Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 06:17 PM JST

PDB ID	:	9JMG / pdb_00009jmg
EMDB ID	:	EMD-61601
Title	:	Cryo-EM structure of EU-HedgehogCoV (Erinaceus/VMC/DEU/2012) S-trimer in a locked-2 conformation
Authors	:	Yuan, H.; Xiong, X.
Deposited on	:	2024-09-20
Resolution	:	3.00 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:

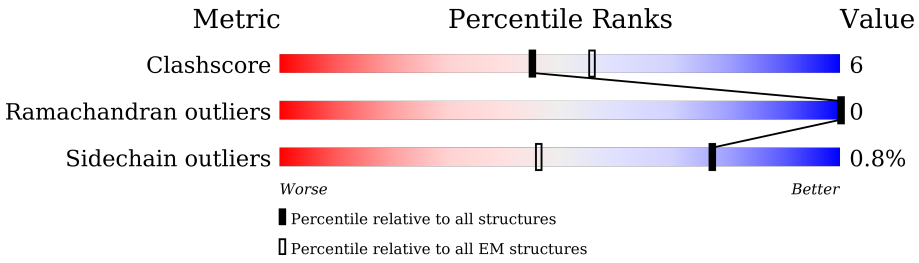
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1353	71% 12% 17%
1	B	1353	70% 13% 17%
1	C	1353	73% 10% 17%
2	D	3	33% 67%
2	E	3	33% 33% 33%
2	F	3	33% 67%
2	H	3	67% 33%
2	I	3	67% 33%

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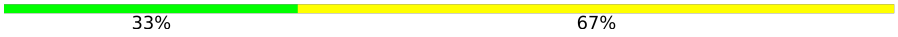
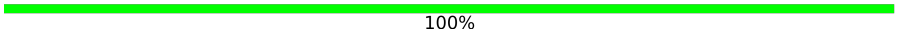
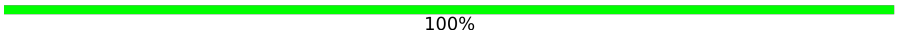
Mol	Chain	Length	Quality of chain
2	K	3	
3	G	2	
3	J	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 27340 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	1126	Total	C	N	O	S	0	0
			8792	5591	1456	1688	57		
1	B	1126	Total	C	N	O	S	0	0
			8792	5591	1456	1688	57		
1	C	1126	Total	C	N	O	S	0	0
			8792	5591	1456	1688	57		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1275	GLY	-	linker	UNP U5LMM7
A	1276	SER	-	linker	UNP U5LMM7
A	1298	LEU	PHE	conflict	UNP P10104
A	1304	LEU	-	expression tag	UNP P10104
A	1305	GLU	-	expression tag	UNP P10104
A	1306	VAL	-	expression tag	UNP P10104
A	1307	LEU	-	expression tag	UNP P10104
A	1308	PHE	-	expression tag	UNP P10104
A	1309	GLN	-	expression tag	UNP P10104
A	1310	GLY	-	expression tag	UNP P10104
A	1311	PRO	-	expression tag	UNP P10104
A	1312	GLY	-	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	HIS	-	expression tag	UNP P10104
A	1318	HIS	-	expression tag	UNP P10104
A	1319	HIS	-	expression tag	UNP P10104
A	1320	HIS	-	expression tag	UNP P10104
A	1321	SER	-	expression tag	UNP P10104
A	1322	ALA	-	expression tag	UNP P10104
A	1323	TRP	-	expression tag	UNP P10104
A	1324	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1325	HIS	-	expression tag	UNP P10104
A	1326	PRO	-	expression tag	UNP P10104
A	1327	GLN	-	expression tag	UNP P10104
A	1328	PHE	-	expression tag	UNP P10104
A	1329	GLU	-	expression tag	UNP P10104
A	1330	LYS	-	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	SER	-	expression tag	UNP P10104
A	1335	GLY	-	expression tag	UNP P10104
A	1336	GLY	-	expression tag	UNP P10104
A	1337	GLY	-	expression tag	UNP P10104
A	1338	GLY	-	expression tag	UNP P10104
A	1339	SER	-	expression tag	UNP P10104
A	1340	GLY	-	expression tag	UNP P10104
A	1341	GLY	-	expression tag	UNP P10104
A	1342	SER	-	expression tag	UNP P10104
A	1343	ALA	-	expression tag	UNP P10104
A	1344	TRP	-	expression tag	UNP P10104
A	1345	SER	-	expression tag	UNP P10104
A	1346	HIS	-	expression tag	UNP P10104
A	1347	PRO	-	expression tag	UNP P10104
A	1348	GLN	-	expression tag	UNP P10104
A	1349	PHE	-	expression tag	UNP P10104
A	1350	GLU	-	expression tag	UNP P10104
A	1351	LYS	-	expression tag	UNP P10104
A	1352	SER	-	expression tag	UNP P10104
A	1353	ALA	-	expression tag	UNP P10104
B	1275	GLY	-	linker	UNP U5LMM7
B	1276	SER	-	linker	UNP U5LMM7
B	1298	LEU	PHE	conflict	UNP P10104
B	1304	LEU	-	expression tag	UNP P10104
B	1305	GLU	-	expression tag	UNP P10104
B	1306	VAL	-	expression tag	UNP P10104
B	1307	LEU	-	expression tag	UNP P10104
B	1308	PHE	-	expression tag	UNP P10104
B	1309	GLN	-	expression tag	UNP P10104
B	1310	GLY	-	expression tag	UNP P10104
B	1311	PRO	-	expression tag	UNP P10104
B	1312	GLY	-	expression tag	UNP P10104
B	1313	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1314	HIS	-	expression tag	UNP P10104
B	1315	HIS	-	expression tag	UNP P10104
B	1316	HIS	-	expression tag	UNP P10104
B	1317	HIS	-	expression tag	UNP P10104
B	1318	HIS	-	expression tag	UNP P10104
B	1319	HIS	-	expression tag	UNP P10104
B	1320	HIS	-	expression tag	UNP P10104
B	1321	SER	-	expression tag	UNP P10104
B	1322	ALA	-	expression tag	UNP P10104
B	1323	TRP	-	expression tag	UNP P10104
B	1324	SER	-	expression tag	UNP P10104
B	1325	HIS	-	expression tag	UNP P10104
B	1326	PRO	-	expression tag	UNP P10104
B	1327	GLN	-	expression tag	UNP P10104
B	1328	PHE	-	expression tag	UNP P10104
B	1329	GLU	-	expression tag	UNP P10104
B	1330	LYS	-	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	SER	-	expression tag	UNP P10104
B	1335	GLY	-	expression tag	UNP P10104
B	1336	GLY	-	expression tag	UNP P10104
B	1337	GLY	-	expression tag	UNP P10104
B	1338	GLY	-	expression tag	UNP P10104
B	1339	SER	-	expression tag	UNP P10104
B	1340	GLY	-	expression tag	UNP P10104
B	1341	GLY	-	expression tag	UNP P10104
B	1342	SER	-	expression tag	UNP P10104
B	1343	ALA	-	expression tag	UNP P10104
B	1344	TRP	-	expression tag	UNP P10104
B	1345	SER	-	expression tag	UNP P10104
B	1346	HIS	-	expression tag	UNP P10104
B	1347	PRO	-	expression tag	UNP P10104
B	1348	GLN	-	expression tag	UNP P10104
B	1349	PHE	-	expression tag	UNP P10104
B	1350	GLU	-	expression tag	UNP P10104
B	1351	LYS	-	expression tag	UNP P10104
B	1352	SER	-	expression tag	UNP P10104
B	1353	ALA	-	expression tag	UNP P10104
C	1275	GLY	-	linker	UNP U5LMM7
C	1276	SER	-	linker	UNP U5LMM7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1298	LEU	PHE	conflict	UNP P10104
C	1304	LEU	-	expression tag	UNP P10104
C	1305	GLU	-	expression tag	UNP P10104
C	1306	VAL	-	expression tag	UNP P10104
C	1307	LEU	-	expression tag	UNP P10104
C	1308	PHE	-	expression tag	UNP P10104
C	1309	GLN	-	expression tag	UNP P10104
C	1310	GLY	-	expression tag	UNP P10104
C	1311	PRO	-	expression tag	UNP P10104
C	1312	GLY	-	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	HIS	-	expression tag	UNP P10104
C	1318	HIS	-	expression tag	UNP P10104
C	1319	HIS	-	expression tag	UNP P10104
C	1320	HIS	-	expression tag	UNP P10104
C	1321	SER	-	expression tag	UNP P10104
C	1322	ALA	-	expression tag	UNP P10104
C	1323	TRP	-	expression tag	UNP P10104
C	1324	SER	-	expression tag	UNP P10104
C	1325	HIS	-	expression tag	UNP P10104
C	1326	PRO	-	expression tag	UNP P10104
C	1327	GLN	-	expression tag	UNP P10104
C	1328	PHE	-	expression tag	UNP P10104
C	1329	GLU	-	expression tag	UNP P10104
C	1330	LYS	-	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	SER	-	expression tag	UNP P10104
C	1335	GLY	-	expression tag	UNP P10104
C	1336	GLY	-	expression tag	UNP P10104
C	1337	GLY	-	expression tag	UNP P10104
C	1338	GLY	-	expression tag	UNP P10104
C	1339	SER	-	expression tag	UNP P10104
C	1340	GLY	-	expression tag	UNP P10104
C	1341	GLY	-	expression tag	UNP P10104
C	1342	SER	-	expression tag	UNP P10104
C	1343	ALA	-	expression tag	UNP P10104
C	1344	TRP	-	expression tag	UNP P10104

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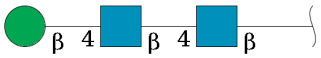
Chain	Residue	Modelled	Actual	Comment	Reference
C	1345	SER	-	expression tag	UNP P10104
C	1346	HIS	-	expression tag	UNP P10104
C	1347	PRO	-	expression tag	UNP P10104
C	1348	GLN	-	expression tag	UNP P10104
C	1349	PHE	-	expression tag	UNP P10104
C	1350	GLU	-	expression tag	UNP P10104
C	1351	LYS	-	expression tag	UNP P10104
C	1352	SER	-	expression tag	UNP P10104
C	1353	ALA	-	expression tag	UNP P10104

- Molecule 2 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
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	H	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 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
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

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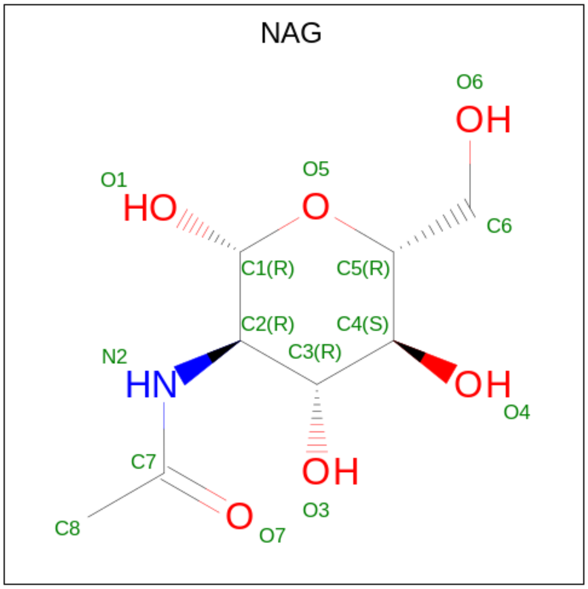
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	J	2	28	16	2	10	0	0

- Molecule 4 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
			Total	C	N	O	
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0
4	A	1	14	8	1	5	0

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

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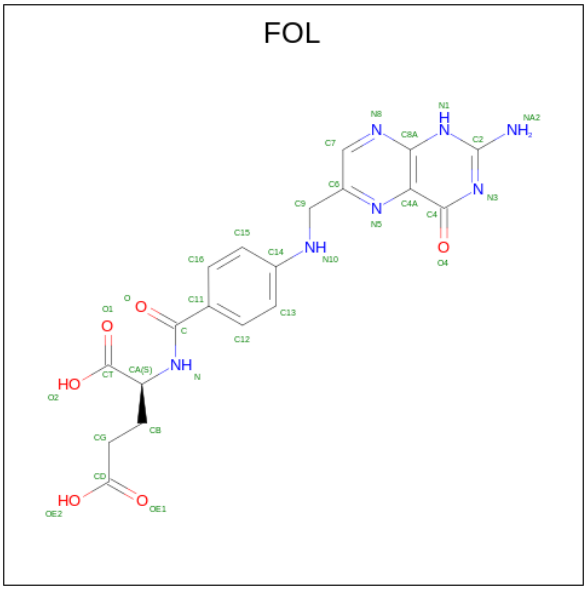
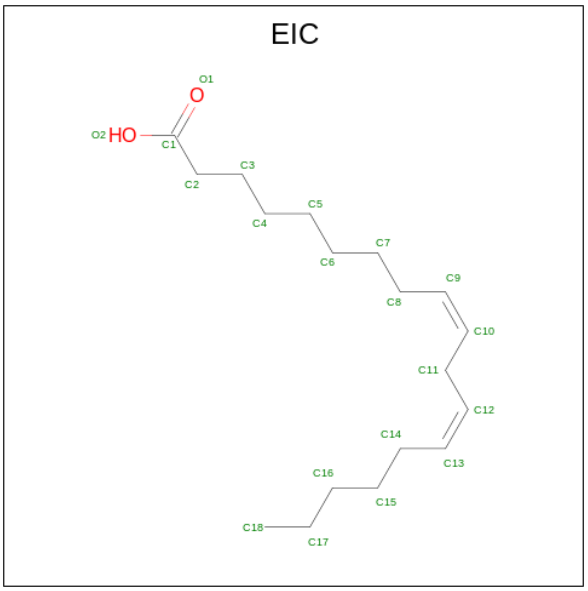
Mol	Chain	Residues	Atoms	AltConf
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0

- Molecule 5 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
5	A	1	Total C N O 32 19 7 6	0
5	B	1	Total C N O 32 19 7 6	0
5	C	1	Total C N O 32 19 7 6	0

- Molecule 6 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



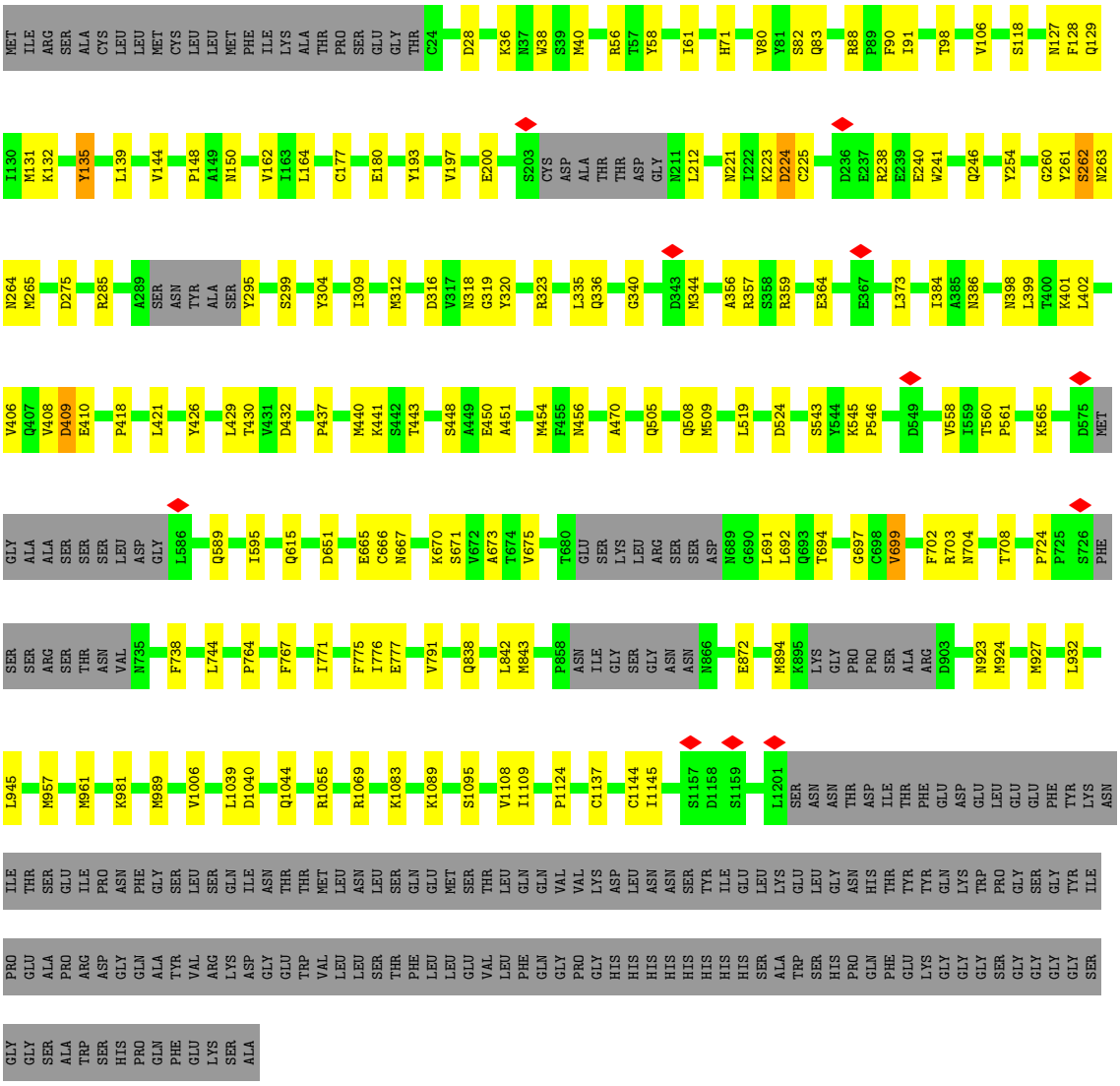
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			20	18	2	
6	B	1	Total	C	O	0
			20	18	2	
6	C	1	Total	C	O	0
			20	18	2	

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.

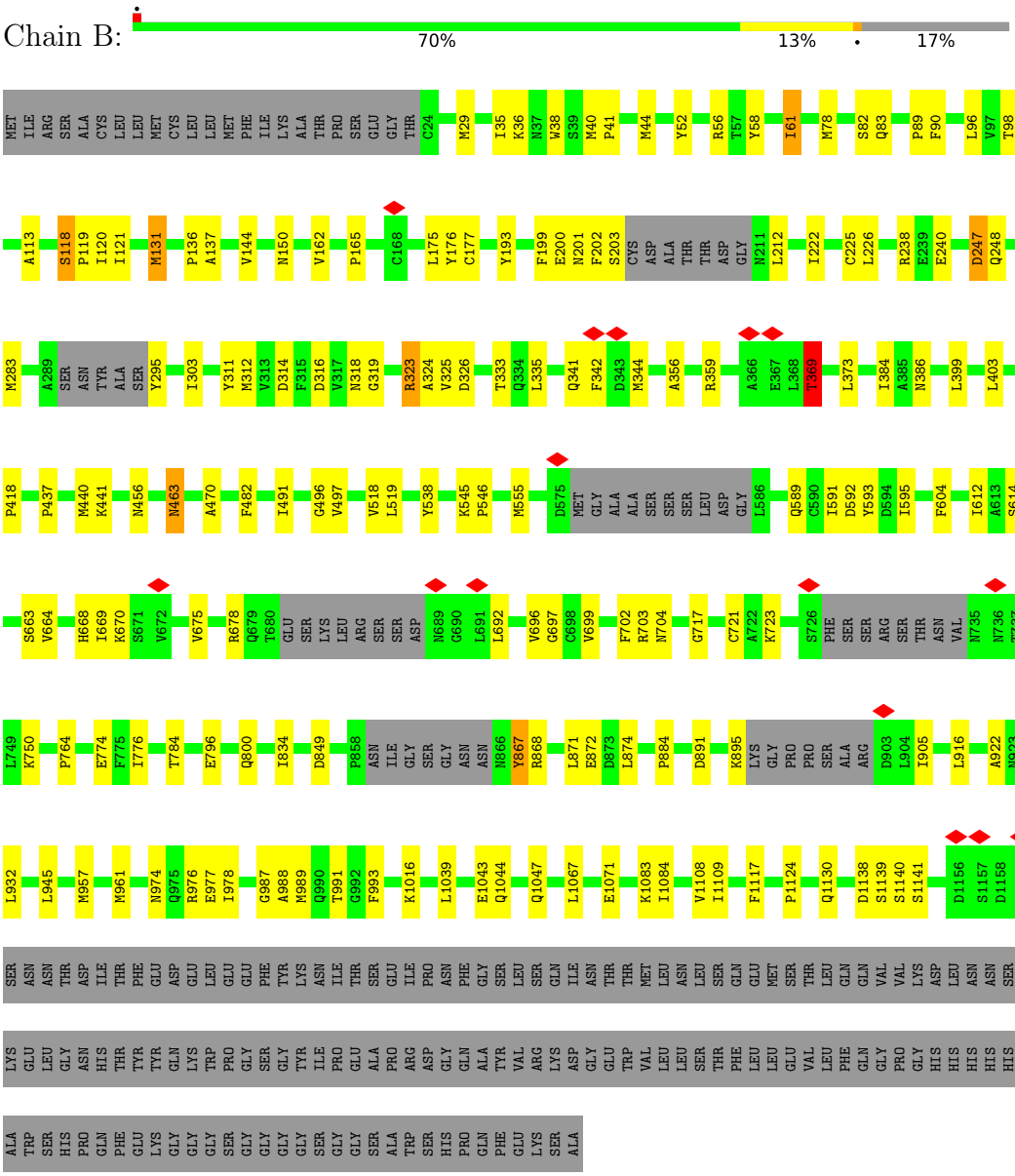
• Molecule 1: Spike glycoprotein,Fibritin

Chain A:



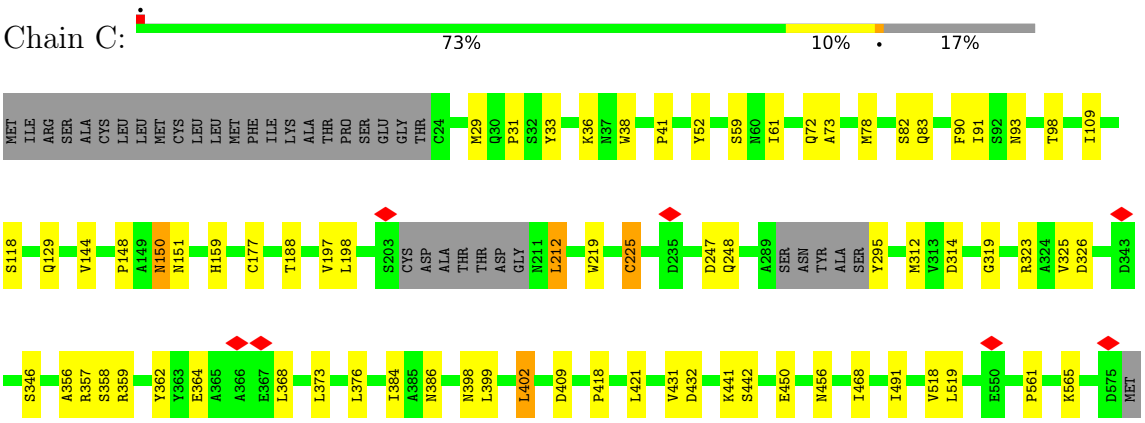
• Molecule 1: Spike glycoprotein,Fibritin

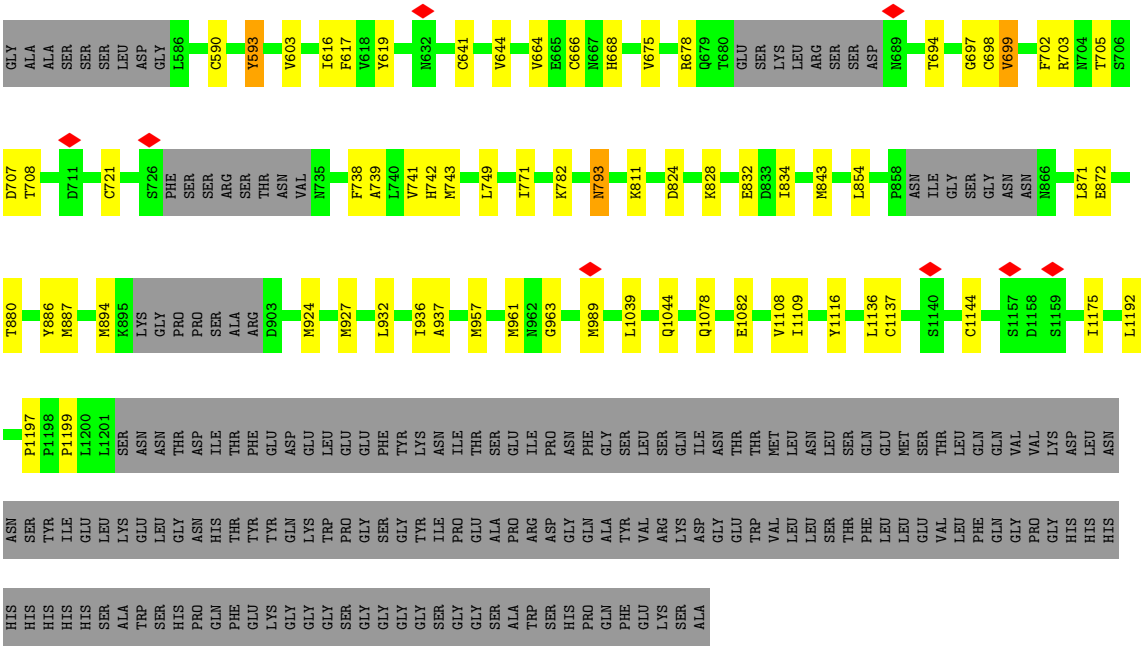
Chain B:



• Molecule 1: Spike glycoprotein,Fibritin

Chain C:



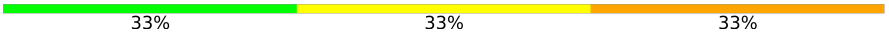


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

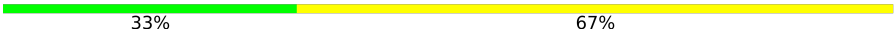
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain F:



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

Chain H:

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

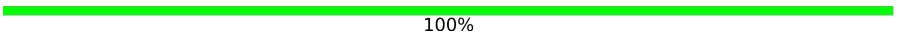
Chain I:

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

Chain K:

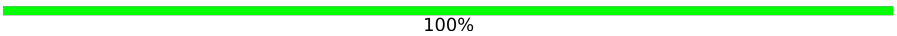
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82386	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	0.214	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0253	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: EIC, NAG, FOL, BMA

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	0.33	3/8989 (0.0%)	0.50	11/12197 (0.1%)
1	B	0.39	2/8989 (0.0%)	0.53	6/12197 (0.0%)
1	C	0.32	0/8989	0.49	7/12197 (0.1%)
All	All	0.34	5/26967 (0.0%)	0.51	24/36591 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	ASP	CA-C	-5.50	1.45	1.53
1	B	312	MET	CA-C	-5.45	1.46	1.52
1	B	247	ASP	CA-C	-5.38	1.47	1.53
1	A	409	ASP	CA-CB	-5.23	1.47	1.53
1	A	409	ASP	C-O	-5.11	1.18	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1140	SER	N-CA-C	7.77	119.75	111.28
1	A	224	ASP	CA-C-N	-7.72	112.07	122.72
1	A	224	ASP	C-N-CA	-7.72	112.07	122.72
1	C	963	GLY	N-CA-C	-7.62	105.20	114.66
1	B	496	GLY	O-C-N	-7.09	116.71	122.81
1	A	260	GLY	N-CA-C	7.03	123.72	111.50
1	C	1197	PRO	CA-C-N	-6.96	113.21	120.38
1	C	1197	PRO	C-N-CA	-6.96	113.21	120.38
1	B	369	THR	N-CA-C	6.53	119.70	110.50
1	A	148	PRO	N-CA-C	6.10	122.01	113.53
1	B	991	THR	N-CA-C	-6.06	106.14	112.93
1	A	224	ASP	CB-CA-C	-5.98	102.67	112.06
1	A	148	PRO	CB-CA-C	-5.69	103.23	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	118	SER	N-CA-C	5.57	116.83	109.93
1	A	262	SER	N-CA-C	5.49	115.27	108.19
1	A	135	TYR	CA-C-N	5.48	125.46	120.03
1	A	135	TYR	C-N-CA	5.48	125.46	120.03
1	C	699	VAL	N-CA-C	5.48	116.62	108.46
1	C	148	PRO	CB-CA-C	-5.38	103.74	112.62
1	C	886	TYR	N-CA-C	-5.26	101.36	109.52
1	A	410	GLU	N-CA-C	5.12	117.58	109.50
1	B	593	TYR	N-CA-C	5.06	116.68	109.14
1	C	593	TYR	N-CA-C	5.06	116.88	109.24
1	A	842	LEU	N-CA-C	5.01	119.04	113.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8792	0	8478	110	0
1	B	8792	0	8478	129	0
1	C	8792	0	8478	98	0
2	D	39	0	34	0	0
2	E	39	0	34	6	0
2	F	39	0	34	3	0
2	H	39	0	34	0	0
2	I	39	0	34	0	0
2	K	39	0	34	0	0
3	G	28	0	25	0	0
3	J	28	0	25	0	0
4	A	182	0	169	0	0
4	B	168	0	156	2	0
4	C	168	0	156	1	0
5	A	32	0	17	3	0
5	B	32	0	17	5	0
5	C	32	0	17	3	0
6	A	20	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	20	0	31	3	0
6	C	20	0	31	5	0
All	All	27340	0	26313	326	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (326) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASN:HD22	1:A:401:LYS:HE2	1.43	0.82
1:A:401:LYS:HG3	2:E:1:NAG:HN2	1.42	0.82
1:B:200:GLU:HG2	1:B:201:ASN:H	1.50	0.75
1:A:429:LEU:HD21	6:C:1401:EIC:H121	1.69	0.74
1:A:409:ASP:O	1:C:442:SER:HB2	1.88	0.74
1:A:1137:CYS:HB3	1:A:1144:CYS:HA	1.70	0.73
1:B:867:TYR:CD2	1:B:927:MET:HG2	2.26	0.71
1:C:118:SER:H	5:C:1414:FOL:HN1	1.38	0.71
1:A:401:LYS:HA	2:E:1:NAG:H82	1.73	0.70
1:A:699:VAL:HG21	1:A:702:PHE:CD2	2.25	0.70
1:A:118:SER:O	5:A:1414:FOL:NA2	2.25	0.70
6:A:1415:EIC:H51	1:B:418:PRO:HB3	1.75	0.68
1:C:872:GLU:HG2	1:C:1109:ILE:HG23	1.76	0.68
1:B:591:ILE:HD11	1:B:604:PHE:CD2	2.29	0.68
1:A:241:TRP:HB3	1:A:265:MET:HE2	1.74	0.67
1:B:247:ASP:CG	1:B:248:GLN:H	2.02	0.67
1:B:867:TYR:CE2	1:B:927:MET:HG2	2.29	0.67
1:A:923:ASN:O	1:A:927:MET:HG3	1.95	0.66
1:B:98:THR:HG21	1:B:144:VAL:HG11	1.75	0.66
1:A:359:ARG:HG3	1:A:589:GLN:HB3	1.76	0.66
1:B:200:GLU:HG2	1:B:201:ASN:N	2.11	0.65
6:B:1414:EIC:H41	1:C:418:PRO:HB3	1.78	0.65
1:A:28:ASP:HB2	1:A:88:ARG:HE	1.61	0.65
1:C:843:MET:HE1	1:C:936:ILE:HG13	1.79	0.65
1:C:1137:CYS:HB3	1:C:1144:CYS:HA	1.79	0.65
1:C:1078:GLN:NE2	1:C:1082:GLU:OE1	2.31	0.64
1:C:924:MET:HA	1:C:927:MET:HG3	1.81	0.63
1:C:41:PRO:HD2	5:C:1414:FOL:HB1	1.80	0.62
1:C:177:CYS:HB3	1:C:225:CYS:HA	1.81	0.62
1:A:180:GLU:HB2	1:A:221:ASN:HB2	1.82	0.62
1:A:421:LEU:HB3	6:C:1401:EIC:H91	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:TYR:HB3	1:B:61:ILE:HD12	1.83	0.61
1:C:312:MET:HE1	1:C:323:ARG:NH2	2.15	0.61
1:C:699:VAL:HG21	1:C:702:PHE:CD2	2.35	0.61
1:B:40:MET:HG2	5:B:1412:FOL:H16	1.81	0.61
1:C:314:ASP:OD1	1:C:323:ARG:HG3	2.01	0.61
1:B:796:GLU:OE2	1:B:800:GLN:NE2	2.32	0.61
1:A:409:ASP:OD2	1:A:441:LYS:NZ	2.30	0.60
1:C:957:MET:O	1:C:961:MET:HG3	2.01	0.60
1:B:987:GLY:O	1:B:988:ALA:C	2.43	0.59
1:A:771:ILE:HG21	1:A:989:MET:HG3	1.86	0.57
1:B:409:ASP:OD2	1:B:441:LYS:NZ	2.37	0.57
1:C:708:THR:HG22	1:C:742:HIS:HB2	1.87	0.57
1:B:118:SER:H	5:B:1412:FOL:HN1	1.52	0.57
1:C:705:THR:HG22	1:C:707:ASP:H	1.68	0.57
1:C:699:VAL:CG2	1:C:702:PHE:HD2	2.17	0.57
1:C:98:THR:HG21	1:C:144:VAL:HG11	1.85	0.57
1:C:666:CYS:N	1:C:698:CYS:SG	2.78	0.56
1:A:443:THR:HG22	1:A:450:GLU:HG3	1.88	0.56
1:C:129:GLN:HE22	1:C:295:TYR:HB2	1.71	0.56
1:C:356:ALA:HA	1:C:675:VAL:HG11	1.88	0.56
1:A:135:TYR:HE1	1:A:240:GLU:OE2	1.89	0.56
1:C:771:ILE:HG21	1:C:989:MET:HG3	1.87	0.56
6:A:1415:EIC:H22	1:B:408:VAL:HG21	1.88	0.56
1:A:401:LYS:HG3	2:E:1:NAG:N2	2.19	0.56
1:A:945:LEU:HD21	1:A:1089:LYS:HD3	1.88	0.56
1:C:83:GLN:HE22	1:C:295:TYR:HA	1.71	0.56
1:A:666:CYS:HB3	1:A:691:LEU:HD23	1.88	0.55
1:A:838:GLN:HG2	1:C:749:LEU:HB2	1.89	0.55
1:B:314:ASP:OD1	1:B:323:ARG:NH1	2.40	0.55
1:C:323:ARG:NH1	1:C:325:VAL:HG23	2.21	0.55
1:B:326:ASP:OD1	1:B:678:ARG:NH2	2.36	0.55
1:B:356:ALA:HA	1:B:675:VAL:HG11	1.88	0.55
1:A:359:ARG:NH2	1:A:671:SER:O	2.40	0.55
1:B:1196:LEU:HB2	1:B:1201:LEU:HD13	1.87	0.55
1:B:748:PRO:O	1:B:750:LYS:NZ	2.38	0.55
1:A:40:MET:HG2	5:A:1414:FOL:H16	1.89	0.55
1:C:82:SER:OG	1:C:90:PHE:O	2.23	0.55
1:B:884:PRO:HA	1:B:905:ILE:HD13	1.88	0.55
1:C:247:ASP:OD1	1:C:248:GLN:N	2.35	0.55
1:B:83:GLN:HE22	1:B:295:TYR:HA	1.72	0.55
1:A:357:ARG:C	1:A:357:ARG:HD2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:THR:OG1	1:C:697:GLY:O	2.25	0.54
1:B:41:PRO:HD2	5:B:1412:FOL:HB1	1.88	0.54
1:B:165:PRO:O	1:B:212:LEU:HD12	2.07	0.54
1:B:1039:LEU:O	1:B:1044:GLN:NE2	2.41	0.54
1:A:127:ASN:O	1:A:129:GLN:NE2	2.40	0.54
1:C:373:LEU:HD13	1:C:402:LEU:HD21	1.90	0.54
1:C:644:VAL:HG13	1:C:664:VAL:HG21	1.88	0.54
1:C:312:MET:HE1	1:C:323:ARG:CZ	2.37	0.54
1:A:177:CYS:HB3	1:A:225:CYS:HA	1.89	0.54
1:A:83:GLN:HE22	1:A:295:TYR:HA	1.72	0.54
1:A:703:ARG:HG2	1:A:738:PHE:O	2.09	0.54
1:C:1039:LEU:O	1:C:1044:GLN:NE2	2.41	0.53
1:B:868:ARG:HG3	1:B:872:GLU:CB	2.38	0.53
1:C:398:ASN:O	1:C:402:LEU:HD13	2.09	0.53
1:B:323:ARG:HH21	1:B:325:VAL:CG2	2.22	0.53
1:B:849:ASP:OD2	1:B:976:ARG:NH1	2.40	0.53
1:A:82:SER:OG	1:A:90:PHE:O	2.27	0.53
1:A:699:VAL:CG2	1:A:702:PHE:CD2	2.90	0.53
1:A:164:LEU:HD13	1:A:212:LEU:HD23	1.91	0.53
1:A:356:ALA:HA	1:A:675:VAL:HG11	1.89	0.53
1:B:867:TYR:CD2	1:B:867:TYR:N	2.77	0.53
1:A:58:TYR:HB3	1:A:61:ILE:HD13	1.91	0.53
1:B:107:ILE:HG12	1:B:303:ILE:HG12	1.91	0.52
1:C:150:ASN:O	1:C:151:ASN:HB2	2.08	0.52
1:A:418:PRO:HB3	6:C:1401:EIC:H51	1.90	0.52
1:B:692:LEU:HD11	1:B:704:ASN:HB2	1.89	0.52
1:B:1016:LYS:HE2	1:C:811:LYS:HD3	1.92	0.52
1:B:177:CYS:SG	1:B:222:ILE:HG23	2.49	0.52
1:B:325:VAL:HG13	1:B:333:THR:HG22	1.91	0.52
1:C:59:SER:H	1:C:61:ILE:HD12	1.74	0.52
6:A:1415:EIC:H72	1:B:399:LEU:HD21	1.91	0.52
1:B:335:LEU:HG	1:B:344:MET:HE1	1.91	0.52
1:B:162:VAL:HB	1:B:175:LEU:HB2	1.91	0.51
1:B:699:VAL:HG21	1:B:702:PHE:CD2	2.46	0.51
1:C:616:ILE:HG22	1:C:617:PHE:HD1	1.74	0.51
1:A:139:LEU:HD13	1:A:162:VAL:HG22	1.92	0.51
1:C:409:ASP:OD2	1:C:441:LYS:NZ	2.34	0.51
1:A:565:LYS:HB2	1:B:56:ARG:HD3	1.92	0.51
1:B:721:CYS:HB2	1:B:741:VAL:HG23	1.93	0.51
1:C:312:MET:HE1	1:C:323:ARG:NH1	2.25	0.51
1:A:106:VAL:HG23	1:A:304:TYR:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HD21	1:A:561:PRO:HG3	1.93	0.51
1:A:357:ARG:HD2	1:A:357:ARG:O	2.10	0.50
1:A:924:MET:HE1	1:C:743:MET:HB3	1.92	0.50
1:B:113:ALA:HB3	2:F:1:NAG:H82	1.92	0.50
1:C:314:ASP:CG	1:C:323:ARG:HG3	2.36	0.50
1:C:854:LEU:HD22	1:C:871:LEU:HD13	1.93	0.50
1:B:150:ASN:HD22	1:B:193:TYR:HB3	1.76	0.50
1:A:401:LYS:HG2	2:E:1:NAG:C8	2.41	0.50
1:B:44:MET:HB2	1:B:324:ALA:O	2.11	0.50
1:B:776:ILE:HD11	1:B:1083:LYS:HD2	1.93	0.50
1:A:437:PRO:HG2	1:A:440:MET:HG3	1.92	0.50
1:C:188:THR:HG23	1:C:219:TRP:HE3	1.77	0.50
1:C:198:LEU:HB3	1:C:212:LEU:HD22	1.93	0.50
1:B:491:ILE:HG12	1:B:518:VAL:HG21	1.93	0.50
1:B:663:SER:H	1:B:697:GLY:HA3	1.76	0.50
1:A:364:GLU:HB3	1:A:595:ILE:HA	1.94	0.49
1:B:703:ARG:HG2	1:B:738:PHE:O	2.11	0.49
1:A:238:ARG:NH1	1:A:261:TYR:HD1	2.10	0.49
1:A:384:ILE:HG13	1:A:456:ASN:HB3	1.94	0.49
1:C:33:TYR:O	1:C:36:LYS:NZ	2.45	0.49
1:B:644:VAL:HG13	1:B:664:VAL:HG11	1.93	0.49
1:C:703:ARG:NH2	1:C:739:ALA:HB2	2.26	0.49
1:A:386:ASN:HB2	1:A:519:LEU:HD11	1.93	0.49
1:B:119:PRO:O	1:B:121:ILE:N	2.41	0.49
1:A:894:MET:HG2	1:C:668:HIS:NE2	2.28	0.49
1:C:699:VAL:CG2	1:C:702:PHE:CD2	2.96	0.49
1:C:932:LEU:HD23	1:C:1108:VAL:HG11	1.95	0.49
1:A:791:VAL:O	1:A:1055:ARG:NH1	2.41	0.49
1:C:834:ILE:HG23	1:C:932:LEU:HD22	1.95	0.49
1:A:335:LEU:HG	1:A:344:MET:HE2	1.94	0.49
1:A:262:SER:OG	1:A:263:ASN:N	2.45	0.48
1:A:505:GLN:HB2	1:A:508:GLN:HG3	1.95	0.48
1:B:868:ARG:NH2	1:B:922:ALA:HB1	2.28	0.48
1:B:82:SER:OG	1:B:90:PHE:O	2.30	0.48
1:C:78:MET:HE3	1:C:78:MET:HB3	1.73	0.48
1:A:56:ARG:HD3	1:C:565:LYS:HG3	1.96	0.48
1:B:834:ILE:HG23	1:B:932:LEU:HD22	1.95	0.48
6:B:1414:EIC:H82	1:C:399:LEU:HD13	1.95	0.48
1:C:384:ILE:HG13	1:C:456:ASN:HB3	1.96	0.48
1:A:651:ASP:OD2	1:A:724:PRO:HG3	2.13	0.48
1:B:589:GLN:O	1:B:591:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:GLN:N	1:C:326:ASP:OD2	2.46	0.48
1:C:793:ASN:O	1:C:793:ASN:ND2	2.31	0.48
1:C:880:THR:O	1:C:880:THR:OG1	2.30	0.48
1:B:109:ILE:HD12	1:B:136:PRO:HG3	1.96	0.48
1:B:176:TYR:CD2	1:B:226:LEU:HD12	2.49	0.48
1:B:463:ASN:OD1	1:B:463:ASN:N	2.45	0.47
1:C:323:ARG:HD2	1:C:323:ARG:C	2.39	0.47
1:B:670:LYS:HE2	1:B:670:LYS:H	1.78	0.47
1:C:1109:ILE:HB	1:C:1116:TYR:HB3	1.96	0.47
1:B:109:ILE:HB	1:B:240:GLU:HG2	1.95	0.47
1:B:386:ASN:HB2	1:B:519:LEU:HD11	1.96	0.47
1:A:670:LYS:HA	1:A:673:ALA:HB2	1.96	0.47
1:A:708:THR:HB	1:A:744:LEU:HB2	1.95	0.47
1:A:957:MET:O	1:A:961:MET:HG3	2.14	0.47
1:B:612:ILE:HG22	1:B:614:SER:H	1.80	0.47
1:A:373:LEU:HB3	1:A:402:LEU:HD11	1.96	0.47
1:B:52:TYR:OH	1:B:319:GLY:O	2.31	0.47
1:B:545:LYS:HD3	1:B:546:PRO:HD2	1.96	0.47
6:C:1401:EIC:H81	6:C:1401:EIC:H112	1.72	0.47
1:A:200:GLU:OE1	1:A:285:ARG:NH2	2.48	0.47
1:A:545:LYS:HD3	1:A:546:PRO:HD2	1.96	0.47
6:A:1415:EIC:H142	1:B:373:LEU:HD13	1.97	0.47
1:B:261:TYR:HD2	2:F:3:BMA:H5	1.79	0.47
1:A:432:ASP:HB2	1:A:558:VAL:HB	1.97	0.47
1:B:238:ARG:HH12	1:B:261:TYR:HB3	1.80	0.47
1:B:437:PRO:HG2	1:B:440:MET:HG2	1.97	0.47
1:B:764:PRO:HB3	1:B:1124:PRO:HB3	1.96	0.46
1:B:774:GLU:HG3	1:B:1117:PHE:HB2	1.97	0.46
1:B:868:ARG:HG3	1:B:872:GLU:HB2	1.96	0.46
1:C:52:TYR:OH	1:C:319:GLY:O	2.31	0.46
1:B:497:VAL:HA	1:B:538:TYR:HE2	1.80	0.46
1:A:1040:ASP:OD1	1:A:1040:ASP:N	2.49	0.46
1:A:150:ASN:HD22	1:A:193:TYR:HB3	1.80	0.46
1:B:591:ILE:HD11	1:B:604:PHE:HD2	1.78	0.46
1:A:98:THR:HG21	1:A:144:VAL:HG21	1.98	0.46
1:B:118:SER:C	1:B:120:ILE:H	2.23	0.46
1:B:868:ARG:HG3	1:B:872:GLU:HB3	1.98	0.46
1:A:401:LYS:HG2	2:E:1:NAG:H82	1.98	0.46
1:C:326:ASP:OD1	1:C:678:ARG:NH1	2.40	0.46
1:A:872:GLU:HG2	1:A:1109:ILE:HG23	1.97	0.46
1:B:323:ARG:NH2	1:B:342:PHE:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:SER:N	5:C:1414:FOL:HN1	2.11	0.46
1:B:702:PHE:CE1	1:B:738:PHE:HB2	2.52	0.45
1:B:137:ALA:HB1	1:B:283:MET:HE3	1.99	0.45
1:C:843:MET:SD	1:C:937:ALA:HB2	2.56	0.45
1:A:694:THR:OG1	1:A:697:GLY:O	2.32	0.45
1:B:384:ILE:HG13	1:B:456:ASN:HB3	1.97	0.45
1:A:651:ASP:OD1	1:A:651:ASP:C	2.60	0.45
1:A:692:LEU:HD11	1:A:704:ASN:HB2	1.98	0.45
1:C:491:ILE:HG12	1:C:518:VAL:HG21	1.99	0.45
1:B:314:ASP:HB2	1:B:323:ARG:HG2	1.96	0.45
1:A:989:MET:HE3	1:A:989:MET:HB3	1.71	0.45
1:B:150:ASN:HA	4:B:1404:NAG:H82	1.99	0.45
1:B:247:ASP:CG	1:B:248:GLN:N	2.68	0.45
1:C:432:ASP:OD1	1:C:432:ASP:N	2.48	0.45
1:A:406:VAL:HB	1:A:470:ALA:HB1	1.99	0.45
1:A:894:MET:HE1	1:C:603:VAL:HG21	1.98	0.45
1:B:202:PHE:CD1	1:B:203:SER:N	2.84	0.45
1:B:314:ASP:CG	1:B:323:ARG:NH1	2.75	0.45
1:B:323:ARG:CZ	1:B:342:PHE:HB3	2.46	0.45
1:B:399:LEU:HG	1:B:403:LEU:HD23	1.98	0.45
1:B:1130:GLN:HA	4:B:1411:NAG:H82	1.98	0.45
1:C:36:LYS:HG3	1:C:38:TRP:CH2	2.52	0.45
1:A:223:LYS:O	1:A:224:ASP:C	2.57	0.44
1:B:987:GLY:C	1:B:989:MET:N	2.74	0.44
1:A:1095:SER:HB2	1:B:945:LEU:HD11	2.00	0.44
1:C:421:LEU:HD21	1:C:561:PRO:HG3	1.98	0.44
1:B:131:MET:HE1	5:B:1412:FOL:C4A	2.47	0.44
1:C:362:TYR:OH	1:C:364:GLU:OE2	2.31	0.44
1:C:565:LYS:HB2	1:C:619:TYR:CZ	2.52	0.44
1:A:264:ASN:HD22	1:A:320:TYR:HD1	1.66	0.44
1:A:316:ASP:OD1	1:A:318:ASN:N	2.51	0.44
1:B:699:VAL:CG2	1:B:702:PHE:HD2	2.31	0.44
1:C:782:LYS:NZ	1:C:824:ASP:OD1	2.44	0.44
1:B:89:PRO:HG3	1:B:199:PHE:CD1	2.53	0.44
1:B:359:ARG:HD3	1:B:589:GLN:HB3	2.00	0.44
1:B:668:HIS:NE2	1:C:894:MET:HG2	2.33	0.44
1:C:109:ILE:HD13	1:C:109:ILE:HA	1.86	0.44
1:A:426:TYR:HE1	1:A:429:LEU:HB2	1.83	0.43
1:A:665:GLU:OE1	1:A:667:ASN:ND2	2.51	0.43
1:B:238:ARG:HE	1:B:238:ARG:HB2	1.57	0.43
1:A:312:MET:HE2	1:A:323:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH1	1:A:359:ARG:HA	2.33	0.43
1:B:323:ARG:HH21	1:B:325:VAL:HG21	1.84	0.43
1:A:131:MET:HE2	1:A:131:MET:HB2	1.90	0.43
1:A:767:PHE:O	1:A:981:LYS:NZ	2.43	0.43
1:B:723:LYS:HB2	1:B:723:LYS:HE3	1.80	0.43
1:B:924:MET:HA	1:B:927:MET:HE3	2.00	0.43
6:B:1414:EIC:H32	1:C:468:ILE:HD13	2.00	0.43
1:C:312:MET:HE1	1:C:323:ARG:HH22	1.81	0.43
1:A:316:ASP:OD1	1:A:316:ASP:C	2.61	0.43
1:B:176:TYR:HD2	1:B:226:LEU:HD12	1.84	0.43
1:B:482:PHE:HZ	1:B:555:MET:HE2	1.83	0.43
1:C:150:ASN:HA	4:C:1405:NAG:H82	2.00	0.43
1:C:887:MET:HE2	1:C:887:MET:HB3	1.85	0.43
1:C:91:ILE:HD13	1:C:197:VAL:HG22	2.00	0.43
1:A:40:MET:HA	5:A:1414:FOL:HG2	2.01	0.43
1:A:1039:LEU:O	1:A:1044:GLN:NE2	2.52	0.43
1:B:36:LYS:HG3	1:B:38:TRP:CH2	2.53	0.43
1:C:29:MET:HG2	1:C:31:PRO:HD3	2.01	0.43
1:C:1136:LEU:HD22	1:C:1192:LEU:HD11	1.99	0.43
1:A:36:LYS:HG3	1:A:38:TRP:CH2	2.54	0.43
1:A:777:GLU:OE2	1:A:1069:ARG:NH2	2.52	0.43
1:B:957:MET:O	1:B:961:MET:HG3	2.18	0.43
1:C:159:HIS:CD2	1:C:177:CYS:HA	2.54	0.43
1:C:590:CYS:HB2	1:C:641:CYS:HB2	1.97	0.43
1:A:764:PRO:HB3	1:A:1124:PRO:HB3	2.01	0.43
1:B:40:MET:HE3	5:B:1412:FOL:HB2	2.01	0.43
1:B:1138:ASP:OD2	1:B:1141:SER:HB3	2.18	0.43
1:C:150:ASN:O	1:C:151:ASN:CB	2.66	0.43
1:C:1175:ILE:HG22	1:C:1199:PRO:HG2	2.01	0.43
1:A:91:ILE:HD13	1:A:197:VAL:HG22	2.00	0.42
1:A:127:ASN:O	1:A:128:PHE:C	2.61	0.42
1:A:408:VAL:HG21	6:C:1401:EIC:H32	2.00	0.42
1:B:774:GLU:OE1	1:B:1083:LYS:HD3	2.19	0.42
1:B:311:TYR:CE2	1:B:324:ALA:HB1	2.54	0.42
1:C:989:MET:HB3	1:C:989:MET:HE3	1.60	0.42
1:A:776:ILE:HD11	1:A:1083:LYS:HD2	2.01	0.42
1:B:118:SER:C	1:B:120:ILE:N	2.77	0.42
1:A:509:MET:HE2	1:B:274:TYR:HB2	2.01	0.42
1:C:41:PRO:HB2	1:C:73:ALA:HA	2.01	0.42
1:C:386:ASN:HB2	1:C:519:LEU:HD11	2.00	0.42
1:A:38:TRP:HZ3	1:A:80:VAL:HG11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:PHE:HE2	1:A:1006:VAL:HG21	1.84	0.42
1:C:721:CYS:HB2	1:C:741:VAL:HG23	2.01	0.42
1:A:316:ASP:OD1	1:A:319:GLY:N	2.53	0.42
1:A:398:ASN:ND2	1:A:401:LYS:HE2	2.22	0.42
1:A:524:ASP:OD1	1:A:543:SER:OG	2.35	0.42
1:B:316:ASP:OD1	1:B:318:ASN:N	2.53	0.42
1:B:595:ILE:H	1:B:595:ILE:HG12	1.63	0.42
1:B:891:ASP:O	1:B:895:LYS:HG2	2.20	0.42
1:C:828:LYS:O	1:C:832:GLU:HG2	2.19	0.42
1:B:872:GLU:HG3	1:B:1109:ILE:HD12	2.02	0.42
1:C:957:MET:HE3	1:C:957:MET:HB3	1.88	0.42
1:B:696:VAL:HG11	1:B:717:GLY:HA3	2.00	0.41
1:A:246:GLN:NE2	1:A:275:ASP:O	2.50	0.41
1:A:615:GLN:HG2	1:B:56:ARG:O	2.20	0.41
1:B:834:ILE:HG12	1:B:1084:ILE:HD13	2.03	0.41
1:A:430:THR:HB	1:A:560:THR:HB	2.00	0.41
1:B:247:ASP:OD2	1:B:248:GLN:N	2.52	0.41
1:C:31:PRO:HB3	1:C:93:ASN:HB2	2.00	0.41
1:C:357:ARG:NH2	1:C:359:ARG:HE	2.19	0.41
1:A:448:SER:OG	6:A:1415:EIC:O1	2.33	0.41
1:A:399:LEU:HD12	1:A:399:LEU:HA	1.87	0.41
1:B:238:ARG:HB3	2:F:1:NAG:H3	2.02	0.41
1:B:1043:GLU:O	1:B:1047:GLN:HG2	2.21	0.41
1:B:314:ASP:CG	1:B:323:ARG:HH11	2.29	0.41
1:B:341:GLN:HG3	1:B:344:MET:HG2	2.02	0.41
1:B:406:VAL:HB	1:B:470:ALA:HB1	2.02	0.41
1:B:974:ASN:HB2	1:B:977:GLU:HB2	2.03	0.41
1:B:1067:LEU:O	1:B:1071:GLU:HG2	2.20	0.41
1:A:451:ALA:HA	1:A:454:MET:HG2	2.03	0.41
1:A:254:TYR:HB3	1:A:265:MET:HB3	2.02	0.40
1:C:376:LEU:HD21	1:C:431:VAL:HG11	2.02	0.40
1:C:593:TYR:CD1	1:C:593:TYR:C	2.99	0.40
1:A:401:LYS:CG	2:E:1:NAG:H82	2.50	0.40
1:B:871:LEU:HD12	1:B:871:LEU:HA	1.95	0.40
1:B:874:LEU:HD23	1:B:993:PHE:CD1	2.57	0.40
1:C:368:LEU:HD23	1:C:368:LEU:HA	1.92	0.40
1:A:132:LYS:O	1:A:299:SER:N	2.46	0.40
1:B:29:MET:HE1	1:B:96:LEU:HD11	2.02	0.40
1:B:109:ILE:HD12	1:B:136:PRO:CD	2.51	0.40
1:C:357:ARG:NH1	1:C:358:SER:O	2.54	0.40
1:C:961:MET:HE2	1:C:961:MET:HB3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:HE1	1:A:309:ILE:HG21	1.86	0.40
1:A:932:LEU:HD23	1:A:1108:VAL:HG11	2.03	0.40
1:B:369:THR:H	1:B:369:THR:HG22	1.60	0.40
1:A:336:GLN:O	1:A:340:GLY:N	2.54	0.40
1:B:78:MET:HE3	1:B:78:MET:HB3	1.84	0.40
1:B:784:THR:HG23	1:B:916:LEU:HD11	2.04	0.40
1:B:974:ASN:O	1:B:978:ILE:HG12	2.22	0.40
1:C:702:PHE:CE1	1:C:738:PHE:HB2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1110/1353 (82%)	1077 (97%)	33 (3%)	0	100	100
1	B	1110/1353 (82%)	1067 (96%)	43 (4%)	0	100	100
1	C	1110/1353 (82%)	1066 (96%)	44 (4%)	0	100	100
All	All	3330/4059 (82%)	3210 (96%)	120 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	971/1162 (84%)	968 (100%)	3 (0%)	91 96
1	B	971/1162 (84%)	959 (99%)	12 (1%)	67 86
1	C	971/1162 (84%)	964 (99%)	7 (1%)	81 91
All	All	2913/3486 (84%)	2891 (99%)	22 (1%)	77 90

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	699	VAL
1	A	843	MET
1	A	1145	ILE
1	B	35	ILE
1	B	61	ILE
1	B	131	MET
1	B	225	CYS
1	B	323	ARG
1	B	369	THR
1	B	463	ASN
1	B	592	ASP
1	B	669	ILE
1	B	867	TYR
1	B	1108	VAL
1	B	1139	SER
1	C	150	ASN
1	C	212	LEU
1	C	225	CYS
1	C	346	SER
1	C	402	LEU
1	C	450	GLU
1	C	793	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	159	HIS
1	A	221	ASN
1	A	589	GLN
1	A	668	HIS
1	A	693	GLN
1	A	765	GLN

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Mol	Chain	Res	Type
1	A	781	GLN
1	A	789	GLN
1	A	823	GLN
1	A	1001	GLN
1	A	1125	GLN
1	B	71	HIS
1	B	159	HIS
1	B	249	GLN
1	B	307	HIS
1	B	355	ASN
1	B	533	GLN
1	B	667	ASN
1	B	679	GLN
1	B	742	HIS
1	B	746	GLN
1	B	781	GLN
1	B	1001	GLN
1	B	1047	GLN
1	B	1066	GLN
1	B	1078	GLN
1	B	1085	ASN
1	B	1091	GLN
1	C	129	GLN
1	C	310	ASN
1	C	533	GLN
1	C	693	GLN
1	C	765	GLN
1	C	781	GLN
1	C	823	GLN
1	C	962	ASN
1	C	969	ASN
1	C	998	GLN
1	C	1001	GLN
1	C	1044	GLN
1	C	1125	GLN
1	C	1155	ASN
1	C	1190	GLN

5.3.3 RNA

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)

22 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.18	0	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.42	0	17,19,21	1.04	1 (5%)
2	BMA	D	3	2	11,11,12	0.46	0	15,15,17	1.16	2 (13%)
2	NAG	E	1	2,1	14,14,15	0.87	1 (7%)	17,19,21	0.95	1 (5%)
2	NAG	E	2	2	14,14,15	0.22	0	17,19,21	0.53	0
2	BMA	E	3	2	11,11,12	0.84	1 (9%)	15,15,17	1.23	2 (13%)
2	NAG	F	1	2,1	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	BMA	F	3	2	11,11,12	0.66	0	15,15,17	0.85	0
3	NAG	G	1	3,1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	G	2	3	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	H	1	2,1	14,14,15	0.29	0	17,19,21	0.58	0
2	NAG	H	2	2	14,14,15	0.26	0	17,19,21	0.46	0
2	BMA	H	3	2	11,11,12	0.57	0	15,15,17	0.88	1 (6%)
2	NAG	I	1	2,1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.20	0	17,19,21	0.41	0
2	BMA	I	3	2	11,11,12	0.63	0	15,15,17	1.04	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.49	0	17,19,21	0.64	0
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	0.44	0
2	NAG	K	1	2,1	14,14,15	0.24	0	17,19,21	0.66	1 (5%)
2	NAG	K	2	2	14,14,15	0.23	0	17,19,21	0.46	0
2	BMA	K	3	2	11,11,12	0.59	0	15,15,17	0.87	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	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-3.09	1.38	1.43
2	E	3	BMA	C1-C2	2.30	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	BMA	C1-O5-C5	3.32	116.69	112.19
2	D	2	NAG	C1-O5-C5	3.05	116.33	112.19
2	I	3	BMA	C1-O5-C5	2.41	115.46	112.19
2	E	3	BMA	C1-O5-C5	2.29	115.30	112.19
2	E	1	NAG	C3-C4-C5	2.17	114.11	110.24
2	K	1	NAG	C1-O5-C5	2.12	115.06	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	3	BMA	C1-O5-C5	2.09	115.02	112.19
2	H	3	BMA	C1-O5-C5	2.06	114.98	112.19
2	E	3	BMA	O2-C2-C3	-2.05	106.02	110.14
2	D	3	BMA	O2-C2-C3	-2.05	106.04	110.14

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C1-C2-N2-C7
2	H	1	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C3-C2-N2-C7

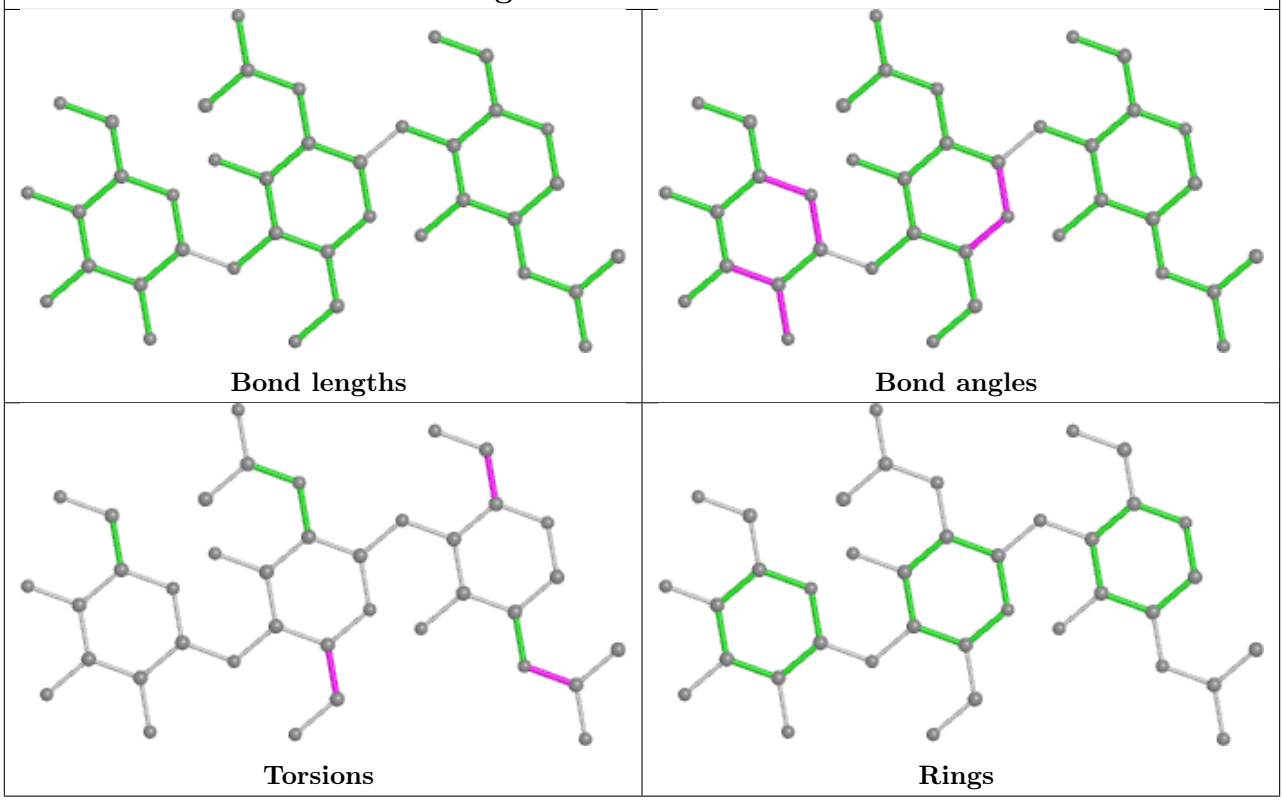
There are no ring outliers.

3 monomers are involved in 9 short contacts:

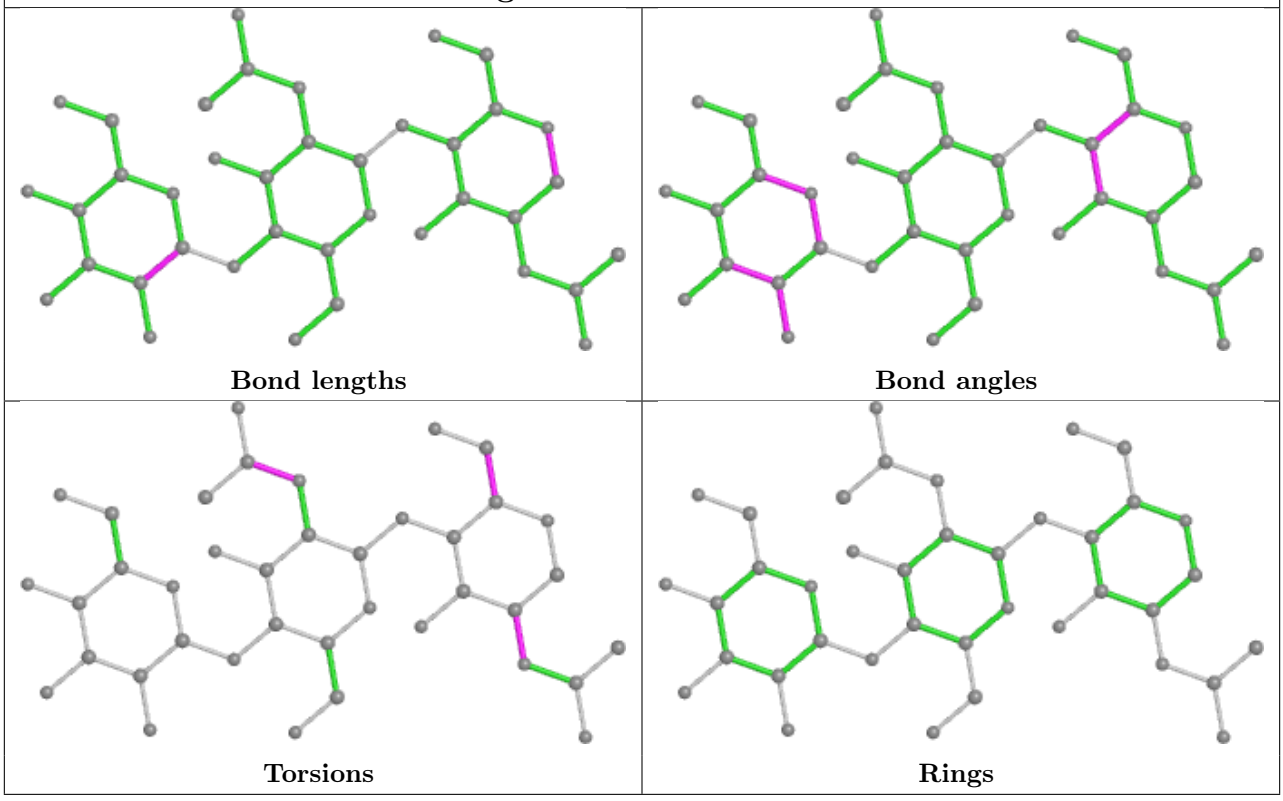
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	BMA	1	0
2	F	1	NAG	2	0
2	E	1	NAG	6	0

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

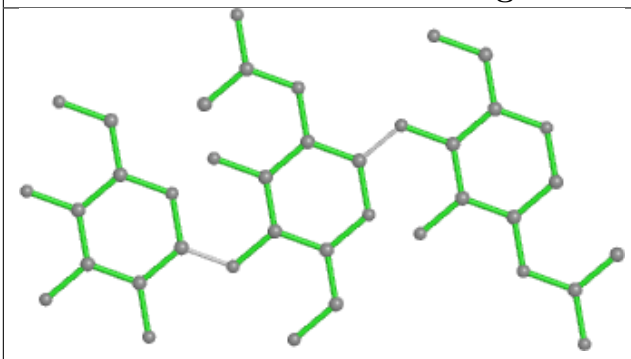
Oligosaccharide Chain D



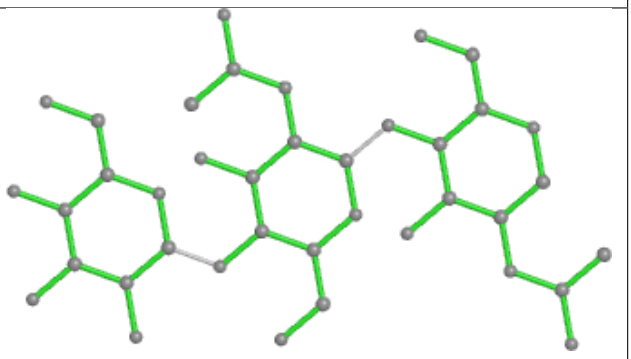
Oligosaccharide Chain E



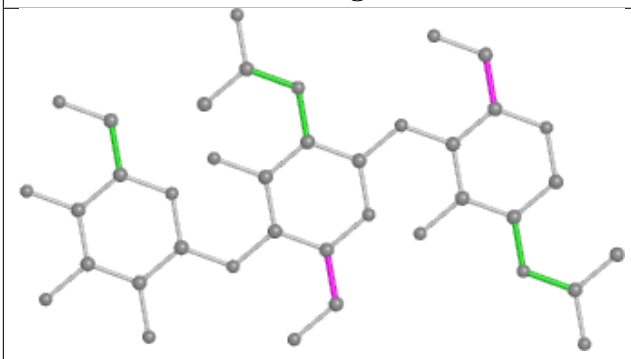
Oligosaccharide Chain F



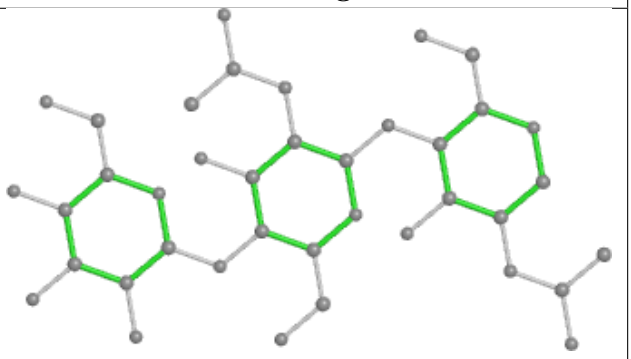
Bond lengths



Bond angles

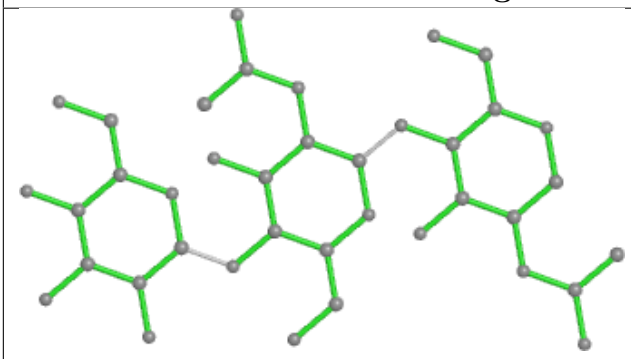


Torsions

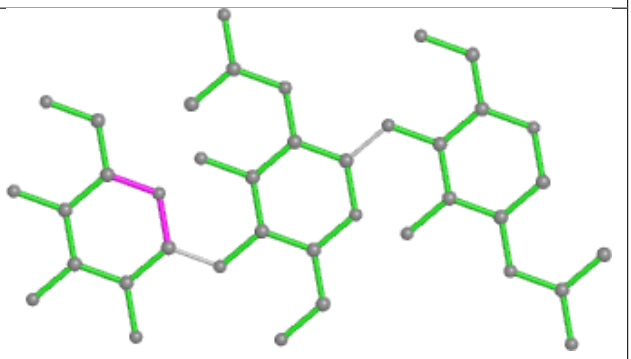


Rings

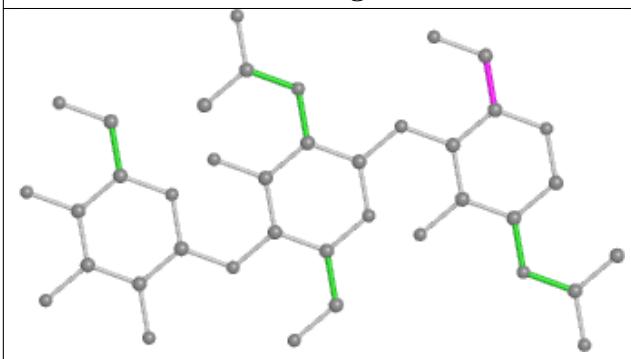
Oligosaccharide Chain H



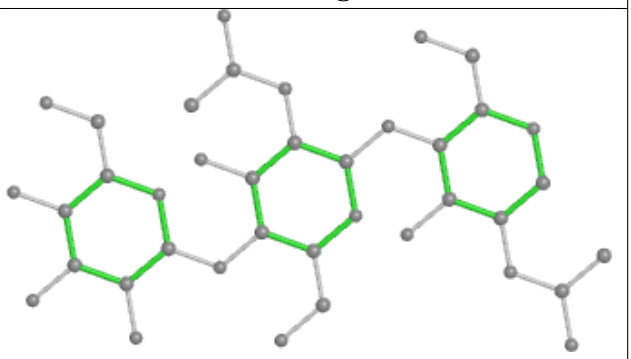
Bond lengths



Bond angles

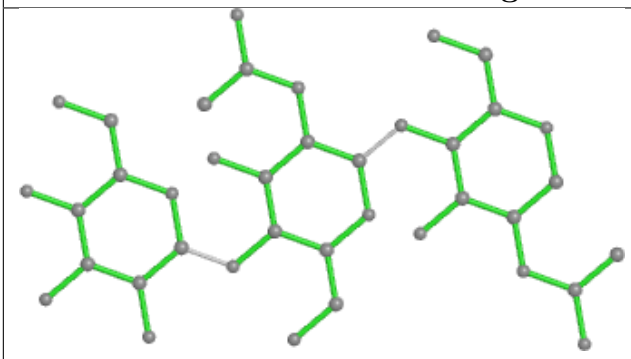


Torsions

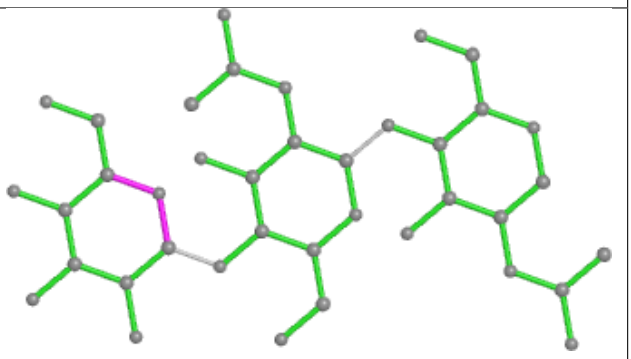


Rings

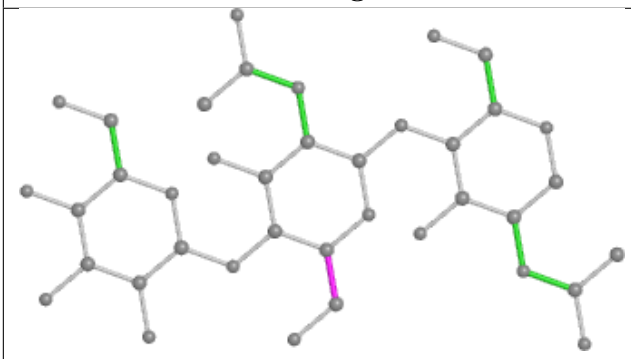
Oligosaccharide Chain I



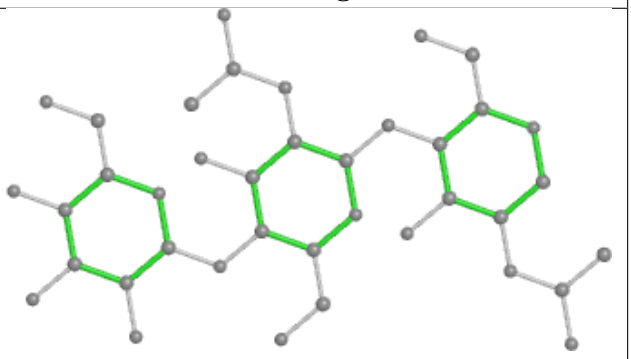
Bond lengths



Bond angles

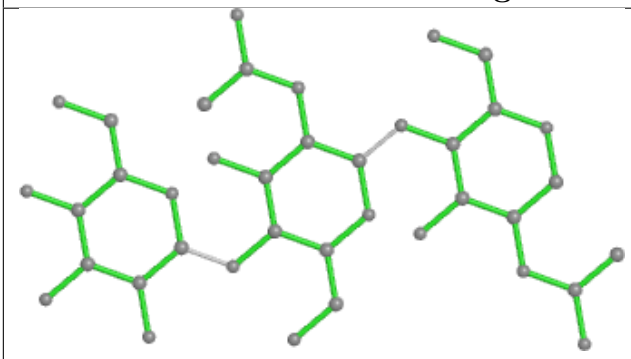


Torsions

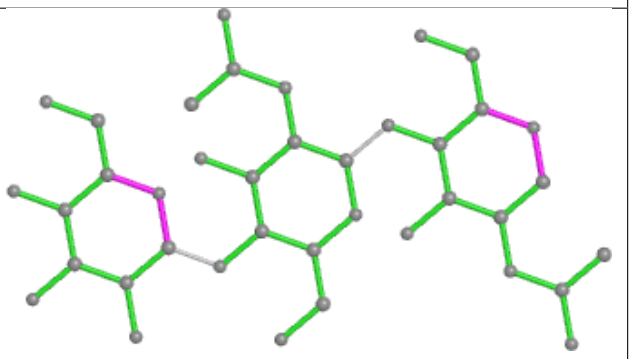


Rings

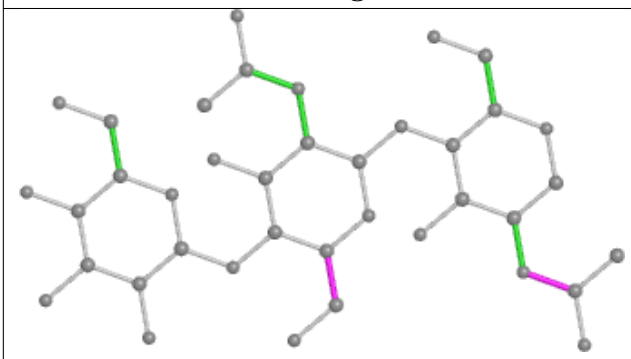
Oligosaccharide Chain K



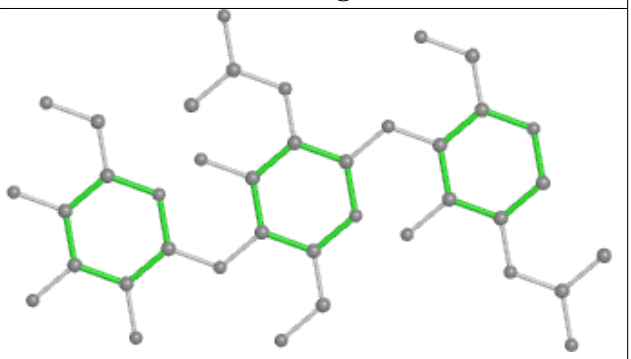
Bond lengths



Bond angles

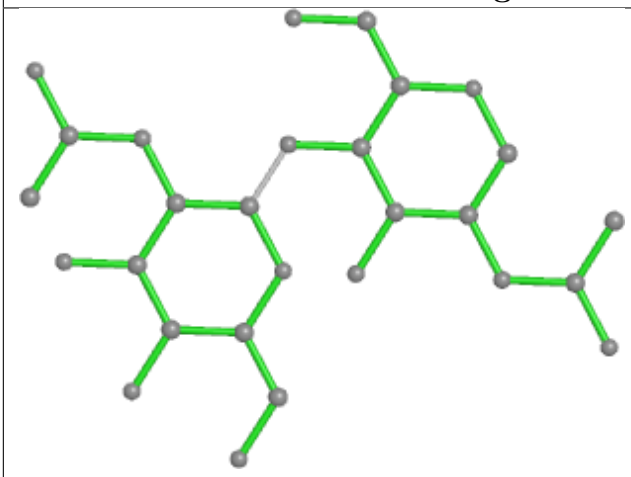


Torsions

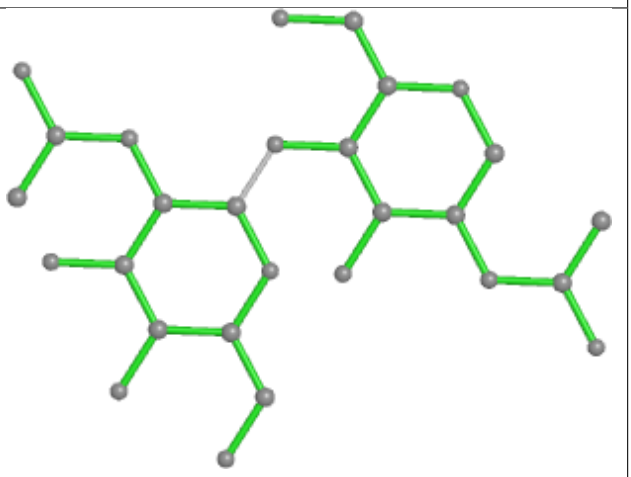


Rings

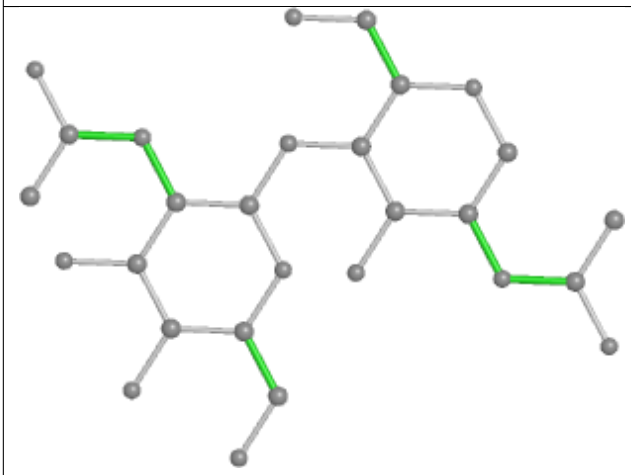
Oligosaccharide Chain G



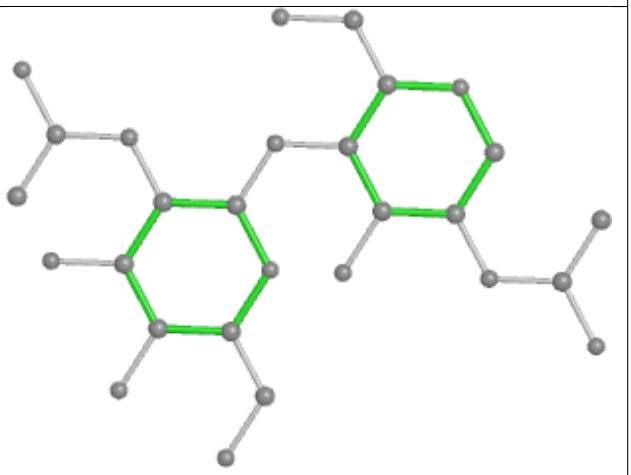
Bond lengths



Bond angles

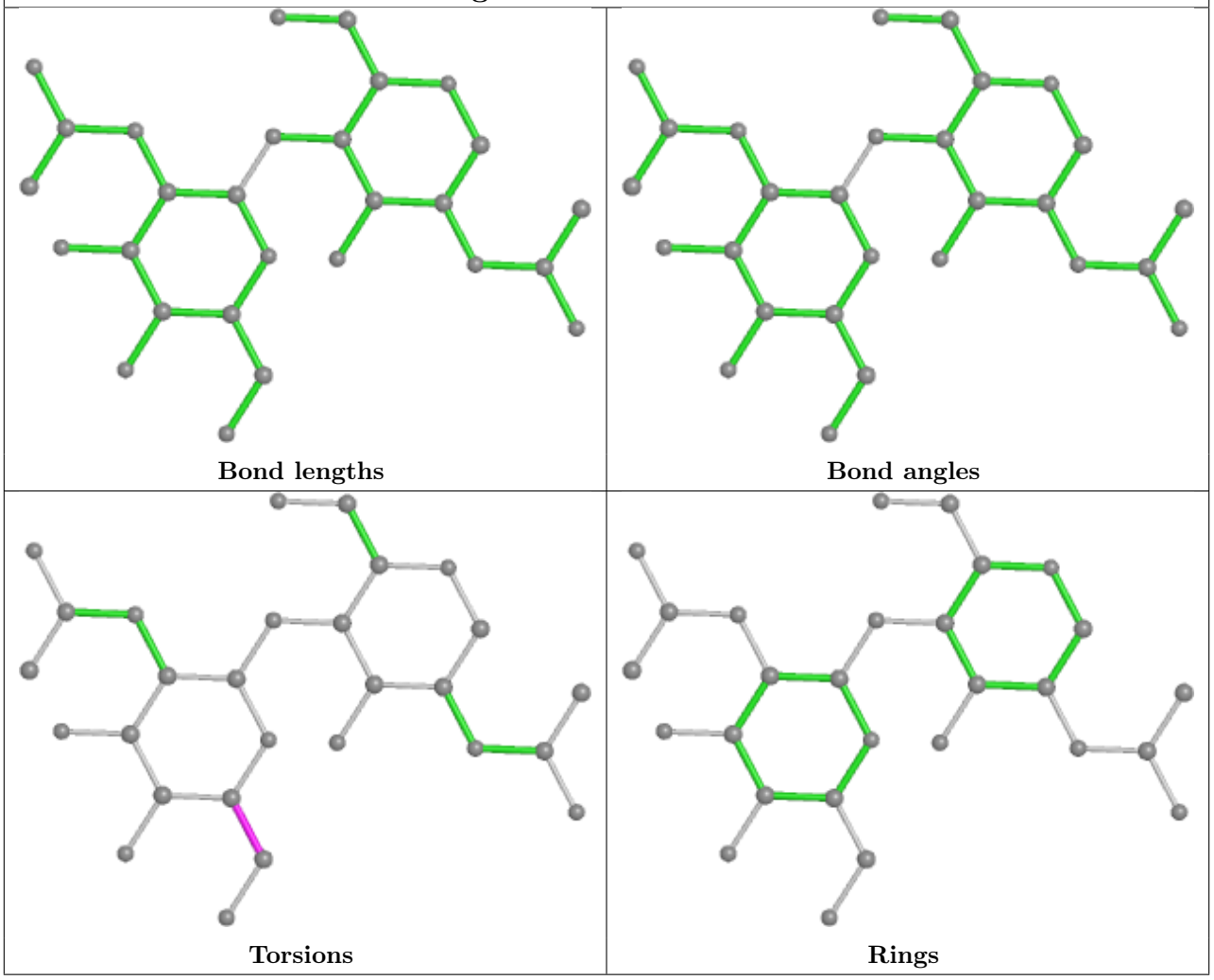


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry (i)

43 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	$\#\|Z\| > 2$
4	NAG	A	1405	1	14,14,15	0.27	0	17,19,21	0.49	0
5	FOL	B	1412	-	34,34,34	1.24	2 (5%)	44,47,47	2.02	8 (18%)
4	NAG	C	1402	1	14,14,15	0.22	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1405	1	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	C	1404	1	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	B	1408	1	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	C	1412	1	14,14,15	0.33	0	17,19,21	0.55	0
4	NAG	B	1410	1	14,14,15	0.36	0	17,19,21	0.52	0
4	NAG	B	1413	1	14,14,15	0.40	0	17,19,21	1.00	1 (5%)
5	FOL	A	1414	-	34,34,34	1.23	2 (5%)	44,47,47	2.07	11 (25%)
4	NAG	A	1412	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	1403	1	14,14,15	0.25	0	17,19,21	0.42	0
6	EIC	C	1401	-	19,19,19	0.45	0	19,19,19	1.03	1 (5%)
4	NAG	A	1402	1	14,14,15	0.25	0	17,19,21	0.54	0
4	NAG	C	1411	1	14,14,15	0.34	0	17,19,21	0.48	0
4	NAG	A	1413	1	14,14,15	0.22	0	17,19,21	0.52	0
4	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	B	1409	1	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	C	1409	1	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	A	1408	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	B	1402	1	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	A	1409	1	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	C	1406	1	14,14,15	0.27	0	17,19,21	0.49	0
5	FOL	C	1414	-	34,34,34	1.22	2 (5%)	44,47,47	2.14	9 (20%)
4	NAG	B	1404	1	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	C	1403	1	14,14,15	0.37	0	17,19,21	0.49	0
4	NAG	C	1408	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	B	1406	1	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	A	1404	1	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	C	1410	1	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	B	1411	1	14,14,15	0.36	0	17,19,21	0.56	0
4	NAG	A	1407	1	14,14,15	0.26	0	17,19,21	0.46	0
6	EIC	A	1415	-	19,19,19	0.45	0	19,19,19	0.90	1 (5%)
4	NAG	A	1403	1	14,14,15	0.29	0	17,19,21	0.44	0
6	EIC	B	1414	-	19,19,19	0.46	0	19,19,19	0.84	0
4	NAG	A	1410	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	A	1411	1	14,14,15	0.32	0	17,19,21	0.49	0
4	NAG	C	1405	1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	A	1401	1	14,14,15	0.18	0	17,19,21	0.51	0
4	NAG	B	1401	1	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	C	1407	1	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	C	1413	1	14,14,15	0.46	0	17,19,21	0.75	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
5	FOL	B	1412	-	-	2/22/22/22	0/3/3/3
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1412	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1413	1	-	2/6/23/26	0/1/1/1
5	FOL	A	1414	-	-	3/22/22/22	0/3/3/3
4	NAG	A	1412	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
6	EIC	C	1401	-	-	6/17/17/17	-
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1411	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1413	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	FOL	C	1414	-	-	6/22/22/22	0/3/3/3
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1411	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	2/6/23/26	0/1/1/1
6	EIC	A	1415	-	-	3/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
6	EIC	B	1414	-	-	6/17/17/17	-
4	NAG	A	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1411	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1413	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1414	FOL	C4A-C4	3.86	1.48	1.41
5	B	1412	FOL	C4A-C4	3.86	1.48	1.41
5	C	1414	FOL	C4A-C4	3.79	1.47	1.41
5	A	1414	FOL	C4A-C8A	3.76	1.47	1.40
5	B	1412	FOL	C4A-C8A	3.69	1.47	1.40
5	C	1414	FOL	C4A-C8A	3.57	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1414	FOL	C2-N1-C8A	6.33	122.58	115.36
5	C	1414	FOL	N8-C8A-N1	5.99	122.66	115.82
5	B	1412	FOL	N8-C8A-N1	5.93	122.59	115.82
5	B	1412	FOL	C2-N1-C8A	5.69	121.85	115.36
5	A	1414	FOL	C2-N1-C8A	5.33	121.45	115.36
5	A	1414	FOL	N8-C8A-N1	5.28	121.84	115.82
5	C	1414	FOL	C8A-C4A-C4	-5.07	116.59	119.95
5	A	1414	FOL	C8A-C4A-C4	-4.90	116.71	119.95
5	B	1412	FOL	C8A-C4A-C4	-4.47	117.00	119.95
5	C	1414	FOL	C4-C4A-N5	4.03	123.20	118.60
5	A	1414	FOL	C4-C4A-N5	3.91	123.06	118.60
5	A	1414	FOL	C4A-C4-N3	-3.88	118.12	123.43
5	B	1412	FOL	C4A-C4-N3	-3.83	118.19	123.43
5	A	1414	FOL	C2-N3-C4	3.67	121.77	115.93
5	C	1414	FOL	N1-C2-N3	-3.67	122.33	127.22
5	B	1412	FOL	C4-C4A-N5	3.56	122.67	118.60
5	A	1414	FOL	C6-C9-N10	-3.55	105.21	113.07
5	B	1412	FOL	C2-N3-C4	3.49	121.47	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1414	FOL	C4A-C4-N3	-3.41	118.77	123.43
5	B	1412	FOL	N1-C2-N3	-3.36	122.73	127.22
5	C	1414	FOL	C2-N3-C4	3.36	121.27	115.93
6	C	1401	EIC	C3-C2-C1	-3.24	106.31	114.47
5	A	1414	FOL	N1-C2-N3	-3.10	123.08	127.22
5	B	1412	FOL	C7-N8-C8A	2.72	119.42	116.69
4	C	1413	NAG	C1-O5-C5	2.68	115.82	112.19
5	C	1414	FOL	C7-N8-C8A	2.68	119.38	116.69
6	A	1415	EIC	C3-C2-C1	-2.40	108.43	114.47
5	A	1414	FOL	C7-N8-C8A	2.26	118.97	116.69
4	B	1413	NAG	C1-O5-C5	2.19	115.16	112.19
5	A	1414	FOL	C9-C6-N5	2.16	120.49	116.66
5	A	1414	FOL	C9-C6-C7	-2.13	117.84	121.55
5	C	1414	FOL	C11-C-N	2.08	121.05	117.06

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1413	NAG	C8-C7-N2-C2
4	B	1413	NAG	O7-C7-N2-C2
4	C	1402	NAG	O5-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	A	1405	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	A	1413	NAG	O5-C5-C6-O6
4	C	1410	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	C	1403	NAG	O5-C5-C6-O6
4	B	1405	NAG	C4-C5-C6-O6
4	A	1410	NAG	O5-C5-C6-O6
4	A	1405	NAG	C4-C5-C6-O6
4	C	1402	NAG	C4-C5-C6-O6
4	C	1410	NAG	C4-C5-C6-O6
4	C	1406	NAG	C4-C5-C6-O6
4	B	1410	NAG	O5-C5-C6-O6
4	A	1410	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1405	NAG	C4-C5-C6-O6
4	A	1401	NAG	C4-C5-C6-O6
4	C	1403	NAG	C4-C5-C6-O6
4	A	1409	NAG	C8-C7-N2-C2
4	A	1409	NAG	O7-C7-N2-C2
4	A	1413	NAG	C8-C7-N2-C2
4	A	1413	NAG	O7-C7-N2-C2
4	B	1407	NAG	C8-C7-N2-C2
4	B	1407	NAG	O7-C7-N2-C2
5	A	1414	FOL	C11-C-N-CA
4	A	1407	NAG	C4-C5-C6-O6
4	A	1413	NAG	C4-C5-C6-O6
4	B	1410	NAG	C4-C5-C6-O6
4	C	1408	NAG	C4-C5-C6-O6
4	A	1404	NAG	C4-C5-C6-O6
4	B	1409	NAG	O5-C5-C6-O6
5	A	1414	FOL	O-C-N-CA
4	B	1409	NAG	C4-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	A	1407	NAG	O5-C5-C6-O6
4	A	1412	NAG	O5-C5-C6-O6
5	C	1414	FOL	N-CA-CT-O1
5	C	1414	FOL	N-CA-CT-O2
6	B	1414	EIC	C5-C6-C7-C8
6	C	1401	EIC	C2-C3-C4-C5
5	A	1414	FOL	CT-CA-CB-CG
4	C	1409	NAG	C4-C5-C6-O6
6	B	1414	EIC	C9-C10-C11-C12
6	B	1414	EIC	C2-C3-C4-C5
4	A	1402	NAG	C4-C5-C6-O6
4	B	1401	NAG	C4-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
6	C	1401	EIC	C4-C5-C6-C7
4	B	1408	NAG	C4-C5-C6-O6
4	B	1402	NAG	C4-C5-C6-O6
5	C	1414	FOL	CB-CA-CT-O2
6	C	1401	EIC	C3-C4-C5-C6
5	C	1414	FOL	CB-CA-CT-O1
4	A	1406	NAG	C4-C5-C6-O6
4	C	1409	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	1414	FOL	OE1-CD-CG-CB
5	B	1412	FOL	OE1-CD-CG-CB
5	C	1414	FOL	OE2-CD-CG-CB
4	A	1406	NAG	O5-C5-C6-O6
5	B	1412	FOL	OE2-CD-CG-CB
6	B	1414	EIC	O2-C1-C2-C3
6	B	1414	EIC	O1-C1-C2-C3
6	A	1415	EIC	O1-C1-C2-C3
6	A	1415	EIC	O2-C1-C2-C3
6	A	1415	EIC	C7-C8-C9-C10
6	B	1414	EIC	C12-C13-C14-C15
4	C	1411	NAG	C4-C5-C6-O6
6	C	1401	EIC	O1-C1-C2-C3
6	C	1401	EIC	O2-C1-C2-C3
4	B	1408	NAG	O5-C5-C6-O6
6	C	1401	EIC	C12-C13-C14-C15
4	C	1411	NAG	O5-C5-C6-O6

There are no ring outliers.

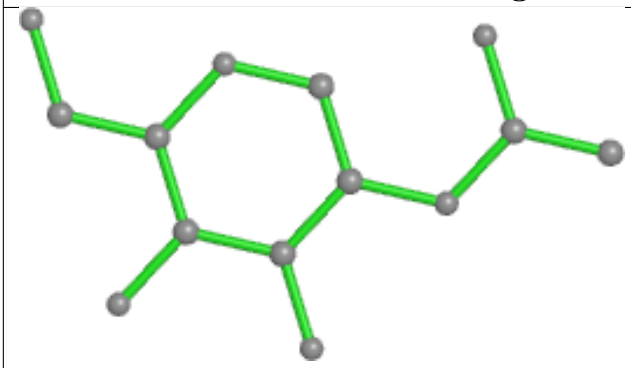
9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1412	FOL	5	0
5	A	1414	FOL	3	0
6	C	1401	EIC	5	0
5	C	1414	FOL	3	0
4	B	1404	NAG	1	0
4	B	1411	NAG	1	0
6	A	1415	EIC	5	0
6	B	1414	EIC	3	0
4	C	1405	NAG	1	0

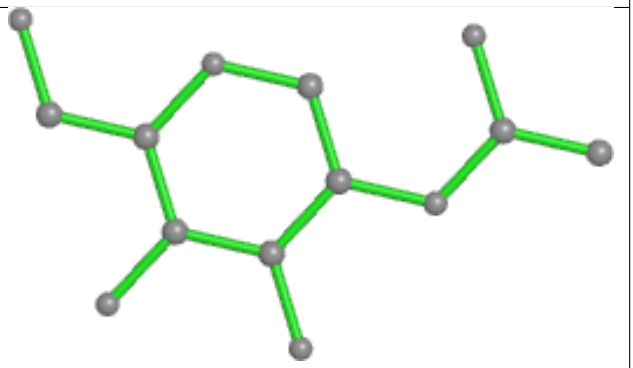
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

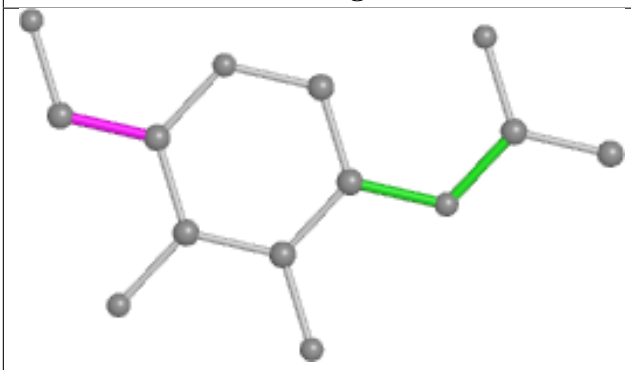
Ligand NAG A 1405



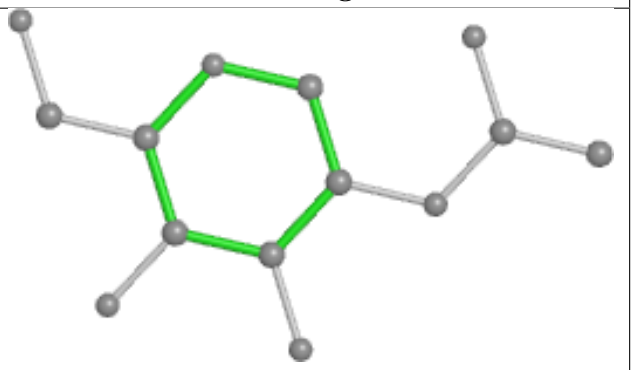
Bond lengths



Bond angles

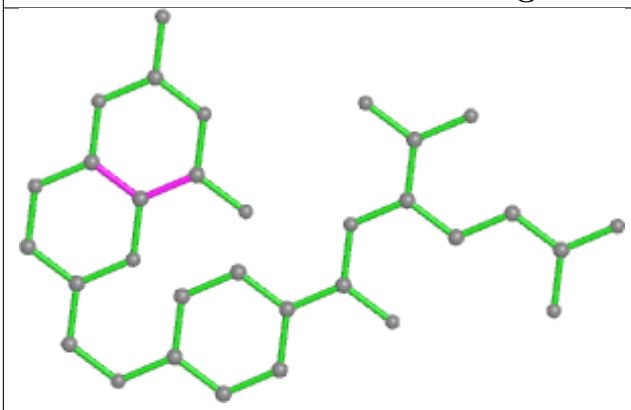


Torsions

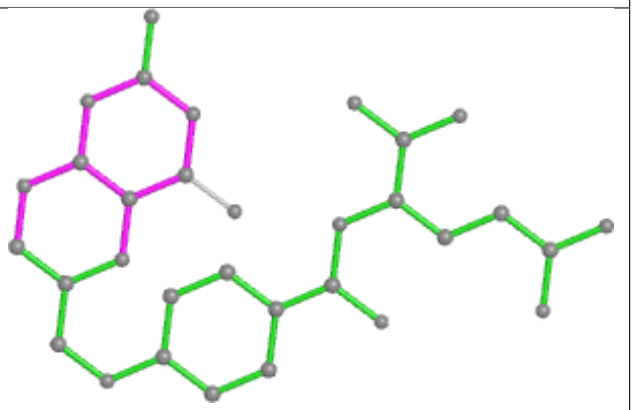


Rings

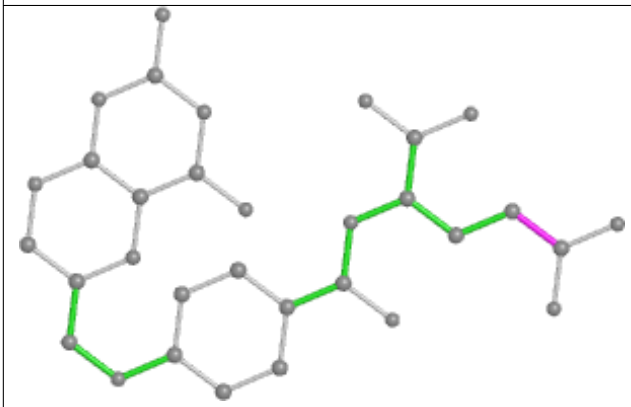
Ligand FOL B 1412



Bond lengths



Bond angles



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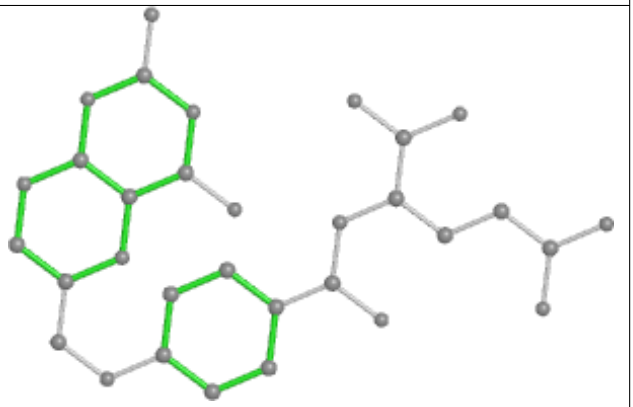
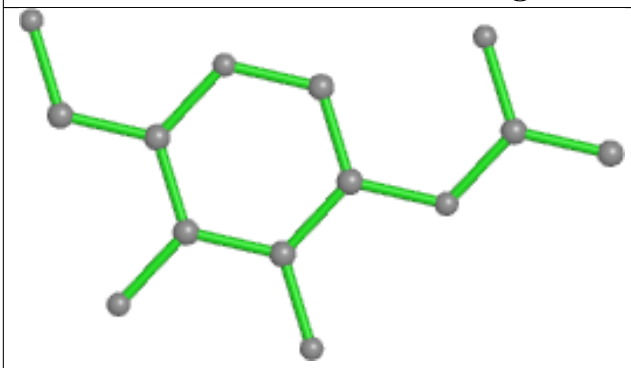
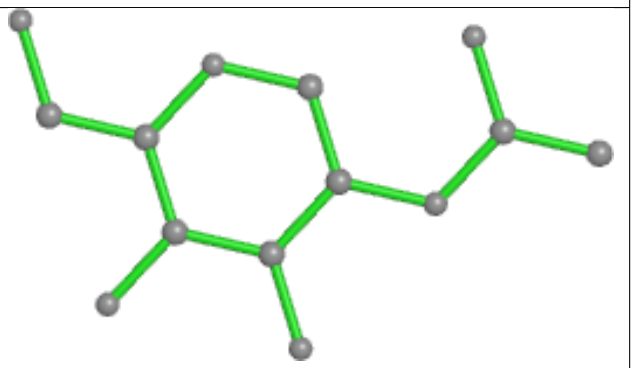


Rings

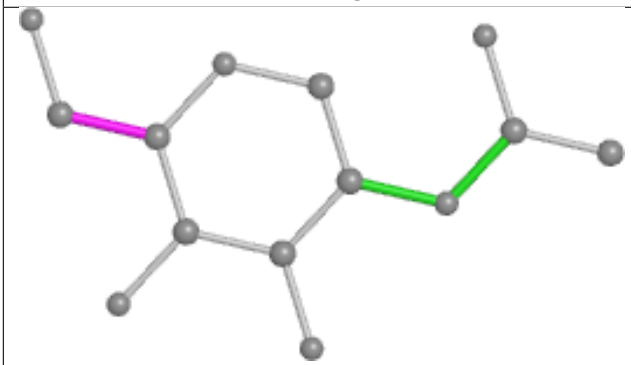
Ligand NAG C 1402



Bond lengths



Bond angles



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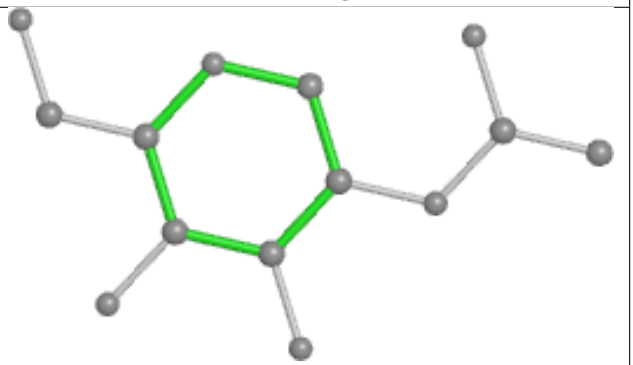
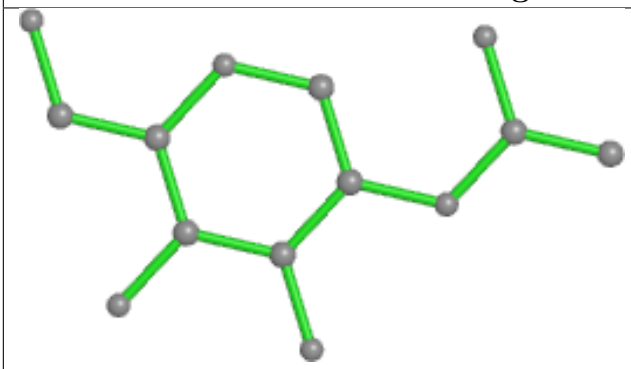
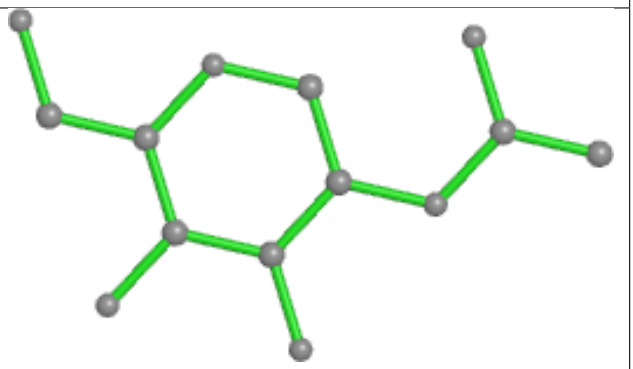


Rings

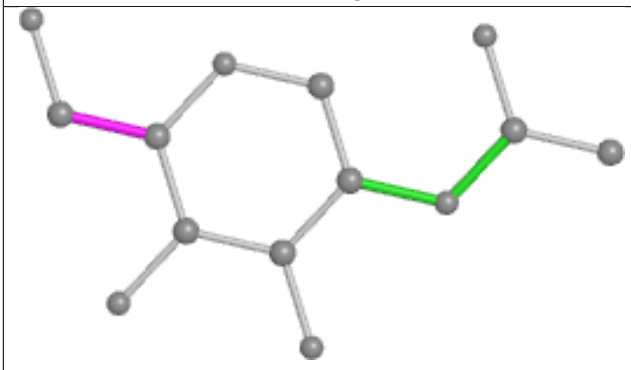
Ligand NAG B 1405



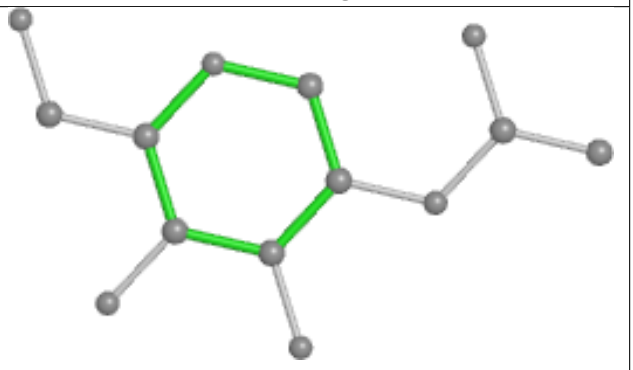
Bond lengths



Bond angles

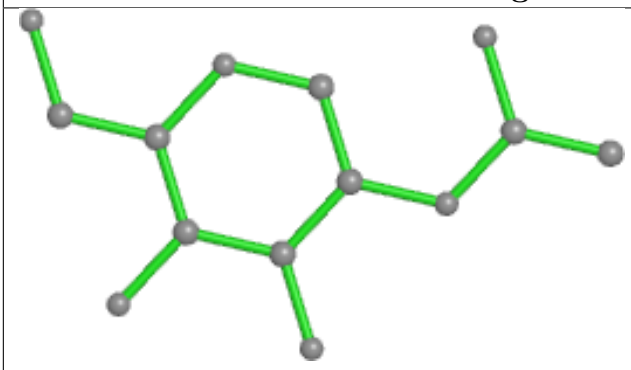


Torsions

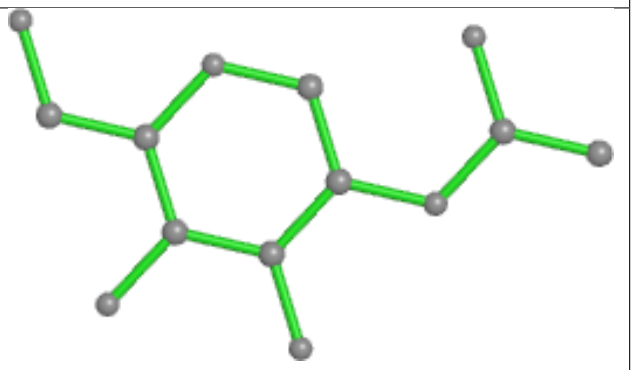


Rings

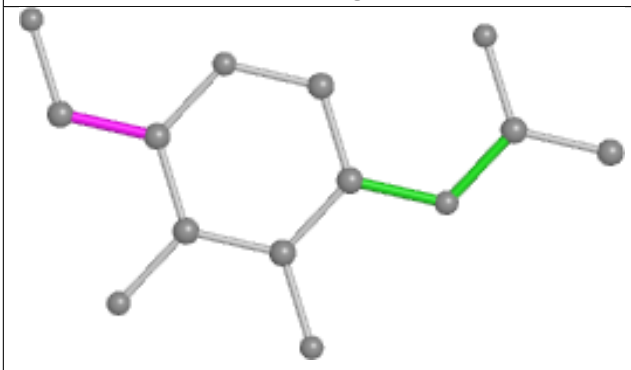
Ligand NAG C 1404



Bond lengths



Bond angles



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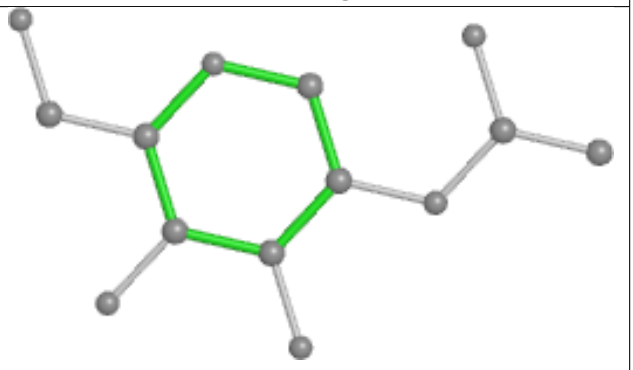
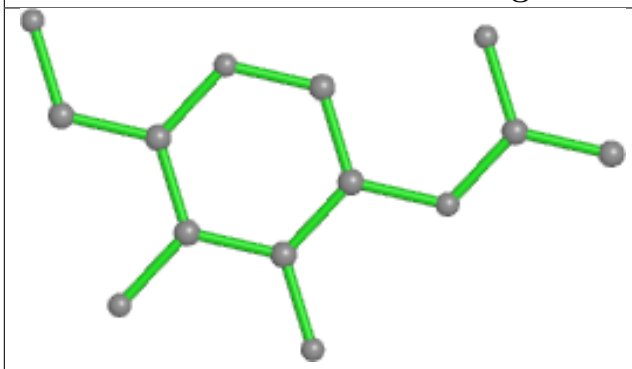
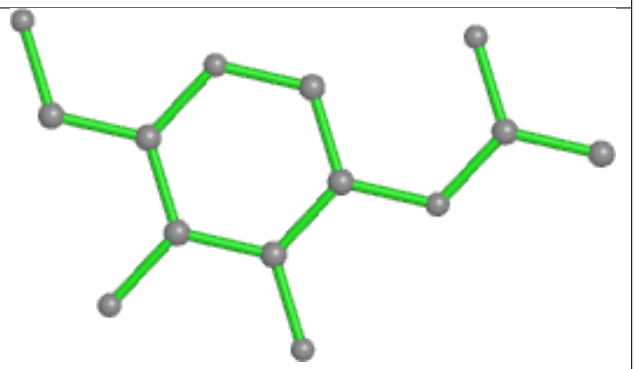


Rings

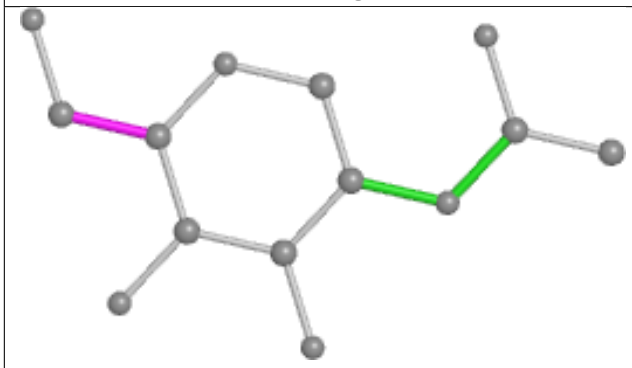
Ligand NAG A 1406



Bond lengths



Bond angles



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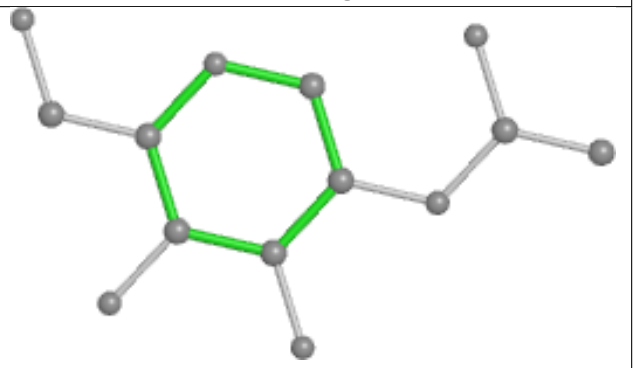
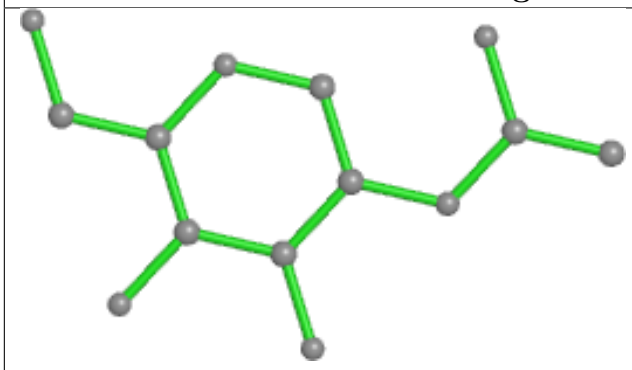
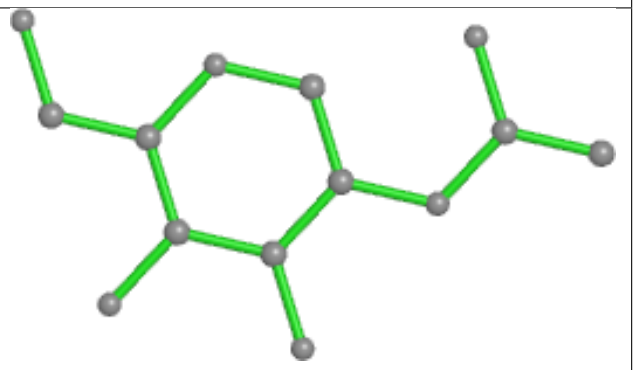


Rings

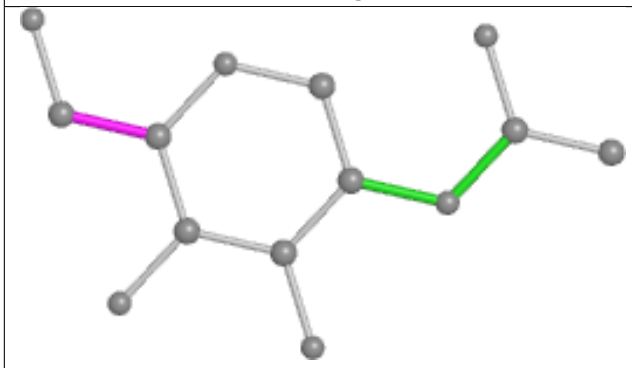
Ligand NAG B 1408



Bond lengths



Bond angles



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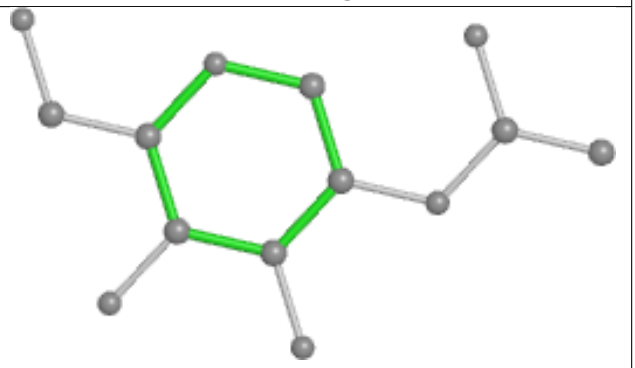
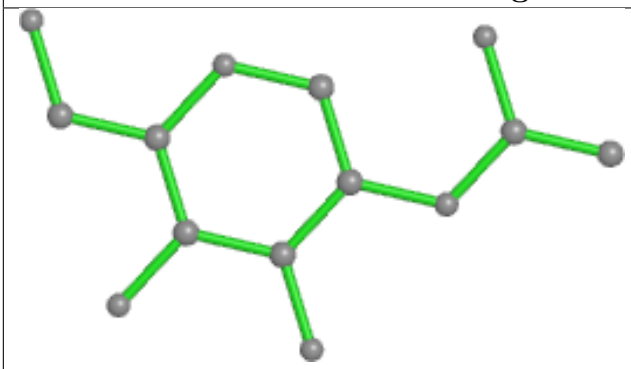
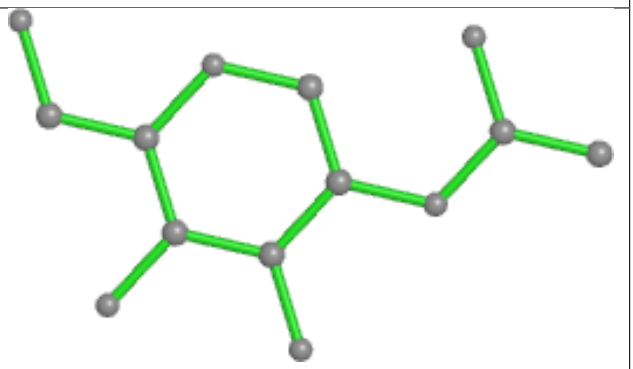


Rings

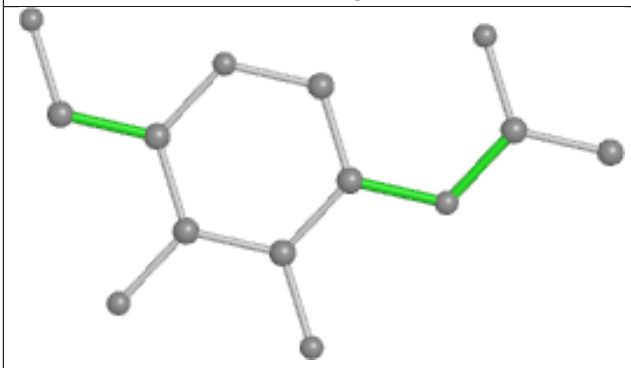
Ligand NAG C 1412



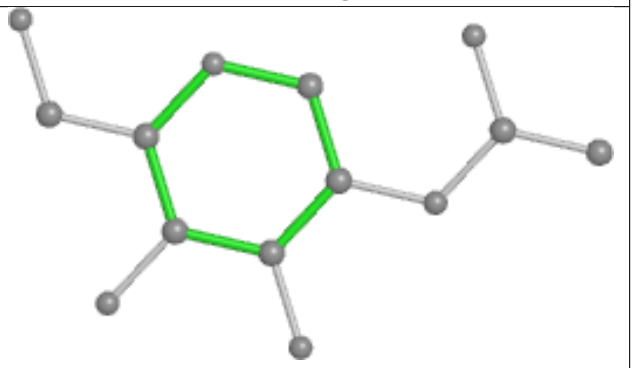
Bond lengths



Bond angles

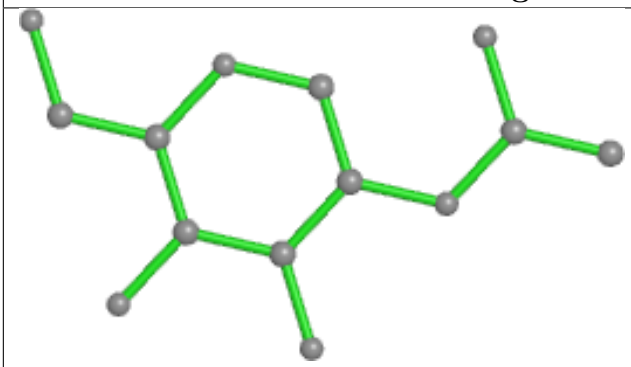


Torsions

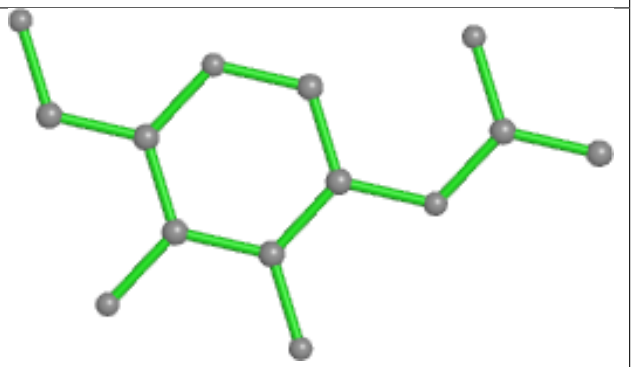


Rings

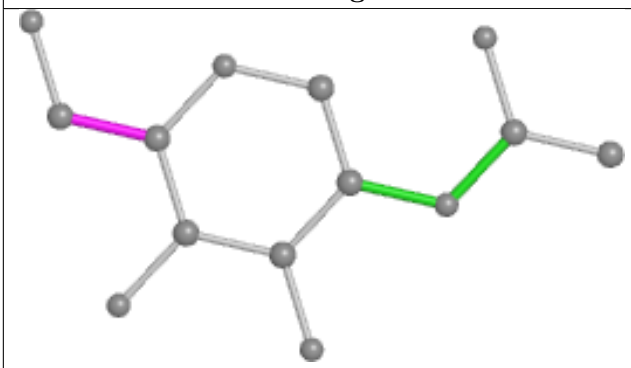
Ligand NAG B 1410



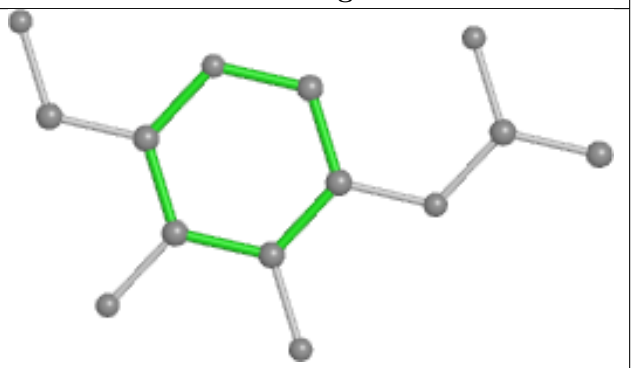
Bond lengths



Bond angles

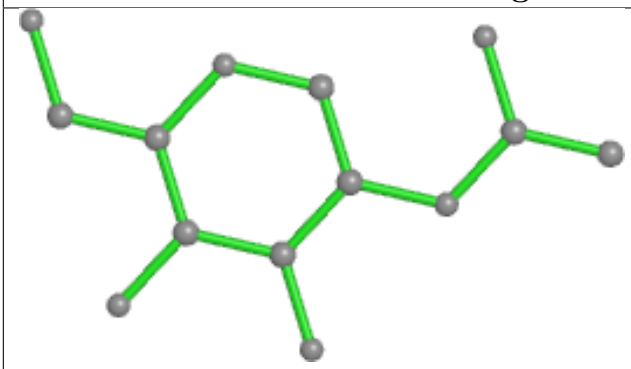


Torsions



Rings

Ligand NAG B 1413



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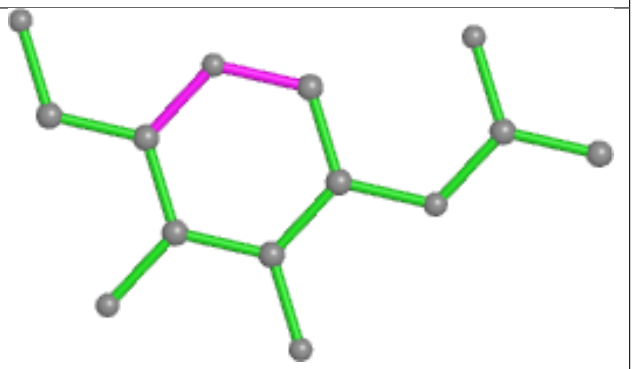
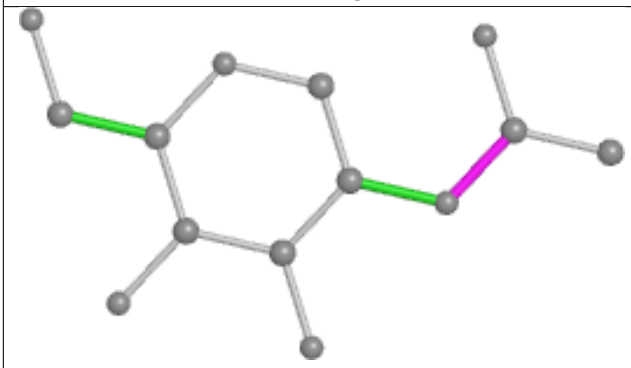
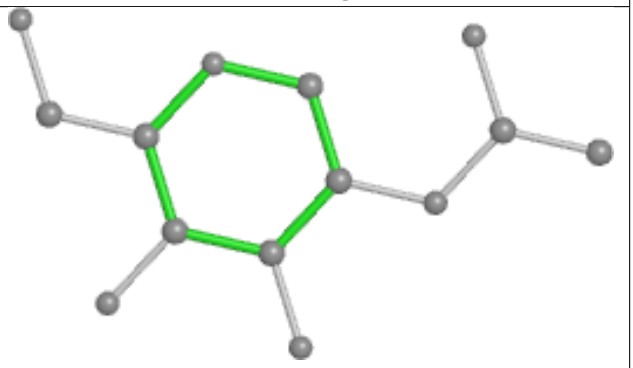


Bond angles

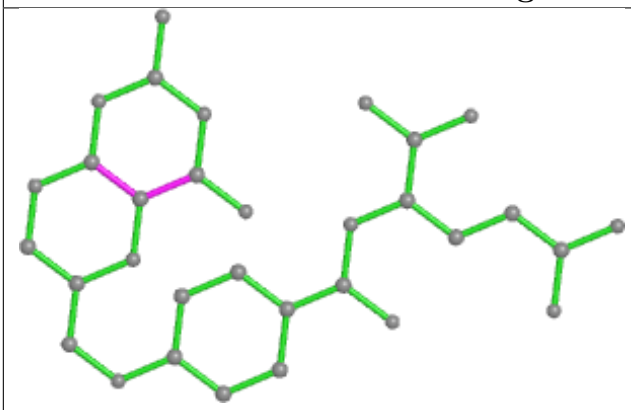


Torsions



Rings

Ligand FOL A 1414



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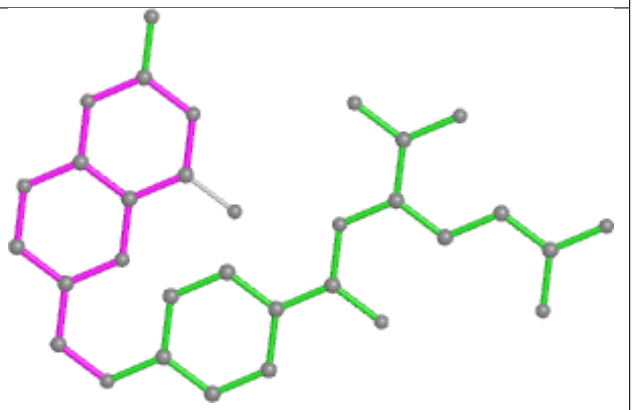
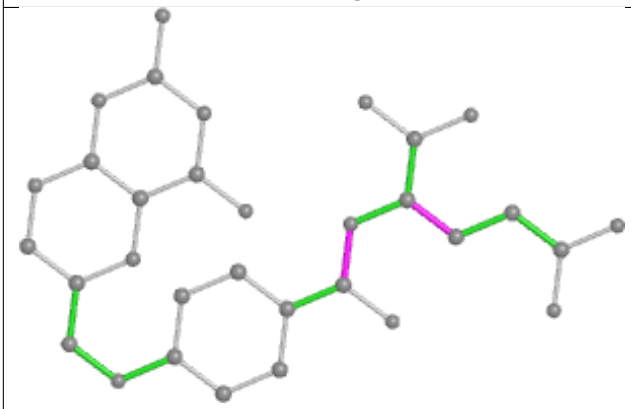
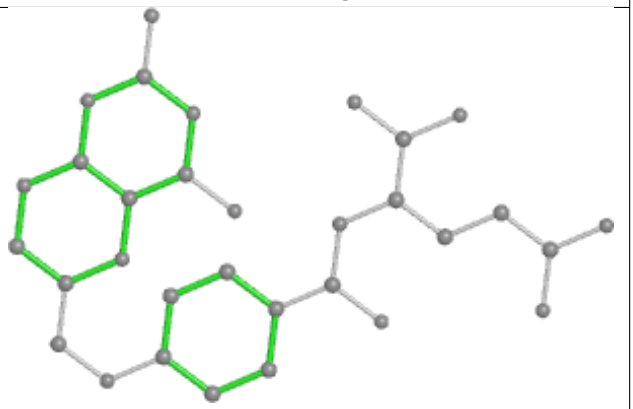


Bond angles

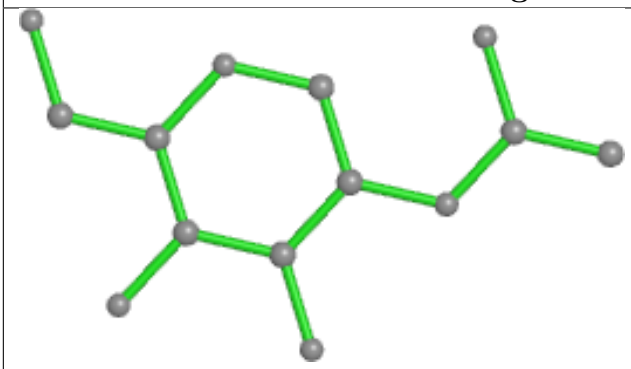


Torsions

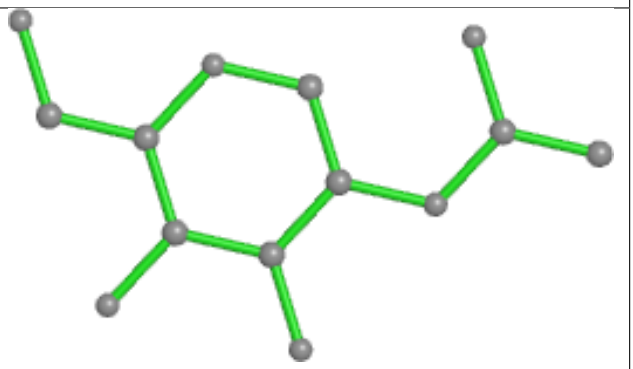


Rings

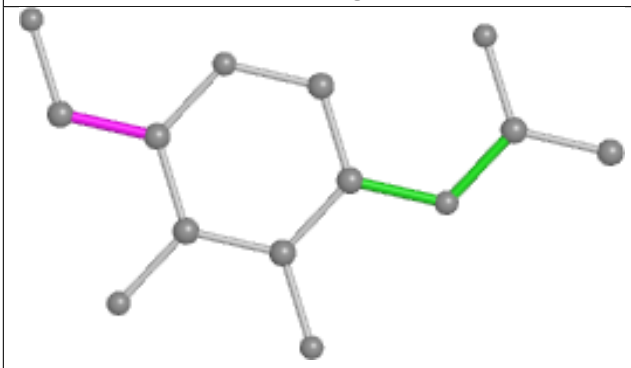
Ligand NAG A 1412



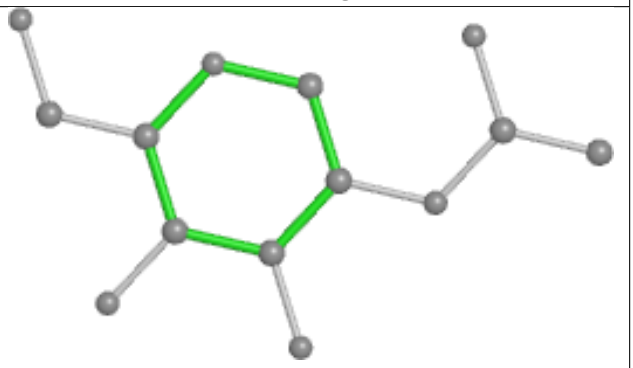
Bond lengths



Bond angles

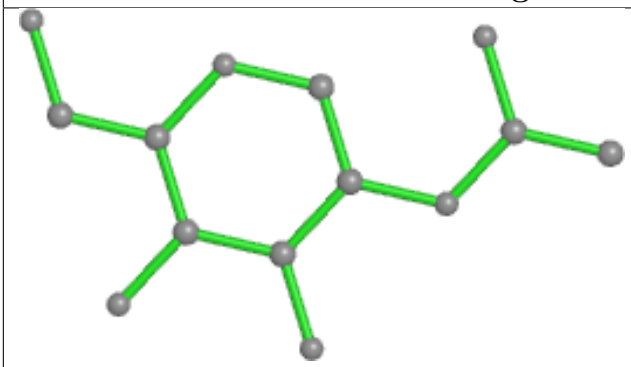


Torsions



Rings

Ligand NAG B 1403



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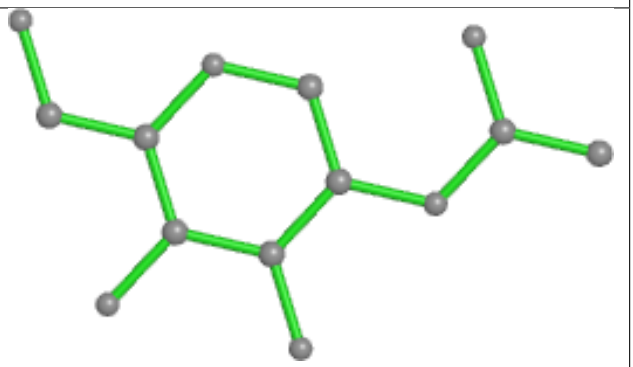
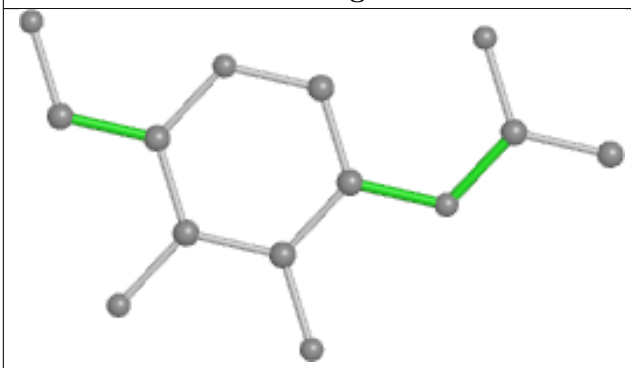
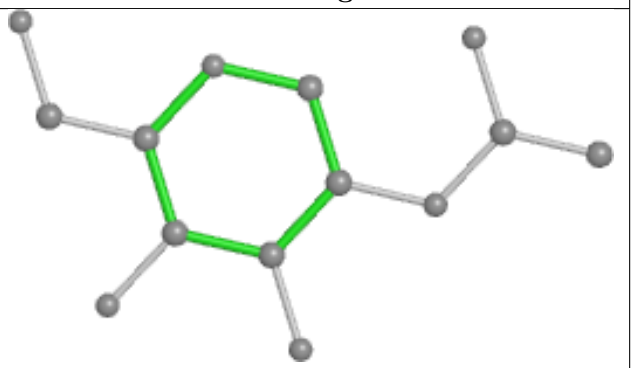


Bond angles

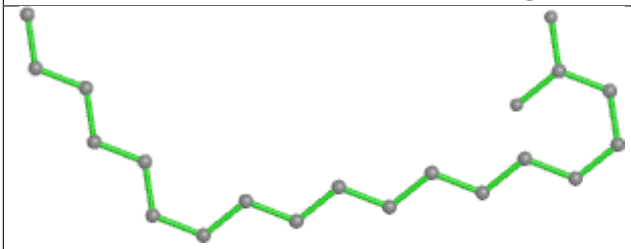


Torsions

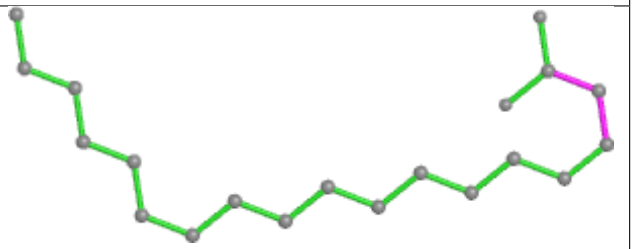


Rings

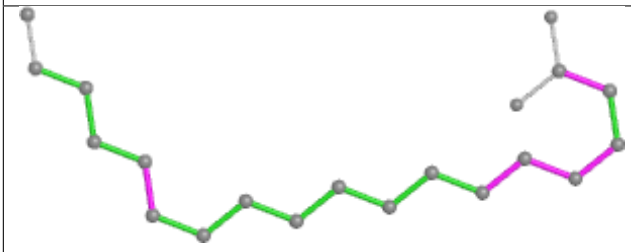
Ligand EIC C 1401



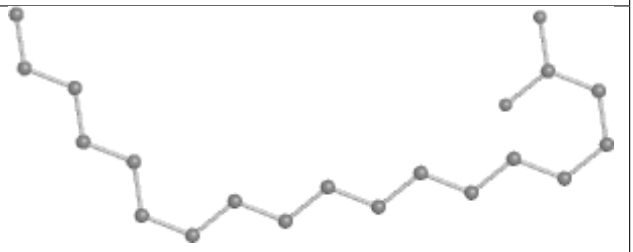
Bond lengths



Bond angles

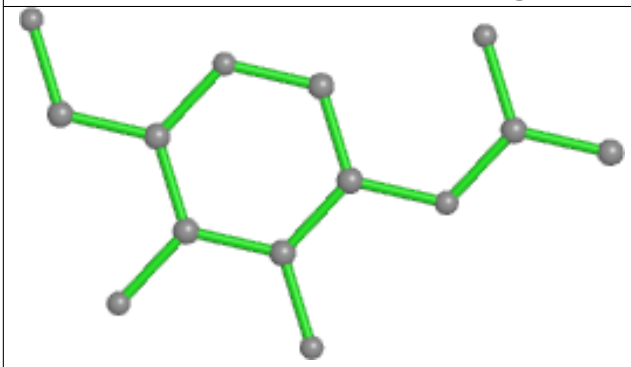


Torsions



Rings

Ligand NAG A 1402



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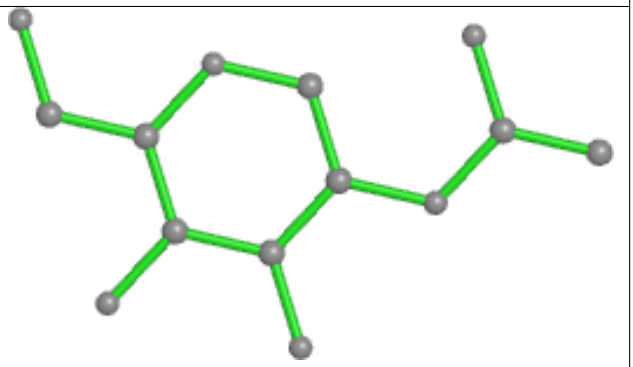
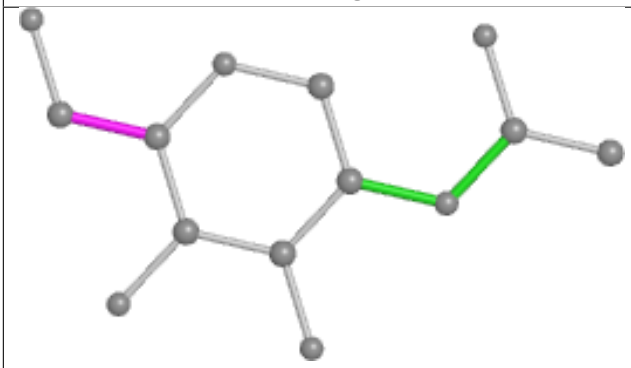
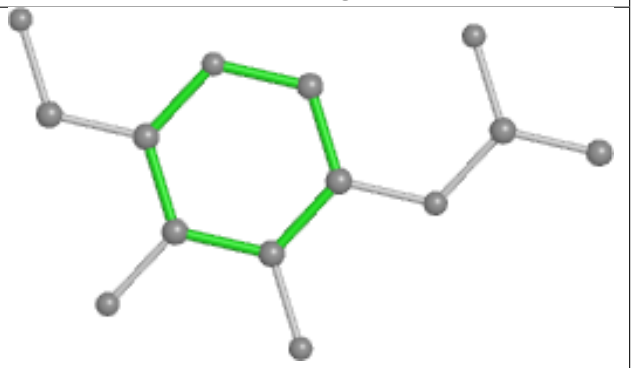


Bond angles

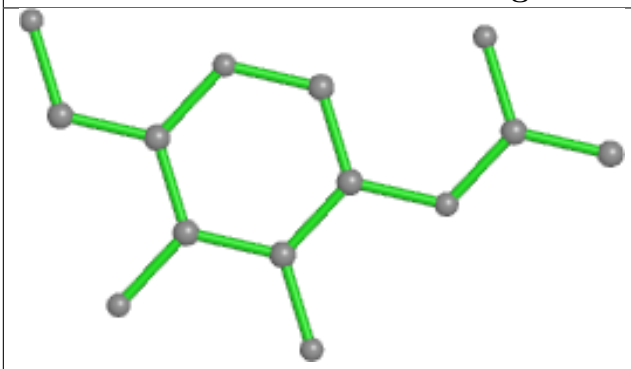


Torsions



Rings

Ligand NAG C 1411



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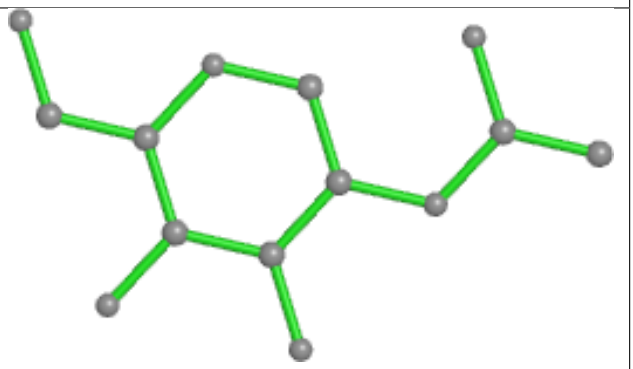
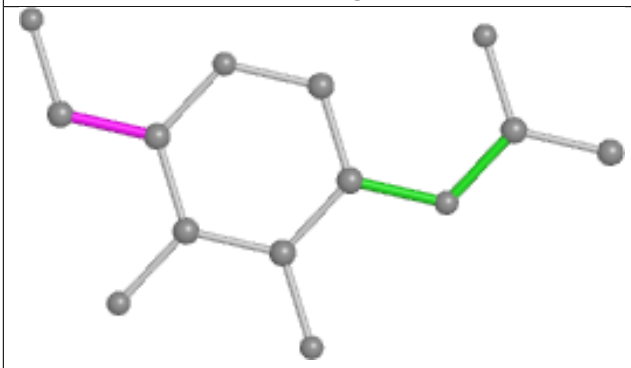
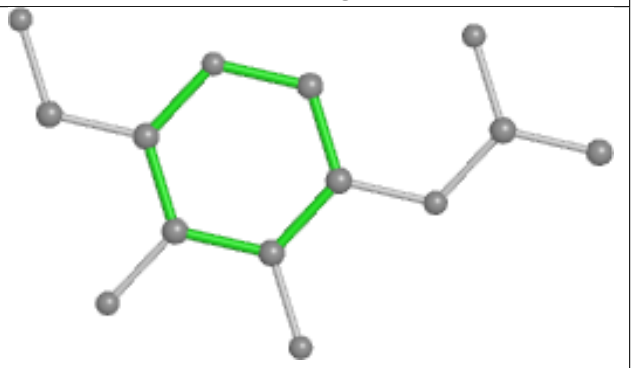


Bond angles

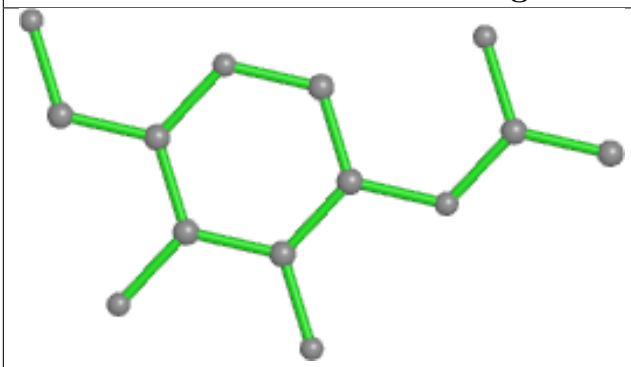


Torsions



Rings

Ligand NAG A 1413



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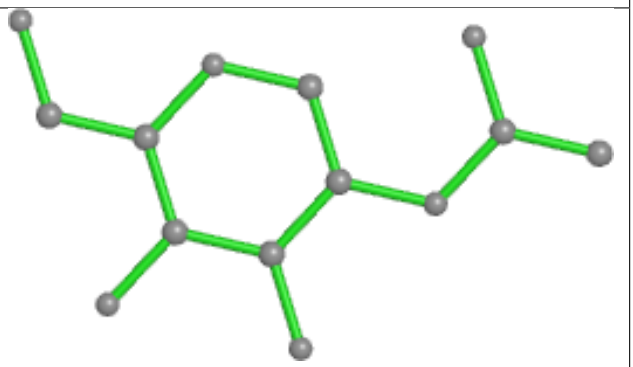
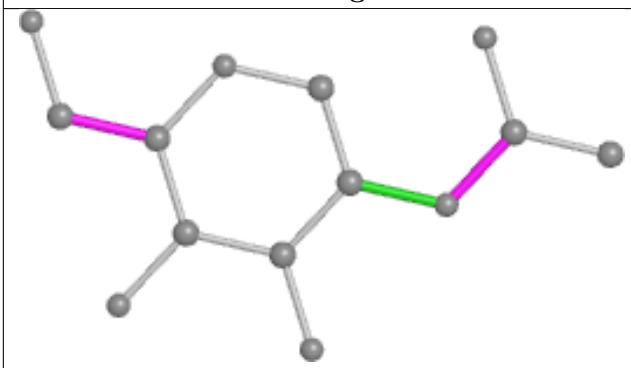
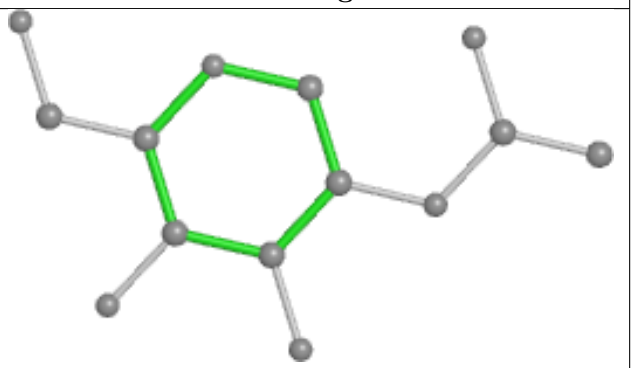


Bond angles

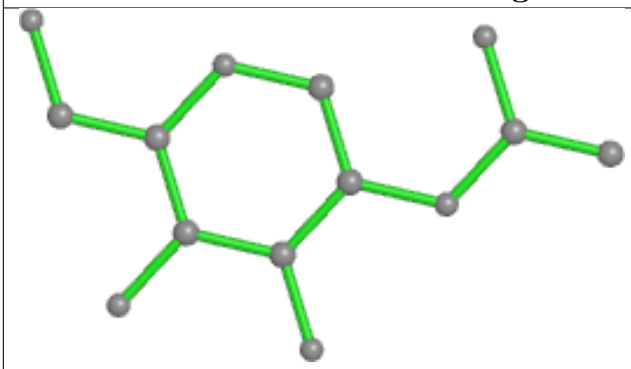


Torsions

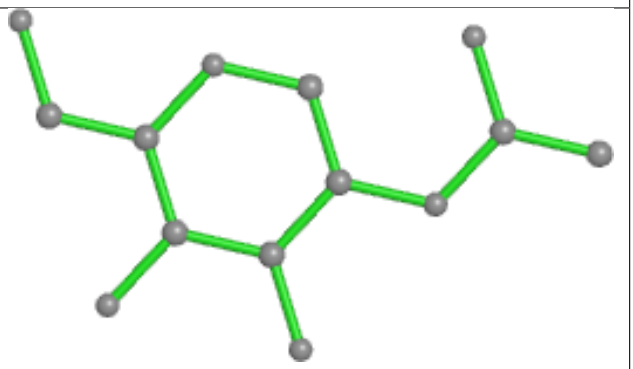


Rings

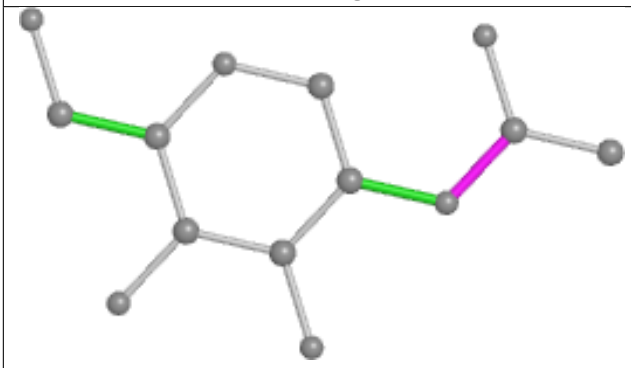
Ligand NAG B 1407



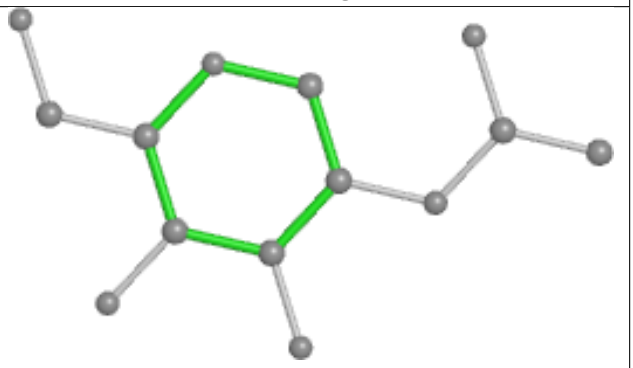
Bond lengths



Bond angles

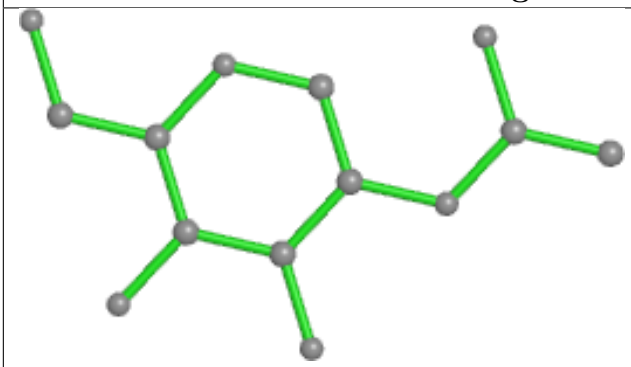


Torsions



Rings

Ligand NAG B 1409



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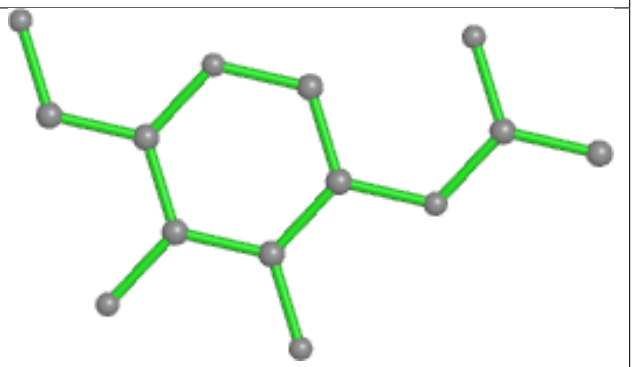
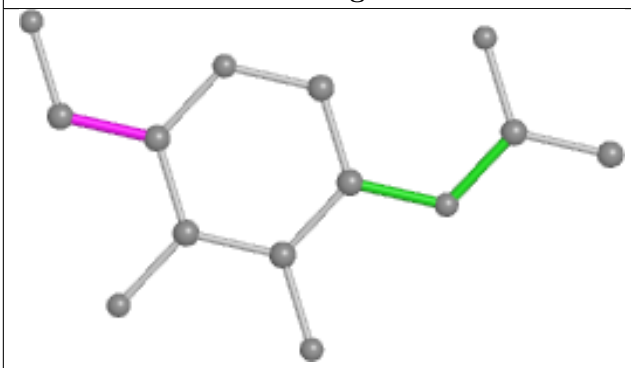
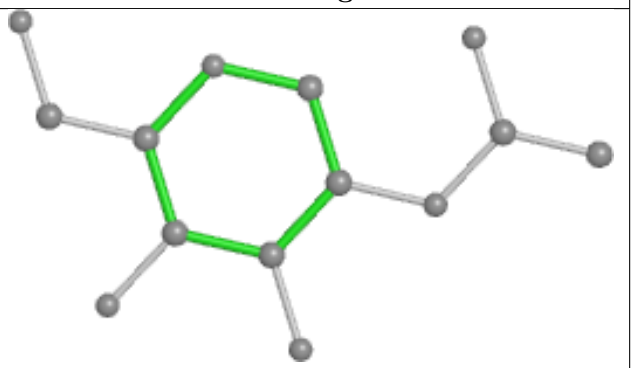


Bond angles

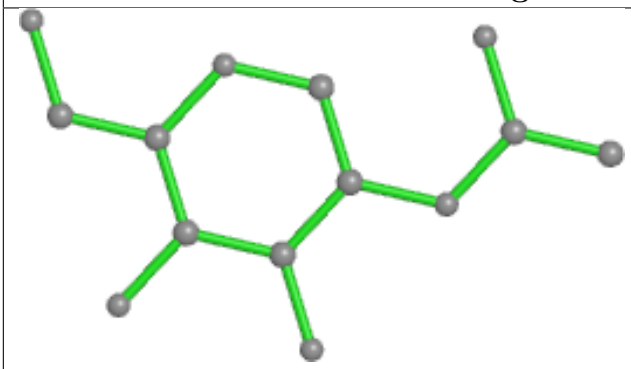


Torsions



Rings

Ligand NAG C 1409



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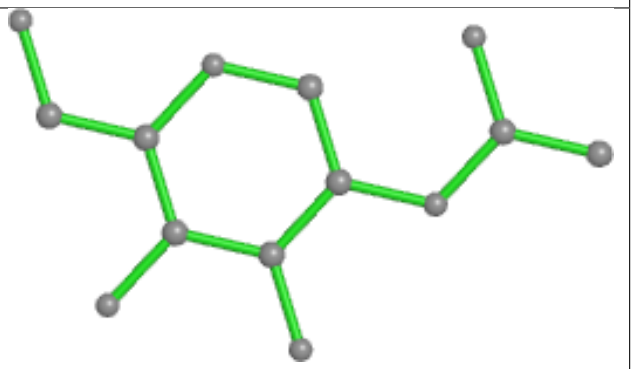
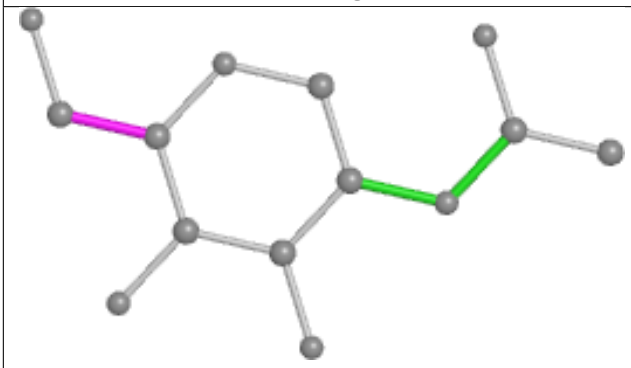
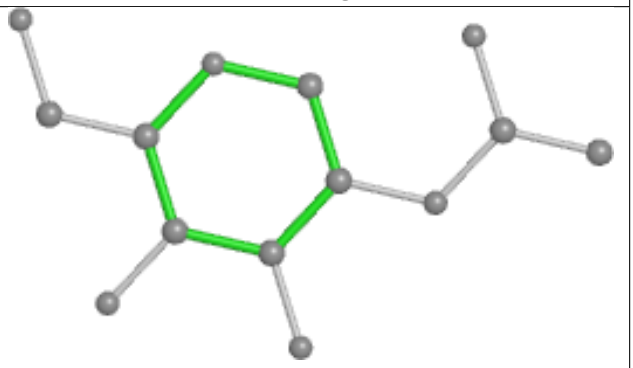


Bond angles

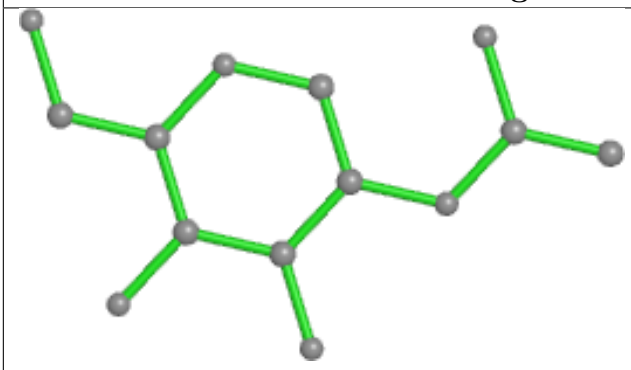


Torsions

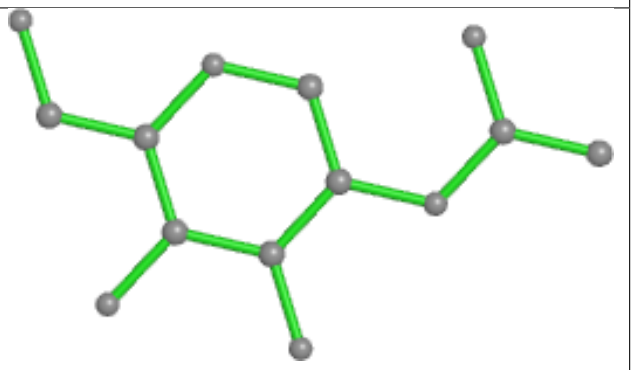


Rings

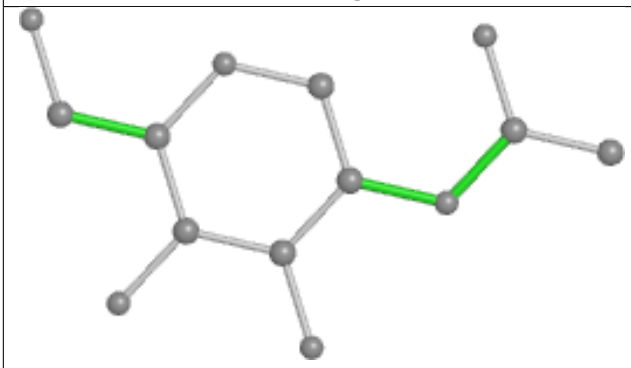
Ligand NAG A 1408



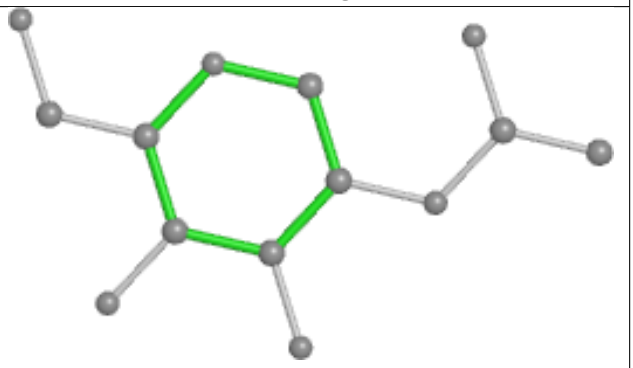
Bond lengths



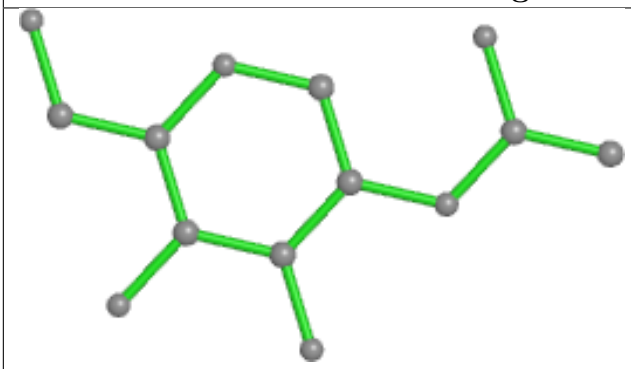
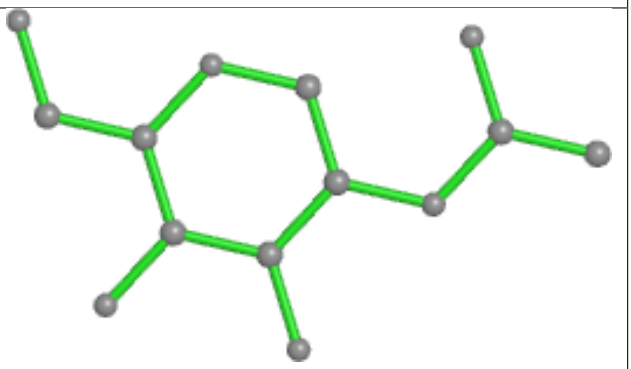
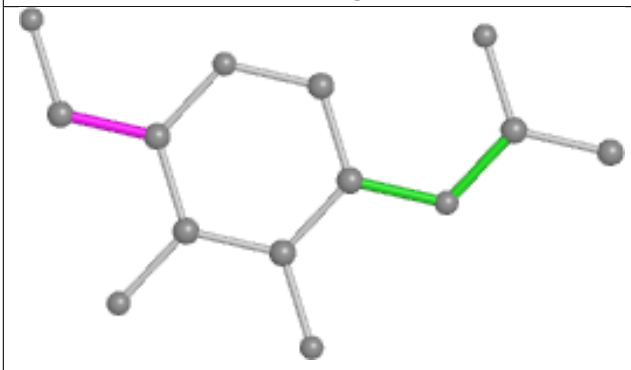
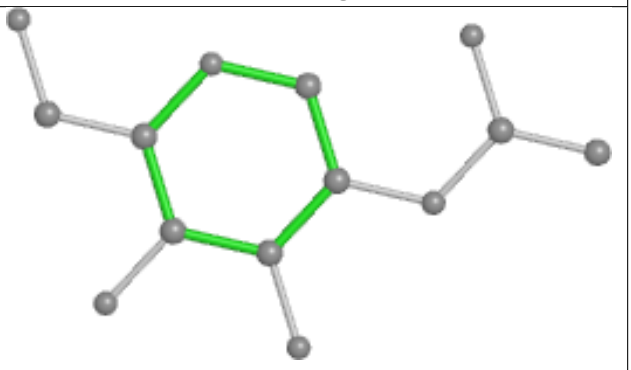
Bond angles

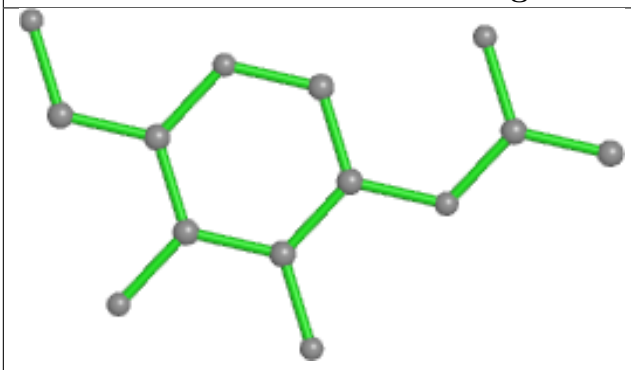
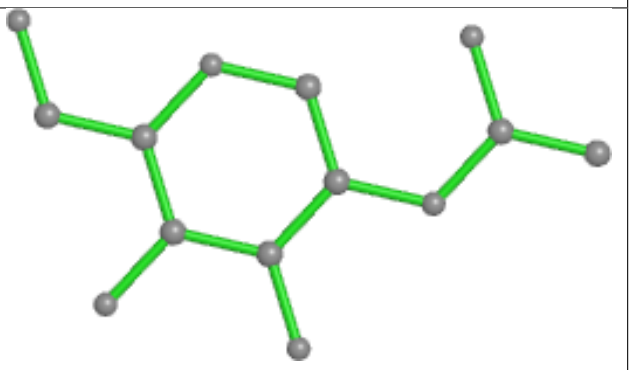
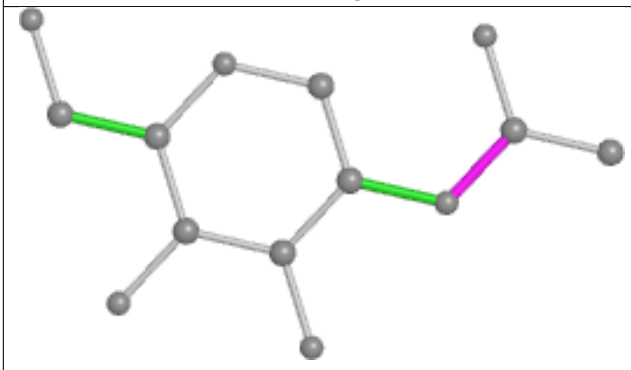
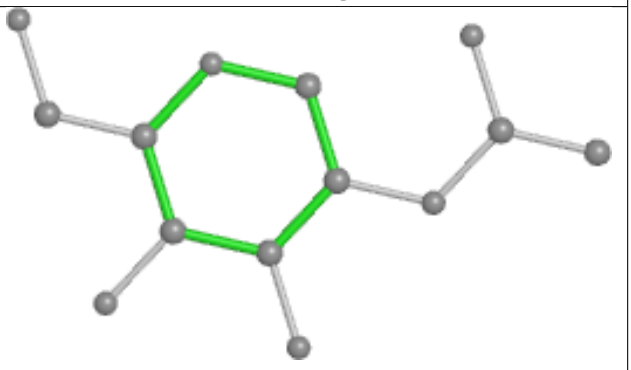


Torsions

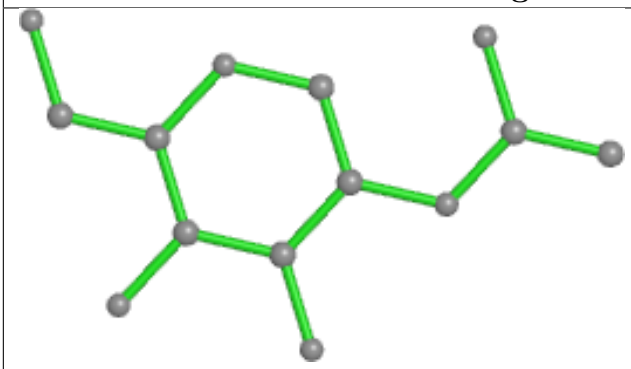


Rings

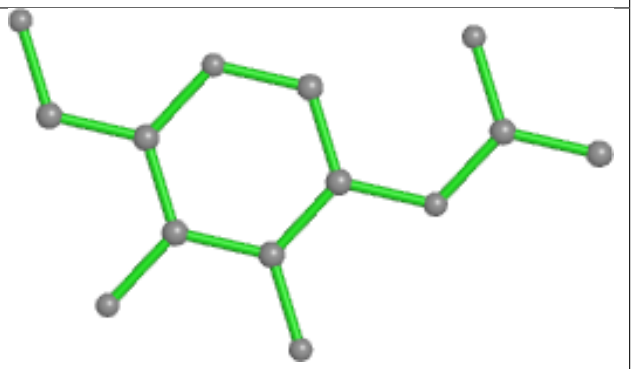
Ligand NAG B 1402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1409	
 Bond lengths	 Bond angles
 Torsions	 Rings

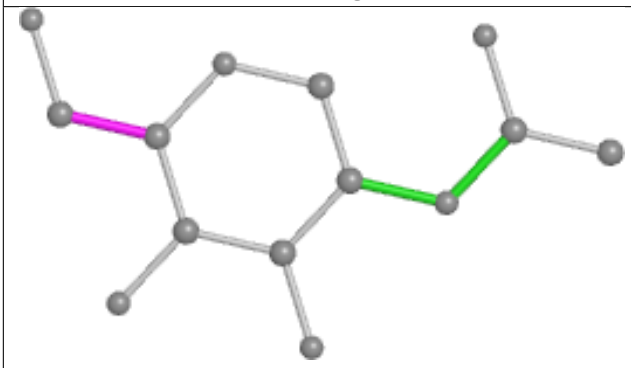
Ligand NAG C 1406



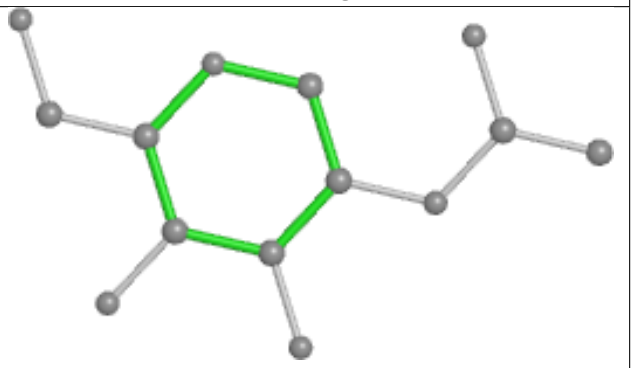
Bond lengths



Bond angles

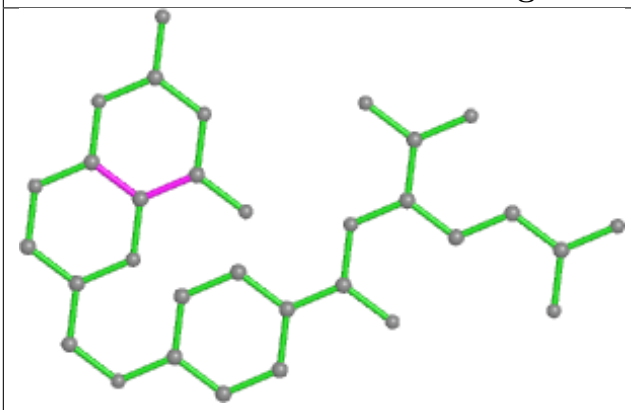


Torsions



Rings

Ligand FOL C 1414



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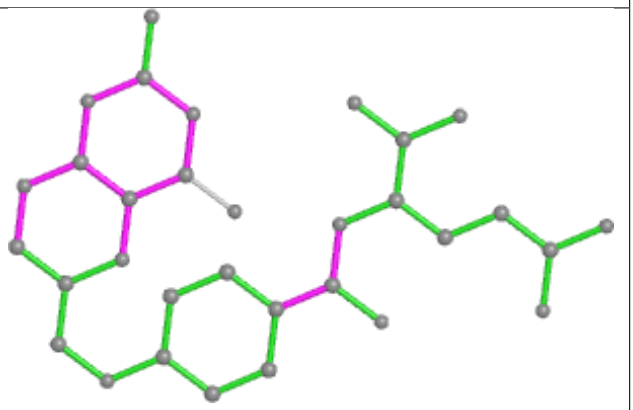
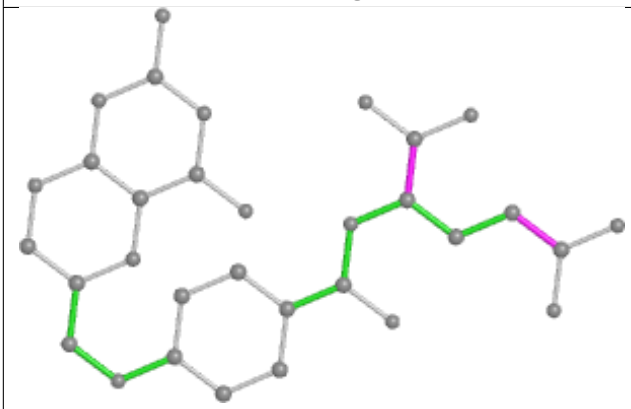


Bond angles



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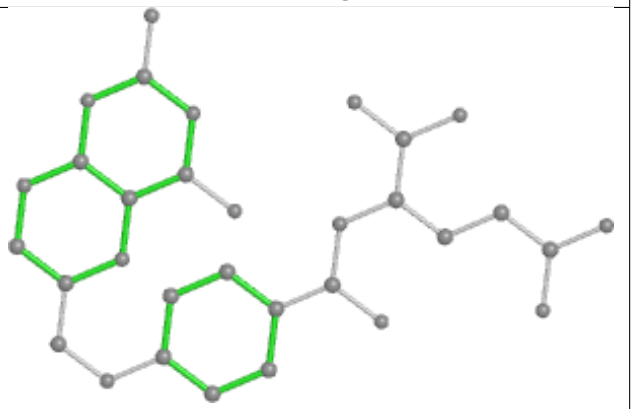
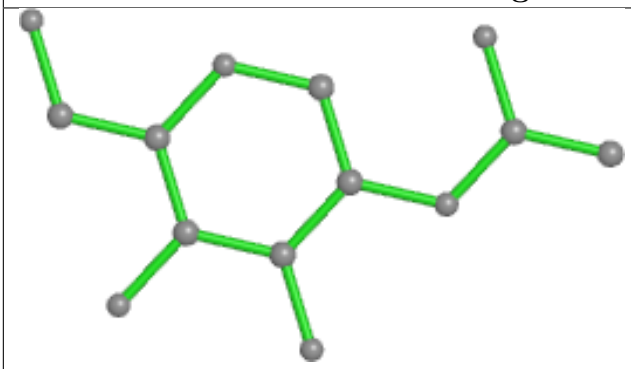


Rings

Ligand NAG B 1404



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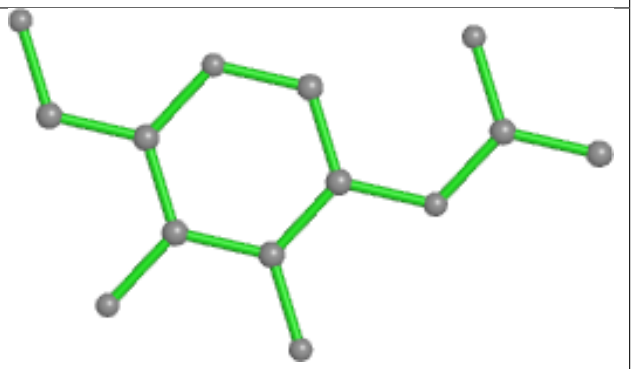
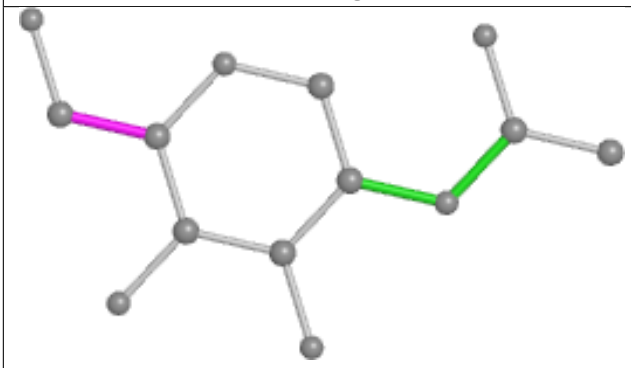


Bond angles



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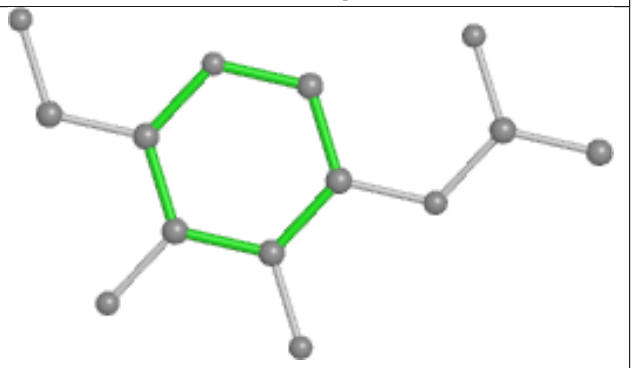
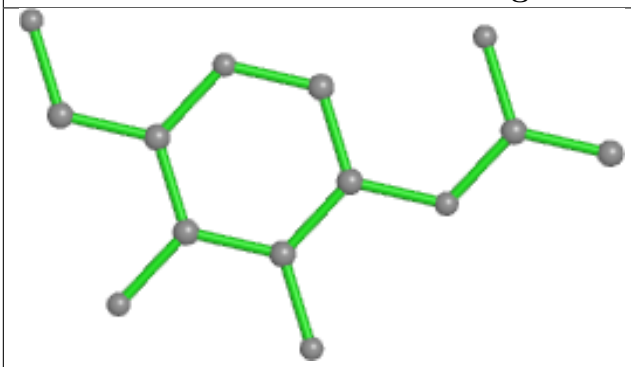
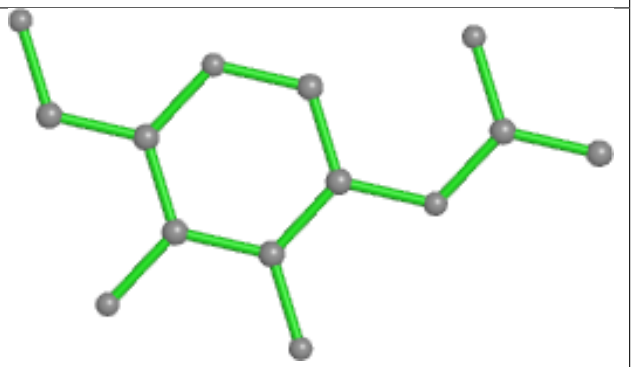


Rings

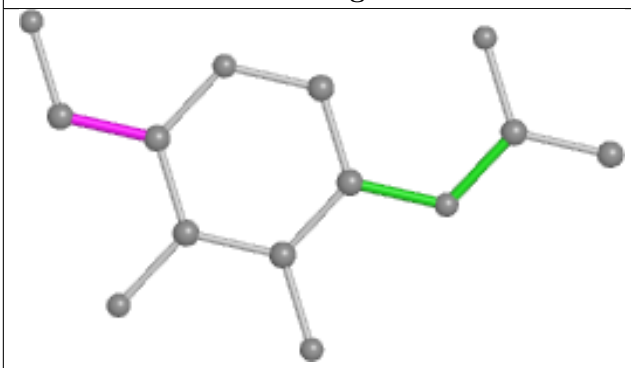
Ligand NAG C 1403



Bond lengths



Bond angles



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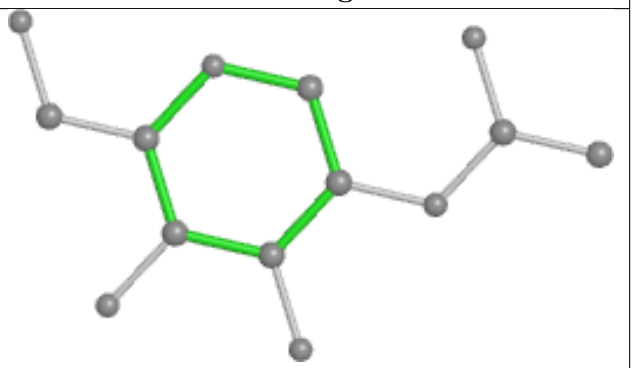
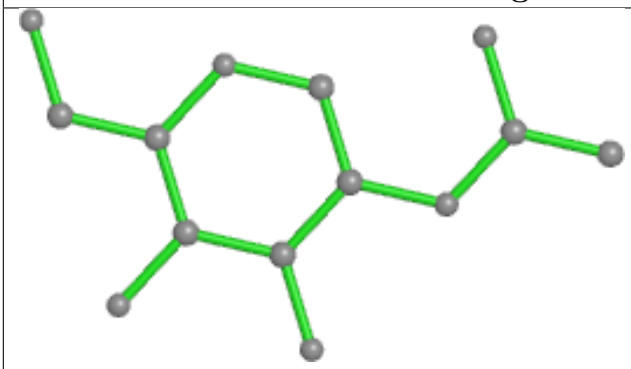


Rings

Ligand NAG C 1408



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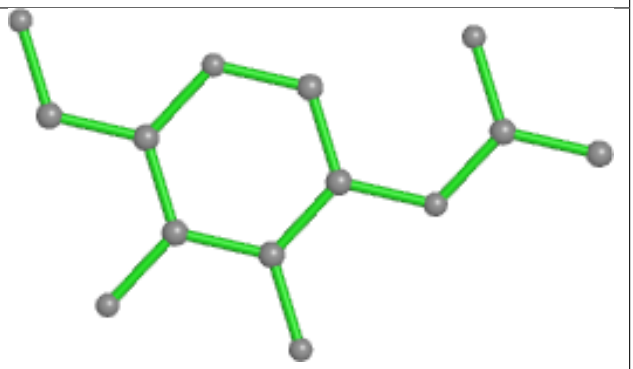
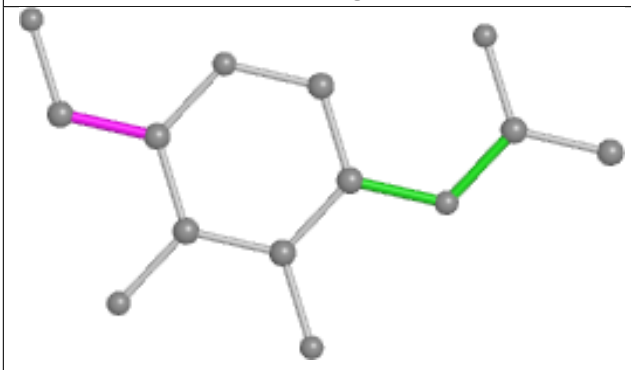


Bond angles



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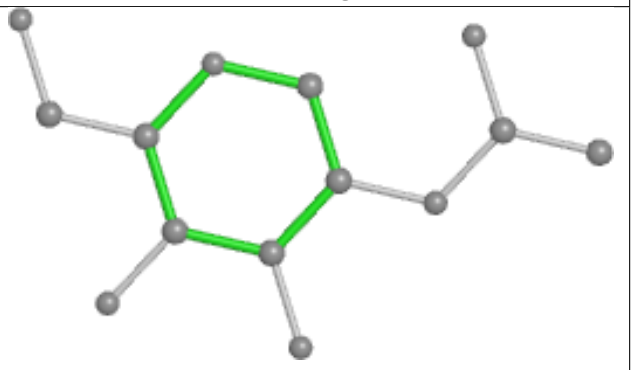
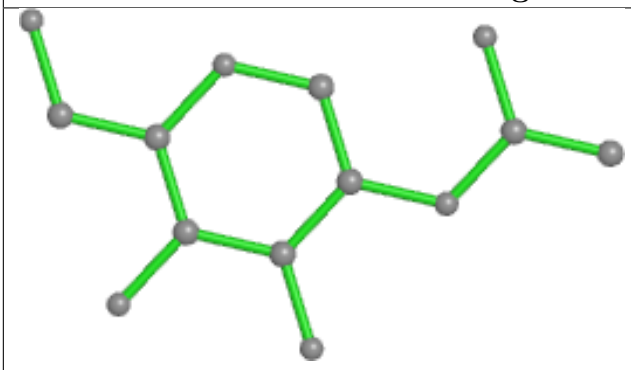
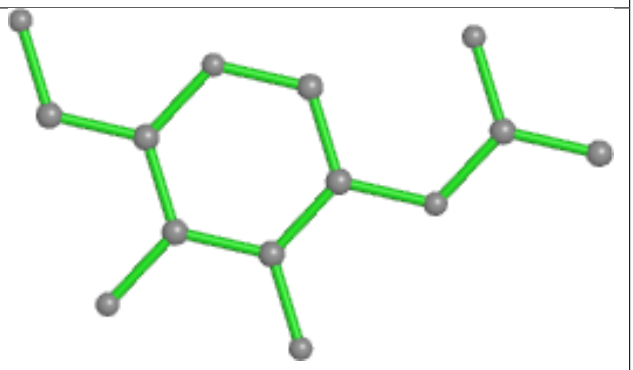


Rings

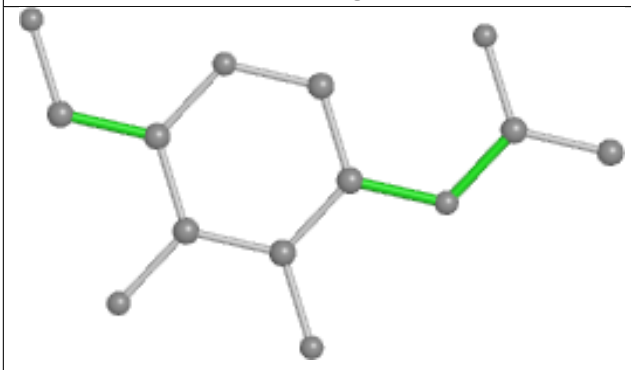
Ligand NAG B 1406



Bond lengths



Bond angles



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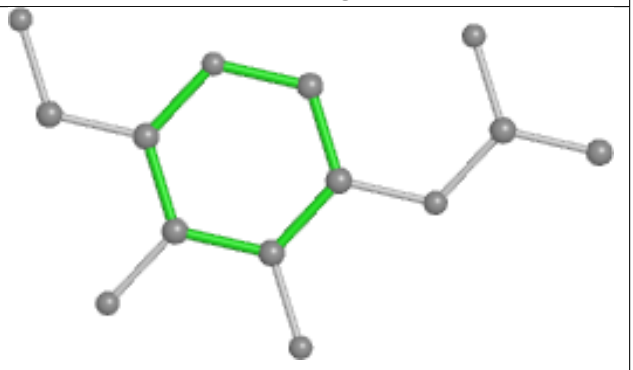
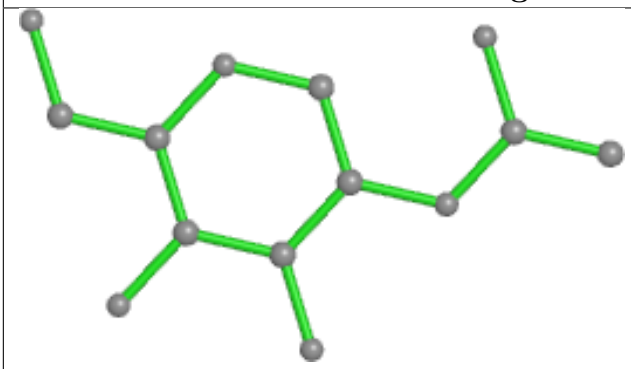


Rings

Ligand NAG A 1404



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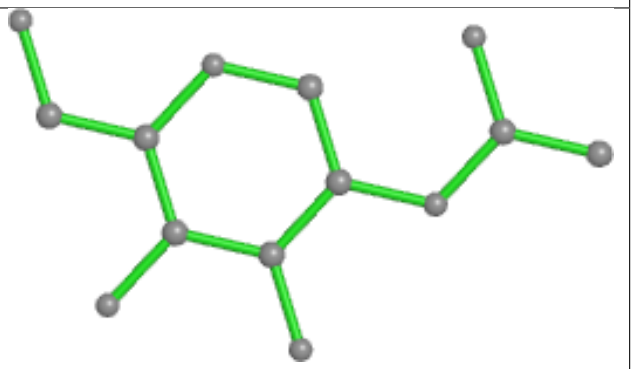
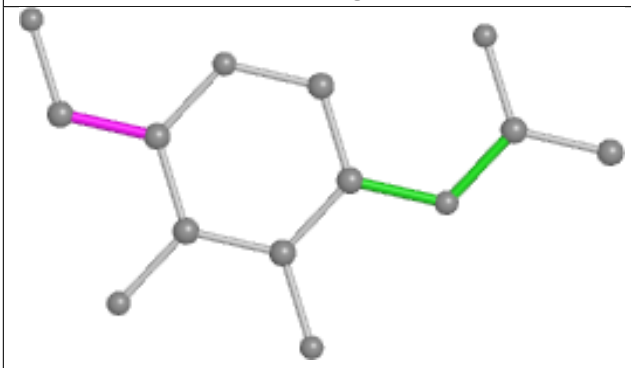


Bond angles



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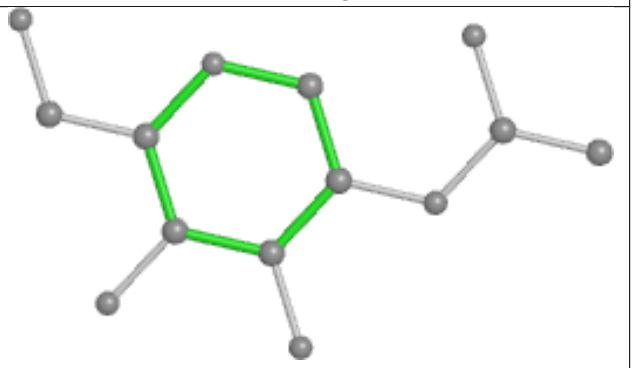
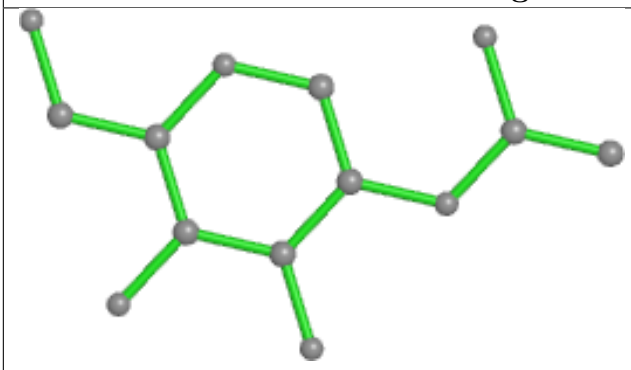


Rings

Ligand NAG C 1410



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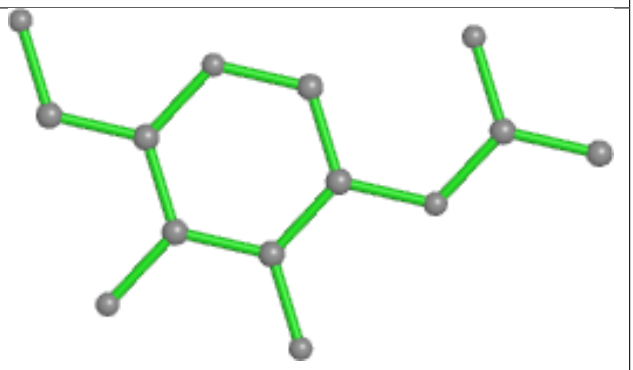
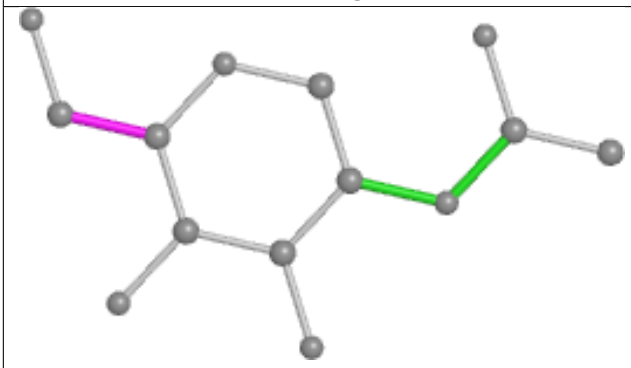
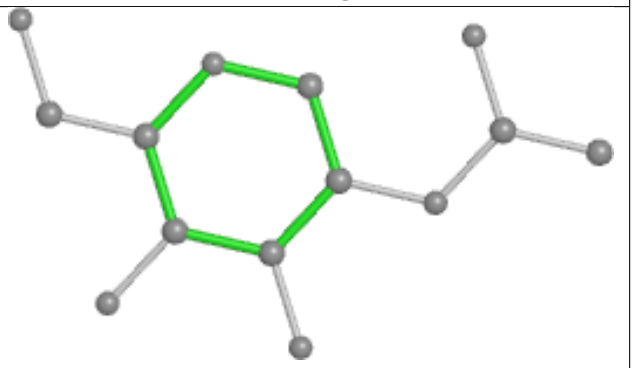


Bond angles

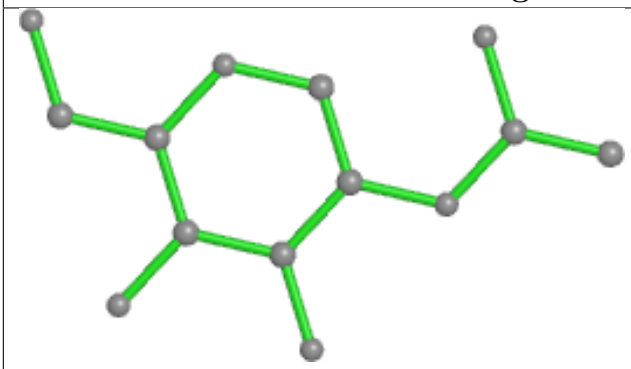


Torsions



Rings

Ligand NAG B 1411



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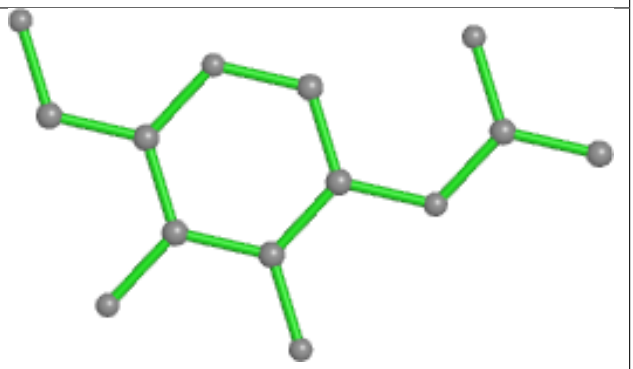
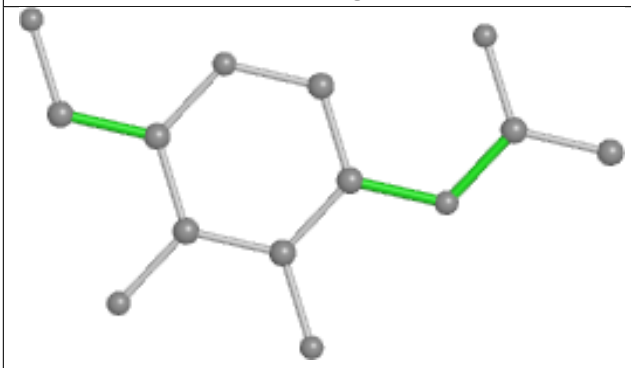
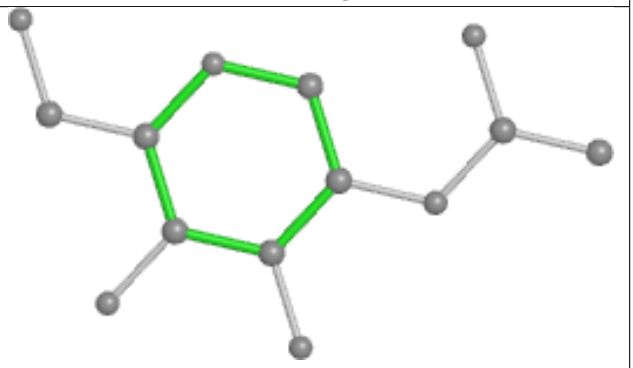


Bond angles

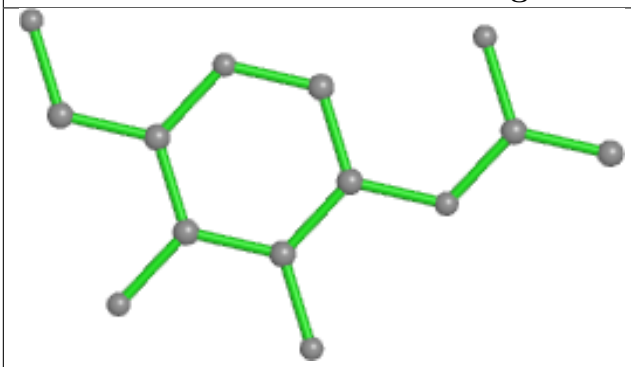


Torsions



Rings

Ligand NAG A 1407



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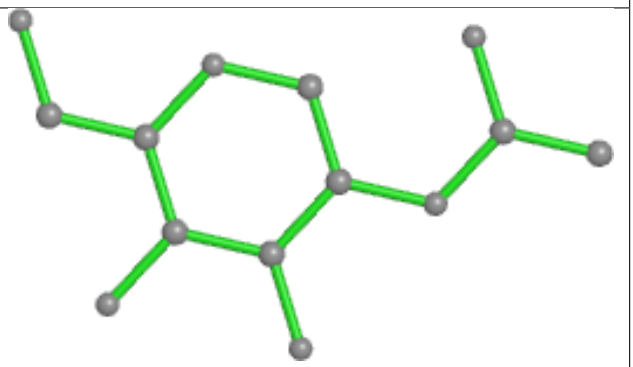
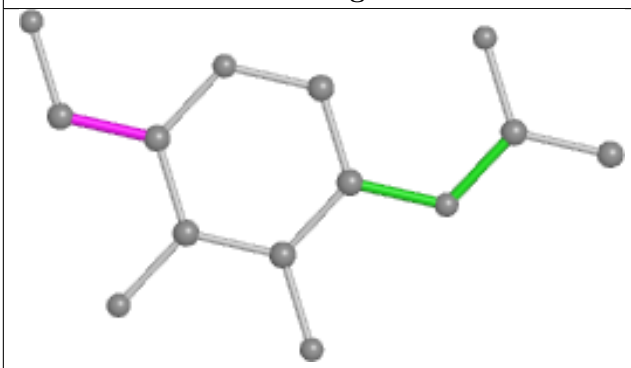
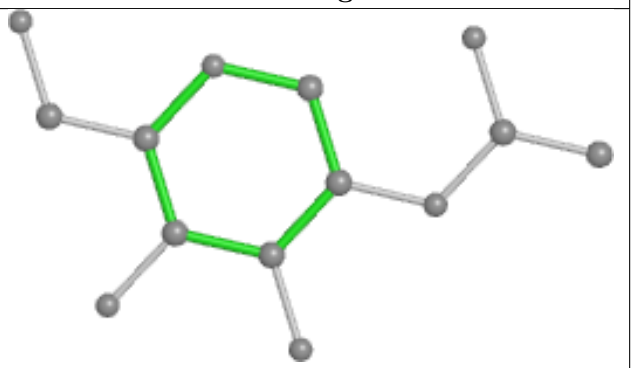


Bond angles

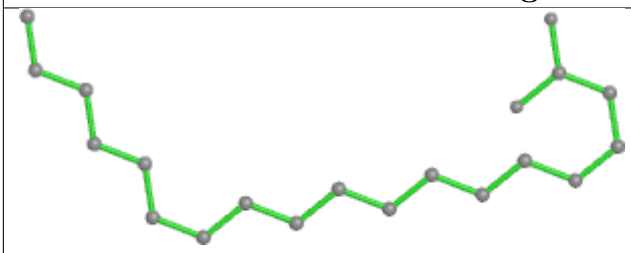


Torsions



Rings

Ligand EIC A 1415



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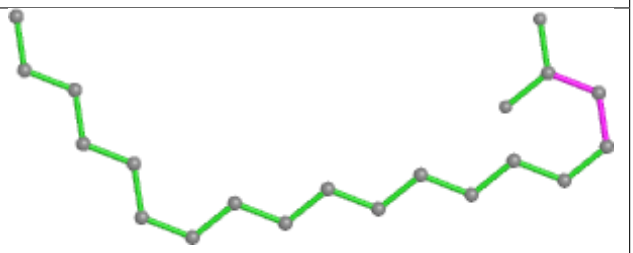
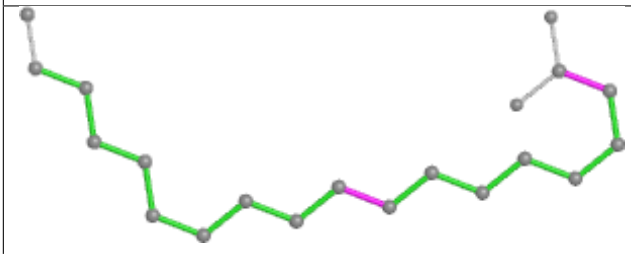


Bond angles



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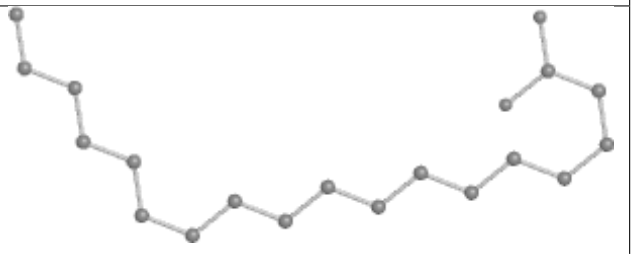
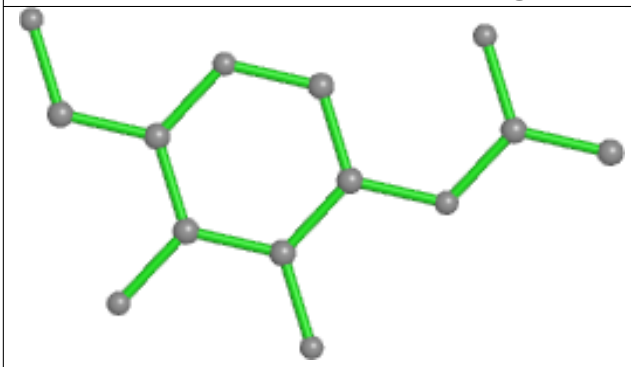
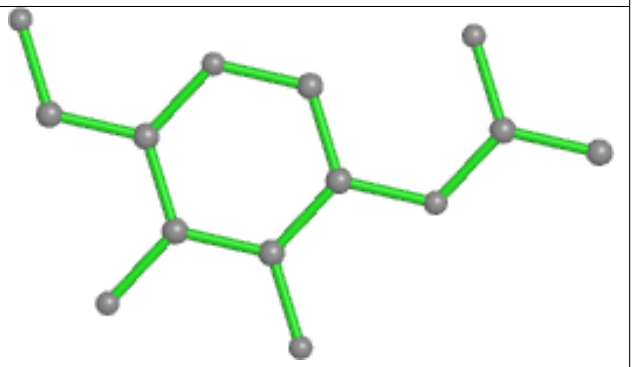


Rings

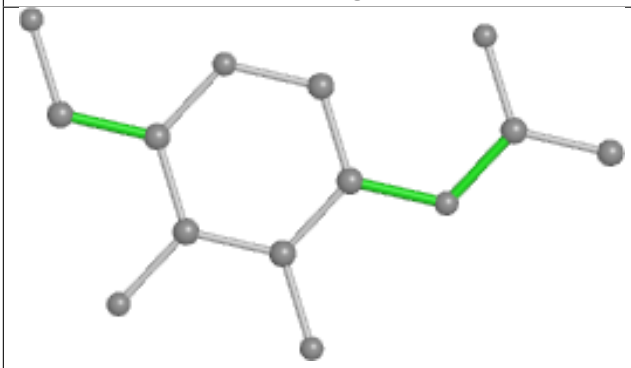
Ligand NAG A 1403



Bond lengths



Bond angles



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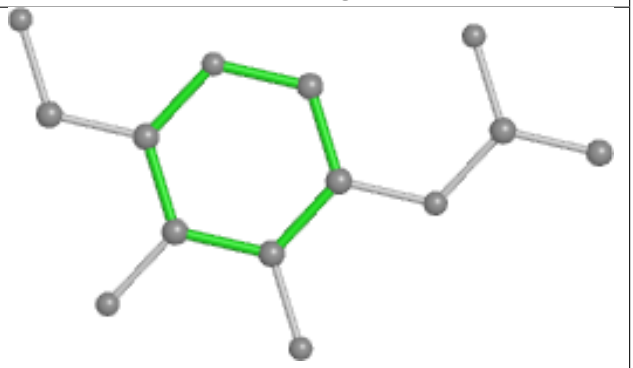
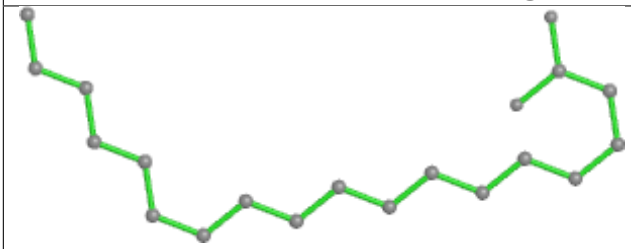
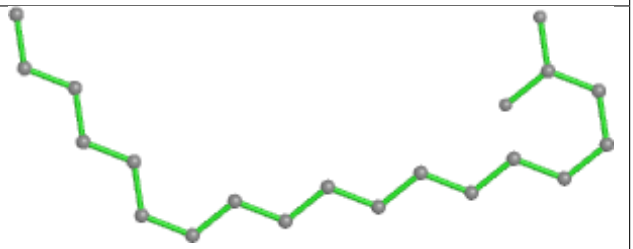


Rings

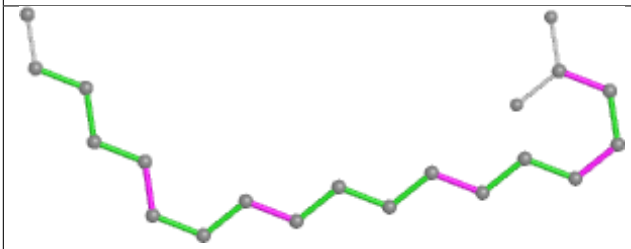
Ligand EIC B 1414



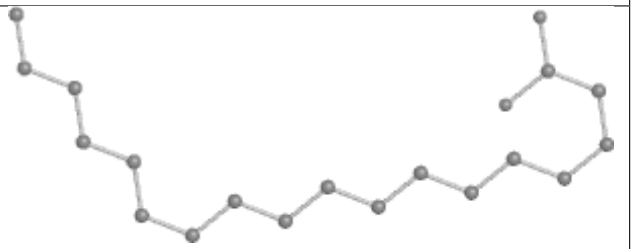
Bond lengths



Bond angles

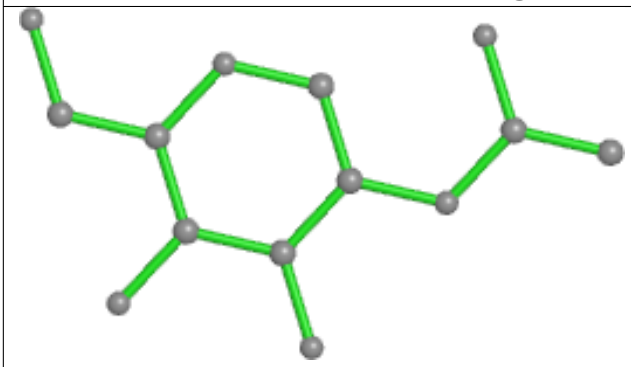


Torsions

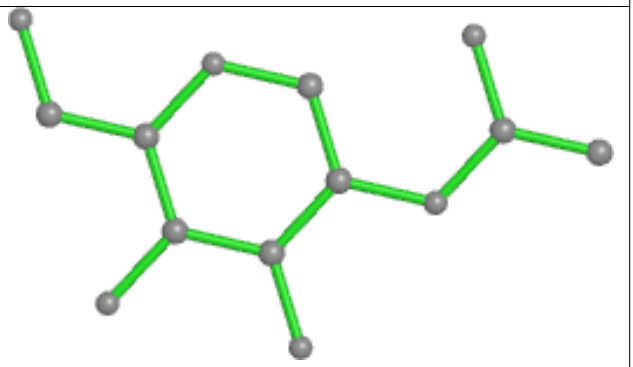


Rings

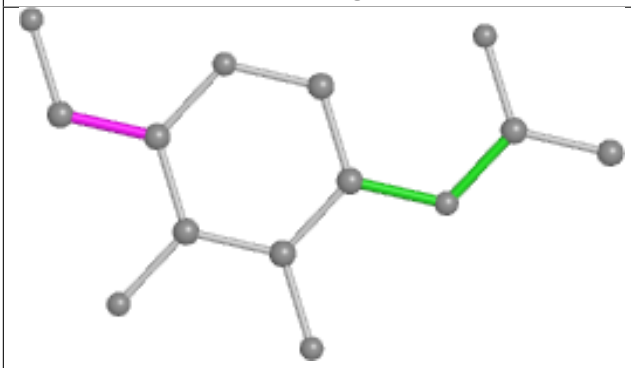
Ligand NAG A 1410



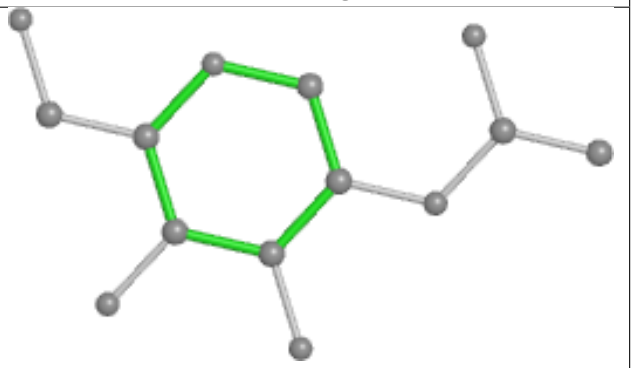
Bond lengths



Bond angles

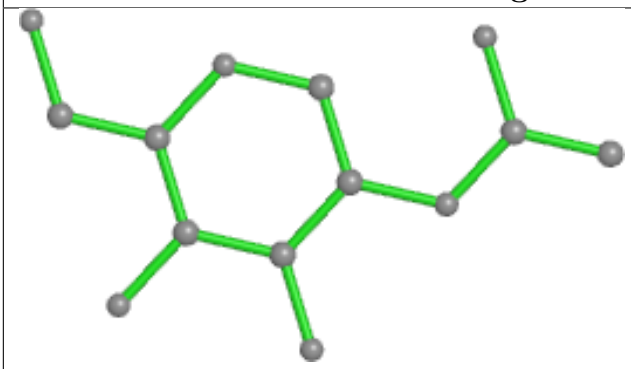


Torsions

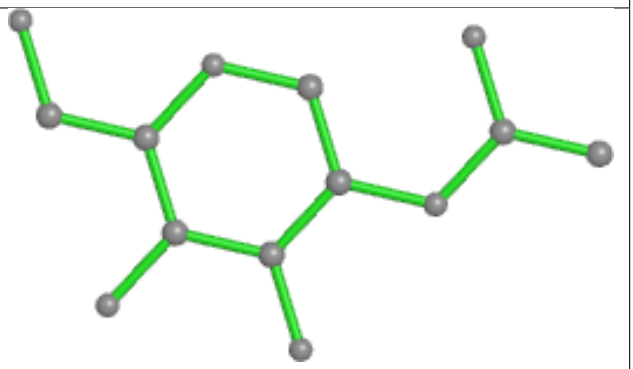


Rings

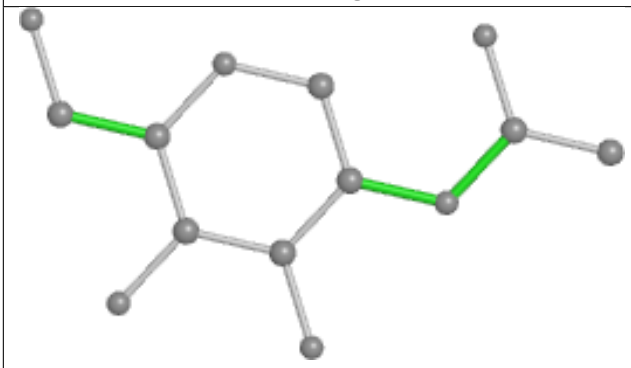
Ligand NAG A 1411



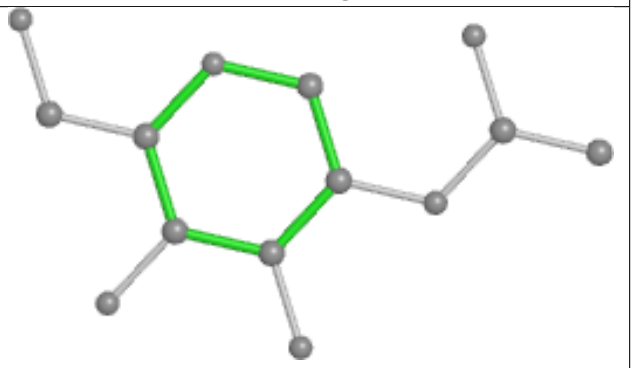
Bond lengths



Bond angles

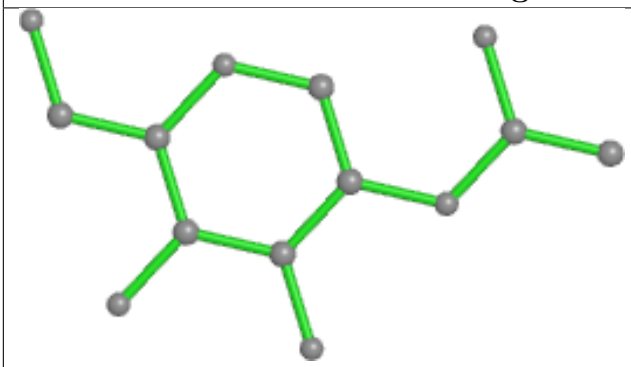


Torsions

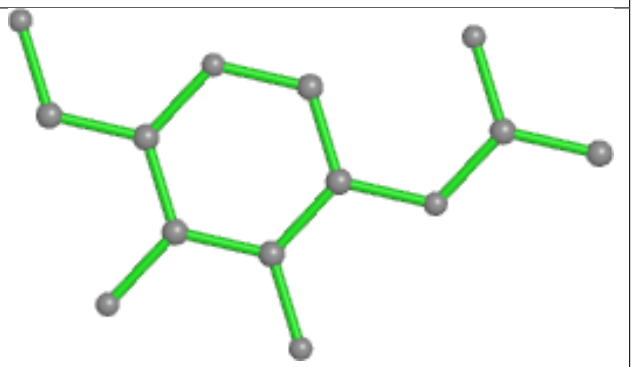


Rings

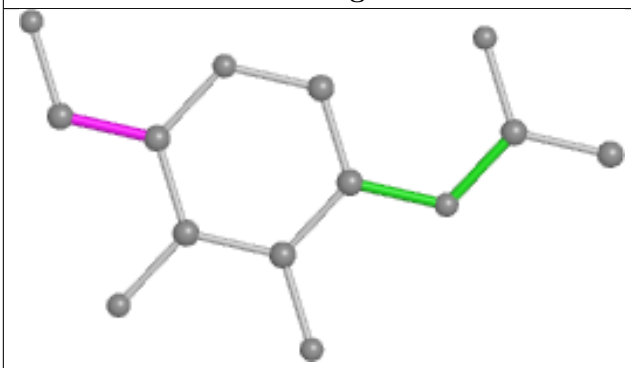
Ligand NAG C 1405



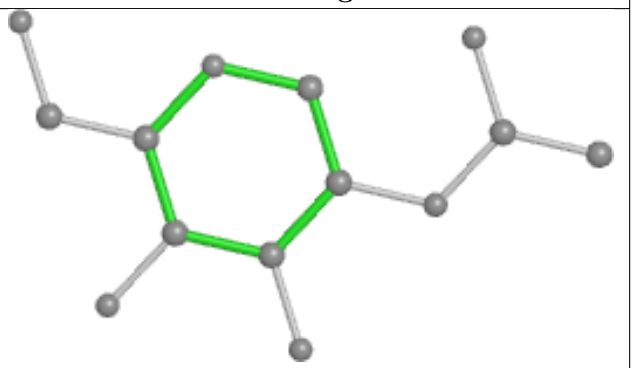
Bond lengths



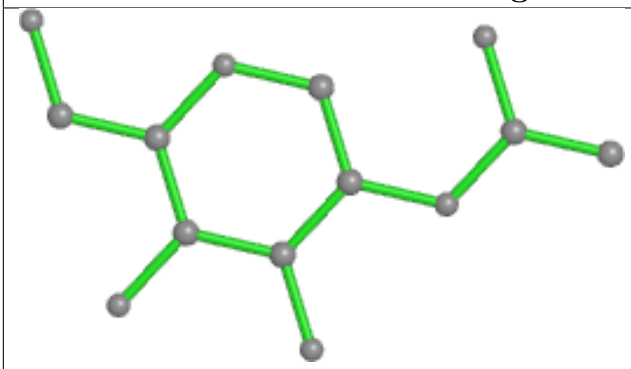
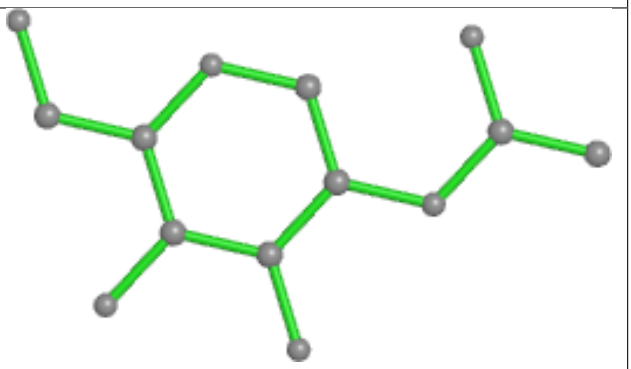
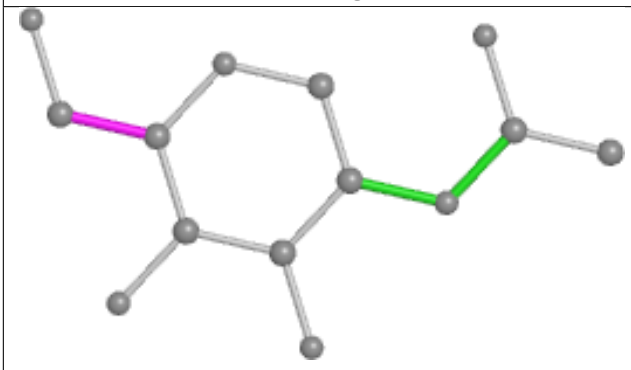
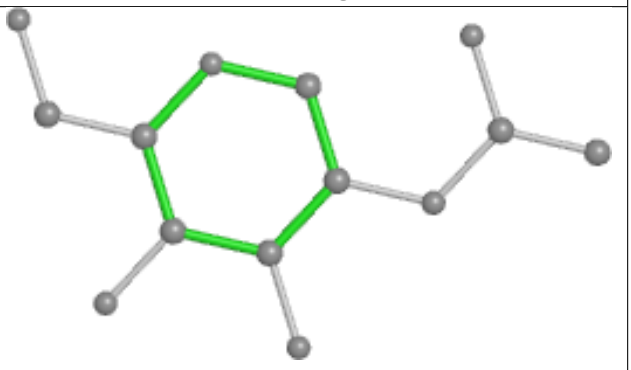
Bond angles

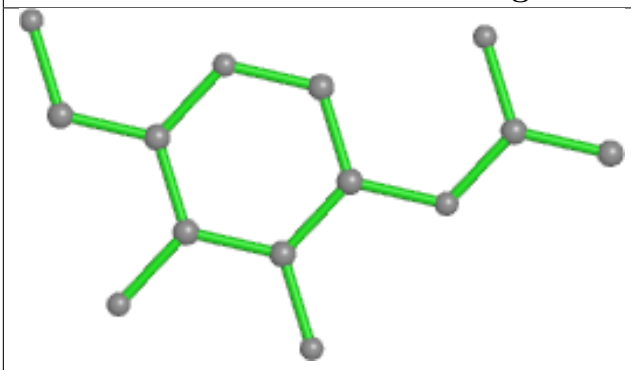
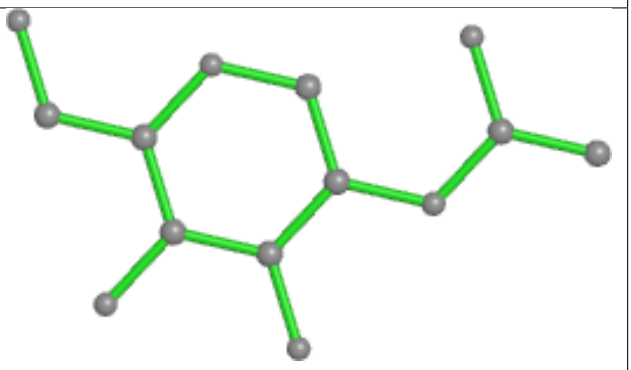
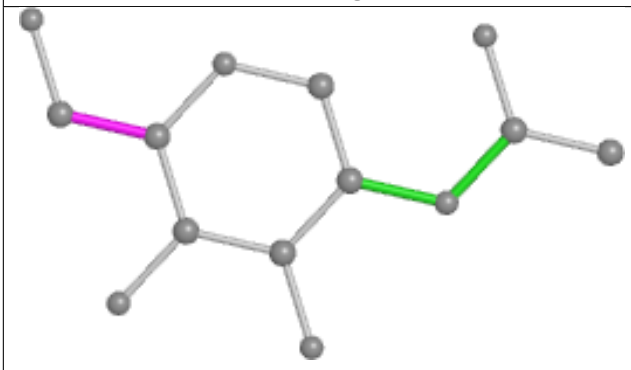
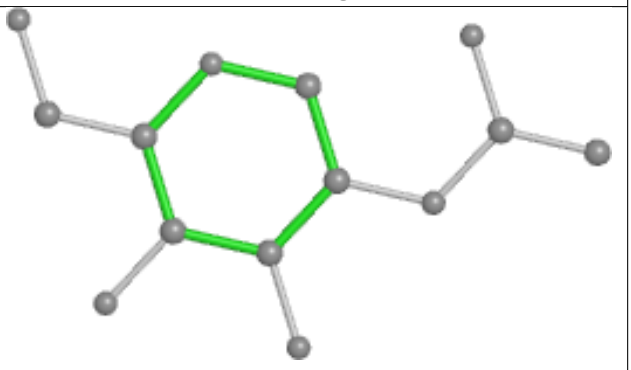


Torsions

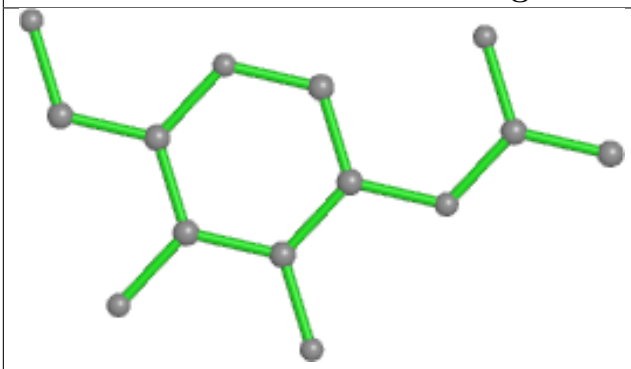


Rings

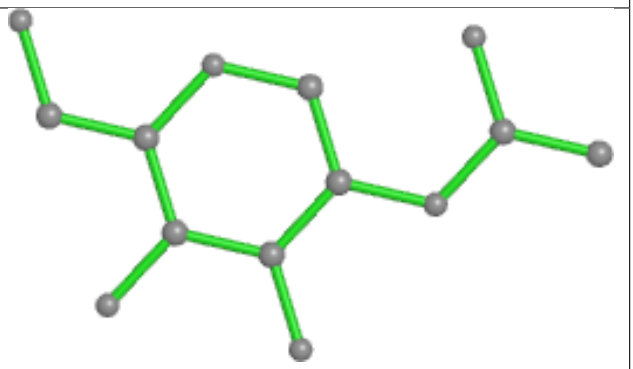
Ligand NAG A 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1401	
 Bond lengths	 Bond angles
 Torsions	 Rings

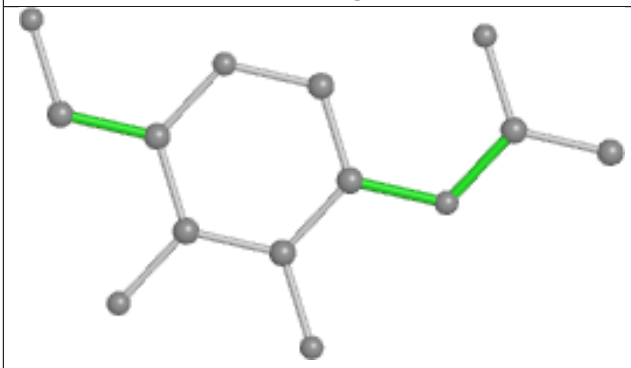
Ligand NAG C 1407



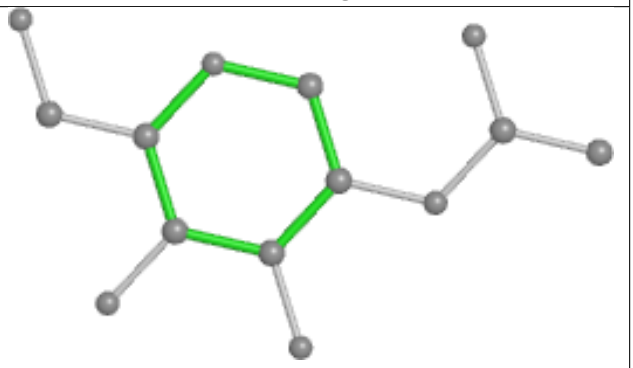
Bond lengths



Bond angles

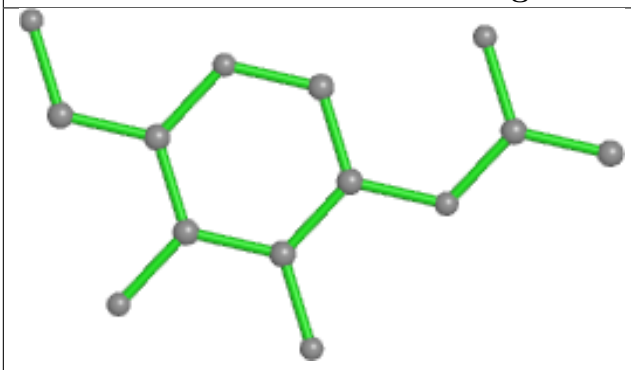


Torsions

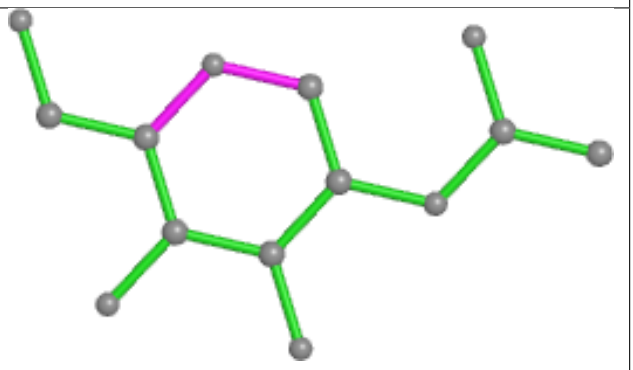


Rings

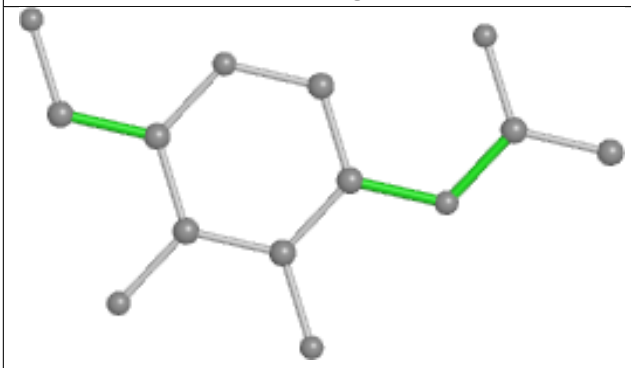
Ligand NAG C 1413



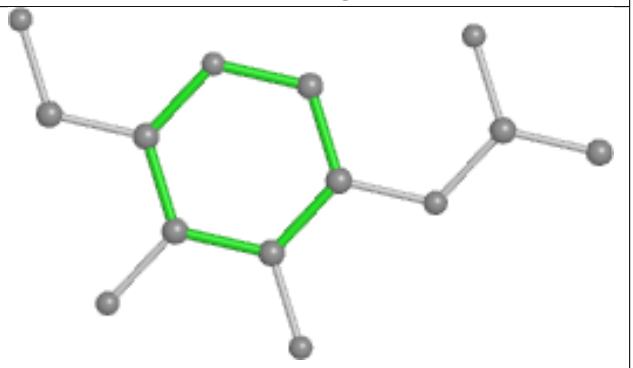
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

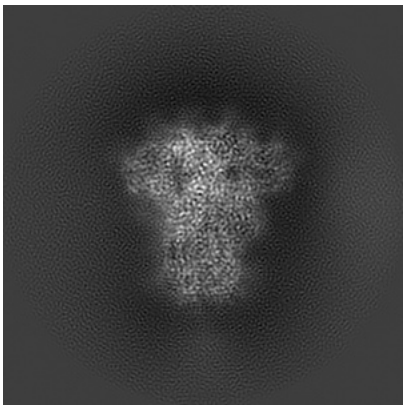
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61601. These allow visual inspection of the internal detail of the map and identification of artifacts.

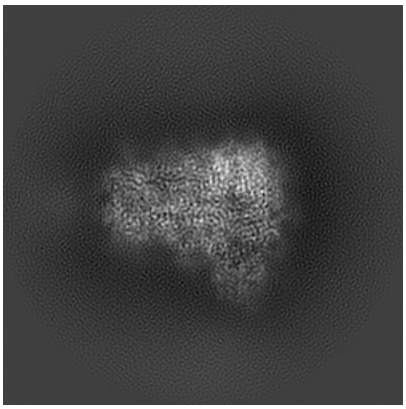
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

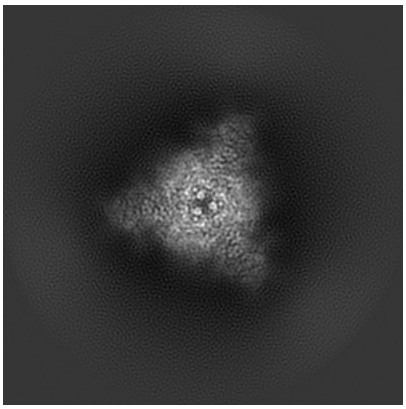
6.1.1 Primary map



X

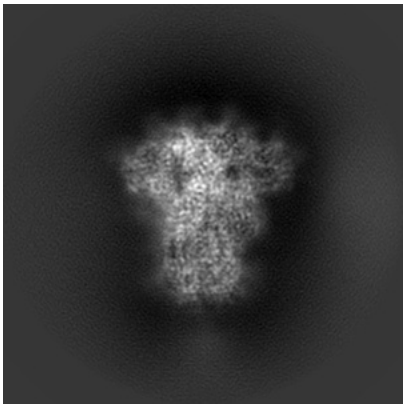


Y

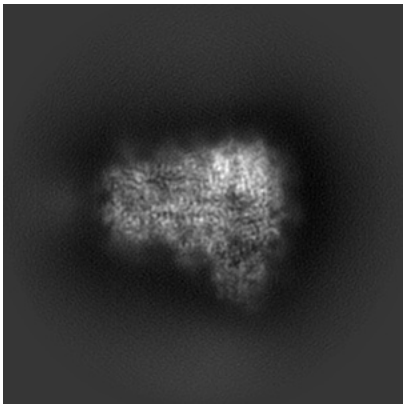


Z

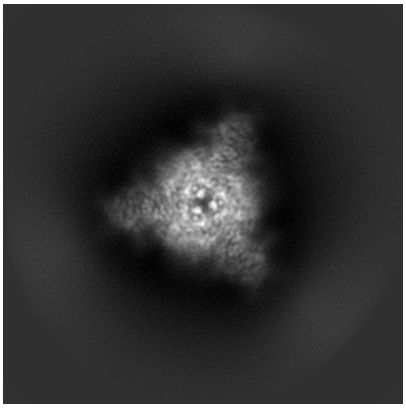
6.1.2 Raw map



X



Y

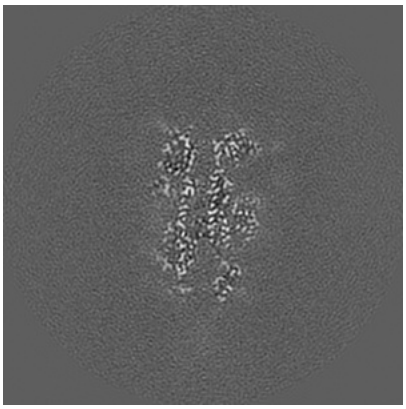


Z

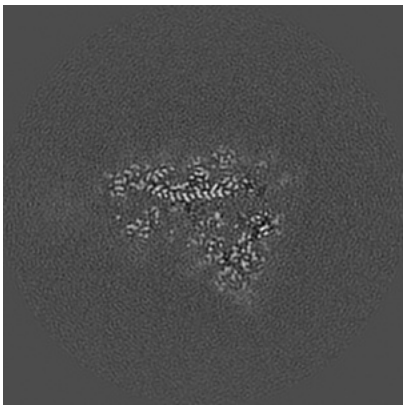
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

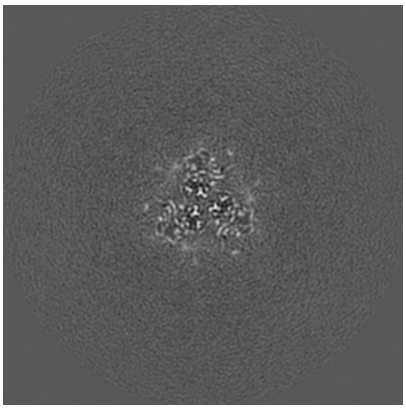
6.2.1 Primary map



X Index: 120

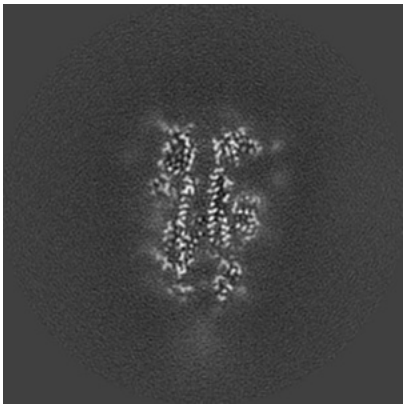


Y Index: 120

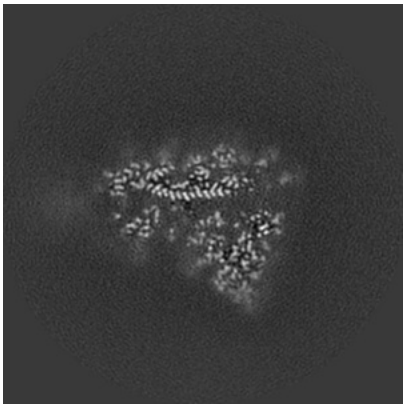


Z Index: 120

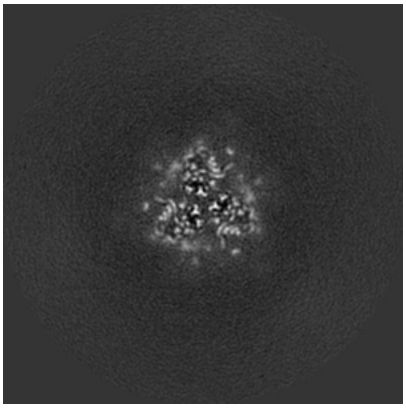
6.2.2 Raw map



X Index: 120



Y Index: 120

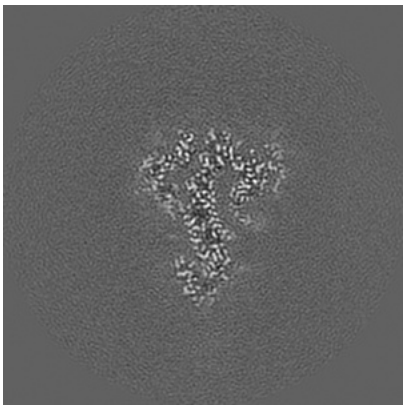


Z Index: 120

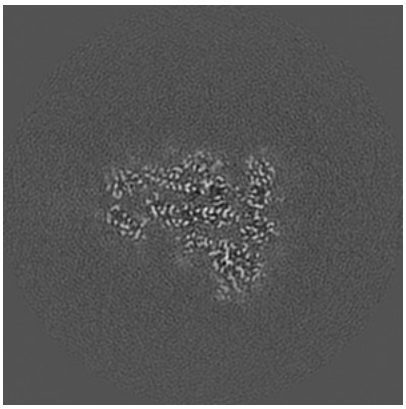
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

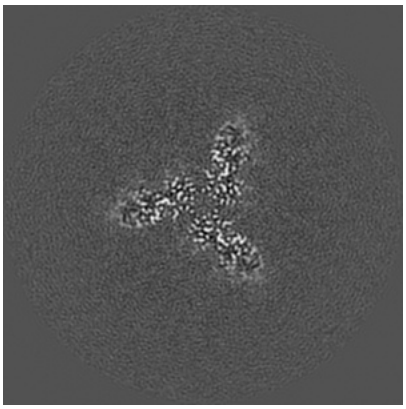
6.3.1 Primary map



X Index: 131

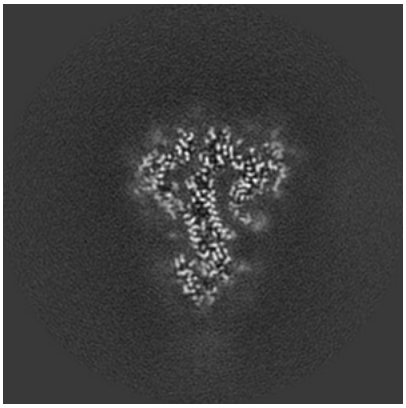


Y Index: 114

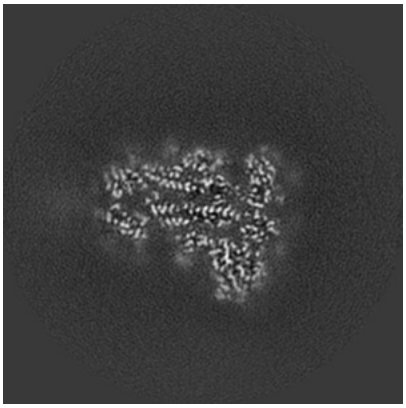


Z Index: 144

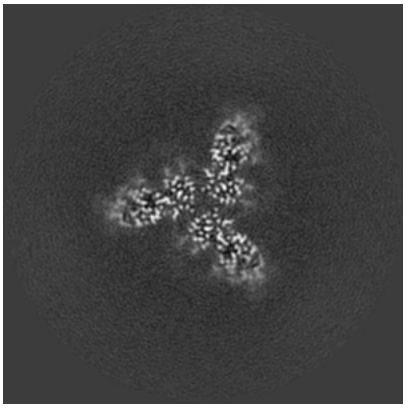
6.3.2 Raw map



X Index: 131



Y Index: 114

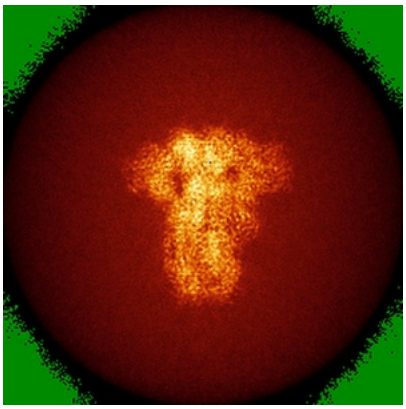


Z Index: 144

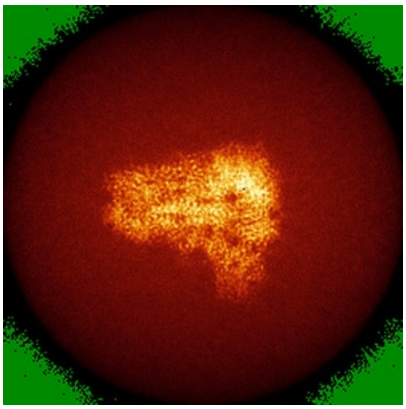
The images above show the largest variance slices of the map in three orthogonal directions.

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

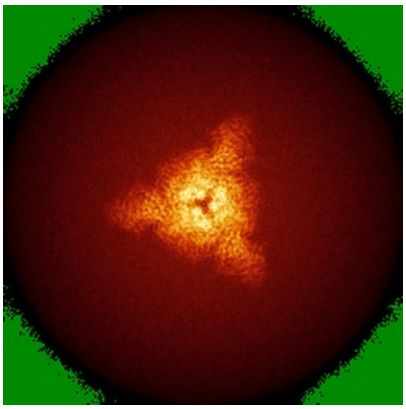
6.4.1 Primary map



X

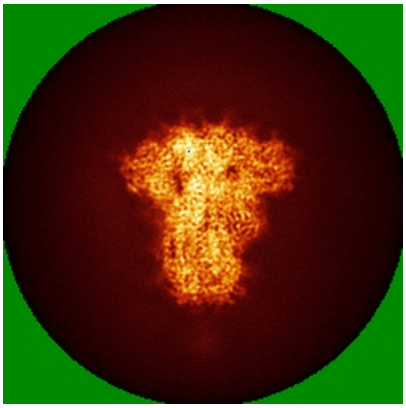


Y

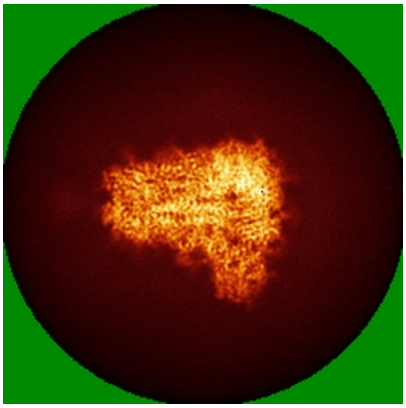


Z

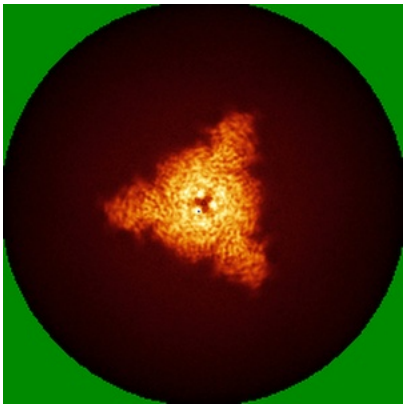
6.4.2 Raw map



X



Y

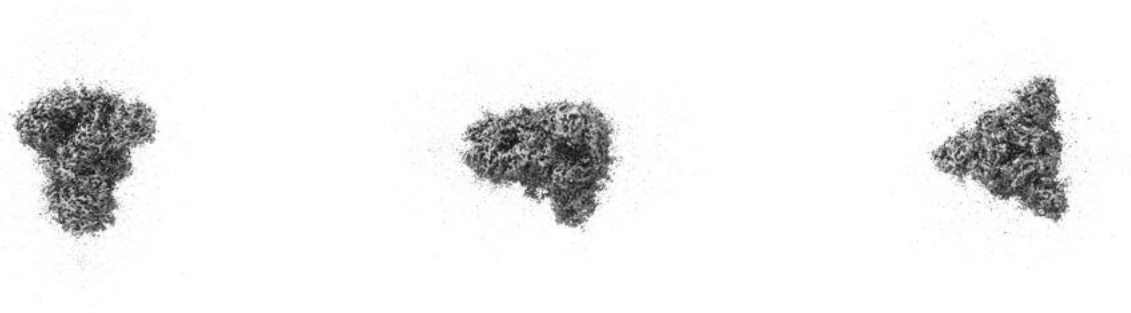


Z

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 0.0253. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

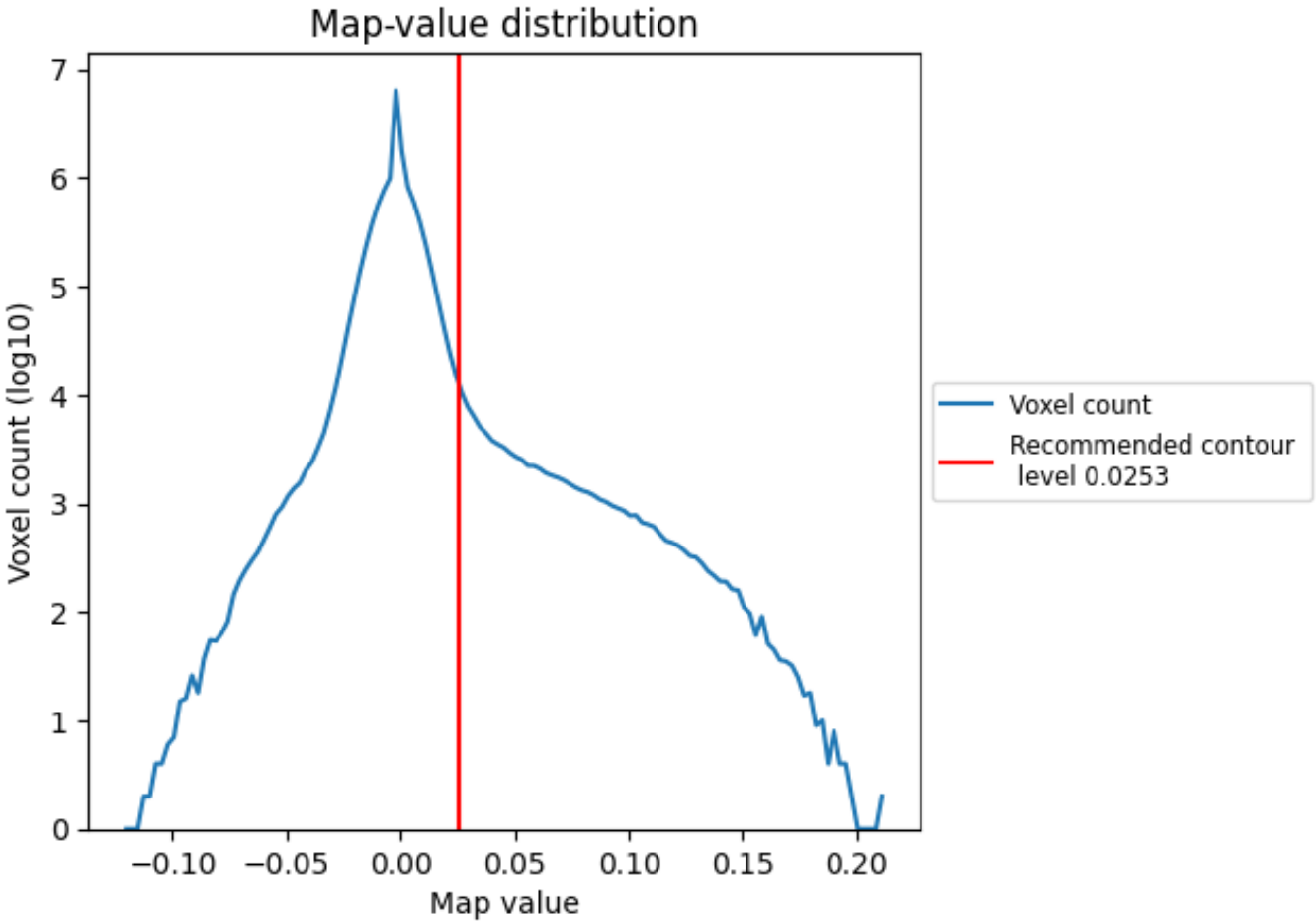
6.6 Mask visualisation (i)

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

7 Map analysis

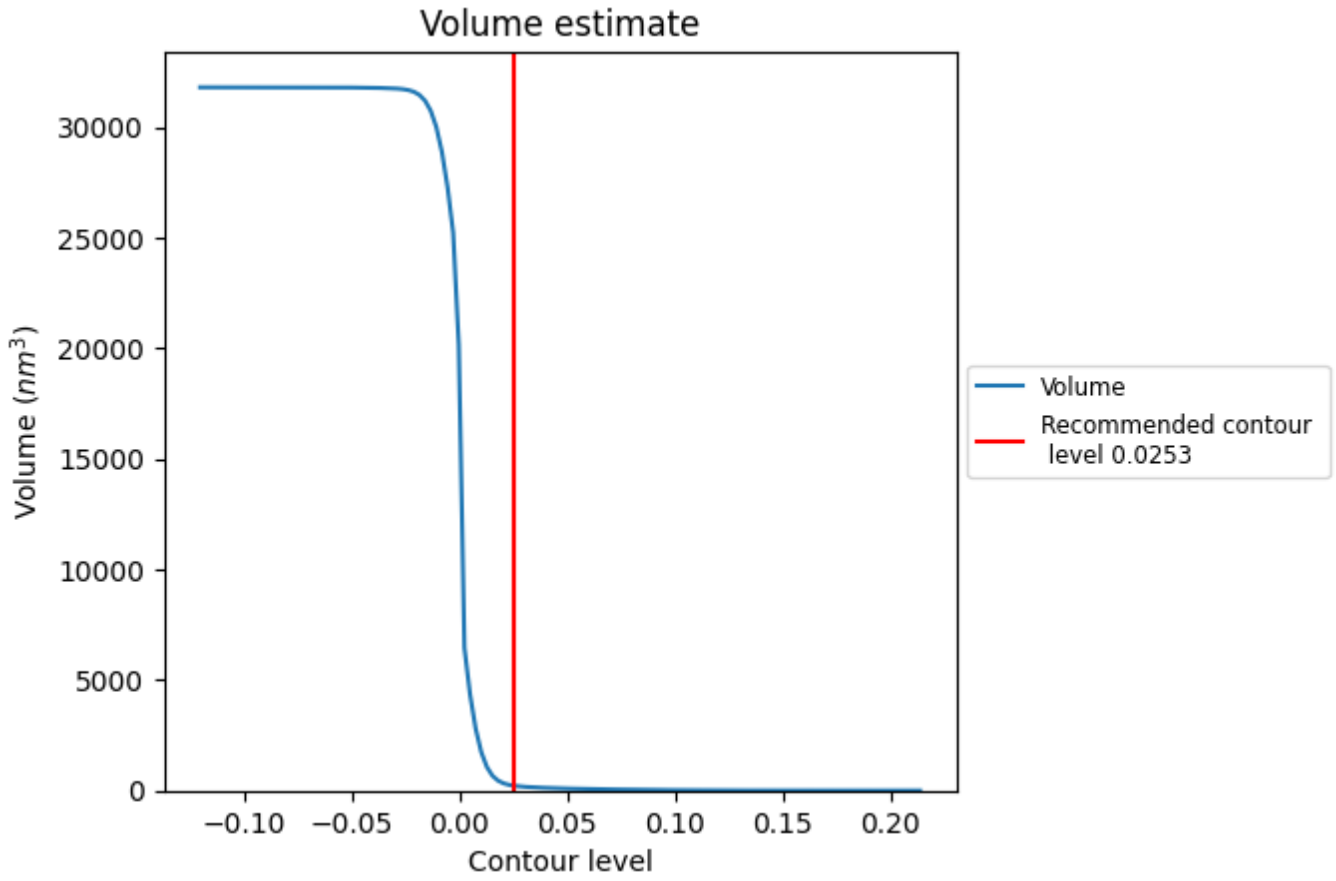
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

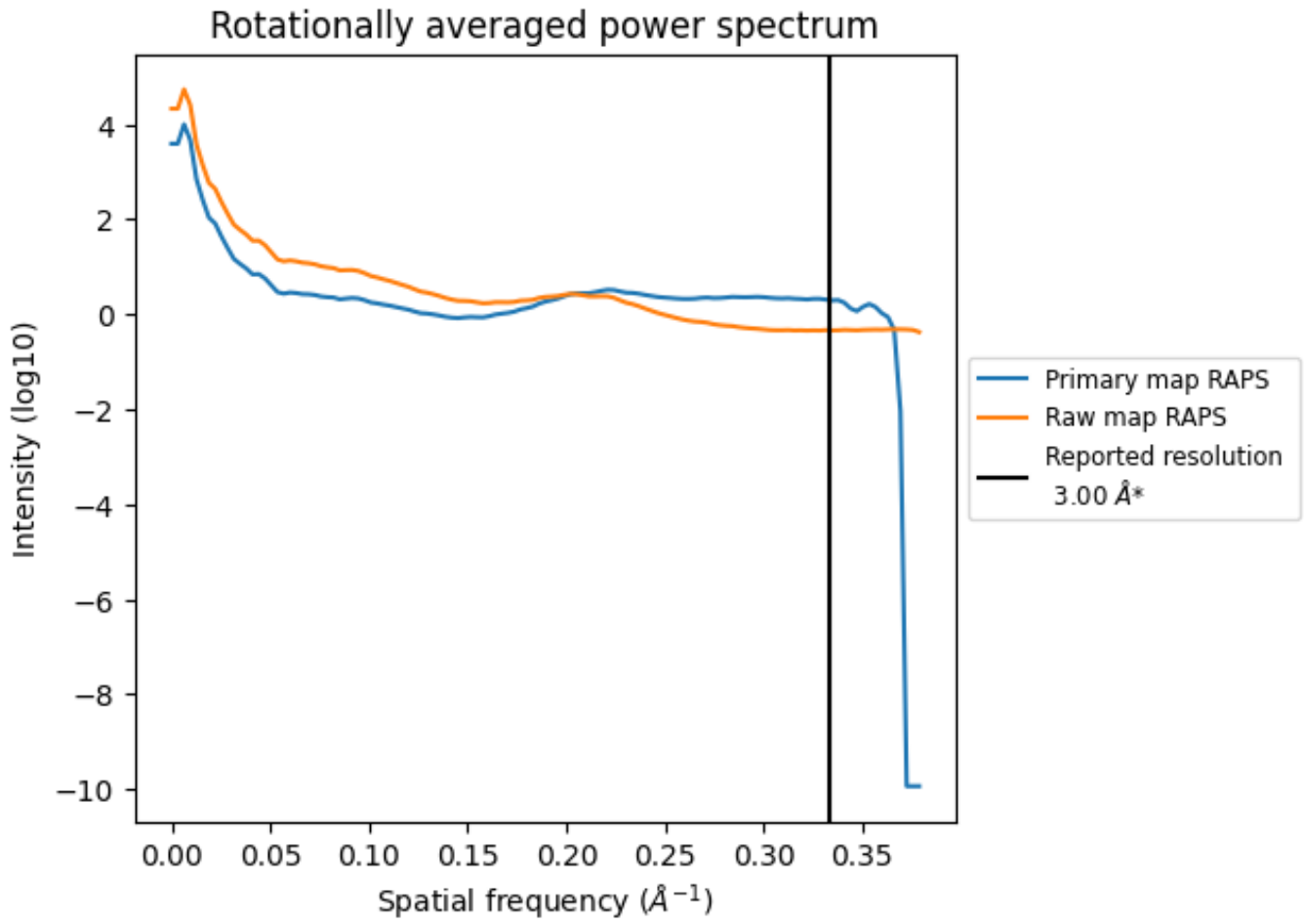
7.2 Volume estimate



The volume at the recommended contour level is 220 nm^3; this corresponds to an approximate mass of 198 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)

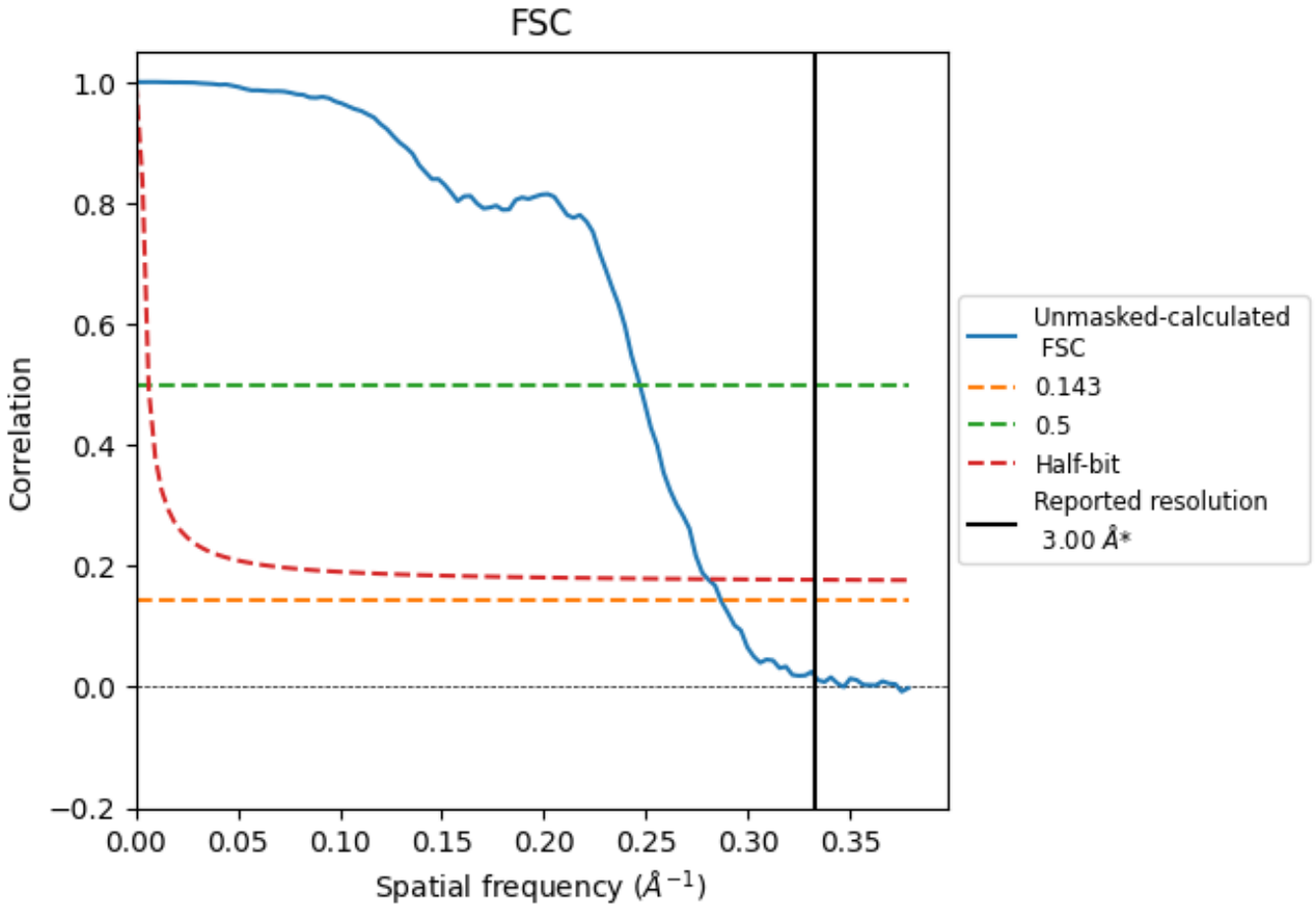


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

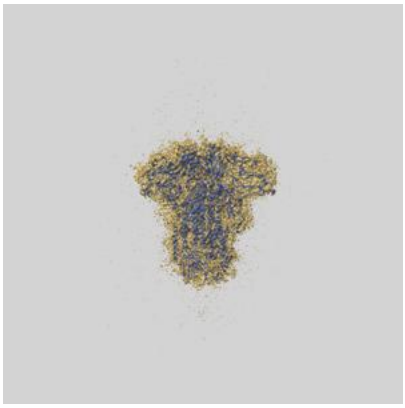
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	4.05	3.56

*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 3.48 differs from the reported value 3.0 by more than 10 %

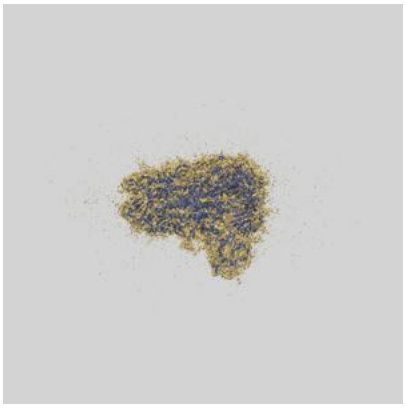
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61601 and PDB model 9JMG. Per-residue inclusion information can be found in section 3 on page 13.

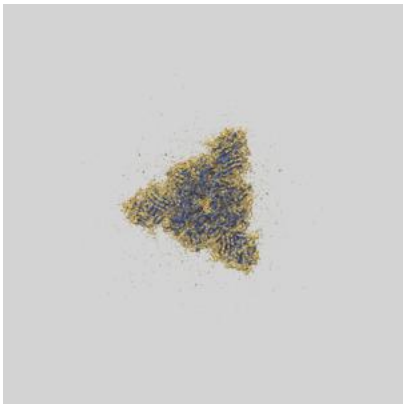
9.1 Map-model overlay



X



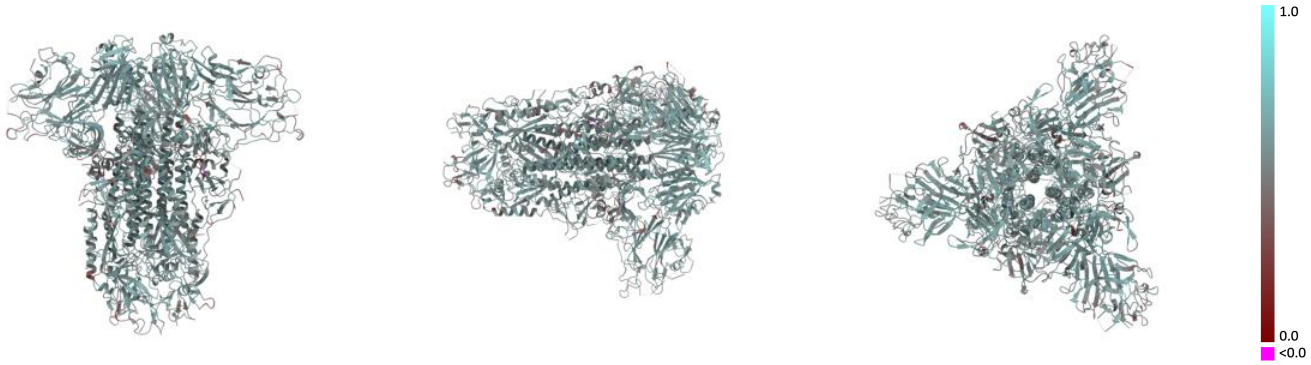
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

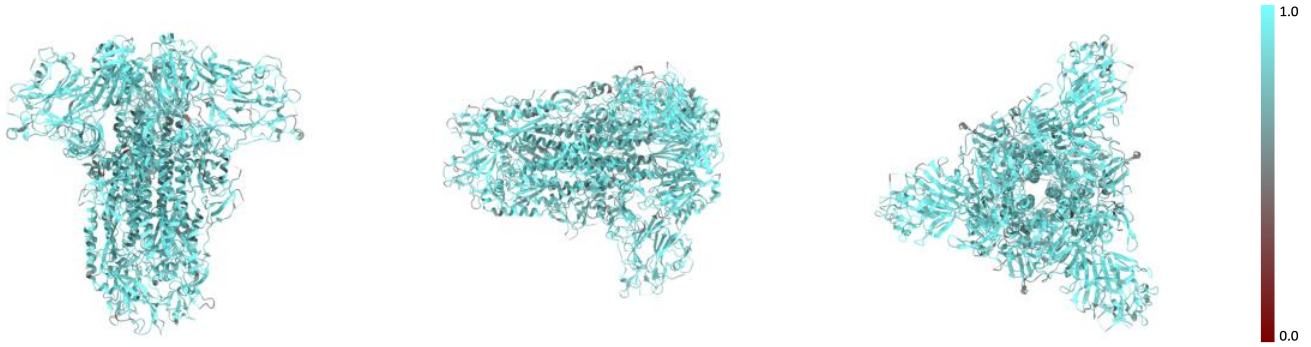
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

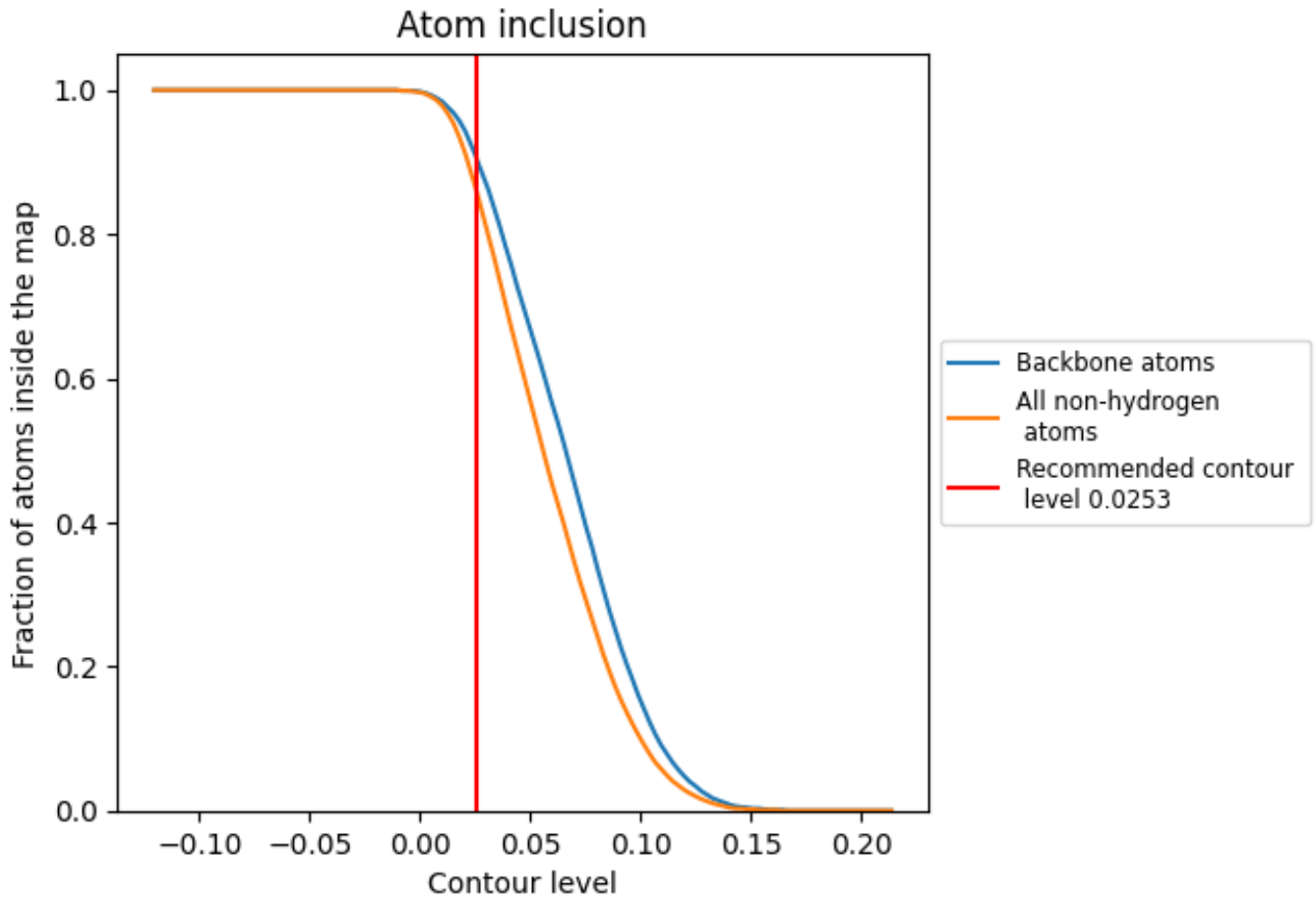
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0253).

9.4 Atom inclusion (i)



At the recommended contour level, 91% 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 (0.0253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8650	0.5540
A	0.8680	0.5590
B	0.8650	0.5550
C	0.8660	0.5530
D	0.6410	0.3330
E	0.7180	0.3840
F	0.7690	0.4330
G	0.6430	0.5060
H	0.8460	0.5080
I	0.7440	0.4730
J	0.7140	0.4530
K	0.8460	0.5420