wwPDB EM Validation Summary Report (i)

Nov 22, 2022 – 02:21 AM JST

PDB ID	:	7DX8
EMDB ID	:	EMD-30899
Title	:	Trypsin-digested S protein of SARS-CoV-2 bound with PD of ACE2 in the conformation 2 (2 up RBD and 2 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	:	2.90 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:

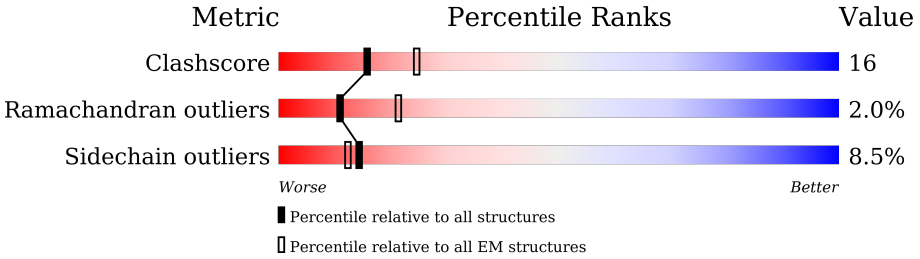
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.90 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	13% 52% 21% • 22%
1	B	1283	9% 51% 20% • • 24%
1	C	1283	15% 54% 20% • • 22%
2	D	817	73% 65% 7% 27%
2	E	817	73% 65% 7% 27%
3	F	2	50% 100%
3	G	2	50% 50% 50%
3	H	2	100%

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

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Mol	Chain	Length	Quality of chain
3	h	2	100% 50% 50%
3	i	2	100% 100%
3	j	2	100% 100%
3	k	2	100% 50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 34338 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	1006	7866	5022	1309	1499	36	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
2	E	595	4857	3108	804	916	29	0	0

There are 26 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
E	-11	MET	-	expression tag	UNP Q9BYF1
E	-10	ALA	-	expression tag	UNP Q9BYF1
E	-9	SER	-	expression tag	UNP Q9BYF1
E	-8	GLY	-	expression tag	UNP Q9BYF1
E	-7	ARG	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	TRP	-	insertion	UNP Q9BYF1
E	11	SER	-	insertion	UNP Q9BYF1
E	12	HIS	-	insertion	UNP Q9BYF1
E	13	PRO	-	insertion	UNP Q9BYF1
E	14	GLN	-	insertion	UNP Q9BYF1
E	15	PHE	-	insertion	UNP Q9BYF1
E	16	GLU	-	insertion	UNP Q9BYF1
E	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	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

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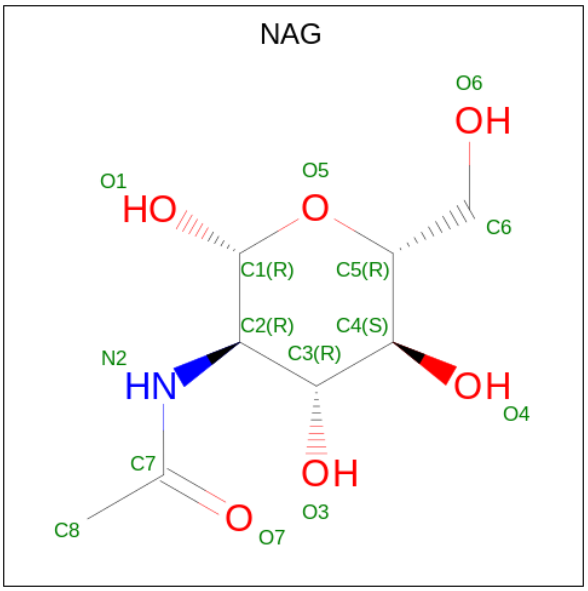
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	R	2	28	16	2	10	0	0
3	S	2	28	16	2	10	0	0
3	T	2	28	16	2	10	0	0
3	U	2	28	16	2	10	0	0
3	V	2	28	16	2	10	0	0
3	W	2	28	16	2	10	0	0
3	X	2	28	16	2	10	0	0
3	Y	2	28	16	2	10	0	0
3	Z	2	28	16	2	10	0	0
3	a	2	28	16	2	10	0	0
3	b	2	28	16	2	10	0	0
3	c	2	28	16	2	10	0	0
3	d	2	28	16	2	10	0	0
3	e	2	28	16	2	10	0	0
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

- 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
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	A	1	126	72	9	45	0
			Total	C	N	O	
4	B	1	140	80	10	50	0
			Total	C	N	O	
4	B	1	140	80	10	50	0
			Total	C	N	O	
4	B	1	140	80	10	50	0
			Total	C	N	O	
4	B	1	140	80	10	50	0
			Total	C	N	O	
4	B	1	140	80	10	50	0

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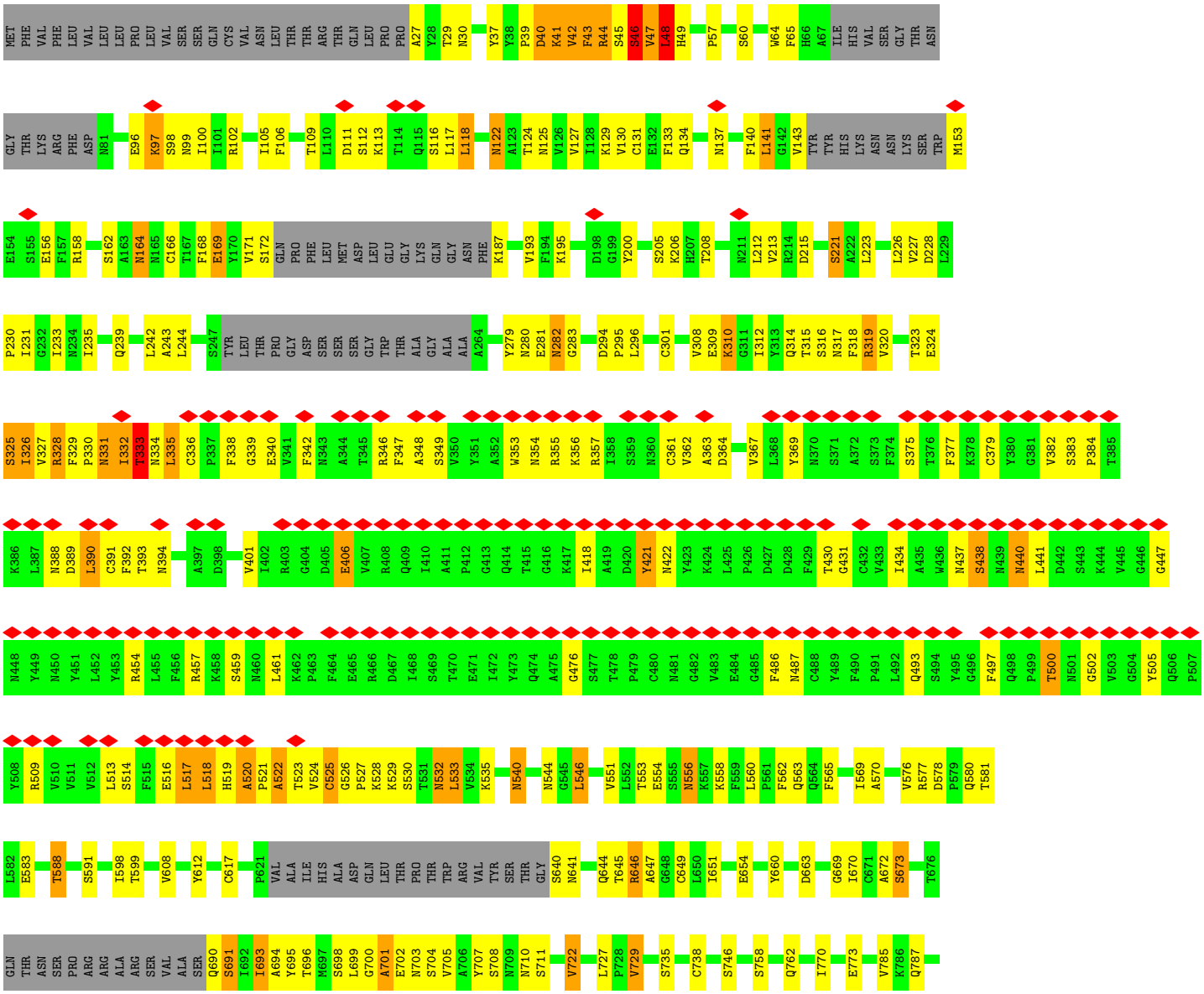
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	B	1	140	80	10	50	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	D	1	14	8	1	5	0
4	E	1	14	8	1	5	0

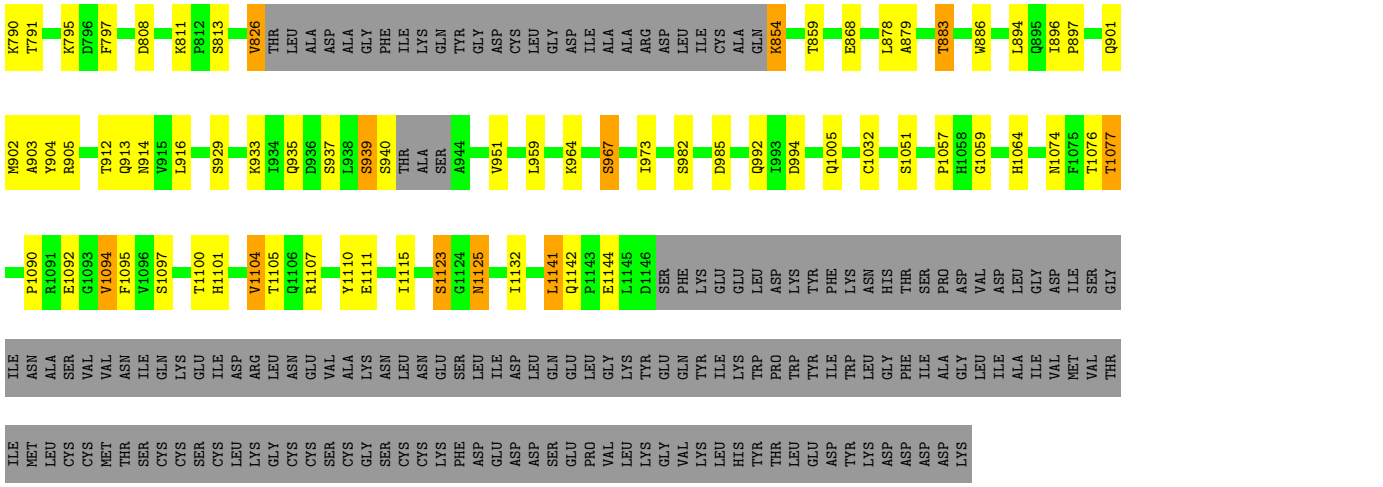
3 Residue-property plots (i)

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

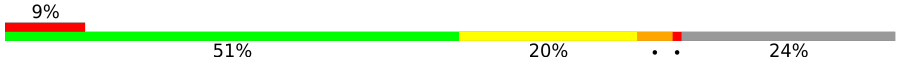
Chain A: 13% 52% 21% • 22%

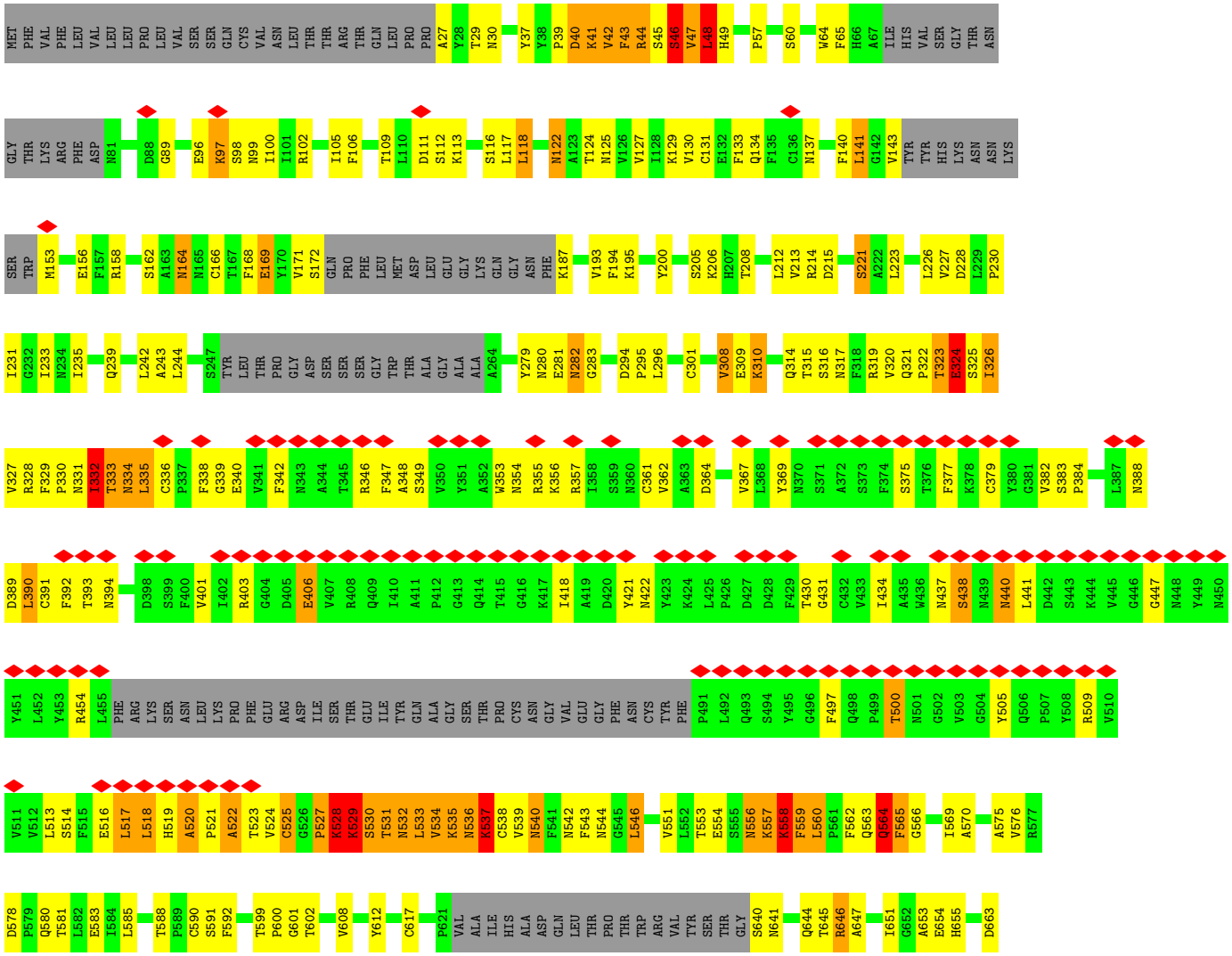


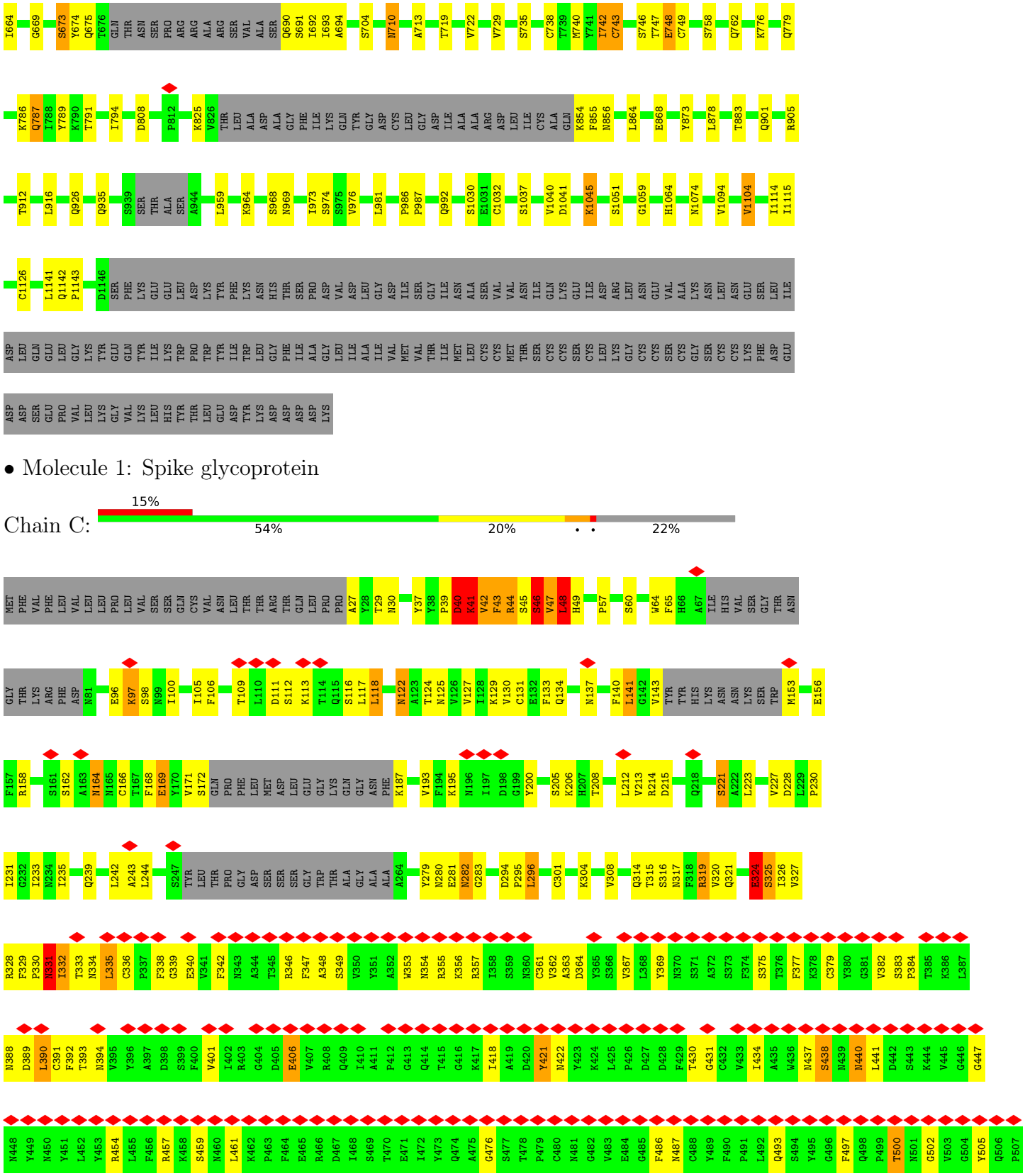


- Molecule 1: Spike glycoprotein

Chain B:

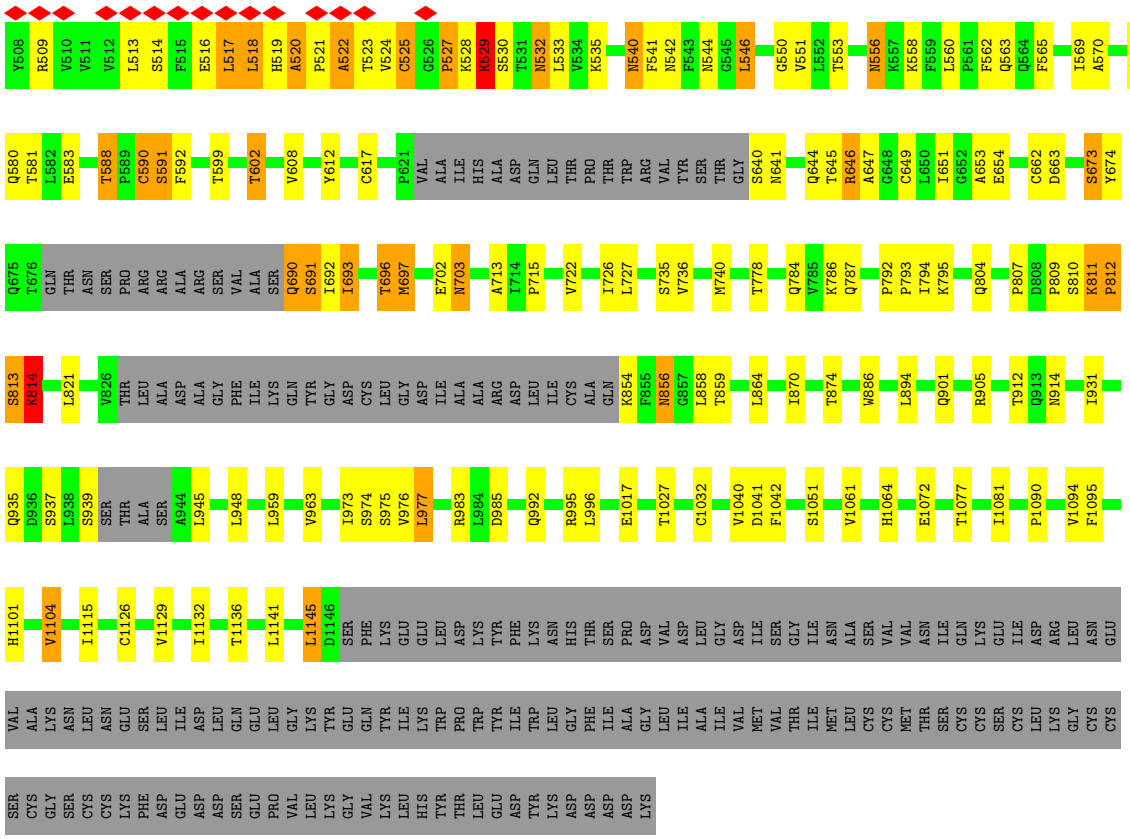






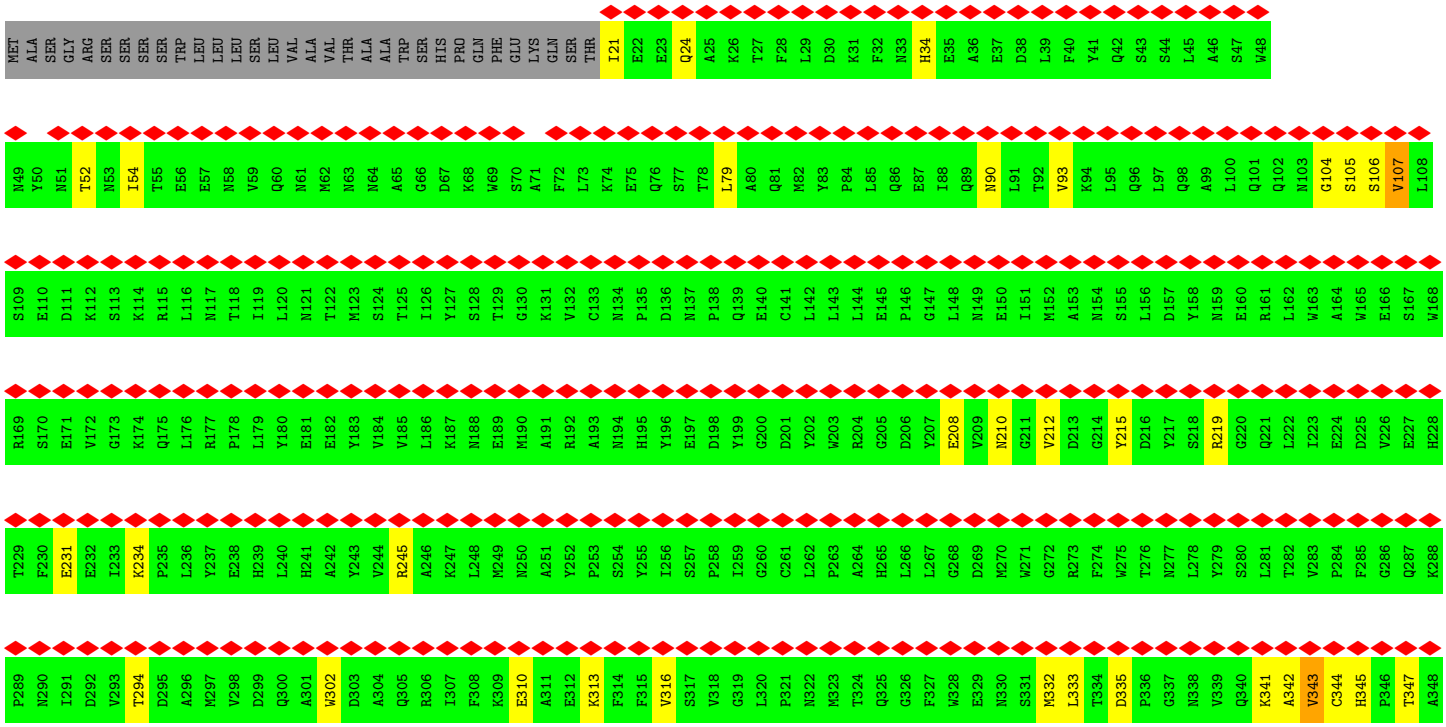
- Molecule 1: Spike glycoprotein

Chain C:



- Molecule 2: Angiotensin-converting enzyme 2

Chain D:



W349 D350 L351 G352 K353 G354 D355 F356 R357 I358 L359 M360 C361 T362 K363 V364 T365 M366 D367 D368 F369 L370 T371 A372 H373 H374 E375 M376 G377 H378 I379 Q380 Y381 D382 M383 A384 Y385 A386 A387 Q388 P389 F390 L391 L392 R393 N394 G395 A396 N397 E398 G399 F400 H401 E402 A403 V404 G405 E406 I407 M408

S409 L410 S411 A412 A413 T414 P415 K416 H417 L418 K419 S420 I421 G422 L423 L424 S425 P426 D427 F428 Q429 E430 D431 M432 E433 T434 E435 I436 N437 F438 L439 L440 K441 Q442 A443 L444 T445 I446 V447 G448 T449 L450 P451 F452 T453 Y454 M455 L456 E457 K458 W459 R460 W461 M462 V463 F464 K465 G466 E467 I468

P469 K470 D471 Q472 W473 M474 K475 K476 W477 W478 E479 M480 K481 R482 E483 I484 V485 G486 V487 V488 E489 P490 V491 P492 H493 D494 E495 T496 Y497 C498 D499 P500 A501 S502 L503 F504 H505 V506 S507 N508 D509 Y510 S511 F512 T513 R514 Y515 Y516 T517 R518 T519 L520 Y521 Q522 F523 Q524 F525 Q526 E527 A528

L529 C530 Q531 A532 A533 K534 H535 E536 G537 P538 L539 H540 K541 C542 D543 I544 S545 N546 S547 T548 E549 A550 G551 Q552 K553 L554 F555 N556 M557 L558 R559 L560 G561 K562 S563 E564 P565 W566 T567 L568 A569 L570 E571 N572 V573 V574 G575 A576 K577 N578 M579 N580 V581 R582 P583 L584 L585 N586 Y587 F588

E589 P590 L591 F592 T593 W594 L595 K596 D597 Q598 N599 K600 N601 S602 F603 V604 G605 W606 S607 T608 D609 W610 S611 P612 Y613 A614 D615 GLN SER ILE LYS VAL ARG ILE SER LEU LYS SER ALA LEU GLY ASP LYS ALA TYR GLU TRP ASN ASP ASN GLU MET TYR LEU PHE ARG SER SER VAL ALA

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

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

LYS LYS LYS ASN LYS ALA ARG SER GLY GLU ASN PRO TYR ALA SER ILE ASP ILE SER LYS GLY GLU ASN ASN PRO GLY PHE GLN ASN THR ASP ASP VAL GLN THR SER PHE

- Molecule 2: Angiotensin-converting enzyme 2

Chain E:

MET ALA SER GLY ARG SER SER SER SER TRP LEU LEU LEU LEU SER LEU VAL ALA VAL THR ALA ALA TRP SER HIS PRO GLN PHE GLU LYS GLN SER THR I21 E22 E23 Q24 A25 K26 T27 F28 L29 D30 K31 F32 N33 H34 E35 A36 E37 D38 L39 F40 Y41 Q42 S43 S44 L45 A46 S47 W48

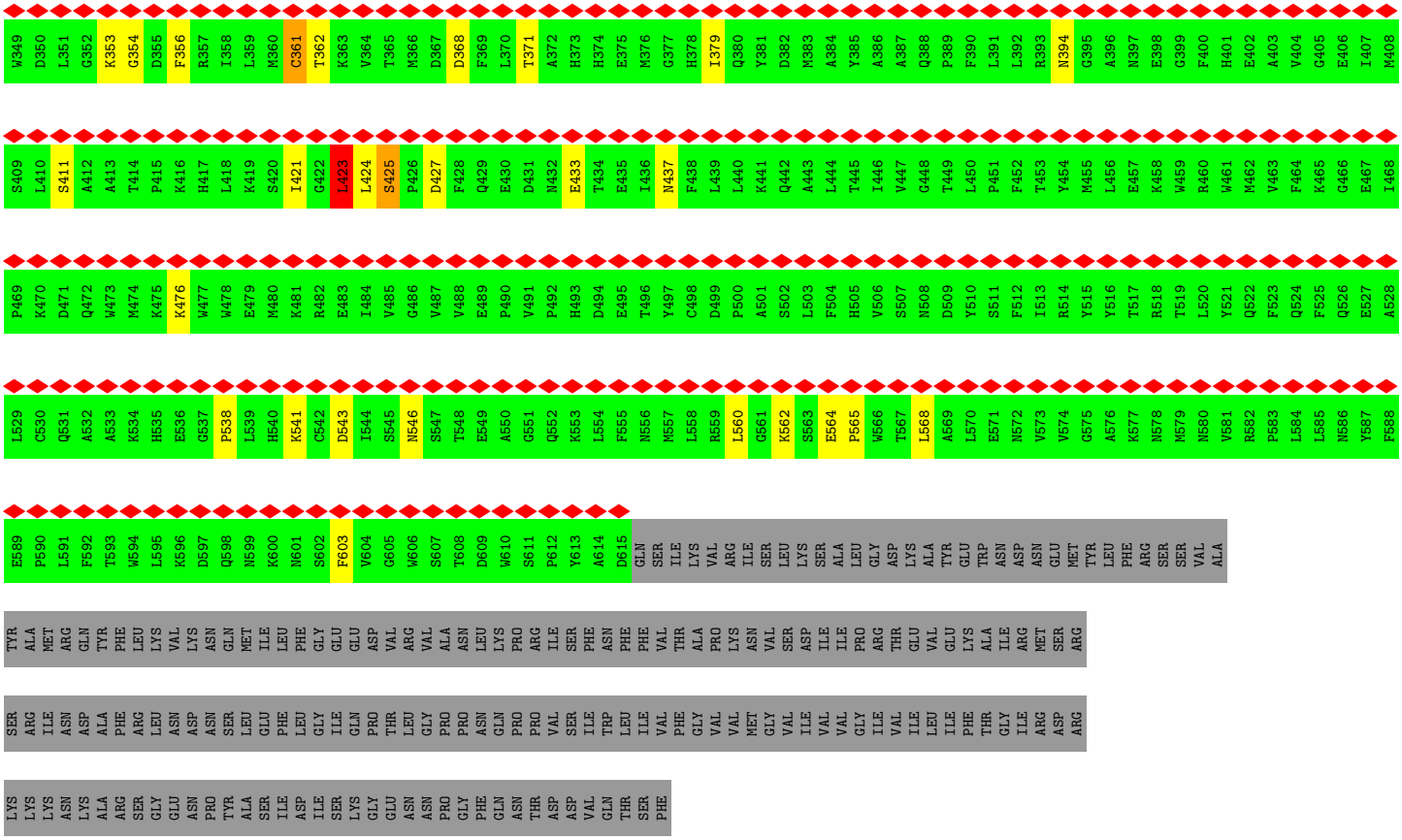
N49 Y50 N51 T52 N53 I54 T55 E56 E57 N58 V59 Q60 N61 M62 N63 N64 A65 G66 D67 K68 W69 S70 A71 F72 L73 K74 E75 Q76 S77 T78 L79 A80 Q81 M82 Y83 P84 L85 Q86 E87 I88 Q89 N90 L91 T92 V93 K94 L95 Q96 L97 Q98 A99 L100 Q101 Q102 N103 G104 S105 S106 V107 L108

S109 E110 D111 K112 S113 K114 R115 L116 N117 T118 I119 L120 N121 T122 M123 S124 T125 I126 Y127 S128 T129 G130 K131 V132 C133 N134 P135 D136 N137 P138 Q139 E140 C141 L142 L143 L144 E145 P146 G147 L148 N149 E150 I151 M152 A153 N154 S155 L156 D157 Y158 N159 E160 R161 L162 W163 A164 W165 E166 S167 W168

R169 S170 E171 V172 G173 K174 Q175 L176 R177 P178 L179 Y180 E181 E182 Y183 V184 V185 L186 K187 N188 E189 M190 A191 R192 A193 N194 H195 Y196 E197 D198 Y199 G200 D201 Y202 W203 R204 G205 D206 Y207 E208 V209 N210 G211 V212 D213 G214 Y215 D216 Y217 S218 R219 G220 Q221 L222 I223 E224 D225 V226 E227 H228

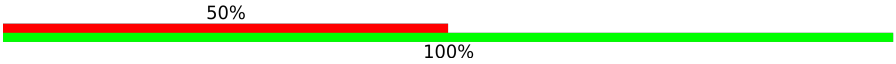
T229 F230 E231 E232 I233 K234 P235 L236 Y237 E238 H239 L240 H241 A242 Y243 V244 R245 A246 K247 L248 M249 N250 A251 Y252 P253 S254 Y255 I256 S257 P258 I259 G260 C261 L262 P263 A264 H265 L266 L267 G268 D269 M270 W271 G272 R273 F274 W275 T276 N277 L278 Y279 S280 L281 T282 V283 P284 F285 Q286 Q287 K288

P289 N290 I291 D292 V293 T294 D295 A296 M297 V298 D299 Q300 A301 W302 D303 A304 Q305 R306 I307 F308 K309 E310 A311 E312 K313 F314 F315 V316 S317 V318 G319 L320 P321 N322 M323 T324 Q325 G326 F327 W328 E329 N330 S331 M332 L333 T334 D335 P336 G337 N338 V339 Q340 K341 A342 V343 C344 H345 P346 T347 A348



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

Chain F:

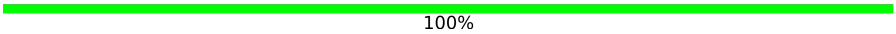


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

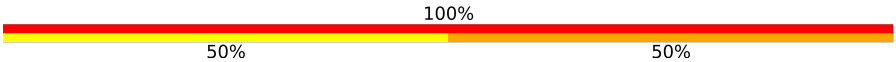
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

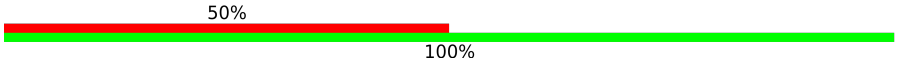
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

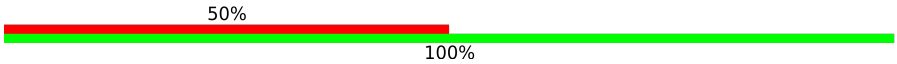
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

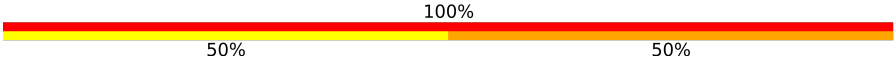
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

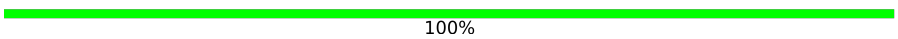
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

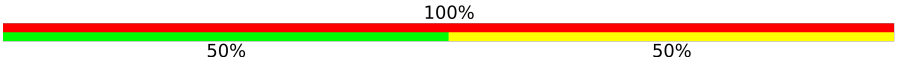
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

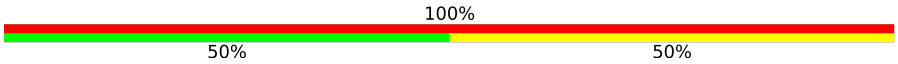
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

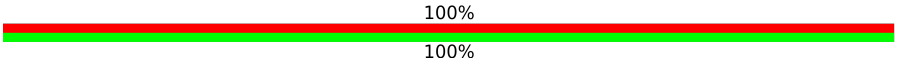
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

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

Chain c: 

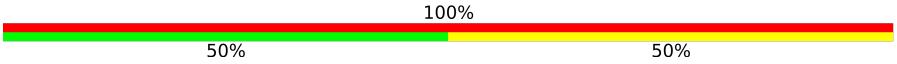
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 

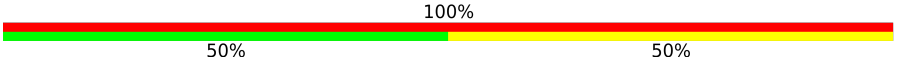
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

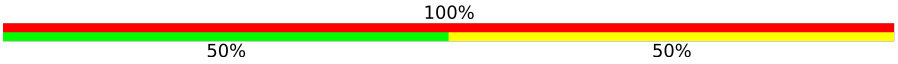
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: 

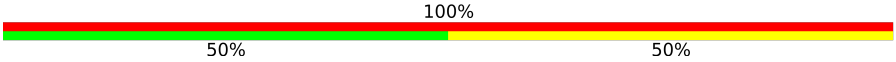
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208455	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	0.198	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	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	0.57	0/7751	0.55	0/10544
1	C	0.58	0/8042	0.54	0/10939
2	D	0.35	0/4994	0.50	0/6785
2	E	0.35	0/4994	0.50	0/6785
All	All	0.52	0/33829	0.54	0/46000

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	7668	335	0
1	B	7584	0	7402	364	0
1	C	7866	0	7663	373	0
2	D	4857	0	4624	66	0
2	E	4857	0	4624	67	0
3	F	28	0	25	0	0
3	G	28	0	25	3	0
3	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	28	0	25	6	0
3	J	28	0	25	1	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	2	0
3	N	28	0	25	3	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	4	0
3	V	28	0	25	1	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	1	0
3	Z	28	0	25	2	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
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	0	0
3	i	28	0	25	0	0
3	j	28	0	25	0	0
3	k	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
4	E	14	0	13	0	0
All	All	34338	0	33157	1090	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 16.

The worst 5 of 1090 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:C:654:GLU:HG3	1:C:693:ILE:CG2	1.37	1.50
4:B:1409:NAG:O4	4:B:1410:NAG:C1	1.63	1.46
1:A:230:PRO:CB	1:C:521:PRO:HG2	1.47	1.44
1:A:703:ASN:HB2	1:B:787:GLN:OE1	1.28	1.28
1:A:486:PHE:CE1	2:D:79:LEU:HD22	1.75	1.21

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%)	876 (89%)	91 (9%)	22 (2%)	6 24
1	B	951/1283 (74%)	823 (86%)	98 (10%)	30 (3%)	4 16
1	C	988/1283 (77%)	866 (88%)	96 (10%)	26 (3%)	5 20
2	D	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	41 71
2	E	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	41 71
All	All	4114/5483 (75%)	3691 (90%)	341 (8%)	82 (2%)	11 27

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	331	ASN
1	A	332	ILE
1	A	333	THR
1	A	518	LEU

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%)	776 (88%)	106 (12%)	5 15
1	B	850/1122 (76%)	746 (88%)	104 (12%)	5 15
1	C	881/1122 (78%)	792 (90%)	89 (10%)	7 23
2	D	525/721 (73%)	518 (99%)	7 (1%)	69 90
2	E	525/721 (73%)	518 (99%)	7 (1%)	69 90
All	All	3663/4808 (76%)	3350 (92%)	313 (8%)	14 31

5 of 313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	301	CYS
1	C	974	SER
1	C	331	ASN
1	C	540	ASN
2	D	344	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	188	ASN
1	C	703	ASN
2	E	472	GLN
1	C	317	ASN
1	C	540	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)

64 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	F	1	1,3	14,14,15	0.55	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.58	0
3	NAG	G	1	1,3	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	H	1	1,3	14,14,15	0.31	0	17,19,21	0.62	0
3	NAG	H	2	3	14,14,15	0.53	0	17,19,21	0.48	0
3	NAG	I	1	1,3	14,14,15	0.37	0	17,19,21	0.73	0
3	NAG	I	2	3	14,14,15	0.28	0	17,19,21	1.32	2 (11%)
3	NAG	J	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
3	NAG	J	2	3	14,14,15	0.39	0	17,19,21	1.40	3 (17%)
3	NAG	K	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.67	0
3	NAG	K	2	3	14,14,15	0.30	0	17,19,21	0.65	0
3	NAG	L	1	1,3	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
3	NAG	L	2	3	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	M	1	1,3	14,14,15	0.56	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	N	1	1,3	14,14,15	0.57	1 (7%)	17,19,21	0.56	0
3	NAG	N	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	O	1	1,3	14,14,15	0.32	0	17,19,21	0.40	0
3	NAG	O	2	3	14,14,15	0.37	0	17,19,21	0.35	0
3	NAG	P	1	1,3	14,14,15	0.35	0	17,19,21	1.14	1 (5%)
3	NAG	P	2	3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	Q	1	1,3	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
3	NAG	Q	2	3	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	R	1	1,3	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	R	2	3	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
3	NAG	S	1	1,3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	S	2	3	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	T	1	1,3	14,14,15	0.55	0	17,19,21	0.49	0
3	NAG	T	2	3	14,14,15	0.25	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	U	1	1,3	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
3	NAG	U	2	3	14,14,15	0.29	0	17,19,21	0.46	0
3	NAG	V	1	1,3	14,14,15	0.23	0	17,19,21	1.36	1 (5%)
3	NAG	V	2	3	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	W	1	1,3	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
3	NAG	W	2	3	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	X	1	1,3	14,14,15	0.36	0	17,19,21	0.39	0
3	NAG	X	2	3	14,14,15	0.20	0	17,19,21	0.74	0
3	NAG	Y	1	1,3	14,14,15	0.36	0	17,19,21	0.48	0
3	NAG	Y	2	3	14,14,15	0.53	0	17,19,21	1.30	1 (5%)
3	NAG	Z	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.43	0
3	NAG	Z	2	3	14,14,15	0.32	0	17,19,21	1.36	2 (11%)
3	NAG	a	1	1,3	14,14,15	0.40	0	17,19,21	0.44	0
3	NAG	a	2	3	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	b	1	2,3	14,14,15	0.62	1 (7%)	17,19,21	0.73	0
3	NAG	b	2	3	14,14,15	0.54	0	17,19,21	0.36	0
3	NAG	c	1	2,3	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	c	2	3	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
3	NAG	d	1	2,3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	d	2	3	14,14,15	0.30	0	17,19,21	0.63	0
3	NAG	e	1	2,3	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	e	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	f	1	2,3	14,14,15	0.23	0	17,19,21	0.62	0
3	NAG	f	2	3	14,14,15	0.33	0	17,19,21	0.59	1 (5%)
3	NAG	g	1	2,3	14,14,15	0.62	1 (7%)	17,19,21	0.73	0
3	NAG	g	2	3	14,14,15	0.54	0	17,19,21	0.36	0
3	NAG	h	1	2,3	14,14,15	0.42	0	17,19,21	0.65	0
3	NAG	h	2	3	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
3	NAG	i	1	2,3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	i	2	3	14,14,15	0.29	0	17,19,21	0.63	0
3	NAG	j	1	2,3	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	j	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	k	1	2,3	14,14,15	0.22	0	17,19,21	0.62	0
3	NAG	k	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	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	5/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	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	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	5/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	4/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	0/6/23/26	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	-	2/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	4/6/23/26	0/1/1/1
3	NAG	e	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	NAG	f	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	i	2	3	-	4/6/23/26	0/1/1/1
3	NAG	j	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	j	2	3	-	0/6/23/26	0/1/1/1
3	NAG	k	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	k	2	3	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C1	-2.68	1.39	1.43
3	K	1	NAG	O5-C1	-2.55	1.39	1.43
3	J	1	NAG	O5-C1	-2.33	1.40	1.43
3	b	1	NAG	O5-C1	-2.19	1.40	1.43
3	g	1	NAG	O5-C1	-2.17	1.40	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	V	1	NAG	C2-N2-C7	4.64	129.52	122.90
3	J	2	NAG	C2-N2-C7	4.43	129.21	122.90
3	Z	2	NAG	C2-N2-C7	4.35	129.10	122.90
3	I	2	NAG	C2-N2-C7	4.29	129.00	122.90
3	Y	2	NAG	C2-N2-C7	4.28	128.99	122.90

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

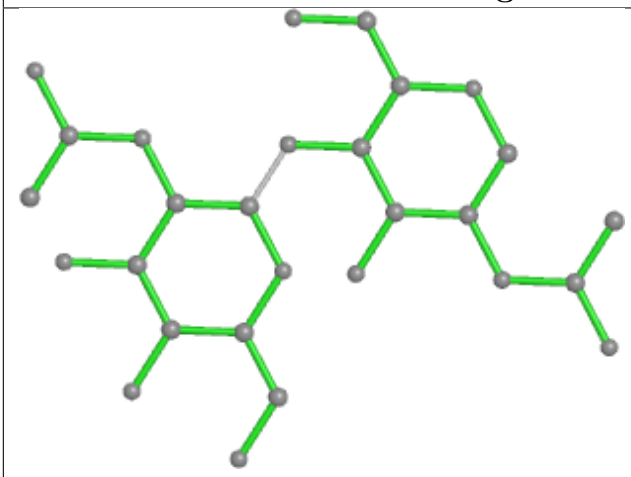
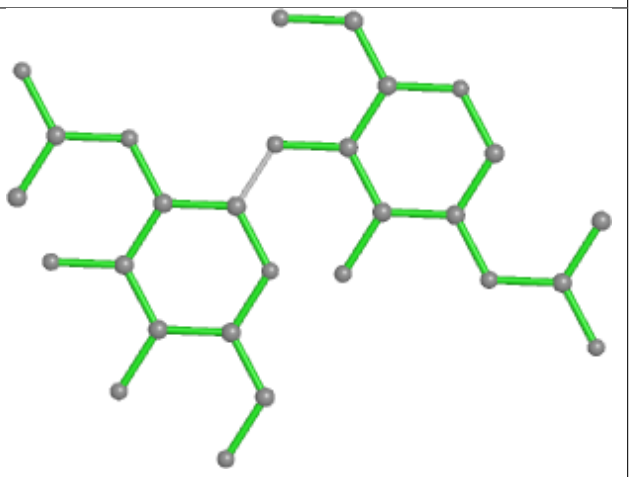
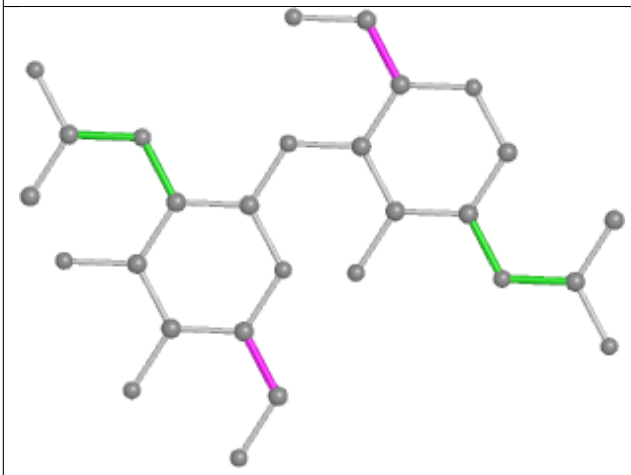
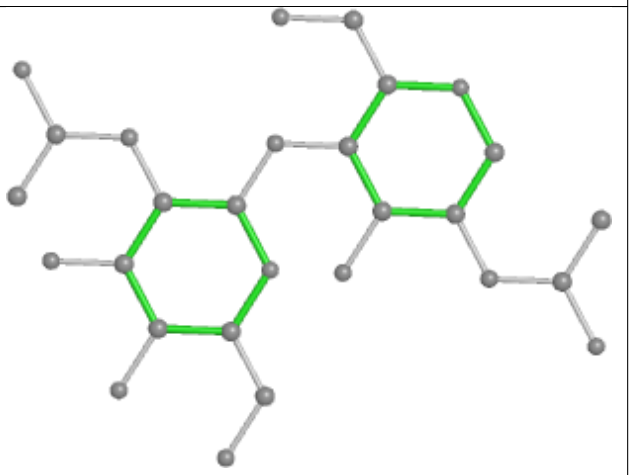
Mol	Chain	Res	Type	Atoms
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	d	2	NAG	C3-C2-N2-C7
3	d	2	NAG	C8-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2

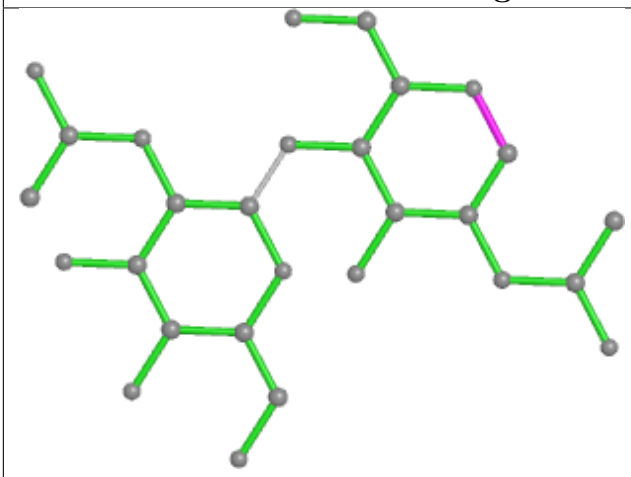
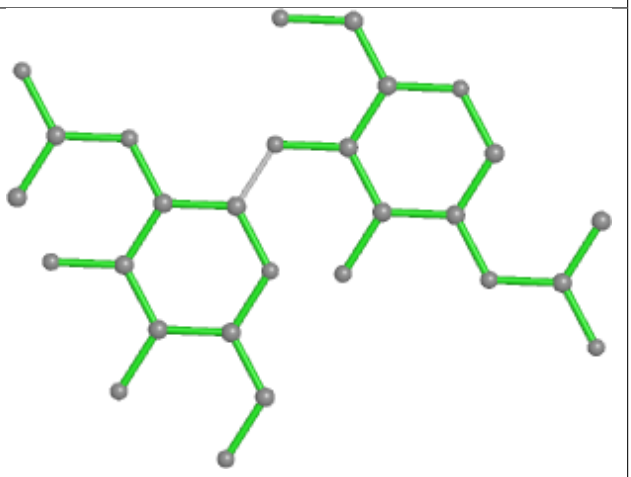
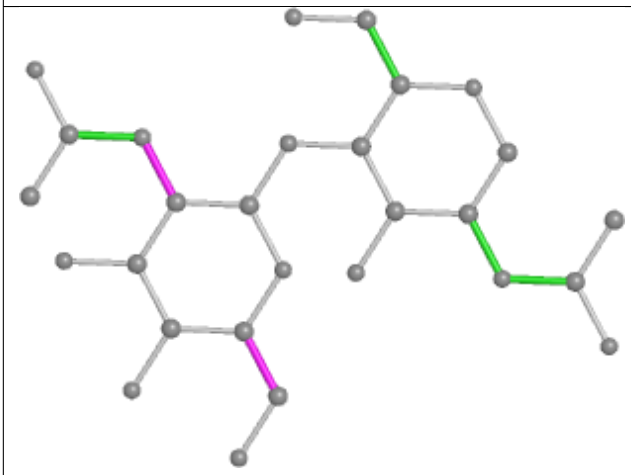
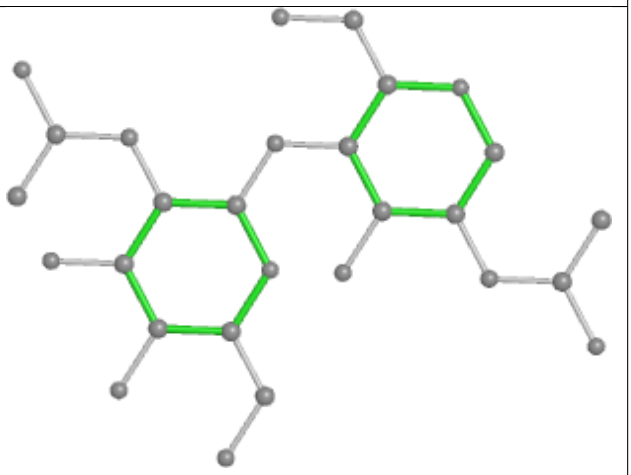
There are no ring outliers.

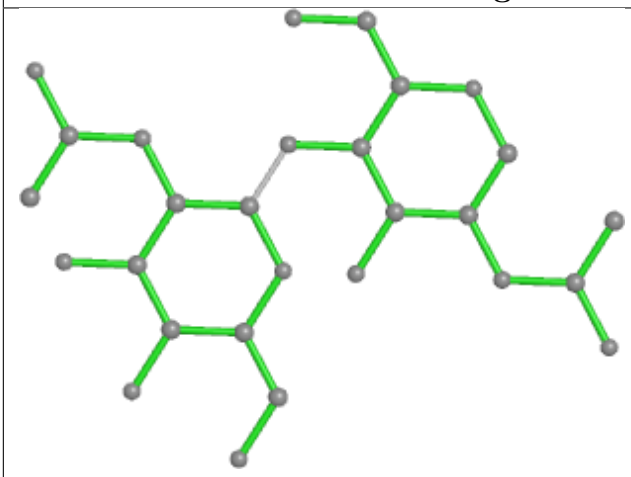
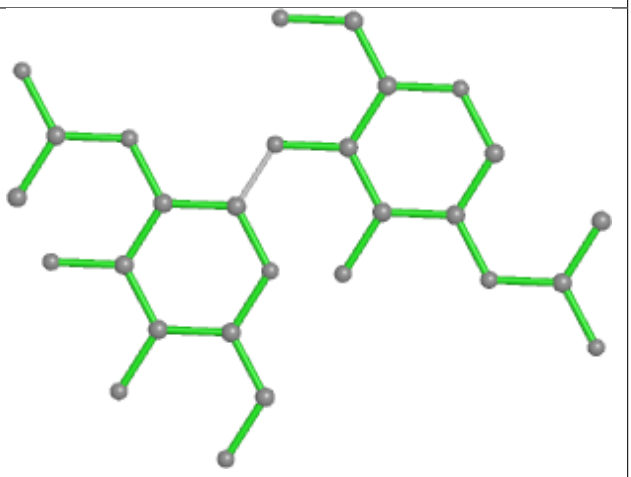
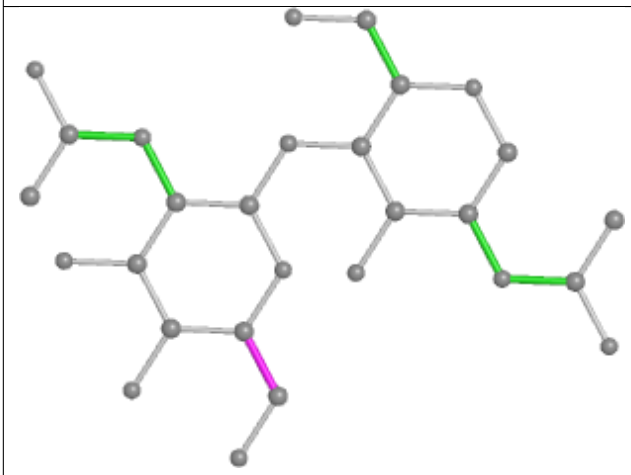
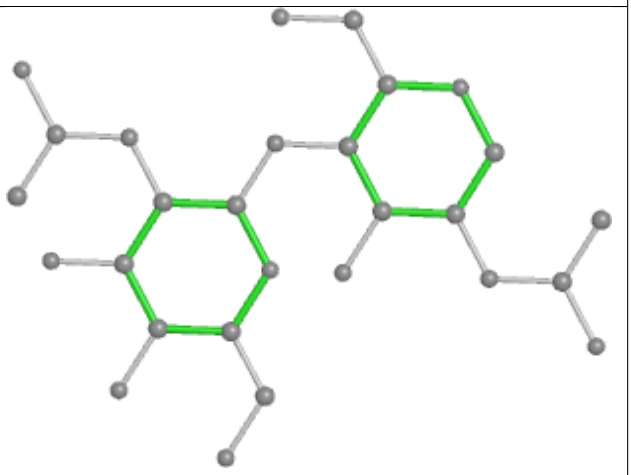
16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	2	NAG	2	0
3	G	1	NAG	3	0
3	I	1	NAG	4	0
3	R	2	NAG	1	0
3	Z	1	NAG	1	0
3	Z	2	NAG	1	0
3	V	1	NAG	1	0
3	M	1	NAG	2	0
3	J	2	NAG	1	0
3	G	2	NAG	2	0
3	U	1	NAG	4	0
3	R	1	NAG	1	0
3	U	2	NAG	2	0
3	I	2	NAG	6	0
3	Y	2	NAG	1	0
3	N	1	NAG	3	0

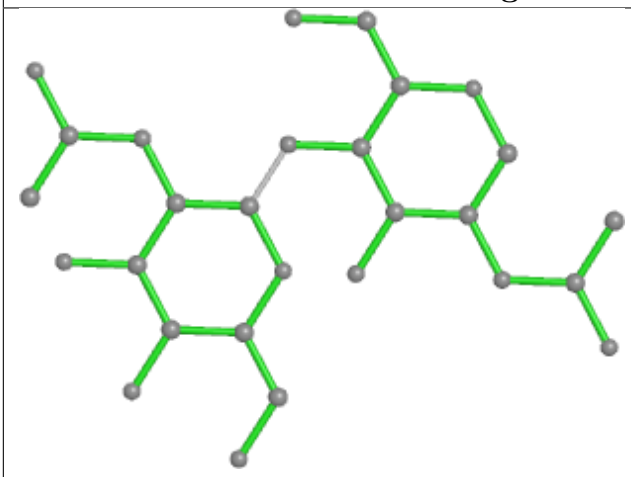
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

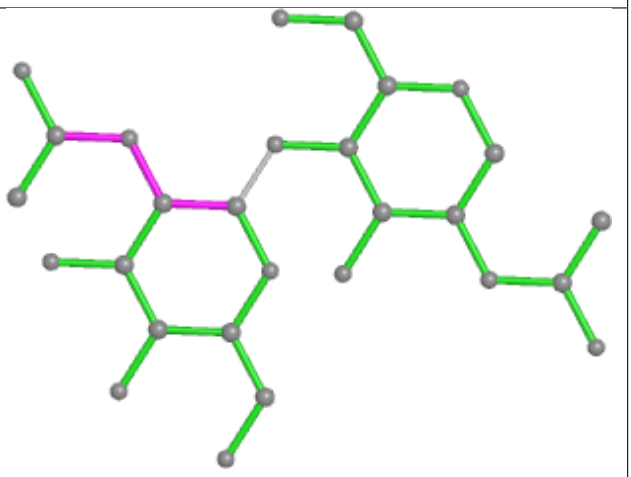
Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

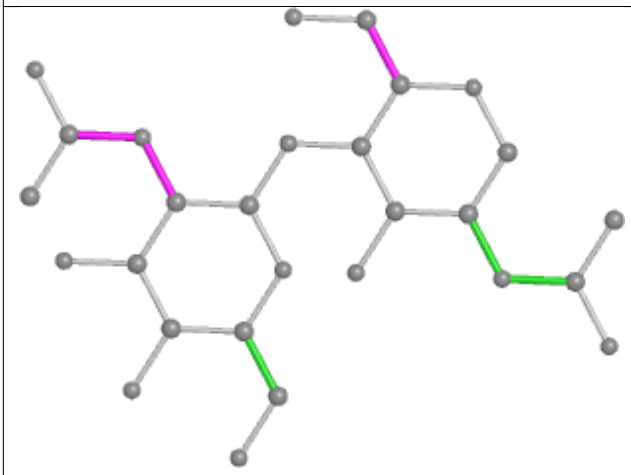
Oligosaccharide Chain I



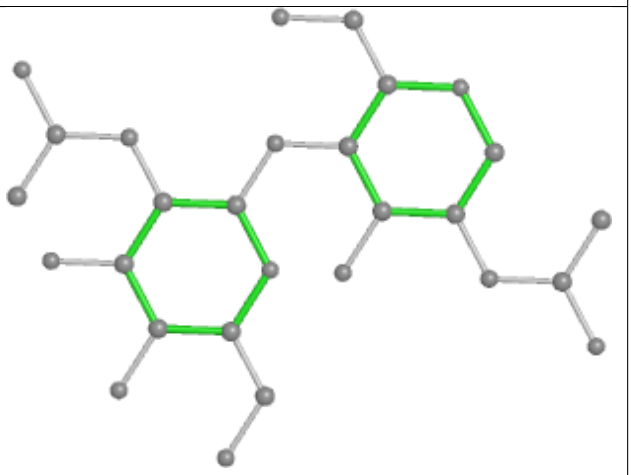
Bond lengths



Bond angles

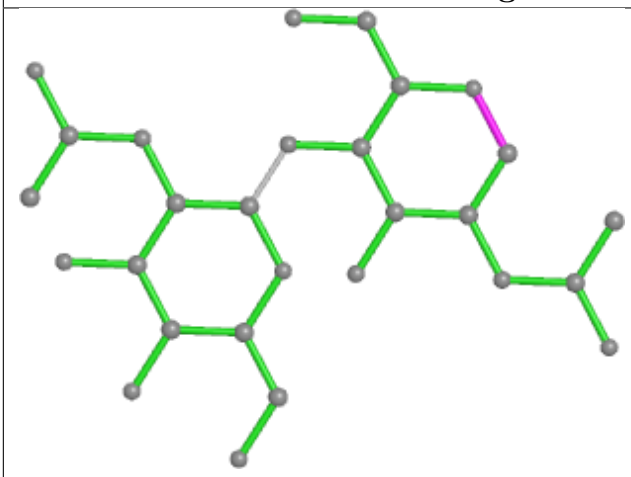


Torsions

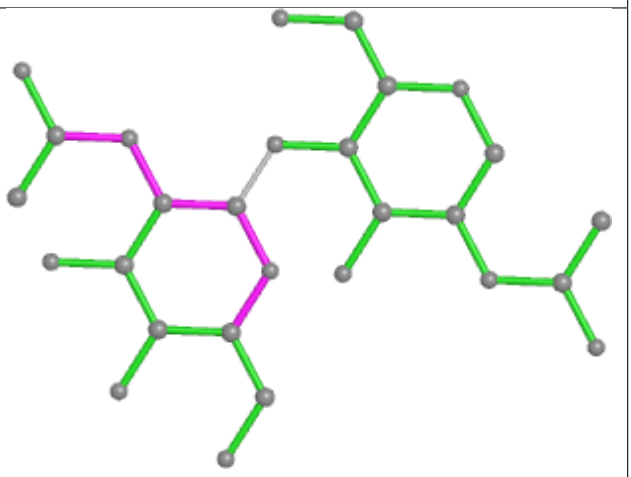


Rings

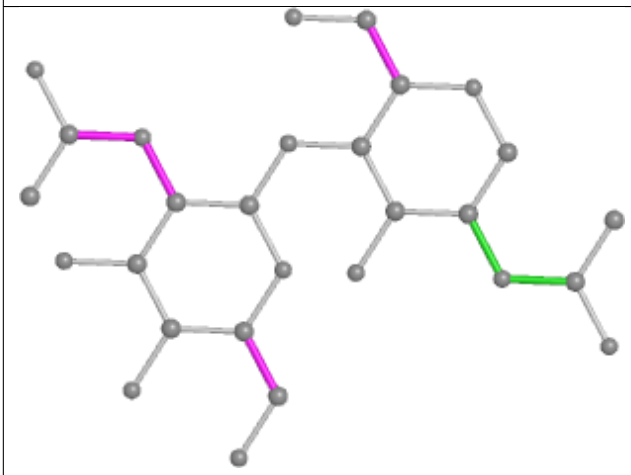
Oligosaccharide Chain J



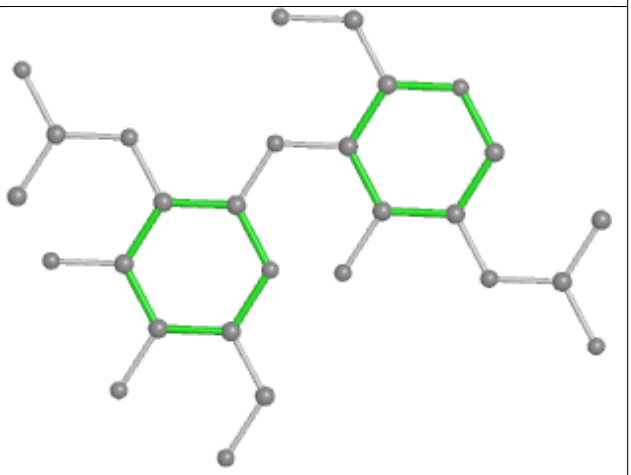
Bond lengths



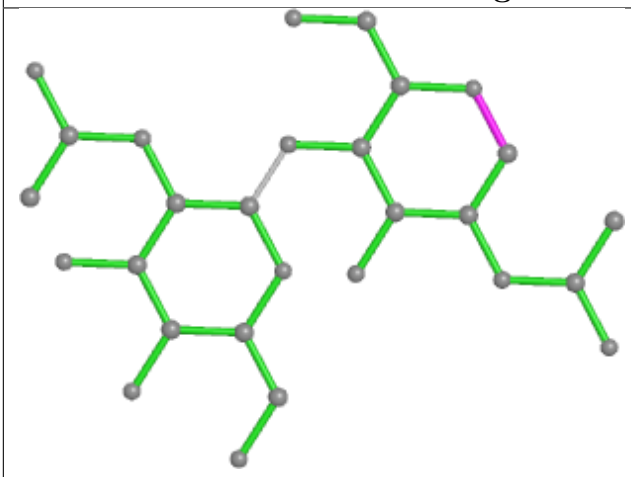
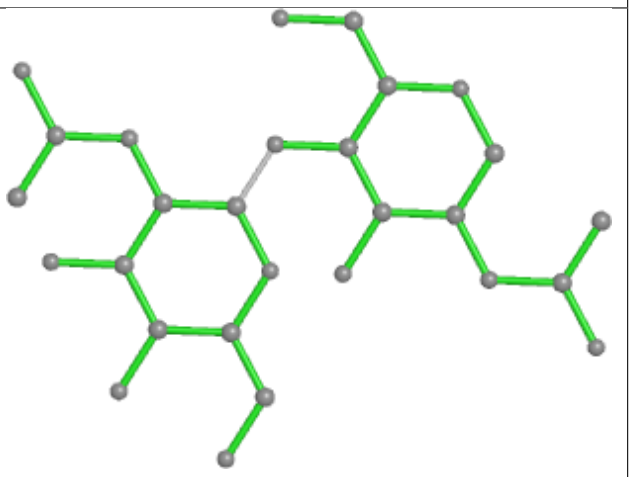
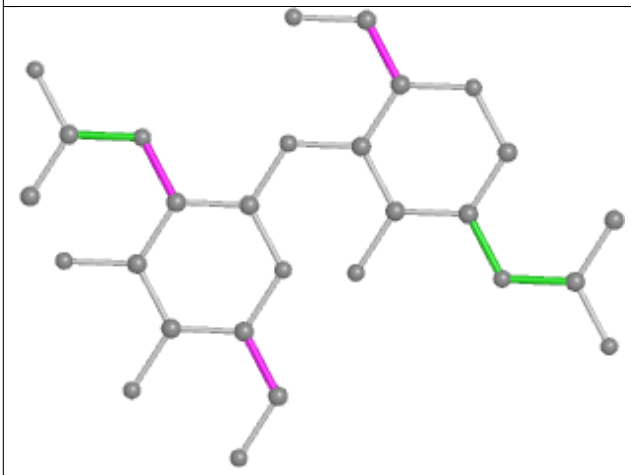
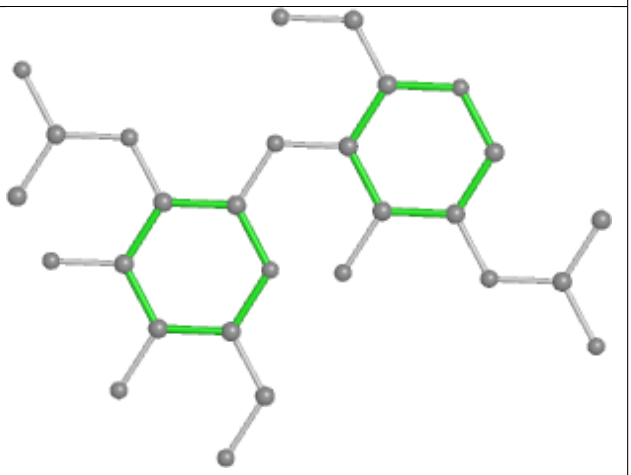
Bond angles

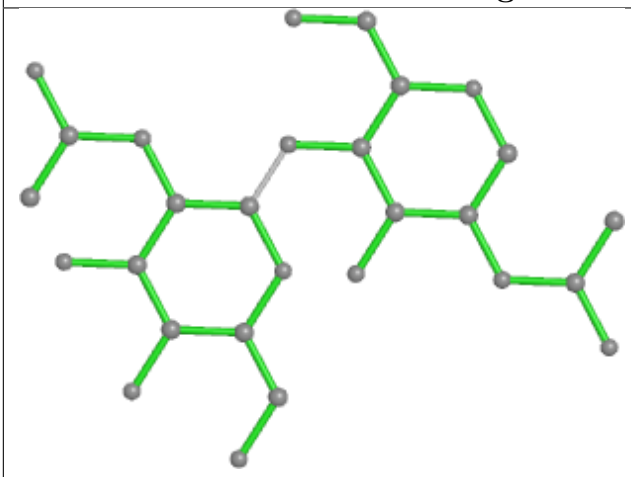
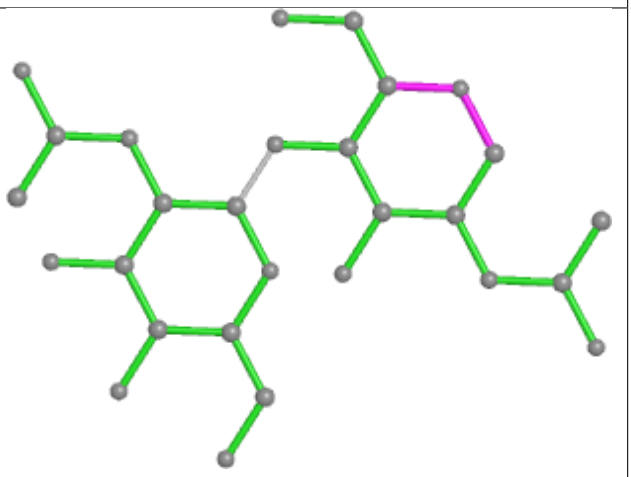
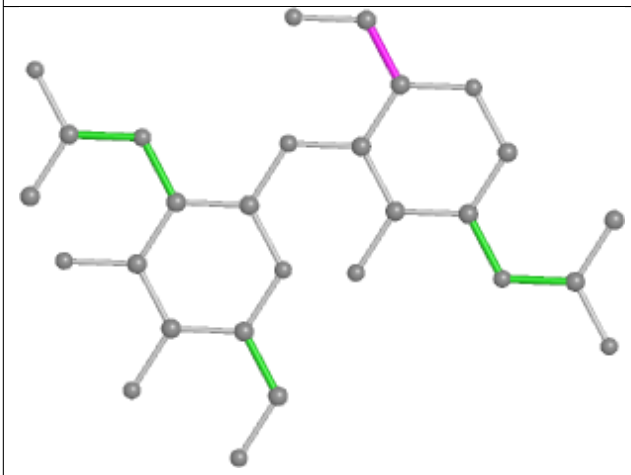
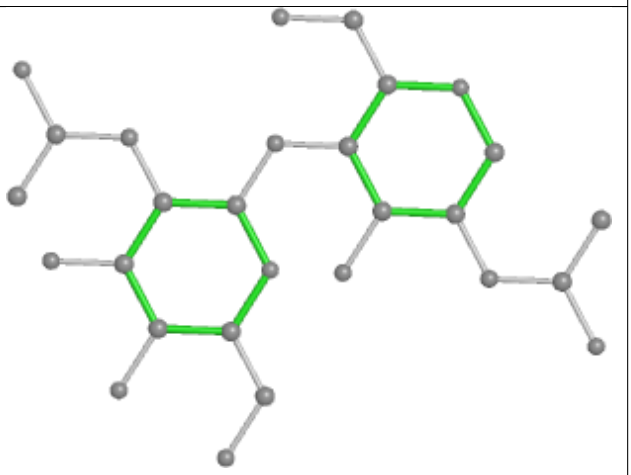


Torsions



Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

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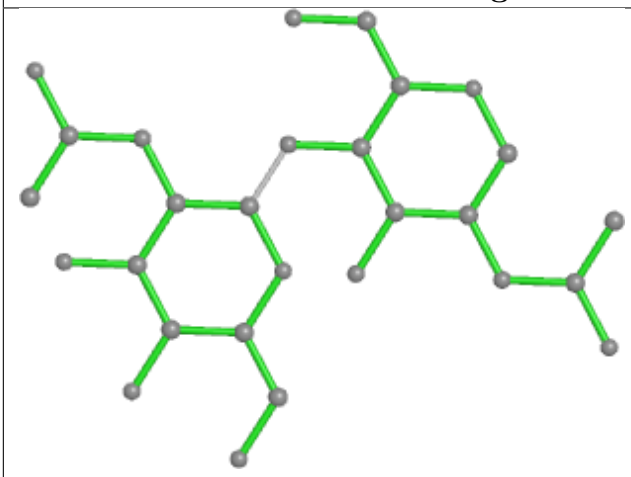
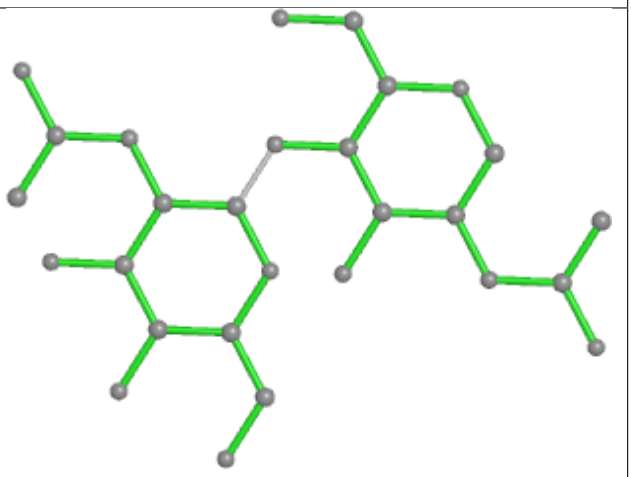
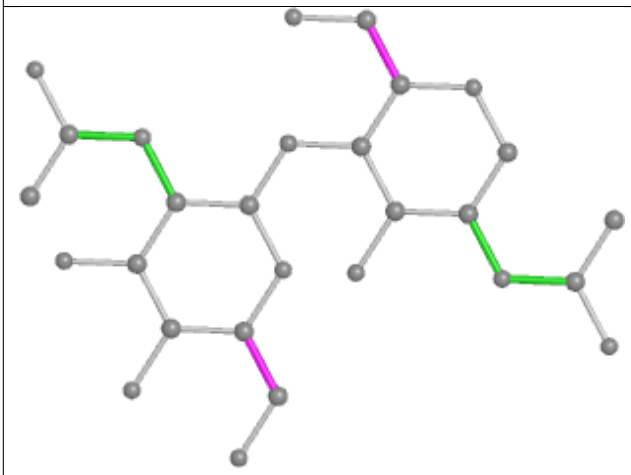
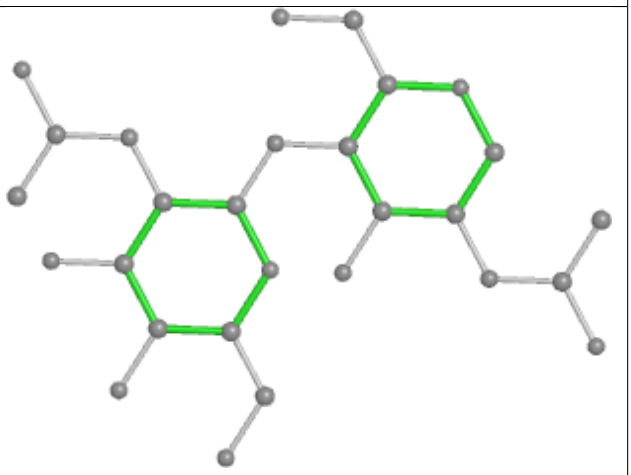
 Bond lengths	 Bond angles
 Torsions	 Rings

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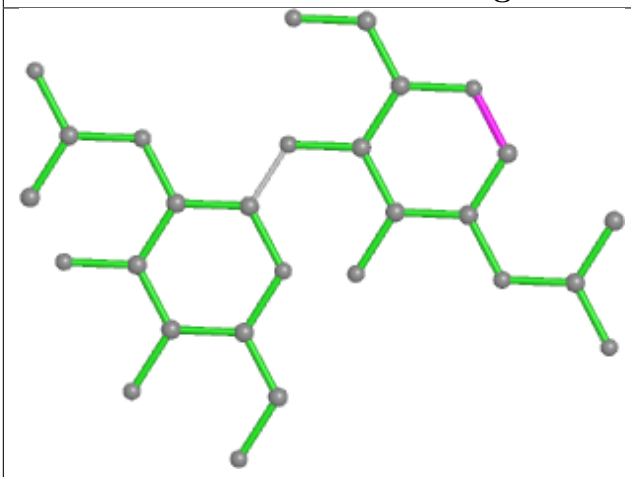
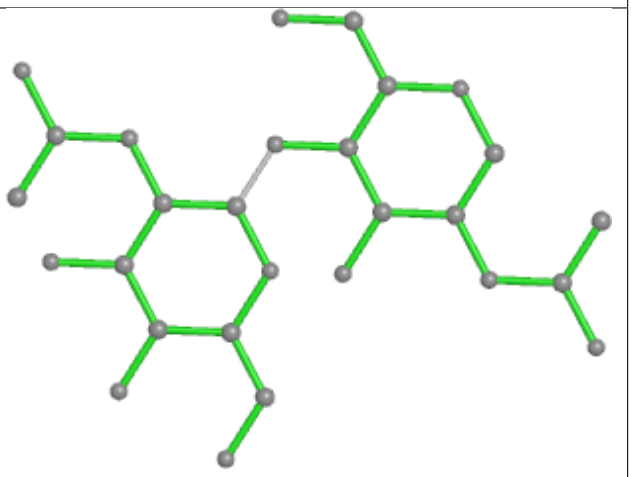
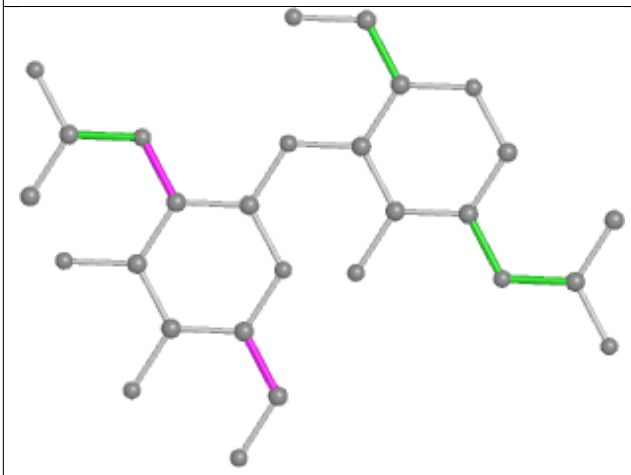
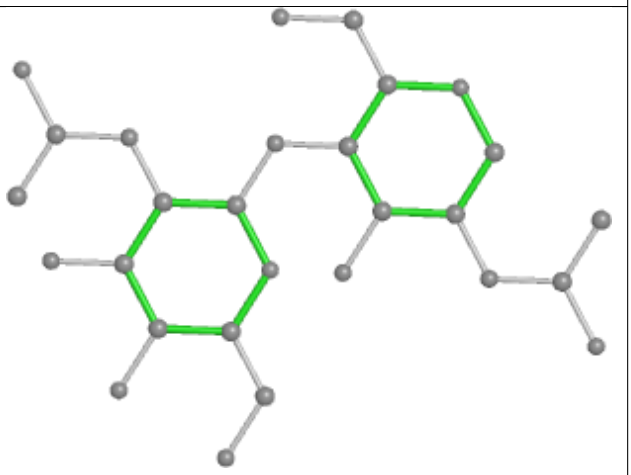
 Bond lengths	 Bond angles
 Torsions	 Rings

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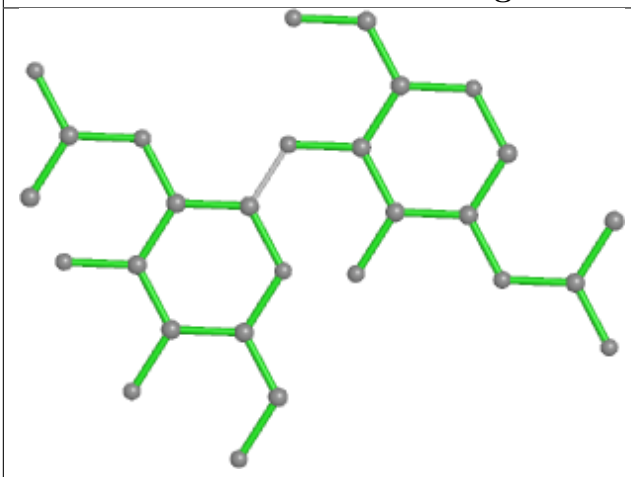
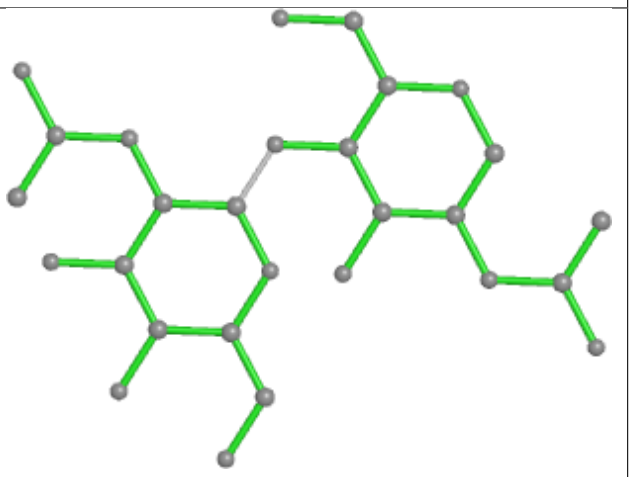
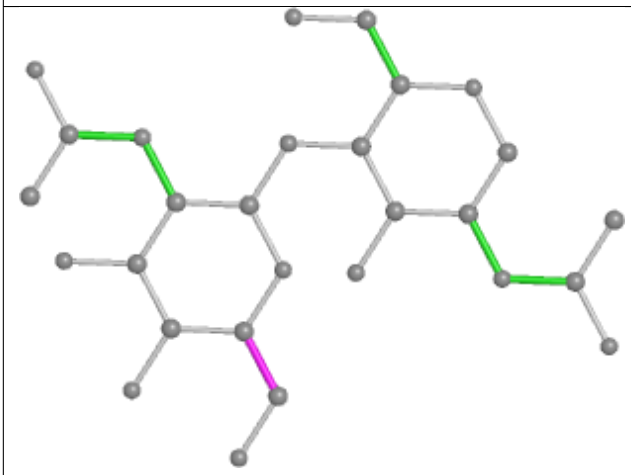
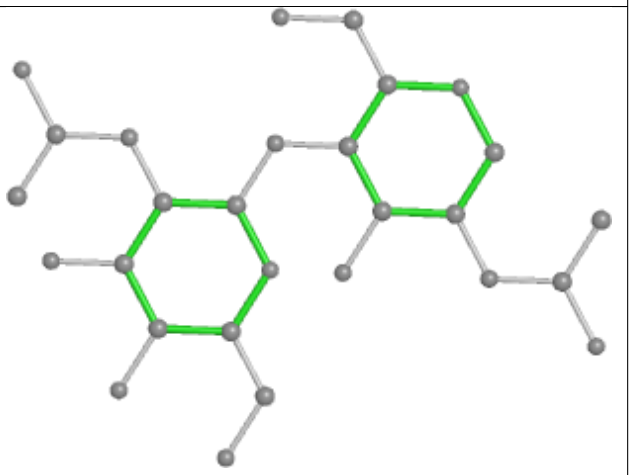
 Bond lengths	 Bond angles
 Torsions	 Rings

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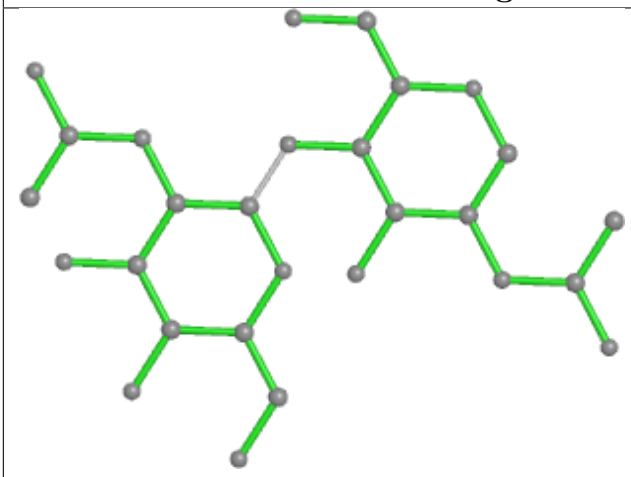
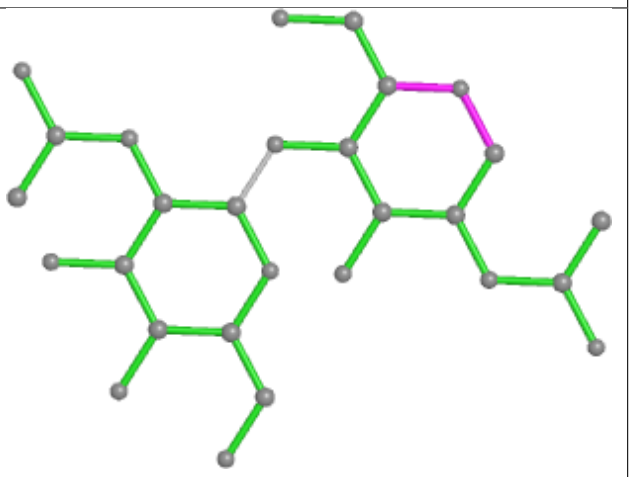
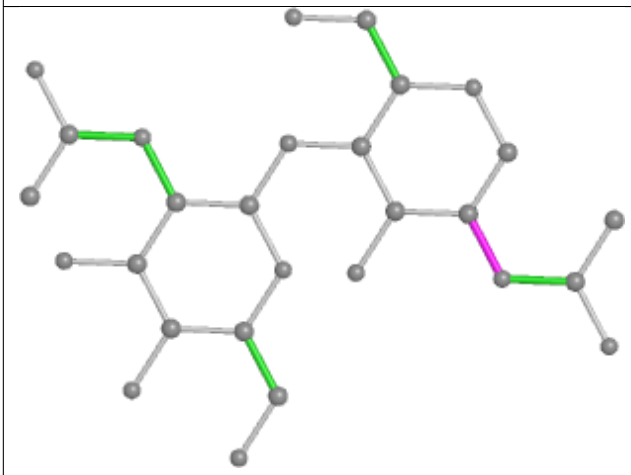
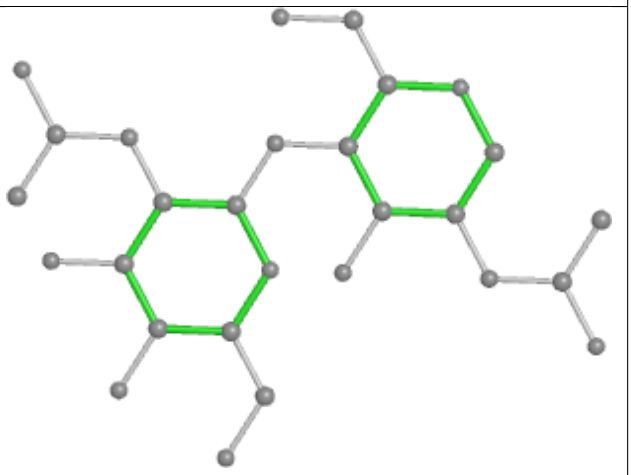
 Bond lengths	 Bond angles
 Torsions	 Rings

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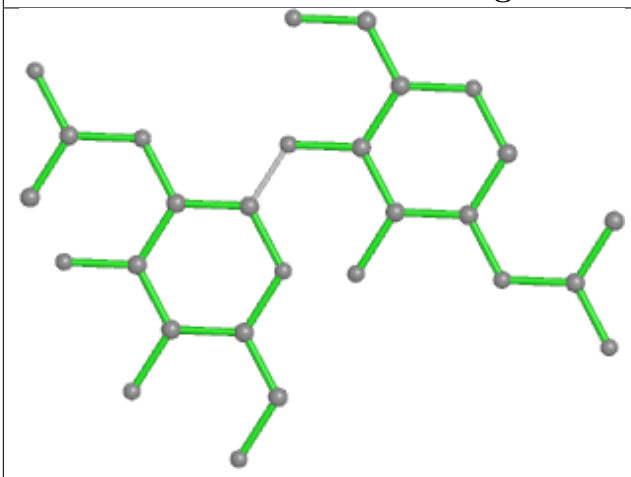
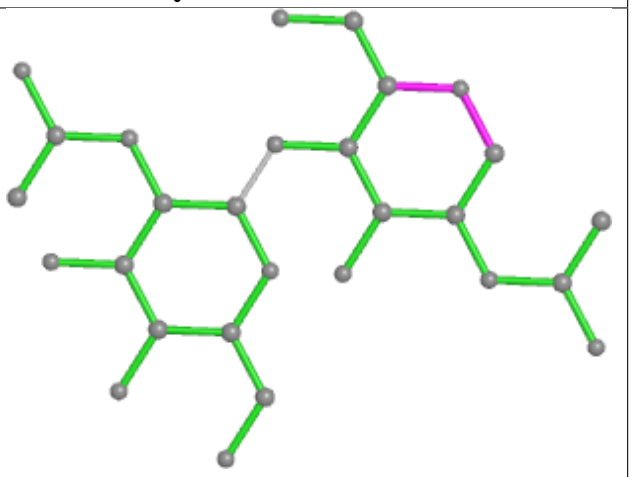
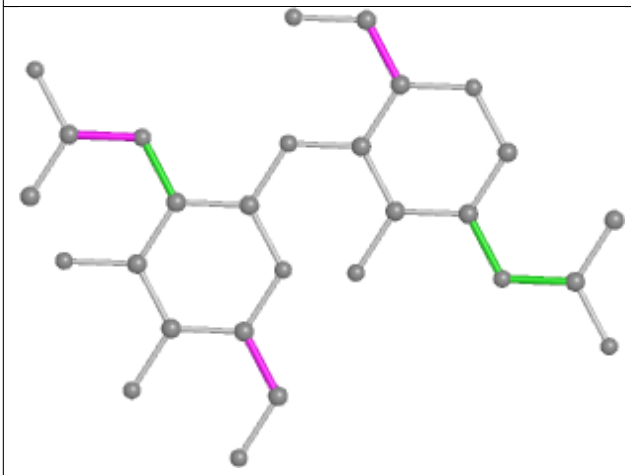
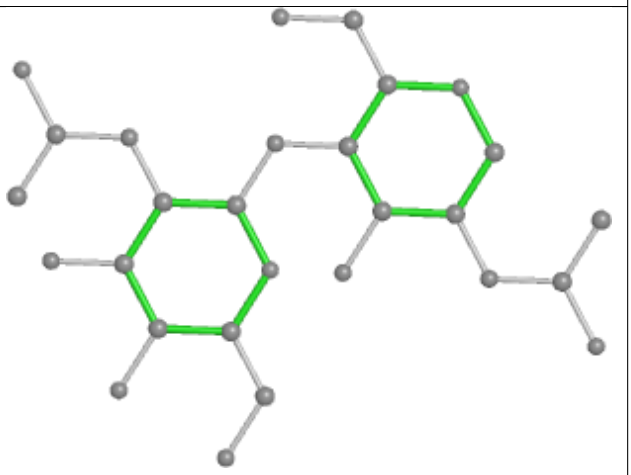
 Bond lengths	 Bond angles
 Torsions	 Rings

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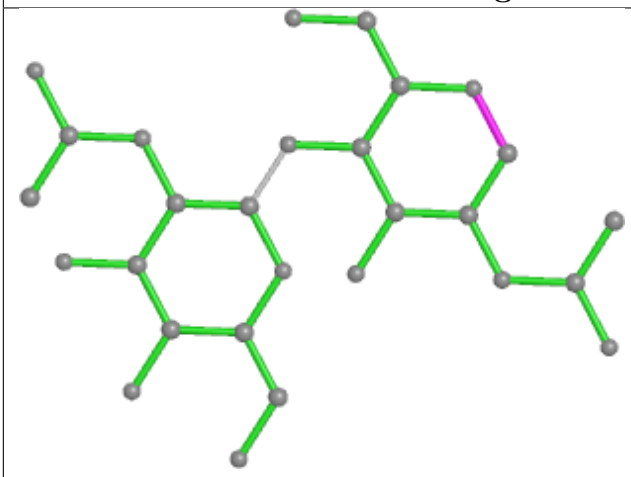
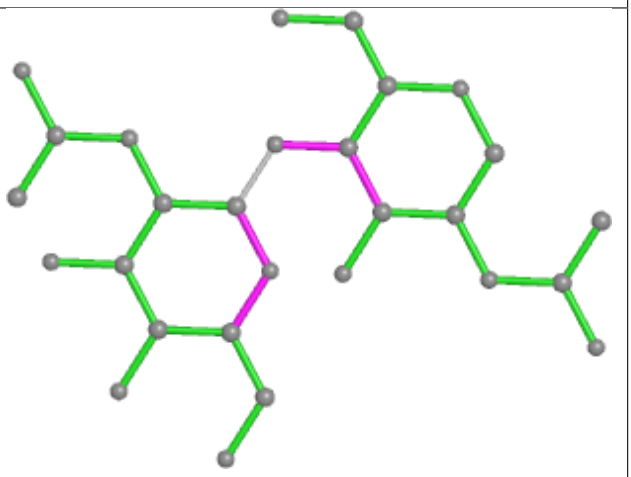
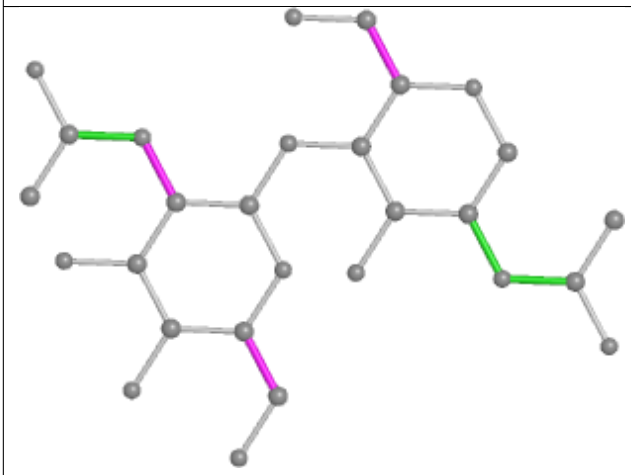
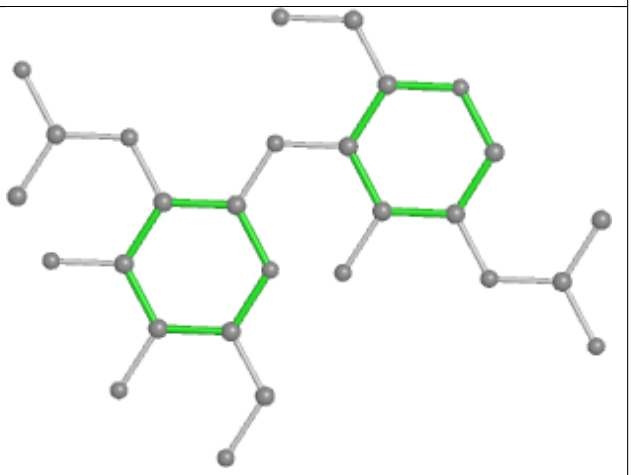
 Bond lengths	 Bond angles
 Torsions	 Rings

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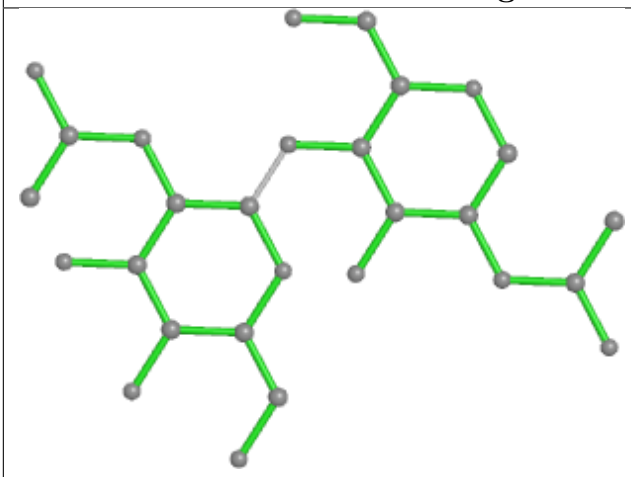
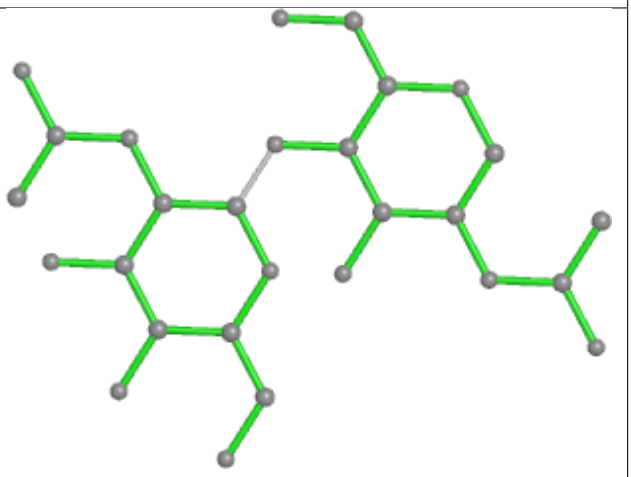
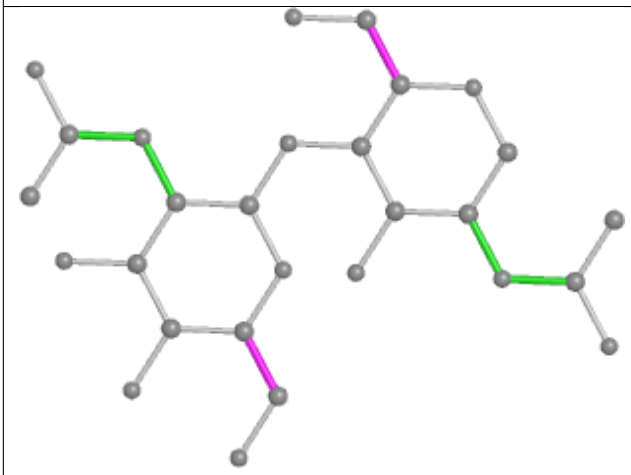
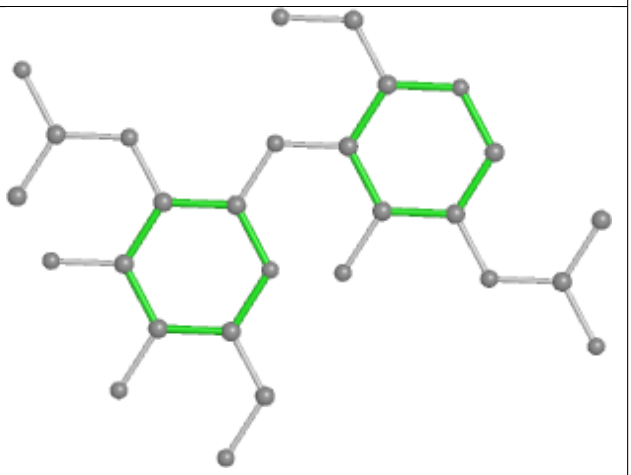
 Bond lengths	 Bond angles
 Torsions	 Rings

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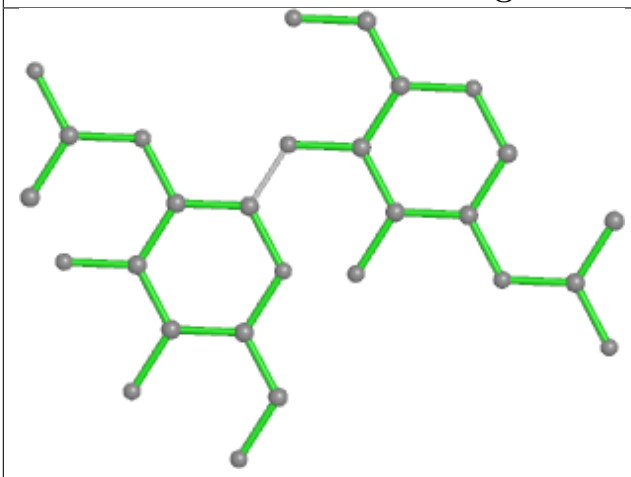
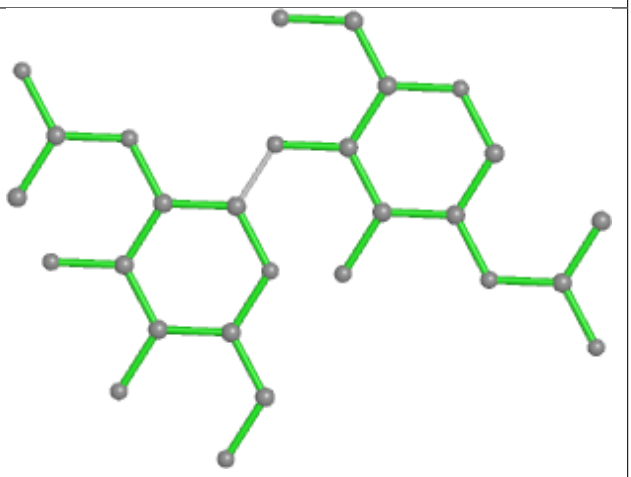
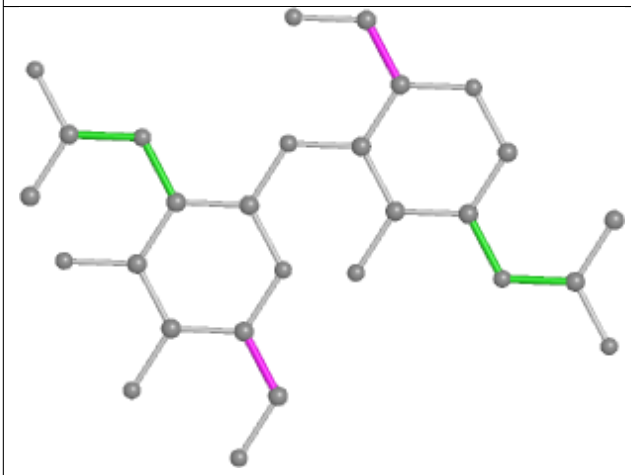
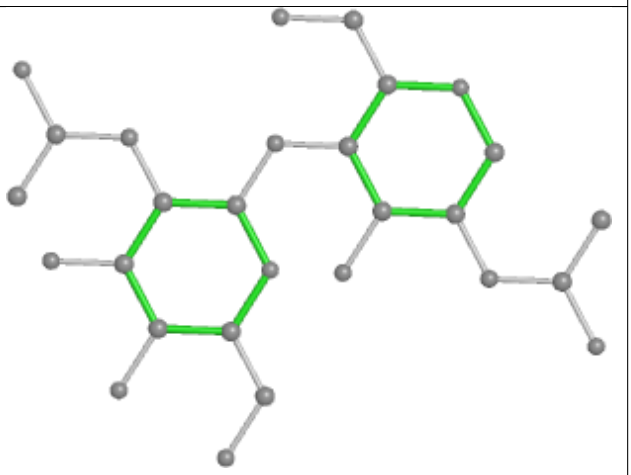
 Bond lengths	 Bond angles
 Torsions	 Rings

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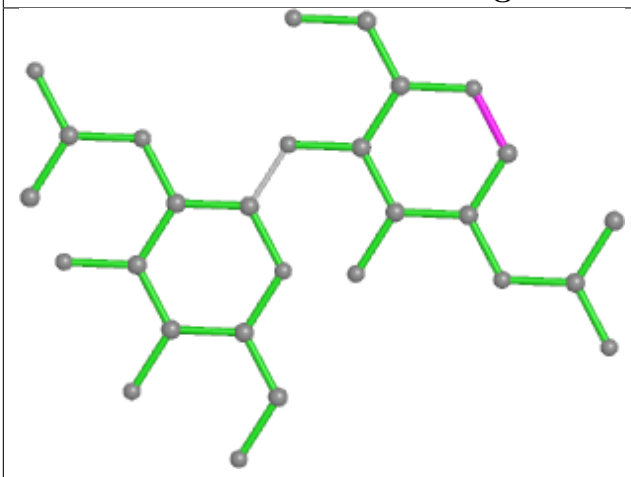
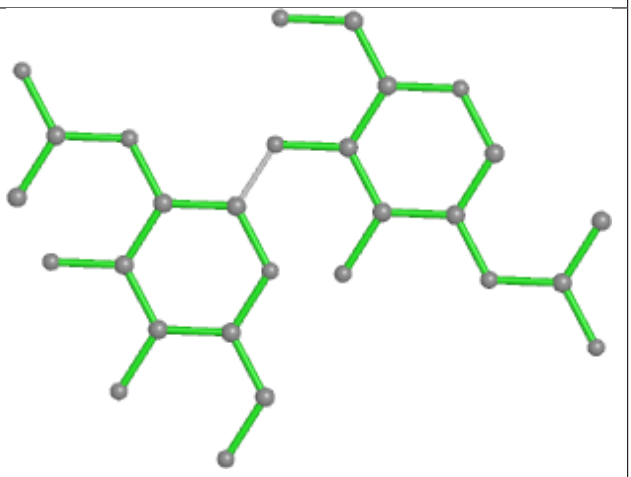
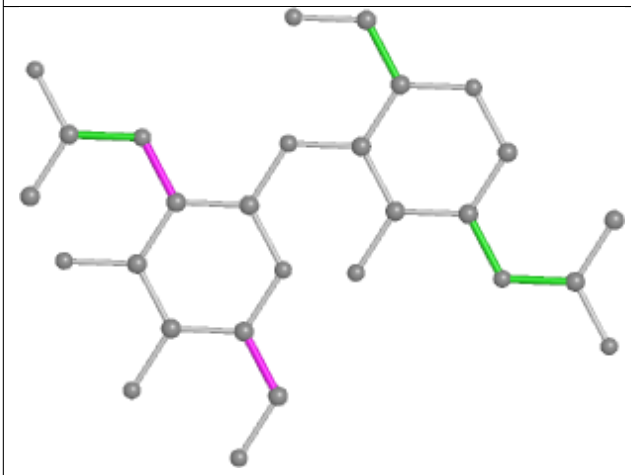
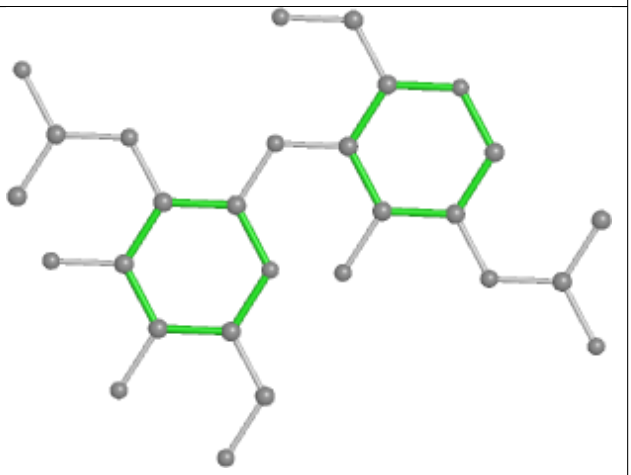
 Bond lengths	 Bond angles
 Torsions	 Rings

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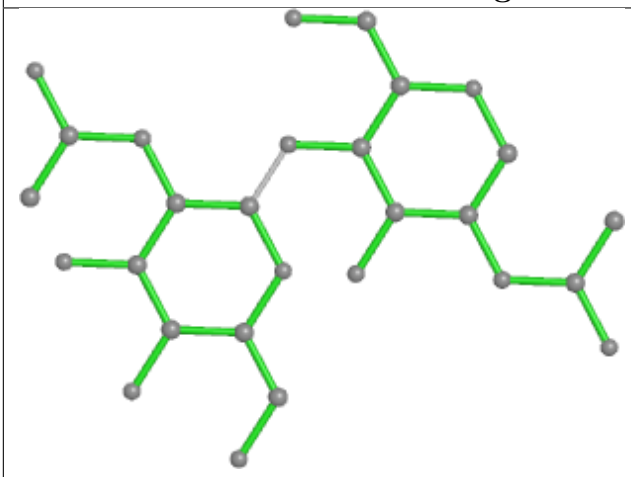
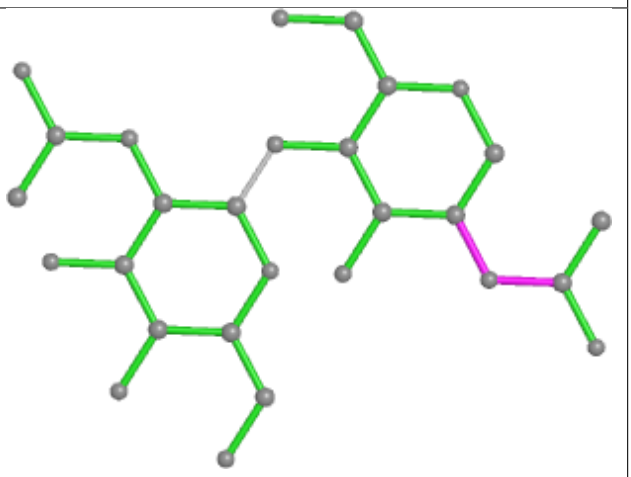
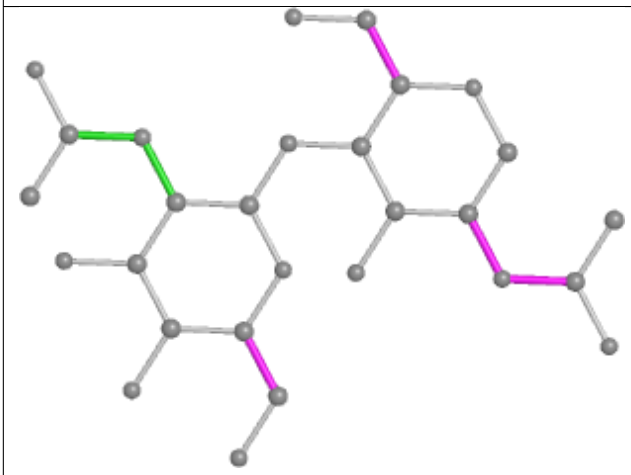
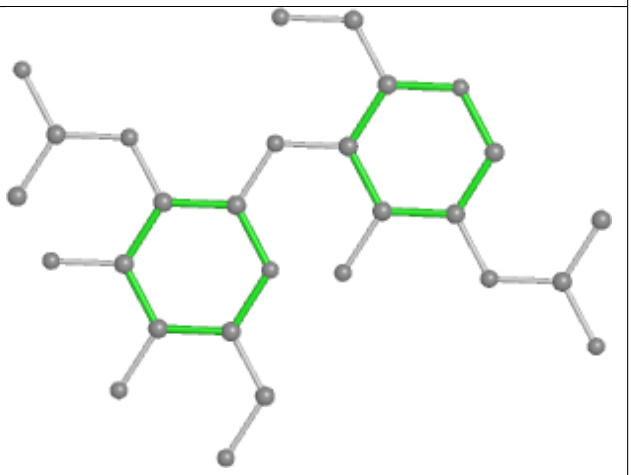
 Bond lengths	 Bond angles
 Torsions	 Rings

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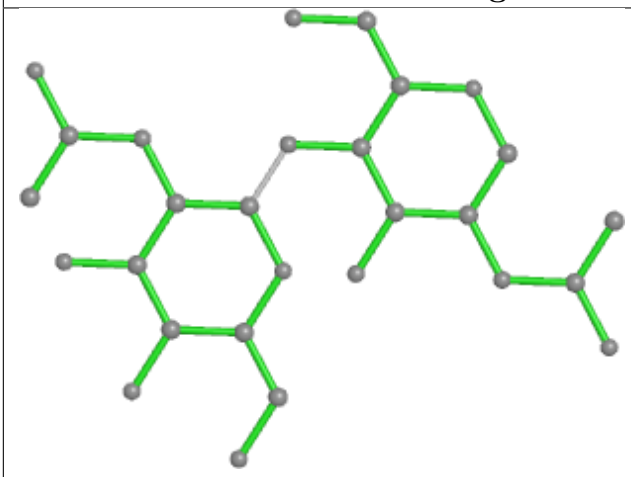
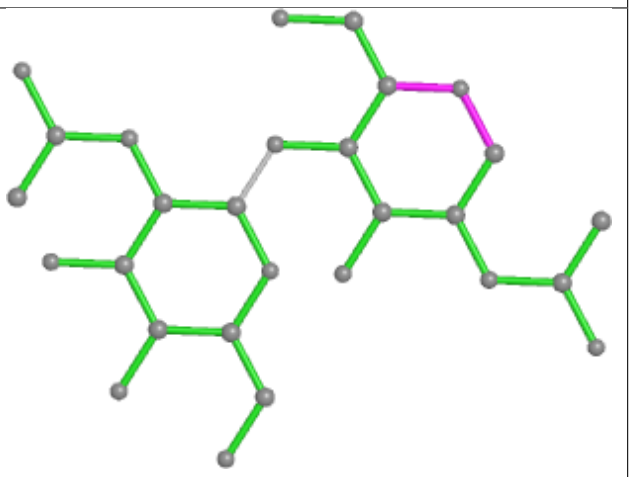
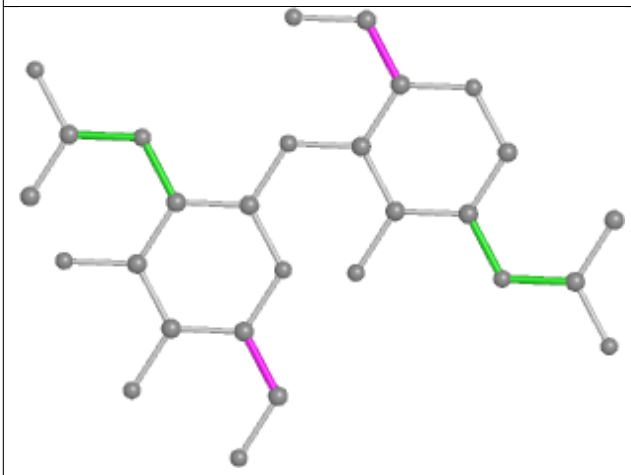
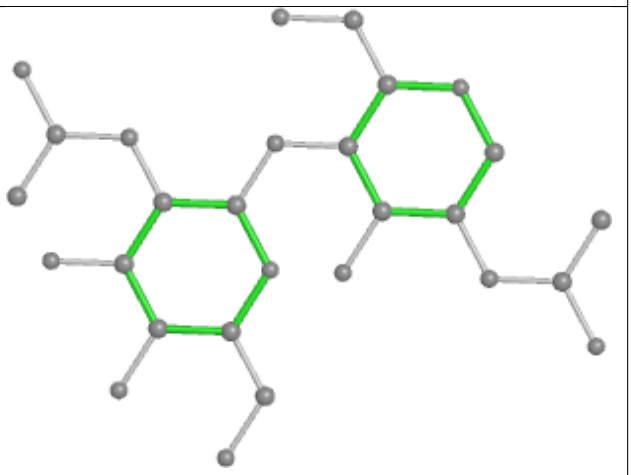
 Bond lengths	 Bond angles
 Torsions	 Rings

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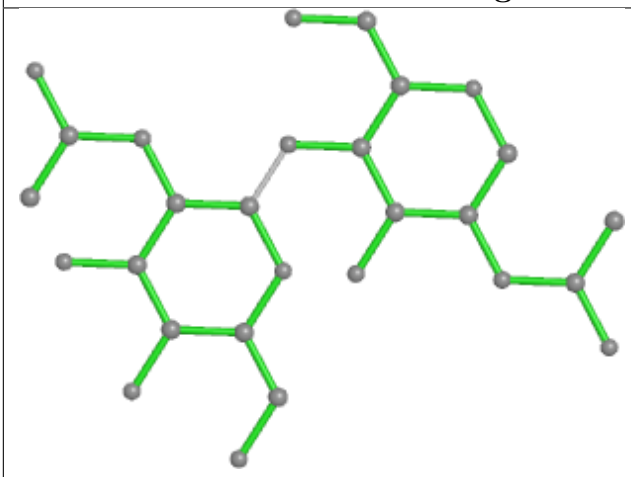
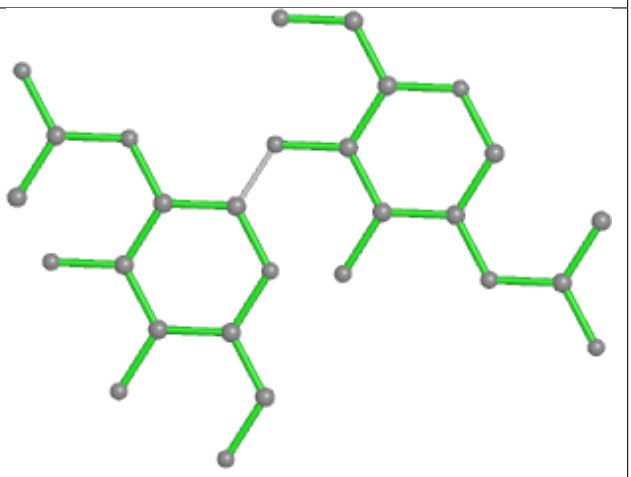
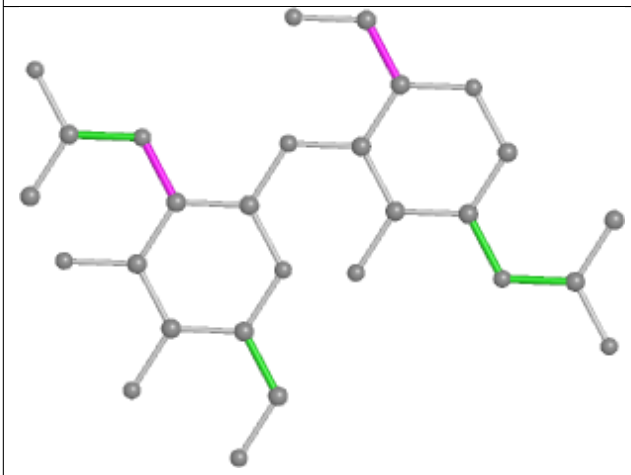
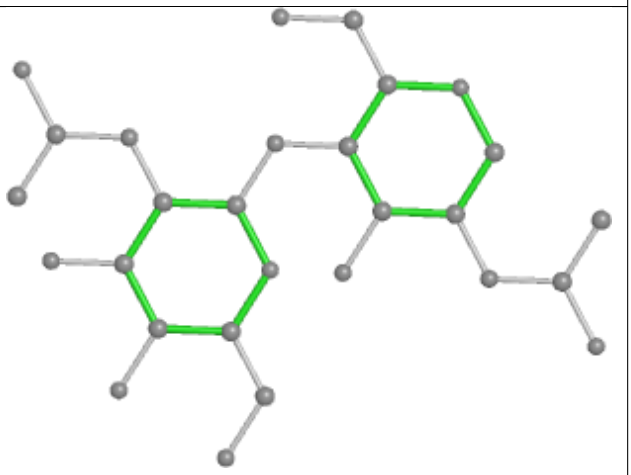
 Bond lengths	 Bond angles
 Torsions	 Rings

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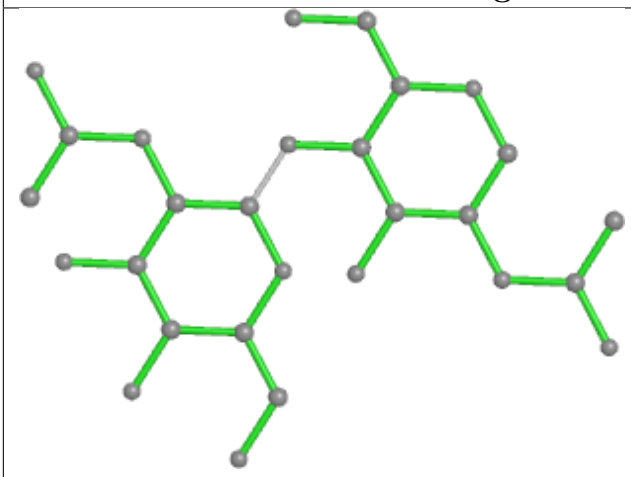
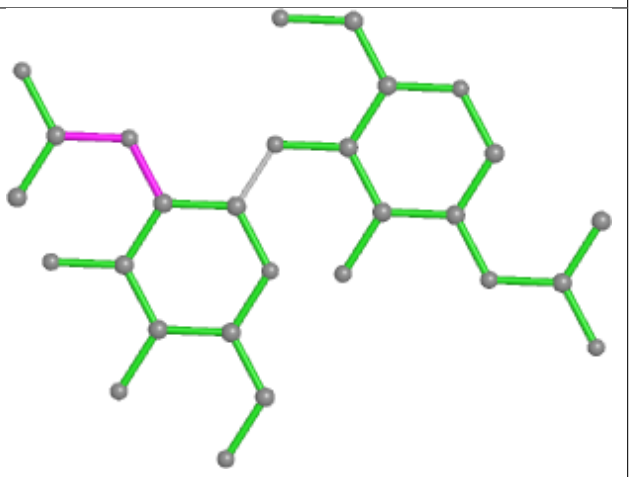
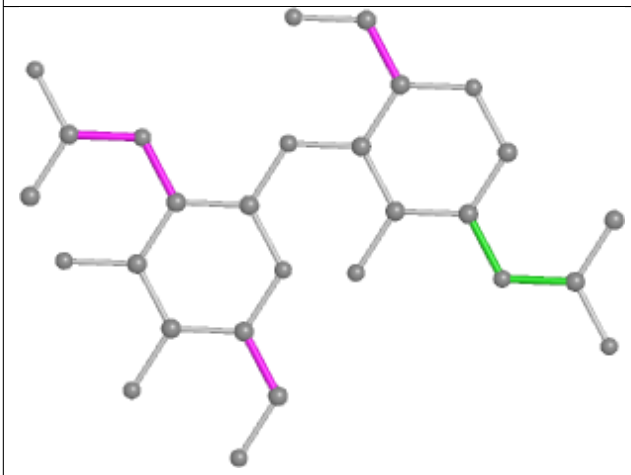
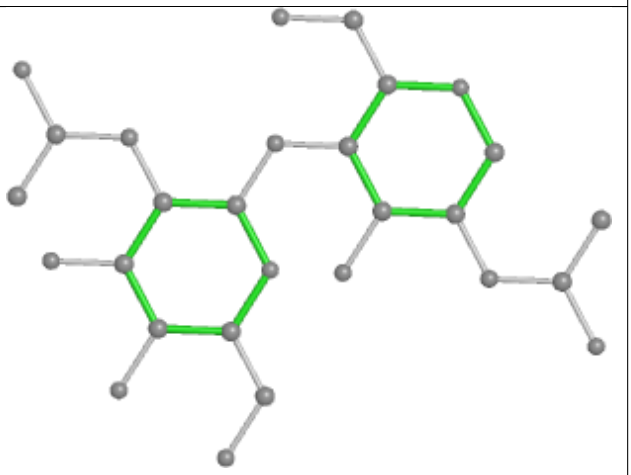
 Bond lengths	 Bond angles
 Torsions	 Rings

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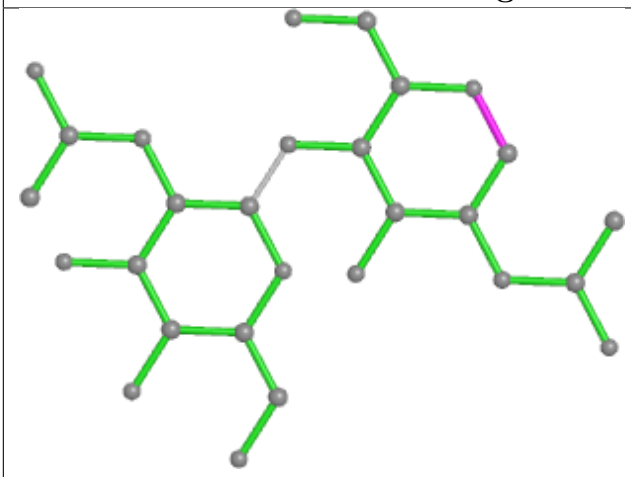
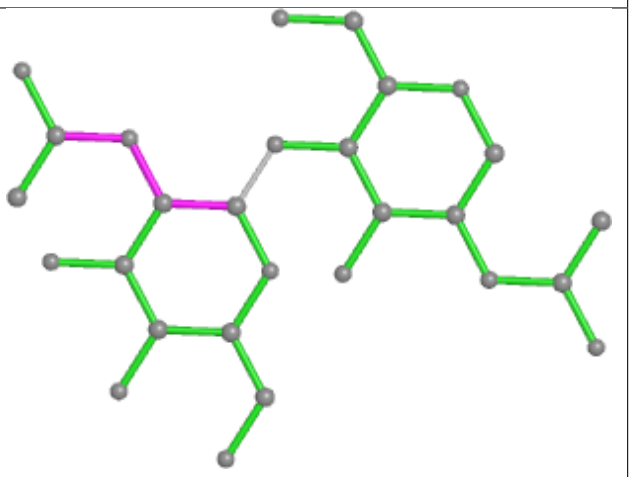
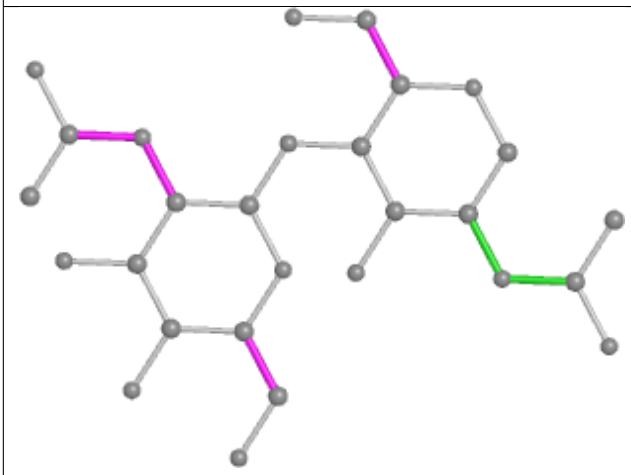
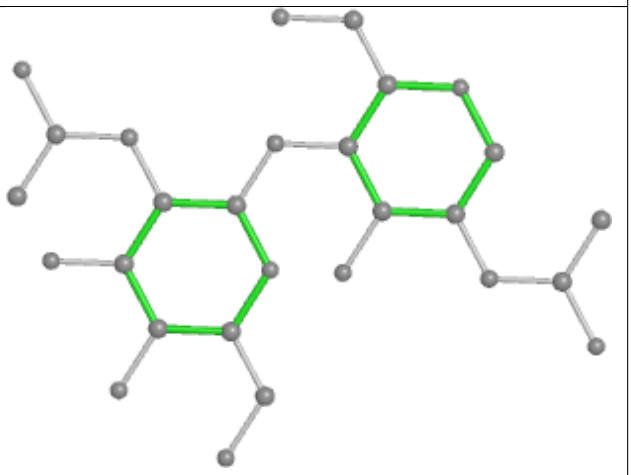
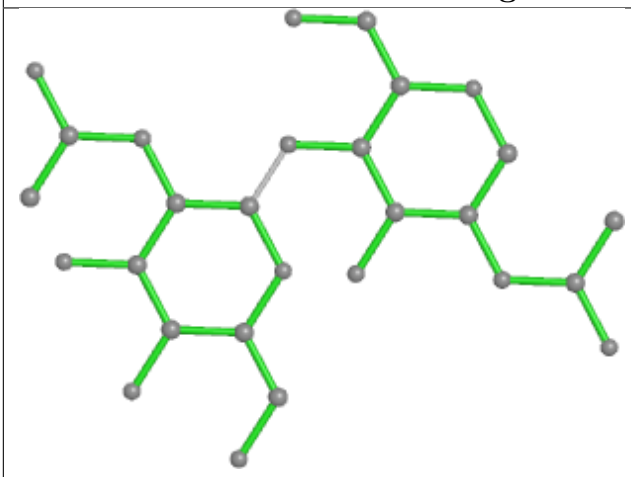
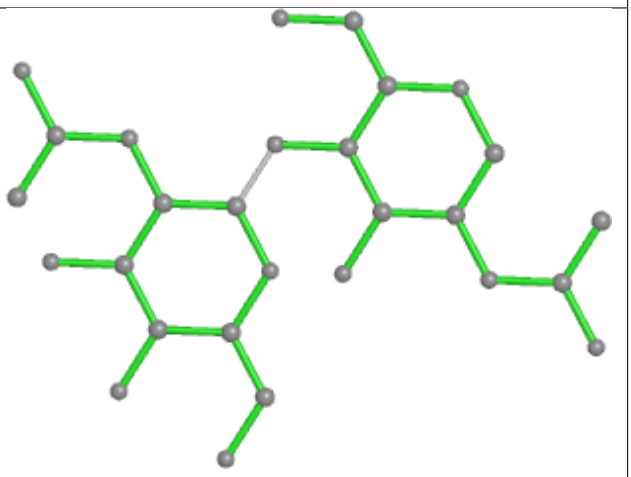
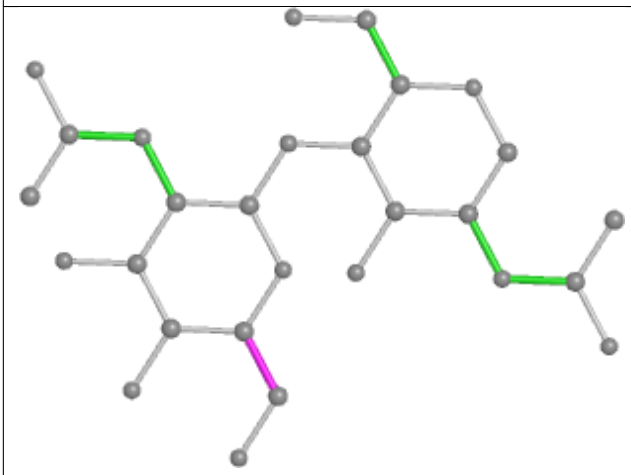
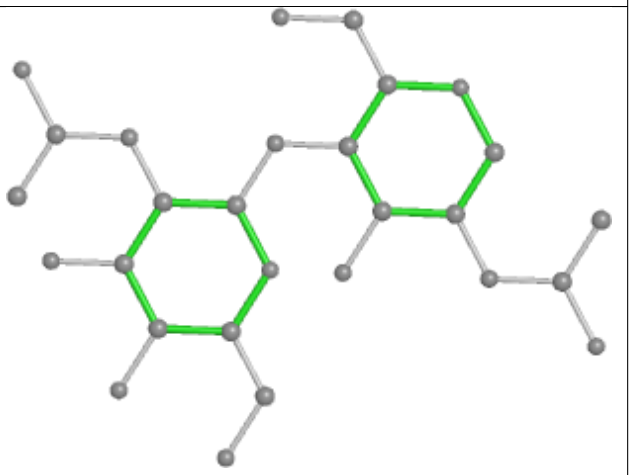
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain a	
 Bond lengths	 Bond angles
 Torsions	 Rings

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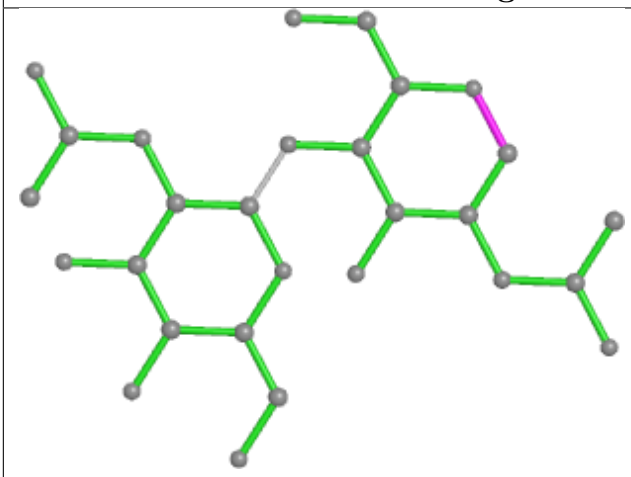
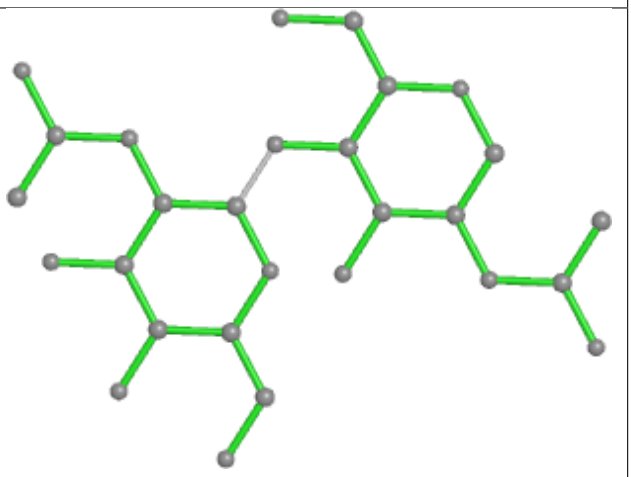
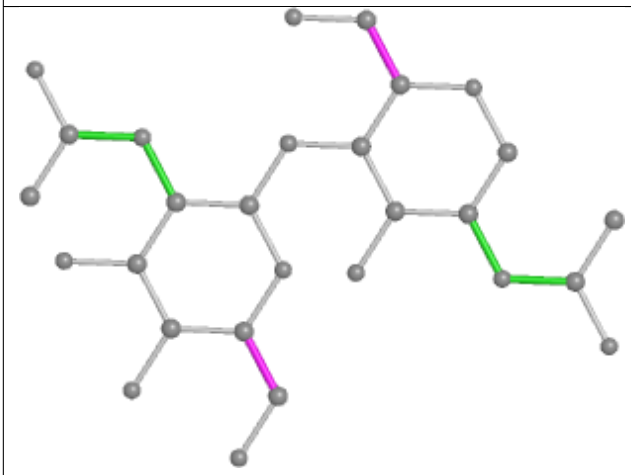
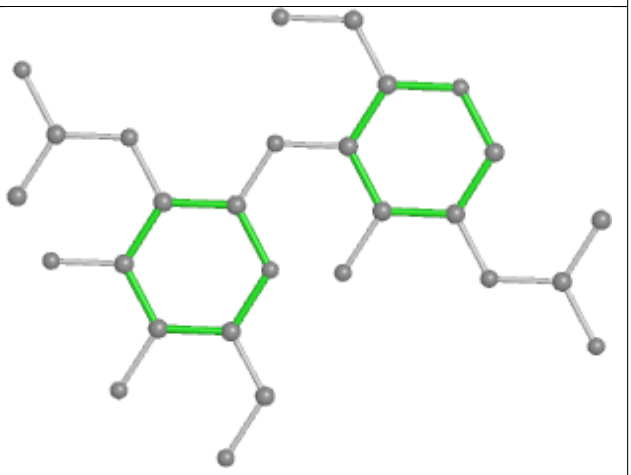
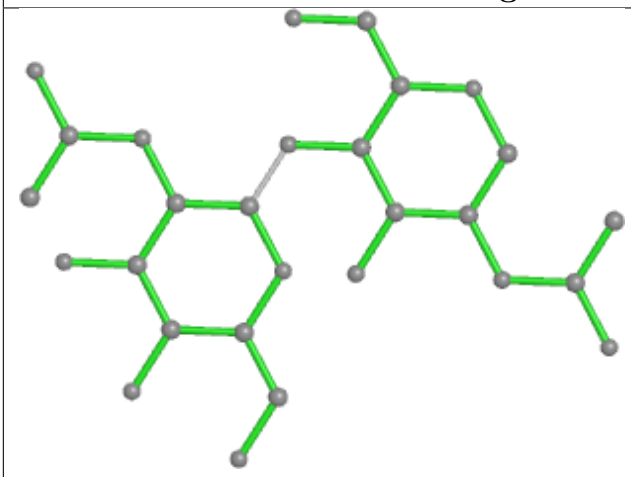
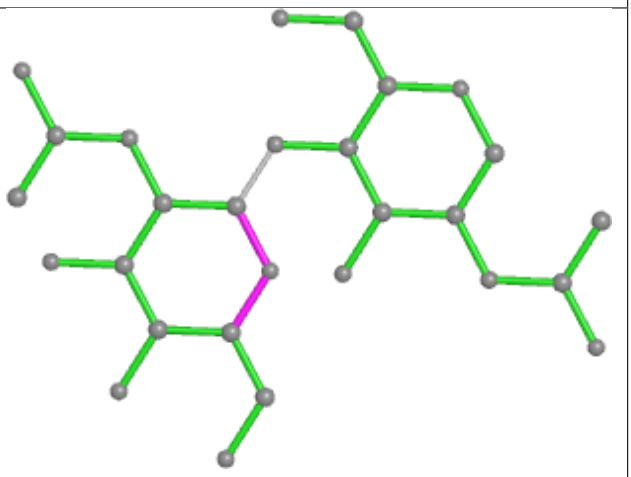
 Bond lengths	 Bond angles
 Torsions	 Rings

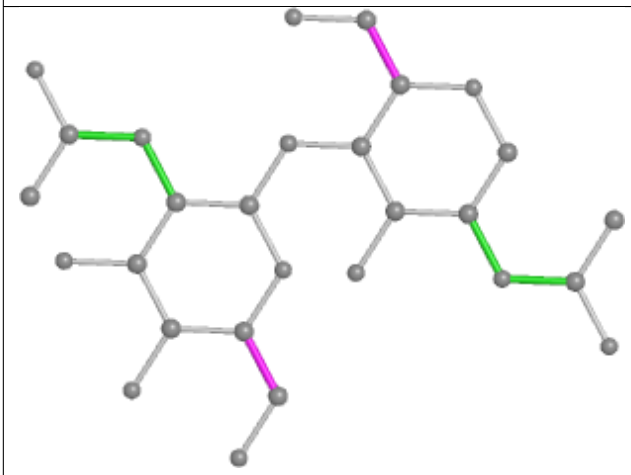
Oligosaccharide Chain c



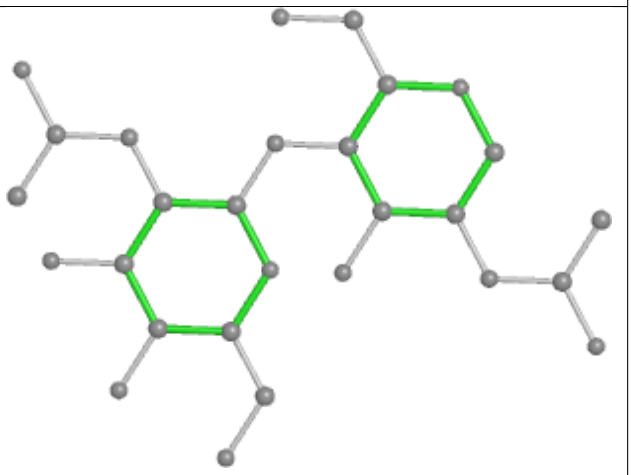
Bond lengths



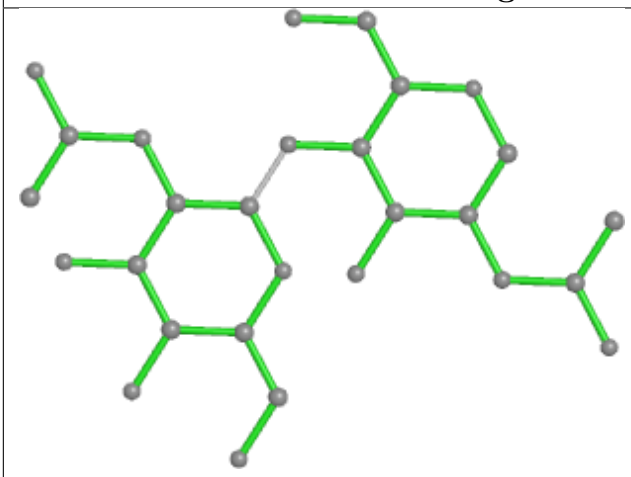
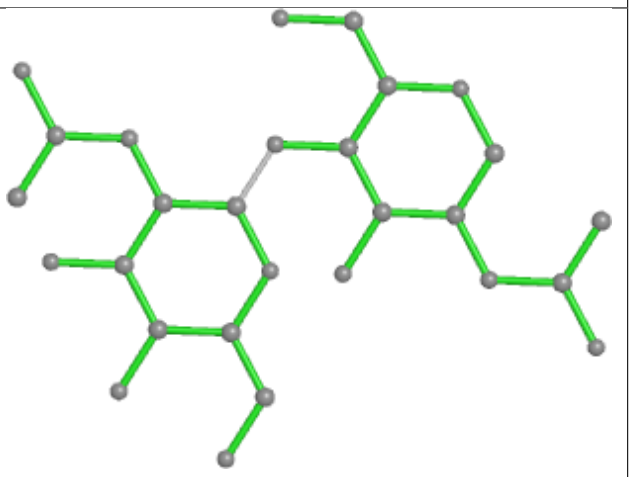
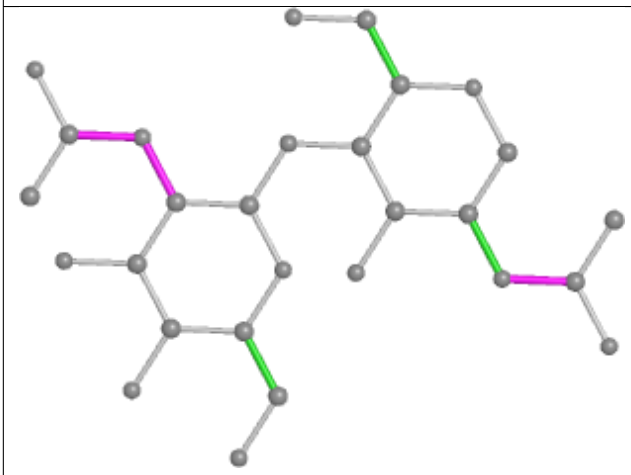
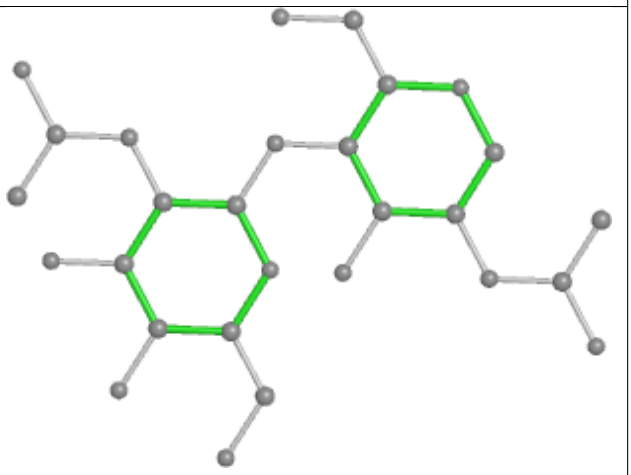
Bond angles



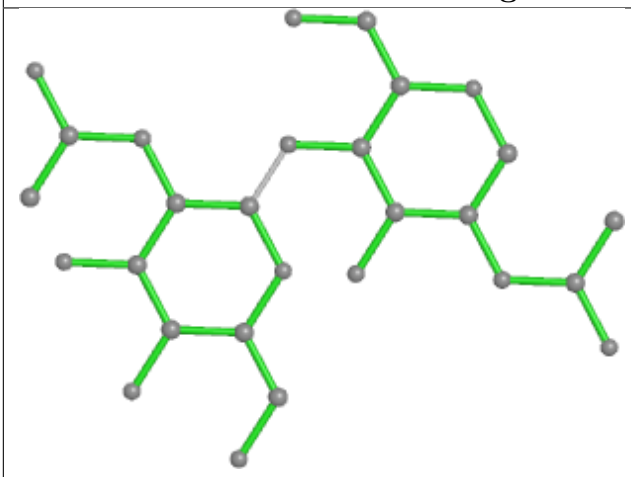
Torsions



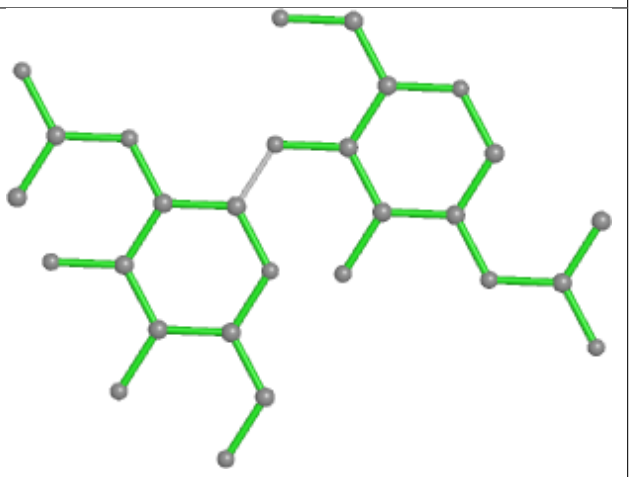
Rings

Oligosaccharide Chain d	
 Bond lengths	 Bond angles
 Torsions	 Rings

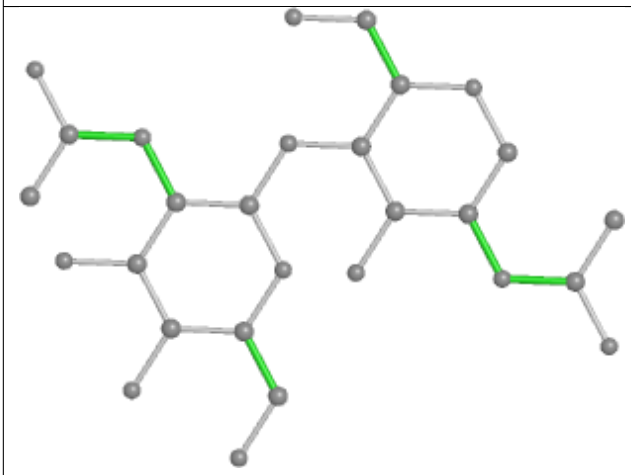
Oligosaccharide Chain e



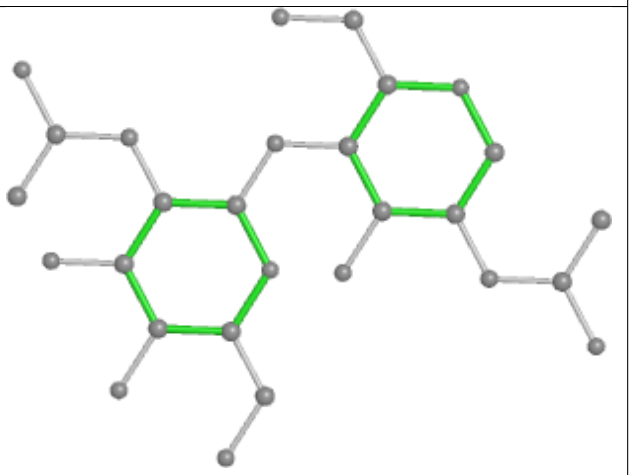
Bond lengths



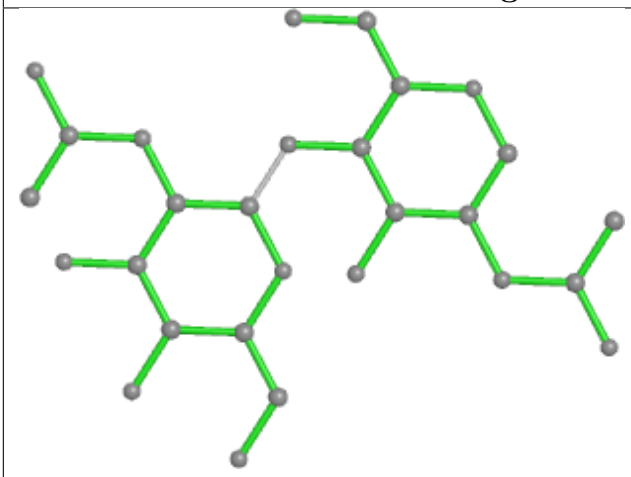
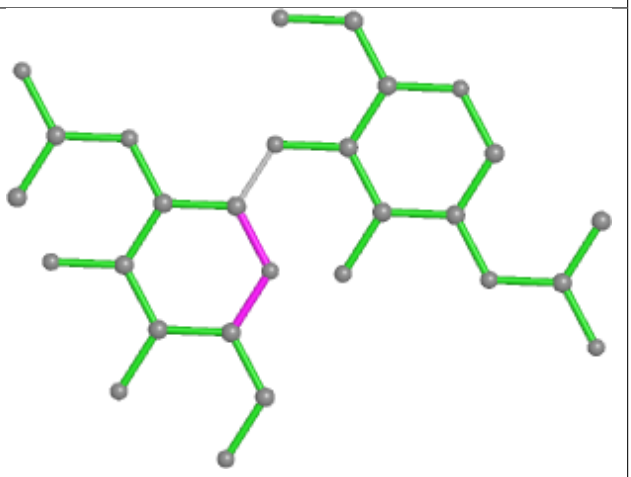
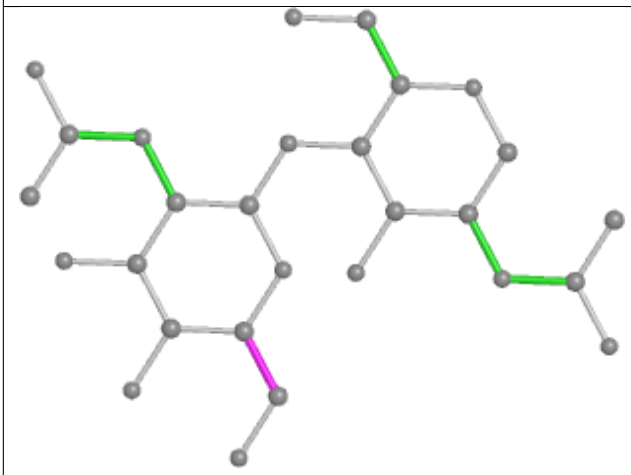
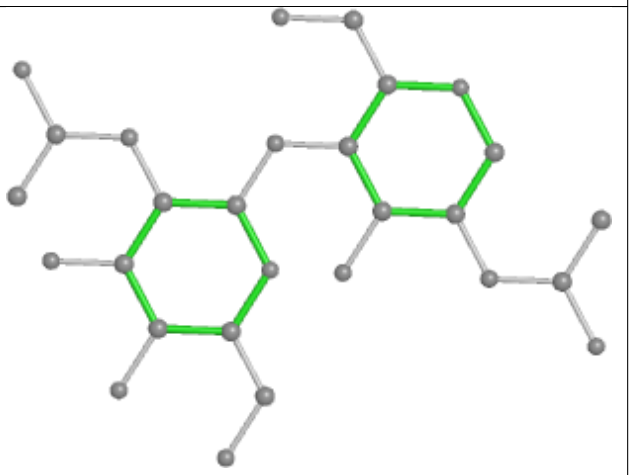
Bond angles

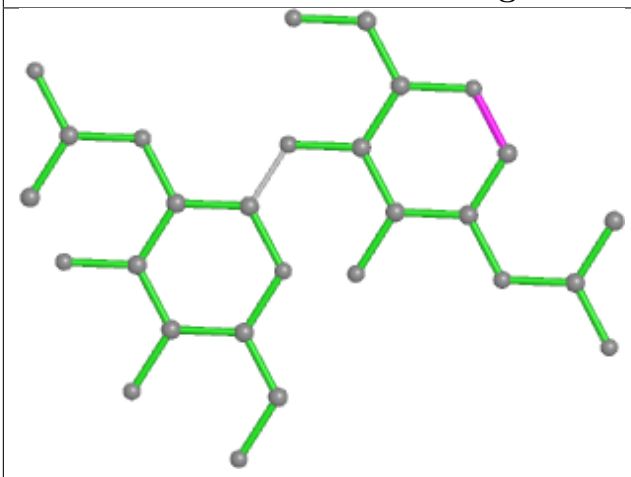
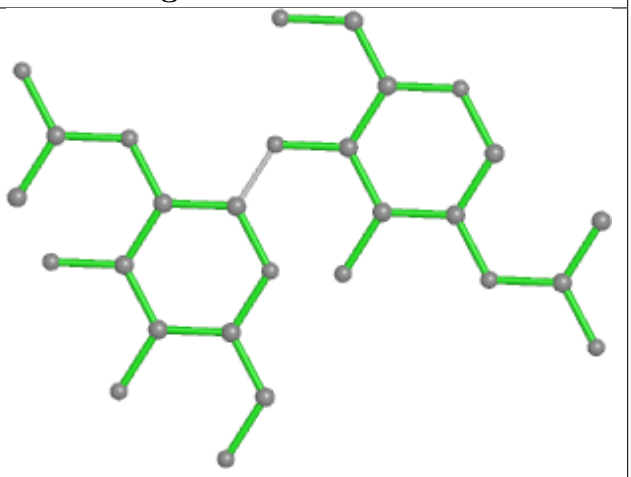
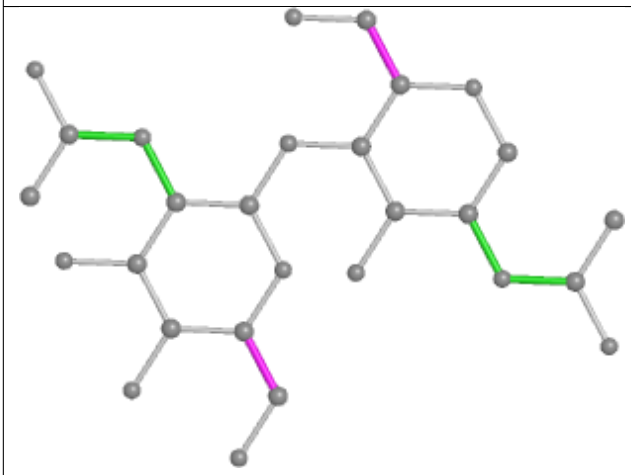
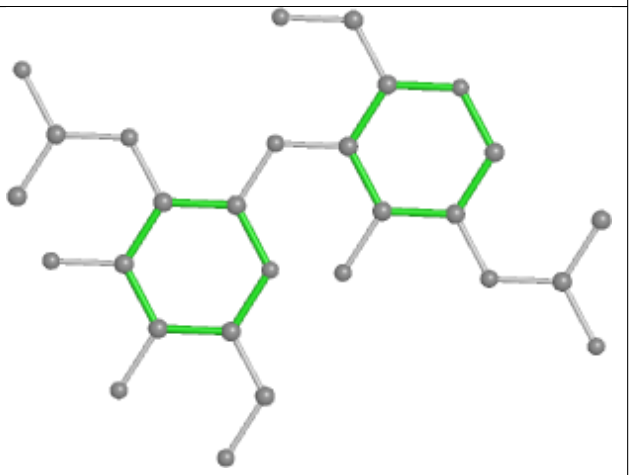


Torsions

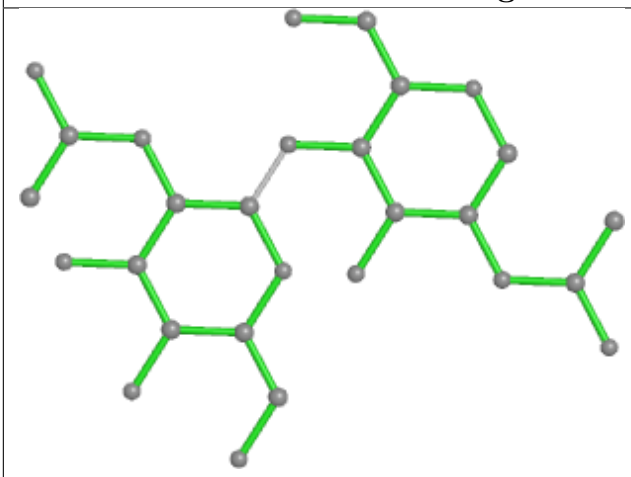


Rings

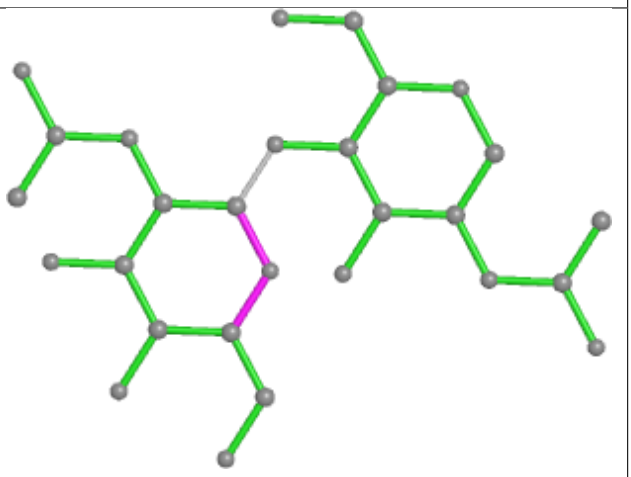
Oligosaccharide Chain f	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain g	
 Bond lengths	 Bond angles
 Torsions	 Rings

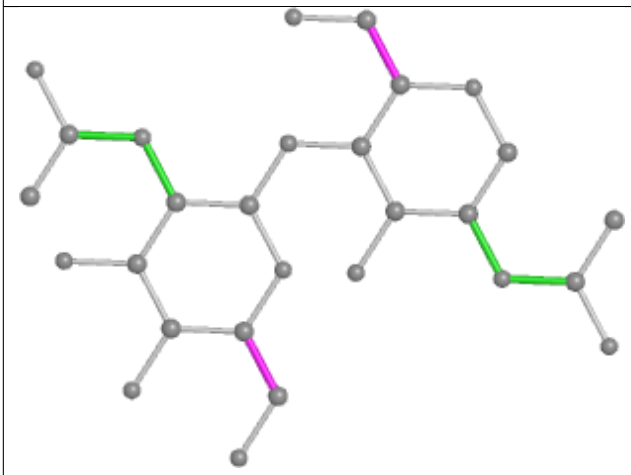
Oligosaccharide Chain h



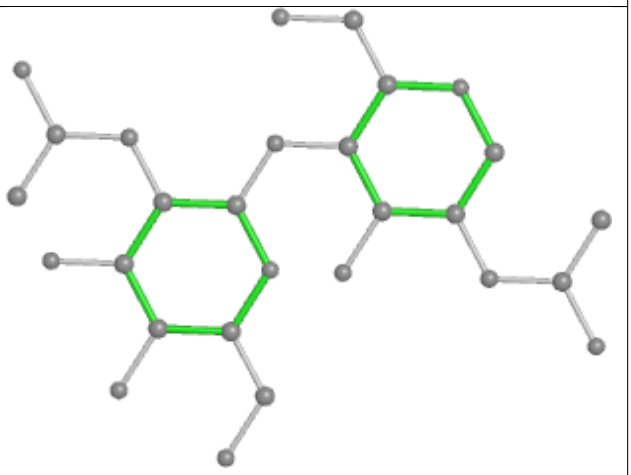
Bond lengths



Bond angles

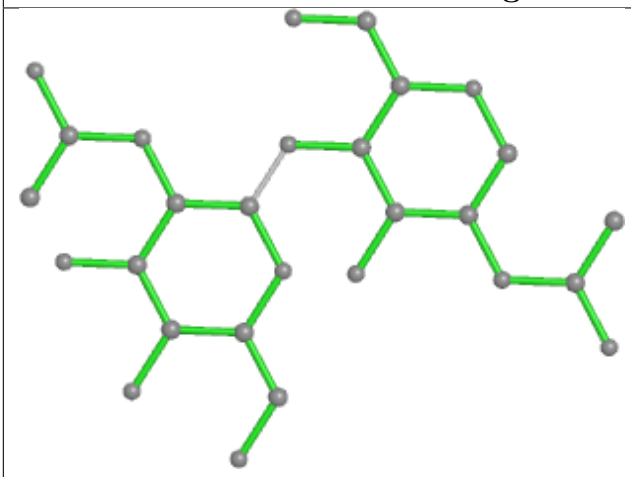


Torsions

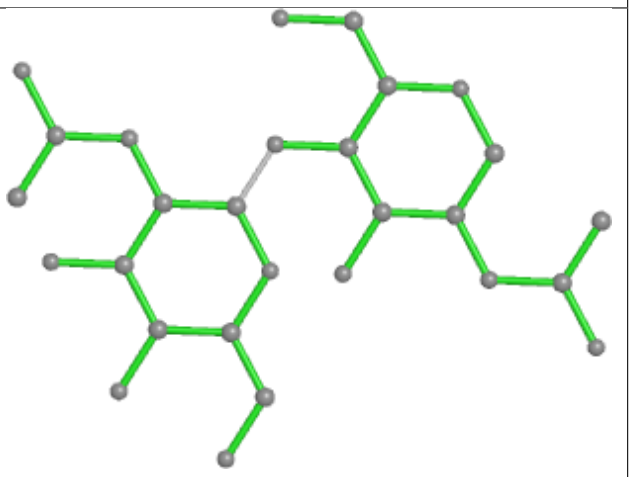


Rings

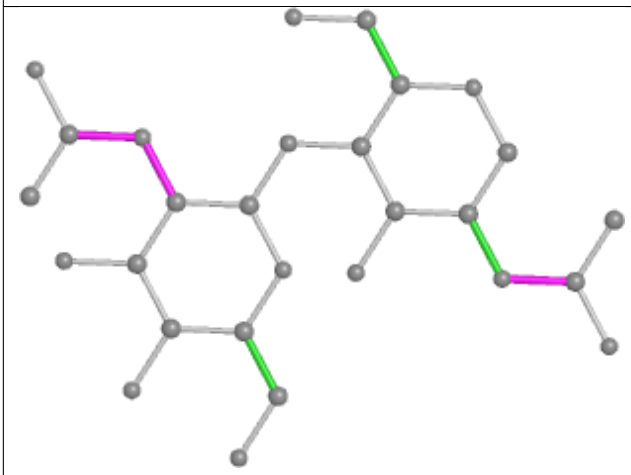
Oligosaccharide Chain i



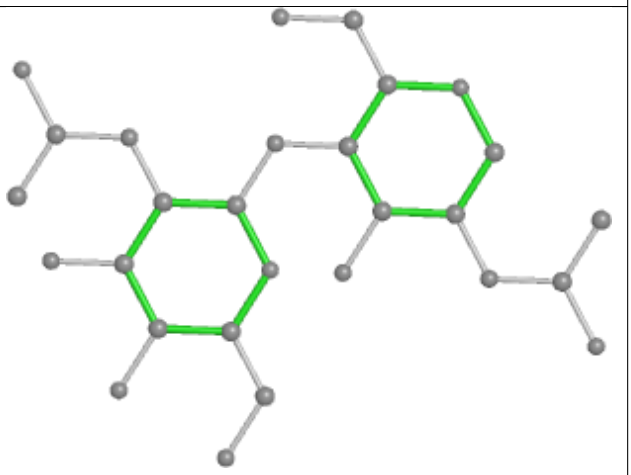
Bond lengths



Bond angles

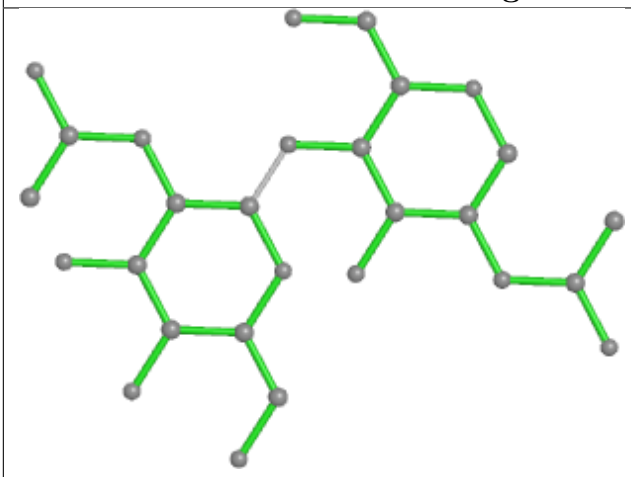


Torsions

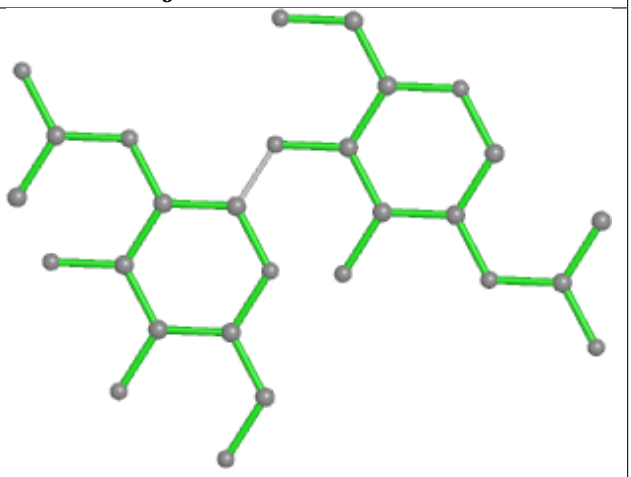


Rings

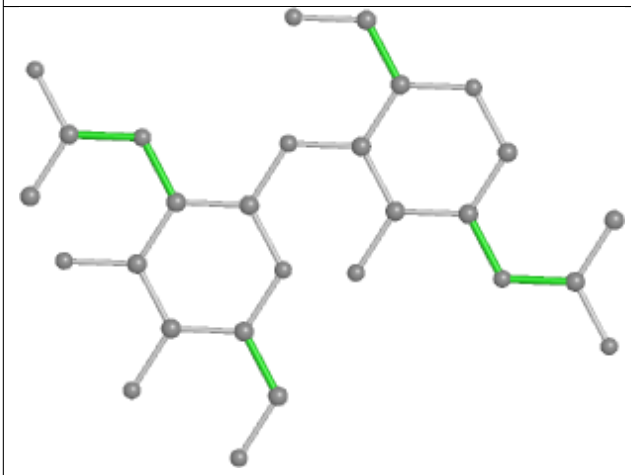
Oligosaccharide Chain j



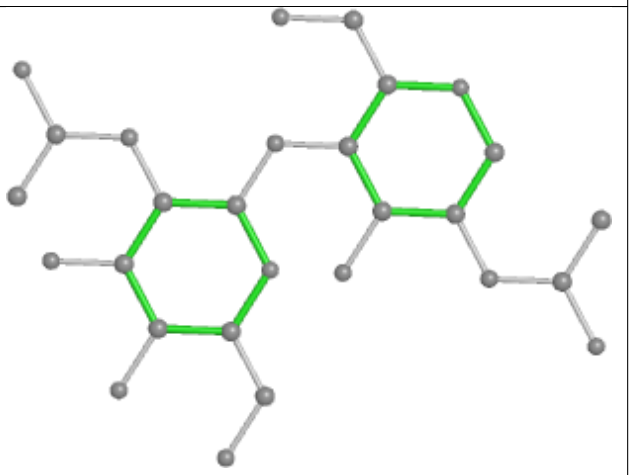
Bond lengths



Bond angles

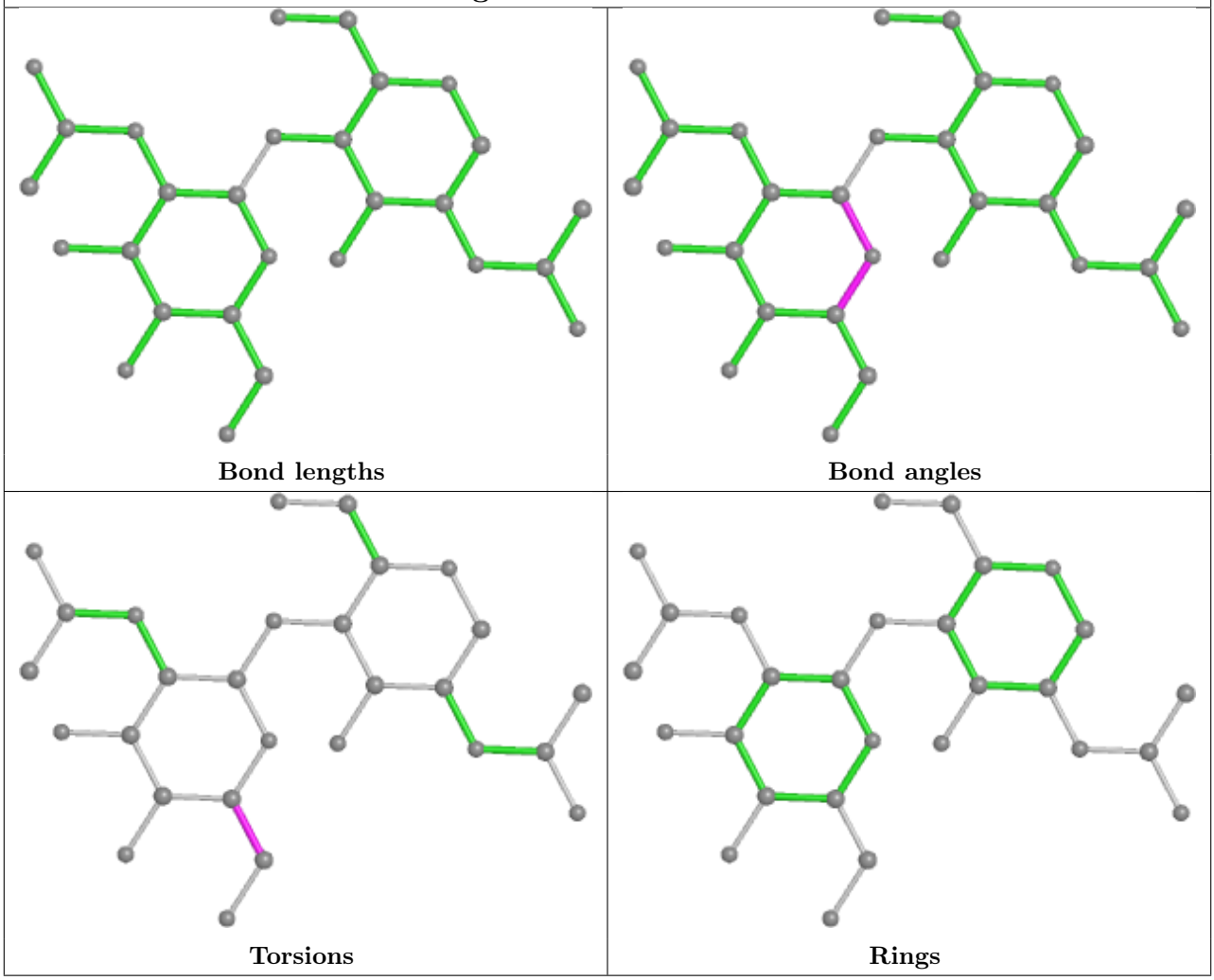


Torsions



Rings

Oligosaccharide Chain k



5.6 Ligand geometry (i)

29 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	B	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	A	1409	1	14,14,15	0.52	0	17,19,21	0.36	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	A	1407	1	14,14,15	0.23	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	A	1401	1	14,14,15	0.31	0	17,19,21	0.33	0
4	NAG	C	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	C	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	E	901	2	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	B	1410	-	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	B	1402	1	14,14,15	0.20	0	17,19,21	0.64	0
4	NAG	C	1401	1	14,14,15	0.30	0	17,19,21	0.34	0
4	NAG	D	901	2	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	B	1404	1	14,14,15	0.47	0	17,19,21	0.53	0
4	NAG	C	1406	1	14,14,15	0.30	0	17,19,21	0.39	0
4	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.33	0
4	NAG	A	1405	1	14,14,15	0.55	0	17,19,21	1.26	1 (5%)
4	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	C	1404	1	14,14,15	0.48	0	17,19,21	0.54	0
4	NAG	C	1408	1	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	A	1404	1	14,14,15	0.47	0	17,19,21	0.54	0
4	NAG	B	1409	1	14,14,15	0.41	0	17,19,21	1.15	2 (11%)
4	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.64	0
4	NAG	C	1403	1	14,14,15	0.20	0	17,19,21	0.42	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	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	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1405	NAG	C2-N2-C7	4.34	129.08	122.90
4	A	1405	NAG	C2-N2-C7	4.32	129.05	122.90
4	B	1405	NAG	C2-N2-C7	4.29	129.02	122.90
4	B	1409	NAG	C8-C7-N2	2.29	119.97	116.10
4	E	901	NAG	C1-O5-C5	2.09	115.02	112.19

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

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

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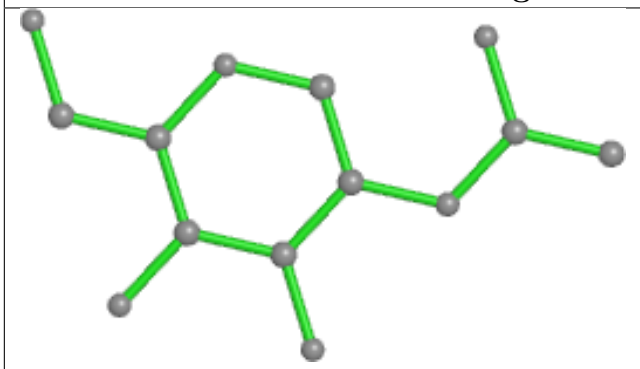
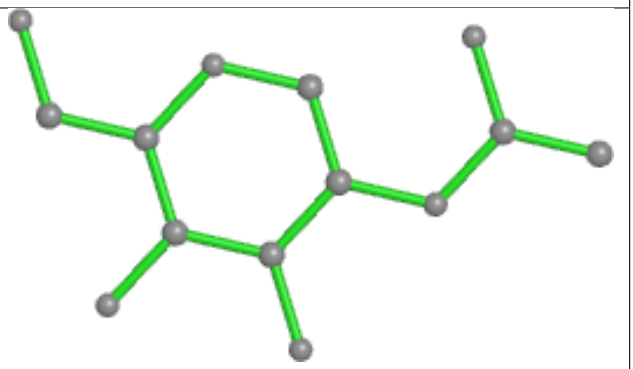
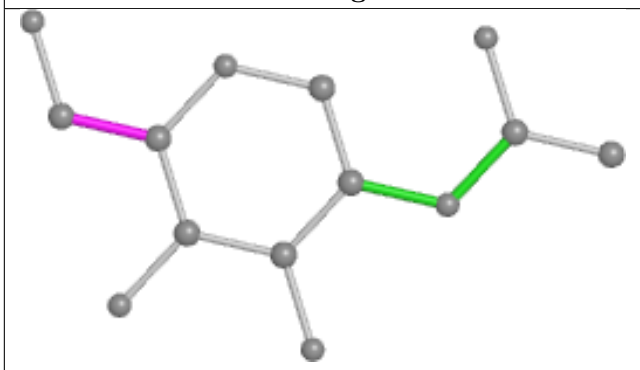
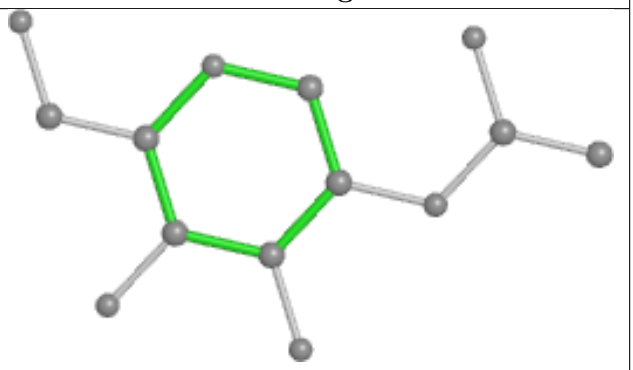
Mol	Chain	Res	Type	Atoms
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1402	NAG	3	0
4	C	1405	NAG	1	0
4	B	1410	NAG	4	0
4	B	1402	NAG	3	0
4	A	1405	NAG	1	0
4	B	1409	NAG	4	0
4	B	1405	NAG	1	0
4	A	1402	NAG	3	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 B 1406	
 Bond lengths	 Bond angles
 Torsions	 Rings

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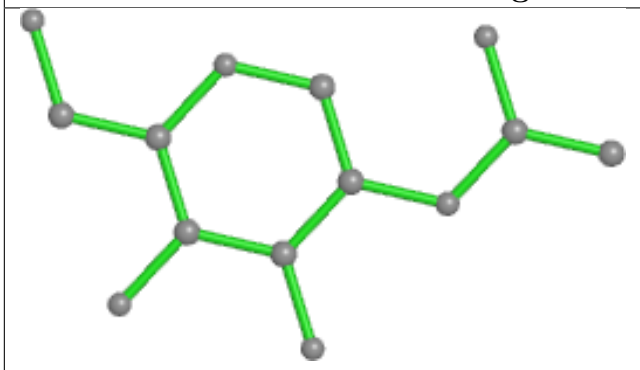
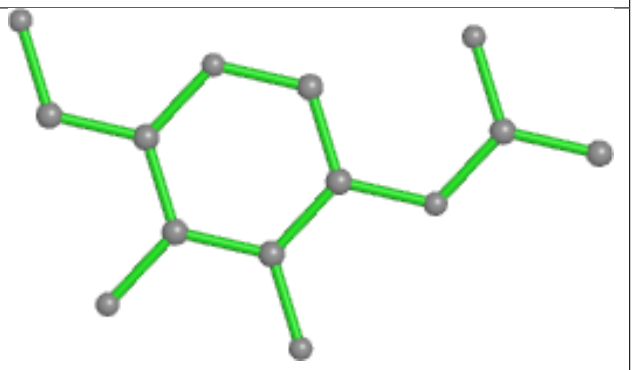
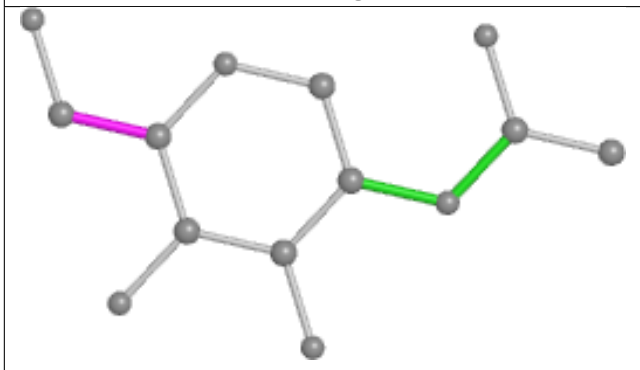
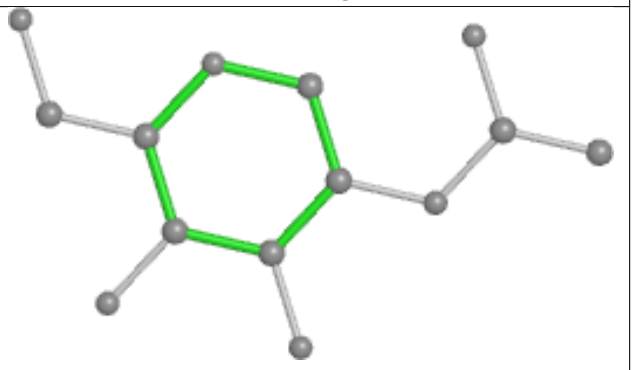
 Bond lengths	 Bond angles
 Torsions	 Rings

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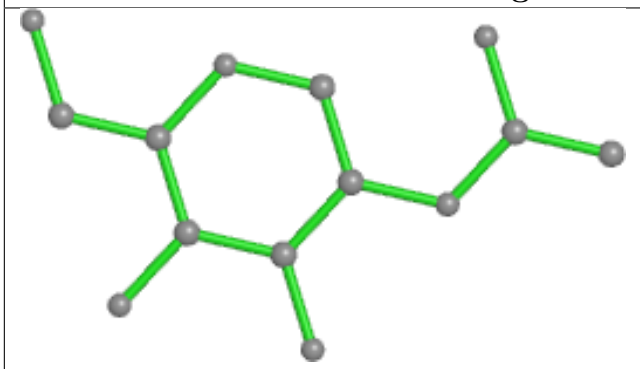
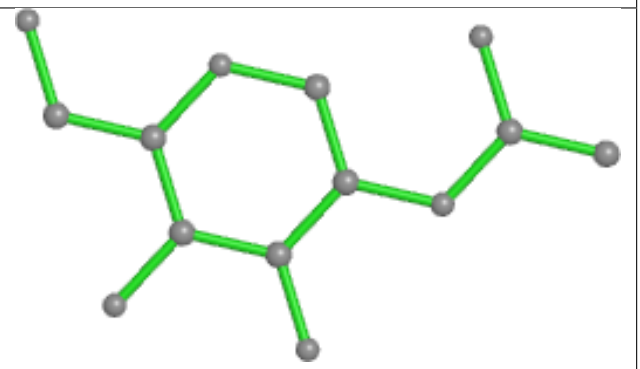
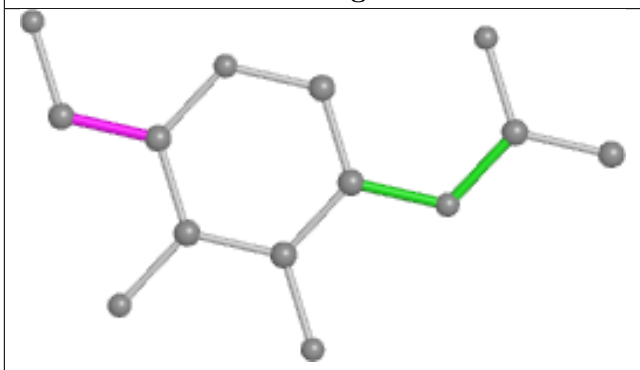
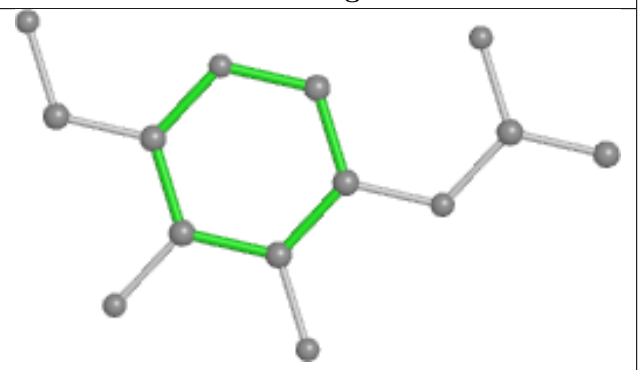
 Bond lengths	 Bond angles
 Torsions	 Rings

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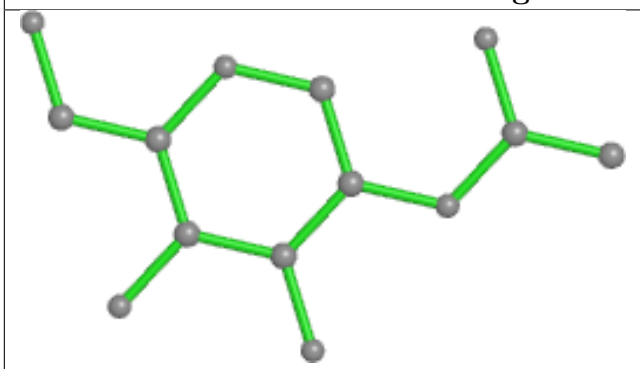
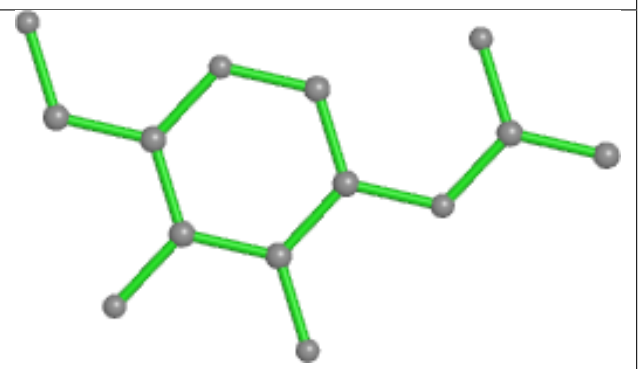
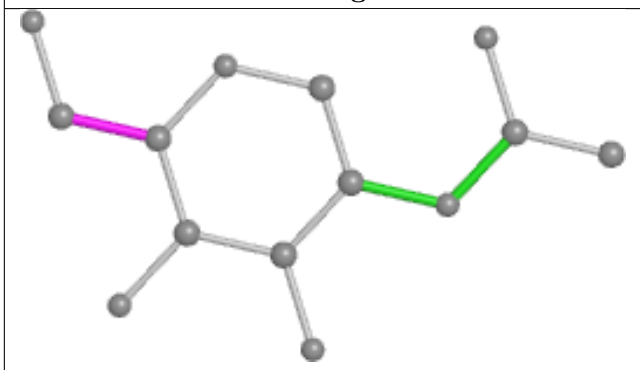
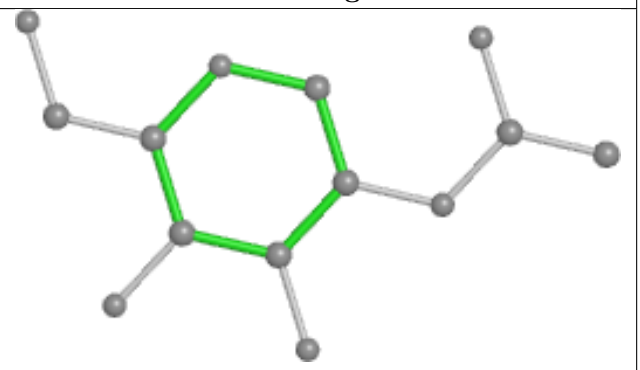
 Bond lengths	 Bond angles
 Torsions	 Rings

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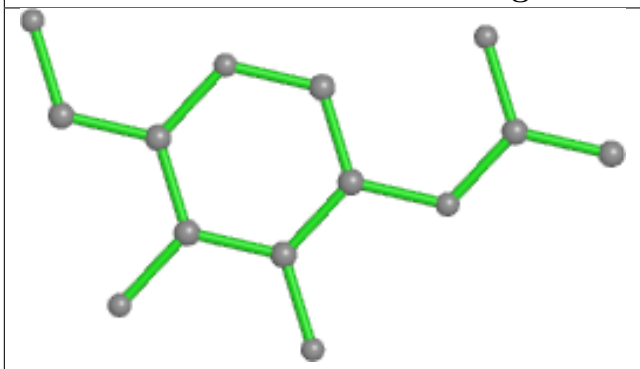
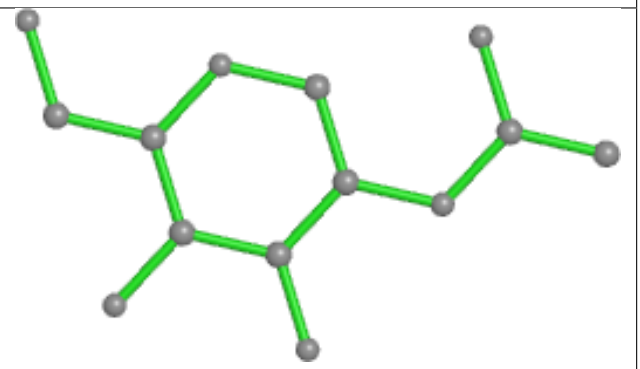
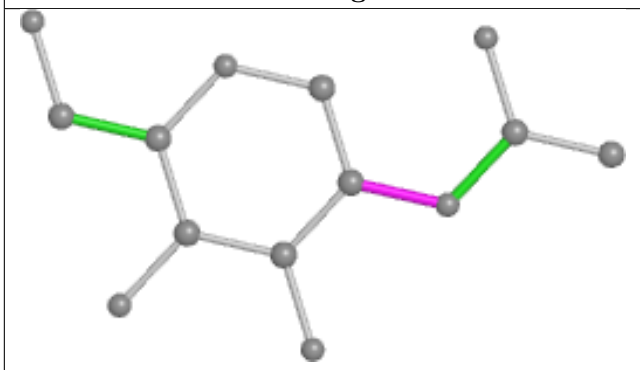
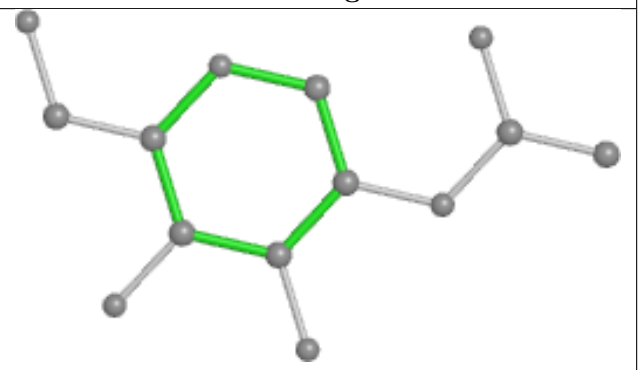
 Bond lengths	 Bond angles
 Torsions	 Rings

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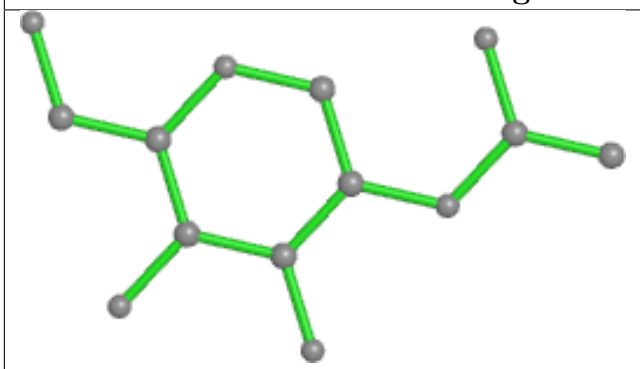
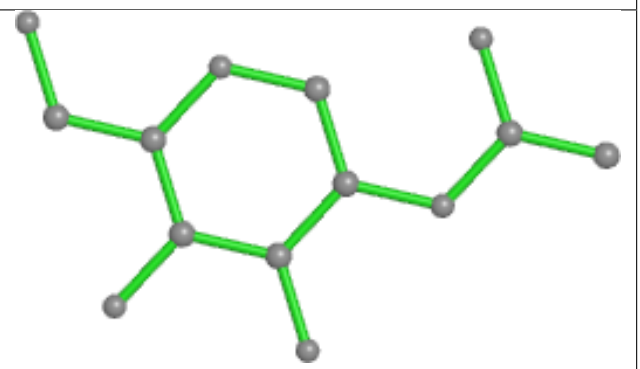
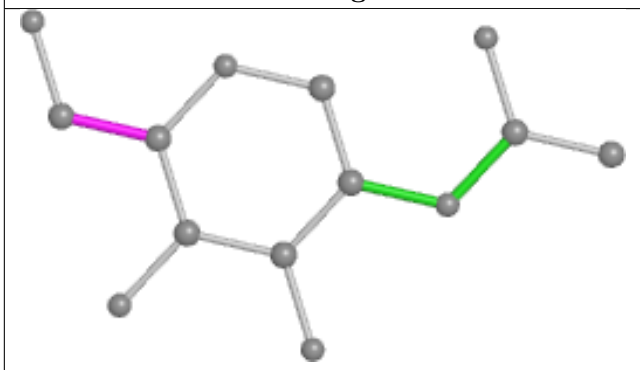
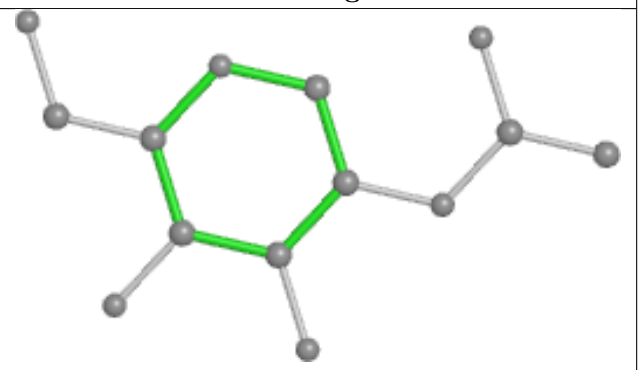
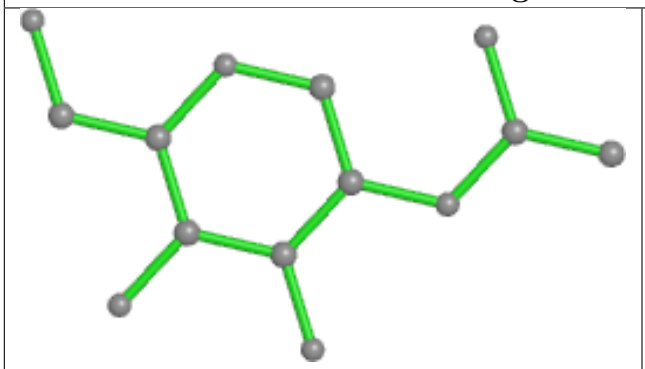
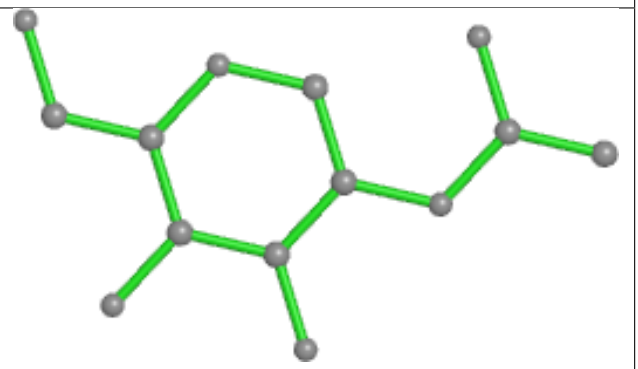
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1401



Bond lengths



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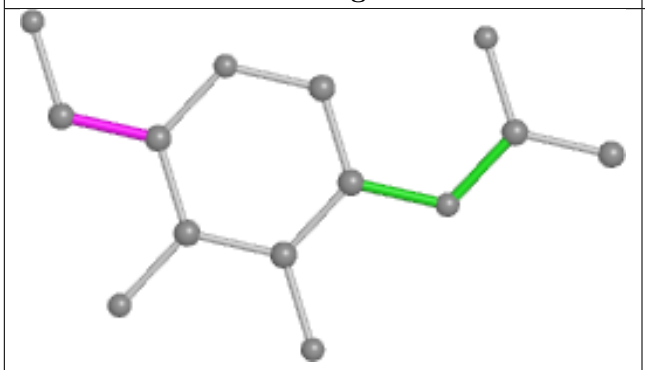
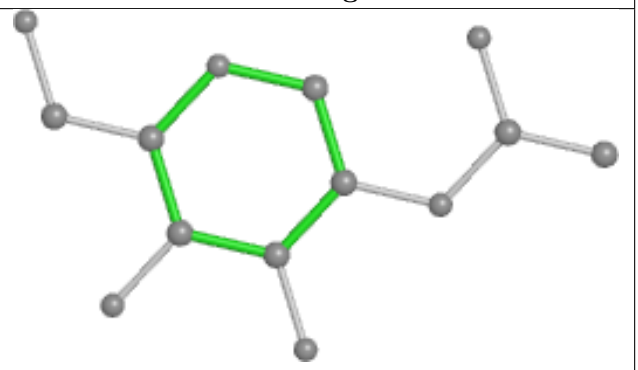
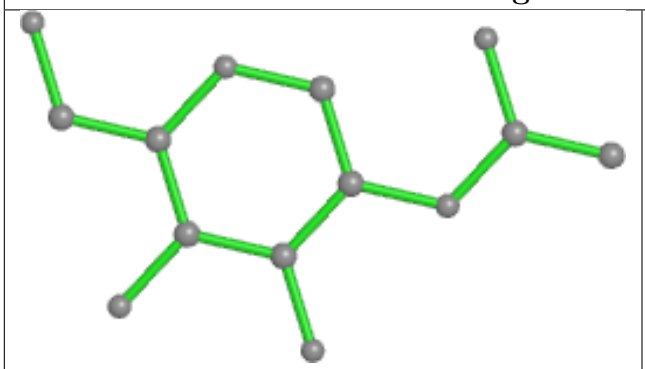


Torsions



Rings

Ligand NAG C 1405



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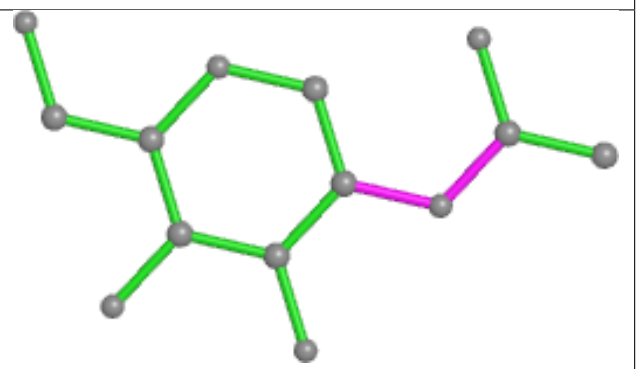

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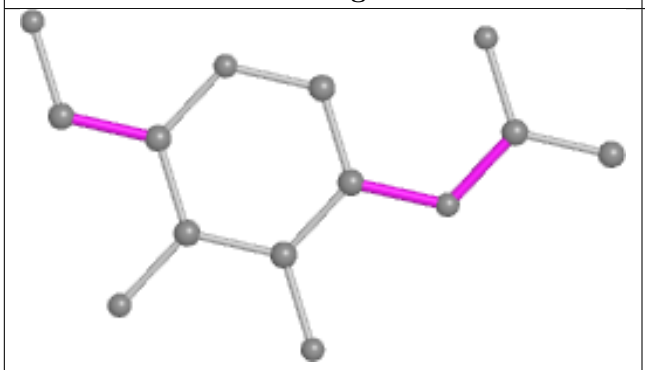

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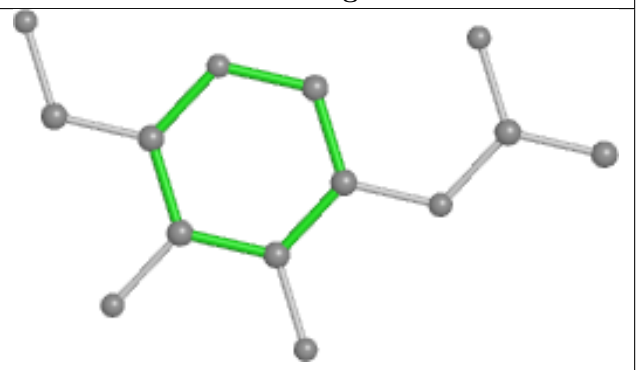
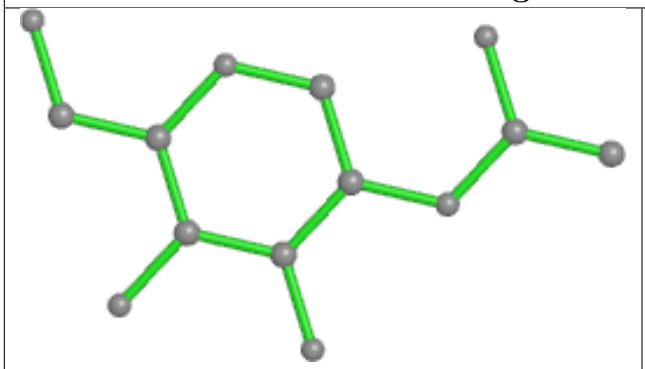


Rings

Ligand NAG C 1407



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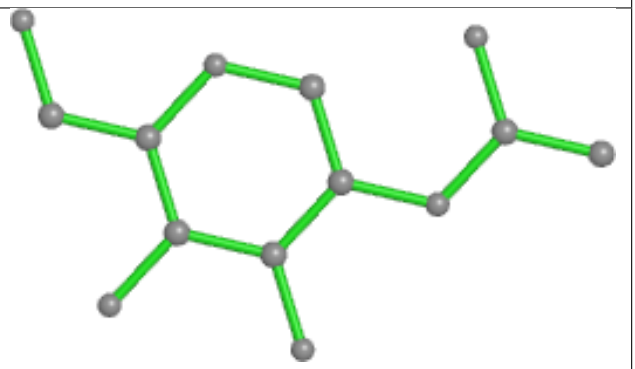

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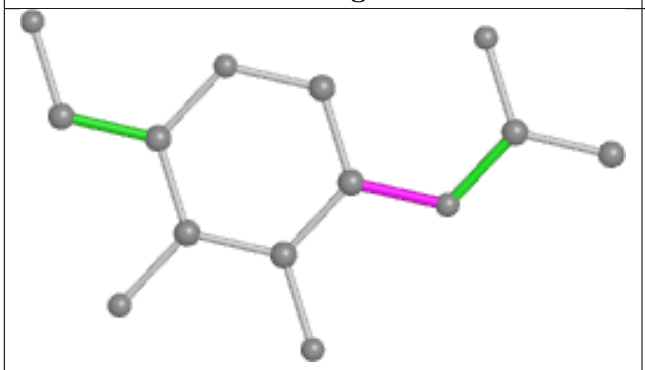

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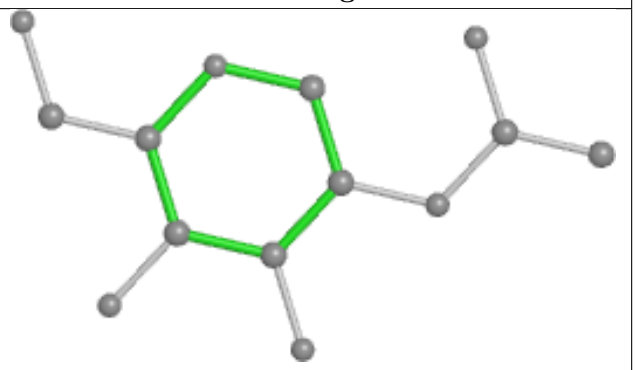
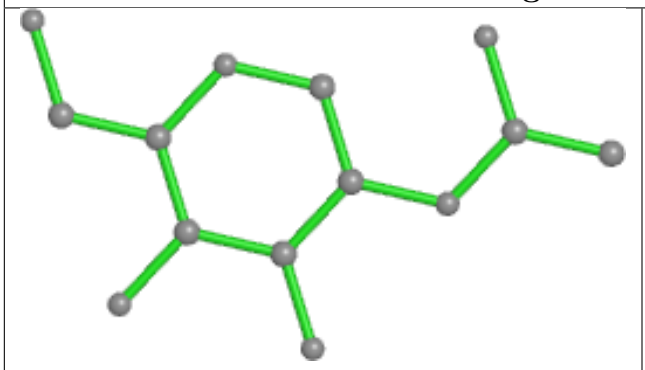


Rings

Ligand NAG E 901



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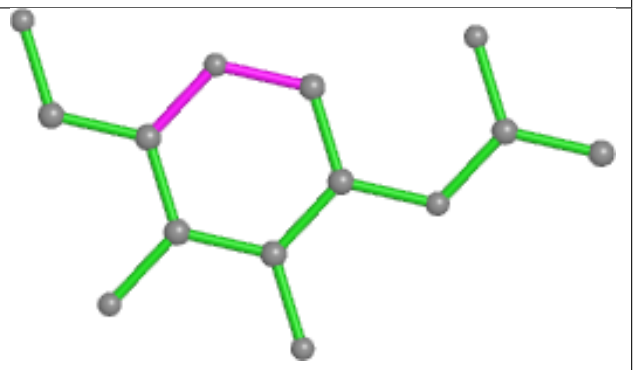
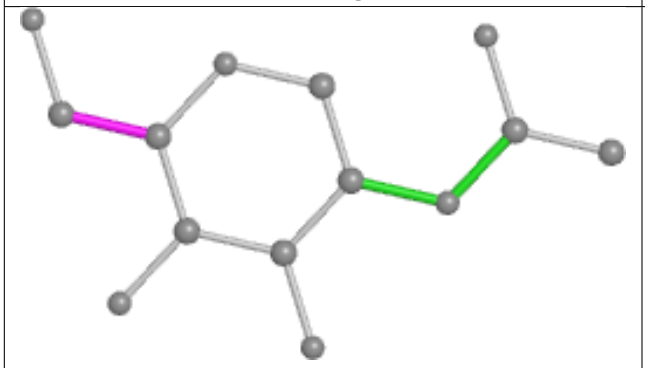
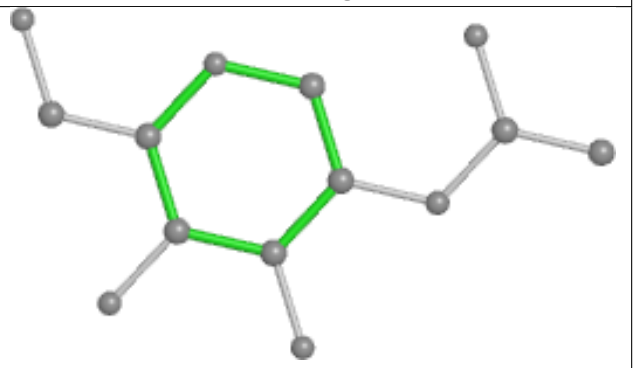


Bond angles



Torsions



Rings

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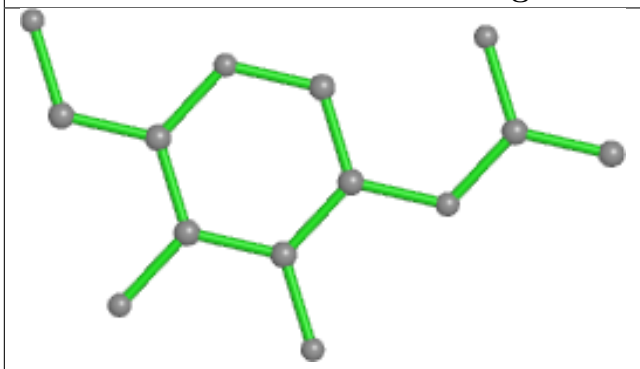
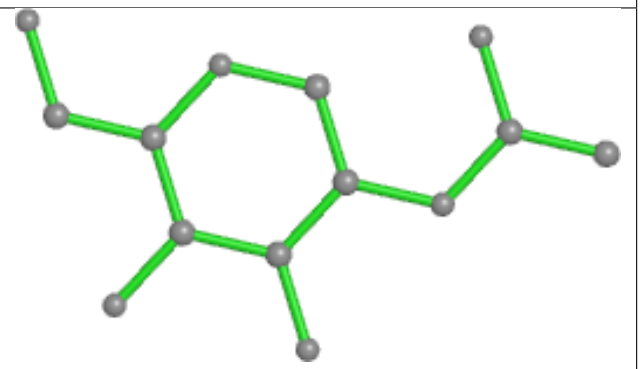
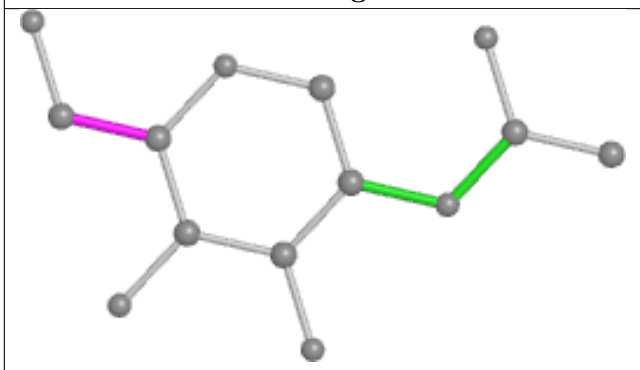
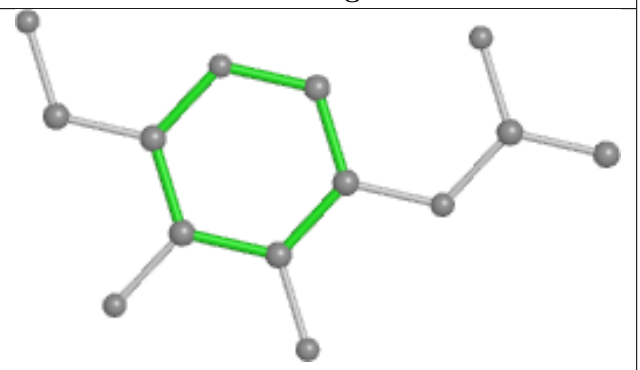
 Bond lengths	 Bond angles
 Torsions	 Rings

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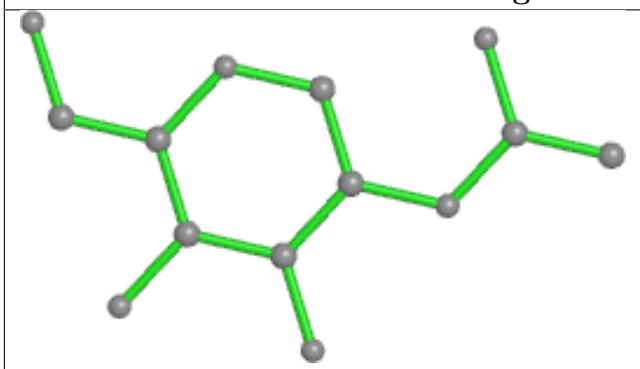
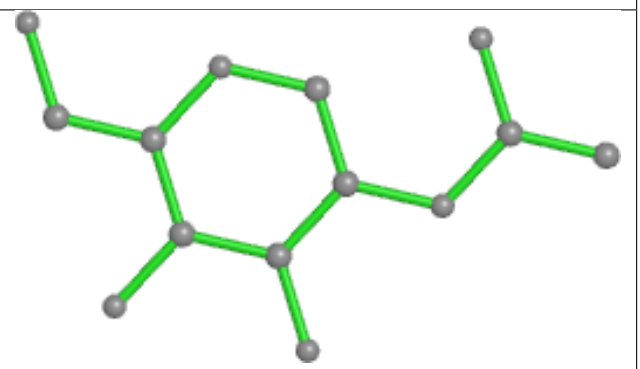
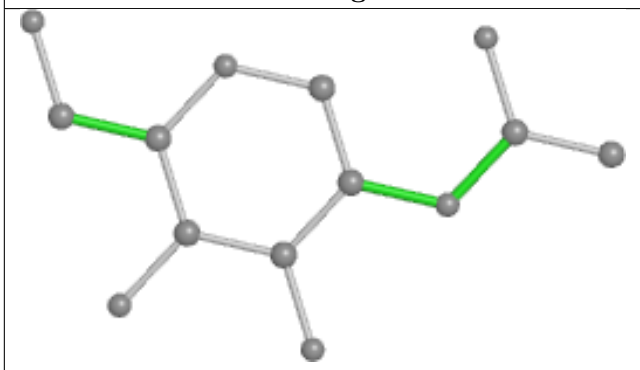
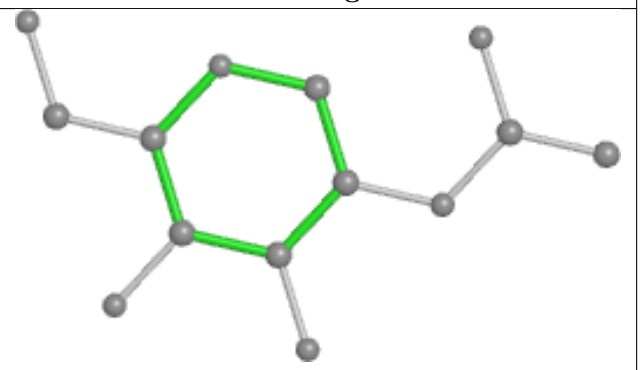
 Bond lengths	 Bond angles
 Torsions	 Rings

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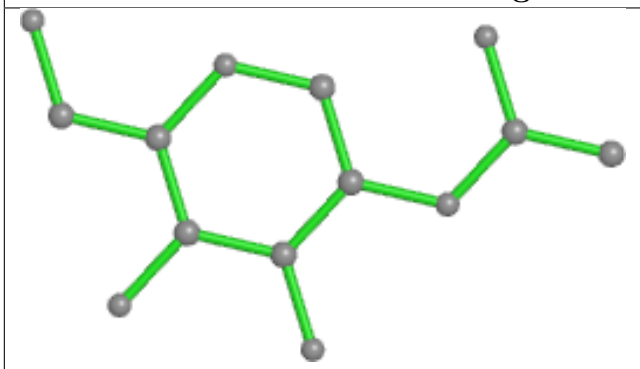
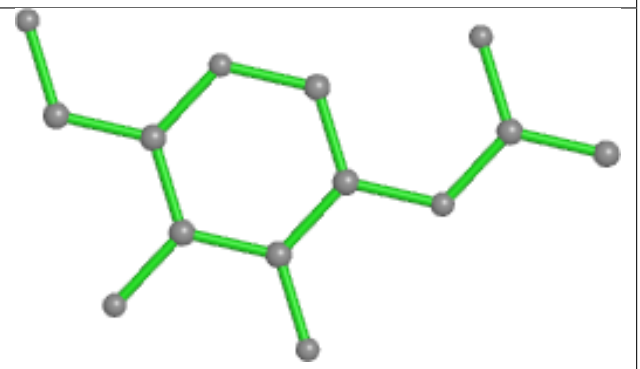
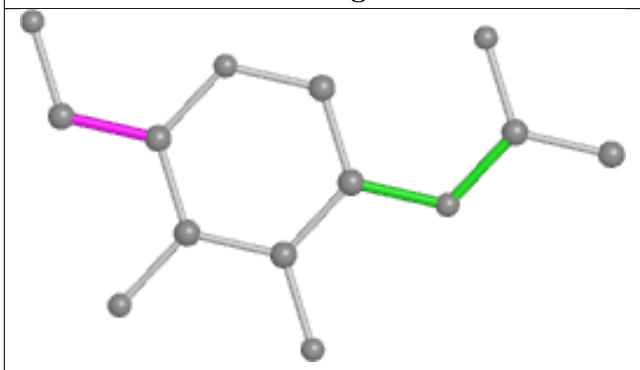
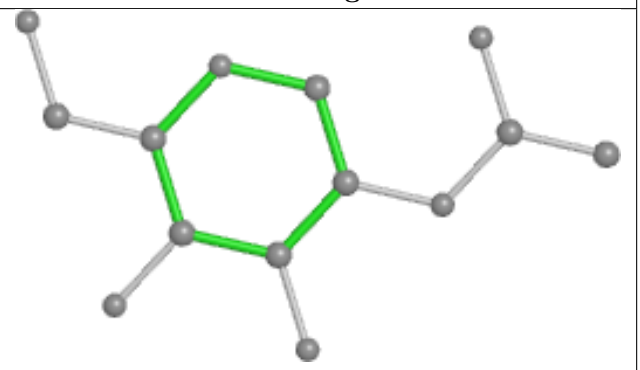
 Bond lengths	 Bond angles
 Torsions	 Rings

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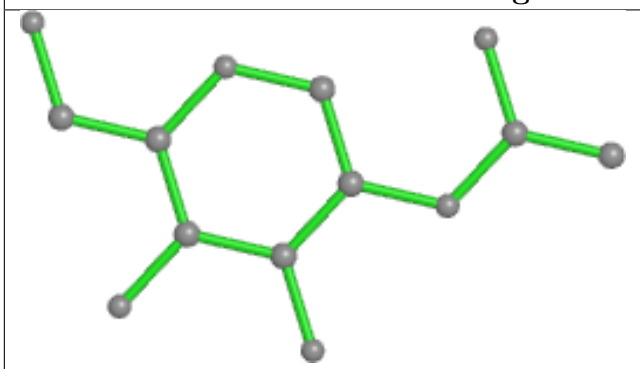
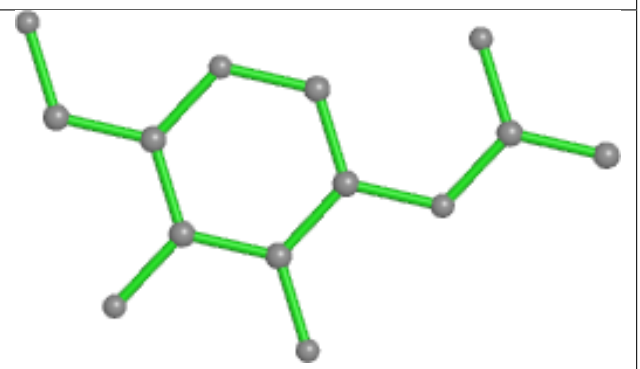
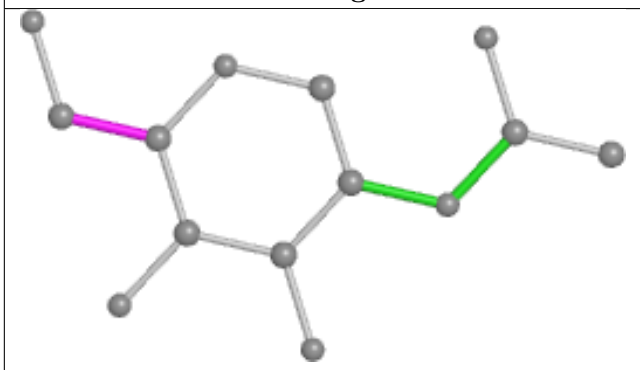
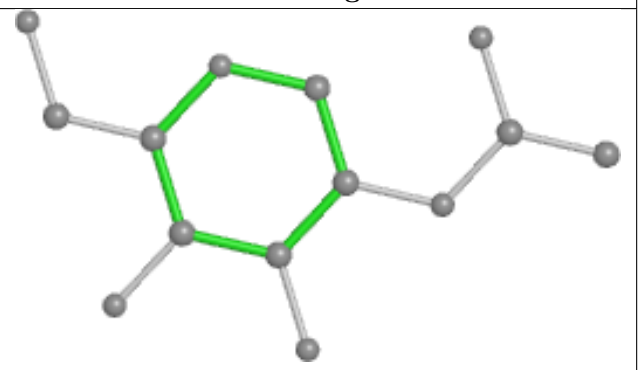
 Bond lengths	 Bond angles
 Torsions	 Rings

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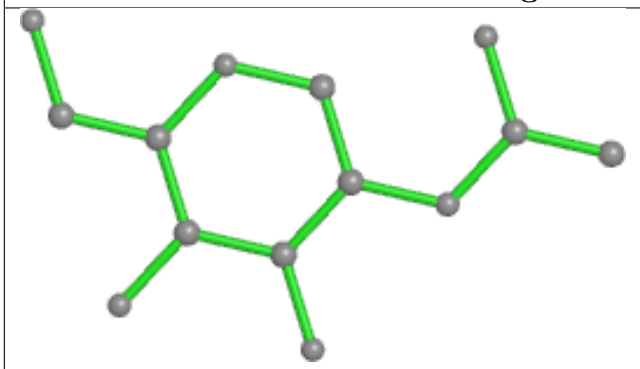
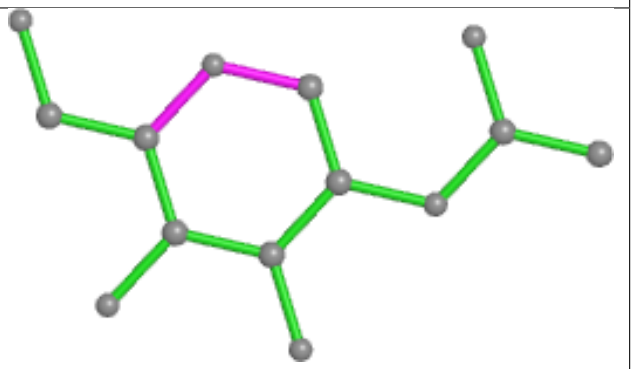
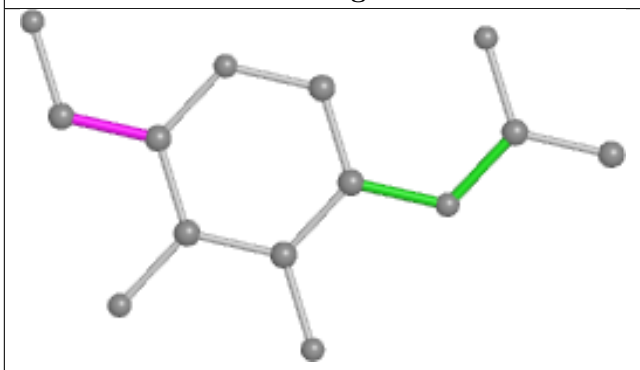
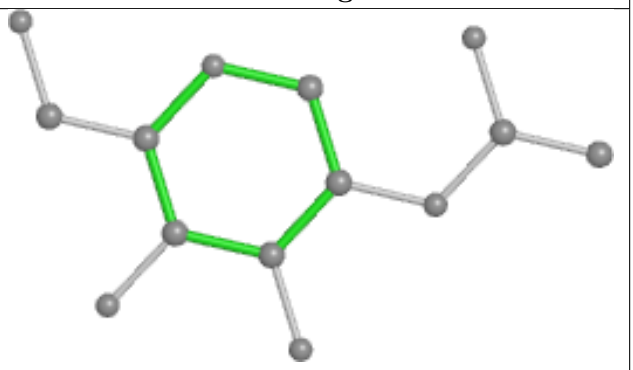
 Bond lengths	 Bond angles
 Torsions	 Rings

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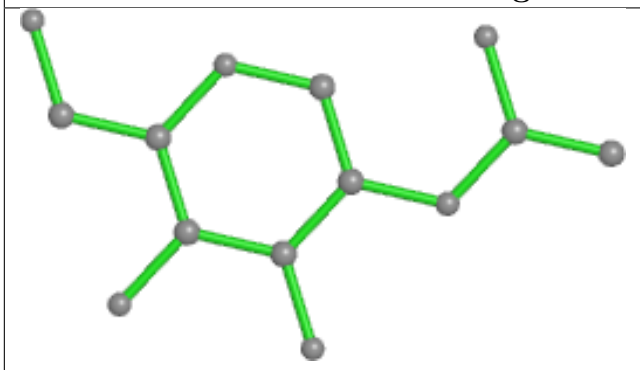
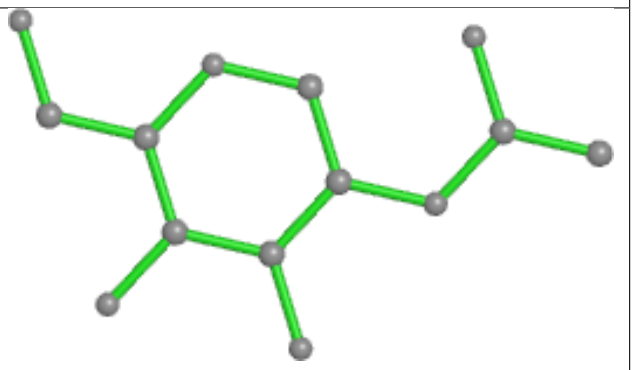
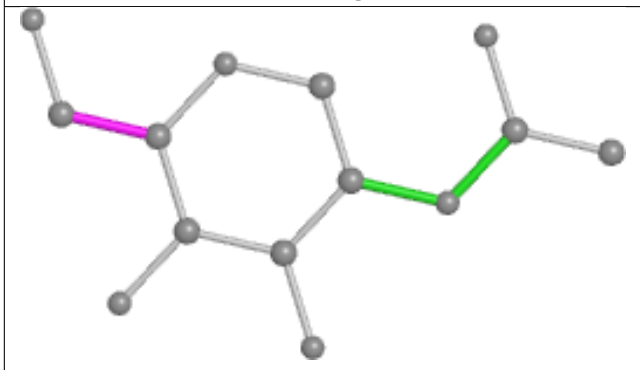
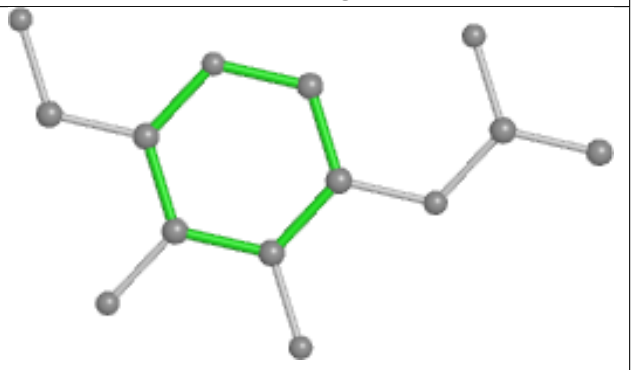
 Bond lengths	 Bond angles
 Torsions	 Rings

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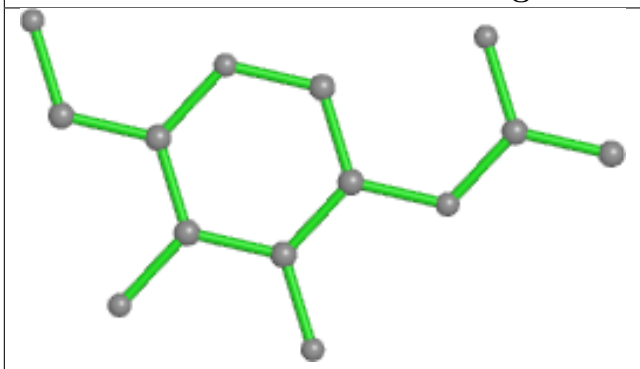
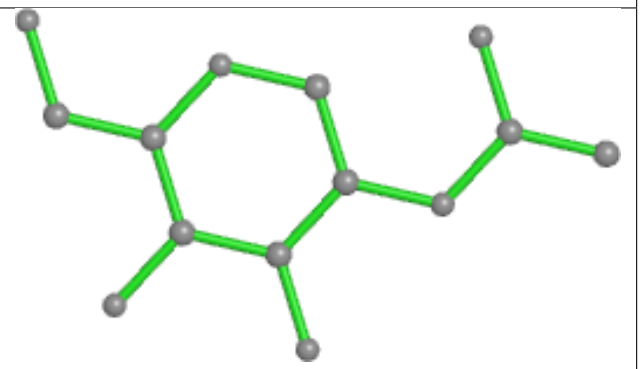
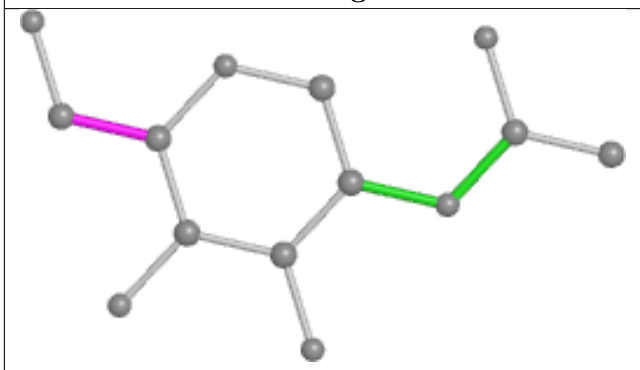
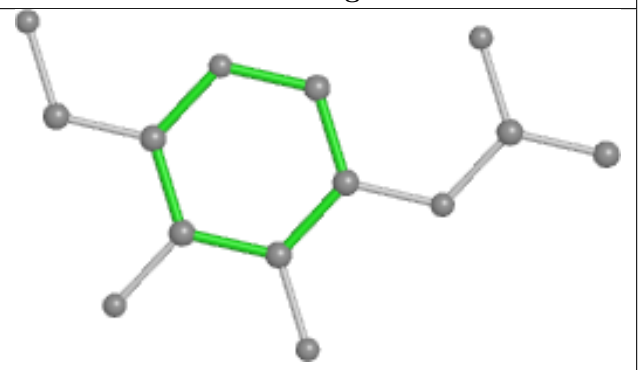
 Bond lengths	 Bond angles
 Torsions	 Rings

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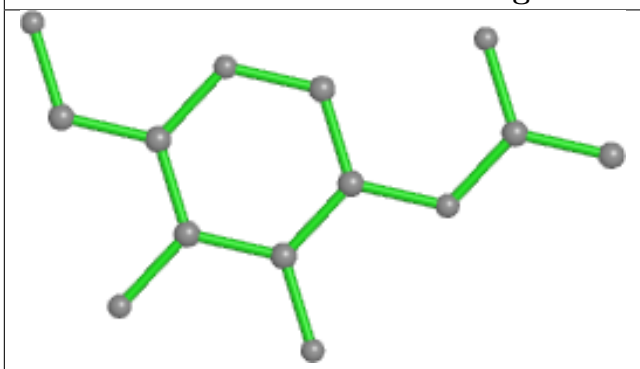
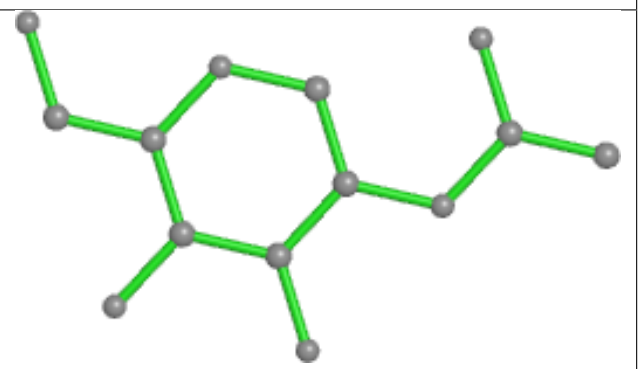
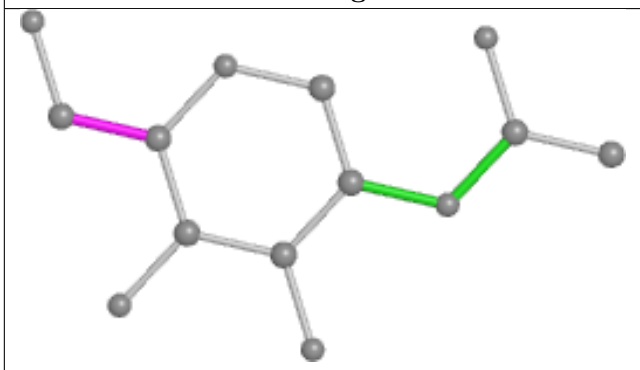
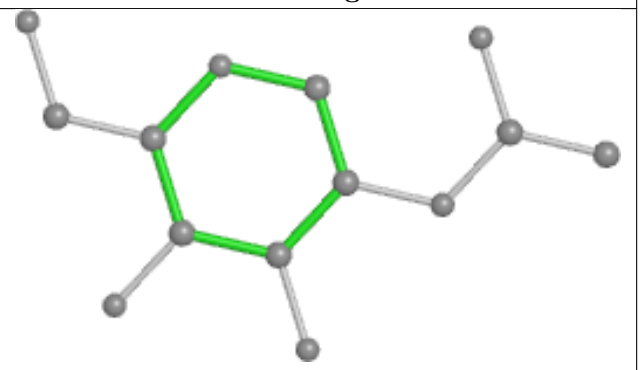
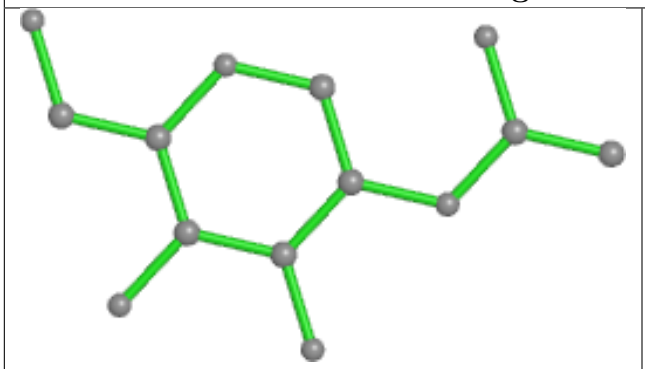
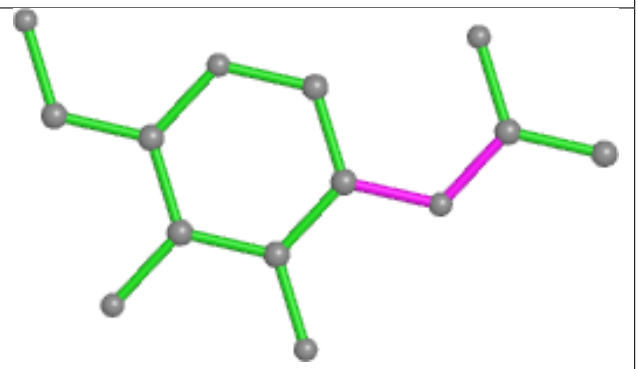
 Bond lengths	 Bond angles
 Torsions	 Rings

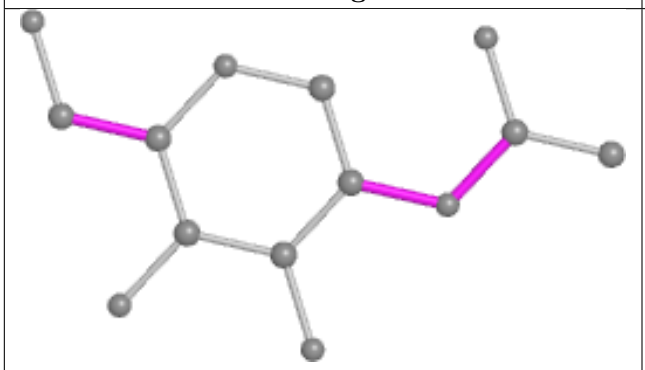
Ligand NAG A 1405



Bond lengths



Bond angles



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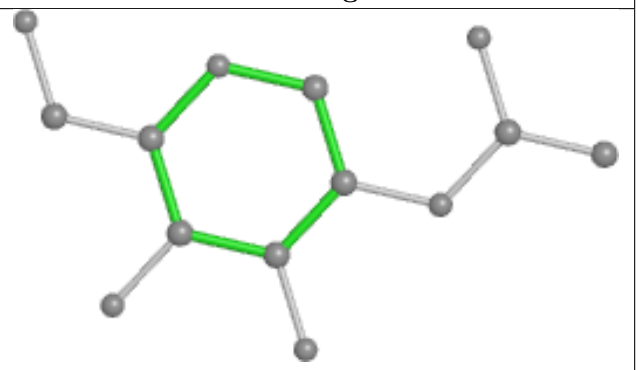
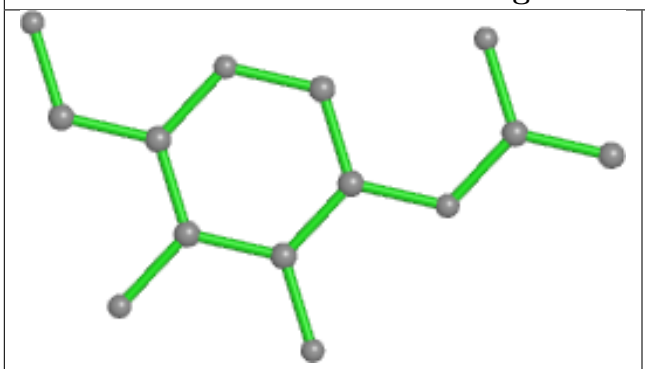


Rings

Ligand NAG B 1408



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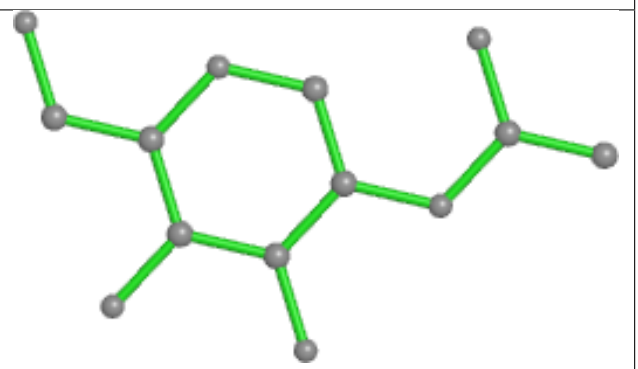

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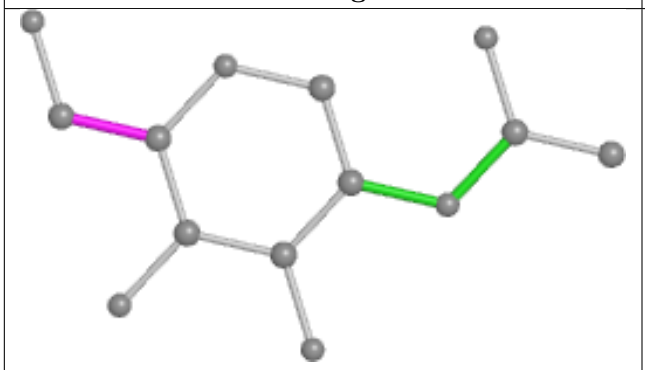

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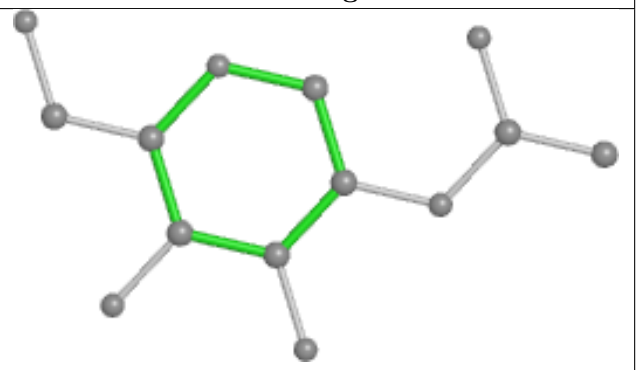

Rings

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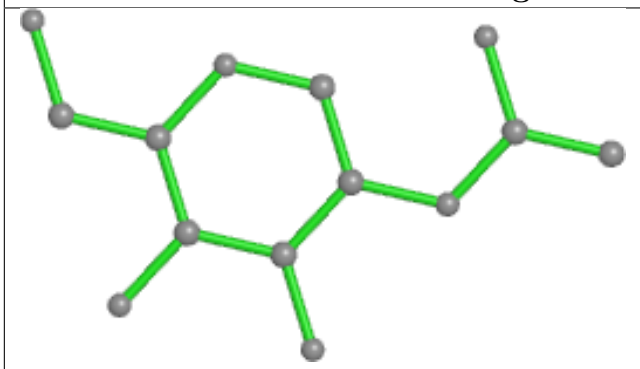
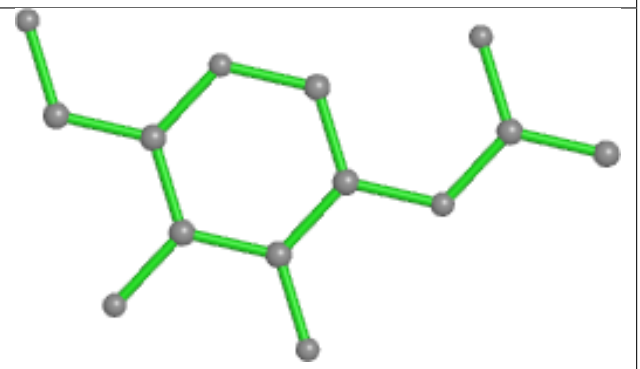
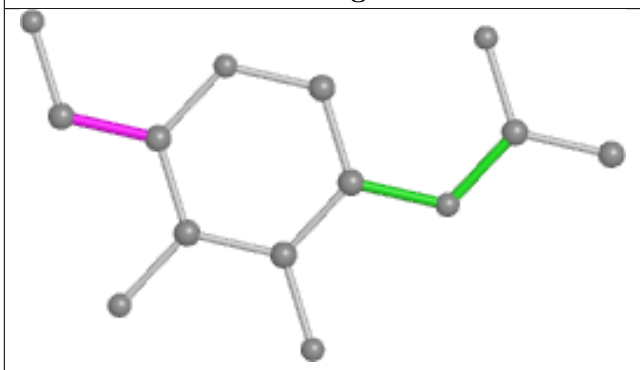
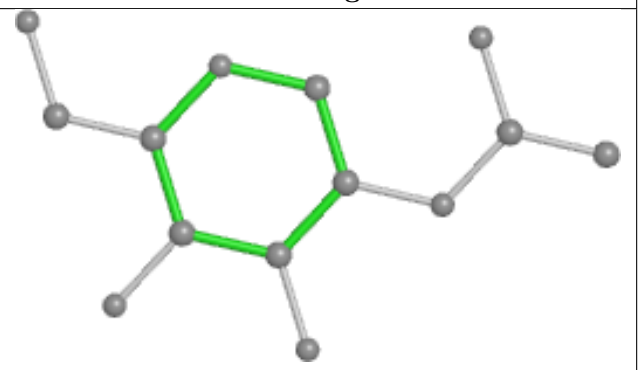
 Bond lengths	 Bond angles
 Torsions	 Rings

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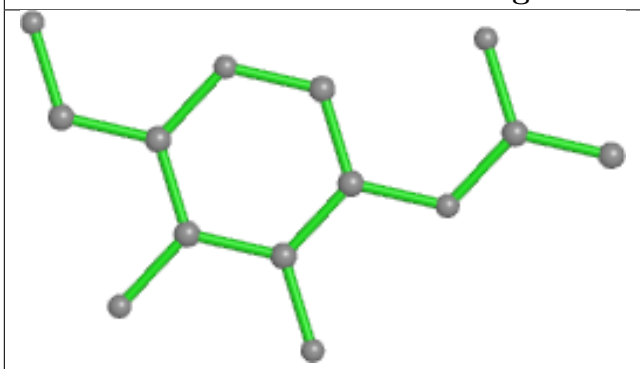
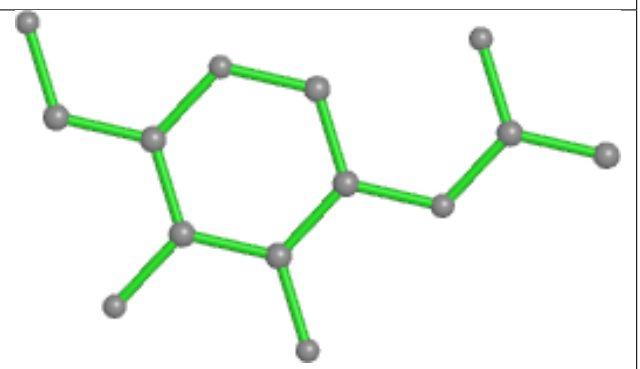
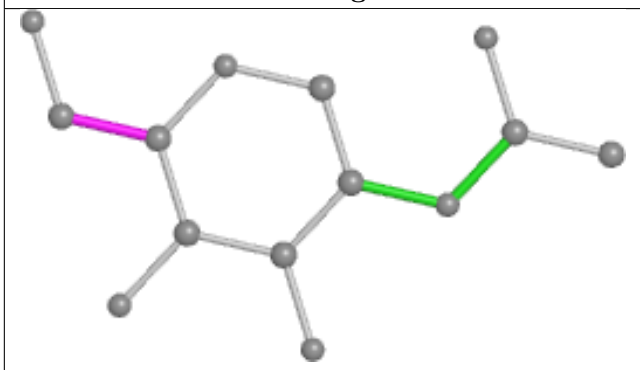
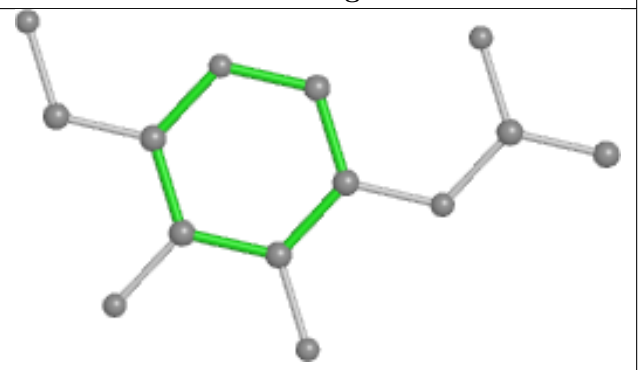
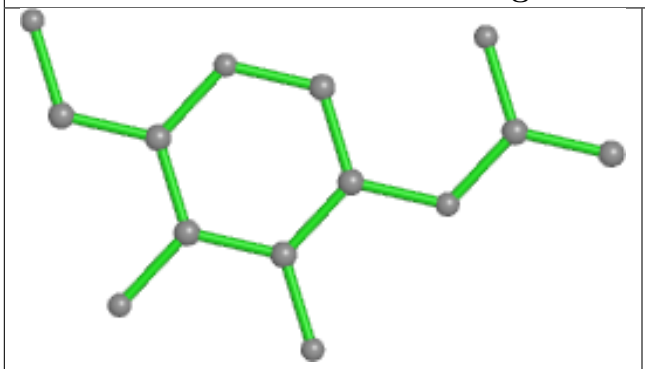
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1404



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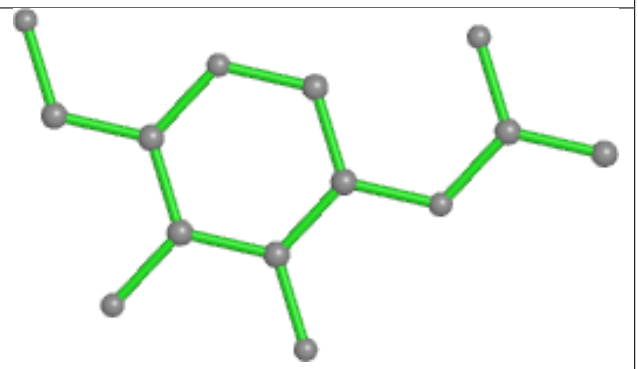
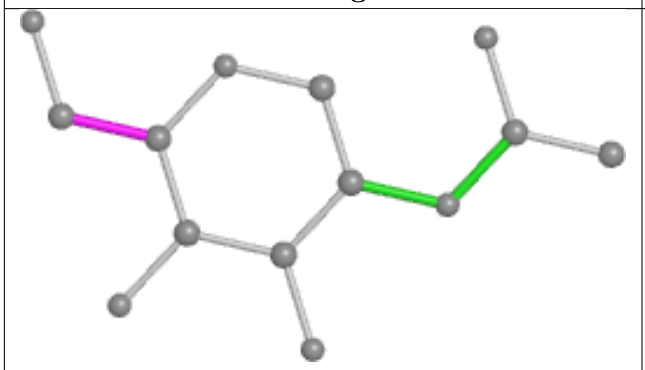


Bond angles



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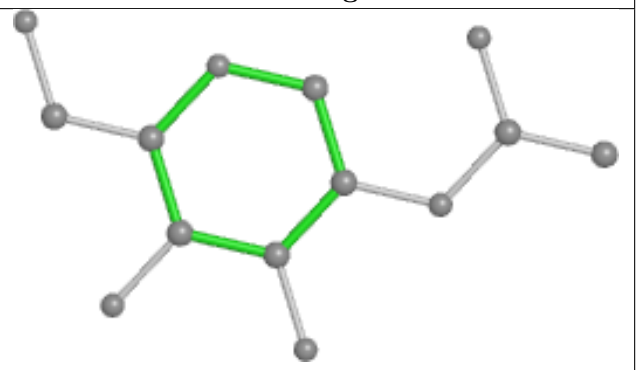
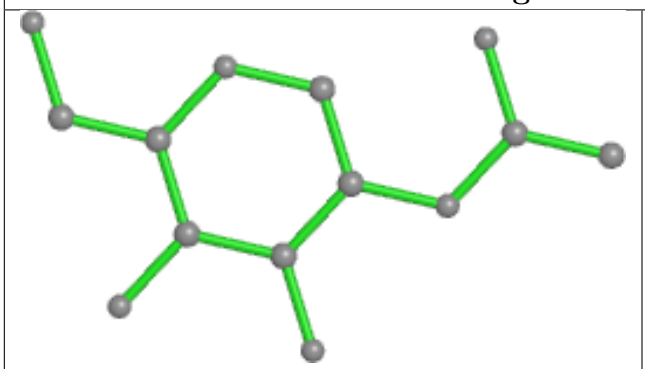
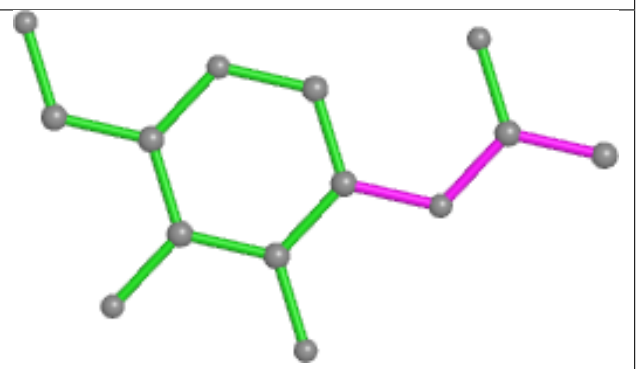


Rings

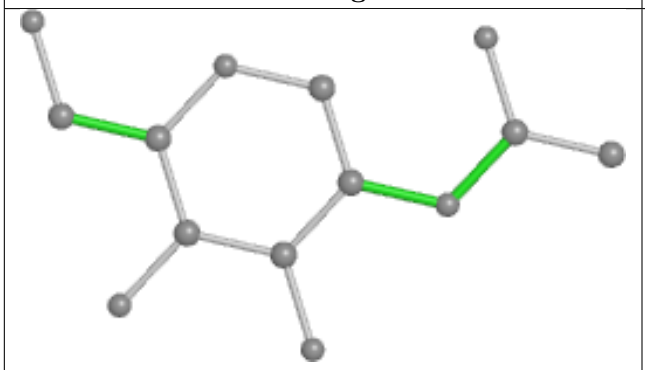
Ligand NAG B 1409



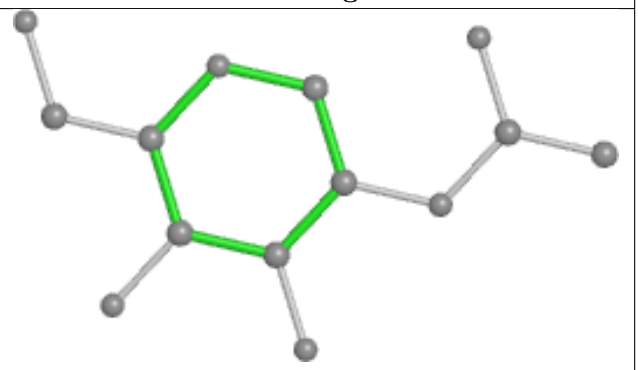
Bond lengths



Bond angles

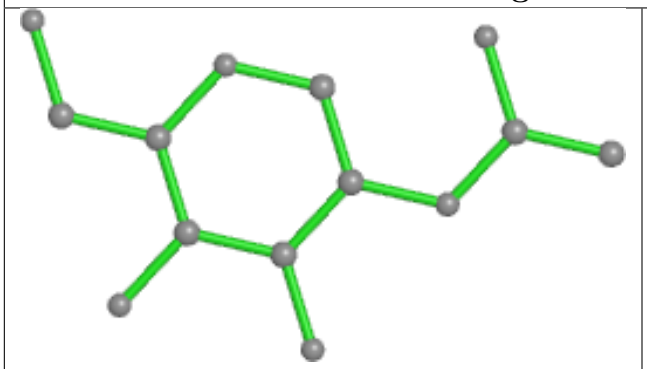


Torsions

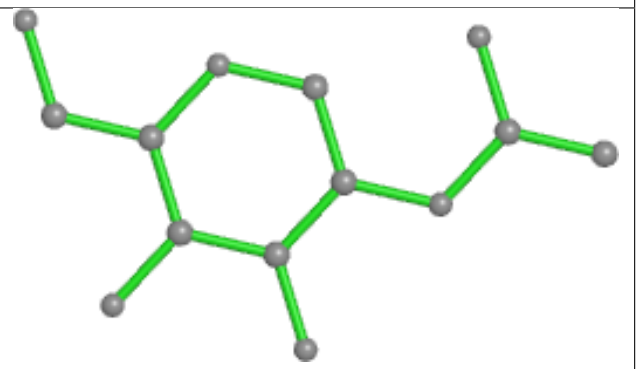


Rings

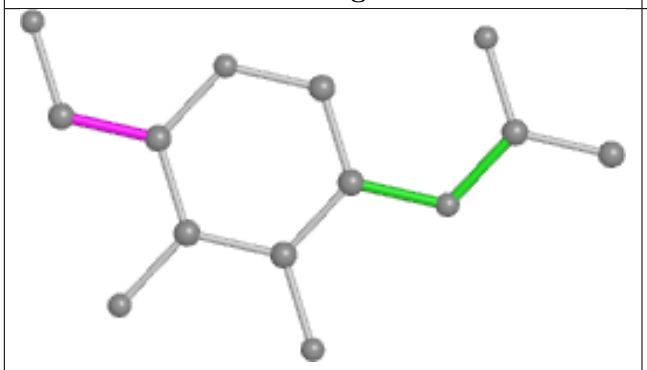
Ligand NAG A 1406



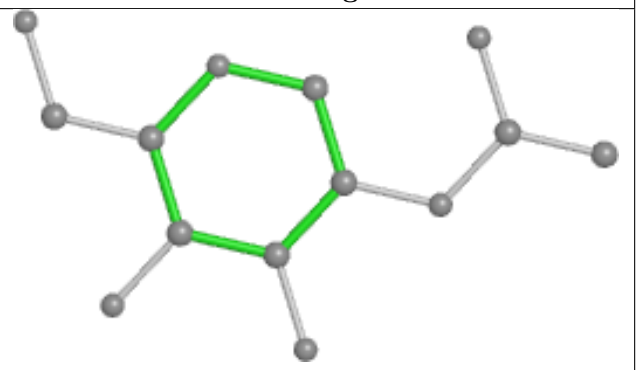
Bond lengths



Bond angles

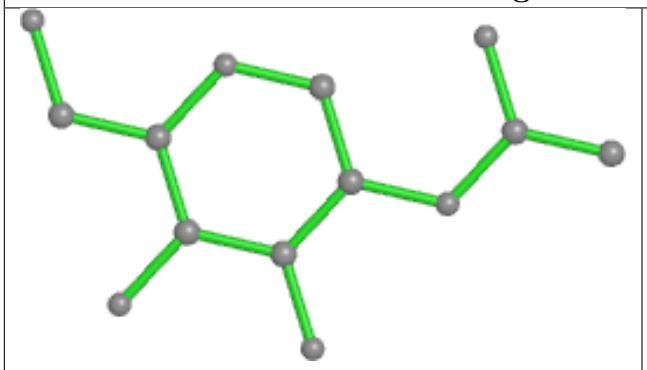


Torsions

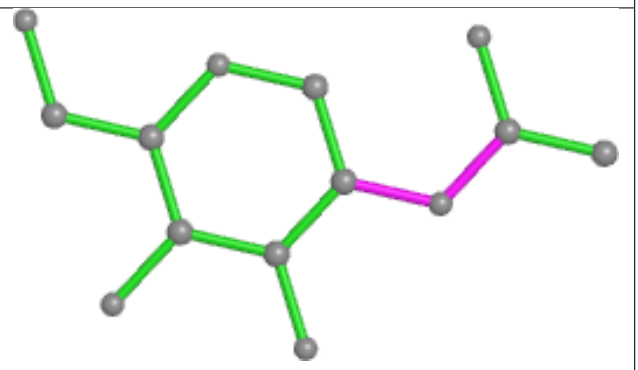


Rings

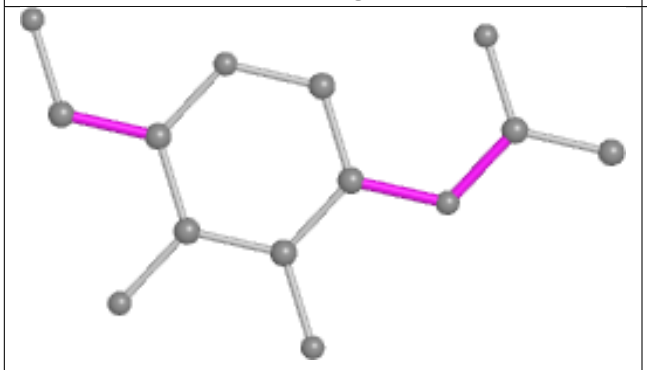
Ligand NAG B 1405



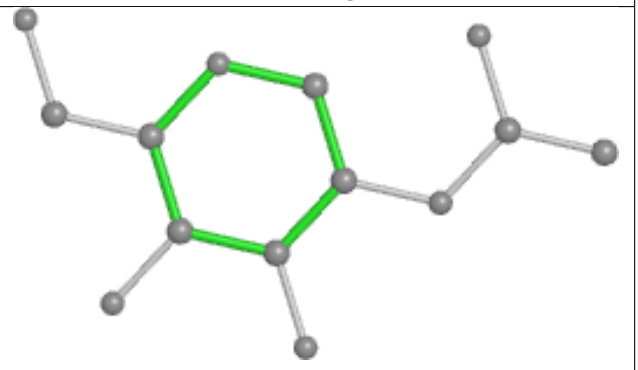
Bond lengths



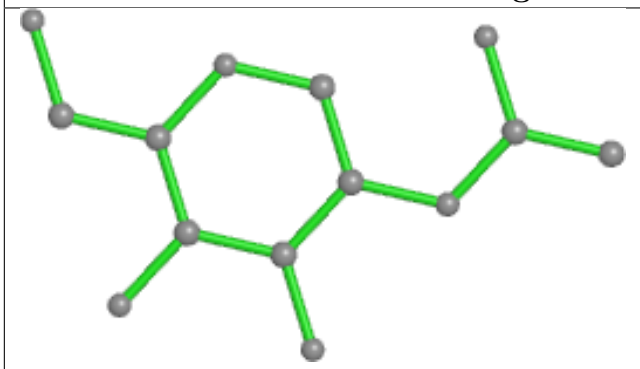
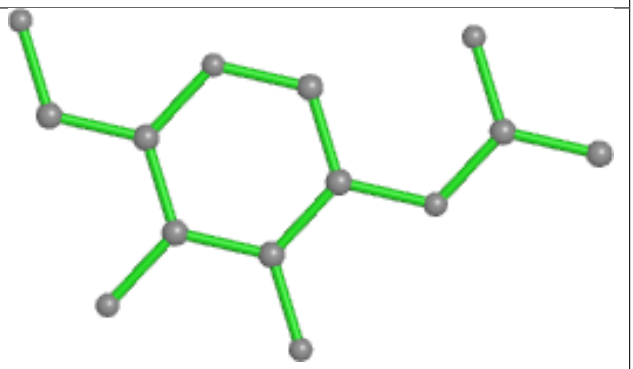
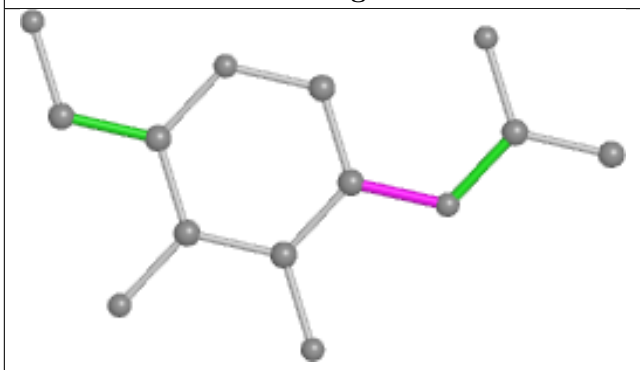
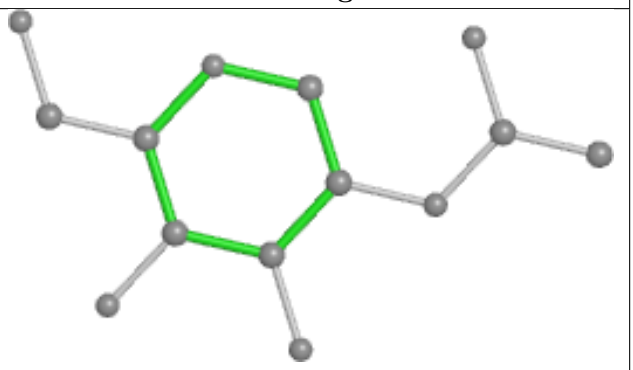
Bond angles

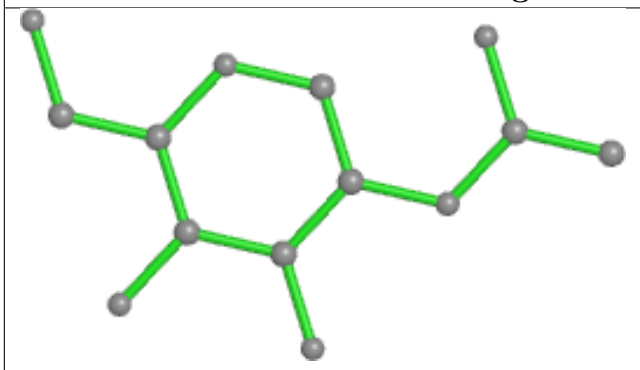
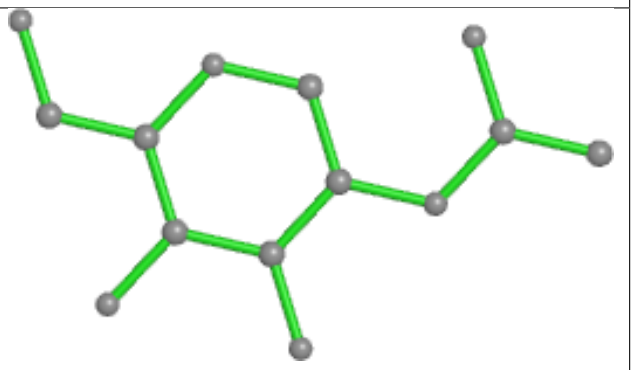
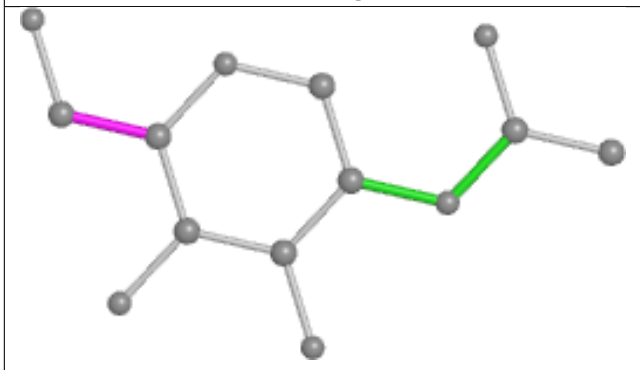
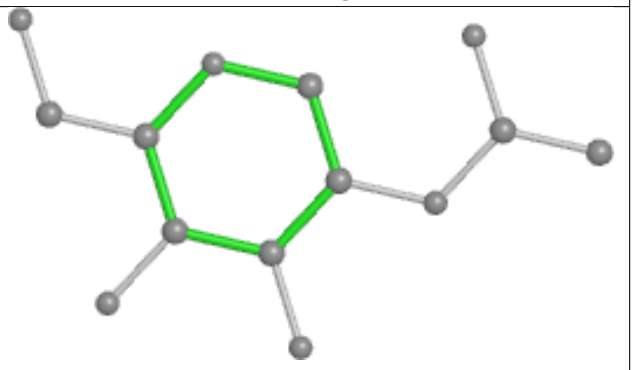


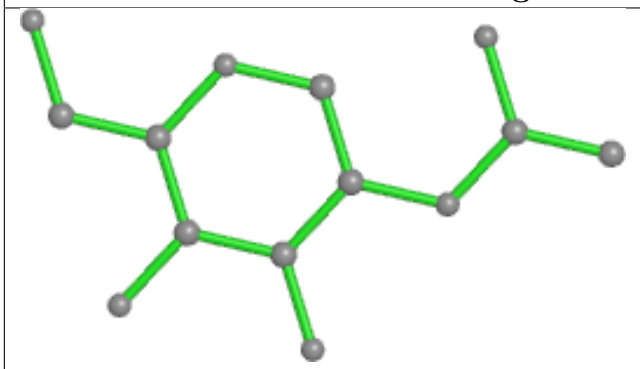
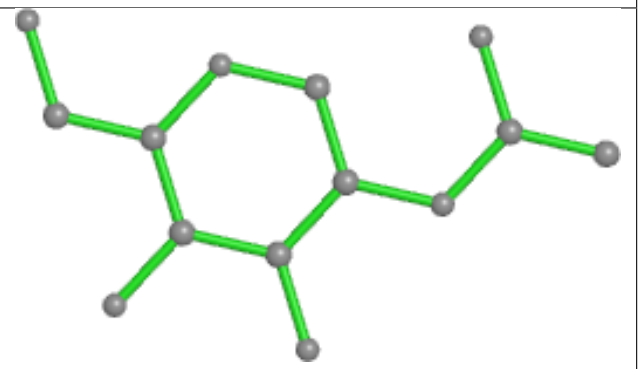
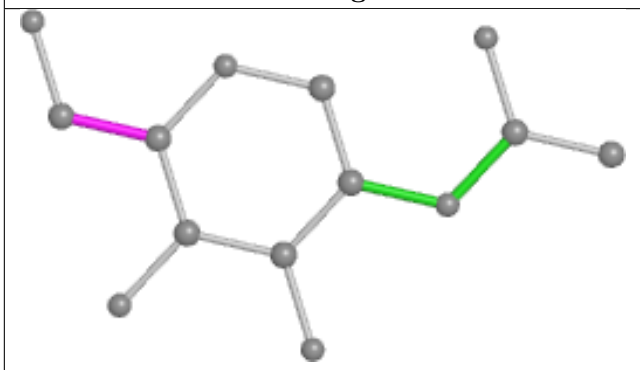
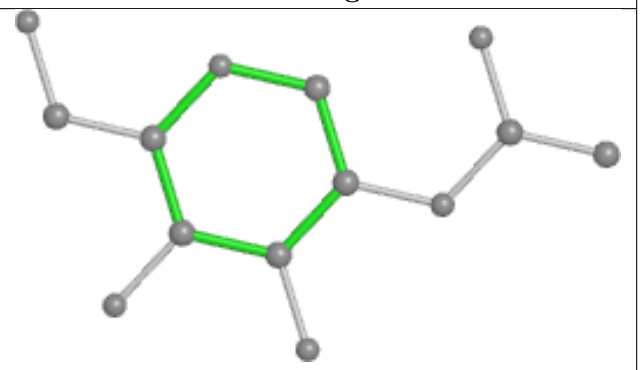
Torsions



Rings

Ligand NAG B 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1403	
 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.

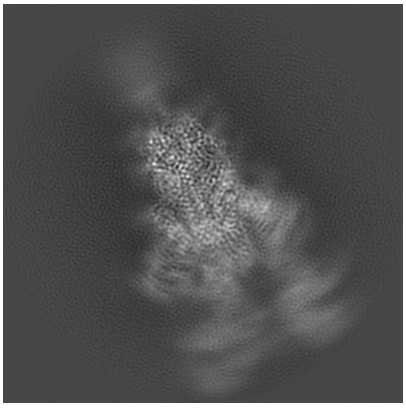
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30899. These allow visual inspection of the internal detail of the map and identification of artifacts.

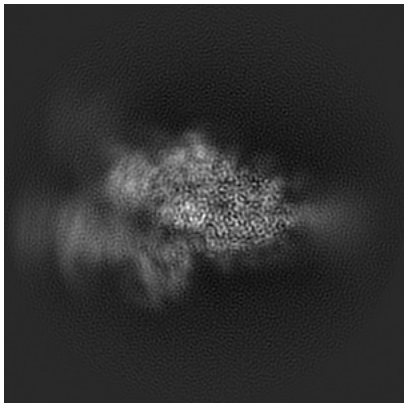
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

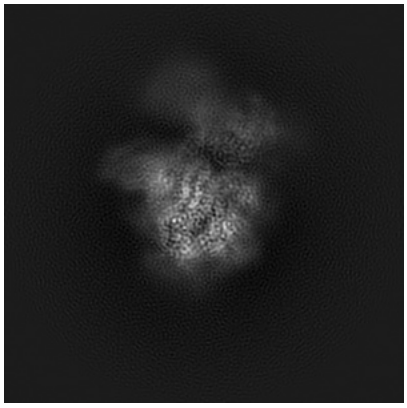
6.1.1 Primary map



X



Y

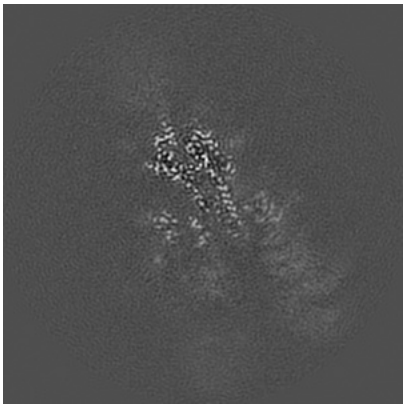


Z

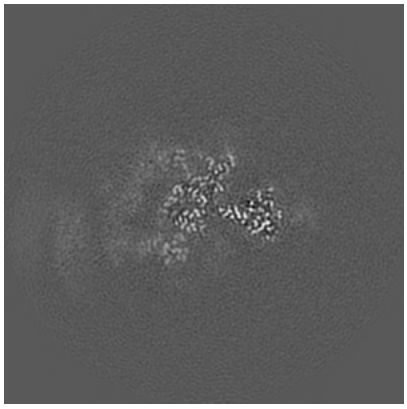
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

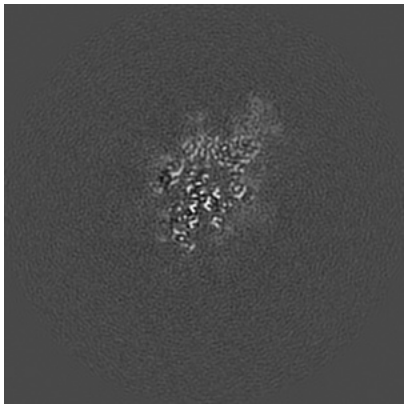
6.2.1 Primary map



X Index: 144



Y Index: 144

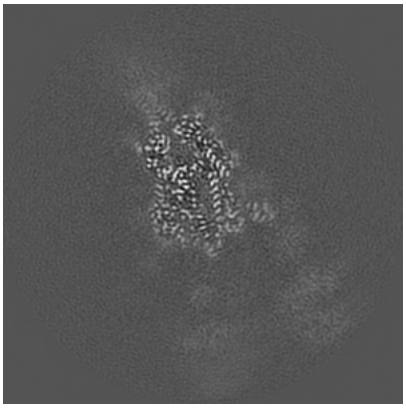


Z Index: 144

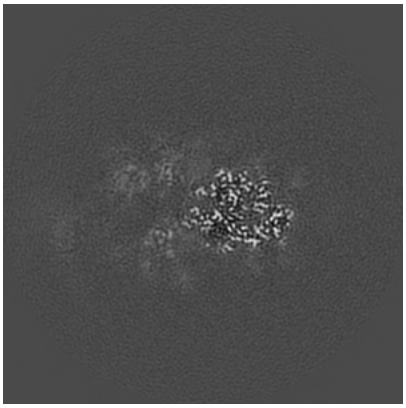
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

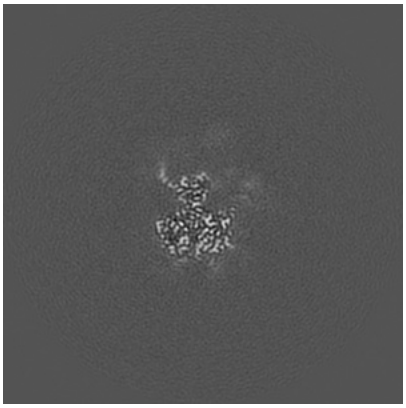
6.3.1 Primary map



X Index: 132



Y Index: 133

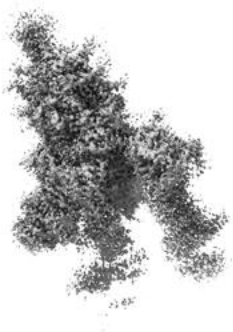


Z Index: 167

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

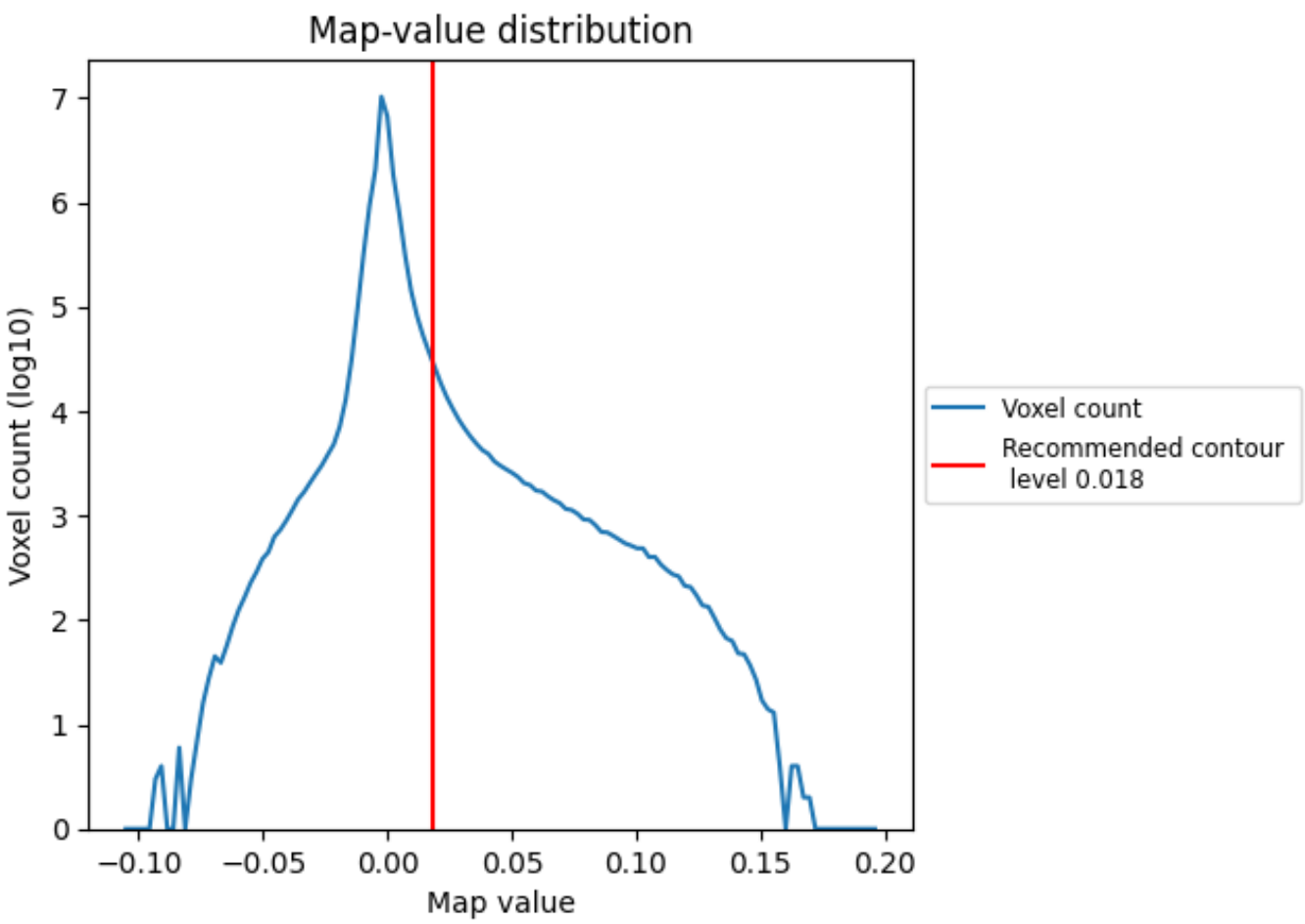
6.5 Mask visualisation (i)

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

7 Map analysis (i)

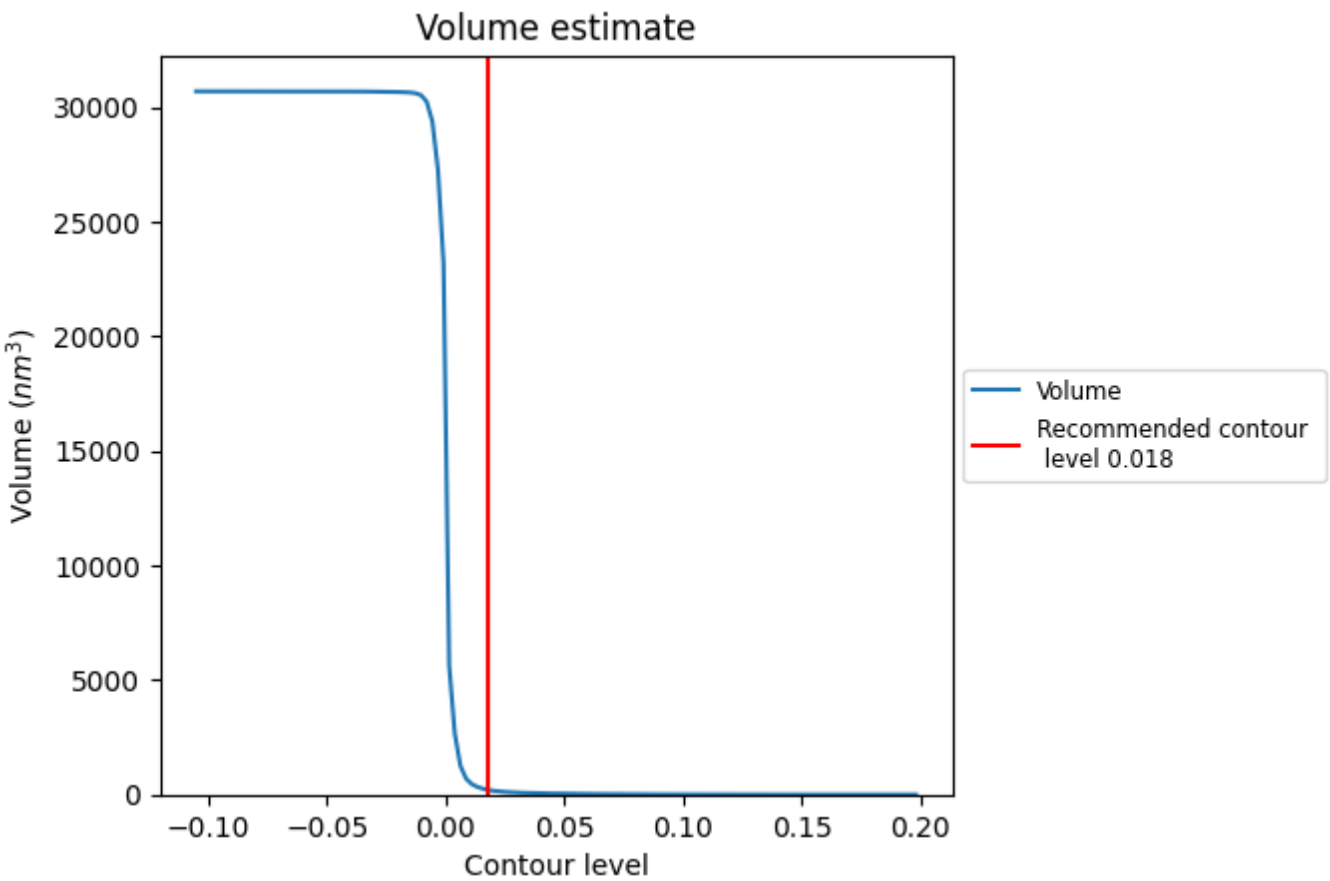
This section contains the results of statistical analysis of the map.

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.

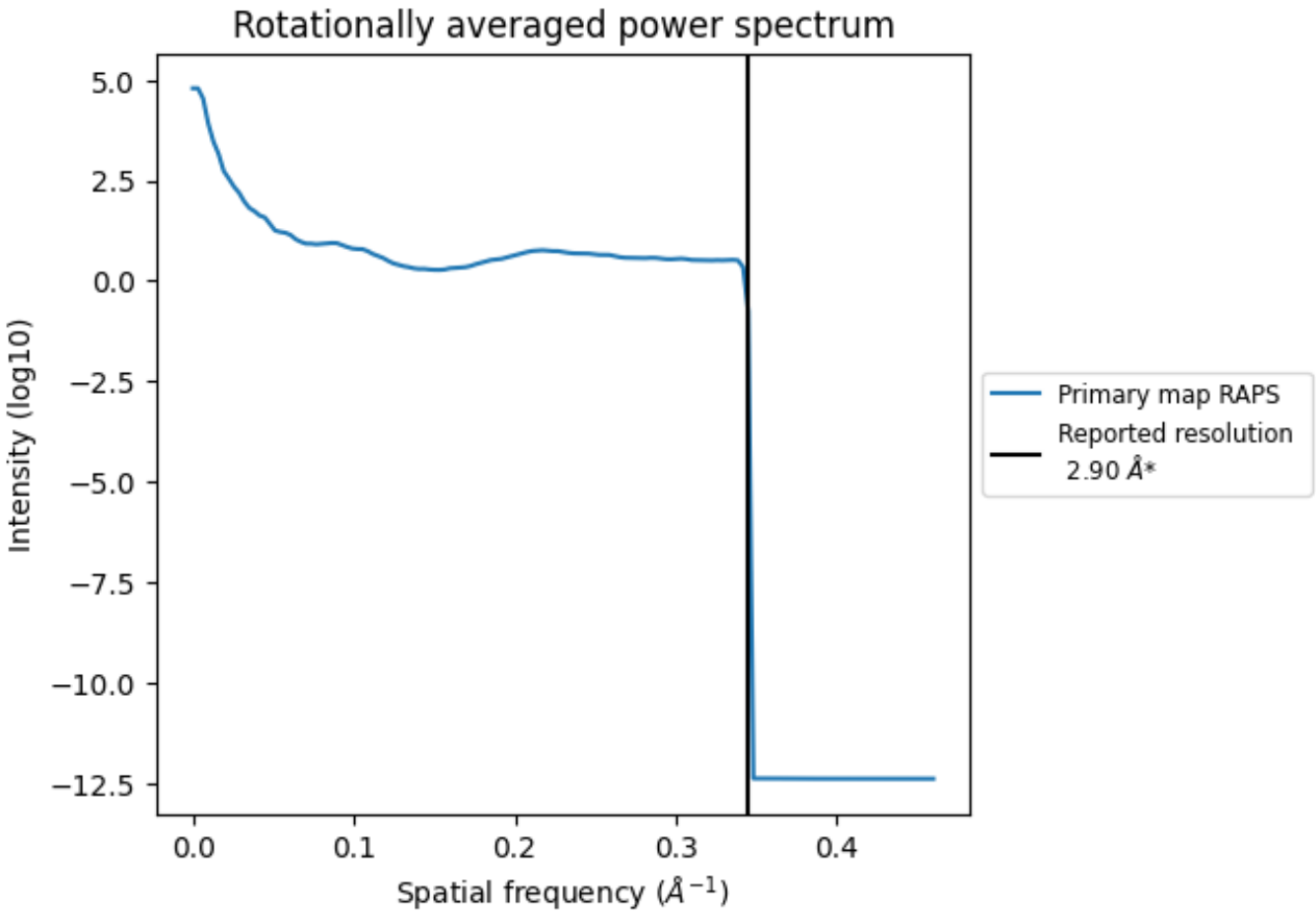
7.2 Volume estimate (i)



The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 184 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 0.345 Å^{-1}

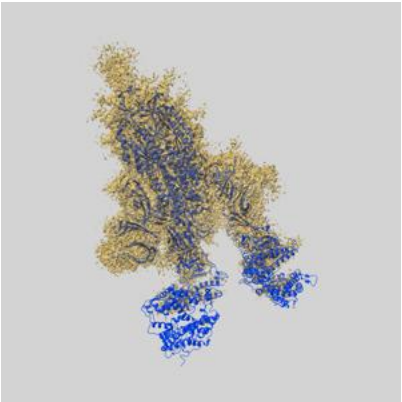
8 Fourier-Shell correlation (i)

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

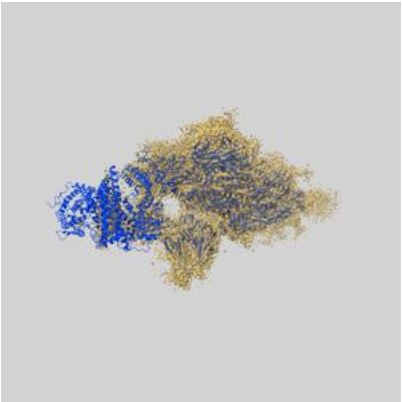
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30899 and PDB model 7DX8. Per-residue inclusion information can be found in section 3 on page 11.

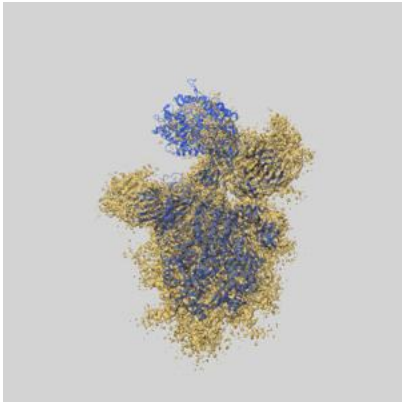
9.1 Map-model overlay (i)



X



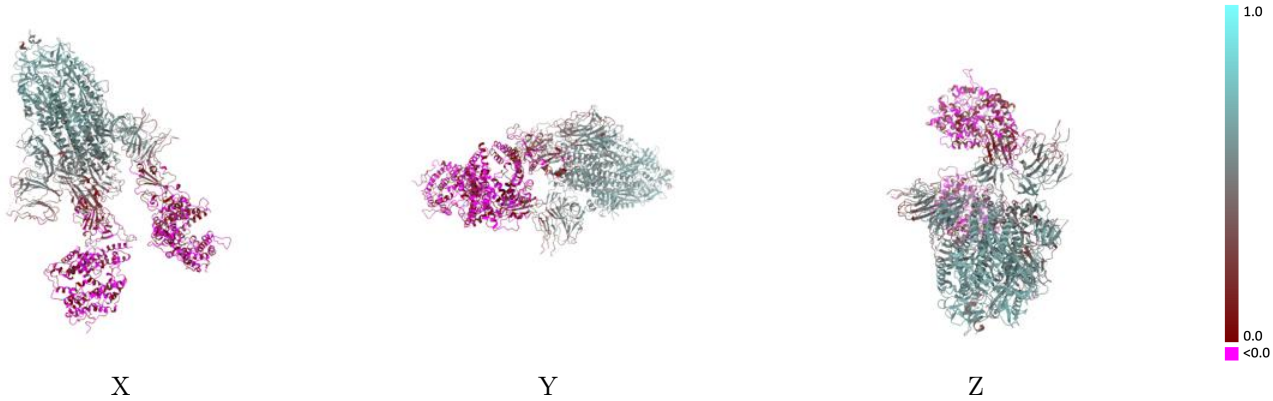
Y



Z

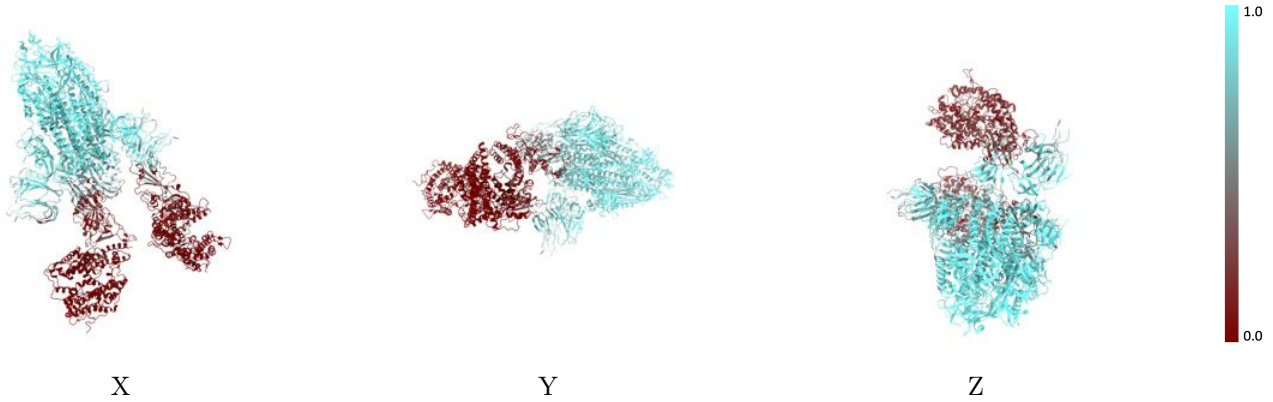
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



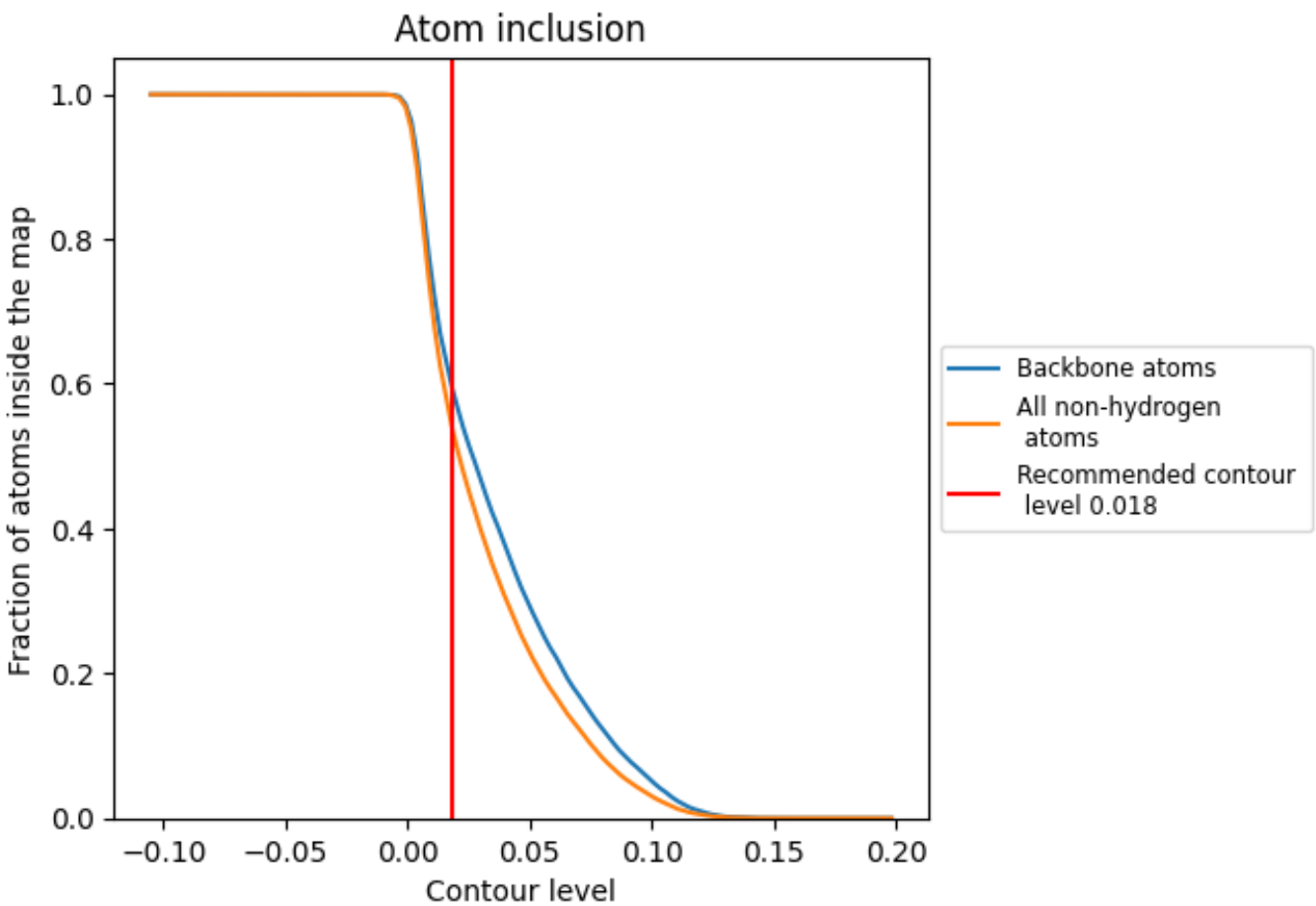
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 54% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5440	0.3260
A	0.7549	0.4550
B	0.7953	0.4820
C	0.7388	0.4400
D	0.0272	0.0150
E	0.0130	0.0070
F	0.5000	0.2070
G	0.2857	0.2920
H	0.9286	0.5270
I	0.8214	0.3920
J	0.6786	0.4650
K	0.8571	0.4920
L	0.7857	0.3800
M	0.4286	0.1450
N	0.1071	0.0750
O	0.6429	0.2710
P	0.8929	0.4990
Q	0.7857	0.3950
R	0.7500	0.4590
S	0.7500	0.3730
T	0.4286	0.2830
U	0.0714	-0.0220
V	0.6429	0.3330
W	0.8571	0.5040
X	0.7500	0.4480
Y	0.6429	0.3680
Z	0.8214	0.4550
a	0.7500	0.4460
b	0.0357	0.0860
c	0.0000	-0.0140
d	0.0000	0.0290
e	0.0000	0.0820
f	0.0000	-0.0280
g	0.0000	-0.0920
h	0.0000	0.0400

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.0000	0.1070
j	0.0000	-0.0520
k	0.0000	0.0290