Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 08:26 AM EST

PDB ID	:	7TM0
EMDB ID	:	EMD-25992
Title	:	SARS-CoV-2 S B.1.1.529 Omicron variant + S309 + S2L20 Global Refinement
Authors	:	McCallum, M.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2022-01-19
Resolution	:	3.10 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:

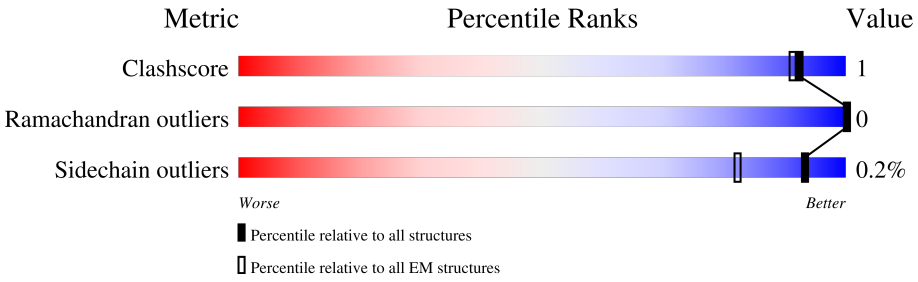
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1274	33% 77% · 20%
1	B	1274	40% 78% · 20%
1	C	1274	40% 77% · 21%
2	D	107	97% 97% ·
2	F	107	97% 94% · ·
2	H	107	97% 95% · ·
3	E	122	98% 98% ·
3	G	122	98% 98% ·

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Mol	Chain	Length	Quality of chain
3	I	122	69% 98%
4	J	127	99% 99%
4	L	127	100% 100%
4	N	127	100% 100%
5	K	104	97% 97%
5	M	104	97% 97%
5	O	104	100% 98%
6	P	2	50% 100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 27963 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	1016	Total	C	N	O	S	0	0
			7054	4518	1220	1279	37		
1	B	1015	Total	C	N	O	S	0	0
			6746	4272	1186	1252	36		
1	C	1012	Total	C	N	O	S	0	0
			6652	4207	1174	1234	37		

There are 369 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	VAL	-	insertion	UNP P0DTC2
A	214	ARG	-	insertion	UNP P0DTC2
A	9215	GLU	-	insertion	UNP P0DTC2
A	9216	PRO	-	insertion	UNP P0DTC2
A	9217	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	SER	ARG	variant	UNP P0DTC2
A	683	GLY	ARG	variant	UNP P0DTC2
A	685	GLY	ARG	variant	UNP P0DTC2
A	707	CYS	TYR	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	883	CYS	THR	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1206	TYR	-	expression tag	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	ASN	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	ILE	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	TRP	-	expression tag	UNP P0DTC2
A	1265	HIS	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	HIS	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	HIS	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	VAL	-	insertion	UNP P0DTC2
B	214	ARG	-	insertion	UNP P0DTC2
B	9215	GLU	-	insertion	UNP P0DTC2
B	9216	PRO	-	insertion	UNP P0DTC2
B	9217	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	SER	ARG	variant	UNP P0DTC2
B	683	GLY	ARG	variant	UNP P0DTC2
B	685	GLY	ARG	variant	UNP P0DTC2
B	707	CYS	TYR	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	883	CYS	THR	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1206	TYR	-	expression tag	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	GLY	-	expression tag	UNP P0DTC2
B	1252	GLY	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	ASN	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	ILE	-	expression tag	UNP P0DTC2
B	1257	PHE	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	GLN	-	expression tag	UNP P0DTC2
B	1261	LYS	-	expression tag	UNP P0DTC2
B	1262	ILE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	TRP	-	expression tag	UNP P0DTC2
B	1265	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	HIS	-	expression tag	UNP P0DTC2
B	1271	HIS	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	HIS	-	expression tag	UNP P0DTC2
B	1274	HIS	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	VAL	-	insertion	UNP P0DTC2
C	214	ARG	-	insertion	UNP P0DTC2
C	9215	GLU	-	insertion	UNP P0DTC2
C	9216	PRO	-	insertion	UNP P0DTC2
C	9217	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	SER	ARG	variant	UNP P0DTC2
C	683	GLY	ARG	variant	UNP P0DTC2
C	685	GLY	ARG	variant	UNP P0DTC2
C	707	CYS	TYR	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	883	CYS	THR	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1206	TYR	-	expression tag	UNP P0DTC2
C	1207	GLU	-	expression tag	UNP P0DTC2
C	1208	GLN	-	expression tag	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	GLY	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	ASN	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	ILE	-	expression tag	UNP P0DTC2
C	1257	PHE	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	GLN	-	expression tag	UNP P0DTC2
C	1261	LYS	-	expression tag	UNP P0DTC2
C	1262	ILE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	TRP	-	expression tag	UNP P0DTC2
C	1265	HIS	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	HIS	-	expression tag	UNP P0DTC2
C	1271	HIS	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	HIS	-	expression tag	UNP P0DTC2
C	1274	HIS	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called S2L20 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	104	Total	C	N	O	S	0	0
			528	318	104	104	2		
2	F	104	Total	C	N	O	S	0	0
			528	318	104	104	2		
2	H	104	Total	C	N	O	S	0	0
			528	318	104	104	2		

- Molecule 3 is a protein called S2L20 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	120	Total	C	N	O	S	0	0
			592	349	120	121	2		
3	G	120	Total	C	N	O	S	0	0
			592	349	120	121	2		
3	I	120	Total	C	N	O	S	0	0
			592	349	120	121	2		

- Molecule 4 is a protein called S309 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	126	Total	C	N	O	S	0	0
			624	369	126	127	2		
4	L	127	Total	C	N	O	S	0	0
			630	372	127	129	2		
4	N	127	Total	C	N	O	S	0	0
			630	372	127	129	2		

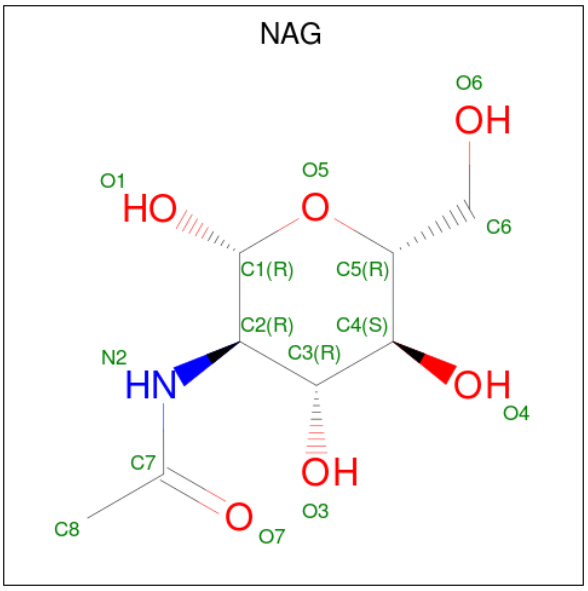
- Molecule 5 is a protein called S309 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	101	Total	C	N	O	S	0	0
			508	304	101	101	2		
5	M	101	Total	C	N	O	S	0	0
			508	304	101	101	2		
5	O	104	Total	C	N	O	S	0	0
			523	313	104	104	2		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	

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Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	A	1	Total	C	N	O	0
			238	136	17	85	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	

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Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	B	1	Total	C	N	O	0
			224	128	16	80	
7	C	1	Total	C	N	O	0
			238	136	17	85	
7	C	1	Total	C	N	O	0
			238	136	17	85	
7	C	1	Total	C	N	O	0
			238	136	17	85	
7	C	1	Total	C	N	O	0
			238	136	17	85	
7	C	1	Total	C	N	O	0
			238	136	17	85	
7	C	1	Total	C	N	O	0
			238	136	17	85	
7	C	1	Total	C	N	O	0
			238	136	17	85	
7	C	1	Total	C	N	O	0
			238	136	17	85	
7	C	1	Total	C	N	O	0
			238	136	17	85	

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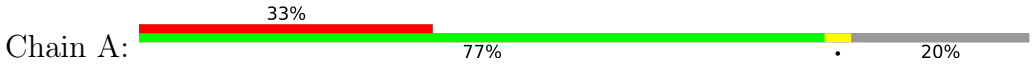
Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total 238	C 136	N 17	O 85	0
7	C	1	Total 238	C 136	N 17	O 85	0
7	C	1	Total 238	C 136	N 17	O 85	0
7	C	1	Total 238	C 136	N 17	O 85	0
7	C	1	Total 238	C 136	N 17	O 85	0
7	C	1	Total 238	C 136	N 17	O 85	0

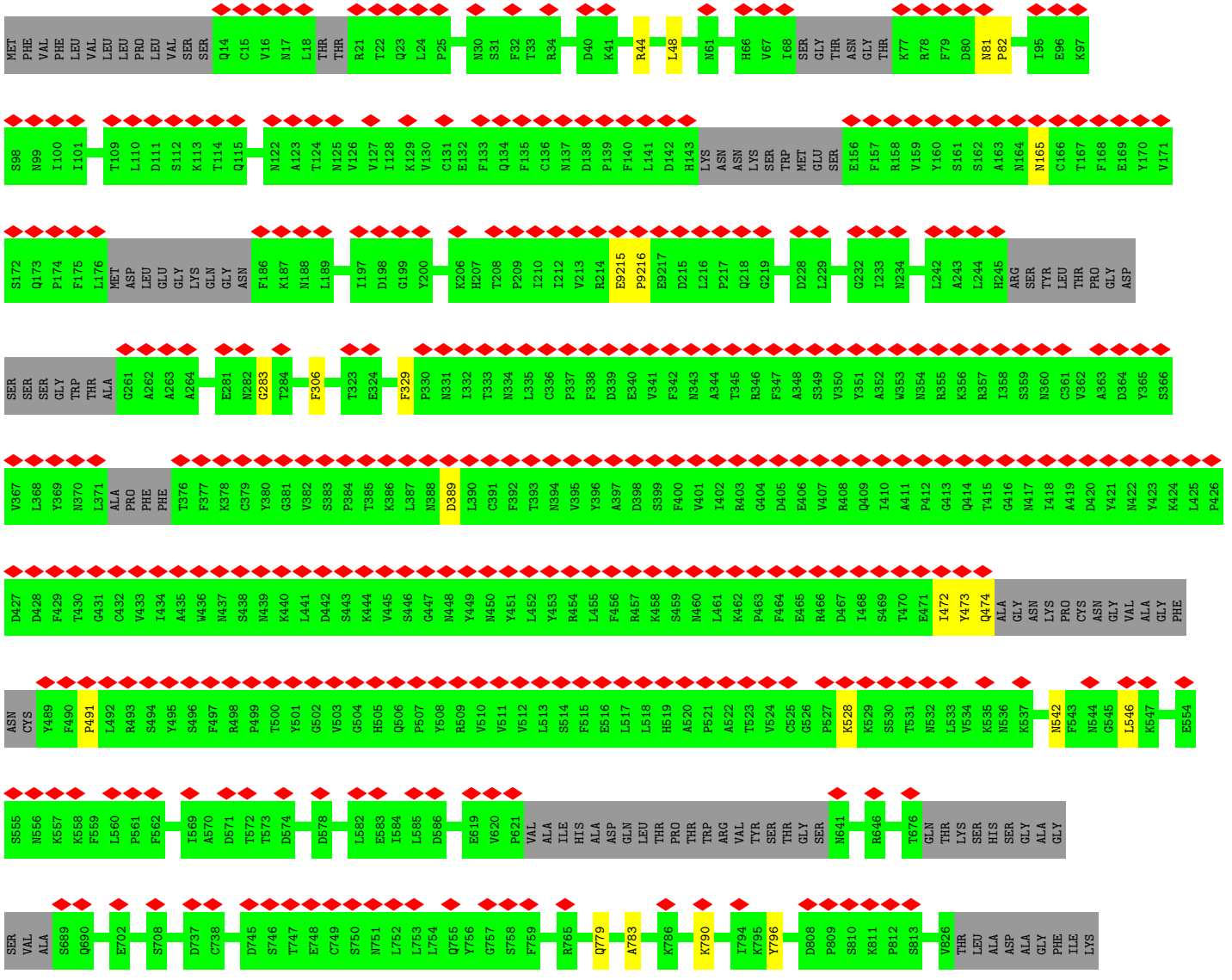
3 Residue-property plots (i)

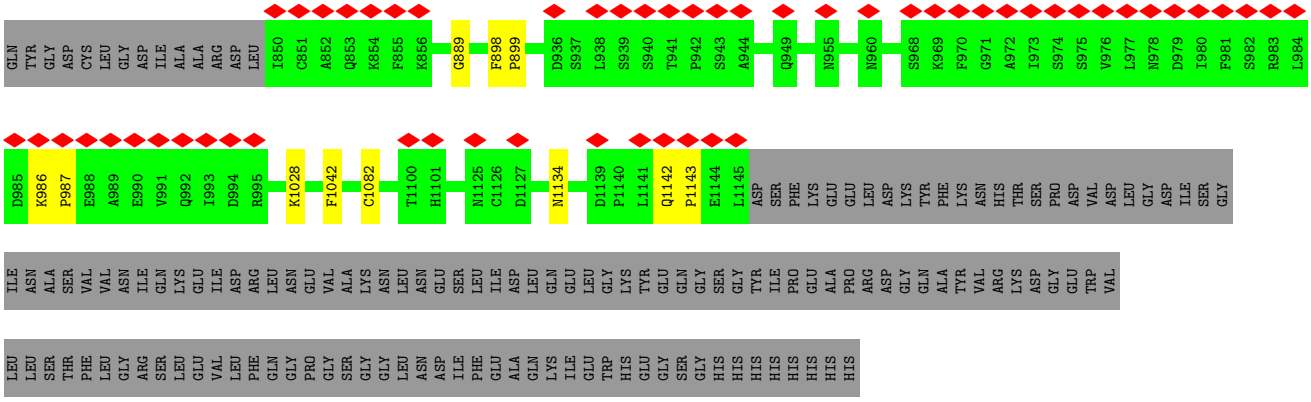
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Spike glycoprotein

Chain A:

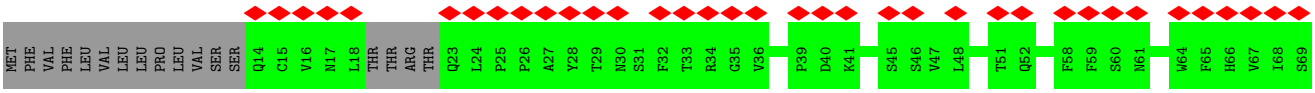


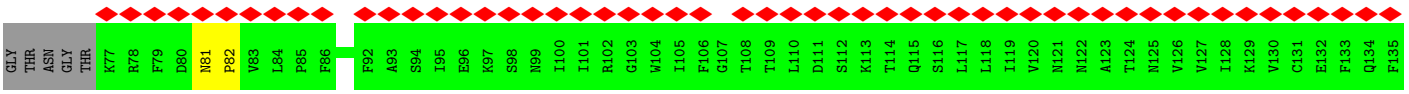


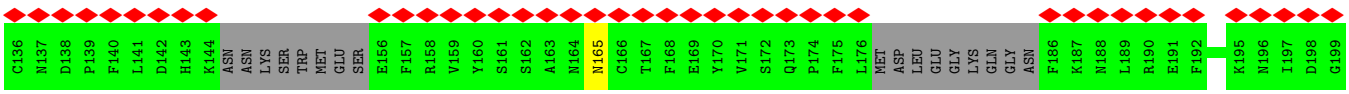


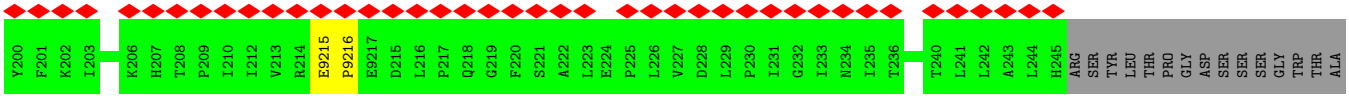
• Molecule 1: Spike glycoprotein

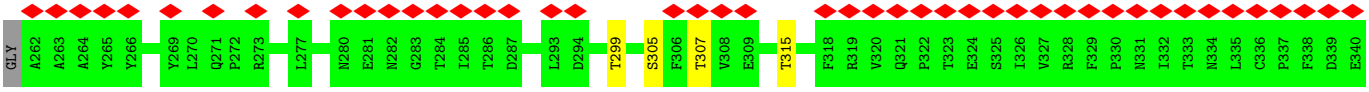
Chain B:

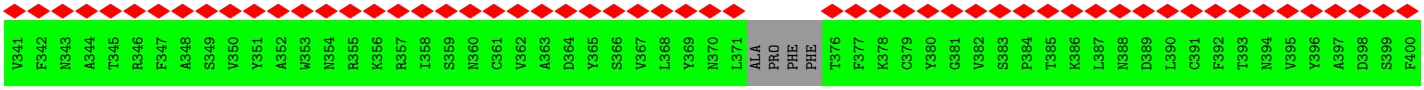


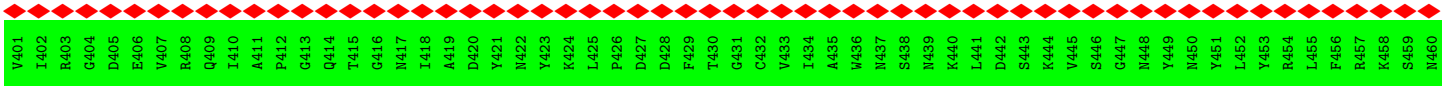


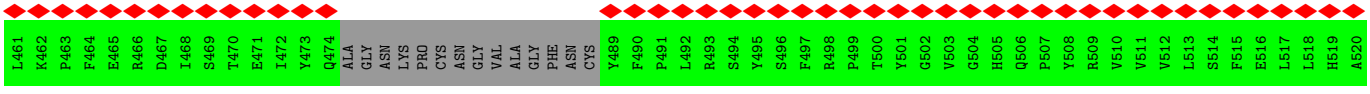


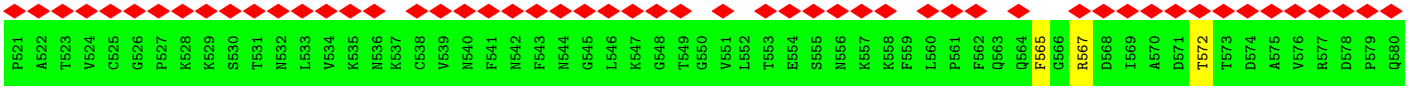


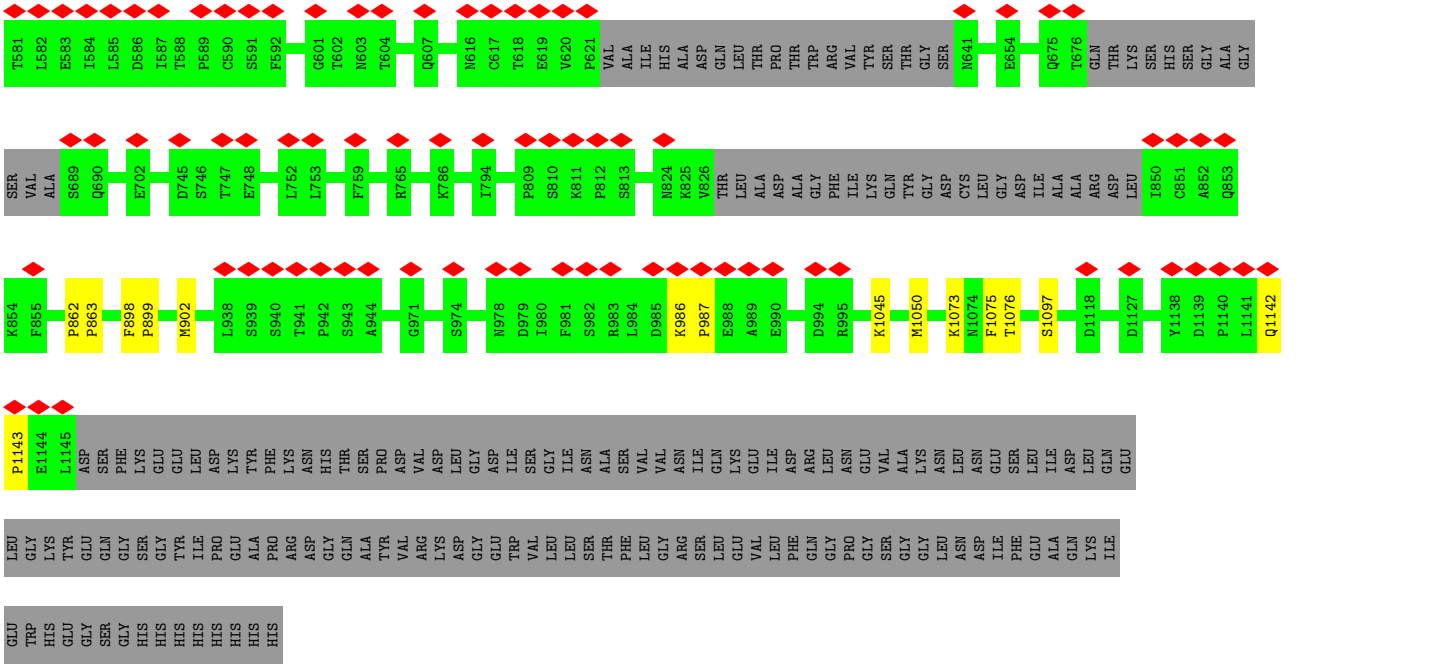




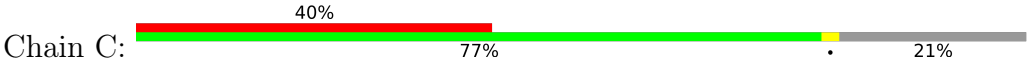


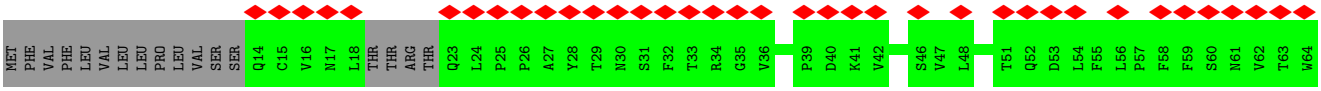


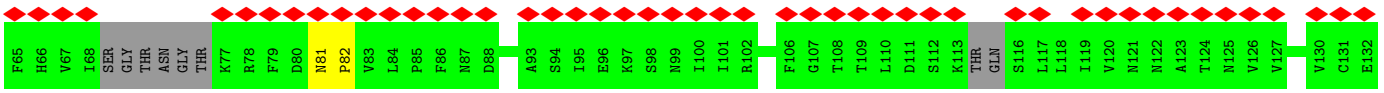


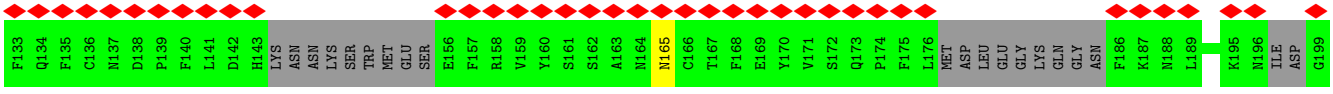


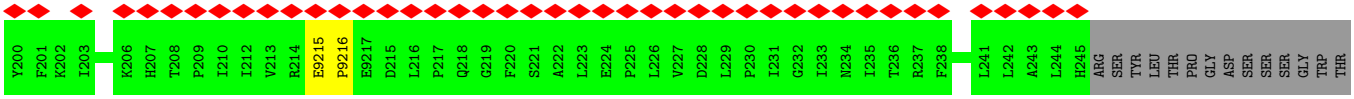
• Molecule 1: Spike glycoprotein

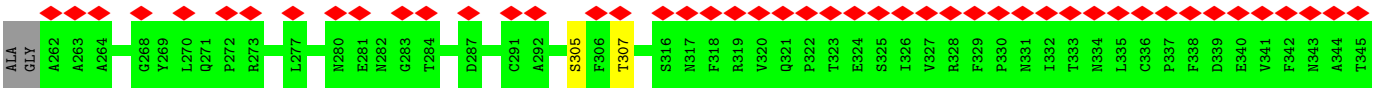


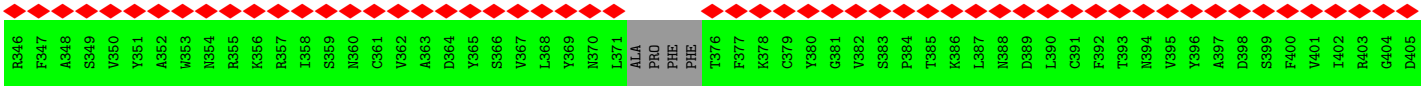


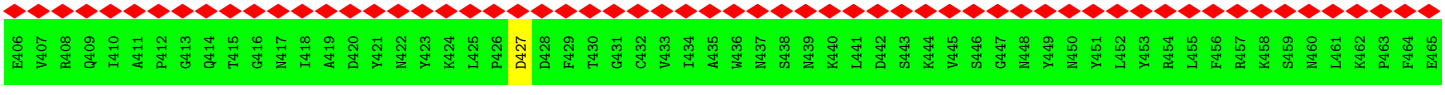


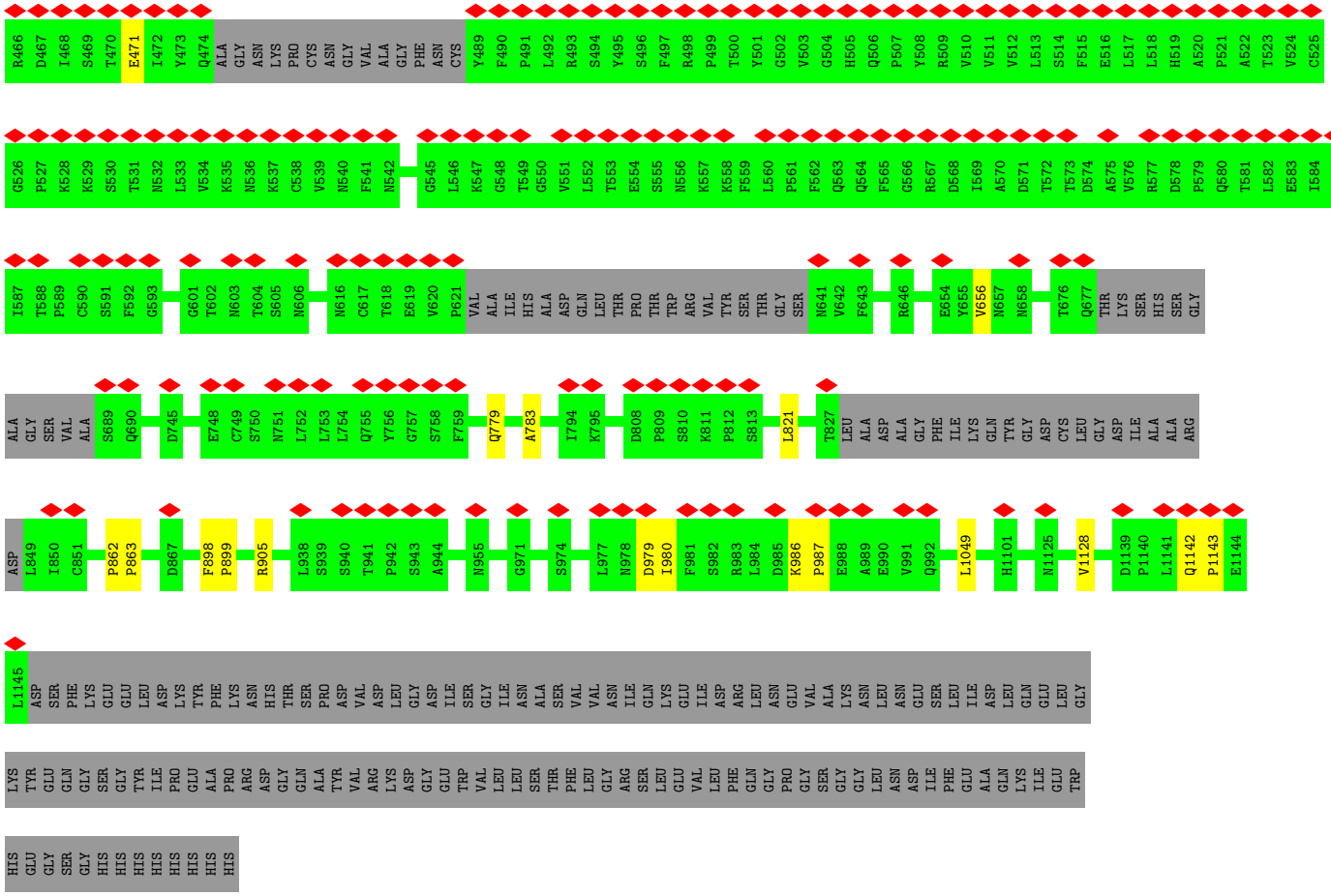






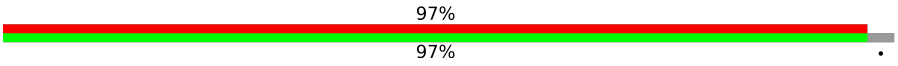






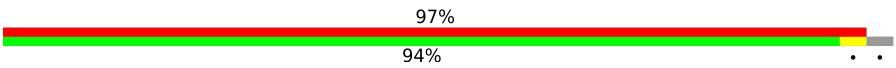
• Molecule 2: S2L20 Fab light chain

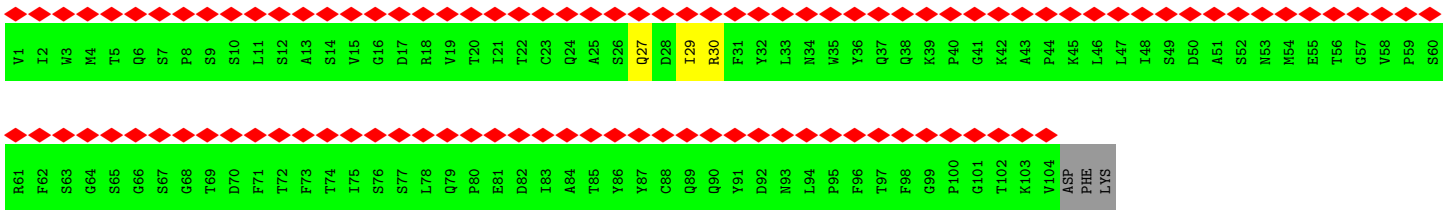
Chain D:



• Molecule 2: S2L20 Fab light chain

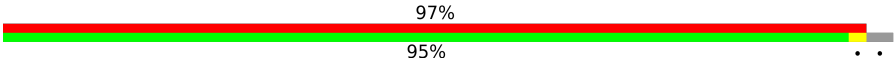
Chain F:





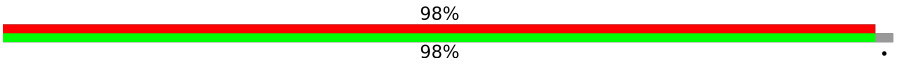
• Molecule 2: S2L20 Fab light chain

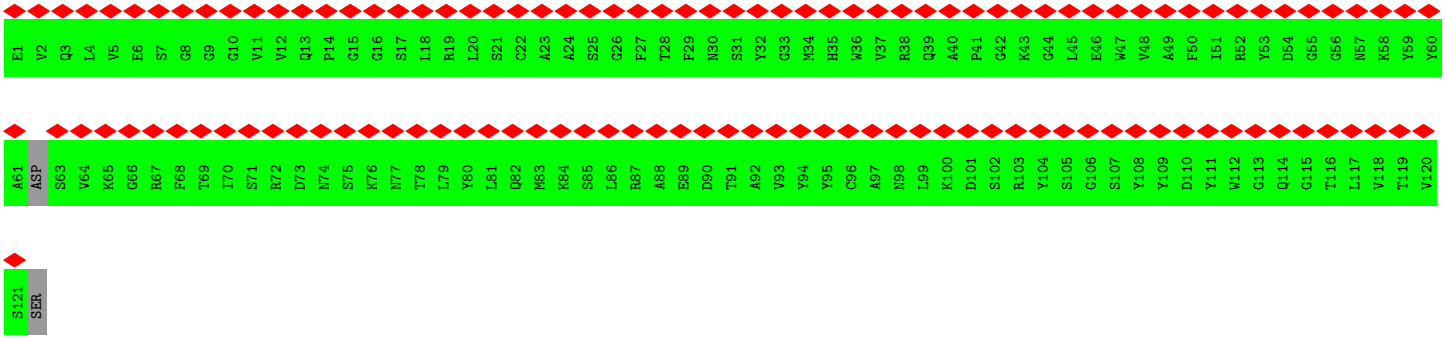
Chain H:



• Molecule 3: S2L20 Fab heavy chain

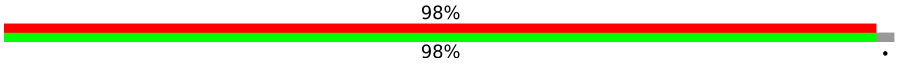
Chain E:

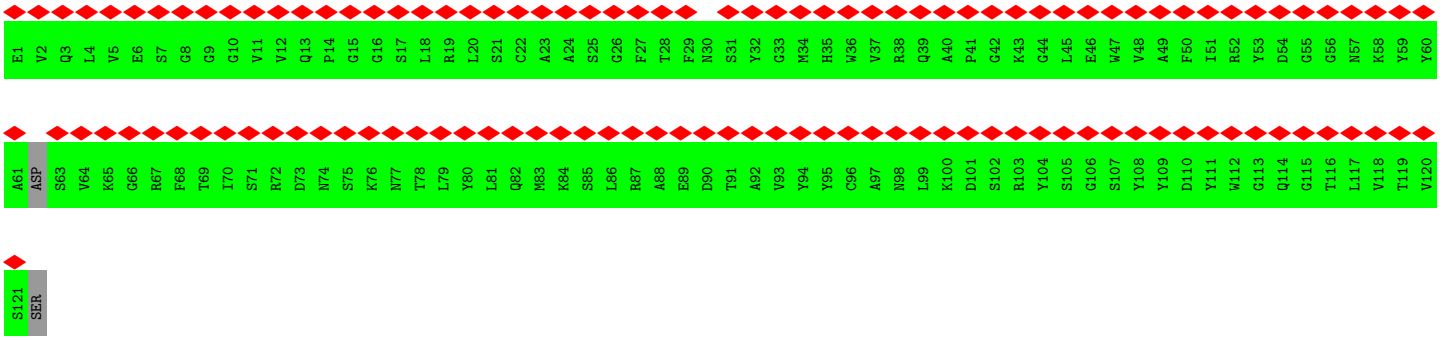




• Molecule 3: S2L20 Fab heavy chain

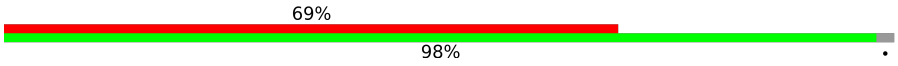
Chain G:

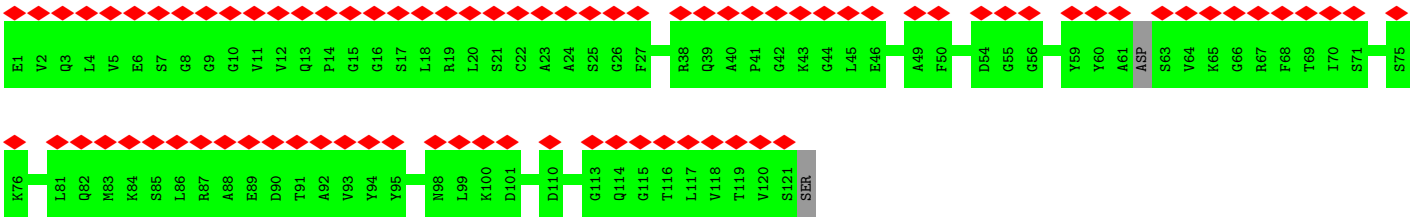




• Molecule 3: S2L20 Fab heavy chain

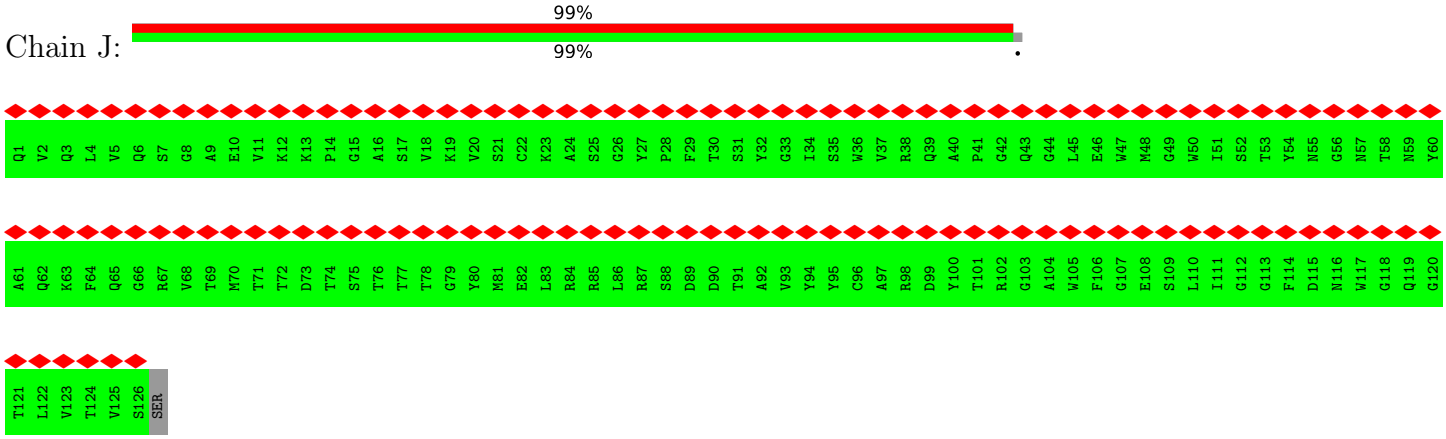
Chain I:





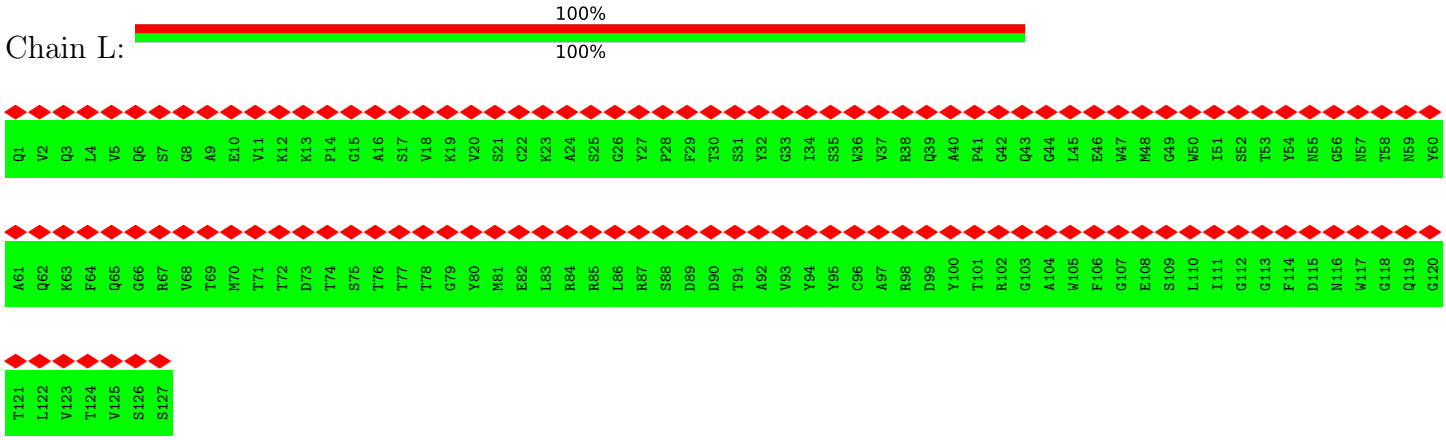
• Molecule 4: S309 Fab Heavy Chain

Chain J:



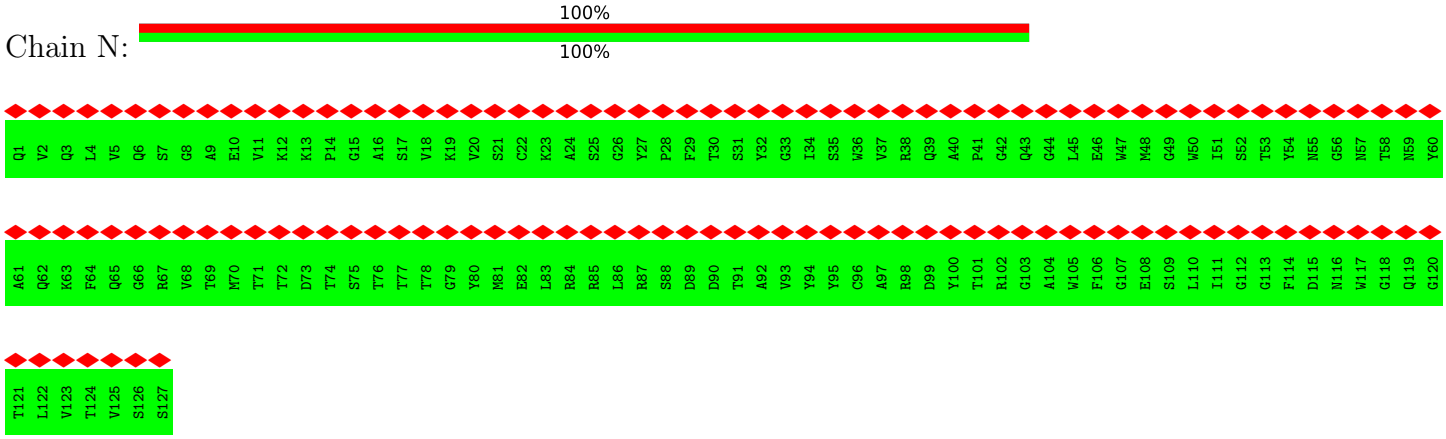
• Molecule 4: S309 Fab Heavy Chain

Chain L:



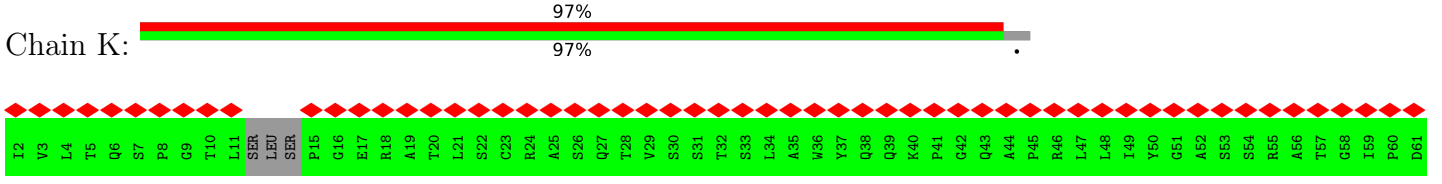
• Molecule 4: S309 Fab Heavy Chain

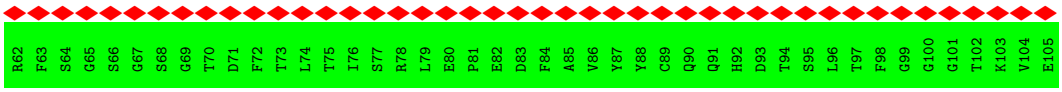
Chain N:



• Molecule 5: S309 Fab light chain

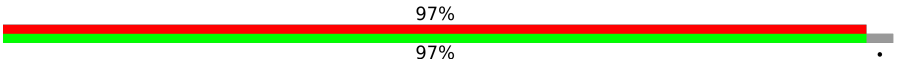
Chain K:

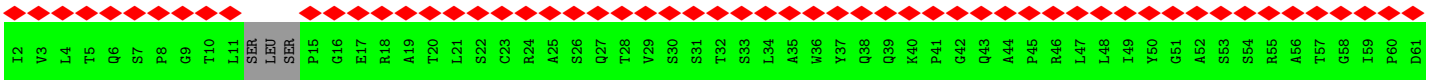


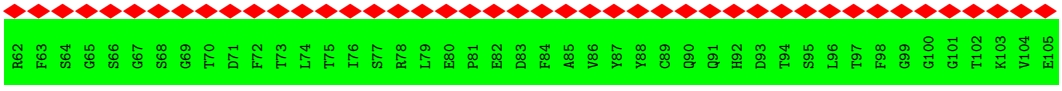


• Molecule 5: S309 Fab light chain

Chain M:

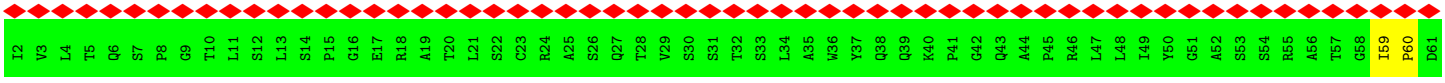


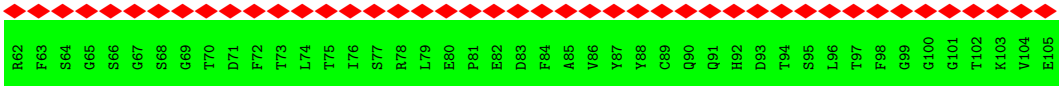




• Molecule 5: S309 Fab light chain

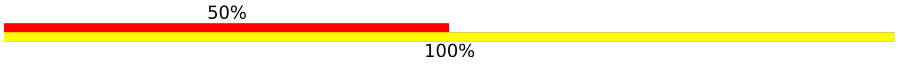
Chain O:





• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74826	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 ($e^-/Å^2$)	63	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.255	Depositor
Minimum map value	-2.465	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	431.616, 431.616, 431.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.843, 0.843, 0.843	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	0.49	0/7200	0.56	0/9861
1	B	0.50	0/6875	0.56	0/9441
1	C	0.50	0/6777	0.57	0/9314
2	D	0.31	0/534	0.48	0/746
2	F	0.39	0/534	0.55	0/746
2	H	0.31	0/534	0.48	0/746
3	E	0.33	0/592	0.48	0/817
3	G	0.33	0/592	0.48	0/817
3	I	0.33	0/592	0.48	0/817
4	J	0.28	0/626	0.44	0/867
4	L	0.28	0/632	0.44	0/874
4	N	0.28	0/632	0.44	0/874
5	K	0.34	0/512	0.53	0/710
5	M	0.34	0/512	0.53	0/710
5	O	0.34	0/528	0.52	0/735
All	All	0.46	0/27672	0.54	0/38075

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7054	0	6154	26	0
1	B	6746	0	5516	21	0
1	C	6652	0	5358	23	0
2	D	528	0	272	0	0
2	F	528	0	272	4	0
2	H	528	0	272	1	0
3	E	592	0	297	0	0
3	G	592	0	297	0	0
3	I	592	0	297	0	0
4	J	624	0	318	0	0
4	L	630	0	320	0	0
4	N	630	0	320	0	0
5	K	508	0	267	0	0
5	M	508	0	267	0	0
5	O	523	0	273	1	0
6	P	28	0	25	0	0
7	A	238	0	221	1	0
7	B	224	0	208	0	0
7	C	238	0	221	1	0
All	All	27963	0	21175	68	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 1.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:GLU:HA	2:F:27:GLN:HA	1.53	0.90
1:B:902:MET:HE1	1:B:1050:MET:HE3	1.58	0.83
1:A:790:LYS:HE2	1:A:790:LYS:HA	1.65	0.79
1:C:471:GLU:HA	2:F:27:GLN:CA	2.17	0.74
1:A:779:GLN:NE2	1:A:783:ALA:CB	2.50	0.74
1:B:902:MET:CE	1:B:1050:MET:HE3	2.18	0.74
1:A:779:GLN:NE2	1:A:783:ALA:HB3	2.03	0.73
1:C:305:SER:C	1:C:307:THR:H	1.97	0.67
1:A:779:GLN:HE21	1:A:783:ALA:HB3	1.61	0.64
1:B:902:MET:CE	1:B:1050:MET:CE	2.75	0.63
1:A:986:LYS:HD2	1:C:427:ASP:CB	2.29	0.63
1:C:779:GLN:HG3	1:C:783:ALA:HB3	1.81	0.62
1:C:471:GLU:HA	2:F:27:GLN:CB	2.29	0.62
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.01	0.61
1:A:986:LYS:HZ3	1:C:427:ASP:C	2.07	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.67	0.58
1:A:986:LYS:CD	1:C:427:ASP:CB	2.82	0.57
1:C:979:ASP:OD1	1:C:980:ILE:N	2.38	0.56
1:A:1142:GLN:N	1:A:1143:PRO:CD	2.68	0.56
1:A:473:TYR:O	1:A:474:GLN:C	2.45	0.56
1:B:565:PHE:HE1	1:B:567:ARG:HE	1.54	0.56
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.68	0.56
1:A:389:ASP:HA	1:A:528:LYS:HD2	1.90	0.54
1:C:305:SER:C	1:C:307:THR:N	2.61	0.53
1:B:305:SER:C	1:B:307:THR:H	2.13	0.50
1:A:329:PHE:CZ	1:A:528:LYS:HD3	2.47	0.50
1:A:472:ILE:HA	1:A:491:PRO:HD3	1.93	0.49
1:A:898:PHE:N	1:A:899:PRO:CD	2.75	0.49
1:B:81:ASN:N	1:B:82:PRO:CD	2.75	0.49
1:C:81:ASN:N	1:C:82:PRO:CD	2.75	0.48
1:A:81:ASN:N	1:A:82:PRO:CD	2.75	0.48
1:B:898:PHE:N	1:B:899:PRO:CD	2.76	0.48
1:C:1128:VAL:HG22	1:C:1128:VAL:O	2.14	0.48
1:C:898:PHE:N	1:C:899:PRO:CD	2.77	0.47
1:A:889:GLY:O	1:B:1045:LYS:NZ	2.44	0.46
1:A:81:ASN:N	1:A:82:PRO:HD3	2.32	0.45
1:C:81:ASN:N	1:C:82:PRO:HD3	2.32	0.45
2:F:29:ILE:O	2:F:30:ARG:C	2.54	0.45
1:B:9215:GLU:N	1:B:9216:PRO:CD	2.80	0.44
1:B:81:ASN:N	1:B:82:PRO:HD3	2.32	0.44
1:B:862:PRO:HA	1:B:863:PRO:HD3	1.87	0.44
1:A:48:LEU:HD22	1:A:306:PHE:HE1	1.82	0.44
1:A:9215:GLU:N	1:A:9216:PRO:CD	2.80	0.44
1:C:9215:GLU:N	1:C:9216:PRO:CD	2.81	0.43
1:B:902:MET:HE2	1:B:1050:MET:CE	2.48	0.43
1:B:902:MET:HE2	1:B:1050:MET:HE1	1.98	0.43
1:A:796:TYR:CG	7:A:9312:NAG:H82	2.53	0.43
1:B:986:LYS:N	1:B:987:PRO:HD2	2.32	0.43
1:B:1073:LYS:HD3	1:B:1075:PHE:CZ	2.53	0.43
1:C:862:PRO:HA	1:C:863:PRO:HD3	1.86	0.43
1:A:779:GLN:HE22	1:A:783:ALA:CB	2.29	0.43
1:A:542:ASN:HA	1:A:546:LEU:O	2.19	0.42
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.51	0.42
1:C:986:LYS:N	1:C:987:PRO:HD2	2.34	0.42
1:C:656:VAL:HA	7:C:9309:NAG:H82	2.01	0.42
1:A:986:LYS:HZ2	1:C:427:ASP:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:CYS:HB3	1:A:1134:ASN:OD1	2.19	0.42
1:B:299:THR:OG1	1:B:315:THR:HG21	2.20	0.42
1:B:1076:THR:HB	1:B:1097:SER:HB3	2.00	0.42
1:B:567:ARG:HA	1:B:572:THR:O	2.20	0.42
1:A:986:LYS:N	1:A:987:PRO:HD2	2.35	0.41
1:B:902:MET:CE	1:B:1050:MET:HE1	2.50	0.41
1:C:821:LEU:C	1:C:821:LEU:HD23	2.42	0.40
5:O:59:ILE:HA	5:O:60:PRO:HD3	1.90	0.40
2:H:58:VAL:HA	2:H:59:PRO:HD3	1.93	0.40
1:A:44:ARG:O	1:A:283:GLY:HA2	2.22	0.40
1:C:305:SER:CB	1:C:307:THR:O	2.69	0.40
1:B:898:PHE:HB3	1:B:899:PRO:HD3	2.03	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	994/1274 (78%)	973 (98%)	21 (2%)	0	100	100
1	B	993/1274 (78%)	967 (97%)	26 (3%)	0	100	100
1	C	986/1274 (77%)	959 (97%)	27 (3%)	0	100	100
2	D	102/107 (95%)	99 (97%)	3 (3%)	0	100	100
2	F	102/107 (95%)	99 (97%)	3 (3%)	0	100	100
2	H	102/107 (95%)	99 (97%)	3 (3%)	0	100	100
3	E	116/122 (95%)	114 (98%)	2 (2%)	0	100	100
3	G	116/122 (95%)	114 (98%)	2 (2%)	0	100	100
3	I	116/122 (95%)	114 (98%)	2 (2%)	0	100	100
4	J	124/127 (98%)	122 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
4	N	125/127 (98%)	123 (98%)	2 (2%)	0	100	100
5	K	97/104 (93%)	94 (97%)	3 (3%)	0	100	100
5	M	97/104 (93%)	94 (97%)	3 (3%)	0	100	100
5	O	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
All	All	4297/5202 (83%)	4193 (98%)	104 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	611/1110 (55%)	610 (100%)	1 (0%)	93	97
1	B	524/1110 (47%)	523 (100%)	1 (0%)	93	97
1	C	504/1110 (45%)	503 (100%)	1 (0%)	93	97
2	D	9/94 (10%)	9 (100%)	0	100	100
2	F	9/94 (10%)	9 (100%)	0	100	100
2	H	9/94 (10%)	9 (100%)	0	100	100
3	E	5/99 (5%)	5 (100%)	0	100	100
3	G	5/99 (5%)	5 (100%)	0	100	100
3	I	5/99 (5%)	5 (100%)	0	100	100
4	J	6/103 (6%)	6 (100%)	0	100	100
4	L	6/103 (6%)	6 (100%)	0	100	100
4	N	6/103 (6%)	6 (100%)	0	100	100
5	K	8/86 (9%)	8 (100%)	0	100	100
5	M	8/86 (9%)	8 (100%)	0	100	100
5	O	8/86 (9%)	8 (100%)	0	100	100
All	All	1723/4476 (38%)	1720 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	B	165	ASN
1	C	165	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	779	GLN
1	B	1101	HIS
1	C	314	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	P	1	6,1	14,14,15	1.13	1 (7%)	17,19,21	1.15	1 (5%)
6	NAG	P	2	6	14,14,15	1.08	1 (7%)	17,19,21	1.00	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	P	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	1	NAG	C1-C2	3.30	1.57	1.52
6	P	2	NAG	C1-C2	2.87	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	1	NAG	C8-C7-N2	2.76	120.77	116.10
6	P	2	NAG	C8-C7-N2	2.36	120.09	116.10

There are no chirality outliers.

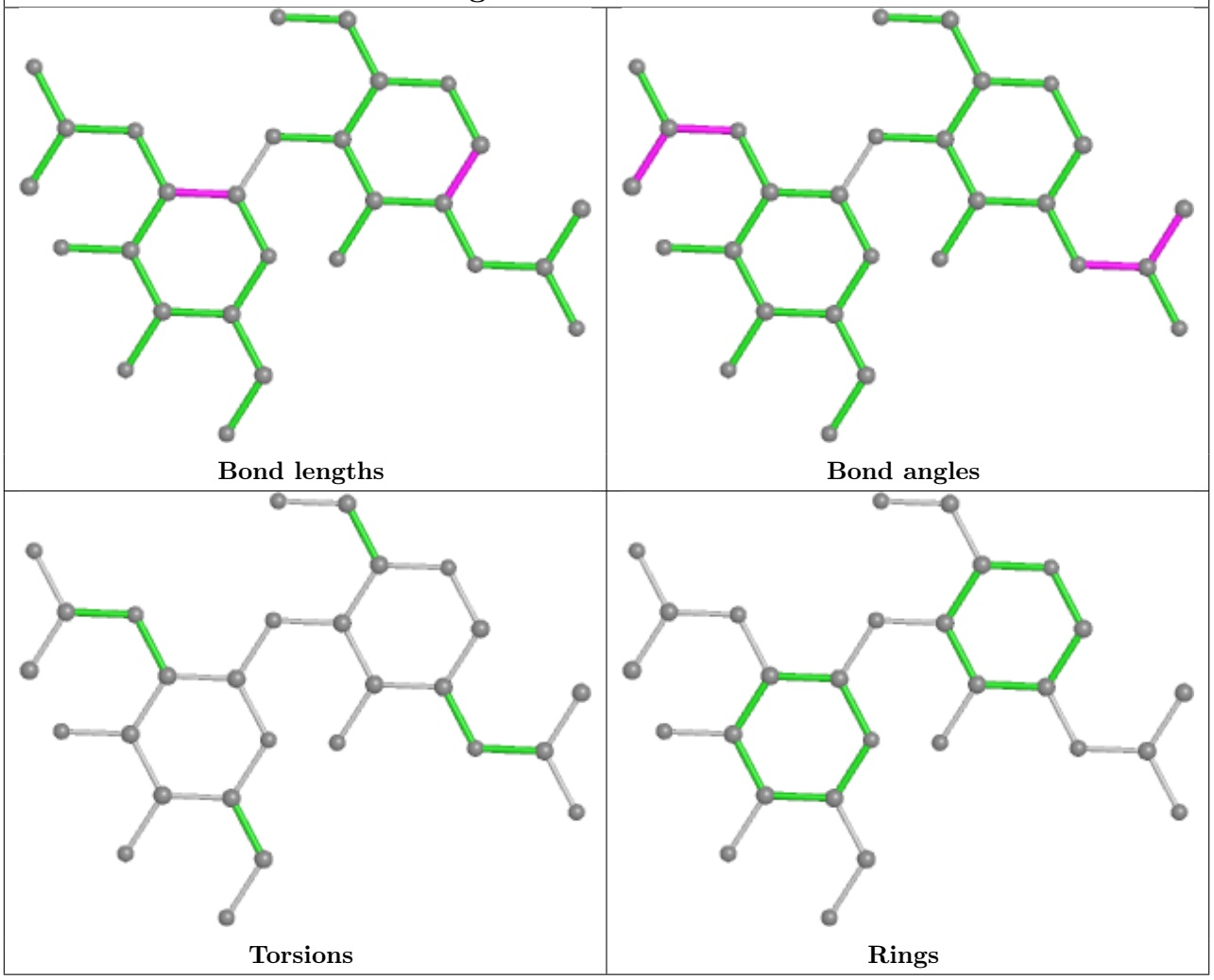
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain P



5.6 Ligand geometry (i)

50 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	$\#\|Z\| > 2$
7	NAG	B	9306	1	14,14,15	1.28	1 (7%)	17,19,21	1.12	2 (11%)
7	NAG	C	9306	1	14,14,15	1.28	1 (7%)	17,19,21	1.12	2 (11%)
7	NAG	A	9305	1	14,14,15	1.13	1 (7%)	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	A	9301	1	14,14,15	0.91	1 (7%)	17,19,21	1.15	2 (11%)
7	NAG	B	9302	1	14,14,15	1.33	2 (14%)	17,19,21	1.22	1 (5%)
7	NAG	B	9313	1	14,14,15	1.18	1 (7%)	17,19,21	1.04	1 (5%)
7	NAG	B	9305	1	14,14,15	1.13	1 (7%)	17,19,21	1.10	1 (5%)
7	NAG	C	9313	1	14,14,15	1.14	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	B	9308	1	14,14,15	1.14	1 (7%)	17,19,21	1.04	1 (5%)
7	NAG	A	9306	1	14,14,15	1.28	1 (7%)	17,19,21	1.11	2 (11%)
7	NAG	A	9307	1	14,14,15	1.19	2 (14%)	17,19,21	1.06	1 (5%)
7	NAG	A	9314	1	14,14,15	1.13	1 (7%)	17,19,21	1.07	1 (5%)
7	NAG	C	9316	1	14,14,15	1.19	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	C	9303	1	14,14,15	1.07	1 (7%)	17,19,21	1.09	1 (5%)
7	NAG	B	9316	1	14,14,15	1.22	1 (7%)	17,19,21	0.76	0
7	NAG	C	9312	1	14,14,15	1.15	1 (7%)	17,19,21	1.02	1 (5%)
7	NAG	C	9317	1	14,14,15	1.09	1 (7%)	17,19,21	1.08	1 (5%)
7	NAG	B	9303	1	14,14,15	1.05	1 (7%)	17,19,21	1.08	1 (5%)
7	NAG	B	9304	1	14,14,15	1.23	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	A	9303	1	14,14,15	1.05	1 (7%)	17,19,21	1.10	1 (5%)
7	NAG	C	9304	1	14,14,15	1.23	1 (7%)	17,19,21	0.93	1 (5%)
7	NAG	A	9313	1	14,14,15	1.10	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	A	9308	1	14,14,15	1.14	1 (7%)	17,19,21	1.02	1 (5%)
7	NAG	A	9312	1	14,14,15	1.16	1 (7%)	17,19,21	1.15	1 (5%)
7	NAG	C	9307	1	14,14,15	1.19	2 (14%)	17,19,21	1.07	1 (5%)
7	NAG	B	9311	1	14,14,15	1.09	1 (7%)	17,19,21	1.08	1 (5%)
7	NAG	B	9315	1	14,14,15	1.19	1 (7%)	17,19,21	1.03	1 (5%)
7	NAG	C	9315	1	14,14,15	1.14	1 (7%)	17,19,21	1.07	1 (5%)
7	NAG	C	9301	1	14,14,15	0.91	1 (7%)	17,19,21	1.17	2 (11%)
7	NAG	A	9315	1	14,14,15	1.15	1 (7%)	17,19,21	1.01	1 (5%)
7	NAG	B	9307	1	14,14,15	1.18	2 (14%)	17,19,21	1.06	1 (5%)
7	NAG	C	9310	1	14,14,15	1.14	1 (7%)	17,19,21	1.04	1 (5%)
7	NAG	C	9302	1	14,14,15	1.32	2 (14%)	17,19,21	1.22	1 (5%)
7	NAG	B	9314	1	14,14,15	1.23	2 (14%)	17,19,21	1.32	3 (17%)
7	NAG	A	9310	1	14,14,15	1.16	1 (7%)	17,19,21	1.03	1 (5%)
7	NAG	C	9314	1	14,14,15	1.17	1 (7%)	17,19,21	1.10	1 (5%)
7	NAG	C	9308	1	14,14,15	1.14	2 (14%)	17,19,21	1.00	1 (5%)
7	NAG	A	9302	1	14,14,15	1.34	2 (14%)	17,19,21	1.24	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	B	9310	1	14,14,15	1.17	1 (7%)	17,19,21	1.08	1 (5%)
7	NAG	B	9312	1	14,14,15	1.17	1 (7%)	17,19,21	1.13	1 (5%)
7	NAG	A	9316	1	14,14,15	1.13	1 (7%)	17,19,21	1.10	1 (5%)
7	NAG	C	9309	1	14,14,15	1.18	1 (7%)	17,19,21	1.08	1 (5%)
7	NAG	A	9304	1	14,14,15	1.24	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	A	9309	1	14,14,15	1.21	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	C	9305	1	14,14,15	1.13	1 (7%)	17,19,21	1.10	1 (5%)
7	NAG	A	9317	1	14,14,15	1.18	1 (7%)	17,19,21	1.13	1 (5%)
7	NAG	B	9309	1	14,14,15	1.21	1 (7%)	17,19,21	1.03	1 (5%)
7	NAG	C	9311	1	14,14,15	1.15	1 (7%)	17,19,21	1.14	1 (5%)
7	NAG	B	9301	1	14,14,15	0.90	1 (7%)	17,19,21	1.14	2 (11%)
7	NAG	A	9311	1	14,14,15	1.08	1 (7%)	17,19,21	1.09	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	9306	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9306	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9305	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9301	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9302	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9313	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9305	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9313	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9308	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9306	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9307	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9314	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9316	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9303	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9316	1	-	2/6/23/26	0/1/1/1
7	NAG	C	9312	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9317	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9303	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9304	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9303	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9304	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	9313	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9308	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9312	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9307	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9311	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9315	1	-	2/6/23/26	0/1/1/1
7	NAG	C	9315	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9315	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9307	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9310	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9302	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9314	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9310	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9314	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9308	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9302	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9310	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9312	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9316	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9309	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9304	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9309	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9305	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9317	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9309	1	-	0/6/23/26	0/1/1/1
7	NAG	C	9311	1	-	0/6/23/26	0/1/1/1
7	NAG	B	9301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	9311	1	-	0/6/23/26	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	9302	NAG	C1-C2	3.92	1.58	1.52
7	B	9302	NAG	C1-C2	3.84	1.58	1.52
7	C	9302	NAG	C1-C2	3.79	1.58	1.52
7	A	9309	NAG	C1-C2	3.64	1.57	1.52
7	B	9309	NAG	C1-C2	3.54	1.57	1.52
7	B	9306	NAG	C1-C2	3.54	1.57	1.52
7	A	9306	NAG	C1-C2	3.53	1.57	1.52
7	C	9306	NAG	C1-C2	3.52	1.57	1.52
7	B	9315	NAG	C1-C2	3.51	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	9312	NAG	C1-C2	3.50	1.57	1.52
7	C	9316	NAG	C1-C2	3.48	1.57	1.52
7	A	9304	NAG	C1-C2	3.48	1.57	1.52
7	B	9304	NAG	C1-C2	3.46	1.57	1.52
7	B	9313	NAG	C1-C2	3.45	1.57	1.52
7	C	9304	NAG	C1-C2	3.44	1.57	1.52
7	A	9317	NAG	C1-C2	3.43	1.57	1.52
7	A	9312	NAG	C1-C2	3.43	1.57	1.52
7	C	9312	NAG	C1-C2	3.38	1.57	1.52
7	C	9309	NAG	C1-C2	3.38	1.57	1.52
7	B	9314	NAG	C1-C2	3.36	1.57	1.52
7	A	9305	NAG	C1-C2	3.35	1.57	1.52
7	B	9305	NAG	C1-C2	3.35	1.57	1.52
7	C	9305	NAG	C1-C2	3.34	1.57	1.52
7	C	9313	NAG	C1-C2	3.33	1.57	1.52
7	B	9310	NAG	C1-C2	3.33	1.57	1.52
7	C	9307	NAG	C1-C2	3.33	1.57	1.52
7	A	9310	NAG	C1-C2	3.33	1.57	1.52
7	C	9314	NAG	C1-C2	3.32	1.57	1.52
7	C	9311	NAG	C1-C2	3.32	1.57	1.52
7	C	9315	NAG	C1-C2	3.31	1.57	1.52
7	B	9316	NAG	C1-C2	3.31	1.57	1.52
7	A	9307	NAG	C1-C2	3.31	1.57	1.52
7	B	9307	NAG	C1-C2	3.25	1.57	1.52
7	A	9315	NAG	C1-C2	3.24	1.57	1.52
7	A	9308	NAG	C1-C2	3.23	1.57	1.52
7	A	9314	NAG	C1-C2	3.21	1.57	1.52
7	A	9313	NAG	C1-C2	3.21	1.57	1.52
7	C	9310	NAG	C1-C2	3.21	1.57	1.52
7	B	9308	NAG	C1-C2	3.20	1.57	1.52
7	C	9317	NAG	C1-C2	3.12	1.57	1.52
7	B	9311	NAG	C1-C2	3.08	1.56	1.52
7	A	9311	NAG	C1-C2	3.04	1.56	1.52
7	A	9316	NAG	C1-C2	3.01	1.56	1.52
7	C	9303	NAG	C1-C2	2.80	1.56	1.52
7	A	9303	NAG	C1-C2	2.73	1.56	1.52
7	A	9301	NAG	C1-C2	2.69	1.56	1.52
7	B	9303	NAG	C1-C2	2.66	1.56	1.52
7	C	9301	NAG	C1-C2	2.66	1.56	1.52
7	C	9308	NAG	C1-C2	2.63	1.56	1.52
7	B	9301	NAG	C1-C2	2.62	1.56	1.52
7	B	9314	NAG	O5-C5	2.23	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	9308	NAG	O5-C5	2.22	1.48	1.43
7	B	9307	NAG	O5-C5	2.14	1.47	1.43
7	C	9307	NAG	O5-C5	2.13	1.47	1.43
7	A	9307	NAG	O5-C5	2.13	1.47	1.43
7	A	9302	NAG	O5-C5	2.12	1.47	1.43
7	C	9302	NAG	O5-C5	2.11	1.47	1.43
7	B	9302	NAG	O5-C5	2.11	1.47	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	9314	NAG	C8-C7-N2	2.87	120.95	116.10
7	C	9301	NAG	C8-C7-N2	2.81	120.86	116.10
7	A	9301	NAG	C8-C7-N2	2.78	120.81	116.10
7	B	9301	NAG	C8-C7-N2	2.75	120.76	116.10
7	A	9317	NAG	C8-C7-N2	2.74	120.73	116.10
7	C	9311	NAG	C8-C7-N2	2.70	120.67	116.10
7	A	9312	NAG	C8-C7-N2	2.70	120.67	116.10
7	C	9309	NAG	C8-C7-N2	2.67	120.61	116.10
7	A	9302	NAG	C8-C7-N2	2.64	120.57	116.10
7	B	9302	NAG	C8-C7-N2	2.63	120.56	116.10
7	C	9302	NAG	C8-C7-N2	2.62	120.53	116.10
7	B	9312	NAG	C8-C7-N2	2.61	120.52	116.10
7	C	9314	NAG	C8-C7-N2	2.58	120.47	116.10
7	A	9303	NAG	C8-C7-N2	2.56	120.44	116.10
7	B	9311	NAG	C8-C7-N2	2.55	120.42	116.10
7	A	9311	NAG	C8-C7-N2	2.54	120.39	116.10
7	C	9303	NAG	C8-C7-N2	2.53	120.39	116.10
7	B	9305	NAG	C8-C7-N2	2.52	120.37	116.10
7	C	9310	NAG	C8-C7-N2	2.51	120.36	116.10
7	A	9305	NAG	C8-C7-N2	2.51	120.35	116.10
7	B	9313	NAG	C8-C7-N2	2.50	120.33	116.10
7	C	9305	NAG	C8-C7-N2	2.50	120.33	116.10
7	B	9310	NAG	C8-C7-N2	2.49	120.31	116.10
7	B	9303	NAG	C8-C7-N2	2.48	120.30	116.10
7	C	9313	NAG	C8-C7-N2	2.48	120.30	116.10
7	B	9308	NAG	C8-C7-N2	2.47	120.29	116.10
7	A	9304	NAG	C8-C7-N2	2.47	120.28	116.10
7	C	9315	NAG	C8-C7-N2	2.46	120.27	116.10
7	A	9316	NAG	C8-C7-N2	2.46	120.27	116.10
7	B	9304	NAG	C8-C7-N2	2.46	120.26	116.10
7	A	9308	NAG	C8-C7-N2	2.45	120.25	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	9307	NAG	C8-C7-N2	2.45	120.25	116.10
7	C	9304	NAG	C8-C7-N2	2.44	120.23	116.10
7	A	9310	NAG	C8-C7-N2	2.44	120.22	116.10
7	A	9314	NAG	C8-C7-N2	2.43	120.21	116.10
7	B	9309	NAG	C8-C7-N2	2.43	120.21	116.10
7	B	9315	NAG	C8-C7-N2	2.42	120.20	116.10
7	B	9307	NAG	C8-C7-N2	2.40	120.17	116.10
7	A	9307	NAG	C8-C7-N2	2.40	120.16	116.10
7	A	9306	NAG	C8-C7-N2	2.39	120.14	116.10
7	C	9306	NAG	C8-C7-N2	2.38	120.13	116.10
7	A	9315	NAG	C8-C7-N2	2.37	120.11	116.10
7	B	9306	NAG	C8-C7-N2	2.34	120.07	116.10
7	A	9313	NAG	C8-C7-N2	2.31	120.01	116.10
7	B	9306	NAG	C1-C2-N2	-2.30	106.56	110.49
7	C	9306	NAG	C1-C2-N2	-2.28	106.59	110.49
7	C	9317	NAG	C8-C7-N2	2.28	119.96	116.10
7	A	9309	NAG	C8-C7-N2	2.27	119.94	116.10
7	C	9316	NAG	C8-C7-N2	2.27	119.94	116.10
7	A	9306	NAG	C1-C2-N2	-2.27	106.61	110.49
7	C	9312	NAG	C8-C7-N2	2.23	119.88	116.10
7	A	9301	NAG	C2-N2-C7	-2.22	119.74	122.90
7	B	9301	NAG	C2-N2-C7	-2.22	119.75	122.90
7	C	9301	NAG	C2-N2-C7	-2.22	119.75	122.90
7	C	9308	NAG	C8-C7-N2	2.06	119.58	116.10
7	B	9314	NAG	C4-C3-C2	-2.01	108.07	111.02
7	B	9314	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	9315	NAG	O5-C5-C6-O6
7	B	9316	NAG	O5-C5-C6-O6
7	B	9316	NAG	C4-C5-C6-O6
7	B	9315	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	9312	NAG	1	0

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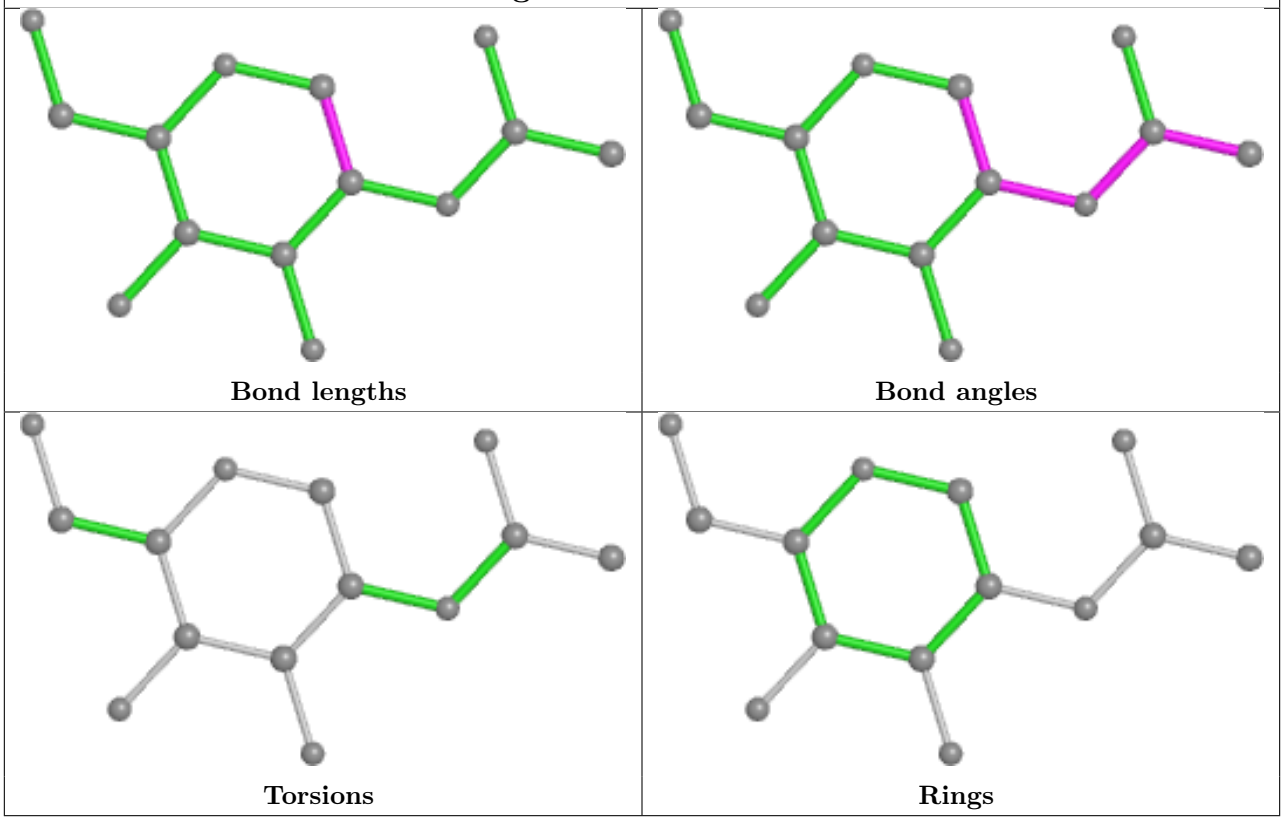
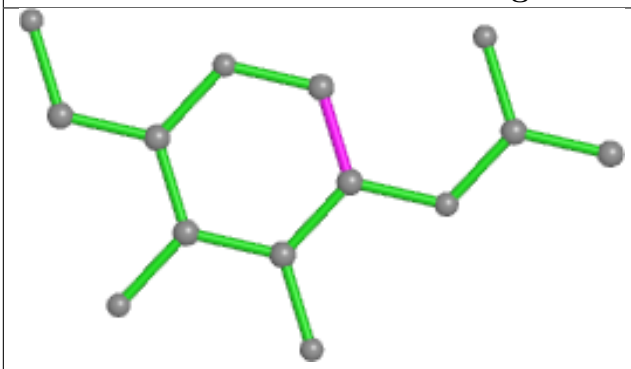
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	9309	NAG	1	0

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

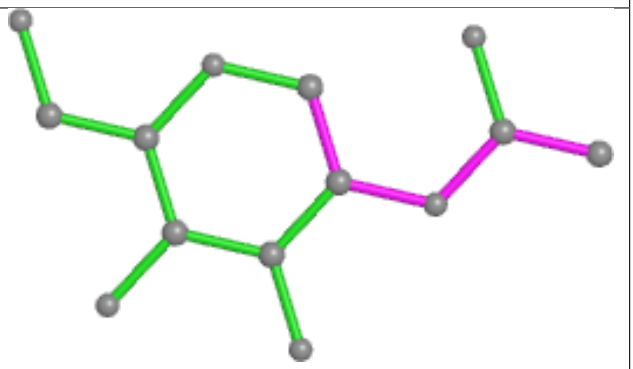
Ligand NAG B 9306



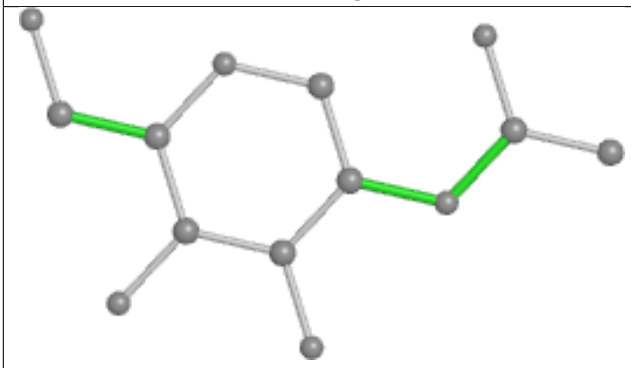
Ligand NAG C 9306



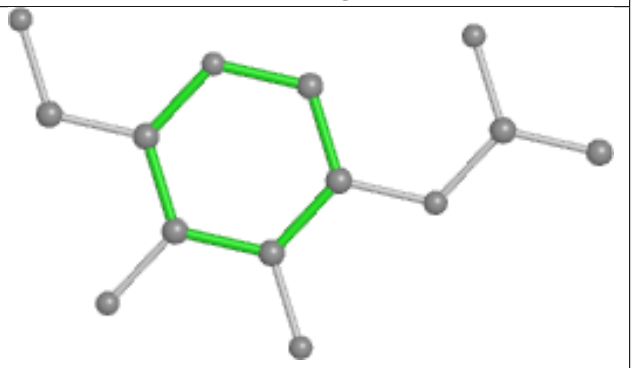
Bond lengths



Bond angles

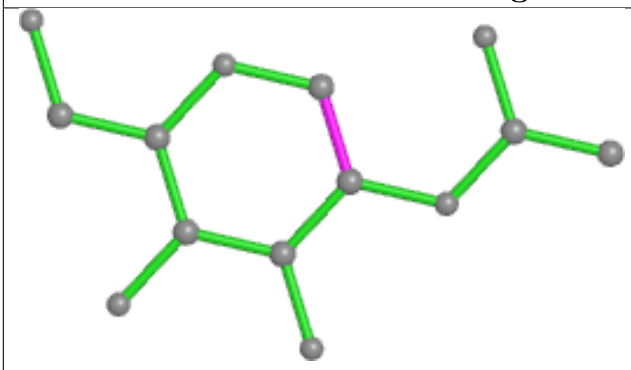


Torsions



Rings

Ligand NAG A 9305



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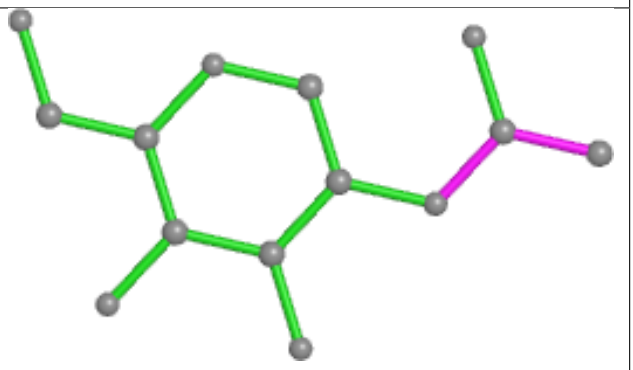
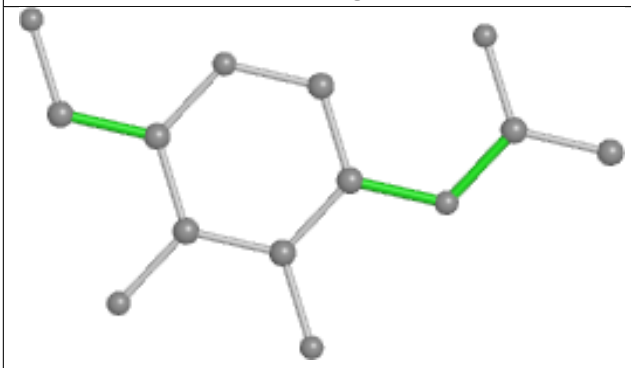


Bond angles



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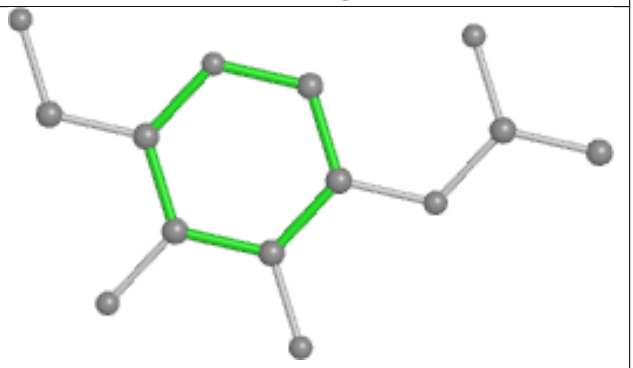
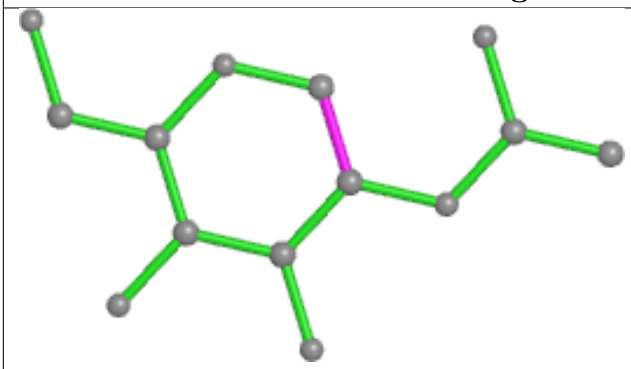


Rings

Ligand NAG A 9301



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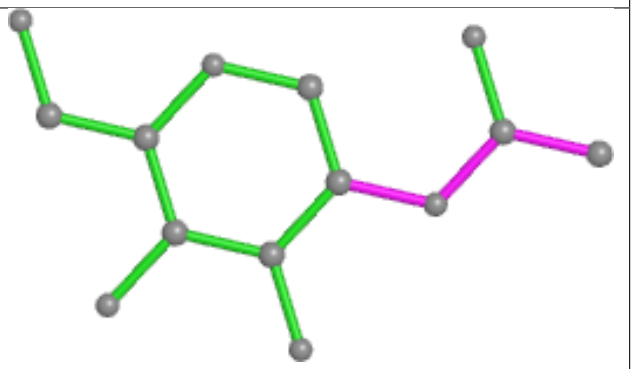
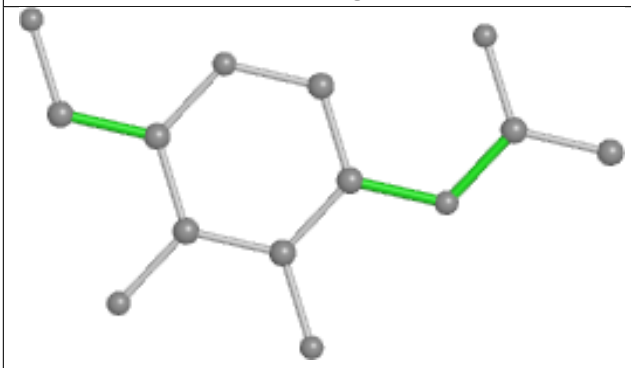
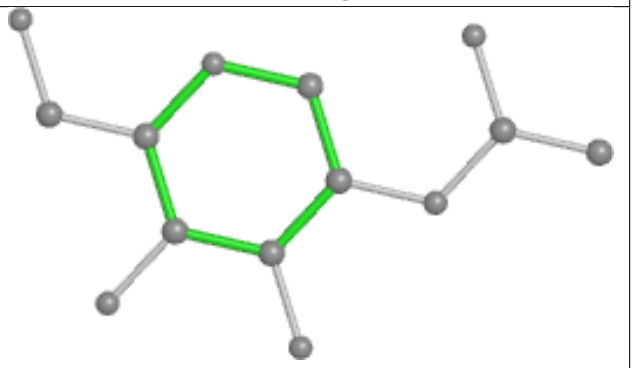


Bond angles

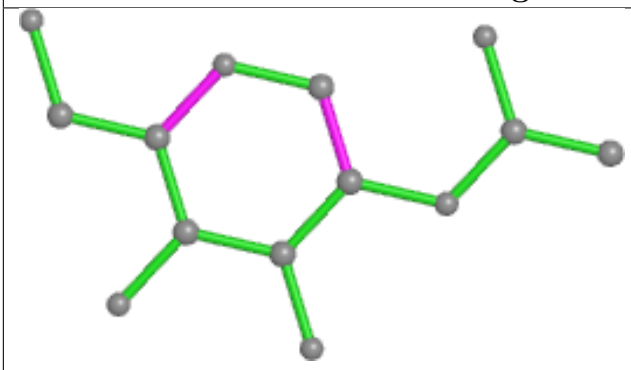


Torsions



Rings

Ligand NAG B 9302



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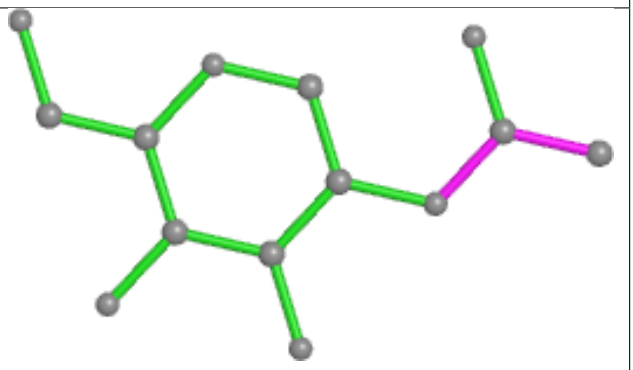
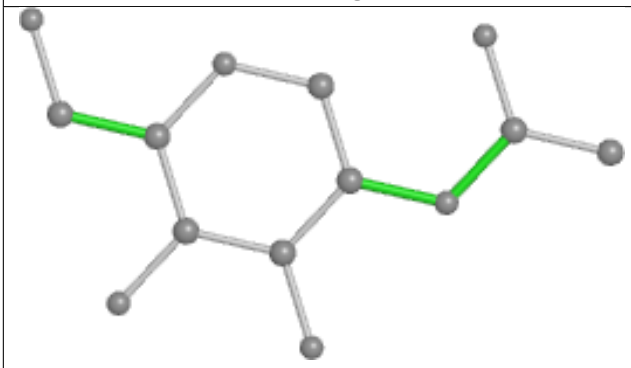


Bond angles



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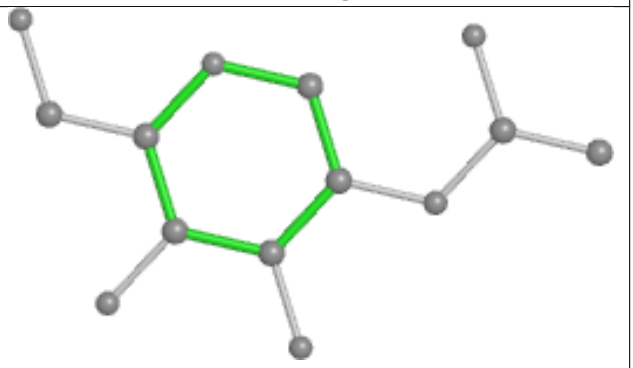
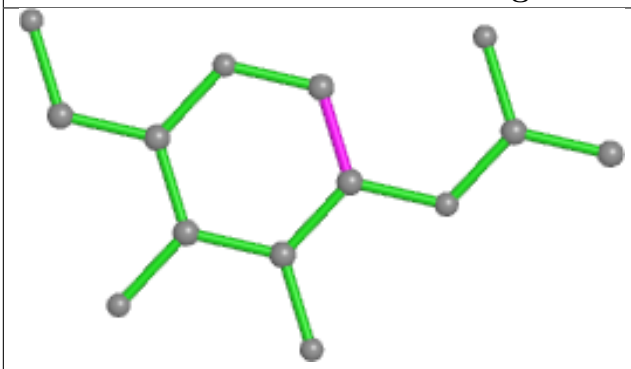


Rings

Ligand NAG B 9313



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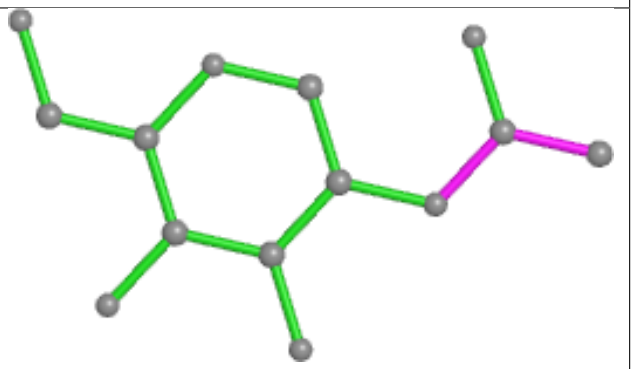

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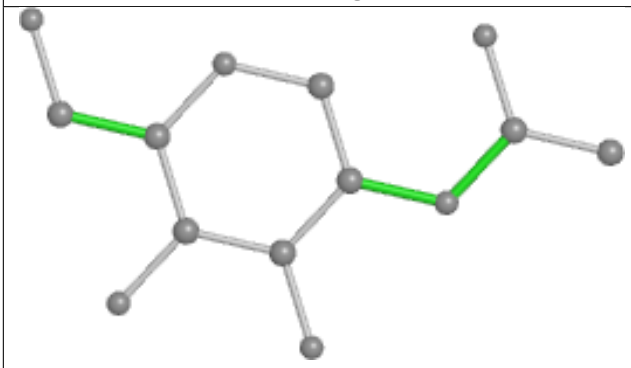

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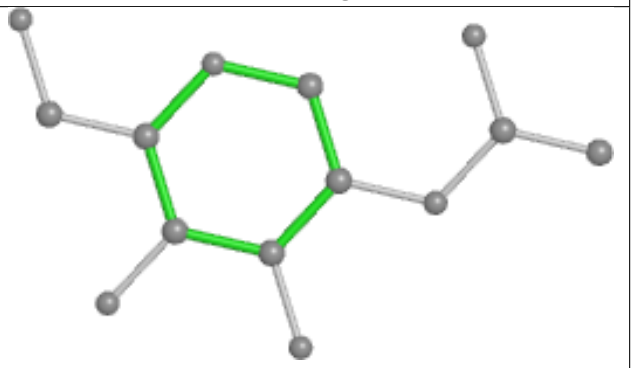

Rings

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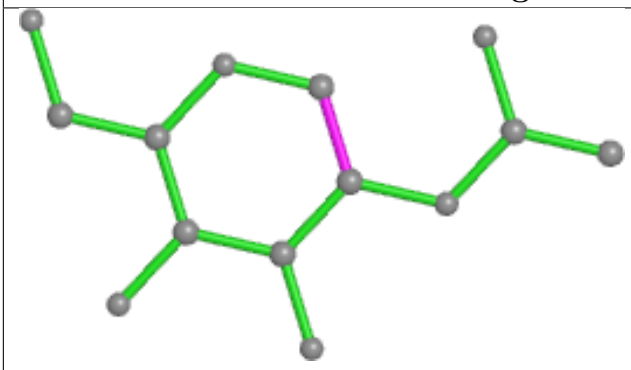

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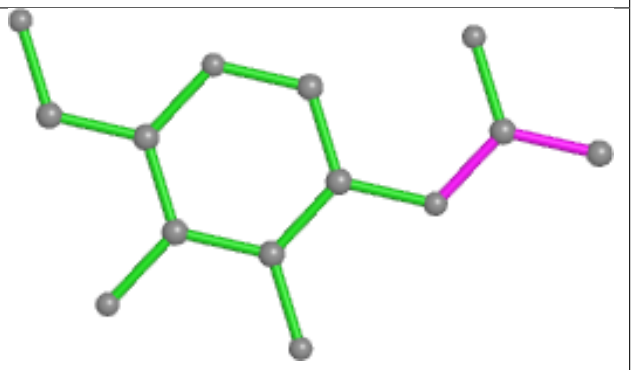

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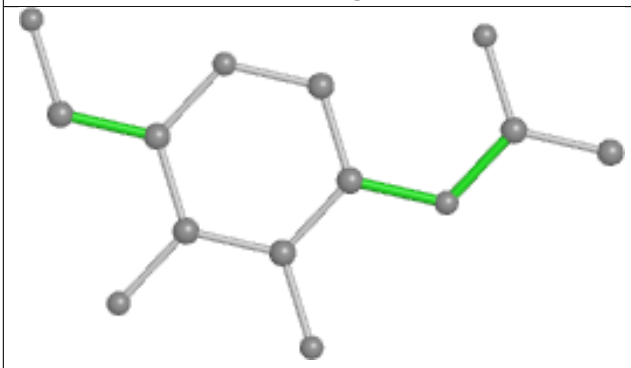

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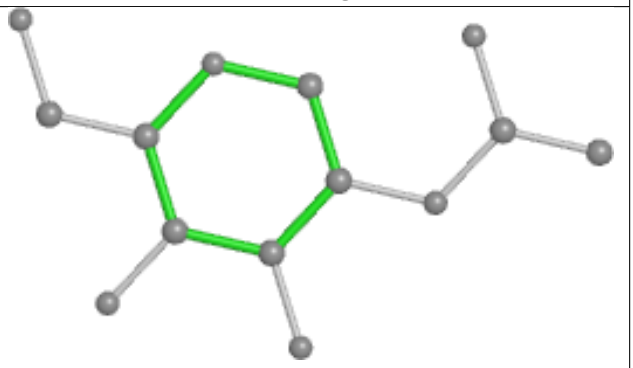
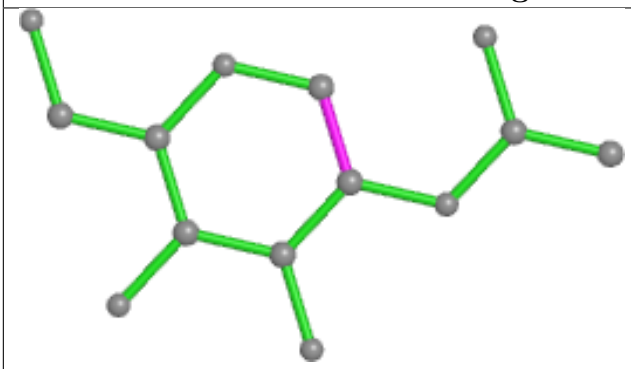


Rings

Ligand NAG C 9313



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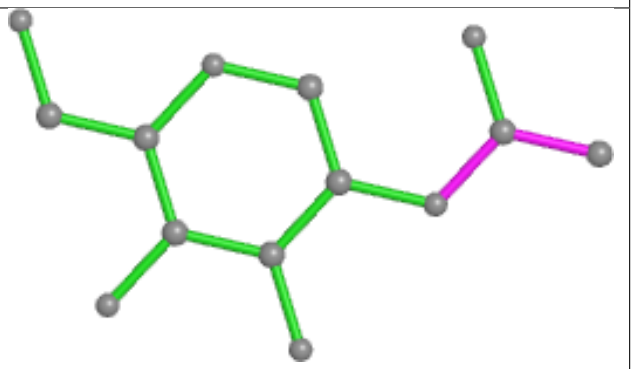

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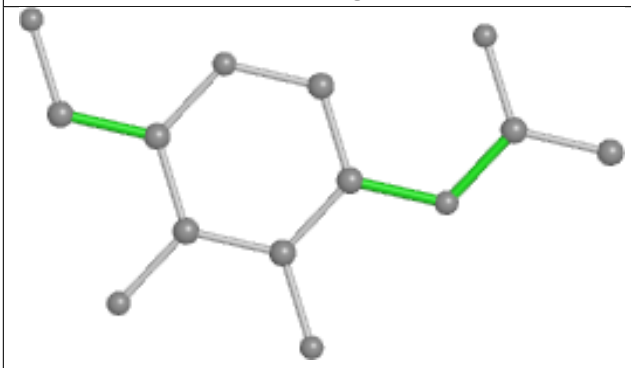

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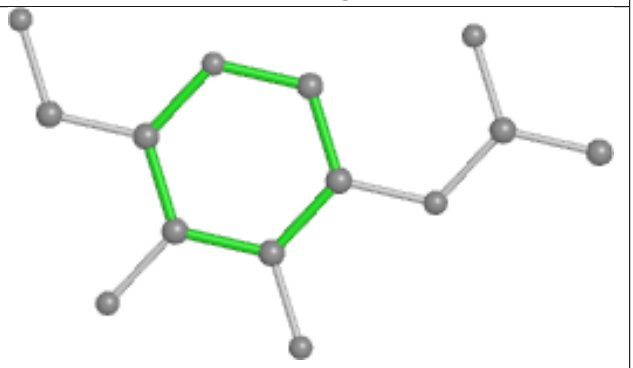
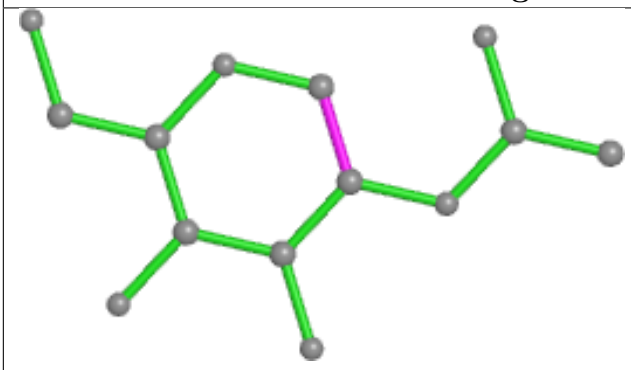


Rings

Ligand NAG B 9308



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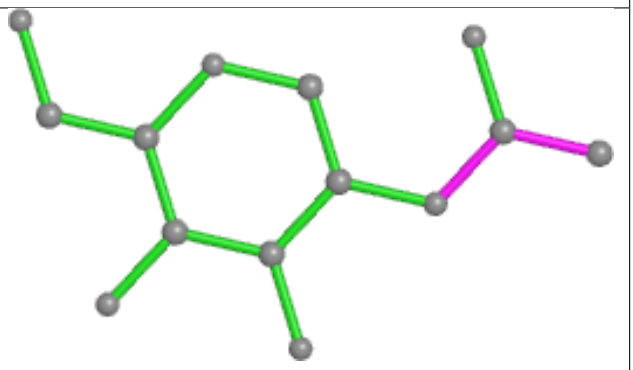

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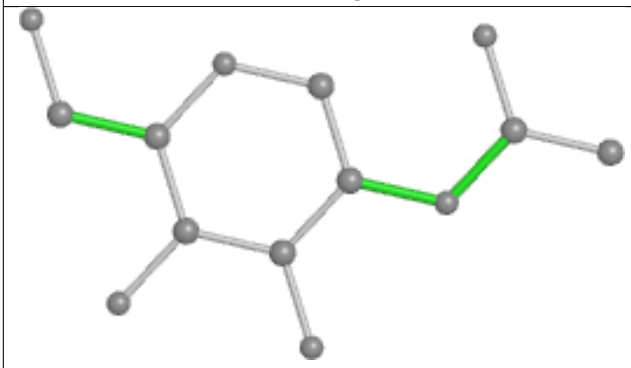
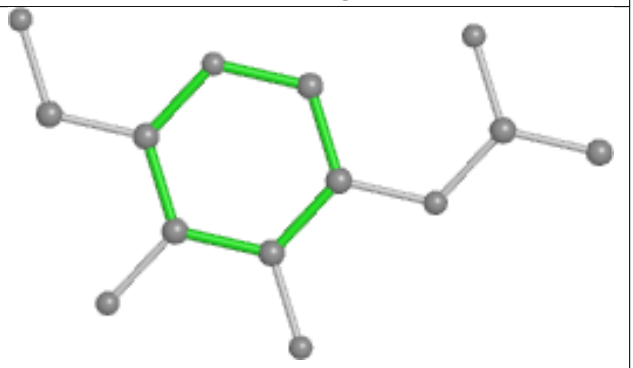
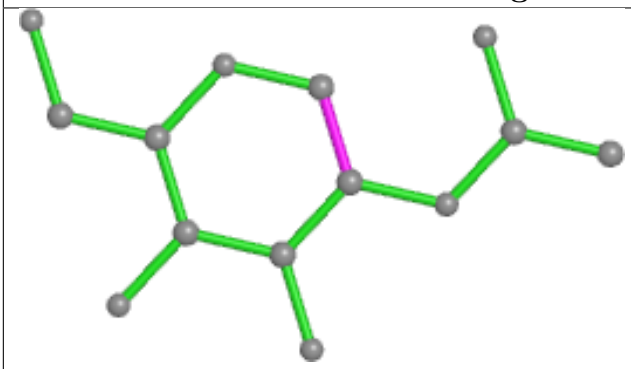


Torsions



Rings

Ligand NAG A 9306



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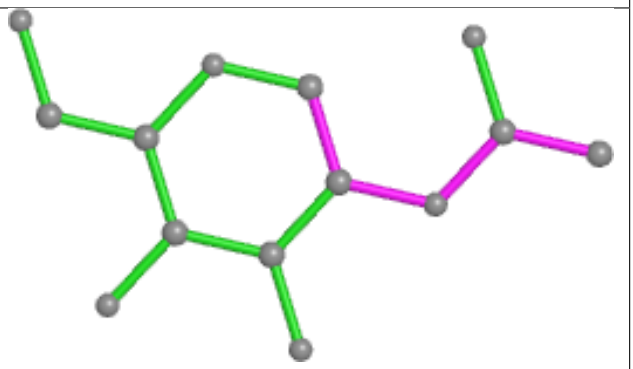

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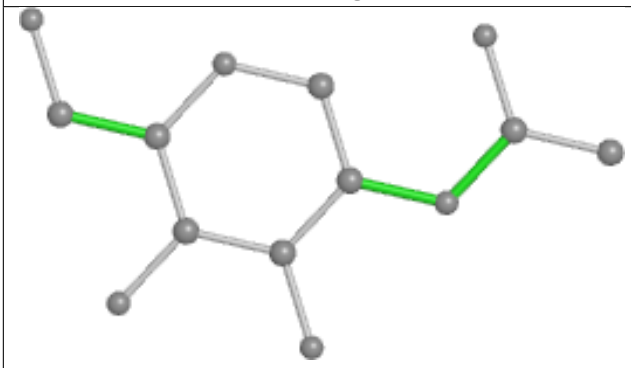

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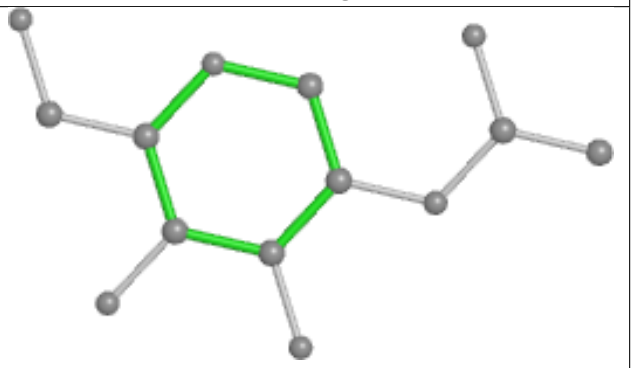
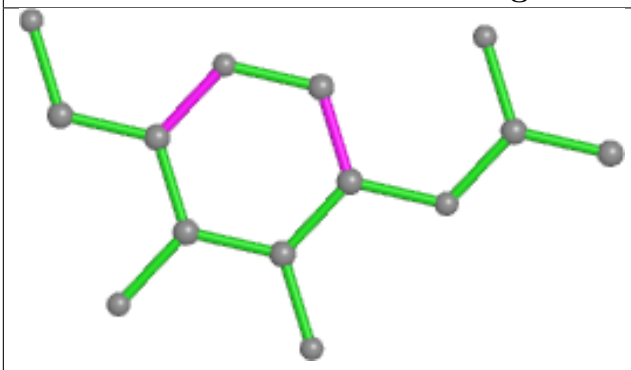


Rings

Ligand NAG A 9307



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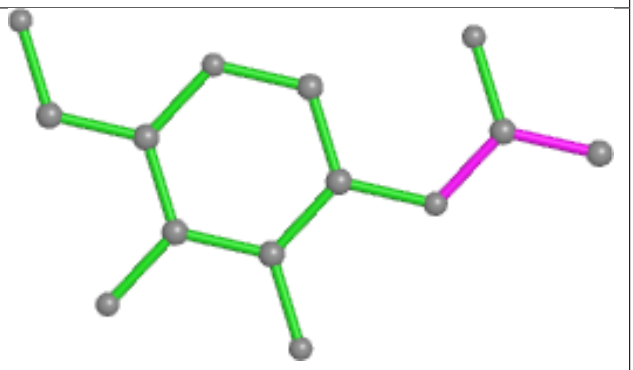

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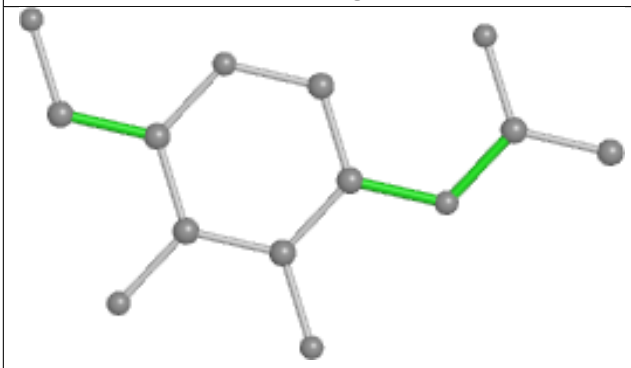

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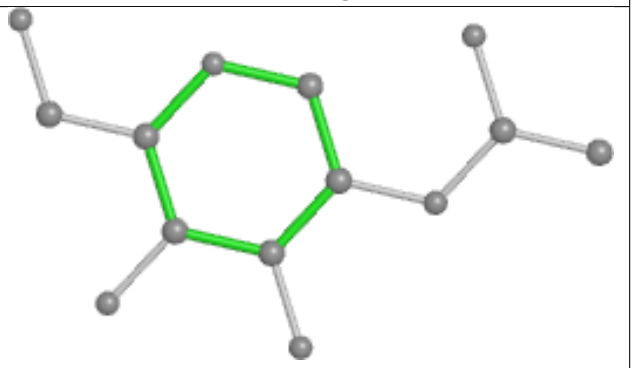
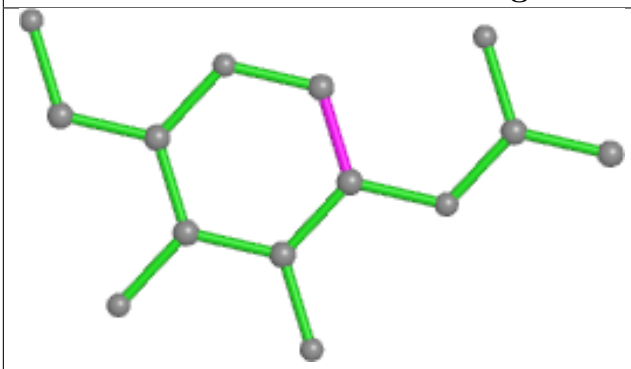


Rings

Ligand NAG A 9314



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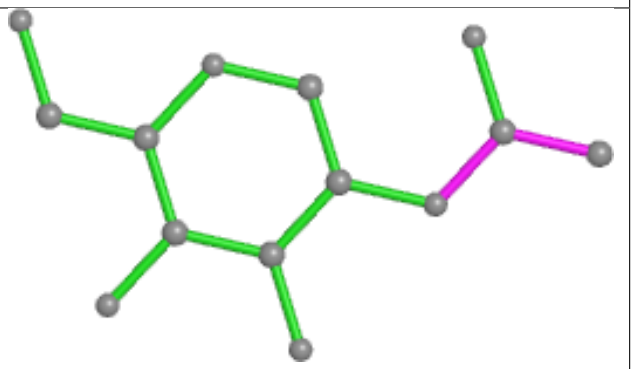
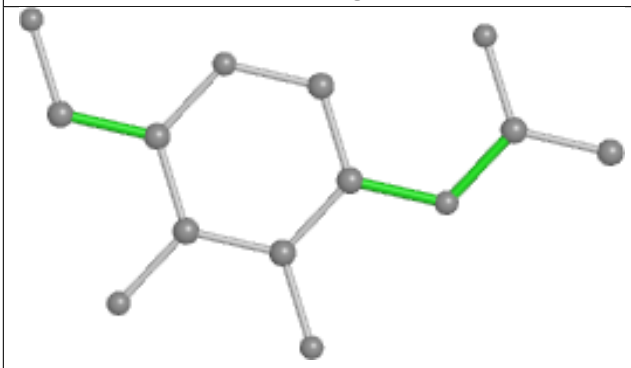


Bond angles



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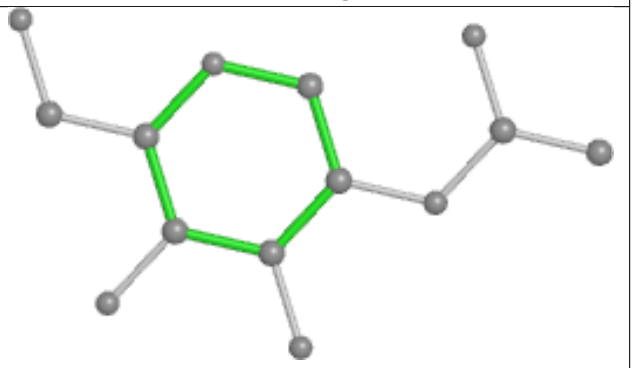
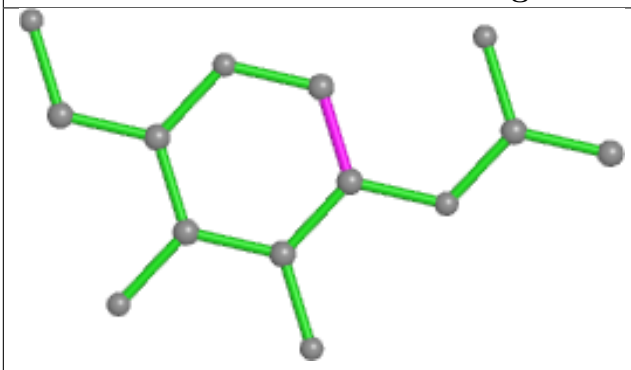


Rings

Ligand NAG C 9316



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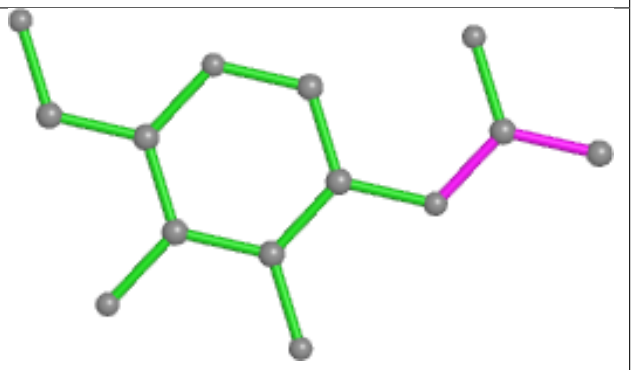
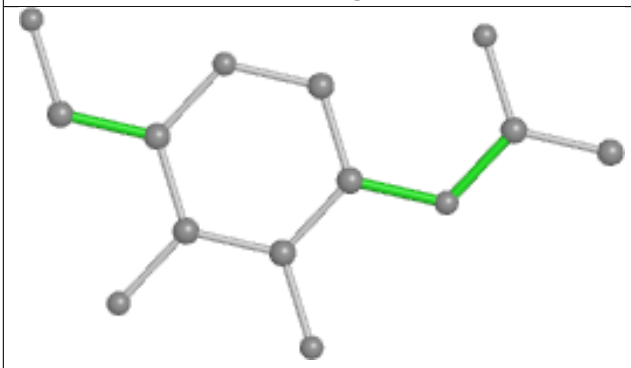


Bond angles



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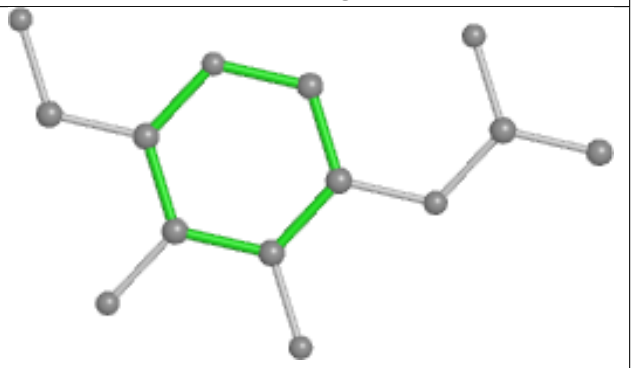
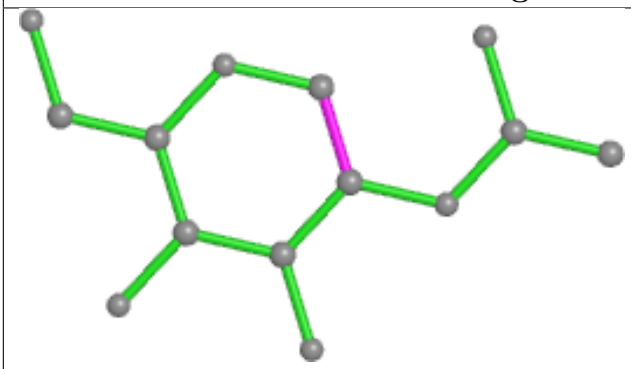


Rings

Ligand NAG C 9303



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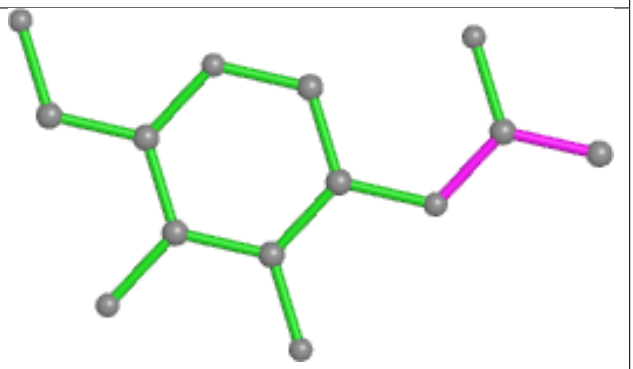
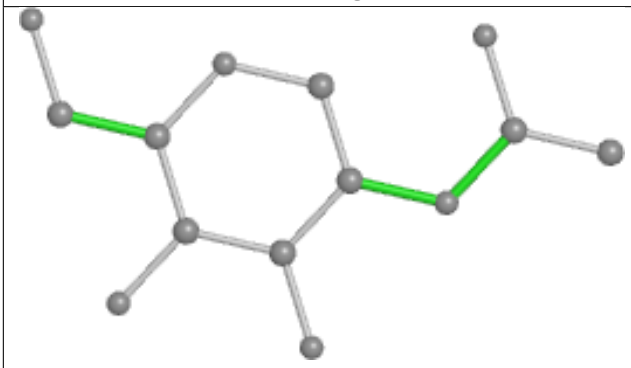


Bond angles



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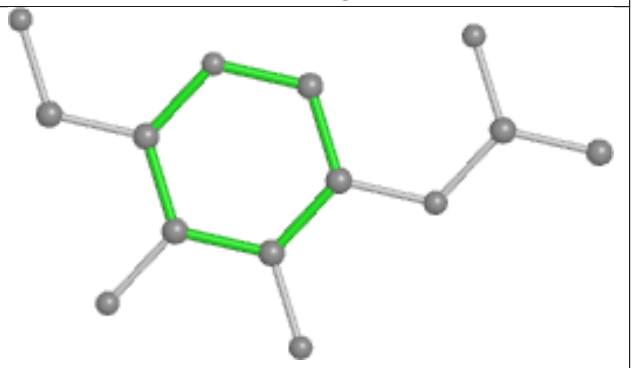
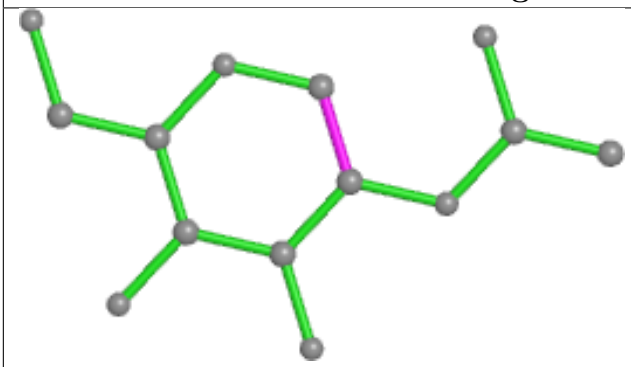
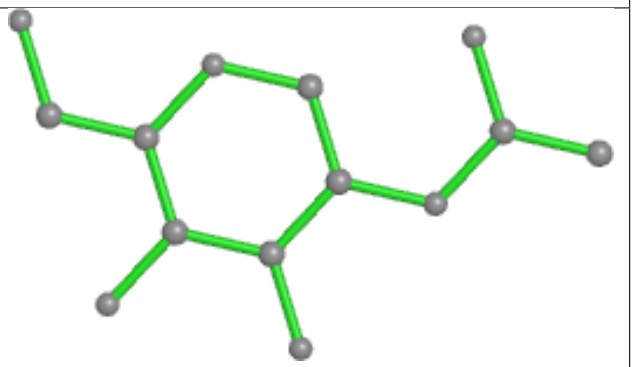


Rings

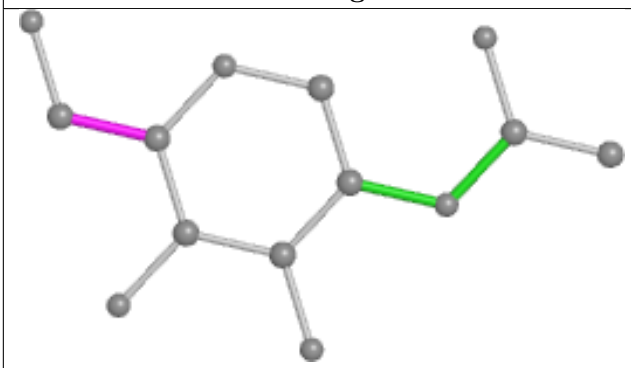
Ligand NAG B 9316



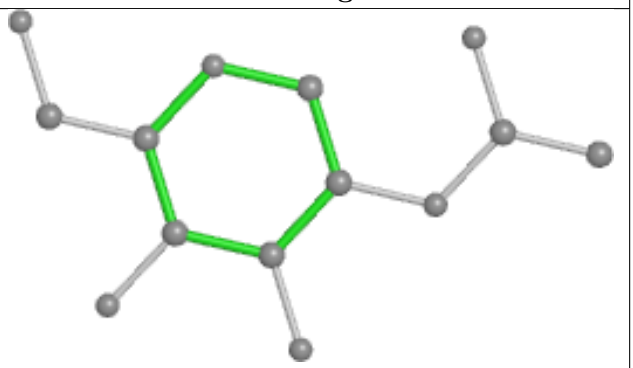
Bond lengths



Bond angles

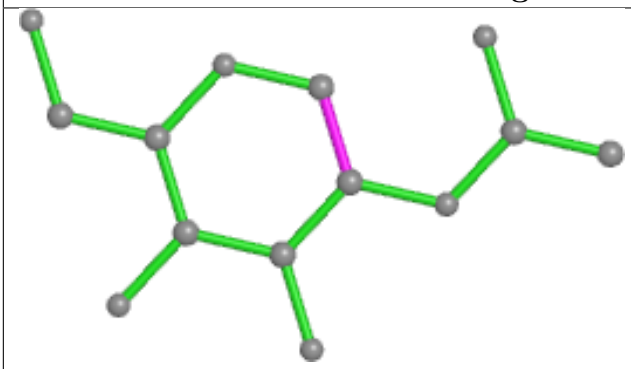


Torsions



Rings

Ligand NAG C 9312



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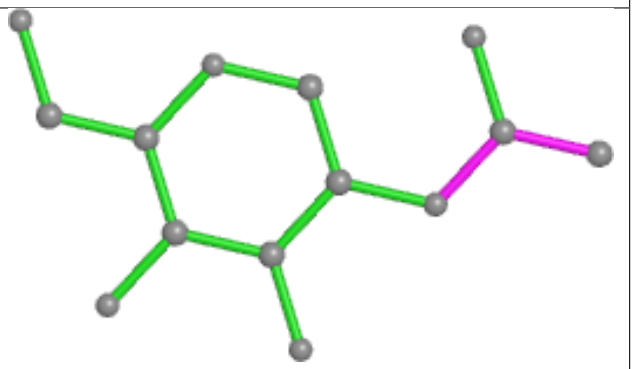
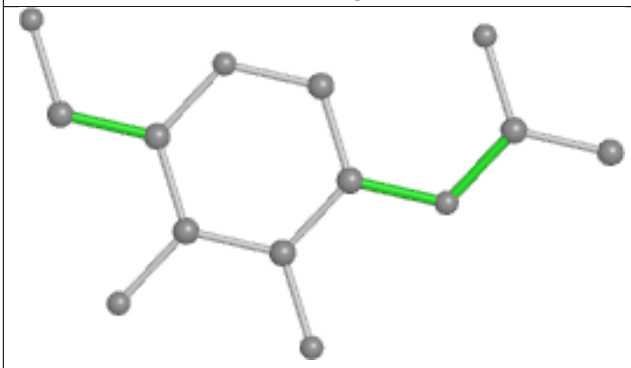


Bond angles



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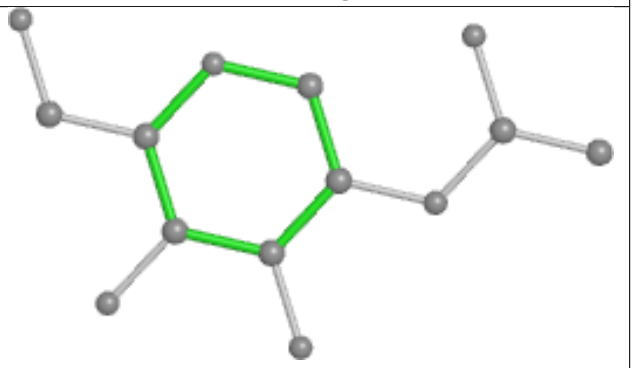
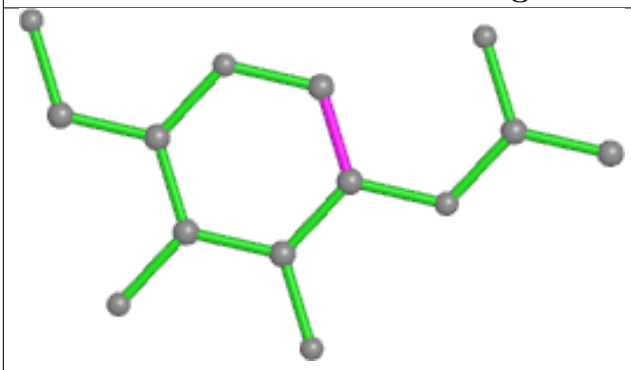


Rings

Ligand NAG C 9317



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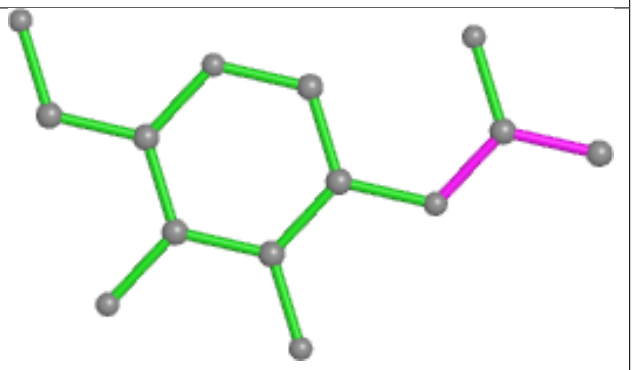
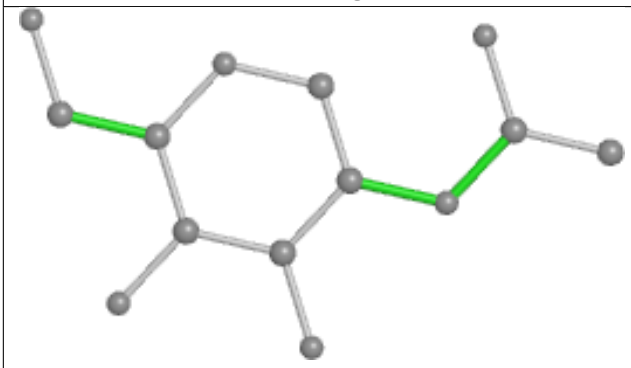


Bond angles



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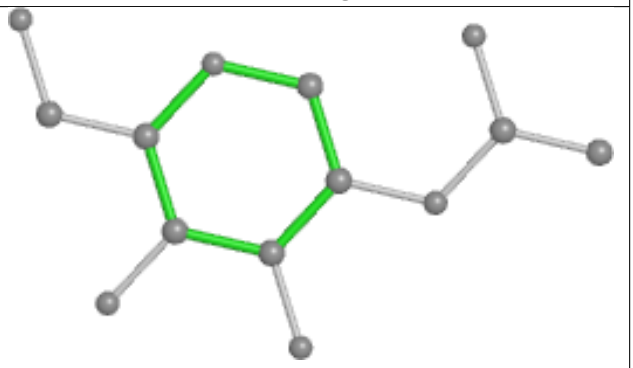
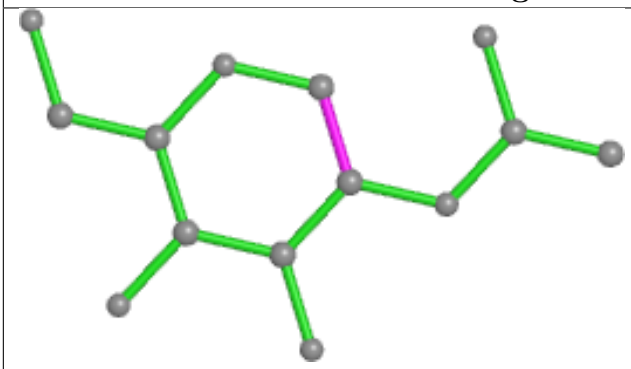


Rings

Ligand NAG B 9303



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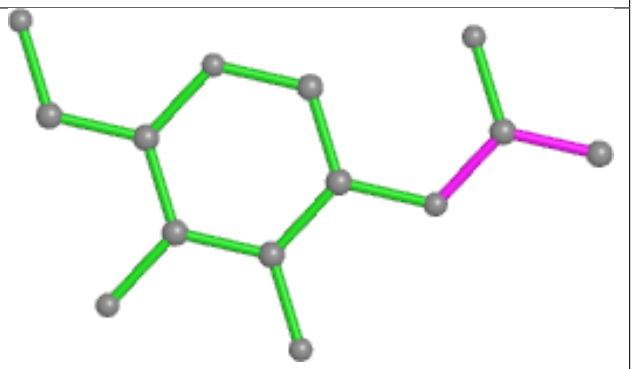
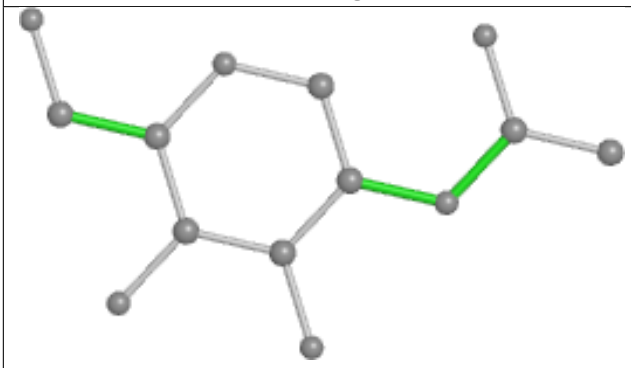


Bond angles



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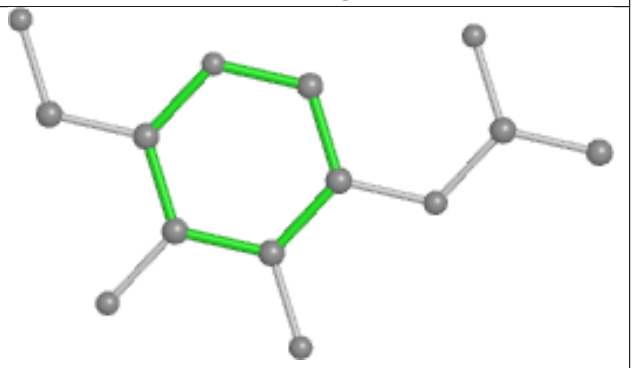
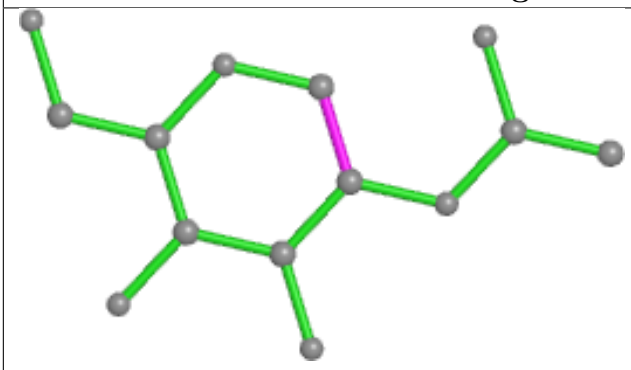


Rings

Ligand NAG B 9304



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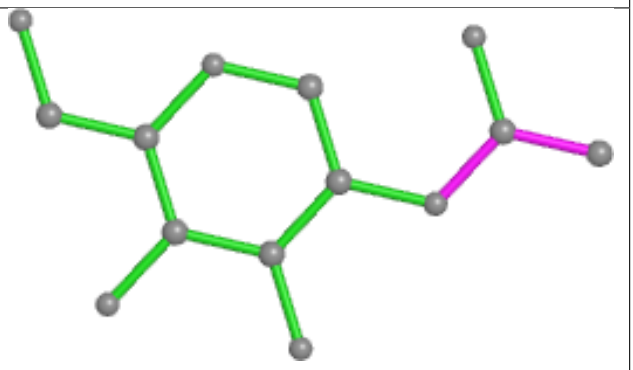
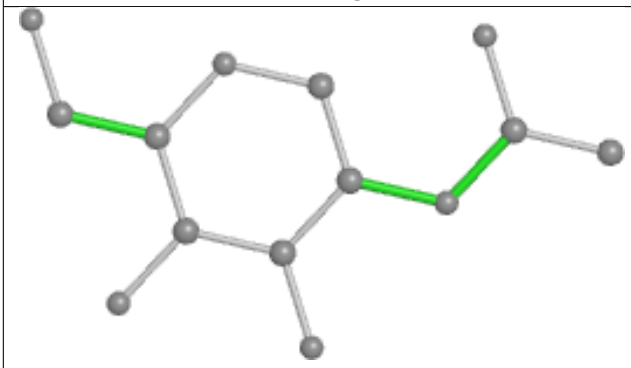


Bond angles



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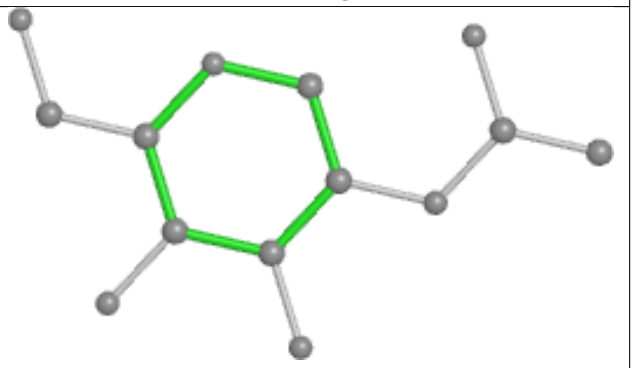
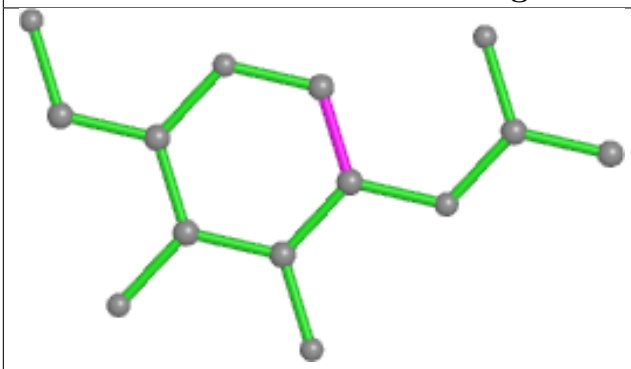


Rings

Ligand NAG A 9303



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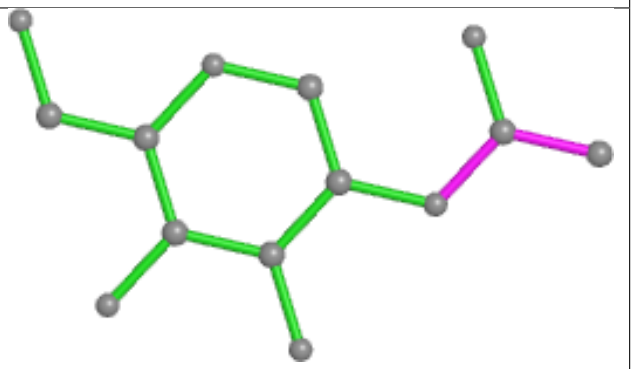
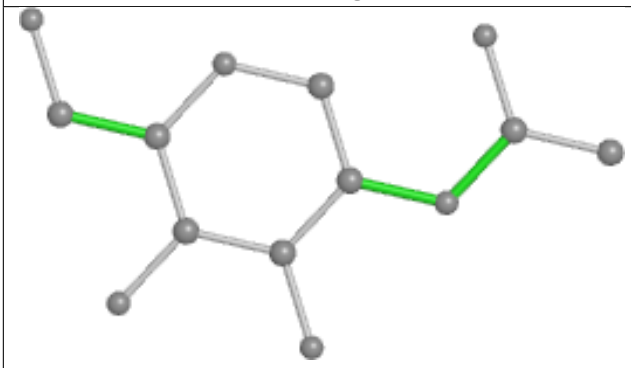


Bond angles



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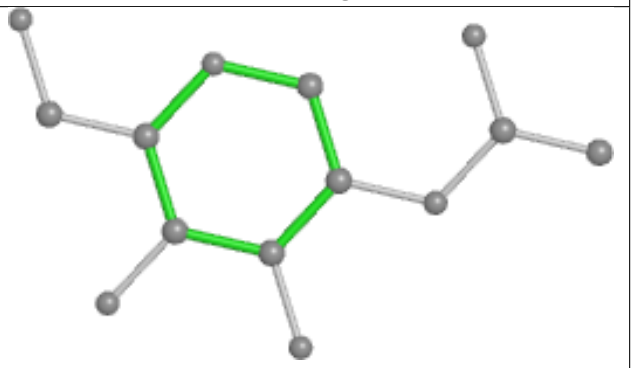
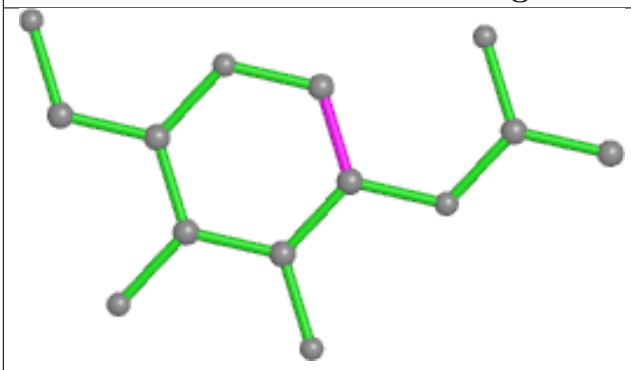
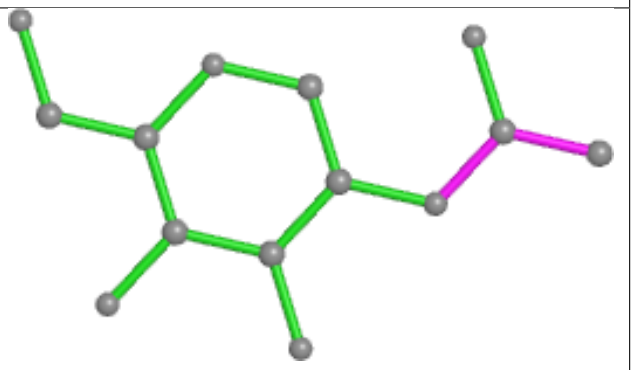


Rings

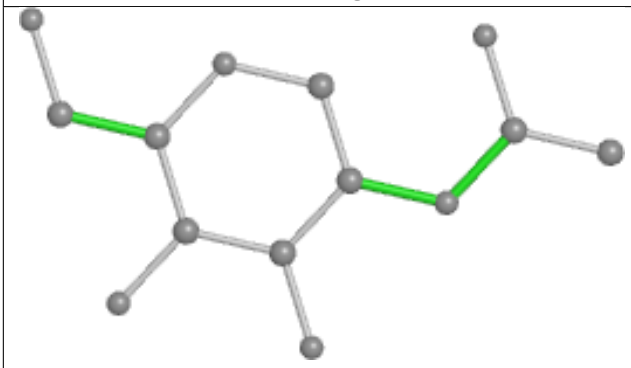
Ligand NAG C 9304



Bond lengths



Bond angles



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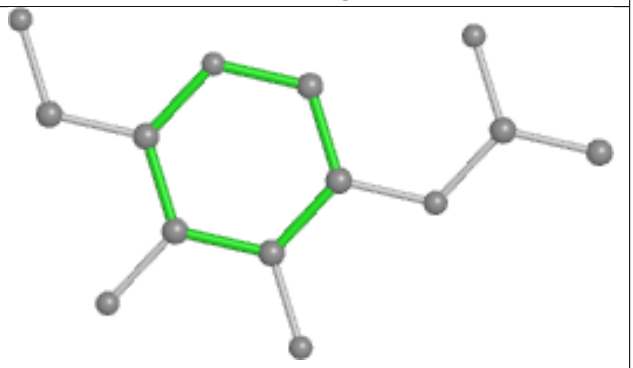
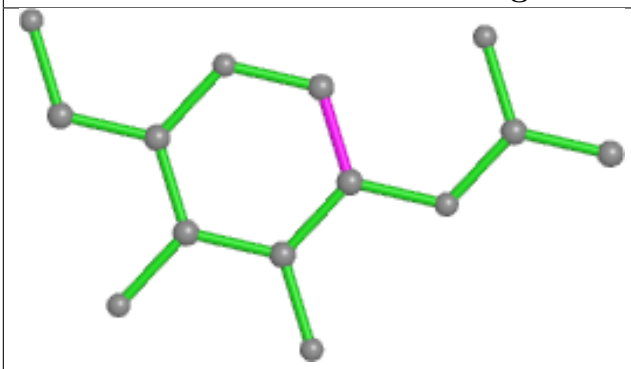


Rings

Ligand NAG A 9313



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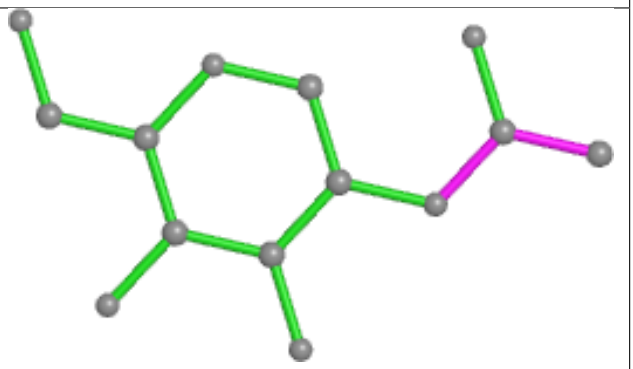
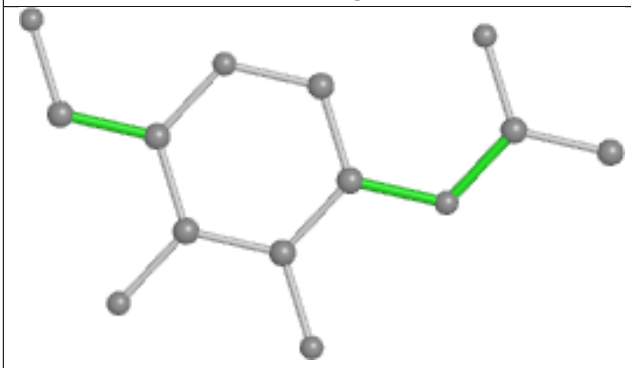
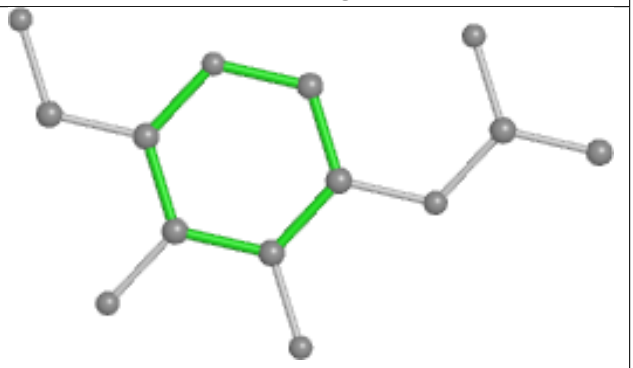


Bond angles

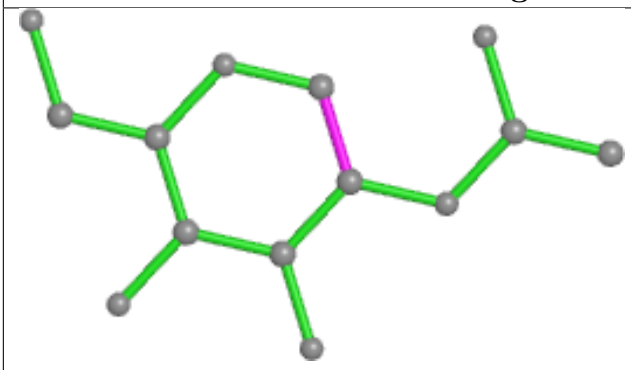


Torsions



Rings

Ligand NAG A 9308



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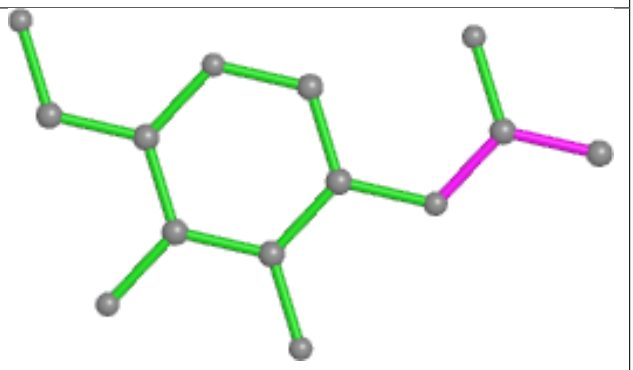
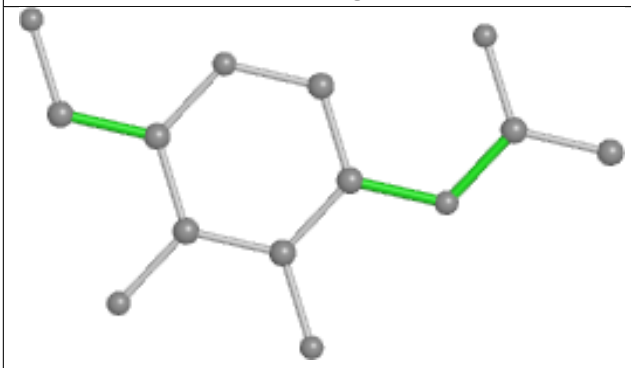


Bond angles



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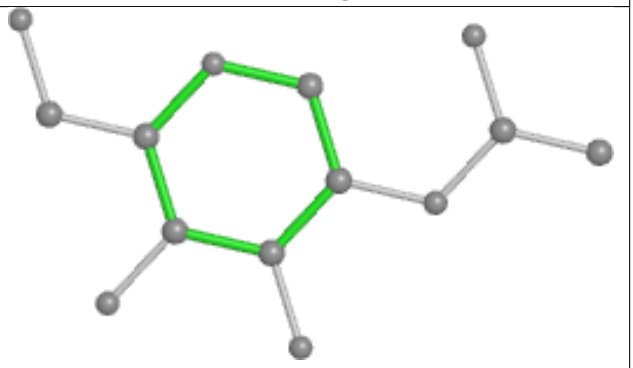
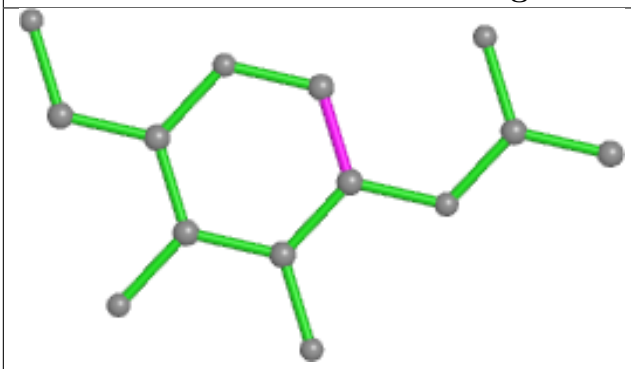


Rings

Ligand NAG A 9312



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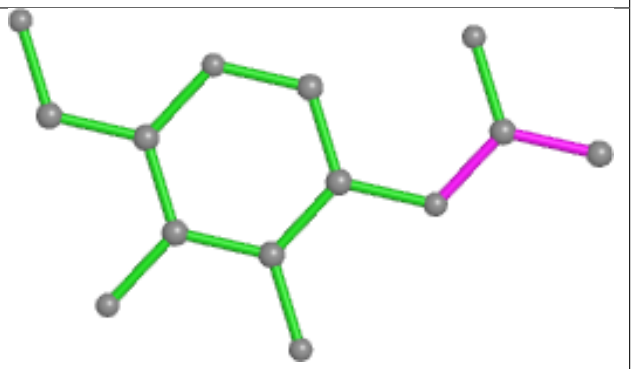
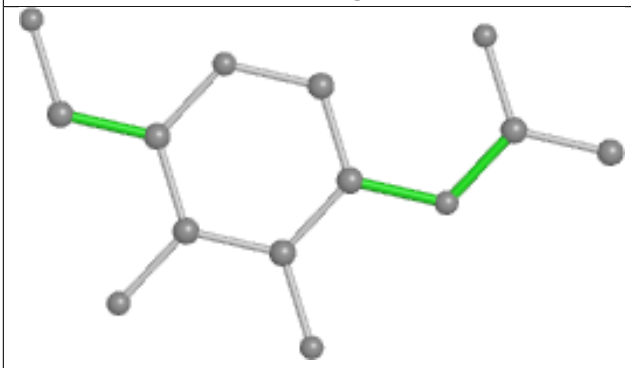


Bond angles



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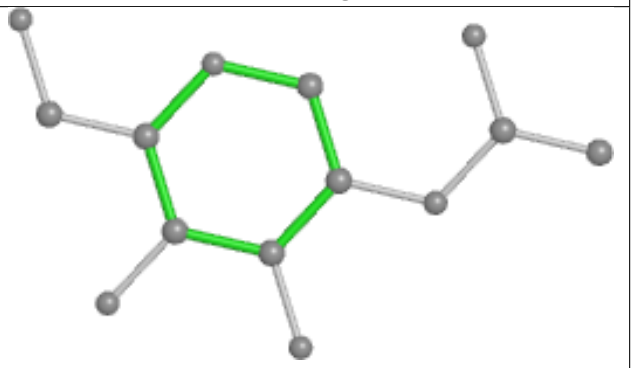
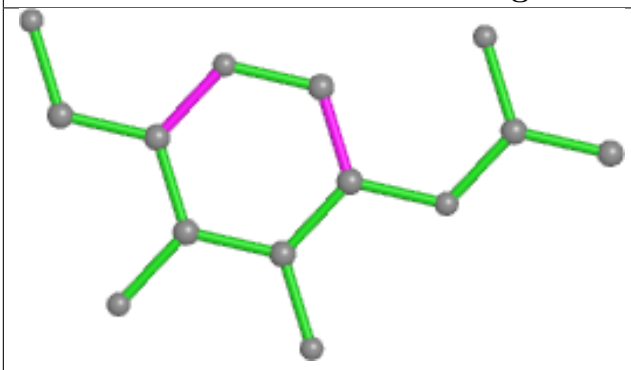


Rings

Ligand NAG C 9307



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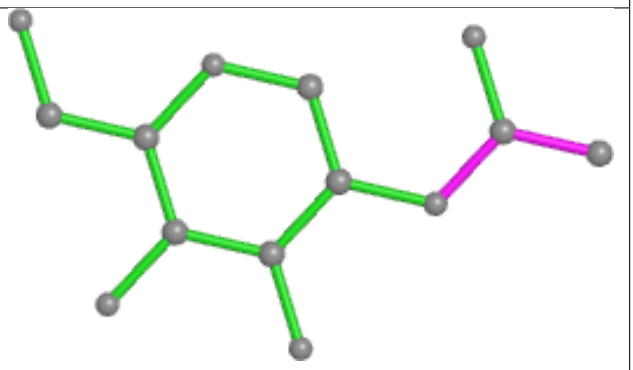
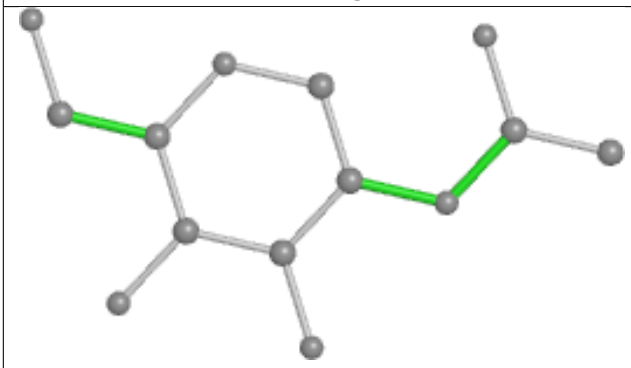


Bond angles



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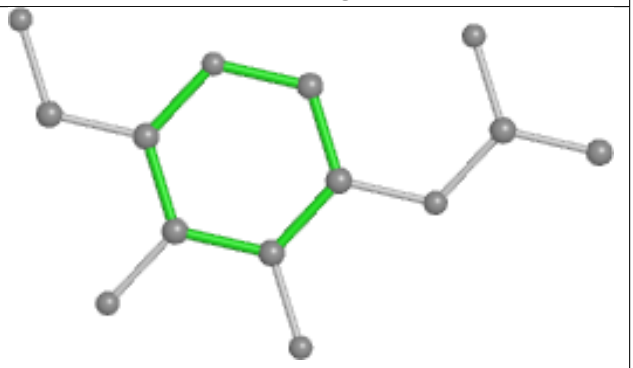
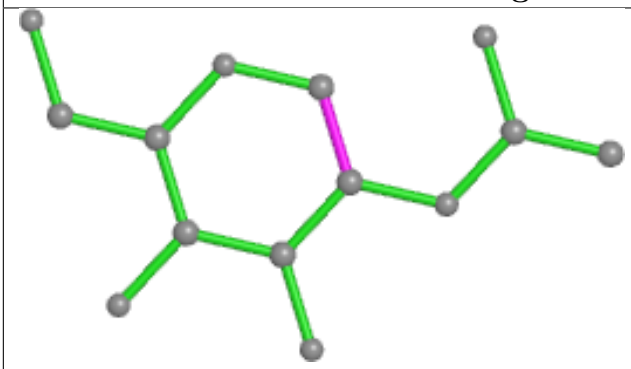
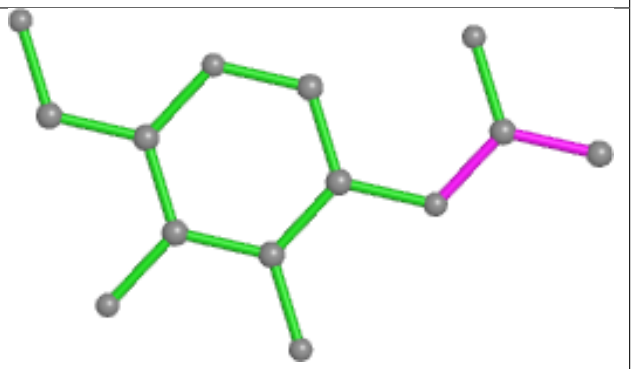


Rings

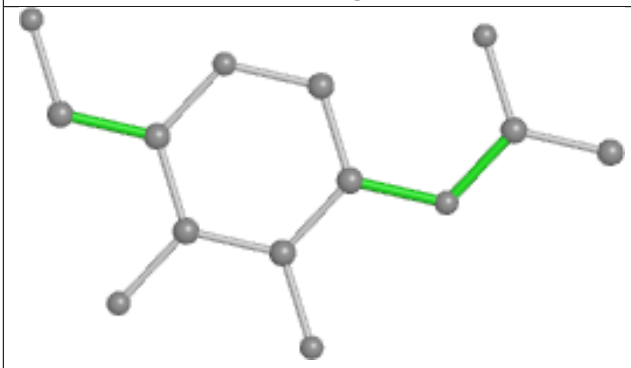
Ligand NAG B 9311



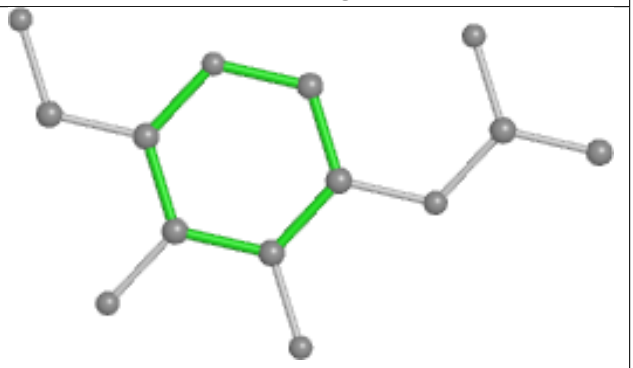
Bond lengths



Bond angles

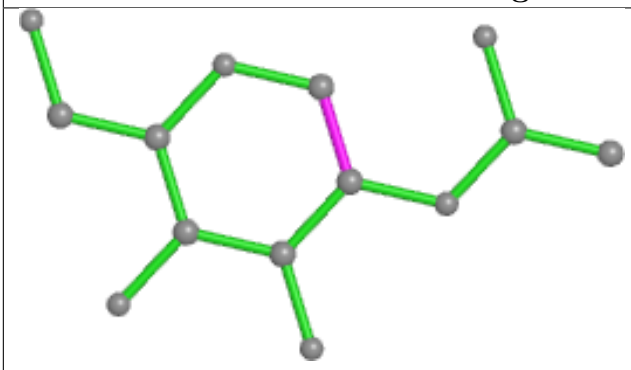


Torsions



Rings

Ligand NAG B 9315



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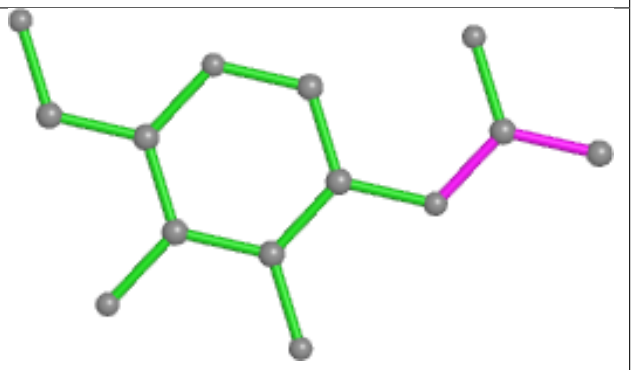
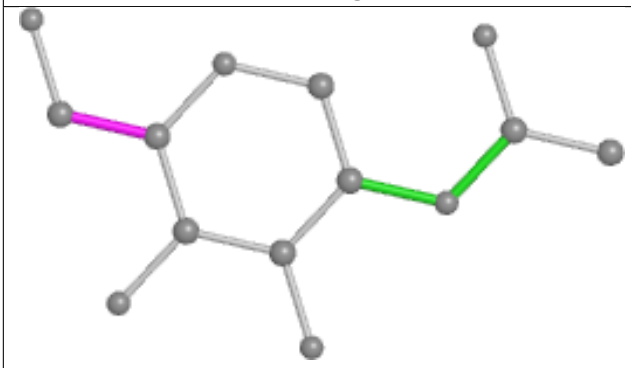


Bond angles



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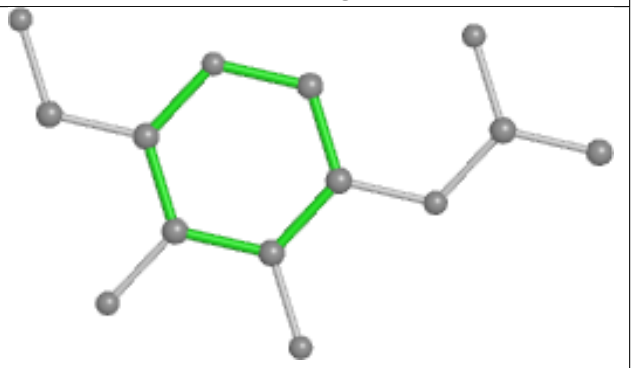
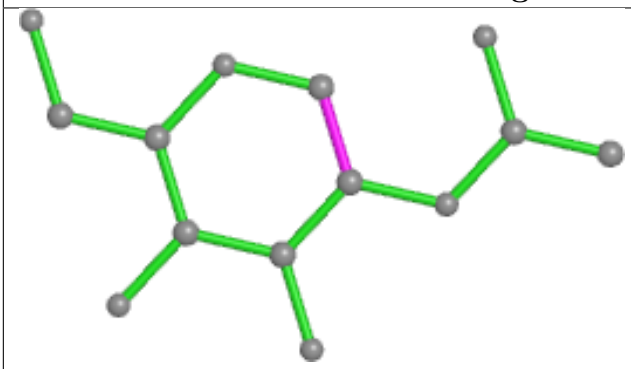


Rings

Ligand NAG C 9315



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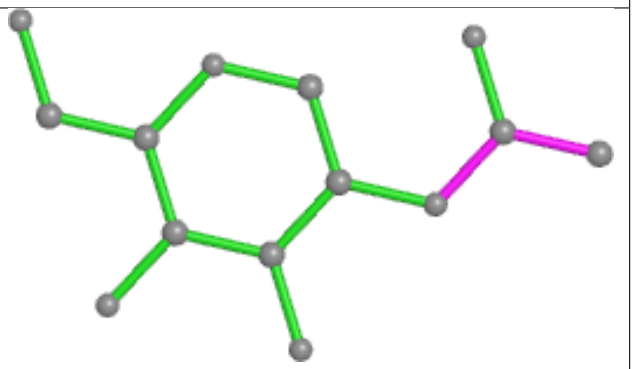
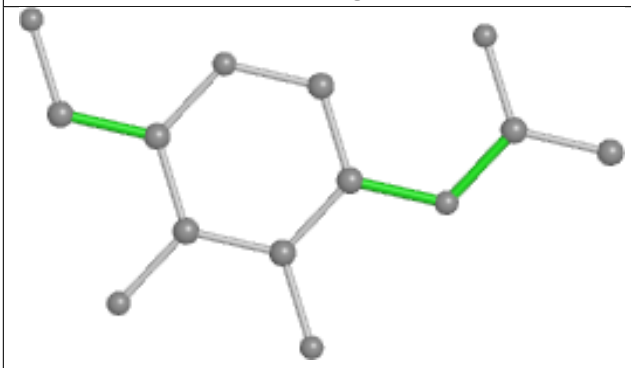
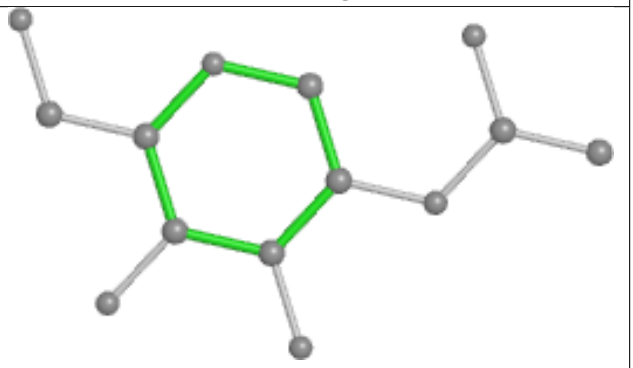


Bond angles

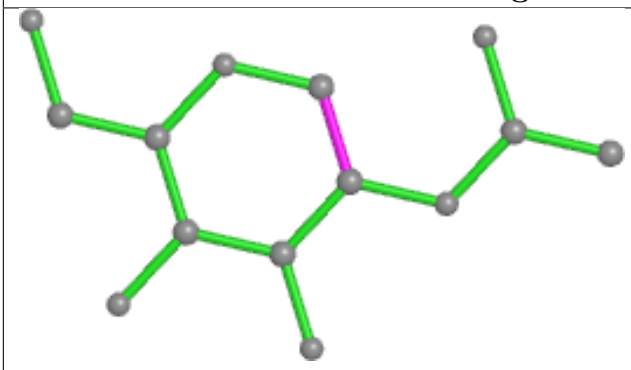


Torsions

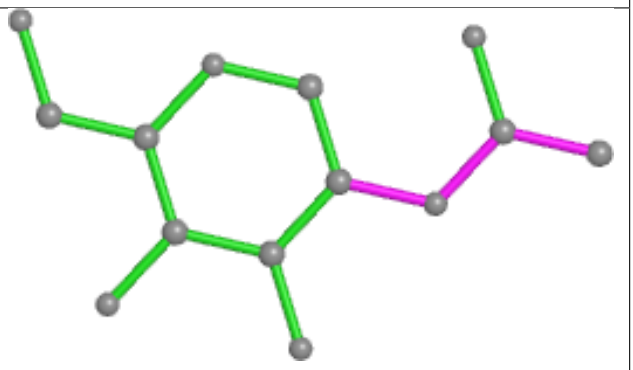


Rings

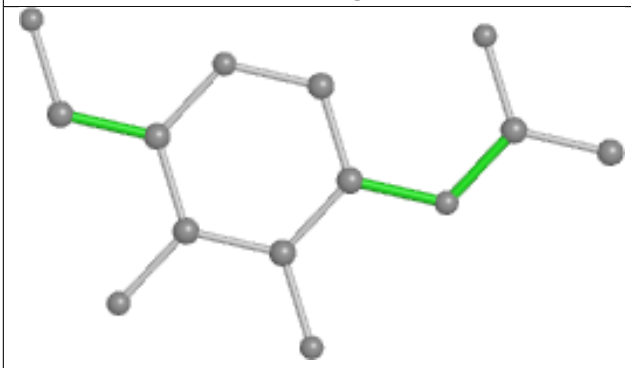
Ligand NAG C 9301



Bond lengths



Bond angles



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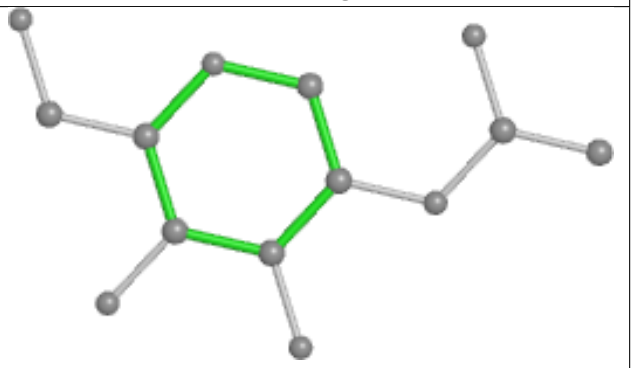
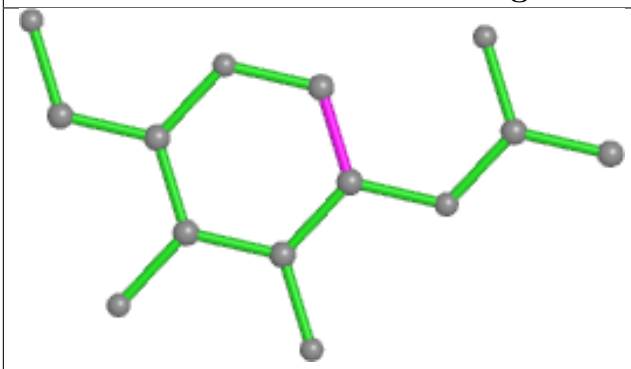


Rings

Ligand NAG A 9315



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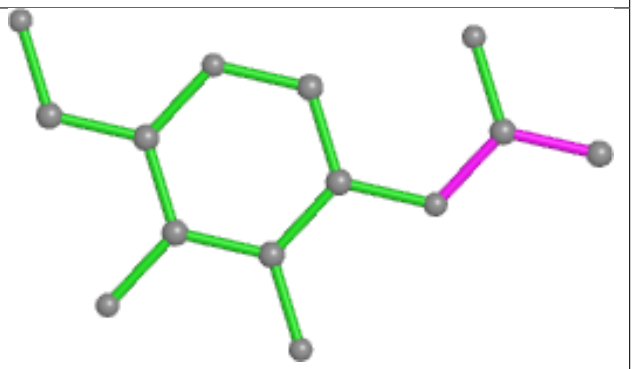
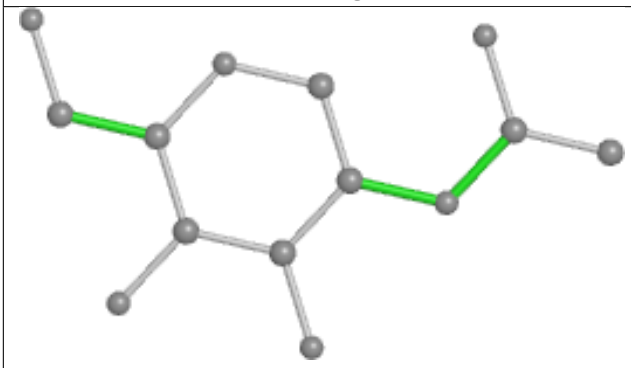


Bond angles



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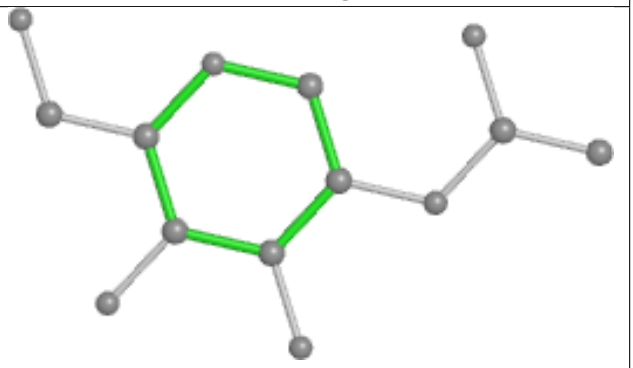
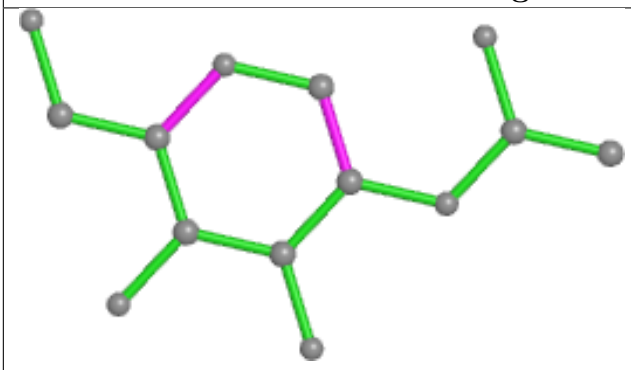


Rings

Ligand NAG B 9307



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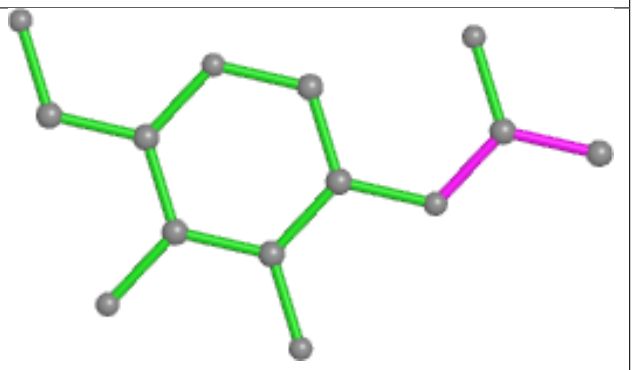
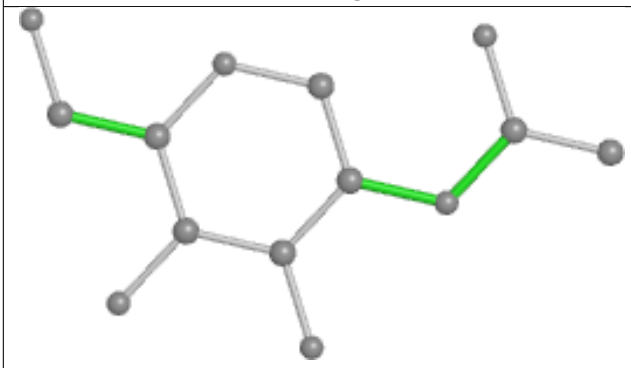


Bond angles



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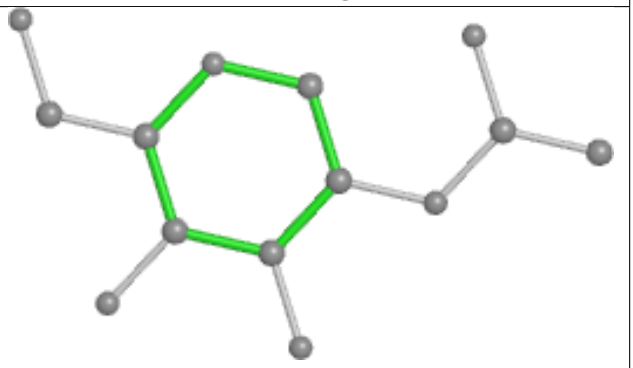
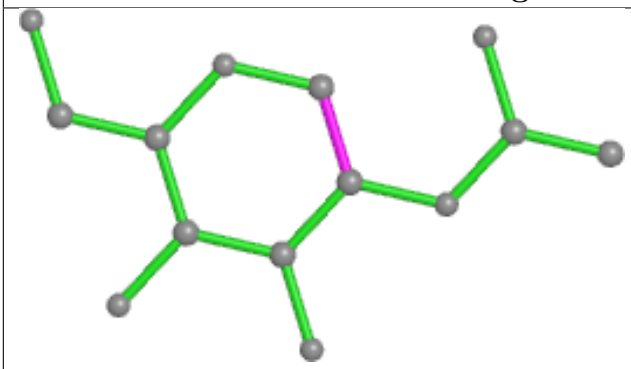


Rings

Ligand NAG C 9310



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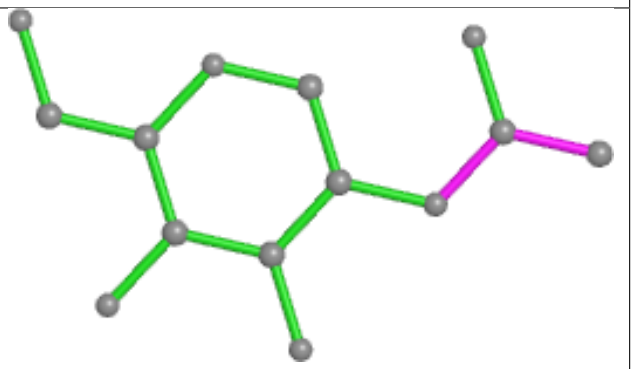
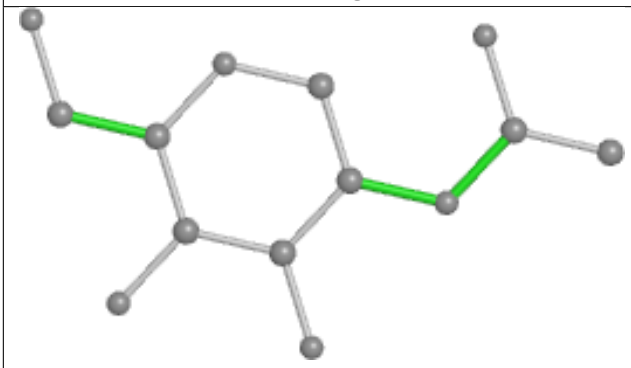


Bond angles



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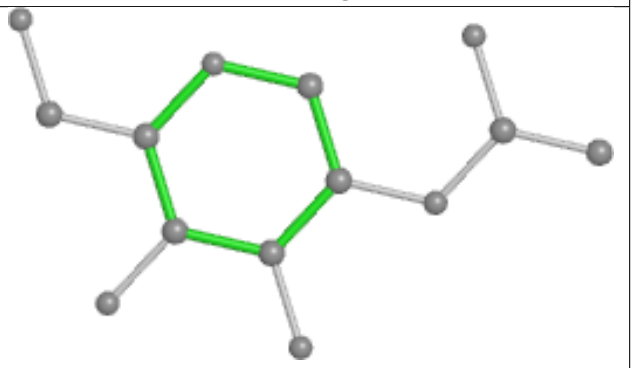
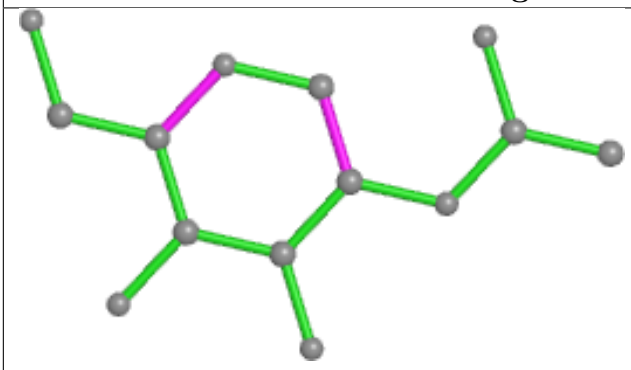


Rings

Ligand NAG C 9302



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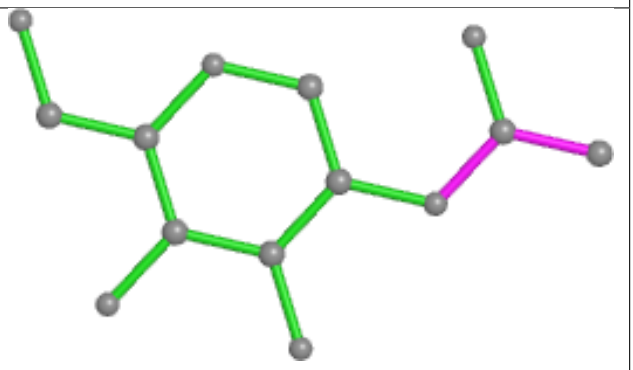
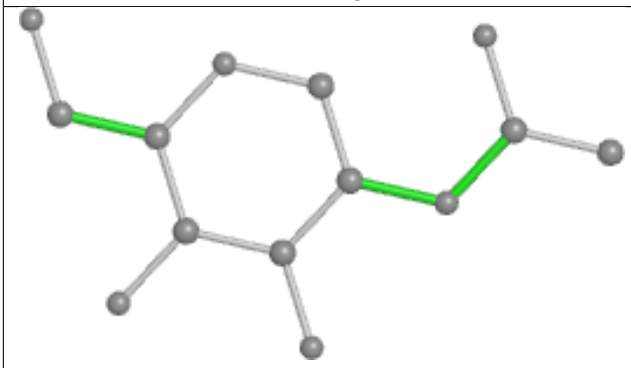


Bond angles



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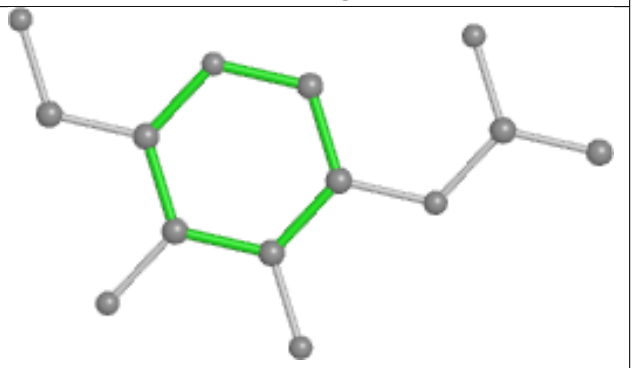
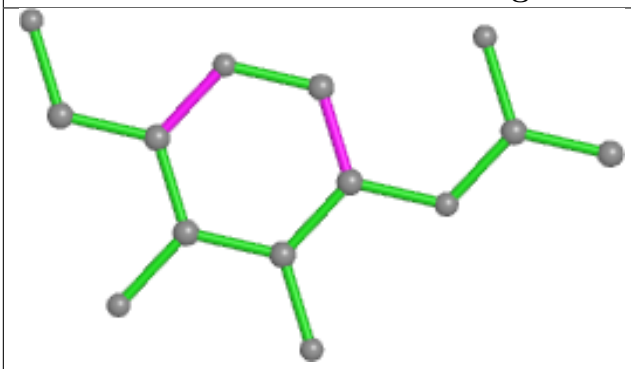


Rings

Ligand NAG B 9314



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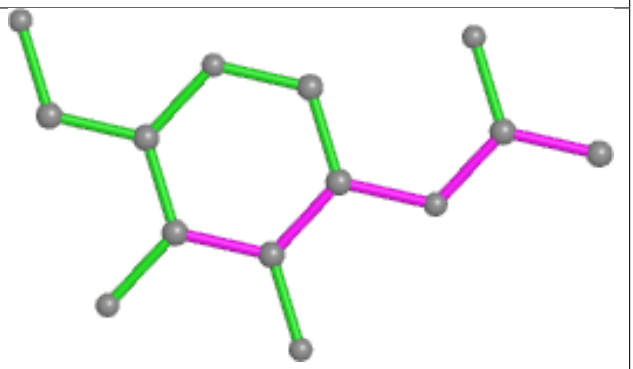
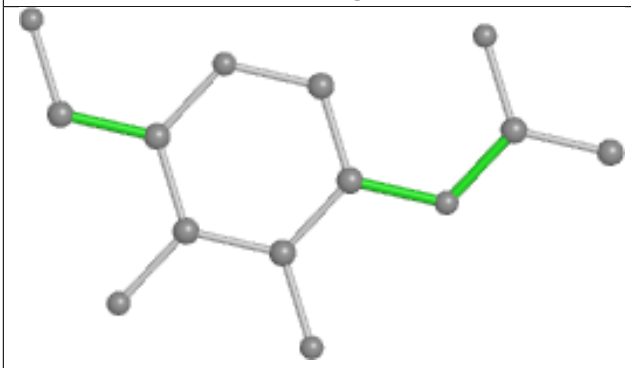


Bond angles



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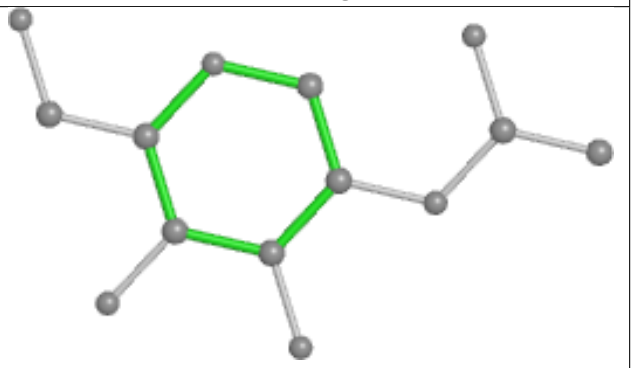
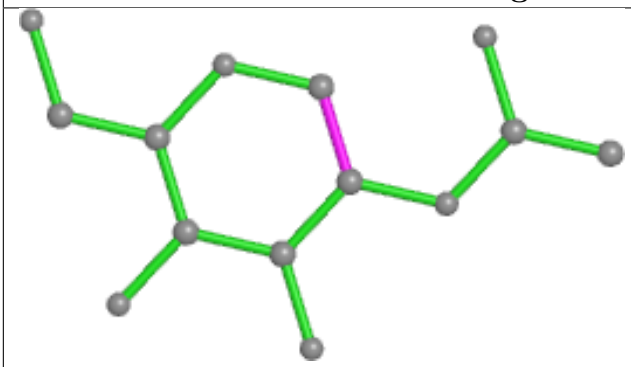


Rings

Ligand NAG A 9310



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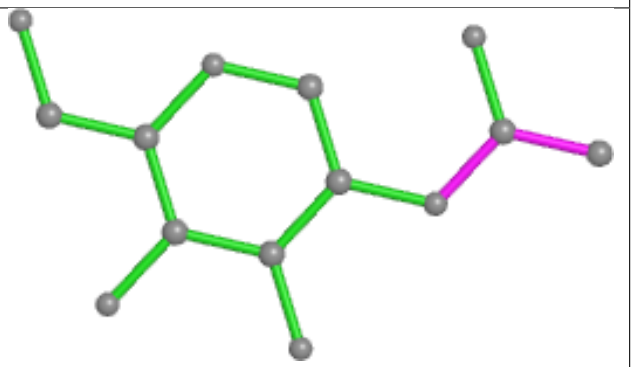

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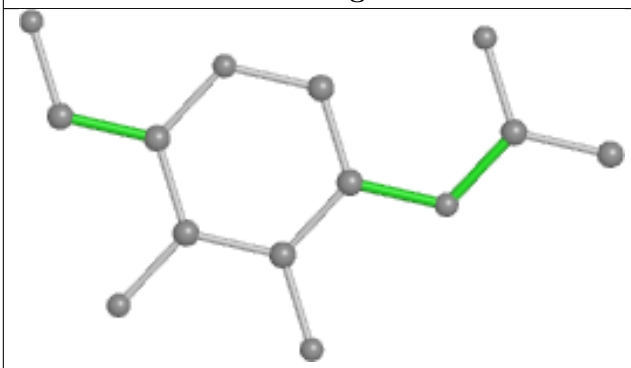

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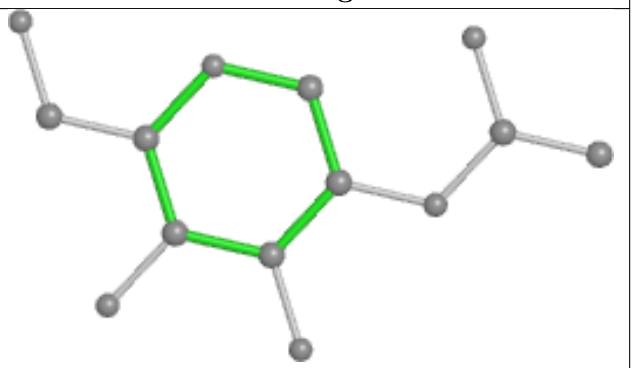
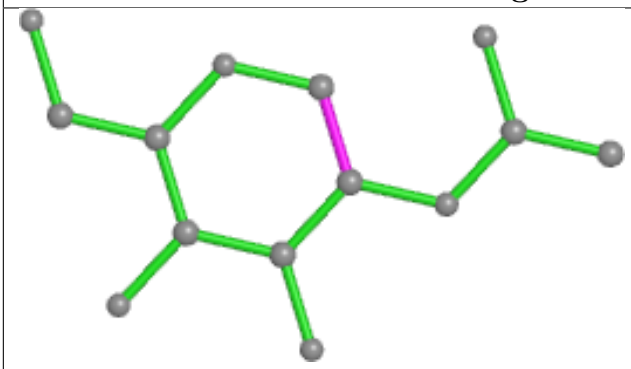


Rings

Ligand NAG C 9314



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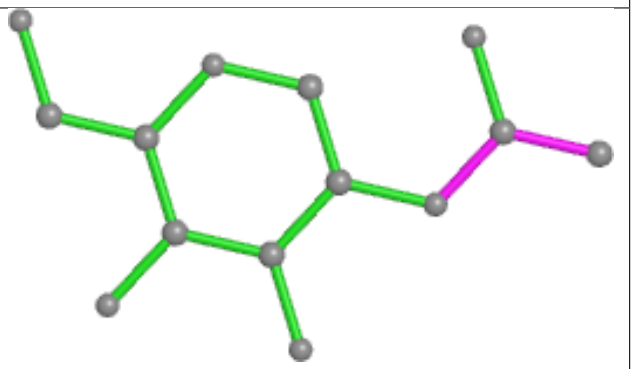
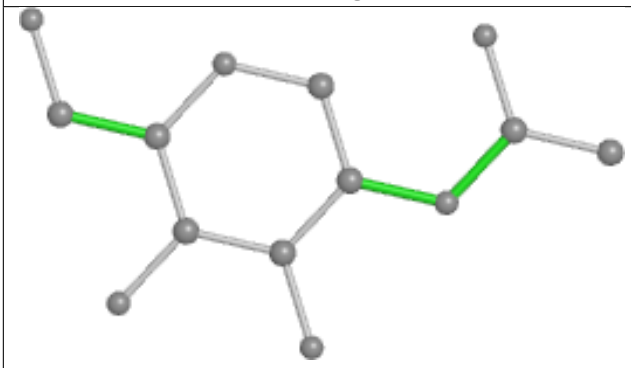


Bond angles



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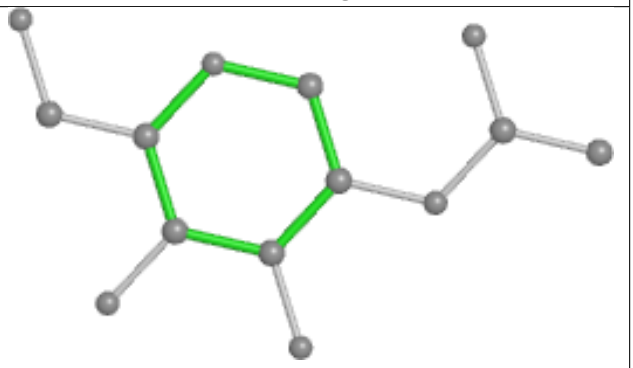
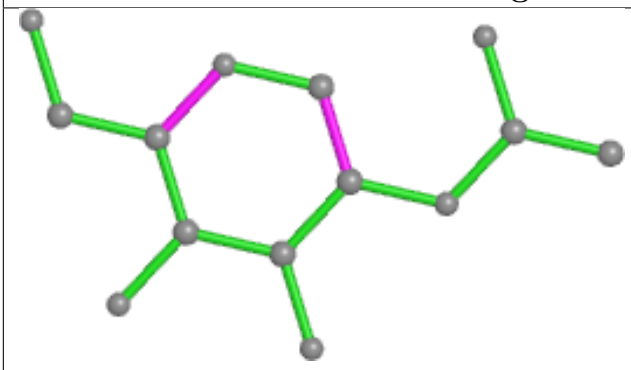


Rings

Ligand NAG C 9308



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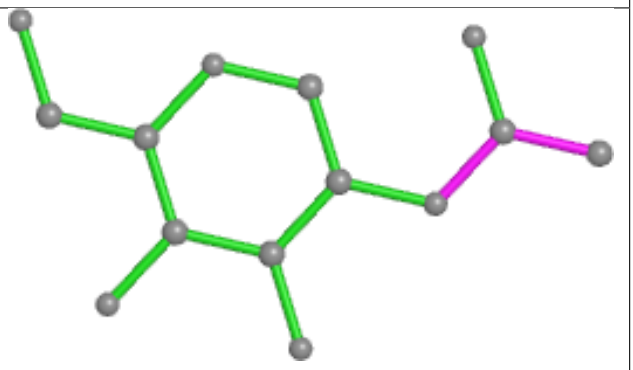
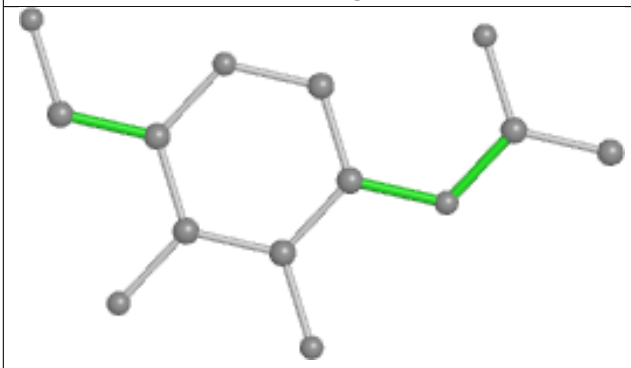


Bond angles



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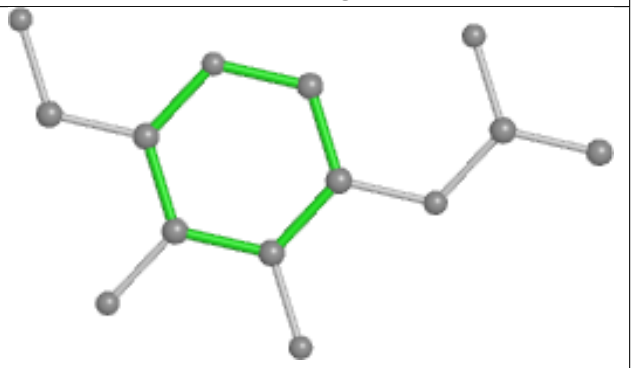
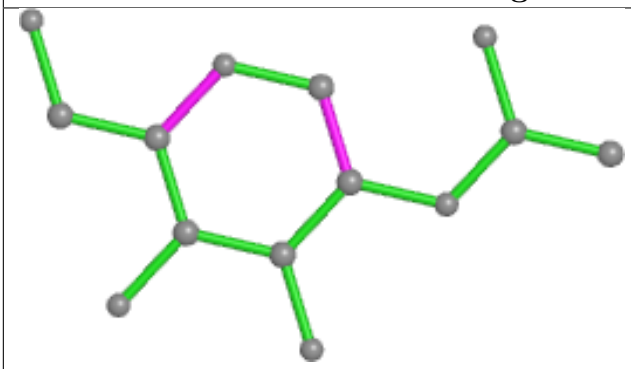


Rings

Ligand NAG A 9302



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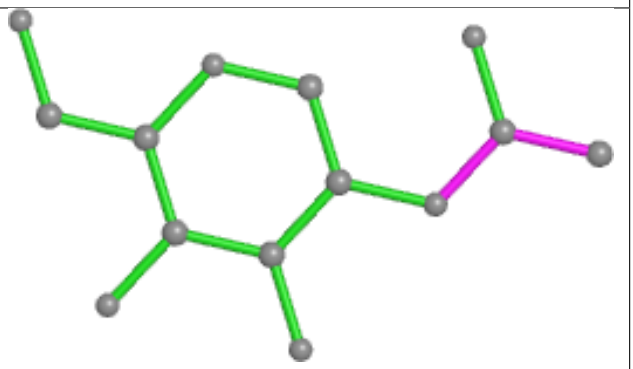
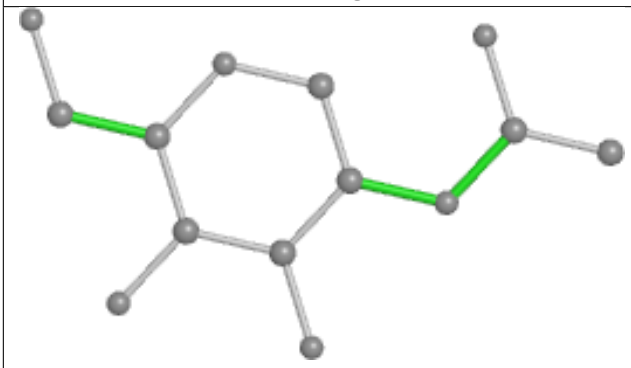


Bond angles



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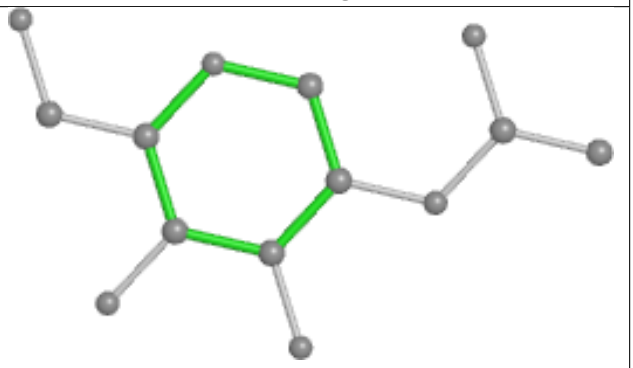
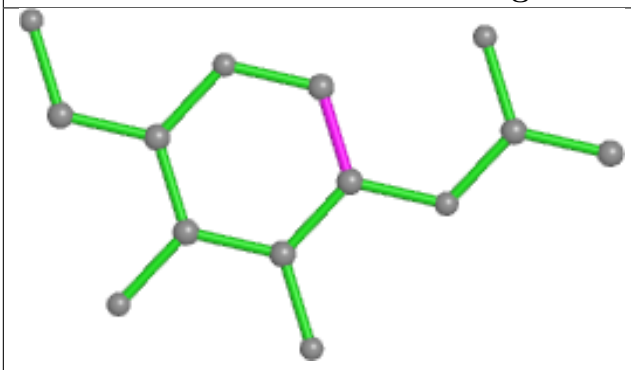


Rings

Ligand NAG B 9310



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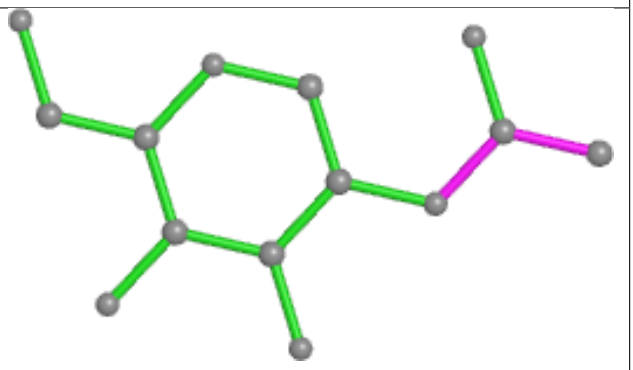
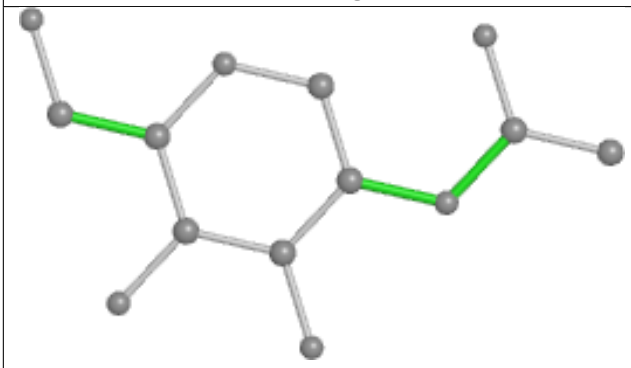


Bond angles



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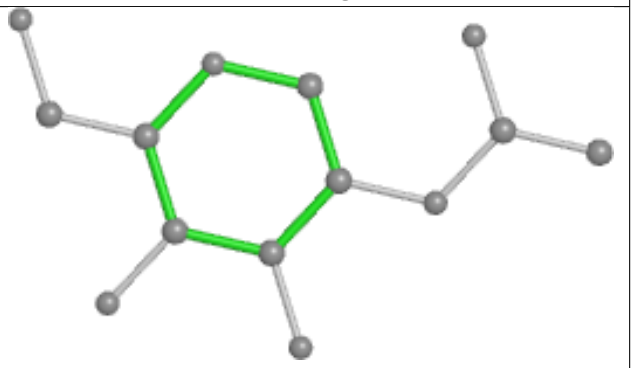
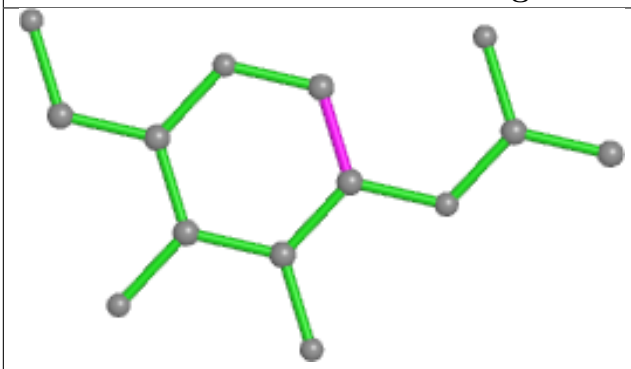


Rings

Ligand NAG B 9312



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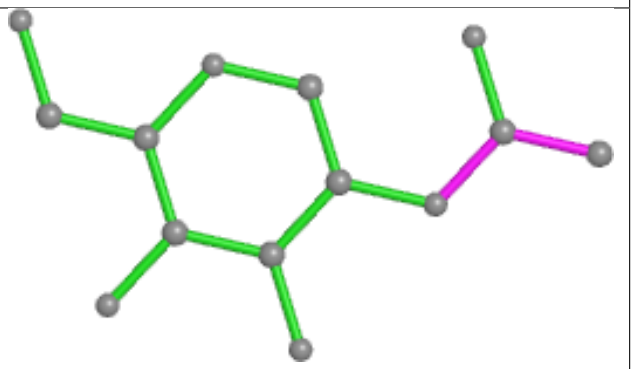
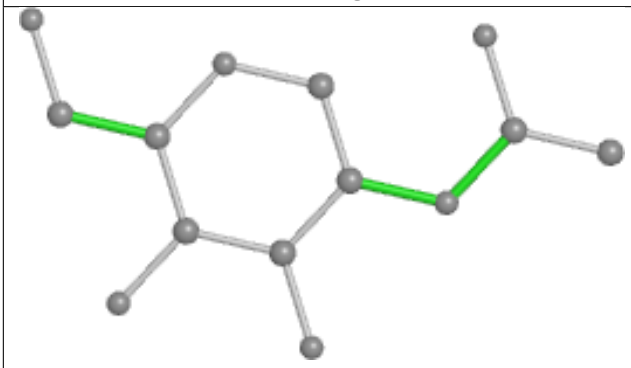
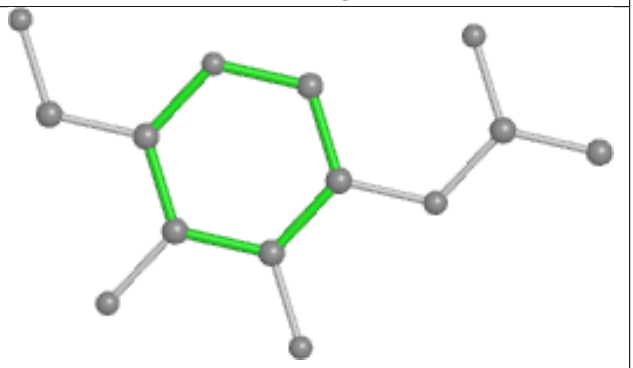


Bond angles

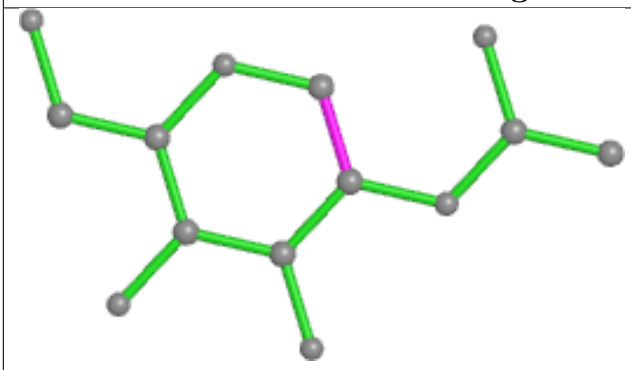


Torsions



Rings

Ligand NAG A 9316



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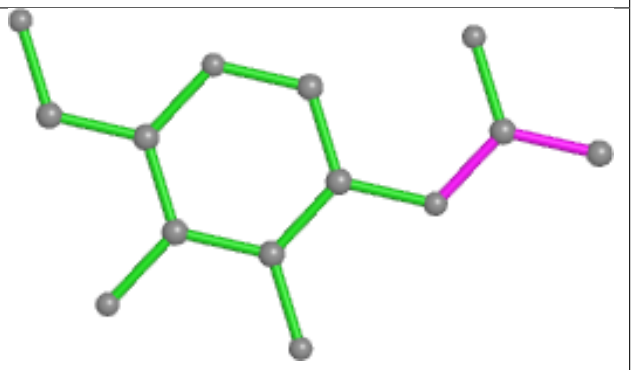
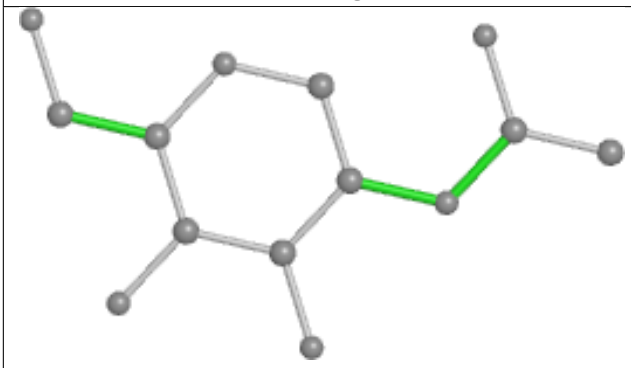


Bond angles



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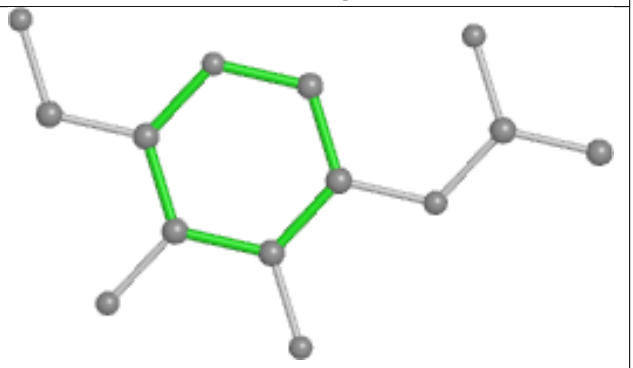
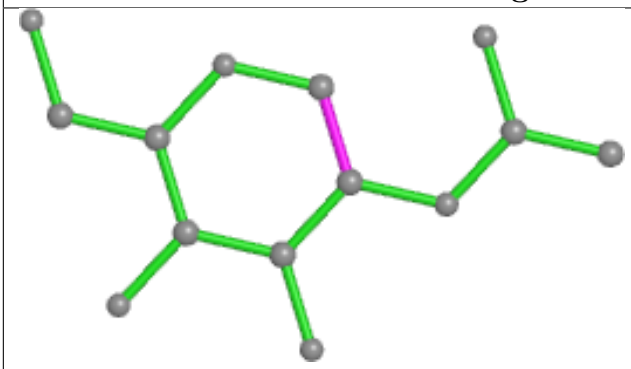
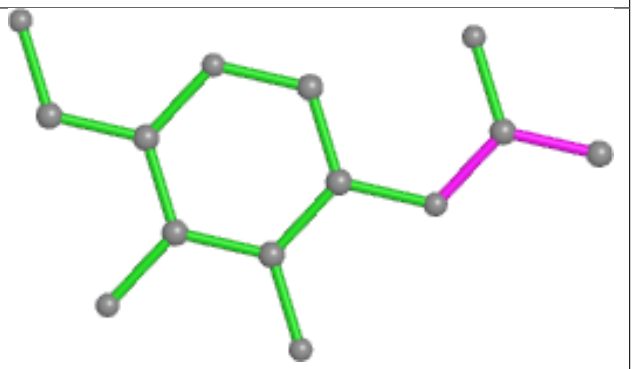


Rings

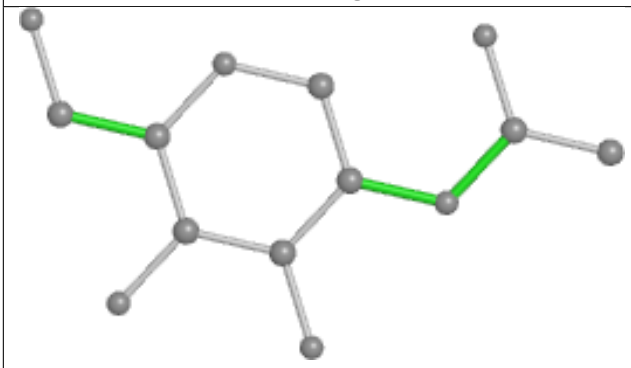
Ligand NAG C 9309



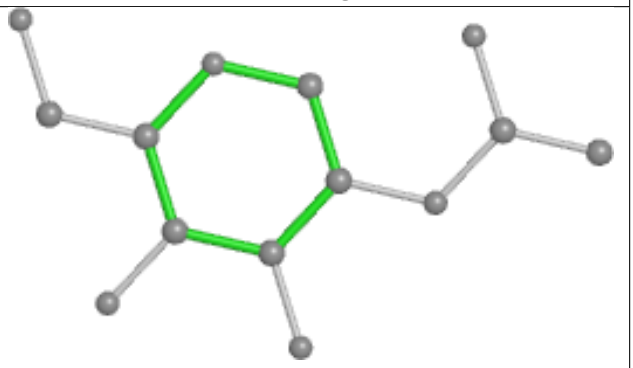
Bond lengths



Bond angles

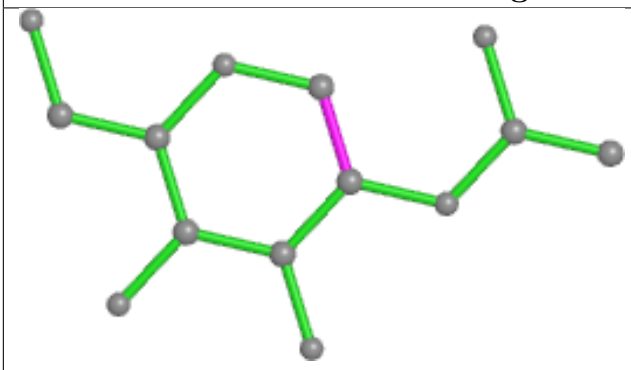


Torsions

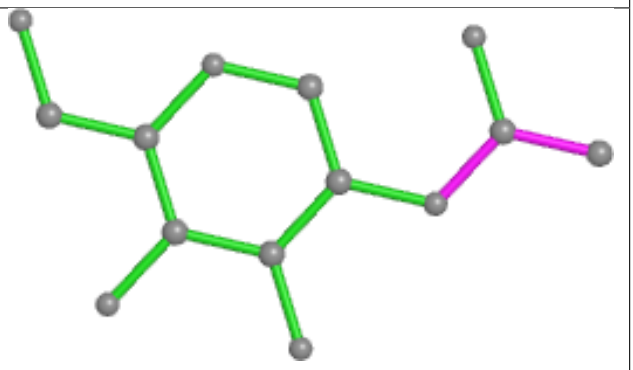


Rings

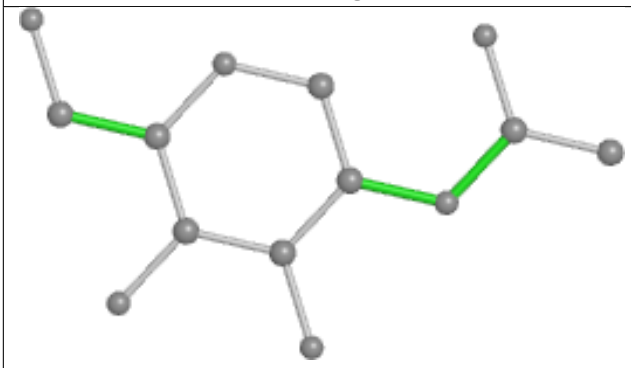
Ligand NAG A 9304



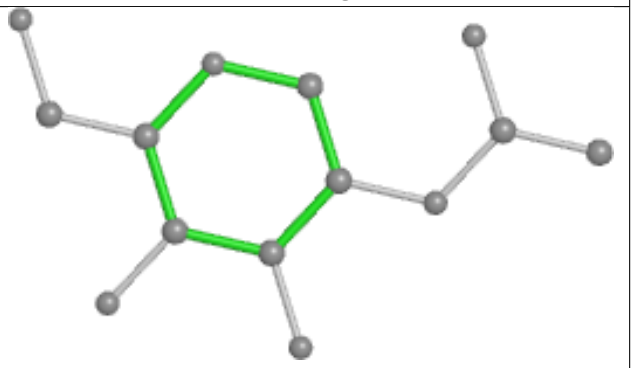
Bond lengths



Bond angles

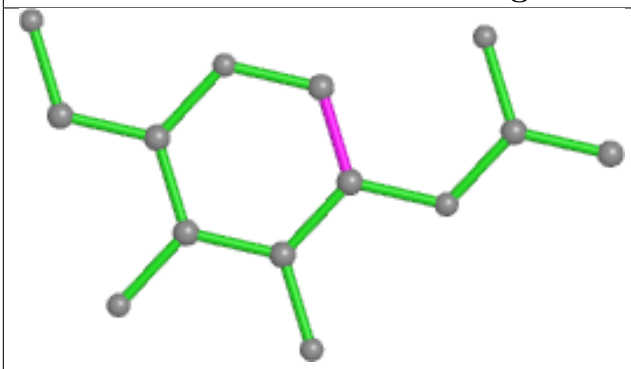


Torsions

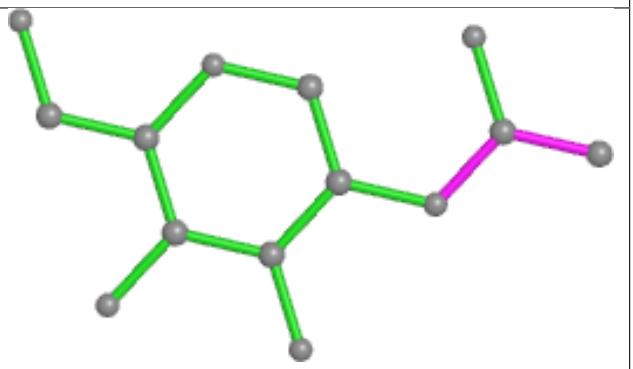


Rings

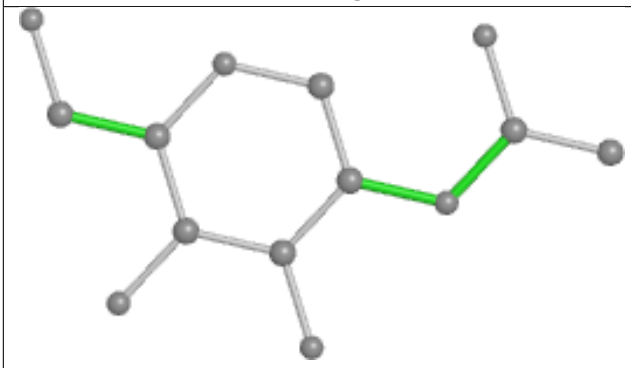
Ligand NAG A 9309



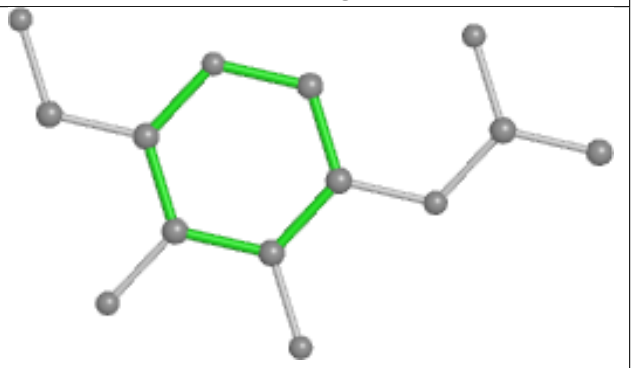
Bond lengths



Bond angles

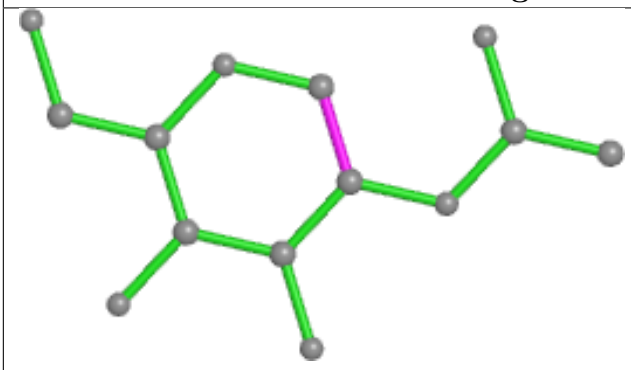


Torsions

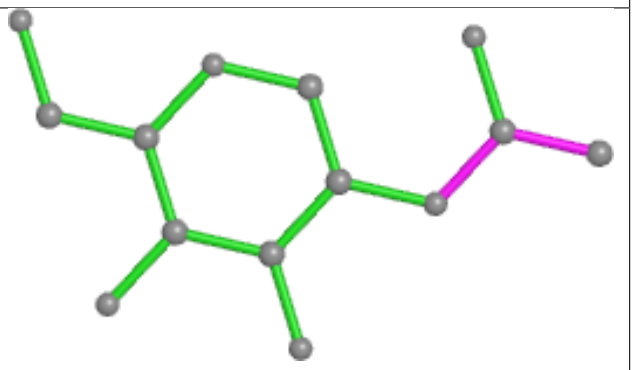


Rings

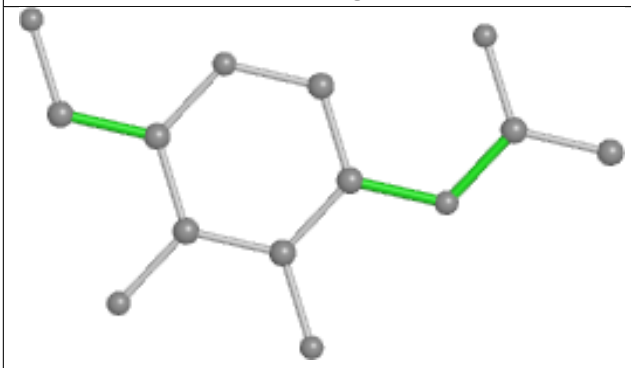
Ligand NAG C 9305



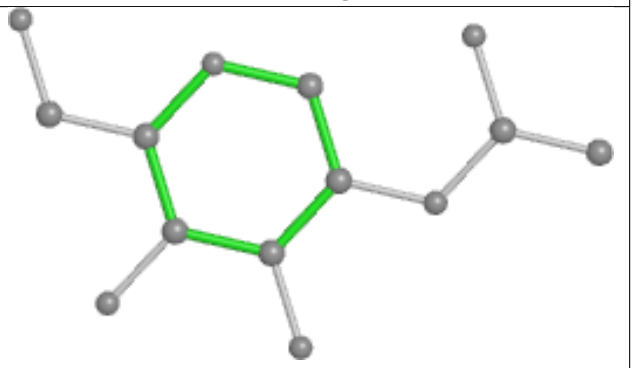
Bond lengths



Bond angles

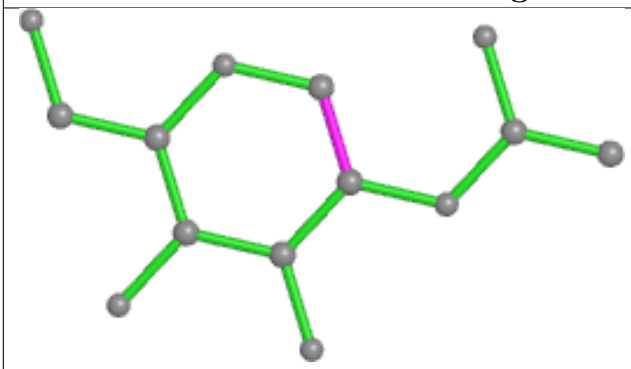


Torsions

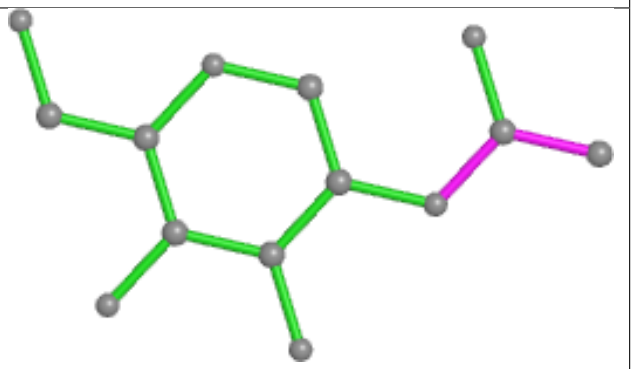


Rings

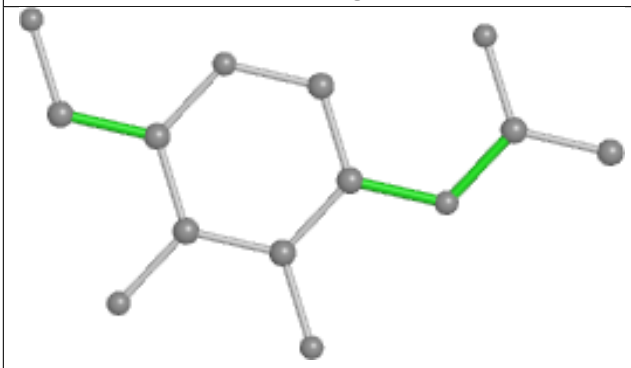
Ligand NAG A 9317



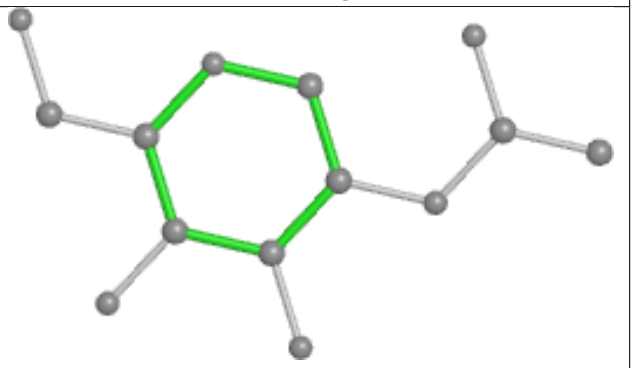
Bond lengths



Bond angles

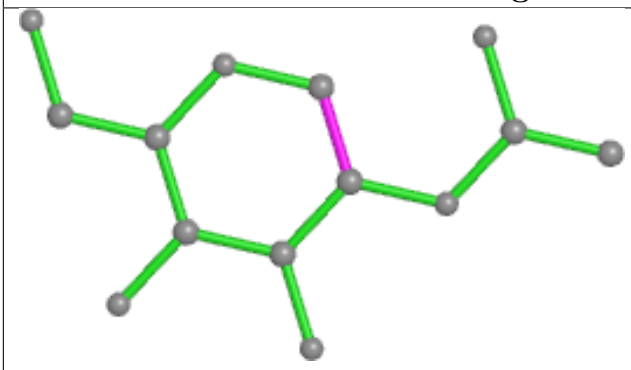


Torsions

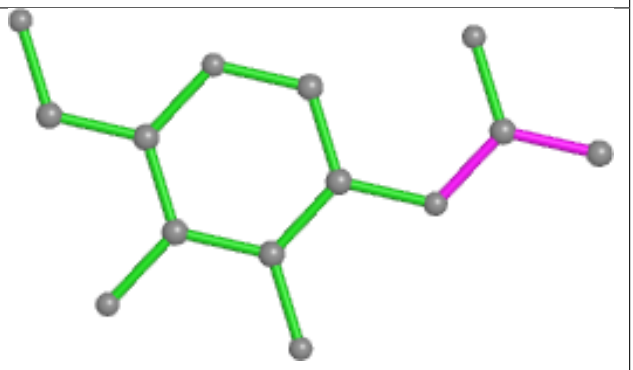


Rings

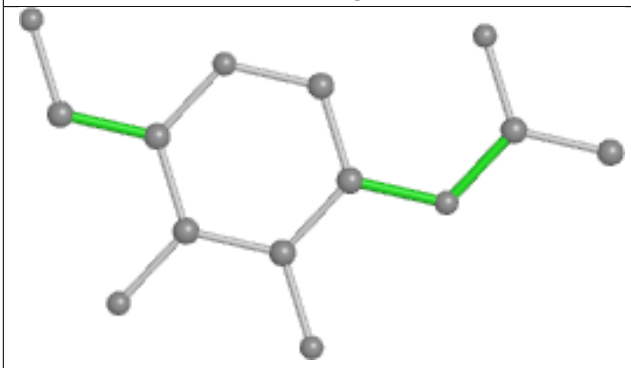
Ligand NAG B 9309



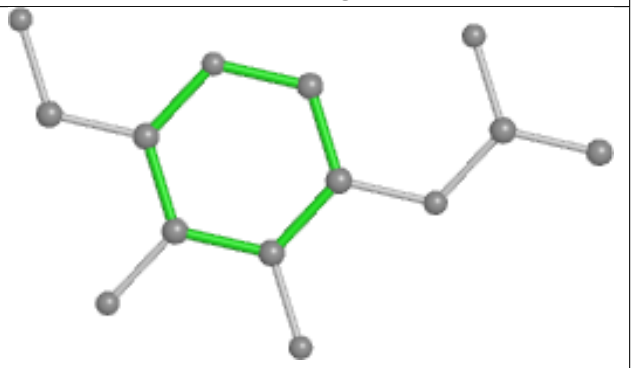
Bond lengths



Bond angles

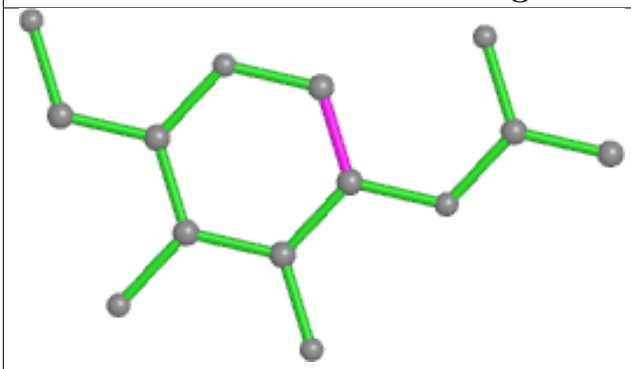


Torsions

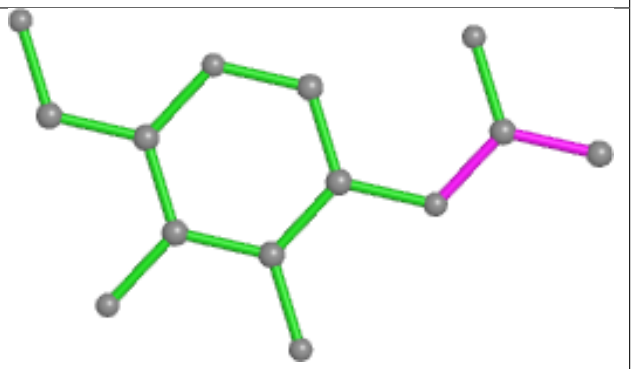


Rings

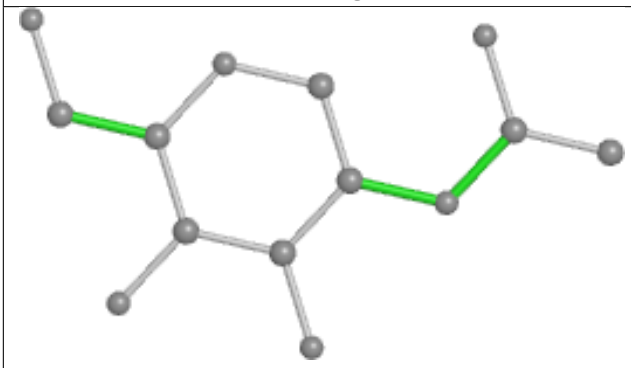
Ligand NAG C 9311



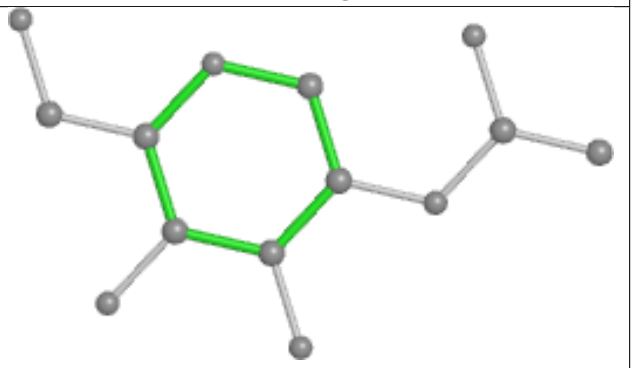
Bond lengths



Bond angles

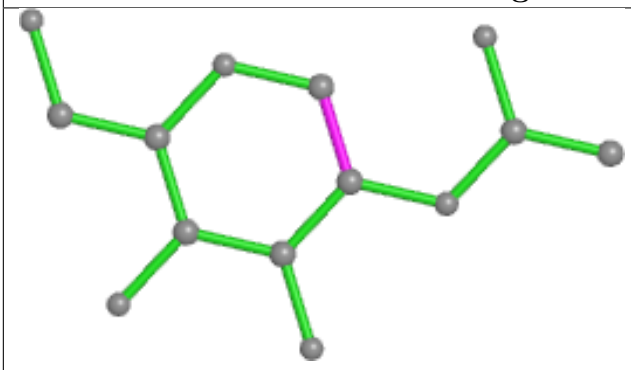


Torsions

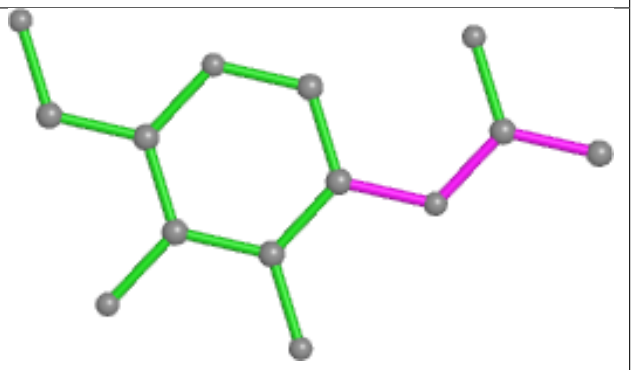


Rings

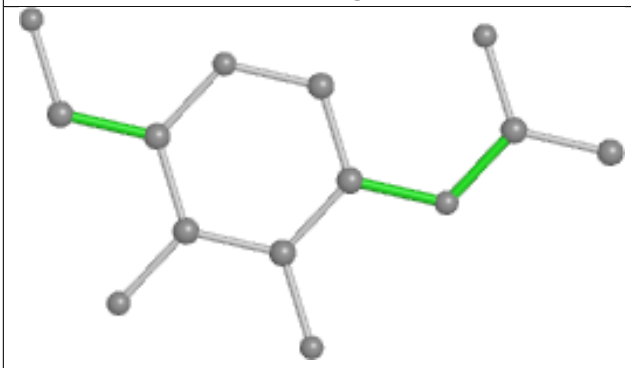
Ligand NAG B 9301



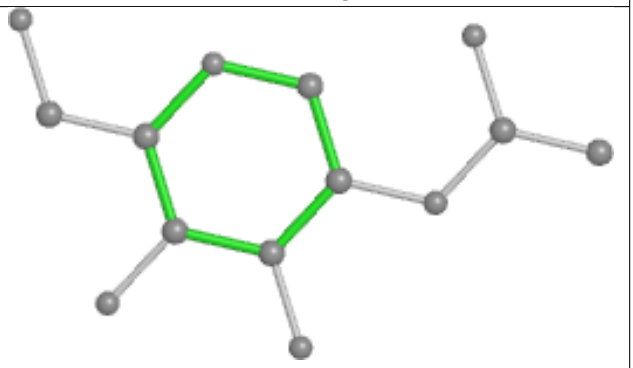
Bond lengths



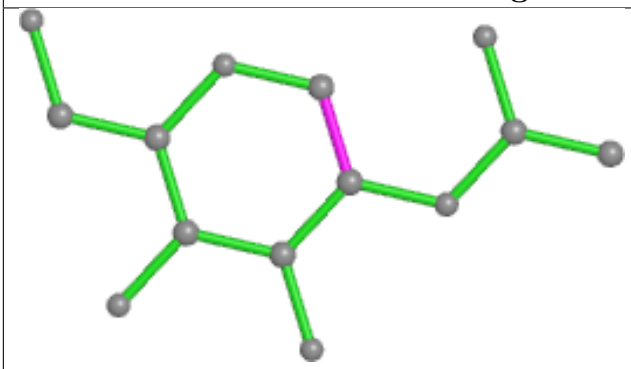
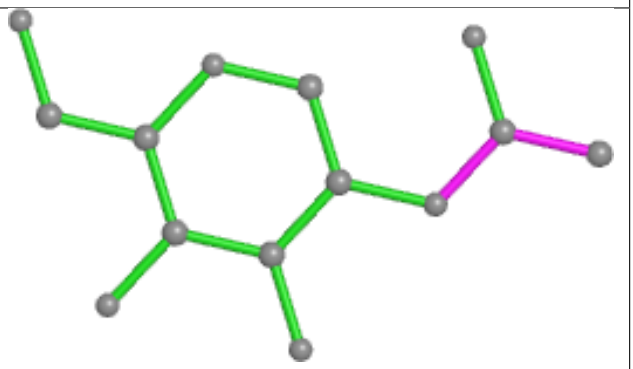
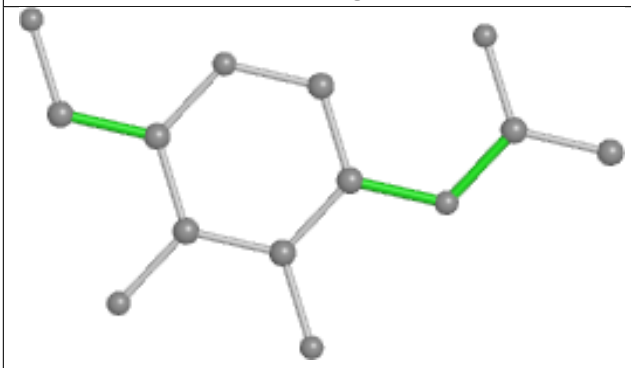
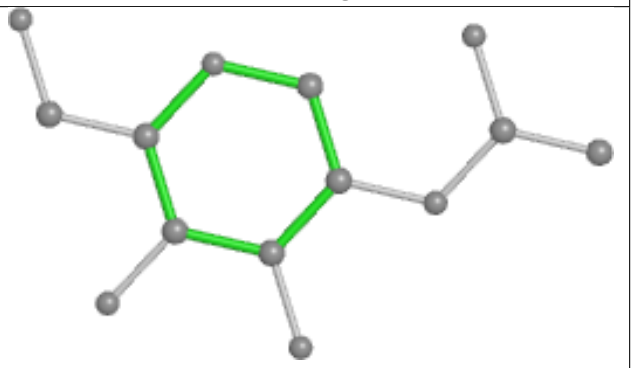
Bond angles



Torsions



Rings

Ligand NAG A 9311	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

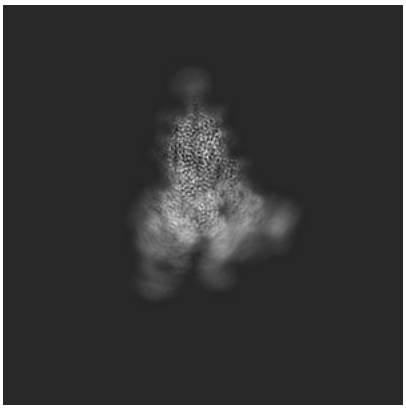
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25992. These allow visual inspection of the internal detail of the map and identification of artifacts.

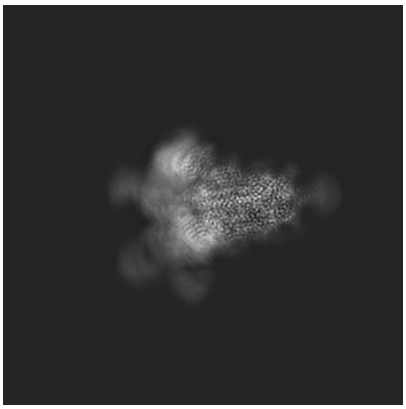
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

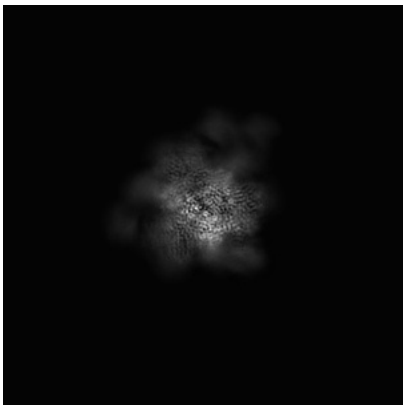
6.1.1 Primary map



X

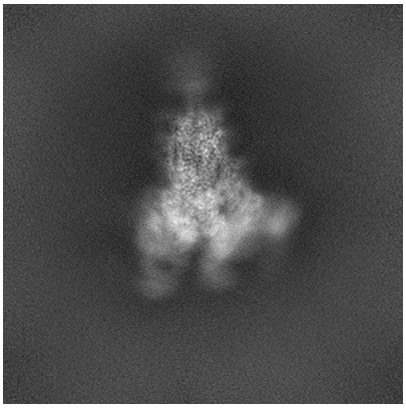


Y

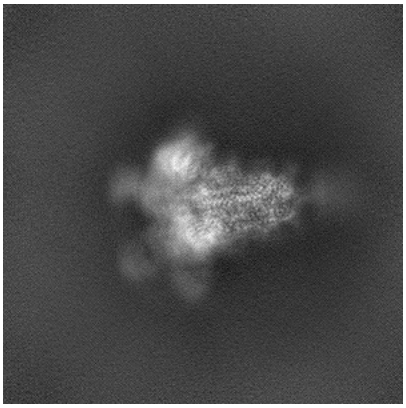


Z

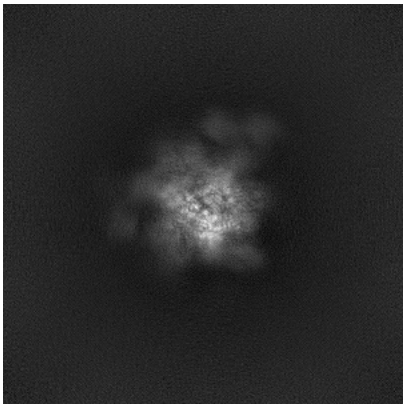
6.1.2 Raw map



X



Y

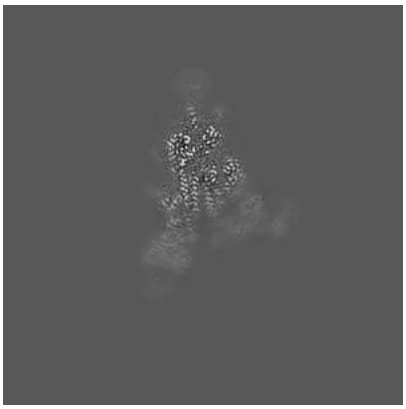


Z

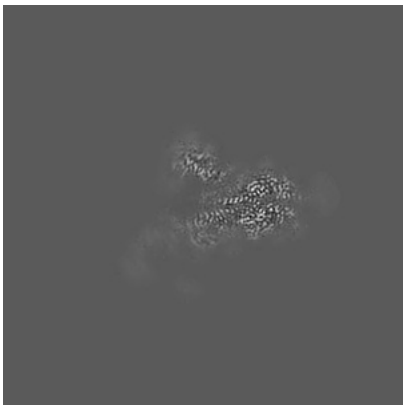
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

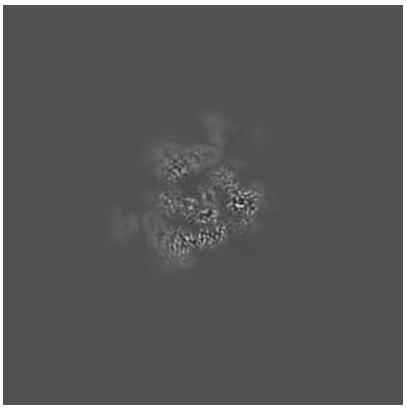
6.2.1 Primary map



X Index: 256

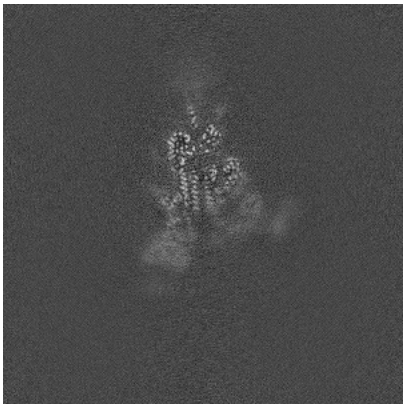


Y Index: 256

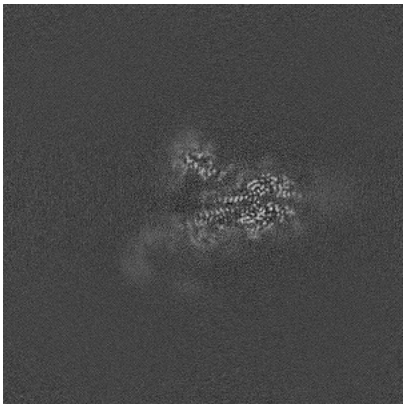


Z Index: 256

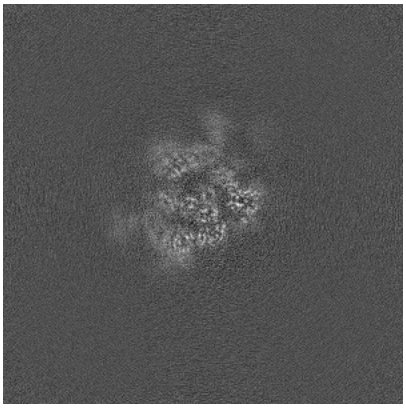
6.2.2 Raw map



X Index: 256



Y Index: 256

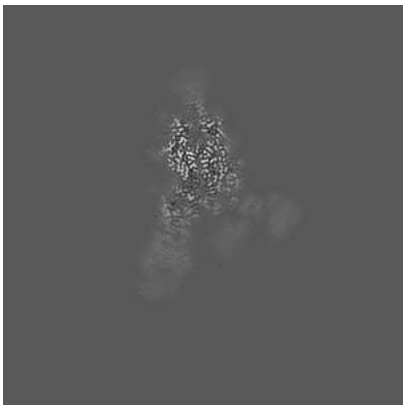


Z Index: 256

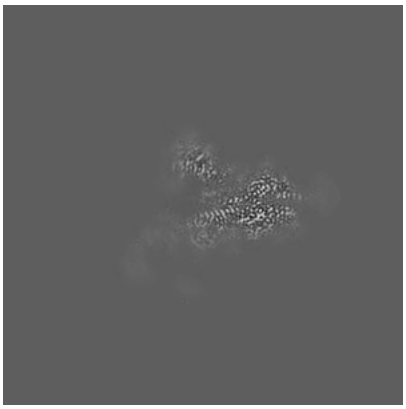
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

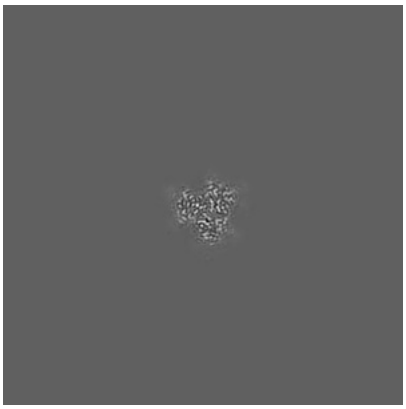
6.3.1 Primary map



X Index: 265

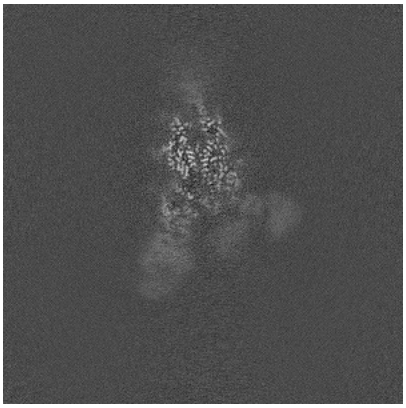


Y Index: 255

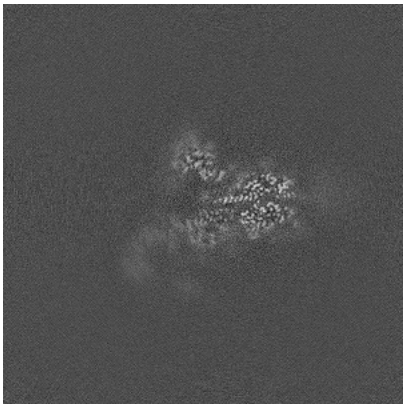


Z Index: 329

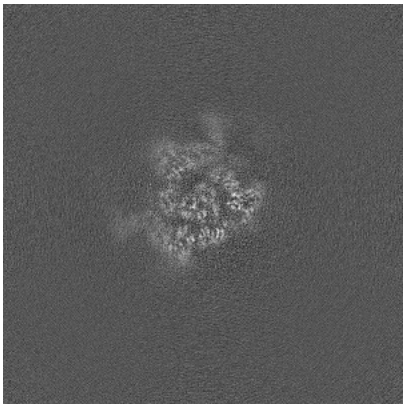
6.3.2 Raw map



X Index: 265



Y Index: 257



Z Index: 258

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

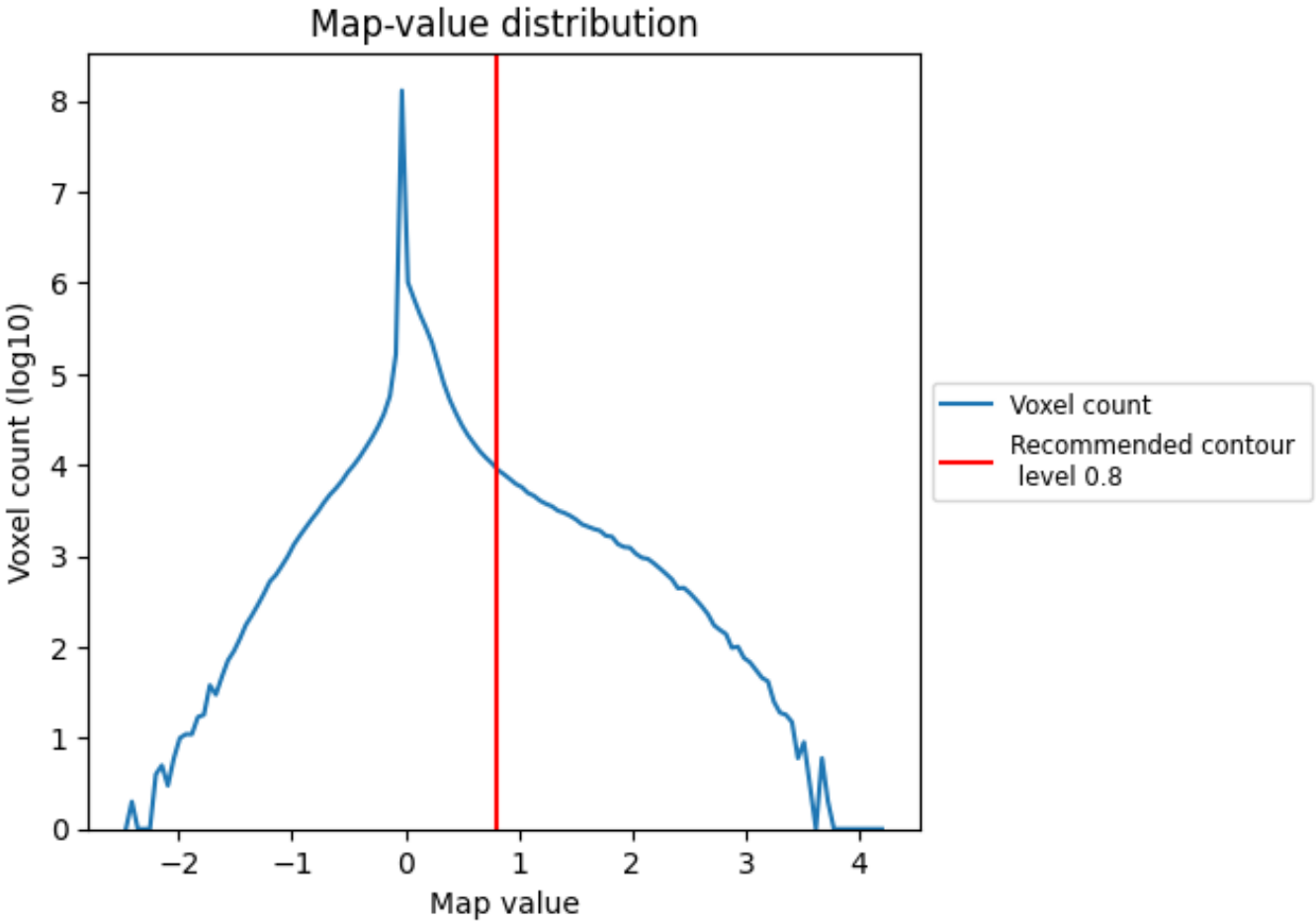
6.5 Mask visualisation (i)

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

7 Map analysis

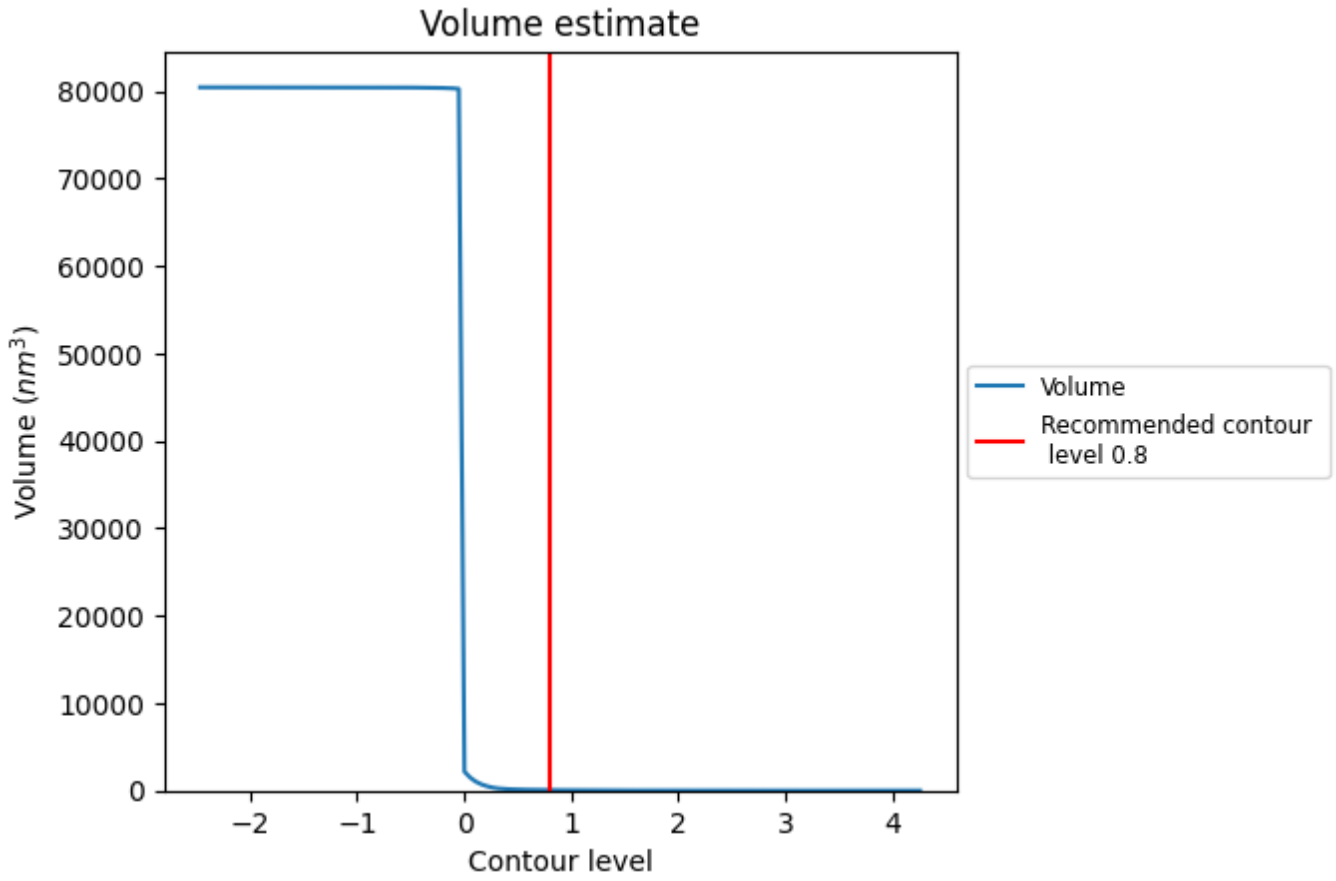
This section contains the results of statistical analysis of the map.

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.

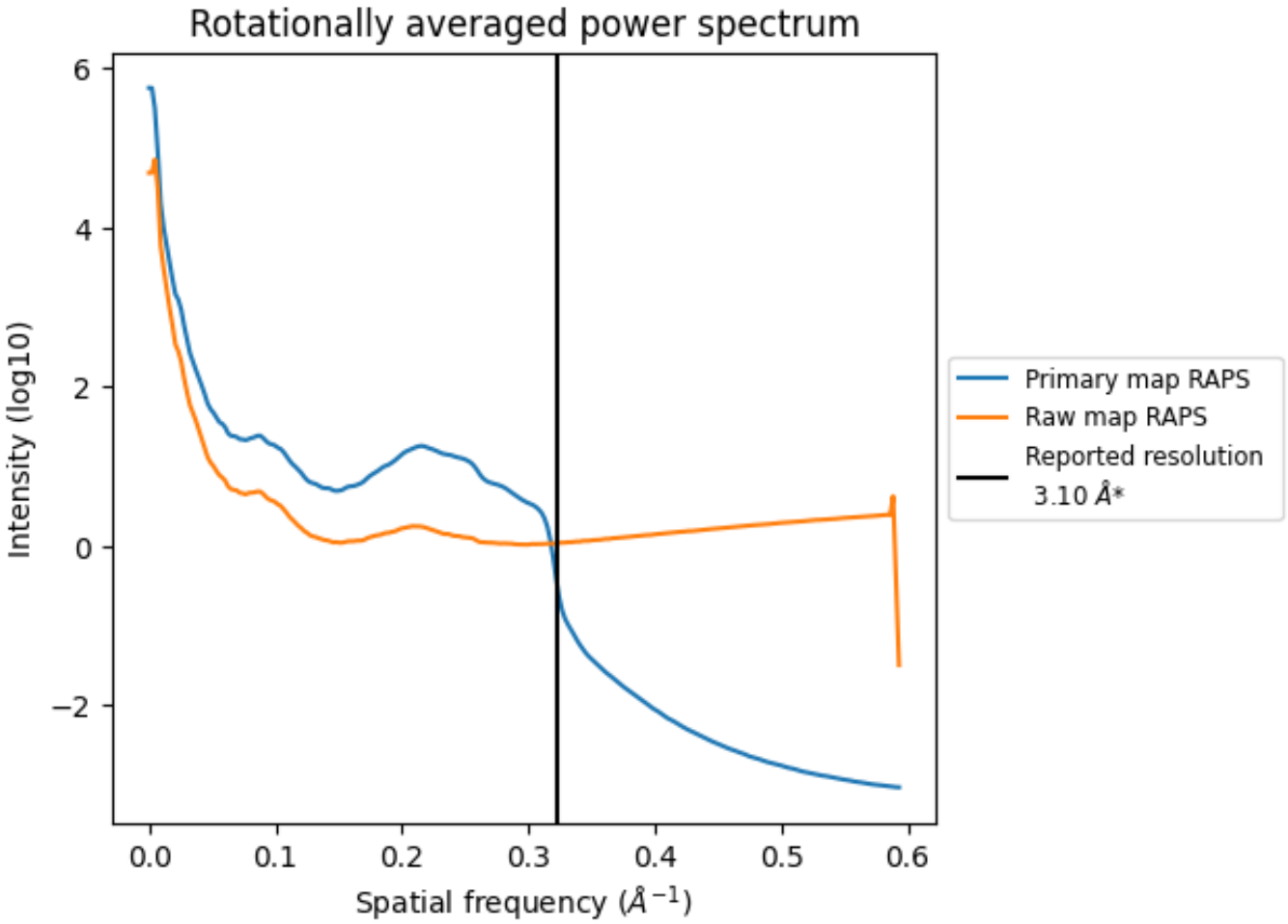
7.2 Volume estimate



The volume at the recommended contour level is 57 nm^3; this corresponds to an approximate mass of 52 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)

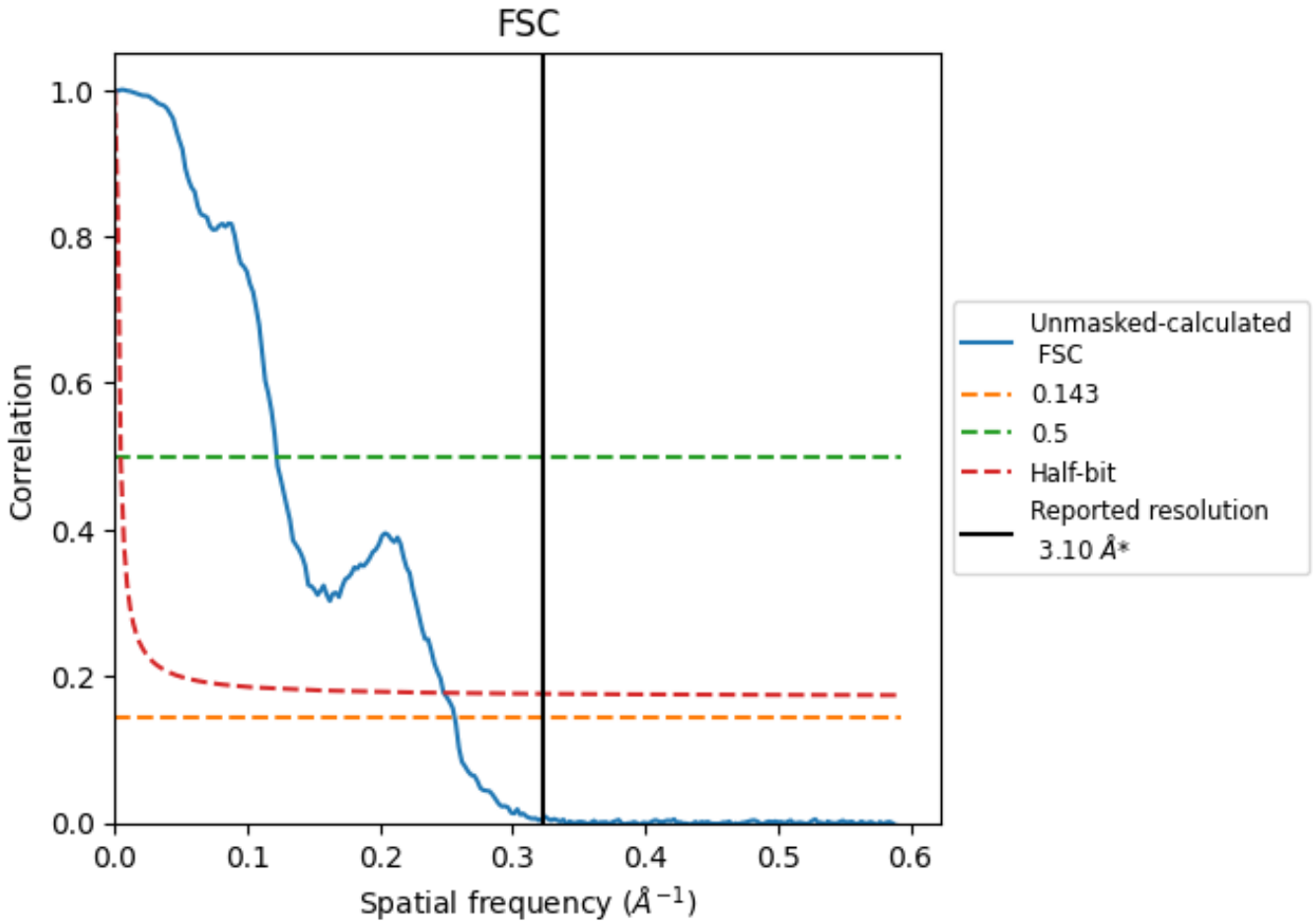


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

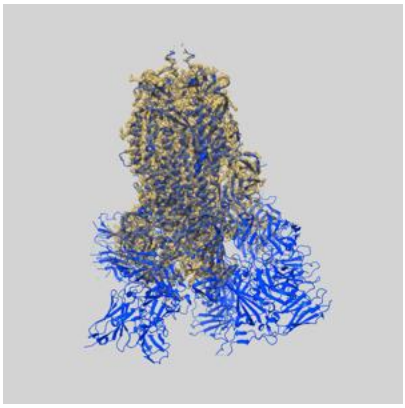
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.90	8.19	4.03

*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 3.90 differs from the reported value 3.1 by more than 10 %

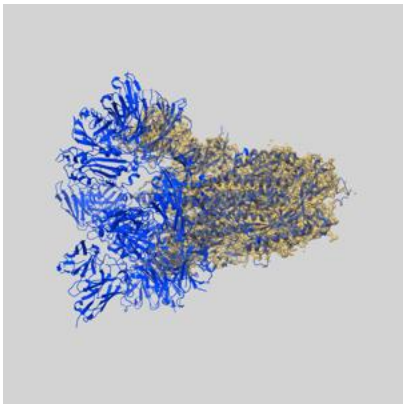
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25992 and PDB model 7TM0. Per-residue inclusion information can be found in section 3 on page 18.

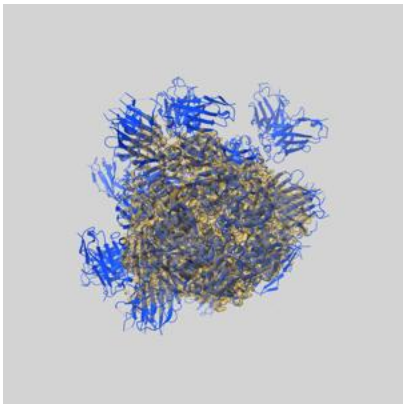
9.1 Map-model overlay



X



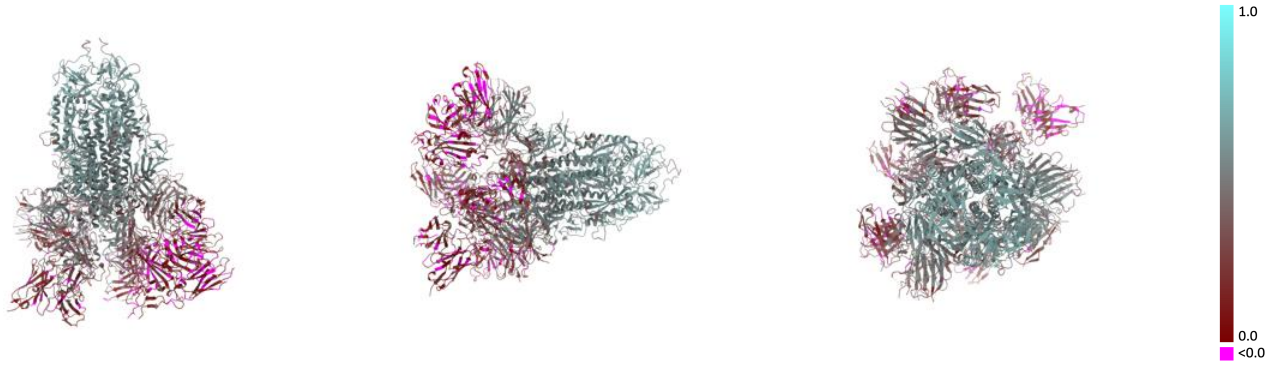
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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.

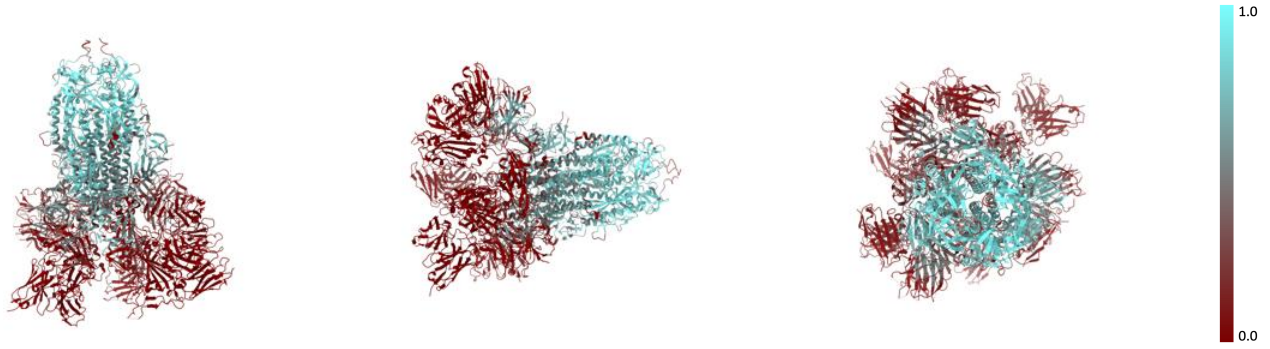
9.2 Q-score mapped to coordinate model



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.

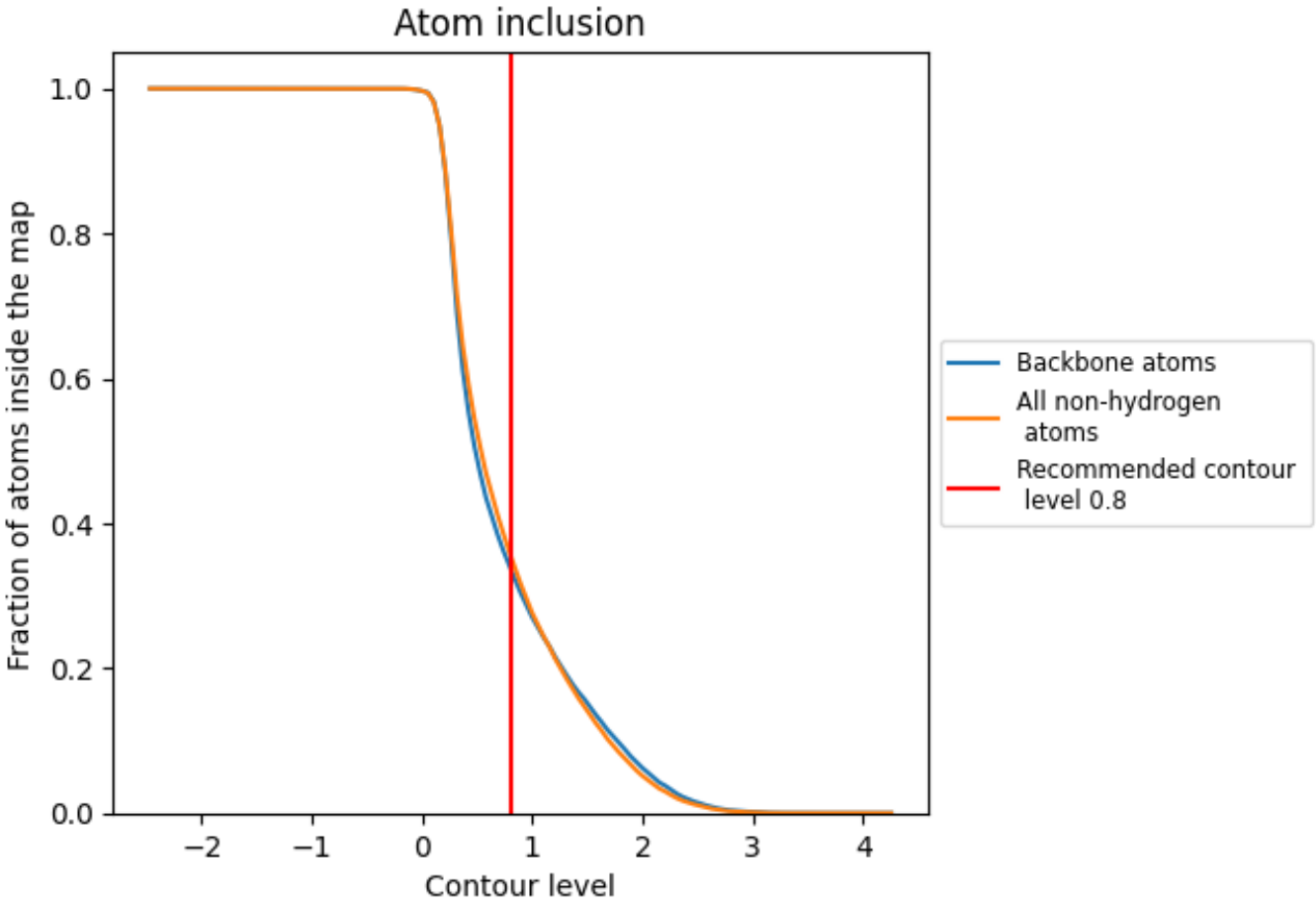
9.3 Atom inclusion mapped to coordinate model



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 (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 34% of all backbone atoms, 36% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3573	0.4010
A	0.4977	0.4920
B	0.4368	0.4380
C	0.4572	0.4650
D	0.0000	0.1690
E	0.0000	0.1950
F	0.0000	0.1850
G	0.0101	0.2260
H	0.0398	0.3460
I	0.2601	0.3900
J	0.0000	0.0750
K	0.0000	0.0740
L	0.0000	0.1420
M	0.0000	0.1710
N	0.0000	0.2120
O	0.0000	0.2020
P	0.2143	0.4160