wwPDB EM Validation Summary Report

Oct 14, 2024 – 03:03 PM JST

PDB ID	:	7CZZ
EMDB ID	:	EMD-30522
Title	:	S protein of SARS-CoV-2 in complex bound with P5A-2F11_3B
Authors	:	Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Zhou, Q.
Deposited on	:	2020-09-09
Resolution	:	3.20 Å(reported)

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 ⓘ 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 ⓘ) were used in the production of this report:

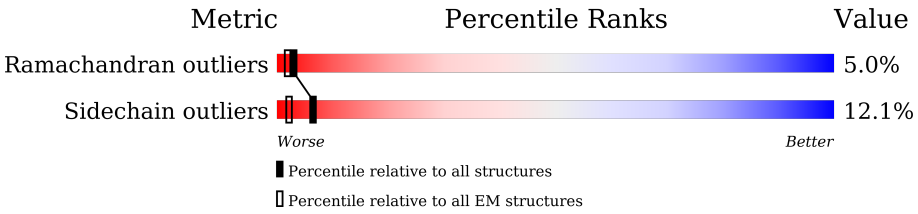
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	207382	16835
Sidechain outliers	206894	16415

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	1283	11% 69% 9% 22%
1	B	1283	15% 67% 11% • 22%
1	C	1283	14% 68% 9% • 22%
2	H	452	49% 42% 7% • 50%
2	I	452	50% 42% 7% • 50%
2	J	452	50% 42% 7% • 50%
3	K	220	100% 84% 12% •
3	M	220	100% 84% 12% •
3	N	220	100% 84% 12% •

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Mol	Chain	Length	Quality of chain
4	D	2	100%
4	E	2	100% 100%
4	F	2	50% 50%
4	G	2	50% 50%
4	L	2	100%
4	O	2	50% 50%
4	P	2	50% 50%
4	Q	2	50% 50% 50%
4	R	2	100% 100%
4	S	2	50% 100%
4	T	2	50% 50%
4	U	2	50% 50%
4	V	2	50% 50%
4	W	2	100%
4	X	2	50% 100%
4	Y	2	100% 100%
4	Z	2	50% 50% 50%
4	a	2	50% 50%
4	b	2	50% 100%
4	c	2	50% 50% 50%
4	d	2	100%
4	e	2	100%
5	f	3	100% 33% 67%
5	g	3	100% 33% 67%
5	h	3	100% 33% 67%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 34771 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
1	A	1006	Total	C	N	O	S	0	0
			7863	5019	1308	1500	36		
1	B	1007	Total	C	N	O	S	0	0
			7870	5023	1310	1501	36		
1	C	1004	Total	C	N	O	S	0	0
			7853	5014	1307	1496	36		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_3B,Epididymis luminal protein 214,Epididymis luminal protein 214.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	224	Total	C	N	O	S	0	0
			1670	1053	281	328	8		
2	I	224	Total	C	N	O	S	0	0
			1670	1053	281	328	8		
2	J	224	Total	C	N	O	S	0	0
			1670	1053	281	328	8		

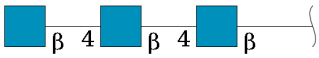
- Molecule 3 is a protein called IG c168_light_IGKV4-1_IGKJ4,Immunoglobulin kappa constant.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	220	Total	C	N	O	S	0	0
			1685	1055	278	346	6		
3	M	220	Total	C	N	O	S	0	0
			1685	1055	278	346	6		
3	N	220	Total	C	N	O	S	0	0
			1685	1055	278	346	6		

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

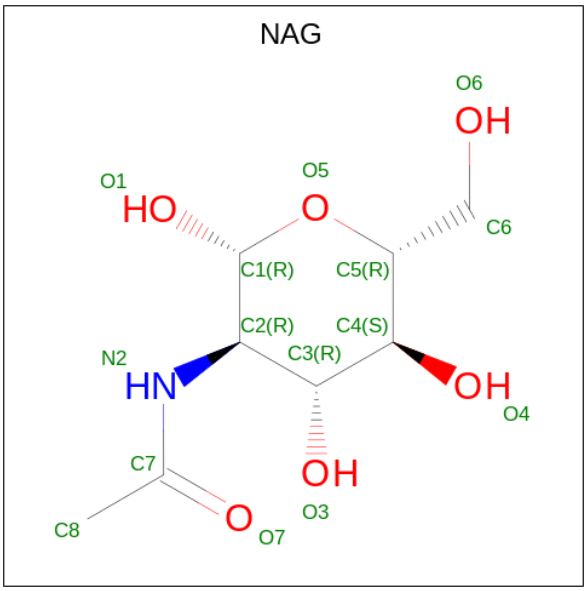
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms	AltConf	Trace
5	f	3	Total C N O 42 24 3 15	0	0
5	g	3	Total C N O 42 24 3 15	0	0
5	h	3	Total C N O 42 24 3 15	0	0

- Molecule 6 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
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0
6	A	1	Total C N O 14 8 1 5	0

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

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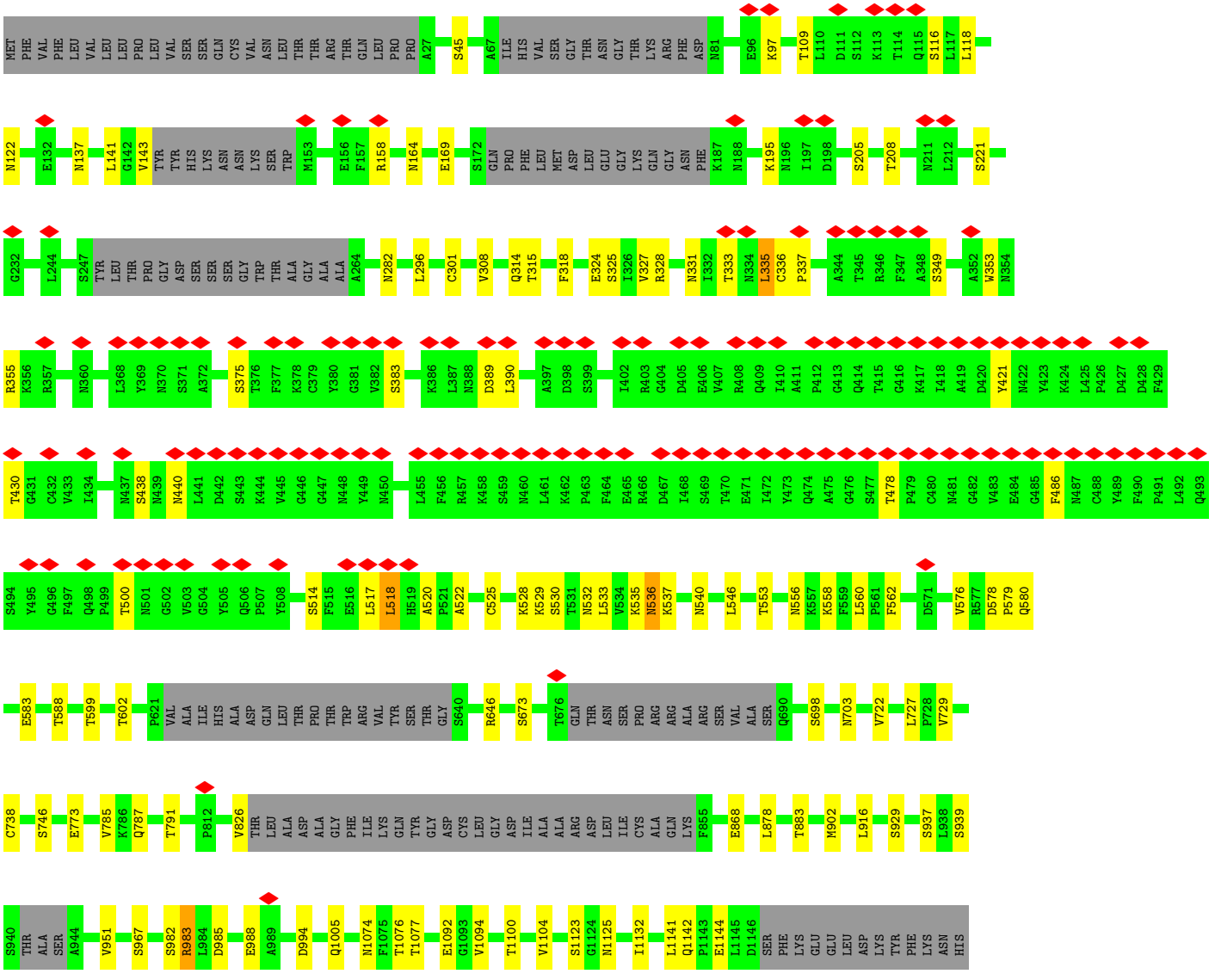
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	

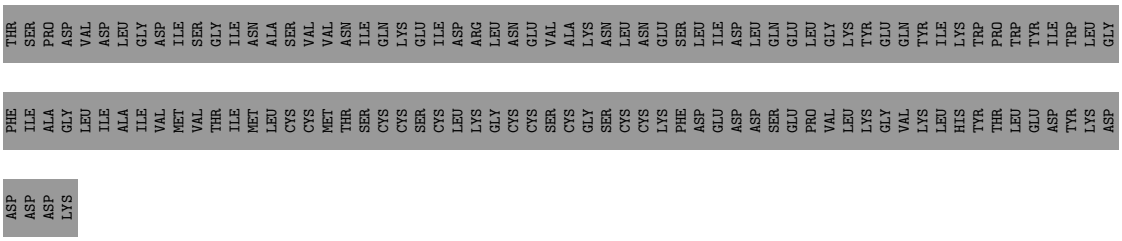
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

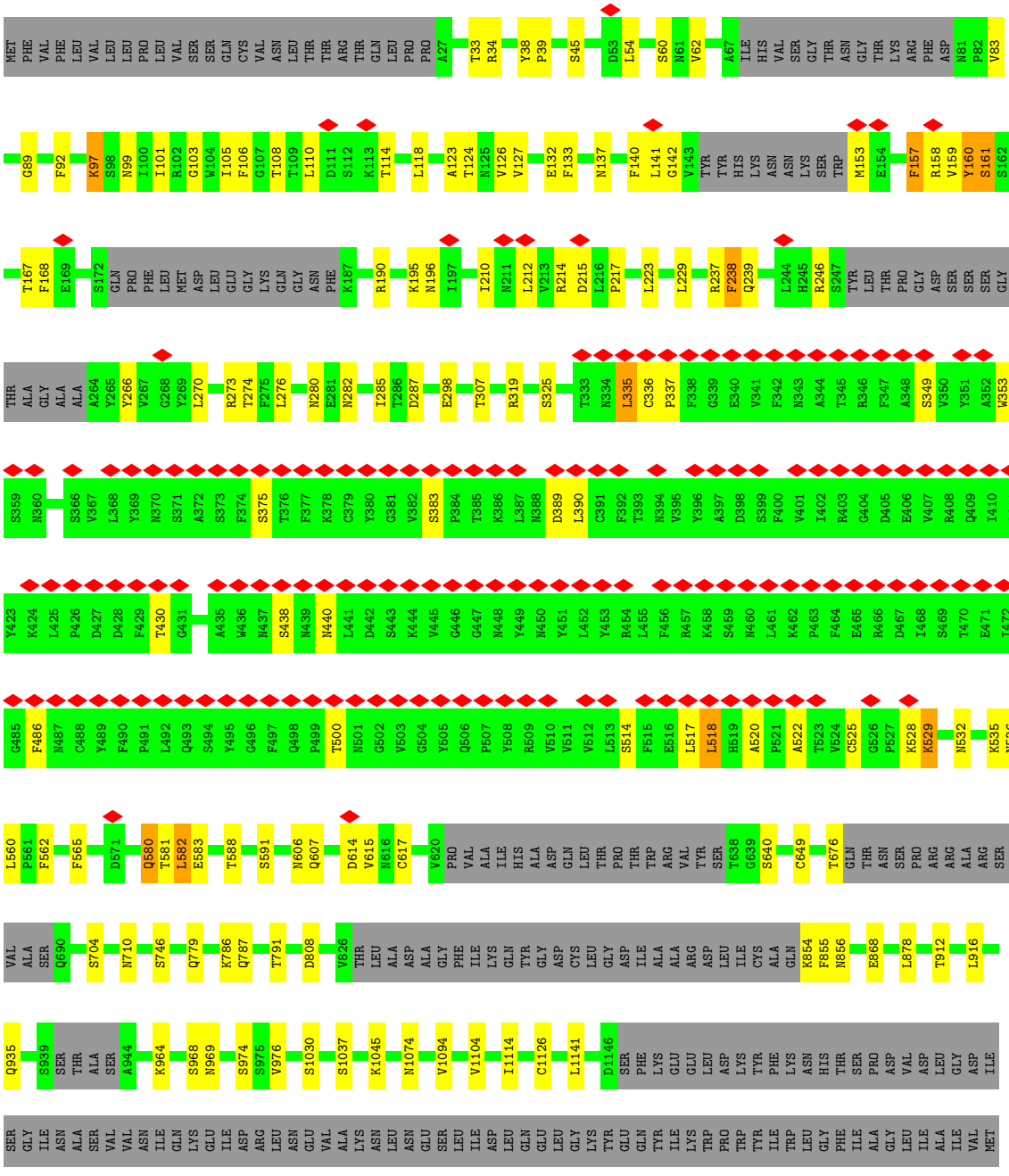
Chain A:

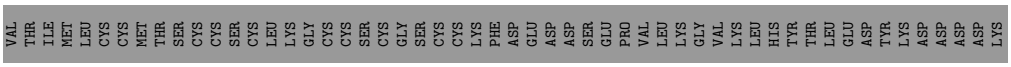




• Molecule 1: Spike glycoprotein

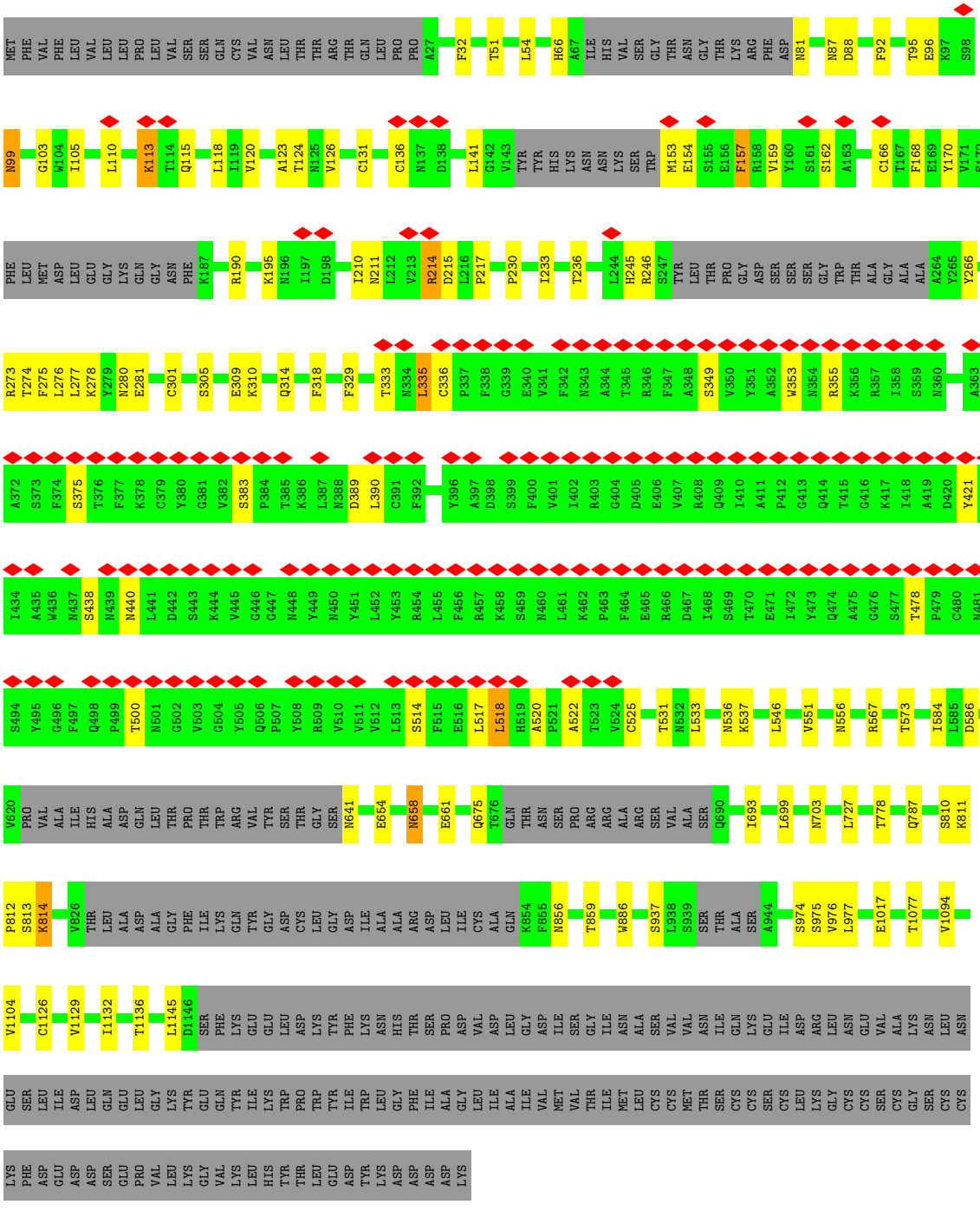
Chain B:





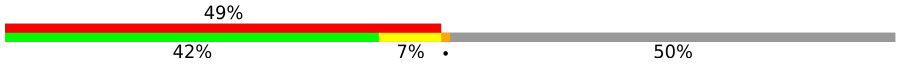
• Molecule 1: Spike glycoprotein

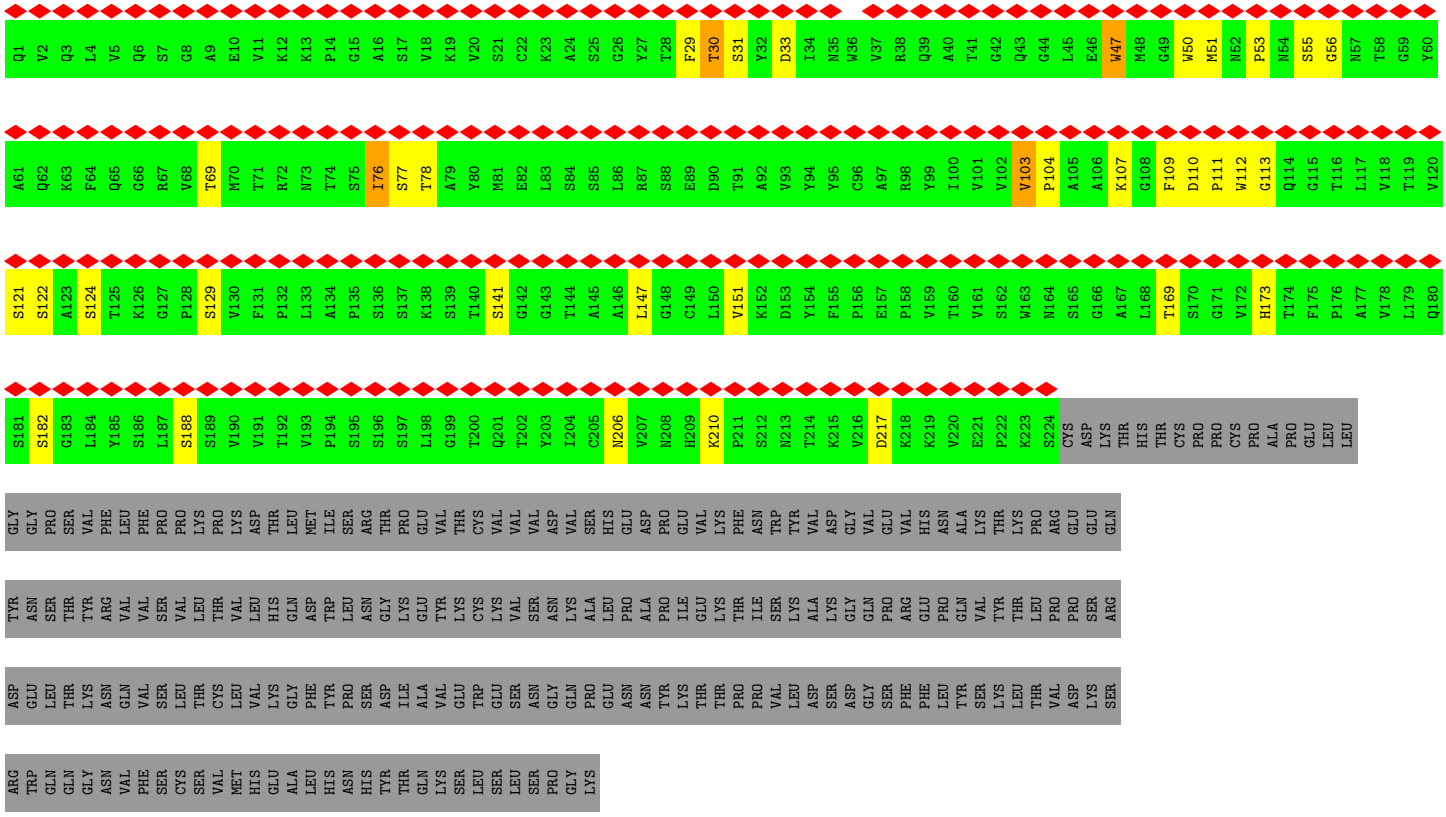
Chain C:



• Molecule 2: Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_3B,Epididymis luminal protein 214,Epididymis luminal protein 214

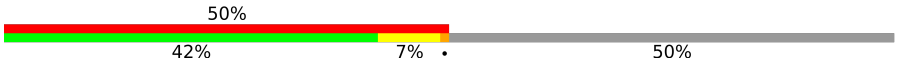
Chain H:

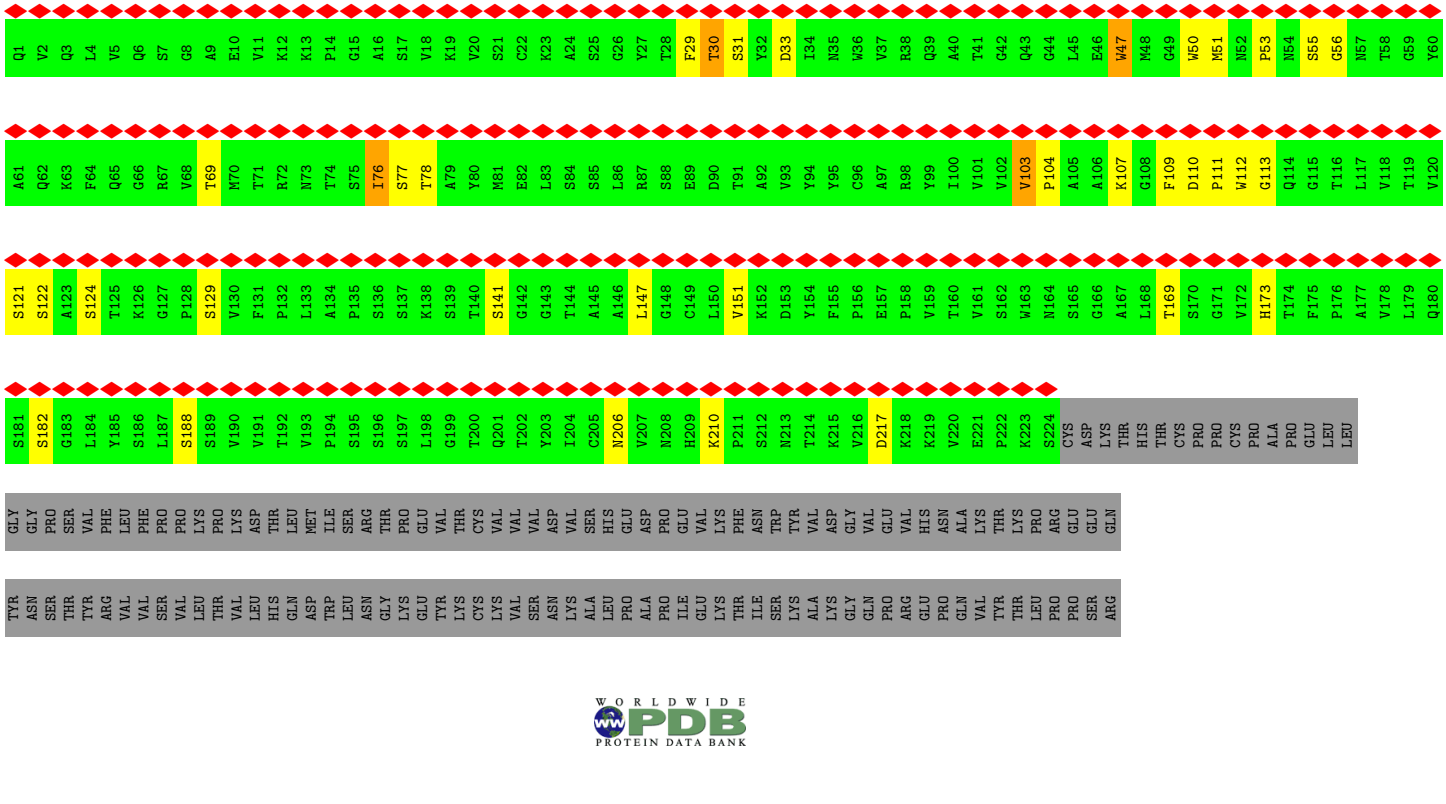


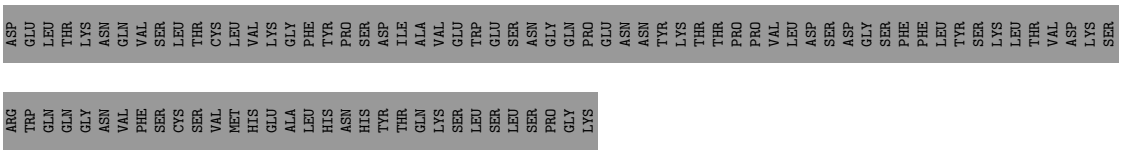


• Molecule 2: Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_3B,Epididymis luminal protein 214,Epididymis luminal protein 214

Chain I:

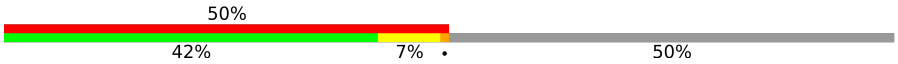


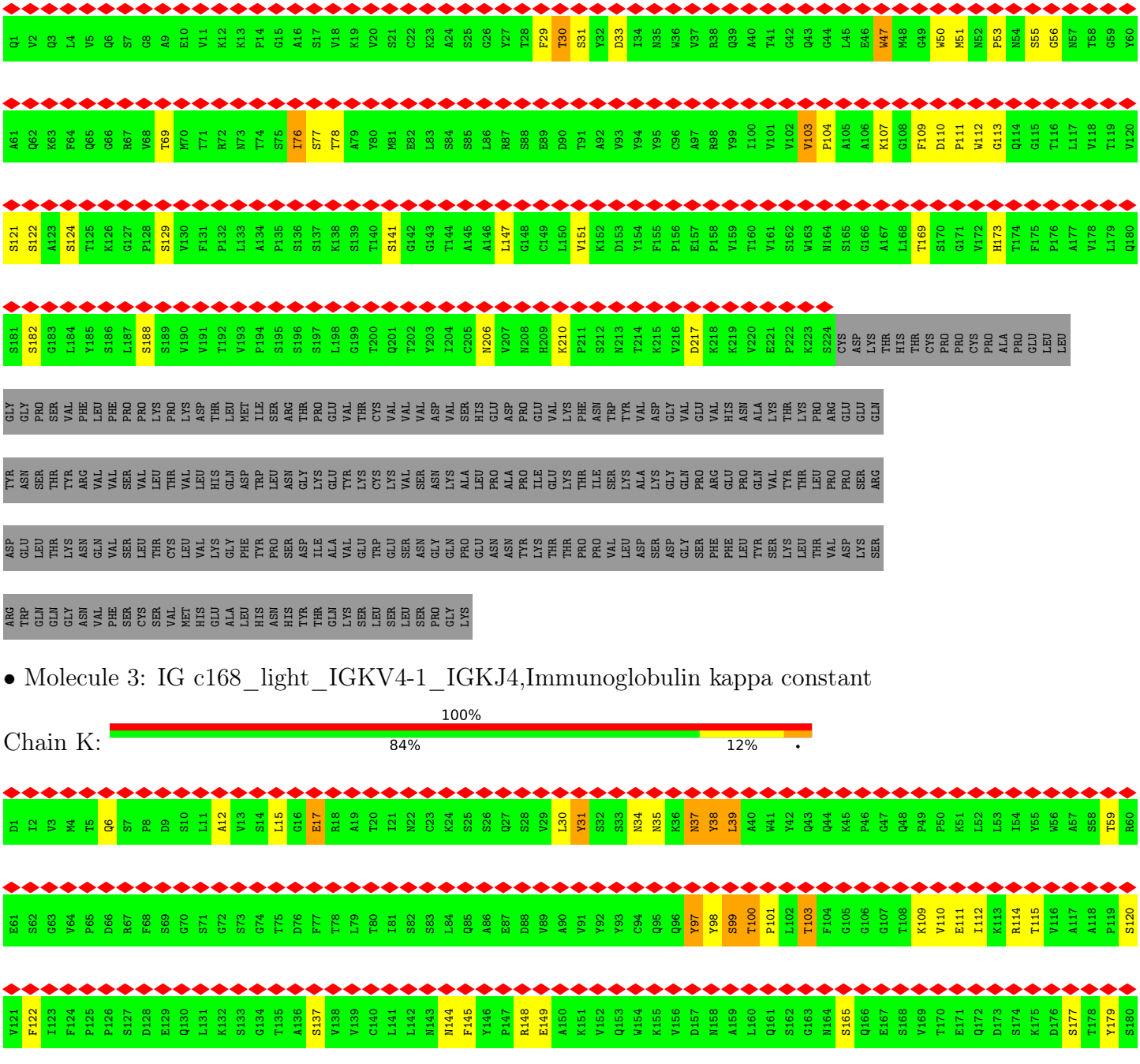




• Molecule 2: Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_3B,Epididymis luminal protein 214,Epididymis luminal protein 214

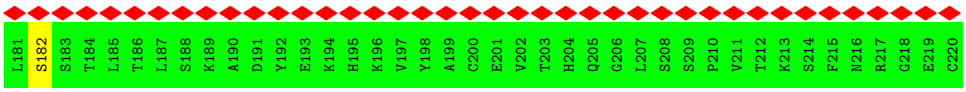
Chain J:





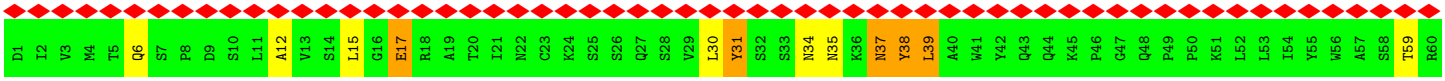
• Molecule 3: IG c168_light_IGKV4-1_IGKJ4,Immunoglobulin kappa constant

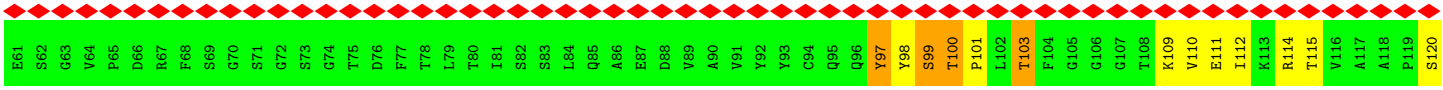
Chain K:

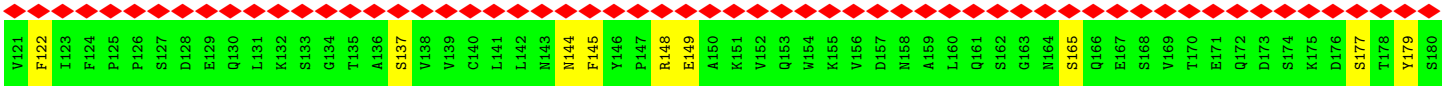


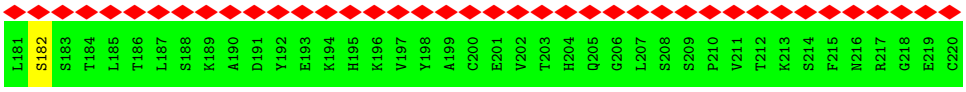
• Molecule 3: IG c168_light_IGKV4-1_IGKJ4,Immunoglobulin kappa constant

Chain M:



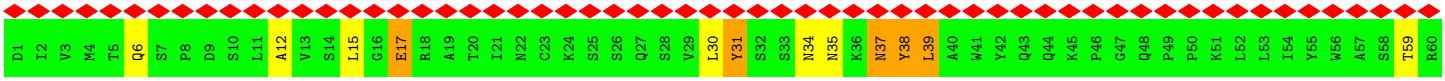


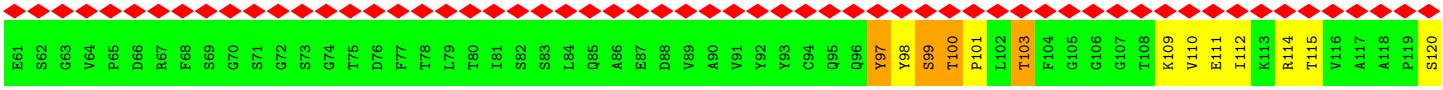


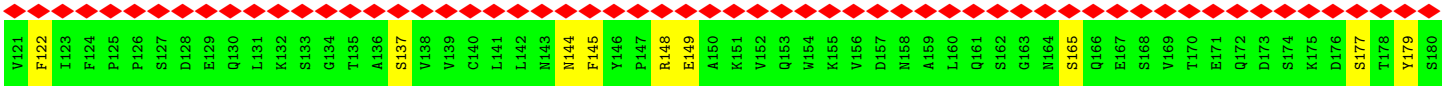


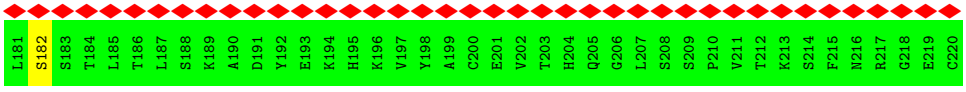
• Molecule 3: IG c168_light_IGKV4-1_IGKJ4,Immunoglobulin kappa constant

Chain N:



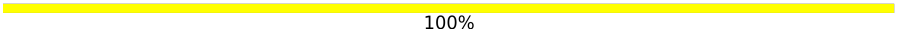






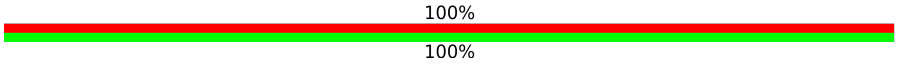
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain E:



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

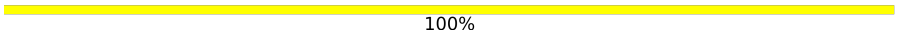
Chain F:

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

Chain G:

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

Chain L:



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

Chain O:

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

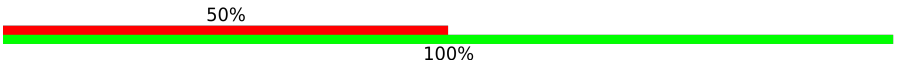
Chain P:

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

Chain Q:

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

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

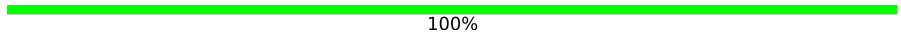


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

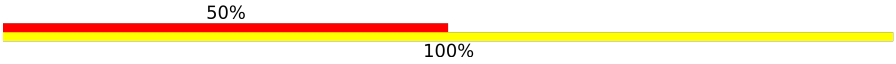
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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



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

Chain X:



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

Chain Y:

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

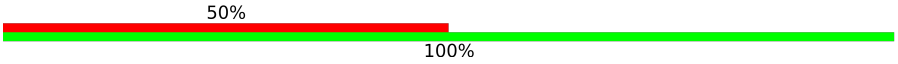
Chain Z:

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

Chain a:

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

Chain b:

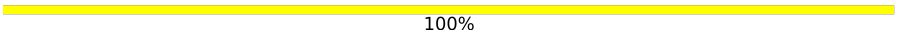


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

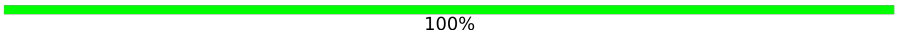
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



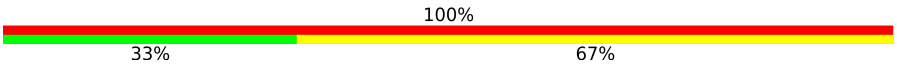
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

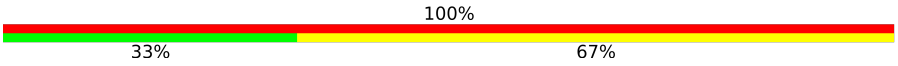


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55704	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.60	0/8039	0.56	0/10936
1	B	0.71	0/8045	0.74	0/10942
1	C	0.71	0/8028	0.73	0/10919
2	H	0.36	0/1710	0.52	0/2331
2	I	0.36	0/1710	0.52	0/2331
2	J	0.36	0/1710	0.52	0/2331
3	K	0.46	0/1722	0.58	0/2343
3	M	0.46	0/1722	0.58	0/2343
3	N	0.46	0/1722	0.58	0/2343
All	All	0.61	0/34408	0.65	0/46819

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	988/1283 (77%)	870 (88%)	103 (10%)	15 (2%)	8 38
1	B	989/1283 (77%)	837 (85%)	111 (11%)	41 (4%)	2 17
1	C	986/1283 (77%)	850 (86%)	96 (10%)	40 (4%)	2 17
2	H	222/452 (49%)	175 (79%)	31 (14%)	16 (7%)	1 6
2	I	222/452 (49%)	175 (79%)	31 (14%)	16 (7%)	1 6
2	J	222/452 (49%)	175 (79%)	31 (14%)	16 (7%)	1 6
3	K	218/220 (99%)	162 (74%)	33 (15%)	23 (11%)	0 2
3	M	218/220 (99%)	162 (74%)	33 (15%)	23 (11%)	0 2
3	N	218/220 (99%)	162 (74%)	33 (15%)	23 (11%)	0 2
All	All	4283/5865 (73%)	3568 (83%)	502 (12%)	213 (5%)	3 13

5 of 213 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	LEU
1	A	518	LEU
1	A	983	ARG
1	B	97	LYS
1	B	133	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	881/1122 (78%)	774 (88%)	107 (12%)	4 19
1	B	881/1122 (78%)	763 (87%)	118 (13%)	3 15
1	C	879/1122 (78%)	780 (89%)	99 (11%)	4 22
2	H	188/399 (47%)	164 (87%)	24 (13%)	3 17
2	I	188/399 (47%)	164 (87%)	24 (13%)	3 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	188/399 (47%)	164 (87%)	24 (13%)	3	17
3	K	191/194 (98%)	170 (89%)	21 (11%)	5	23
3	M	191/194 (98%)	170 (89%)	21 (11%)	5	23
3	N	191/194 (98%)	170 (89%)	21 (11%)	5	23
All	All	3778/5145 (73%)	3319 (88%)	459 (12%)	6	19

5 of 459 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	95	THR
3	N	38	TYR
1	C	537	LYS
3	N	6	GLN
3	M	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	914	ASN
1	C	360	ASN
3	K	96	GLN
1	B	920	GLN
1	C	87	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)

53 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	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.41	0	17,19,21	1.17	1 (5%)
4	NAG	D	2	4	14,14,15	0.42	0	17,19,21	1.16	1 (5%)
4	NAG	E	1	4,1	14,14,15	0.54	0	17,19,21	0.57	0
4	NAG	E	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	F	1	4,1	14,14,15	0.36	0	17,19,21	0.63	1 (5%)
4	NAG	F	2	4	14,14,15	0.52	0	17,19,21	0.46	0
4	NAG	G	1	4,1	14,14,15	0.39	0	17,19,21	0.73	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
4	NAG	L	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
4	NAG	L	2	4	14,14,15	0.40	0	17,19,21	1.38	3 (17%)
4	NAG	O	1	4,1	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
4	NAG	O	2	4	14,14,15	0.30	0	17,19,21	0.65	0
4	NAG	P	1	4,1	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
4	NAG	P	2	4	14,14,15	0.15	0	17,19,21	0.44	0
4	NAG	Q	1	4,1	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
4	NAG	Q	2	4	14,14,15	0.31	0	17,19,21	0.61	0
4	NAG	R	1	4,1	14,14,15	0.56	0	17,19,21	0.57	0
4	NAG	R	2	4	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	S	1	4,1	14,14,15	0.33	0	17,19,21	0.41	0
4	NAG	S	2	4	14,14,15	0.38	0	17,19,21	0.36	0
4	NAG	T	1	4,1	14,14,15	0.34	0	17,19,21	1.10	1 (5%)
4	NAG	T	2	4	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	U	1	4,1	14,14,15	0.31	0	17,19,21	0.69	1 (5%)
4	NAG	U	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	V	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	V	2	4	14,14,15	0.30	0	17,19,21	0.67	0
4	NAG	W	1	4,1	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	W	2	4	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	X	1	4,1	14,14,15	0.40	0	17,19,21	1.16	2 (11%)
4	NAG	X	2	4	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
4	NAG	Y	1	4,1	14,14,15	0.56	0	17,19,21	0.57	0
4	NAG	Y	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	Z	1	4,1	14,14,15	0.21	0	17,19,21	1.35	1 (5%)
4	NAG	Z	2	4	14,14,15	0.19	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	a	1	4,1	14,14,15	0.52	0	17,19,21	0.71	1 (5%)
4	NAG	a	2	4	14,14,15	0.41	0	17,19,21	0.46	0
4	NAG	b	1	4,1	14,14,15	0.34	0	17,19,21	0.42	0
4	NAG	b	2	4	14,14,15	0.23	0	17,19,21	0.72	0
4	NAG	c	1	4,1	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	c	2	4	14,14,15	0.55	0	17,19,21	1.31	1 (5%)
4	NAG	d	1	4,1	14,14,15	0.63	1 (7%)	17,19,21	0.45	0
4	NAG	d	2	4	14,14,15	0.30	0	17,19,21	1.34	2 (11%)
4	NAG	e	1	4,1	14,14,15	0.41	0	17,19,21	0.43	0
4	NAG	e	2	4	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	f	1	2,5	14,14,15	0.41	0	17,19,21	1.17	1 (5%)
5	NAG	f	2	5	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
5	NAG	f	3	5	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	g	1	2,5	14,14,15	0.41	0	17,19,21	1.18	1 (5%)
5	NAG	g	2	5	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
5	NAG	g	3	5	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	h	1	2,5	14,14,15	0.40	0	17,19,21	1.17	1 (5%)
5	NAG	h	2	5	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
5	NAG	h	3	5	14,14,15	0.29	0	17,19,21	0.62	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
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	5/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	5/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	3/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	4/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	1/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	c	2	4	-	5/6/23/26	0/1/1/1
4	NAG	d	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	4/6/23/26	0/1/1/1
4	NAG	e	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
5	NAG	f	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	f	2	5	-	4/6/23/26	0/1/1/1
5	NAG	f	3	5	-	2/6/23/26	0/1/1/1
5	NAG	g	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	g	2	5	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	g	3	5	-	2/6/23/26	0/1/1/1
5	NAG	h	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	h	2	5	-	4/6/23/26	0/1/1/1
5	NAG	h	3	5	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	NAG	O5-C1	-2.79	1.39	1.43
4	O	1	NAG	O5-C1	-2.55	1.39	1.43
4	L	1	NAG	O5-C1	-2.37	1.39	1.43
4	d	1	NAG	O5-C1	-2.12	1.40	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	1	NAG	C2-N2-C7	4.59	129.44	122.90
4	c	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	d	2	NAG	C2-N2-C7	4.32	129.06	122.90
4	L	2	NAG	C2-N2-C7	4.29	129.01	122.90
4	G	2	NAG	C2-N2-C7	4.28	129.00	122.90

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

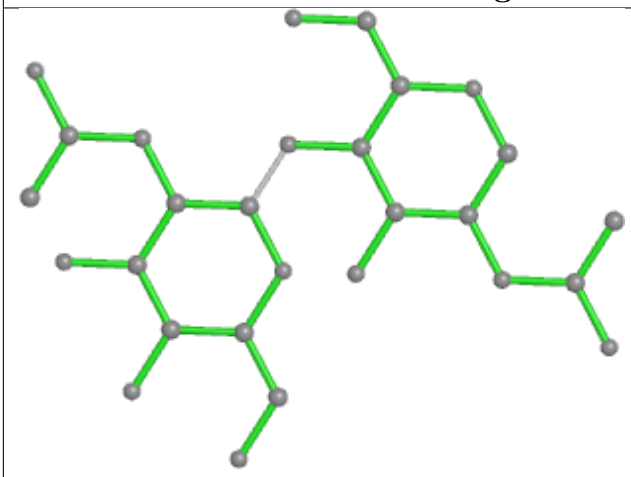
Mol	Chain	Res	Type	Atoms
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
5	f	2	NAG	C8-C7-N2-C2
5	f	2	NAG	O7-C7-N2-C2
5	g	2	NAG	C8-C7-N2-C2

There are no ring outliers.

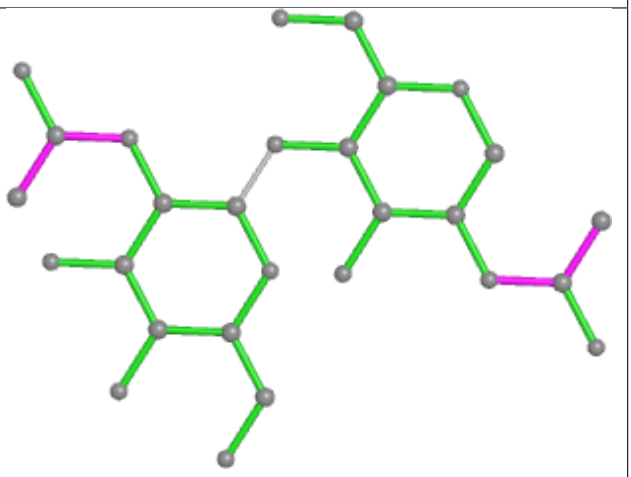
No monomer is involved in short contacts.

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

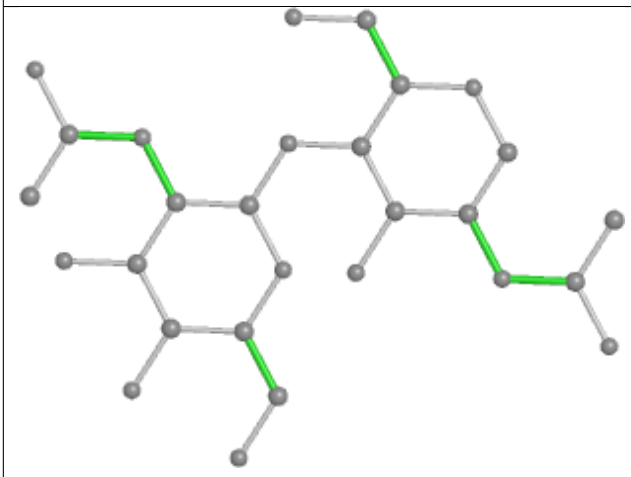
Oligosaccharide Chain D



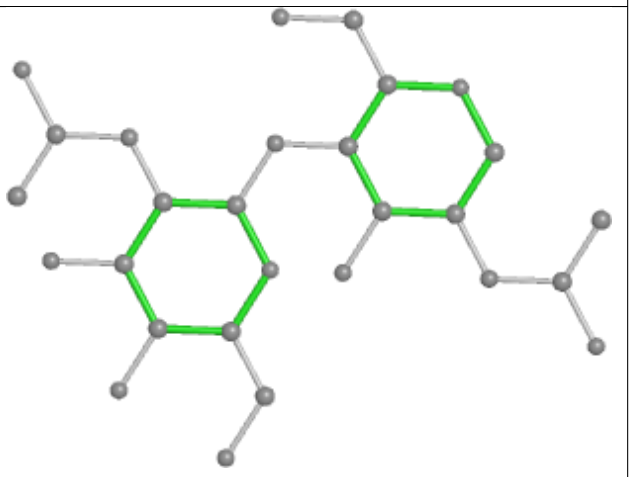
Bond lengths



Bond angles

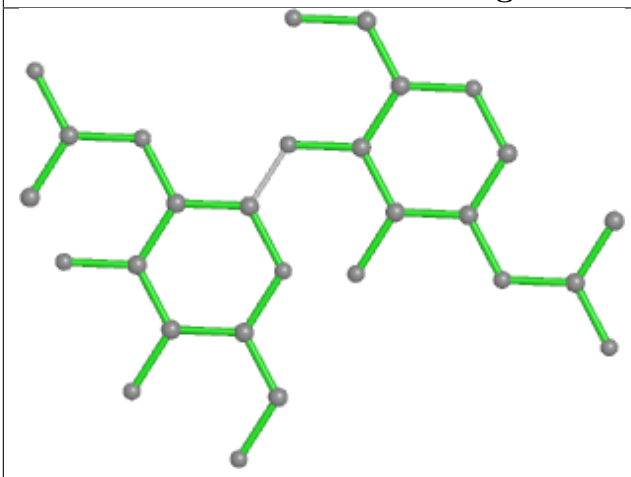


Torsions

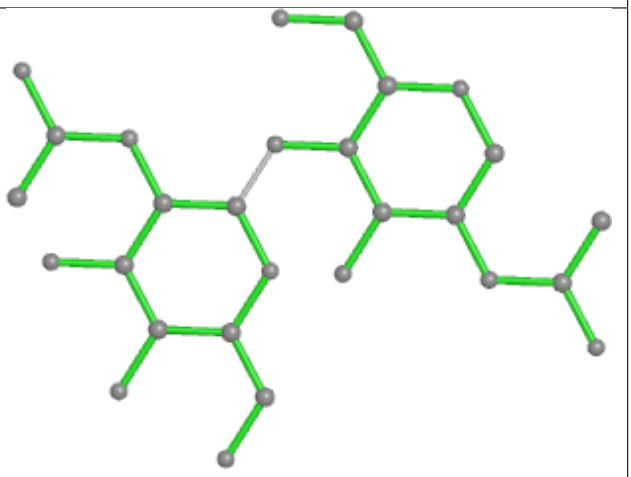


Rings

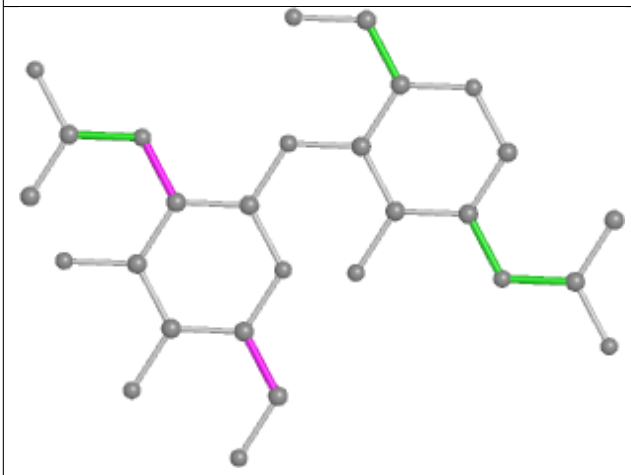
Oligosaccharide Chain E



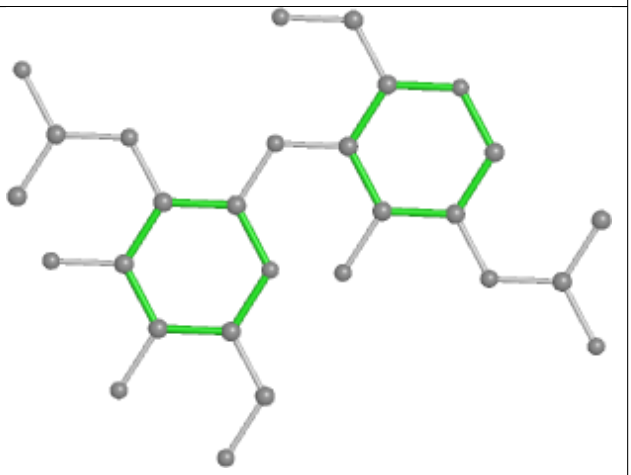
Bond lengths



Bond angles

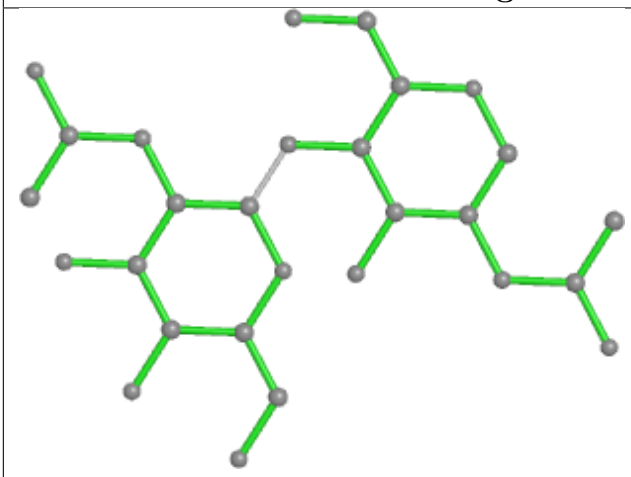


Torsions

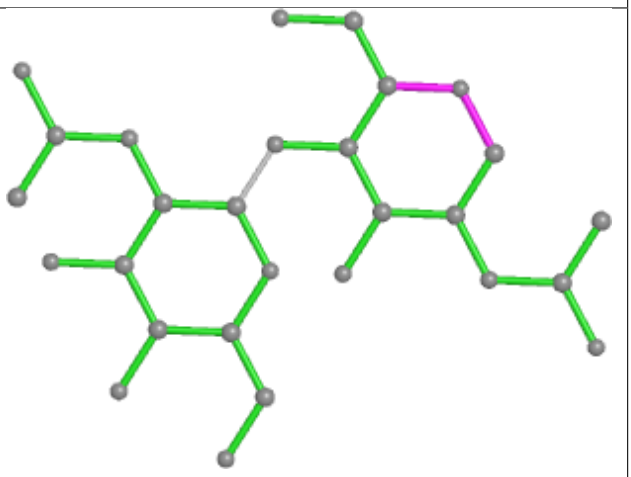


Rings

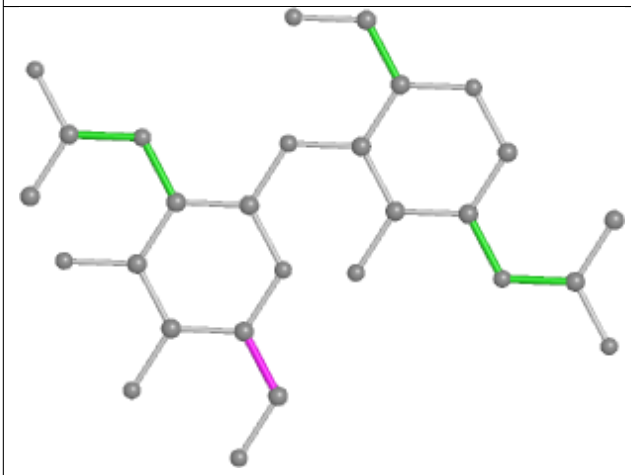
Oligosaccharide Chain F



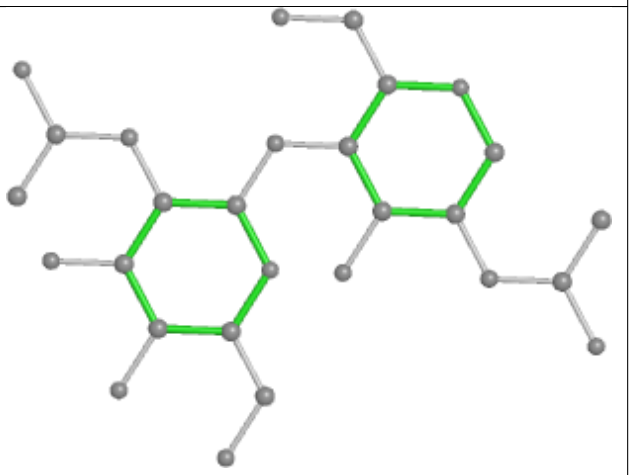
Bond lengths



Bond angles

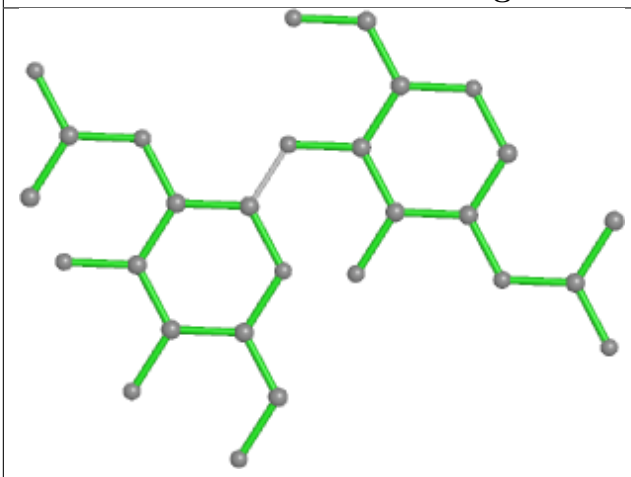


Torsions

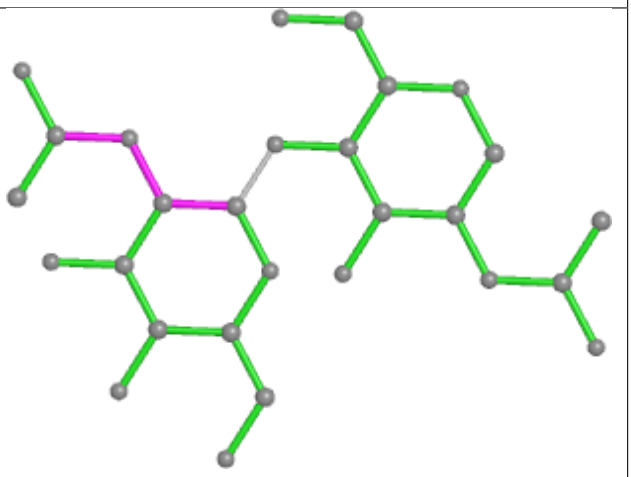


Rings

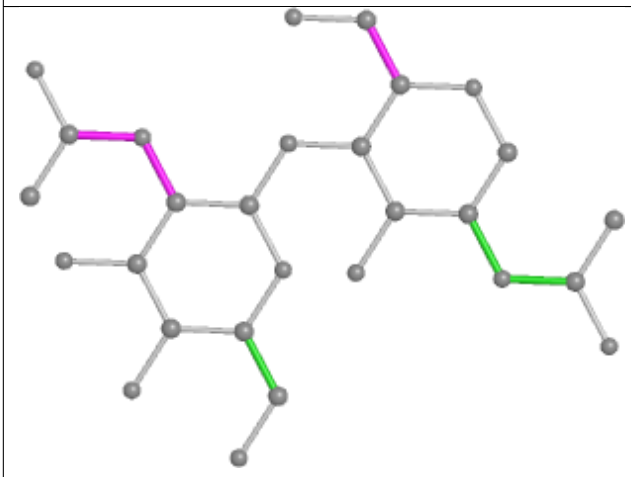
Oligosaccharide Chain G



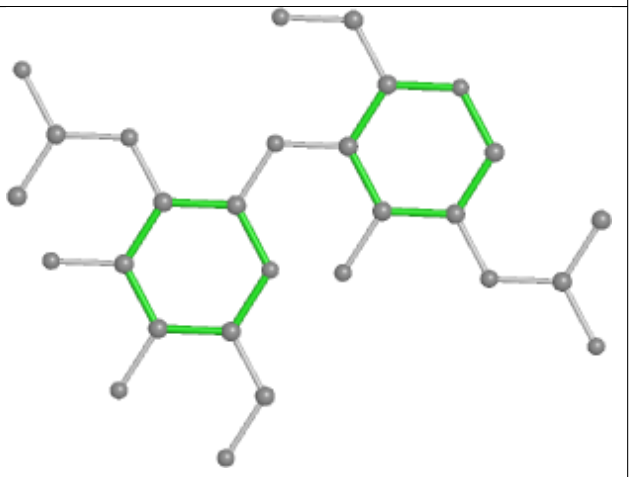
Bond lengths



Bond angles

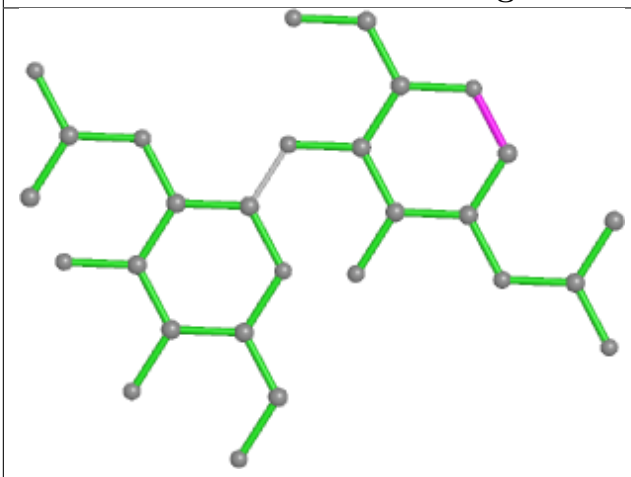


Torsions

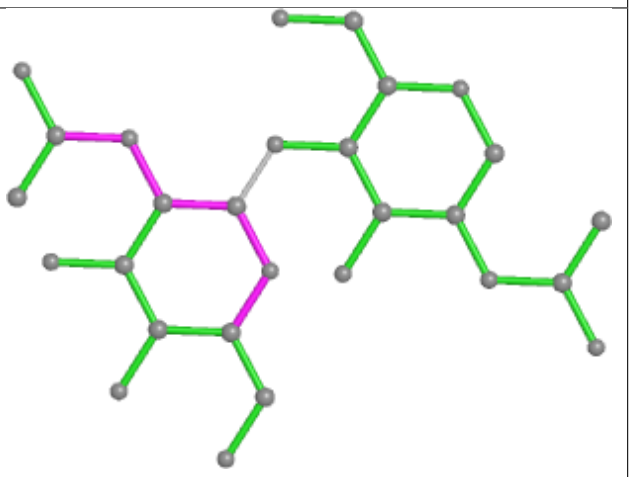


Rings

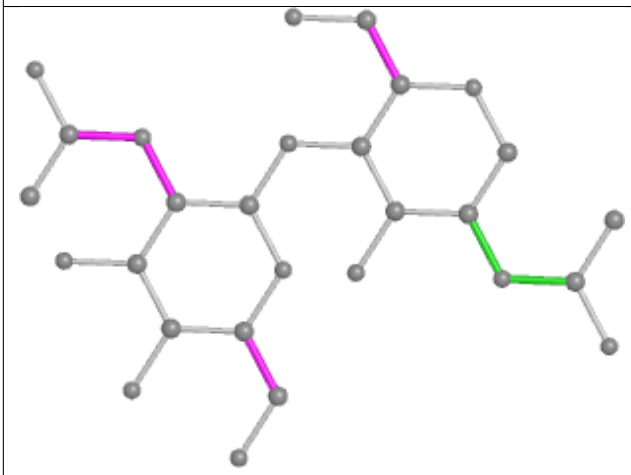
Oligosaccharide Chain L



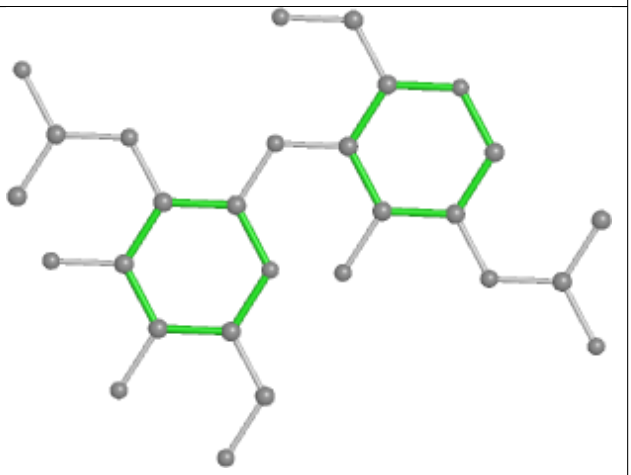
Bond lengths



Bond angles

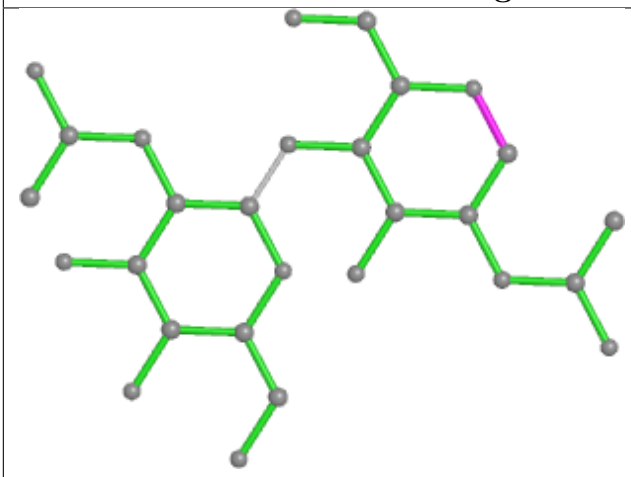


Torsions



Rings

Oligosaccharide Chain O



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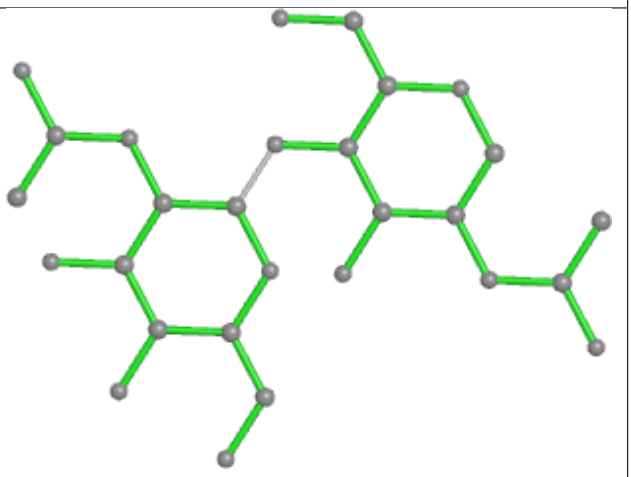
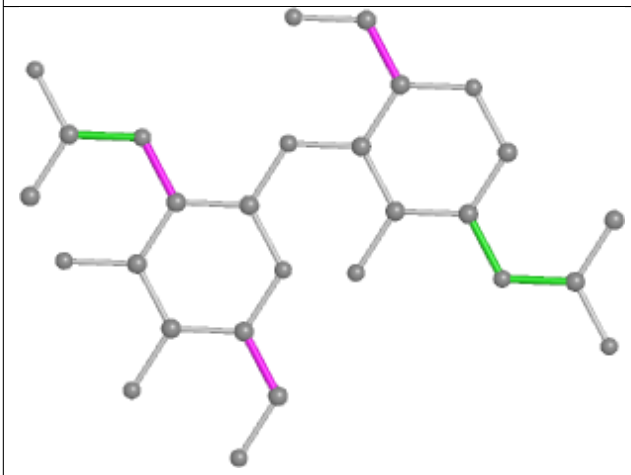
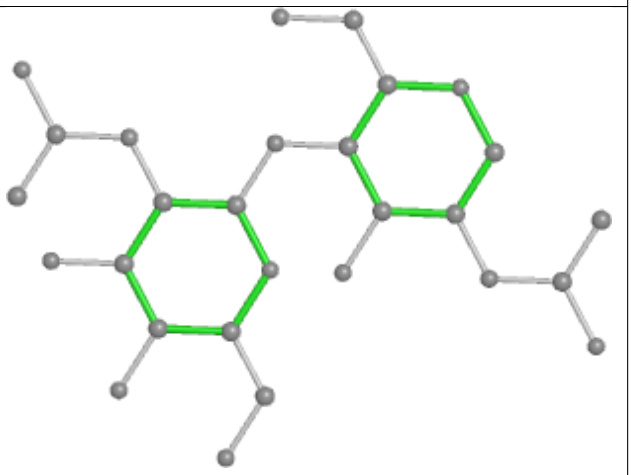


Bond angles

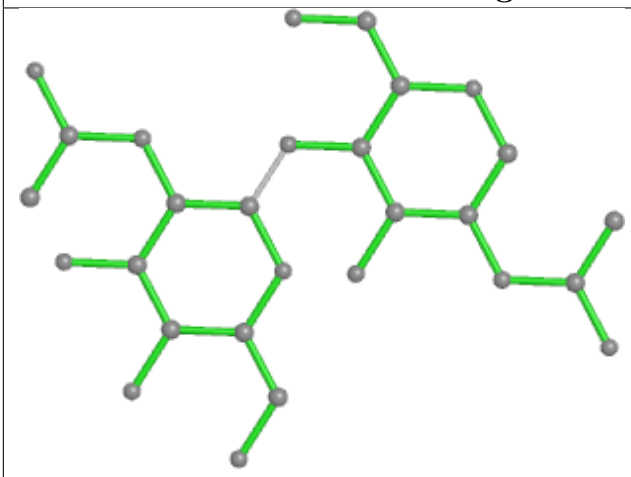


Torsions



Rings

Oligosaccharide Chain P



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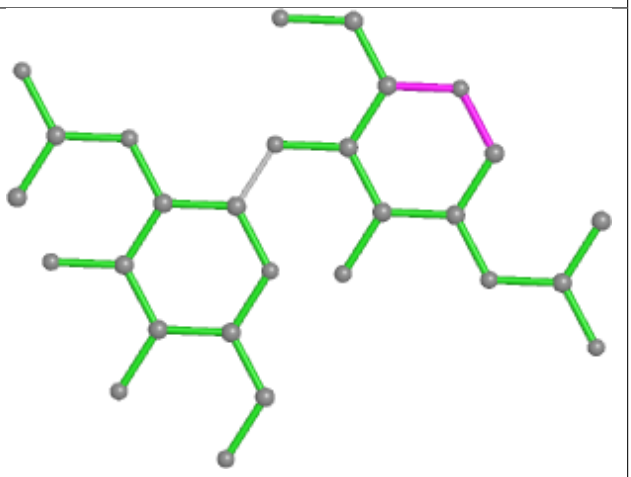
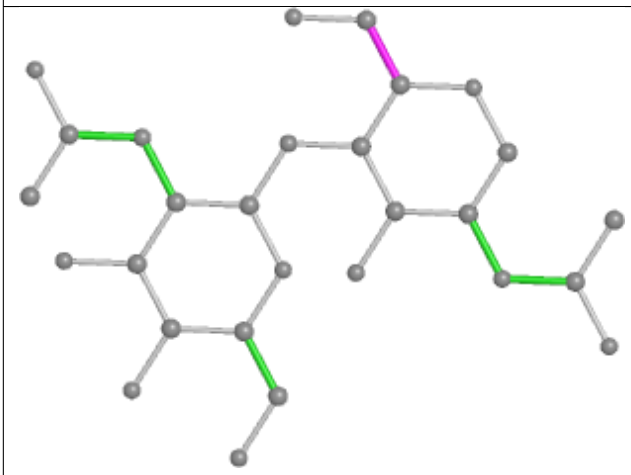
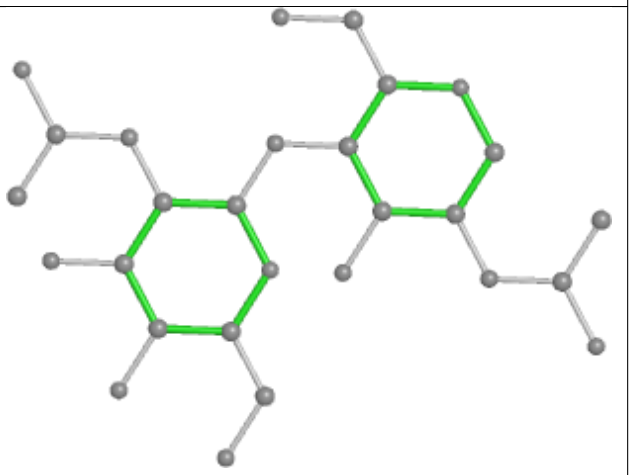


Bond angles

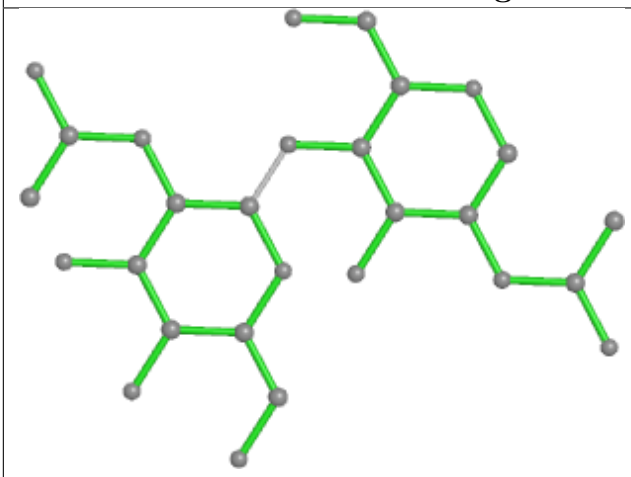


Torsions



Rings

Oligosaccharide Chain Q



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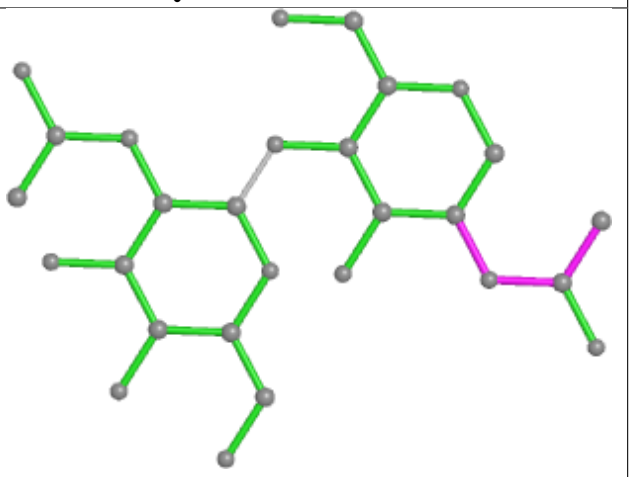
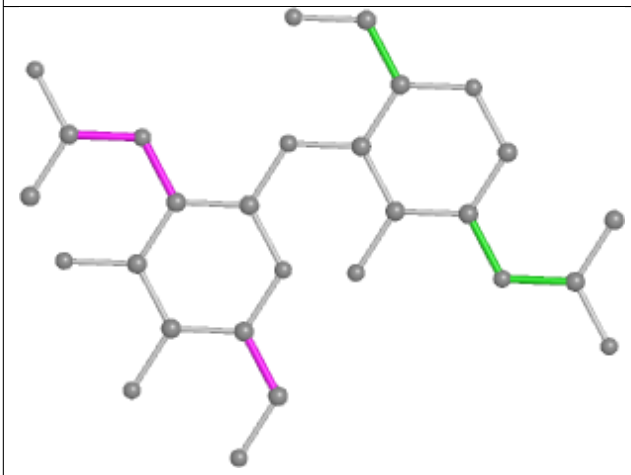


Bond angles



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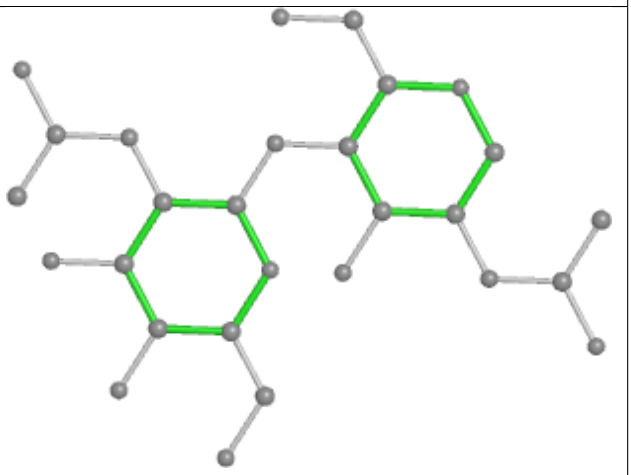
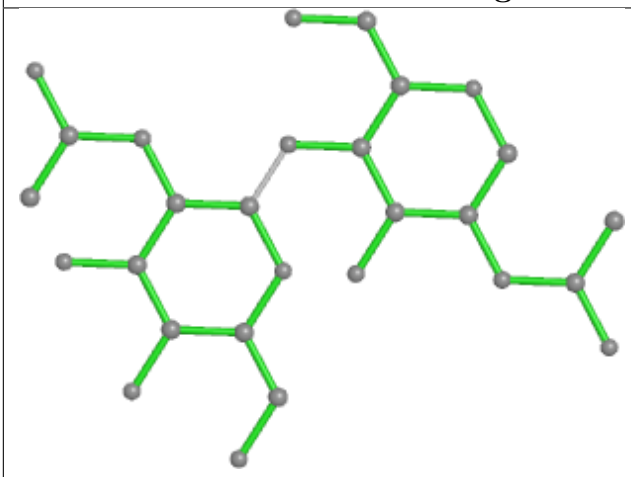


Rings

Oligosaccharide Chain R



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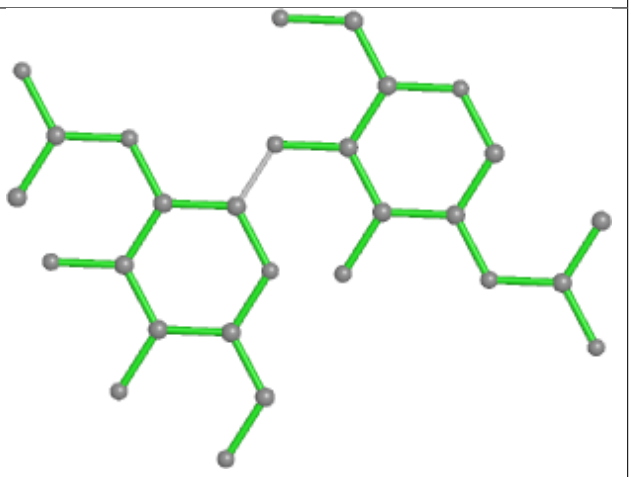
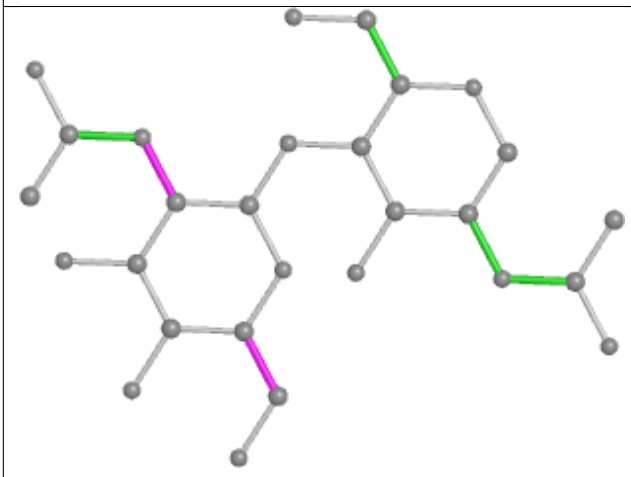
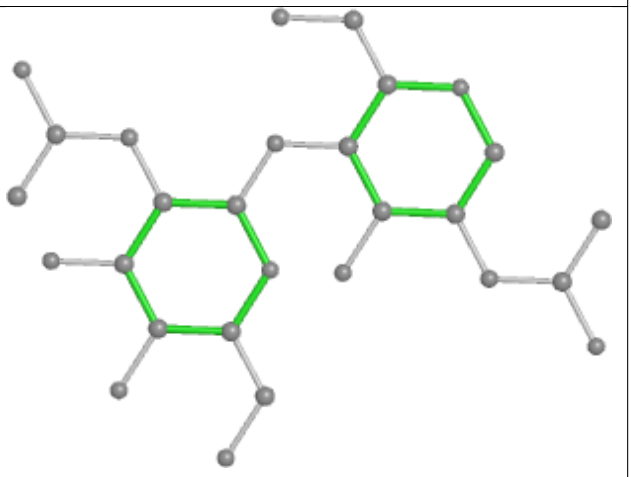


Bond angles

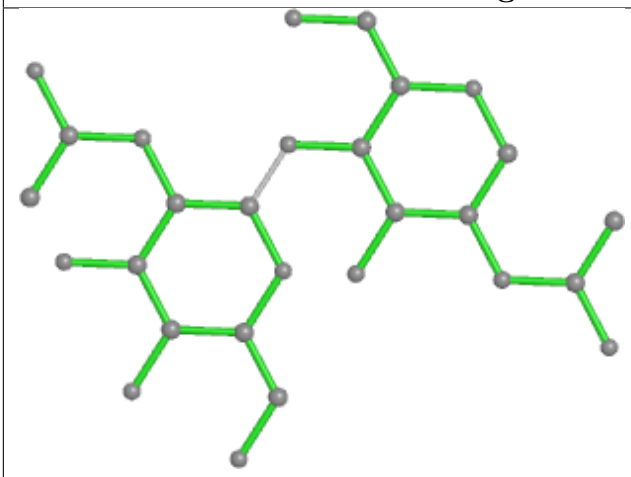


Torsions

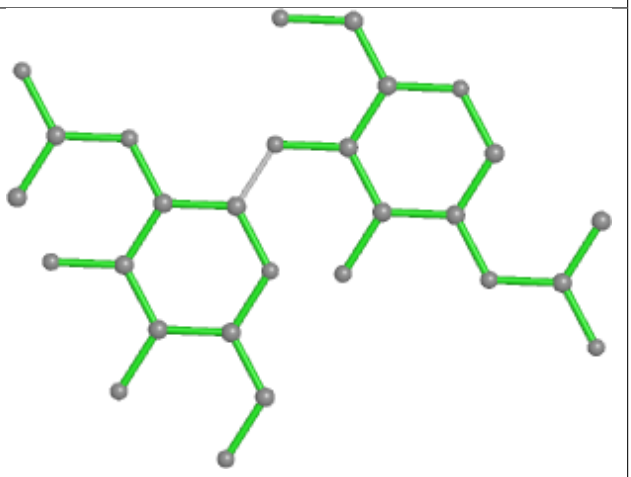


Rings

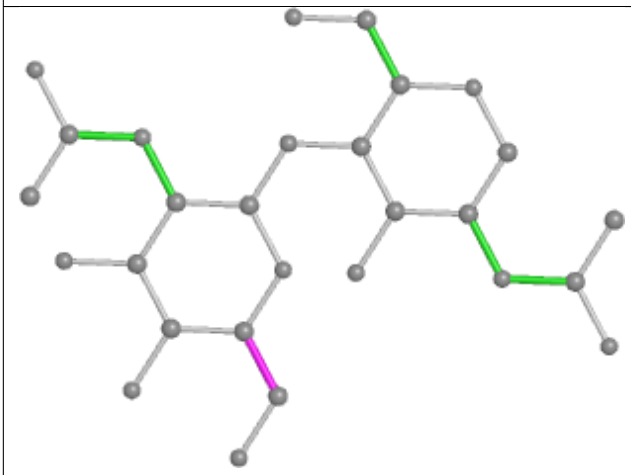
Oligosaccharide Chain S



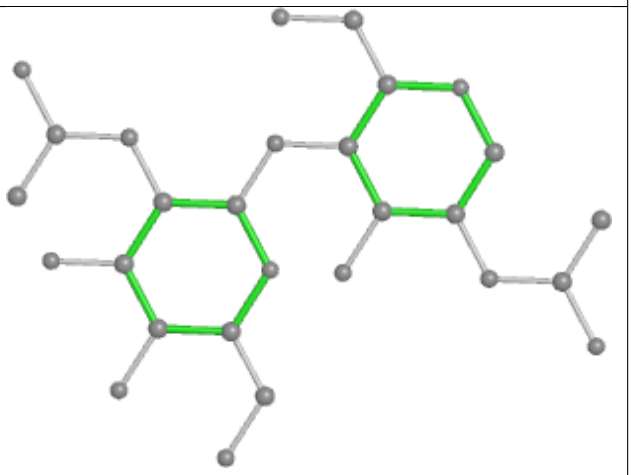
Bond lengths



Bond angles

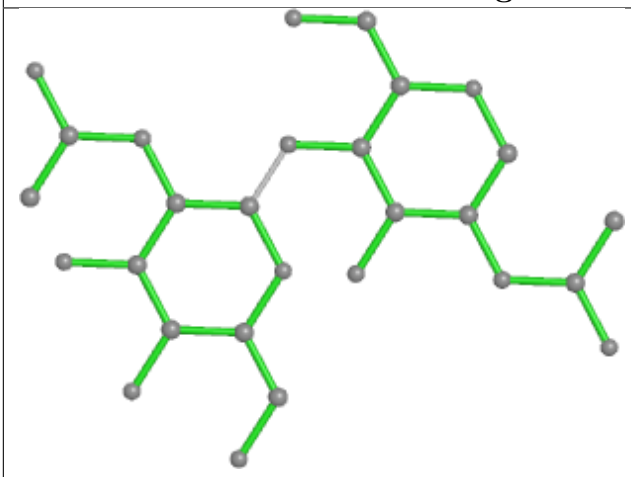


Torsions



Rings

Oligosaccharide Chain T



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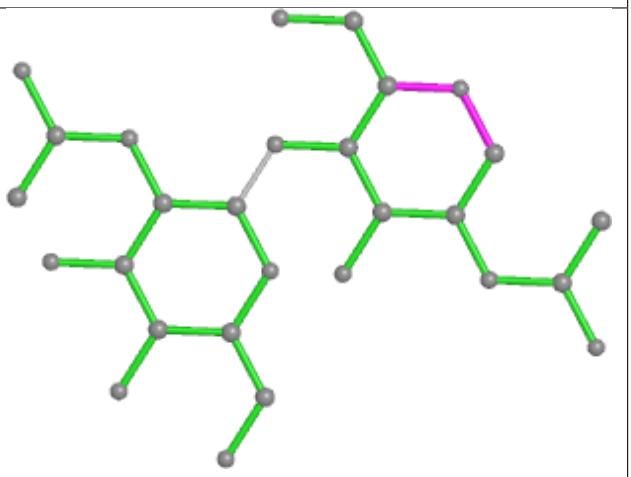
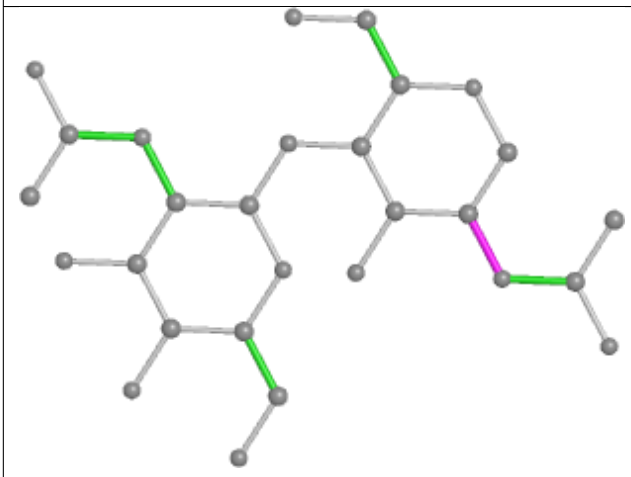
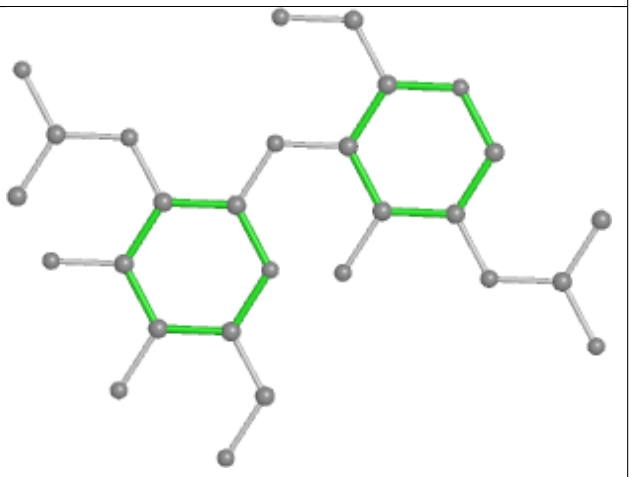


Bond angles

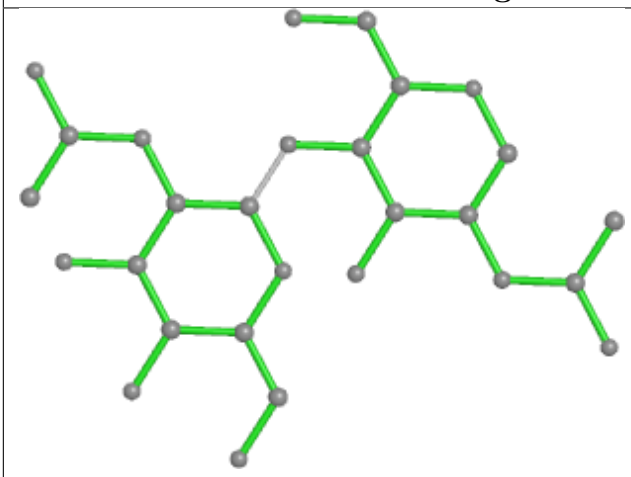


Torsions



Rings

Oligosaccharide Chain U



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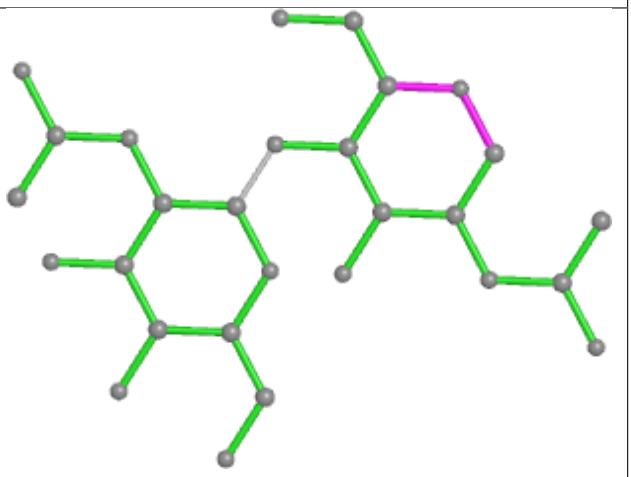
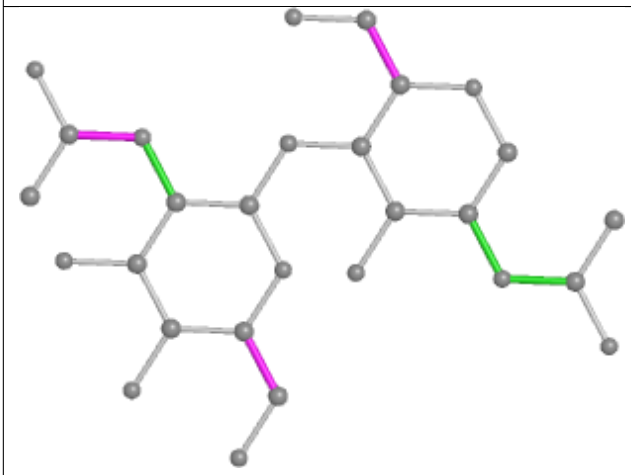


Bond angles



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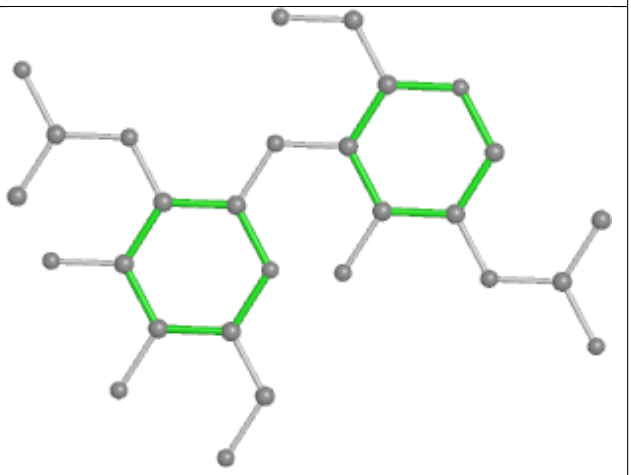
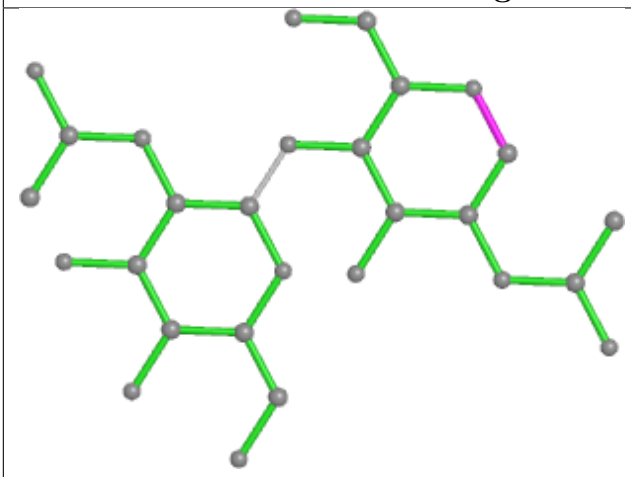


Rings

Oligosaccharide Chain V



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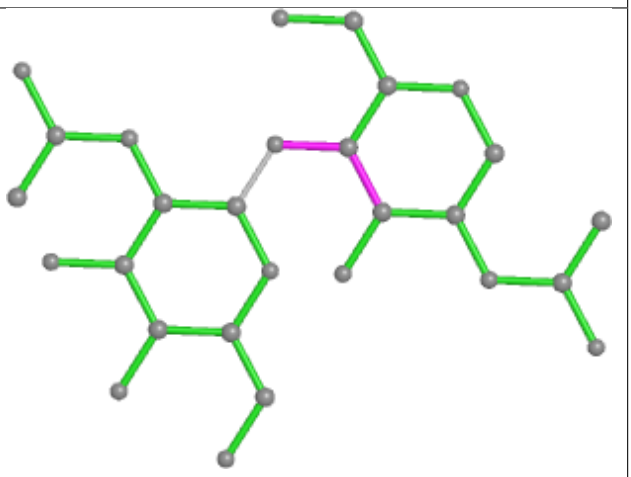

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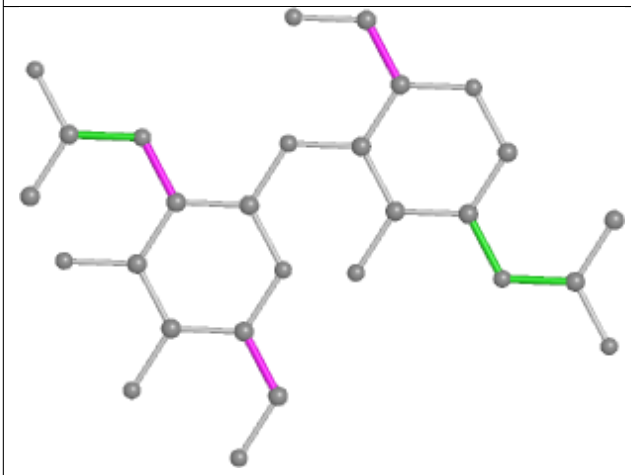

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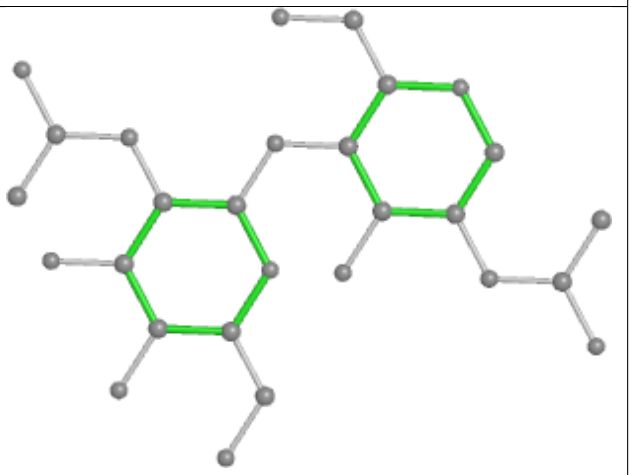
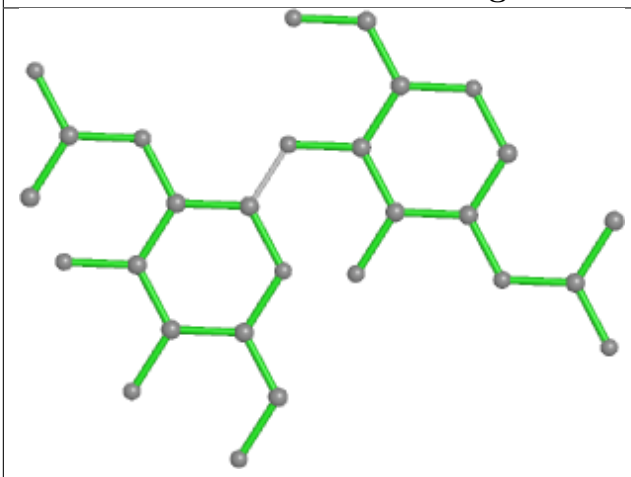


Rings

Oligosaccharide Chain W



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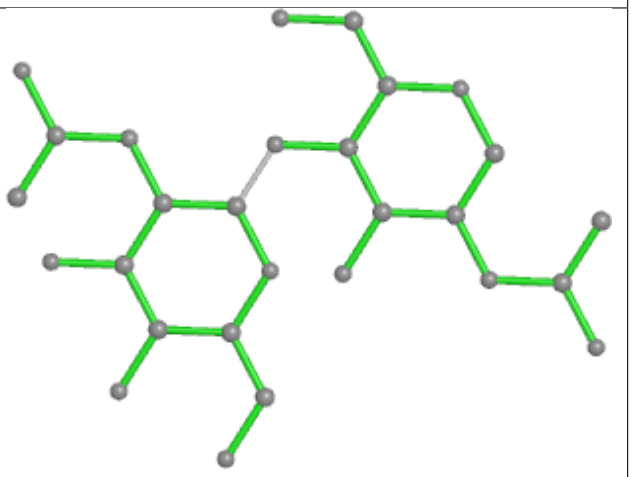

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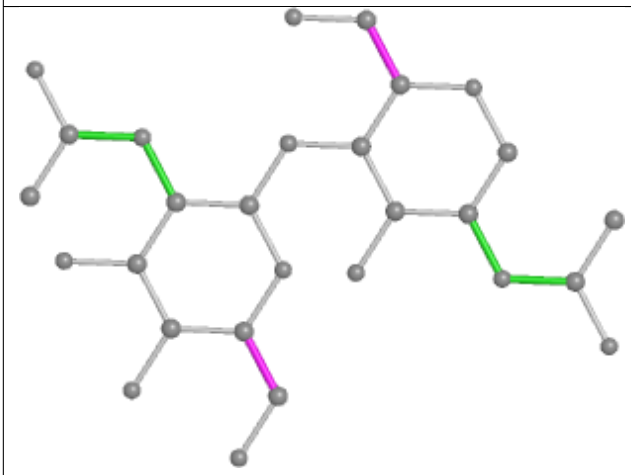

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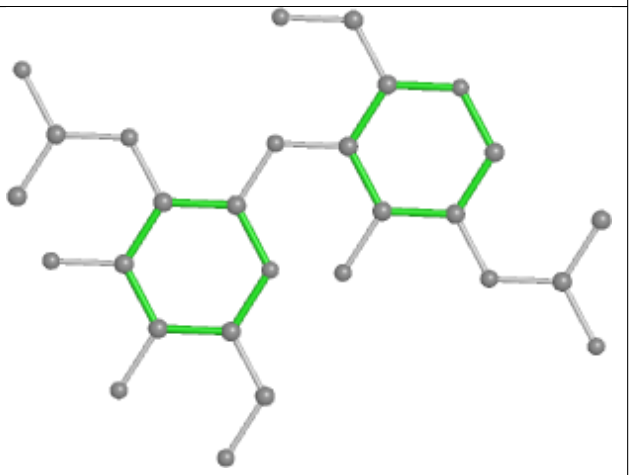
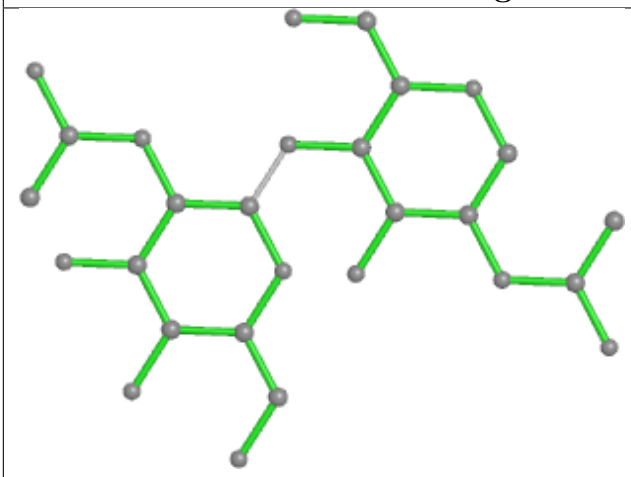


Rings

Oligosaccharide Chain X



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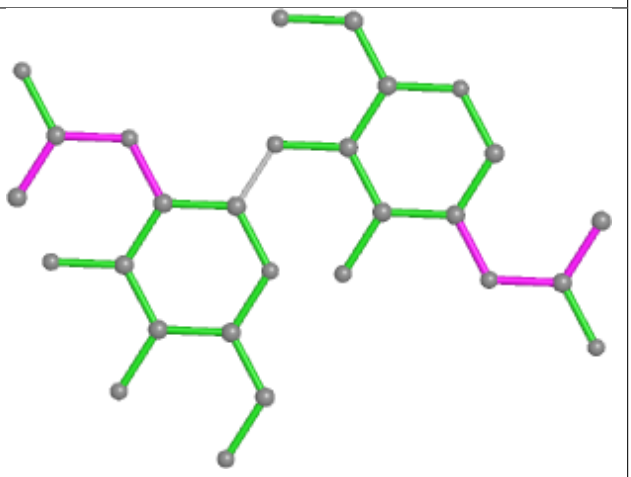
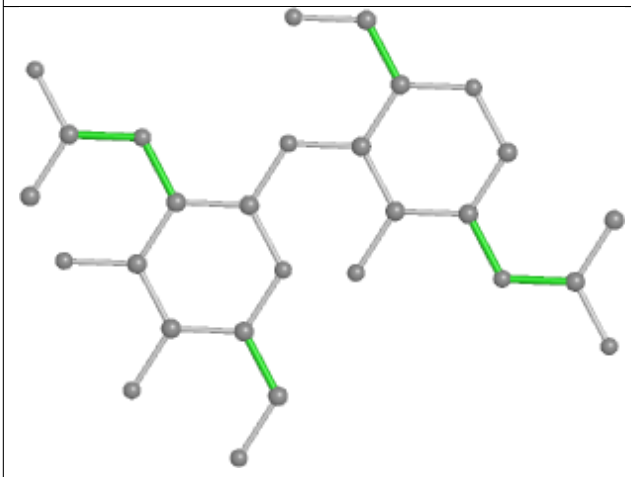


Bond angles



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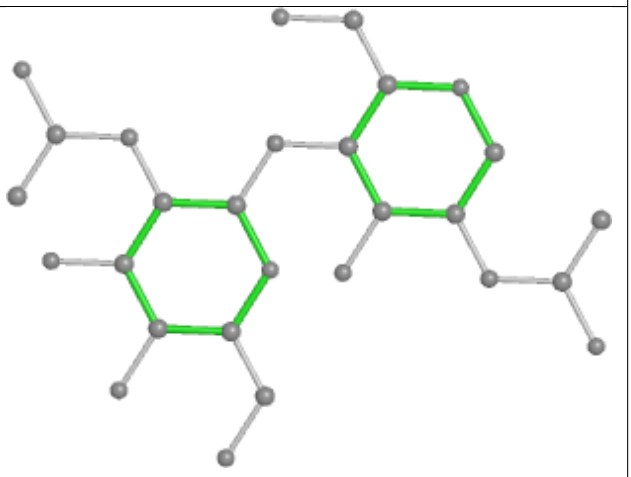
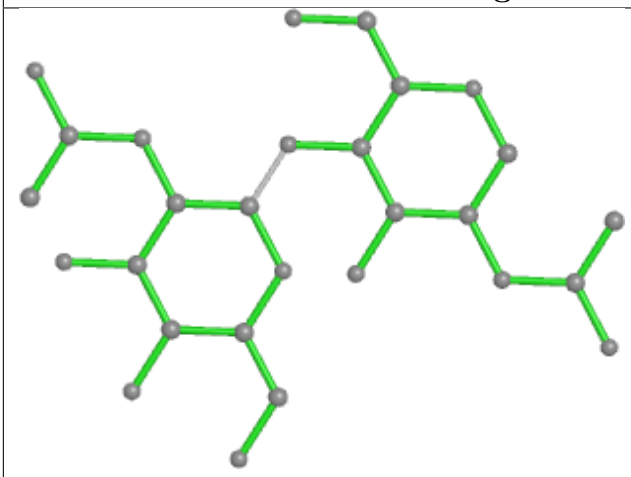


Rings

Oligosaccharide Chain Y



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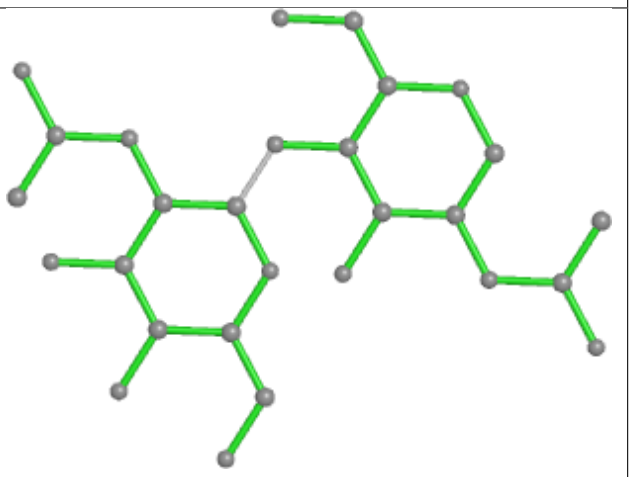

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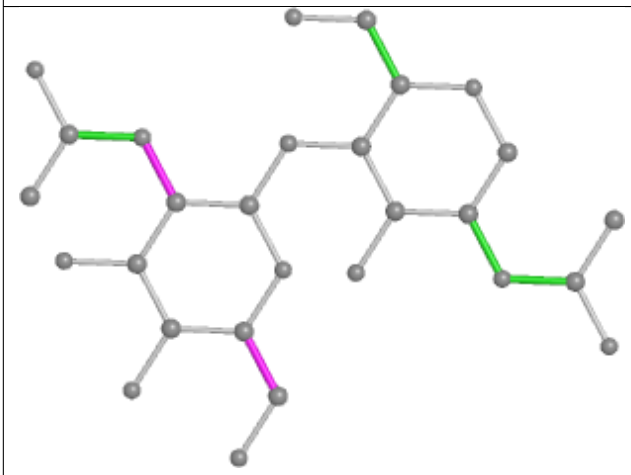

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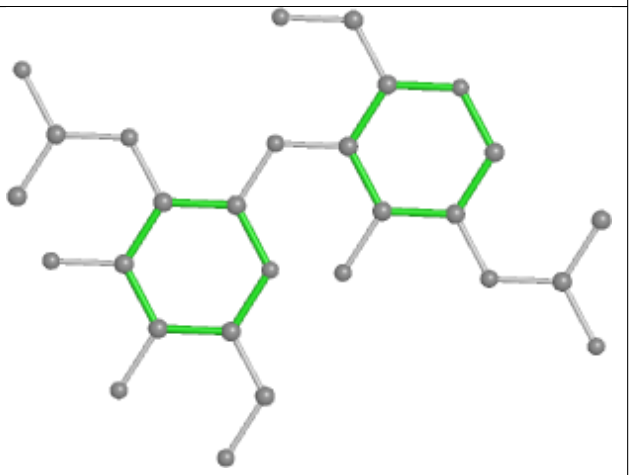

Rings

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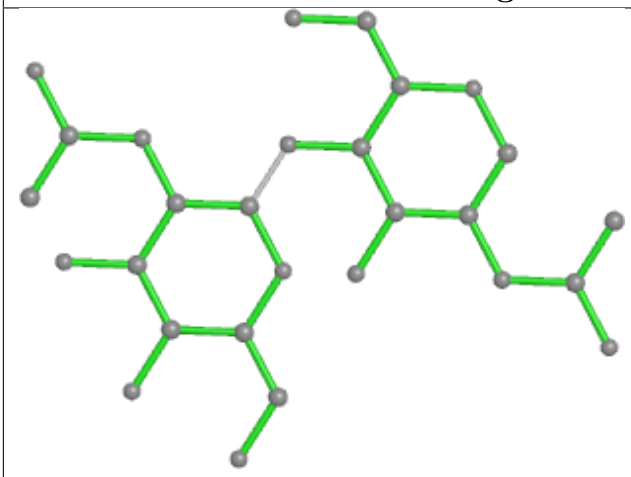

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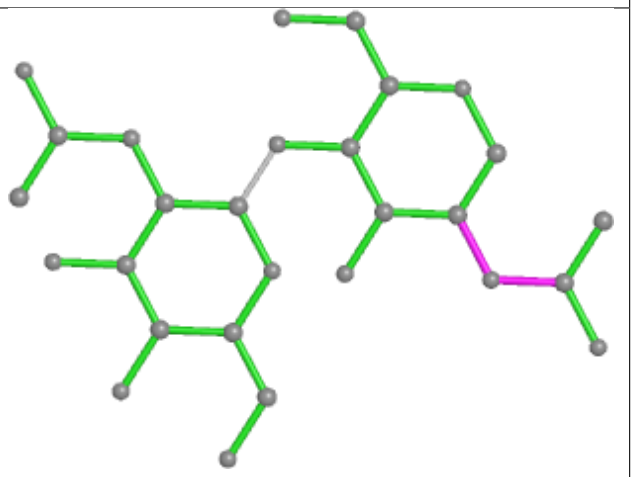

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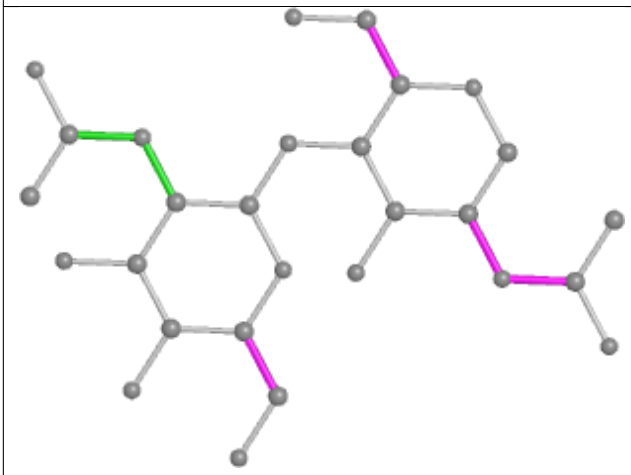

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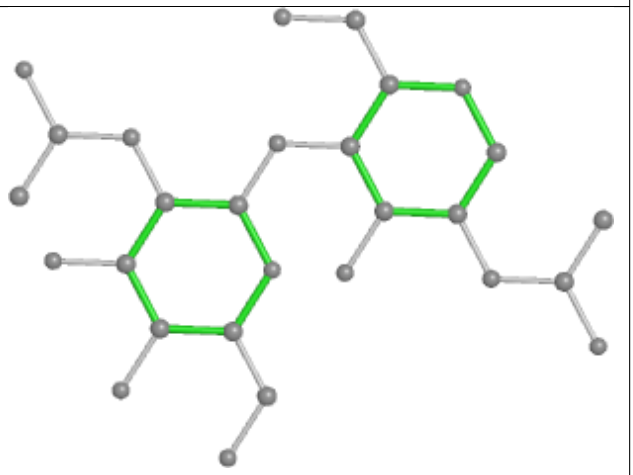
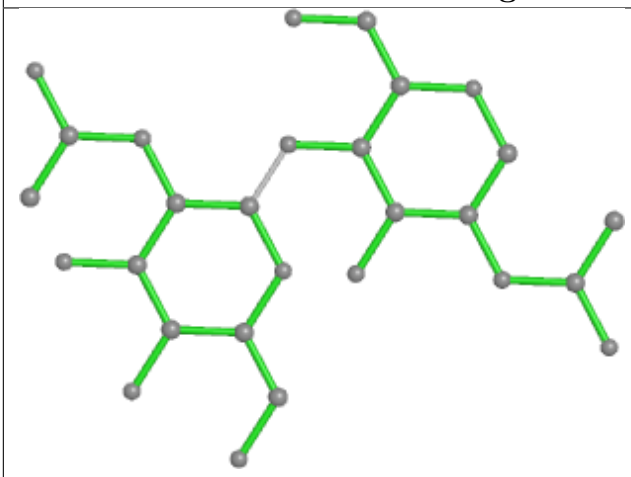


Rings

Oligosaccharide Chain a



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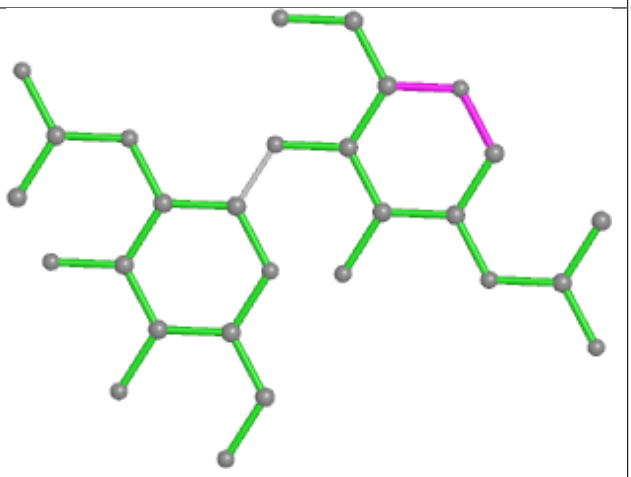

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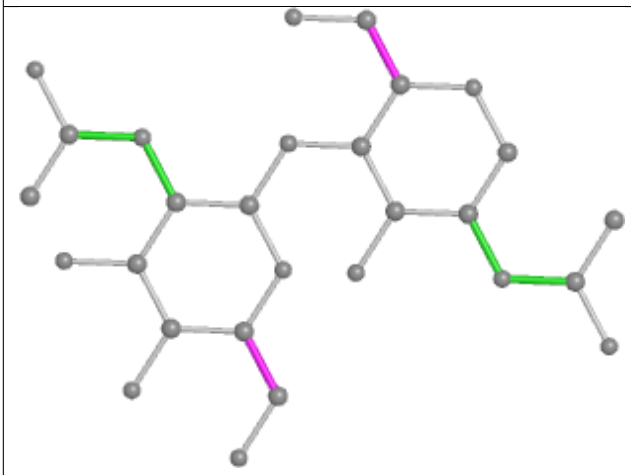

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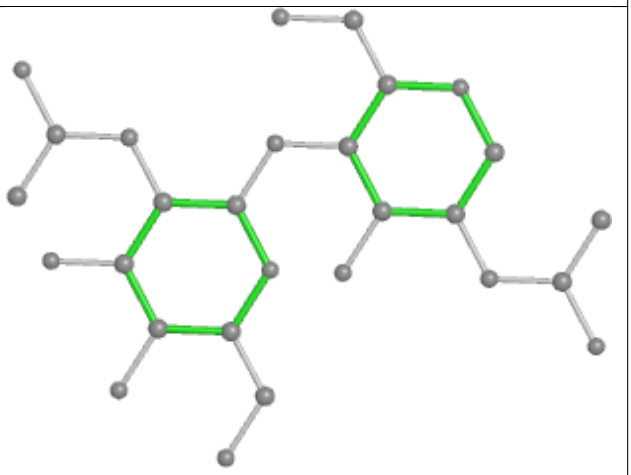
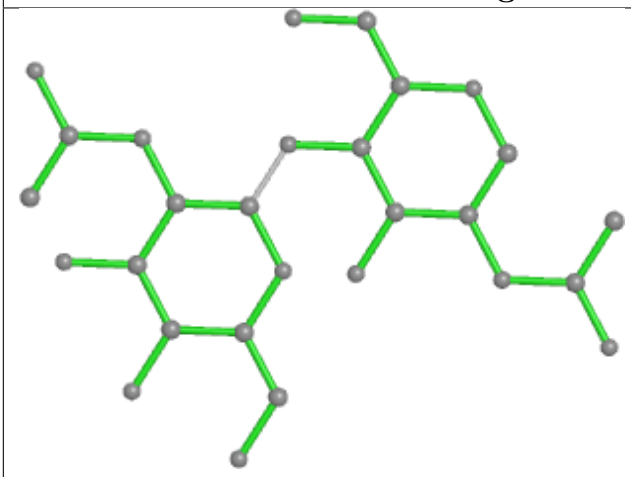


Rings

Oligosaccharide Chain b



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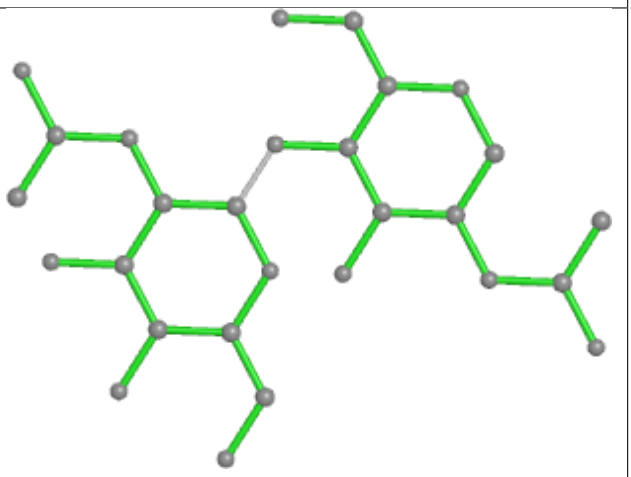
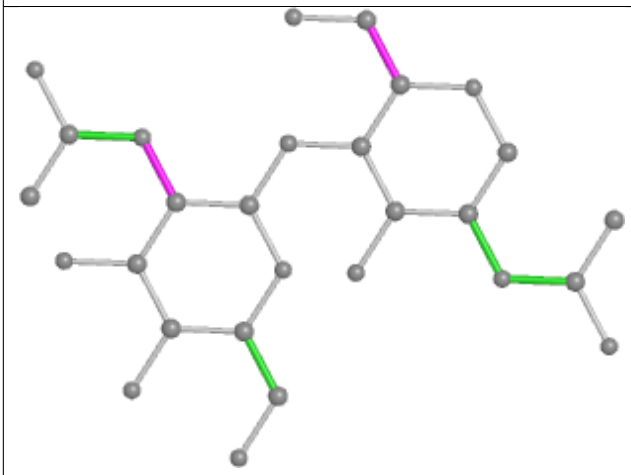


Bond angles



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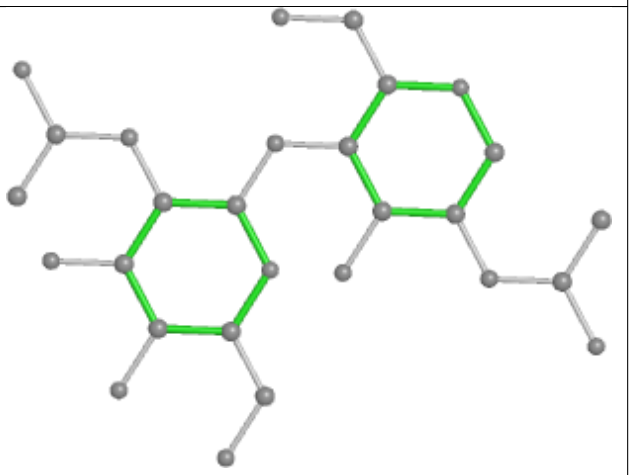
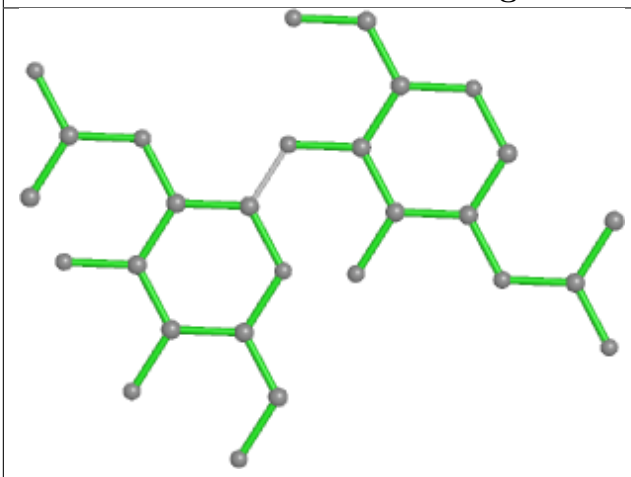


Rings

Oligosaccharide Chain c



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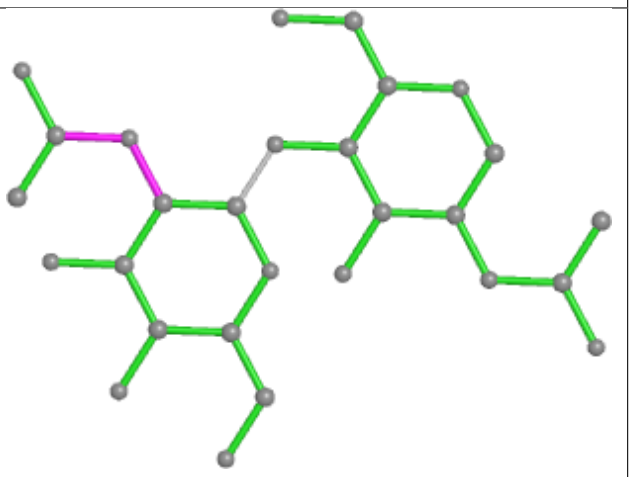

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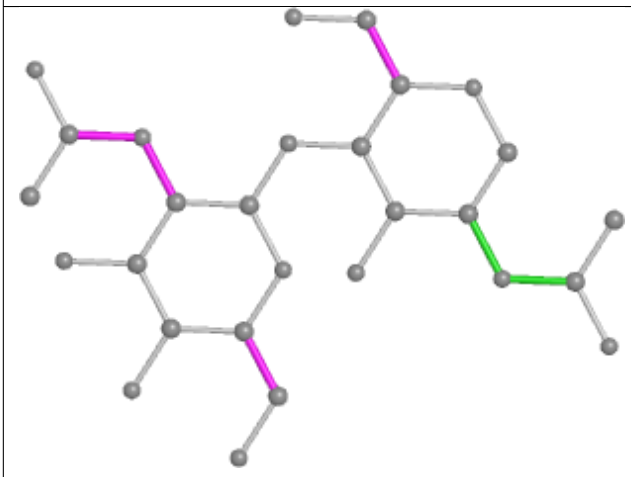

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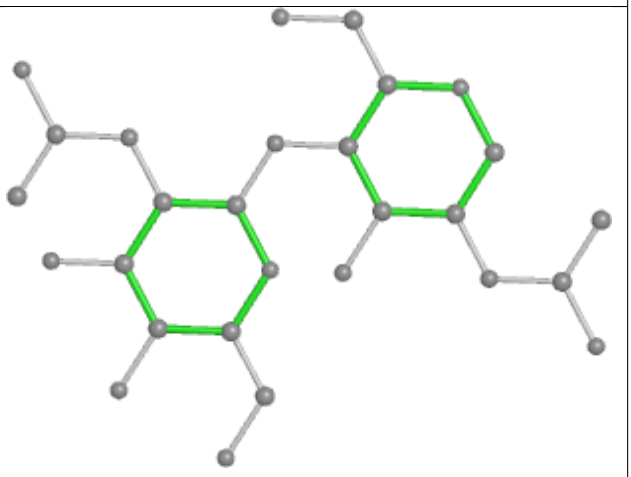
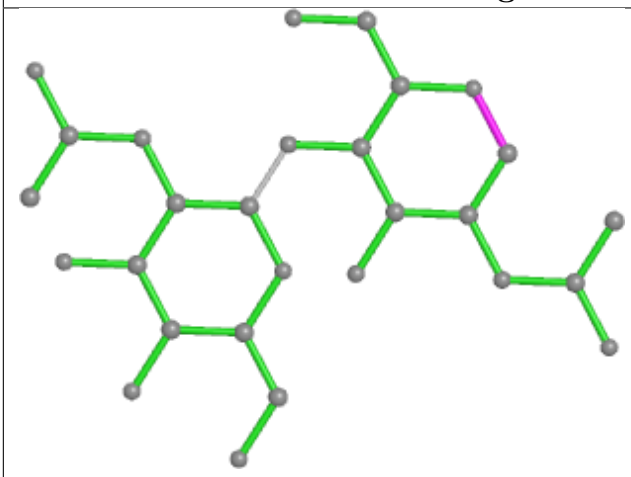


Rings

Oligosaccharide Chain d



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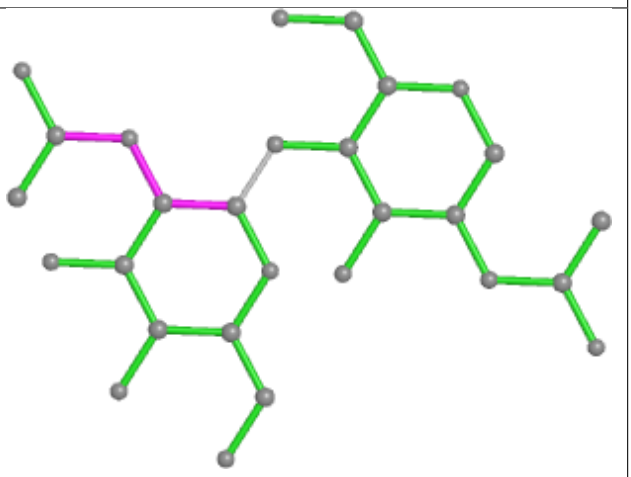

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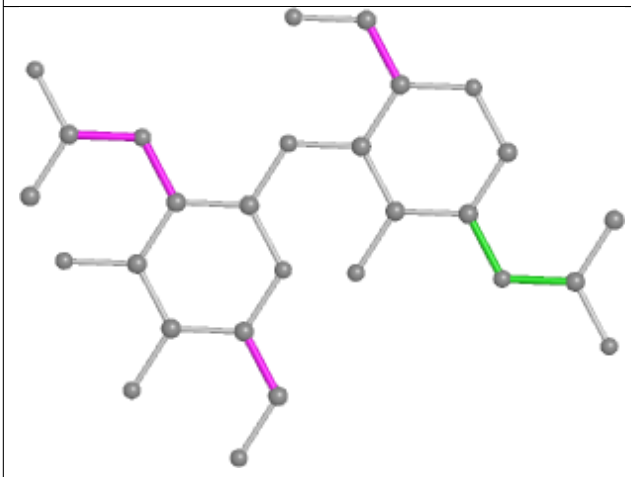

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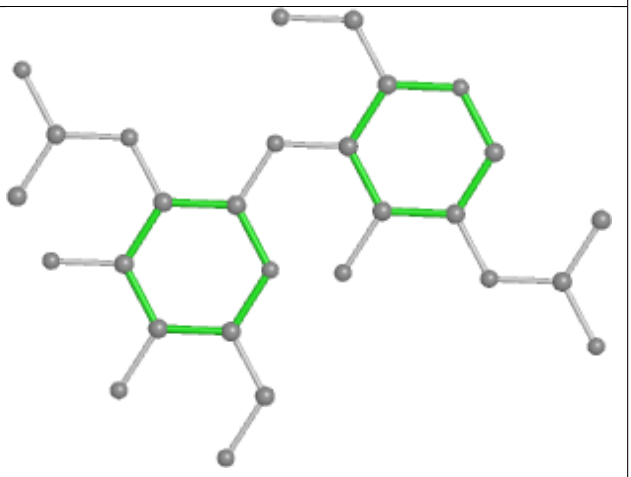
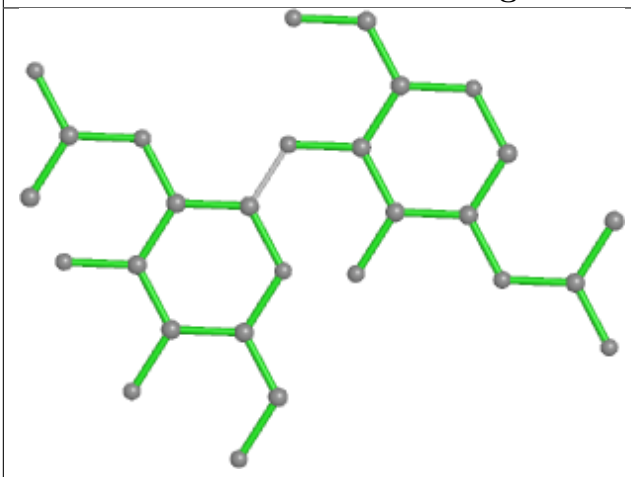


Rings

Oligosaccharide Chain e



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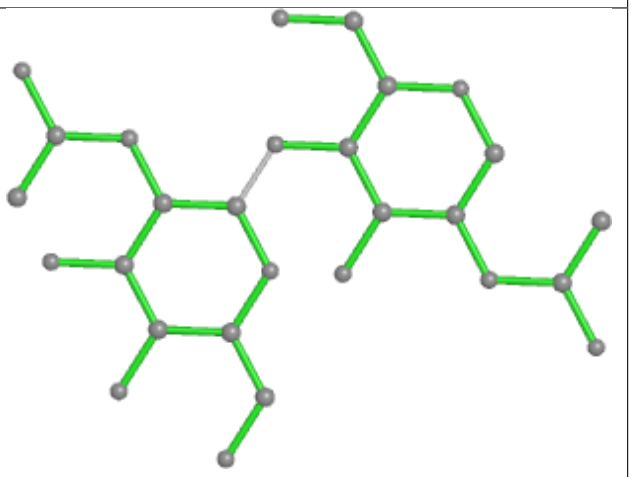
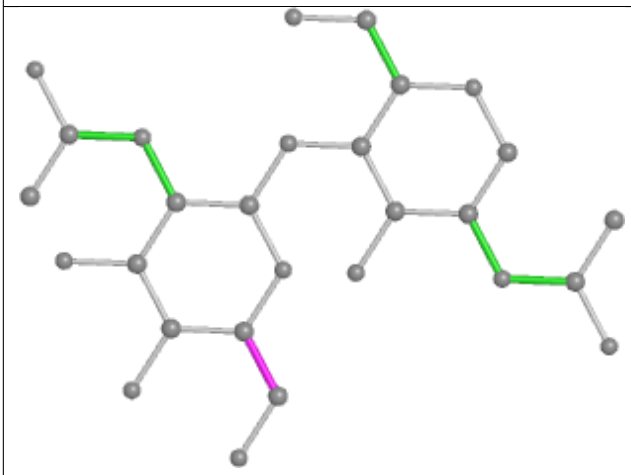


Bond angles



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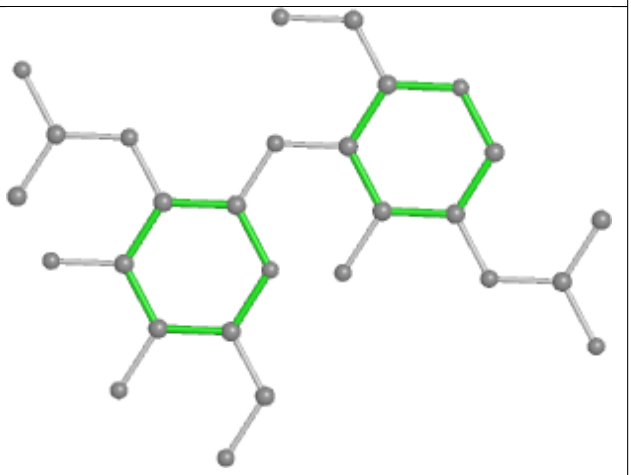
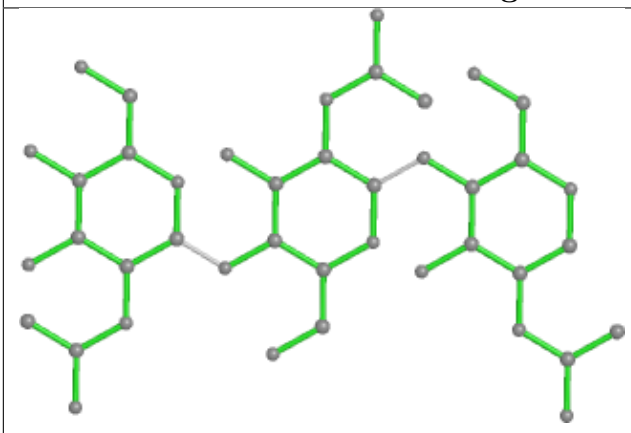


Rings

Oligosaccharide Chain f



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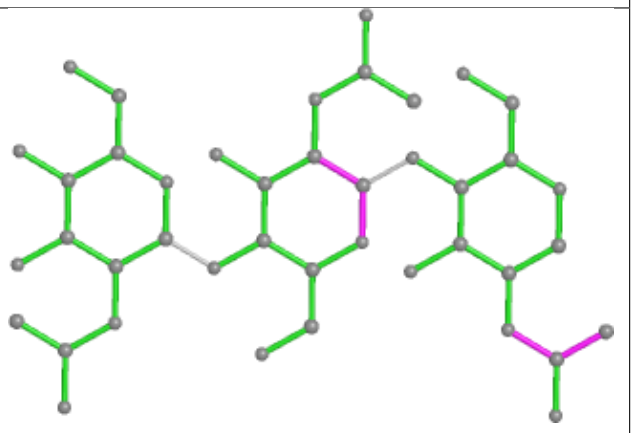
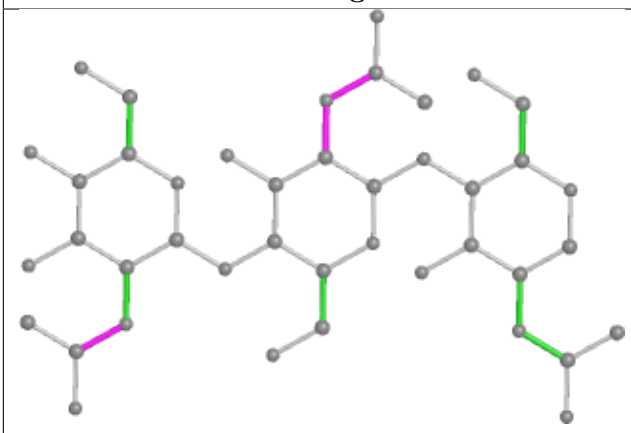


Bond angles



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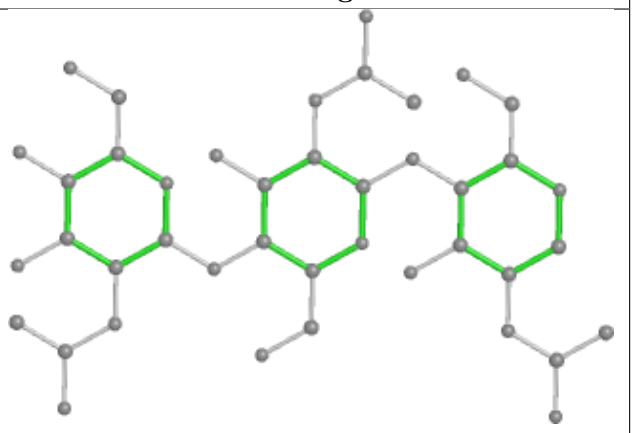
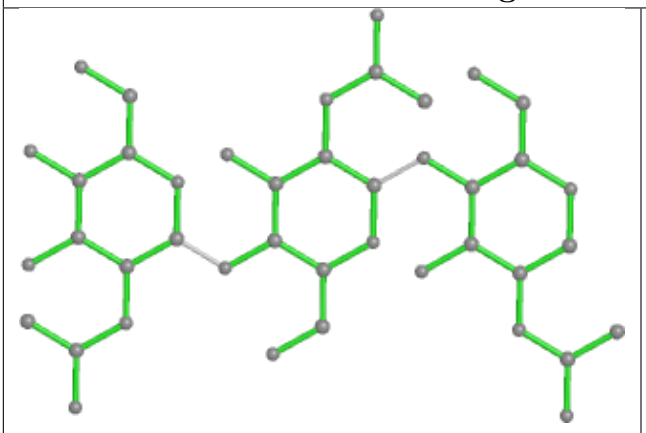


Rings

Oligosaccharide Chain g



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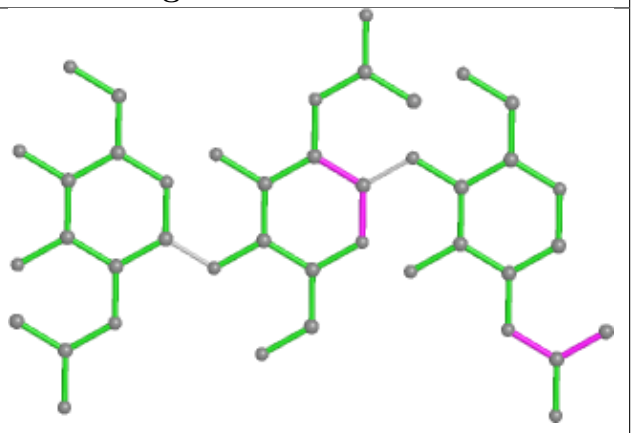
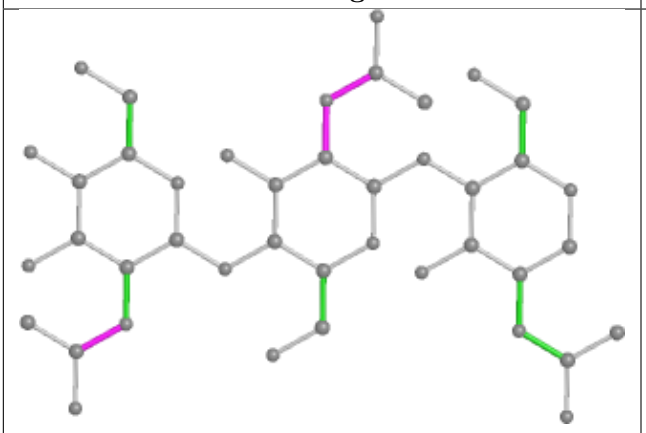


Bond angles



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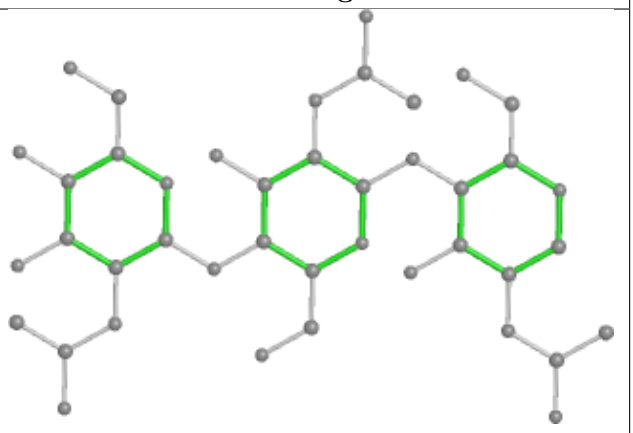
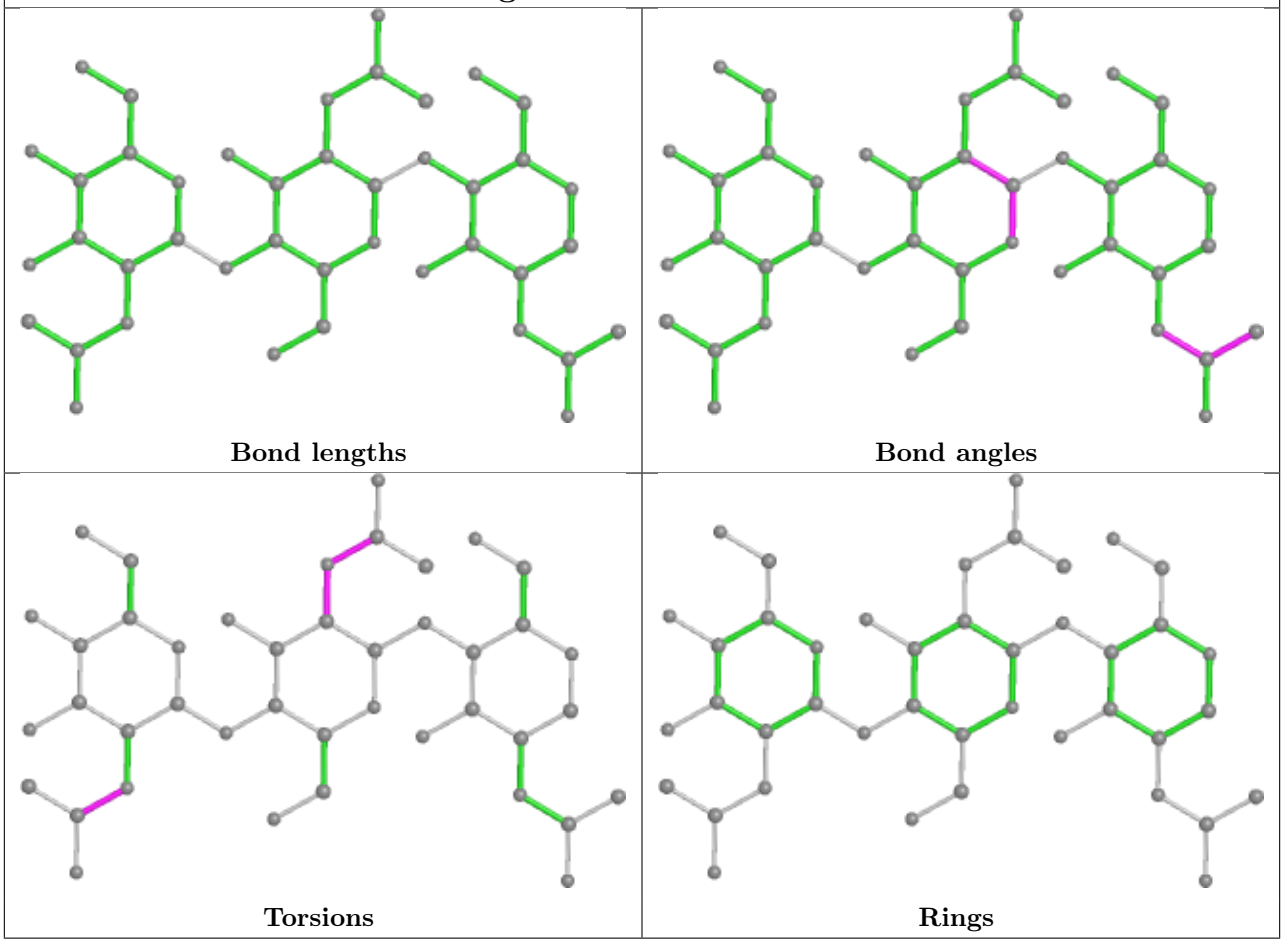


Rings

Oligosaccharide Chain h



5.6 Ligand geometry (i)

27 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	$\#\|Z\| > 2$
6	NAG	B	1403	1	14,14,15	0.40	0	17,19,21	1.17	2 (11%)
6	NAG	B	1408	1	14,14,15	0.22	0	17,19,21	0.39	0
6	NAG	B	1406	1	14,14,15	0.43	0	17,19,21	0.73	1 (5%)
6	NAG	C	1403	1	14,14,15	0.55	0	17,19,21	0.44	0
6	NAG	A	1405	1	14,14,15	0.55	0	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.39	0
6	NAG	C	1405	1	14,14,15	0.39	0	17,19,21	1.29	2 (11%)
6	NAG	B	1407	1	14,14,15	0.33	0	17,19,21	0.40	0
6	NAG	B	1402	1	14,14,15	0.34	0	17,19,21	0.64	0
6	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
6	NAG	B	1409	1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
6	NAG	B	1405	1	14,14,15	0.30	0	17,19,21	0.61	0
6	NAG	A	1407	1	14,14,15	0.26	0	17,19,21	0.49	0
6	NAG	C	1402	1	14,14,15	0.45	0	17,19,21	0.56	0
6	NAG	B	1401	1	14,14,15	0.32	0	17,19,21	0.55	0
6	NAG	B	1404	1	14,14,15	0.29	0	17,19,21	0.62	0
6	NAG	C	1404	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	A	1409	1	14,14,15	0.53	0	17,19,21	0.35	0
6	NAG	B	1410	-	14,14,15	0.33	0	17,19,21	0.42	0
6	NAG	A	1403	1	14,14,15	0.21	0	17,19,21	0.40	0
6	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.62	0
6	NAG	C	1408	1	14,14,15	0.15	0	17,19,21	0.57	0
6	NAG	C	1401	1	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
6	NAG	C	1406	1	14,14,15	0.20	0	17,19,21	0.37	0
6	NAG	A	1404	1	14,14,15	0.44	0	17,19,21	0.55	0
6	NAG	A	1401	1	14,14,15	0.29	0	17,19,21	0.34	0
6	NAG	C	1407	1	14,14,15	0.33	0	17,19,21	0.63	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
6	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
6	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1405	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1409	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1405	NAG	C2-N2-C7	4.34	129.09	122.90
6	C	1405	NAG	C2-N2-C7	4.33	129.06	122.90
6	C	1401	NAG	C1-O5-C5	2.86	116.06	112.19
6	B	1406	NAG	C1-O5-C5	2.36	115.38	112.19
6	B	1409	NAG	C8-C7-N2	2.31	120.01	116.10

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

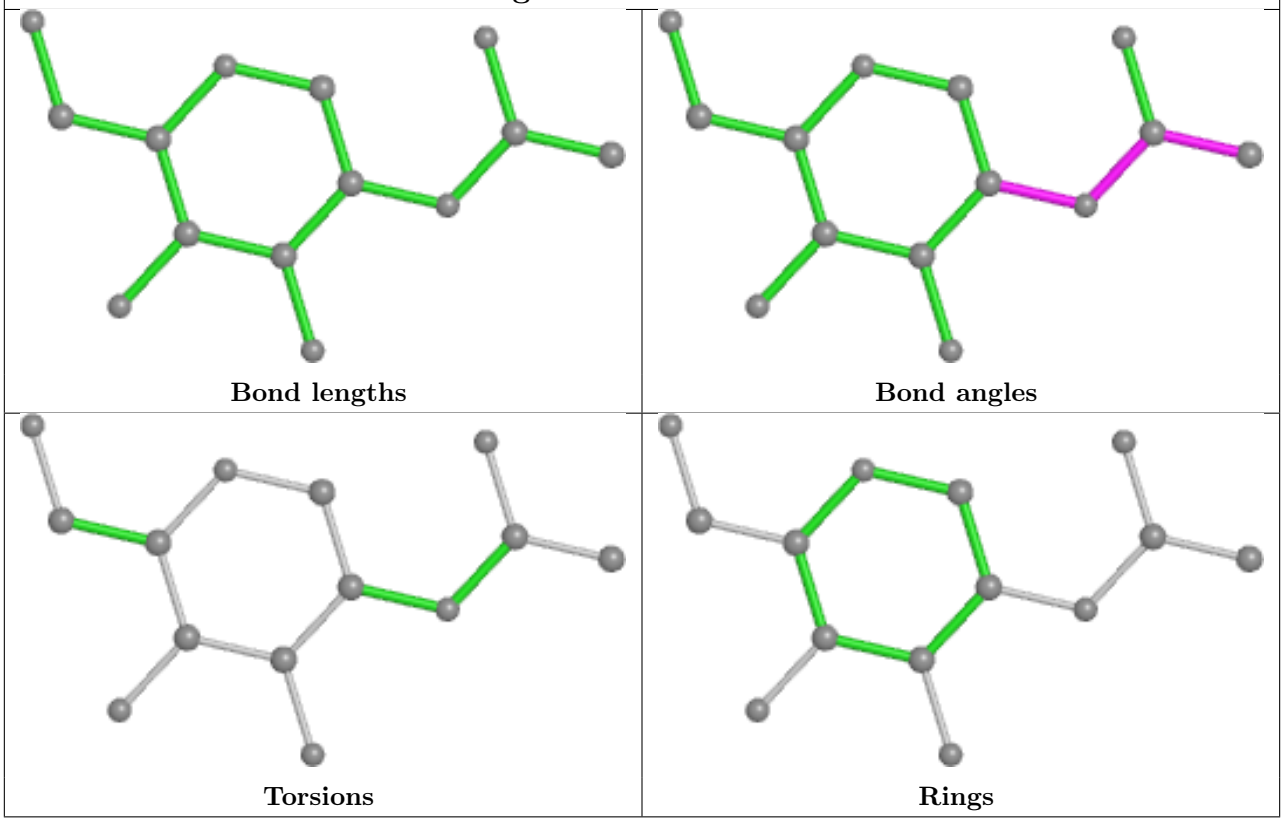
Mol	Chain	Res	Type	Atoms
6	B	1405	NAG	C8-C7-N2-C2
6	B	1405	NAG	O7-C7-N2-C2
6	B	1407	NAG	O5-C5-C6-O6
6	B	1401	NAG	O5-C5-C6-O6
6	A	1406	NAG	O5-C5-C6-O6

There are no ring outliers.

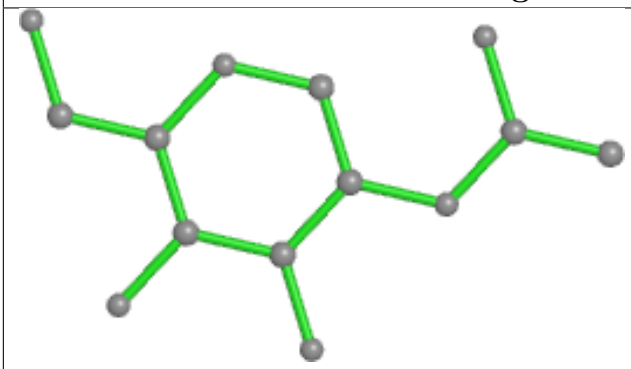
No monomer is involved in short contacts.

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



Ligand NAG B 1408



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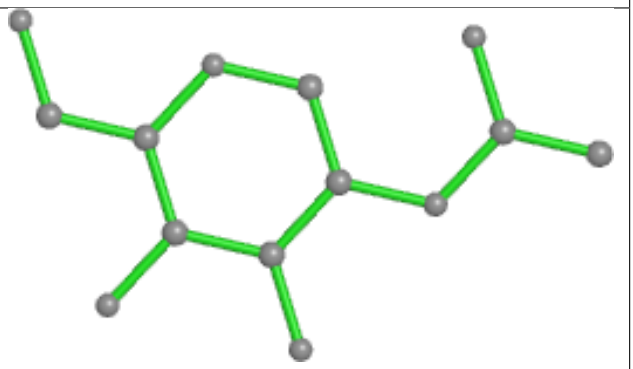
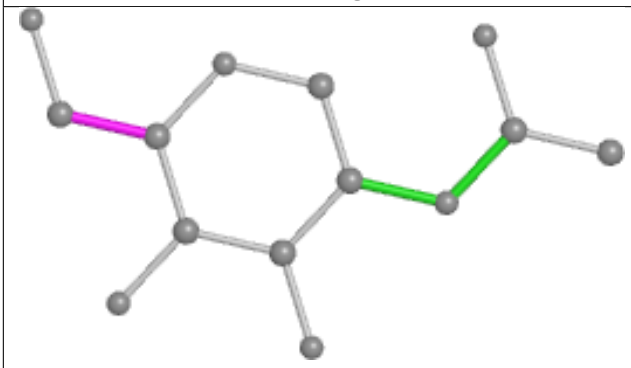
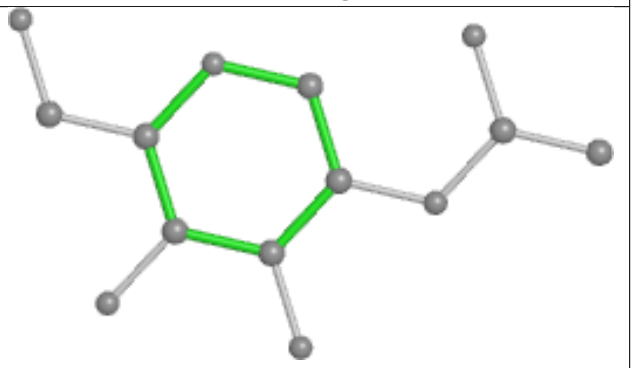


Bond angles

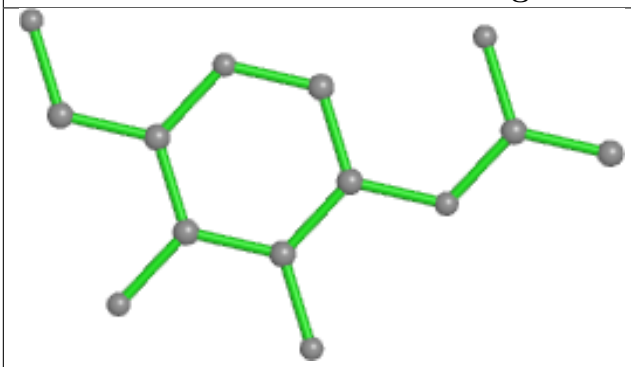


Torsions



Rings

Ligand NAG B 1406



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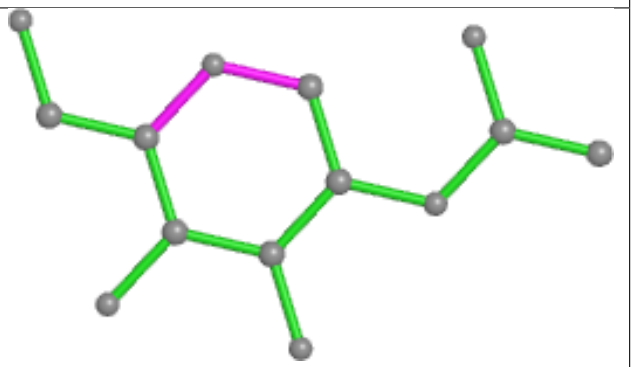

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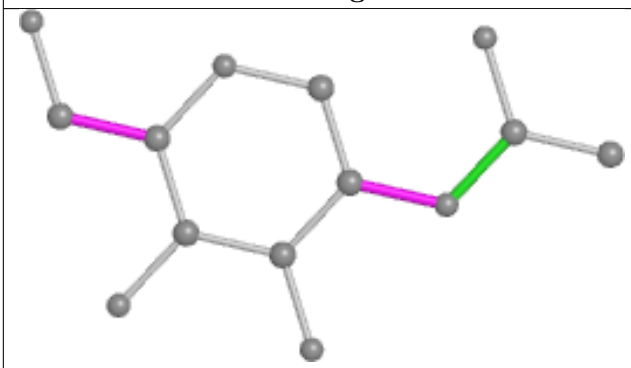

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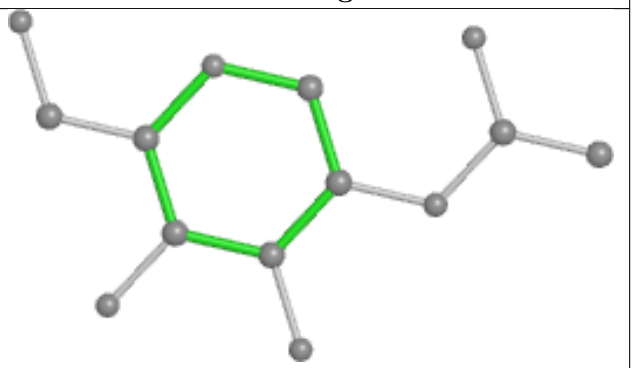

Rings

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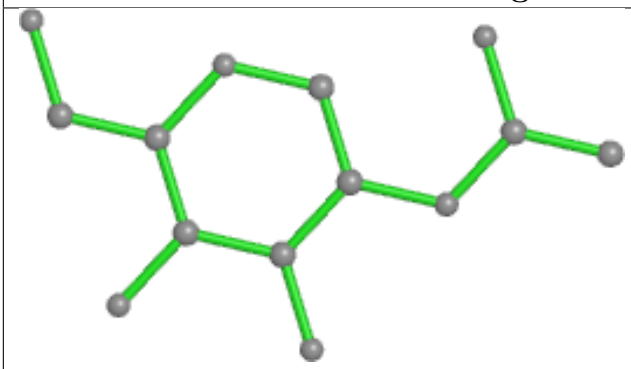
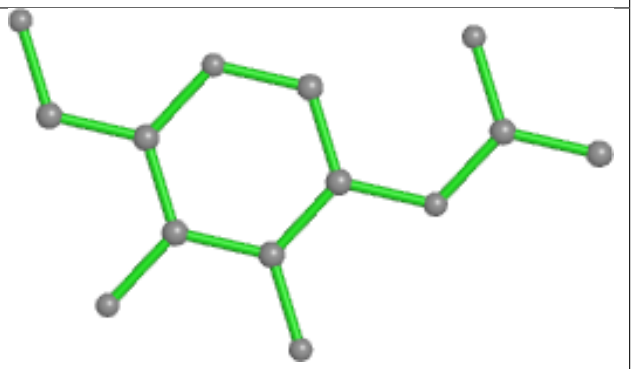
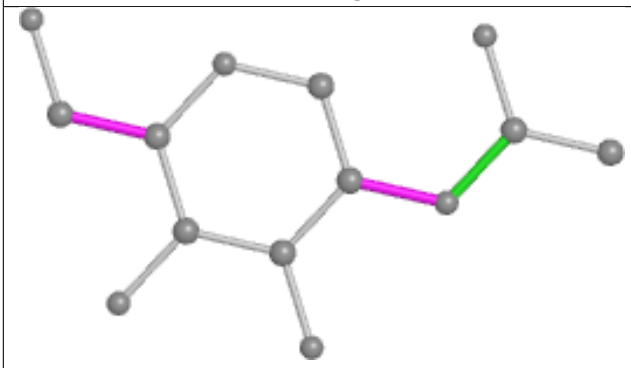


Bond lengths



Bond angles



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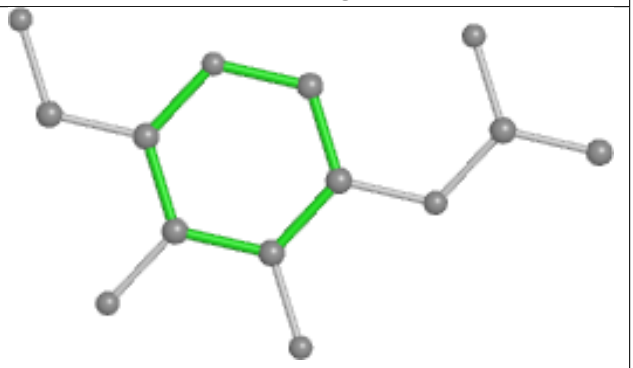
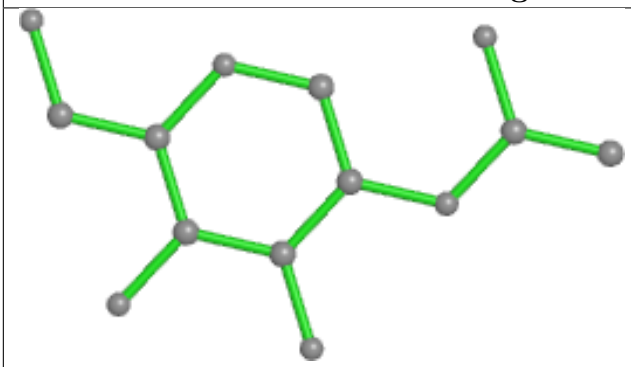
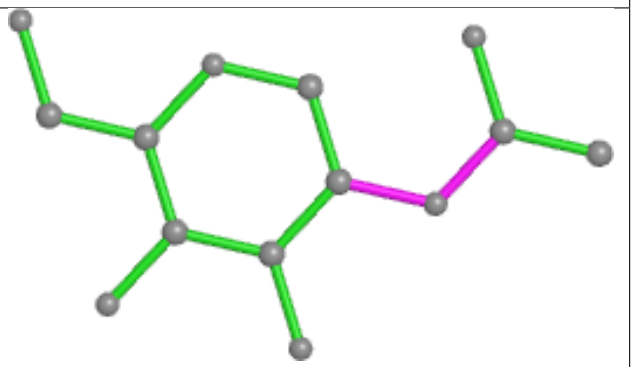


Rings

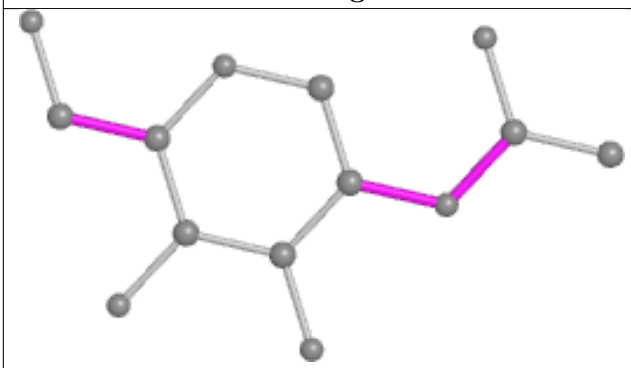
Ligand NAG A 1405



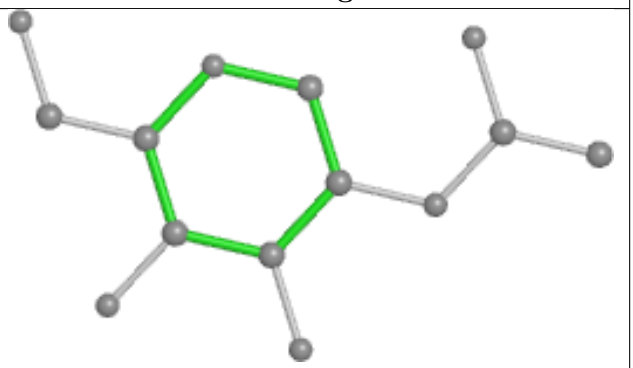
Bond lengths



Bond angles



Torsions



Rings

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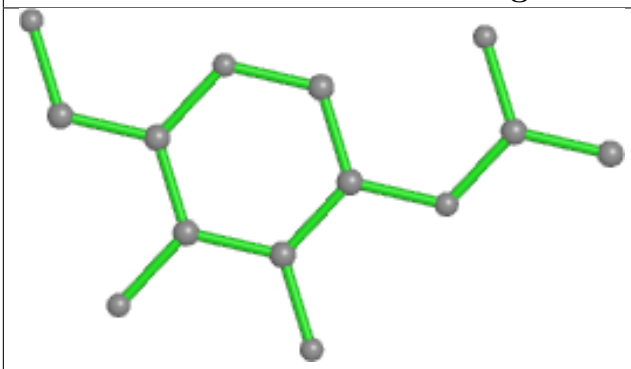

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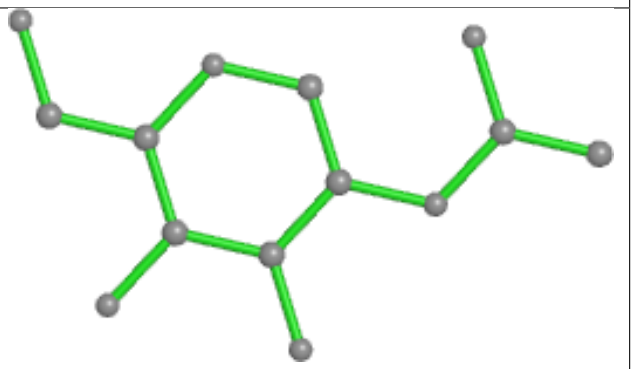

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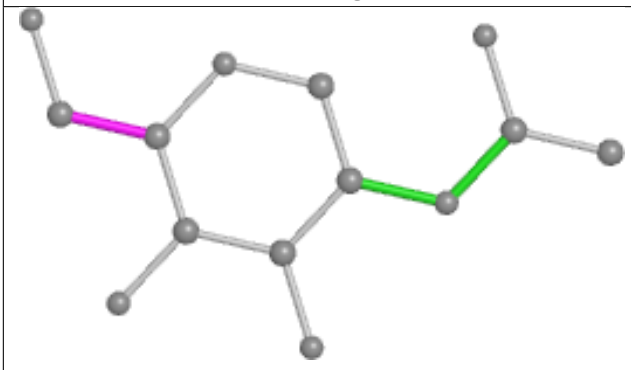

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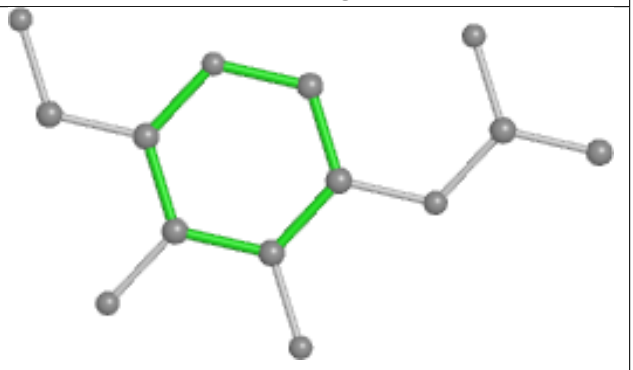
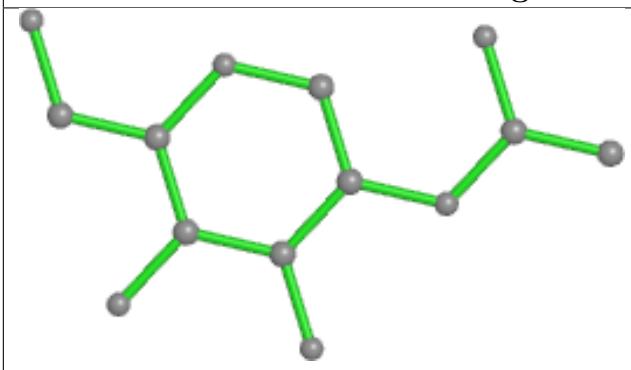


Rings

Ligand NAG C 1405



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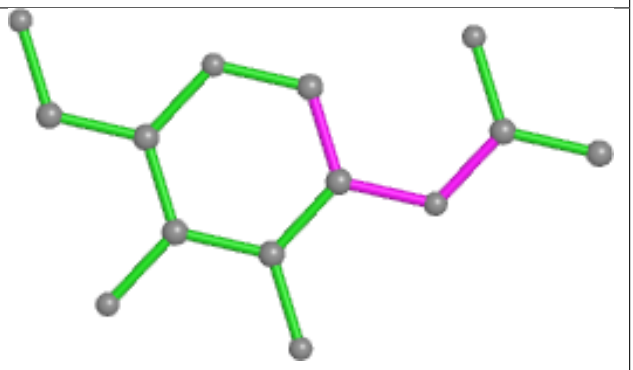
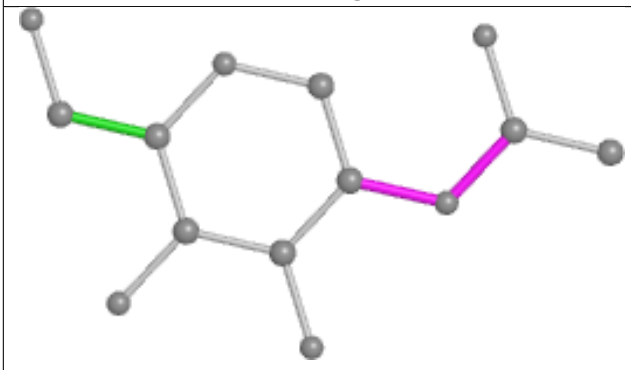


Bond angles



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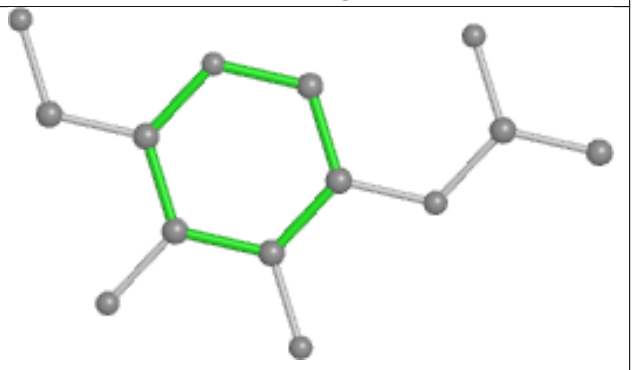
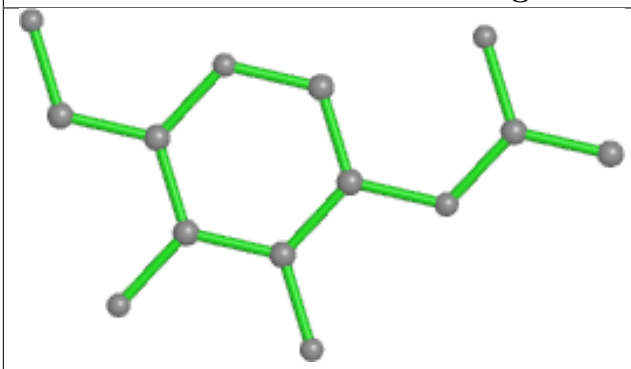


Rings

Ligand NAG B 1407



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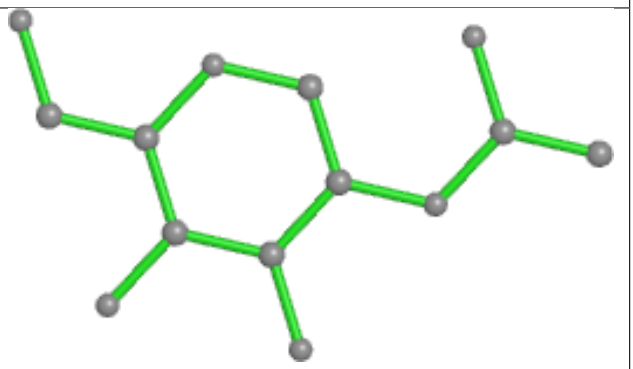
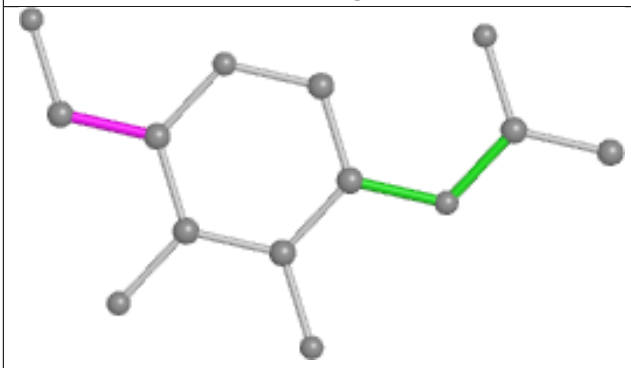


Bond angles



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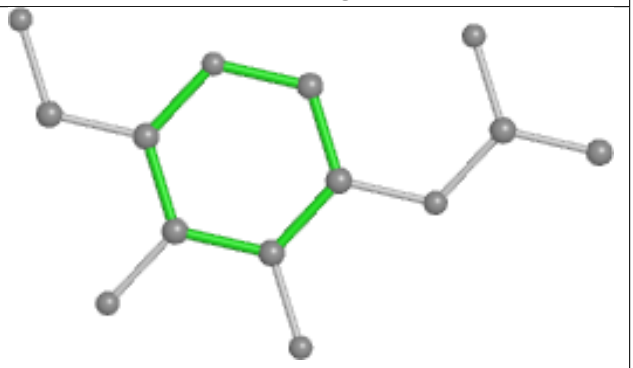
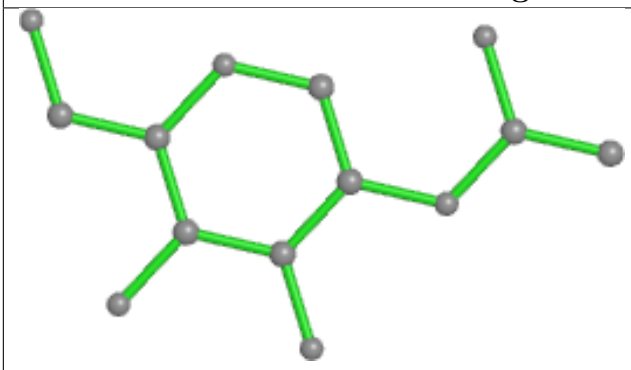


Rings

Ligand NAG B 1402



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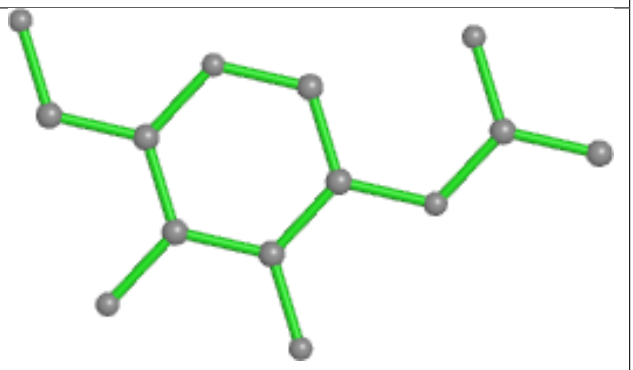
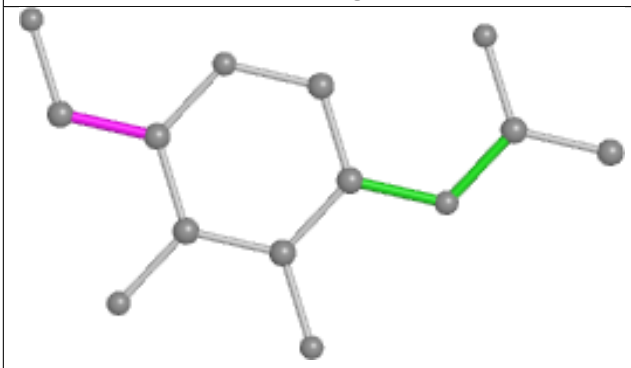
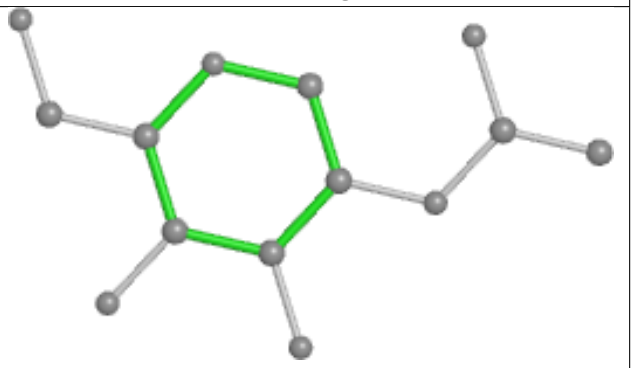


Bond angles

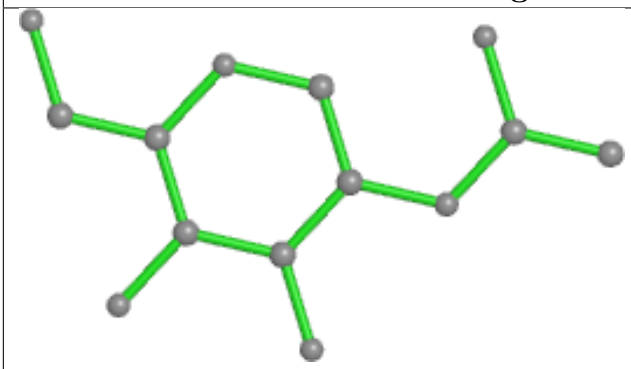


Torsions

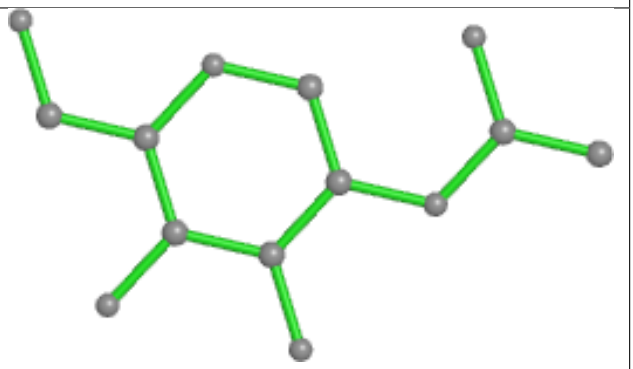


Rings

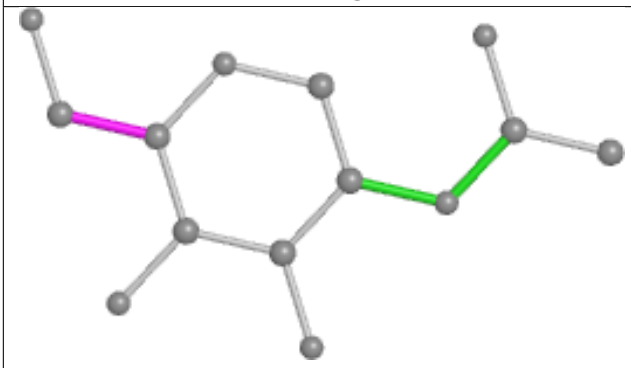
Ligand NAG A 1406



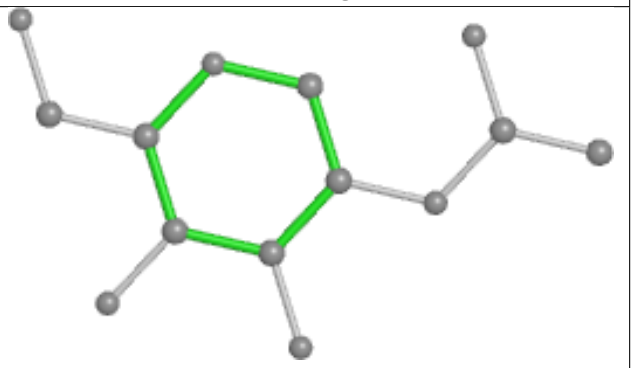
Bond lengths



Bond angles

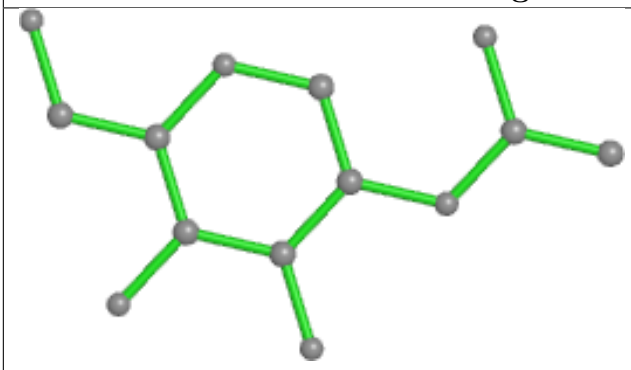


Torsions

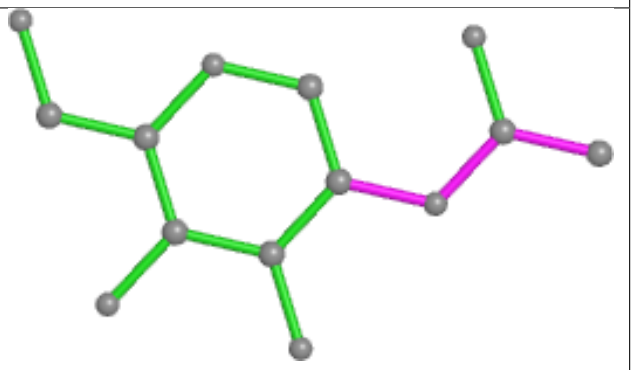


Rings

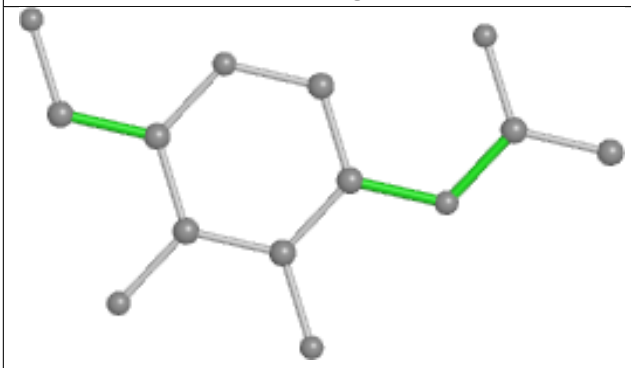
Ligand NAG B 1409



Bond lengths



Bond angles



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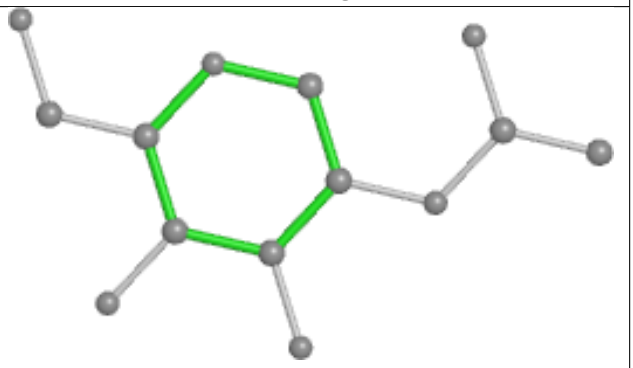
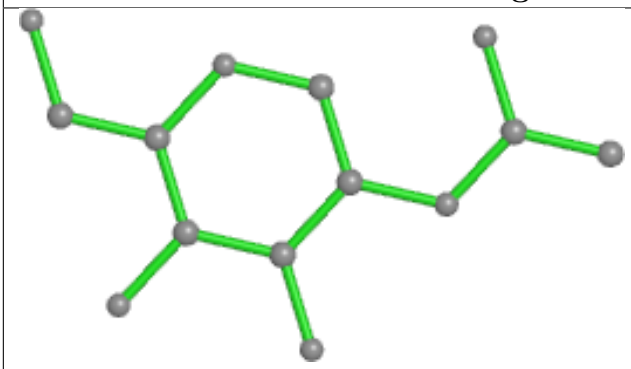


Rings

Ligand NAG B 1405



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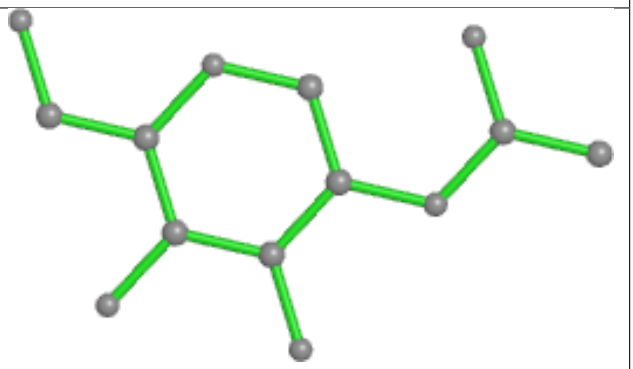
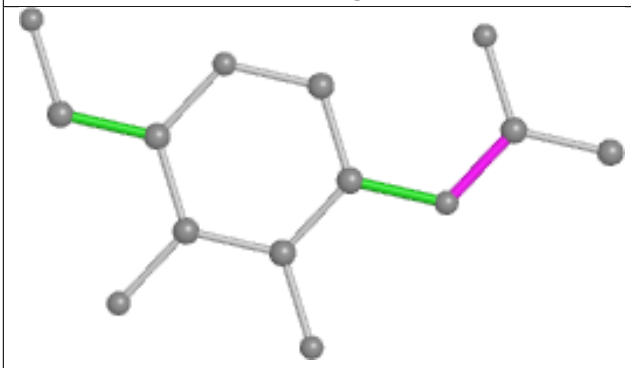


Bond angles



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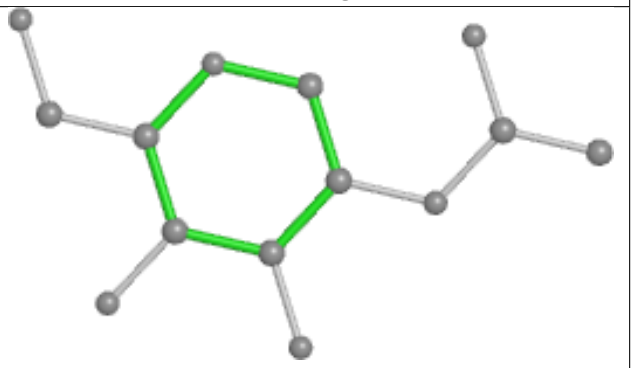
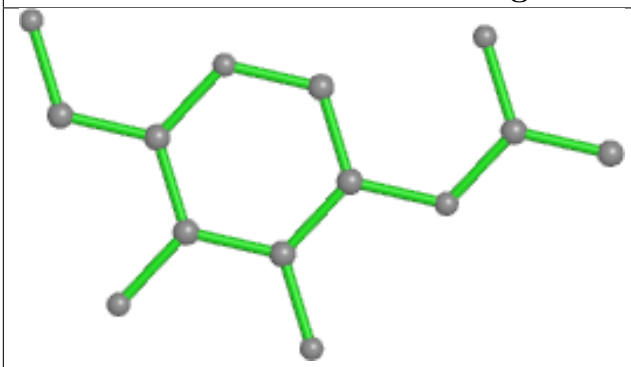


Rings

Ligand NAG A 1407



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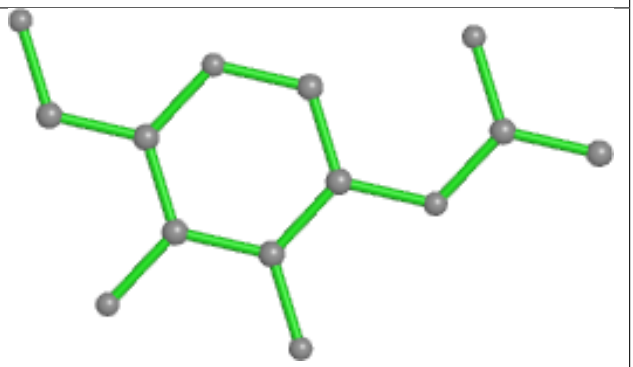
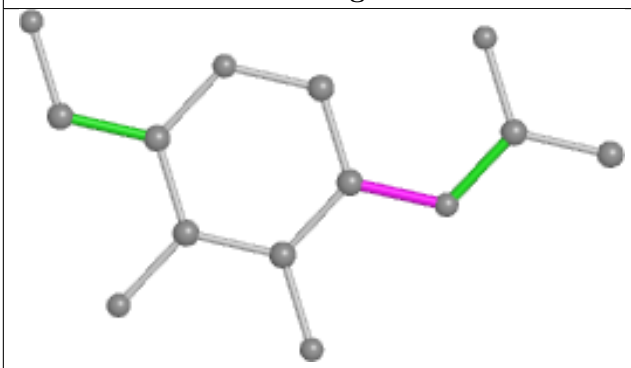


Bond angles



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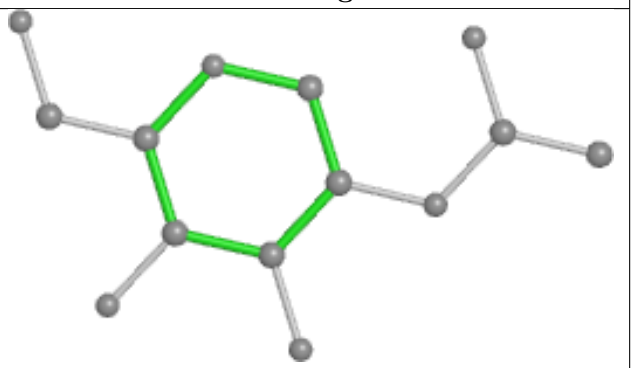
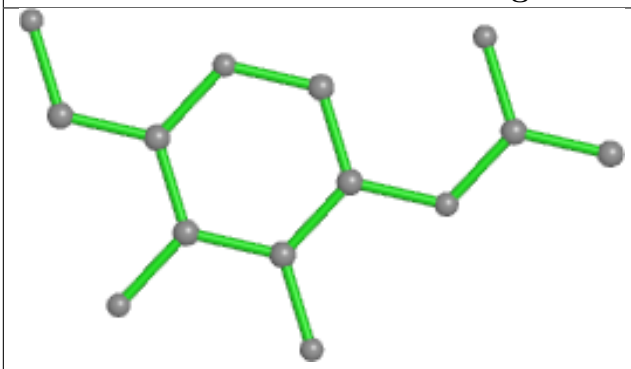


Rings

Ligand NAG C 1402



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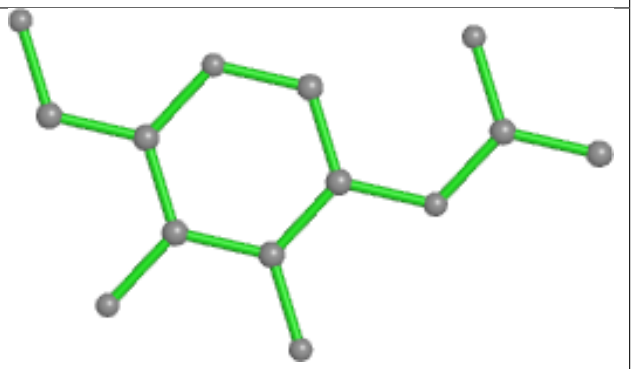
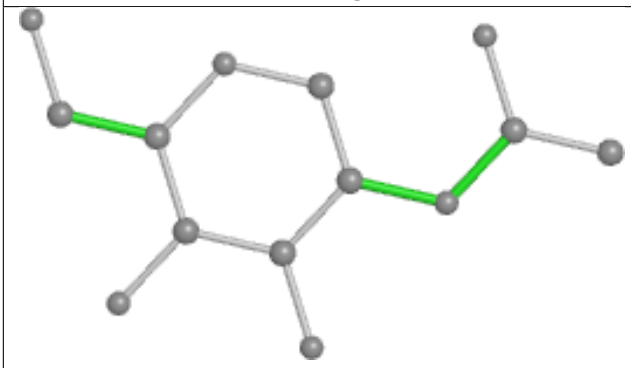


Bond angles



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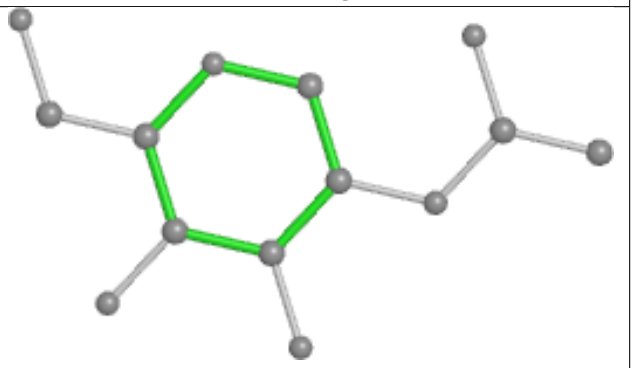
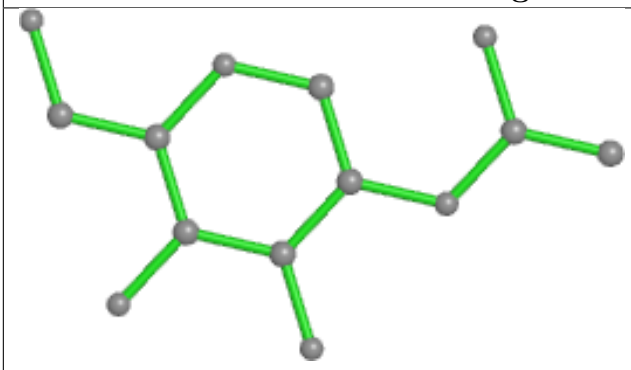


Rings

Ligand NAG B 1401



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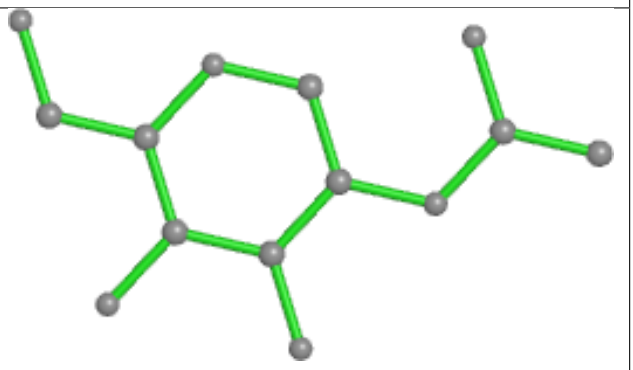
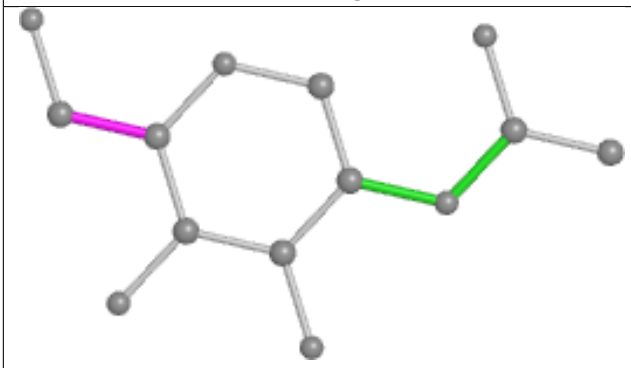


Bond angles



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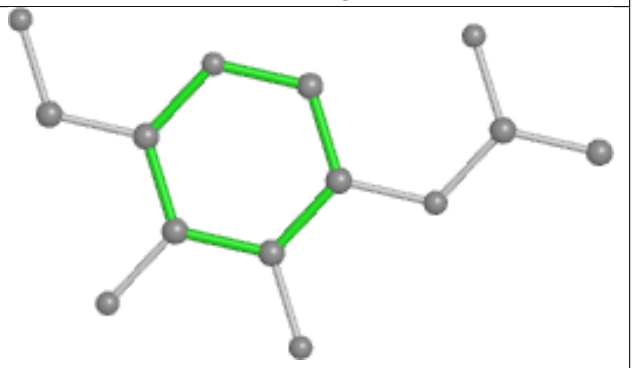
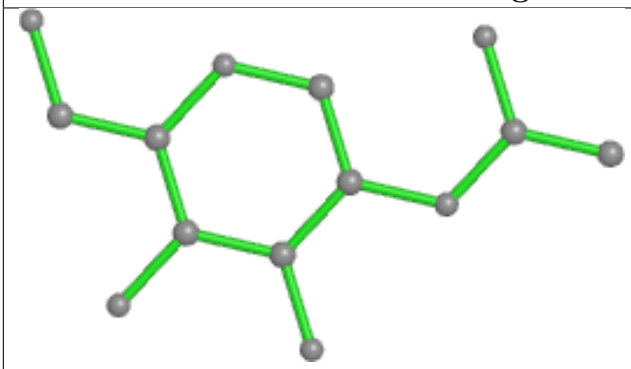


Rings

Ligand NAG B 1404



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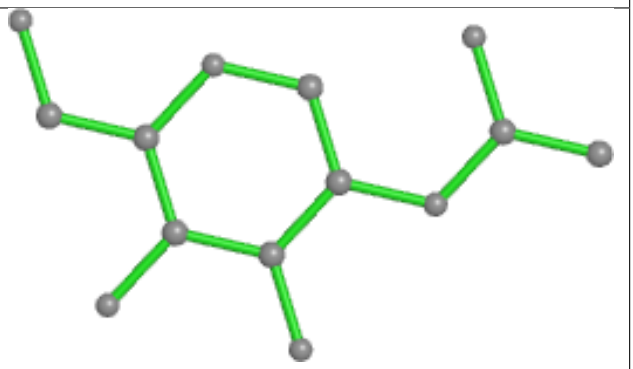
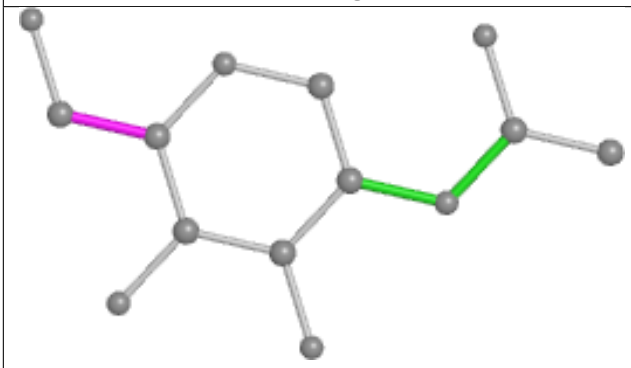


Bond angles



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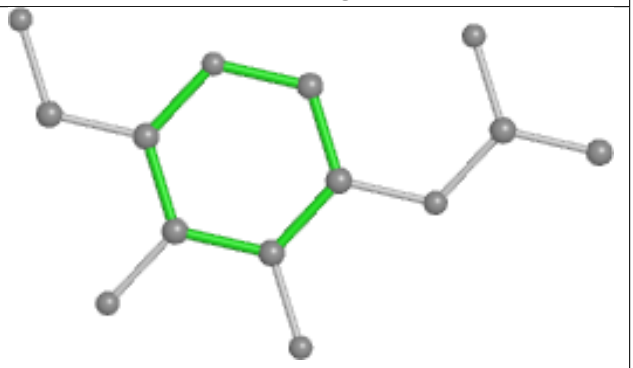
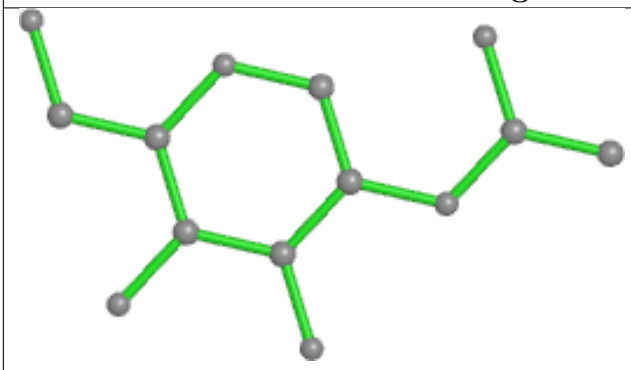


Rings

Ligand NAG C 1404



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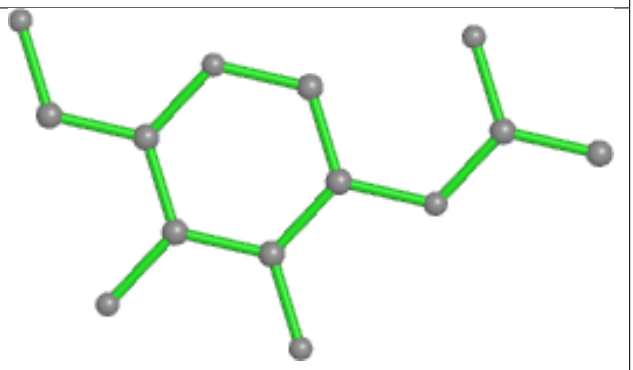

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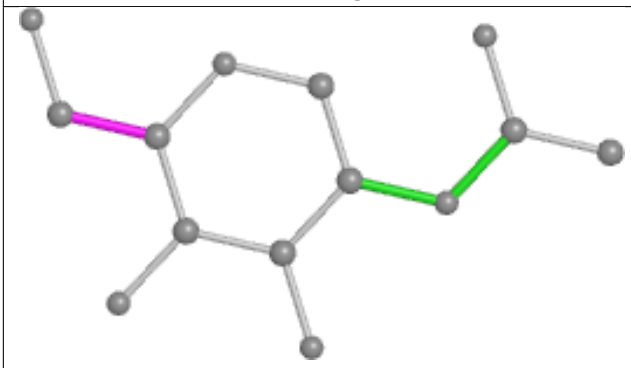

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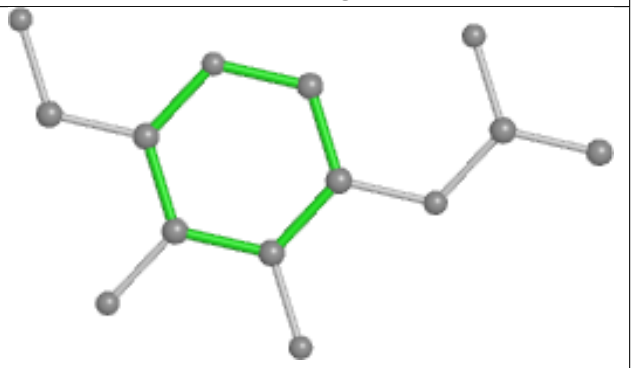
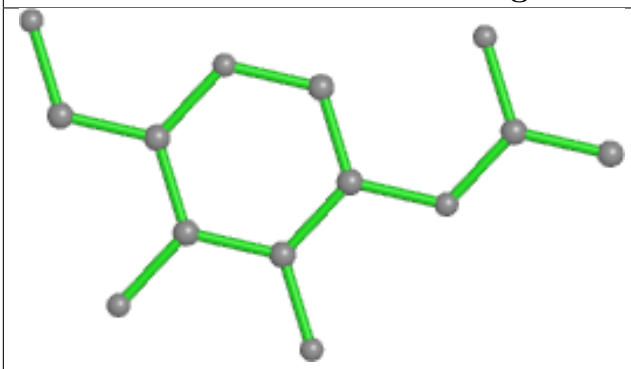


Rings

Ligand NAG A 1409



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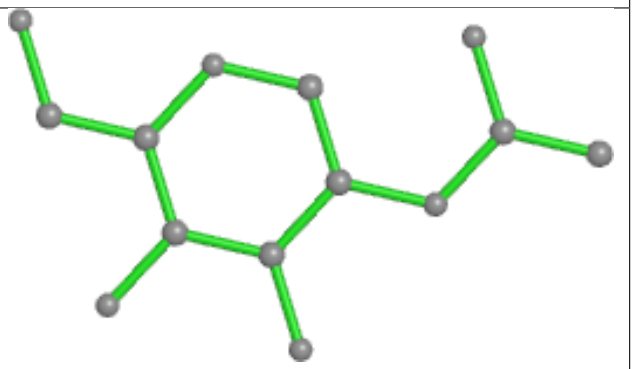
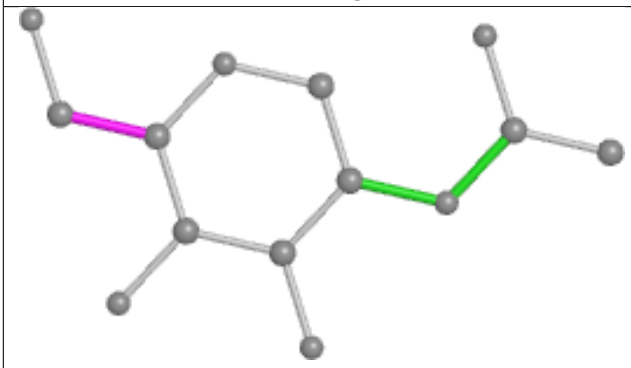


Bond angles



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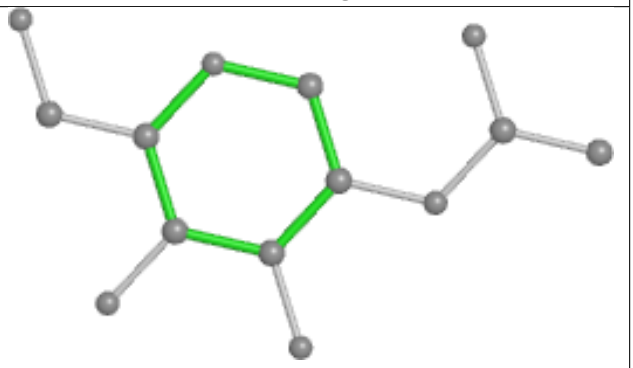
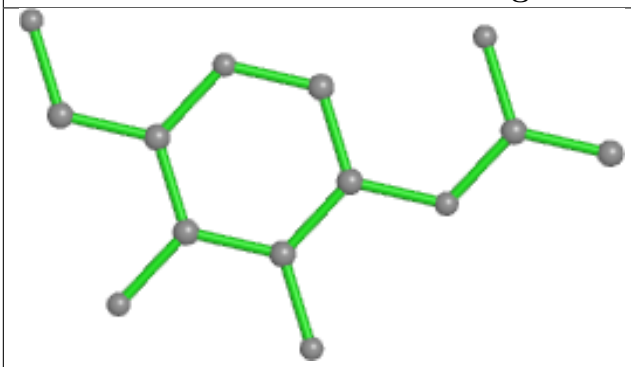


Rings

Ligand NAG B 1410



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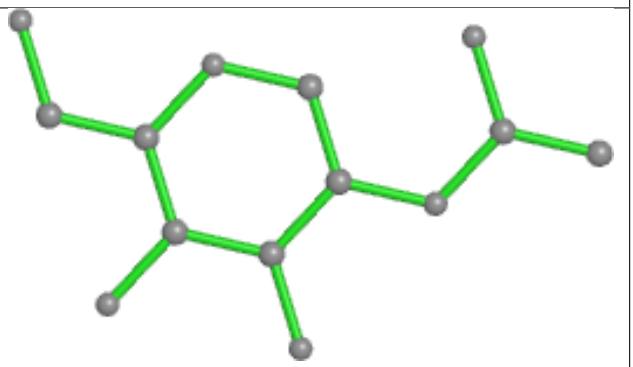
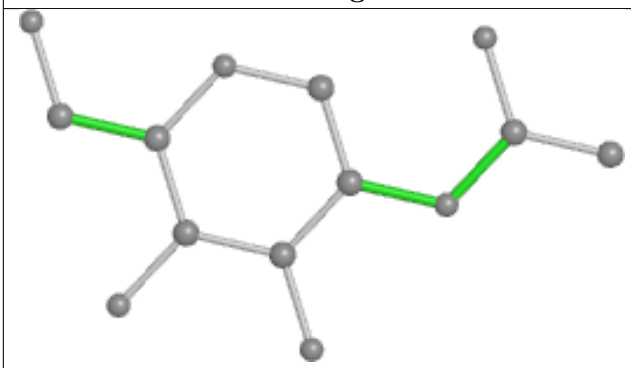


Bond angles



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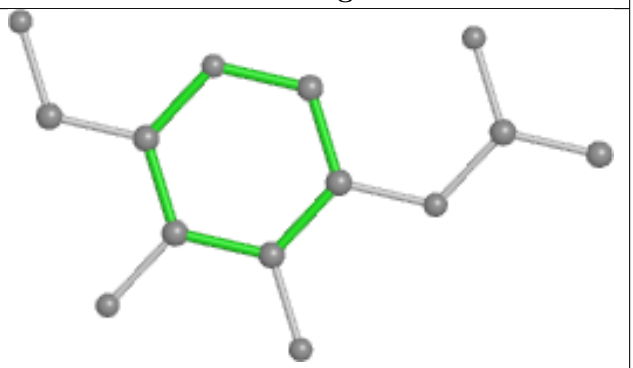
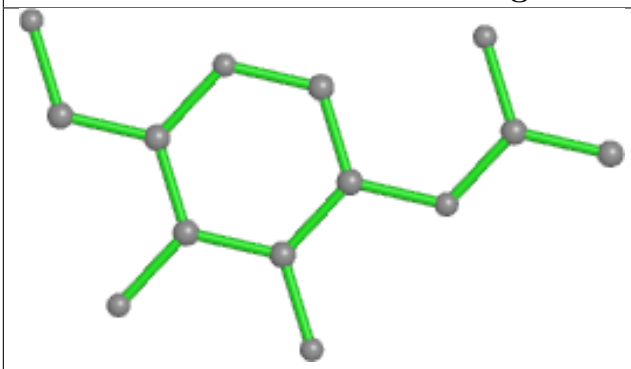


Rings

Ligand NAG A 1403



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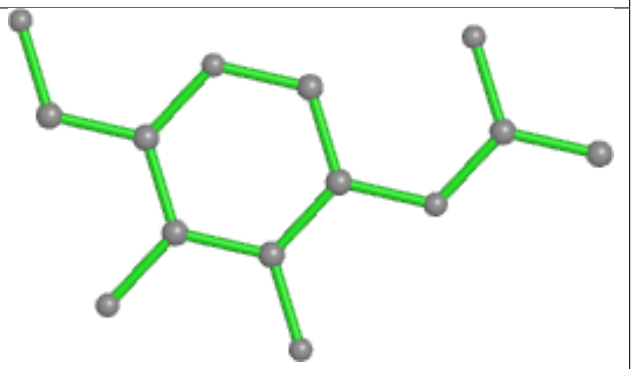
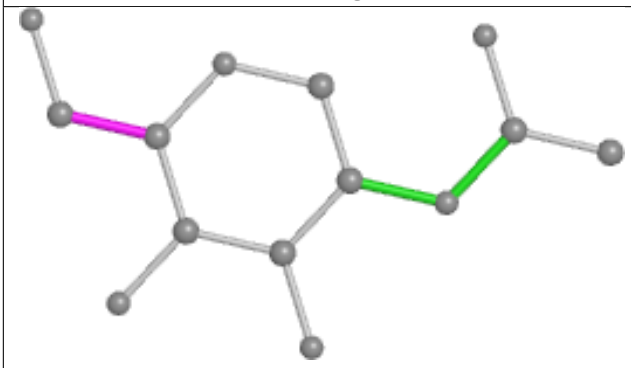


Bond angles



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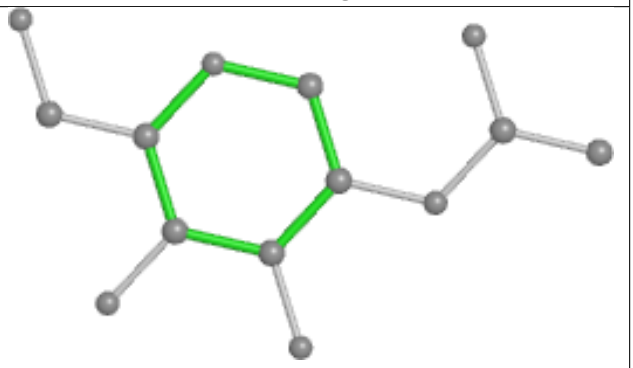
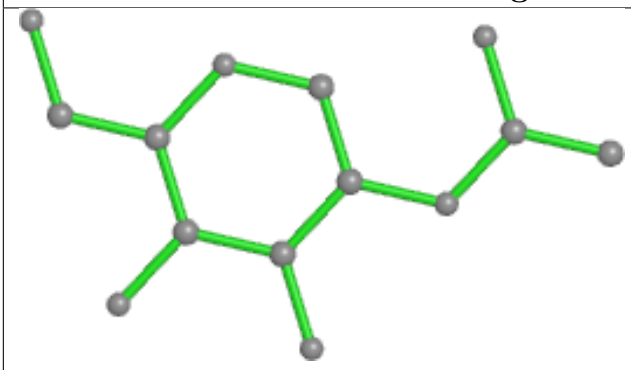


Rings

Ligand NAG A 1402



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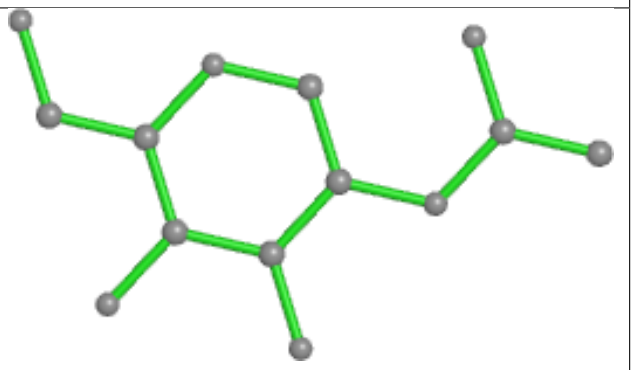
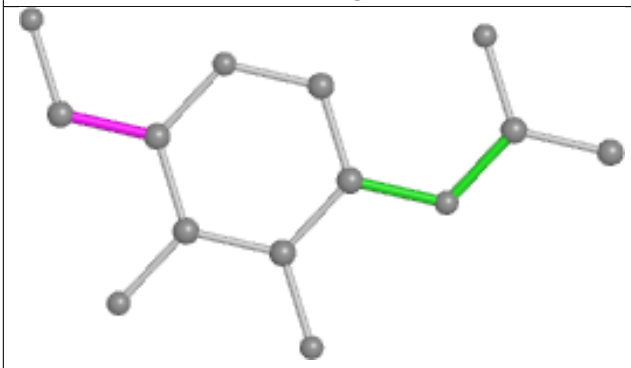


Bond angles



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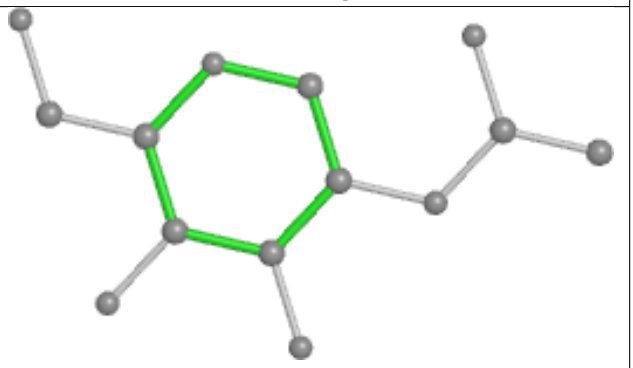
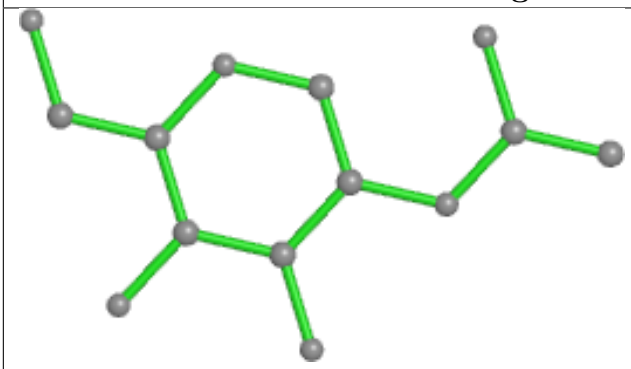
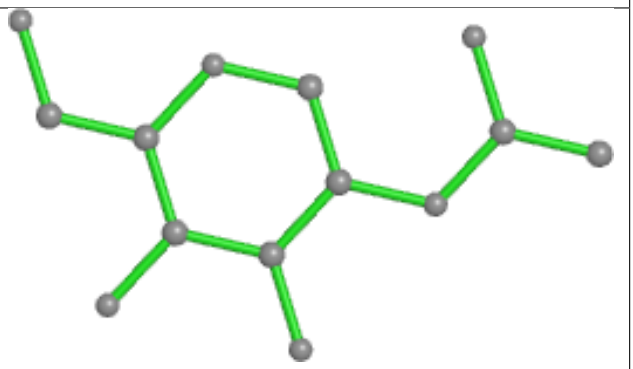
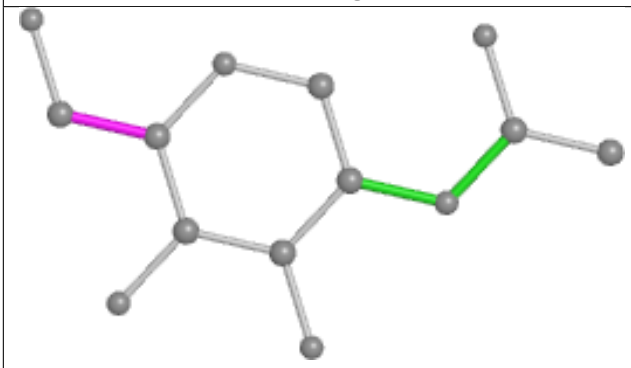
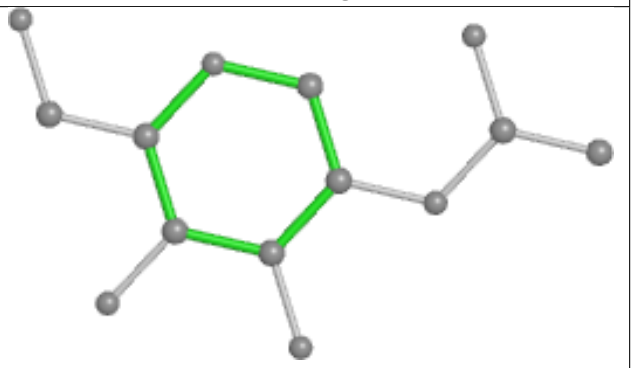


Rings

Ligand NAG C 1408	
 Bond lengths	 Bond angles
 Torsions	 Rings

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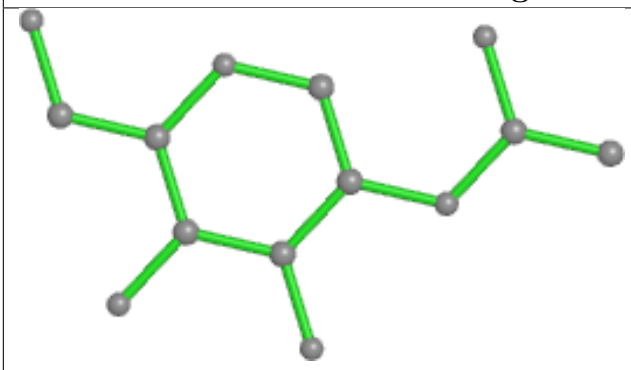
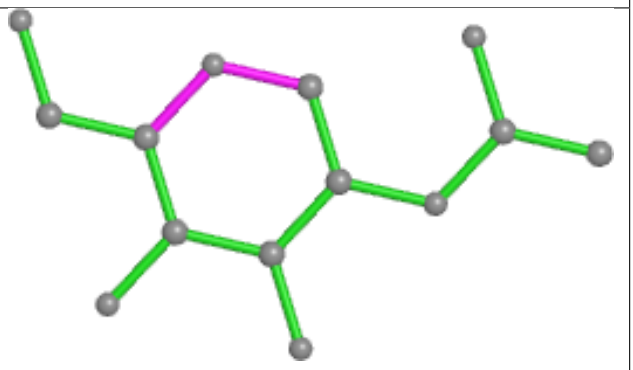
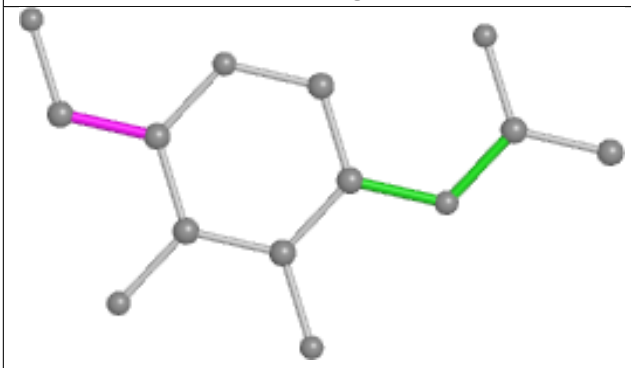
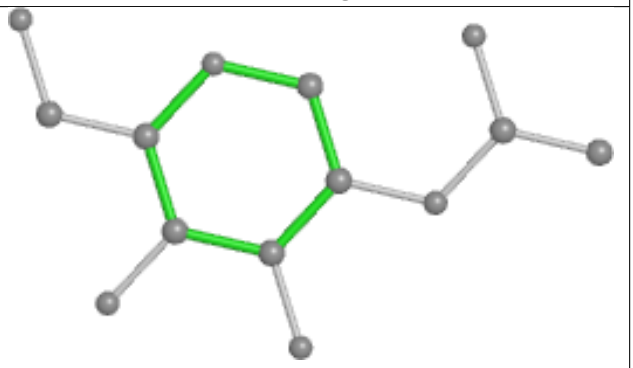
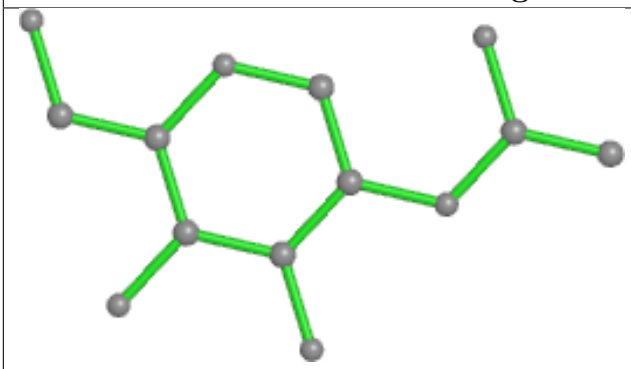
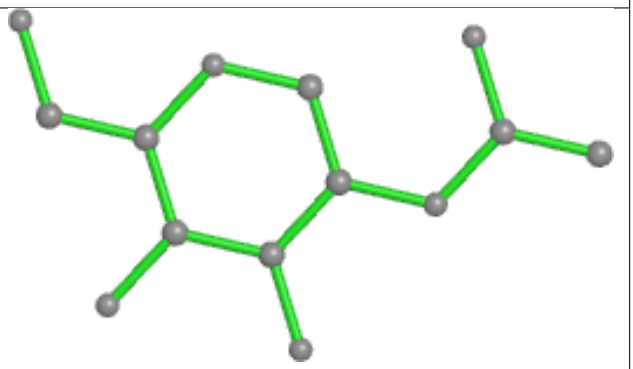
 Bond lengths	 Bond angles
 Torsions	 Rings

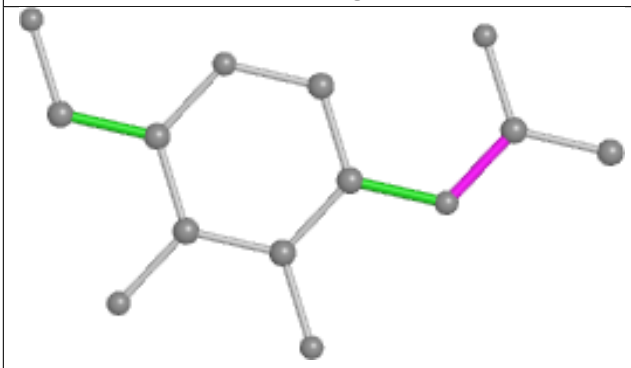
Ligand NAG C 1406



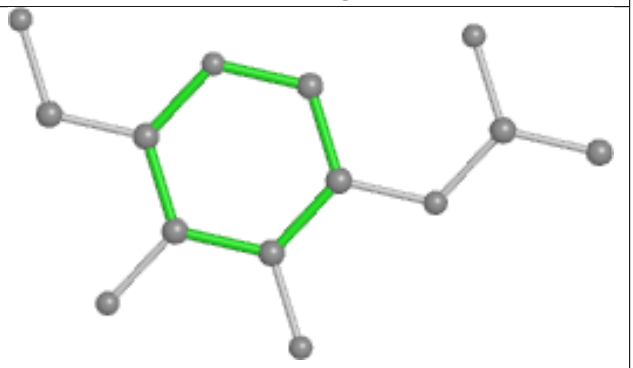
Bond lengths



Bond angles

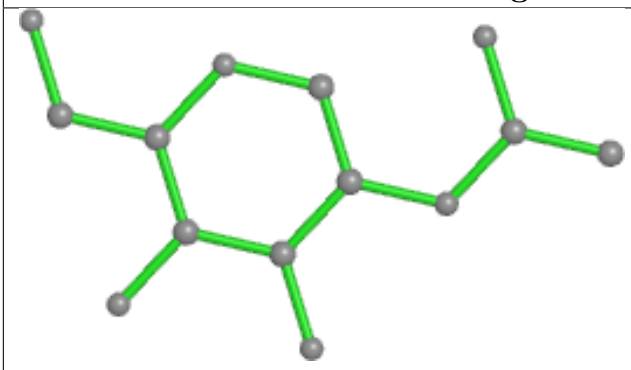


Torsions

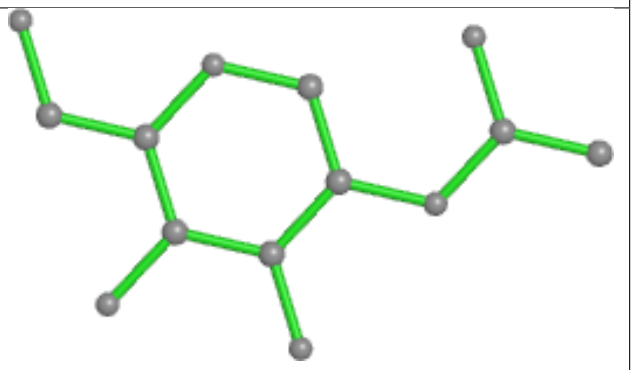


Rings

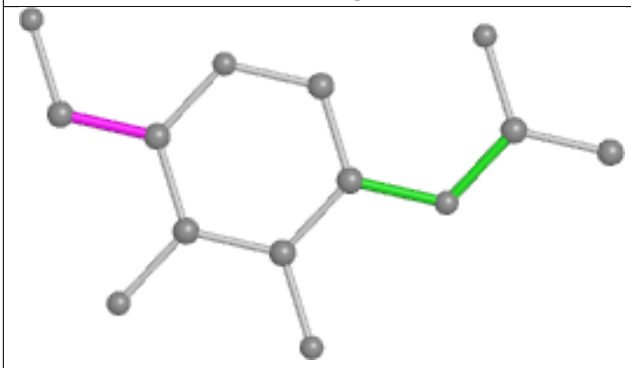
Ligand NAG A 1404



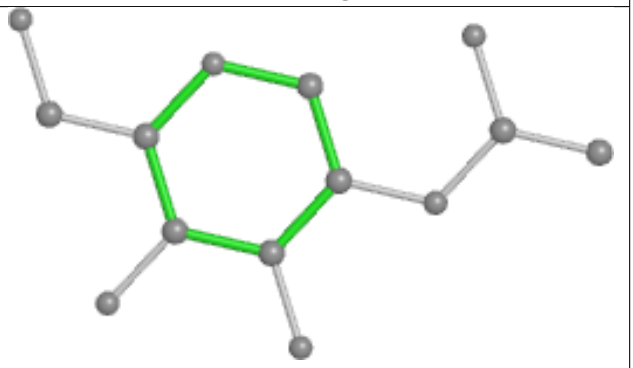
Bond lengths



Bond angles

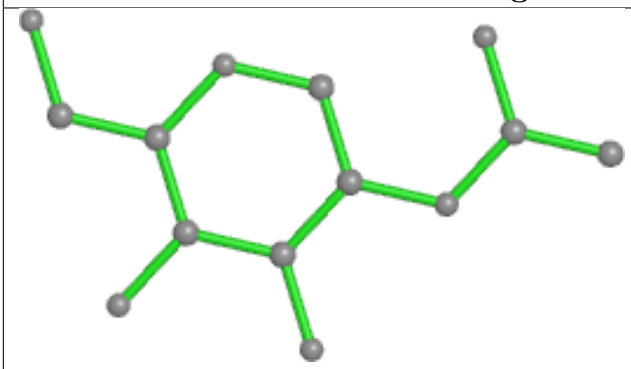


Torsions

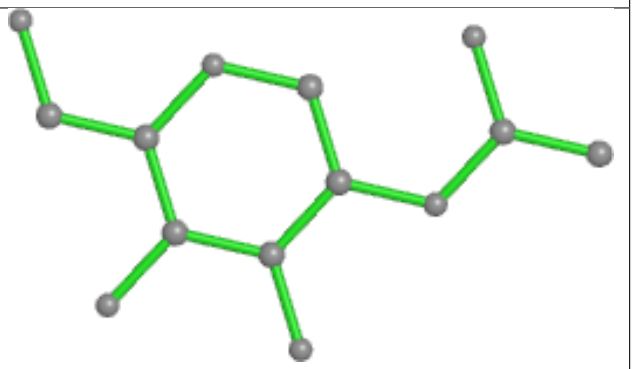


Rings

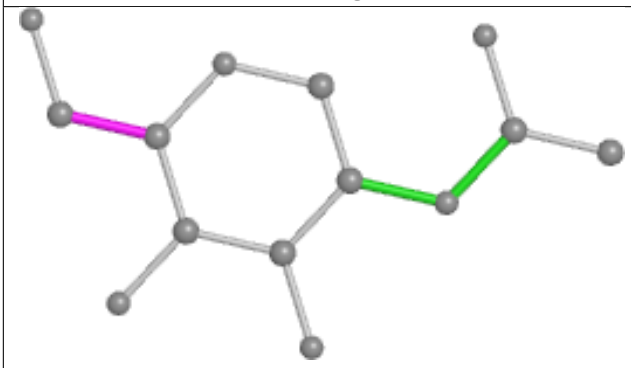
Ligand NAG A 1401



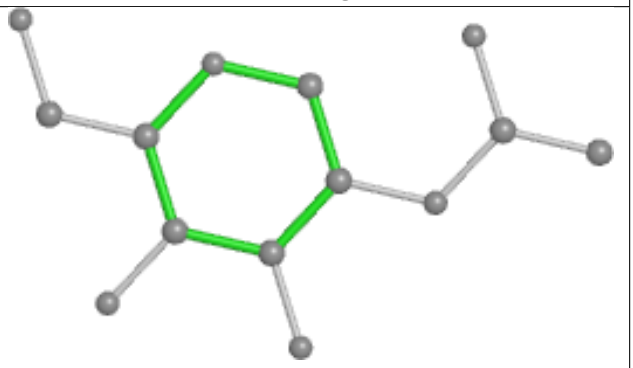
Bond lengths



Bond angles

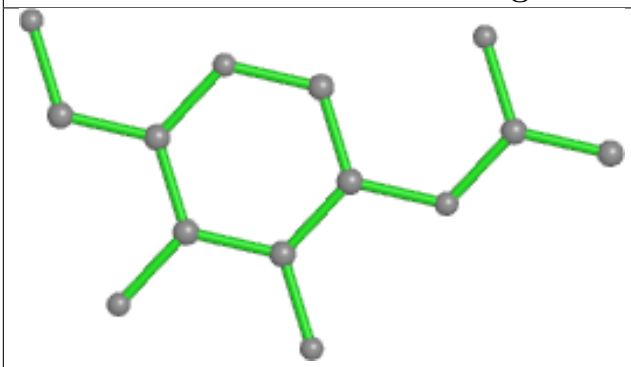


Torsions

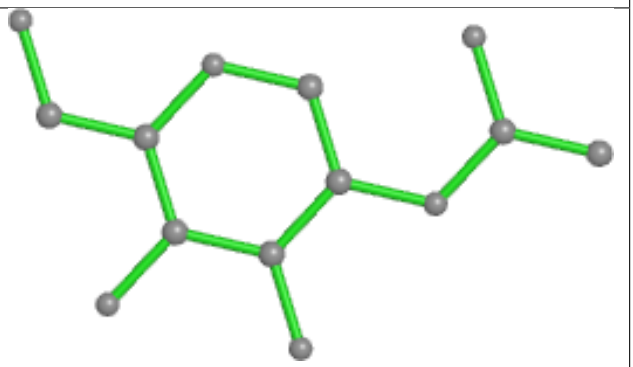


Rings

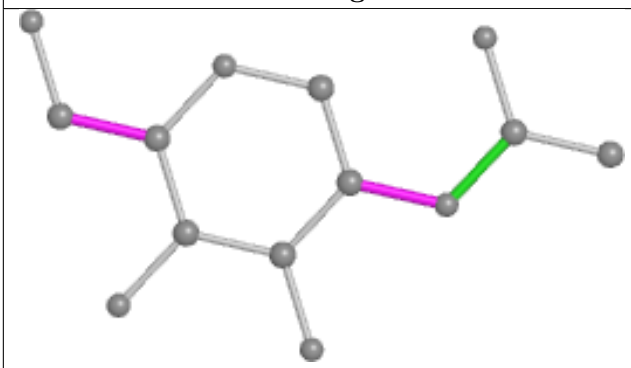
Ligand NAG C 1407



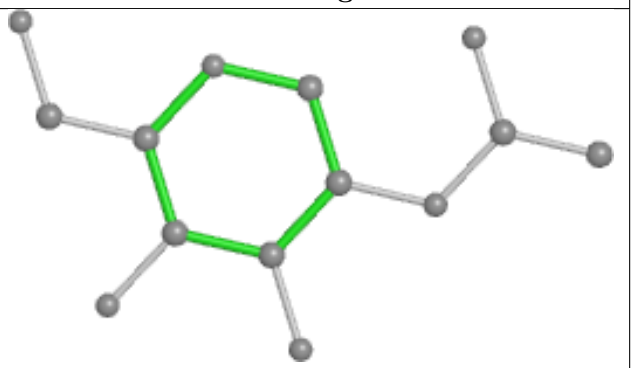
Bond lengths



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.

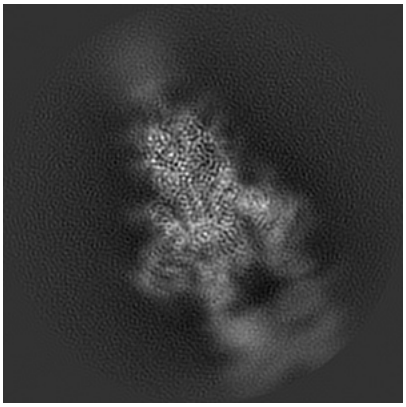
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30522. These allow visual inspection of the internal detail of the map and identification of artifacts.

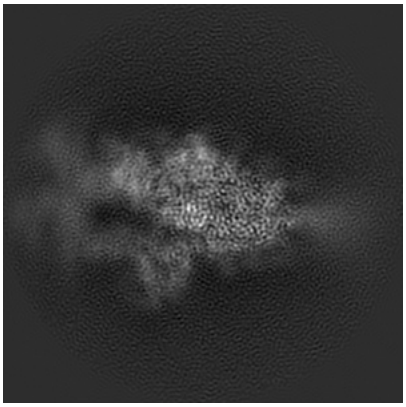
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

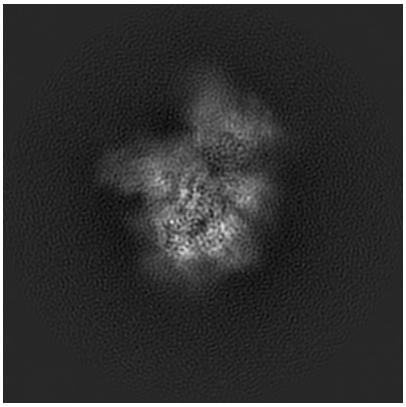
6.1.1 Primary map



X



Y

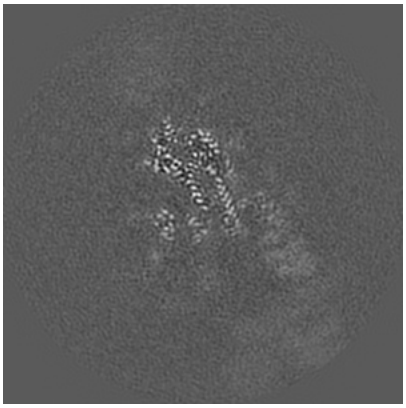


Z

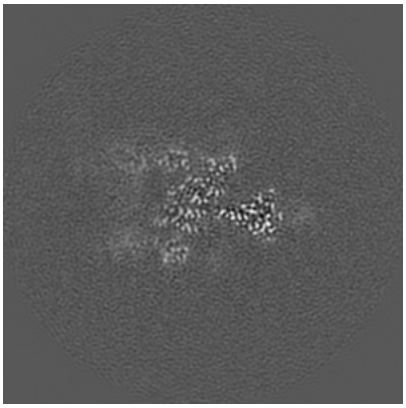
The images above show the map projected in three orthogonal directions.

6.2 Central slices

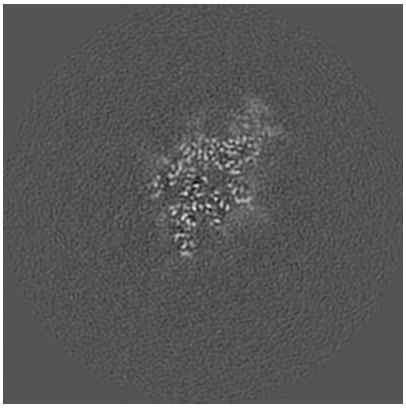
6.2.1 Primary map



X Index: 144



Y Index: 144

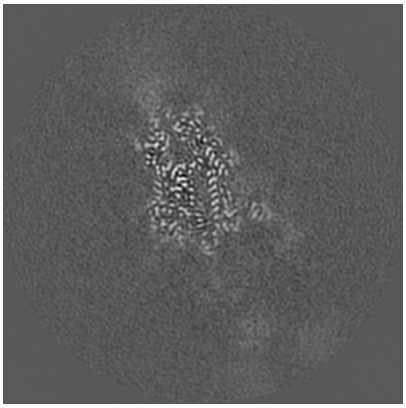


Z Index: 144

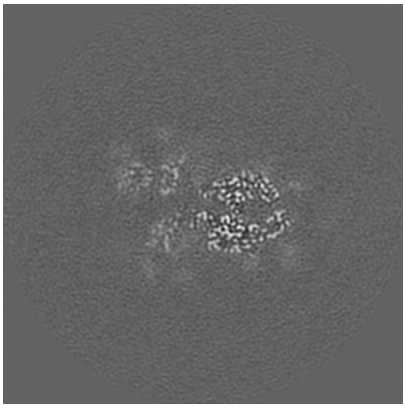
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

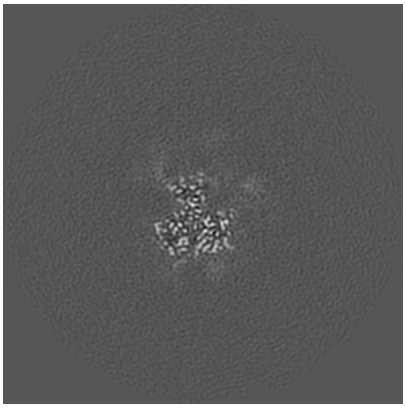
6.3.1 Primary map



X Index: 131



Y Index: 129

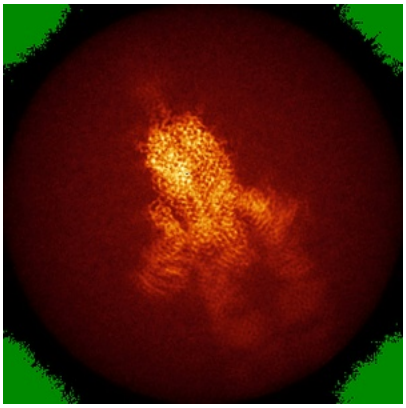


Z Index: 169

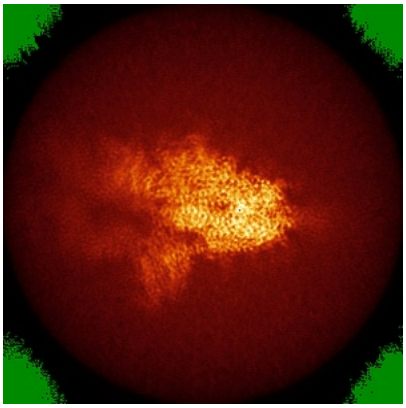
The images above show the largest variance slices of the map in three orthogonal directions.

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

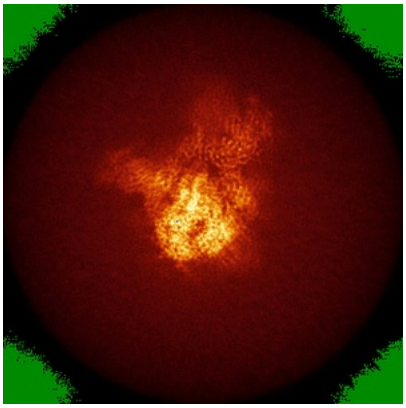
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

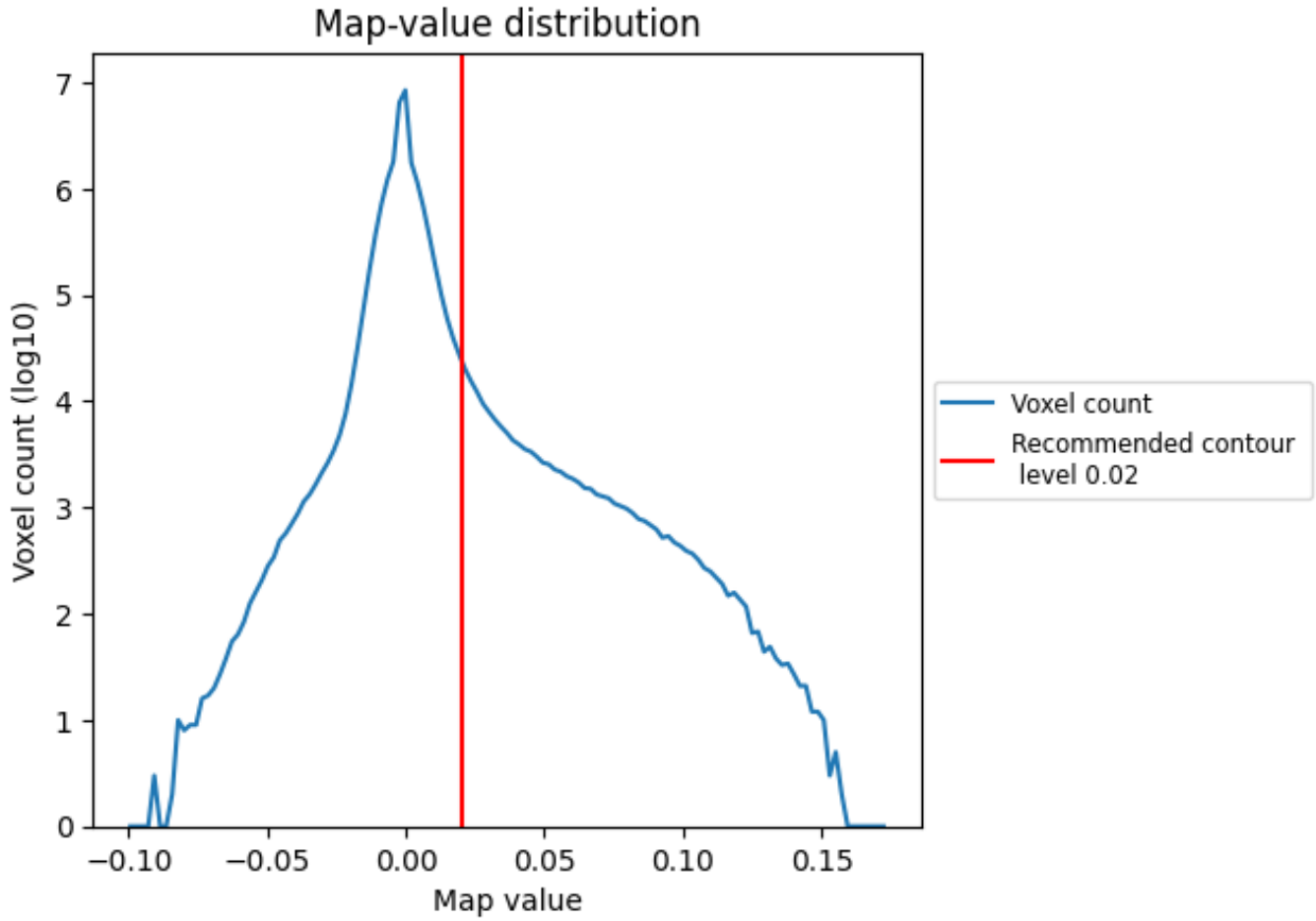
6.6 Mask visualisation (i)

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

7 Map analysis

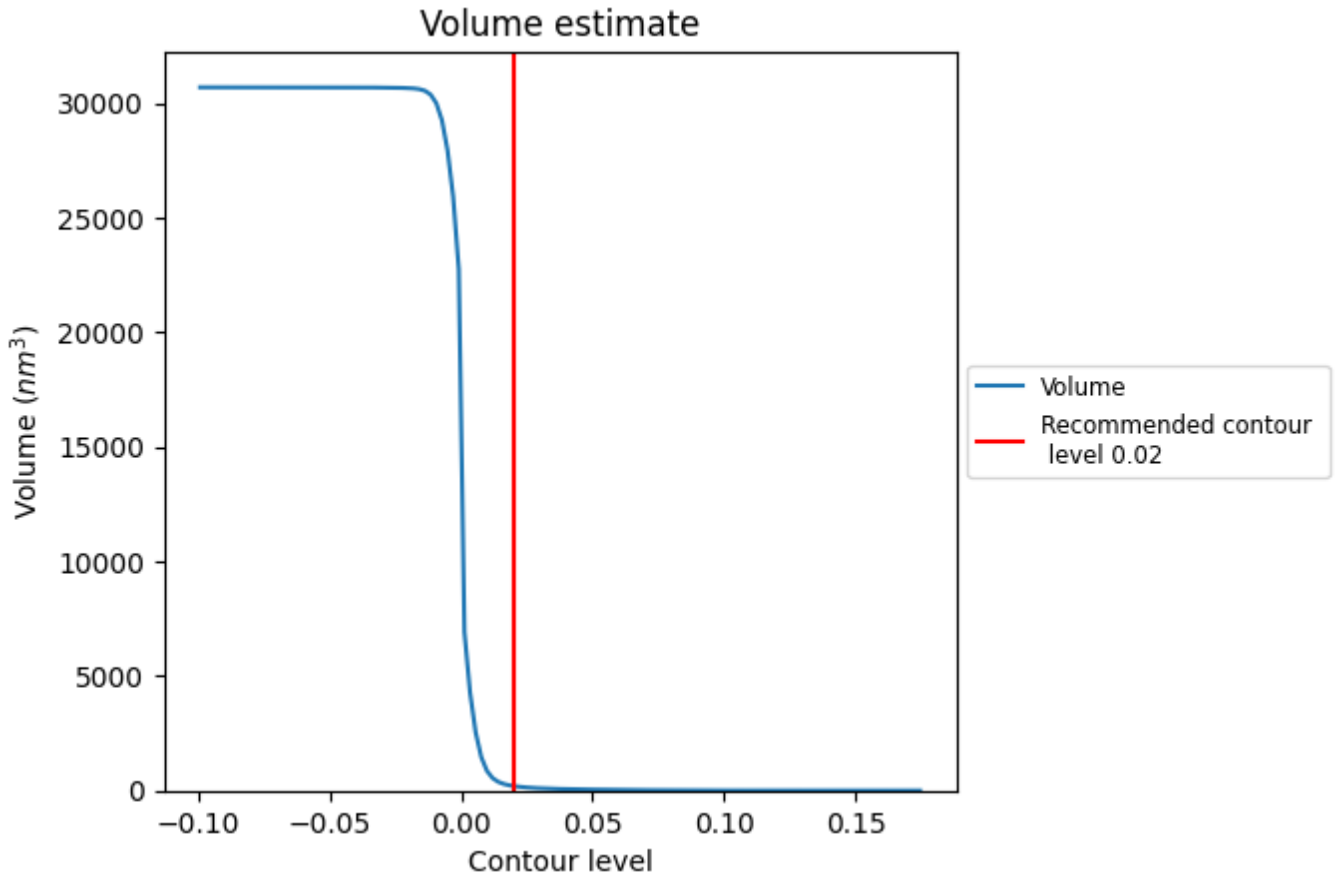
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

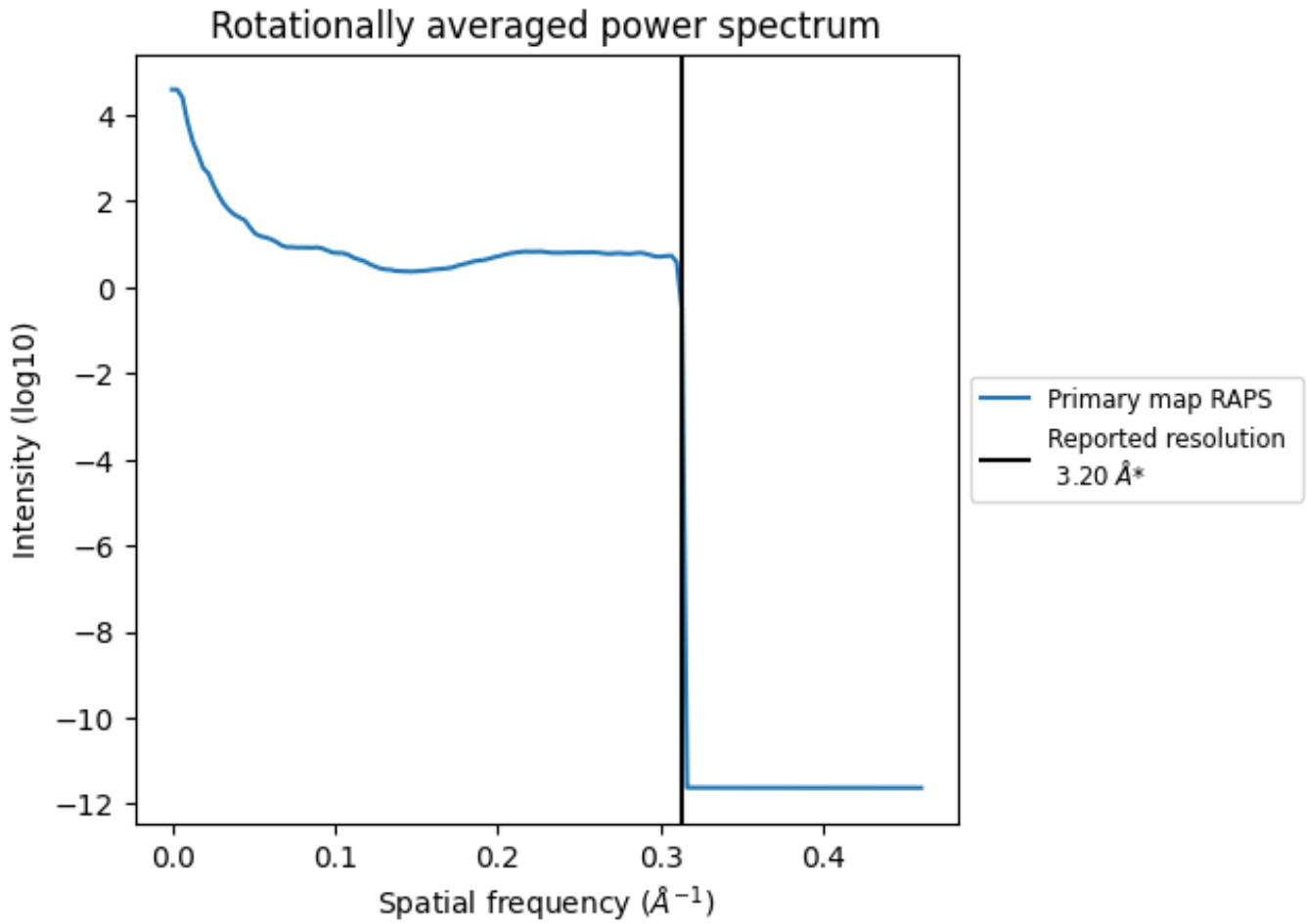
7.2 Volume estimate (i)



The volume at the recommended contour level is 196 nm^3; this corresponds to an approximate mass of 177 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}

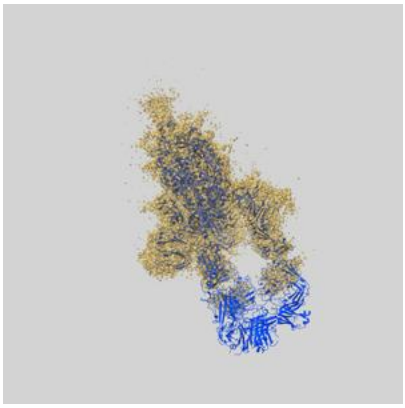
8 Fourier-Shell correlation (i)

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

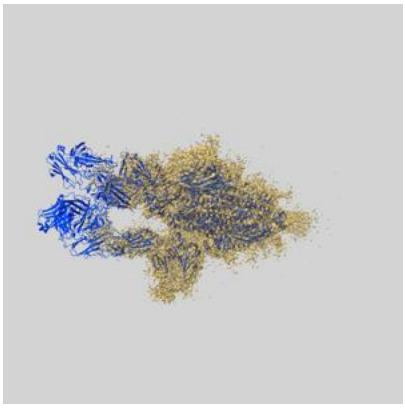
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30522 and PDB model 7CZZ. Per-residue inclusion information can be found in section 3 on page 10.

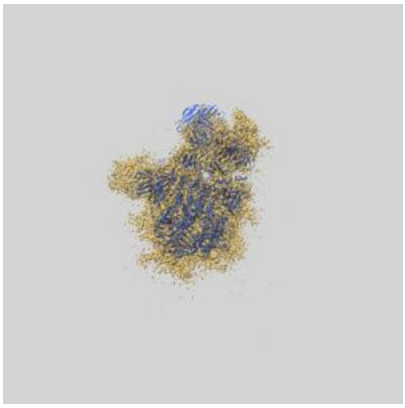
9.1 Map-model overlay



X



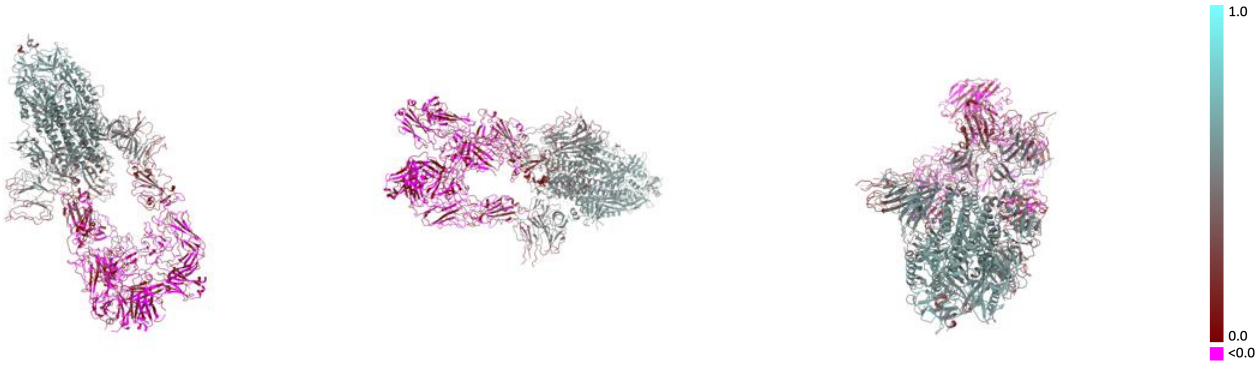
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

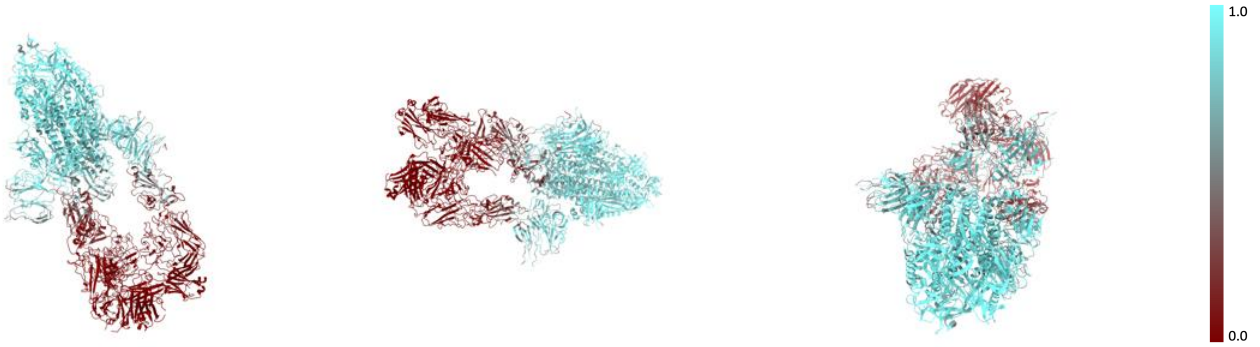
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

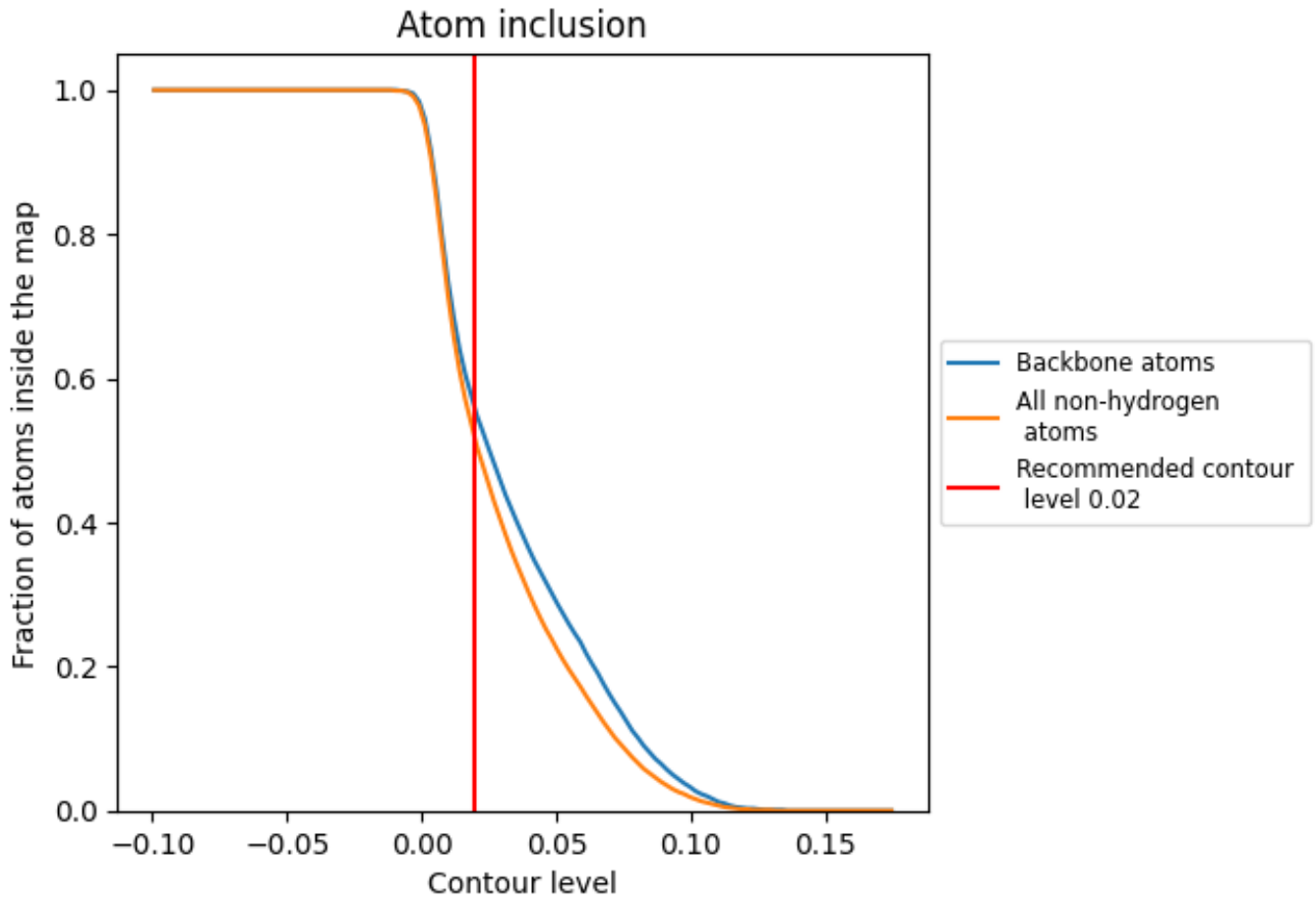
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5140	0.2980
A	0.7430	0.4250
B	0.7190	0.4140
C	0.7120	0.4100
D	0.6430	0.3110
E	0.1790	-0.0190
F	0.9290	0.5400
G	0.6790	0.4140
H	0.0330	0.0050
I	0.0060	0.0290
J	0.0050	0.0110
K	0.0190	0.0170
L	0.6430	0.4500
M	0.0020	0.0250
N	0.0070	0.0120
O	0.8570	0.4810
P	0.7140	0.4180
Q	0.4640	0.0560
R	0.0360	0.0810
S	0.5000	0.3050
T	0.8210	0.4580
U	0.7140	0.3550
V	0.8210	0.4550
W	0.7140	0.4210
X	0.4640	0.1860
Y	0.1070	0.1330
Z	0.4640	0.2380
a	0.7860	0.5020
b	0.6070	0.2540
c	0.5360	0.3130
d	0.8570	0.4710
e	0.7140	0.3100
f	0.0240	0.1740
g	0.0240	0.0230
h	0.0000	0.0210