Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 03:00 PM JST

PDB ID	:	8ZC4
EMDB ID	:	EMD-39922
Title	:	SARS-CoV-2 Omicron BA.4 spike trimer (6P) in complex with 3 D1F6 Fabs (2 RBD up)
Authors	:	Liu, B.; Gao, X.; Li, Z.; Chen, Q.; He, J.; Xiong, X.
Deposited on	:	2024-04-28
Resolution	:	3.95 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:

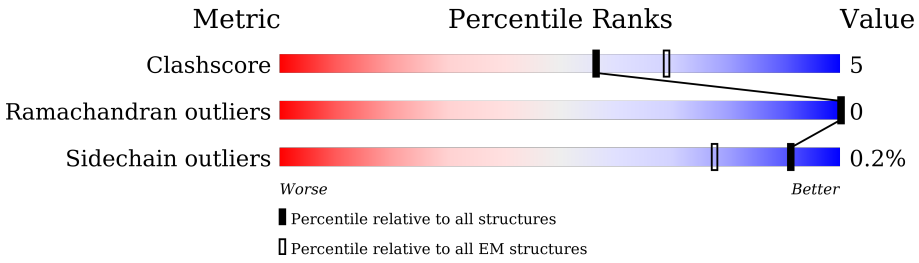
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.95 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%

Mol	Chain	Length	Quality of chain
1	A	1238	71% 9% 20%
1	B	1238	70% 10% 20%
1	C	1238	70% 10% 20%
2	G	223	86% 9% .
2	M	223	79% 17% .
2	N	223	87% 9% .
3	H	230	82% 14% .
3	Q	230	78% 18% .
3	R	230	83% 12% .

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Mol	Chain	Length	Quality of chain
4	D	2	100%
4	E	2	50% 50%
4	F	2	100%
4	I	2	100%
4	J	2	100%
4	K	2	100%
4	L	2	100%
4	O	2	100%
4	P	2	100%
4	S	2	100%
4	T	2	100%
4	U	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33840 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	994	Total	C	N	O	S	0	0
			7790	4994	1293	1469	34		
1	B	994	Total	C	N	O	S	0	0
			7790	4994	1293	1469	34		
1	C	993	Total	C	N	O	S	0	0
			7778	4988	1288	1468	34		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	683	LYS	ASN	variant	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	683	LYS	ASN	variant	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	683	LYS	ASN	variant	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Light chain of D1F6 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		
2	M	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		
2	N	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		

- Molecule 3 is a protein called Heavy chain of D1F6 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	Q	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	R	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		

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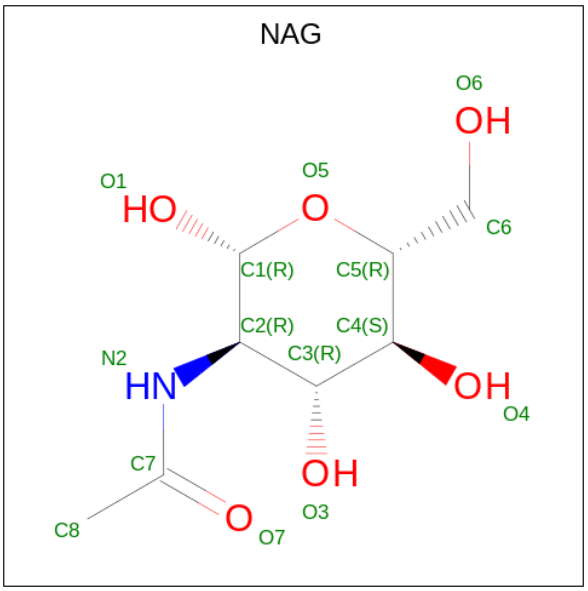
Mol	Chain	Residues	Atoms	AltConf	Trace
4	P	2	Total C N O 28 16 2 10	0	0
4	S	2	Total C N O 28 16 2 10	0	0
4	T	2	Total C N O 28 16 2 10	0	0
4	U	2	Total C N O 28 16 2 10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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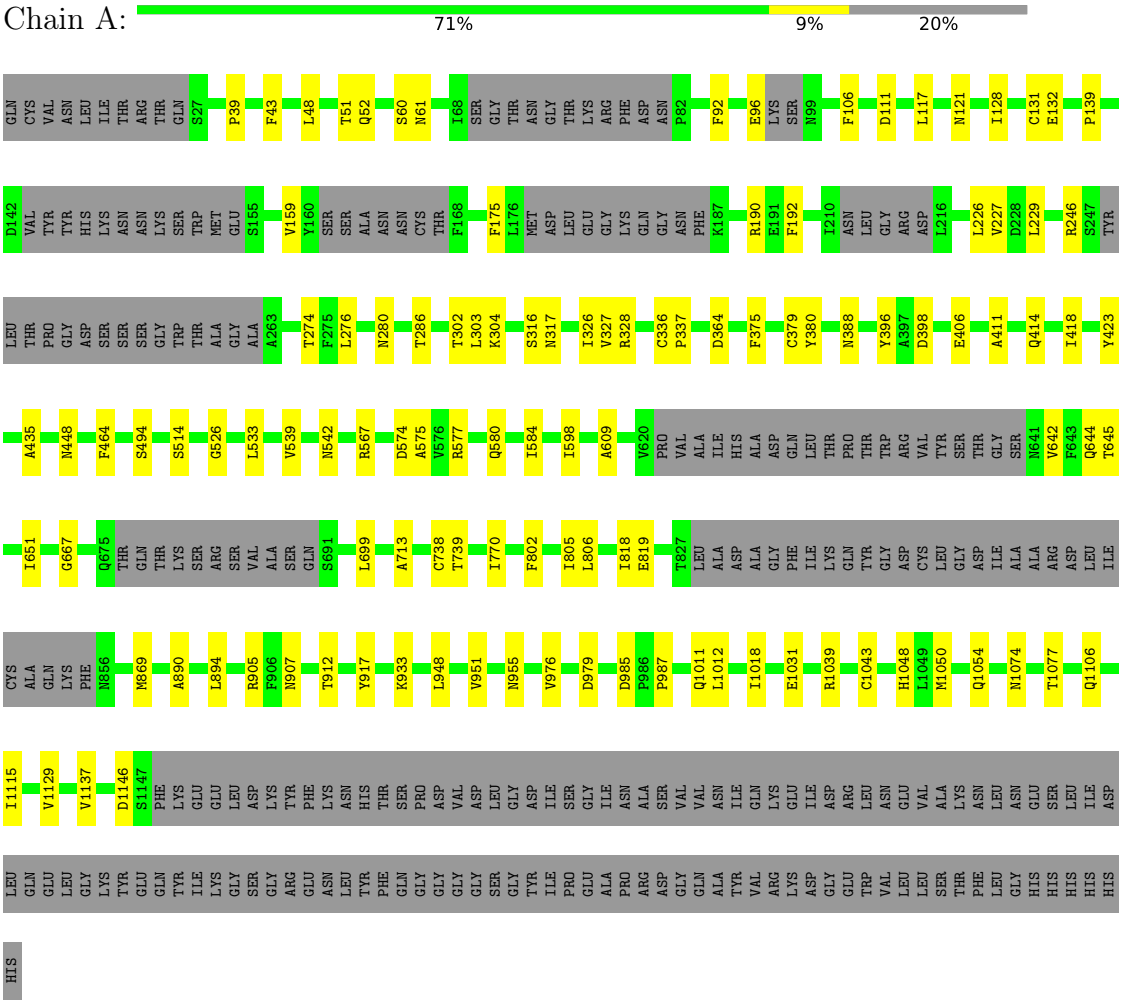
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C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

3 Residue-property plots (i)

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

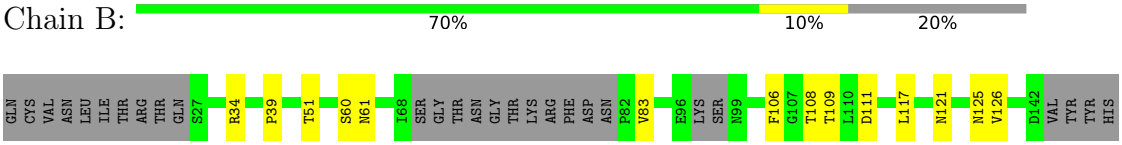
- Molecule 1: Spike glycoprotein

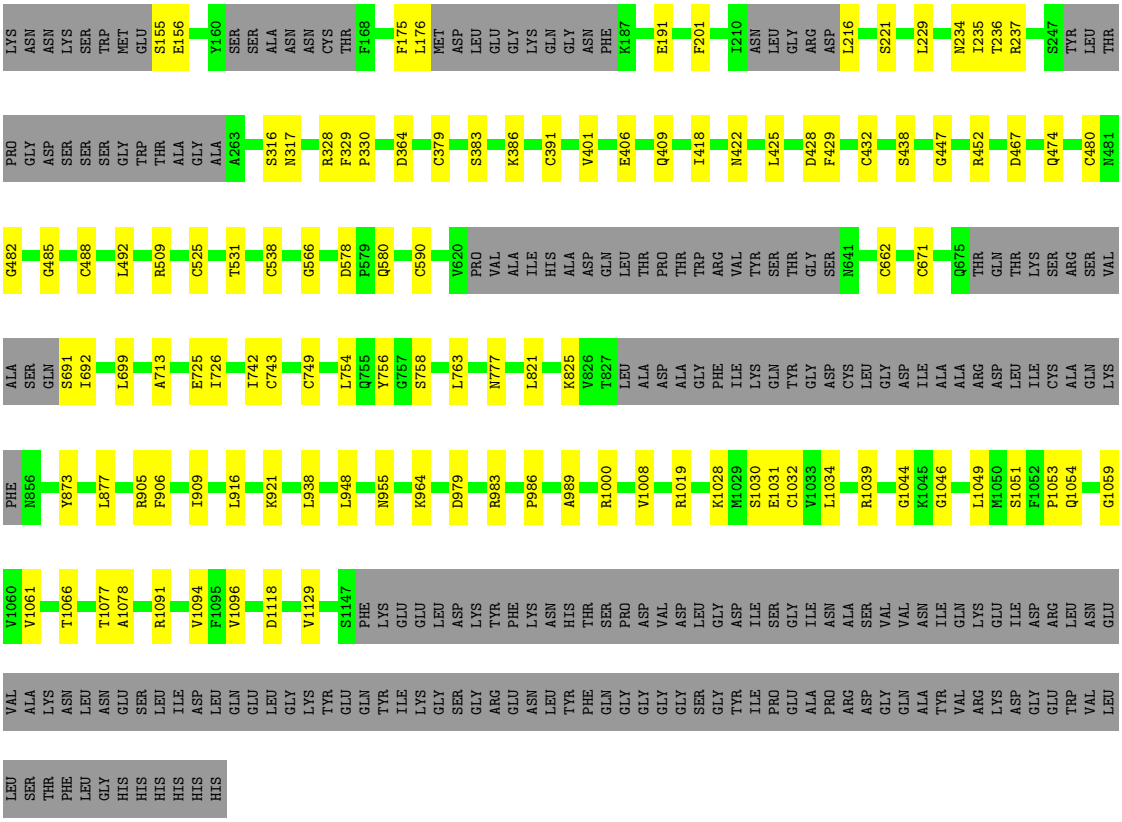
Chain A:



- Molecule 1: Spike glycoprotein

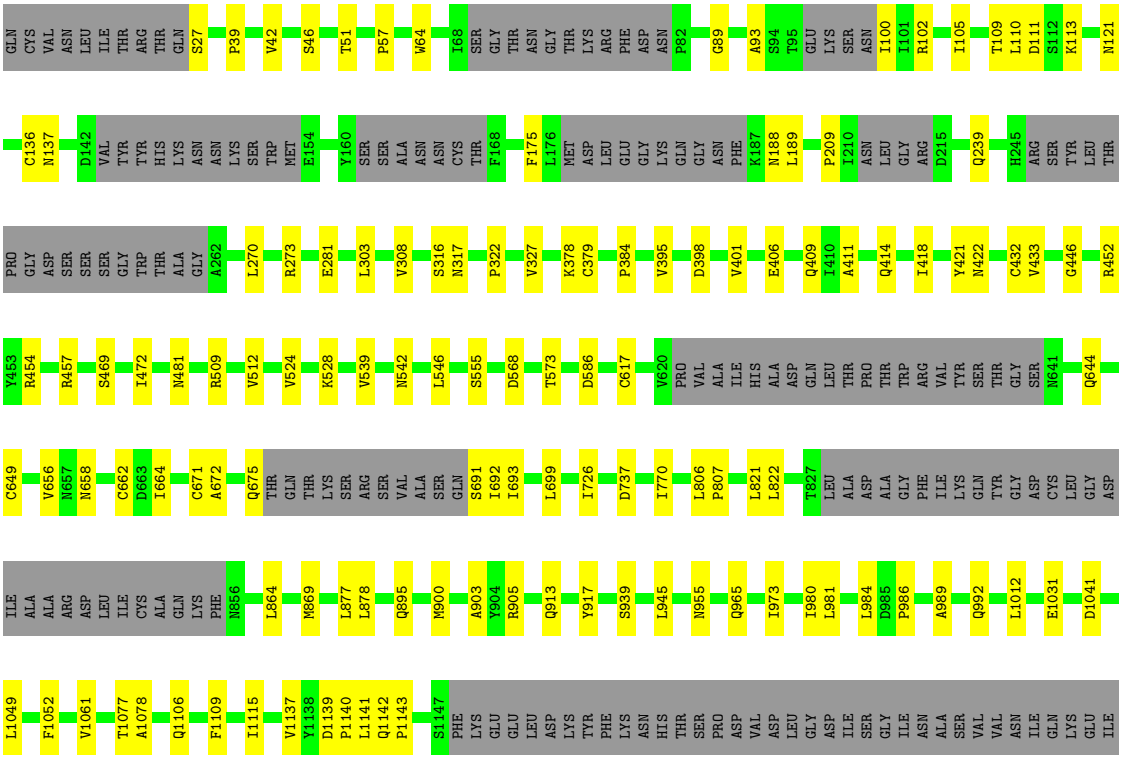
Chain B:

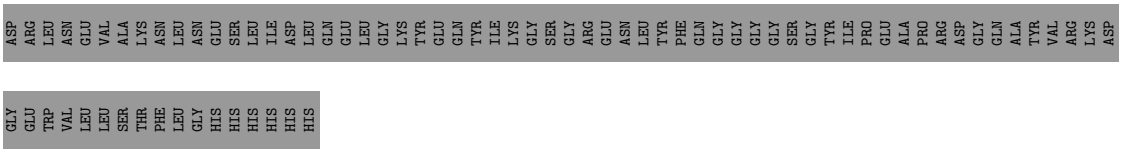




• Molecule 1: Spike glycoprotein

Chain C:



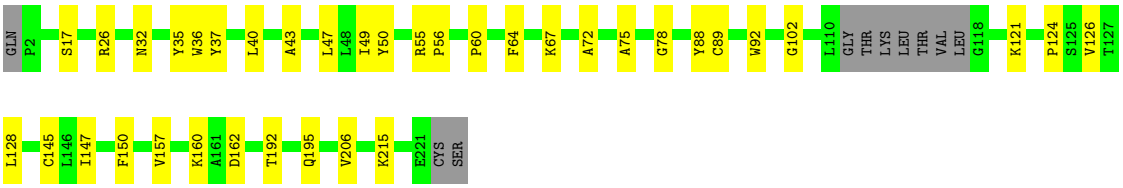


• Molecule 2: Light chain of D1F6 Fab

Chain G:

• Molecule 2: Light chain of D1F6 Fab

Chain M:

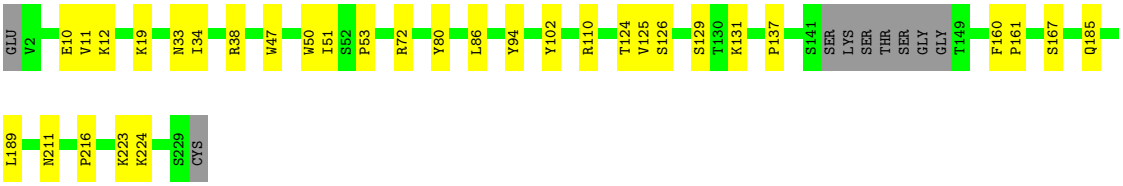


• Molecule 2: Light chain of D1F6 Fab

Chain N:

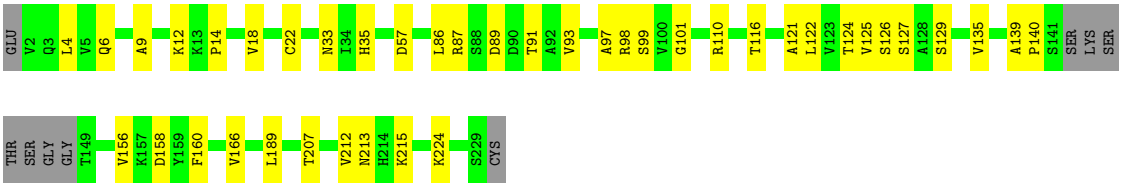
• Molecule 3: Heavy chain of D1F6 Fab

Chain H:



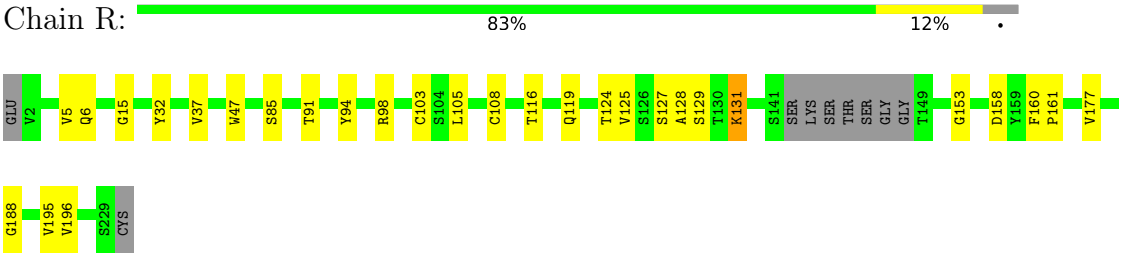
• Molecule 3: Heavy chain of D1F6 Fab

Chain Q:



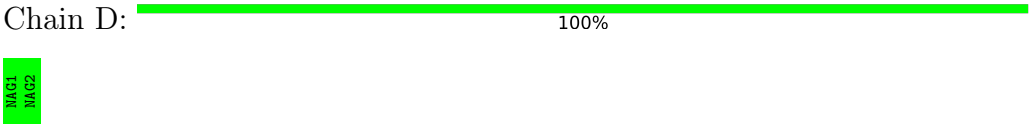
• Molecule 3: Heavy chain of D1F6 Fab

Chain R:



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

Chain D:

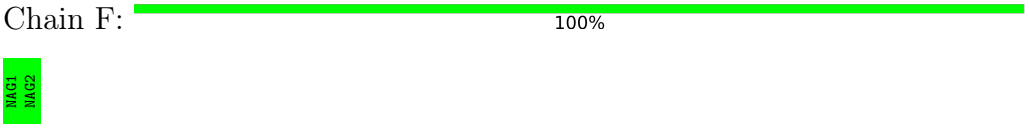


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F:

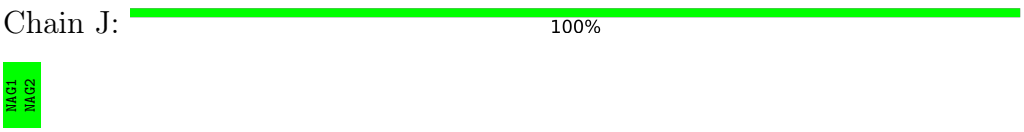


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



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

Chain K: 100%

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

Chain L: 100%

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

Chain O: 100%

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

Chain P: 100%

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

Chain S: 100%

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

Chain T: 100%

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

Chain U: 100%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251455	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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/7972	0.51	0/10845
1	B	0.27	0/7972	0.52	0/10845
1	C	0.27	0/7960	0.53	0/10830
2	G	0.25	0/1633	0.48	0/2229
2	M	0.25	0/1633	0.50	0/2229
2	N	0.25	0/1633	0.50	0/2229
3	H	0.25	0/1722	0.50	0/2349
3	Q	0.26	0/1722	0.57	0/2349
3	R	0.28	0/1722	0.59	0/2349
All	All	0.26	0/33969	0.52	0/46254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7790	0	7618	67	0
1	B	7790	0	7616	78	0
1	C	7778	0	7602	77	0
2	G	1591	0	1539	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1591	0	1539	21	0
2	N	1591	0	1539	13	0
3	H	1679	0	1624	23	0
3	Q	1679	0	1624	28	0
3	R	1679	0	1624	20	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	A	98	0	91	1	0
5	B	112	0	104	1	0
5	C	126	0	117	0	0
All	All	33840	0	32937	316	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 5.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:ASP:O	1:B:983:ARG:HB2	1.81	0.81
3:R:128:ALA:HB3	3:R:160:PHE:CE1	2.18	0.78
2:N:34:VAL:H	2:N:52:ASN:HD21	1.30	0.76
3:Q:86:LEU:HB3	3:Q:125:VAL:HG21	1.73	0.70
2:M:160:LYS:HG3	2:M:162:ASP:H	1.59	0.67
2:M:124:PRO:HB2	2:M:147:ILE:HD11	1.78	0.65
1:C:878:LEU:HD11	1:C:1052:PHE:HB3	1.78	0.64
2:M:40:LEU:HB3	2:M:43:ALA:HB3	1.80	0.64
1:A:128:ILE:HD13	1:A:229:LEU:HD21	1.81	0.62
1:A:276:LEU:HD11	1:A:304:LYS:HA	1.82	0.62
1:A:131:CYS:SG	1:A:132:GLU:N	2.73	0.61
1:B:1030:SER:HA	1:B:1034:LEU:HD12	1.82	0.61
1:B:1031:GLU:OE1	1:B:1039:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ILE:HG12	1:C:1061:VAL:HG23	1.82	0.61
3:Q:98:ARG:HB2	3:Q:116:THR:H	1.66	0.61
1:B:106:PHE:HB2	1:B:117:LEU:HB2	1.83	0.61
2:G:40:LEU:HB3	2:G:43:ALA:HB3	1.82	0.60
1:C:1142:GLN:HB3	1:C:1143:PRO:HD3	1.83	0.60
2:M:36:TRP:HD1	2:M:49:ILE:HB	1.67	0.60
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.83	0.59
1:B:447:GLY:H	3:Q:101:GLY:HA2	1.67	0.59
3:H:126:SER:HB2	3:H:160:PHE:CZ	2.38	0.59
2:N:34:VAL:O	2:N:52:ASN:ND2	2.36	0.58
3:Q:86:LEU:HB3	3:Q:125:VAL:CG2	2.34	0.58
3:H:86:LEU:HB2	3:H:125:VAL:HG21	1.85	0.57
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.69	0.57
1:A:917:TYR:HB3	1:B:1129:VAL:HG23	1.86	0.57
1:A:327:VAL:HG23	1:A:542:ASN:HB3	1.86	0.57
2:M:128:LEU:HD13	2:M:145:CYS:HB3	1.87	0.57
3:R:91:THR:HG22	3:R:125:VAL:H	1.69	0.56
3:Q:158:ASP:HA	3:Q:189:LEU:HD22	1.87	0.56
1:A:644:GLN:NE2	1:A:645:THR:O	2.39	0.56
1:C:418:ILE:HG23	1:C:422:ASN:HB2	1.88	0.56
1:B:236:THR:HG21	5:B:1302:NAG:H62	1.88	0.55
1:B:825:LYS:NZ	1:B:938:LEU:O	2.36	0.55
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.37	0.55
1:C:452:ARG:HH12	3:R:105:LEU:HD22	1.71	0.55
1:C:986:PRO:HA	1:C:989:ALA:HB3	1.89	0.55
1:C:821:LEU:HD21	1:C:939:SER:HB2	1.89	0.55
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.40	0.54
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.39	0.54
3:Q:129:SER:O	3:Q:160:PHE:HD2	1.90	0.54
1:C:316:SER:OG	1:C:317:ASN:N	2.39	0.54
1:A:955:ASN:OD1	1:A:1011:GLN:NE2	2.41	0.54
3:R:124:THR:HG22	3:R:125:VAL:N	2.22	0.54
3:Q:4:LEU:HD21	3:Q:98:ARG:HD3	1.90	0.54
1:A:423:TYR:HE1	1:A:464:PHE:H	1.54	0.54
3:H:11:VAL:HG22	3:H:124:THR:HB	1.90	0.53
1:A:411:ALA:HB3	1:A:414:GLN:HB3	1.89	0.53
1:C:406:GLU:HA	1:C:409:GLN:HG3	1.90	0.53
2:M:55:ARG:NH2	2:M:60:PRO:O	2.42	0.53
3:Q:6:GLN:HB3	3:Q:22:CYS:HA	1.90	0.53
1:A:1129:VAL:HG23	1:C:917:TYR:HB3	1.90	0.53
2:M:37:TYR:HB2	2:M:88:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:160:LYS:HG3	2:G:162:ASP:H	1.72	0.53
3:H:19:LYS:HD2	3:H:80:TYR:HB3	1.90	0.53
3:R:128:ALA:HB3	3:R:160:PHE:CZ	2.44	0.53
3:Q:87:ARG:O	3:Q:125:VAL:HB	2.09	0.53
3:H:86:LEU:HB2	3:H:125:VAL:CG2	2.39	0.52
2:G:25:SER:OG	2:G:26:ARG:N	2.42	0.52
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.92	0.52
2:M:32:ASN:HD22	2:M:92:TRP:HB3	1.74	0.52
1:B:121:ASN:HD21	1:B:175:PHE:HB2	1.75	0.52
1:B:406:GLU:OE1	1:B:409:GLN:NE2	2.40	0.52
2:G:55:ARG:HG3	2:G:61:GLU:HG3	1.92	0.52
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.92	0.52
1:C:89:GLY:HA3	1:C:270:LEU:HG	1.91	0.52
1:C:110:LEU:O	1:C:110:LEU:HD23	2.10	0.52
3:Q:135:VAL:HG21	3:Q:156:VAL:HG23	1.91	0.52
3:H:53:PRO:HA	3:H:72:ARG:HD3	1.92	0.51
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.92	0.51
1:A:60:SER:OG	1:A:61:ASN:N	2.43	0.51
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.43	0.51
1:A:667:GLY:HA2	1:C:864:LEU:HA	1.92	0.51
1:B:1030:SER:HB3	1:C:1041:ASP:HB3	1.92	0.51
3:R:131:LYS:NZ	3:R:158:ASP:OD1	2.37	0.51
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.44	0.51
1:A:642:VAL:HG22	1:A:651:ILE:HG12	1.92	0.51
1:A:912:THR:OG1	1:A:1106:GLN:OE1	2.22	0.51
1:B:986:PRO:HA	1:B:989:ALA:HB3	1.92	0.51
1:B:474:GLN:NE2	1:B:480:CYS:O	2.43	0.51
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.93	0.51
3:R:177:VAL:HA	3:R:196:VAL:HG12	1.92	0.51
1:A:43:PHE:H	1:B:566:GLY:HA2	1.76	0.50
1:B:428:ASP:OD1	1:B:428:ASP:N	2.45	0.50
2:G:132:SER:OG	2:G:133:SER:N	2.43	0.50
3:H:124:THR:HG22	3:H:125:VAL:H	1.76	0.50
1:C:822:LEU:HD11	1:C:945:LEU:HD11	1.94	0.50
2:M:35:TYR:OH	3:Q:110:ARG:O	2.29	0.50
3:Q:4:LEU:HD11	3:Q:98:ARG:HG2	1.93	0.50
3:H:34:ILE:HB	3:H:51:ILE:HD11	1.93	0.50
2:N:55:ARG:NH1	2:N:61:GLU:OE1	2.45	0.50
1:B:467:ASP:OD1	1:B:467:ASP:N	2.45	0.50
1:C:421:TYR:HD1	1:C:457:ARG:HB2	1.76	0.49
1:C:664:ILE:HB	1:C:672:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:OG1	1:B:234:ASN:O	2.30	0.49
1:C:675:GLN:HG2	1:C:693:ILE:HD11	1.93	0.49
3:H:86:LEU:HB2	3:H:125:VAL:CB	2.41	0.49
3:H:86:LEU:HB2	3:H:125:VAL:HB	1.94	0.49
3:R:127:SER:O	3:R:188:GLY:HA3	2.13	0.49
3:H:33:ASN:ND2	3:H:102:TYR:O	2.43	0.49
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.95	0.49
1:C:433:VAL:HG12	1:C:512:VAL:HG12	1.94	0.49
3:H:137:PRO:HG3	3:H:223:LYS:HB3	1.94	0.49
1:B:121:ASN:HD22	1:B:176:LEU:HG	1.78	0.48
2:G:35:TYR:OH	3:H:110:ARG:O	2.30	0.48
1:A:226:LEU:HG	1:A:227:VAL:HG13	1.95	0.48
1:A:985:ASP:OD1	1:A:985:ASP:N	2.45	0.48
1:C:395:VAL:HG13	1:C:524:VAL:HG11	1.95	0.48
1:C:100:ILE:O	1:C:102:ARG:NH1	2.46	0.48
3:H:12:LYS:O	3:H:125:VAL:HG23	2.13	0.48
1:A:567:ARG:HD2	1:C:42:VAL:HG11	1.96	0.48
1:C:980:ILE:HD11	1:C:992:GLN:HB3	1.95	0.48
1:B:125:ASN:OD1	1:B:126:VAL:N	2.47	0.48
1:B:155:SER:OG	1:B:156:GLU:N	2.45	0.48
1:C:1139:ASP:OD1	1:C:1140:PRO:HD2	2.13	0.48
3:H:38:ARG:HH21	3:H:94:TYR:HE2	1.62	0.48
1:C:327:VAL:HG12	1:C:542:ASN:HB3	1.95	0.48
3:R:91:THR:CG2	3:R:125:VAL:HG22	2.44	0.48
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.42	0.48
1:C:303:LEU:HD23	1:C:308:VAL:HG12	1.96	0.47
2:N:93:ASP:N	2:N:93:ASP:OD1	2.47	0.47
1:C:546:LEU:HD21	1:C:573:THR:HG21	1.96	0.47
1:A:48:LEU:HD23	1:A:276:LEU:HD21	1.95	0.47
3:R:5:VAL:HG23	3:R:119:GLN:HE21	1.79	0.47
1:C:903:ALA:HB1	1:C:913:GLN:HB2	1.96	0.47
3:H:129:SER:C	3:H:131:LYS:H	2.18	0.47
1:A:388:ASN:HA	1:A:526:GLY:HA3	1.96	0.47
1:C:691:SER:OG	1:C:692:ILE:N	2.46	0.47
1:A:139:PRO:HB2	1:A:159:VAL:HG12	1.95	0.47
1:A:280:ASN:ND2	1:A:286:THR:OG1	2.47	0.47
1:B:316:SER:OG	1:B:317:ASN:N	2.48	0.47
1:B:425:LEU:HD22	1:B:429:PHE:HE1	1.80	0.47
1:C:109:THR:O	1:C:110:LEU:HB3	2.13	0.47
1:C:454:ARG:NH2	1:C:469:SER:O	2.48	0.47
1:A:894:LEU:HB3	1:B:713:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASN:HA	1:C:209:PRO:HA	1.97	0.47
2:N:147:ILE:HG12	2:N:206:VAL:HG11	1.96	0.47
1:A:375:PHE:N	1:A:435:ALA:O	2.46	0.47
1:C:446:GLY:HA3	3:R:32:TYR:HE1	1.80	0.47
1:A:699:LEU:HD11	1:C:869:MET:HG2	1.97	0.46
2:G:64:PHE:HB2	2:G:75:ALA:HB3	1.97	0.46
3:Q:213:ASN:O	3:Q:215:LYS:NZ	2.48	0.46
1:B:777:ASN:HD21	1:B:1019:ARG:HA	1.79	0.46
2:M:157:VAL:HG22	2:M:206:VAL:HG12	1.97	0.46
3:R:103:CYS:HB3	3:R:108:CYS:HB3	1.85	0.46
1:A:1146:ASP:OD1	1:A:1146:ASP:N	2.47	0.46
1:C:973:ILE:HG13	1:C:984:LEU:HD21	1.97	0.46
3:R:37:VAL:HG12	3:R:47:TRP:HA	1.98	0.46
1:A:364:ASP:N	1:A:364:ASP:OD1	2.49	0.46
1:B:578:ASP:OD1	1:B:578:ASP:N	2.45	0.46
1:C:1140:PRO:O	1:C:1141:LEU:HG	2.15	0.46
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.98	0.46
3:R:153:GLY:HA2	3:R:195:VAL:HA	1.96	0.46
3:Q:91:THR:HG23	3:Q:124:THR:HG22	1.98	0.46
1:B:60:SER:OG	1:B:61:ASN:N	2.48	0.46
1:C:46:SER:HB2	1:C:281:GLU:HG3	1.97	0.46
1:A:121:ASN:HD21	1:A:175:PHE:HD2	1.63	0.45
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.98	0.45
1:B:474:GLN:HE21	1:B:480:CYS:HB2	1.80	0.45
1:A:52:GLN:HG3	1:A:274:THR:HB	1.98	0.45
1:A:302:THR:HG23	1:A:303:LEU:HD12	1.98	0.45
1:A:819:GLU:HG3	1:A:1054:GLN:HE21	1.81	0.45
1:B:364:ASP:OD1	1:B:364:ASP:N	2.49	0.45
3:Q:93:VAL:HG12	3:Q:122:LEU:HA	1.99	0.45
1:A:326:ILE:HG12	1:A:539:VAL:HG21	1.97	0.45
1:B:383:SER:HB3	1:B:386:LYS:HG2	1.99	0.45
2:G:4:LEU:HD21	2:G:29:ILE:HD11	1.98	0.45
2:N:175:PRO:HG3	2:N:185:ALA:HB2	1.98	0.45
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.99	0.45
1:A:317:ASN:ND2	1:C:737:ASP:OD1	2.50	0.45
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.28	0.45
3:H:185:GLN:HG3	3:H:189:LEU:HG	1.99	0.44
1:A:106:PHE:HB2	1:A:117:LEU:HB2	1.98	0.44
1:C:57:PRO:HG3	1:C:273:ARG:HE	1.82	0.44
1:C:398:ASP:HB2	1:C:512:VAL:HG22	1.99	0.44
1:C:1115:ILE:HG22	1:C:1137:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:906:PHE:HA	1:B:909:ILE:HG12	2.00	0.44
2:G:147:ILE:HG12	2:G:206:VAL:HG11	1.99	0.44
3:H:47:TRP:HH2	3:H:50:TRP:HE3	1.65	0.44
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.98	0.44
1:B:34:ARG:NH1	1:B:221:SER:OG	2.51	0.44
1:B:482:GLY:HA3	2:M:26:ARG:HB2	2.00	0.44
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.82	0.44
3:Q:35:HIS:HB2	3:Q:97:ALA:HB3	2.00	0.44
1:A:316:SER:OG	1:A:317:ASN:N	2.51	0.44
1:A:577:ARG:HB2	1:A:584:ILE:HG22	2.00	0.44
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.98	0.44
1:B:754:LEU:C	1:B:756:TYR:N	2.71	0.44
1:B:873:TYR:HE1	1:C:699:LEU:HB3	1.82	0.44
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.99	0.44
1:C:322:PRO:HB3	1:C:539:VAL:HA	2.00	0.44
1:C:1077:THR:OG1	1:C:1078:ALA:N	2.51	0.44
2:G:32:ASN:HB3	3:H:110:ARG:HG3	1.99	0.44
1:A:92:PHE:HB3	1:A:192:PHE:HB2	1.99	0.44
1:B:758:SER:N	1:C:965:GLN:OE1	2.44	0.44
1:C:568:ASP:N	1:C:568:ASP:OD1	2.50	0.44
2:N:197:LYS:HA	2:N:197:LYS:HD2	1.82	0.44
1:A:96:GLU:OE1	1:A:190:ARG:NH1	2.47	0.44
1:A:713:ALA:HA	1:A:1074:ASN:HA	1.99	0.44
1:A:738:CYS:SG	1:A:739:THR:N	2.91	0.44
1:B:538:CYS:HB2	1:B:590:CYS:HB3	1.74	0.44
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.91	0.44
1:B:964:LYS:HB2	1:B:964:LYS:HE2	1.81	0.44
1:C:1142:GLN:HB3	1:C:1143:PRO:CD	2.45	0.44
2:G:2:PRO:HA	2:G:25:SER:HB3	1.98	0.44
2:G:48:LEU:HD12	2:G:48:LEU:HA	1.90	0.44
1:A:111:ASP:OD1	1:A:111:ASP:N	2.50	0.43
3:Q:207:THR:HG23	3:Q:224:LYS:HE3	2.00	0.43
1:B:921:LYS:HA	1:B:921:LYS:HD3	1.72	0.43
2:N:86:ASP:OD2	2:N:86:ASP:N	2.50	0.43
2:N:124:PRO:HG3	2:N:208:HIS:HB3	1.99	0.43
1:A:805:ILE:HG22	1:A:818:ILE:HD12	2.00	0.43
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.99	0.43
1:C:401:VAL:HG12	1:C:509:ARG:HA	2.00	0.43
2:M:89:CYS:O	2:M:102:GLY:N	2.50	0.43
1:A:398:ASP:OD1	1:A:398:ASP:N	2.51	0.43
1:A:770:ILE:HD11	1:A:1012:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:PHE:HB3	1:B:229:LEU:HB2	2.01	0.43
3:Q:14:PRO:HG3	3:Q:125:VAL:HG12	2.01	0.43
3:R:129:SER:O	3:R:160:PHE:CD2	2.72	0.43
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.84	0.43
1:B:1094:VAL:HG13	1:B:1096:VAL:HG23	2.01	0.43
5:A:1306:NAG:H82	1:C:895:GLN:HE22	1.83	0.43
1:C:472:ILE:HD11	2:N:31:THR:HG22	2.00	0.43
1:C:111:ASP:OD1	1:C:113:LYS:HB2	2.19	0.43
1:C:93:ALA:HB1	1:C:189:LEU:HD11	2.00	0.43
1:A:328:ARG:HH12	1:A:533:LEU:HD13	1.84	0.43
3:Q:12:LYS:HG3	3:Q:18:VAL:HB	2.00	0.43
1:B:691:SER:OG	1:B:692:ILE:N	2.52	0.43
2:N:127:THR:HA	2:N:215:LYS:HE2	2.00	0.43
1:A:448:ASN:O	1:A:494:SER:OG	2.36	0.42
1:C:379:CYS:HB2	1:C:384:PRO:HD3	2.01	0.42
1:A:985:ASP:HB2	1:A:987:PRO:HD2	2.01	0.42
1:B:106:PHE:HB3	1:B:235:ILE:HD12	2.00	0.42
3:H:167:SER:HB2	3:H:211:ASN:HB3	2.01	0.42
1:A:905:ARG:HD3	1:A:1050:MET:HB3	2.02	0.42
1:B:328:ARG:HD2	1:B:580:GLN:HG3	2.01	0.42
1:B:1032:CYS:O	1:B:1051:SER:OG	2.31	0.42
1:C:981:LEU:HD23	1:C:981:LEU:HA	1.91	0.42
2:M:17:SER:HA	2:M:78:GLY:H	1.84	0.42
3:Q:57:ASP:OD1	3:Q:57:ASP:N	2.52	0.42
1:B:401:VAL:HG12	1:B:509:ARG:HA	2.02	0.42
3:R:160:PHE:HA	3:R:161:PRO:HA	1.89	0.42
1:B:328:ARG:NE	1:B:531:THR:O	2.49	0.42
1:C:617:CYS:N	1:C:649:CYS:SG	2.93	0.42
3:H:10:GLU:OE2	3:H:12:LYS:NZ	2.44	0.42
2:N:28:ASN:HD21	2:N:100:VAL:HG21	1.84	0.42
1:C:27:SER:OG	1:C:64:TRP:O	2.34	0.42
1:A:1115:ILE:HG22	1:A:1137:VAL:HG23	2.02	0.42
1:B:418:ILE:HG23	1:B:422:ASN:HB2	2.01	0.42
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	2.01	0.42
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.53	0.42
1:C:528:LYS:HA	1:C:528:LYS:HD2	1.86	0.42
1:C:877:LEU:HD23	1:C:877:LEU:HA	1.93	0.42
3:Q:166:VAL:HG22	3:Q:212:VAL:HG22	2.01	0.42
1:B:485:GLY:H	1:B:488:CYS:HB2	1.84	0.42
2:M:47:LEU:HD21	2:M:50:TYR:HB3	2.02	0.42
1:A:336:CYS:HA	1:A:337:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:GLU:OE2	1:B:1039:ARG:HD2	2.20	0.42
1:B:906:PHE:CD2	1:B:916:LEU:HD12	2.53	0.42
1:C:973:ILE:HG21	1:C:984:LEU:HD11	2.02	0.42
2:G:27:SER:O	2:G:27:SER:OG	2.36	0.42
2:N:215:LYS:HB3	2:N:215:LYS:HE3	1.88	0.42
1:A:976:VAL:HG12	1:A:979:ASP:H	1.85	0.41
1:A:1039:ARG:NE	1:C:1031:GLU:OE2	2.53	0.41
1:C:121:ASN:HD21	1:C:175:PHE:H	1.68	0.41
2:M:192:THR:HG23	2:M:195:GLN:H	1.84	0.41
1:A:869:MET:HG2	1:B:699:LEU:HD21	2.01	0.41
1:B:329:PHE:HD1	1:B:330:PRO:HD2	1.84	0.41
1:B:438:SER:O	1:B:438:SER:OG	2.36	0.41
1:B:1044:GLY:HA3	1:B:1066:THR:HG21	2.02	0.41
2:M:67:LYS:HA	2:M:72:ALA:HA	2.02	0.41
3:Q:9:ALA:H	3:Q:121:ALA:HB1	1.85	0.41
1:B:34:ARG:HD2	1:B:216:LEU:HD23	2.01	0.41
1:C:644:GLN:HA	1:C:649:CYS:HA	2.02	0.41
1:C:662:CYS:HB2	1:C:671:CYS:HB3	1.79	0.41
2:M:124:PRO:HB3	2:M:150:PHE:HB3	2.02	0.41
3:Q:87:ARG:HG3	3:Q:89:ASP:H	1.84	0.41
1:A:1077:THR:HG21	1:C:900:MET:HE1	2.02	0.41
3:R:6:GLN:NE2	3:R:94:TYR:O	2.45	0.41
3:R:98:ARG:NH2	3:R:116:THR:OG1	2.43	0.41
1:B:662:CYS:HB2	1:B:671:CYS:HB3	1.80	0.41
3:Q:126:SER:OG	3:Q:127:SER:N	2.53	0.41
3:R:15:GLY:HA2	3:R:85:SER:HA	2.02	0.41
1:A:406:GLU:HG2	1:A:418:ILE:HG13	2.02	0.41
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.51	0.41
1:B:429:PHE:HE2	1:B:432:CYS:HA	1.85	0.41
1:B:754:LEU:C	1:B:756:TYR:H	2.23	0.41
2:M:64:PHE:HB3	2:M:75:ALA:HB3	2.02	0.41
1:A:1043:CYS:HB2	1:A:1048:HIS:CD2	2.56	0.41
1:A:379:CYS:SG	1:A:380:TYR:N	2.93	0.41
1:A:574:ASP:OD1	1:A:575:ALA:N	2.54	0.41
1:A:890:ALA:HA	1:B:1046:GLY:HA2	2.02	0.41
1:B:83:VAL:HG11	1:B:237:ARG:HE	1.85	0.41
1:C:105:ILE:HB	1:C:239:GLN:HB3	2.03	0.41
1:C:136:CYS:SG	1:C:137:ASN:N	2.94	0.41
1:C:481:ASN:OD1	1:C:481:ASN:N	2.53	0.41
1:C:806:LEU:HA	1:C:807:PRO:HD3	1.95	0.41
3:H:124:THR:HG22	3:H:125:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:VAL:HG12	1:C:658:ASN:H	1.86	0.41
1:A:802:PHE:HB3	1:A:806:LEU:HD23	2.04	0.40
1:B:821:LEU:HG	1:B:825:LYS:HE2	2.03	0.40
2:M:55:ARG:HA	2:M:56:PRO:HD3	1.94	0.40
1:C:878:LEU:HD13	1:C:878:LEU:HA	1.92	0.40
3:Q:86:LEU:C	3:Q:125:VAL:HG11	2.42	0.40
1:A:948:LEU:HA	1:A:951:VAL:HG12	2.03	0.40
1:B:452:ARG:HD2	1:B:492:LEU:HD23	2.03	0.40
2:M:121:LYS:HE3	2:M:121:LYS:HB3	1.97	0.40
3:Q:139:ALA:HA	3:Q:140:PRO:HD3	1.96	0.40
3:R:91:THR:HG23	3:R:125:VAL:HG22	2.02	0.40
1:A:1018:ILE:HD13	1:A:1018:ILE:HA	1.96	0.40
3:H:161:PRO:HD2	3:H:216:PRO:HG2	2.04	0.40
3:Q:33:ASN:O	3:Q:99:SER:OG	2.40	0.40
3:Q:91:THR:HA	3:Q:124:THR:HA	2.04	0.40
2:M:126:VAL:HG13	2:M:215:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	972/1238 (78%)	930 (96%)	42 (4%)	0	100	100
1	B	972/1238 (78%)	917 (94%)	55 (6%)	0	100	100
1	C	971/1238 (78%)	920 (95%)	51 (5%)	0	100	100
2	G	209/223 (94%)	204 (98%)	5 (2%)	0	100	100
2	M	209/223 (94%)	200 (96%)	9 (4%)	0	100	100
2	N	209/223 (94%)	200 (96%)	9 (4%)	0	100	100
3	H	217/230 (94%)	205 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	217/230 (94%)	206 (95%)	11 (5%)	0	100	100
3	R	217/230 (94%)	206 (95%)	11 (5%)	0	100	100
All	All	4193/5073 (83%)	3988 (95%)	205 (5%)	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	871/1075 (81%)	868 (100%)	3 (0%)	91	92
1	B	871/1075 (81%)	870 (100%)	1 (0%)	92	95
1	C	869/1075 (81%)	867 (100%)	2 (0%)	92	94
2	G	178/187 (95%)	178 (100%)	0	100	100
2	M	178/187 (95%)	178 (100%)	0	100	100
2	N	178/187 (95%)	177 (99%)	1 (1%)	84	88
3	H	191/198 (96%)	190 (100%)	1 (0%)	86	89
3	Q	191/198 (96%)	191 (100%)	0	100	100
3	R	191/198 (96%)	190 (100%)	1 (0%)	86	89
All	All	3718/4380 (85%)	3709 (100%)	9 (0%)	91	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	A	907	ASN
1	A	933	LYS
1	B	955	ASN
1	C	378	LYS
1	C	955	ASN
3	H	224	LYS
2	N	80	ARG

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Mol	Chain	Res	Type
3	R	131	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	474	GLN
1	B	755	GLN
1	B	1083	HIS
1	C	394	ASN
1	C	1119	ASN
2	N	52	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 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	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	D	2	4	14,14,15	0.30	0	17,19,21	0.45	0
4	NAG	E	1	4,1	14,14,15	0.29	0	17,19,21	0.82	1 (5%)
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	F	1	4,1	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	F	2	4	14,14,15	0.28	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	I	1	4,1	14,14,15	0.39	0	17,19,21	0.59	0
4	NAG	I	2	4	14,14,15	0.40	0	17,19,21	0.44	0
4	NAG	J	1	4,1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	J	2	4	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	K	1	4,1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	K	2	4	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	L	1	4,1	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	L	2	4	14,14,15	0.30	0	17,19,21	0.42	0
4	NAG	O	1	4,1	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	P	1	4,1	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	P	2	4	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	S	1	4,1	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	S	2	4	14,14,15	0.30	0	17,19,21	0.43	0
4	NAG	T	1	4,1	14,14,15	0.44	0	17,19,21	0.82	1 (5%)
4	NAG	T	2	4	14,14,15	0.26	0	17,19,21	0.58	1 (5%)
4	NAG	U	1	4,1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	U	2	4	14,14,15	0.30	0	17,19,21	0.45	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	T	1	NAG	C1-O5-C5	2.75	115.92	112.19
4	E	1	NAG	C2-N2-C7	2.47	126.42	122.90
4	T	2	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2

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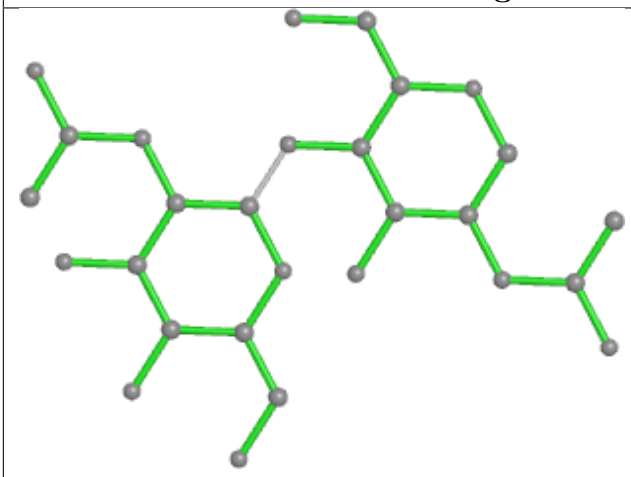
Mol	Chain	Res	Type	Atoms
4	U	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7

There are no ring outliers.

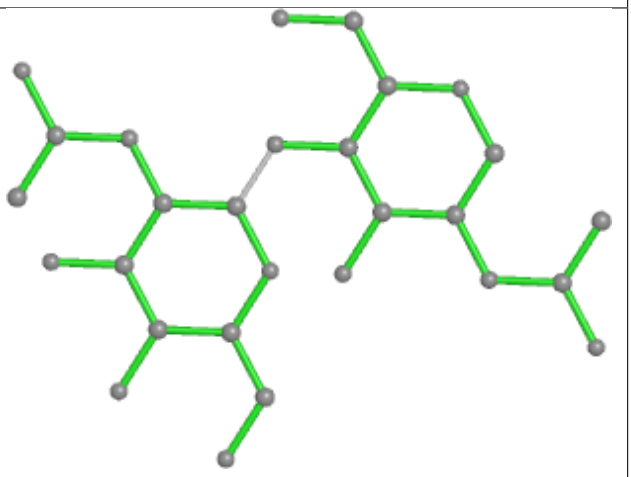
No monomer is involved in short contacts.

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

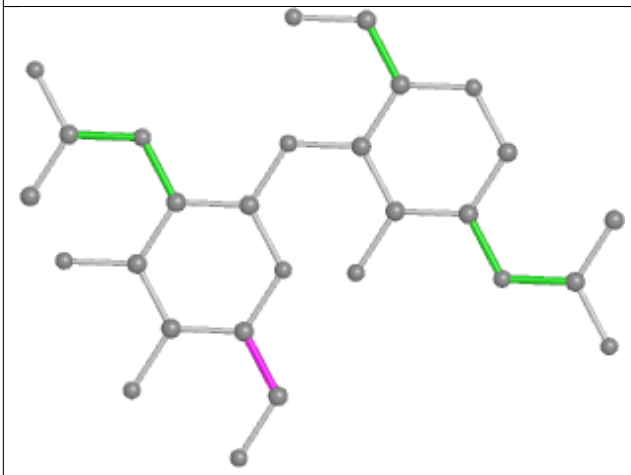
Oligosaccharide Chain D



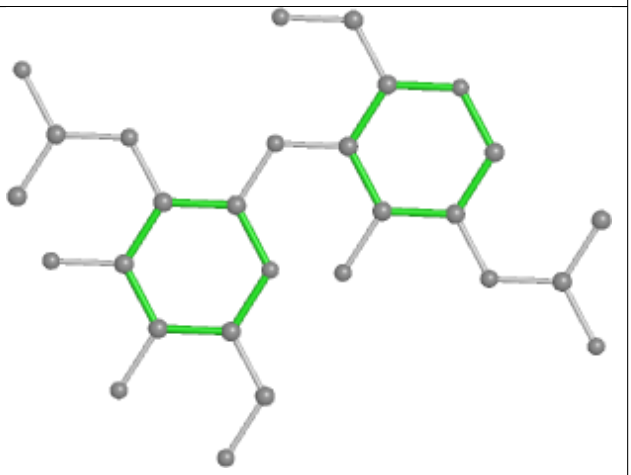
Bond lengths



Bond angles

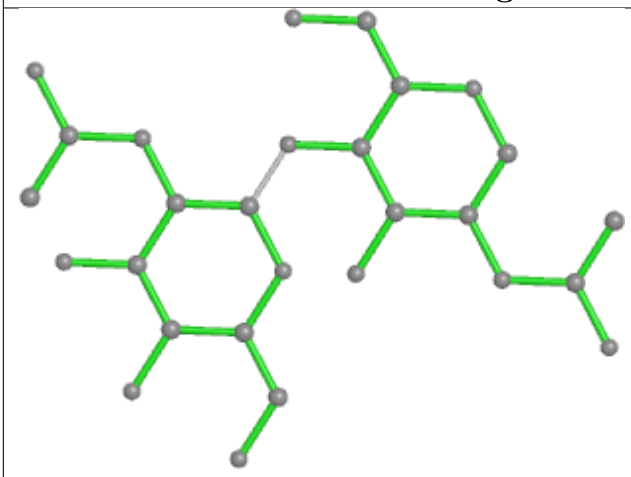


Torsions

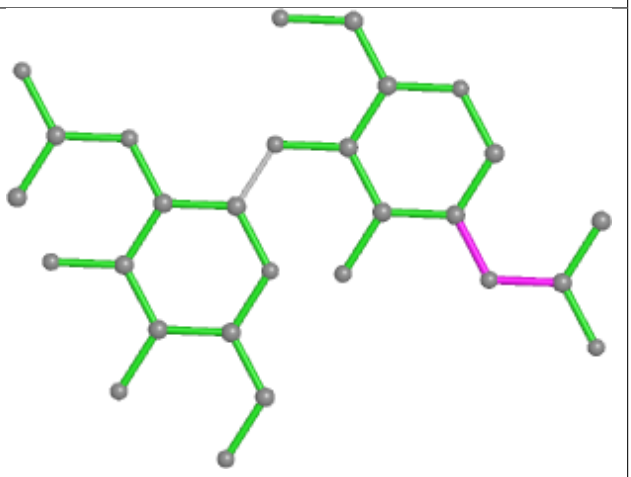


Rings

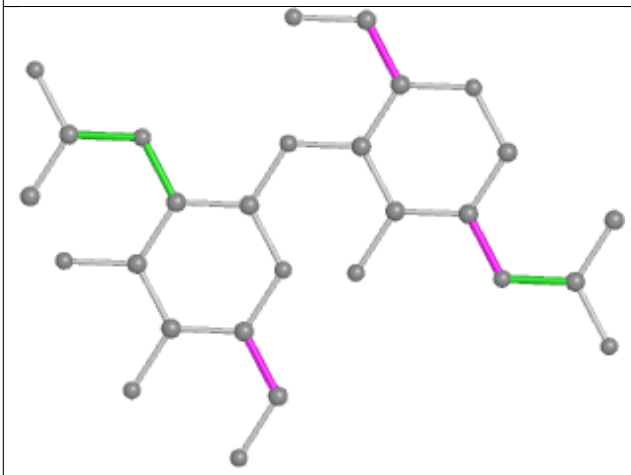
Oligosaccharide Chain E



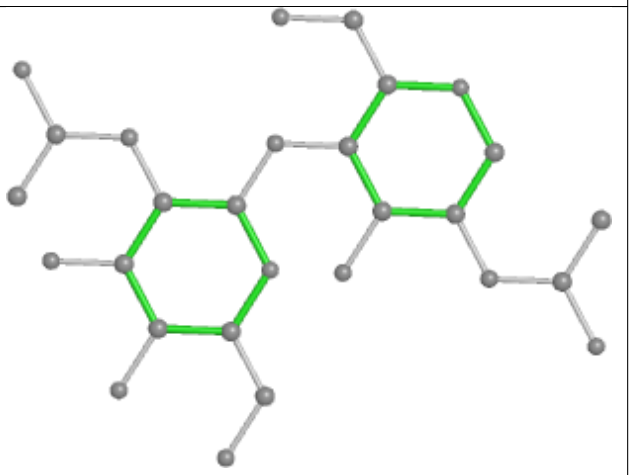
Bond lengths



Bond angles

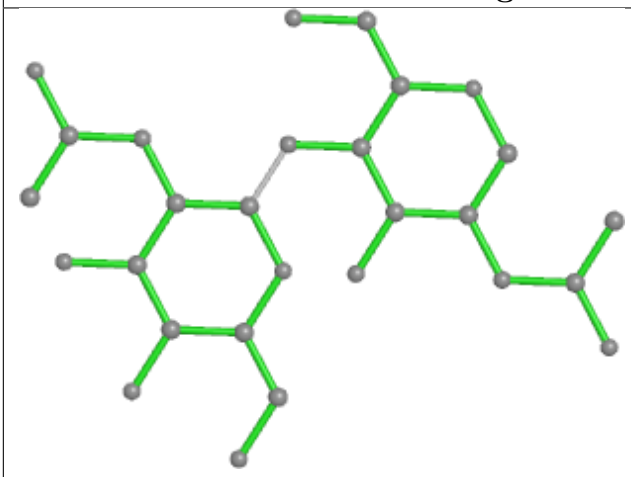


Torsions

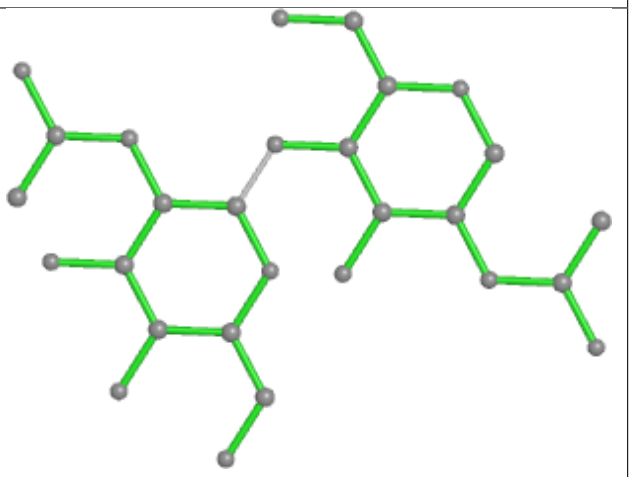


Rings

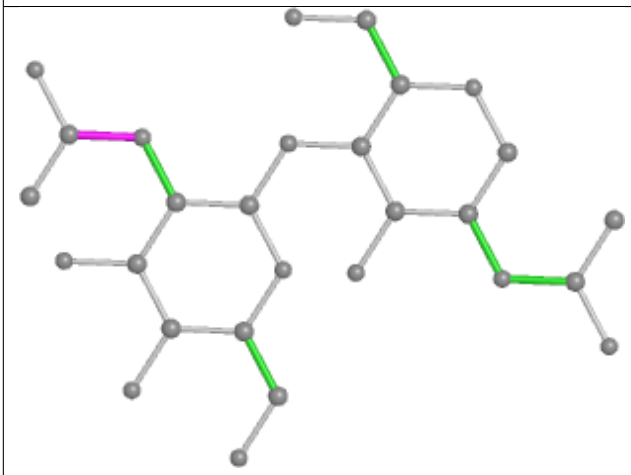
Oligosaccharide Chain F



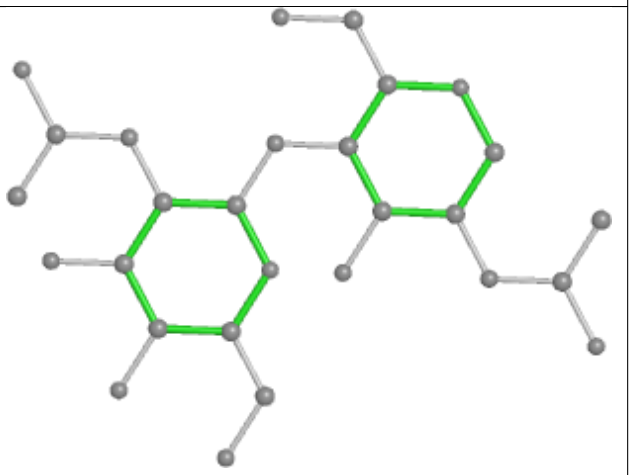
Bond lengths



Bond angles

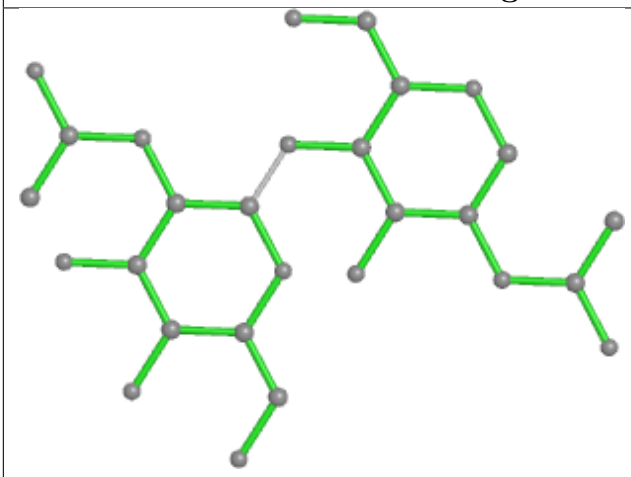


Torsions

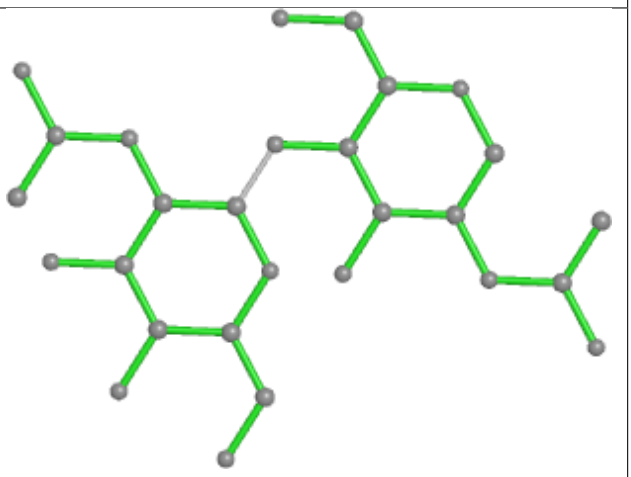


Rings

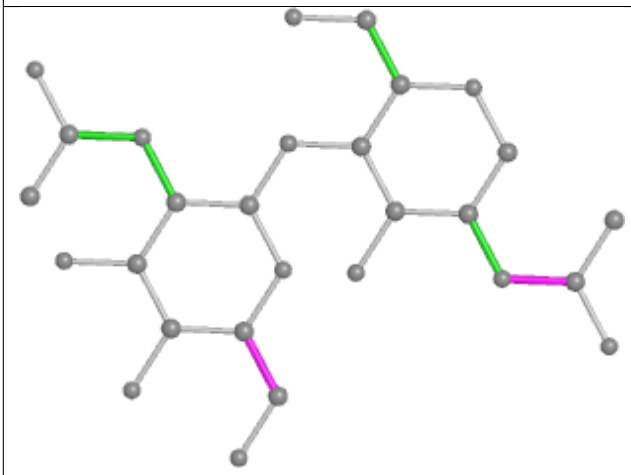
Oligosaccharide Chain I



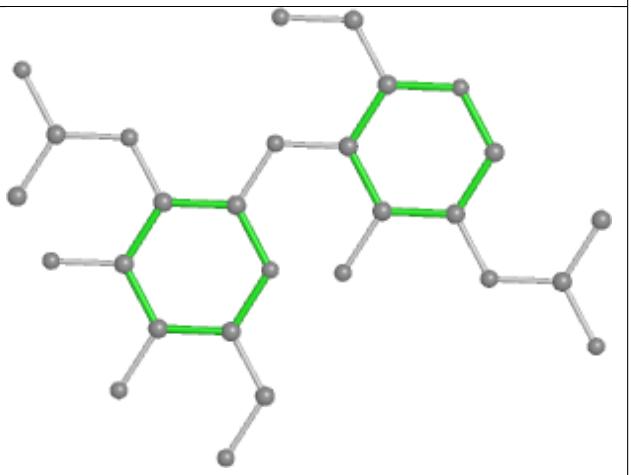
Bond lengths



Bond angles

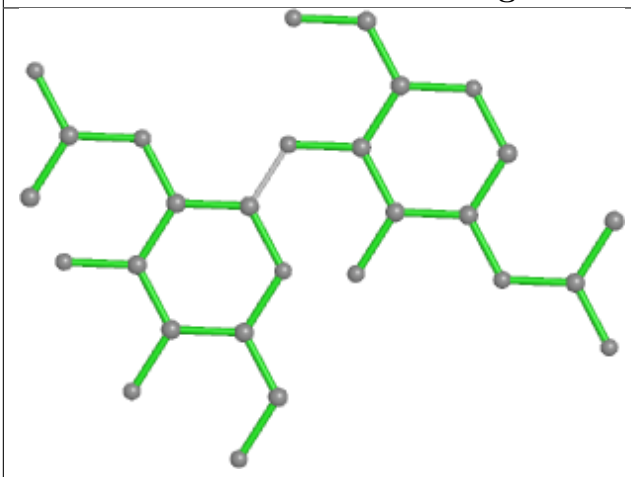


Torsions

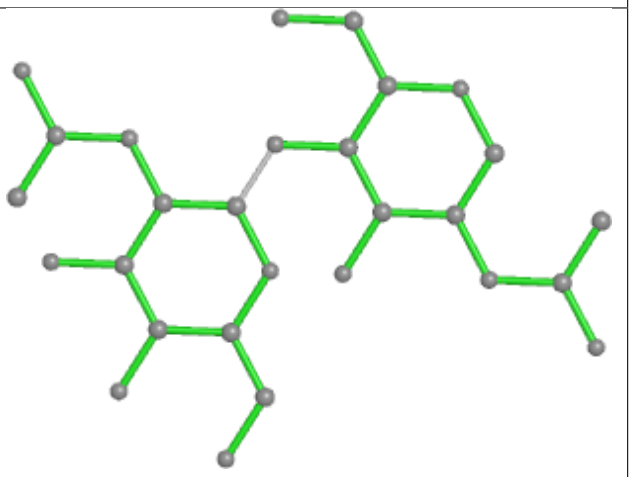


Rings

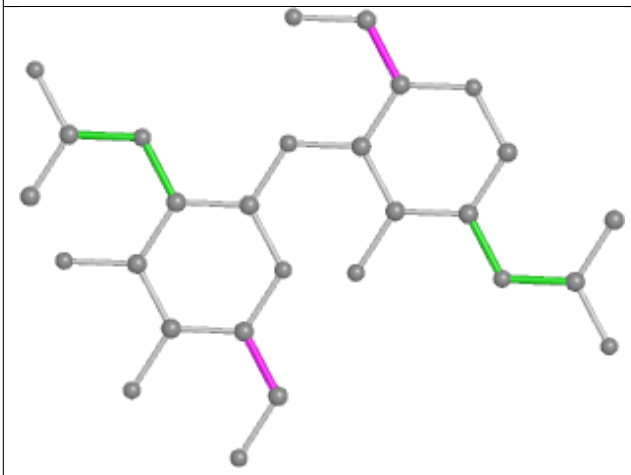
Oligosaccharide Chain J



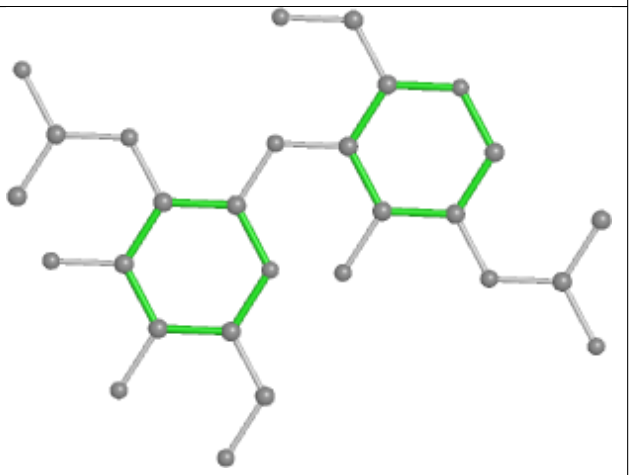
Bond lengths



Bond angles

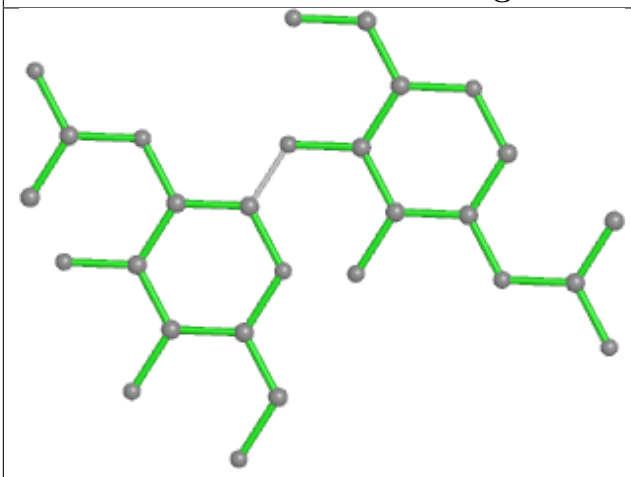


Torsions

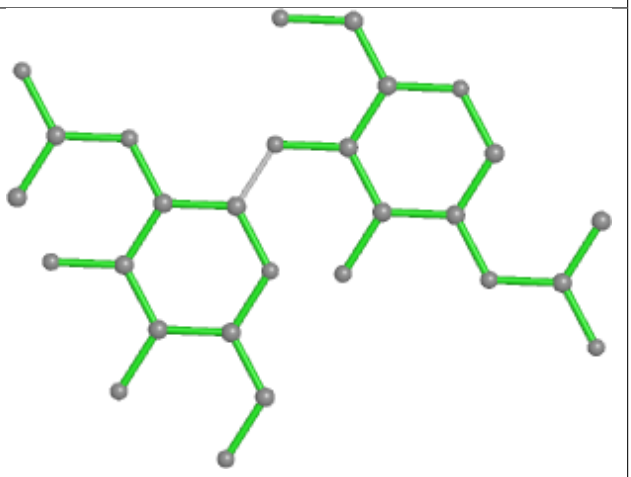


Rings

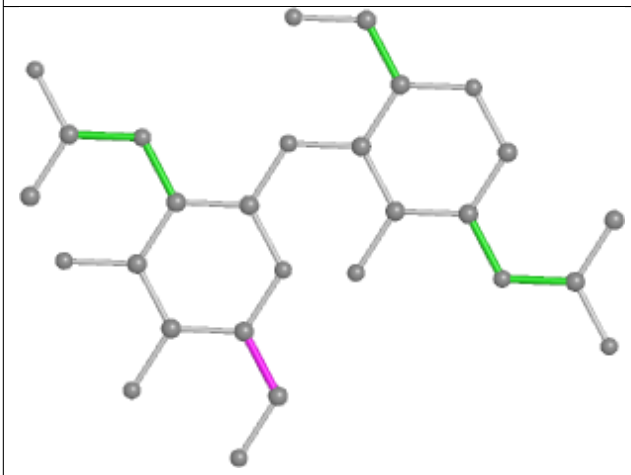
Oligosaccharide Chain K



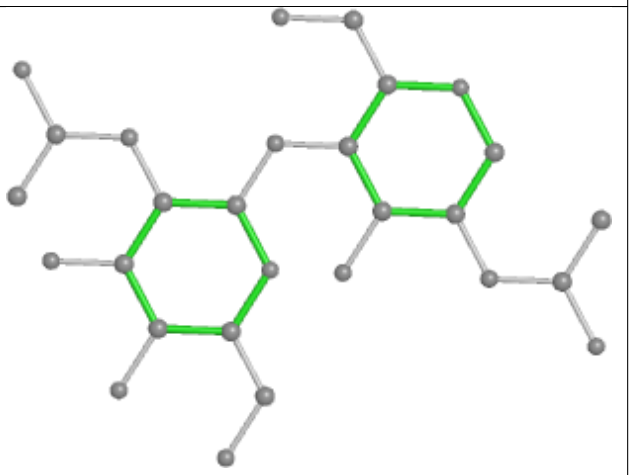
Bond lengths



Bond angles

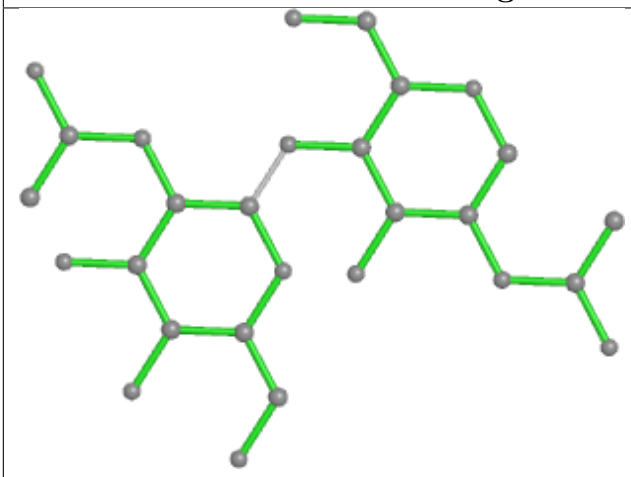


Torsions

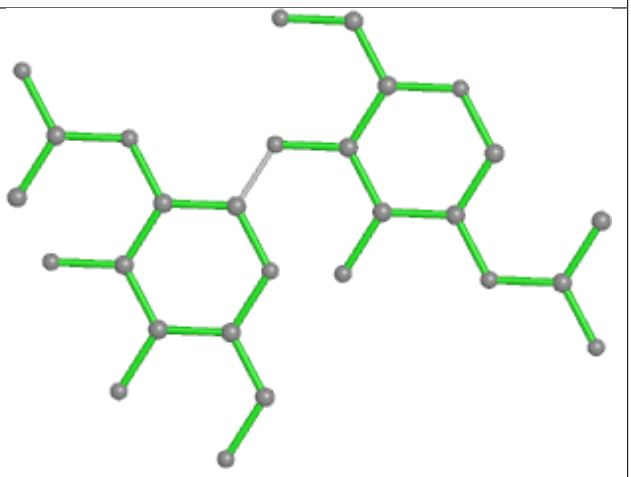


Rings

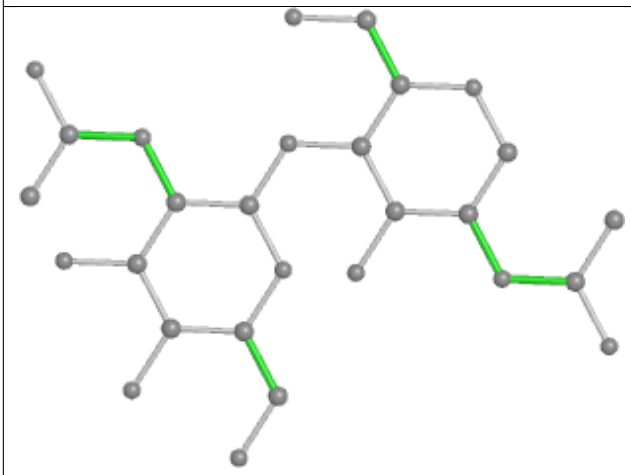
Oligosaccharide Chain L



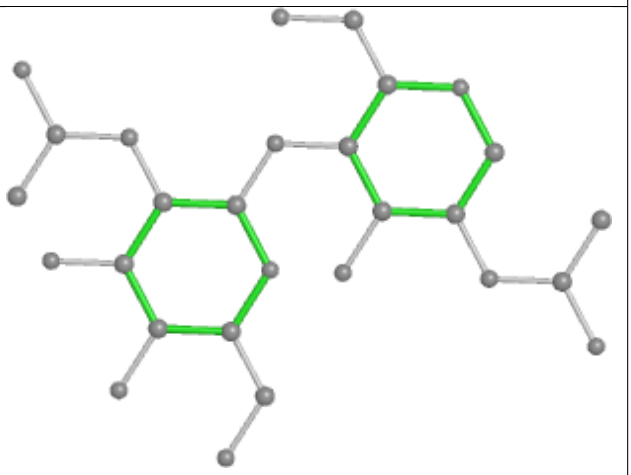
Bond lengths



Bond angles

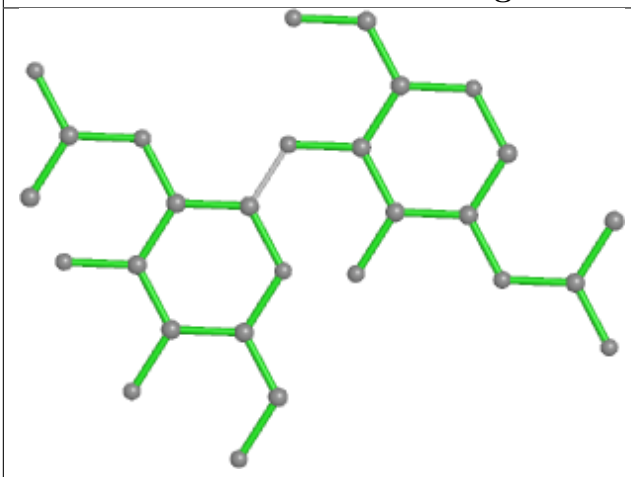


Torsions

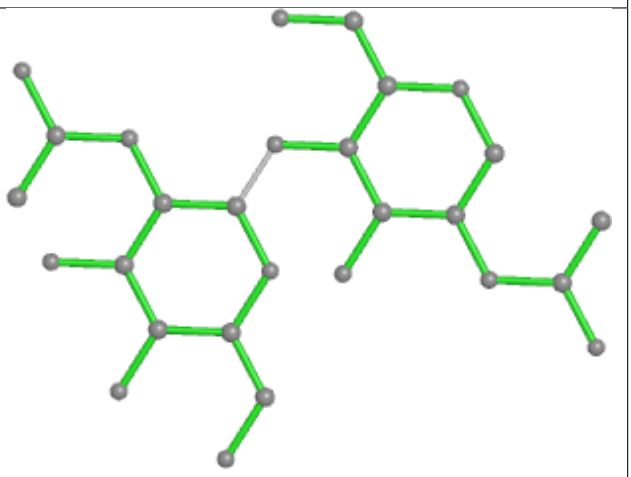


Rings

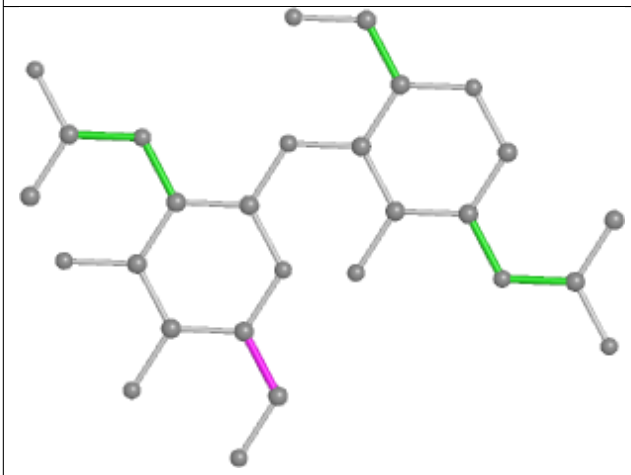
Oligosaccharide Chain O



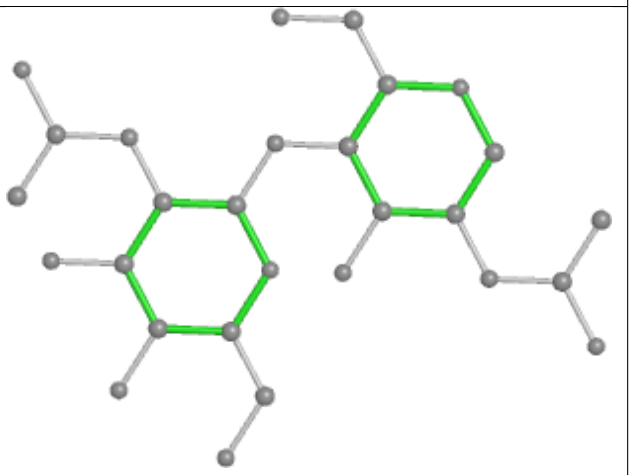
Bond lengths



Bond angles

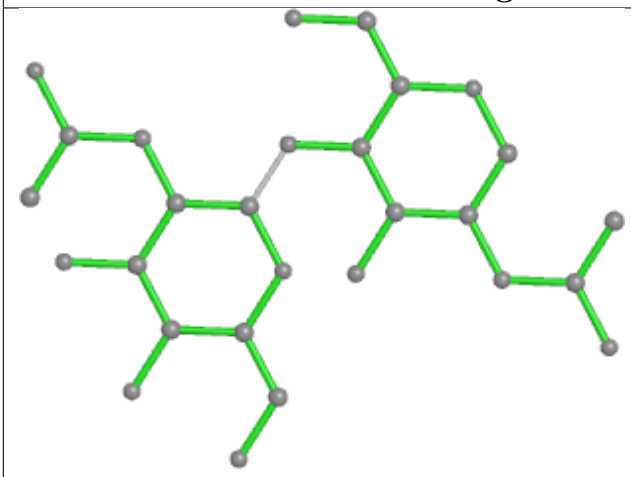


Torsions

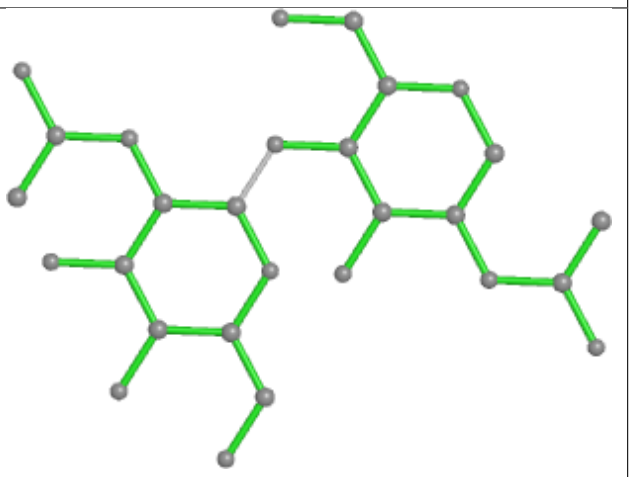


Rings

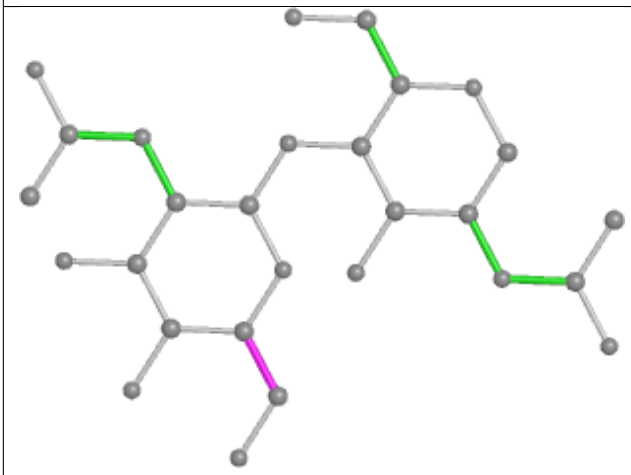
Oligosaccharide Chain P



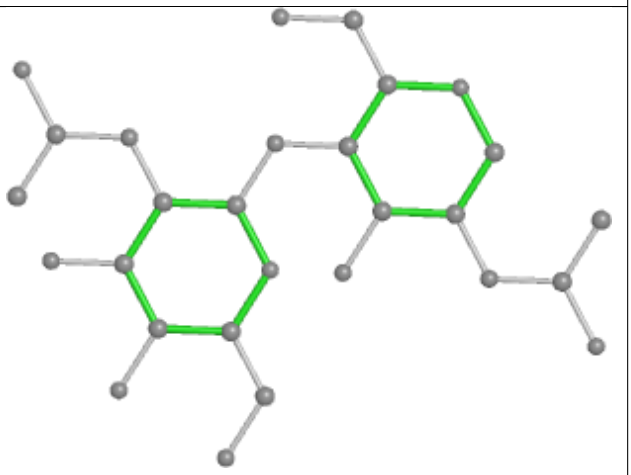
Bond lengths



Bond angles

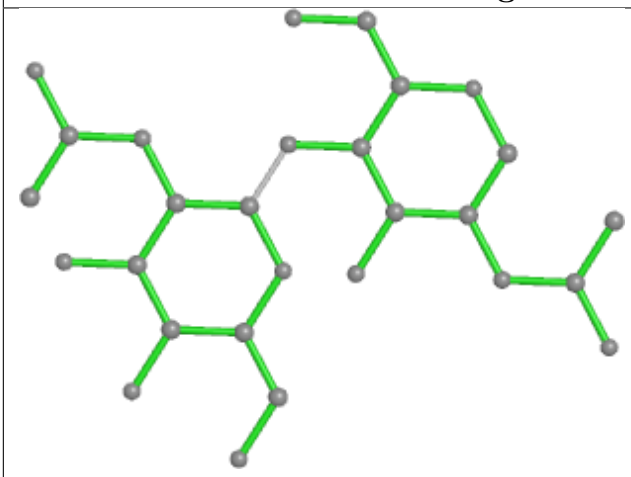


Torsions

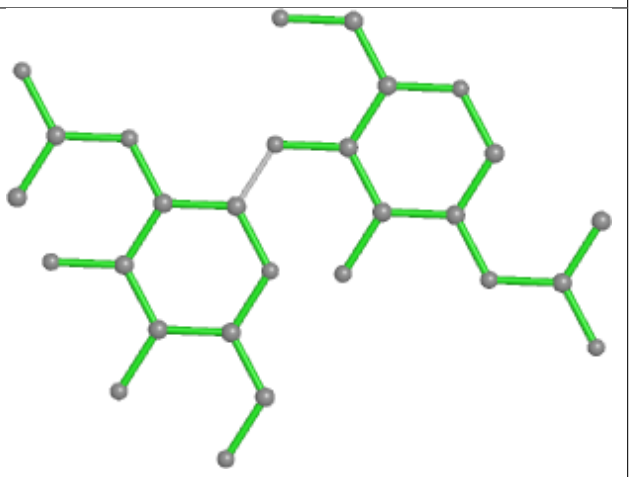


Rings

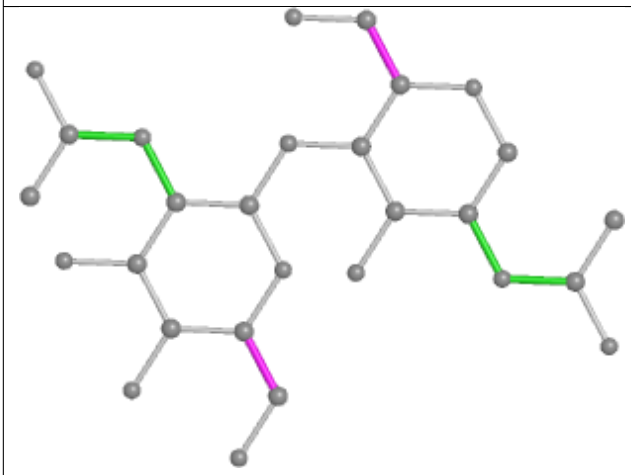
Oligosaccharide Chain S



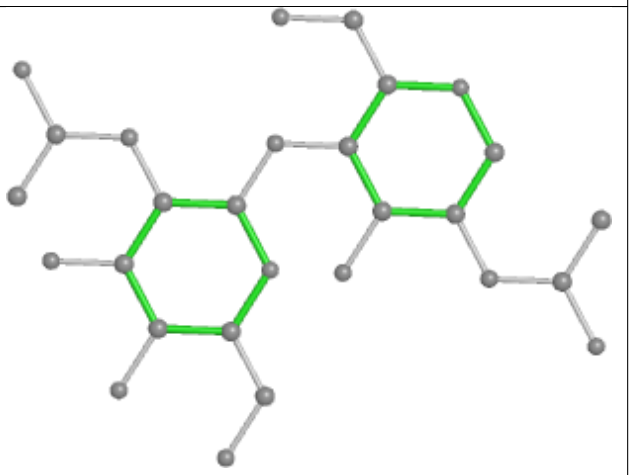
Bond lengths



Bond angles

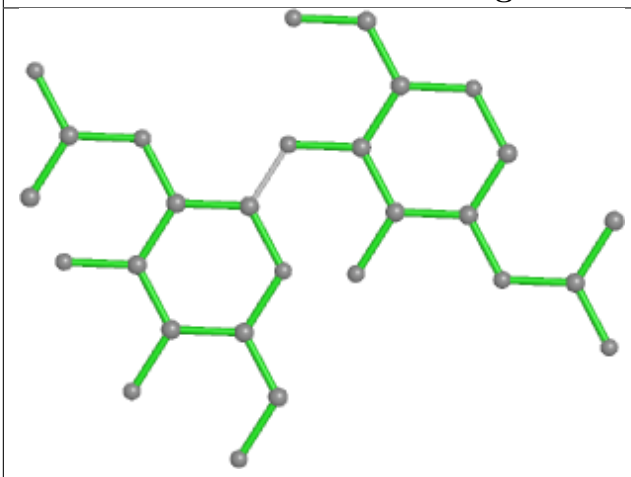


Torsions

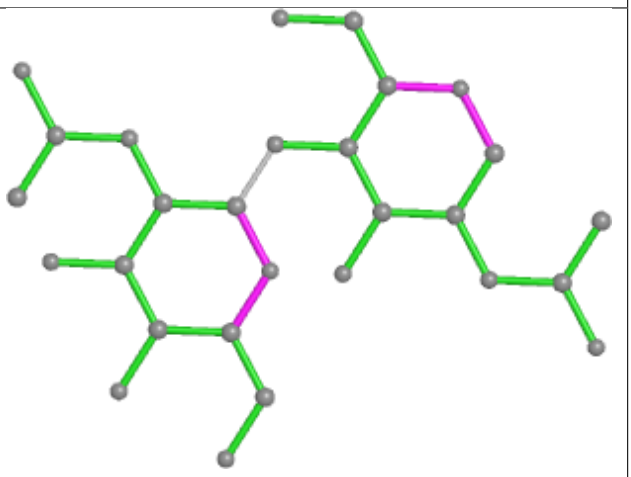


Rings

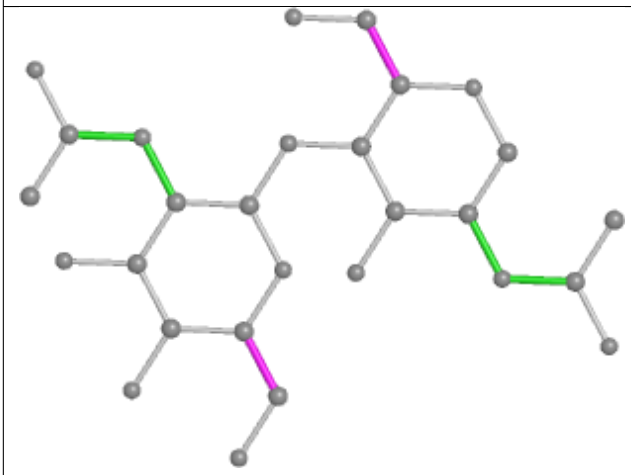
Oligosaccharide Chain T



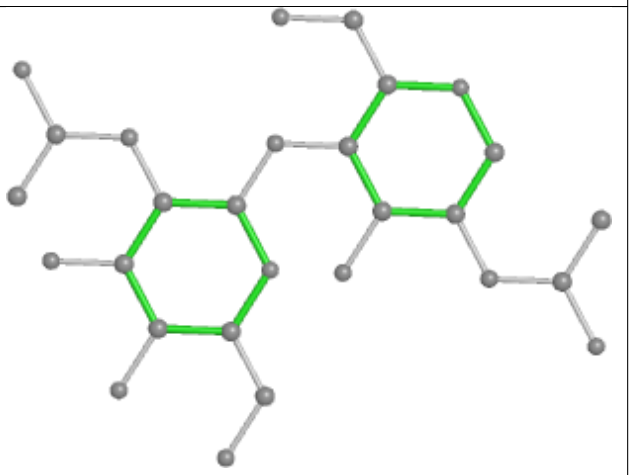
Bond lengths



Bond angles

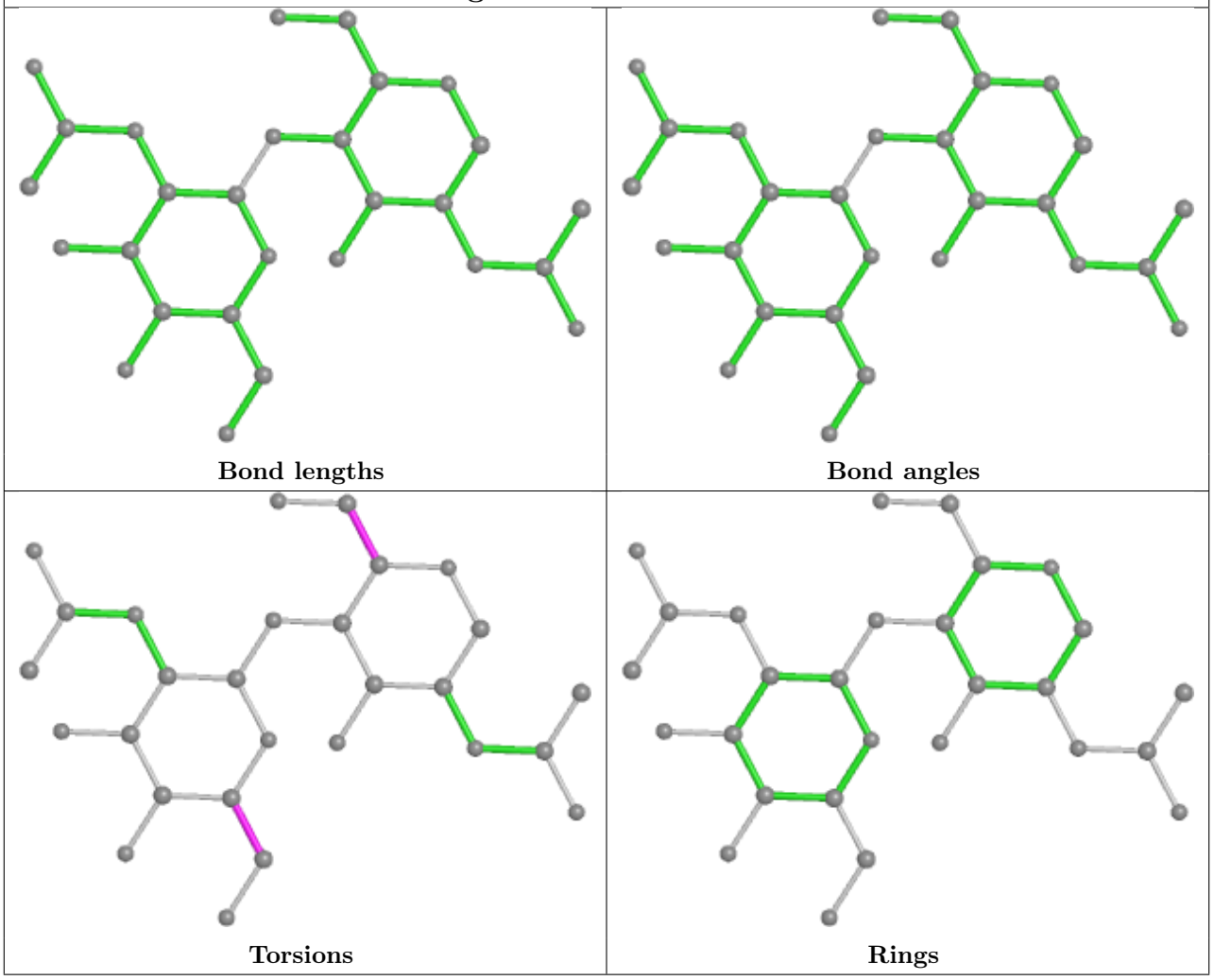


Torsions



Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.52	0
5	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	0.54	0
5	NAG	B	1303	1	14,14,15	0.31	0	17,19,21	0.53	0
5	NAG	A	1303	1	14,14,15	0.32	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	A	1301	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	B	1307	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	B	1302	1	14,14,15	0.28	0	17,19,21	0.48	0
5	NAG	C	1304	1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	C	1306	1	14,14,15	0.45	0	17,19,21	0.40	0
5	NAG	A	1307	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	C	1302	1	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	B	1301	1	14,14,15	0.32	0	17,19,21	0.51	0
5	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	A	1305	1	14,14,15	0.37	0	17,19,21	0.53	0
5	NAG	A	1306	1	14,14,15	0.25	0	17,19,21	0.39	0
5	NAG	B	1308	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	C	1307	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	C	1303	1	14,14,15	0.29	0	17,19,21	0.42	0
5	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	B	1306	1	14,14,15	0.22	0	17,19,21	0.38	0
5	NAG	C	1305	1	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	C	1309	1	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	B	1304	1	14,14,15	0.30	0	17,19,21	0.48	0
5	NAG	A	1302	1	14,14,15	0.27	0	17,19,21	0.44	0

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	B	1305	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	B	1307	NAG	C4-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6

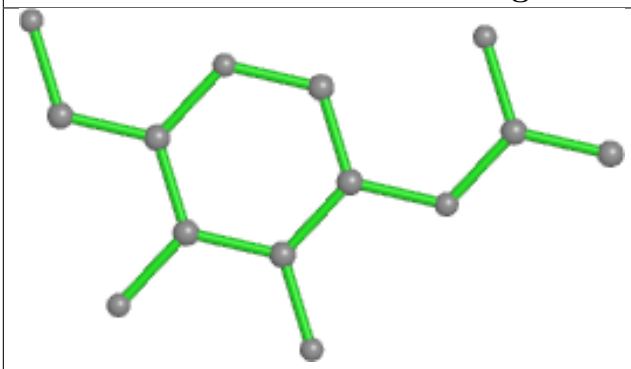
There are no ring outliers.

2 monomers are involved in 2 short contacts:

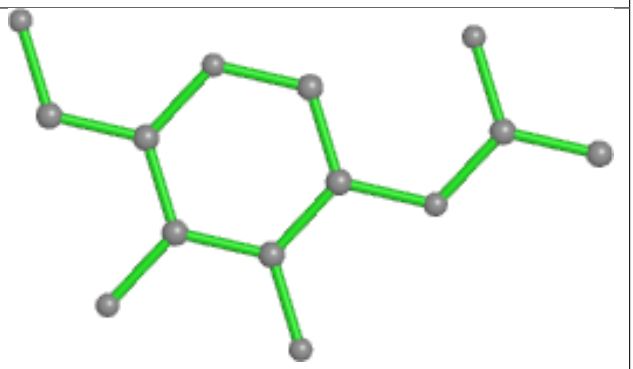
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1302	NAG	1	0
5	A	1306	NAG	1	0

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

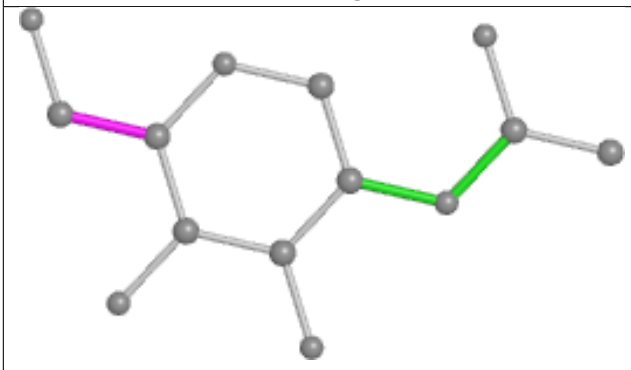
Ligand NAG B 1305



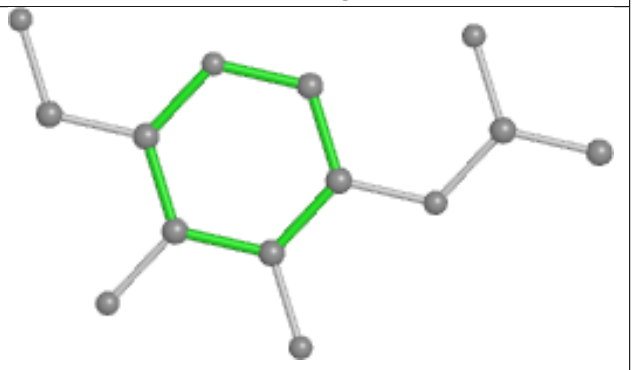
Bond lengths



Bond angles

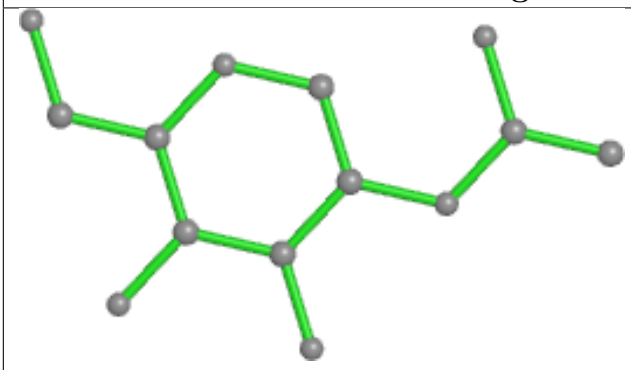


Torsions

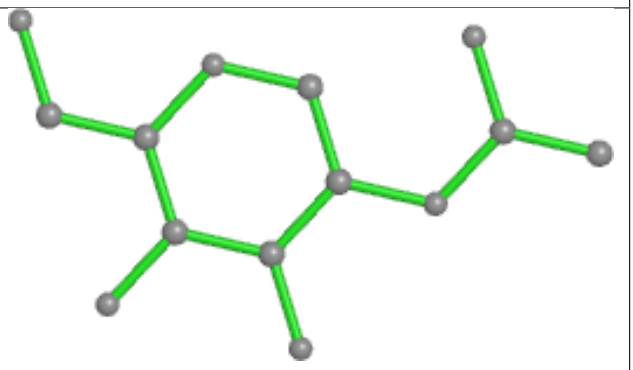


Rings

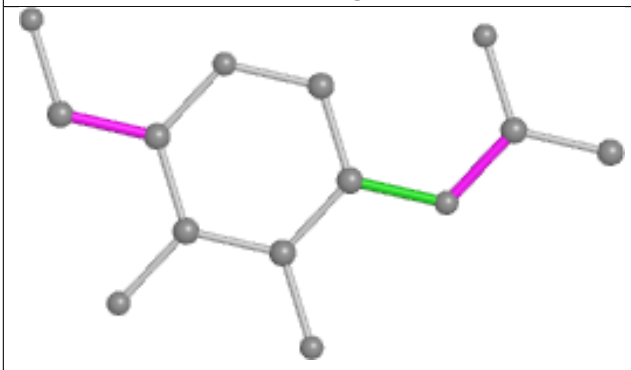
Ligand NAG C 1301



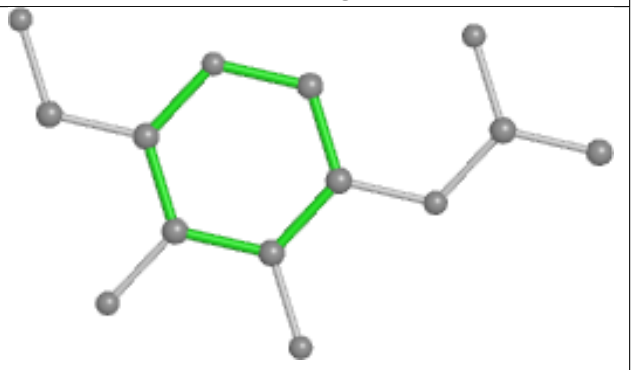
Bond lengths



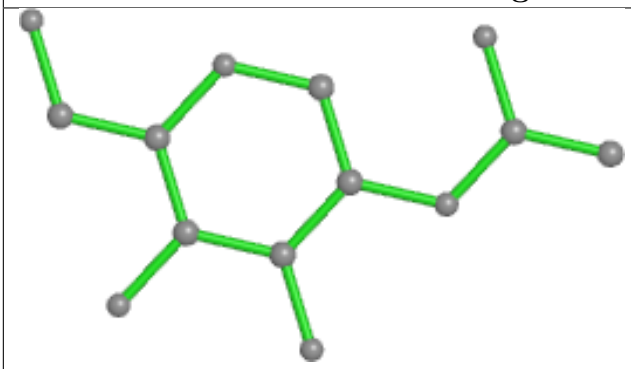
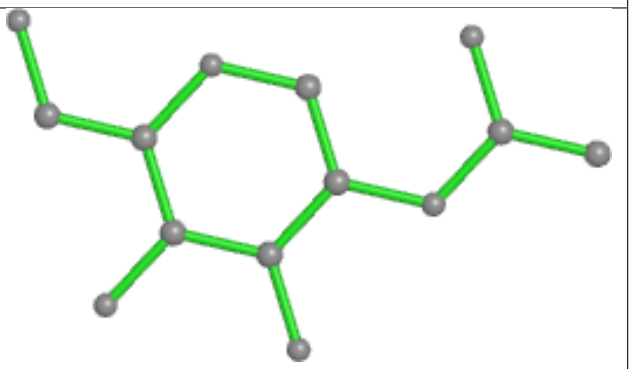
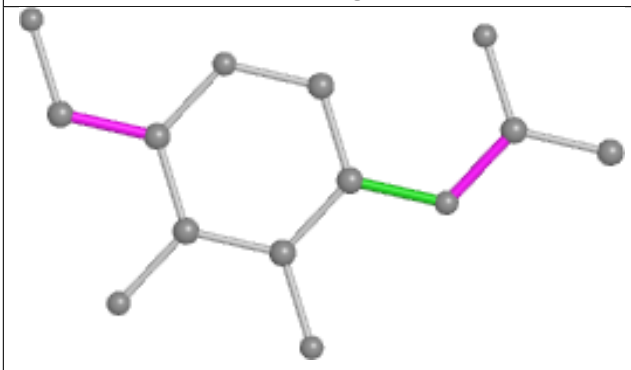
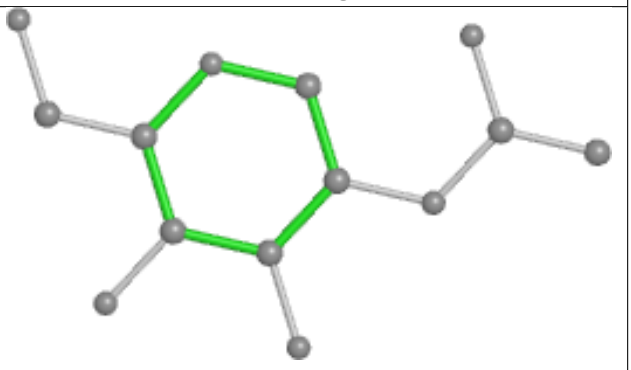
Bond angles

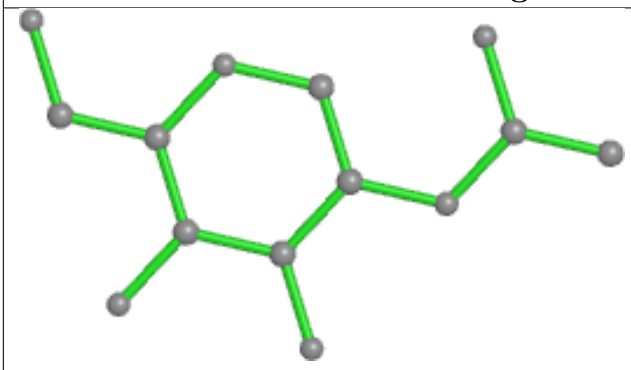
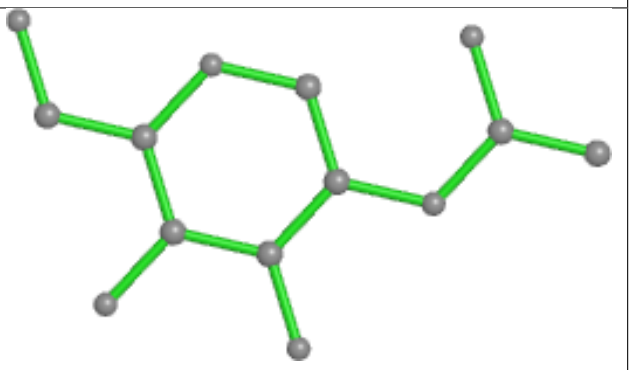
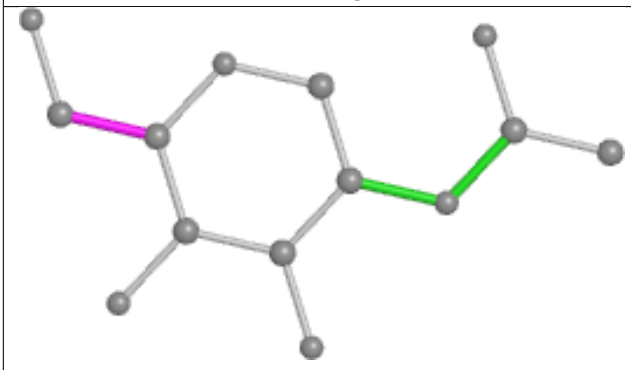
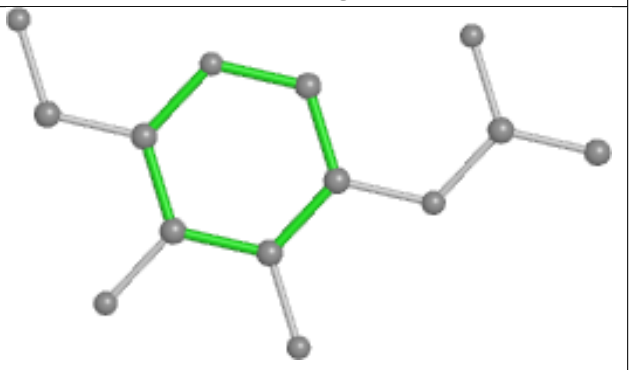


Torsions

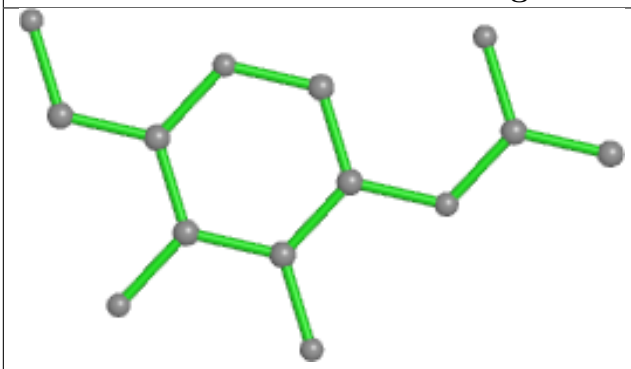


Rings

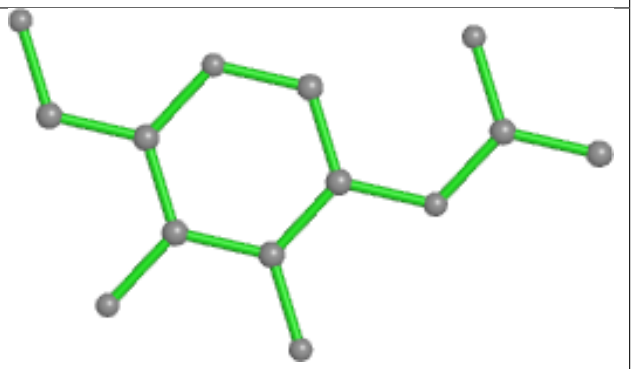
Ligand NAG B 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

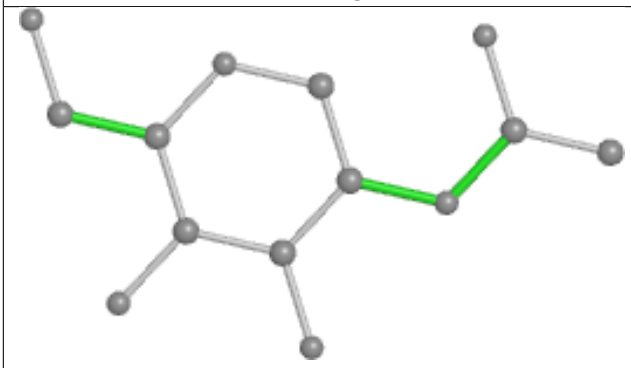
Ligand NAG A 1301



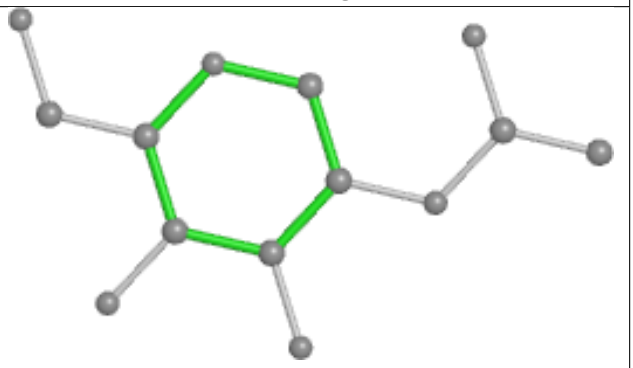
Bond lengths



Bond angles

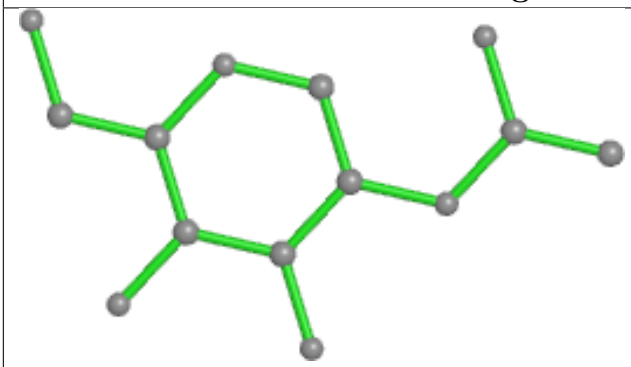


Torsions

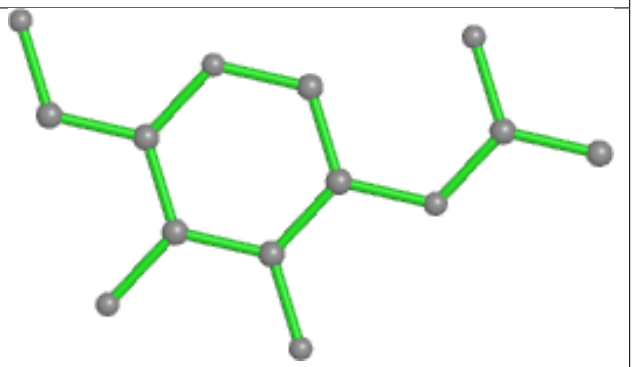


Rings

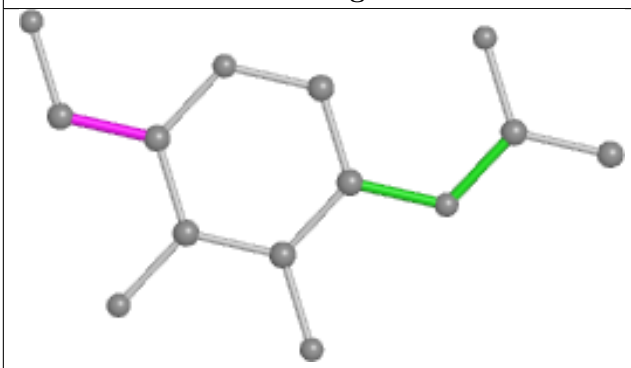
Ligand NAG B 1307



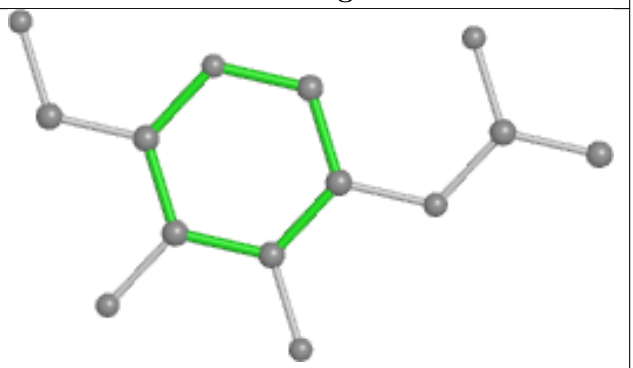
Bond lengths



Bond angles

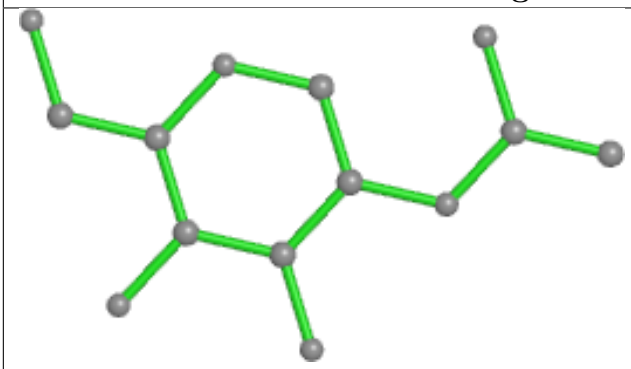


Torsions

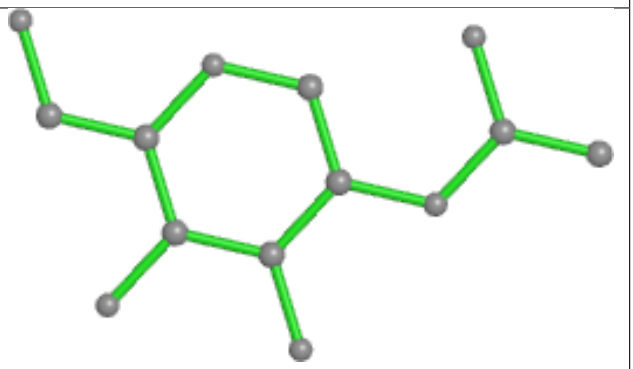


Rings

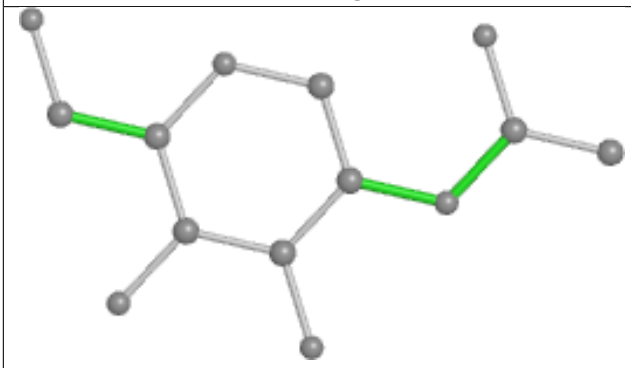
Ligand NAG B 1302



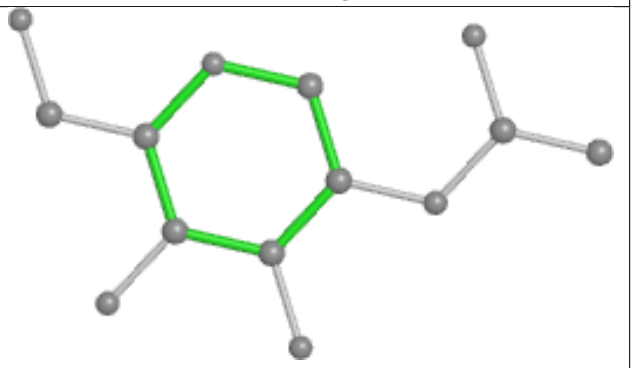
Bond lengths



Bond angles

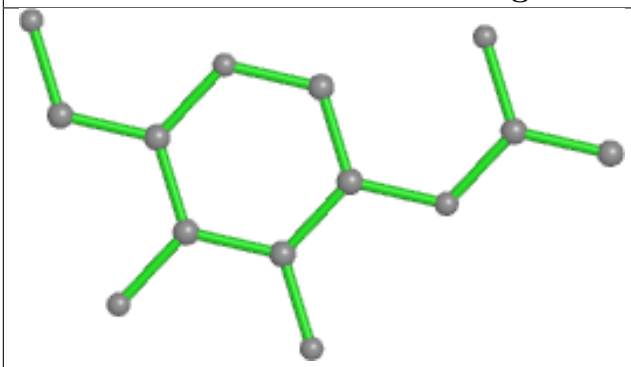


Torsions

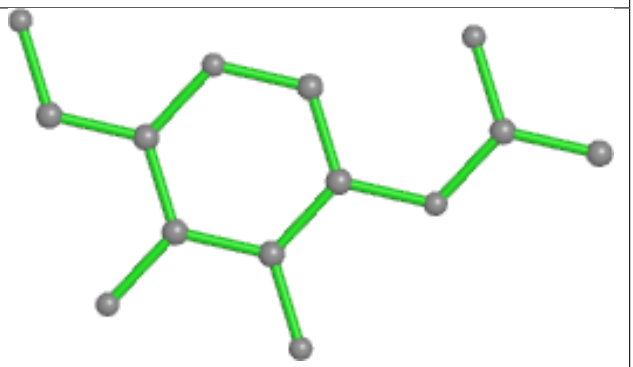


Rings

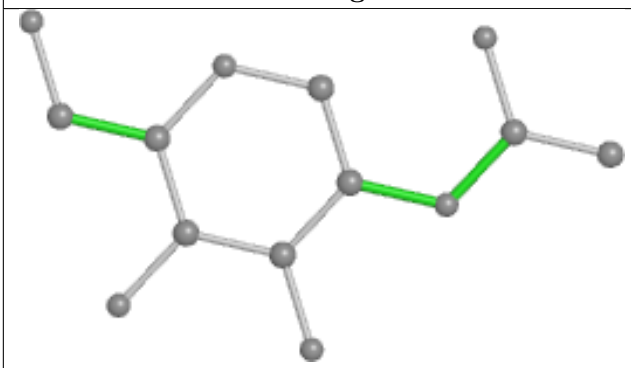
Ligand NAG C 1304



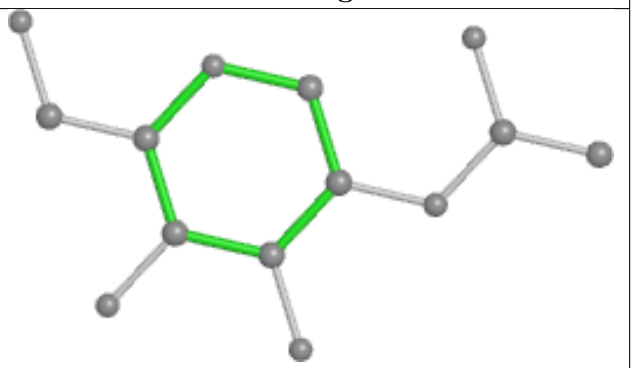
Bond lengths



Bond angles

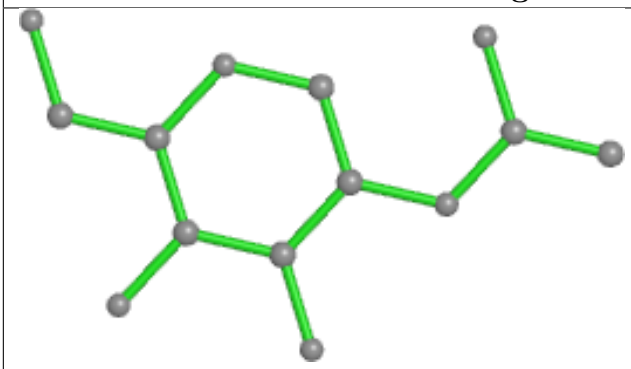


Torsions



Rings

Ligand NAG C 1306



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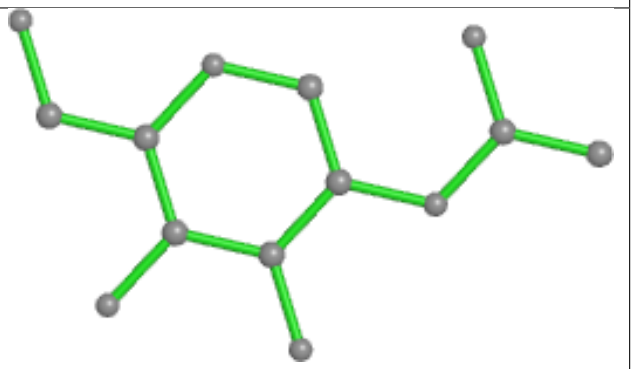
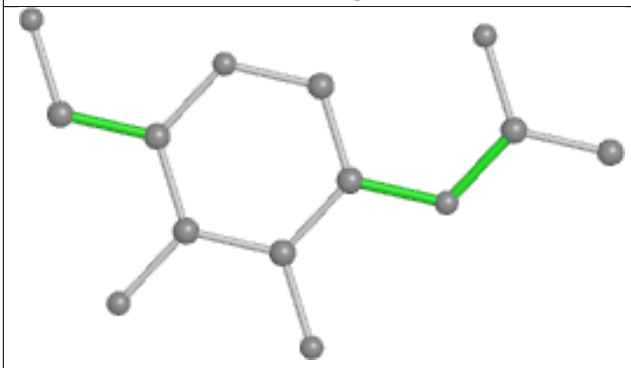


Bond angles



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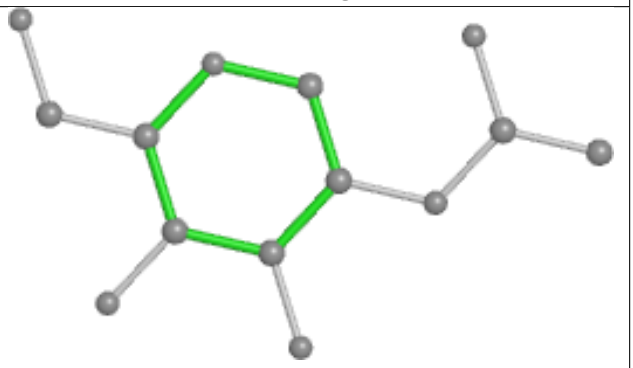
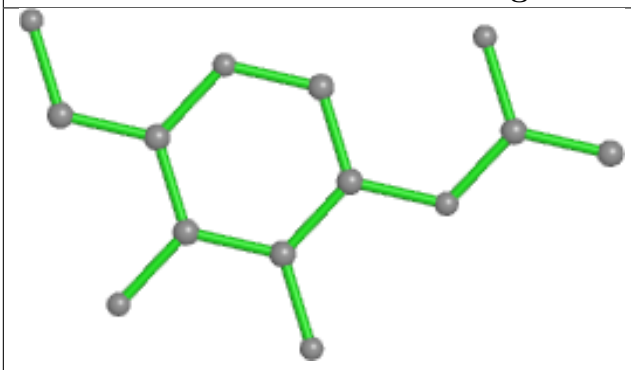


Rings

Ligand NAG A 1307



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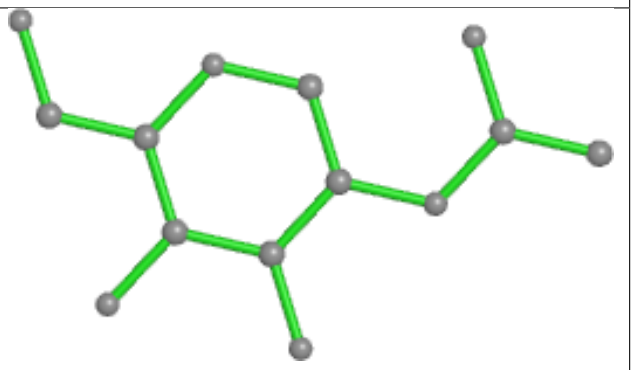
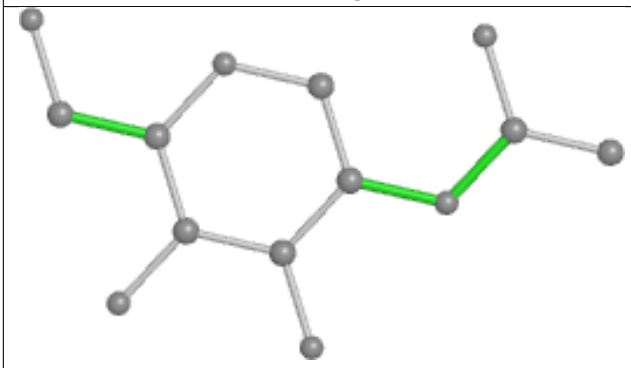
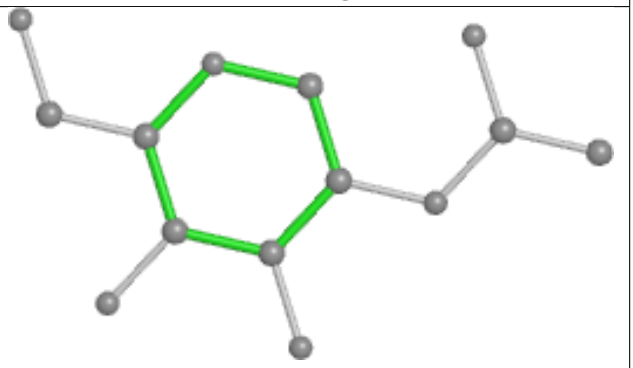


Bond angles

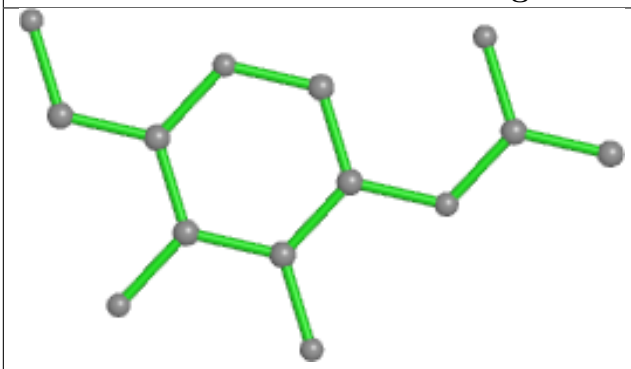


Torsions



Rings

Ligand NAG C 1302



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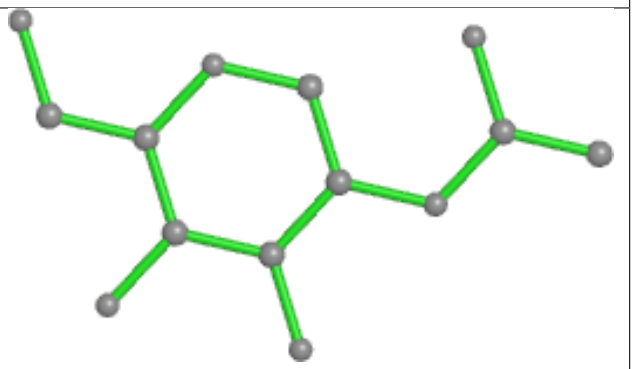
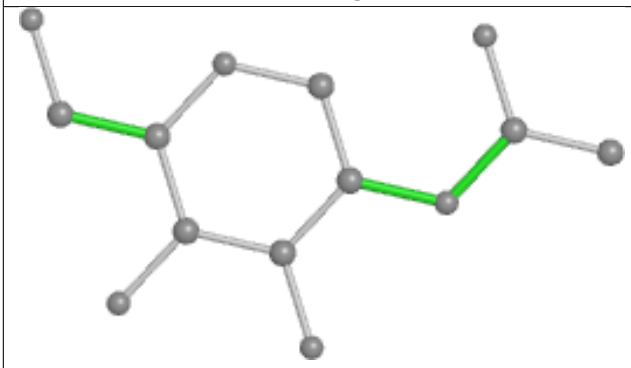
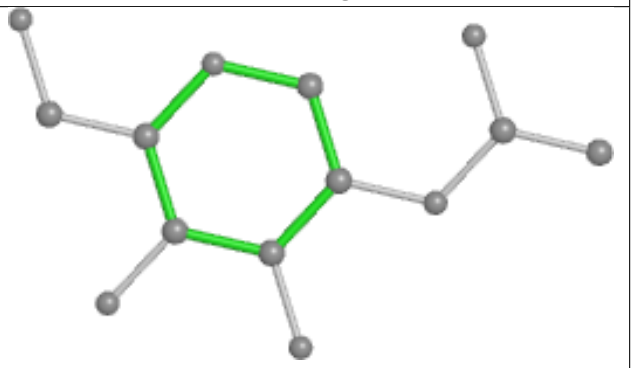


Bond angles

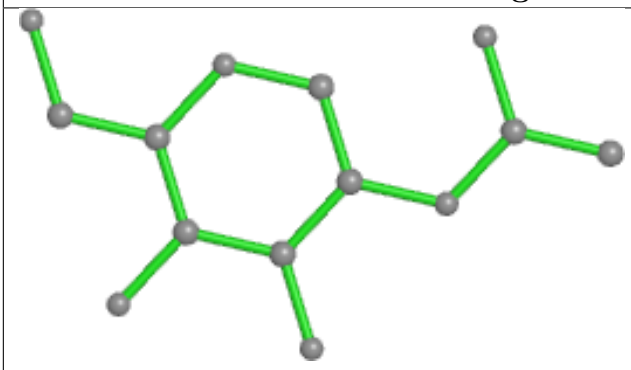


Torsions



Rings

Ligand NAG B 1301



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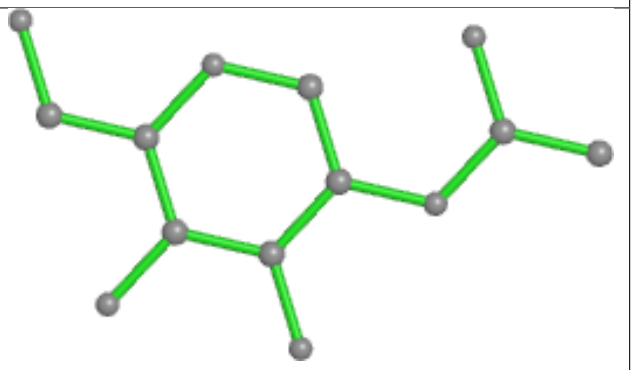
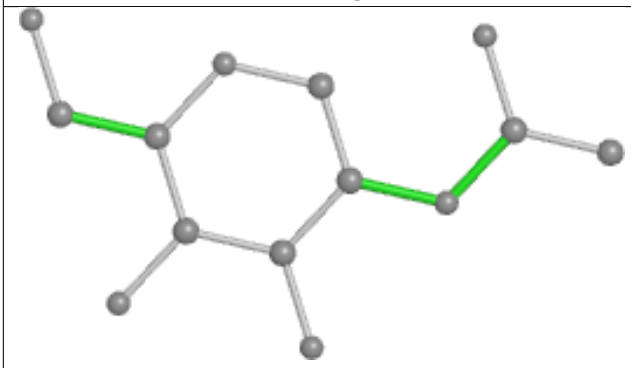
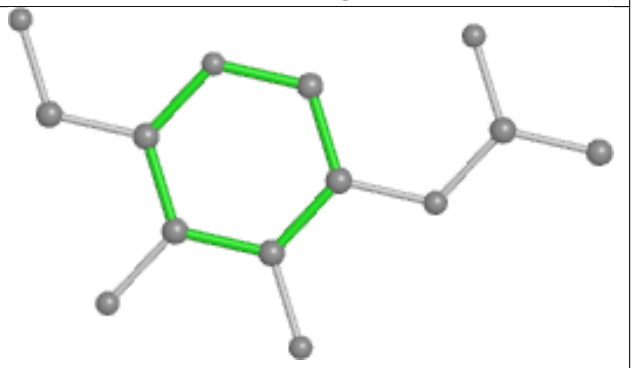


Bond angles

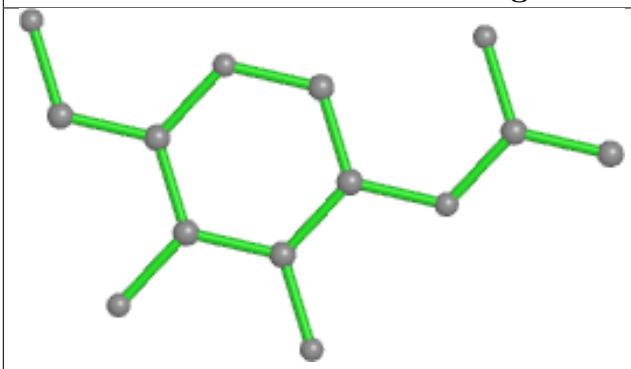


Torsions



Rings

Ligand NAG A 1304



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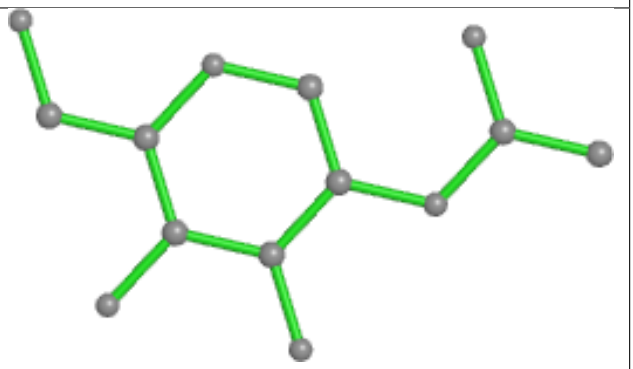
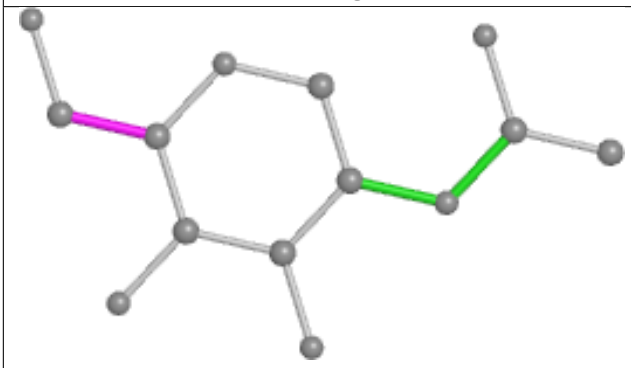


Bond angles



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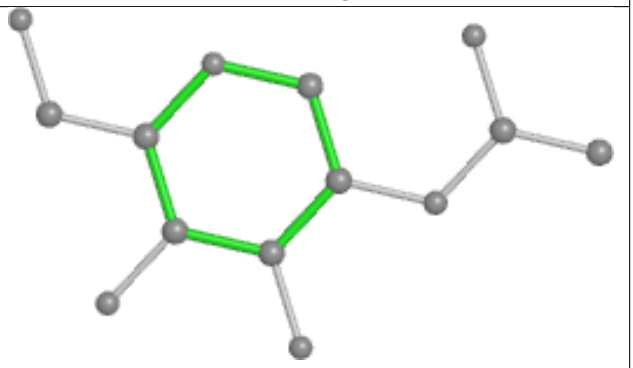
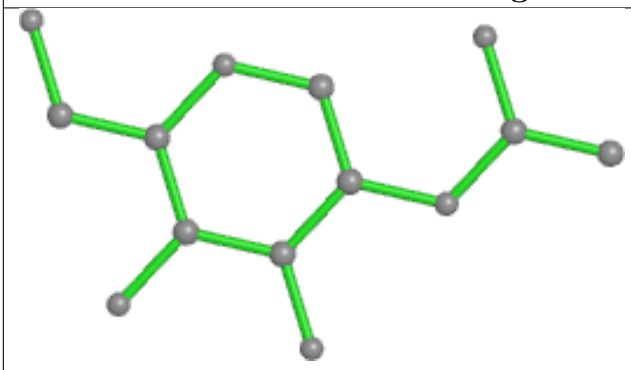


Rings

Ligand NAG A 1305



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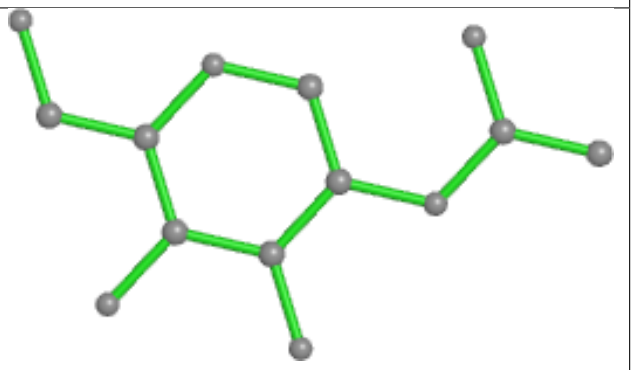
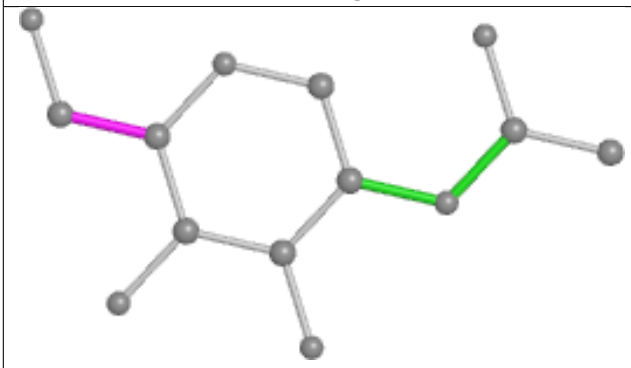


Bond angles



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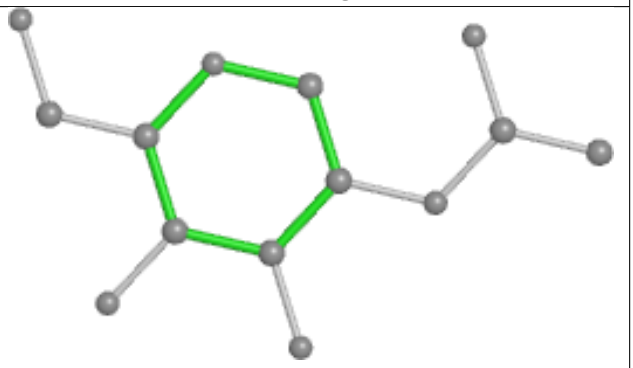
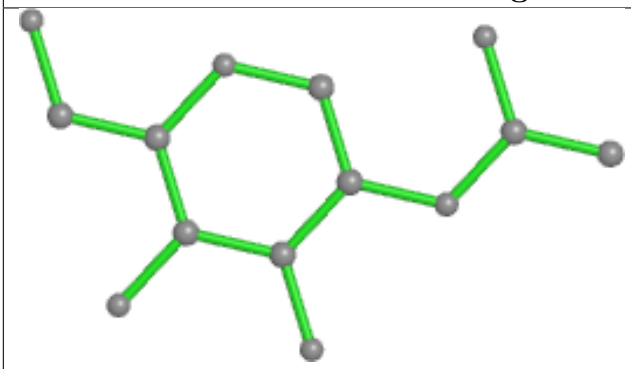


Rings

Ligand NAG A 1306



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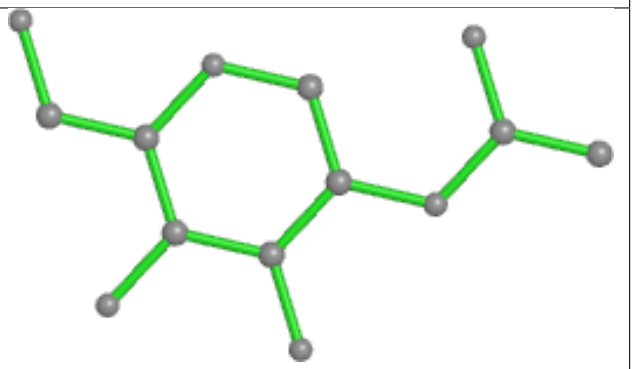
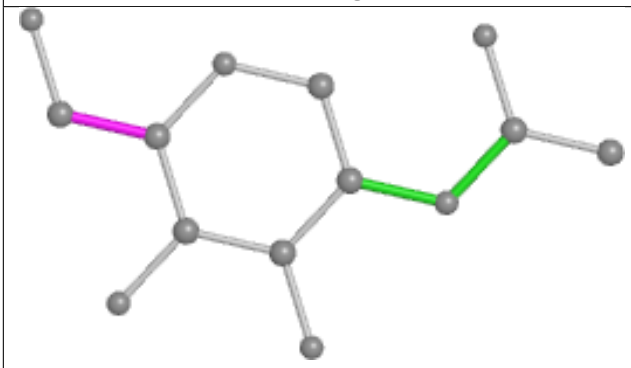
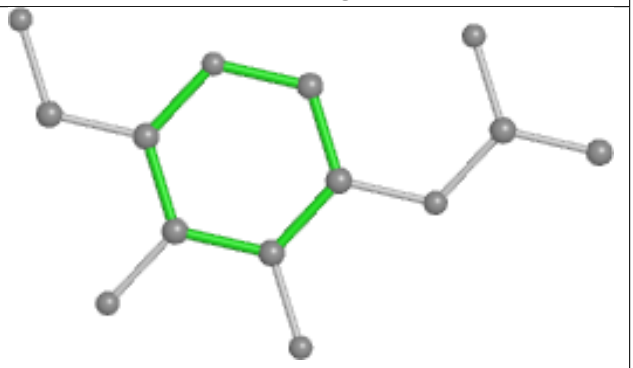


Bond angles

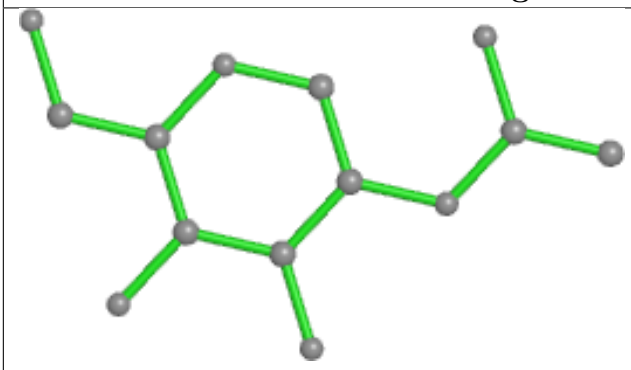


Torsions



Rings

Ligand NAG B 1308



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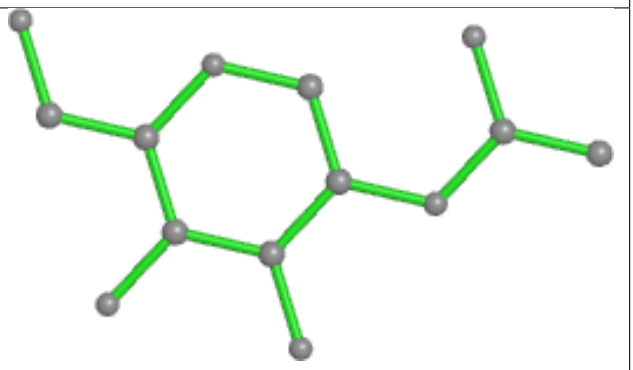
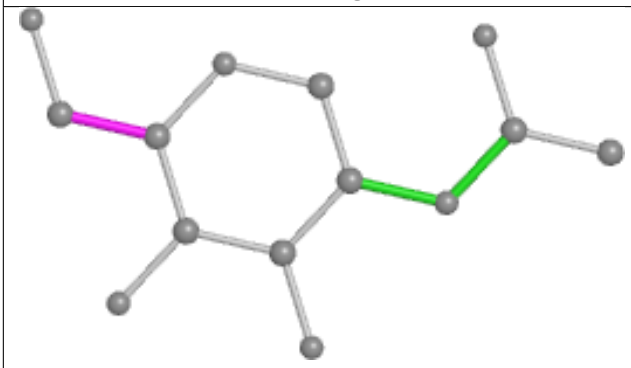
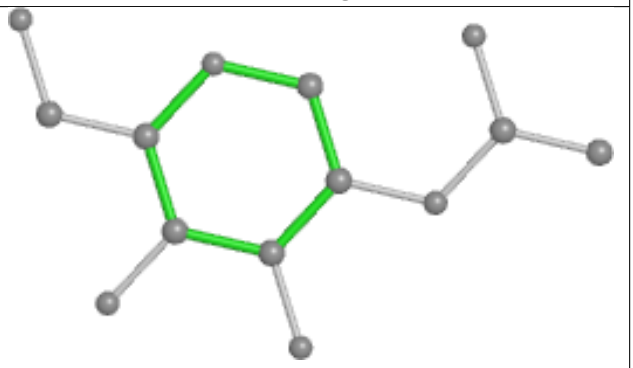


Bond angles

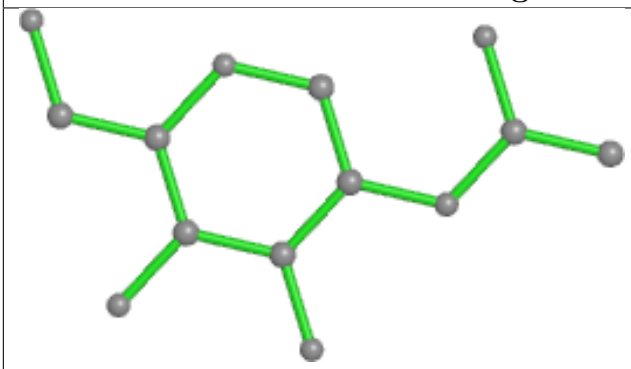


Torsions



Rings

Ligand NAG C 1307



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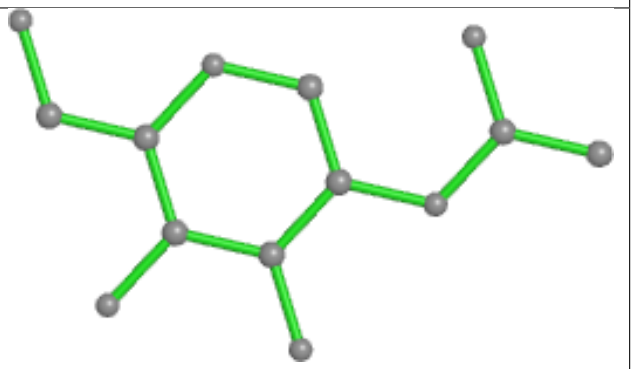
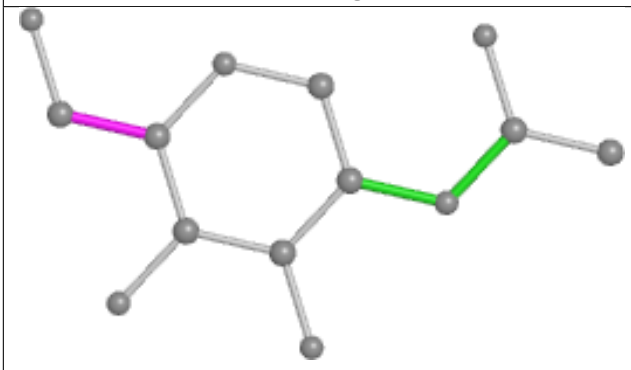
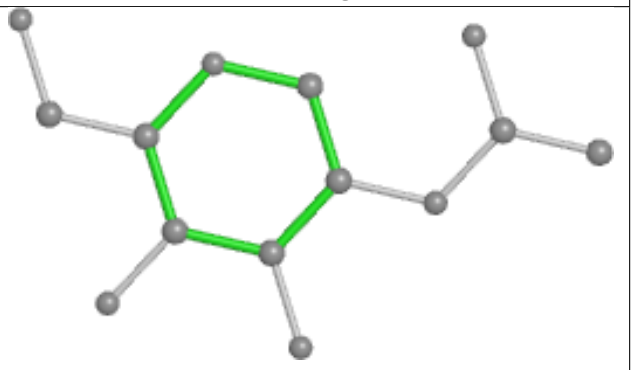


Bond angles

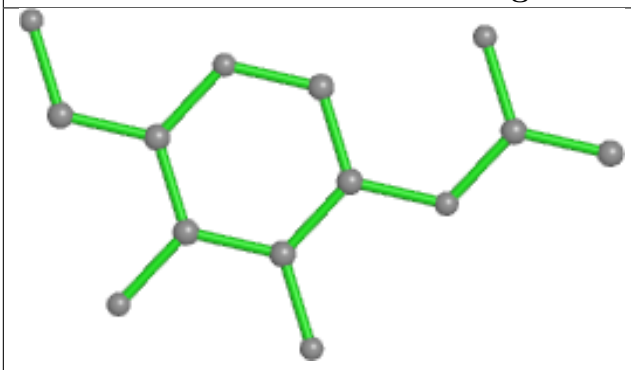


Torsions



Rings

Ligand NAG C 1303



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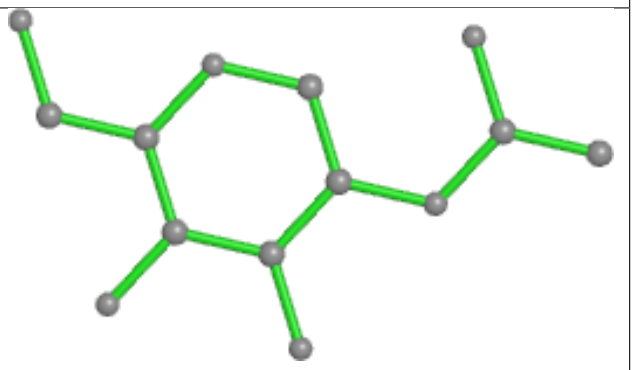
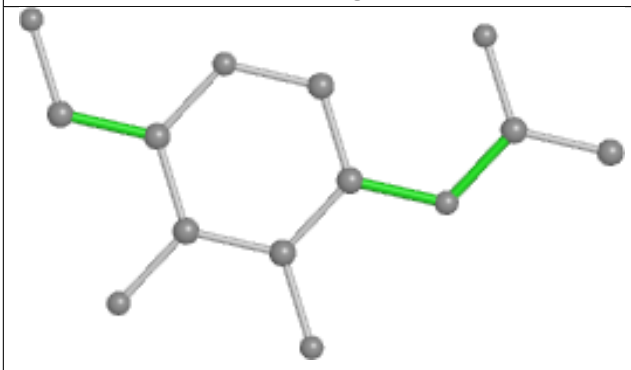


Bond angles



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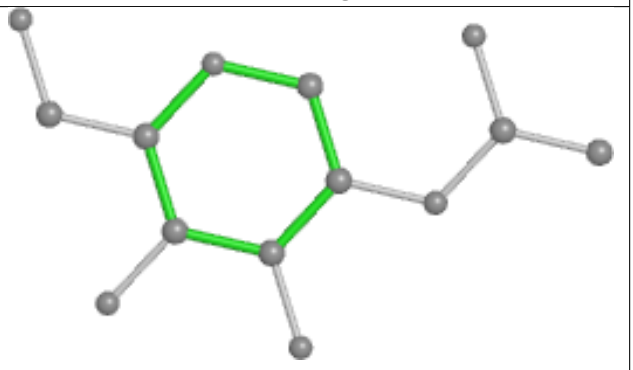
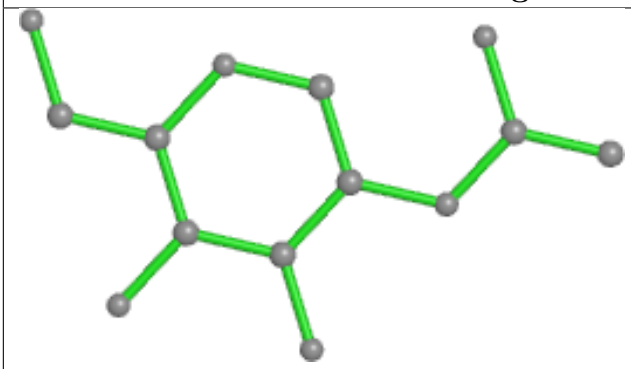


Rings

Ligand NAG C 1308



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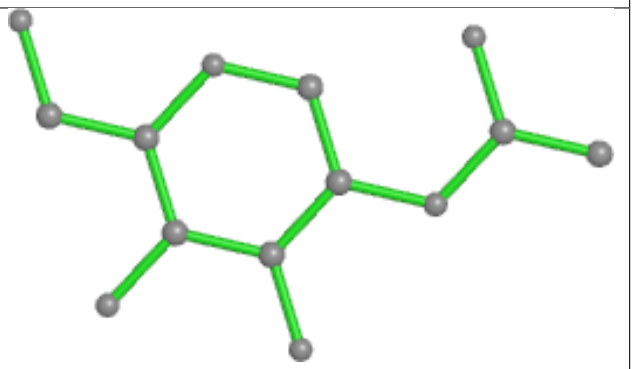
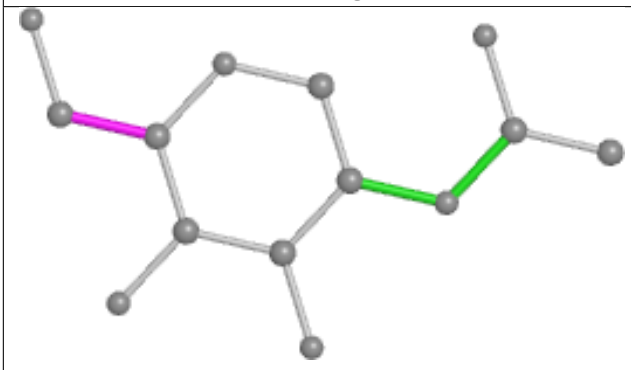
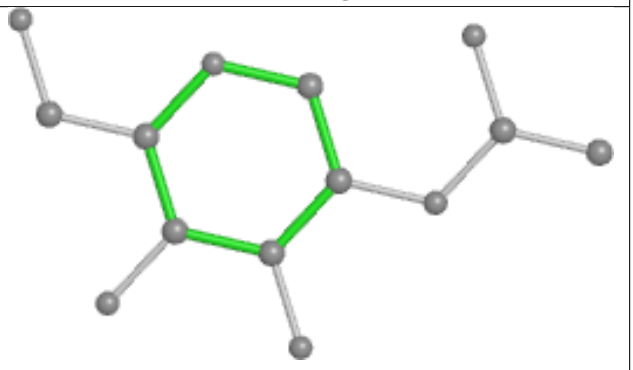


Bond angles

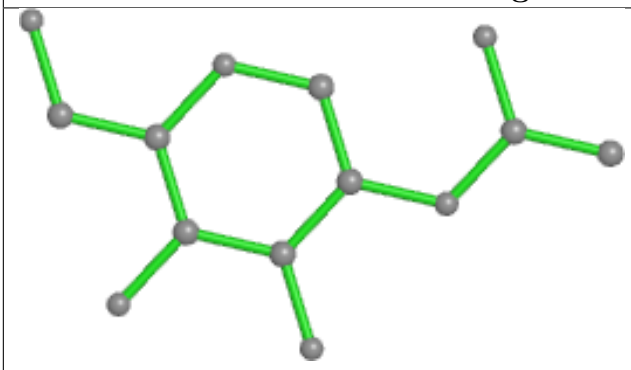


Torsions

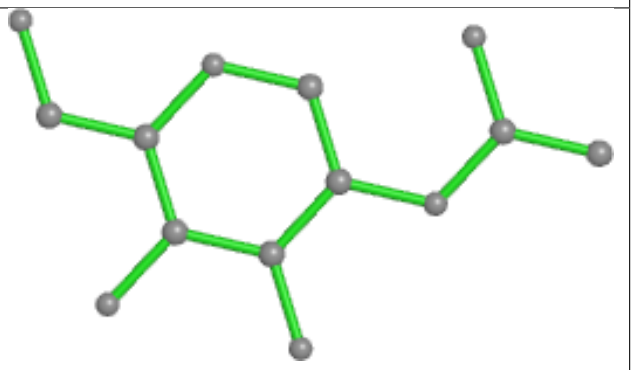


Rings

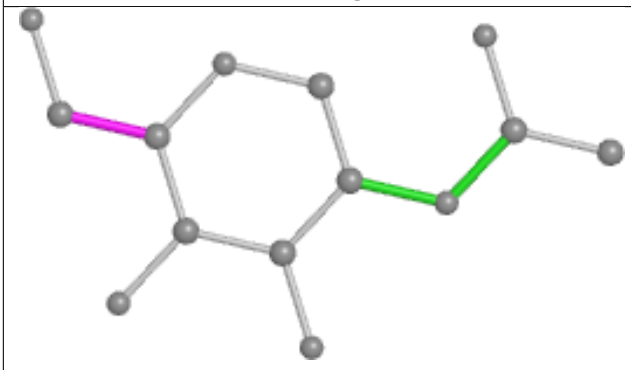
Ligand NAG B 1306



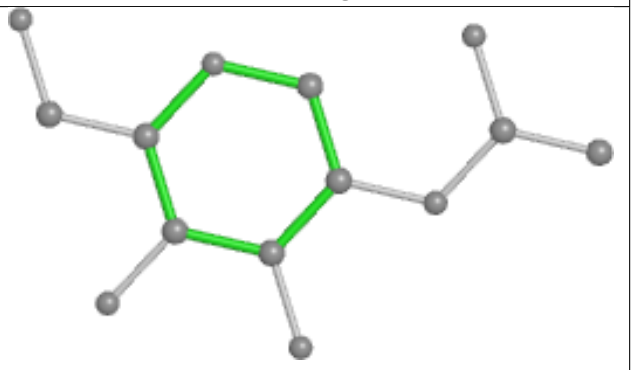
Bond lengths



Bond angles

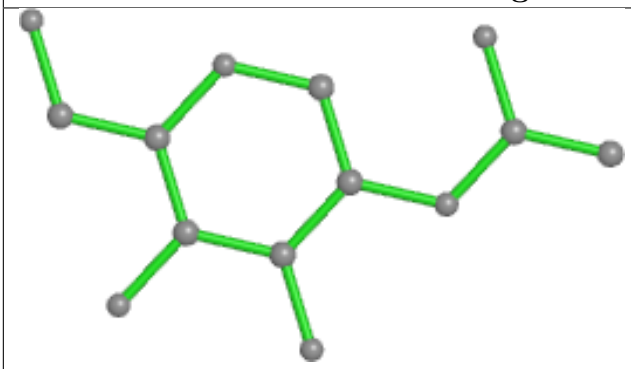


Torsions

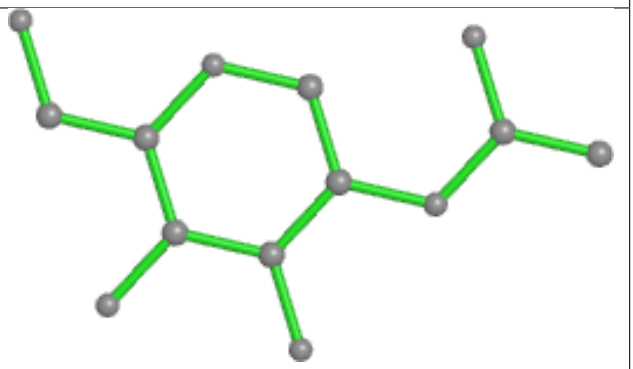


Rings

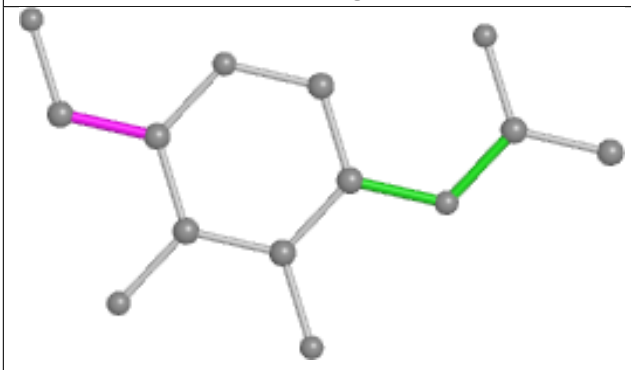
Ligand NAG C 1305



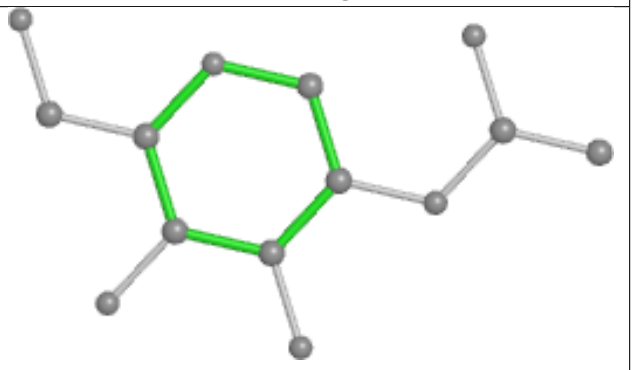
Bond lengths



Bond angles

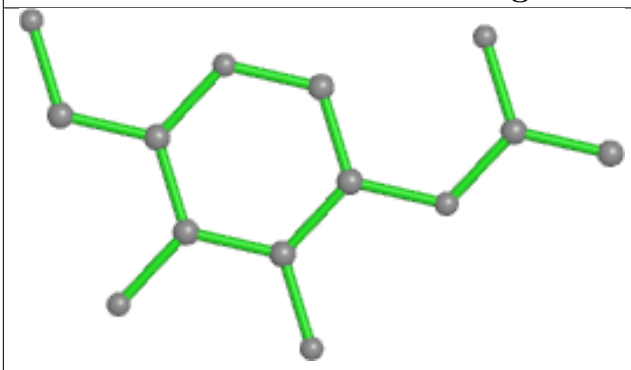


Torsions

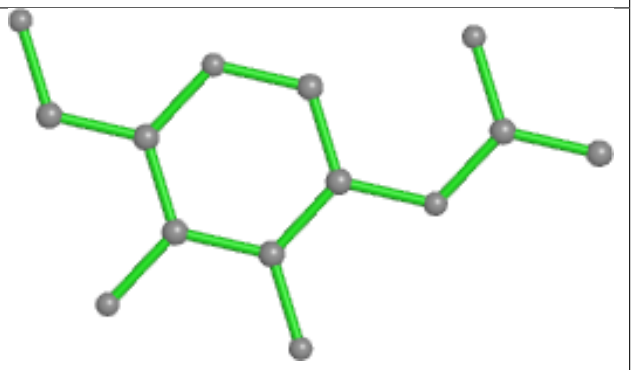


Rings

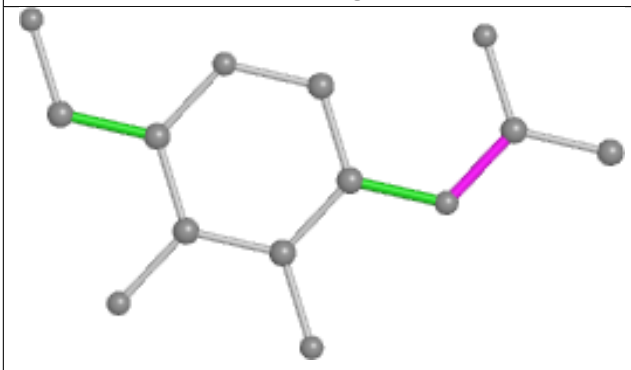
Ligand NAG C 1309



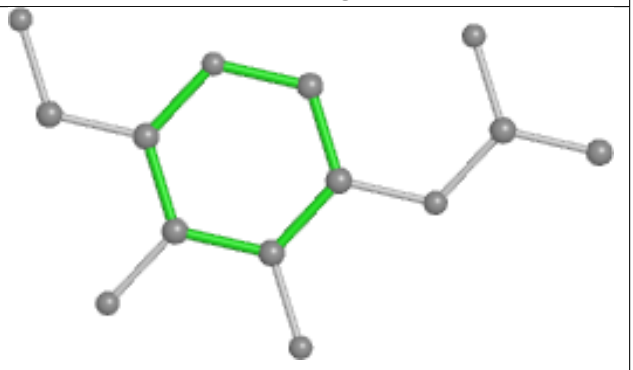
Bond lengths



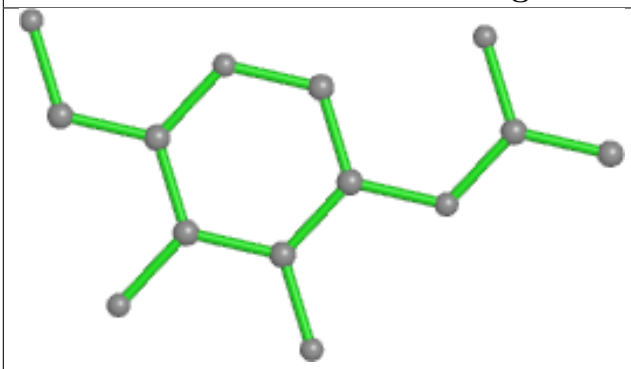
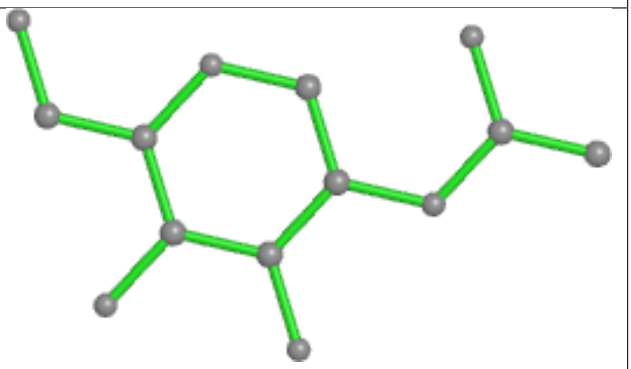
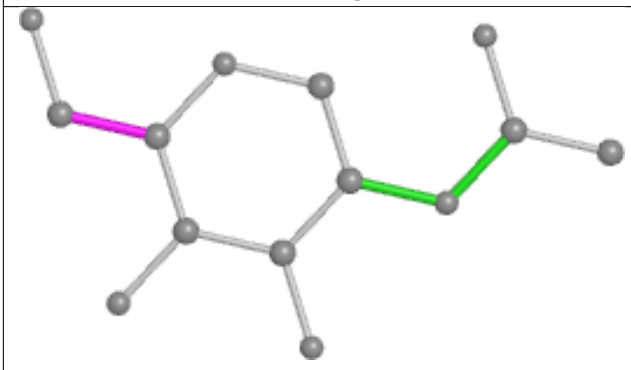
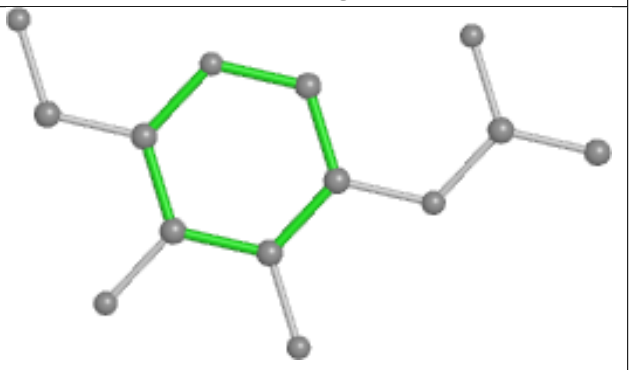
Bond angles

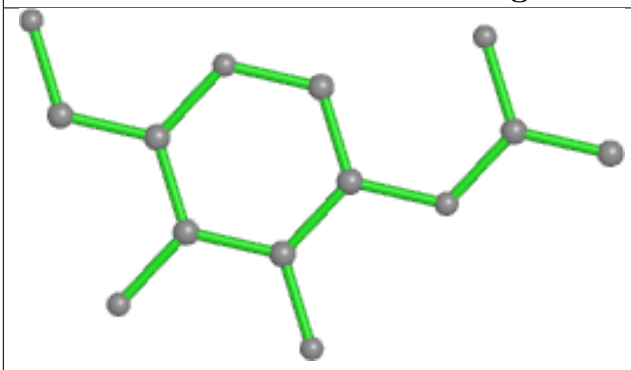
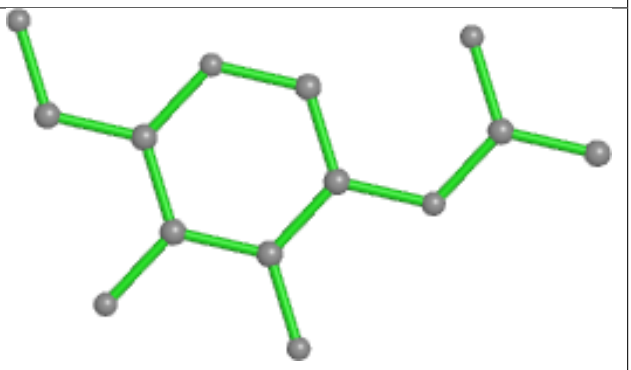
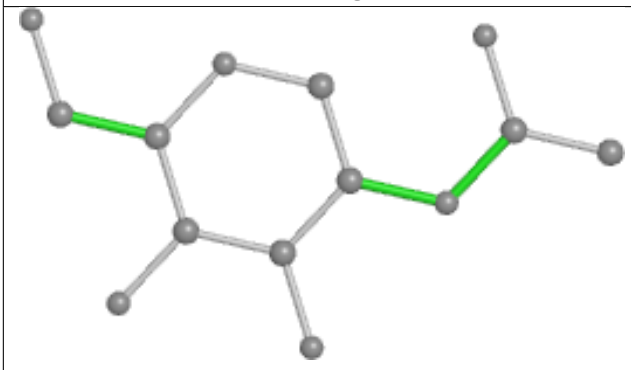
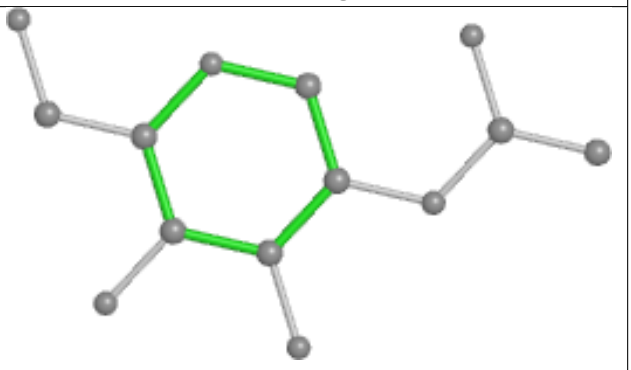


Torsions



Rings

Ligand NAG B 1304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1302	
 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.