Full wwPDB EM Validation Report ⓘ

Apr 15, 2024 – 03:22 PM EDT

PDB ID	:	8FU8
EMDB ID	:	EMD-29455
Title	:	Structure of Covid Spike variant deltaN135 with one erect RBD
Authors	:	Yu, X.; Juraszek, J.; Rutten, L.; Bakkers, M.J.G.; Blokland, S.; Van den Broek, N.J.F.; Verwilligen, A.Y.W.; Abeywickrema, P.; Vingerhoets, J.; Neefs, J.; Bakhash, S.A.M.; Roychoudhury, P.; Greninger, A.; Sharma, S.; Langedijk, J.P.M.
Deposited on	:	2023-01-16
Resolution	:	3.08 Å(reported)

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

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

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

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

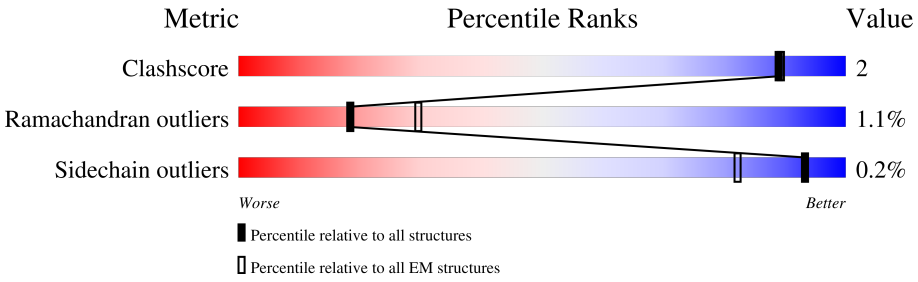
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 3.08 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1192	9% 83% 5% • 12%
1	B	1192	15% 84% 5% 10%
1	C	1192	11% 84% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1206	X	-	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25469 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	1046	Total	C	N	O	S	0	0
			8183	5229	1363	1555	36		
1	B	1069	Total	C	N	O	S	0	0
			8360	5335	1398	1591	36		
1	C	1050	Total	C	N	O	S	0	0
			8211	5244	1368	1562	37		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	LEU	PRO	conflict	UNP P0DTC2
A	?	-	CYS	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	ASP	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TRP	deletion	UNP P0DTC2
A	?	-	THR	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	468	LYS	GLU	conflict	UNP P0DTC2
A	478	PRO	SER	conflict	UNP P0DTC2
A	598	GLY	ASP	conflict	UNP P0DTC2
A	666	SER	ARG	conflict	UNP P0DTC2
A	669	GLY	ARG	conflict	UNP P0DTC2
A	876	PRO	ALA	engineered mutation	UNP P0DTC2
A	926	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	971	PRO	VAL	engineered mutation	UNP P0DTC2
A	1160	PHE	VAL	conflict	UNP P0DTC2
B	9	LEU	PRO	conflict	UNP P0DTC2
B	?	-	CYS	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	ASP	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TRP	deletion	UNP P0DTC2
B	?	-	THR	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	468	LYS	GLU	conflict	UNP P0DTC2
B	478	PRO	SER	conflict	UNP P0DTC2
B	598	GLY	ASP	conflict	UNP P0DTC2
B	666	SER	ARG	conflict	UNP P0DTC2
B	669	GLY	ARG	conflict	UNP P0DTC2
B	876	PRO	ALA	engineered mutation	UNP P0DTC2
B	926	PRO	ALA	engineered mutation	UNP P0DTC2
B	971	PRO	VAL	engineered mutation	UNP P0DTC2
B	1160	PHE	VAL	conflict	UNP P0DTC2
C	9	LEU	PRO	conflict	UNP P0DTC2
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TRP	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2

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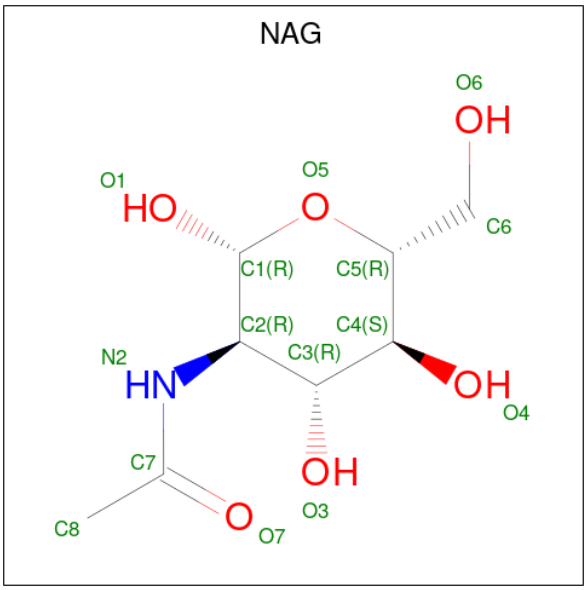
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	468	LYS	GLU	conflict	UNP P0DTC2
C	478	PRO	SER	conflict	UNP P0DTC2
C	598	GLY	ASP	conflict	UNP P0DTC2
C	666	SER	ARG	conflict	UNP P0DTC2
C	669	GLY	ARG	conflict	UNP P0DTC2
C	876	PRO	ALA	engineered mutation	UNP P0DTC2
C	926	PRO	ALA	engineered mutation	UNP P0DTC2
C	971	PRO	VAL	engineered mutation	UNP P0DTC2
C	1160	PHE	VAL	conflict	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			15	8	1	6	
2	A	1	Total	C	N	O	0
			15	8	1	6	
2	A	1	Total	C	N	O	0
			15	8	1	6	
2	A	1	Total	C	N	O	0
			15	8	1	6	
2	A	1	Total	C	N	O	0
			15	8	1	6	

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C N O 14 8 1 5	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 14 8 1 5	0
2	A	1	Total C N O 15 8 1 6	0
2	A	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0

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Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C N O 14 8 1 5	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	B	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 14 8 1 5	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 14 8 1 5	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0
2	C	1	Total C N O 15 8 1 6	0

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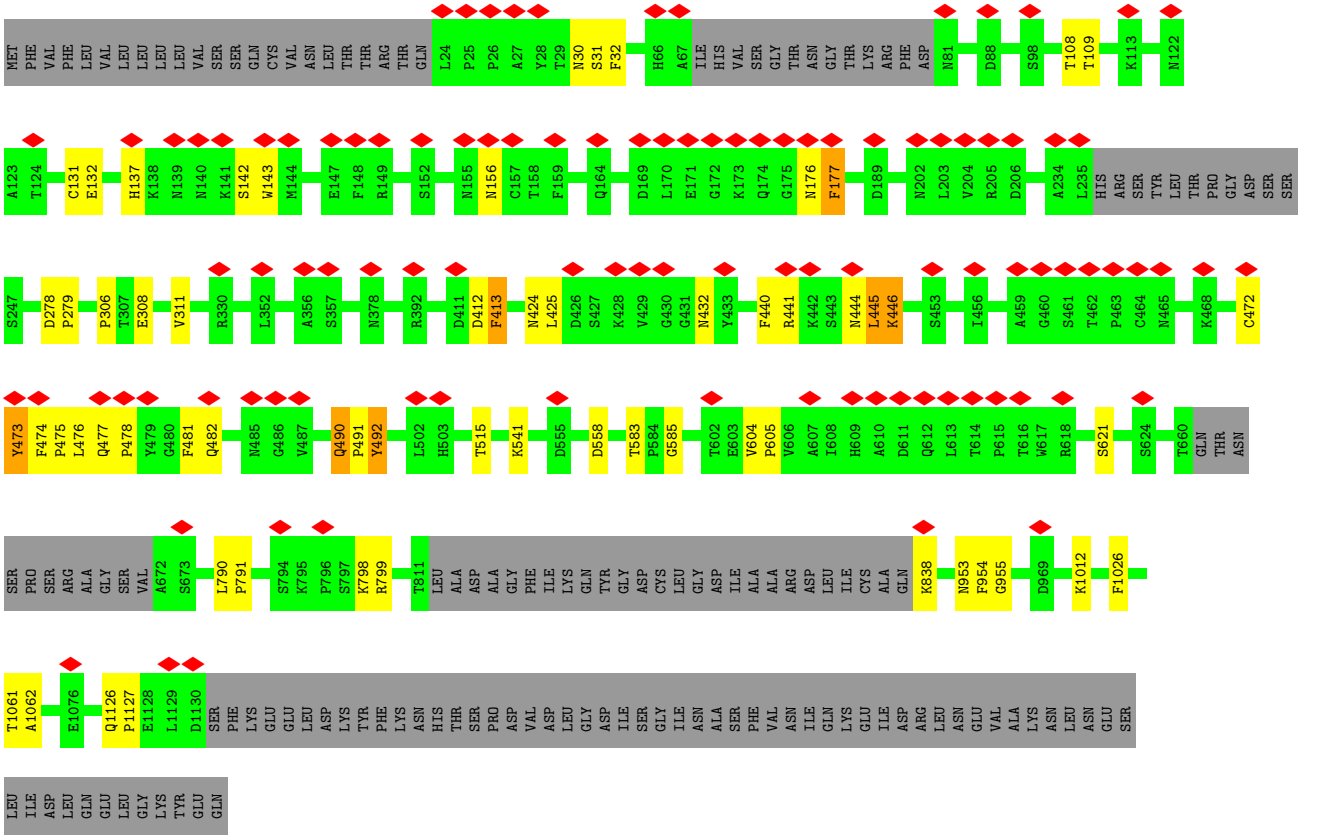
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			15	8	1	6	

3 Residue-property plots (i)

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

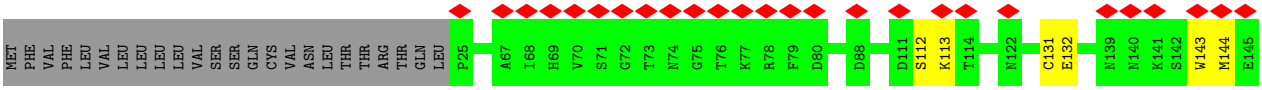
• Molecule 1: Spike glycoprotein

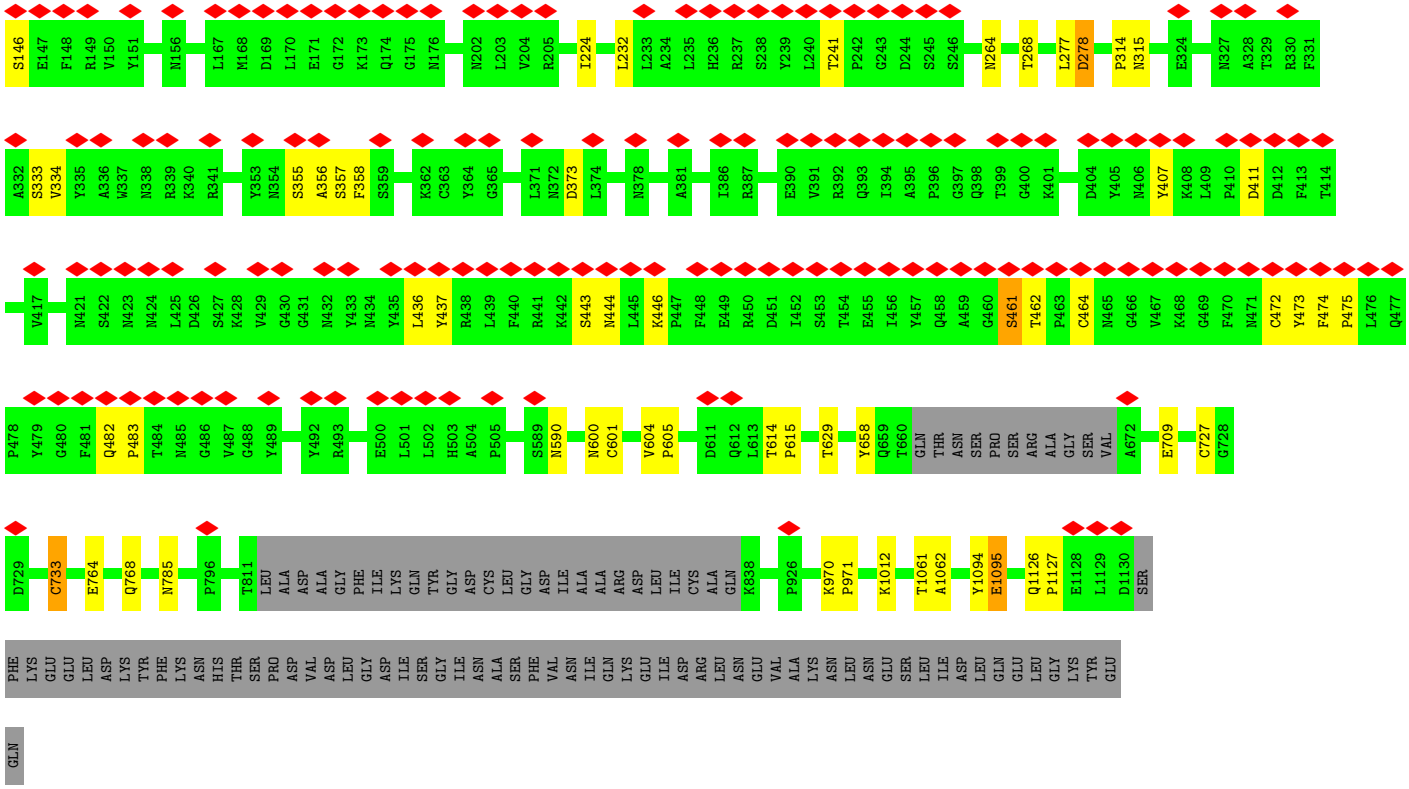
Chain A:



• Molecule 1: Spike glycoprotein

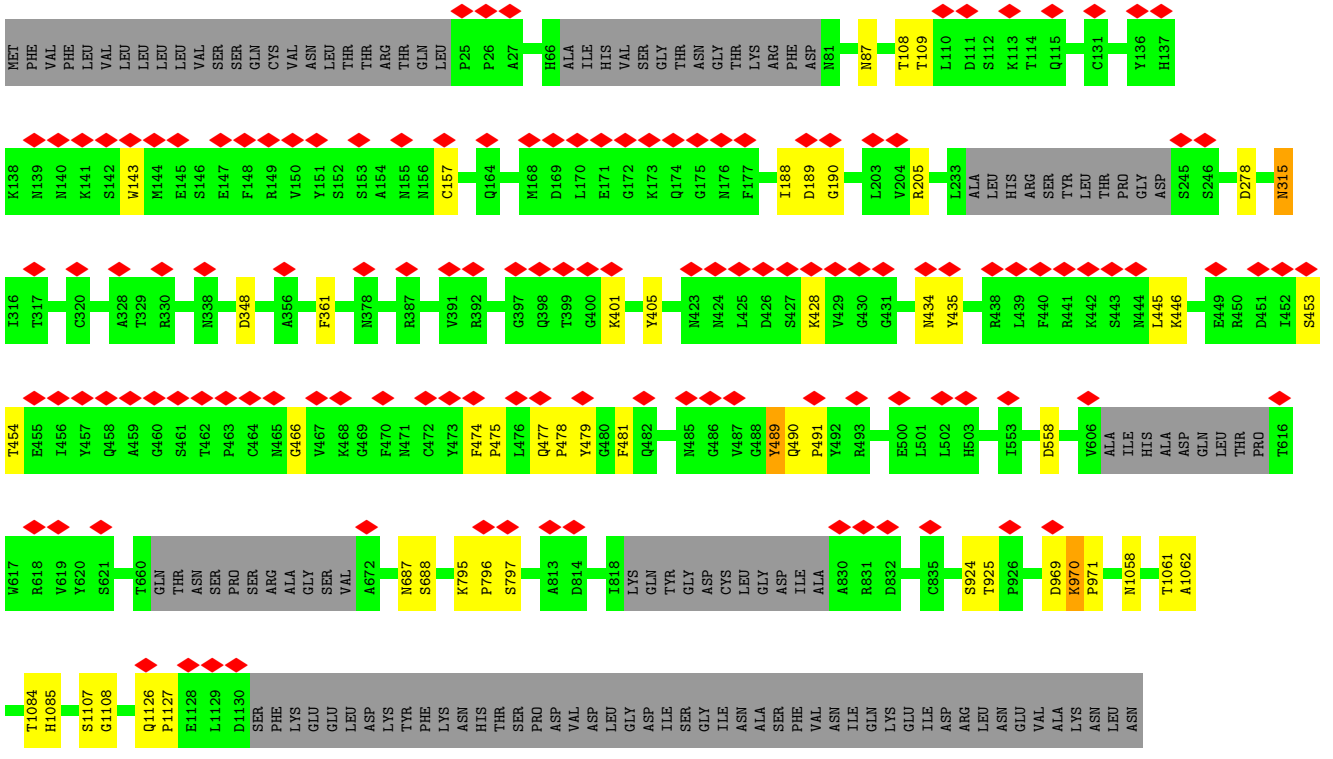
Chain B:





- Molecule 1: Spike glycoprotein

Chain C:



GLU
SER
LEU
ILE
ASP
LEU
GLN
GLU
LEU
GLY
LYS
TYR
GLU
GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	378064	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0084	Depositor
Map size (Å)	366.168, 366.168, 366.168	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8322, 0.8322, 0.8322	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	0.66	0/8376	0.59	0/11402
1	B	0.67	1/8560 (0.0%)	0.58	0/11653
1	C	0.68	0/8402	0.59	0/11431
All	All	0.67	1/25338 (0.0%)	0.59	0/34486

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	733	CYS	CB-SG	-7.20	1.70	1.82

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	8183	0	8028	32	0
1	B	8360	0	8194	29	0
1	C	8211	0	8051	29	0
2	A	253	0	251	0	0
2	B	224	0	223	2	0
2	C	238	0	236	1	0
All	All	25469	0	24983	89	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 2.

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:GLU:OE2	1:B:1012:LYS:NZ	2.34	0.60
1:A:541:LYS:NZ	1:A:558:ASP:OD2	2.34	0.60
1:B:590:ASN:ND2	1:B:658:TYR:OH	2.34	0.59
1:A:490:GLN:N	1:A:491:PRO:CD	2.66	0.59
1:A:481:PHE:O	1:A:482:GLN:C	2.41	0.58
1:C:490:GLN:N	1:C:491:PRO:HD3	2.18	0.57
1:A:838:LYS:NZ	1:C:558:ASP:OD1	2.38	0.56
1:C:428:LYS:NZ	1:C:489:TYR:O	2.39	0.55
1:A:798:LYS:HA	1:A:799:ARG:HB3	1.90	0.54
1:A:477:GLN:N	1:A:478:PRO:CD	2.70	0.54
1:B:1094:TYR:O	1:B:1095:GLU:C	2.46	0.53
1:B:264:ASN:ND2	1:B:268:THR:OG1	2.42	0.51
1:B:1126:GLN:N	1:B:1127:PRO:HD2	2.25	0.51
1:B:727:CYS:CB	1:B:733:CYS:HG	2.24	0.51
1:A:108:THR:O	1:A:109:THR:C	2.49	0.50
1:A:1012:LYS:NZ	1:A:1026:PHE:O	2.43	0.50
1:B:131:CYS:SG	1:B:132:GLU:N	2.85	0.50
1:B:461:SER:OG	1:B:462:THR:N	2.45	0.50
1:B:436:LEU:O	1:B:437:TYR:C	2.50	0.50
1:C:970:LYS:HB3	1:C:971:PRO:HD3	1.94	0.49
1:C:1107:SER:OG	1:C:1108:GLY:N	2.45	0.49
1:B:355:SER:OG	1:B:356:ALA:N	2.46	0.49
1:C:428:LYS:NZ	1:C:481:PHE:O	2.36	0.48
1:B:600:ASN:OD1	1:B:601:CYS:N	2.46	0.48
1:A:604:VAL:N	1:A:605:PRO:HD2	2.29	0.48
1:B:357:SER:OG	1:B:358:PHE:N	2.46	0.48
1:A:142:SER:OG	1:A:143:TRP:N	2.44	0.48
1:C:1126:GLN:N	1:C:1127:PRO:HD2	2.29	0.48
1:B:604:VAL:N	1:B:605:PRO:CD	2.77	0.47
1:B:474:PHE:N	1:B:475:PRO:CD	2.77	0.47
1:B:764:GLU:O	1:B:768:GLN:NE2	2.48	0.47
1:A:953:ASN:O	1:A:955:GLY:N	2.47	0.47
1:A:491:PRO:O	1:A:492:TYR:HB2	2.14	0.47
1:C:453:SER:OG	1:C:454:THR:N	2.45	0.47
1:C:490:GLN:N	1:C:491:PRO:CD	2.78	0.46
1:A:1126:GLN:N	1:A:1127:PRO:HD2	2.29	0.46
1:A:444:ASN:O	1:A:445:LEU:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:O	1:A:441:ARG:HB2	2.16	0.46
1:A:472:CYS:O	1:A:473:TYR:CB	2.64	0.46
1:B:333:SER:OG	1:B:334:VAL:N	2.48	0.46
1:B:482:GLN:HB2	1:B:483:PRO:CD	2.45	0.46
1:C:969:ASP:O	1:C:970:LYS:CB	2.65	0.45
1:A:412:ASP:O	1:A:413:PHE:C	2.55	0.45
1:C:315:ASN:OD1	1:C:315:ASN:N	2.45	0.45
1:C:479:TYR:CG	1:C:479:TYR:O	2.70	0.45
1:C:1058:ASN:HD21	2:C:1210:NAG:H82	1.82	0.45
1:B:970:LYS:HB3	1:B:971:PRO:HD3	1.99	0.45
1:A:306:PRO:O	1:A:308:GLU:N	2.50	0.44
1:B:112:SER:OG	1:B:113:LYS:N	2.49	0.44
1:C:969:ASP:N	1:C:969:ASP:OD1	2.46	0.44
1:C:108:THR:O	1:C:109:THR:C	2.56	0.44
1:A:583:THR:HG22	1:A:585:GLY:H	1.83	0.44
1:A:176:ASN:O	1:A:177:PHE:HB2	2.18	0.44
1:A:474:PHE:N	1:A:475:PRO:HD2	2.34	0.43
1:A:445:LEU:O	1:A:446:LYS:HB2	2.18	0.43
1:A:311:VAL:H	1:A:515:THR:HG22	1.82	0.43
1:B:143:TRP:N	1:B:146:SER:OG	2.52	0.43
1:B:315:ASN:ND2	2:B:1211:NAG:O1	2.51	0.43
1:B:472:CYS:O	1:B:473:TYR:HB3	2.18	0.43
1:C:474:PHE:N	1:C:475:PRO:HD2	2.33	0.43
1:C:477:GLN:HB2	1:C:478:PRO:HD3	2.01	0.43
1:C:795:LYS:O	1:C:797:SER:N	2.52	0.42
1:B:474:PHE:N	1:B:475:PRO:HD3	2.34	0.42
1:C:445:LEU:O	1:C:446:LYS:HB2	2.20	0.42
1:A:131:CYS:SG	1:A:132:GLU:N	2.92	0.42
1:B:443:SER:O	1:B:444:ASN:C	2.58	0.42
1:A:31:SER:OG	1:A:32:PHE:N	2.52	0.42
1:A:1061:THR:OG1	1:A:1062:ALA:N	2.52	0.42
1:C:477:GLN:CB	1:C:478:PRO:CD	2.97	0.42
1:B:143:TRP:CG	1:B:144:MET:N	2.88	0.42
1:B:277:LEU:O	1:B:278:ASP:HB3	2.20	0.42
1:C:348:ASP:OD1	1:C:348:ASP:N	2.48	0.42
1:C:687:ASN:OD1	1:C:688:SER:N	2.53	0.41
1:C:924:SER:O	1:C:925:THR:C	2.59	0.41
1:A:30:ASN:HB3	1:A:32:PHE:CE1	2.56	0.41
1:A:278:ASP:HB2	1:A:279:PRO:HD2	2.03	0.41
1:B:1061:THR:OG1	1:B:1062:ALA:N	2.53	0.41
1:A:424:ASN:O	1:A:425:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:LYS:HA	1:A:799:ARG:CB	2.49	0.41
1:C:434:ASN:O	1:C:435:TYR:HB2	2.20	0.41
1:A:490:GLN:N	1:A:491:PRO:HD2	2.34	0.41
1:C:1061:THR:OG1	1:C:1062:ALA:N	2.54	0.41
1:A:790:LEU:HA	1:A:791:PRO:HD3	1.94	0.41
1:C:188:ILE:O	1:C:190:GLY:N	2.54	0.41
1:C:1084:THR:OG1	1:C:1085:HIS:N	2.52	0.40
1:C:401:LYS:O	1:C:405:TYR:CD2	2.74	0.40
1:B:614:THR:HA	1:B:615:PRO:HD3	1.96	0.40
1:B:785:ASN:ND2	2:B:1208:NAG:O5	2.54	0.40
1:C:477:GLN:HB2	1:C:478:PRO:CD	2.50	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	1036/1192 (87%)	964 (93%)	61 (6%)	11 (1%)	14	44
1	B	1063/1192 (89%)	999 (94%)	52 (5%)	12 (1%)	14	44
1	C	1038/1192 (87%)	973 (94%)	55 (5%)	10 (1%)	15	47
All	All	3137/3576 (88%)	2936 (94%)	168 (5%)	33 (1%)	18	44

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	954	PHE
1	C	970	LYS
1	A	413	PHE
1	A	445	LEU
1	A	492	TYR

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Mol	Chain	Res	Type
1	B	224	ILE
1	B	232	LEU
1	B	411	ASP
1	B	464	CYS
1	C	87	ASN
1	A	473	TYR
1	C	189	ASP
1	C	205	ARG
1	B	407	TYR
1	B	446	LYS
1	B	461	SER
1	C	361	PHE
1	C	796	PRO
1	A	177	PHE
1	A	432	ASN
1	C	157	CYS
1	A	621	SER
1	B	373	ASP
1	C	143	TRP
1	C	466	GLY
1	A	490	GLN
1	B	278	ASP
1	B	241	THR
1	A	446	LYS
1	B	314	PRO
1	B	1095	GLU
1	C	278	ASP

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	916/1044 (88%)	914 (100%)	2 (0%)	93 97
1	B	936/1044 (90%)	935 (100%)	1 (0%)	93 97
1	C	919/1044 (88%)	917 (100%)	2 (0%)	93 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2771/3132 (88%)	2766 (100%)	5 (0%)	93 97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	HIS
1	A	476	LEU
1	B	629	THR
1	C	315	ASN
1	C	489	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	768	GLN
1	B	994	GLN
1	C	490	GLN
1	C	639	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

48 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	A	1206	1	14,14,15	1.29	2 (14%)	17,19,21	1.10	1 (5%)
2	NAG	A	1208	-	15,15,15	1.32	2 (13%)	21,21,21	0.92	1 (4%)
2	NAG	C	1216	-	15,15,15	1.27	2 (13%)	21,21,21	0.98	2 (9%)
2	NAG	A	1214	-	15,15,15	1.30	2 (13%)	21,21,21	0.92	1 (4%)
2	NAG	A	1210	-	15,15,15	1.24	2 (13%)	21,21,21	0.98	1 (4%)
2	NAG	C	1213	-	15,15,15	1.29	2 (13%)	21,21,21	0.97	2 (9%)
2	NAG	B	1204	-	15,15,15	1.28	2 (13%)	21,21,21	1.02	2 (9%)
2	NAG	B	1208	-	15,15,15	1.27	2 (13%)	21,21,21	0.92	1 (4%)
2	NAG	C	1210	-	15,15,15	1.29	2 (13%)	21,21,21	0.97	1 (4%)
2	NAG	B	1209	-	15,15,15	1.26	2 (13%)	21,21,21	0.97	1 (4%)
2	NAG	B	1210	1	14,14,15	1.15	2 (14%)	17,19,21	1.05	1 (5%)
2	NAG	A	1202	-	15,15,15	1.32	2 (13%)	21,21,21	0.93	1 (4%)
2	NAG	A	1211	-	15,15,15	1.35	2 (13%)	21,21,21	0.96	1 (4%)
2	NAG	A	1217	-	15,15,15	1.31	2 (13%)	21,21,21	1.06	1 (4%)
2	NAG	A	1213	-	15,15,15	1.33	2 (13%)	21,21,21	0.91	1 (4%)
2	NAG	A	1205	-	15,15,15	1.31	2 (13%)	21,21,21	0.93	1 (4%)
2	NAG	C	1209	-	15,15,15	1.26	2 (13%)	21,21,21	1.00	1 (4%)
2	NAG	C	1201	-	15,15,15	1.36	2 (13%)	21,21,21	1.07	2 (9%)
2	NAG	B	1215	-	15,15,15	1.31	2 (13%)	21,21,21	1.03	2 (9%)
2	NAG	C	1204	1	14,14,15	1.43	2 (14%)	17,19,21	1.28	2 (11%)
2	NAG	B	1206	-	15,15,15	1.29	2 (13%)	21,21,21	1.01	2 (9%)
2	NAG	C	1208	-	15,15,15	1.21	2 (13%)	21,21,21	0.96	1 (4%)
2	NAG	C	1215	-	15,15,15	1.32	2 (13%)	21,21,21	0.96	1 (4%)
2	NAG	A	1207	-	15,15,15	1.29	2 (13%)	21,21,21	0.94	1 (4%)
2	NAG	A	1216	-	15,15,15	1.31	2 (13%)	21,21,21	0.92	1 (4%)
2	NAG	A	1203	-	15,15,15	1.32	2 (13%)	21,21,21	0.95	1 (4%)
2	NAG	B	1212	-	15,15,15	1.30	2 (13%)	21,21,21	0.98	1 (4%)
2	NAG	C	1206	-	15,15,15	1.35	2 (13%)	21,21,21	0.93	1 (4%)
2	NAG	B	1205	-	15,15,15	1.32	2 (13%)	21,21,21	0.96	1 (4%)
2	NAG	B	1207	-	15,15,15	1.26	2 (13%)	21,21,21	0.93	1 (4%)
2	NAG	C	1202	-	15,15,15	1.34	2 (13%)	21,21,21	0.93	1 (4%)
2	NAG	B	1201	-	15,15,15	1.32	2 (13%)	21,21,21	0.96	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	1204	-	15,15,15	1.30	2 (13%)	21,21,21	1.01	2 (9%)
2	NAG	C	1214	-	15,15,15	1.27	2 (13%)	21,21,21	0.97	2 (9%)
2	NAG	C	1212	1	14,14,15	1.34	2 (14%)	17,19,21	1.12	1 (5%)
2	NAG	C	1211	-	15,15,15	1.30	2 (13%)	21,21,21	0.99	2 (9%)
2	NAG	C	1205	-	15,15,15	1.28	2 (13%)	21,21,21	0.95	1 (4%)
2	NAG	A	1209	-	15,15,15	1.30	2 (13%)	21,21,21	0.94	1 (4%)
2	NAG	B	1203	-	15,15,15	1.40	2 (13%)	21,21,21	0.98	1 (4%)
2	NAG	B	1202	-	15,15,15	1.30	2 (13%)	21,21,21	0.93	1 (4%)
2	NAG	C	1207	-	15,15,15	1.30	2 (13%)	21,21,21	0.98	1 (4%)
2	NAG	B	1214	-	15,15,15	1.30	2 (13%)	21,21,21	0.97	1 (4%)
2	NAG	C	1203	-	15,15,15	1.29	2 (13%)	21,21,21	0.96	1 (4%)
2	NAG	B	1213	-	15,15,15	1.35	2 (13%)	21,21,21	0.95	1 (4%)
2	NAG	B	1211	-	15,15,15	1.29	2 (13%)	21,21,21	0.91	1 (4%)
2	NAG	A	1215	1	14,14,15	1.25	2 (14%)	17,19,21	1.03	1 (5%)
2	NAG	A	1212	-	15,15,15	1.26	2 (13%)	21,21,21	0.97	1 (4%)
2	NAG	A	1201	-	15,15,15	1.32	2 (13%)	21,21,21	1.01	2 (9%)

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	A	1206	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1208	-	-	1/6/26/26	0/1/1/1
2	NAG	C	1216	-	-	0/6/26/26	0/1/1/1
2	NAG	A	1214	-	-	1/6/26/26	0/1/1/1
2	NAG	A	1210	-	-	1/6/26/26	0/1/1/1
2	NAG	C	1213	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1204	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1208	-	-	0/6/26/26	0/1/1/1
2	NAG	C	1210	-	-	2/6/26/26	0/1/1/1
2	NAG	B	1209	-	-	2/6/26/26	0/1/1/1
2	NAG	B	1210	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1202	-	-	0/6/26/26	0/1/1/1
2	NAG	A	1211	-	-	0/6/26/26	0/1/1/1
2	NAG	A	1217	-	-	1/6/26/26	0/1/1/1
2	NAG	A	1213	-	-	1/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1205	-	-	1/6/26/26	0/1/1/1
2	NAG	C	1209	-	-	0/6/26/26	0/1/1/1
2	NAG	C	1201	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1215	-	-	2/6/26/26	0/1/1/1
2	NAG	C	1204	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1206	-	-	1/6/26/26	0/1/1/1
2	NAG	C	1208	-	-	0/6/26/26	0/1/1/1
2	NAG	C	1215	-	-	0/6/26/26	0/1/1/1
2	NAG	A	1207	-	-	1/6/26/26	0/1/1/1
2	NAG	A	1216	-	-	1/6/26/26	0/1/1/1
2	NAG	A	1203	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1212	-	-	1/6/26/26	0/1/1/1
2	NAG	C	1206	-	-	0/6/26/26	0/1/1/1
2	NAG	B	1205	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1207	-	-	0/6/26/26	0/1/1/1
2	NAG	C	1202	-	-	0/6/26/26	0/1/1/1
2	NAG	B	1201	-	-	1/6/26/26	0/1/1/1
2	NAG	A	1204	-	-	1/6/26/26	0/1/1/1
2	NAG	C	1214	-	-	0/6/26/26	0/1/1/1
2	NAG	C	1212	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1211	-	-	2/6/26/26	0/1/1/1
2	NAG	C	1205	-	-	1/6/26/26	0/1/1/1
2	NAG	A	1209	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1203	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1202	-	-	1/6/26/26	0/1/1/1
2	NAG	C	1207	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1214	-	-	1/6/26/26	0/1/1/1
2	NAG	C	1203	-	-	0/6/26/26	0/1/1/1
2	NAG	B	1213	-	-	1/6/26/26	0/1/1/1
2	NAG	B	1211	-	-	1/6/26/26	0/1/1/1
2	NAG	A	1215	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1212	-	-	0/6/26/26	0/1/1/1
2	NAG	A	1201	-	-	2/6/26/26	0/1/1/1

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1204	NAG	C1-C2	3.92	1.58	1.52
2	C	1212	NAG	C1-C2	3.80	1.58	1.52
2	A	1206	NAG	C1-C2	3.75	1.57	1.52
2	B	1203	NAG	C1-C2	3.64	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1211	NAG	C1-C2	3.58	1.57	1.52
2	B	1213	NAG	C1-C2	3.58	1.57	1.52
2	C	1206	NAG	C1-C2	3.56	1.57	1.52
2	A	1215	NAG	C1-C2	3.55	1.57	1.52
2	A	1213	NAG	C1-C2	3.54	1.57	1.52
2	C	1201	NAG	C1-C2	3.50	1.57	1.52
2	A	1202	NAG	C1-C2	3.47	1.57	1.52
2	A	1208	NAG	C1-C2	3.45	1.57	1.52
2	C	1215	NAG	C1-C2	3.43	1.57	1.52
2	A	1209	NAG	C1-C2	3.43	1.57	1.52
2	B	1201	NAG	C1-C2	3.42	1.57	1.52
2	A	1201	NAG	C1-C2	3.41	1.57	1.52
2	C	1202	NAG	C1-C2	3.40	1.57	1.52
2	C	1207	NAG	C1-C2	3.38	1.57	1.52
2	B	1205	NAG	C1-C2	3.35	1.56	1.52
2	A	1216	NAG	C1-C2	3.34	1.56	1.52
2	B	1215	NAG	C1-C2	3.33	1.56	1.52
2	C	1210	NAG	C1-C2	3.33	1.56	1.52
2	A	1214	NAG	C1-C2	3.32	1.56	1.52
2	C	1211	NAG	C1-C2	3.32	1.56	1.52
2	A	1203	NAG	C1-C2	3.32	1.56	1.52
2	B	1214	NAG	C1-C2	3.31	1.56	1.52
2	C	1205	NAG	C1-C2	3.31	1.56	1.52
2	B	1212	NAG	C1-C2	3.31	1.56	1.52
2	B	1211	NAG	C1-C2	3.31	1.56	1.52
2	C	1203	NAG	C1-C2	3.31	1.56	1.52
2	A	1205	NAG	C1-C2	3.31	1.56	1.52
2	B	1202	NAG	C1-C2	3.29	1.56	1.52
2	A	1204	NAG	C1-C2	3.28	1.56	1.52
2	B	1206	NAG	C1-C2	3.28	1.56	1.52
2	B	1207	NAG	C1-C2	3.27	1.56	1.52
2	A	1207	NAG	C1-C2	3.27	1.56	1.52
2	A	1217	NAG	C1-C2	3.26	1.56	1.52
2	B	1208	NAG	C1-C2	3.26	1.56	1.52
2	C	1209	NAG	C1-C2	3.24	1.56	1.52
2	B	1209	NAG	C1-C2	3.23	1.56	1.52
2	C	1213	NAG	C1-C2	3.21	1.56	1.52
2	A	1212	NAG	C1-C2	3.19	1.56	1.52
2	B	1204	NAG	C1-C2	3.13	1.56	1.52
2	C	1214	NAG	C1-C2	3.13	1.56	1.52
2	C	1216	NAG	C1-C2	3.12	1.56	1.52
2	A	1210	NAG	C1-C2	3.08	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1210	NAG	C1-C2	3.08	1.56	1.52
2	C	1208	NAG	C1-C2	2.97	1.56	1.52
2	B	1203	NAG	O1-C1	2.86	1.48	1.39
2	B	1204	NAG	O1-C1	2.83	1.48	1.39
2	C	1215	NAG	O1-C1	2.82	1.48	1.39
2	A	1211	NAG	O1-C1	2.82	1.48	1.39
2	C	1213	NAG	O1-C1	2.81	1.48	1.39
2	B	1212	NAG	O1-C1	2.80	1.48	1.39
2	C	1202	NAG	O1-C1	2.80	1.48	1.39
2	C	1206	NAG	O1-C1	2.79	1.48	1.39
2	A	1204	NAG	O1-C1	2.79	1.48	1.39
2	A	1205	NAG	O1-C1	2.78	1.48	1.39
2	A	1213	NAG	O1-C1	2.78	1.48	1.39
2	C	1203	NAG	O1-C1	2.77	1.48	1.39
2	C	1211	NAG	O1-C1	2.77	1.48	1.39
2	B	1201	NAG	O1-C1	2.77	1.48	1.39
2	B	1205	NAG	O1-C1	2.77	1.48	1.39
2	A	1216	NAG	O1-C1	2.76	1.48	1.39
2	A	1209	NAG	O1-C1	2.76	1.48	1.39
2	B	1208	NAG	O1-C1	2.76	1.48	1.39
2	B	1214	NAG	O1-C1	2.75	1.48	1.39
2	C	1214	NAG	O1-C1	2.75	1.48	1.39
2	C	1209	NAG	O1-C1	2.75	1.48	1.39
2	A	1203	NAG	O1-C1	2.75	1.48	1.39
2	B	1202	NAG	O1-C1	2.75	1.48	1.39
2	C	1216	NAG	O1-C1	2.75	1.48	1.39
2	A	1214	NAG	O1-C1	2.74	1.48	1.39
2	A	1201	NAG	O1-C1	2.74	1.48	1.39
2	A	1207	NAG	O1-C1	2.74	1.48	1.39
2	A	1217	NAG	O1-C1	2.73	1.48	1.39
2	B	1211	NAG	O1-C1	2.73	1.48	1.39
2	B	1213	NAG	O1-C1	2.73	1.48	1.39
2	A	1210	NAG	O1-C1	2.73	1.48	1.39
2	A	1208	NAG	O1-C1	2.73	1.48	1.39
2	C	1208	NAG	O1-C1	2.72	1.48	1.39
2	B	1207	NAG	O1-C1	2.72	1.48	1.39
2	A	1202	NAG	O1-C1	2.71	1.48	1.39
2	C	1207	NAG	O1-C1	2.71	1.48	1.39
2	B	1206	NAG	O1-C1	2.71	1.48	1.39
2	C	1210	NAG	O1-C1	2.70	1.48	1.39
2	B	1215	NAG	O1-C1	2.70	1.48	1.39
2	C	1201	NAG	O1-C1	2.67	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1205	NAG	O1-C1	2.66	1.48	1.39
2	B	1209	NAG	O1-C1	2.65	1.48	1.39
2	A	1212	NAG	O1-C1	2.63	1.48	1.39
2	C	1212	NAG	O5-C5	2.36	1.48	1.43
2	C	1204	NAG	O5-C5	2.30	1.48	1.43
2	B	1210	NAG	O5-C5	2.03	1.47	1.43
2	A	1206	NAG	O5-C5	2.03	1.47	1.43
2	A	1215	NAG	O5-C5	2.01	1.47	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1204	NAG	C8-C7-N2	3.17	121.46	116.10
2	C	1212	NAG	C8-C7-N2	2.76	120.76	116.10
2	A	1217	NAG	C8-C7-N2	2.75	120.75	116.10
2	C	1209	NAG	C8-C7-N2	2.66	120.60	116.10
2	A	1211	NAG	C8-C7-N2	2.65	120.59	116.10
2	B	1210	NAG	C8-C7-N2	2.63	120.56	116.10
2	C	1210	NAG	C8-C7-N2	2.61	120.51	116.10
2	C	1207	NAG	C8-C7-N2	2.60	120.49	116.10
2	A	1201	NAG	C8-C7-N2	2.58	120.47	116.10
2	C	1205	NAG	C8-C7-N2	2.57	120.45	116.10
2	C	1208	NAG	C8-C7-N2	2.55	120.42	116.10
2	A	1207	NAG	C8-C7-N2	2.55	120.41	116.10
2	B	1209	NAG	C8-C7-N2	2.53	120.38	116.10
2	B	1214	NAG	C8-C7-N2	2.53	120.38	116.10
2	A	1210	NAG	C8-C7-N2	2.53	120.38	116.10
2	B	1206	NAG	C8-C7-N2	2.51	120.35	116.10
2	B	1212	NAG	C8-C7-N2	2.51	120.34	116.10
2	B	1215	NAG	C8-C7-N2	2.50	120.34	116.10
2	A	1209	NAG	C8-C7-N2	2.49	120.31	116.10
2	A	1212	NAG	C8-C7-N2	2.47	120.29	116.10
2	C	1215	NAG	C8-C7-N2	2.47	120.28	116.10
2	A	1204	NAG	C8-C7-N2	2.46	120.27	116.10
2	B	1202	NAG	C8-C7-N2	2.45	120.25	116.10
2	B	1201	NAG	C8-C7-N2	2.45	120.25	116.10
2	A	1215	NAG	C8-C7-N2	2.45	120.25	116.10
2	A	1205	NAG	C8-C7-N2	2.45	120.25	116.10
2	B	1207	NAG	C8-C7-N2	2.44	120.24	116.10
2	B	1204	NAG	C8-C7-N2	2.44	120.23	116.10
2	C	1201	NAG	C1-C2-N2	-2.43	107.91	110.73
2	A	1202	NAG	C8-C7-N2	2.43	120.22	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1206	NAG	C8-C7-N2	2.43	120.21	116.10
2	A	1208	NAG	C8-C7-N2	2.43	120.21	116.10
2	B	1205	NAG	C8-C7-N2	2.43	120.21	116.10
2	C	1213	NAG	C8-C7-N2	2.41	120.19	116.10
2	C	1202	NAG	C8-C7-N2	2.41	120.18	116.10
2	C	1216	NAG	C8-C7-N2	2.39	120.15	116.10
2	A	1214	NAG	C8-C7-N2	2.39	120.14	116.10
2	C	1206	NAG	C8-C7-N2	2.38	120.12	116.10
2	B	1203	NAG	C8-C7-N2	2.35	120.08	116.10
2	C	1211	NAG	C8-C7-N2	2.35	120.07	116.10
2	B	1213	NAG	C8-C7-N2	2.35	120.07	116.10
2	A	1203	NAG	C8-C7-N2	2.34	120.06	116.10
2	C	1203	NAG	C8-C7-N2	2.34	120.06	116.10
2	A	1213	NAG	C8-C7-N2	2.33	120.05	116.10
2	C	1201	NAG	C8-C7-N2	2.29	119.98	116.10
2	B	1204	NAG	C1-C2-N2	-2.29	108.08	110.73
2	A	1216	NAG	C8-C7-N2	2.27	119.95	116.10
2	B	1208	NAG	C8-C7-N2	2.25	119.91	116.10
2	B	1215	NAG	C1-C2-N2	-2.24	108.14	110.73
2	C	1214	NAG	C8-C7-N2	2.21	119.83	116.10
2	C	1216	NAG	C1-C2-N2	-2.18	108.20	110.73
2	C	1214	NAG	C1-C2-N2	-2.18	108.20	110.73
2	B	1211	NAG	C8-C7-N2	2.15	119.73	116.10
2	C	1211	NAG	C1-C2-N2	-2.13	108.26	110.73
2	B	1206	NAG	C1-C2-N2	-2.10	108.30	110.73
2	C	1204	NAG	O7-C7-C8	-2.09	118.17	122.06
2	A	1204	NAG	C1-C2-N2	-2.07	108.33	110.73
2	A	1201	NAG	C1-C2-N2	-2.04	108.36	110.73
2	C	1213	NAG	C1-C2-N2	-2.00	108.41	110.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1206	NAG	C1

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1204	NAG	O5-C5-C6-O6
2	C	1204	NAG	C4-C5-C6-O6
2	A	1201	NAG	C1-C2-N2-C7
2	A	1207	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	1209	NAG	O5-C5-C6-O6
2	A	1213	NAG	O5-C5-C6-O6
2	A	1217	NAG	O5-C5-C6-O6
2	A	1203	NAG	O5-C5-C6-O6
2	B	1204	NAG	O5-C5-C6-O6
2	B	1205	NAG	O5-C5-C6-O6
2	A	1208	NAG	O5-C5-C6-O6
2	A	1214	NAG	O5-C5-C6-O6
2	A	1201	NAG	O5-C5-C6-O6
2	A	1205	NAG	O5-C5-C6-O6
2	B	1202	NAG	O5-C5-C6-O6
2	B	1211	NAG	O5-C5-C6-O6
2	C	1207	NAG	O5-C5-C6-O6
2	B	1213	NAG	O5-C5-C6-O6
2	B	1214	NAG	O5-C5-C6-O6
2	B	1215	NAG	O5-C5-C6-O6
2	A	1204	NAG	O5-C5-C6-O6
2	A	1210	NAG	O5-C5-C6-O6
2	A	1215	NAG	O5-C5-C6-O6
2	A	1216	NAG	O5-C5-C6-O6
2	B	1201	NAG	O5-C5-C6-O6
2	B	1212	NAG	O5-C5-C6-O6
2	C	1201	NAG	O5-C5-C6-O6
2	C	1205	NAG	O5-C5-C6-O6
2	C	1211	NAG	O5-C5-C6-O6
2	C	1213	NAG	O5-C5-C6-O6
2	B	1203	NAG	O5-C5-C6-O6
2	B	1209	NAG	C4-C5-C6-O6
2	B	1209	NAG	O5-C5-C6-O6
2	B	1206	NAG	C1-C2-N2-C7
2	B	1215	NAG	C1-C2-N2-C7
2	C	1211	NAG	C1-C2-N2-C7
2	C	1210	NAG	C4-C5-C6-O6
2	C	1210	NAG	O5-C5-C6-O6

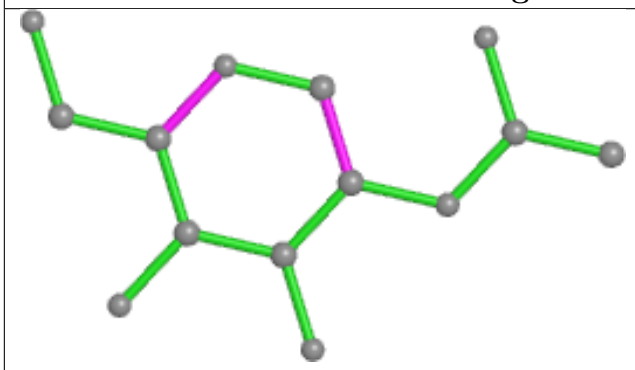
There are no ring outliers.

3 monomers are involved in 3 short contacts:

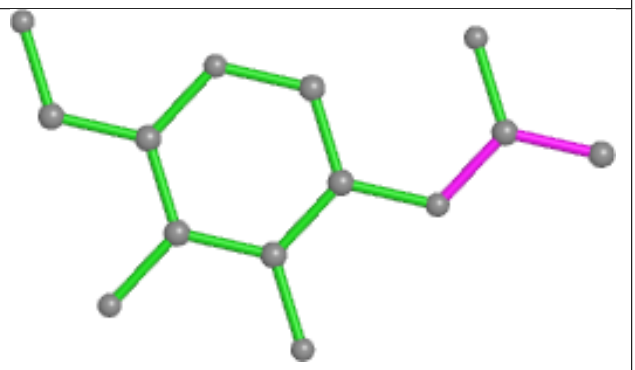
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1208	NAG	1	0
2	C	1210	NAG	1	0
2	B	1211	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

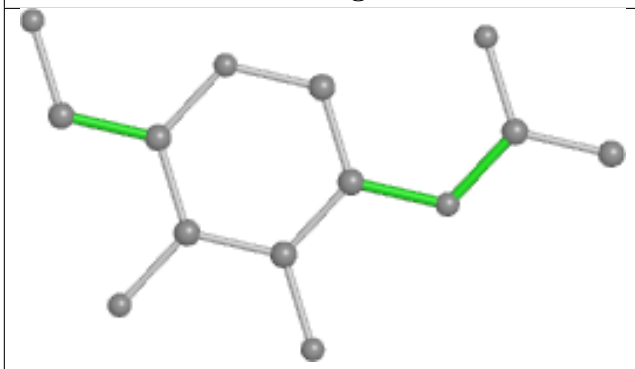
Ligand NAG A 1206



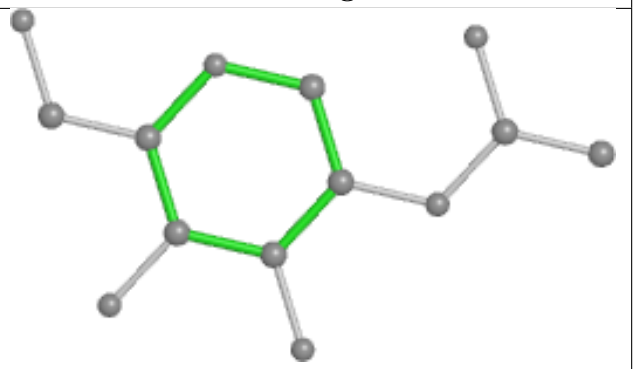
Bond lengths



Bond angles

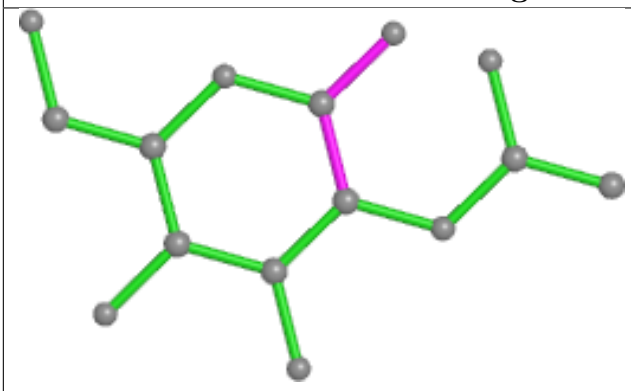


Torsions

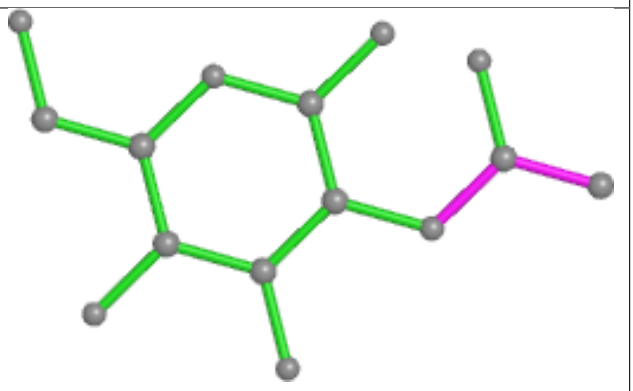


Rings

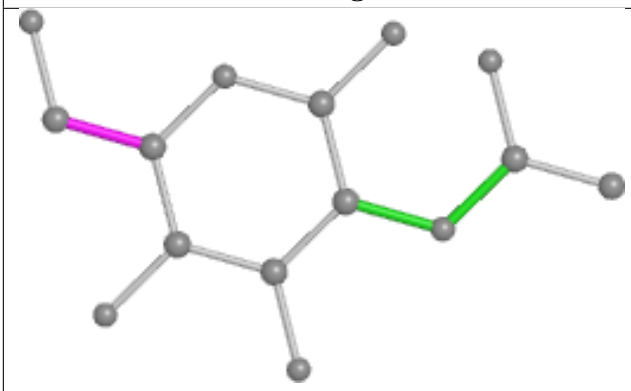
Ligand NAG A 1208



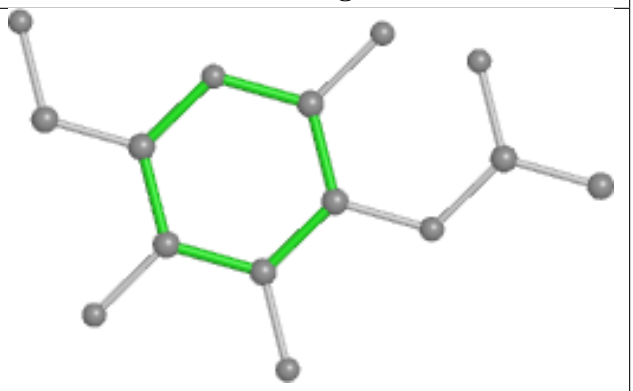
Bond lengths



Bond angles

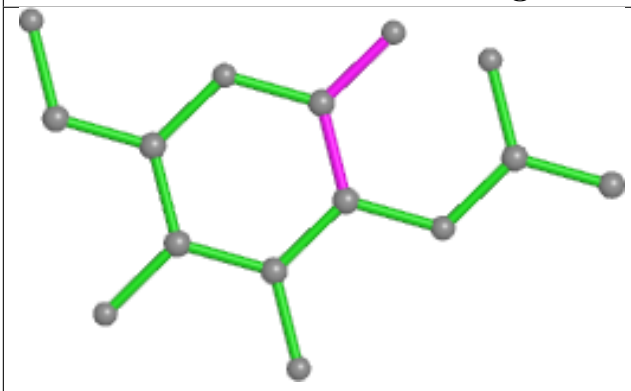


Torsions

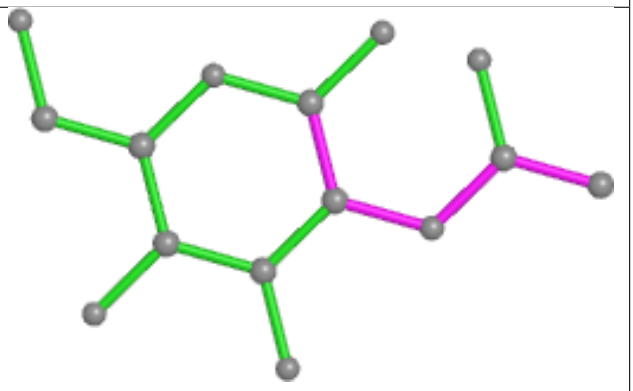


Rings

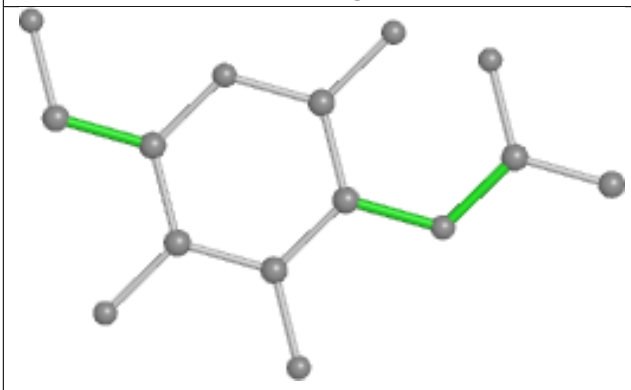
Ligand NAG C 1216



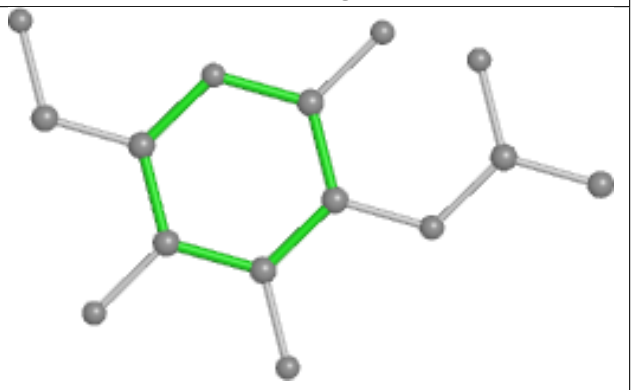
Bond lengths



Bond angles

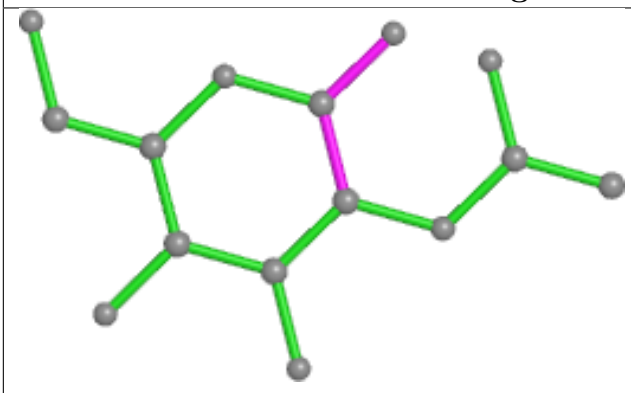


Torsions

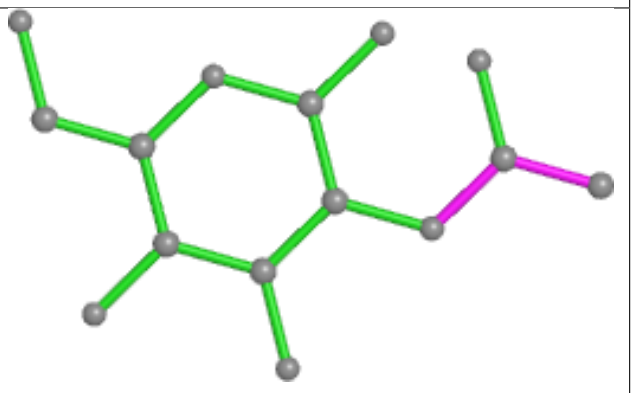


Rings

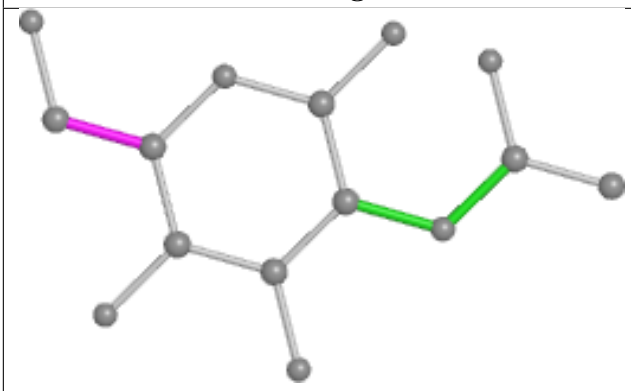
Ligand NAG A 1214



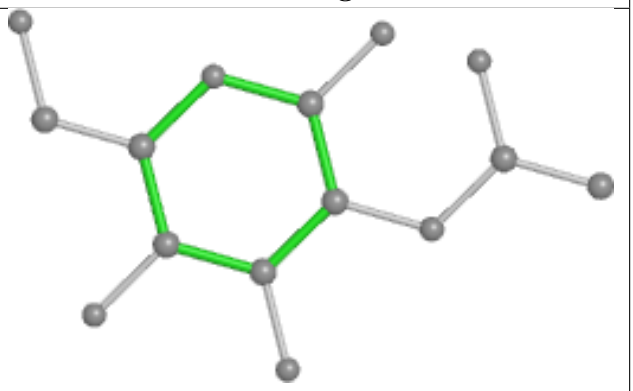
Bond lengths



Bond angles

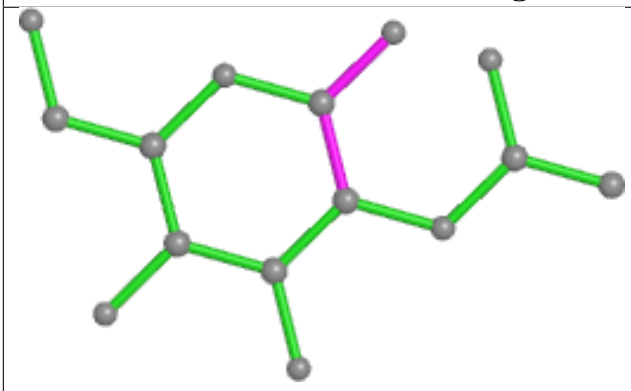


Torsions

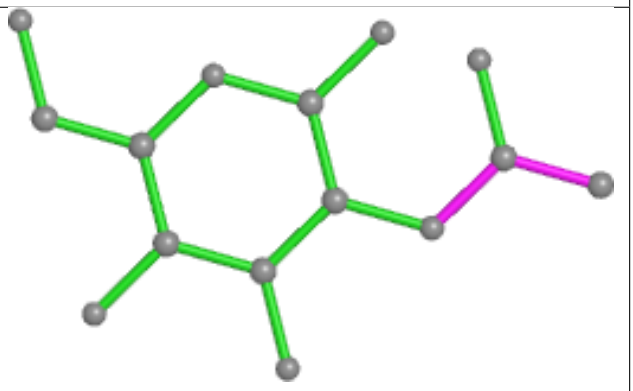


Rings

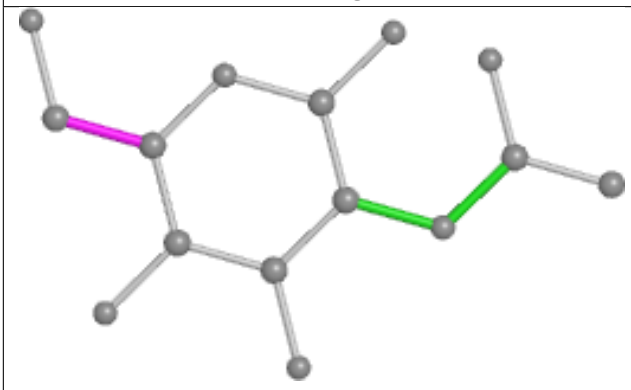
Ligand NAG A 1210



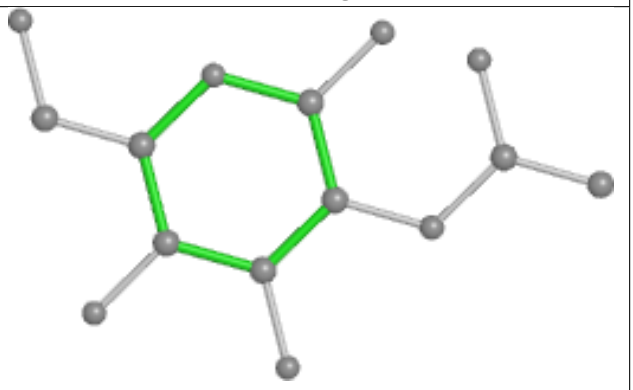
Bond lengths



Bond angles

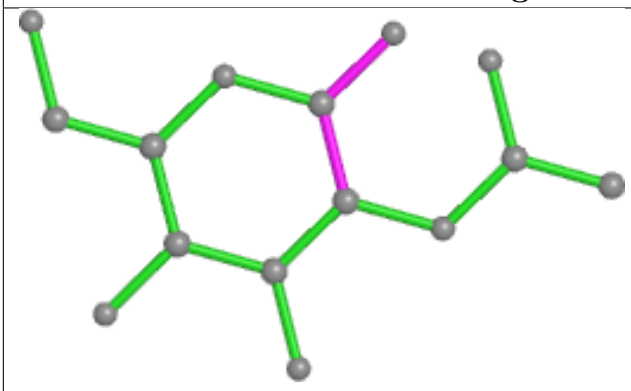


Torsions

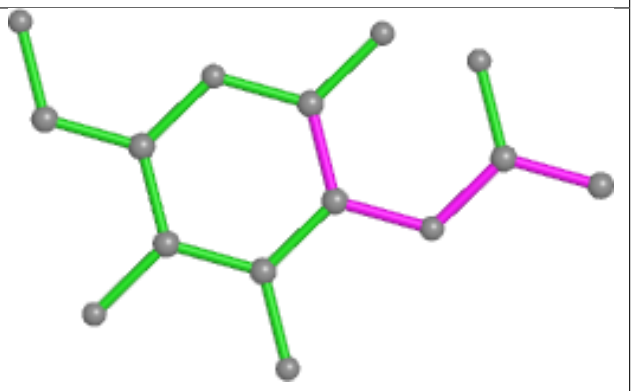


Rings

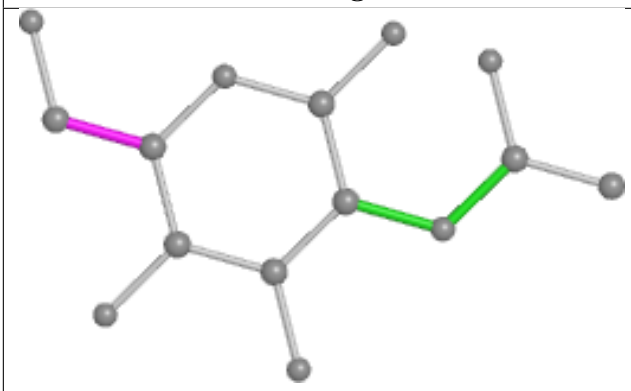
Ligand NAG C 1213



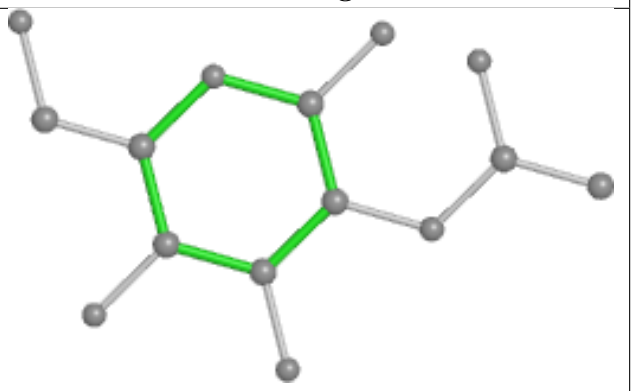
Bond lengths



Bond angles

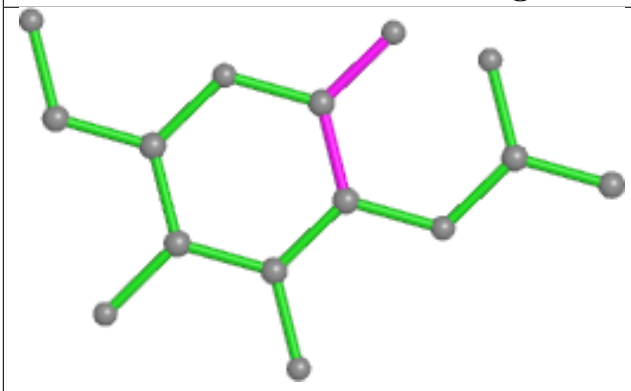


Torsions

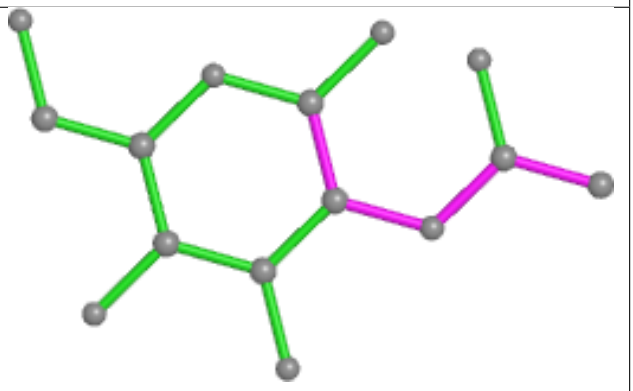


Rings

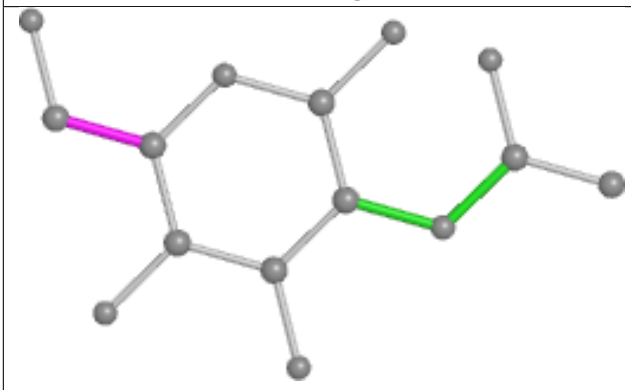
Ligand NAG B 1204



Bond lengths



Bond angles



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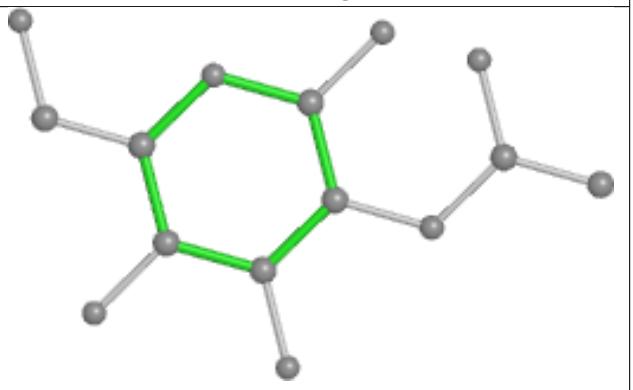
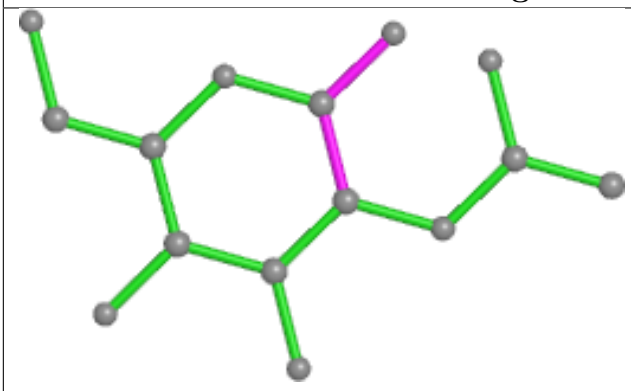
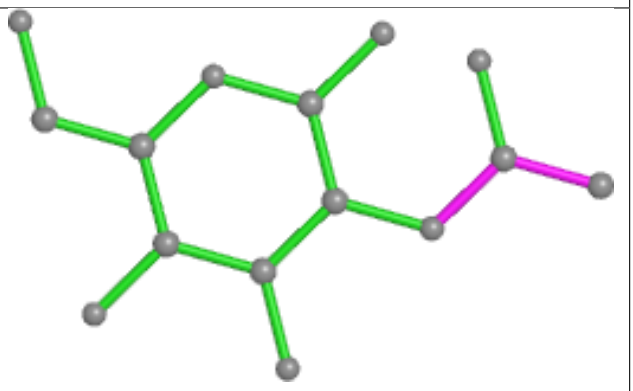


Rings

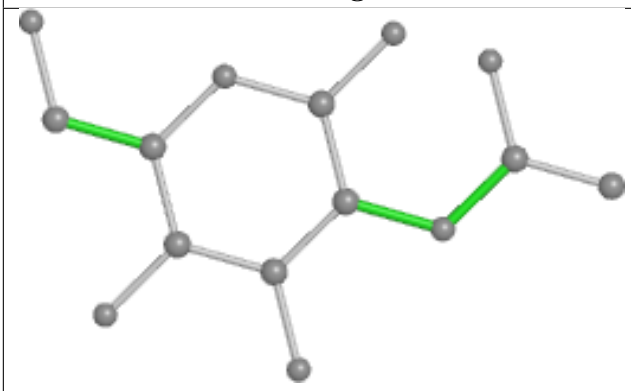
Ligand NAG B 1208



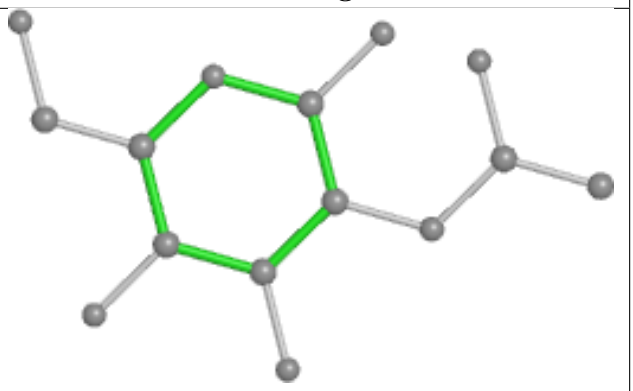
Bond lengths



Bond angles

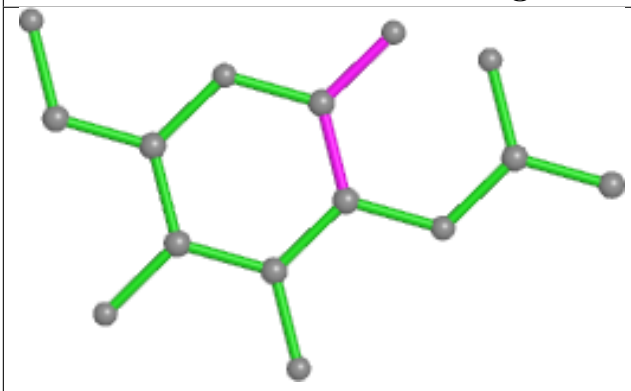


Torsions



Rings

Ligand NAG C 1210



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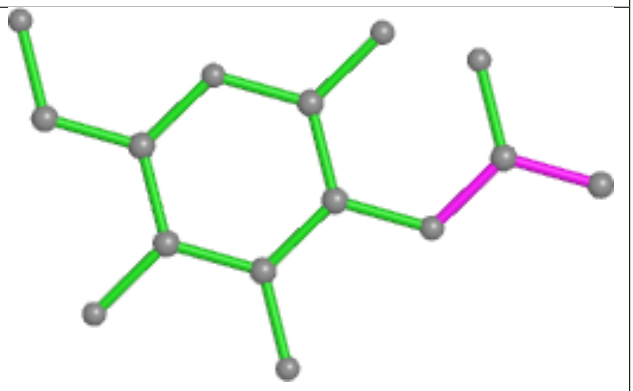
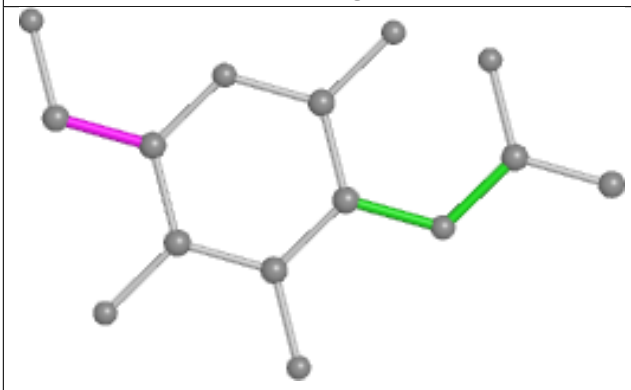
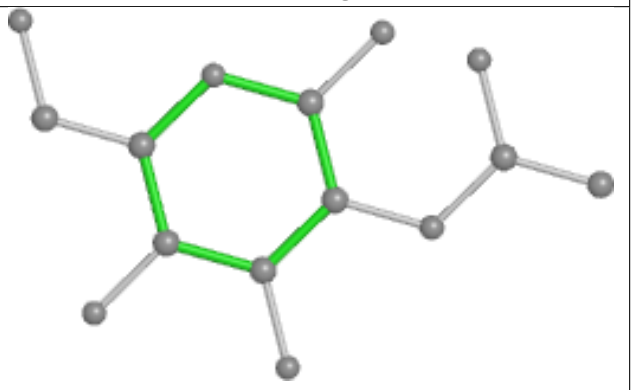


Bond angles

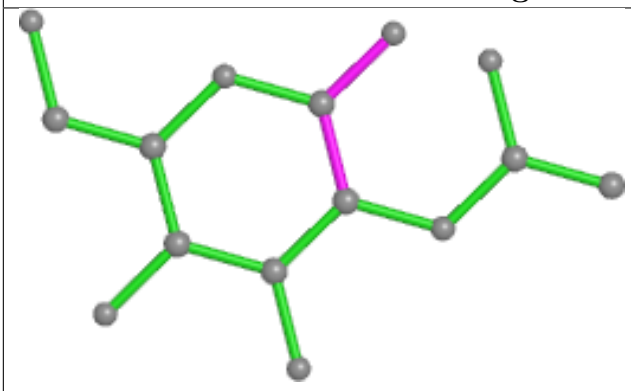


Torsions

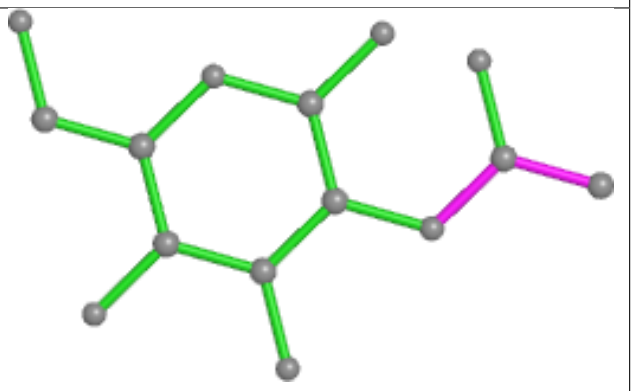


Rings

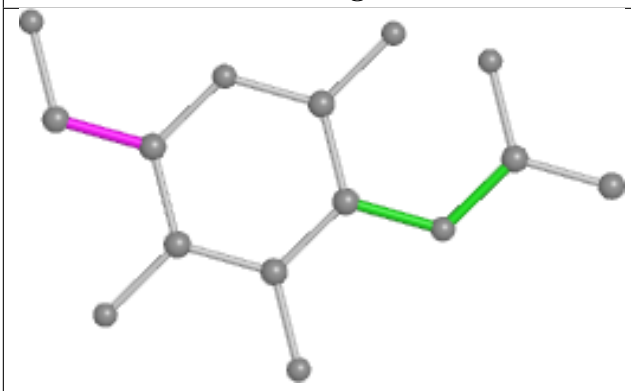
Ligand NAG B 1209



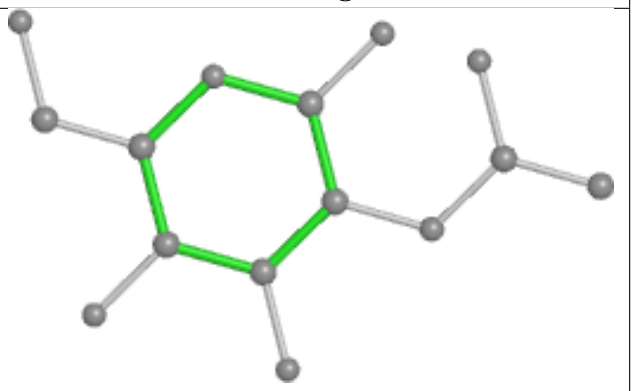
Bond lengths



Bond angles

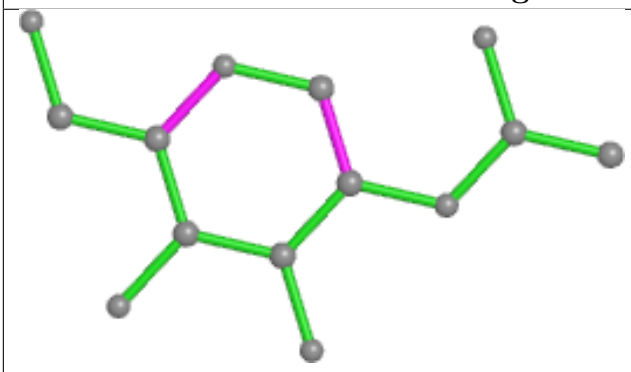


Torsions



Rings

Ligand NAG B 1210



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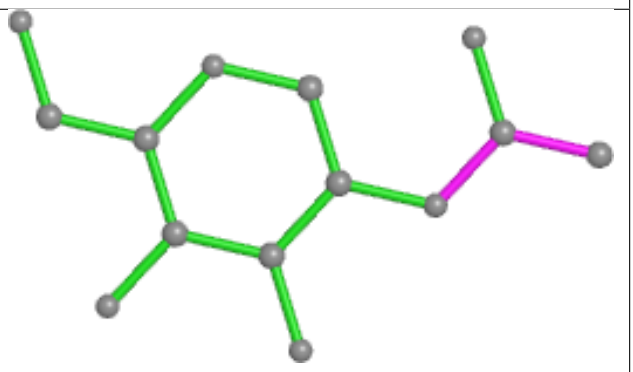
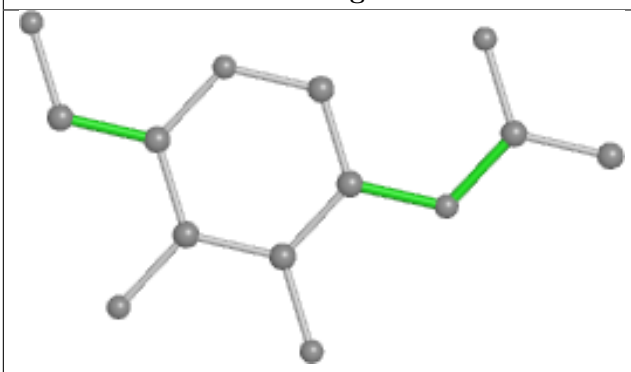
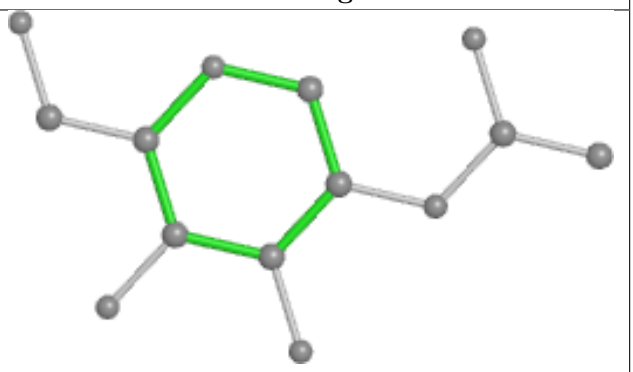


Bond angles

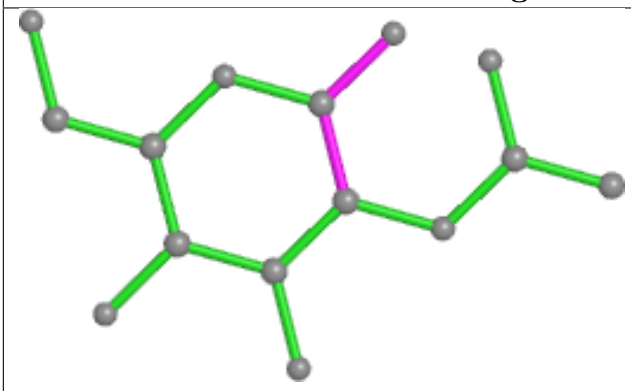


Torsions



Rings

Ligand NAG A 1202



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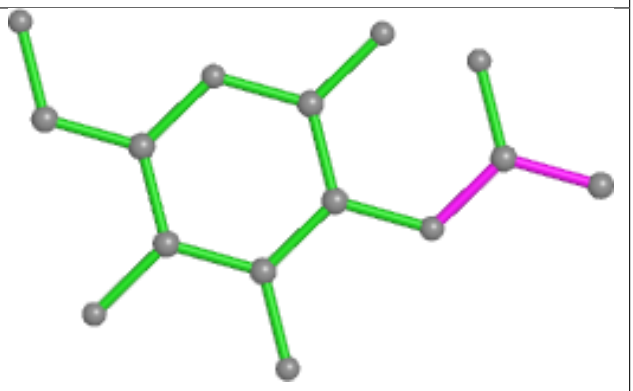
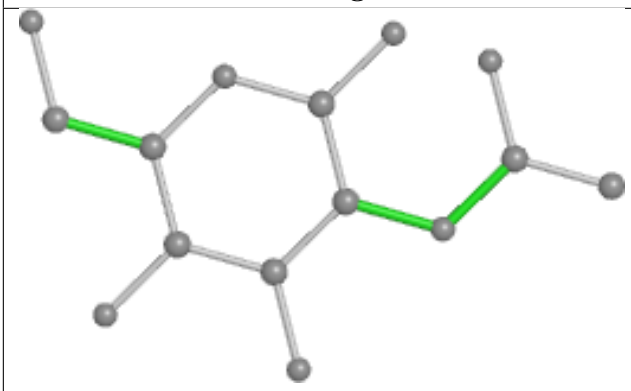
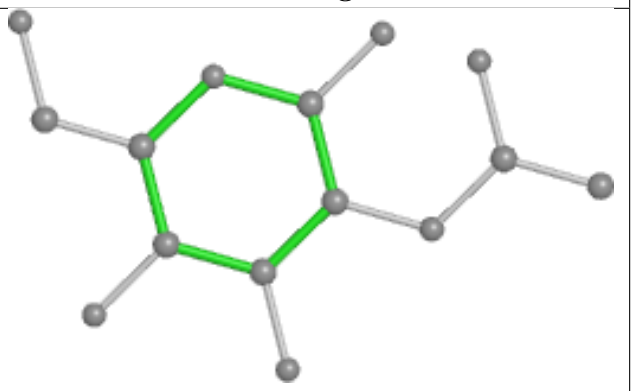


Bond angles

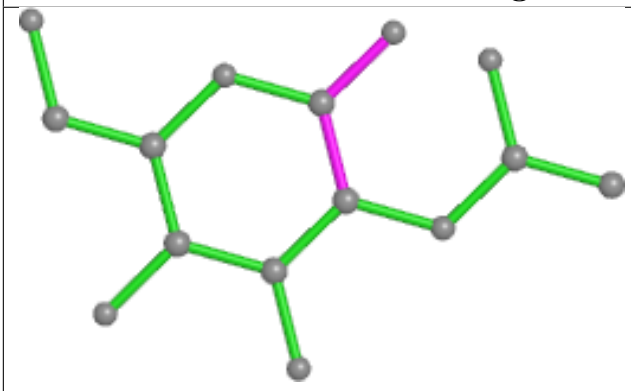


Torsions



Rings

Ligand NAG A 1211



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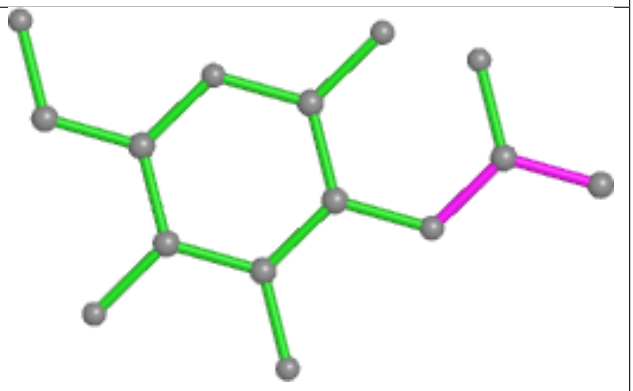
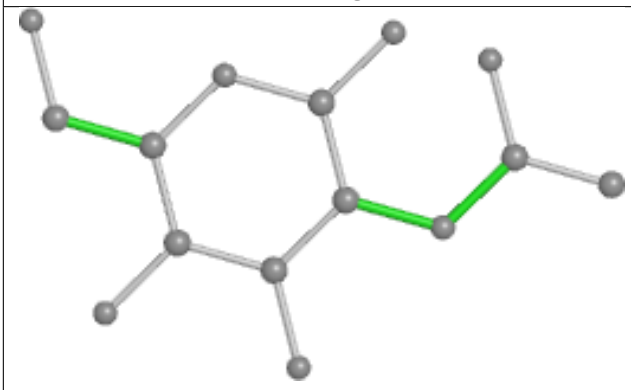


Bond angles



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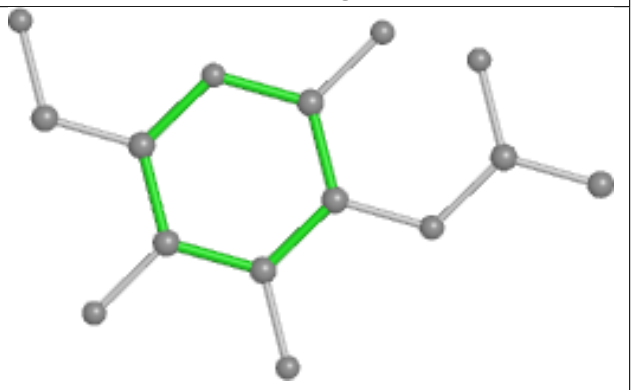
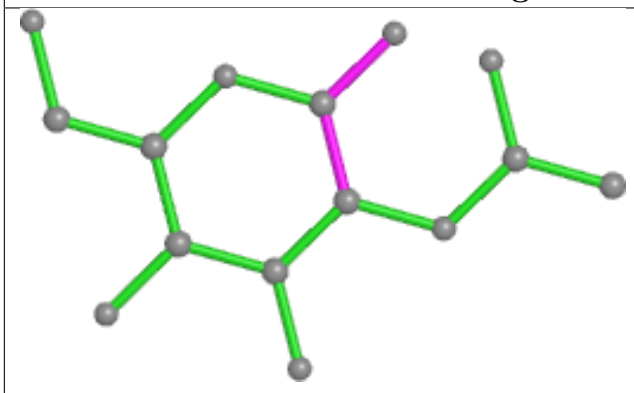


Rings

Ligand NAG A 1217



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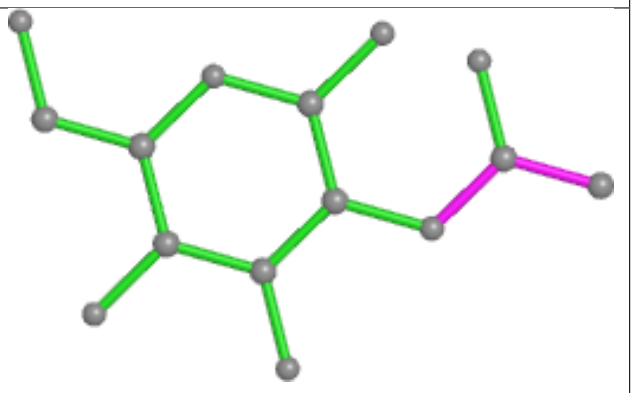
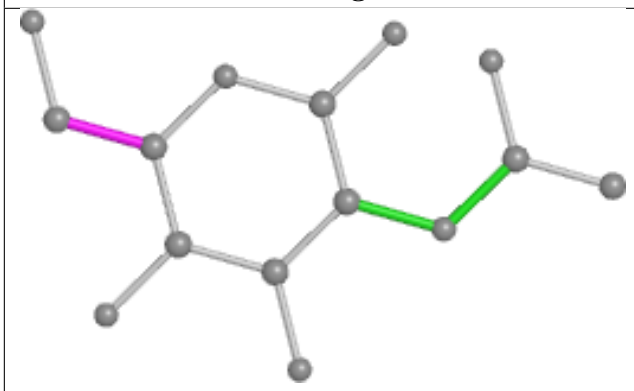
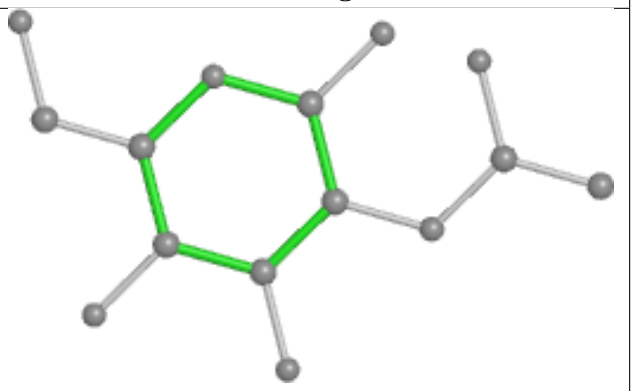


Bond angles

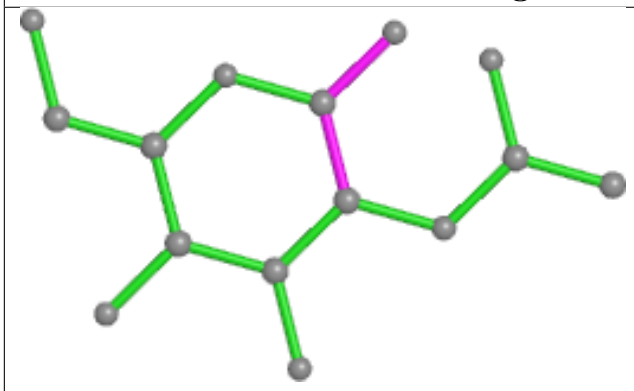


Torsions



Rings

Ligand NAG A 1213



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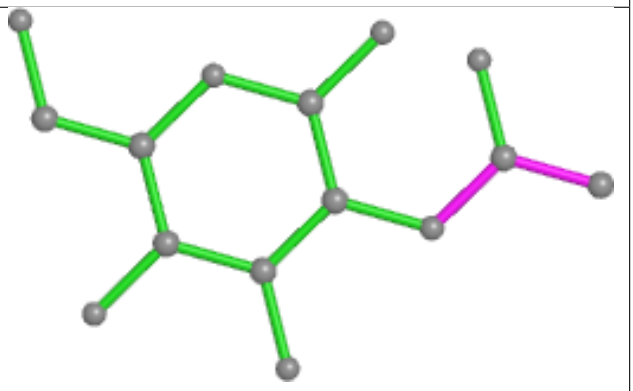
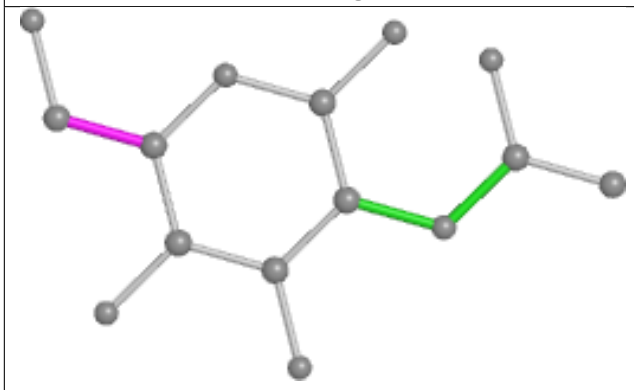


Bond angles



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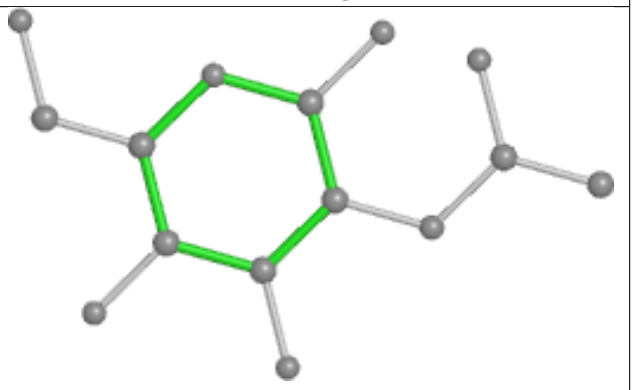
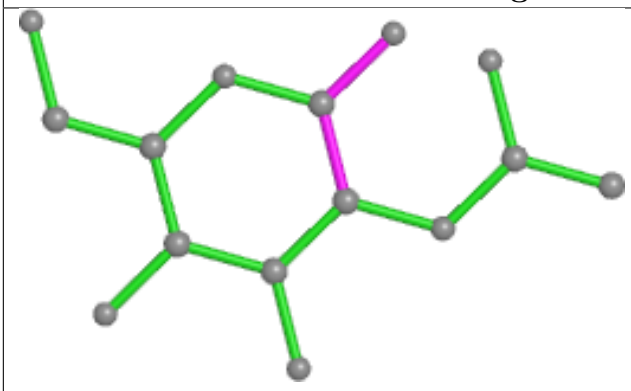


Rings

Ligand NAG A 1205



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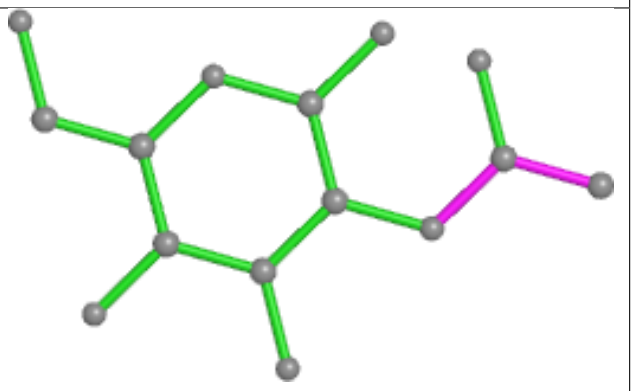
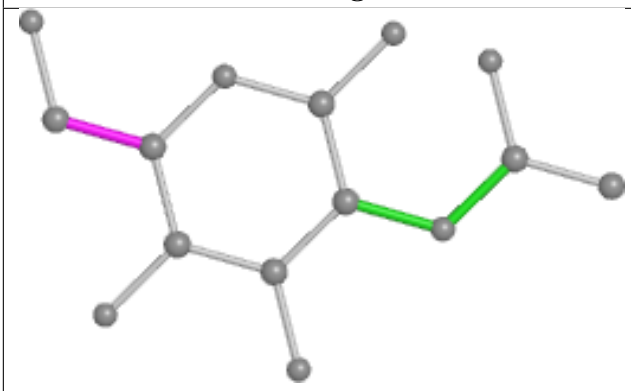
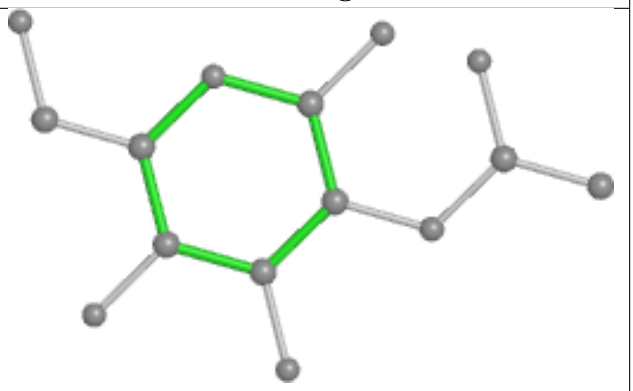


Bond angles

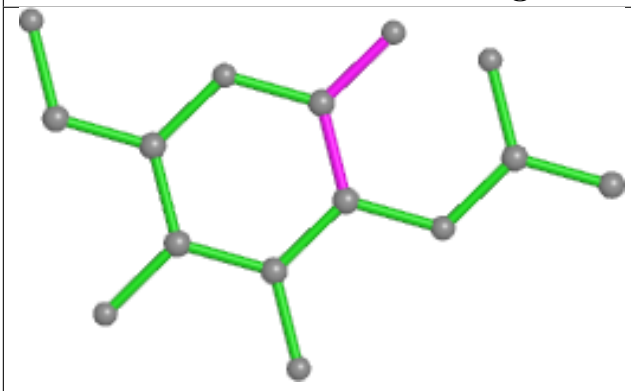


Torsions



Rings

Ligand NAG C 1209



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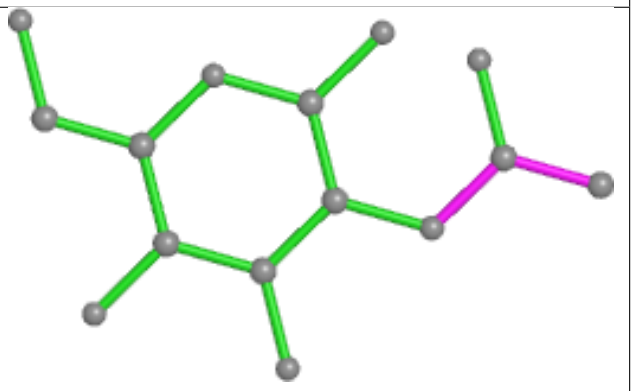
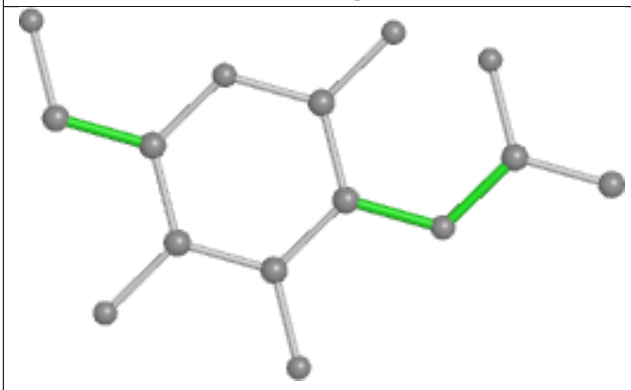
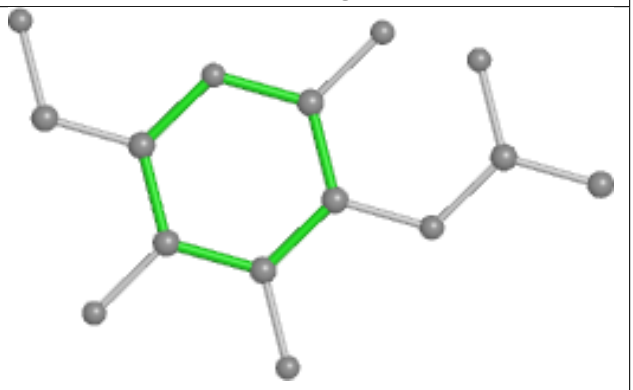


Bond angles

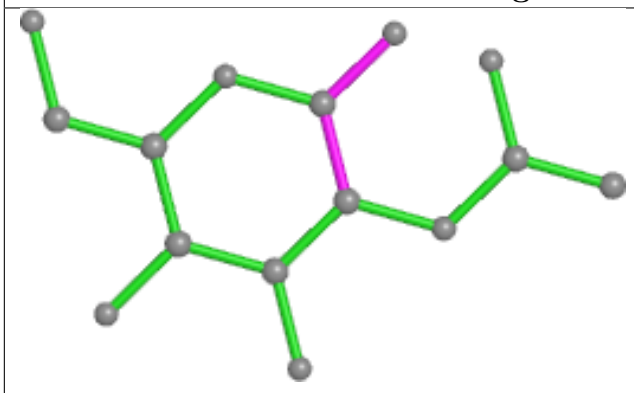


Torsions



Rings

Ligand NAG C 1201



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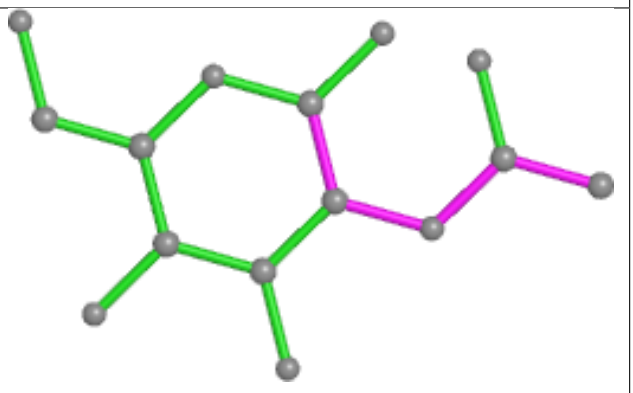
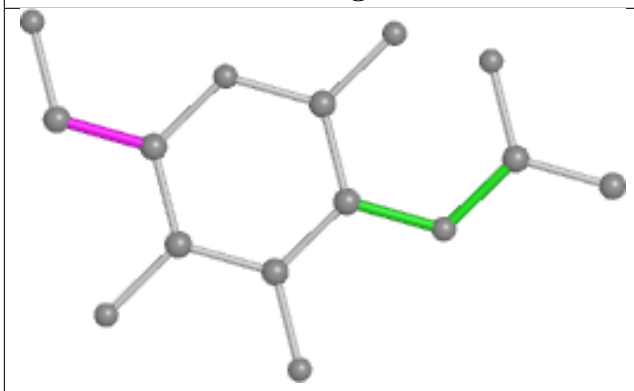
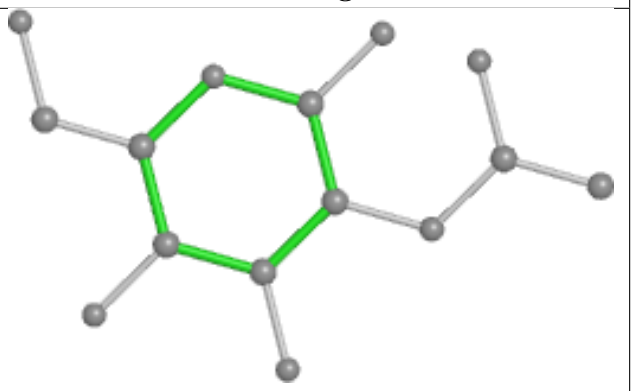


Bond angles

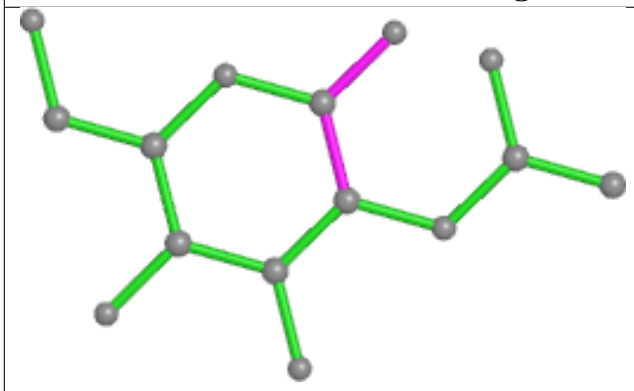


Torsions

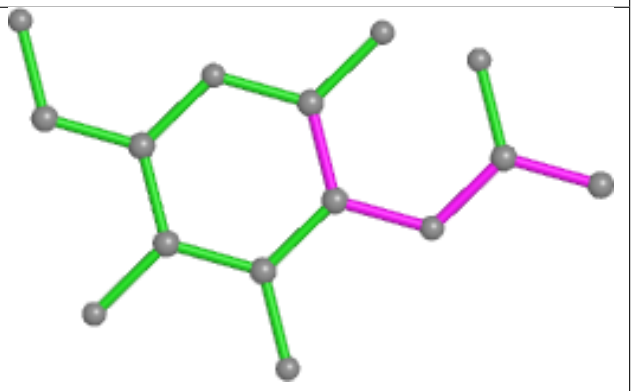


Rings

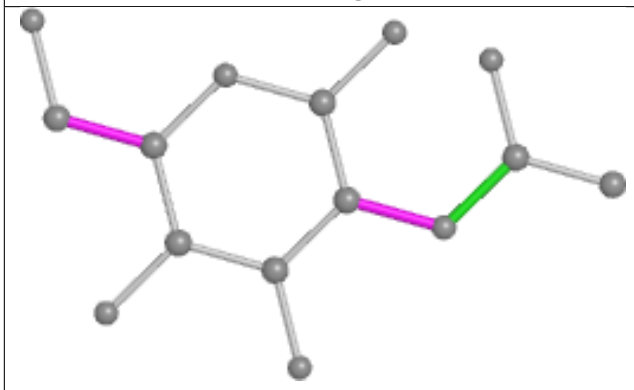
Ligand NAG B 1215



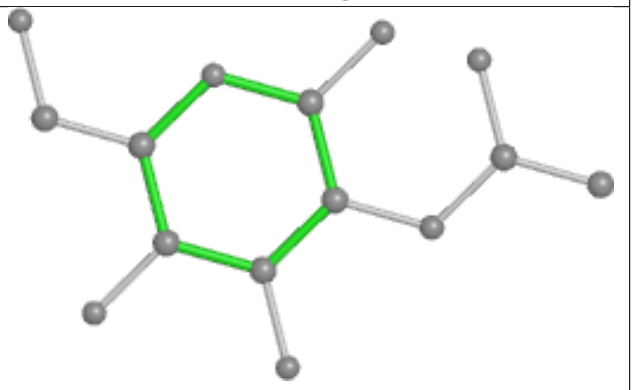
Bond lengths



Bond angles

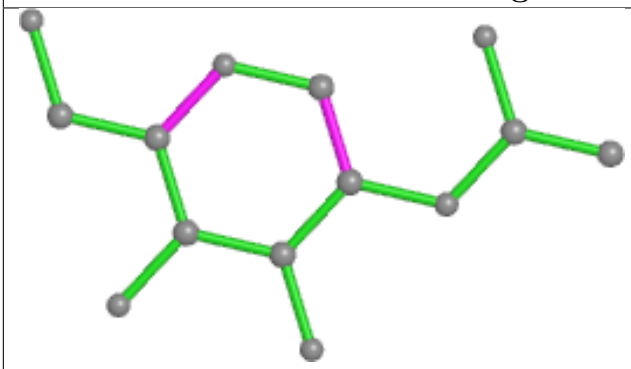


Torsions

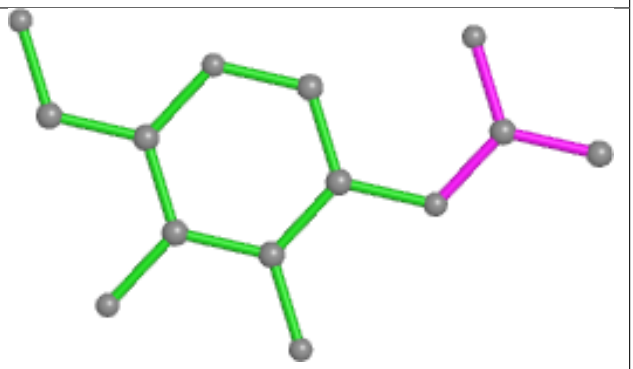


Rings

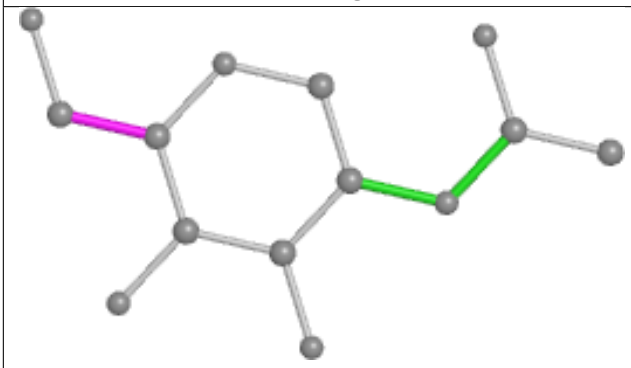
Ligand NAG C 1204



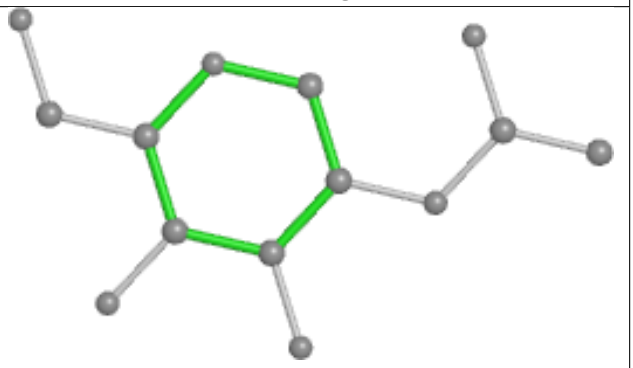
Bond lengths



Bond angles

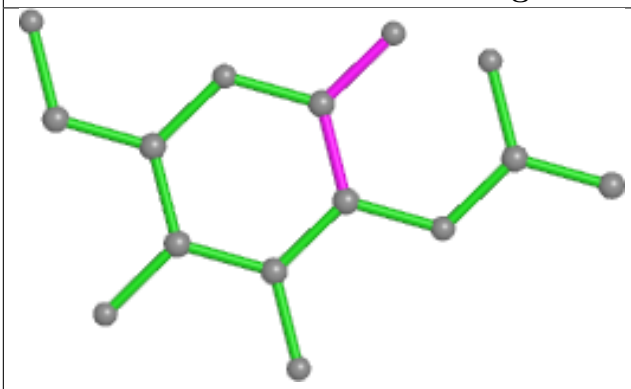


Torsions

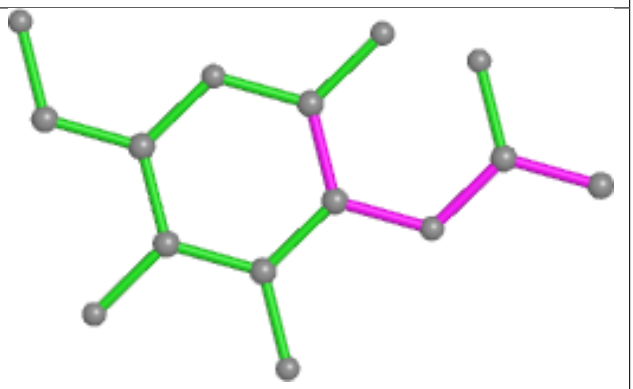


Rings

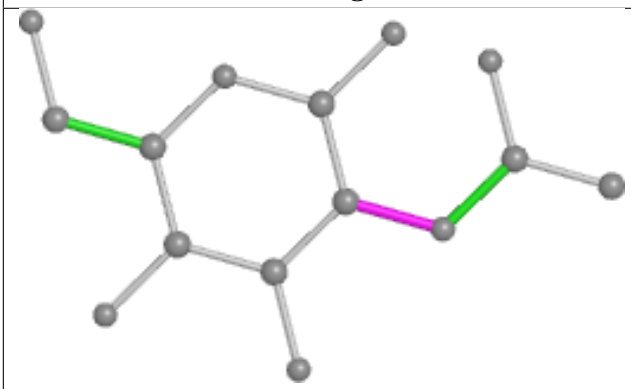
Ligand NAG B 1206



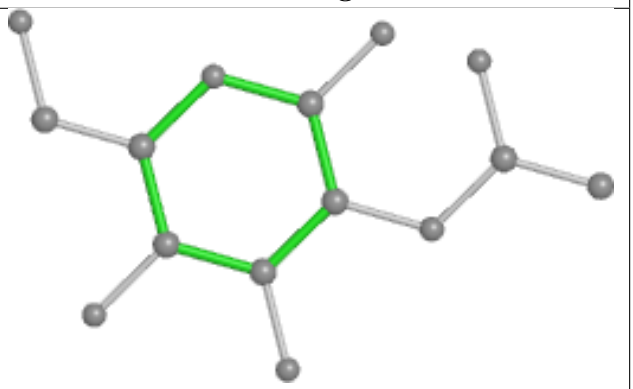
Bond lengths



Bond angles

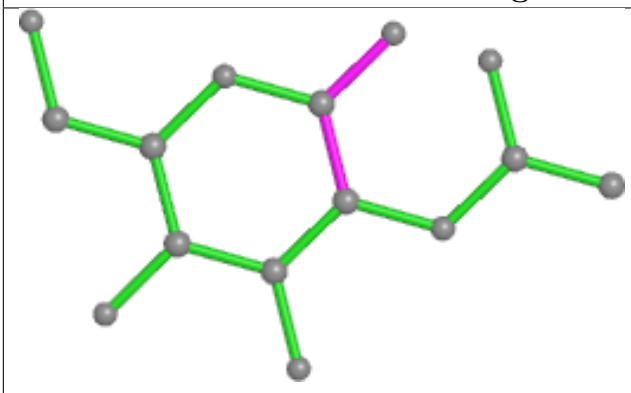


Torsions

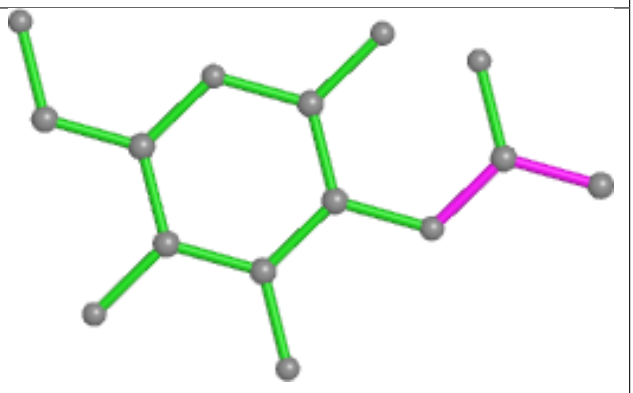


Rings

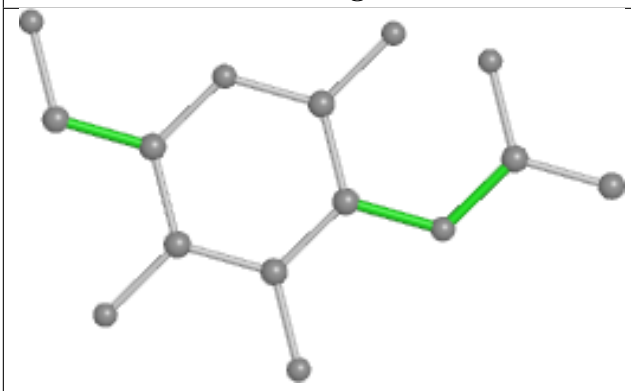
Ligand NAG C 1208



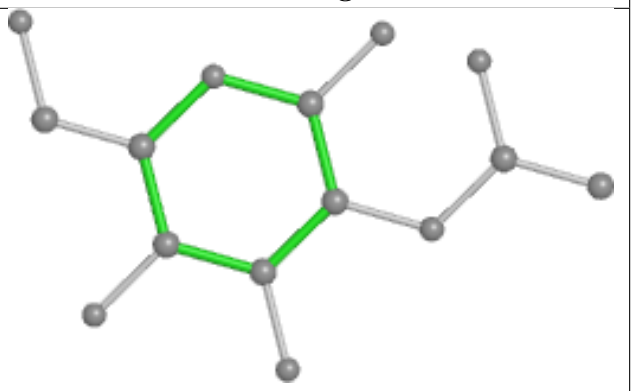
Bond lengths



Bond angles

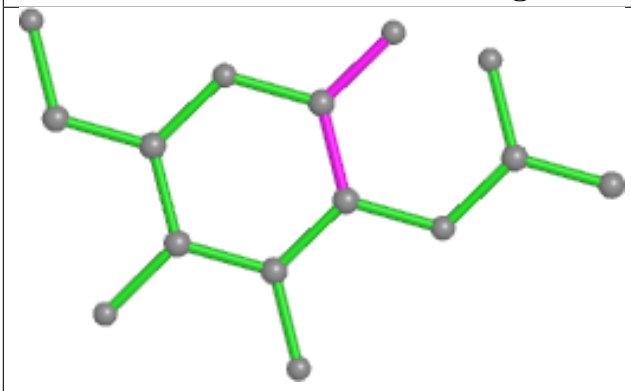


Torsions

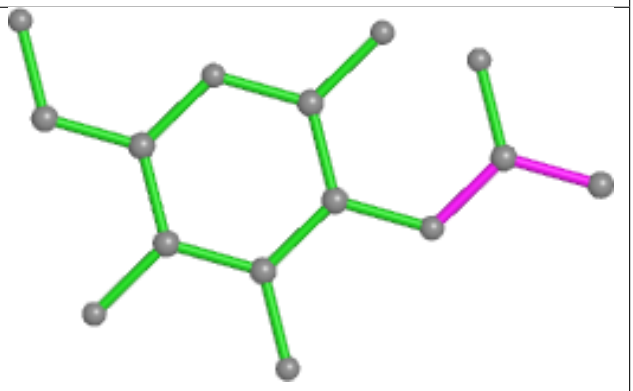


Rings

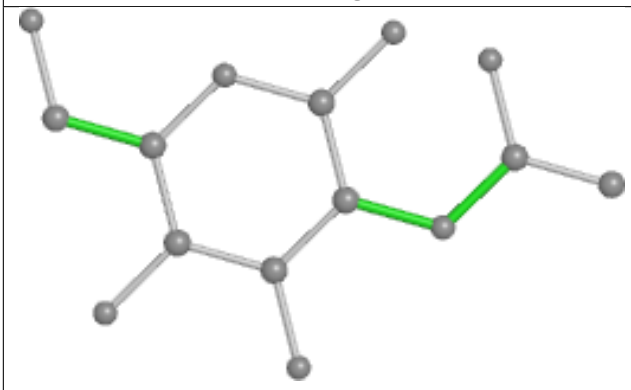
Ligand NAG C 1215



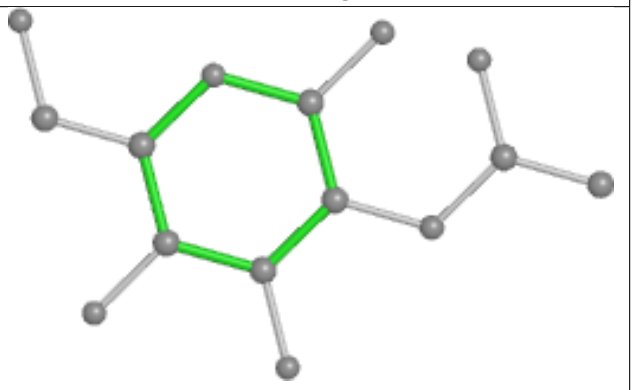
Bond lengths



Bond angles

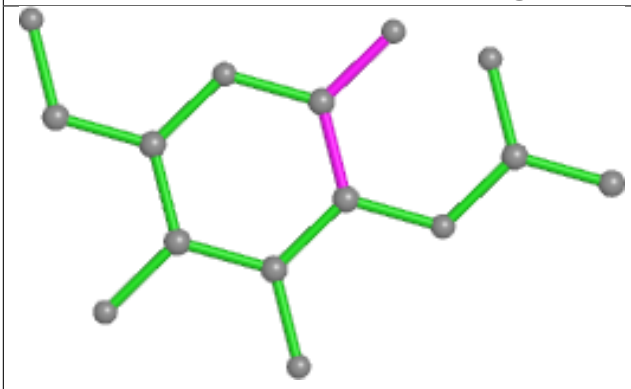


Torsions

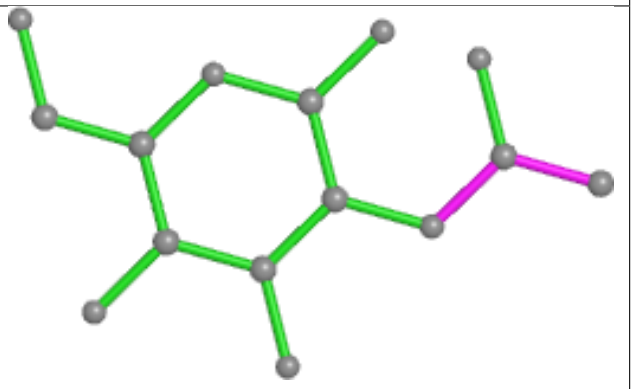


Rings

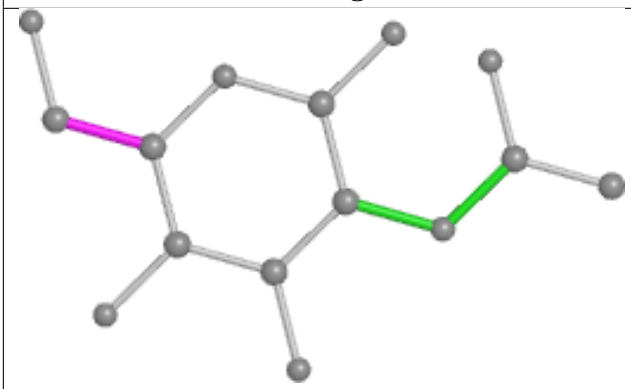
Ligand NAG A 1207



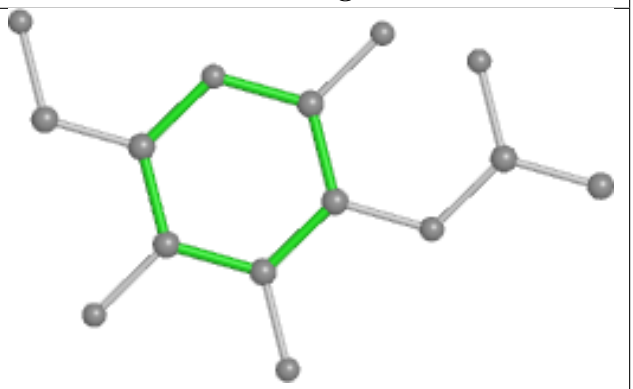
Bond lengths



Bond angles

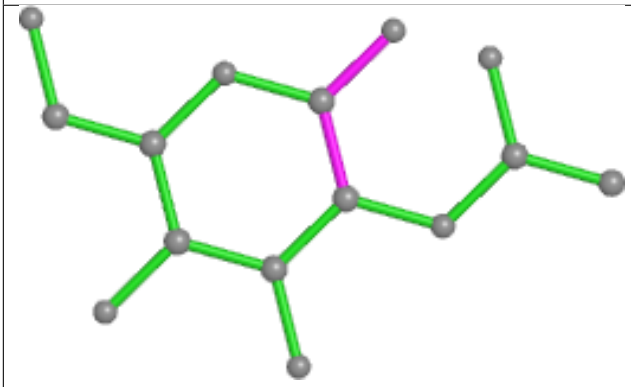


Torsions



Rings

Ligand NAG A 1216



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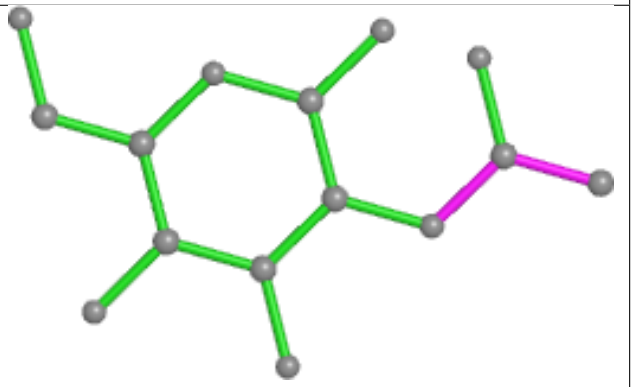
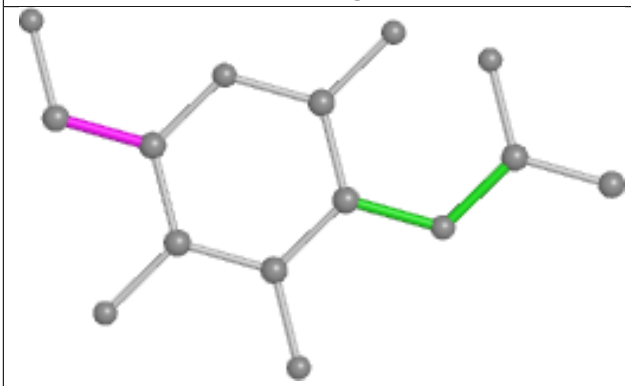
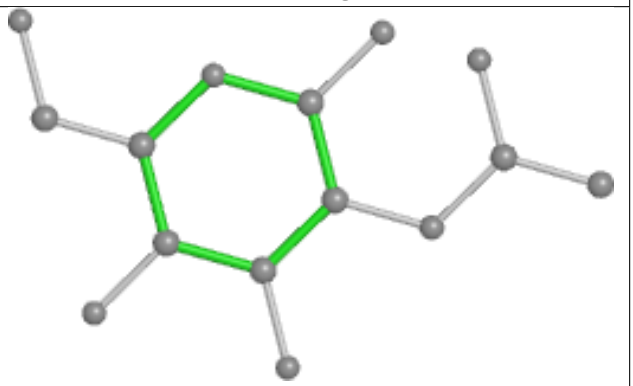


Bond angles

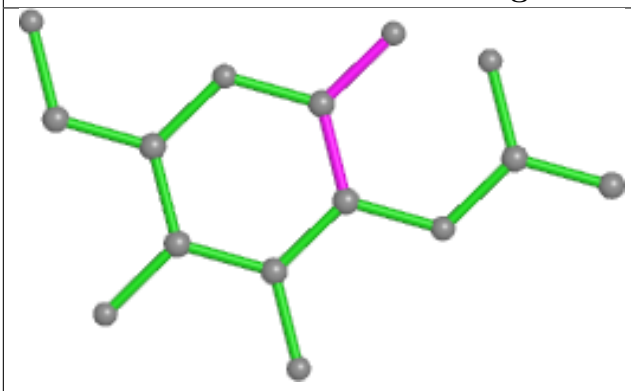


Torsions



Rings

Ligand NAG A 1203



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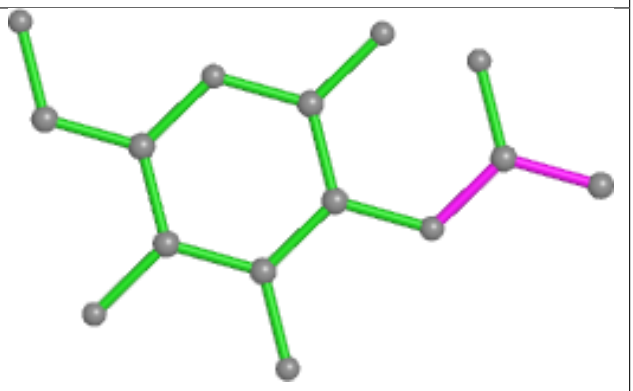
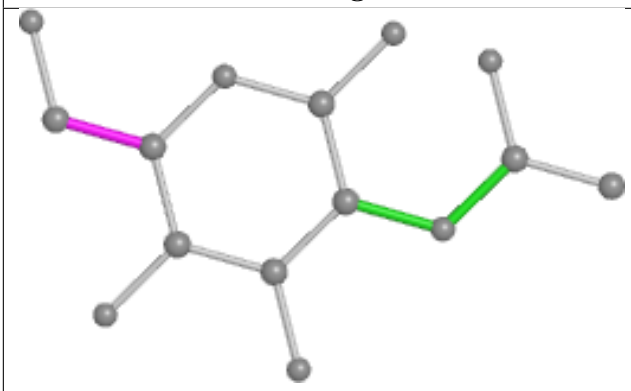
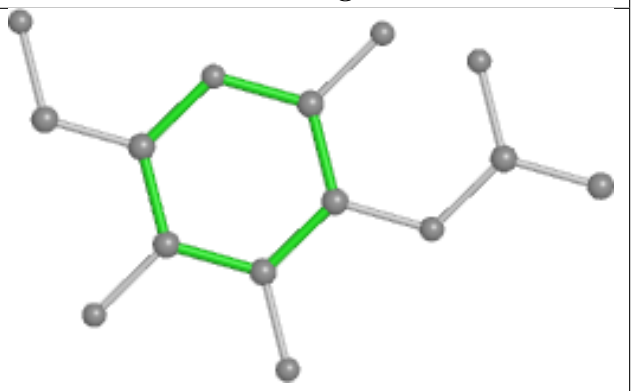


Bond angles

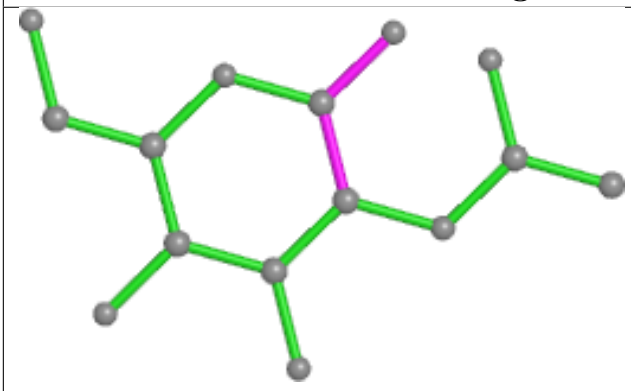


Torsions



Rings

Ligand NAG B 1212



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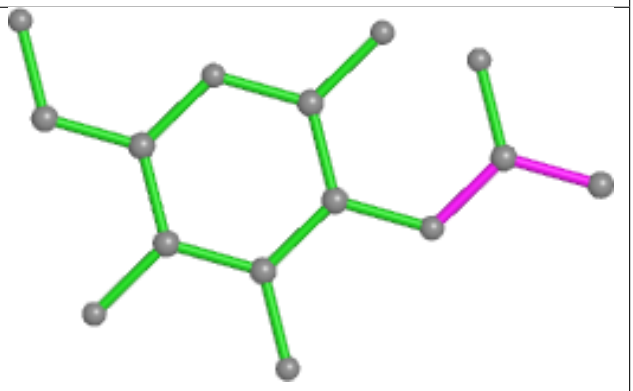
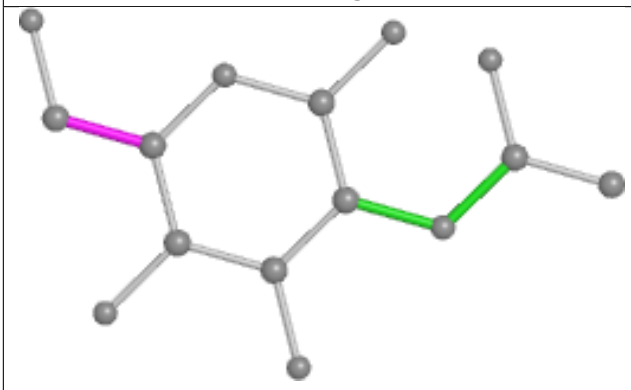
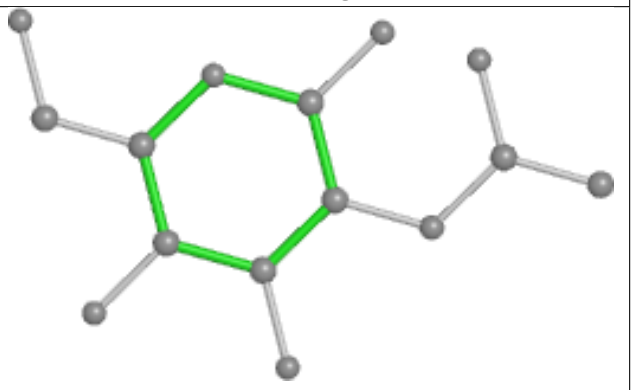


Bond angles

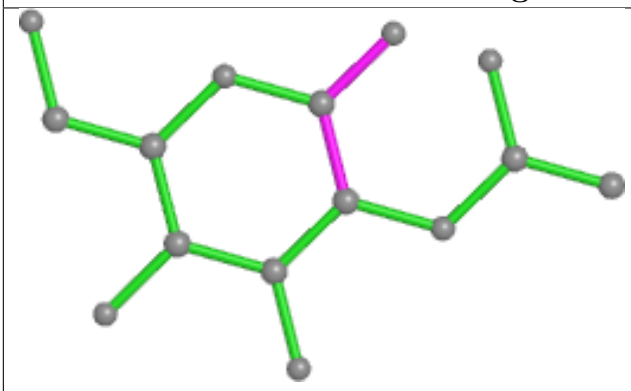


Torsions



Rings

Ligand NAG C 1206



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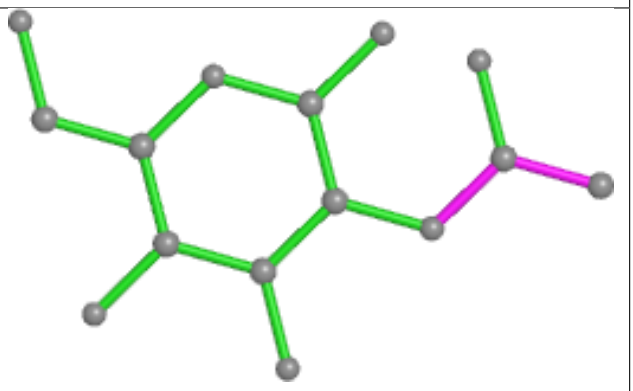
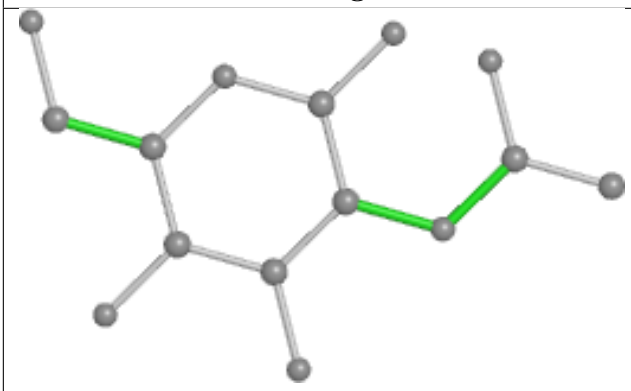
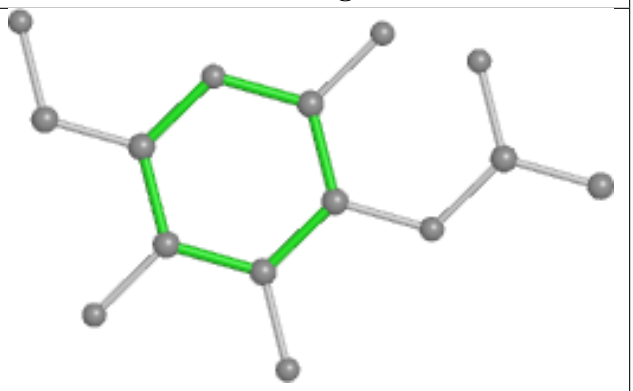


Bond angles

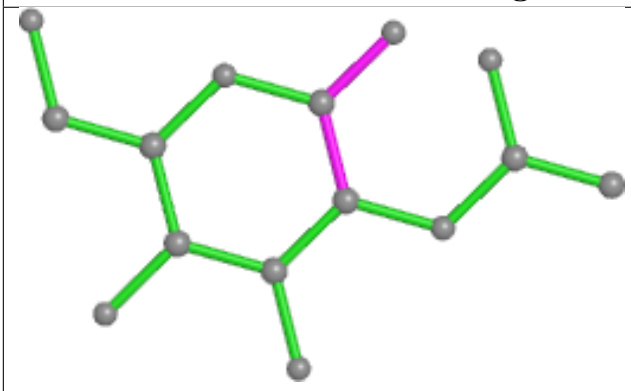


Torsions



Rings

Ligand NAG B 1205



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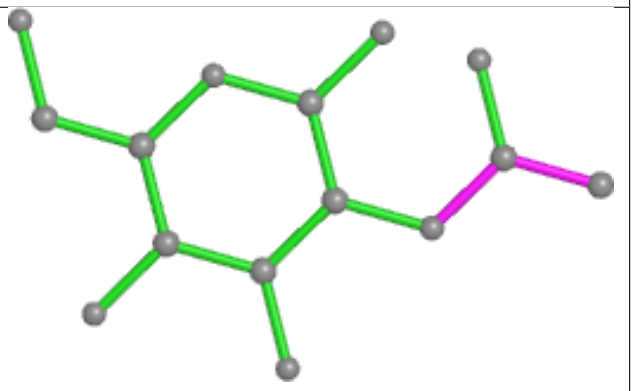
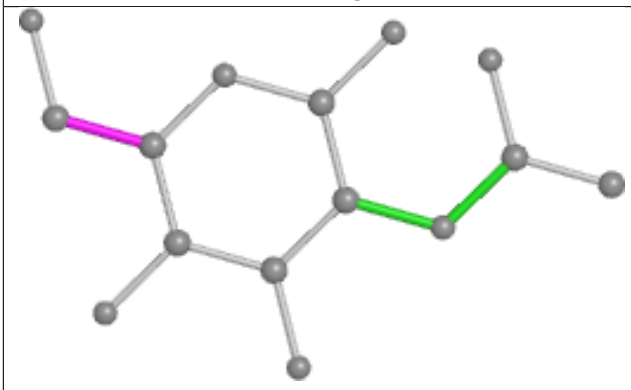
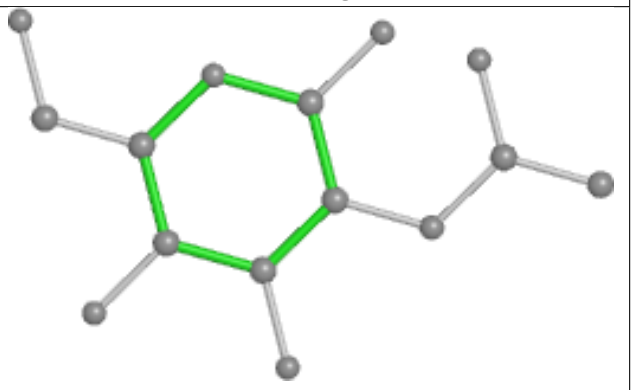


Bond angles

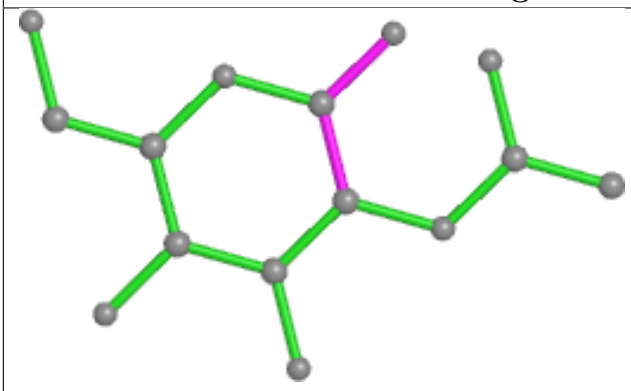


Torsions



Rings

Ligand NAG B 1207



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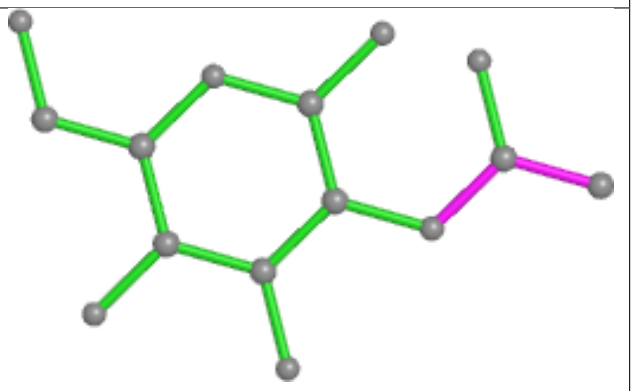
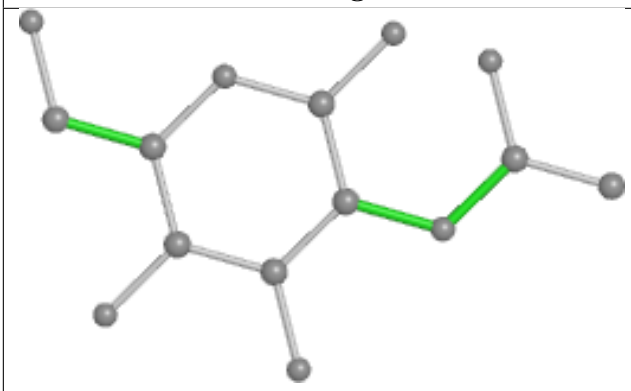
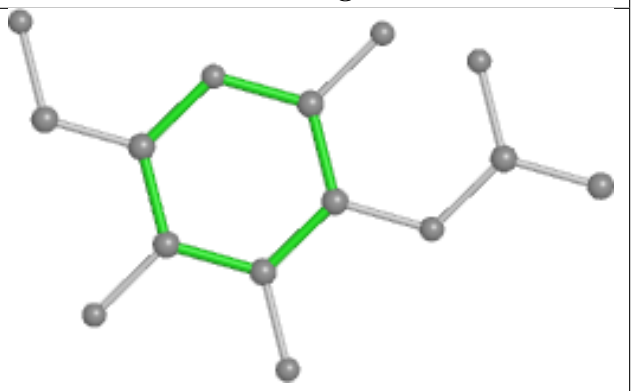


Bond angles

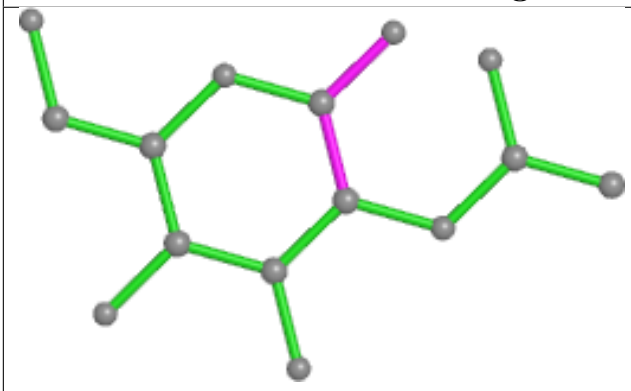


Torsions

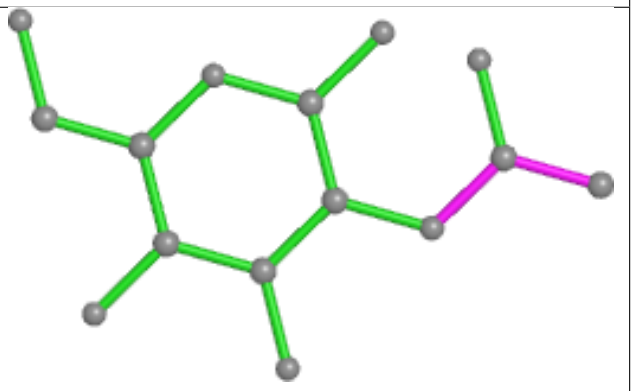


Rings

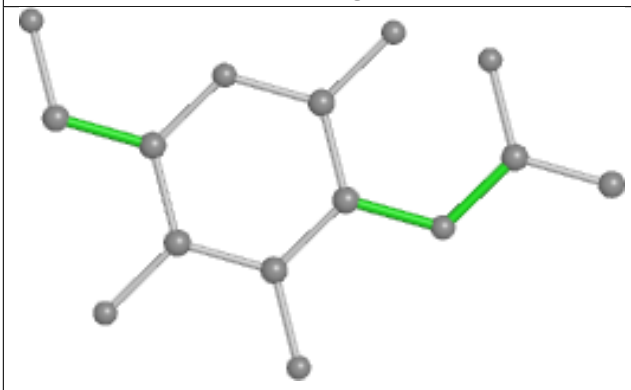
Ligand NAG C 1202



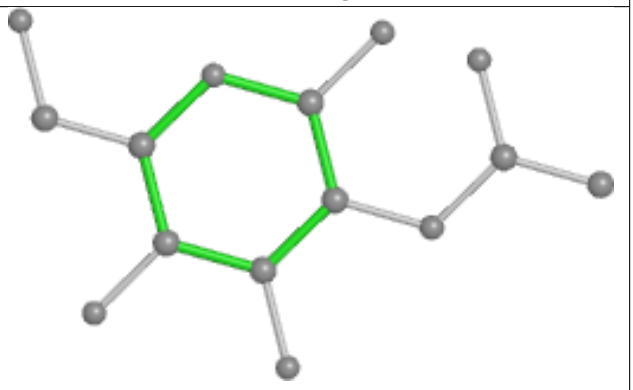
Bond lengths



Bond angles

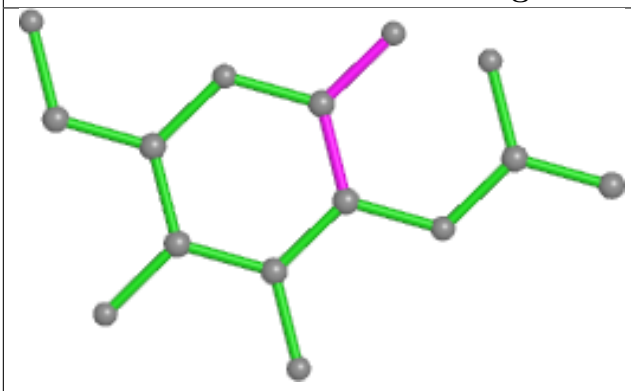


Torsions



Rings

Ligand NAG B 1201



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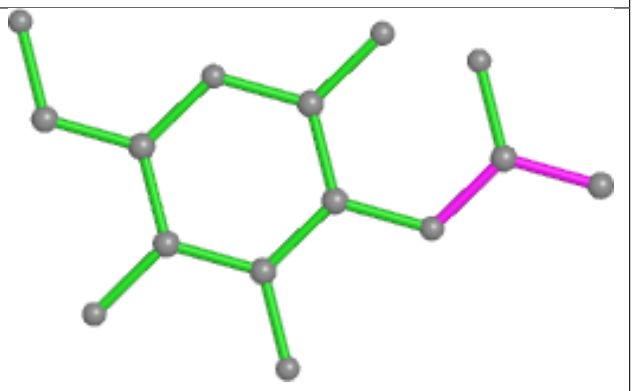
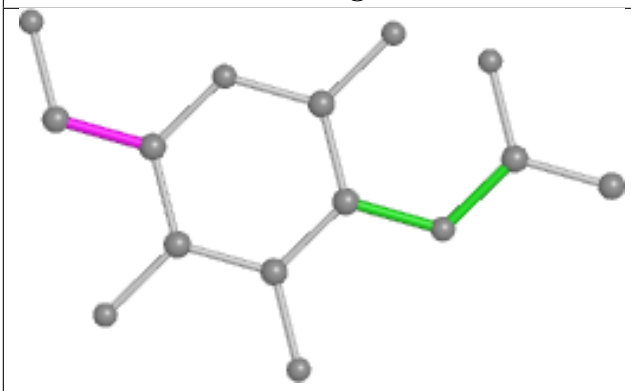


Bond angles



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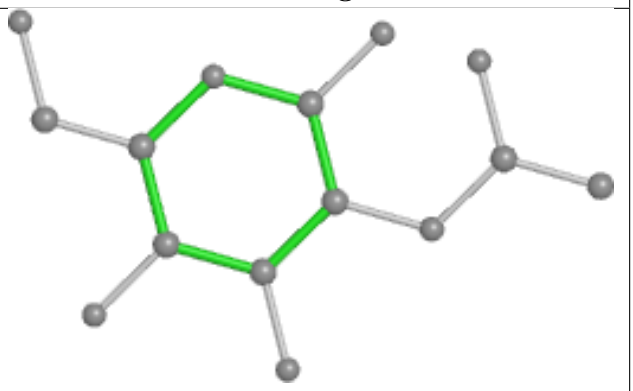
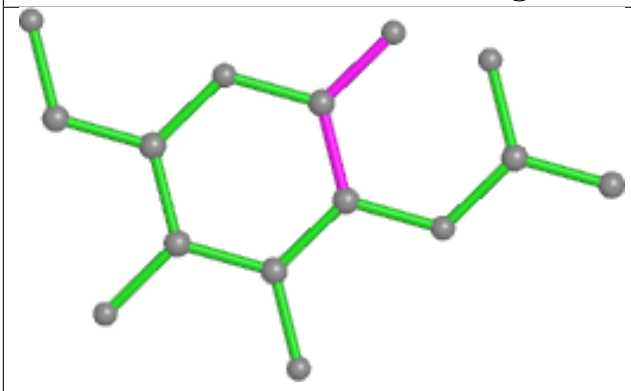


Rings

Ligand NAG A 1204



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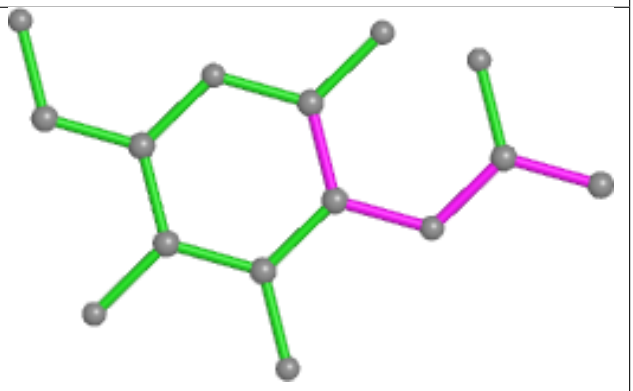
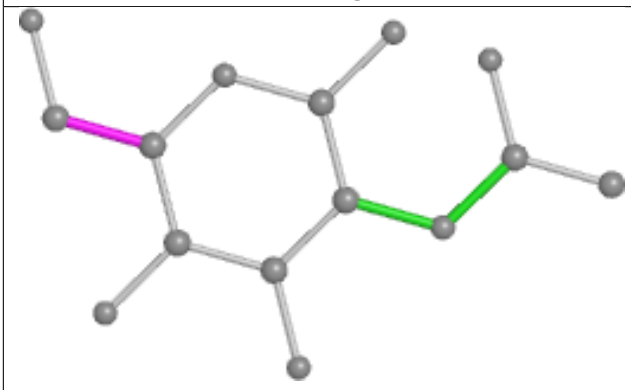


Bond angles



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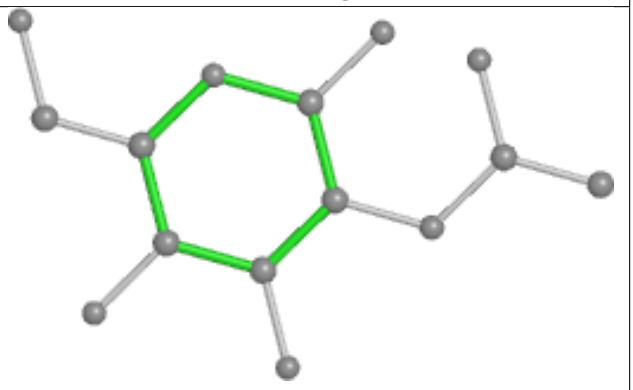
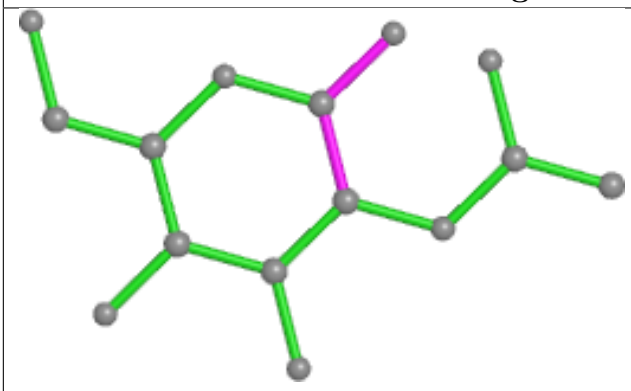


Rings

Ligand NAG C 1214



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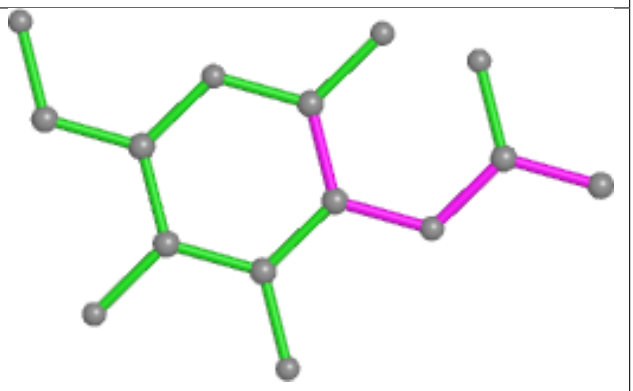
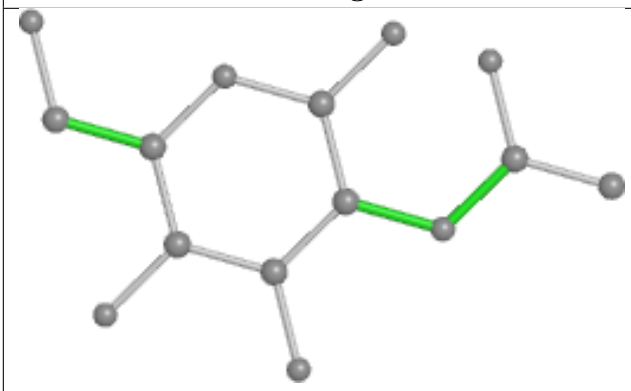
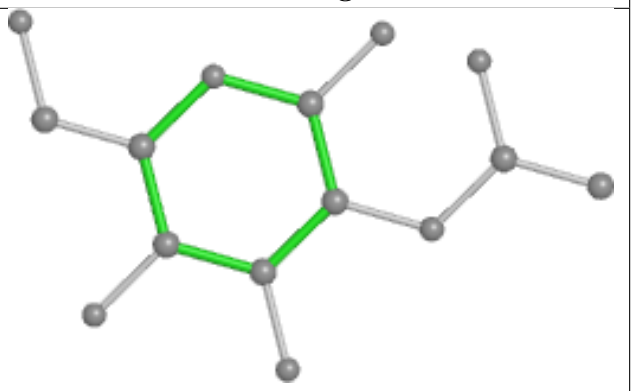


Bond angles

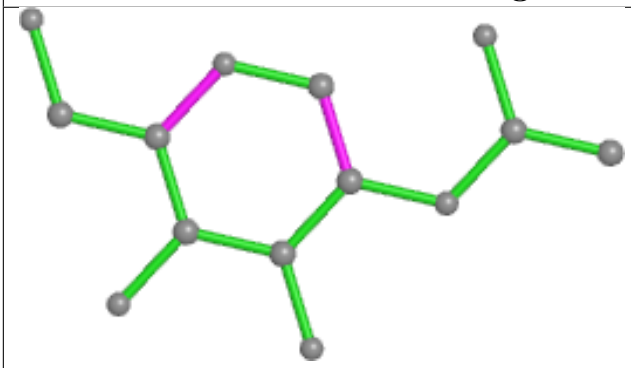


Torsions

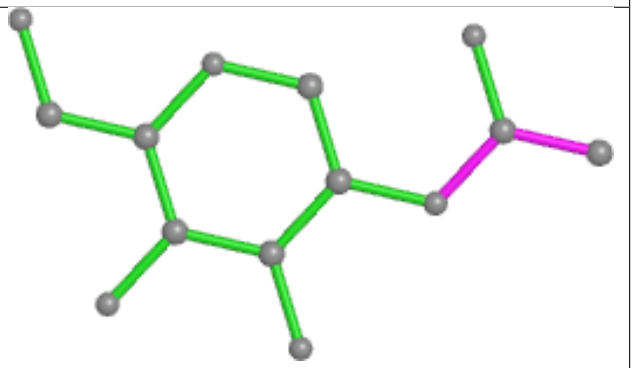


Rings

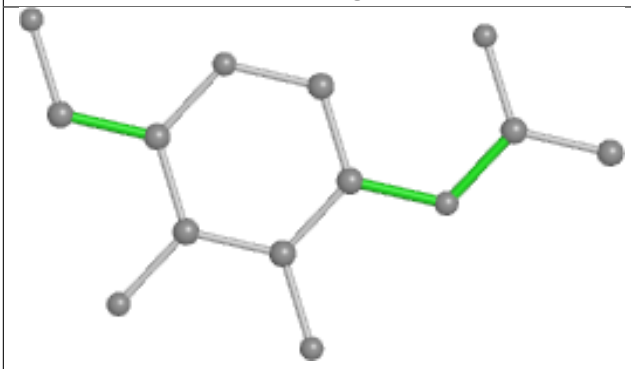
Ligand NAG C 1212



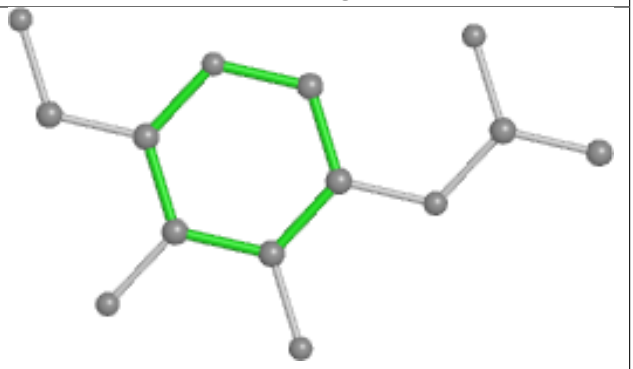
Bond lengths



Bond angles

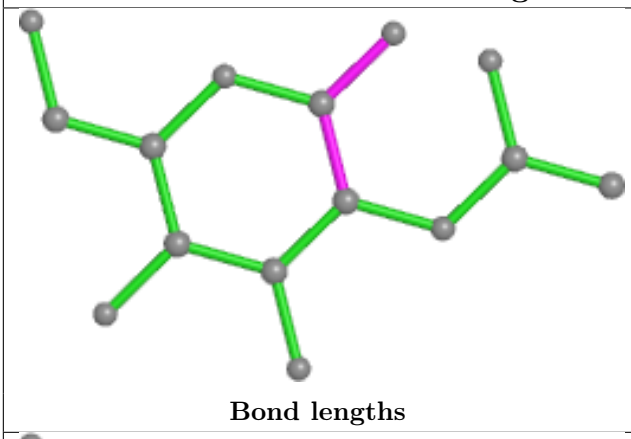


Torsions

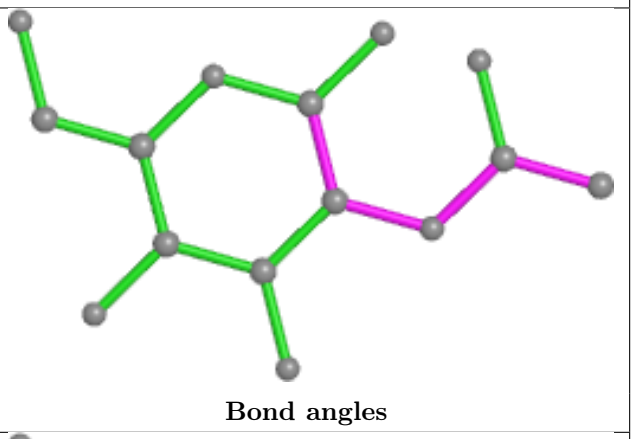


Rings

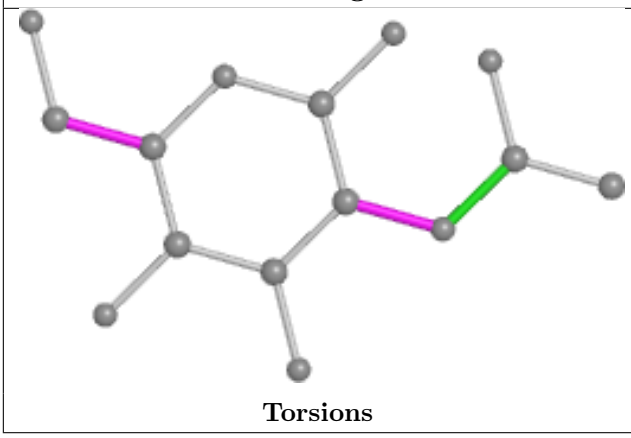
Ligand NAG C 1211



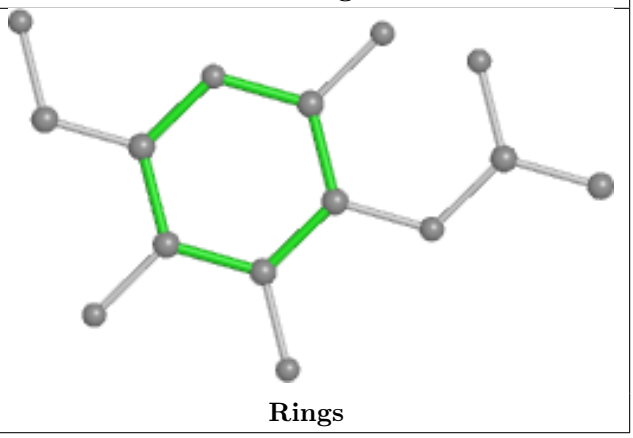
Bond lengths



Bond angles

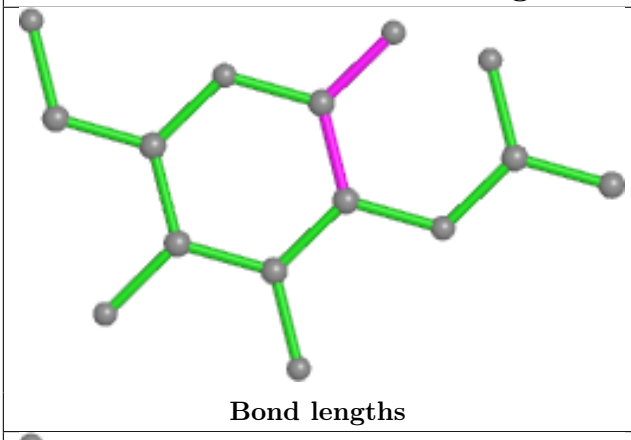


Torsions

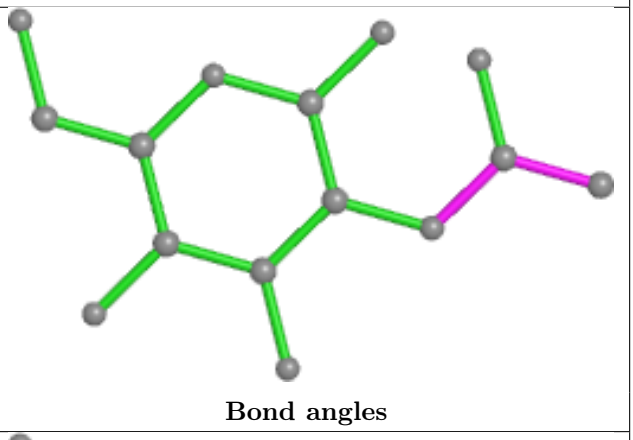


Rings

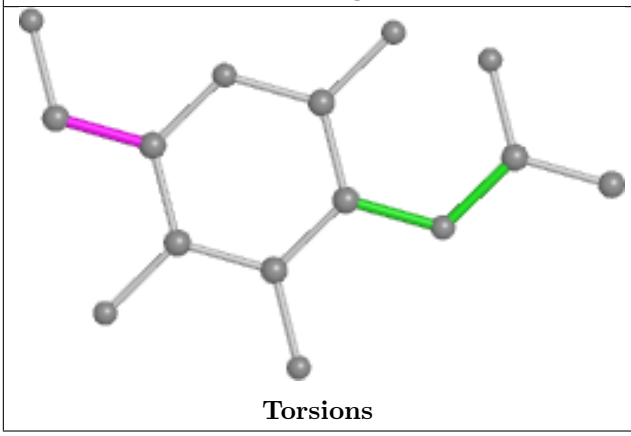
Ligand NAG C 1205



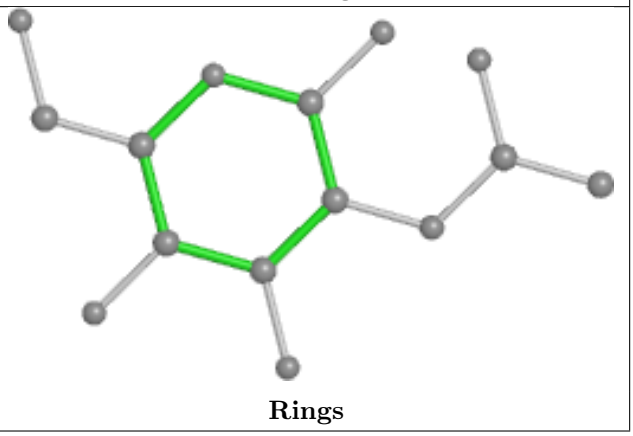
Bond lengths



Bond angles

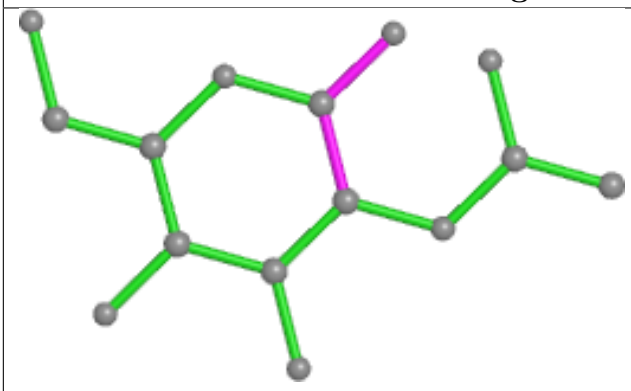


Torsions

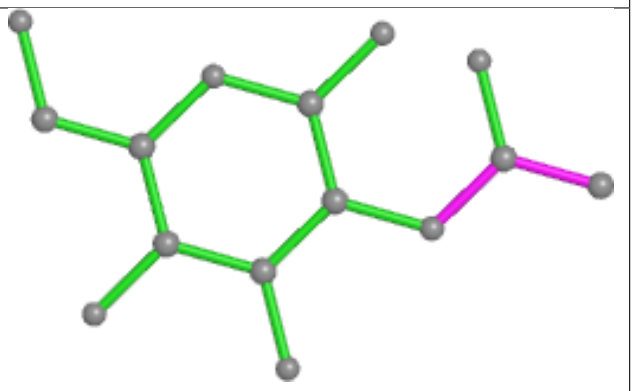


Rings

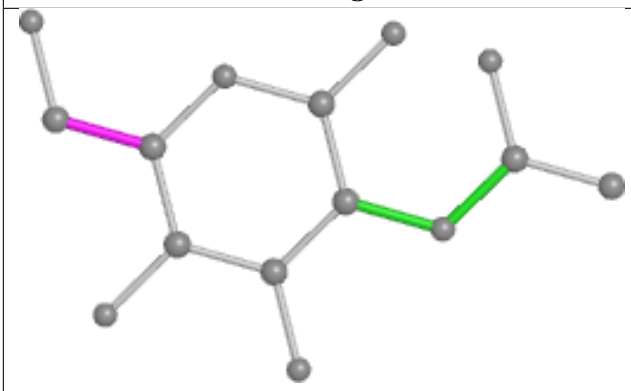
Ligand NAG A 1209



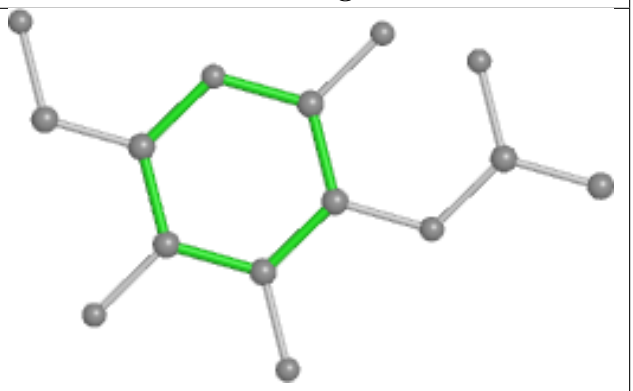
Bond lengths



Bond angles

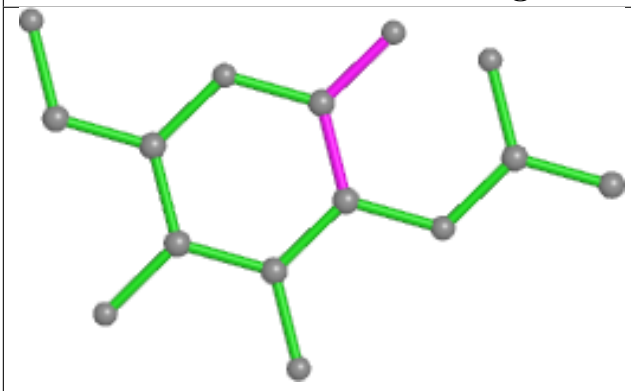


Torsions

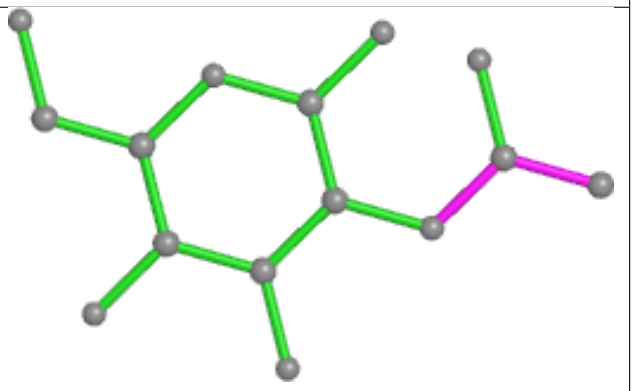


Rings

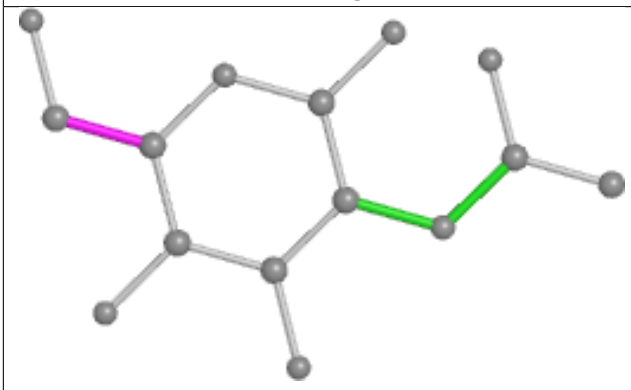
Ligand NAG B 1203



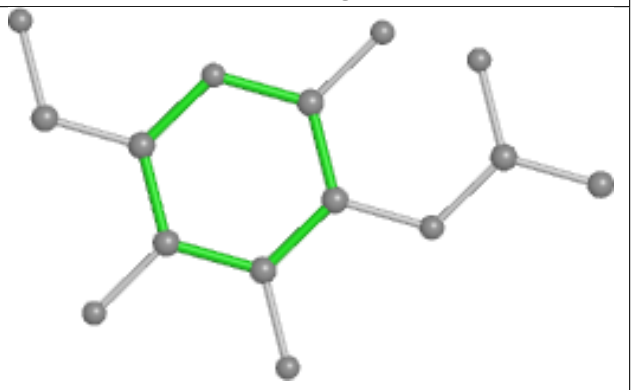
Bond lengths



Bond angles

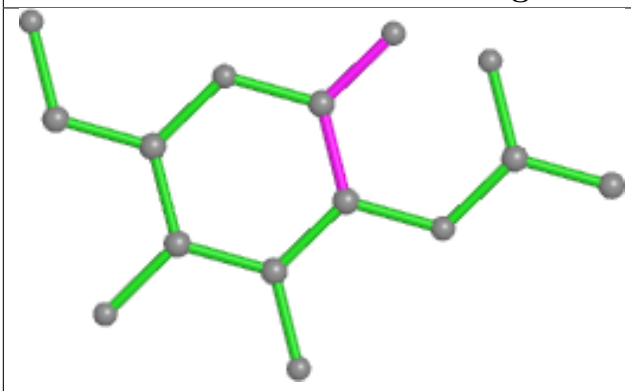


Torsions

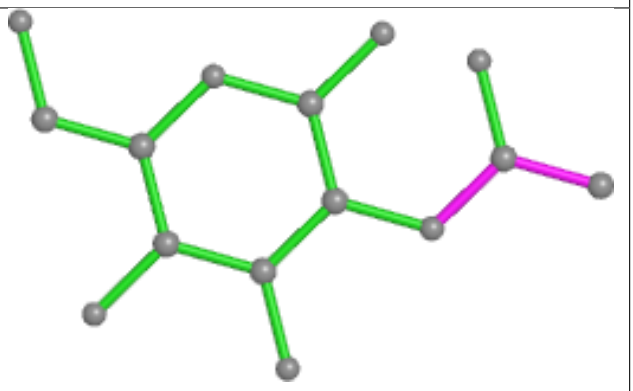


Rings

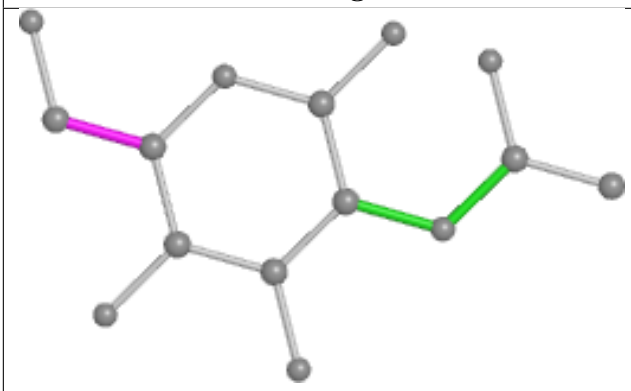
Ligand NAG B 1202



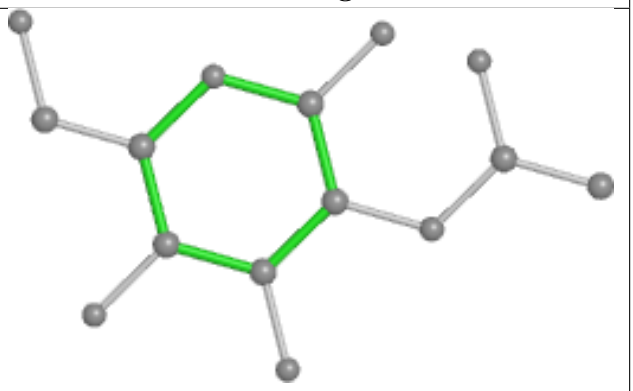
Bond lengths



Bond angles

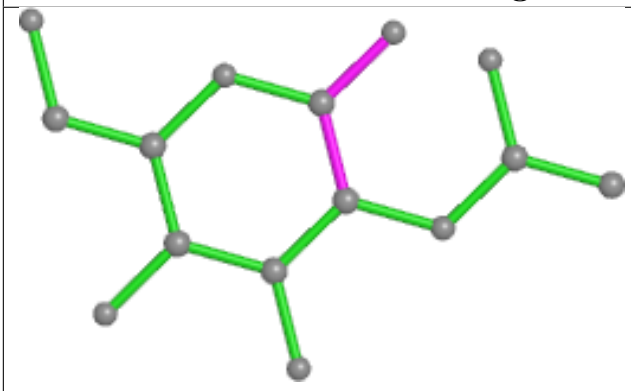


Torsions

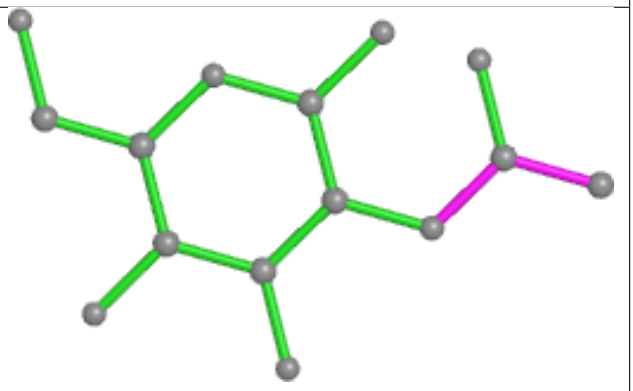


Rings

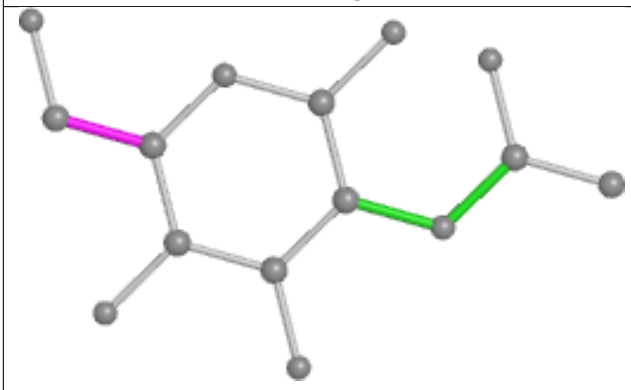
Ligand NAG C 1207



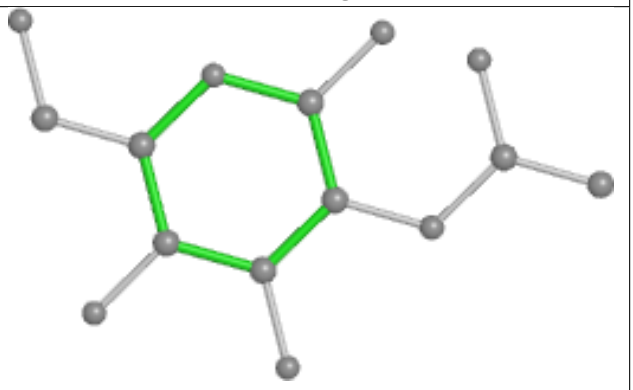
Bond lengths



Bond angles

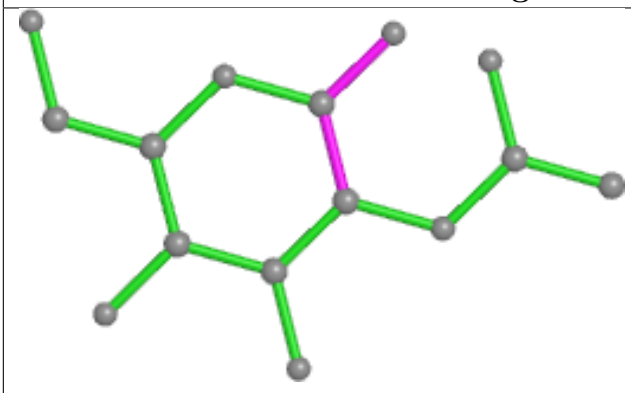


Torsions

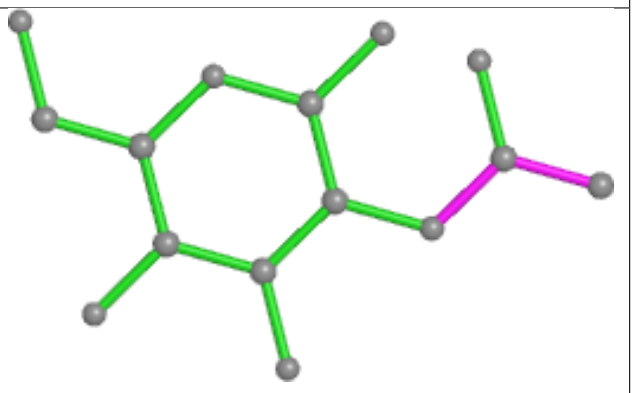


Rings

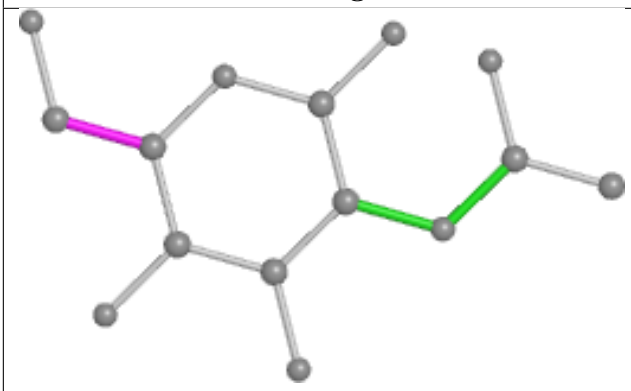
Ligand NAG B 1214



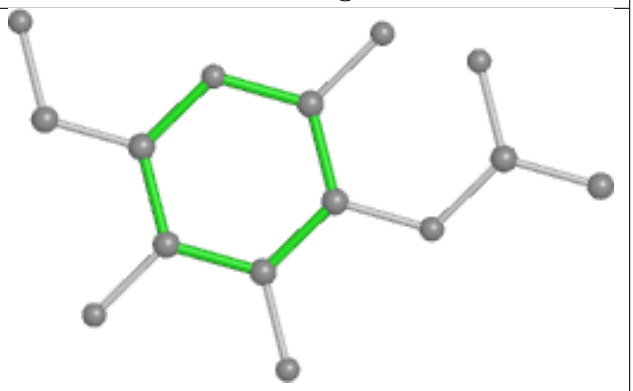
Bond lengths



Bond angles

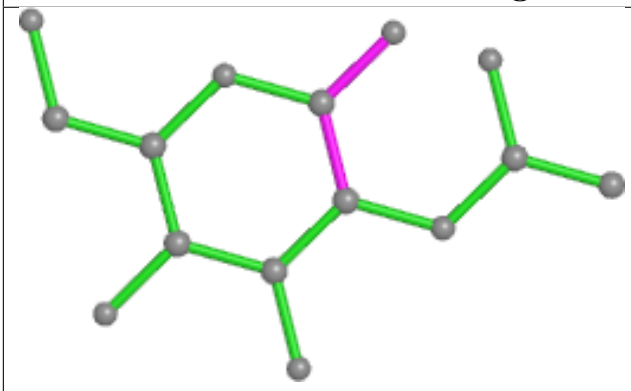


Torsions

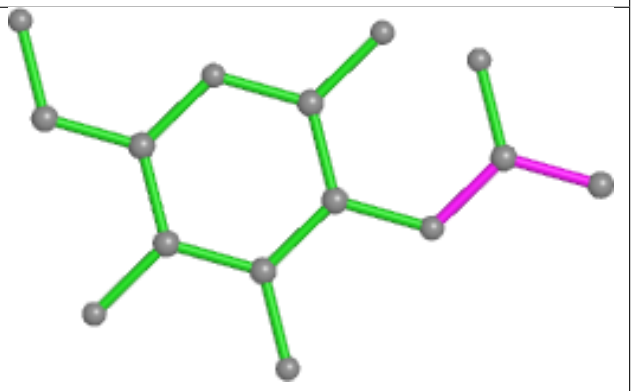


Rings

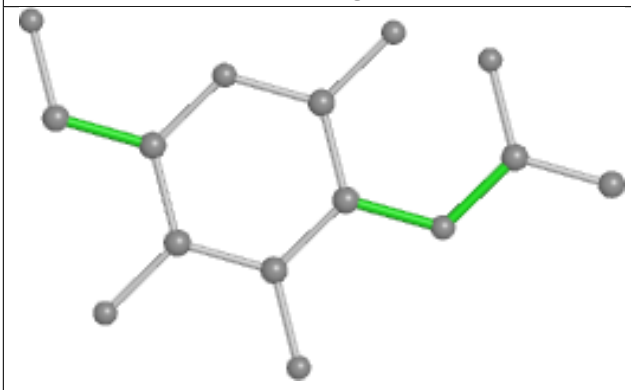
Ligand NAG C 1203



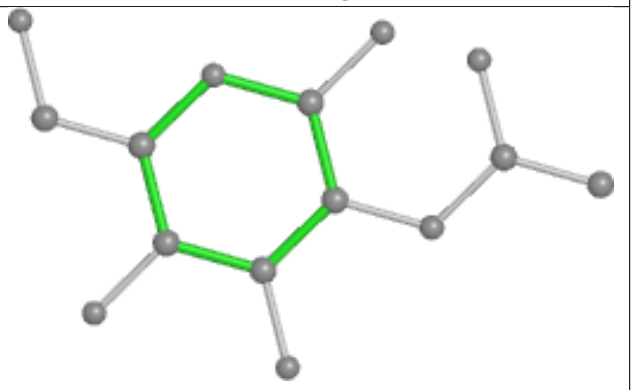
Bond lengths



Bond angles

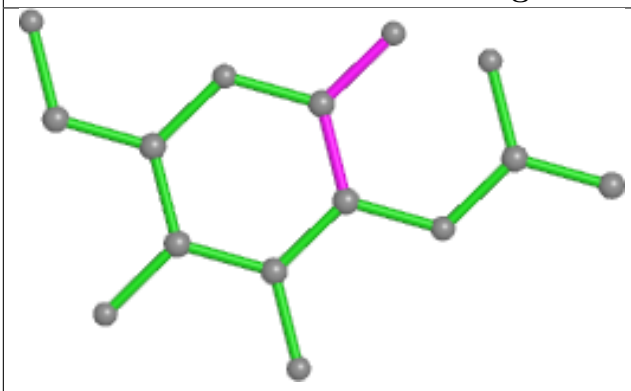


Torsions

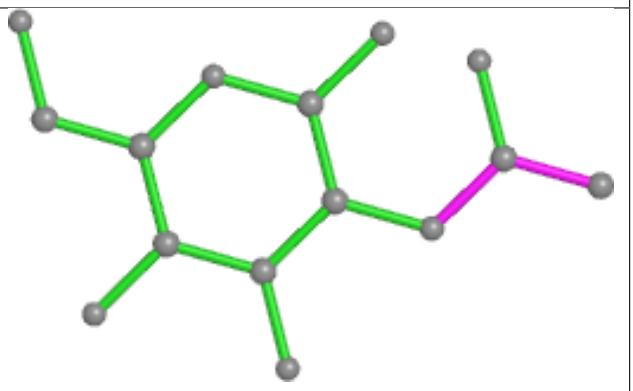


Rings

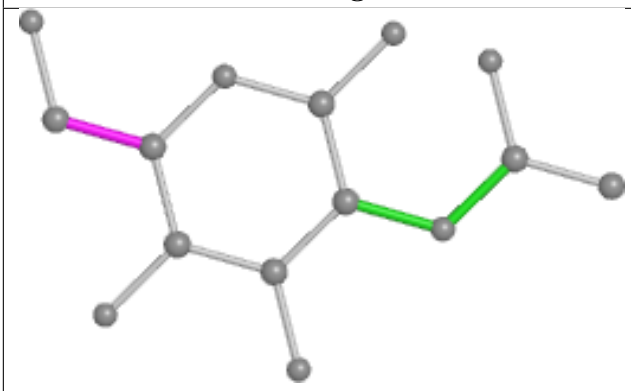
Ligand NAG B 1213



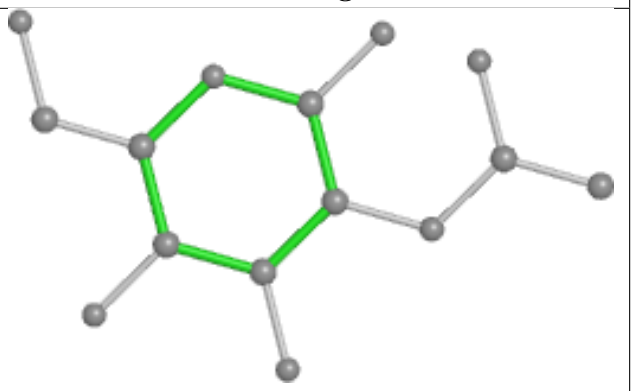
Bond lengths



Bond angles

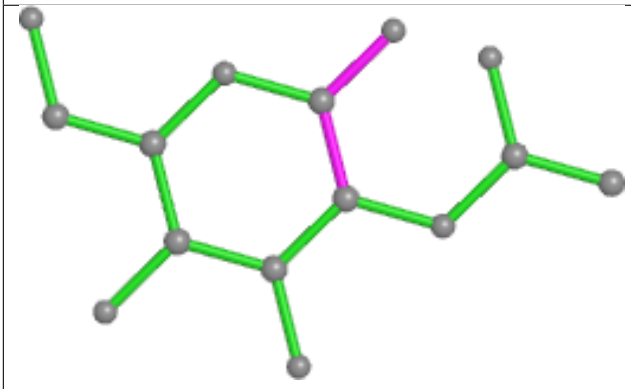


Torsions

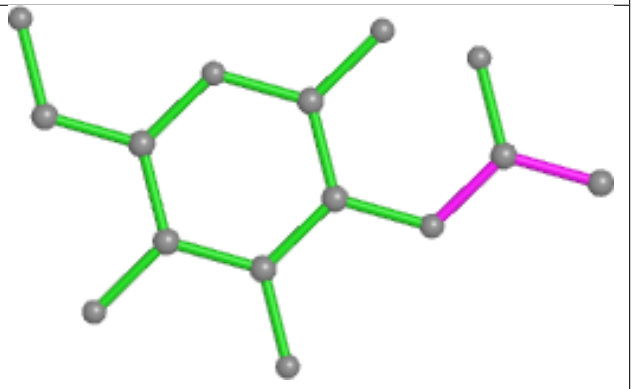


Rings

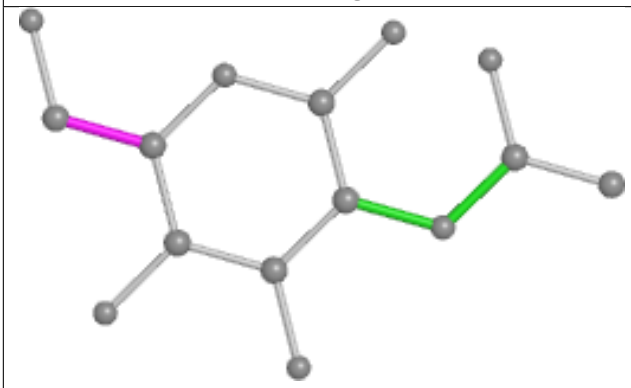
Ligand NAG B 1211



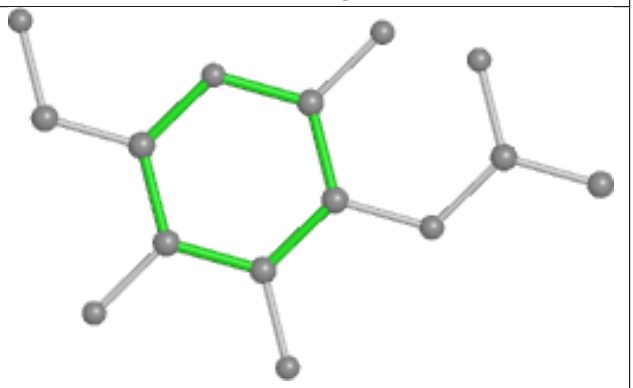
Bond lengths



Bond angles

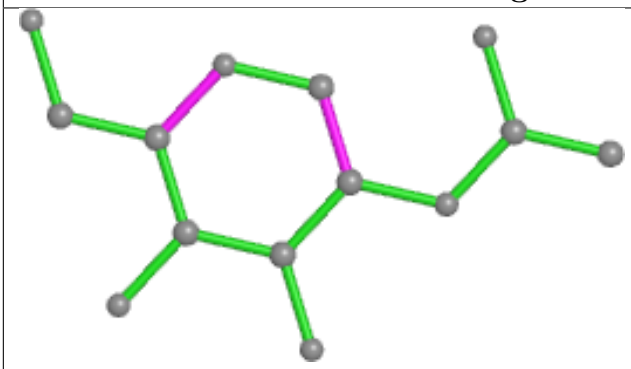


Torsions

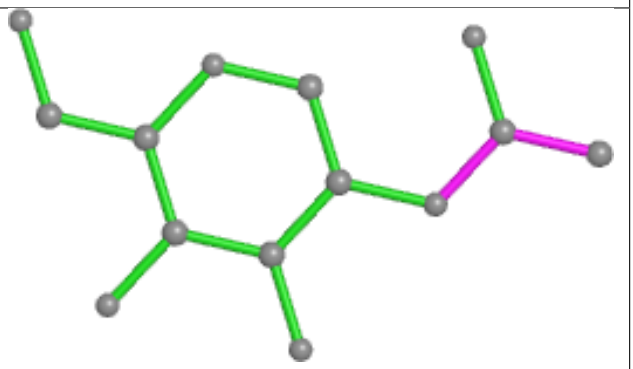


Rings

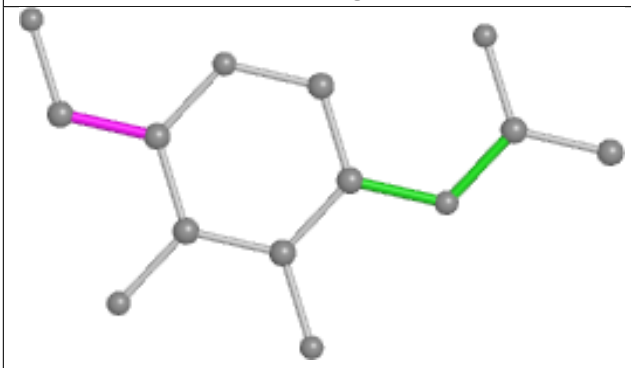
Ligand NAG A 1215



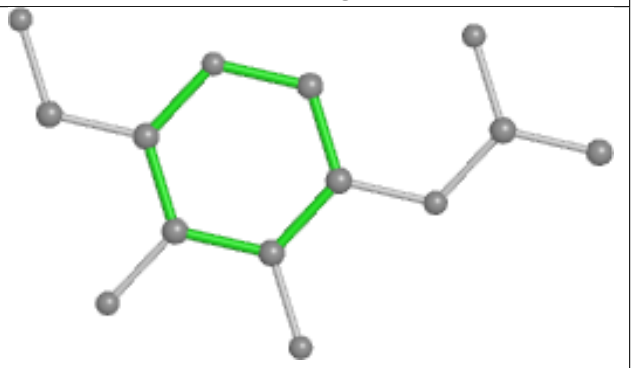
Bond lengths



Bond angles

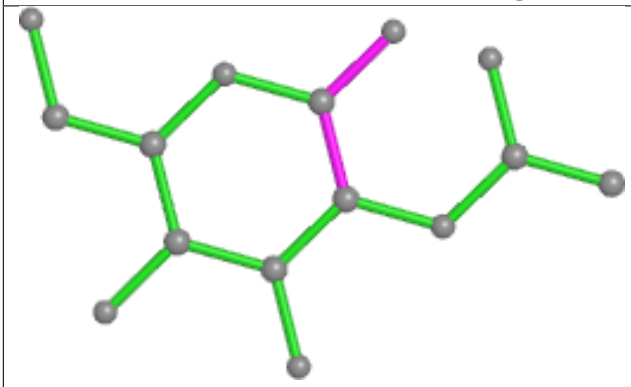


Torsions

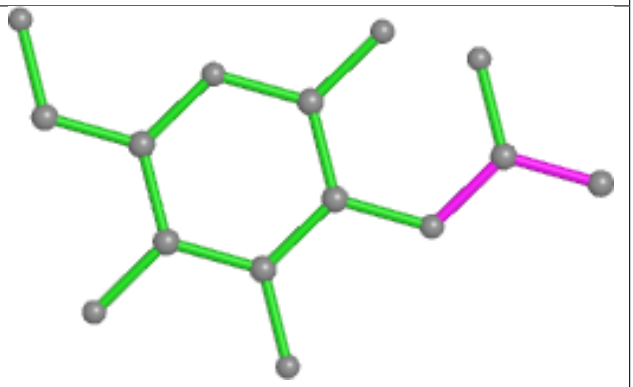


Rings

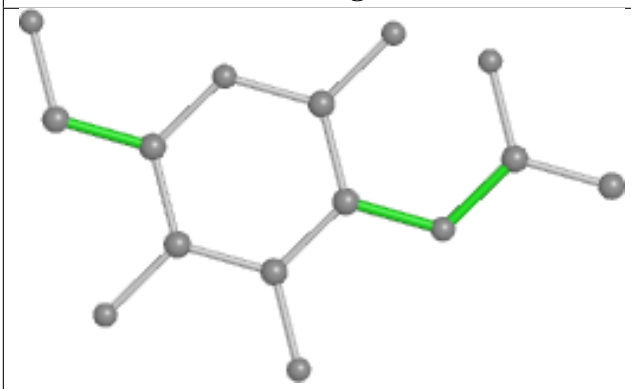
Ligand NAG A 1212



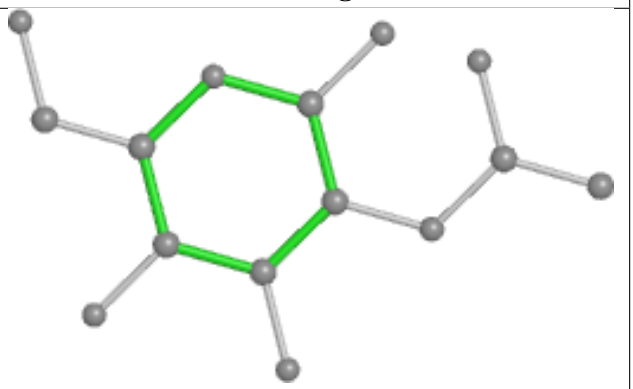
Bond lengths



Bond angles

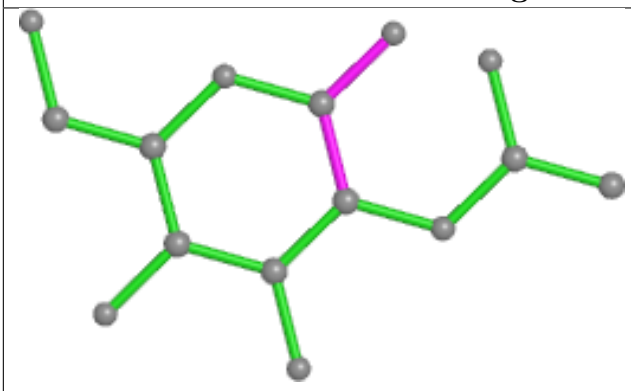


Torsions

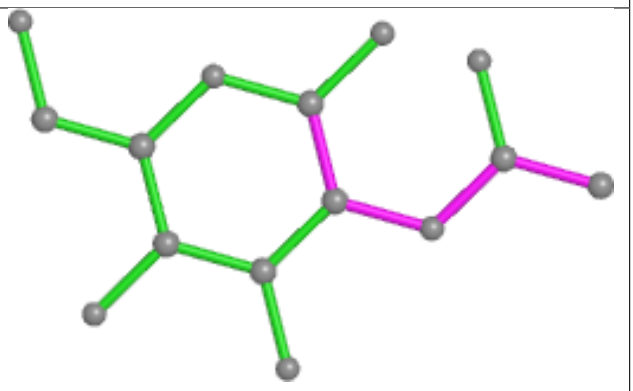


Rings

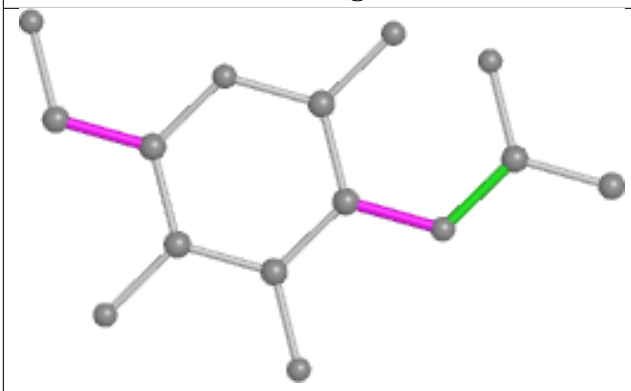
Ligand NAG A 1201



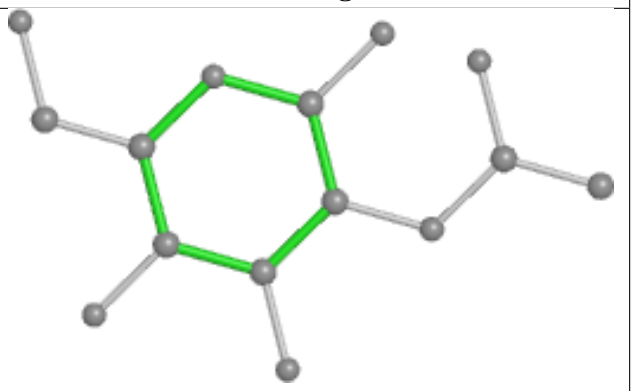
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

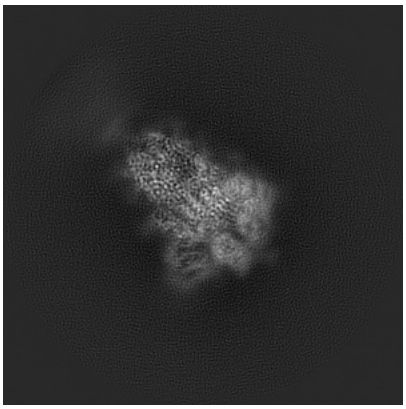
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29455. These allow visual inspection of the internal detail of the map and identification of artifacts.

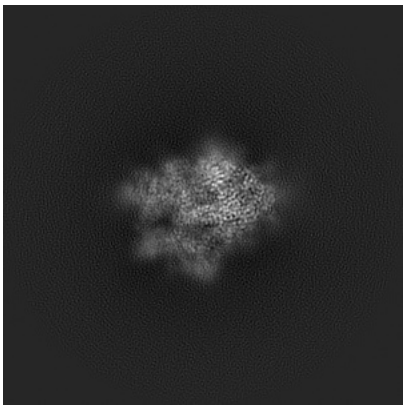
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

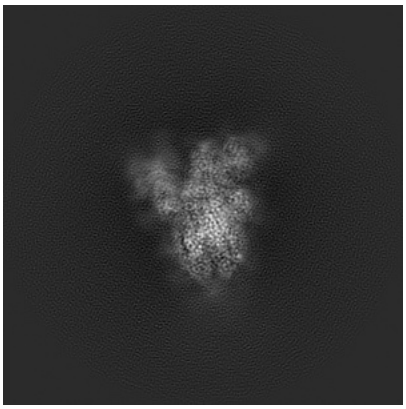
6.1.1 Primary map



X

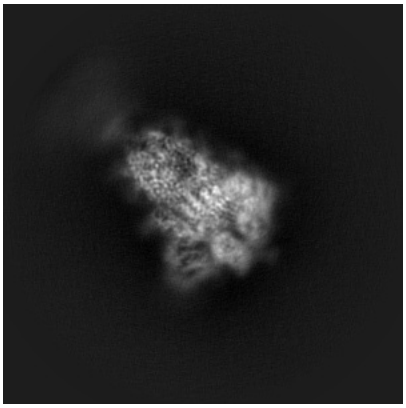


Y

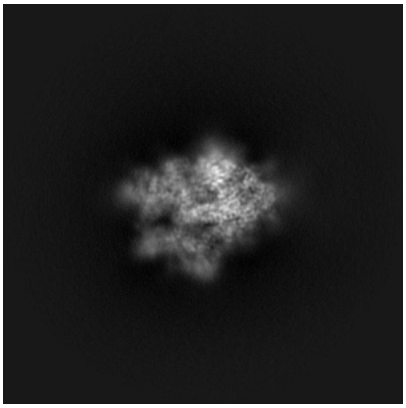


Z

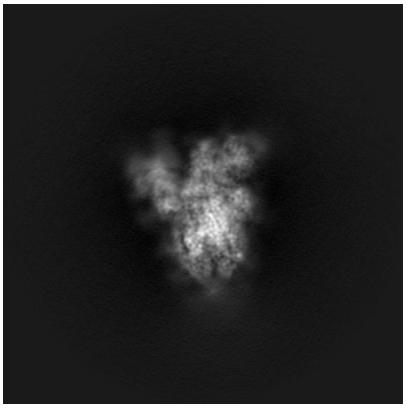
6.1.2 Raw map



X



Y

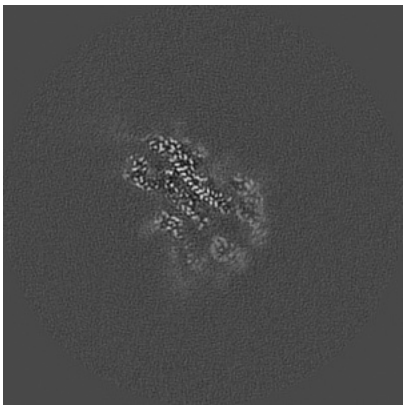


Z

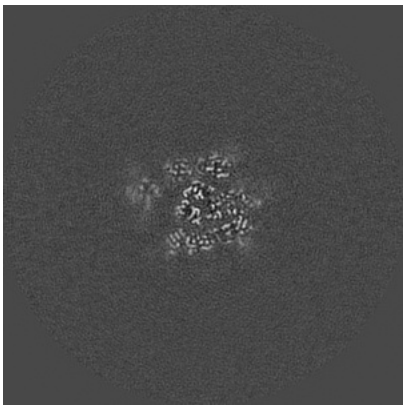
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

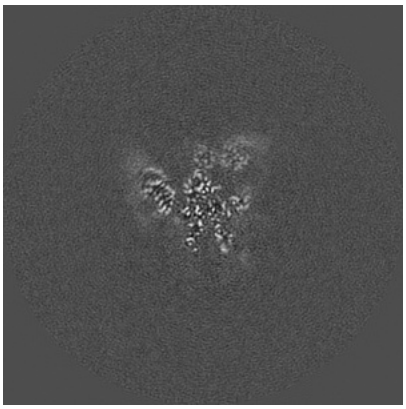
6.2.1 Primary map



X Index: 220

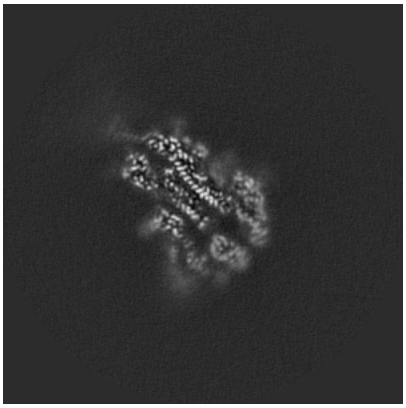


Y Index: 220

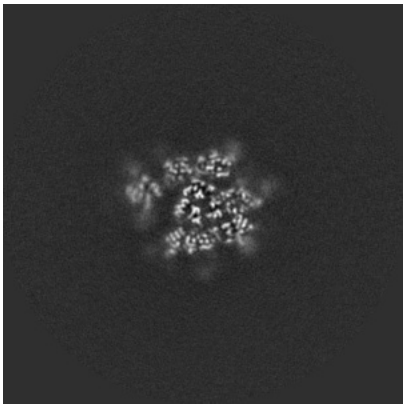


Z Index: 220

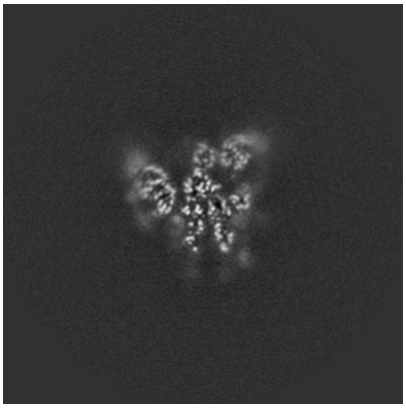
6.2.2 Raw map



X Index: 220



Y Index: 220

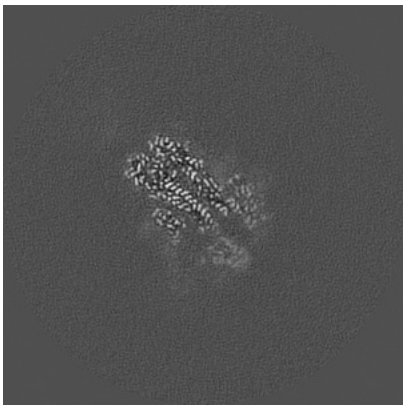


Z Index: 220

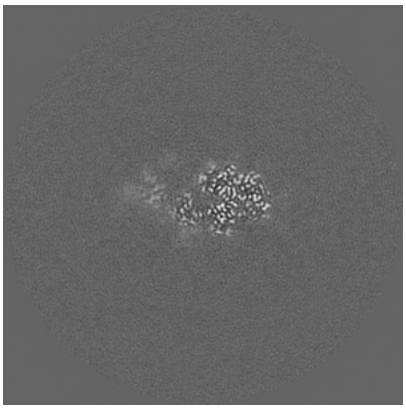
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

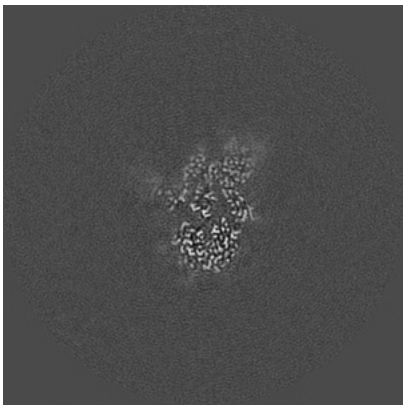
6.3.1 Primary map



X Index: 215

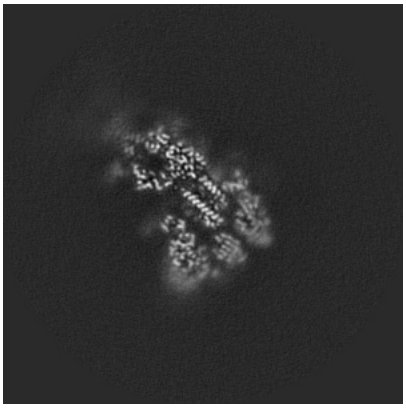


Y Index: 185

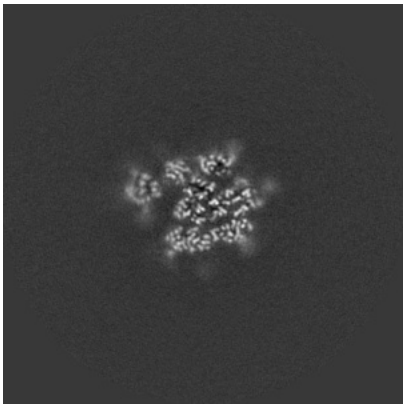


Z Index: 239

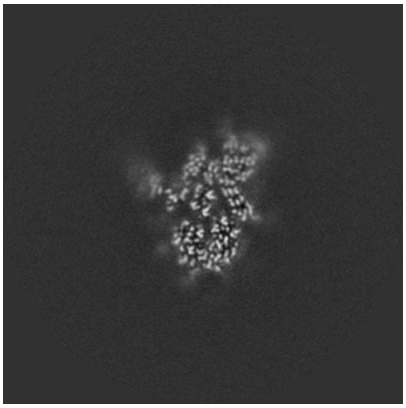
6.3.2 Raw map



X Index: 228



Y Index: 217

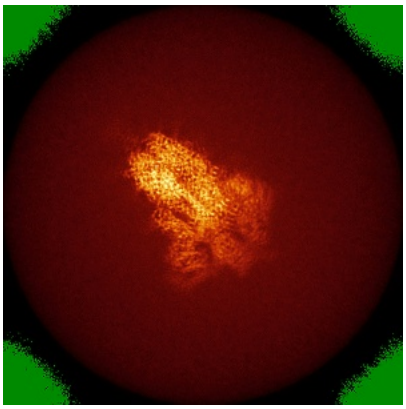


Z Index: 238

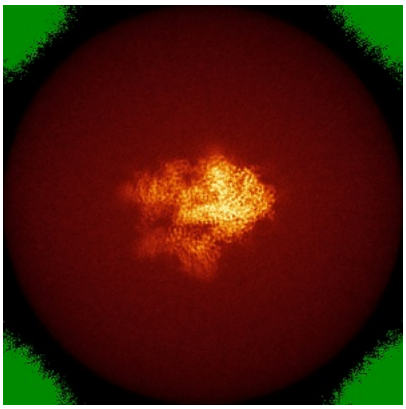
The images above show the largest variance slices of the map in three orthogonal directions.

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

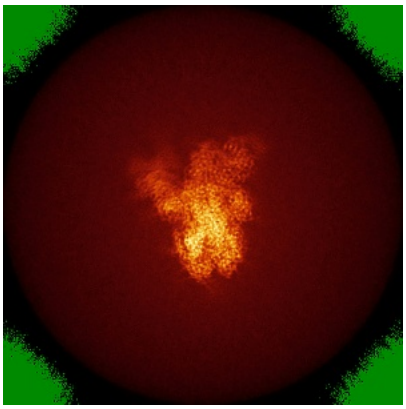
6.4.1 Primary map



X

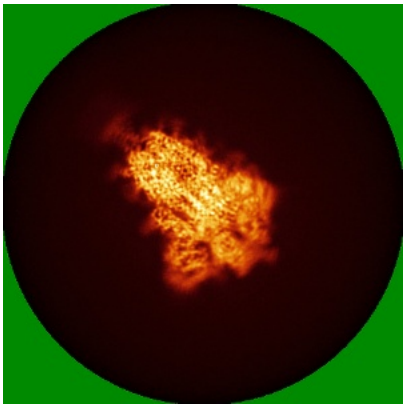


Y

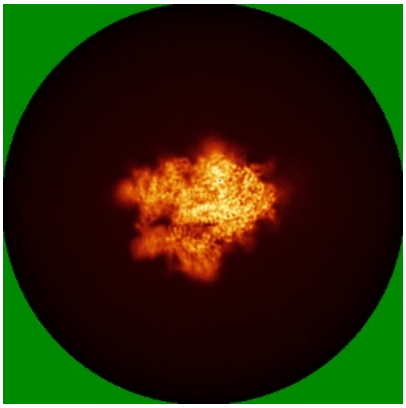


Z

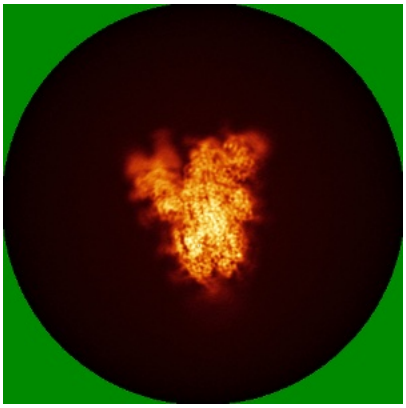
6.4.2 Raw map



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

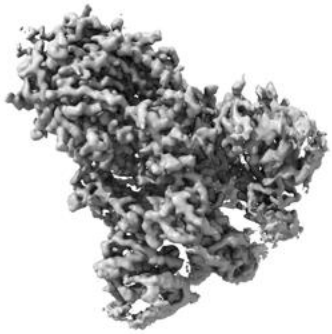
X

Y

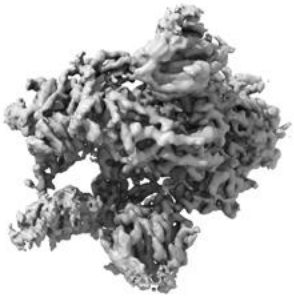
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0084. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

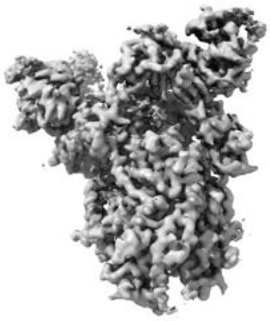
6.5.2 Raw map



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.

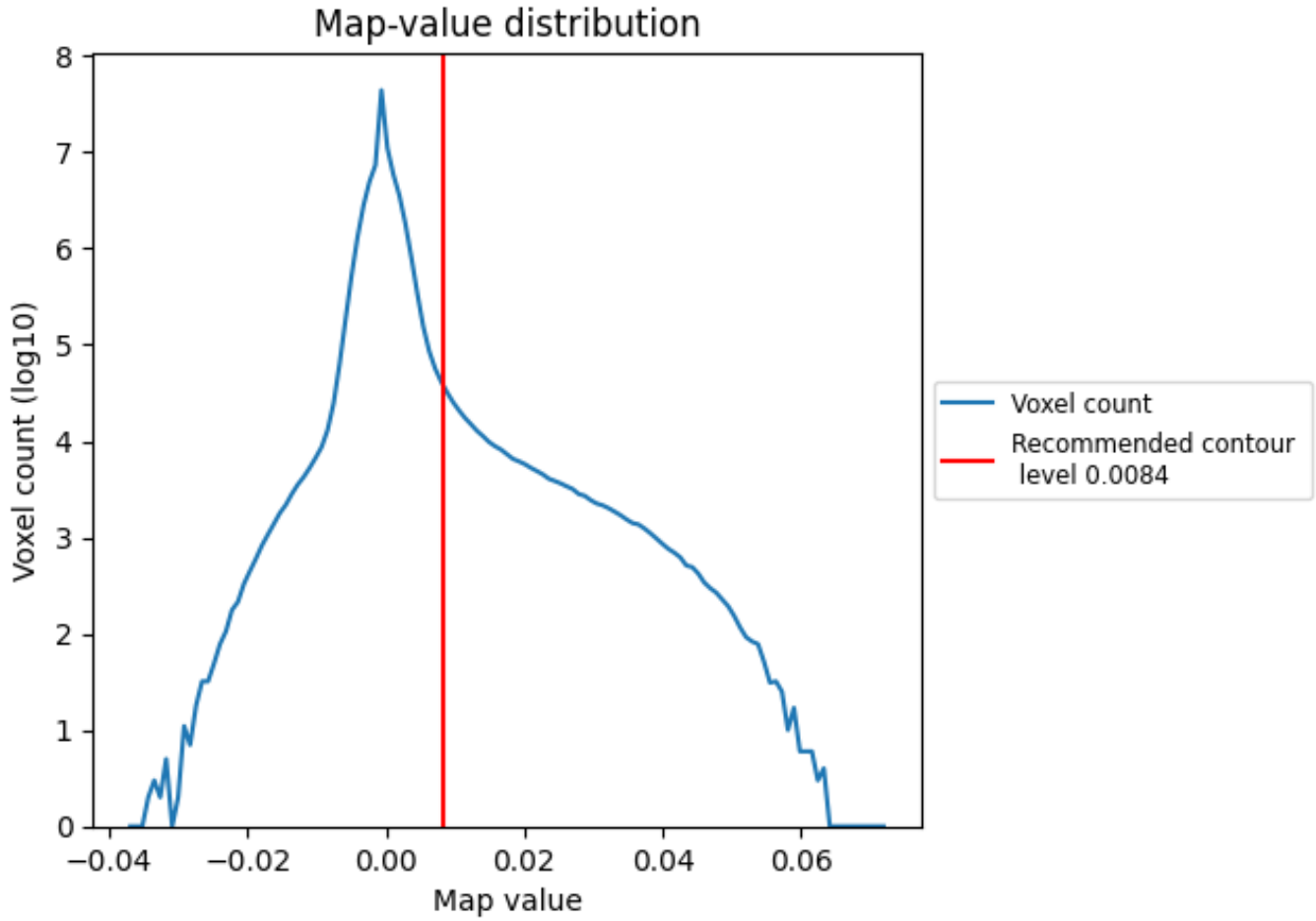
6.6 Mask visualisation (i)

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

7 Map analysis

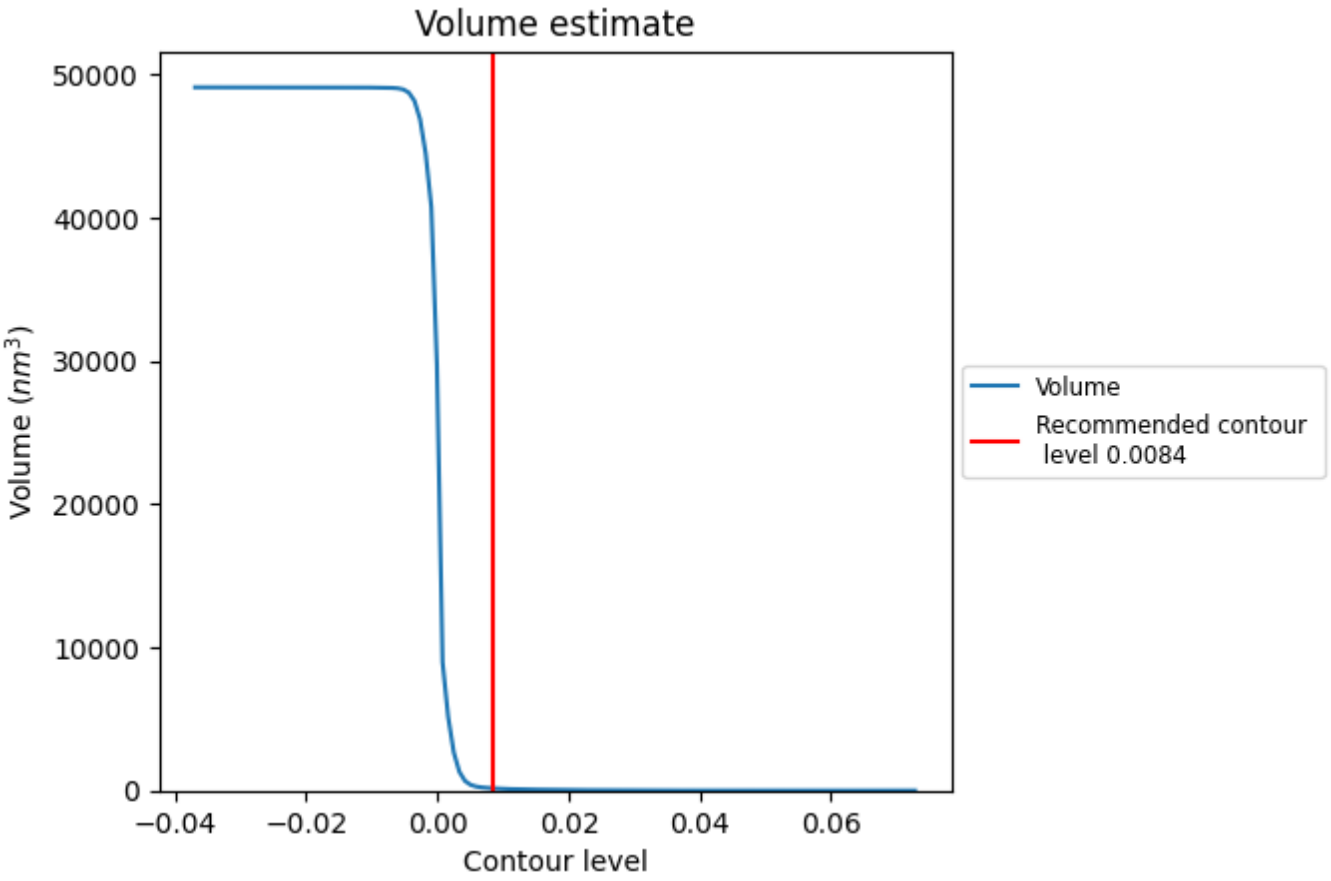
This section contains the results of statistical analysis of the map.

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.

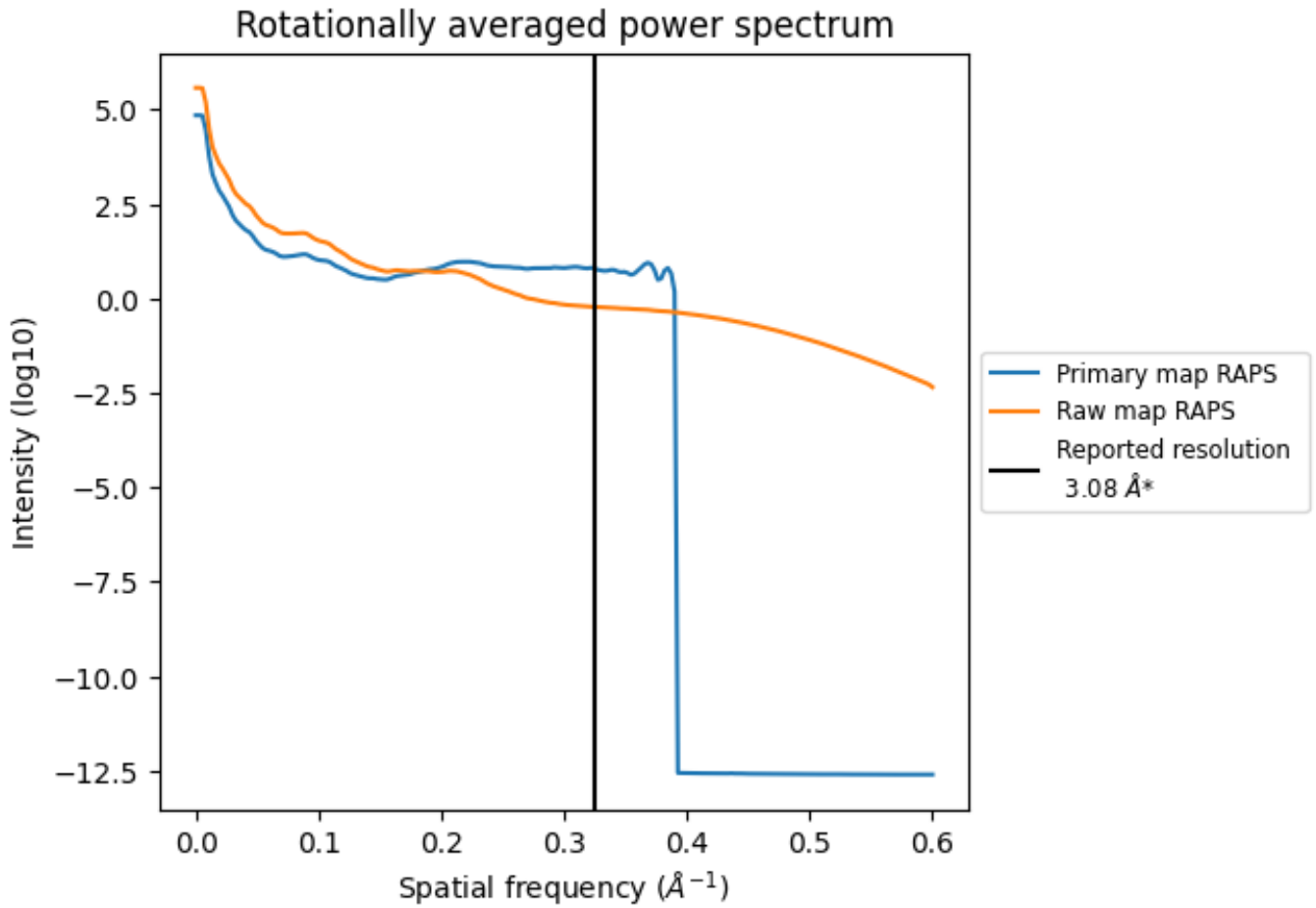
7.2 Volume estimate



The volume at the recommended contour level is 157 nm^3; this corresponds to an approximate mass of 142 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)

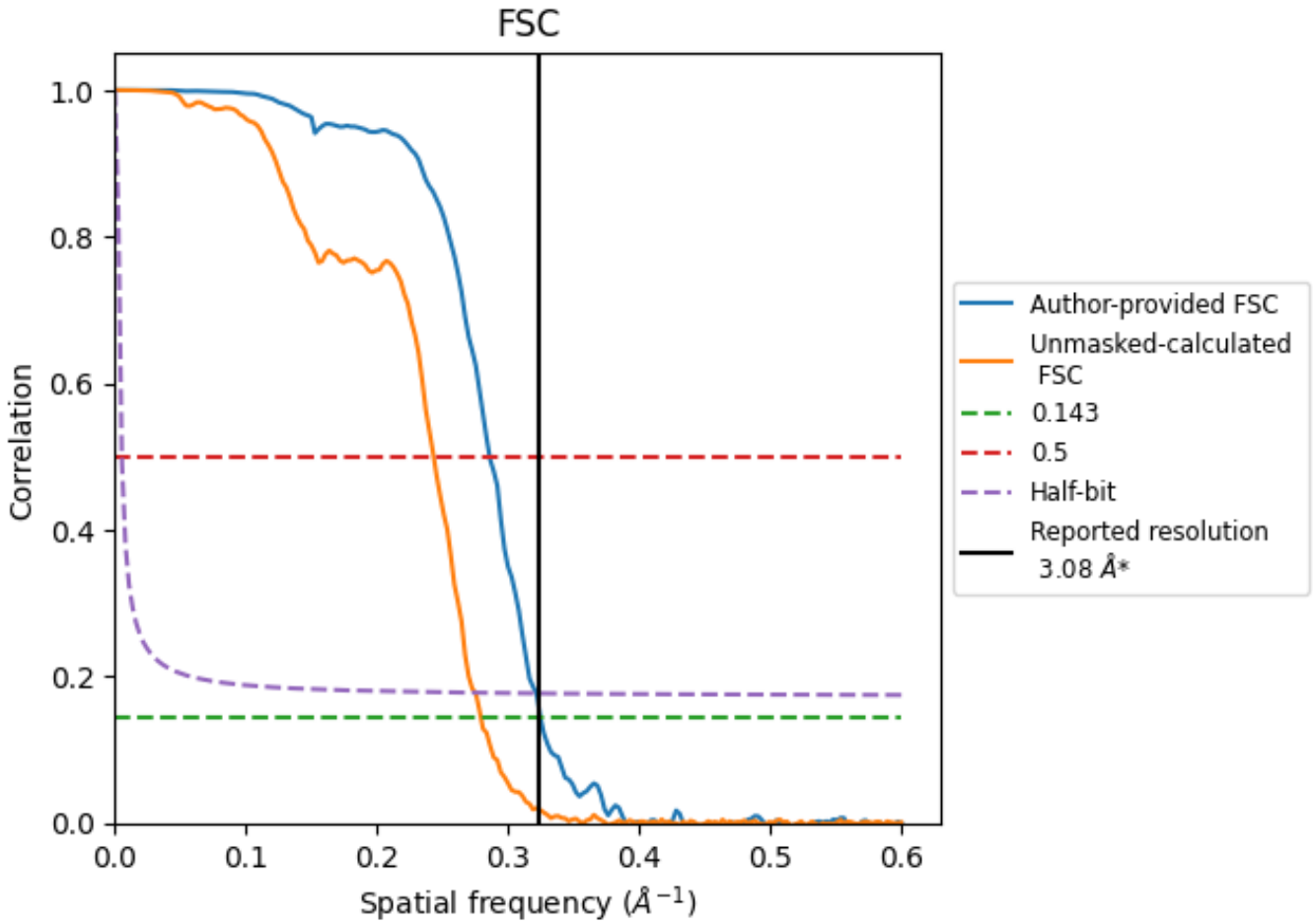


*Reported resolution corresponds to spatial frequency of 0.325 Å^{-1}

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 0.325 Å^{-1}

8.2 Resolution estimates (i)

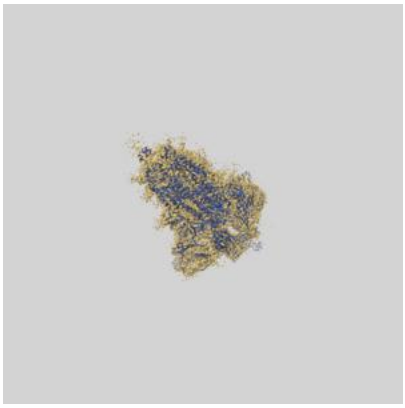
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.49	3.11
Unmasked-calculated*	3.58	4.11	3.63

*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 3.58 differs from the reported value 3.08 by more than 10 %

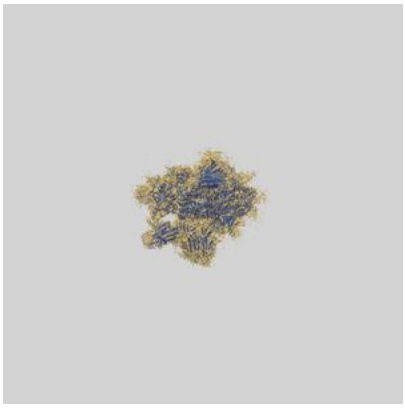
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29455 and PDB model 8FU8. Per-residue inclusion information can be found in section 3 on page 9.

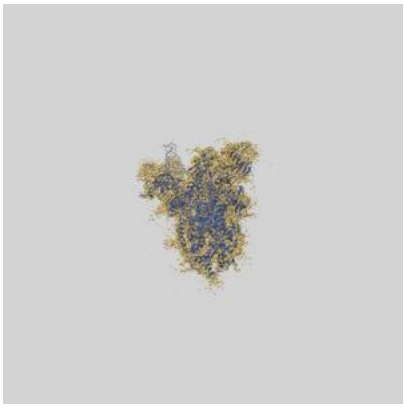
9.1 Map-model overlay



X



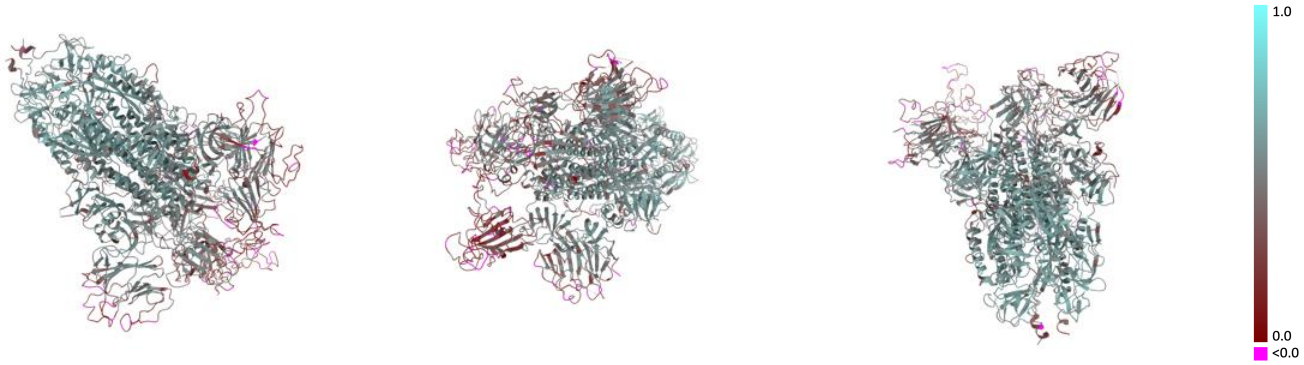
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0084 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.

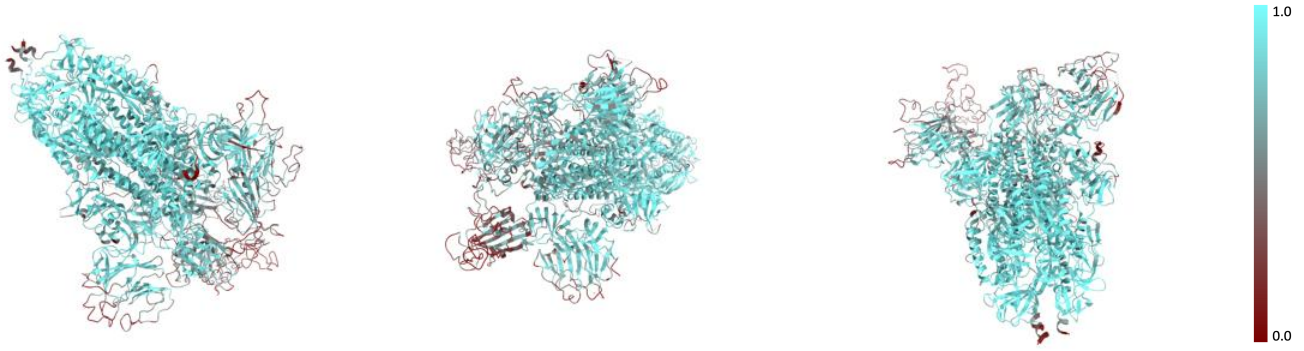
9.2 Q-score mapped to coordinate model (i)



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.

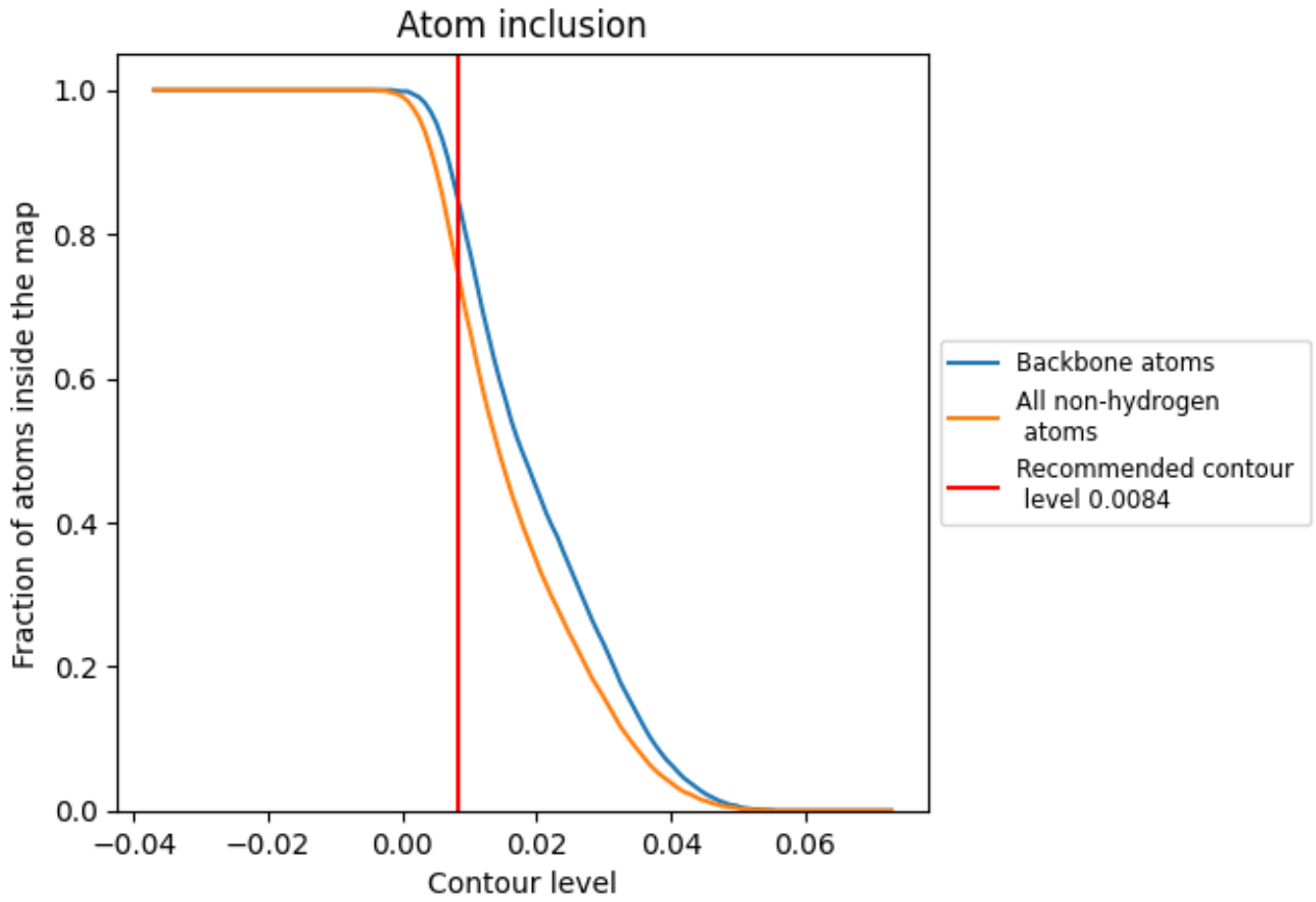
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0084).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.0084) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.4570
A	0.7570	0.4600
B	0.7180	0.4500
C	0.7460	0.4600