wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 02:10 AM JST

PDB ID	:	7DX7
EMDB ID	:	EMD-30898
Title	:	Trypsin-digested S protein of SARS-CoV-2 bound with PD of ACE2 in the conformation 1 (1 up RBD and 1 PD bound)
Authors	:	Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.
Deposited on	:	2021-01-18
Resolution	:	3.40 Å(reported)

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

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

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

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

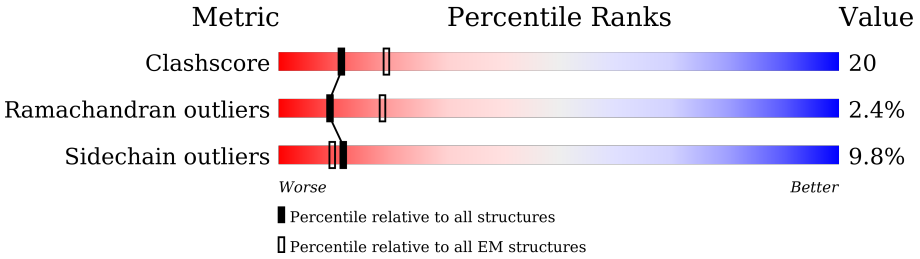
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

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 3.40 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)
Clashscore	158937	4297
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	1283	7%; 51%, 22%, 5%, 22%
1	B	1283	11%; 51%, 19%, 5% •, 24%
1	C	1283	13%; 50%, 21%, •, 24%
2	D	817	59%; 65%, 7%, 27%
3	E	2	50%, 50%
3	F	2	50%; 50%, 50%
3	G	2	100%
3	H	2	50%, 50%

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Mol	Chain	Length	Quality of chain
3	I	2	50% 50% 50%
3	J	2	50% 50%
3	K	2	50% 50%
3	L	2	100% 100%
3	M	2	100% 50% 50%
3	N	2	50% 100%
3	O	2	50% 50%
3	P	2	50% 50%
3	Q	2	100%
3	R	2	100%
3	S	2	100% 100%
3	T	2	100% 50% 50%
3	U	2	50% 50% 50%
3	V	2	50% 50%
3	W	2	100%
3	X	2	50% 50% 50%
3	Y	2	100%
3	Z	2	100%
3	a	2	100% 50% 50%
3	b	2	100% 50% 50%
3	c	2	100% 100%
3	d	2	100% 100%
3	e	2	100% 50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1007	7872	5025	1310	1501	36	0	0
1	B	971	7584	4843	1262	1445	34	0	0
1	C	971	7584	4843	1262	1445	34	0	0

There are 36 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	595	4857	3108	804	916	29	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP Q9BYF1
D	-10	ALA	-	expression tag	UNP Q9BYF1
D	-9	SER	-	expression tag	UNP Q9BYF1
D	-8	GLY	-	expression tag	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	2	28	16	2	10	0	0
3	F	2	28	16	2	10	0	0
3	G	2	28	16	2	10	0	0
3	H	2	28	16	2	10	0	0
3	I	2	28	16	2	10	0	0
3	J	2	28	16	2	10	0	0
3	K	2	28	16	2	10	0	0
3	L	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0
3	N	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0
3	Q	2	28	16	2	10	0	0
3	R	2	28	16	2	10	0	0
3	S	2	28	16	2	10	0	0
3	T	2	28	16	2	10	0	0
3	U	2	28	16	2	10	0	0
3	V	2	28	16	2	10	0	0
3	W	2	28	16	2	10	0	0
3	X	2	28	16	2	10	0	0
3	Y	2	28	16	2	10	0	0
3	Z	2	28	16	2	10	0	0

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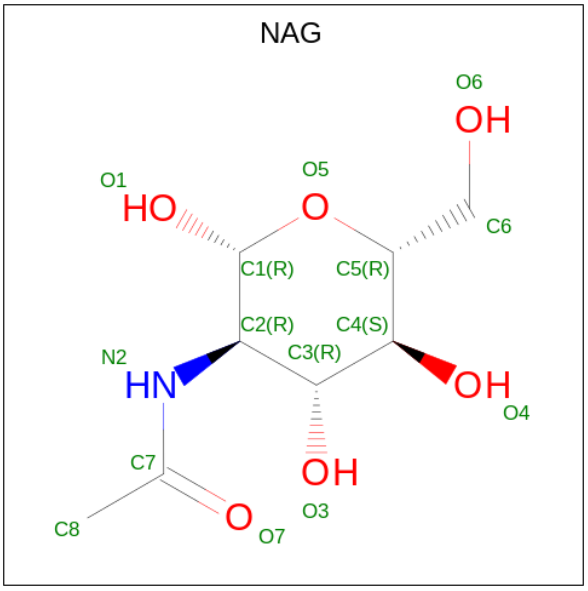
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	a	2	28	16	2	10	0	0
3	b	2	28	16	2	10	0	0
3	c	2	28	16	2	10	0	0
3	d	2	28	16	2	10	0	0
3	e	2	28	16	2	10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	126	72	9	45	0
4	A	1	126	72	9	45	0
4	A	1	126	72	9	45	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0

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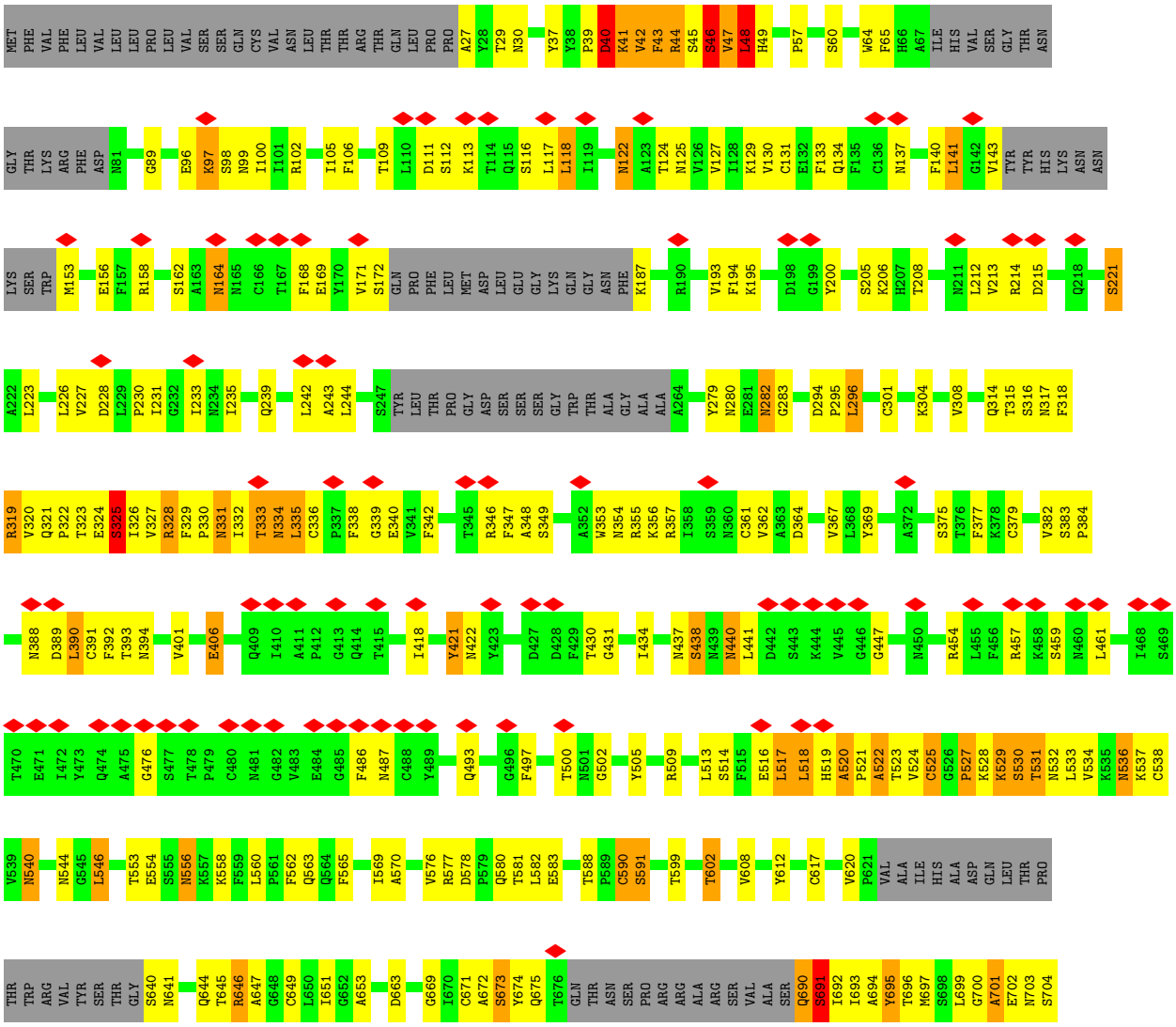
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	D	1	14	8	1	5	0

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: 7% 51% 22% 5% 22%



V705 A706 Y707 S708 N709 N710 S711 V722 L727 P728 V729 S735 C738 T739 M740 D745 S746 S758 Q762 E773 V785 K786 Q787 K790 T791 K795 D796 F797 D808 K811 P812 S813 V826 THR LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP

CYS LEU GLY ASP ILE ALA ALA ARG ASP LEU ILE CYS ALA GLN K854 F855 N856 T859 E868 L878 T883 W886 L894 Q895 I896 P897 Q901 M902 A903 Y904 R905 T912 Q913 N914 V915 L916 S929 K933 I934 Q935 D936 S937 L938 S939 S940 THR ALA SER A944

V951 L959 V963 K964 Q965 L966 S967 G971 A972 I973 N978 D979 I980 L981 S982 R983 L984 D985 P987 E988 V991 Q992 I993 D994 R995 Q1005 C1032 S1051 P1057 H1058 G1059 H1064 N1074 F1075 T1076 T1077 P1090 R1091 E1092 G1093 V1094 F1095 V1096 S1097 T1100 H1101

V1104 T1105 Q1106 R1107 Y1110 E1111 I1115 S1123 G1124 N1125 I1132 L1141 Q1142 P1143 E1144 L1145 D1146 SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE

ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO TRP TYR ILE TRP LEU GLY PHE ILE ALA GLY LEU ILE ALA ILE VAL MET VAL THR ILE MET LEU CYS CYS MET THR SER CYS CYS SER CYS

LEU LYS GLY CYS CYS SER CYS GLY SER CYS LYS PHE ASP GLU ASP ASP SER GLU PRO VAL LEU LYS GLY VAL LYS LEU HIS TYR THR LEU GLU ASP TYR LYS ASP ASP ASP ASP LYS

- Molecule 1: Spike glycoprotein

Chain B:

MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU THR THR ARG THR GLN LEU PRO PRO A27 Y28 T29 N30 Y37 Y38 P39 D40 K41 V42 F43 R44 S45 S46 V47 L48 H49 P57 S60 W64 F65 H66 A67 ILE HIS VAL SER GLY THR ASN

GLY THR LYS ARG PHE ASP N81 G89 E96 K97 S98 N99 I100 I101 R102 I105 F106 T109 L110 D111 S112 K113 S116 L117 L118 N122 A123 T124 N125 V126 V127 I128 K129 V130 C131 E132 F133 Q134 N137 F140 L141 G142 V143 TYR TYR HIS LYS ASN ASN LYS SER TRP

M153 E156 F157 R158 S162 A163 N164 N165 C166 T167 F168 E169 Y170 V171 S172 GLN PRO PHE LEU MET ASP LEU GLU GLY LYS GLN GLY ASN PHE K187 V193 F194 K195 S205 K206 H207 T208 N211 L212 V213 R214 D215 S221 A222 L223 L226 V227 D228 I231 G232 I233 N234

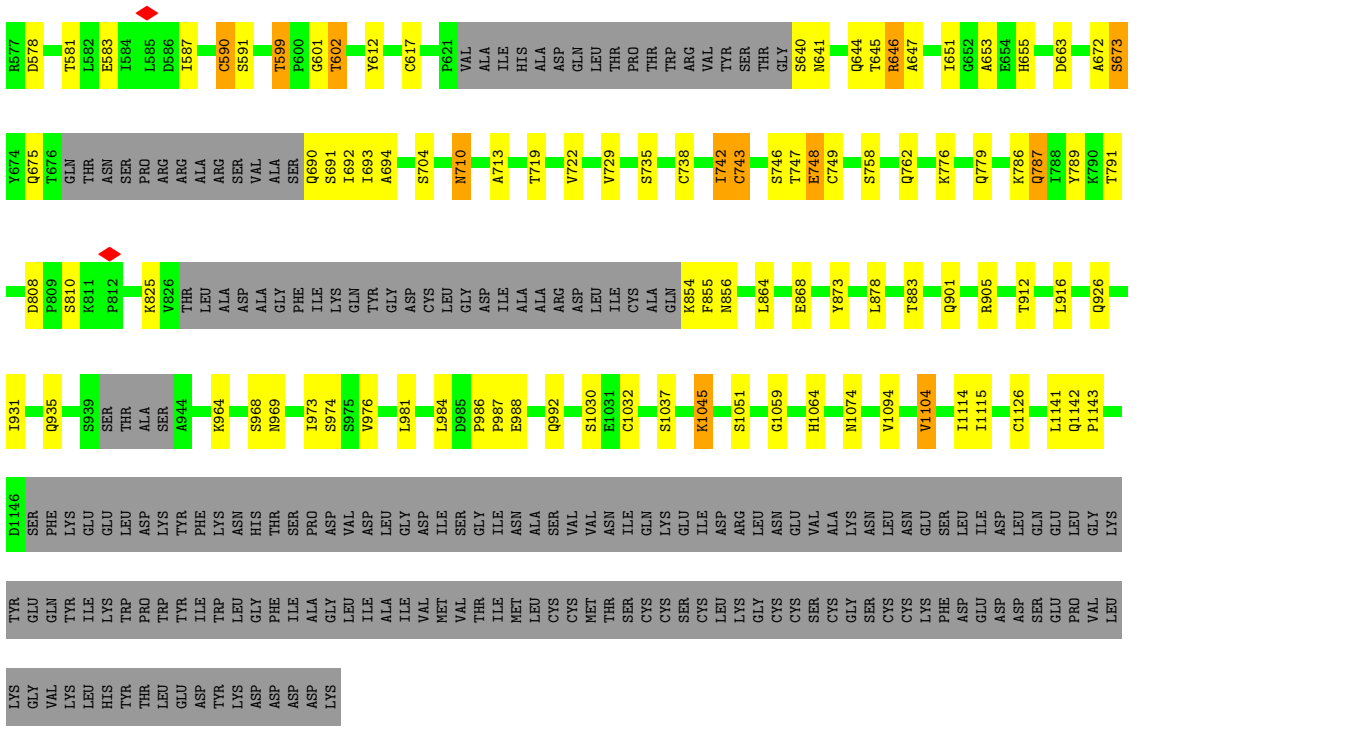
I235 Q239 L242 A243 L244 S247 TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA ALA A264 Y279 N280 E281 N282 G283 D294 P296 L296 C301 T307 V308 E309 K310 Q314 T315 S316 N317 F318 R319 V320 Q321 P322 T323 E324 S325 I326 V327 R328 F329

P330 N331 I332 T333 N334 L335 C336 P337 F338 G339 E340 V341 F342 N343 A344 T345 R346 F347 A348 S349 V350 Y351 A352 W353 N354 R355 K356 R357 N360 C361 V362 A363 D364 Y365 S366 V367 L368 Y369 N370 S371 A372 S373 F374 S375 T376 F377 K378 C379 Y380 G381 V382 S383 P384 T385 K386 L387 N388 D389 L390

C391 F392 T393 N394 V395 Y396 A397 D398 S399 F400 V401 I402 R403 G404 D405 E406 V407 R408 Q409 I410 A411 P412 G413 Q414 T415 G416 K417 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 C432 V433 I434 A435 W436 N437 S438 N439 N440 L441 D442 S443 K444 V445 G446 G447 M448 Y449 N450

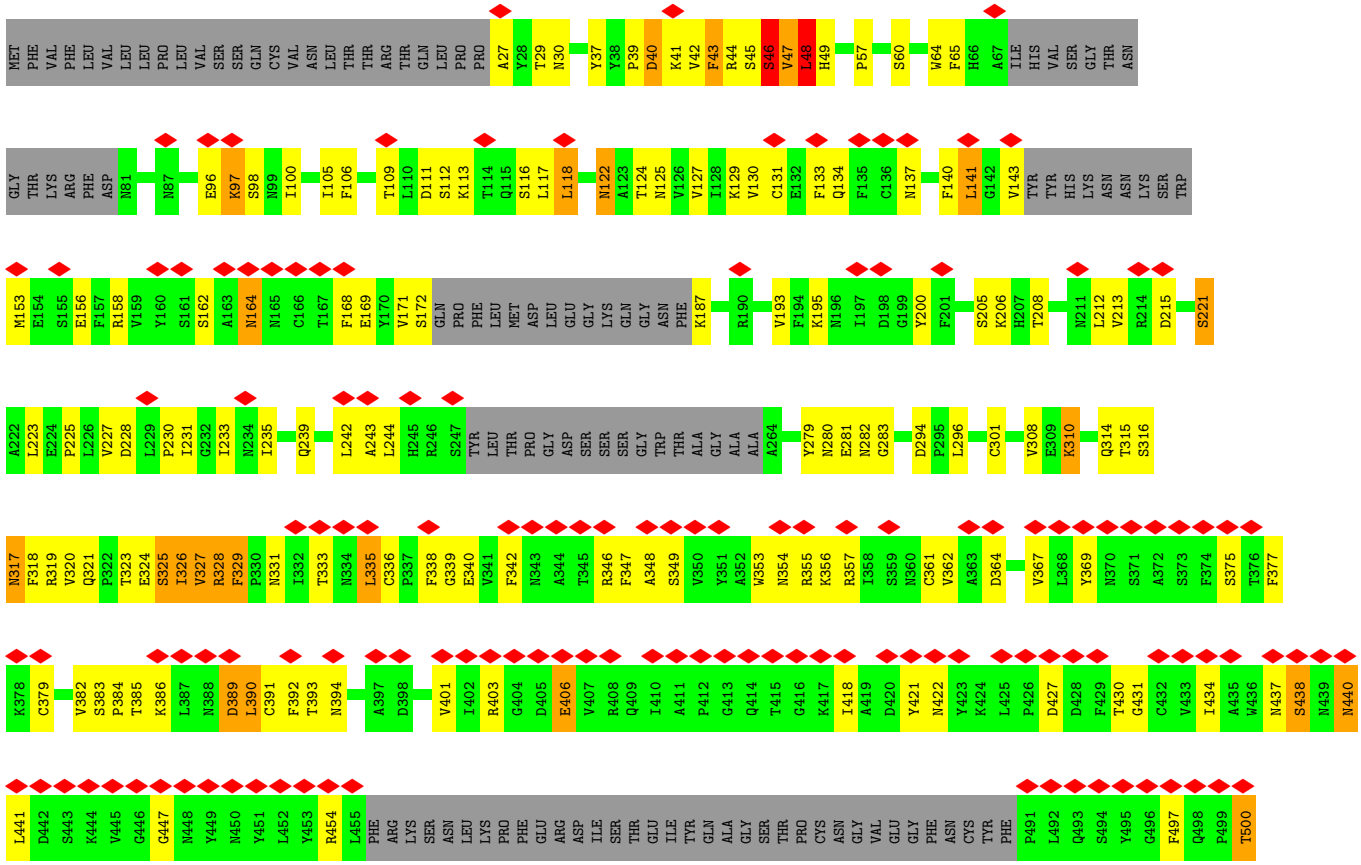
Y451 L452 Y453 R454 L455 PHE ARG LYS SER ASN LEU LYS PRO PHE GLU ARG ASP ILE SER THR GLU ILE TYR GLN ALA GLY SER THR PRO CYS ASN GLY VAL GLU GLY PHE ASN CYS TYR PHE P491 L492 Q493 S494 Y495 G496 F497 Q498 P499 T500 N501 G502 V503 G504 Y505 Q506 P507 Y508 R509 V510

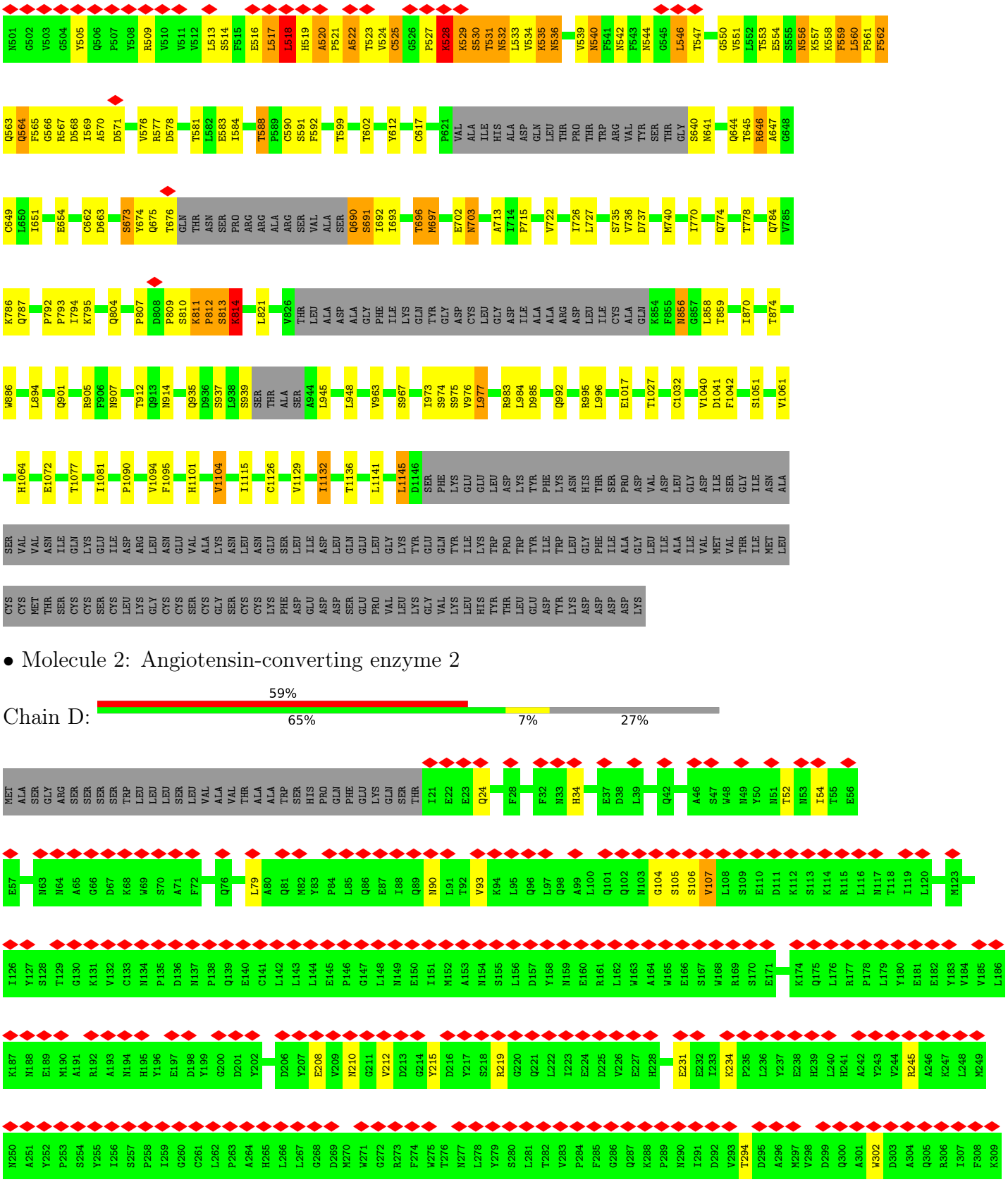
V511 V512 L513 S514 F515 E516 L517 L518 H519 A520 P521 A522 T523 V524 C525 C526 P527 K528 K529 S530 T531 N532 L533 V534 K535 C538 V539 N540 F541 N542 F543 N544 G545 L546 T549 L552 T553 E554 S555 N556 K557 K558 F559 L560 P561 F562 Q563 Q564 F565 D568 I569 A570 D571 A575 V576



- Molecule 1: Spike glycoprotein

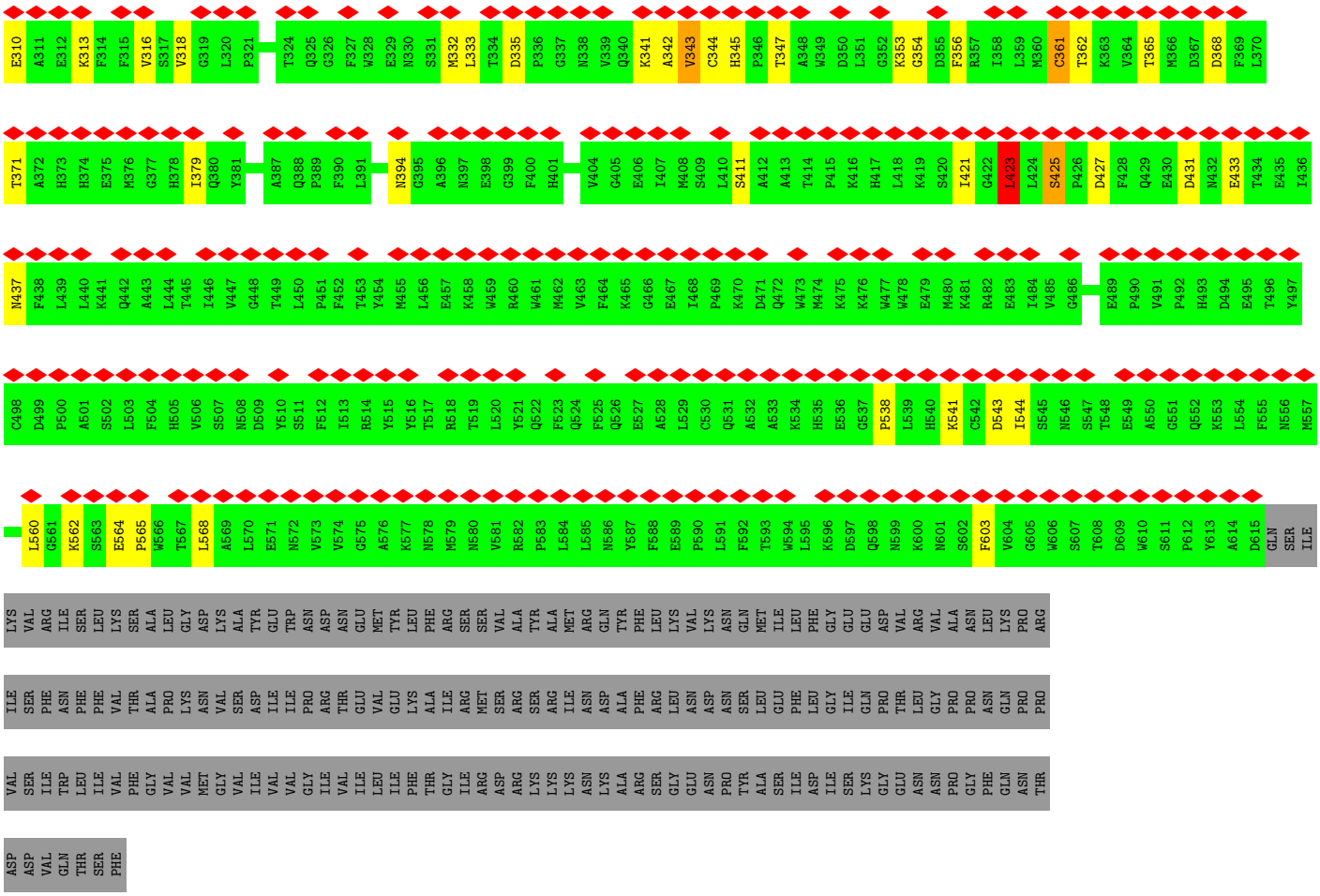
Chain C:





- Molecule 2: Angiotensin-converting enzyme 2

Chain D:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

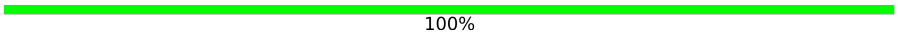
Chain E:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

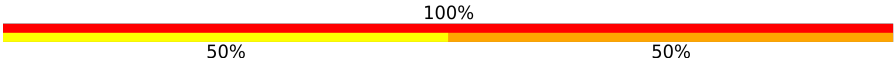
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

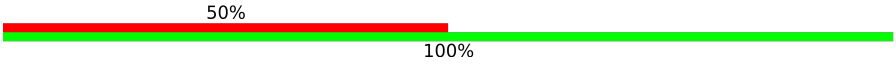
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

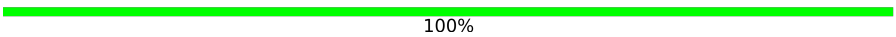
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

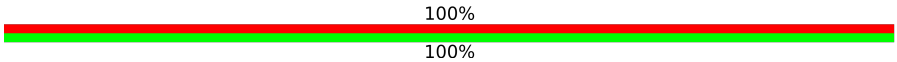
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

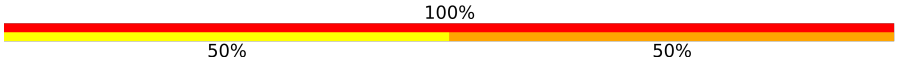
Chain R: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

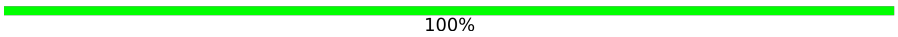
Chain U:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



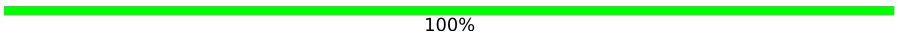
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

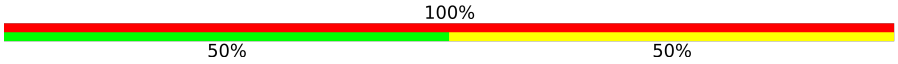
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

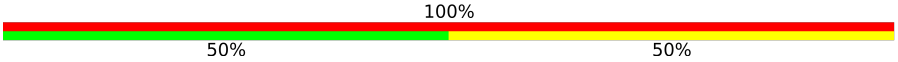
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

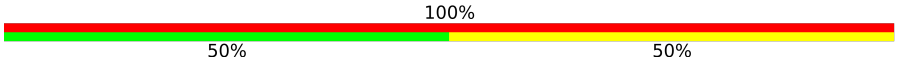
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 

NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23551	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.58	0/8048	0.55	0/10947
1	B	0.58	0/7751	0.55	0/10544
1	C	0.58	0/7751	0.54	0/10544
2	D	0.35	0/4994	0.50	0/6785
All	All	0.54	0/28544	0.54	0/38820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7872	0	7671	376	0
1	B	7584	0	7405	389	0
1	C	7584	0	7405	428	0
2	D	4857	0	4624	66	0
3	E	28	0	25	1	0
3	F	28	0	25	3	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	3	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	1	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	4	0
3	U	28	0	25	1	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	1	0
3	Y	28	0	25	2	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
4	A	126	0	117	4	0
4	B	140	0	129	8	0
4	C	112	0	104	4	0
4	D	14	0	13	0	0
All	All	29045	0	28143	1150	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 1150 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HG13	1:B:362:VAL:CG2	1.41	1.46
4:B:1409:NAG:O4	4:B:1410:NAG:C1	1.63	1.45
1:B:332:ILE:CG1	1:B:362:VAL:HG21	1.46	1.45
1:B:560:LEU:HB2	1:B:563:GLN:CG	1.49	1.41
1:A:703:ASN:HB2	1:B:787:GLN:OE1	1.28	1.32

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	989/1283 (77%)	865 (88%)	96 (10%)	28 (3%)	5 24
1	B	951/1283 (74%)	818 (86%)	103 (11%)	30 (3%)	4 22
1	C	951/1283 (74%)	817 (86%)	109 (12%)	25 (3%)	5 26
2	D	593/817 (73%)	564 (95%)	27 (5%)	2 (0%)	41 72
All	All	3484/4666 (75%)	3064 (88%)	335 (10%)	85 (2%)	9 28

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	331	ASN
1	A	518	LEU
1	A	691	SER
1	A	701	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	882/1122 (79%)	775 (88%)	107 (12%)	5 18
1	B	850/1122 (76%)	750 (88%)	100 (12%)	5 19
1	C	850/1122 (76%)	758 (89%)	92 (11%)	6 24
2	D	525/721 (73%)	518 (99%)	7 (1%)	69 84
All	All	3107/4087 (76%)	2801 (90%)	306 (10%)	11 28

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	317	ASN
1	C	974	SER
1	C	355	ARG
1	C	553	THR
2	D	344	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	239	GLN
1	C	703	ASN
1	C	360	ASN
1	C	540	ASN
1	C	907	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)

54 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	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.55	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.24	0	17,19,21	0.59	0
3	NAG	F	1	3,1	14,14,15	0.58	1 (7%)	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.45	0
3	NAG	G	1	3,1	14,14,15	0.31	0	17,19,21	0.62	0
3	NAG	G	2	3	14,14,15	0.53	0	17,19,21	0.48	0
3	NAG	H	1	3,1	14,14,15	0.38	0	17,19,21	0.72	0
3	NAG	H	2	3	14,14,15	0.28	0	17,19,21	1.32	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.70	1 (7%)	17,19,21	0.71	0
3	NAG	I	2	3	14,14,15	0.40	0	17,19,21	1.40	3 (17%)
3	NAG	J	1	3,1	14,14,15	0.71	1 (7%)	17,19,21	0.67	0
3	NAG	J	2	3	14,14,15	0.29	0	17,19,21	0.65	0
3	NAG	K	1	3,1	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
3	NAG	K	2	3	14,14,15	0.18	0	17,19,21	0.48	0
3	NAG	L	1	3,1	14,14,15	0.53	0	17,19,21	0.50	0
3	NAG	L	2	3	14,14,15	0.24	0	17,19,21	0.58	0
3	NAG	M	1	3,1	14,14,15	0.59	1 (7%)	17,19,21	0.56	0
3	NAG	M	2	3	14,14,15	0.29	0	17,19,21	0.45	0
3	NAG	N	1	3,1	14,14,15	0.32	0	17,19,21	0.41	0
3	NAG	N	2	3	14,14,15	0.36	0	17,19,21	0.36	0
3	NAG	O	1	3,1	14,14,15	0.35	0	17,19,21	1.14	1 (5%)
3	NAG	O	2	3	14,14,15	0.27	0	17,19,21	0.47	0
3	NAG	P	1	3,1	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
3	NAG	P	2	3	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	Q	1	3,1	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	Q	2	3	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	R	2	3	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	S	1	3,1	14,14,15	0.55	0	17,19,21	0.50	0
3	NAG	S	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	T	1	3,1	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
3	NAG	T	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	U	1	3,1	14,14,15	0.23	0	17,19,21	1.37	1 (5%)
3	NAG	U	2	3	14,14,15	0.18	0	17,19,21	0.50	0
3	NAG	V	1	3,1	14,14,15	0.55	0	17,19,21	0.71	1 (5%)
3	NAG	V	2	3	14,14,15	0.38	0	17,19,21	0.47	0
3	NAG	W	1	3,1	14,14,15	0.38	0	17,19,21	0.40	0
3	NAG	W	2	3	14,14,15	0.21	0	17,19,21	0.74	0
3	NAG	X	1	3,1	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	X	2	3	14,14,15	0.55	0	17,19,21	1.30	1 (5%)
3	NAG	Y	1	3,1	14,14,15	0.63	1 (7%)	17,19,21	0.44	0
3	NAG	Y	2	3	14,14,15	0.33	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	Z	1	3,1	14,14,15	0.40	0	17,19,21	0.45	0
3	NAG	Z	2	3	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	a	1	2,3	14,14,15	0.60	1 (7%)	17,19,21	0.73	0
3	NAG	a	2	3	14,14,15	0.53	0	17,19,21	0.36	0
3	NAG	b	1	2,3	14,14,15	0.42	0	17,19,21	0.65	0
3	NAG	b	2	3	14,14,15	0.28	0	17,19,21	0.69	1 (5%)
3	NAG	c	1	2,3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	c	2	3	14,14,15	0.29	0	17,19,21	0.62	0
3	NAG	d	1	2,3	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	d	2	3	14,14,15	0.35	0	17,19,21	0.47	0
3	NAG	e	1	2,3	14,14,15	0.22	0	17,19,21	0.62	0
3	NAG	e	2	3	14,14,15	0.32	0	17,19,21	0.59	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	5/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1

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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	O5-C1	-2.69	1.39	1.43
3	J	1	NAG	O5-C1	-2.58	1.39	1.43
3	I	1	NAG	O5-C1	-2.37	1.39	1.43
3	Y	1	NAG	O5-C1	-2.12	1.40	1.43
3	a	1	NAG	O5-C1	-2.09	1.40	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1	NAG	C2-N2-C7	4.72	129.63	122.90
3	I	2	NAG	C2-N2-C7	4.43	129.21	122.90
3	Y	2	NAG	C2-N2-C7	4.37	129.13	122.90
3	H	2	NAG	C2-N2-C7	4.28	129.00	122.90
3	X	2	NAG	C2-N2-C7	4.28	128.99	122.90

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	c	1	NAG	O7-C7-N2-C2
3	c	2	NAG	C3-C2-N2-C7
3	c	2	NAG	C8-C7-N2-C2
3	c	2	NAG	O7-C7-N2-C2
3	c	1	NAG	C8-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Y	2	NAG	1	0
3	E	1	NAG	1	0
3	T	1	NAG	4	0
3	Q	2	NAG	1	0
3	F	1	NAG	3	0
3	H	2	NAG	1	0
3	T	2	NAG	2	0
3	I	2	NAG	1	0
3	Q	1	NAG	1	0
3	F	2	NAG	2	0
3	U	1	NAG	1	0
3	M	1	NAG	3	0
3	Y	1	NAG	1	0

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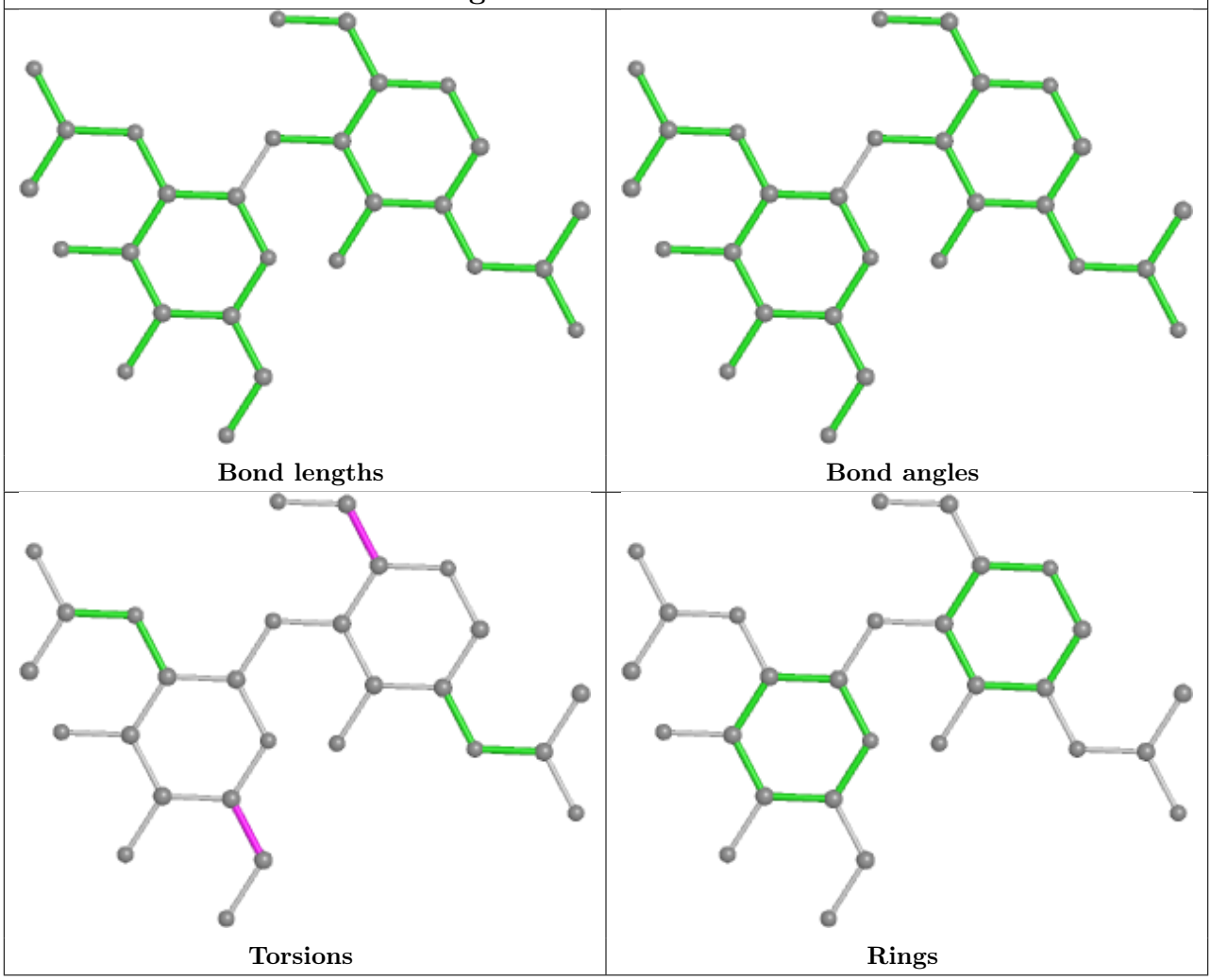
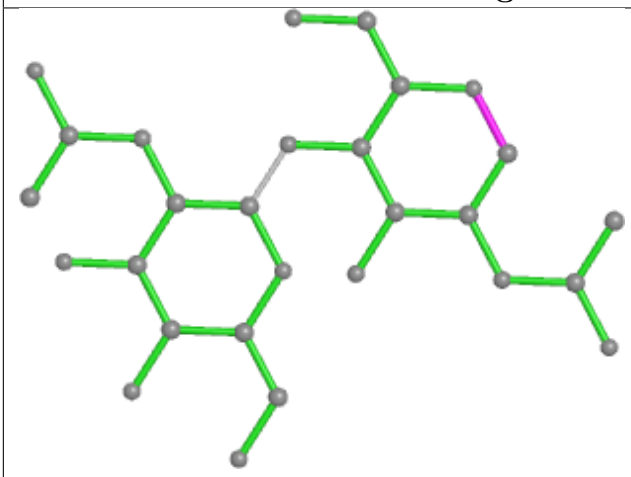
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2	NAG	1	0
3	M	2	NAG	2	0

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

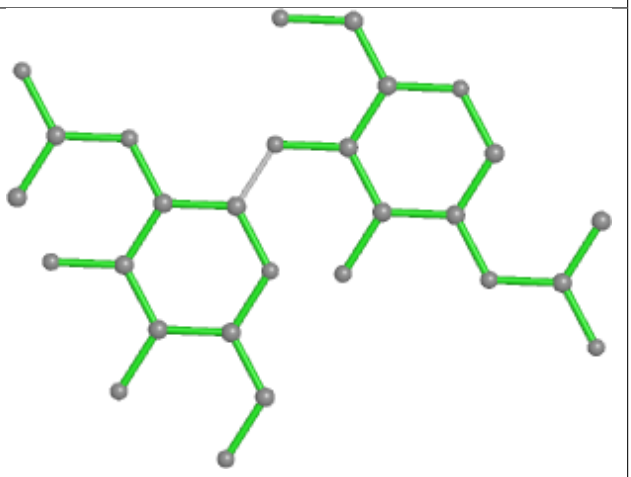
Oligosaccharide Chain E



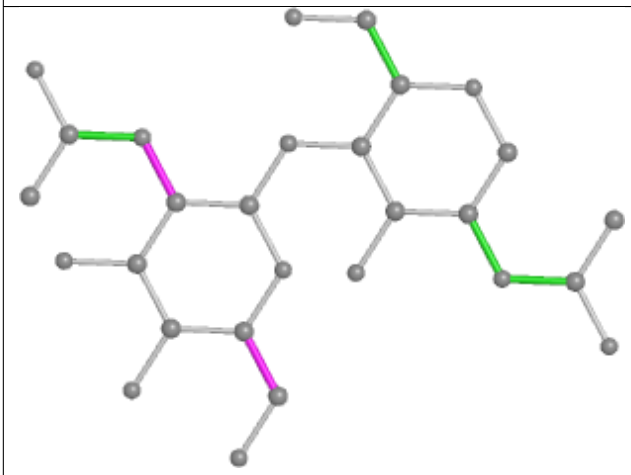
Oligosaccharide Chain F



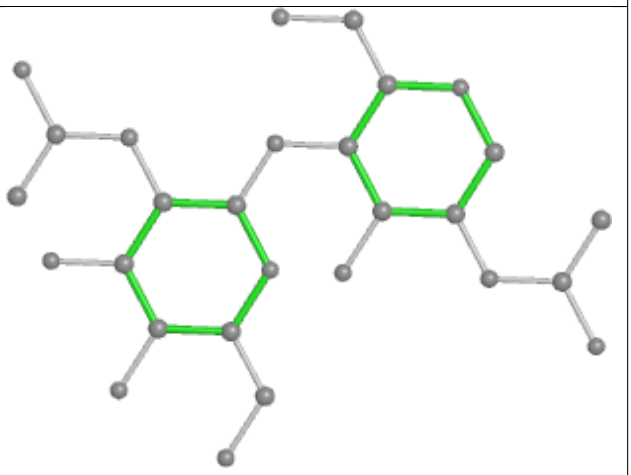
Bond lengths



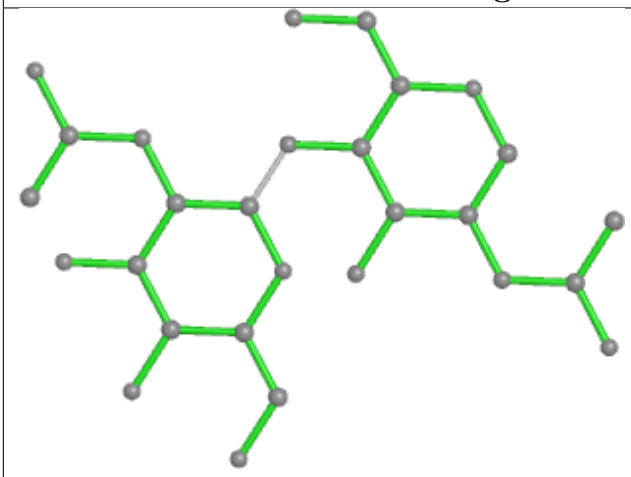
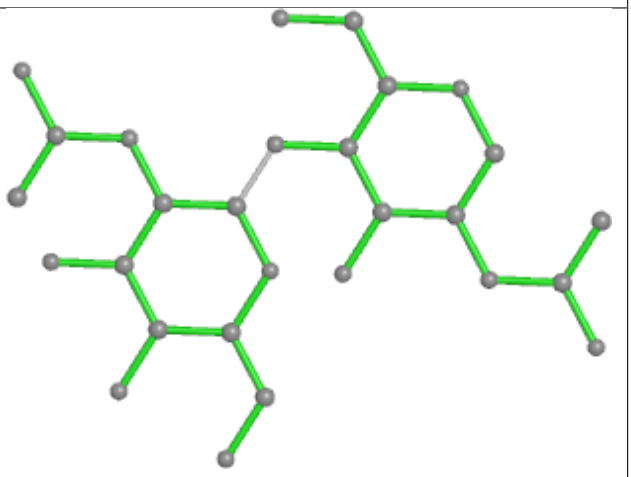
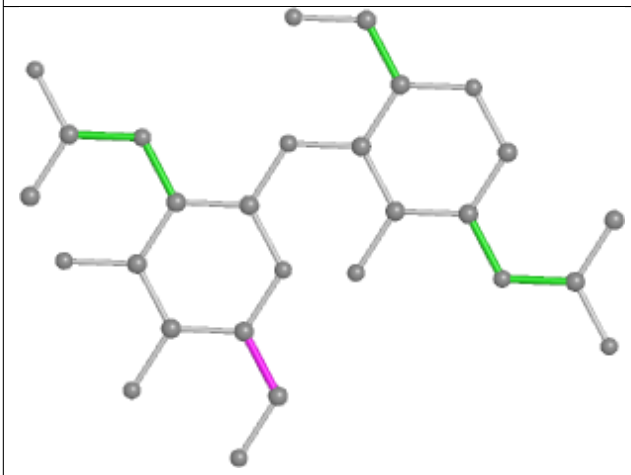
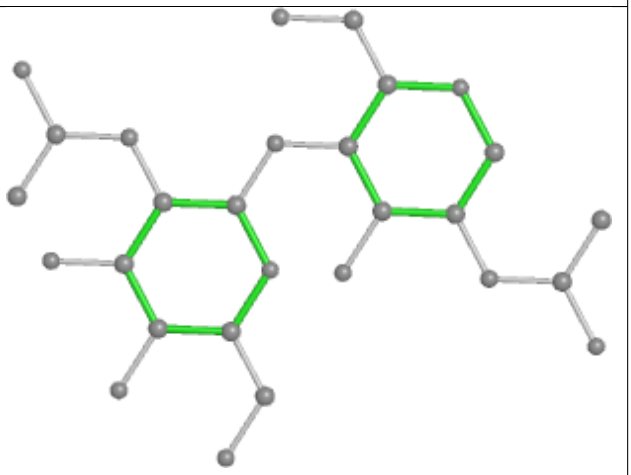
Bond angles

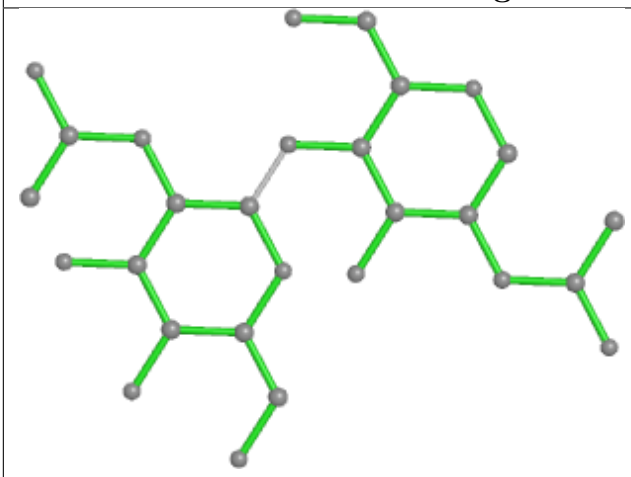
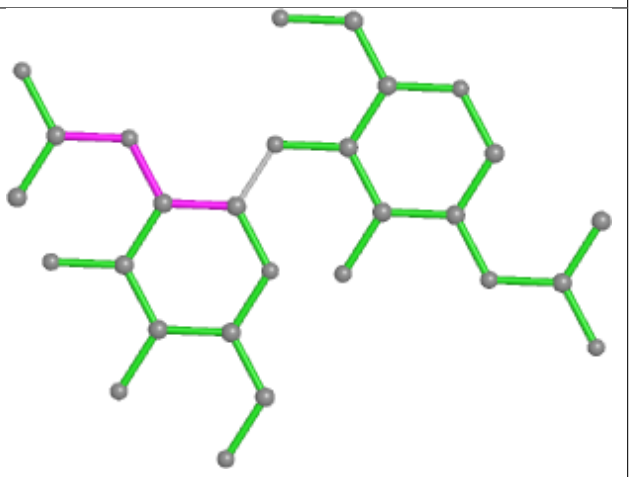
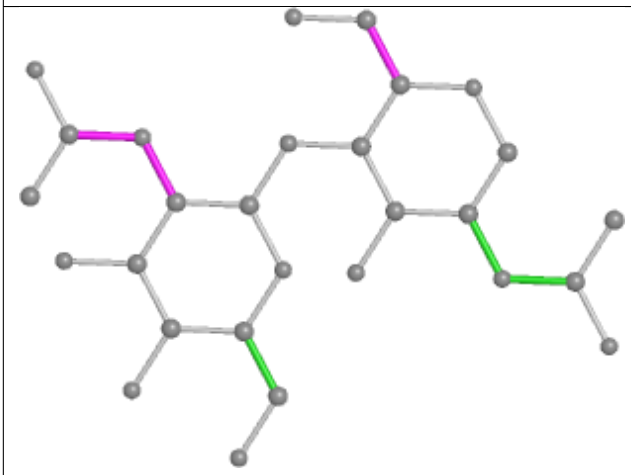
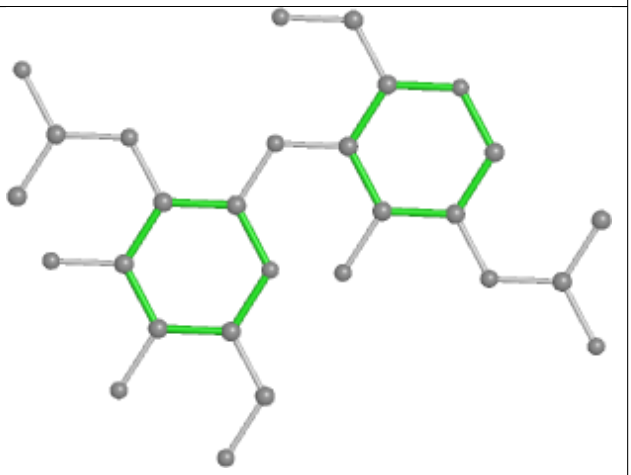


Torsions

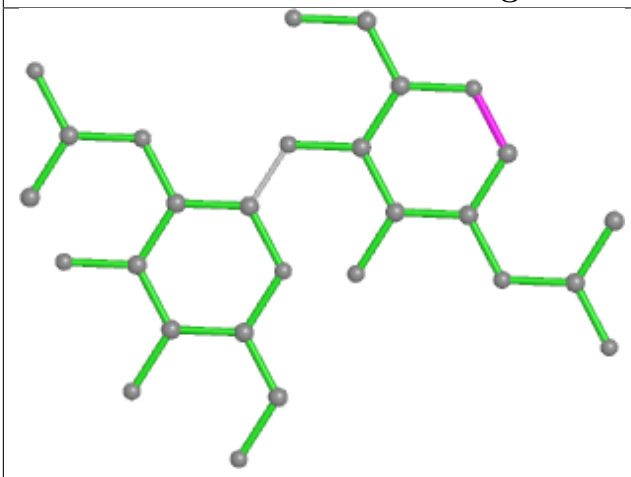


Rings

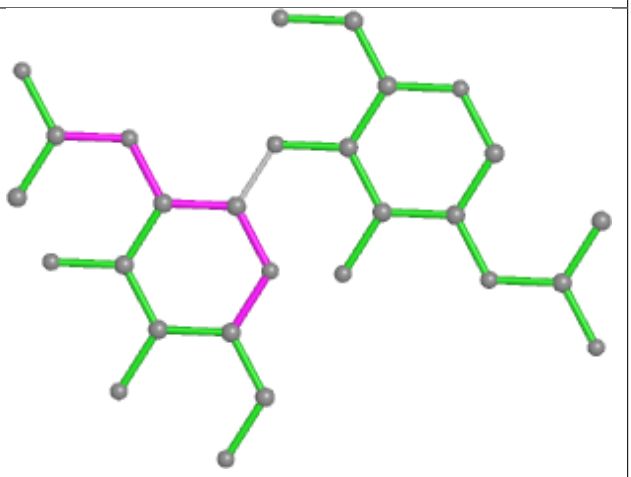
Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

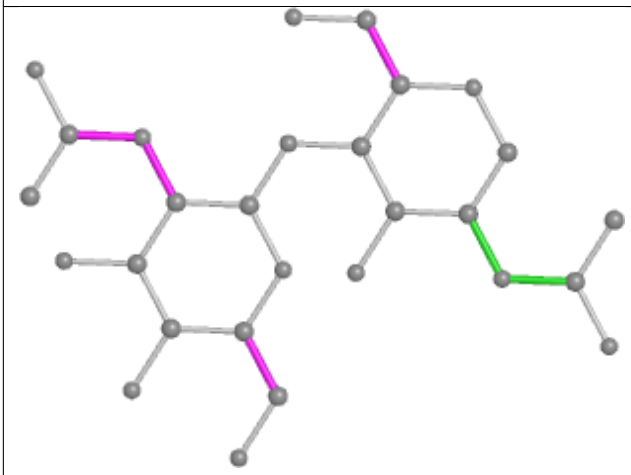
Oligosaccharide Chain I



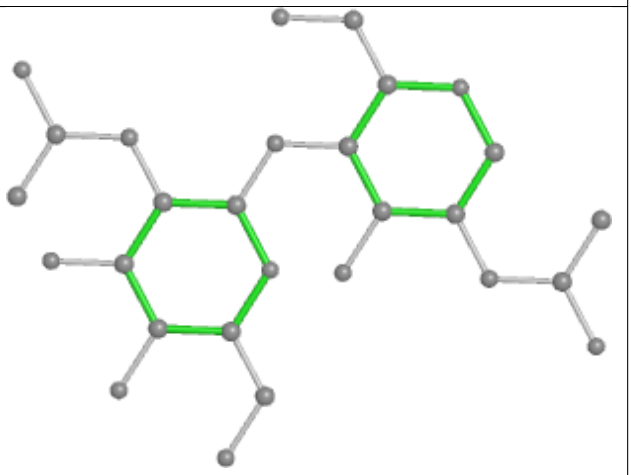
Bond lengths



Bond angles

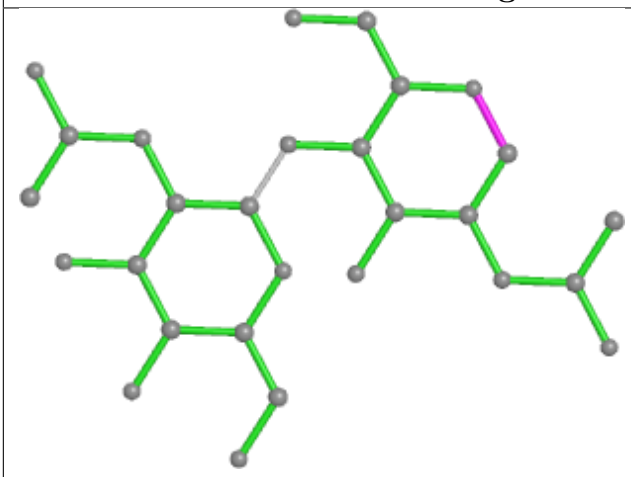


Torsions

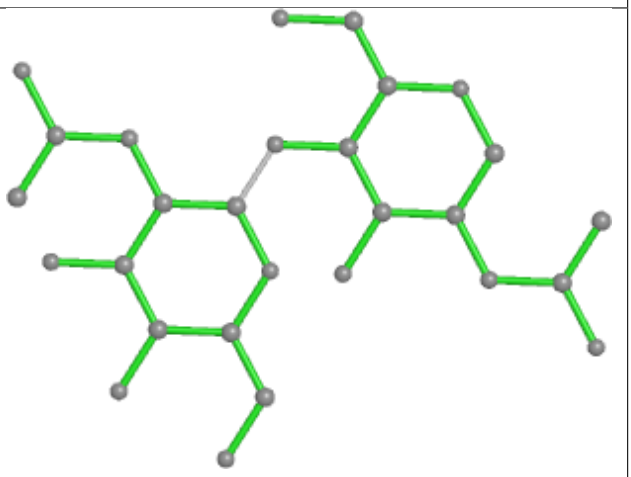


Rings

Oligosaccharide Chain J



Bond lengths



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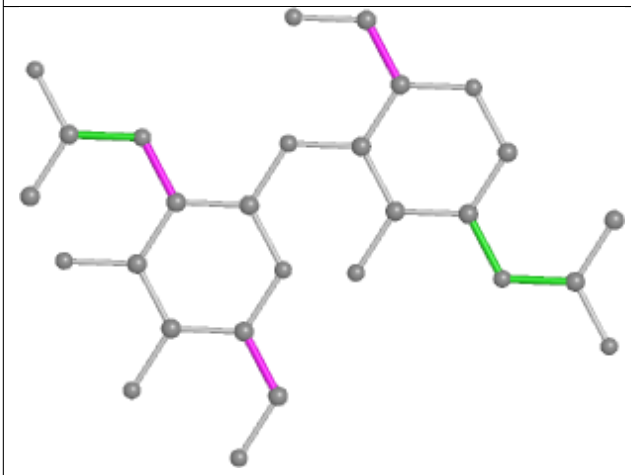

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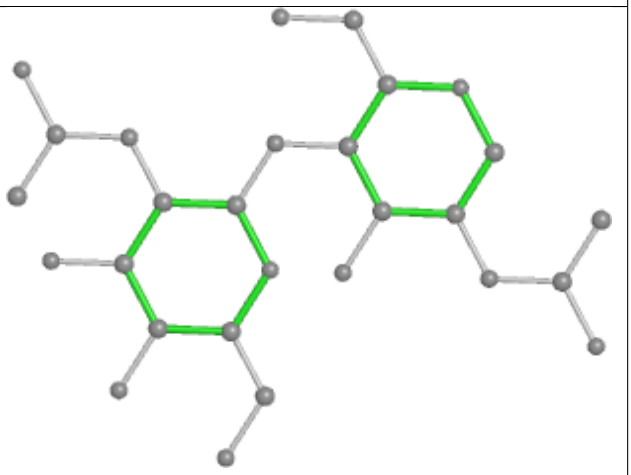
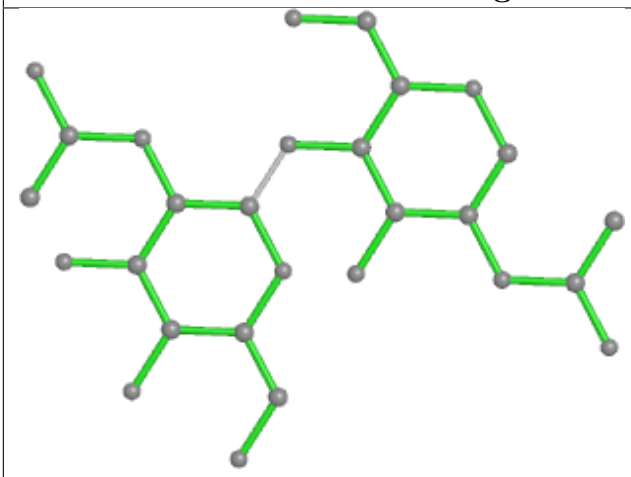
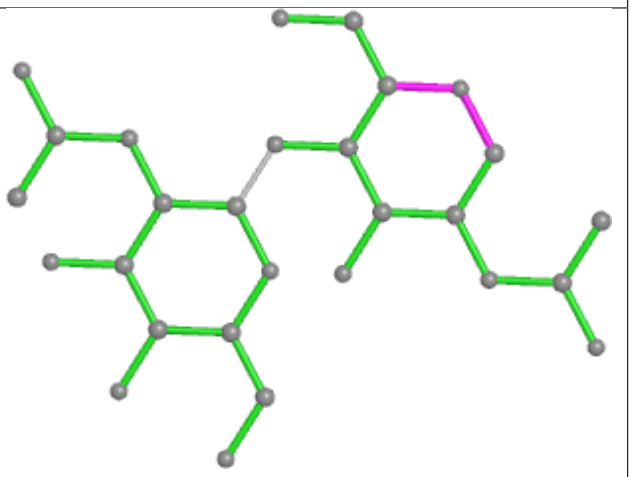
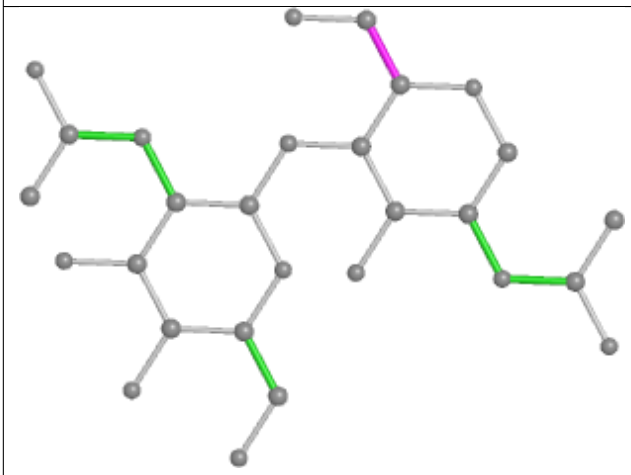
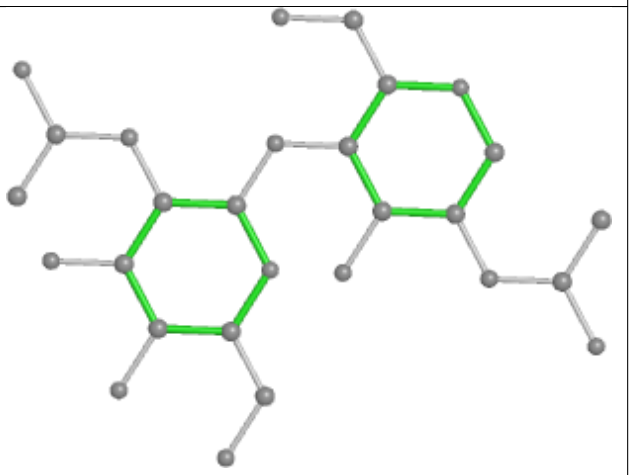
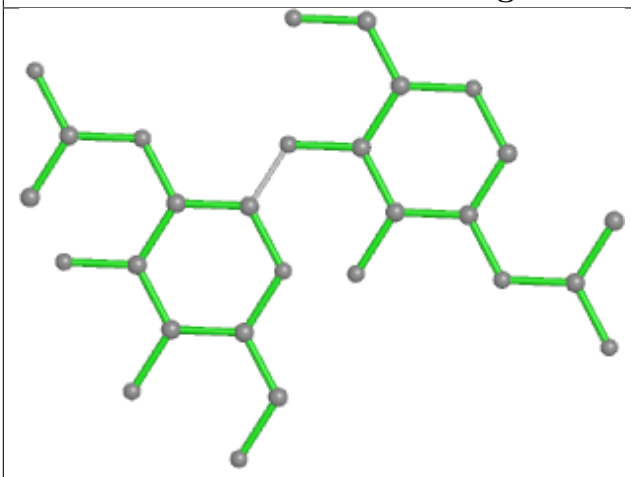


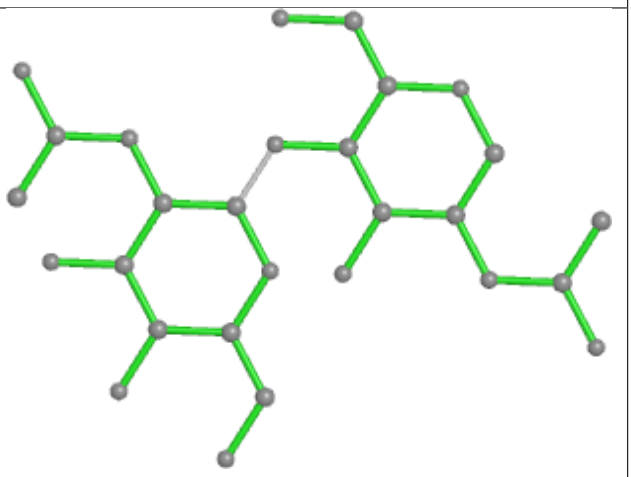
Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

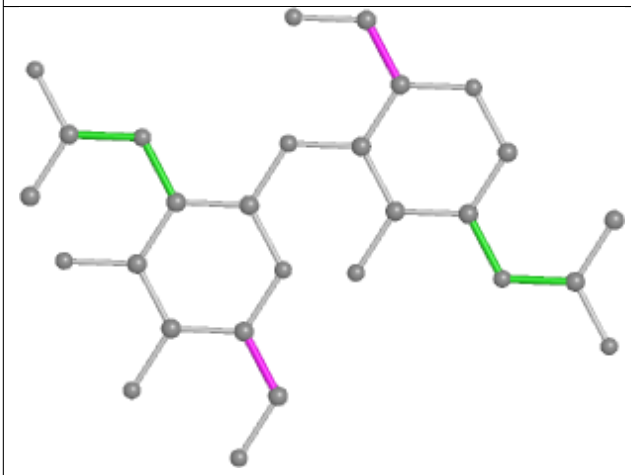
Oligosaccharide Chain L



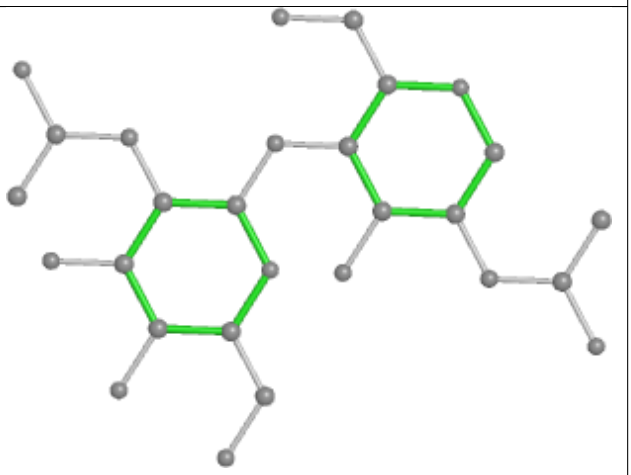
Bond lengths



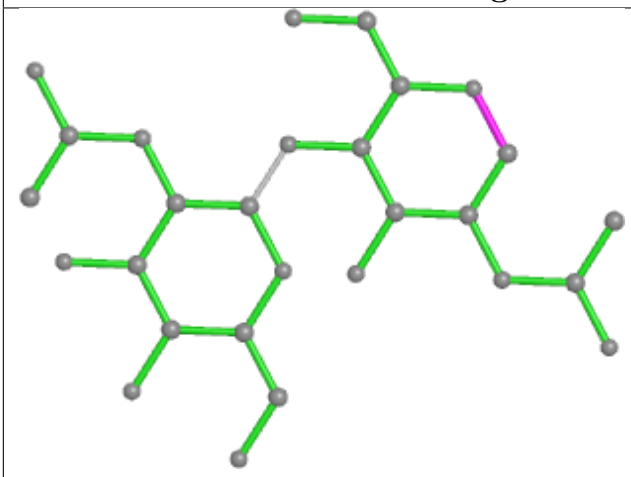
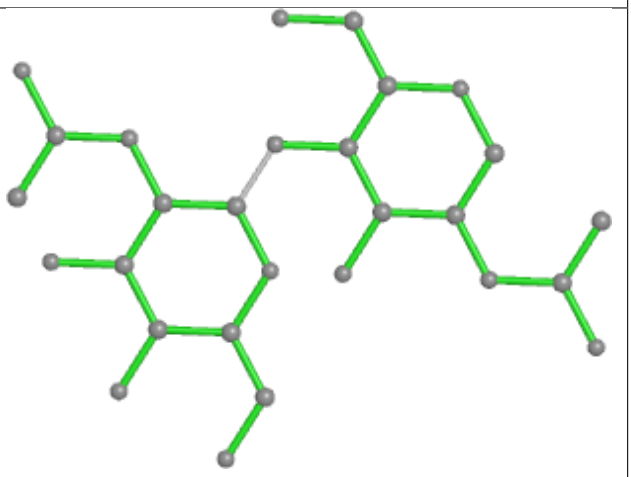
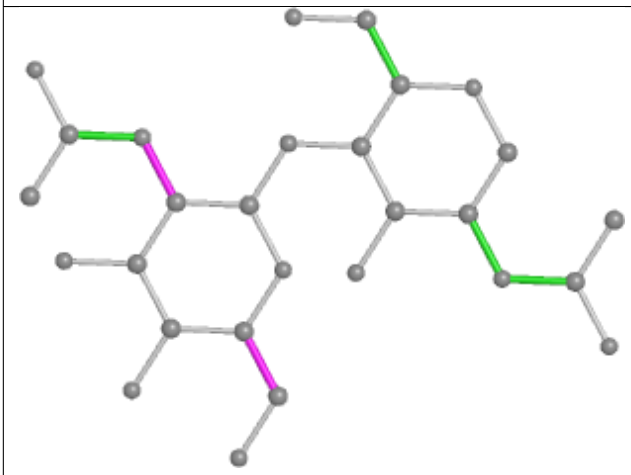
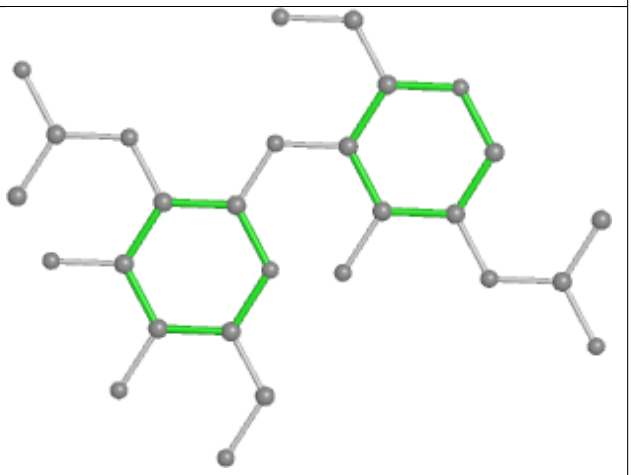
Bond angles

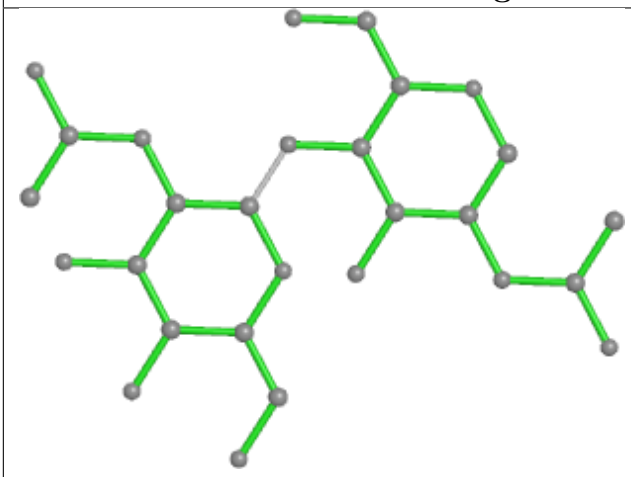
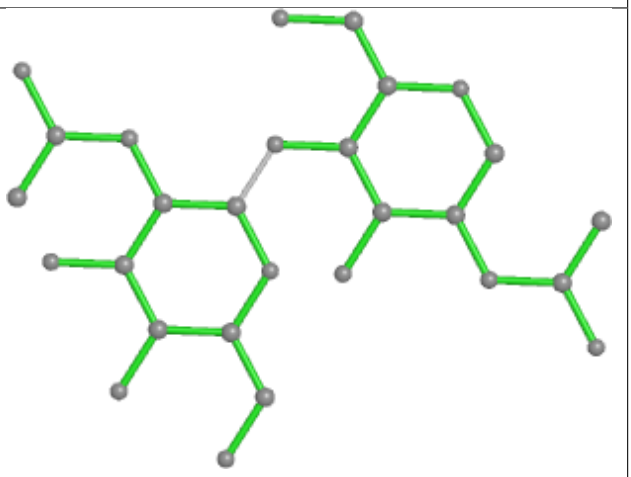
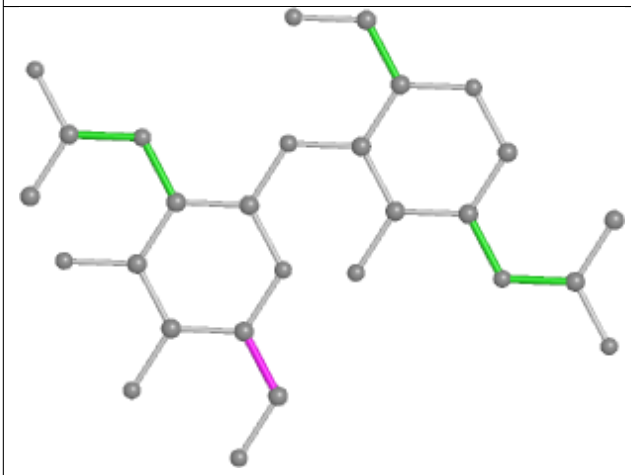
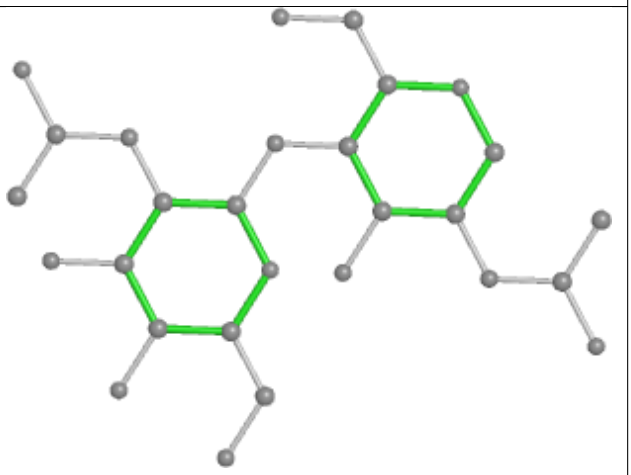


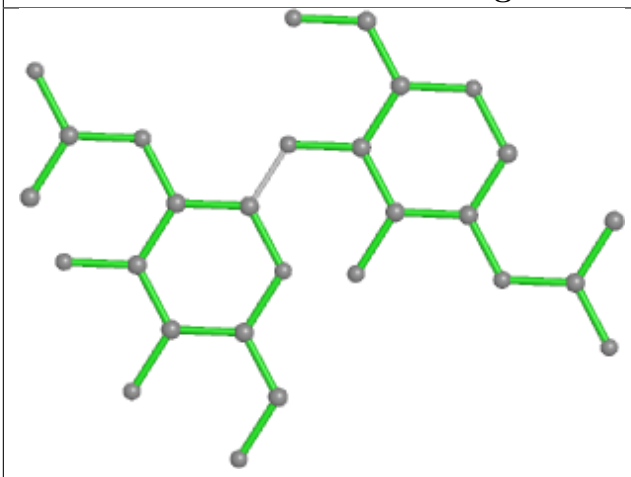
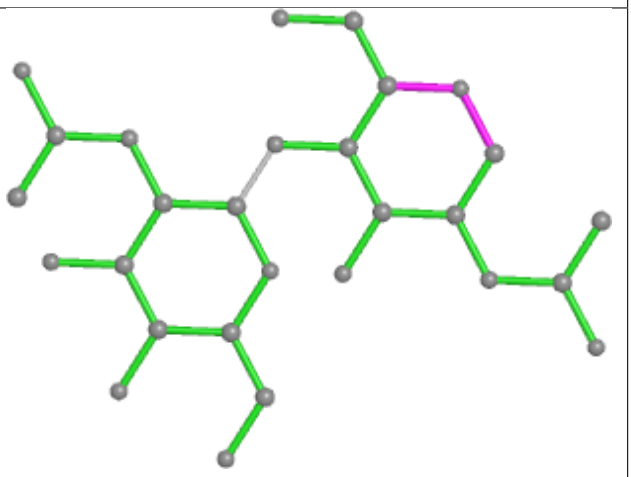
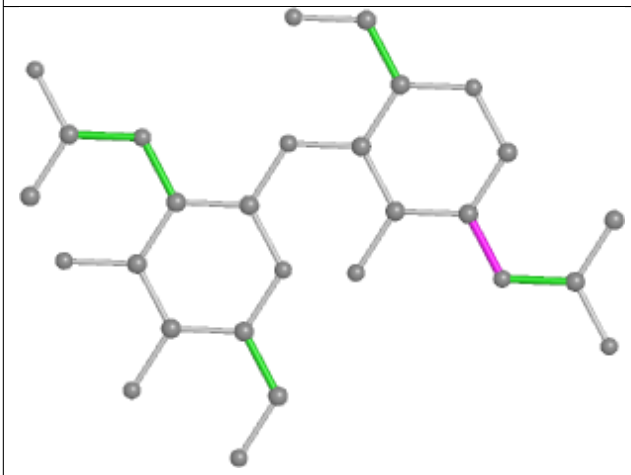
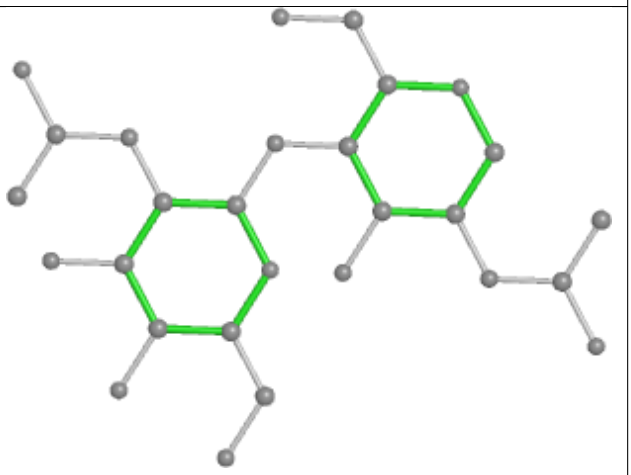
Torsions

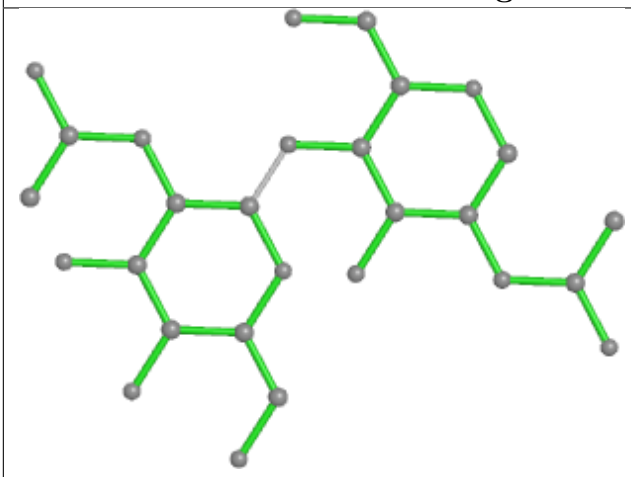
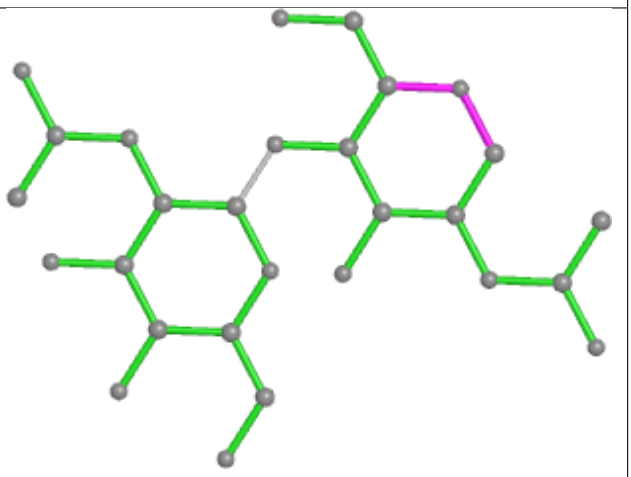
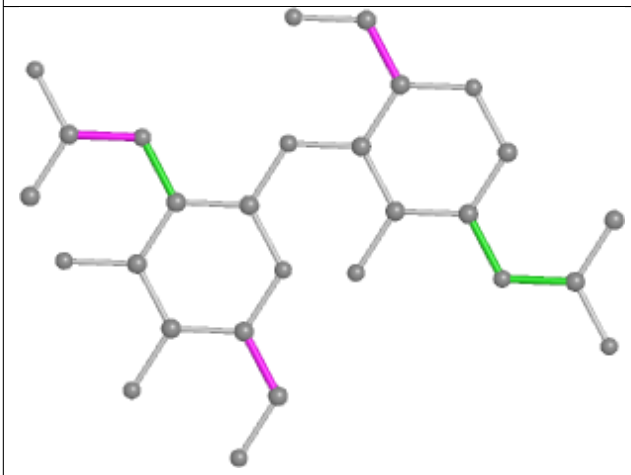
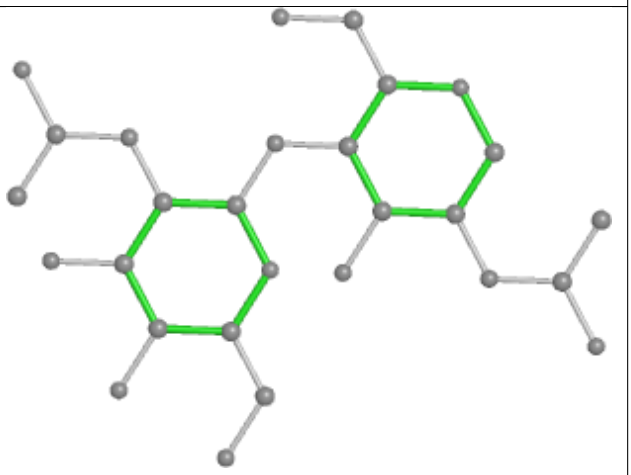


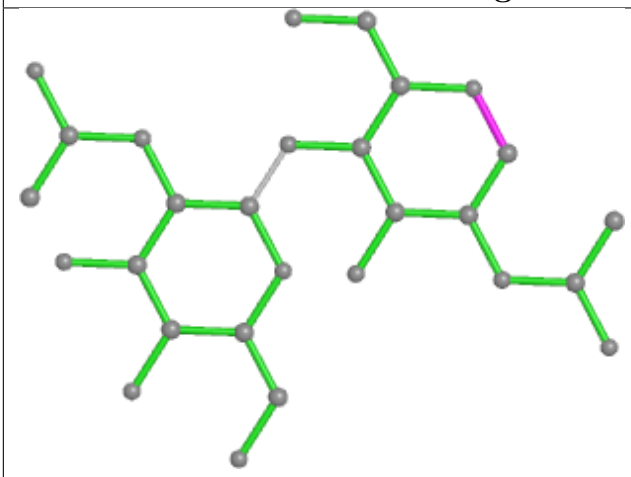
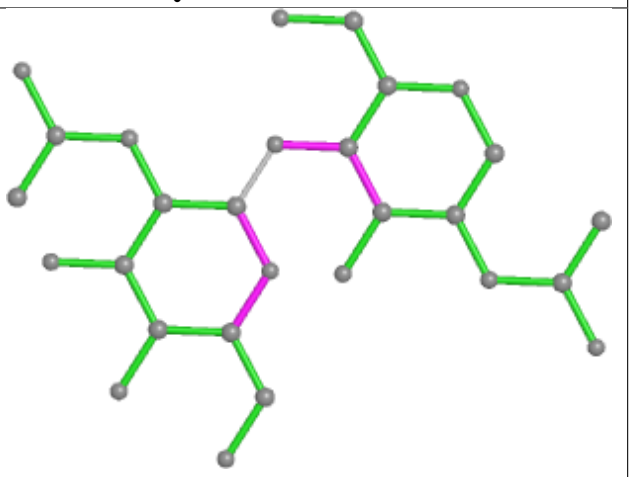
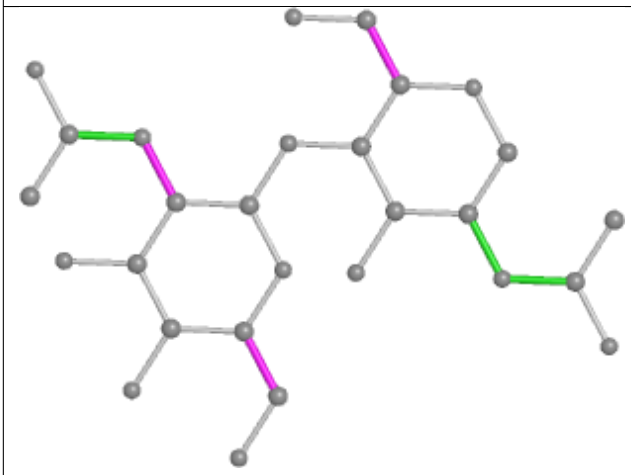
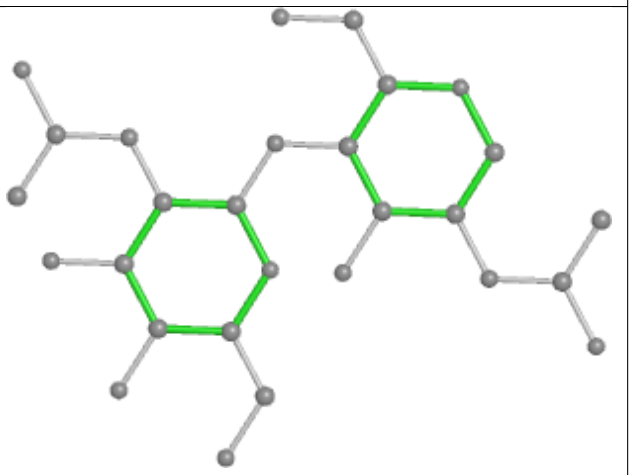
Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

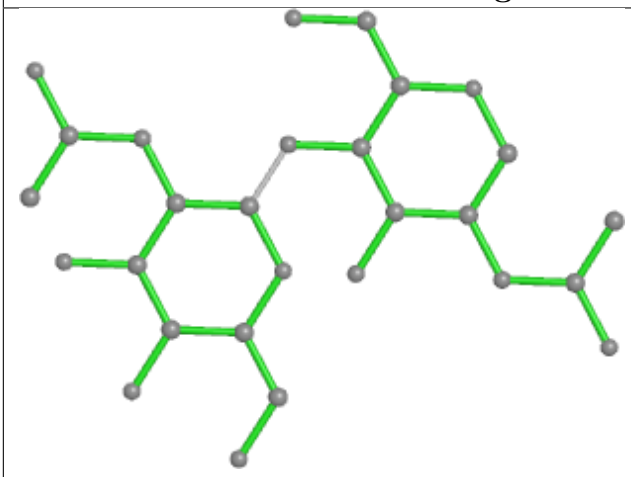
Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain R



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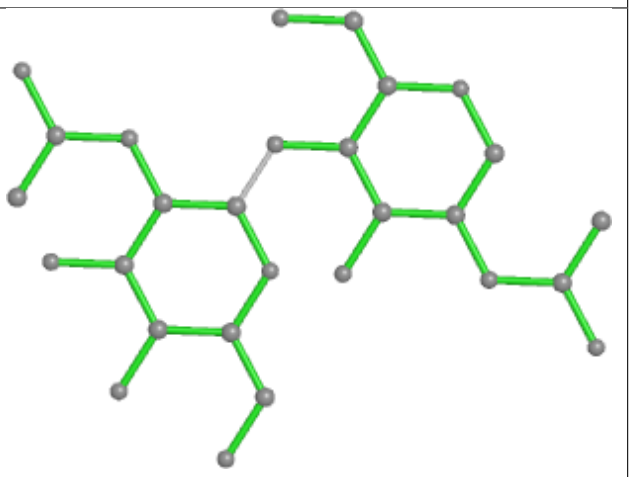

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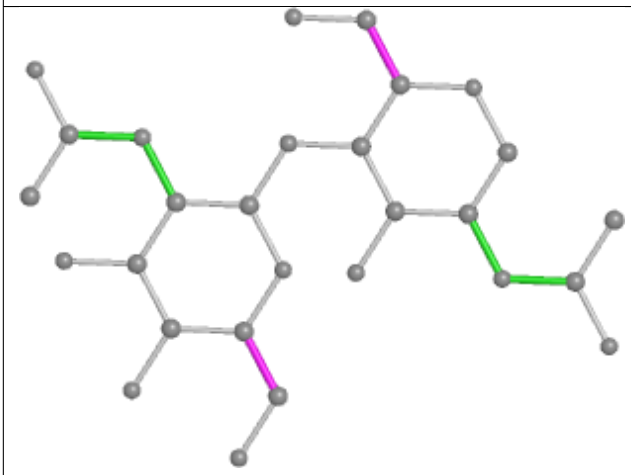

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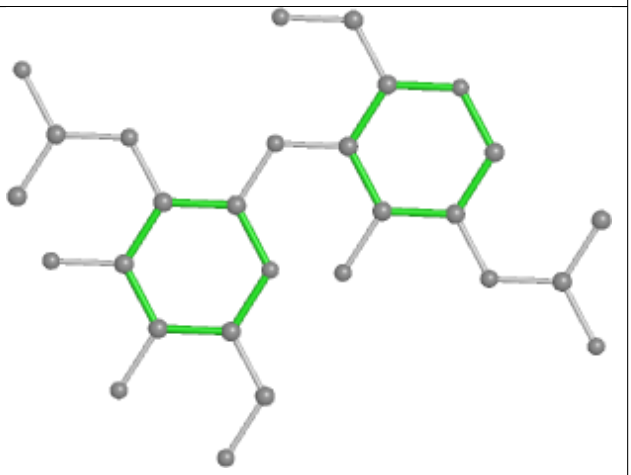

Rings

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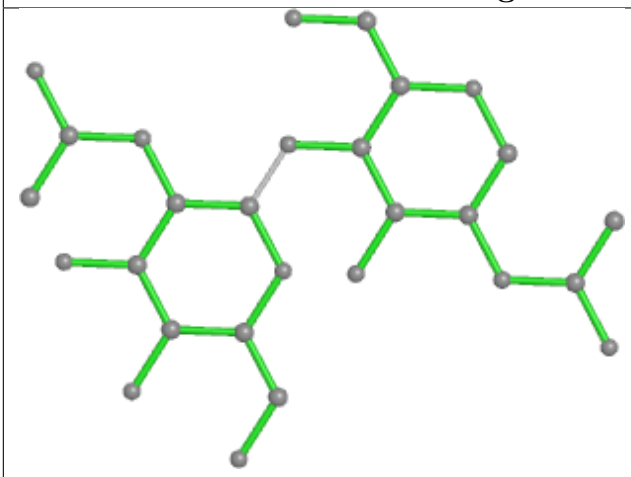
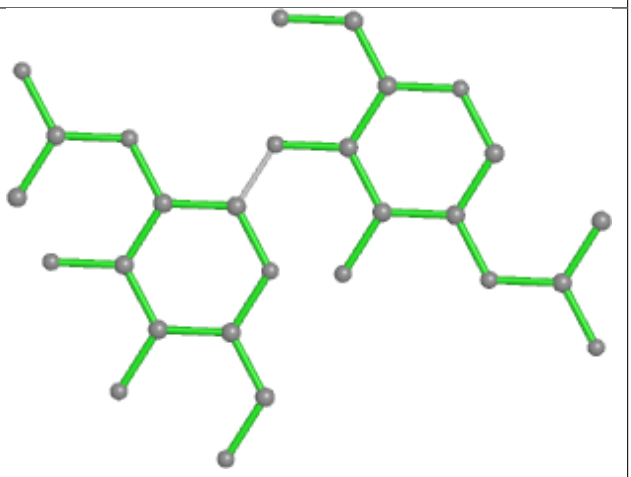
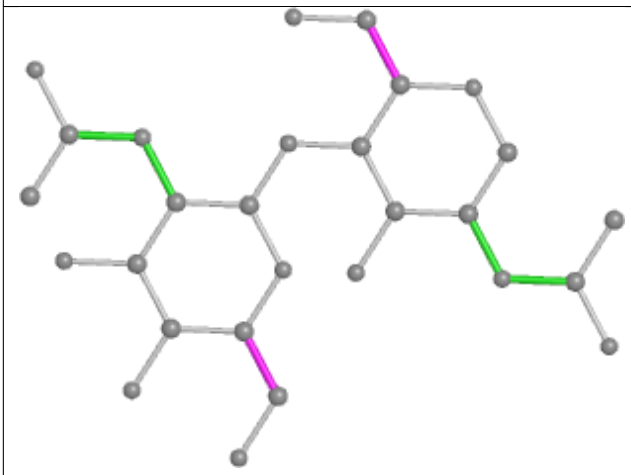
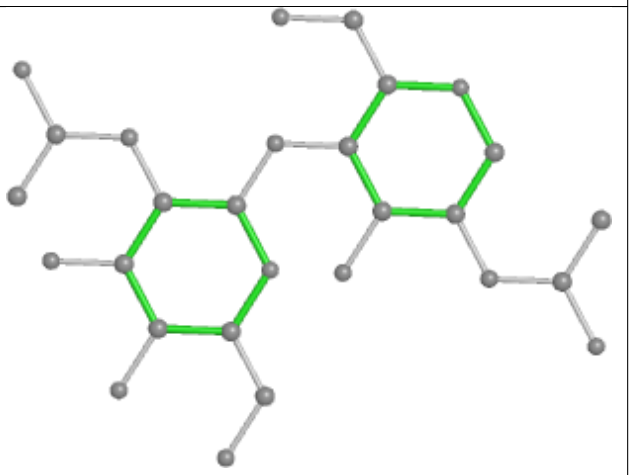
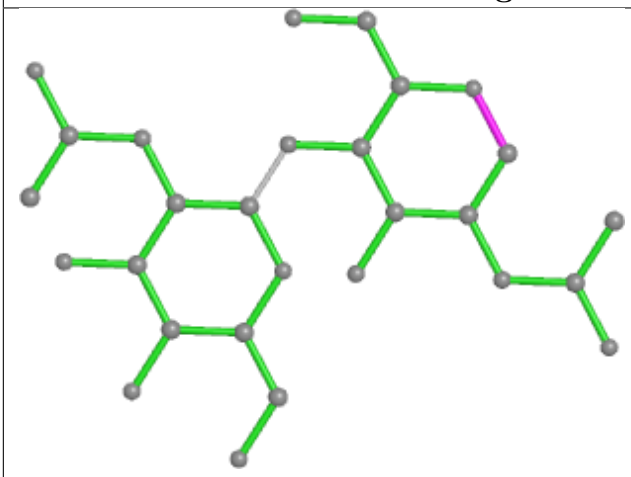
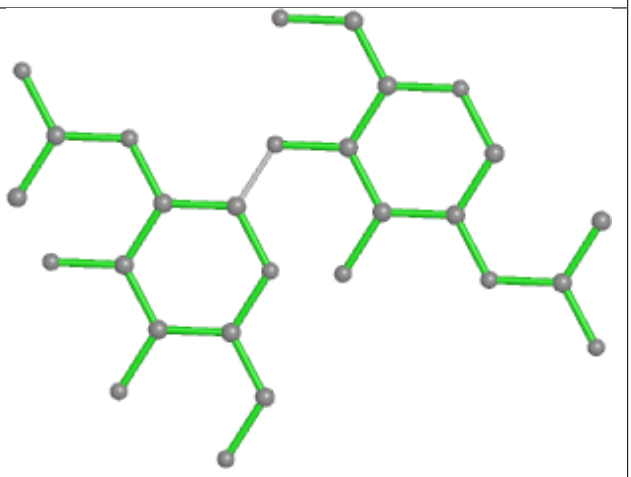
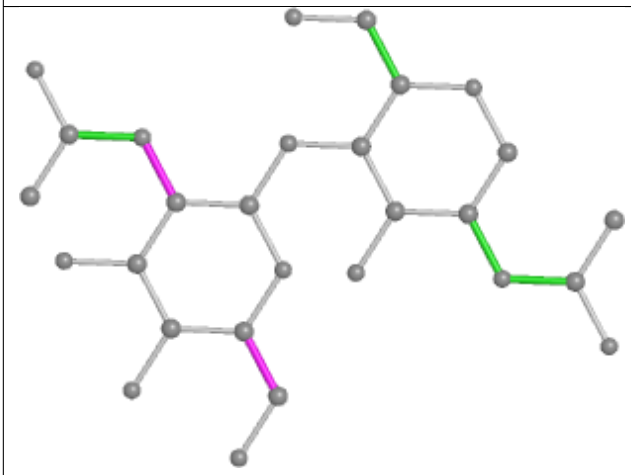
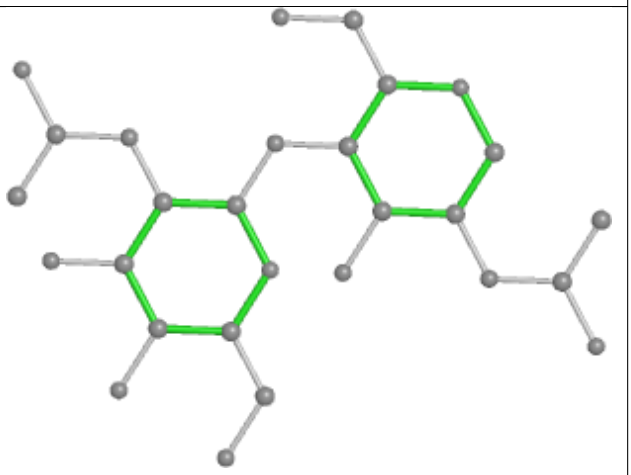
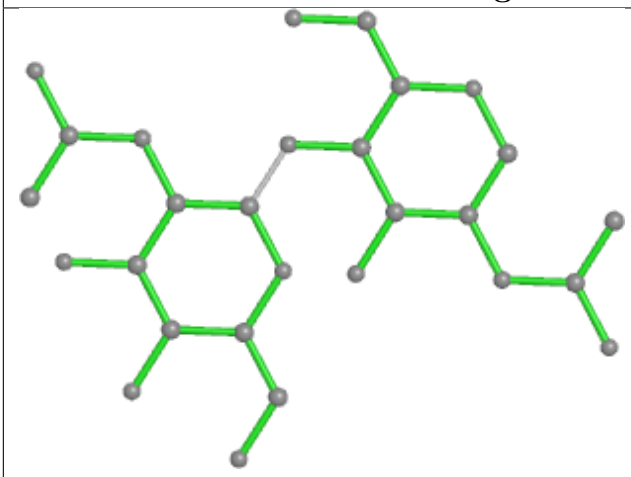
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain T	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain U



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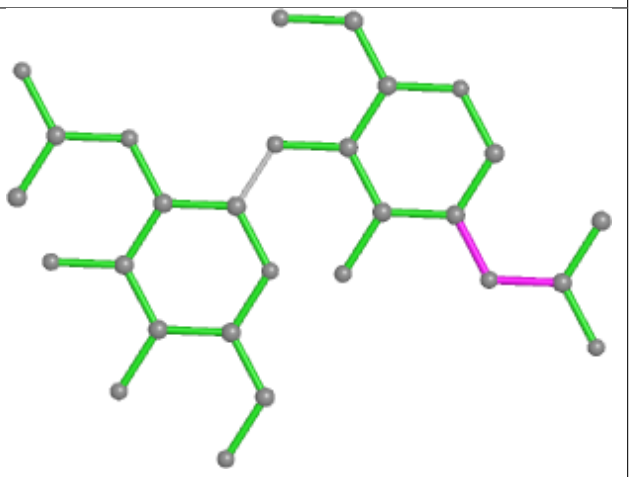

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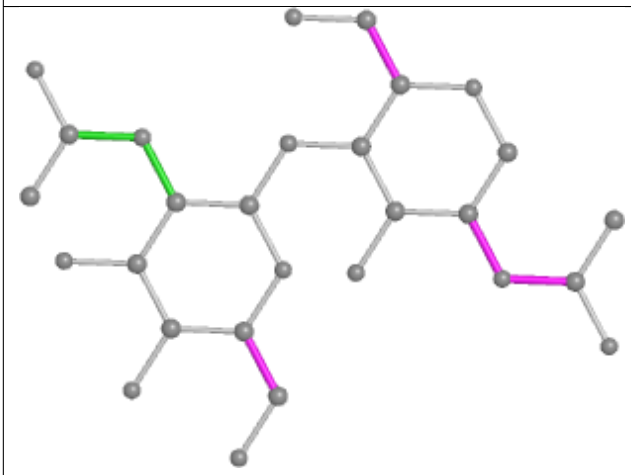

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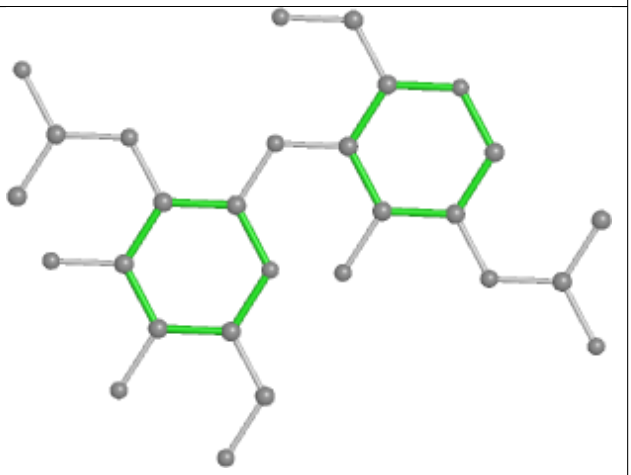

Rings

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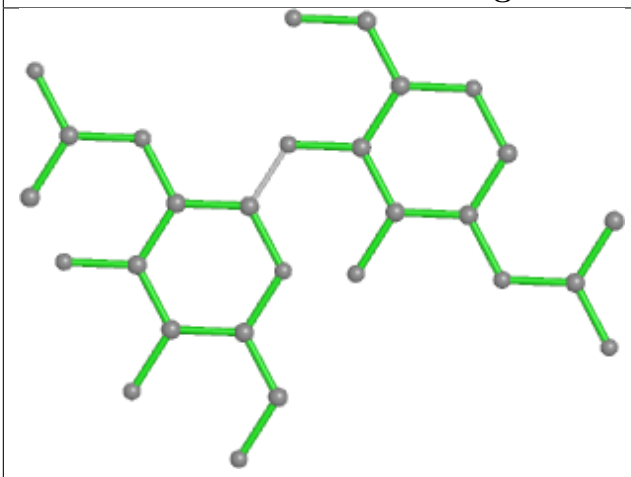
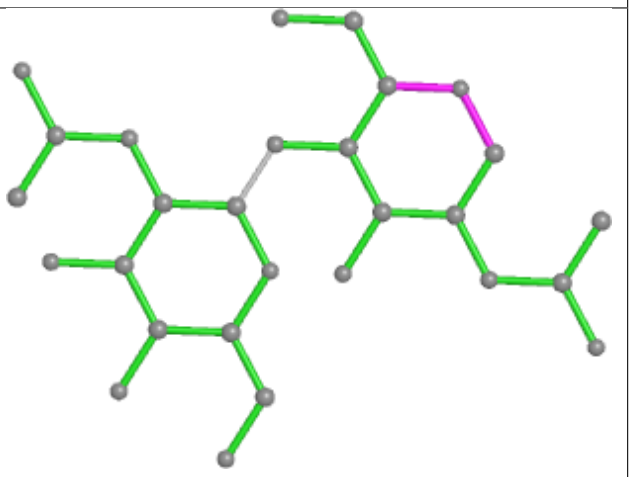
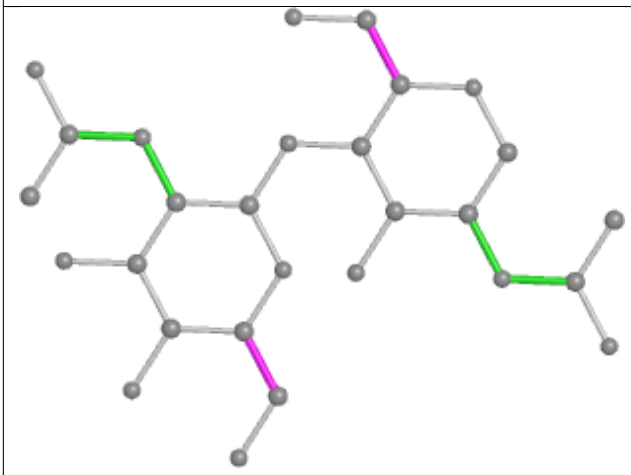
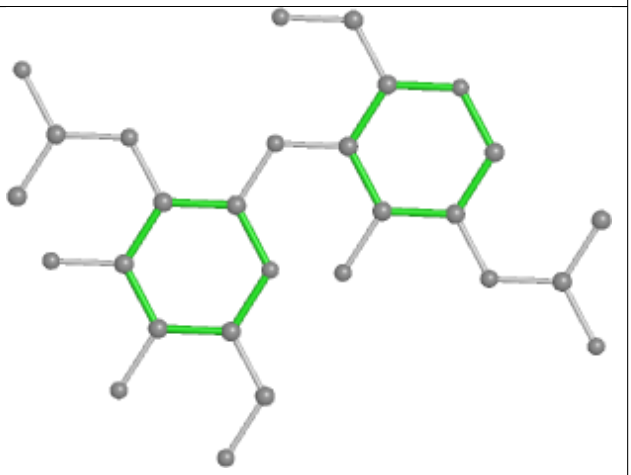
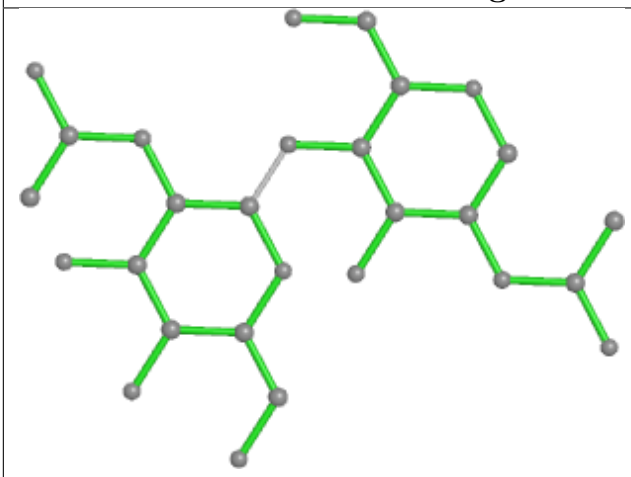
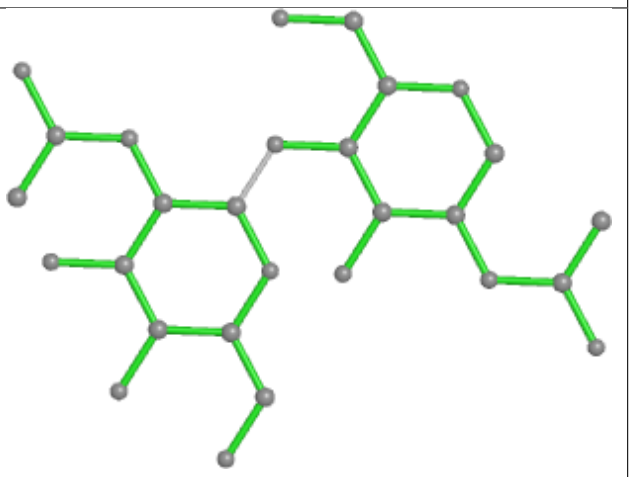
 Bond lengths	 Bond angles
 Torsions	 Rings

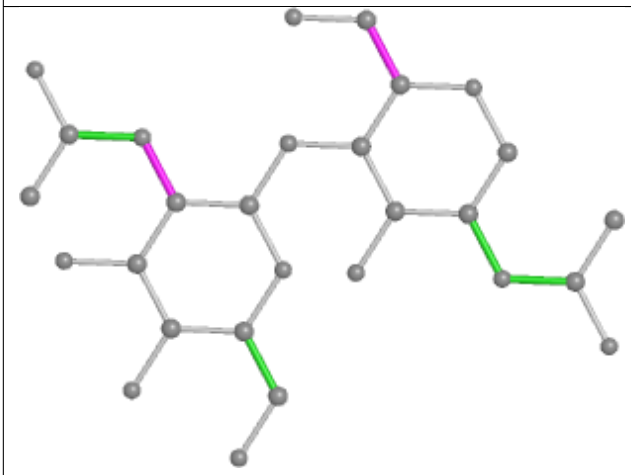
Oligosaccharide Chain W



Bond lengths



Bond angles



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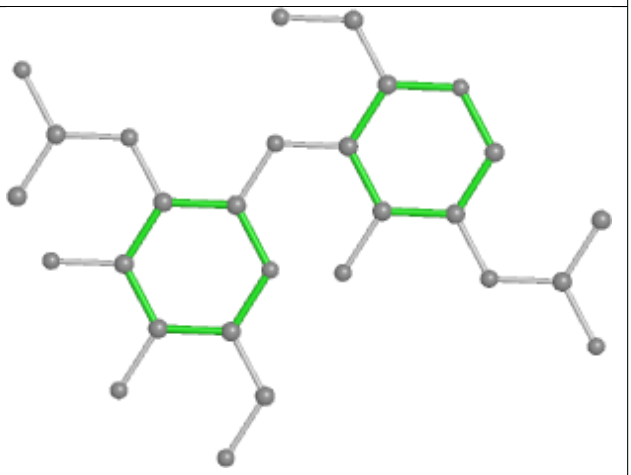
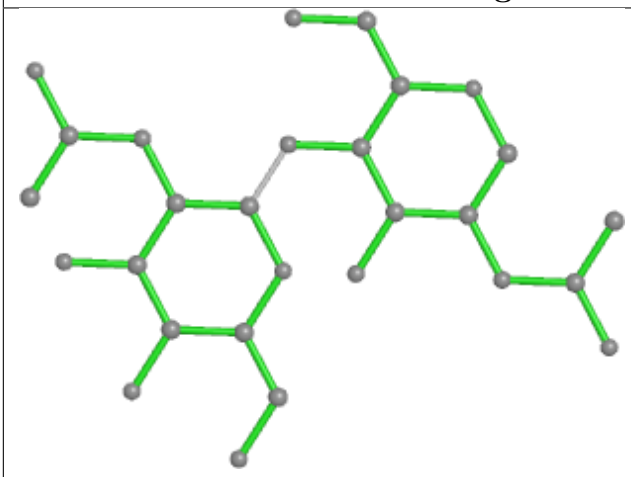
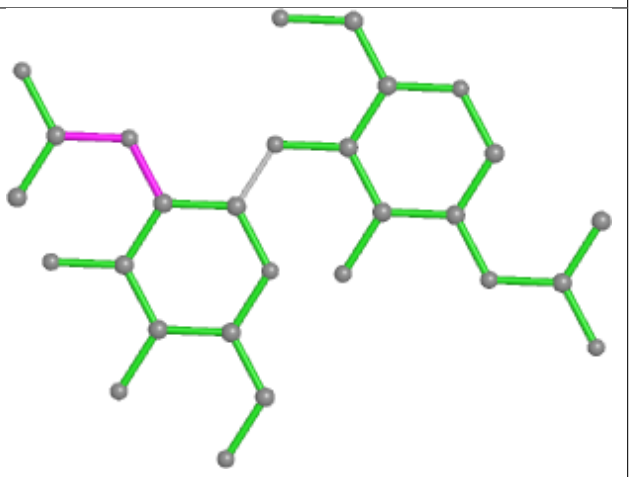
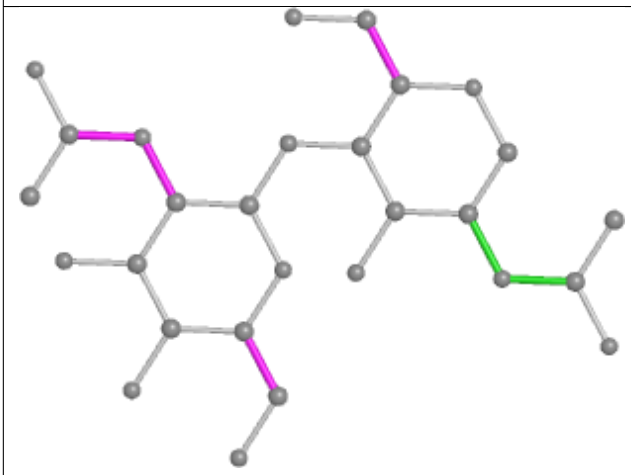
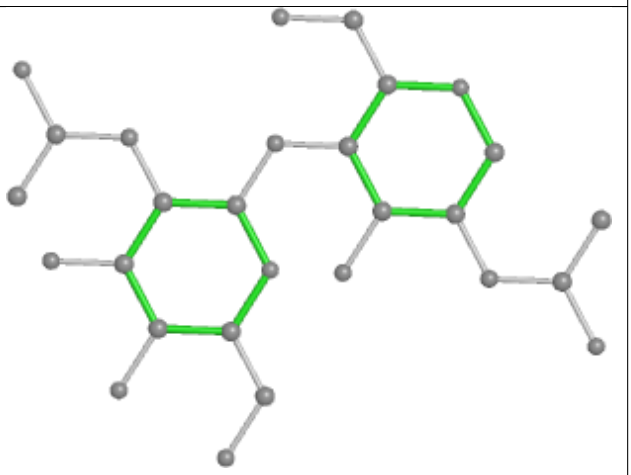
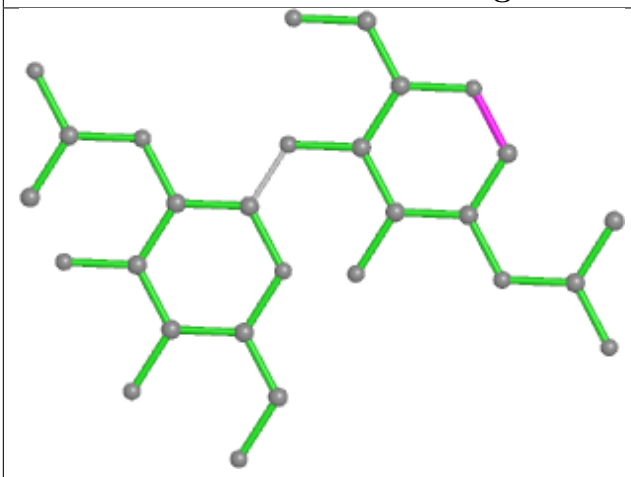


Rings

Oligosaccharide Chain X	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Y



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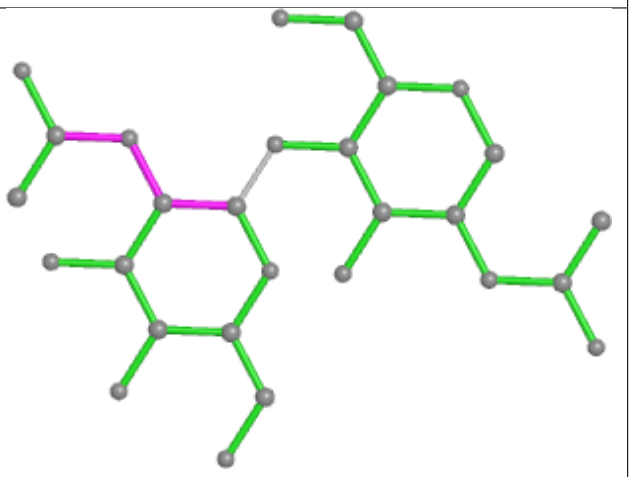

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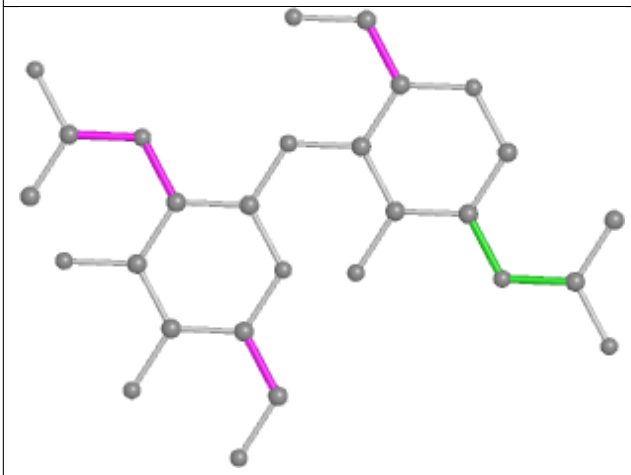

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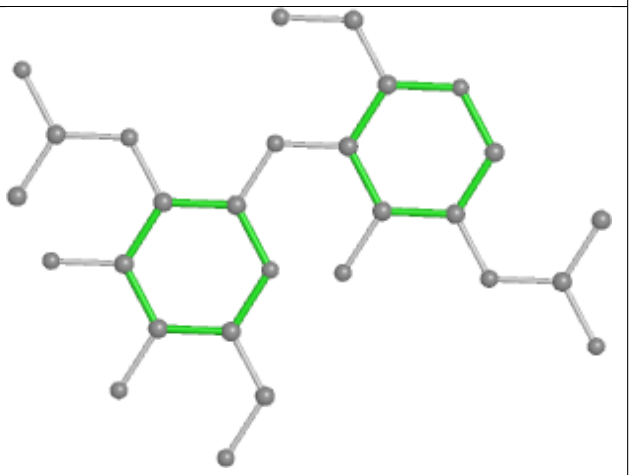

Rings

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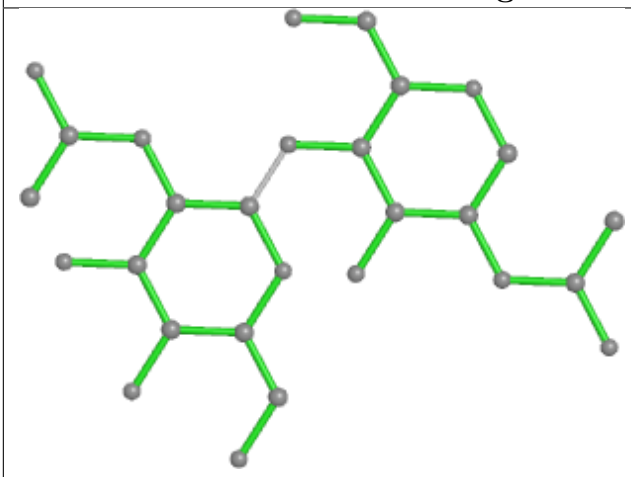
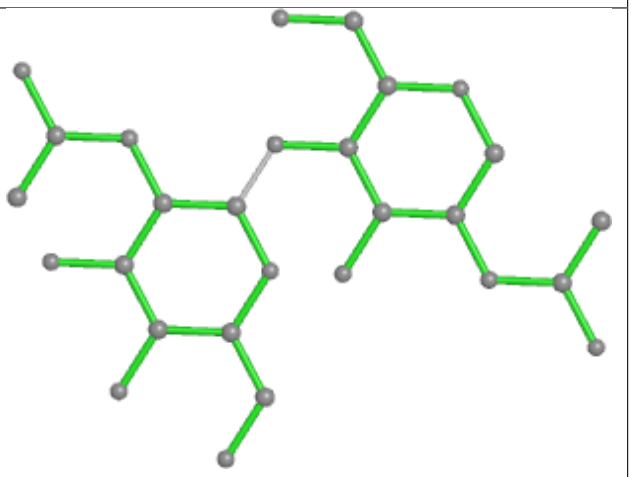
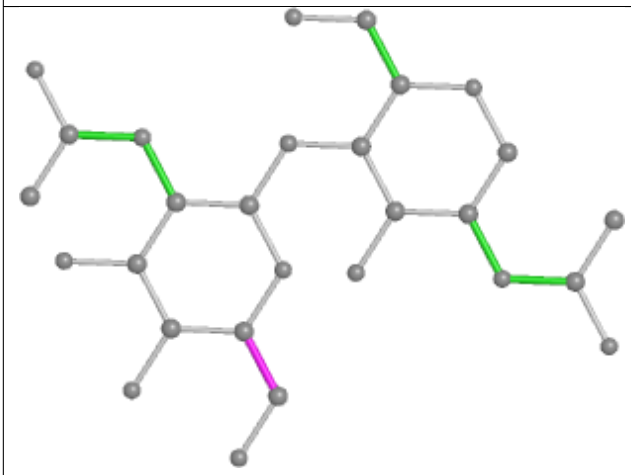
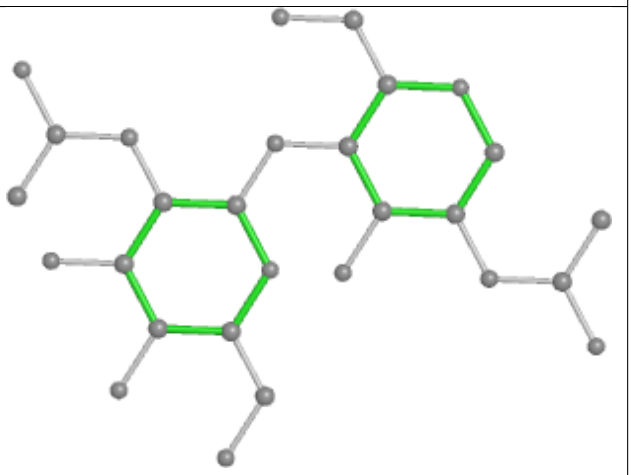
 Bond lengths	 Bond angles
 Torsions	 Rings

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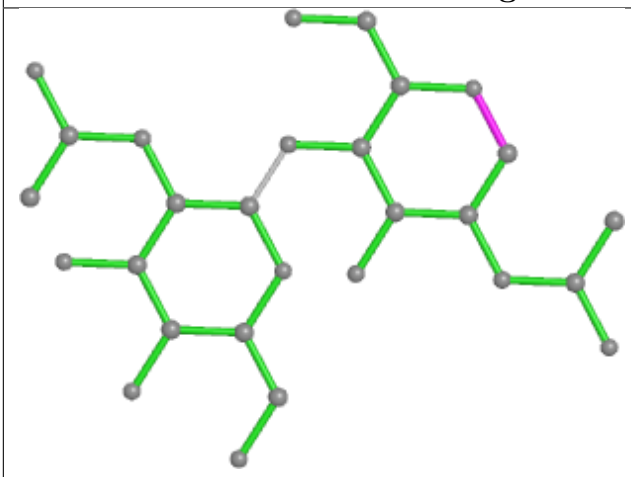
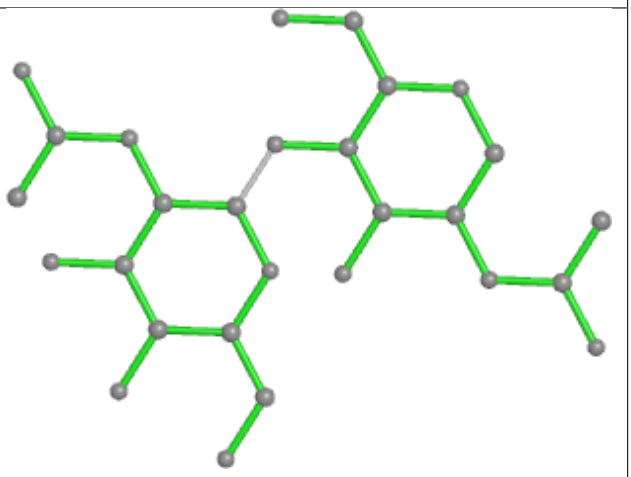
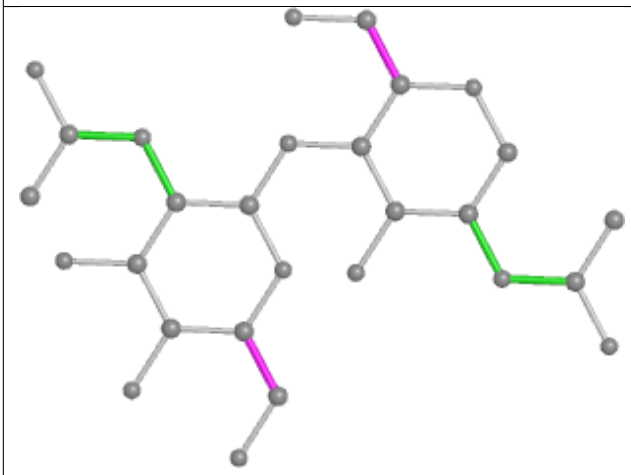
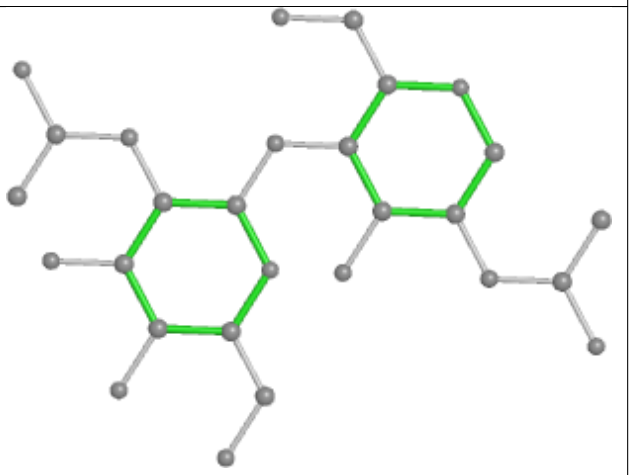
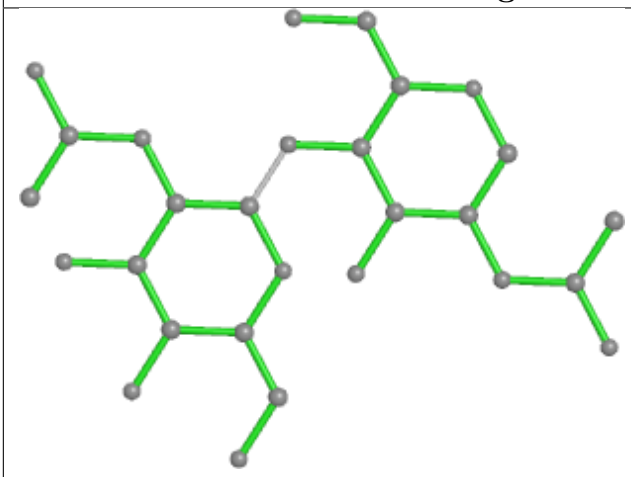
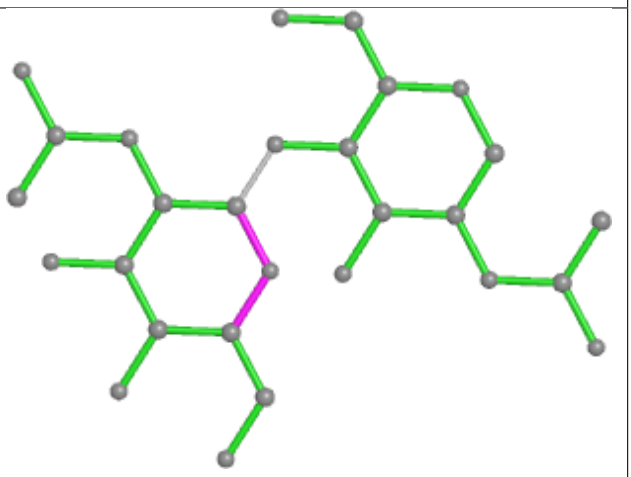
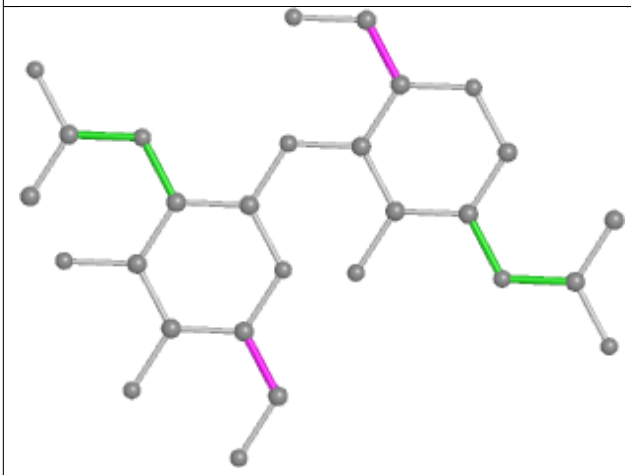
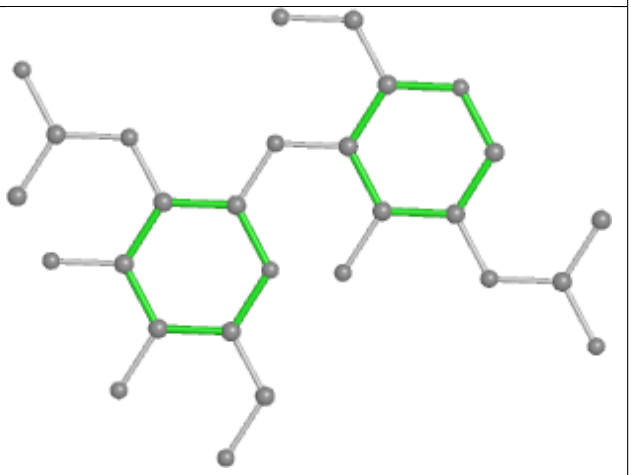
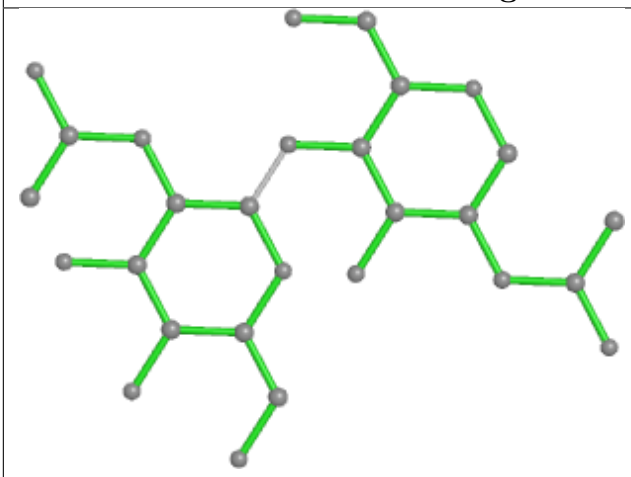
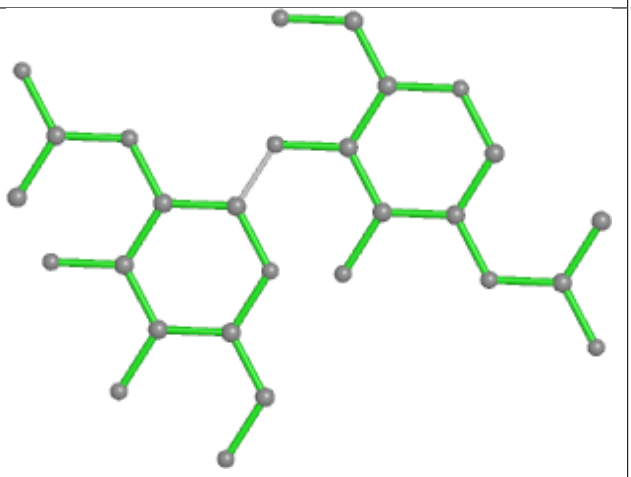
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain b	
 Bond lengths	 Bond angles
 Torsions	 Rings

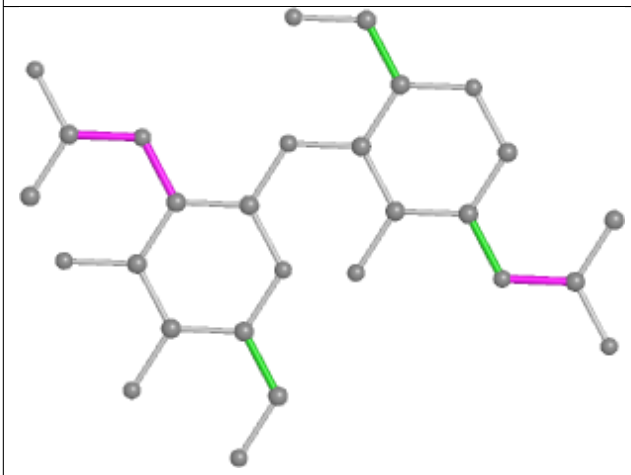
Oligosaccharide Chain c



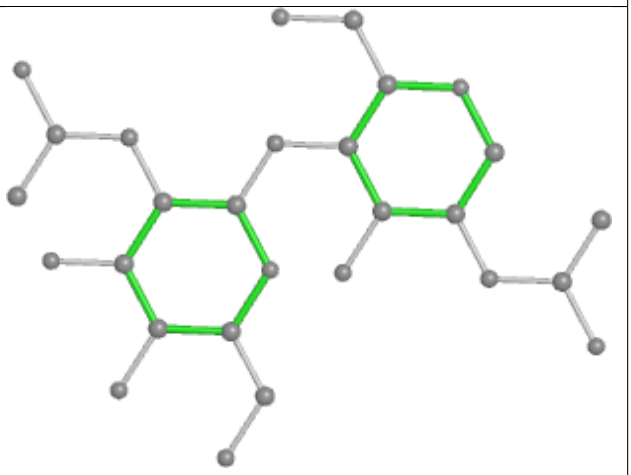
Bond lengths



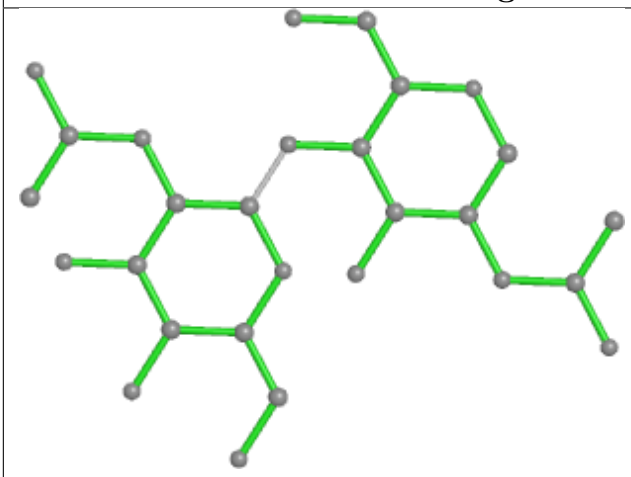
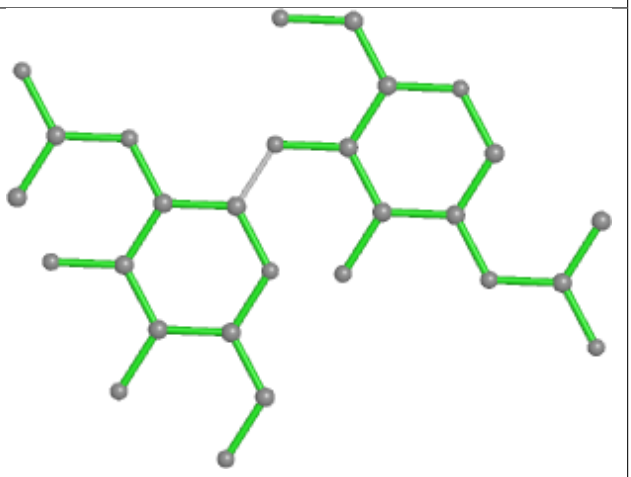
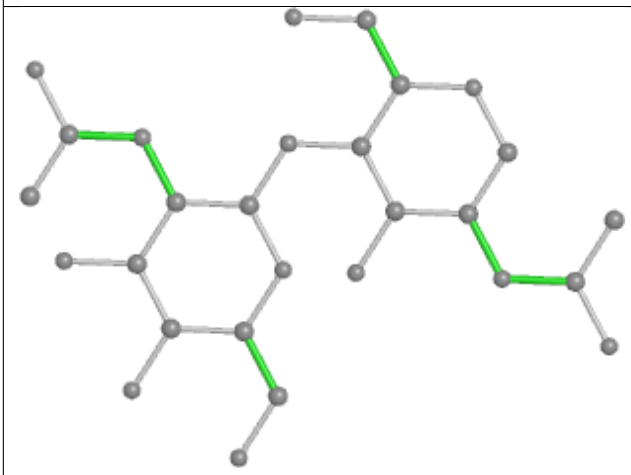
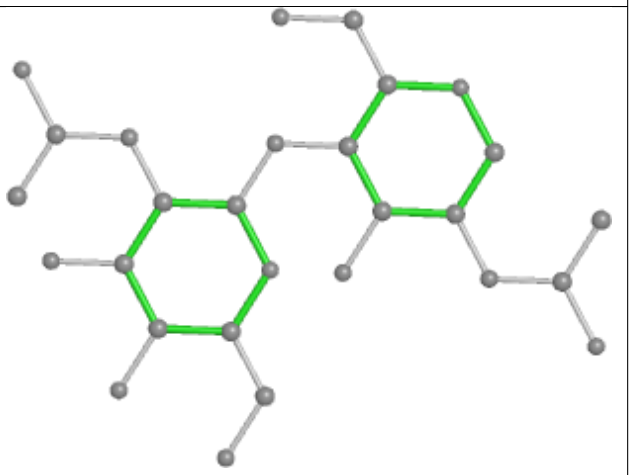
Bond angles



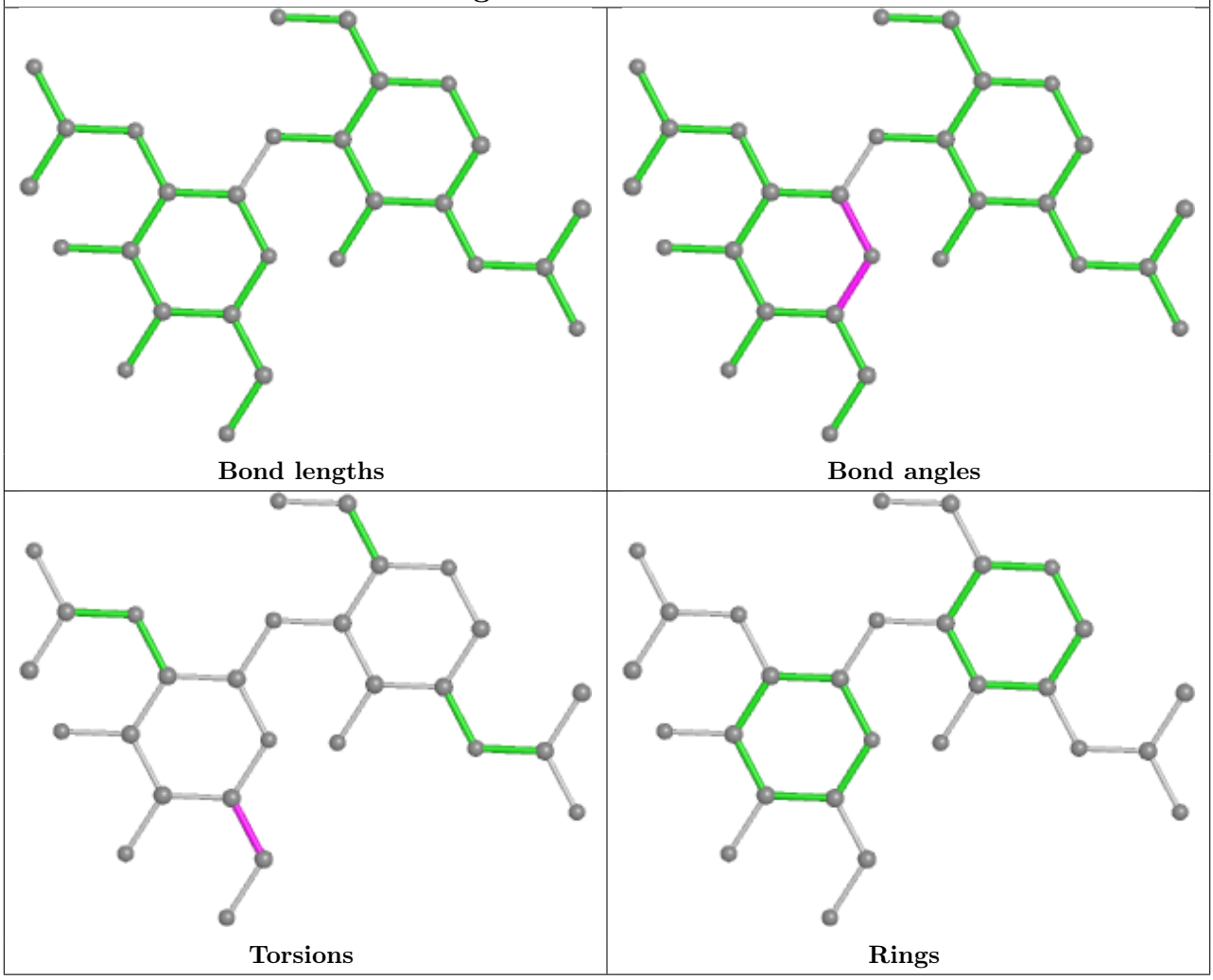
Torsions



Rings

Oligosaccharide Chain d	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain e



5.6 Ligand geometry (i)

28 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	$\#\|Z\| > 2$
4	NAG	A	1404	1	14,14,15	0.48	0	17,19,21	0.54	0
4	NAG	B	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1401	1	14,14,15	0.29	0	17,19,21	0.33	0
4	NAG	A	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	B	1403	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	C	1405	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
4	NAG	C	1403	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1409	1	14,14,15	0.51	0	17,19,21	0.35	0
4	NAG	C	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	A	1408	1	14,14,15	0.31	0	17,19,21	0.38	0
4	NAG	C	1401	1	14,14,15	0.28	0	17,19,21	0.33	0
4	NAG	A	1406	1	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	A	1401	1	14,14,15	0.30	0	17,19,21	0.33	0
4	NAG	B	1410	-	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	C	1408	1	14,14,15	0.30	0	17,19,21	0.39	0
4	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.63	0
4	NAG	C	1404	1	14,14,15	0.46	0	17,19,21	0.54	0
4	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.62	0
4	NAG	B	1409	1	14,14,15	0.41	0	17,19,21	1.15	2 (11%)
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.64	0
4	NAG	D	901	2	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	A	1405	1	14,14,15	0.57	0	17,19,21	1.25	1 (5%)
4	NAG	B	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	1404	1	14,14,15	0.47	0	17,19,21	0.53	0
4	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	C	1407	1	14,14,15	0.22	0	17,19,21	0.50	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	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1405	NAG	C2-N2-C7	4.34	129.08	122.90
4	C	1405	NAG	C2-N2-C7	4.28	129.00	122.90
4	A	1405	NAG	C2-N2-C7	4.28	129.00	122.90
4	B	1409	NAG	C8-C7-N2	2.26	119.93	116.10
4	D	901	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1406	NAG	O5-C5-C6-O6
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1401	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6

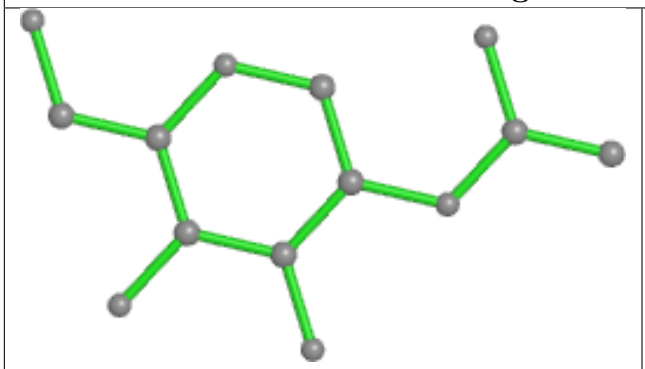
There are no ring outliers.

8 monomers are involved in 16 short contacts:

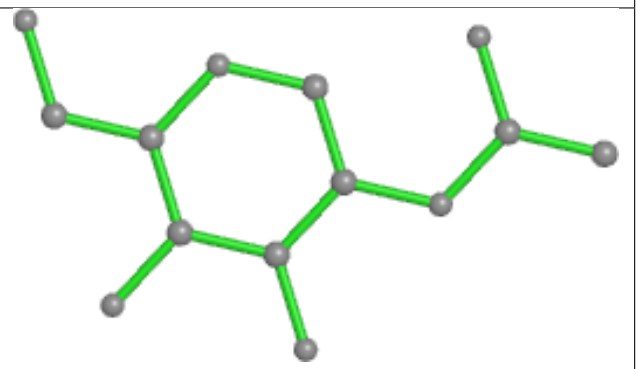
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1405	NAG	1	0
4	C	1405	NAG	1	0
4	B	1410	NAG	4	0
4	A	1402	NAG	3	0
4	B	1402	NAG	3	0
4	B	1409	NAG	4	0
4	C	1402	NAG	3	0
4	A	1405	NAG	1	0

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.

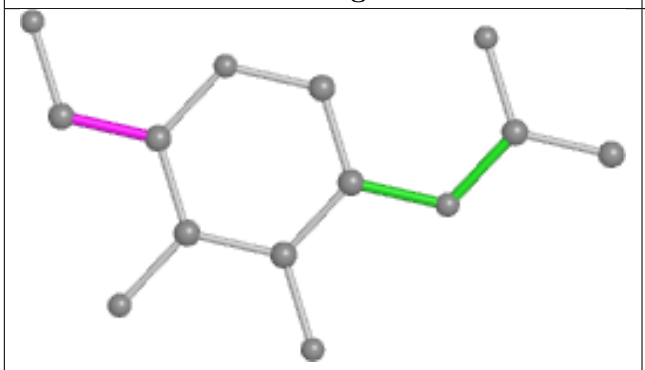
Ligand NAG A 1404



Bond lengths



Bond angles



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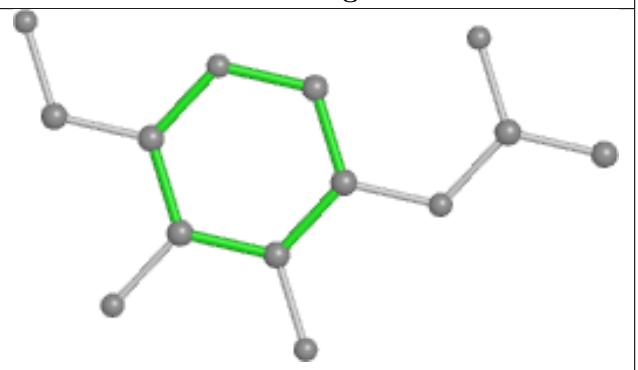
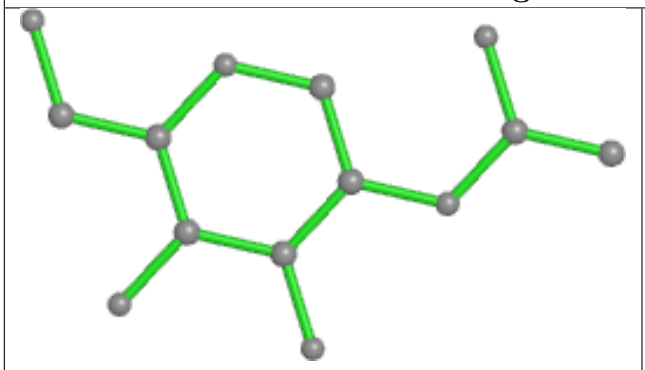


Rings

Ligand NAG B 1405



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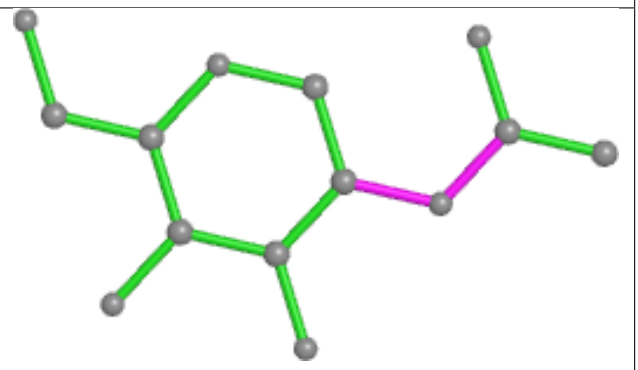

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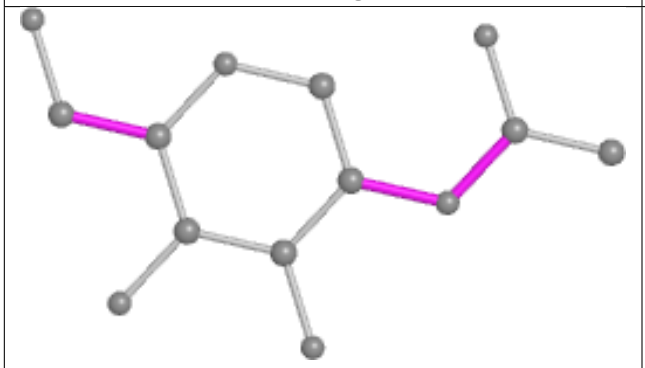
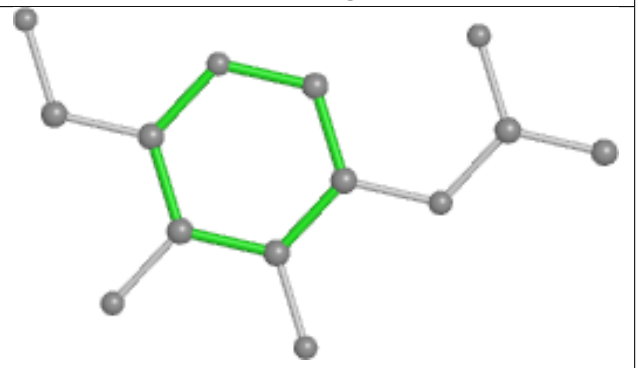


Torsions



Rings

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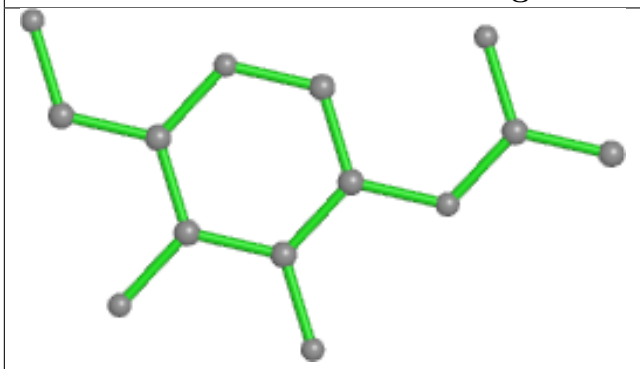
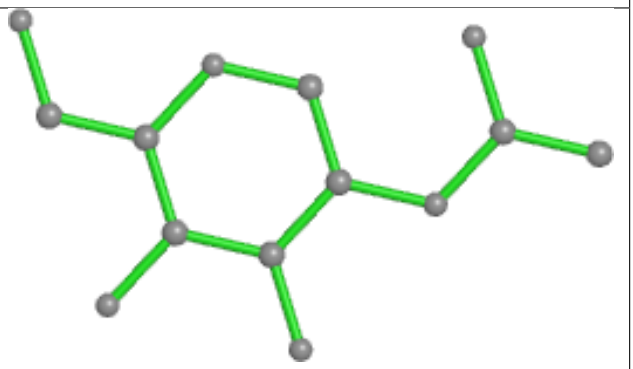
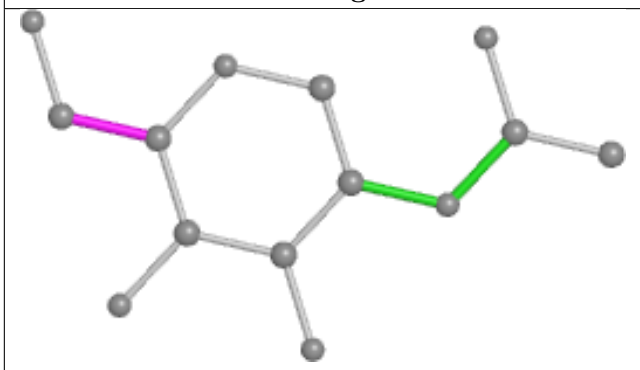
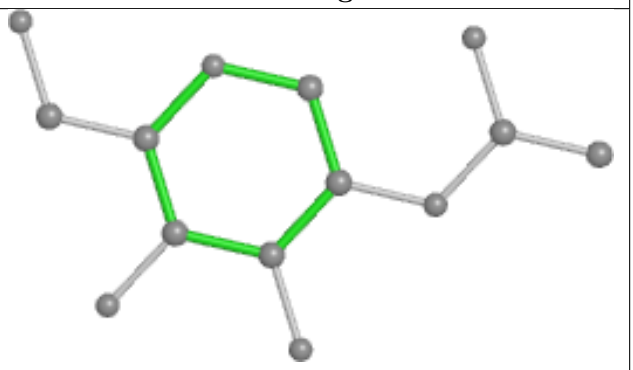
 Bond lengths	 Bond angles
 Torsions	 Rings

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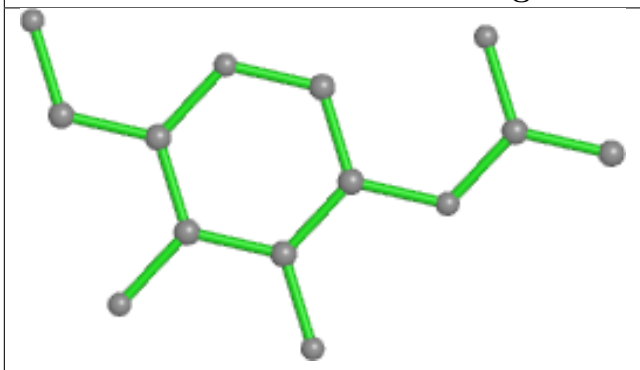
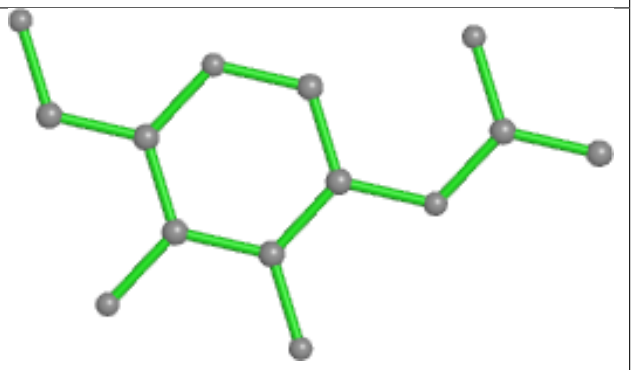
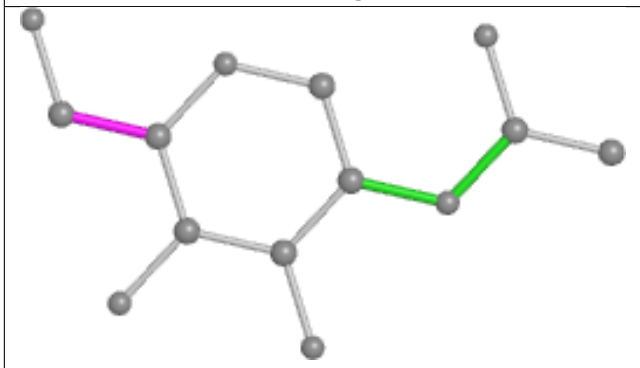
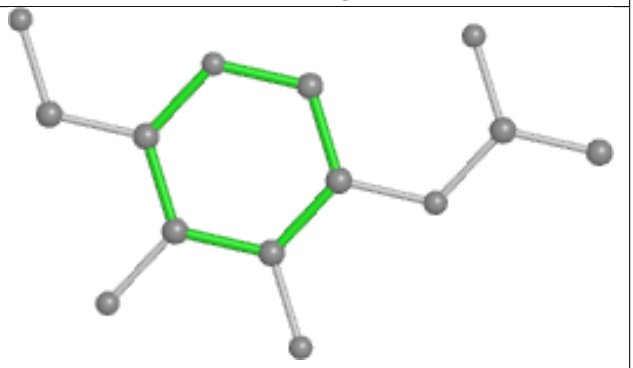
 Bond lengths	 Bond angles
 Torsions	 Rings

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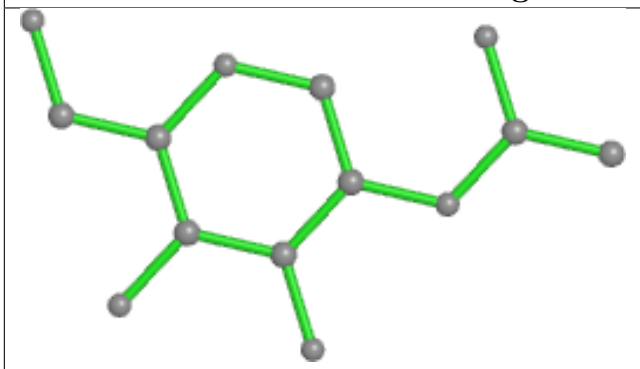
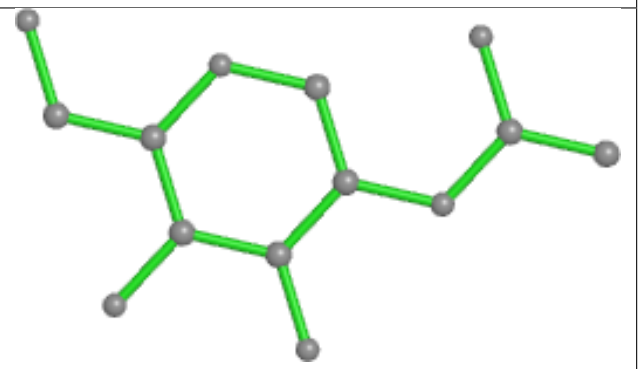
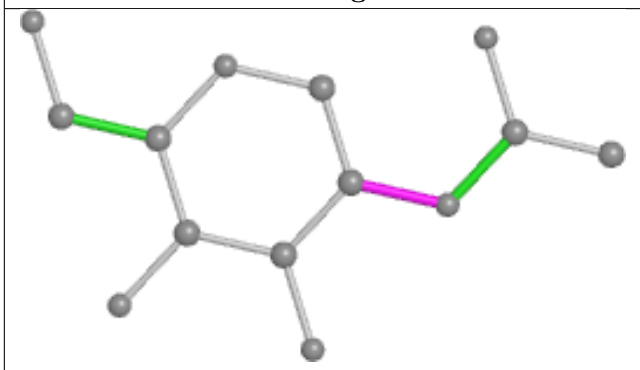
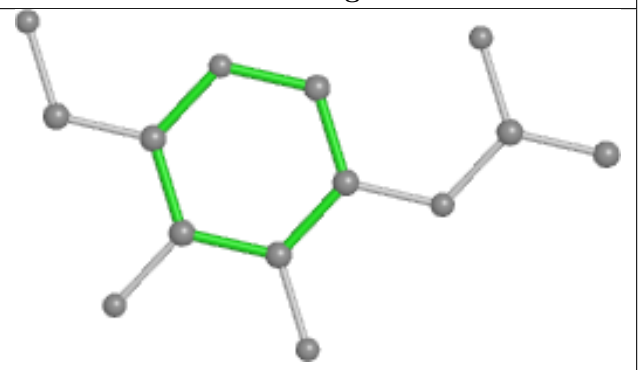
 Bond lengths	 Bond angles
 Torsions	 Rings

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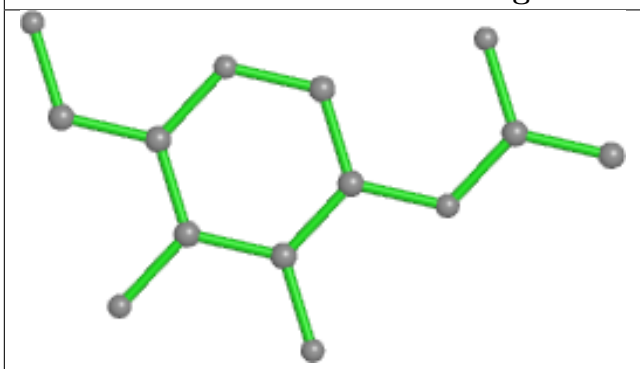
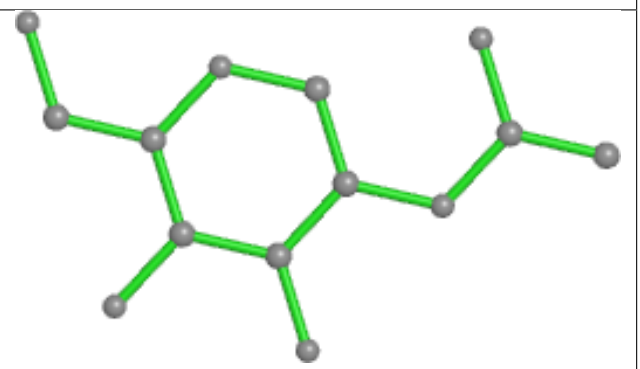
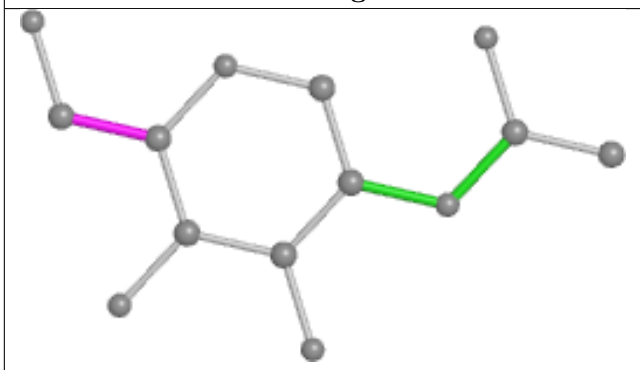
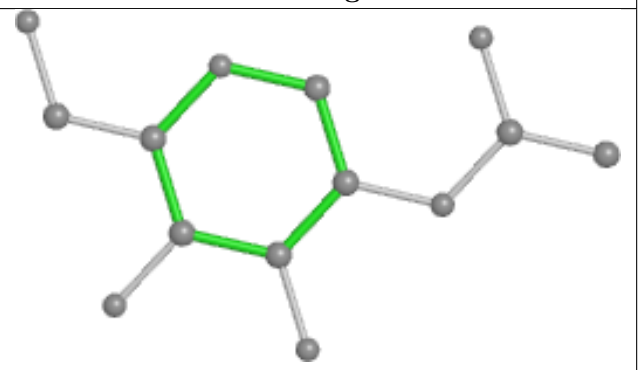
 Bond lengths	 Bond angles
 Torsions	 Rings

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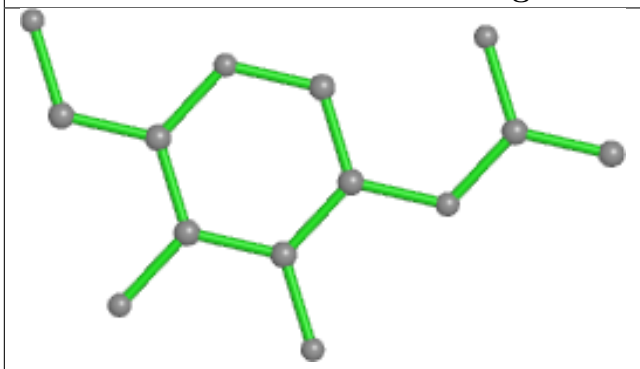
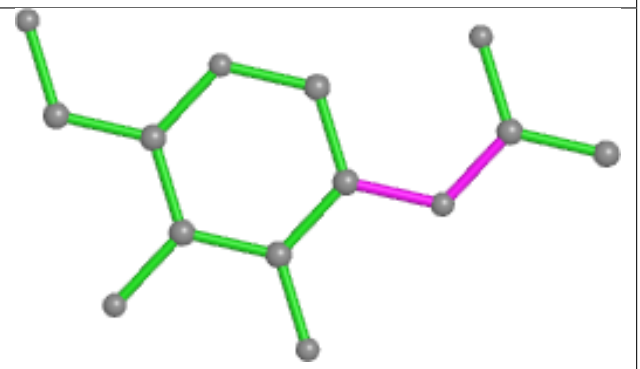
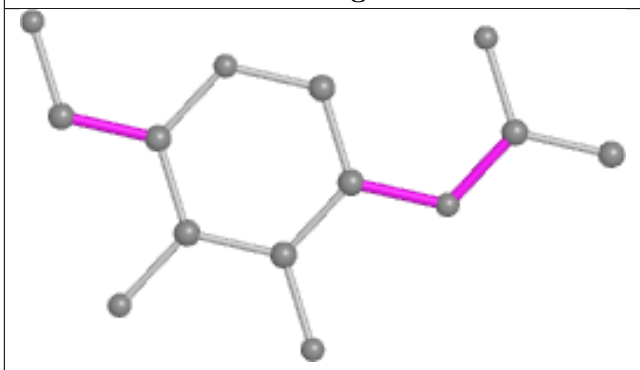
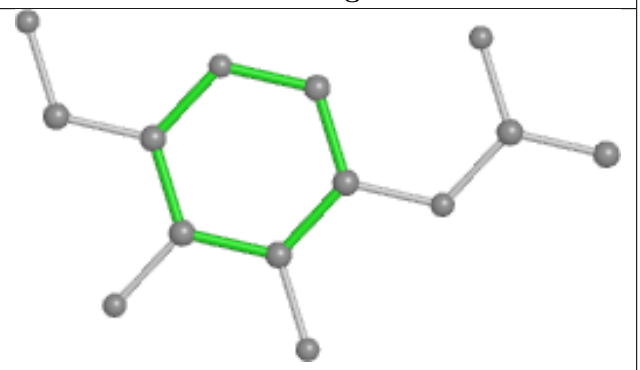
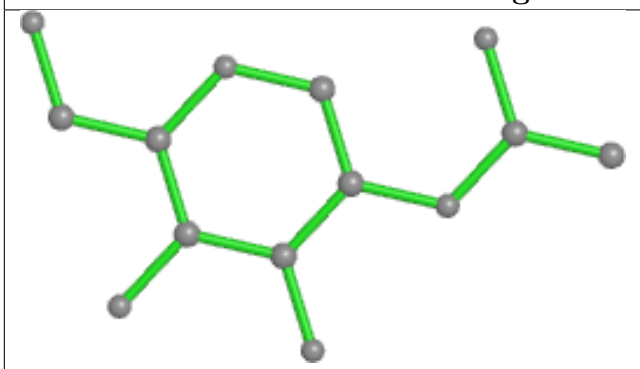
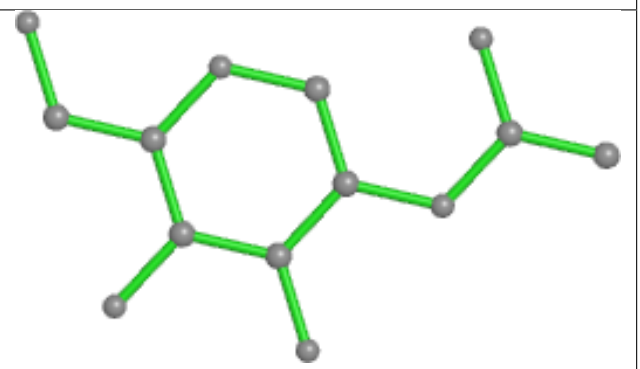
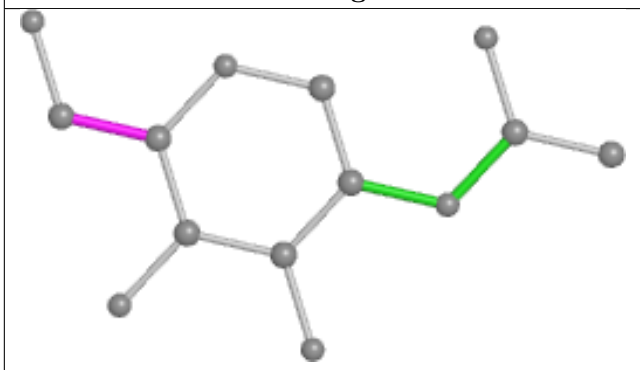
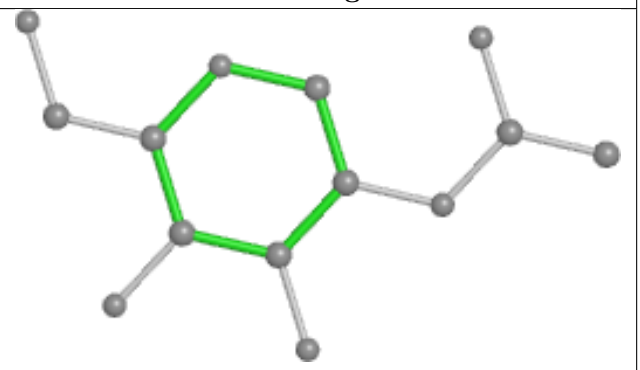
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1403	
 Bond lengths	 Bond angles
 Torsions	 Rings

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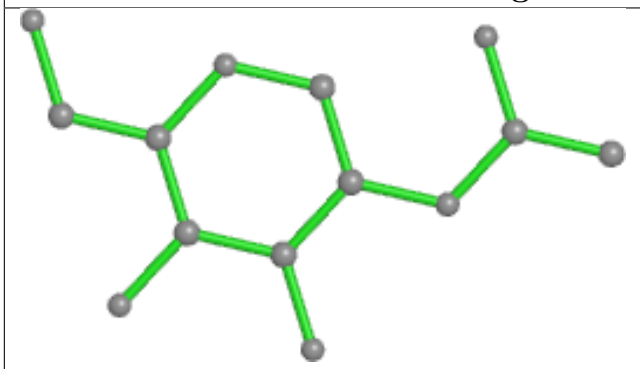
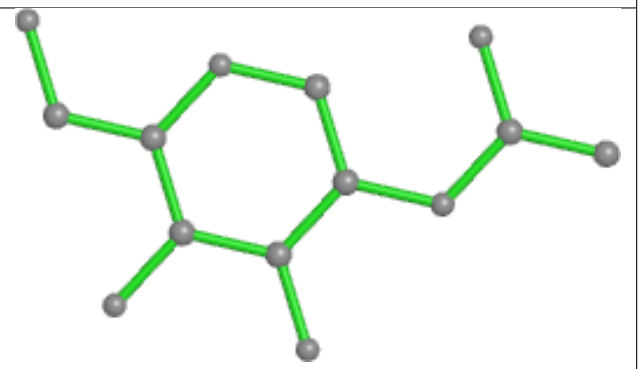
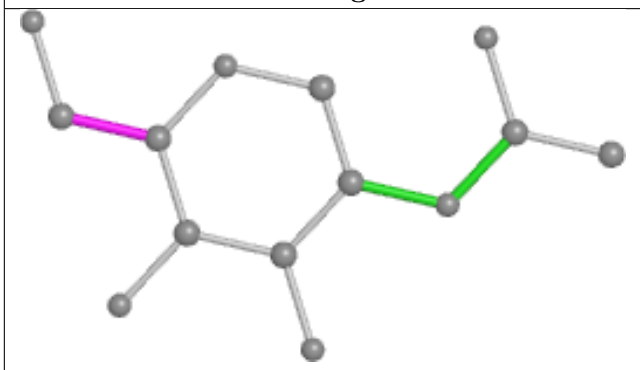
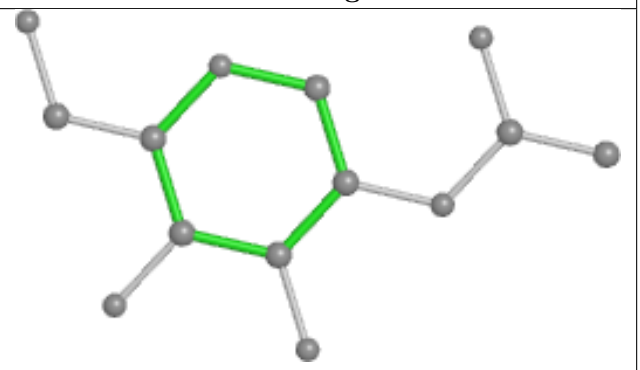
 Bond lengths	 Bond angles
 Torsions	 Rings

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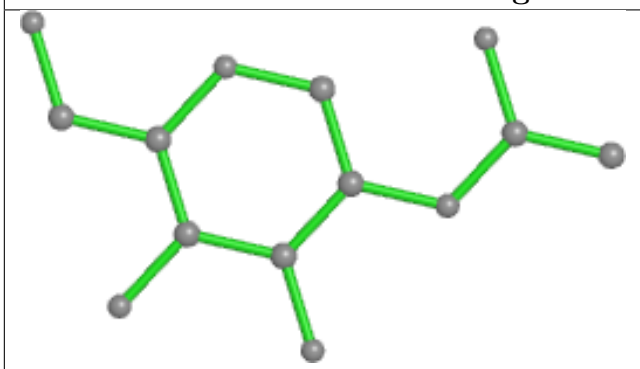
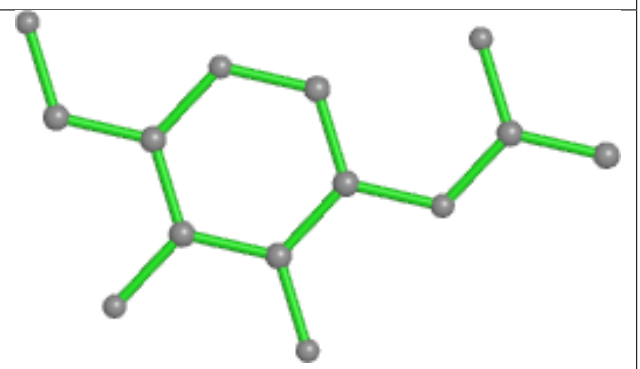
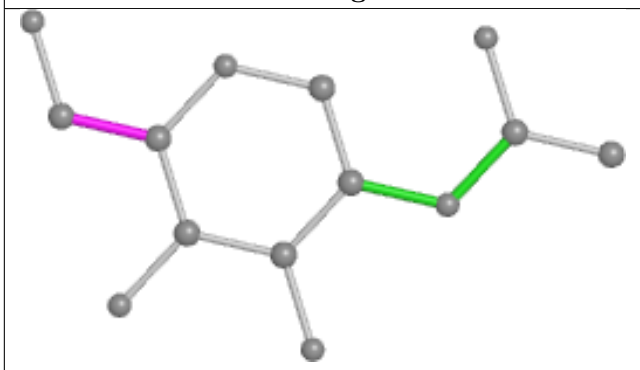
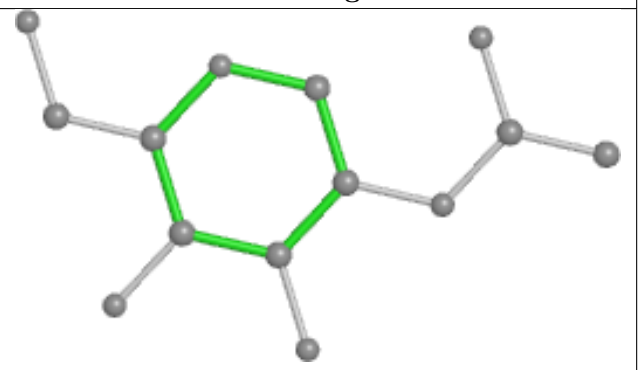
 Bond lengths	 Bond angles
 Torsions	 Rings

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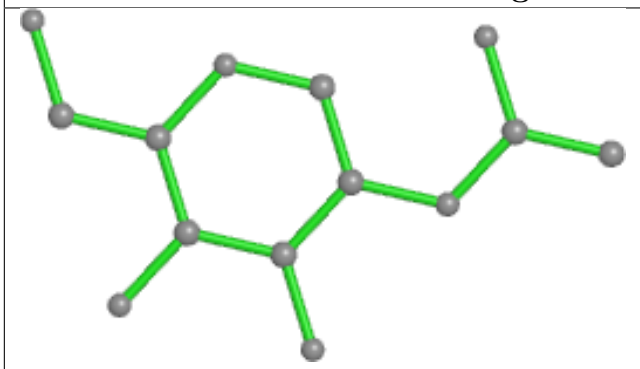
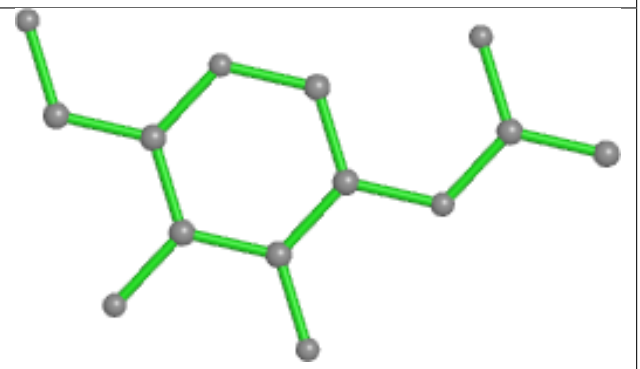
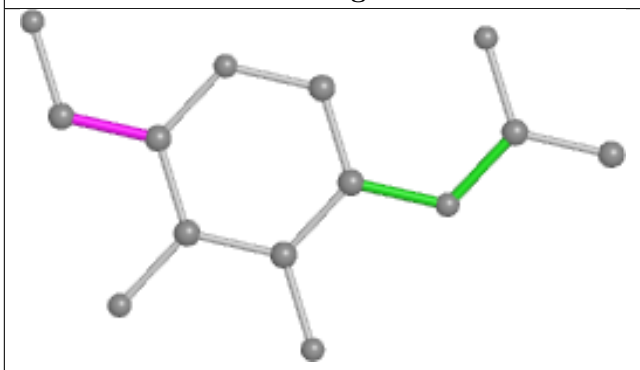
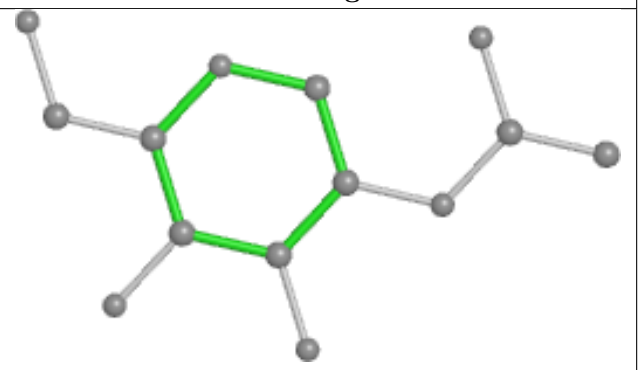
 Bond lengths	 Bond angles
 Torsions	 Rings

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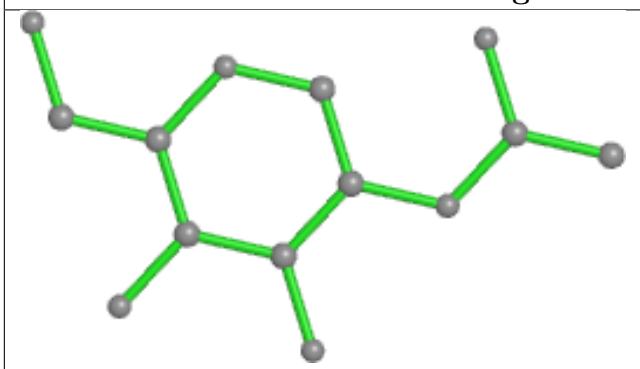
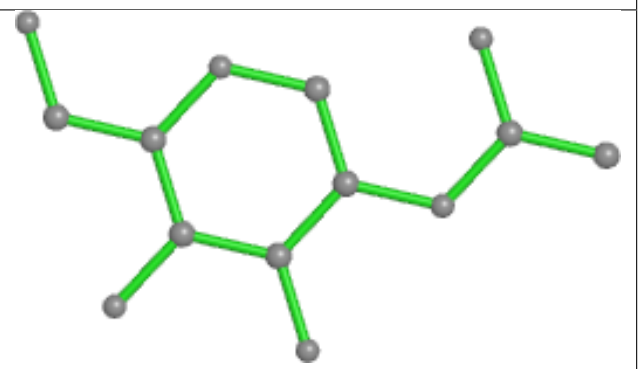
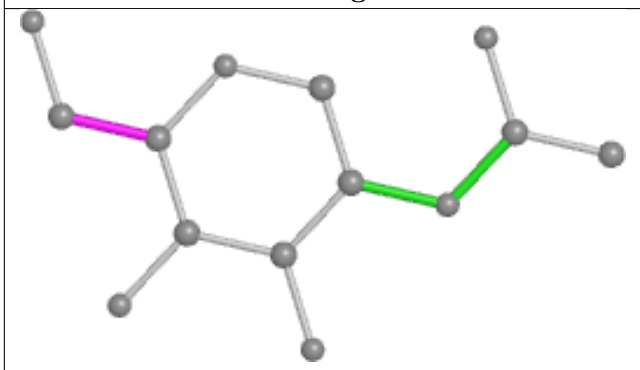
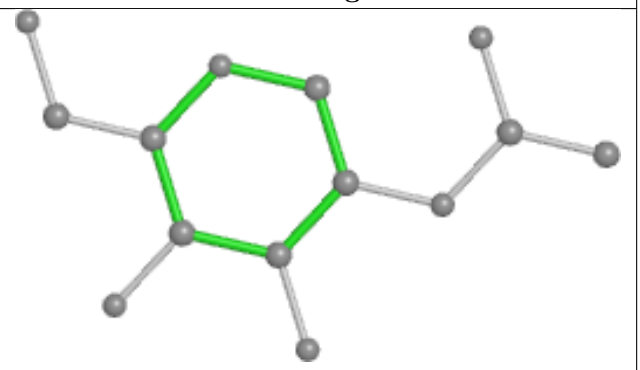
 Bond lengths	 Bond angles
 Torsions	 Rings

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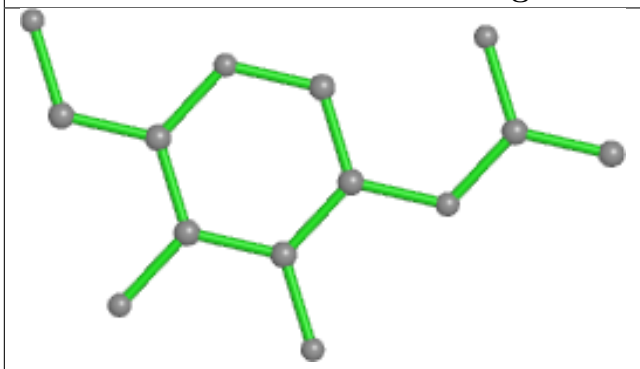
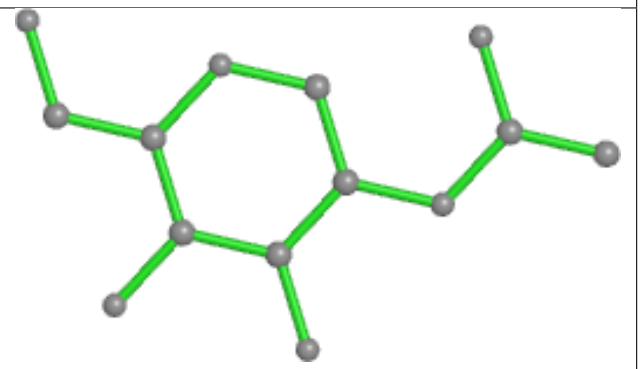
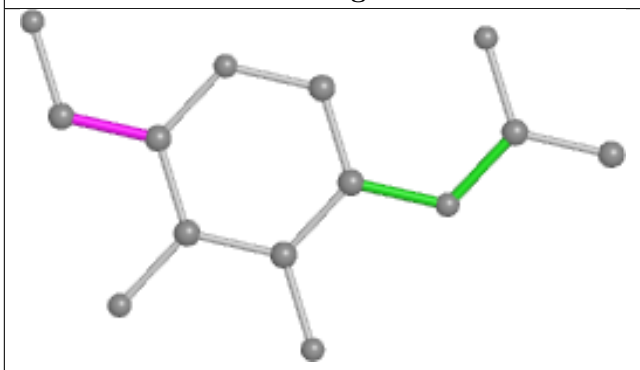
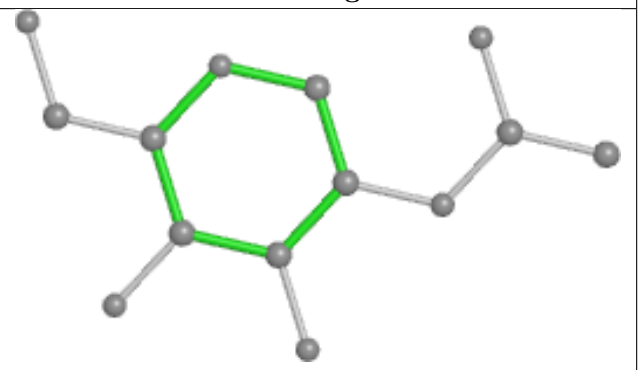
 Bond lengths	 Bond angles
 Torsions	 Rings

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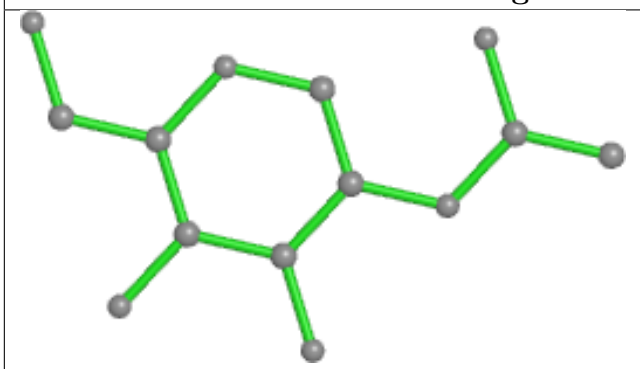
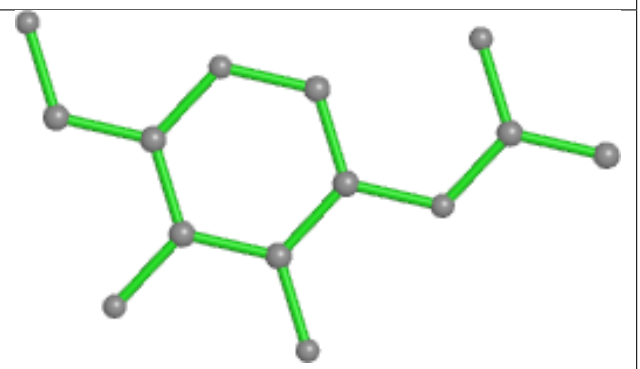
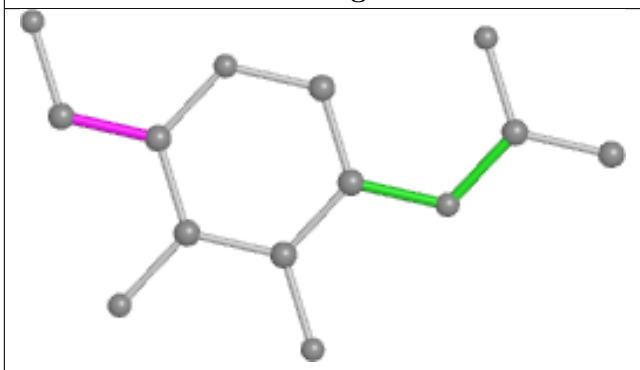
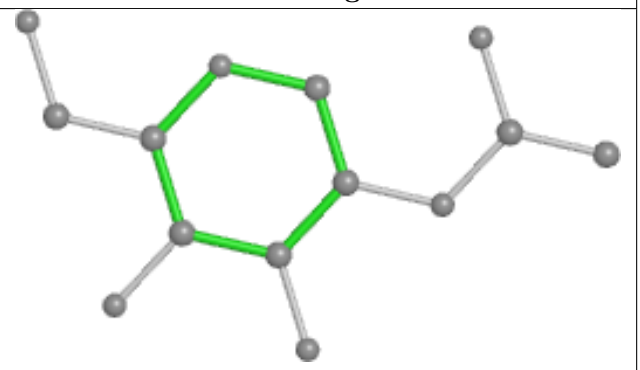
 Bond lengths	 Bond angles
 Torsions	 Rings

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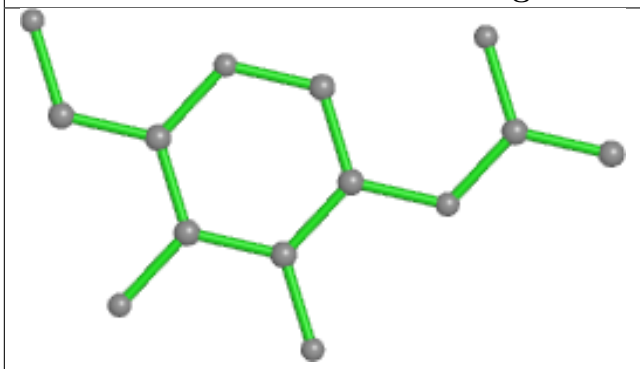
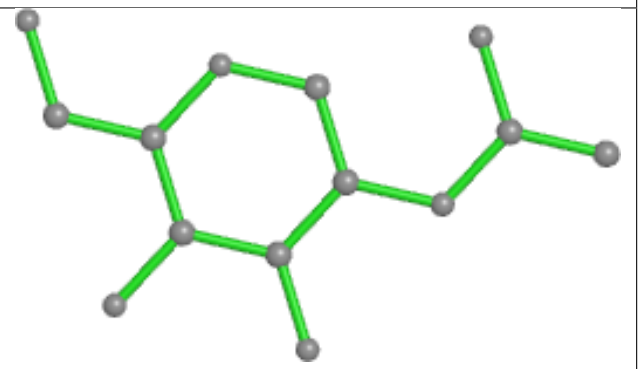
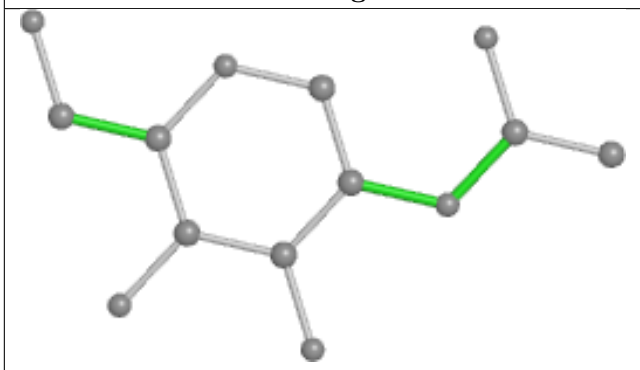
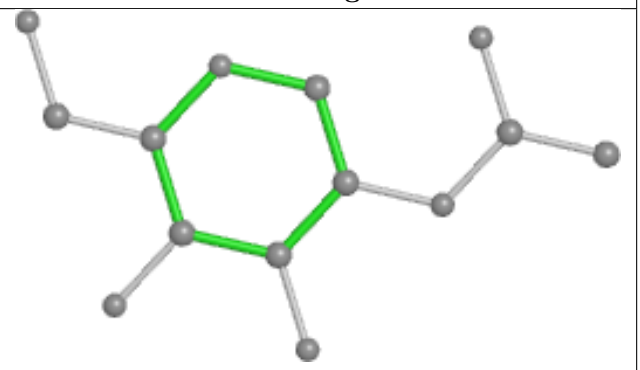
 Bond lengths	 Bond angles
 Torsions	 Rings

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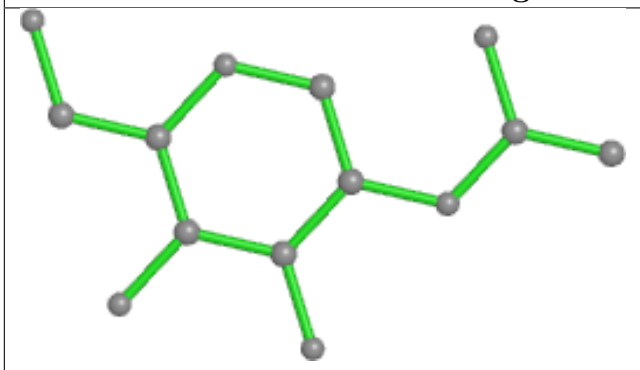
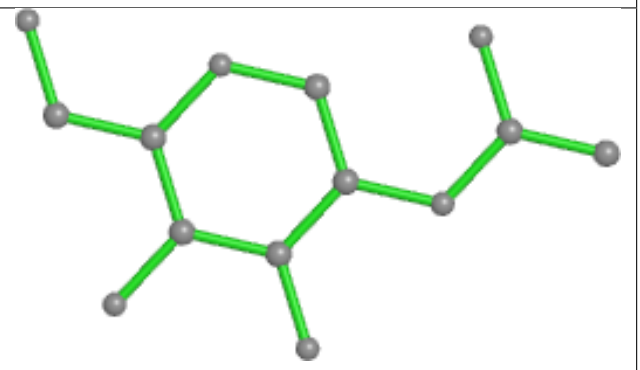
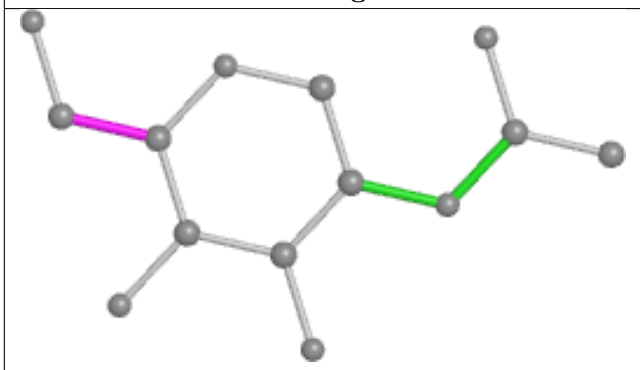
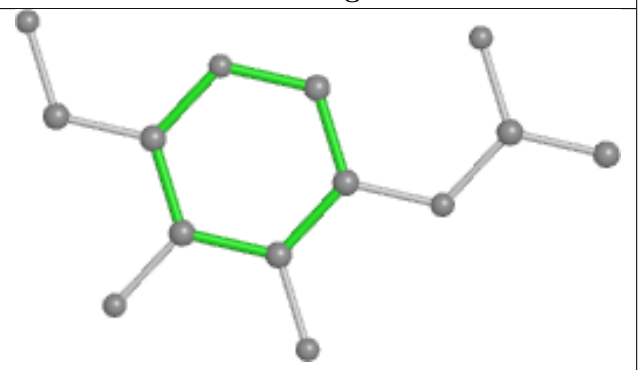
 Bond lengths	 Bond angles
 Torsions	 Rings

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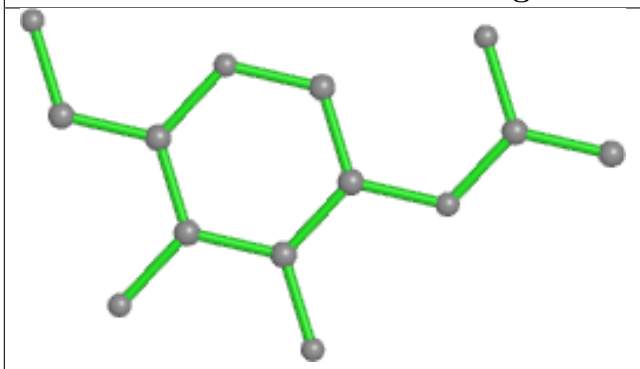
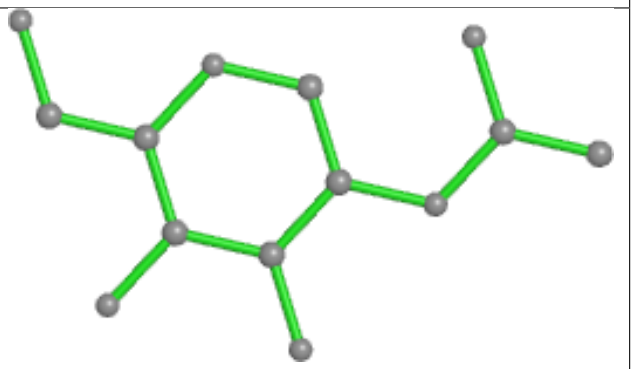
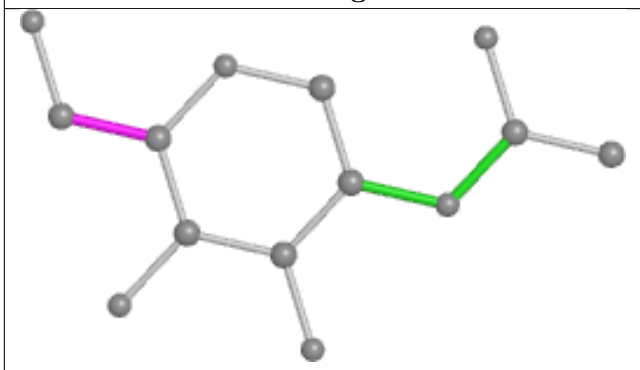
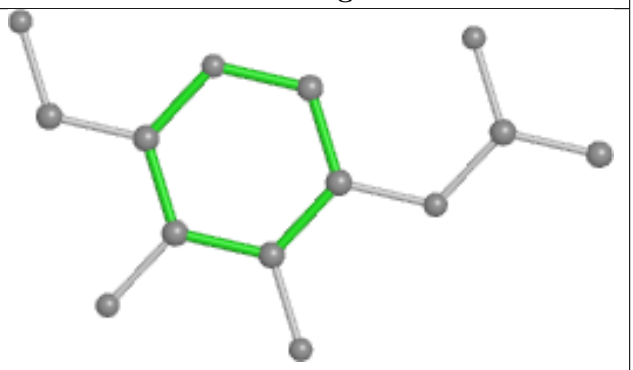
 Bond lengths	 Bond angles
 Torsions	 Rings

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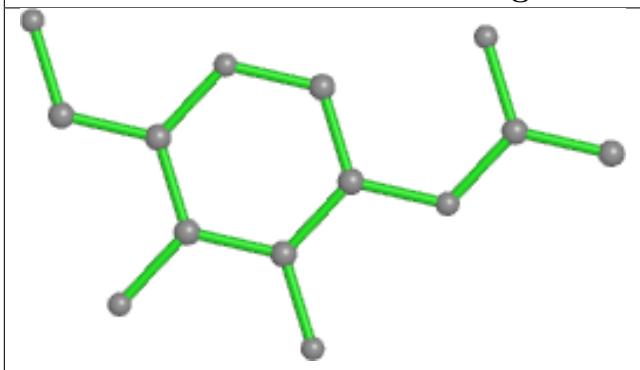
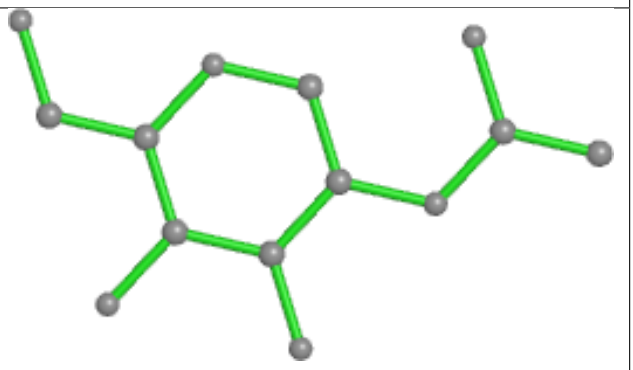
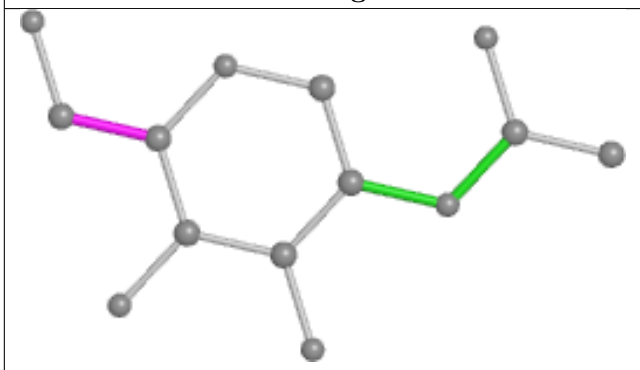
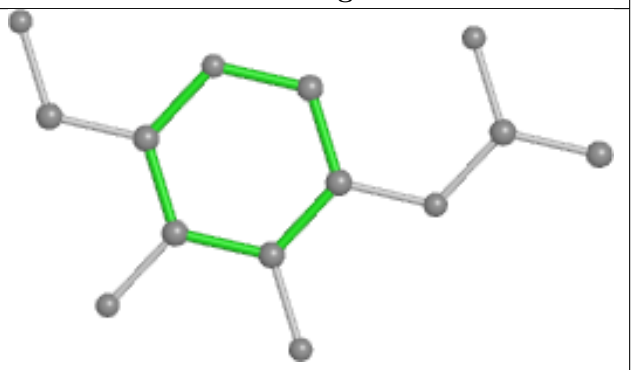
 Bond lengths	 Bond angles
 Torsions	 Rings

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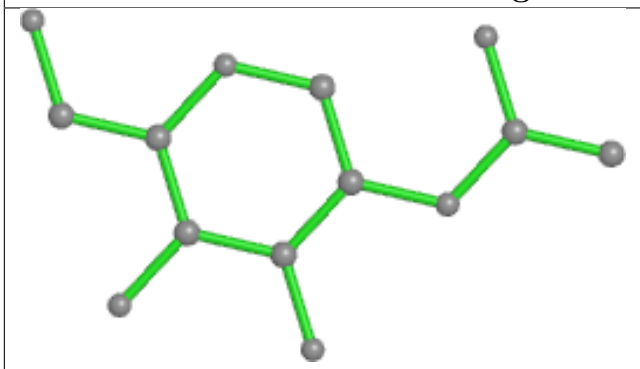
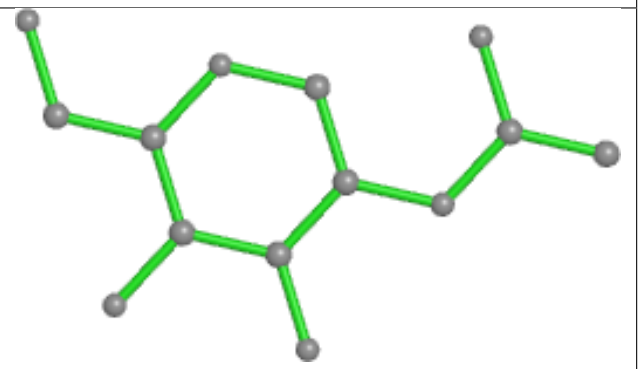
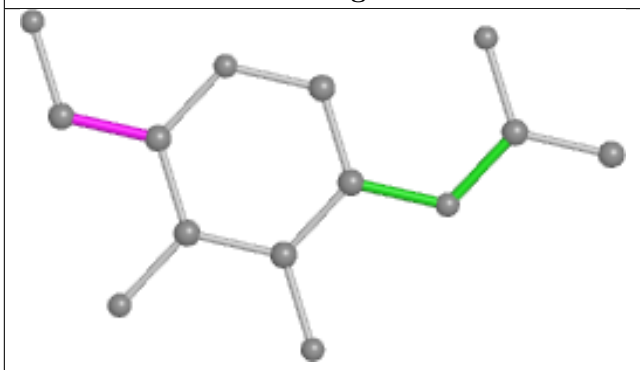
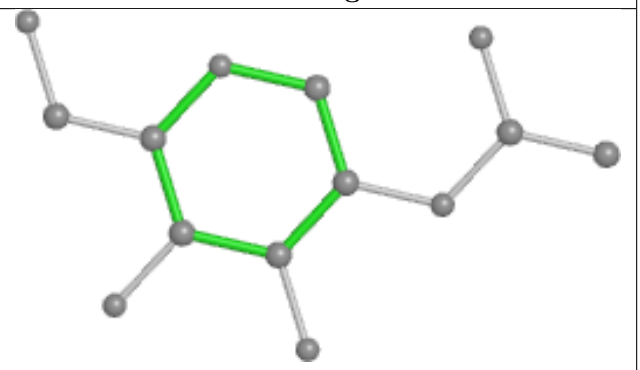
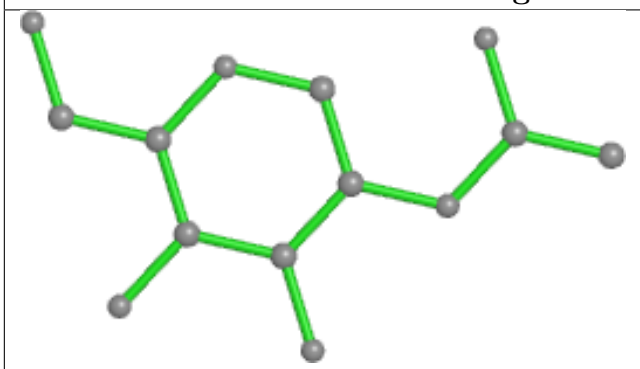
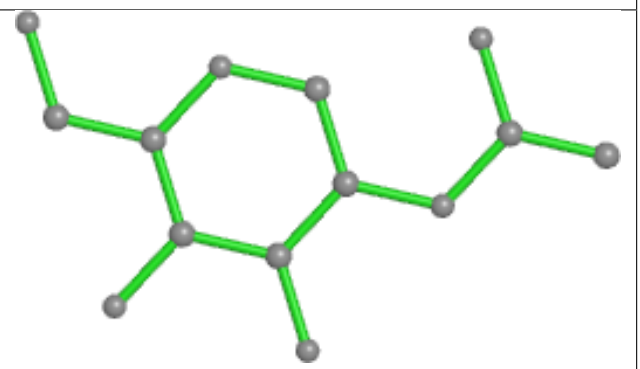
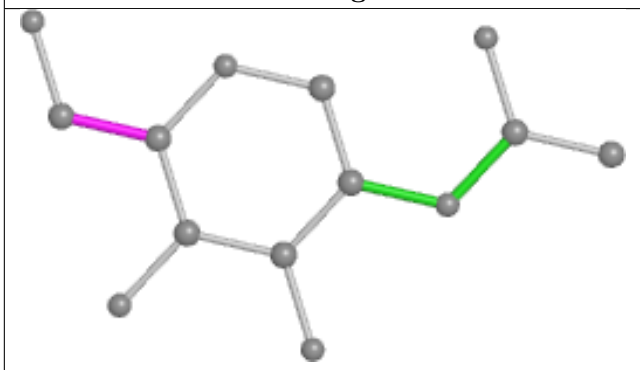
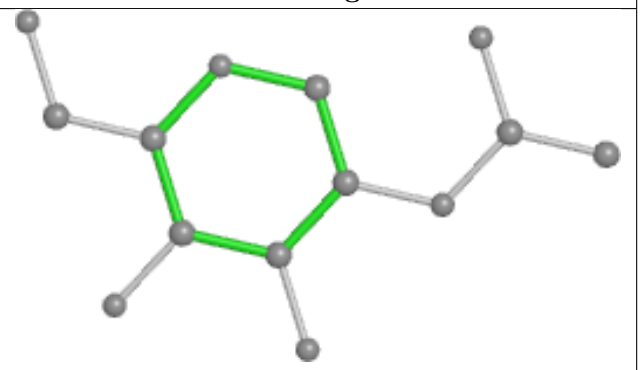
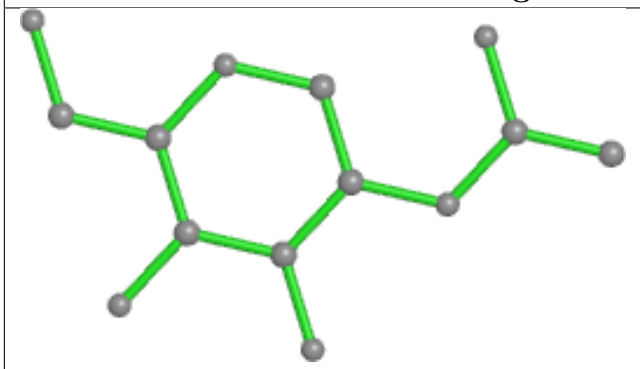
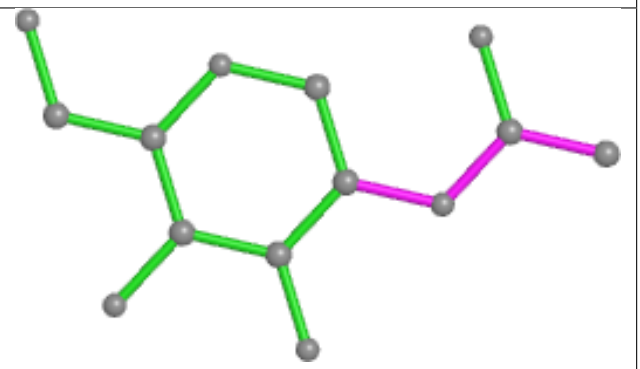
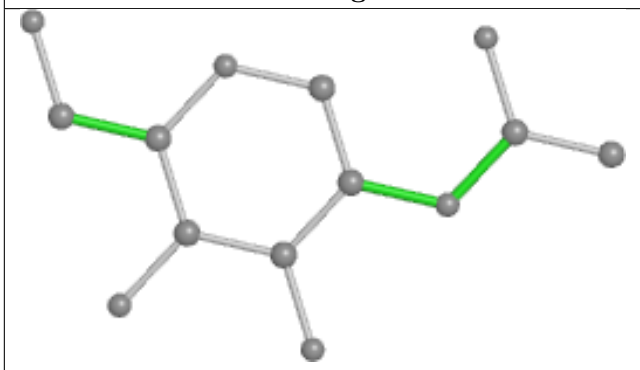
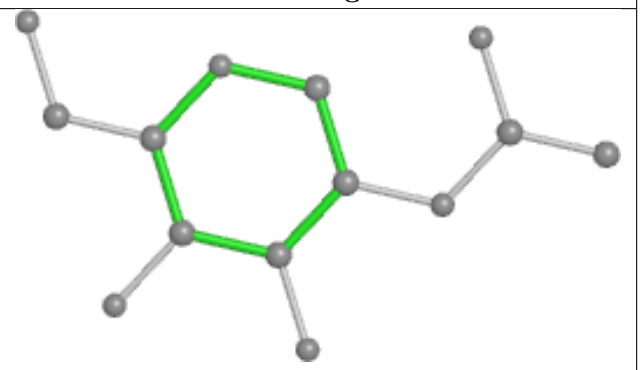
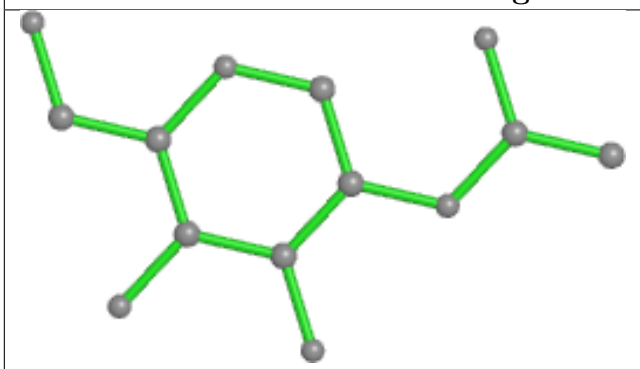
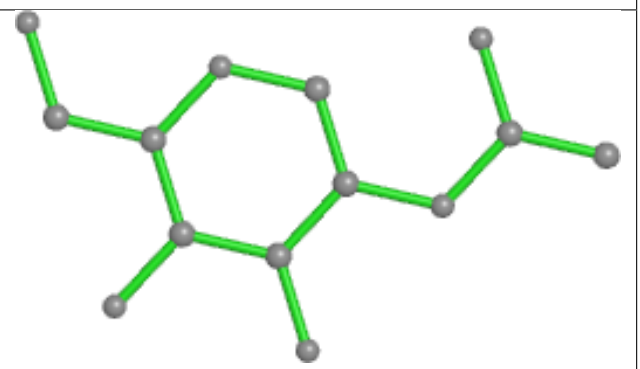
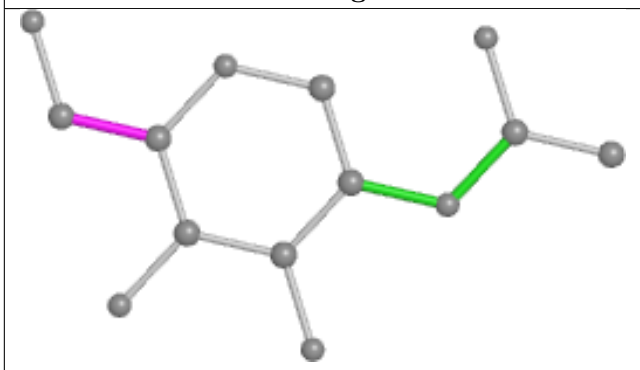
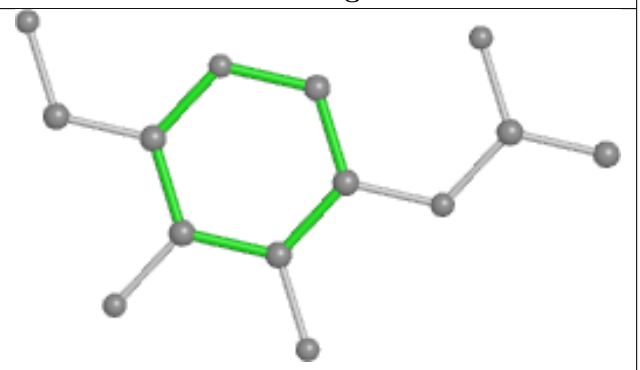
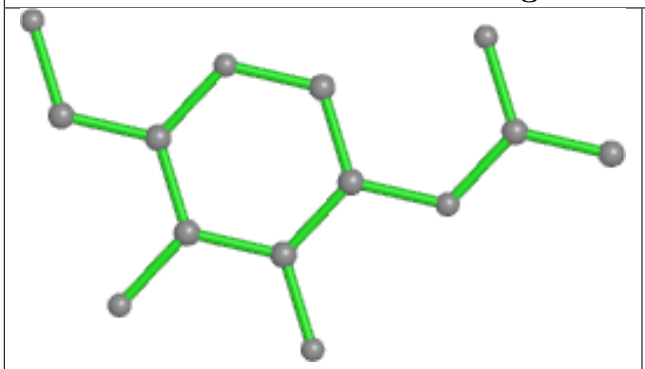
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

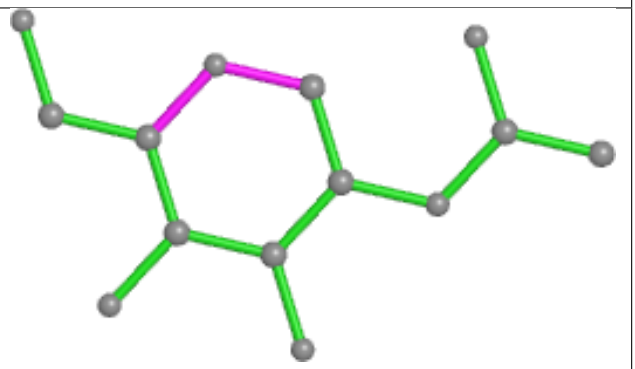
Ligand NAG B 1409	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

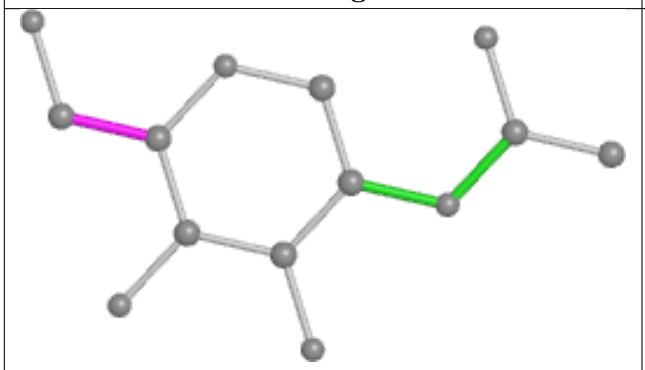
Ligand NAG D 901



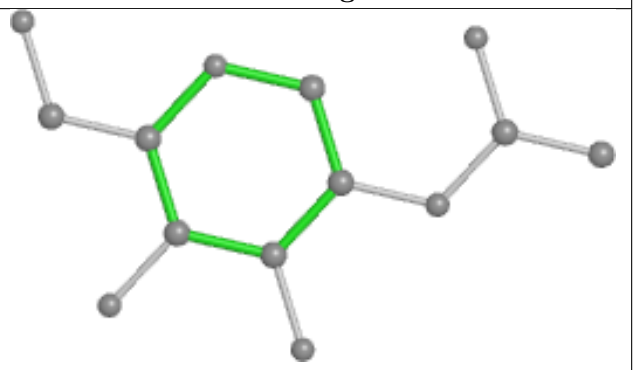
Bond lengths



Bond angles

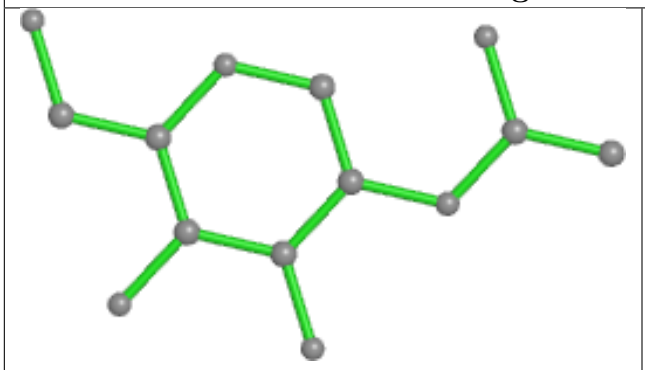


Torsions

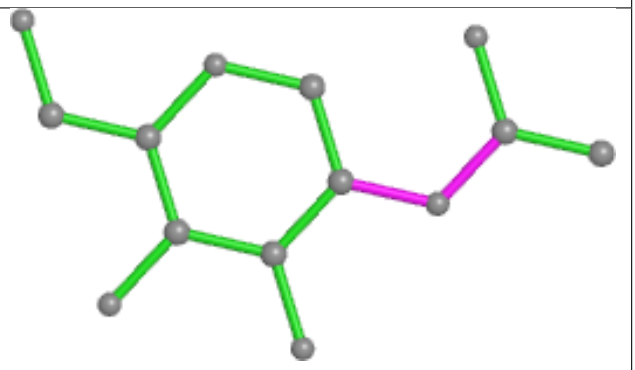


Rings

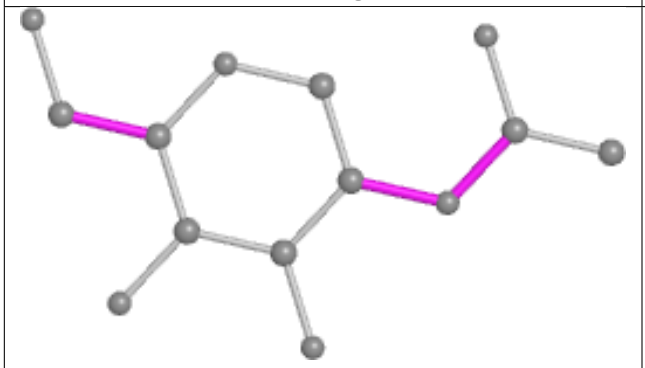
Ligand NAG A 1405



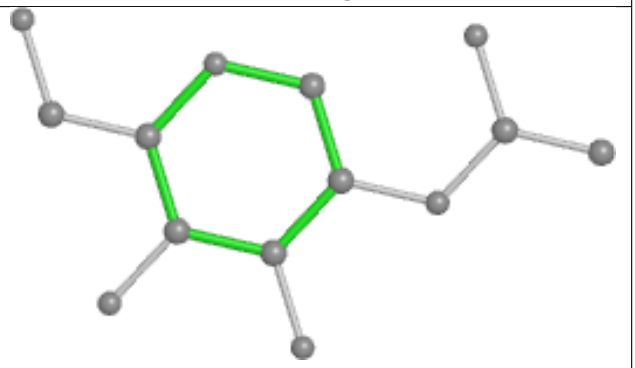
Bond lengths



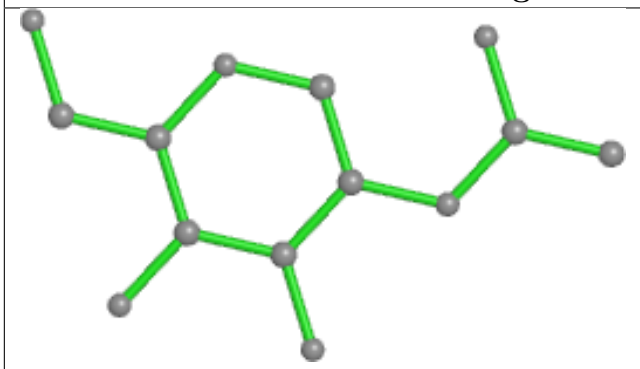
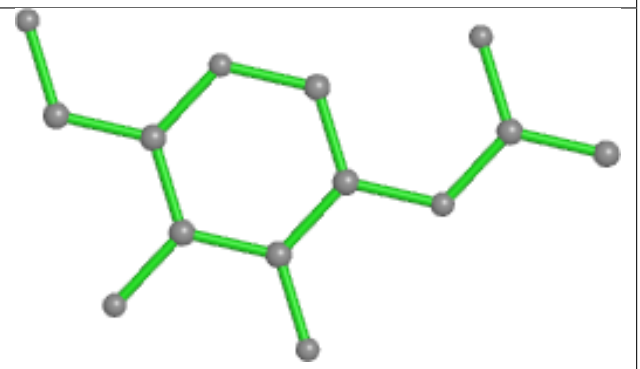
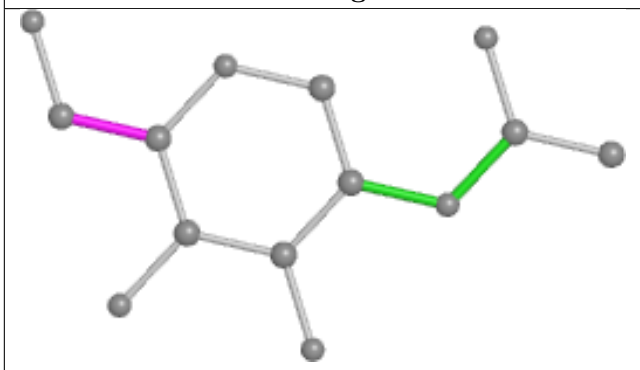
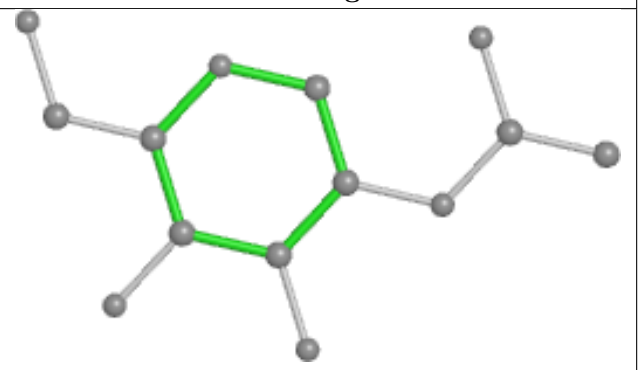
Bond angles

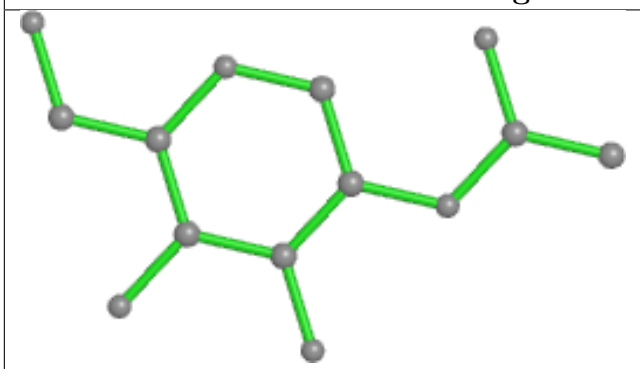
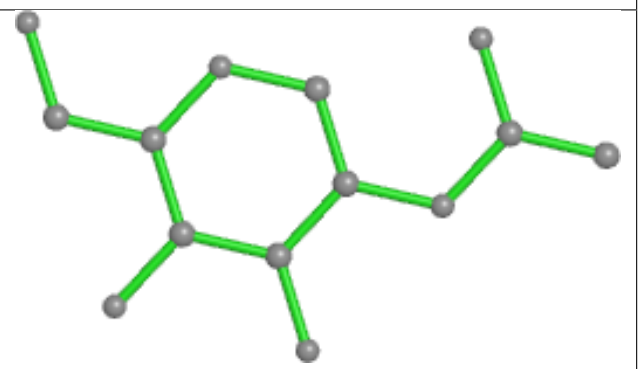
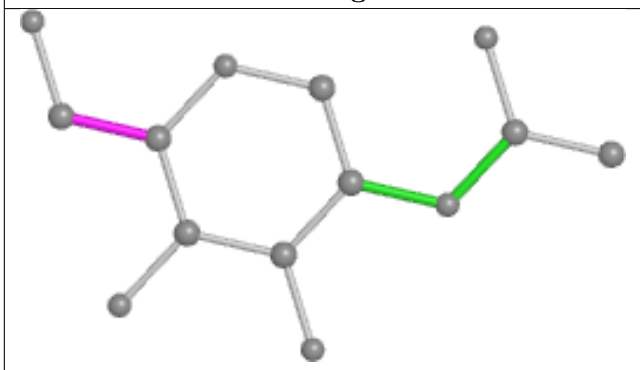
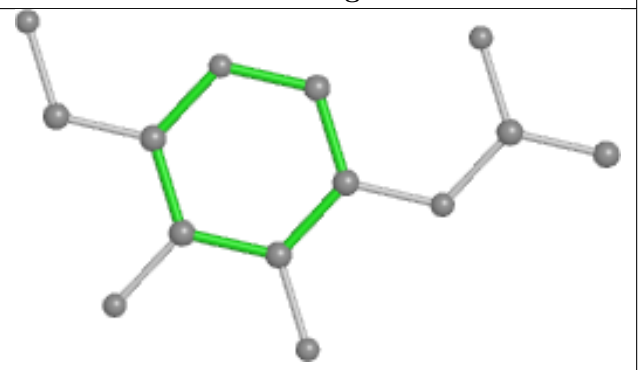


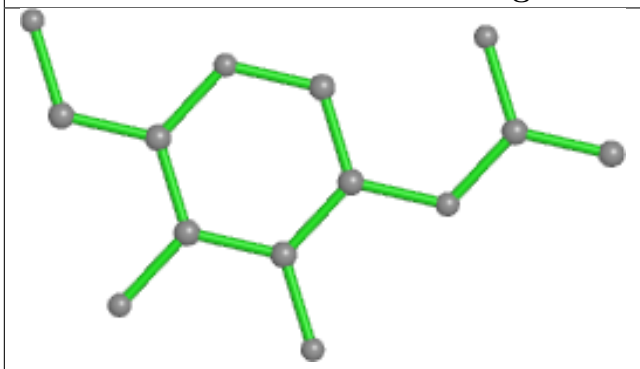
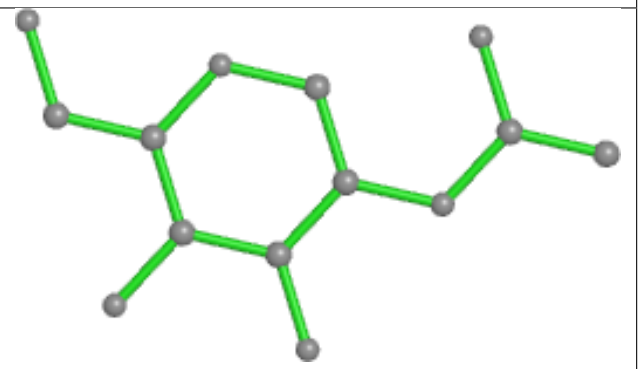
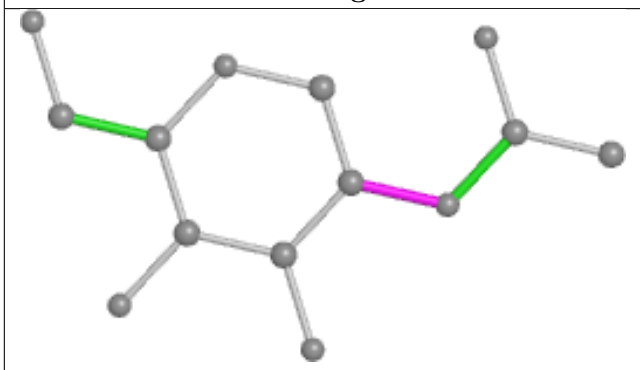
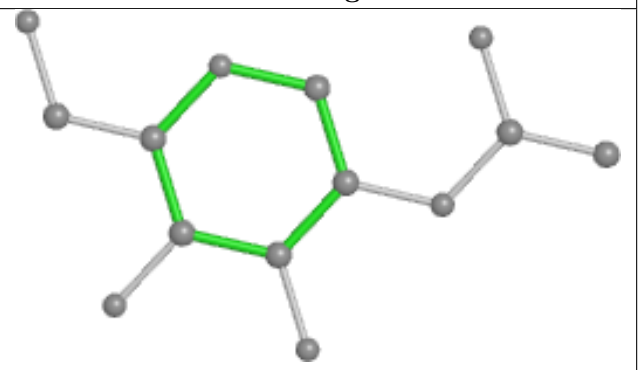
Torsions

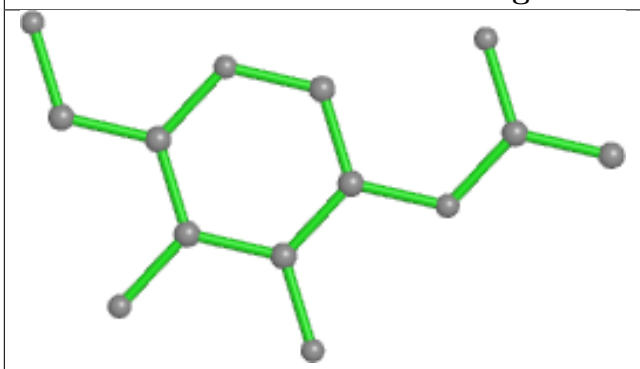
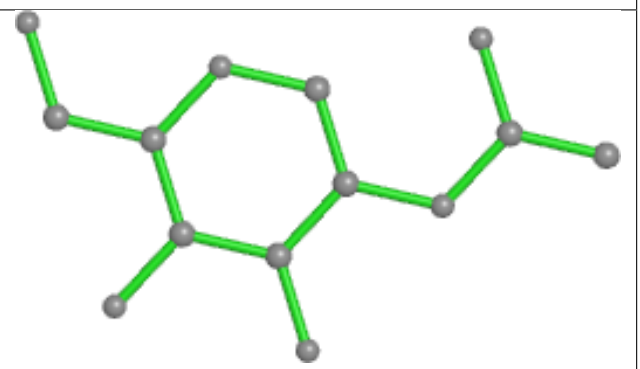
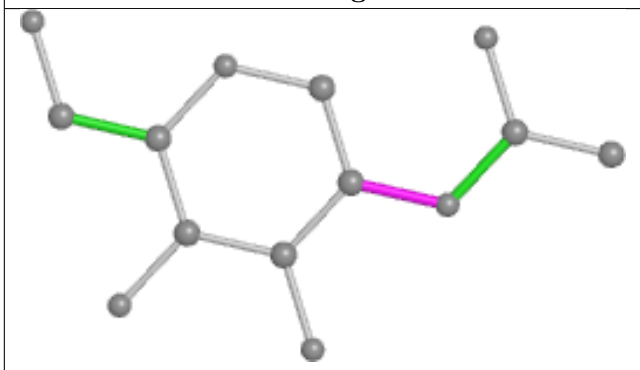
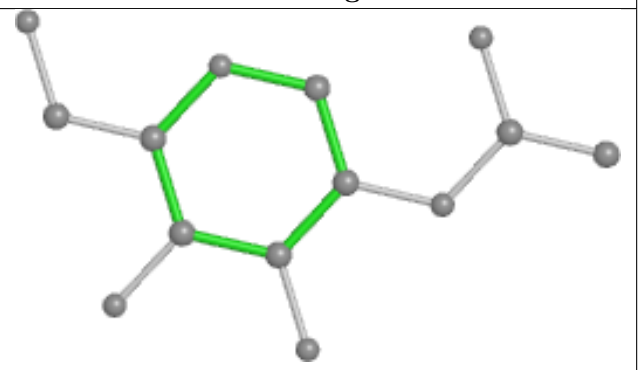


Rings

Ligand NAG B 1406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

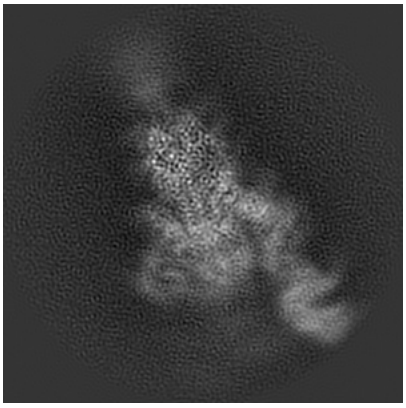
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30898. These allow visual inspection of the internal detail of the map and identification of artifacts.

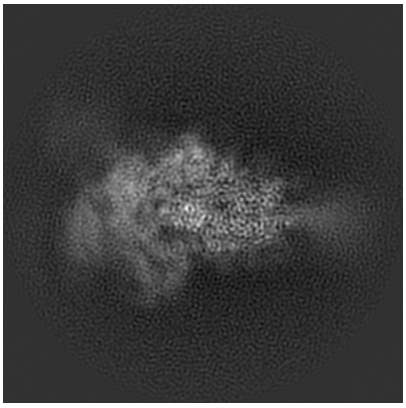
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

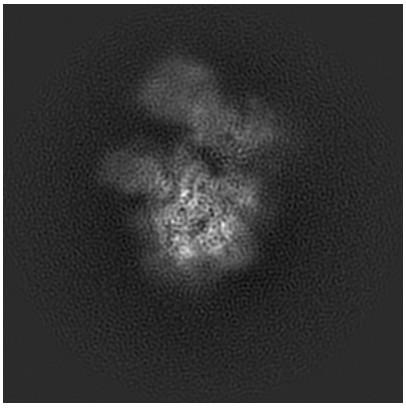
6.1.1 Primary map



X



Y

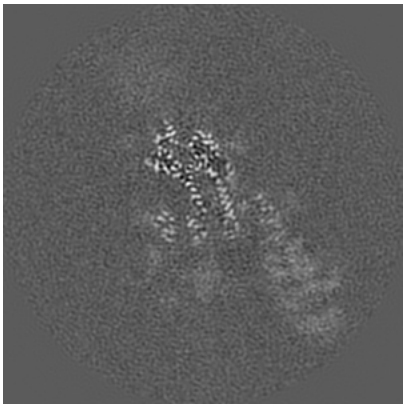


Z

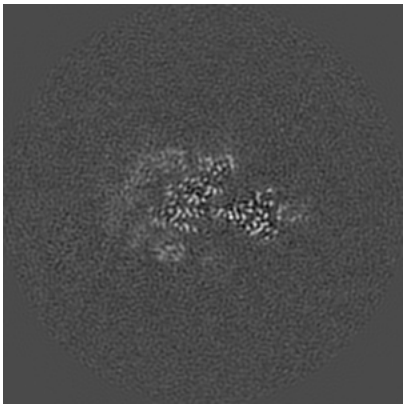
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

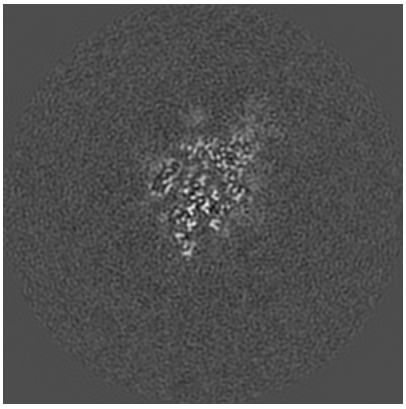
6.2.1 Primary map



X Index: 144



Y Index: 144

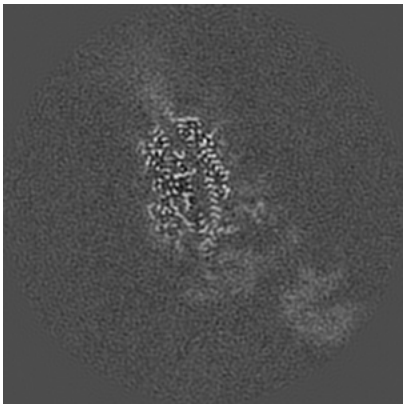


Z Index: 144

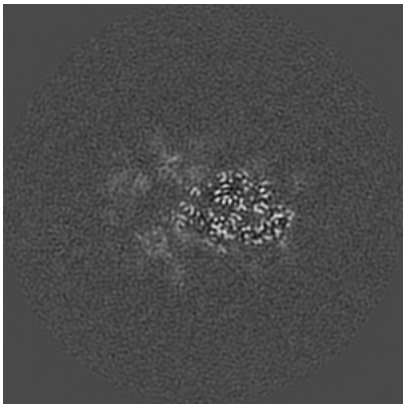
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

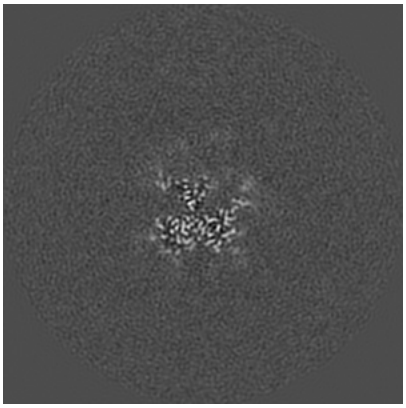
6.3.1 Primary map



X Index: 129



Y Index: 134



Z Index: 164

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

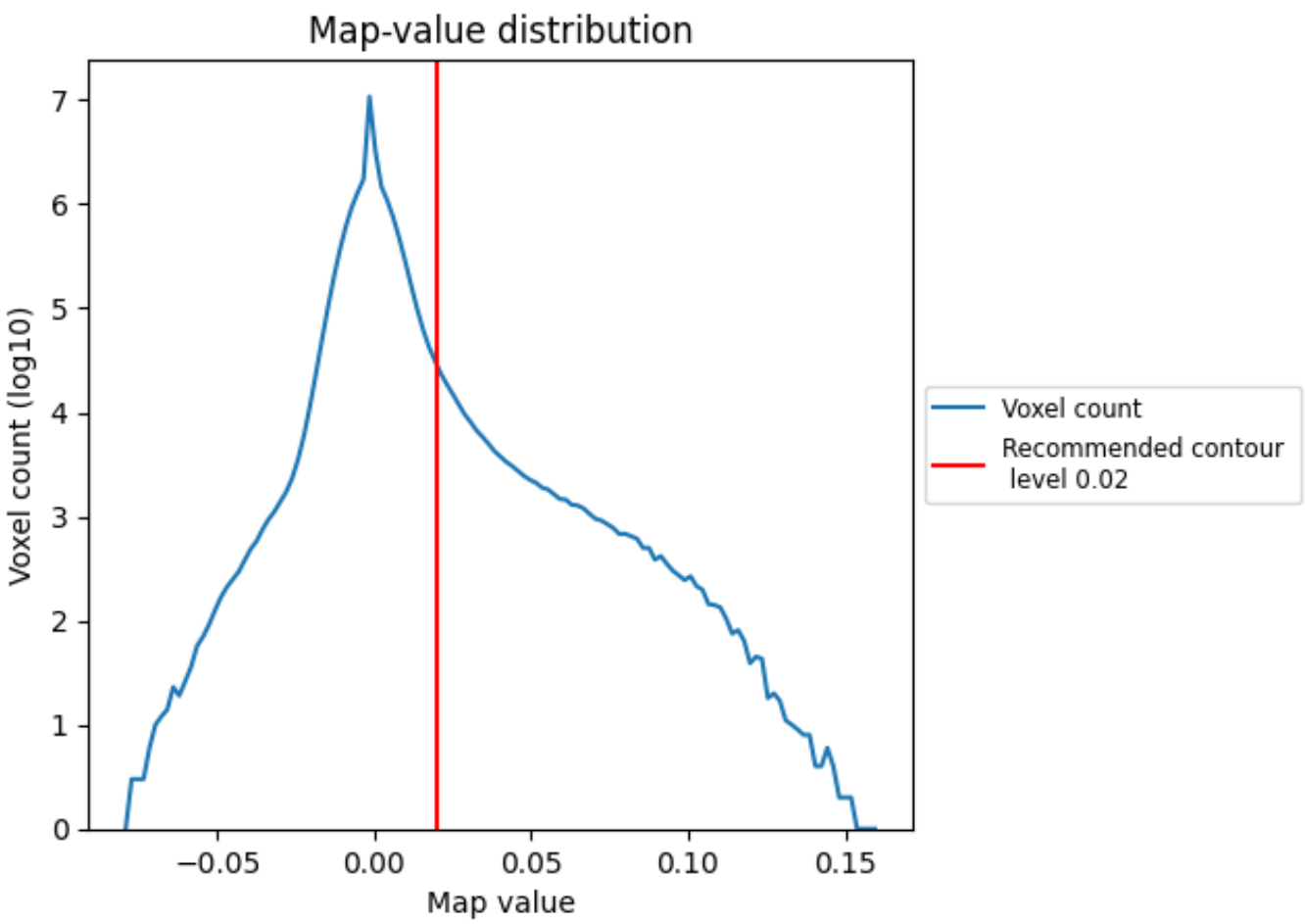
6.5 Mask visualisation (i)

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

7 Map analysis (i)

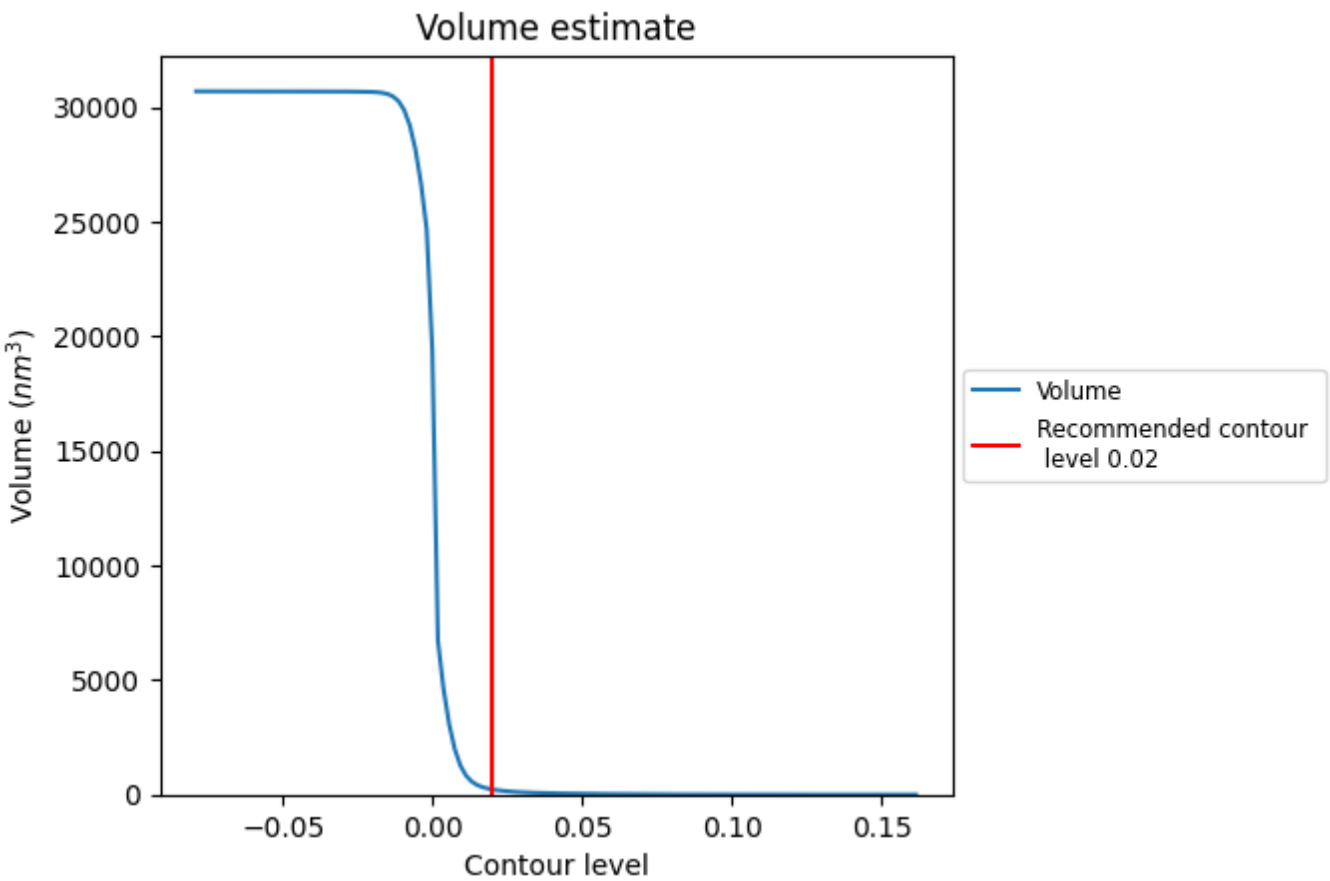
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

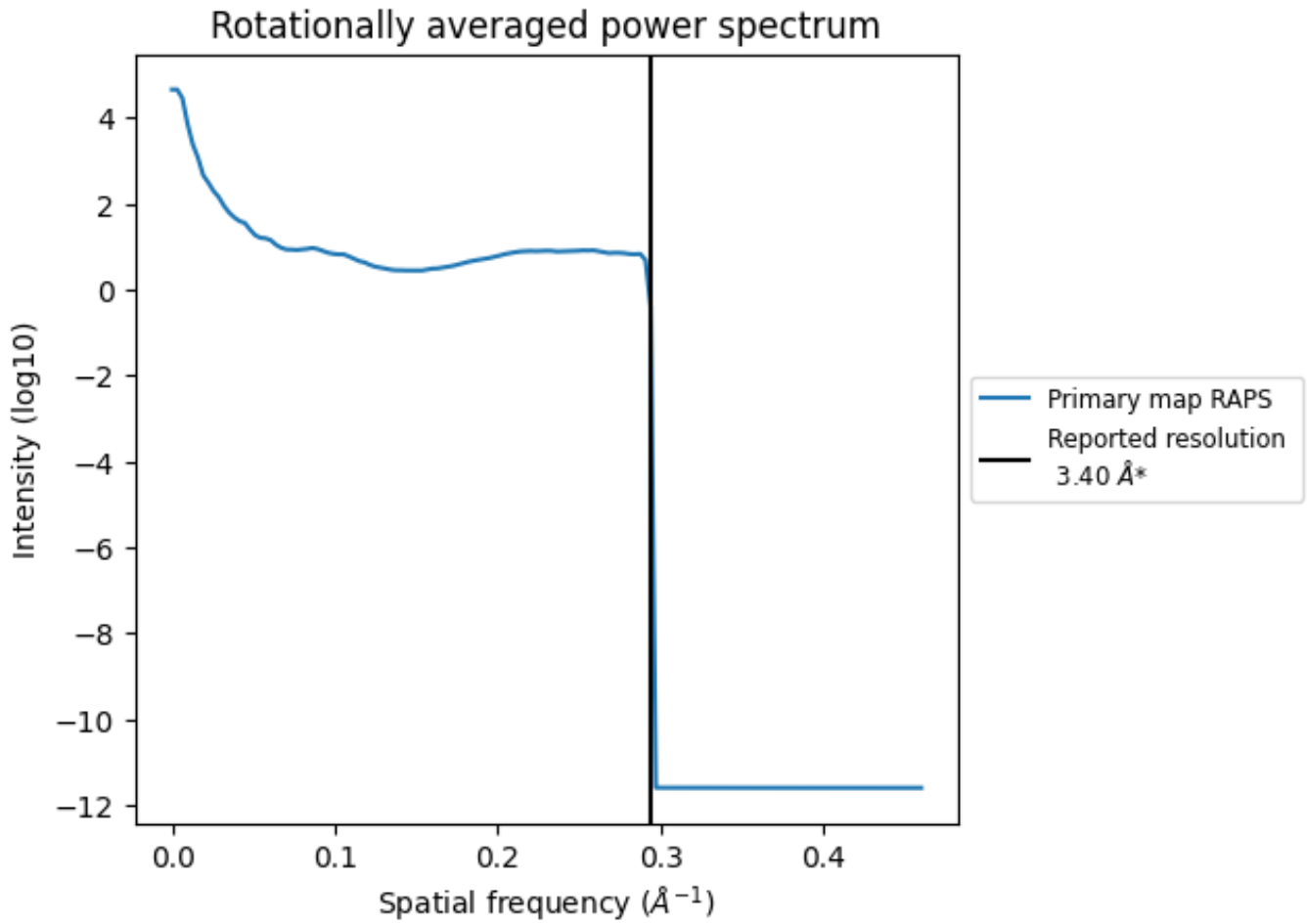
7.2 Volume estimate (i)



The volume at the recommended contour level is 222 nm^3; this corresponds to an approximate mass of 200 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 0.294 Å^{-1}

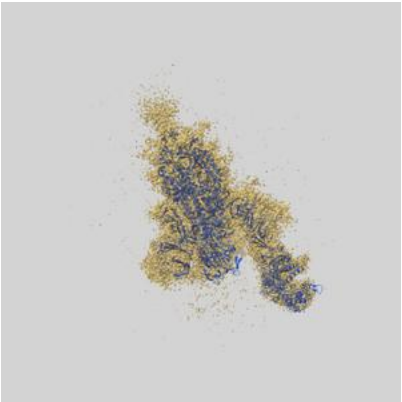
8 Fourier-Shell correlation (i)

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

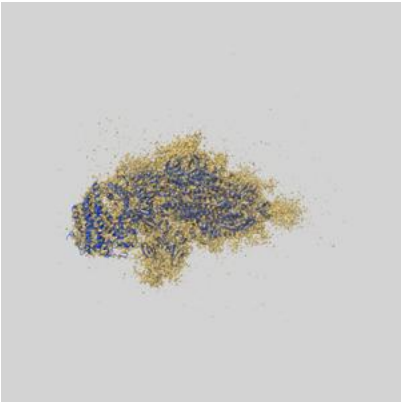
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30898 and PDB model 7DX7. Per-residue inclusion information can be found in section 3 on page 10.

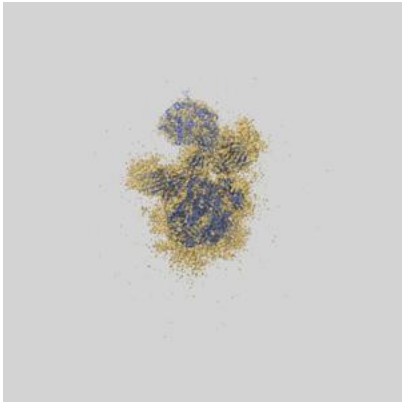
9.1 Map-model overlay (i)



X



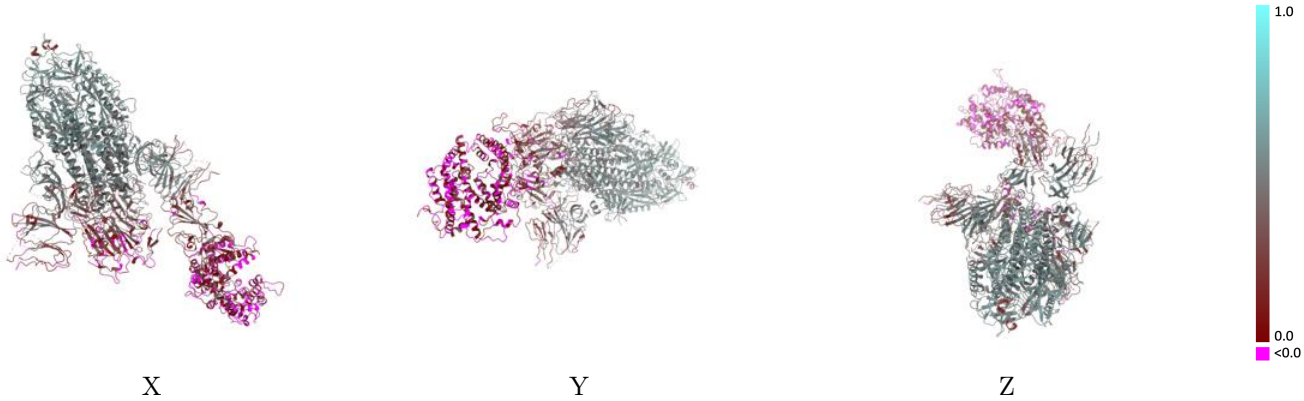
Y



Z

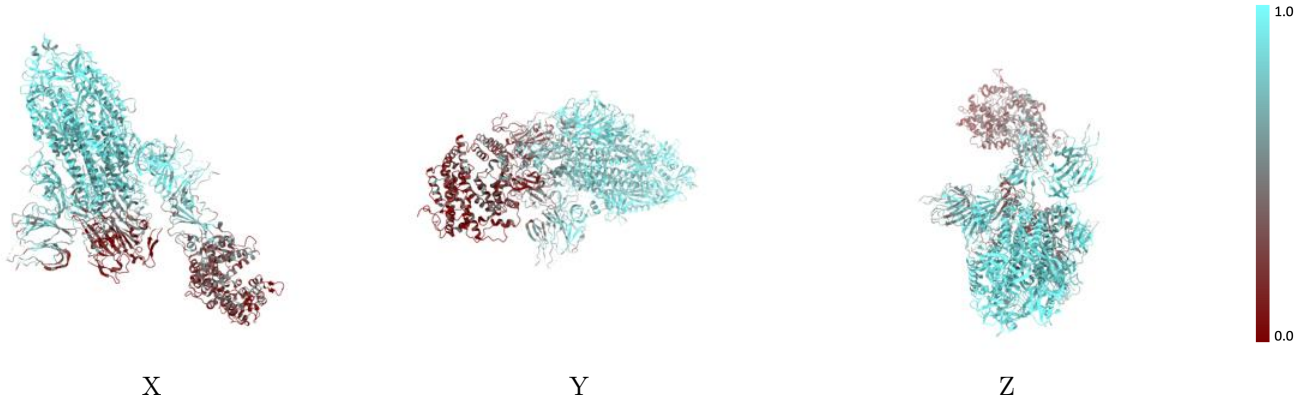
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



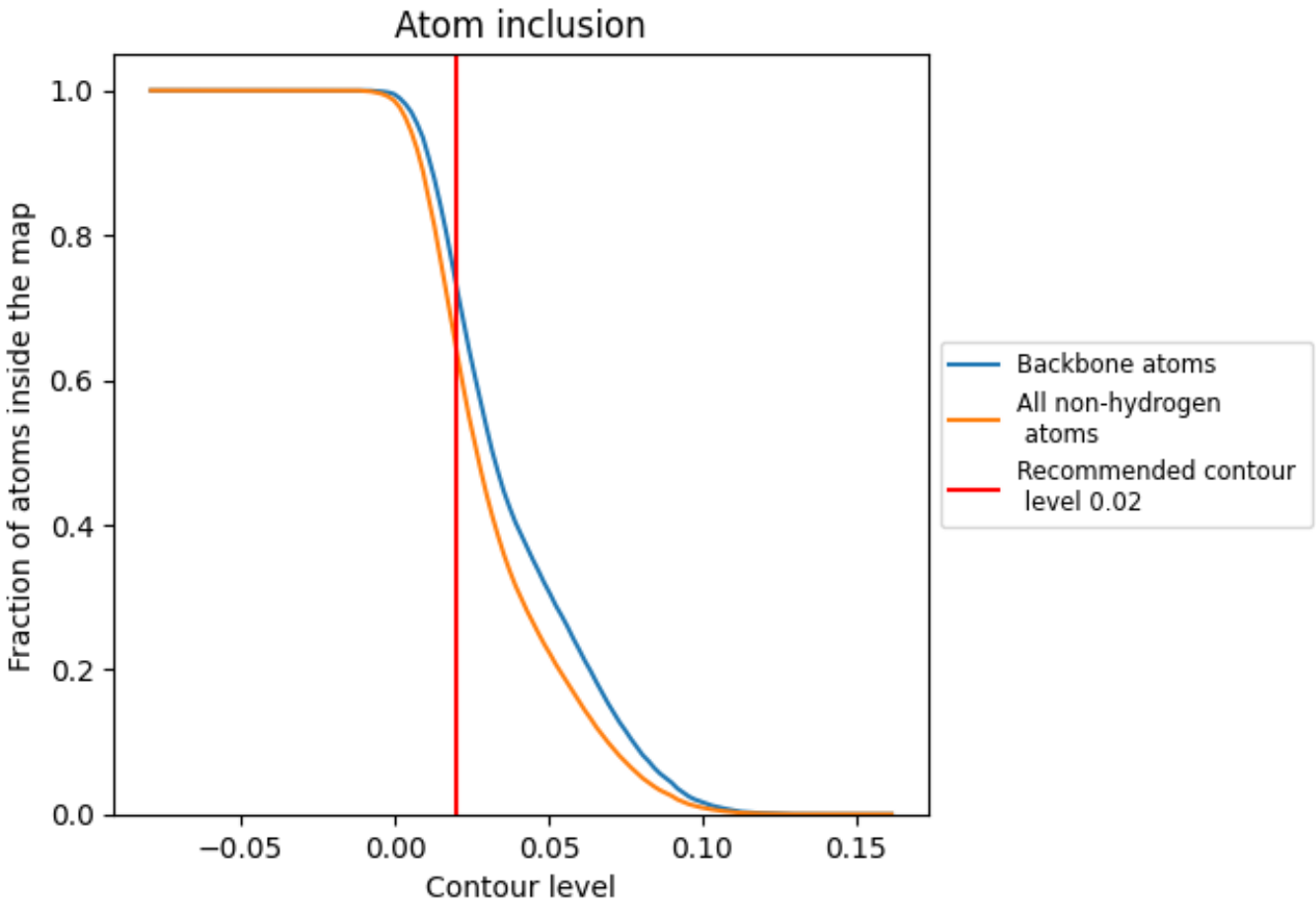
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.6439	0.3490
A	0.7635	0.4190
B	0.7387	0.4230
C	0.7023	0.4000
D	0.2308	0.0540
E	0.6786	0.3240
F	0.3214	0.1500
G	0.7857	0.4750
H	0.8214	0.3830
I	0.5000	0.3560
J	0.6429	0.3970
K	0.7143	0.4260
L	0.1786	0.1090
M	0.2857	0.2380
N	0.3571	0.2300
O	0.7500	0.3320
P	0.7500	0.3700
Q	0.8214	0.4110
R	0.7500	0.3110
S	0.1429	0.0810
T	0.1786	-0.0060
U	0.4286	0.1640
V	0.8214	0.4470
W	0.7143	0.3790
X	0.4643	0.3240
Y	0.7857	0.3820
Z	0.6786	0.3380
a	0.1071	0.0610
b	0.0000	-0.2300
c	0.0357	-0.0810
d	0.0000	0.2370
e	0.0357	0.1140