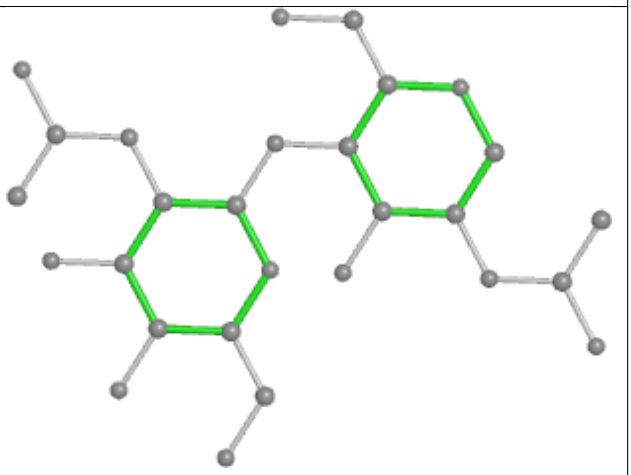

Rings

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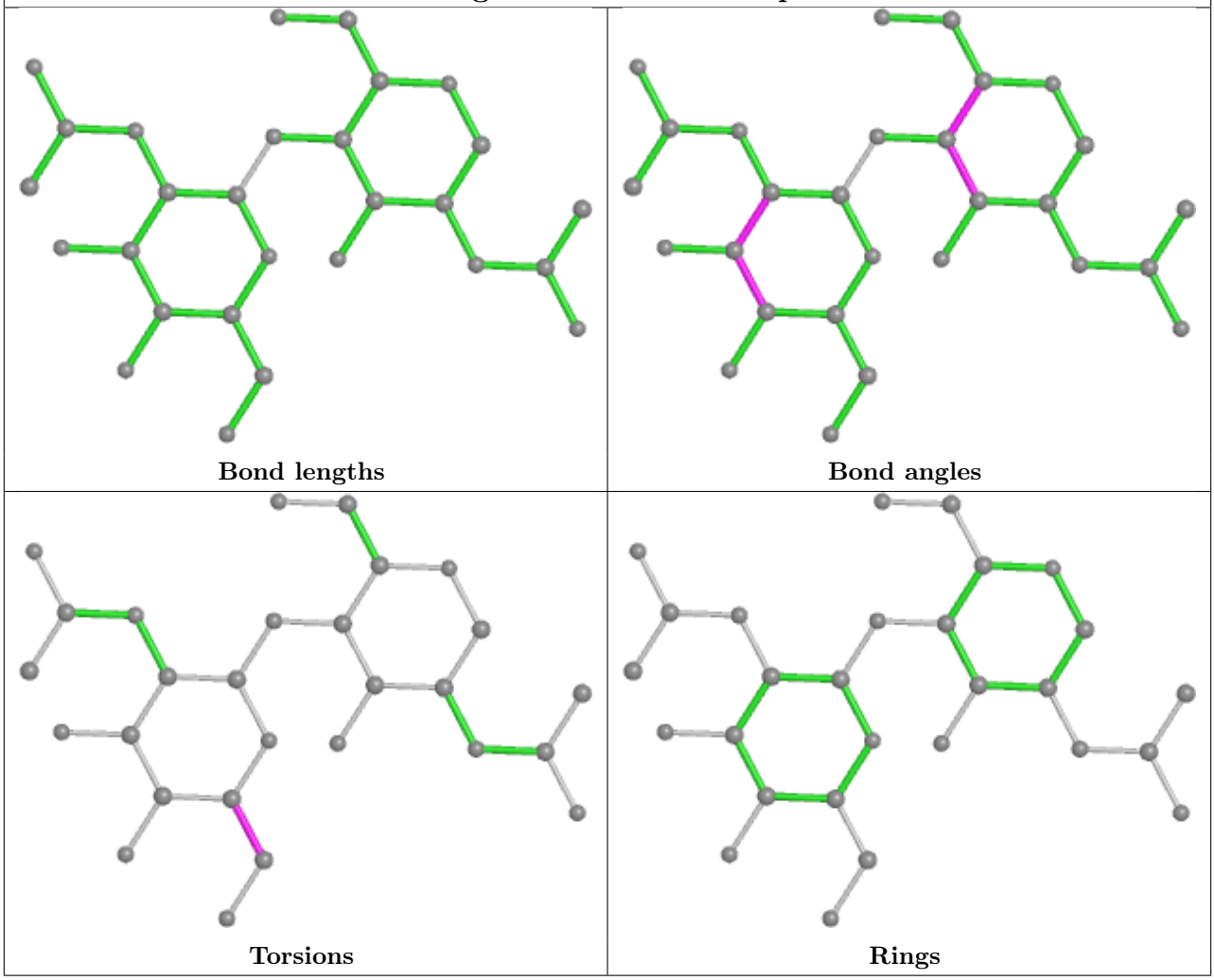
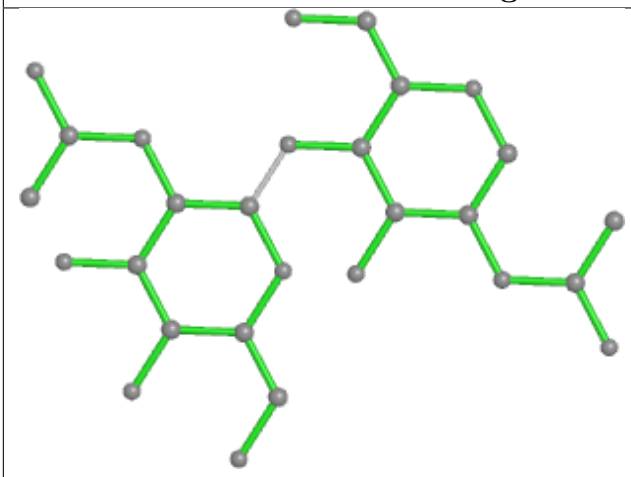
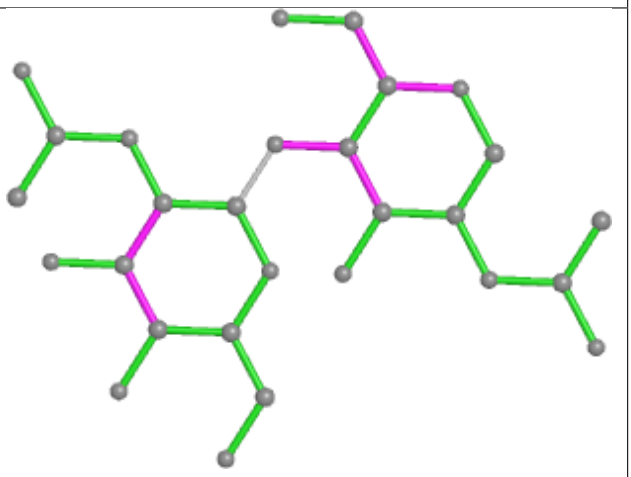


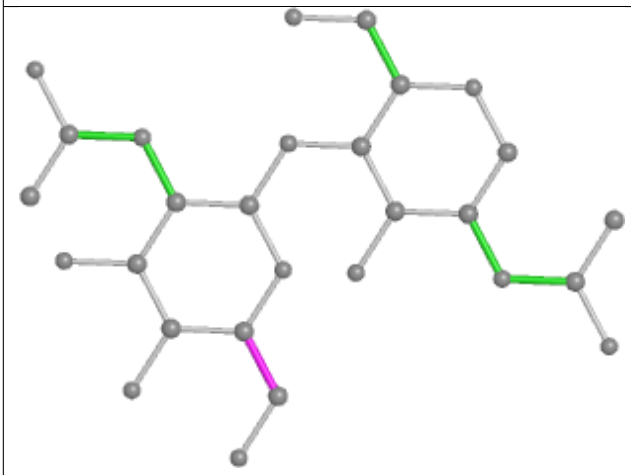
Oligosaccharide Chain r



Bond lengths



Bond angles



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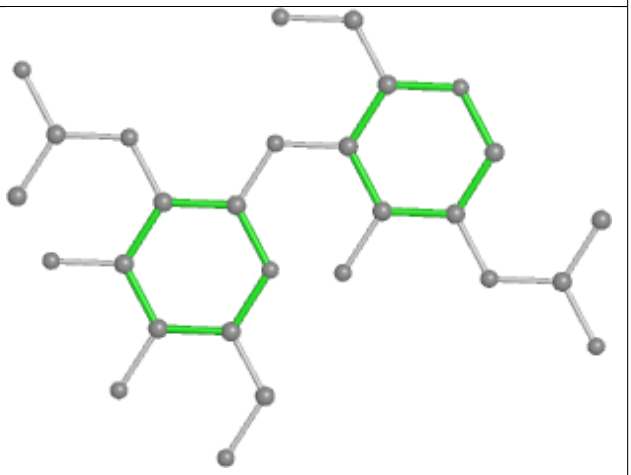
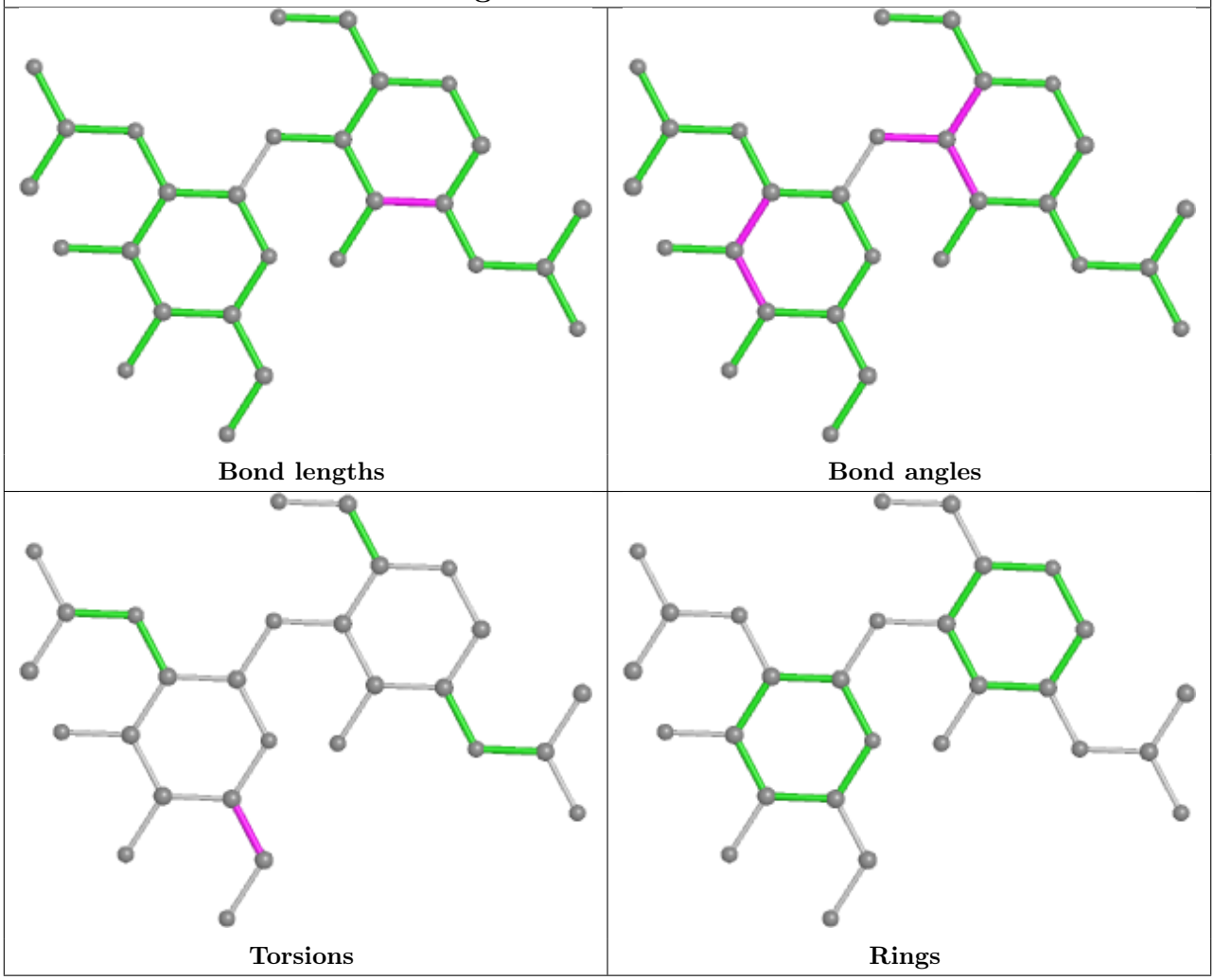


Rings

Oligosaccharide Chain s



5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
7	NAG	D	622	1	14,14,15	0.85	0	17,19,21	0.94	1 (5%)
7	NAG	E	703	2	14,14,15	0.78	0	17,19,21	1.55	3 (17%)
7	NAG	D	619	1	14,14,15	0.84	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	622	1	14,14,15	0.85	0	17,19,21	0.94	1 (5%)
7	NAG	C	622	1	14,14,15	0.85	0	17,19,21	0.94	1 (5%)
7	NAG	C	619	1	14,14,15	0.84	0	17,19,21	0.90	1 (5%)
7	NAG	F	703	2	14,14,15	0.77	0	17,19,21	1.55	3 (17%)
7	NAG	F	702	2	14,14,15	0.75	0	17,19,21	1.38	2 (11%)
7	NAG	D	632	1	14,14,15	0.84	0	17,19,21	0.98	2 (11%)
7	NAG	B	702	2	14,14,15	0.76	0	17,19,21	1.38	2 (11%)
7	NAG	F	701	2	14,14,15	0.76	0	17,19,21	1.62	2 (11%)
7	NAG	A	629	1	14,14,15	0.81	0	17,19,21	0.74	0
7	NAG	C	629	1	14,14,15	0.82	0	17,19,21	0.74	0
7	NAG	A	619	1	14,14,15	0.84	0	17,19,21	0.90	1 (5%)
7	NAG	D	629	1	14,14,15	0.81	0	17,19,21	0.74	0
7	NAG	E	701	2	14,14,15	0.76	0	17,19,21	1.61	2 (11%)
7	NAG	B	703	2	14,14,15	0.79	0	17,19,21	1.55	3 (17%)
7	NAG	A	632	1	14,14,15	0.85	0	17,19,21	0.97	2 (11%)
7	NAG	E	702	2	14,14,15	0.75	0	17,19,21	1.37	2 (11%)
7	NAG	C	632	1	14,14,15	0.85	0	17,19,21	0.97	2 (11%)
7	NAG	B	701	2	14,14,15	0.76	0	17,19,21	1.62	2 (11%)

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
7	NAG	D	622	1	-	1/6/23/26	0/1/1/1
7	NAG	E	703	2	-	2/6/23/26	0/1/1/1
7	NAG	D	619	1	-	1/6/23/26	0/1/1/1
7	NAG	A	622	1	-	1/6/23/26	0/1/1/1
7	NAG	C	622	1	-	1/6/23/26	0/1/1/1
7	NAG	C	619	1	-	1/6/23/26	0/1/1/1
7	NAG	F	703	2	-	2/6/23/26	0/1/1/1
7	NAG	F	702	2	-	2/6/23/26	0/1/1/1
7	NAG	D	632	1	-	2/6/23/26	0/1/1/1
7	NAG	B	702	2	-	2/6/23/26	0/1/1/1
7	NAG	F	701	2	-	2/6/23/26	0/1/1/1
7	NAG	A	629	1	-	1/6/23/26	0/1/1/1
7	NAG	C	629	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	619	1	-	1/6/23/26	0/1/1/1
7	NAG	D	629	1	-	1/6/23/26	0/1/1/1
7	NAG	E	701	2	-	2/6/23/26	0/1/1/1
7	NAG	B	703	2	-	2/6/23/26	0/1/1/1
7	NAG	A	632	1	-	2/6/23/26	0/1/1/1
7	NAG	E	702	2	-	2/6/23/26	0/1/1/1
7	NAG	C	632	1	-	2/6/23/26	0/1/1/1
7	NAG	B	701	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	701	NAG	C4-C3-C2	-4.95	103.76	111.02
7	F	701	NAG	C4-C3-C2	-4.95	103.76	111.02
7	E	701	NAG	C4-C3-C2	-4.93	103.79	111.02
7	B	703	NAG	C4-C3-C2	-4.79	104.00	111.02
7	F	703	NAG	C4-C3-C2	-4.79	104.00	111.02
7	E	703	NAG	C4-C3-C2	-4.78	104.01	111.02
7	F	702	NAG	C4-C3-C2	-4.23	104.82	111.02
7	B	702	NAG	C4-C3-C2	-4.23	104.82	111.02
7	E	702	NAG	C4-C3-C2	-4.21	104.85	111.02
7	A	622	NAG	C4-C3-C2	-2.89	106.79	111.02
7	D	622	NAG	C4-C3-C2	-2.89	106.79	111.02
7	C	622	NAG	C4-C3-C2	-2.86	106.82	111.02
7	A	632	NAG	C4-C3-C2	-2.63	107.16	111.02
7	D	632	NAG	C4-C3-C2	-2.63	107.16	111.02
7	C	632	NAG	C4-C3-C2	-2.62	107.19	111.02
7	D	619	NAG	C4-C3-C2	-2.61	107.20	111.02
7	C	619	NAG	C4-C3-C2	-2.60	107.20	111.02
7	A	619	NAG	C4-C3-C2	-2.60	107.21	111.02
7	F	701	NAG	C2-N2-C7	-2.55	119.28	122.90
7	B	701	NAG	C2-N2-C7	-2.53	119.30	122.90
7	E	701	NAG	C2-N2-C7	-2.53	119.30	122.90
7	F	703	NAG	C1-O5-C5	-2.47	108.85	112.19
7	E	703	NAG	C1-O5-C5	-2.46	108.86	112.19
7	B	703	NAG	C1-O5-C5	-2.46	108.86	112.19
7	B	703	NAG	C2-N2-C7	2.35	126.25	122.90
7	F	703	NAG	C2-N2-C7	2.34	126.23	122.90
7	E	703	NAG	C2-N2-C7	2.32	126.20	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	632	NAG	O5-C1-C2	-2.14	107.90	111.29
7	C	632	NAG	O5-C1-C2	-2.14	107.92	111.29
7	A	632	NAG	O5-C1-C2	-2.13	107.92	111.29
7	E	702	NAG	C2-N2-C7	-2.05	119.99	122.90
7	F	702	NAG	C2-N2-C7	-2.05	119.99	122.90
7	B	702	NAG	C2-N2-C7	-2.04	120.00	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	701	NAG	O5-C5-C6-O6
7	E	701	NAG	O5-C5-C6-O6
7	F	701	NAG	O5-C5-C6-O6
7	A	632	NAG	O5-C5-C6-O6
7	C	632	NAG	O5-C5-C6-O6
7	D	632	NAG	O5-C5-C6-O6
7	A	622	NAG	O5-C5-C6-O6
7	B	702	NAG	O5-C5-C6-O6
7	C	622	NAG	O5-C5-C6-O6
7	E	702	NAG	O5-C5-C6-O6
7	D	622	NAG	O5-C5-C6-O6
7	F	702	NAG	O5-C5-C6-O6
7	A	629	NAG	O5-C5-C6-O6
7	C	629	NAG	O5-C5-C6-O6
7	D	629	NAG	O5-C5-C6-O6
7	B	703	NAG	C1-C2-N2-C7
7	E	703	NAG	C1-C2-N2-C7
7	F	703	NAG	C1-C2-N2-C7
7	A	619	NAG	O5-C5-C6-O6
7	C	619	NAG	O5-C5-C6-O6
7	D	619	NAG	O5-C5-C6-O6
7	B	703	NAG	O5-C5-C6-O6
7	E	703	NAG	O5-C5-C6-O6
7	F	703	NAG	O5-C5-C6-O6
7	B	701	NAG	C4-C5-C6-O6
7	E	701	NAG	C4-C5-C6-O6
7	F	701	NAG	C4-C5-C6-O6
7	A	632	NAG	C4-C5-C6-O6
7	C	632	NAG	C4-C5-C6-O6
7	D	632	NAG	C4-C5-C6-O6
7	B	702	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	E	702	NAG	C4-C5-C6-O6
7	F	702	NAG	C4-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.

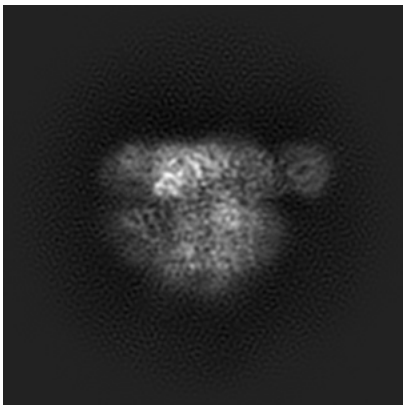
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21246. These allow visual inspection of the internal detail of the map and identification of artifacts.

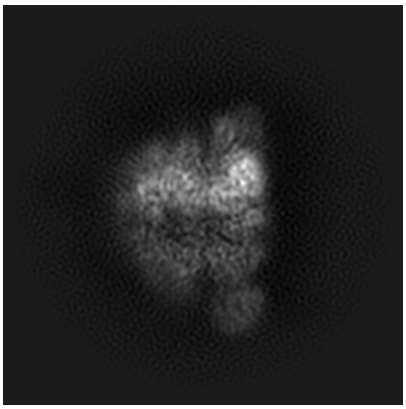
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

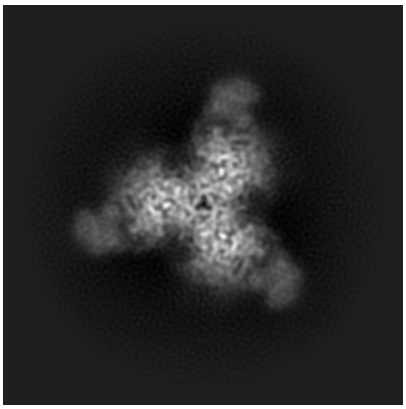
6.1.1 Primary map



X

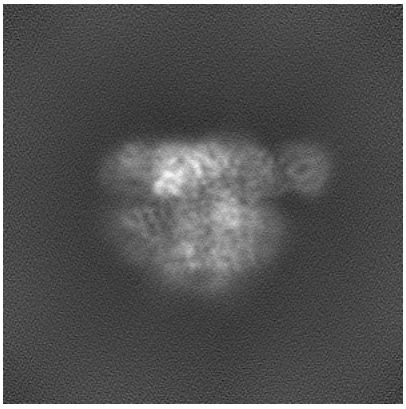


Y

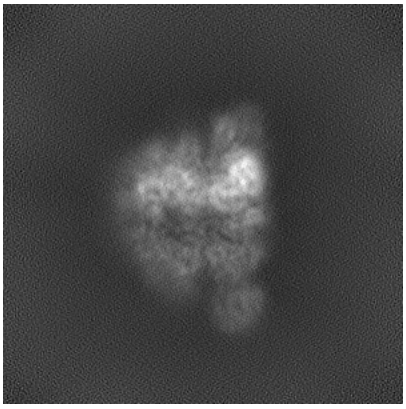


Z

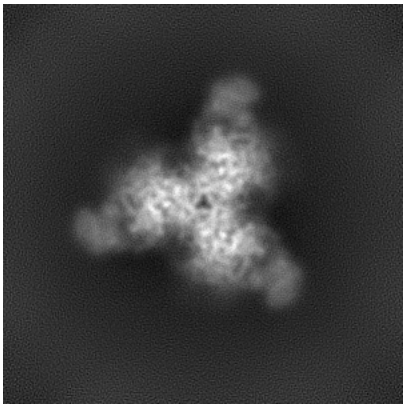
6.1.2 Raw map



X



Y

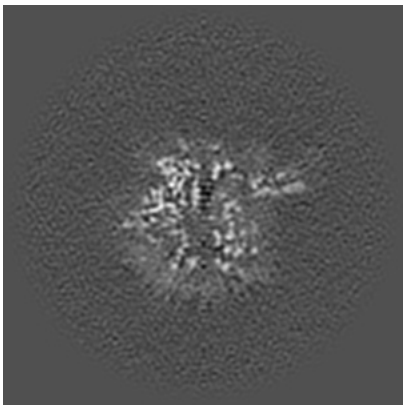


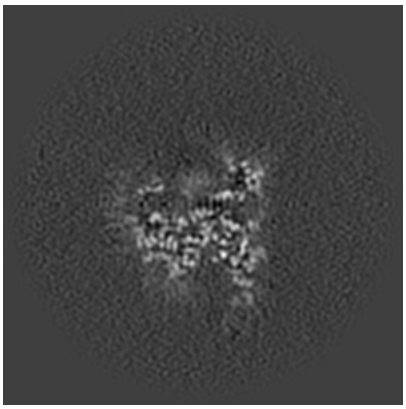
Z

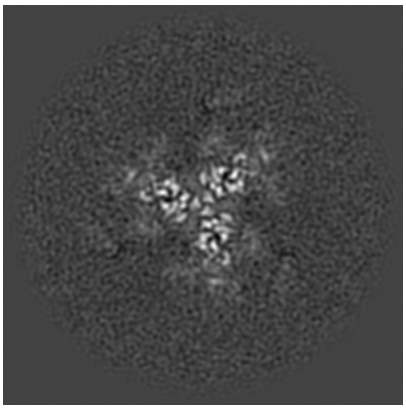
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

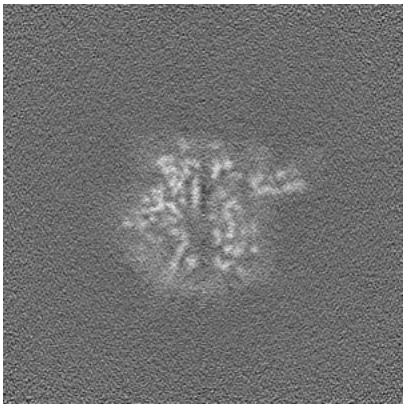
6.2.1 Primary map

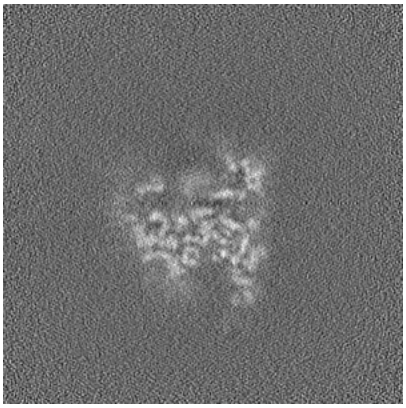

X Index: 150

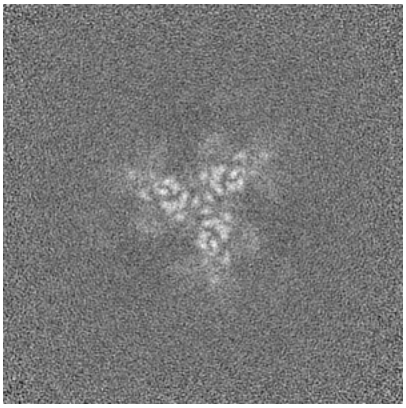

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

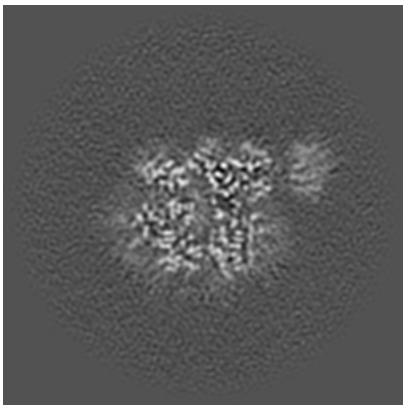

Y Index: 150

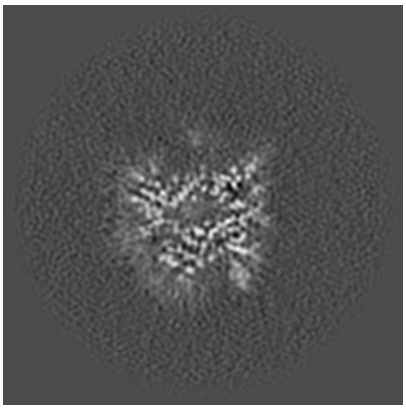

Z Index: 150

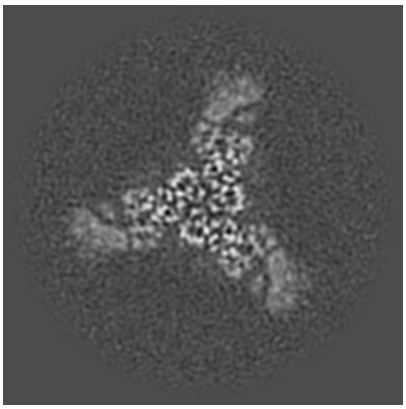
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

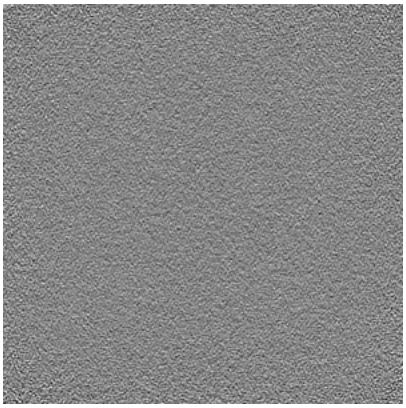
6.3.1 Primary map

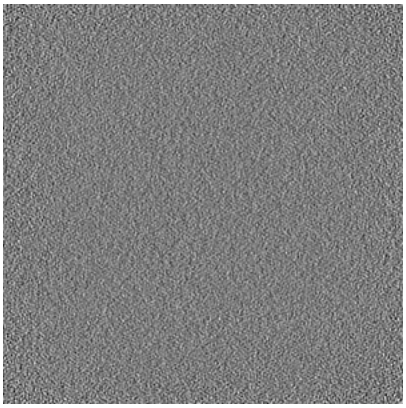

X Index: 165

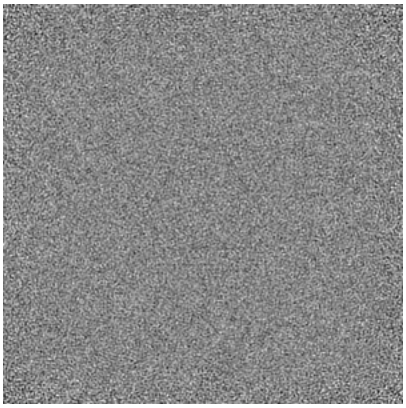

Y Index: 160


Z Index: 172

6.3.2 Raw map


X Index: 0

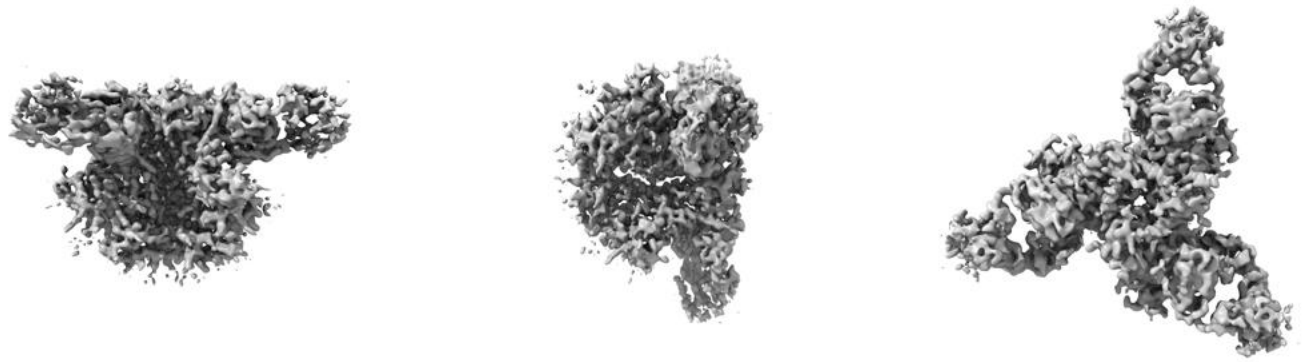

Y Index: 0


Z Index: 0

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

6.4 Orthogonal surface views (i)

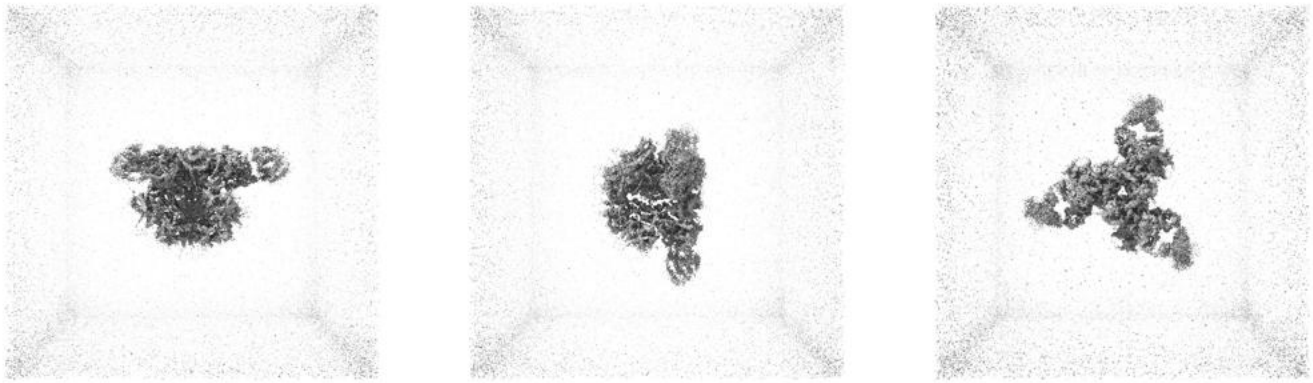
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.31. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

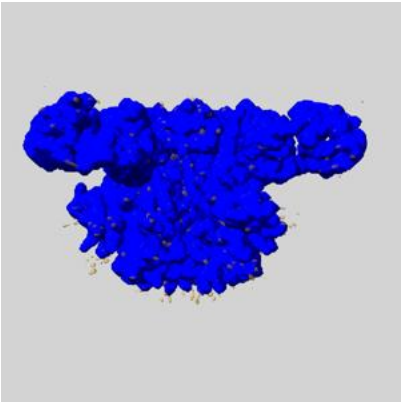
6.5 Mask visualisation (i)

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

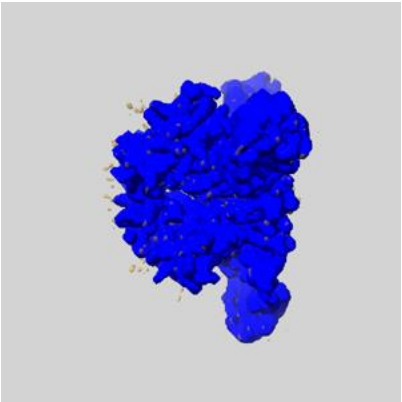
A mask typically either:

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

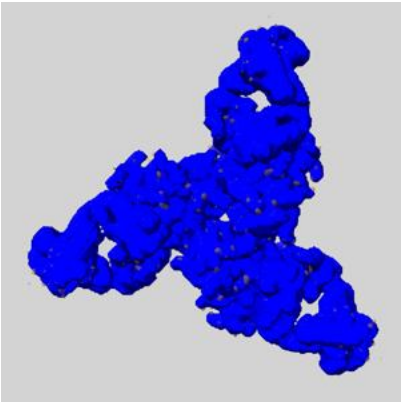
6.5.1 emd_21246_msk_1.map (i)



X



Y

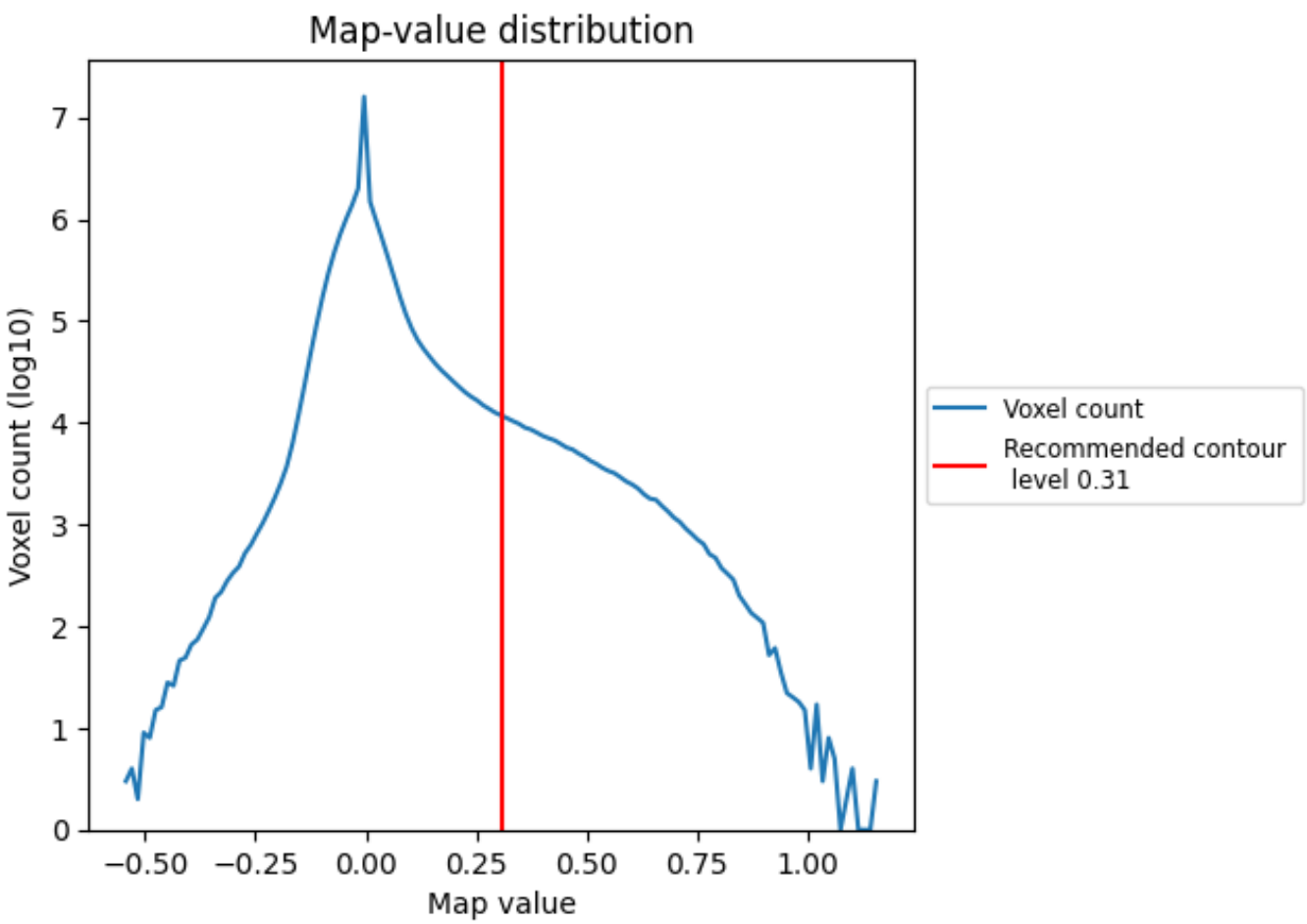


Z

7 Map analysis (i)

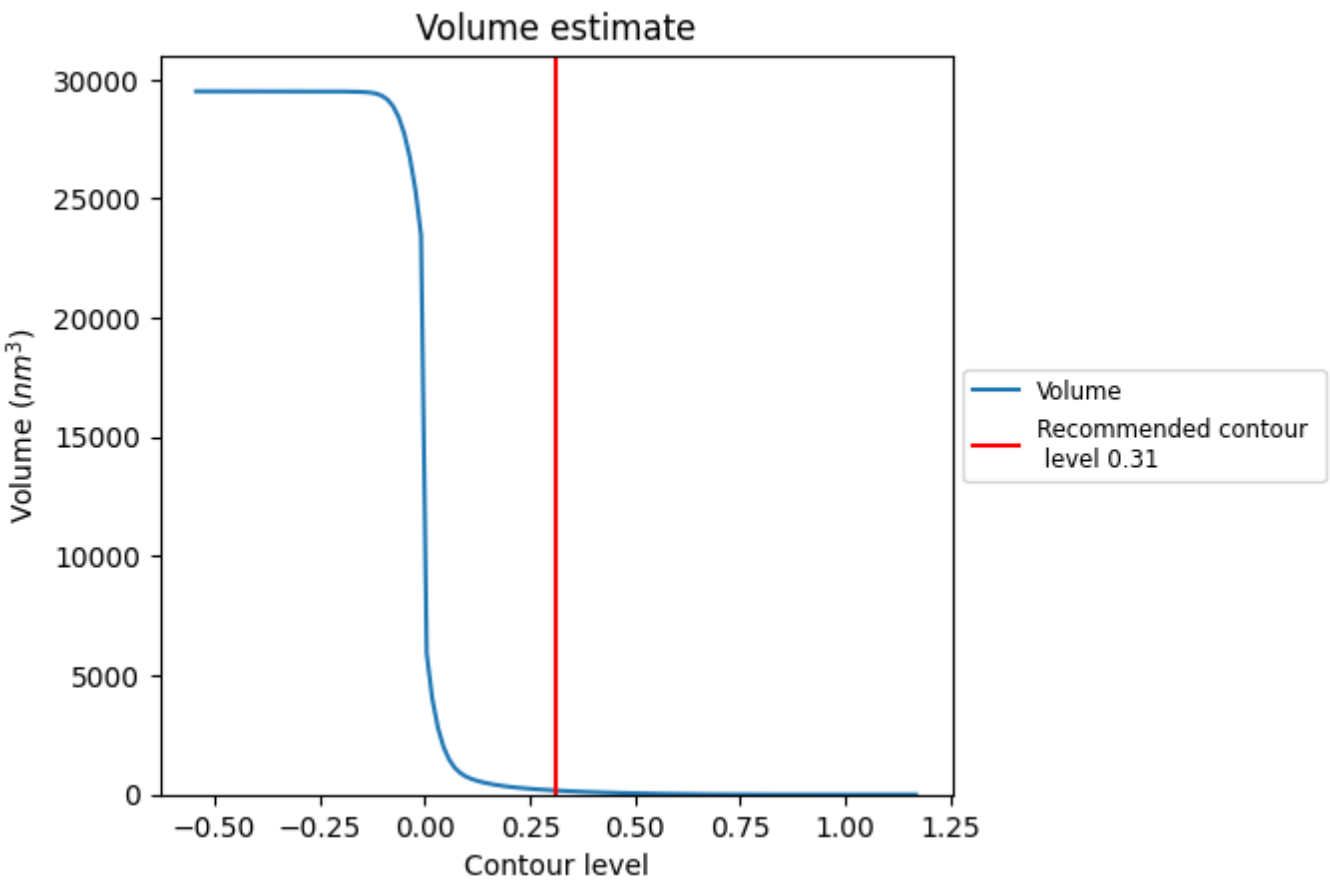
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

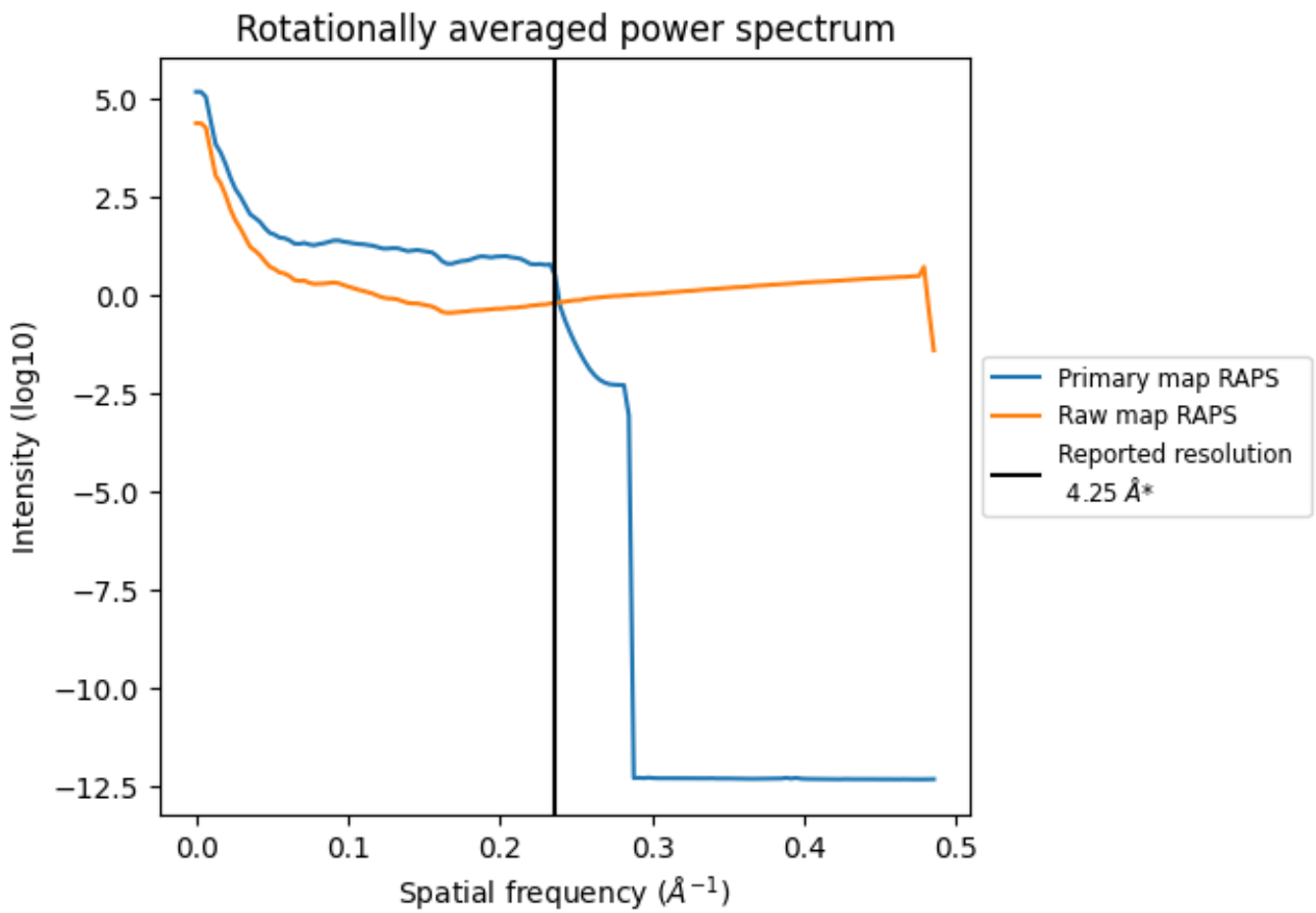
7.2 Volume estimate (i)



The volume at the recommended contour level is 173 nm^3; this corresponds to an approximate mass of 156 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)

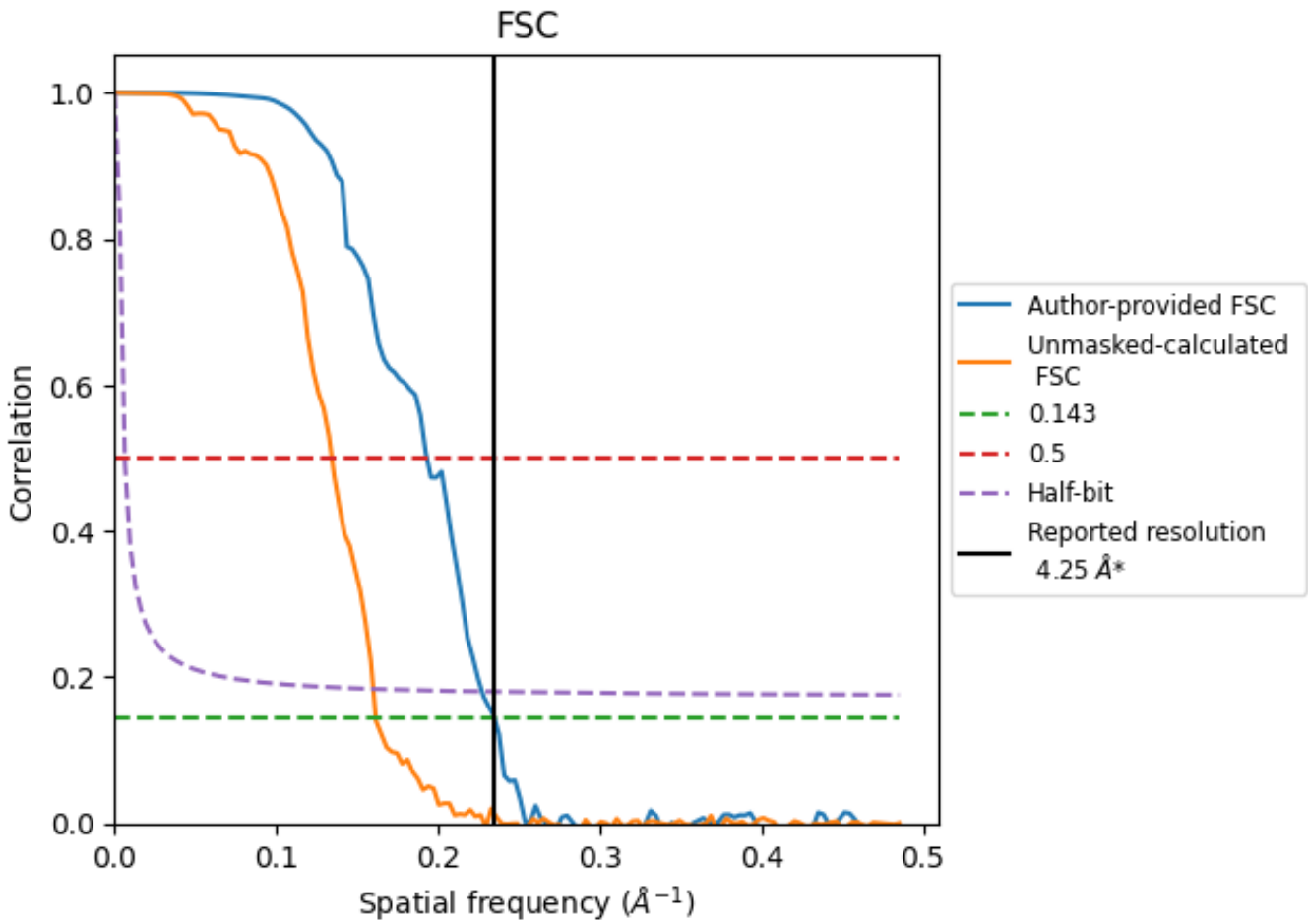


*Reported resolution corresponds to spatial frequency of 0.235 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.235 Å^{-1}

8.2 Resolution estimates (i)

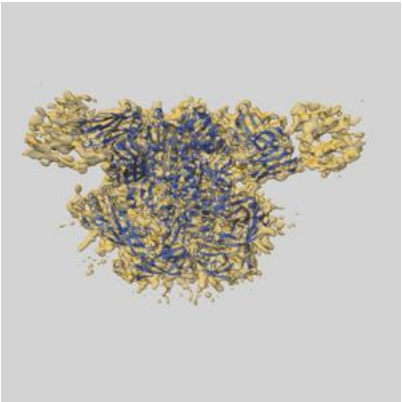
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.25	5.18	4.40
Unmasked-calculated*	6.18	7.44	6.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.18 differs from the reported value 4.25 by more than 10 %

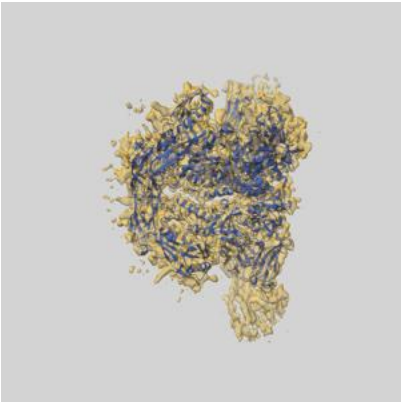
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21246 and PDB model 6VN0. Per-residue inclusion information can be found in section 3 on page 11.

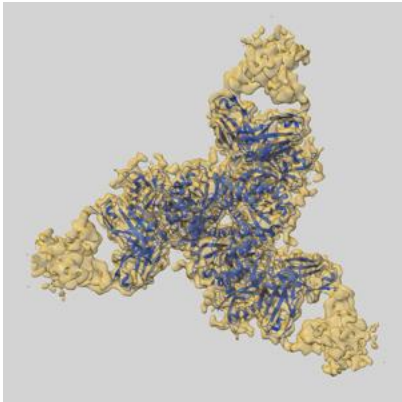
9.1 Map-model overlay (i)



X



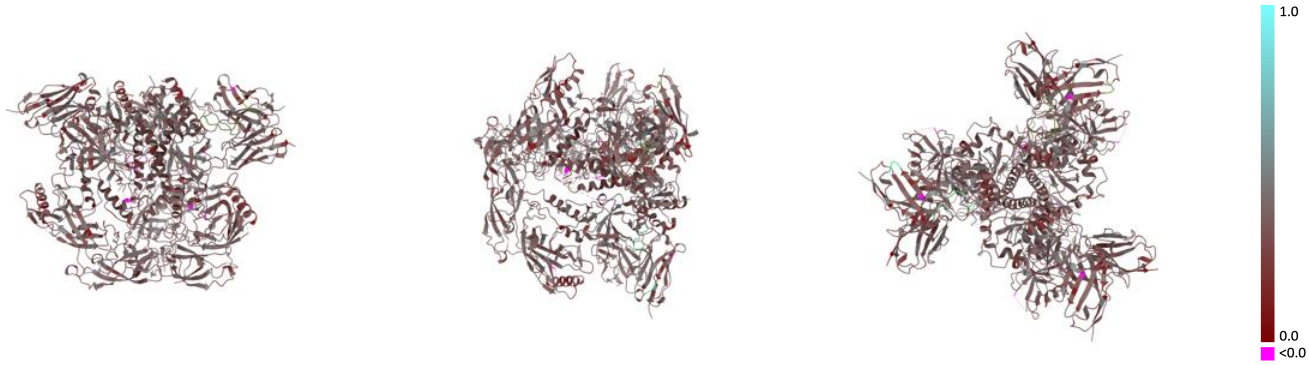
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.31 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

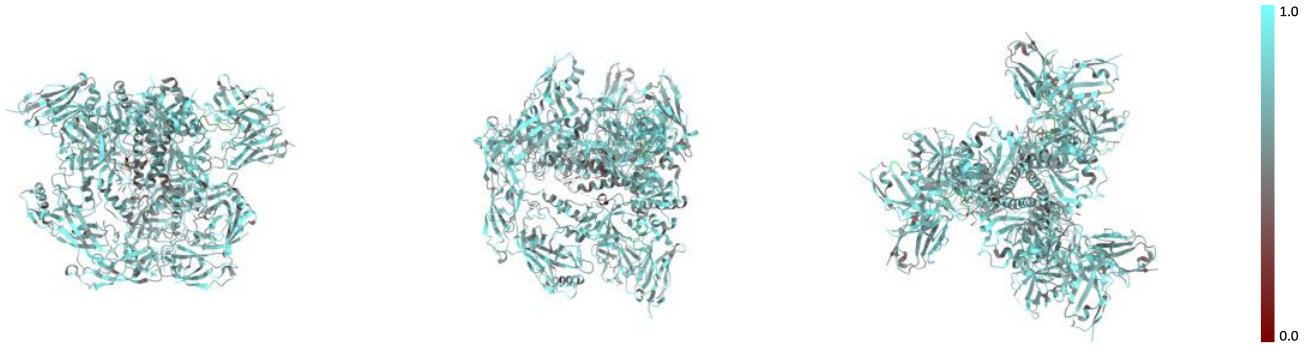
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

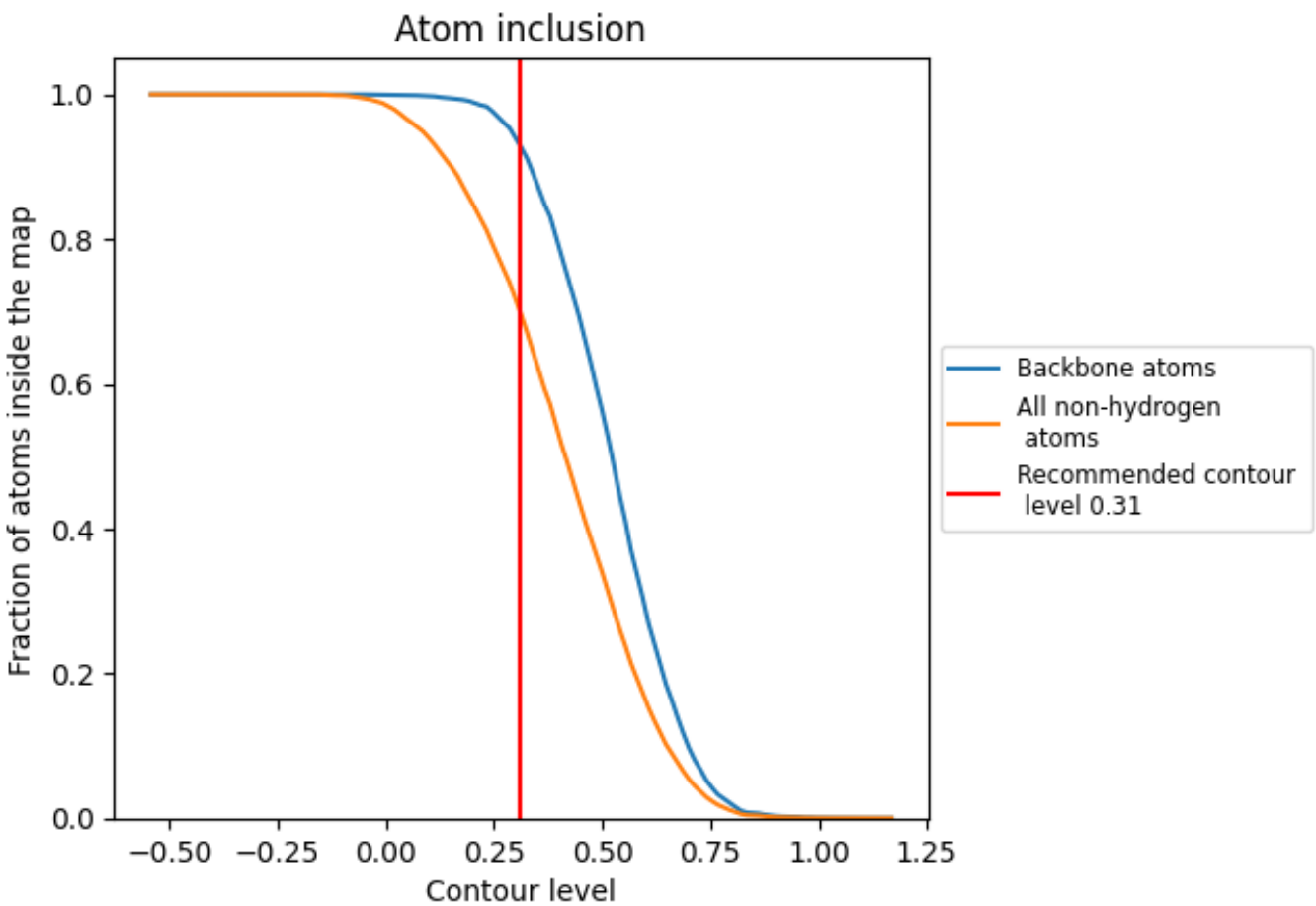
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.31).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6995	0.3450
A	0.7106	0.3490
B	0.6768	0.3210
C	0.7106	0.3490
D	0.7121	0.3490
E	0.6749	0.3200
F	0.6711	0.3240
G	0.7311	0.3470
H	0.7332	0.3450
I	0.7289	0.3460
J	0.6940	0.3440
K	0.6953	0.3430
L	0.6978	0.3440
M	0.6557	0.4060
N	0.6429	0.3550
O	0.3571	0.2310
P	0.3929	0.3280
Q	0.5574	0.3600
R	0.5000	0.4180
S	0.5714	0.3220
T	0.8929	0.3790
U	0.6071	0.4300
V	0.7143	0.4300
W	0.5357	0.3450
X	0.6885	0.4110
Y	0.6429	0.3560
Z	0.3571	0.2350
a	0.4286	0.3250
b	0.5738	0.3570
c	0.5000	0.4080
d	0.6071	0.3240
e	0.8929	0.3940
f	0.6071	0.4140
g	0.7143	0.4450
h	0.5357	0.3480

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Chain	Atom inclusion	Q-score
i	0.6721	0.4100
j	0.6429	0.3730
k	0.3571	0.2310
l	0.4286	0.3380
m	0.5902	0.3630
n	0.5000	0.4090
o	0.6071	0.3240
p	0.8571	0.3750
q	0.5714	0.4310
r	0.7143	0.4290
s	0.5357	0.3600