Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:30 AM UTC

PDB ID	:	9JMI / pdb_00009jmi
EMDB ID	:	EMD-61603
Title	:	Cryo-EM structure of CN-HedgehogCoV (HKU31/Erinaceus amurensis/China/2014) S-trimer in a locked-2 conformation
Authors	:	Yuan, H.; Xiong, X.
Deposited on	:	2024-09-20
Resolution	:	3.30 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:

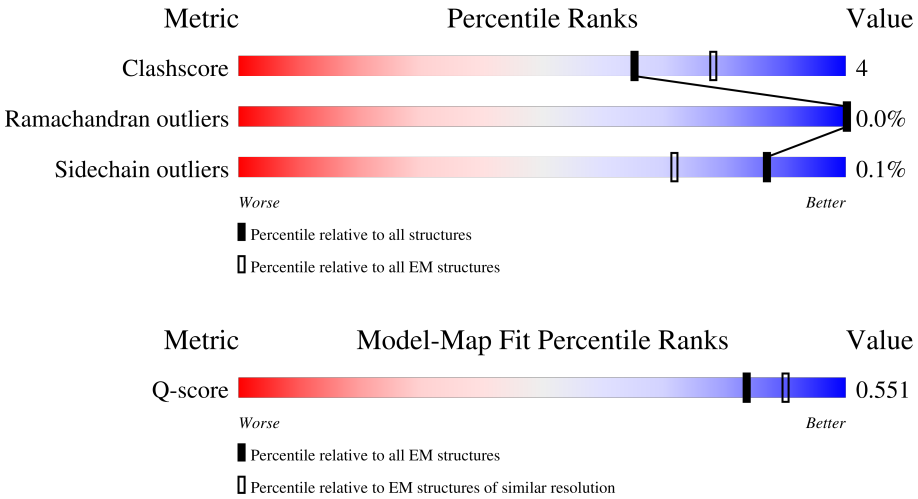
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
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

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	1349	74% 9% 16%
1	B	1349	75% 9% 16%
1	C	1349	76% 8% 16%
2	D	2	100%

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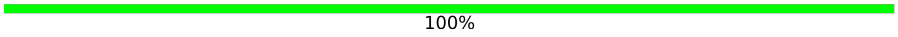
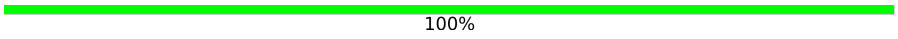
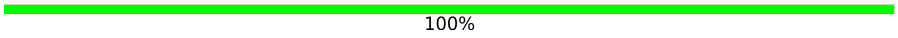
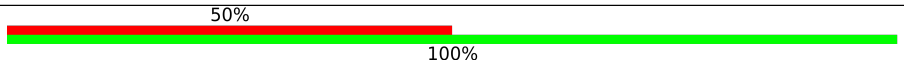
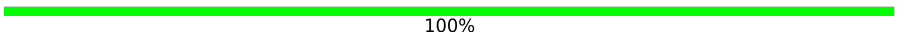
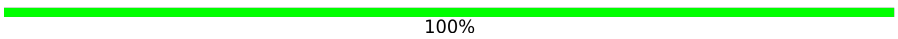
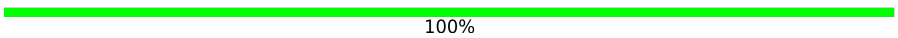
Mol	Chain	Length	Quality of chain
2	E	2	
2	F	2	
2	G	2	
2	H	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	P	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
3	I	3	
3	O	3	
3	U	3	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27732 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1131	Total 8851	C 5607	N 1476	O 1710	S 58	0	0
1	B	1131	Total 8851	C 5607	N 1476	O 1710	S 58	0	0
1	C	1131	Total 8851	C 5607	N 1476	O 1710	S 58	0	0

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	GLY	-	linker	UNP A0A5Q0TVR1
A	1272	SER	-	linker	UNP A0A5Q0TVR1
A	1294	LEU	PHE	conflict	UNP P10104
A	1300	LEU	-	expression tag	UNP P10104
A	1301	GLU	-	expression tag	UNP P10104
A	1302	VAL	-	expression tag	UNP P10104
A	1303	LEU	-	expression tag	UNP P10104
A	1304	PHE	-	expression tag	UNP P10104
A	1305	GLN	-	expression tag	UNP P10104
A	1306	GLY	-	expression tag	UNP P10104
A	1307	PRO	-	expression tag	UNP P10104
A	1308	GLY	-	expression tag	UNP P10104
A	1309	HIS	-	expression tag	UNP P10104
A	1310	HIS	-	expression tag	UNP P10104
A	1311	HIS	-	expression tag	UNP P10104
A	1312	HIS	-	expression tag	UNP P10104
A	1313	HIS	-	expression tag	UNP P10104
A	1314	HIS	-	expression tag	UNP P10104
A	1315	HIS	-	expression tag	UNP P10104
A	1316	HIS	-	expression tag	UNP P10104
A	1317	SER	-	expression tag	UNP P10104
A	1318	ALA	-	expression tag	UNP P10104
A	1319	TRP	-	expression tag	UNP P10104
A	1320	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1321	HIS	-	expression tag	UNP P10104
A	1322	PRO	-	expression tag	UNP P10104
A	1323	GLN	-	expression tag	UNP P10104
A	1324	PHE	-	expression tag	UNP P10104
A	1325	GLU	-	expression tag	UNP P10104
A	1326	LYS	-	expression tag	UNP P10104
A	1327	GLY	-	expression tag	UNP P10104
A	1328	GLY	-	expression tag	UNP P10104
A	1329	GLY	-	expression tag	UNP P10104
A	1330	SER	-	expression tag	UNP P10104
A	1331	GLY	-	expression tag	UNP P10104
A	1332	GLY	-	expression tag	UNP P10104
A	1333	GLY	-	expression tag	UNP P10104
A	1334	GLY	-	expression tag	UNP P10104
A	1335	SER	-	expression tag	UNP P10104
A	1336	GLY	-	expression tag	UNP P10104
A	1337	GLY	-	expression tag	UNP P10104
A	1338	SER	-	expression tag	UNP P10104
A	1339	ALA	-	expression tag	UNP P10104
A	1340	TRP	-	expression tag	UNP P10104
A	1341	SER	-	expression tag	UNP P10104
A	1342	HIS	-	expression tag	UNP P10104
A	1343	PRO	-	expression tag	UNP P10104
A	1344	GLN	-	expression tag	UNP P10104
A	1345	PHE	-	expression tag	UNP P10104
A	1346	GLU	-	expression tag	UNP P10104
A	1347	LYS	-	expression tag	UNP P10104
A	1348	SER	-	expression tag	UNP P10104
A	1349	ALA	-	expression tag	UNP P10104
B	1271	GLY	-	linker	UNP A0A5Q0TVR1
B	1272	SER	-	linker	UNP A0A5Q0TVR1
B	1294	LEU	PHE	conflict	UNP P10104
B	1300	LEU	-	expression tag	UNP P10104
B	1301	GLU	-	expression tag	UNP P10104
B	1302	VAL	-	expression tag	UNP P10104
B	1303	LEU	-	expression tag	UNP P10104
B	1304	PHE	-	expression tag	UNP P10104
B	1305	GLN	-	expression tag	UNP P10104
B	1306	GLY	-	expression tag	UNP P10104
B	1307	PRO	-	expression tag	UNP P10104
B	1308	GLY	-	expression tag	UNP P10104
B	1309	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1310	HIS	-	expression tag	UNP P10104
B	1311	HIS	-	expression tag	UNP P10104
B	1312	HIS	-	expression tag	UNP P10104
B	1313	HIS	-	expression tag	UNP P10104
B	1314	HIS	-	expression tag	UNP P10104
B	1315	HIS	-	expression tag	UNP P10104
B	1316	HIS	-	expression tag	UNP P10104
B	1317	SER	-	expression tag	UNP P10104
B	1318	ALA	-	expression tag	UNP P10104
B	1319	TRP	-	expression tag	UNP P10104
B	1320	SER	-	expression tag	UNP P10104
B	1321	HIS	-	expression tag	UNP P10104
B	1322	PRO	-	expression tag	UNP P10104
B	1323	GLN	-	expression tag	UNP P10104
B	1324	PHE	-	expression tag	UNP P10104
B	1325	GLU	-	expression tag	UNP P10104
B	1326	LYS	-	expression tag	UNP P10104
B	1327	GLY	-	expression tag	UNP P10104
B	1328	GLY	-	expression tag	UNP P10104
B	1329	GLY	-	expression tag	UNP P10104
B	1330	SER	-	expression tag	UNP P10104
B	1331	GLY	-	expression tag	UNP P10104
B	1332	GLY	-	expression tag	UNP P10104
B	1333	GLY	-	expression tag	UNP P10104
B	1334	GLY	-	expression tag	UNP P10104
B	1335	SER	-	expression tag	UNP P10104
B	1336	GLY	-	expression tag	UNP P10104
B	1337	GLY	-	expression tag	UNP P10104
B	1338	SER	-	expression tag	UNP P10104
B	1339	ALA	-	expression tag	UNP P10104
B	1340	TRP	-	expression tag	UNP P10104
B	1341	SER	-	expression tag	UNP P10104
B	1342	HIS	-	expression tag	UNP P10104
B	1343	PRO	-	expression tag	UNP P10104
B	1344	GLN	-	expression tag	UNP P10104
B	1345	PHE	-	expression tag	UNP P10104
B	1346	GLU	-	expression tag	UNP P10104
B	1347	LYS	-	expression tag	UNP P10104
B	1348	SER	-	expression tag	UNP P10104
B	1349	ALA	-	expression tag	UNP P10104
C	1271	GLY	-	linker	UNP A0A5Q0TVR1
C	1272	SER	-	linker	UNP A0A5Q0TVR1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1294	LEU	PHE	conflict	UNP P10104
C	1300	LEU	-	expression tag	UNP P10104
C	1301	GLU	-	expression tag	UNP P10104
C	1302	VAL	-	expression tag	UNP P10104
C	1303	LEU	-	expression tag	UNP P10104
C	1304	PHE	-	expression tag	UNP P10104
C	1305	GLN	-	expression tag	UNP P10104
C	1306	GLY	-	expression tag	UNP P10104
C	1307	PRO	-	expression tag	UNP P10104
C	1308	GLY	-	expression tag	UNP P10104
C	1309	HIS	-	expression tag	UNP P10104
C	1310	HIS	-	expression tag	UNP P10104
C	1311	HIS	-	expression tag	UNP P10104
C	1312	HIS	-	expression tag	UNP P10104
C	1313	HIS	-	expression tag	UNP P10104
C	1314	HIS	-	expression tag	UNP P10104
C	1315	HIS	-	expression tag	UNP P10104
C	1316	HIS	-	expression tag	UNP P10104
C	1317	SER	-	expression tag	UNP P10104
C	1318	ALA	-	expression tag	UNP P10104
C	1319	TRP	-	expression tag	UNP P10104
C	1320	SER	-	expression tag	UNP P10104
C	1321	HIS	-	expression tag	UNP P10104
C	1322	PRO	-	expression tag	UNP P10104
C	1323	GLN	-	expression tag	UNP P10104
C	1324	PHE	-	expression tag	UNP P10104
C	1325	GLU	-	expression tag	UNP P10104
C	1326	LYS	-	expression tag	UNP P10104
C	1327	GLY	-	expression tag	UNP P10104
C	1328	GLY	-	expression tag	UNP P10104
C	1329	GLY	-	expression tag	UNP P10104
C	1330	SER	-	expression tag	UNP P10104
C	1331	GLY	-	expression tag	UNP P10104
C	1332	GLY	-	expression tag	UNP P10104
C	1333	GLY	-	expression tag	UNP P10104
C	1334	GLY	-	expression tag	UNP P10104
C	1335	SER	-	expression tag	UNP P10104
C	1336	GLY	-	expression tag	UNP P10104
C	1337	GLY	-	expression tag	UNP P10104
C	1338	SER	-	expression tag	UNP P10104
C	1339	ALA	-	expression tag	UNP P10104
C	1340	TRP	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1341	SER	-	expression tag	UNP P10104
C	1342	HIS	-	expression tag	UNP P10104
C	1343	PRO	-	expression tag	UNP P10104
C	1344	GLN	-	expression tag	UNP P10104
C	1345	PHE	-	expression tag	UNP P10104
C	1346	GLU	-	expression tag	UNP P10104
C	1347	LYS	-	expression tag	UNP P10104
C	1348	SER	-	expression tag	UNP P10104
C	1349	ALA	-	expression tag	UNP P10104

- 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	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		

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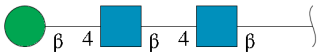
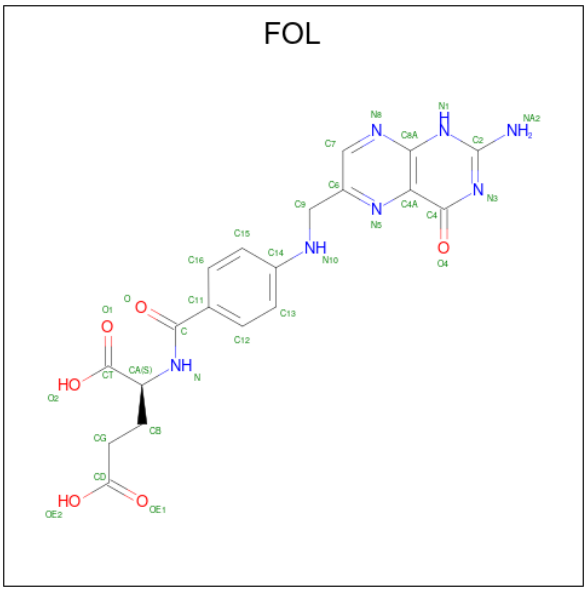
Mol	Chain	Residues	Atoms				AltConf	Trace
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



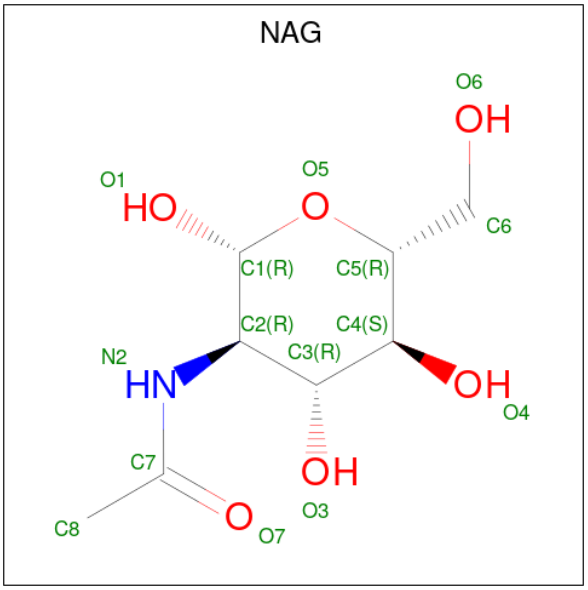
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is FOLIC ACID (CCD ID: FOL) (formula: $C_{19}H_{19}N_7O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 32 19 7 6	0
4	B	1	Total C N O 32 19 7 6	0
4	C	1	Total C N O 32 19 7 6	0

- Molecule 5 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
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0

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

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

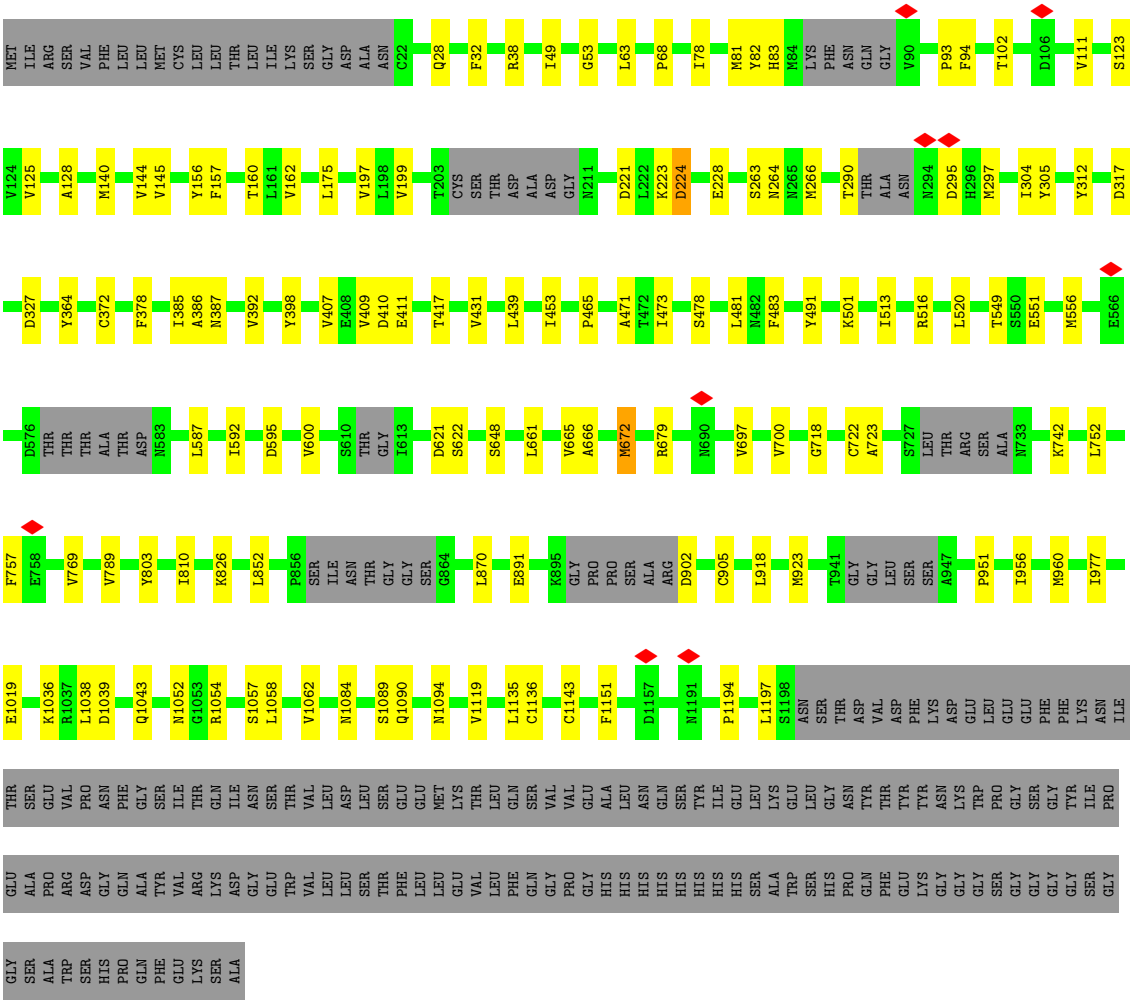
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein,Fibritin

Chain A:

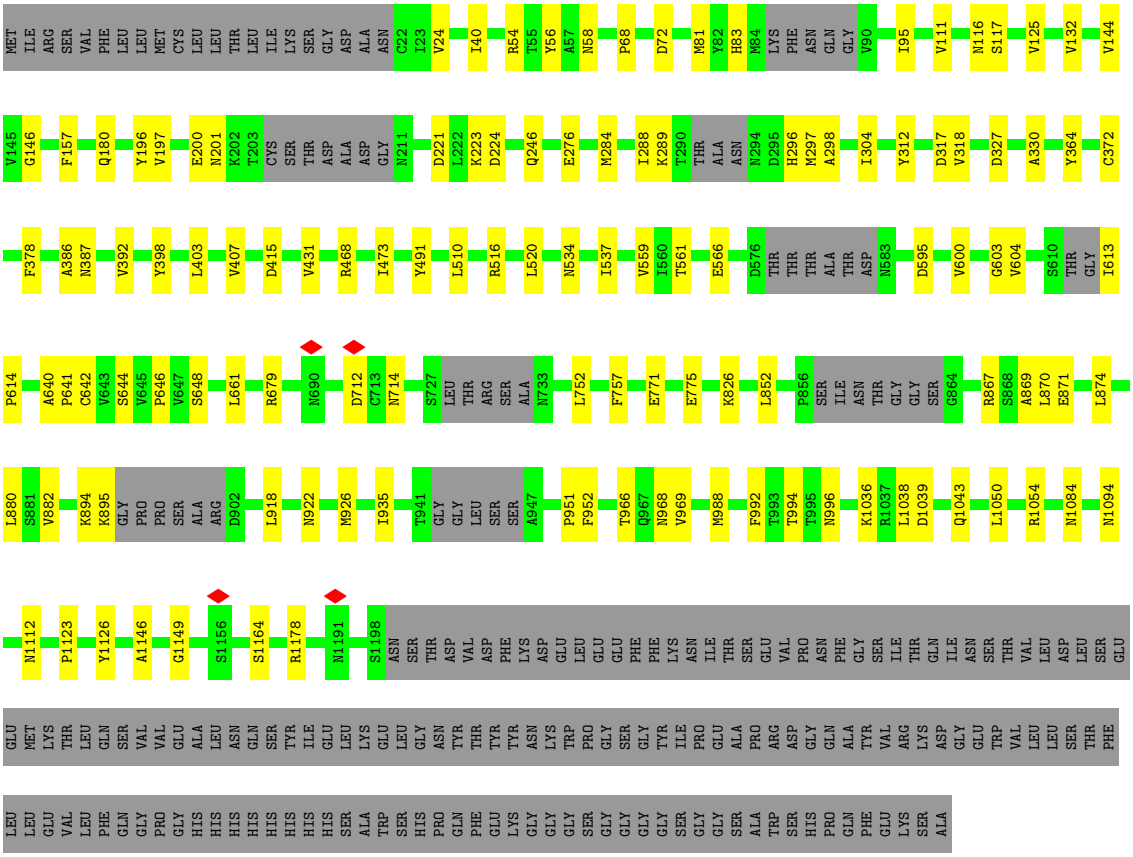




- Molecule 1: Spike glycoprotein,Fibritin

Chain B:

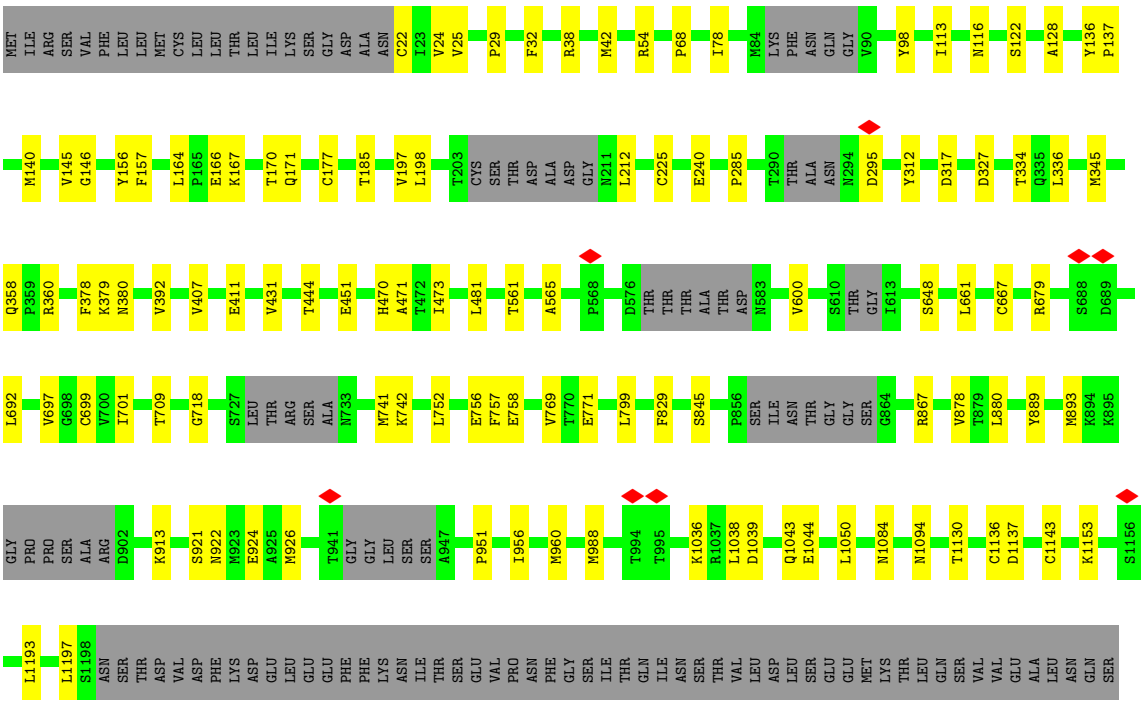




• Molecule 1: Spike glycoprotein,Fibritin

Chain C:





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

HIS HIS HIS SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS SER ALA

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

Chain D: 100%

NAG1 NAG2

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

Chain E: 100%

NAG1 NAG2

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

Chain F: 50% 50%

NAG1 NAG2

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

Chain G: 100%

NAG1 NAG2

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

Chain H: 100%

NAG1 NAG2

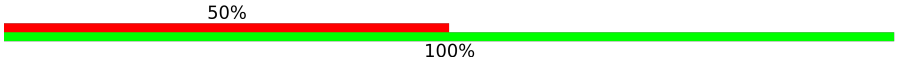
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%

NAG1 NAG2

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

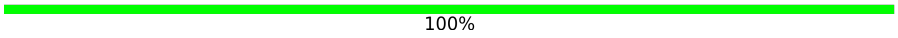
Chain K:





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

Chain L:





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

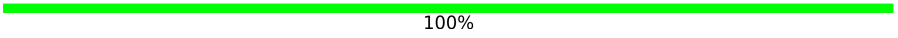
Chain M:





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

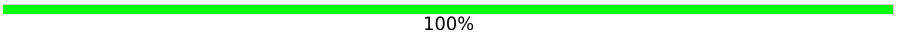
Chain N:





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

Chain P:





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

Chain Q:





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

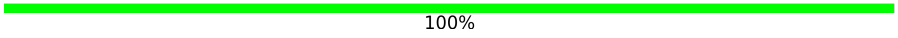
Chain R:





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

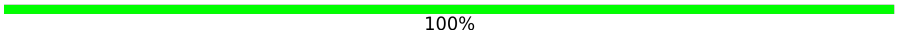
Chain S:





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

Chain T:





• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:





• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:





• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.192	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, BMA, 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	0.25	1/9043 (0.0%)	0.43	1/12272 (0.0%)
1	B	0.22	0/9043	0.40	0/12272
1	C	0.19	0/9043	0.40	0/12272
All	All	0.22	1/27129 (0.0%)	0.41	1/36816 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	ASP	CA-C	-5.63	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	409	VAL	N-CA-C	6.19	116.42	108.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8851	0	8533	80	0
1	B	8851	0	8533	79	0
1	C	8851	0	8533	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
3	I	39	0	34	0	0
3	O	39	0	34	0	0
3	U	39	0	34	0	0
4	A	32	0	17	0	0
4	B	32	0	17	1	0
4	C	32	0	17	2	0
5	A	182	0	169	1	0
5	B	182	0	169	1	0
5	C	182	0	169	1	0
All	All	27732	0	26634	215	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 4.

All (215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:752:LEU:HD13	1:C:757:PHE:HB3	1.71	0.71
1:B:180:GLN:NE2	1:B:223:LYS:HD2	2.05	0.71
1:C:29:PRO:HG2	2:Q:1:NAG:H62	1.75	0.68
1:C:648:SER:HB2	1:C:661:LEU:HB3	1.80	0.62
1:C:198:LEU:HD23	1:C:212:LEU:HD12	1.81	0.62
1:A:513:ILE:HG13	1:A:516:ARG:HH21	1.66	0.61
1:B:752:LEU:HD21	1:C:951:PRO:HD3	1.83	0.61
1:B:752:LEU:HD22	1:B:757:PHE:HB3	1.83	0.61
1:A:81:MET:HE1	1:A:295:ASP:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HG3	1:A:162:VAL:HG12	1.82	0.60
1:B:95:ILE:HD13	1:B:197:VAL:HB	1.83	0.60
1:C:769:VAL:HG21	1:C:988:MET:HB2	1.84	0.60
1:C:758:GLU:HG2	1:C:1130:THR:HG22	1.83	0.59
1:B:81:MET:HE1	1:B:296:HIS:H	1.67	0.59
1:B:83:HIS:HA	1:B:125:VAL:HG21	1.85	0.59
1:A:410:ASP:OD1	1:A:439:LEU:HD11	2.03	0.59
1:A:752:LEU:HD13	1:A:757:PHE:HB3	1.84	0.58
1:C:166:GLU:HB2	1:C:171:GLN:HB3	1.85	0.57
1:B:566:GLU:N	1:B:566:GLU:OE2	2.36	0.57
1:A:951:PRO:HD3	1:C:752:LEU:HD21	1.87	0.57
1:A:378:PHE:HB3	1:A:481:LEU:HD13	1.87	0.57
1:A:327:ASP:OD2	1:A:679:ARG:NH2	2.36	0.57
1:A:478:SER:HB2	1:A:483:PHE:HB3	1.87	0.56
1:A:516:ARG:NH2	1:B:276:GLU:OE2	2.38	0.56
1:C:709:THR:HB	1:C:742:LYS:HB3	1.87	0.56
1:C:878:VAL:HG13	1:C:880:LEU:HD22	1.88	0.56
1:A:1194:PRO:HD2	1:A:1197:LEU:HD12	1.86	0.56
1:B:117:SER:HA	1:B:132:VAL:HG23	1.88	0.55
1:C:122:SER:H	4:C:1401:FOL:HN1	1.54	0.55
1:A:83:HIS:HA	1:A:125:VAL:HG21	1.89	0.55
1:B:935:ILE:HD11	1:B:952:PHE:HE1	1.71	0.55
1:C:411:GLU:HB3	1:C:470:HIS:HB2	1.89	0.55
1:A:68:PRO:O	1:A:312:TYR:OH	2.24	0.55
1:B:771:GLU:OE2	1:B:996:ASN:ND2	2.39	0.55
5:A:1410:NAG:H81	1:B:894:LYS:HD2	1.90	0.54
1:B:327:ASP:OD2	1:B:679:ARG:NH2	2.41	0.54
1:A:722:CYS:SG	1:A:723:ALA:N	2.80	0.54
1:A:1089:SER:OG	1:A:1090:GLN:N	2.41	0.54
1:C:799:LEU:HD21	1:C:1044:GLU:HA	1.90	0.54
1:B:68:PRO:O	1:B:312:TYR:OH	2.27	0.53
1:C:1136:CYS:HB3	1:C:1143:CYS:HA	1.90	0.53
1:C:1136:CYS:HA	1:C:1197:LEU:HD13	1.91	0.53
1:B:407:VAL:HG12	1:B:473:ILE:HG12	1.91	0.52
1:B:1123:PRO:HB2	1:B:1126:TYR:HE1	1.75	0.52
1:B:510:LEU:HD23	1:B:516:ARG:HH12	1.75	0.52
1:C:358:GLN:OE1	1:C:360:ARG:NH2	2.43	0.52
1:A:144:VAL:HG13	1:A:157:PHE:HB2	1.92	0.52
1:B:132:VAL:HG12	1:B:298:ALA:HB3	1.93	0.51
1:C:22:CYS:N	1:C:185:THR:O	2.42	0.51
1:A:410:ASP:OD2	1:A:439:LEU:HD21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:LEU:O	1:A:1043:GLN:NE2	2.44	0.51
1:A:1094:ASN:O	1:B:1084:ASN:ND2	2.44	0.51
1:C:146:GLY:HA3	1:C:157:PHE:HE2	1.76	0.51
1:A:810:ILE:HD12	1:A:1062:VAL:HG21	1.92	0.51
1:A:407:VAL:HG12	1:A:473:ILE:HG12	1.91	0.51
1:A:697:VAL:HG11	1:A:718:GLY:HA3	1.93	0.51
1:B:40:ILE:HG22	1:B:72:ASP:H	1.75	0.51
1:A:290:THR:HA	1:A:297:MET:HE1	1.93	0.50
1:C:697:VAL:HG11	1:C:718:GLY:HA3	1.93	0.50
1:A:385:ILE:HD13	1:A:453:ILE:HD12	1.93	0.50
1:A:410:ASP:CG	1:A:439:LEU:HD11	2.37	0.50
1:A:1084:ASN:ND2	1:C:1094:ASN:O	2.45	0.50
1:B:223:LYS:HG2	1:B:224:ASP:N	2.27	0.50
1:A:410:ASP:O	1:A:411:GLU:HB2	2.11	0.50
1:A:752:LEU:HD21	1:B:951:PRO:HD3	1.94	0.50
1:A:960:MET:HE1	1:A:977:ILE:HG21	1.93	0.50
1:A:128:ALA:HB3	1:A:295:ASP:HB3	1.93	0.49
1:C:327:ASP:OD2	1:C:679:ARG:NH2	2.41	0.49
1:C:378:PHE:HB3	1:C:481:LEU:HD13	1.92	0.49
1:A:102:THR:HG21	1:A:145:VAL:HG11	1.93	0.49
1:A:392:VAL:HG22	1:A:431:VAL:HG22	1.93	0.49
1:B:566:GLU:HG2	1:C:54:ARG:HD2	1.95	0.49
1:C:98:TYR:HB2	1:C:285:PRO:HG3	1.94	0.49
1:B:966:THR:HG22	1:B:968:ASN:H	1.77	0.49
1:B:201:ASN:HA	1:B:289:LYS:HB3	1.95	0.49
1:B:392:VAL:HG22	1:B:431:VAL:HG22	1.94	0.49
1:B:144:VAL:HG13	1:B:157:PHE:HB2	1.94	0.49
1:C:136:TYR:OH	1:C:240:GLU:OE1	2.29	0.49
1:C:752:LEU:HD23	1:C:752:LEU:H	1.77	0.48
1:C:756:GLU:OE2	1:C:1153:LYS:NZ	2.46	0.48
1:A:156:TYR:HB3	1:A:160:THR:HG21	1.95	0.48
1:B:24:VAL:HB	5:B:1405:NAG:H83	1.94	0.48
1:B:1146:ALA:O	1:B:1178:ARG:NH1	2.47	0.48
1:C:1137:ASP:OD1	1:C:1137:ASP:N	2.42	0.48
1:C:392:VAL:HG22	1:C:431:VAL:HG22	1.95	0.48
1:B:431:VAL:HB	1:B:561:THR:HB	1.96	0.47
1:A:661:LEU:HA	1:A:700:VAL:HG12	1.94	0.47
1:A:1036:LYS:HD3	1:C:600:VAL:HG11	1.95	0.47
1:C:407:VAL:HG12	1:C:473:ILE:HG12	1.95	0.47
1:A:648:SER:HB2	1:A:661:LEU:HB3	1.96	0.47
1:C:1193:LEU:HD12	1:C:1197:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:LEU:HD21	1:B:992:PHE:HZ	1.80	0.47
1:A:1019:GLU:HG3	1:A:1057:SER:HB2	1.97	0.47
1:B:874:LEU:HD21	1:B:992:PHE:CZ	2.50	0.47
1:C:128:ALA:HB1	1:C:295:ASP:HB3	1.96	0.46
1:A:407:VAL:HB	1:A:471:ALA:HB1	1.96	0.46
1:B:1149:GLY:HA2	1:B:1164:SER:HB3	1.95	0.46
1:C:25:VAL:HG11	1:C:197:VAL:HG21	1.98	0.46
1:C:692:LEU:HD23	1:C:701:ILE:HB	1.96	0.46
1:A:364:TYR:HD1	1:A:595:ASP:HB3	1.80	0.46
1:B:364:TYR:HD1	1:B:595:ASP:HB3	1.81	0.46
1:B:966:THR:HB	1:B:969:VAL:HG23	1.98	0.46
1:B:752:LEU:HD22	1:B:757:PHE:CB	2.44	0.46
1:B:1094:ASN:O	1:C:1084:ASN:ND2	2.48	0.46
1:A:38:ARG:O	1:A:305:TYR:OH	2.29	0.46
1:C:444:THR:HG22	1:C:451:GLU:HG3	1.98	0.45
1:A:221:ASP:OD1	1:A:221:ASP:N	2.44	0.45
1:A:1136:CYS:HB3	1:A:1143:CYS:HA	1.99	0.45
1:B:468:ARG:HG3	1:B:559:VAL:HG22	1.98	0.45
1:B:874:LEU:HD23	1:B:992:PHE:HE2	1.82	0.45
1:B:895:LYS:HB2	1:B:895:LYS:HE3	1.78	0.45
1:B:58:ASN:HD22	1:B:318:VAL:HG12	1.80	0.45
1:C:38:ARG:HE	1:C:116:ASN:HD21	1.64	0.45
1:A:769:VAL:HG22	1:A:1119:VAL:HG22	1.99	0.45
1:A:923:MET:HE1	1:C:741:MET:HB3	1.99	0.45
1:A:111:VAL:HG22	1:A:304:ILE:HG12	1.99	0.45
1:A:600:VAL:HG21	1:B:1036:LYS:HD2	1.98	0.45
1:A:123:SER:OG	1:A:125:VAL:O	2.35	0.45
1:C:1039:ASP:OD1	1:C:1039:ASP:N	2.47	0.45
1:B:600:VAL:HG21	1:C:1036:LYS:HD2	2.00	0.44
1:C:68:PRO:O	1:C:312:TYR:OH	2.25	0.44
1:C:431:VAL:HB	1:C:561:THR:HB	1.99	0.44
1:A:852:LEU:HG	1:A:870:LEU:HB2	1.99	0.44
1:A:372:CYS:HB2	1:A:398:TYR:HA	1.99	0.44
1:C:317:ASP:OD1	1:C:317:ASP:C	2.60	0.44
1:C:1038:LEU:O	1:C:1043:GLN:NE2	2.49	0.44
1:C:407:VAL:HB	1:C:471:ALA:HB1	2.00	0.44
1:A:386:ALA:HB2	1:A:491:TYR:HA	1.98	0.44
1:A:549:THR:HG23	1:A:551:GLU:H	1.83	0.44
1:C:692:LEU:HB3	1:C:699:CYS:SG	2.58	0.44
1:A:789:VAL:O	1:A:1054:ARG:NH1	2.51	0.44
1:B:922:ASN:O	1:B:926:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLN:NE2	1:B:276:GLU:O	2.42	0.44
1:A:53:GLY:HA2	1:C:565:ALA:HB1	1.99	0.43
1:B:327:ASP:HB3	1:B:330:ALA:HB2	2.00	0.43
1:B:378:PHE:HZ	1:B:403:LEU:HA	1.83	0.43
1:B:386:ALA:HB2	1:B:491:TYR:HA	1.98	0.43
1:A:902:ASP:HB3	1:A:905:CYS:HB2	2.01	0.43
1:B:54:ARG:HG2	1:B:56:TYR:CZ	2.54	0.43
1:A:28:GLN:HB3	1:A:94:PHE:HE1	1.83	0.43
1:B:880:LEU:HB3	1:B:882:VAL:HG23	2.01	0.43
1:C:167:LYS:HB2	1:C:170:THR:HG22	2.01	0.43
1:C:829:PHE:CZ	1:C:924:GLU:HG2	2.53	0.43
1:C:922:ASN:O	1:C:926:MET:HG3	2.18	0.43
1:C:113:ILE:HD13	1:C:137:PRO:HD2	2.00	0.43
1:A:501:LYS:HE2	1:A:501:LYS:HB2	1.82	0.43
1:A:665:VAL:HG22	1:A:666:ALA:H	1.84	0.43
1:C:164:LEU:HD13	1:C:212:LEU:HB3	2.00	0.43
1:A:49:ILE:HD13	1:A:266:MET:HE3	2.00	0.43
1:B:372:CYS:HB2	1:B:398:TYR:HA	2.00	0.43
1:C:177:CYS:HB3	1:C:225:CYS:HA	2.00	0.43
1:C:867:ARG:HH21	1:C:921:SER:HB2	1.83	0.43
1:A:82:TYR:HA	1:A:93:PRO:HA	2.01	0.43
1:A:417:THR:HG23	1:A:465:PRO:HB3	2.00	0.43
1:A:1058:LEU:HD23	1:A:1058:LEU:HA	1.87	0.42
1:B:712:ASP:OD1	1:B:712:ASP:N	2.52	0.42
1:C:667:CYS:HB2	1:C:699:CYS:HB2	1.67	0.42
1:B:111:VAL:HG22	1:B:304:ILE:HG12	2.01	0.42
1:B:852:LEU:HG	1:B:870:LEU:HB2	2.01	0.42
1:C:956:ILE:O	1:C:960:MET:HG3	2.18	0.42
1:A:956:ILE:HG12	1:A:960:MET:HE2	2.02	0.42
1:B:852:LEU:HA	1:B:869:ALA:HB3	2.01	0.42
1:B:146:GLY:HA3	1:B:157:PHE:HE2	1.84	0.42
1:A:803:TYR:OH	1:A:1052:ASN:ND2	2.48	0.42
1:B:196:TYR:HE1	1:B:284:MET:HG2	1.83	0.42
1:B:775:GLU:HG3	1:B:1112:ASN:HB3	2.02	0.42
1:B:988:MET:HE2	1:B:988:MET:HB3	1.97	0.42
1:A:175:LEU:HB3	1:A:228:GLU:HG3	2.02	0.42
1:A:556:MET:HE3	1:A:556:MET:HB3	1.85	0.42
1:A:263:SER:OG	1:A:264:ASN:N	2.52	0.42
1:B:996:ASN:OD1	1:B:996:ASN:N	2.52	0.42
1:C:140:MET:HG2	1:C:156:TYR:CE2	2.55	0.42
1:A:387:ASN:HB2	1:A:520:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ASP:OD1	1:A:622:SER:N	2.51	0.41
1:B:613:ILE:HA	1:B:614:PRO:HD3	1.89	0.41
1:B:867:ARG:HD3	1:B:871:GLU:HB3	2.02	0.41
1:C:379:LYS:HG3	1:C:380:ASN:OD1	2.20	0.41
1:C:845:SER:O	1:C:845:SER:OG	2.34	0.41
1:B:387:ASN:HB2	1:B:520:LEU:HD11	2.03	0.41
1:B:534:ASN:ND2	1:C:145:VAL:O	2.54	0.41
1:B:1039:ASP:N	1:B:1039:ASP:OD1	2.53	0.41
1:A:197:VAL:HG12	1:A:199:VAL:HG13	2.01	0.41
1:A:317:ASP:OD1	1:A:317:ASP:C	2.63	0.41
1:B:648:SER:HB2	1:B:661:LEU:HB3	2.01	0.41
1:C:42:MET:HE1	1:C:334:THR:HG21	2.02	0.41
1:C:889:TYR:CZ	1:C:893:MET:HG3	2.55	0.41
1:A:672:MET:H	1:A:672:MET:HG3	1.66	0.41
1:B:537:ILE:HD13	1:B:537:ILE:HA	1.96	0.41
1:B:646:PRO:HG3	1:C:913:LYS:HD3	2.02	0.41
1:B:1038:LEU:O	1:B:1043:GLN:NE2	2.54	0.41
1:A:742:LYS:HB2	1:A:742:LYS:HE2	1.90	0.41
1:A:1039:ASP:OD1	1:A:1039:ASP:N	2.53	0.41
1:B:297:MET:SD	1:B:297:MET:N	2.94	0.41
1:B:317:ASP:OD1	1:B:317:ASP:C	2.64	0.41
1:B:603:GLY:HA2	1:B:642:CYS:HB2	2.03	0.41
1:C:771:GLU:H	1:C:771:GLU:HG2	1.69	0.41
1:A:264:ASN:N	1:A:264:ASN:OD1	2.46	0.41
1:A:826:LYS:HG3	1:A:918:LEU:HD21	2.02	0.41
1:C:32:PHE:HD2	1:C:78:ILE:HB	1.86	0.41
1:A:587:LEU:HB3	1:A:592:ILE:HG21	2.02	0.41
1:A:1135:LEU:HG	1:A:1151:PHE:CD2	2.56	0.41
4:C:1401:FOL:H15	4:C:1401:FOL:H91	1.87	0.41
1:B:826:LYS:HG3	1:B:918:LEU:HD21	2.03	0.40
1:B:1050:LEU:O	1:B:1054:ARG:HG2	2.21	0.40
1:C:336:LEU:HG	1:C:345:MET:HE3	2.03	0.40
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.92	0.40
1:A:223:LYS:O	1:A:224:ASP:HB3	2.21	0.40
1:B:200:GLU:HG3	1:B:288:ILE:HG23	2.02	0.40
1:B:604:VAL:HG22	1:B:640:ALA:HB3	2.02	0.40
1:B:116:ASN:ND2	4:B:1401:FOL:O4	2.52	0.40
1:A:32:PHE:HA	1:A:78:ILE:HD11	2.03	0.40
1:B:641:PRO:HD2	1:B:644:SER:HB3	2.03	0.40
1:B:714:ASN:OD1	1:B:714:ASN:N	2.53	0.40
1:C:24:VAL:HG23	5:C:1404:NAG:H4	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1050:LEU:HD23	1:C:1050:LEU:HA	1.97	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	1111/1349 (82%)	1059 (95%)	52 (5%)	0	100	100
1	B	1111/1349 (82%)	1062 (96%)	48 (4%)	1 (0%)	48	75
1	C	1111/1349 (82%)	1062 (96%)	49 (4%)	0	100	100
All	All	3333/4047 (82%)	3183 (96%)	149 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	994	THR

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	985/1165 (84%)	983 (100%)	2 (0%)	87	88
1	B	985/1165 (84%)	983 (100%)	2 (0%)	87	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	985/1165 (84%)	985 (100%)	0	100 100
All	All	2955/3495 (84%)	2951 (100%)	4 (0%)	87 90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	672	MET
1	A	891	GLU
1	B	221	ASP
1	B	415	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	107	ASN
1	A	211	ASN
1	A	308	HIS
1	A	524	ASN
1	A	779	GLN
1	A	798	GLN
1	A	811	ASN
1	A	907	GLN
1	A	997	GLN
1	A	1046	GLN
1	A	1109	ASN
1	B	159	HIS
1	B	180	GLN
1	B	311	ASN
1	B	524	ASN
1	B	532	ASN
1	B	570	ASN
1	B	625	ASN
1	B	791	ASN
1	B	798	GLN
1	B	974	GLN
1	B	989	GLN
1	B	1052	ASN
1	B	1077	GLN
1	B	1084	ASN
1	B	1109	ASN

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Mol	Chain	Res	Type
1	B	1174	ASN
1	B	1192	ASN
1	C	107	ASN
1	C	159	HIS
1	C	190	HIS
1	C	384	GLN
1	C	512	ASN
1	C	524	ASN
1	C	563	ASN
1	C	569	ASN
1	C	798	GLN
1	C	1052	ASN
1	C	1084	ASN
1	C	1112	ASN
1	C	1140	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

39 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	1,2	14,14,15	0.30	0	17,19,21	0.50	0
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	E	1	1,2	14,14,15	0.25	0	17,19,21	0.51	0
2	NAG	E	2	2	14,14,15	0.31	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	F	1	1,2	14,14,15	0.32	0	17,19,21	0.96	1 (5%)
2	NAG	F	2	2	14,14,15	0.23	0	17,19,21	0.52	0
2	NAG	G	1	1,2	14,14,15	0.31	0	17,19,21	0.60	0
2	NAG	G	2	2	14,14,15	0.31	0	17,19,21	0.47	0
2	NAG	H	1	1,2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.51	0
3	NAG	I	1	1,3	14,14,15	0.26	0	17,19,21	0.51	0
3	NAG	I	2	3	14,14,15	0.23	0	17,19,21	0.46	0
3	BMA	I	3	3	11,11,12	0.56	0	15,15,17	0.88	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.29	0	17,19,21	0.52	0
2	NAG	J	2	2	14,14,15	0.31	0	17,19,21	0.48	0
2	NAG	K	1	1,2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	K	2	2	14,14,15	0.27	0	17,19,21	0.55	0
2	NAG	L	1	1,2	14,14,15	0.24	0	17,19,21	0.56	0
2	NAG	L	2	2	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	M	1	1,2	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
2	NAG	M	2	2	14,14,15	0.32	0	17,19,21	0.45	0
2	NAG	N	1	1,2	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	N	2	2	14,14,15	0.23	0	17,19,21	0.51	0
3	NAG	O	1	1,3	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	O	2	3	14,14,15	0.21	0	17,19,21	0.45	0
3	BMA	O	3	3	11,11,12	0.54	0	15,15,17	0.92	1 (6%)
2	NAG	P	1	1,2	14,14,15	0.32	0	17,19,21	0.52	0
2	NAG	P	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	NAG	Q	1	1,2	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	Q	2	2	14,14,15	0.43	0	17,19,21	0.51	0
2	NAG	R	1	1,2	14,14,15	0.25	0	17,19,21	0.58	0
2	NAG	R	2	2	14,14,15	0.22	0	17,19,21	0.47	0
2	NAG	S	1	1,2	14,14,15	0.31	0	17,19,21	0.59	0
2	NAG	S	2	2	14,14,15	0.28	0	17,19,21	0.45	0
2	NAG	T	1	1,2	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	T	2	2	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	U	1	1,3	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	U	2	3	14,14,15	0.21	0	17,19,21	0.46	0
3	BMA	U	3	3	11,11,12	0.59	0	15,15,17	0.85	1 (6%)

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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C2-N2-C7	2.67	126.47	122.90
3	O	3	BMA	C1-O5-C5	2.36	115.35	112.19
2	M	1	NAG	C1-O5-C5	2.24	115.19	112.19
3	I	3	BMA	C1-O5-C5	2.18	115.10	112.19
3	U	3	BMA	C1-O5-C5	2.14	115.05	112.19

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6

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Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	T	2	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	P	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C1-C2-N2-C7
3	I	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
2	M	2	NAG	C1-C2-N2-C7
2	Q	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
3	U	3	BMA	O5-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6

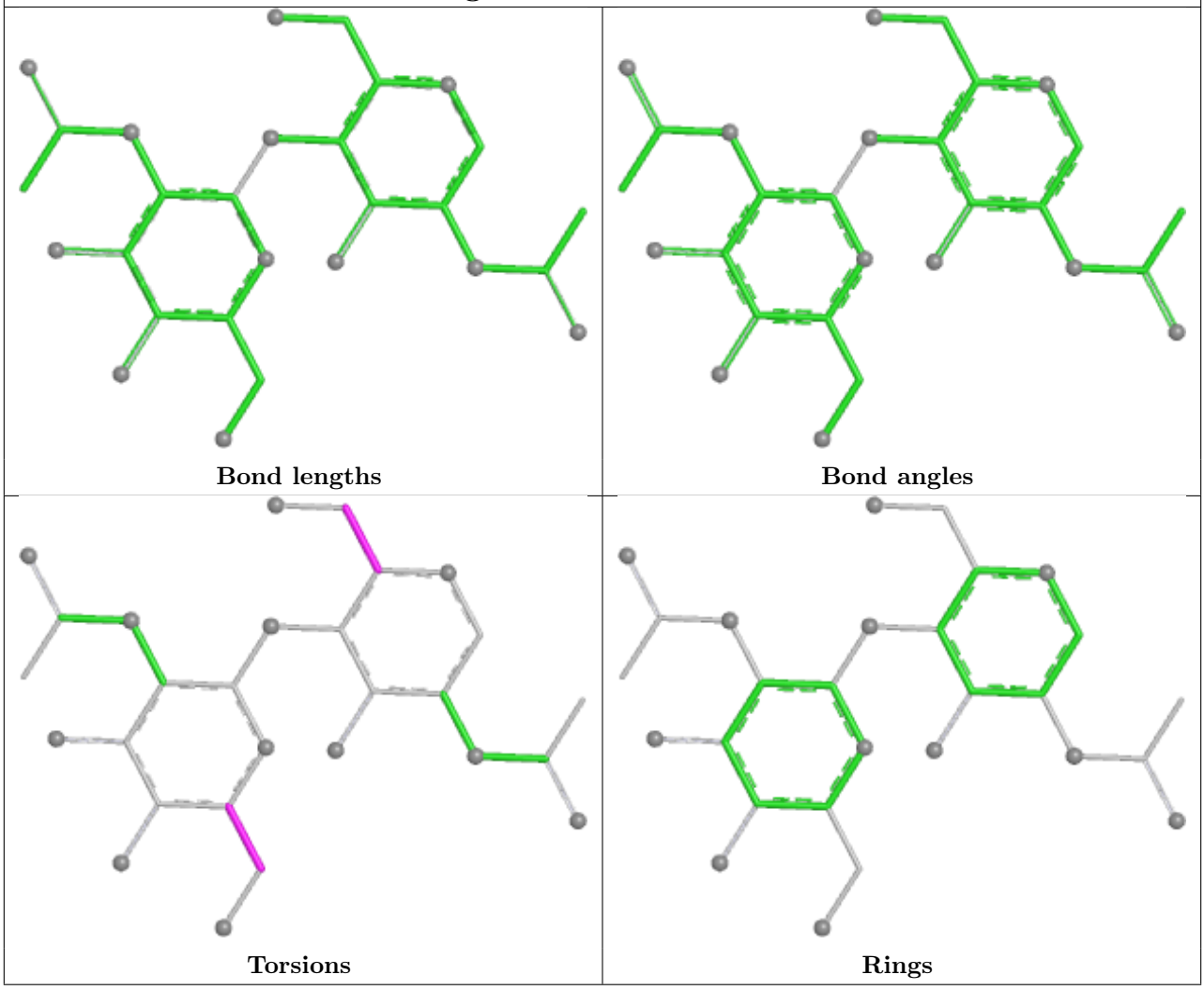
There are no ring outliers.

1 monomer is involved in 1 short contact:

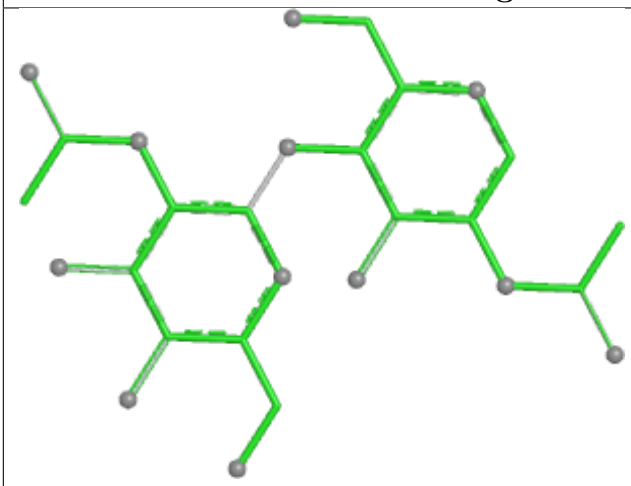
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	1	0

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

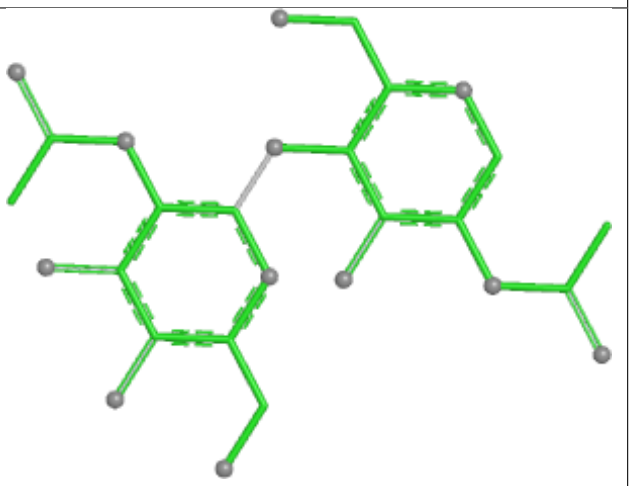
Oligosaccharide Chain D



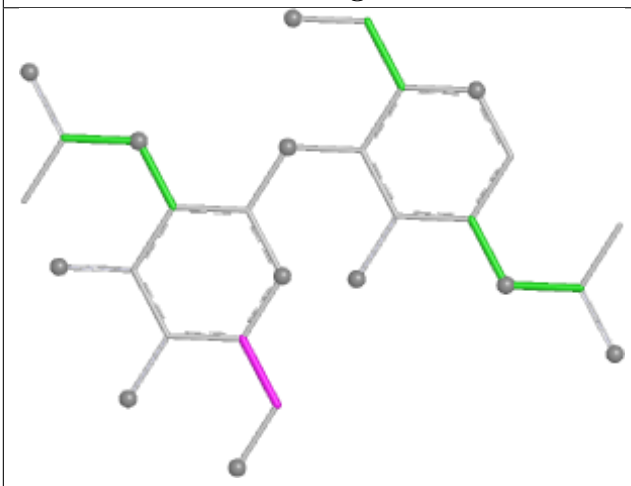
Oligosaccharide Chain E



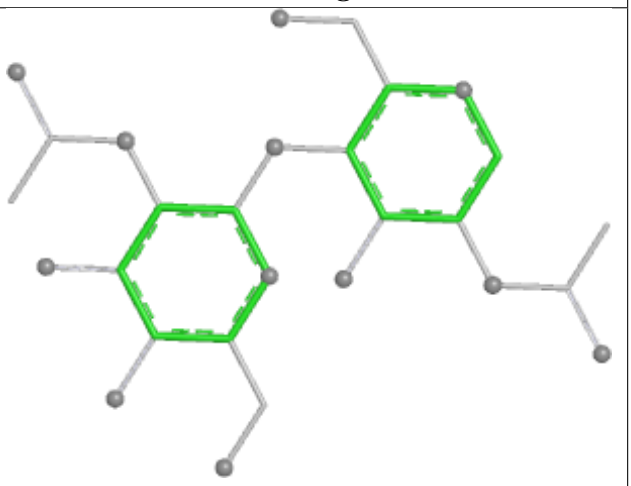
Bond lengths



Bond angles

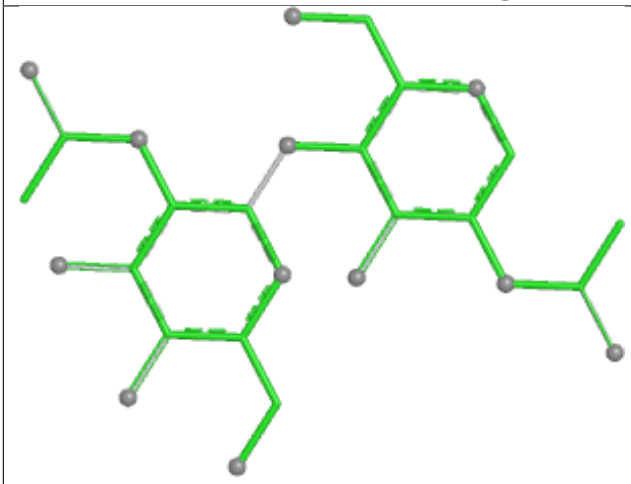


Torsions

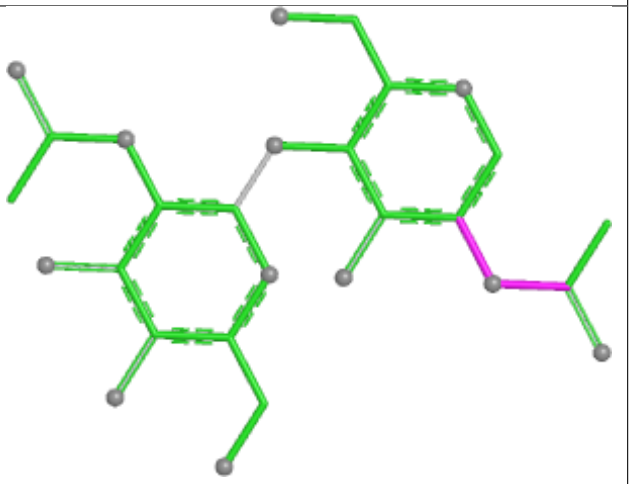


Rings

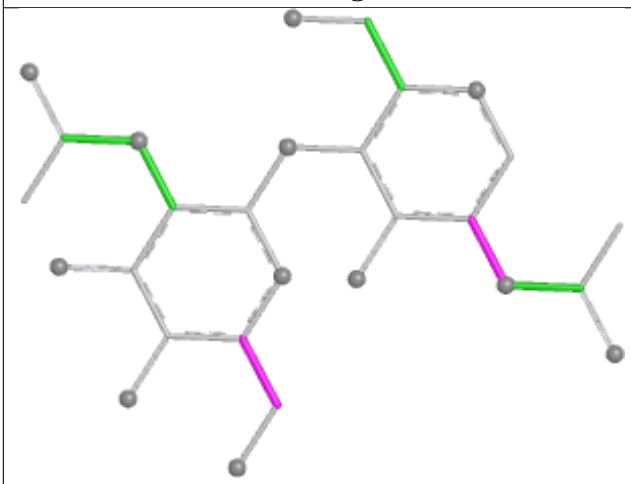
Oligosaccharide Chain F



Bond lengths



Bond angles



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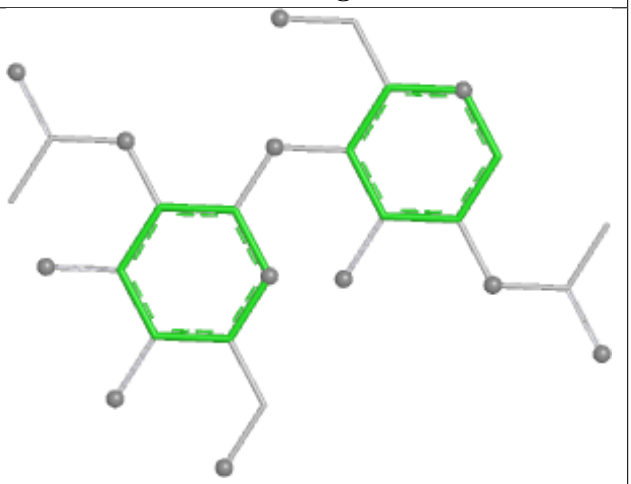
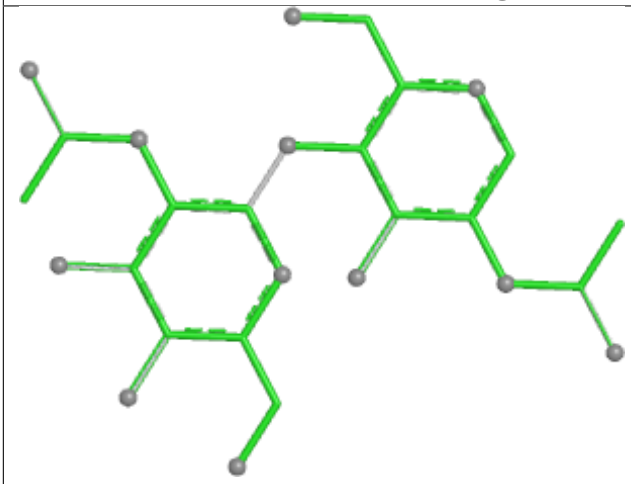
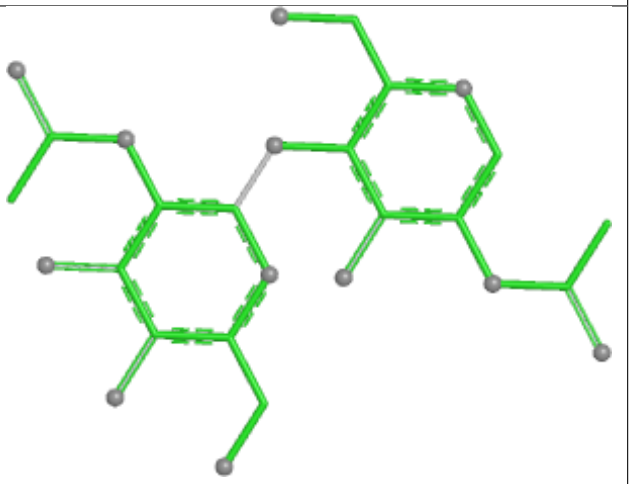


Rings

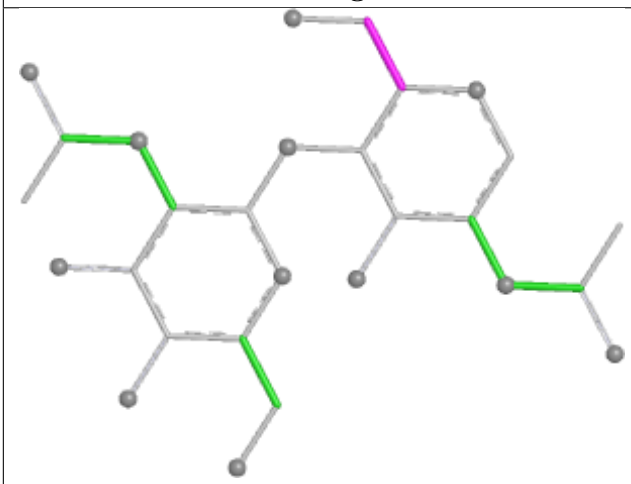
Oligosaccharide Chain G



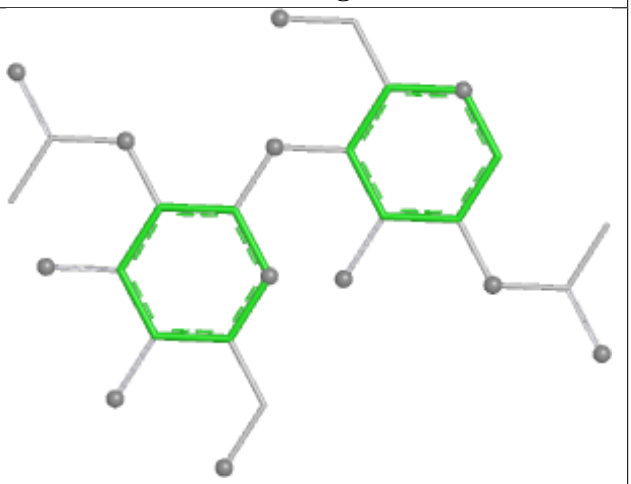
Bond lengths



Bond angles

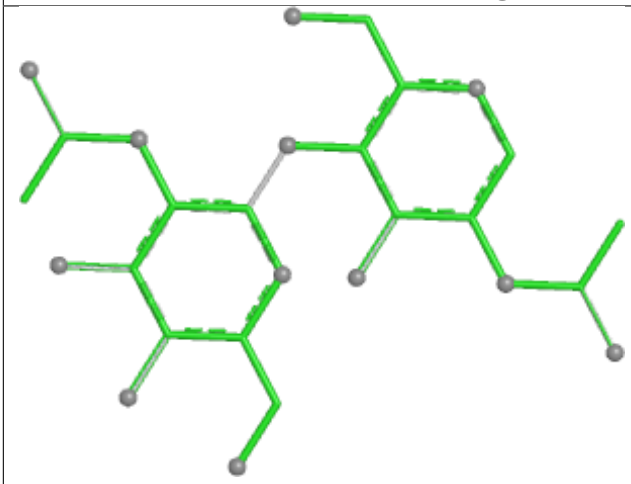


Torsions

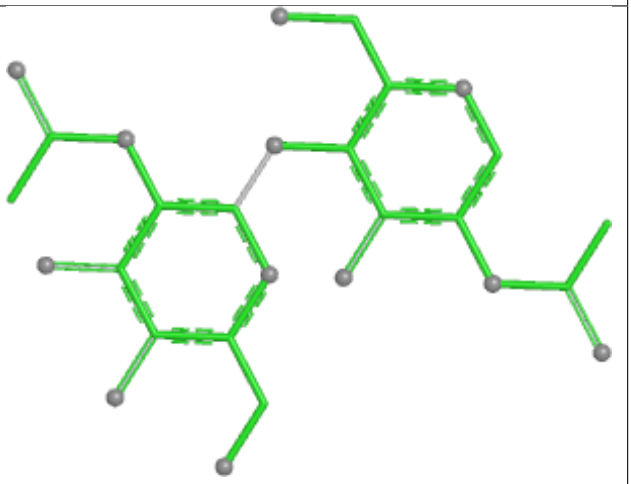


Rings

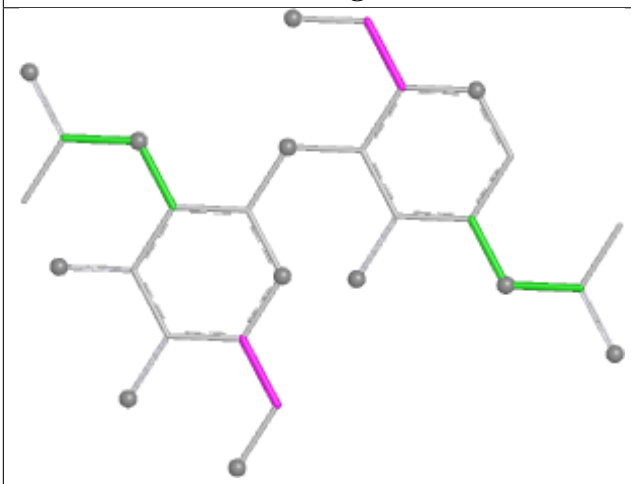
Oligosaccharide Chain H



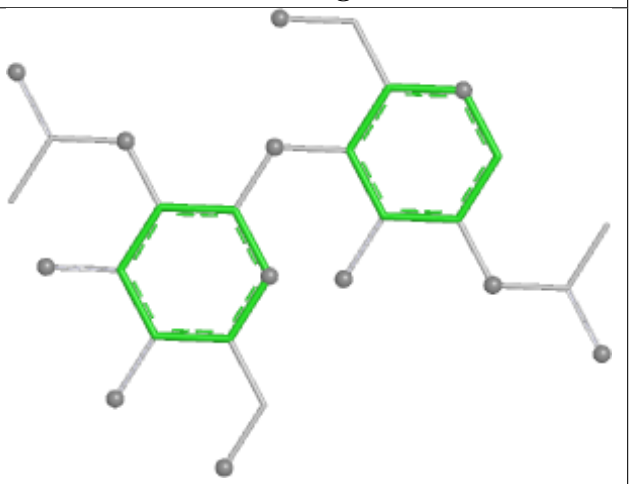
Bond lengths



Bond angles

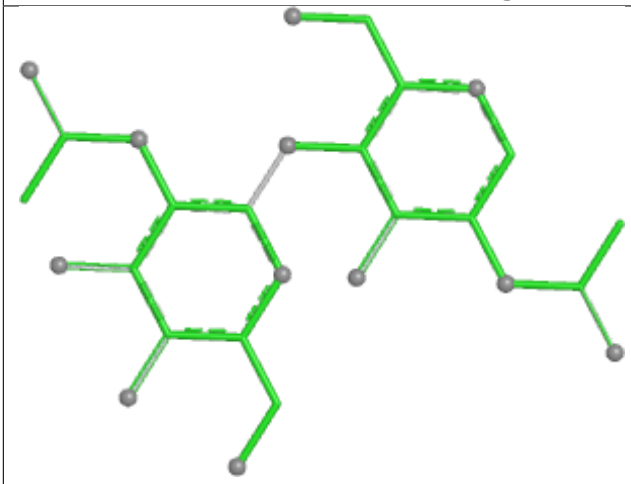


Torsions

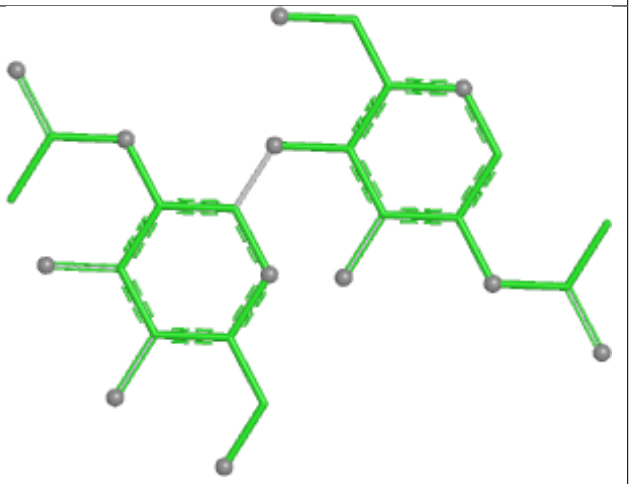


Rings

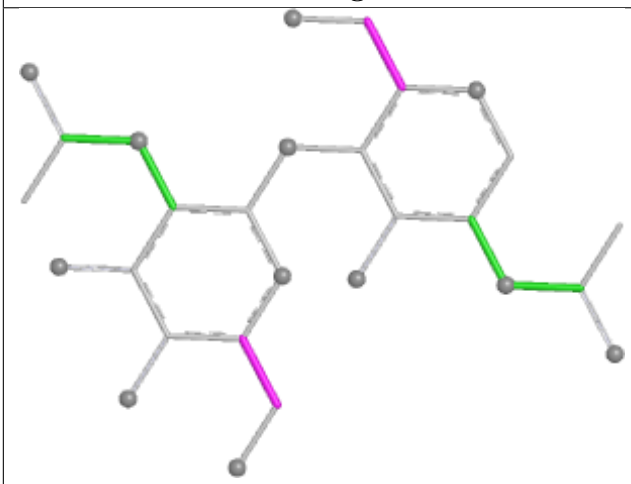
Oligosaccharide Chain J



Bond lengths



Bond angles



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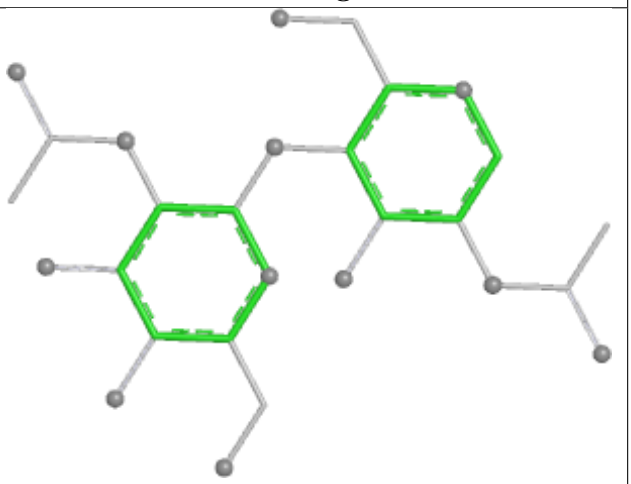
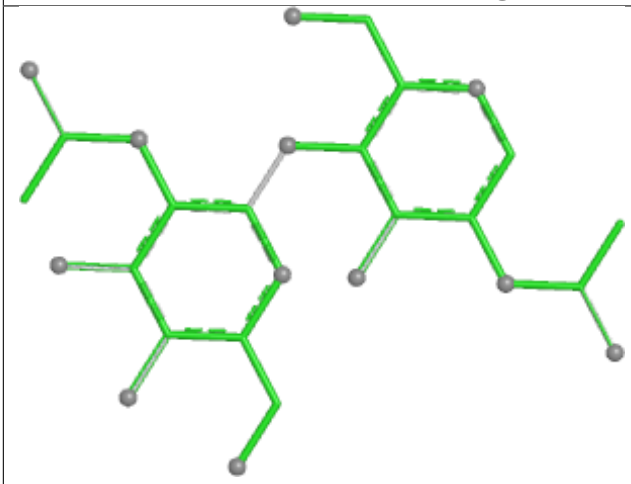


Rings

Oligosaccharide Chain K



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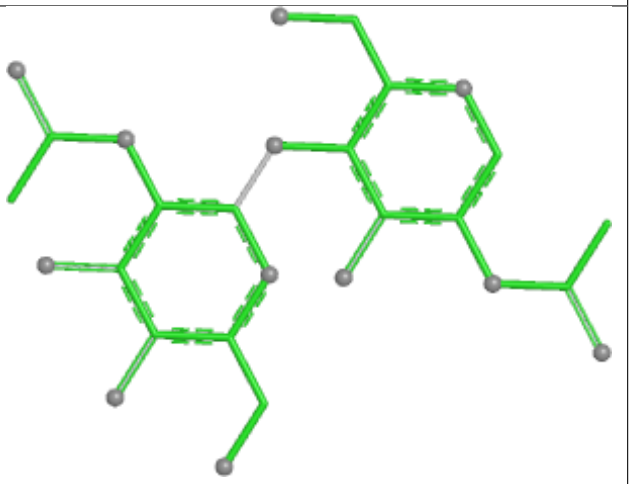
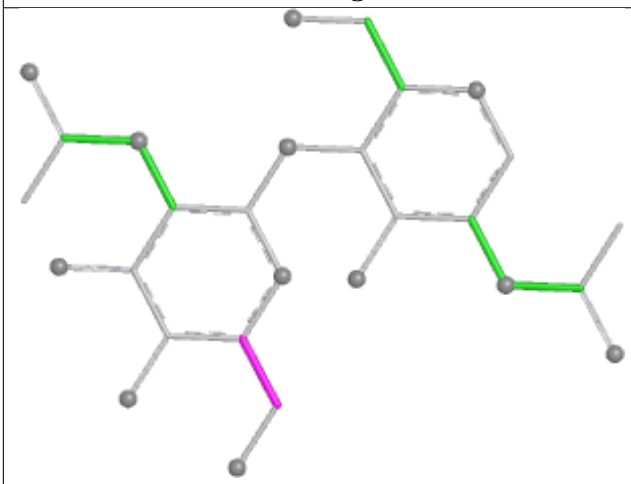


Bond angles



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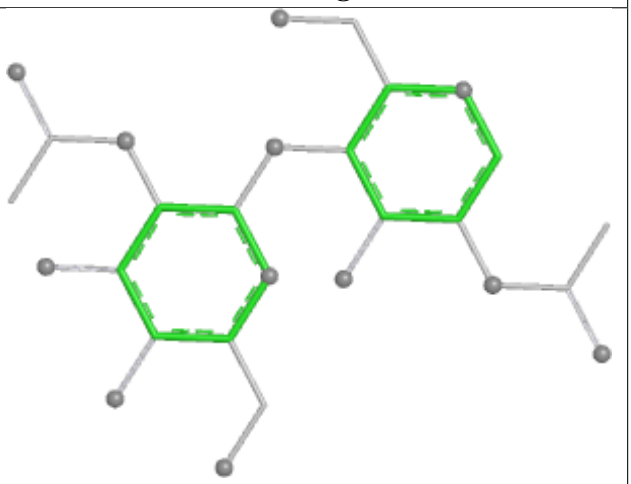
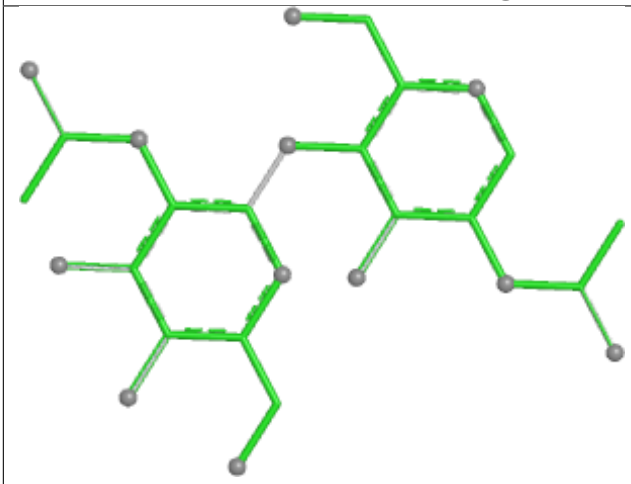


Rings

Oligosaccharide Chain L



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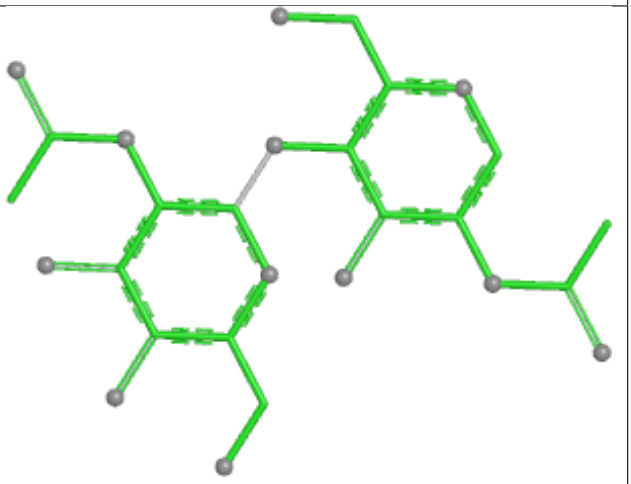
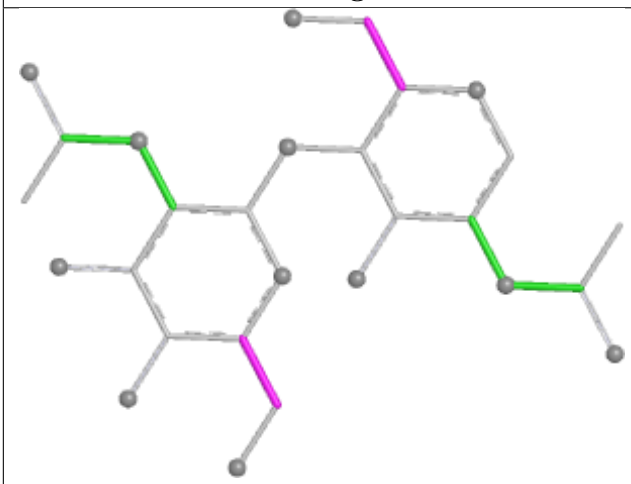


Bond angles



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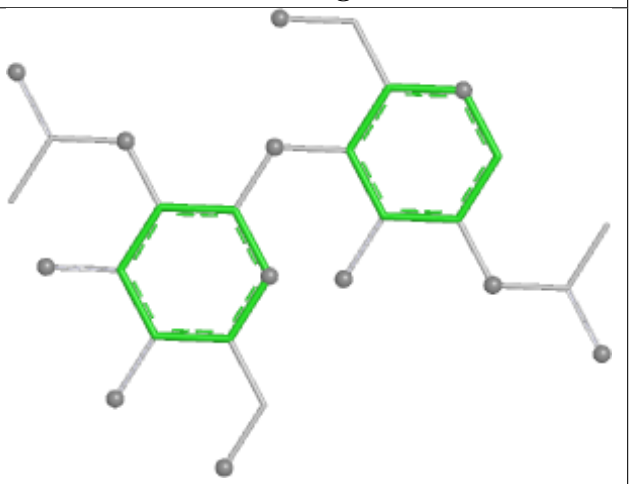
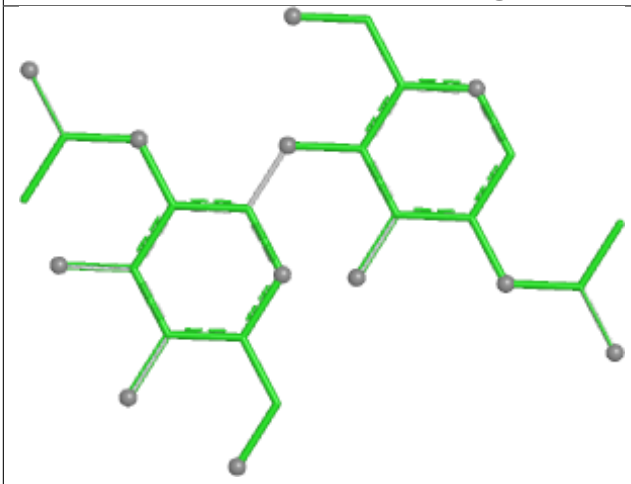


Rings

Oligosaccharide Chain M



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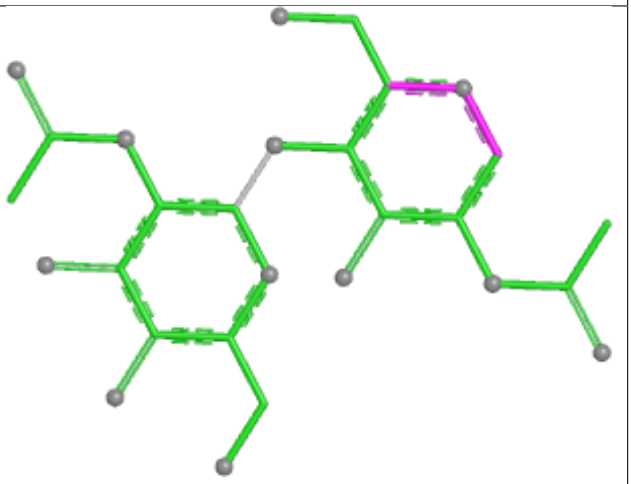
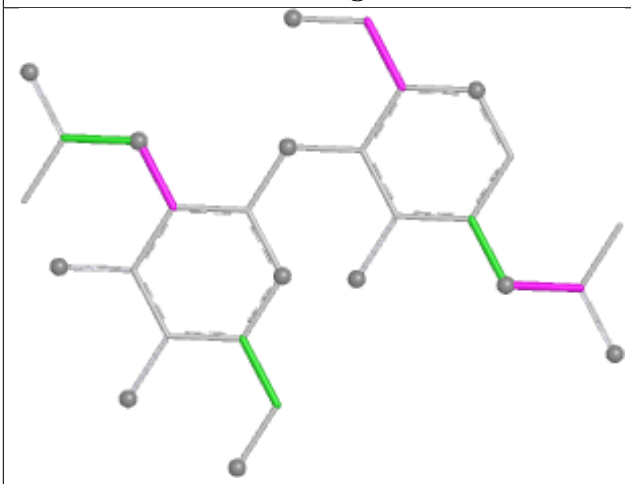


Bond angles



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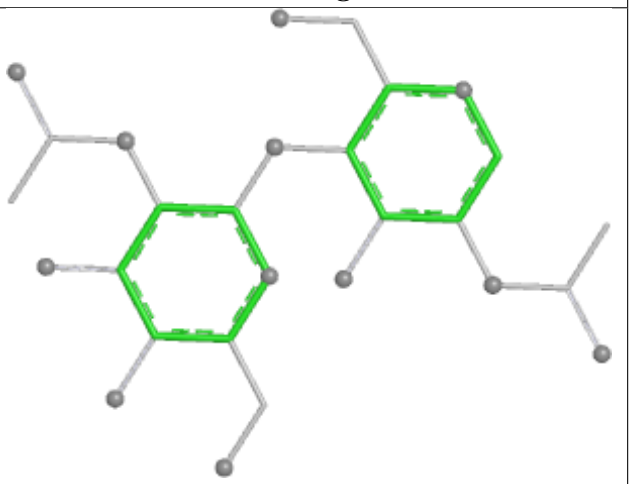
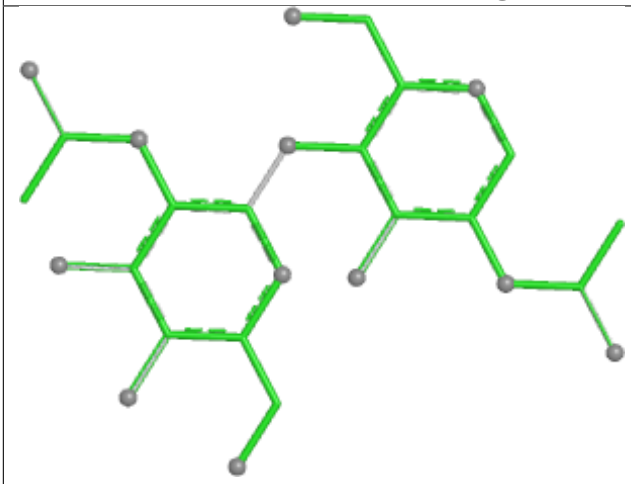
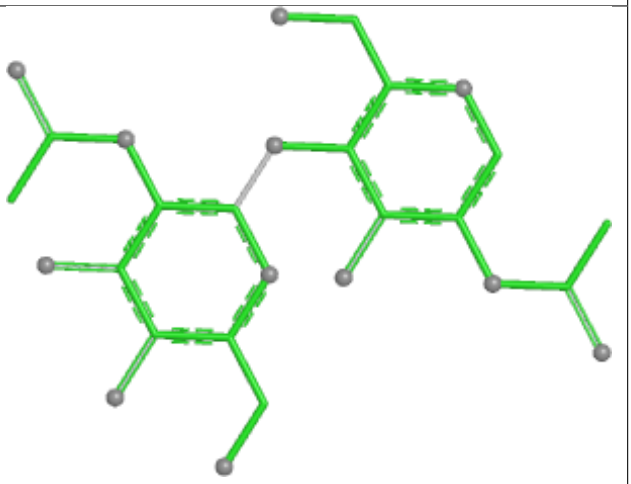


Rings

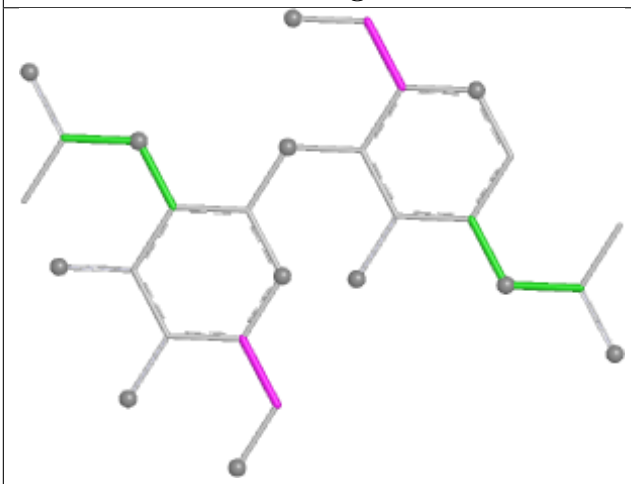
Oligosaccharide Chain N



Bond lengths



Bond angles



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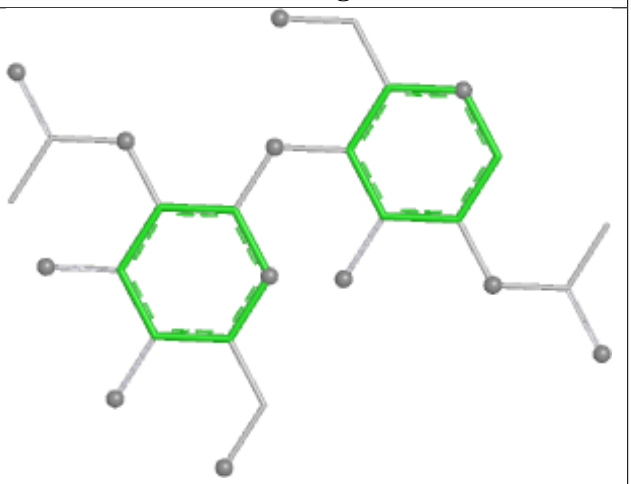
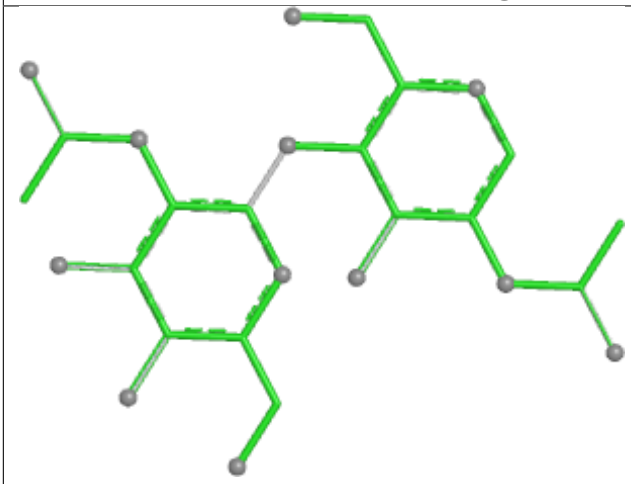


Rings

Oligosaccharide Chain P



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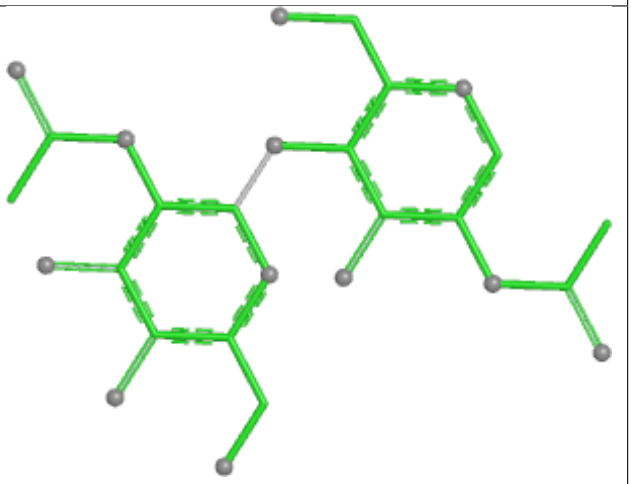

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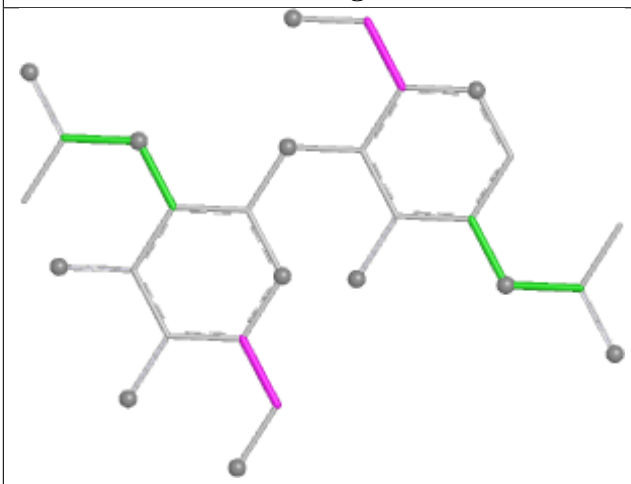

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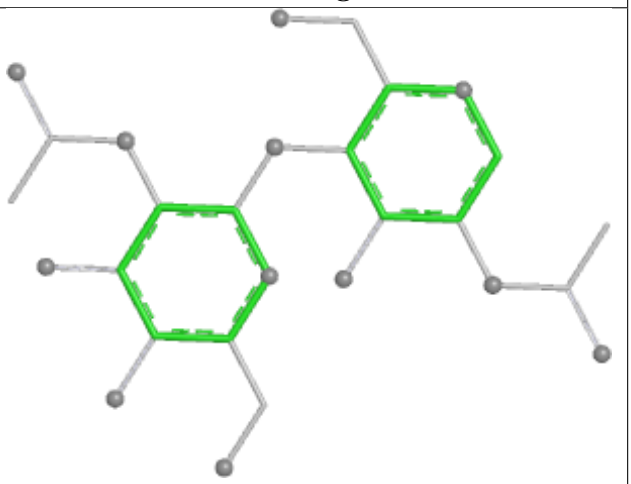
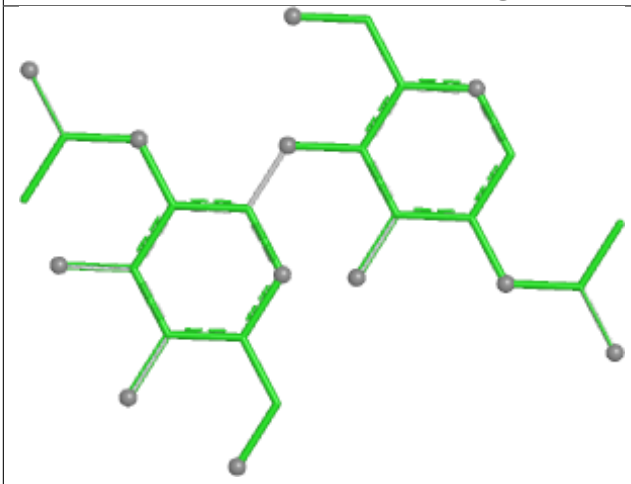


Rings

Oligosaccharide Chain Q



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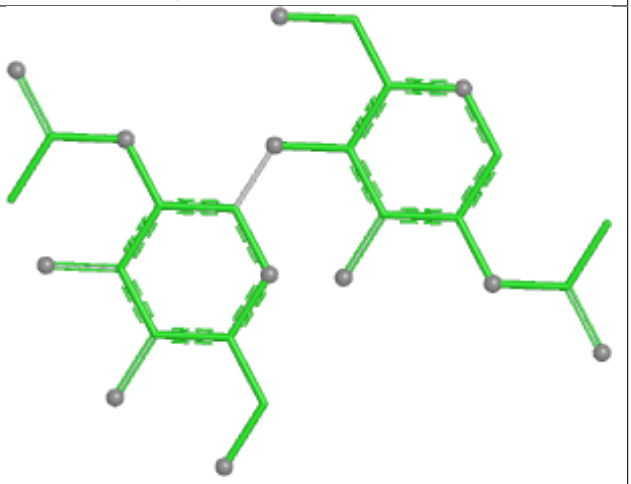
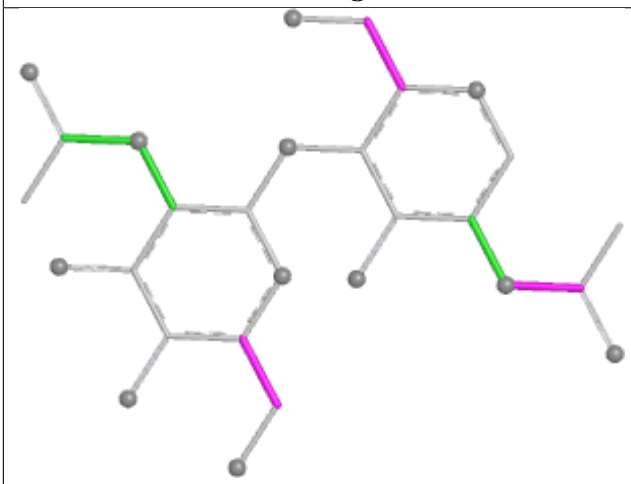


Bond angles



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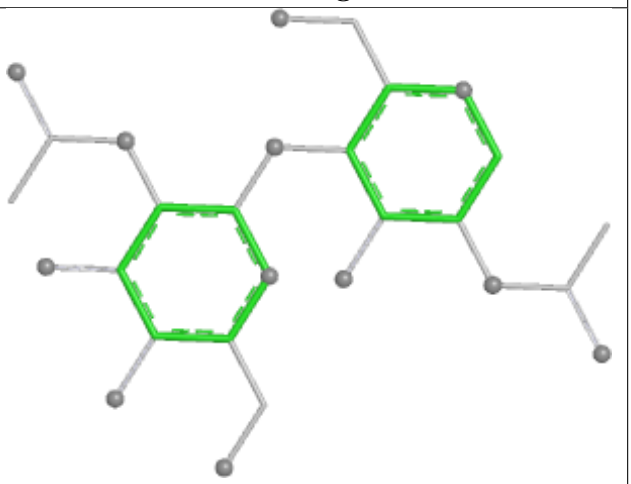
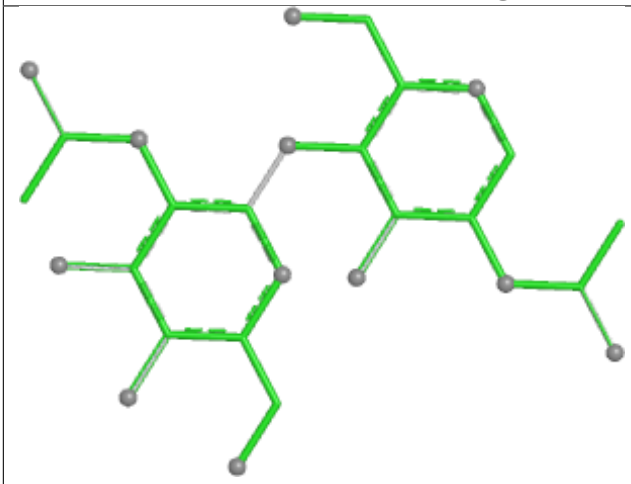
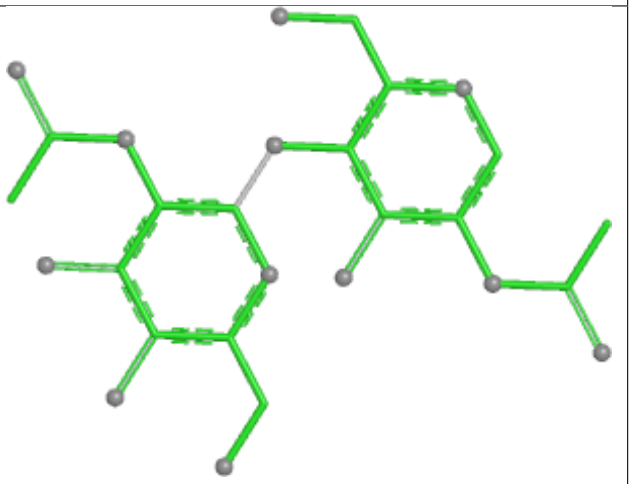


Rings

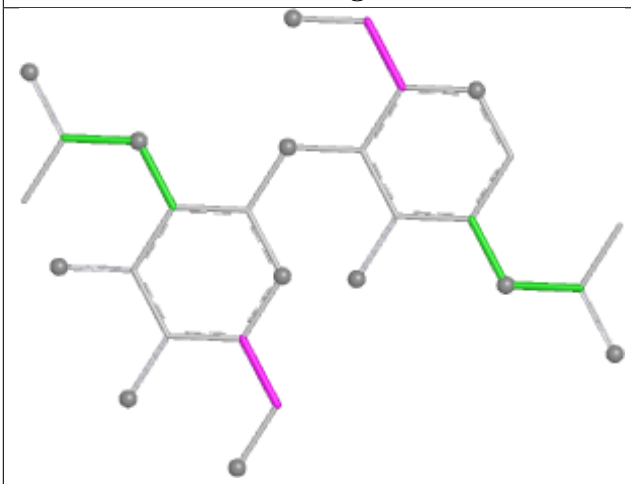
Oligosaccharide Chain R



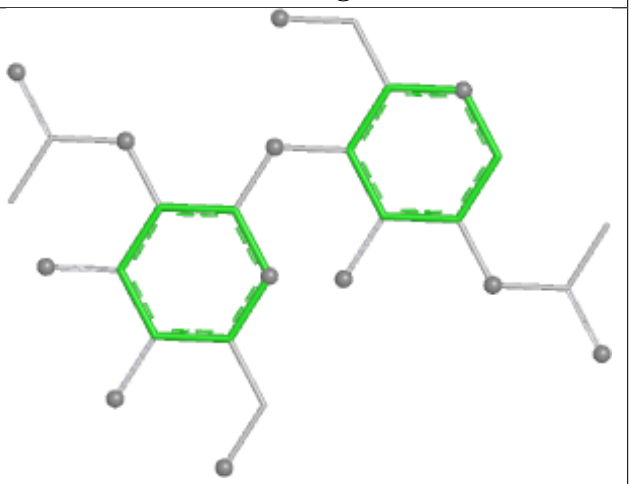
Bond lengths



Bond angles

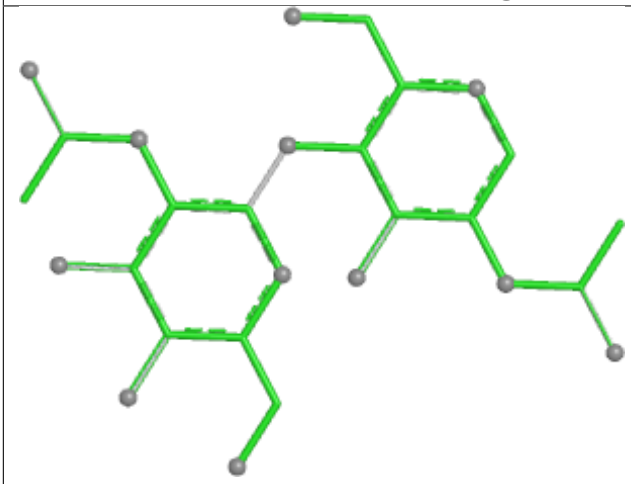


Torsions

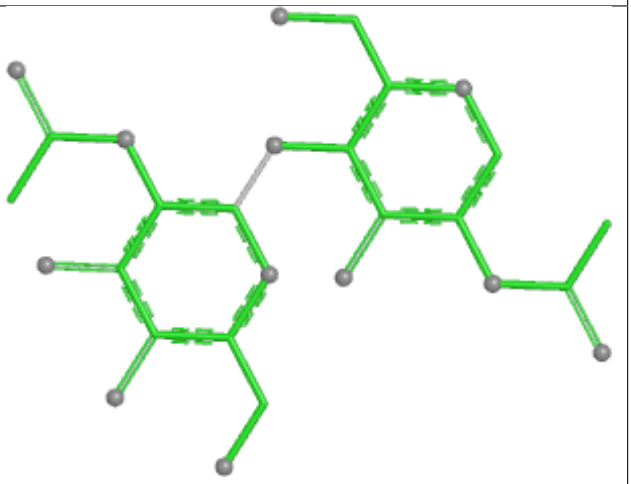


Rings

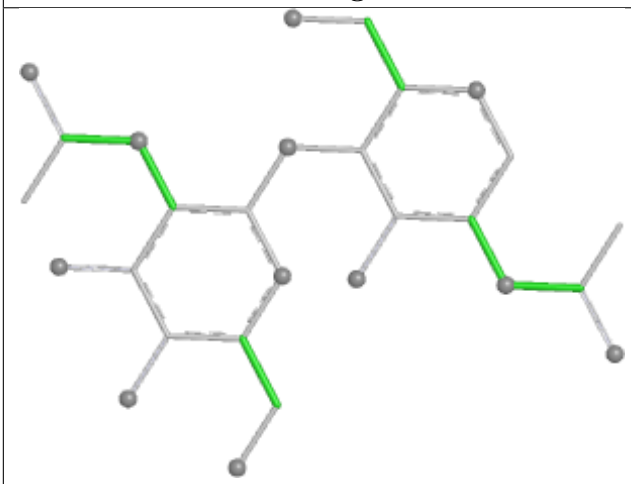
Oligosaccharide Chain S



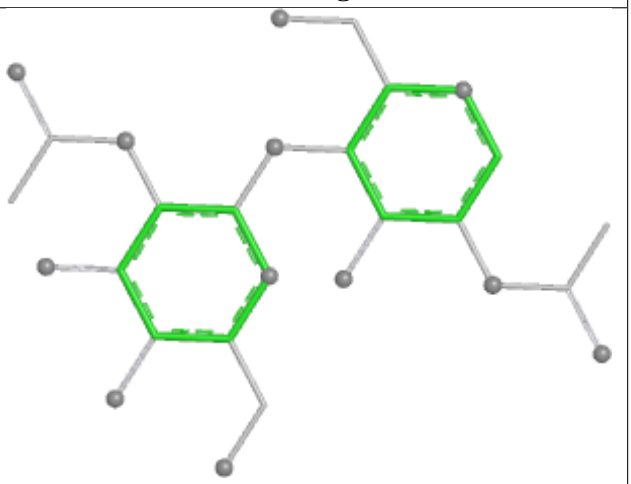
Bond lengths



Bond angles

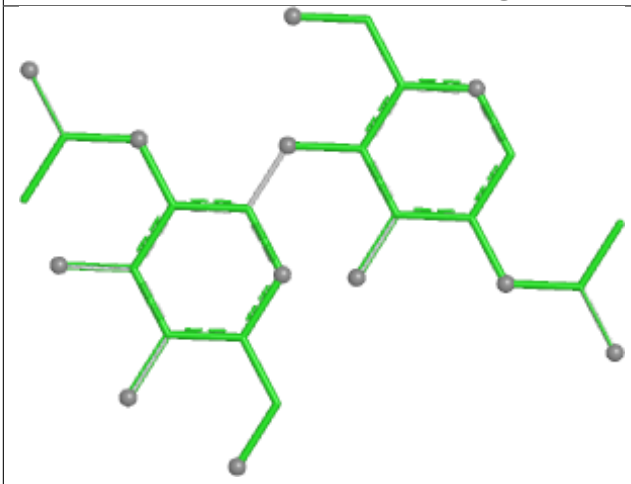


Torsions

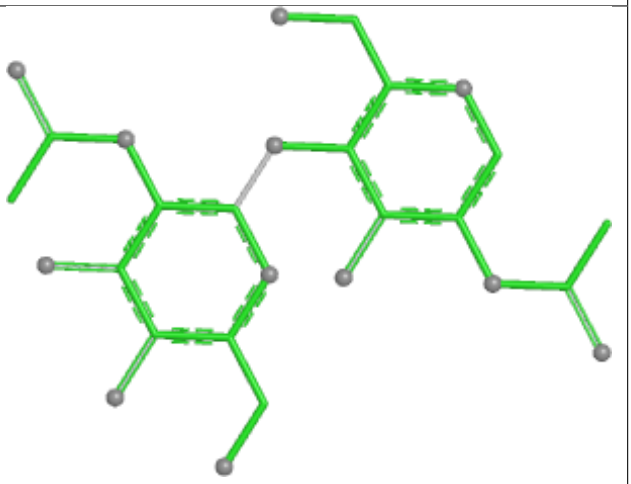


Rings

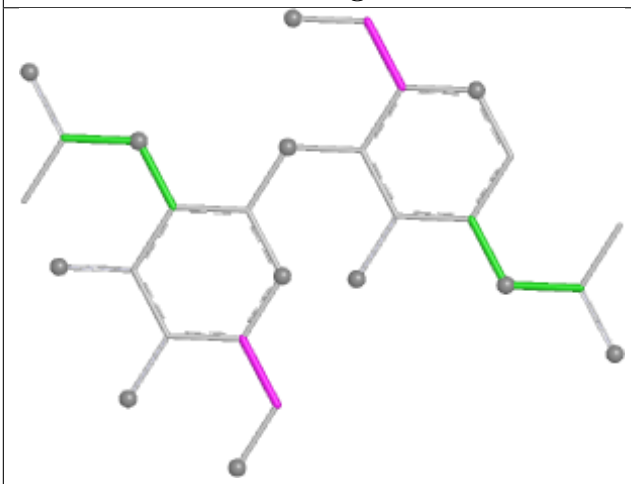
Oligosaccharide Chain T



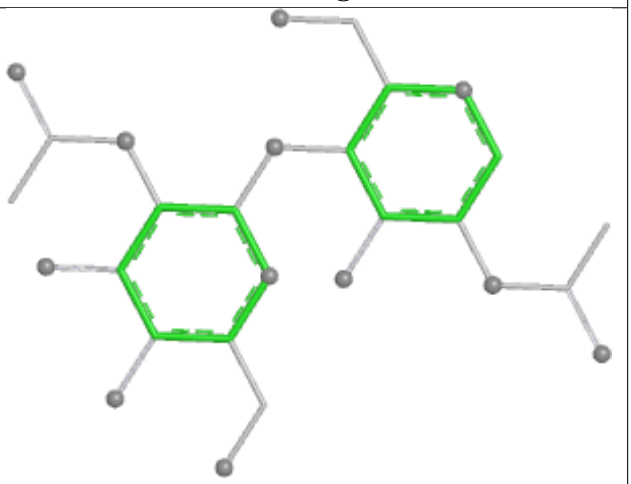
Bond lengths



Bond angles

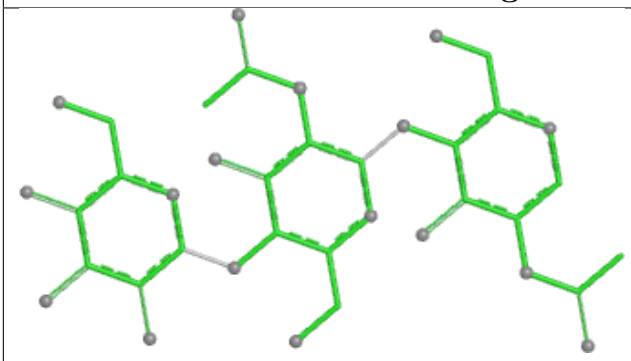


Torsions

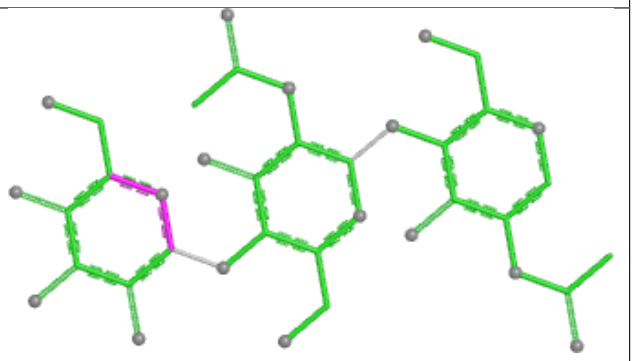


Rings

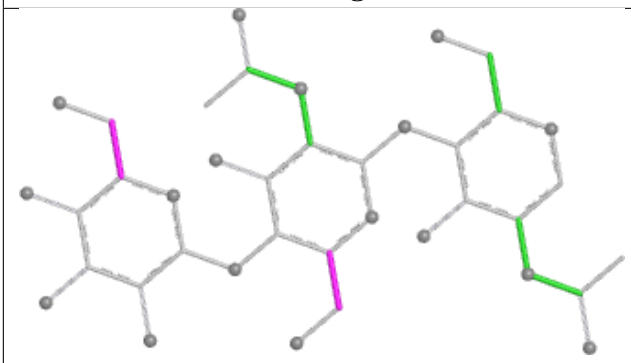
Oligosaccharide Chain I



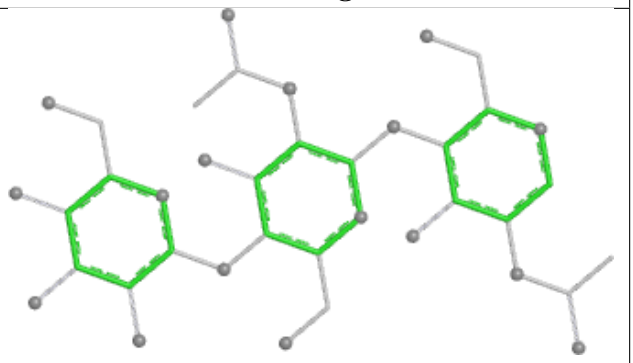
Bond lengths



Bond angles

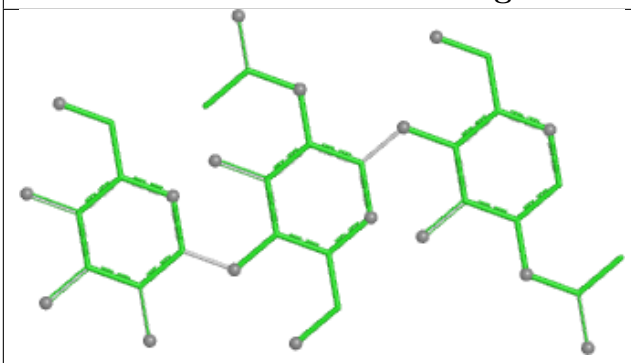


Torsions

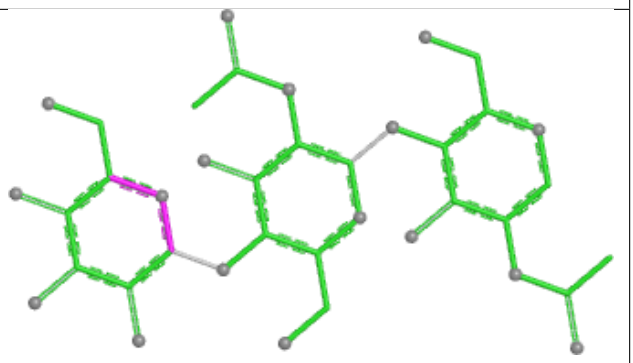


Rings

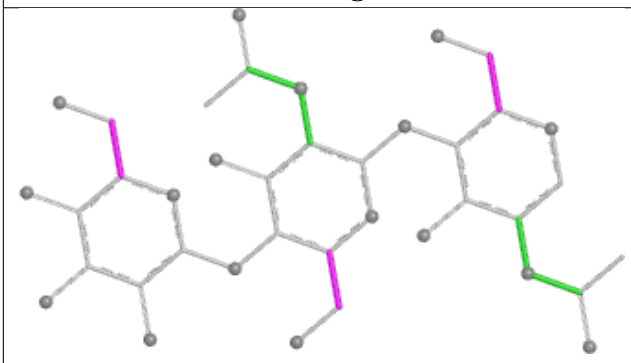
Oligosaccharide Chain O



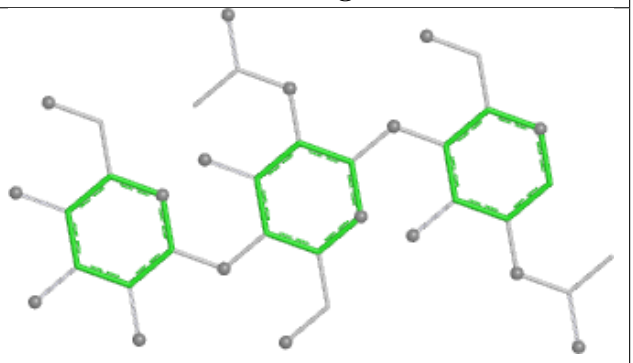
Bond lengths



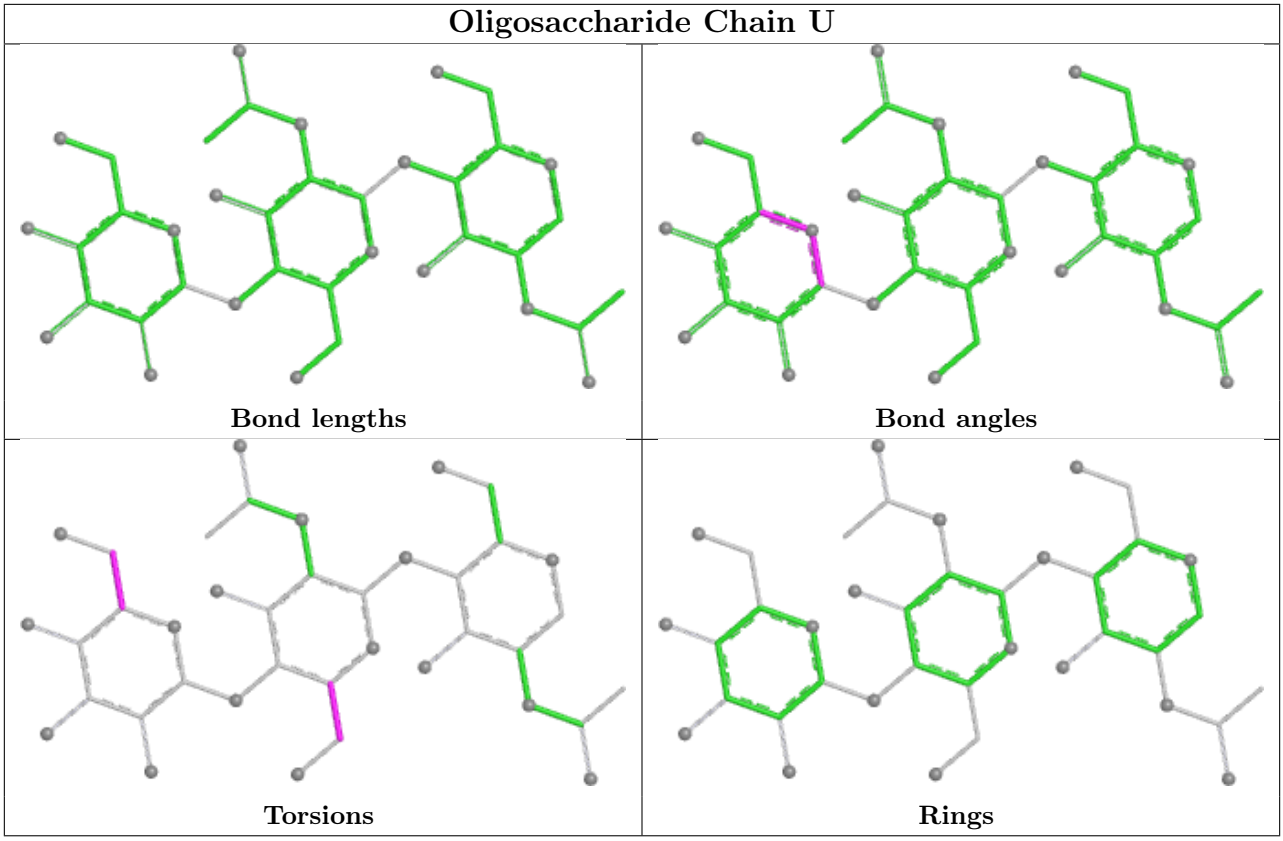
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

42 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	$\#\|Z\| > 2$
5	NAG	B	1407	1	14,14,15	0.26	0	17,19,21	0.47	0
5	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.49	0
5	NAG	A	1413	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	B	1408	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	A	1411	1	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	B	1403	1	14,14,15	0.31	0	17,19,21	0.51	0
5	NAG	A	1403	1	14,14,15	0.30	0	17,19,21	0.49	0
5	NAG	C	1406	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	B	1409	1	14,14,15	0.29	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	1402	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	A	1408	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	A	1405	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	B	1413	1	14,14,15	0.22	0	17,19,21	0.50	0
5	NAG	B	1412	1	14,14,15	0.24	0	17,19,21	0.54	0
4	FOL	A	1401	-	34,34,34	0.97	1 (2%)	43,47,47	1.29	3 (6%)
5	NAG	B	1414	1	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	C	1412	1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	A	1407	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	B	1406	1	14,14,15	0.26	0	17,19,21	0.47	0
5	NAG	B	1404	1	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	B	1411	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	C	1404	1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	C	1414	1	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	B	1410	1	14,14,15	0.32	0	17,19,21	0.50	0
4	FOL	C	1401	-	34,34,34	0.96	1 (2%)	43,47,47	1.24	3 (6%)
5	NAG	A	1402	1	14,14,15	0.63	1 (7%)	17,19,21	1.06	2 (11%)
5	NAG	C	1403	1	14,14,15	0.25	0	17,19,21	0.50	0
5	NAG	C	1410	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	C	1413	1	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	C	1411	1	14,14,15	0.25	0	17,19,21	0.56	0
4	FOL	B	1401	-	34,34,34	0.99	1 (2%)	43,47,47	1.30	3 (6%)
5	NAG	A	1414	1	14,14,15	0.25	0	17,19,21	0.51	0
5	NAG	C	1402	1	14,14,15	0.22	0	17,19,21	0.46	0
5	NAG	C	1408	1	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	A	1410	1	14,14,15	0.32	0	17,19,21	0.49	0
5	NAG	B	1405	1	14,14,15	0.37	0	17,19,21	0.62	0
5	NAG	A	1409	1	14,14,15	0.33	0	17,19,21	0.44	0
5	NAG	A	1404	1	14,14,15	0.25	0	17,19,21	0.53	0
5	NAG	C	1409	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	A	1412	1	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	C	1405	1	14,14,15	0.30	0	17,19,21	0.52	0
5	NAG	C	1407	1	14,14,15	0.26	0	17,19,21	0.46	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
5	NAG	B	1407	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1411	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1412	1	-	2/6/23/26	0/1/1/1
4	FOL	A	1401	-	-	2/22/22/22	0/3/3/3
5	NAG	B	1414	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1412	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1411	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1414	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
4	FOL	C	1401	-	-	6/22/22/22	0/3/3/3
5	NAG	A	1402	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1411	1	-	2/6/23/26	0/1/1/1
4	FOL	B	1401	-	-	4/22/22/22	0/3/3/3
5	NAG	A	1414	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1409	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1412	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1401	FOL	C8A-N1	-3.27	1.33	1.38
4	A	1401	FOL	C8A-N1	-3.19	1.34	1.38
4	C	1401	FOL	C8A-N1	-3.10	1.34	1.38
5	A	1402	NAG	C1-C2	2.03	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1401	FOL	N1-C8A-N8	4.17	122.60	116.38
4	A	1401	FOL	N1-C8A-N8	4.02	122.38	116.38
4	B	1401	FOL	N1-C8A-N8	3.89	122.18	116.38
4	B	1401	FOL	C8A-C4A-C4	-3.73	117.14	119.56
4	A	1401	FOL	C8A-C4A-C4	-3.71	117.15	119.56
4	C	1401	FOL	C8A-C4A-C4	-3.48	117.30	119.56
4	A	1401	FOL	C4-C4A-N5	2.86	123.05	118.55
4	C	1401	FOL	C4-C4A-N5	2.81	122.98	118.55
5	A	1402	NAG	C1-O5-C5	2.81	115.95	112.19
4	B	1401	FOL	C4-C4A-N5	2.76	122.90	118.55
5	A	1402	NAG	C2-N2-C7	2.55	126.32	122.90

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1404	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	B	1413	NAG	O5-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
5	B	1407	NAG	O5-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1403	NAG	O5-C5-C6-O6
5	B	1414	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	C	1410	NAG	O5-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	C	1409	NAG	C4-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	C	1406	NAG	O5-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	B	1413	NAG	C4-C5-C6-O6
5	A	1413	NAG	O5-C5-C6-O6
5	B	1410	NAG	O5-C5-C6-O6
5	C	1405	NAG	O5-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	A	1406	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
5	B	1411	NAG	O5-C5-C6-O6
4	B	1401	FOL	C13-C14-N10-C9
5	C	1408	NAG	O5-C5-C6-O6
5	A	1404	NAG	C4-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	A	1406	NAG	C4-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	B	1411	NAG	C4-C5-C6-O6
5	C	1406	NAG	C4-C5-C6-O6
5	C	1412	NAG	O5-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	B	1407	NAG	C4-C5-C6-O6
5	B	1409	NAG	C4-C5-C6-O6
5	B	1410	NAG	C4-C5-C6-O6
5	A	1411	NAG	O5-C5-C6-O6
5	B	1414	NAG	C4-C5-C6-O6
5	C	1410	NAG	C4-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	A	1410	NAG	O5-C5-C6-O6
5	A	1413	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	1404	NAG	C4-C5-C6-O6
5	C	1405	NAG	C4-C5-C6-O6
5	A	1409	NAG	C8-C7-N2-C2
5	A	1409	NAG	O7-C7-N2-C2
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	B	1409	NAG	C8-C7-N2-C2
5	B	1409	NAG	O7-C7-N2-C2
5	C	1405	NAG	C8-C7-N2-C2
5	C	1405	NAG	O7-C7-N2-C2
5	B	1409	NAG	O5-C5-C6-O6
5	B	1412	NAG	O5-C5-C6-O6
5	C	1409	NAG	O5-C5-C6-O6
5	A	1411	NAG	C4-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	A	1410	NAG	C4-C5-C6-O6
4	B	1401	FOL	C15-C14-N10-C9
5	A	1402	NAG	C4-C5-C6-O6
5	B	1412	NAG	C4-C5-C6-O6
5	A	1409	NAG	O5-C5-C6-O6
5	C	1412	NAG	C4-C5-C6-O6
5	C	1413	NAG	O5-C5-C6-O6
5	C	1413	NAG	C4-C5-C6-O6
4	A	1401	FOL	C11-C-N-CA
4	A	1401	FOL	O-C-N-CA
5	A	1414	NAG	C4-C5-C6-O6
5	A	1414	NAG	O5-C5-C6-O6
5	C	1411	NAG	C4-C5-C6-O6
5	C	1411	NAG	O5-C5-C6-O6
5	A	1412	NAG	C4-C5-C6-O6
5	A	1412	NAG	O5-C5-C6-O6
4	C	1401	FOL	CB-CA-CT-O1
4	C	1401	FOL	CB-CA-CT-O2
5	A	1402	NAG	C3-C2-N2-C7
4	C	1401	FOL	C11-C-N-CA
4	C	1401	FOL	O-C-N-CA
4	C	1401	FOL	OE1-CD-CG-CB
4	C	1401	FOL	OE2-CD-CG-CB
4	B	1401	FOL	OE1-CD-CG-CB
5	A	1402	NAG	C1-C2-N2-C7
5	A	1403	NAG	C1-C2-N2-C7
5	B	1403	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	B	1401	FOL	OE2-CD-CG-CB
5	A	1407	NAG	O5-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6

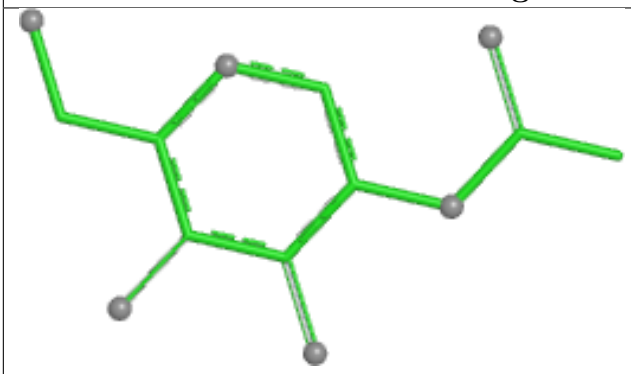
There are no ring outliers.

5 monomers are involved in 6 short contacts:

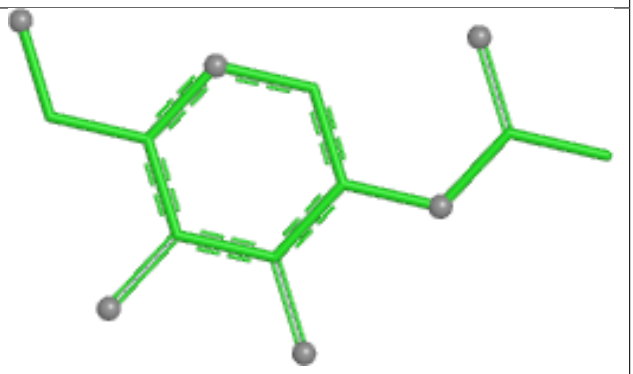
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1404	NAG	1	0
4	C	1401	FOL	2	0
4	B	1401	FOL	1	0
5	A	1410	NAG	1	0
5	B	1405	NAG	1	0

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.

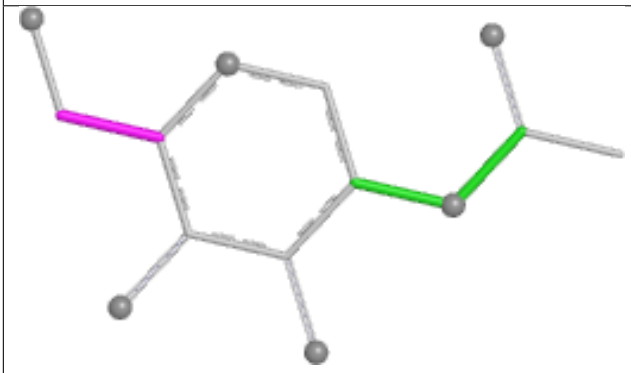
Ligand NAG B 1407



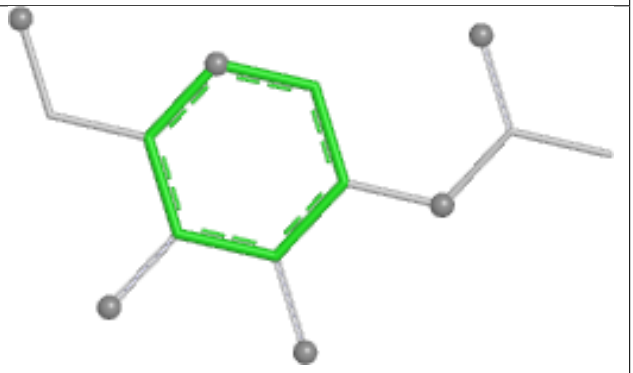
Bond lengths



Bond angles

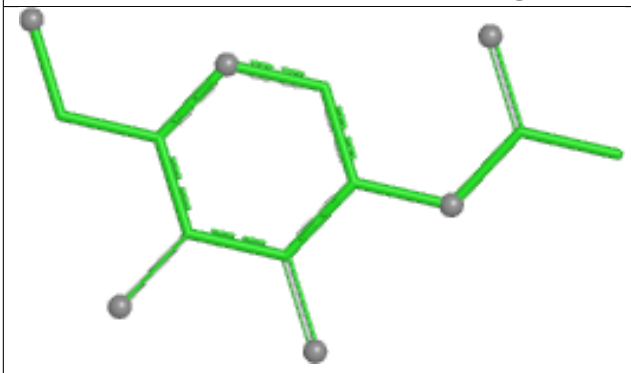


Torsions

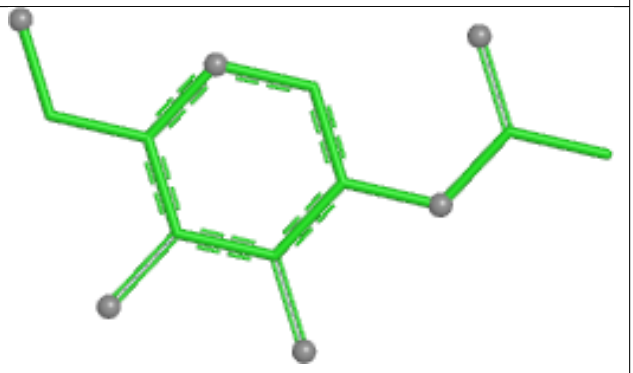


Rings

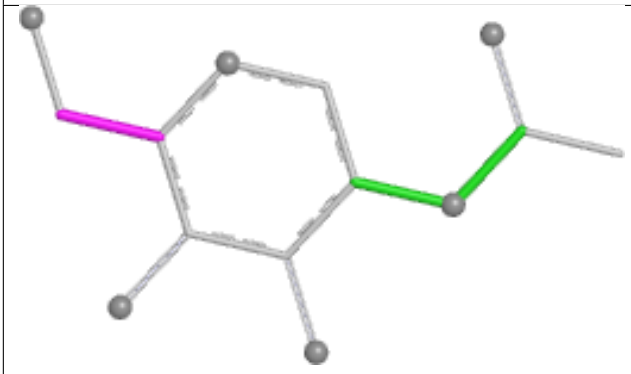
Ligand NAG A 1406



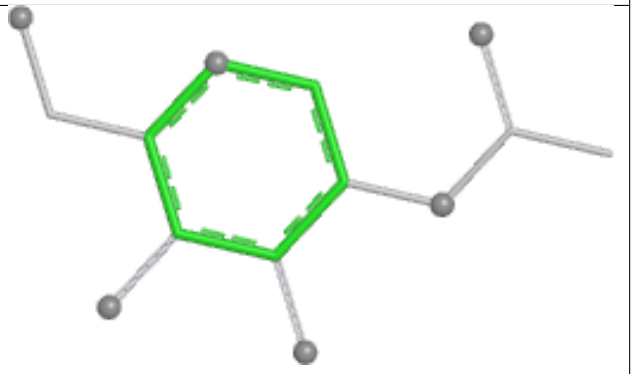
Bond lengths



Bond angles

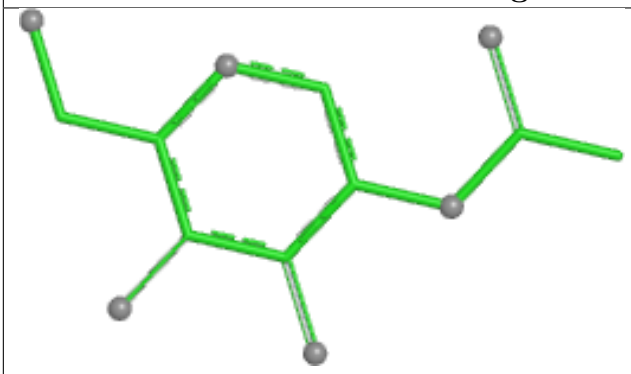


Torsions

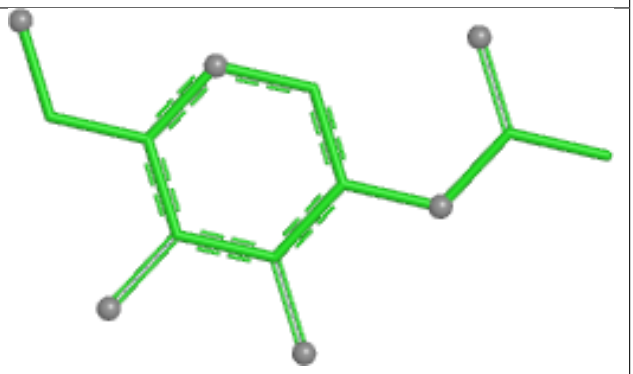


Rings

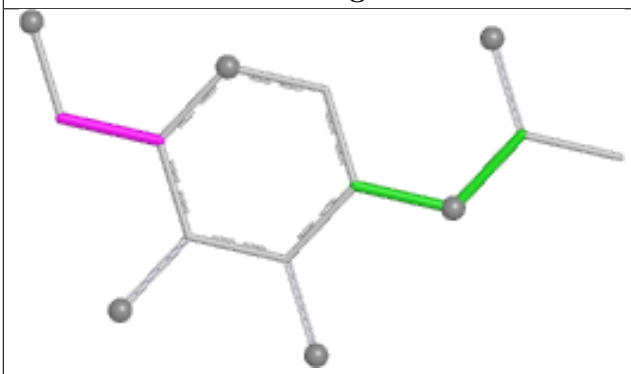
Ligand NAG A 1413



Bond lengths



Bond angles



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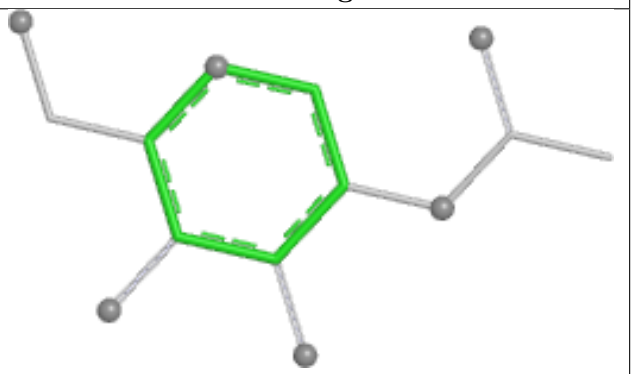
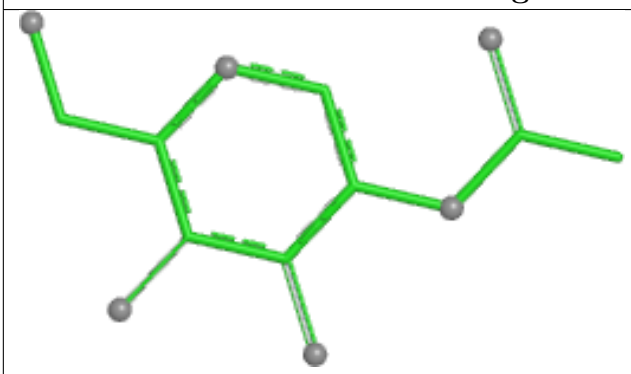


Rings

Ligand NAG B 1408



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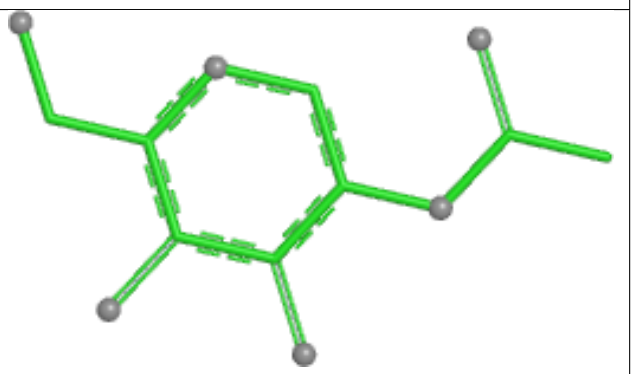

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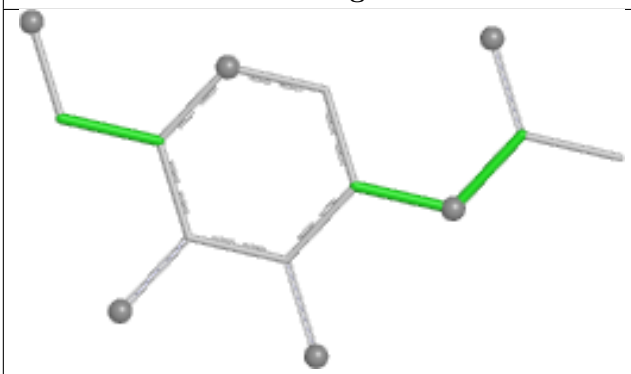

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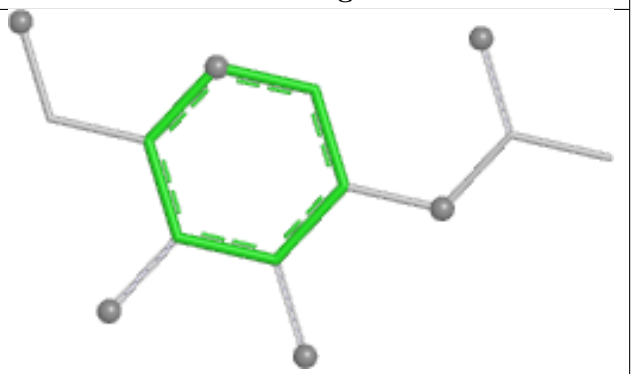
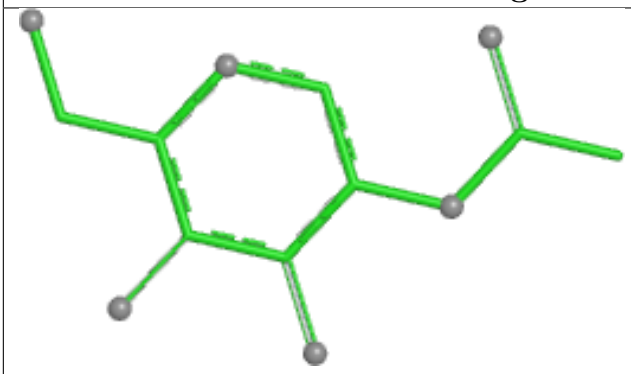


Rings

Ligand NAG A 1411



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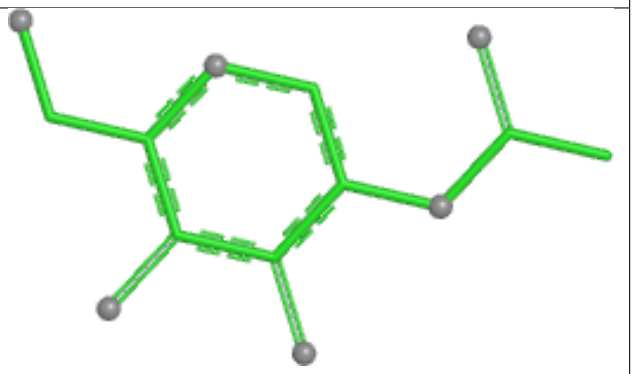

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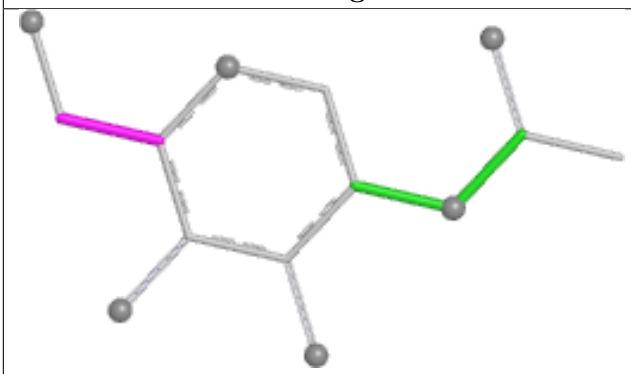

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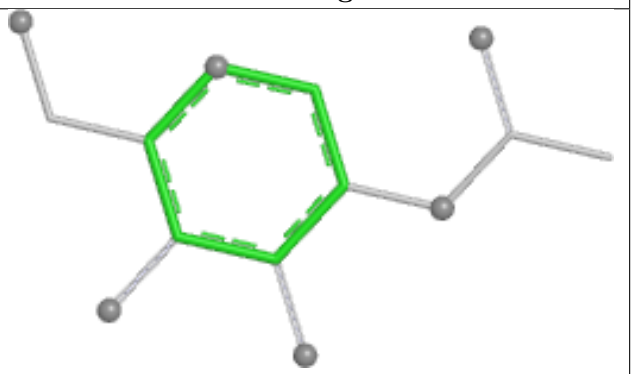
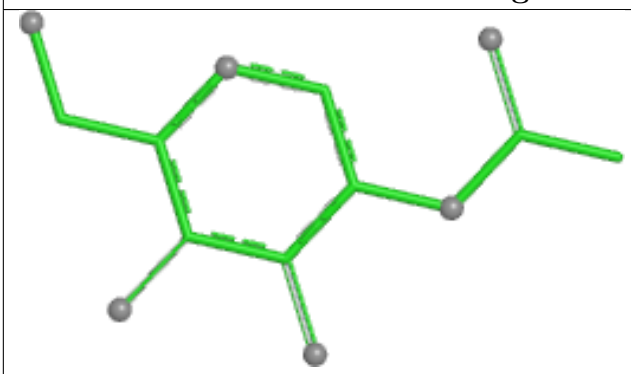


Rings

Ligand NAG B 1403



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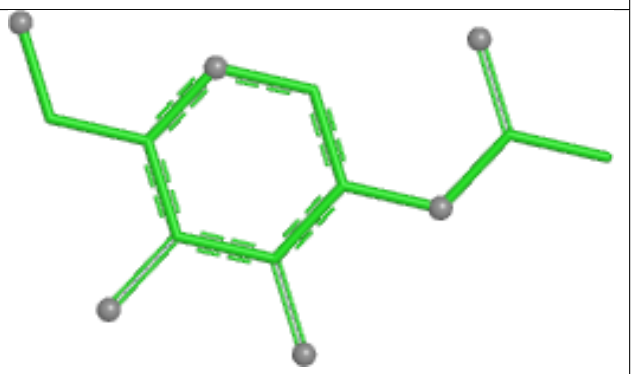

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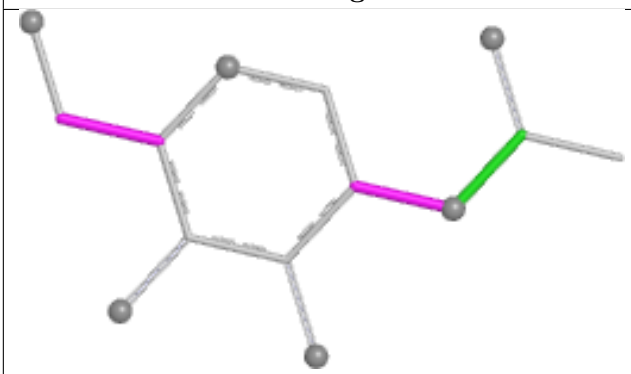

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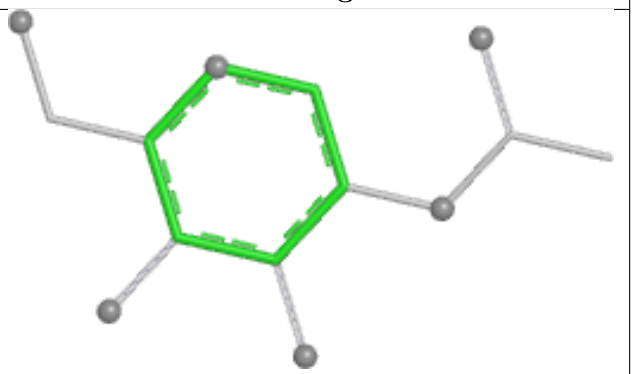
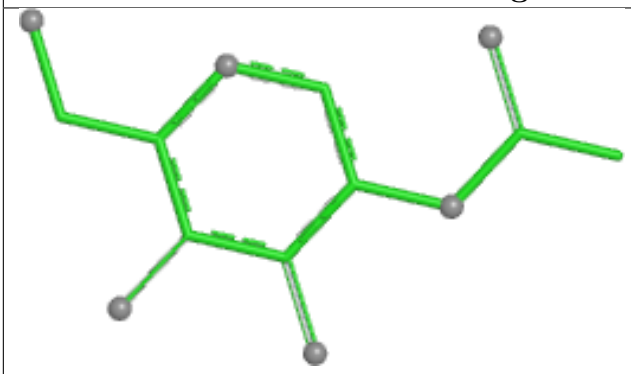


Rings

Ligand NAG A 1403



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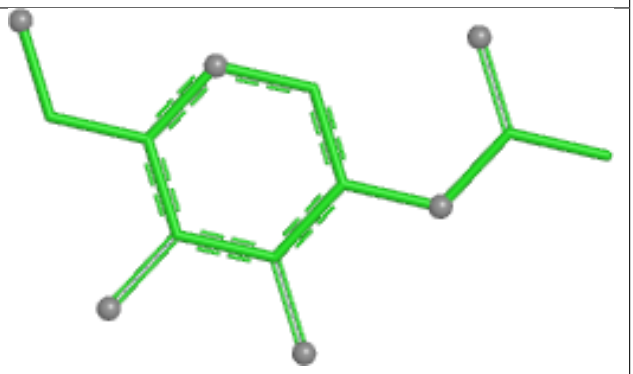

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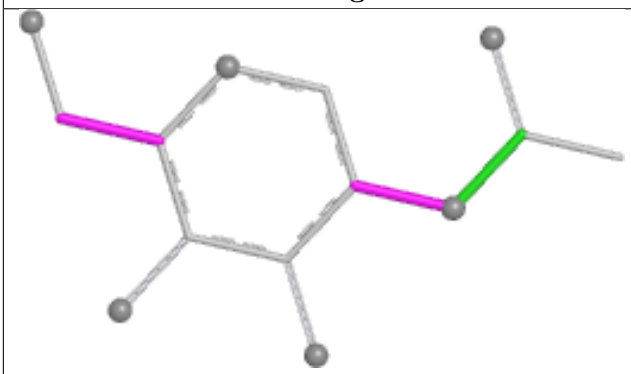

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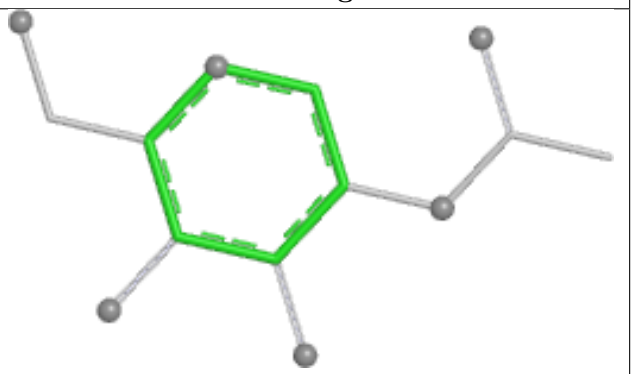
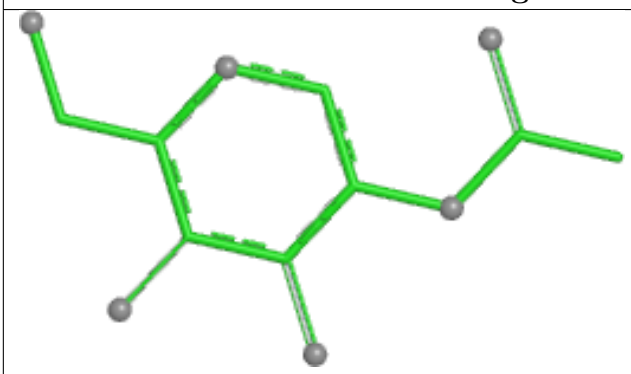


Rings

Ligand NAG C 1406



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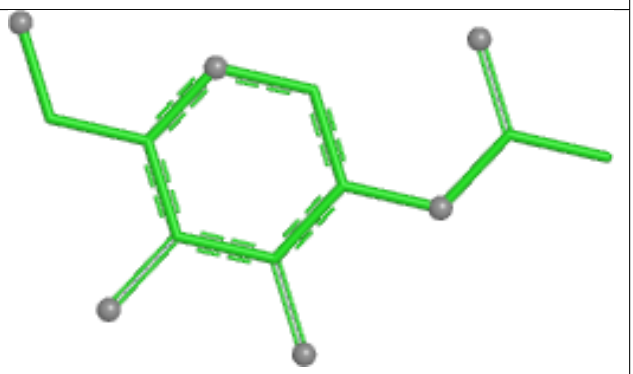

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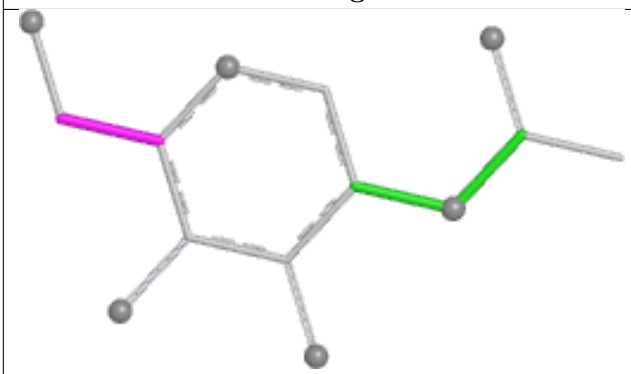

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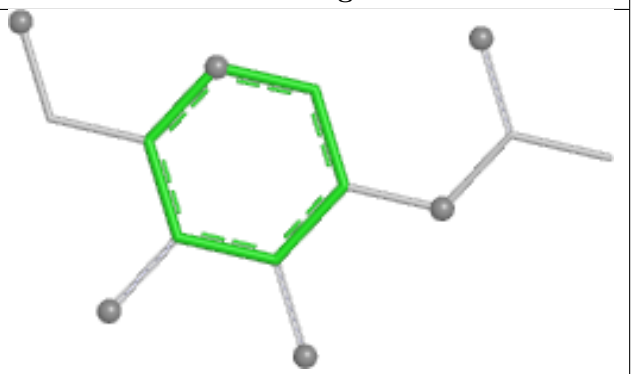
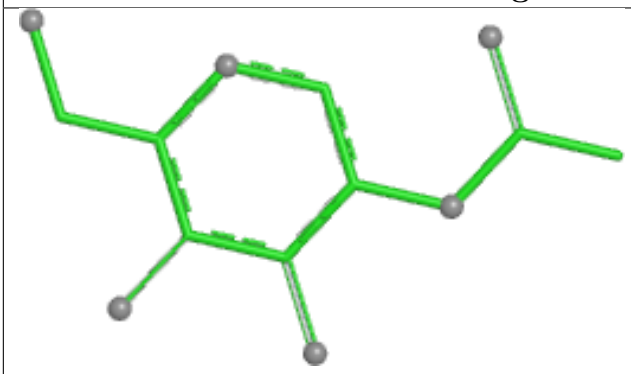


Rings

Ligand NAG B 1409



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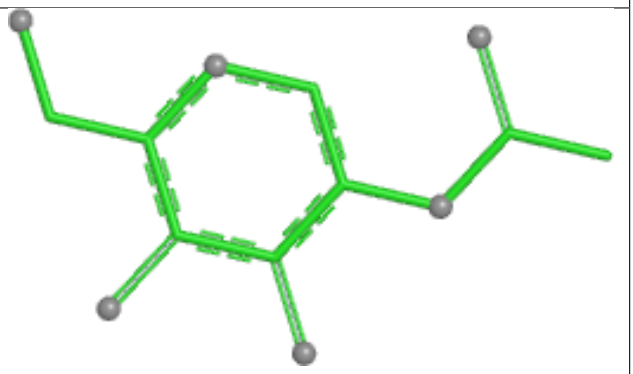
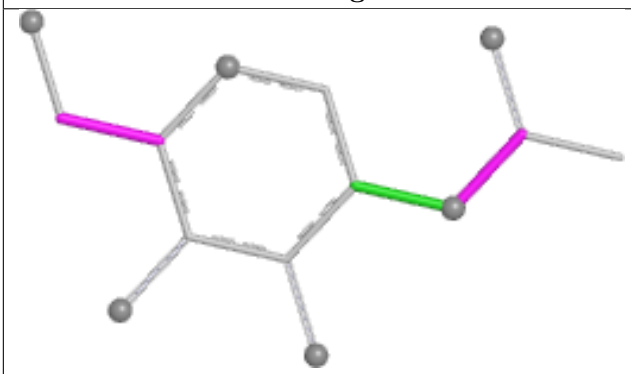


Bond angles



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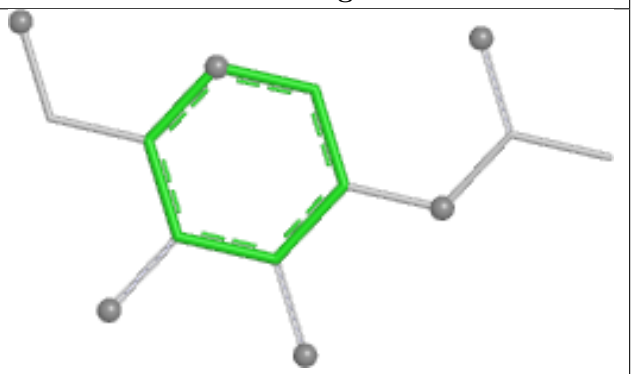
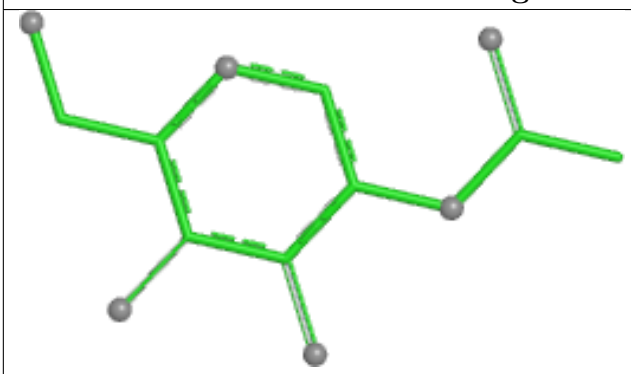


Rings

Ligand NAG B 1402



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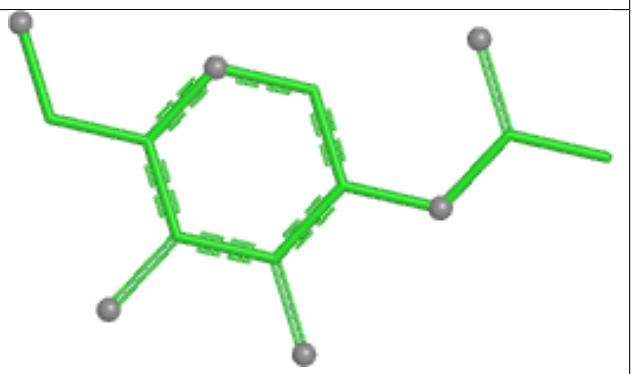

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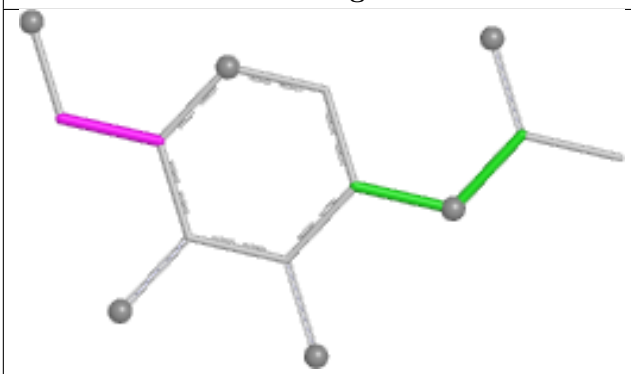

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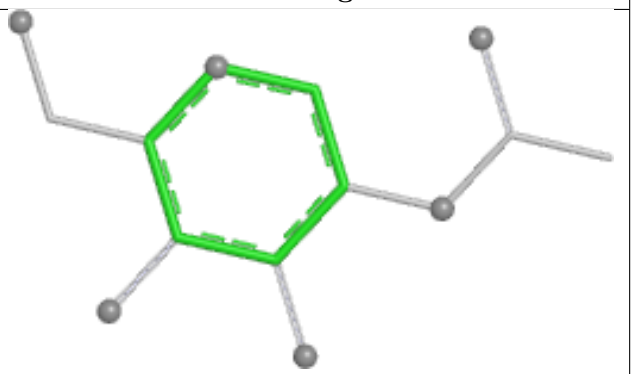
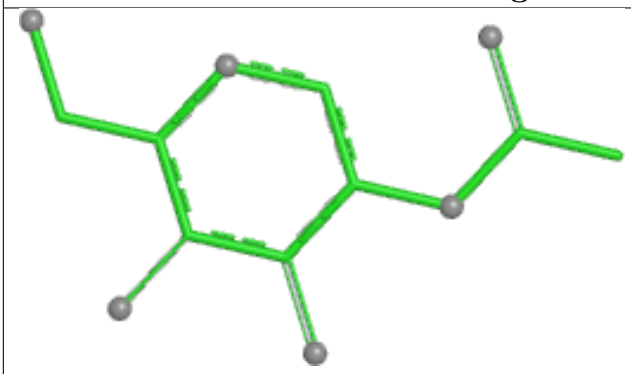


Rings

Ligand NAG A 1408



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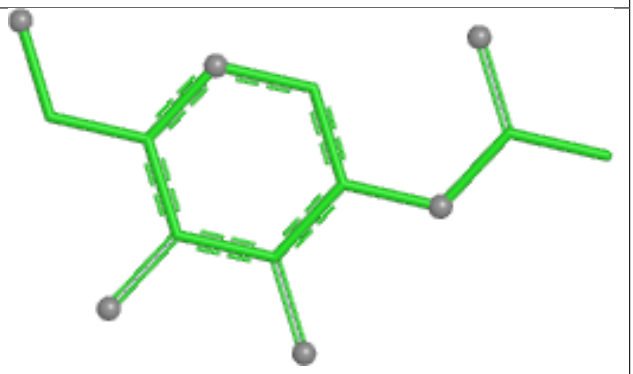

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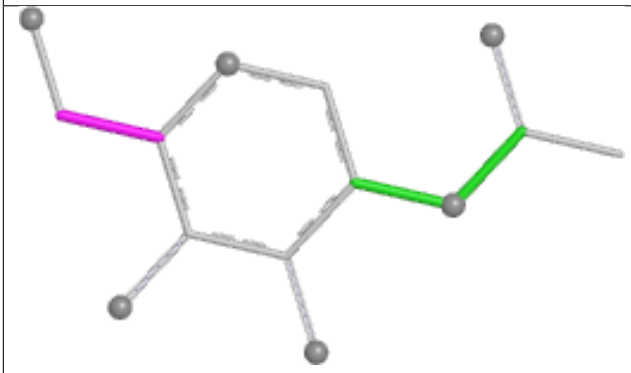

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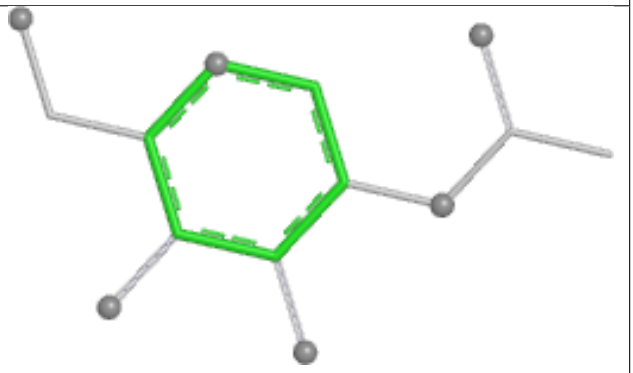
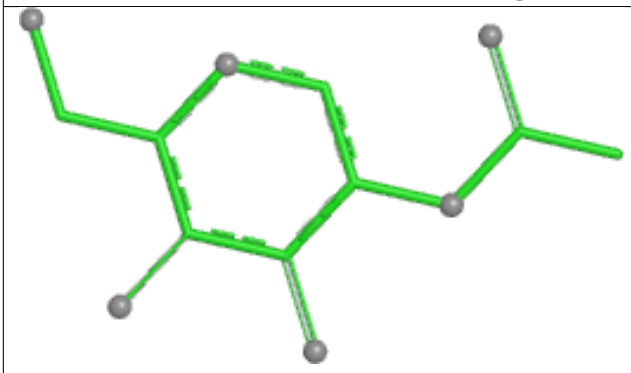


Rings

Ligand NAG A 1405



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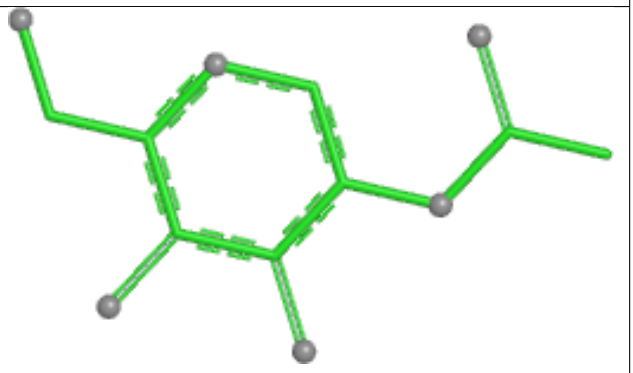

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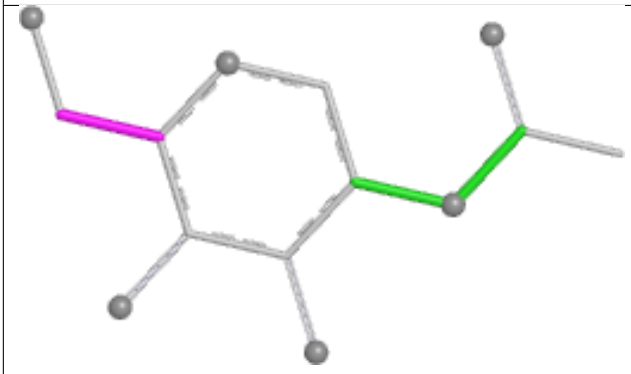

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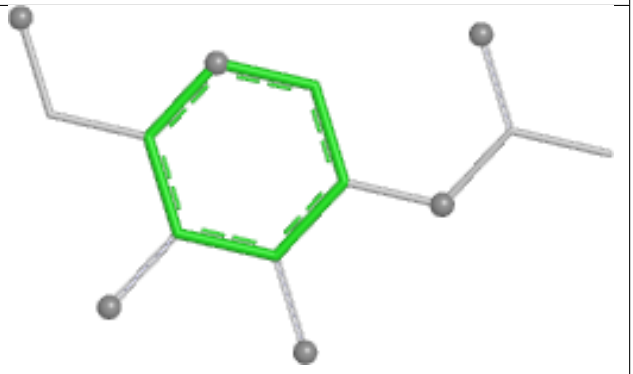
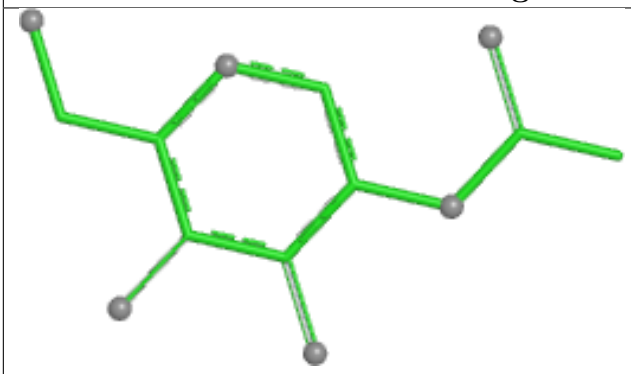


Rings

Ligand NAG B 1413



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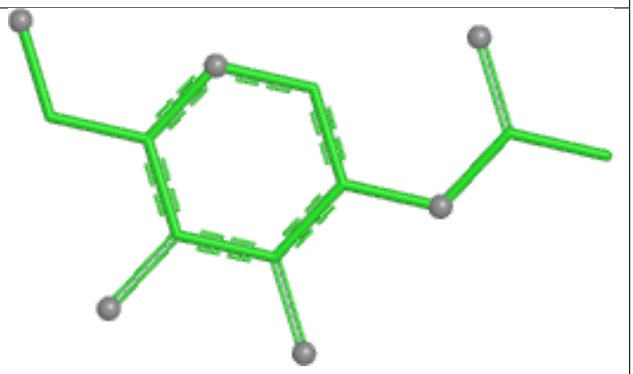
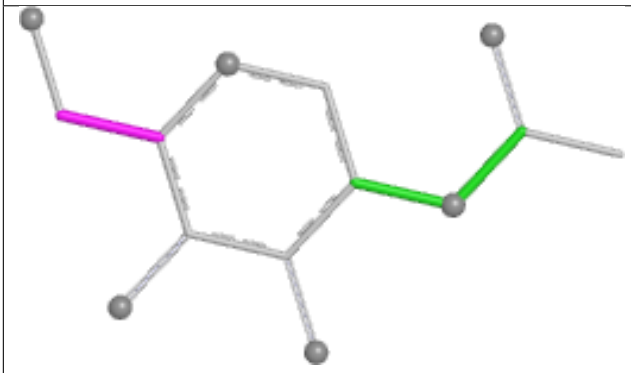


Bond angles



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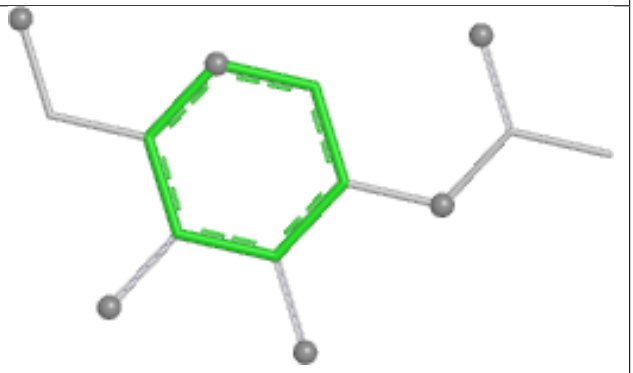
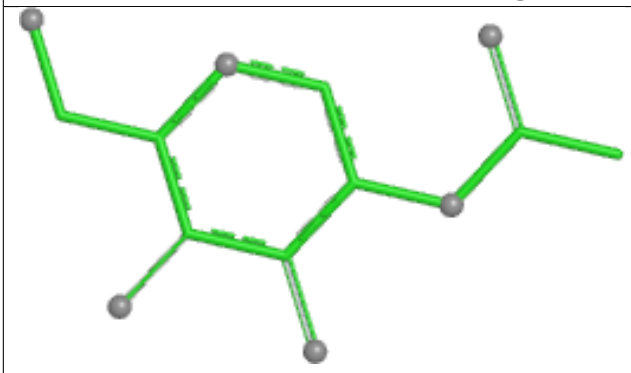
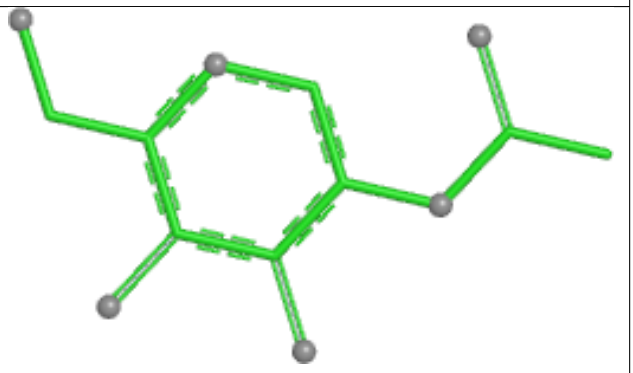


Rings

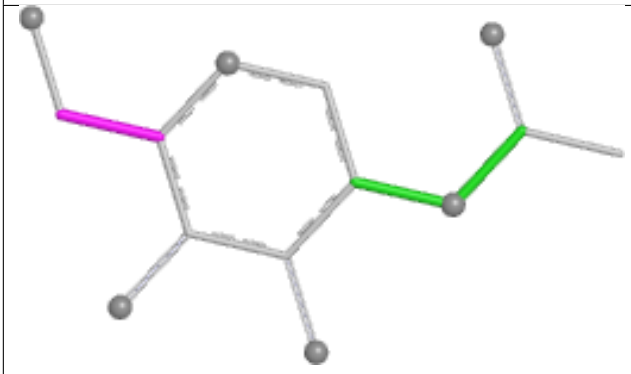
Ligand NAG B 1412



Bond lengths



Bond angles



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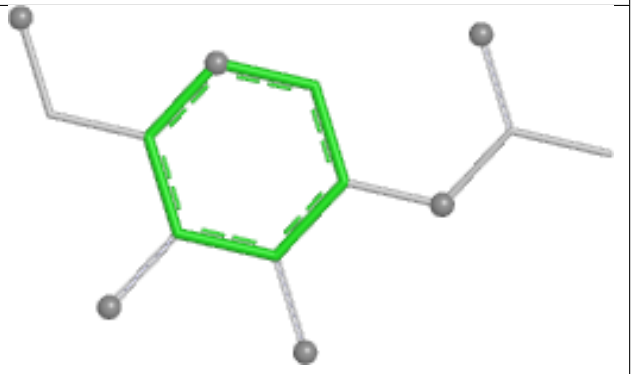
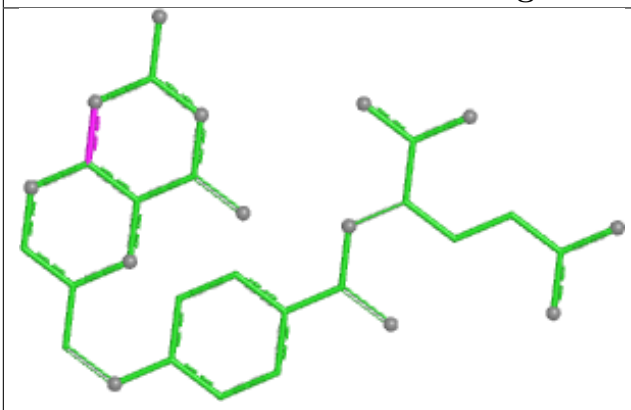


Rings

Ligand FOL A 1401



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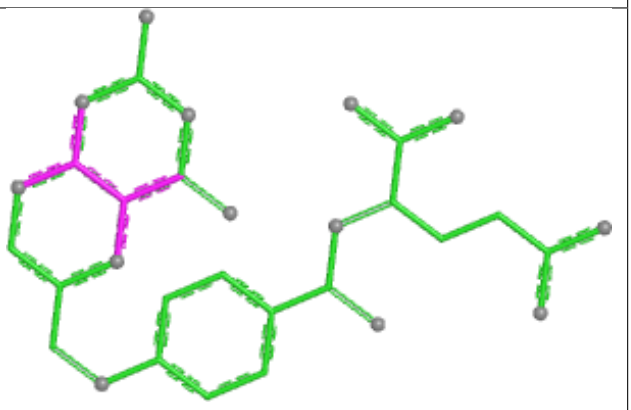
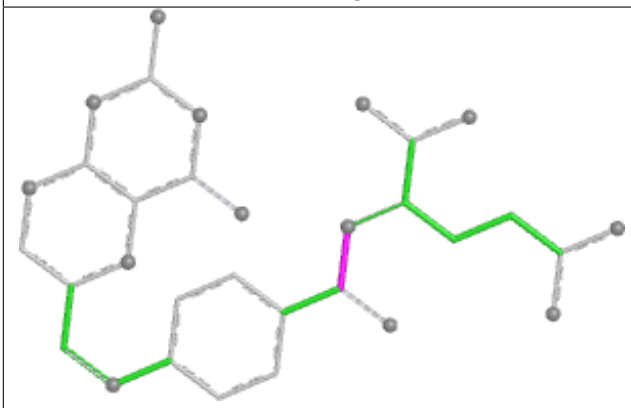
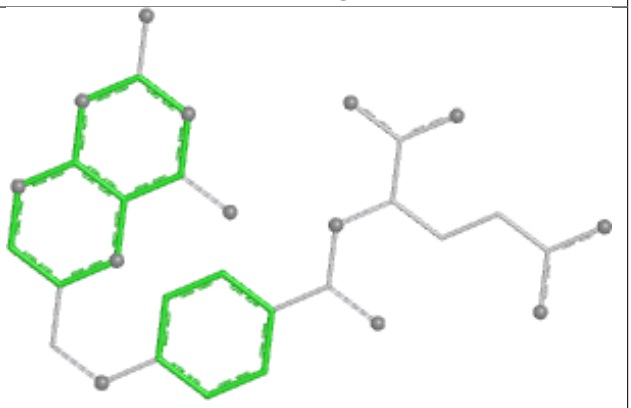


Bond angles

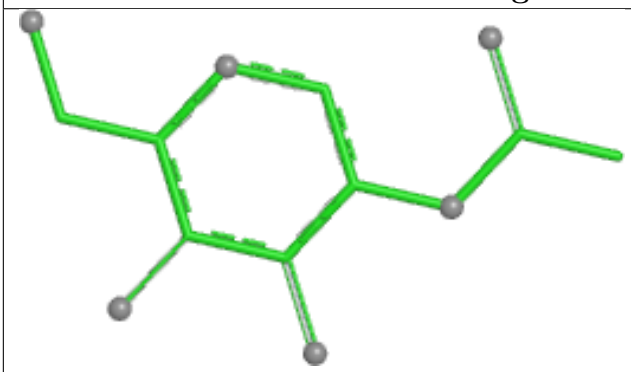


Torsions



Rings

Ligand NAG B 1414



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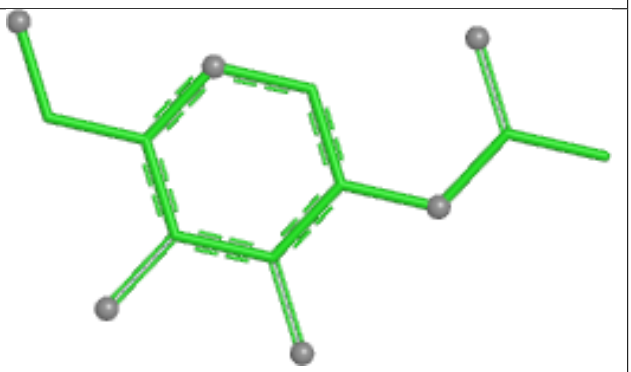

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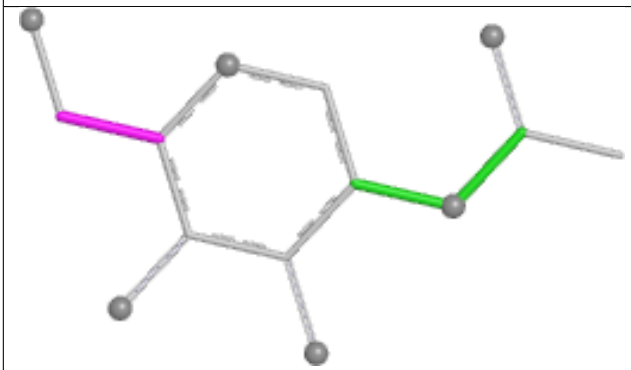

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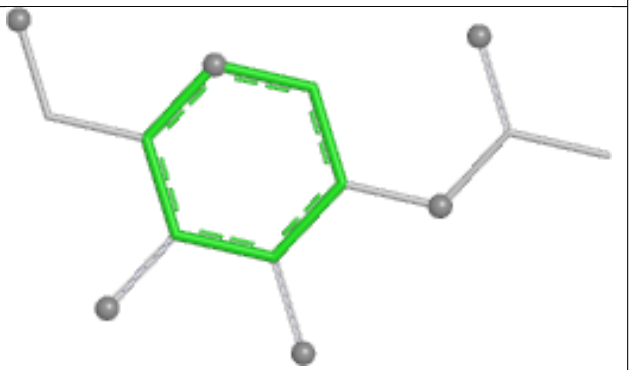
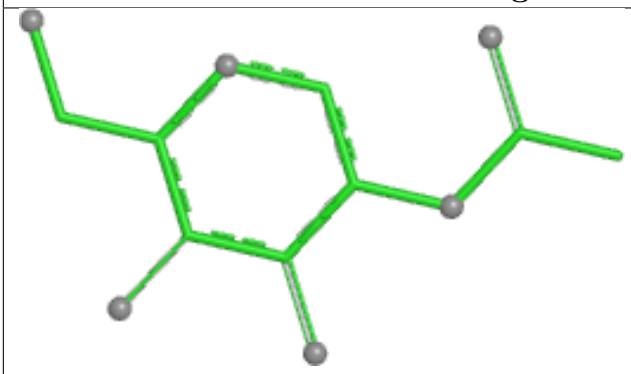


Rings

Ligand NAG C 1412



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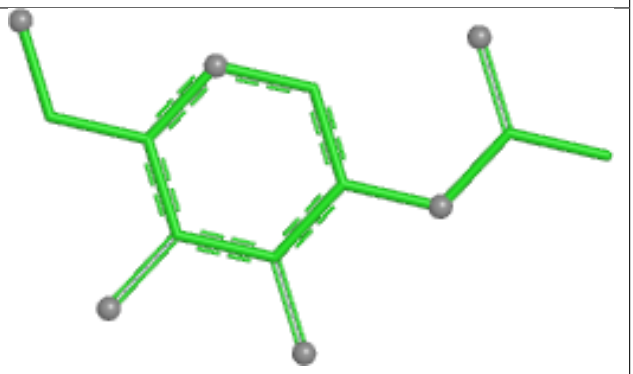

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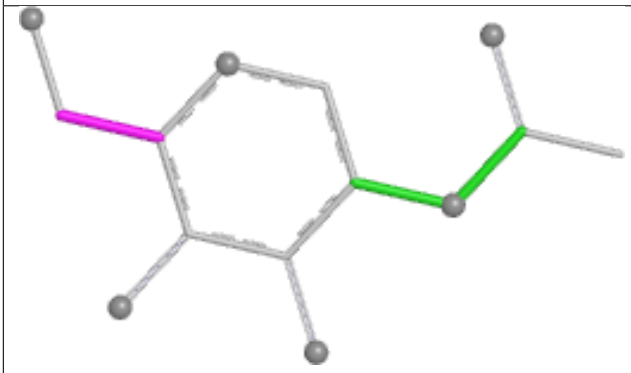

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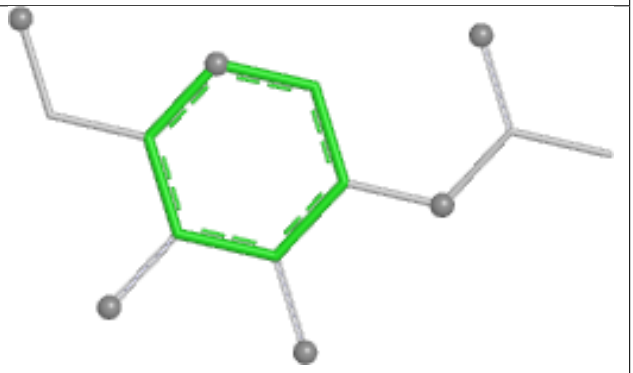
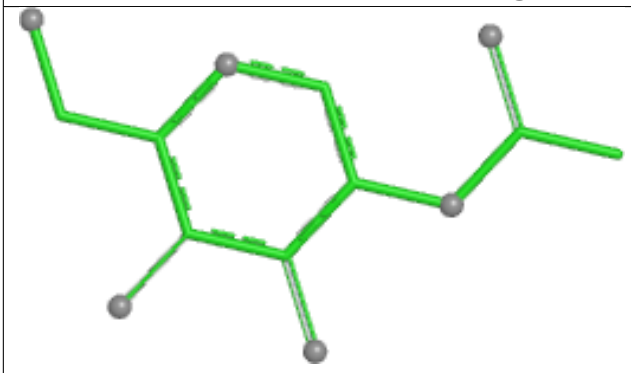


Rings

Ligand NAG A 1407



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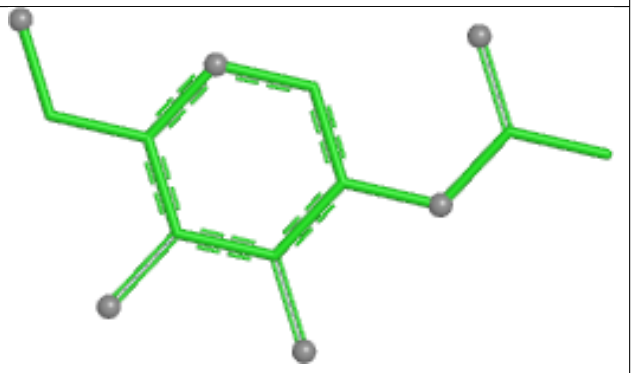

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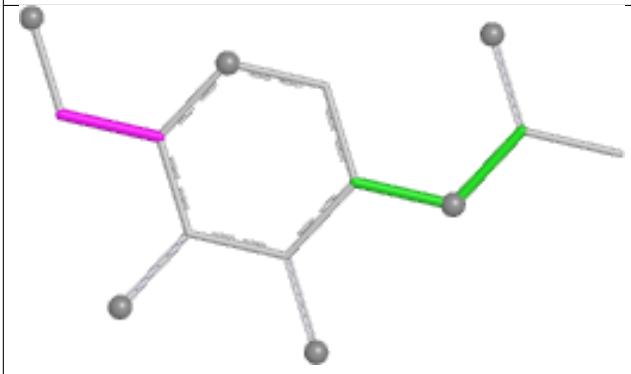

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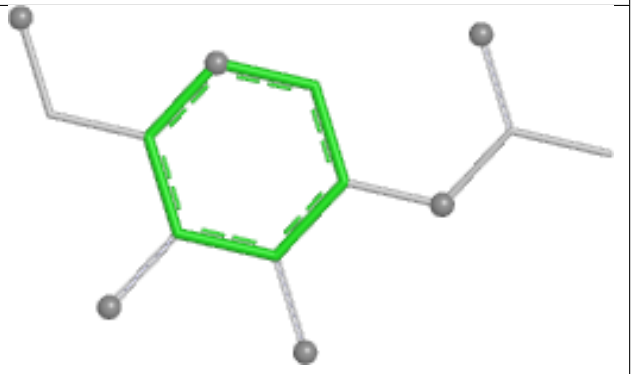
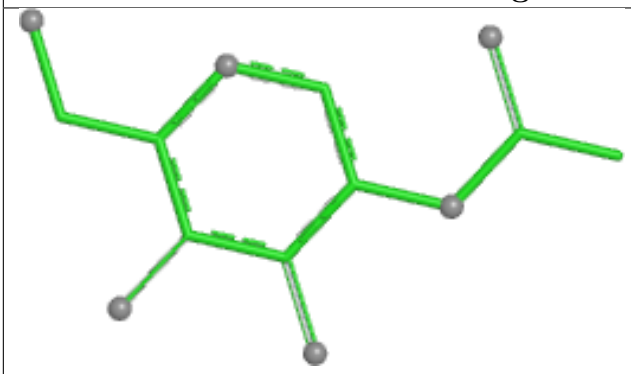


Rings

Ligand NAG B 1406



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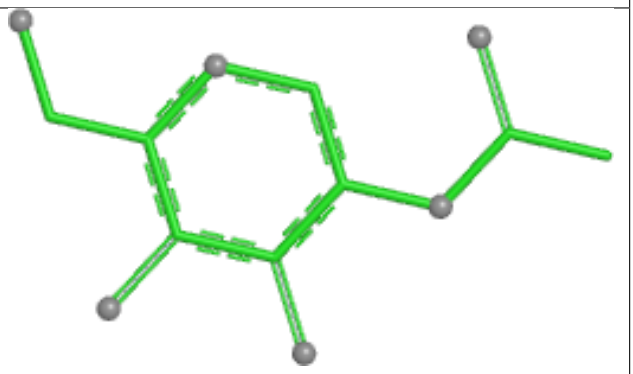

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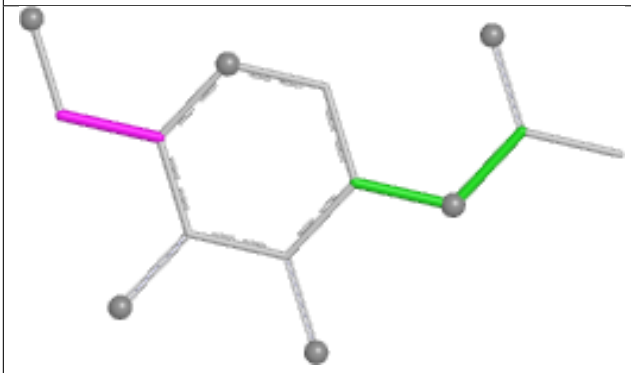

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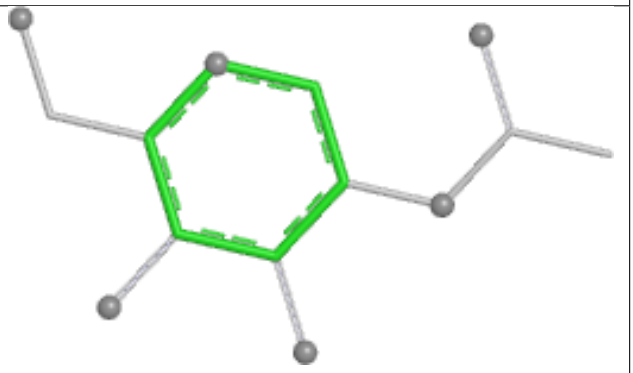
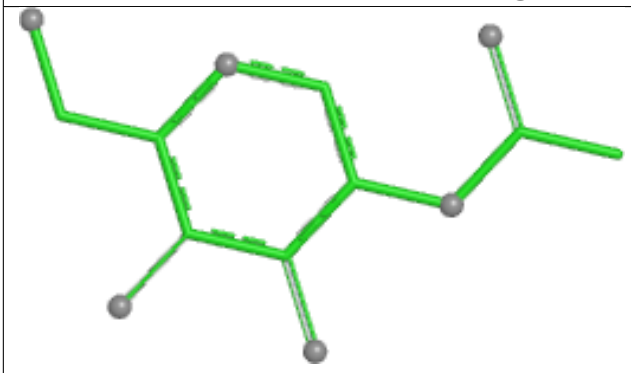


Rings

Ligand NAG B 1404



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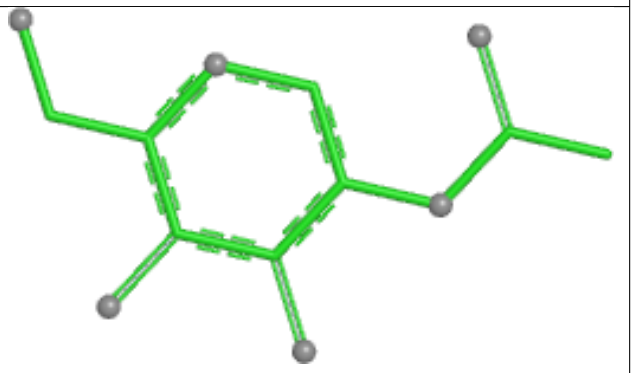

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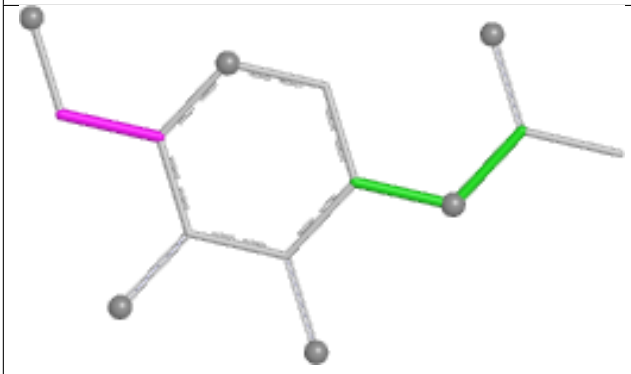

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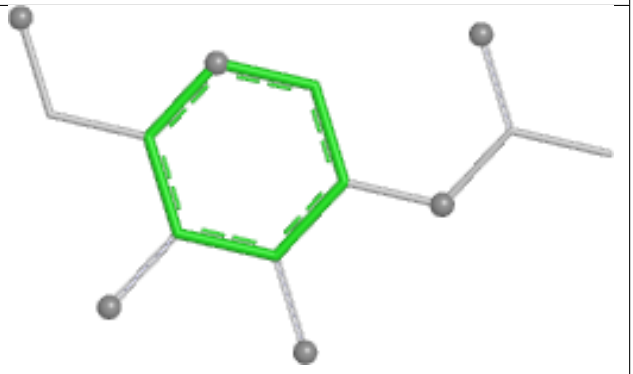

Rings

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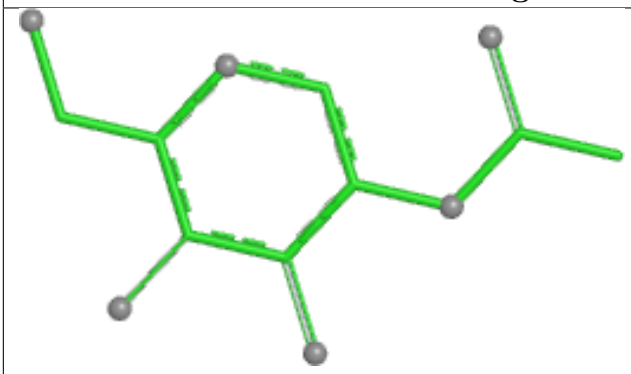

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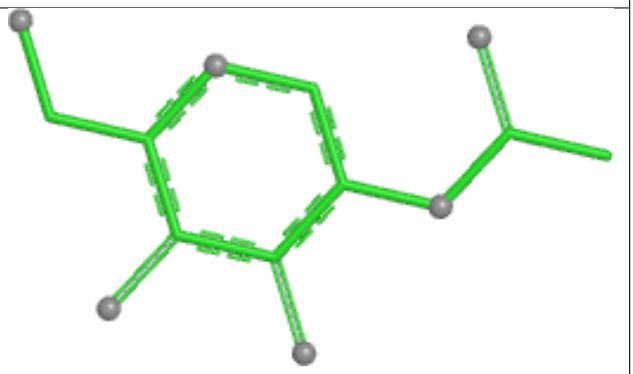

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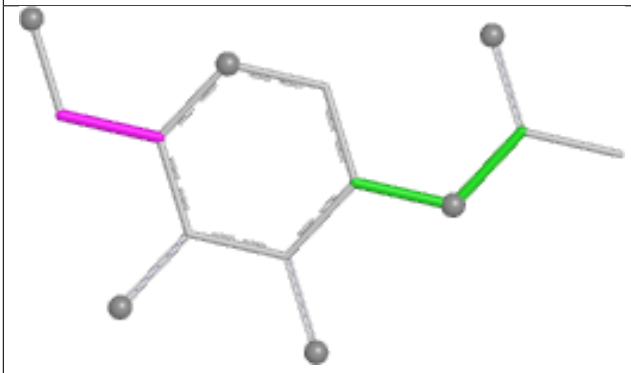

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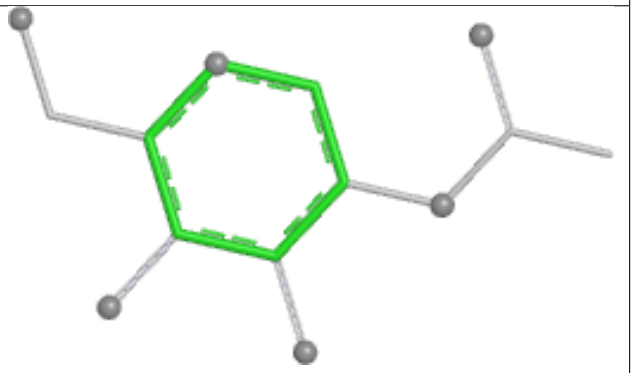
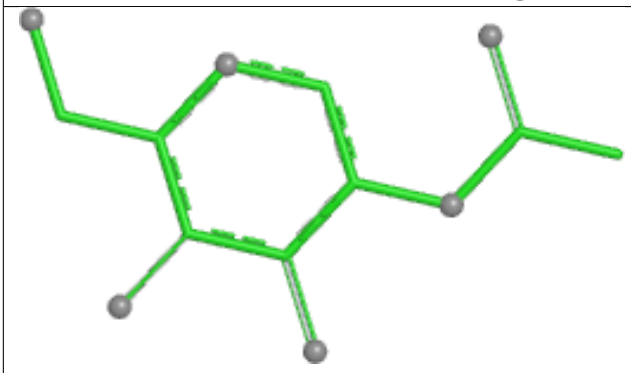


Rings

Ligand NAG C 1404



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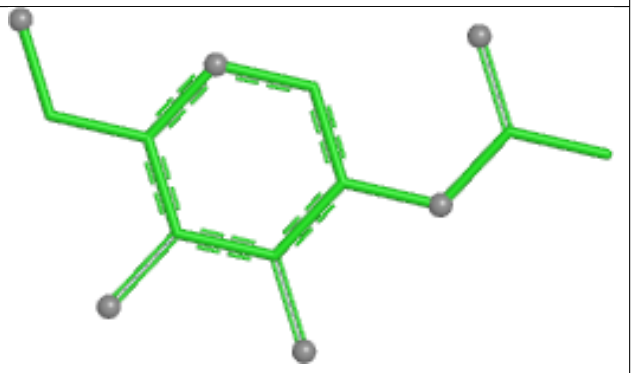

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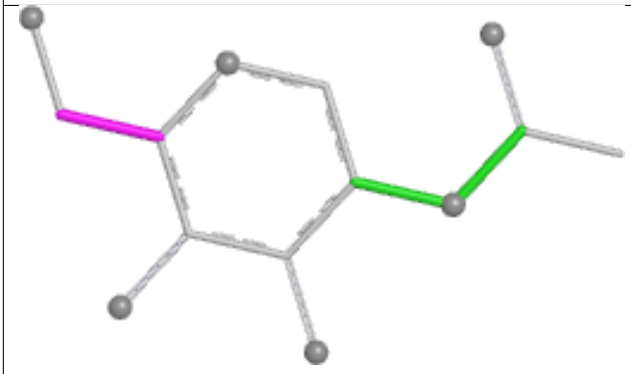

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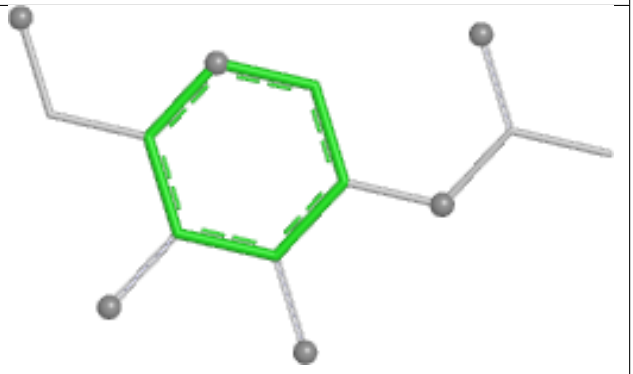

Rings

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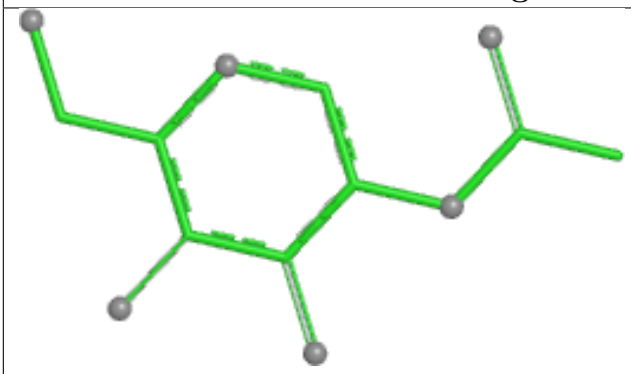

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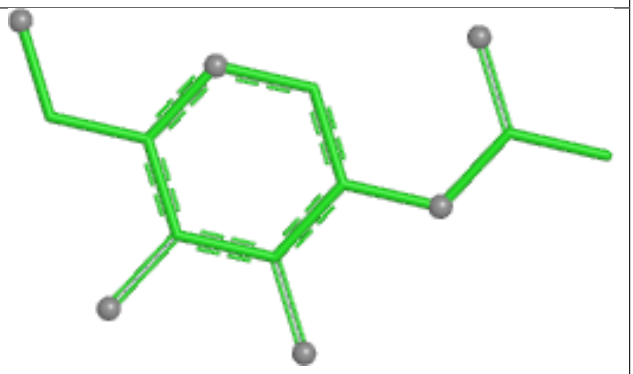
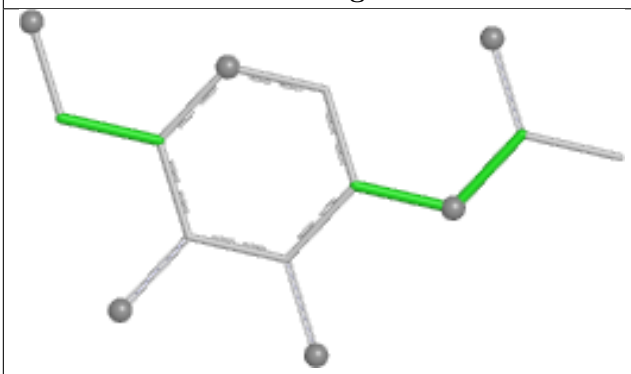


Bond angles



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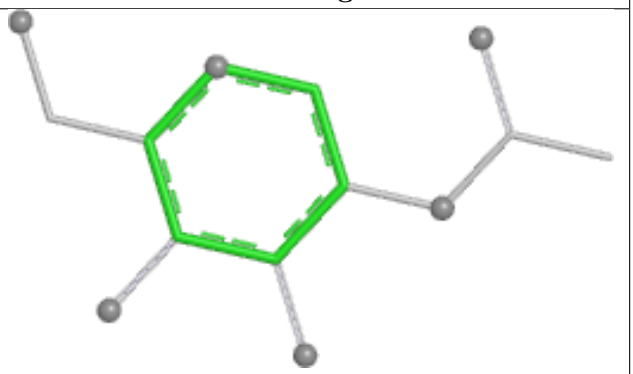
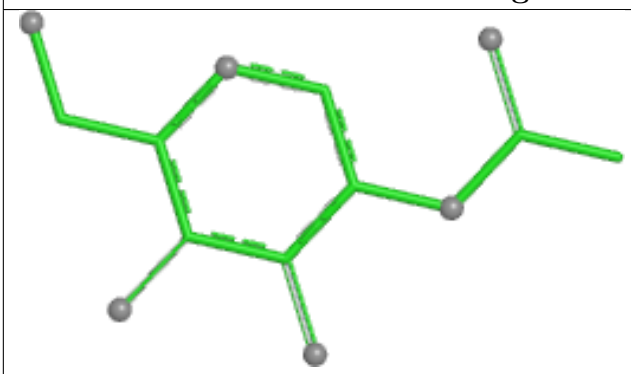


Rings

Ligand NAG B 1410



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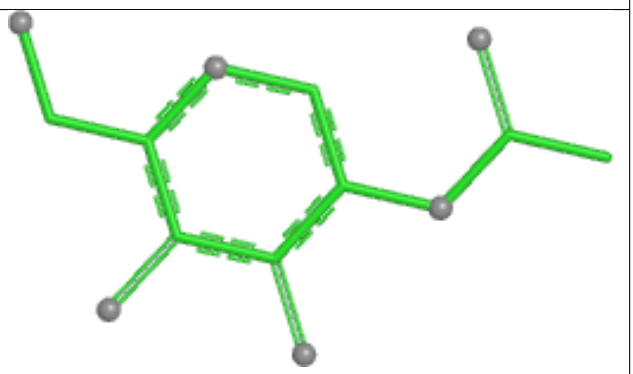

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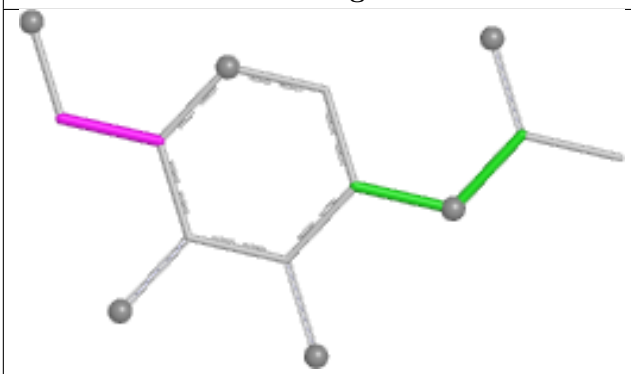

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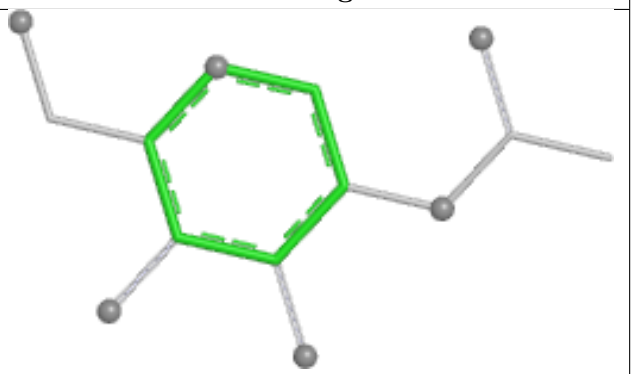
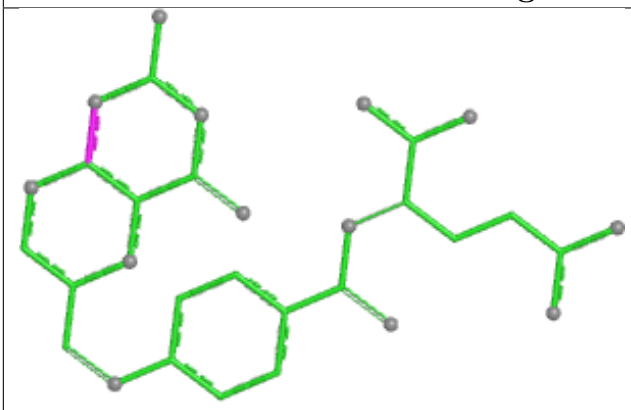


Rings

Ligand FOL C 1401



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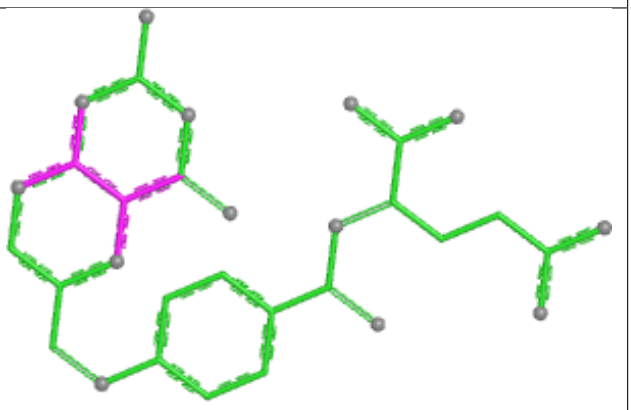
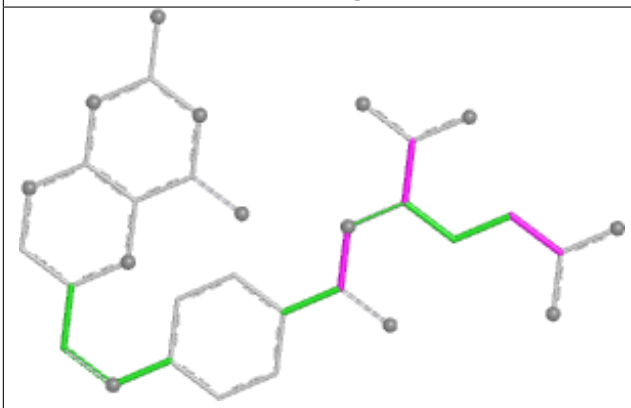


Bond angles



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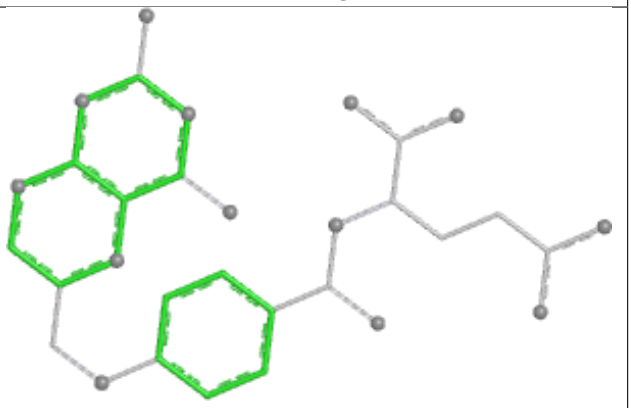
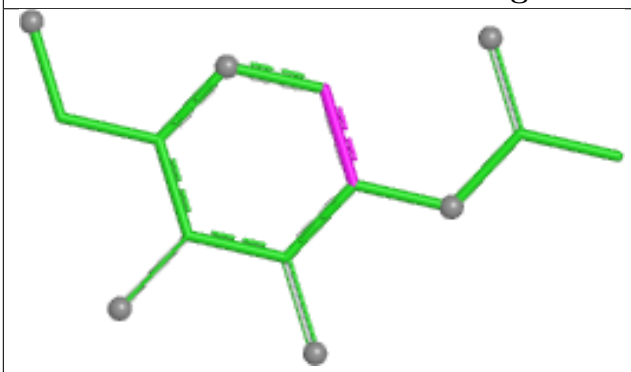


Rings

Ligand NAG A 1402



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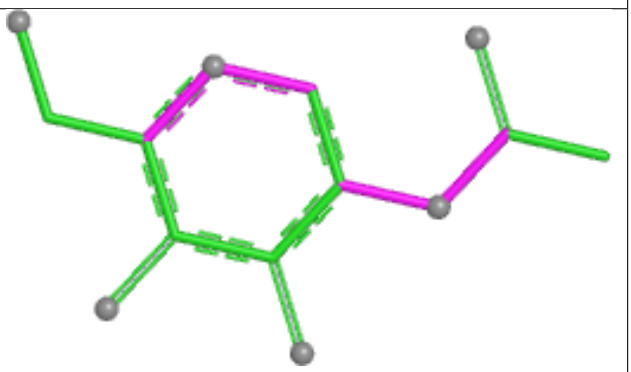
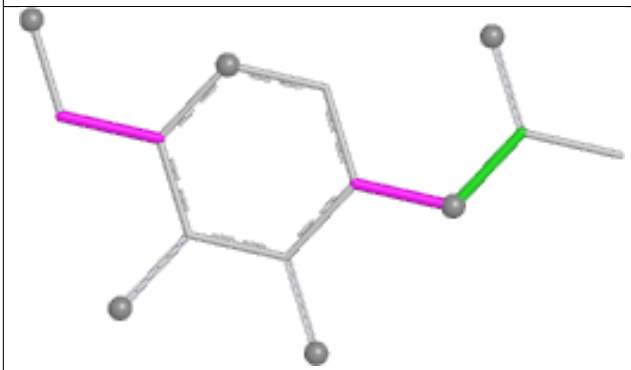


Bond angles



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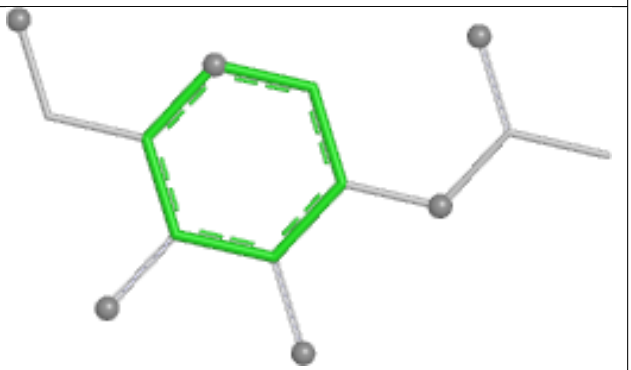
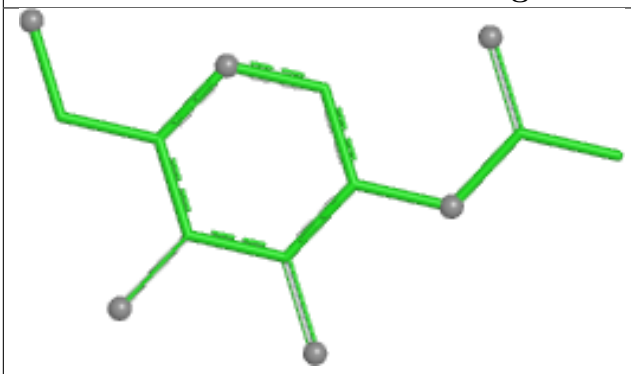
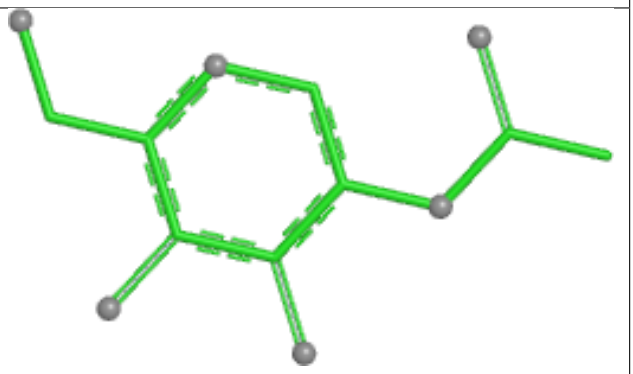


Rings

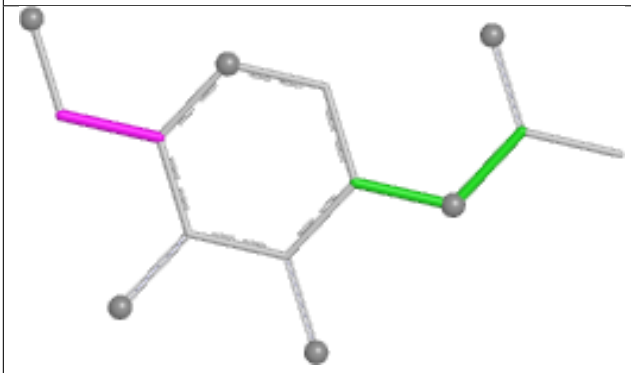
Ligand NAG C 1403



Bond lengths



Bond angles



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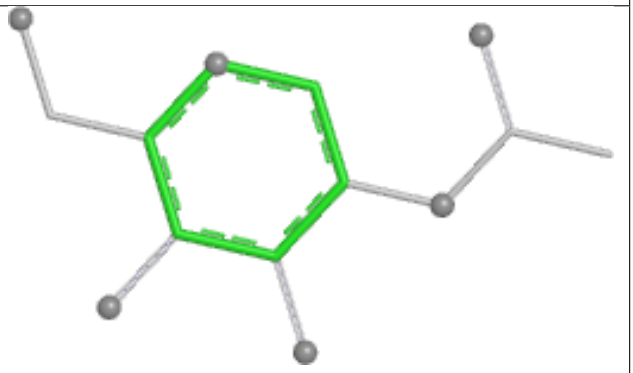
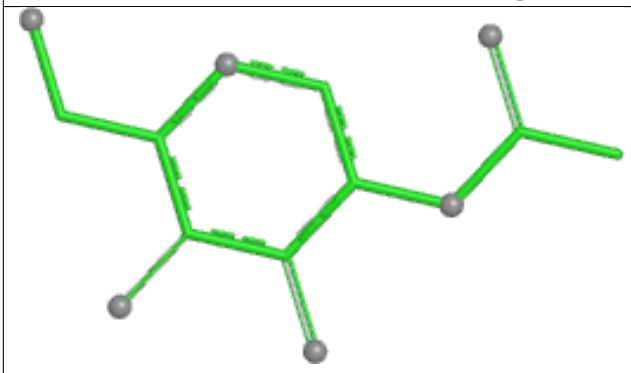
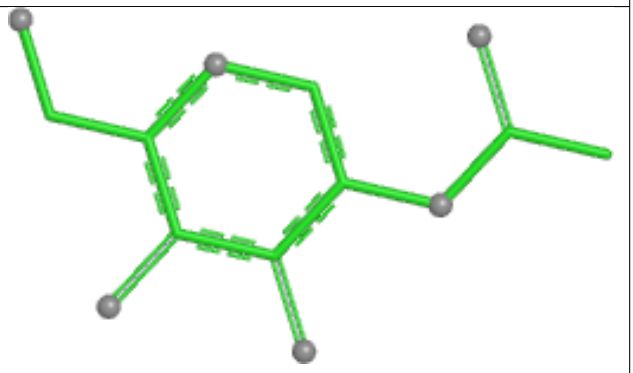


Rings

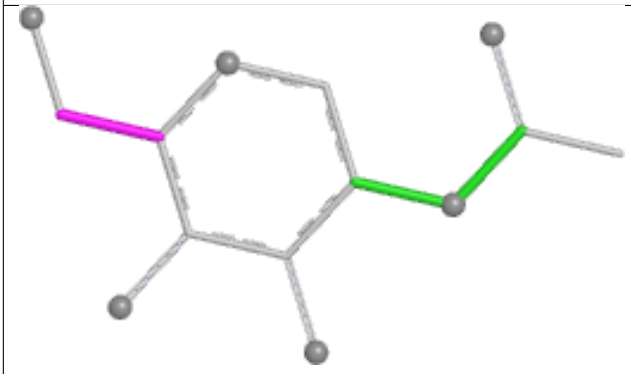
Ligand NAG C 1410



Bond lengths



Bond angles



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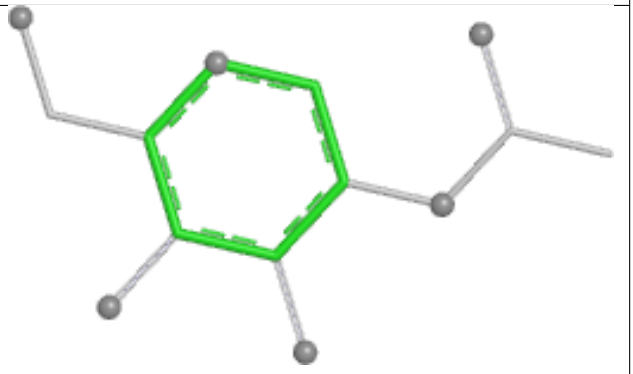
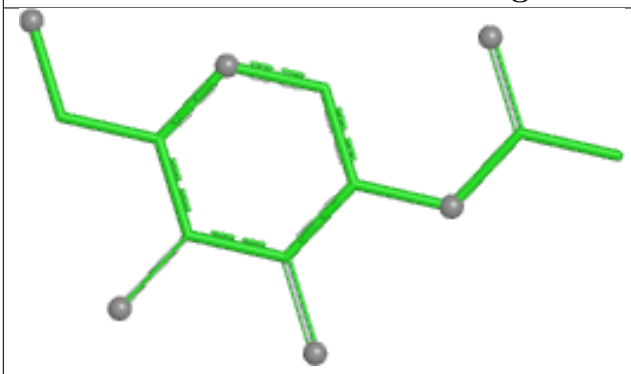
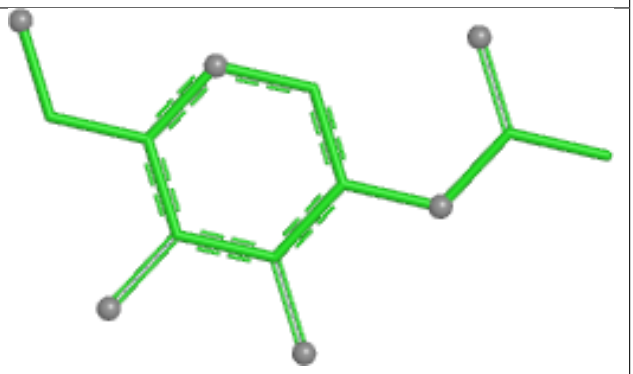


Rings

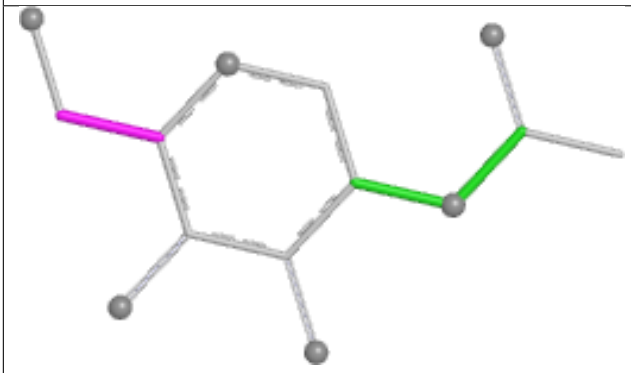
Ligand NAG C 1413



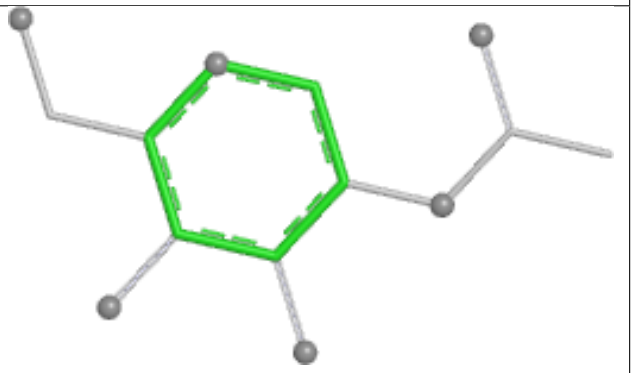
Bond lengths



Bond angles

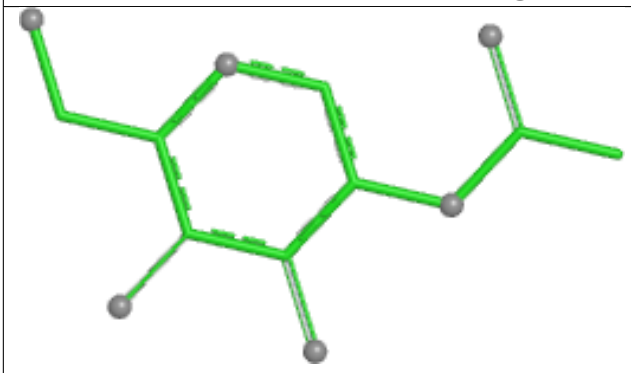


Torsions



Rings

Ligand NAG C 1411



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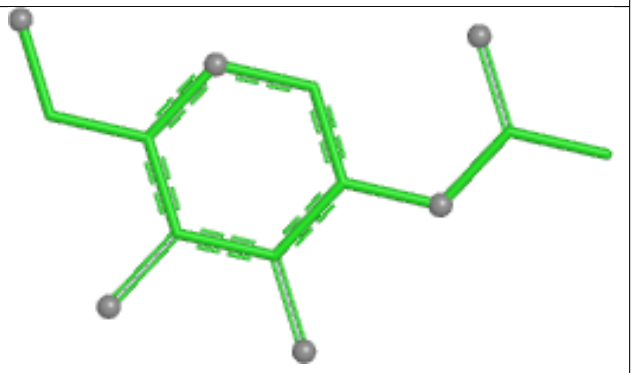
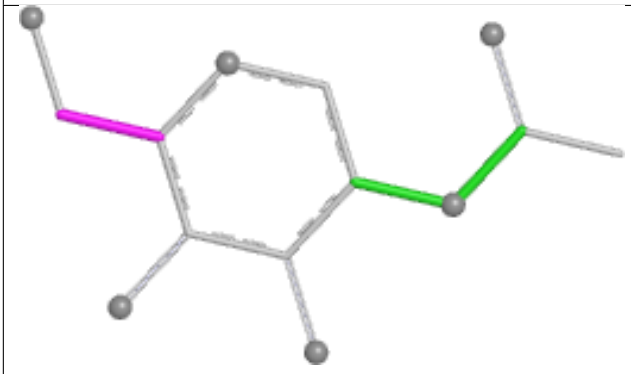


Bond angles



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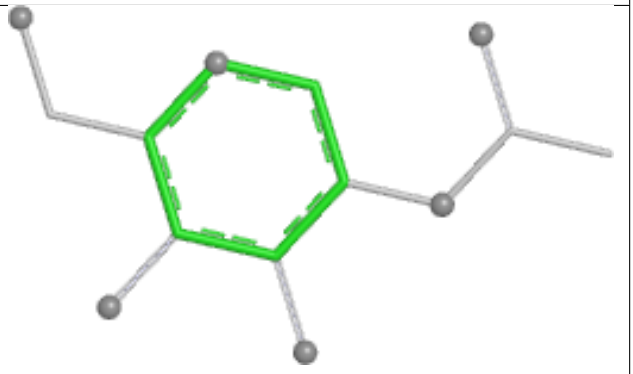
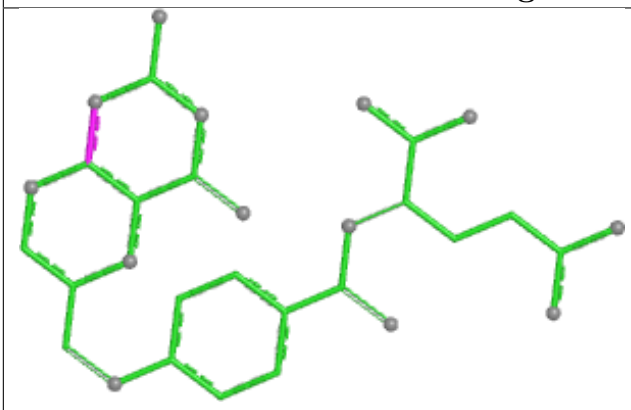


Rings

Ligand FOL B 1401



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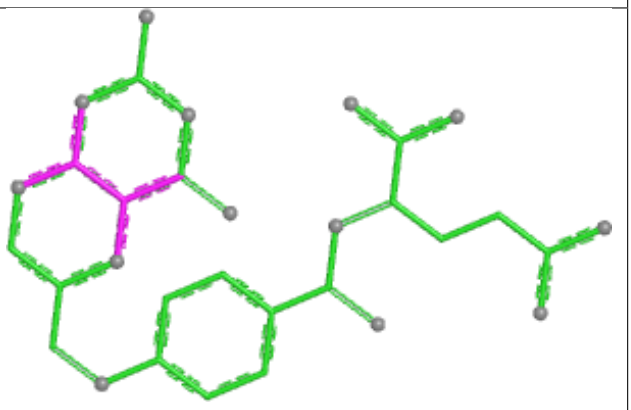

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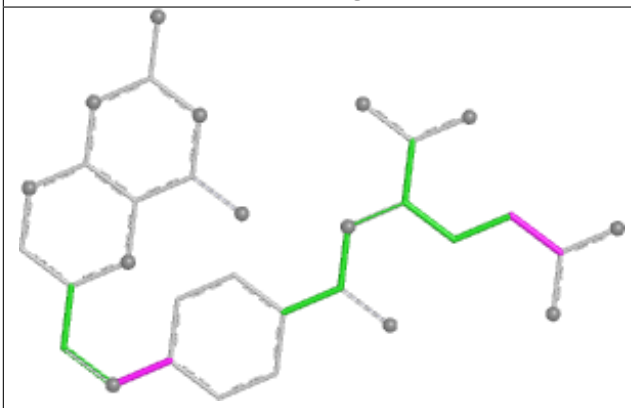

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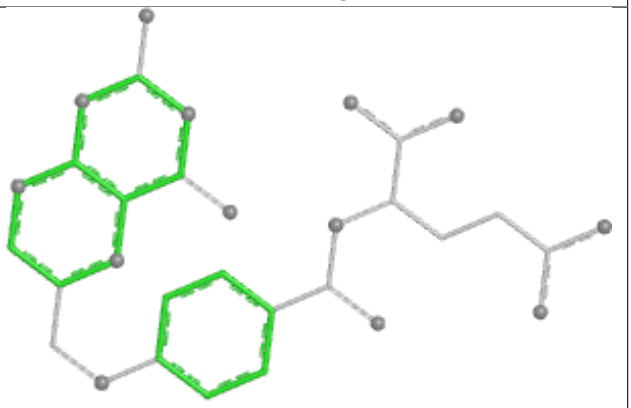
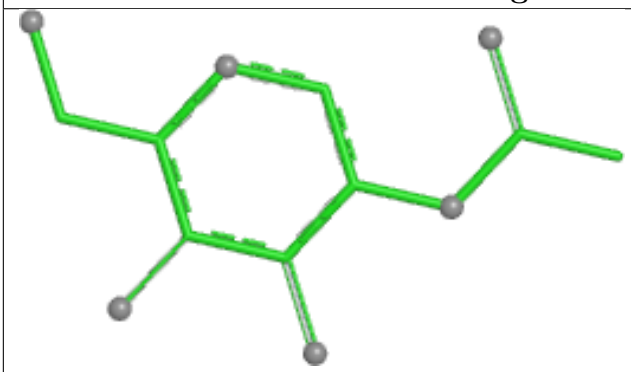


Rings

Ligand NAG A 1414



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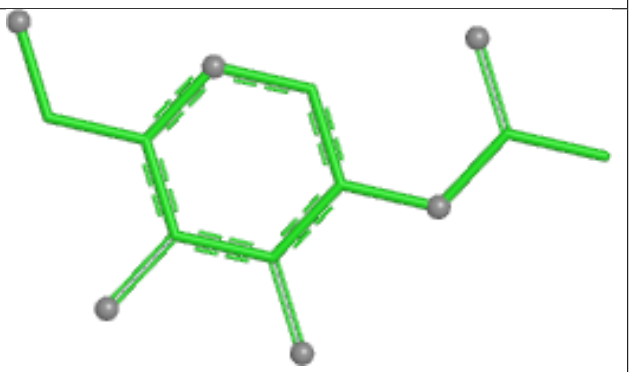
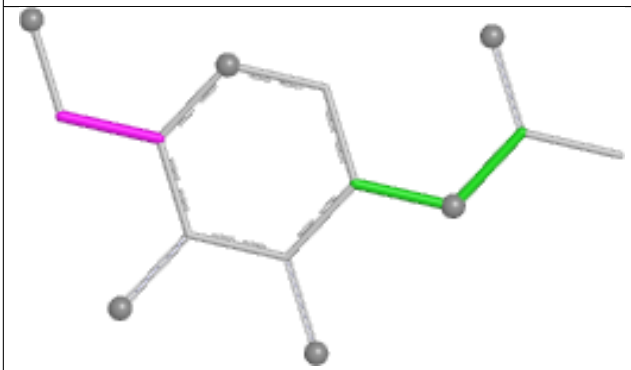


Bond angles



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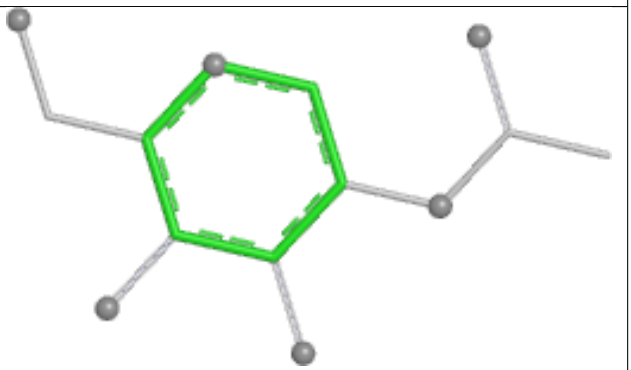
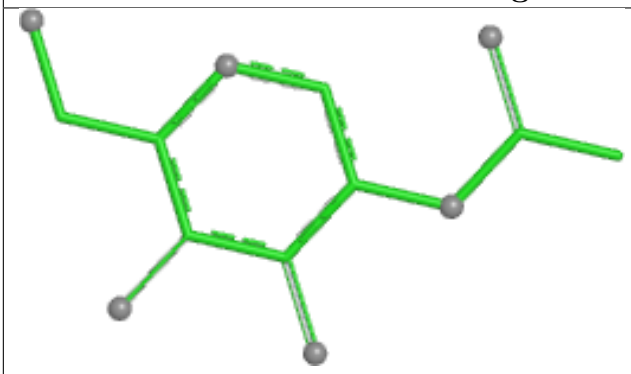


Rings

Ligand NAG C 1402



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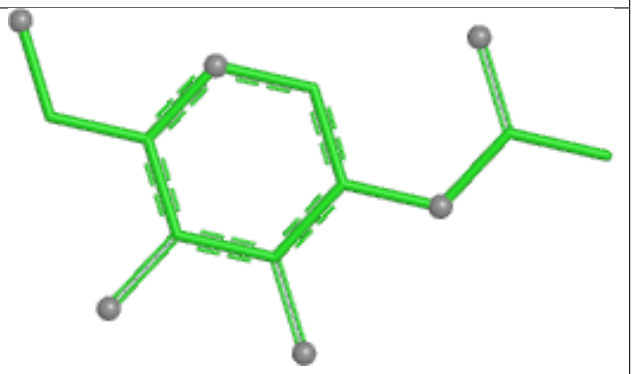

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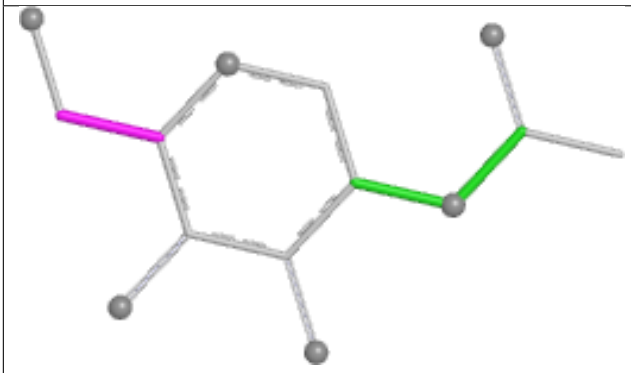

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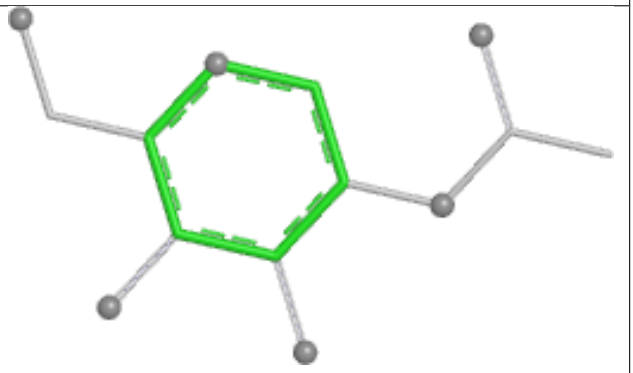
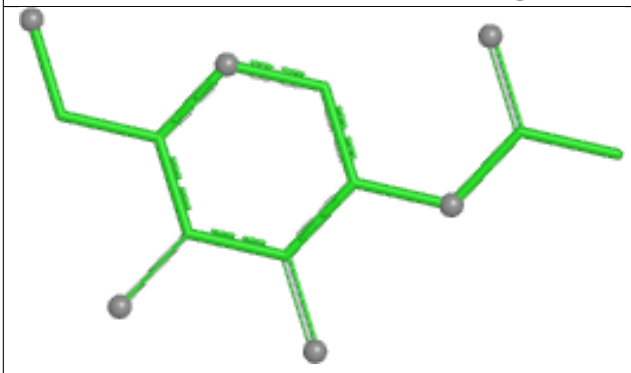


Rings

Ligand NAG C 1408



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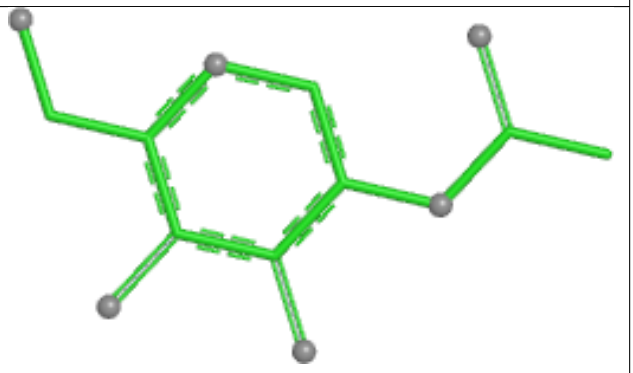
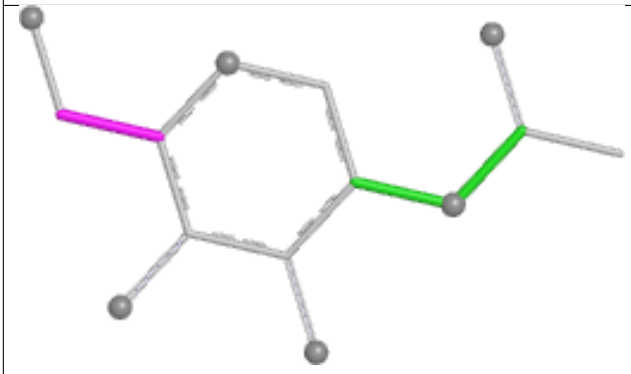


Bond angles



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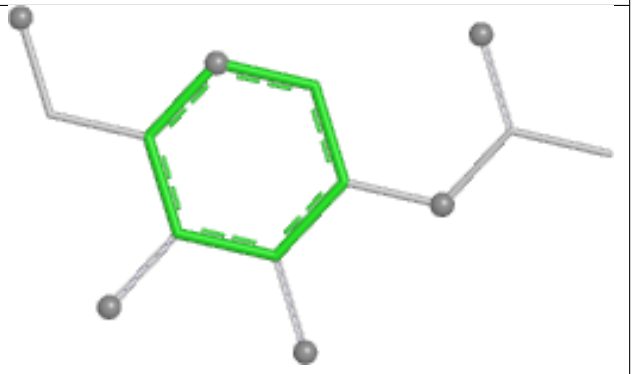
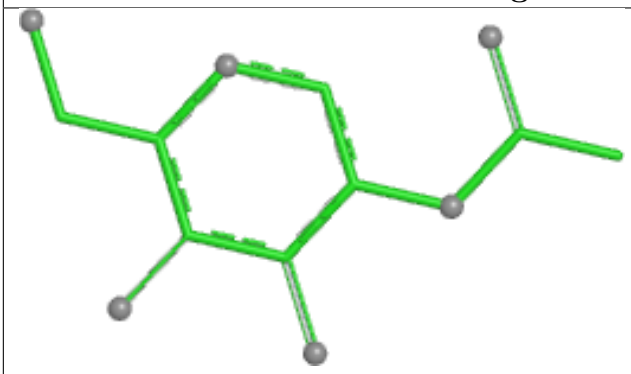


Rings

Ligand NAG A 1410



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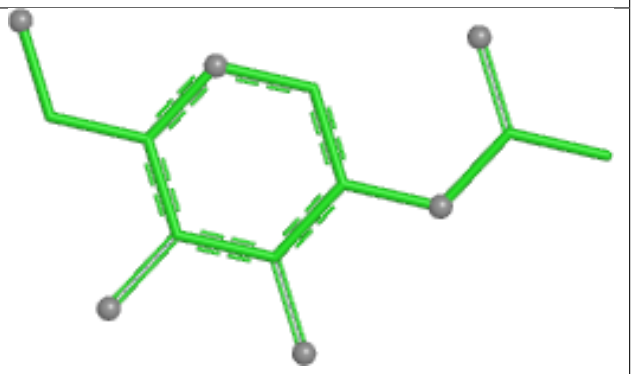
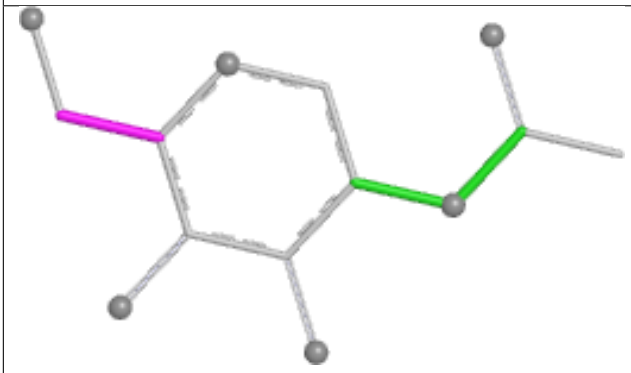


Bond angles



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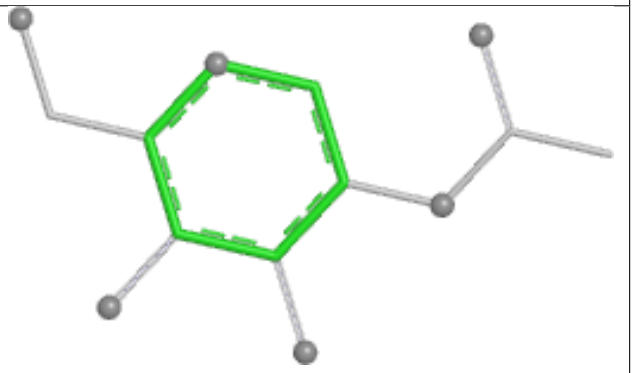
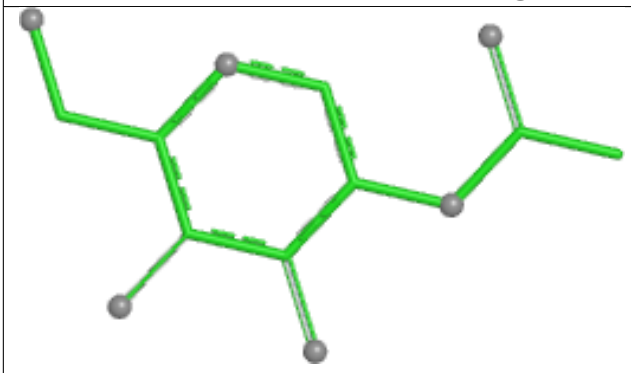


Rings

Ligand NAG B 1405



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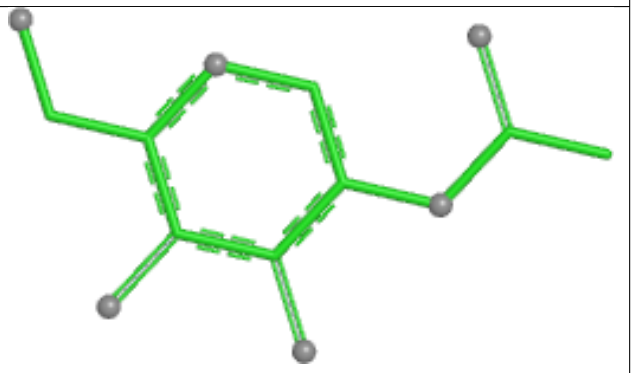
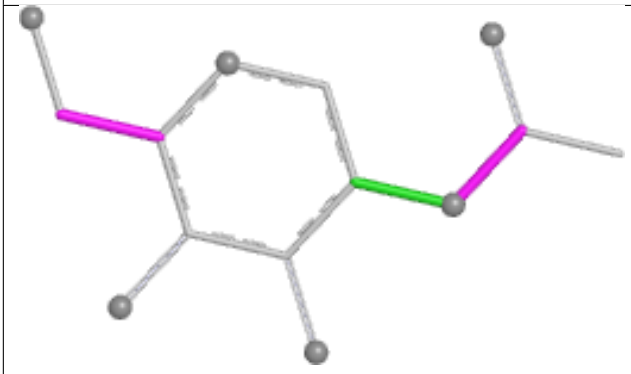


Bond angles



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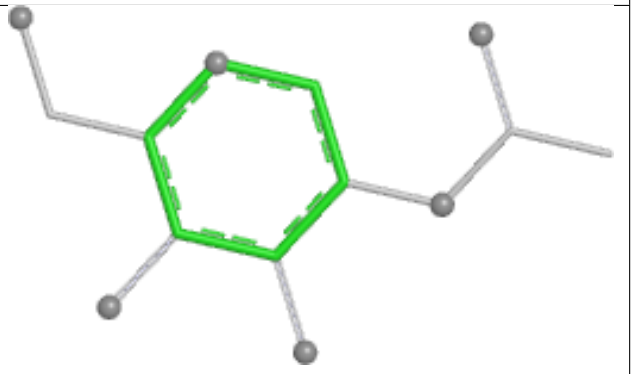
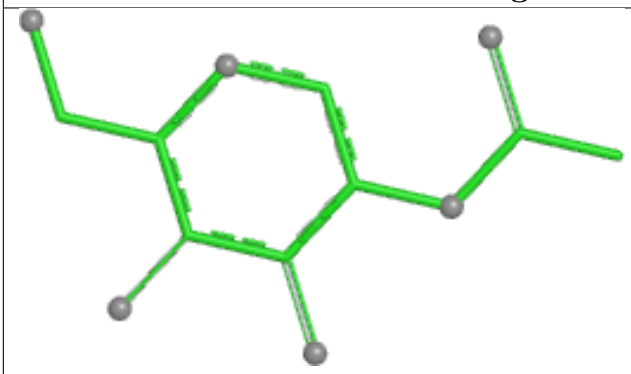


Rings

Ligand NAG A 1409



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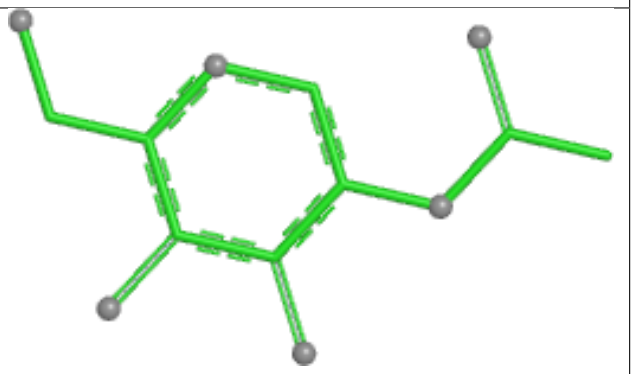
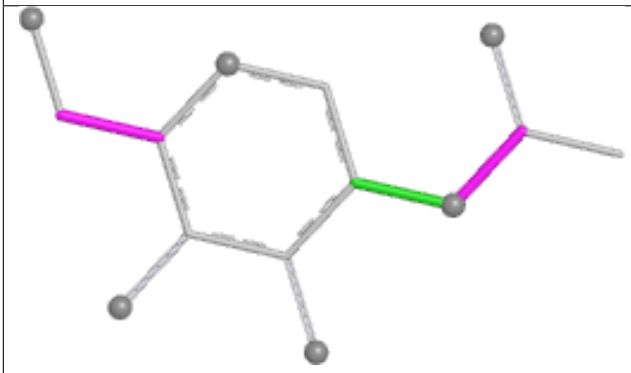


Bond angles



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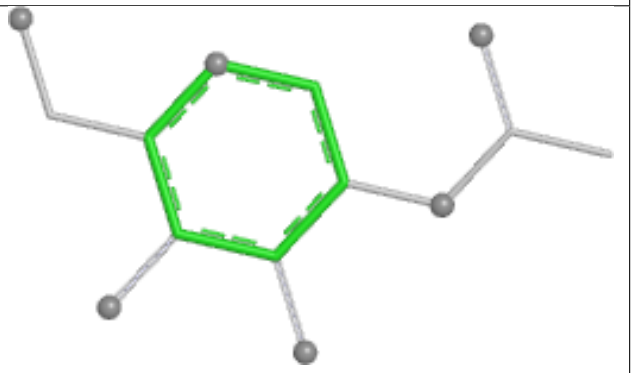
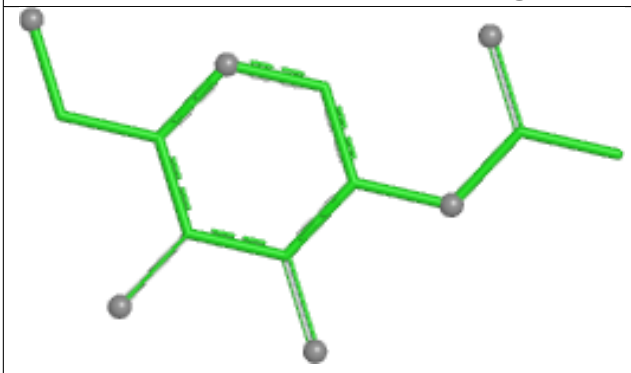


Rings

Ligand NAG A 1404



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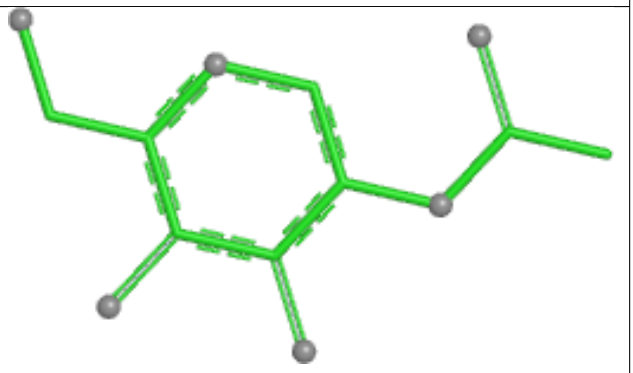
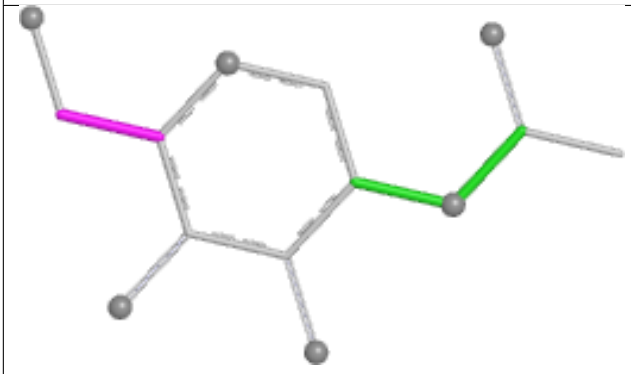


Bond angles



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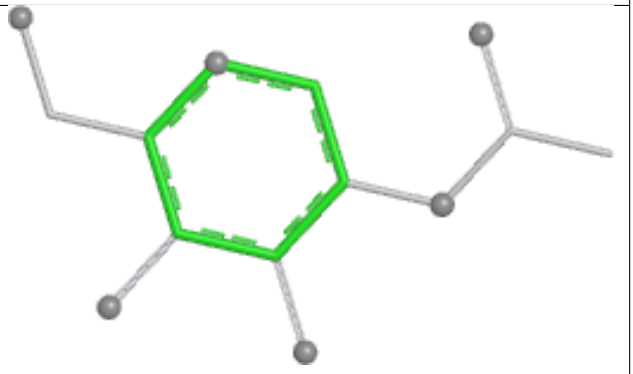
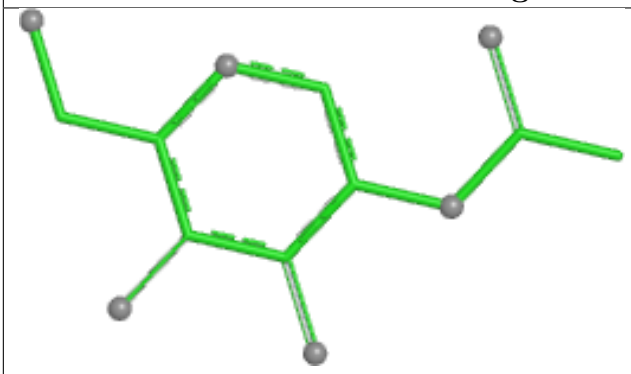


Rings

Ligand NAG C 1409



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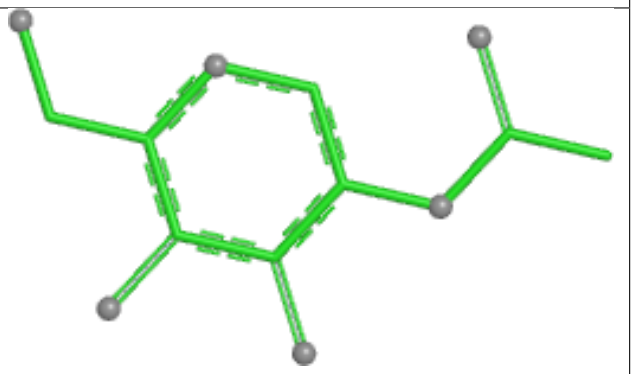

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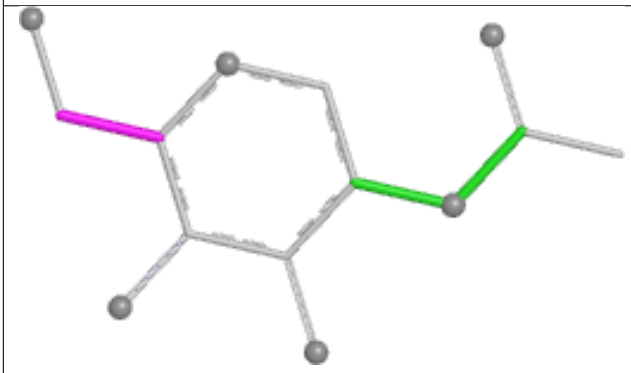

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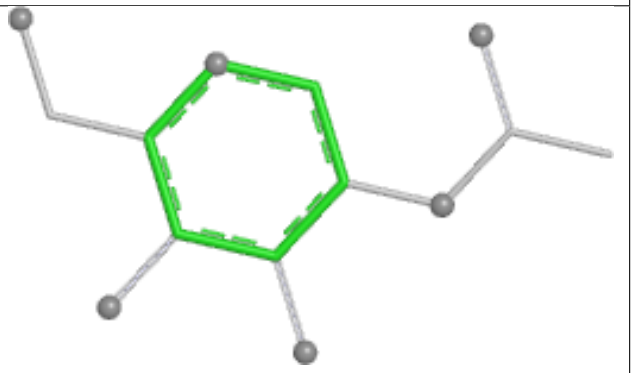
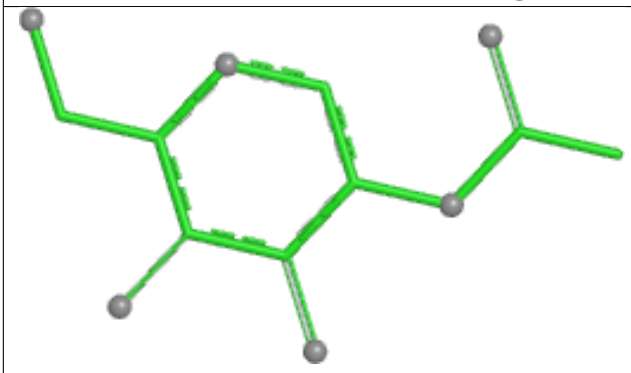


Rings

Ligand NAG A 1412



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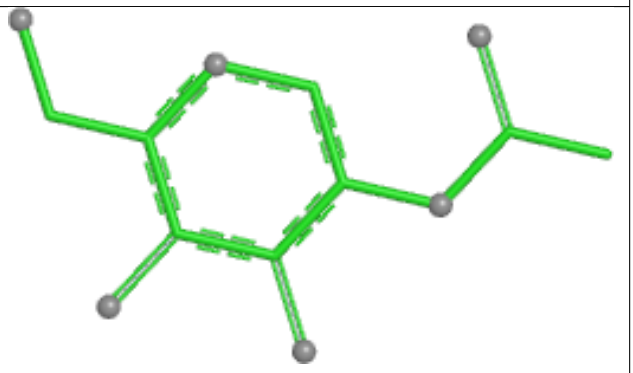
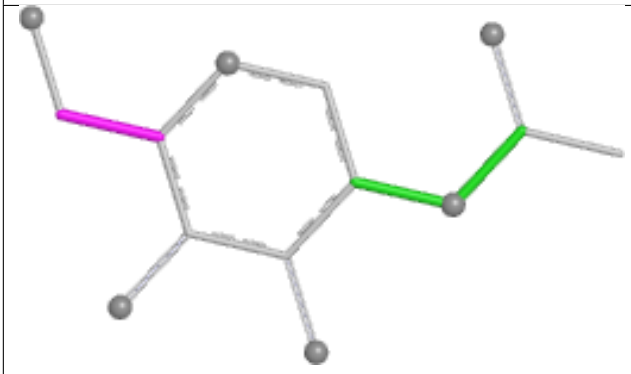


Bond angles



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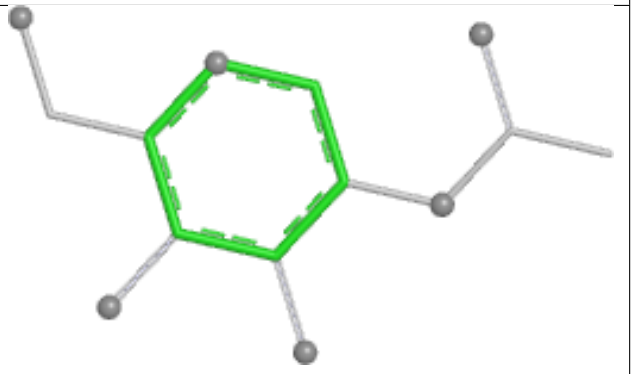
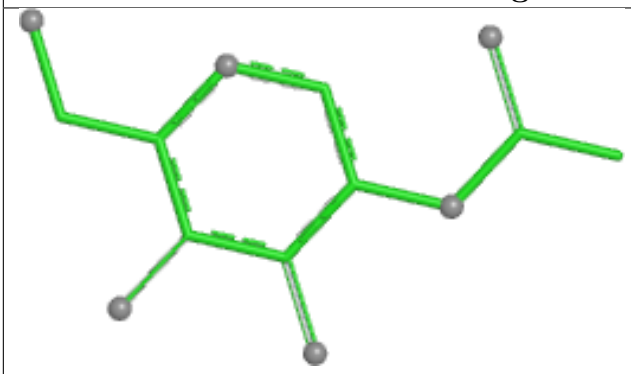


Rings

Ligand NAG C 1405



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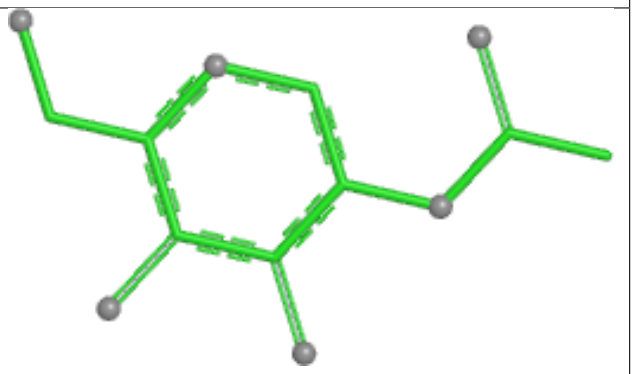
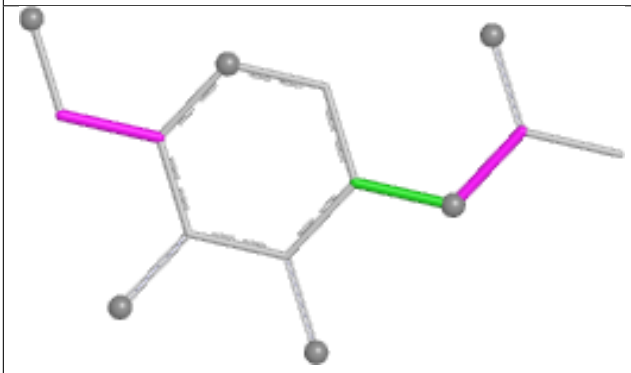


Bond angles



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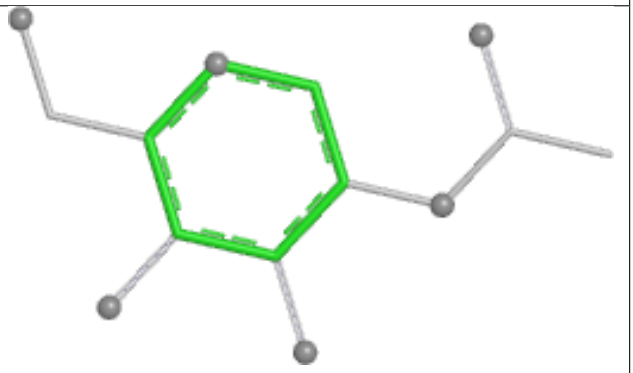
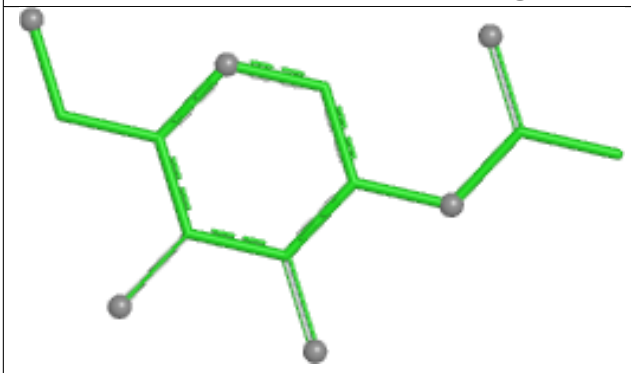


Rings

Ligand NAG C 1407



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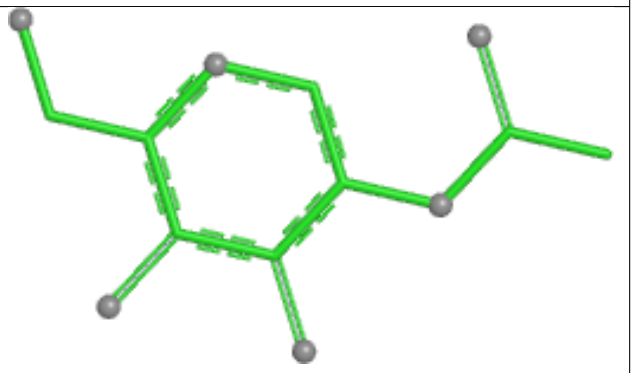
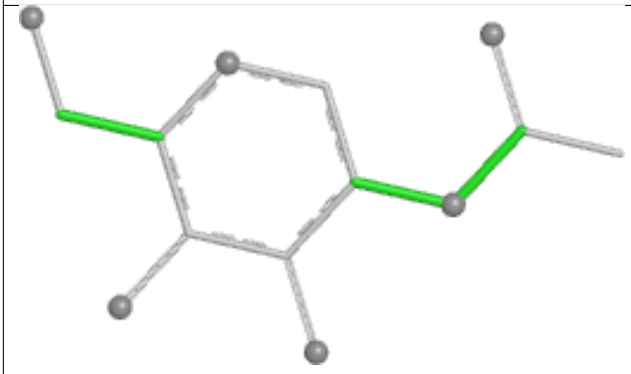


Bond angles



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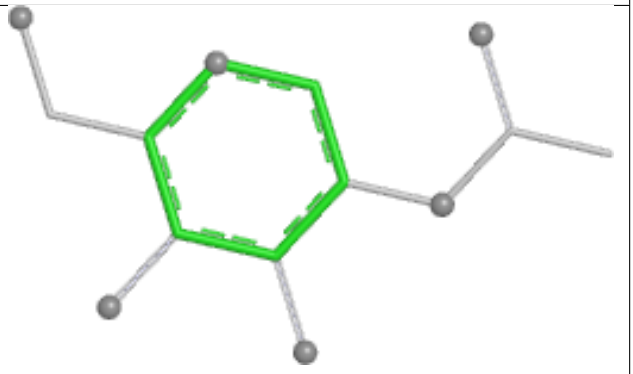


Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

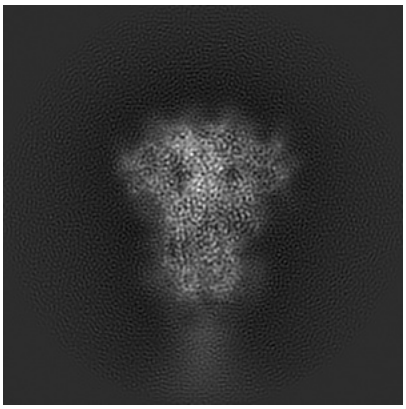
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61603. These allow visual inspection of the internal detail of the map and identification of artifacts.

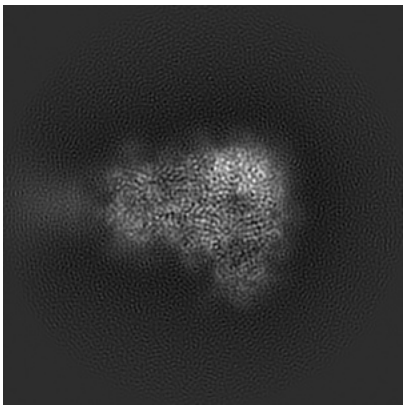
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

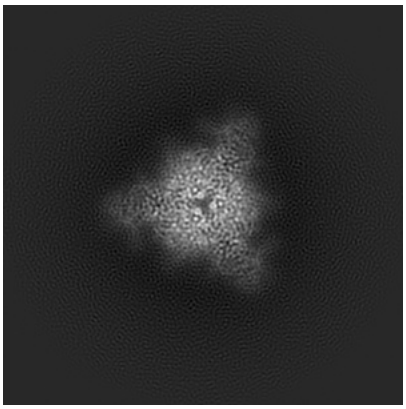
6.1.1 Primary map



X

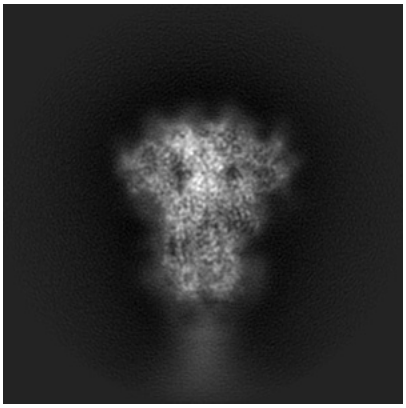


Y

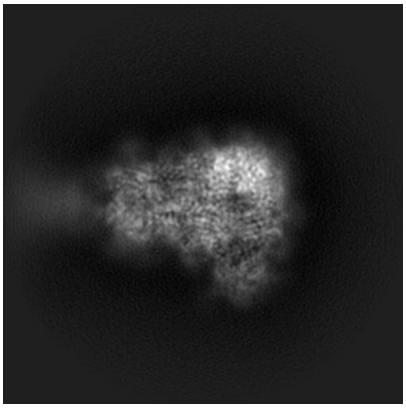


Z

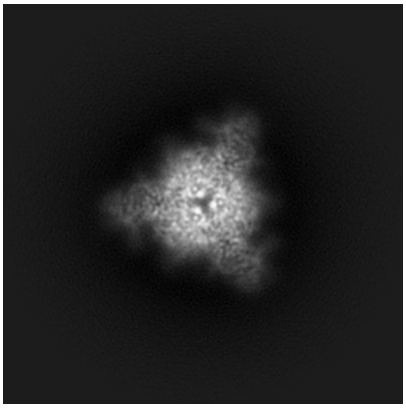
6.1.2 Raw map



X



Y

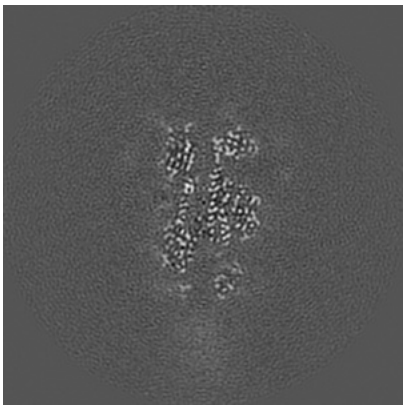


Z

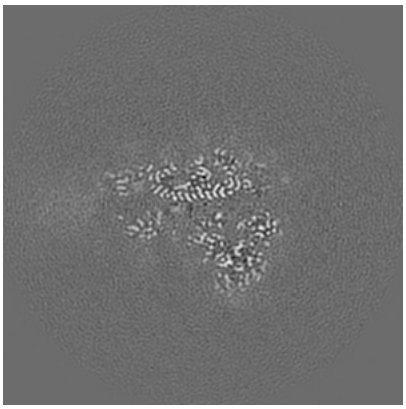
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

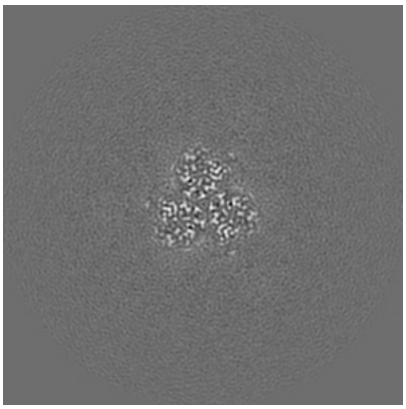
6.2.1 Primary map



X Index: 120

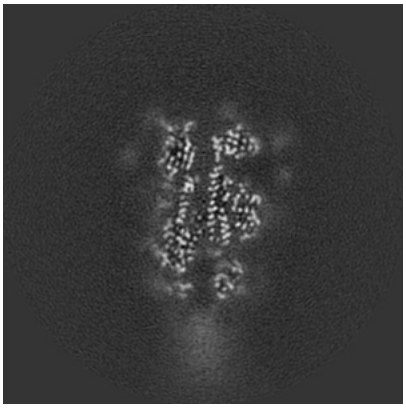


Y Index: 120

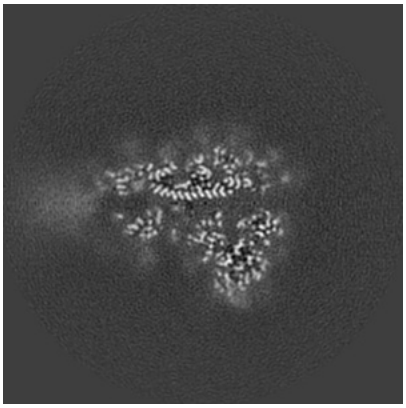


Z Index: 120

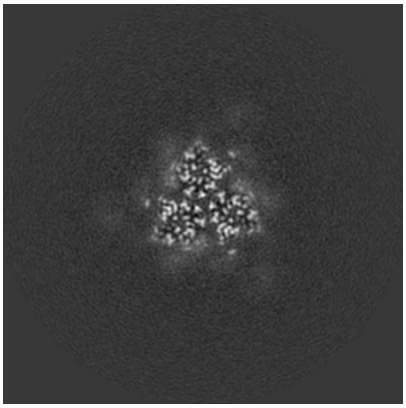
6.2.2 Raw map



X Index: 120



Y Index: 120

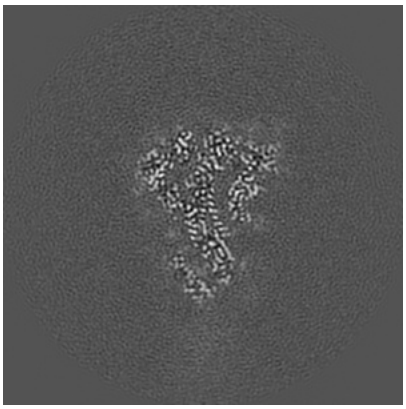


Z Index: 120

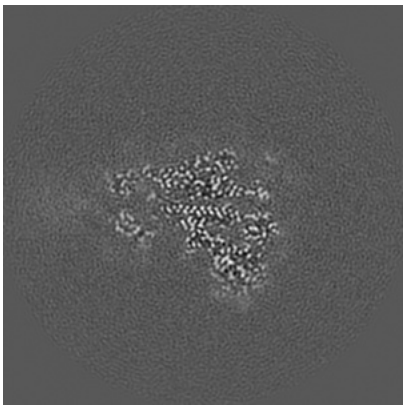
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

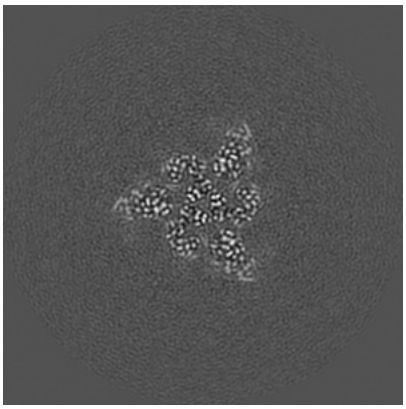
6.3.1 Primary map



X Index: 130

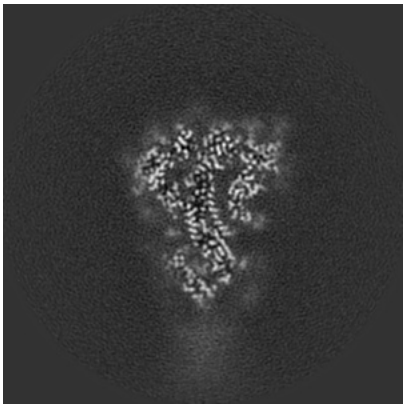


Y Index: 116

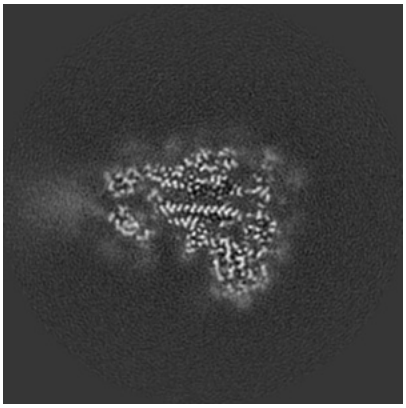


Z Index: 131

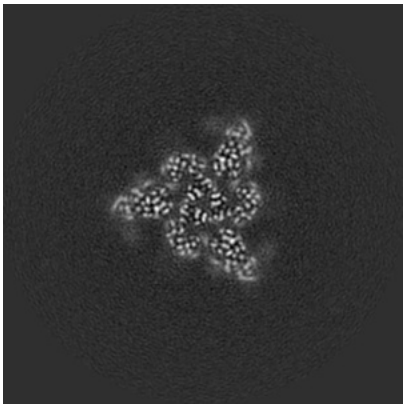
6.3.2 Raw map



X Index: 130



Y Index: 115

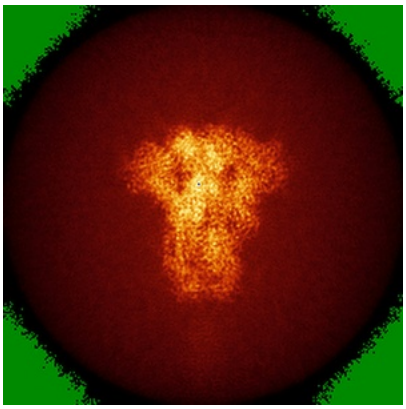


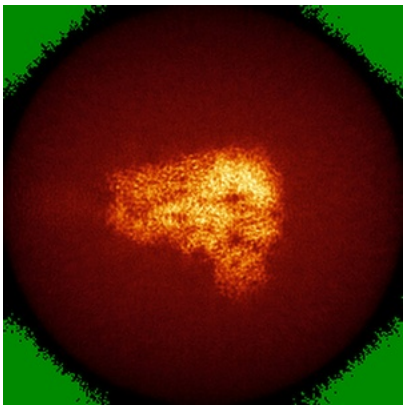
Z Index: 131

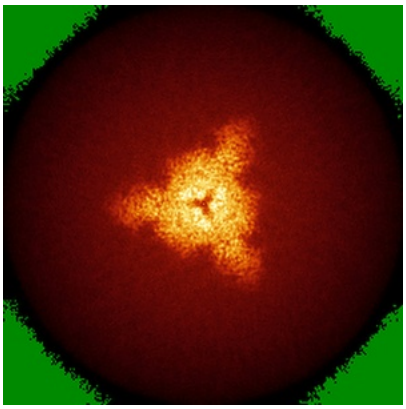
The images above show the largest variance slices of the map in three orthogonal directions.

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

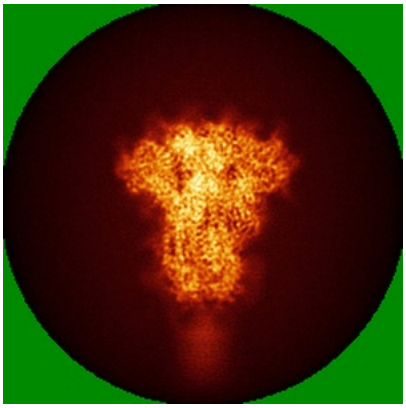
6.4.1 Primary map

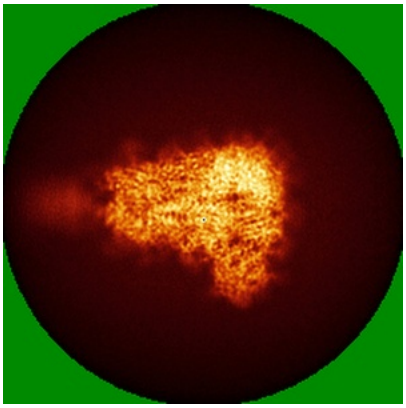

X

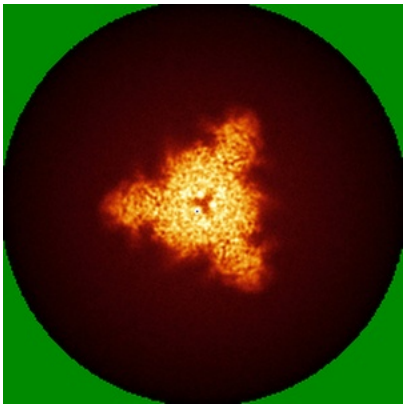

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

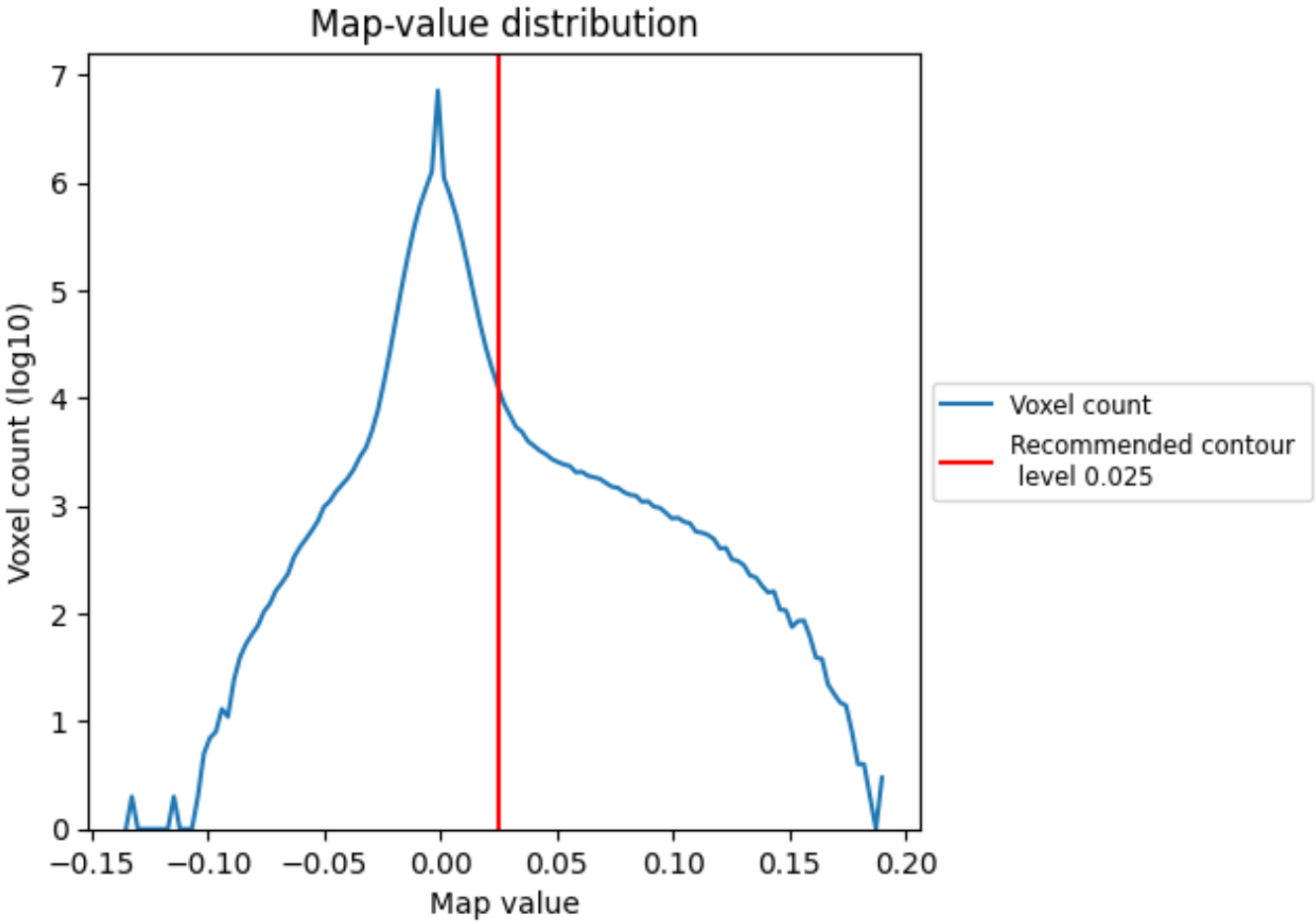
6.6 Mask visualisation (i)

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

7 Map analysis

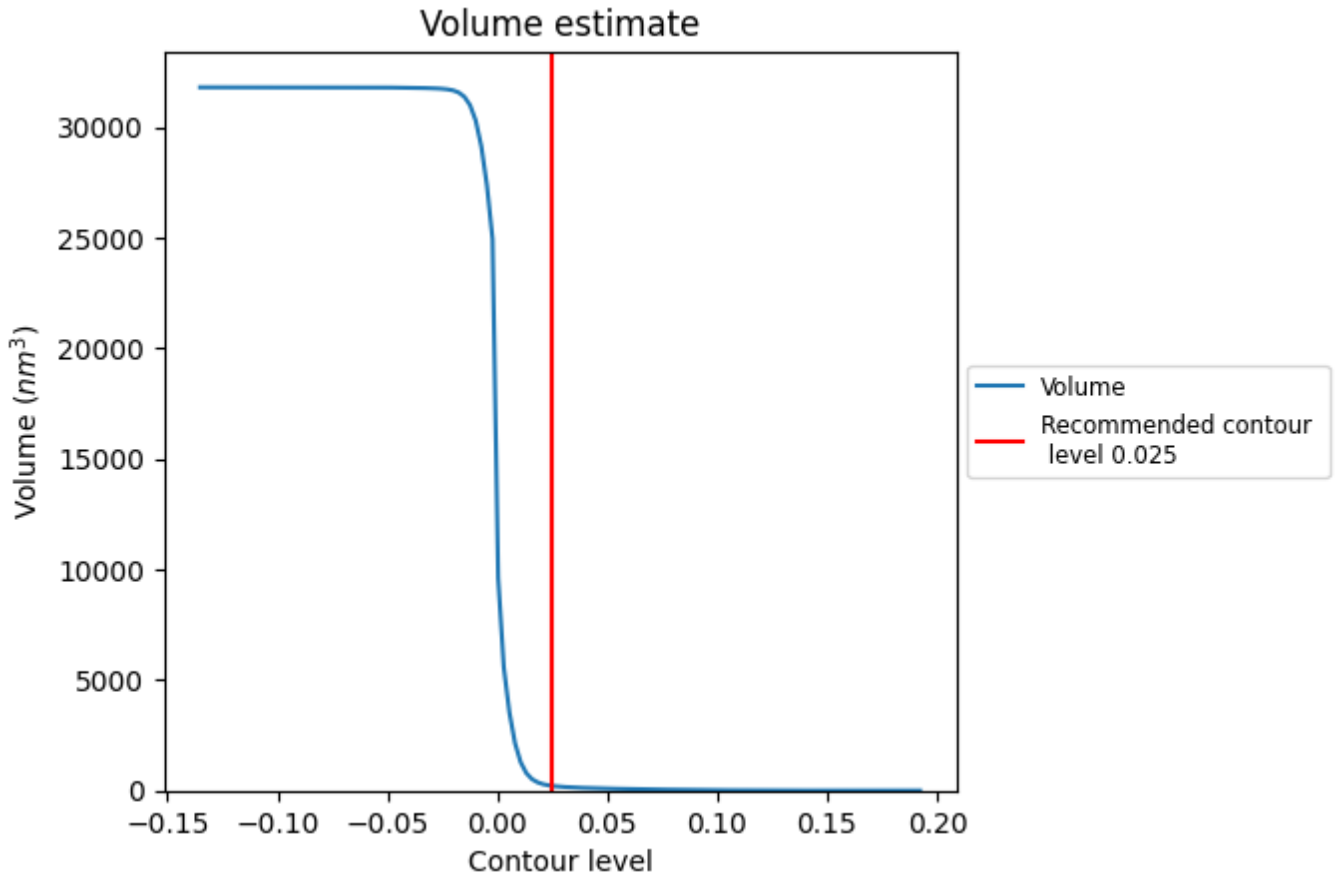
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

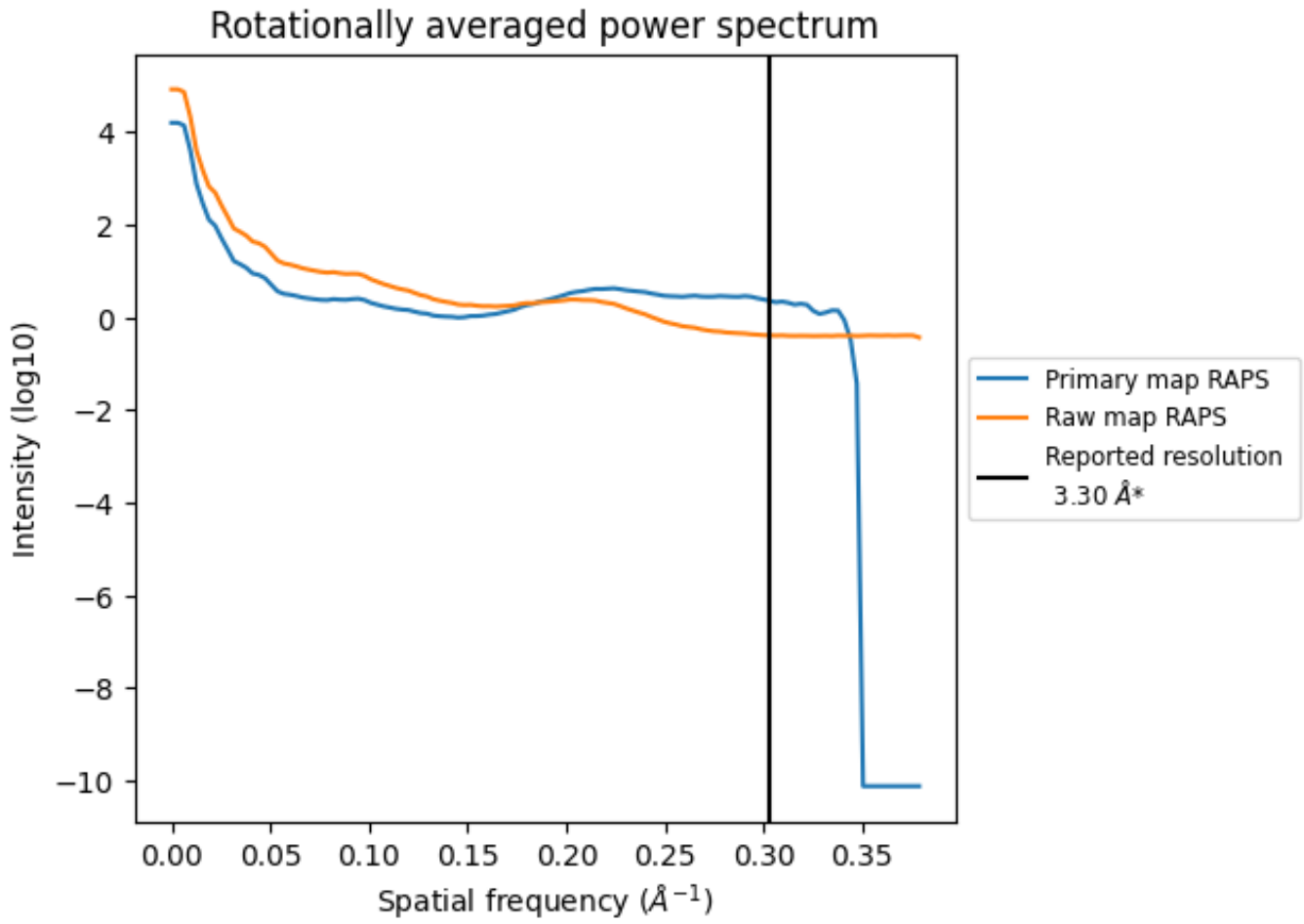
7.2 Volume estimate



The volume at the recommended contour level is 214 nm^3; this corresponds to an approximate mass of 193 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

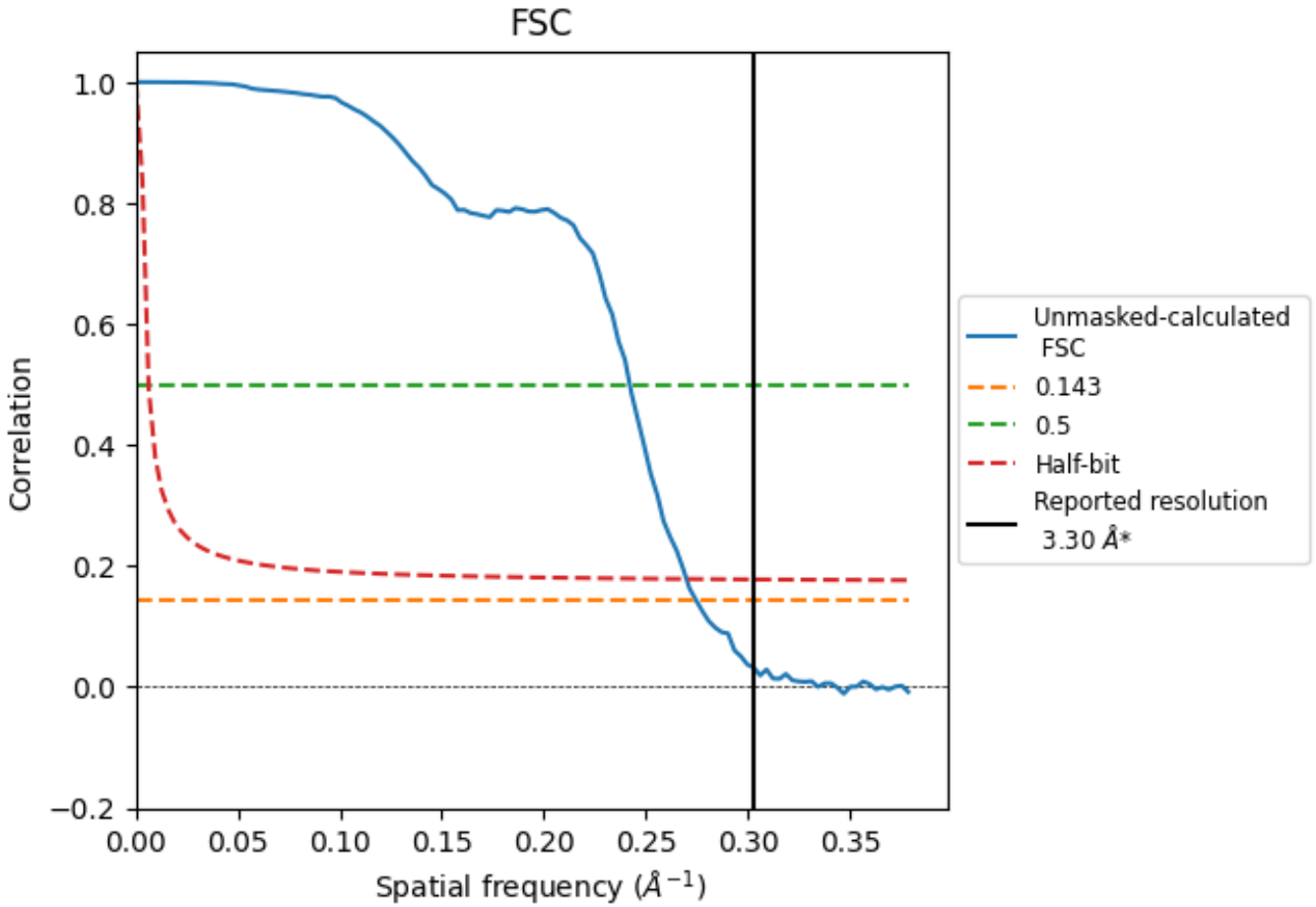


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

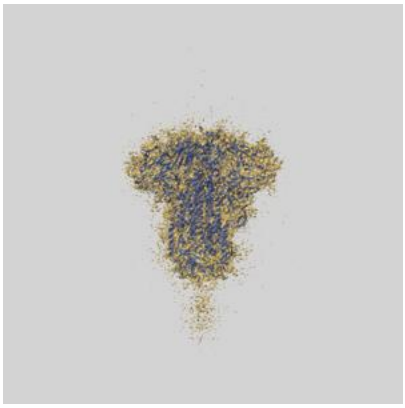
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.64	4.13	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.64 differs from the reported value 3.3 by more than 10 %

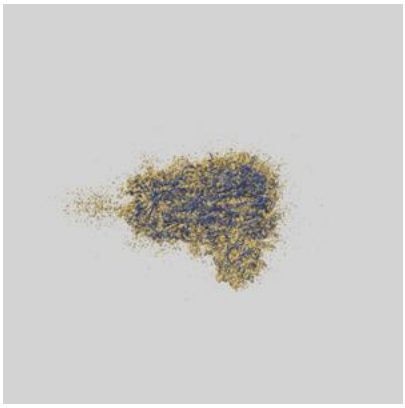
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61603 and PDB model 9JMI. Per-residue inclusion information can be found in section 3 on page 13.

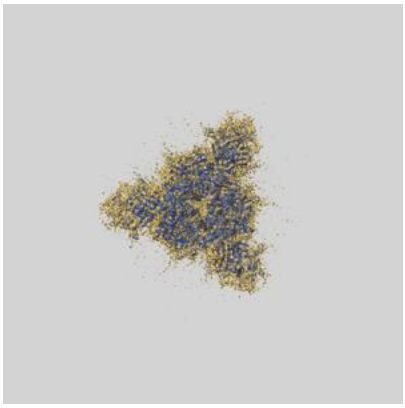
9.1 Map-model overlay



X



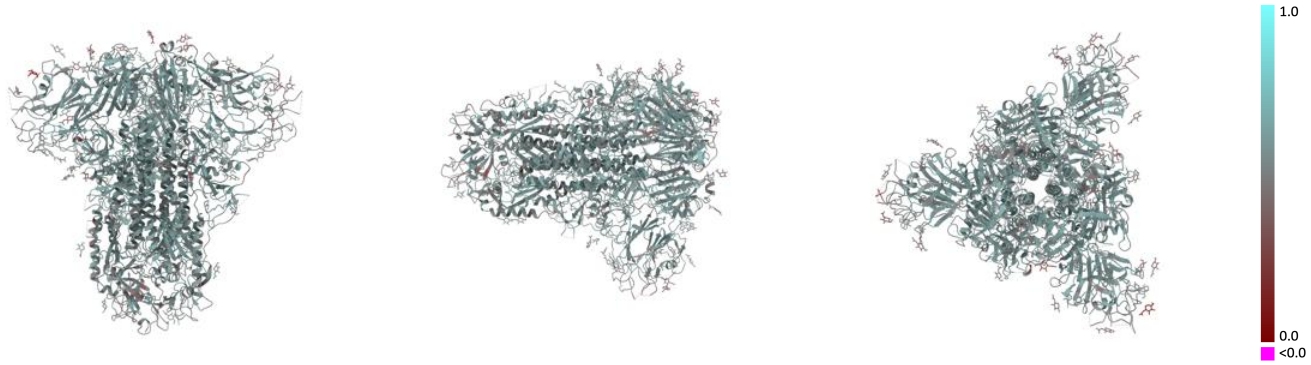
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



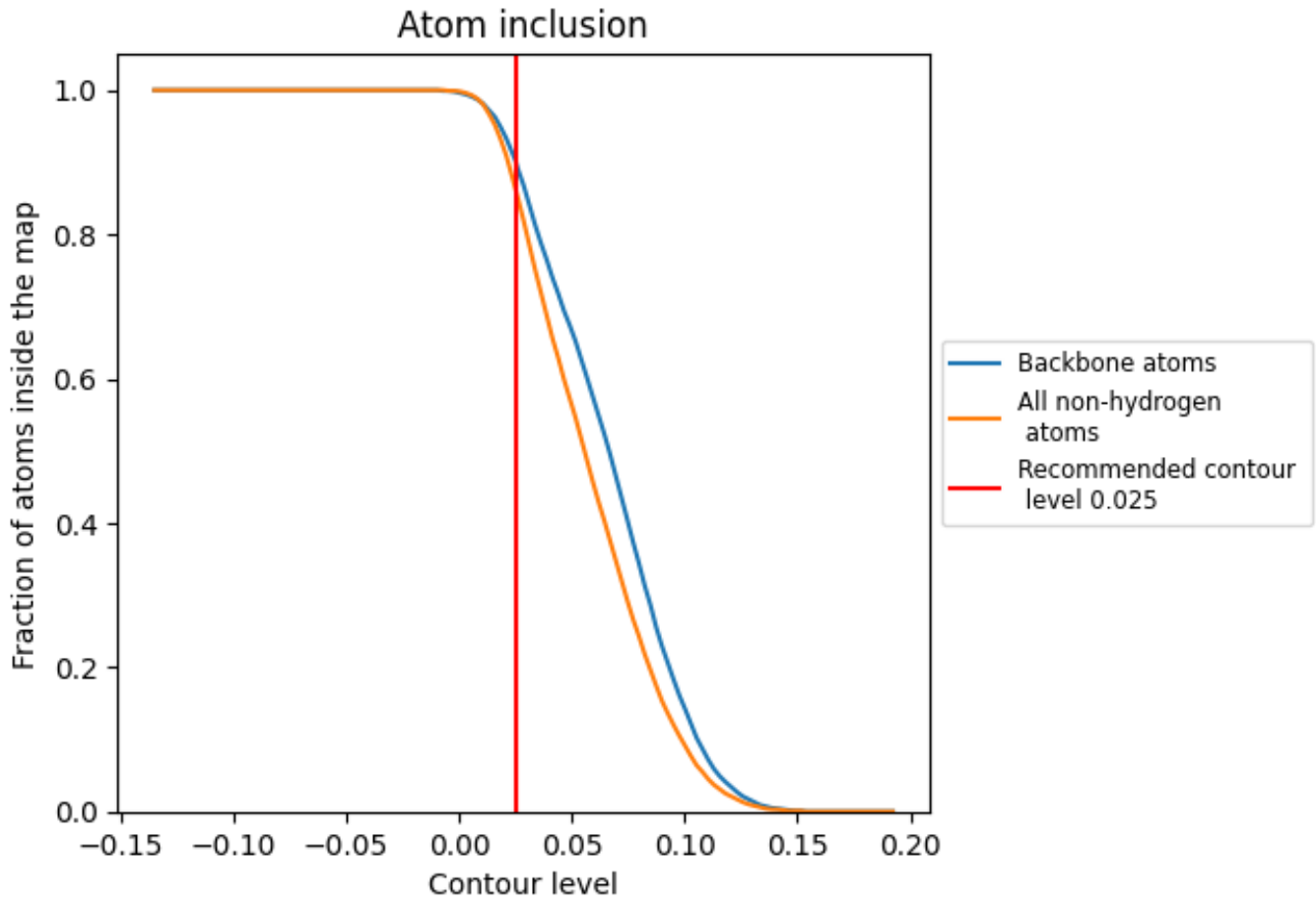
X Y Z

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

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.5510
A	0.8650	0.5520
B	0.8650	0.5520
C	0.8660	0.5520
D	0.7140	0.5180
E	0.6790	0.4730
F	0.7860	0.5360
G	0.7500	0.5190
H	0.8210	0.5390
I	0.8210	0.5180
J	0.7500	0.5140
K	0.6070	0.4390
L	0.8210	0.5460
M	0.7860	0.5220
N	0.8210	0.5320
O	0.8210	0.5290
P	0.7500	0.5340
Q	0.6430	0.3660
R	0.8930	0.5530
S	0.8210	0.5260
T	0.8570	0.5330
U	0.8210	0.5050

