wwPDB EM Validation Summary Report (i)

Nov 16, 2022 – 06:44 AM EST

PDB ID	:	7KRS
EMDB ID	:	EMD-23012
Title	:	Structural impact on SARS-CoV-2 spike protein by D614G substitution
Authors	:	Zhang, J.; Cai, Y.F.; Xiao, T.S.; Lu, J.M.; Peng, H.Q.; Sterling, S.M.; Walsh Jr, R.M.; Volloch, S.R.; Zhu, H.S.; Woosley, A.N.; Yang, W.; Sliz, P.; Chen, B.
Deposited on	:	2020-11-20
Resolution	:	3.20 Å(reported)
Based on initial model	:	6XR8

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

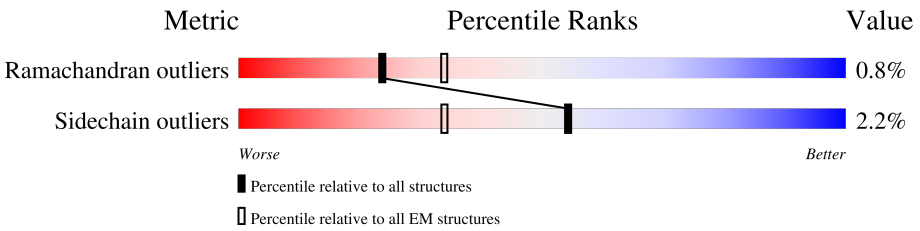
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1310	5%, 82%, •, 15%
1	B	1310	82%, •, 16%
1	C	1310	82%, •, 15%
2	D	2	50%, 50%
2	E	2	50%, 50%
2	F	2	50%, 50%
2	G	2	50%, 50%
2	H	2	50%, 50%
2	I	2	100%

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Mol	Chain	Length	Quality of chain
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	50% 50%
2	O	2	50% 50%
2	P	2	50% 50%
2	Q	2	50% 50%
2	R	2	50% 50%
2	S	2	50% 50% 50%
2	T	2	50% 50%
2	U	2	50% 100%
2	V	2	50% 50% 50%
2	W	2	50% 50%
2	X	2	100%
2	a	2	100%
2	b	2	50% 50%
2	c	2	50% 50%
2	d	2	50% 50%
2	e	2	50% 50%
2	f	2	50% 50%
2	g	2	50% 100%
2	h	2	50% 50%
2	i	2	100%
2	j	2	50% 50%
2	m	2	50% 50%
3	M	3	100%

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Mol	Chain	Length	Quality of chain
3	Y	3	33% 100%
3	k	3	100%
4	N	3	100%
4	Z	3	100%
4	l	3	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27298 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1109	8665	5528	1444	1653	40	0	0
1	B	1098	8590	5485	1431	1635	39	0	0
1	C	1109	8678	5540	1447	1652	39	0	0

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	ALA	-	expression tag	UNP P0DTC2
A	1282	TRP	-	expression tag	UNP P0DTC2
A	1283	SER	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	PRO	-	expression tag	UNP P0DTC2
A	1286	GLN	-	expression tag	UNP P0DTC2
A	1287	PHE	-	expression tag	UNP P0DTC2
A	1288	GLU	-	expression tag	UNP P0DTC2
A	1289	LYS	-	expression tag	UNP P0DTC2
A	1290	GLY	-	expression tag	UNP P0DTC2
A	1291	GLY	-	expression tag	UNP P0DTC2
A	1292	GLY	-	expression tag	UNP P0DTC2
A	1293	SER	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	GLY	-	expression tag	UNP P0DTC2
A	1296	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1297	SER	-	expression tag	UNP P0DTC2
A	1298	GLY	-	expression tag	UNP P0DTC2
A	1299	GLY	-	expression tag	UNP P0DTC2
A	1300	SER	-	expression tag	UNP P0DTC2
A	1301	SER	-	expression tag	UNP P0DTC2
A	1302	ALA	-	expression tag	UNP P0DTC2
A	1303	TRP	-	expression tag	UNP P0DTC2
A	1304	SER	-	expression tag	UNP P0DTC2
A	1305	HIS	-	expression tag	UNP P0DTC2
A	1306	PRO	-	expression tag	UNP P0DTC2
A	1307	GLN	-	expression tag	UNP P0DTC2
A	1308	PHE	-	expression tag	UNP P0DTC2
A	1309	GLU	-	expression tag	UNP P0DTC2
A	1310	LYS	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	ALA	-	expression tag	UNP P0DTC2
B	1282	TRP	-	expression tag	UNP P0DTC2
B	1283	SER	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	PRO	-	expression tag	UNP P0DTC2
B	1286	GLN	-	expression tag	UNP P0DTC2
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B	1288	GLU	-	expression tag	UNP P0DTC2
B	1289	LYS	-	expression tag	UNP P0DTC2
B	1290	GLY	-	expression tag	UNP P0DTC2
B	1291	GLY	-	expression tag	UNP P0DTC2
B	1292	GLY	-	expression tag	UNP P0DTC2
B	1293	SER	-	expression tag	UNP P0DTC2
B	1294	GLY	-	expression tag	UNP P0DTC2
B	1295	GLY	-	expression tag	UNP P0DTC2
B	1296	GLY	-	expression tag	UNP P0DTC2
B	1297	SER	-	expression tag	UNP P0DTC2
B	1298	GLY	-	expression tag	UNP P0DTC2
B	1299	GLY	-	expression tag	UNP P0DTC2
B	1300	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1301	SER	-	expression tag	UNP P0DTC2
B	1302	ALA	-	expression tag	UNP P0DTC2
B	1303	TRP	-	expression tag	UNP P0DTC2
B	1304	SER	-	expression tag	UNP P0DTC2
B	1305	HIS	-	expression tag	UNP P0DTC2
B	1306	PRO	-	expression tag	UNP P0DTC2
B	1307	GLN	-	expression tag	UNP P0DTC2
B	1308	PHE	-	expression tag	UNP P0DTC2
B	1309	GLU	-	expression tag	UNP P0DTC2
B	1310	LYS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	ALA	-	expression tag	UNP P0DTC2
C	1282	TRP	-	expression tag	UNP P0DTC2
C	1283	SER	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	PRO	-	expression tag	UNP P0DTC2
C	1286	GLN	-	expression tag	UNP P0DTC2
C	1287	PHE	-	expression tag	UNP P0DTC2
C	1288	GLU	-	expression tag	UNP P0DTC2
C	1289	LYS	-	expression tag	UNP P0DTC2
C	1290	GLY	-	expression tag	UNP P0DTC2
C	1291	GLY	-	expression tag	UNP P0DTC2
C	1292	GLY	-	expression tag	UNP P0DTC2
C	1293	SER	-	expression tag	UNP P0DTC2
C	1294	GLY	-	expression tag	UNP P0DTC2
C	1295	GLY	-	expression tag	UNP P0DTC2
C	1296	GLY	-	expression tag	UNP P0DTC2
C	1297	SER	-	expression tag	UNP P0DTC2
C	1298	GLY	-	expression tag	UNP P0DTC2
C	1299	GLY	-	expression tag	UNP P0DTC2
C	1300	SER	-	expression tag	UNP P0DTC2
C	1301	SER	-	expression tag	UNP P0DTC2
C	1302	ALA	-	expression tag	UNP P0DTC2
C	1303	TRP	-	expression tag	UNP P0DTC2
C	1304	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1305	HIS	-	expression tag	UNP P0DTC2
C	1306	PRO	-	expression tag	UNP P0DTC2
C	1307	GLN	-	expression tag	UNP P0DTC2
C	1308	PHE	-	expression tag	UNP P0DTC2
C	1309	GLU	-	expression tag	UNP P0DTC2
C	1310	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 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		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0
2	J	2	28	16	2	10	0	0
2	K	2	28	16	2	10	0	0
2	L	2	28	16	2	10	0	0
2	O	2	28	16	2	10	0	0
2	P	2	28	16	2	10	0	0
2	Q	2	28	16	2	10	0	0
2	R	2	28	16	2	10	0	0
2	S	2	28	16	2	10	0	0

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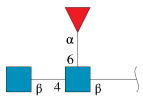
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	T	2	28	16	2	10	0	0
2	U	2	28	16	2	10	0	0
2	V	2	28	16	2	10	0	0
2	W	2	28	16	2	10	0	0
2	X	2	28	16	2	10	0	0
2	a	2	28	16	2	10	0	0
2	b	2	28	16	2	10	0	0
2	c	2	28	16	2	10	0	0
2	d	2	28	16	2	10	0	0
2	e	2	28	16	2	10	0	0
2	f	2	28	16	2	10	0	0
2	g	2	28	16	2	10	0	0
2	h	2	28	16	2	10	0	0
2	i	2	28	16	2	10	0	0
2	j	2	28	16	2	10	0	0
2	m	2	28	16	2	10	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	M	3	38	22	2	14	0	0

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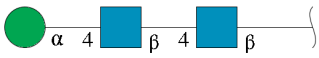
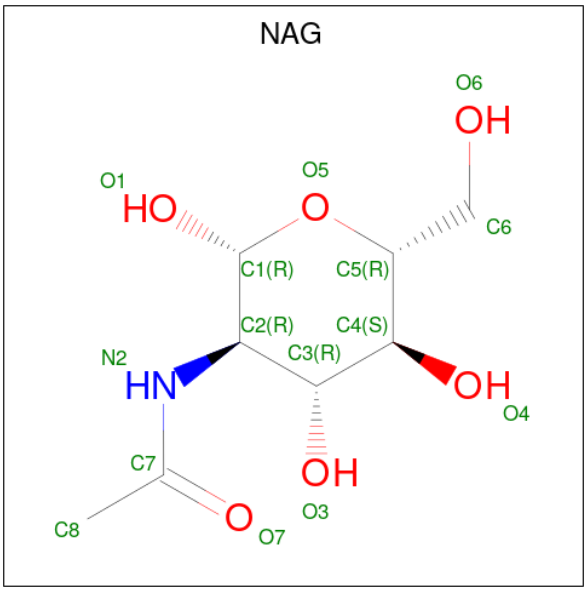
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Y	3	38	22	2	14	0	0
3	k	3	38	22	2	14	0	0

- Molecule 4 is an oligosaccharide called alpha-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		
4	N	3	39	22	2	15	0	0
4	Z	3	39	22	2	15	0	0
4	l	3	39	22	2	15	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	98	56	7	35	0

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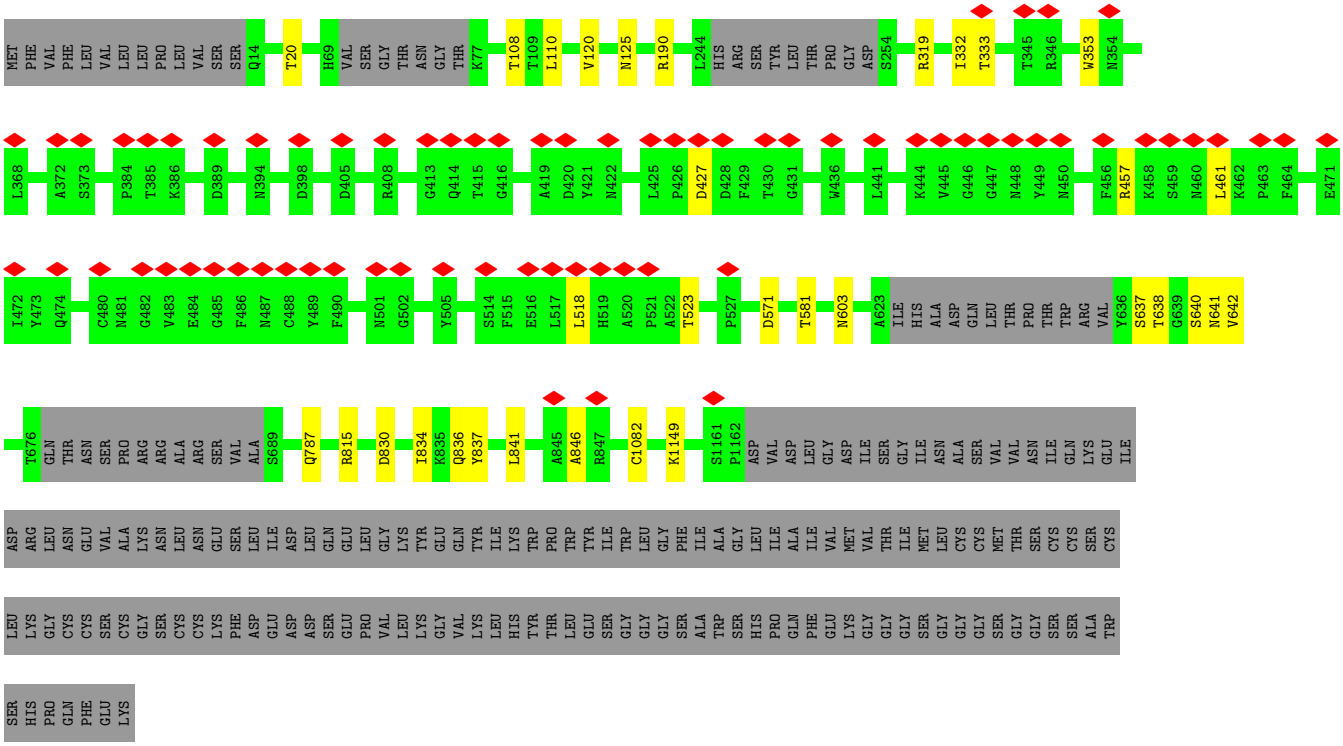
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	98	56	7	35	0
5	A	1	98	56	7	35	0
5	A	1	98	56	7	35	0
5	A	1	98	56	7	35	0
5	A	1	98	56	7	35	0
5	A	1	98	56	7	35	0
5	B	1	98	56	7	35	0
5	B	1	98	56	7	35	0
5	B	1	98	56	7	35	0
5	B	1	98	56	7	35	0
5	B	1	98	56	7	35	0
5	B	1	98	56	7	35	0
5	B	1	98	56	7	35	0
5	C	1	98	56	7	35	0
5	C	1	98	56	7	35	0
5	C	1	98	56	7	35	0
5	C	1	98	56	7	35	0
5	C	1	98	56	7	35	0
5	C	1	98	56	7	35	0
5	C	1	98	56	7	35	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.

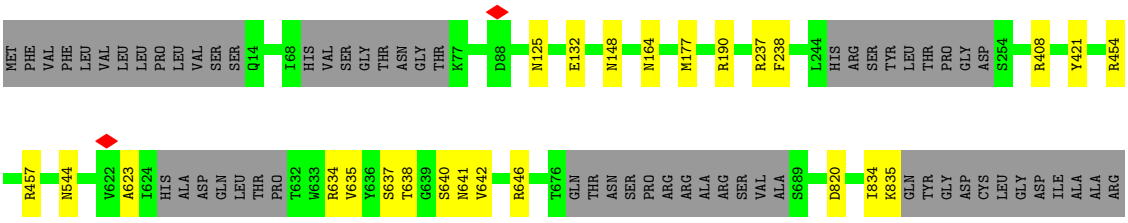
- Molecule 1: Spike glycoprotein

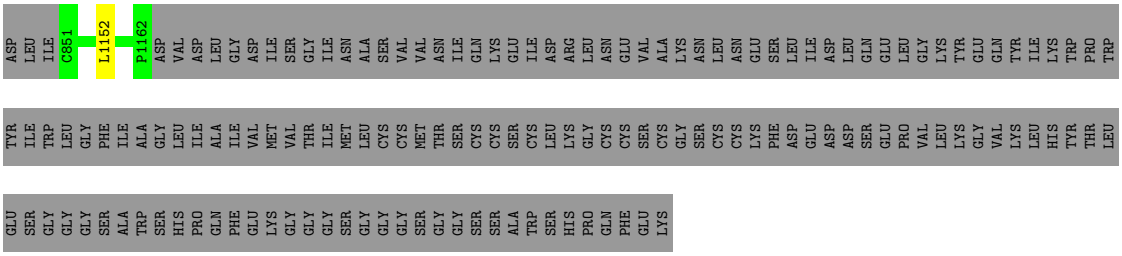
Chain A:



- Molecule 1: Spike glycoprotein

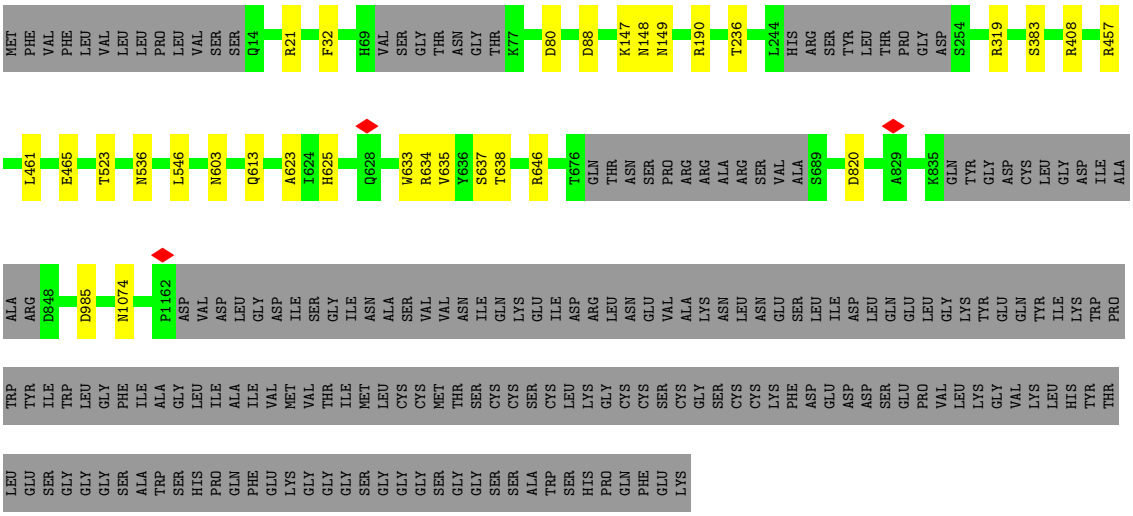
Chain B:





• Molecule 1: Spike glycoprotein

Chain C:



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

Chain D:

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

Chain E:

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

Chain F:

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

Chain G: 50% 50%

NAG1 NAG2

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

Chain H: 50% 50%

NAG1 NAG2

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

Chain I: 100%

NAG1 NAG2

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

Chain J: 50% 50%

NAG1 NAG2

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

Chain K: 50% 50%

NAG1 NAG2

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

Chain L: 50% 50%

NAG1 NAG2

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

Chain O: 50% 50%

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

Chain P: 50% 50%

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

Chain Q: 50% 50%

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

Chain R: 50% 50%

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

Chain S: 50% 50% 50%

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

Chain T: 50% 50%

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

Chain U: 50% 100%

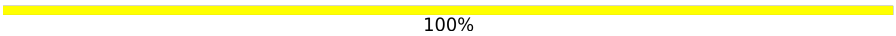
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

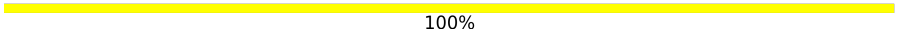
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

Chain X: 

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

Chain a: 

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

Chain b:

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

Chain c:

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

Chain d:

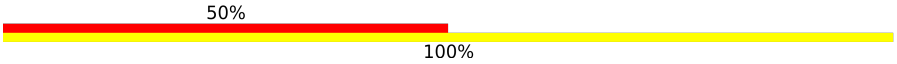
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

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

Chain f:

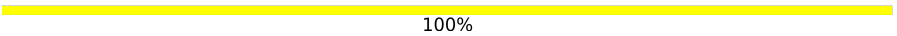
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 

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

Chain h:

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

Chain i: 

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

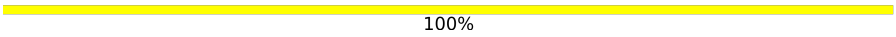
Chain j:

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

Chain m:

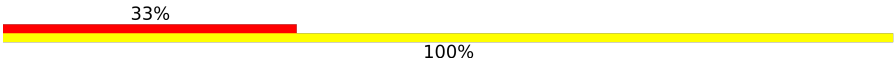
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



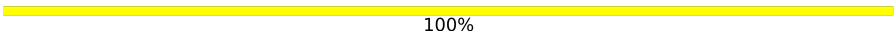
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



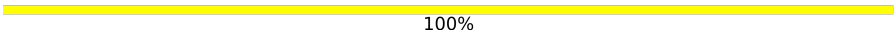
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



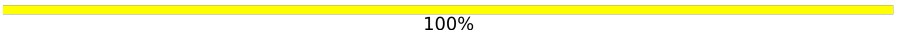
• Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain Z:



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

Chain l: 100%

NAG1
NAG2
MAN3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63040	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 ($e^-/Å^2$)	53.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: FUC, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.63	0/8864	0.91	0/12056
1	B	0.62	0/8788	0.91	0/11953
1	C	0.61	0/8880	0.91	0/12082
All	All	0.62	0/26532	0.91	0/36091

There are no bond length outliers.

There are no bond angle outliers.

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	1099/1310 (84%)	1018 (93%)	72 (7%)	9 (1%)	19 58
1	B	1086/1310 (83%)	1018 (94%)	61 (6%)	7 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1099/1310 (84%)	1031 (94%)	58 (5%)	10 (1%)	17	56
All	All	3284/3930 (84%)	3067 (93%)	191 (6%)	26 (1%)	24	58

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	ASN
1	C	148	ASN
1	A	834	ILE
1	A	846	ALA
1	B	623	ALA

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	965/1135 (85%)	941 (98%)	24 (2%)	47	77
1	B	958/1135 (84%)	939 (98%)	19 (2%)	55	80
1	C	968/1135 (85%)	947 (98%)	21 (2%)	52	79
All	All	2891/3405 (85%)	2827 (98%)	64 (2%)	54	79

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	634	ARG
1	C	638	THR
1	B	125	ASN
1	A	1149	LYS
1	C	646	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	282	ASN
1	C	188	ASN
1	B	658	ASN
1	C	165	ASN
1	B	165	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)

78 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	D	2	2	14,14,15	1.14	1 (7%)	17,19,21	0.63	0
2	NAG	E	1	2,1	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	E	2	2	14,14,15	1.24	2 (14%)	17,19,21	1.18	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.31	0	17,19,21	0.56	0
2	NAG	F	2	2	14,14,15	1.09	1 (7%)	17,19,21	0.80	1 (5%)
2	NAG	G	1	2,1	14,14,15	0.29	0	17,19,21	0.59	0
2	NAG	G	2	2	14,14,15	1.33	2 (14%)	17,19,21	1.14	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.36	0	17,19,21	0.43	0
2	NAG	H	2	2	14,14,15	1.31	2 (14%)	17,19,21	0.90	1 (5%)
2	NAG	I	1	2,1	14,14,15	1.26	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	I	2	2	14,14,15	1.17	1 (7%)	17,19,21	1.00	1 (5%)
2	NAG	J	1	2,1	14,14,15	0.25	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	J	2	2	14,14,15	1.24	2 (14%)	17,19,21	1.34	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.34	0	17,19,21	0.50	0
2	NAG	K	2	2	14,14,15	1.34	2 (14%)	17,19,21	0.58	0
2	NAG	L	1	2,1	14,14,15	0.98	0	17,19,21	0.79	0
2	NAG	L	2	2	14,14,15	1.27	2 (14%)	17,19,21	0.73	0
3	NAG	M	1	3,1	14,14,15	0.15	0	17,19,21	0.83	1 (5%)
3	NAG	M	2	3	14,14,15	1.07	1 (7%)	17,19,21	0.76	1 (5%)
3	FUC	M	3	3	10,10,11	1.67	2 (20%)	14,14,16	1.60	4 (28%)
4	NAG	N	1	1,4	14,14,15	1.38	3 (21%)	17,19,21	0.80	0
4	NAG	N	2	4	14,14,15	1.33	2 (14%)	17,19,21	0.65	0
4	MAN	N	3	4	11,11,12	1.53	2 (18%)	15,15,17	0.95	1 (6%)
2	NAG	O	1	2,1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	O	2	2	14,14,15	1.24	2 (14%)	17,19,21	0.77	0
2	NAG	P	1	2	14,14,15	0.27	0	17,19,21	0.34	0
2	NAG	P	2	2	14,14,15	1.07	1 (7%)	17,19,21	1.02	1 (5%)
2	NAG	Q	1	2,1	14,14,15	0.18	0	17,19,21	0.42	0
2	NAG	Q	2	2	14,14,15	1.26	2 (14%)	17,19,21	0.89	1 (5%)
2	NAG	R	1	2,1	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	R	2	2	14,14,15	0.93	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	S	1	2,1	14,14,15	0.25	0	17,19,21	0.53	0
2	NAG	S	2	2	14,14,15	1.30	2 (14%)	17,19,21	0.91	1 (5%)
2	NAG	T	1	2,1	14,14,15	0.37	0	17,19,21	0.42	0
2	NAG	T	2	2	14,14,15	1.30	2 (14%)	17,19,21	0.91	1 (5%)
2	NAG	U	1	2,1	14,14,15	1.17	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	U	2	2	14,14,15	1.12	1 (7%)	17,19,21	1.43	3 (17%)
2	NAG	V	1	2,1	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	V	2	2	14,14,15	1.36	2 (14%)	17,19,21	0.87	1 (5%)
2	NAG	W	1	2,1	14,14,15	1.13	0	17,19,21	0.90	0
2	NAG	W	2	2	14,14,15	1.40	2 (14%)	17,19,21	0.87	0
2	NAG	X	1	2,1	14,14,15	1.04	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	X	2	2	14,14,15	1.32	2 (14%)	17,19,21	0.62	0
3	NAG	Y	1	3,1	14,14,15	0.26	0	17,19,21	0.89	1 (5%)
3	NAG	Y	2	3	14,14,15	1.07	1 (7%)	17,19,21	0.98	1 (5%)
3	FUC	Y	3	3	10,10,11	1.50	3 (30%)	14,14,16	1.83	2 (14%)
4	NAG	Z	1	1,4	14,14,15	1.36	2 (14%)	17,19,21	0.95	0
4	NAG	Z	2	4	14,14,15	1.43	3 (21%)	17,19,21	0.80	1 (5%)
4	MAN	Z	3	4	11,11,12	1.51	2 (18%)	15,15,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	a	1	2,1	14,14,15	1.11	2 (14%)	17,19,21	1.37	1 (5%)
2	NAG	a	2	2	14,14,15	1.39	2 (14%)	17,19,21	0.96	1 (5%)
2	NAG	b	1	2	14,14,15	0.26	0	17,19,21	0.39	0
2	NAG	b	2	2	14,14,15	1.09	1 (7%)	17,19,21	0.93	0
2	NAG	c	1	2,1	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	c	2	2	14,14,15	1.19	2 (14%)	17,19,21	1.09	2 (11%)
2	NAG	d	1	2,1	14,14,15	0.30	0	17,19,21	0.55	0
2	NAG	d	2	2	14,14,15	1.06	1 (7%)	17,19,21	0.82	0
2	NAG	e	1	2,1	14,14,15	0.25	0	17,19,21	0.54	0
2	NAG	e	2	2	14,14,15	1.36	2 (14%)	17,19,21	1.65	2 (11%)
2	NAG	f	1	2	14,14,15	0.35	0	17,19,21	0.43	0
2	NAG	f	2	2	14,14,15	1.30	2 (14%)	17,19,21	0.91	1 (5%)
2	NAG	g	1	2,1	14,14,15	1.19	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	g	2	2	14,14,15	1.13	1 (7%)	17,19,21	1.36	1 (5%)
2	NAG	h	1	2,1	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	h	2	2	14,14,15	1.24	2 (14%)	17,19,21	1.12	1 (5%)
2	NAG	i	1	2,1	14,14,15	1.09	1 (7%)	17,19,21	0.70	0
2	NAG	i	2	2	14,14,15	1.24	2 (14%)	17,19,21	0.78	0
2	NAG	j	1	2,1	14,14,15	1.08	0	17,19,21	0.80	0
2	NAG	j	2	2	14,14,15	1.29	3 (21%)	17,19,21	0.70	0
3	NAG	k	1	3,1	14,14,15	0.16	0	17,19,21	0.83	1 (5%)
3	NAG	k	2	3	14,14,15	1.09	1 (7%)	17,19,21	0.66	0
3	FUC	k	3	3	10,10,11	1.65	2 (20%)	14,14,16	1.34	3 (21%)
4	NAG	l	1	1,4	14,14,15	1.23	2 (14%)	17,19,21	0.89	0
4	NAG	l	2	4	14,14,15	1.24	2 (14%)	17,19,21	0.69	0
4	MAN	l	3	4	11,11,12	1.37	2 (18%)	15,15,17	0.80	0
2	NAG	m	1	2,1	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	m	2	2	14,14,15	1.29	2 (14%)	17,19,21	1.11	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
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	FUC	M	3	3	-	-	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	MAN	N	3	4	-	1/2/19/22	1/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	U	2	2	-	1/6/23/26	0/1/1/1
2	NAG	V	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	NAG	W	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	NAG	X	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1

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

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	-4.64	1.36	1.43
2	g	1	NAG	O5-C1	-4.38	1.36	1.43
2	U	1	NAG	O5-C1	-4.32	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	3	FUC	C2-C3	3.87	1.58	1.52
2	m	2	NAG	O5-C5	3.39	1.50	1.43

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	2	NAG	C1-O5-C5	5.50	119.65	112.19
2	g	2	NAG	C1-O5-C5	4.85	118.76	112.19
3	Y	3	FUC	C1-C2-C3	4.82	115.60	109.67
2	a	1	NAG	C1-O5-C5	4.78	118.66	112.19
2	J	2	NAG	C1-O5-C5	4.76	118.64	112.19

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Y	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6

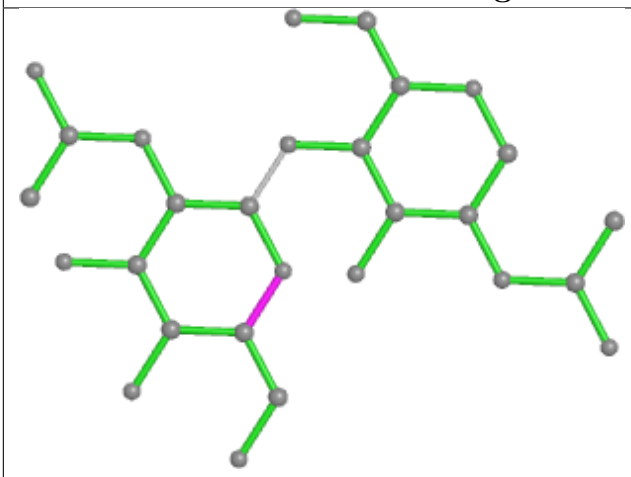
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	3	MAN	C1-C2-C3-C4-C5-O5

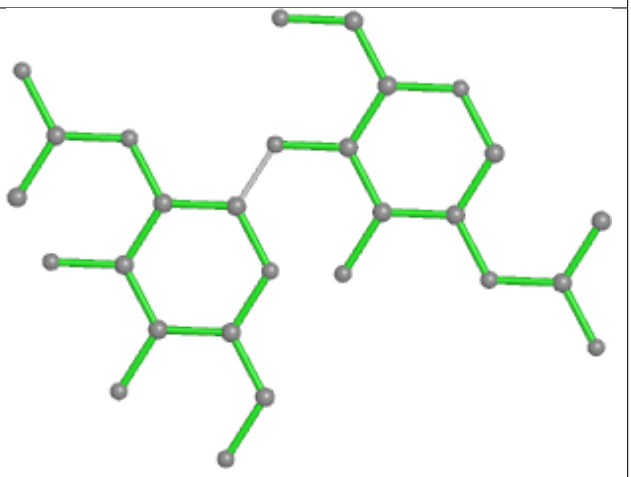
No monomer is involved in short contacts.

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

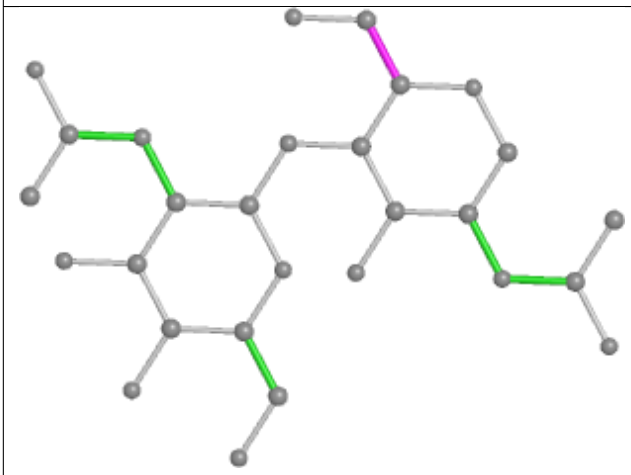
Oligosaccharide Chain D



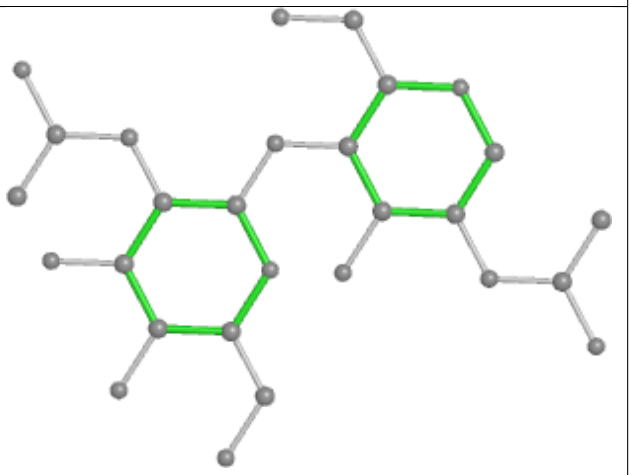
Bond lengths



Bond angles

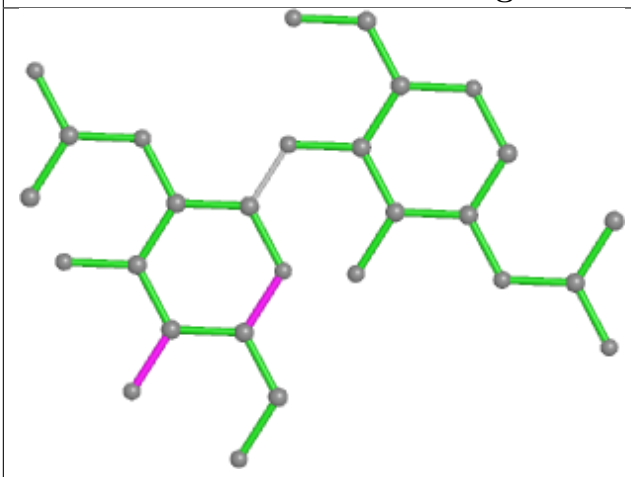


Torsions

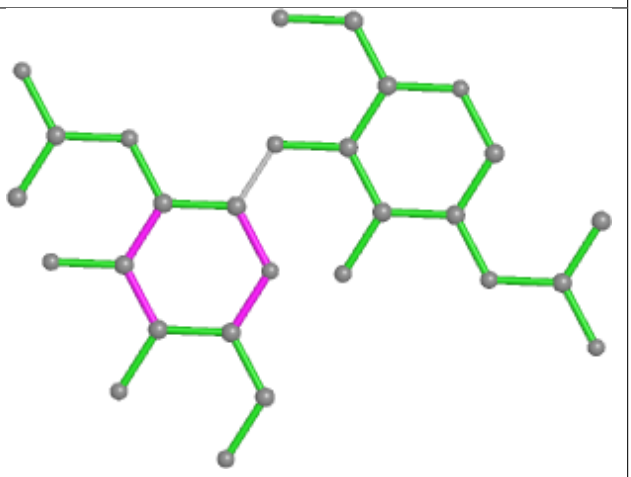


Rings

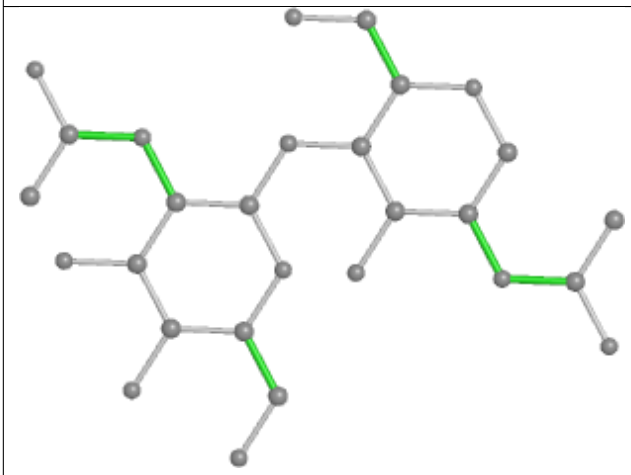
Oligosaccharide Chain E



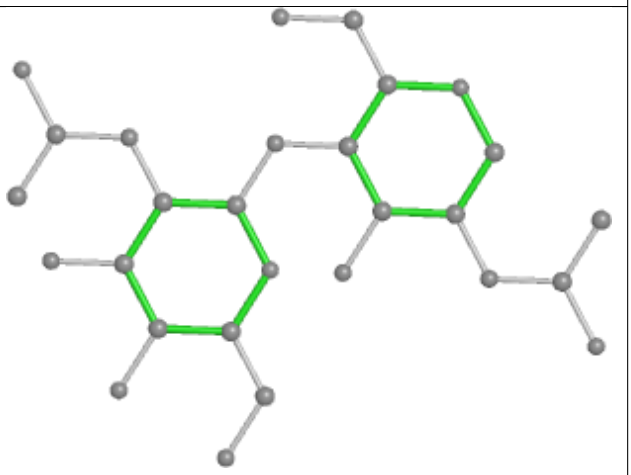
Bond lengths



Bond angles

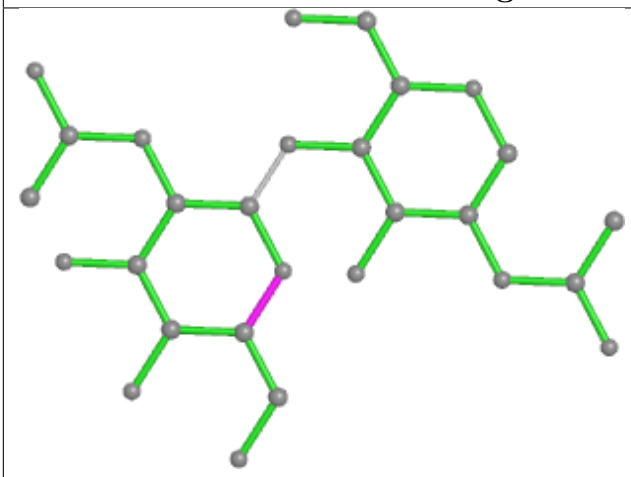


Torsions

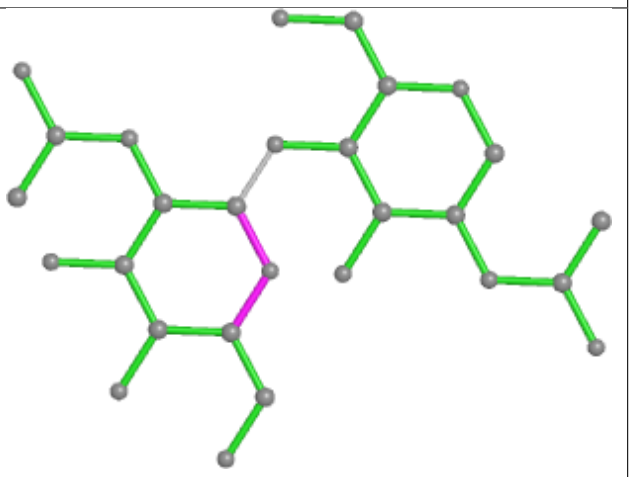


Rings

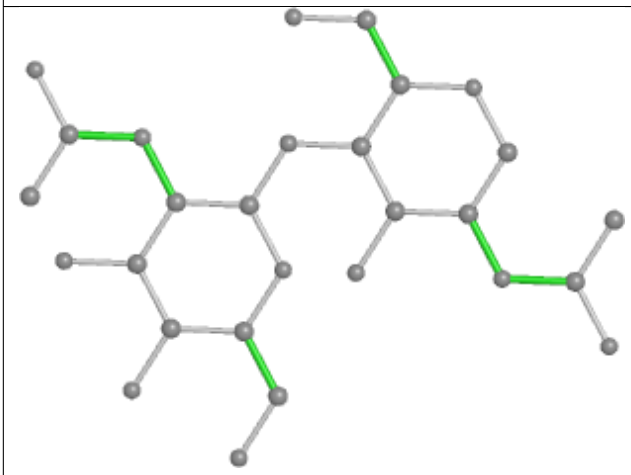
Oligosaccharide Chain F



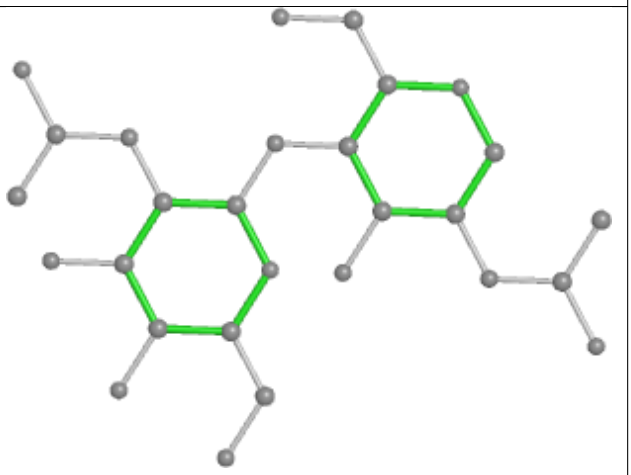
Bond lengths



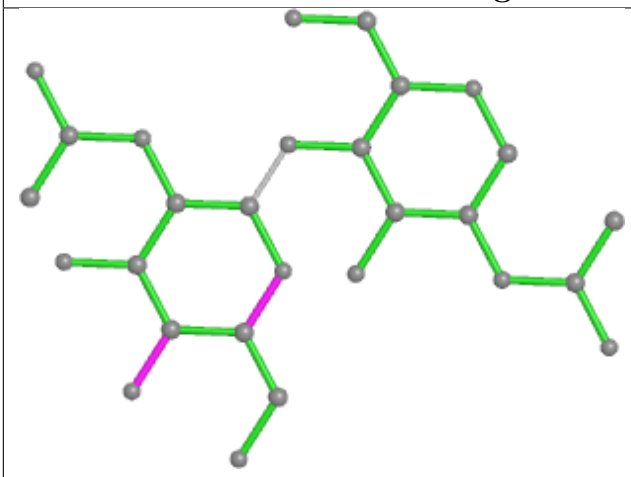
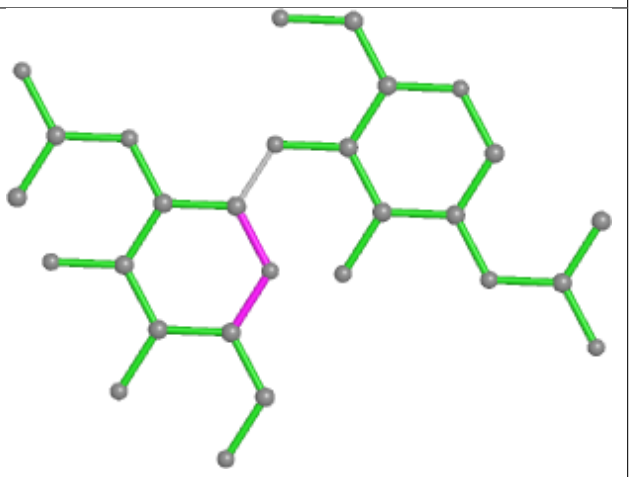
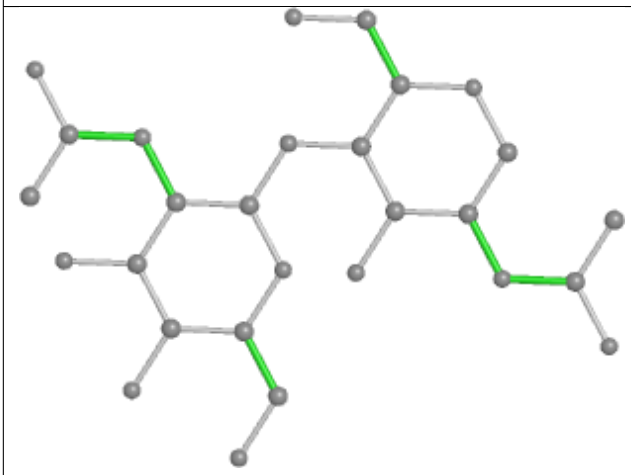
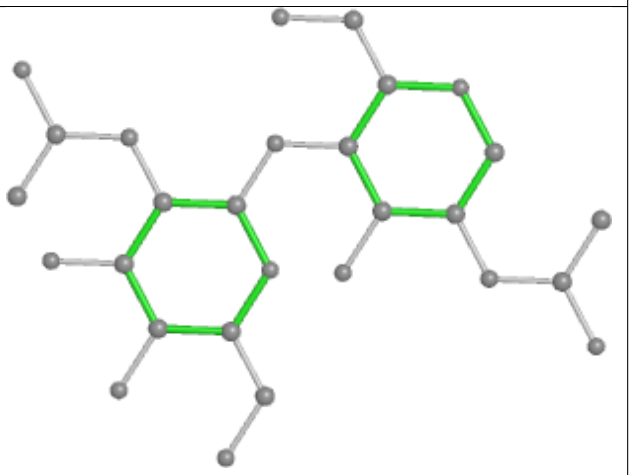
Bond angles

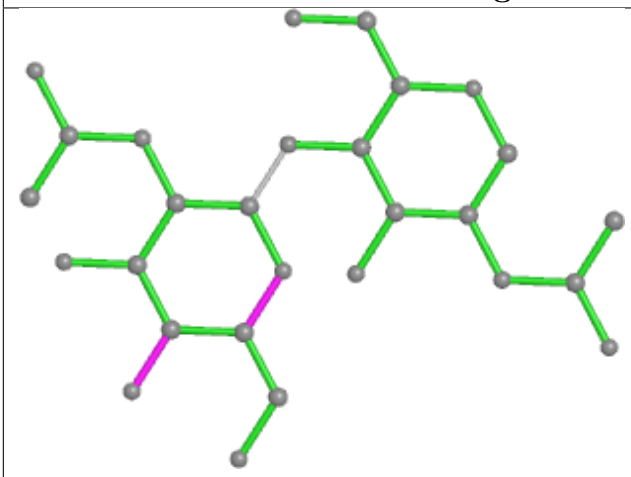
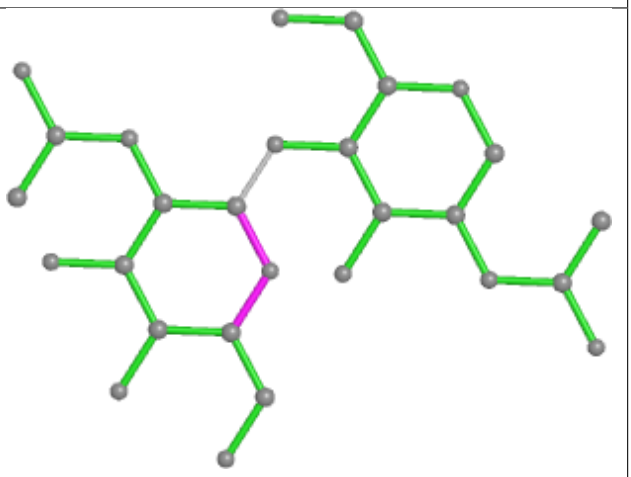
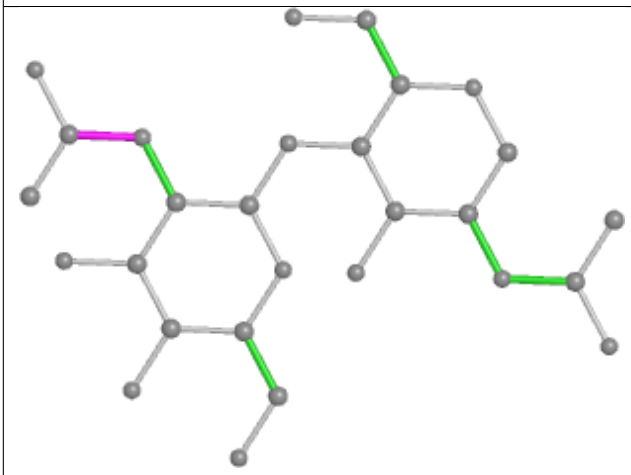
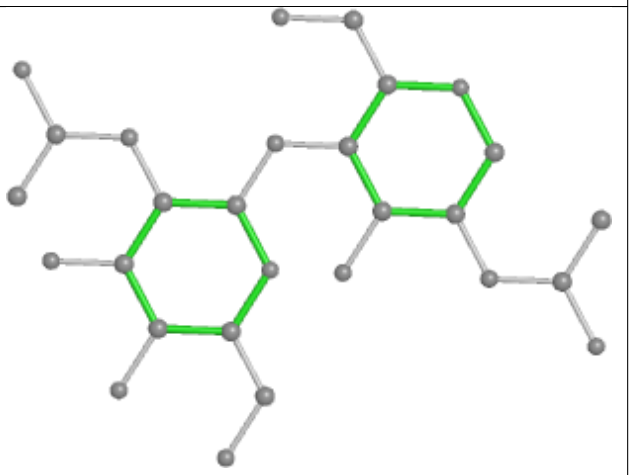


Torsions

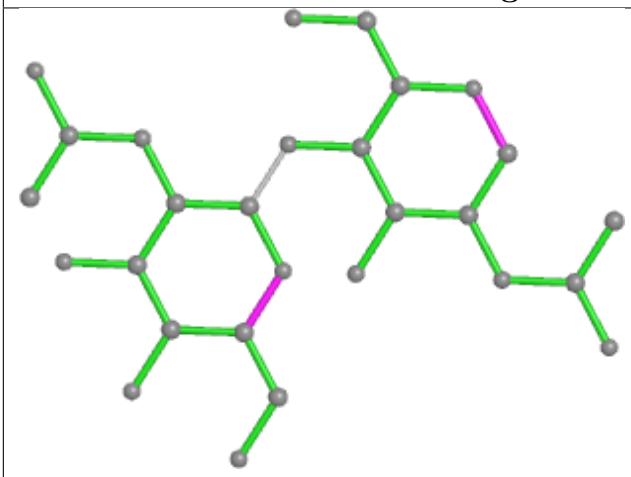


Rings

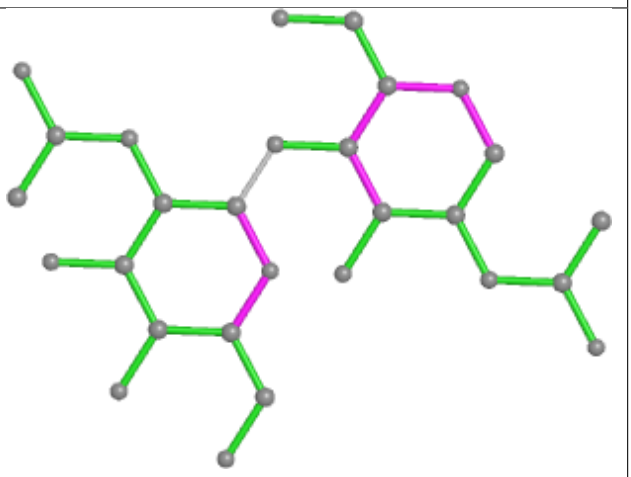
Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

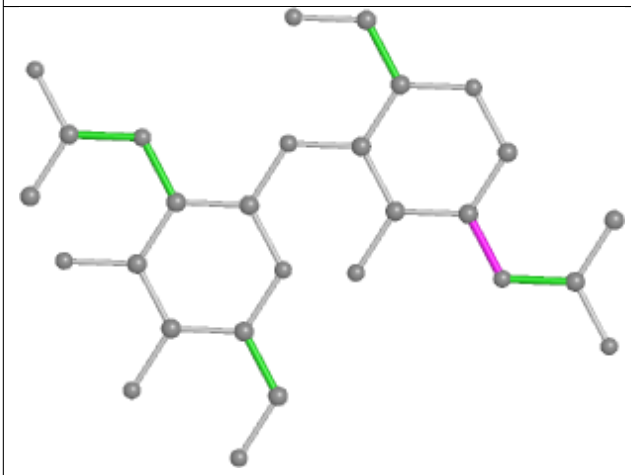
Oligosaccharide Chain I



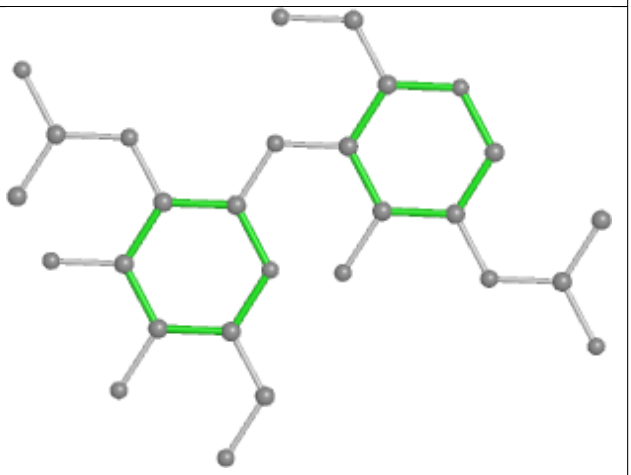
Bond lengths



Bond angles

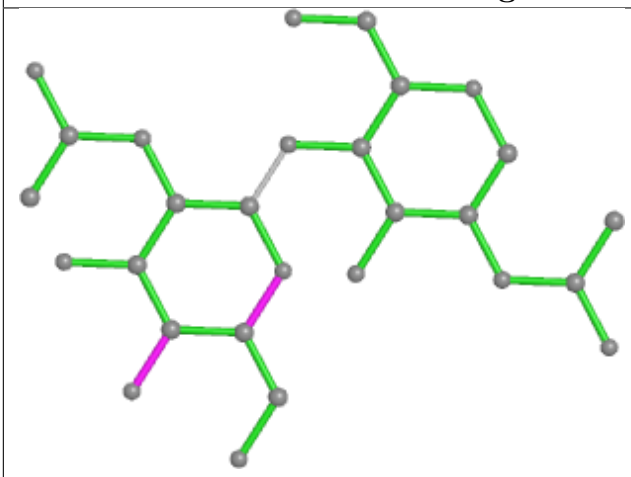


Torsions

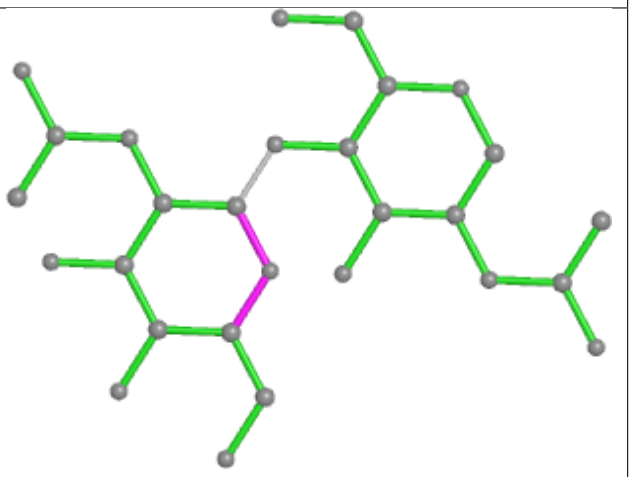


Rings

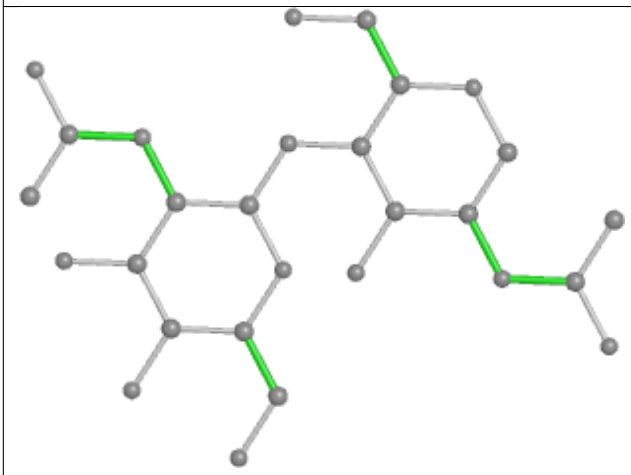
Oligosaccharide Chain J



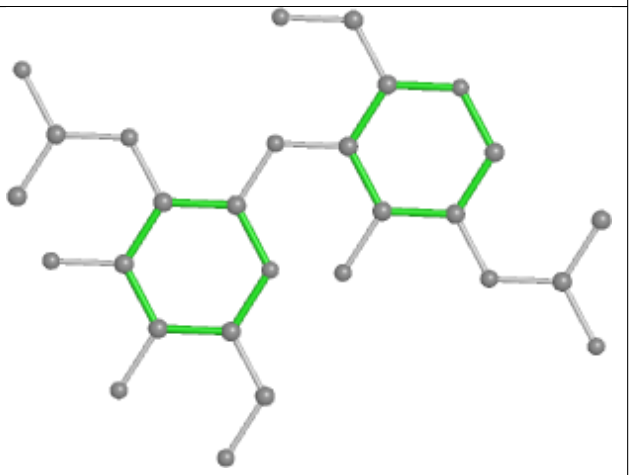
Bond lengths



Bond angles

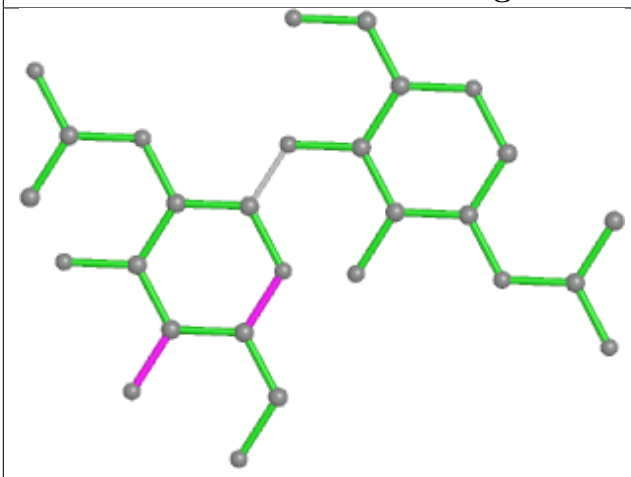


Torsions

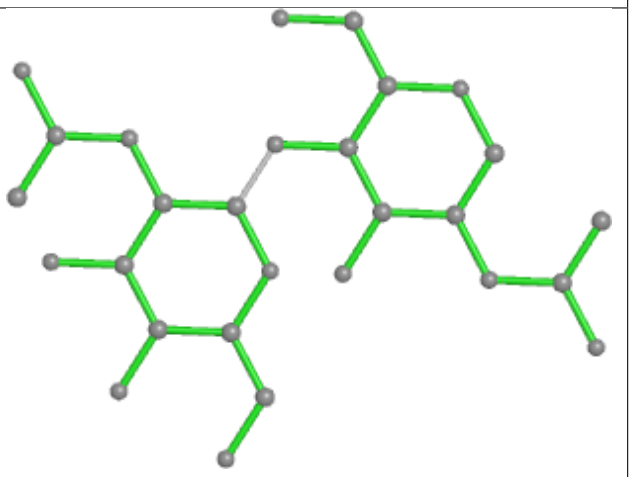


Rings

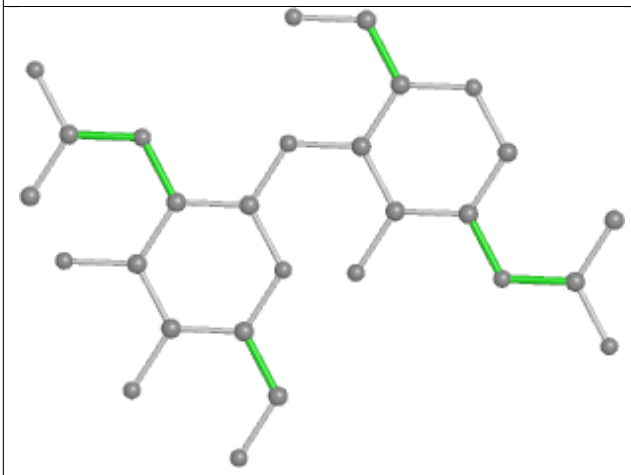
Oligosaccharide Chain K



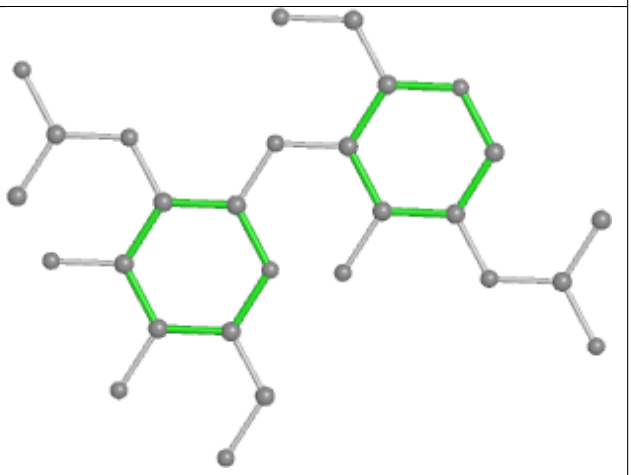
Bond lengths



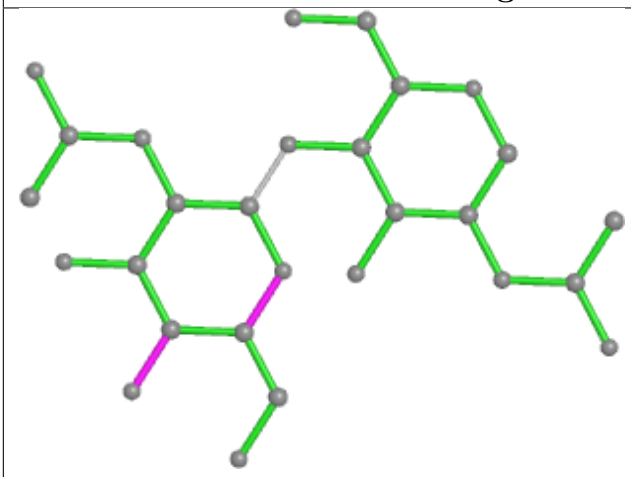
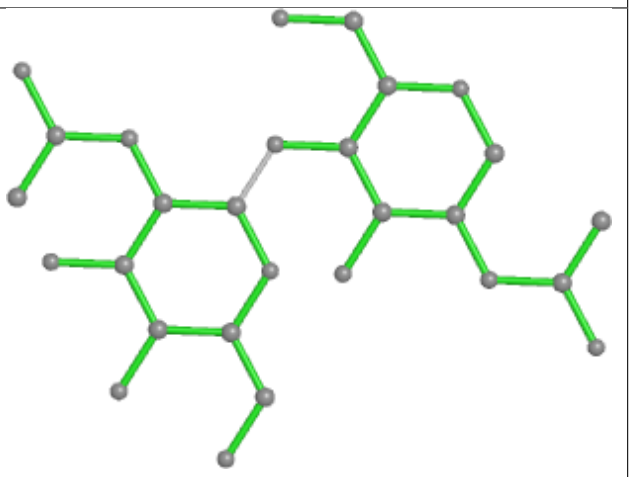
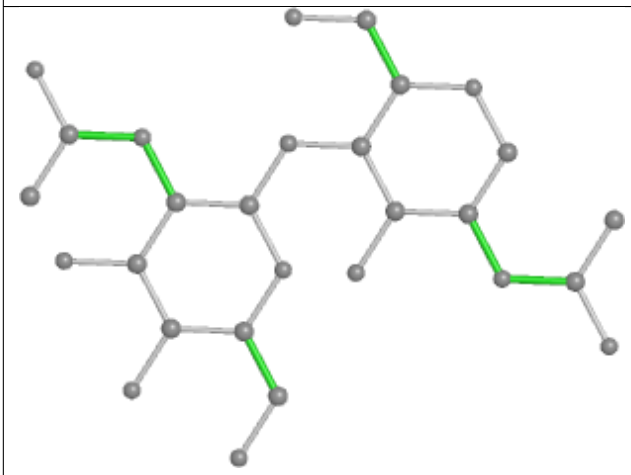
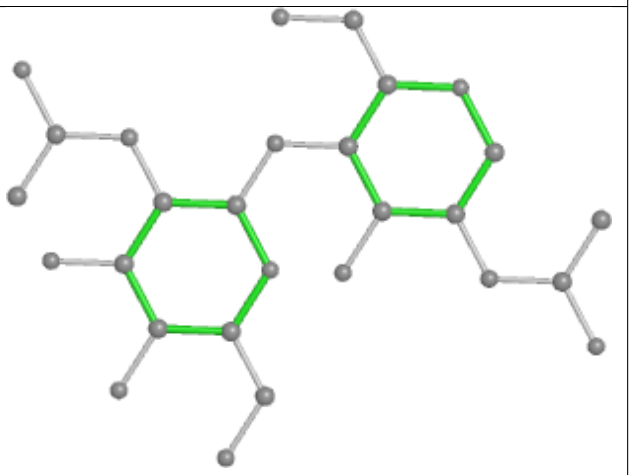
Bond angles



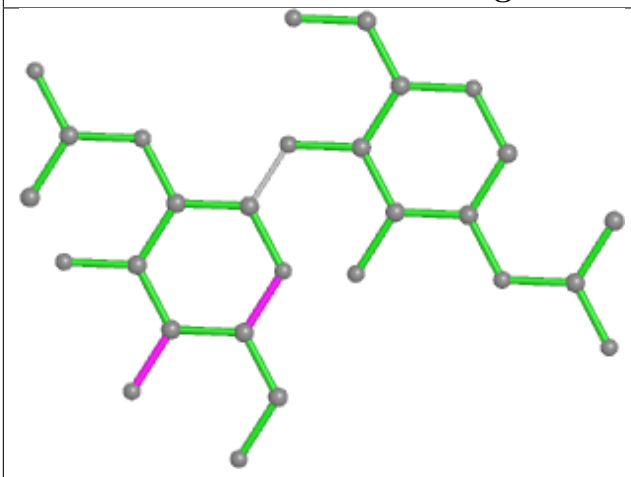
Torsions



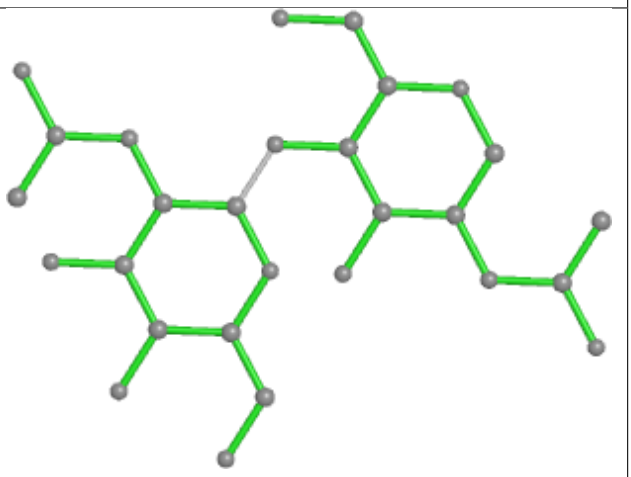
Rings

Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

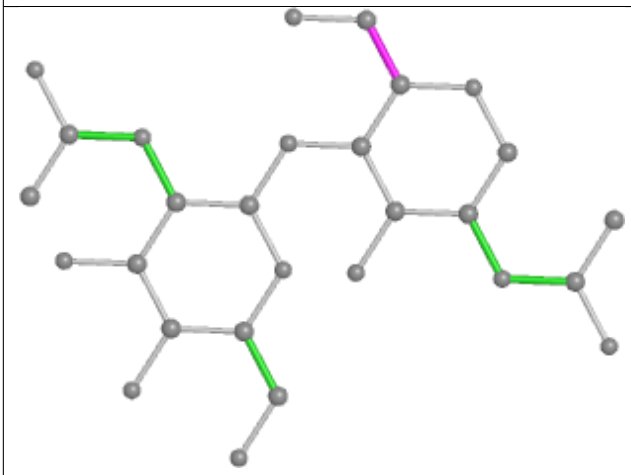
Oligosaccharide Chain O



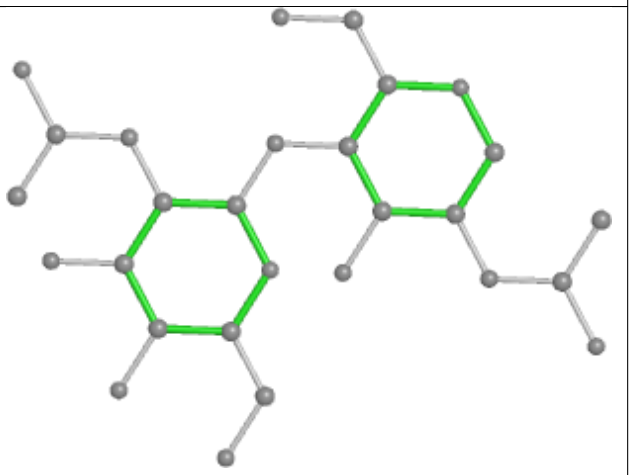
Bond lengths



Bond angles

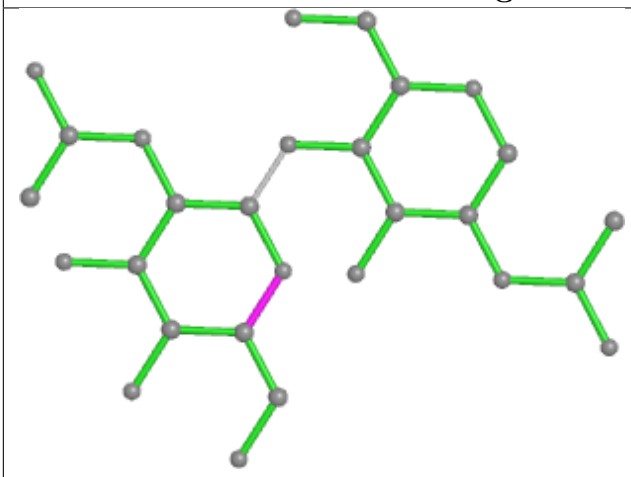


Torsions

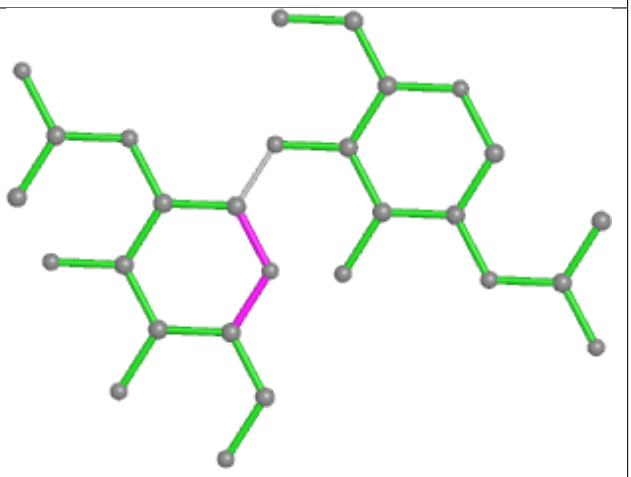


Rings

Oligosaccharide Chain P



Bond lengths



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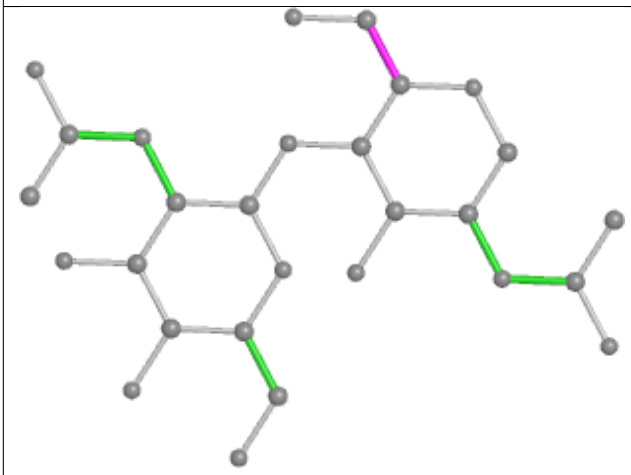

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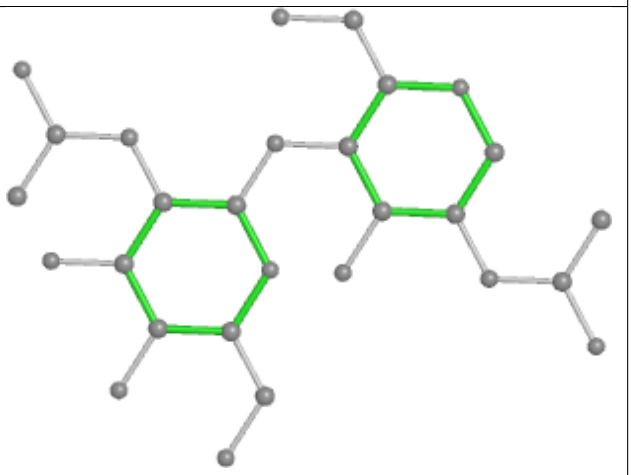
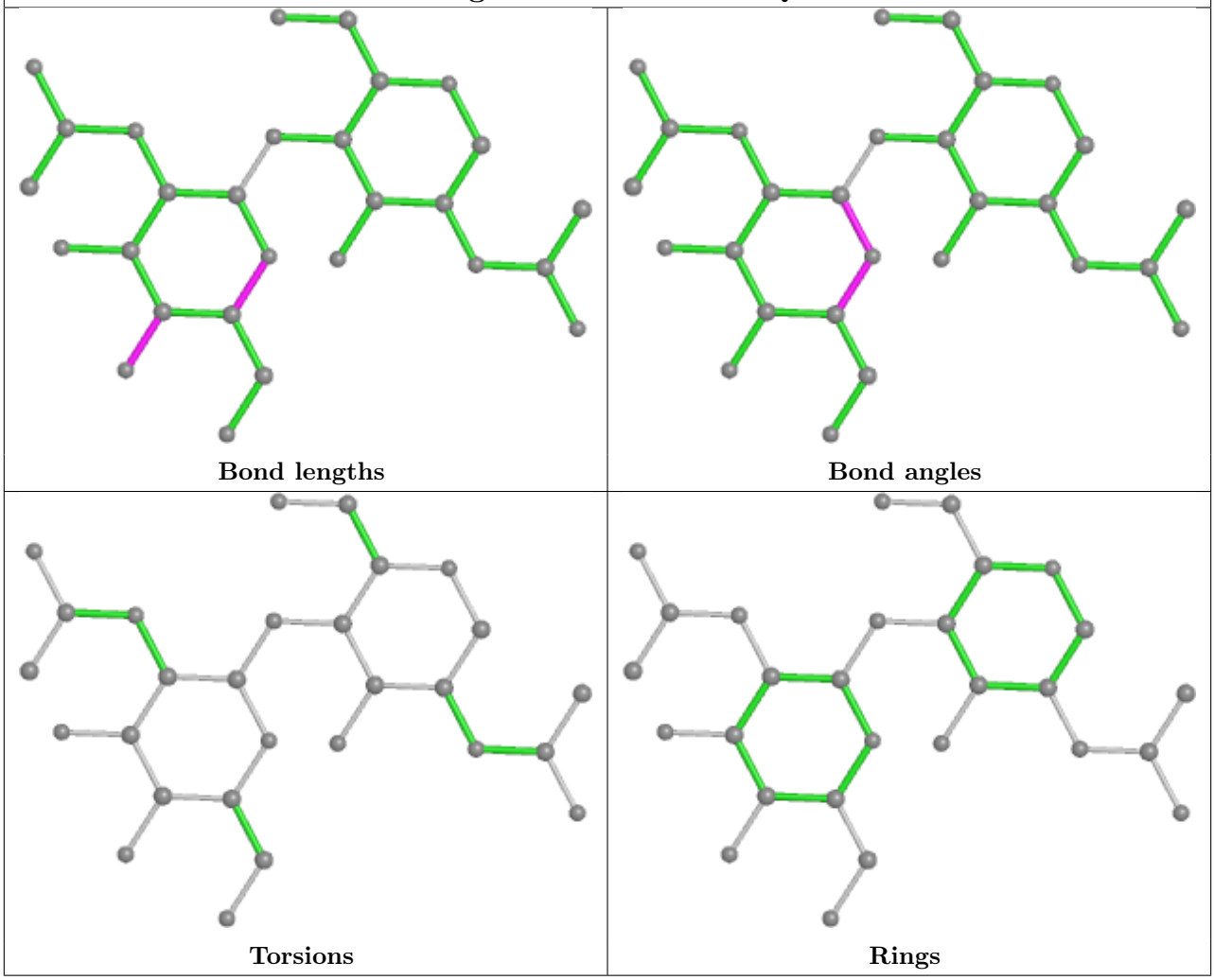
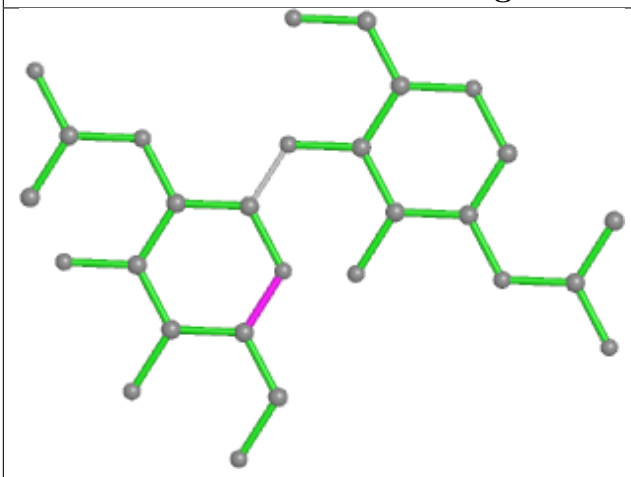


Rings

Oligosaccharide Chain Q



Oligosaccharide Chain R



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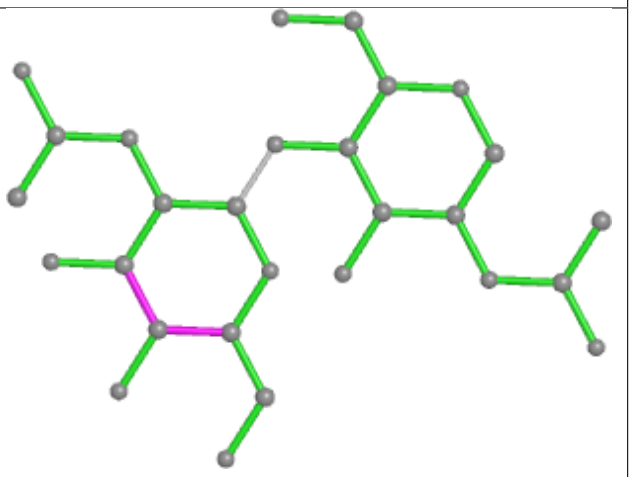
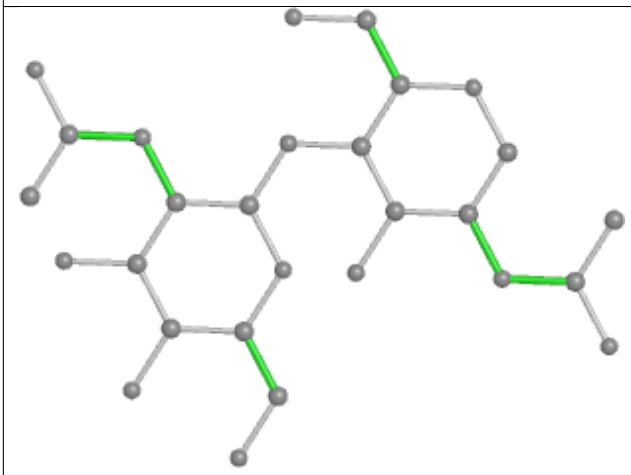


Bond angles



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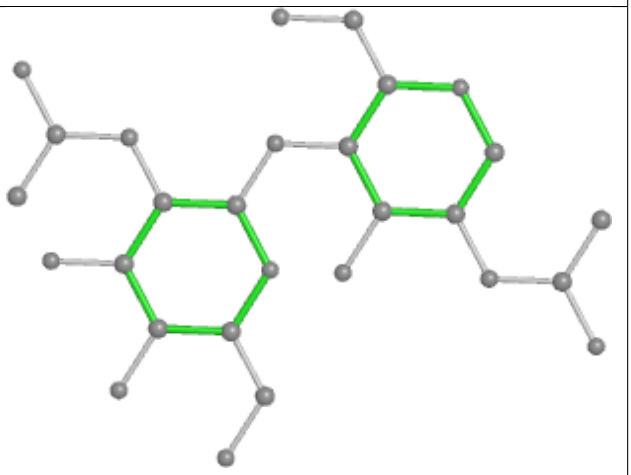
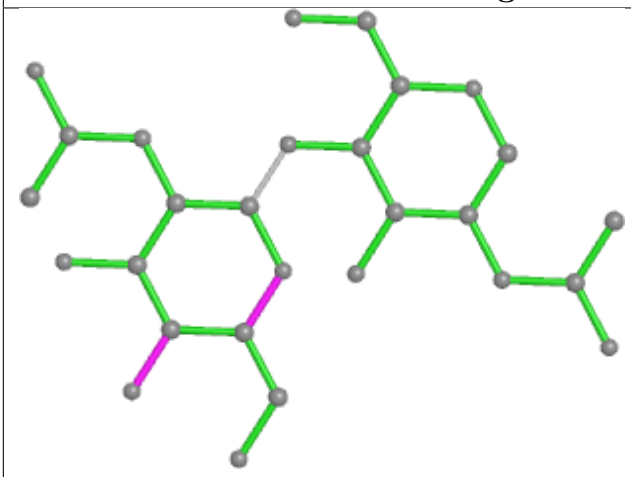


Rings

Oligosaccharide Chain S



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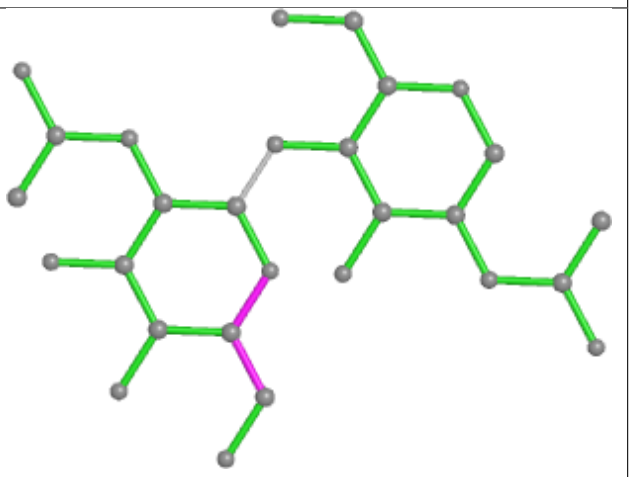

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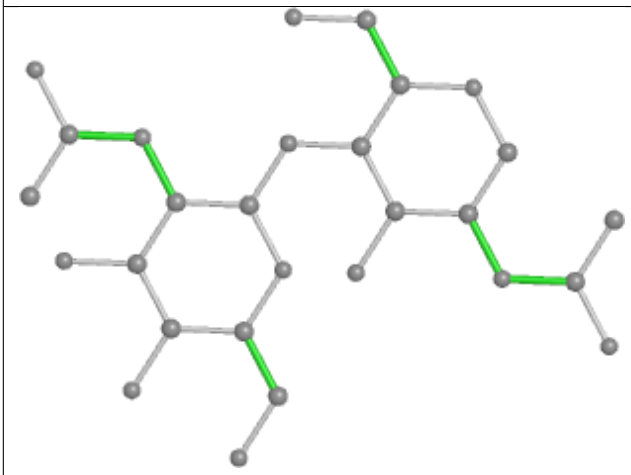

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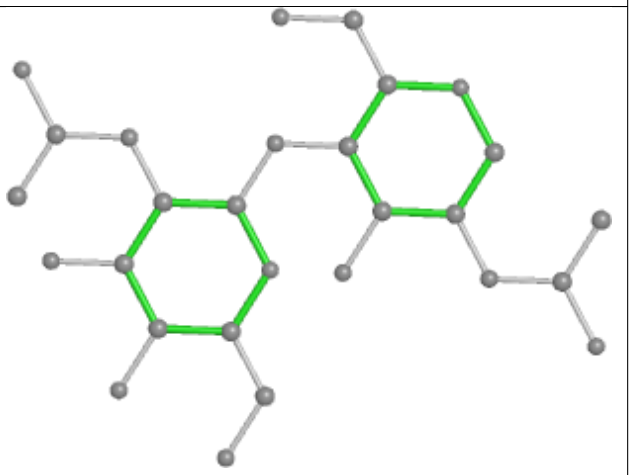
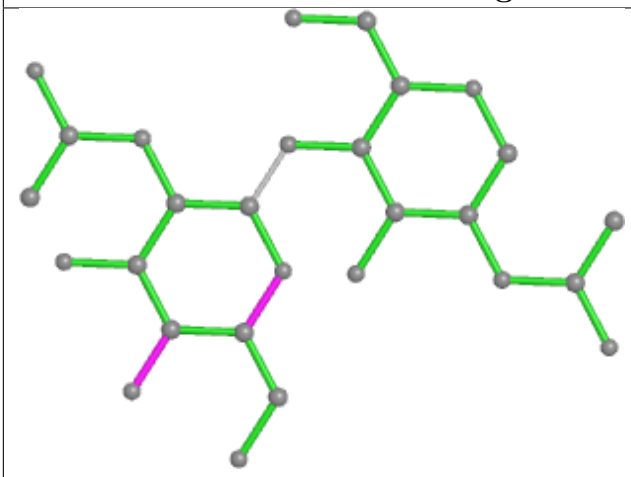


Rings

Oligosaccharide Chain T



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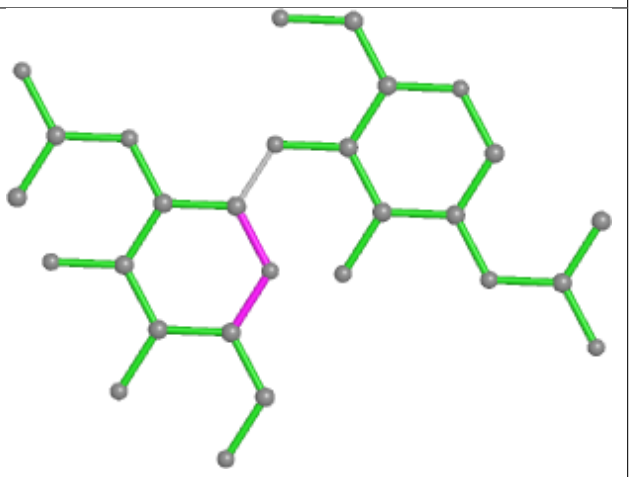

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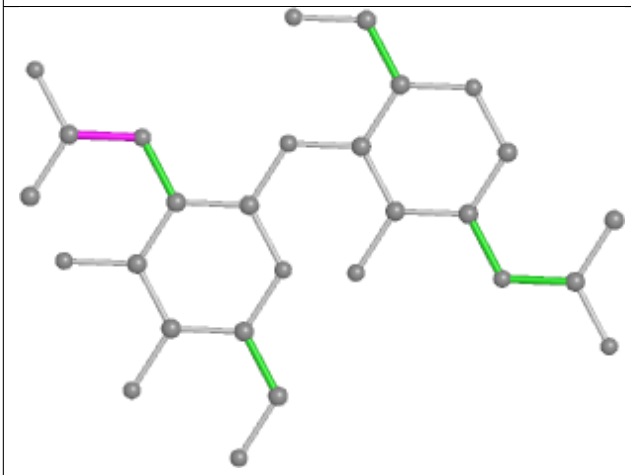

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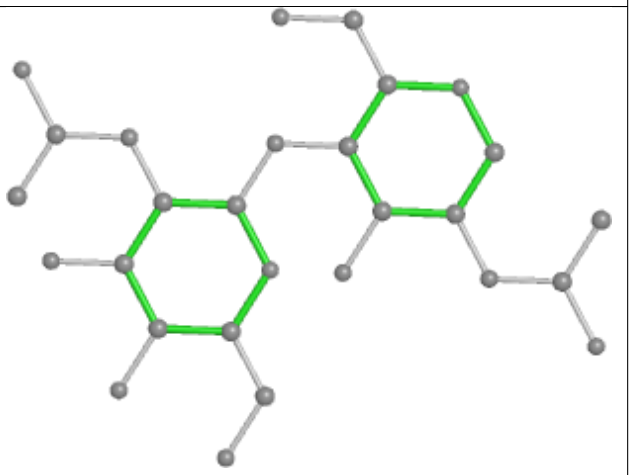
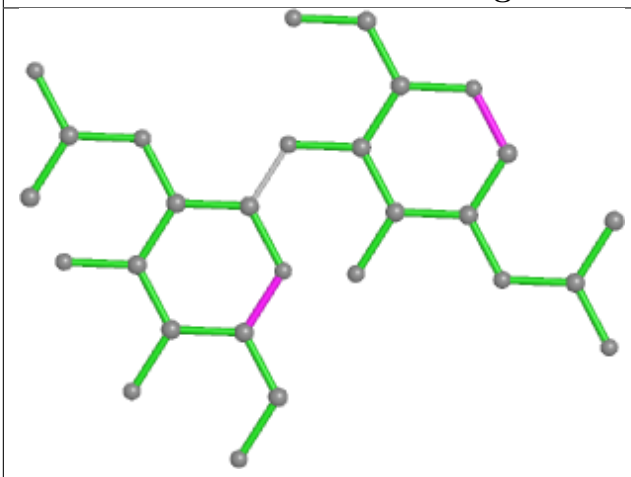


Rings

Oligosaccharide Chain U



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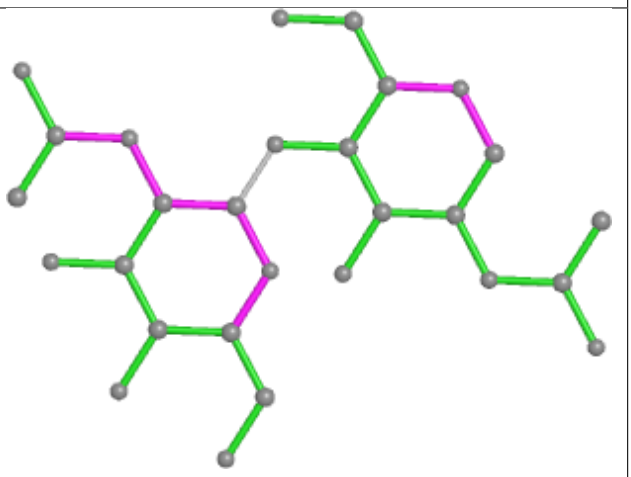

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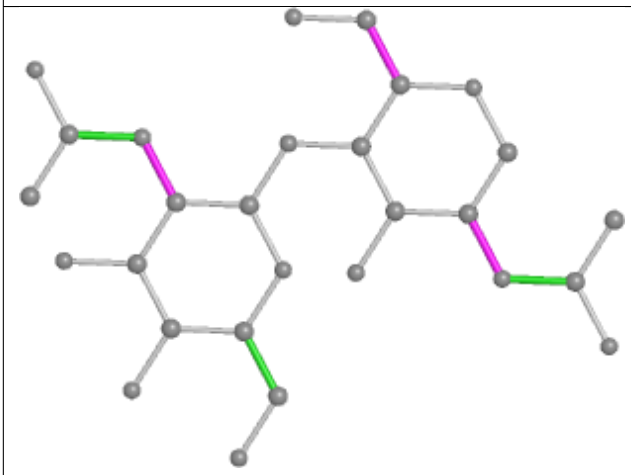

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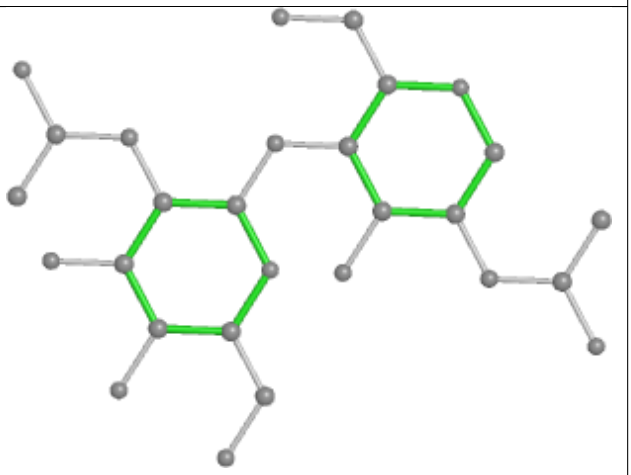
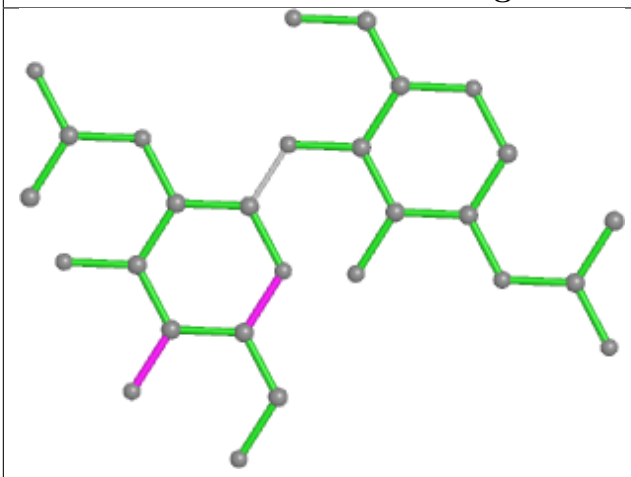


Rings

Oligosaccharide Chain V



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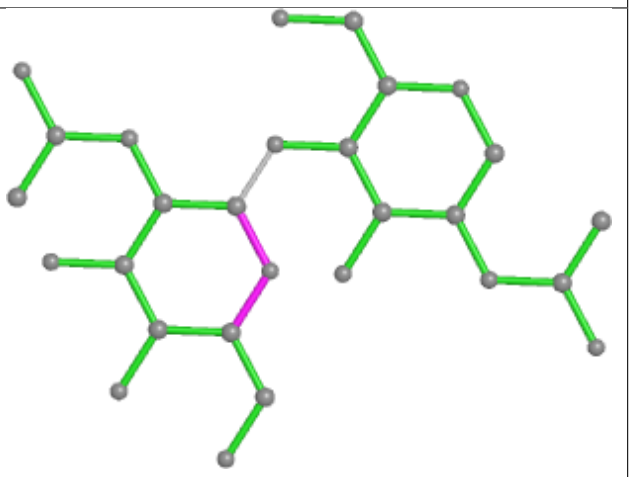

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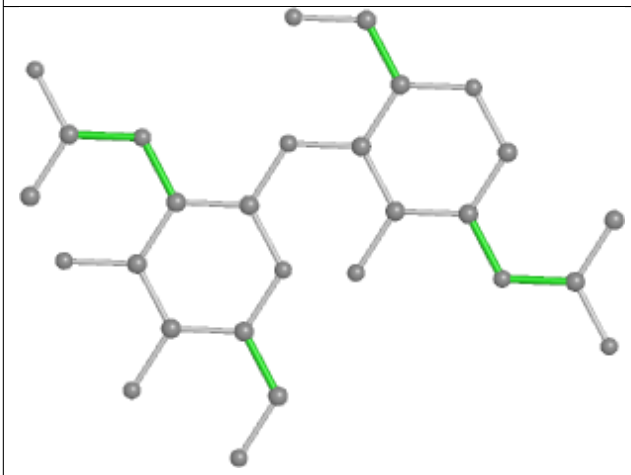

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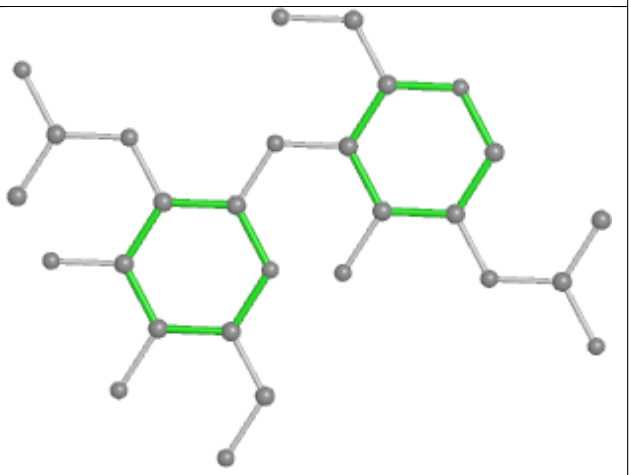
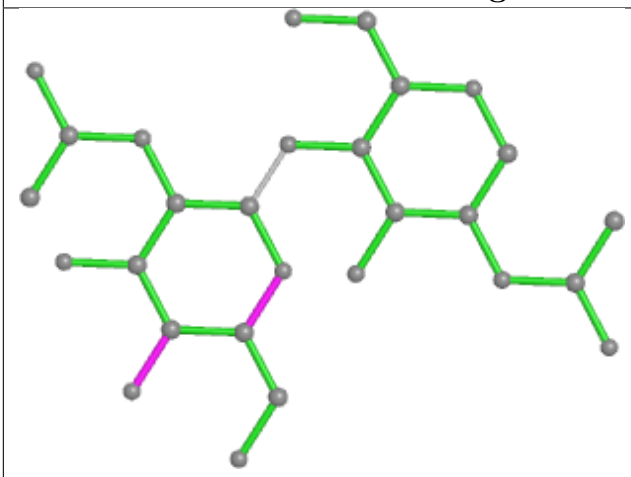


Rings

Oligosaccharide Chain W



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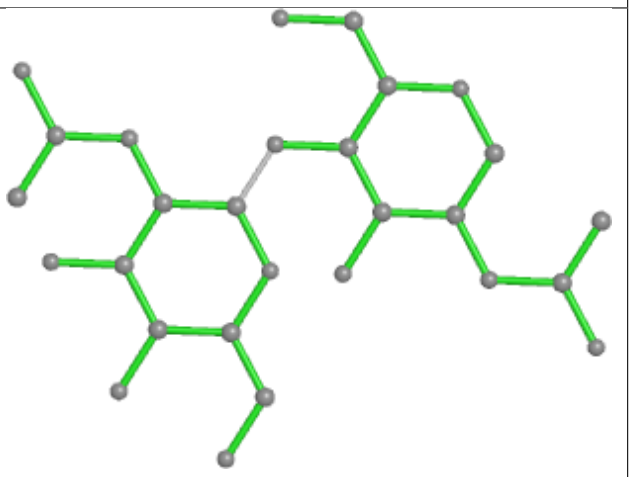

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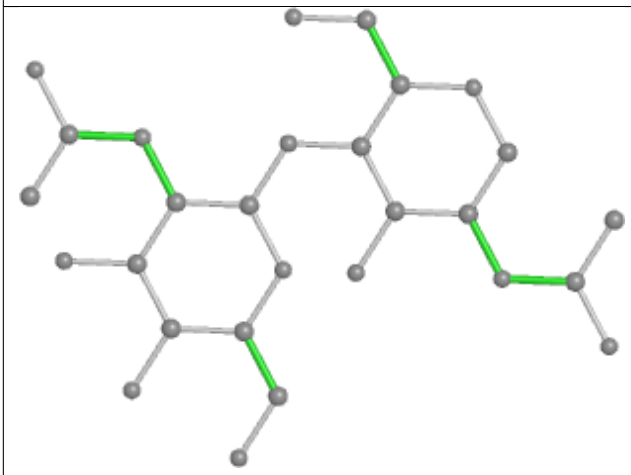

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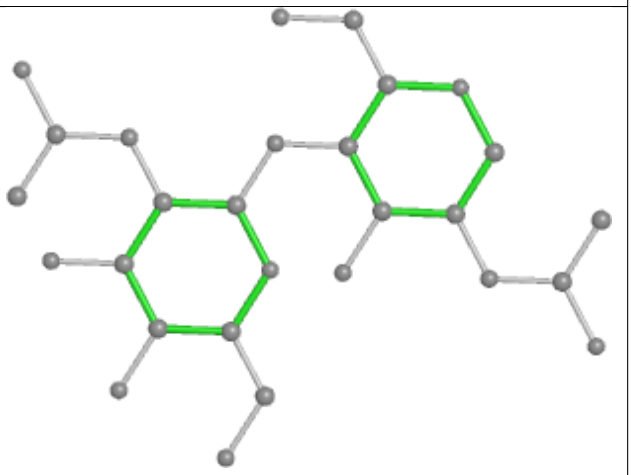

Rings

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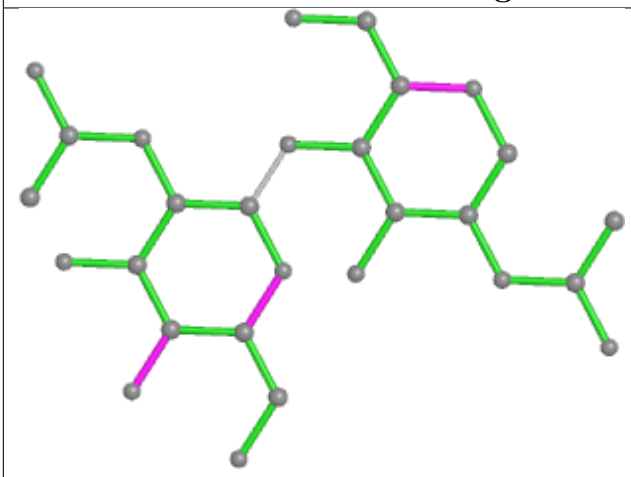

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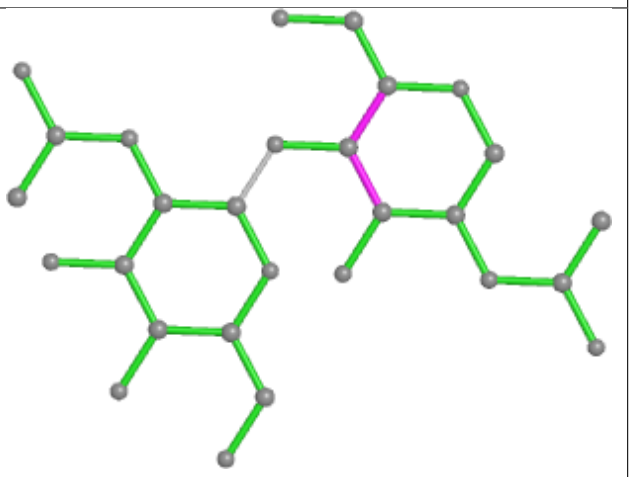

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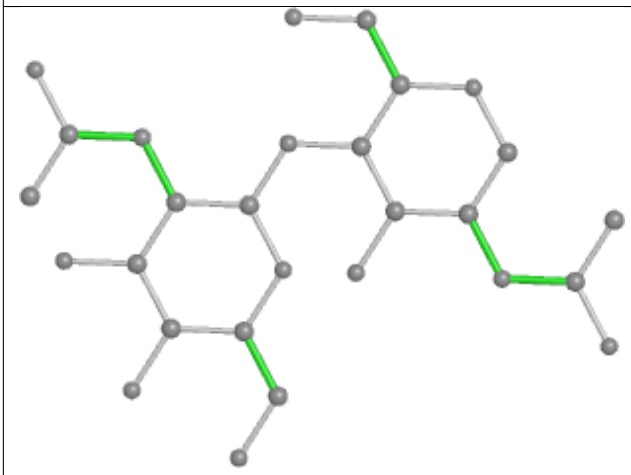

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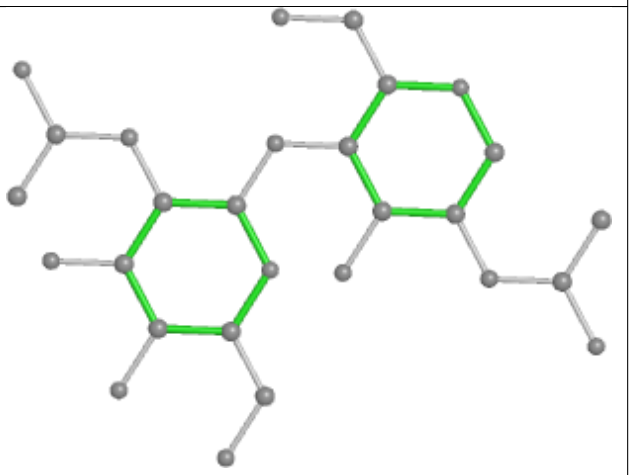
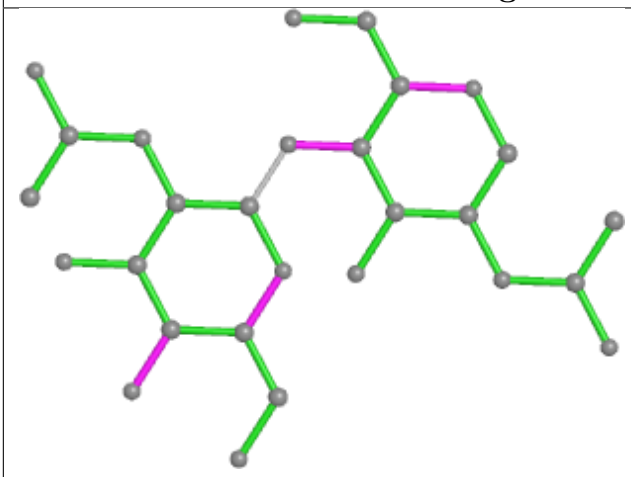


Rings

Oligosaccharide Chain a



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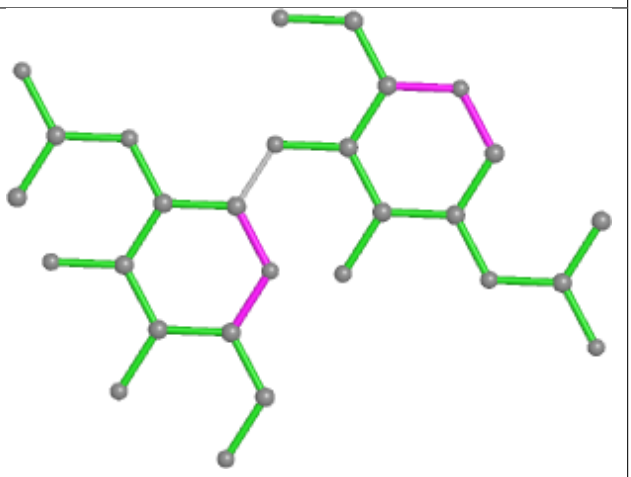

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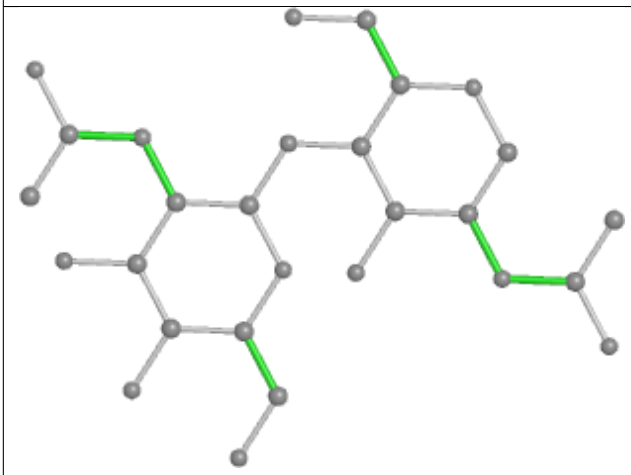

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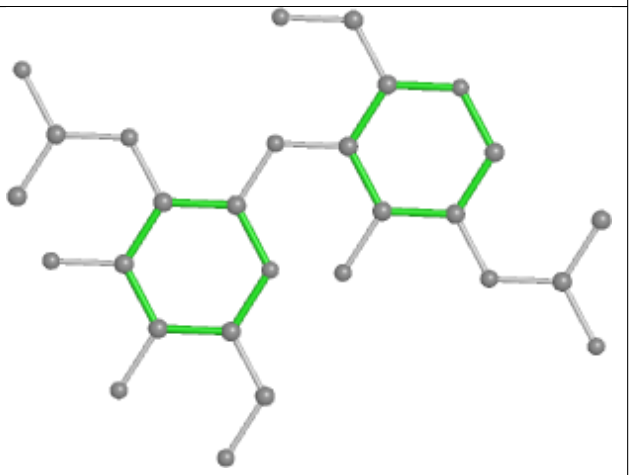
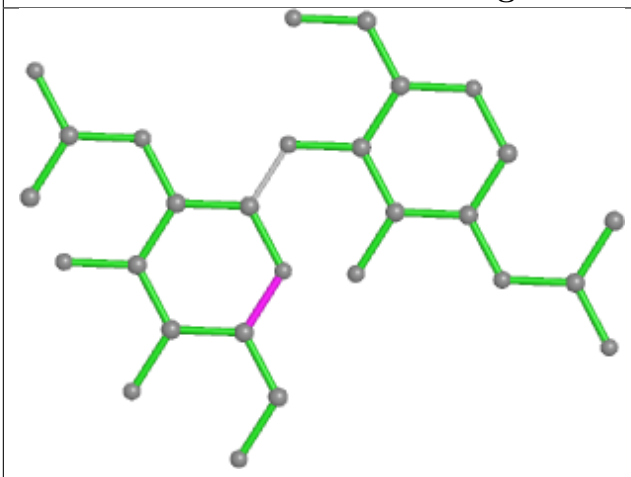


Rings

Oligosaccharide Chain b



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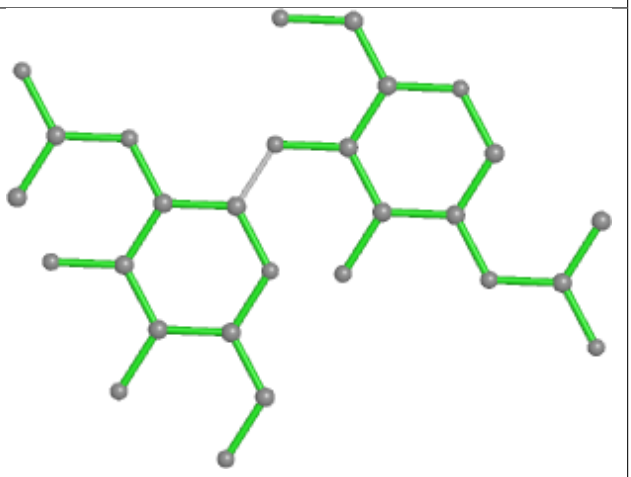

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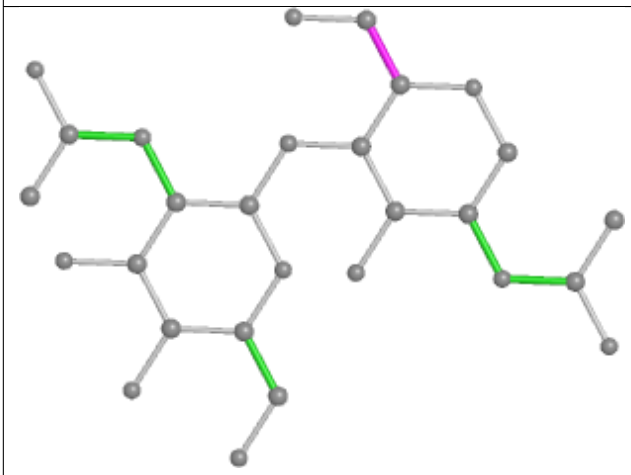

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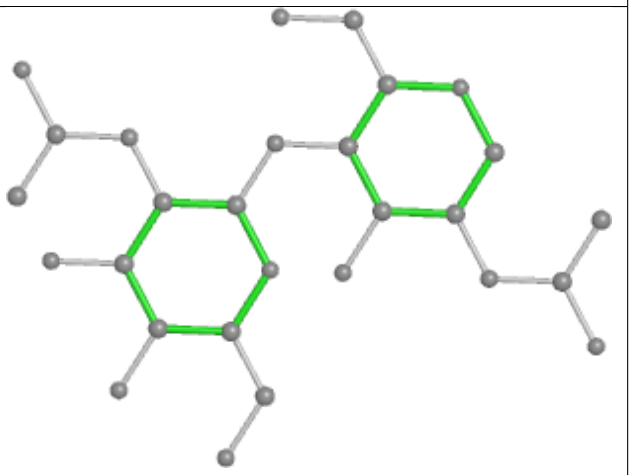
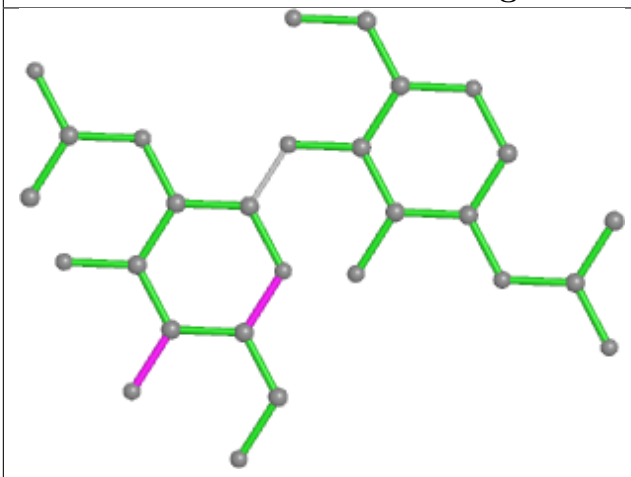


Rings

Oligosaccharide Chain c



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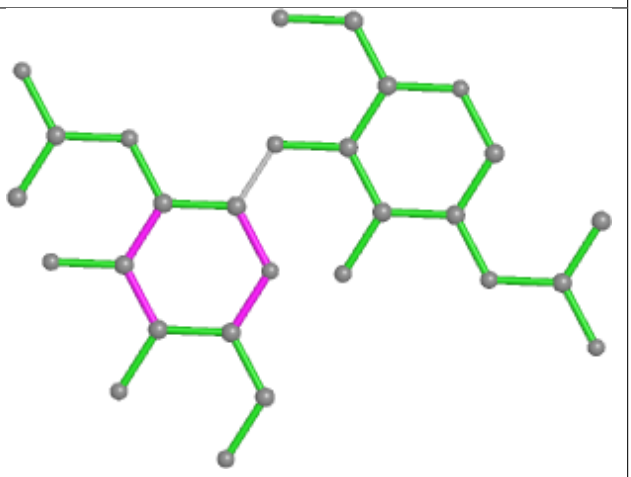

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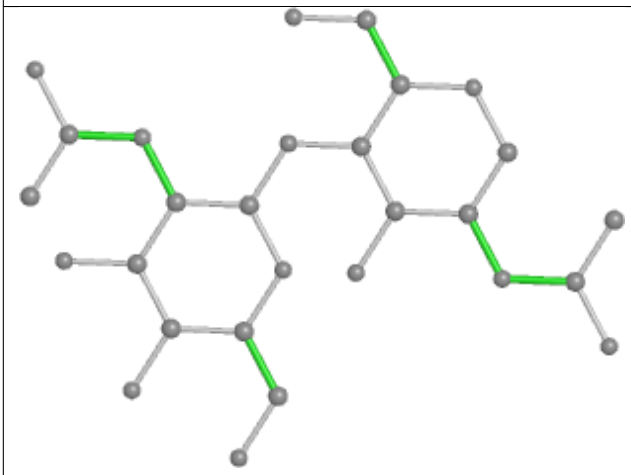

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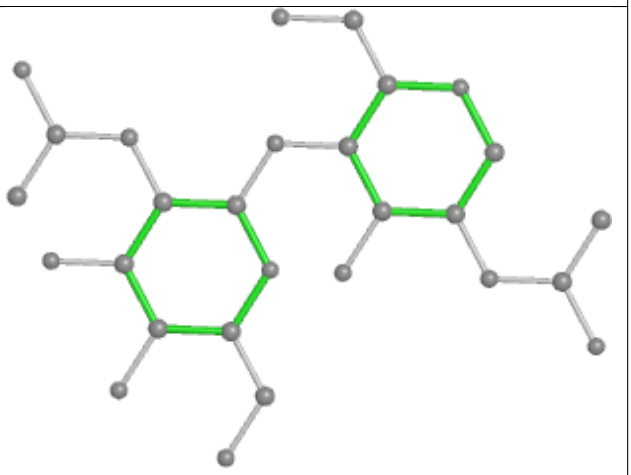
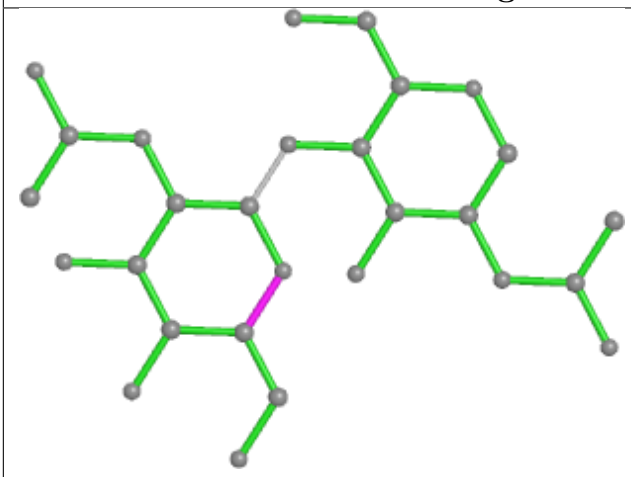
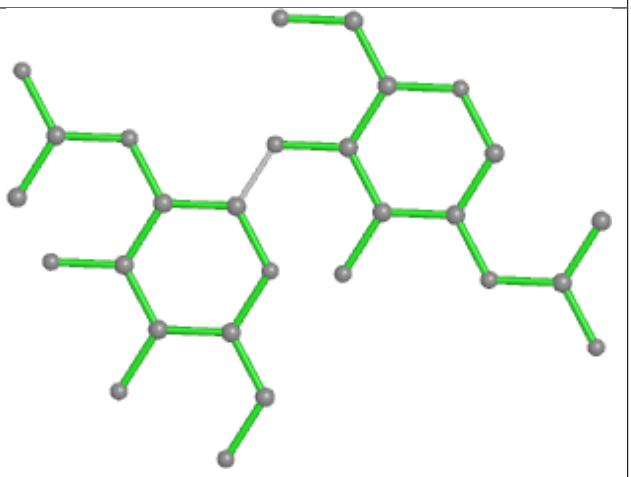
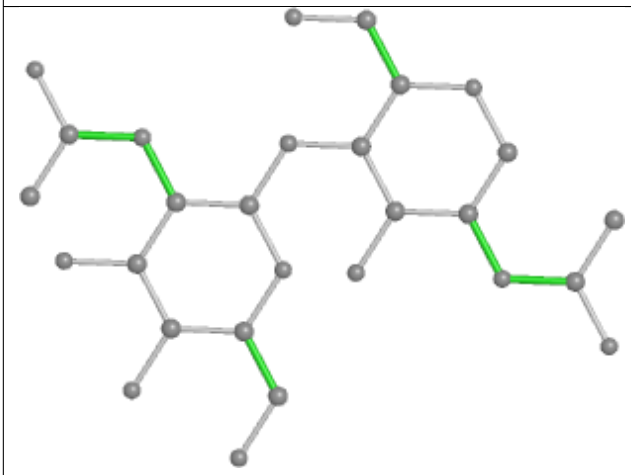
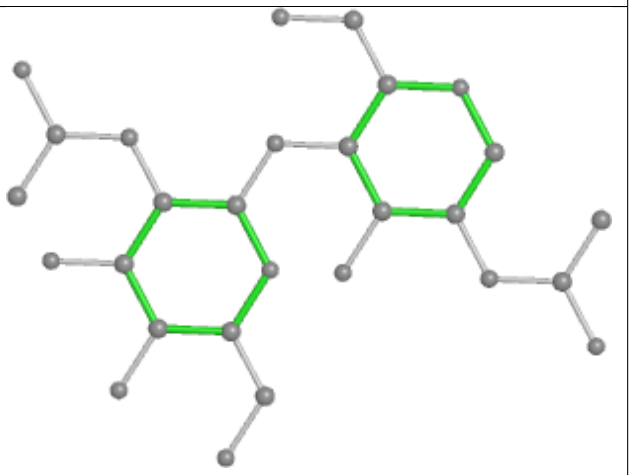


Rings

Oligosaccharide Chain d	
 Bond lengths	 Bond angles
 Torsions	 Rings

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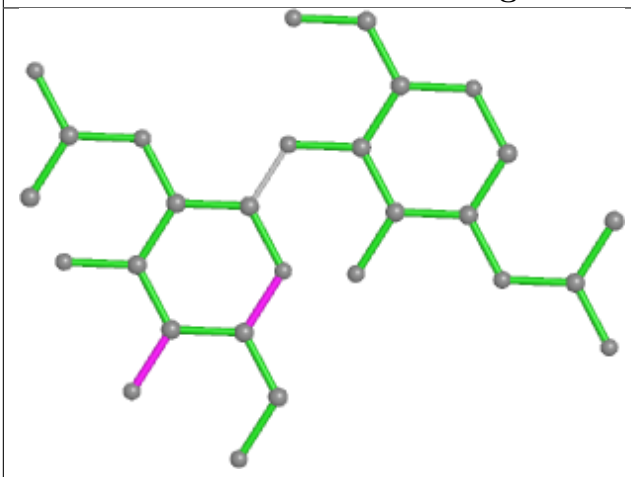

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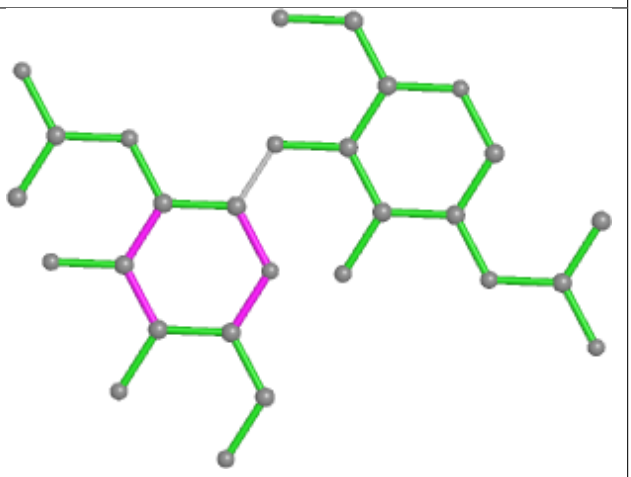
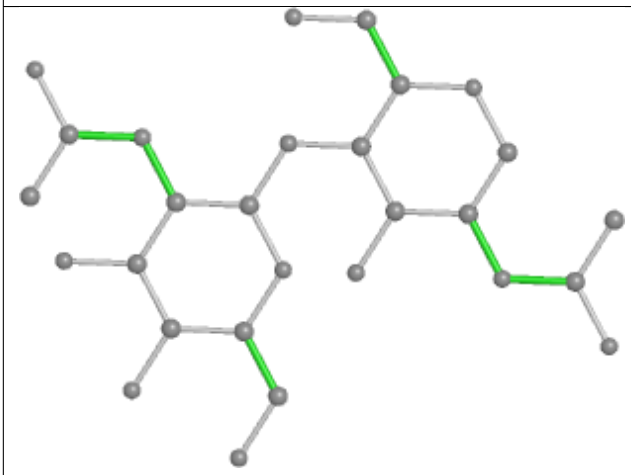
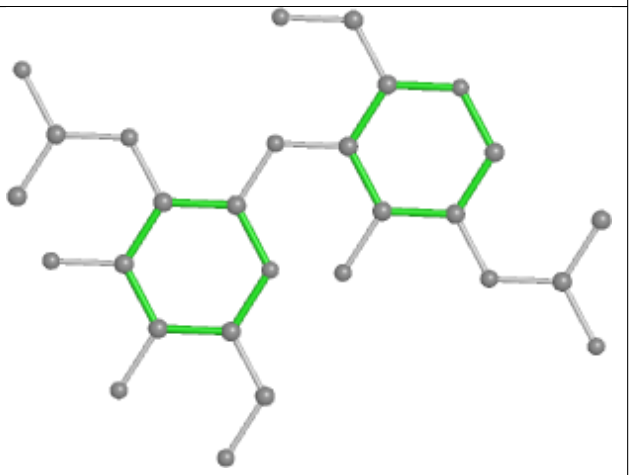


Bond angles

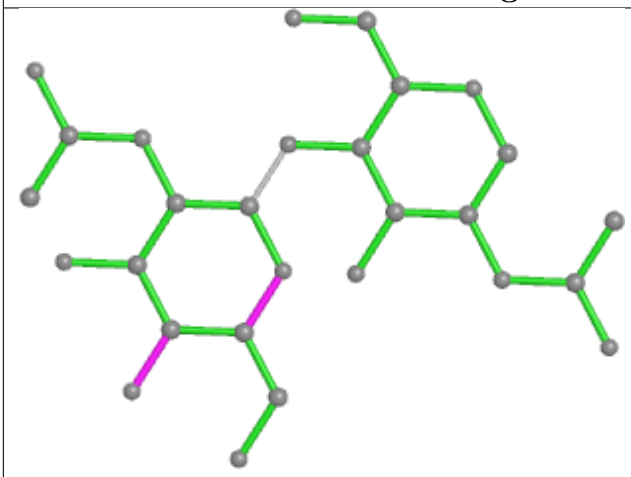


Torsions

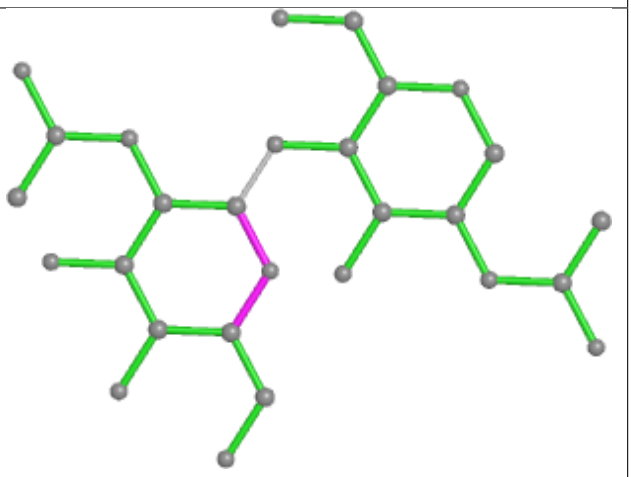


Rings

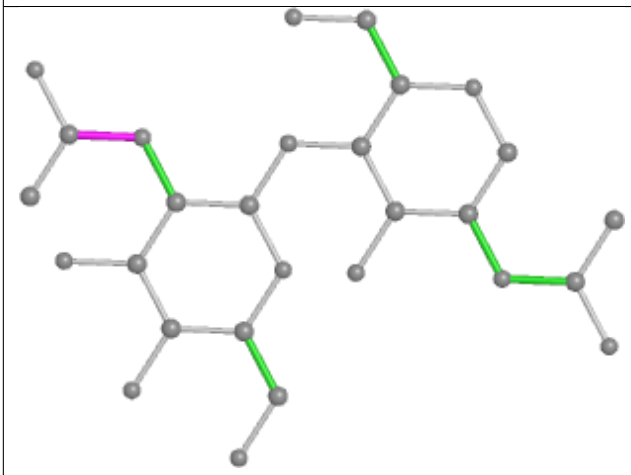
Oligosaccharide Chain f



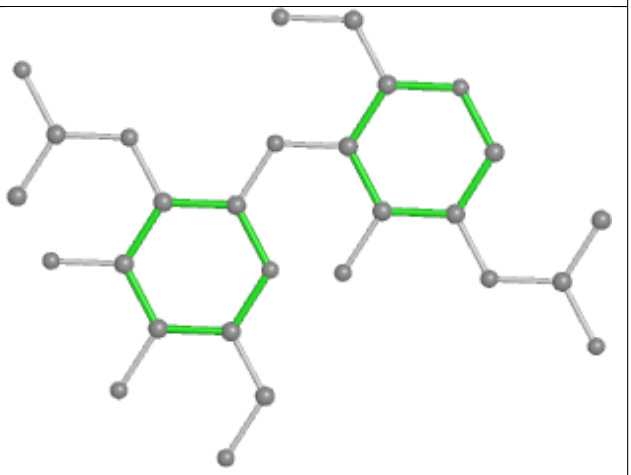
Bond lengths



Bond angles

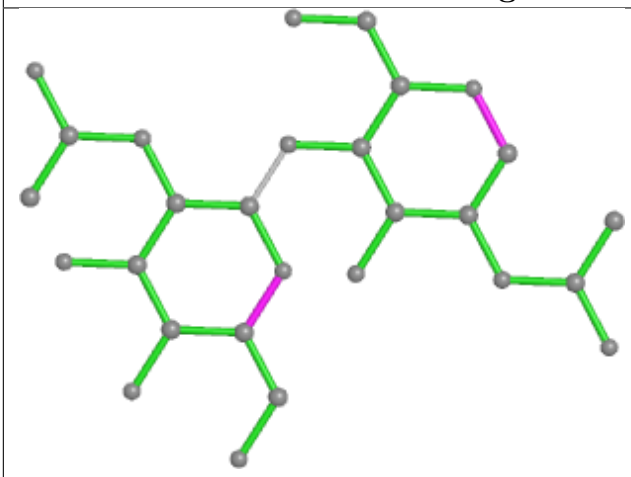


Torsions

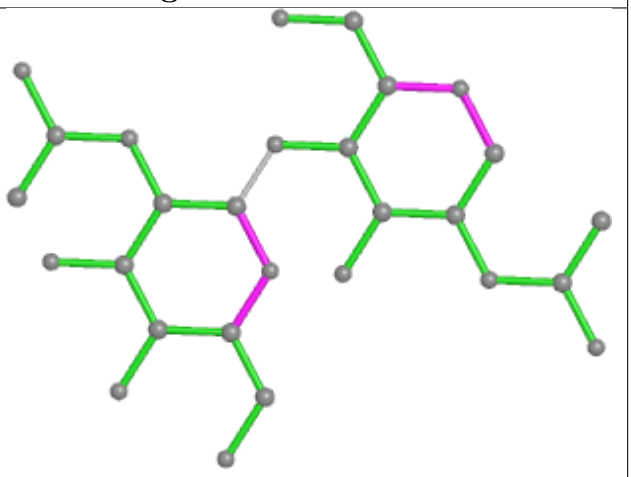


Rings

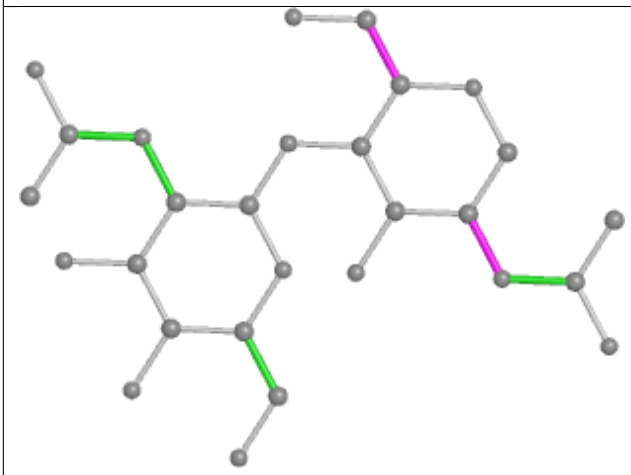
Oligosaccharide Chain g



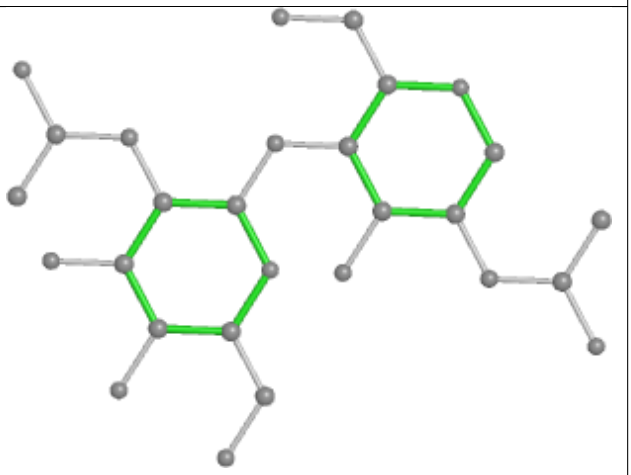
Bond lengths



Bond angles

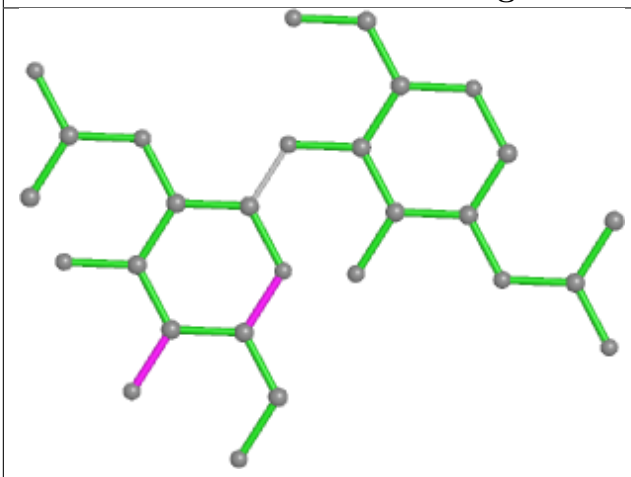


Torsions

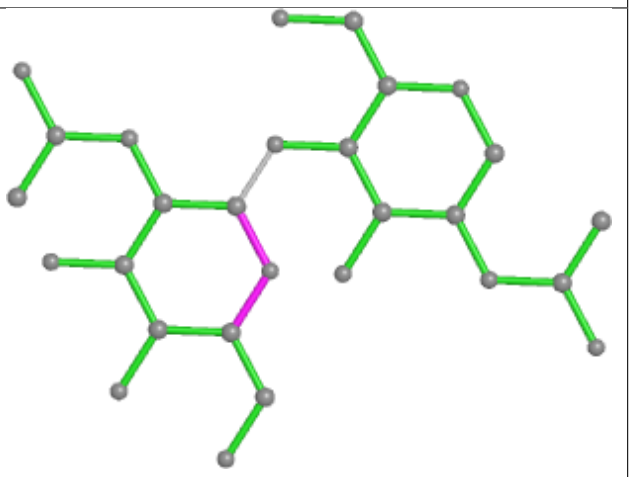


Rings

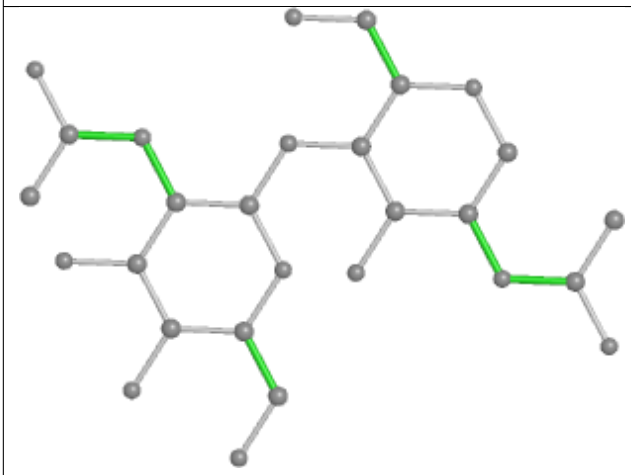
Oligosaccharide Chain h



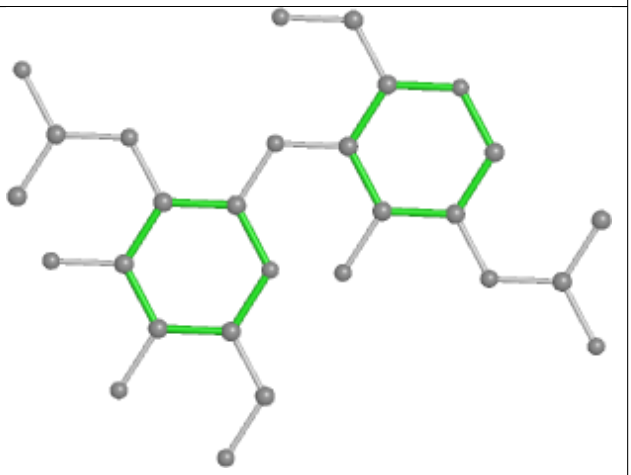
Bond lengths



Bond angles

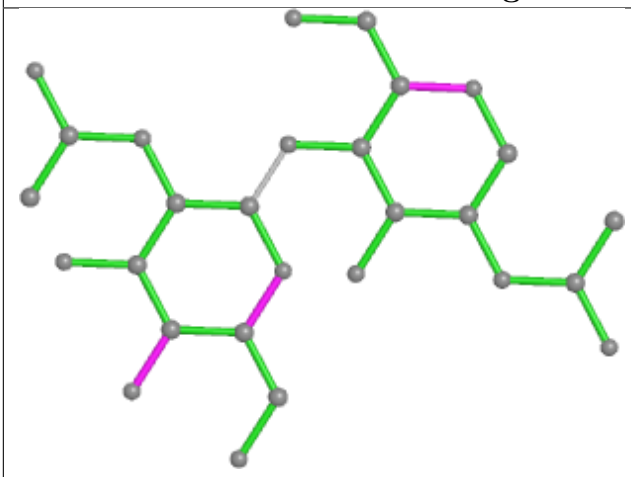


Torsions

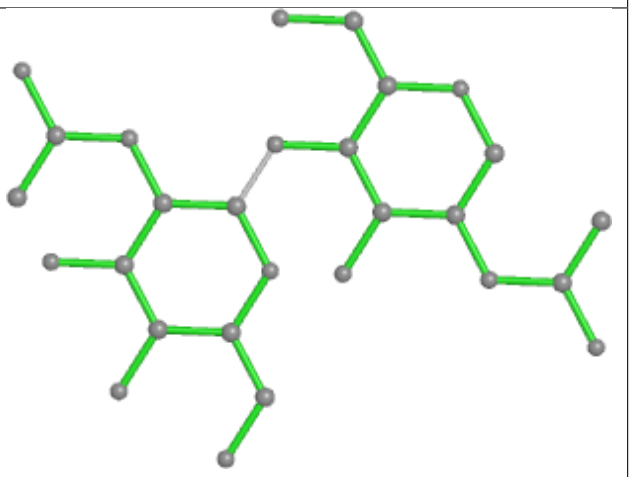


Rings

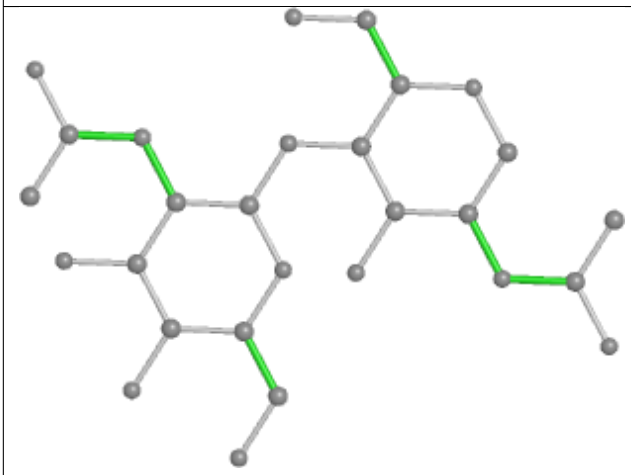
Oligosaccharide Chain i



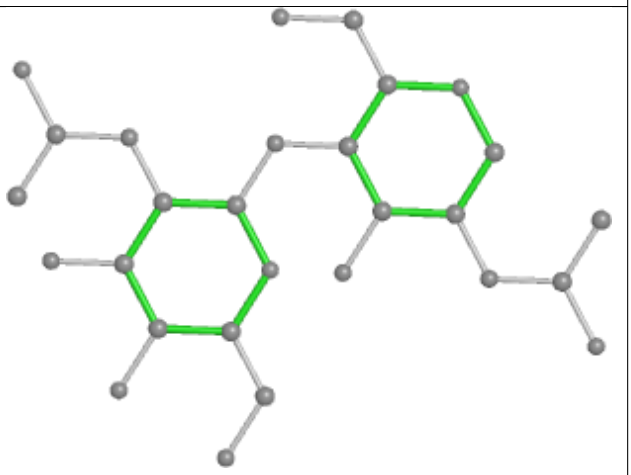
Bond lengths



Bond angles

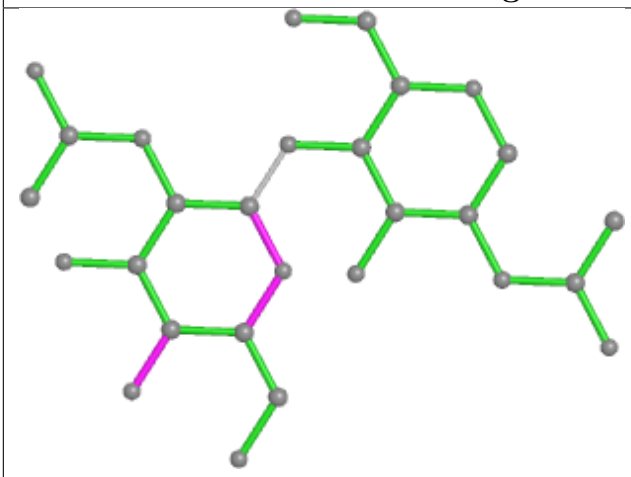


Torsions

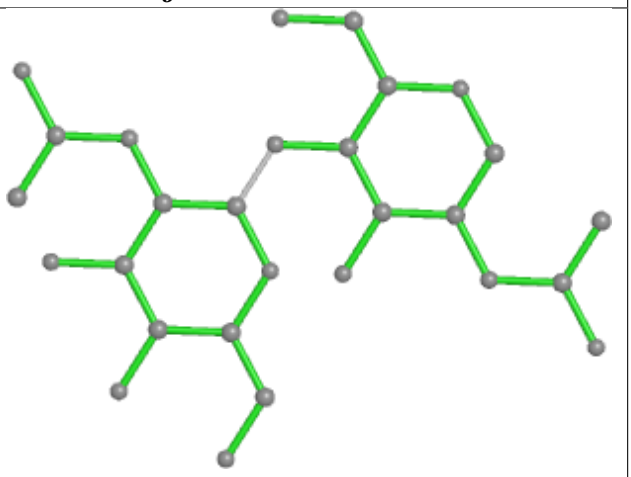


Rings

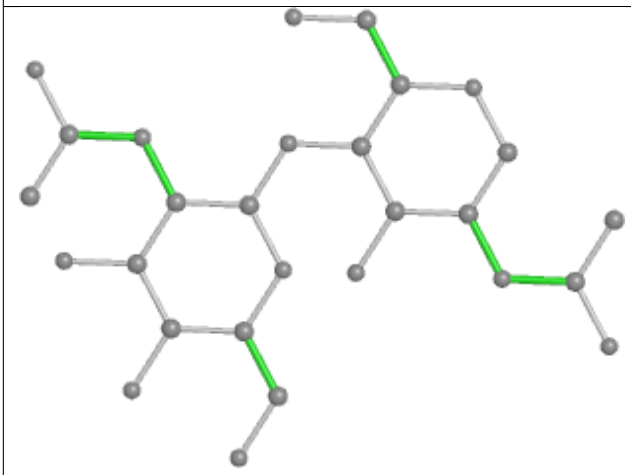
Oligosaccharide Chain j



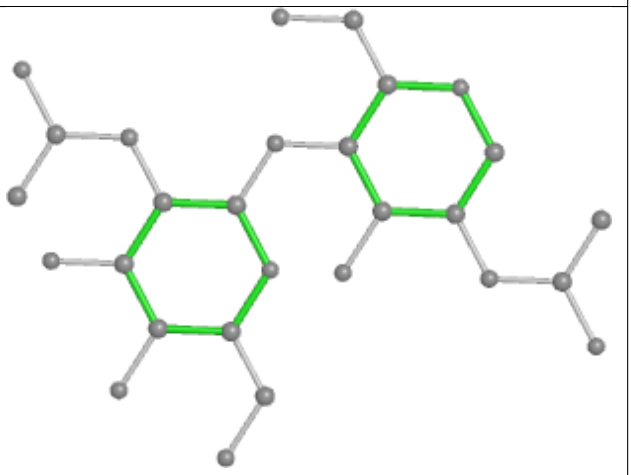
Bond lengths



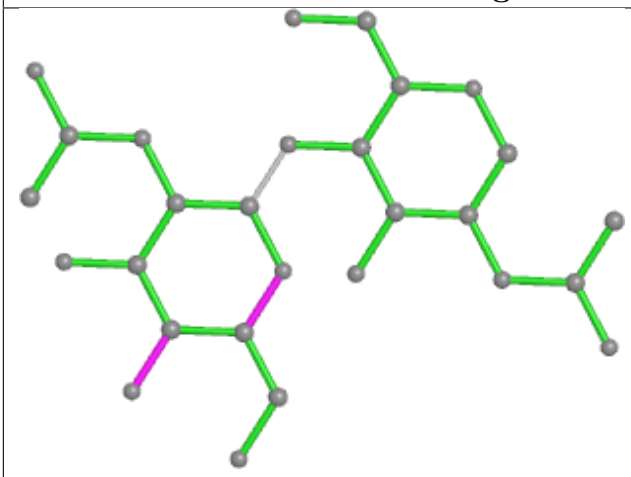
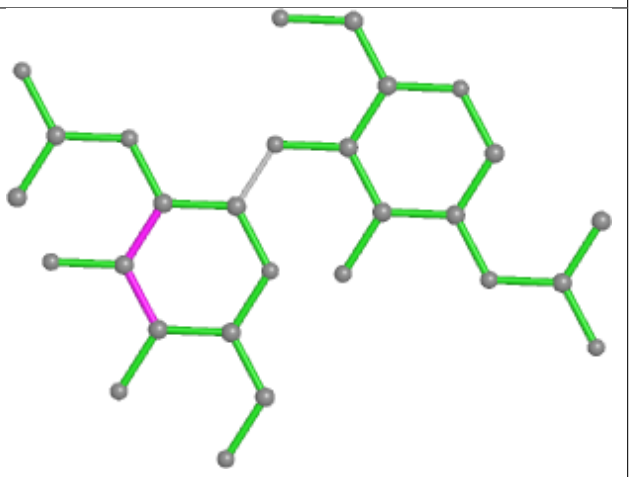
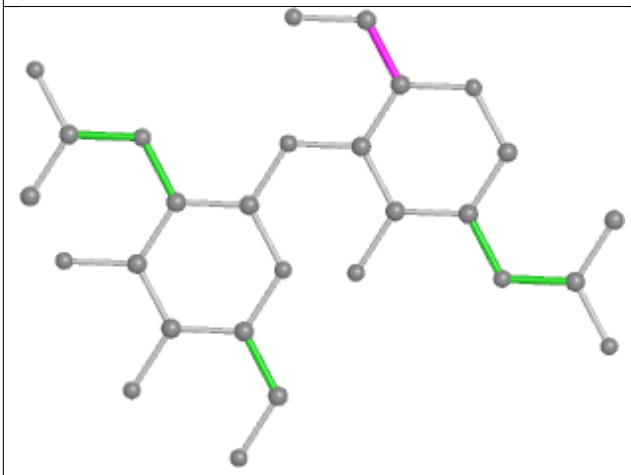
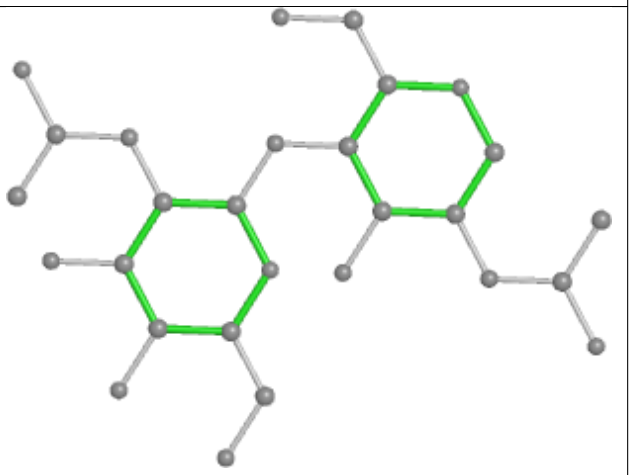
Bond angles

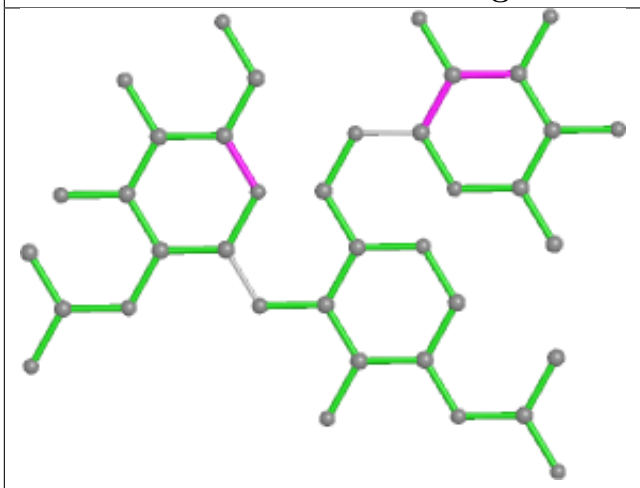
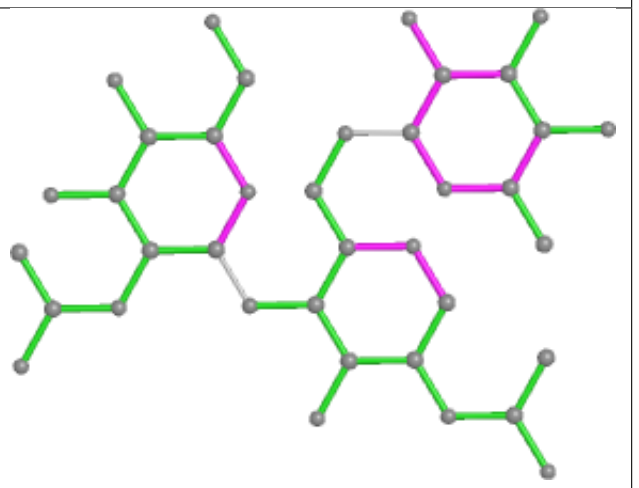
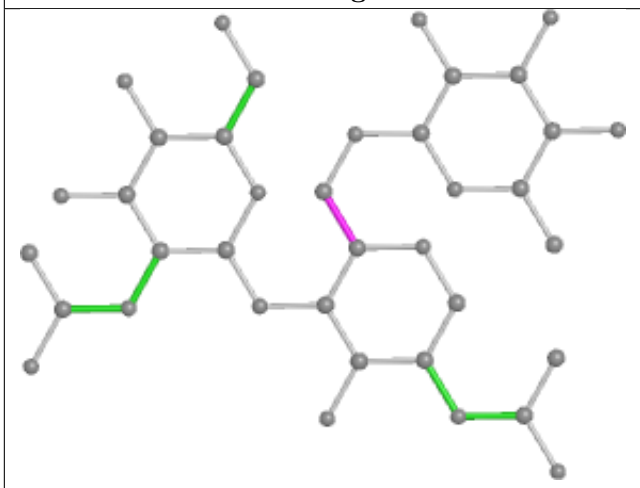
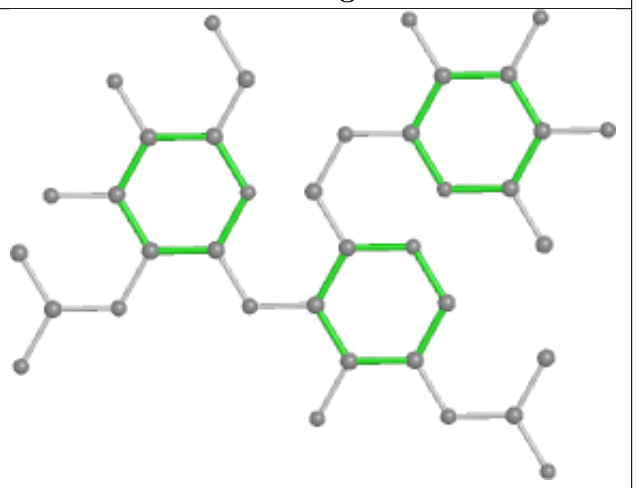


Torsions

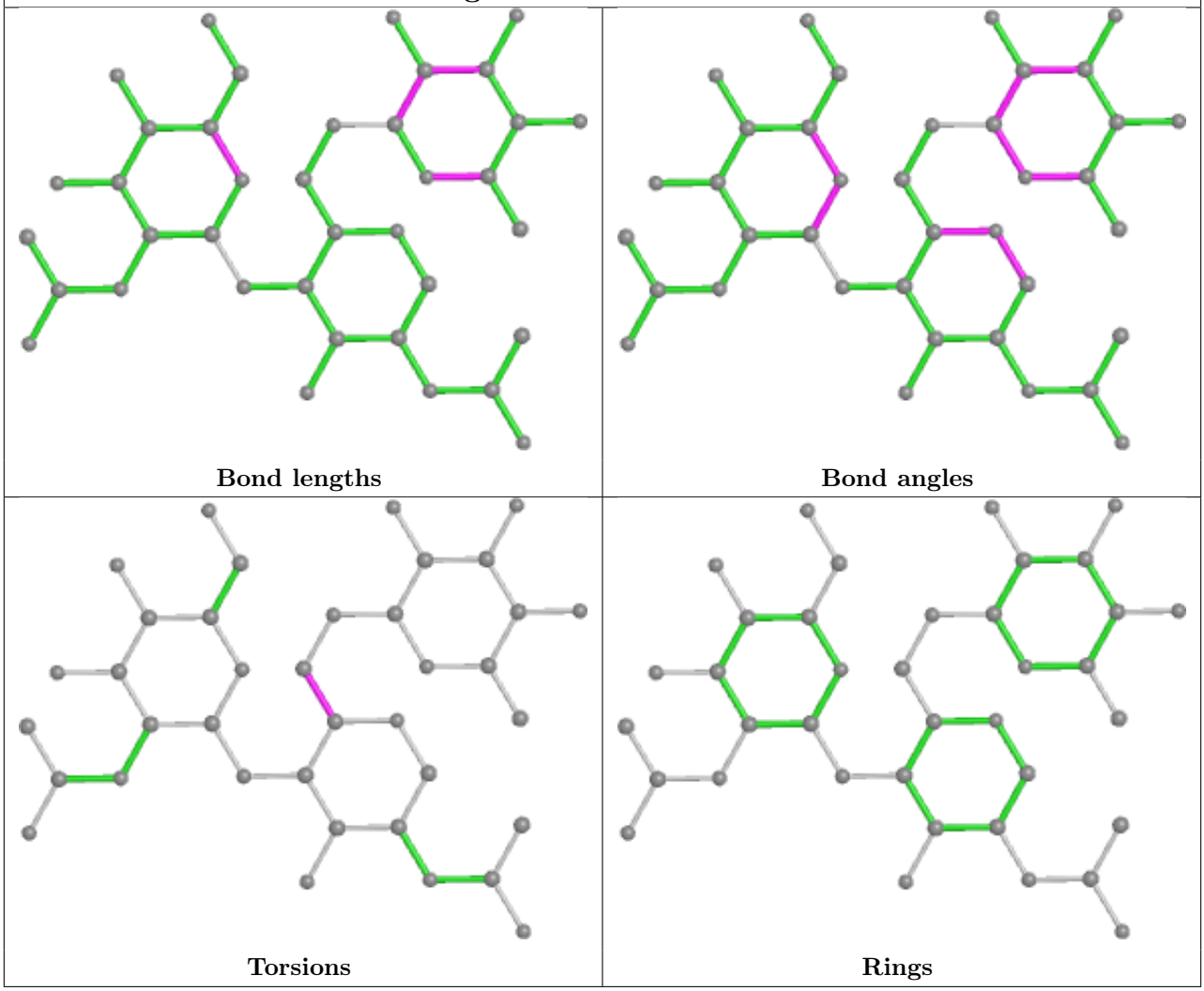


Rings

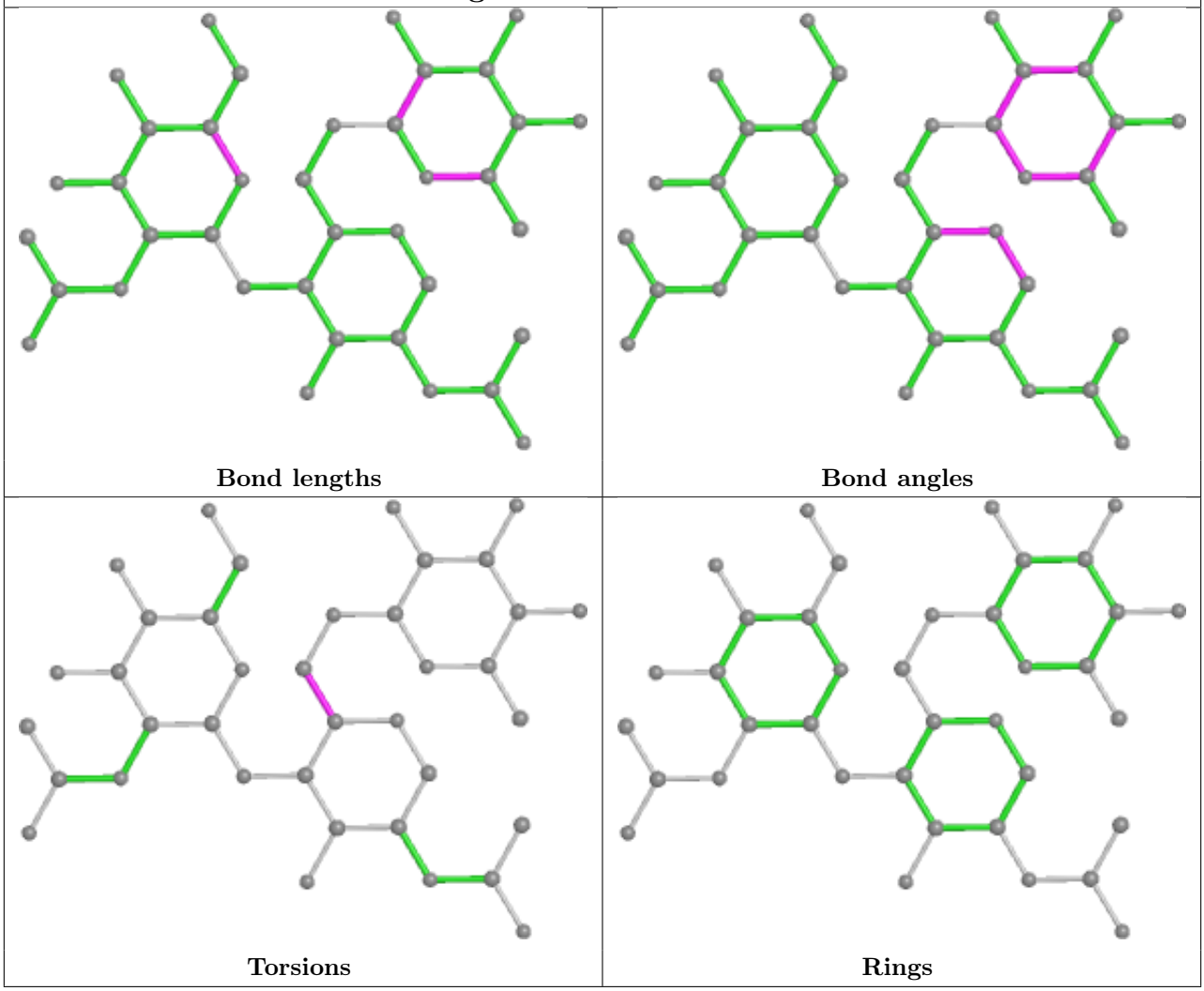
Oligosaccharide Chain m	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Y



Oligosaccharide Chain k



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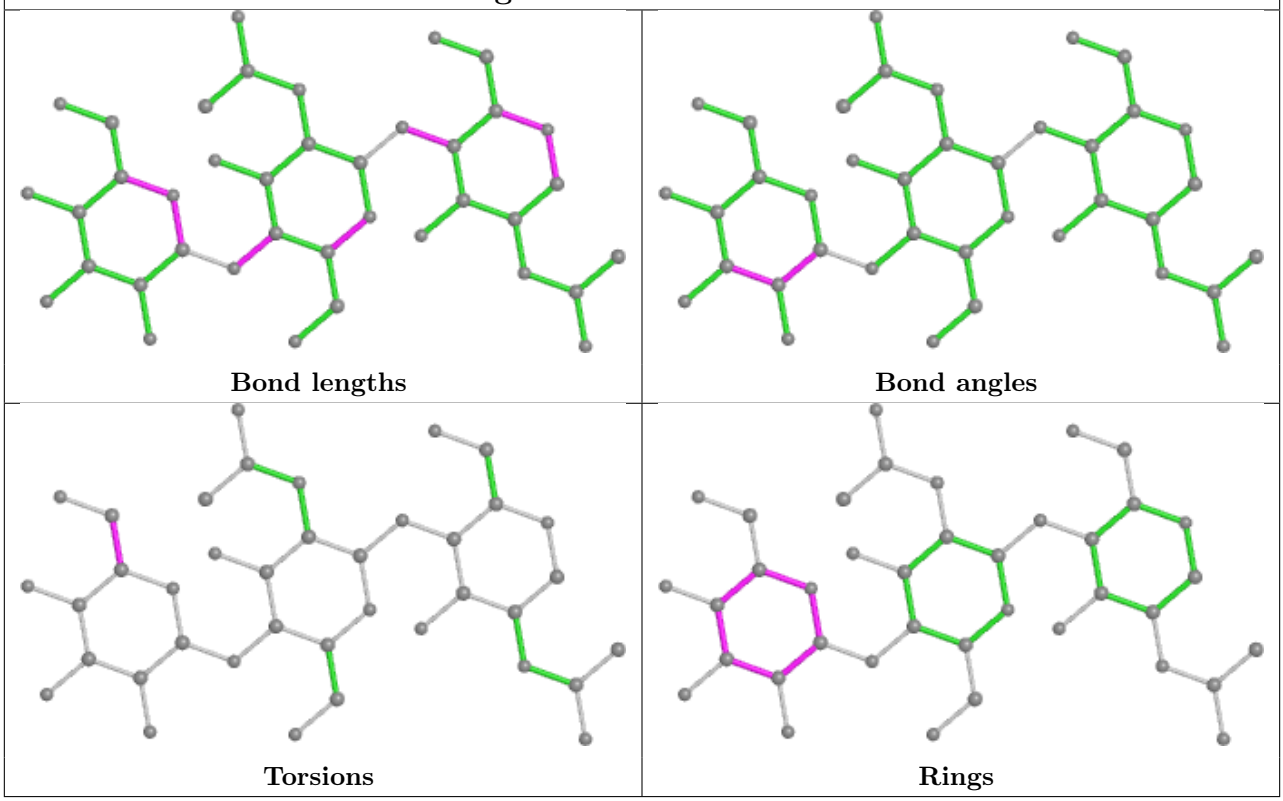
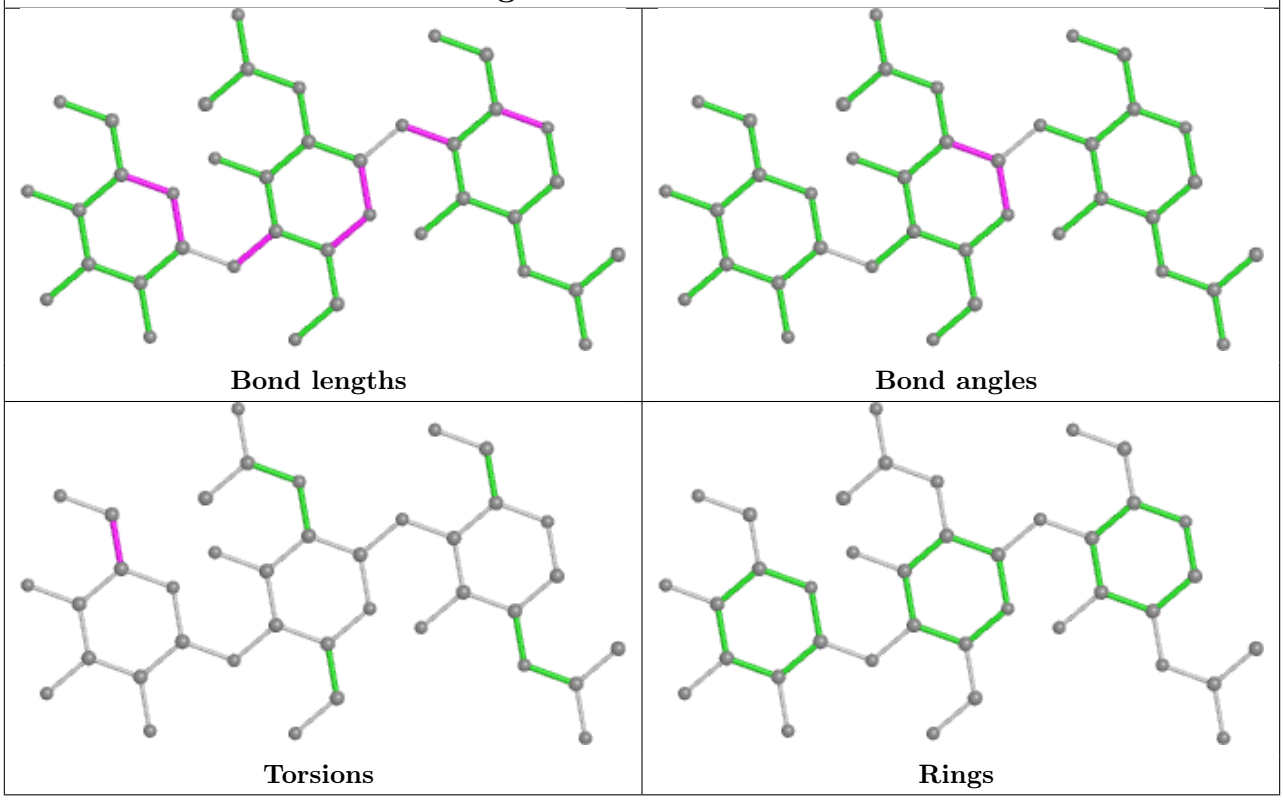
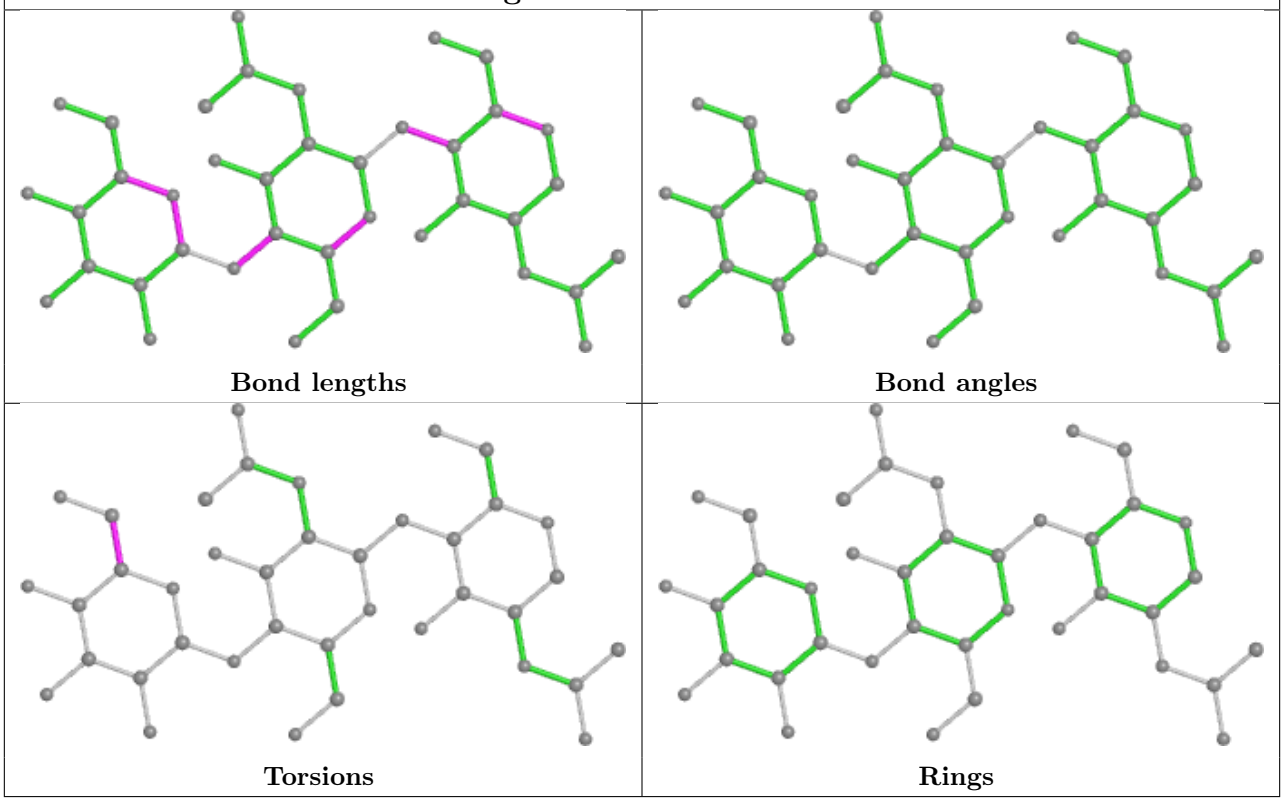


Oligosaccharide Chain Z



Oligosaccharide Chain l



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	$\#\|Z\| > 2$
5	NAG	B	1403	1	14,14,15	0.31	0	17,19,21	0.44	0
5	NAG	B	1406	1	14,14,15	1.19	1 (7%)	17,19,21	0.61	0
5	NAG	C	1401	1	14,14,15	0.57	0	17,19,21	0.45	0
5	NAG	C	1402	1	14,14,15	0.45	0	17,19,21	0.64	1 (5%)
5	NAG	C	1407	1	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	A	1404	1	14,14,15	1.36	3 (21%)	17,19,21	1.12	1 (5%)
5	NAG	A	1403	1	14,14,15	0.31	0	17,19,21	0.46	0
5	NAG	B	1404	1	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	A	1406	1	14,14,15	1.24	2 (14%)	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1405	1	14,14,15	0.26	0	17,19,21	0.36	0
5	NAG	B	1405	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	A	1407	1	14,14,15	1.24	2 (14%)	17,19,21	0.66	0
5	NAG	C	1405	1	14,14,15	0.26	0	17,19,21	0.37	0
5	NAG	B	1407	1	14,14,15	1.23	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	C	1403	1	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	B	1401	1	14,14,15	0.49	0	17,19,21	0.44	0
5	NAG	C	1406	1	14,14,15	1.16	1 (7%)	17,19,21	0.61	0
5	NAG	B	1402	-	14,14,15	1.14	1 (7%)	17,19,21	1.14	1 (5%)
5	NAG	A	1401	1	14,14,15	0.18	0	17,19,21	0.47	0
5	NAG	C	1404	1	14,14,15	1.52	2 (14%)	17,19,21	0.65	0
5	NAG	A	1402	1	14,14,15	1.28	3 (21%)	17,19,21	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1402	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	0/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1404	NAG	C1-C2	4.01	1.58	1.52
5	A	1404	NAG	O5-C5	3.02	1.49	1.43
5	B	1407	NAG	O5-C5	2.90	1.49	1.43
5	B	1402	NAG	O5-C5	2.82	1.49	1.43
5	A	1407	NAG	O5-C5	2.57	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1402	NAG	C1-O5-C5	3.78	117.31	112.19
5	A	1404	NAG	C1-O5-C5	3.53	116.97	112.19
5	C	1402	NAG	C1-O5-C5	2.23	115.22	112.19
5	B	1407	NAG	C3-C4-C5	2.10	113.99	110.24
5	A	1406	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

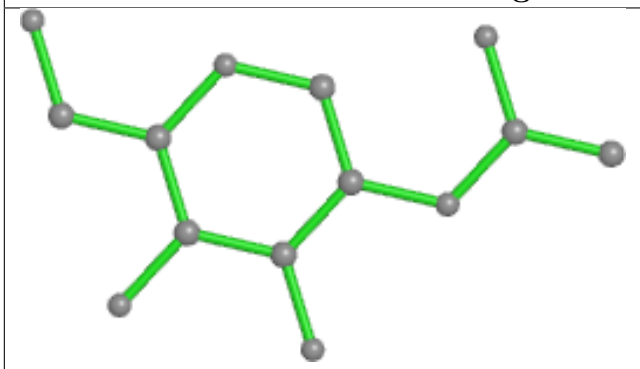
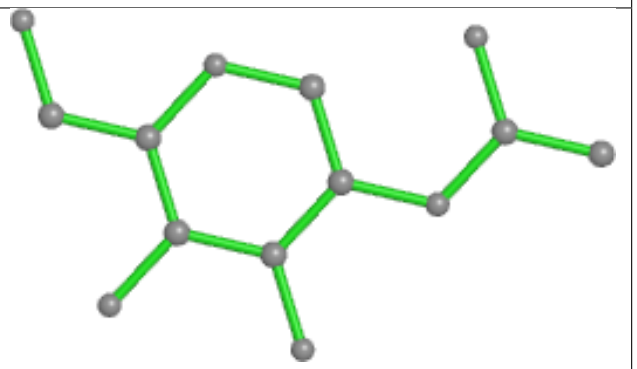
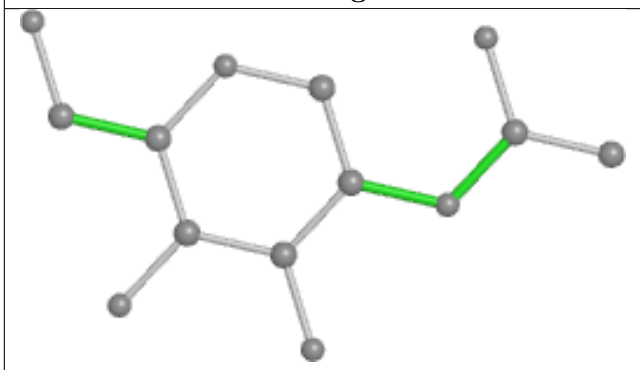
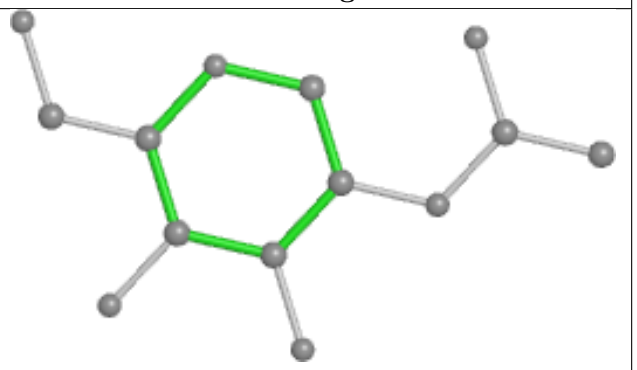
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1401	NAG	O5-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAG B 1403	
 Bond lengths	 Bond angles
 Torsions	 Rings

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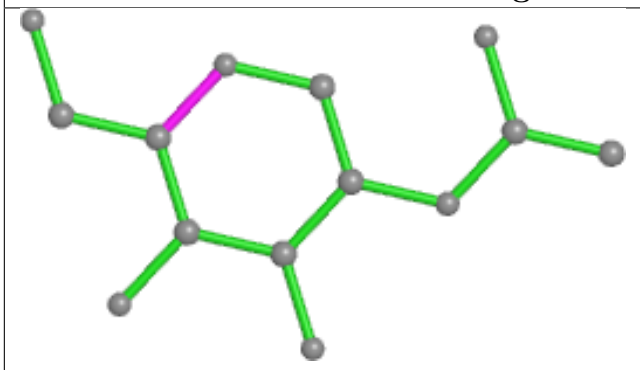
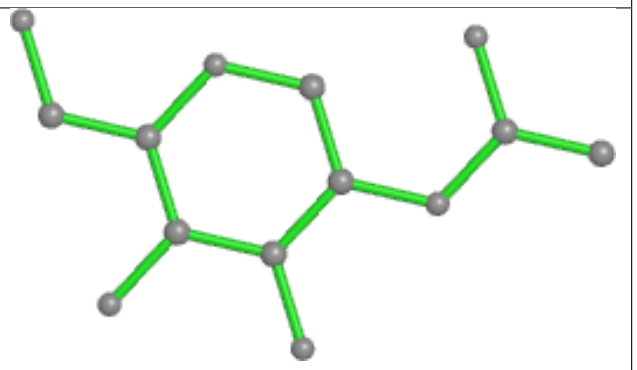
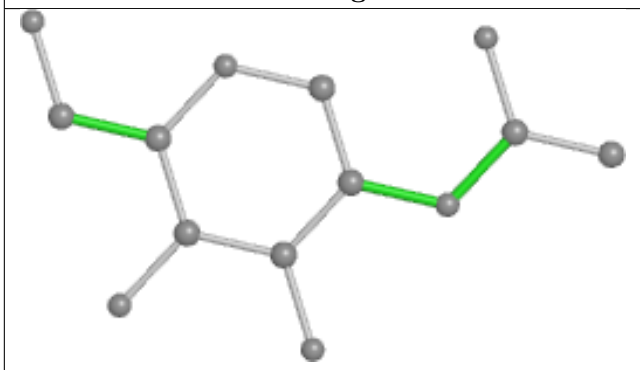
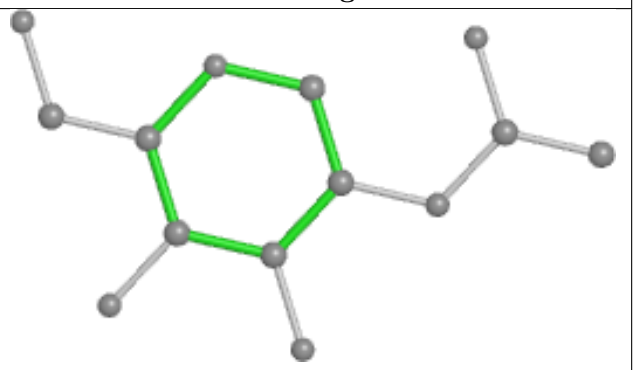
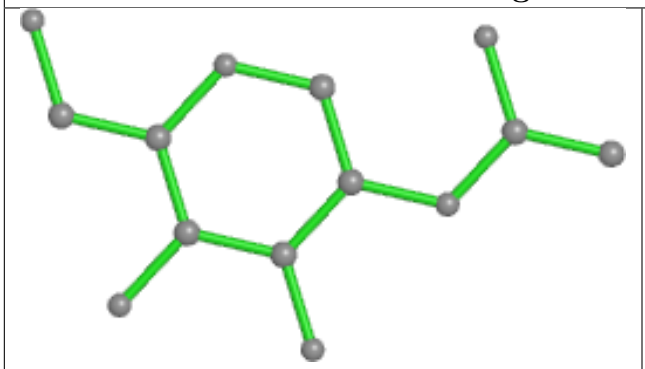
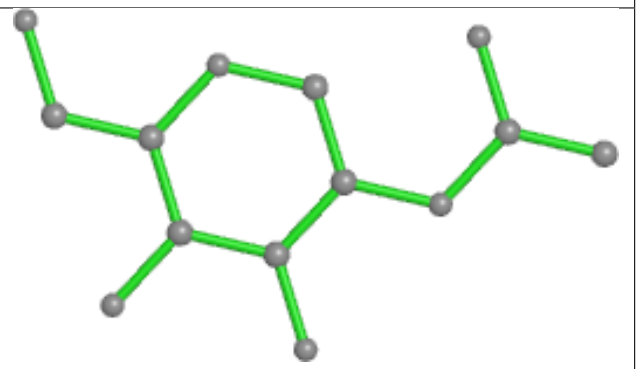
 Bond lengths	 Bond angles
 Torsions	 Rings

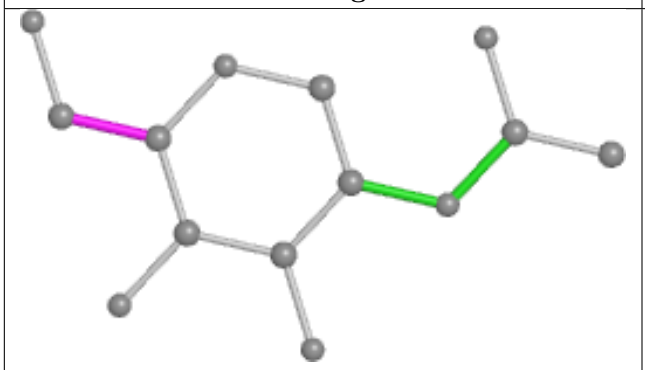
Ligand NAG C 1401



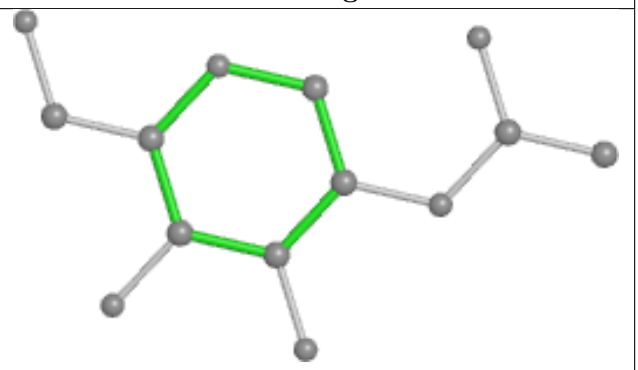
Bond lengths



Bond angles

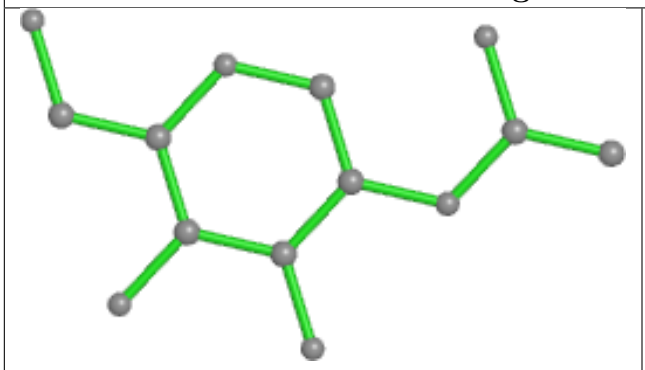


Torsions



Rings

Ligand NAG C 1402



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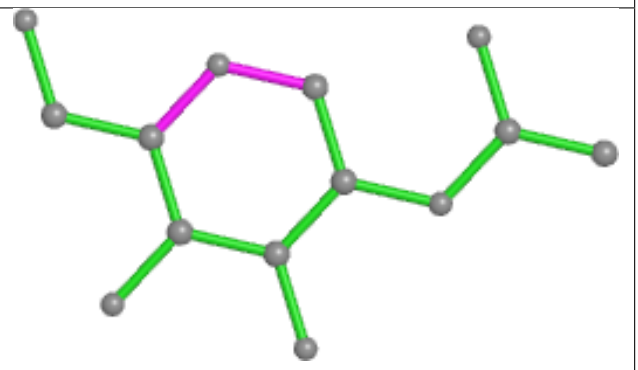

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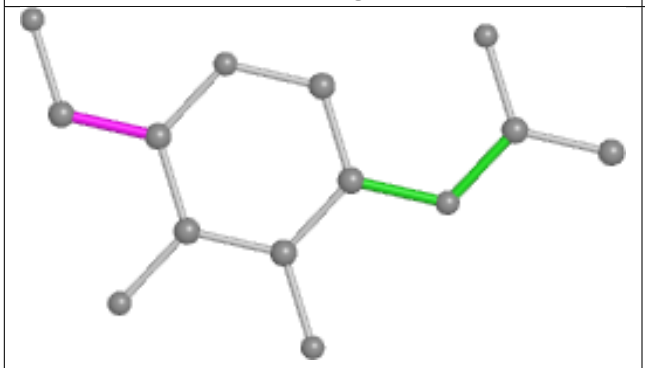
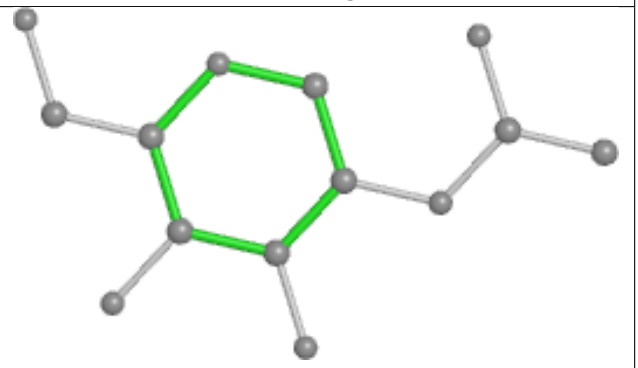
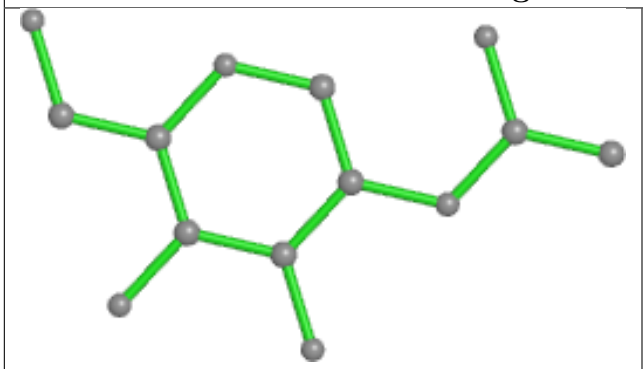


Torsions



Rings

Ligand NAG C 1407



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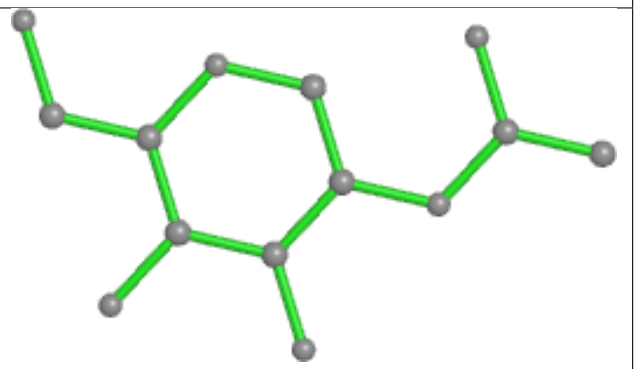

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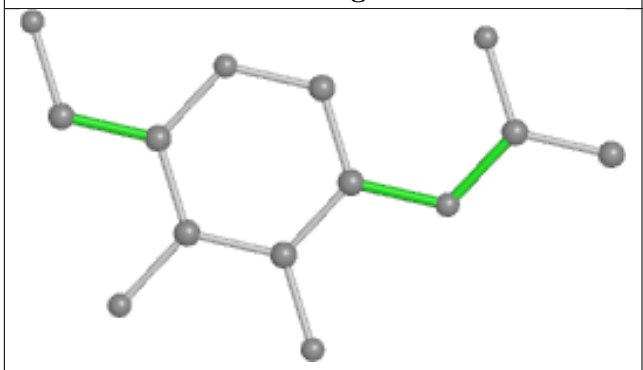

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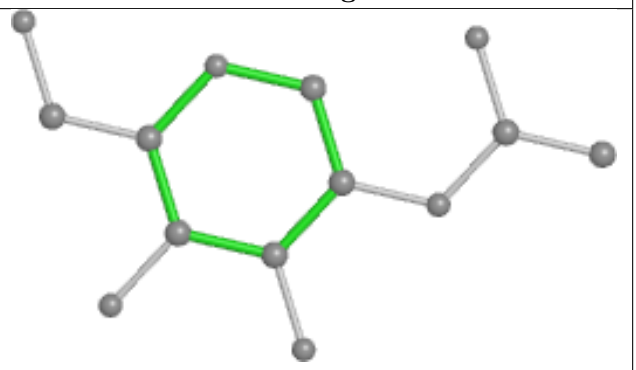
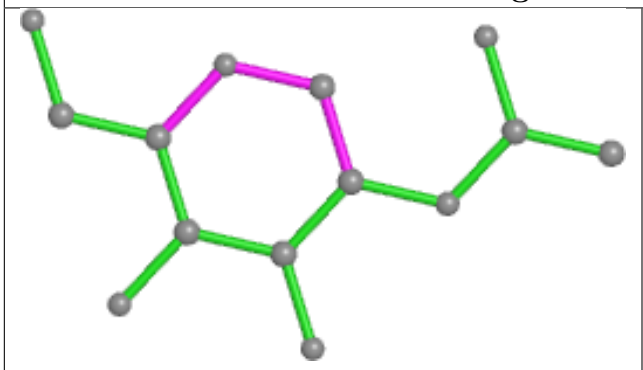


Rings

Ligand NAG A 1404



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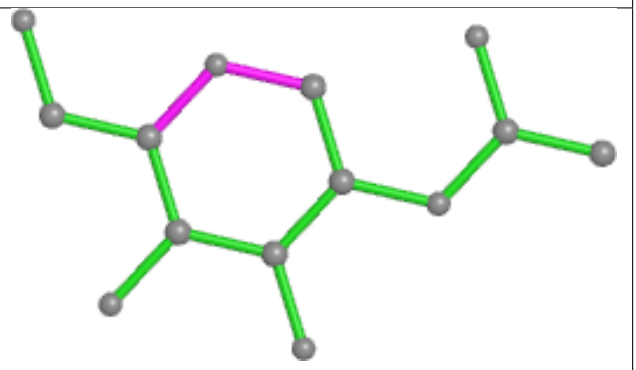

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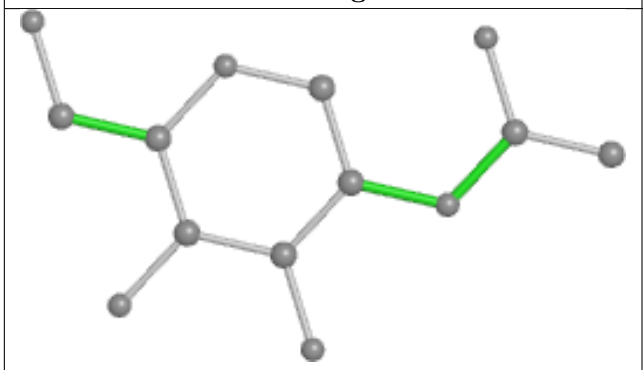

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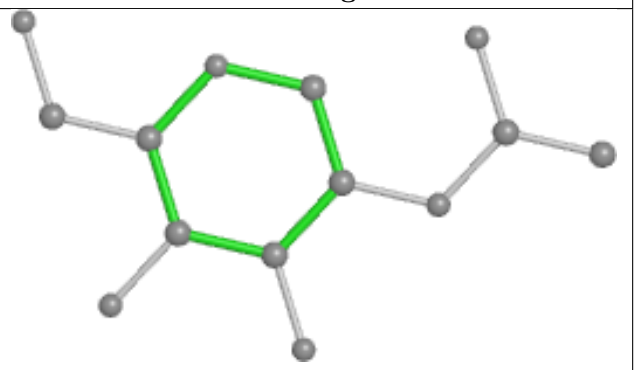

Rings

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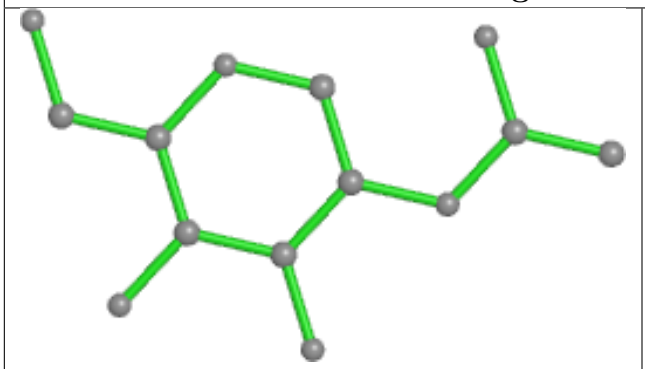

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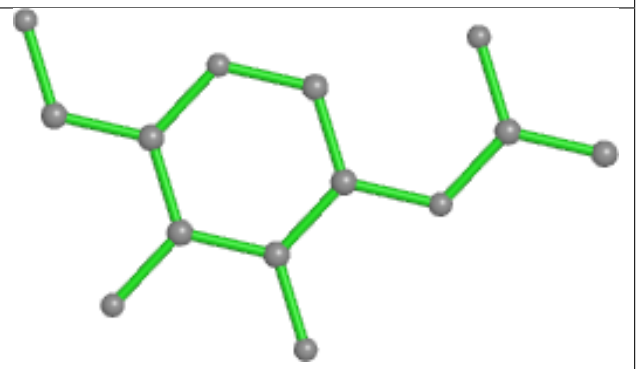

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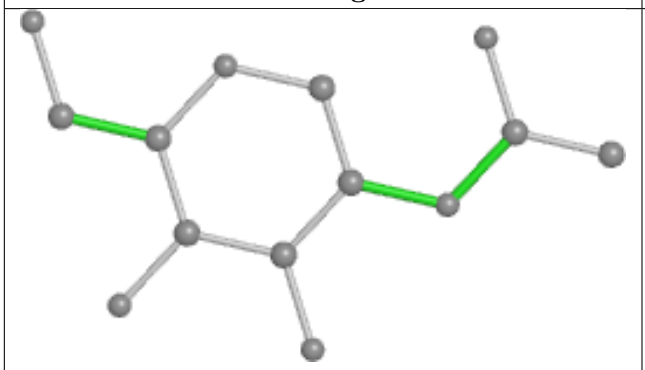

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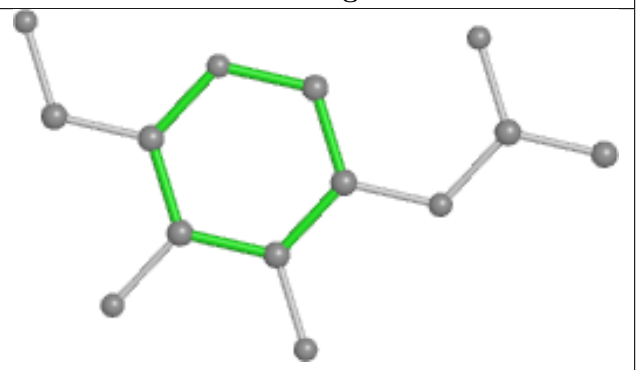

Rings

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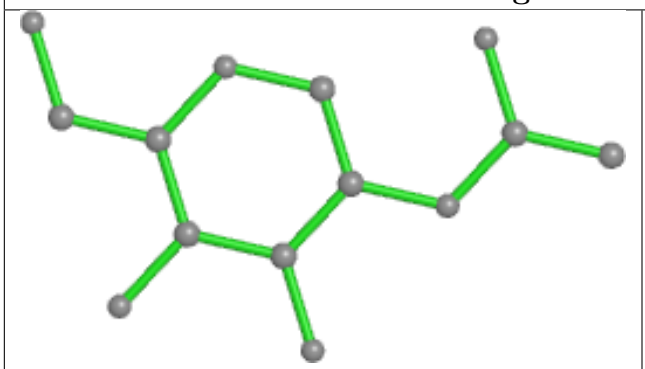

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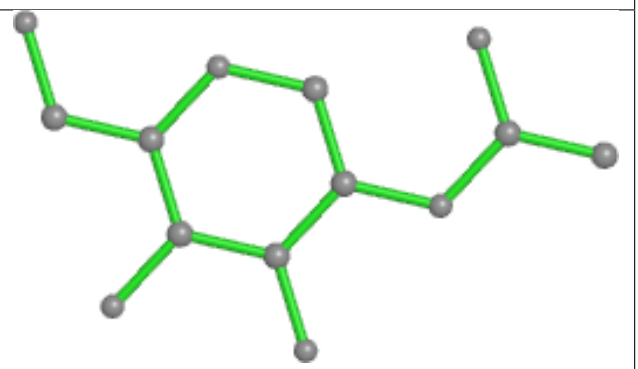

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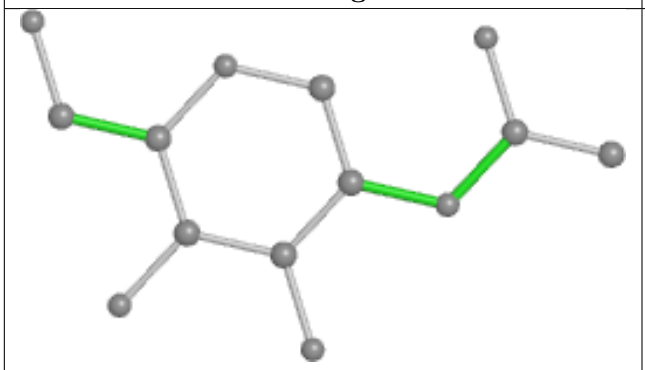

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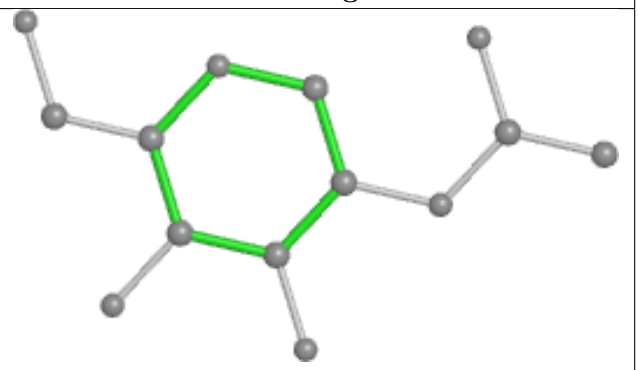
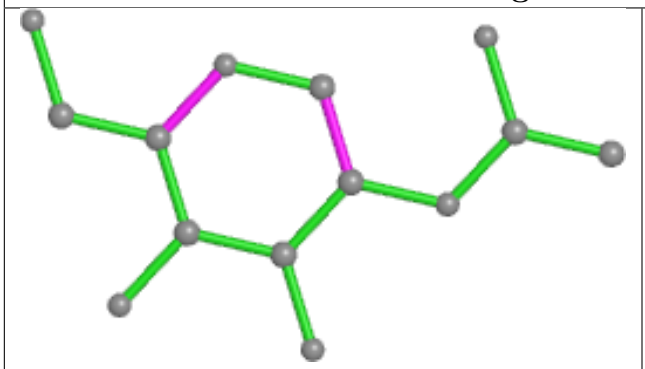


Rings

Ligand NAG A 1406



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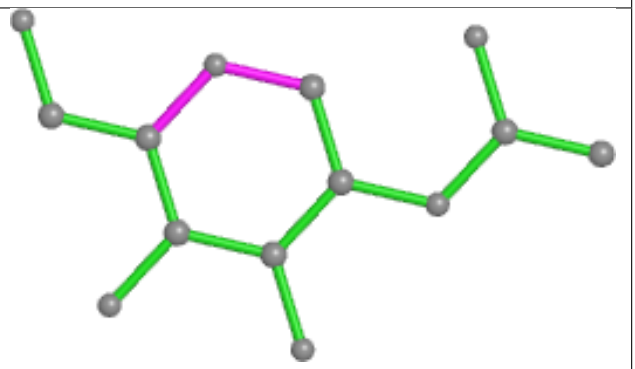

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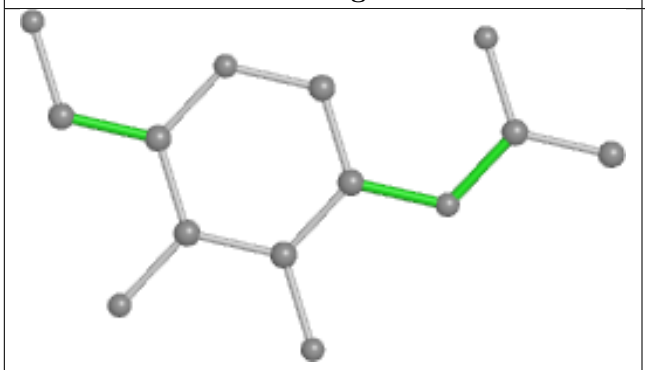

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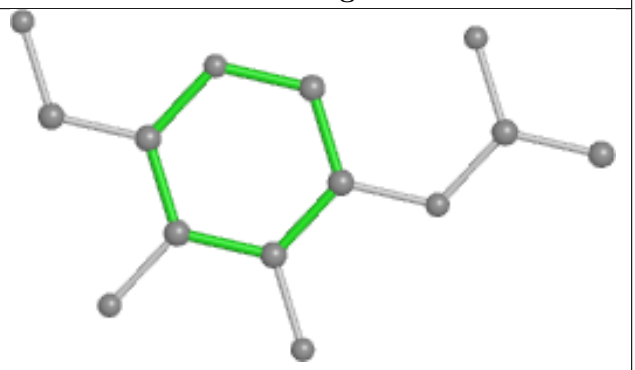
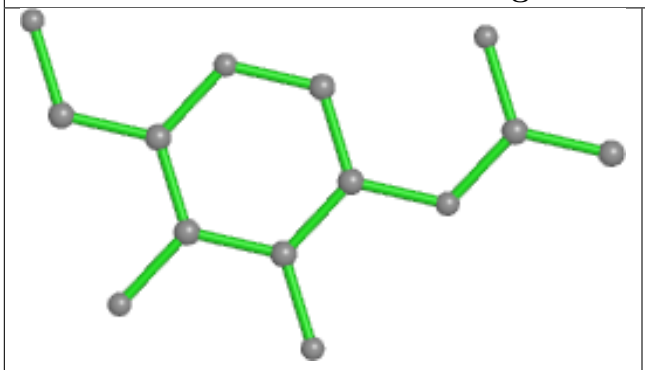


Rings

Ligand NAG A 1405



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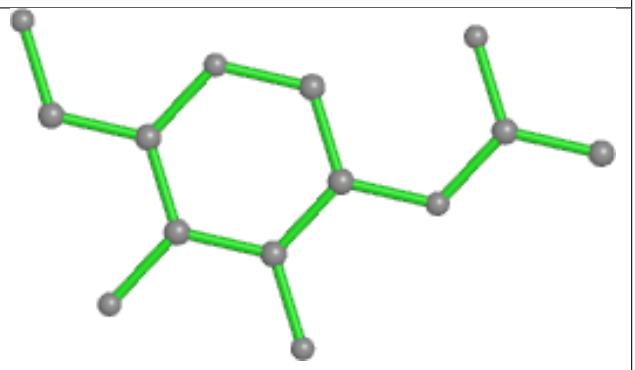

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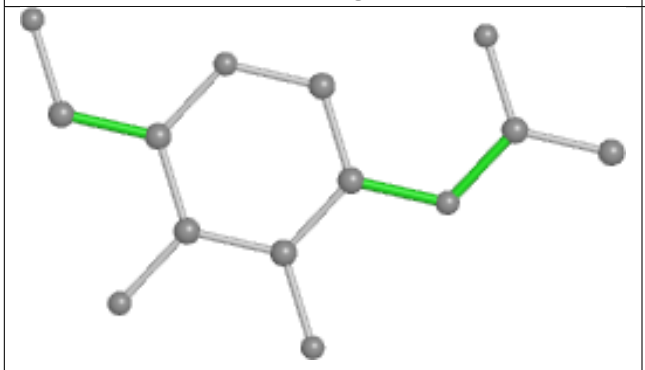

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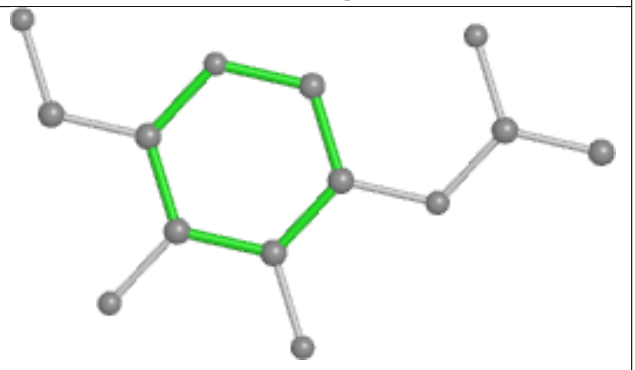
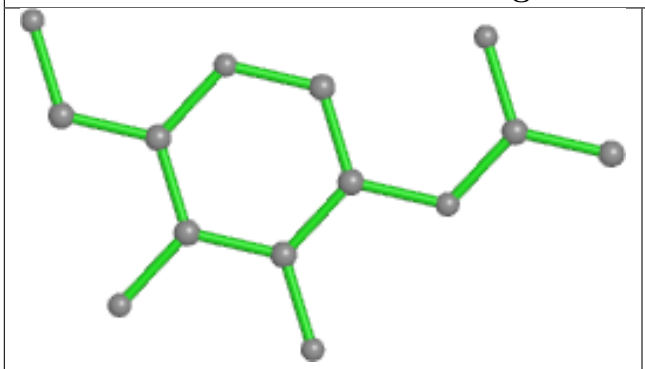


Rings

Ligand NAG B 1405



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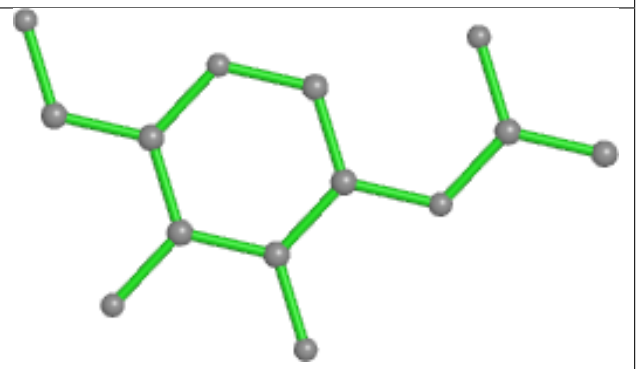
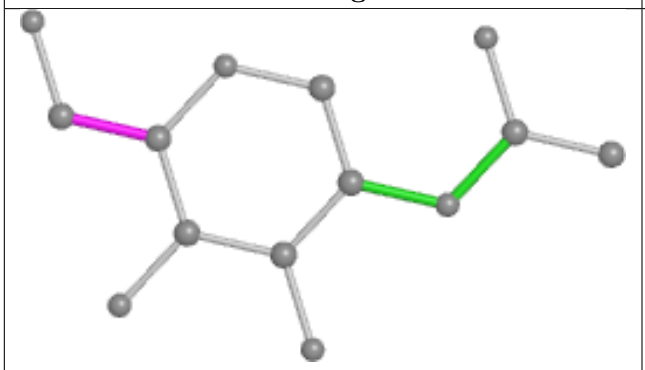


Bond angles



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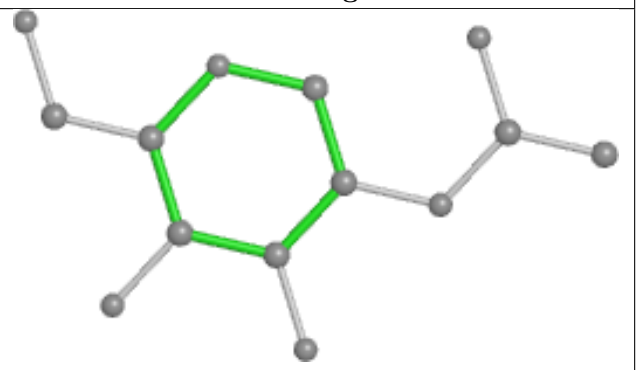
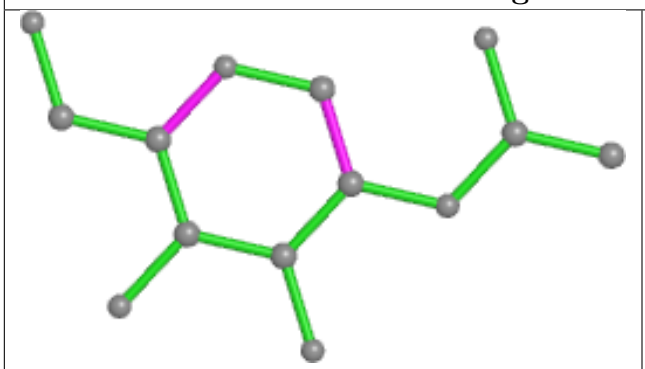


Rings

Ligand NAG A 1407



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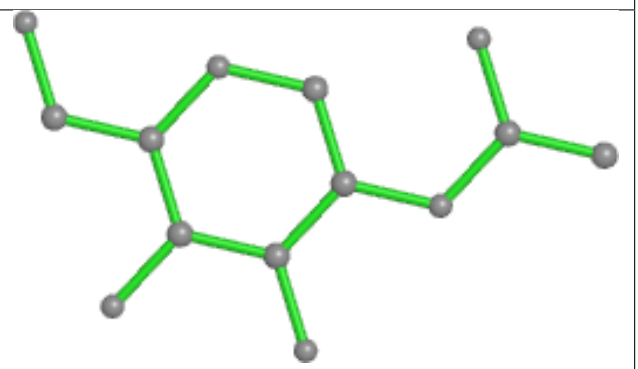
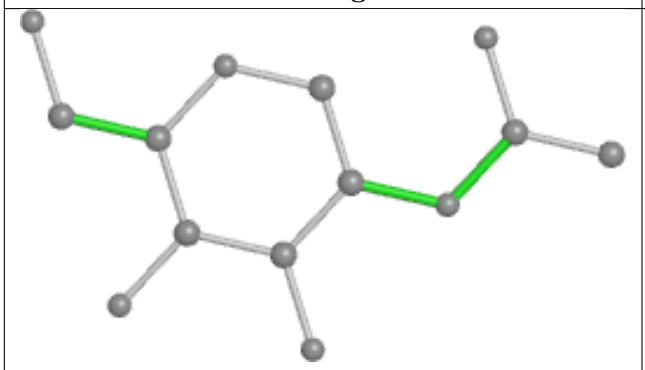


Bond angles



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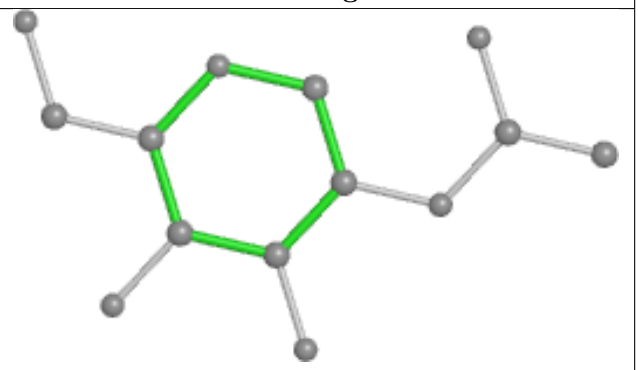
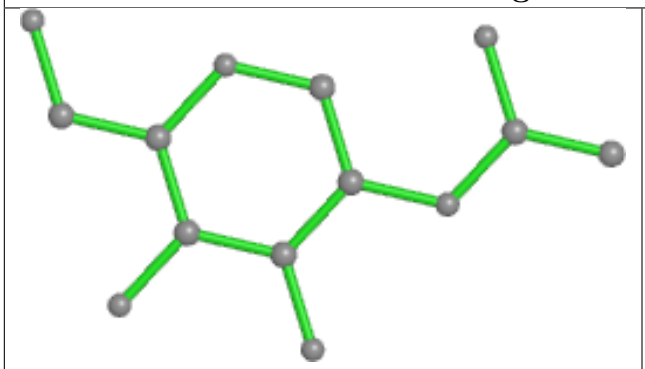


Rings

Ligand NAG C 1405



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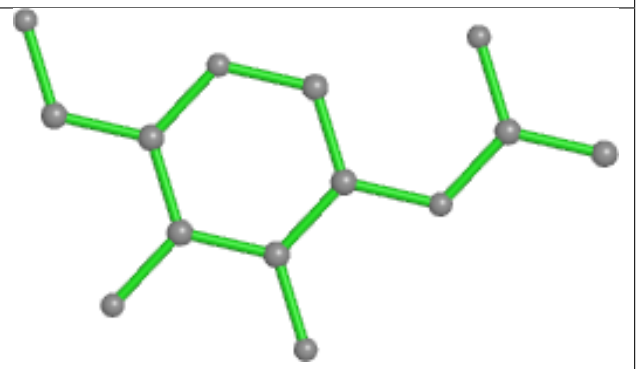
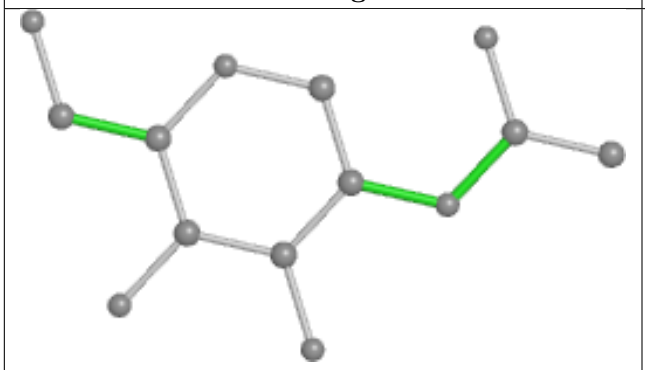


Bond angles



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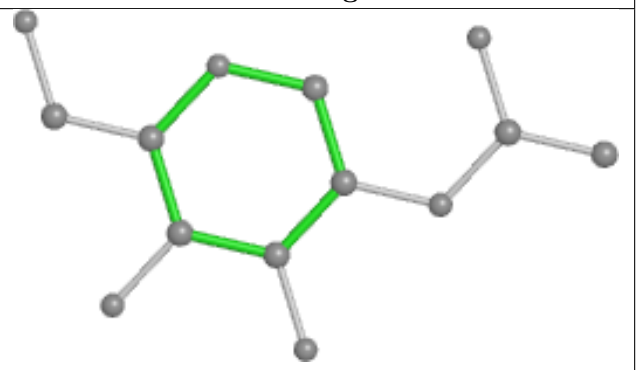
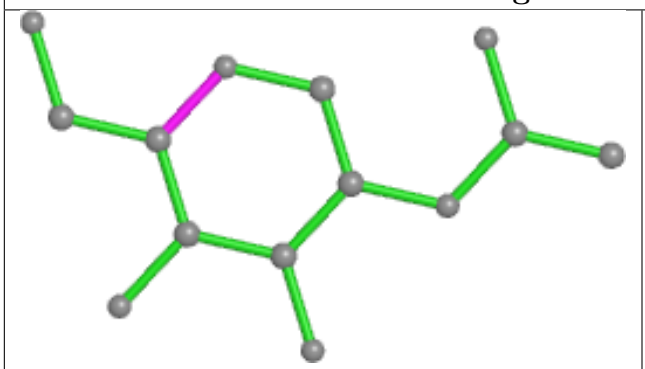
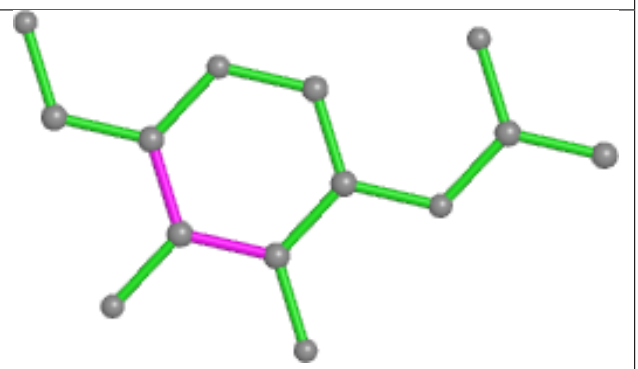


Rings

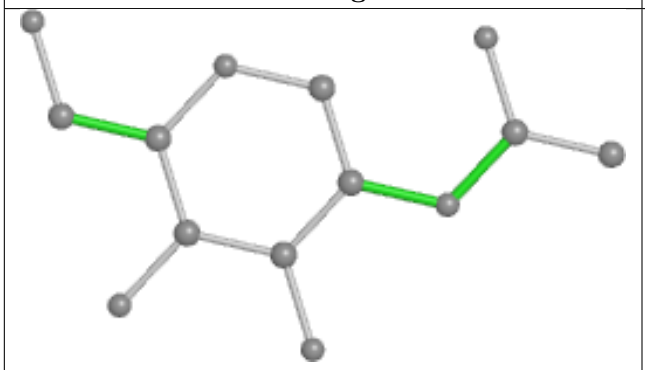
Ligand NAG B 1407



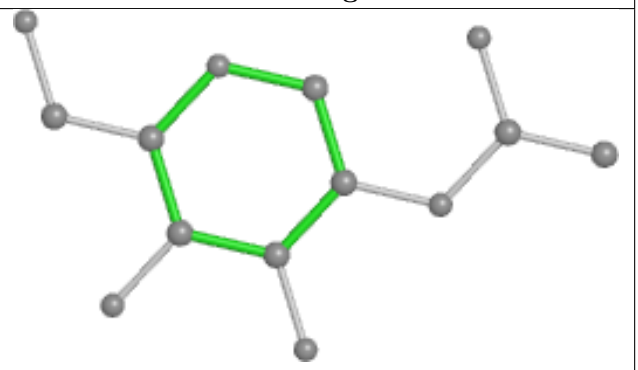
Bond lengths



Bond angles

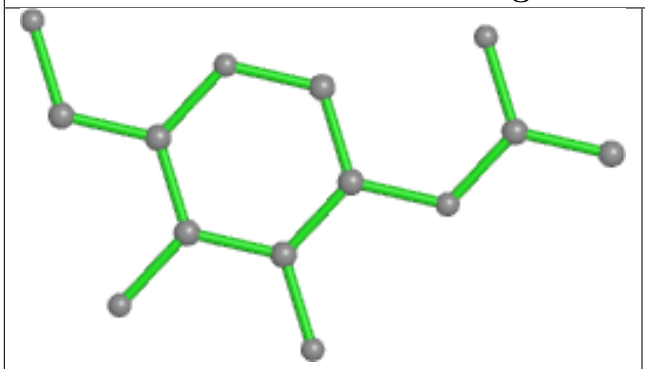


Torsions

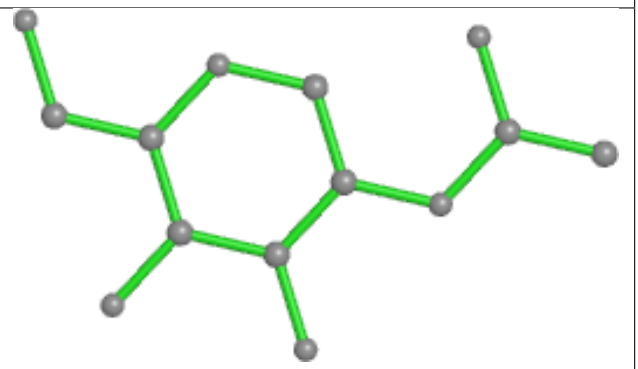


Rings

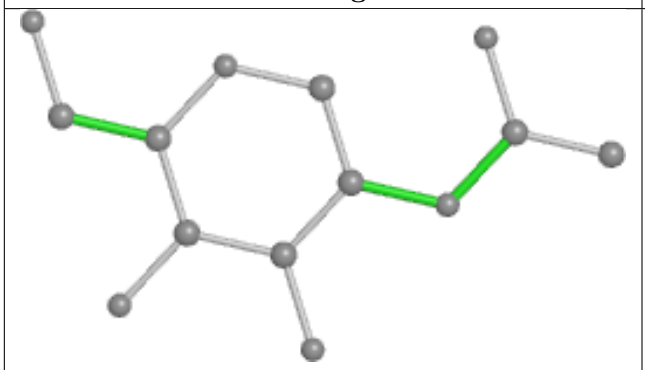
Ligand NAG C 1403



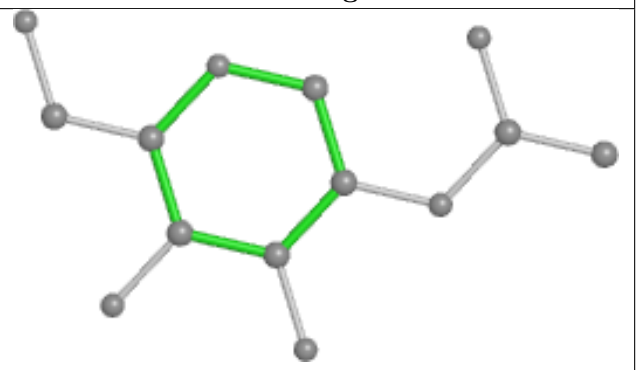
Bond lengths



Bond angles

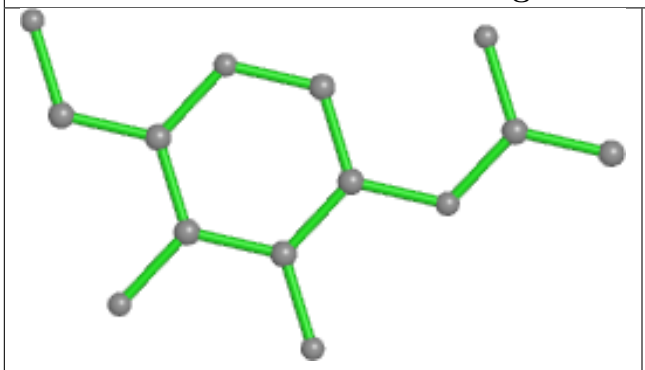


Torsions

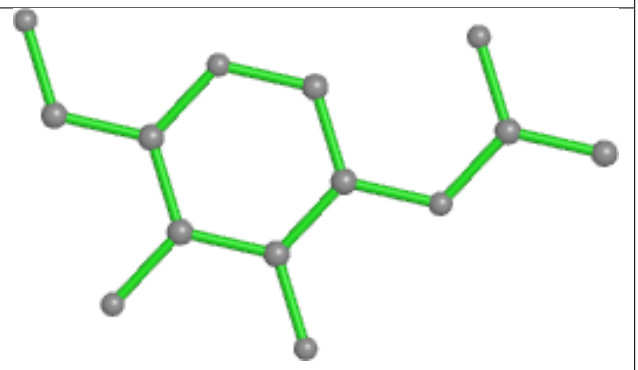


Rings

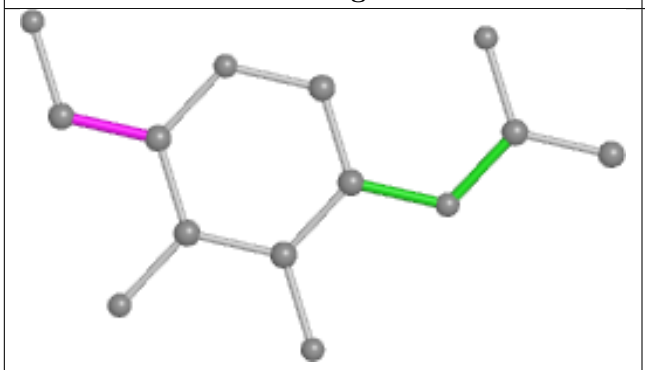
Ligand NAG B 1401



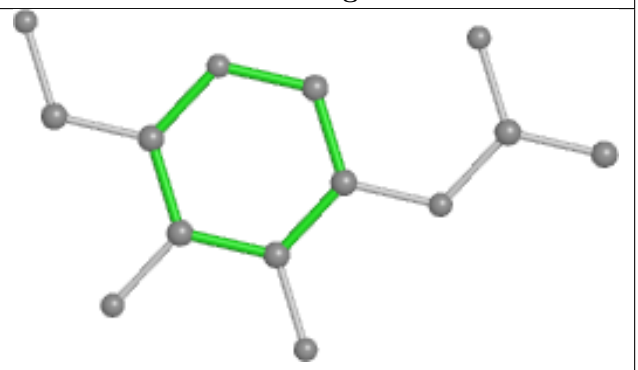
Bond lengths



Bond angles

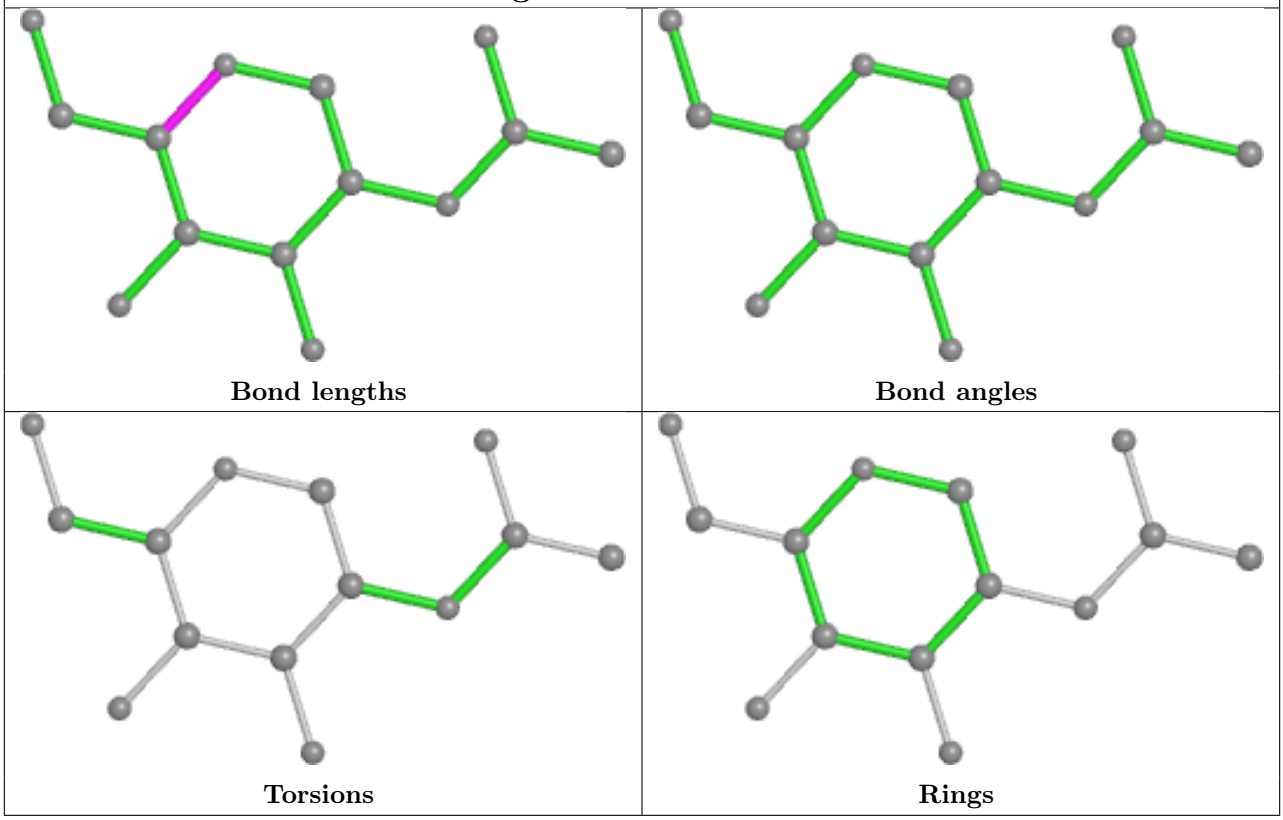


Torsions

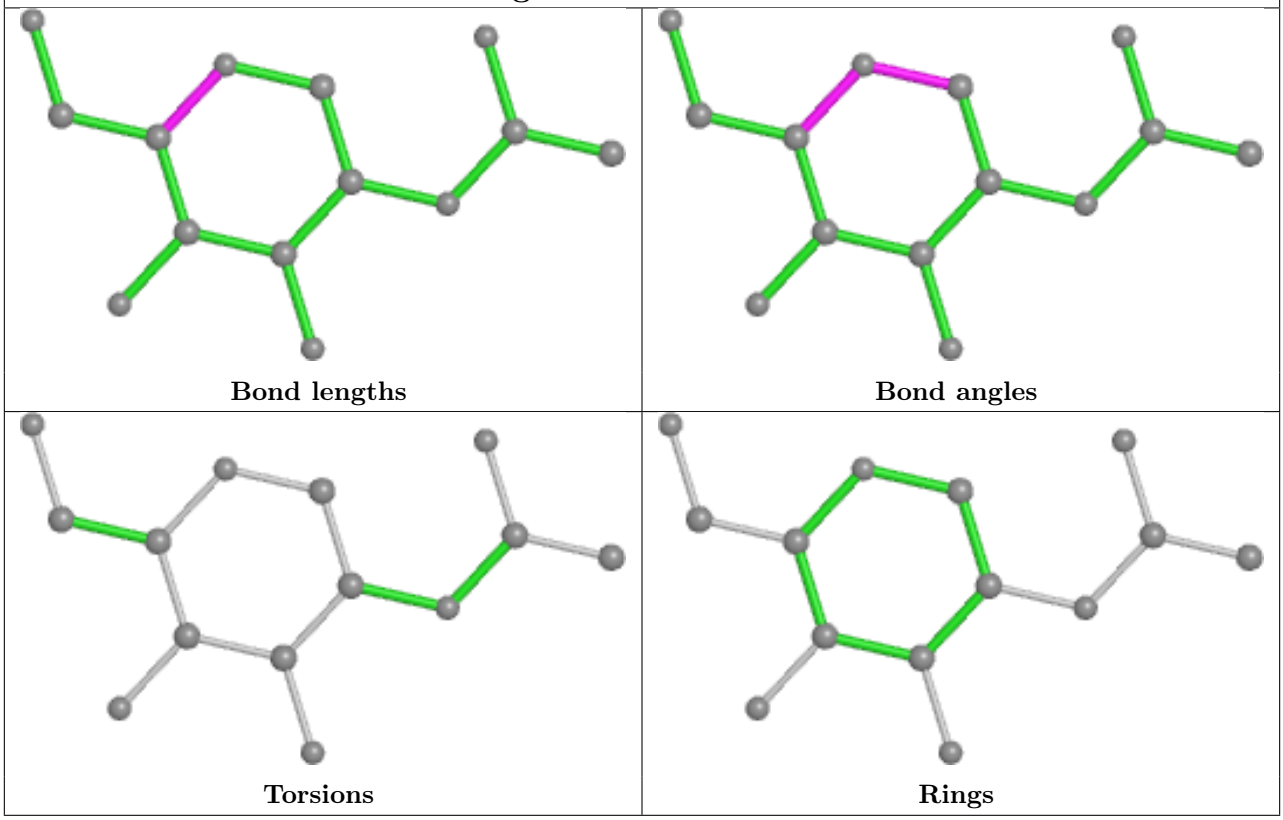


Rings

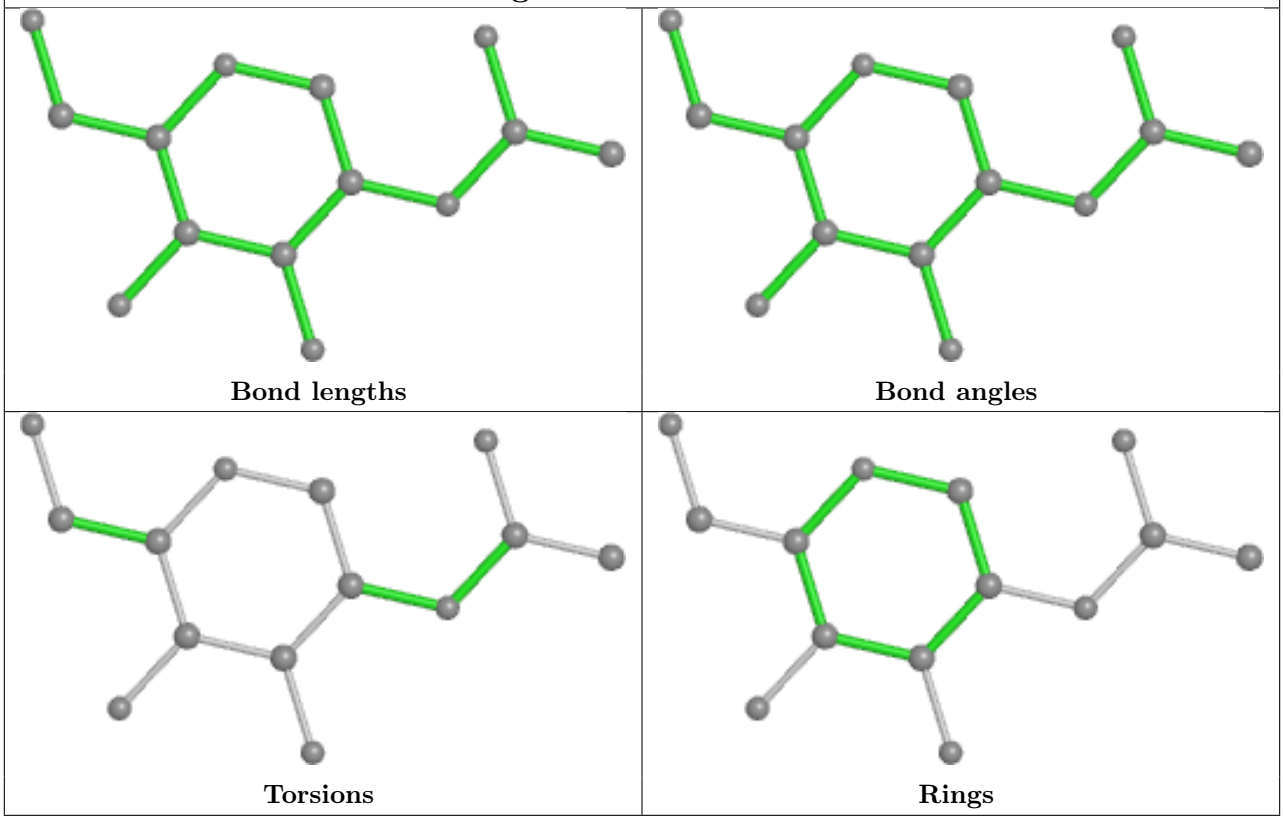
Ligand NAG C 1406



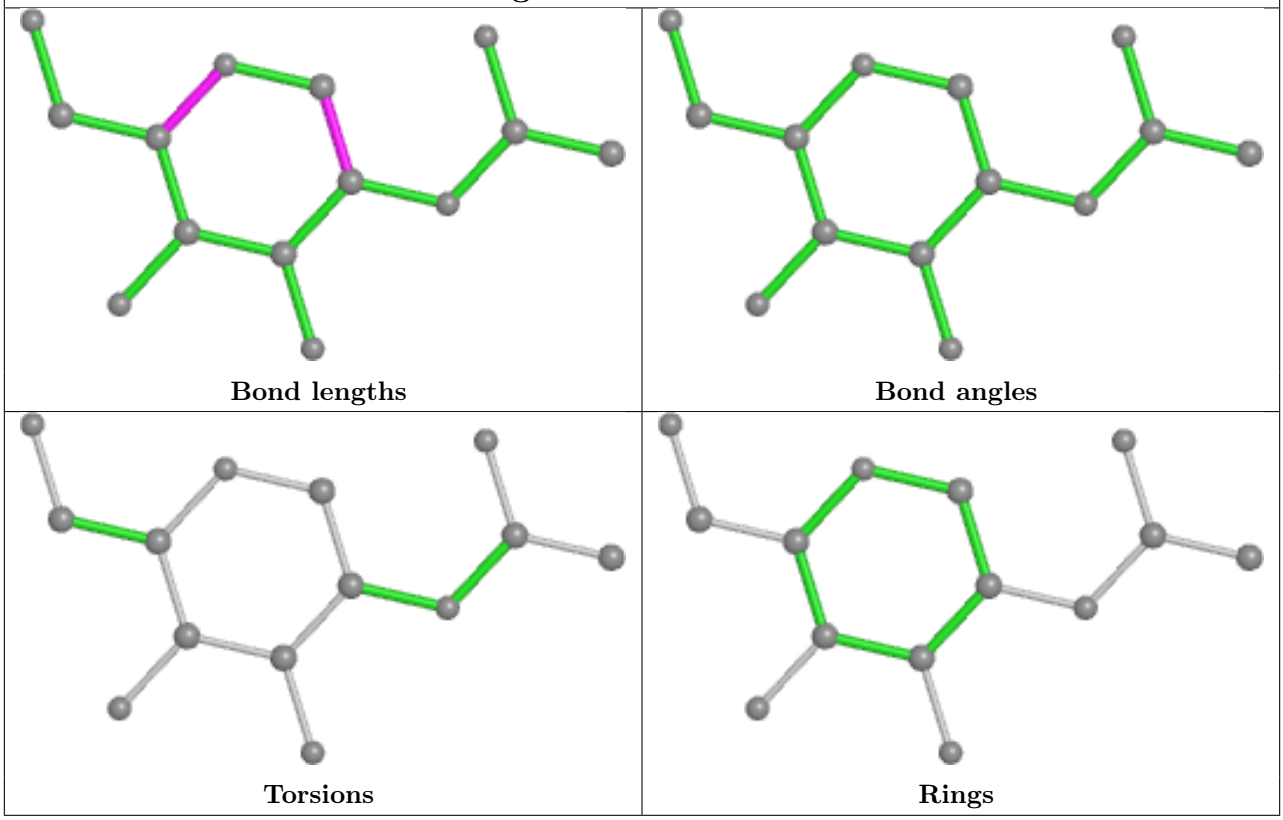
Ligand NAG B 1402

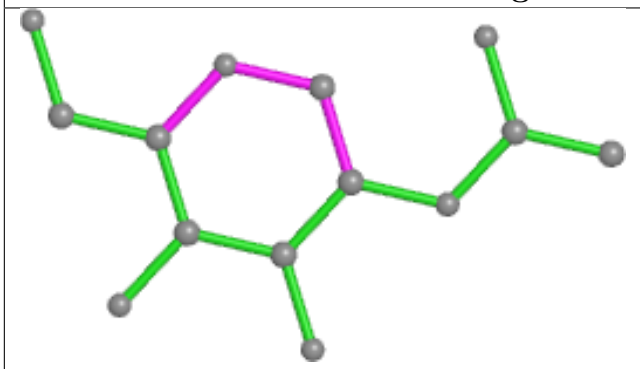
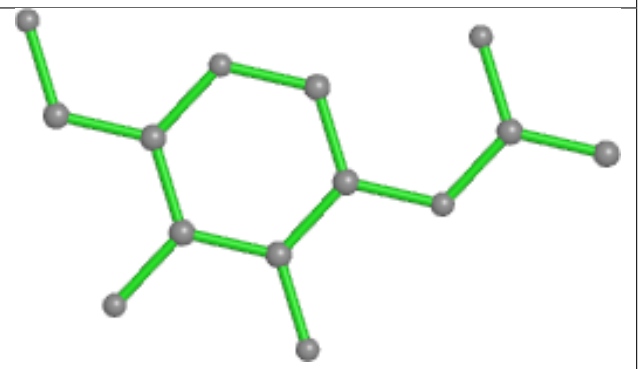
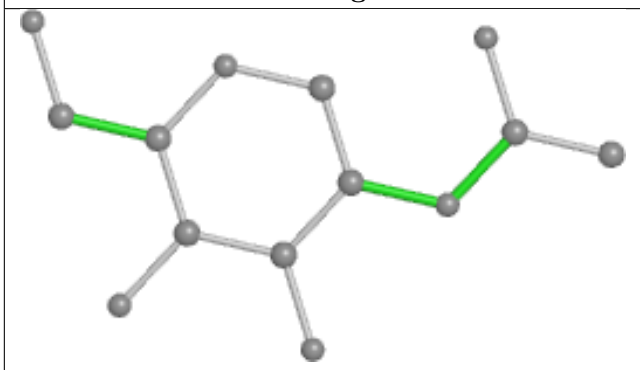
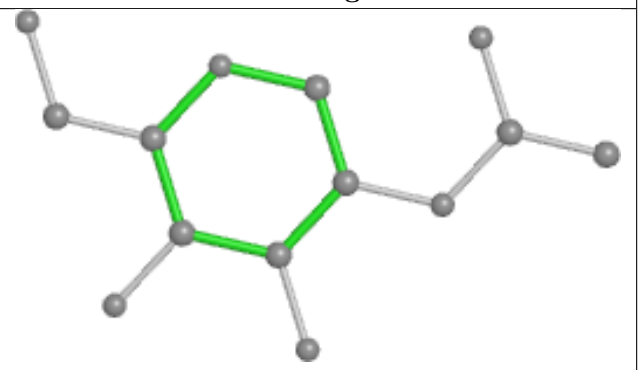


Ligand NAG A 1401



Ligand NAG C 1404



Ligand NAG A 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

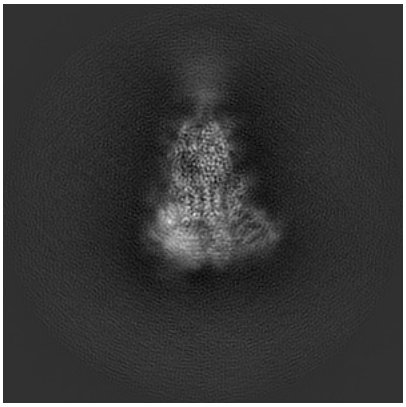
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23012. These allow visual inspection of the internal detail of the map and identification of artifacts.

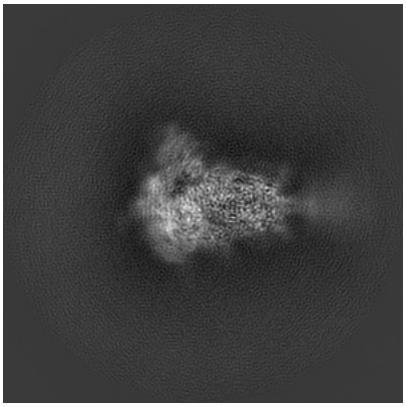
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

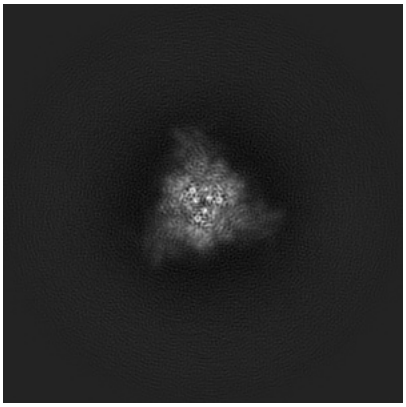
6.1.1 Primary map



X



Y

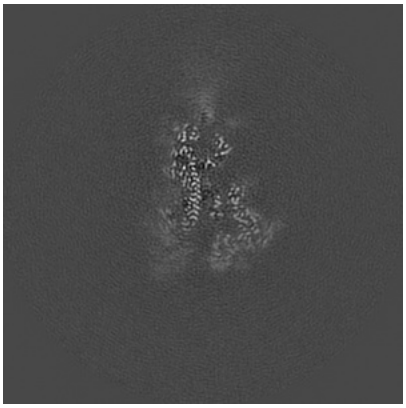


Z

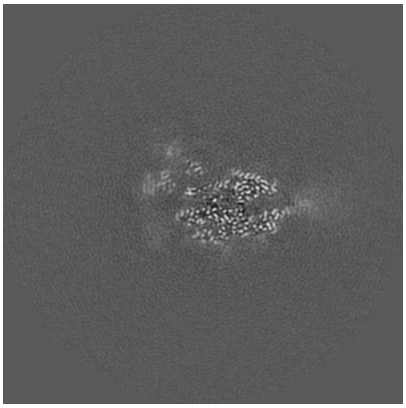
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

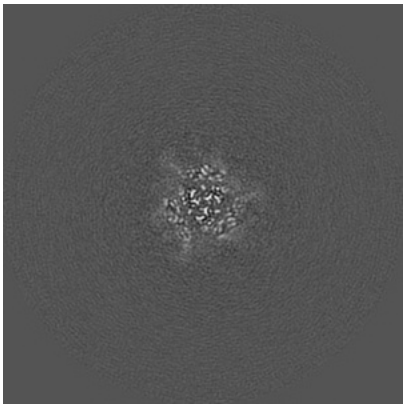
6.2.1 Primary map



X Index: 240



Y Index: 240

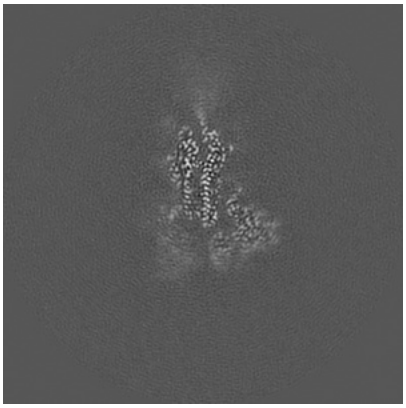


Z Index: 240

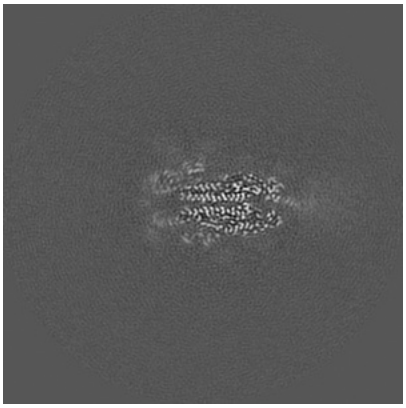
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

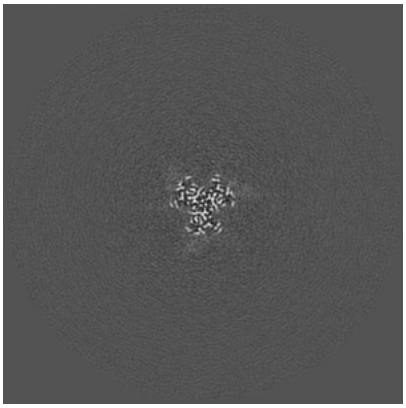
6.3.1 Primary map



X Index: 231



Y Index: 246

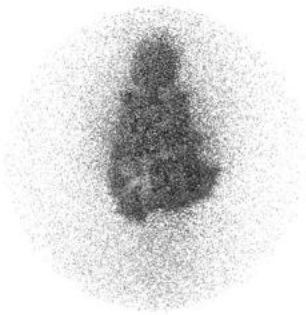


Z Index: 287

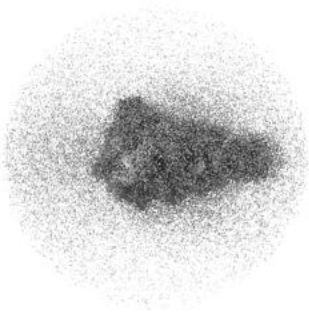
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

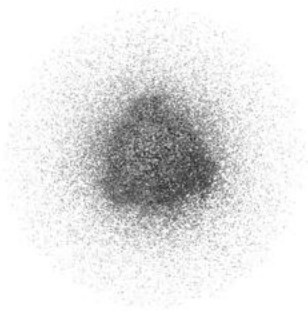
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

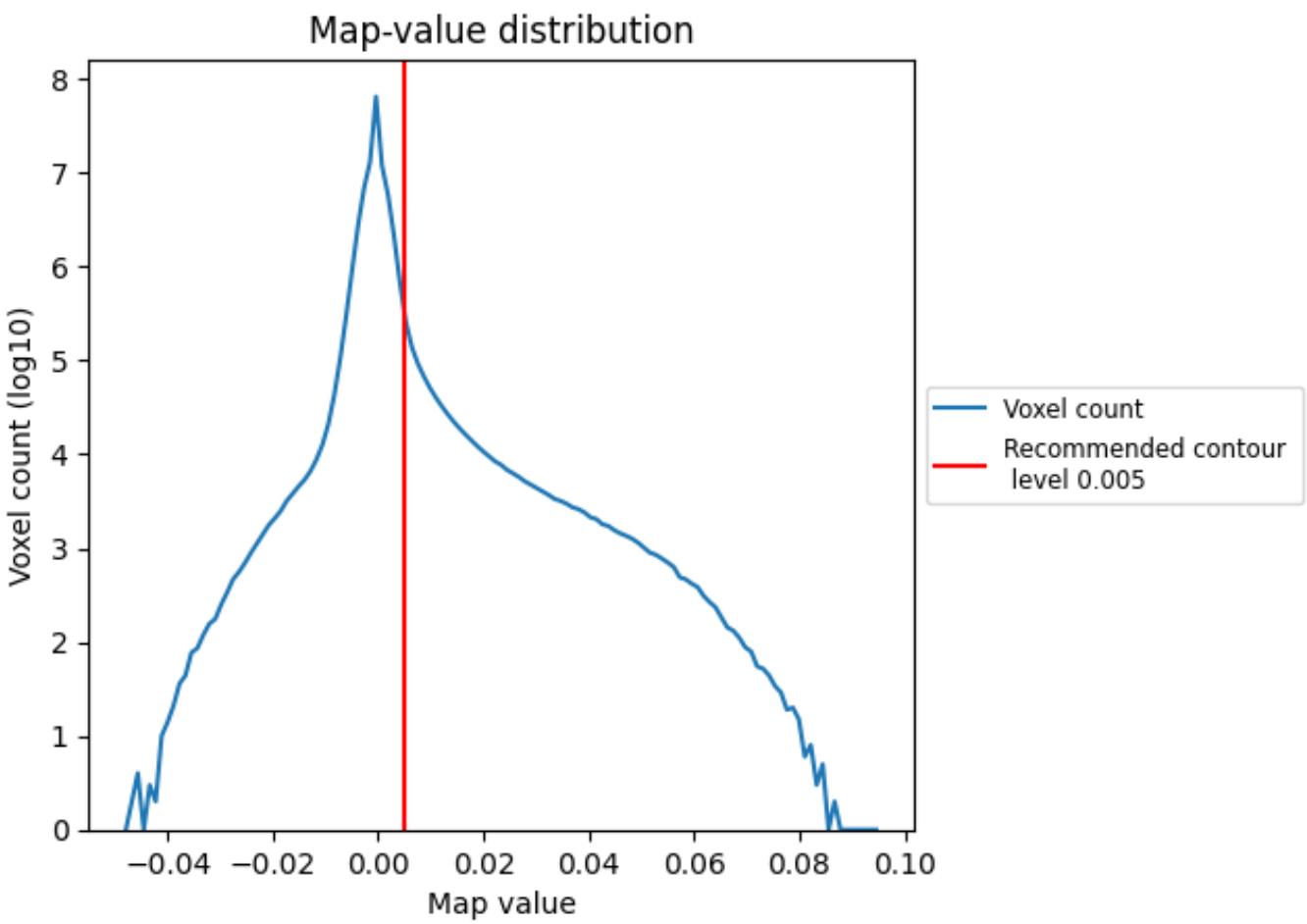
6.5 Mask visualisation (i)

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

7 Map analysis (i)

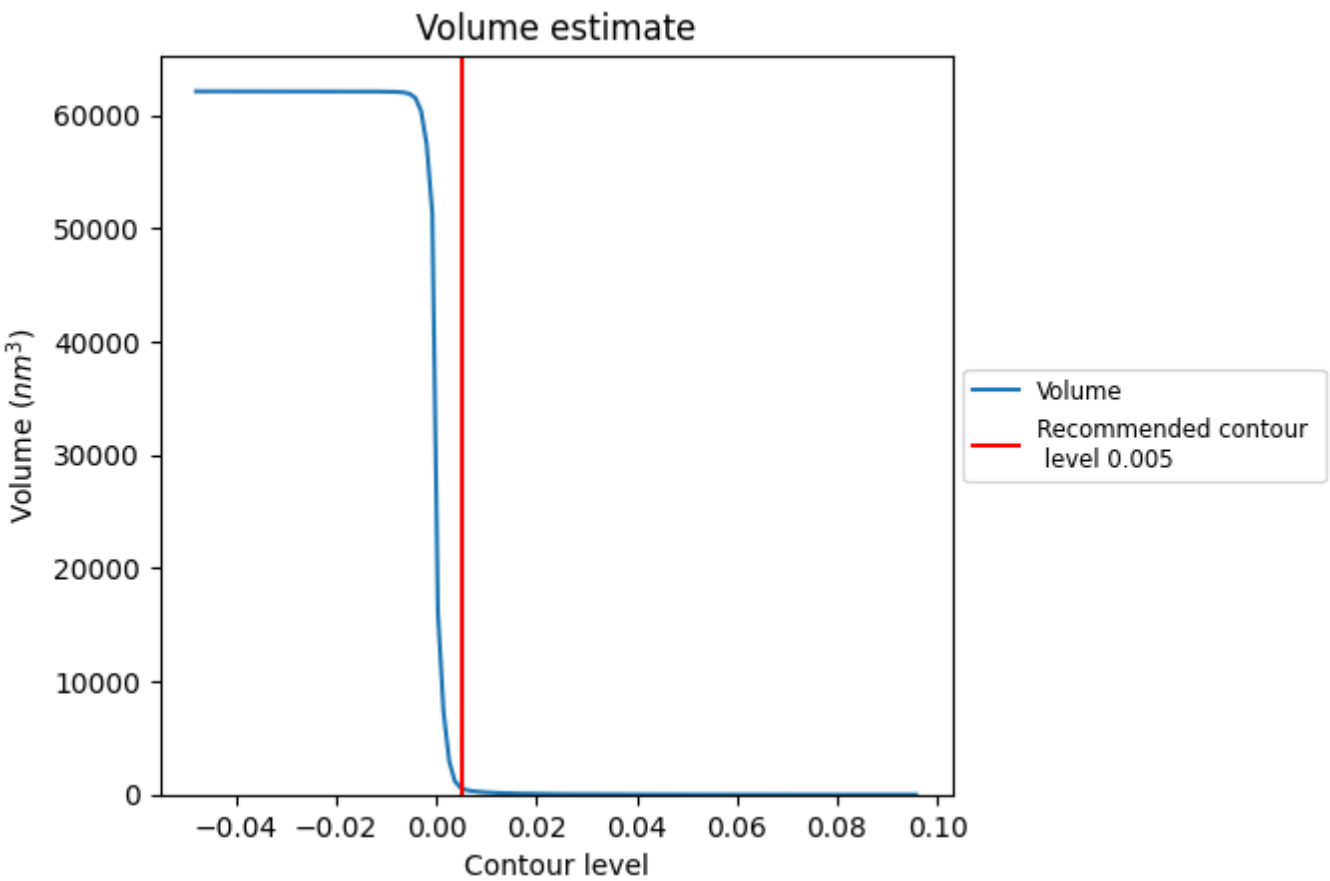
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

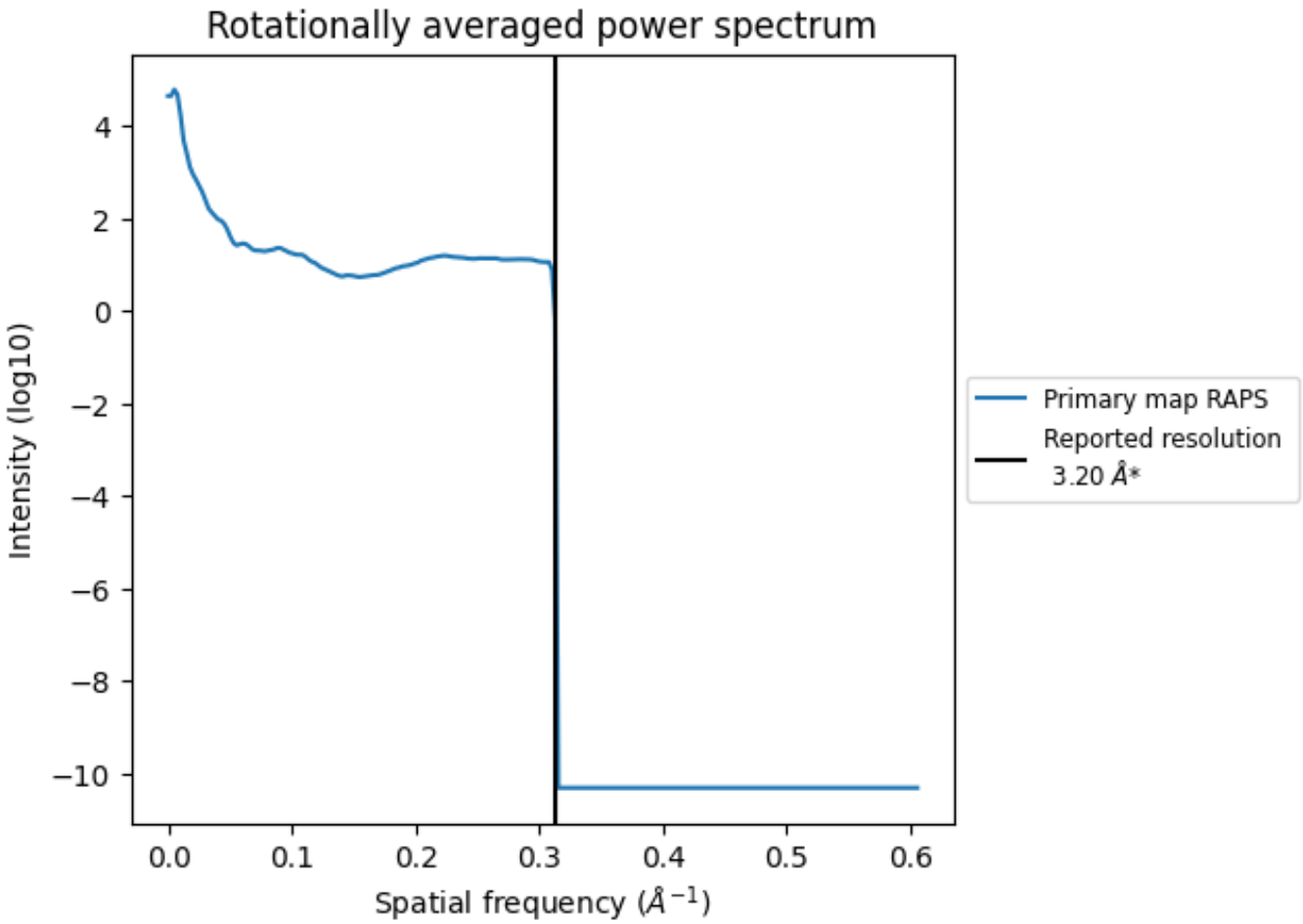
7.2 Volume estimate (i)



The volume at the recommended contour level is 579 nm^3; this corresponds to an approximate mass of 523 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 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

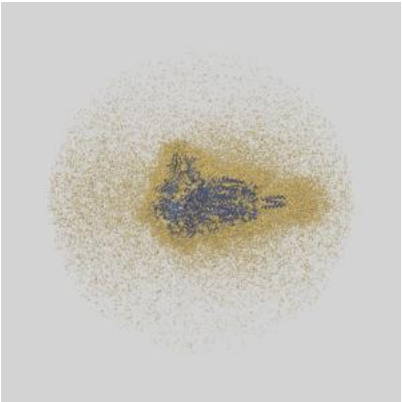
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

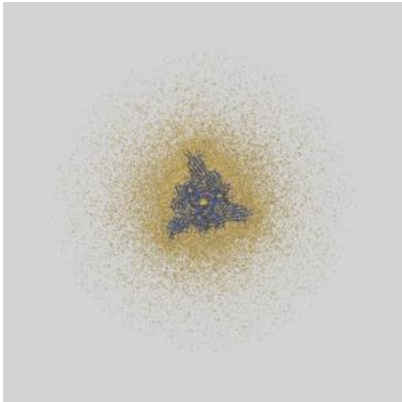
This section contains information regarding the fit between EMDB map EMD-23012 and PDB model 7KRS. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay (i)

X



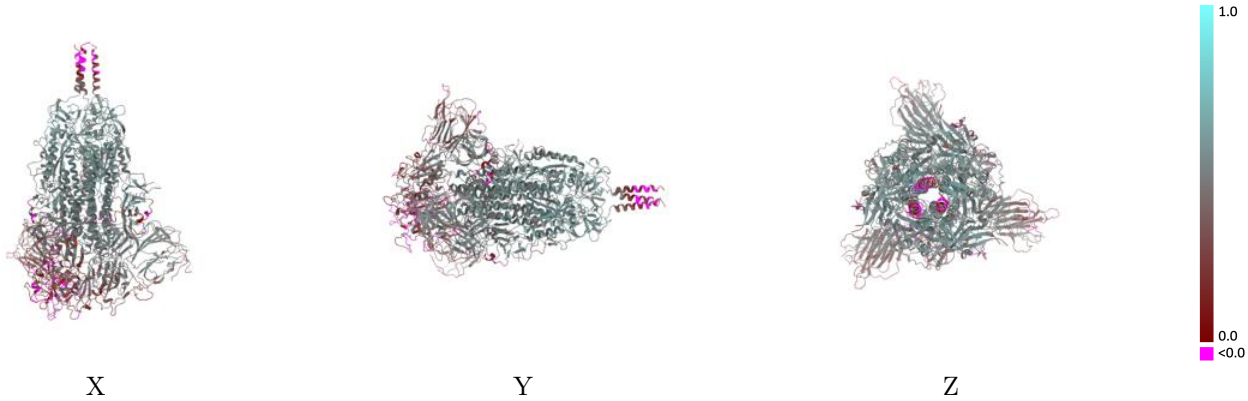
Y



Z

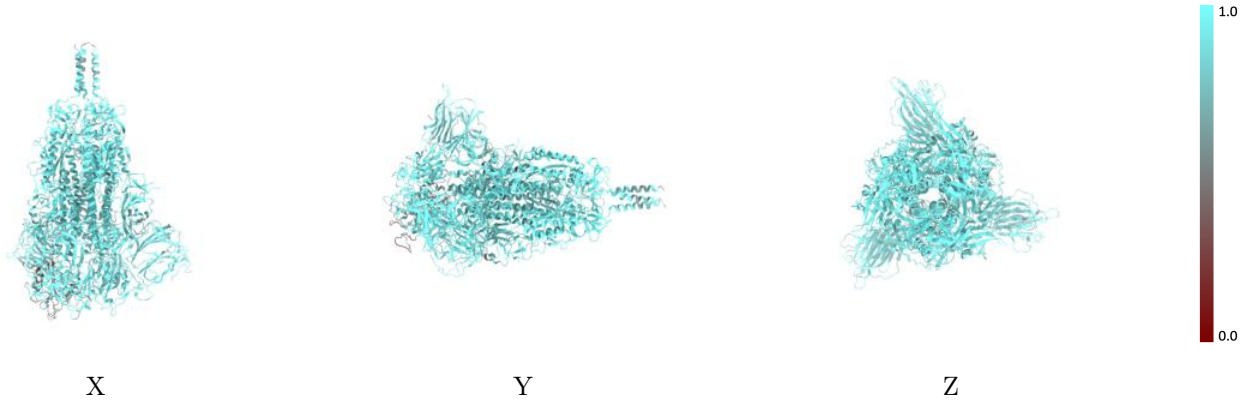
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



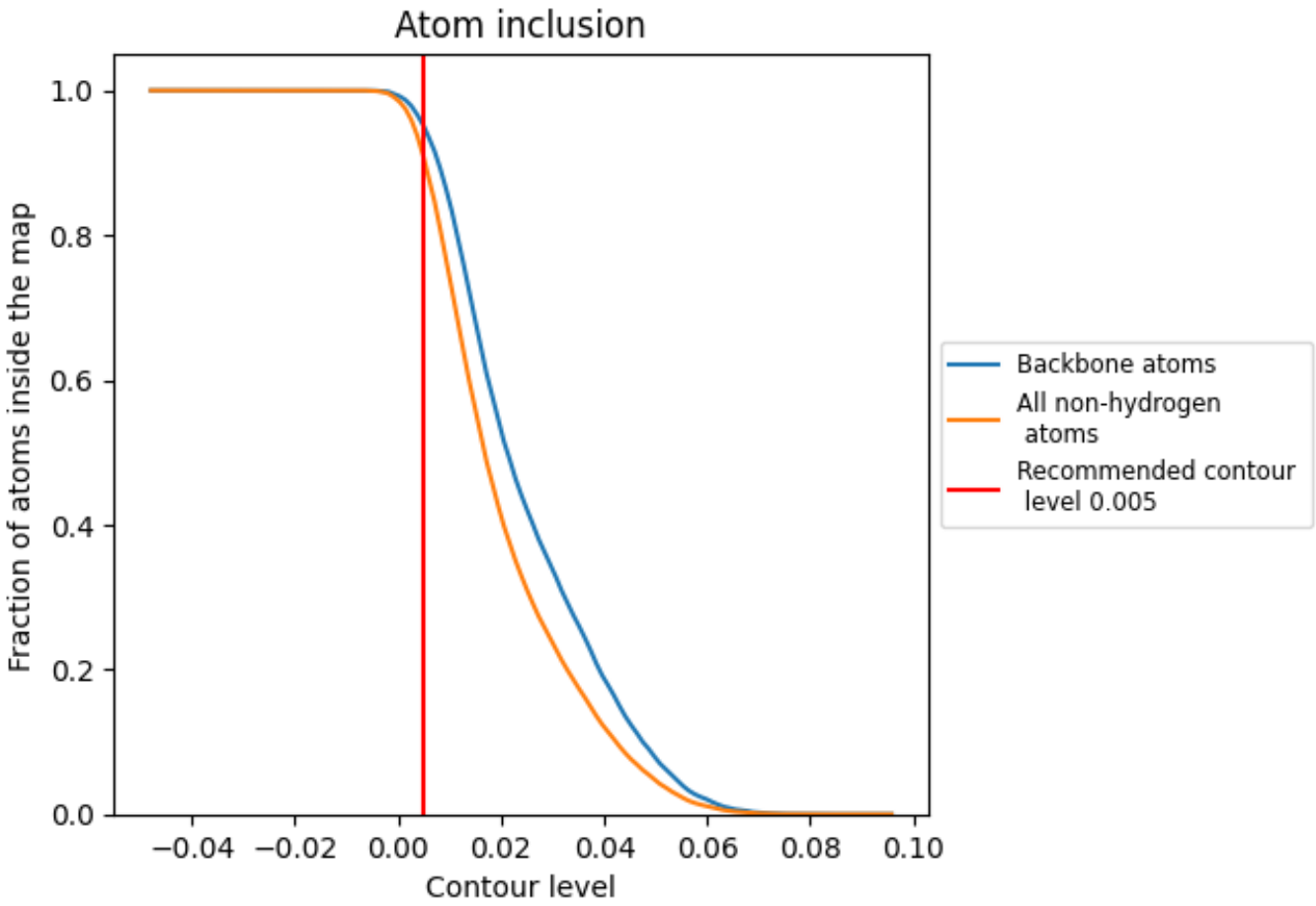
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9068	0.4150
A	0.8588	0.3730
B	0.9367	0.4370
C	0.9410	0.4590
D	0.8214	0.2790
E	0.6429	0.0320
F	0.6071	0.1120
G	0.7500	0.1080
H	0.5714	-0.0360
I	0.6071	0.1110
J	0.7500	0.0710
K	0.9643	0.4180
L	0.8571	0.3120
M	0.7368	0.2370
N	0.9487	0.4000
O	0.8571	0.3190
P	0.6071	-0.0180
Q	0.8214	0.1660
R	0.6071	0.1420
S	0.4286	-0.0470
T	0.7143	0.1330
U	0.5357	0.0380
V	0.6786	0.1880
W	1.0000	0.5240
X	0.9286	0.3620
Y	0.6579	0.2540
Z	0.9231	0.2870
a	0.9286	0.3220
b	0.8929	0.2940
c	0.8929	0.2740
d	0.6429	0.1210
e	0.8214	0.2850
f	0.7857	0.1930
g	0.5357	-0.0480
h	0.8214	0.1730

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Chain	Atom inclusion	Q-score
i	0.8929	0.4080
j	0.9643	0.4270
k	0.8158	0.2340
l	0.9487	0.3570
m	0.8929	0.2410