Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:08 AM UTC

PDB ID	:	8UIR / pdb_00008uir
EMDB ID	:	EMD-42302
Title	:	SARS-CoV-2 Omicron-XBB.1.16 3-RBD down Spike Protein Trimer consensus (S-GSAS-Omicron-XBB.1.16)
Authors	:	Zhang, Q.E.; Acharya, P.
Deposited on	:	2023-10-10
Resolution	:	3.20 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:

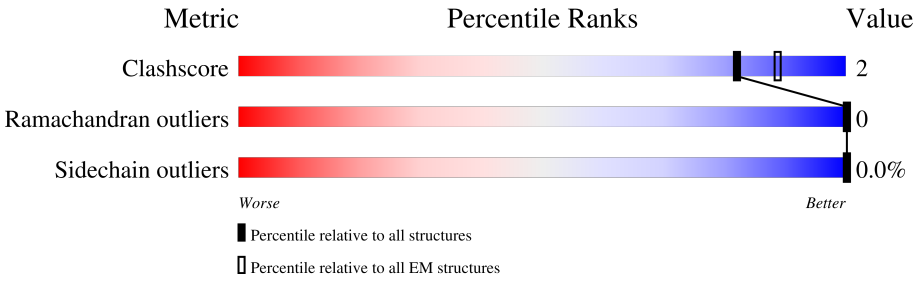
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	NOT EXECUTED
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.20 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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%

Mol	Chain	Length	Quality of chain
1	A	1284	75% 6% 19%
1	B	1284	75% 6% 19%
1	C	1284	75% 6% 19%
2	D	2	100%
2	E	2	50% 50%
2	F	2	100%
2	G	2	100%
2	H	2	100%
2	I	2	100%

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Mol	Chain	Length	Quality of chain
2	J	2	100%
2	K	2	50% 50%
2	L	2	50% 50%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24879 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	1035	Total	C	N	O	S	0	0
			8069	5159	1342	1530	38		
1	B	1035	Total	C	N	O	S	0	0
			8069	5159	1342	1530	38		
1	C	1035	Total	C	N	O	S	0	0
			8069	5159	1342	1530	38		

There are 378 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	83	ALA	VAL	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	180	VAL	GLU	conflict	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	ARG	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	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	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	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	83	ALA	VAL	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	180	VAL	GLU	conflict	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	ARG	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	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	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	180	VAL	GLU	conflict	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	ARG	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	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	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	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
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		

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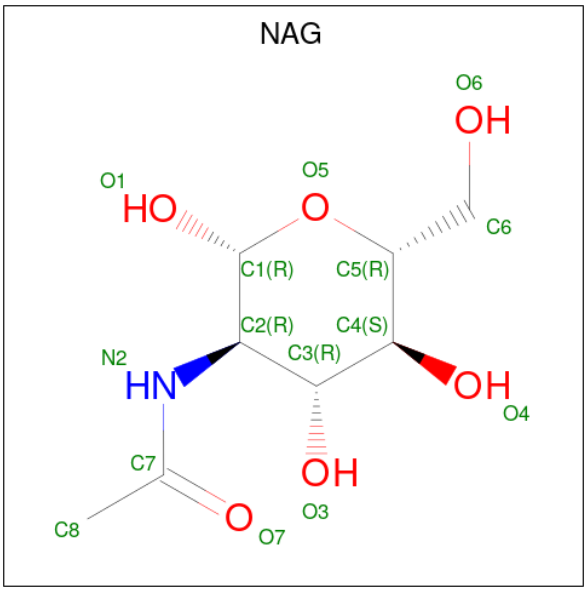
Mol	Chain	Residues	Atoms	AltConf	Trace
2	K	2	Total C N O 28 16 2 10	0	0
2	L	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

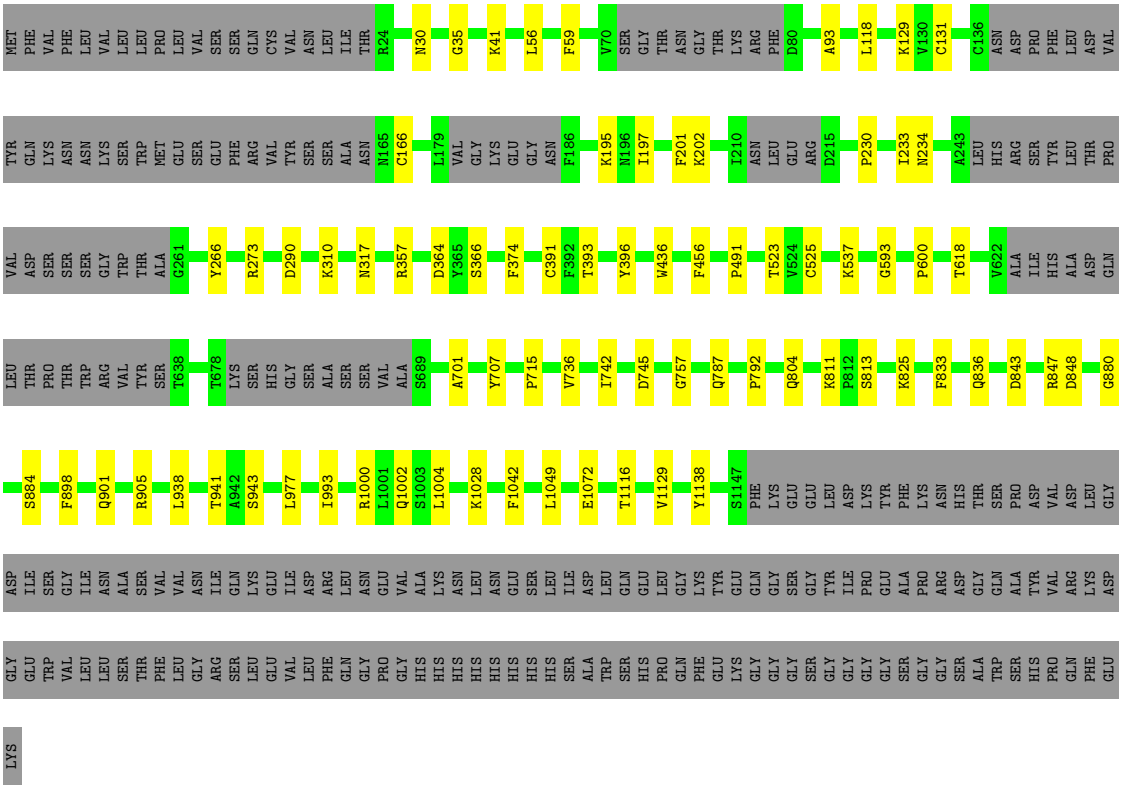
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein

Chain A:

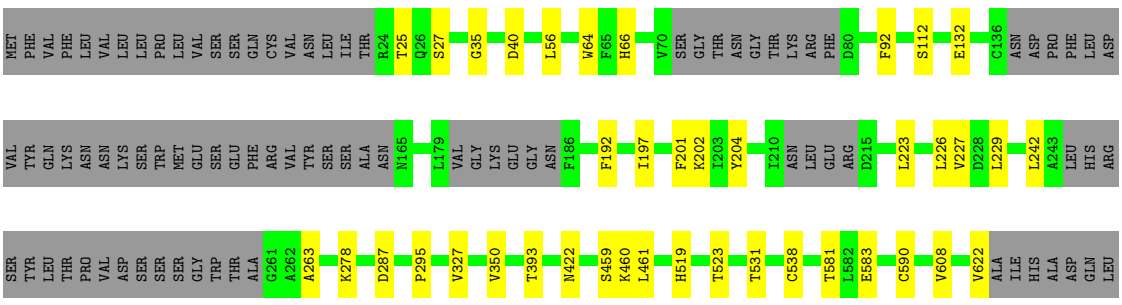


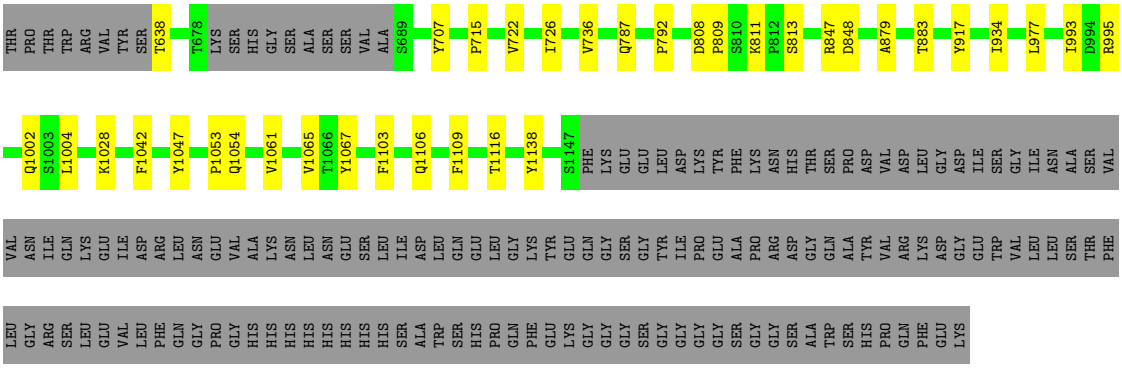


• Molecule 1: Spike glycoprotein

Chain B:



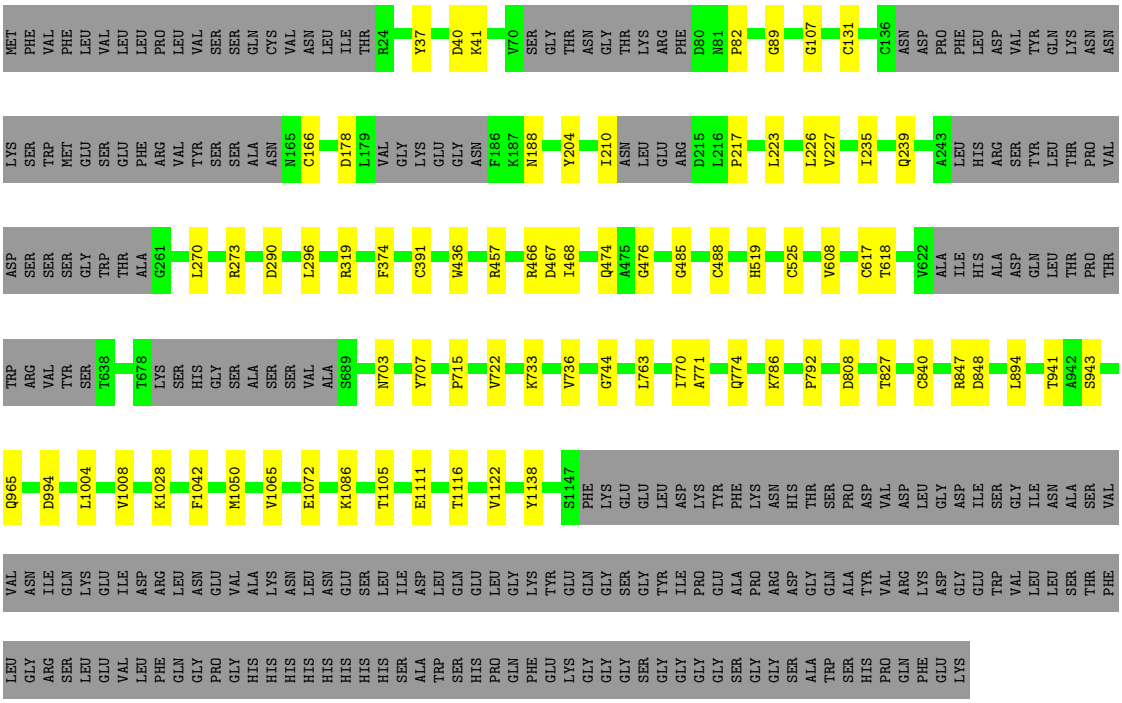




• Molecule 1: Spike glycoprotein

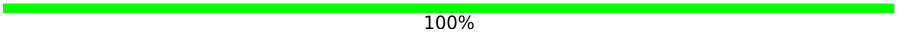
Chain C:





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

Chain D:





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

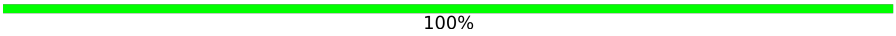
Chain E:





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

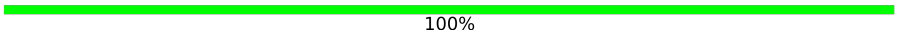
Chain F:





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

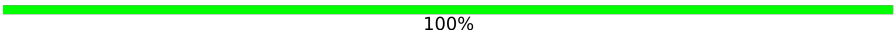
Chain G:





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

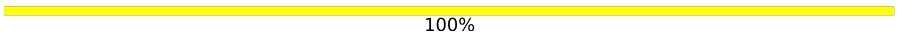
Chain H:





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

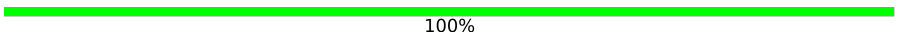
Chain I:





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

Chain J:





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

Chain K:





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

Chain L:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	852149	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 ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	350	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	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	0.16	0/8252	0.40	2/11224 (0.0%)
1	B	0.15	0/8252	0.37	0/11224
1	C	0.16	0/8252	0.39	2/11224 (0.0%)
All	All	0.16	0/24756	0.39	4/33672 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	744	GLY	CA-C-N	5.74	130.56	122.46
1	C	744	GLY	C-N-CA	5.74	130.56	122.46
1	A	197	ILE	CA-C-N	5.41	131.87	121.54
1	A	197	ILE	C-N-CA	5.41	131.87	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	617	CYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8069	0	7891	45	0
1	B	8069	0	7890	45	0
1	C	8069	0	7889	45	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
3	A	126	0	117	1	0
3	B	154	0	143	0	0
3	C	140	0	130	1	0
All	All	24879	0	24285	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:995:ARG:NH2	1:C:994:ASP:OD2	2.34	0.60
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.86	0.57
1:C:1105:THR:HG23	1:C:1111:GLU:H	1.69	0.57
1:C:1116:THR:HG22	1:C:1138:TYR:HB3	1.87	0.56
1:C:457:ARG:NH1	1:C:467:ASP:OD2	2.39	0.56
1:A:787:GLN:OE1	1:C:703:ASN:ND2	2.39	0.55
1:B:736:VAL:HG11	1:B:1004:LEU:HD11	1.87	0.55
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.89	0.55
1:B:201:PHE:HB3	1:B:229:LEU:HB2	1.88	0.54
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.73	0.54
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.89	0.54
1:B:27:SER:HB2	1:B:64:TRP:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:PRO:HG2	1:C:707:TYR:HB3	1.89	0.53
1:A:118:LEU:HD22	1:A:129:LYS:HB2	1.90	0.53
1:A:833:PHE:O	1:A:836:GLN:NE2	2.41	0.53
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.90	0.53
1:A:201:PHE:HB3	1:A:230:PRO:HA	1.91	0.52
1:A:233:ILE:HG13	1:A:234:ASN:H	1.75	0.52
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.90	0.52
1:C:131:CYS:HB3	1:C:166:CYS:HA	1.90	0.52
1:C:210:ILE:HG21	1:C:217:PRO:HG3	1.91	0.52
1:C:82:PRO:HB2	1:C:239:GLN:HG3	1.91	0.52
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.41	0.51
1:A:757:GLY:HA3	1:C:965:GLN:HE22	1.75	0.51
1:C:107:GLY:H	1:C:235:ILE:HG23	1.76	0.51
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.44	0.51
1:B:92:PHE:HB3	1:B:192:PHE:HB2	1.92	0.50
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.92	0.50
1:B:977:LEU:HD22	1:B:993:ILE:HG12	1.94	0.50
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.42	0.50
1:B:25:THR:HB	1:B:66:HIS:HB2	1.93	0.49
1:C:178:ASP:OD2	1:C:188:ASN:ND2	2.45	0.49
1:A:374:PHE:HB3	1:A:436:TRP:HB3	1.95	0.49
1:B:707:TYR:HB3	1:C:792:PRO:HG2	1.95	0.49
1:B:295:PRO:HB2	1:B:608:VAL:HG11	1.93	0.49
1:A:843:ASP:OD1	1:A:847:ARG:NH1	2.45	0.49
1:C:226:LEU:HG	1:C:227:VAL:HG23	1.95	0.48
1:C:941:THR:HG22	1:C:943:SER:H	1.78	0.48
1:B:715:PRO:HD3	1:C:894:LEU:HD21	1.95	0.48
1:A:41:LYS:HB2	1:C:519:HIS:HB2	1.95	0.48
1:A:456:PHE:HB2	1:A:491:PRO:HB3	1.96	0.48
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.41	0.48
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	1.96	0.48
1:A:848:ASP:OD1	1:A:848:ASP:N	2.46	0.47
1:A:745:ASP:OD2	1:C:319:ARG:NH2	2.47	0.47
1:A:357:ARG:HD2	1:A:396:TYR:HE1	1.79	0.47
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.96	0.47
1:A:618:THR:HG21	3:A:1306:NAG:H62	1.96	0.47
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.46	0.46
1:B:242:LEU:HD11	1:B:263:ALA:HB2	1.97	0.46
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.49	0.46
1:B:879:ALA:O	1:B:883:THR:OG1	2.31	0.46
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.97	0.46
1:A:1002:GLN:NE2	1:B:1002:GLN:OE1	2.49	0.46
1:B:538:CYS:HB2	1:B:590:CYS:HB3	1.75	0.46
1:A:364:ASP:OD1	1:A:366:SER:OG	2.33	0.46
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.98	0.46
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.42	0.45
1:C:618:THR:HG21	3:C:1307:NAG:H62	1.98	0.45
1:C:786:LYS:H	1:C:786:LYS:HG2	1.54	0.45
1:C:808:ASP:OD1	1:C:808:ASP:N	2.47	0.45
1:B:327:VAL:H	1:B:531:THR:HB	1.80	0.45
1:A:977:LEU:HD22	1:A:993:ILE:HG12	1.99	0.45
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	1.98	0.45
1:C:848:ASP:OD1	1:C:848:ASP:N	2.45	0.45
1:A:393:THR:O	1:A:523:THR:OG1	2.34	0.45
1:B:112:SER:HA	1:B:132:GLU:HB2	1.99	0.45
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	1.98	0.44
1:A:30:ASN:HD21	1:A:59:PHE:HD1	1.65	0.44
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.51	0.44
1:A:880:GLY:O	1:A:884:SER:OG	2.31	0.44
1:B:278:LYS:HE2	1:B:287:ASP:HB2	1.99	0.44
1:B:622:VAL:HG21	1:B:638:THR:HG21	1.99	0.44
1:B:848:ASP:OD1	1:B:848:ASP:N	2.43	0.44
1:B:811:LYS:HE3	1:B:813:SER:HB3	2.00	0.44
1:C:1050:MET:HE2	1:C:1050:MET:HB3	1.87	0.44
1:A:701:ALA:HB3	1:B:787:GLN:HG2	1.99	0.44
1:C:374:PHE:HB3	1:C:436:TRP:HB3	2.00	0.44
1:C:840:CYS:O	1:C:847:ARG:NH2	2.50	0.44
1:B:519:HIS:HB2	1:C:41:LYS:HB2	2.00	0.43
1:C:466:ARG:HD3	1:C:468:ILE:HD11	2.00	0.43
1:C:733:LYS:HE3	1:C:771:ALA:HB1	2.00	0.43
1:C:485:GLY:H	1:C:488:CYS:HB2	1.83	0.43
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.99	0.43
1:A:707:TYR:HB3	1:B:792:PRO:HG2	2.01	0.43
1:B:35:GLY:HA3	1:B:56:LEU:HB3	2.01	0.43
1:B:393:THR:O	1:B:523:THR:OG1	2.36	0.43
1:C:89:GLY:HA3	1:C:270:LEU:HB2	2.01	0.43
1:B:847:ARG:HA	1:B:847:ARG:HD2	1.88	0.43
1:B:1103:PHE:HZ	2:I:1:NAG:H62	1.84	0.42
1:B:459:SER:OG	1:B:460:LYS:N	2.53	0.42
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.01	0.42
1:A:898:PHE:HA	1:A:901:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASP:OD1	1:B:40:ASP:N	2.50	0.42
1:C:391:CYS:HB2	1:C:525:CYS:HA	2.01	0.42
1:A:391:CYS:HB2	1:A:525:CYS:HA	2.02	0.42
1:B:581:THR:HG23	1:B:583:GLU:HG2	2.01	0.42
1:A:93:ALA:HB3	1:A:266:TYR:HB2	2.02	0.42
1:A:811:LYS:HG2	1:A:813:SER:H	1.84	0.42
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	2.02	0.41
1:A:35:GLY:HA3	1:A:56:LEU:HB3	2.02	0.41
1:C:37:TYR:HA	1:C:223:LEU:H	1.84	0.41
1:A:131:CYS:SG	1:A:166:CYS:N	2.94	0.41
1:A:537:LYS:HE2	1:A:537:LYS:HB2	1.93	0.41
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	2.02	0.41
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.95	0.41
1:A:811:LYS:HE3	1:A:813:SER:HB3	2.03	0.41
1:B:934:ILE:HD13	1:B:934:ILE:HA	1.94	0.41
1:C:474:GLN:NE2	1:C:476:GLY:O	2.44	0.41
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.41
1:C:40:ASP:OD1	1:C:40:ASP:N	2.52	0.41
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.93	0.40
1:C:296:LEU:HB2	1:C:608:VAL:HG21	2.03	0.40
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	2.04	0.40
1:A:825:LYS:HA	1:A:825:LYS:HD3	1.83	0.40
1:B:808:ASP:HA	1:B:809:PRO:HD3	1.94	0.40
1:C:827:THR:O	1:C:827:THR:OG1	2.39	0.40
1:A:195:LYS:HE3	1:A:202:LYS:HD2	2.02	0.40
1:A:317:ASN:ND2	1:A:593:GLY:O	2.54	0.40
1:A:941:THR:HG22	1:A:943:SER:H	1.85	0.40
1:B:197:ILE:O	1:B:202:LYS:NZ	2.55	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	1019/1284 (79%)	972 (95%)	47 (5%)	0	100	100
1	B	1019/1284 (79%)	985 (97%)	34 (3%)	0	100	100
1	C	1019/1284 (79%)	979 (96%)	40 (4%)	0	100	100
All	All	3057/3852 (79%)	2936 (96%)	121 (4%)	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	898/1110 (81%)	897 (100%)	1 (0%)	88	91
1	B	898/1110 (81%)	898 (100%)	0	100	100
1	C	898/1110 (81%)	898 (100%)	0	100	100
All	All	2694/3330 (81%)	2693 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	804	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	122	ASN
1	A	125	ASN
1	A	317	ASN
1	A	388	ASN
1	A	690	GLN
1	A	914	ASN
1	A	935	GLN
1	A	1002	GLN

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Mol	Chain	Res	Type
1	A	1011	GLN
1	A	1054	GLN
1	B	87	ASN
1	B	207	HIS
1	B	370	ASN
1	B	405	ASN
1	B	417	ASN
1	B	450	ASN
1	B	474	GLN
1	B	481	ASN
1	B	607	GLN
1	B	644	GLN
1	B	677	GLN
1	B	856	ASN
1	B	1010	GLN
1	B	1106	GLN
1	C	321	GLN
1	C	493	GLN
1	C	677	GLN
1	C	787	GLN
1	C	856	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

18 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	$\#\|Z\|>2$
2	NAG	D	1	2,1	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	E	1	2,1	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
2	NAG	E	2	2	14,14,15	0.36	0	17,19,21	0.56	0
2	NAG	F	1	2,1	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	F	2	2	14,14,15	0.42	0	17,19,21	0.58	0
2	NAG	G	1	2,1	14,14,15	0.30	0	17,19,21	0.54	0
2	NAG	G	2	2	14,14,15	0.36	0	17,19,21	0.50	0
2	NAG	H	1	2,1	14,14,15	0.37	0	17,19,21	0.50	0
2	NAG	H	2	2	14,14,15	0.34	0	17,19,21	0.52	0
2	NAG	I	1	2,1	14,14,15	0.37	0	17,19,21	0.65	0
2	NAG	I	2	2	14,14,15	0.89	1 (7%)	17,19,21	0.57	0
2	NAG	J	1	2,1	14,14,15	0.34	0	17,19,21	0.57	0
2	NAG	J	2	2	14,14,15	0.37	0	17,19,21	0.51	0
2	NAG	K	1	2,1	14,14,15	0.50	0	17,19,21	1.04	1 (5%)
2	NAG	K	2	2	14,14,15	0.37	0	17,19,21	0.48	0
2	NAG	L	1	2,1	14,14,15	0.36	0	17,19,21	0.61	0
2	NAG	L	2	2	14,14,15	0.98	1 (7%)	17,19,21	0.61	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	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)
2	L	2	NAG	C1-C2	3.23	1.56	1.52
2	I	2	NAG	C1-C2	2.85	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1	NAG	C2-N2-C7	3.23	127.23	122.90
2	E	1	NAG	C2-N2-C7	3.22	127.22	122.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	J	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C1-C2-N2-C7
2	K	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	K	1	NAG	C3-C2-N2-C7
2	I	2	NAG	O5-C5-C6-O6

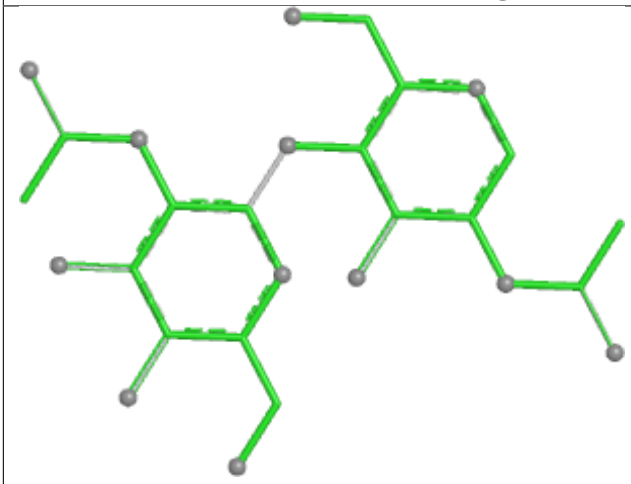
There are no ring outliers.

1 monomer is involved in 1 short contact:

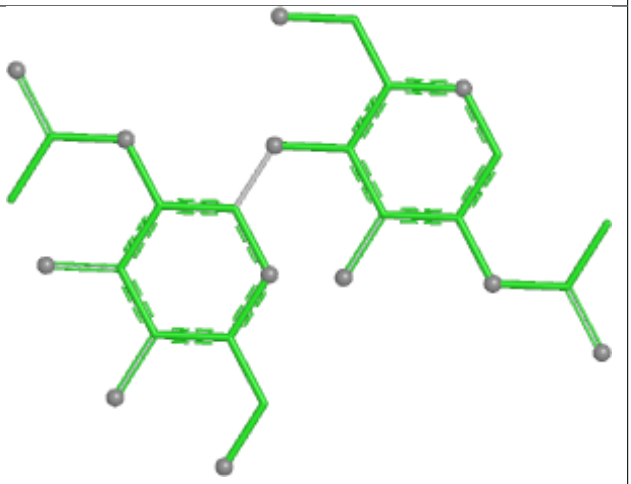
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	1	0

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

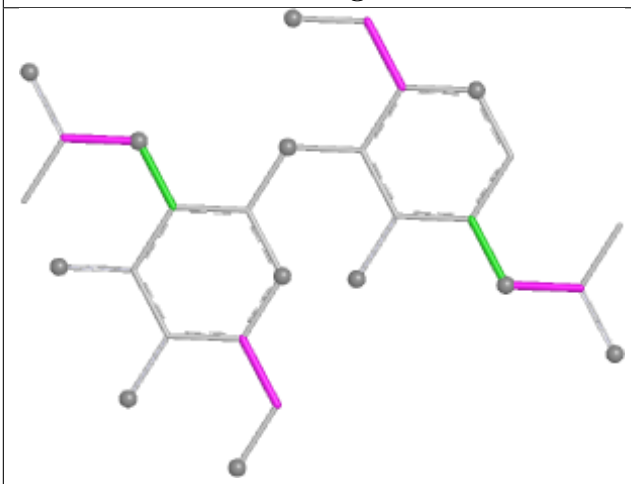
Oligosaccharide Chain D



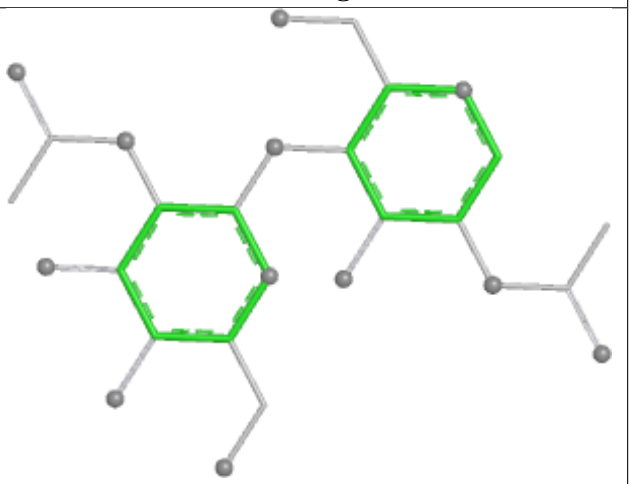
Bond lengths



Bond angles

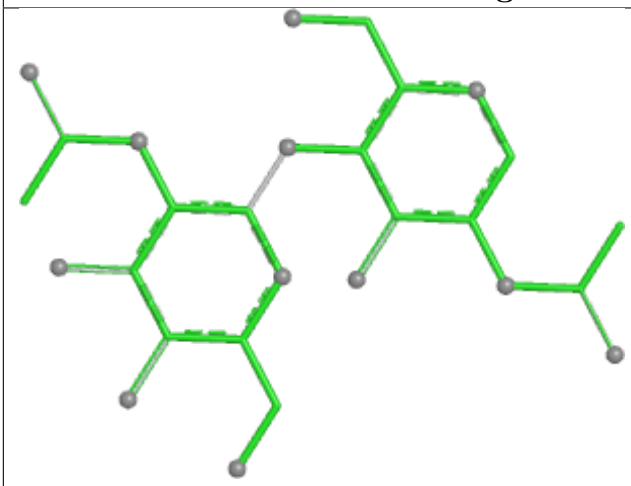


Torsions

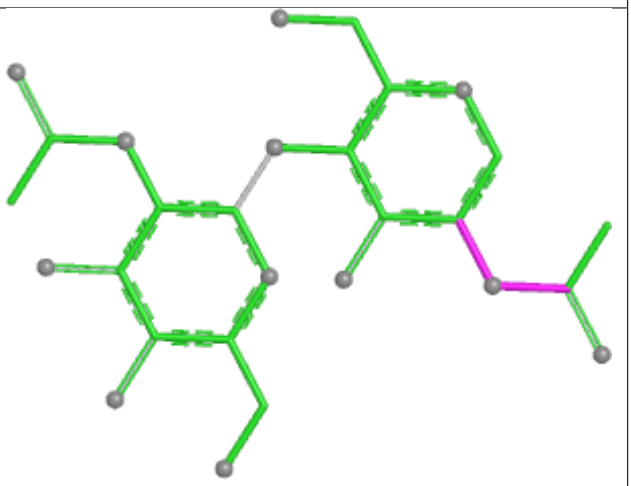


Rings

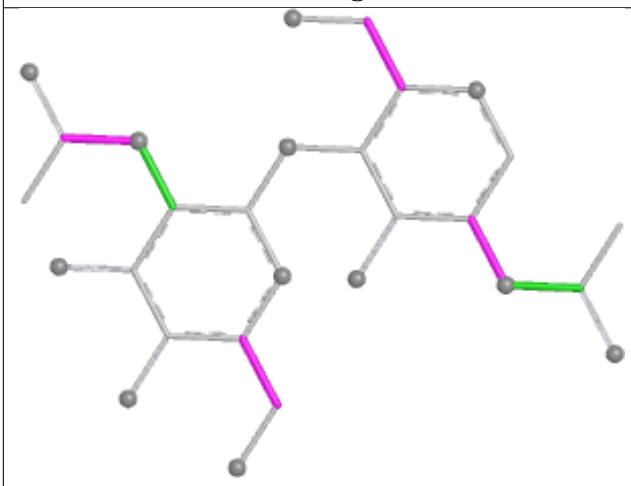
Oligosaccharide Chain E



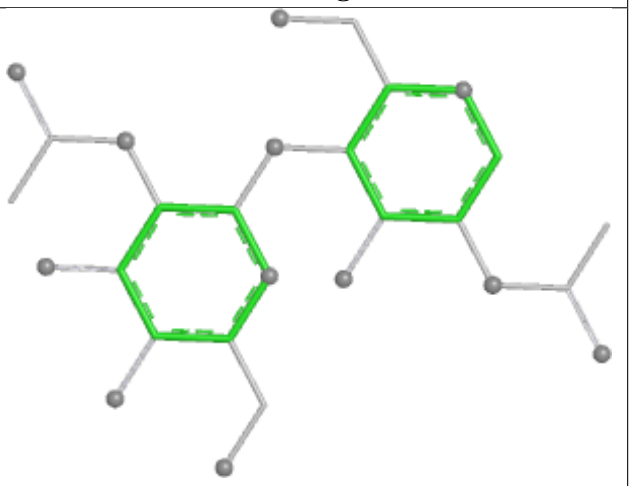
Bond lengths



Bond angles

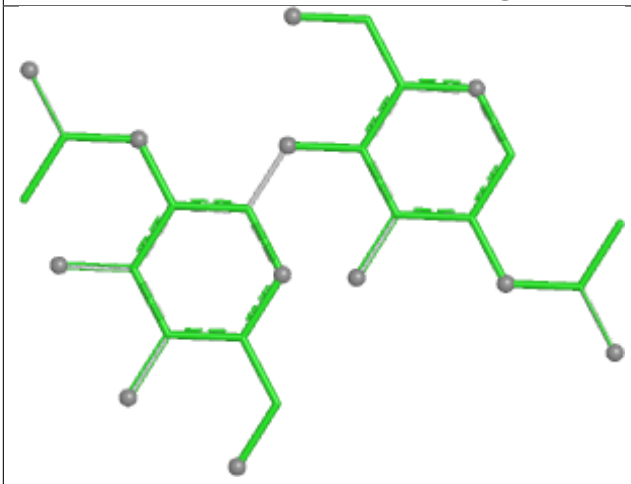


Torsions

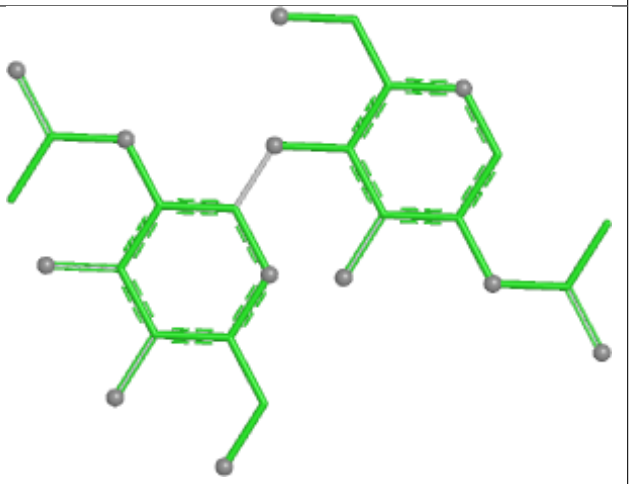


Rings

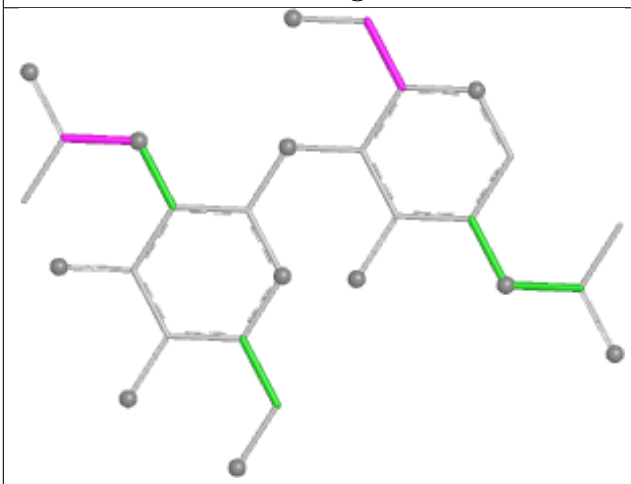
Oligosaccharide Chain F



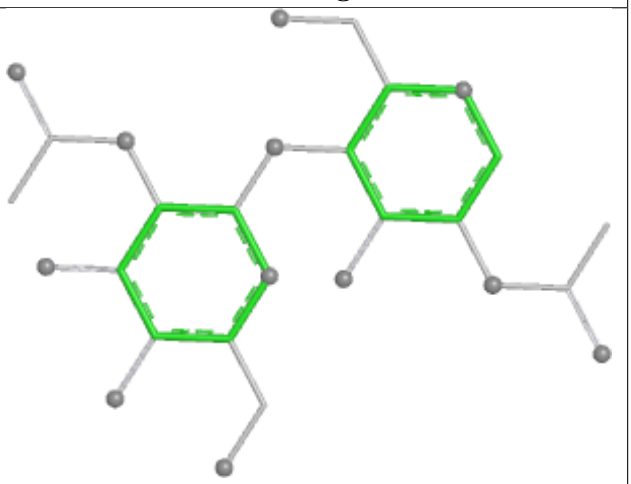
Bond lengths



Bond angles

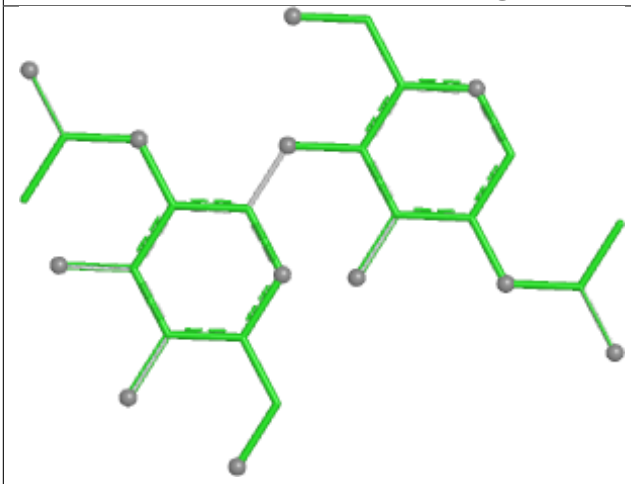


Torsions

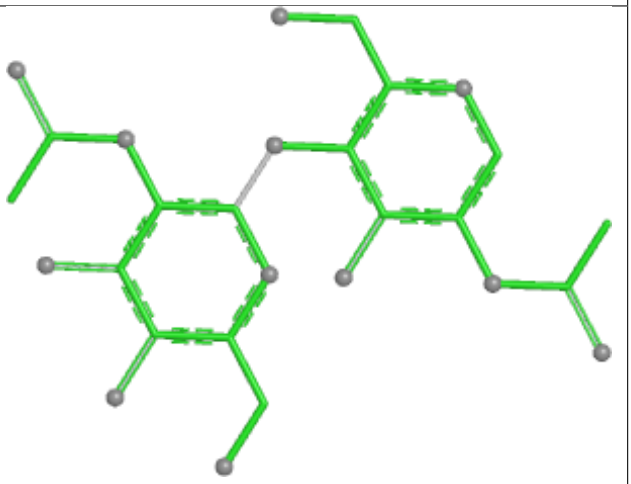


Rings

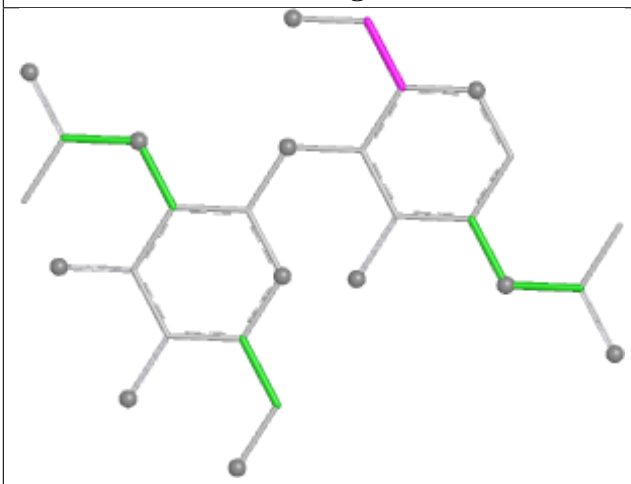
Oligosaccharide Chain G



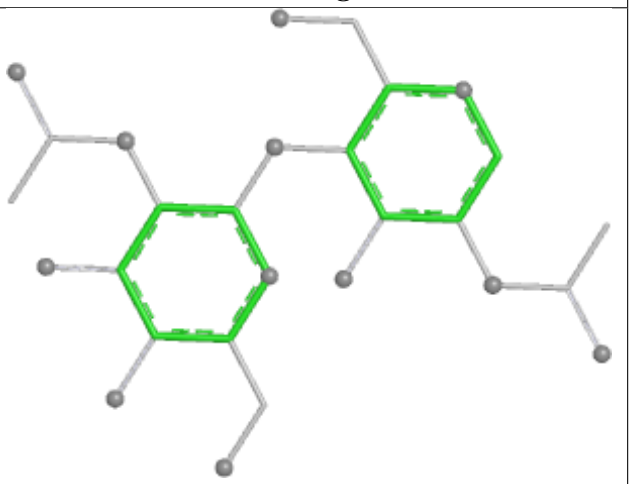
Bond lengths



Bond angles

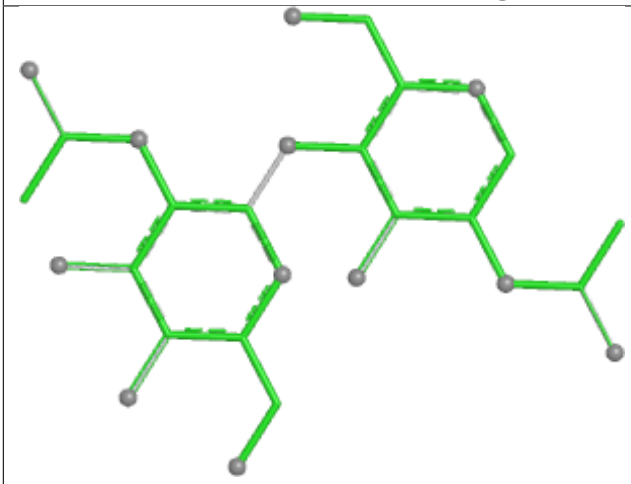


Torsions

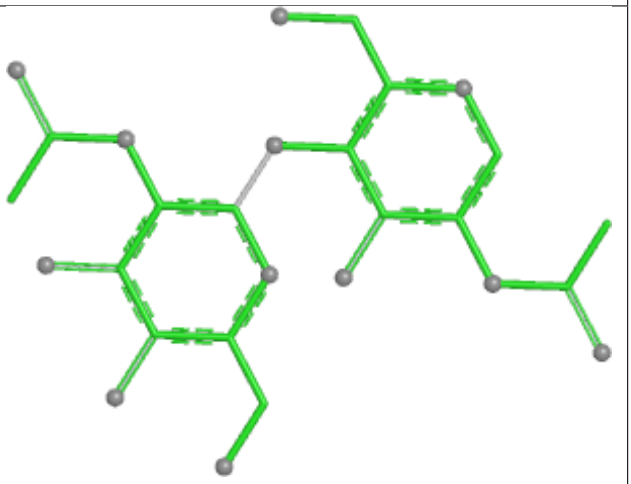


Rings

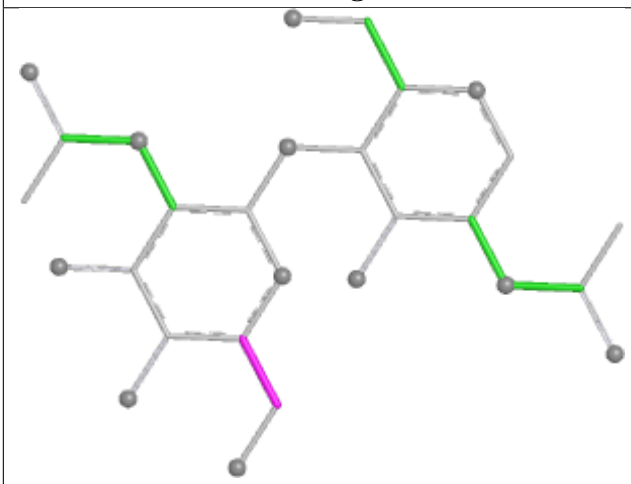
Oligosaccharide Chain H



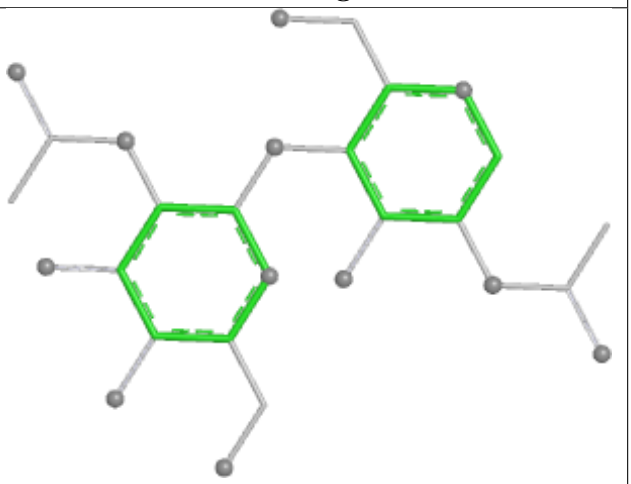
Bond lengths



Bond angles

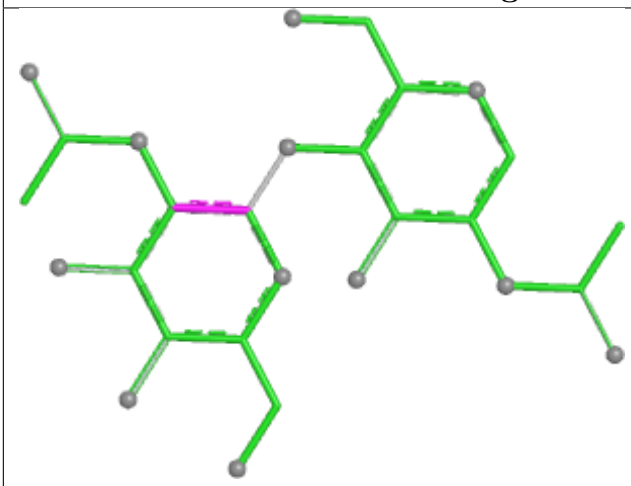


Torsions

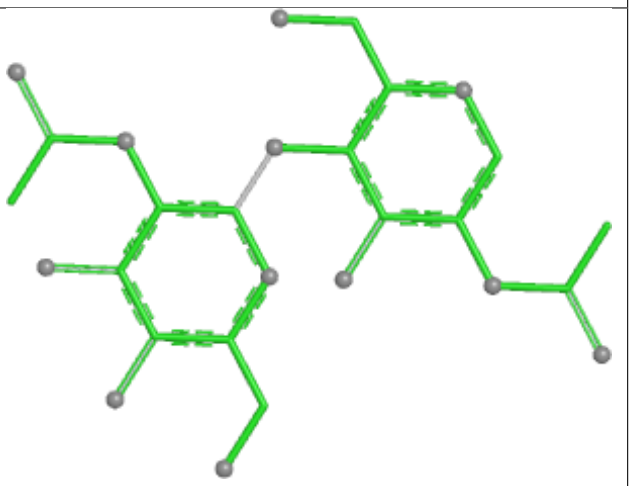


Rings

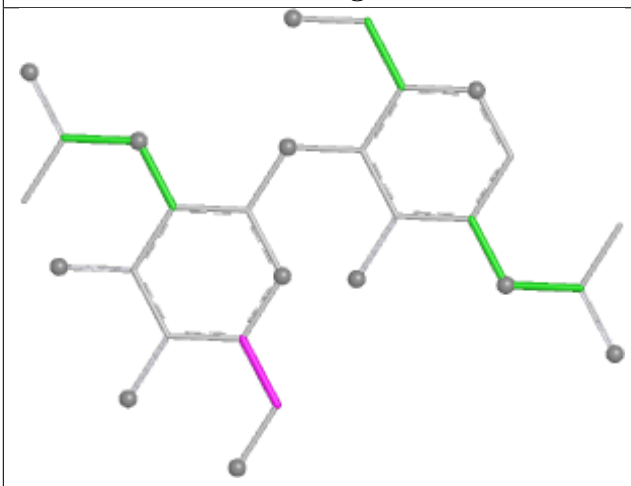
Oligosaccharide Chain I



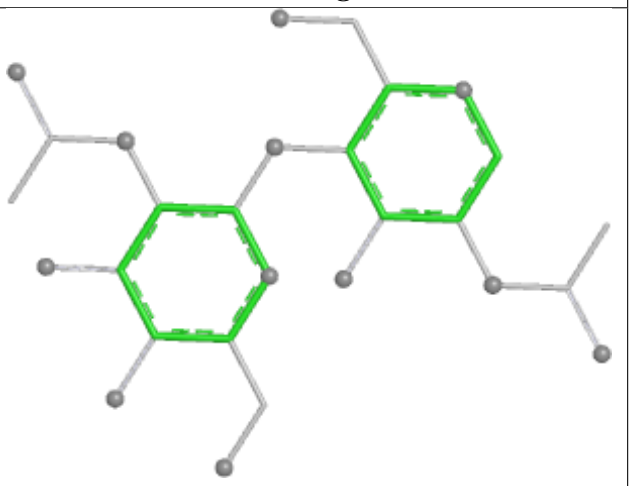
Bond lengths



Bond angles

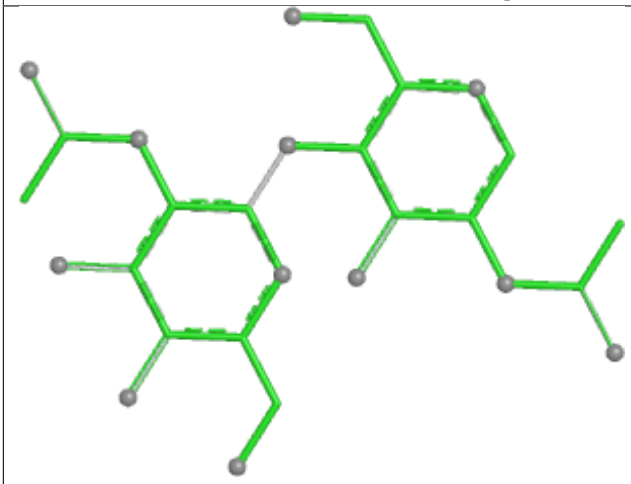


Torsions

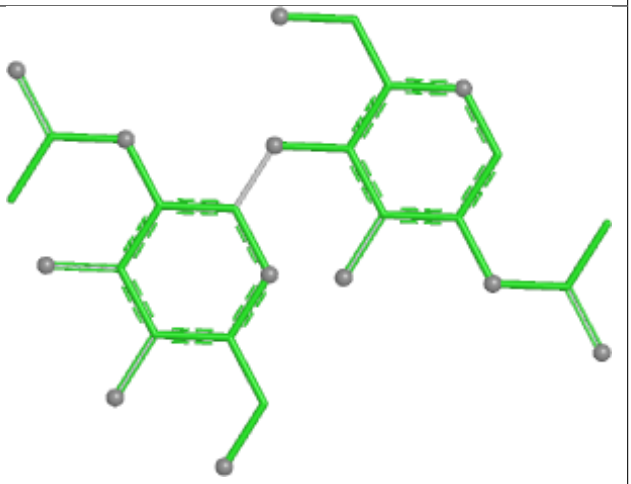


Rings

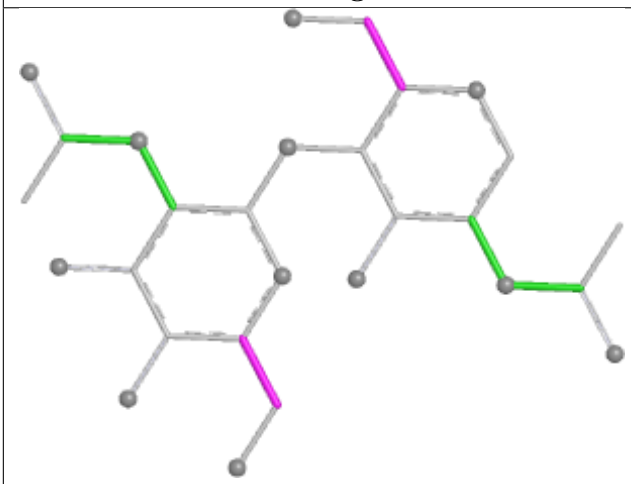
Oligosaccharide Chain J



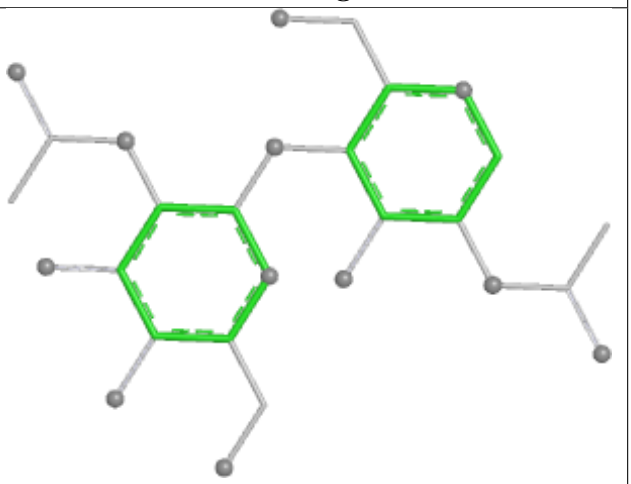
Bond lengths



Bond angles

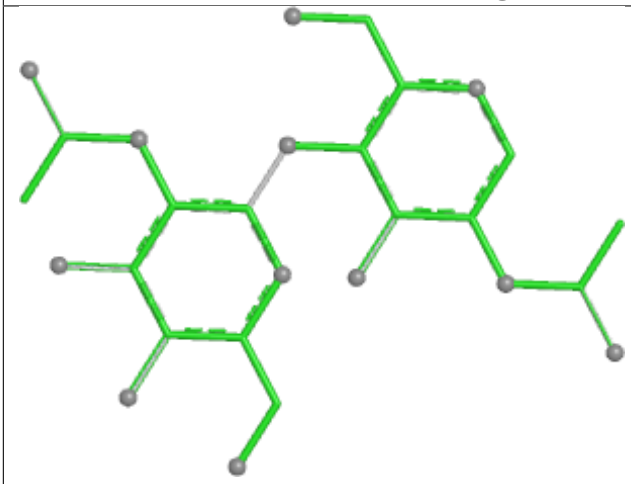


Torsions

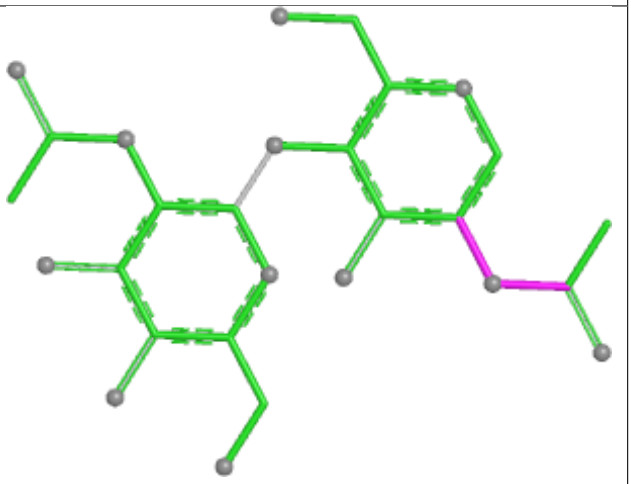


Rings

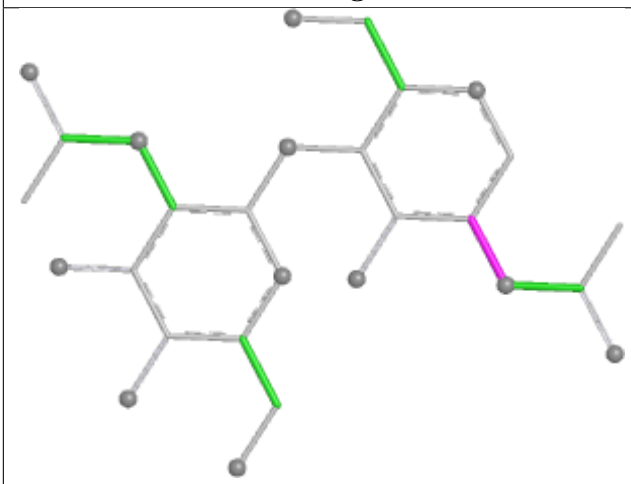
Oligosaccharide Chain K



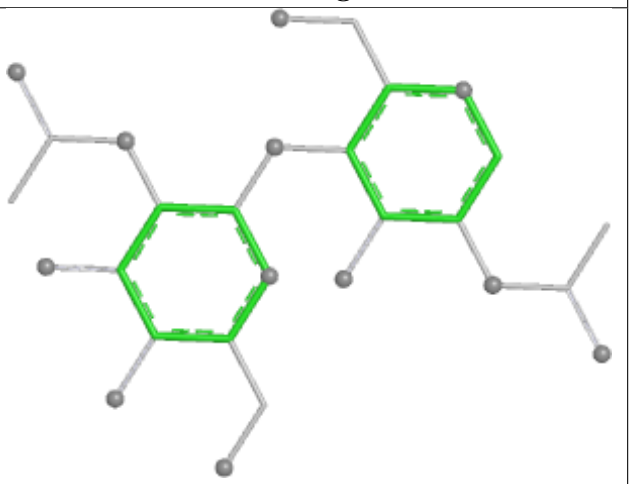
Bond lengths



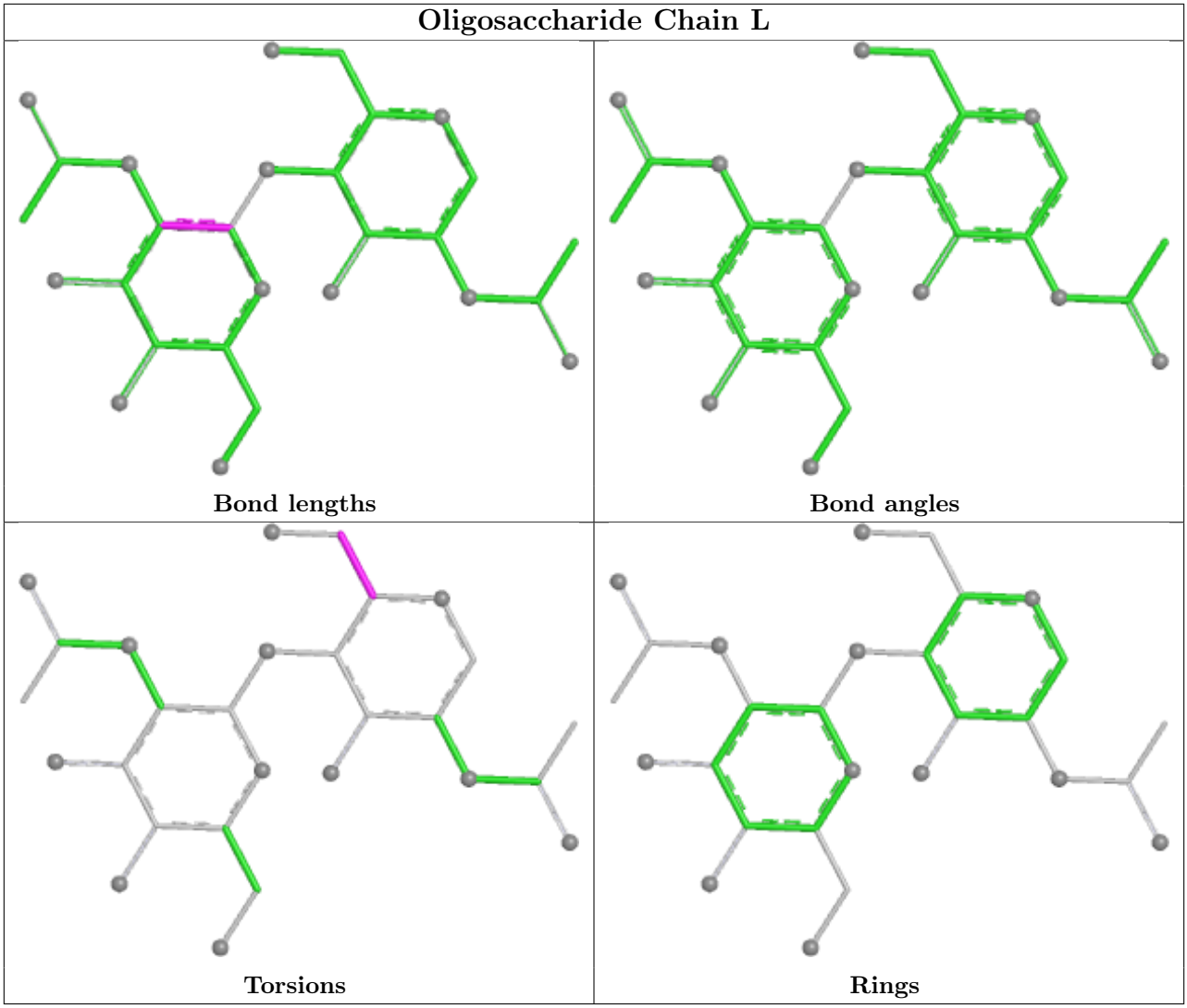
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

30 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	$\#\|Z\| > 2$
3	NAG	B	1302	1	14,14,15	0.38	0	17,19,21	0.52	0
3	NAG	C	1305	1	14,14,15	0.48	0	17,19,21	0.51	0
3	NAG	B	1303	1	14,14,15	0.34	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1311	1	14,14,15	1.08	1 (7%)	17,19,21	2.38	4 (23%)
3	NAG	A	1303	1	14,14,15	0.34	0	17,19,21	0.50	0
3	NAG	C	1301	1	14,14,15	1.09	1 (7%)	17,19,21	2.39	4 (23%)
3	NAG	B	1307	1	14,14,15	0.53	0	17,19,21	1.06	1 (5%)
3	NAG	C	1302	1	14,14,15	0.57	0	17,19,21	0.81	1 (5%)
3	NAG	C	1308	1	14,14,15	0.54	0	17,19,21	1.05	1 (5%)
3	NAG	A	1308	1	14,14,15	0.53	0	17,19,21	1.08	1 (5%)
3	NAG	B	1305	1	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
3	NAG	C	1307	1	14,14,15	0.52	0	17,19,21	1.06	1 (5%)
3	NAG	C	1303	1	14,14,15	0.37	0	17,19,21	0.47	0
3	NAG	C	1309	1	14,14,15	0.48	0	17,19,21	1.08	1 (5%)
3	NAG	C	1310	1	14,14,15	0.33	0	17,19,21	0.51	0
3	NAG	A	1304	1	14,14,15	0.55	0	17,19,21	0.48	0
3	NAG	A	1305	1	14,14,15	0.87	2 (14%)	17,19,21	1.23	2 (11%)
3	NAG	A	1301	1	14,14,15	0.45	0	17,19,21	0.75	1 (5%)
3	NAG	B	1306	1	14,14,15	0.53	0	17,19,21	1.06	1 (5%)
3	NAG	B	1309	1	14,14,15	0.39	0	17,19,21	0.55	0
3	NAG	B	1308	1	14,14,15	0.48	0	17,19,21	1.11	2 (11%)
3	NAG	C	1306	1	14,14,15	0.82	1 (7%)	17,19,21	1.14	2 (11%)
3	NAG	C	1304	1	14,14,15	0.42	0	17,19,21	0.48	0
3	NAG	A	1306	1	14,14,15	0.70	1 (7%)	17,19,21	1.14	2 (11%)
3	NAG	B	1304	1	14,14,15	0.55	0	17,19,21	0.43	0
3	NAG	A	1302	1	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	B	1310	1	14,14,15	0.94	1 (7%)	17,19,21	2.38	3 (17%)
3	NAG	A	1307	1	14,14,15	0.55	0	17,19,21	1.05	1 (5%)
3	NAG	B	1301	1	14,14,15	0.42	0	17,19,21	0.61	0
3	NAG	A	1309	1	14,14,15	0.37	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	5/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1311	NAG	C1-C2	3.39	1.57	1.52
3	C	1301	NAG	C1-C2	3.38	1.56	1.52
3	B	1310	NAG	C1-C2	2.84	1.56	1.52
3	C	1306	NAG	C1-C2	2.63	1.55	1.52
3	A	1305	NAG	C1-C2	2.19	1.55	1.52
3	A	1305	NAG	O5-C1	2.14	1.47	1.43
3	A	1306	NAG	C1-C2	2.08	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1310	NAG	C2-N2-C7	8.30	134.03	122.90
3	C	1301	NAG	C2-N2-C7	8.26	133.97	122.90
3	B	1311	NAG	C2-N2-C7	8.20	133.89	122.90
3	B	1311	NAG	C1-C2-N2	3.95	116.66	110.43
3	C	1301	NAG	C1-C2-N2	3.93	116.63	110.43
3	B	1310	NAG	C1-C2-N2	3.92	116.61	110.43
3	B	1308	NAG	C2-N2-C7	3.31	127.33	122.90
3	B	1305	NAG	C2-N2-C7	3.27	127.29	122.90
3	A	1305	NAG	C1-O5-C5	3.26	116.55	112.19
3	C	1309	NAG	C2-N2-C7	3.25	127.26	122.90
3	A	1308	NAG	C2-N2-C7	3.25	127.25	122.90
3	C	1307	NAG	C2-N2-C7	3.22	127.21	122.90
3	B	1307	NAG	C2-N2-C7	3.21	127.20	122.90
3	B	1306	NAG	C2-N2-C7	3.21	127.20	122.90
3	C	1308	NAG	C2-N2-C7	3.20	127.19	122.90
3	A	1307	NAG	C2-N2-C7	3.18	127.16	122.90
3	A	1306	NAG	C2-N2-C7	3.11	127.06	122.90
3	A	1305	NAG	C2-N2-C7	3.06	127.00	122.90
3	C	1306	NAG	C2-N2-C7	3.03	126.96	122.90
3	C	1306	NAG	C1-O5-C5	2.75	115.87	112.19
3	A	1306	NAG	C1-O5-C5	2.65	115.74	112.19
3	C	1302	NAG	C1-O5-C5	2.64	115.72	112.19
3	A	1301	NAG	C1-O5-C5	2.37	115.36	112.19
3	C	1301	NAG	C1-O5-C5	2.34	115.32	112.19
3	B	1311	NAG	C1-O5-C5	2.28	115.24	112.19
3	B	1310	NAG	C8-C7-N2	2.14	119.67	116.12
3	B	1311	NAG	C8-C7-N2	2.14	119.66	116.12
3	C	1301	NAG	C8-C7-N2	2.14	119.66	116.12
3	B	1308	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1309	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1309	NAG	O5-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	B	1310	NAG	C8-C7-N2-C2
3	B	1310	NAG	O7-C7-N2-C2
3	B	1311	NAG	C8-C7-N2-C2
3	B	1311	NAG	O7-C7-N2-C2
3	C	1301	NAG	C8-C7-N2-C2
3	C	1301	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	B	1304	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1305	NAG	C3-C2-N2-C7
3	A	1306	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7
3	C	1306	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	1307	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1305	NAG	C1-C2-N2-C7
3	A	1306	NAG	C1-C2-N2-C7
3	A	1307	NAG	C1-C2-N2-C7
3	A	1308	NAG	C1-C2-N2-C7
3	B	1305	NAG	C1-C2-N2-C7
3	B	1306	NAG	C1-C2-N2-C7
3	B	1307	NAG	C1-C2-N2-C7
3	B	1308	NAG	C1-C2-N2-C7
3	B	1310	NAG	C1-C2-N2-C7
3	B	1311	NAG	C1-C2-N2-C7
3	C	1301	NAG	C1-C2-N2-C7
3	C	1306	NAG	C1-C2-N2-C7
3	C	1307	NAG	C1-C2-N2-C7
3	C	1308	NAG	C1-C2-N2-C7
3	C	1309	NAG	C1-C2-N2-C7
3	B	1302	NAG	O5-C5-C6-O6
3	A	1307	NAG	C3-C2-N2-C7
3	A	1308	NAG	C3-C2-N2-C7
3	B	1305	NAG	C3-C2-N2-C7
3	B	1306	NAG	C3-C2-N2-C7
3	B	1307	NAG	C3-C2-N2-C7
3	B	1308	NAG	C3-C2-N2-C7
3	B	1310	NAG	C3-C2-N2-C7
3	B	1311	NAG	C3-C2-N2-C7
3	C	1307	NAG	C3-C2-N2-C7
3	C	1308	NAG	C3-C2-N2-C7
3	C	1309	NAG	C3-C2-N2-C7
3	C	1308	NAG	C4-C5-C6-O6

There are no ring outliers.

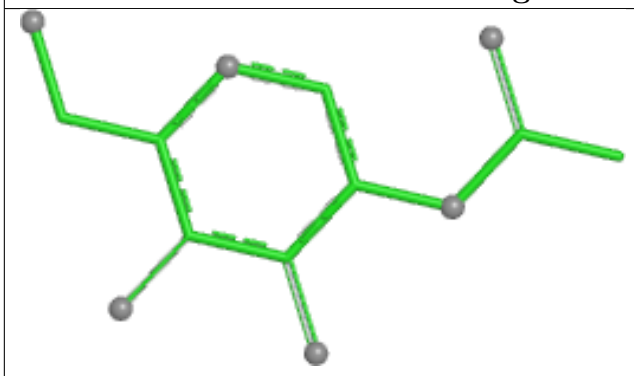
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1307	NAG	1	0
3	A	1306	NAG	1	0

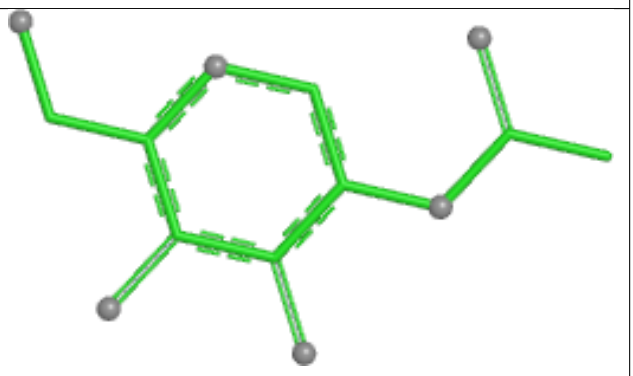
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

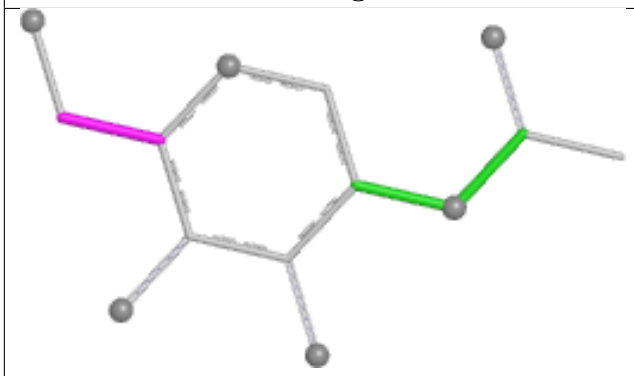
Ligand NAG B 1302



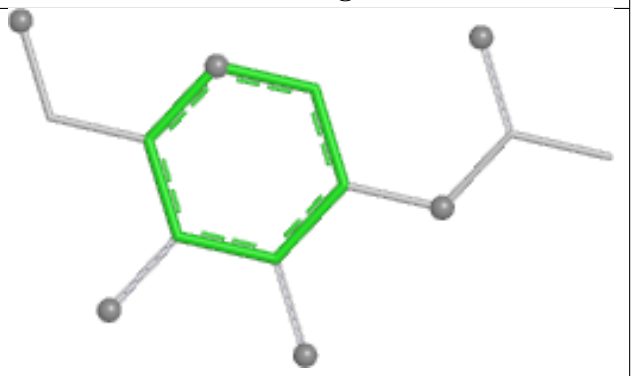
Bond lengths



Bond angles

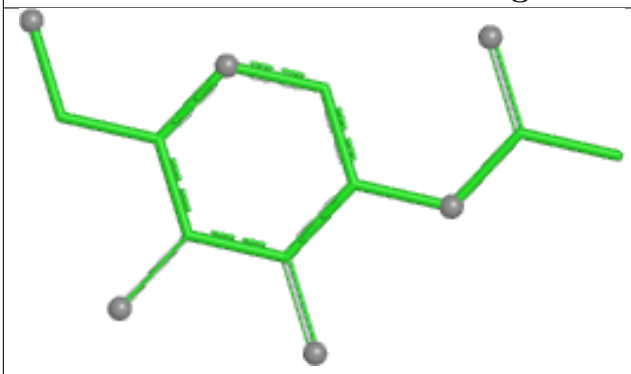


Torsions



Rings

Ligand NAG C 1305



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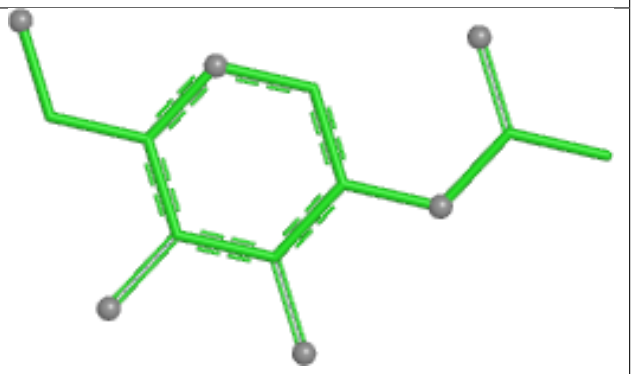

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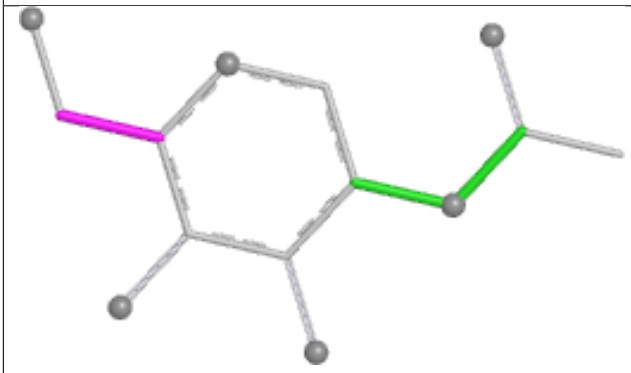

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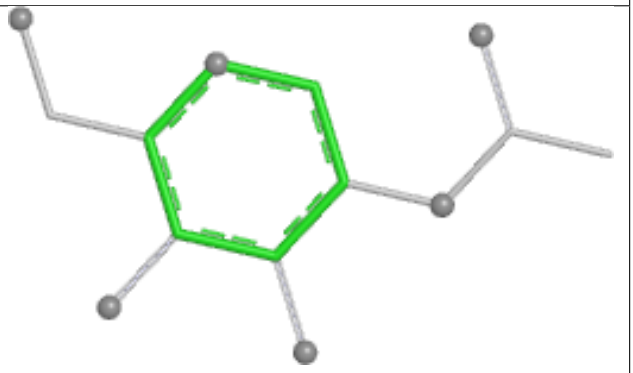
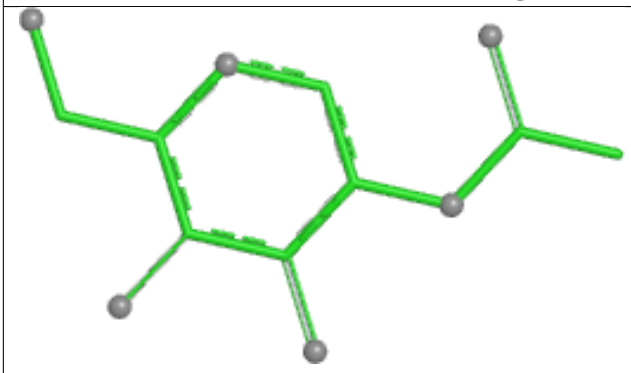


Rings

Ligand NAG B 1303



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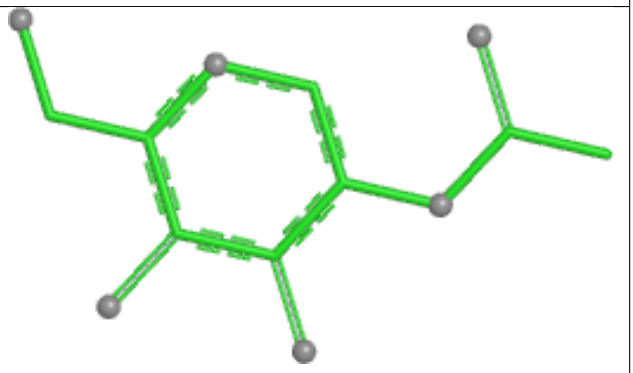
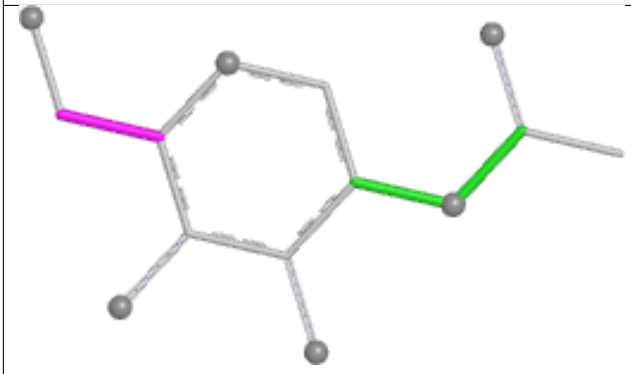


Bond angles



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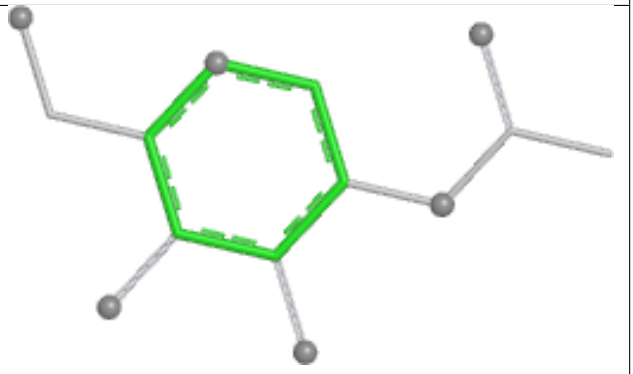
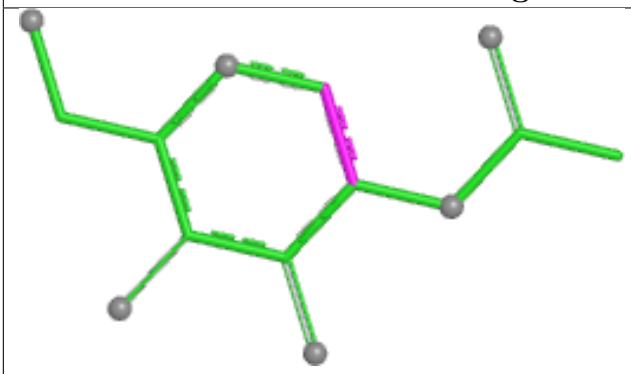


Rings

Ligand NAG B 1311



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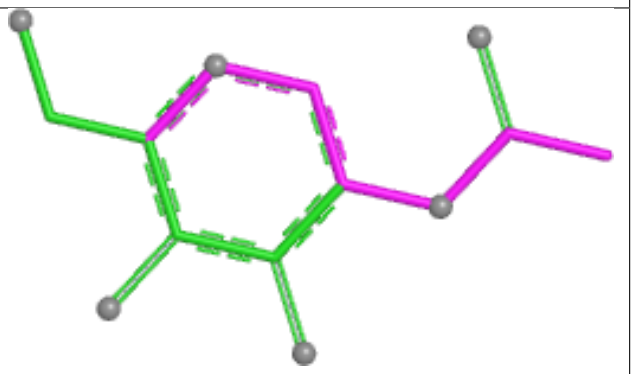
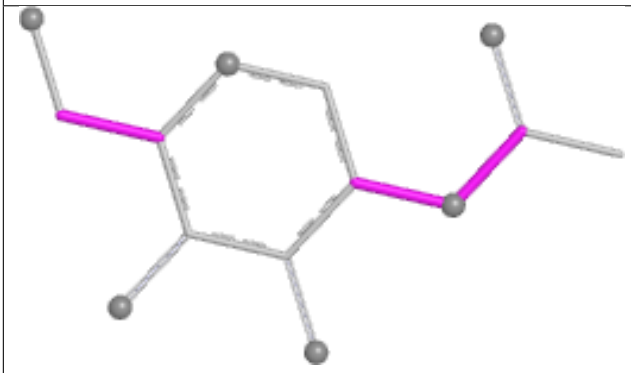


Bond angles



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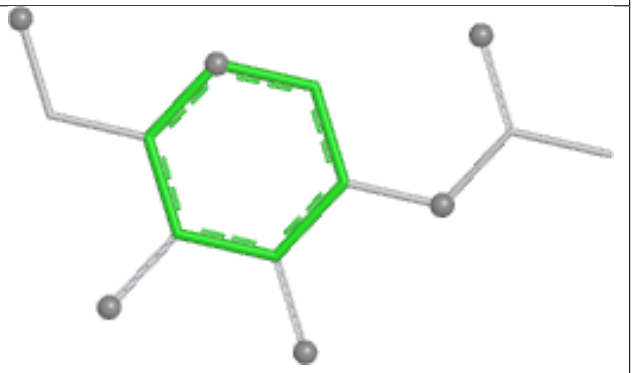
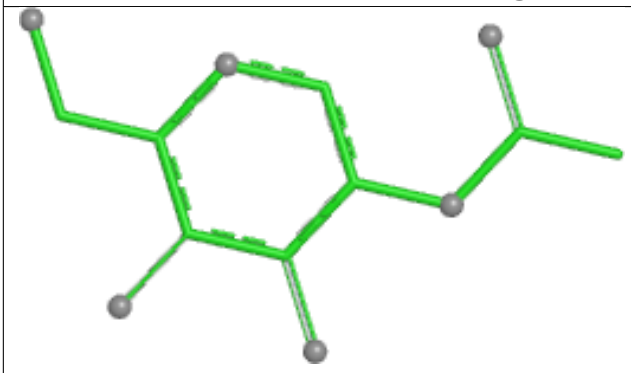


Rings

Ligand NAG A 1303



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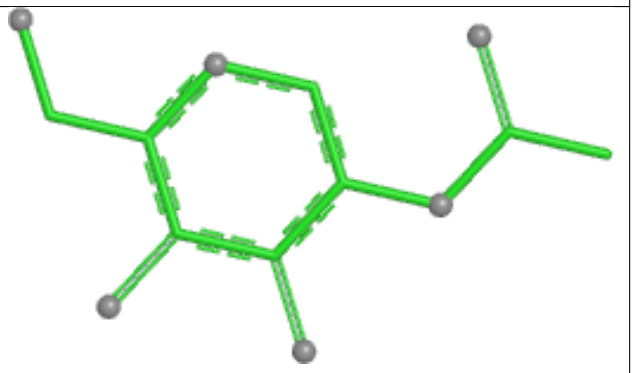

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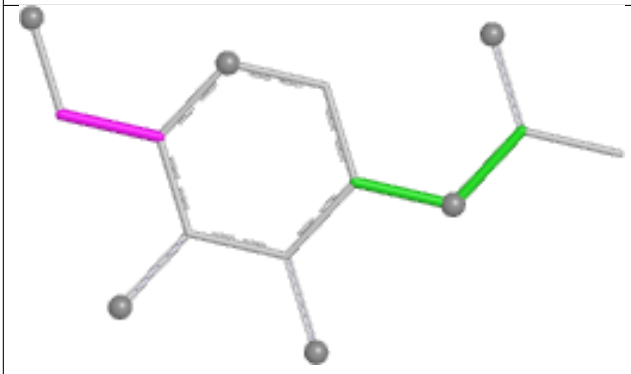

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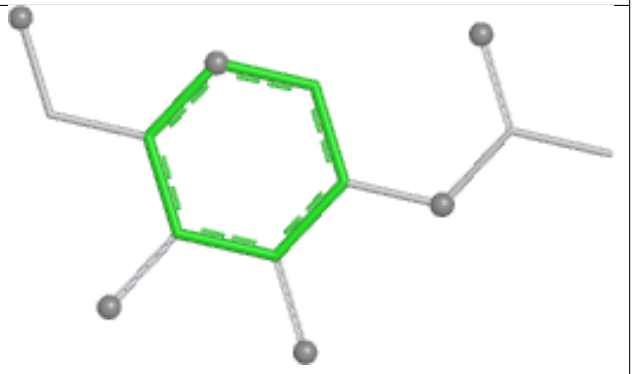
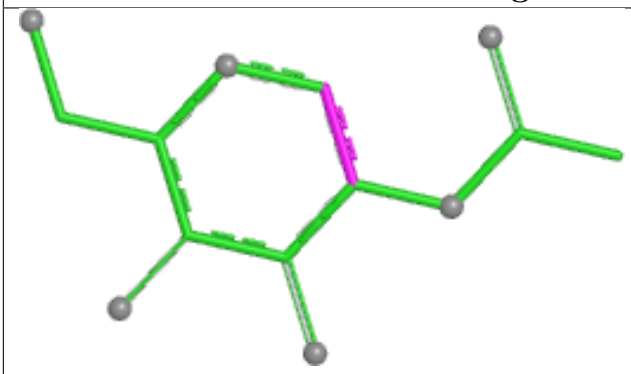


Rings

Ligand NAG C 1301



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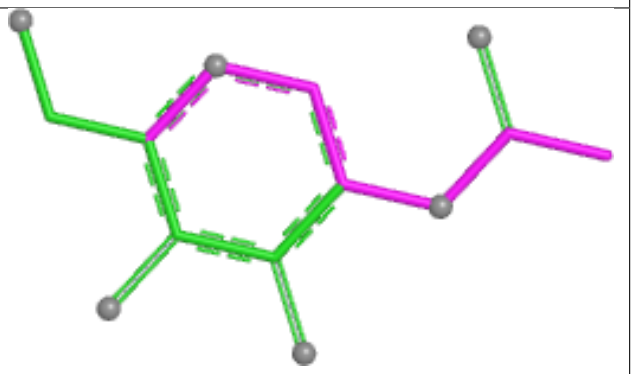

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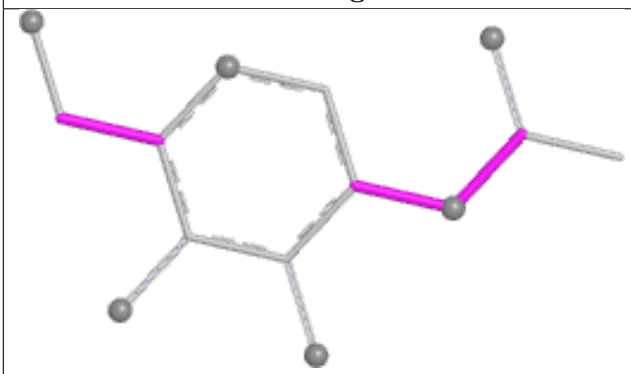

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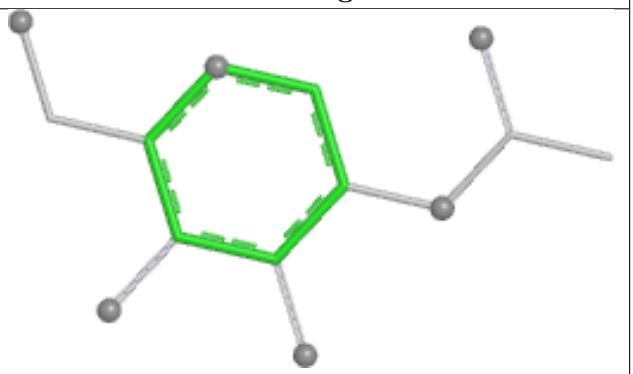
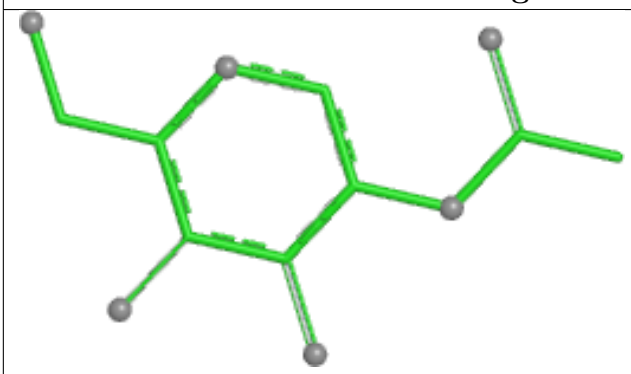


Rings

Ligand NAG B 1307



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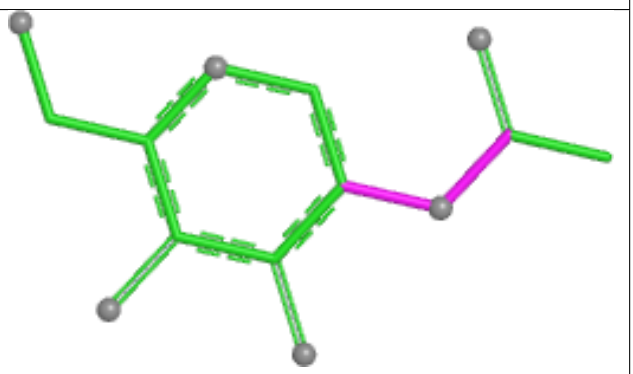

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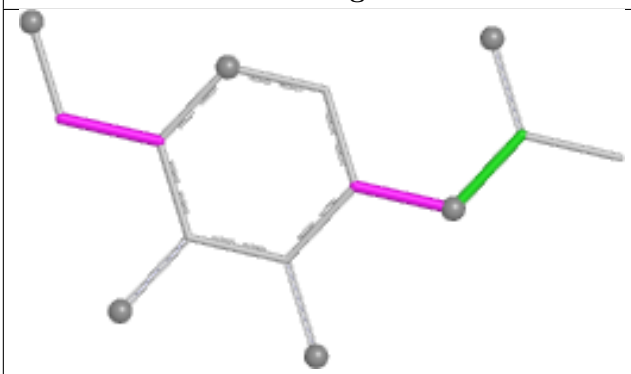

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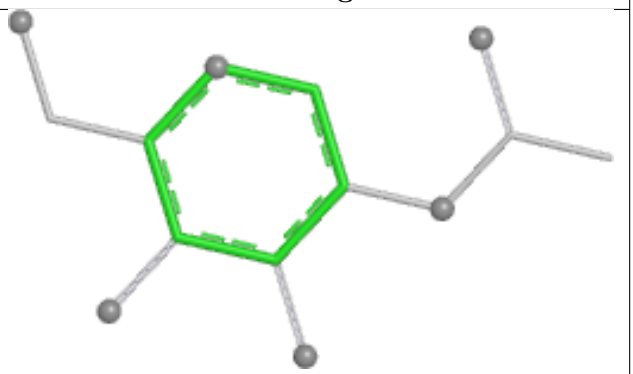
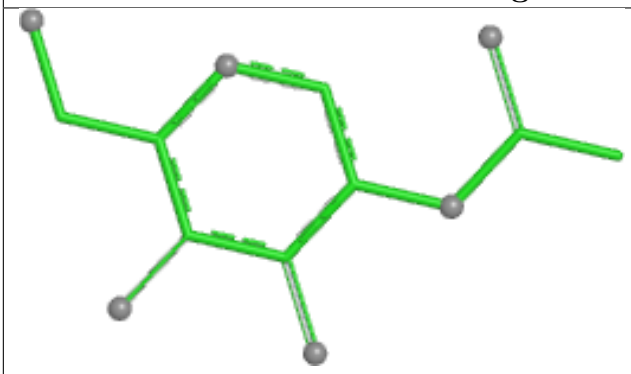


Rings

Ligand NAG C 1302



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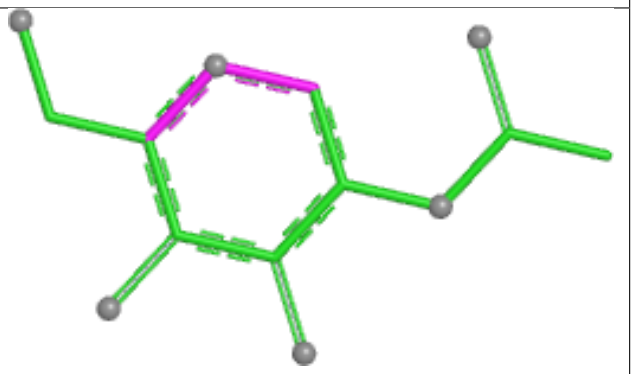

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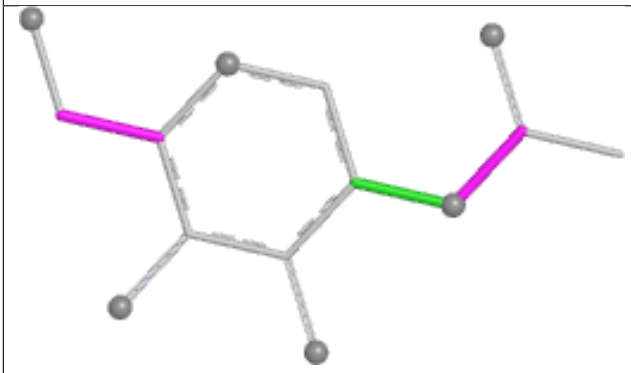

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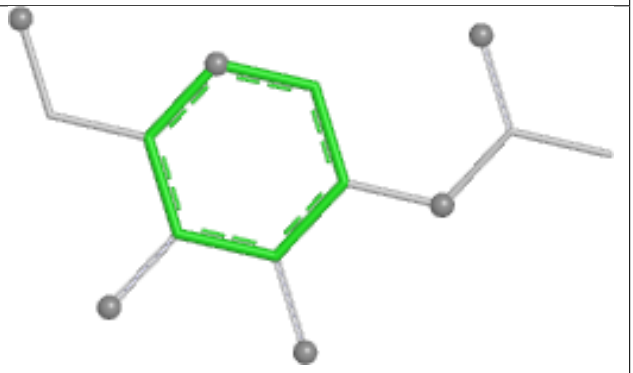
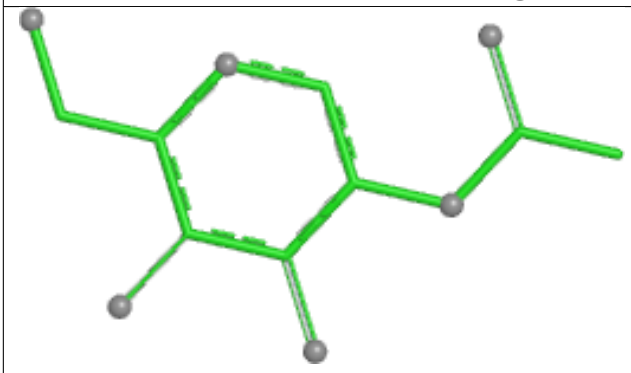


Rings

Ligand NAG C 1308



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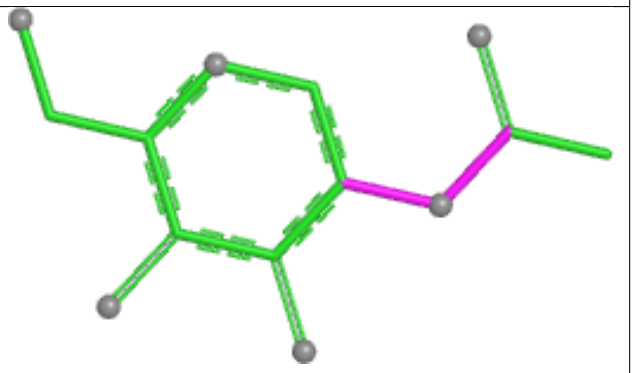
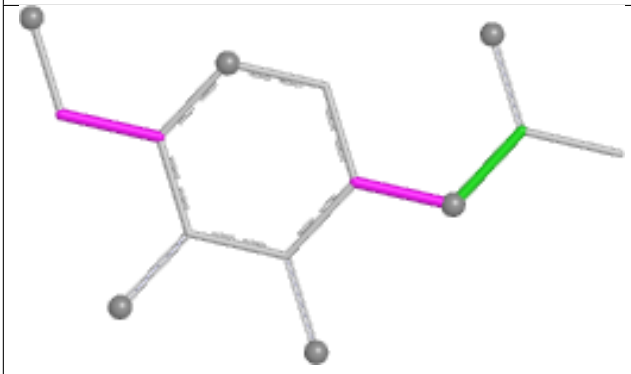


Bond angles



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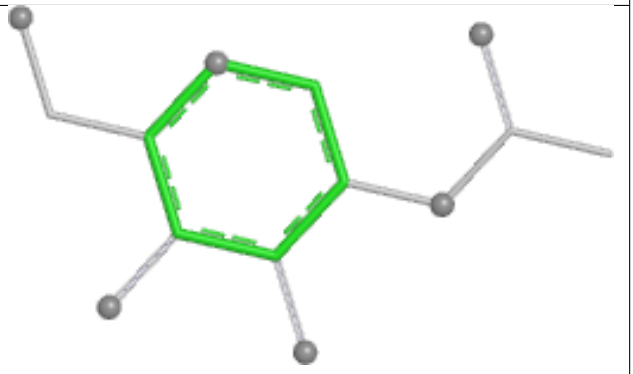
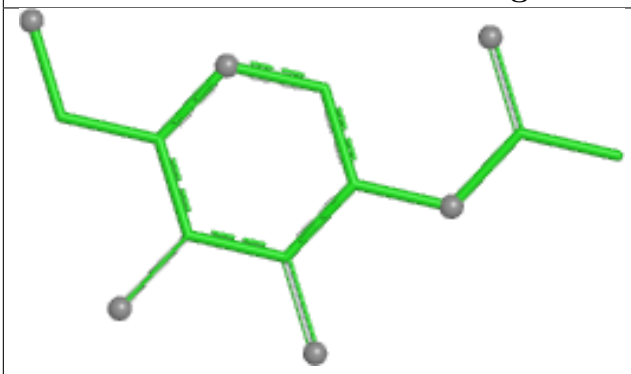


Rings

Ligand NAG A 1308



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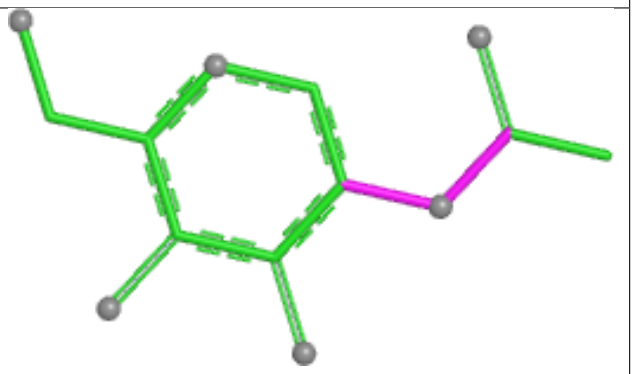

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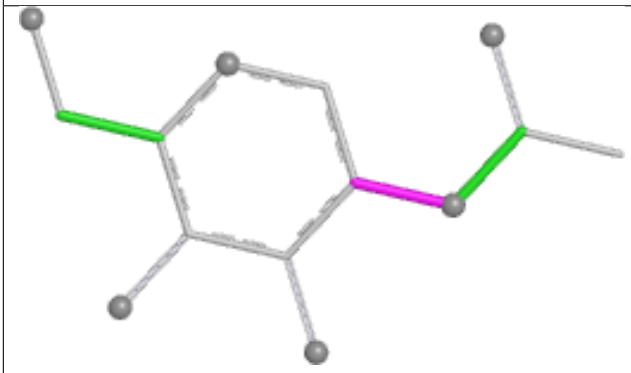

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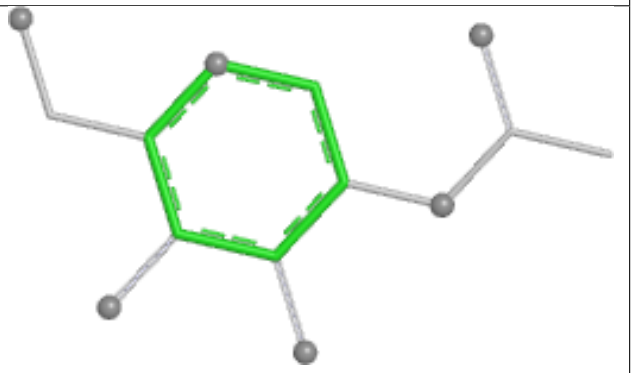
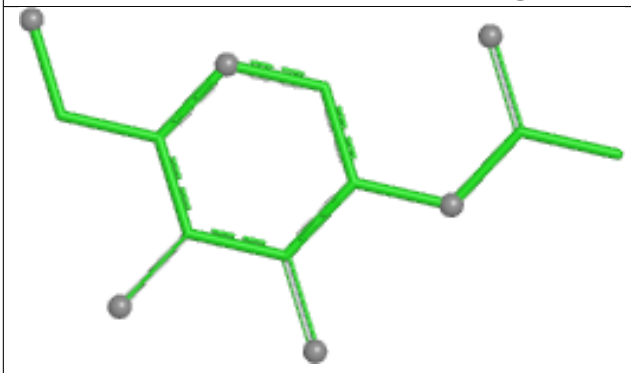


Rings

Ligand NAG B 1305



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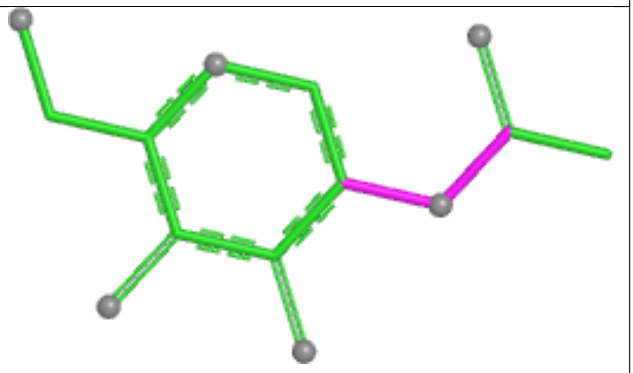

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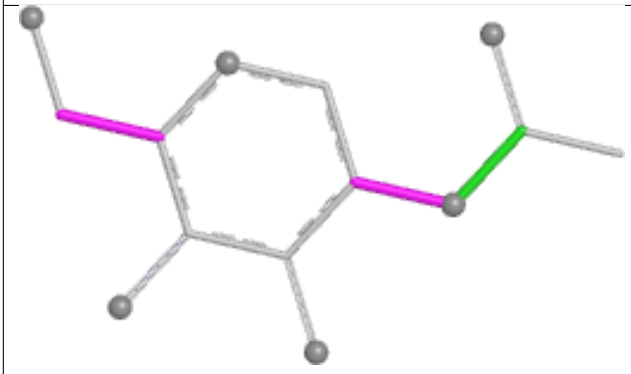

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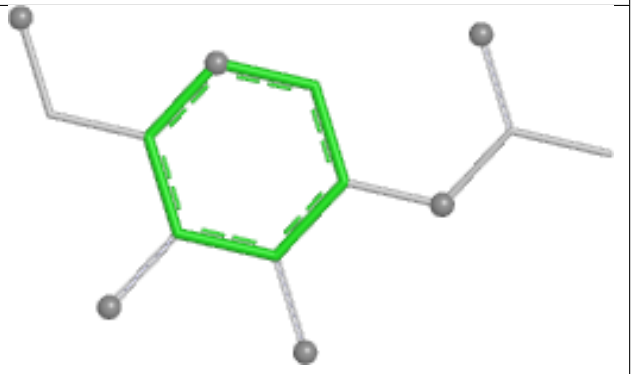
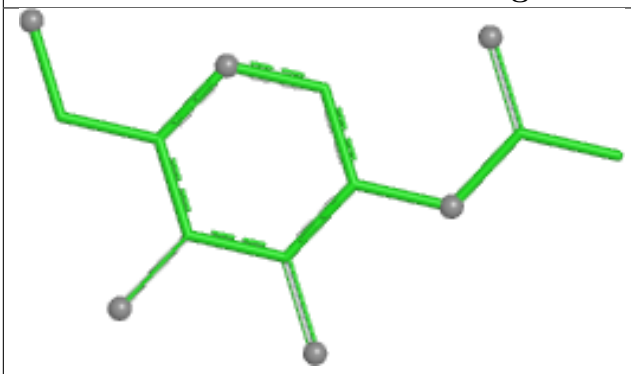


Rings

Ligand NAG C 1307



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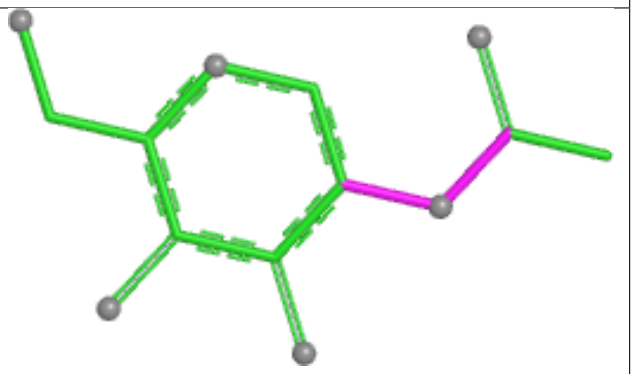
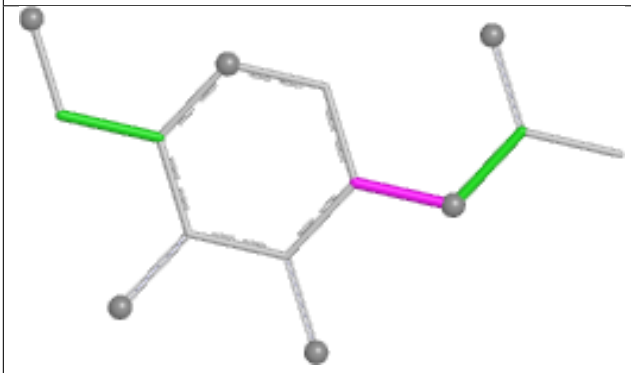


Bond angles



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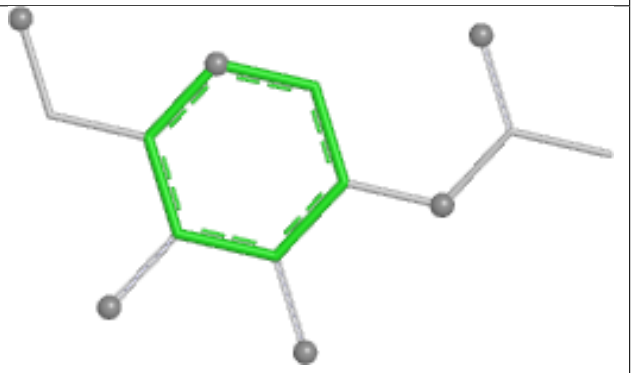
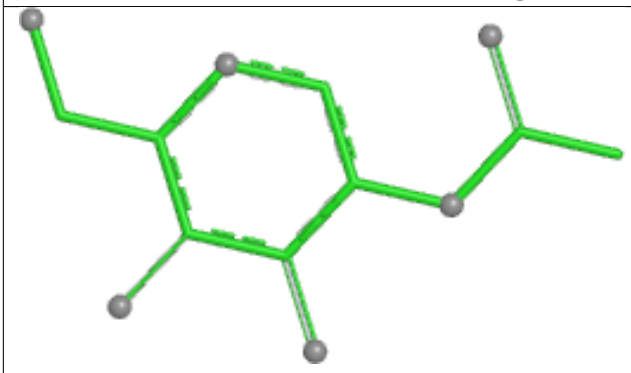
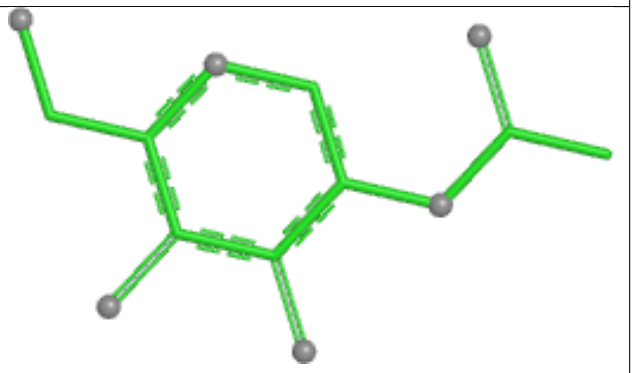


Rings

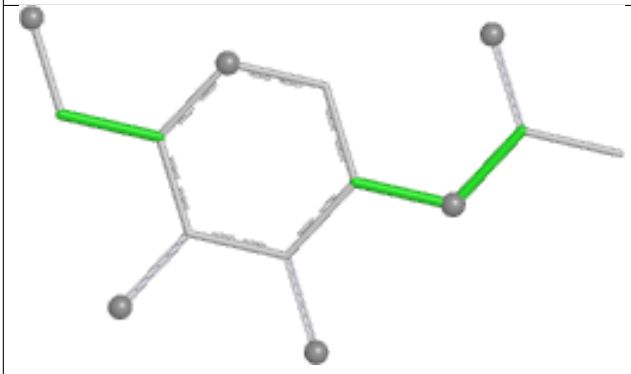
Ligand NAG C 1303



Bond lengths



Bond angles



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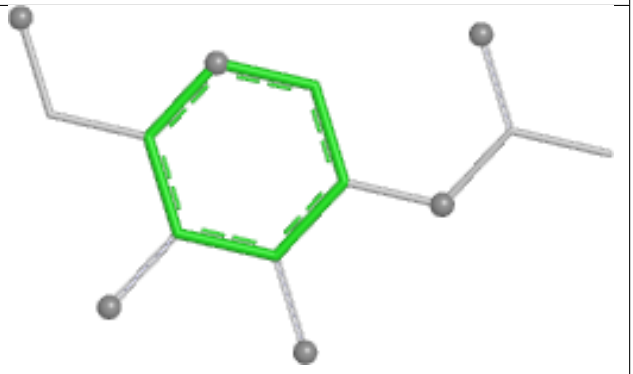
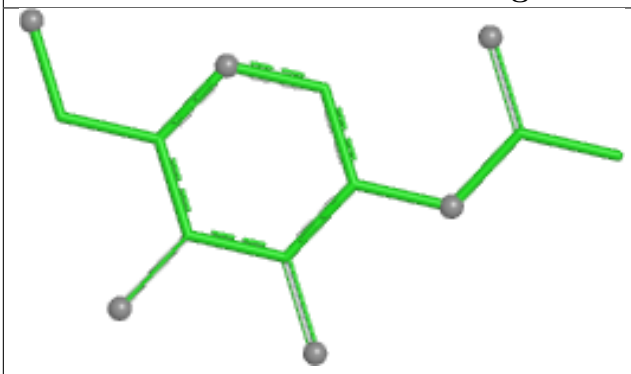
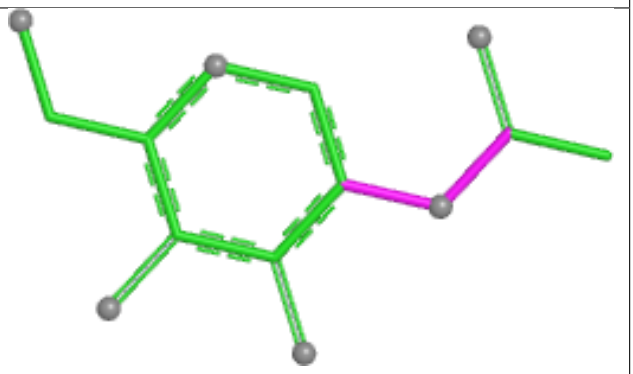


Rings

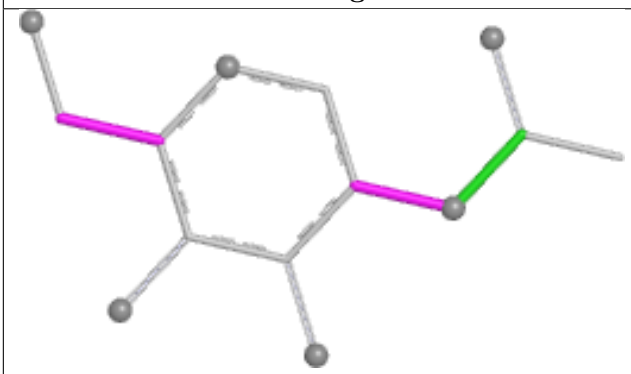
Ligand NAG C 1309



Bond lengths



Bond angles



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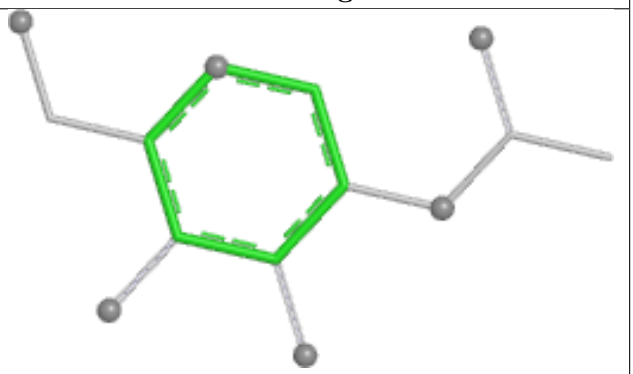
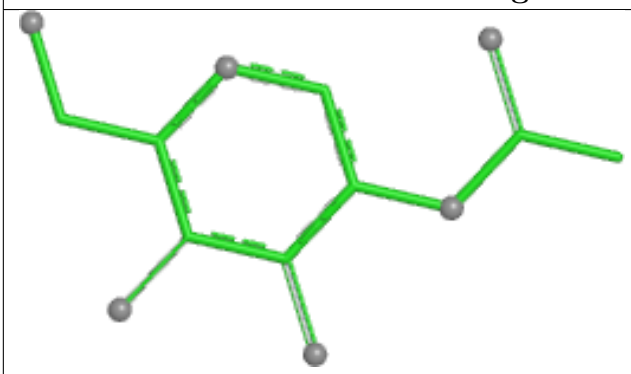
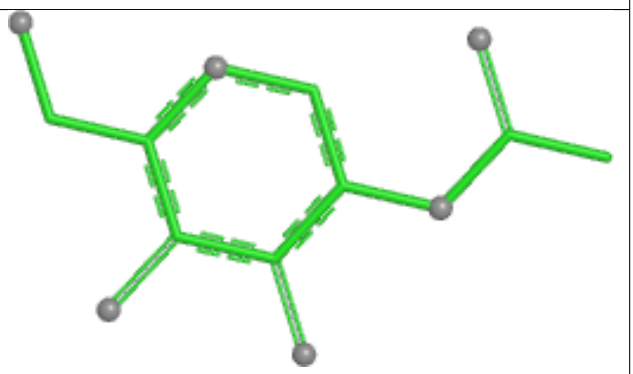


Rings

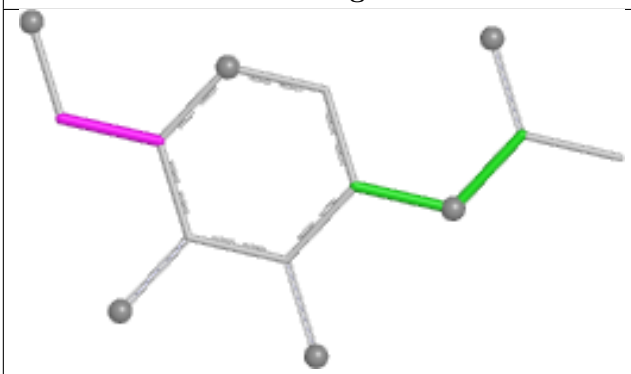
Ligand NAG C 1310



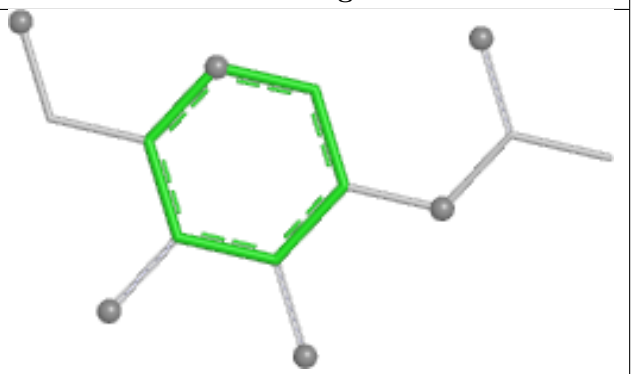
Bond lengths



Bond angles

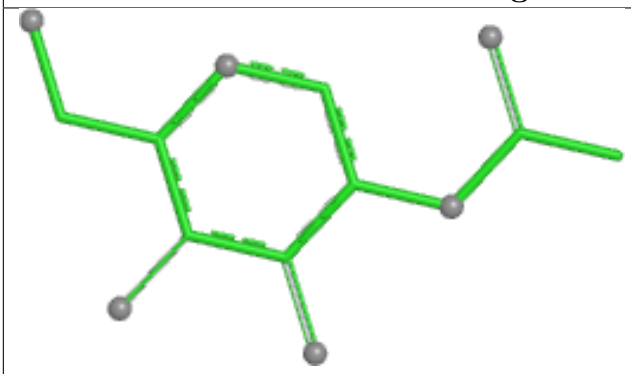


Torsions



Rings

Ligand NAG A 1304



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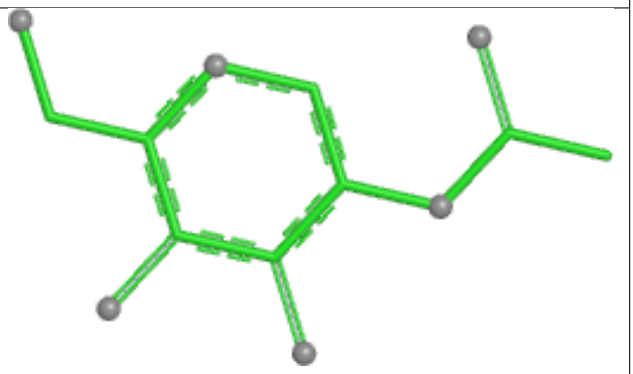
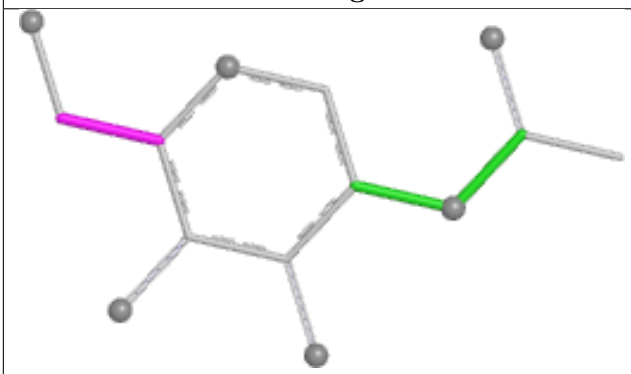


Bond angles



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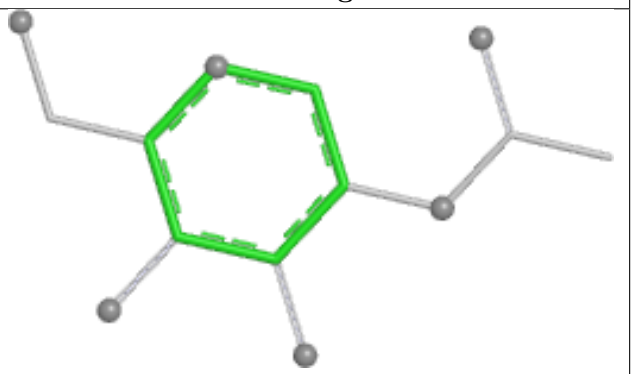
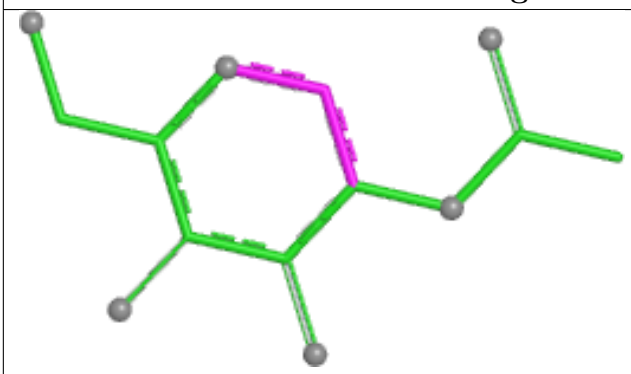


Rings

Ligand NAG A 1305



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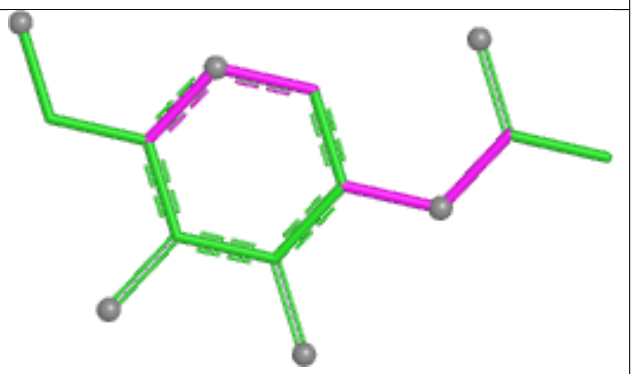

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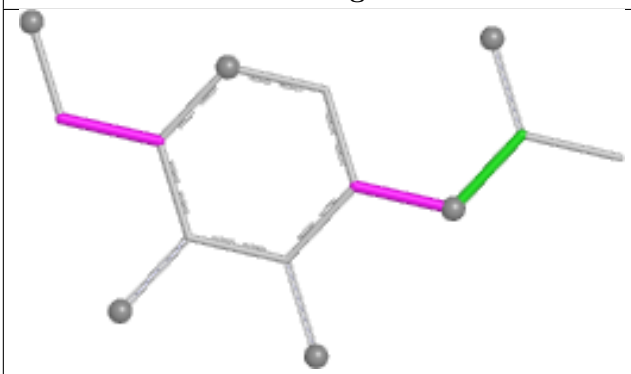

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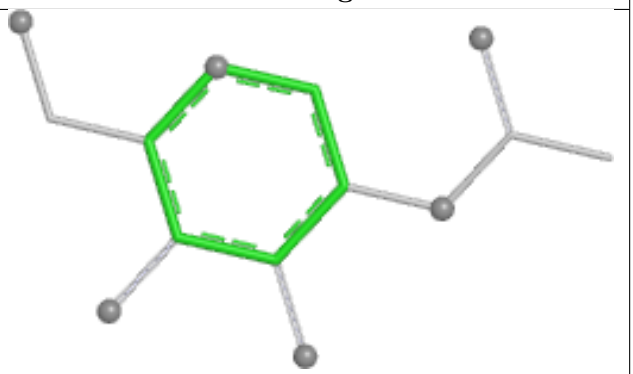
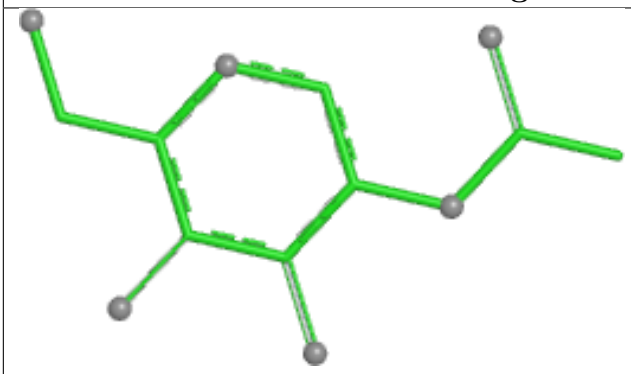


Rings

Ligand NAG A 1301



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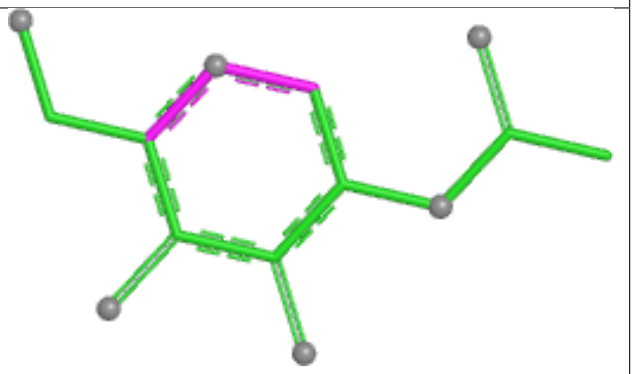
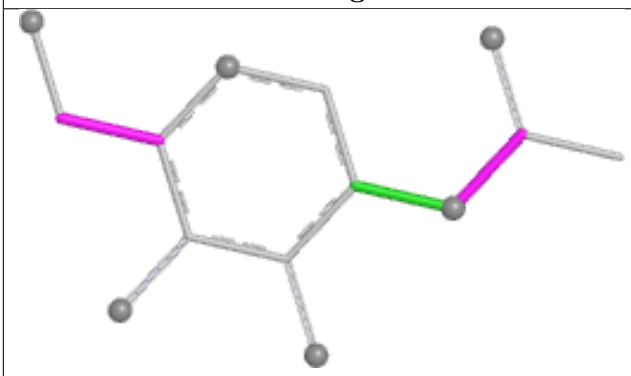


Bond angles



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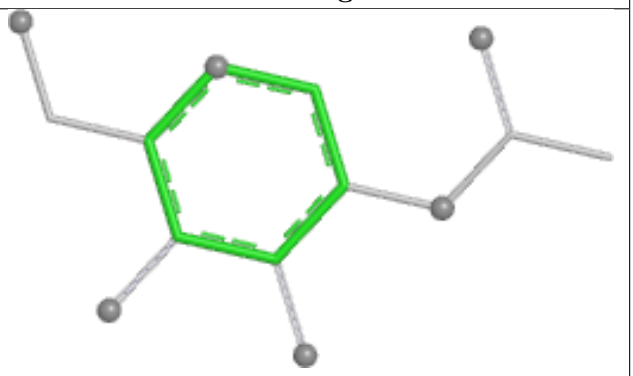
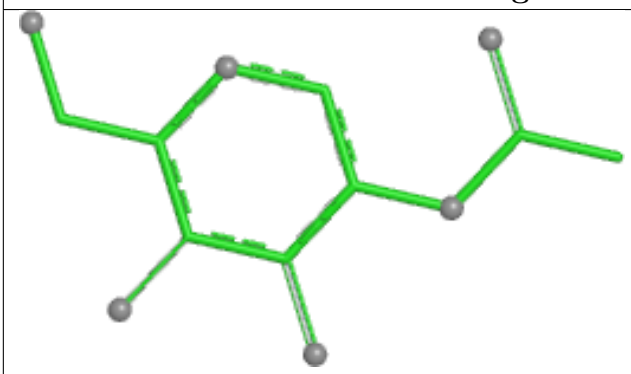


Rings

Ligand NAG B 1306



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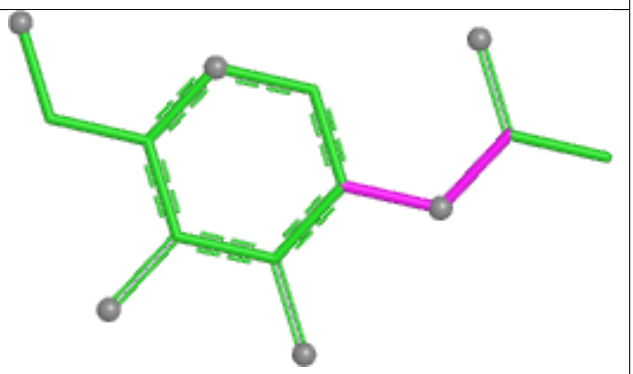

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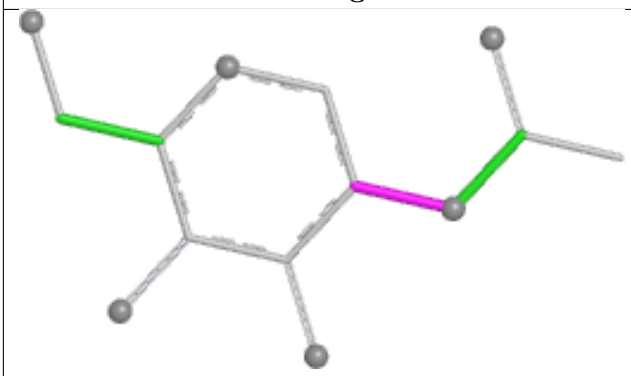

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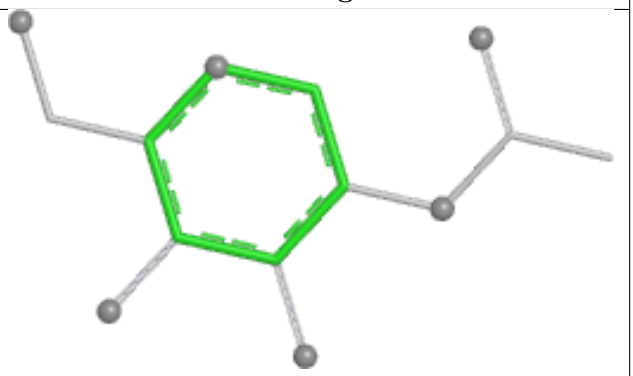
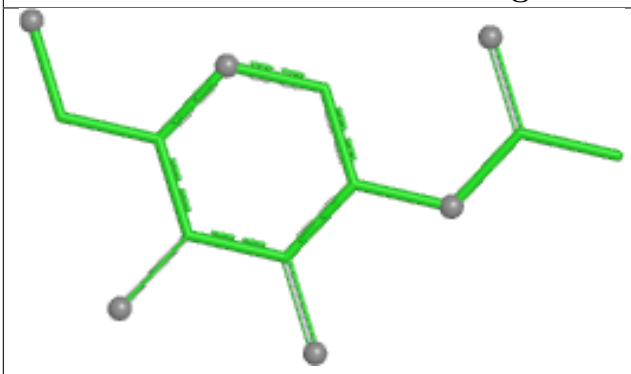


Rings

Ligand NAG B 1309



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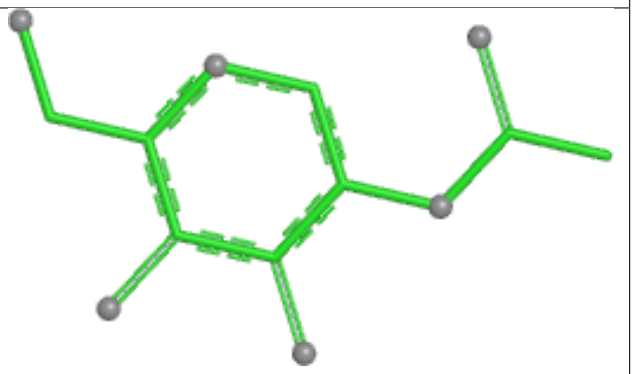

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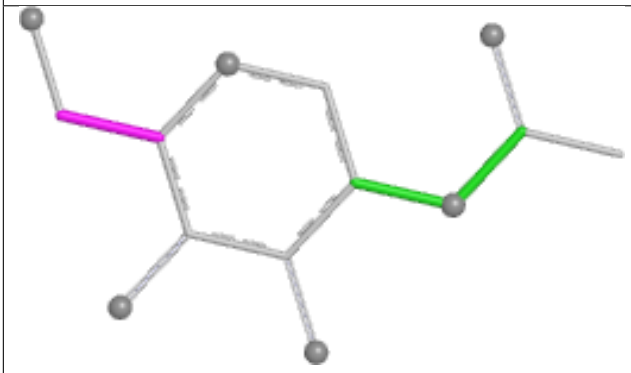

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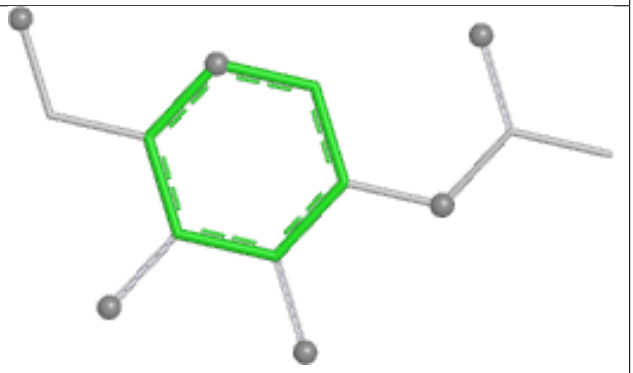
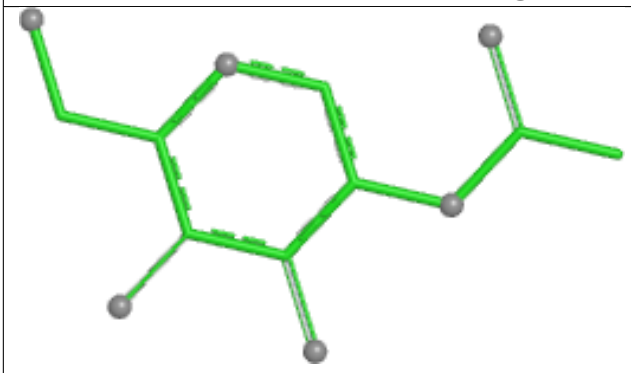


Rings

Ligand NAG B 1308



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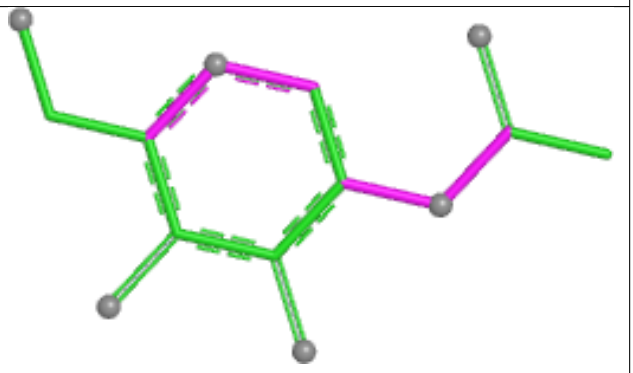
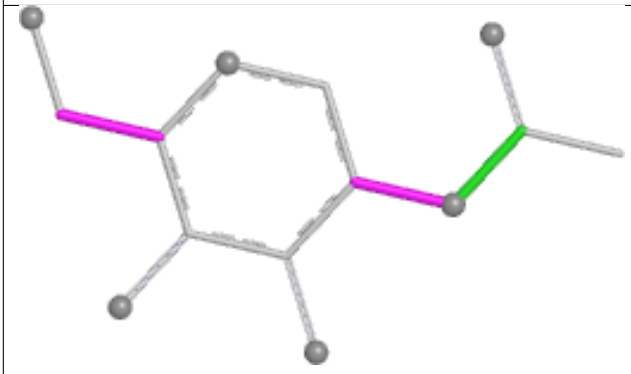


Bond angles



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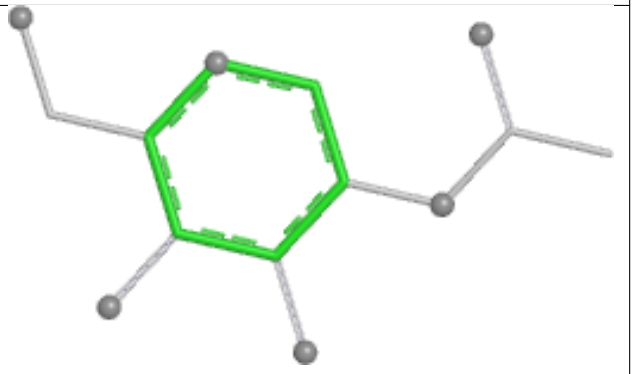
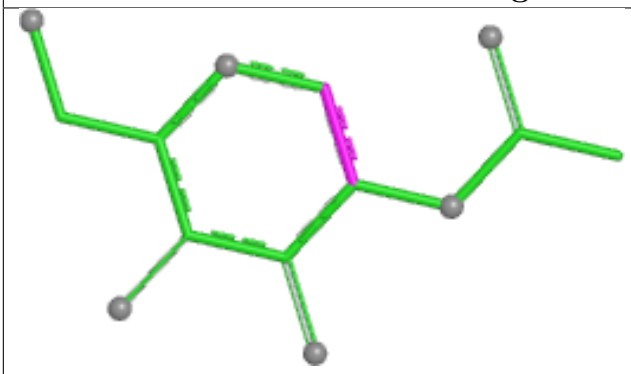


Rings

Ligand NAG C 1306



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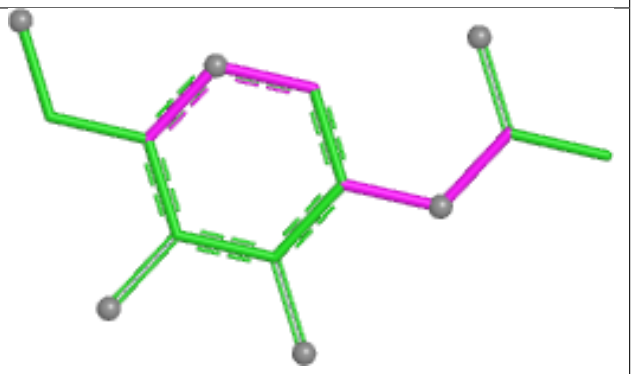
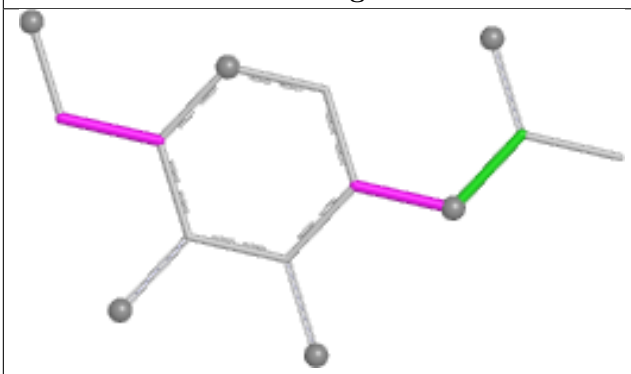


Bond angles



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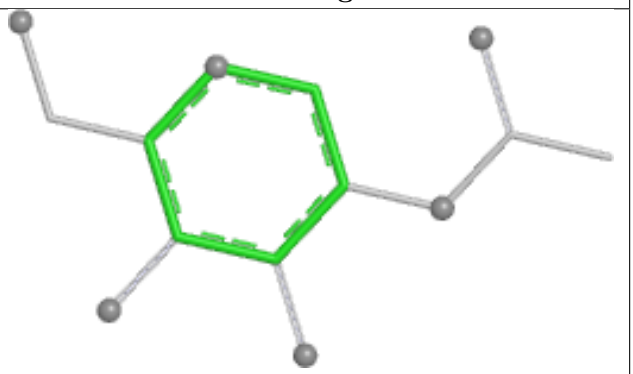
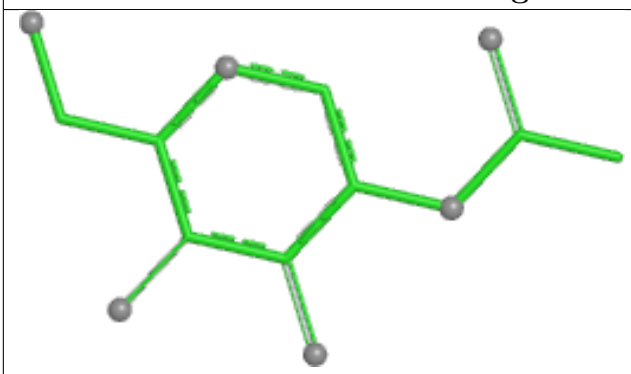


Rings

Ligand NAG C 1304



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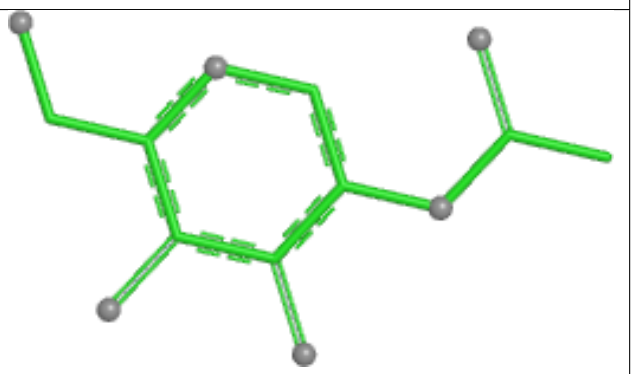
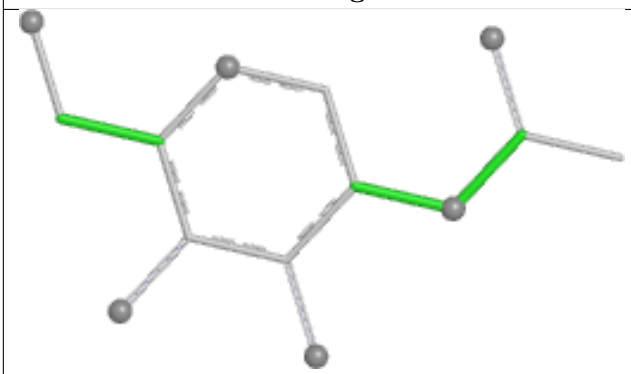


Bond angles



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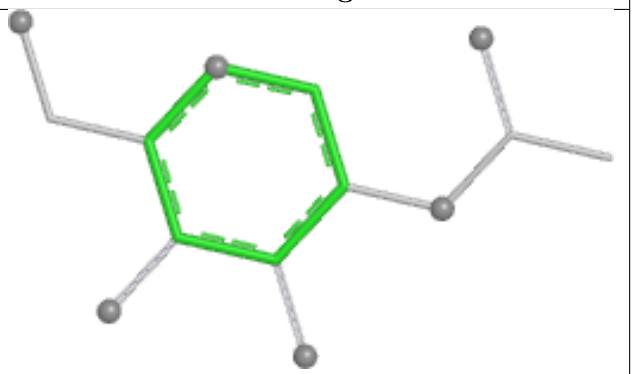
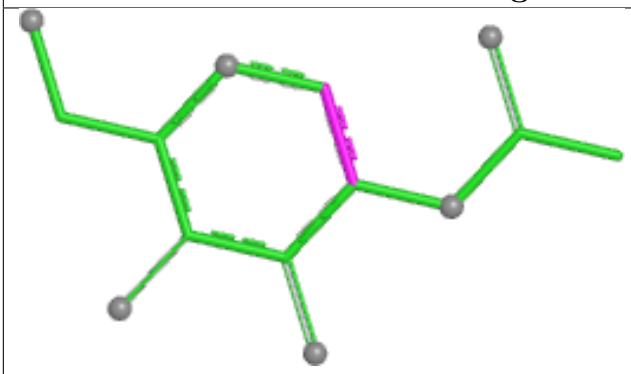


Rings

Ligand NAG A 1306



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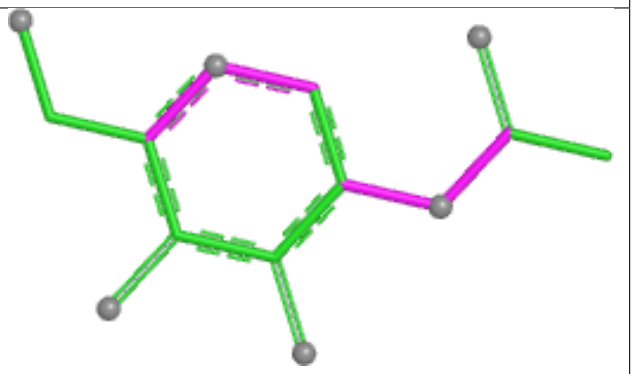
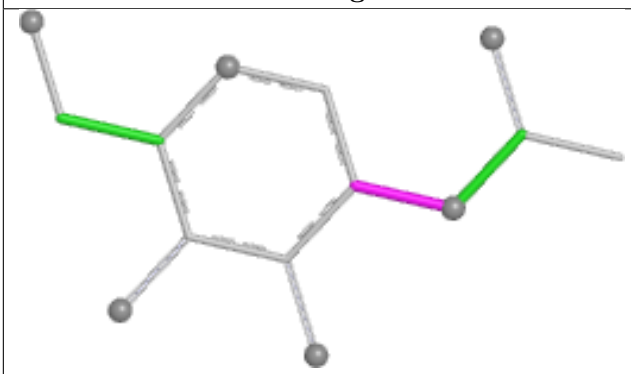


Bond angles



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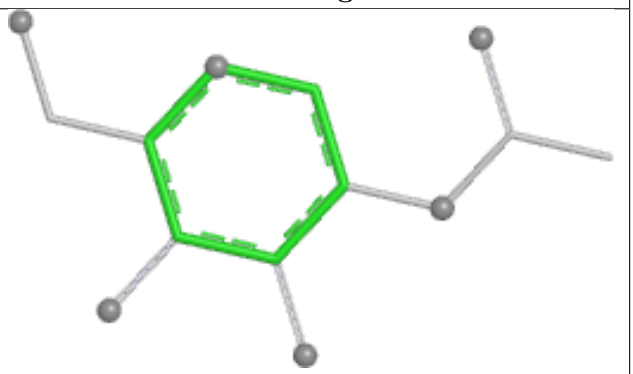
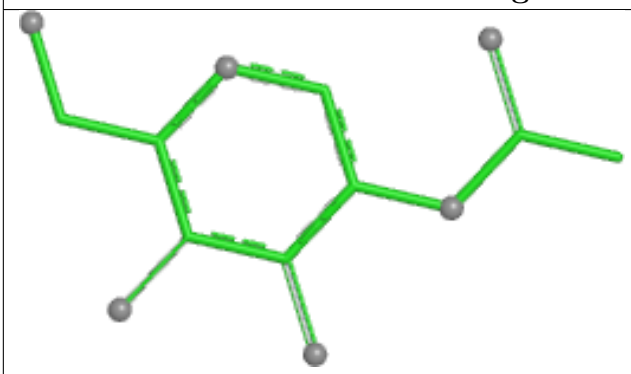


Rings

Ligand NAG B 1304



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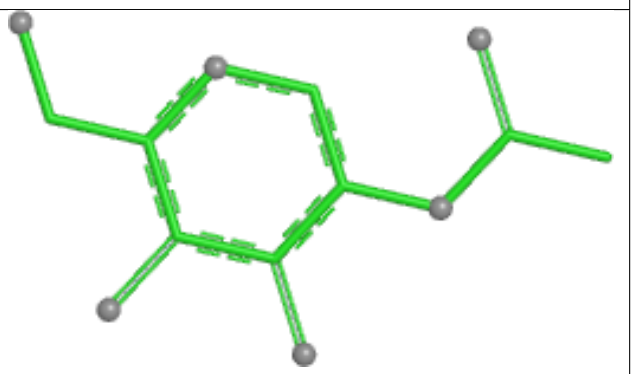

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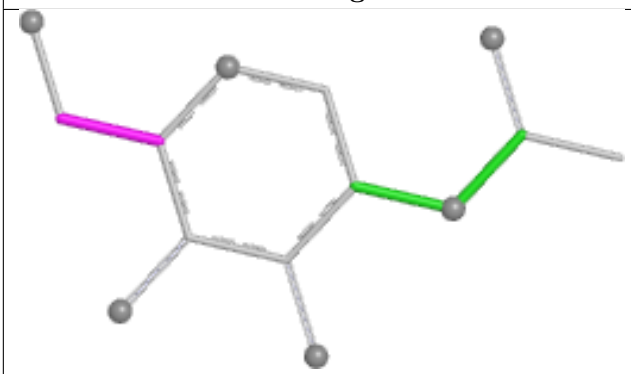

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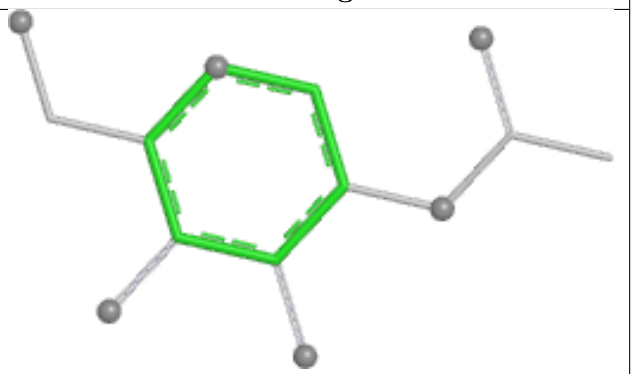
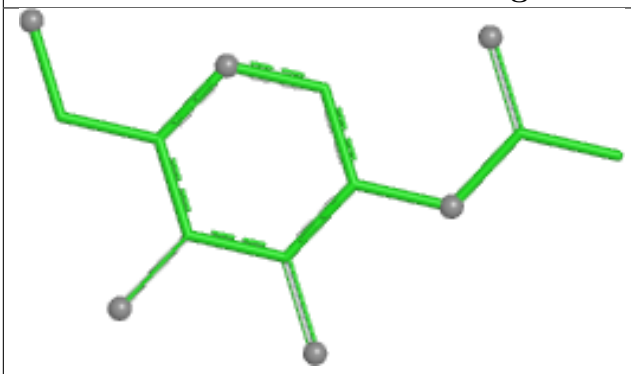


Rings

Ligand NAG A 1302



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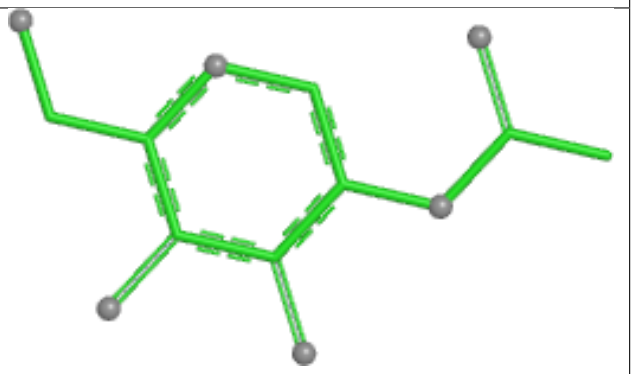
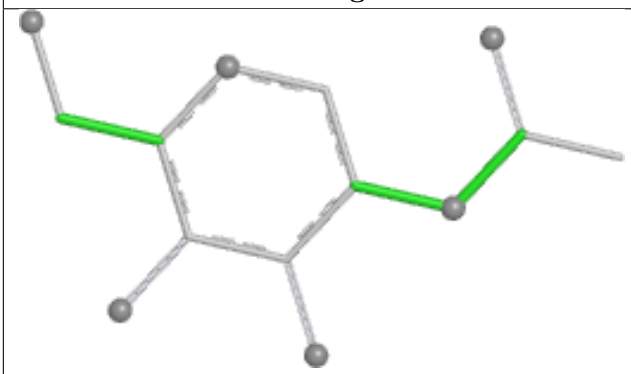


Bond angles



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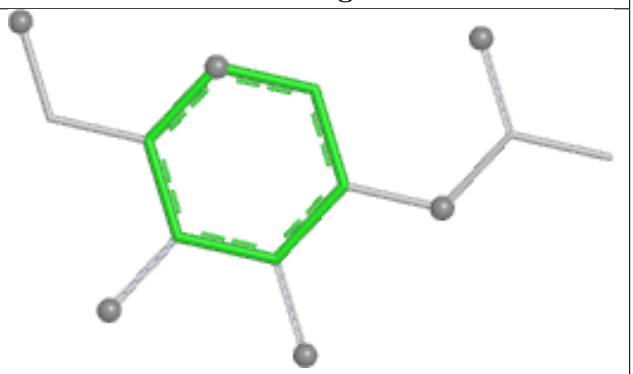
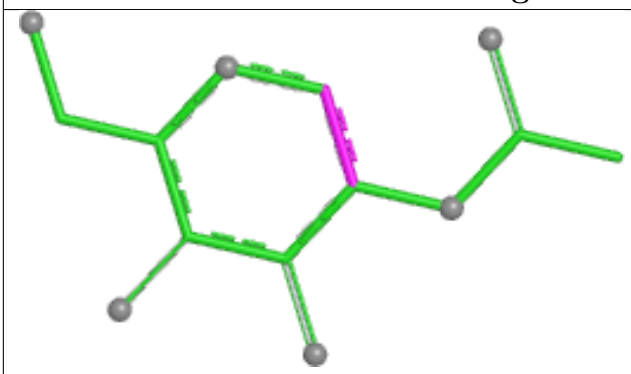


Rings

Ligand NAG B 1310



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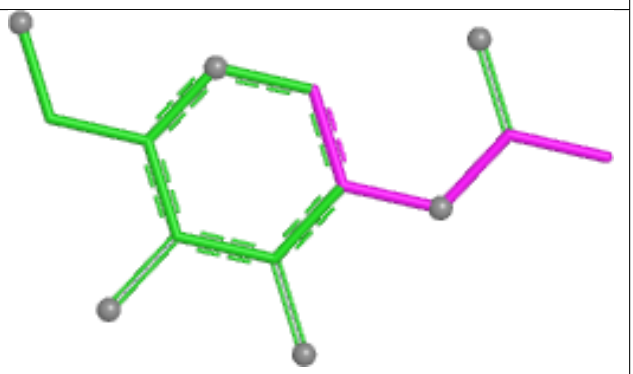
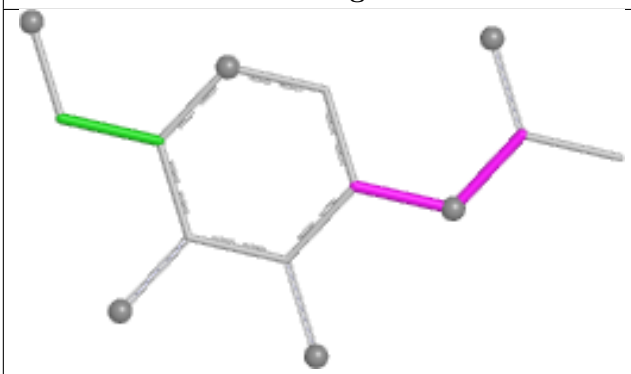


Bond angles



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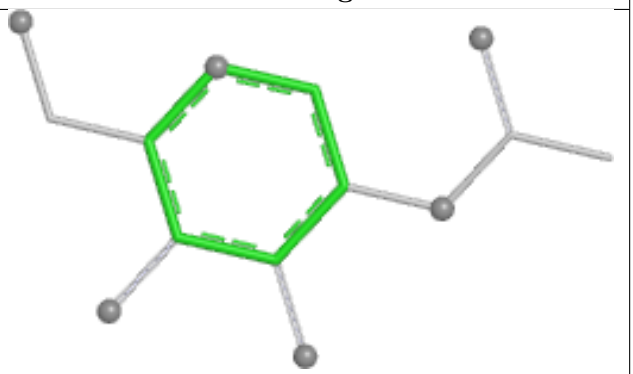
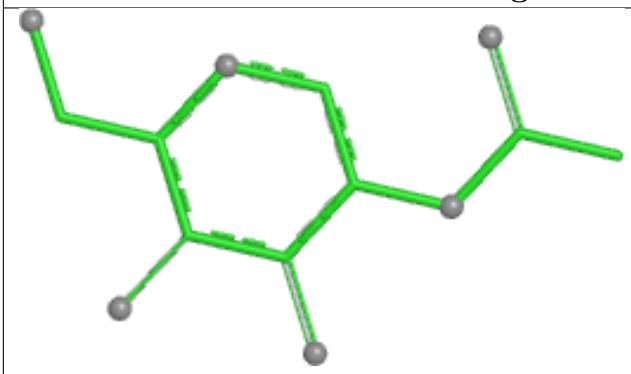
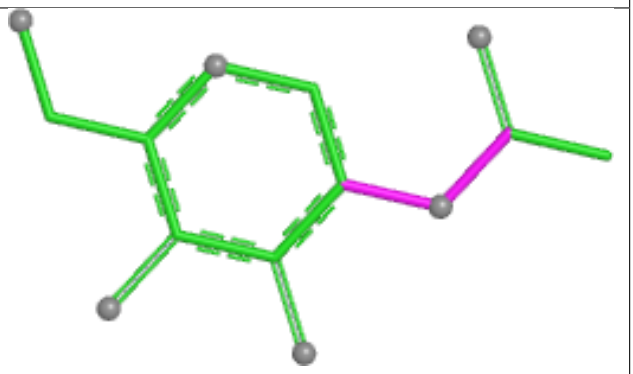


Rings

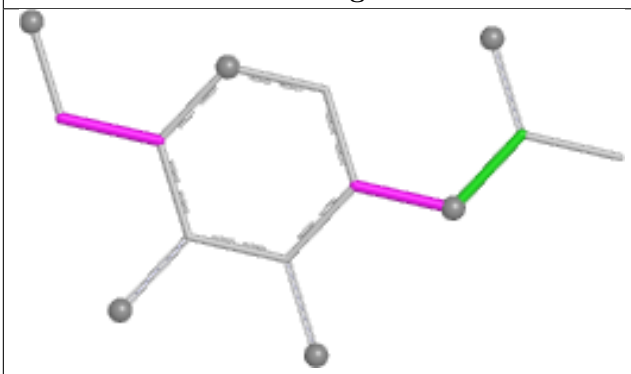
Ligand NAG A 1307



Bond lengths



Bond angles



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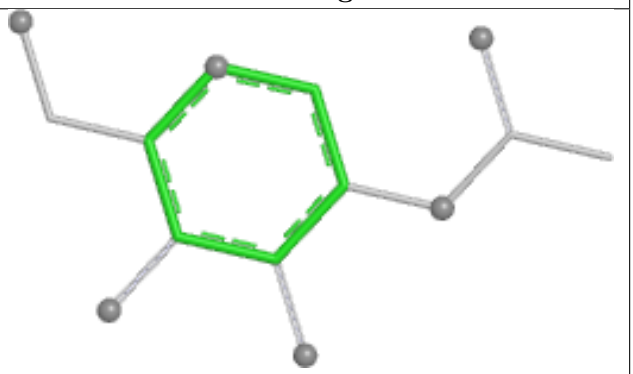
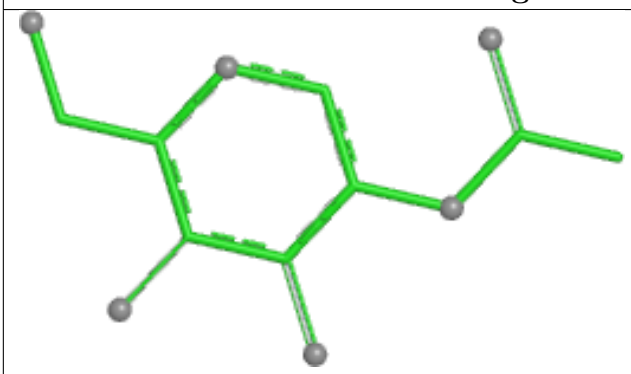
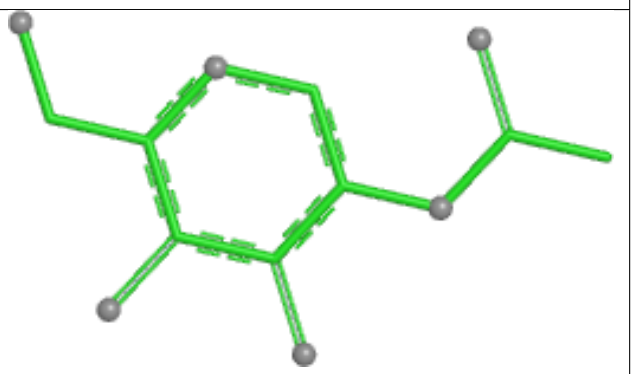


Rings

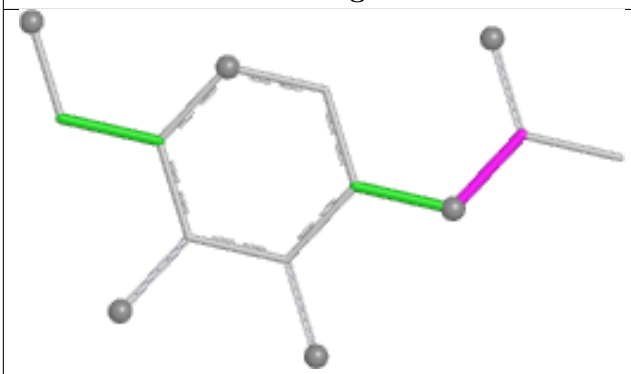
Ligand NAG B 1301



Bond lengths



Bond angles



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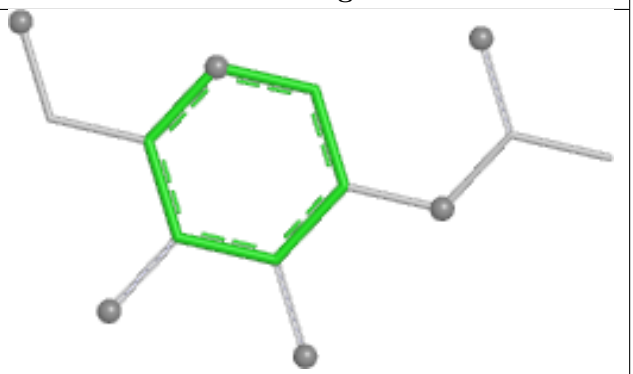
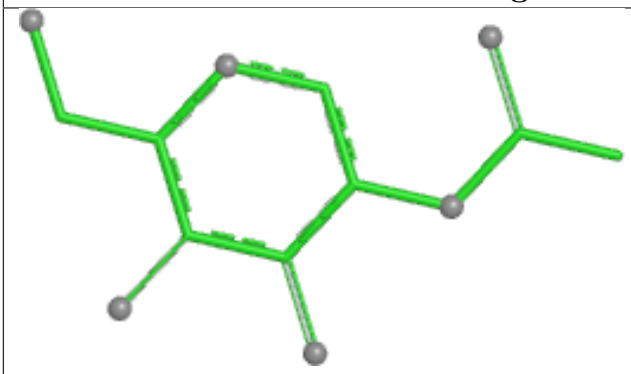
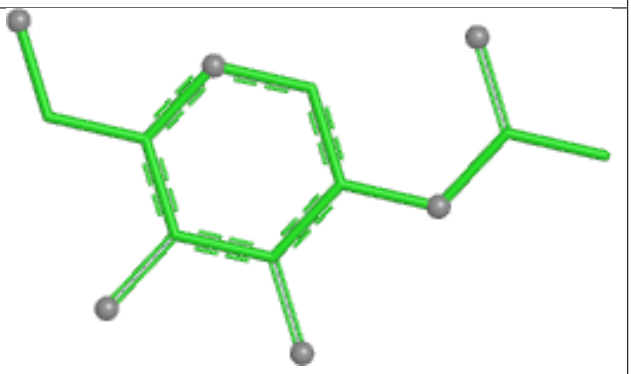
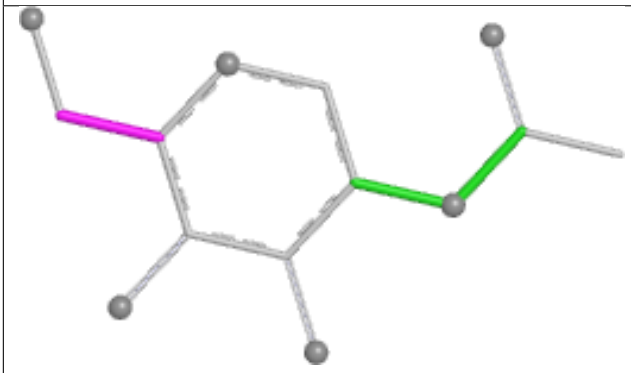
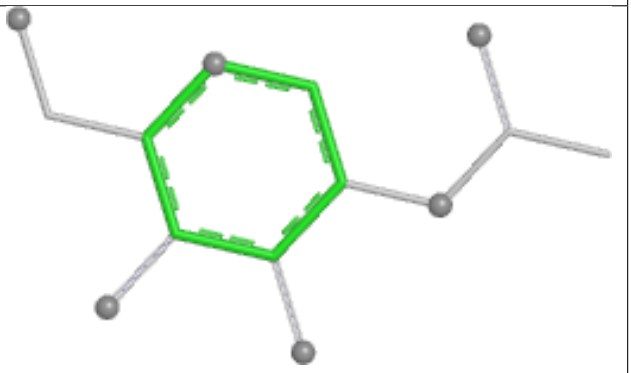


Rings

Ligand NAG A 1309	
 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-42302. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.