Full wwPDB EM Validation Report

Sep 2, 2025 – 01:10 AM JST

PDB ID	:	9K75 / pdb_00009k75
EMDB ID	:	EMD-62145
Title	:	SARS-CoV-2 related bat coronavirus BANAL-103 spike in the closed state
Authors	:	Qingqing, L.; Xiao, C.; Xiaoning, L.; Yibing, Z.; Ru, L.; Zirui, K.; Didi, W.; Jiaxu, W.; Lili, L.; Junxia, Y.; Jianxiang, S.; Shuiling, J.; Ying, P.; Na, Z.; Yushun, W.; Jian, S.
Deposited on	:	2024-10-23
Resolution	:	3.11 Å(reported)

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

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

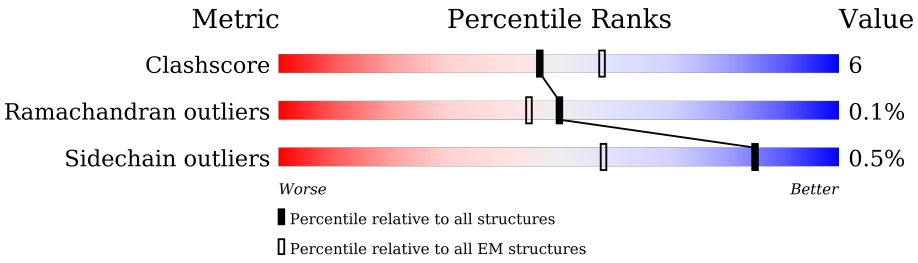
EMDB validation analysis	:	0.0.1.dev126
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

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 3.11 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1243	15% 74% 14% 12%
1	B	1243	15% 74% 14% 12%
1	C	1243	14% 75% 12% 12%

2 Entry composition

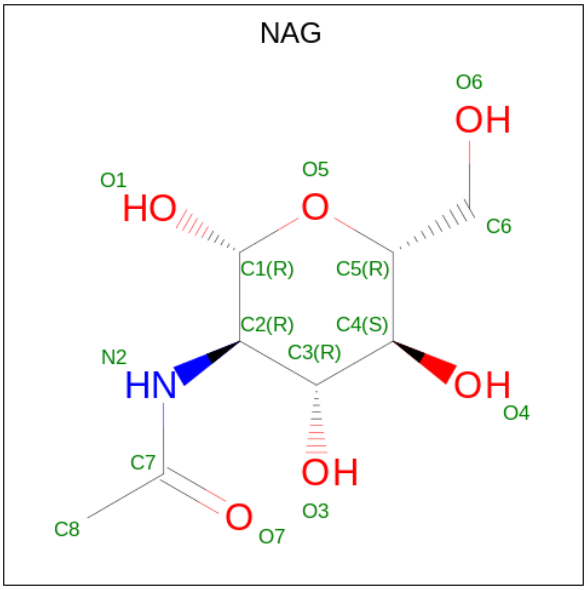
There are 2 unique types of molecules in this entry. The entry contains 26352 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1092	Total	C	N	O	S	0	0
			8504	5422	1414	1628	40		
1	B	1092	Total	C	N	O	S	0	0
			8504	5422	1414	1628	40		
1	C	1092	Total	C	N	O	S	0	0
			8504	5422	1414	1628	40		

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



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

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

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

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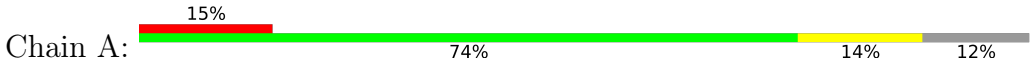
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2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

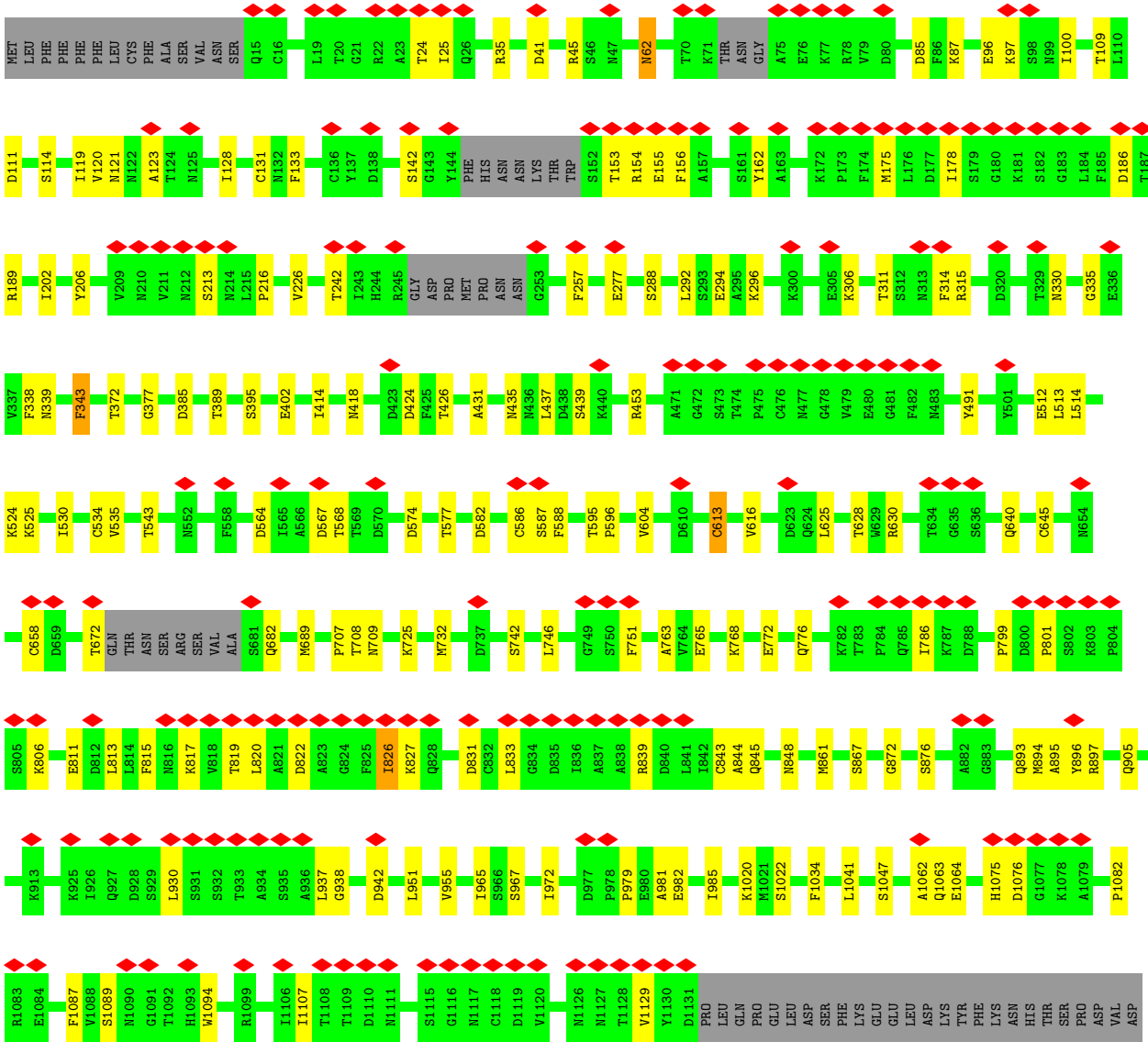
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

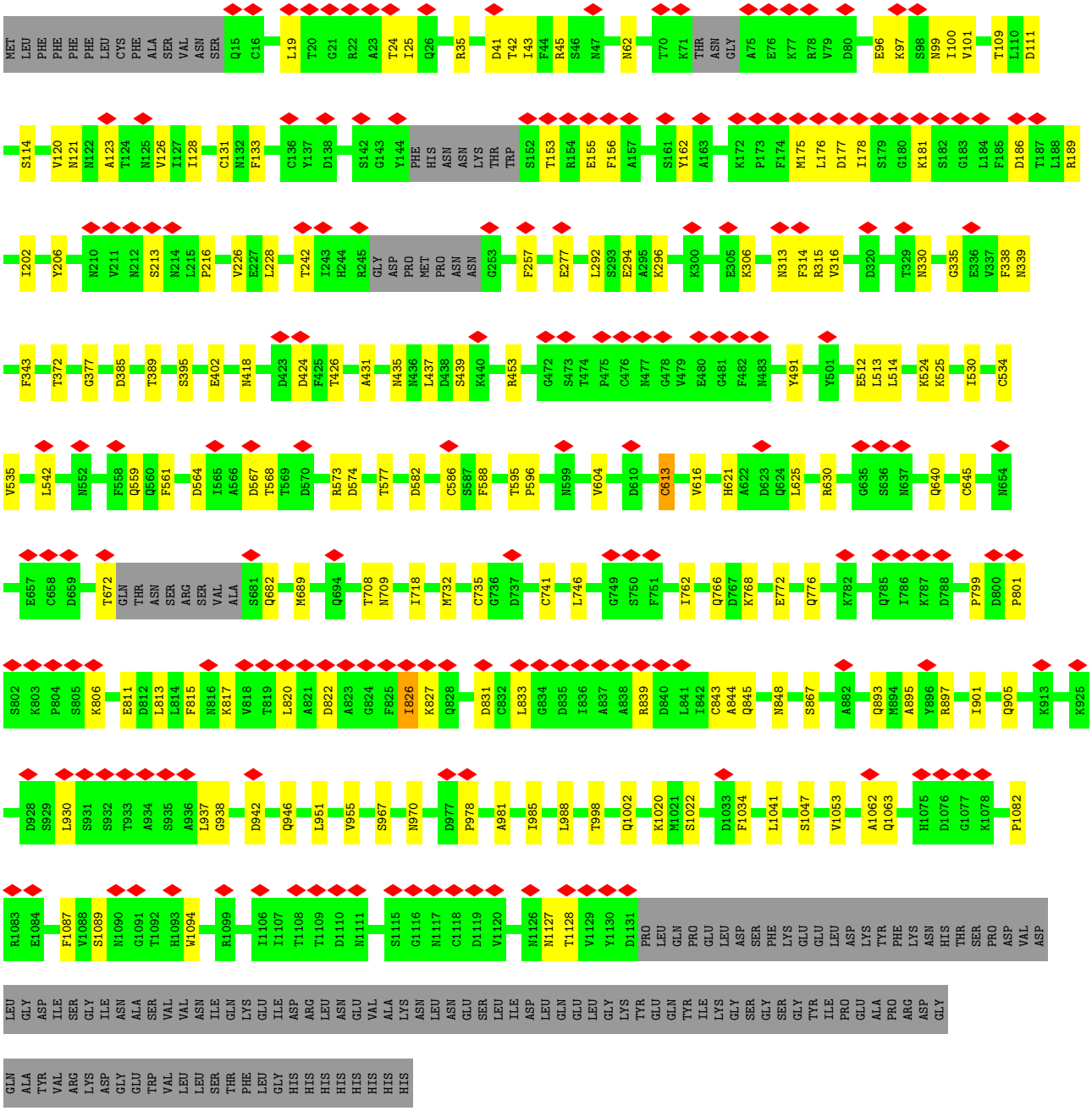
Chain A:





• Molecule 1: Spike glycoprotein

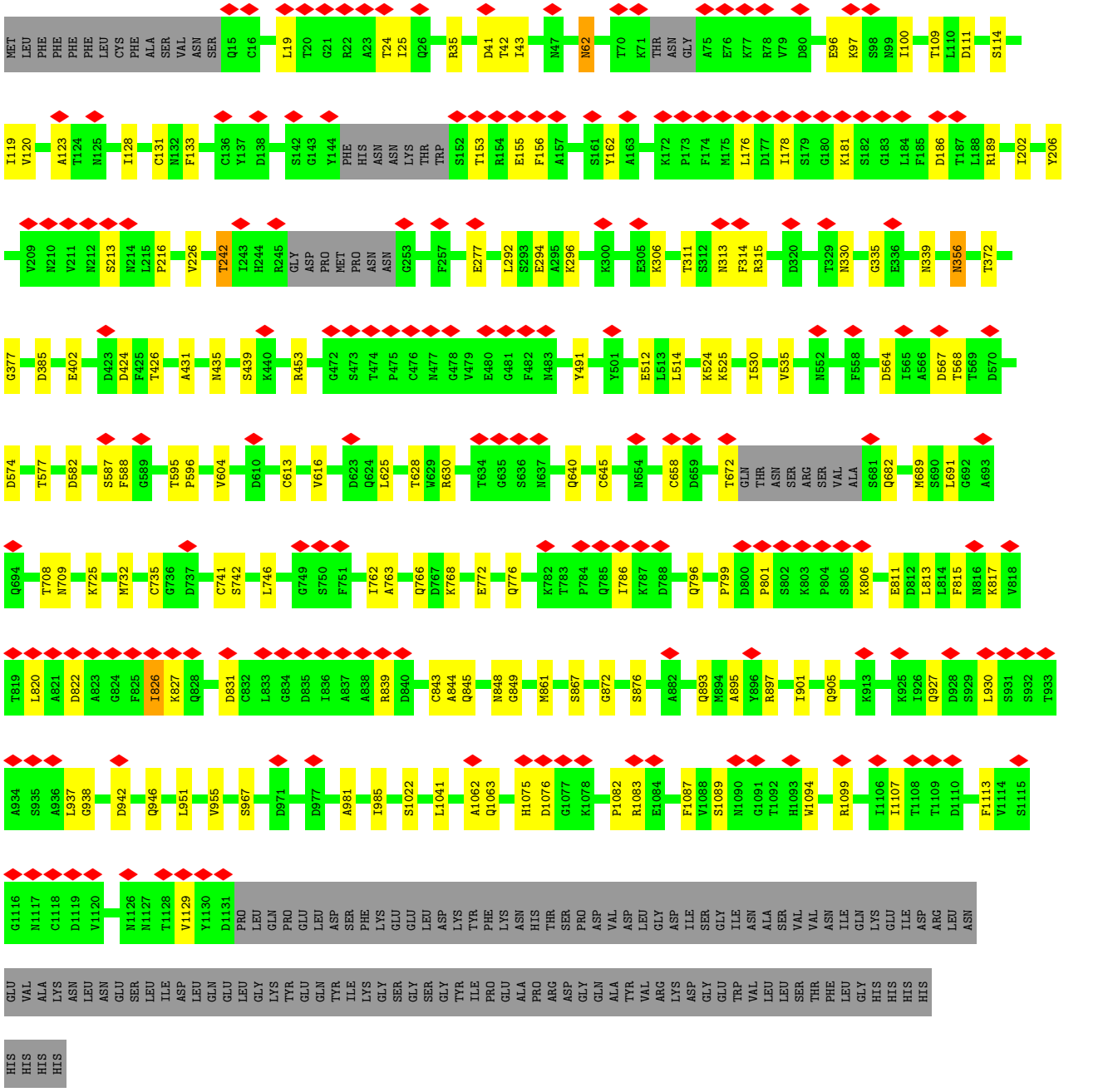
Chain B:



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

• Molecule 1: Spike glycoprotein

Chain C:


MET LEU PHE PHE PHE LEU CYS PHE ALA SER VAL ASN SER Q15 C16 L19 T20 G21 R22 A23 T24 I25 Q26 R35 D41 T42 I43 M47 N62 T70 K71 THR ASN GLY A75 E76 K77 R78 V79 D80 E96 K97 S98 N99 I100 T109 L110 D111 S114
I119 V120 A123 T124 N125 I128 C131 N132 F133 C136 Y137 D138 S142 G143 Y144 PHE HIS ASN ASN LYS THR TRP S152 T153 R154 E155 F156 A157 S161 Y162 A163 K172 P173 F174 M175 L176 D177 I178 S179 G180 K181 S182 G183 L184 F185 D186 T187 L188 R189 I202 Y206
V209 N210 V211 N212 S213 N214 L215 P216 V226 T242 I243 H244 R245 GLY ASP PRO MET PRO ASN ASN G253 F257 E277 L292 S293 E294 A295 K296 K300 E305 K306 T311 S312 N313 F314 R315 D320 T329 N330 G335 E336 N339 N356 T372
G377 D385 E402 D423 D424 F425 T426 A431 N435 S439 K440 R453 G472 S473 T474 P475 C476 N477 G478 V479 E480 G481 F482 N483 Y491 Y501 E512 L513 L514 K524 K525 I530 V535 N552 F558 D564 I565 A566 D567 T568 T569 D570
D574 T577 D582 S587 F588 G589 T595 P596 V604 D610 C613 V616 D623 Q624 L625 T628 W629 R630 T634 G635 S636 N637 Q640 C645 N654 C658 D659 T672 GLN THR ASN SER ARG SER VAL ALA S681 Q682 M689 S690 L691 G692 A693
Q694 T708 N709 K725 M732 C735 G736 D737 C741 S742 L746 G749 S750 F751 I762 A763 Q766 D767 K768 E772 Q776 K782 T783 P784 Q785 I786 K787 D788 Q796 P799 D800 P801 S802 K803 P804 S805 K806 E811 D812 L813 L814 F815 N816 K817 V818
T819 L820 A821 D822 A823 G824 F825 I826 K827 Q828 D831 C832 L833 G834 D835 I836 A837 A838 R839 D840 C843 A844 Q845 N848 G849 M861 S867 G872 S876 A882 Q893 N894 A895 Y896 R897 I901 Q905 K913 K925 I926 Q927 D928 S929 L930 S931 S932 T933
A934 S935 A936 L937 G938 D942 Q946 L951 V955 S967 D971 D977 A981 I985 S1022 L1041 A1062 Q1063 H1075 D1076 G1077 K1078 P1082 R1083 E1084 F1087 V1088 S1089 N1090 G1091 T1092 H1093 W1094 R1099 T1106 I1107 T1108 T1109 D1110 F1113 V1114 S1115
G1116 N1117 C1118 D1119 V1120 N1126 N1127 T1128 V1129 Y1130 D1131 PRO LEU GLN PRO GLU LEU ASP SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN
GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS GLY SER GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLU TRP VAL LEU LEU SER THR PHE LEU GLY HIS HIS HIS HIS
HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.136	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	348.6, 348.6, 348.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.11	0/8697	0.29	0/11838
1	B	0.12	0/8697	0.30	0/11838
1	C	0.11	0/8697	0.29	0/11838
All	All	0.11	0/26091	0.29	0/35514

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	8504	0	8269	107	0
1	B	8504	0	8269	111	0
1	C	8504	0	8269	101	0
2	A	280	0	260	2	0
2	B	280	0	260	2	0
2	C	280	0	260	2	0
All	All	26352	0	25587	308	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 6.

All (308) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:HE1	1:A:588:PHE:H	1.37	0.73
1:C:826:ILE:HG22	1:C:827:LYS:H	1.54	0.71
1:A:820:LEU:HG	1:A:822:ASP:H	1.56	0.71
1:B:820:LEU:HG	1:B:822:ASP:H	1.56	0.71
1:B:826:ILE:HG22	1:B:827:LYS:H	1.55	0.70
1:A:121:ASN:HD22	1:A:175:MET:HB2	1.54	0.70
1:C:820:LEU:HG	1:C:822:ASP:H	1.56	0.70
1:A:894:MET:HB3	1:A:908:LEU:HD11	1.74	0.69
1:A:97:LYS:HE2	1:A:186:ASP:HB2	1.75	0.69
1:B:97:LYS:HE2	1:B:186:ASP:HB2	1.75	0.69
1:C:109:THR:HG1	1:C:114:SER:HG	1.40	0.68
1:C:97:LYS:HE2	1:C:186:ASP:HB2	1.74	0.68
1:A:895:ALA:HB1	1:A:905:GLN:HB2	1.75	0.67
1:C:356:ASN:ND2	1:C:356:ASN:O	2.27	0.66
1:C:314:PHE:HE1	1:C:588:PHE:H	1.44	0.66
1:A:826:ILE:HG22	1:A:827:LYS:H	1.62	0.65
1:A:109:THR:HG1	1:A:114:SER:HG	1.46	0.64
1:C:895:ALA:HB1	1:C:905:GLN:HB2	1.79	0.63
1:A:453:ARG:NH2	2:B:1319:NAG:O7	2.32	0.63
1:A:732:MET:SD	1:C:587:SER:OG	2.56	0.63
1:C:817:LYS:HD2	1:C:937:LEU:HD13	1.80	0.63
1:B:314:PHE:HE1	1:B:588:PHE:H	1.46	0.62
2:A:1319:NAG:O7	1:C:453:ARG:NH2	2.33	0.62
1:B:453:ARG:NH2	2:C:1319:NAG:O7	2.33	0.62
1:A:613:CYS:HA	1:A:616:VAL:HG23	1.82	0.62
1:B:640:GLN:HA	1:B:645:CYS:HB2	1.81	0.62
1:B:817:LYS:HD2	1:B:937:LEU:HD13	1.82	0.60
1:B:895:ALA:HB1	1:B:905:GLN:HB2	1.83	0.60
1:A:213:SER:O	1:A:213:SER:OG	2.20	0.60
1:A:640:GLN:HA	1:A:645:CYS:HB2	1.82	0.59
1:A:402:GLU:OE1	1:A:491:TYR:OH	2.21	0.59
1:B:613:CYS:HA	1:B:616:VAL:HG23	1.84	0.58
1:A:817:LYS:HD2	1:A:937:LEU:HD13	1.85	0.58
1:B:435:ASN:O	1:B:439:SER:OG	2.21	0.58
1:C:640:GLN:HA	1:C:645:CYS:HB2	1.84	0.58
1:B:845:GLN:HG2	1:B:955:VAL:HG21	1.86	0.58
1:A:587:SER:OG	1:B:732:MET:SD	2.62	0.57
1:A:896:TYR:CE1	1:C:1099:ARG:HD2	2.39	0.57
1:A:1075:HIS:ND1	1:A:1076:ASP:OD1	2.38	0.56
1:A:435:ASN:O	1:A:439:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:GLU:OE1	1:B:491:TYR:OH	2.22	0.56
1:B:123:ALA:HB3	2:B:1302:NAG:H82	1.87	0.56
1:B:998:THR:O	1:B:1002:GLN:HG2	2.05	0.56
1:A:277:GLU:N	1:A:277:GLU:OE1	2.39	0.56
1:A:1020:LYS:NZ	1:A:1034:PHE:O	2.33	0.56
1:C:732:MET:HE3	1:C:849:GLY:HA2	1.88	0.55
1:B:277:GLU:OE1	1:B:277:GLU:N	2.39	0.55
1:C:123:ALA:HB3	2:C:1302:NAG:H82	1.88	0.55
1:C:435:ASN:O	1:C:439:SER:OG	2.24	0.55
1:A:845:GLN:HG2	1:A:955:VAL:HG21	1.87	0.55
1:C:845:GLN:HG2	1:C:955:VAL:HG21	1.88	0.55
1:B:424:ASP:OD1	1:B:424:ASP:N	2.38	0.55
1:C:313:ASN:O	1:C:315:ARG:HD3	2.07	0.55
1:C:189:ARG:HG2	1:C:206:TYR:HD1	1.72	0.55
1:C:277:GLU:N	1:C:277:GLU:OE1	2.39	0.55
1:B:189:ARG:HG2	1:B:206:TYR:HD1	1.70	0.55
1:C:335:GLY:O	1:C:339:ASN:HB2	2.07	0.55
1:B:559:GLN:NE2	1:B:561:PHE:O	2.40	0.54
1:C:844:ALA:O	1:C:848:ASN:ND2	2.33	0.54
1:A:896:TYR:HE1	1:C:1099:ARG:HD2	1.71	0.54
1:A:189:ARG:HG2	1:A:206:TYR:HD1	1.73	0.54
1:B:951:LEU:O	1:B:955:VAL:HG23	2.08	0.54
1:C:951:LEU:O	1:C:955:VAL:HG23	2.07	0.54
1:A:330:ASN:OD1	1:A:330:ASN:N	2.41	0.54
1:A:839:ARG:HB3	1:A:843:CYS:HB2	1.90	0.54
1:A:1107:ILE:HG22	1:A:1129:VAL:HG13	1.89	0.54
1:C:424:ASP:OD1	1:C:424:ASP:N	2.38	0.54
1:A:123:ALA:HB3	2:A:1302:NAG:H82	1.90	0.54
1:A:844:ALA:O	1:A:848:ASN:ND2	2.31	0.54
1:B:306:LYS:HG3	1:B:596:PRO:HA	1.90	0.54
1:C:613:CYS:HA	1:C:616:VAL:HG23	1.90	0.54
1:B:41:ASP:OD1	1:B:43:ILE:N	2.39	0.53
1:B:827:LYS:HD3	1:B:831:ASP:HB2	1.90	0.53
1:A:178:ILE:HG21	1:A:242:THR:HG21	1.91	0.53
1:C:306:LYS:HG3	1:C:596:PRO:HA	1.91	0.53
1:C:708:THR:HB	1:C:1063:GLN:HG3	1.91	0.53
1:B:121:ASN:ND2	1:B:175:MET:HB2	2.22	0.53
1:A:827:LYS:HD3	1:A:831:ASP:HB2	1.91	0.53
1:A:1075:HIS:HD1	1:A:1076:ASP:H	1.56	0.53
1:A:424:ASP:OD1	1:A:424:ASP:N	2.38	0.53
1:B:1127:ASN:OD1	1:B:1128:THR:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1075:HIS:ND1	1:C:1076:ASP:OD1	2.41	0.53
1:A:708:THR:HB	1:A:1063:GLN:HG3	1.91	0.52
1:B:844:ALA:O	1:B:848:ASN:ND2	2.33	0.52
1:B:175:MET:SD	1:B:189:ARG:NE	2.82	0.52
1:B:811:GLU:OE2	1:B:1047:SER:OG	2.27	0.52
1:C:213:SER:O	1:C:213:SER:OG	2.20	0.52
1:B:213:SER:O	1:B:213:SER:OG	2.20	0.52
1:A:564:ASP:N	1:A:568:THR:O	2.40	0.52
1:B:315:ARG:HD3	1:B:315:ARG:N	2.25	0.52
1:C:827:LYS:HD3	1:C:831:ASP:HB2	1.91	0.52
1:A:625:LEU:O	1:A:630:ARG:NH2	2.42	0.51
1:A:799:PRO:HG3	1:A:867:SER:OG	2.10	0.51
1:A:306:LYS:HG3	1:A:596:PRO:HA	1.91	0.51
1:B:708:THR:HB	1:B:1063:GLN:HG3	1.93	0.51
1:A:335:GLY:O	1:A:339:ASN:HB2	2.10	0.51
1:B:799:PRO:HG3	1:B:867:SER:OG	2.10	0.51
1:C:178:ILE:HG21	1:C:242:THR:HG21	1.93	0.51
1:C:372:THR:HB	1:C:431:ALA:HB3	1.93	0.50
1:B:709:ASN:HB3	1:B:1062:ALA:HB3	1.93	0.50
1:C:35:ARG:HH21	1:C:216:PRO:HB2	1.77	0.50
1:C:625:LEU:O	1:C:630:ARG:NH2	2.45	0.50
1:A:142:SER:OG	1:A:154:ARG:O	2.22	0.50
1:A:709:ASN:HB3	1:A:1062:ALA:HB3	1.94	0.50
1:B:335:GLY:O	1:B:339:ASN:HB2	2.11	0.50
1:B:530:ILE:HD11	1:B:535:VAL:HG11	1.94	0.50
1:C:41:ASP:OD1	1:C:43:ILE:N	2.40	0.50
1:B:96:GLU:OE2	1:B:100:ILE:N	2.45	0.49
1:C:799:PRO:HG3	1:C:867:SER:OG	2.11	0.49
1:A:372:THR:HB	1:A:431:ALA:HB3	1.94	0.49
1:A:512:GLU:HG2	1:A:514:LEU:HD23	1.92	0.49
1:C:709:ASN:HB3	1:C:1062:ALA:HB3	1.95	0.49
1:A:530:ILE:HD11	1:A:535:VAL:HG11	1.95	0.49
1:B:343:PHE:CD2	1:B:395:SER:HB3	2.48	0.49
1:B:938:GLY:O	1:B:942:ASP:HB2	2.12	0.49
1:B:153:THR:OG1	1:B:155:GLU:OE1	2.22	0.49
1:A:35:ARG:HH21	1:A:216:PRO:HB2	1.78	0.49
1:A:776:GLN:OE1	1:A:1022:SER:OG	2.29	0.49
1:B:120:VAL:HG11	1:B:156:PHE:HE1	1.77	0.49
1:B:101:VAL:O	1:B:175:MET:HE3	2.13	0.48
1:B:893:GLN:OE1	1:B:897:ARG:NH2	2.43	0.48
1:C:776:GLN:OE1	1:C:1022:SER:OG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:938:GLY:O	1:C:942:ASP:HB2	2.12	0.48
1:B:372:THR:HB	1:B:431:ALA:HB3	1.94	0.48
1:C:530:ILE:HD11	1:C:535:VAL:HG11	1.94	0.48
1:B:35:ARG:HH21	1:B:216:PRO:HB2	1.78	0.48
1:B:672:THR:HA	1:B:682:GLN:HA	1.95	0.48
1:B:121:ASN:HA	1:B:126:VAL:HA	1.96	0.48
1:A:811:GLU:OE2	1:A:1047:SER:OG	2.30	0.48
1:A:938:GLY:O	1:A:942:ASP:HB2	2.13	0.48
1:B:595:THR:HB	1:B:604:VAL:HG12	1.96	0.48
1:A:153:THR:OG1	1:A:155:GLU:OE1	2.22	0.48
1:C:564:ASP:N	1:C:568:THR:O	2.42	0.48
1:A:96:GLU:OE2	1:A:100:ILE:N	2.47	0.47
1:C:512:GLU:HG2	1:C:514:LEU:HD23	1.95	0.47
1:B:100:ILE:HD11	1:B:257:PHE:HB2	1.96	0.47
1:C:981:ALA:O	1:C:985:ILE:HG12	2.15	0.47
1:A:41:ASP:OD2	1:A:45:ARG:NH2	2.46	0.47
1:B:389:THR:OG1	1:B:513:LEU:O	2.28	0.47
1:B:574:ASP:HB3	1:B:577:THR:O	2.15	0.47
1:B:625:LEU:O	1:B:630:ARG:NH2	2.48	0.47
1:A:202:ILE:HB	1:A:226:VAL:HG12	1.97	0.47
1:A:819:THR:O	1:A:819:THR:OG1	2.32	0.47
1:B:512:GLU:HG2	1:B:514:LEU:HD23	1.95	0.47
1:B:735:CYS:HB3	1:B:741:CYS:HB3	1.70	0.47
1:C:202:ILE:HB	1:C:226:VAL:HG12	1.95	0.47
1:C:402:GLU:OE1	1:C:491:TYR:OH	2.20	0.47
1:A:294:GLU:OE1	1:A:314:PHE:HA	2.14	0.47
1:A:672:THR:HA	1:A:682:GLN:HA	1.96	0.47
1:A:377:GLY:HA3	1:A:426:THR:HG23	1.97	0.47
1:A:389:THR:OG1	1:A:513:LEU:O	2.27	0.47
1:A:414:ILE:HD13	1:A:418:ASN:HD21	1.80	0.47
1:A:595:THR:HB	1:A:604:VAL:HG12	1.97	0.47
1:B:313:ASN:O	1:B:315:ARG:HD3	2.14	0.47
1:C:574:ASP:HB3	1:C:577:THR:O	2.15	0.47
1:A:574:ASP:HB3	1:A:577:THR:O	2.15	0.47
1:A:861:MET:HE1	1:C:689:MET:HG2	1.98	0.46
1:B:811:GLU:O	1:B:815:PHE:HD1	1.99	0.46
1:B:981:ALA:O	1:B:985:ILE:HG12	2.15	0.46
1:C:96:GLU:OE2	1:C:100:ILE:N	2.48	0.46
1:C:582:ASP:OD1	1:C:582:ASP:N	2.41	0.46
1:C:672:THR:HA	1:C:682:GLN:HA	1.96	0.46
1:A:343:PHE:CD2	1:A:395:SER:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ASP:OD2	1:B:967:SER:OG	2.34	0.46
1:A:979:PRO:HA	1:A:982:GLU:OE1	2.15	0.46
1:C:1107:ILE:HG22	1:C:1129:VAL:HG13	1.97	0.46
1:B:689:MET:HG2	1:C:861:MET:HE1	1.98	0.46
1:C:294:GLU:OE1	1:C:314:PHE:HA	2.15	0.46
1:A:120:VAL:HG11	1:A:156:PHE:HE1	1.81	0.46
1:C:377:GLY:HA3	1:C:426:THR:HG23	1.98	0.46
1:C:1082:PRO:HD3	1:C:1087:PHE:CE2	2.51	0.46
1:C:628:THR:O	1:C:628:THR:OG1	2.34	0.45
1:B:41:ASP:OD2	1:B:45:ARG:NH2	2.48	0.45
1:B:801:PRO:HA	1:B:806:LYS:HD2	1.99	0.45
1:A:582:ASP:OD1	1:A:582:ASP:N	2.36	0.45
1:B:567:ASP:OD2	1:C:967:SER:OG	2.33	0.45
1:B:292:LEU:HG	1:B:296:LYS:HE3	1.98	0.45
1:C:893:GLN:OE1	1:C:897:ARG:NH2	2.46	0.45
1:A:811:GLU:O	1:A:815:PHE:HD2	1.99	0.45
1:A:967:SER:OG	1:C:567:ASP:OD2	2.33	0.45
1:B:99:ASN:ND2	1:B:177:ASP:O	2.43	0.45
1:C:120:VAL:HG11	1:C:156:PHE:HE1	1.81	0.45
1:C:525:LYS:HB2	1:C:525:LYS:HE2	1.79	0.45
1:C:897:ARG:O	1:C:901:ILE:HG23	2.17	0.45
1:B:128:ILE:HD13	1:B:228:LEU:HD11	1.99	0.45
1:C:292:LEU:HG	1:C:296:LYS:HE3	1.97	0.45
1:A:897:ARG:HD2	1:A:1041:LEU:O	2.17	0.45
1:B:377:GLY:HA3	1:B:426:THR:HG23	1.99	0.44
1:B:1094:TRP:HD1	1:B:1127:ASN:HD22	1.63	0.44
1:C:811:GLU:O	1:C:815:PHE:HD2	2.00	0.44
1:B:559:GLN:O	1:B:573:ARG:NH1	2.49	0.44
1:B:1082:PRO:HD3	1:B:1087:PHE:CE2	2.52	0.44
1:B:202:ILE:HB	1:B:226:VAL:HG12	1.99	0.44
1:C:181:LYS:HA	1:C:181:LYS:HD3	1.90	0.44
1:A:292:LEU:HG	1:A:296:LYS:HE3	1.99	0.44
1:A:294:GLU:HG2	1:A:311:THR:HB	2.00	0.44
1:B:542:LEU:HD21	1:B:561:PHE:CE1	2.52	0.44
1:B:776:GLN:OE1	1:B:1022:SER:OG	2.30	0.44
1:C:62:ASN:OD1	1:C:62:ASN:N	2.51	0.44
1:C:189:ARG:HG2	1:C:206:TYR:CD1	2.52	0.44
1:A:893:GLN:OE1	1:A:897:ARG:NH2	2.50	0.44
1:C:897:ARG:HD2	1:C:1041:LEU:O	2.18	0.44
1:A:437:LEU:H	1:A:437:LEU:HD23	1.83	0.44
1:B:897:ARG:HD2	1:B:1041:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:LEU:HD23	1:B:988:LEU:HA	1.85	0.44
1:C:872:GLY:O	1:C:876:SER:OG	2.34	0.44
1:A:62:ASN:OD1	1:A:62:ASN:N	2.51	0.44
1:B:24:THR:HG22	1:B:25:ILE:N	2.33	0.44
1:C:131:CYS:SG	1:C:162:TYR:HB2	2.57	0.44
1:C:330:ASN:OD1	1:C:330:ASN:N	2.51	0.44
1:A:861:MET:HE2	1:C:691:LEU:HD21	2.00	0.43
1:C:839:ARG:HB3	1:C:843:CYS:HB2	1.99	0.43
1:A:85:ASP:HB3	1:A:87:LYS:HE3	1.99	0.43
1:A:628:THR:O	1:A:628:THR:OG1	2.34	0.43
1:A:1082:PRO:HD3	1:A:1087:PHE:CE2	2.53	0.43
1:B:534:CYS:HB2	1:B:586:CYS:HB3	1.86	0.43
1:B:978:PRO:O	1:B:981:ALA:N	2.50	0.43
1:A:543:THR:O	1:B:970:ASN:ND2	2.51	0.43
1:C:735:CYS:HB3	1:C:741:CYS:HB3	1.69	0.43
1:C:762:ILE:O	1:C:766:GLN:HG2	2.18	0.43
1:B:294:GLU:OE1	1:B:314:PHE:HA	2.18	0.43
1:B:1089:SER:HB3	1:B:1094:TRP:CD2	2.53	0.43
1:A:24:THR:HG22	1:A:25:ILE:N	2.33	0.43
1:A:786:ILE:HD12	1:A:786:ILE:HA	1.91	0.43
1:B:131:CYS:SG	1:B:162:TYR:HB2	2.59	0.43
1:B:189:ARG:HG2	1:B:206:TYR:CD1	2.52	0.43
1:B:762:ILE:O	1:B:766:GLN:HG2	2.18	0.43
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.87	0.43
1:C:24:THR:HG22	1:C:25:ILE:N	2.33	0.43
1:C:595:THR:HB	1:C:604:VAL:HG12	1.99	0.43
1:A:111:ASP:OD2	1:A:111:ASP:C	2.62	0.43
1:A:742:SER:O	1:A:746:LEU:HD13	2.19	0.43
1:A:525:LYS:HB2	1:A:525:LYS:HE2	1.79	0.43
1:B:897:ARG:O	1:B:901:ILE:HG23	2.19	0.43
1:A:981:ALA:O	1:A:985:ILE:HG12	2.18	0.43
1:B:564:ASP:N	1:B:568:THR:O	2.40	0.43
1:B:768:LYS:O	1:B:772:GLU:HG3	2.18	0.43
1:C:742:SER:O	1:C:746:LEU:HD13	2.19	0.43
1:C:951:LEU:HD23	1:C:951:LEU:HA	1.80	0.43
1:B:437:LEU:HD23	1:B:437:LEU:H	1.84	0.42
1:A:288:SER:HA	1:A:315:ARG:HG3	2.00	0.42
1:A:1089:SER:HB3	1:A:1094:TRP:CD2	2.54	0.42
1:B:109:THR:OG1	1:B:114:SER:OG	2.34	0.42
1:B:839:ARG:HB3	1:B:843:CYS:HB2	2.01	0.42
1:C:786:ILE:HD12	1:C:786:ILE:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:PRO:HA	1:A:1064:GLU:HA	2.00	0.42
1:A:725:LYS:HD2	1:A:763:ALA:HB1	2.00	0.42
1:B:525:LYS:HB2	1:B:525:LYS:HE2	1.78	0.42
1:B:542:LEU:HD21	1:B:561:PHE:CZ	2.54	0.42
1:C:176:LEU:HD13	1:C:176:LEU:HA	1.91	0.42
1:C:1089:SER:HB3	1:C:1094:TRP:CD2	2.55	0.42
1:A:801:PRO:HA	1:A:806:LYS:HD2	2.02	0.42
1:B:176:LEU:HD13	1:B:176:LEU:HA	1.92	0.42
1:B:831:ASP:OD1	1:B:831:ASP:N	2.51	0.42
1:C:119:ILE:HG12	1:C:128:ILE:HG12	2.02	0.42
1:C:111:ASP:OD2	1:C:111:ASP:C	2.63	0.42
1:C:133:PHE:CD1	1:C:162:TYR:HB3	2.55	0.42
1:C:768:LYS:O	1:C:772:GLU:HG3	2.20	0.42
1:A:35:ARG:NH2	1:A:216:PRO:HB2	2.35	0.42
1:A:951:LEU:HD23	1:A:951:LEU:HA	1.81	0.42
1:B:133:PHE:CD1	1:B:162:TYR:HB3	2.54	0.42
1:B:330:ASN:OD1	1:B:330:ASN:N	2.52	0.42
1:B:833:LEU:HD23	1:B:833:LEU:HA	1.84	0.42
1:A:768:LYS:O	1:A:772:GLU:HG3	2.20	0.42
1:B:35:ARG:NH2	1:B:216:PRO:HB2	2.34	0.42
1:C:813:LEU:HD23	1:C:930:LEU:HB3	2.02	0.42
1:C:1083:ARG:NH1	1:C:1113:PHE:HB3	2.35	0.42
1:A:813:LEU:HD23	1:A:930:LEU:HB3	2.02	0.41
1:B:41:ASP:OD1	1:B:42:THR:N	2.53	0.41
1:B:111:ASP:C	1:B:111:ASP:OD2	2.63	0.41
1:C:153:THR:OG1	1:C:155:GLU:OE1	2.22	0.41
1:C:796:GLN:OE1	1:C:927:GLN:NE2	2.53	0.41
1:C:831:ASP:OD1	1:C:831:ASP:N	2.53	0.41
1:A:131:CYS:SG	1:A:162:TYR:HB2	2.60	0.41
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.87	0.41
1:B:178:ILE:HG21	1:B:242:THR:HG21	2.01	0.41
1:C:41:ASP:OD1	1:C:42:THR:N	2.53	0.41
1:C:294:GLU:HG2	1:C:311:THR:HB	2.02	0.41
1:A:833:LEU:HD23	1:A:833:LEU:HA	1.85	0.41
1:B:62:ASN:OD1	1:B:62:ASN:N	2.51	0.41
1:C:625:LEU:HD23	1:C:625:LEU:HA	1.93	0.41
1:A:872:GLY:O	1:A:876:SER:OG	2.34	0.41
1:B:625:LEU:HD23	1:B:625:LEU:HA	1.92	0.41
1:A:658:CYS:HB2	1:A:689:MET:HE3	2.02	0.41
1:A:951:LEU:O	1:A:955:VAL:HG23	2.20	0.41
1:B:718:ILE:HG13	1:B:1053:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1020:LYS:NZ	1:B:1034:PHE:O	2.33	0.41
1:A:385:ASP:OD1	1:A:524:LYS:HD2	2.21	0.41
1:B:121:ASN:HD22	1:B:175:MET:HB2	1.86	0.41
1:A:100:ILE:HD11	1:A:257:PHE:HB2	2.03	0.41
1:A:534:CYS:HB2	1:A:586:CYS:HB3	1.88	0.41
1:C:801:PRO:HA	1:C:806:LYS:HD2	2.02	0.41
1:B:181:LYS:HA	1:B:181:LYS:HD3	1.90	0.41
1:B:813:LEU:HD23	1:B:930:LEU:HB3	2.01	0.41
1:A:338:PHE:N	1:A:338:PHE:CD1	2.89	0.40
1:B:338:PHE:N	1:B:338:PHE:CD1	2.90	0.40
1:C:35:ARG:NH2	1:C:216:PRO:HB2	2.36	0.40
1:C:97:LYS:HA	1:C:97:LYS:HD3	1.95	0.40
1:B:385:ASP:OD1	1:B:524:LYS:HD2	2.21	0.40
1:A:119:ILE:HG12	1:A:128:ILE:HG12	2.03	0.40
1:A:831:ASP:OD1	1:A:831:ASP:N	2.53	0.40
1:A:965:ILE:HD11	1:A:972:ILE:HG12	2.03	0.40
1:B:316:VAL:HG21	1:B:621:HIS:HB2	2.04	0.40
1:C:658:CYS:HB2	1:C:689:MET:HE3	2.04	0.40
1:C:725:LYS:HD2	1:C:763:ALA:HB1	2.02	0.40
1:A:133:PHE:CD1	1:A:162:TYR:HB3	2.56	0.40
1:B:582:ASP:OD1	1:B:582:ASP:N	2.40	0.40
1:C:385:ASP:OD1	1:C:524:LYS:HD2	2.21	0.40

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	1082/1243 (87%)	1030 (95%)	51 (5%)	1 (0%)	48	78
1	B	1082/1243 (87%)	1029 (95%)	52 (5%)	1 (0%)	48	78
1	C	1082/1243 (87%)	1028 (95%)	53 (5%)	1 (0%)	48	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3246/3729 (87%)	3087 (95%)	156 (5%)	3 (0%)	50 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	826	ILE
1	B	826	ILE
1	C	826	ILE

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	945/1079 (88%)	940 (100%)	5 (0%)	86 92
1	B	945/1079 (88%)	941 (100%)	4 (0%)	89 94
1	C	945/1079 (88%)	941 (100%)	4 (0%)	89 94
All	All	2835/3237 (88%)	2822 (100%)	13 (0%)	85 92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	343	PHE
1	A	613	CYS
1	A	751	PHE
1	A	765	GLU
1	B	418	ASN
1	B	613	CYS
1	B	746	LEU
1	B	946	GLN
1	C	62	ASN
1	C	242	THR
1	C	356	ASN
1	C	946	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	390	ASN
1	A	927	GLN
1	A	994	GLN
1	A	1046	GLN
1	A	1111	ASN
1	B	53	GLN
1	B	121	ASN
1	B	927	GLN
1	B	1046	GLN
1	B	1098	GLN
1	B	1111	ASN
1	C	418	ASN
1	C	747	GLN
1	C	927	GLN
1	C	994	GLN
1	C	1098	GLN
1	C	1111	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

60 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	$\#\|Z\| > 2$
2	NAG	B	1303	1	14,14,15	0.32	0	17,19,21	0.34	0
2	NAG	B	1317	1	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	B	1316	1	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	C	1316	1	14,14,15	0.25	0	17,19,21	0.46	0
2	NAG	A	1306	1	14,14,15	0.26	0	17,19,21	0.35	0
2	NAG	A	1314	1	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	C	1310	1	14,14,15	0.39	0	17,19,21	0.55	0
2	NAG	C	1320	1	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	B	1304	1	14,14,15	0.41	0	17,19,21	0.40	0
2	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	A	1303	1	14,14,15	0.32	0	17,19,21	0.34	0
2	NAG	A	1302	1	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	B	1320	1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	A	1310	1	14,14,15	0.36	0	17,19,21	0.52	0
2	NAG	C	1317	1	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	C	1318	1	14,14,15	0.26	0	17,19,21	0.46	0
2	NAG	B	1319	1	14,14,15	0.29	0	17,19,21	0.52	0
2	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.45	0
2	NAG	B	1302	1	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	B	1310	1	14,14,15	0.36	0	17,19,21	0.52	0
2	NAG	C	1311	1	14,14,15	0.43	0	17,19,21	0.60	0
2	NAG	A	1319	1	14,14,15	0.28	0	17,19,21	0.51	0
2	NAG	A	1309	1	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	B	1318	1	14,14,15	0.28	0	17,19,21	0.45	0
2	NAG	A	1316	1	14,14,15	0.25	0	17,19,21	0.46	0
2	NAG	B	1311	1	14,14,15	0.42	0	17,19,21	0.58	0
2	NAG	A	1308	1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	C	1305	1	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	C	1309	1	14,14,15	0.29	0	17,19,21	0.52	0
2	NAG	C	1315	1	14,14,15	0.20	0	17,19,21	0.40	0
2	NAG	C	1302	1	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	A	1312	1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	B	1313	1	14,14,15	0.21	0	17,19,21	0.39	0
2	NAG	A	1311	1	14,14,15	0.47	0	17,19,21	0.60	1 (5%)
2	NAG	C	1301	1	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	A	1304	1	14,14,15	0.43	0	17,19,21	0.46	0
2	NAG	B	1314	1	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	C	1303	1	14,14,15	0.32	0	17,19,21	0.34	0
2	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1307	1	14,14,15	0.28	0	17,19,21	0.45	0
2	NAG	C	1314	1	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	C	1304	1	14,14,15	0.45	0	17,19,21	0.49	0
2	NAG	A	1315	1	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	C	1307	1	14,14,15	0.28	0	17,19,21	0.45	0
2	NAG	B	1312	1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	A	1313	1	14,14,15	0.21	0	17,19,21	0.39	0
2	NAG	C	1313	1	14,14,15	0.21	0	17,19,21	0.39	0
2	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	A	1305	1	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	C	1319	1	14,14,15	0.28	0	17,19,21	0.51	0
2	NAG	A	1320	1	14,14,15	0.24	0	17,19,21	0.50	0
2	NAG	C	1312	1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	A	1317	1	14,14,15	0.27	0	17,19,21	0.49	0
2	NAG	B	1309	1	14,14,15	0.30	0	17,19,21	0.52	0
2	NAG	A	1318	1	14,14,15	0.26	0	17,19,21	0.46	0
2	NAG	B	1306	1	14,14,15	0.26	0	17,19,21	0.36	0
2	NAG	B	1308	1	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	B	1315	1	14,14,15	0.20	0	17,19,21	0.40	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
2	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1317	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1314	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1320	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1320	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1317	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1318	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1319	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1319	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1318	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1315	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1314	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1314	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1315	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1319	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1320	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1317	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1318	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1315	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1311	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1304	NAG	O5-C5-C6-O6
2	A	1305	NAG	C4-C5-C6-O6
2	C	1305	NAG	C4-C5-C6-O6
2	A	1304	NAG	O5-C5-C6-O6
2	B	1305	NAG	C4-C5-C6-O6
2	B	1312	NAG	O5-C5-C6-O6
2	A	1317	NAG	C4-C5-C6-O6
2	B	1317	NAG	C4-C5-C6-O6
2	C	1317	NAG	C4-C5-C6-O6
2	A	1312	NAG	O5-C5-C6-O6
2	B	1308	NAG	O5-C5-C6-O6
2	C	1305	NAG	O5-C5-C6-O6
2	C	1312	NAG	O5-C5-C6-O6
2	A	1312	NAG	C4-C5-C6-O6
2	C	1312	NAG	C4-C5-C6-O6
2	A	1305	NAG	O5-C5-C6-O6
2	A	1318	NAG	O5-C5-C6-O6
2	B	1305	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	1320	NAG	O5-C5-C6-O6
2	C	1320	NAG	O5-C5-C6-O6
2	B	1312	NAG	C4-C5-C6-O6
2	A	1308	NAG	O5-C5-C6-O6
2	A	1319	NAG	O5-C5-C6-O6
2	A	1320	NAG	O5-C5-C6-O6
2	B	1318	NAG	O5-C5-C6-O6
2	B	1319	NAG	O5-C5-C6-O6
2	C	1308	NAG	O5-C5-C6-O6
2	C	1318	NAG	O5-C5-C6-O6
2	C	1319	NAG	O5-C5-C6-O6
2	A	1304	NAG	C4-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	B	1307	NAG	O5-C5-C6-O6
2	C	1302	NAG	O5-C5-C6-O6
2	C	1304	NAG	C4-C5-C6-O6
2	B	1304	NAG	C4-C5-C6-O6
2	B	1311	NAG	O5-C5-C6-O6
2	A	1302	NAG	C4-C5-C6-O6
2	A	1320	NAG	C4-C5-C6-O6
2	B	1302	NAG	C4-C5-C6-O6
2	B	1320	NAG	C4-C5-C6-O6
2	C	1302	NAG	C4-C5-C6-O6
2	C	1320	NAG	C4-C5-C6-O6
2	A	1311	NAG	O5-C5-C6-O6
2	C	1311	NAG	O5-C5-C6-O6
2	B	1308	NAG	C4-C5-C6-O6
2	B	1304	NAG	O5-C5-C6-O6
2	A	1318	NAG	C4-C5-C6-O6
2	B	1317	NAG	O5-C5-C6-O6
2	C	1317	NAG	O5-C5-C6-O6
2	B	1307	NAG	C4-C5-C6-O6
2	B	1311	NAG	C4-C5-C6-O6
2	B	1318	NAG	C4-C5-C6-O6
2	A	1307	NAG	O5-C5-C6-O6
2	A	1317	NAG	O5-C5-C6-O6
2	C	1307	NAG	O5-C5-C6-O6
2	C	1318	NAG	C4-C5-C6-O6
2	A	1311	NAG	C4-C5-C6-O6
2	C	1311	NAG	C4-C5-C6-O6
2	C	1307	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	1309	NAG	O5-C5-C6-O6
2	C	1309	NAG	C4-C5-C6-O6
2	B	1309	NAG	O5-C5-C6-O6
2	B	1309	NAG	C4-C5-C6-O6
2	A	1308	NAG	C4-C5-C6-O6
2	C	1319	NAG	C4-C5-C6-O6
2	A	1319	NAG	C4-C5-C6-O6
2	A	1307	NAG	C4-C5-C6-O6
2	C	1308	NAG	C4-C5-C6-O6
2	A	1303	NAG	C1-C2-N2-C7
2	B	1303	NAG	C1-C2-N2-C7
2	C	1303	NAG	C1-C2-N2-C7
2	A	1314	NAG	O5-C5-C6-O6
2	B	1314	NAG	O5-C5-C6-O6
2	C	1314	NAG	O5-C5-C6-O6
2	B	1304	NAG	C1-C2-N2-C7
2	B	1319	NAG	C4-C5-C6-O6
2	A	1309	NAG	C4-C5-C6-O6
2	A	1309	NAG	O5-C5-C6-O6
2	C	1304	NAG	C1-C2-N2-C7
2	A	1304	NAG	C1-C2-N2-C7
2	A	1303	NAG	C3-C2-N2-C7
2	B	1303	NAG	C3-C2-N2-C7
2	B	1304	NAG	C3-C2-N2-C7
2	C	1303	NAG	C3-C2-N2-C7
2	C	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

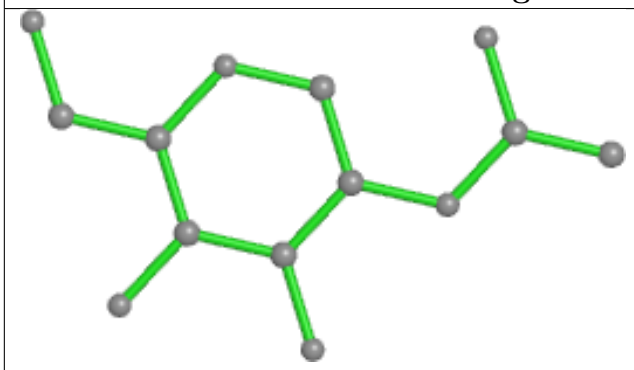
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1302	NAG	1	0
2	B	1319	NAG	1	0
2	B	1302	NAG	1	0
2	A	1319	NAG	1	0
2	C	1302	NAG	1	0
2	C	1319	NAG	1	0

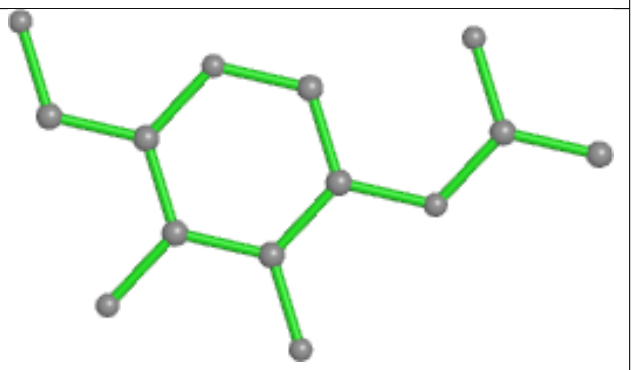
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

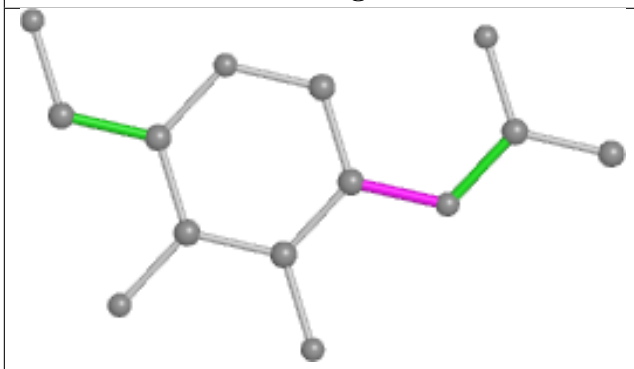
Ligand NAG B 1303



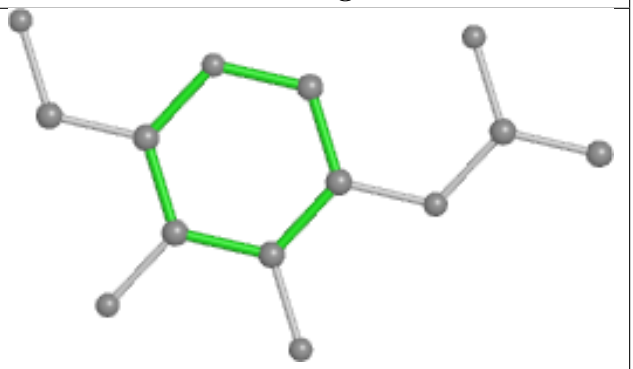
Bond lengths



Bond angles

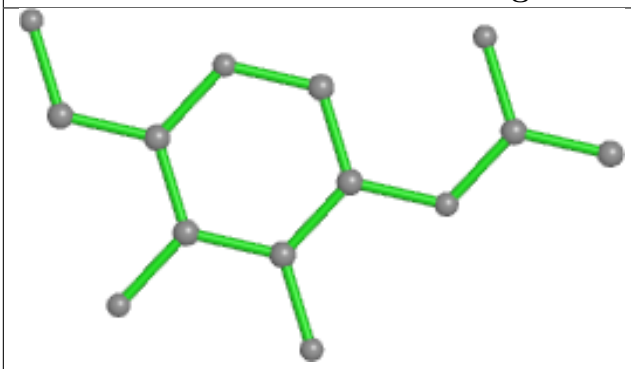


Torsions

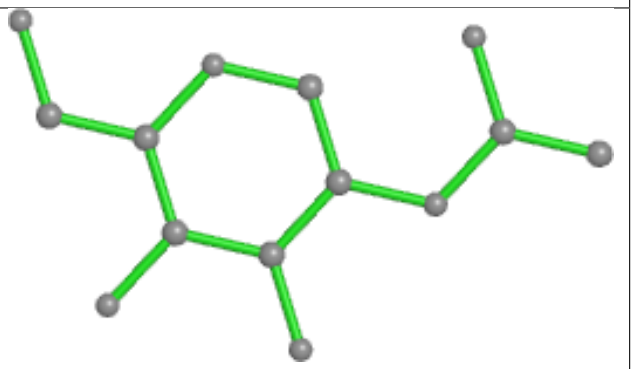


Rings

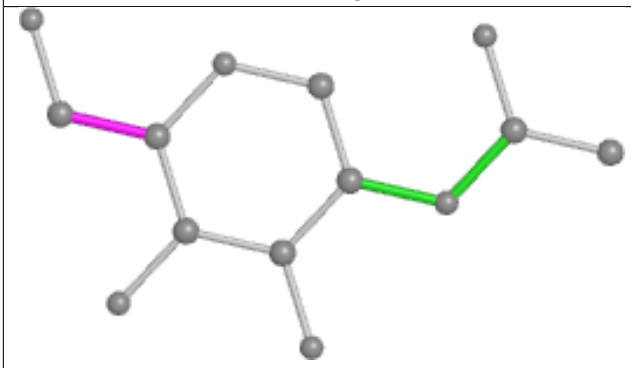
Ligand NAG B 1317



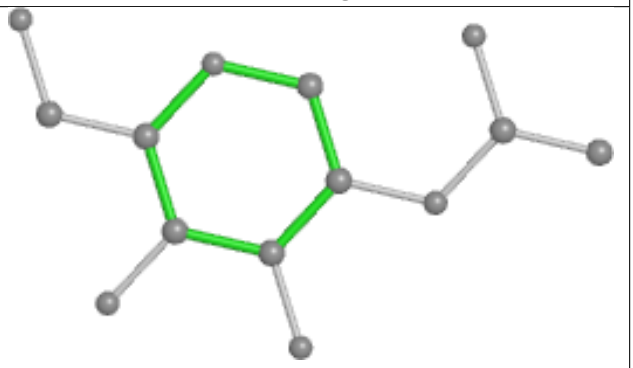
Bond lengths



Bond angles

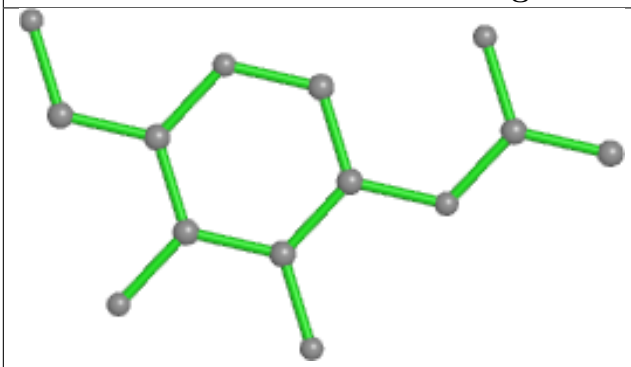


Torsions

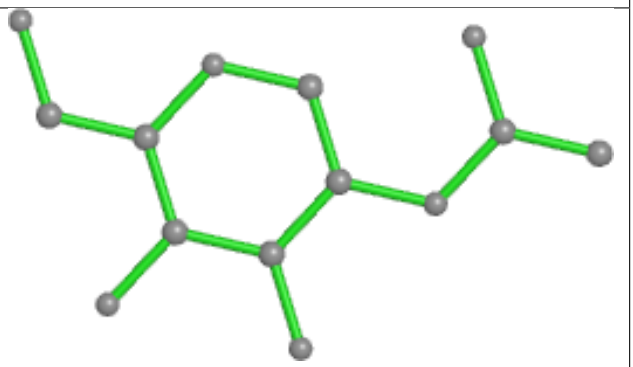


Rings

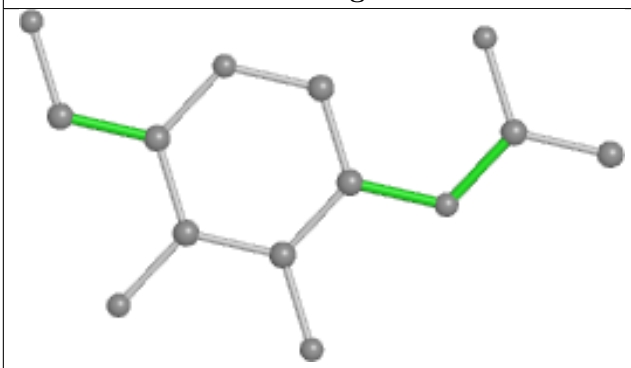
Ligand NAG B 1316



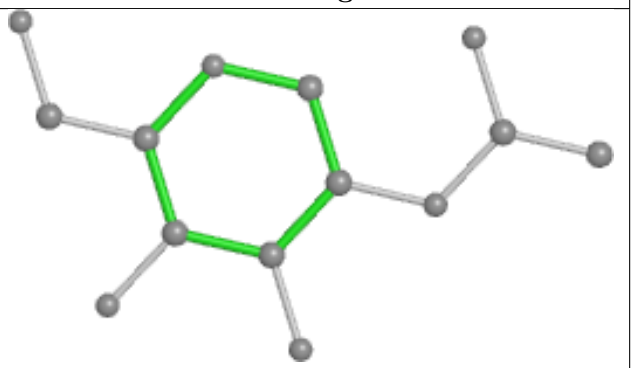
Bond lengths



Bond angles

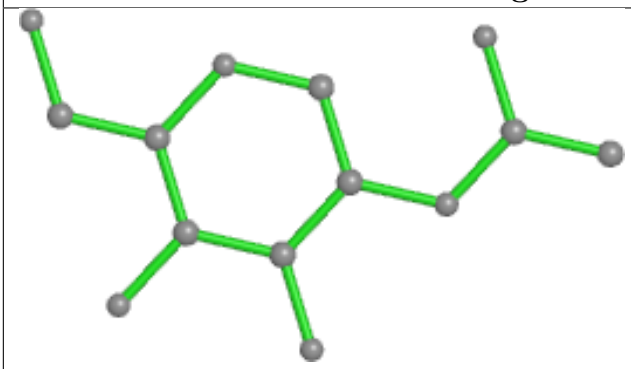


Torsions

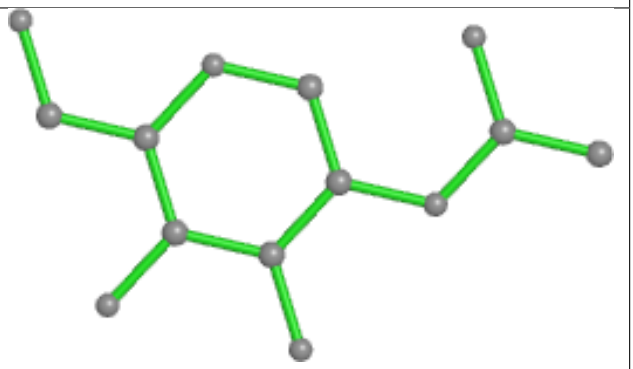


Rings

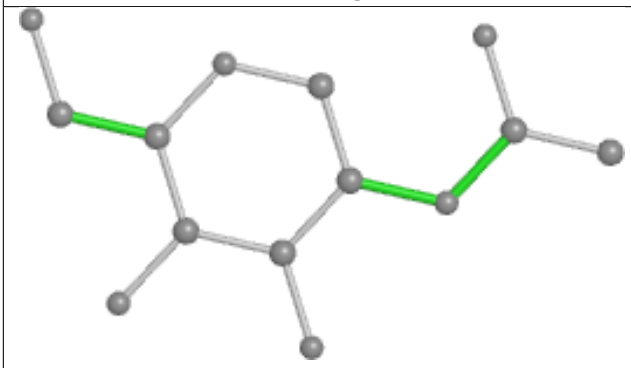
Ligand NAG C 1316



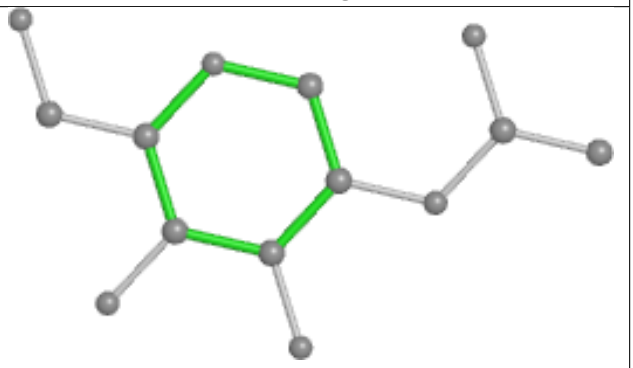
Bond lengths



Bond angles

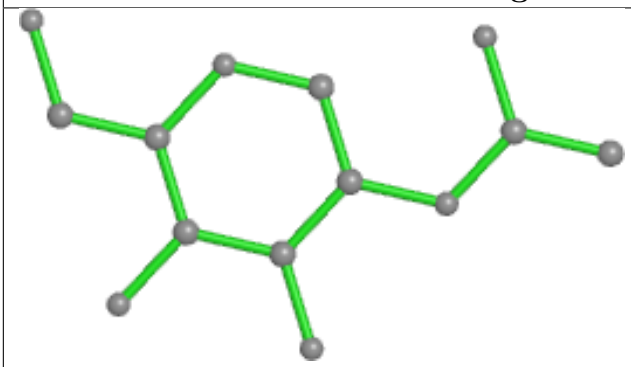


Torsions



Rings

Ligand NAG A 1306



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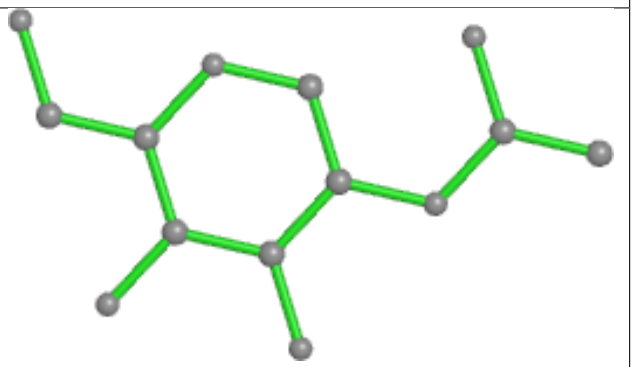

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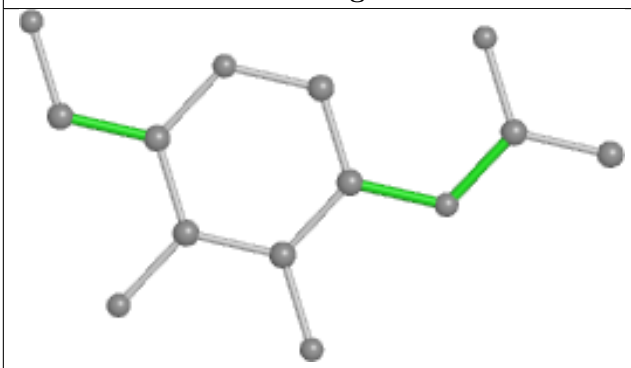

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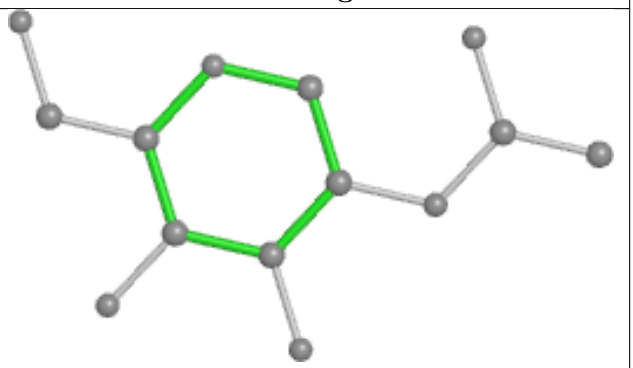
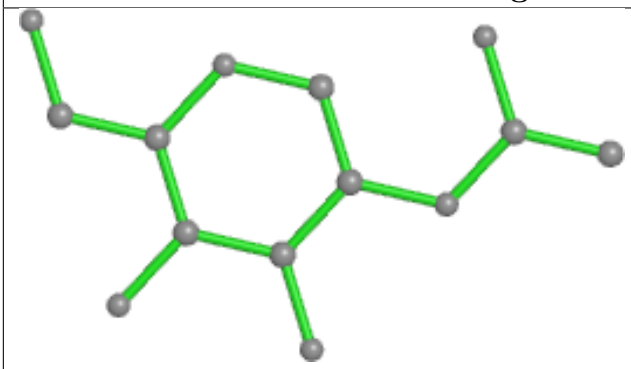


Rings

Ligand NAG A 1314



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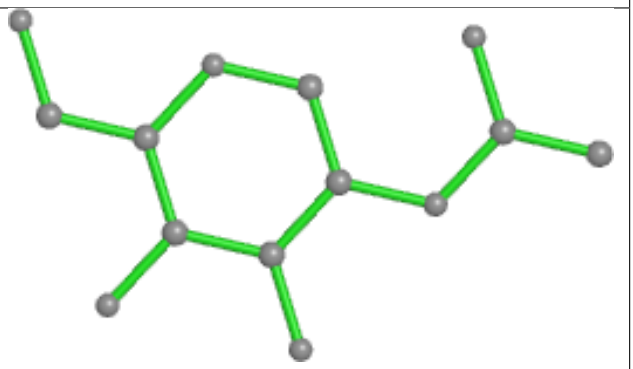
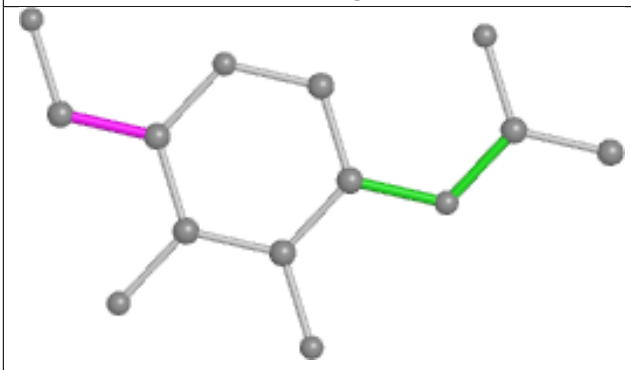


Bond angles



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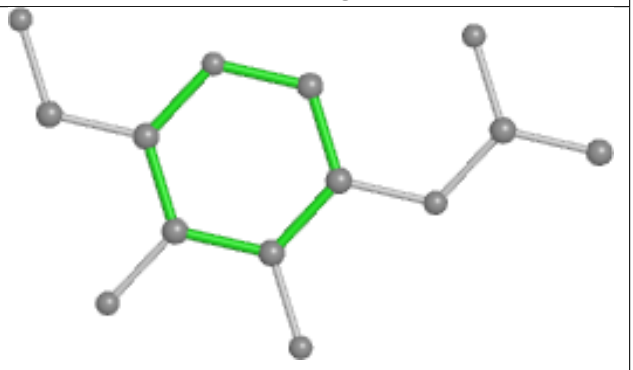
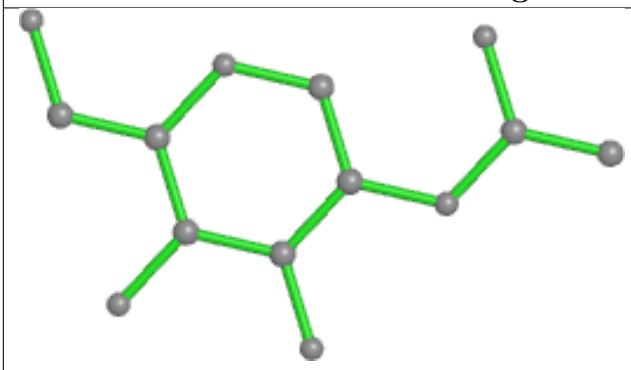


Rings

Ligand NAG C 1310



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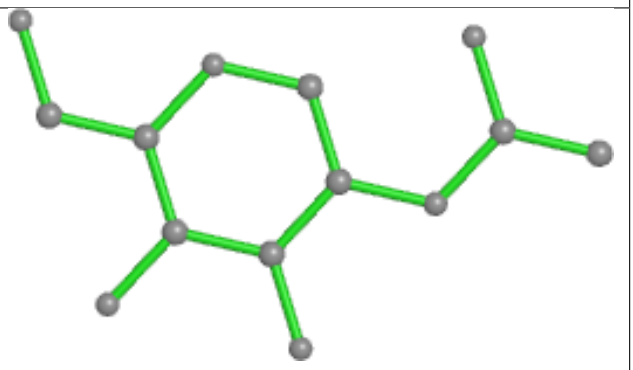
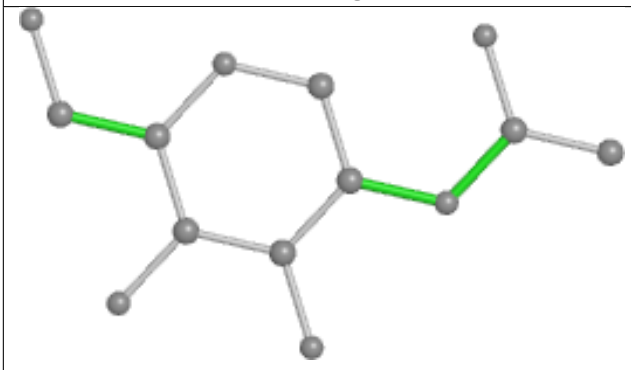


Bond angles



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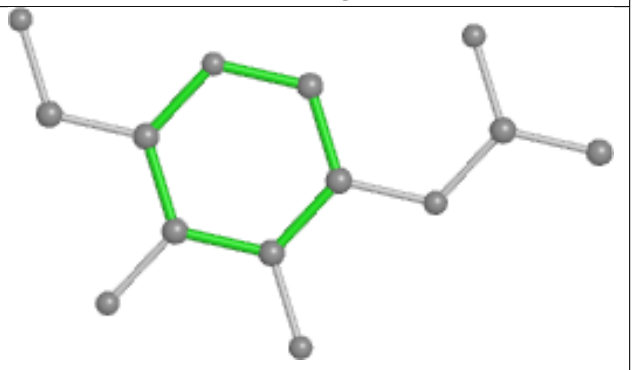
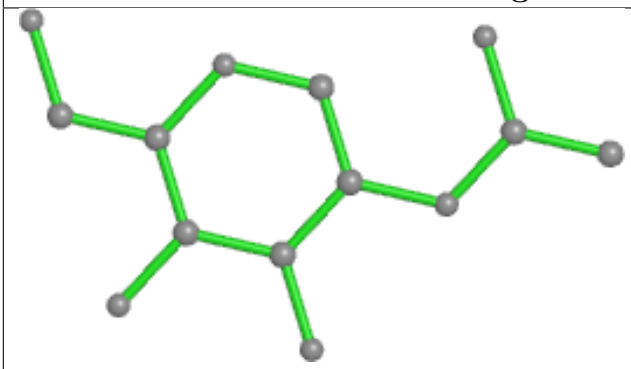


Rings

Ligand NAG C 1320



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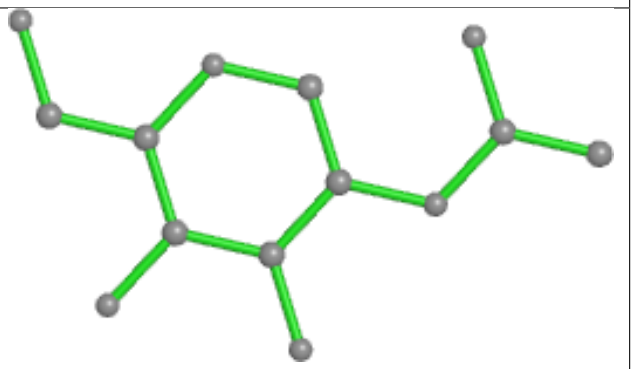
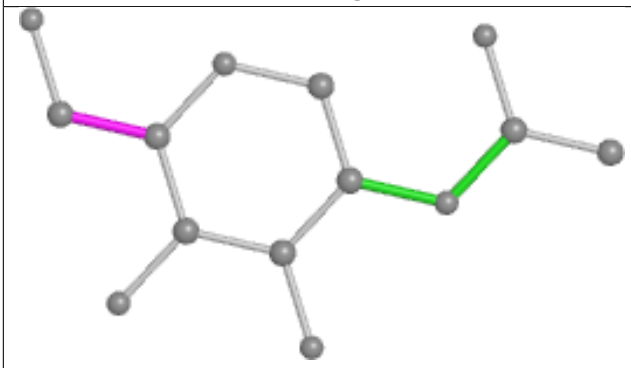
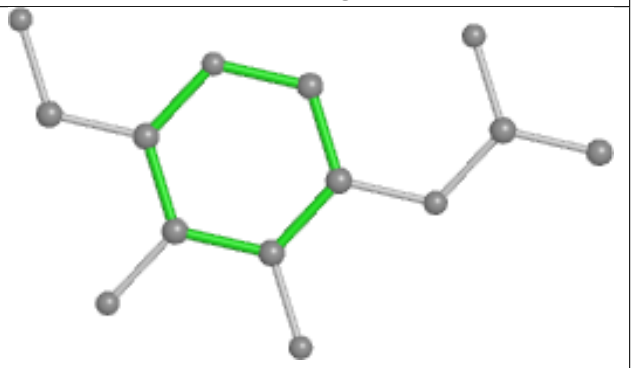


Bond angles

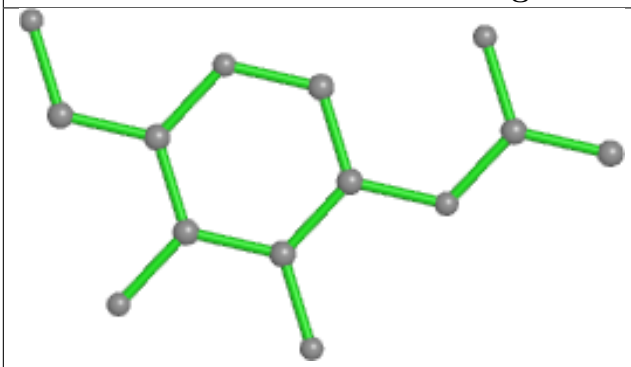


Torsions

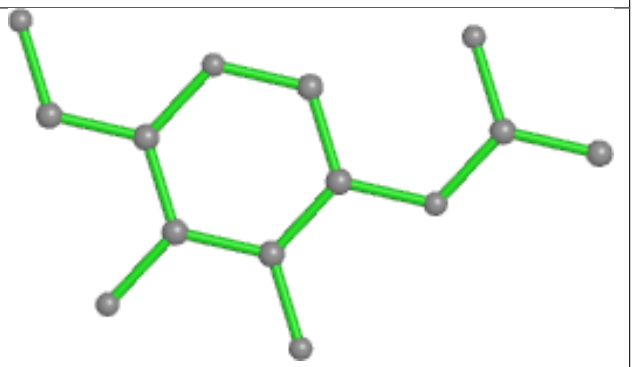


Rings

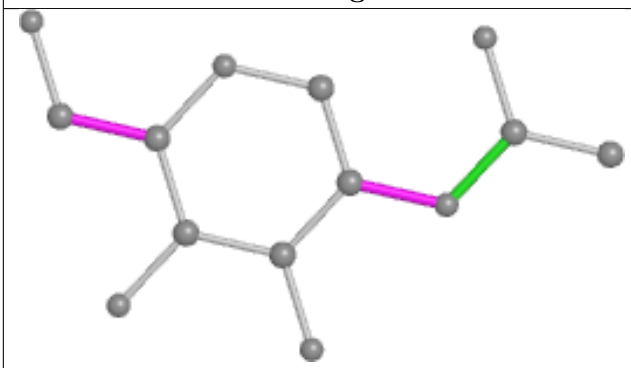
Ligand NAG B 1304



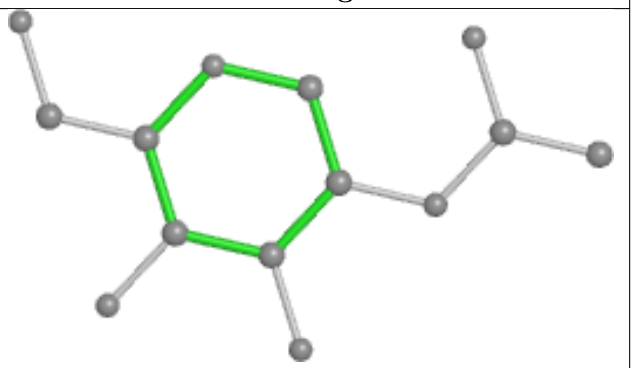
Bond lengths



Bond angles

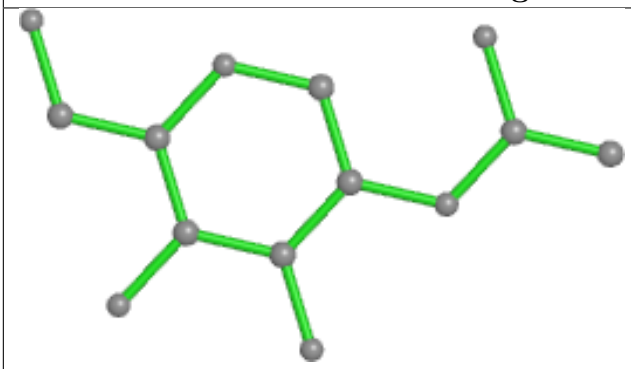


Torsions



Rings

Ligand NAG C 1308



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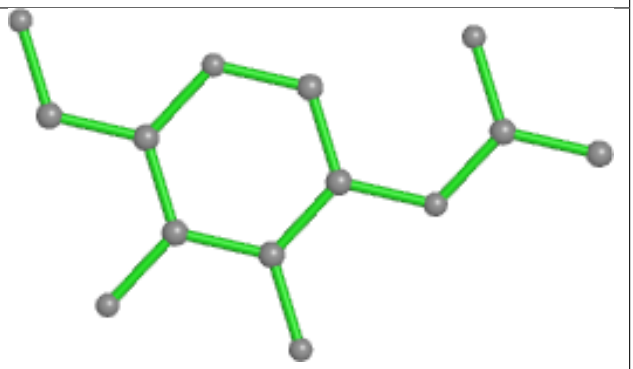
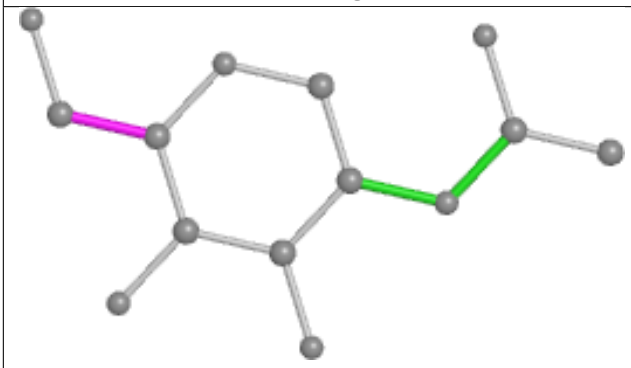
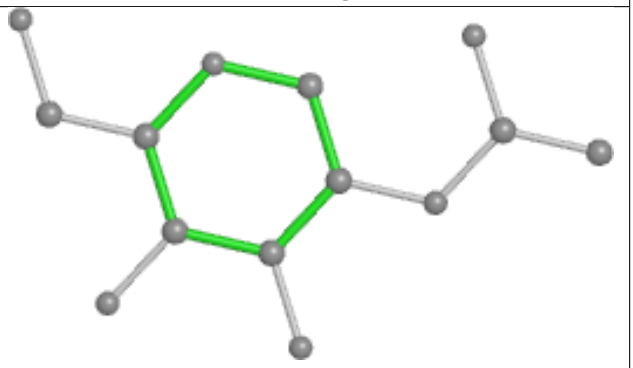


Bond angles

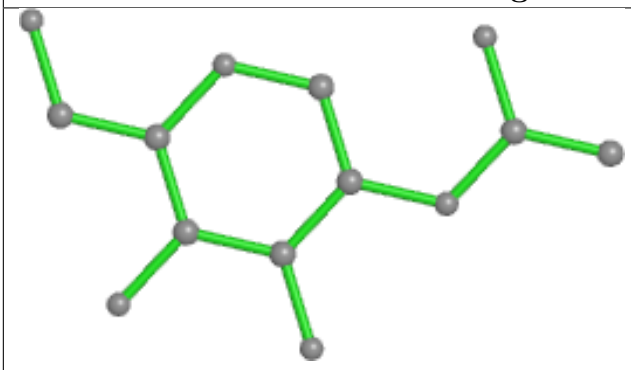


Torsions



Rings

Ligand NAG A 1303



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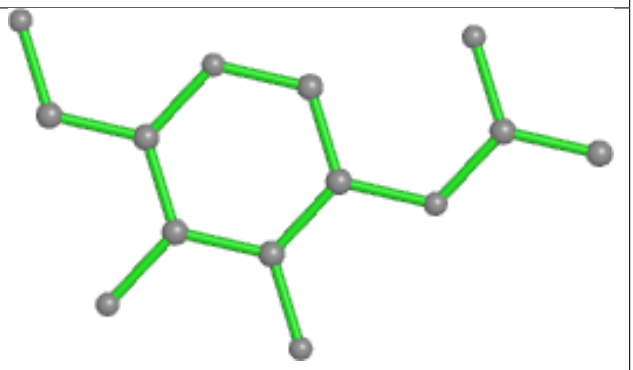
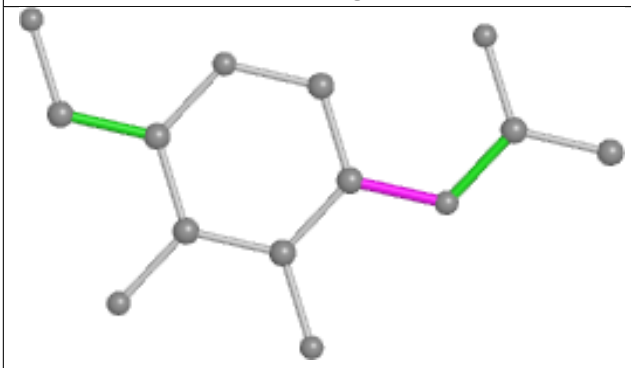


Bond angles



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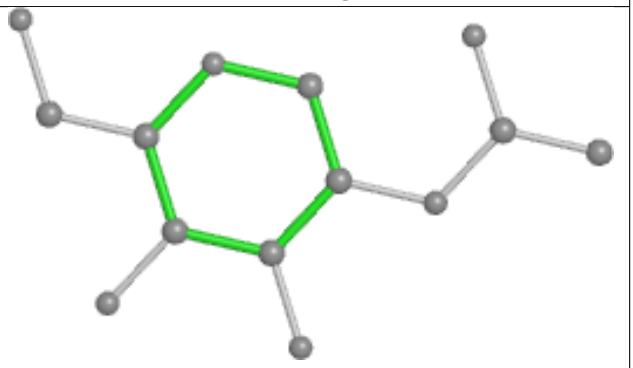
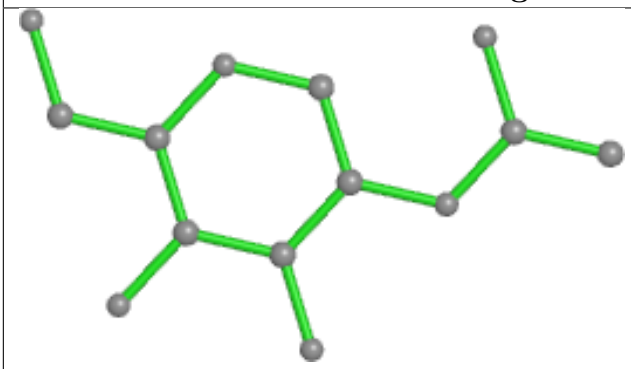


Rings

Ligand NAG A 1302



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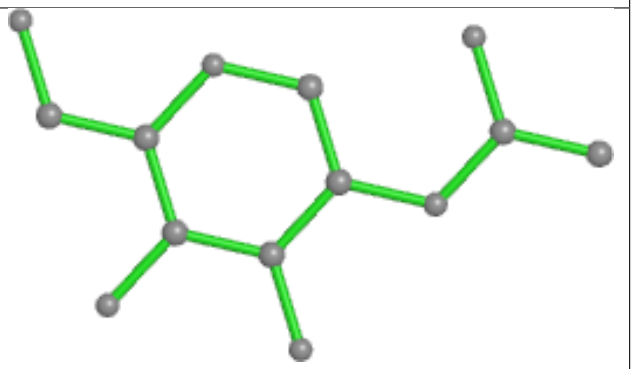
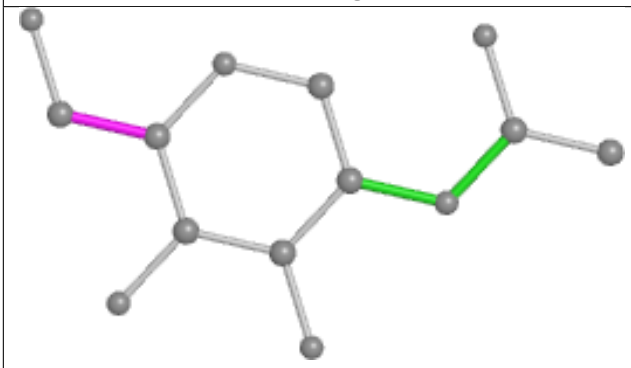


Bond angles



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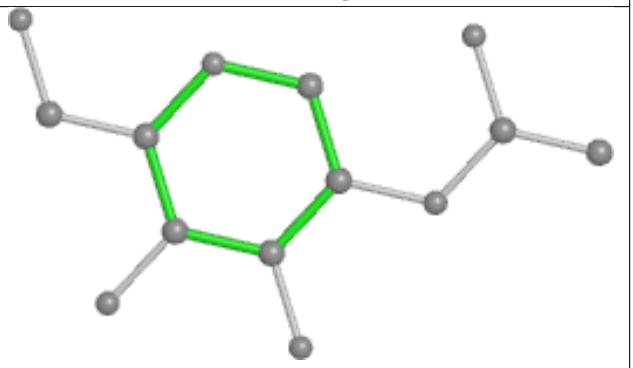
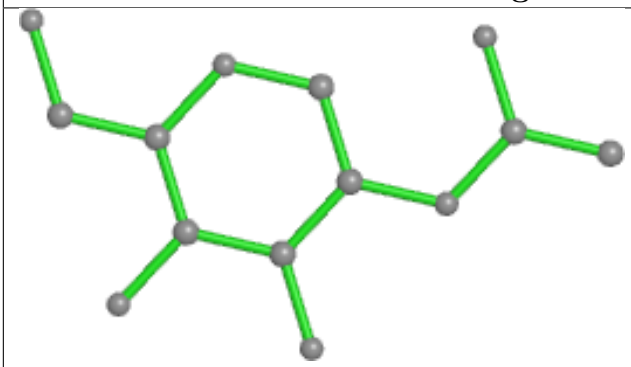
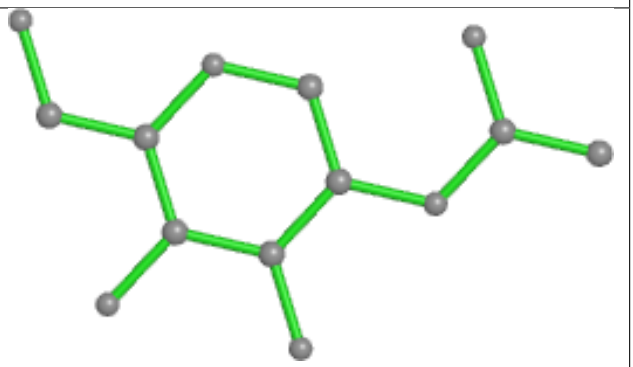


Rings

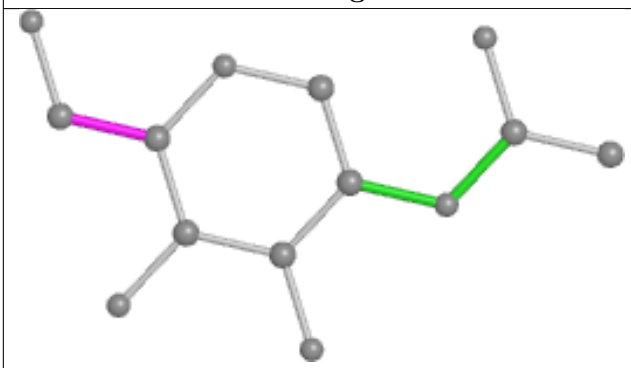
Ligand NAG B 1320



Bond lengths



Bond angles



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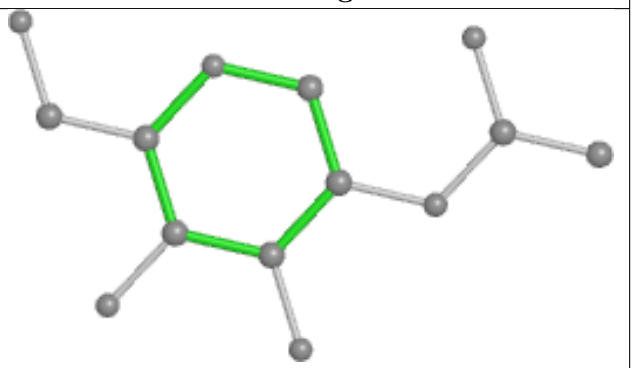
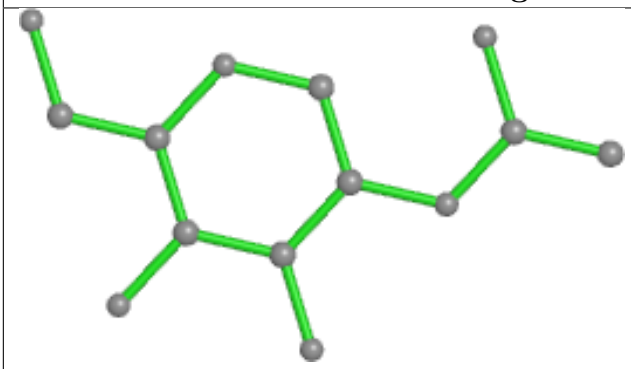
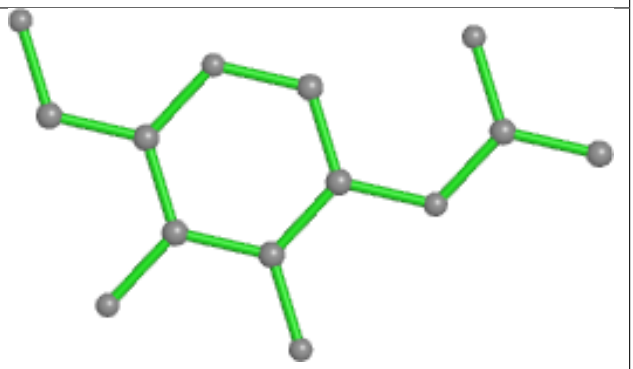


Rings

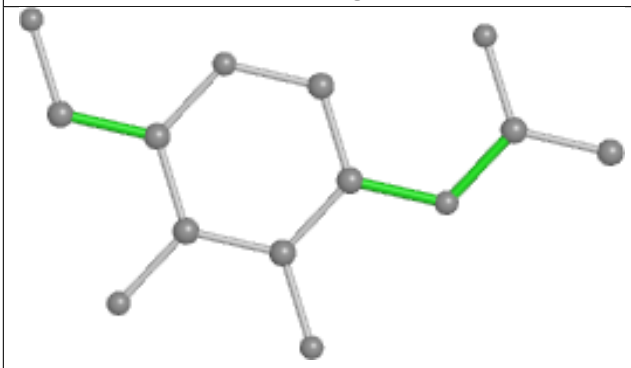
Ligand NAG A 1310



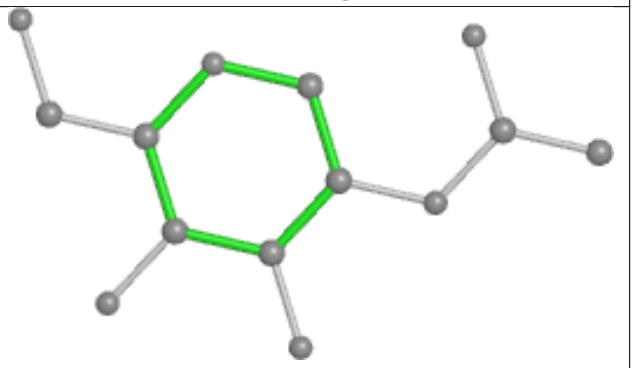
Bond lengths



Bond angles

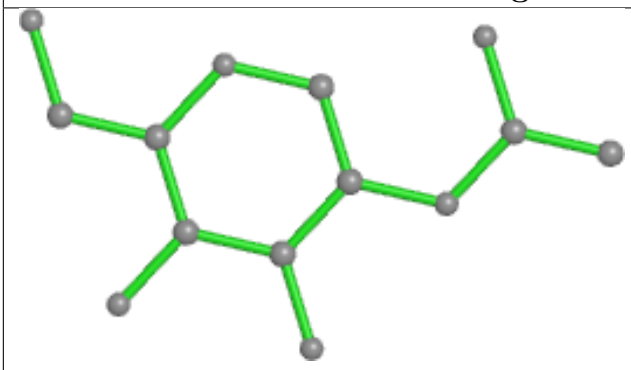


Torsions

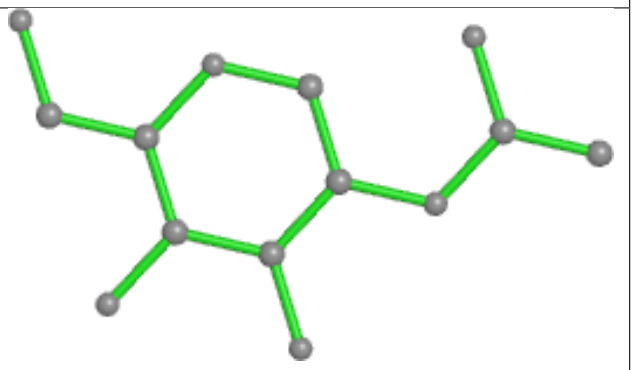


Rings

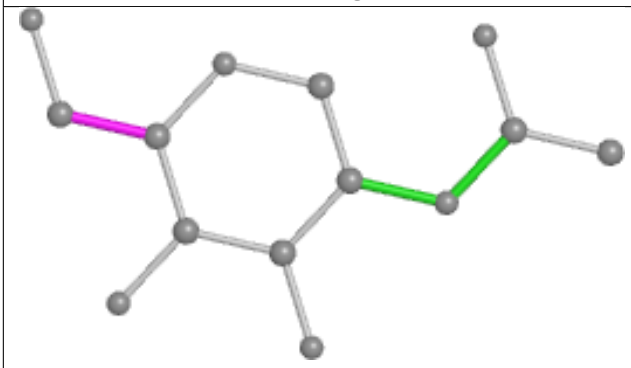
Ligand NAG C 1317



Bond lengths



Bond angles



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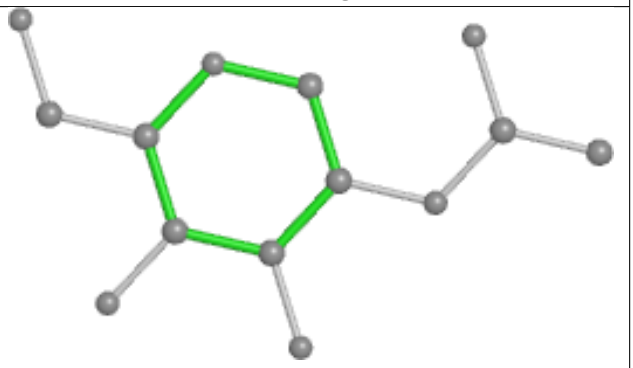
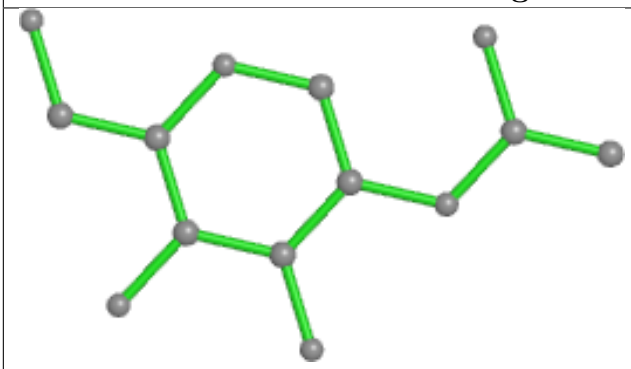
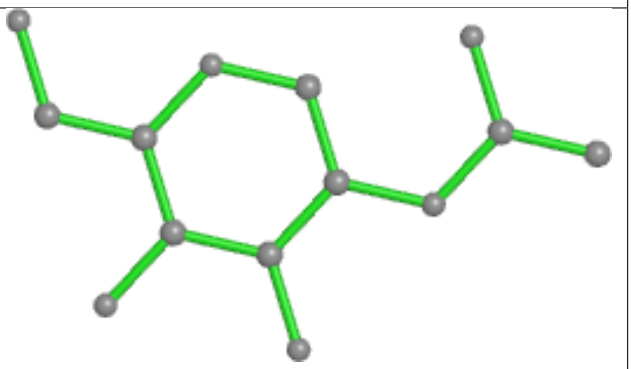
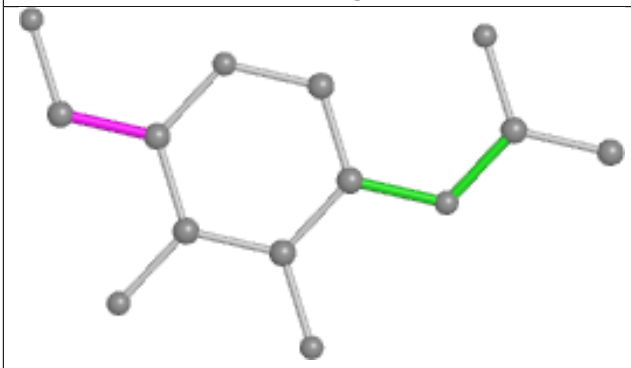
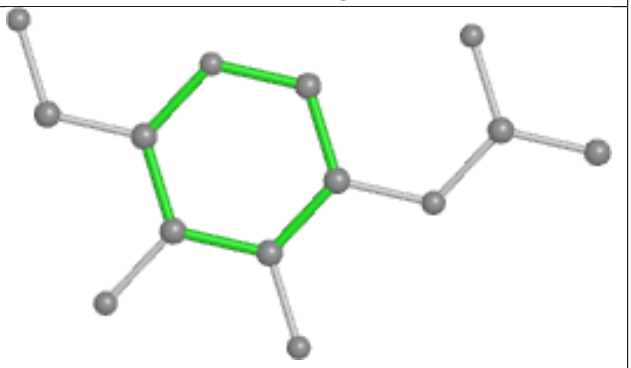
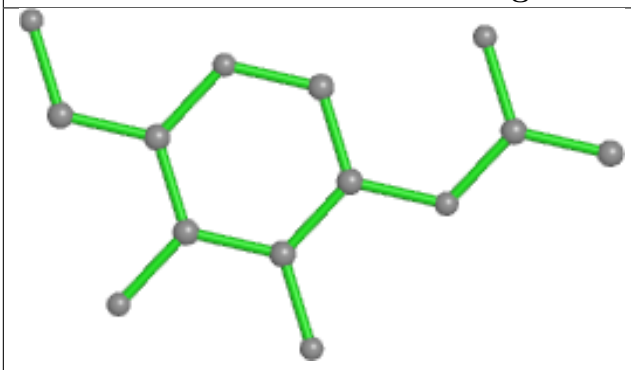
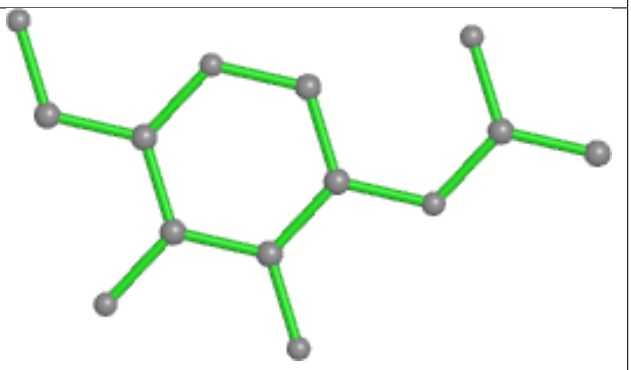
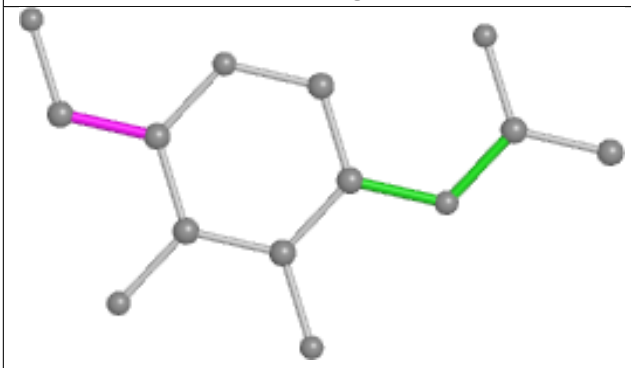
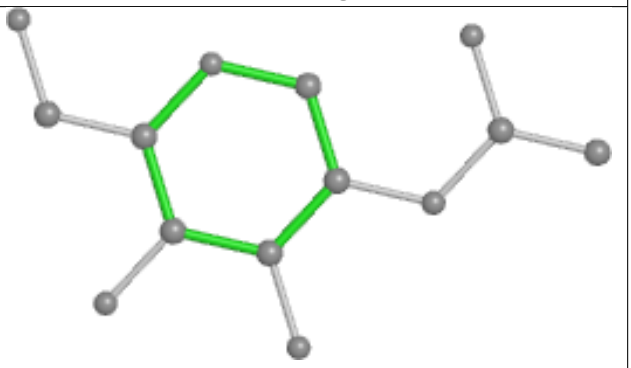
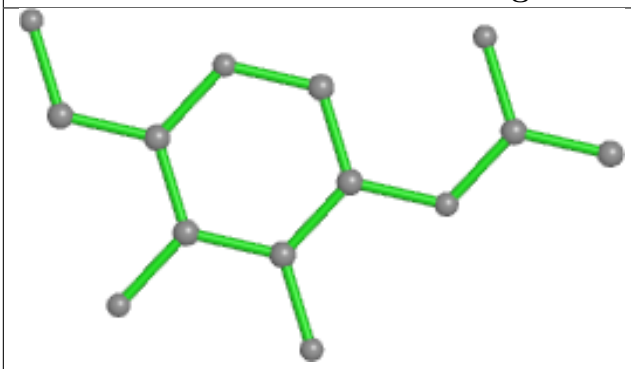


Rings

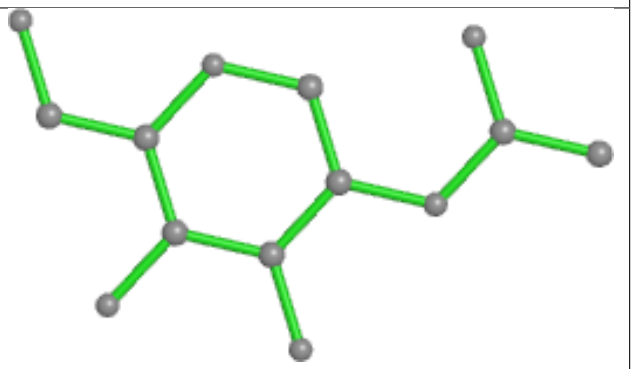
Ligand NAG C 1318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1319	
 Bond lengths	 Bond angles
 Torsions	 Rings

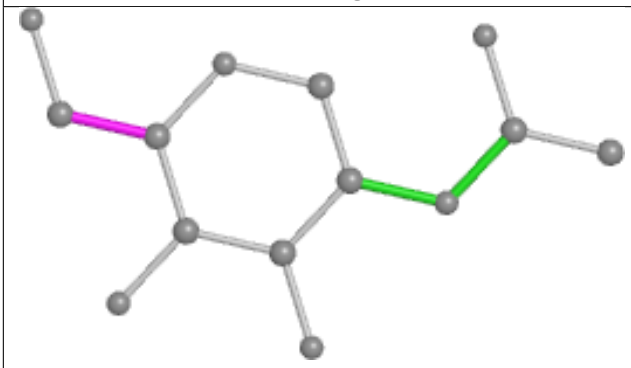
Ligand NAG B 1307



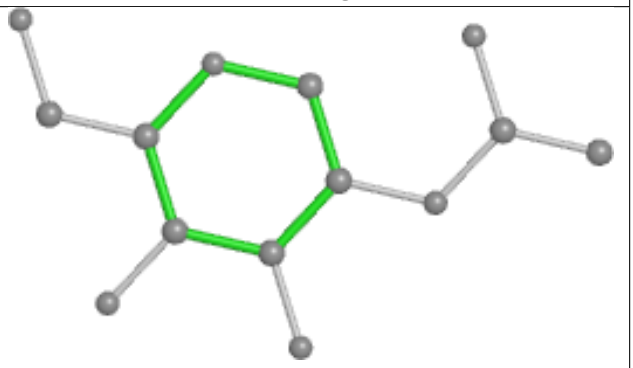
Bond lengths



Bond angles

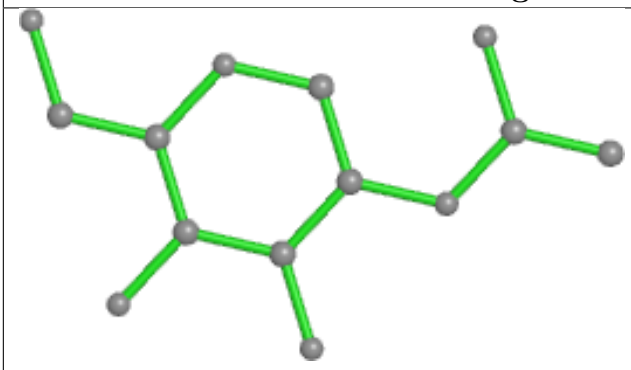


Torsions



Rings

Ligand NAG B 1302



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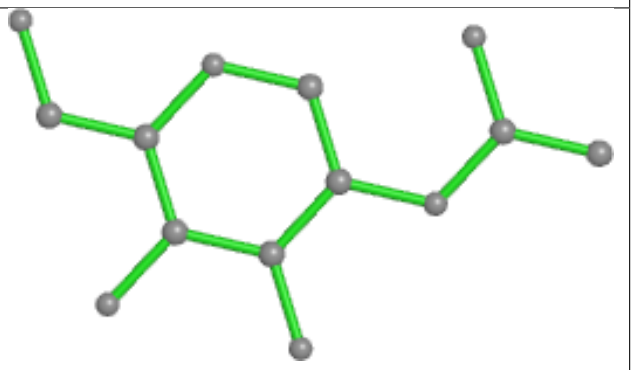
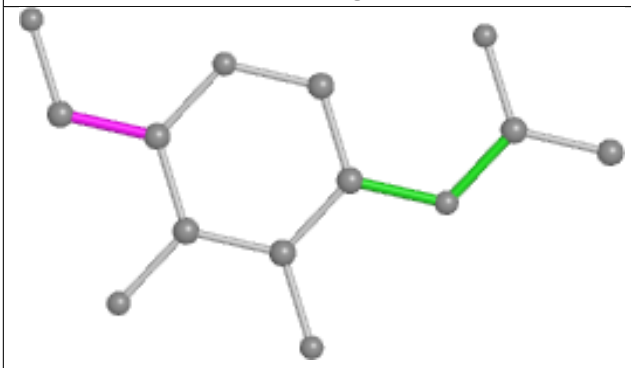


Bond angles



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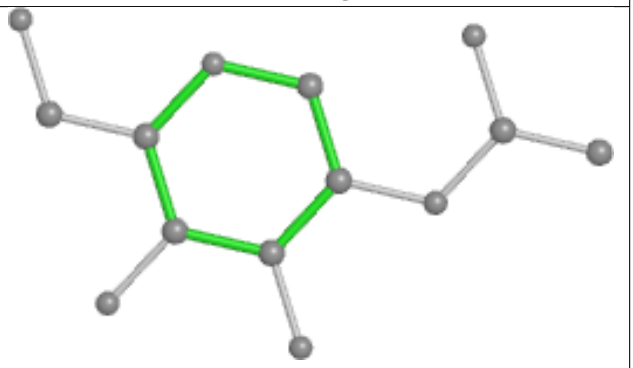
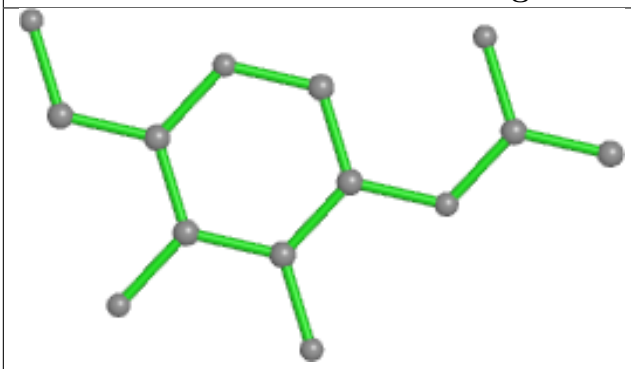


Rings

Ligand NAG B 1310



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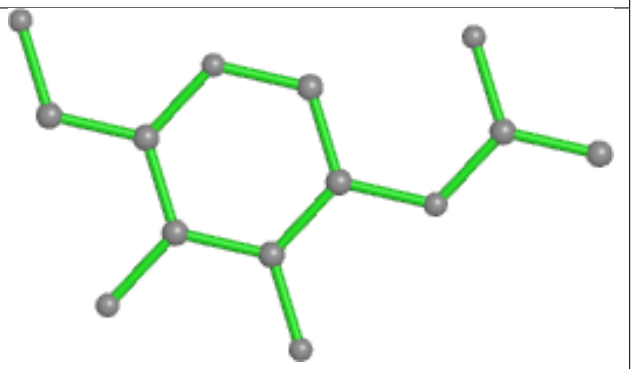
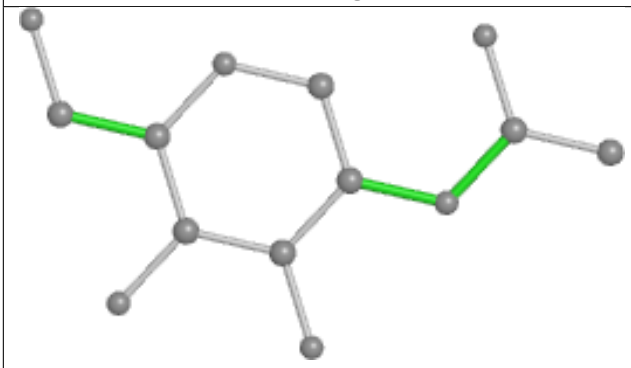


Bond angles



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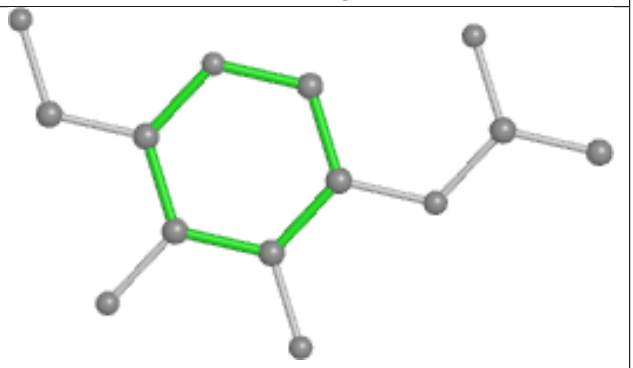
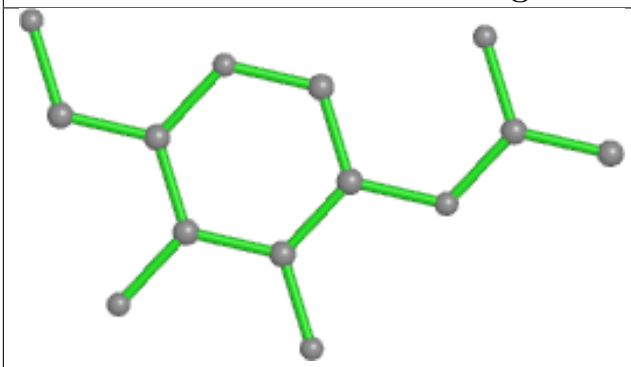


Rings

Ligand NAG C 1311



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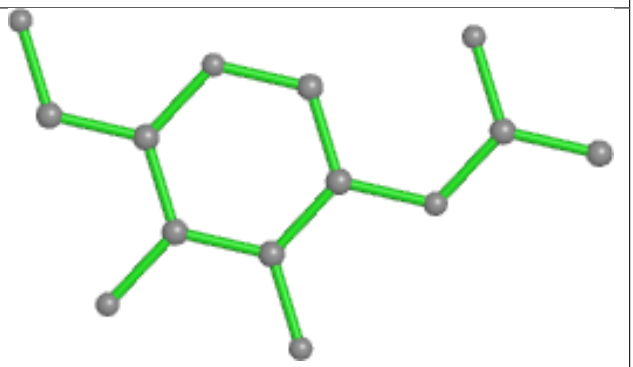

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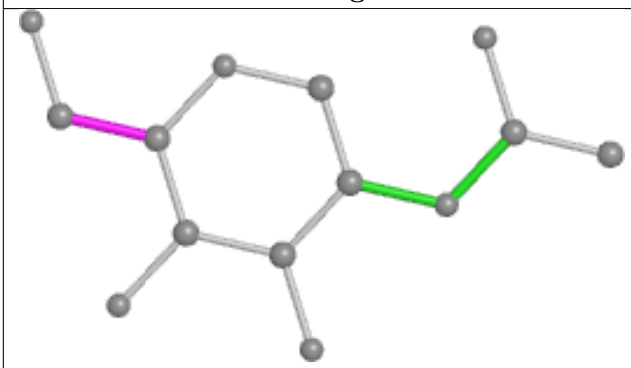

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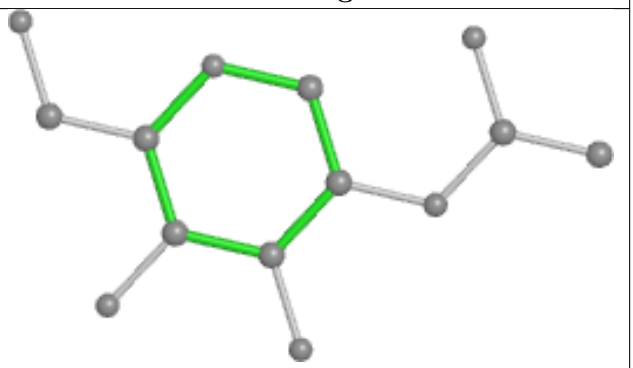
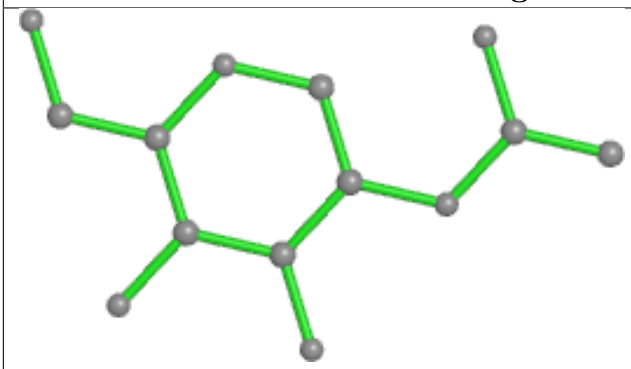


Rings

Ligand NAG A 1319



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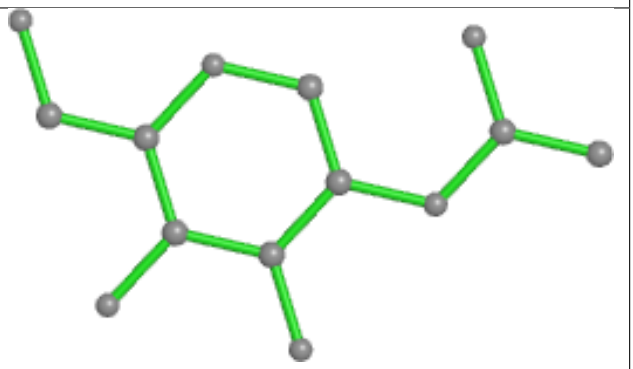
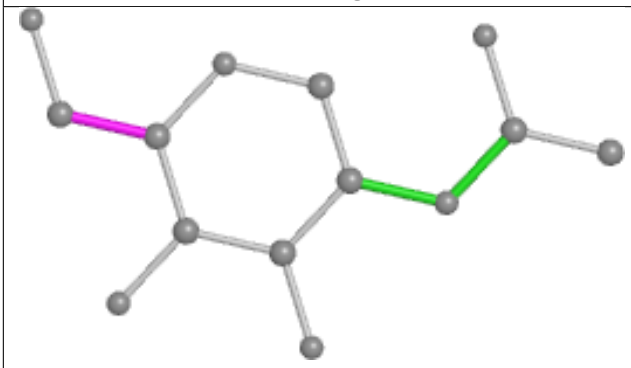


Bond angles



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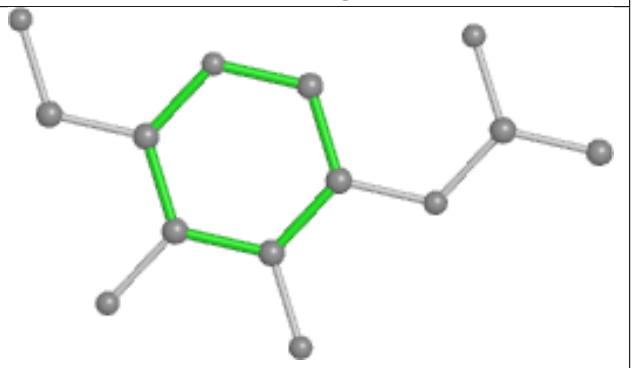
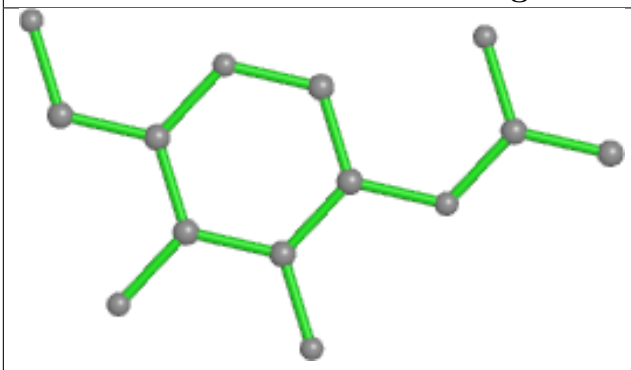


Rings

Ligand NAG A 1309



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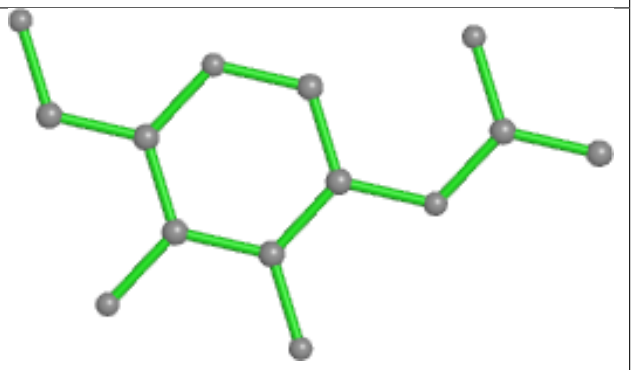
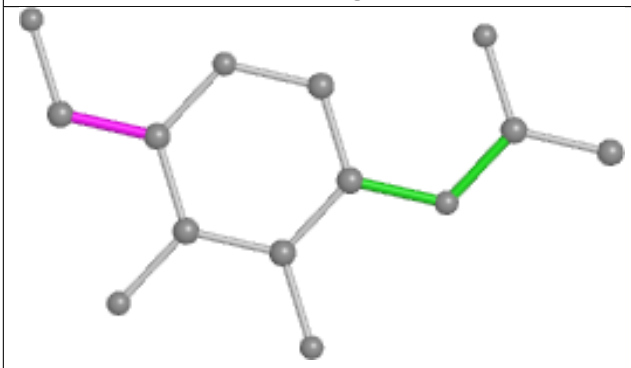


Bond angles



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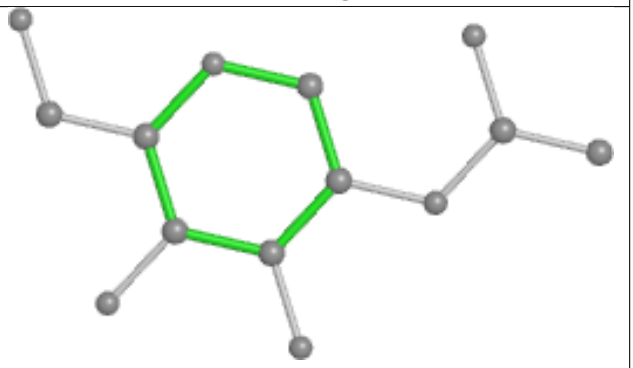
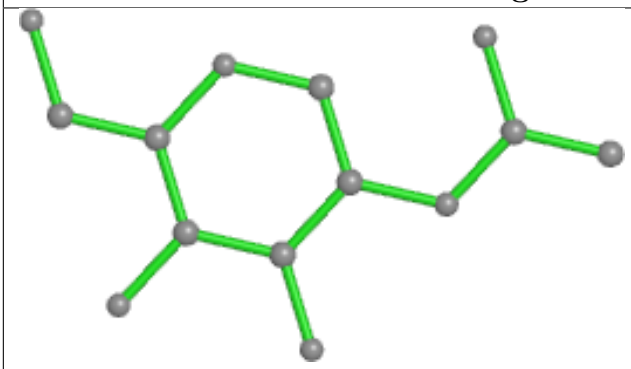


Rings

Ligand NAG B 1318



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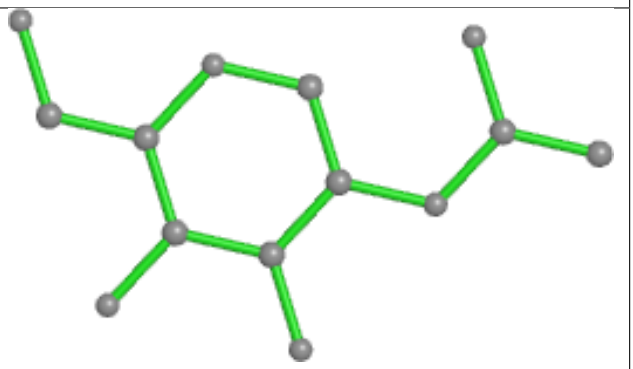
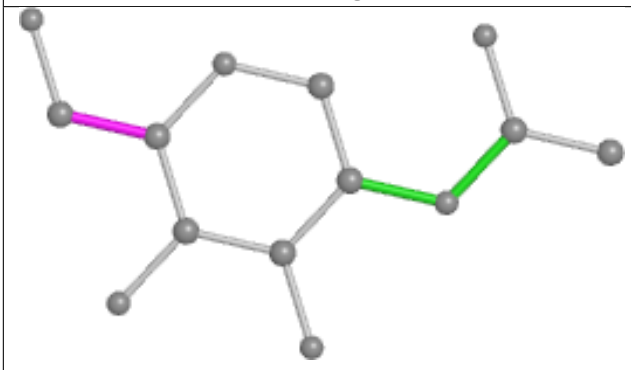


Bond angles



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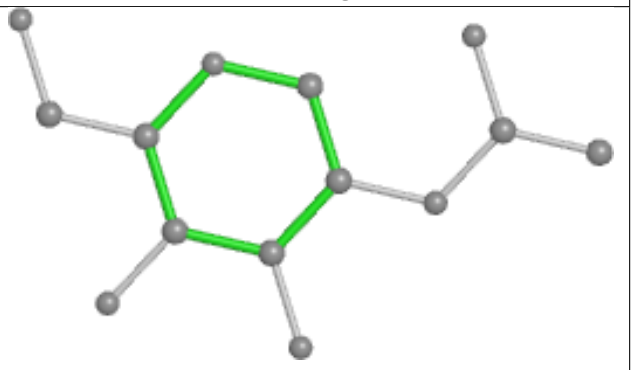
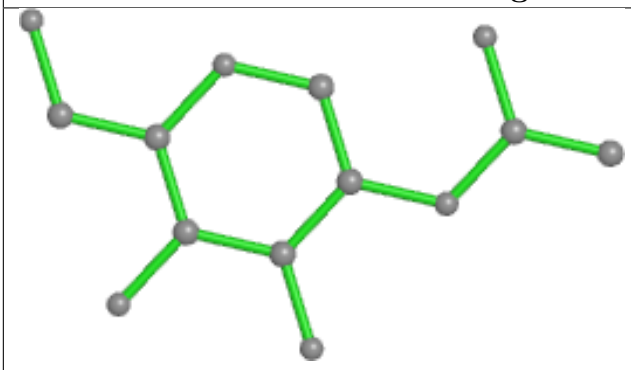


Rings

Ligand NAG A 1316



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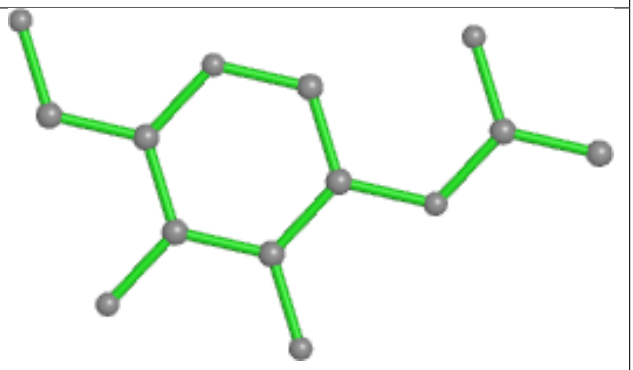
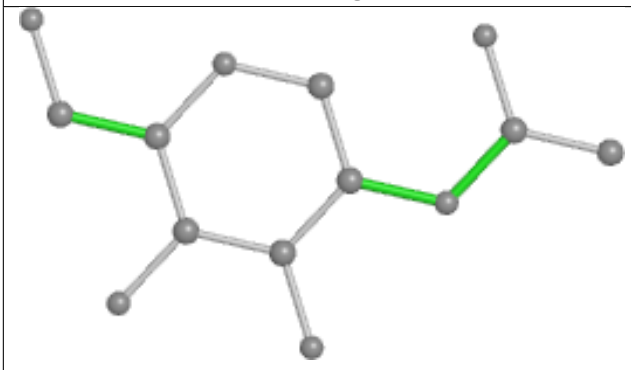


Bond angles



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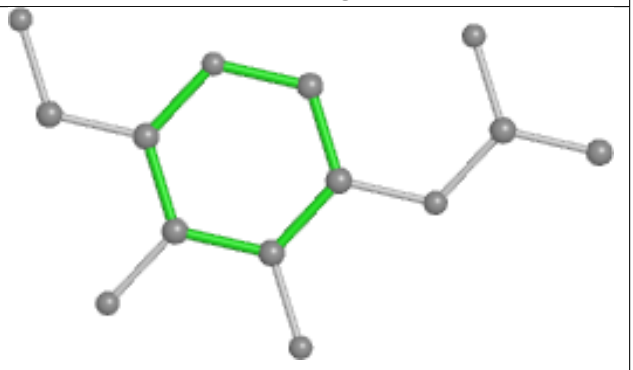
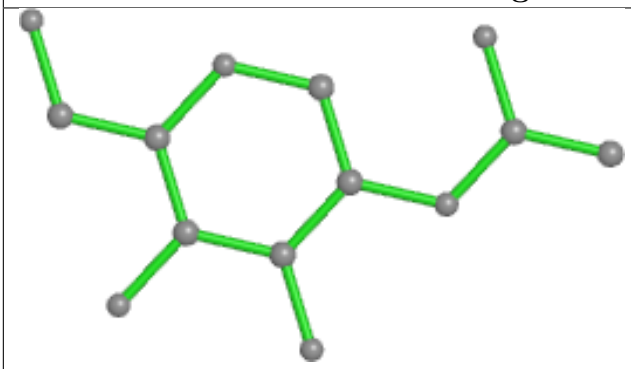


Rings

Ligand NAG B 1311



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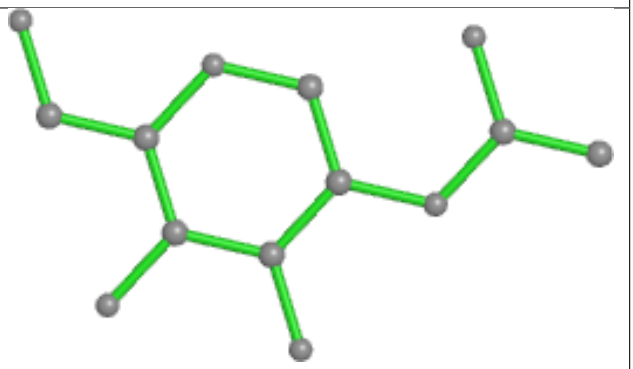
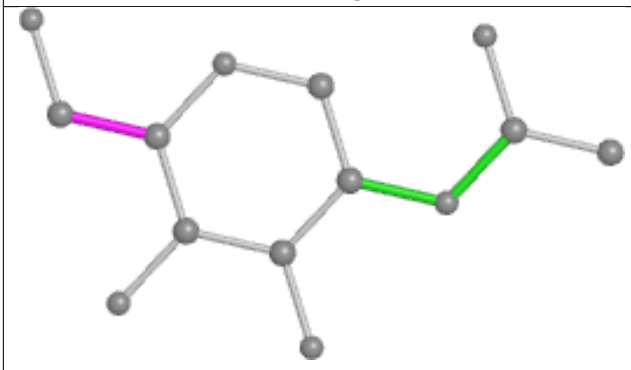


Bond angles



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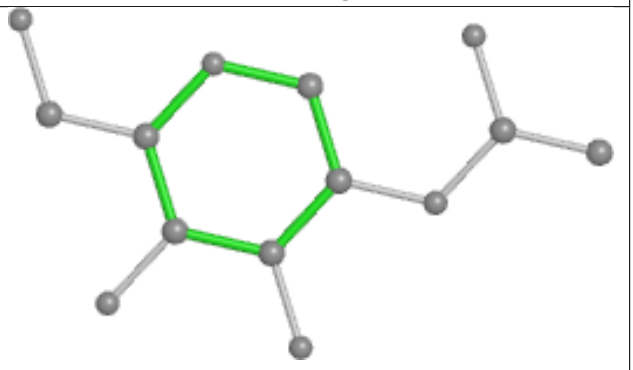
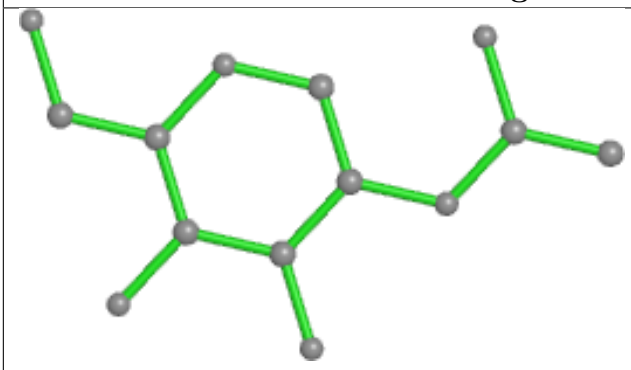


Rings

Ligand NAG A 1308



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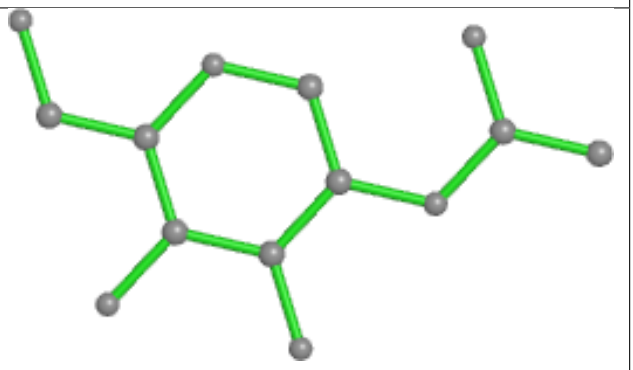
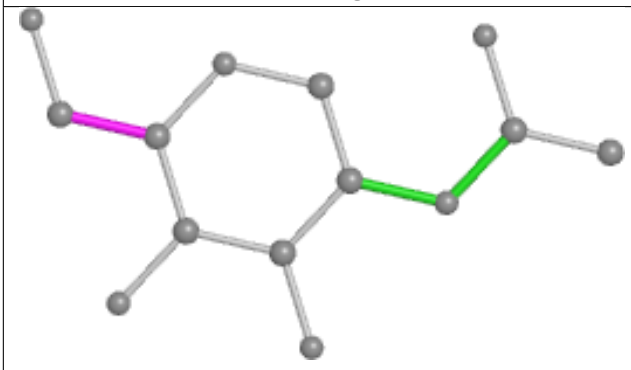


Bond angles



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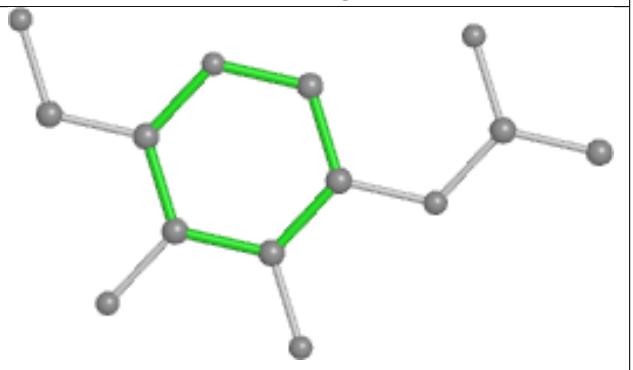
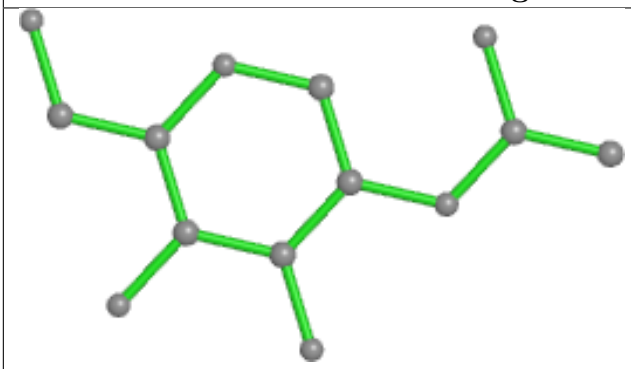
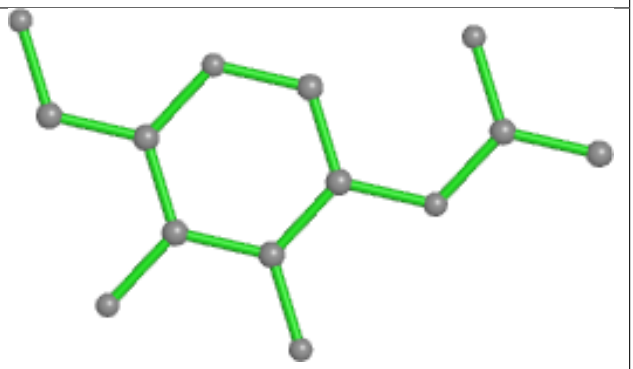


Rings

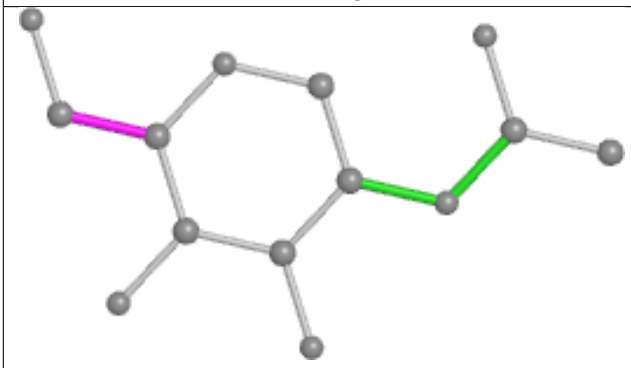
Ligand NAG C 1305



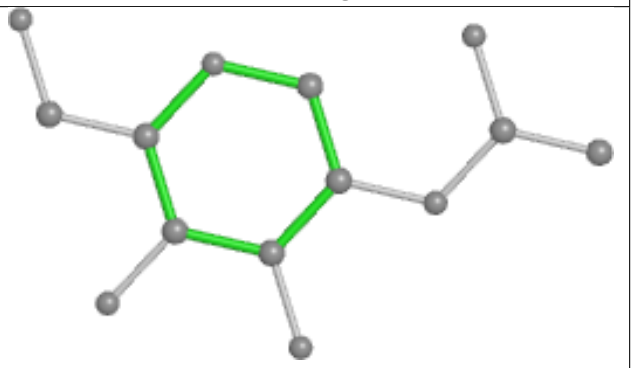
Bond lengths



Bond angles

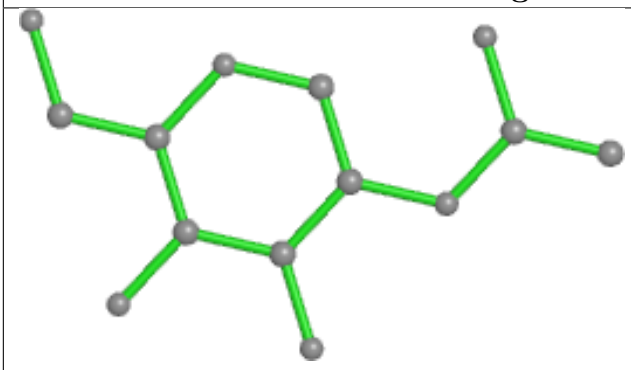


Torsions

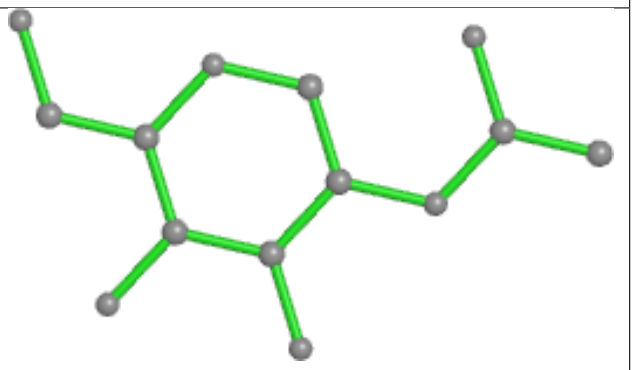


Rings

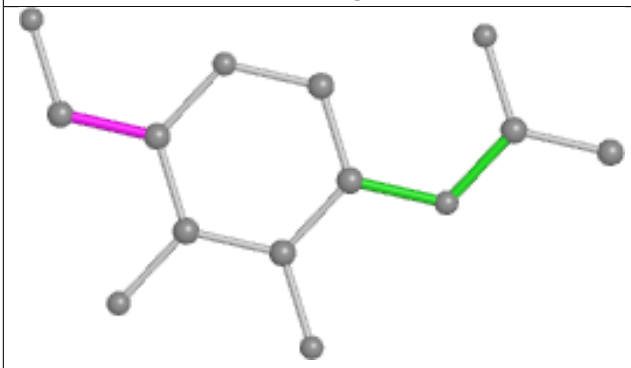
Ligand NAG C 1309



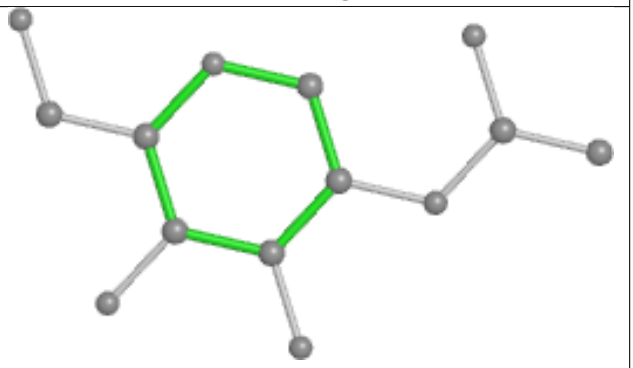
Bond lengths



Bond angles

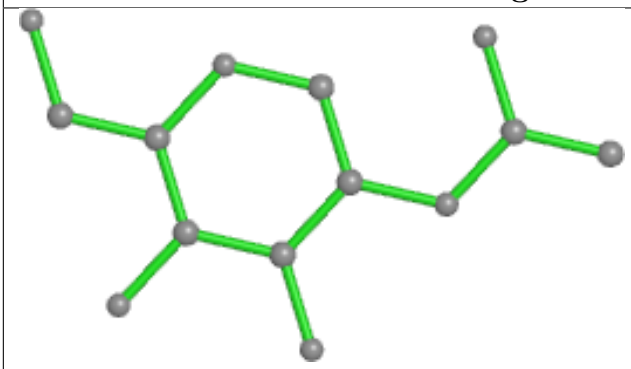


Torsions

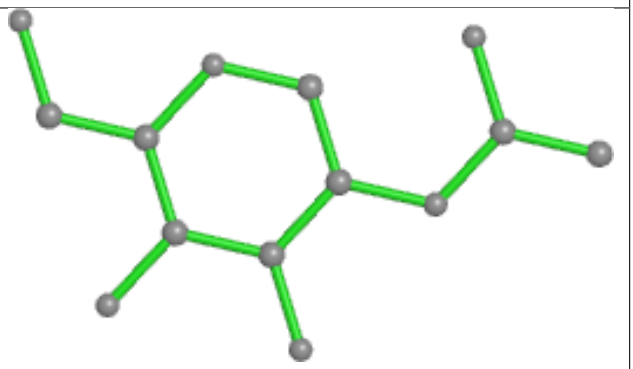


Rings

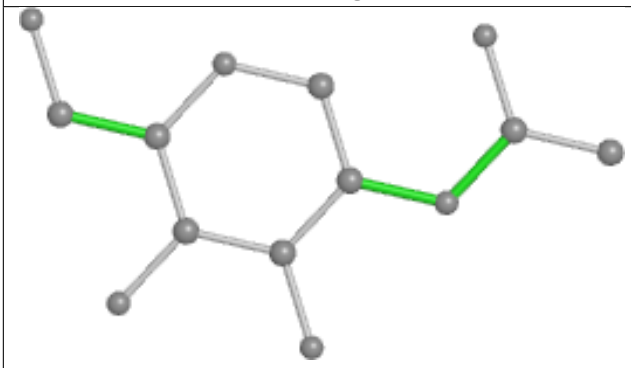
Ligand NAG C 1315



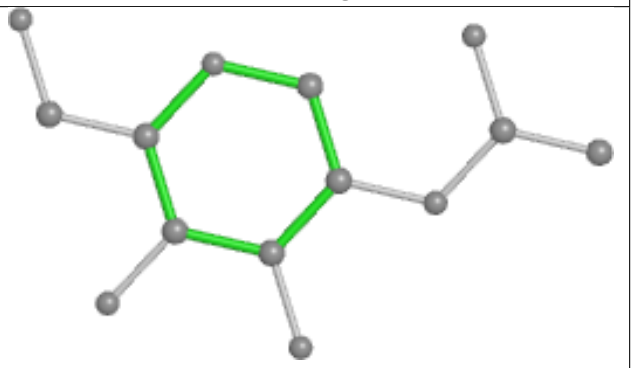
Bond lengths



Bond angles

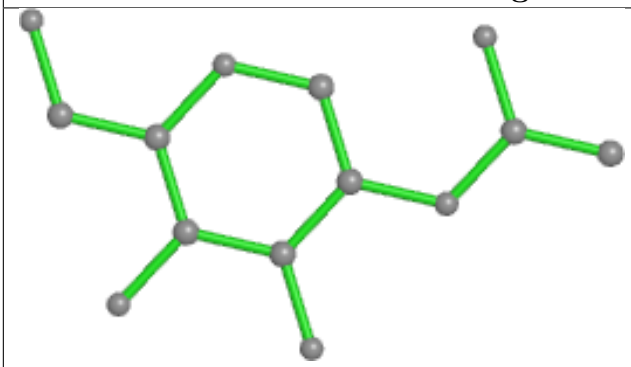


Torsions

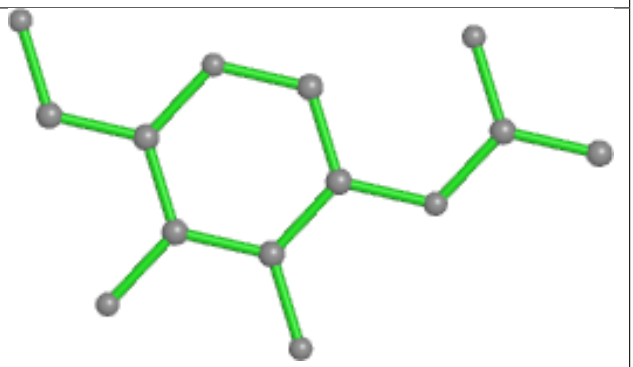


Rings

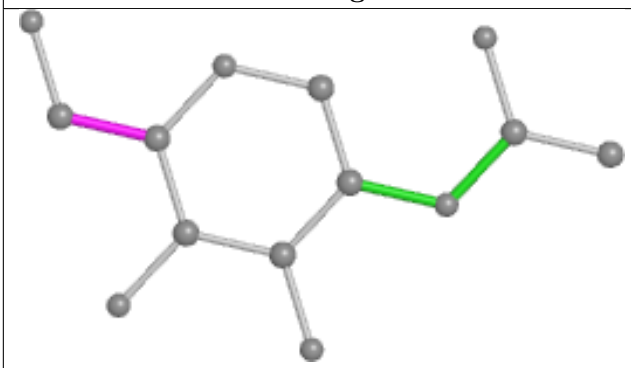
Ligand NAG C 1302



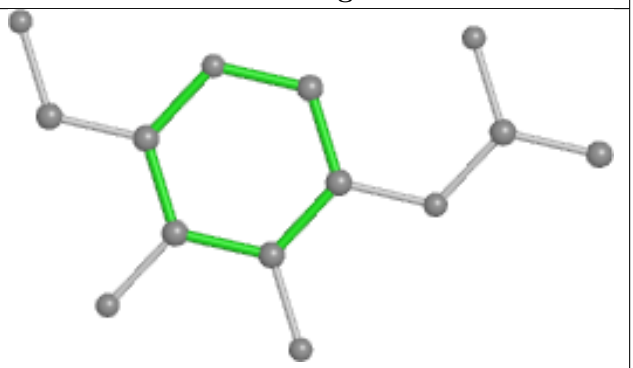
Bond lengths



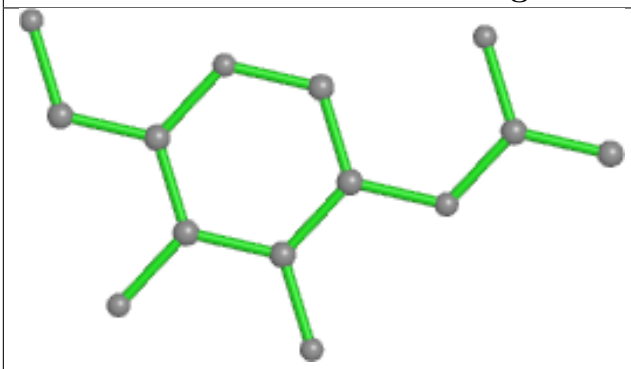
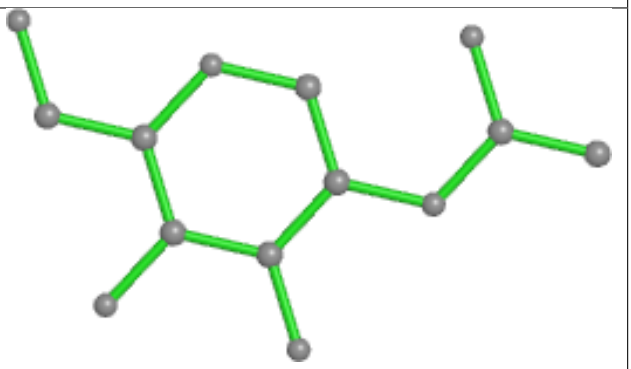
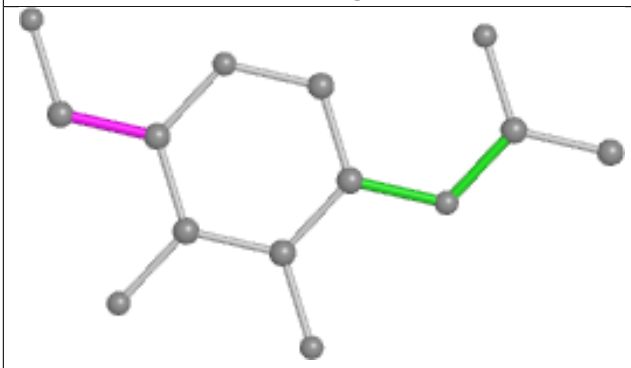
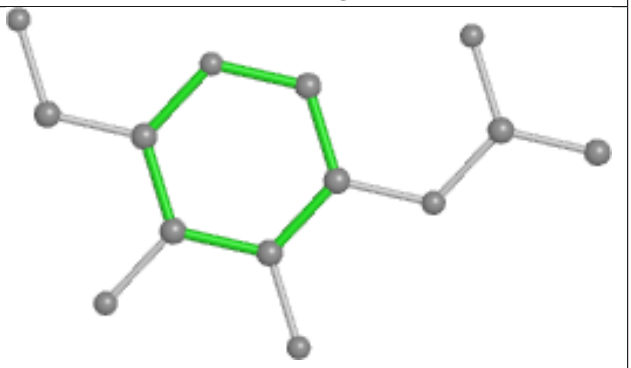
Bond angles

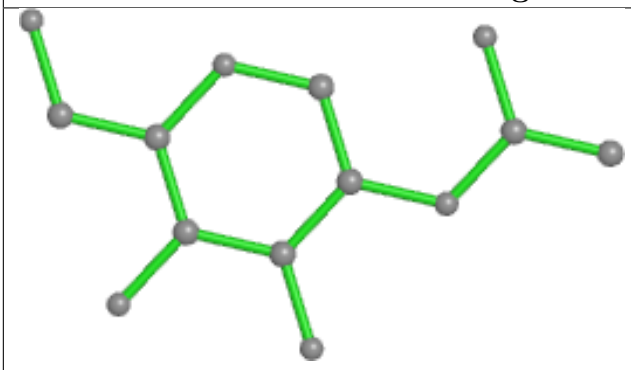
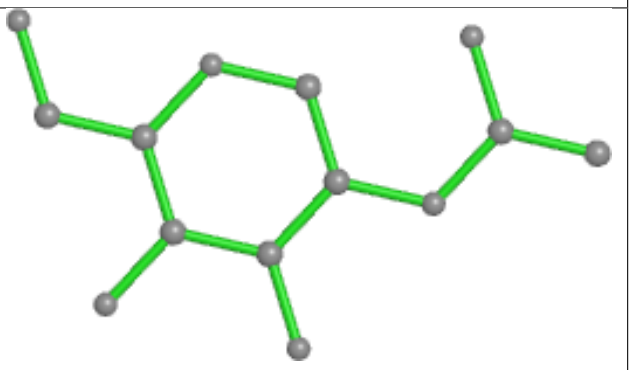
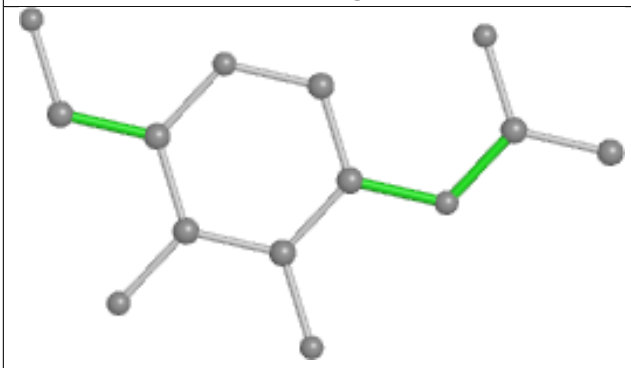
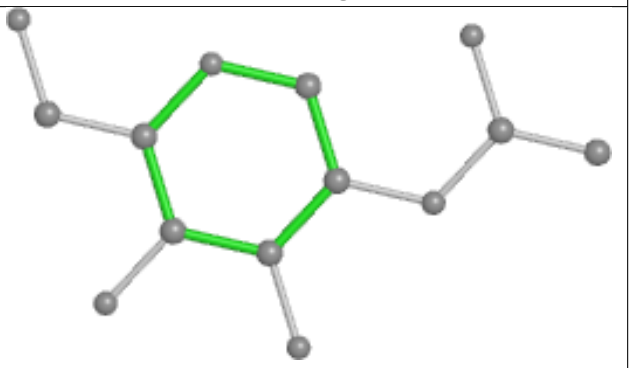


Torsions

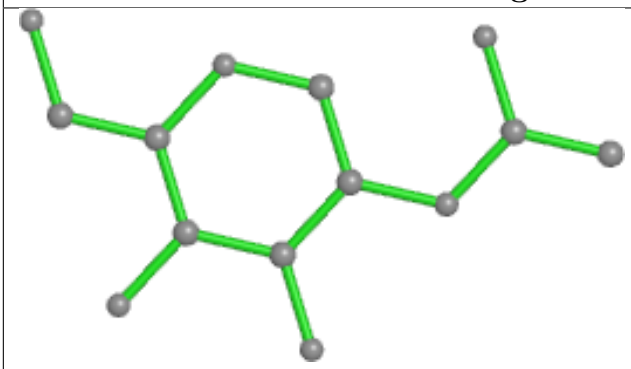


Rings

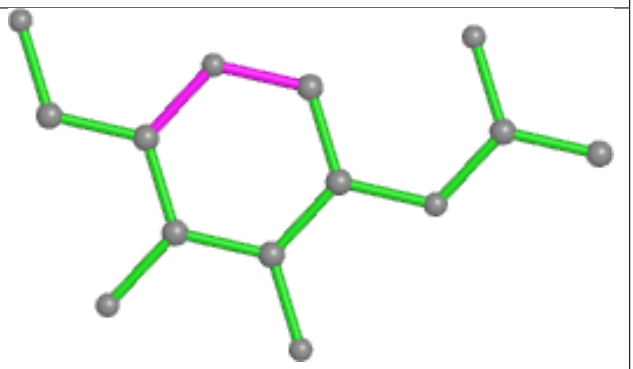
Ligand NAG A 1312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1313	
 Bond lengths	 Bond angles
 Torsions	 Rings

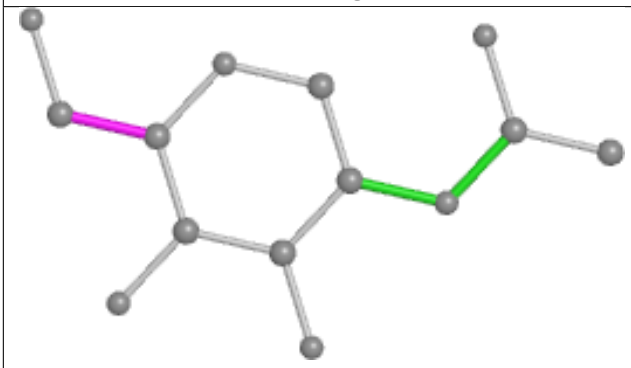
Ligand NAG A 1311



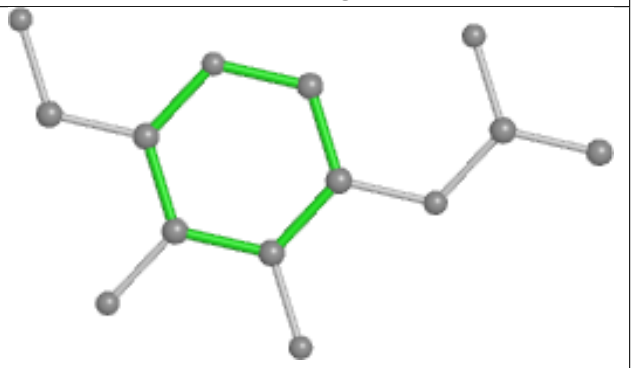
Bond lengths



Bond angles

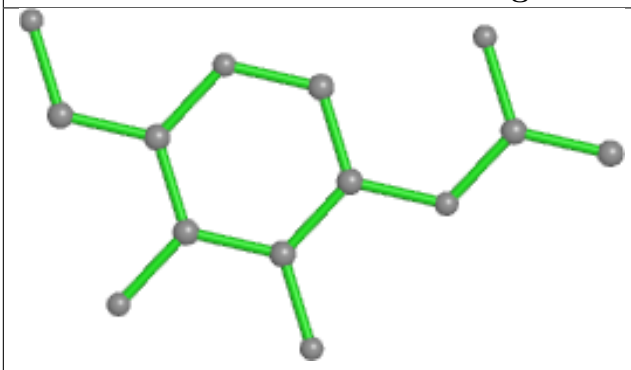


Torsions

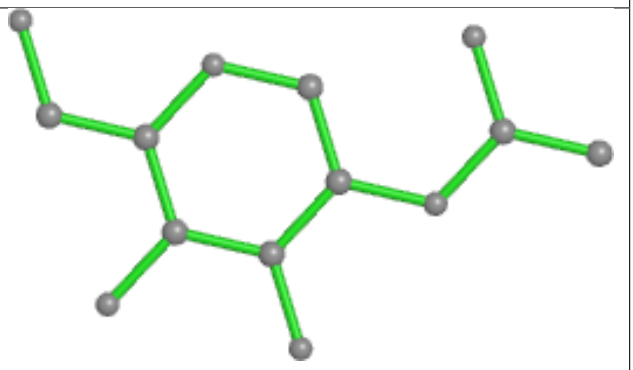


Rings

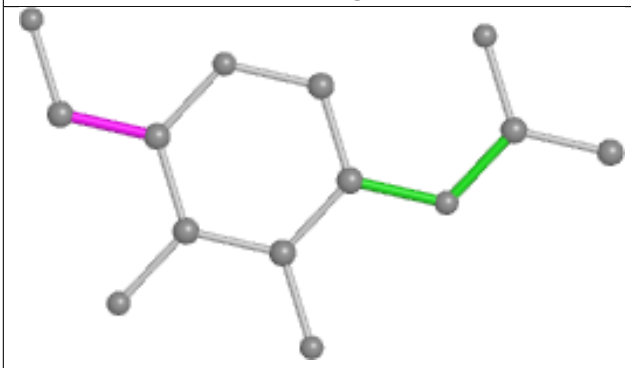
Ligand NAG C 1301



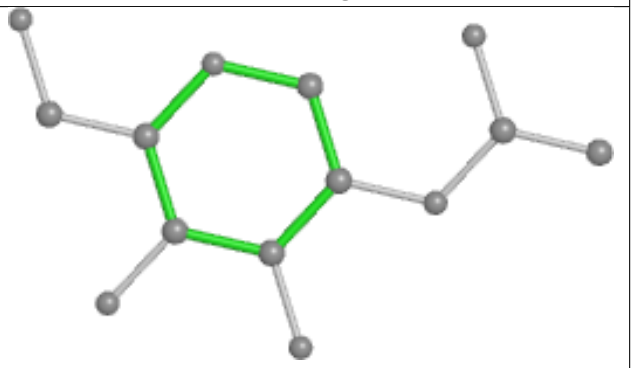
Bond lengths



Bond angles

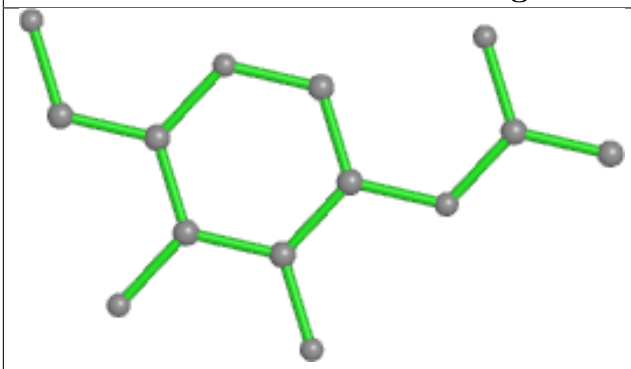


Torsions

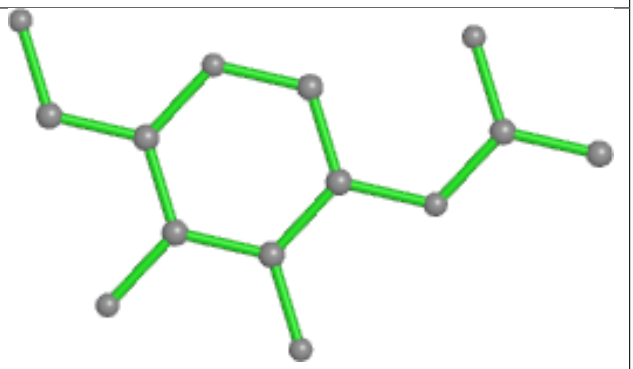


Rings

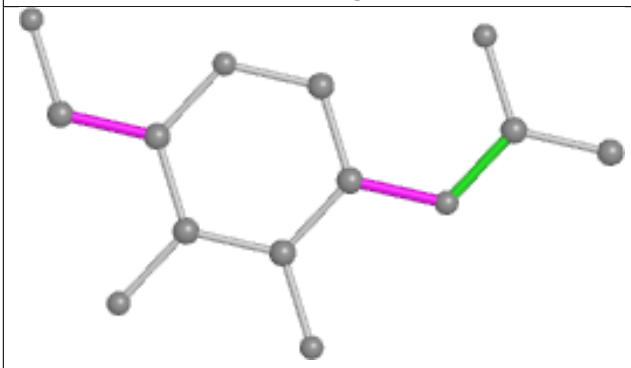
Ligand NAG A 1304



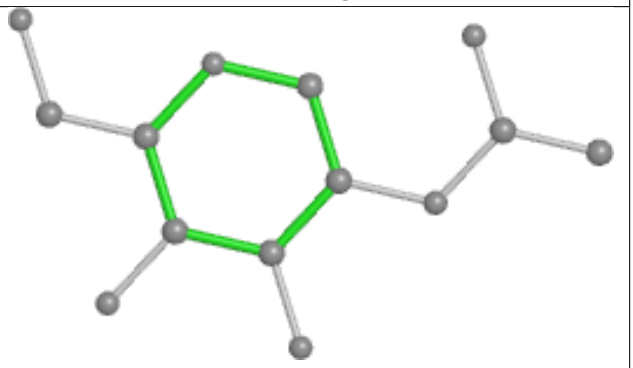
Bond lengths



Bond angles

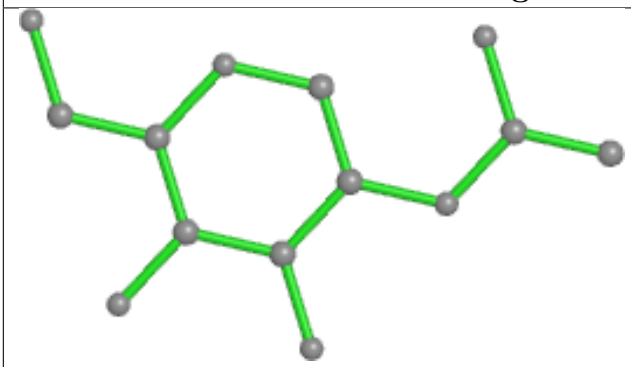


Torsions



Rings

Ligand NAG B 1314



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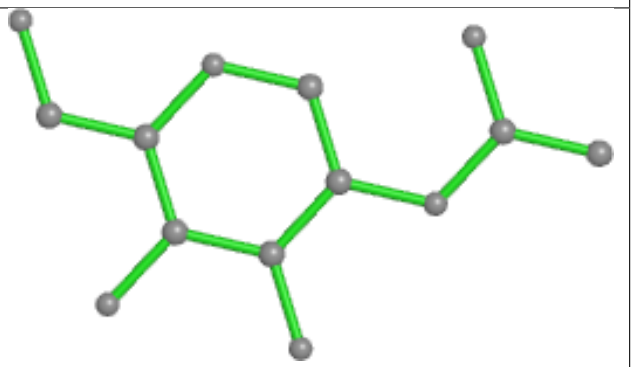
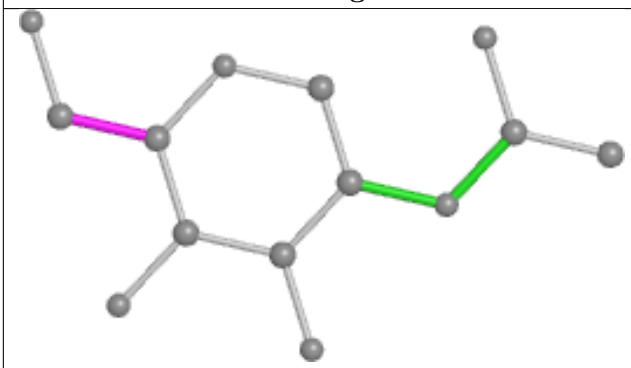


Bond angles



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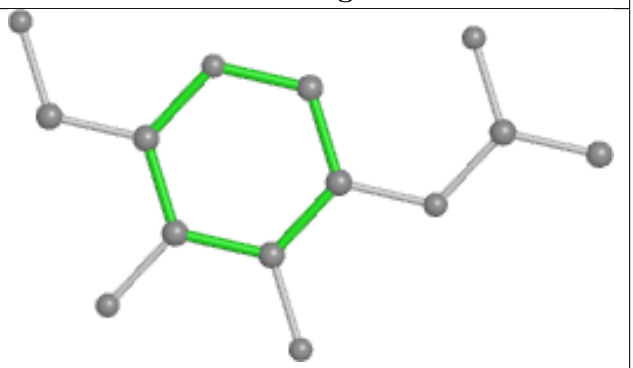
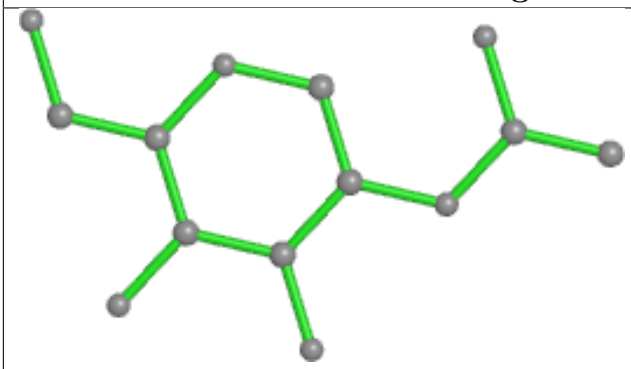


Rings

Ligand NAG C 1303



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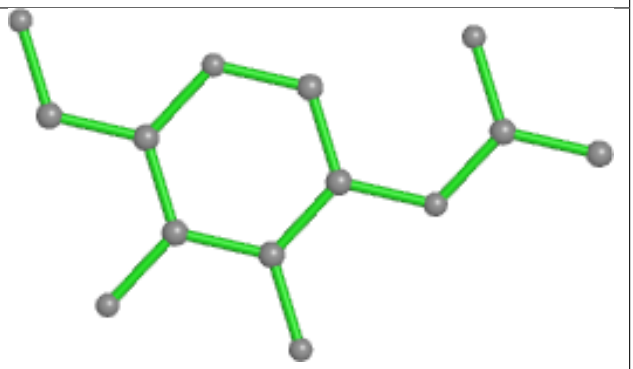
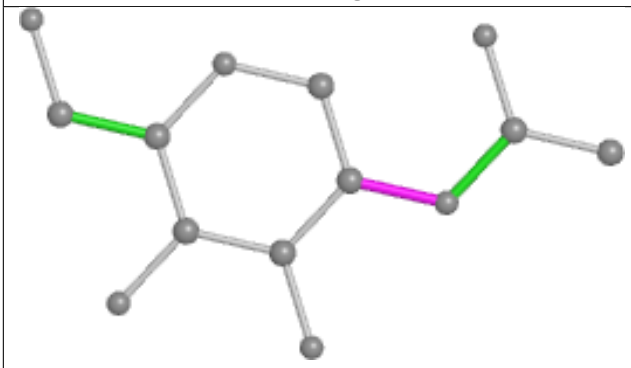
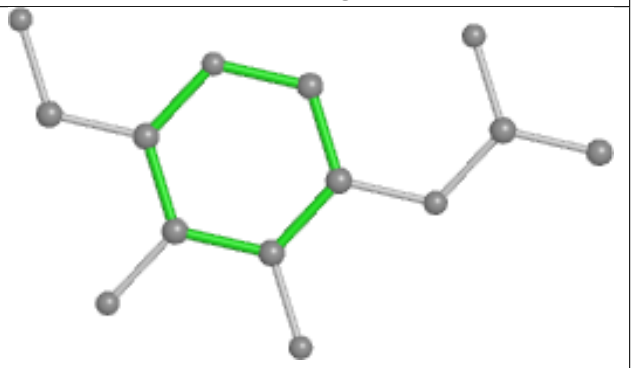


Bond angles

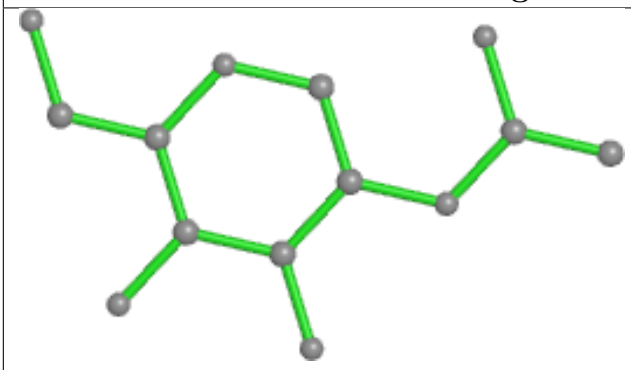


Torsions



Rings

Ligand NAG C 1306



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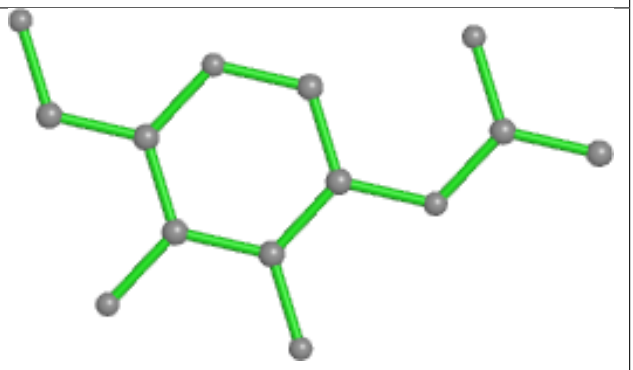
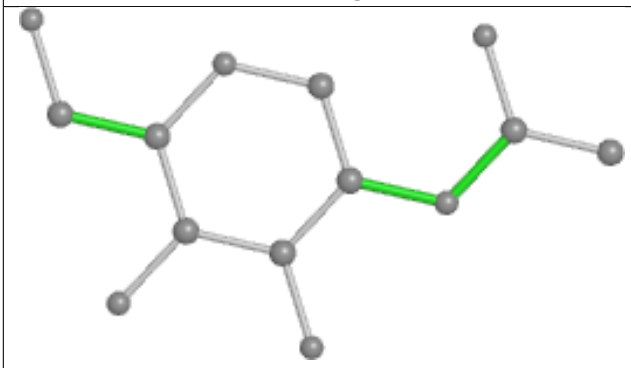
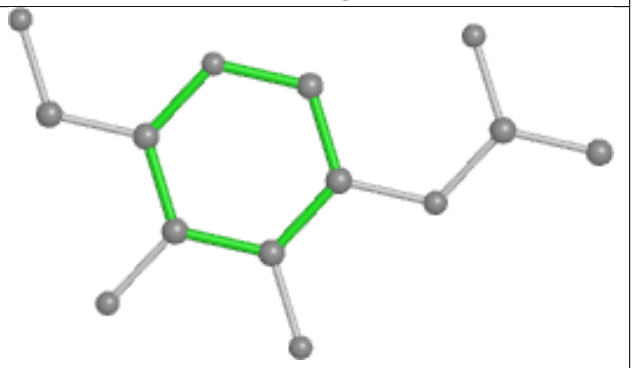


Bond angles

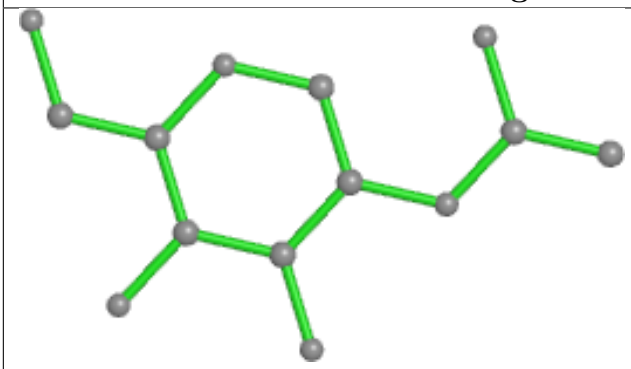


Torsions

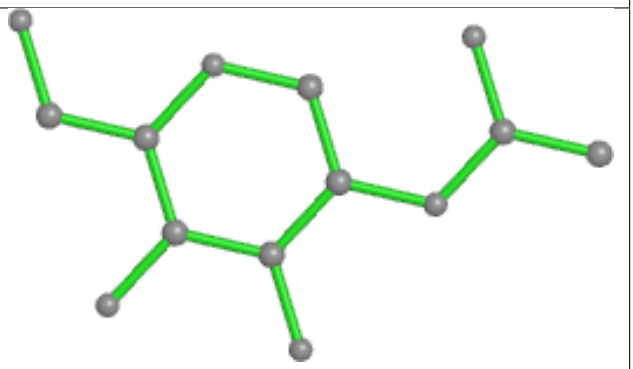


Rings

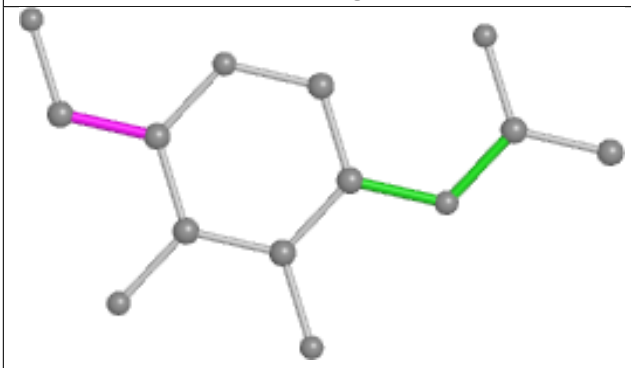
Ligand NAG A 1307



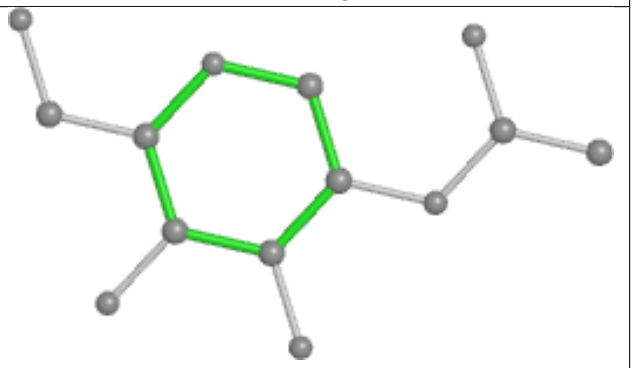
Bond lengths



Bond angles

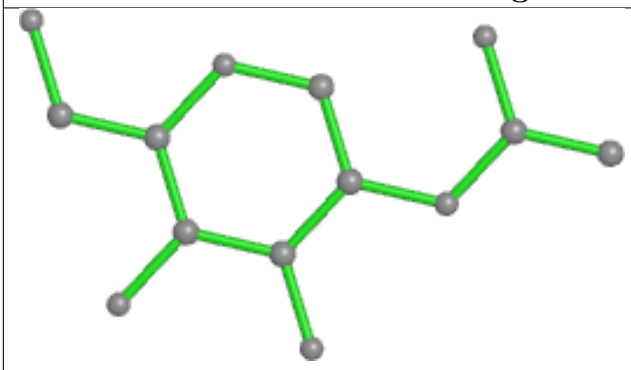


Torsions



Rings

Ligand NAG C 1314



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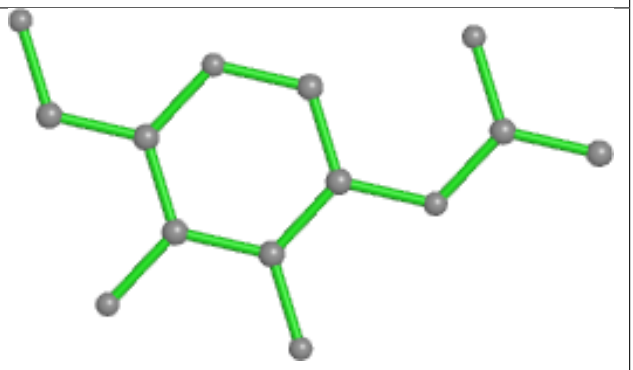
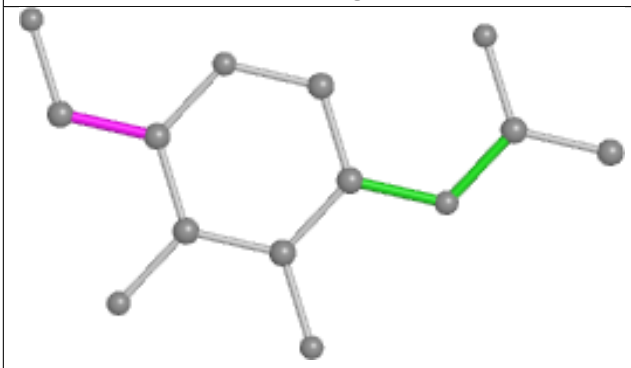
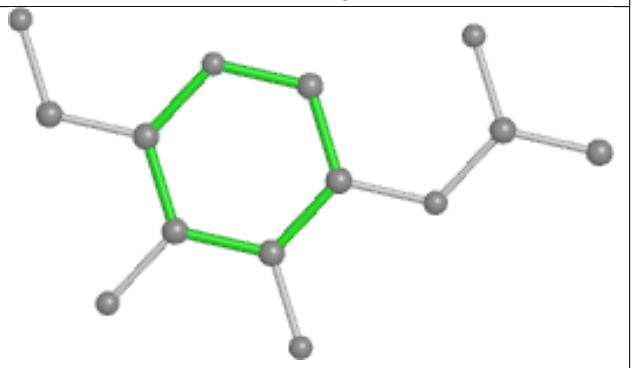


Bond angles

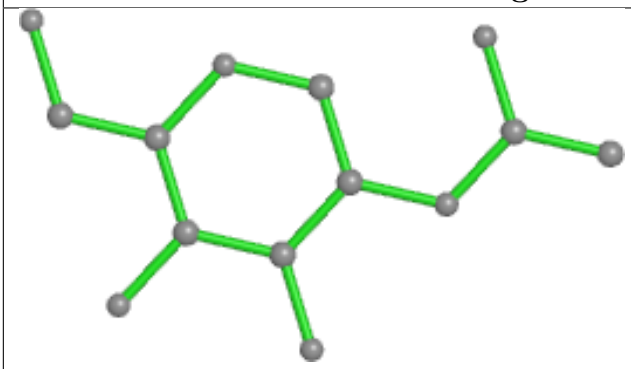


Torsions

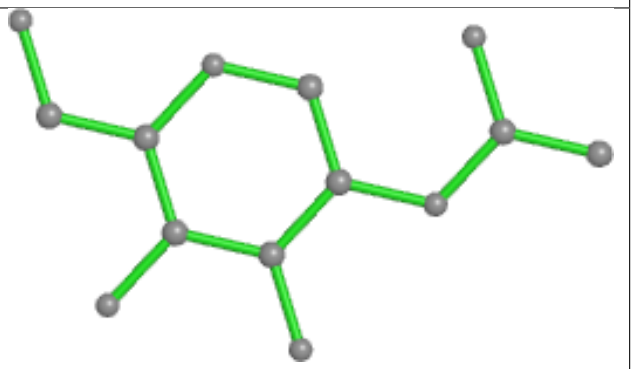


Rings

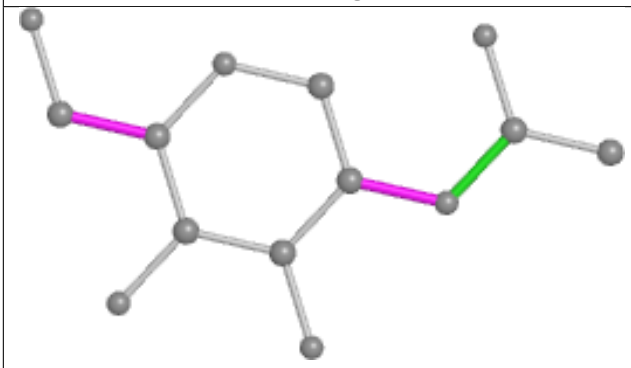
Ligand NAG C 1304



Bond lengths



Bond angles



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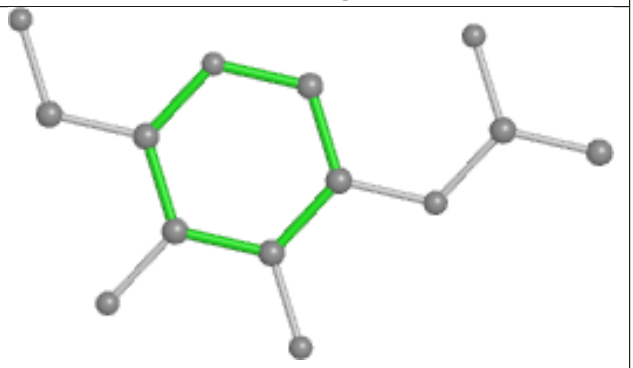
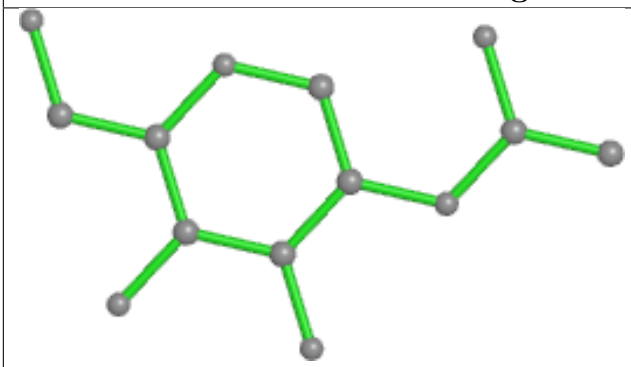


Rings

Ligand NAG A 1315



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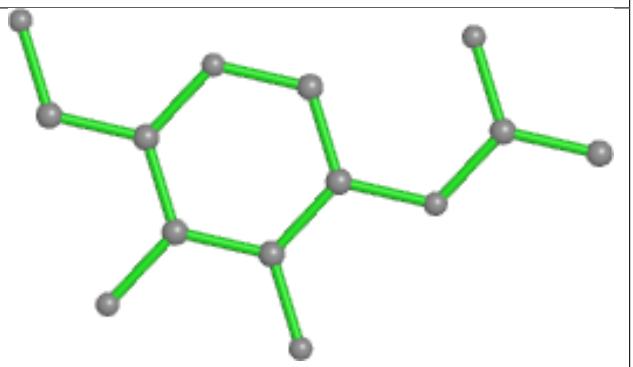
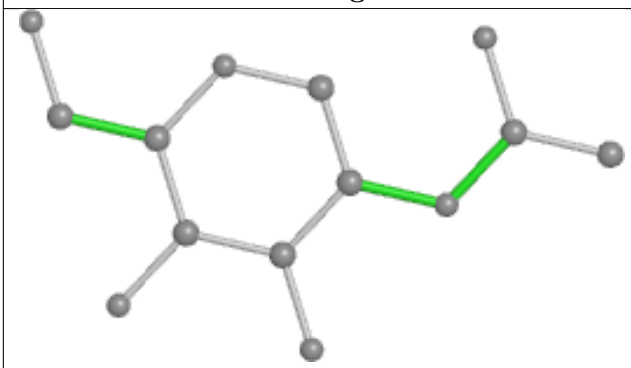


Bond angles



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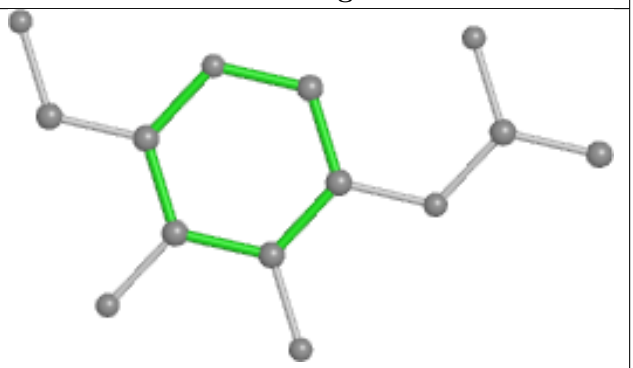
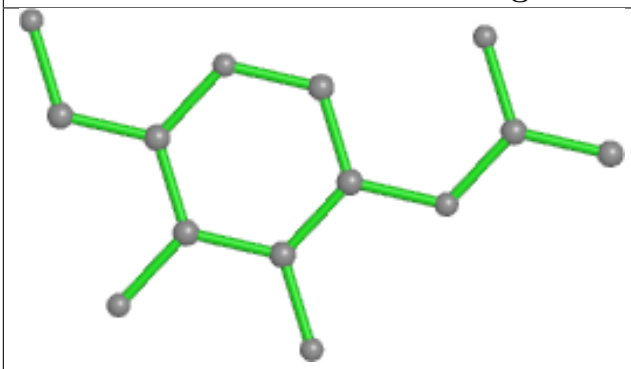


Rings

Ligand NAG C 1307



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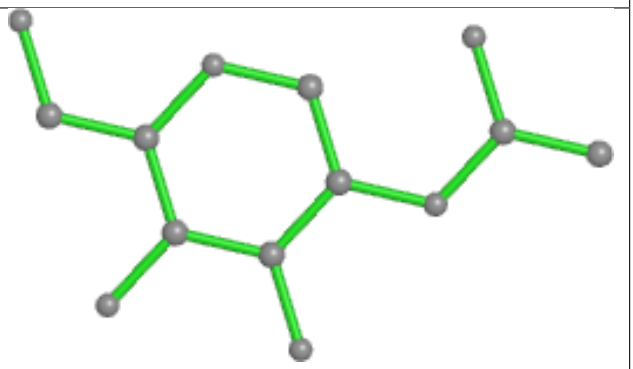
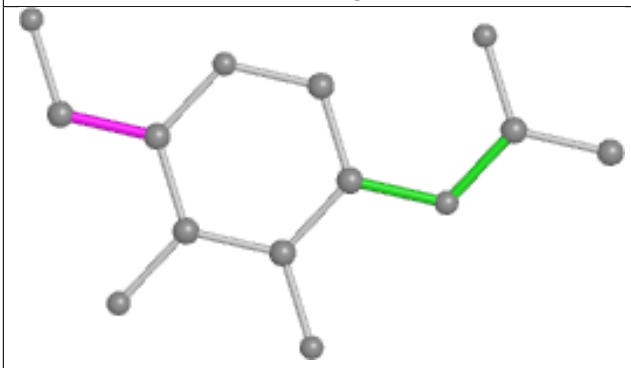


Bond angles



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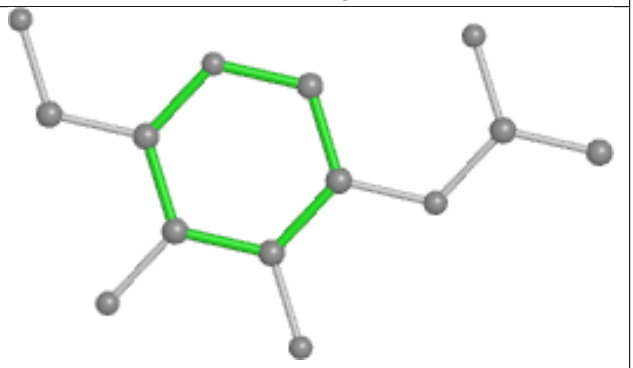
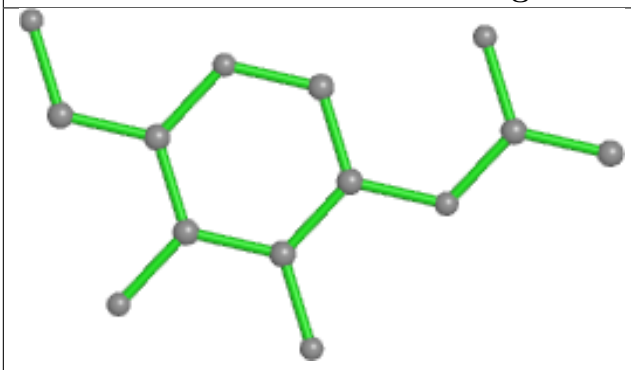


Rings

Ligand NAG B 1312



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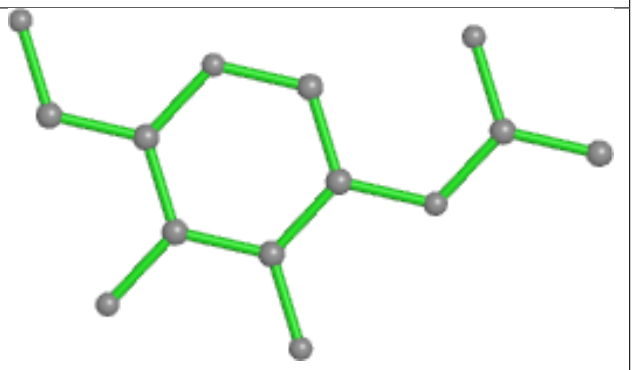
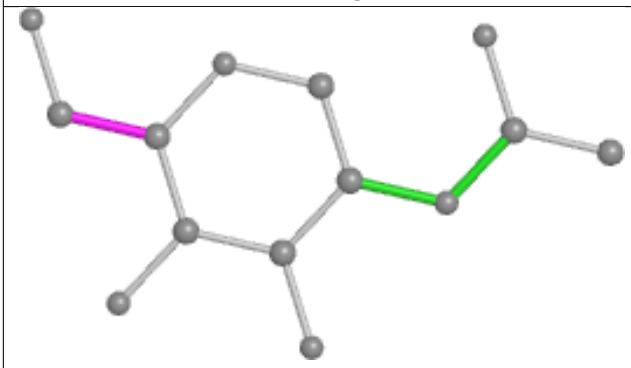


Bond angles



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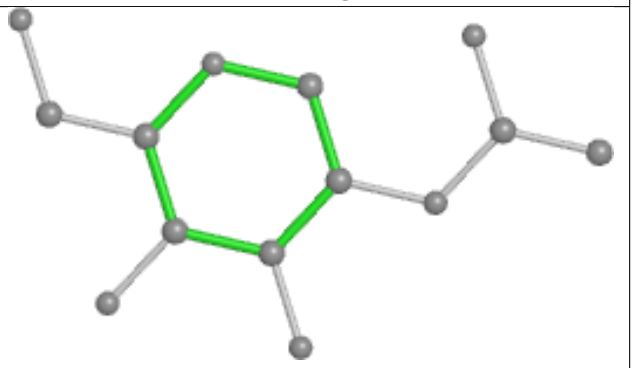
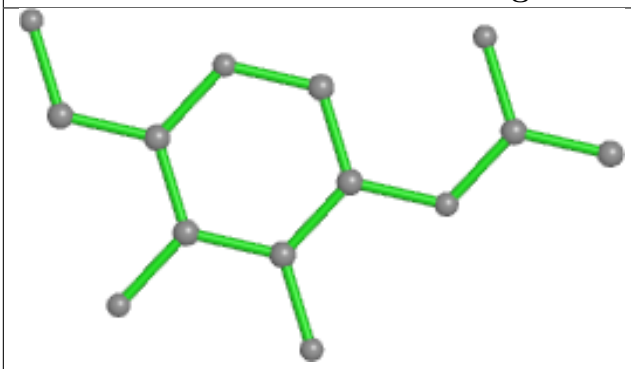
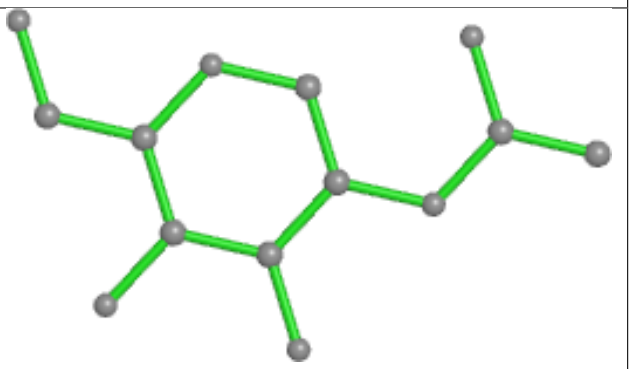
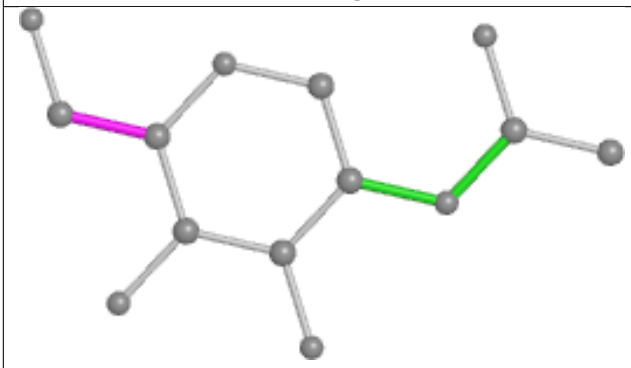
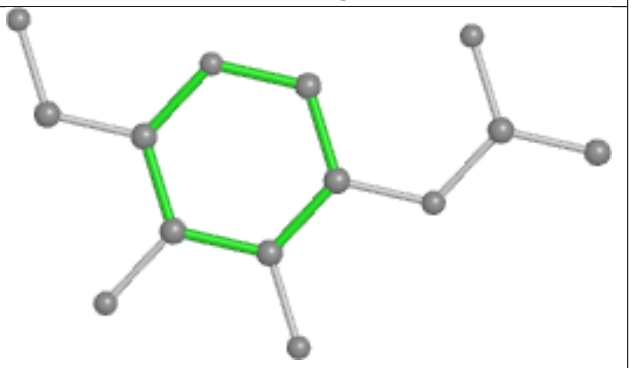
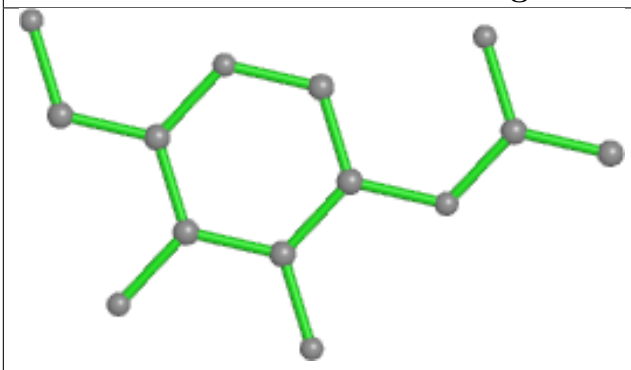
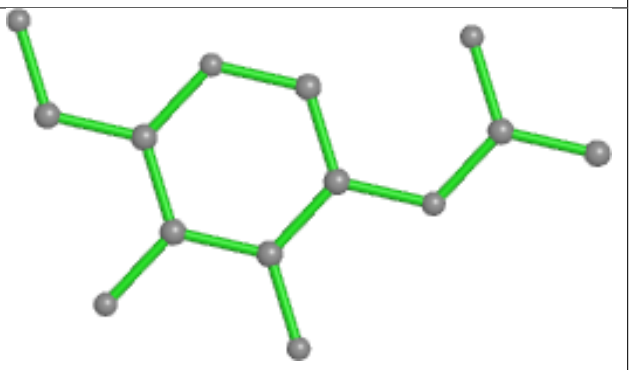
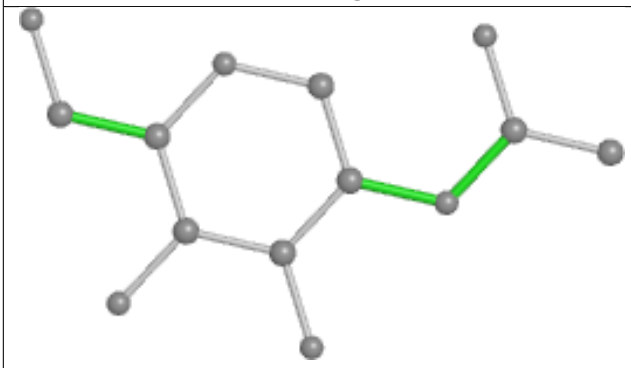
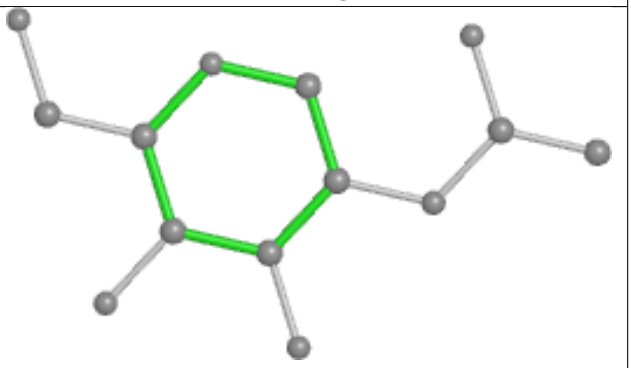
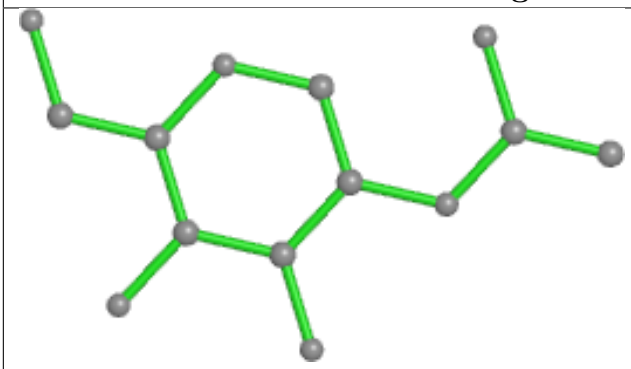


Rings

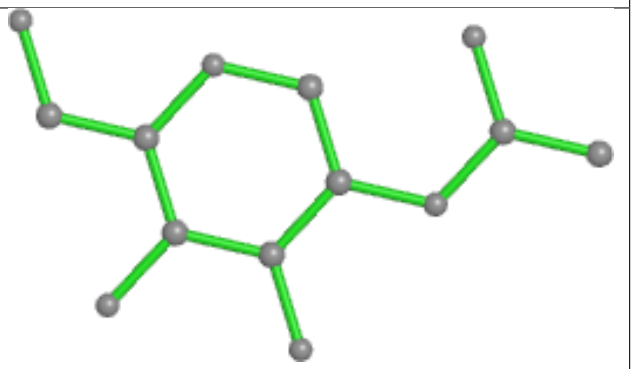
Ligand NAG B 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1313	
 Bond lengths	 Bond angles
 Torsions	 Rings

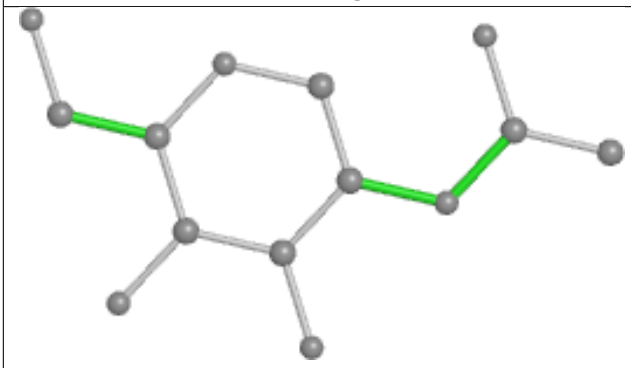
Ligand NAG C 1313



Bond lengths



Bond angles



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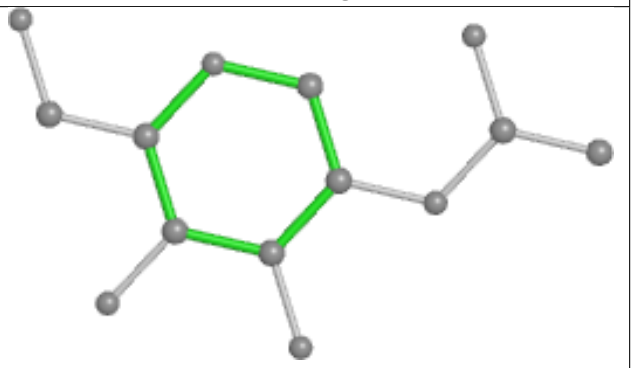
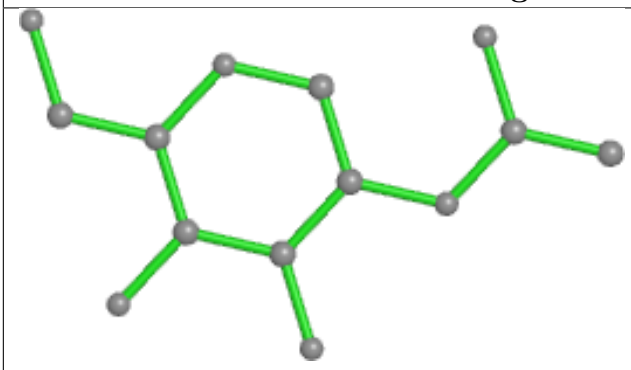


Rings

Ligand NAG A 1301



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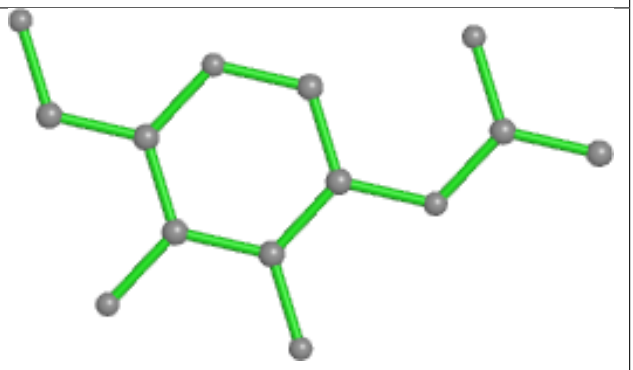
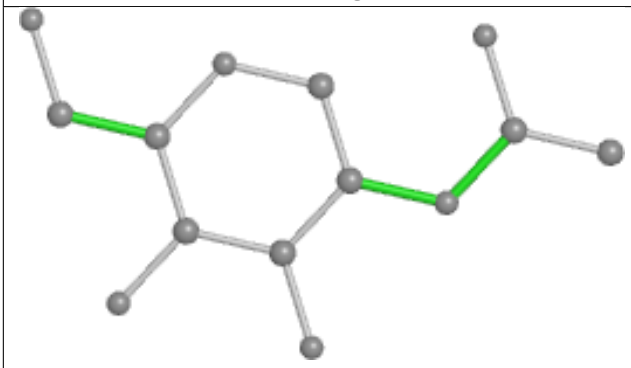


Bond angles



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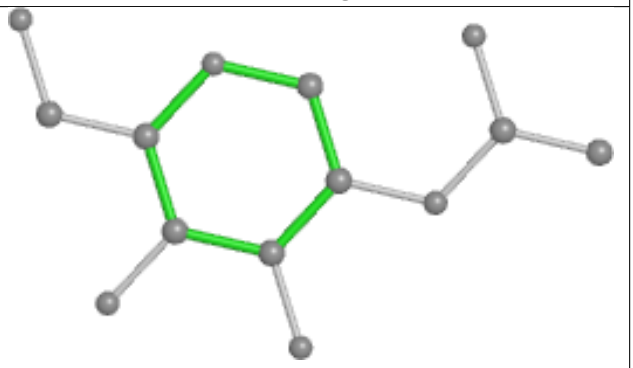
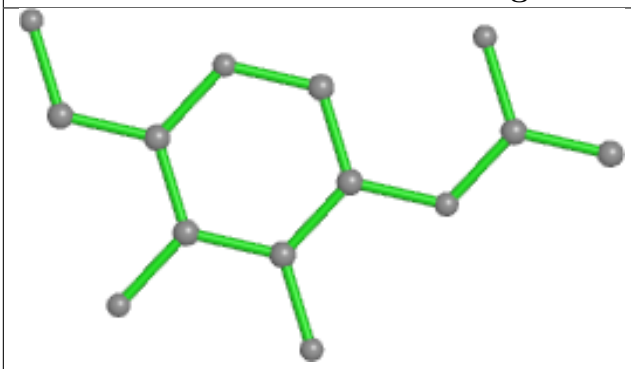


Rings

Ligand NAG A 1305



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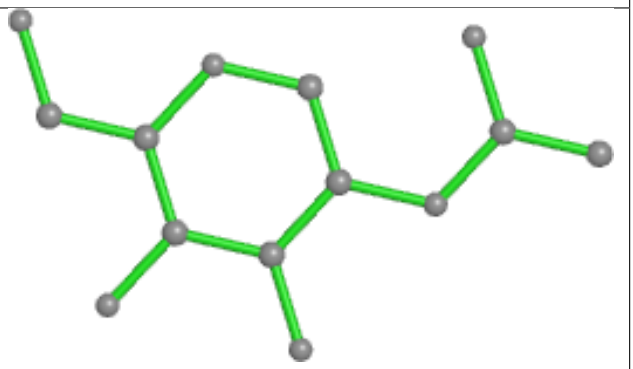
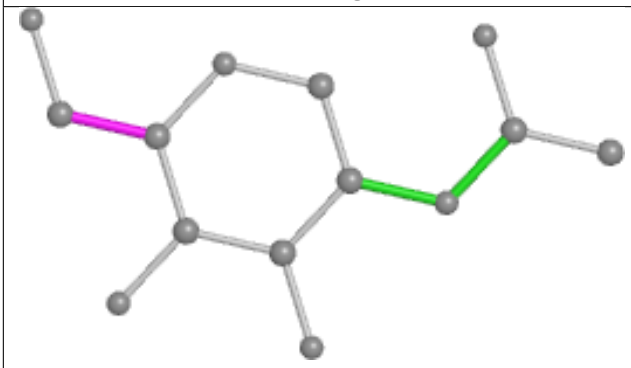


Bond angles



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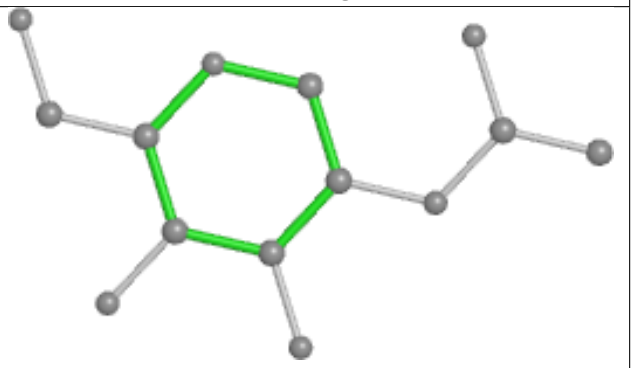
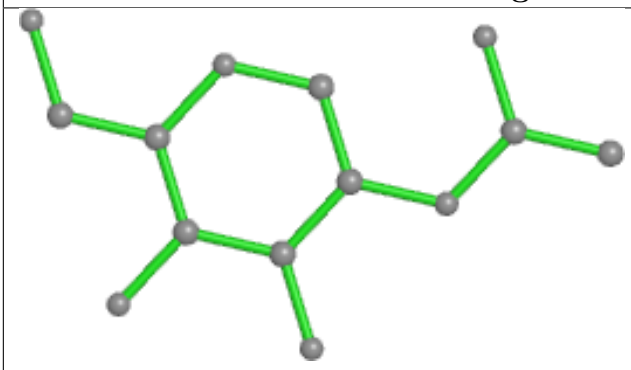


Rings

Ligand NAG B 1301



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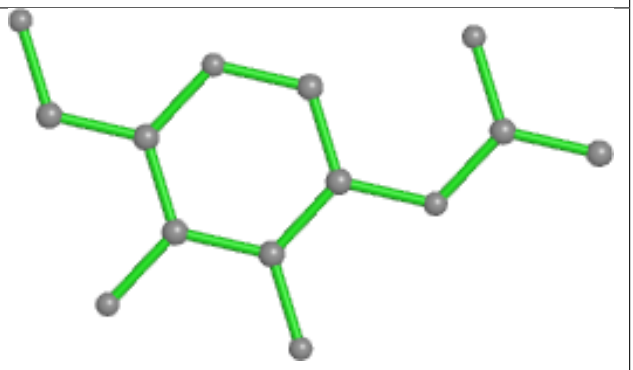
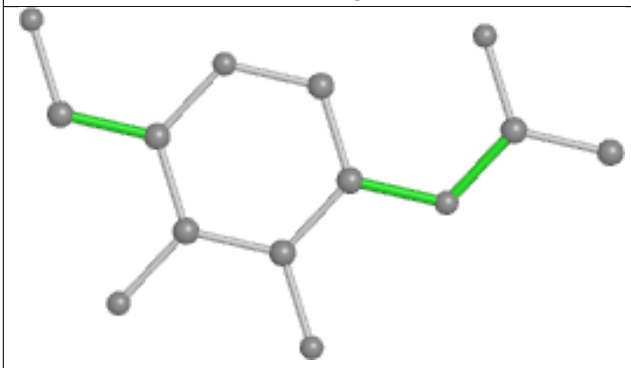


Bond angles



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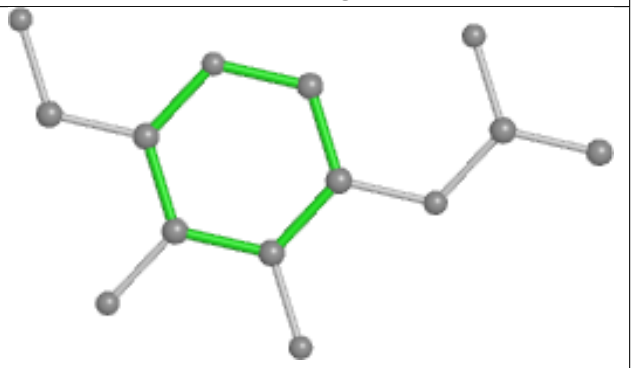
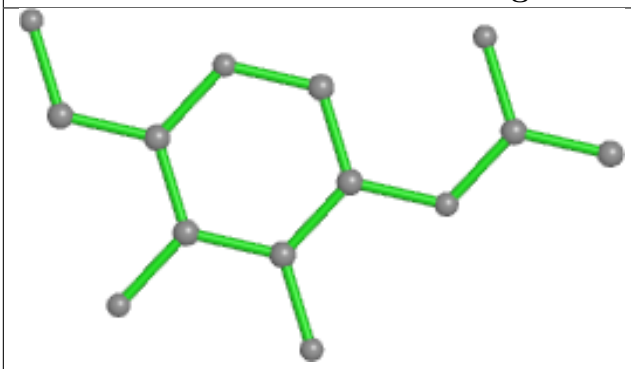


Rings

Ligand NAG C 1319



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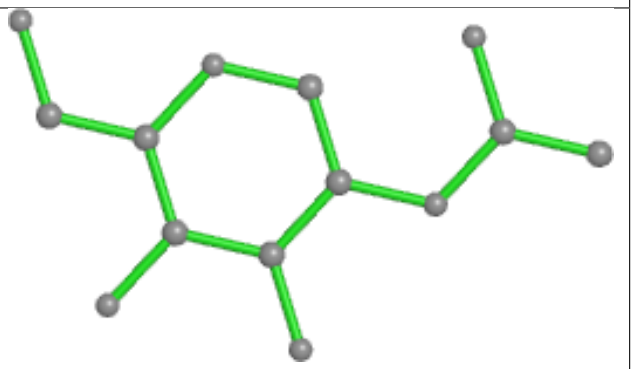
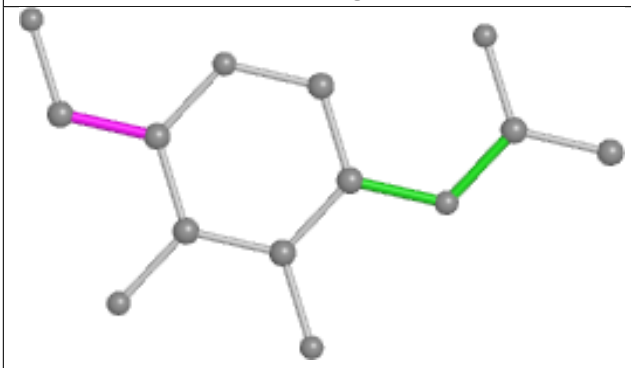


Bond angles



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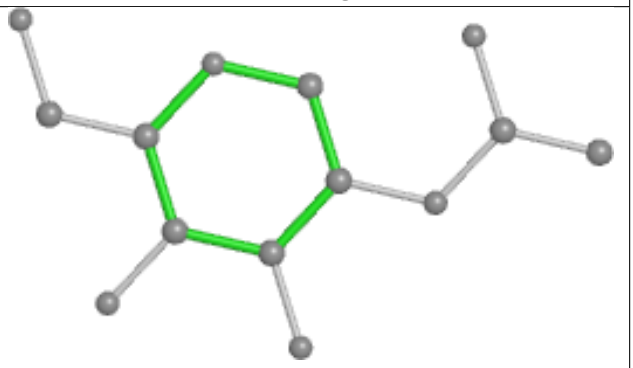
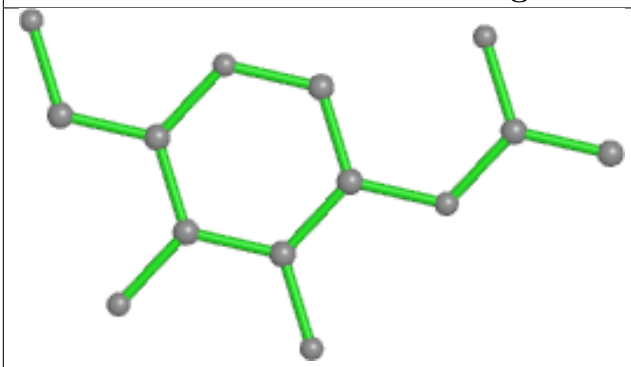


Rings

Ligand NAG A 1320



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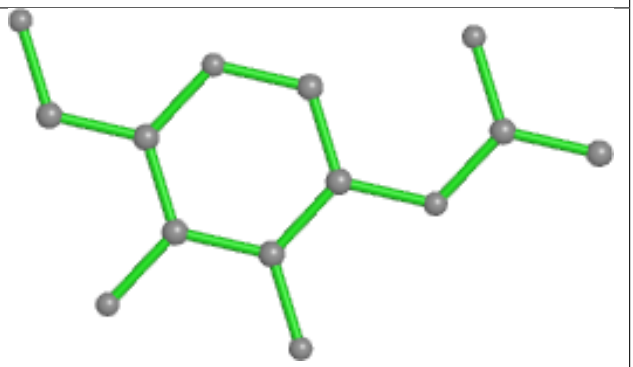
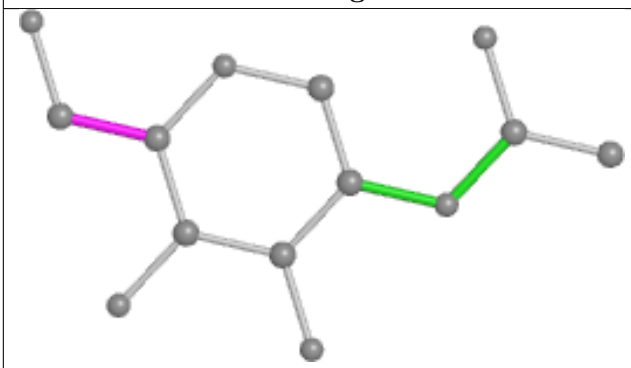


Bond angles



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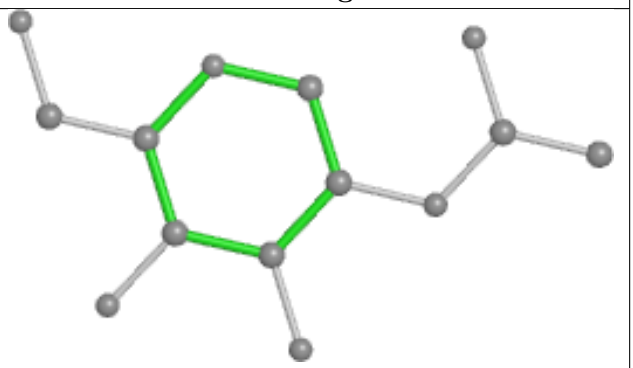
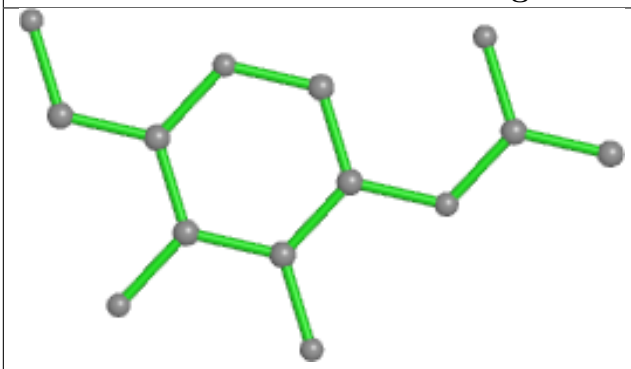


Rings

Ligand NAG C 1312



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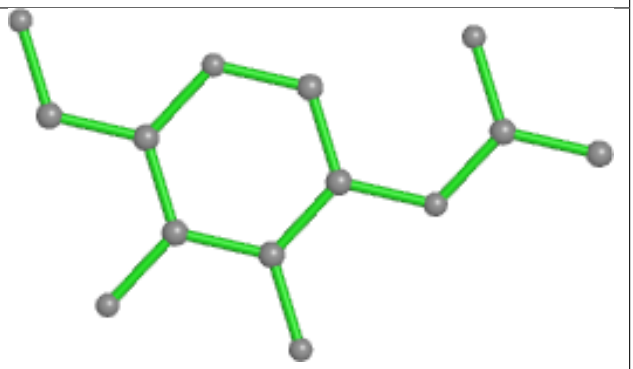
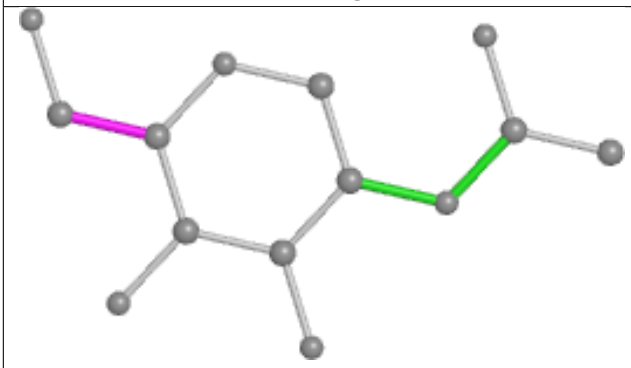
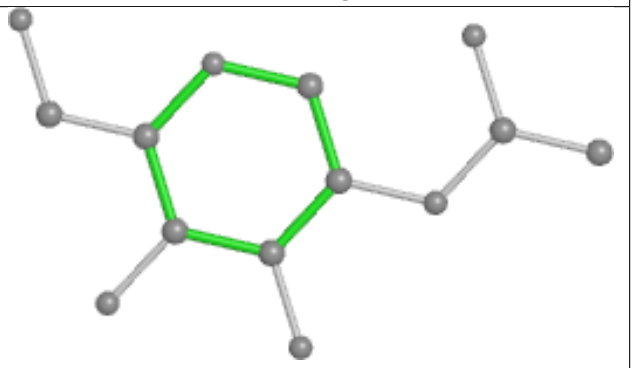


Bond angles

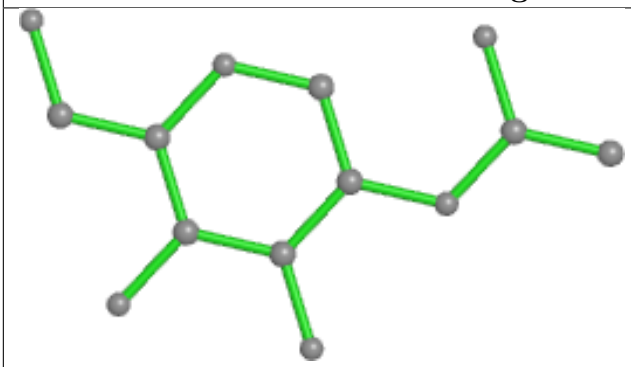


Torsions



Rings

Ligand NAG A 1317



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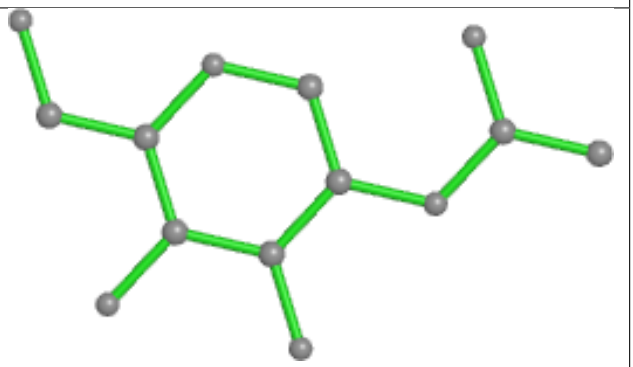
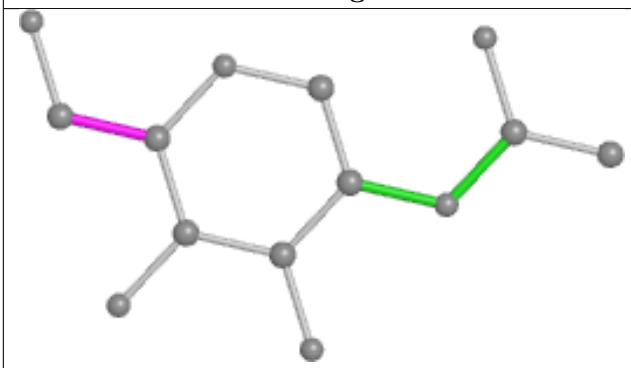
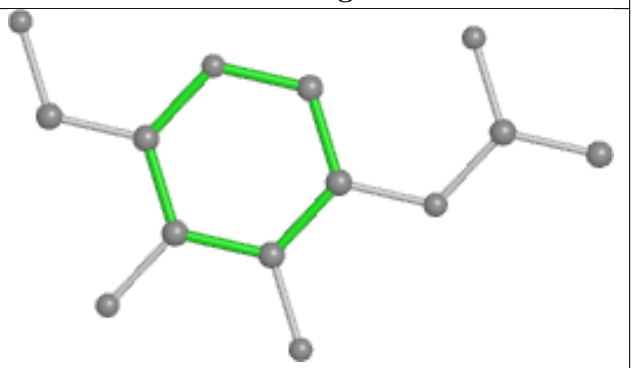


Bond angles

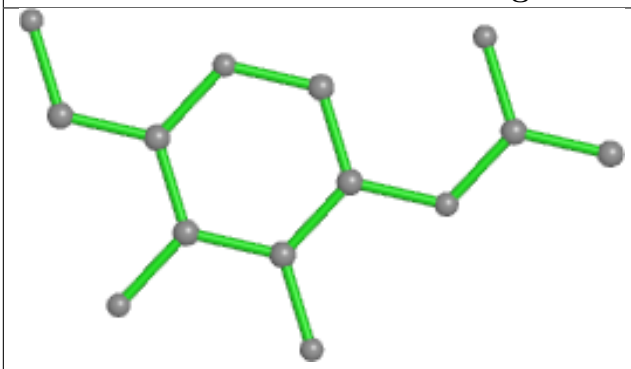


Torsions

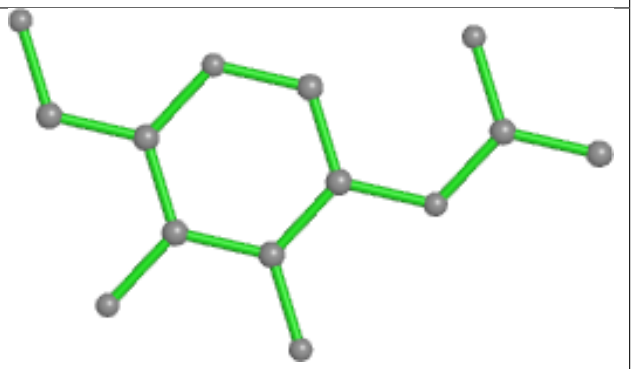


Rings

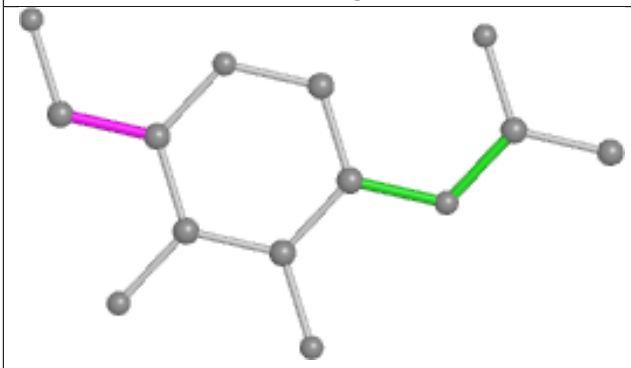
Ligand NAG B 1309



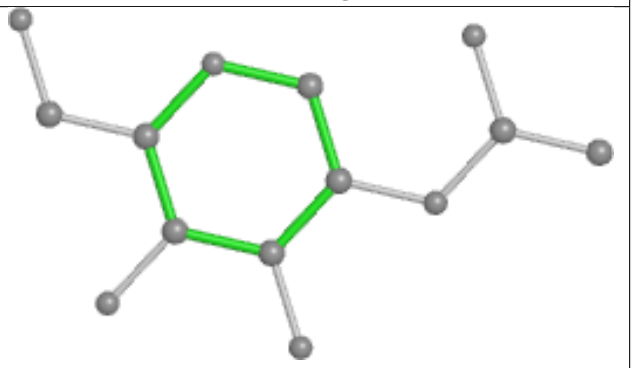
Bond lengths



Bond angles

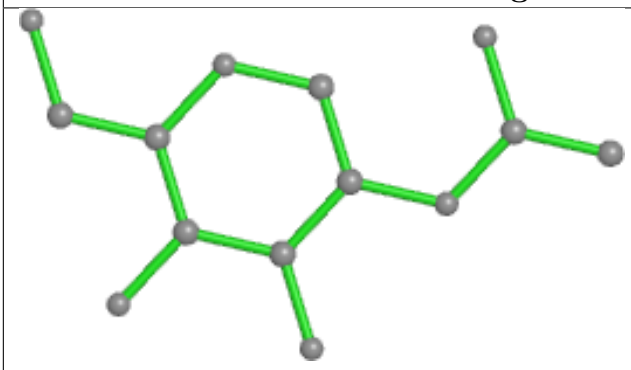


Torsions

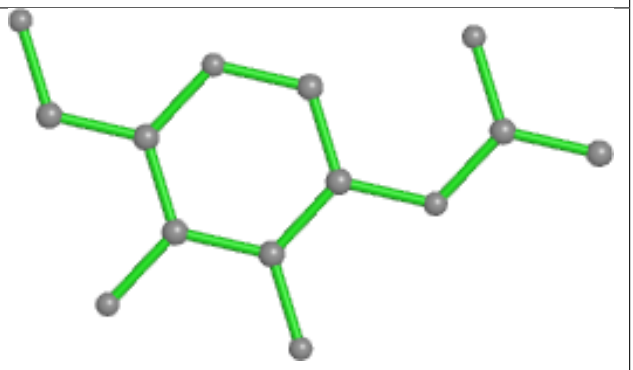


Rings

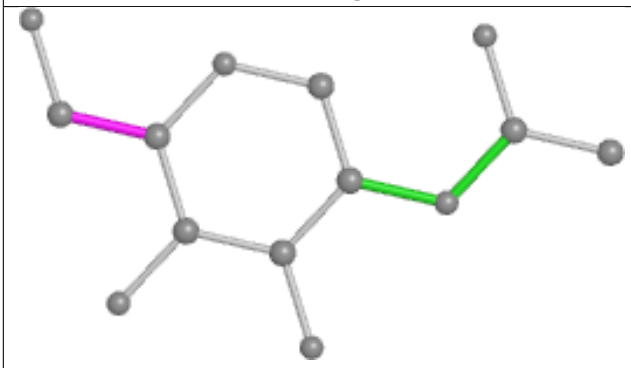
Ligand NAG A 1318



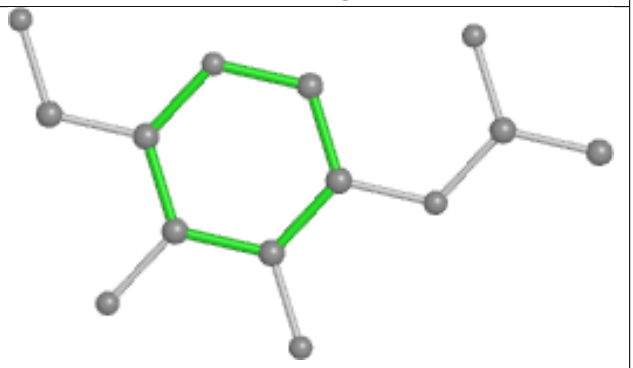
Bond lengths



Bond angles

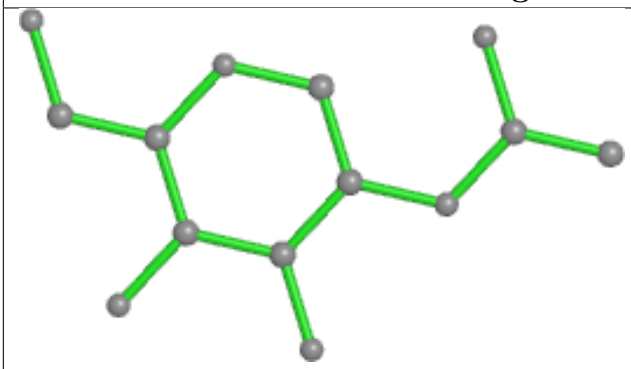


Torsions

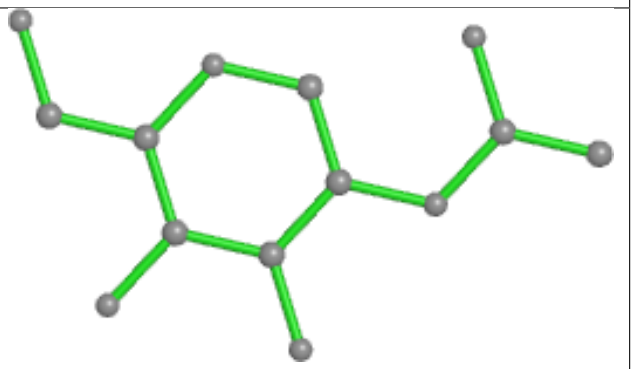


Rings

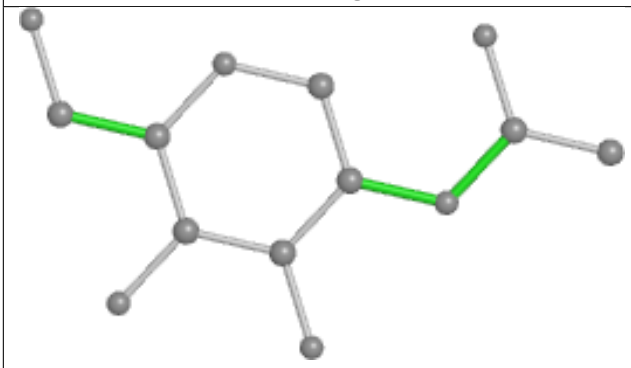
Ligand NAG B 1306



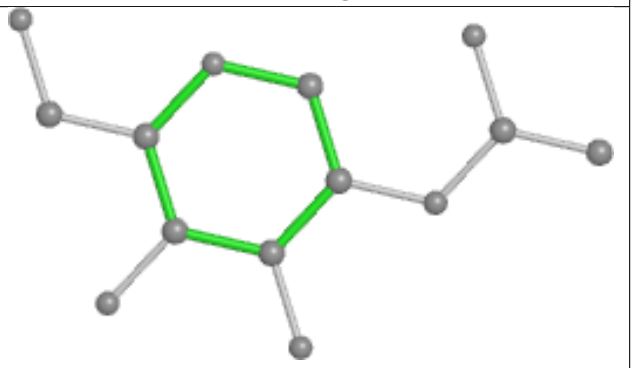
Bond lengths



Bond angles

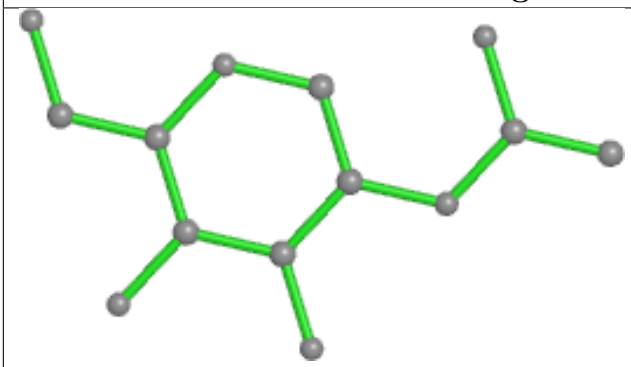


Torsions

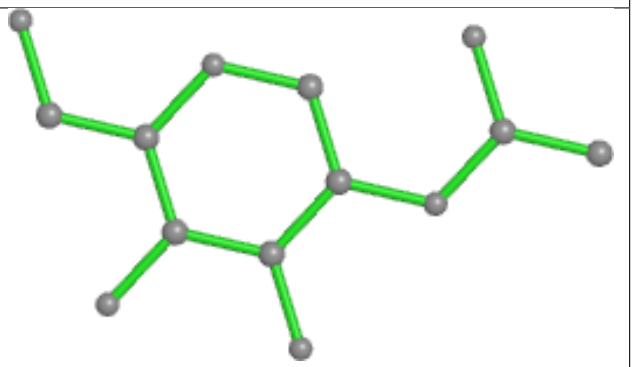


Rings

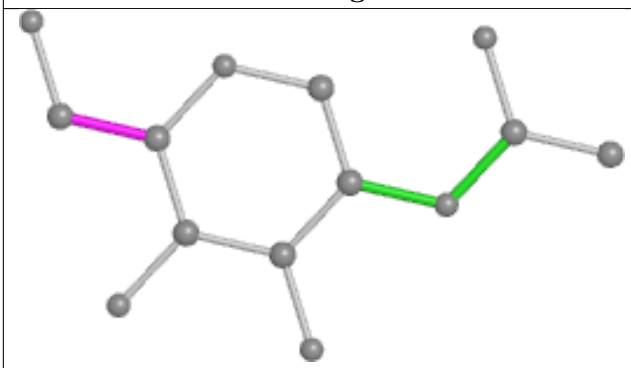
Ligand NAG B 1308



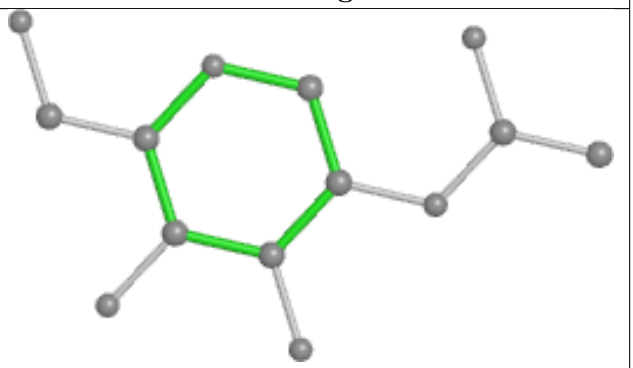
Bond lengths



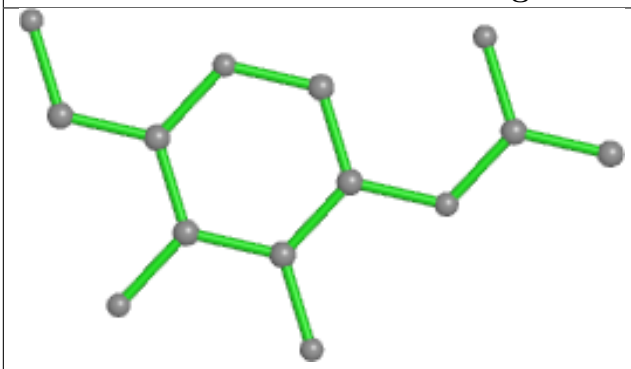
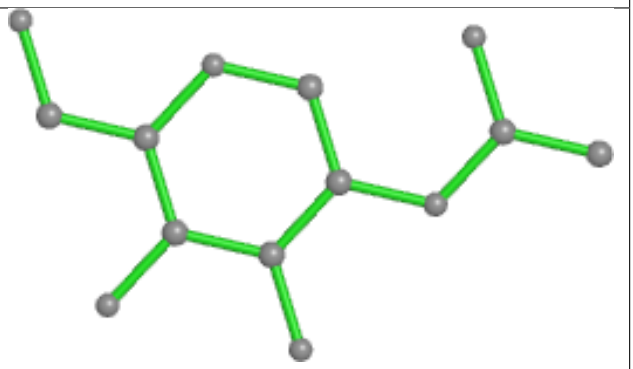
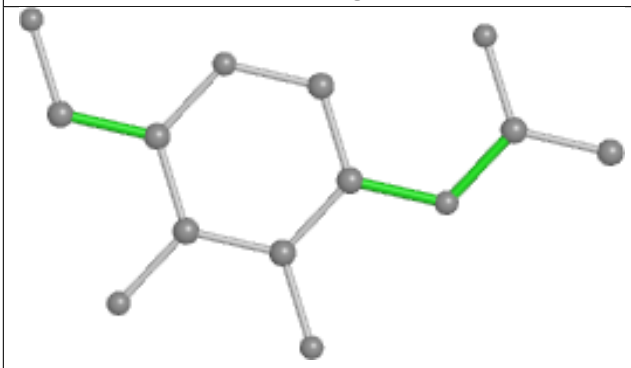
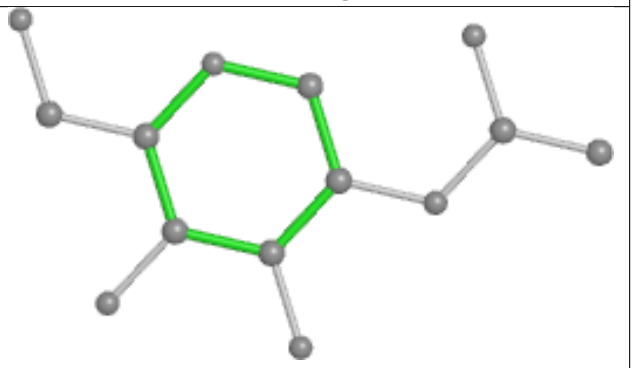
Bond angles



Torsions



Rings

Ligand NAG B 1315	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

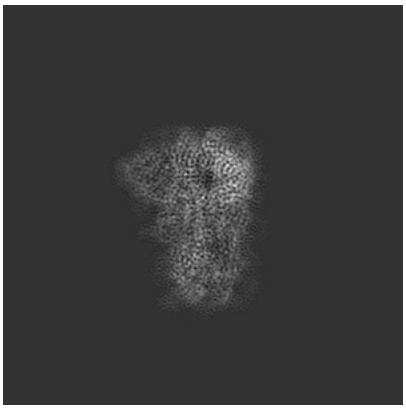
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62145. These allow visual inspection of the internal detail of the map and identification of artifacts.

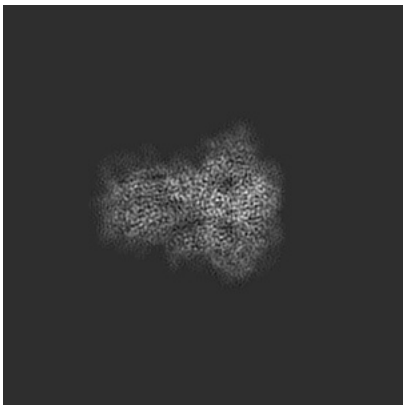
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

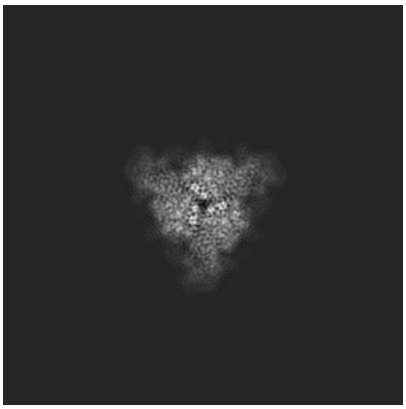
6.1.1 Primary map



X

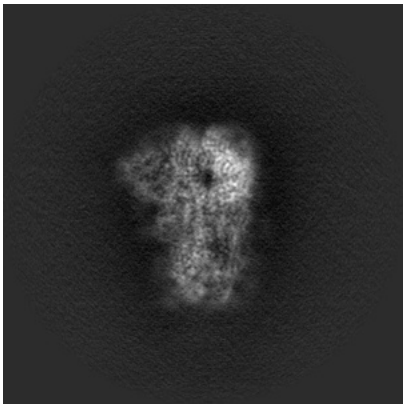


Y

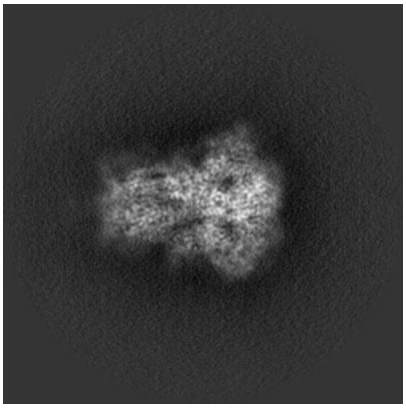


Z

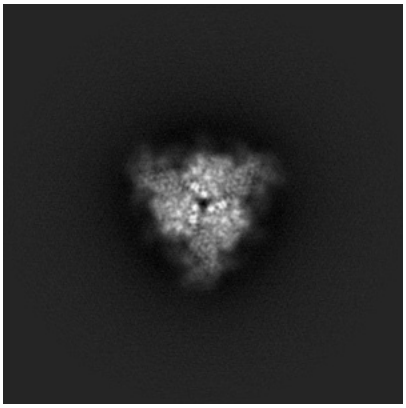
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

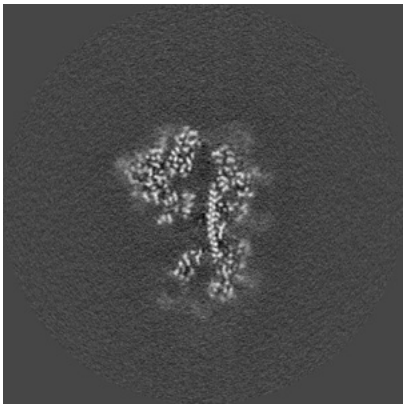
6.2.1 Primary map

X Index: 210

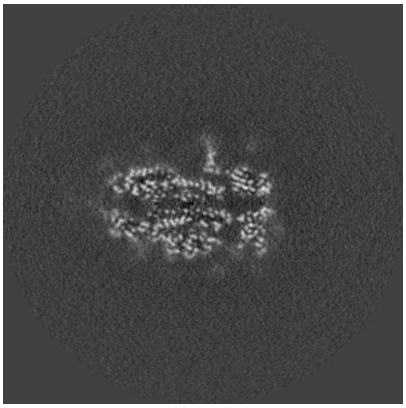
Y Index: 210

Z Index: 210

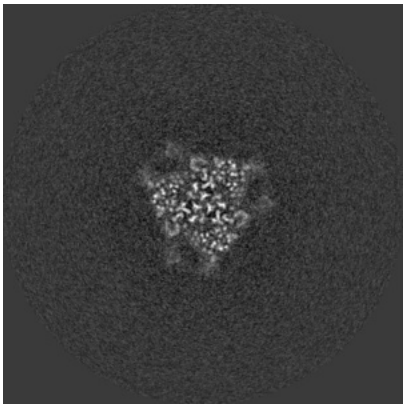
6.2.2 Raw map



X Index: 210



Y Index: 210

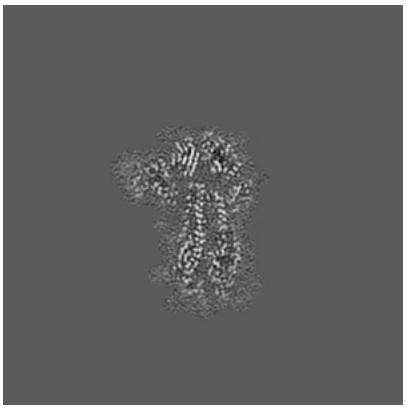


Z Index: 210

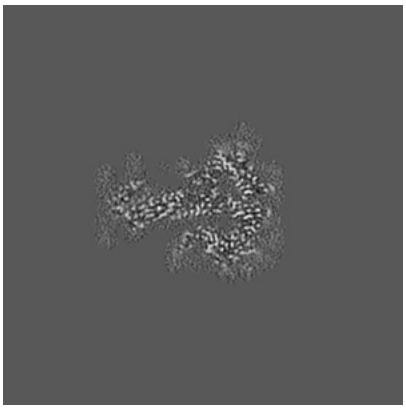
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



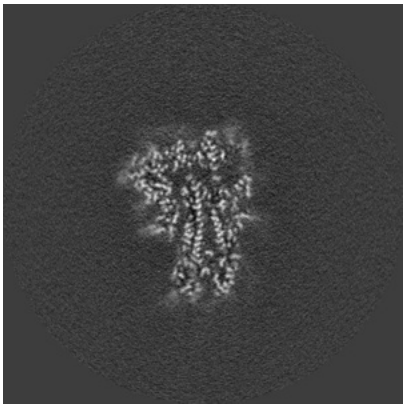
X Index: 201



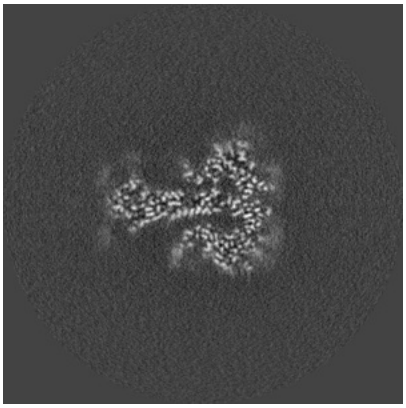
Y Index: 227

Z Index: 247

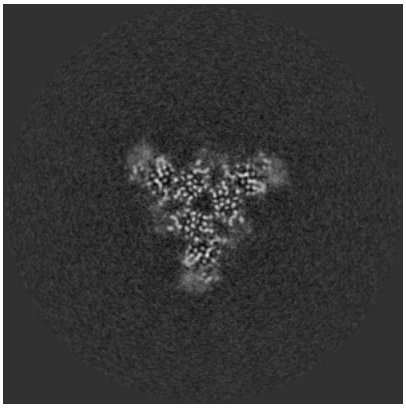
6.3.2 Raw map



X Index: 220



Y Index: 228

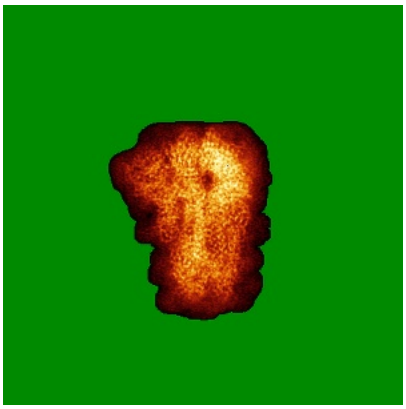


Z Index: 248

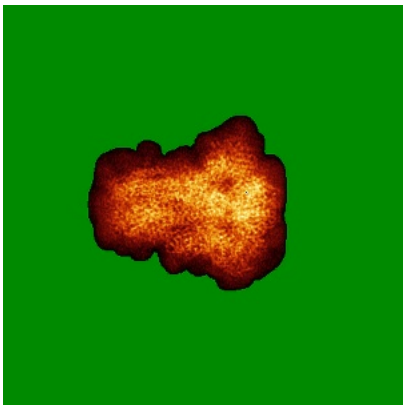
The images above show the largest variance slices of the map in three orthogonal directions.

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

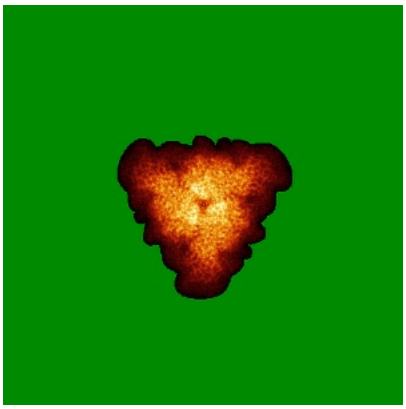
6.4.1 Primary map



X

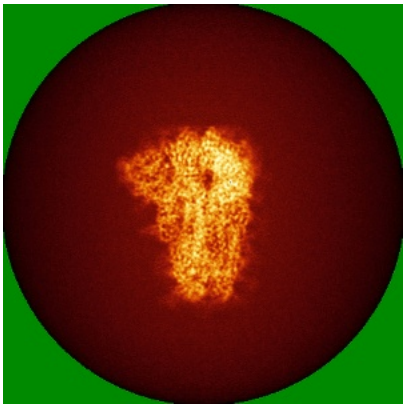


Y

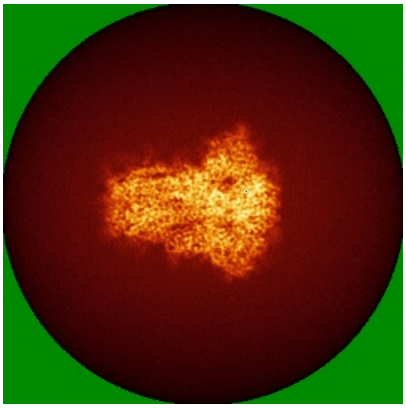


Z

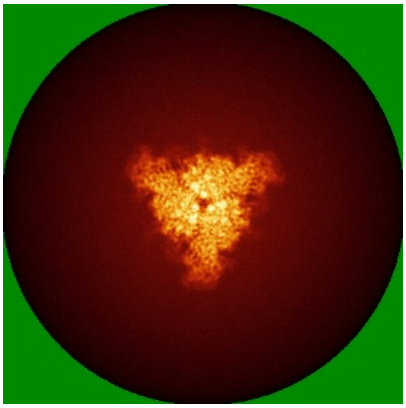
6.4.2 Raw map



X



Y



Z

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

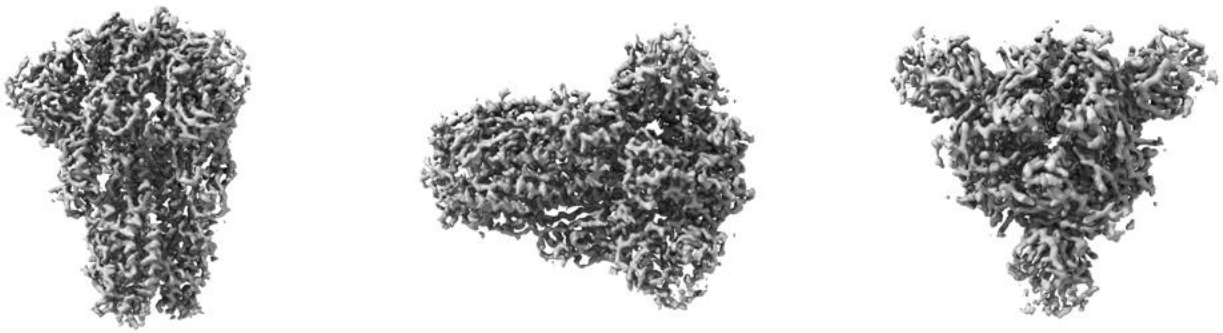
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

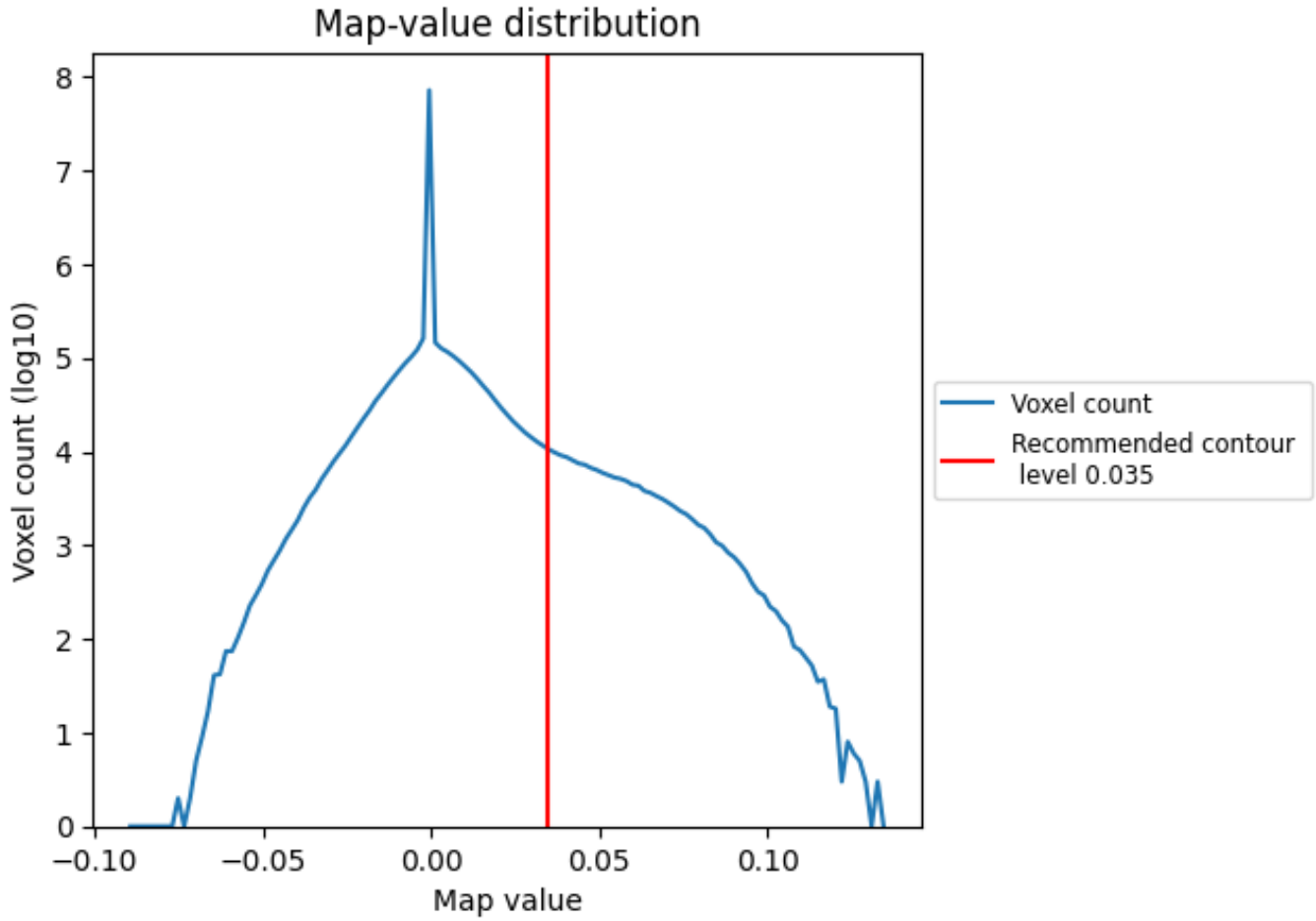
6.6 Mask visualisation (i)

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

7 Map analysis

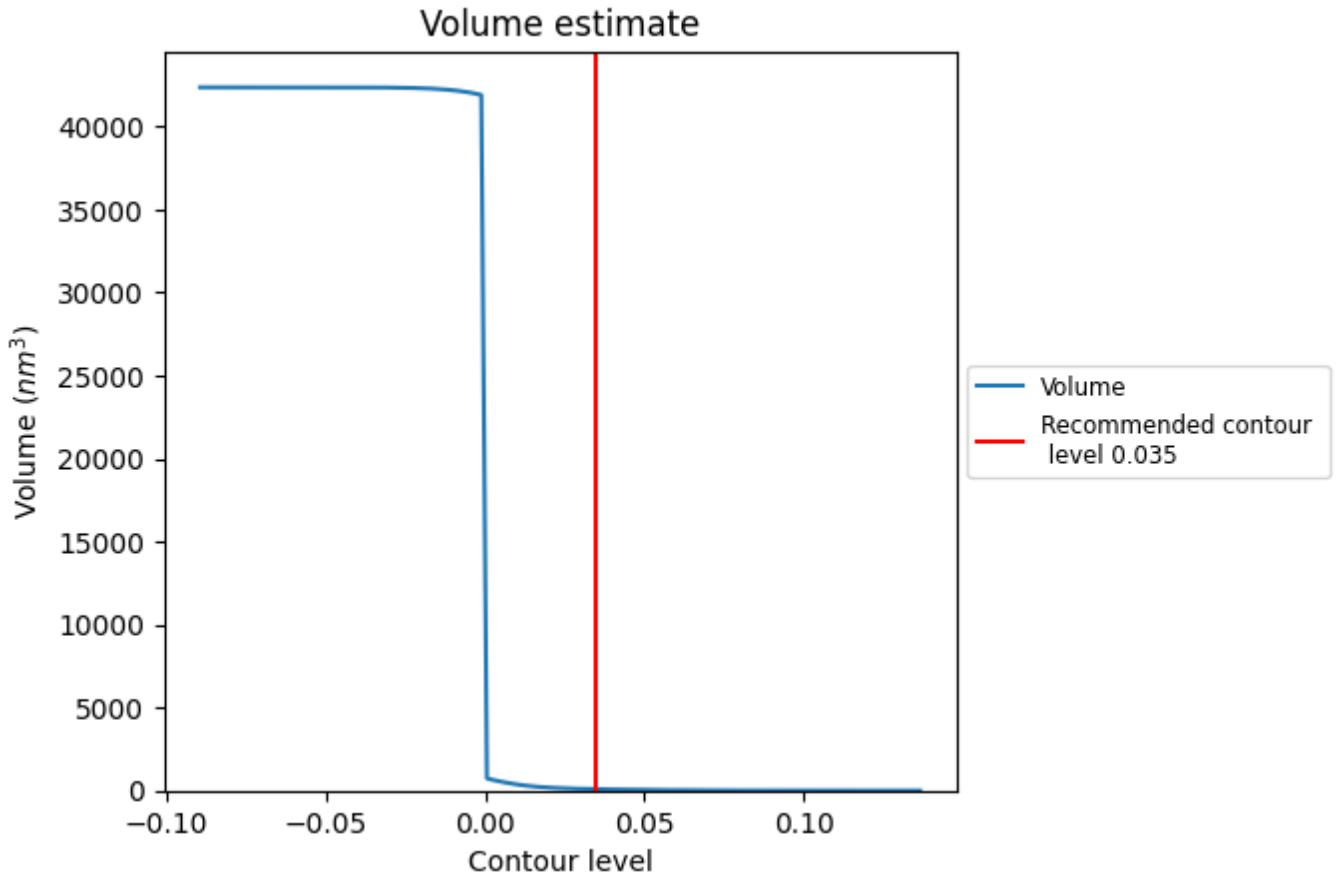
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

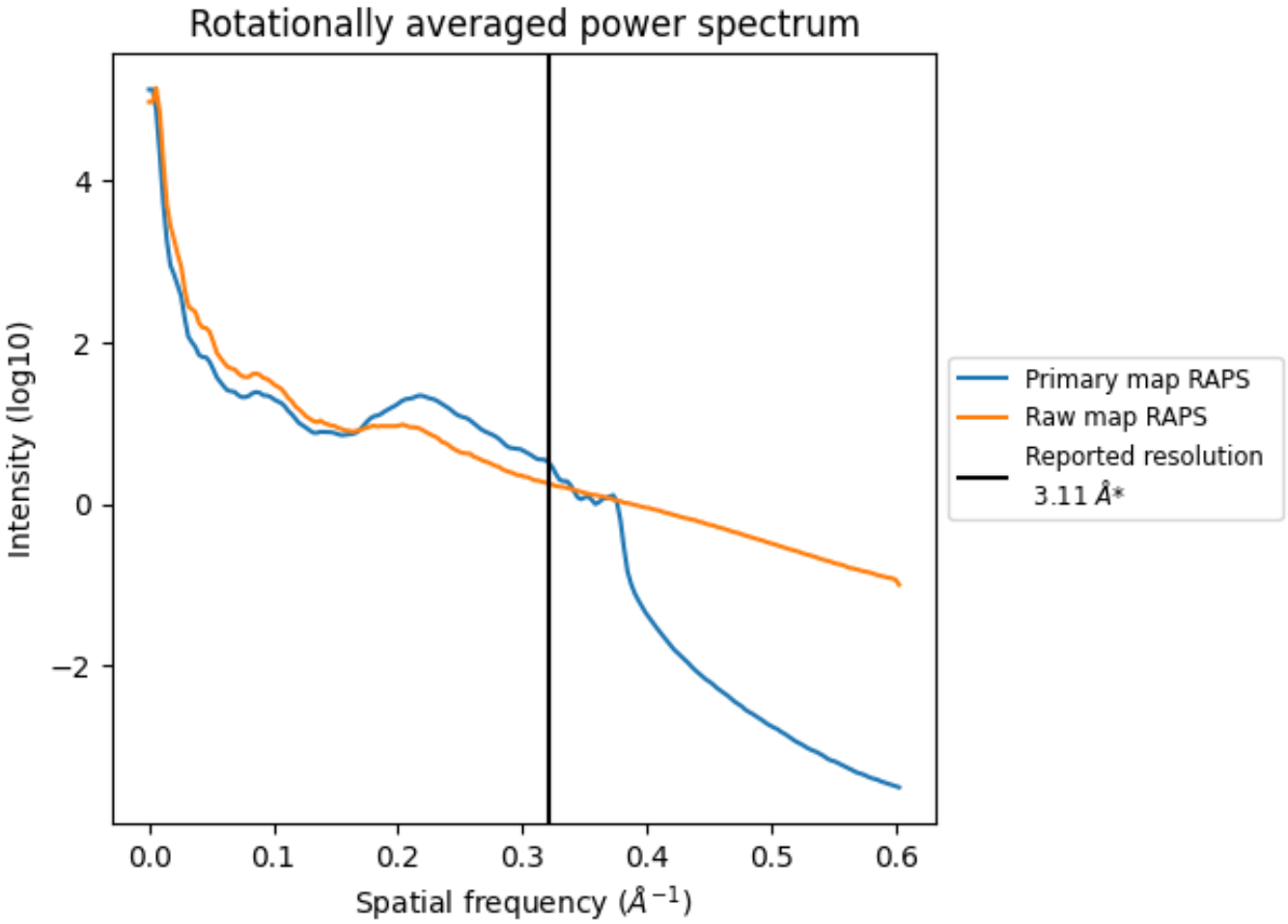
7.2 Volume estimate (i)



The volume at the recommended contour level is 84 nm^3; this corresponds to an approximate mass of 76 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)

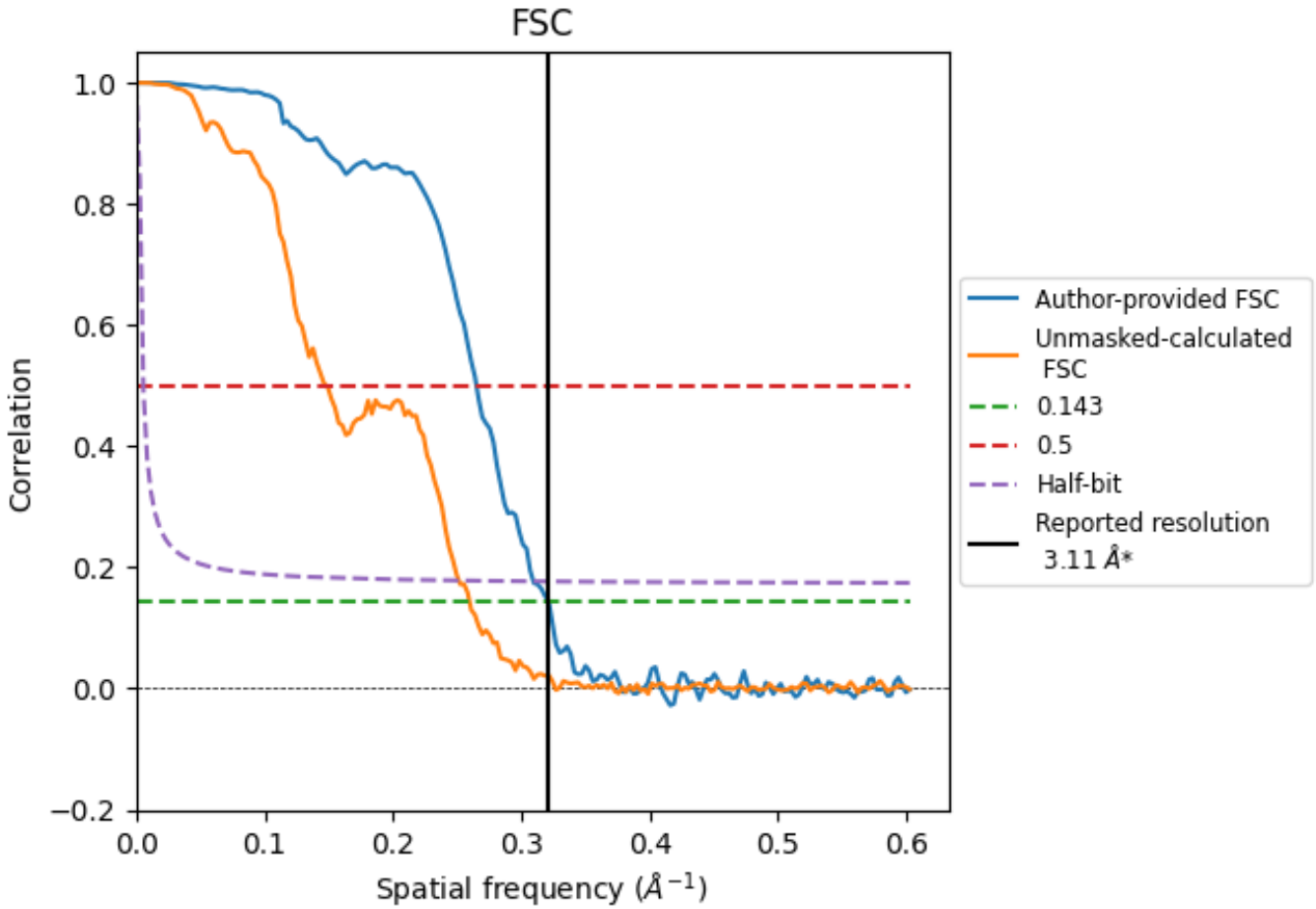


*Reported resolution corresponds to spatial frequency of 0.322 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.322 Å^{-1}

8.2 Resolution estimates (i)

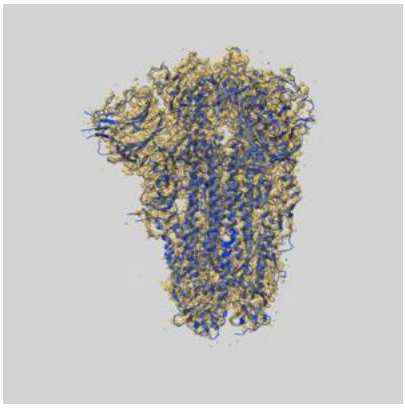
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.77	3.23
Unmasked-calculated*	3.85	6.75	3.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.11 by more than 10 %

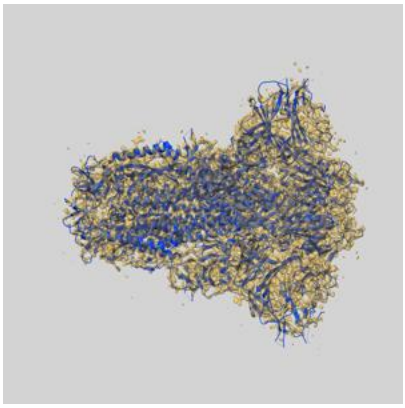
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62145 and PDB model 9K75. Per-residue inclusion information can be found in section 3 on page 7.

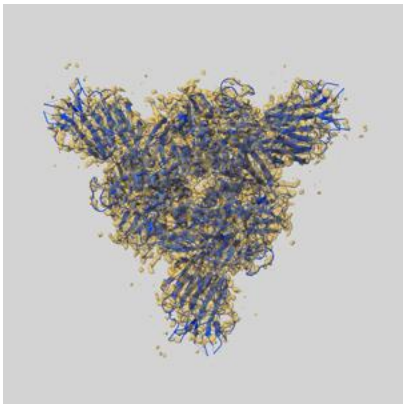
9.1 Map-model overlay



X



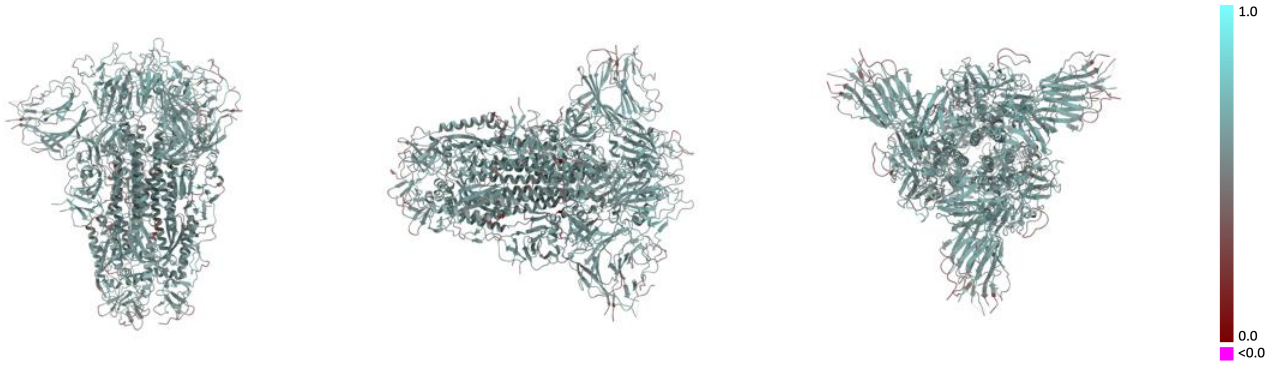
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

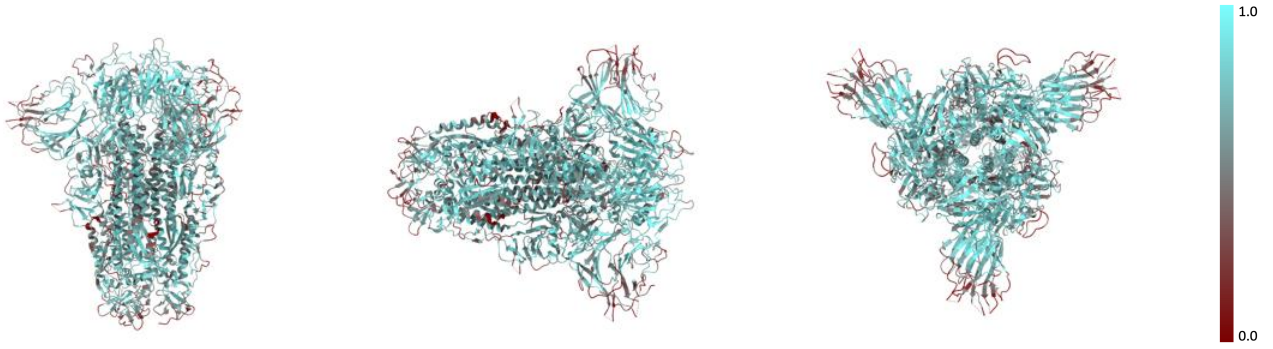
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

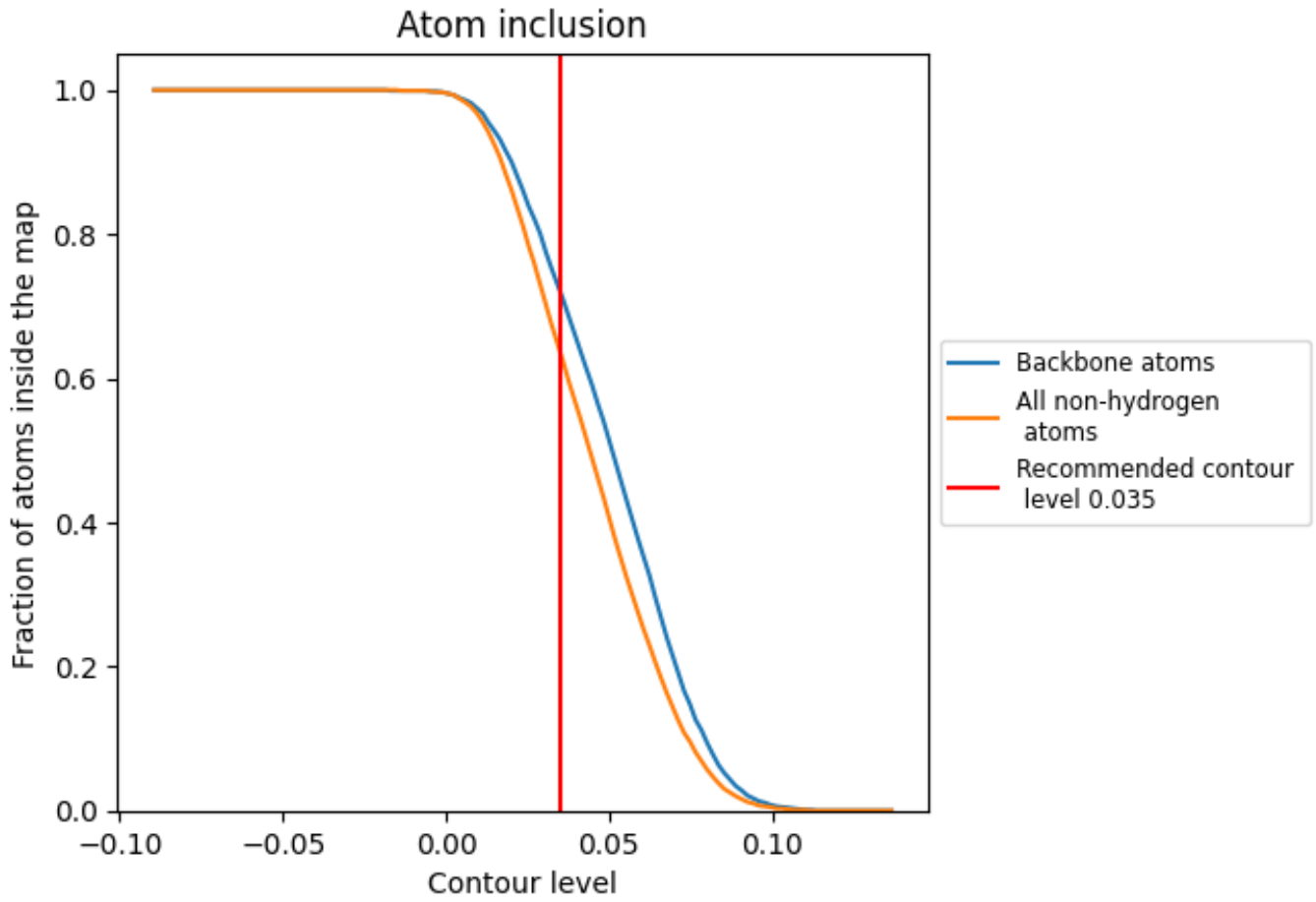
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.5610
A	0.6360	0.5620
B	0.6350	0.5610
C	0.6370	0.5610