Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 07:59 PM JST

PDB ID	:	7WWL
EMDB ID	:	EMD-32869
Title	:	S protein of Delta variant in complex with ZWD12
Authors	:	Guo, Y.Y.; Zhang, Y.Y.; Zhou, Q.
Deposited on	:	2022-02-13
Resolution	:	3.00 Å(reported)

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

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

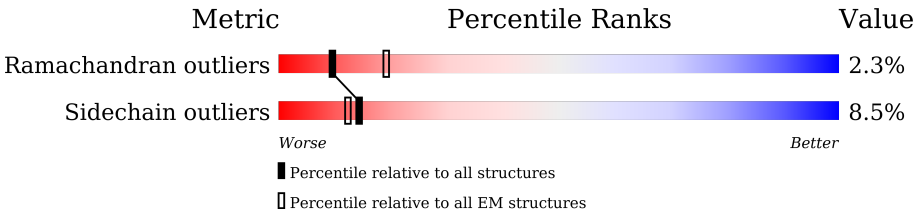
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1271	20% 69% 9% · 22%
1	B	1271	9% 70% 7% · 22%
1	C	1271	8% 71% 6% · 22%
2	H	123	33% 97% ·
2	I	123	93% 97% ·
2	J	123	97% 97% ·
3	L	108	20% 99% ·
3	M	108	92% 94% 6%
3	N	108	99% 98% ·

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

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29704 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	994	Total	C	N	O	S	0	0
			7765	4958	1294	1478	35		
1	B	993	Total	C	N	O	S	0	0
			7759	4955	1293	1476	35		
1	C	993	Total	C	N	O	S	0	0
			7759	4955	1293	1476	35		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	THR	variant	UNP P0DTC2
A	144	ASP	GLY	variant	UNP P0DTC2
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	158	GLY	ARG	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	950	ASN	ASP	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	19	ARG	THR	variant	UNP P0DTC2
B	144	ASP	GLY	variant	UNP P0DTC2
B	?	-	GLU	deletion	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	158	GLY	ARG	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	ARG	PRO	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	950	ASN	ASP	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	19	ARG	THR	variant	UNP P0DTC2
C	144	ASP	GLY	variant	UNP P0DTC2
C	?	-	GLU	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	950	ASN	ASP	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called heavy chain of ZWD12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	123	Total	C	N	O	S	0	0
			967	609	170	184	4		
2	I	123	Total	C	N	O	S	0	0
			967	609	170	184	4		
2	J	123	Total	C	N	O	S	0	0
			967	609	170	184	4		

- Molecule 3 is a protein called light chain of ZWD12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total	C	N	O	S	0	0
			842	532	143	164	3		
3	M	108	Total	C	N	O	S	0	0
			842	532	143	164	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	108	Total	C	N	O	S	0	0
			842	532	143	164	3		

- 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	K	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		

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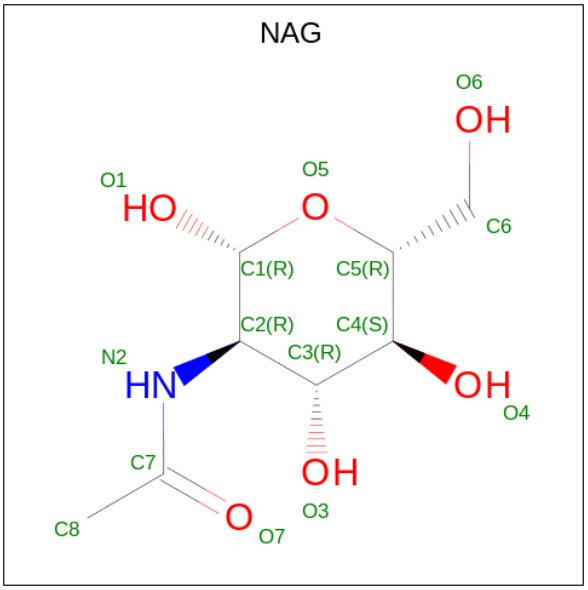
Mol	Chain	Residues	Atoms	AltConf	Trace
4	Z	2	Total C N O 28 16 2 10	0	0
4	a	2	Total C N O 28 16 2 10	0	0
4	b	2	Total C N O 28 16 2 10	0	0
4	c	2	Total C N O 28 16 2 10	0	0
4	d	2	Total C N O 28 16 2 10	0	0
4	e	2	Total C N O 28 16 2 10	0	0
4	f	2	Total C N O 28 16 2 10	0	0

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



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 126 72 9 45	0
5	A	1	Total C N O 126 72 9 45	0
5	A	1	Total C N O 126 72 9 45	0
5	A	1	Total C N O 126 72 9 45	0

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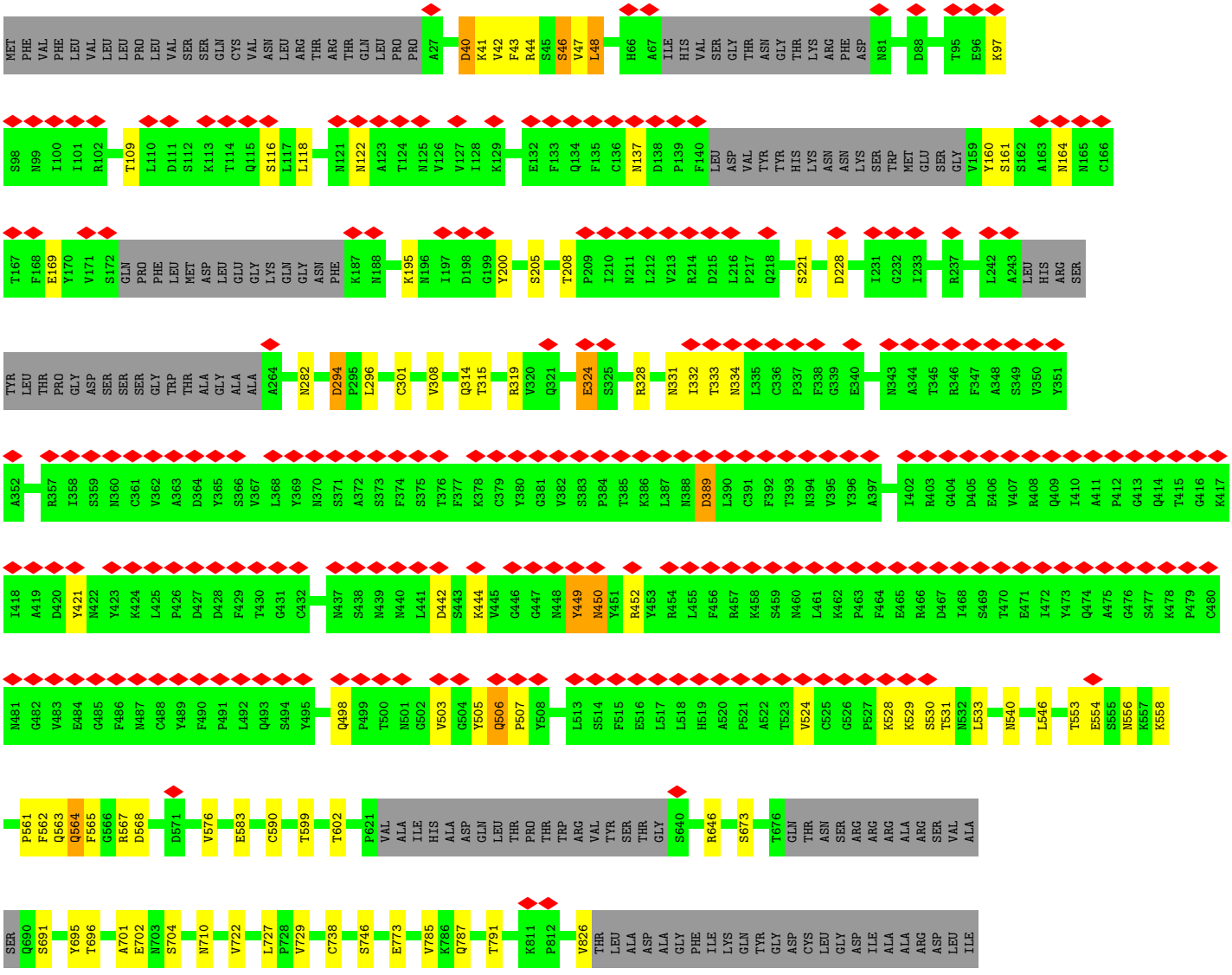
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	A	1	Total 126	C 72	N 9	O 45	0
5	B	1	Total 112	C 64	N 8	O 40	0
5	B	1	Total 112	C 64	N 8	O 40	0
5	B	1	Total 112	C 64	N 8	O 40	0
5	B	1	Total 112	C 64	N 8	O 40	0
5	B	1	Total 112	C 64	N 8	O 40	0
5	B	1	Total 112	C 64	N 8	O 40	0
5	B	1	Total 112	C 64	N 8	O 40	0
5	B	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0
5	C	1	Total 112	C 64	N 8	O 40	0

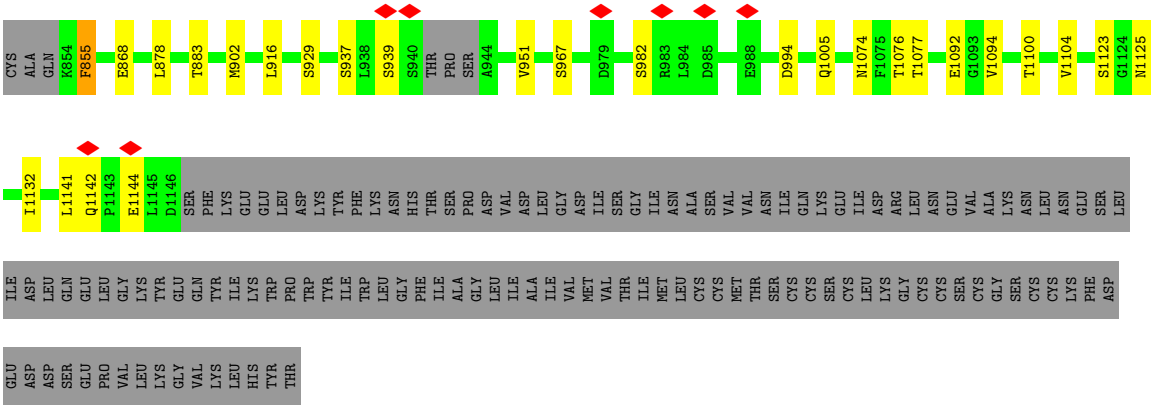
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

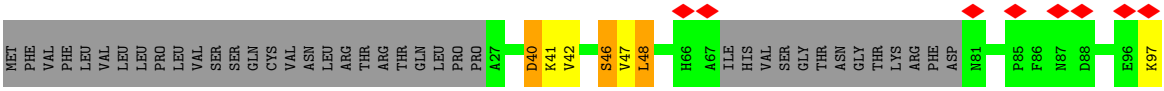
Chain A:

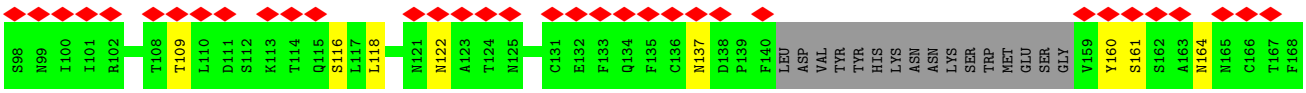


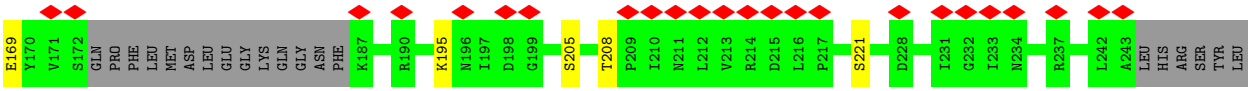


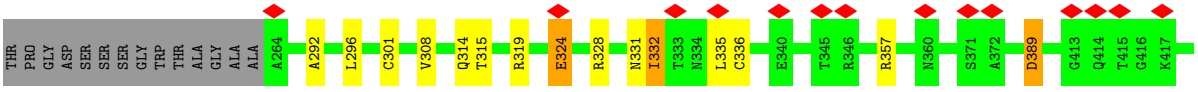
• Molecule 1: Spike glycoprotein

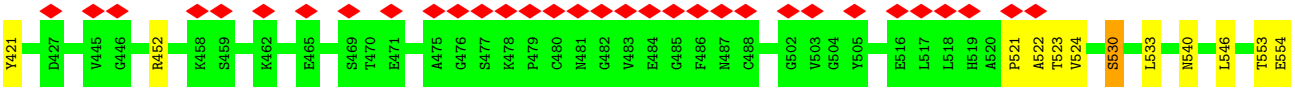
Chain B:

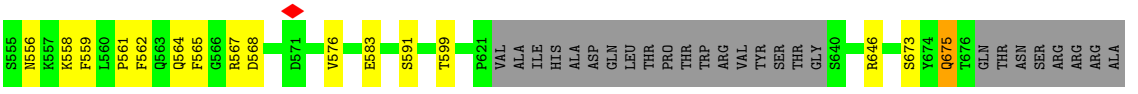


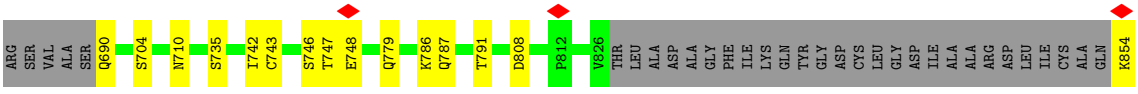


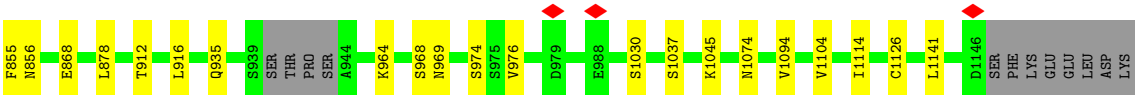


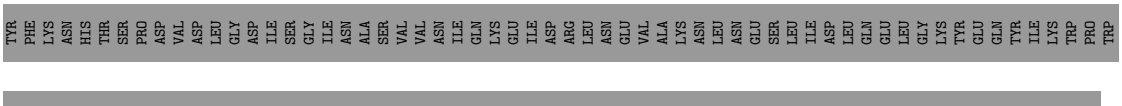






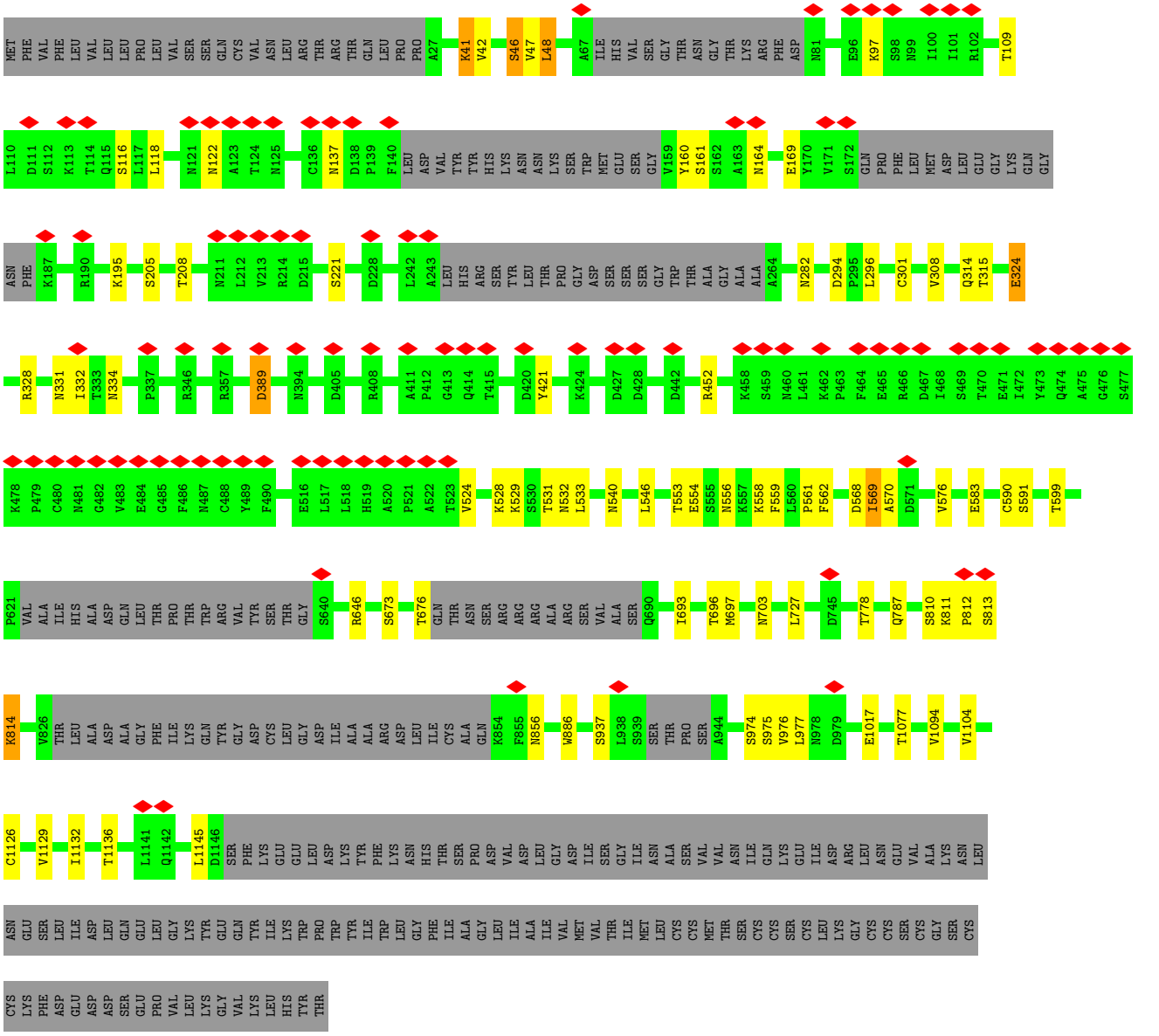






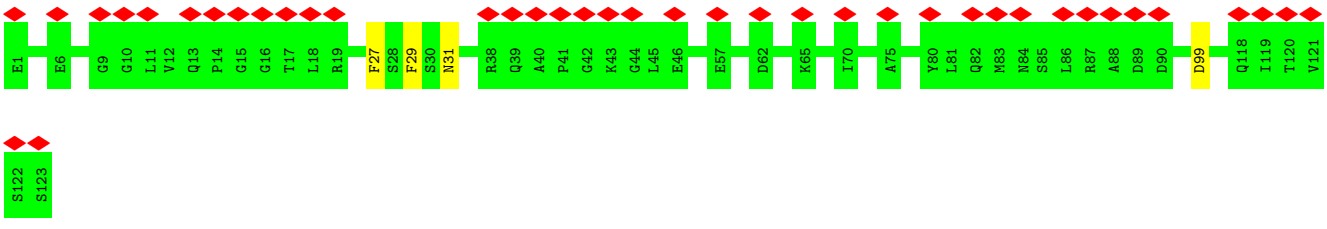
• Molecule 1: Spike glycoprotein

Chain C:



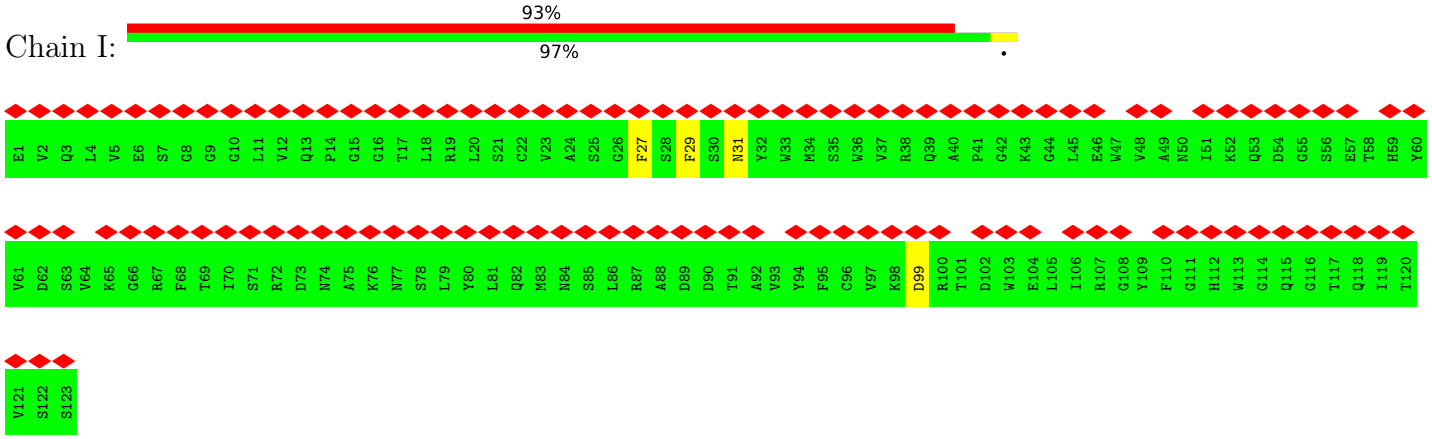
• Molecule 2: heavy chain of ZWD12

Chain H:



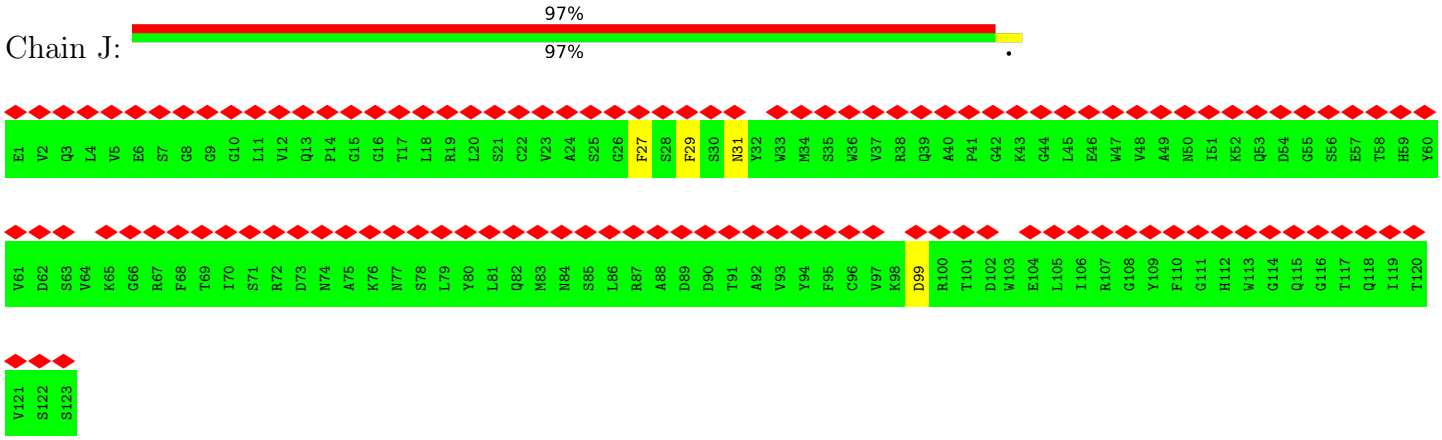
• Molecule 2: heavy chain of ZWD12

Chain I:



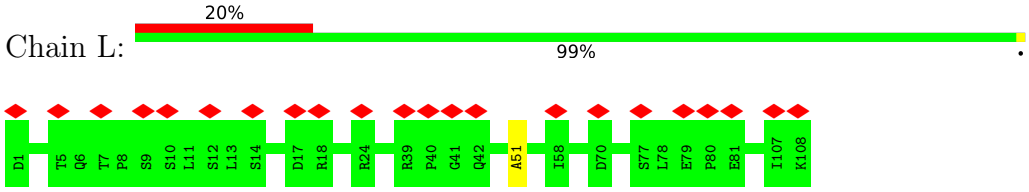
• Molecule 2: heavy chain of ZWD12

Chain J:



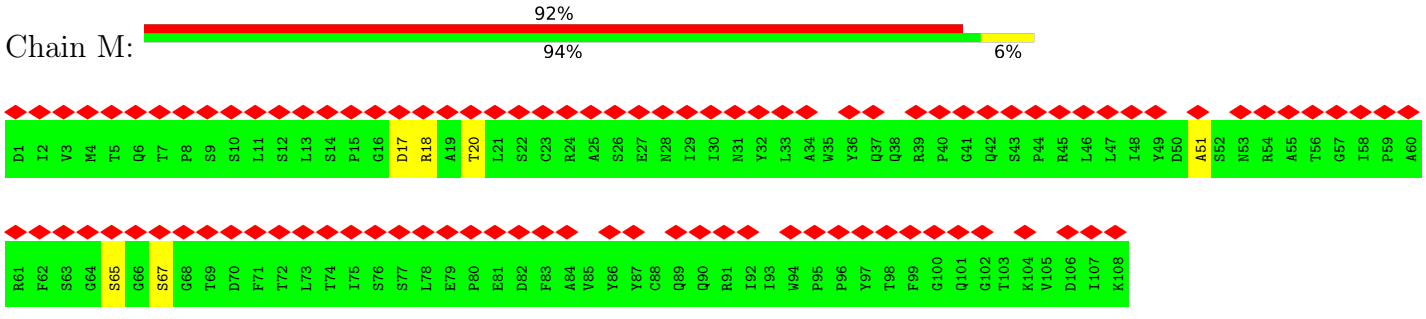
• Molecule 3: light chain of ZWD12

Chain L:



• Molecule 3: light chain of ZWD12

Chain M:

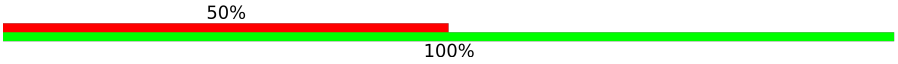


• Molecule 3: light chain of ZWD12

Chain N:

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

Chain D:

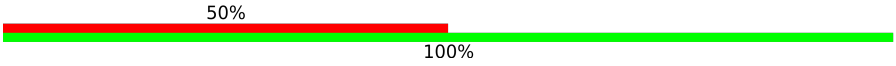


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:

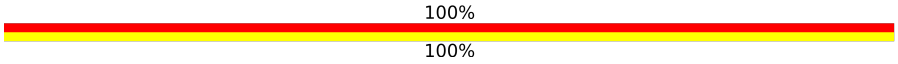


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain K:



• 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

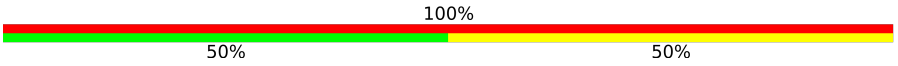
Chain P:

• 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

Chain R:



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

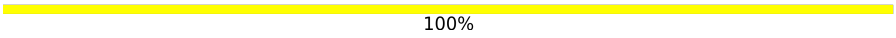
Chain S:

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

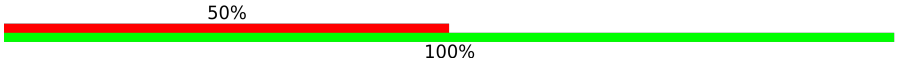
Chain T:

• 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

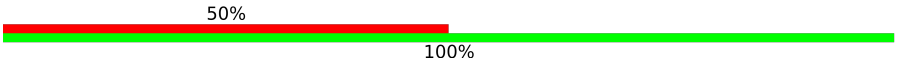
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

Chain a:

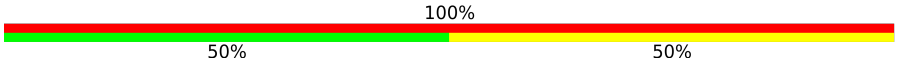
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



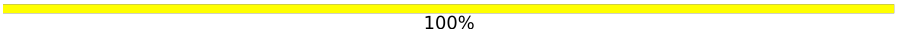
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



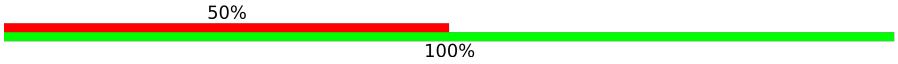
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



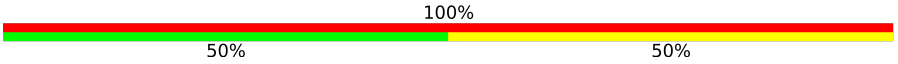
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



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

Chain f:




NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159808	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	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	0.49	0/7941	0.55	0/10805
1	B	0.49	0/7935	0.55	0/10797
1	C	0.49	0/7935	0.54	0/10797
2	H	0.41	0/990	0.61	0/1340
2	I	0.41	0/990	0.61	0/1340
2	J	0.41	0/990	0.61	0/1340
3	L	0.33	0/863	0.52	0/1176
3	M	0.32	0/863	0.51	0/1176
3	N	0.33	0/863	0.51	0/1176
All	All	0.47	0/29370	0.55	0/39947

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	976/1271 (77%)	857 (88%)	90 (9%)	29 (3%)	4	24
1	B	975/1271 (77%)	862 (88%)	91 (9%)	22 (2%)	6	30
1	C	975/1271 (77%)	861 (88%)	91 (9%)	23 (2%)	6	29
2	H	121/123 (98%)	104 (86%)	16 (13%)	1 (1%)	19	57
2	I	121/123 (98%)	104 (86%)	16 (13%)	1 (1%)	19	57
2	J	121/123 (98%)	104 (86%)	16 (13%)	1 (1%)	19	57
3	L	106/108 (98%)	98 (92%)	7 (7%)	1 (1%)	17	55
3	M	106/108 (98%)	96 (91%)	7 (7%)	3 (3%)	5	25
3	N	106/108 (98%)	96 (91%)	8 (8%)	2 (2%)	8	36
All	All	3607/4506 (80%)	3182 (88%)	342 (10%)	83 (2%)	9	30

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	389	ASP
1	A	449	TYR
1	A	450	ASN
1	A	524	VAL
1	A	562	PHE
1	A	564	GLN
1	A	590	CYS
1	A	701	ALA
1	A	855	PHE
1	B	41	LYS
1	B	48	LEU
1	B	332	ILE
1	B	389	ASP
1	B	524	VAL
1	B	530	SER
1	B	562	PHE
1	C	41	LYS
1	C	42	VAL
1	C	48	LEU
1	C	389	ASP
1	C	524	VAL
1	C	562	PHE

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Mol	Chain	Res	Type
1	C	814	LYS
3	M	67	SER
1	A	41	LYS
1	A	46	SER
1	A	160	TYR
1	A	332	ILE
1	B	46	SER
1	B	160	TYR
1	B	522	ALA
1	B	742	ILE
1	B	743	CYS
1	C	46	SER
1	C	160	TYR
1	C	331	ASN
1	C	697	MET
1	C	810	SER
3	L	51	ALA
3	M	51	ALA
3	N	51	ALA
1	A	43	PHE
1	A	695	TYR
1	A	710	ASN
1	B	42	VAL
3	M	65	SER
1	A	44	ARG
1	A	324	GLU
1	A	331	ASN
1	A	561	PRO
1	A	691	SER
1	B	324	GLU
1	B	561	PRO
1	B	675	GLN
1	B	746	SER
1	C	324	GLU
1	C	561	PRO
1	C	570	ALA
1	C	590	CYS
1	C	813	SER
2	H	29	PHE
2	I	29	PHE
2	J	29	PHE
1	A	40	ASP

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Mol	Chain	Res	Type
1	A	42	VAL
1	A	47	VAL
1	A	294	ASP
1	A	503	VAL
1	A	506	GLN
1	A	507	PRO
1	B	40	ASP
1	B	47	VAL
1	B	292	ALA
1	C	47	VAL
1	C	294	ASP
1	C	812	PRO
3	N	17	ASP
1	C	332	ILE
1	C	811	LYS
1	B	336	CYS
1	C	569	ILE
1	B	521	PRO

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	871/1112 (78%)	769 (88%)	102 (12%)	5 22
1	B	870/1112 (78%)	785 (90%)	85 (10%)	8 30
1	C	870/1112 (78%)	798 (92%)	72 (8%)	11 39
2	H	103/103 (100%)	100 (97%)	3 (3%)	42 76
2	I	103/103 (100%)	100 (97%)	3 (3%)	42 76
2	J	103/103 (100%)	100 (97%)	3 (3%)	42 76
3	L	93/93 (100%)	93 (100%)	0	100 100
3	M	93/93 (100%)	90 (97%)	3 (3%)	39 74
3	N	93/93 (100%)	93 (100%)	0	100 100
All	All	3199/3924 (82%)	2928 (92%)	271 (8%)	14 38

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	46	SER
1	A	48	LEU
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	137	ASN
1	A	161	SER
1	A	164	ASN
1	A	169	GLU
1	A	195	LYS
1	A	200	TYR
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	228	ASP
1	A	282	ASN
1	A	294	ASP
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	319	ARG
1	A	324	GLU
1	A	328	ARG
1	A	333	THR
1	A	334	ASN
1	A	389	ASP
1	A	421	TYR
1	A	442	ASP
1	A	444	LYS
1	A	449	TYR
1	A	450	ASN
1	A	452	ARG
1	A	498	GLN
1	A	505	TYR
1	A	506	GLN
1	A	528	LYS
1	A	529	LYS

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Mol	Chain	Res	Type
1	A	530	SER
1	A	531	THR
1	A	533	LEU
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	558	LYS
1	A	563	GLN
1	A	564	GLN
1	A	565	PHE
1	A	567	ARG
1	A	568	ASP
1	A	576	VAL
1	A	583	GLU
1	A	599	THR
1	A	602	THR
1	A	646	ARG
1	A	673	SER
1	A	696	THR
1	A	702	GLU
1	A	704	SER
1	A	722	VAL
1	A	727	LEU
1	A	729	VAL
1	A	738	CYS
1	A	746	SER
1	A	773	GLU
1	A	785	VAL
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	855	PHE
1	A	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU
1	A	929	SER
1	A	937	SER
1	A	939	SER

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Mol	Chain	Res	Type
1	A	951	VAL
1	A	967	SER
1	A	982	SER
1	A	994	ASP
1	A	1005	GLN
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1123	SER
1	A	1125	ASN
1	A	1132	ILE
1	A	1141	LEU
1	A	1142	GLN
1	A	1144	GLU
1	B	40	ASP
1	B	46	SER
1	B	48	LEU
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	137	ASN
1	B	161	SER
1	B	164	ASN
1	B	169	GLU
1	B	195	LYS
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL
1	B	314	GLN
1	B	315	THR
1	B	319	ARG
1	B	324	GLU
1	B	328	ARG

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Mol	Chain	Res	Type
1	B	331	ASN
1	B	332	ILE
1	B	335	LEU
1	B	357	ARG
1	B	389	ASP
1	B	421	TYR
1	B	452	ARG
1	B	523	THR
1	B	530	SER
1	B	533	LEU
1	B	540	ASN
1	B	546	LEU
1	B	553	THR
1	B	554	GLU
1	B	556	ASN
1	B	558	LYS
1	B	559	PHE
1	B	564	GLN
1	B	565	PHE
1	B	567	ARG
1	B	568	ASP
1	B	576	VAL
1	B	583	GLU
1	B	591	SER
1	B	599	THR
1	B	646	ARG
1	B	673	SER
1	B	675	GLN
1	B	690	GLN
1	B	704	SER
1	B	710	ASN
1	B	735	SER
1	B	747	THR
1	B	748	GLU
1	B	779	GLN
1	B	786	LYS
1	B	787	GLN
1	B	791	THR
1	B	808	ASP
1	B	854	LYS
1	B	855	PHE
1	B	856	ASN

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Mol	Chain	Res	Type
1	B	868	GLU
1	B	878	LEU
1	B	912	THR
1	B	916	LEU
1	B	935	GLN
1	B	964	LYS
1	B	968	SER
1	B	969	ASN
1	B	974	SER
1	B	976	VAL
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1141	LEU
1	C	41	LYS
1	C	46	SER
1	C	48	LEU
1	C	97	LYS
1	C	109	THR
1	C	116	SER
1	C	118	LEU
1	C	122	ASN
1	C	137	ASN
1	C	161	SER
1	C	164	ASN
1	C	169	GLU
1	C	195	LYS
1	C	205	SER
1	C	208	THR
1	C	221	SER
1	C	282	ASN
1	C	296	LEU
1	C	301	CYS
1	C	308	VAL
1	C	314	GLN
1	C	315	THR
1	C	324	GLU

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Mol	Chain	Res	Type
1	C	328	ARG
1	C	334	ASN
1	C	389	ASP
1	C	421	TYR
1	C	452	ARG
1	C	528	LYS
1	C	529	LYS
1	C	531	THR
1	C	532	ASN
1	C	533	LEU
1	C	540	ASN
1	C	546	LEU
1	C	553	THR
1	C	554	GLU
1	C	556	ASN
1	C	558	LYS
1	C	559	PHE
1	C	568	ASP
1	C	569	ILE
1	C	576	VAL
1	C	583	GLU
1	C	591	SER
1	C	599	THR
1	C	646	ARG
1	C	673	SER
1	C	676	THR
1	C	693	ILE
1	C	696	THR
1	C	703	ASN
1	C	727	LEU
1	C	778	THR
1	C	787	GLN
1	C	814	LYS
1	C	856	ASN
1	C	886	TRP
1	C	937	SER
1	C	974	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1017	GLU
1	C	1077	THR

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Mol	Chain	Res	Type
1	C	1094	VAL
1	C	1104	VAL
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU
2	H	27	PHE
2	H	31	ASN
2	H	99	ASP
2	I	27	PHE
2	I	31	ASN
2	I	99	ASP
3	M	17	ASP
3	M	18	ARG
3	M	20	THR
2	J	27	PHE
2	J	31	ASN
2	J	99	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	239	GLN
1	A	317	ASN
1	A	422	ASN
1	A	450	ASN
1	A	493	GLN
1	A	498	GLN
1	A	506	GLN
1	A	519	HIS
1	A	540	ASN
1	A	544	ASN
1	A	556	ASN
1	A	564	GLN
1	A	644	GLN
1	A	658	ASN
1	A	690	GLN
1	A	703	ASN

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Mol	Chain	Res	Type
1	A	762	GLN
1	A	787	GLN
1	A	901	GLN
1	A	914	ASN
1	A	919	ASN
1	A	926	GLN
1	A	955	ASN
1	A	969	ASN
1	A	992	GLN
1	A	1125	ASN
1	A	1142	GLN
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	239	GLN
1	B	317	ASN
1	B	422	ASN
1	B	450	ASN
1	B	540	ASN
1	B	556	ASN
1	B	564	GLN
1	B	644	GLN
1	B	658	ASN
1	B	675	GLN
1	B	690	GLN
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	920	GLN
1	B	926	GLN
1	B	992	GLN
1	B	1054	GLN
1	C	134	GLN
1	C	137	ASN
1	C	188	ASN
1	C	239	GLN
1	C	317	ASN
1	C	422	ASN
1	C	450	ASN
1	C	519	HIS

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Mol	Chain	Res	Type
1	C	540	ASN
1	C	544	ASN
1	C	556	ASN
1	C	564	GLN
1	C	644	GLN
1	C	658	ASN
1	C	703	ASN
1	C	784	GLN
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	926	GLN
1	C	935	GLN
1	C	969	ASN
1	C	992	GLN
1	C	1010	GLN
1	C	1071	GLN
1	C	1101	HIS
1	C	1106	GLN
2	H	31	ASN
2	I	31	ASN
2	J	31	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)

46 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	0.54	0	17,19,21	0.49	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.57	0
4	NAG	E	1	4,1	14,14,15	0.20	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.24	0	17,19,21	0.60	1 (5%)
4	NAG	F	1	4,1	14,14,15	0.32	0	17,19,21	0.62	0
4	NAG	F	2	4	14,14,15	0.52	0	17,19,21	0.48	0
4	NAG	G	1	4,1	14,14,15	0.38	0	17,19,21	0.72	0
4	NAG	G	2	4	14,14,15	0.28	0	17,19,21	1.31	2 (11%)
4	NAG	K	1	4,1	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
4	NAG	K	2	4	14,14,15	0.39	0	17,19,21	1.40	3 (17%)
4	NAG	O	1	4,1	14,14,15	0.72	1 (7%)	17,19,21	0.66	0
4	NAG	O	2	4	14,14,15	0.29	0	17,19,21	0.65	0
4	NAG	P	1	4,1	14,14,15	0.24	0	17,19,21	0.68	1 (5%)
4	NAG	P	2	4	14,14,15	0.17	0	17,19,21	0.47	0
4	NAG	Q	1	4,1	14,14,15	0.54	0	17,19,21	0.49	0
4	NAG	Q	2	4	14,14,15	0.26	0	17,19,21	0.58	0
4	NAG	R	1	4,1	14,14,15	0.19	0	17,19,21	0.56	0
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	0.60	1 (5%)
4	NAG	S	1	4,1	14,14,15	0.32	0	17,19,21	0.40	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	1.14	1 (5%)
4	NAG	T	2	4	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	U	1	4,1	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
4	NAG	U	2	4	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	V	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	V	2	4	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
4	NAG	W	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	W	2	4	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	X	1	4,1	14,14,15	0.56	0	17,19,21	0.49	0
4	NAG	X	2	4	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	Y	1	4,1	14,14,15	0.19	0	17,19,21	0.56	0
4	NAG	Y	2	4	14,14,15	0.24	0	17,19,21	0.60	1 (5%)
4	NAG	Z	1	4,1	14,14,15	0.22	0	17,19,21	1.36	1 (5%)
4	NAG	Z	2	4	14,14,15	0.18	0	17,19,21	0.50	0
4	NAG	a	1	4,1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
4	NAG	a	2	4	14,14,15	0.39	0	17,19,21	0.47	0
4	NAG	b	1	4,1	14,14,15	0.38	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	b	2	4	14,14,15	0.20	0	17,19,21	0.74	0
4	NAG	c	1	4,1	14,14,15	0.38	0	17,19,21	0.49	0
4	NAG	c	2	4	14,14,15	0.55	0	17,19,21	1.30	1 (5%)
4	NAG	d	1	4,1	14,14,15	0.62	1 (7%)	17,19,21	0.42	0
4	NAG	d	2	4	14,14,15	0.34	0	17,19,21	1.35	2 (11%)
4	NAG	e	1	4,1	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	e	2	4	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	f	1	4,1	14,14,15	0.40	0	17,19,21	1.14	2 (11%)
4	NAG	f	2	4	14,14,15	0.35	0	17,19,21	0.42	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	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	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	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	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
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	-	1/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	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
4	NAG	f	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	f	2	4	-	0/6/23/26	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	-2.71	1.39	1.43
4	O	1	NAG	O5-C1	-2.61	1.39	1.43
4	K	1	NAG	O5-C1	-2.33	1.40	1.43
4	d	1	NAG	O5-C1	-2.11	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Z	1	NAG	C2-N2-C7	4.68	129.57	122.90
4	K	2	NAG	C2-N2-C7	4.44	129.23	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	2	NAG	C2-N2-C7	4.33	129.07	122.90
4	c	2	NAG	C2-N2-C7	4.28	129.00	122.90
4	G	2	NAG	C2-N2-C7	4.26	128.97	122.90
4	T	1	NAG	C1-O5-C5	3.33	116.71	112.19
4	K	2	NAG	C1-C2-N2	2.38	114.56	110.49
4	V	1	NAG	O4-C4-C3	-2.38	104.84	110.35
4	G	2	NAG	C1-C2-N2	2.36	114.52	110.49
4	U	1	NAG	C1-O5-C5	2.29	115.29	112.19
4	f	1	NAG	C8-C7-N2	2.25	119.91	116.10
4	a	1	NAG	C1-O5-C5	2.25	115.24	112.19
4	d	2	NAG	C1-C2-N2	2.21	114.27	110.49
4	R	2	NAG	C1-O5-C5	2.11	115.05	112.19
4	Y	2	NAG	C1-O5-C5	2.10	115.03	112.19
4	E	2	NAG	C1-O5-C5	2.10	115.03	112.19
4	P	1	NAG	C1-O5-C5	2.09	115.02	112.19
4	K	2	NAG	C1-O5-C5	2.07	115.00	112.19
4	V	2	NAG	C1-O5-C5	2.05	114.97	112.19
4	f	1	NAG	C2-N2-C7	-2.05	119.98	122.90

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Z	2	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	a	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
4	Z	1	NAG	C8-C7-N2-C2
4	Z	1	NAG	O7-C7-N2-C2
4	c	2	NAG	C8-C7-N2-C2
4	c	2	NAG	O7-C7-N2-C2
4	d	2	NAG	C8-C7-N2-C2
4	d	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

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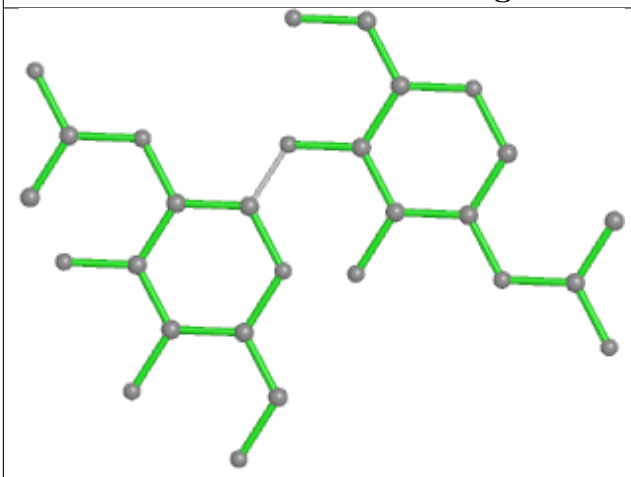
Mol	Chain	Res	Type	Atoms
4	R	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C3-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	V	2	NAG	C3-C2-N2-C7
4	b	2	NAG	C3-C2-N2-C7
4	d	2	NAG	C3-C2-N2-C7
4	K	2	NAG	C4-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	C1-C2-N2-C7
4	U	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7
4	K	2	NAG	C3-C2-N2-C7
4	Z	1	NAG	C3-C2-N2-C7
4	c	2	NAG	C3-C2-N2-C7

There are no ring outliers.

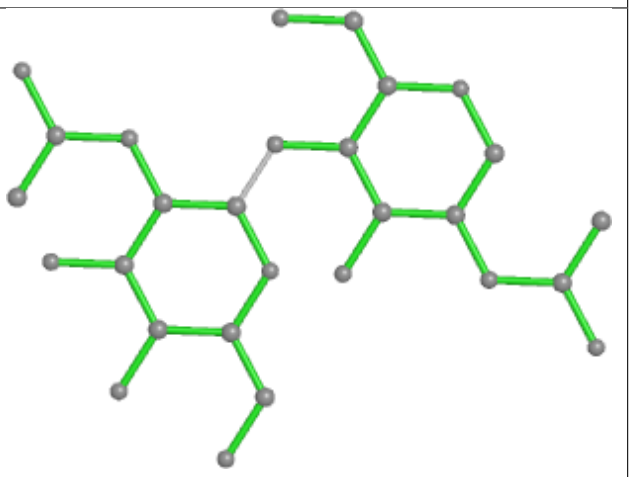
No monomer is involved in short contacts.

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

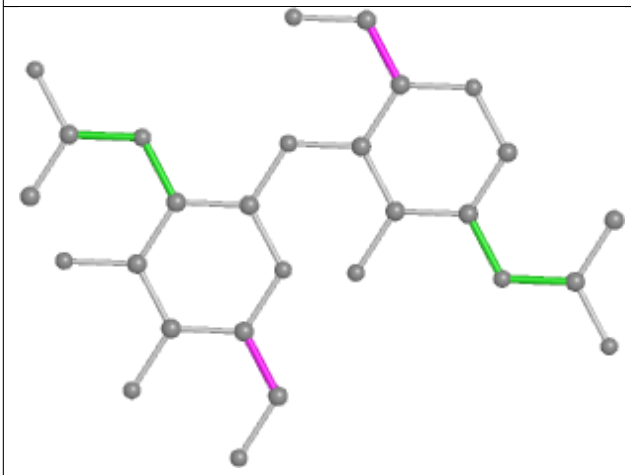
Oligosaccharide Chain D



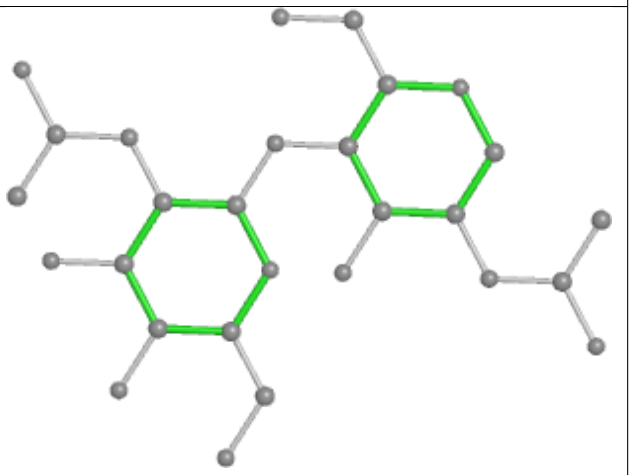
Bond lengths



Bond angles

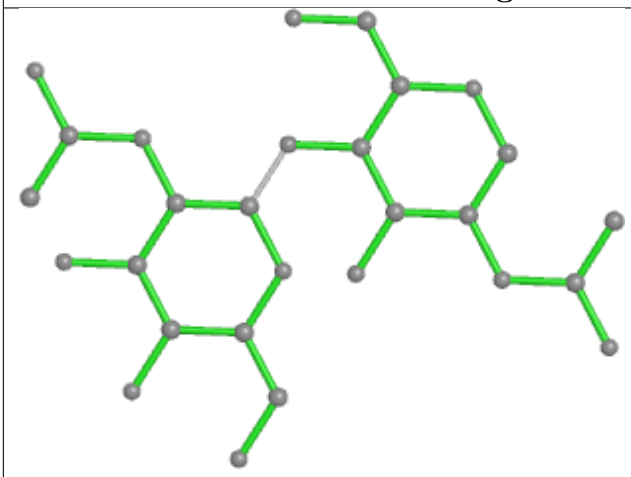


Torsions

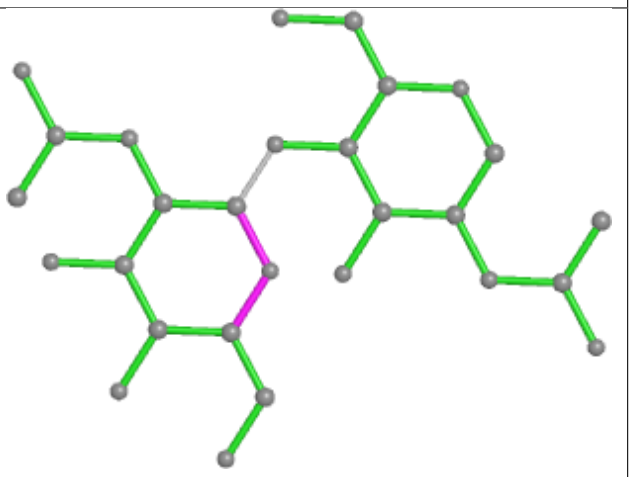


Rings

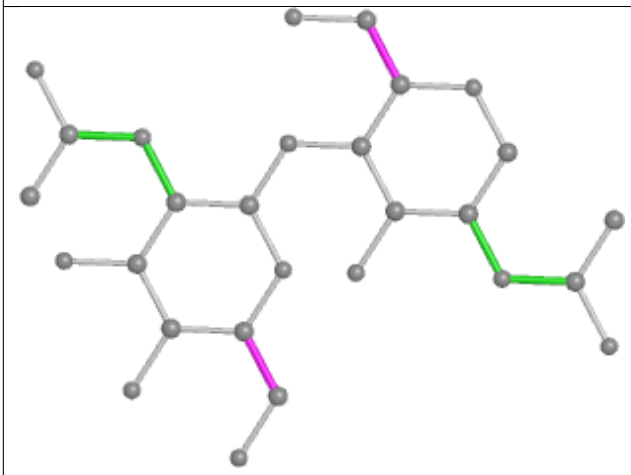
Oligosaccharide Chain E



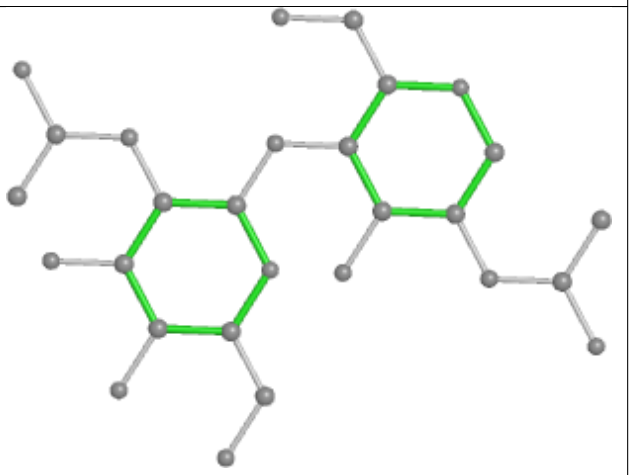
Bond lengths



Bond angles

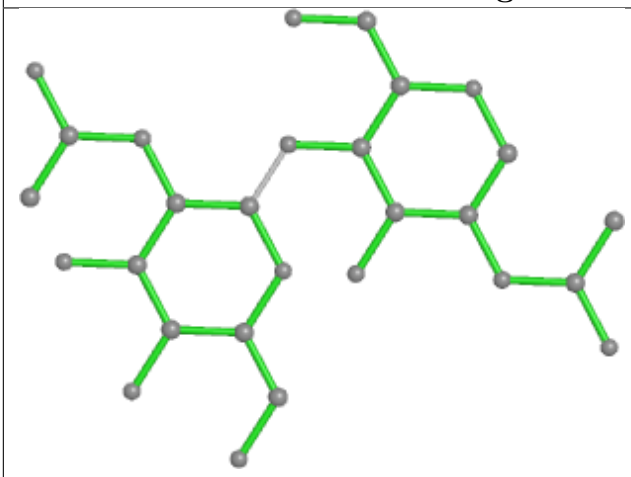


Torsions

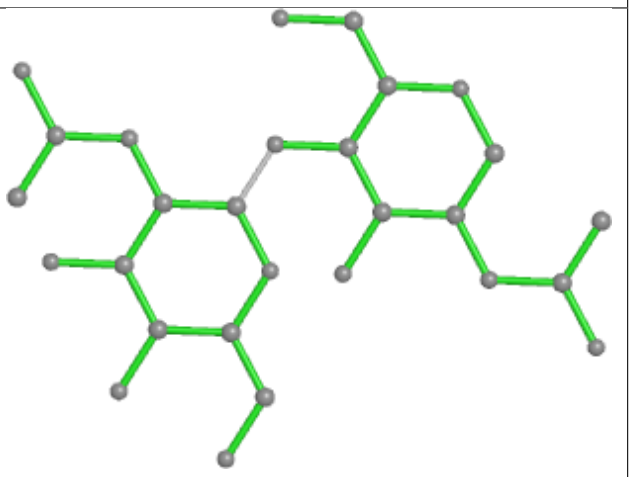


Rings

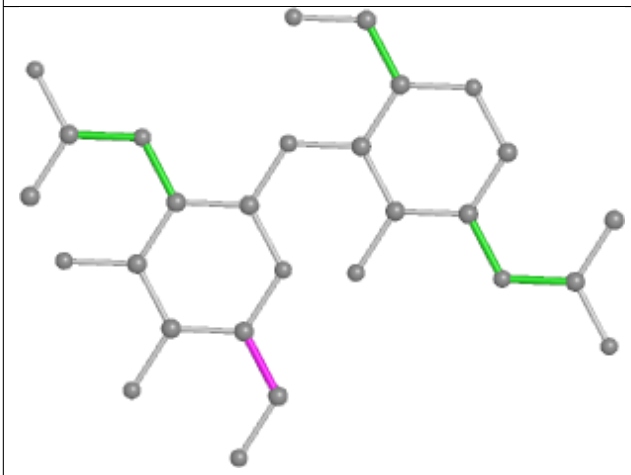
Oligosaccharide Chain F



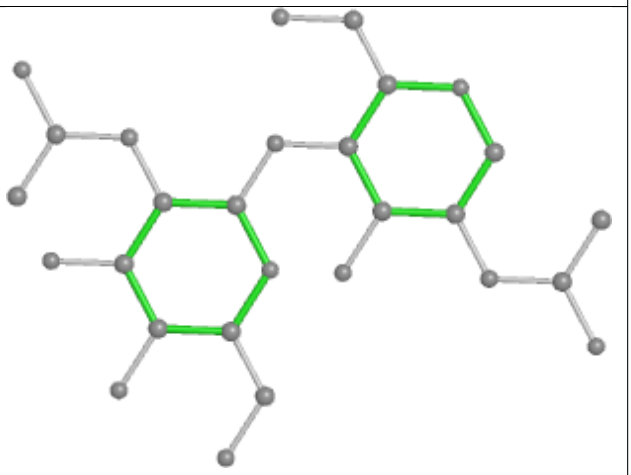
Bond lengths



Bond angles

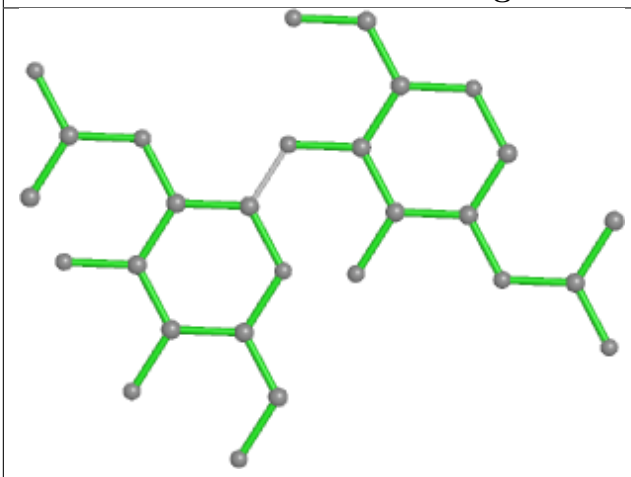


Torsions

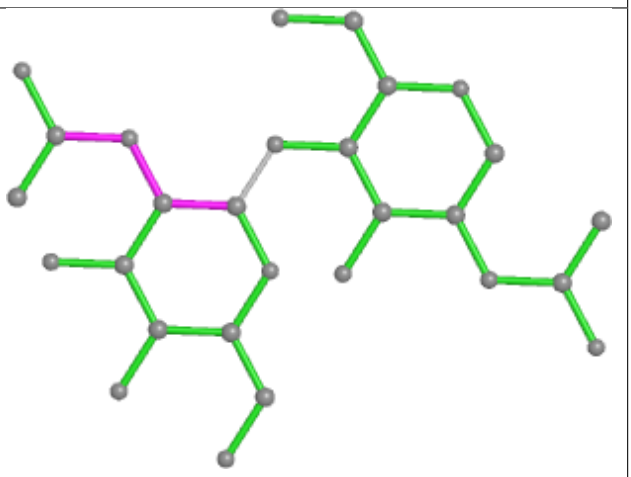


Rings

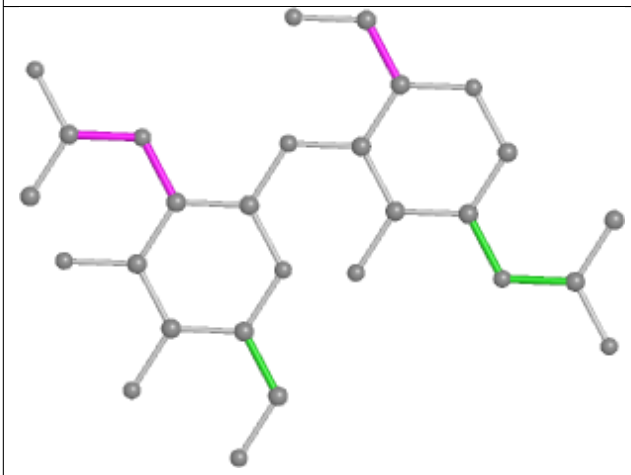
Oligosaccharide Chain G



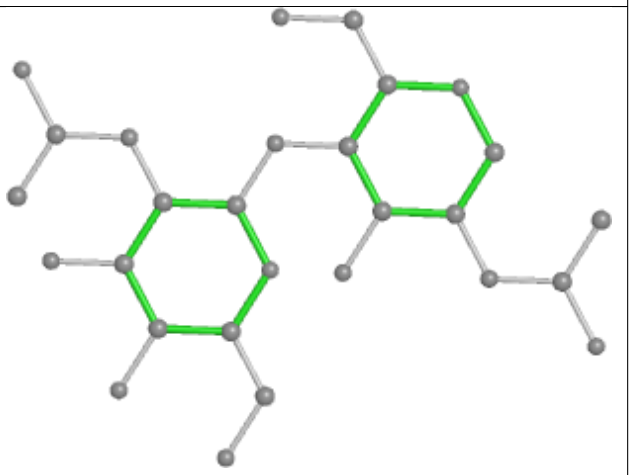
Bond lengths



Bond angles

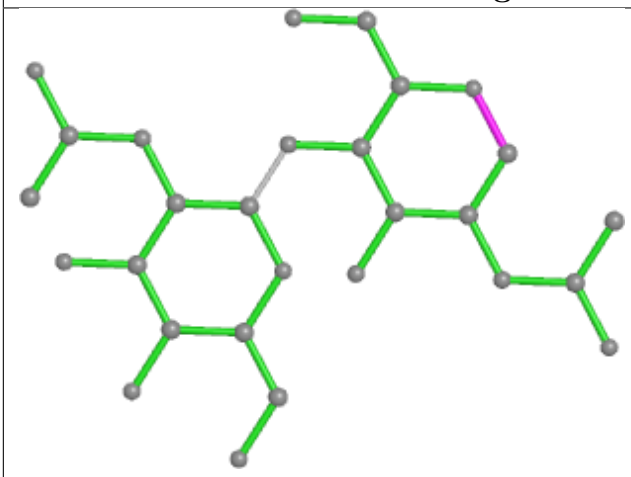


Torsions



Rings

Oligosaccharide Chain K



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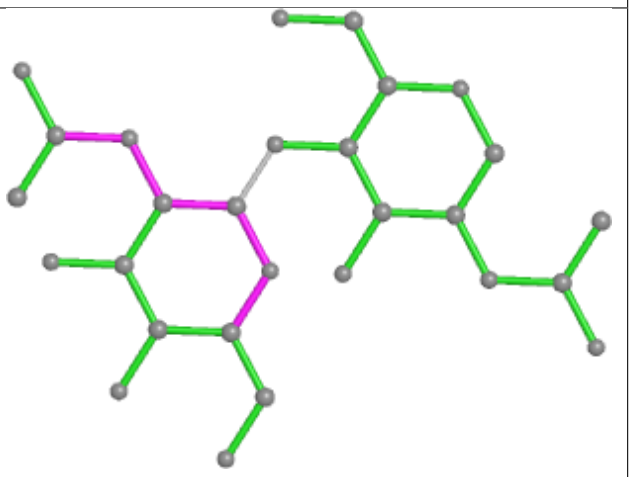
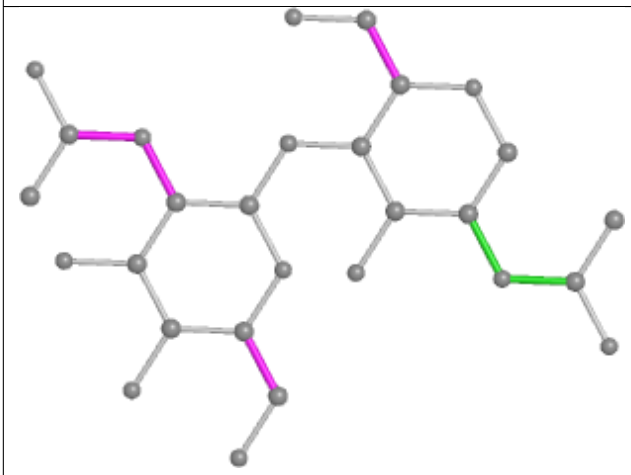


Bond angles



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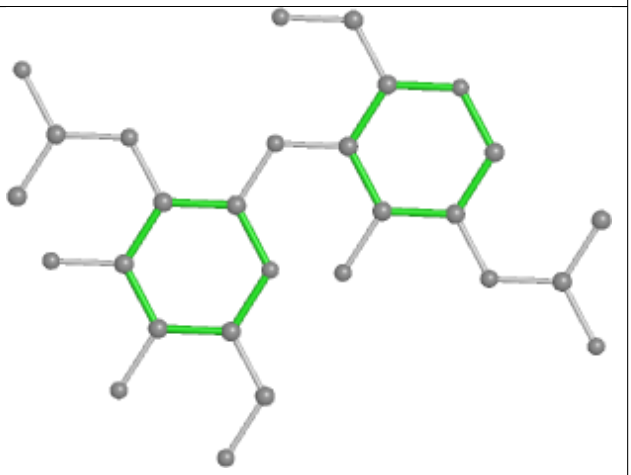
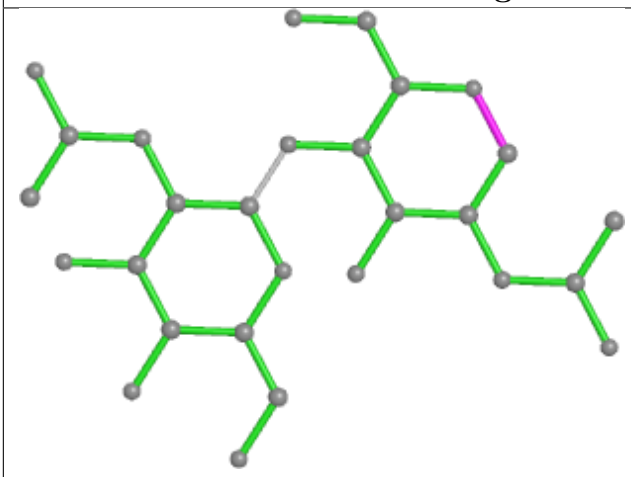


Rings

Oligosaccharide Chain O



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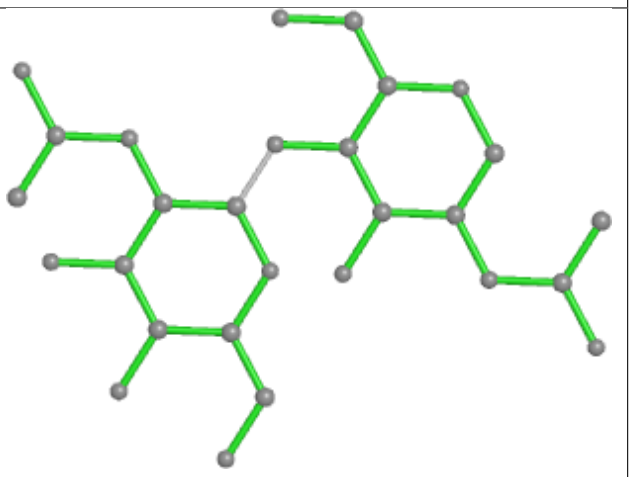

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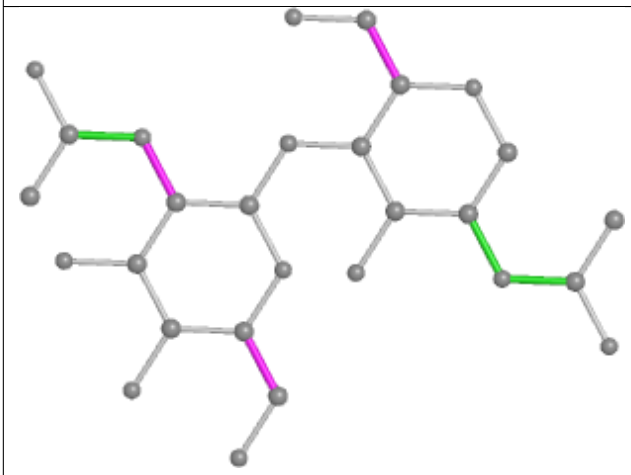

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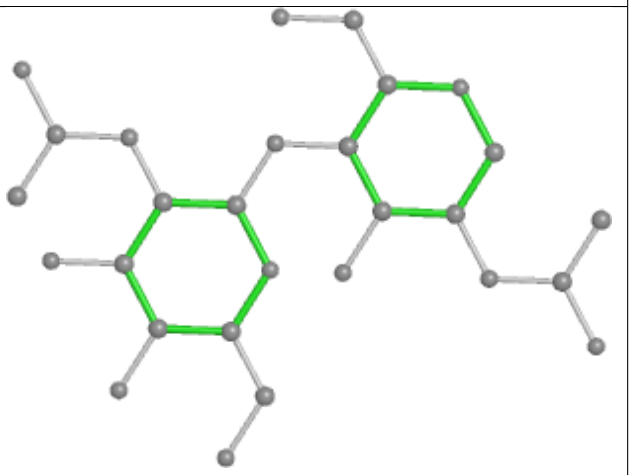
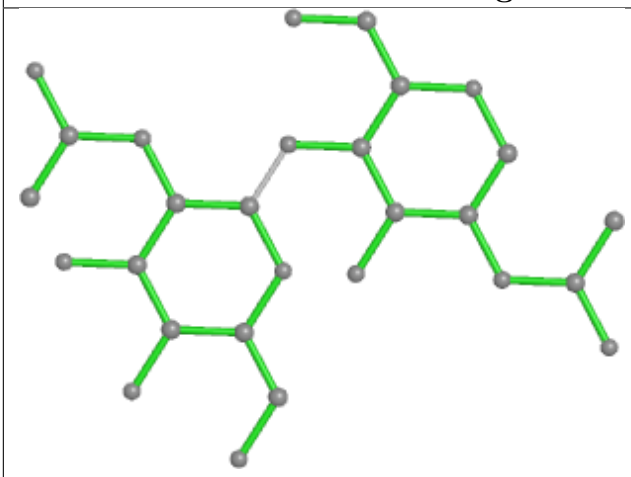


Rings

Oligosaccharide Chain P



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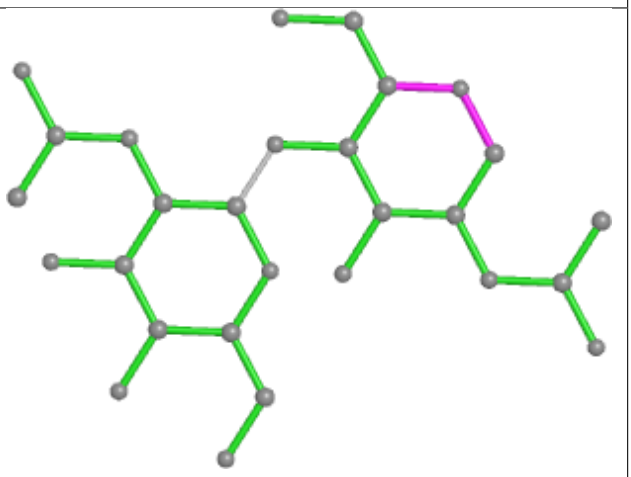

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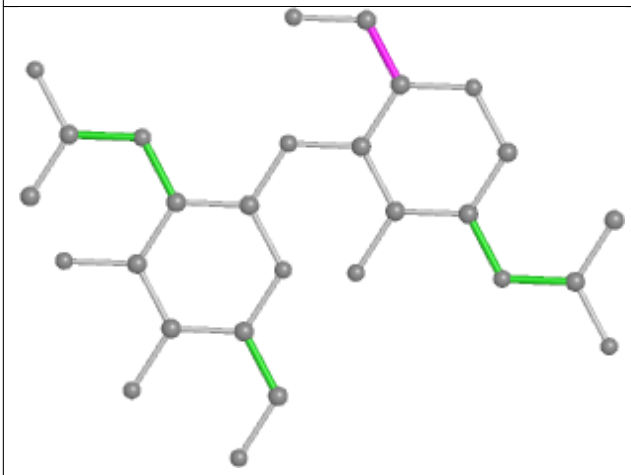

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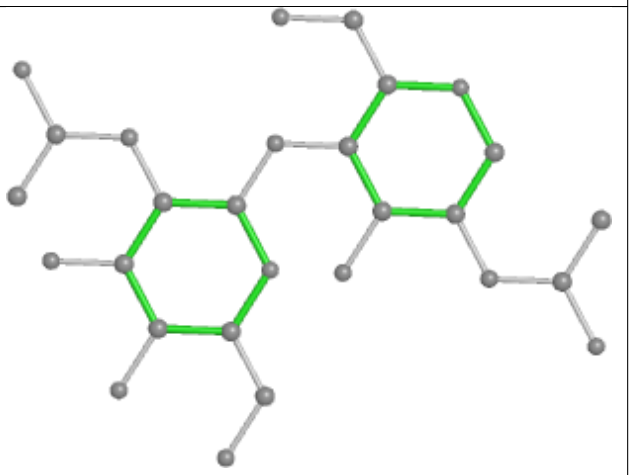
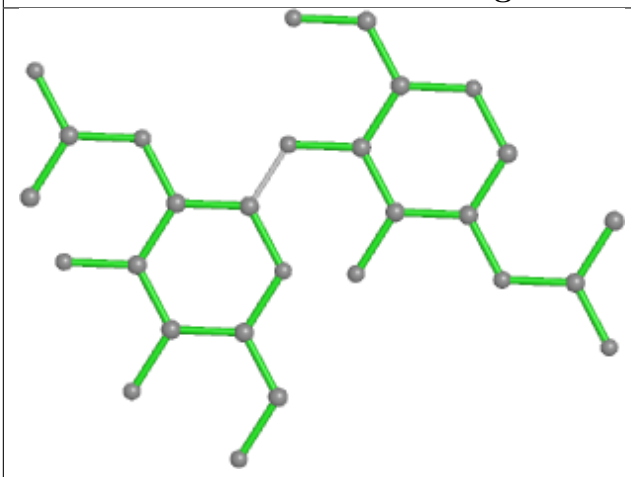


Rings

Oligosaccharide Chain Q



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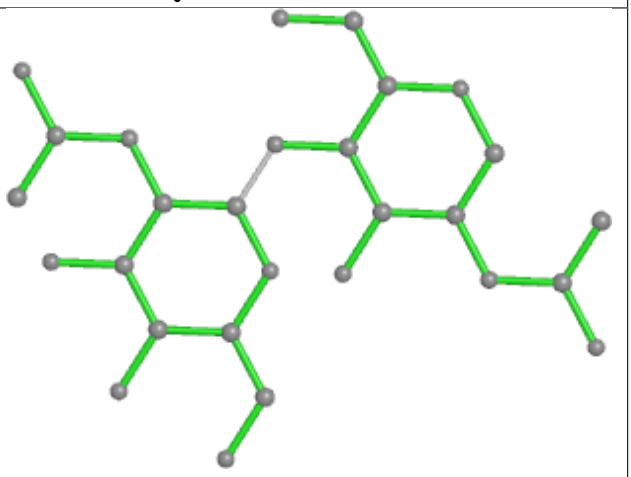

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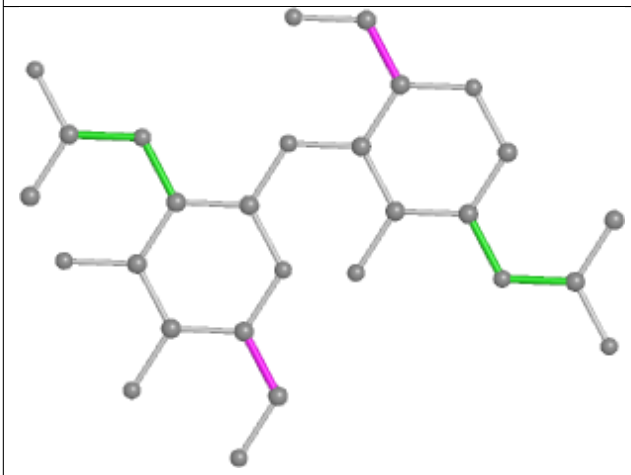

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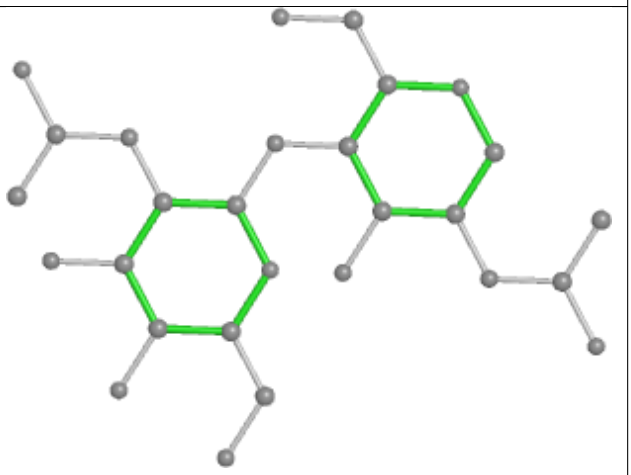
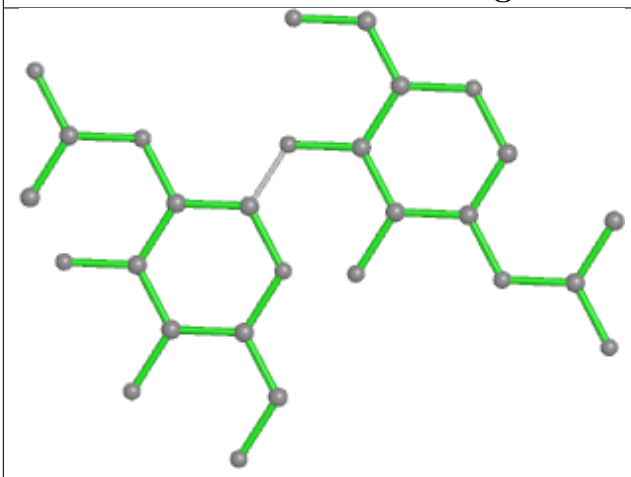


Rings

Oligosaccharide Chain R



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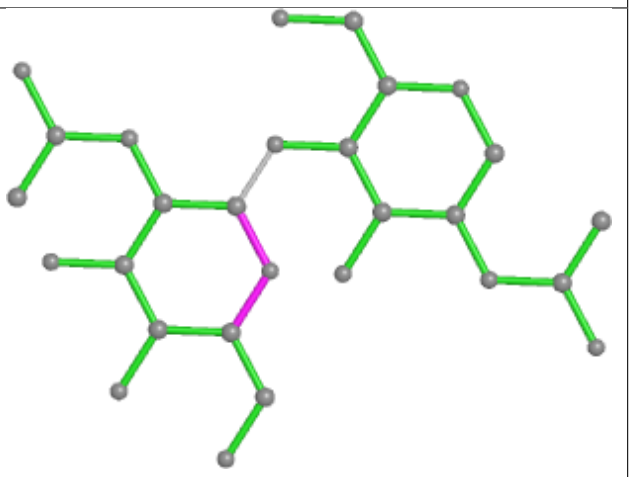
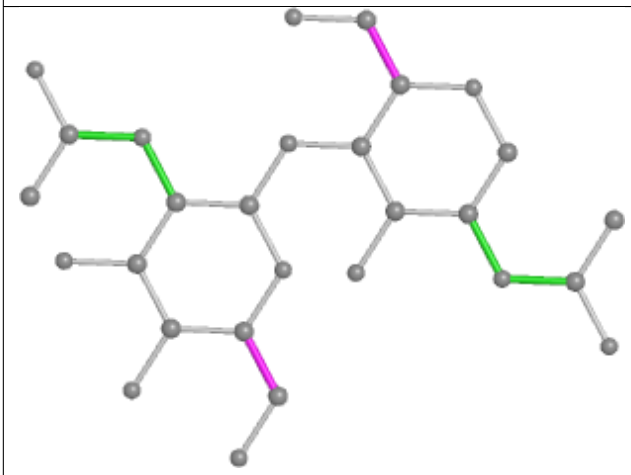


Bond angles



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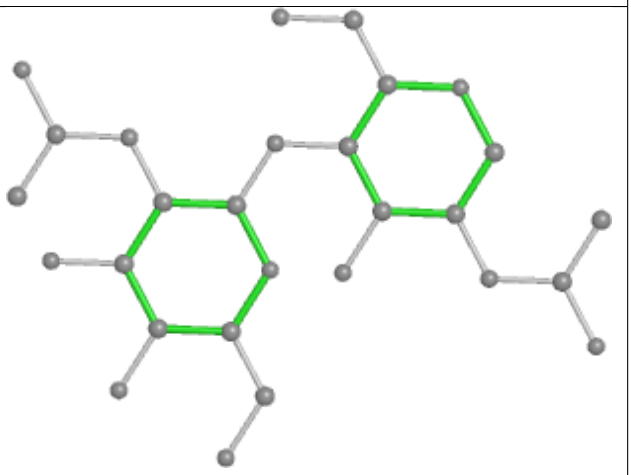
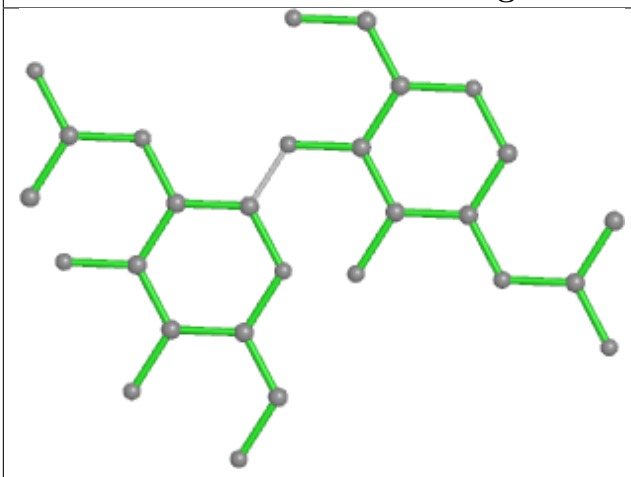


Rings

Oligosaccharide Chain S



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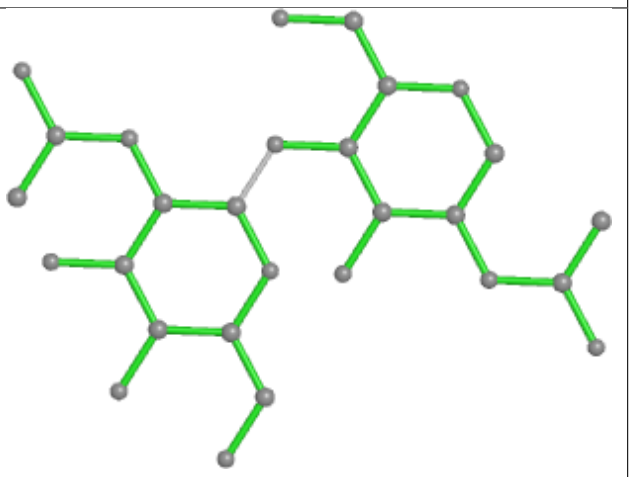
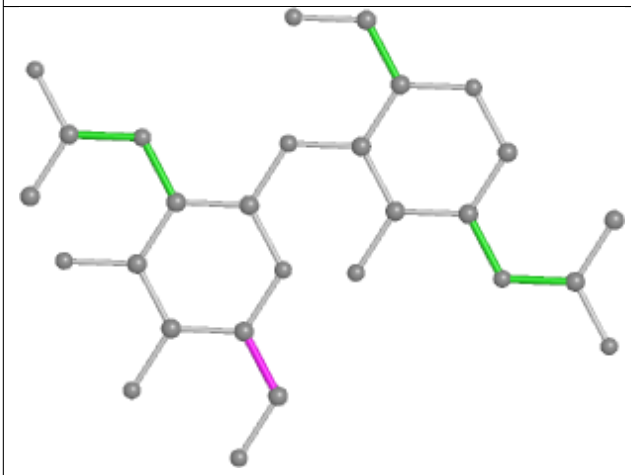


Bond angles



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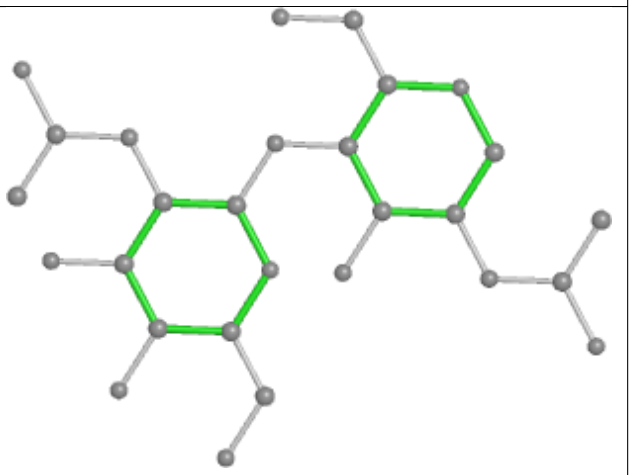
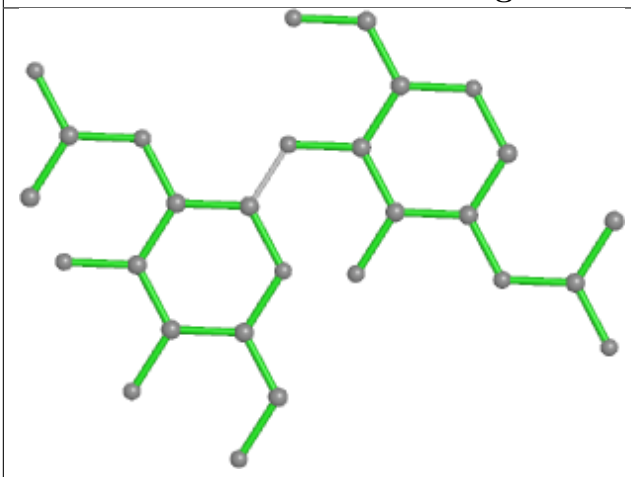


Rings

Oligosaccharide Chain T



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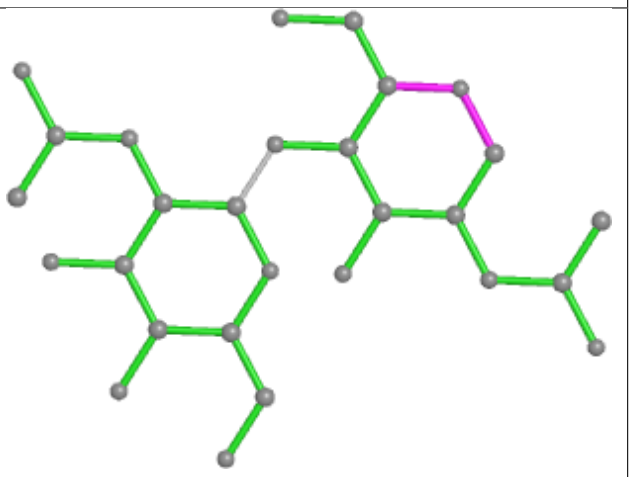
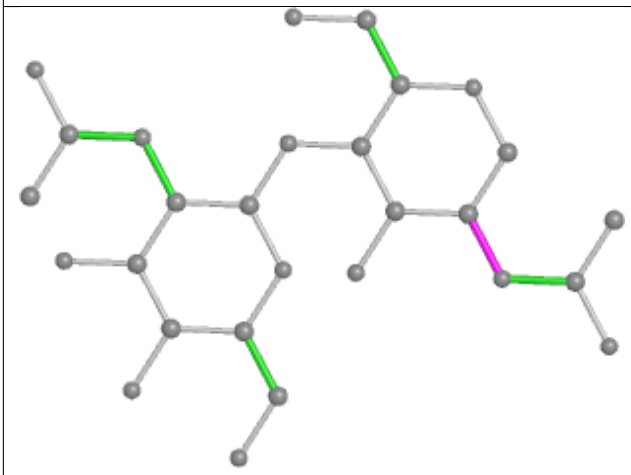


Bond angles



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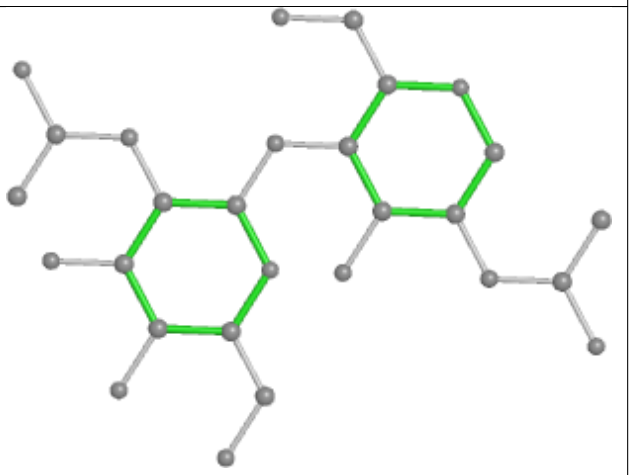
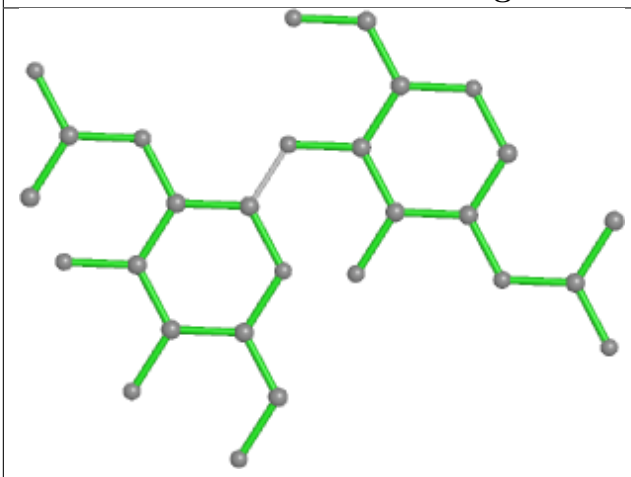


Rings

Oligosaccharide Chain U



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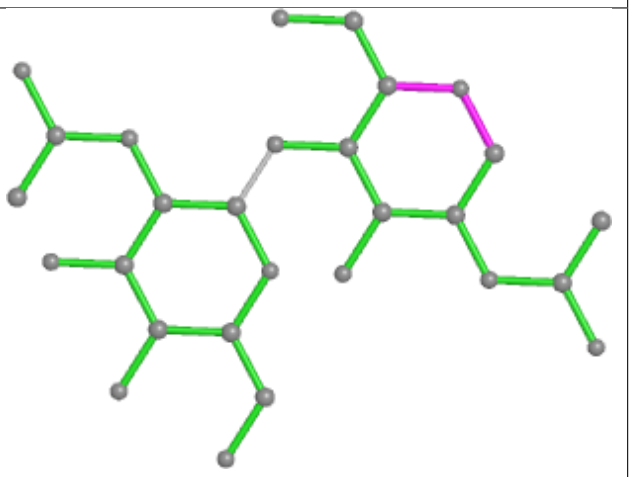
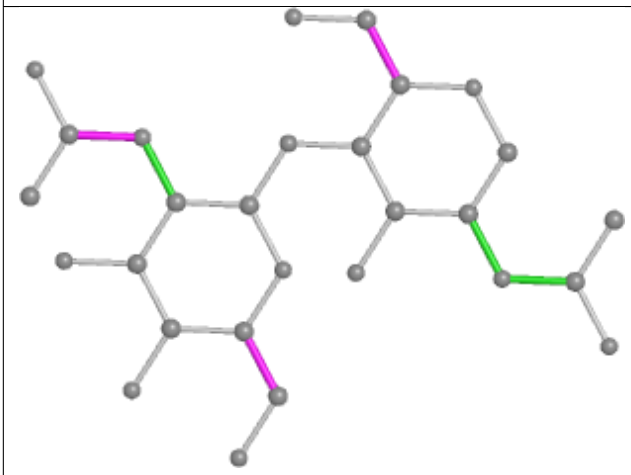


Bond angles



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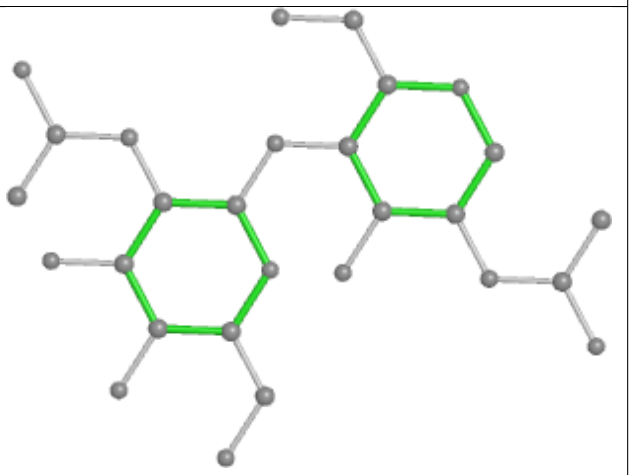
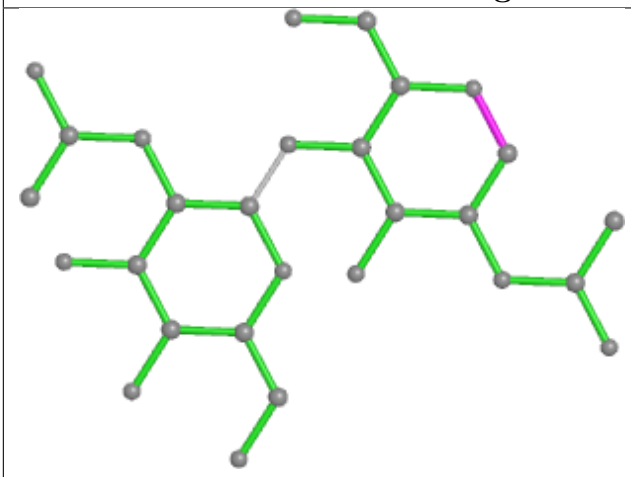


Rings

Oligosaccharide Chain V



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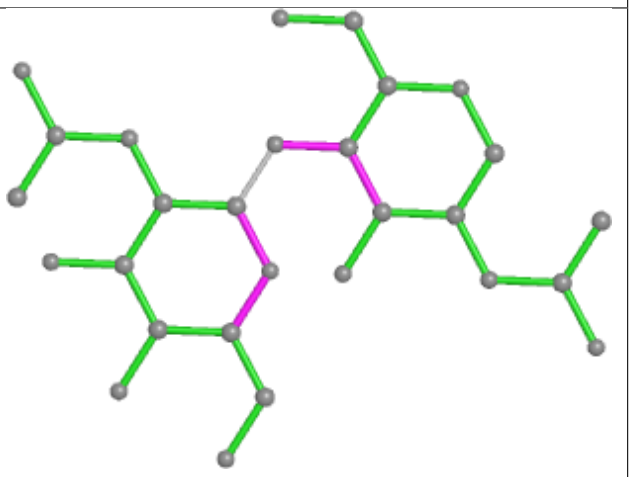
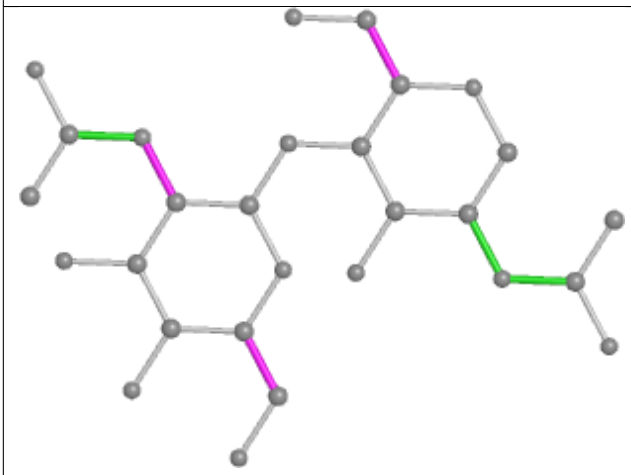
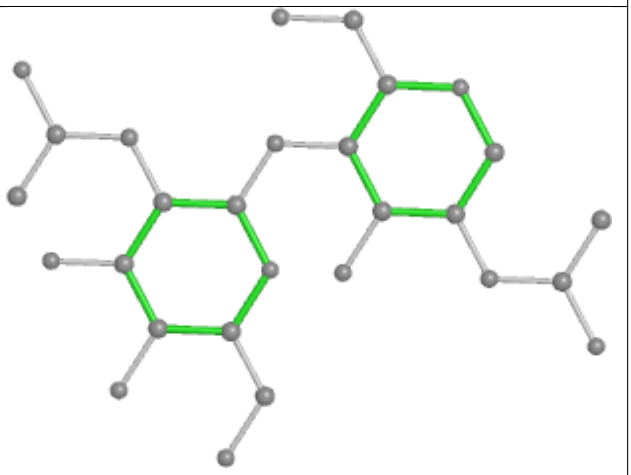


Bond angles

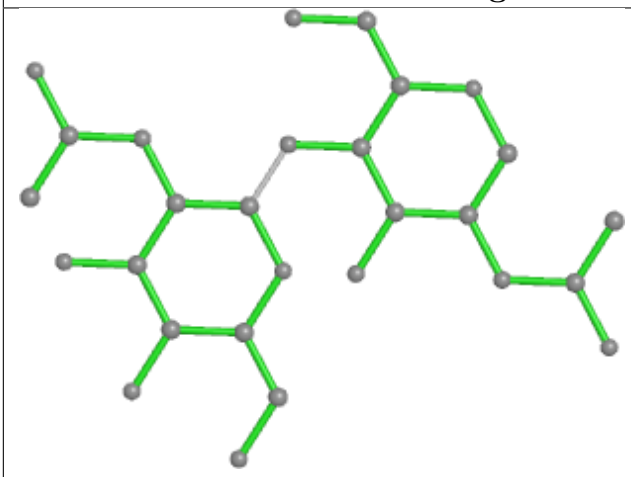


Torsions



Rings

Oligosaccharide Chain W



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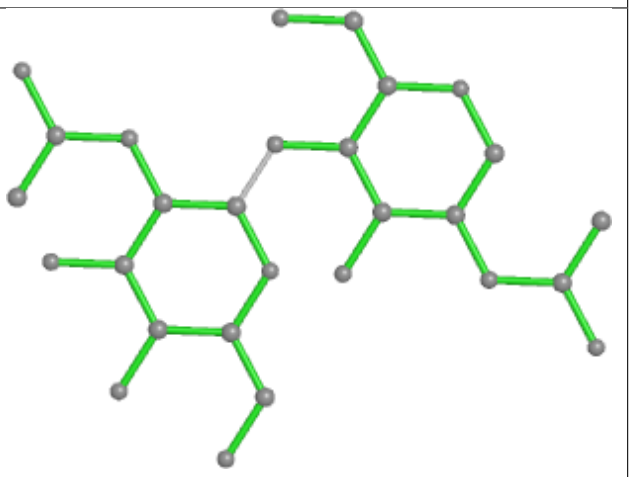
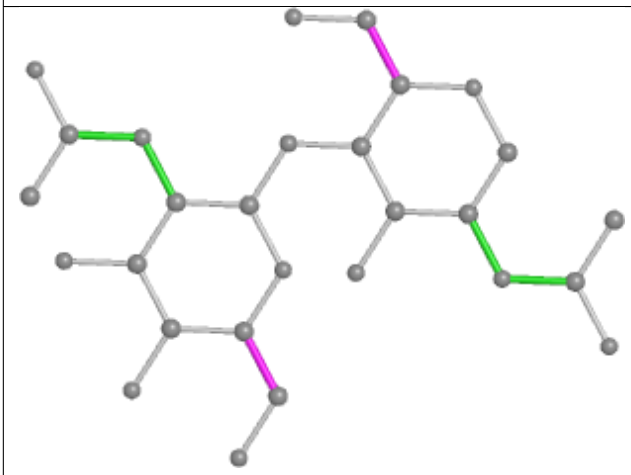


Bond angles



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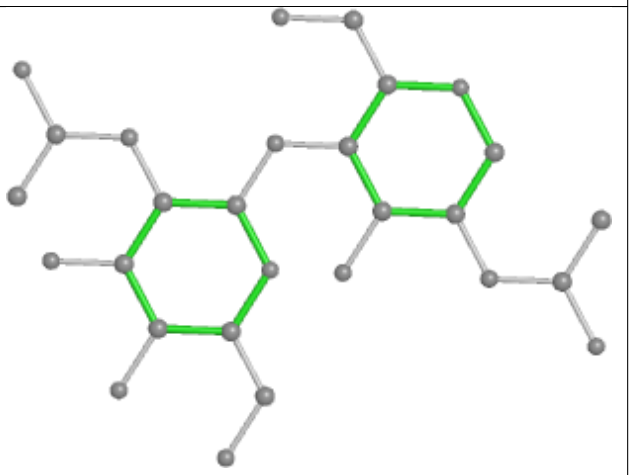
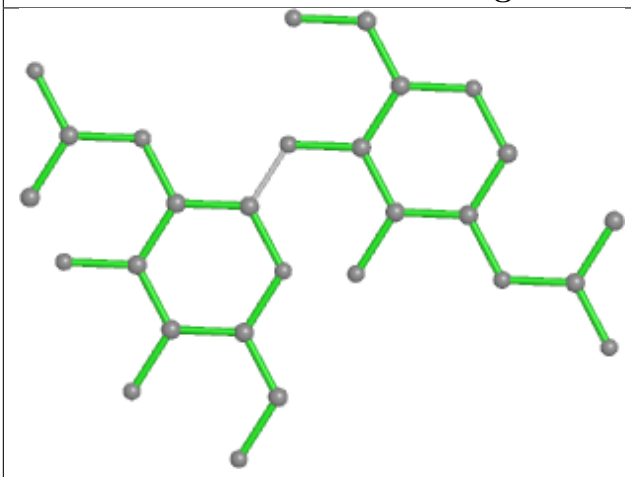


Rings

Oligosaccharide Chain X



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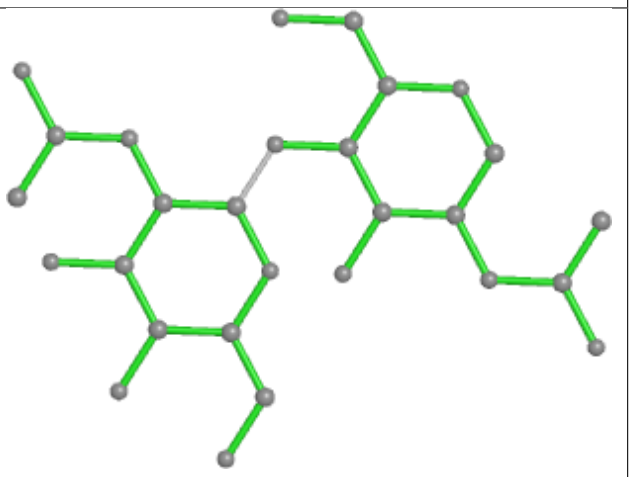
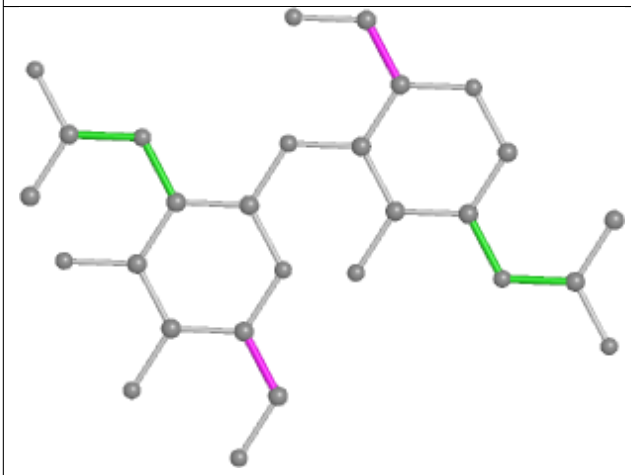


Bond angles



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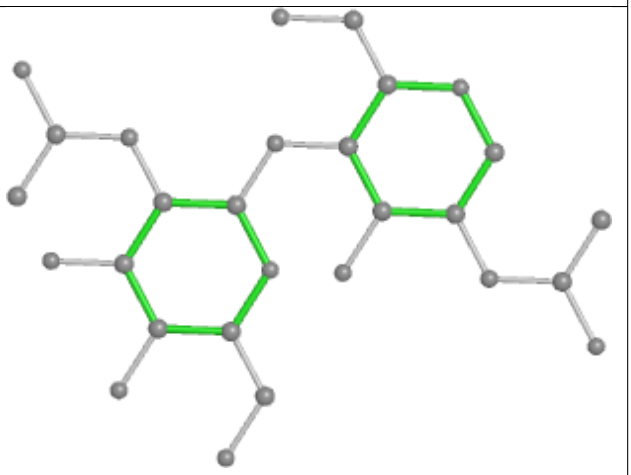
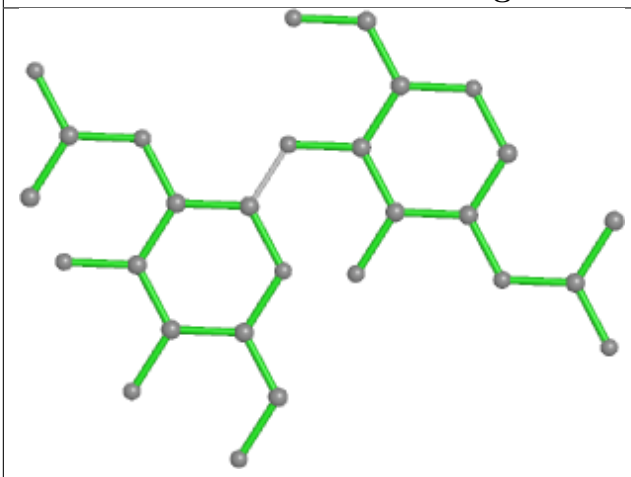


Rings

Oligosaccharide Chain Y



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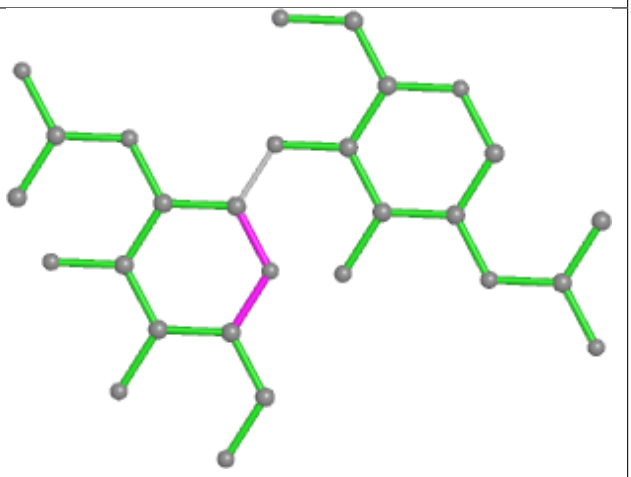
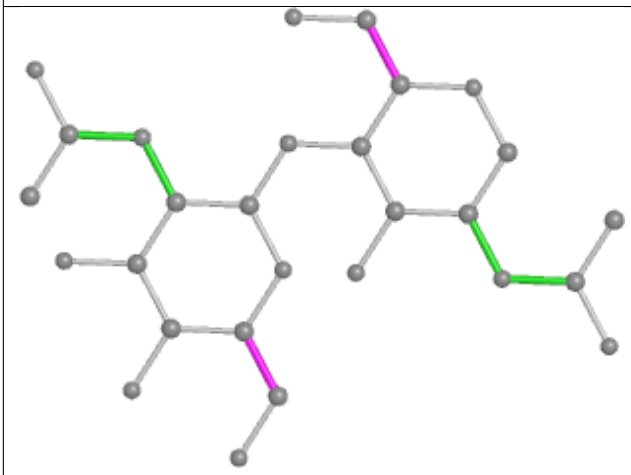


Bond angles



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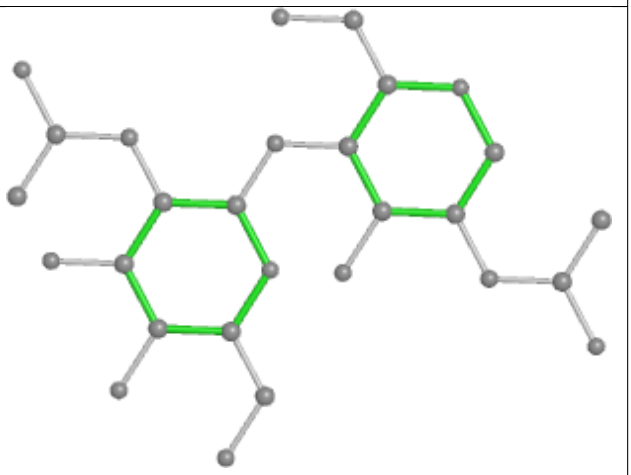
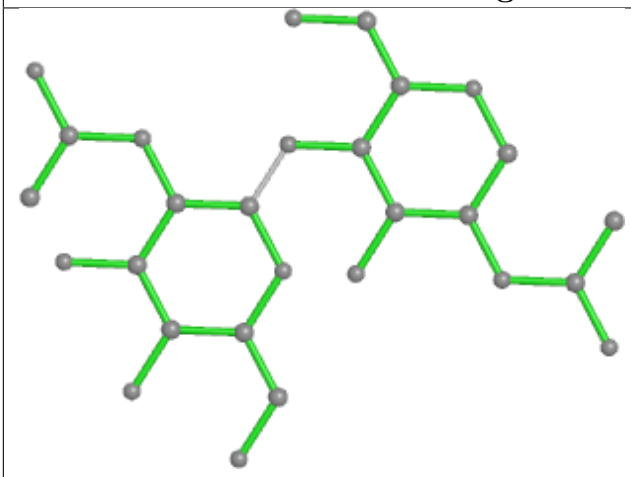


Rings

Oligosaccharide Chain Z



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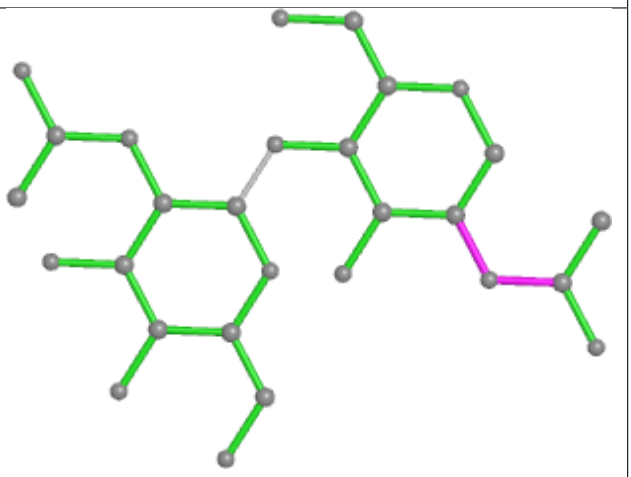
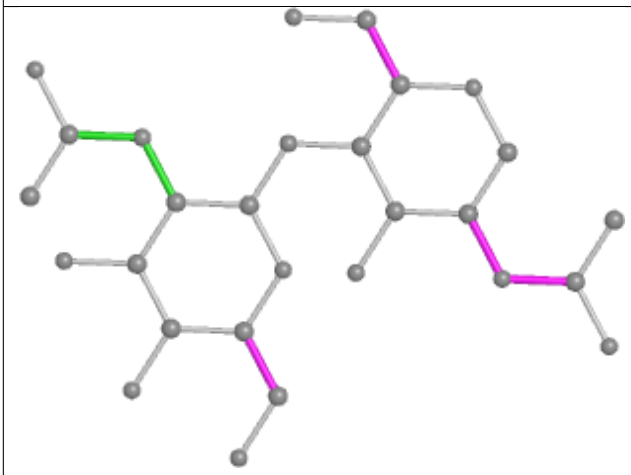


Bond angles



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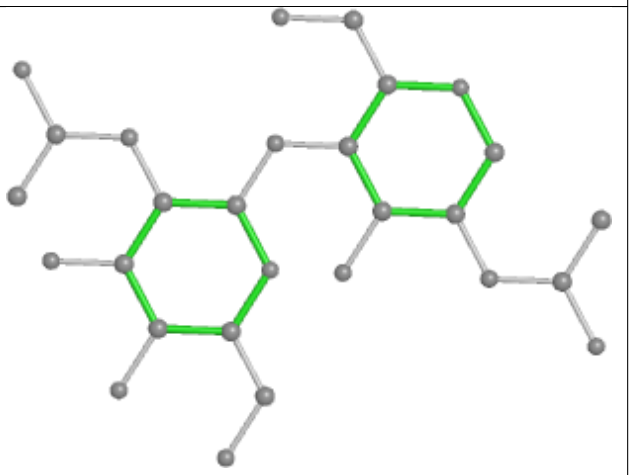
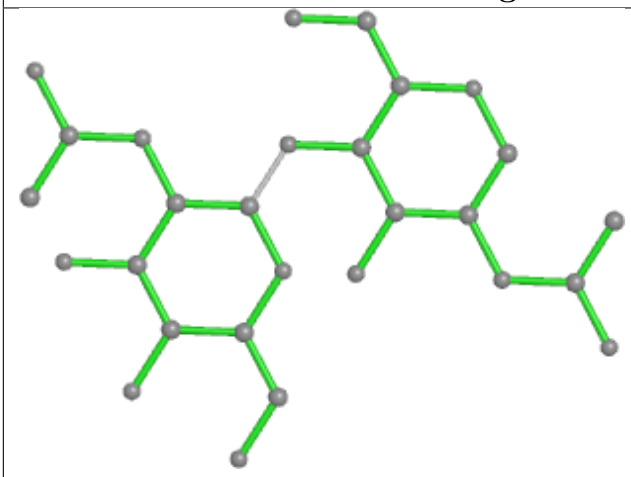


Rings

Oligosaccharide Chain a



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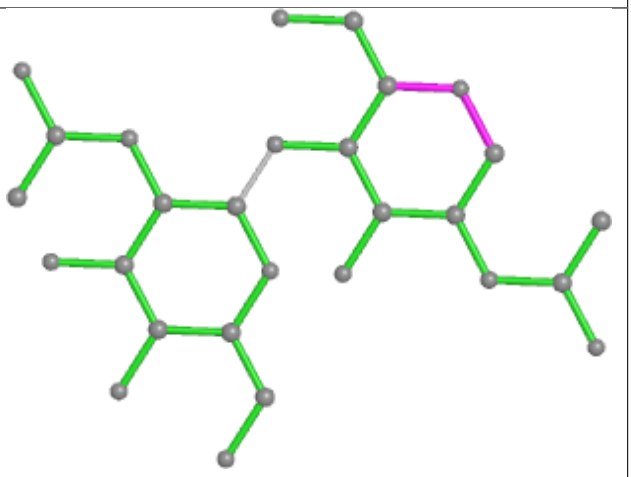
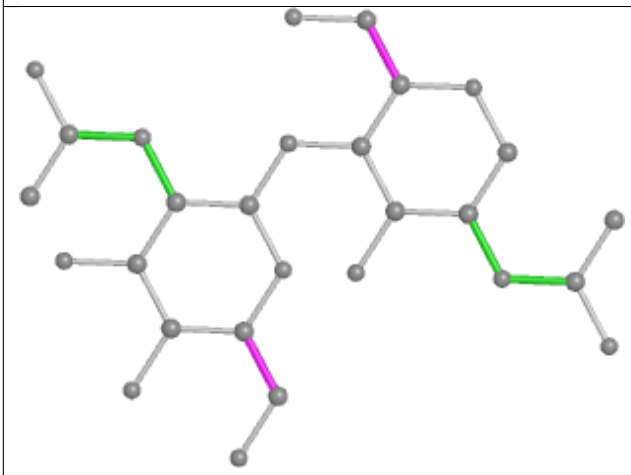
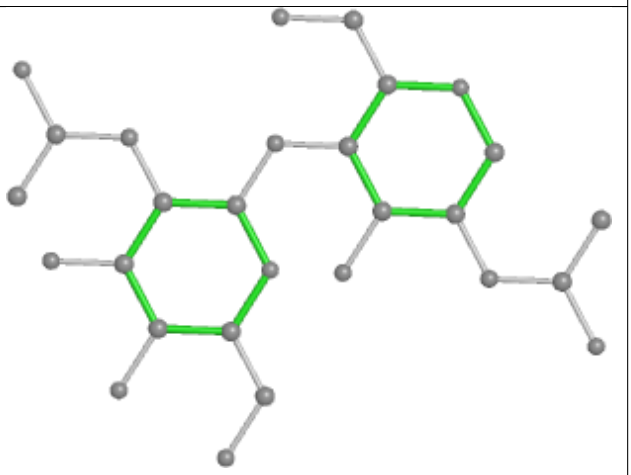


Bond angles

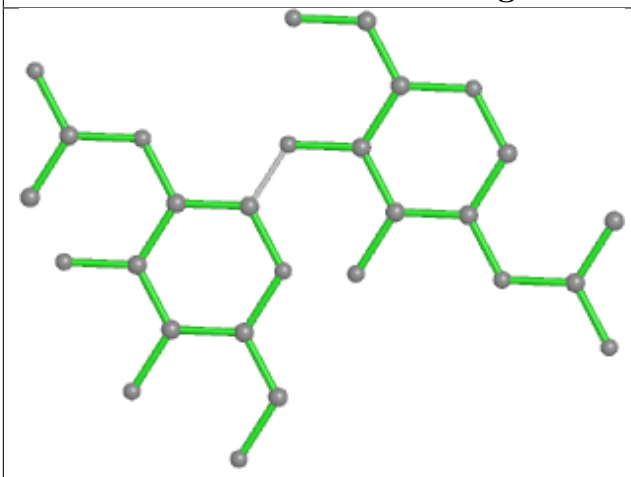


Torsions

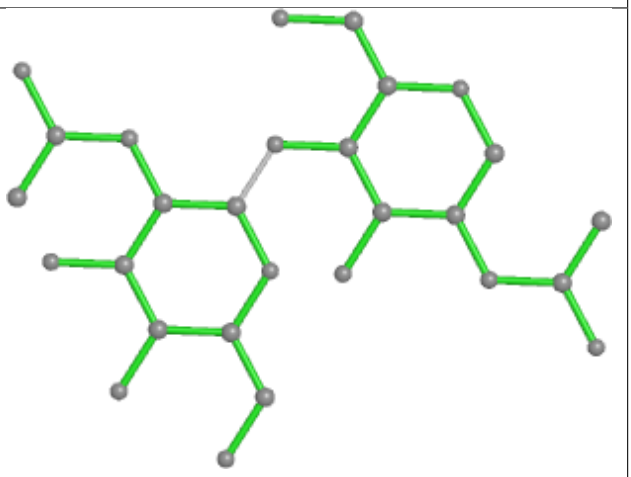


Rings

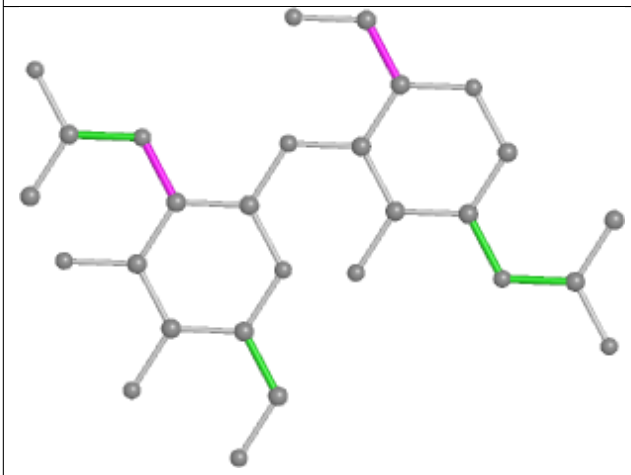
Oligosaccharide Chain b



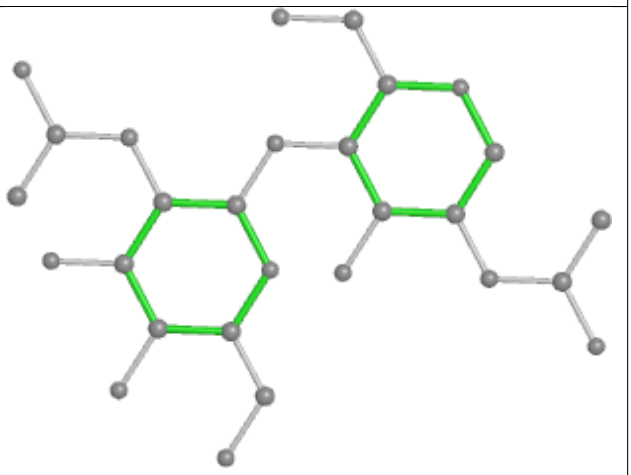
Bond lengths



Bond angles

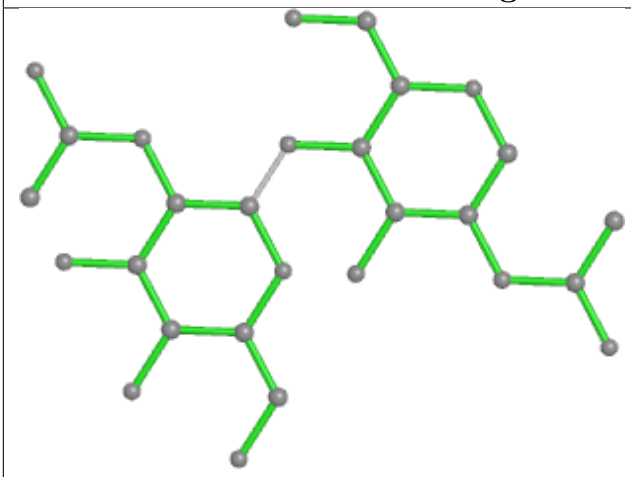


Torsions

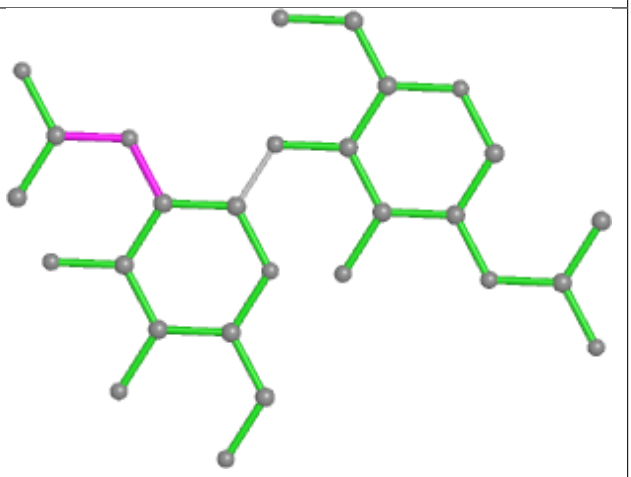


Rings

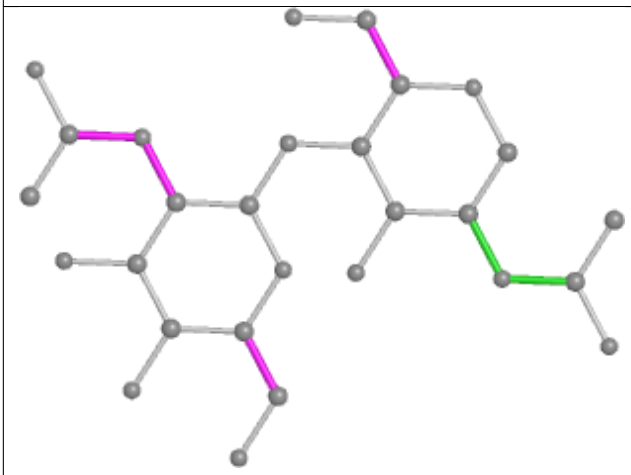
Oligosaccharide Chain c



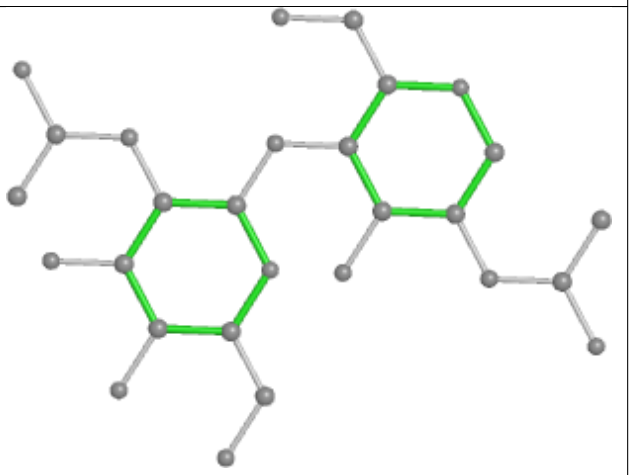
Bond lengths



Bond angles

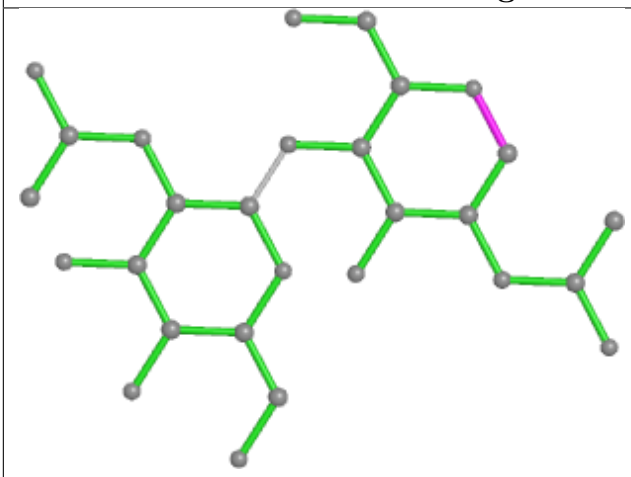


Torsions

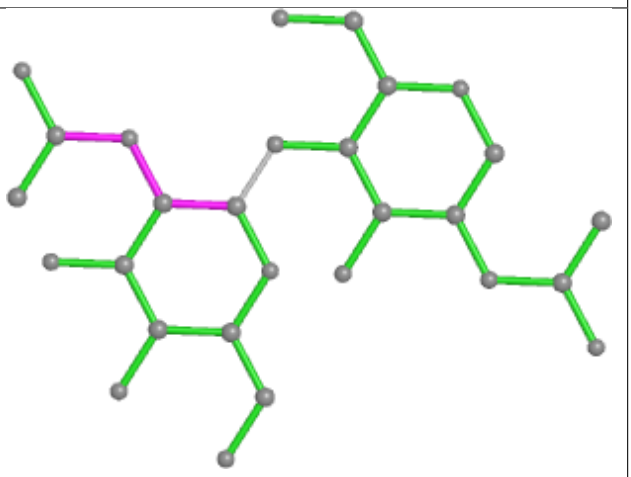


Rings

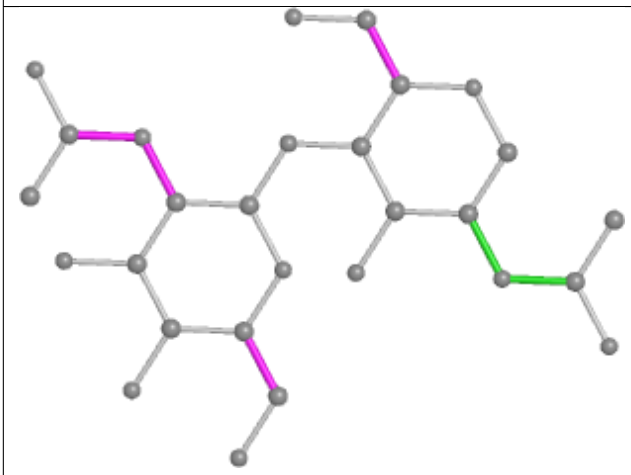
Oligosaccharide Chain d



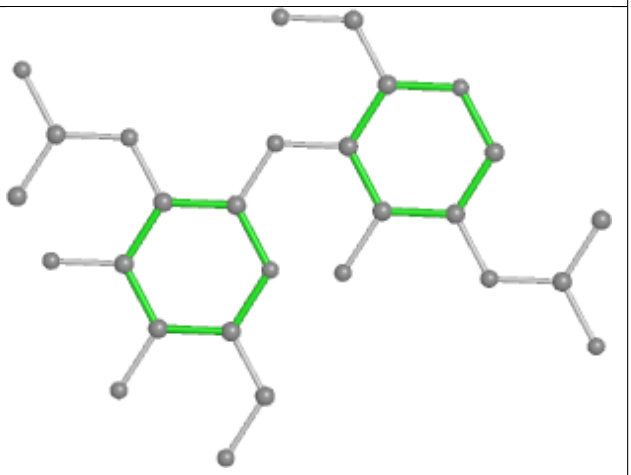
Bond lengths



Bond angles

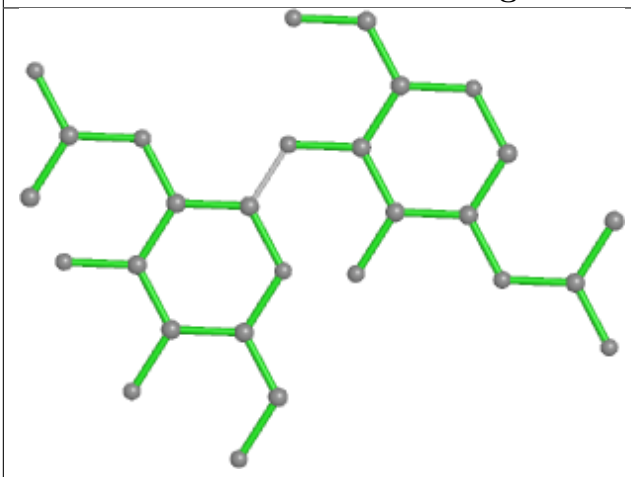


Torsions

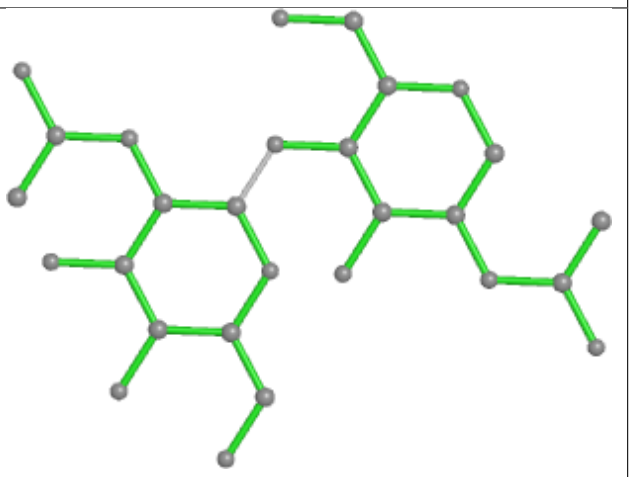


Rings

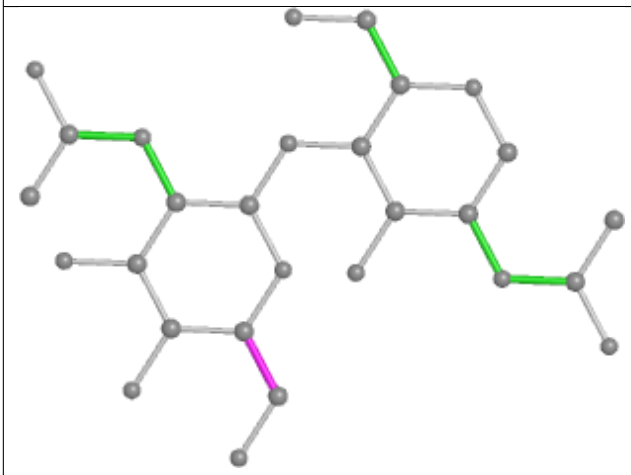
Oligosaccharide Chain e



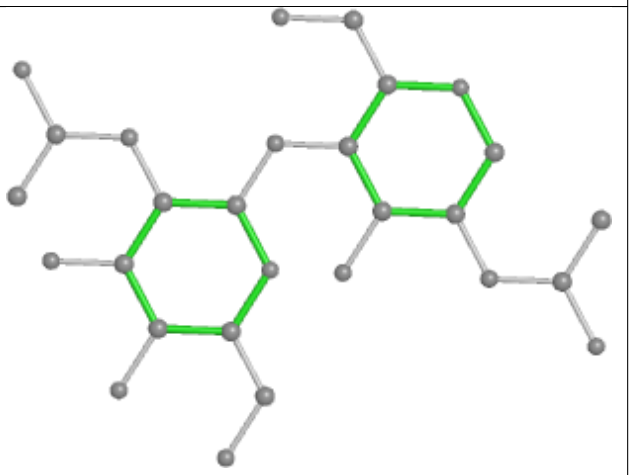
Bond lengths



Bond angles

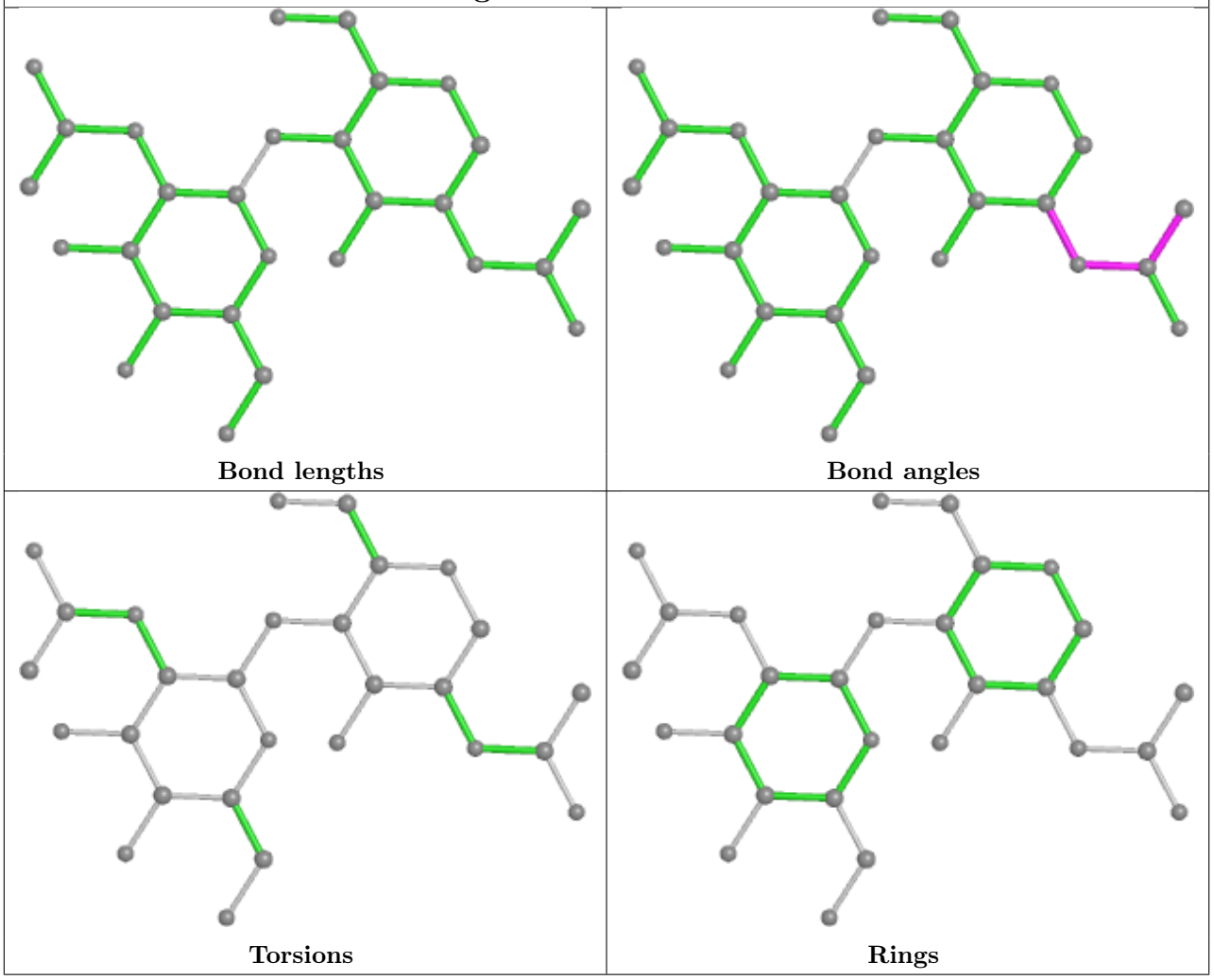


Torsions



Rings

Oligosaccharide Chain f



5.6 Ligand geometry (i)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.63	0
5	NAG	B	1403	1	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	B	1405	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	1405	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
5	NAG	C	1407	1	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	C	1401	1	14,14,15	0.31	0	17,19,21	0.33	0
5	NAG	A	1409	1	14,14,15	0.52	0	17,19,21	0.36	0
5	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.38	0
5	NAG	C	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
5	NAG	B	1402	1	14,14,15	0.20	0	17,19,21	0.64	0
5	NAG	B	1404	1	14,14,15	0.48	0	17,19,21	0.53	0
5	NAG	C	1403	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.38	0
5	NAG	B	1401	1	14,14,15	0.30	0	17,19,21	0.33	0
5	NAG	A	1401	1	14,14,15	0.31	0	17,19,21	0.33	0
5	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.63	0
5	NAG	C	1405	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
5	NAG	A	1404	1	14,14,15	0.46	0	17,19,21	0.54	0
5	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	C	1404	1	14,14,15	0.47	0	17,19,21	0.53	0
5	NAG	C	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	A	1403	1	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	A	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	B	1406	1	14,14,15	0.30	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1405	NAG	C2-N2-C7	4.34	129.08	122.90
5	C	1405	NAG	C2-N2-C7	4.33	129.07	122.90
5	A	1405	NAG	C2-N2-C7	4.33	129.07	122.90

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1406	NAG	O5-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	C	1406	NAG	O5-C5-C6-O6
5	A	1401	NAG	O5-C5-C6-O6
5	B	1401	NAG	O5-C5-C6-O6
5	C	1401	NAG	O5-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	A	1404	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1402	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	C	1405	NAG	O5-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
5	A	1409	NAG	C4-C5-C6-O6
5	A	1408	NAG	O5-C5-C6-O6
5	B	1408	NAG	O5-C5-C6-O6
5	C	1408	NAG	O5-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	C	1405	NAG	C4-C5-C6-O6
5	A	1405	NAG	C8-C7-N2-C2
5	A	1405	NAG	O7-C7-N2-C2
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	C	1405	NAG	C8-C7-N2-C2
5	C	1405	NAG	O7-C7-N2-C2
5	A	1409	NAG	O5-C5-C6-O6
5	A	1406	NAG	C4-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	C	1406	NAG	C4-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	C	1404	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6
5	B	1408	NAG	C4-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6
5	A	1401	NAG	C4-C5-C6-O6
5	B	1401	NAG	C4-C5-C6-O6
5	C	1401	NAG	C4-C5-C6-O6
5	A	1407	NAG	C1-C2-N2-C7
5	B	1407	NAG	C1-C2-N2-C7
5	C	1407	NAG	C1-C2-N2-C7

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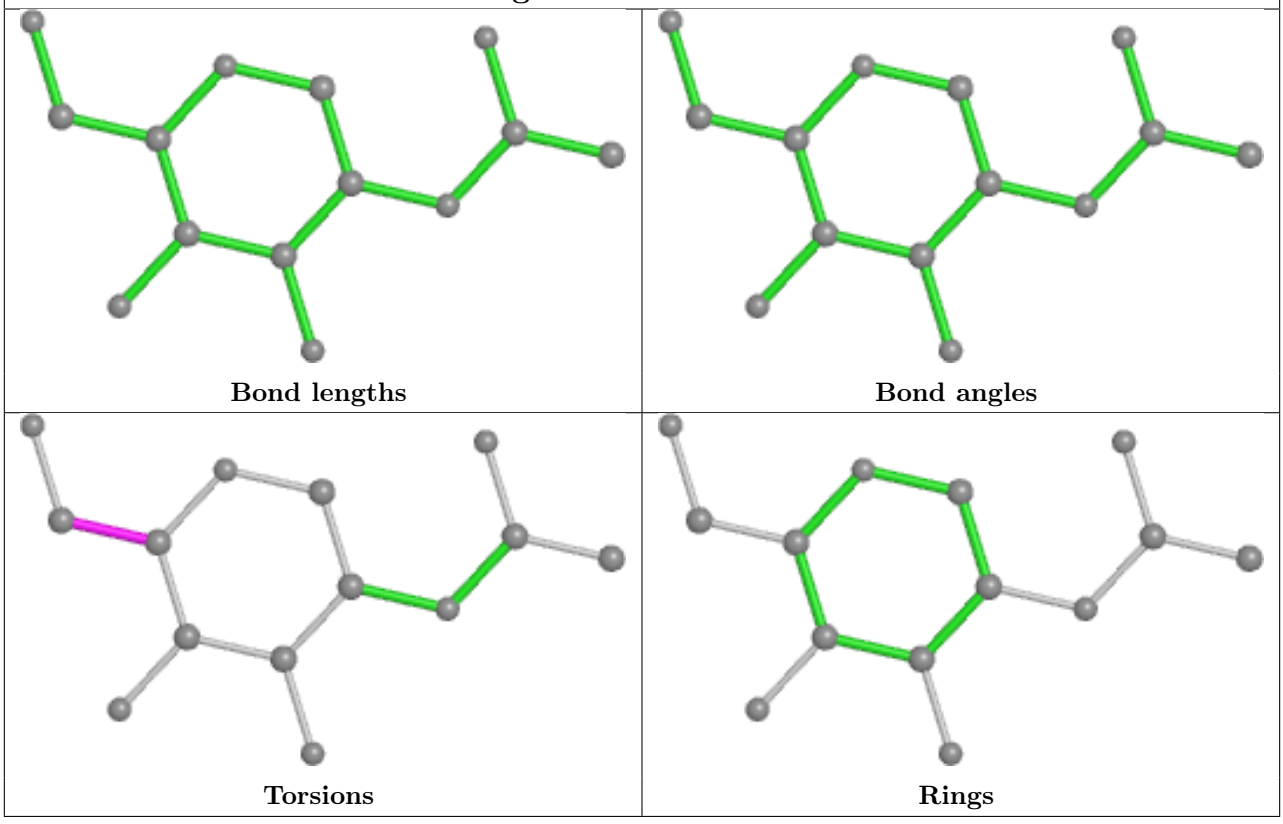
Mol	Chain	Res	Type	Atoms
5	A	1405	NAG	C3-C2-N2-C7
5	B	1405	NAG	C3-C2-N2-C7
5	C	1405	NAG	C3-C2-N2-C7

There are no ring outliers.

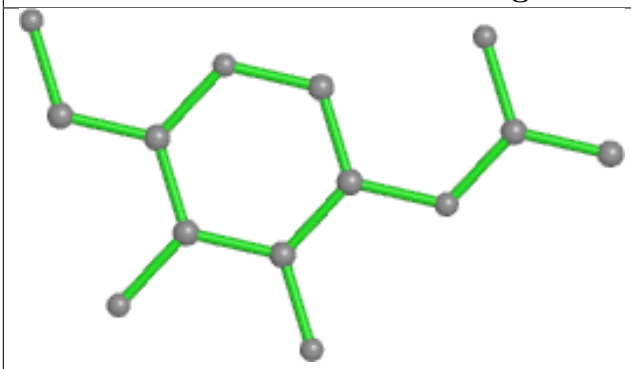
No monomer is involved in short contacts.

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.

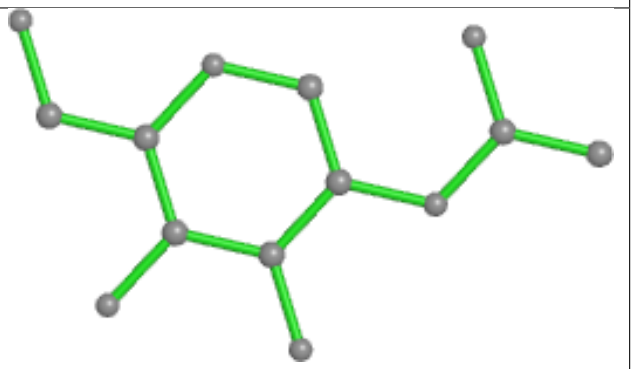
Ligand NAG C 1402



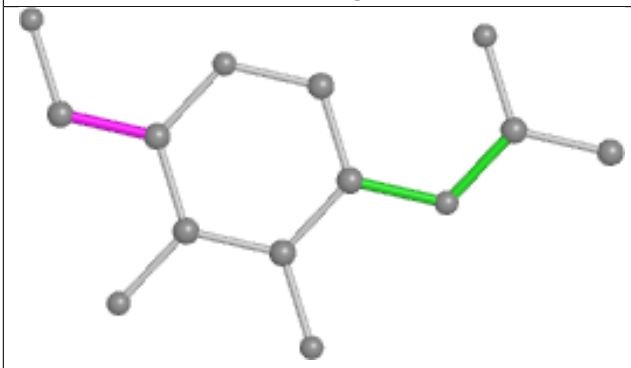
Ligand NAG B 1403



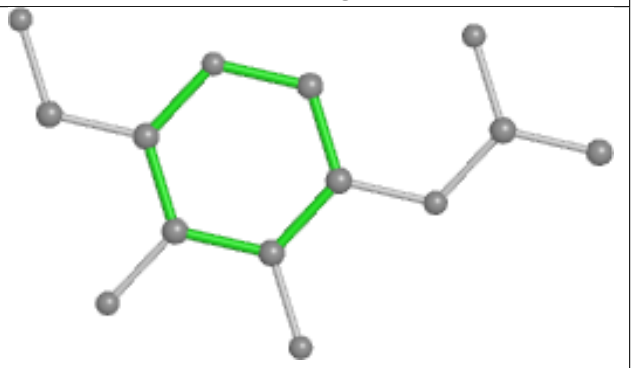
Bond lengths



Bond angles

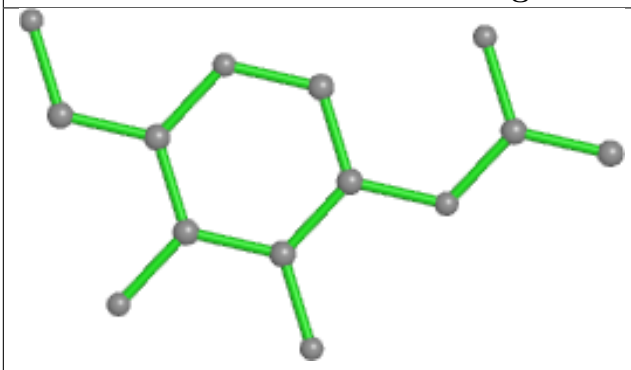


Torsions

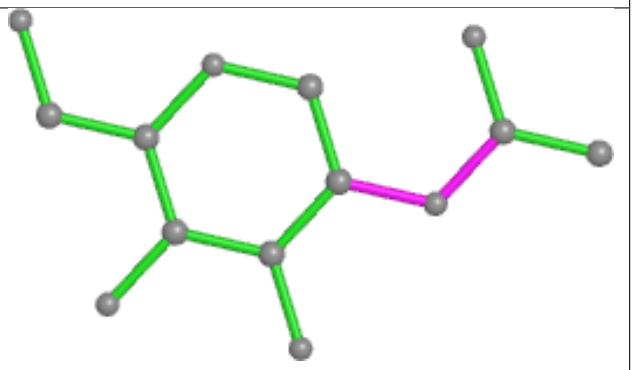


Rings

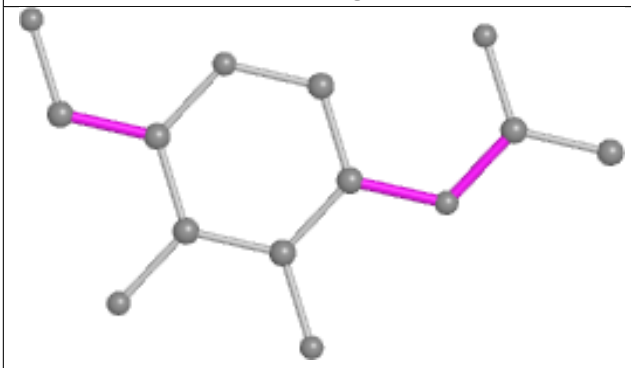
Ligand NAG B 1405



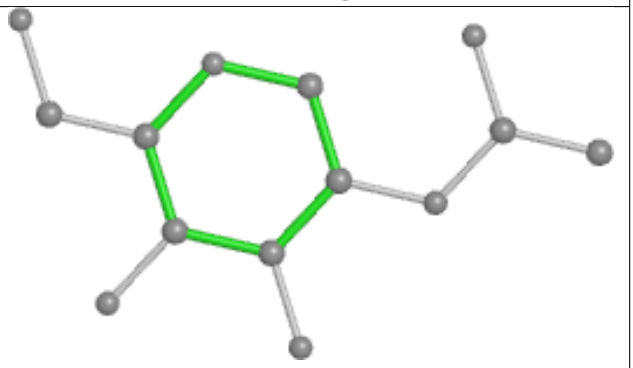
Bond lengths



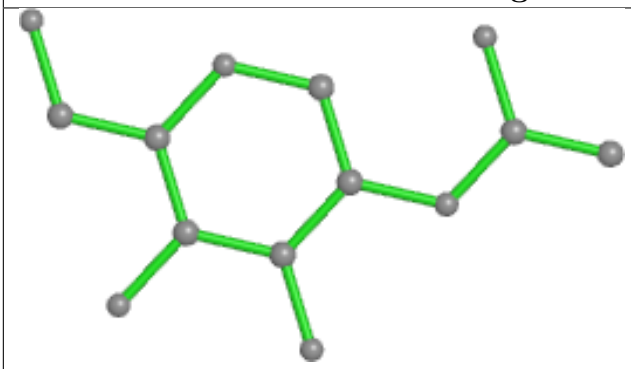
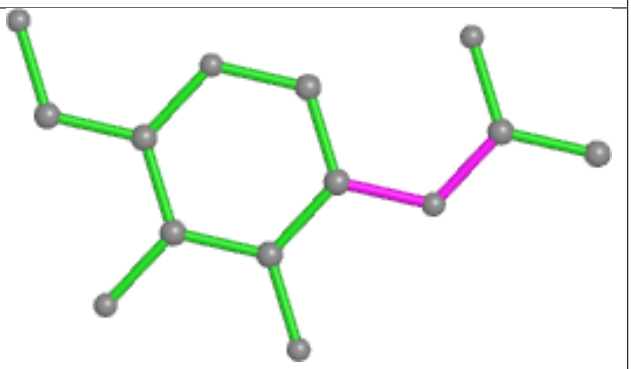
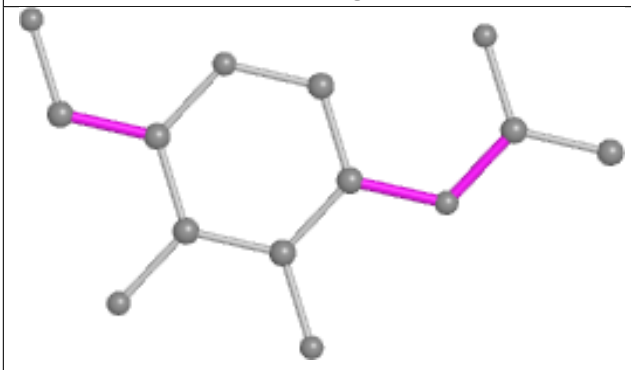
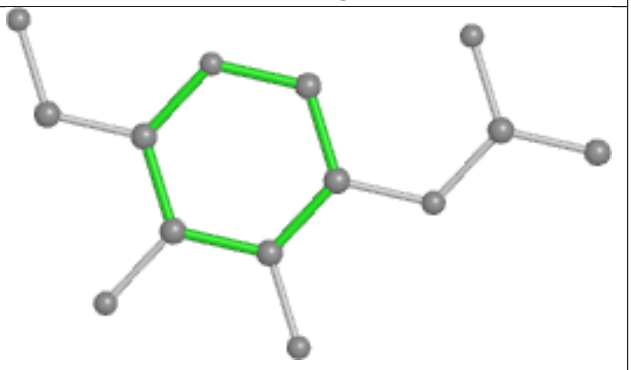
Bond angles



Torsions



Rings

Ligand NAG A 1405	
 Bond lengths	 Bond angles
 Torsions	 Rings

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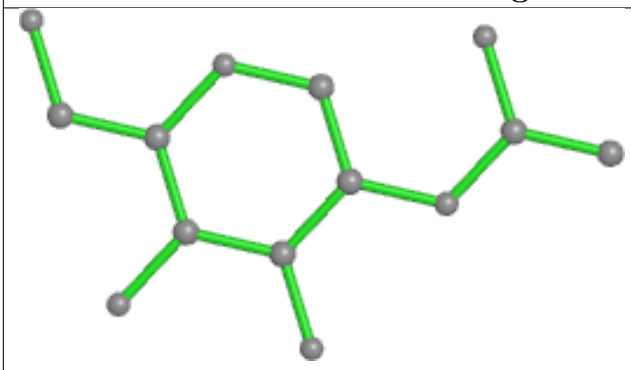
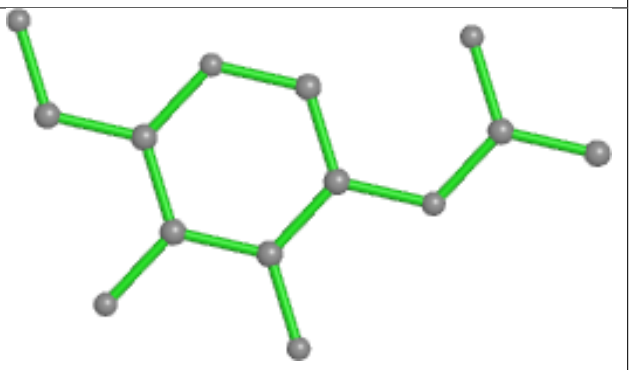
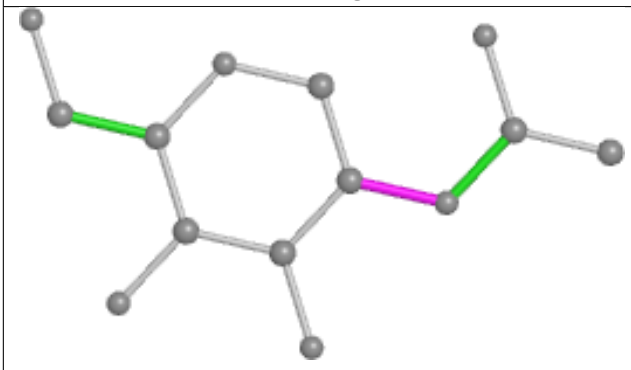
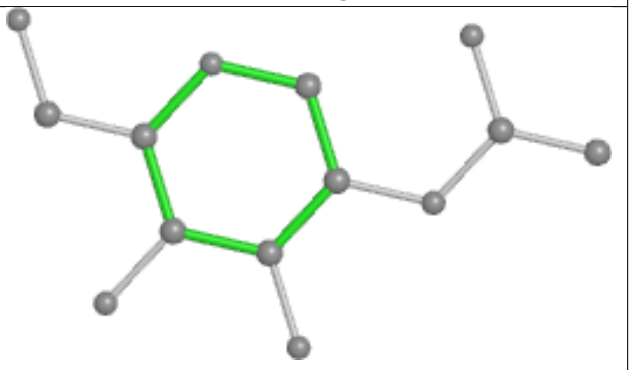
 Bond lengths	 Bond angles
 Torsions	 Rings

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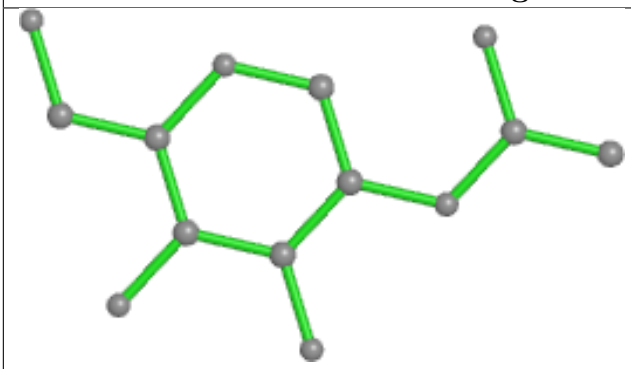
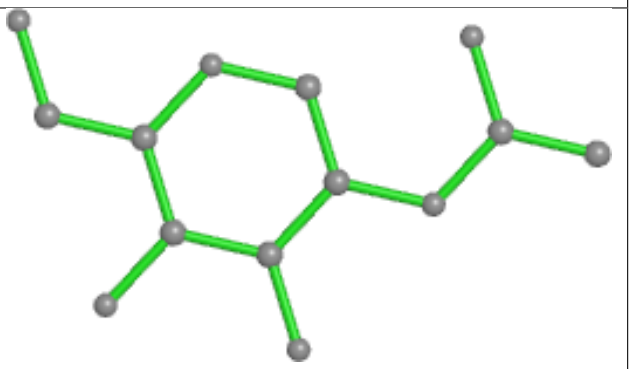
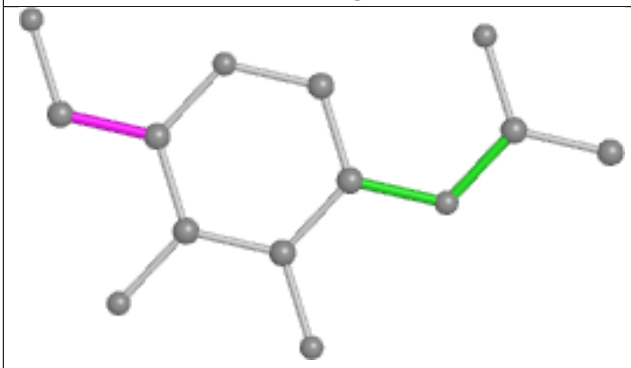
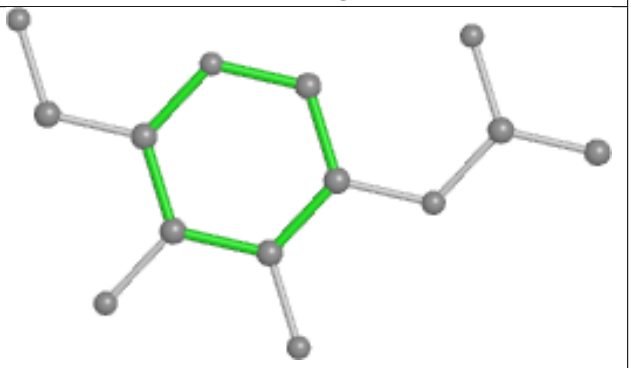
 Bond lengths	 Bond angles
 Torsions	 Rings

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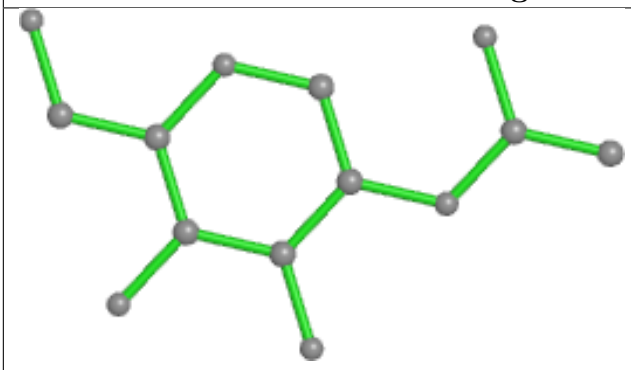
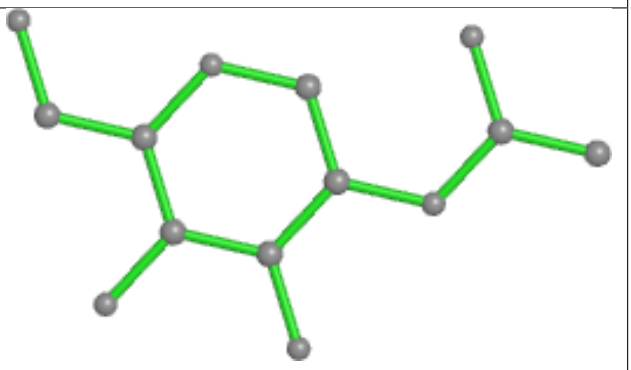
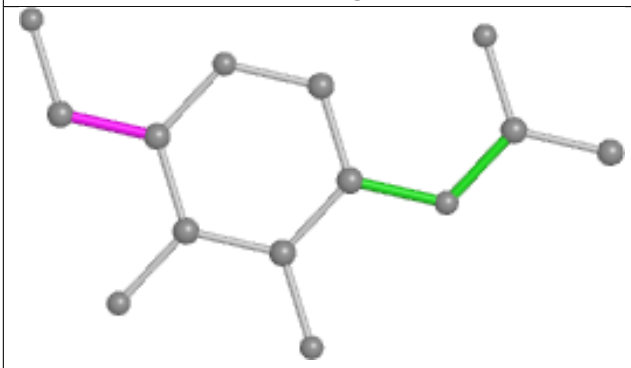
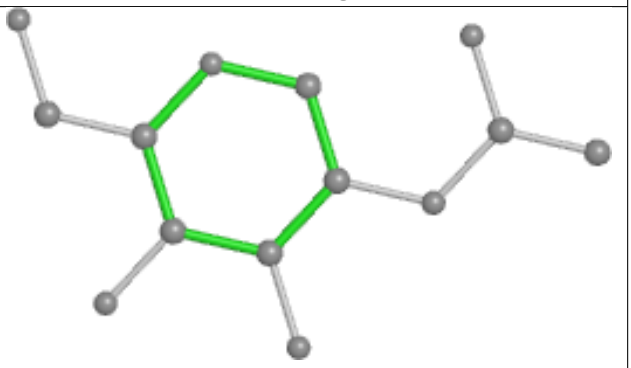
 Bond lengths	 Bond angles
 Torsions	 Rings

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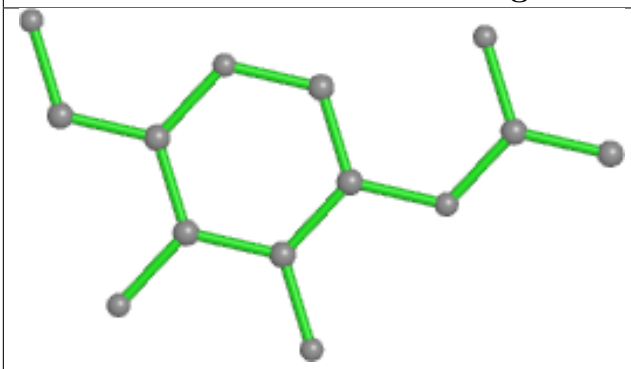
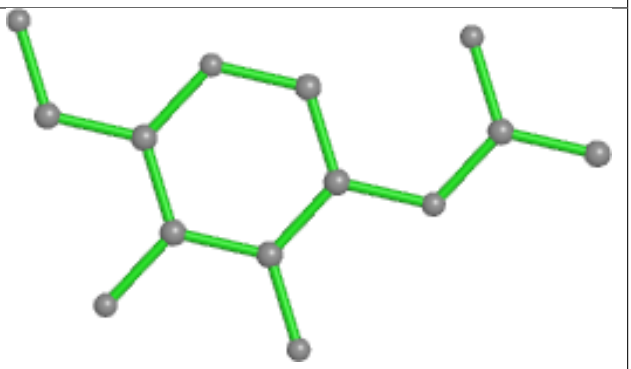
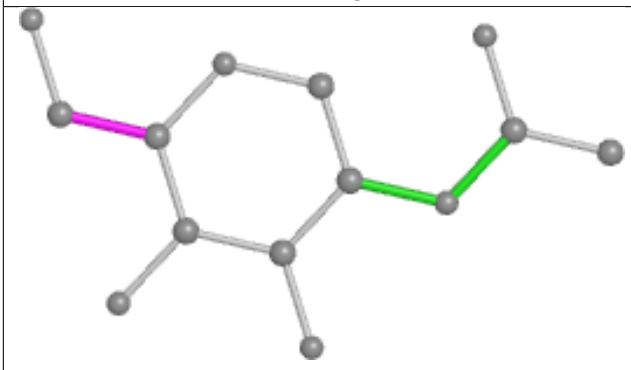
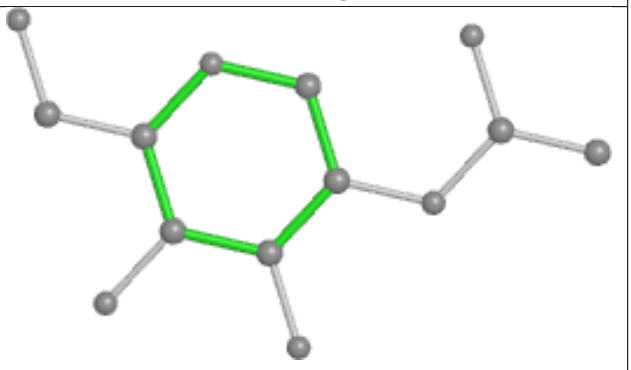
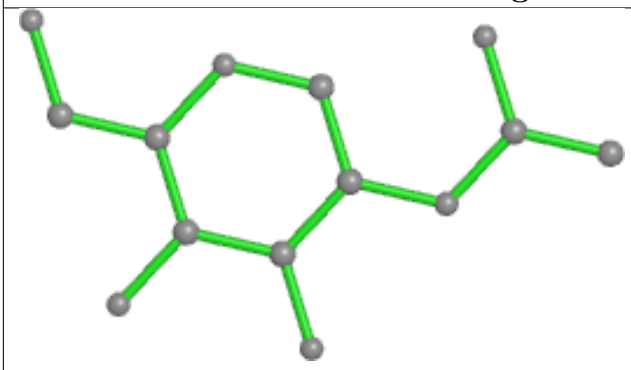
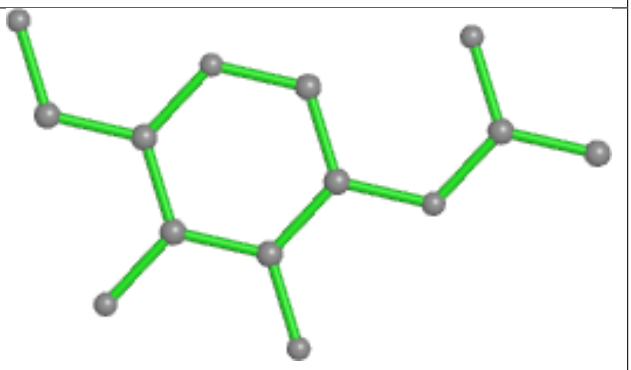
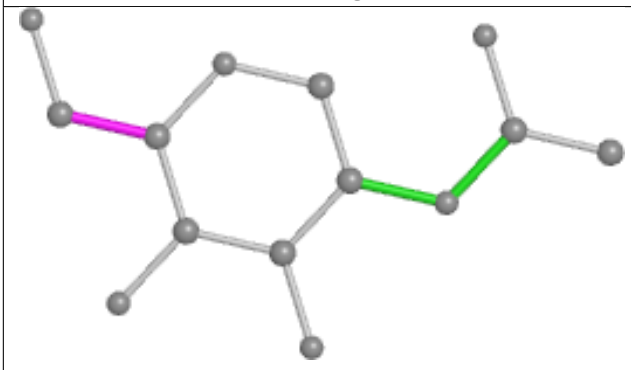
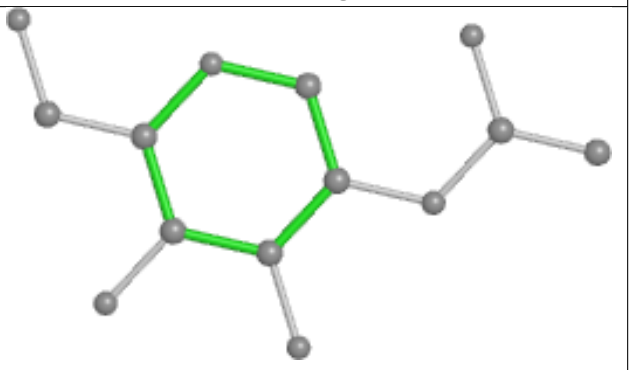
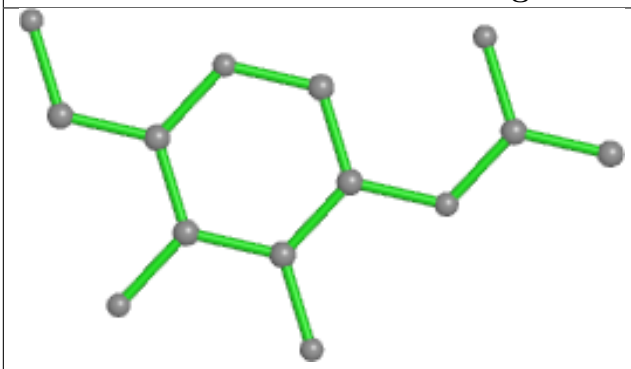
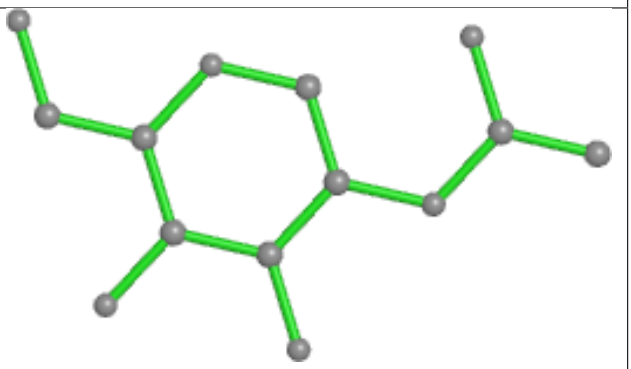
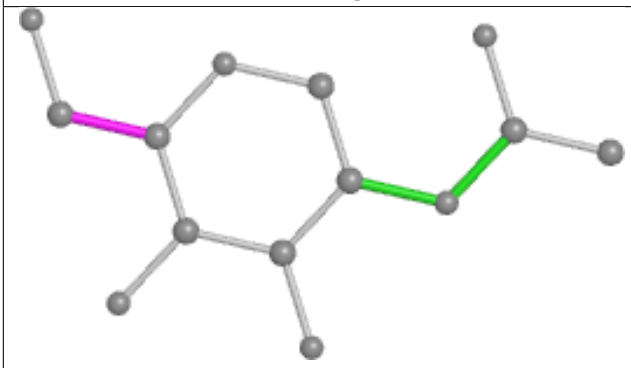
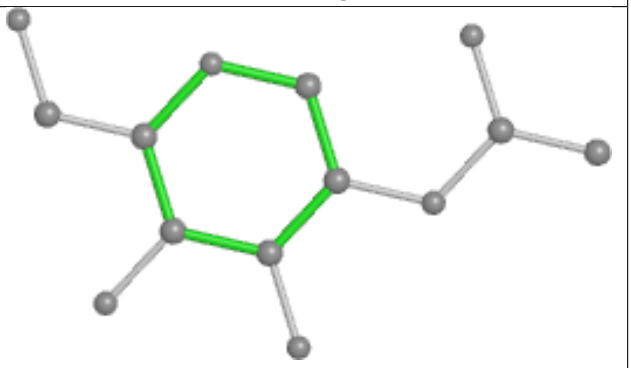
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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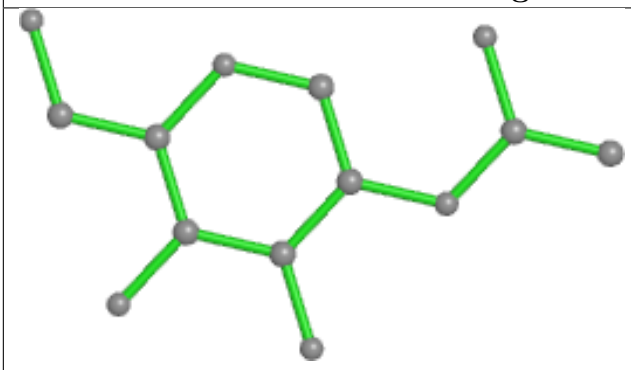
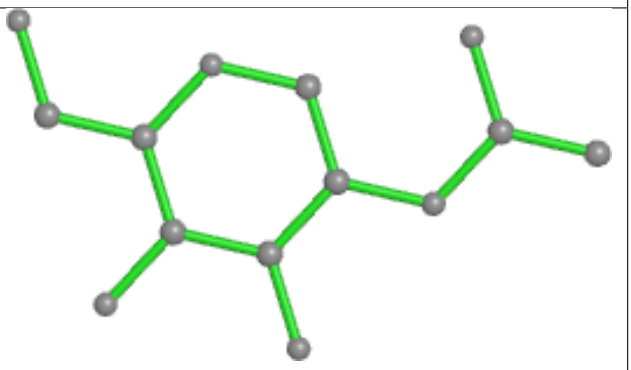
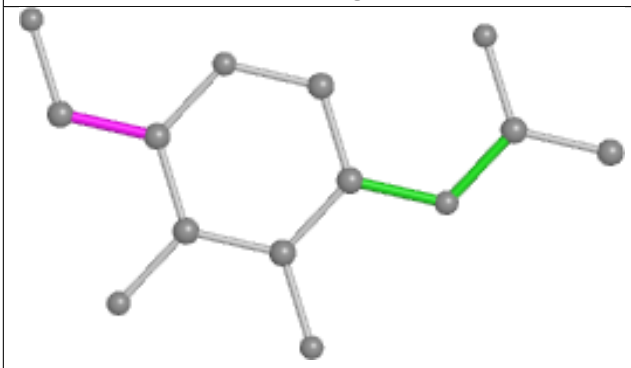
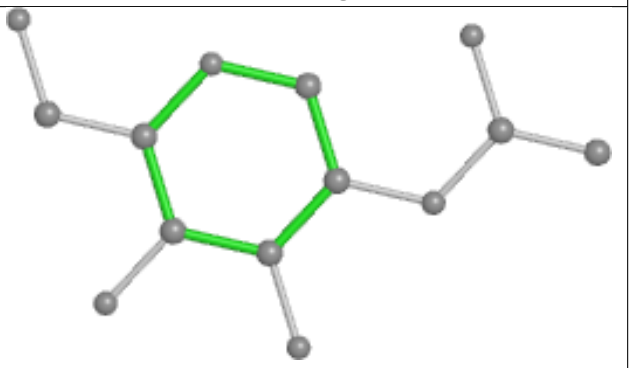
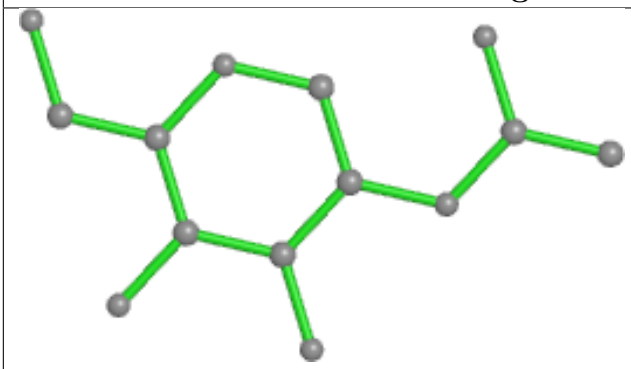
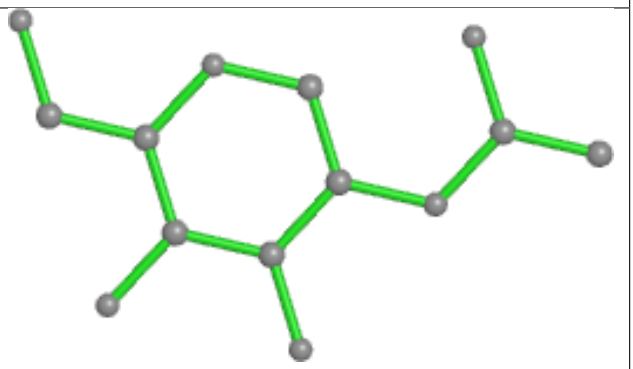
 Bond lengths	 Bond angles
 Torsions	 Rings

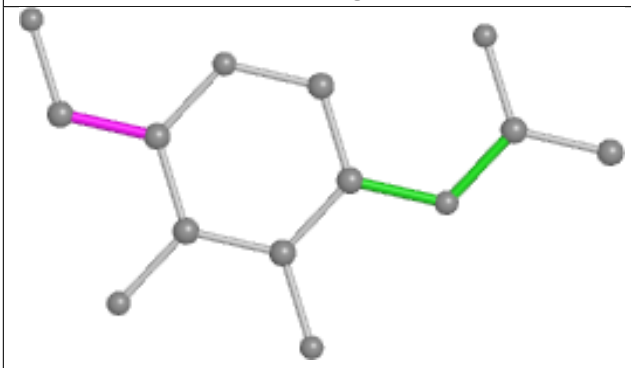
Ligand NAG C 1403



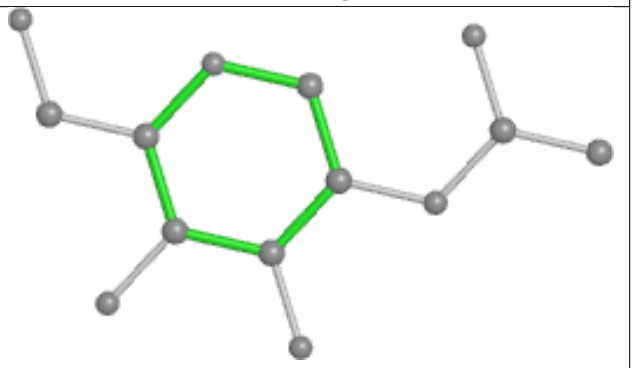
Bond lengths



Bond angles

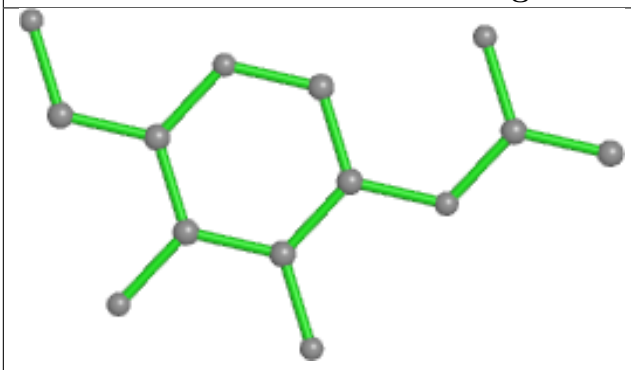


Torsions



Rings

Ligand NAG B 1408



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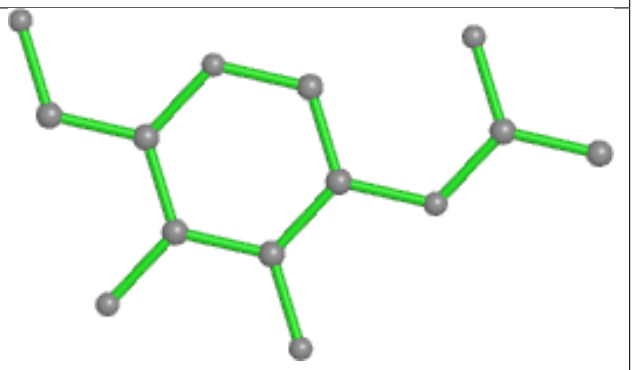

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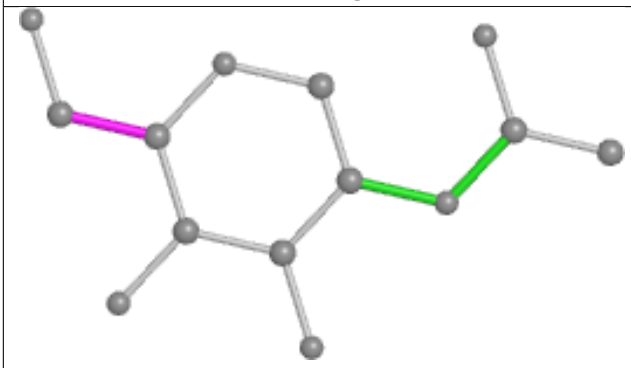

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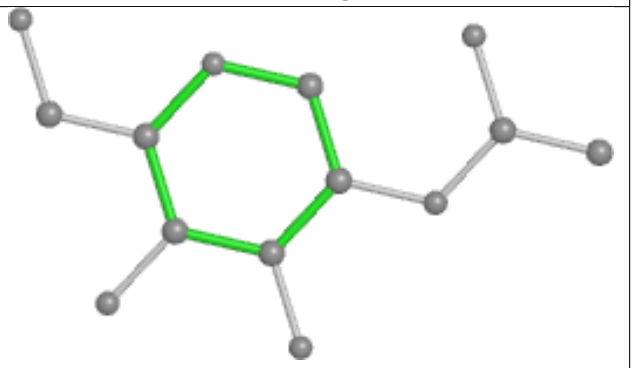
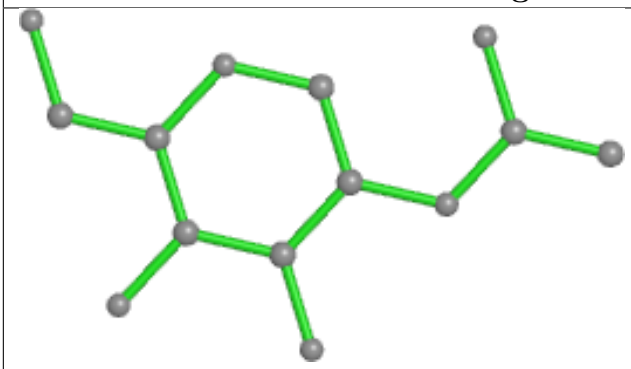
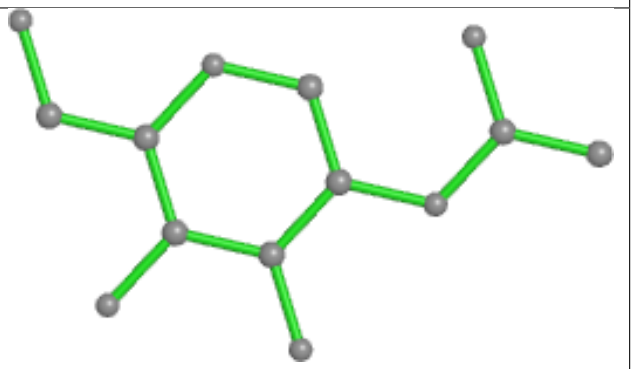


Rings

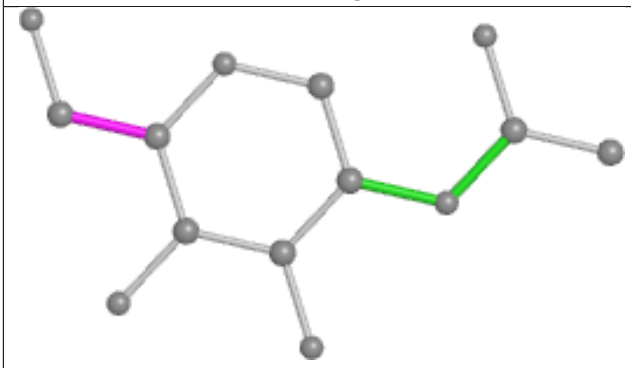
Ligand NAG B 1401



Bond lengths



Bond angles



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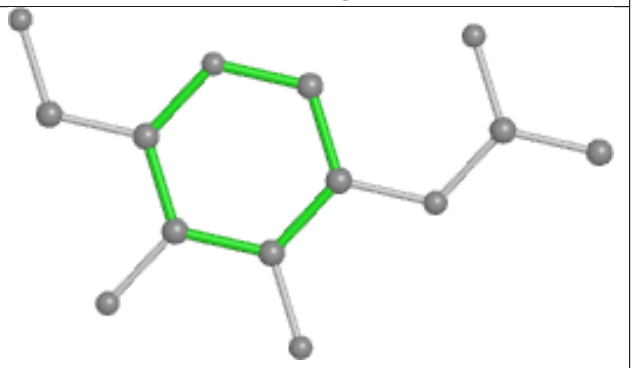
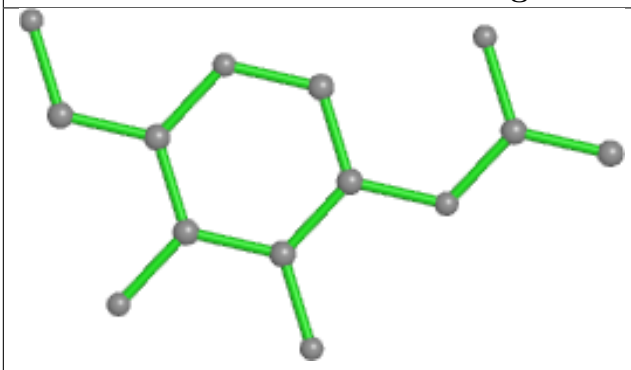


Rings

Ligand NAG A 1401



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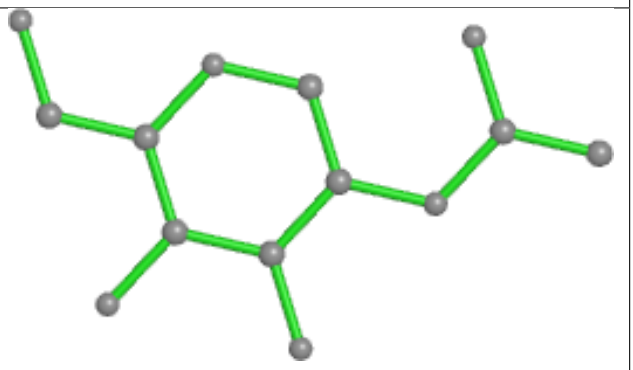
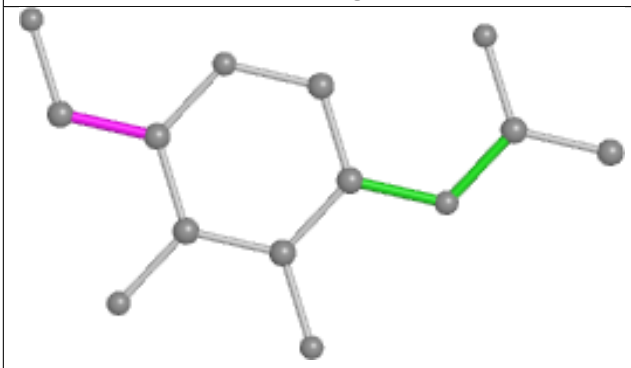


Bond angles



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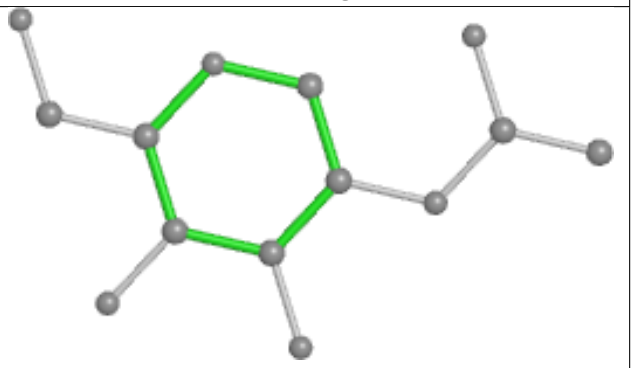
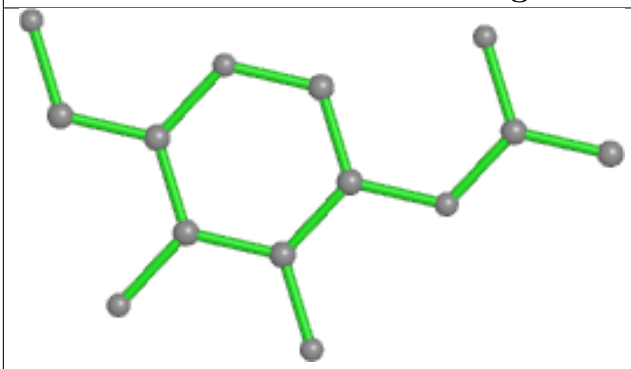
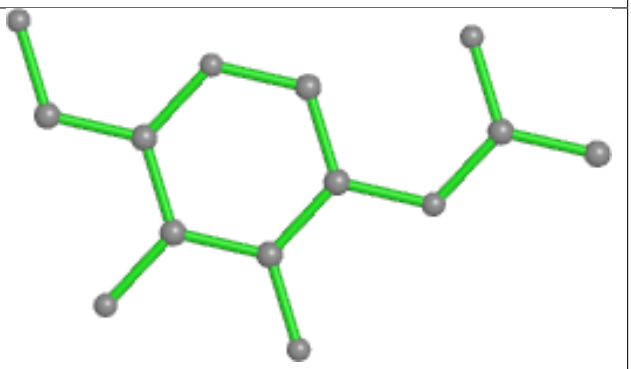
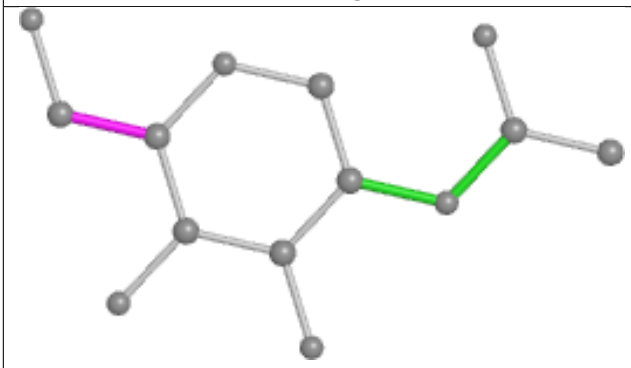
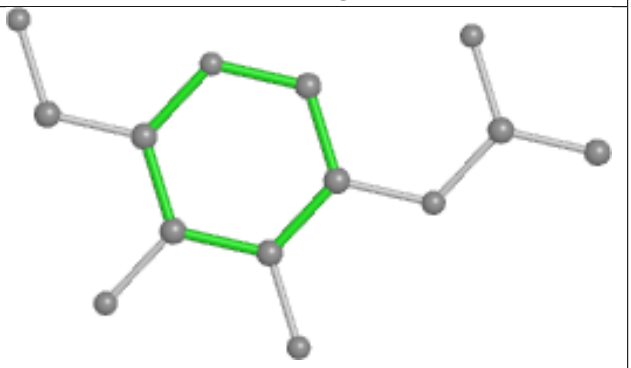
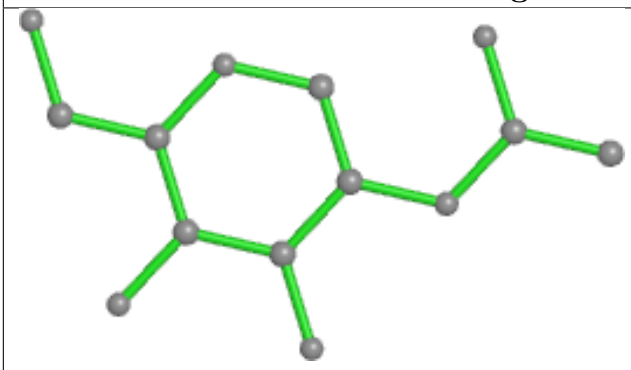
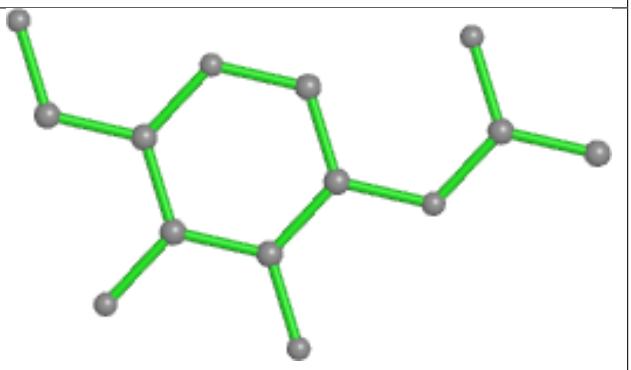
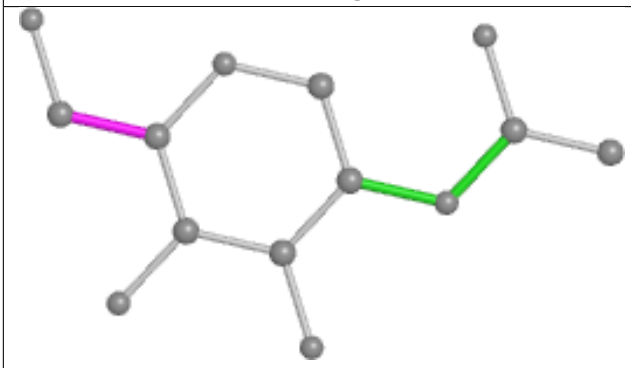
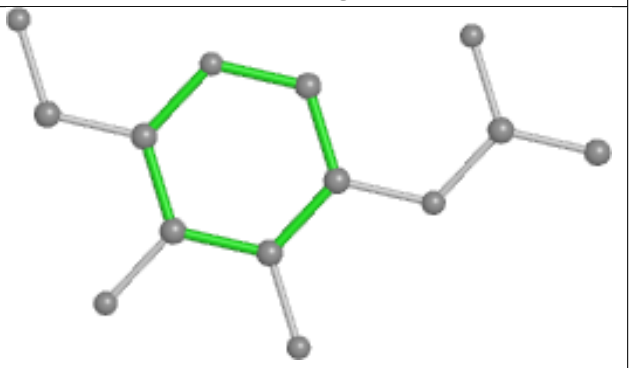
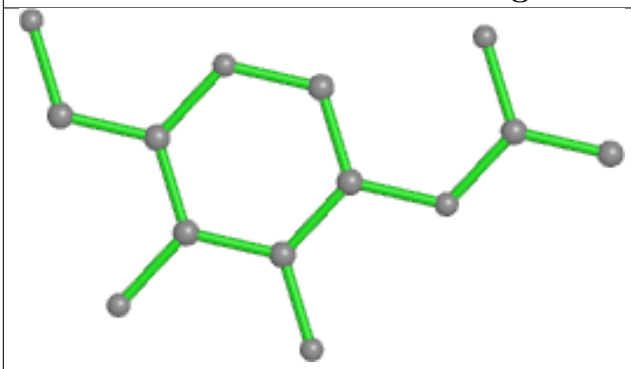


Rings

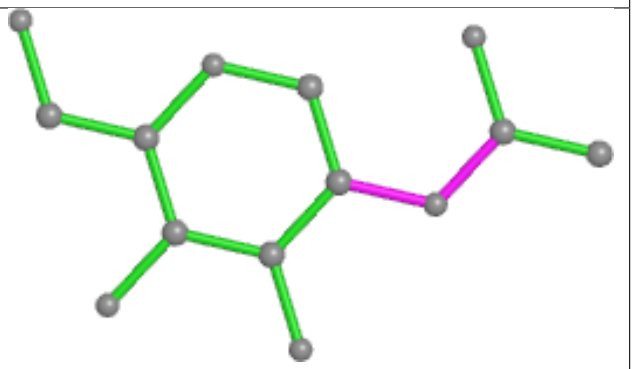
Ligand NAG A 1408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

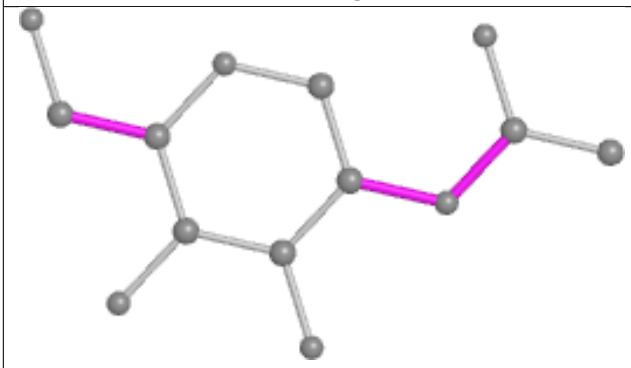
Ligand NAG C 1405



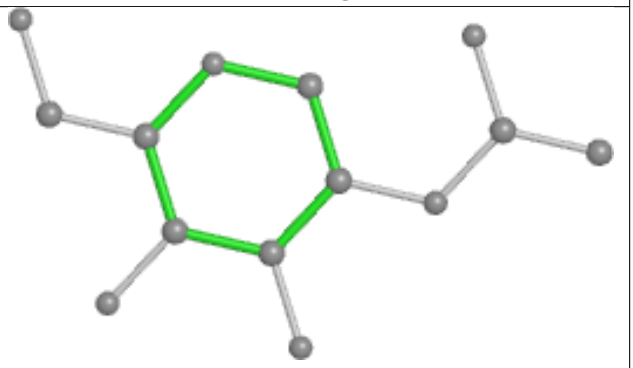
Bond lengths



Bond angles

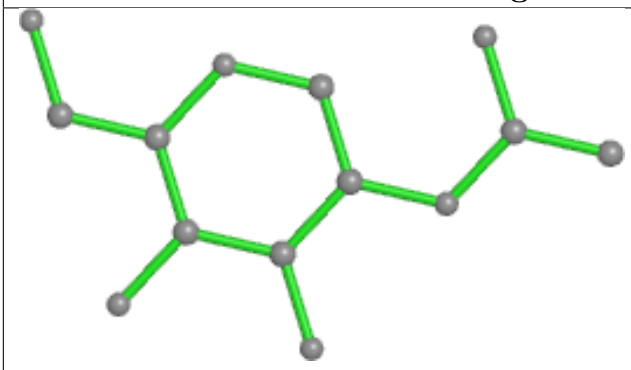


Torsions

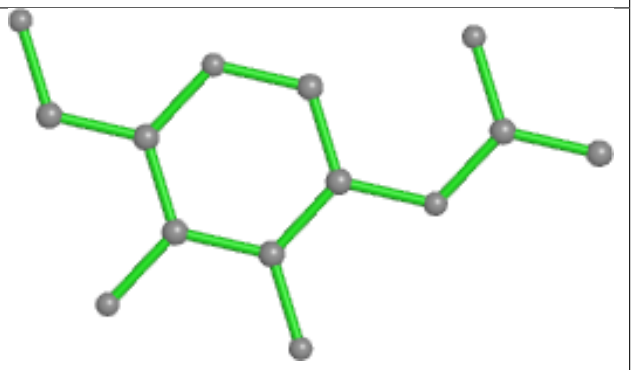


Rings

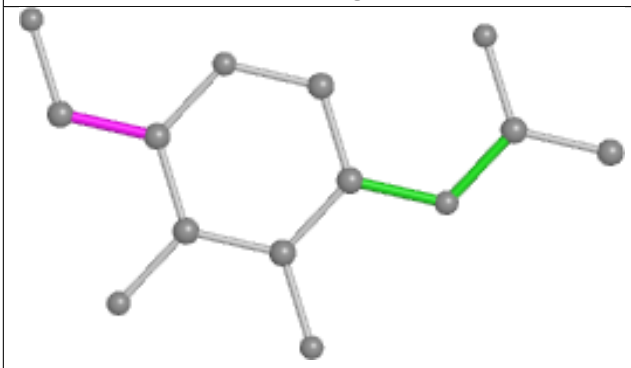
Ligand NAG A 1404



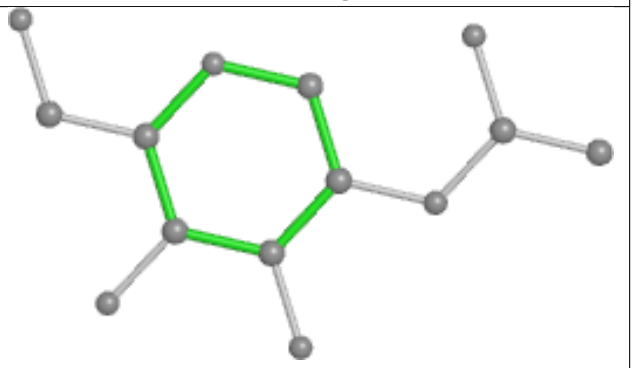
Bond lengths



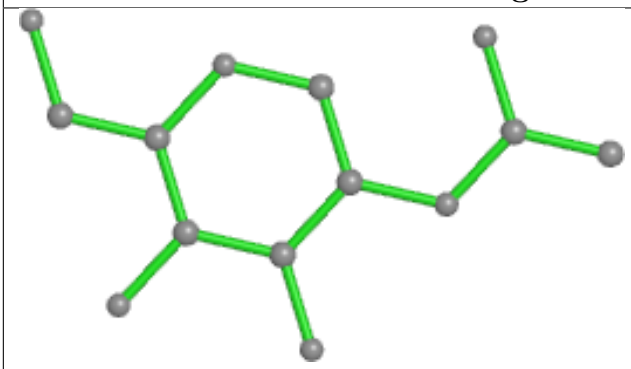
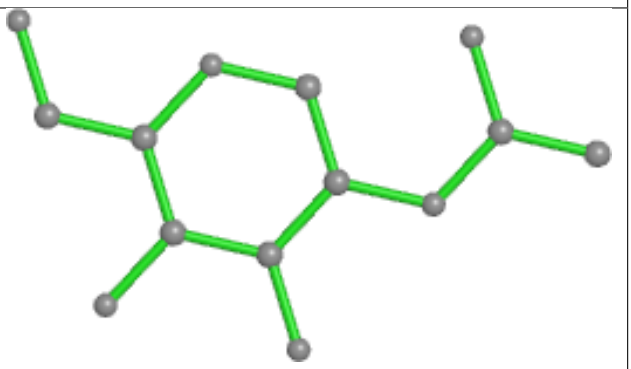
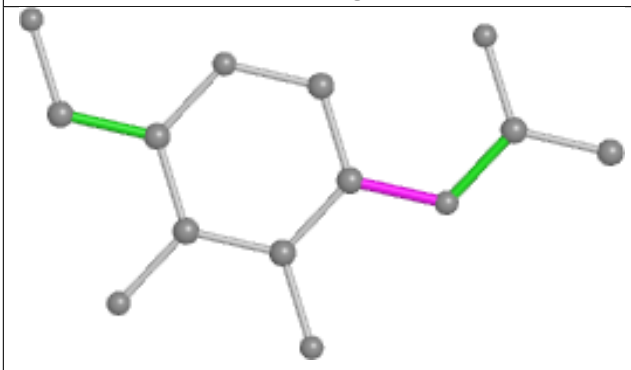
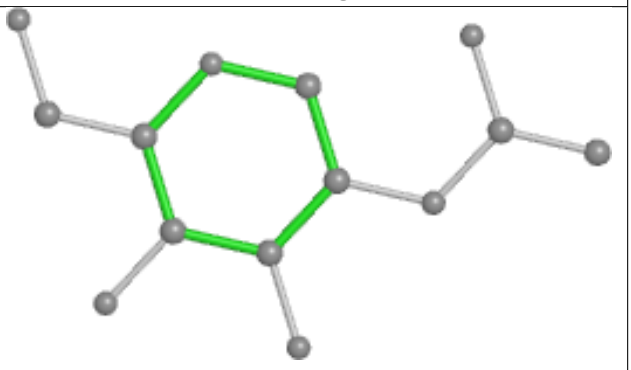
Bond angles

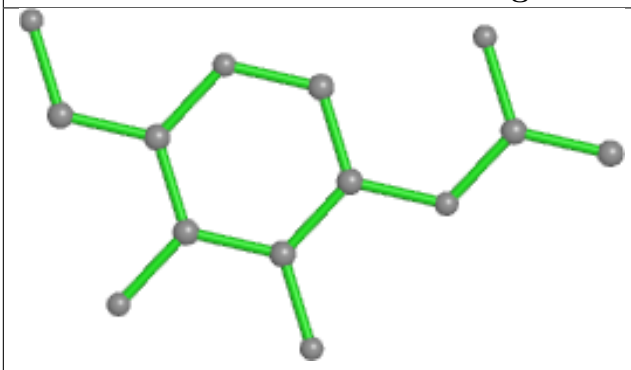
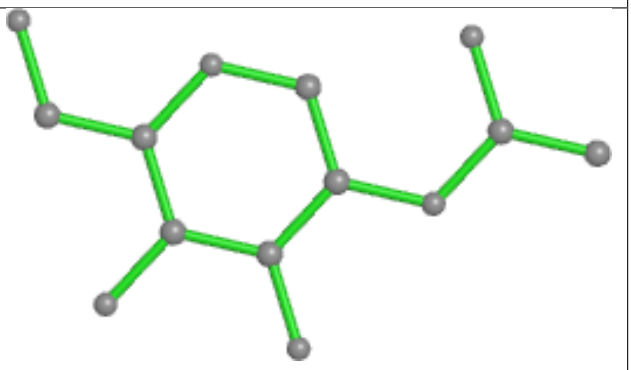
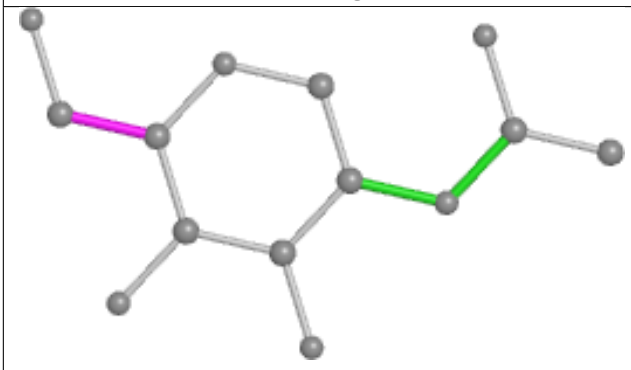
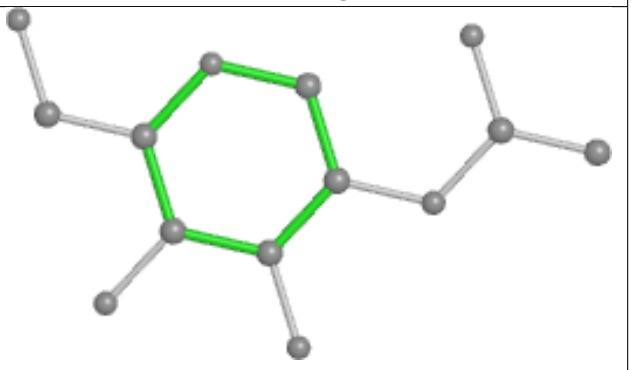


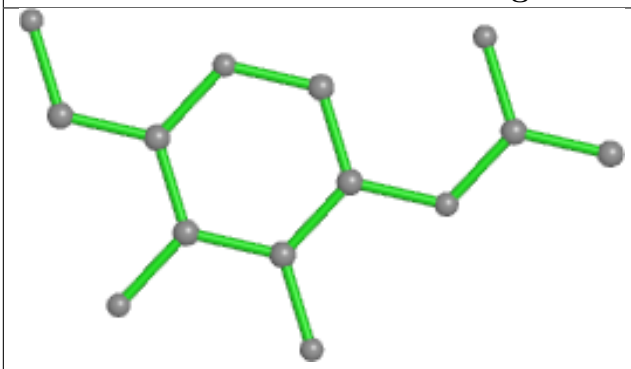
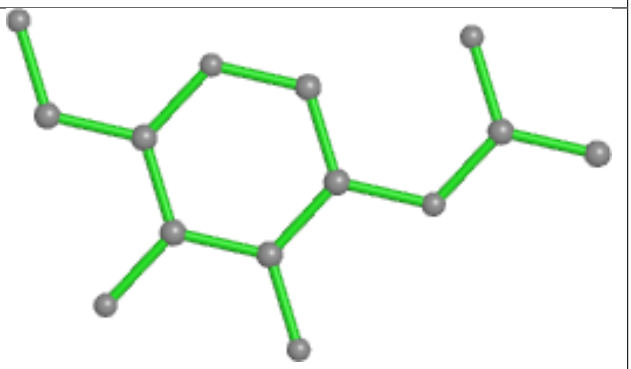
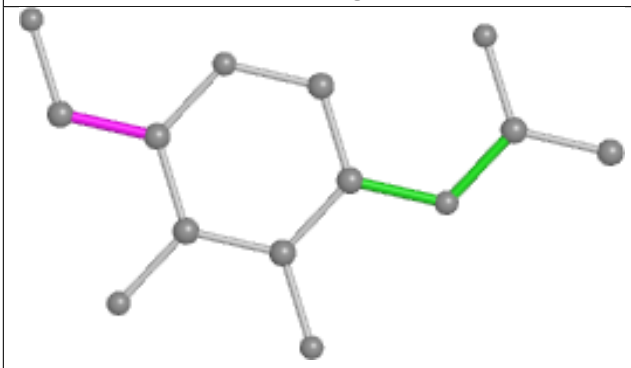
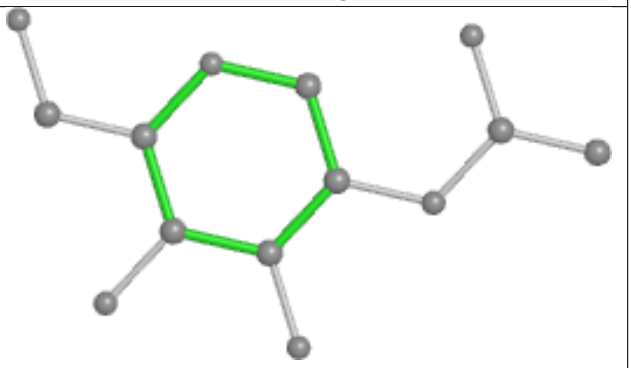
Torsions

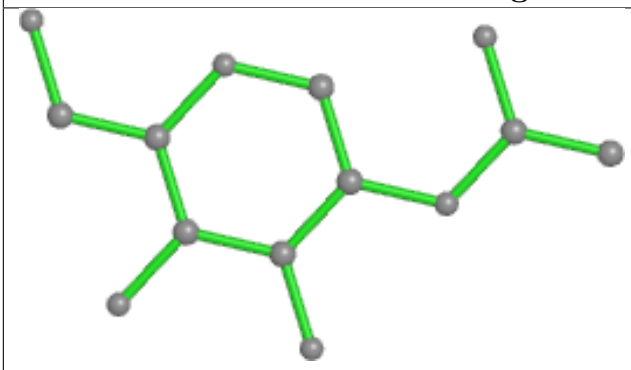
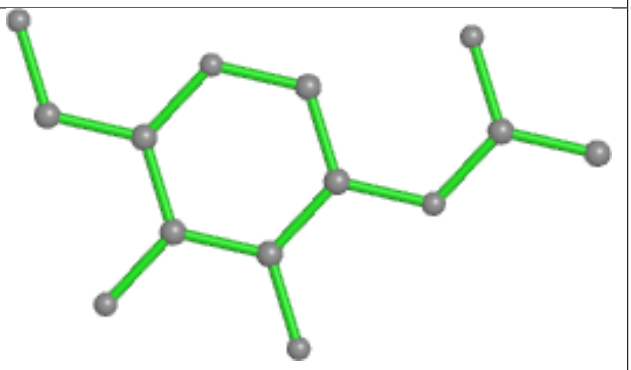
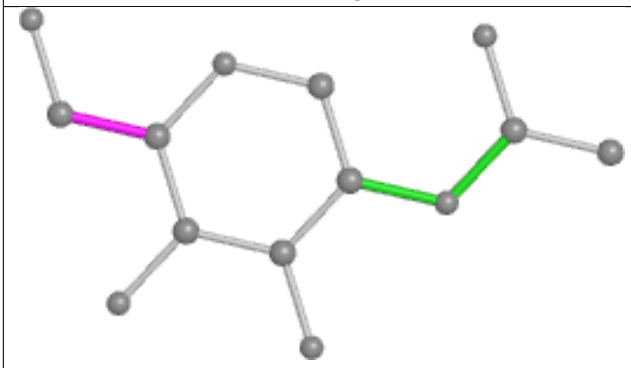
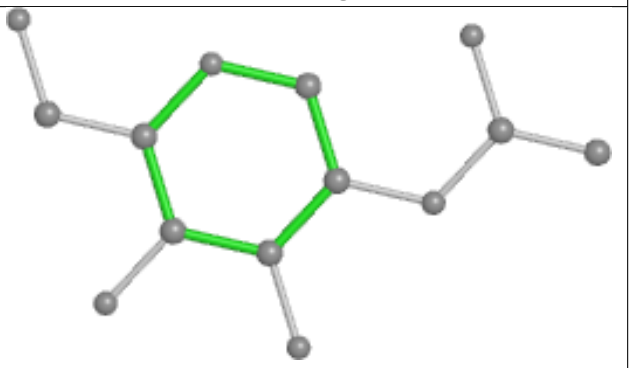


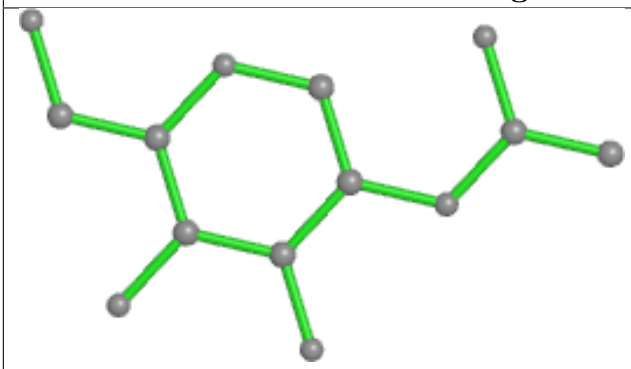
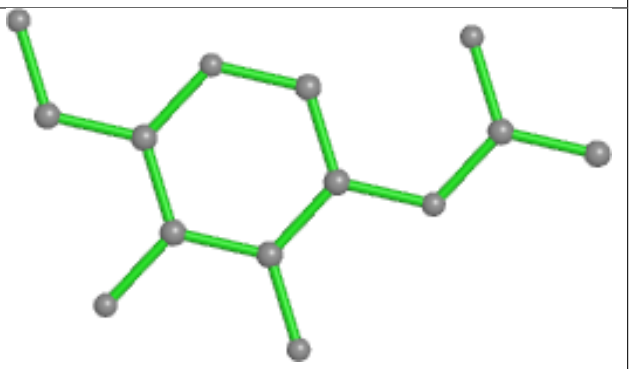
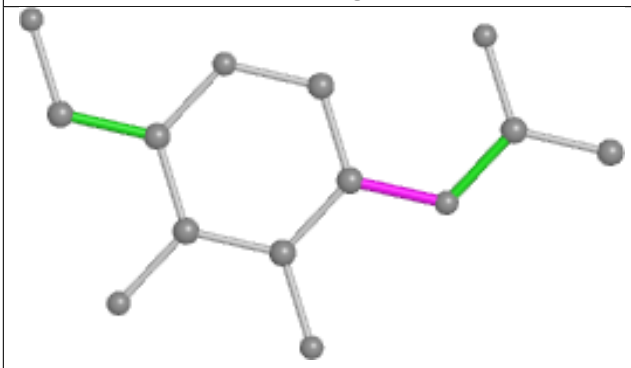
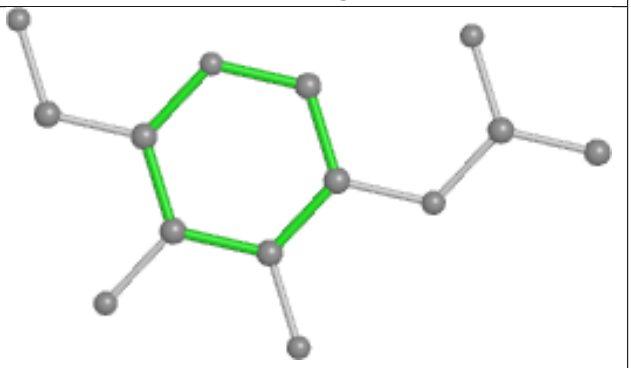
Rings

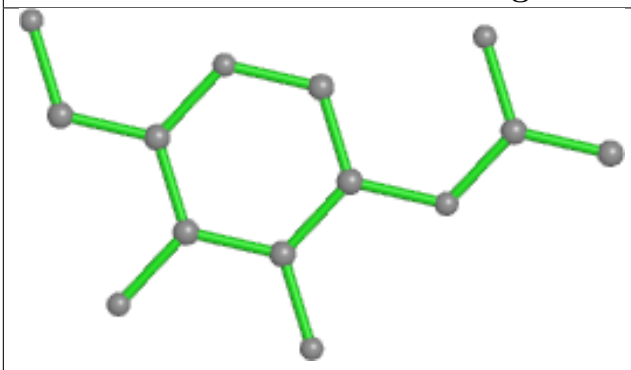
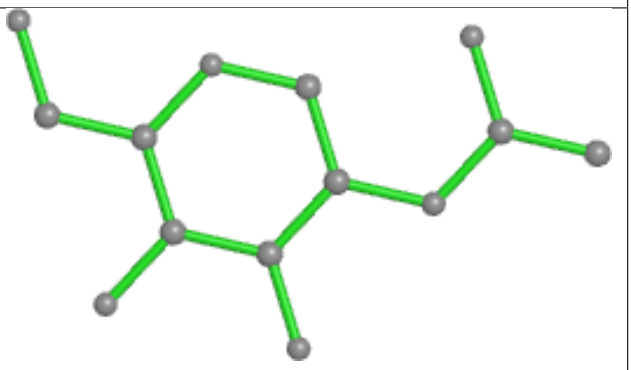
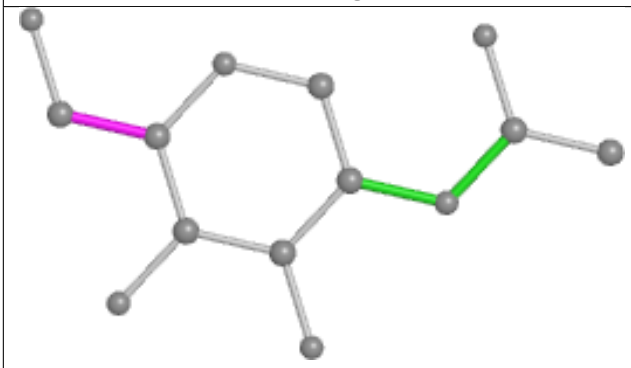
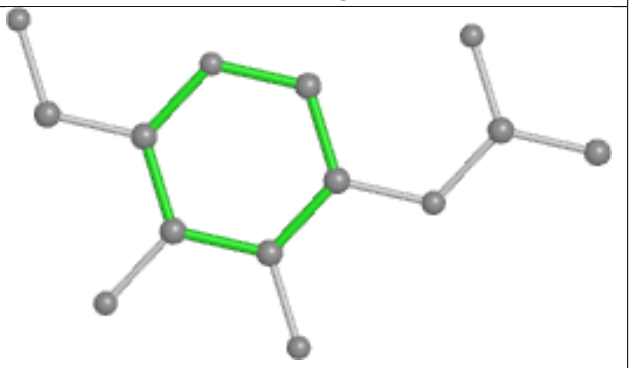
Ligand NAG B 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1406	
 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.

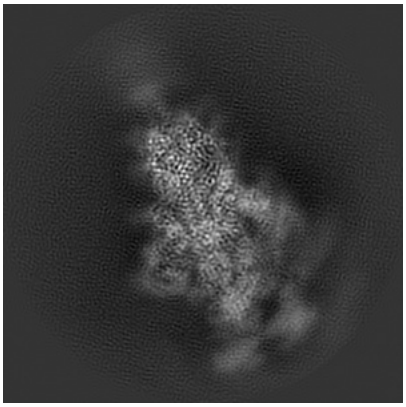
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32869. These allow visual inspection of the internal detail of the map and identification of artifacts.

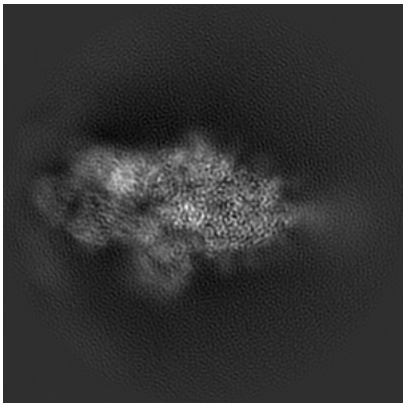
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

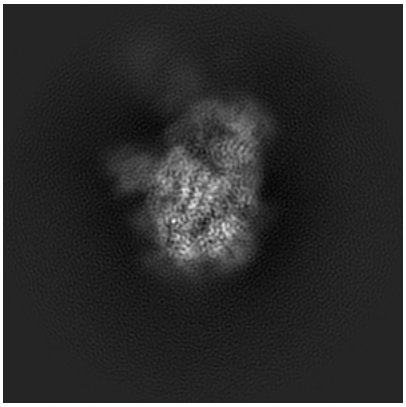
6.1.1 Primary map



X



Y

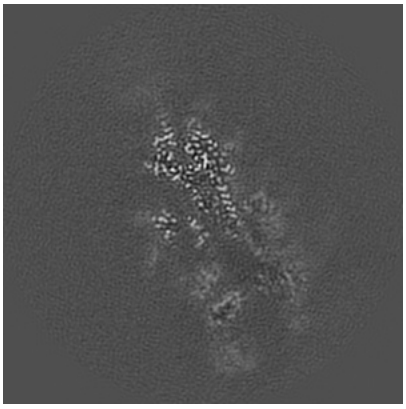


Z

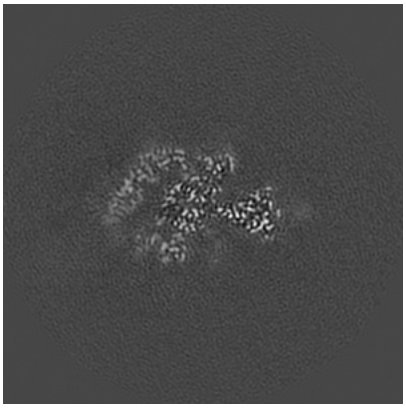
The images above show the map projected in three orthogonal directions.

6.2 Central slices

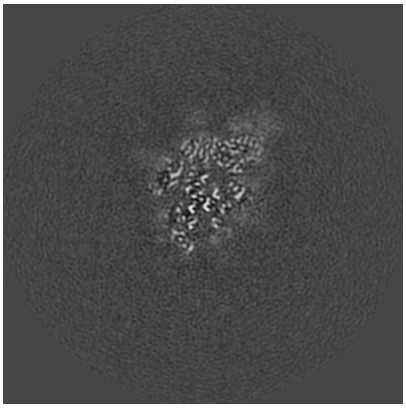
6.2.1 Primary map



X Index: 144



Y Index: 144

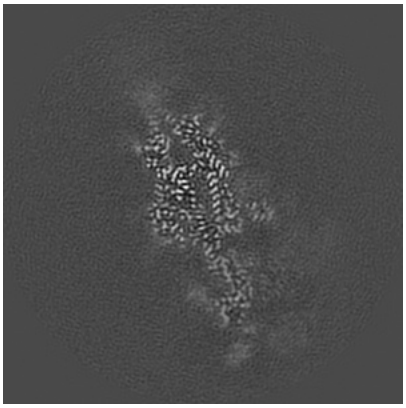


Z Index: 144

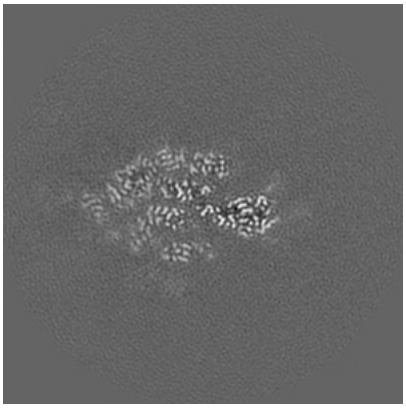
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

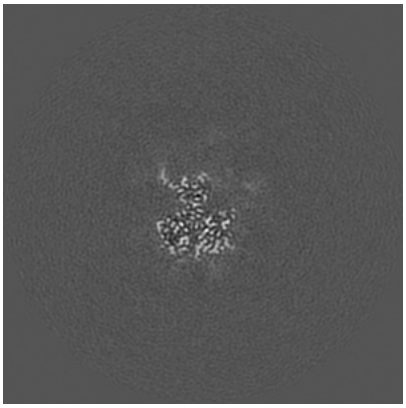
6.3.1 Primary map



X Index: 132



Y Index: 149

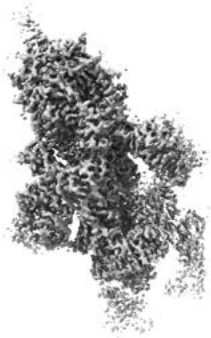


Z Index: 167

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

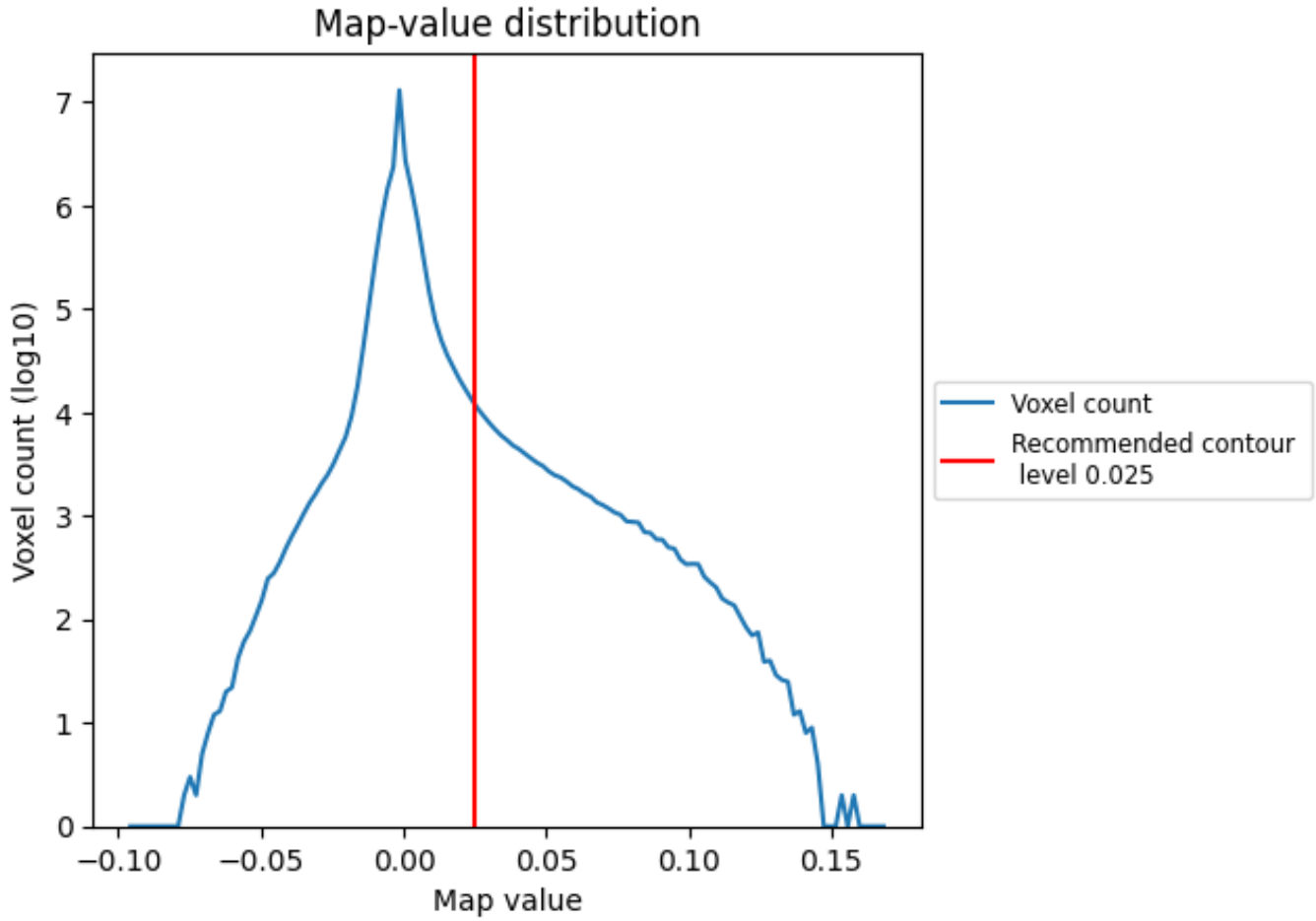
6.5 Mask visualisation (i)

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

7 Map analysis

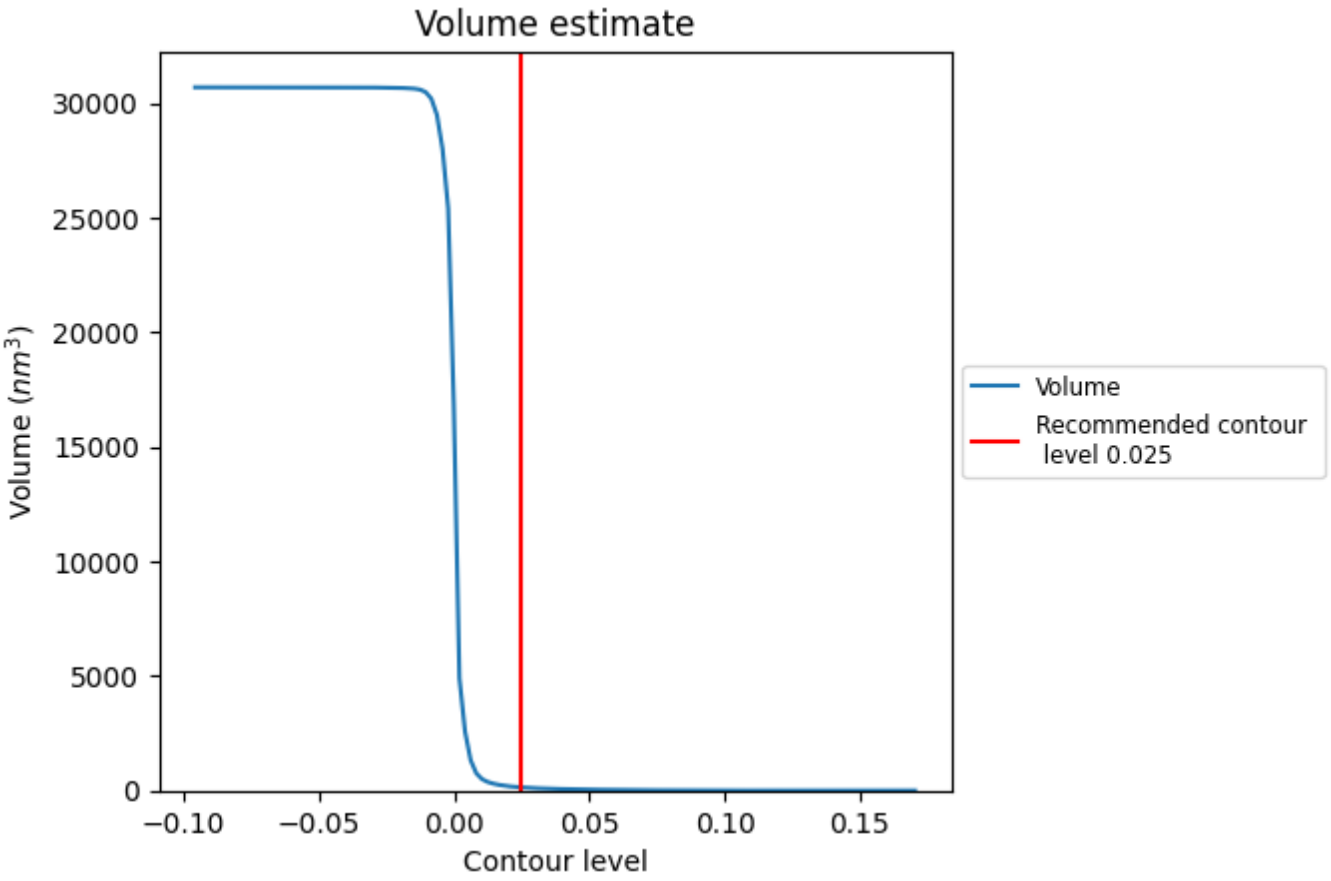
This section contains the results of statistical analysis of the map.

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.

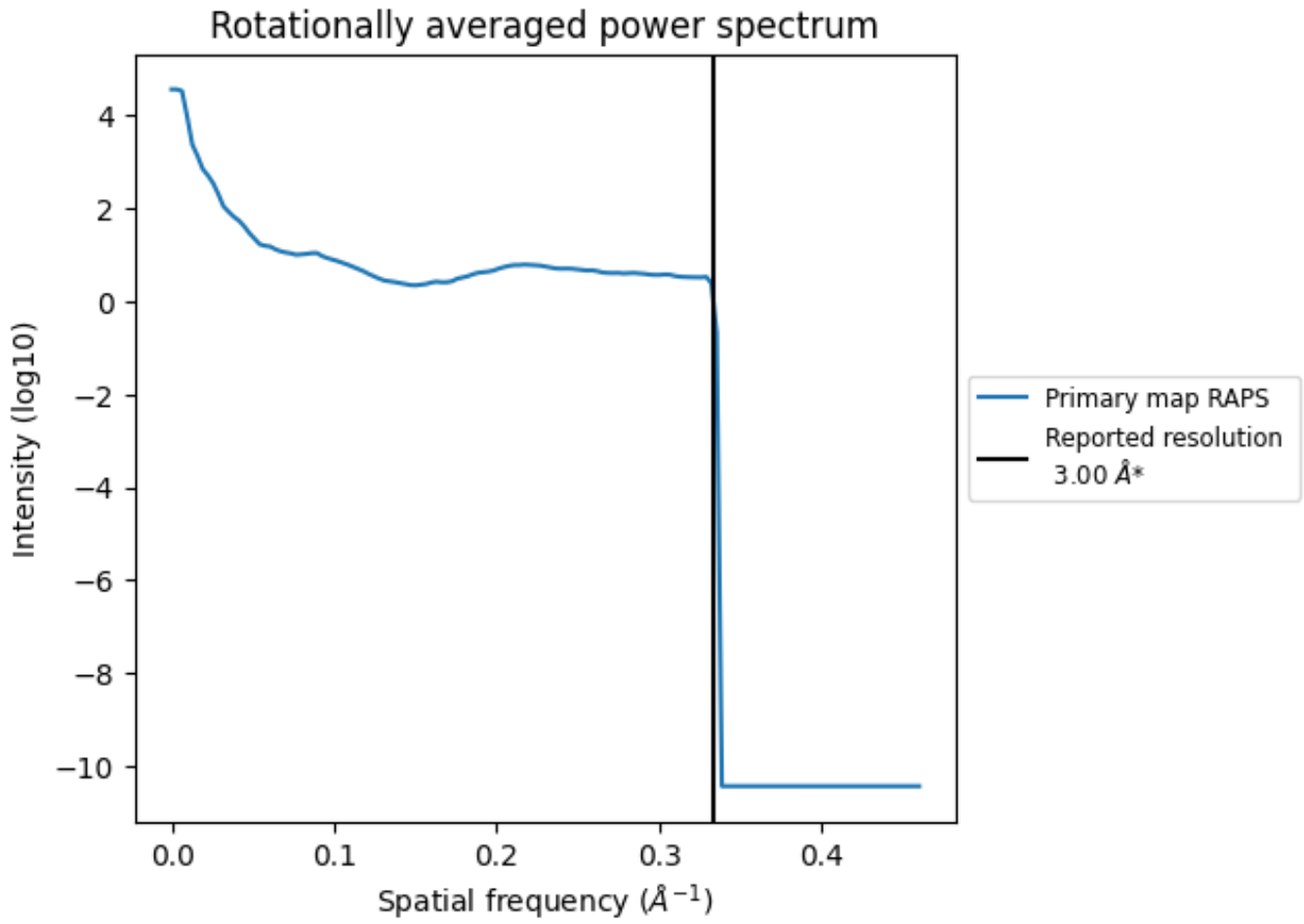
7.2 Volume estimate



The volume at the recommended contour level is 137 nm^3; this corresponds to an approximate mass of 124 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 0.333 Å^{-1}

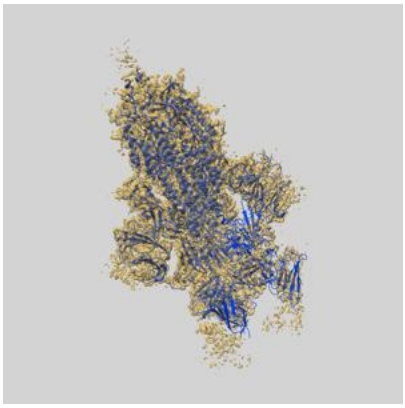
8 Fourier-Shell correlation (i)

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

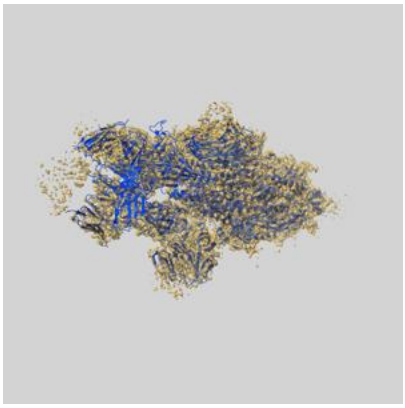
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32869 and PDB model 7WWL. Per-residue inclusion information can be found in section 3 on page 9.

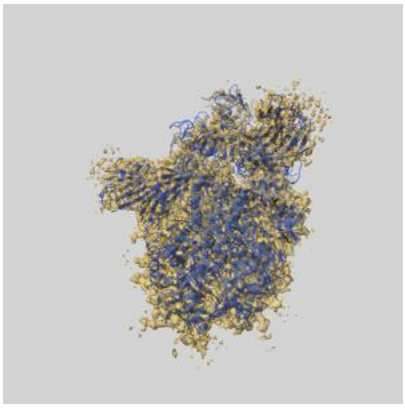
9.1 Map-model overlay



X



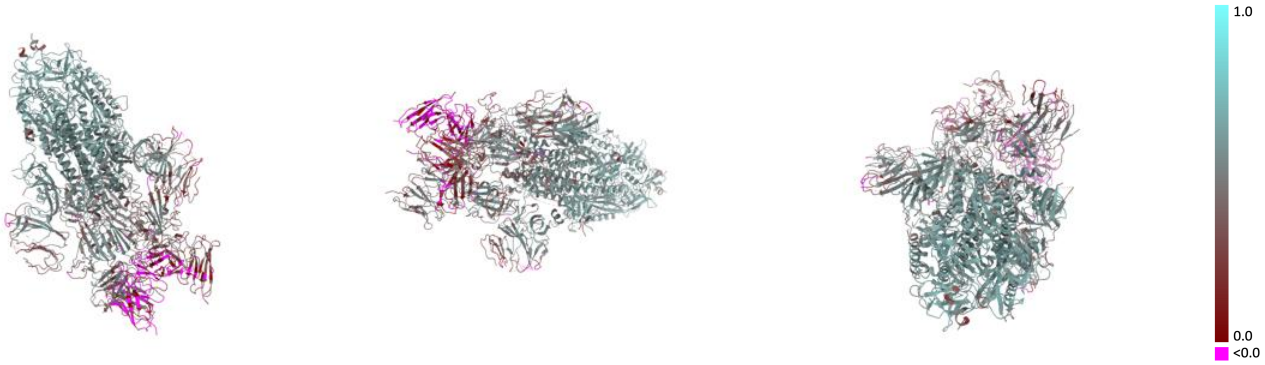
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

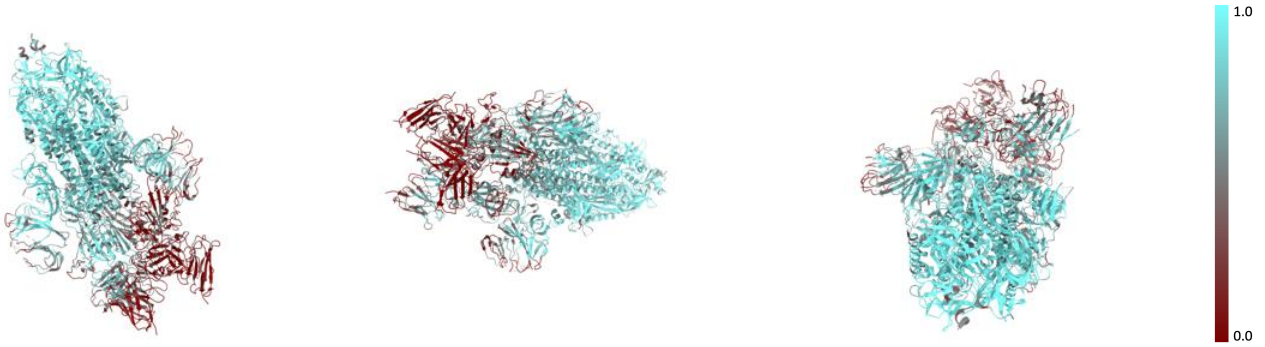
9.2 Q-score mapped to coordinate model (i)



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.

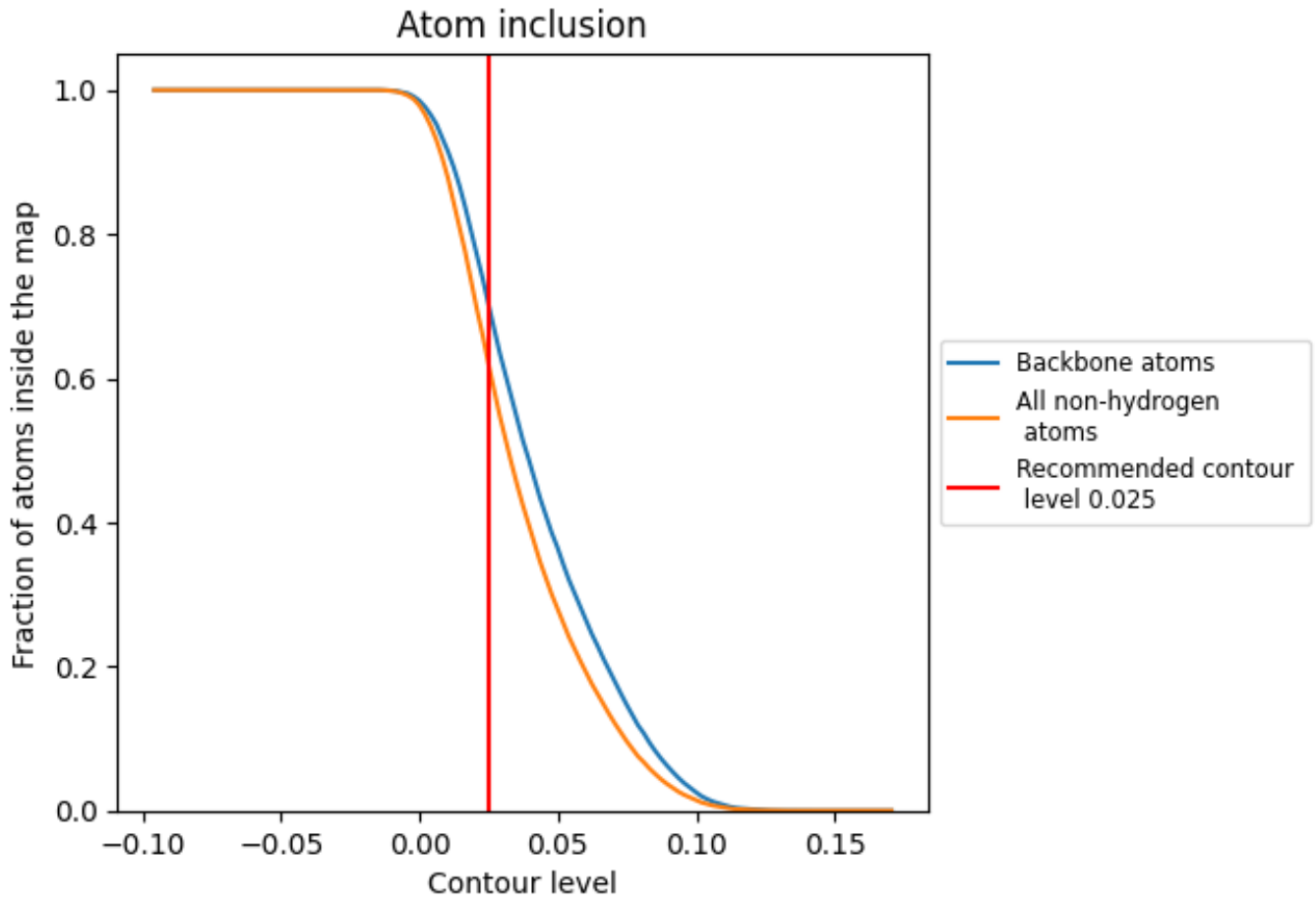
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 62% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6182	0.4440
A	0.6368	0.4820
B	0.7337	0.4950
C	0.7518	0.5150
D	0.2500	0.2320
E	0.3214	0.2900
F	0.5714	0.5210
G	0.6071	0.3750
H	0.5217	0.4300
I	0.1166	-0.0010
J	0.0923	0.2190
K	0.1786	0.4010
L	0.6146	0.4740
M	0.1463	0.0200
N	0.0207	0.1860
O	0.5357	0.3820
P	0.4643	0.3610
Q	0.0714	0.2000
R	0.2143	0.1480
S	0.3214	0.3690
T	0.5714	0.4330
U	0.5357	0.4360
V	0.6071	0.5060
W	0.3571	0.4550
X	0.1429	0.1670
Y	0.6429	0.4450
Z	0.4643	0.3790
a	0.7500	0.4970
b	0.4286	0.2940
c	0.1786	0.3670
d	0.5714	0.4280
e	0.4643	0.4470
f	0.1071	0.3340