wwPDB EM Validation Summary Report (i)

Nov 21, 2022 – 02:30 PM JST

PDB ID	:	7CZY
EMDB ID	:	EMD-30521
Title	:	S protein of SARS-CoV-2 in complex bound with P5A-2F11_2B
Authors	:	Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Zhou, Q.
Deposited on	:	2020-09-09
Resolution	:	3.30 Å(reported)

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

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

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

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

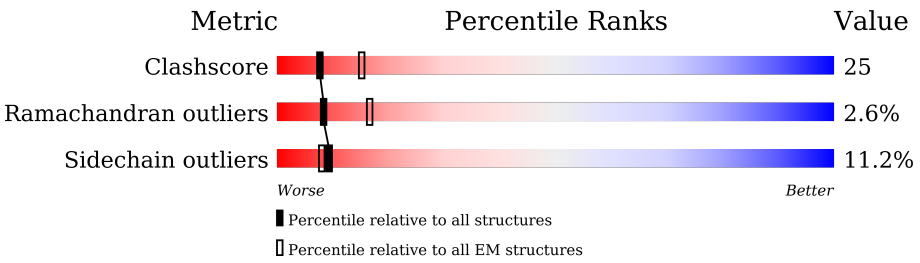
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	21% 56% 19% • 22%
1	B	1283	7% 58% 17% • 23%
1	C	1283	19% 57% 19% • 22%
2	H	452	49% 23% 21% 5% • 50%
2	J	452	50% 23% 21% 5% • 50%
3	K	220	100% 49% 38% 10% •
3	N	220	100% 48% 38% 10% •
4	D	2	100%

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

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31186 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	1006	7863	5019	1308	1500	36	0	0
1	B	982	7696	4920	1279	1462	35	0	0
1	C	1004	7853	5014	1307	1496	36	0	0

There are 36 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_2B,Epididymis luminal protein 214,Epididymis luminal protein 214.

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0

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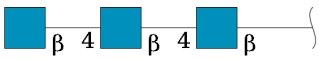
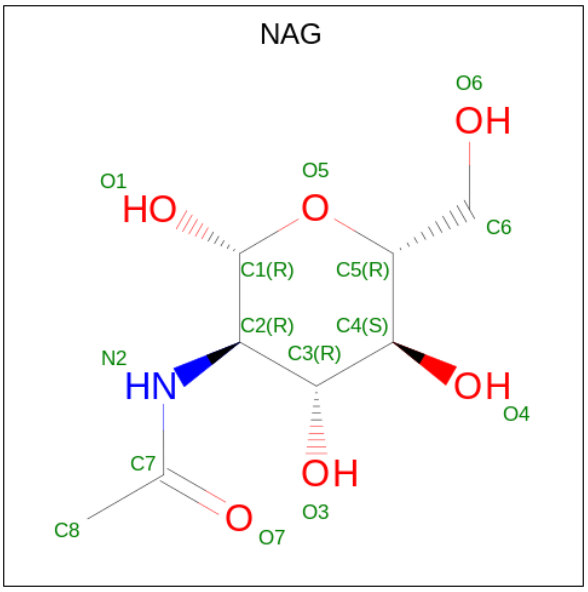
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	2	28	16	2	10	0	0
4	F	2	28	16	2	10	0	0
4	G	2	28	16	2	10	0	0
4	I	2	28	16	2	10	0	0
4	L	2	28	16	2	10	0	0
4	M	2	28	16	2	10	0	0
4	O	2	28	16	2	10	0	0
4	P	2	28	16	2	10	0	0
4	Q	2	28	16	2	10	0	0
4	R	2	28	16	2	10	0	0
4	S	2	28	16	2	10	0	0
4	T	2	28	16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

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	c	3	42	24	3	15	0	0
5	d	3	42	24	3	15	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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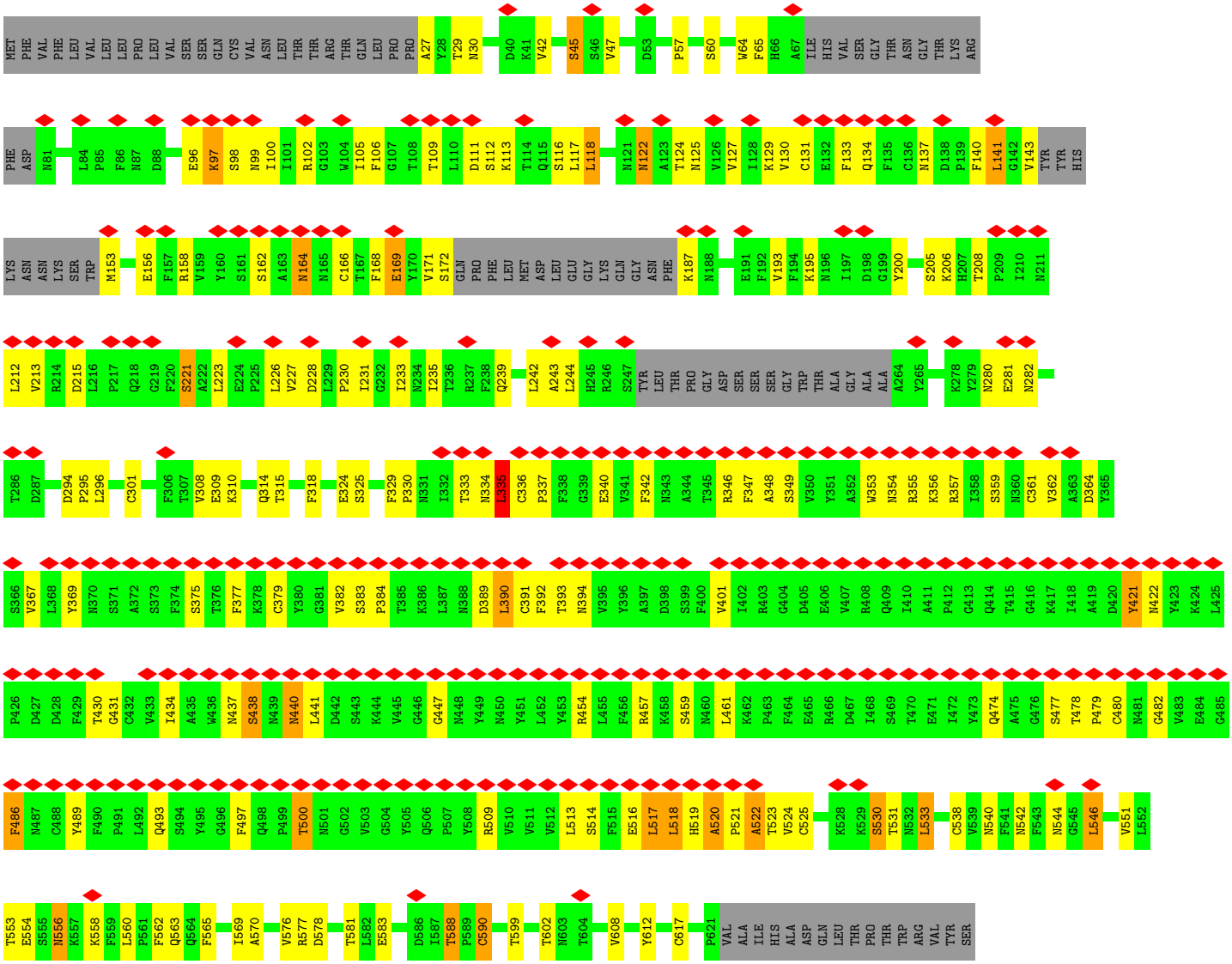
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	126	72	9	45	0
			Total	C	N	O	
6	A	1	126	72	9	45	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	B	1	154	88	11	55	0
			Total	C	N	O	
6	C	1	112	64	8	40	0
			Total	C	N	O	
6	C	1	112	64	8	40	0
			Total	C	N	O	
6	C	1	112	64	8	40	0
			Total	C	N	O	
6	C	1	112	64	8	40	0
			Total	C	N	O	
6	C	1	112	64	8	40	0
			Total	C	N	O	
6	C	1	112	64	8	40	0
			Total	C	N	O	
6	C	1	112	64	8	40	0
			Total	C	N	O	
6	C	1	112	64	8	40	0

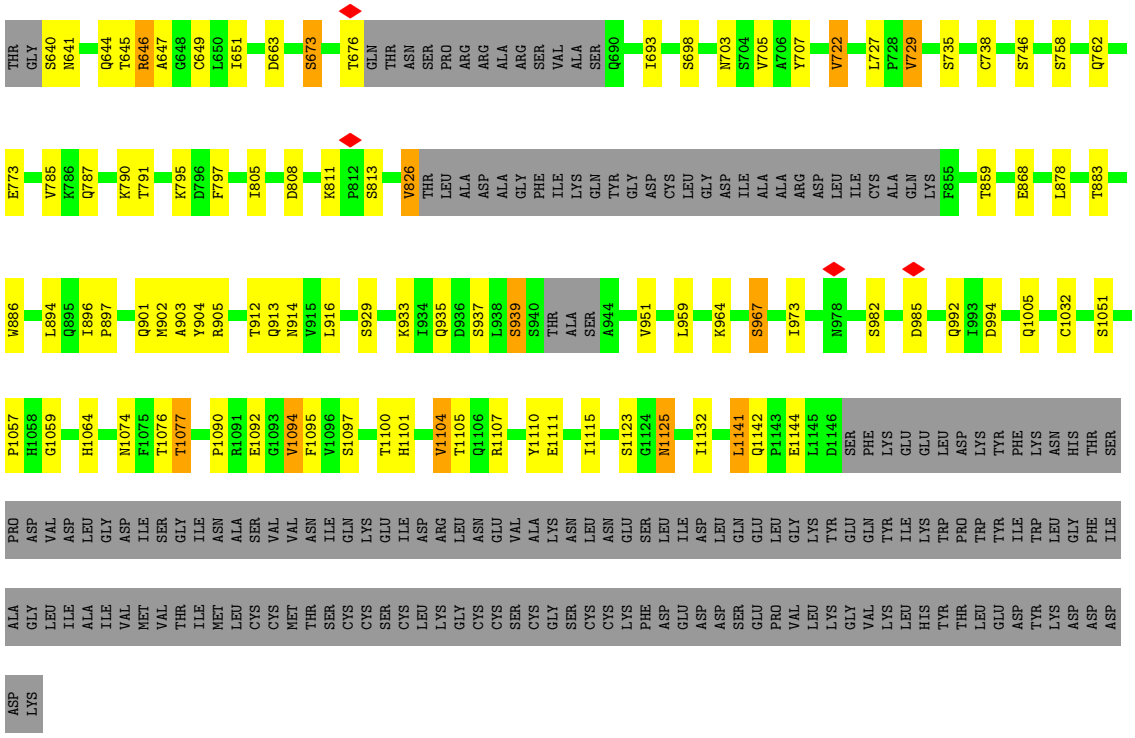
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

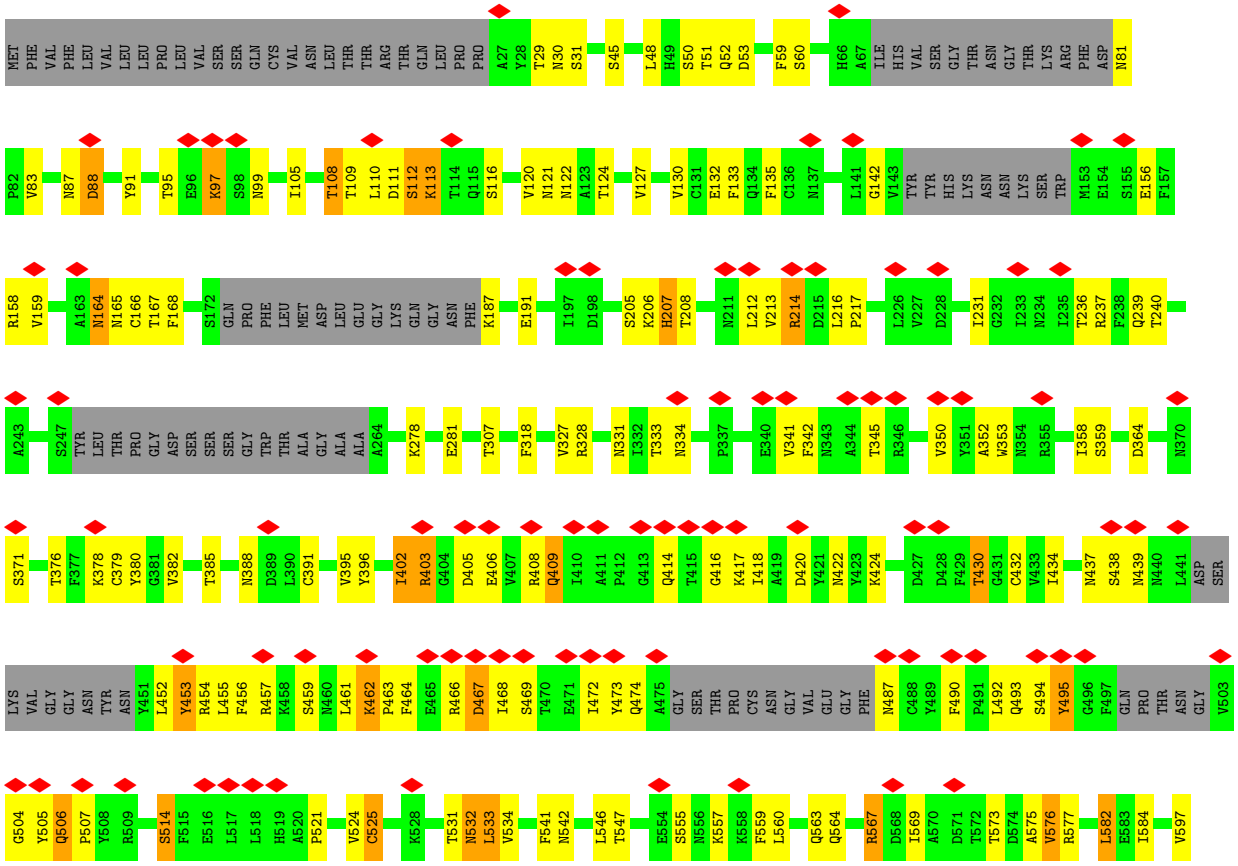
Chain A: 21% 56% 19% 22%

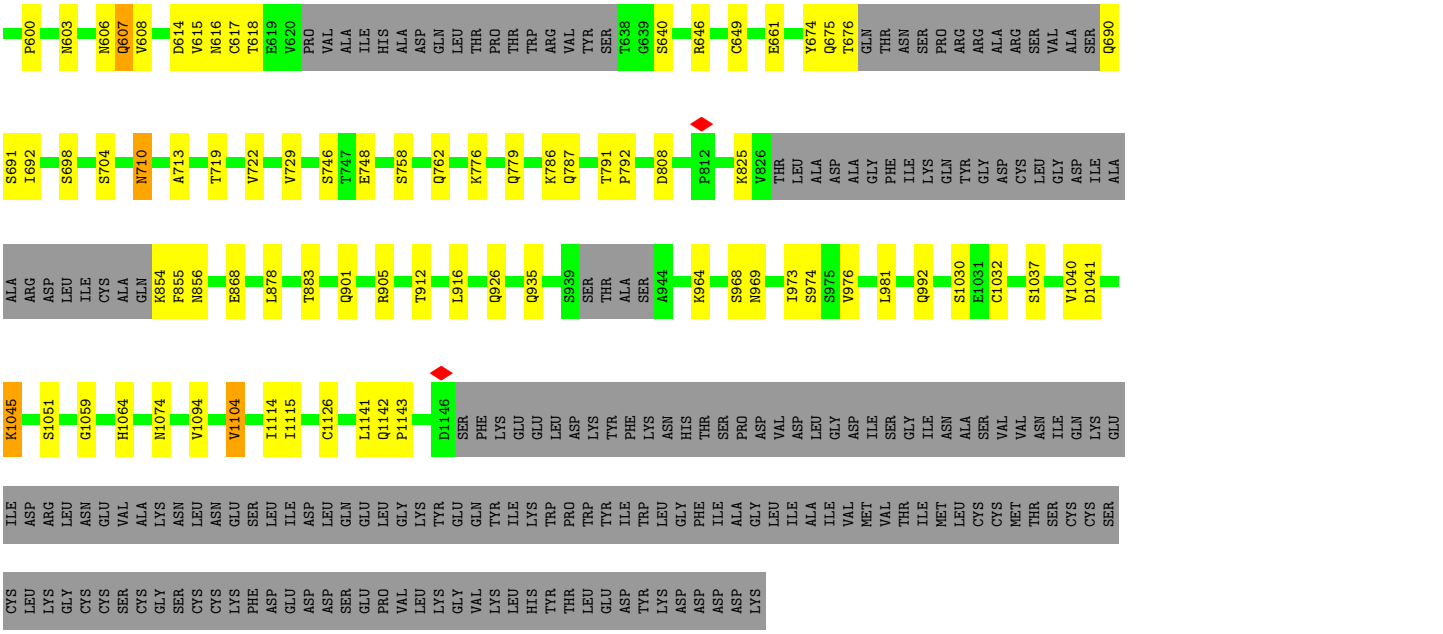




- Molecule 1: Spike glycoprotein

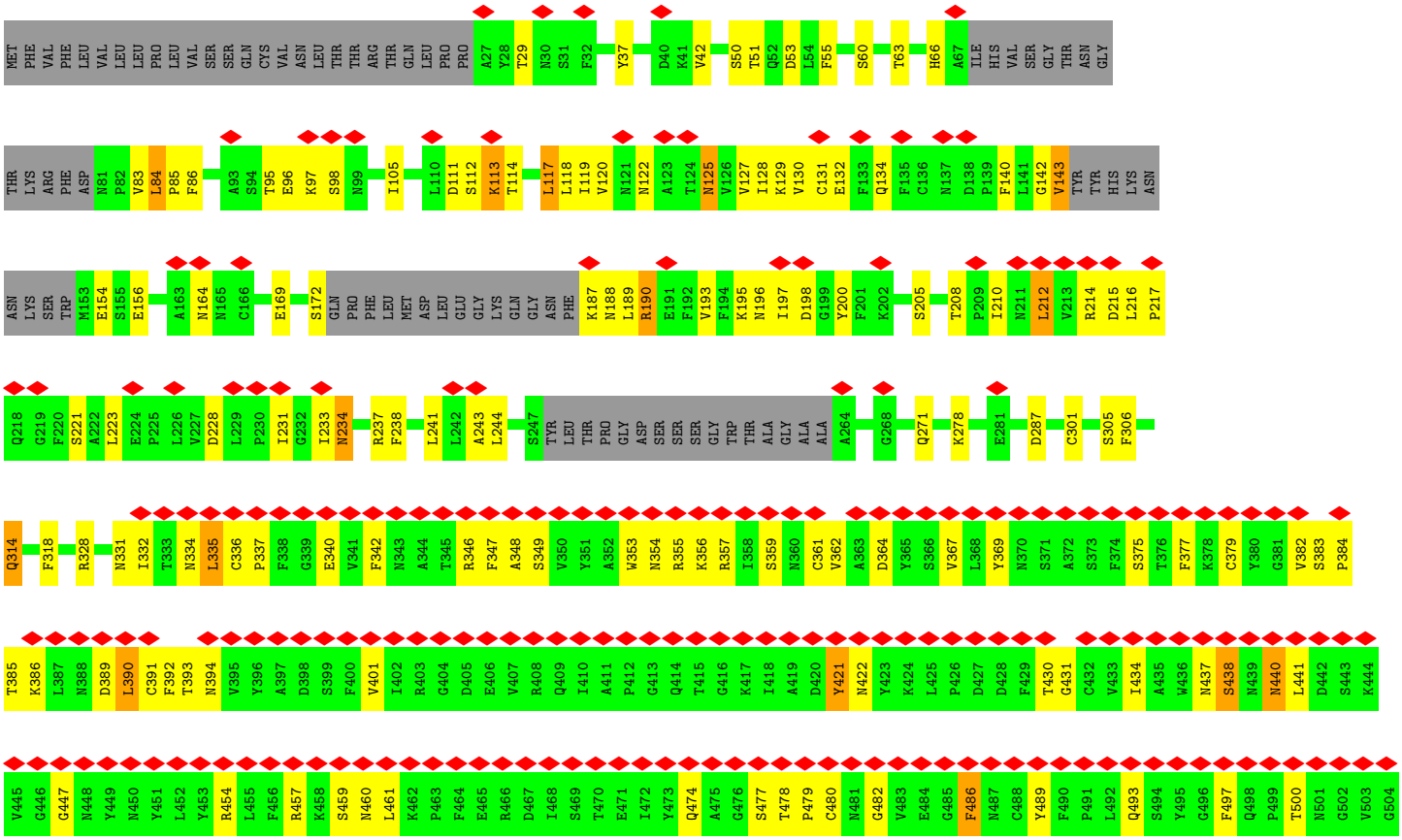
Chain B:

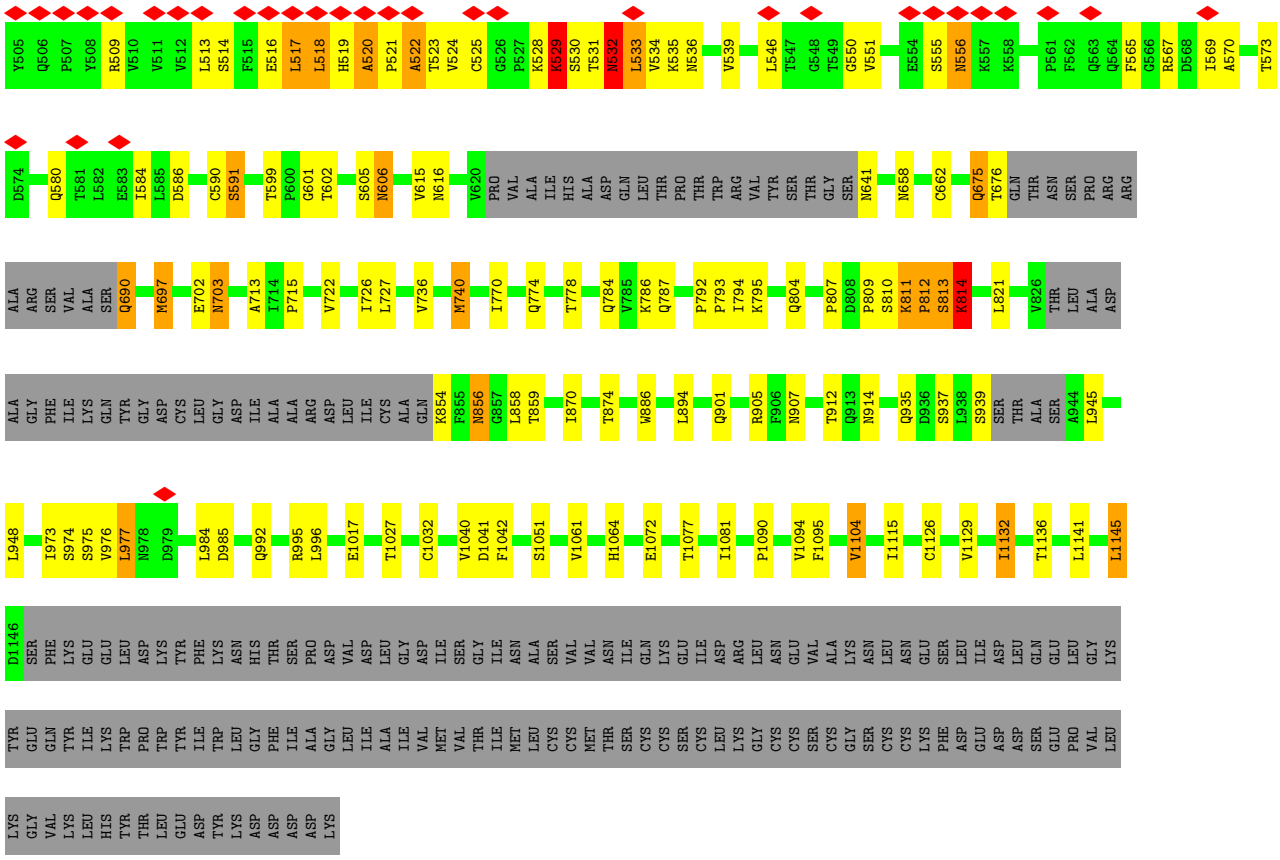




- Molecule 1: Spike glycoprotein

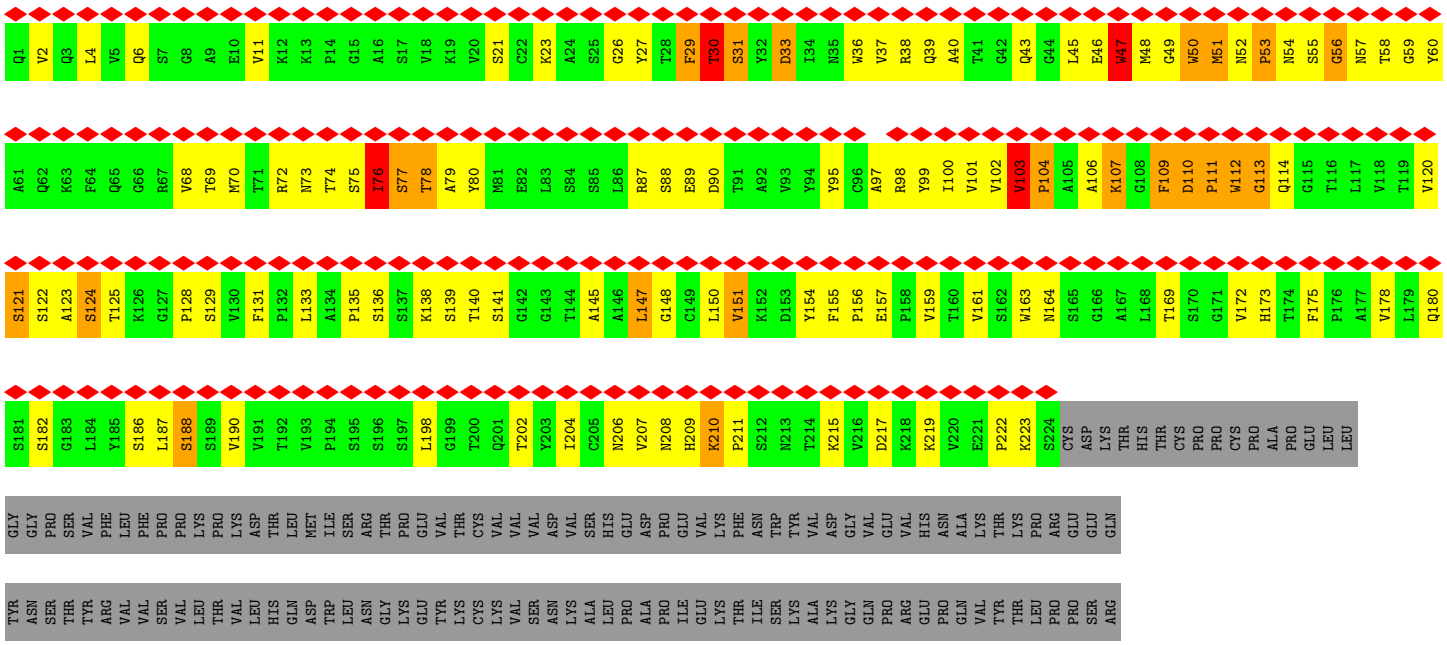
Chain C:





• Molecule 2: Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_2B,Epididymis luminal protein 214,Epididymis luminal protein 214

Chain H: 49% 23% 21% 5% • 50%



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

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

• Molecule 2: Immunoglobulin heavy variable 1-8,Immunoglobulin heavy variable 1-8,chain H of P5A-2F11_2B,Epididymis luminal protein 214,Epididymis luminal protein 214

Chain J: 50% 23% 21% 5% • 50%

Q1 V2 Q3 L4 V5 Q6 S7 G8 A9 E10 V11 K12 K13 P14 G15 A16 S17 V18 K19 V20 S21 C22 K23 A24 S25 G26 Y27 T28 F29 T30 S31 Y32 D33 I34 N35 W36 V37 R38 Q39 A40 T41 G42 Q43 G44 L45 E46 W47 M48 G49 W50 M51 N52 P53 N54 S55 G56 N57 T58 G59 Y60

A61 Q62 K63 F64 Q65 G66 R67 V68 T69 M70 T71 R72 N73 T74 S75 I76 S77 T78 A79 Y80 M81 E82 L83 S84 S85 L86 R87 S88 E89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 Y99 I100 V101 V102 V103 P104 A105 A106 K107 G108 F109 D110 P111 W112 G113 Q114 G115 T116 L117 V118 T119 V120

S121 S122 A123 S124 T125 K126 G127 P128 S129 V130 F131 P132 L133 A134 P135 S136 S137 K138 S139 T140 S141 G142 G143 T144 A145 A146 L147 G148 C149 L150 V151 K152 D153 Y154 F155 P156 E157 P158 V159 T160 V161 S162 W163 N164 S165 G166 A167 L168 T169 S170 G171 V172 H173 T174 F175 P176 A177 V178 L179 Q180

S181 S182 G183 L184 Y185 S186 L187 S188 S189 V190 V191 T192 V193 P194 S195 S196 S197 L198 G199 T200 Q201 T202 Y203 I204 C205 N206 V207 N208 H209 K210 P211 S212 N213 T214 K215 V216 D217 K218 K219 V220 E221 P222 K223 S224 CYS ASP LYS THR HIS THR CYS PRO PRO CYS PRO ALA PRO GLU LEU LEU

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

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

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

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

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

Chain K: 100% 49% 38% 10% •

D1 I2 V3 M4 T5 Q6 S7 P8 D9 S10 L11 A12 V13 S14 L15 G16 E17 R18 A19 T20 I21 N22 C23 K24 S25 S26 Q27 S28 V29 L30 Y31 S32 S33 M34 N35 K36 M37 Y38 L39 A40 W41 Y42 Q43 Q44 K45 P46 G47 Q48 P49 P50 K51 L52 L53 I54 Y55 W56 A57 S58 T59 R60

E61 S62 G63 V64 P65 D66 R67 F68 S69 G70 S71 G72 S73 G74 T75 D76 F77 T78 L79 T80 I81 S82 S83 L84 Q85 A86 E87 D88 V89 A90 V91 Y92 Y93 C94 Q95 Q96 Y97 Y98 S99 T100 P101 L102 T103 F104 G105 G106 G107 T108 K109 V110 E111 I112 K113 R114 T115 V116 A117 A118 P119 S120

V121 F122 I123 F124 P125 P126 S127 D128 E129 Q130 L131 K132 S133 G134 T135 A136 S137 V138 V139 C140 L141 L142 N143 N144 F145 Y146 P147 R148 E149 A150 K151 V152 Q153 W154 K155 V156 D157 N158 A159 L160 Q161 S162 G163 N164 S165 Q166 E167 S168 V169 T170 E171 Q172 D173 S174 K175 D176 S177 T178 Y179 S180

L181 S182 S183 T184 L185 T186 L187 S188 K189 A190 D191 Y192 E193 K194 H195 K196 V197 Y198 A199 C200 E201 V202 T203 H204 Q205 G206 L207 S208 S209 P210 V211 T212 K213 S214 F215 N216 R217 G218 E219 C220

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

Chain N: 100% 48% 38% 10%

D1 I2 V3 M4 T5 Q6 S7 P8 D9 S10 L11 A12 V13 S14 L15 G16 E17 R18 A19 T20 I21 N22 C23 K24 S25 S26 Q27 S28 V29 L30 Y31 S32 S33 M34 N35 K36 M37 Y38 L39 A40 W41 Y42 Q43 Q44 K45 P46 G47 Q48 P49 P50 K51 L52 L53 I54 Y55 W56 A57 S58 T59 R60

E61 S62 G63 V64 P65 D66 R67 F68 S69 G70 S71 G72 S73 G74 T75 D76 F77 T78 L79 T80 I81 S82 S83 L84 Q85 A86 E87 D88 V89 A90 V91 Y92 Y93 C94 Q95 Q96 Y97 Y98 S99 T100 P101 L102 T103 F104 G105 G106 G107 T108 K109 V110 E111 I112 K113 R114 T115 V116 A117 A118 P119 S120

V121 F122 I123 F124 P125 P126 S127 D128 E129 Q130 L131 K132 S133 G134 T135 A136 S137 V138 V139 C140 L141 L142 N143 N144 F145 Y146 P147 R148 E149 A150 K151 V152 Q153 W154 K155 V156 D157 N158 A159 L160 Q161 S162 G163 N164 S165 Q166 E167 S168 V169 T170 E171 Q172 D173 S174 K175 D176 S177 T178 Y179 S180

L181 S182 S183 T184 L185 T186 L187 S188 K189 A190 D191 Y192 E193 K194 H195 K196 V197 Y198 A199 C200 E201 V202 T203 H204 Q205 G206 L207 S208 S209 P210 V211 T212 K213 S214 F215 N216 R217 G218 E219 C220

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

Chain D: 100%

NAG1 NAG2

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

Chain E: 100% 100%

NAG1 NAG2

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

Chain F: 50% 50%

NAG1 NAG2

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

Chain G: 50% 50%

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

Chain I:

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

Chain L:

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

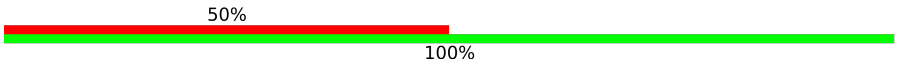
Chain M:

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

Chain O:

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

Chain P:



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

Chain Q:

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

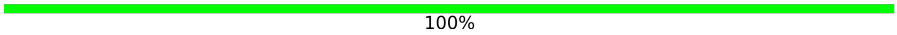
Chain R:

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

Chain S:

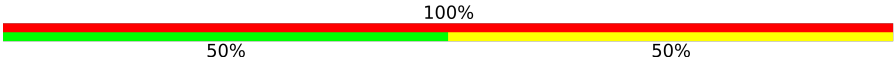
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



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

Chain U:



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

Chain V:

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

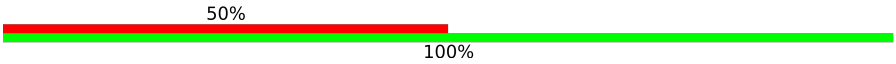
Chain W:

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

Chain X:

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

Chain Y:

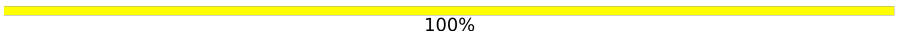


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

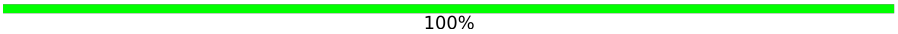
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



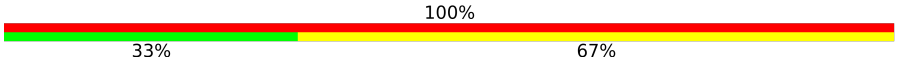
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



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

Chain c:



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

Chain d:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39337	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	0.157	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality (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	0.59	1/8039 (0.0%)	0.56	0/10936
1	B	0.49	0/7864	0.55	0/10691
1	C	0.59	0/8028	0.55	0/10919
2	H	0.36	0/1710	0.52	0/2331
2	J	0.36	0/1710	0.52	0/2331
3	K	0.46	0/1722	0.58	0/2343
3	N	0.46	0/1722	0.58	0/2343
All	All	0.53	1/30795 (0.0%)	0.55	0/41894

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	805	ILE	C-N	-5.00	1.22	1.34

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	7863	0	7656	212	0
1	B	7696	0	7514	135	0
1	C	7853	0	7652	204	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1670	0	1647	270	0
2	J	1670	0	1647	261	0
3	K	1685	0	1616	316	0
3	N	1685	0	1616	314	0
4	D	28	0	25	2	0
4	E	28	0	25	3	0
4	F	28	0	25	0	0
4	G	28	0	25	1	0
4	I	28	0	25	1	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	0	0
4	U	28	0	25	1	0
4	V	28	0	25	4	0
4	W	28	0	25	1	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	1	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
5	c	42	0	37	0	0
5	d	42	0	37	0	0
6	A	126	0	117	5	0
6	B	154	0	142	10	0
6	C	112	0	104	2	0
All	All	31186	0	30310	1558	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 25.

The worst 5 of 1558 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)
3:N:110:VAL:CG1	3:N:177:SER:HB2	1.36	1.51
3:K:110:VAL:CG1	3:K:177:SER:HB2	1.36	1.51
6:B:1410:NAG:O4	6:B:1411:NAG:C1	1.63	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:110:VAL:HG11	3:N:177:SER:CB	1.51	1.41
3:K:110:VAL:HG11	3:K:177:SER:CB	1.51	1.39

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	988/1283 (77%)	891 (90%)	90 (9%)	7 (1%)	22 54
1	B	958/1283 (75%)	868 (91%)	89 (9%)	1 (0%)	51 81
1	C	986/1283 (77%)	885 (90%)	86 (9%)	15 (2%)	10 38
2	H	222/452 (49%)	175 (79%)	31 (14%)	16 (7%)	1 7
2	J	222/452 (49%)	175 (79%)	31 (14%)	16 (7%)	1 7
3	K	218/220 (99%)	162 (74%)	33 (15%)	23 (11%)	0 3
3	N	218/220 (99%)	162 (74%)	33 (15%)	23 (11%)	0 3
All	All	3812/5193 (73%)	3318 (87%)	393 (10%)	101 (3%)	8 27

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	LEU
1	C	518	LEU
1	C	814	LYS
2	H	55	SER
2	H	103	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	881/1122 (78%)	783 (89%)	98 (11%)	6	23
1	B	862/1122 (77%)	762 (88%)	100 (12%)	5	22
1	C	879/1122 (78%)	787 (90%)	92 (10%)	7	25
2	H	188/399 (47%)	164 (87%)	24 (13%)	4	18
2	J	188/399 (47%)	164 (87%)	24 (13%)	4	18
3	K	191/194 (98%)	170 (89%)	21 (11%)	6	24
3	N	191/194 (98%)	170 (89%)	21 (11%)	6	24
All	All	3380/4552 (74%)	3000 (89%)	380 (11%)	9	23

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	355	ARG
1	C	1129	VAL
1	C	438	SER
1	C	602	THR
2	H	109	PHE

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

Mol	Chain	Res	Type
1	C	271	GLN
1	C	675	GLN
1	C	321	GLN
1	C	493	GLN
1	C	804	GLN

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)

48 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.51	0	17,19,21	0.51	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.59	0
4	NAG	E	1	4,1	14,14,15	0.55	0	17,19,21	0.57	0
4	NAG	E	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	F	1	4,1	14,14,15	0.34	0	17,19,21	0.63	1 (5%)
4	NAG	F	2	4	14,14,15	0.53	0	17,19,21	0.46	0
4	NAG	G	1	4,1	14,14,15	0.39	0	17,19,21	0.72	0
4	NAG	G	2	4	14,14,15	0.31	0	17,19,21	1.31	2 (11%)
4	NAG	I	1	4,1	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
4	NAG	I	2	4	14,14,15	0.40	0	17,19,21	1.40	3 (17%)
4	NAG	L	1	4,1	14,14,15	0.71	1 (7%)	17,19,21	0.66	0
4	NAG	L	2	4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	M	1	4,1	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
4	NAG	M	2	4	14,14,15	0.14	0	17,19,21	0.46	0
4	NAG	O	1	4,1	14,14,15	0.32	0	17,19,21	0.41	0
4	NAG	O	2	4	14,14,15	0.17	0	17,19,21	0.47	0
4	NAG	P	1	4,1	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	P	2	4	14,14,15	0.37	0	17,19,21	0.37	0
4	NAG	Q	1	4,1	14,14,15	0.35	0	17,19,21	1.11	1 (5%)
4	NAG	Q	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	R	1	4,1	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
4	NAG	R	2	4	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	S	1	4,1	14,14,15	0.76	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	S	2	4	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
4	NAG	T	1	4,1	14,14,15	0.27	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	T	2	4	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	U	1	4,1	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	U	2	4	14,14,15	0.31	0	17,19,21	0.61	0
4	NAG	V	1	4,1	14,14,15	0.56	0	17,19,21	0.56	0
4	NAG	V	2	4	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	W	1	4,1	14,14,15	0.23	0	17,19,21	1.35	1 (5%)
4	NAG	W	2	4	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	X	1	4,1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
4	NAG	X	2	4	14,14,15	0.38	0	17,19,21	0.46	0
4	NAG	Y	1	4,1	14,14,15	0.34	0	17,19,21	0.42	0
4	NAG	Y	2	4	14,14,15	0.19	0	17,19,21	0.73	0
4	NAG	Z	1	4,1	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	Z	2	4	14,14,15	0.57	0	17,19,21	1.31	1 (5%)
4	NAG	a	1	4,1	14,14,15	0.66	1 (7%)	17,19,21	0.43	0
4	NAG	a	2	4	14,14,15	0.31	0	17,19,21	1.36	2 (11%)
4	NAG	b	1	4,1	14,14,15	0.42	0	17,19,21	0.44	0
4	NAG	b	2	4	14,14,15	0.24	0	17,19,21	0.48	0
5	NAG	c	1	5,2	14,14,15	0.41	0	17,19,21	1.17	1 (5%)
5	NAG	c	2	5	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
5	NAG	c	3	5	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	d	1	5,2	14,14,15	0.41	0	17,19,21	1.18	1 (5%)
5	NAG	d	2	5	14,14,15	0.29	0	17,19,21	0.99	1 (5%)
5	NAG	d	3	5	14,14,15	0.29	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	O5-C1	-2.77	1.39	1.43
4	L	1	NAG	O5-C1	-2.59	1.39	1.43
4	I	1	NAG	O5-C1	-2.32	1.40	1.43
4	a	1	NAG	O5-C1	-2.18	1.40	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	W	1	NAG	C2-N2-C7	4.65	129.52	122.90
4	a	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	I	2	NAG	C2-N2-C7	4.34	129.09	122.90
4	Z	2	NAG	C2-N2-C7	4.33	129.07	122.90
4	G	2	NAG	C2-N2-C7	4.32	129.06	122.90

There are no chirality outliers.

5 of 103 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	c	2	NAG	C8-C7-N2-C2
5	c	2	NAG	O7-C7-N2-C2
5	d	2	NAG	C8-C7-N2-C2
5	d	2	NAG	O7-C7-N2-C2
4	W	2	NAG	O5-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0
4	E	2	NAG	2	0
4	O	1	NAG	1	0
4	W	1	NAG	1	0
4	E	1	NAG	3	0

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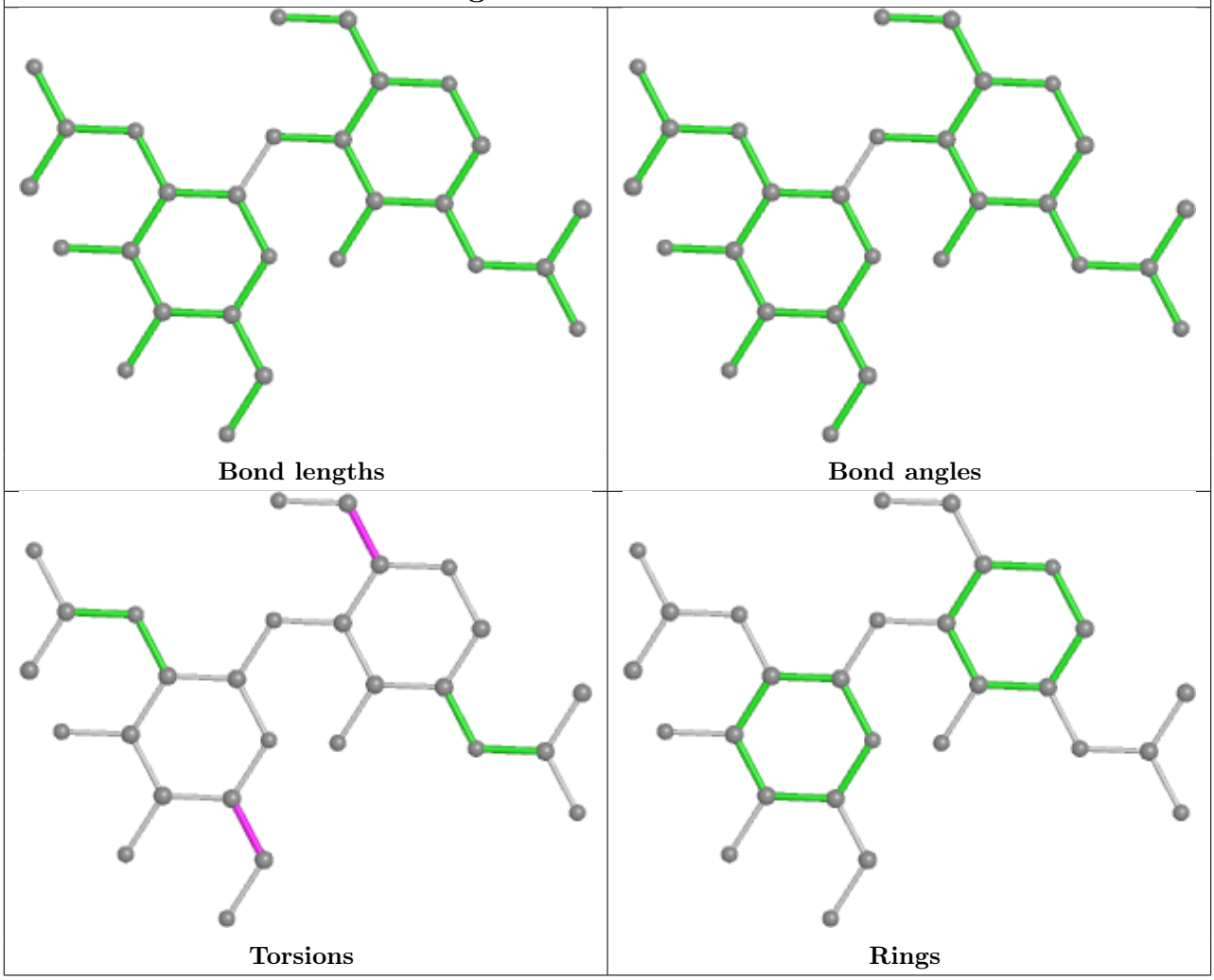
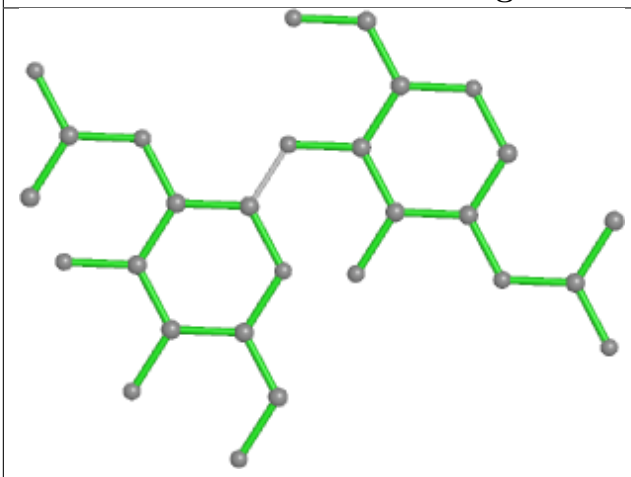
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	V	1	NAG	4	0
4	S	1	NAG	1	0
4	D	2	NAG	2	0
4	S	2	NAG	1	0
4	Z	2	NAG	1	0
4	I	2	NAG	1	0
4	V	2	NAG	2	0
4	U	1	NAG	1	0
4	D	1	NAG	2	0

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

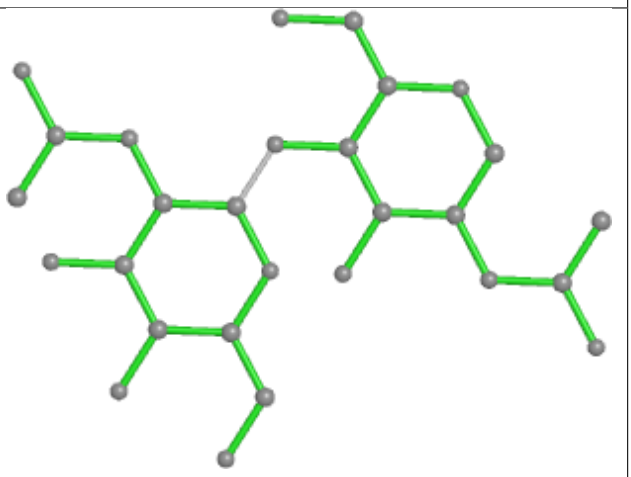
Oligosaccharide Chain D



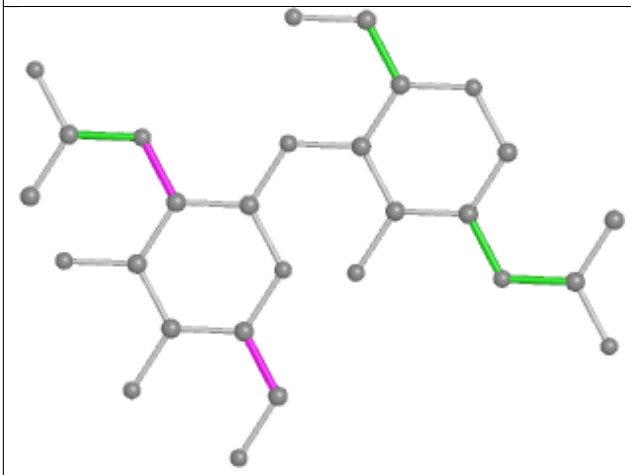
Oligosaccharide Chain E



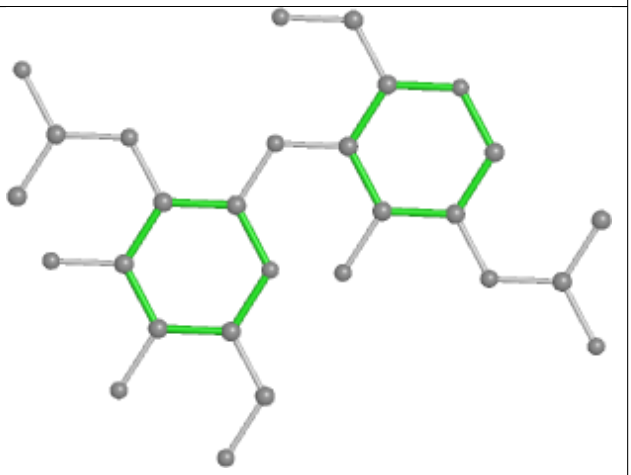
Bond lengths



Bond angles

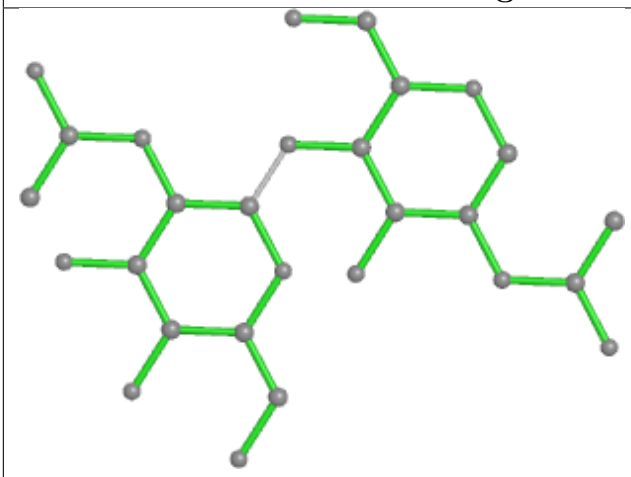


Torsions

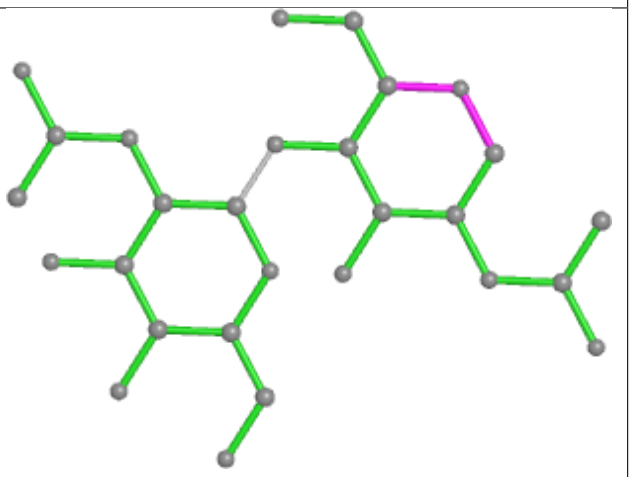


Rings

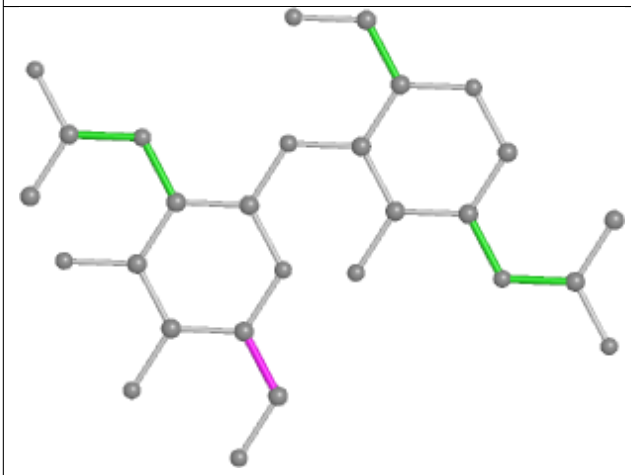
Oligosaccharide Chain F



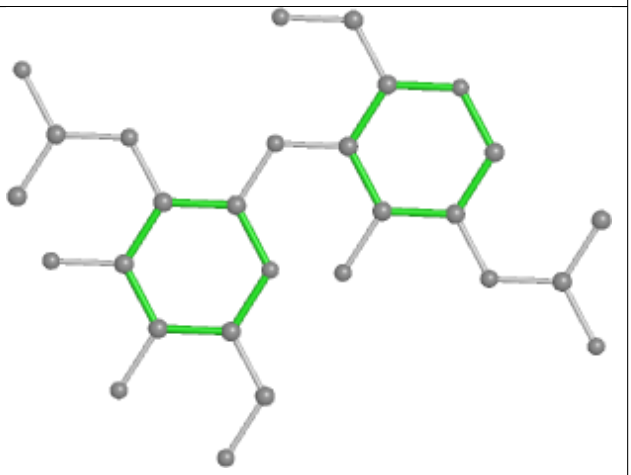
Bond lengths



Bond angles

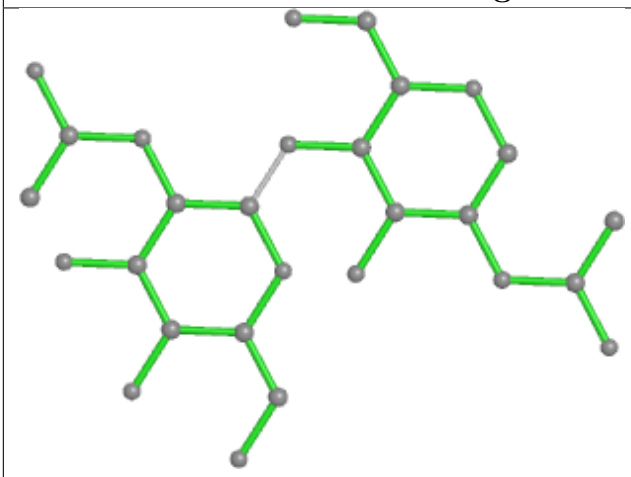


Torsions

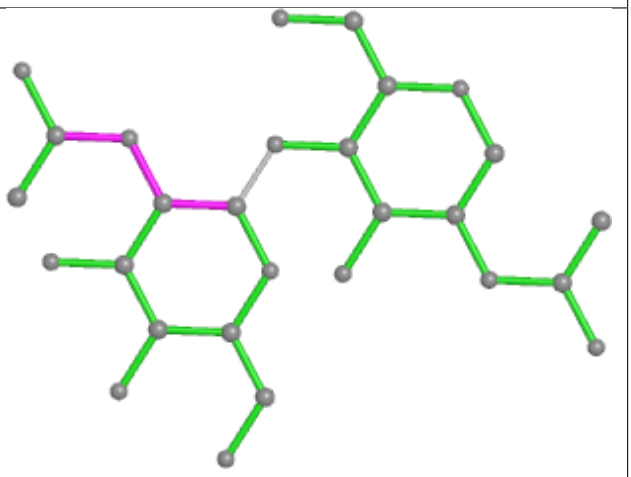


Rings

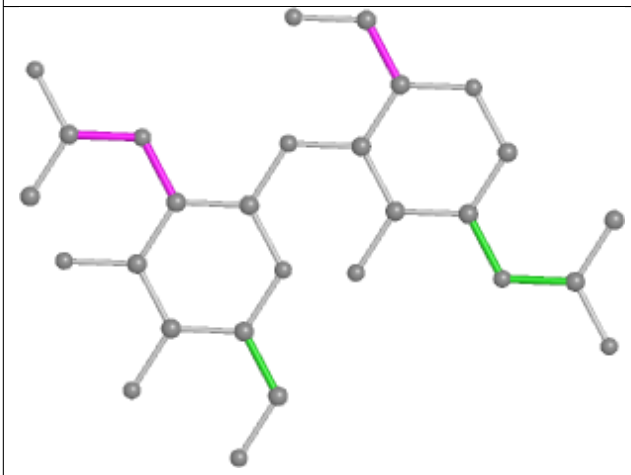
Oligosaccharide Chain G



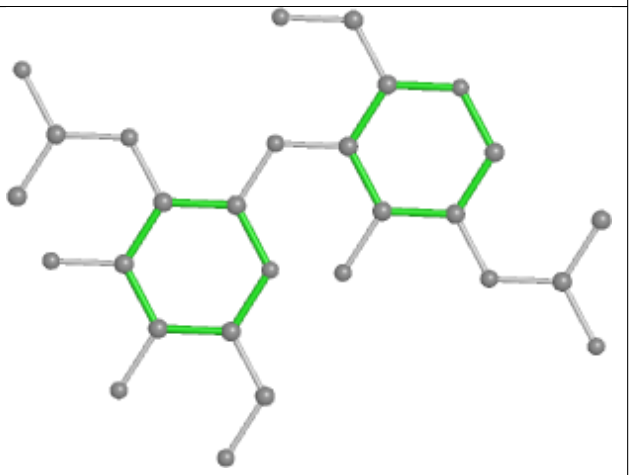
Bond lengths



Bond angles

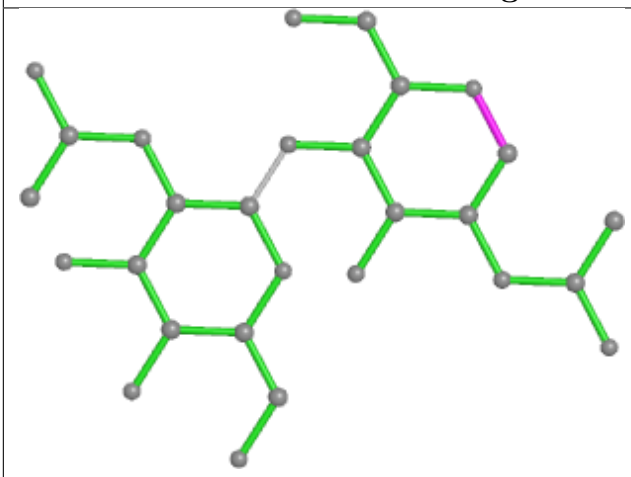


Torsions

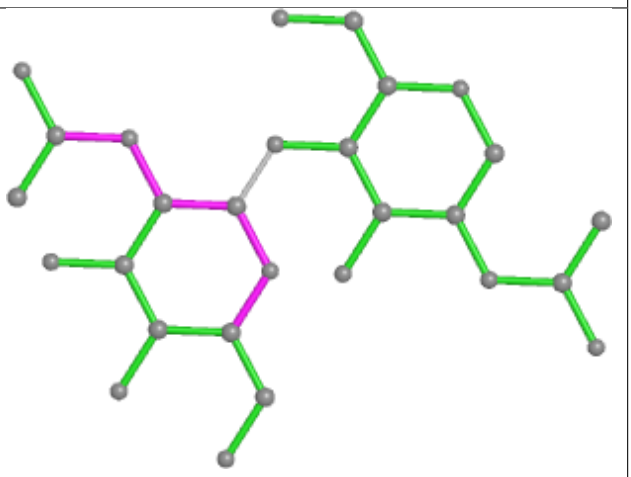


Rings

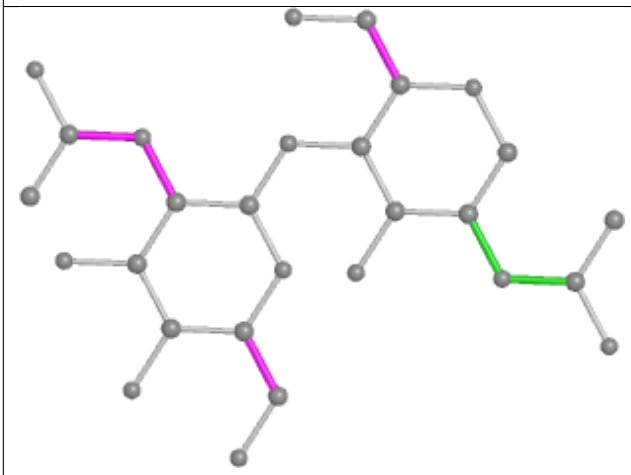
Oligosaccharide Chain I



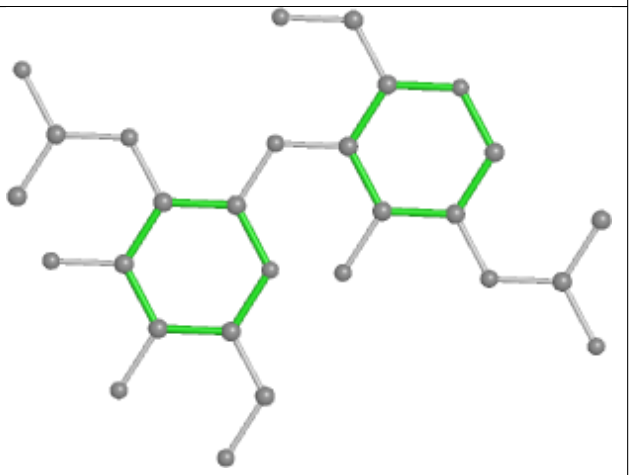
Bond lengths



Bond angles

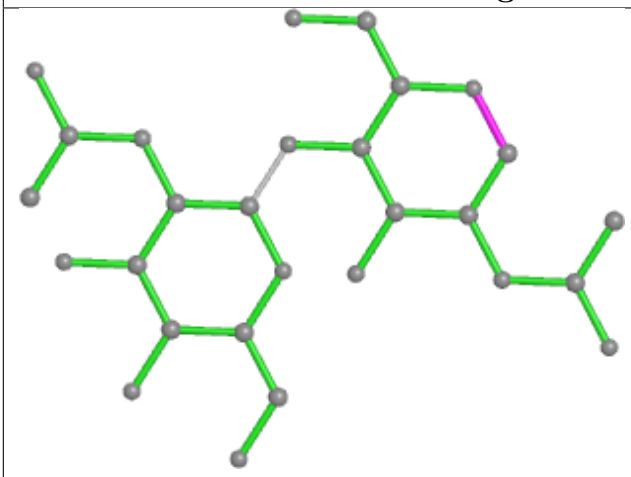


Torsions



Rings

Oligosaccharide Chain L



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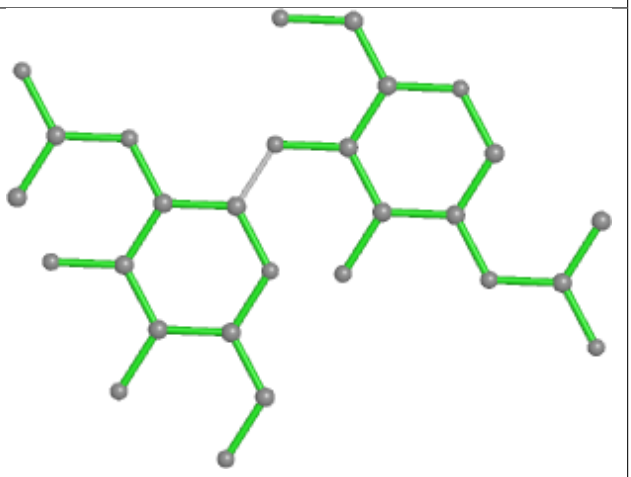

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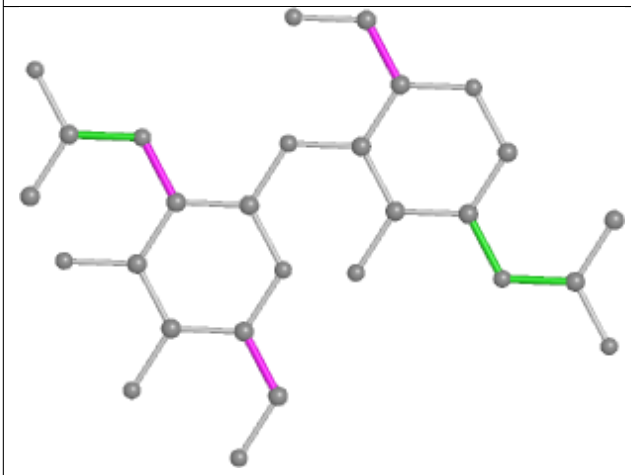

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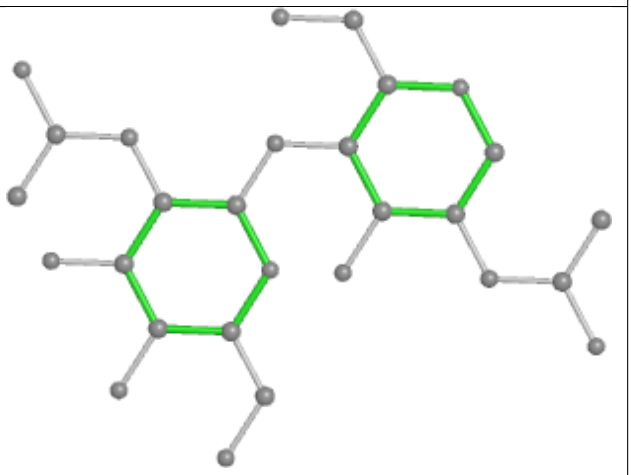
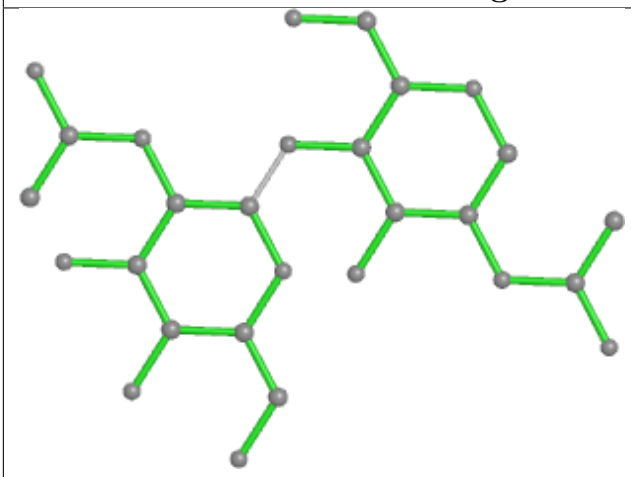


Rings

Oligosaccharide Chain M



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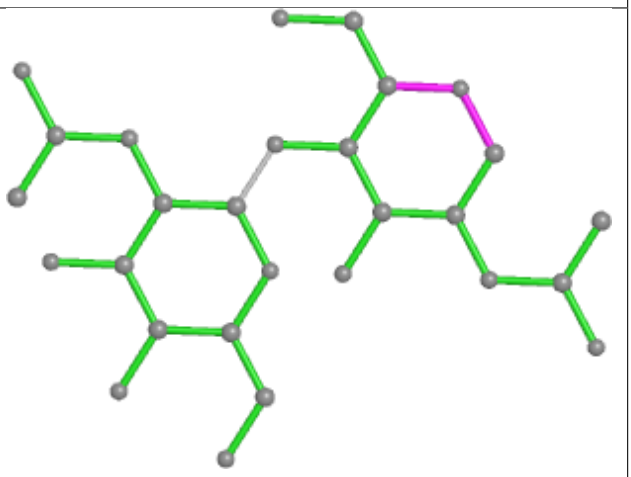
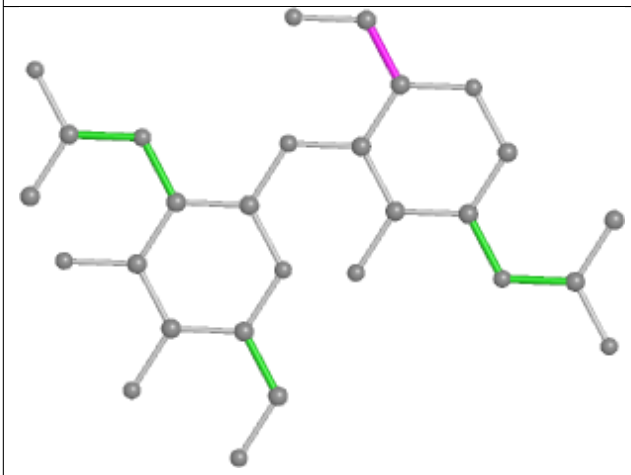


Bond angles



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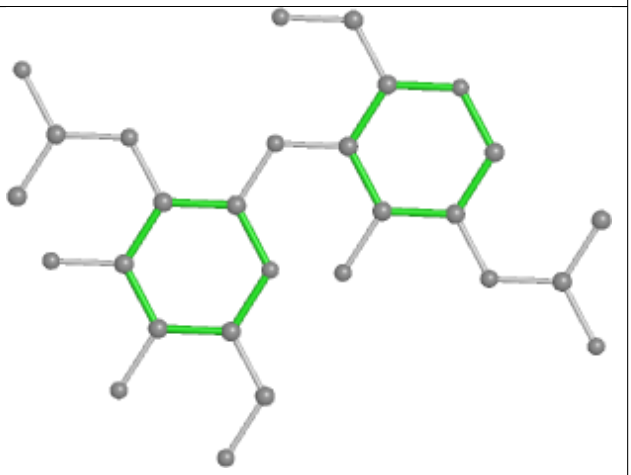
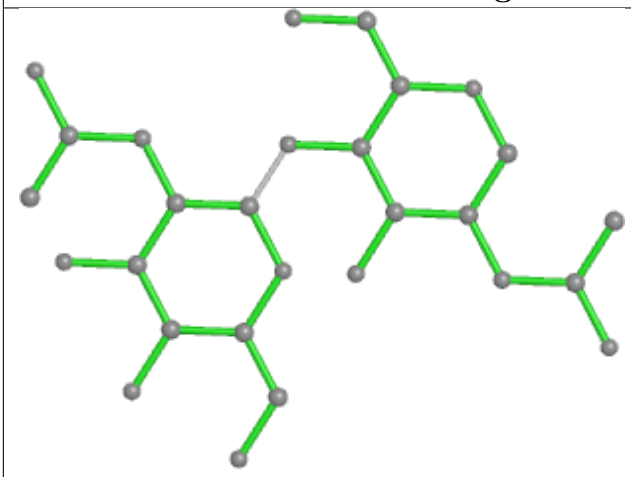


Rings

Oligosaccharide Chain O



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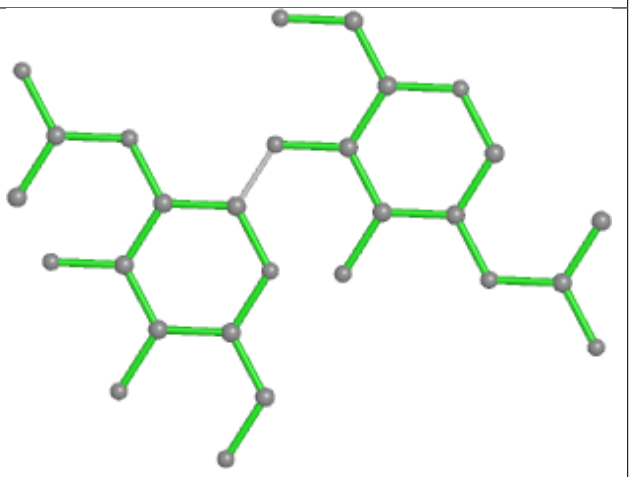

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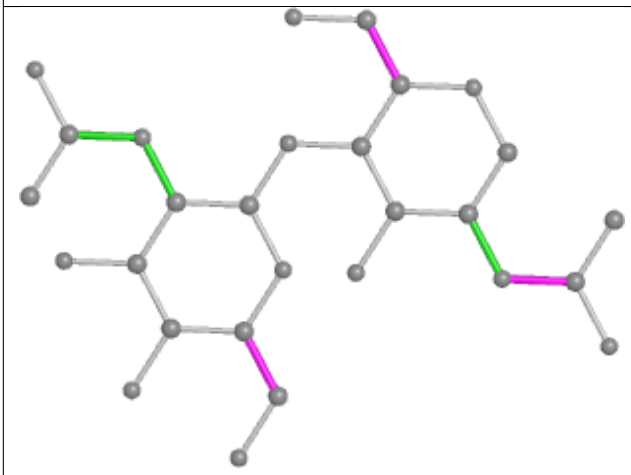

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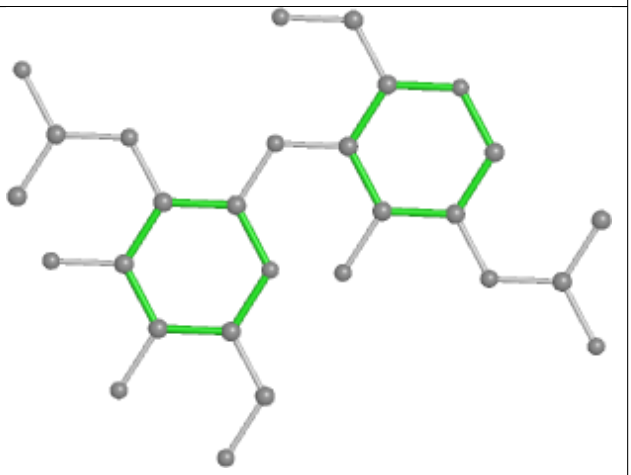
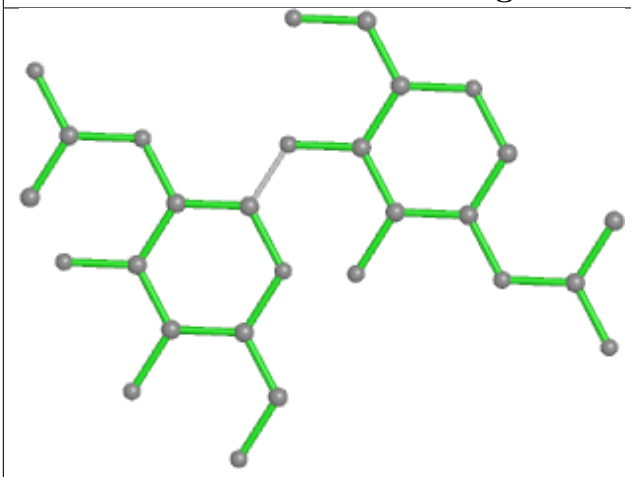


Rings

Oligosaccharide Chain P



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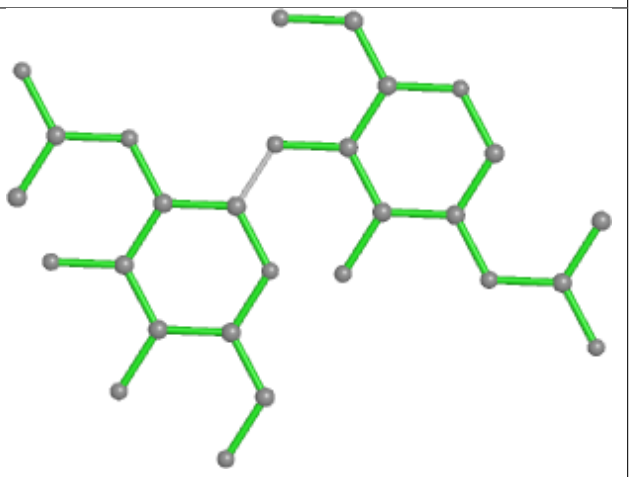
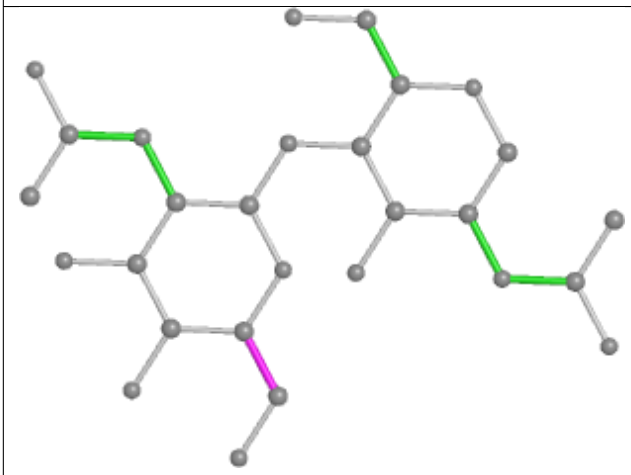
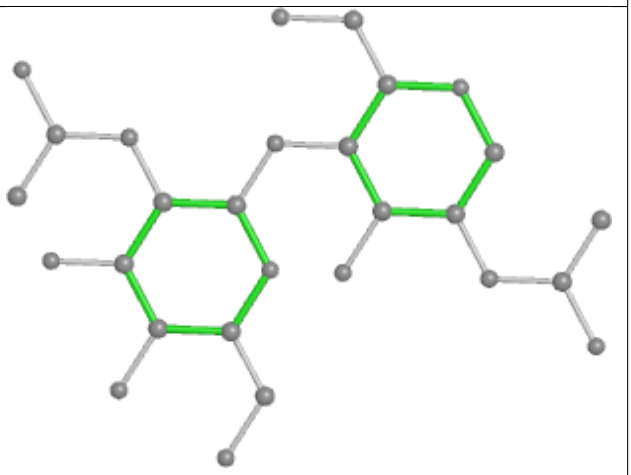


Bond angles

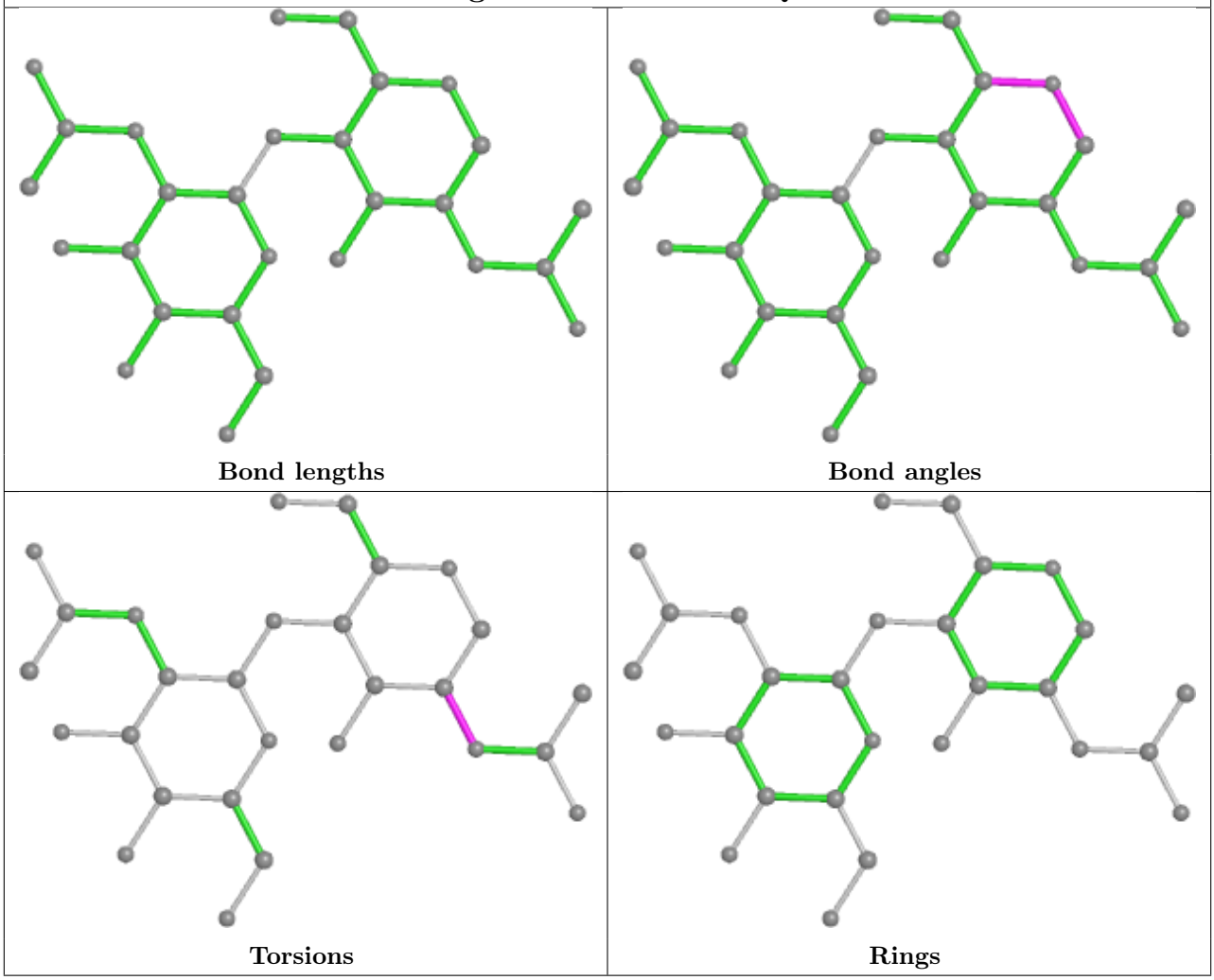


Torsions

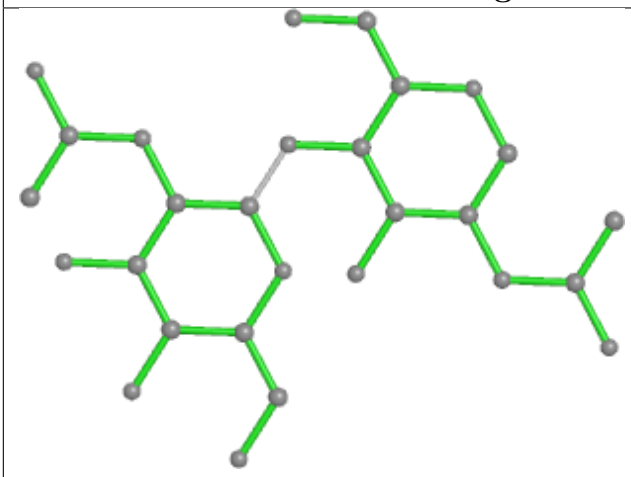


Rings

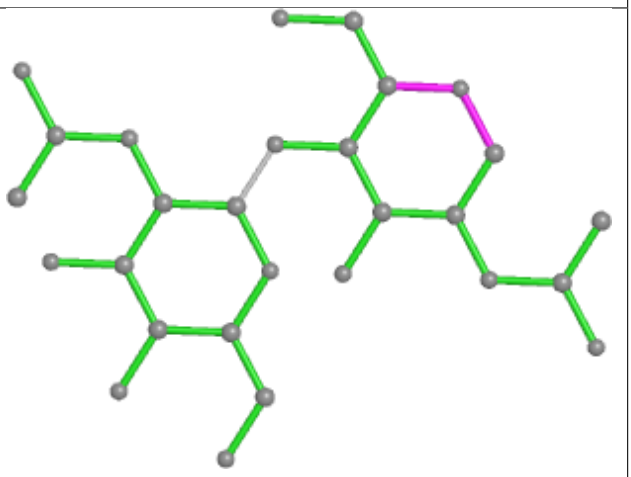
Oligosaccharide Chain Q



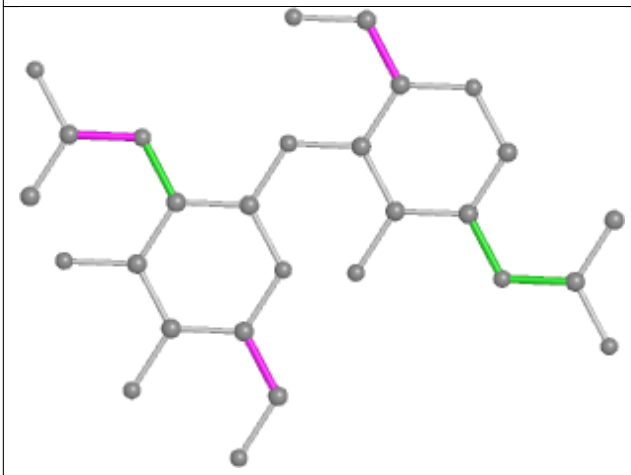
Oligosaccharide Chain R



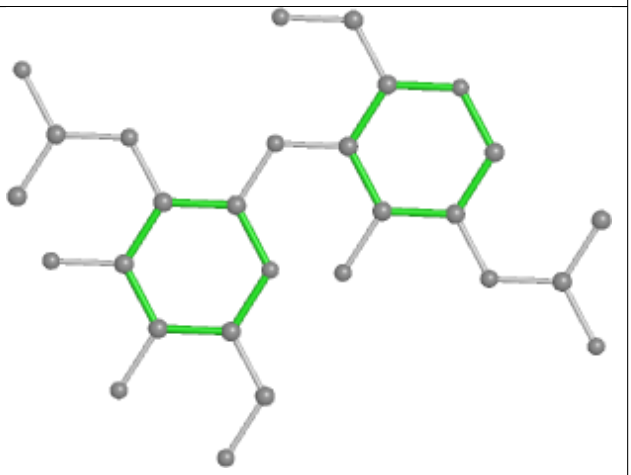
Bond lengths



Bond angles

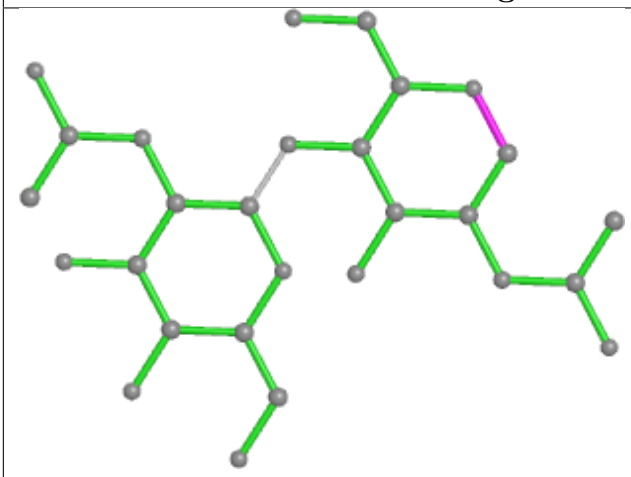


Torsions

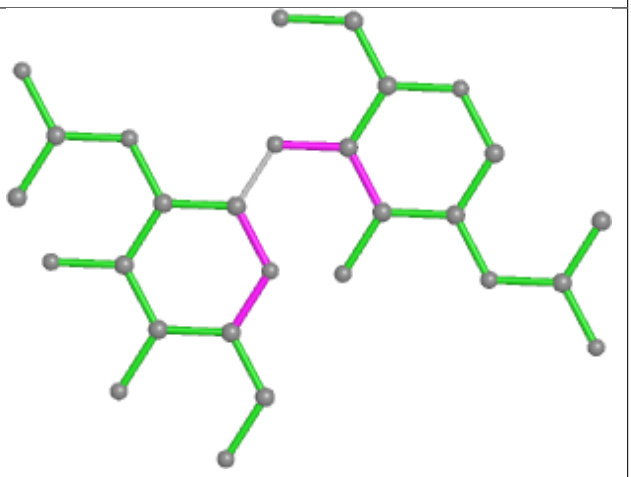


Rings

Oligosaccharide Chain S



Bond lengths



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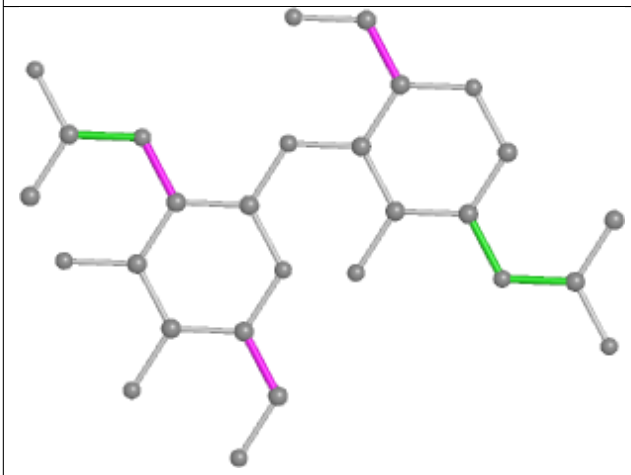

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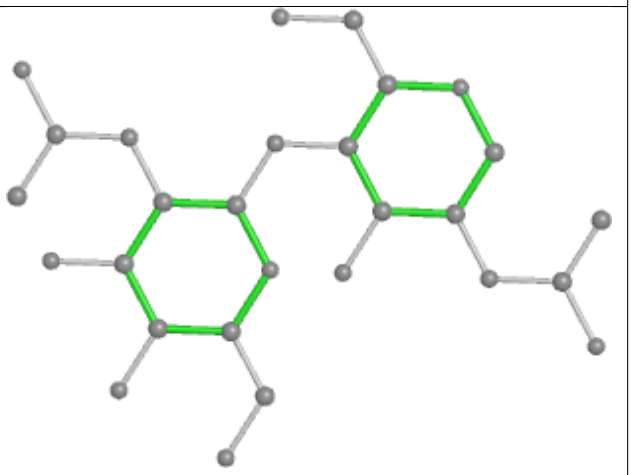
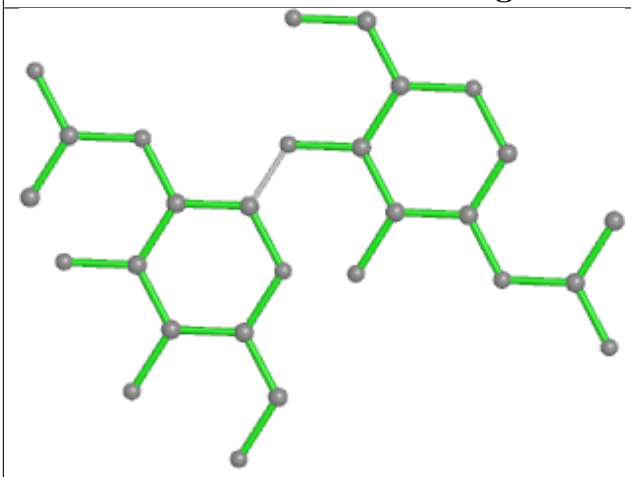
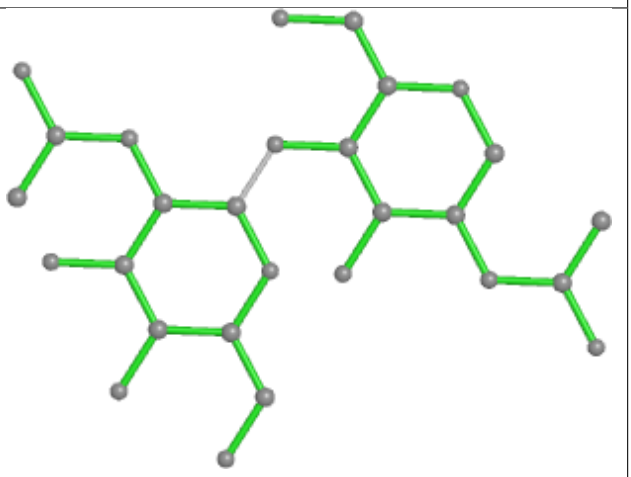


Rings

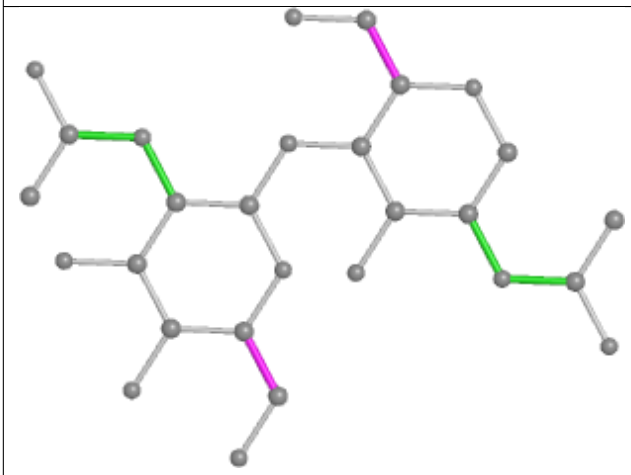
Oligosaccharide Chain T



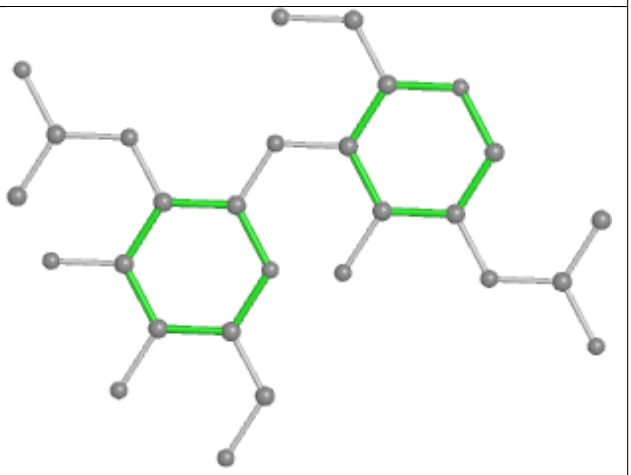
Bond lengths



Bond angles

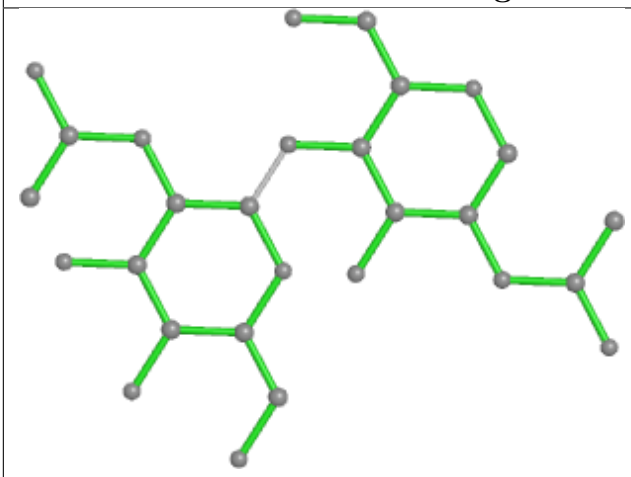


Torsions

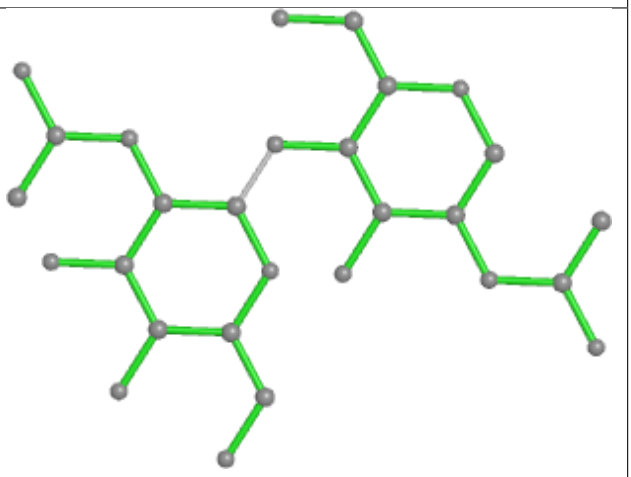


Rings

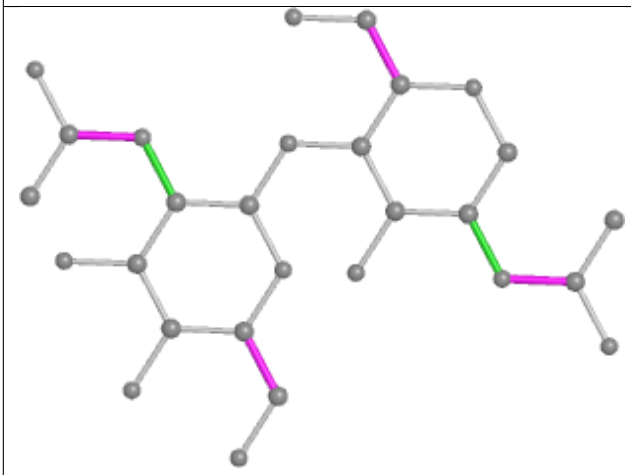
Oligosaccharide Chain U



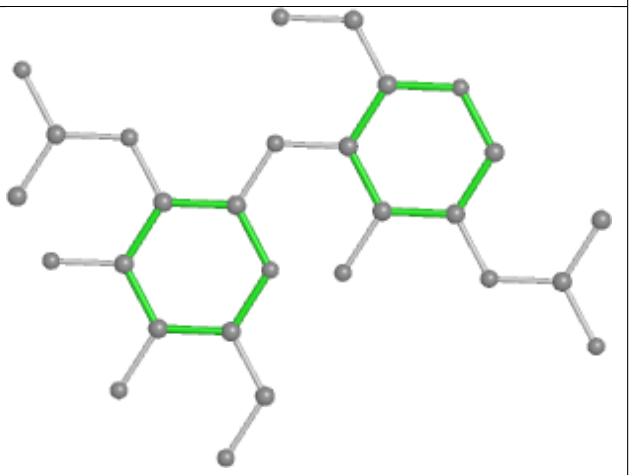
Bond lengths



Bond angles

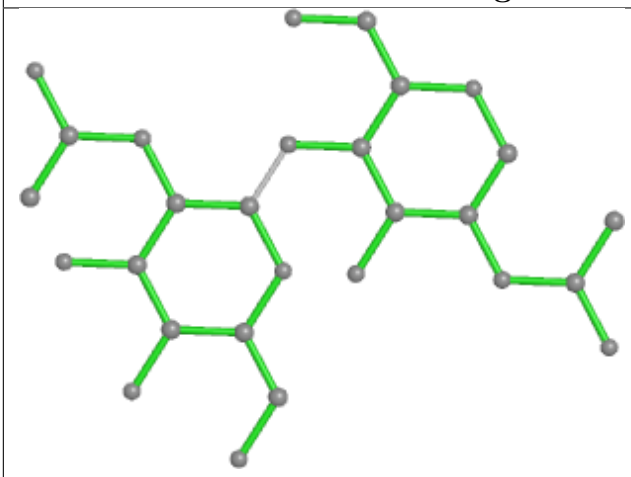


Torsions

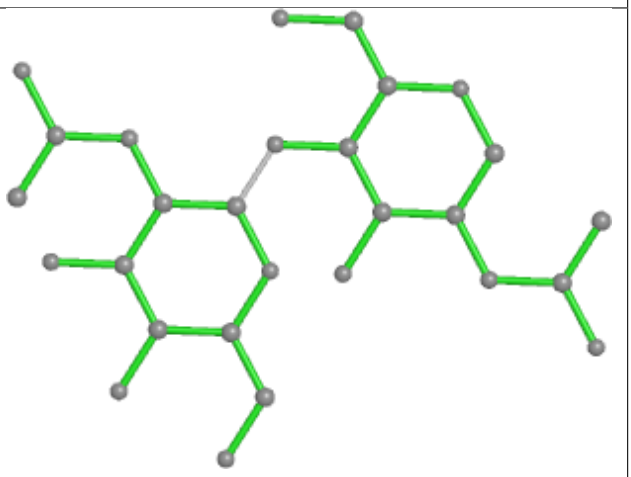


Rings

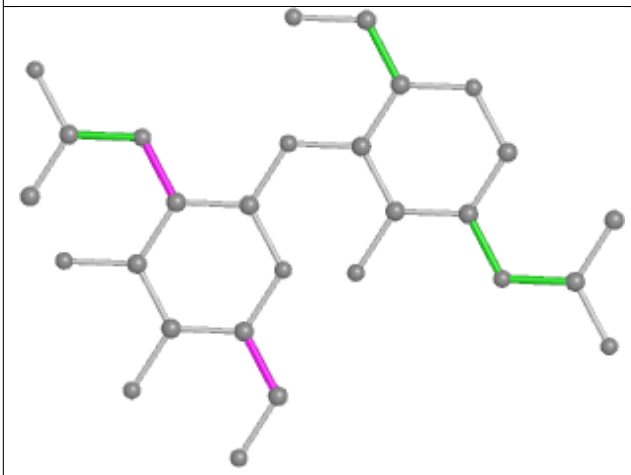
Oligosaccharide Chain V



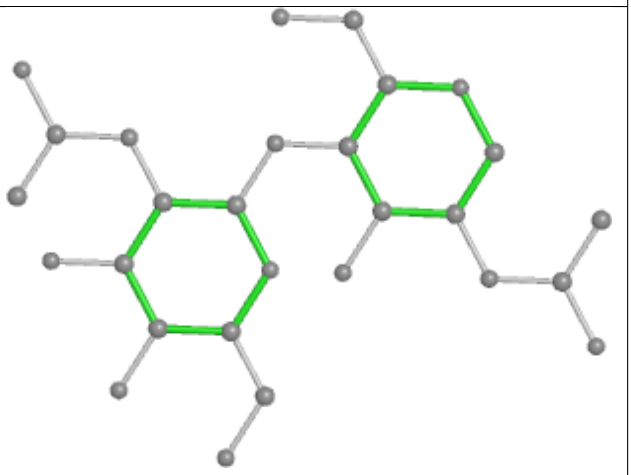
Bond lengths



Bond angles

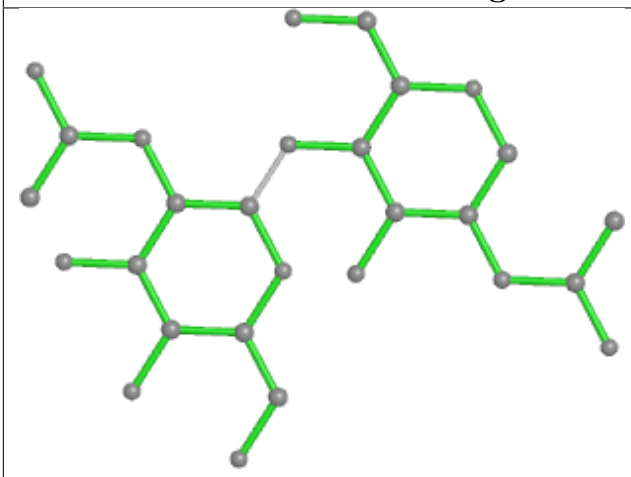


Torsions

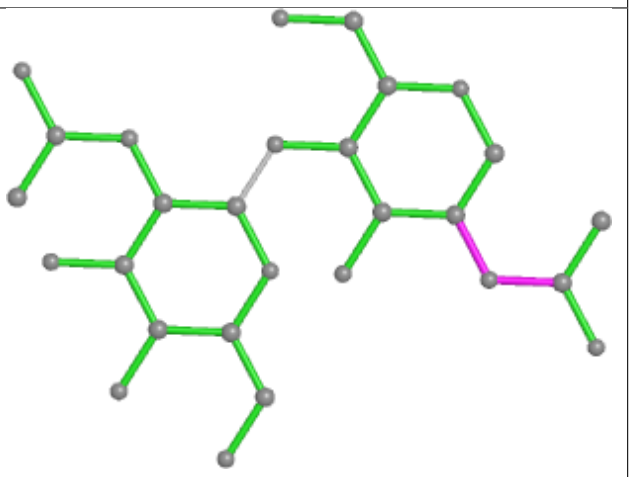


Rings

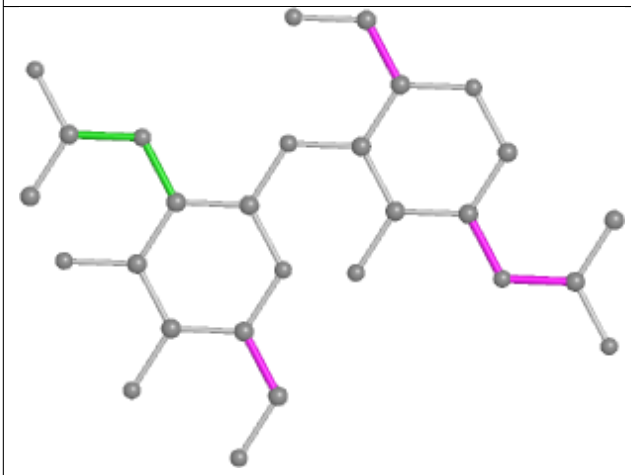
Oligosaccharide Chain W



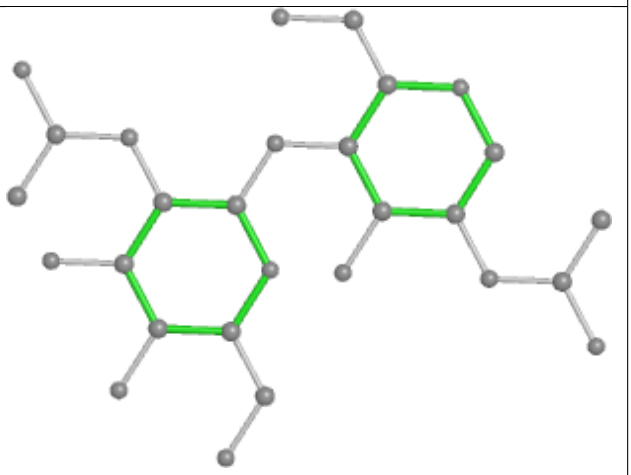
Bond lengths



Bond angles

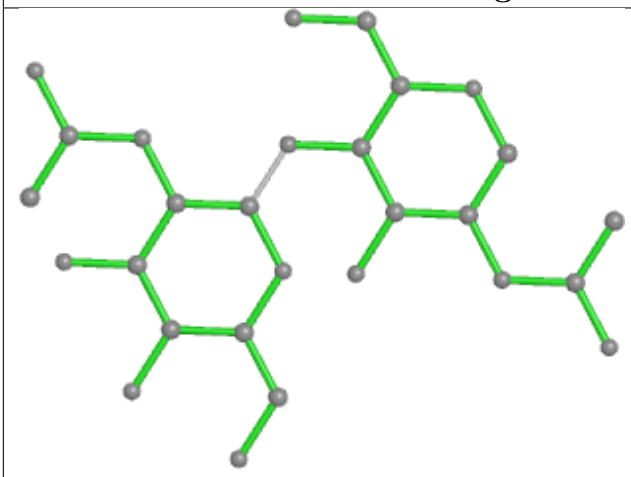


Torsions

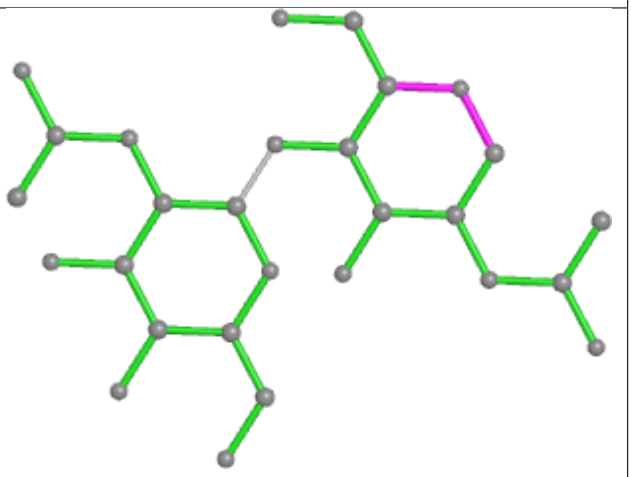


Rings

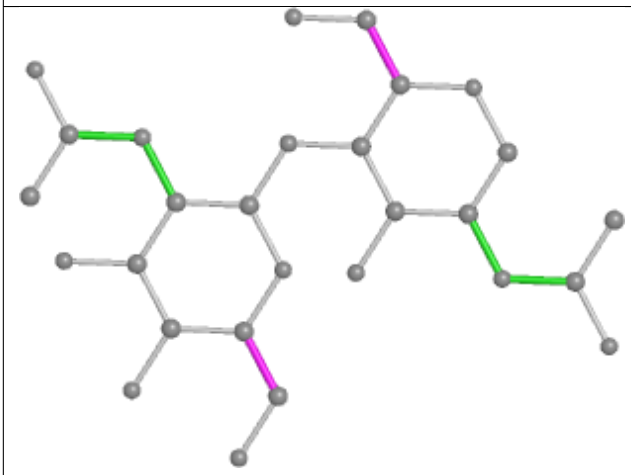
Oligosaccharide Chain X



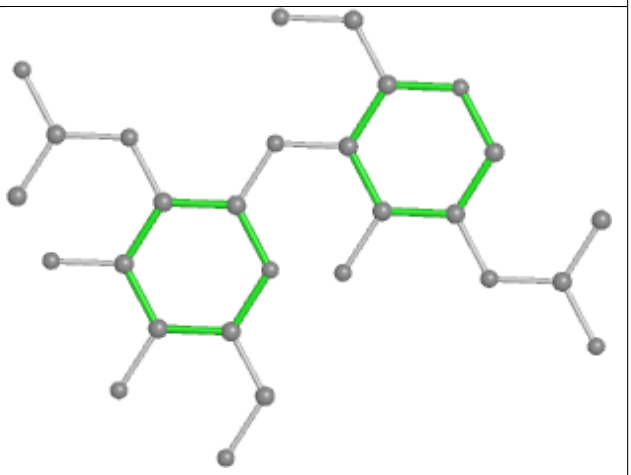
Bond lengths



Bond angles

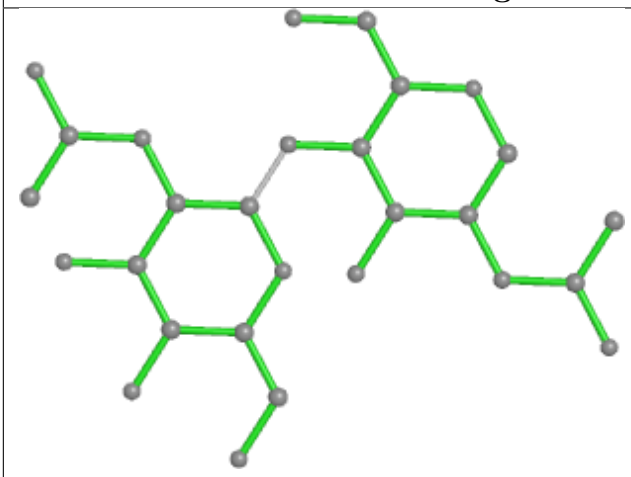


Torsions

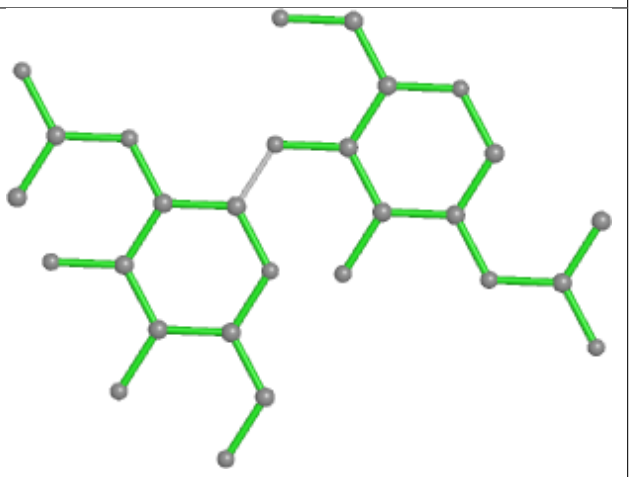


Rings

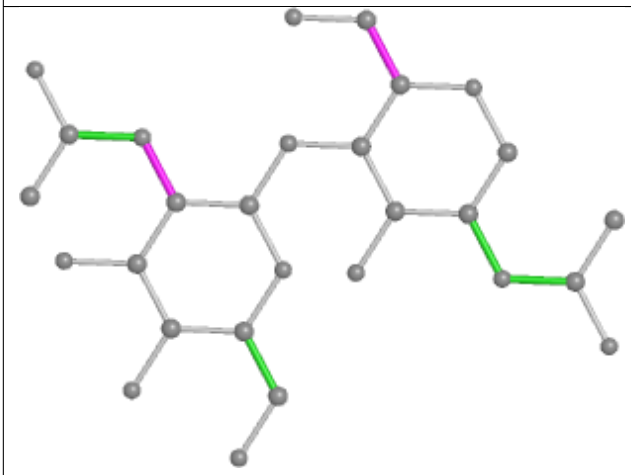
Oligosaccharide Chain Y



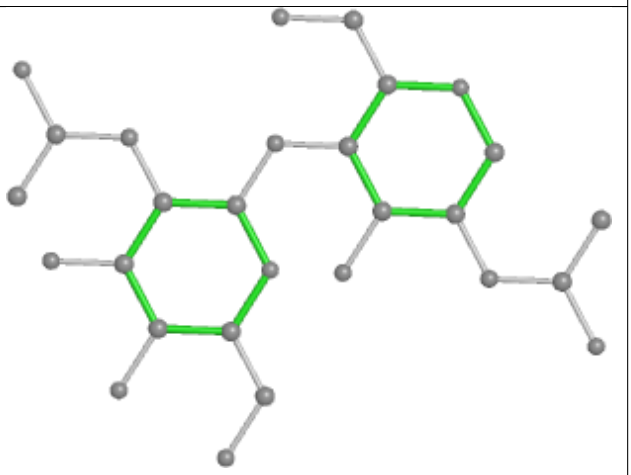
Bond lengths



Bond angles

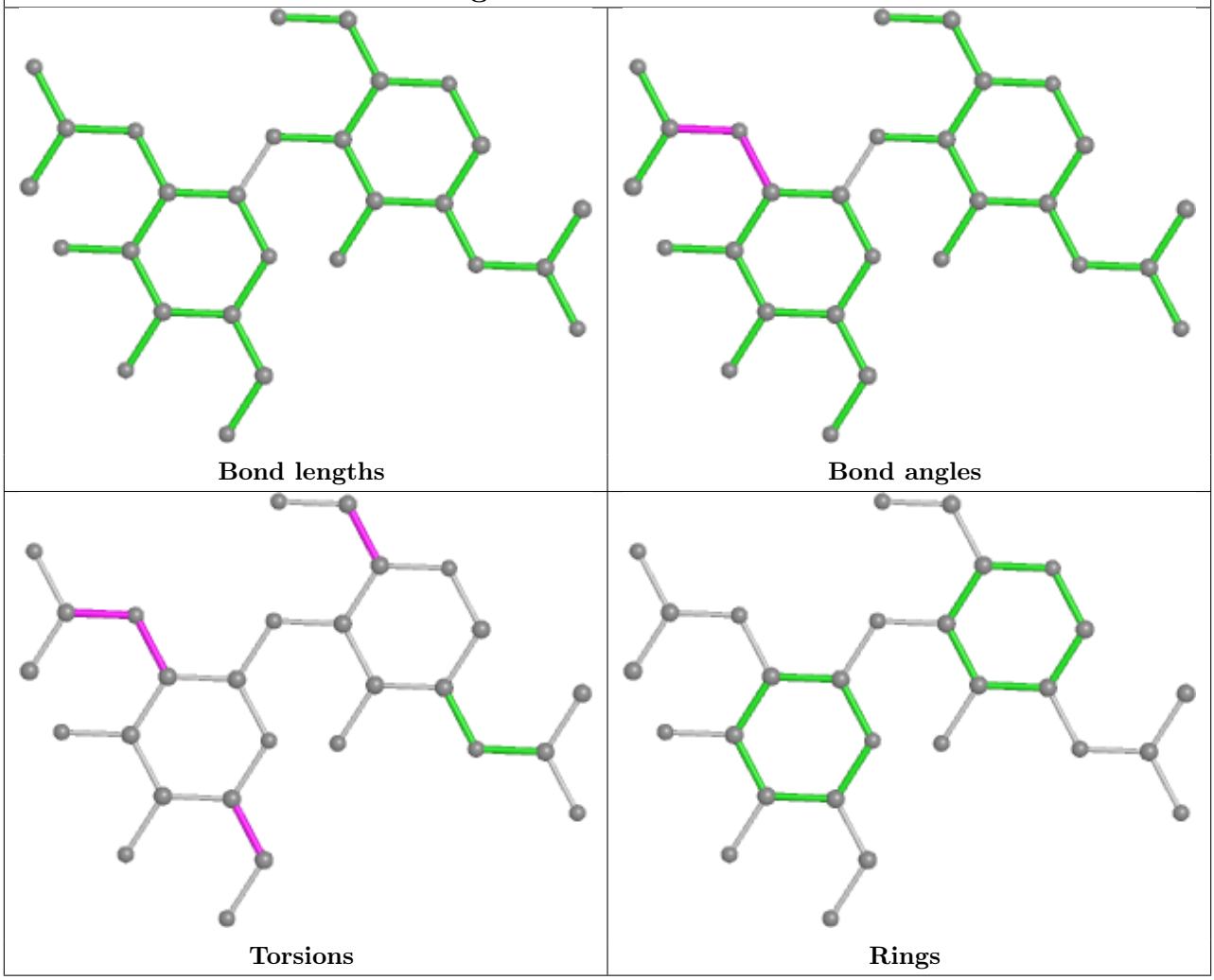


Torsions

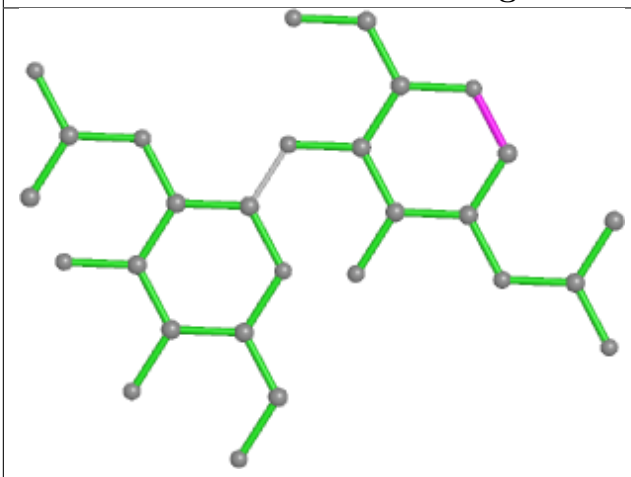


Rings

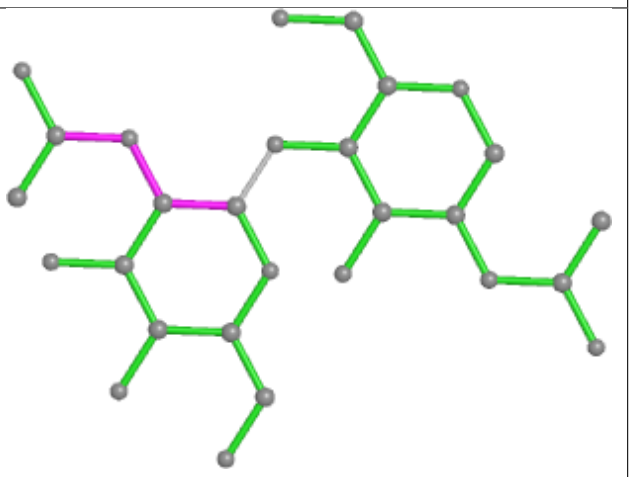
Oligosaccharide Chain Z



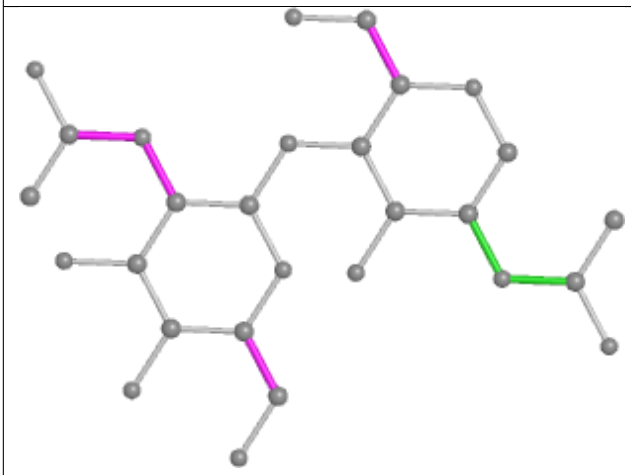
Oligosaccharide Chain a



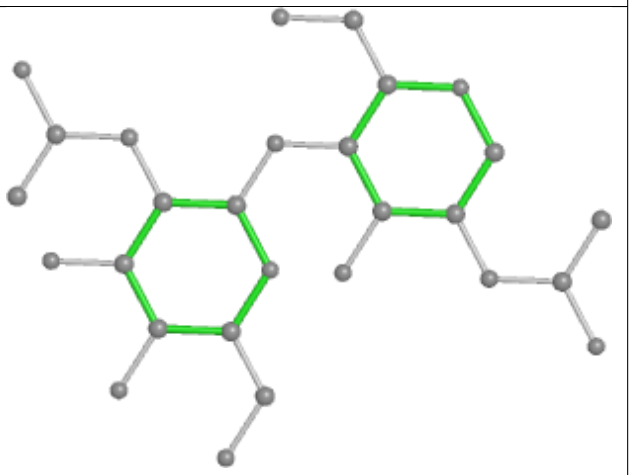
Bond lengths



Bond angles

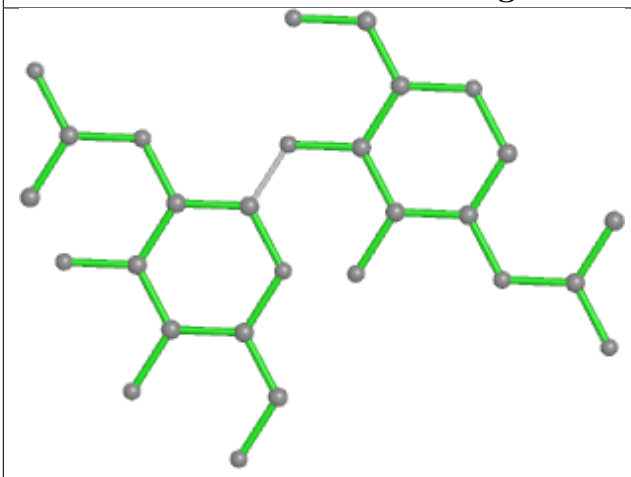


Torsions

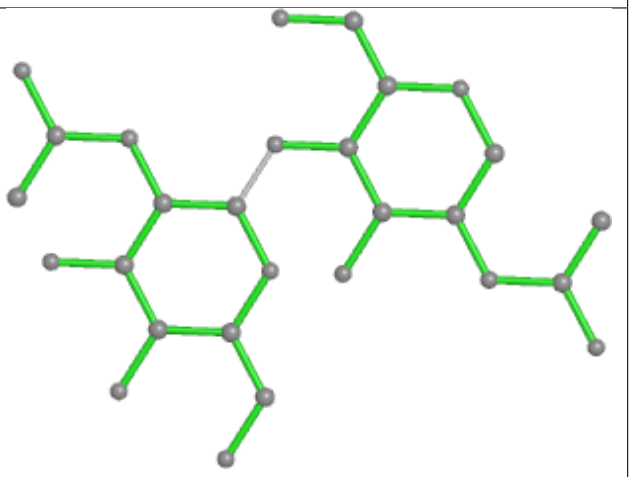


Rings

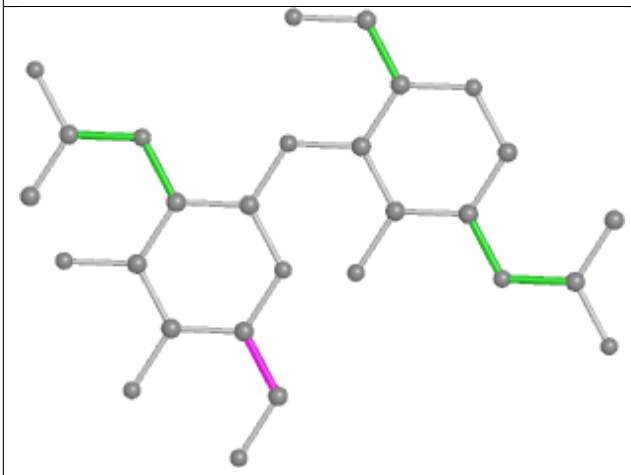
Oligosaccharide Chain b



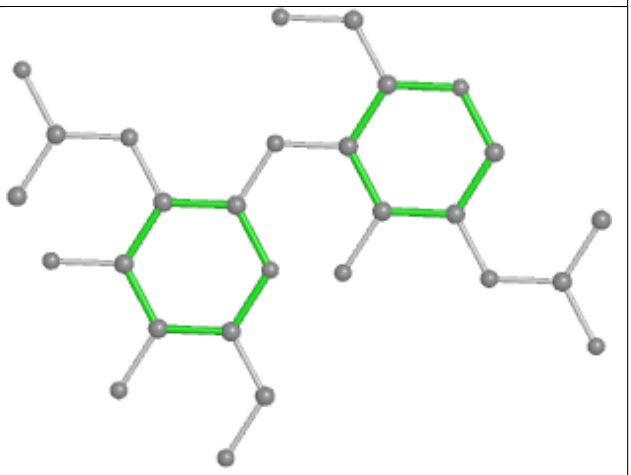
Bond lengths



Bond angles

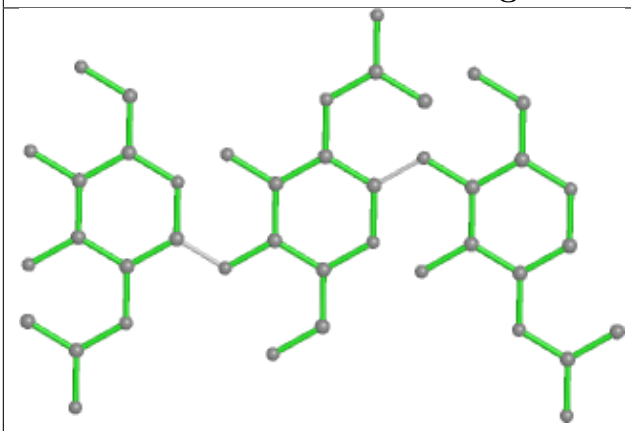


Torsions

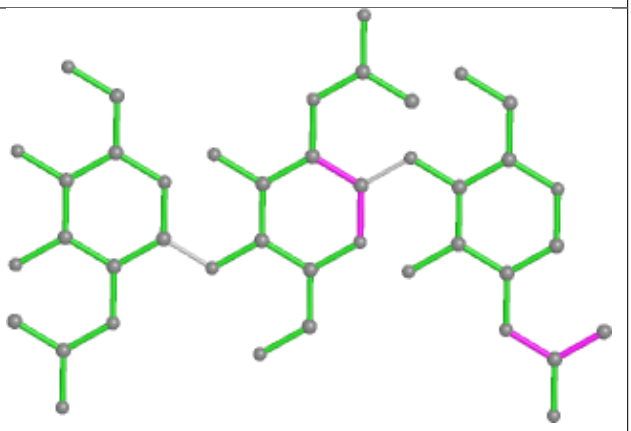


Rings

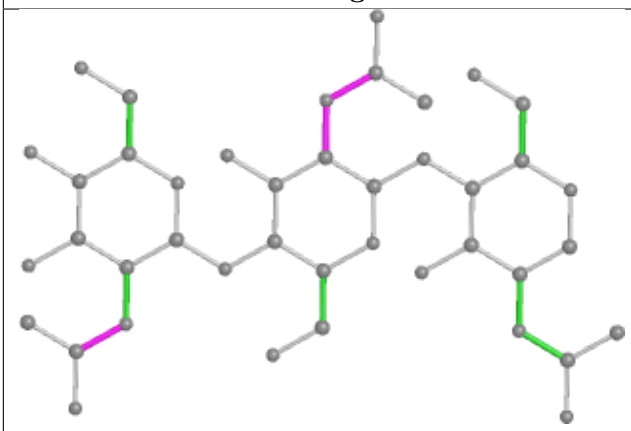
Oligosaccharide Chain c



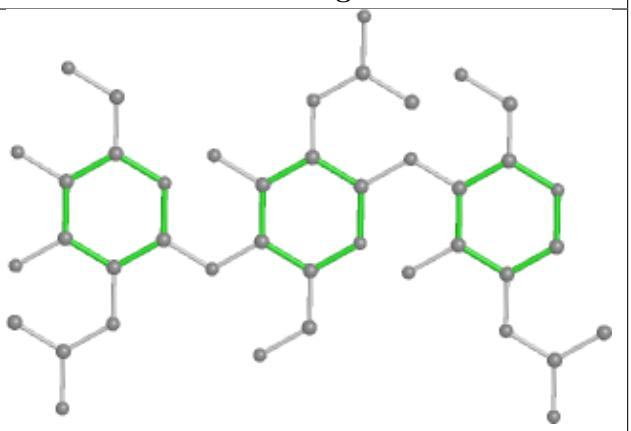
Bond lengths



Bond angles

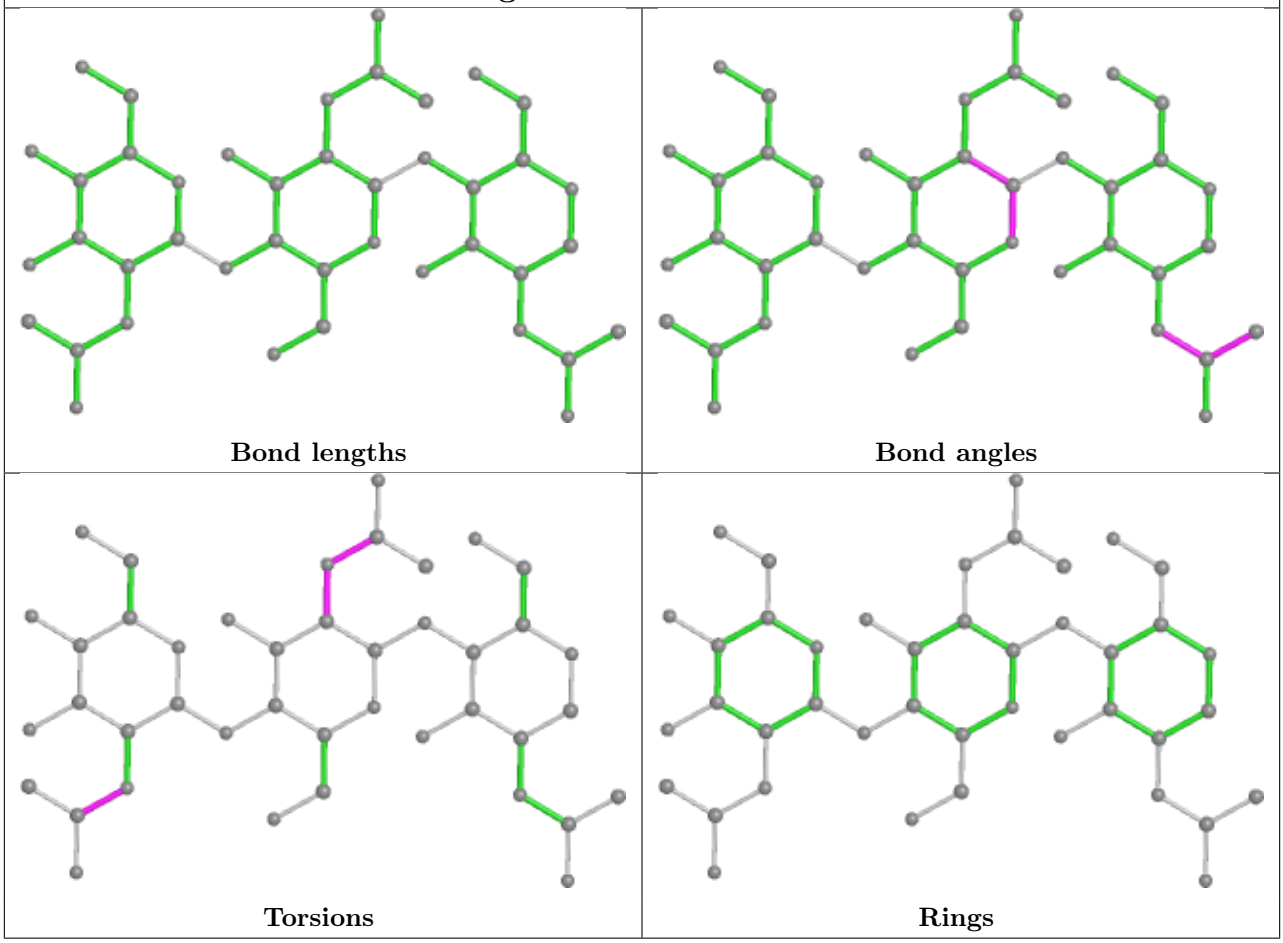


Torsions



Rings

Oligosaccharide Chain d



5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.43	0
6	NAG	C	1406	1	14,14,15	0.22	0	17,19,21	0.36	0
6	NAG	B	1401	1	14,14,15	0.30	0	17,19,21	0.55	0
6	NAG	A	1403	1	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	B	1405	1	14,14,15	0.38	0	17,19,21	1.28	2 (11%)
6	NAG	A	1407	1	14,14,15	0.26	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	B	1410	1	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
6	NAG	C	1402	1	14,14,15	0.45	0	17,19,21	0.57	0
6	NAG	A	1401	1	14,14,15	0.29	0	17,19,21	0.33	0
6	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.39	0
6	NAG	B	1411	-	14,14,15	0.33	0	17,19,21	0.42	0
6	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
6	NAG	B	1402	1	14,14,15	0.31	0	17,19,21	0.64	0
6	NAG	B	1404	1	14,14,15	0.32	0	17,19,21	0.59	0
6	NAG	C	1403	1	14,14,15	0.55	0	17,19,21	0.46	0
6	NAG	C	1405	1	14,14,15	0.36	0	17,19,21	1.30	2 (11%)
6	NAG	A	1404	1	14,14,15	0.44	0	17,19,21	0.54	0
6	NAG	A	1405	1	14,14,15	0.55	0	17,19,21	1.25	1 (5%)
6	NAG	B	1407	1	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
6	NAG	B	1406	1	14,14,15	0.40	0	17,19,21	0.80	1 (5%)
6	NAG	C	1401	1	14,14,15	0.44	0	17,19,21	0.78	1 (5%)
6	NAG	B	1409	1	14,14,15	0.20	0	17,19,21	0.39	0
6	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
6	NAG	C	1408	1	14,14,15	0.15	0	17,19,21	0.57	0
6	NAG	C	1404	1	14,14,15	0.29	0	17,19,21	0.37	0
6	NAG	B	1403	1	14,14,15	0.30	0	17,19,21	0.41	0
6	NAG	A	1409	1	14,14,15	0.49	0	17,19,21	0.35	0
6	NAG	C	1407	1	14,14,15	0.36	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1411	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1405	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
6	NAG	B	1407	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1406	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1405	NAG	C2-N2-C7	4.32	129.06	122.90
6	A	1405	NAG	C2-N2-C7	4.30	129.02	122.90
6	B	1405	NAG	C2-N2-C7	4.13	128.78	122.90
6	C	1401	NAG	C1-O5-C5	2.83	116.03	112.19
6	B	1406	NAG	C1-O5-C5	2.57	115.68	112.19

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1408	NAG	O5-C5-C6-O6
6	B	1401	NAG	O5-C5-C6-O6
6	A	1406	NAG	O5-C5-C6-O6
6	B	1402	NAG	O5-C5-C6-O6
6	C	1408	NAG	O5-C5-C6-O6

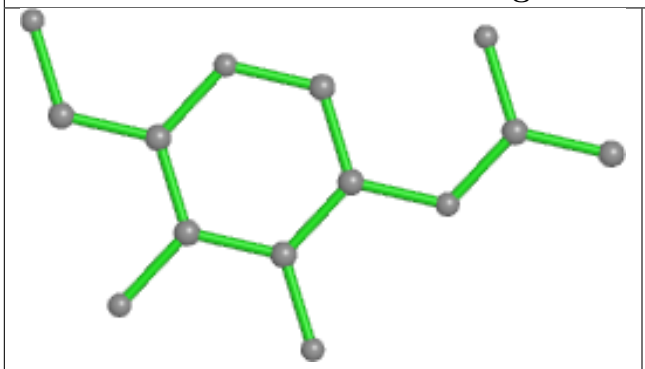
There are no ring outliers.

11 monomers are involved in 17 short contacts:

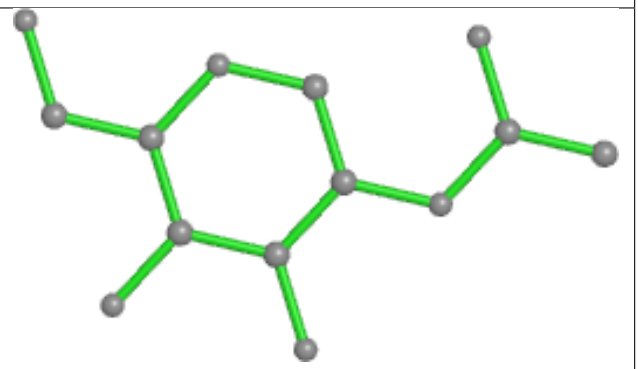
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1405	NAG	2	0
6	B	1410	NAG	4	0
6	C	1402	NAG	1	0
6	B	1411	NAG	4	0
6	A	1402	NAG	3	0
6	B	1402	NAG	1	0
6	C	1405	NAG	1	0
6	A	1404	NAG	1	0
6	A	1405	NAG	1	0
6	B	1407	NAG	1	0
6	B	1403	NAG	2	0

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

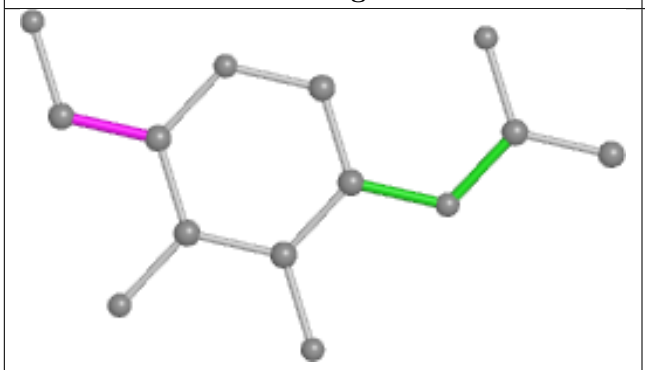
Ligand NAG B 1408



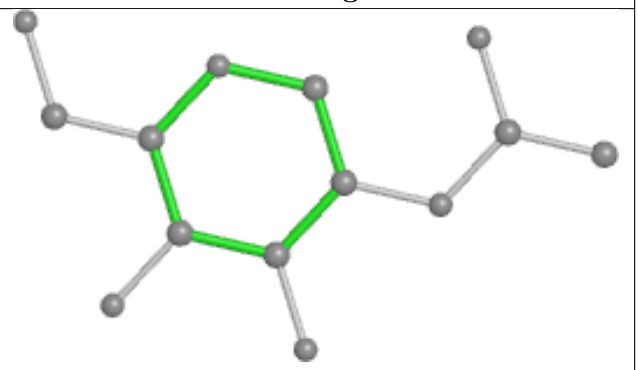
Bond lengths



Bond angles

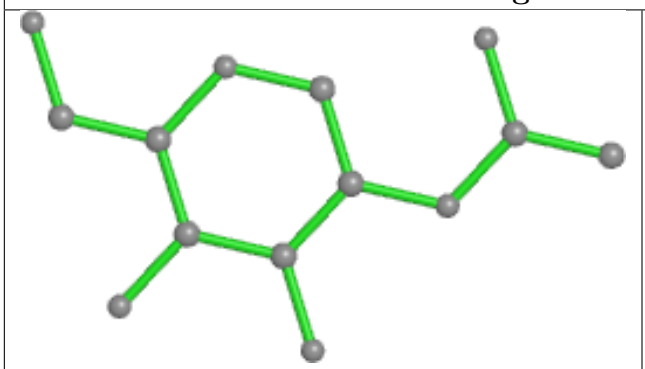


Torsions



Rings

Ligand NAG C 1406



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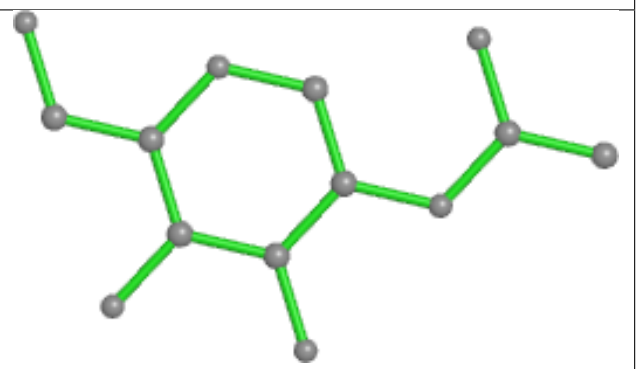
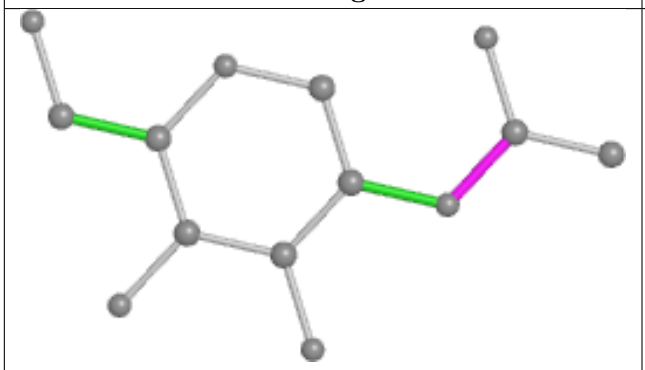


Bond angles



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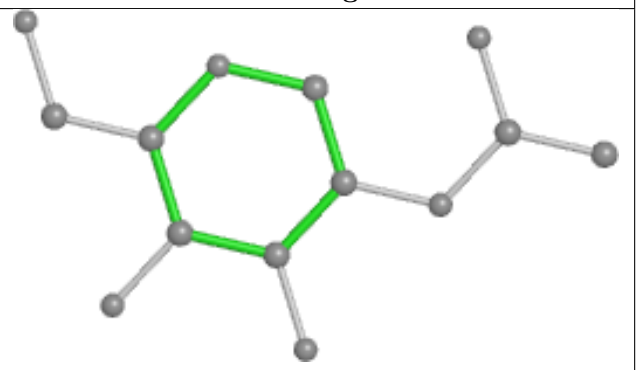

Rings

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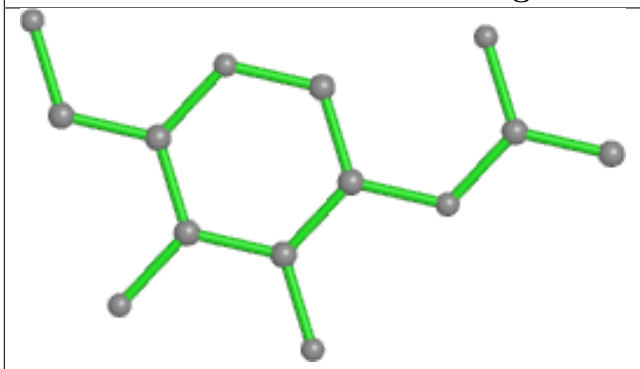
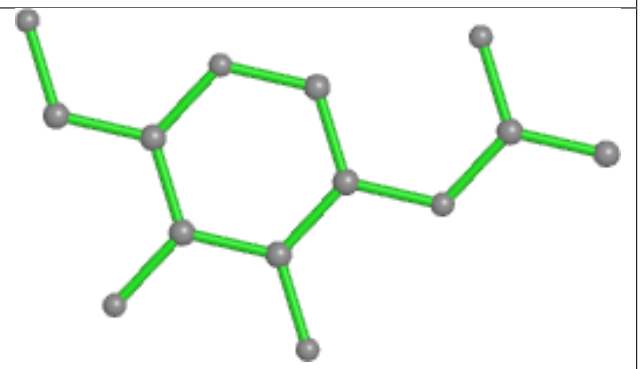
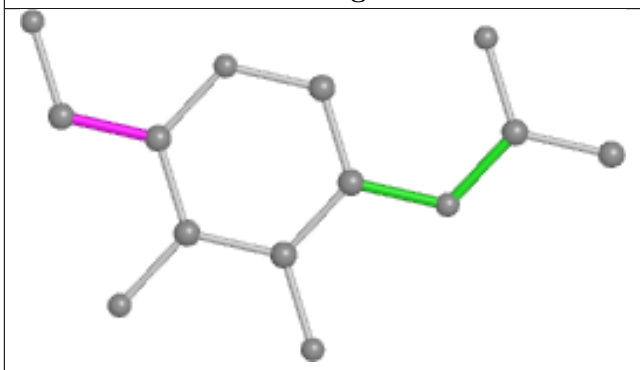
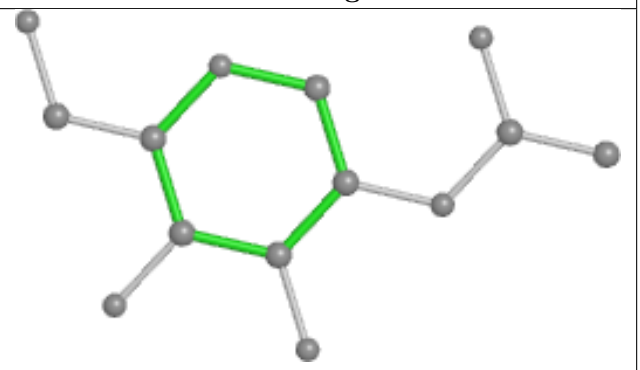
 Bond lengths	 Bond angles
 Torsions	 Rings

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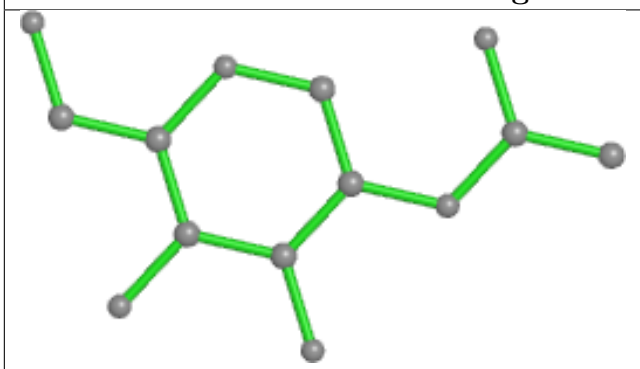
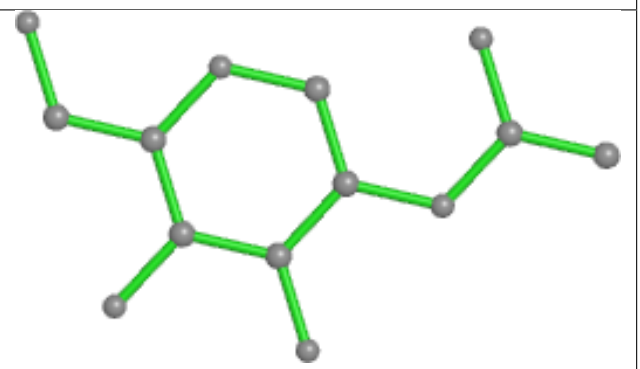
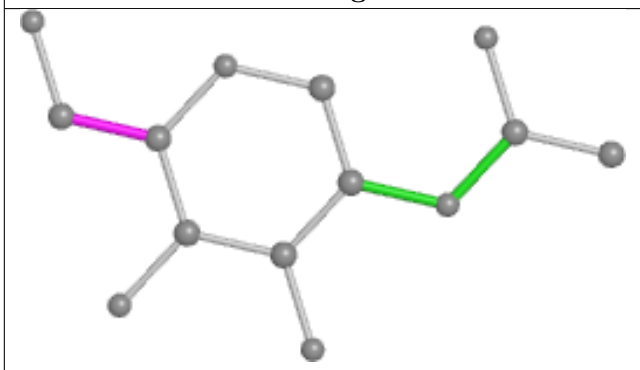
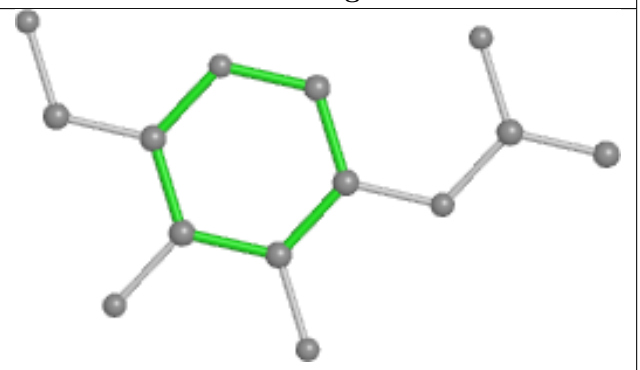
 Bond lengths	 Bond angles
 Torsions	 Rings

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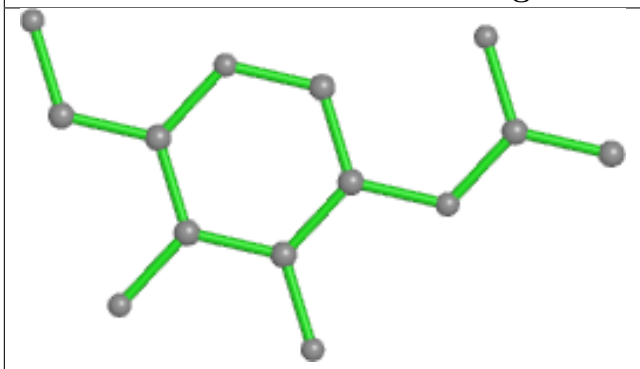
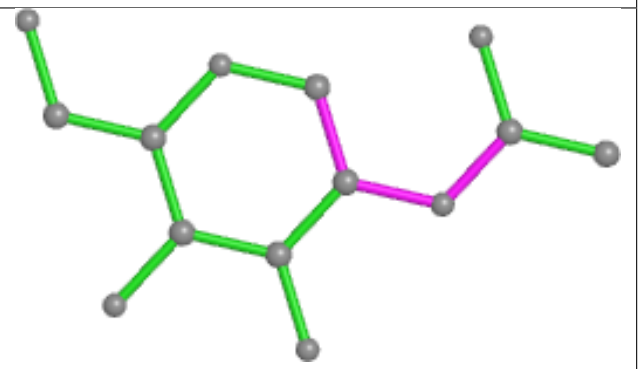
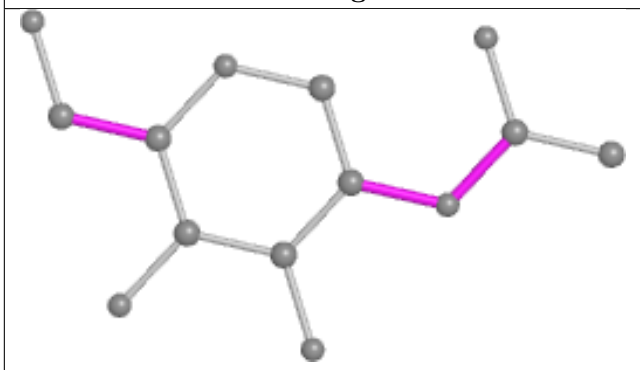
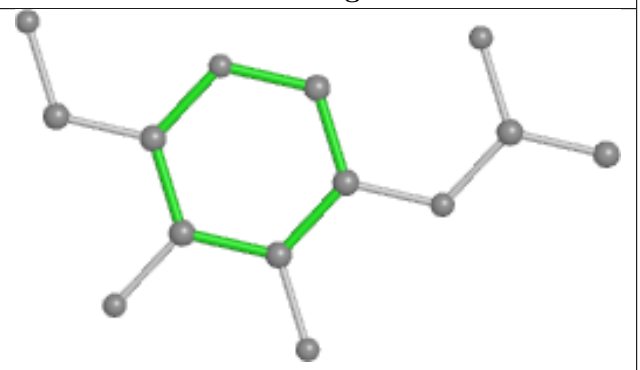
 Bond lengths	 Bond angles
 Torsions	 Rings

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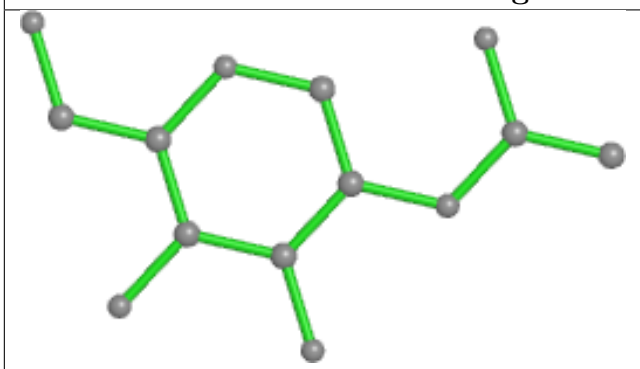
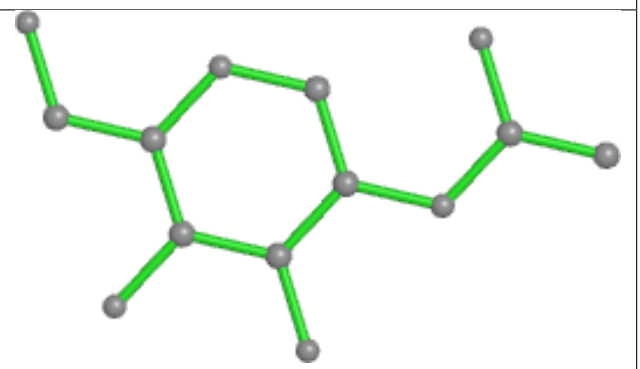
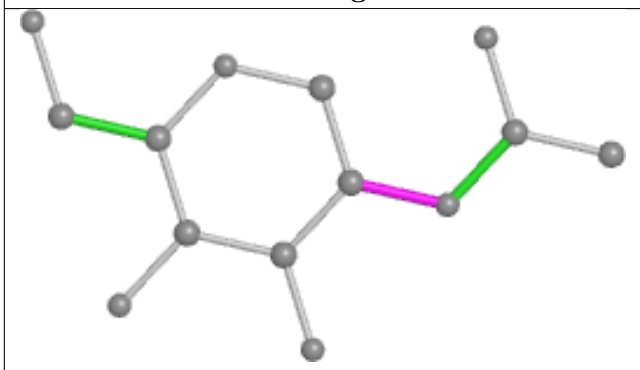
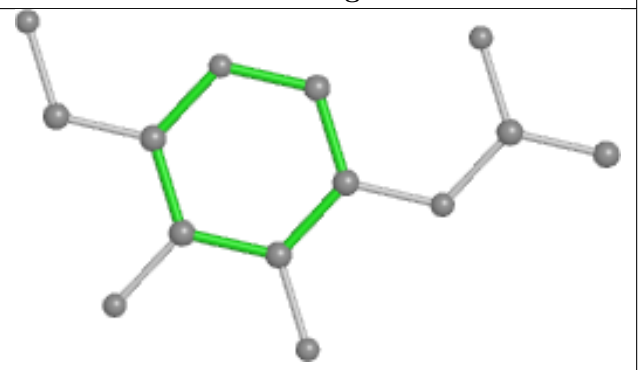
 Bond lengths	 Bond angles
 Torsions	 Rings

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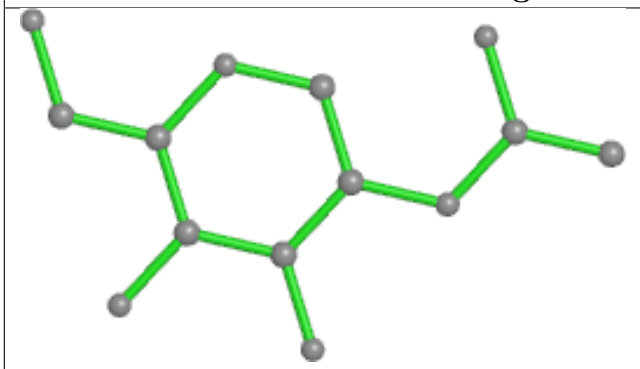
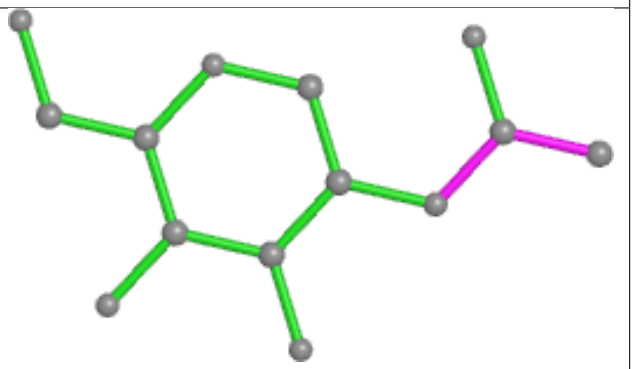
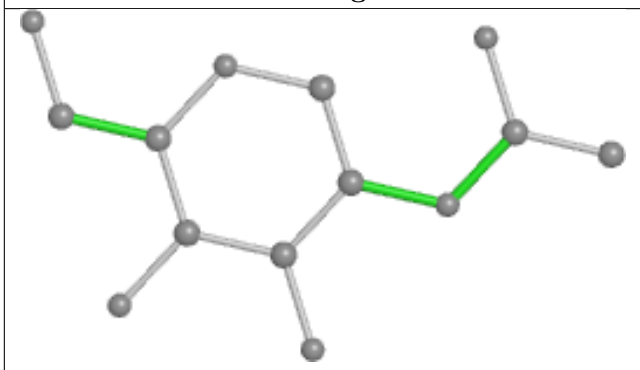
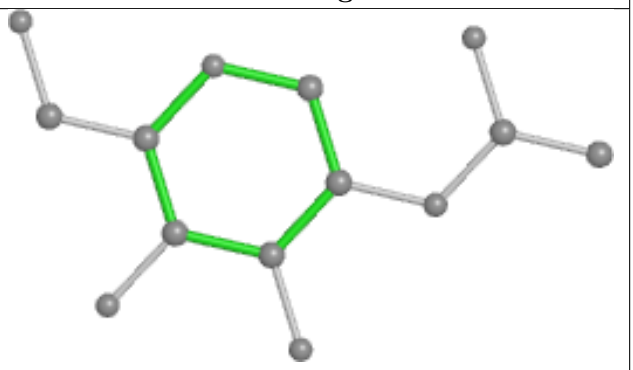
 Bond lengths	 Bond angles
 Torsions	 Rings

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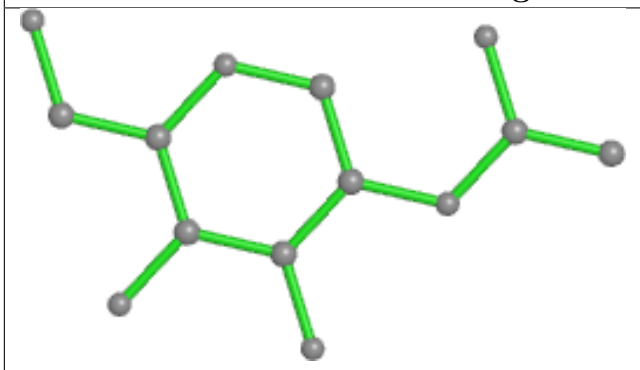
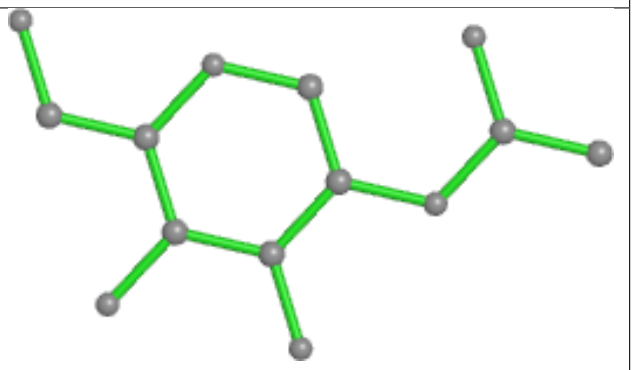
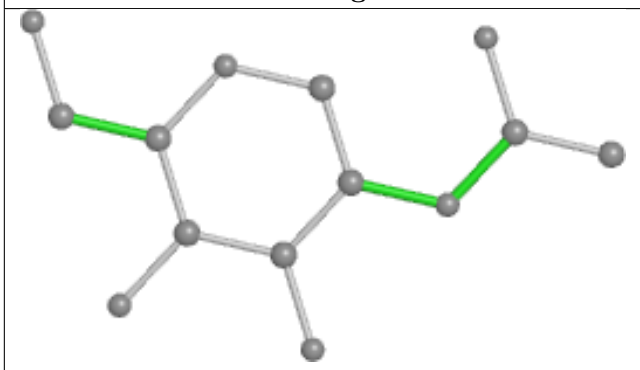
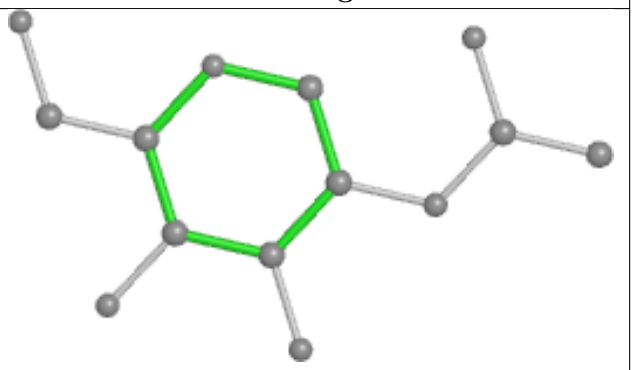
 Bond lengths	 Bond angles
 Torsions	 Rings

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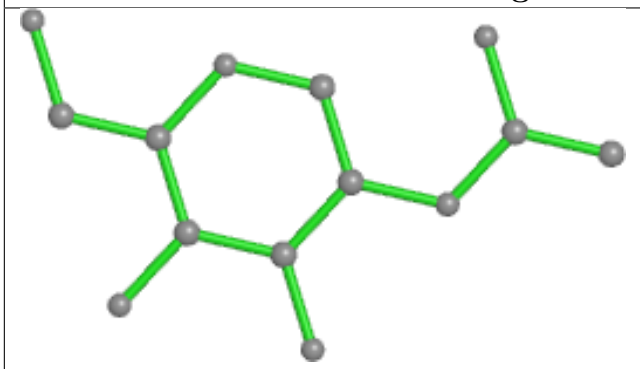
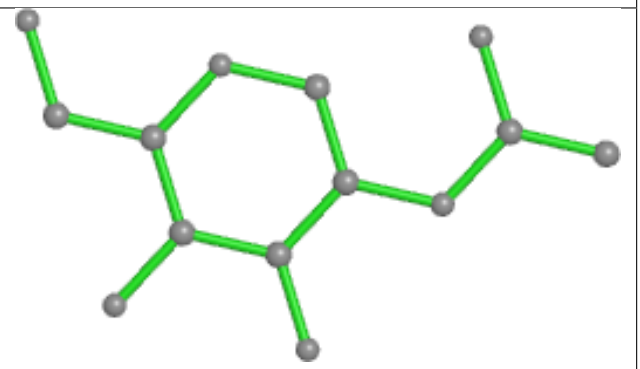
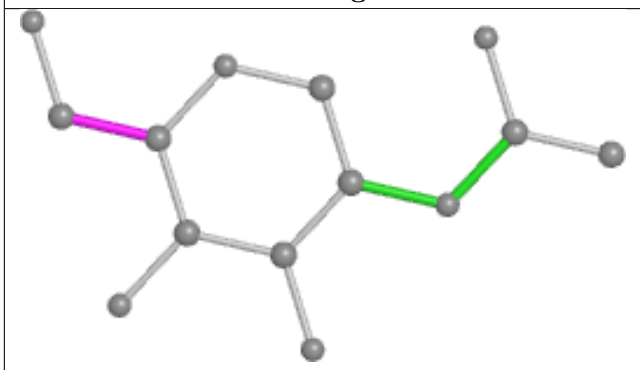
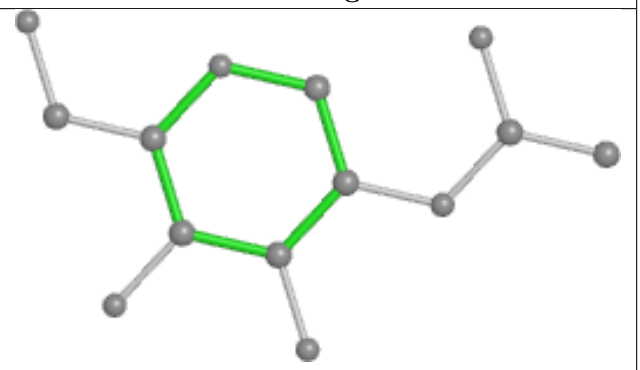
 Bond lengths	 Bond angles
 Torsions	 Rings

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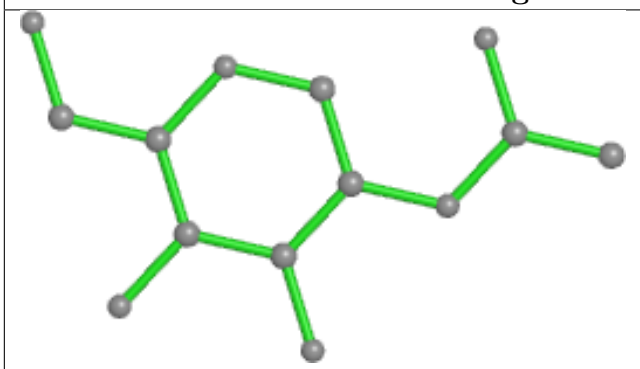
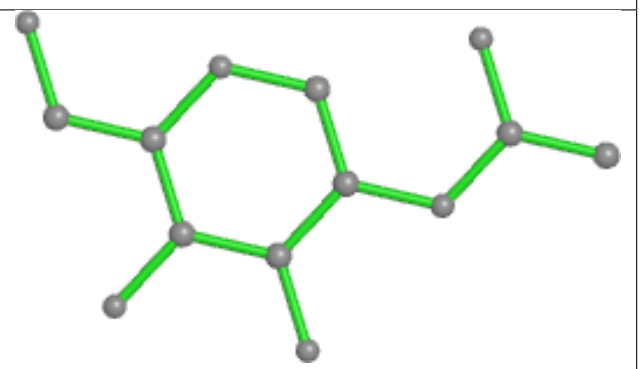
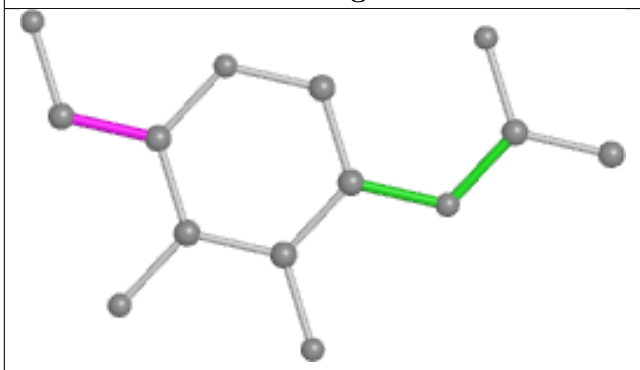
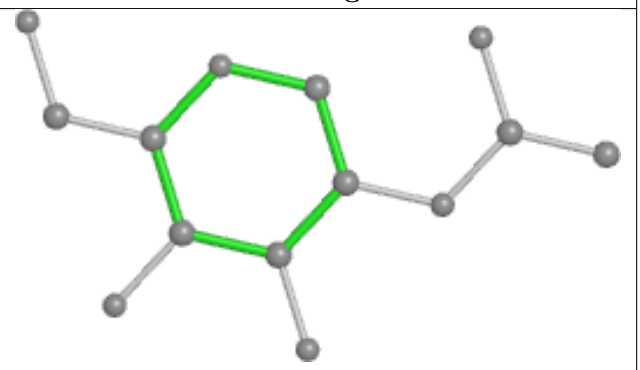
 Bond lengths	 Bond angles
 Torsions	 Rings

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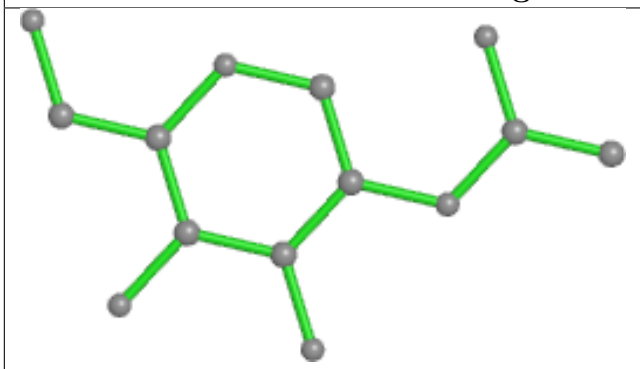
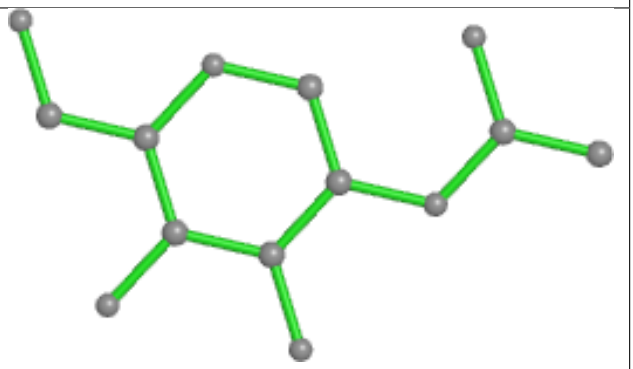
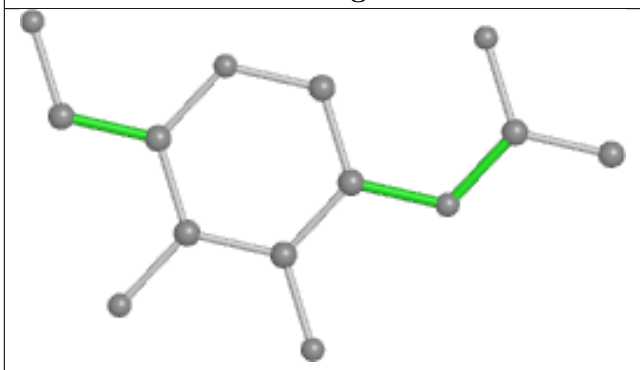
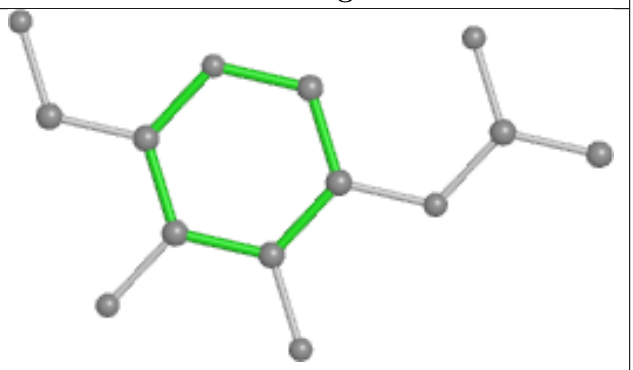
 Bond lengths	 Bond angles
 Torsions	 Rings

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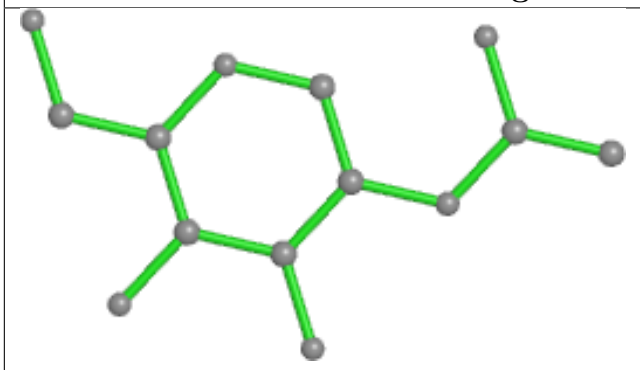
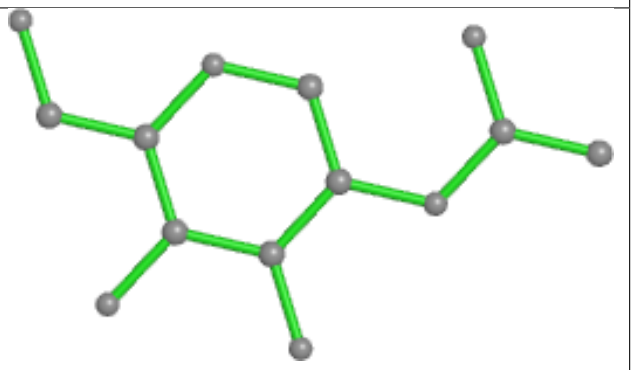
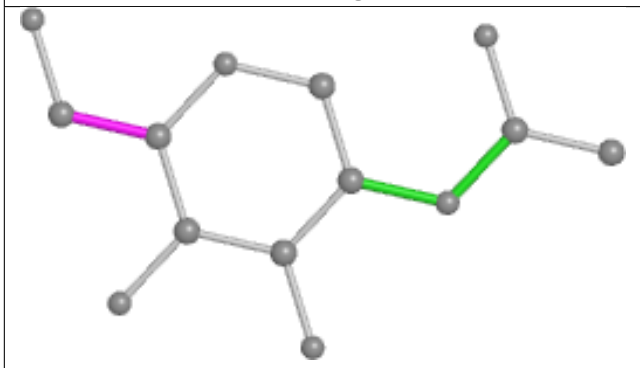
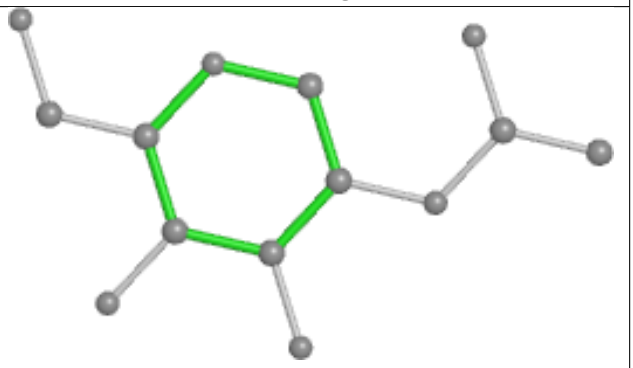
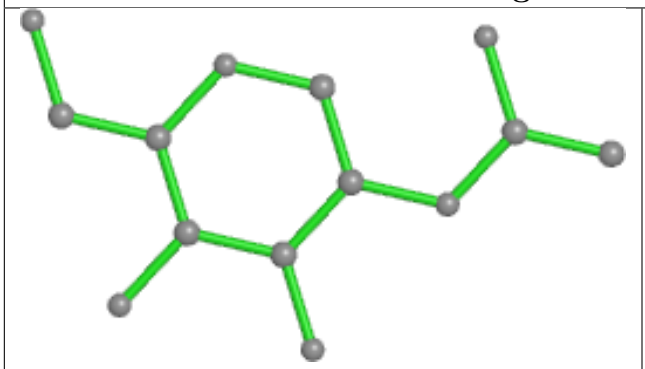
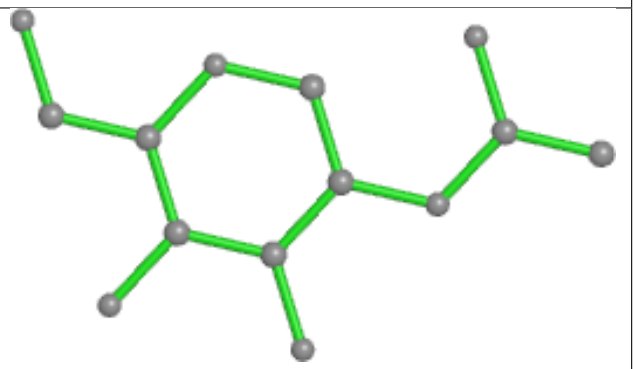
 Bond lengths	 Bond angles
 Torsions	 Rings

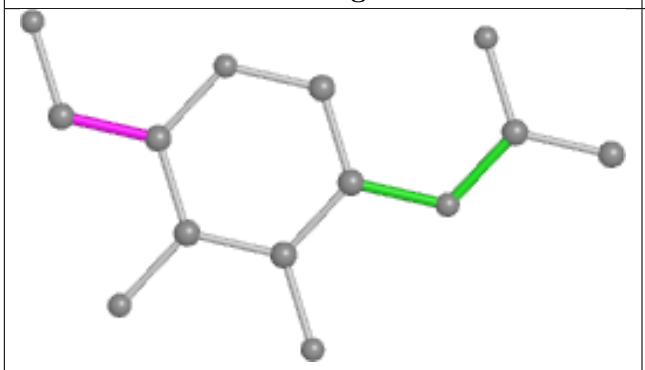
Ligand NAG B 1402



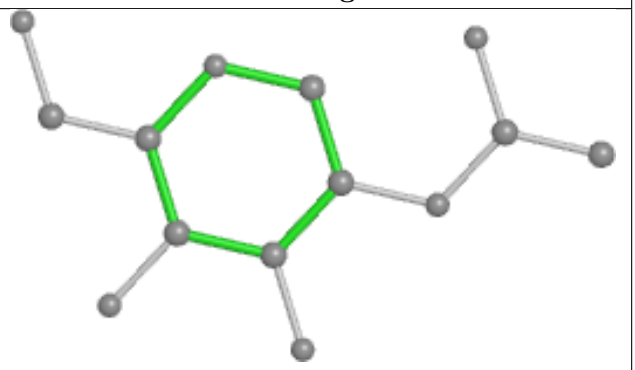
Bond lengths



Bond angles

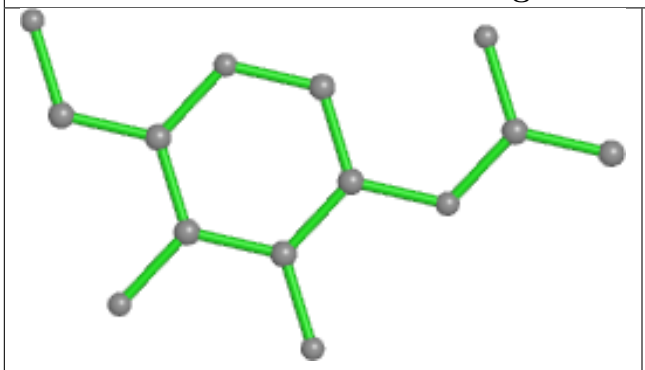


Torsions

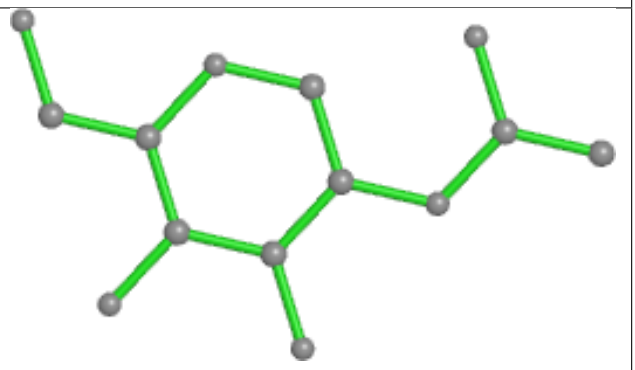


Rings

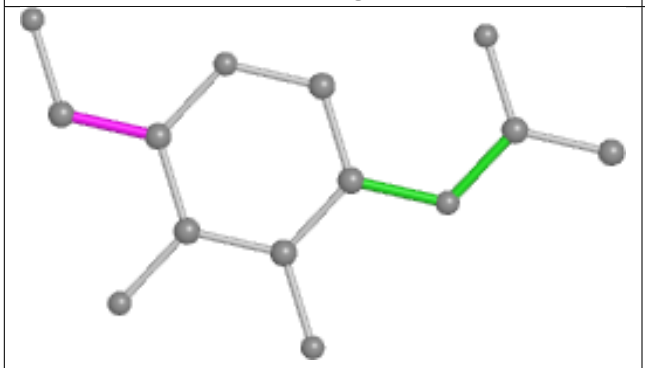
Ligand NAG B 1404



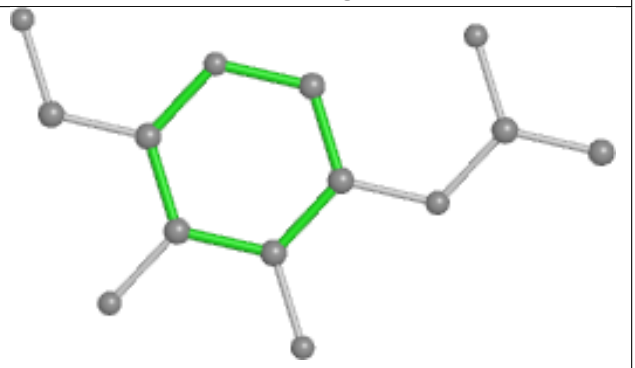
Bond lengths



Bond angles

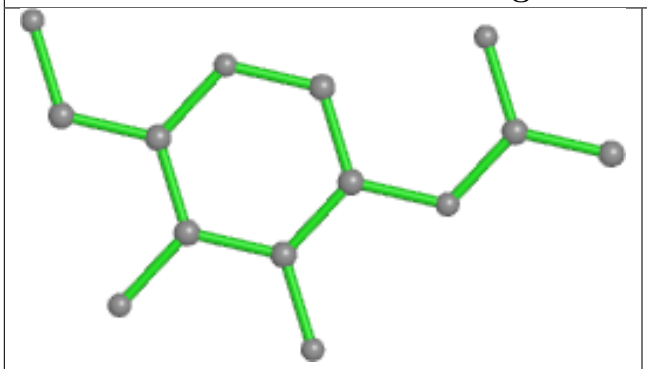


Torsions

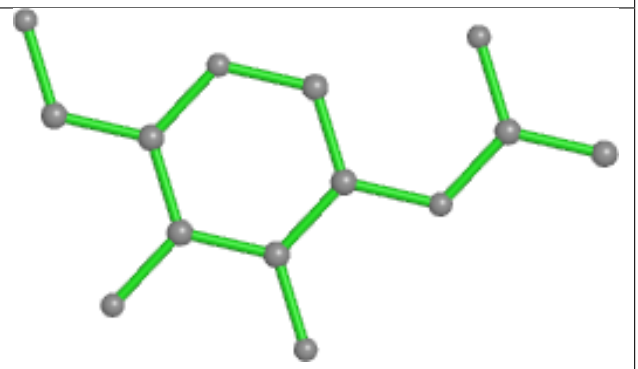


Rings

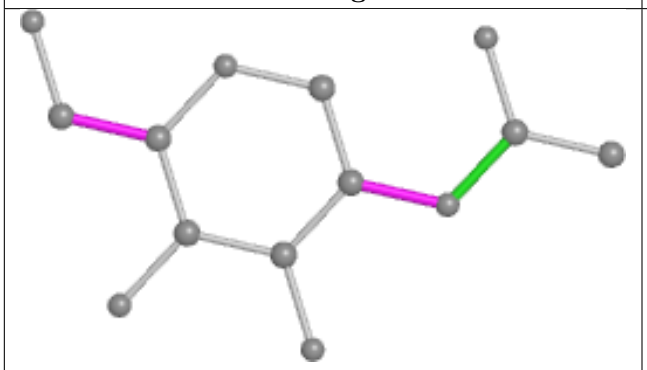
Ligand NAG C 1403



Bond lengths



Bond angles



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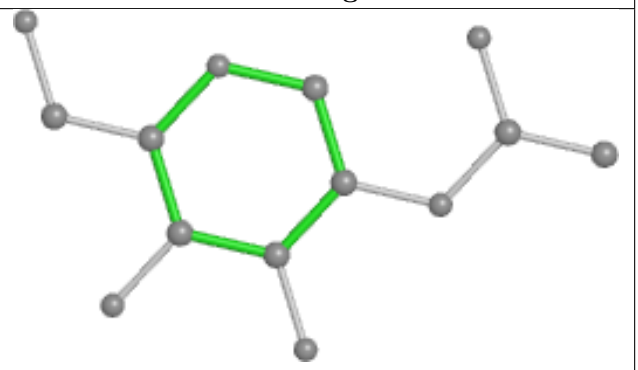
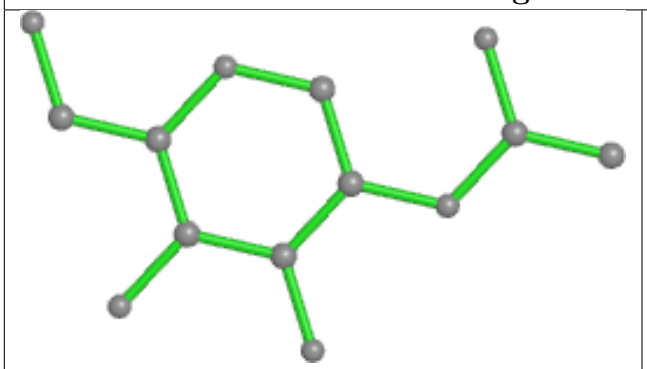


Rings

Ligand NAG C 1405



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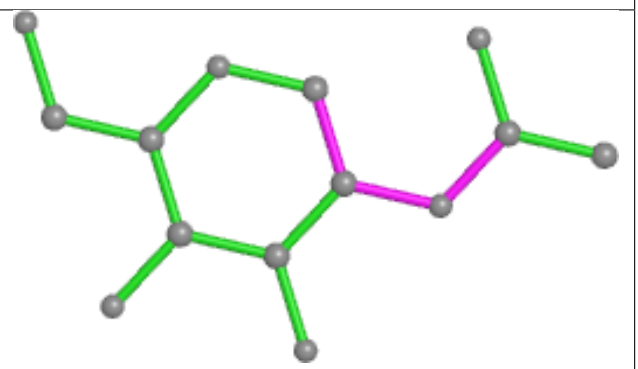
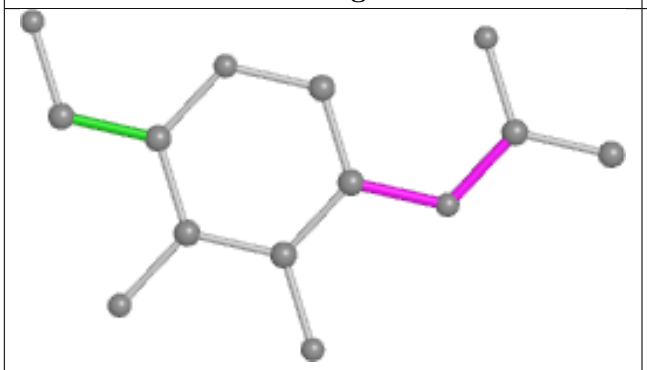


Bond angles



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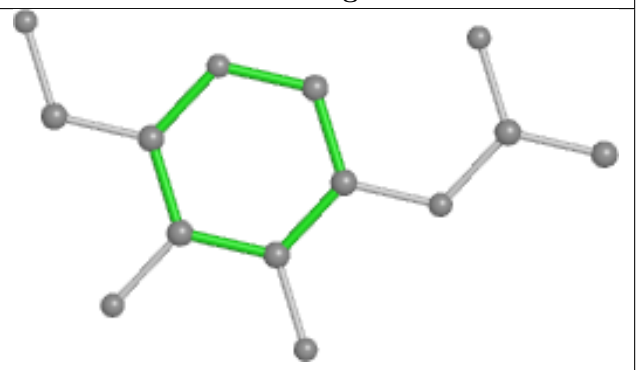
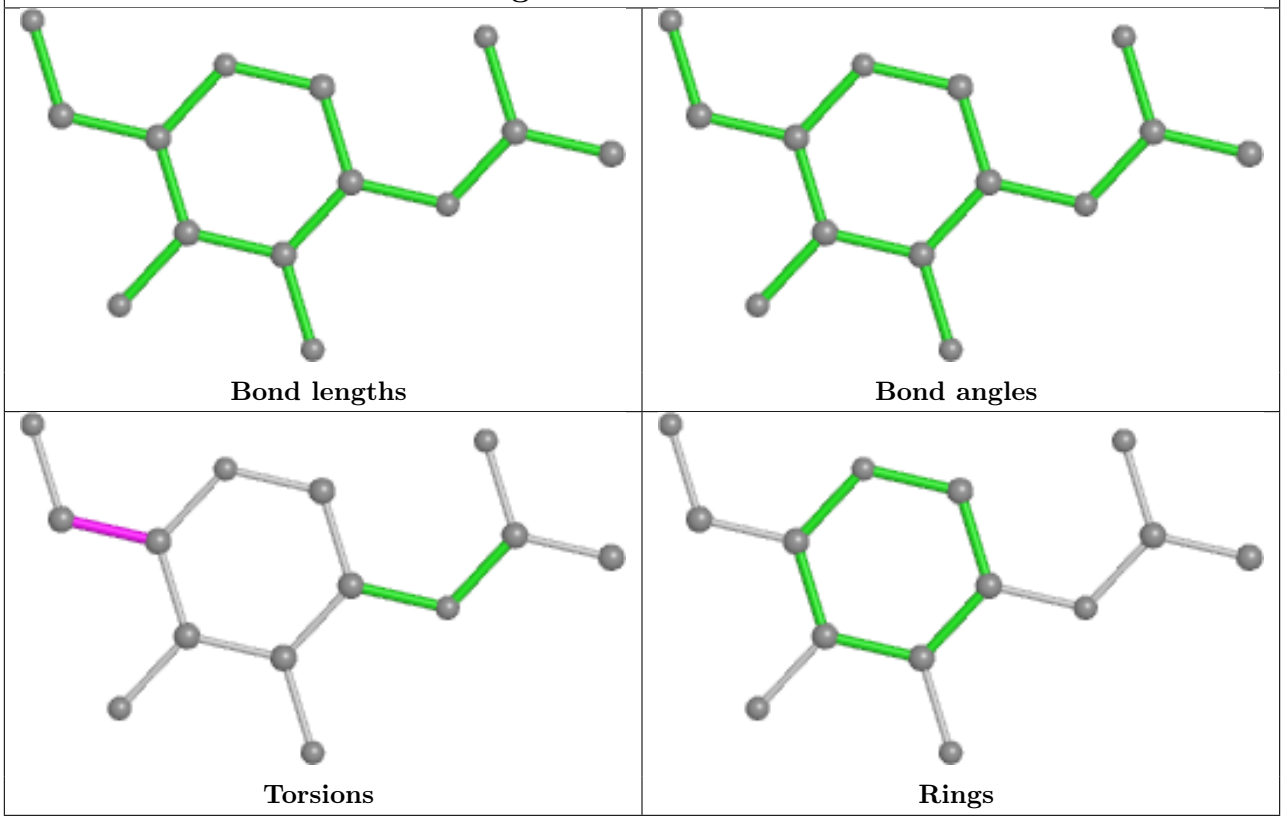


Rings

Ligand NAG A 1404



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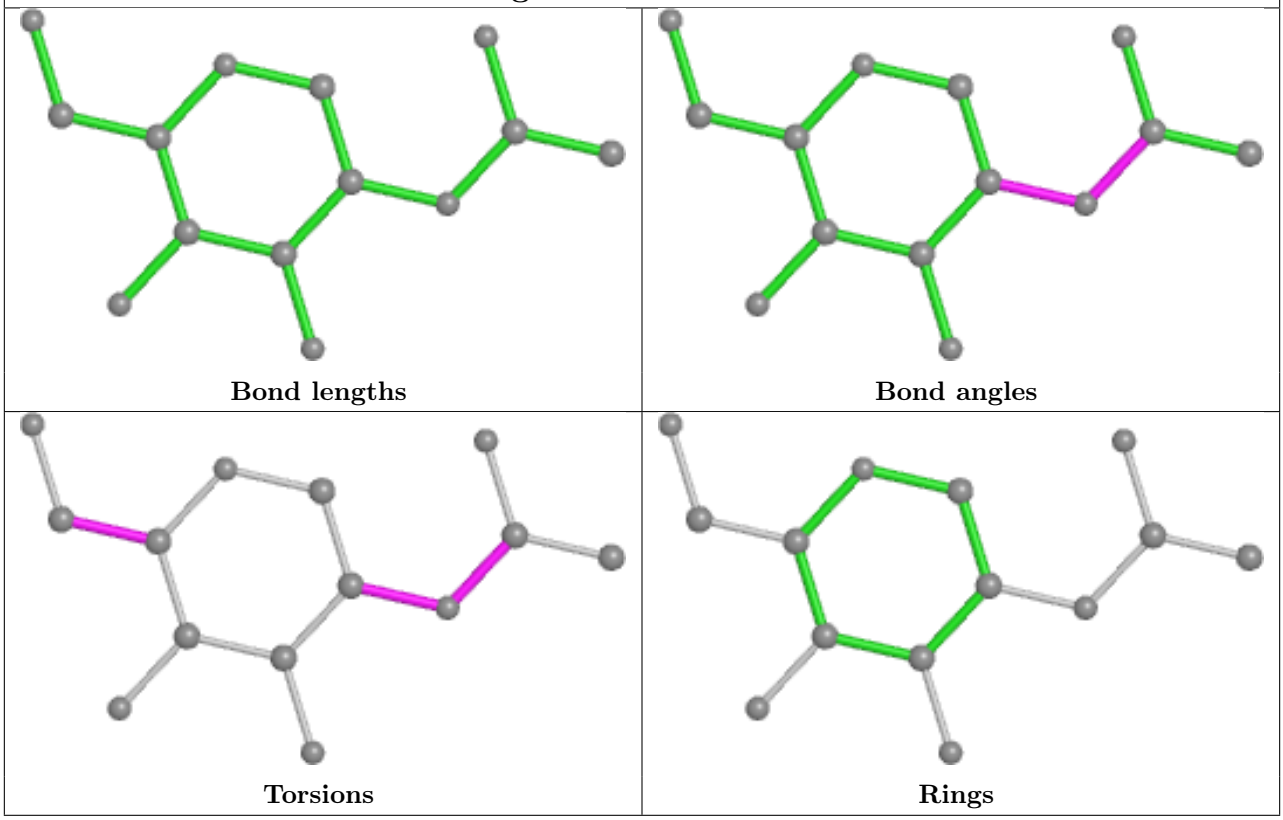
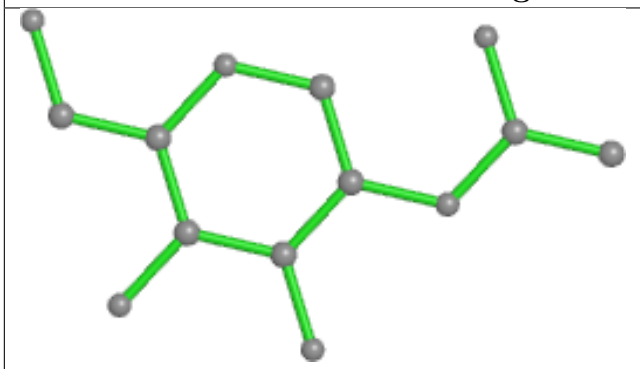
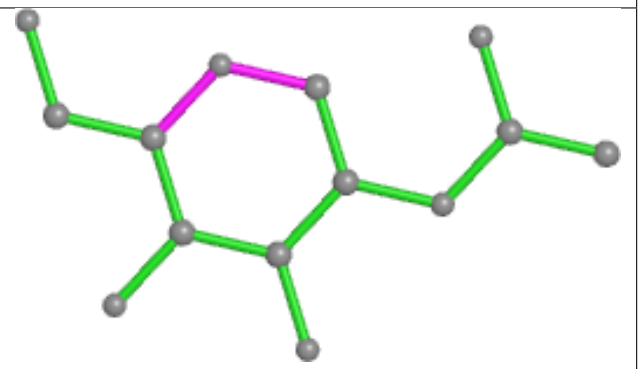
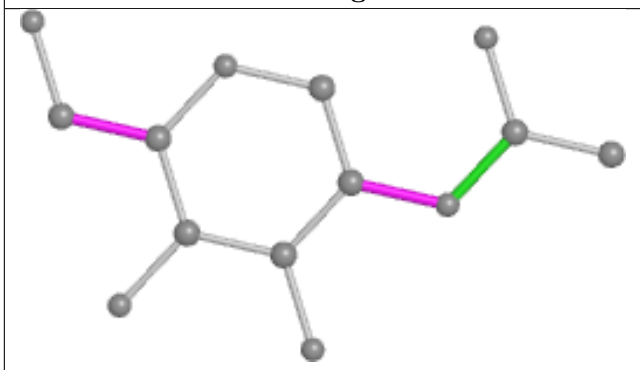
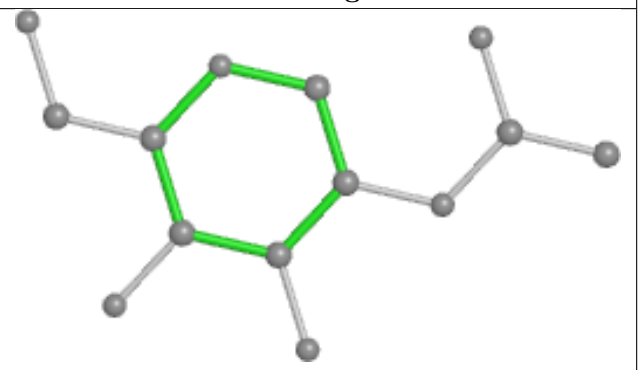


Ligand NAG B 1407	
 Bond lengths	 Bond angles
 Torsions	 Rings

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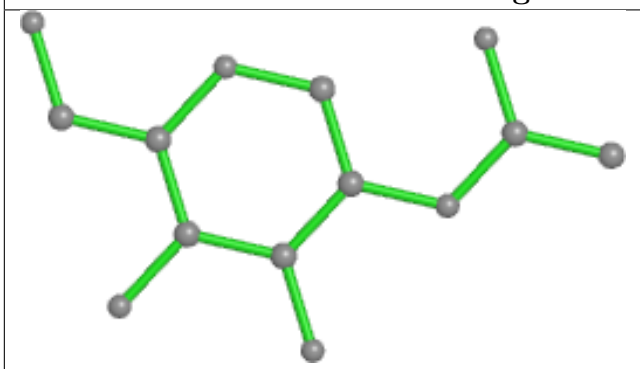
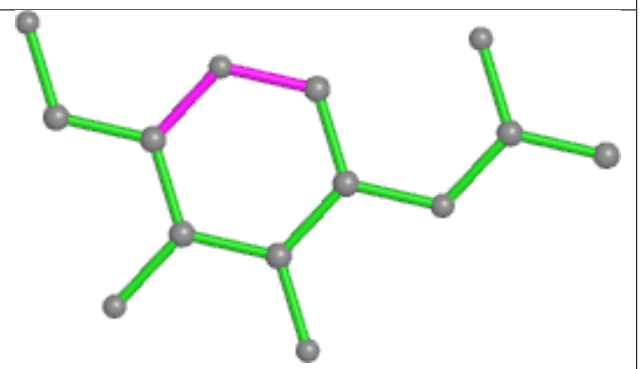
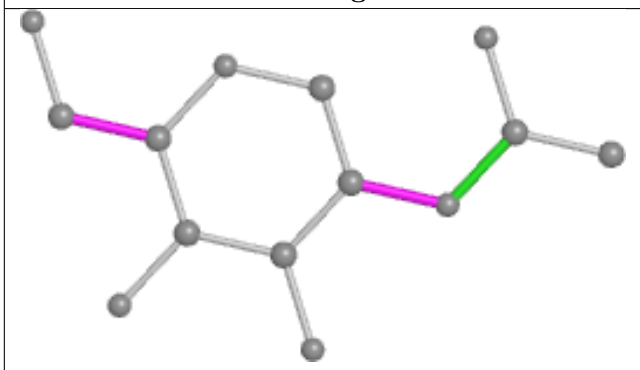
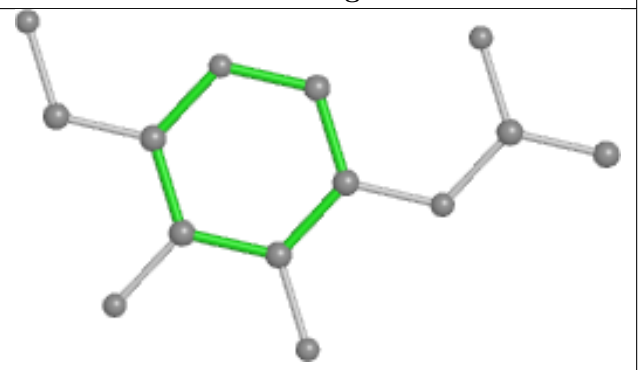
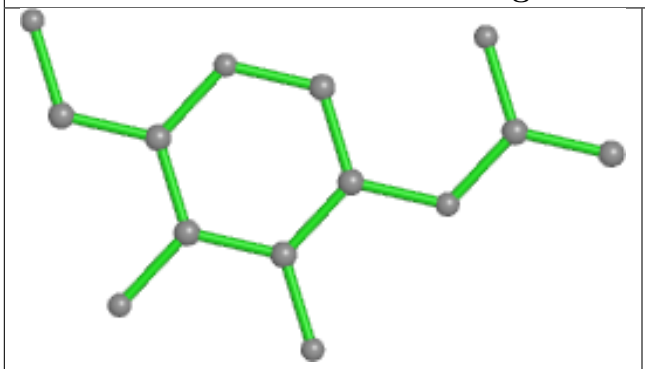
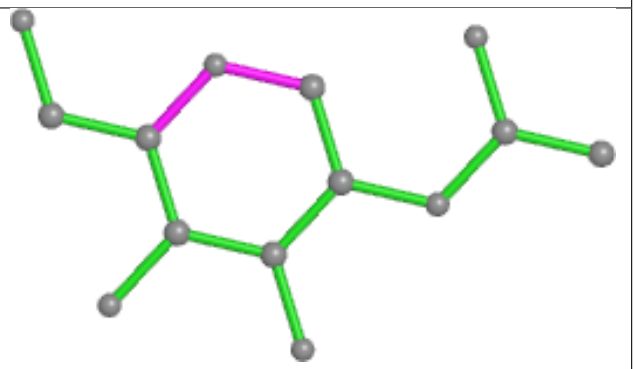
 Bond lengths	 Bond angles
 Torsions	 Rings

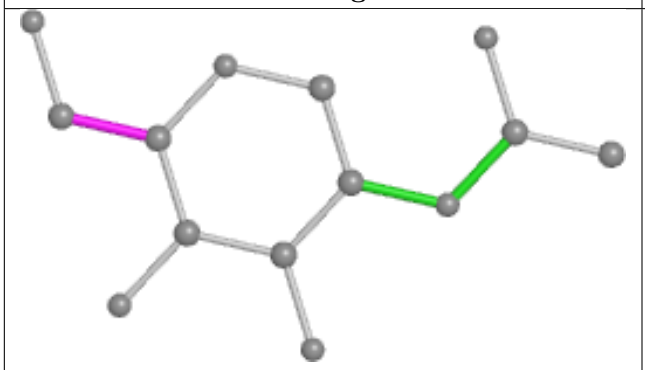
Ligand NAG C 1401



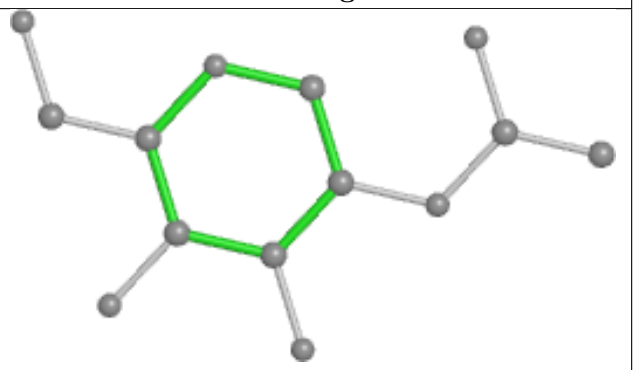
Bond lengths



Bond angles

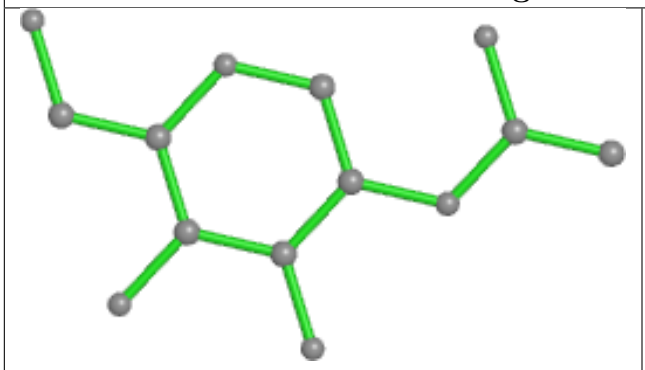


Torsions



Rings

Ligand NAG B 1409



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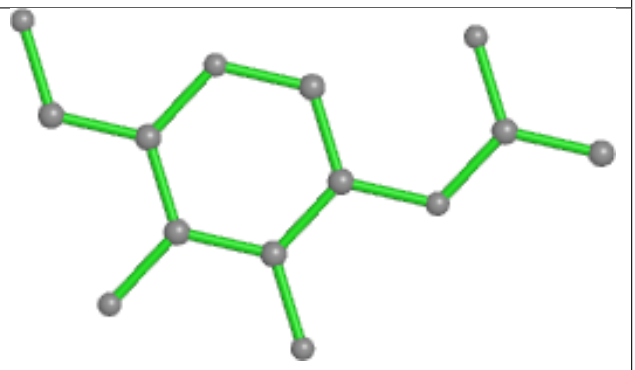
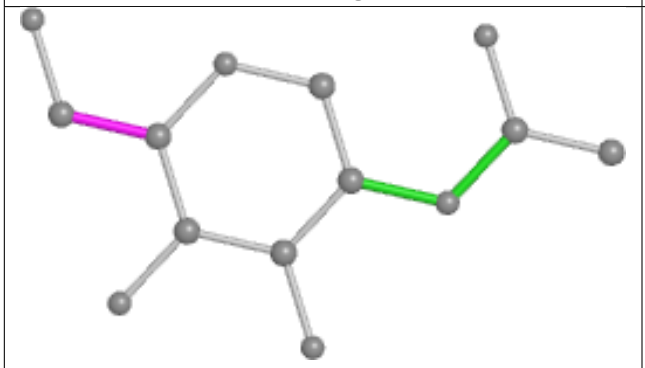


Bond angles



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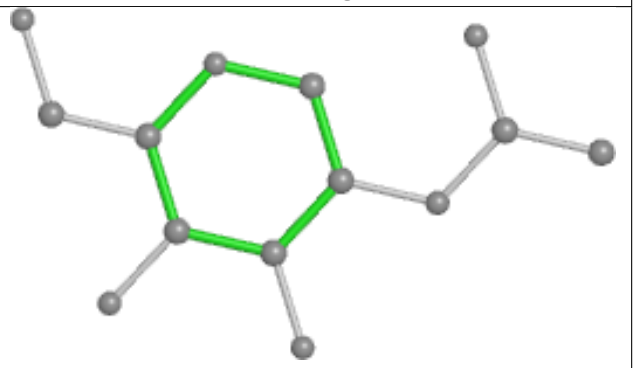
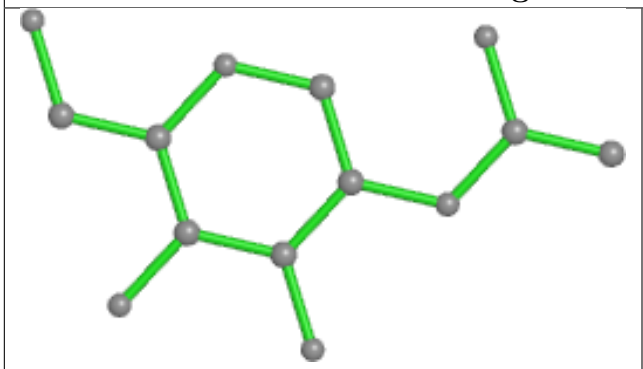
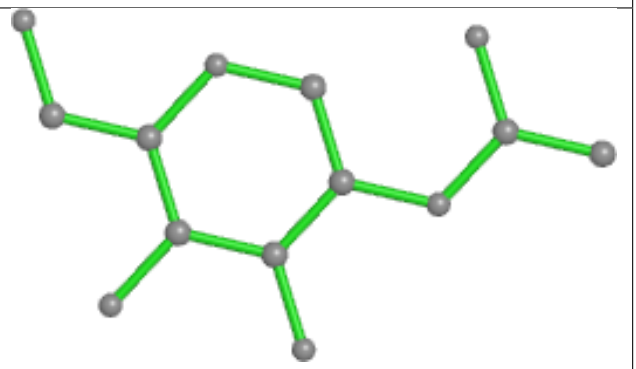


Rings

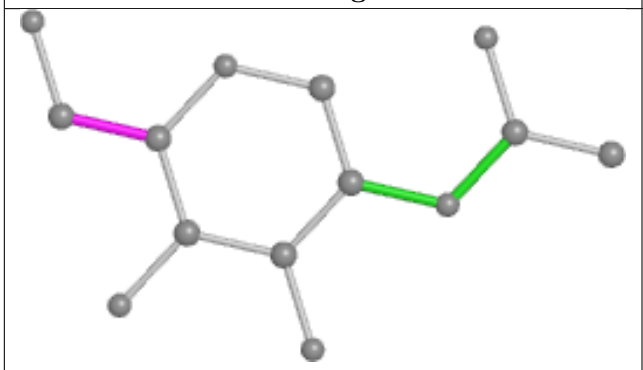
Ligand NAG A 1406



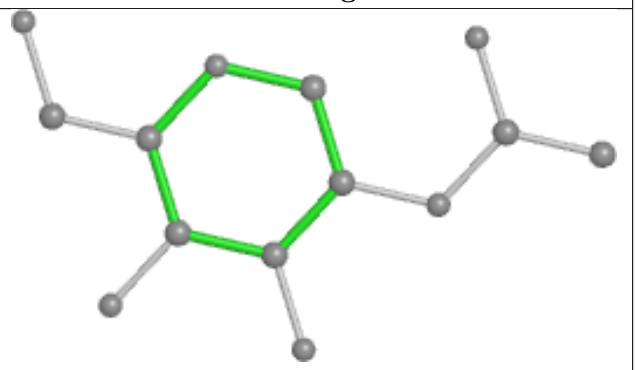
Bond lengths



Bond angles

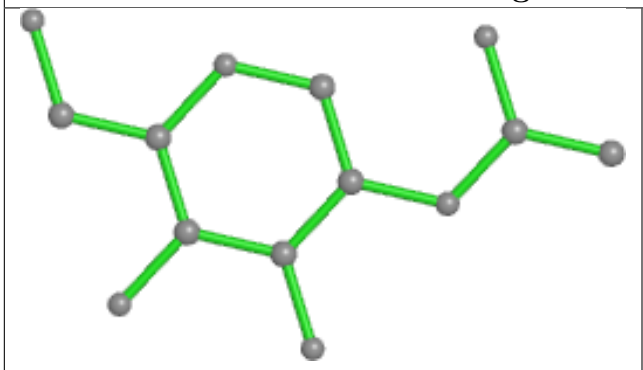


Torsions



Rings

Ligand NAG C 1408



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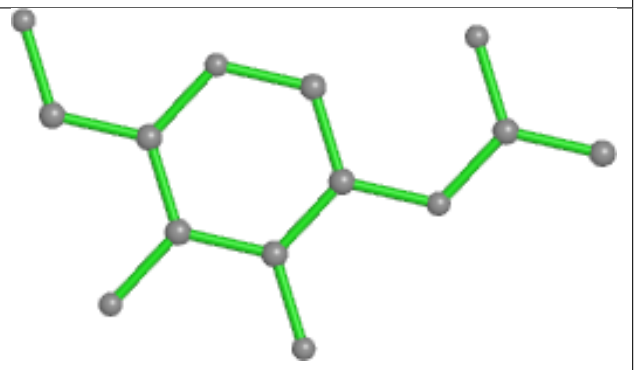
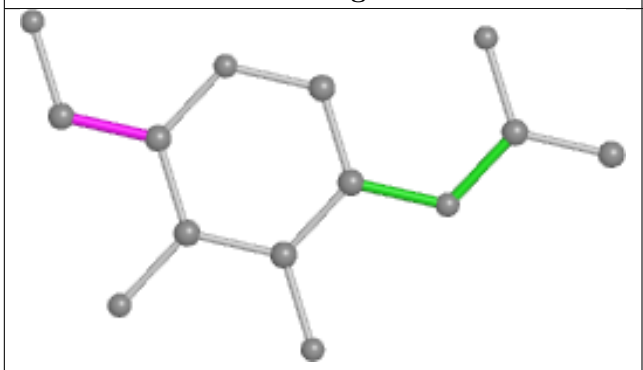


Bond angles



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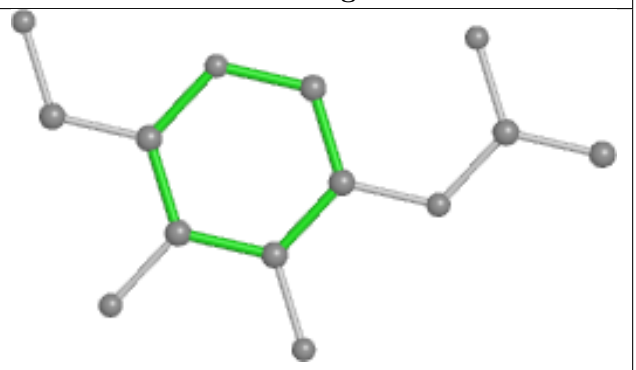
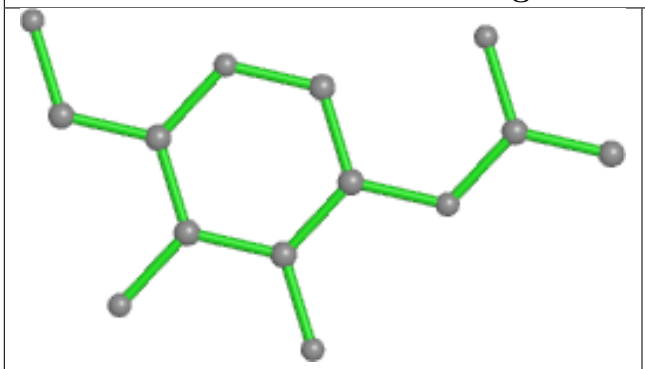


Rings

Ligand NAG C 1404



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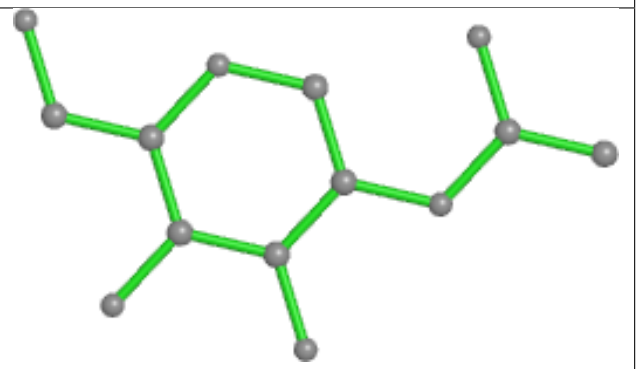
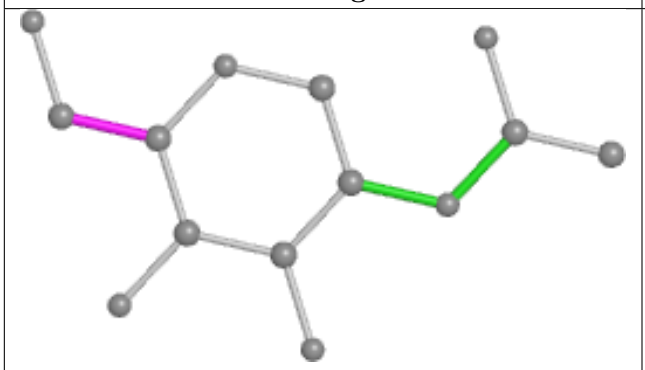
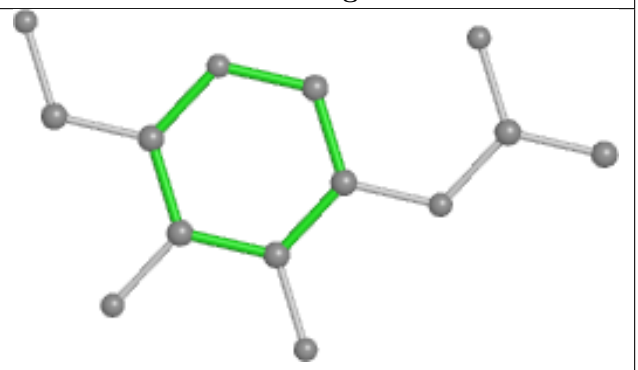


Bond angles

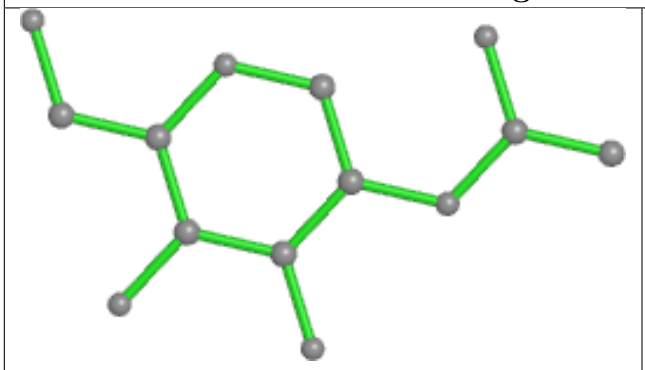


Torsions



Rings

Ligand NAG B 1403



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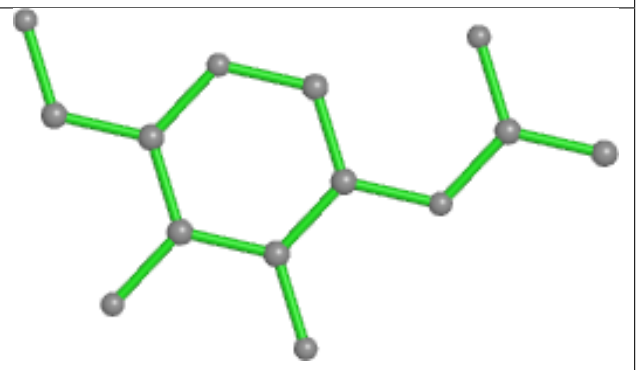
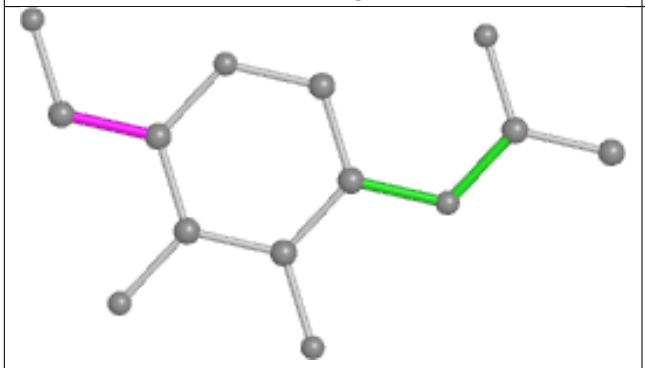
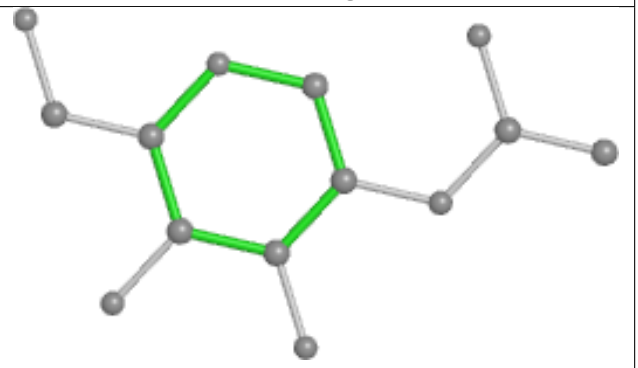


Bond angles

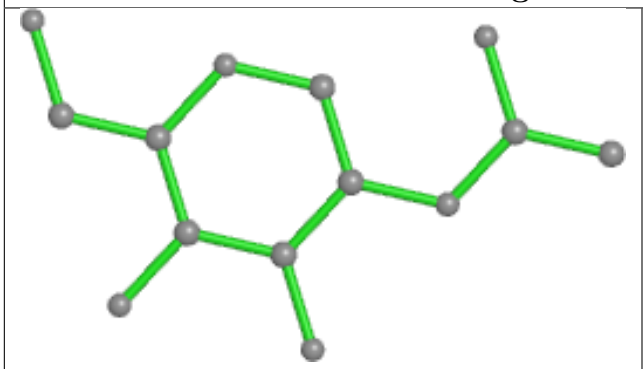


Torsions



Rings

Ligand NAG A 1409



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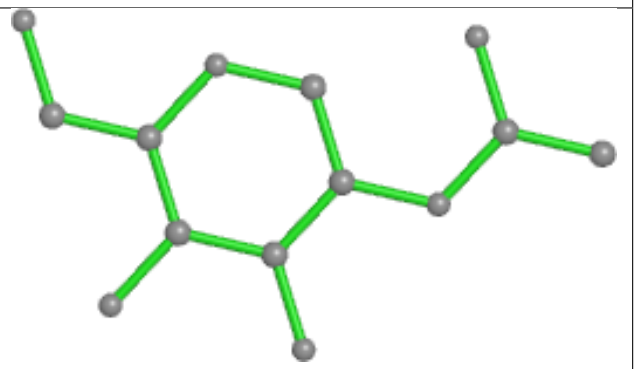
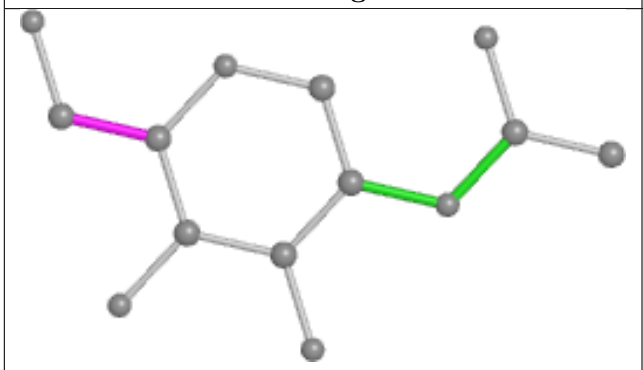
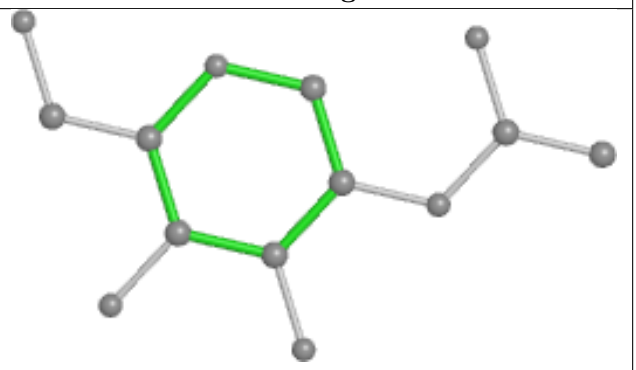


Bond angles

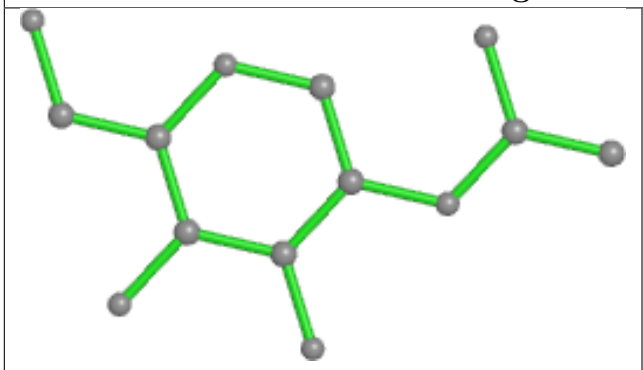


Torsions

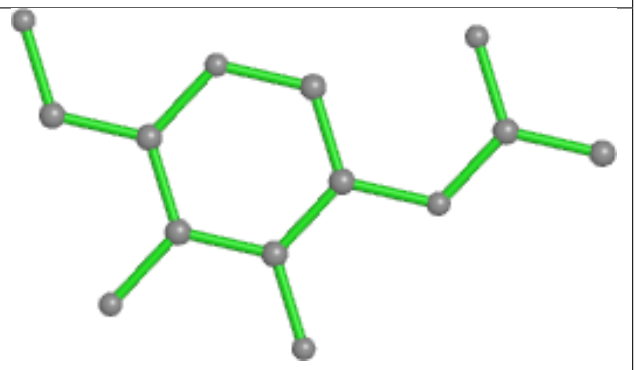


Rings

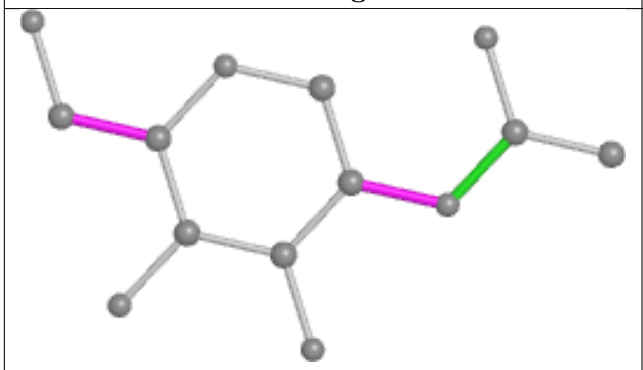
Ligand NAG C 1407



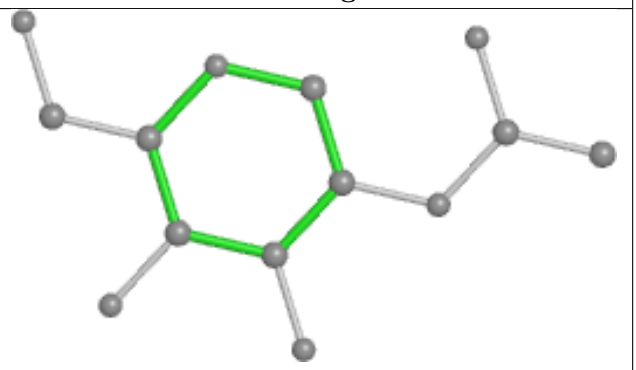
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

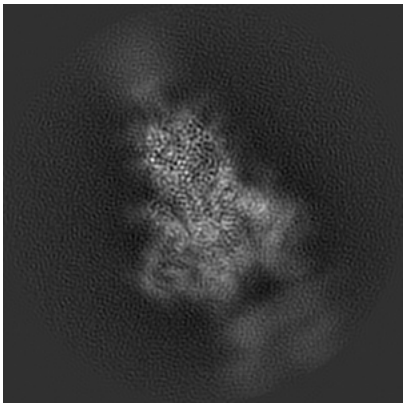
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30521. These allow visual inspection of the internal detail of the map and identification of artifacts.

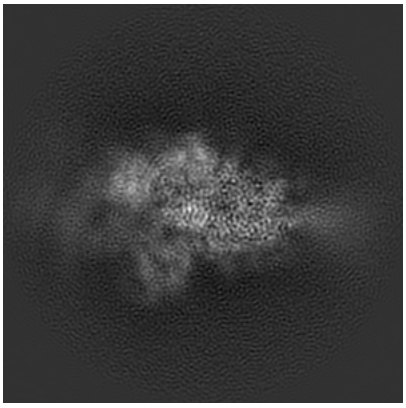
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

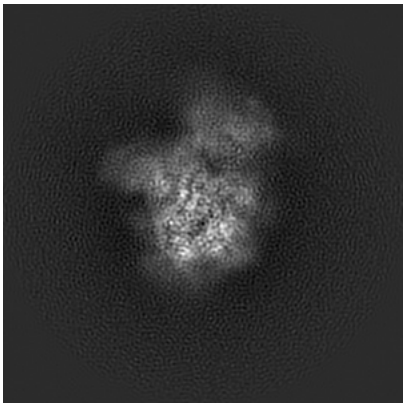
6.1.1 Primary map



X



Y

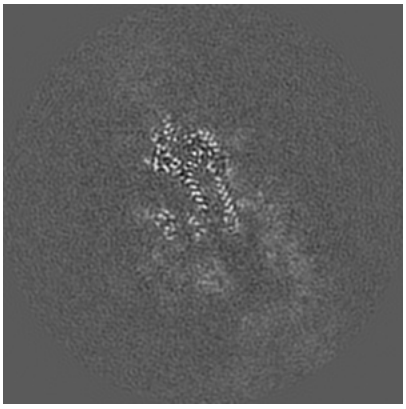


Z

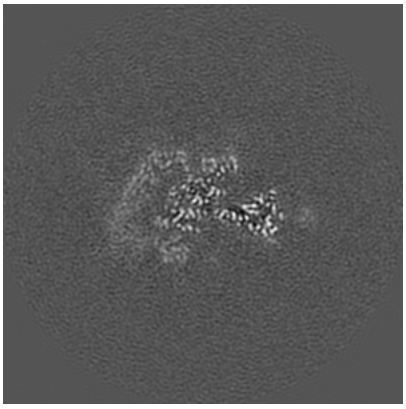
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

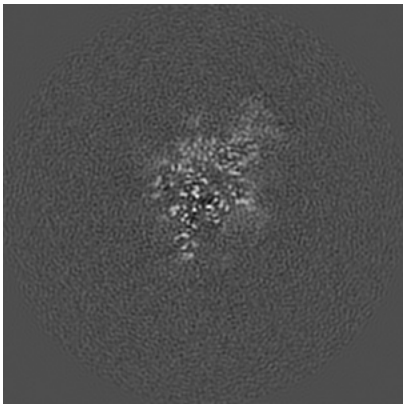
6.2.1 Primary map



X Index: 144



Y Index: 144

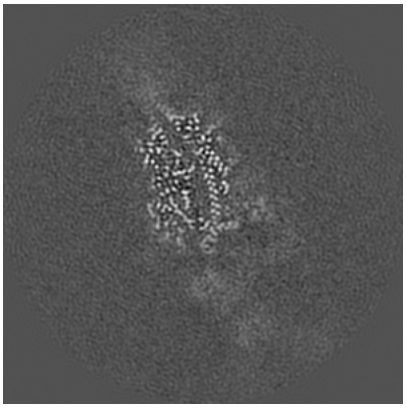


Z Index: 144

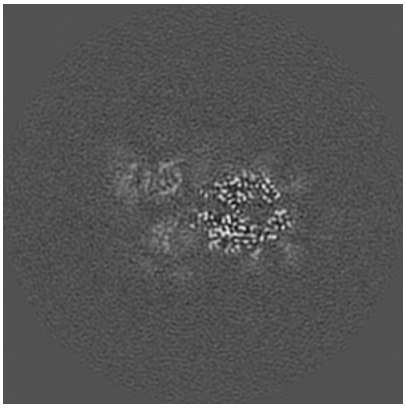
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

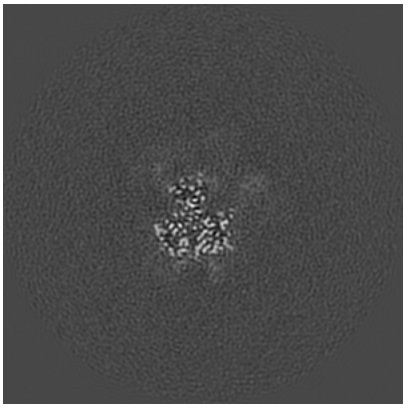
6.3.1 Primary map



X Index: 129



Y Index: 129



Z Index: 170

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

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

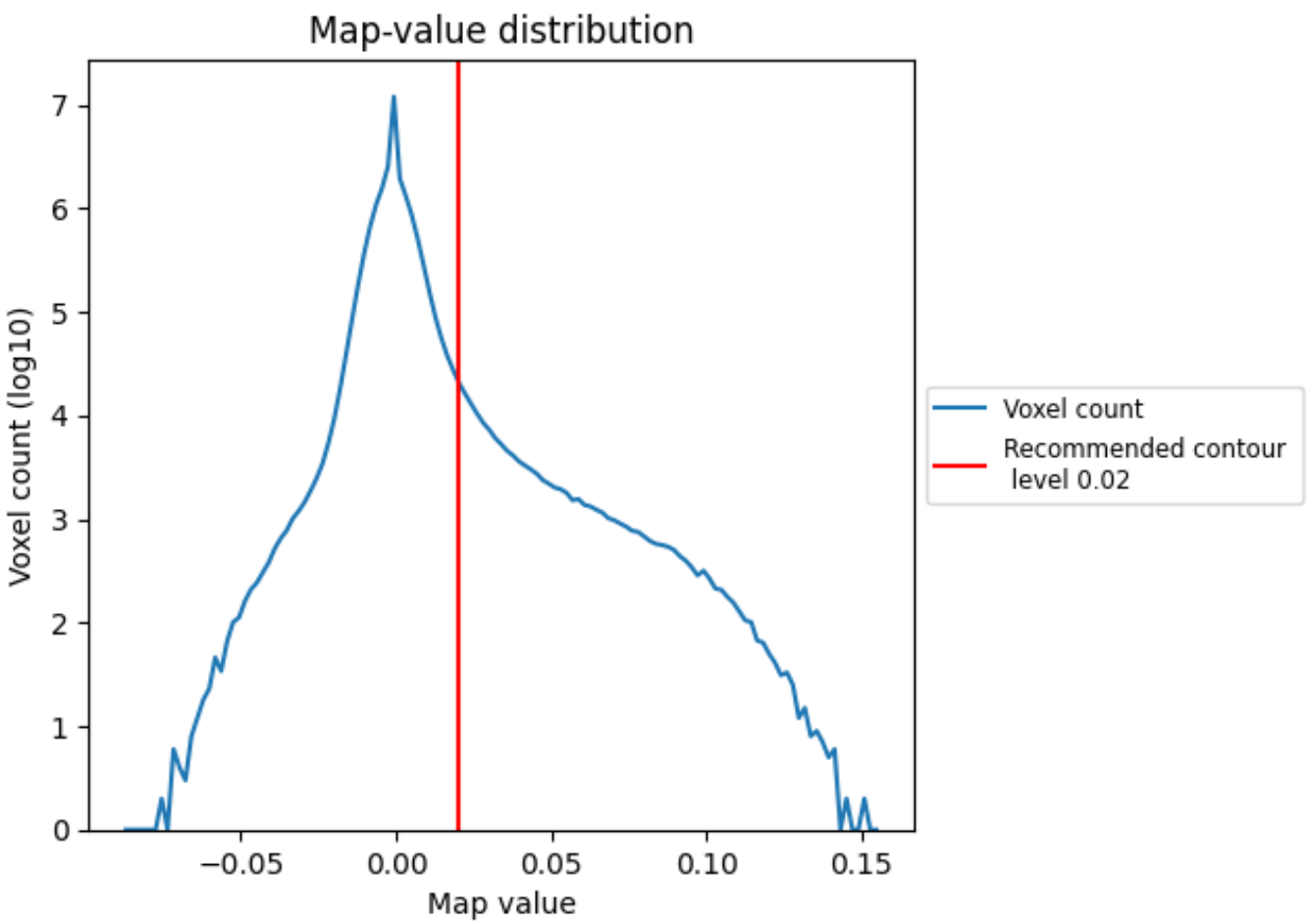
6.5 Mask visualisation (i)

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

7 Map analysis (i)

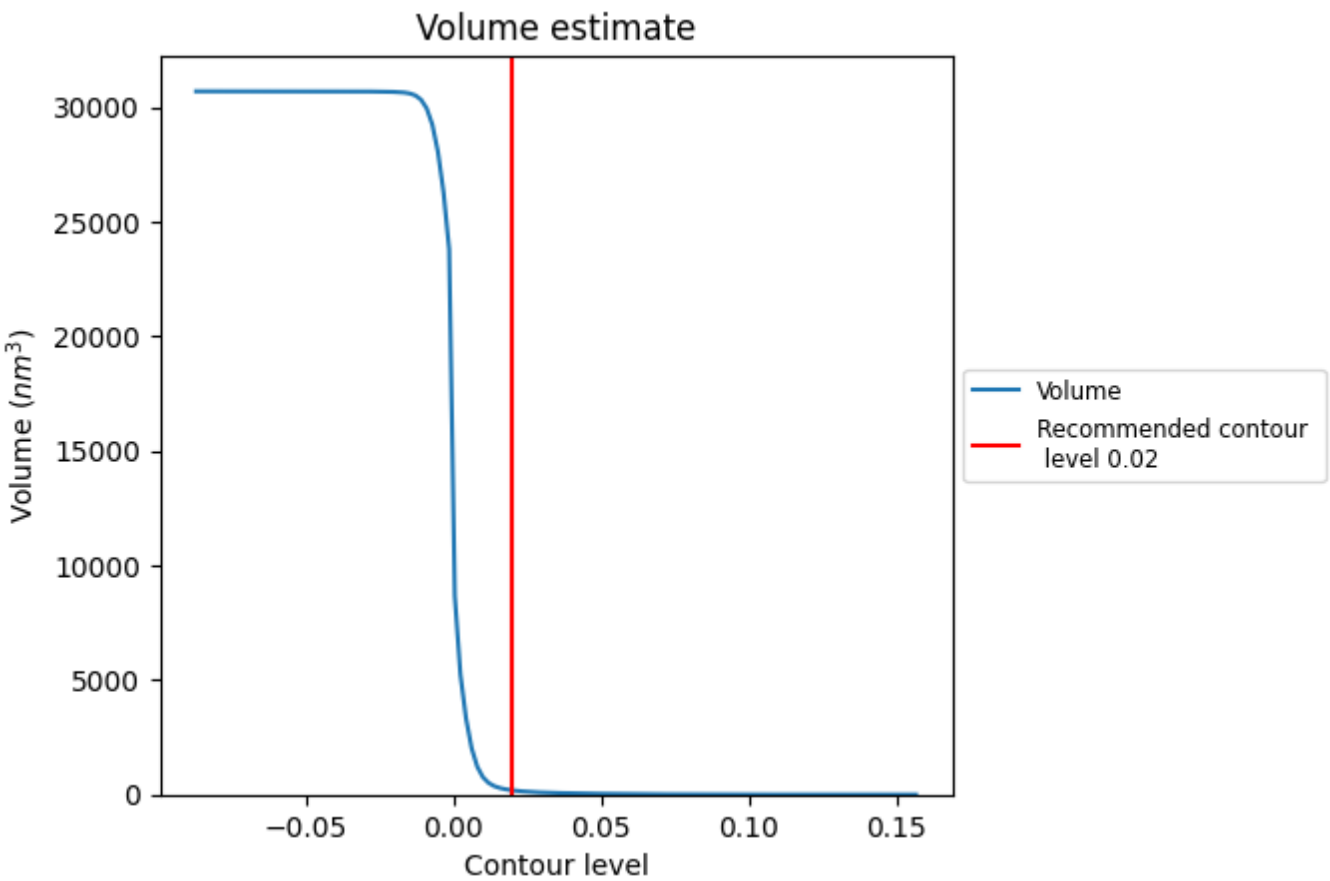
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

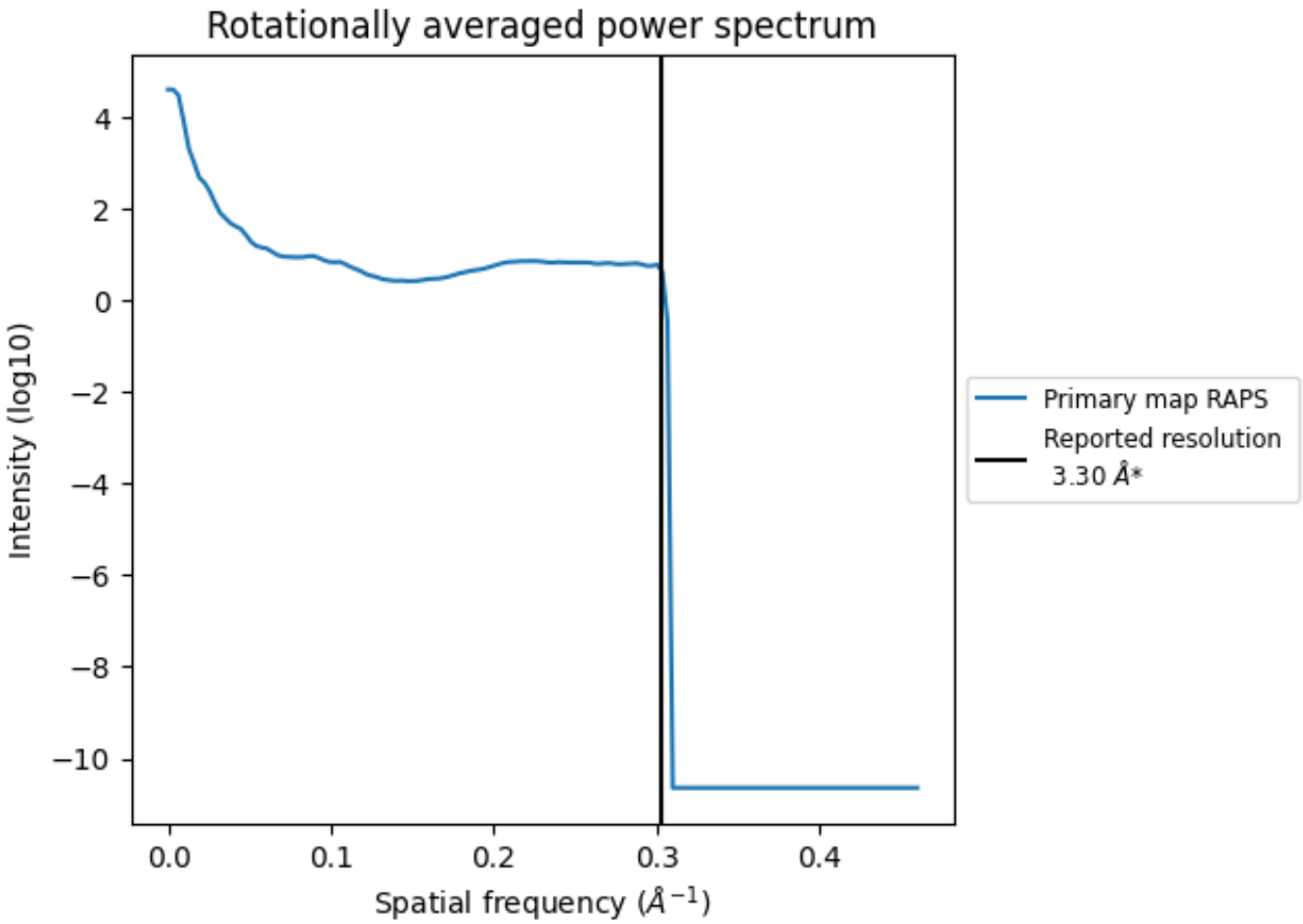
7.2 Volume estimate (i)



The volume at the recommended contour level is 186 nm^3; this corresponds to an approximate mass of 168 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 0.303 Å^{-1}

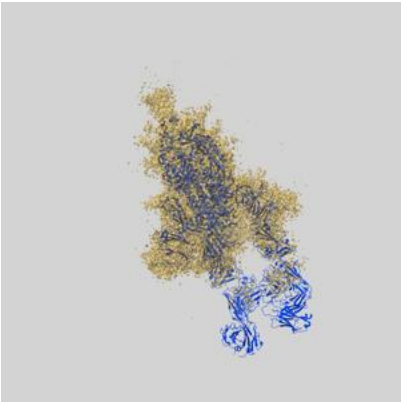
8 Fourier-Shell correlation (i)

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

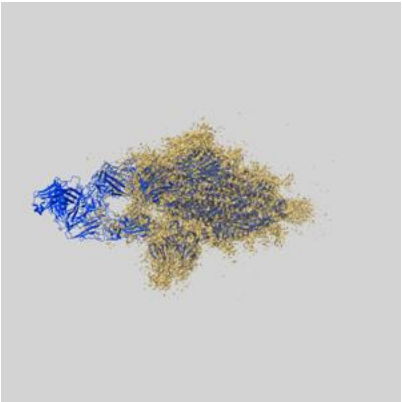
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30521 and PDB model 7CZY. Per-residue inclusion information can be found in section 3 on page 9.

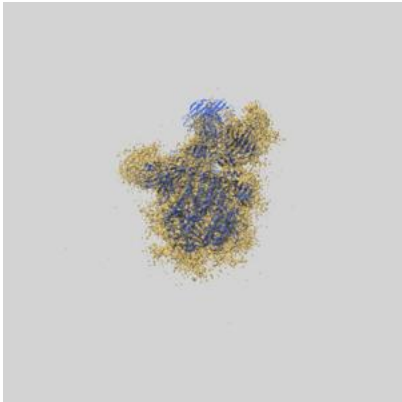
9.1 Map-model overlay (i)



X



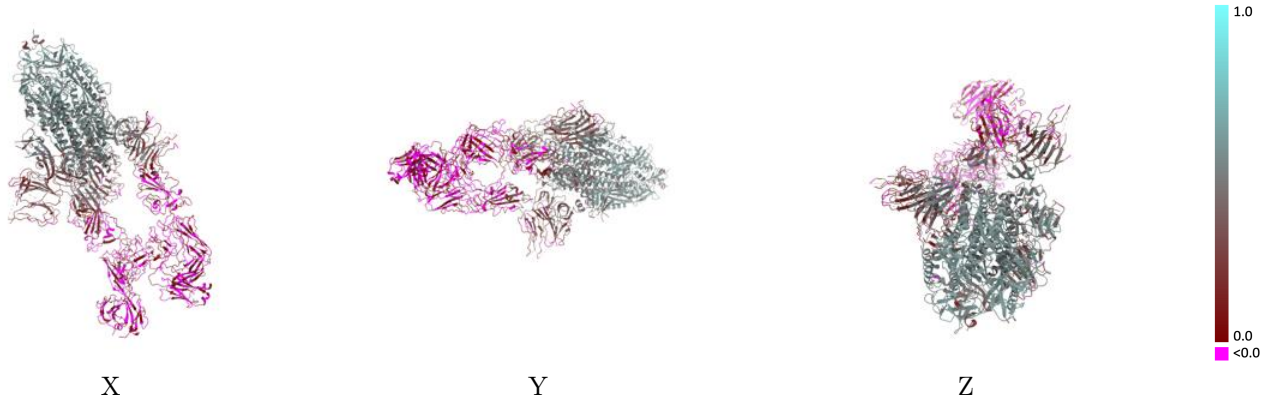
Y



Z

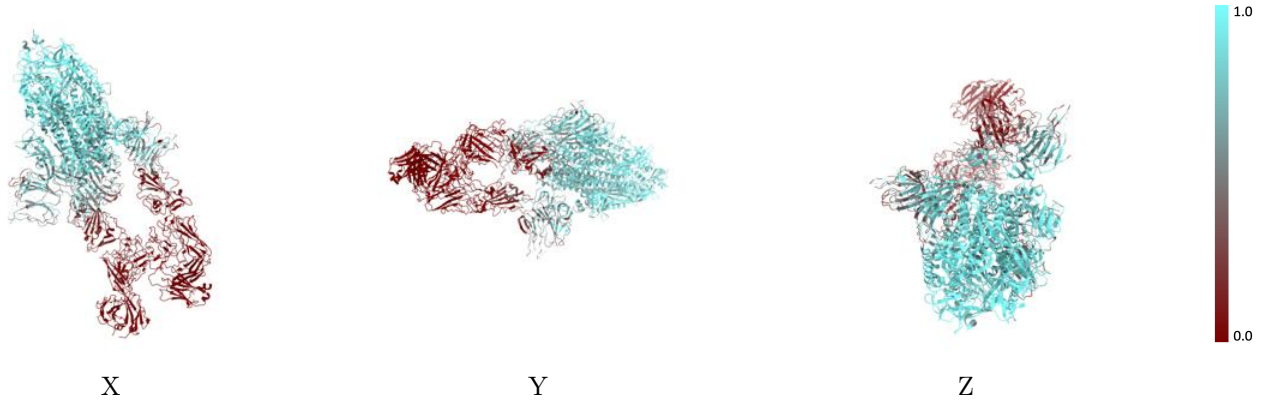
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



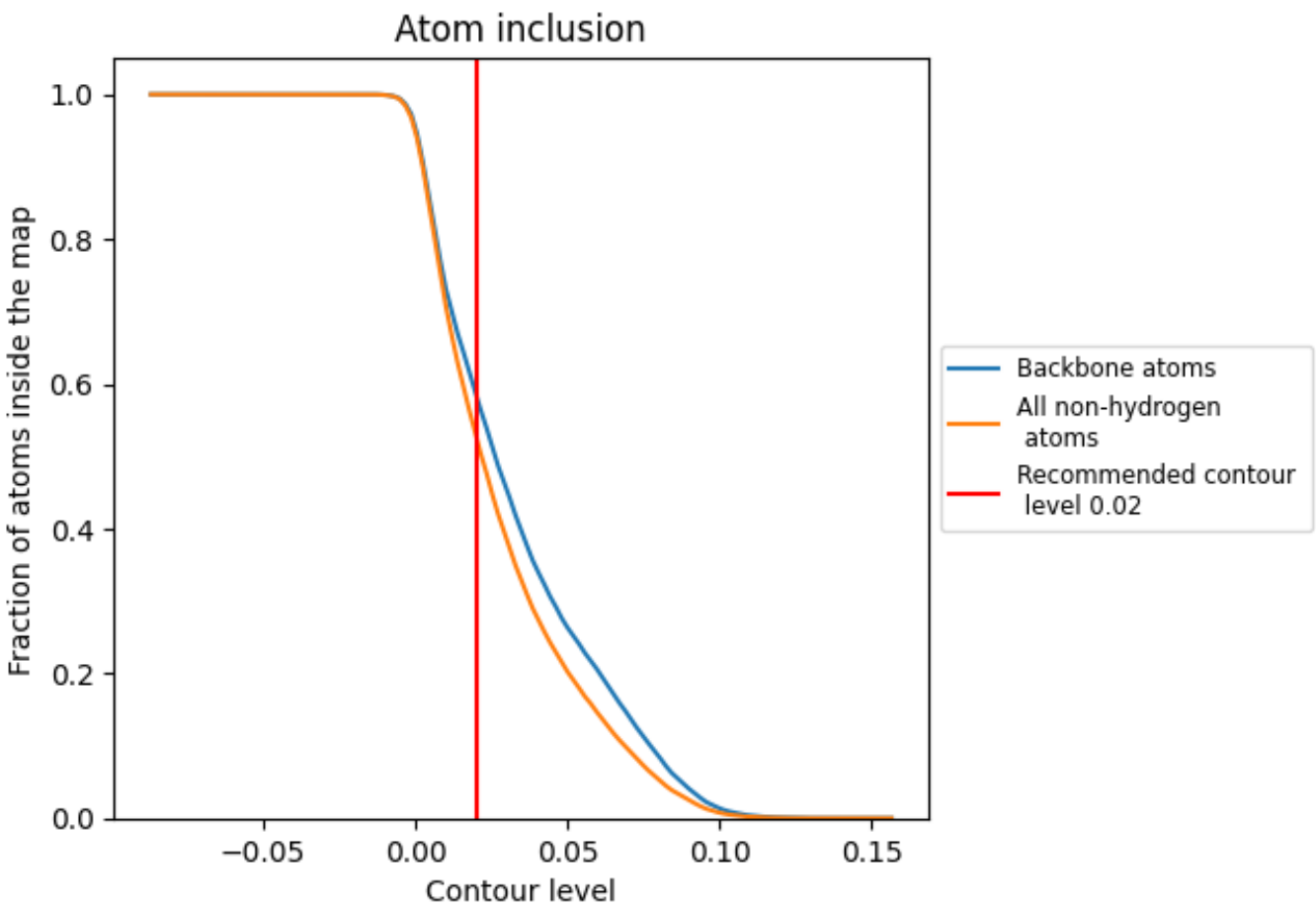
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.5276	0.3010
A	0.6304	0.3540
B	0.7606	0.4320
C	0.6372	0.3570
D	0.5000	0.2670
E	0.1429	0.1280
F	0.7500	0.4190
G	0.7143	0.3640
H	0.0061	0.0440
I	0.5000	0.2790
J	0.0061	0.0110
K	0.0108	0.0080
L	0.7857	0.4520
M	0.5714	0.3310
N	0.0048	0.0070
O	0.3214	0.1200
P	0.4643	0.3040
Q	0.7500	0.3940
R	0.6429	0.3320
S	0.7857	0.4030
T	0.7500	0.4350
U	0.1429	0.0590
V	0.0357	0.0550
W	0.5000	0.3600
X	0.8214	0.4360
Y	0.5357	0.2740
Z	0.3929	0.2840
a	0.7857	0.3800
b	0.6071	0.3050
c	0.0476	0.1150
d	0.0000	0.1400