Full wwPDB EM Validation Report ⓘ

Apr 14, 2024 – 12:11 AM JST

PDB ID	:	8WGV
EMDB ID	:	EMD-37516
Title	:	BA.2(S375) Spike (S6P)/hACE2 complex
Authors	:	Wei, X.; Zhang, Z.
Deposited on	:	2023-09-22
Resolution	:	2.92 Å(reported)
Based on initial model	:	7XO8

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:

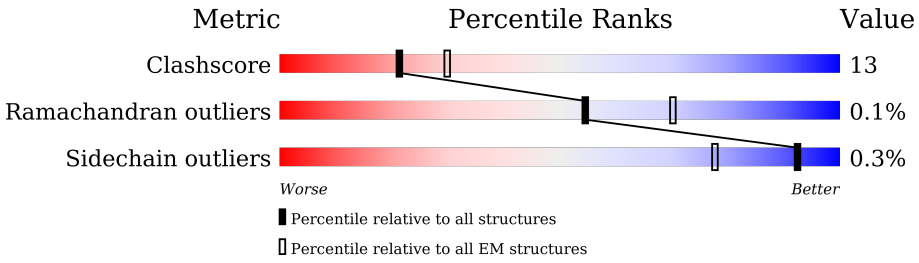
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.92 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1244	60% 19% 20%
1	B	1244	60% 19% 20%
1	C	1244	60% 19% 20%
2	D	614	58% 38% .
2	E	614	55% 42% . .
2	F	614	60% 36% .
3	G	2	100%
3	H	2	100%
3	I	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 38688 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	993	Total	C	N	O	S	1	0
			7773	4971	1293	1475	34		
1	B	992	Total	C	N	O	S	1	0
			7770	4969	1293	1473	35		
1	C	991	Total	C	N	O	S	1	0
			7761	4964	1292	1470	35		

There are 234 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	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	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	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	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	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	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	HIS	-	expression tag	UNP P0DTC2
B	1241	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	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	142	ASP	GLY	variant	UNP P0DTC2
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	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	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	HIS	-	expression tag	UNP P0DTC2
C	1241	HIS	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2

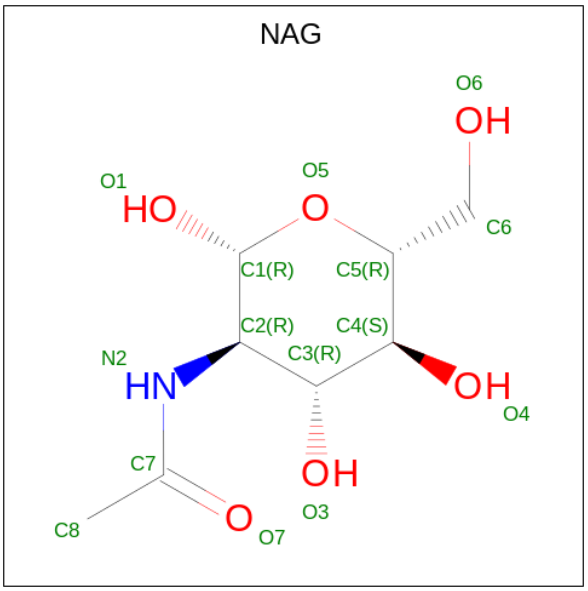
- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		
2	E	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		
2	F	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		

- 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		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		

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

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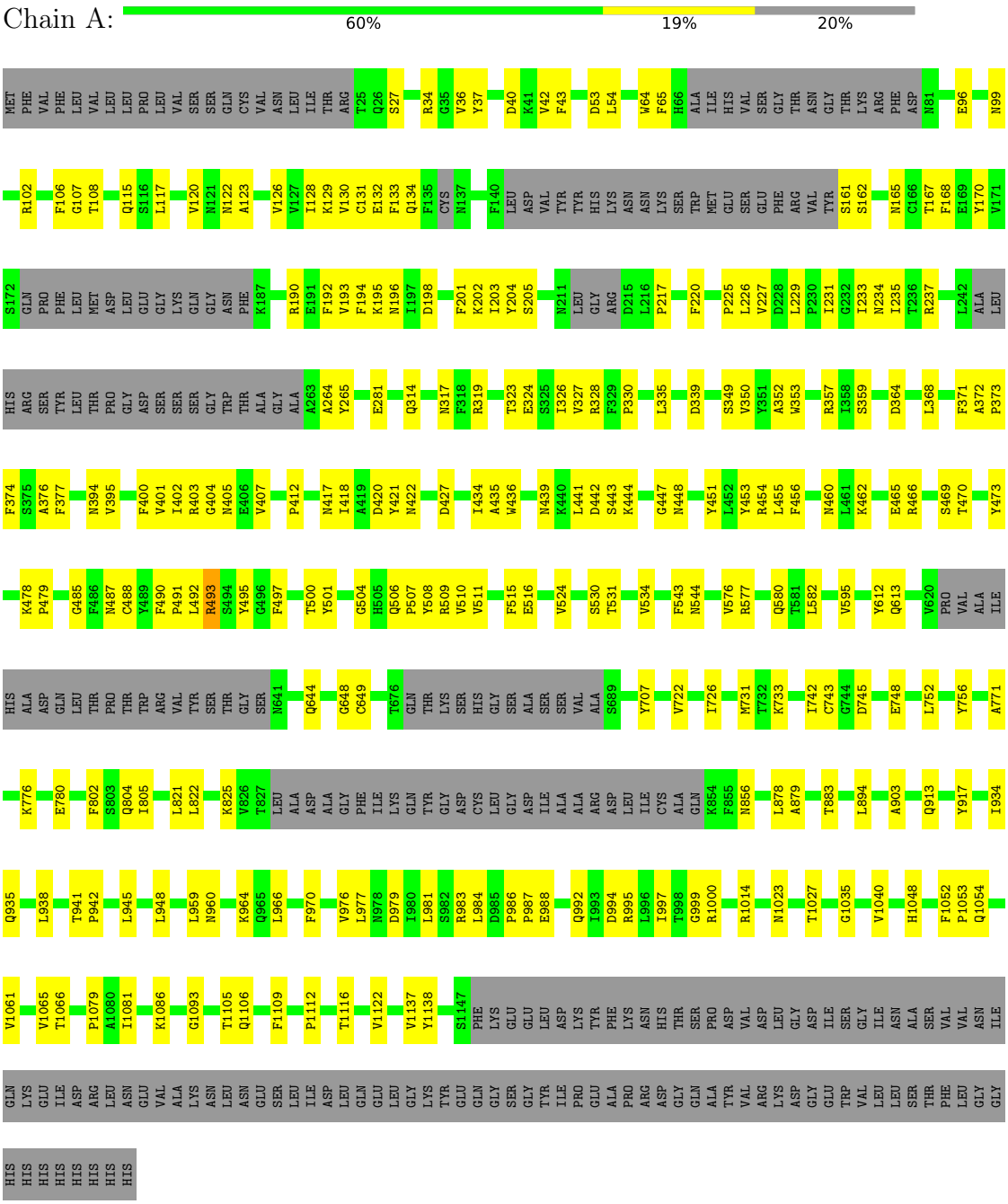
Mol	Chain	Residues	Atoms				AltConf
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

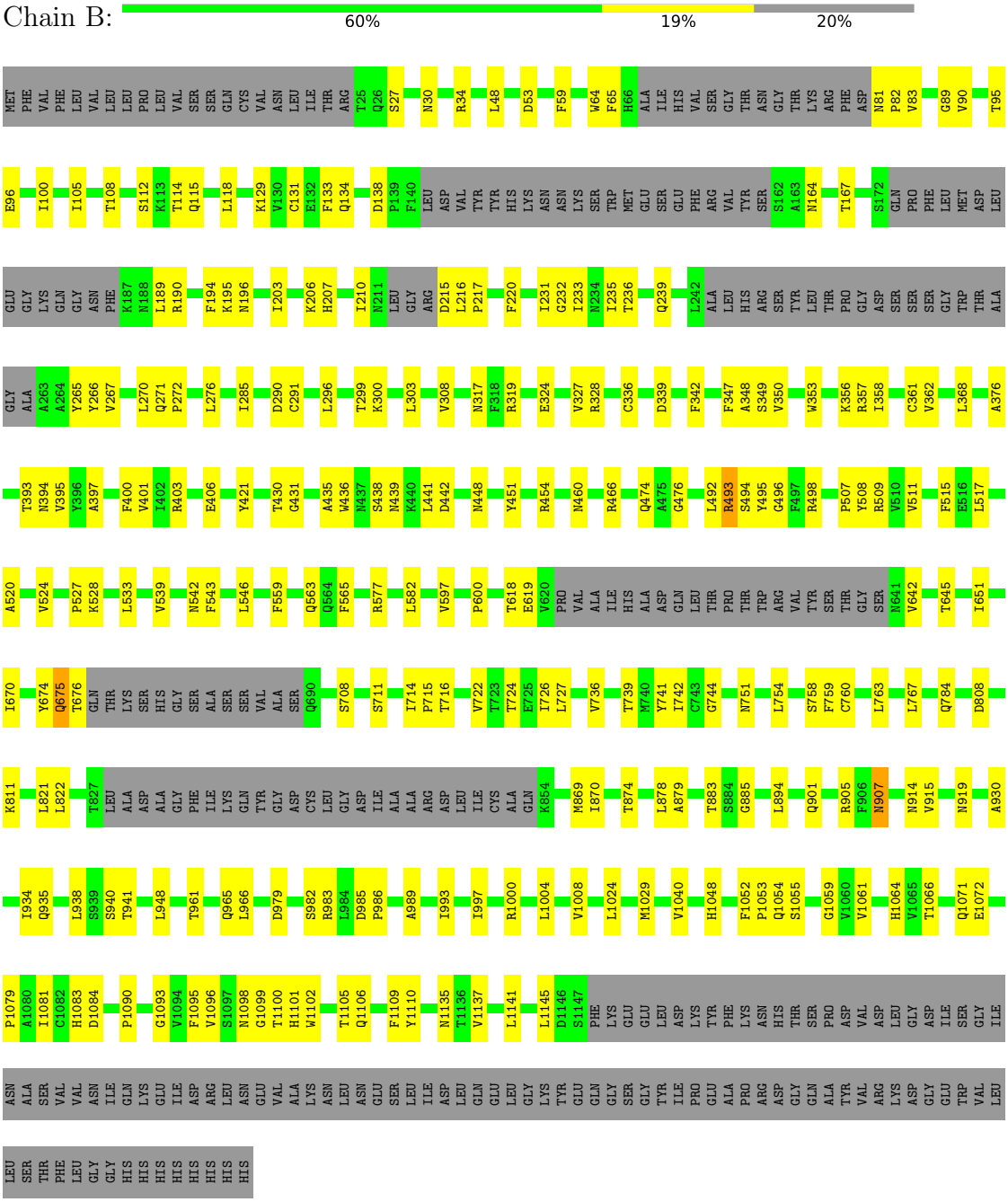
- Molecule 1: Spike glycoprotein

Chain A:



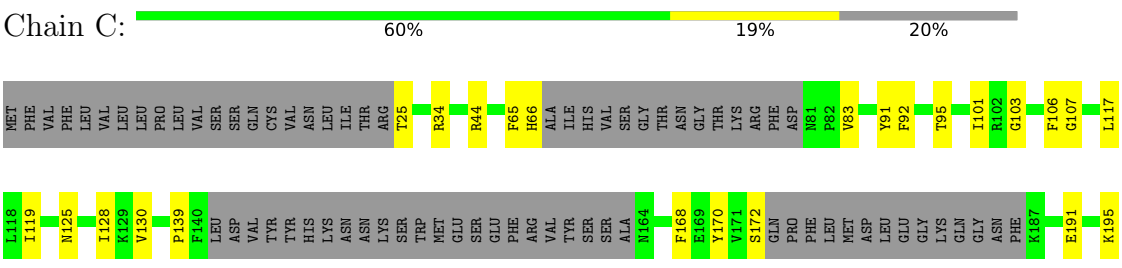
• Molecule 1: Spike glycoprotein

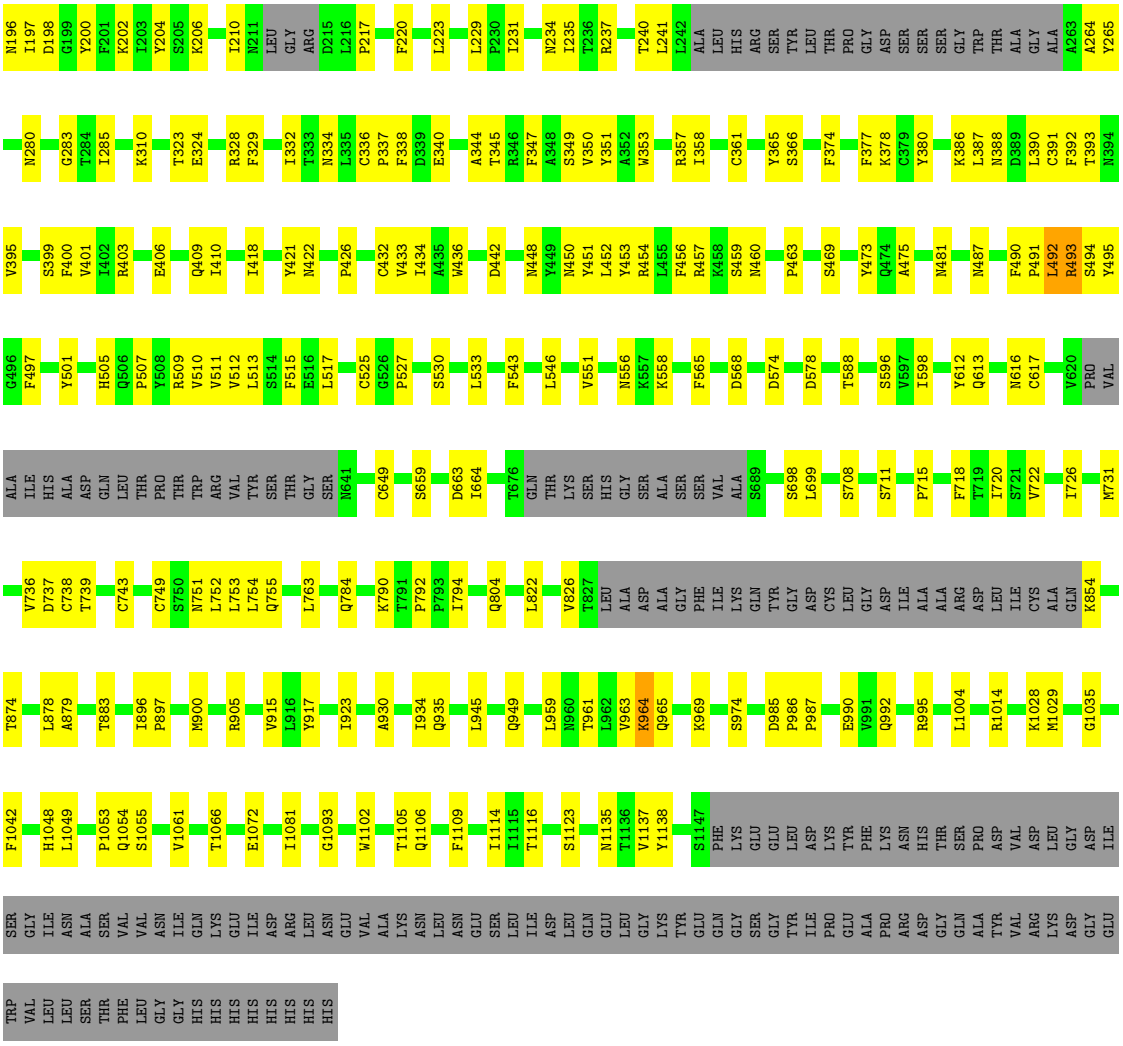
Chain B:



• Molecule 1: Spike glycoprotein

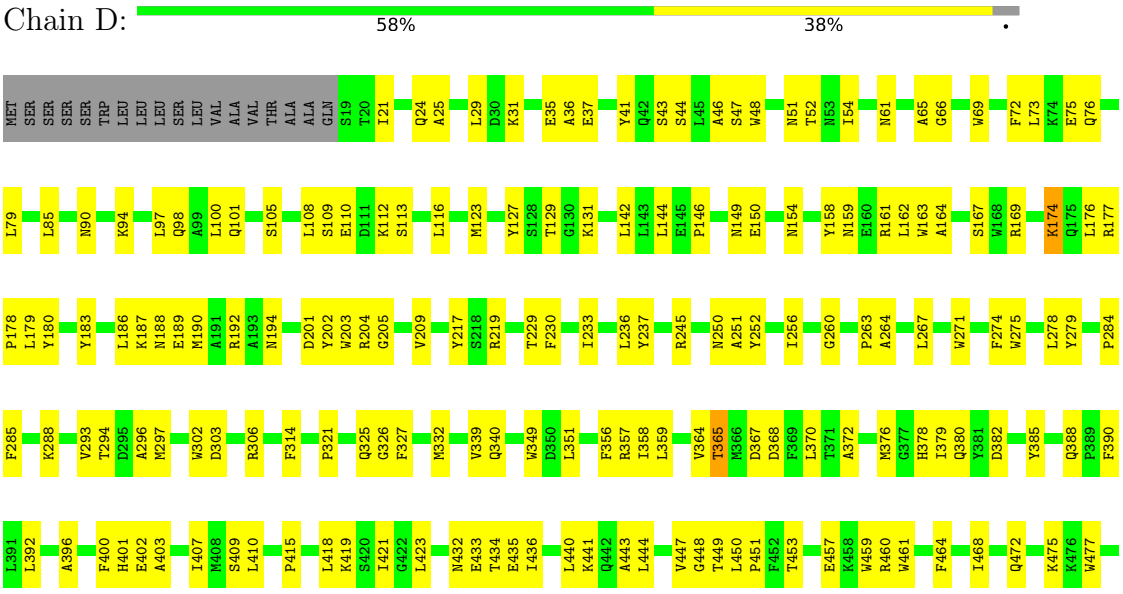
Chain C:

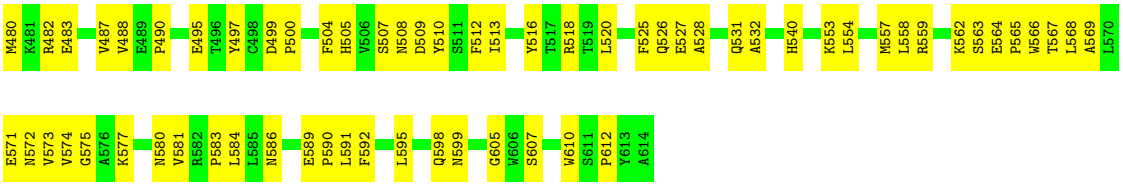




• Molecule 2: Angiotensin-converting enzyme 2

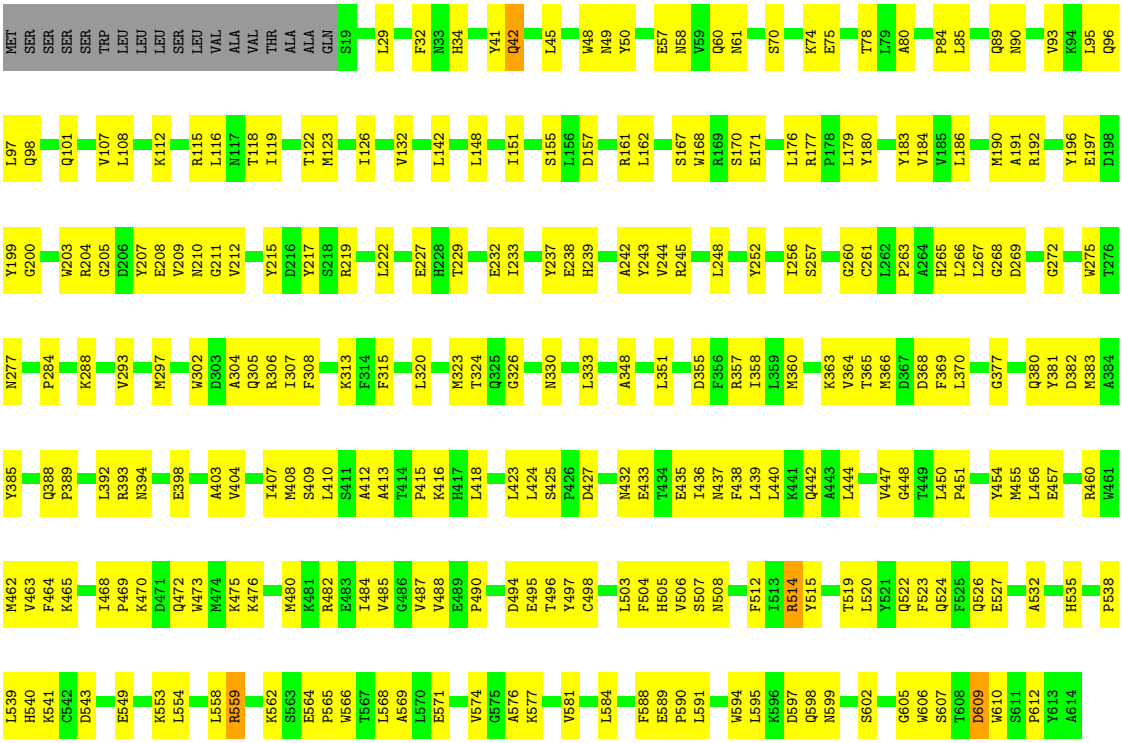
Chain D:





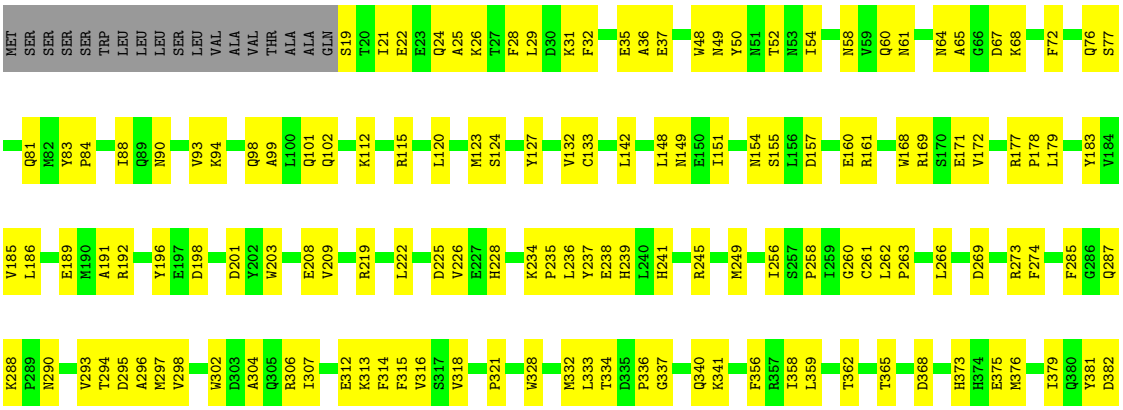
• Molecule 2: Angiotensin-converting enzyme 2

Chain E:



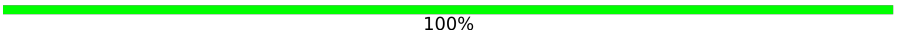
• Molecule 2: Angiotensin-converting enzyme 2

Chain F:



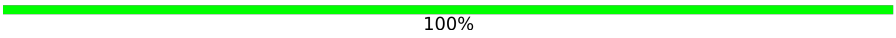
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



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

Chain I:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74518	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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	0.28	0/7952	0.50	0/10818
1	B	0.28	0/7950	0.49	0/10817
1	C	0.28	0/7941	0.50	1/10805 (0.0%)
2	D	0.24	0/4999	0.46	0/6792
2	E	0.25	0/4999	0.47	0/6792
2	F	0.30	1/4999 (0.0%)	0.51	3/6792 (0.0%)
All	All	0.28	1/38840 (0.0%)	0.49	4/52816 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	321	PRO	CG-CD	-11.73	1.11	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	321	PRO	N-CD-CG	-14.40	81.59	103.20
2	F	321	PRO	CA-N-CD	-7.80	100.58	111.50
2	F	321	PRO	CA-CB-CG	-7.35	90.04	104.00
1	C	492	LEU	CA-CB-CG	6.67	130.65	115.30

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	7773	0	7598	162	0
1	B	7770	0	7596	158	0
1	C	7761	0	7586	173	0
2	D	4862	0	4639	169	0
2	E	4862	0	4639	193	0
2	F	4862	0	4639	166	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	1	0
4	A	154	0	143	2	0
4	B	154	0	143	0	0
4	C	196	0	182	5	0
4	D	70	0	65	1	0
4	E	70	0	65	3	0
4	F	70	0	65	3	0
All	All	38688	0	37435	997	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 13.

All (997) 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:215:ASP:N	1:B:266:TYR:HH	1.66	0.93
1:A:400:PHE:O	1:A:510:VAL:HB	1.75	0.86
1:A:330:PRO:HD3	1:A:544:ASN:HD21	1.37	0.86
1:B:190:ARG:HD2	1:B:207:HIS:HD2	1.41	0.85
1:A:1093:GLY:HA3	1:A:1105:THR:O	1.77	0.83
1:A:226:LEU:HG	1:A:227:VAL:HG23	1.60	0.81
2:E:482:ARG:HH21	2:E:610:TRP:HB2	1.45	0.80
2:D:75:GLU:HG3	2:D:79:LEU:HD12	1.64	0.79
1:A:402:ILE:HG13	1:A:403:ARG:H	1.47	0.79
1:C:65:PHE:HB3	1:C:265:TYR:HD2	1.46	0.79
2:D:297:MET:HB3	2:D:302:TRP:HB2	1.65	0.78
2:F:54:ILE:HB	2:F:341:LYS:HB3	1.64	0.77
1:C:763:LEU:HD13	1:C:1004:LEU:HD22	1.66	0.77
2:E:200:GLY:HA2	2:E:203:TRP:HE3	1.49	0.77
1:B:474:GLN:NE2	1:B:476:GLY:O	2.18	0.77
2:F:302:TRP:HB3	2:F:307:ILE:HG13	1.67	0.77
1:B:350:VAL:HA	1:B:400:PHE:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PHE:HE1	1:C:170:TYR:HB2	1.53	0.73
2:D:230:PHE:HA	2:D:233:ILE:HB	1.70	0.72
2:E:237:TYR:HE1	2:E:448:GLY:HA2	1.54	0.72
2:F:356:PHE:HB3	2:F:379:ILE:HD12	1.71	0.72
2:D:356:PHE:HB3	2:D:379:ILE:HD11	1.72	0.72
1:B:393:THR:HG22	1:B:517:LEU:HA	1.72	0.71
2:D:472:GLN:HA	2:D:475:LYS:HG2	1.71	0.71
2:E:233:ILE:HD11	2:E:584:LEU:HD22	1.73	0.71
2:F:416:LYS:HD3	2:F:542:CYS:HA	1.73	0.71
2:D:396:ALA:HA	2:D:562:LYS:HG3	1.73	0.70
2:E:436:ILE:HG13	4:E:702:NAG:H62	1.72	0.70
2:E:126:ILE:HD12	2:E:176:LEU:HG	1.73	0.69
2:E:242:ALA:HB2	2:E:605:GLY:H	1.57	0.69
2:F:132:VAL:HB	2:F:142:LEU:H	1.56	0.69
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.75	0.69
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.57	0.69
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.74	0.69
1:A:120:VAL:HG11	1:A:129:LYS:HE3	1.74	0.68
1:A:456:PHE:HZ	2:D:31:LYS:HD2	1.59	0.68
1:B:327:VAL:HG13	1:B:542:ASN:HB3	1.76	0.68
1:B:131:CYS:HA	1:B:167:THR:H	1.58	0.68
1:B:376:ALA:HB3	1:B:435:ALA:HB3	1.73	0.68
1:B:353:TRP:O	1:B:466:ARG:NH1	2.27	0.68
2:D:161:ARG:NH1	2:D:252:TYR:OH	2.26	0.68
2:F:52:THR:O	2:F:340:GLN:NE2	2.27	0.68
1:A:1106:GLN:HE21	1:A:1109:PHE:HB3	1.58	0.68
1:B:115:GLN:NE2	1:B:164:ASN:O	2.27	0.68
2:D:37:GLU:HB2	2:D:390:PHE:HB2	1.74	0.68
2:D:294:THR:HG23	2:D:365:THR:HA	1.76	0.68
1:C:350:VAL:HG23	1:C:400:PHE:HB2	1.73	0.67
1:A:335:LEU:HD12	1:A:364:ASP:HB2	1.75	0.67
2:D:573:VAL:HG13	2:D:574:VAL:HG23	1.74	0.67
1:B:885:GLY:HA2	1:B:901:GLN:NE2	2.10	0.67
2:F:565:PRO:HG2	2:F:568:LEU:HB2	1.77	0.67
1:C:197:ILE:HG13	1:C:198:ASP:H	1.60	0.67
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	1.75	0.67
2:E:204:ARG:HG2	2:E:222:LEU:HD21	1.76	0.67
2:F:101:GLN:NE2	2:F:102:GLN:OE1	2.28	0.67
2:F:358:ILE:HD11	2:F:376:MET:HB3	1.76	0.67
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.28	0.66
2:E:237:TYR:CE1	2:E:448:GLY:HA2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:58:ASN:O	2:F:61:ASN:HB2	1.95	0.66
2:F:404:VAL:HA	2:F:407:ILE:HG12	1.78	0.66
1:C:421:TYR:HB3	1:C:454:ARG:HB3	1.77	0.65
2:F:394:ASN:OD1	2:F:401:HIS:ND1	2.29	0.65
1:B:210:ILE:HG21	1:B:217:PRO:HG2	1.77	0.65
2:D:457:GLU:HG2	2:D:513:ILE:HB	1.76	0.65
2:E:232:GLU:HB3	2:E:581:VAL:HG11	1.78	0.65
2:E:243:TYR:HB2	2:E:599:ASN:HD21	1.61	0.65
1:B:808:ASP:HB3	1:B:811:LYS:HD2	1.77	0.65
1:C:454:ARG:HA	1:C:492:LEU:HA	1.77	0.65
2:E:204:ARG:HD3	2:E:219:ARG:HG2	1.79	0.65
1:B:358:ILE:HB	1:B:395:VAL:HB	1.79	0.64
2:D:365:THR:HB	2:D:368:ASP:HB2	1.78	0.64
2:F:451:PRO:HA	2:F:454:TYR:HB3	1.77	0.64
1:A:420:ASP:OD1	1:A:460:ASN:ND2	2.31	0.64
2:F:482:ARG:HB3	2:F:608:THR:HB	1.79	0.64
1:A:405:ASN:H	1:A:504:GLY:HA2	1.63	0.64
1:C:130:VAL:HG21	1:C:231:ILE:HG21	1.80	0.64
1:B:356:LYS:HB3	1:B:397:ALA:HB3	1.79	0.64
1:C:1116:THR:HG22	1:C:1138:TYR:HB3	1.80	0.64
2:E:108:LEU:HD13	2:E:116:LEU:HD22	1.79	0.64
2:F:312:GLU:HA	2:F:315:PHE:HB2	1.79	0.64
2:E:538:PRO:HG2	2:E:541:LYS:HB2	1.78	0.64
2:F:269:ASP:HB2	2:F:274:PHE:H	1.62	0.64
2:E:381:TYR:HB2	2:E:404:VAL:HG11	1.78	0.64
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.30	0.63
4:A:1306:NAG:H4	1:C:794:ILE:HG21	1.79	0.63
1:C:345:THR:O	1:C:509:ARG:NH2	2.30	0.63
2:E:209:VAL:H	2:E:217:TYR:HB3	1.64	0.63
2:E:85:LEU:HD12	2:E:97:LEU:HB2	1.80	0.63
2:E:275:TRP:HB2	2:E:444:LEU:HD22	1.79	0.63
2:D:109:SER:HB2	2:D:112:LYS:HE2	1.81	0.63
1:C:117:LEU:HD21	1:C:119:ILE:HG13	1.79	0.63
2:E:485:VAL:HG13	2:E:487:VAL:H	1.63	0.63
1:C:103:GLY:H	1:C:241:LEU:HB2	1.63	0.63
1:A:353:TRP:O	1:A:466:ARG:NH1	2.32	0.63
2:F:529:LEU:HD22	2:F:544:ILE:HG21	1.81	0.63
1:A:198:ASP:OD1	1:A:202:LYS:NZ	2.31	0.63
1:A:577:ARG:HH11	1:A:582:LEU:HD12	1.63	0.63
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.16	0.63
2:D:520:LEU:HG	2:D:581:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASP:O	1:B:448:ASN:ND2	2.32	0.62
1:B:577:ARG:HH11	1:B:582:LEU:HD12	1.63	0.62
2:D:418:LEU:HD22	2:D:423:LEU:HD12	1.79	0.62
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.27	0.62
1:B:438:SER:HB2	1:B:441:LEU:HD13	1.80	0.62
1:B:439:ASN:HA	1:B:507:PRO:HD2	1.81	0.62
2:D:201:ASP:O	2:D:205:GLY:N	2.23	0.62
2:F:236:LEU:HD12	2:F:592:PHE:HB2	1.82	0.62
2:D:229:THR:OG1	2:D:580:ASN:OD1	2.17	0.62
2:F:157:ASP:HB3	2:F:160:GLU:HB2	1.80	0.62
1:B:675:GLN:HG3	1:B:676:THR:HG22	1.82	0.62
2:D:460:ARG:NH2	2:D:509:ASP:OD1	2.32	0.62
2:D:123:MET:HG2	2:D:507:SER:HA	1.82	0.62
1:A:1040:VAL:HG21	1:C:1035:GLY:HA3	1.81	0.62
1:B:190:ARG:HD2	1:B:207:HIS:CD2	2.31	0.62
2:E:119:ILE:O	2:E:123:MET:HG2	2.00	0.62
1:B:961:THR:O	1:B:965:GLN:HG2	2.00	0.62
1:C:432:CYS:H	1:C:513:LEU:HB2	1.64	0.62
2:D:571:GLU:HB2	2:D:577:LYS:NZ	2.15	0.62
1:A:233:ILE:HG22	1:A:234:ASN:H	1.64	0.61
1:C:393:THR:HG23	1:C:517:LEU:HD12	1.81	0.61
1:B:339:ASP:HB3	1:B:368:LEU:HD11	1.82	0.61
2:F:234:LYS:O	2:F:238:GLU:HB3	2.00	0.61
1:A:454:ARG:NH1	1:A:469:SER:OG	2.33	0.61
1:A:752:LEU:HD23	1:A:997:ILE:HD12	1.81	0.61
2:E:261:CYS:SG	2:E:482:ARG:NH2	2.74	0.61
2:E:488:VAL:HG21	2:E:610:TRP:HB3	1.83	0.61
2:F:454:TYR:HE2	2:F:484:ILE:HG13	1.66	0.61
2:E:108:LEU:HD23	2:E:112:LYS:HB3	1.83	0.61
2:F:373:HIS:HB2	2:F:409:SER:HA	1.82	0.60
2:F:356:PHE:HB2	2:F:379:ILE:HG23	1.82	0.60
2:F:446:ILE:HD12	2:F:523:PHE:HZ	1.66	0.60
1:A:128:ILE:HD13	1:A:170:TYR:HD2	1.66	0.60
2:D:66:GLY:HA2	2:D:69:TRP:HB3	1.82	0.60
1:A:903:ALA:HB1	1:A:913:GLN:HB2	1.84	0.60
1:B:164:ASN:HD21	1:C:357:ARG:HH12	1.50	0.60
2:E:597:ASP:OD1	2:E:598:GLN:N	2.34	0.60
1:B:271:GLN:OE1	1:B:272:PRO:HD2	2.01	0.60
1:C:493[A]:ARG:NH2	1:C:494:SER:O	2.33	0.60
2:E:261:CYS:SG	2:E:606:TRP:HB2	2.41	0.60
1:B:357:ARG:NH1	1:B:394:ASN:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ASN:HD22	1:A:506:GLN:HB3	1.66	0.60
1:B:27:SER:HB3	1:B:64:TRP:HB3	1.82	0.60
1:C:616:ASN:OD1	1:C:617:CYS:N	2.34	0.60
1:A:42:VAL:O	1:B:563:GLN:NE2	2.34	0.60
1:C:543:PHE:O	1:C:546:LEU:HD23	2.02	0.60
2:D:403:ALA:HB2	2:D:518:ARG:HB2	1.84	0.60
2:F:168:TRP:O	2:F:172:VAL:HG12	2.02	0.60
1:A:115:GLN:HA	1:A:132:GLU:HG2	1.84	0.59
1:B:546:LEU:HD22	1:B:565:PHE:HE2	1.65	0.59
2:E:244:VAL:O	2:E:248:LEU:HB2	2.02	0.59
2:E:413:ALA:HB1	2:E:438:PHE:HE2	1.67	0.59
2:D:142:LEU:HD21	2:D:164:ALA:HA	1.84	0.59
2:D:209:VAL:HB	2:D:217:TYR:HB3	1.83	0.59
2:F:37:GLU:OE1	2:F:393:ARG:NH1	2.35	0.59
2:D:174:LYS:HB3	2:D:497:TYR:HA	1.84	0.59
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.84	0.59
2:E:49:ASN:O	2:E:58:ASN:ND2	2.35	0.59
2:D:237:TYR:CE2	2:D:451:PRO:HD3	2.37	0.59
1:A:357:ARG:NH1	1:A:359:SER:OG	2.36	0.59
2:E:505:HIS:HB3	2:E:512:PHE:HZ	1.67	0.59
1:C:403:ARG:HB3	1:C:406:GLU:HG2	1.85	0.58
2:E:385:TYR:HB3	2:E:559:ARG:HA	1.85	0.58
1:C:65:PHE:HB3	1:C:265:TYR:CD2	2.35	0.58
2:D:44:SER:HB3	2:D:48:TRP:HZ3	1.67	0.58
2:D:144:LEU:HD11	2:D:271:TRP:HZ2	1.68	0.58
2:D:31:LYS:NZ	2:D:35:GLU:OE2	2.32	0.58
2:F:60:GLN:HE21	2:F:64:ASN:HD22	1.51	0.58
2:D:339:VAL:HG23	2:D:340:GLN:HG3	1.85	0.58
2:F:312:GLU:HB3	2:F:316:VAL:HG23	1.84	0.58
2:F:460:ARG:NH2	2:F:506:VAL:O	2.37	0.58
1:C:358:ILE:HB	1:C:395:VAL:HB	1.85	0.58
1:A:447:GLY:O	1:A:497:PHE:N	2.37	0.58
2:E:191:ALA:HB1	2:E:196:TYR:HB2	1.85	0.58
1:C:344:ALA:HB3	1:C:436:TRP:HZ2	1.69	0.58
1:C:399:SER:HA	1:C:510:VAL:O	2.03	0.58
2:E:200:GLY:HA2	2:E:203:TRP:CE3	2.35	0.58
2:E:239:HIS:CD2	2:E:599:ASN:HD22	2.21	0.58
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.19	0.57
1:C:125:ASN:HD22	4:C:1302:NAG:H5	1.68	0.57
2:D:508:ASN:HB2	2:D:510:TYR:CE2	2.39	0.57
2:F:382:ASP:OD1	2:F:401:HIS:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.68	0.57
2:D:204:ARG:HG3	2:D:219:ARG:HD2	1.87	0.57
2:F:22:GLU:HG3	2:F:88:ILE:HG13	1.86	0.57
1:C:784:GLN:HG3	1:C:1029:MET:HG2	1.86	0.57
1:C:959:LEU:O	1:C:963:VAL:HG23	2.05	0.57
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.36	0.57
2:D:177:ARG:NH2	2:D:495:GLU:O	2.37	0.57
1:B:133:PHE:HD2	1:B:134:GLN:HG2	1.68	0.57
2:E:394:ASN:HB2	2:E:562:LYS:HE3	1.85	0.57
2:F:238:GLU:HG2	2:F:604:VAL:HG12	1.86	0.57
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.69	0.57
2:D:528:ALA:HB2	2:D:574:VAL:HG22	1.86	0.57
1:C:490:PHE:O	1:C:493[B]:ARG:NH2	2.37	0.57
2:F:132:VAL:HG21	2:F:142:LEU:HB2	1.87	0.57
2:F:196:TYR:HB3	2:F:201:ASP:HB3	1.87	0.57
1:B:543:PHE:O	1:B:546:LEU:HD23	2.05	0.57
1:B:1098:ASN:OD1	1:B:1101:HIS:N	2.29	0.57
2:D:372:ALA:O	2:D:376:MET:HG3	2.04	0.57
2:E:229:THR:HG21	2:E:520:LEU:HD21	1.87	0.57
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.38	0.57
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.87	0.57
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.87	0.57
1:B:435:ALA:HB1	1:B:508:TYR:HE1	1.70	0.57
4:E:703:NAG:H3	4:E:703:NAG:H83	1.87	0.57
1:C:386:LYS:O	1:C:390:LEU:N	2.38	0.56
1:C:388:ASN:HA	1:C:527:PRO:HD2	1.87	0.56
2:D:264:ALA:HB3	2:D:490:PRO:HD3	1.85	0.56
2:E:565:PRO:HD2	2:E:568:LEU:HD23	1.87	0.56
1:A:530:SER:OG	1:A:580:GLN:NE2	2.38	0.56
2:F:385:TYR:HB3	2:F:559:ARG:HA	1.86	0.56
1:A:108:THR:O	1:A:237:ARG:NH1	2.36	0.56
1:B:716:THR:OG1	1:B:1071:GLN:O	2.21	0.56
1:C:328:ARG:NH1	1:C:578:ASP:OD1	2.38	0.56
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.38	0.56
2:D:150:GLU:HA	2:D:154:ASN:HD22	1.69	0.56
1:A:317:ASN:ND2	1:C:737:ASP:OD1	2.38	0.56
1:B:48:LEU:HB3	1:B:276:LEU:HD21	1.87	0.56
1:C:426:PRO:HB3	1:C:463:PRO:HB3	1.88	0.56
2:F:65:ALA:HA	2:F:68:LYS:HE2	1.87	0.56
2:F:249:MET:HA	2:F:256:ILE:HG13	1.87	0.56
2:F:328:TRP:NE1	4:F:701:NAG:O7	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASP:OD2	1:B:448:ASN:ND2	2.34	0.56
1:B:763:LEU:HD13	1:B:1004:LEU:HD22	1.86	0.56
1:C:378:LYS:HB3	1:C:433:VAL:HB	1.87	0.56
1:C:475:ALA:O	2:F:19:SER:N	2.39	0.56
2:D:508:ASN:HB2	2:D:510:TYR:HE2	1.69	0.56
1:C:659:SER:HB3	1:C:698:SER:HB2	1.88	0.56
2:E:227:GLU:OE2	2:E:454:TYR:OH	2.24	0.56
2:E:267:LEU:HD12	2:E:269:ASP:H	1.71	0.56
2:E:598:GLN:NE2	2:E:599:ASN:OD1	2.39	0.56
2:D:444:LEU:HA	2:D:448:GLY:HA3	1.88	0.56
4:D:703:NAG:H83	4:D:703:NAG:H3	1.87	0.56
2:D:332:MET:HB3	2:D:359:LEU:HG	1.87	0.56
2:E:297:MET:HB2	2:E:302:TRP:HB3	1.88	0.56
2:F:455:MET:HE1	2:F:481:LYS:HG2	1.88	0.56
1:B:760:CYS:HA	1:B:763:LEU:HD12	1.88	0.55
1:C:366:SER:HB3	1:C:387:LEU:HD22	1.87	0.55
1:C:751:ASN:O	1:C:754:LEU:HG	2.05	0.55
1:A:167:THR:HG23	1:B:357:ARG:HH21	1.70	0.55
1:B:784:GLN:HG3	1:B:1029:MET:HG2	1.88	0.55
2:D:592:PHE:HA	2:D:595:LEU:HB2	1.86	0.55
2:E:351:LEU:HB2	2:E:355:ASP:HB3	1.88	0.55
1:A:168:PHE:CE2	1:A:170:TYR:HB2	2.41	0.55
1:A:454:ARG:NE	1:A:456:PHE:O	2.37	0.55
1:B:914:ASN:ND2	1:C:1123:SER:OG	2.39	0.55
1:C:351:TYR:HB2	1:C:454:ARG:HB2	1.88	0.55
1:C:720:ILE:HG13	1:C:923:ILE:HG23	1.87	0.55
2:D:46:ALA:HB1	2:D:61:ASN:HB3	1.88	0.55
2:F:304:ALA:HB2	2:F:362:THR:H	1.71	0.55
2:E:256:ILE:HD11	2:E:266:LEU:HG	1.87	0.55
1:B:403:ARG:HG2	1:B:406:GLU:HB2	1.89	0.55
4:C:1306:NAG:H83	4:C:1306:NAG:H3	1.89	0.55
1:A:776:LYS:O	1:A:780:GLU:HG2	2.06	0.55
2:F:333:LEU:HG	2:F:334:THR:HG23	1.89	0.55
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.42	0.55
1:B:89:GLY:HA3	1:B:270:LEU:HD12	1.87	0.55
1:B:112:SER:HA	1:B:133:PHE:CD2	2.41	0.55
1:A:281:GLU:OE2	4:A:1303:NAG:O3	2.19	0.55
1:B:493[A]:ARG:HD3	2:E:34:HIS:HB3	1.88	0.55
1:B:982:SER:OG	1:B:983:ARG:NH1	2.35	0.55
2:D:29:LEU:HD21	2:D:100:LEU:HD22	1.88	0.55
2:F:375:GLU:O	2:F:379:ILE:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLN:H	1:A:161:SER:HB3	1.71	0.55
2:E:284:PRO:HD3	2:E:440:LEU:HD13	1.88	0.55
2:D:163:TRP:O	2:D:167:SER:OG	2.24	0.54
2:E:549:GLU:OE2	2:E:553:LYS:NZ	2.40	0.54
1:B:869:MET:HG2	1:C:699:LEU:HD21	1.88	0.54
1:C:128:ILE:HG21	1:C:229:LEU:HD21	1.89	0.54
1:C:365:TYR:HD2	1:C:387:LEU:HA	1.72	0.54
2:D:236:LEU:HD11	2:D:592:PHE:CD1	2.42	0.54
2:D:460:ARG:HH22	2:D:509:ASP:HA	1.72	0.54
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.90	0.54
2:D:159:ASN:HA	2:D:162:LEU:HD12	1.88	0.54
2:D:410:LEU:HD11	2:D:526:GLN:HG2	1.90	0.54
1:A:983:ARG:HG2	1:A:984:LEU:HD22	1.88	0.54
1:B:618:THR:OG1	1:B:619:GLU:OE1	2.26	0.54
2:F:373:HIS:HA	2:F:376:MET:HG2	1.88	0.54
1:C:210:ILE:HG22	1:C:217:PRO:HG3	1.89	0.54
2:E:315:PHE:HD1	2:E:320:LEU:HD12	1.73	0.54
2:F:392:LEU:HB3	2:F:562:LYS:HB2	1.88	0.54
1:A:422:ASN:HD21	1:A:453:TYR:HD2	1.55	0.54
1:A:743:CYS:HB2	1:A:977:LEU:HD12	1.90	0.54
2:F:467:GLU:OE2	2:F:468:ILE:HG12	2.08	0.54
1:B:348:ALA:HB1	1:B:353:TRP:HA	1.90	0.54
1:A:327:VAL:HB	1:A:531:THR:HG23	1.89	0.54
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	1.89	0.54
2:D:25:ALA:HA	2:D:29:LEU:HB2	1.90	0.54
1:A:350:VAL:HG21	1:A:418:ILE:HD12	1.88	0.54
1:B:303:LEU:HD22	1:B:308:VAL:HG12	1.89	0.54
1:B:930:ALA:O	1:B:934:ILE:HG12	2.08	0.54
2:E:457:GLU:HG3	2:E:512:PHE:HB2	1.90	0.54
1:A:374:PHE:CD1	1:A:436:TRP:HB3	2.43	0.53
1:B:739:THR:O	1:B:744:GLY:N	2.41	0.53
1:C:457:ARG:NH1	1:C:460:ASN:O	2.40	0.53
1:A:314:GLN:OE1	1:A:613:GLN:NE2	2.38	0.53
1:B:559:PHE:HB2	1:B:577:ARG:HH21	1.74	0.53
1:B:1141:LEU:HD23	1:B:1145:LEU:HD23	1.89	0.53
1:C:92:PHE:HZ	1:C:101:ILE:HG21	1.73	0.53
2:F:149:ASN:O	2:F:154:ASN:N	2.41	0.53
2:F:553:LYS:HG3	2:F:554:LEU:HD12	1.89	0.53
2:F:313:LYS:HE3	3:I:1:NAG:HN2	1.74	0.53
1:A:96:GLU:HG2	1:A:99:ASN:H	1.74	0.53
1:B:299:THR:OG1	1:B:597:VAL:HG21	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:HG12	1:C:202:LYS:HZ1	1.73	0.53
2:F:155:SER:HB3	2:F:161:ARG:HG3	1.89	0.53
1:A:326:ILE:HD11	1:A:534:VAL:HG12	1.90	0.53
1:A:960:ASN:O	1:A:964:LYS:HG2	2.09	0.53
1:C:930:ALA:O	1:C:934:ILE:HG12	2.09	0.53
2:F:101:GLN:HB2	4:F:703:NAG:H81	1.91	0.53
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.23	0.53
2:D:435:GLU:HG2	2:D:540:HIS:ND1	2.23	0.53
2:E:90:ASN:HB3	2:E:93:VAL:HG22	1.89	0.53
2:E:472:GLN:HA	2:E:475:LYS:HE2	1.91	0.53
1:A:487:ASN:ND2	2:D:24:GLN:OE1	2.41	0.53
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.91	0.53
2:D:267:LEU:HA	2:D:278:LEU:HD11	1.91	0.53
2:E:32:PHE:HE2	2:E:80:ALA:HB2	1.72	0.53
2:E:288:LYS:H	2:E:433:GLU:HG2	1.73	0.53
2:E:330:ASN:HB3	2:E:357:ARG:HE	1.73	0.53
2:E:503:LEU:HD23	2:E:505:HIS:H	1.74	0.53
2:E:591:LEU:HG	2:E:595:LEU:HG	1.91	0.53
1:A:34:ARG:HH21	1:A:217:PRO:HG2	1.74	0.53
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.41	0.53
2:D:392:LEU:HA	2:D:562:LYS:HD3	1.90	0.53
2:D:105:SER:HB2	2:D:108:LEU:HD22	1.91	0.53
2:E:357:ARG:HG2	2:E:358:ILE:H	1.73	0.53
1:A:1023:ASN:O	1:A:1027:THR:HG23	2.09	0.52
1:B:758:SER:HB3	1:C:964:LYS:NZ	2.24	0.52
1:C:433:VAL:HA	1:C:512:VAL:HG23	1.90	0.52
2:D:482:ARG:HG2	2:D:488:VAL:HG23	1.92	0.52
2:F:222:LEU:O	2:F:226:VAL:HG23	2.09	0.52
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.92	0.52
2:D:44:SER:HB3	2:D:48:TRP:CZ3	2.43	0.52
1:B:194:PHE:HD1	1:B:203:ILE:HG12	1.74	0.52
2:D:116:LEU:HD12	2:D:186:LEU:HB3	1.92	0.52
2:D:400:PHE:CZ	2:D:566:TRP:HB2	2.44	0.52
2:F:421:ILE:HG13	2:F:423:LEU:HG	1.91	0.52
2:D:557:MET:HG3	2:D:569:ALA:HB1	1.92	0.52
2:F:287:GLN:HG2	2:F:288:LYS:HG2	1.91	0.52
1:B:296:LEU:O	1:B:300:LYS:HG2	2.10	0.52
1:B:894:LEU:HD13	1:C:715:PRO:HD3	1.91	0.52
1:C:718:PHE:HE2	1:C:923:ILE:HG12	1.73	0.52
2:F:450:LEU:HB2	2:F:519:THR:HG21	1.91	0.52
1:A:349:SER:HB2	1:A:352:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.92	0.52
2:D:443:ALA:O	2:D:448:GLY:N	2.42	0.52
2:E:308:PHE:HB3	2:E:333:LEU:HD13	1.91	0.52
2:E:463:VAL:HA	2:E:468:ILE:HB	1.90	0.52
1:A:53:ASP:OD1	1:A:54:LEU:N	2.35	0.52
1:B:328:ARG:HH11	1:B:533:LEU:HB3	1.74	0.52
2:E:75:GLU:HA	2:E:78:THR:HG22	1.90	0.52
2:E:535:HIS:NE2	2:E:538:PRO:O	2.39	0.52
1:A:745:ASP:N	1:A:745:ASP:OD1	2.43	0.52
1:A:879:ALA:O	1:A:883:THR:OG1	2.21	0.52
1:C:896:ILE:HD11	1:C:900:MET:HE2	1.91	0.52
2:E:167:SER:O	2:E:171:GLU:HG3	2.10	0.52
2:F:263:PRO:HD2	2:F:266:LEU:HD22	1.92	0.52
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.92	0.52
2:D:407:ILE:O	2:D:526:GLN:NE2	2.42	0.52
2:E:161:ARG:HH11	2:E:252:TYR:HE2	1.58	0.52
2:E:456:LEU:HD21	2:E:506:VAL:HB	1.93	0.52
2:F:185:VAL:HG12	2:F:186:LEU:HD23	1.92	0.52
1:C:234:ASN:HB3	4:C:1303:NAG:H83	1.92	0.51
2:F:392:LEU:HA	2:F:562:LYS:HD3	1.93	0.51
2:F:433:GLU:O	2:F:437:ASN:N	2.34	0.51
1:A:612:TYR:HB2	1:A:649:CYS:SG	2.50	0.51
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.28	0.51
1:B:985:ASP:OD1	1:B:986:PRO:HD2	2.10	0.51
1:C:168:PHE:CE1	1:C:170:TYR:HB2	2.39	0.51
1:C:612:TYR:HB2	1:C:649:CYS:SG	2.50	0.51
2:E:524:GLN:HG3	2:E:574:VAL:HG11	1.92	0.51
2:F:50:TYR:HA	2:F:58:ASN:HB3	1.92	0.51
2:E:85:LEU:O	2:E:89:GLN:NE2	2.44	0.51
2:F:588:PHE:O	2:F:592:PHE:N	2.32	0.51
2:D:146:PRO:O	2:D:149:ASN:ND2	2.44	0.51
2:E:122:THR:HB	2:E:179:LEU:HD13	1.91	0.51
2:F:295:ASP:O	2:F:298:VAL:HB	2.09	0.51
1:A:323:THR:OG1	1:A:324:GLU:OE1	2.18	0.51
1:B:645:THR:HG23	1:B:670:ILE:HG13	1.93	0.51
2:D:432:ASN:OD1	2:D:433:GLU:N	2.44	0.51
2:F:290:ASN:HA	2:F:434:THR:HG23	1.93	0.51
2:F:389:PRO:HG2	2:F:392:LEU:HD12	1.92	0.51
1:A:417:ASN:HA	1:A:421:TYR:CZ	2.46	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.93	0.51
1:C:107:GLY:H	1:C:235:ILE:HG23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ASP:HB3	1:C:507:PRO:HG2	1.93	0.51
2:D:459:TRP:HB2	2:D:480:MET:HE1	1.91	0.51
2:E:180:TYR:HB3	2:E:498:CYS:SG	2.50	0.51
2:E:212:VAL:HG23	2:E:215:TYR:HB2	1.91	0.51
2:F:396:ALA:HB1	2:F:566:TRP:HB2	1.92	0.51
1:A:122:ASN:OD1	1:A:123:ALA:N	2.44	0.51
1:B:317:ASN:O	1:B:319:ARG:NH1	2.44	0.51
1:B:361:CYS:H	1:B:524:VAL:HG22	1.75	0.51
1:C:220:PHE:HE2	1:C:285:ILE:HG22	1.75	0.51
2:D:407:ILE:HG21	2:D:525:PHE:HB2	1.92	0.51
2:D:553:LYS:HG2	2:D:573:VAL:HG23	1.93	0.51
2:E:564:GLU:HB3	2:E:569:ALA:HB2	1.93	0.51
2:F:177:ARG:HH22	2:F:501:ALA:HB3	1.75	0.51
1:A:36:VAL:HG11	1:A:220:PHE:CZ	2.46	0.50
1:A:444:LYS:N	1:A:448:ASN:OD1	2.45	0.50
1:C:736:VAL:HG21	1:C:1004:LEU:HD11	1.92	0.50
2:D:285:PHE:HZ	2:D:436:ILE:HB	1.75	0.50
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.45	0.50
2:E:155:SER:OG	2:E:157:ASP:OD1	2.28	0.50
2:E:377:GLY:HA2	2:E:408:MET:SD	2.50	0.50
2:E:382:ASP:HA	2:E:385:TYR:CE2	2.46	0.50
1:B:642:VAL:HG12	1:B:651:ILE:HG12	1.93	0.50
1:C:822:LEU:HD23	1:C:945:LEU:HD13	1.94	0.50
2:D:127:TYR:CE2	2:D:504:PHE:HB2	2.46	0.50
2:E:177:ARG:NH1	2:E:495:GLU:O	2.42	0.50
2:E:450:LEU:HD11	2:E:519:THR:HG21	1.93	0.50
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.42	0.50
2:E:199:TYR:HD2	2:E:203:TRP:CZ3	2.29	0.50
2:F:398:GLU:HB3	2:F:514:ARG:HB2	1.93	0.50
2:D:365:THR:HG22	2:D:367:ASP:N	2.27	0.50
2:E:257:SER:HB3	2:E:260:GLY:HA3	1.93	0.50
2:E:416:LYS:HE3	2:E:543:ASP:HB2	1.93	0.50
2:E:460:ARG:NH1	2:E:506:VAL:O	2.45	0.50
2:F:241:HIS:CE1	2:F:245:ARG:HH21	2.30	0.50
1:A:203:ILE:HB	1:A:227:VAL:HB	1.92	0.50
2:D:527:GLU:HG2	2:D:583:PRO:HG3	1.94	0.50
2:E:184:VAL:HG22	2:E:464:PHE:HE1	1.77	0.50
1:A:402:ILE:HG13	1:A:403:ARG:N	2.23	0.50
2:D:110:GLU:HA	2:D:113:SER:HB3	1.94	0.50
2:D:365:THR:HG22	2:D:367:ASP:H	1.76	0.50
2:D:370:LEU:HD12	2:D:409:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:589:GLU:HA	2:D:592:PHE:CE1	2.47	0.50
2:E:177:ARG:HA	2:E:498:CYS:SG	2.51	0.50
1:A:27:SER:HB2	1:A:64:TRP:HB3	1.94	0.50
2:F:123:MET:HB3	2:F:179:LEU:HD22	1.93	0.50
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.77	0.49
1:B:215:ASP:N	1:B:266:TYR:OH	2.40	0.49
1:B:220:PHE:HE2	1:B:285:ILE:HG22	1.75	0.49
2:D:85:LEU:HD11	2:D:101:GLN:HB3	1.94	0.49
2:D:190:MET:SD	2:D:194:ASN:ND2	2.77	0.49
2:D:302:TRP:CG	2:D:306:ARG:HG2	2.47	0.49
2:F:416:LYS:HB3	2:F:541:LYS:NZ	2.27	0.49
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.94	0.49
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.45	0.49
2:E:210:ASN:OD1	2:E:211:GLY:N	2.44	0.49
2:E:269:ASP:HB3	2:E:272:GLY:H	1.77	0.49
2:F:332:MET:HG3	2:F:336:PRO:HB3	1.94	0.49
2:D:351:LEU:HD11	2:D:357:ARG:HG2	1.94	0.49
2:E:418:LEU:HA	2:E:423:LEU:HB2	1.94	0.49
1:B:167:THR:HG21	1:B:233:ILE:HD11	1.93	0.49
1:C:879:ALA:O	1:C:883:THR:OG1	2.25	0.49
2:D:327:PHE:CE1	2:D:356:PHE:HB2	2.47	0.49
2:D:418:LEU:HB3	2:D:423:LEU:HB2	1.93	0.49
2:E:132:VAL:HG21	2:E:142:LEU:HD23	1.94	0.49
2:F:48:TRP:HZ3	2:F:359:LEU:HB2	1.78	0.49
2:F:177:ARG:NH2	2:F:498:CYS:SG	2.85	0.49
2:F:439:LEU:HD21	2:F:540:HIS:CG	2.48	0.49
1:C:456:PHE:HB2	1:C:491:PRO:HB3	1.94	0.49
2:D:288:LYS:HG2	2:D:434:THR:HG22	1.94	0.49
2:E:199:TYR:HD2	2:E:203:TRP:CH2	2.31	0.49
2:F:191:ALA:HB1	2:F:196:TYR:HB2	1.95	0.49
1:B:164:ASN:ND2	1:C:357:ARG:HH12	2.10	0.49
1:C:992:GLN:NE2	1:C:995:ARG:HH21	2.10	0.49
2:E:148:LEU:HD22	2:E:168:TRP:HZ2	1.77	0.49
2:E:504:PHE:O	2:E:508:ASN:ND2	2.44	0.49
2:F:98:GLN:HE22	2:F:209:VAL:HG22	1.77	0.49
1:A:462:LYS:O	1:A:465:GLU:HG2	2.12	0.49
1:A:577:ARG:NH1	1:A:582:LEU:HD12	2.27	0.49
1:A:856:ASN:HD22	1:A:966:LEU:HD12	1.77	0.49
1:B:336:CYS:SG	1:B:361:CYS:HB2	2.52	0.49
1:C:34:ARG:NH2	1:C:191:GLU:OE2	2.46	0.49
2:E:95:LEU:HA	2:E:98:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:ARG:HH12	2:E:197:GLU:HG3	1.77	0.49
2:E:324:THR:HG22	2:E:326:GLY:H	1.77	0.49
1:A:395:VAL:HG22	1:A:515:PHE:CD1	2.47	0.49
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.47	0.49
1:A:644:GLN:NE2	1:A:648:GLY:O	2.45	0.49
1:C:826:VAL:O	1:C:949:GLN:NE2	2.41	0.49
2:E:304:ALA:HA	2:E:307:ILE:HG22	1.95	0.49
2:F:25:ALA:HA	2:F:28:PHE:CE1	2.48	0.49
2:F:169:ARG:HH22	2:F:478:TRP:HH2	1.61	0.49
2:F:433:GLU:OE2	2:F:594:TRP:NE1	2.46	0.49
1:A:107:GLY:H	1:A:235:ILE:HG23	1.78	0.49
1:A:395:VAL:HG23	1:A:524:VAL:HG21	1.94	0.49
2:E:388:GLN:HB3	2:E:392:LEU:HB2	1.95	0.49
2:F:235:PRO:O	2:F:239:HIS:ND1	2.35	0.49
1:A:451:TYR:HB2	1:A:495:TYR:HB2	1.94	0.49
1:B:53:ASP:OD1	1:B:195:LYS:NZ	2.45	0.49
1:B:108:THR:HA	1:B:236:THR:HB	1.95	0.49
1:C:310:LYS:NZ	1:C:663:ASP:OD1	2.41	0.49
2:E:263:PRO:HD2	2:E:266:LEU:HD23	1.95	0.49
2:E:381:TYR:HD1	2:E:558:LEU:HD22	1.78	0.49
2:F:226:VAL:HG21	2:F:461:TRP:HZ3	1.78	0.49
2:E:364:VAL:O	2:E:365:THR:OG1	2.26	0.48
2:F:403:ALA:O	2:F:407:ILE:HG23	2.13	0.48
1:B:118:LEU:HB3	1:B:129:LYS:O	2.13	0.48
2:D:392:LEU:HG	2:D:562:LYS:HB3	1.95	0.48
2:E:115:ARG:NH1	2:E:118:THR:OG1	2.46	0.48
1:A:436:TRP:CE2	1:A:509:ARG:HG3	2.48	0.48
1:B:30:ASN:HD21	1:B:59:PHE:HD1	1.61	0.48
1:B:600:PRO:HB3	1:B:674:TYR:HB2	1.95	0.48
1:C:366:SER:H	1:C:387:LEU:HD13	1.78	0.48
1:C:551:VAL:HB	1:C:588:THR:HB	1.93	0.48
2:D:382:ASP:HA	2:D:385:TYR:CZ	2.48	0.48
2:E:170:SER:HA	2:E:497:TYR:HE2	1.78	0.48
2:E:366:MET:HA	2:E:369:PHE:HB3	1.94	0.48
2:F:32:PHE:HA	2:F:35:GLU:HG2	1.95	0.48
2:F:416:LYS:HB3	2:F:541:LYS:HZ2	1.77	0.48
1:B:196:ASN:HD22	1:B:235:ILE:HG12	1.79	0.48
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.13	0.48
2:D:528:ALA:O	2:D:553:LYS:NZ	2.38	0.48
1:C:337:PRO:HG2	1:C:358:ILE:HG12	1.95	0.48
2:D:553:LYS:HE3	2:D:573:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:403:ALA:O	2:E:407:ILE:HG23	2.12	0.48
1:C:1106:GLN:NE2	1:C:1109:PHE:HB3	2.28	0.48
2:D:129:THR:O	2:D:131:LYS:NZ	2.47	0.48
2:E:180:TYR:HA	2:E:183:TYR:CD2	2.49	0.48
1:A:442:ASP:O	1:A:451:TYR:OH	2.26	0.48
1:B:1081:ILE:HD11	1:B:1137:VAL:HG22	1.95	0.48
1:C:139:PRO:HB2	1:C:241:LEU:HD13	1.95	0.48
1:C:378:LYS:HE2	1:C:380:TYR:HB2	1.96	0.48
2:E:439:LEU:HD23	2:E:588:PHE:HD1	1.77	0.48
2:F:169:ARG:NH1	2:F:499:ASP:OD1	2.47	0.48
2:F:293:VAL:HG12	2:F:423:LEU:HB3	1.96	0.48
1:C:197:ILE:HG13	1:C:198:ASP:N	2.26	0.48
1:C:340:GLU:HG3	1:C:347:PHE:HZ	1.78	0.48
1:C:487:ASN:OD1	2:F:83:TYR:OH	2.32	0.48
2:D:245:ARG:NH2	2:D:605:GLY:O	2.32	0.48
2:E:463:VAL:HG22	2:E:468:ILE:HG21	1.94	0.48
2:F:556:ASN:HA	2:F:559:ARG:HG2	1.95	0.48
1:B:349:SER:HB3	1:B:451:TYR:HA	1.95	0.48
1:B:979:ASP:O	1:B:983:ARG:HB2	2.13	0.48
2:D:48:TRP:HZ2	2:D:349:TRP:HB2	1.79	0.48
2:D:158:TYR:HE1	2:D:263:PRO:HG2	1.77	0.48
2:F:189:GLU:HA	2:F:192:ARG:HB2	1.94	0.48
1:B:34:ARG:HG3	1:B:216:LEU:HD12	1.95	0.47
1:C:65:PHE:O	1:C:265:TYR:HB3	2.13	0.47
2:E:41:TYR:HA	2:E:351:LEU:O	2.13	0.47
2:F:120:LEU:HD11	2:F:183:TYR:HE1	1.78	0.47
1:A:231:ILE:HG21	1:B:520:ALA:HB1	1.94	0.47
1:A:377:PHE:HD1	1:A:434:ILE:HG12	1.77	0.47
1:B:493[A]:ARG:NH1	2:E:34:HIS:O	2.47	0.47
1:C:986:PRO:N	1:C:987:PRO:HD2	2.30	0.47
2:E:302:TRP:HE1	2:E:307:ILE:HG13	1.77	0.47
2:E:571:GLU:HG3	2:E:577:LYS:HD3	1.95	0.47
1:A:485:GLY:H	1:A:488:CYS:HB2	1.79	0.47
1:C:598:ILE:HG23	1:C:664:ILE:HG21	1.95	0.47
1:C:896:ILE:HD12	1:C:897:PRO:HD2	1.97	0.47
2:E:363:LYS:HE3	2:E:364:VAL:HG22	1.96	0.47
2:F:225:ASP:HA	2:F:228:HIS:CD2	2.49	0.47
2:D:581:VAL:HG21	2:D:584:LEU:HD13	1.96	0.47
2:E:29:LEU:HD11	2:E:96:GLN:HB3	1.96	0.47
2:F:127:TYR:OH	2:F:502:SER:O	2.29	0.47
1:A:99:ASN:O	1:A:102:ARG:NH2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASN:ND2	4:C:1304:NAG:O7	2.47	0.47
1:C:392:PHE:HD2	1:C:395:VAL:HG22	1.80	0.47
1:C:874:THR:HG21	1:C:1055:SER:HB3	1.97	0.47
2:F:396:ALA:HB2	2:F:560:LEU:HD11	1.95	0.47
2:E:204:ARG:O	2:E:208:GLU:HG2	2.14	0.47
2:E:333:LEU:HA	2:E:360:MET:HB2	1.95	0.47
2:F:307:ILE:HG21	2:F:362:THR:HG21	1.95	0.47
2:F:541:LYS:HD2	2:F:541:LYS:O	2.15	0.47
1:A:407:VAL:HG21	1:A:508:TYR:CE2	2.49	0.47
1:B:65:PHE:HB2	1:B:265:TYR:CD2	2.49	0.47
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.96	0.47
1:C:596:SER:OG	1:C:613:GLN:OE1	2.32	0.47
2:D:285:PHE:CE2	2:D:433:GLU:HB3	2.50	0.47
2:E:48:TRP:CH2	2:E:348:ALA:HB1	2.50	0.47
2:E:179:LEU:HB3	2:E:183:TYR:CZ	2.50	0.47
2:E:594:TRP:HB2	4:E:702:NAG:H61	1.96	0.47
2:F:48:TRP:CZ3	2:F:359:LEU:HB2	2.50	0.47
2:F:245:ARG:HG2	2:F:258:PRO:HA	1.95	0.47
2:F:318:VAL:HG22	2:F:544:ILE:HG13	1.96	0.47
1:A:493[B]:ARG:HA	1:A:493[B]:ARG:HD3	1.49	0.47
1:A:941:THR:N	1:A:942:PRO:HD2	2.30	0.47
1:B:81:ASN:HB3	1:B:82:PRO:HD3	1.97	0.47
2:D:388:GLN:HG2	2:D:563:SER:HB2	1.97	0.47
2:E:415:PRO:HG3	2:E:541:LYS:HD2	1.96	0.47
2:E:490:PRO:HA	2:E:612:PRO:HG2	1.96	0.47
2:F:67:ASP:OD1	2:F:68:LYS:N	2.48	0.47
2:F:302:TRP:CD1	2:F:306:ARG:HG2	2.50	0.47
1:C:456:PHE:HB3	1:C:473:TYR:HB2	1.97	0.47
2:D:25:ALA:HB2	2:D:97:LEU:HD12	1.96	0.47
2:D:358:ILE:HG12	2:D:379:ILE:HG21	1.96	0.47
2:F:112:LYS:O	2:F:115:ARG:HG2	2.15	0.47
1:A:412:PRO:HB3	1:A:427:ASP:HA	1.97	0.47
1:B:493[A]:ARG:NH2	1:B:494:SER:O	2.34	0.47
2:D:190:MET:HG3	2:D:202:TYR:OH	2.14	0.47
2:D:260:GLY:HA2	2:D:607:SER:OG	2.15	0.47
2:D:415:PRO:O	2:D:419:LYS:HB3	2.15	0.47
2:E:468:ILE:HG23	2:E:472:GLN:NE2	2.30	0.47
2:E:554:LEU:O	2:E:558:LEU:HG	2.15	0.47
1:B:342:PHE:CE1	1:B:511:VAL:HG11	2.50	0.46
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.50	0.46
1:C:349:SER:HA	1:C:451:TYR:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:203:TRP:HD1	2:D:513:ILE:HG22	1.80	0.46
2:D:293:VAL:HA	2:D:296:ALA:HB3	1.96	0.46
1:A:404:GLY:N	1:A:506:GLN:O	2.42	0.46
1:A:976:VAL:HB	1:A:979:ASP:HB2	1.96	0.46
1:B:290:ASP:OD1	1:B:291:CYS:N	2.45	0.46
1:C:511:VAL:HG12	1:C:511:VAL:O	2.15	0.46
2:D:583:PRO:HA	2:D:586:ASN:HD21	1.79	0.46
2:D:112:LYS:HD2	2:D:189:GLU:HG3	1.97	0.46
2:E:470:LYS:O	2:E:473:TRP:NE1	2.49	0.46
2:F:36:ALA:HB2	2:F:72:PHE:HE2	1.80	0.46
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.98	0.46
1:C:497:PHE:HA	1:C:501:TYR:HE2	1.80	0.46
2:E:540:HIS:HD1	2:E:540:HIS:H	1.62	0.46
2:F:237:TYR:CZ	2:F:451:PRO:HG2	2.50	0.46
1:A:196:ASN:ND2	1:A:235:ILE:HD12	2.30	0.46
1:A:441:LEU:H	1:A:441:LEU:HD23	1.80	0.46
1:B:1098:ASN:OD1	1:B:1100:THR:N	2.42	0.46
1:C:945:LEU:HD23	1:C:945:LEU:H	1.80	0.46
2:D:183:TYR:O	2:D:187:LYS:HG2	2.15	0.46
2:E:116:LEU:HD13	2:E:186:LEU:HD12	1.98	0.46
1:A:339:ASP:OD1	1:A:339:ASP:N	2.47	0.46
1:B:83:VAL:HA	1:B:239:GLN:HE22	1.79	0.46
2:D:150:GLU:HG2	2:D:154:ASN:HD22	1.80	0.46
2:E:589:GLU:HG3	2:E:590:PRO:HD3	1.96	0.46
2:F:263:PRO:HB2	2:F:266:LEU:HD13	1.97	0.46
2:F:527:GLU:HG2	2:F:582:ARG:HH12	1.79	0.46
1:A:117:LEU:HG	1:A:130:VAL:HG23	1.97	0.46
2:E:115:ARG:O	2:E:119:ILE:HG12	2.15	0.46
2:F:198:ASP:OD2	2:F:464:PHE:HB3	2.15	0.46
1:B:1098:ASN:OD1	1:B:1099:GLY:N	2.49	0.46
2:D:236:LEU:HD12	2:D:236:LEU:HA	1.78	0.46
2:D:245:ARG:NH1	2:D:260:GLY:O	2.49	0.46
2:E:435:GLU:HB2	2:E:540:HIS:NE2	2.31	0.46
2:E:469:PRO:HD2	2:E:472:GLN:HE21	1.81	0.46
1:B:993:ILE:O	1:B:997:ILE:HG23	2.16	0.46
1:C:448:ASN:OD1	1:C:450:ASN:ND2	2.48	0.46
2:D:610:TRP:CH2	2:D:612:PRO:HB3	2.51	0.46
1:A:40:ASP:OD1	1:A:40:ASP:N	2.49	0.46
1:A:133:PHE:HB2	1:A:162:SER:O	2.16	0.46
1:A:733:LYS:HE3	1:A:771:ALA:HB1	1.98	0.46
1:B:736:VAL:HG21	1:B:1004:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:LYS:HB2	2:D:31:LYS:HE2	1.70	0.46
2:E:267:LEU:HD13	2:E:272:GLY:N	2.31	0.46
2:E:413:ALA:HB1	2:E:438:PHE:CE2	2.49	0.46
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.81	0.45
1:A:986:PRO:N	1:A:987:PRO:HD2	2.31	0.45
1:B:336:CYS:N	1:B:362:VAL:O	2.39	0.45
2:D:209:VAL:HG21	2:D:567:THR:HG23	1.98	0.45
2:D:418:LEU:HA	2:D:421:ILE:HG12	1.98	0.45
2:E:302:TRP:HA	2:E:306:ARG:HD3	1.98	0.45
2:F:302:TRP:HD1	2:F:306:ARG:HG2	1.81	0.45
1:B:822:LEU:HD21	1:B:938:LEU:HD13	1.96	0.45
1:B:878:LEU:HD21	1:B:1052:PHE:HB3	1.98	0.45
1:C:401:VAL:HG22	1:C:509:ARG:HG3	1.97	0.45
2:D:44:SER:HA	2:D:47:SER:HB3	1.98	0.45
2:E:97:LEU:O	2:E:101:GLN:HB2	2.15	0.45
1:B:759:PHE:O	1:B:763:LEU:HG	2.16	0.45
2:D:176:LEU:HG	2:D:179:LEU:HB3	1.97	0.45
2:D:252:TYR:O	2:D:256:ILE:HG12	2.17	0.45
1:C:1093:GLY:HA3	1:C:1105:THR:O	2.17	0.45
2:D:90:ASN:HB3	2:D:94:LYS:H	1.82	0.45
2:D:112:LYS:NZ	2:D:189:GLU:OE1	2.43	0.45
2:E:305:GLN:HA	2:E:333:LEU:HB2	1.99	0.45
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.98	0.45
1:C:353:TRP:HB3	1:C:400:PHE:HB3	1.98	0.45
1:C:708:SER:OG	1:C:711:SER:HB3	2.17	0.45
2:D:72:PHE:HA	2:D:75:GLU:OE1	2.16	0.45
1:A:748:GLU:HG3	1:A:981:LEU:HD11	1.98	0.45
2:E:407:ILE:HG22	2:E:522:GLN:HE21	1.82	0.45
2:E:494:ASP:OD2	2:E:496:THR:OG1	2.24	0.45
1:A:130:VAL:HG13	1:A:131:CYS:N	2.31	0.45
2:D:453:THR:HA	2:D:512:PHE:CE2	2.51	0.45
1:A:368:LEU:HD22	1:A:377:PHE:CZ	2.52	0.45
1:B:821:LEU:HD13	1:B:935:GLN:OE1	2.16	0.45
1:C:91:TYR:CG	1:C:91:TYR:O	2.68	0.45
2:E:180:TYR:HE1	2:E:507:SER:HA	1.82	0.45
2:D:54:ILE:HD12	2:D:54:ILE:H	1.82	0.45
2:F:26:LYS:HE3	2:F:88:ILE:HD11	1.97	0.45
2:F:414:THR:HG22	2:F:416:LYS:HG2	1.97	0.45
1:A:508:TYR:HD2	1:A:510:VAL:HG23	1.82	0.45
1:A:878:LEU:HD21	1:A:1052:PHE:HB3	1.99	0.45
1:B:90:VAL:HG13	1:B:267:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLU:HB3	1:C:418:ILE:HG13	1.98	0.45
2:E:57:GLU:O	2:E:60:GLN:HG3	2.17	0.45
2:E:209:VAL:HG13	2:E:565:PRO:HB3	1.99	0.45
2:E:523:PHE:O	2:E:526:GLN:HB3	2.17	0.45
1:B:496:GLY:O	1:B:498:ARG:NH1	2.50	0.44
1:C:195:LYS:HD3	1:C:204:TYR:HE1	1.80	0.44
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.88	0.44
2:D:267:LEU:HD11	2:D:487:VAL:HG21	1.98	0.44
2:E:162:LEU:HA	2:E:265:HIS:CD2	2.52	0.44
2:F:90:ASN:HB2	4:F:704:NAG:O5	2.18	0.44
2:F:417:HIS:O	2:F:420:SER:OG	2.31	0.44
1:A:37:TYR:OH	1:A:54:LEU:O	2.22	0.44
1:A:1035:GLY:HA3	1:B:1040:VAL:HG21	1.99	0.44
1:B:403:ARG:HE	1:B:495:TYR:HE1	1.65	0.44
1:C:459:SER:OG	1:C:460:ASN:N	2.50	0.44
2:D:177:ARG:HB2	2:D:178:PRO:HD3	1.98	0.44
2:D:275:TRP:CE3	2:D:444:LEU:HB2	2.52	0.44
2:E:209:VAL:HB	2:E:217:TYR:HB2	2.00	0.44
2:E:482:ARG:HG2	2:E:609:ASP:HA	2.00	0.44
2:F:381:TYR:CD2	2:F:558:LEU:HG	2.52	0.44
1:B:878:LEU:HD11	1:B:1054:GLN:HE22	1.82	0.44
1:B:985:ASP:O	1:B:989:ALA:N	2.45	0.44
1:C:493[B]:ARG:HE	1:C:493[B]:ARG:HB2	1.59	0.44
2:F:101:GLN:NE2	2:F:196:TYR:OH	2.47	0.44
1:A:371:PHE:HB3	1:A:374:PHE:CE1	2.53	0.44
1:A:456:PHE:HB3	1:A:473:TYR:CD1	2.53	0.44
1:B:751:ASN:HA	1:B:754:LEU:HG	2.00	0.44
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.28	0.44
1:C:365:TYR:H	1:C:387:LEU:HB2	1.81	0.44
2:E:404:VAL:HA	2:E:407:ILE:HG12	2.00	0.44
2:E:410:LEU:HD22	2:E:522:GLN:HE22	1.82	0.44
2:E:433:GLU:HG3	2:E:437:ASN:OD1	2.18	0.44
1:A:894:LEU:HD13	1:B:715:PRO:HD3	1.99	0.44
1:C:722:VAL:O	1:C:934:ILE:HD11	2.17	0.44
1:C:752:LEU:HD11	1:C:990:GLU:HG2	1.99	0.44
2:D:457:GLU:OE2	2:D:461:TRP:NE1	2.50	0.44
2:E:238:GLU:HG3	2:E:605:GLY:HA3	1.99	0.44
2:F:419:LYS:HE2	2:F:424:LEU:HD23	1.99	0.44
1:B:915:VAL:O	1:B:919:ASN:ND2	2.47	0.44
1:B:940:SER:OG	1:B:941:THR:N	2.50	0.44
1:C:349:SER:HA	1:C:451:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:ASN:O	2:D:192:ARG:NH1	2.51	0.44
1:A:455:LEU:N	1:A:491:PRO:O	2.33	0.44
1:B:727:LEU:HD21	1:B:1024:LEU:HD23	2.00	0.44
1:C:731:MET:HE1	1:C:1014:ARG:HB3	2.00	0.44
1:C:878:LEU:HD11	1:C:1054:GLN:HE22	1.82	0.44
2:E:268:GLY:O	2:E:277:ASN:ND2	2.45	0.44
2:F:294:THR:HA	2:F:297:MET:HE2	2.00	0.44
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.99	0.44
2:E:432:ASN:O	2:E:436:ILE:HG12	2.18	0.44
2:F:21:ILE:HG21	2:F:84:PRO:HD2	1.99	0.44
2:F:439:LEU:HD21	2:F:540:HIS:CD2	2.52	0.44
1:C:551:VAL:N	1:C:588:THR:O	2.44	0.44
1:C:1102:TRP:HB2	1:C:1135:ASN:HD22	1.82	0.44
2:D:480:MET:HA	2:D:483:GLU:HG2	1.99	0.44
2:D:532:ALA:HB2	2:D:553:LYS:NZ	2.33	0.44
2:F:112:LYS:HE3	2:F:186:LEU:HD13	2.00	0.44
2:F:314:PHE:HB3	2:F:417:HIS:CE1	2.53	0.44
1:A:501:TYR:HB2	1:A:506:GLN:HG3	2.00	0.43
1:B:328:ARG:NH1	1:B:533:LEU:HB3	2.33	0.43
1:B:436:TRP:CZ3	1:B:438:SER:HB3	2.52	0.43
1:B:1093:GLY:HA3	1:B:1105:THR:O	2.18	0.43
1:C:391:CYS:HA	1:C:525:CYS:HA	1.99	0.43
1:C:515:PHE:CE2	1:C:517:LEU:HB2	2.53	0.43
2:D:284:PRO:HD3	2:D:440:LEU:HD22	2.00	0.43
2:D:325:GLN:HG2	2:D:326:GLY:N	2.33	0.43
2:D:400:PHE:CE2	2:D:566:TRP:HB2	2.53	0.43
2:E:482:ARG:NH2	2:E:607:SER:O	2.50	0.43
2:F:273:ARG:O	2:F:449:THR:OG1	2.30	0.43
1:A:190:ARG:HG2	1:A:192:PHE:CZ	2.53	0.43
1:A:500:THR:HG1	2:D:41:TYR:HH	1.49	0.43
1:C:475:ALA:HB3	2:F:24:GLN:OE1	2.18	0.43
1:C:854:LYS:HB2	1:C:959:LEU:HD13	1.99	0.43
2:D:380:GLN:HE22	2:D:558:LEU:HD13	1.83	0.43
2:D:595:LEU:O	2:D:599:ASN:N	2.51	0.43
2:E:389:PRO:O	2:E:393:ARG:N	2.51	0.43
2:E:439:LEU:HD21	2:E:590:PRO:HD2	1.99	0.43
2:F:120:LEU:HD11	2:F:183:TYR:CE1	2.52	0.43
2:F:236:LEU:HD11	2:F:588:PHE:HB2	1.98	0.43
2:F:245:ARG:NE	2:F:262:LEU:HD23	2.32	0.43
1:A:401:VAL:HG13	1:A:508:TYR:H	1.83	0.43
1:A:822:LEU:HD22	1:A:945:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:PHE:CD2	1:A:999:GLY:HA3	2.54	0.43
1:B:105:ILE:HG12	1:B:239:GLN:HB2	1.99	0.43
1:C:196:ASN:OD1	1:C:235:ILE:HD12	2.18	0.43
1:C:378:LYS:O	1:C:433:VAL:N	2.50	0.43
1:C:556:ASN:HB3	1:C:558:LYS:NZ	2.33	0.43
1:C:915:VAL:HG21	1:C:1106:GLN:HE22	1.82	0.43
2:D:279:TYR:CE1	2:D:441:LYS:HB3	2.53	0.43
2:F:415:PRO:HD2	2:F:541:LYS:HD3	1.99	0.43
1:A:374:PHE:HD1	1:A:436:TRP:HB3	1.82	0.43
1:A:490:PHE:CE2	1:A:492:LEU:HB3	2.53	0.43
1:B:339:ASP:OD1	1:B:339:ASP:N	2.52	0.43
1:C:985:ASP:OD1	1:C:985:ASP:N	2.49	0.43
2:D:303:ASP:H	2:D:306:ARG:HB2	1.83	0.43
2:E:205:GLY:HA2	2:E:208:GLU:CG	2.49	0.43
2:E:315:PHE:CE1	2:E:380:GLN:HG2	2.54	0.43
2:F:124:SER:HB2	2:F:508:ASN:HD21	1.84	0.43
2:F:177:ARG:HB2	2:F:178:PRO:HD3	2.01	0.43
2:F:365:THR:HB	2:F:368:ASP:HB2	2.00	0.43
1:B:1106:GLN:NE2	1:B:1109:PHE:HB3	2.31	0.43
1:C:497:PHE:HA	1:C:501:TYR:CE2	2.54	0.43
1:C:969:LYS:HZ1	1:C:974:SER:HA	1.84	0.43
2:D:396:ALA:HB3	2:D:566:TRP:HB3	2.00	0.43
2:D:554:LEU:O	2:D:558:LEU:N	2.35	0.43
2:E:245:ARG:HH22	2:E:602:SER:HB2	1.84	0.43
1:B:95:THR:OG1	1:B:189:LEU:HD13	2.19	0.43
1:B:714:ILE:HD12	1:B:1096:VAL:HG11	1.99	0.43
1:C:453:TYR:HB3	1:C:495:TYR:HE1	1.83	0.43
1:C:493[A]:ARG:HE	1:C:493[A]:ARG:HB3	1.46	0.43
2:D:378:HIS:CE1	2:D:402:GLU:HA	2.53	0.43
2:D:450:LEU:HG	2:D:516:TYR:HD1	1.84	0.43
2:D:568:LEU:O	2:D:572:ASN:ND2	2.42	0.43
2:E:480:MET:O	2:E:484:ILE:HB	2.19	0.43
1:A:825:LYS:NZ	1:A:938:LEU:O	2.42	0.43
1:B:206:LYS:HA	1:B:206:LYS:HD2	1.77	0.43
1:B:401:VAL:HG21	1:B:451:TYR:CZ	2.54	0.43
1:B:741:TYR:CD2	1:B:1004:LEU:HD12	2.54	0.43
1:C:738:CYS:HB3	1:C:753:LEU:HD21	2.01	0.43
2:D:477:TRP:CE3	2:D:500:PRO:HG3	2.54	0.43
2:E:151:ILE:O	2:E:155:SER:HB2	2.19	0.43
2:E:438:PHE:CZ	2:E:442:GLN:HG3	2.53	0.43
2:F:540:HIS:HB3	2:F:587:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:557:MET:HA	2:F:560:LEU:HD23	1.99	0.43
1:C:206:LYS:HB2	1:C:223:LEU:HA	2.01	0.43
1:C:752:LEU:HA	1:C:755:GLN:OE1	2.19	0.43
2:F:88:ILE:HD13	2:F:93:VAL:HG11	2.01	0.43
1:B:430:THR:HG22	1:B:515:PHE:CE1	2.54	0.43
1:B:879:ALA:O	1:B:883:THR:OG1	2.30	0.43
1:C:546:LEU:HD22	1:C:565:PHE:CE1	2.54	0.43
2:E:50:TYR:HD1	2:E:58:ASN:HB3	1.84	0.43
2:E:70:SER:O	2:E:74:LYS:HG2	2.18	0.43
2:E:527:GLU:HG3	2:E:539:LEU:HD11	2.01	0.43
2:F:260:GLY:HA2	2:F:607:SER:H	1.84	0.43
2:F:453:THR:O	2:F:457:GLU:HB2	2.18	0.43
1:A:394:ASN:OD1	1:A:516:GLU:HB3	2.18	0.43
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.84	0.43
1:A:917:TYR:CE1	1:B:1079:PRO:HB3	2.54	0.43
1:A:945:LEU:HD12	1:A:948:LEU:HD12	2.01	0.43
1:A:1093:GLY:CA	1:A:1105:THR:O	2.58	0.43
1:B:114:THR:OG1	1:B:115:GLN:N	2.50	0.43
2:F:94:LYS:NZ	2:F:98:GLN:OE1	2.50	0.43
1:A:376:ALA:H	1:A:435:ALA:HB3	1.84	0.42
1:A:543:PHE:CG	1:A:576:VAL:HG11	2.53	0.42
1:B:231:ILE:HG13	1:B:232:GLY:N	2.34	0.42
1:B:716:THR:HG22	1:B:1110:TYR:HB3	2.01	0.42
2:D:21:ILE:HD12	2:D:24:GLN:HE21	1.84	0.42
2:D:169:ARG:HH11	2:D:499:ASP:HB3	1.84	0.42
2:E:48:TRP:CZ2	2:E:357:ARG:HB3	2.54	0.42
2:E:514:ARG:NH1	2:E:515:TYR:HB2	2.34	0.42
1:A:456:PHE:CZ	2:D:31:LYS:HD2	2.48	0.42
1:A:470:THR:HB	1:A:490:PHE:CE1	2.53	0.42
1:A:707:TYR:HB3	1:C:792:PRO:HG3	2.01	0.42
1:A:821:LEU:HD13	1:A:935:GLN:HG3	2.00	0.42
1:C:410:ILE:O	1:C:410:ILE:HG22	2.19	0.42
2:D:48:TRP:O	2:D:52:THR:HG22	2.19	0.42
2:E:532:ALA:HB2	2:E:553:LYS:HD2	2.00	0.42
2:D:505:HIS:O	2:D:510:TYR:N	2.51	0.42
2:D:564:GLU:HB2	2:D:565:PRO:HD2	2.01	0.42
2:E:392:LEU:HD23	2:E:562:LYS:HB2	2.02	0.42
2:F:527:GLU:O	2:F:531:GLN:HG2	2.19	0.42
1:B:736:VAL:HG12	1:B:767:LEU:HD12	2.00	0.42
1:C:961:THR:O	1:C:965:GLN:HB2	2.18	0.42
2:D:43:SER:HA	2:D:65:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:589:GLU:HB3	2:D:590:PRO:HD3	2.02	0.42
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.83	0.42
1:B:1083:HIS:CE1	1:B:1137:VAL:H	2.38	0.42
1:C:334:ASN:HB2	1:C:361:CYS:HA	2.00	0.42
1:C:350:VAL:HG22	1:C:422:ASN:HD22	1.84	0.42
1:C:1081:ILE:HD11	1:C:1137:VAL:HG22	2.02	0.42
1:C:1114:ILE:H	1:C:1114:ILE:HD12	1.84	0.42
2:E:84:PRO:O	2:E:85:LEU:HB3	2.20	0.42
2:E:157:ASP:OD1	2:E:157:ASP:N	2.52	0.42
2:E:407:ILE:HG22	2:E:522:GLN:HG2	2.01	0.42
2:F:32:PHE:CD1	2:F:76:GLN:HG3	2.55	0.42
1:A:192:PHE:HD1	1:A:205:SER:HG	1.64	0.42
1:B:138:ASP:OD1	1:B:138:ASP:N	2.53	0.42
1:B:874:THR:HG21	1:B:1055:SER:HB3	2.02	0.42
1:C:328:ARG:HD2	1:C:533:LEU:HD13	2.01	0.42
2:D:237:TYR:OH	2:D:447:VAL:HG12	2.19	0.42
2:E:207:TYR:HE1	2:E:398:GLU:HB2	1.84	0.42
2:F:237:TYR:CE1	2:F:451:PRO:HG2	2.55	0.42
1:A:1081:ILE:HD11	1:A:1137:VAL:HG22	2.01	0.42
1:B:493[A]:ARG:HE	1:B:493[A]:ARG:HB3	1.55	0.42
1:B:527:PRO:O	1:B:528:LYS:HE2	2.20	0.42
1:C:44:ARG:O	1:C:283:GLY:HA2	2.20	0.42
1:C:726:ILE:HD13	1:C:945:LEU:HA	2.01	0.42
2:D:36:ALA:HB2	2:D:72:PHE:HE2	1.84	0.42
1:A:350:VAL:O	1:A:353:TRP:HD1	2.03	0.42
1:C:452:LEU:HB3	1:C:492:LEU:HD12	2.01	0.42
2:D:85:LEU:HD23	2:D:98:GLN:HG3	2.02	0.42
2:E:48:TRP:CZ3	2:E:348:ALA:HB1	2.55	0.42
1:A:195:LYS:HE3	1:A:195:LYS:HB2	1.80	0.42
1:B:901:GLN:HE21	1:B:905:ARG:HH21	1.67	0.42
2:D:21:ILE:HA	2:D:24:GLN:HE21	1.85	0.42
2:D:48:TRP:HA	2:D:51:ASN:HB2	2.01	0.42
2:E:242:ALA:HB2	2:E:605:GLY:N	2.32	0.42
2:F:285:PHE:CD2	2:F:433:GLU:HG3	2.54	0.42
1:A:194:PHE:CD1	1:A:203:ILE:HG12	2.55	0.41
1:A:493[A]:ARG:HE	1:A:493[A]:ARG:HB3	1.57	0.41
2:E:369:PHE:HE2	2:E:412:ALA:HB2	1.84	0.41
2:E:450:LEU:HB2	2:E:451:PRO:HD3	2.02	0.41
1:A:722:VAL:O	1:A:934:ILE:HD11	2.20	0.41
1:C:83:VAL:HG11	1:C:237:ARG:NH1	2.35	0.41
1:C:406:GLU:OE1	1:C:409:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:ASN:OD1	2:D:251:ALA:N	2.53	0.41
2:E:574:VAL:HG12	2:E:576:ALA:H	1.85	0.41
2:F:29:LEU:HD12	2:F:93:VAL:HG23	2.02	0.41
1:A:731:MET:HE1	1:A:1014:ARG:HB3	2.02	0.41
1:C:454:ARG:NH1	1:C:469:SER:O	2.37	0.41
2:D:378:HIS:NE2	2:D:401:HIS:O	2.53	0.41
2:D:457:GLU:HG3	2:D:461:TRP:CE2	2.56	0.41
2:E:238:GLU:O	2:E:605:GLY:HA2	2.20	0.41
2:F:77:SER:O	2:F:81:GLN:HG2	2.21	0.41
2:D:314:PHE:HE1	2:D:421:ILE:HG21	1.85	0.41
2:F:403:ALA:O	2:F:406:GLU:HG3	2.21	0.41
1:A:319:ARG:NH1	1:C:739:THR:HG23	2.36	0.41
1:B:454:ARG:HA	1:B:492:LEU:HA	2.03	0.41
1:C:790:LYS:HB2	1:C:790:LYS:HE2	1.75	0.41
2:F:25:ALA:HA	2:F:28:PHE:CD1	2.55	0.41
2:F:133:CYS:H	2:F:171:GLU:HG3	1.85	0.41
2:F:208:GLU:HG3	2:F:219:ARG:HG3	2.02	0.41
2:F:518:ARG:HH12	2:F:522:GLN:HG3	1.85	0.41
2:F:539:LEU:O	2:F:540:HIS:CG	2.73	0.41
1:A:407:VAL:HG21	1:A:508:TYR:CZ	2.55	0.41
1:A:443:SER:HB3	1:A:507:PRO:HG2	2.02	0.41
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	2.02	0.41
1:B:96:GLU:HG2	1:B:100:ILE:HG22	2.03	0.41
2:D:209:VAL:O	2:D:209:VAL:HG12	2.21	0.41
2:E:293:VAL:HG12	2:E:418:LEU:HD22	2.02	0.41
2:E:313:LYS:HD3	2:E:313:LYS:HA	1.80	0.41
2:F:442:GLN:O	2:F:446:ILE:HG12	2.20	0.41
2:F:485:VAL:HG12	2:F:487:VAL:HG23	2.01	0.41
1:A:988:GLU:O	1:A:992:GLN:HG2	2.21	0.41
1:B:421:TYR:HE1	1:B:460:ASN:H	1.68	0.41
1:B:724:THR:HG21	1:B:938:LEU:HD21	2.03	0.41
1:C:240:THR:OG1	1:C:265:TYR:HE1	2.04	0.41
2:E:42:GLN:O	2:E:45:LEU:HG	2.21	0.41
2:F:148:LEU:HA	2:F:151:ILE:HG12	2.02	0.41
2:F:398:GLU:O	2:F:514:ARG:HG3	2.21	0.41
2:F:406:GLU:O	2:F:409:SER:OG	2.22	0.41
1:C:34:ARG:HA	1:C:34:ARG:HD2	1.94	0.41
1:C:568:ASP:HB3	1:C:574:ASP:OD1	2.21	0.41
4:C:1314:NAG:O7	4:C:1314:NAG:O3	2.34	0.41
2:E:107:VAL:HG11	2:E:190:MET:O	2.21	0.41
2:E:407:ILE:HG13	2:E:408:MET:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:416:LYS:HA	2:E:416:LYS:HD3	1.72	0.41
2:E:447:VAL:HG23	2:E:450:LEU:HD12	2.02	0.41
2:E:514:ARG:HH11	2:E:515:TYR:HB2	1.86	0.41
2:F:337:GLY:O	2:F:340:GLN:N	2.35	0.41
1:A:372:ALA:N	1:A:373:PRO:HD2	2.35	0.41
1:A:478:LYS:HD2	1:A:479:PRO:HD2	2.03	0.41
1:A:595:VAL:HG22	1:A:612:TYR:CD1	2.56	0.41
1:B:722:VAL:HA	1:B:1064:HIS:O	2.21	0.41
1:B:870:ILE:O	1:B:874:THR:HG23	2.21	0.41
1:B:907:ASN:HD22	1:B:907:ASN:HA	1.62	0.41
1:C:336:CYS:SG	1:C:338:PHE:HB2	2.61	0.41
1:C:377:PHE:CD1	1:C:434:ILE:HG23	2.56	0.41
2:D:187:LYS:HG3	2:D:464:PHE:CZ	2.55	0.41
2:D:595:LEU:HA	2:D:598:GLN:HG2	2.03	0.41
2:E:209:VAL:HG21	2:E:566:TRP:HB3	2.02	0.41
2:E:462:MET:HG3	2:E:465:LYS:NZ	2.36	0.41
2:F:49:ASN:OD1	2:F:58:ASN:ND2	2.54	0.41
2:F:236:LEU:HD13	2:F:585:LEU:HA	2.02	0.41
2:F:245:ARG:NH2	2:F:261:CYS:HA	2.36	0.41
2:F:529:LEU:HD23	2:F:554:LEU:HD13	2.03	0.41
2:F:539:LEU:HG	2:F:540:HIS:H	1.86	0.41
1:A:165:ASN:OD1	1:A:165:ASN:N	2.54	0.41
1:A:203:ILE:O	1:A:226:LEU:HD23	2.21	0.41
2:D:528:ALA:O	2:D:531:GLN:HG3	2.21	0.41
2:E:42:GLN:HE21	2:E:42:GLN:HB3	1.76	0.41
2:E:323:MET:HA	2:E:383:MET:SD	2.61	0.41
2:F:203:TRP:HH2	2:F:461:TRP:HE1	1.70	0.41
2:F:385:TYR:CD2	2:F:388:GLN:HG3	2.56	0.41
1:A:65:PHE:HD2	1:A:265:TYR:HH	1.68	0.40
1:A:193:VAL:HB	1:A:204:TYR:HD2	1.86	0.40
1:B:431:GLY:HA2	1:B:515:PHE:CE2	2.56	0.40
1:B:454:ARG:HB2	1:B:492:LEU:HD12	2.03	0.40
1:B:763:LEU:HB3	1:B:1008:VAL:HG21	2.03	0.40
1:C:95:THR:H	1:C:264:ALA:HB3	1.86	0.40
1:C:198:ASP:O	1:C:200:TYR:HD1	2.04	0.40
2:D:571:GLU:HA	2:D:575:GLY:HA2	2.03	0.40
2:E:496:THR:O	2:E:497:TYR:HD1	2.04	0.40
2:F:245:ARG:HH12	2:F:260:GLY:C	2.24	0.40
2:F:293:VAL:O	2:F:296:ALA:HB3	2.20	0.40
1:A:371:PHE:CE2	1:A:436:TRP:HB2	2.56	0.40
1:B:708:SER:HB3	1:B:711:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:VAL:HG12	1:C:512:VAL:H	1.86	0.40
2:D:274:PHE:CE1	2:D:449:THR:HG21	2.55	0.40
2:D:357:ARG:HA	2:D:357:ARG:HD3	1.77	0.40
2:E:248:LEU:O	2:E:256:ILE:HG13	2.21	0.40
2:E:302:TRP:HE1	2:E:307:ILE:CG1	2.34	0.40
2:E:424:LEU:HD12	2:E:425:SER:H	1.85	0.40
2:F:50:TYR:O	2:F:54:ILE:HD13	2.21	0.40
1:A:1079:PRO:HB3	1:C:917:TYR:CE1	2.57	0.40
1:B:324:GLU:HB3	1:B:539:VAL:HG23	2.03	0.40
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.56	0.40
1:B:758:SER:HB3	1:C:964:LYS:HZ3	1.86	0.40
1:B:966:LEU:HD23	1:B:966:LEU:HA	1.93	0.40
1:C:25:THR:OG1	1:C:66:HIS:ND1	2.54	0.40
2:D:177:ARG:HA	2:D:177:ARG:HD2	1.86	0.40
2:D:436:ILE:HG23	2:D:591:LEU:HD12	2.02	0.40
2:E:370:LEU:HG	2:E:409:SER:HB2	2.04	0.40
2:E:468:ILE:HG12	2:E:472:GLN:HE22	1.85	0.40
2:E:523:PHE:O	2:E:527:GLU:OE1	2.38	0.40
1:A:43:PHE:CG	1:A:43:PHE:O	2.75	0.40
1:C:329:PHE:N	1:C:530:SER:OG	2.37	0.40
1:C:456:PHE:CZ	2:F:31:LYS:HD3	2.56	0.40
2:D:176:LEU:O	2:D:180:TYR:HB2	2.22	0.40
2:D:321:PRO:HD2	2:D:380:GLN:NE2	2.37	0.40
2:D:468:ILE:HA	2:D:472:GLN:HG2	2.03	0.40
2:E:365:THR:HG22	2:E:368:ASP:H	1.87	0.40
2:E:427:ASP:OD1	2:E:427:ASP:N	2.53	0.40
2:E:455:MET:SD	2:E:456:LEU:N	2.95	0.40
2:F:29:LEU:HD23	2:F:29:LEU:HA	1.93	0.40
1:A:436:TRP:HH2	1:A:511:VAL:HB	1.86	0.40
1:A:995:ARG:HE	1:A:995:ARG:HB2	1.69	0.40
1:C:170:TYR:HE2	1:C:172:SER:HB3	1.87	0.40
1:C:374:PHE:HD2	1:C:436:TRP:HA	1.86	0.40
2:D:73:LEU:HA	2:D:76:GLN:OE1	2.22	0.40
2:E:60:GLN:NE2	2:E:61:ASN:OD1	2.55	0.40
2:E:288:LYS:HB2	2:E:433:GLU:HB3	2.04	0.40
2:F:99:ALA:HA	2:F:102:GLN:HE22	1.87	0.40
2:F:381:TYR:HD1	2:F:385:TYR:HE1	1.67	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	974/1244 (78%)	883 (91%)	90 (9%)	1 (0%)	51	81
1	B	975/1244 (78%)	890 (91%)	84 (9%)	1 (0%)	51	81
1	C	974/1244 (78%)	897 (92%)	75 (8%)	2 (0%)	47	77
2	D	594/614 (97%)	540 (91%)	52 (9%)	2 (0%)	41	70
2	E	594/614 (97%)	550 (93%)	43 (7%)	1 (0%)	47	77
2	F	594/614 (97%)	547 (92%)	47 (8%)	0	100	100
All	All	4705/5574 (84%)	4307 (92%)	391 (8%)	7 (0%)	54	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	675	GLN
1	C	332	ILE
2	D	364	VAL
1	C	481	ASN
2	D	365	THR
2	E	609	ASP
1	A	126	VAL

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	871/1083 (80%)	869 (100%)	2 (0%)	93	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	871/1083 (80%)	868 (100%)	3 (0%)	92 98
1	C	870/1083 (80%)	867 (100%)	3 (0%)	92 98
2	D	526/541 (97%)	524 (100%)	2 (0%)	91 97
2	E	526/541 (97%)	522 (99%)	4 (1%)	81 93
2	F	526/541 (97%)	523 (99%)	3 (1%)	86 95
All	All	4190/4872 (86%)	4173 (100%)	17 (0%)	92 97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	493[A]	ARG
1	A	493[B]	ARG
1	B	493[A]	ARG
1	B	493[B]	ARG
1	B	907	ASN
1	C	493[A]	ARG
1	C	493[B]	ARG
1	C	964	LYS
2	D	174	LYS
2	D	559	ARG
2	E	42	GLN
2	E	476	LYS
2	E	514	ARG
2	E	559	ARG
2	F	518	ARG
2	F	541	LYS
2	F	553	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	439	ASN
1	A	487	ASN
1	A	544	ASN
1	B	207	HIS
1	B	901	GLN
1	B	1002	GLN
1	B	1106	GLN

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Mol	Chain	Res	Type
1	C	992	GLN
2	D	24	GLN
2	D	49	ASN
2	D	58	ASN
2	D	154	ASN
2	E	58	ASN
2	E	60	GLN
2	E	101	GLN
2	E	472	GLN
2	E	522	GLN
2	E	598	GLN
2	E	599	ASN
2	F	64	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)

6 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	$\#\|Z\| > 2$
3	NAG	G	1	3,2	14,14,15	0.43	0	17,19,21	0.36	0
3	NAG	G	2	3	14,14,15	0.41	0	17,19,21	0.34	0
3	NAG	H	1	3,2	14,14,15	0.49	0	17,19,21	0.38	0
3	NAG	H	2	3	14,14,15	0.37	0	17,19,21	0.37	0
3	NAG	I	1	3,2	14,14,15	0.43	0	17,19,21	0.36	0
3	NAG	I	2	3	14,14,15	0.38	0	17,19,21	0.35	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6

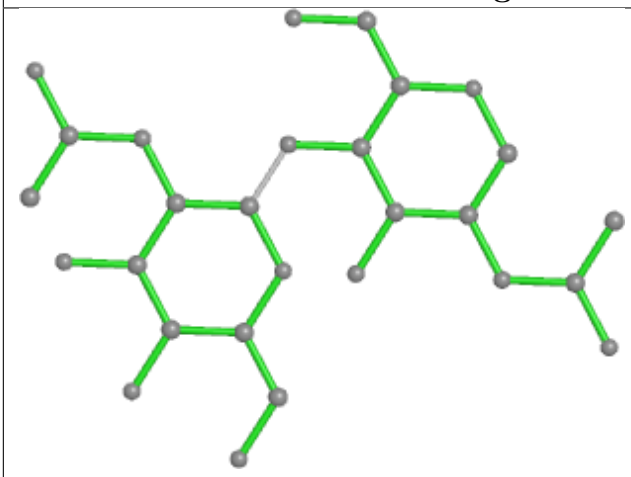
There are no ring outliers.

1 monomer is involved in 1 short contact:

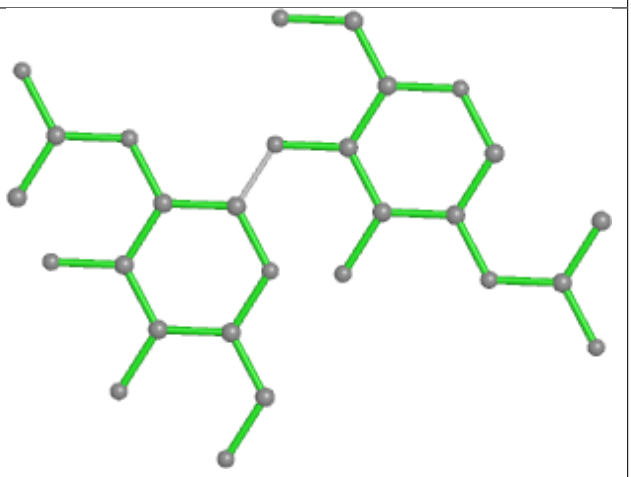
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	1	0

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

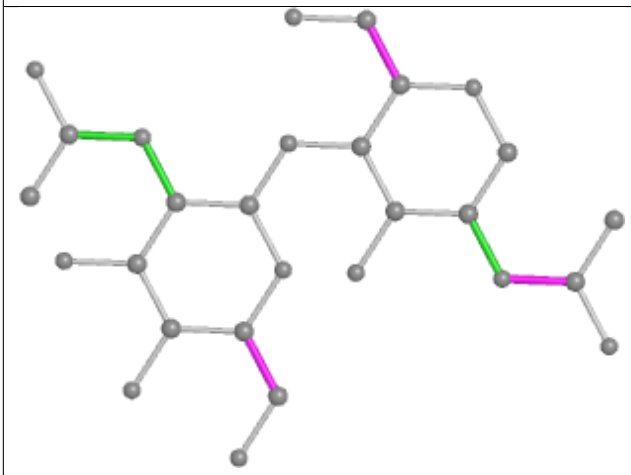
Oligosaccharide Chain G



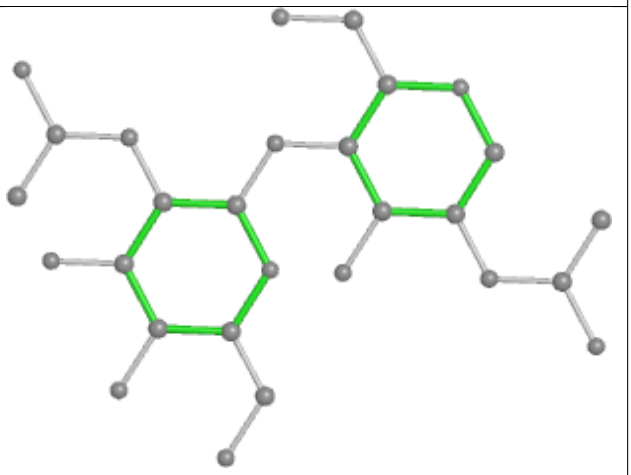
Bond lengths



Bond angles

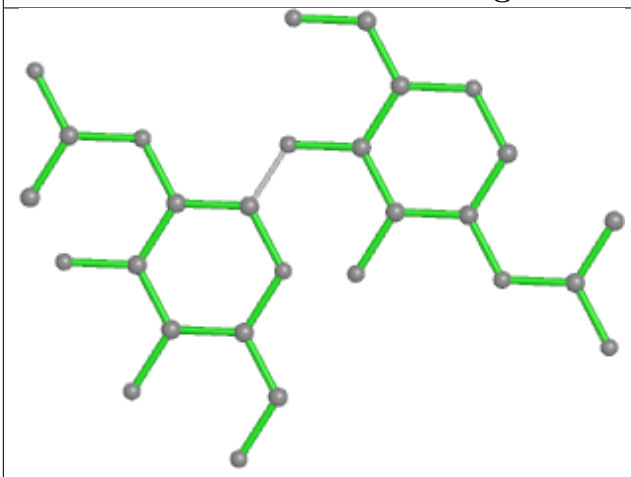


Torsions

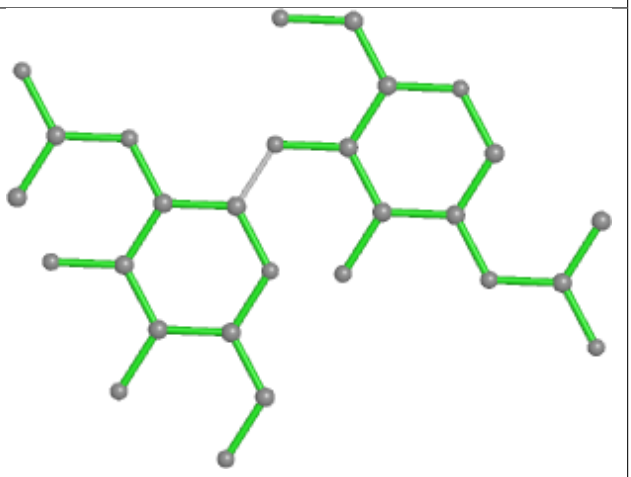


Rings

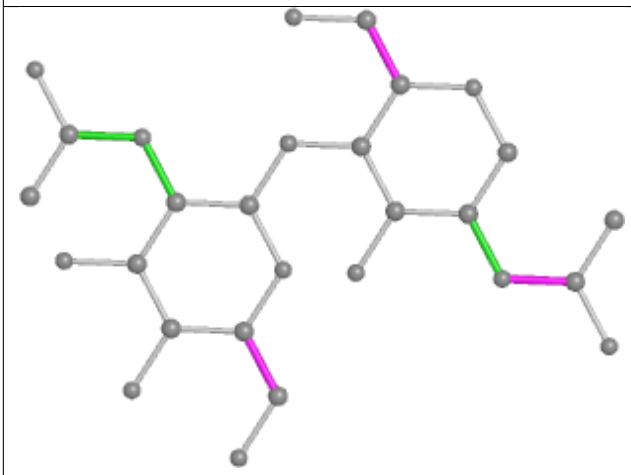
Oligosaccharide Chain H



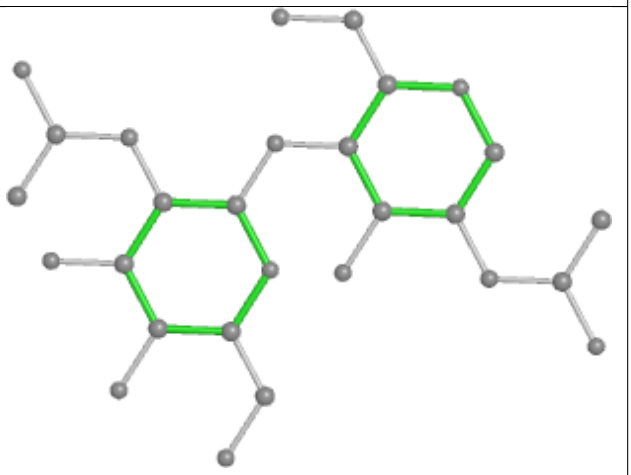
Bond lengths



Bond angles

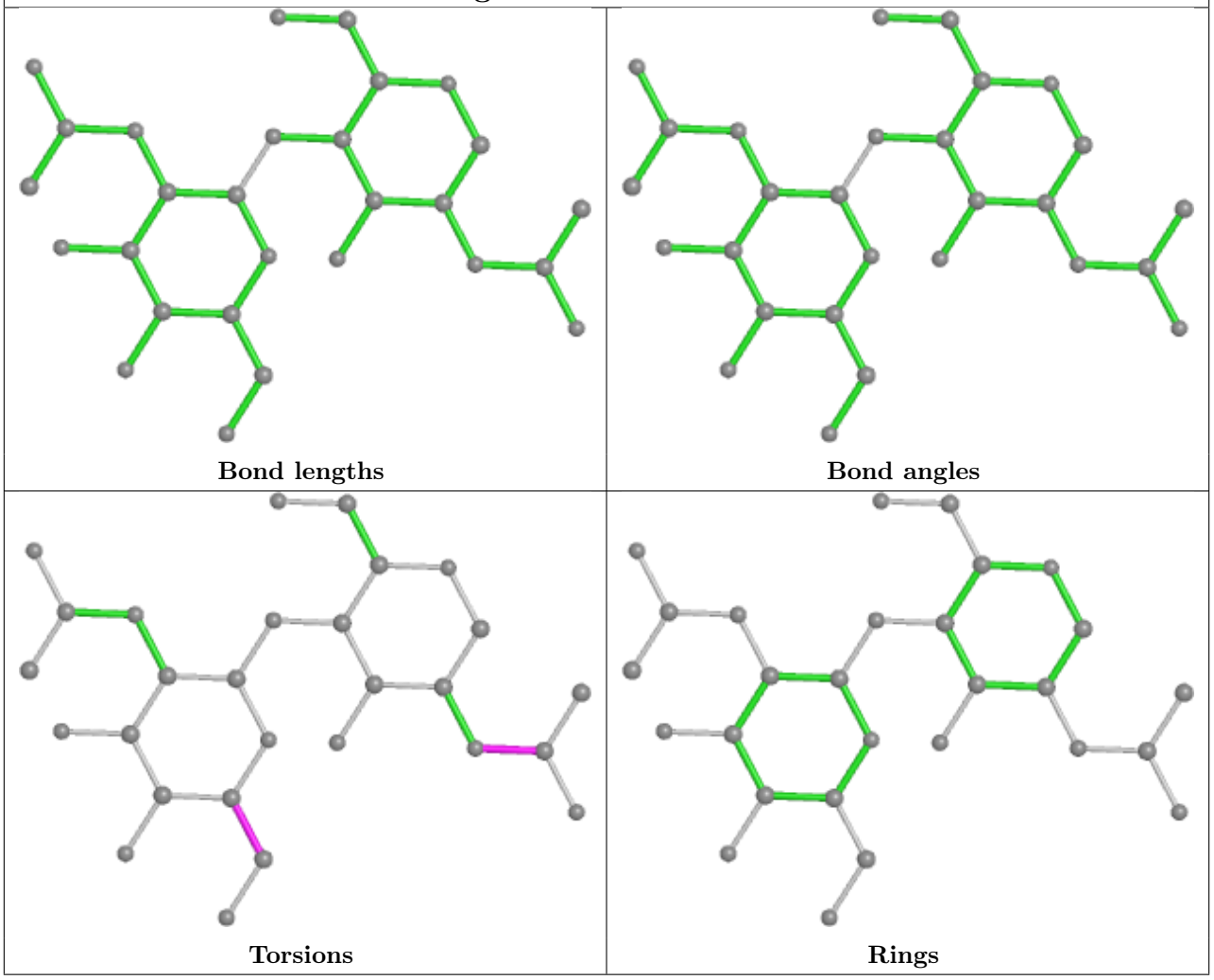


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

51 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	E	702	2	14,14,15	0.33	0	17,19,21	0.34	0
4	NAG	C	1304	1	14,14,15	0.42	0	17,19,21	0.37	0
4	NAG	B	1310	1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	B	1309	1	14,14,15	0.20	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	1306	1	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	A	1307	1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	D	701	2	14,14,15	0.50	0	17,19,21	0.41	0
4	NAG	F	704	2	14,14,15	0.31	0	17,19,21	0.38	0
4	NAG	F	705	2	14,14,15	0.37	0	17,19,21	0.35	0
4	NAG	C	1310	1	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	E	704	2	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	E	705	2	14,14,15	0.40	0	17,19,21	0.34	0
4	NAG	F	701	2	14,14,15	0.45	0	17,19,21	0.39	0
4	NAG	B	1311	1	14,14,15	0.23	0	17,19,21	0.34	0
4	NAG	A	1301	1	14,14,15	0.78	1 (7%)	17,19,21	0.97	1 (5%)
4	NAG	D	702	2	14,14,15	0.85	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	A	1309	1	14,14,15	0.31	0	17,19,21	0.58	0
4	NAG	D	705	2	14,14,15	0.89	2 (14%)	17,19,21	0.91	1 (5%)
4	NAG	F	702	2	14,14,15	0.40	0	17,19,21	0.36	0
4	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.52	0
4	NAG	C	1314	1	14,14,15	0.30	0	17,19,21	0.40	0
4	NAG	B	1308	1	14,14,15	0.52	0	17,19,21	0.42	0
4	NAG	B	1305	1	14,14,15	0.32	0	17,19,21	0.46	0
4	NAG	A	1303	1	14,14,15	0.36	0	17,19,21	0.36	0
4	NAG	A	1302	1	14,14,15	0.39	0	17,19,21	0.35	0
4	NAG	C	1303	1	14,14,15	0.83	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	C	1306	1	14,14,15	0.40	0	17,19,21	1.27	1 (5%)
4	NAG	B	1303	1	14,14,15	0.92	1 (7%)	17,19,21	1.21	1 (5%)
4	NAG	A	1308	1	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	C	1307	1	14,14,15	0.38	0	17,19,21	0.39	0
4	NAG	A	1305	1	14,14,15	0.44	0	17,19,21	0.38	0
4	NAG	A	1311	1	14,14,15	0.85	1 (7%)	17,19,21	1.34	1 (5%)
4	NAG	C	1302	1	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	D	703	2	14,14,15	0.47	0	17,19,21	1.25	2 (11%)
4	NAG	C	1313	1	14,14,15	0.30	0	17,19,21	1.37	2 (11%)
4	NAG	F	703	2	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	B	1301	1	14,14,15	0.38	0	17,19,21	0.45	0
4	NAG	A	1304	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	C	1308	1	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	B	1304	1	14,14,15	0.33	0	17,19,21	0.62	0
4	NAG	E	701	2	14,14,15	0.39	0	17,19,21	0.38	0
4	NAG	C	1301	1	14,14,15	0.26	0	17,19,21	0.34	0
4	NAG	C	1311	1	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	A	1306	1	14,14,15	0.41	0	17,19,21	0.35	0
4	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1305	1	14,14,15	0.30	0	17,19,21	0.36	0
4	NAG	E	703	2	14,14,15	0.47	0	17,19,21	1.26	1 (5%)
4	NAG	A	1310	1	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	D	704	2	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	C	1312	1	14,14,15	0.84	1 (7%)	17,19,21	1.30	1 (5%)
4	NAG	C	1309	1	14,14,15	0.35	0	17,19,21	0.57	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	E	702	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	D	701	2	-	2/6/23/26	0/1/1/1
4	NAG	F	704	2	-	0/6/23/26	0/1/1/1
4	NAG	F	705	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	E	704	2	-	3/6/23/26	0/1/1/1
4	NAG	E	705	2	-	2/6/23/26	0/1/1/1
4	NAG	F	701	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	D	702	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	D	705	2	-	2/6/23/26	0/1/1/1
4	NAG	F	702	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1314	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	D	703	2	-	3/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	F	703	2	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	E	701	2	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	E	703	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	D	704	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	3/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1303	NAG	O5-C1	3.17	1.48	1.43
4	A	1311	NAG	O5-C1	3.10	1.48	1.43
4	C	1312	NAG	O5-C1	3.04	1.48	1.43
4	C	1303	NAG	O5-C1	2.64	1.47	1.43
4	D	702	NAG	O5-C1	2.50	1.47	1.43
4	D	705	NAG	O5-C1	2.48	1.47	1.43
4	A	1301	NAG	O5-C1	2.25	1.47	1.43
4	D	705	NAG	C1-C2	2.04	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1311	NAG	C1-O5-C5	5.26	119.32	112.19
4	C	1312	NAG	C1-O5-C5	5.14	119.16	112.19
4	C	1313	NAG	C1-O5-C5	4.95	118.90	112.19
4	B	1303	NAG	C1-O5-C5	4.58	118.40	112.19
4	C	1306	NAG	C2-N2-C7	4.32	129.05	122.90
4	E	703	NAG	C2-N2-C7	4.29	129.02	122.90
4	D	703	NAG	C2-N2-C7	4.27	128.99	122.90
4	A	1301	NAG	C1-O5-C5	3.81	117.35	112.19
4	C	1303	NAG	C1-O5-C5	3.79	117.32	112.19
4	D	702	NAG	C1-O5-C5	3.48	116.91	112.19
4	D	705	NAG	C1-O5-C5	3.38	116.77	112.19
4	C	1313	NAG	C3-C4-C5	2.07	113.92	110.24
4	D	703	NAG	C1-C2-N2	2.03	113.95	110.49

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	C4-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	E	702	NAG	C4-C5-C6-O6
4	E	704	NAG	O5-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	C	1314	NAG	O5-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	E	702	NAG	O5-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	A	1311	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	B	1311	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	F	701	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1309	NAG	O5-C5-C6-O6
4	C	1314	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	C	1312	NAG	O5-C5-C6-O6
4	D	705	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	E	705	NAG	O5-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	E	704	NAG	C4-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	A	1311	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1312	NAG	C4-C5-C6-O6
4	A	1301	NAG	C8-C7-N2-C2
4	A	1301	NAG	O7-C7-N2-C2
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	A	1303	NAG	C8-C7-N2-C2
4	A	1303	NAG	O7-C7-N2-C2
4	A	1305	NAG	C8-C7-N2-C2
4	A	1305	NAG	O7-C7-N2-C2
4	A	1308	NAG	C8-C7-N2-C2
4	A	1308	NAG	O7-C7-N2-C2
4	A	1309	NAG	C8-C7-N2-C2
4	A	1309	NAG	O7-C7-N2-C2
4	A	1311	NAG	C8-C7-N2-C2
4	A	1311	NAG	O7-C7-N2-C2
4	B	1301	NAG	C8-C7-N2-C2
4	B	1301	NAG	O7-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	1307	NAG	C8-C7-N2-C2
4	C	1307	NAG	O7-C7-N2-C2
4	D	703	NAG	C8-C7-N2-C2
4	D	703	NAG	O7-C7-N2-C2
4	E	703	NAG	C8-C7-N2-C2
4	E	703	NAG	O7-C7-N2-C2
4	F	701	NAG	C8-C7-N2-C2
4	F	701	NAG	O7-C7-N2-C2
4	F	705	NAG	C8-C7-N2-C2
4	F	705	NAG	O7-C7-N2-C2
4	B	1308	NAG	O5-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	C	1311	NAG	O5-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	E	705	NAG	C4-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1314	NAG	C1-C2-N2-C7
4	D	701	NAG	C4-C5-C6-O6
4	F	701	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	E	703	NAG	O5-C5-C6-O6
4	D	702	NAG	C4-C5-C6-O6
4	D	702	NAG	O5-C5-C6-O6
4	C	1311	NAG	C4-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	D	705	NAG	C4-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	E	701	NAG	O5-C5-C6-O6
4	D	704	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	C	1309	NAG	C1-C2-N2-C7
4	B	1302	NAG	C3-C2-N2-C7
4	B	1303	NAG	C3-C2-N2-C7
4	B	1304	NAG	C3-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	B	1310	NAG	C3-C2-N2-C7
4	D	704	NAG	C3-C2-N2-C7
4	E	704	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	F	703	NAG	C3-C2-N2-C7
4	C	1306	NAG	C3-C2-N2-C7
4	C	1314	NAG	C3-C2-N2-C7
4	D	703	NAG	C3-C2-N2-C7
4	E	703	NAG	C3-C2-N2-C7
4	A	1308	NAG	C4-C5-C6-O6

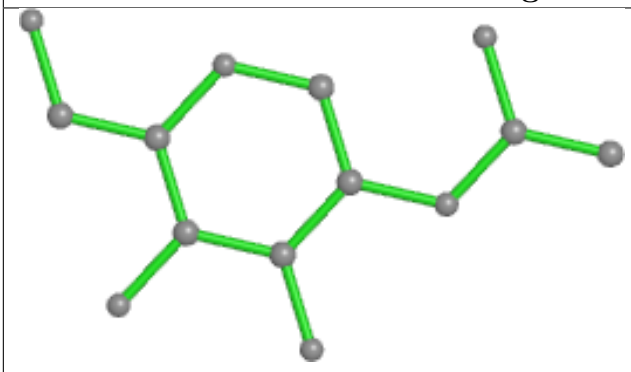
There are no ring outliers.

13 monomers are involved in 14 short contacts:

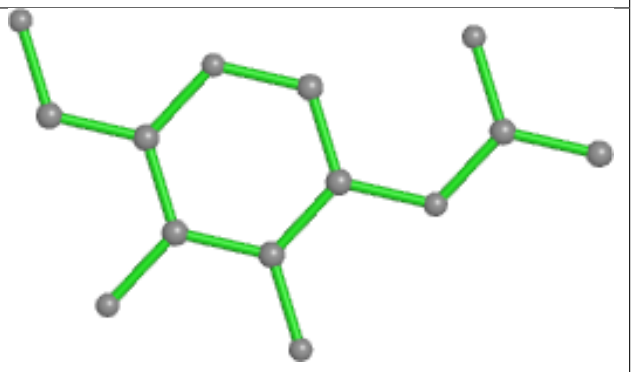
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	702	NAG	2	0
4	C	1304	NAG	1	0
4	F	704	NAG	1	0
4	F	701	NAG	1	0
4	C	1314	NAG	1	0
4	A	1303	NAG	1	0
4	C	1303	NAG	1	0
4	C	1306	NAG	1	0
4	C	1302	NAG	1	0
4	D	703	NAG	1	0
4	F	703	NAG	1	0
4	A	1306	NAG	1	0
4	E	703	NAG	1	0

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.

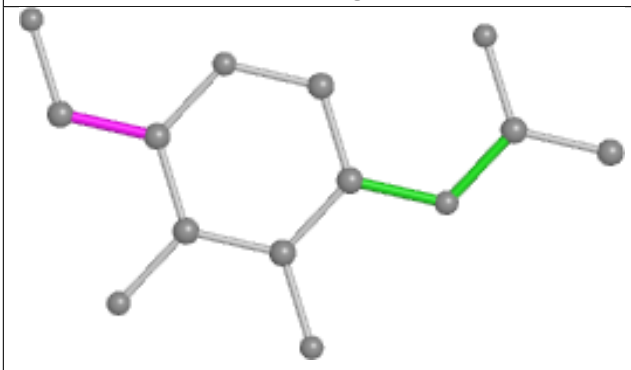
Ligand NAG E 702



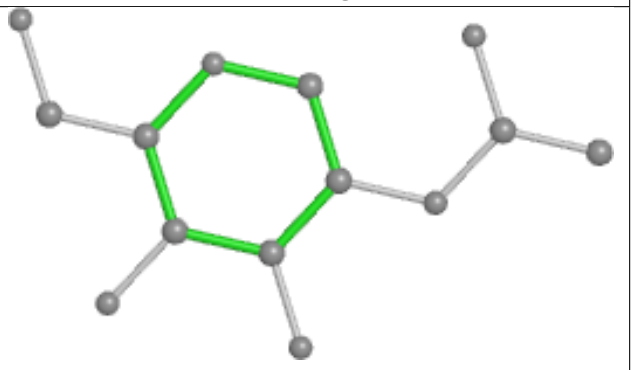
Bond lengths



Bond angles

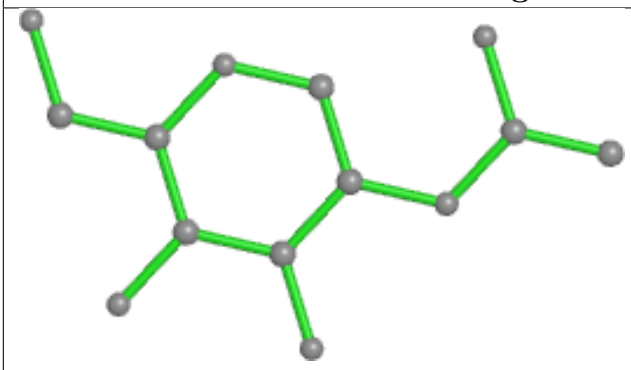


Torsions

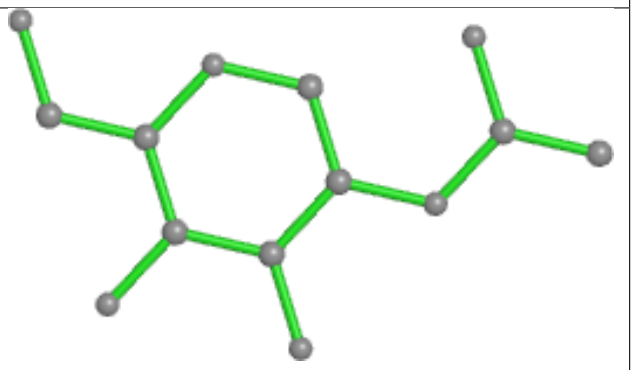


Rings

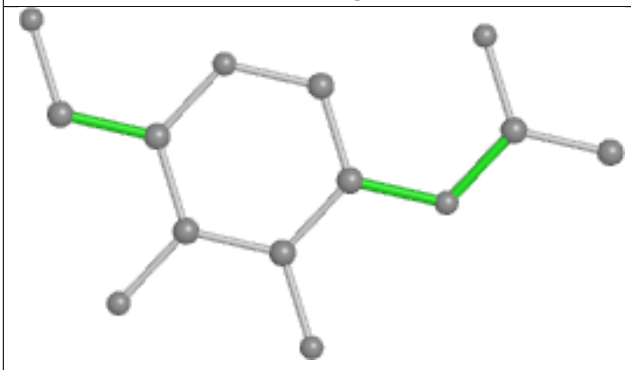
Ligand NAG C 1304



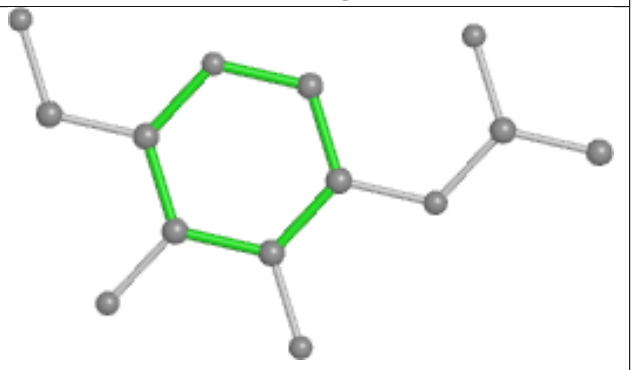
Bond lengths



Bond angles

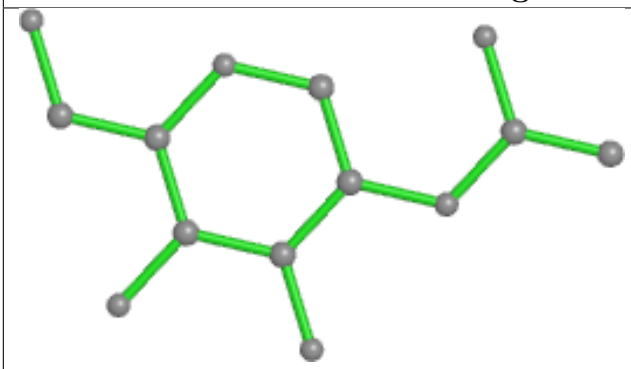


Torsions

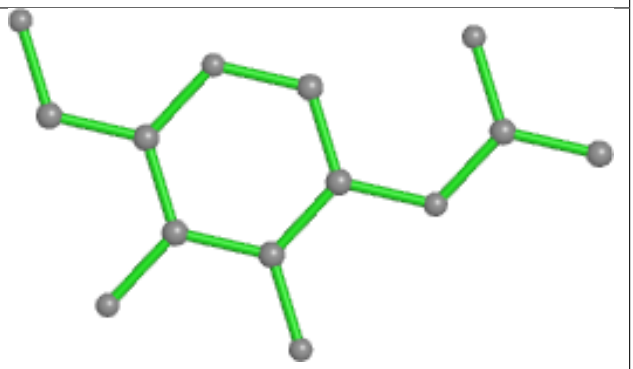


Rings

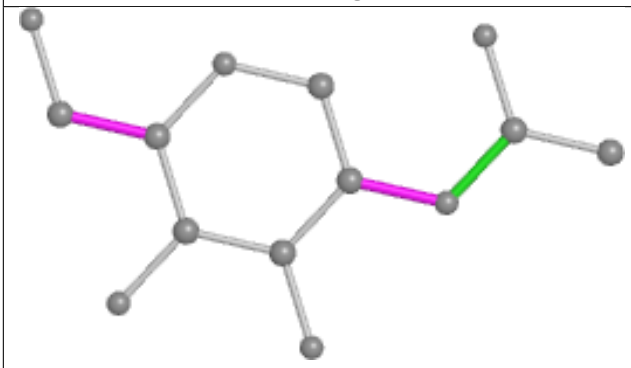
Ligand NAG B 1310



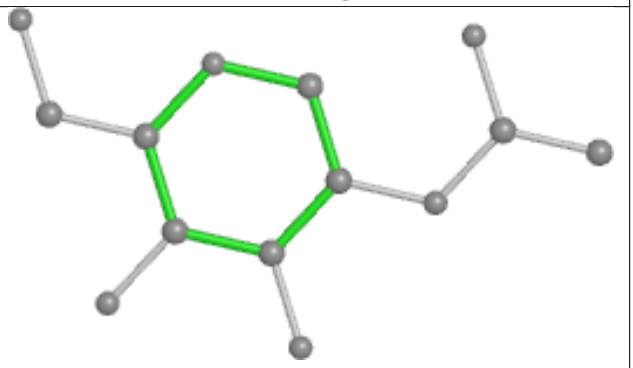
Bond lengths



Bond angles

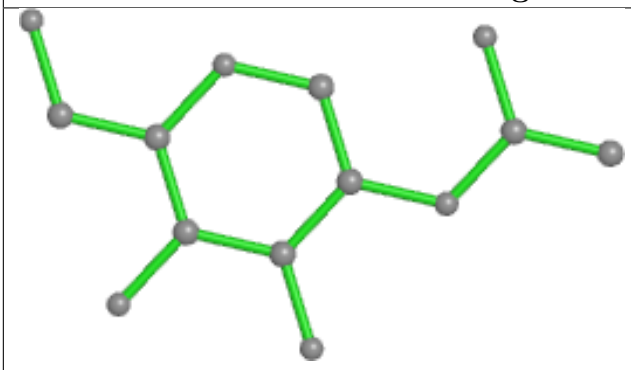


Torsions

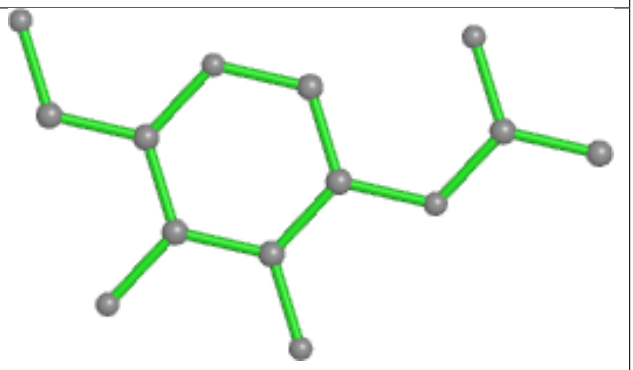


Rings

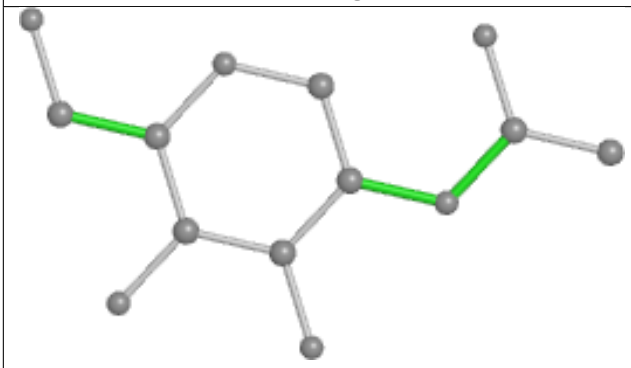
Ligand NAG B 1309



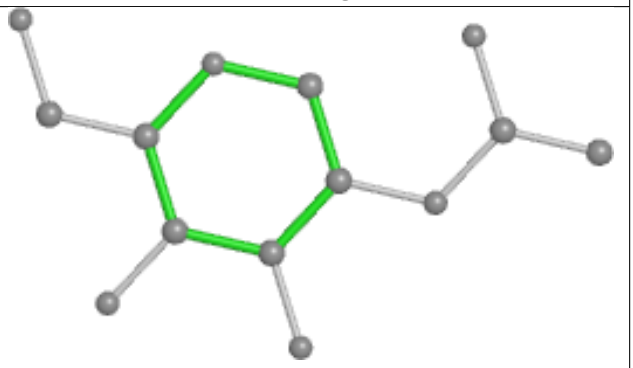
Bond lengths



Bond angles

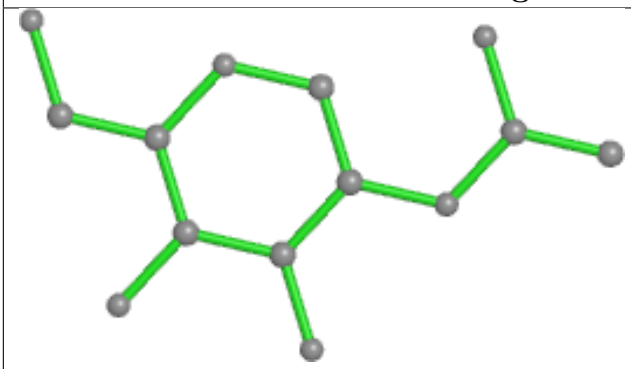


Torsions

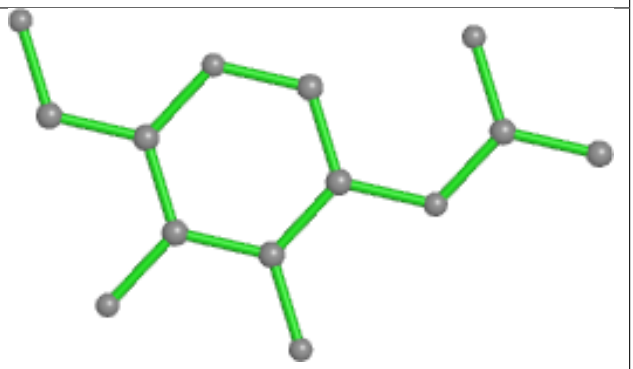


Rings

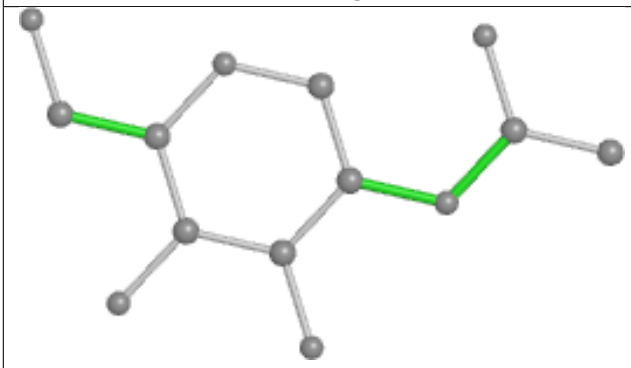
Ligand NAG B 1306



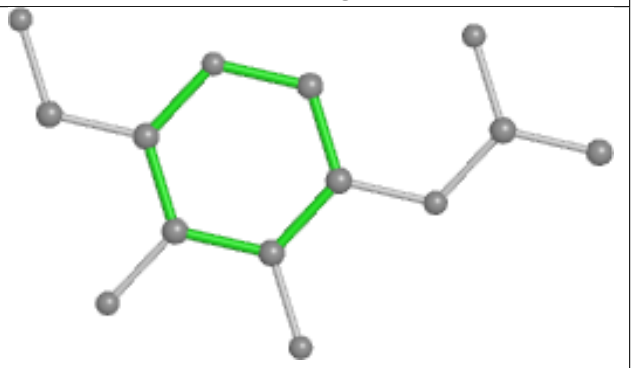
Bond lengths



Bond angles

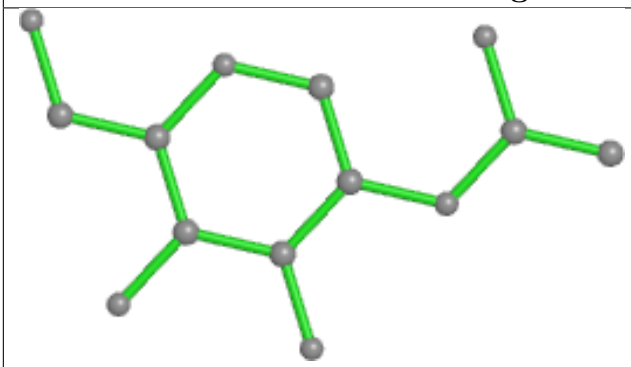


Torsions

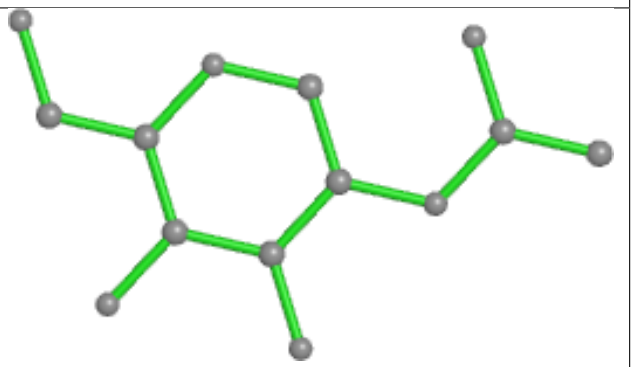


Rings

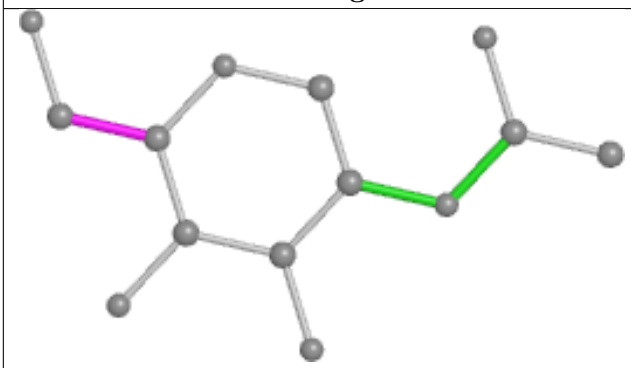
Ligand NAG A 1307



Bond lengths



Bond angles



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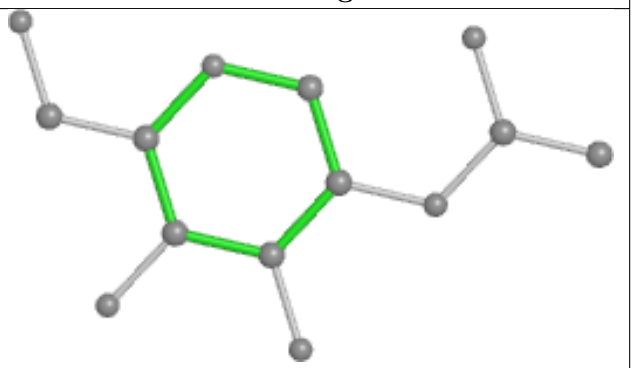
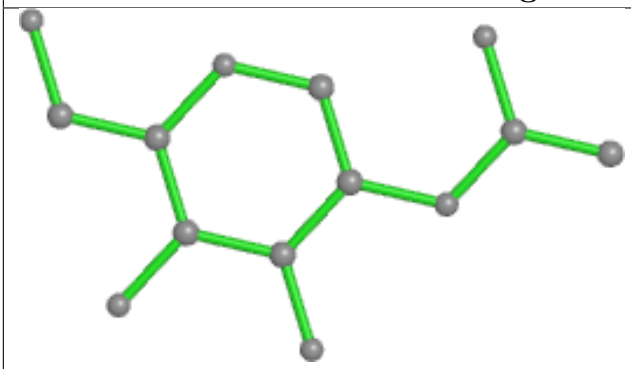


Rings

Ligand NAG D 701



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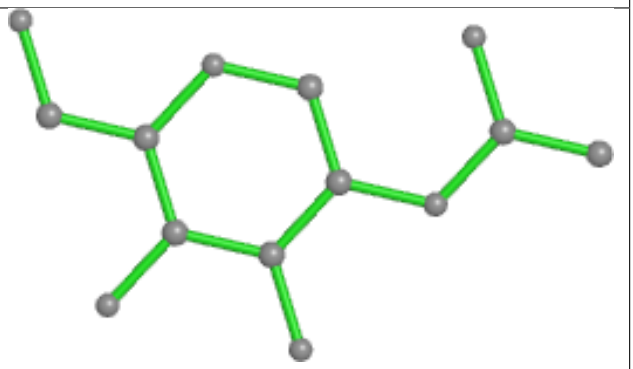
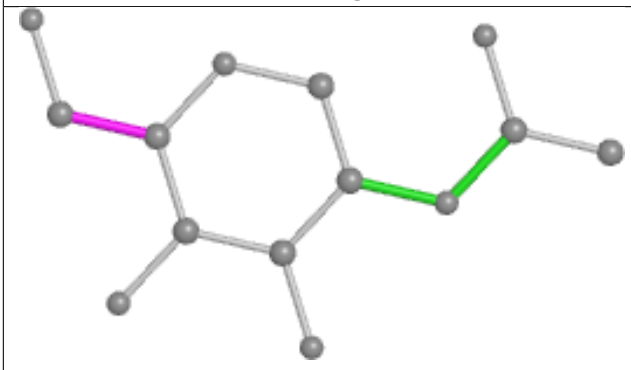


Bond angles



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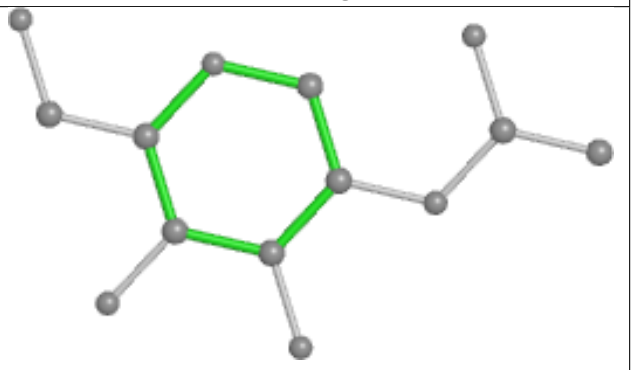
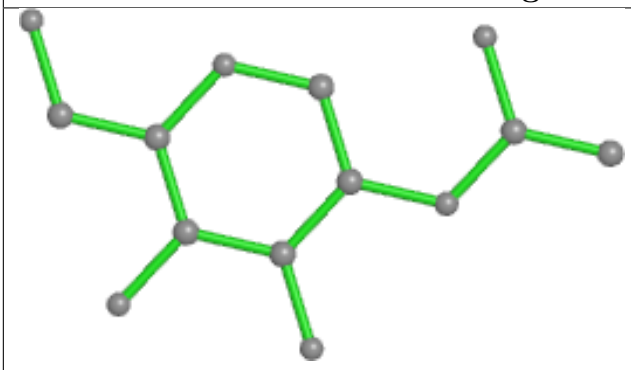


Rings

Ligand NAG F 704



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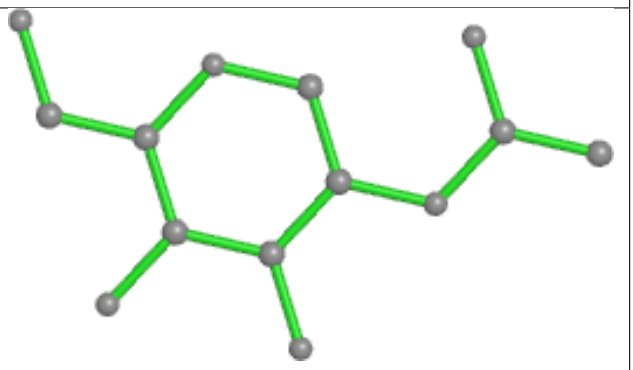
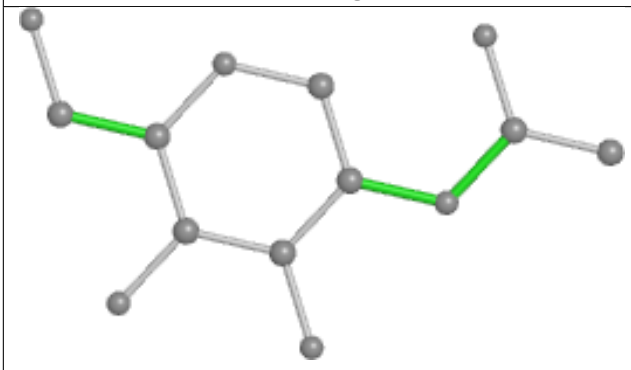


Bond angles



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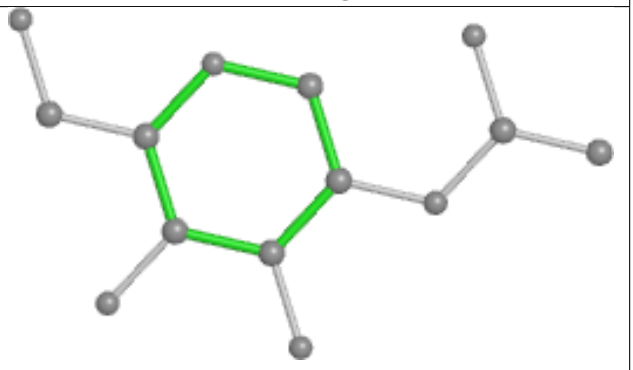
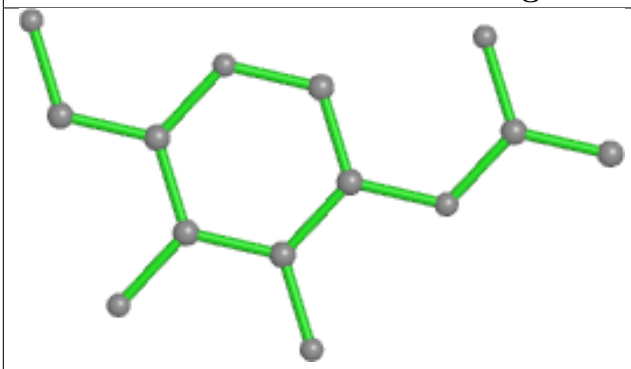


Rings

Ligand NAG F 705



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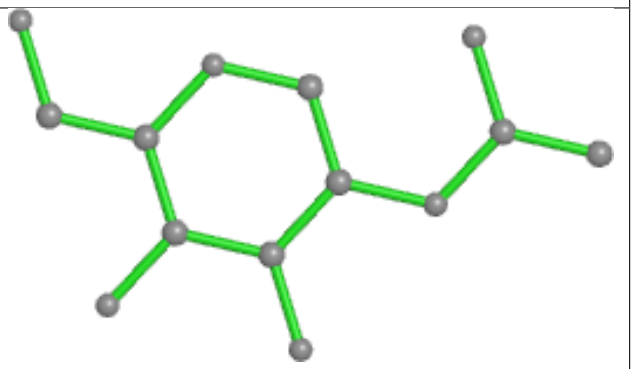
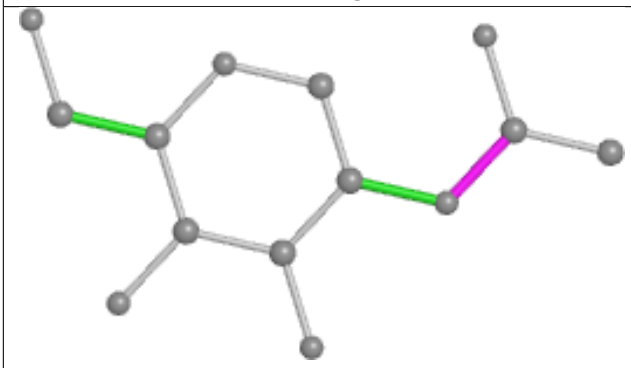


Bond angles



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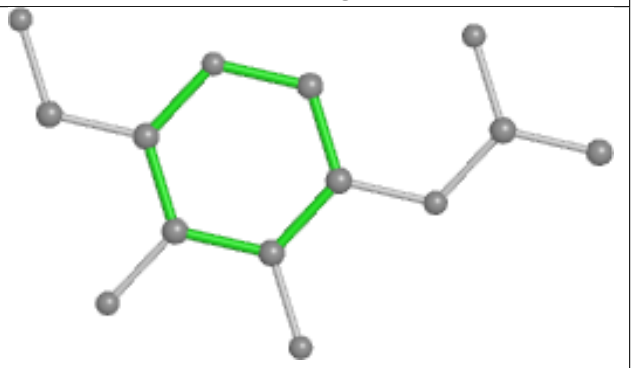
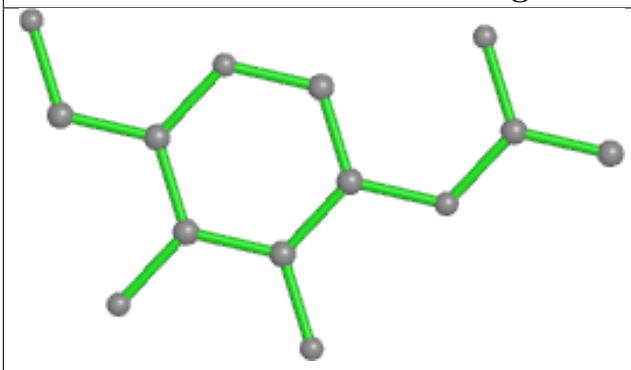
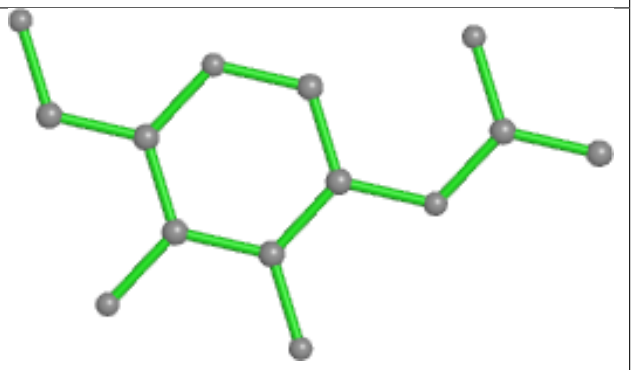


Rings

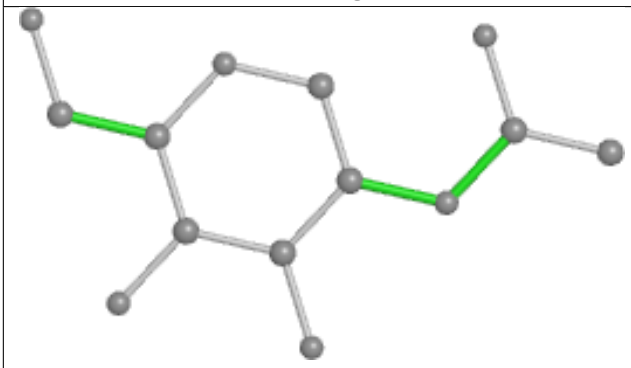
Ligand NAG C 1310



Bond lengths



Bond angles



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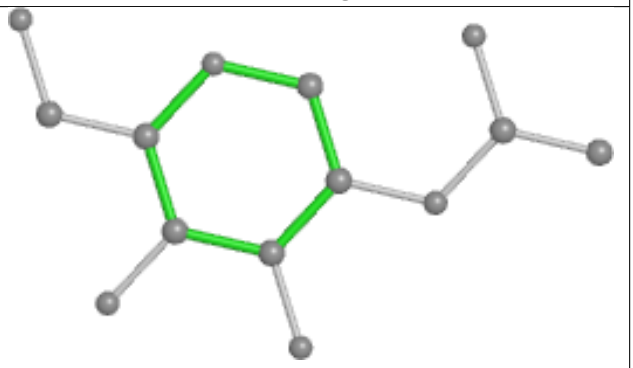
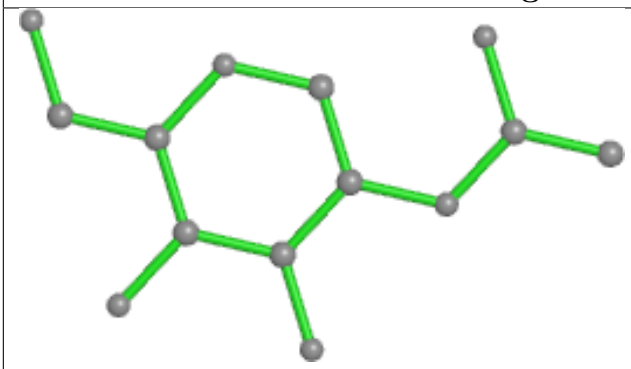
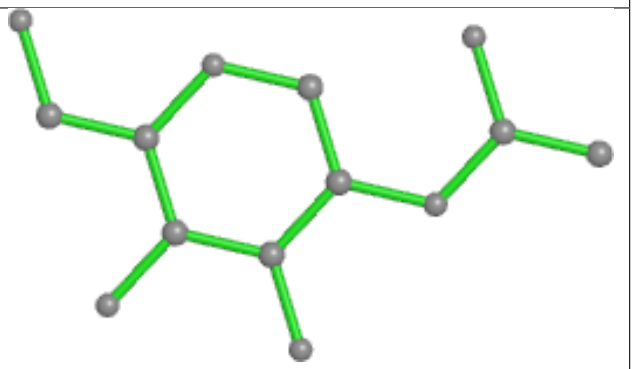


Rings

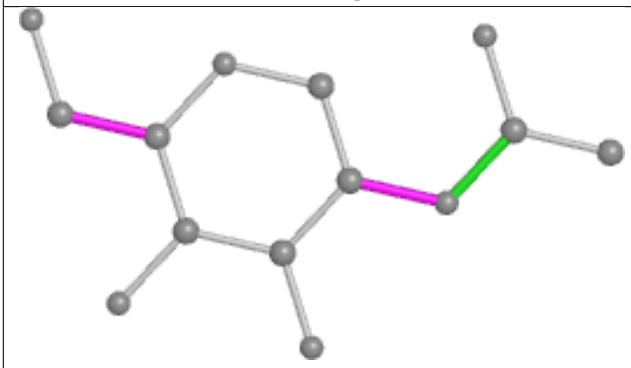
Ligand NAG E 704



Bond lengths



Bond angles



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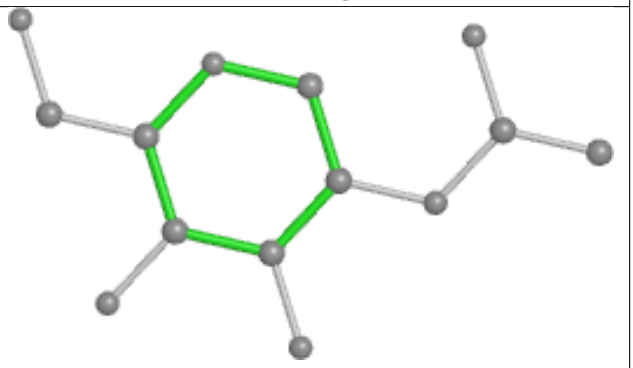
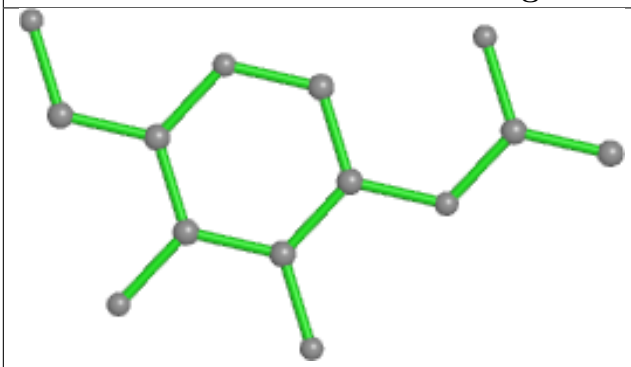
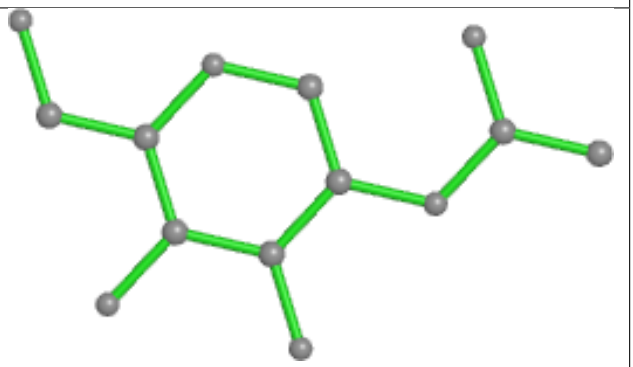


Rings

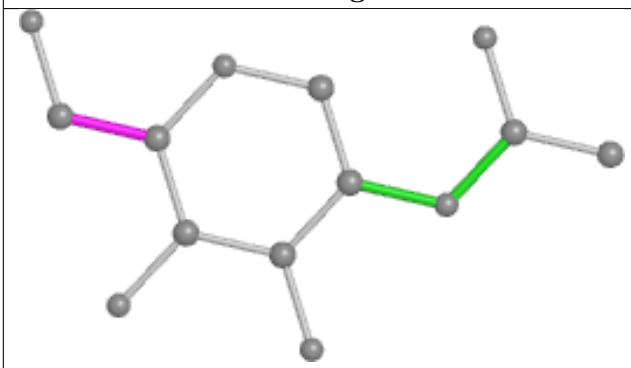
Ligand NAG E 705



Bond lengths



Bond angles



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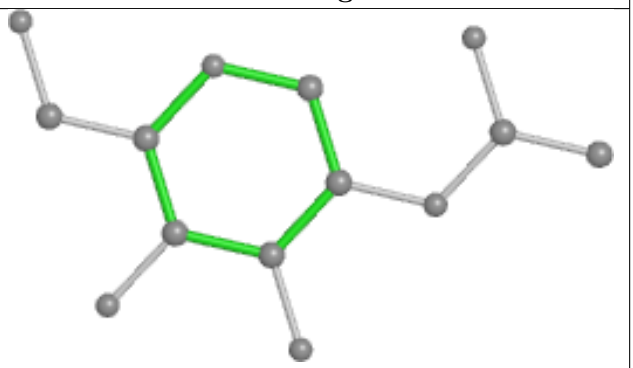
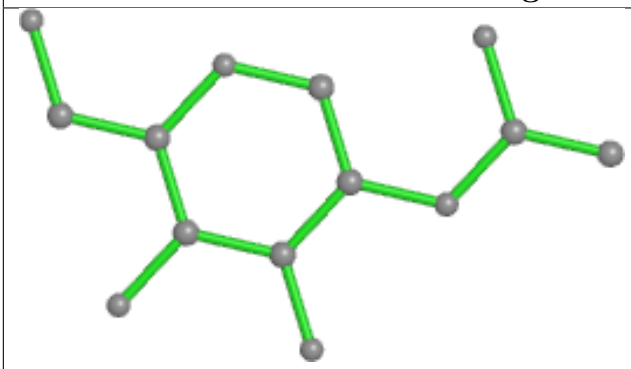
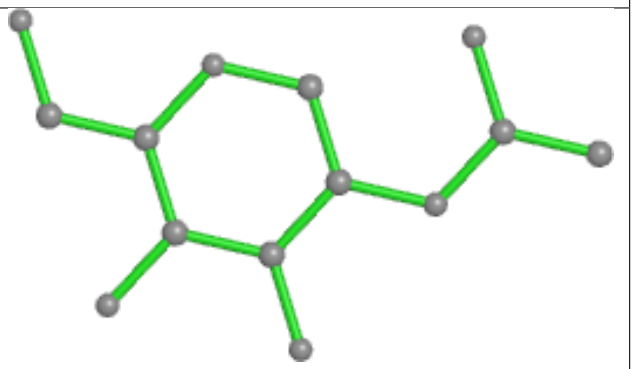
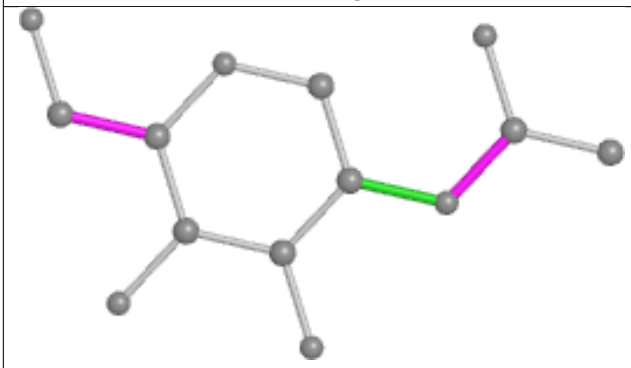
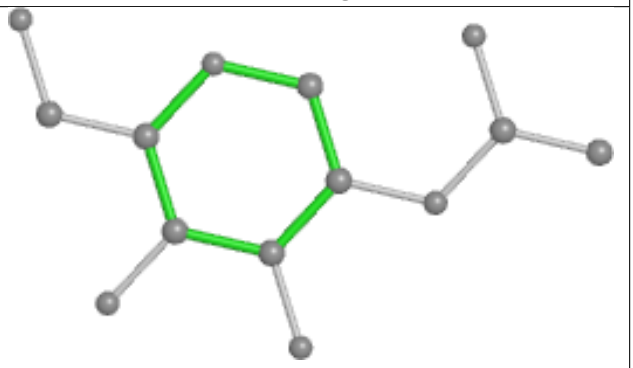
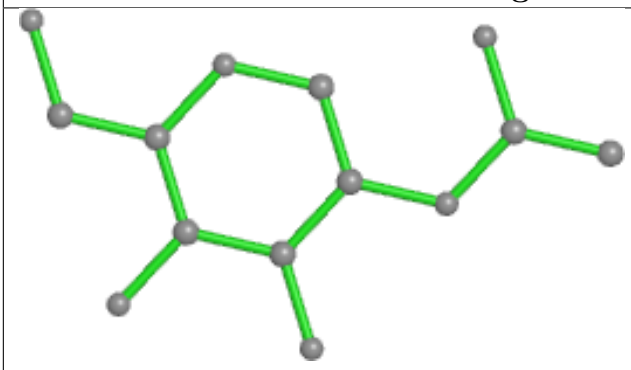
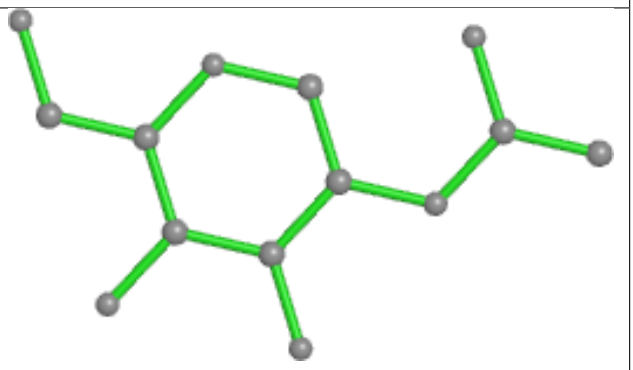
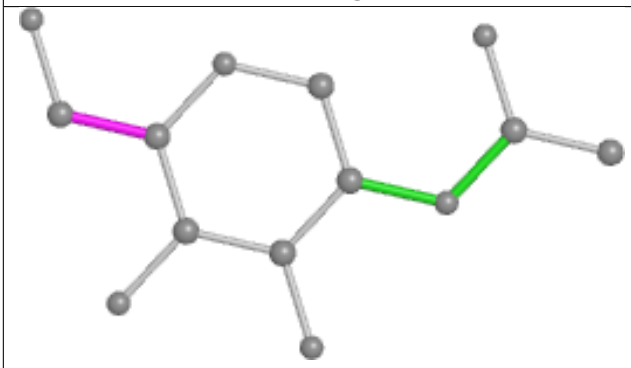
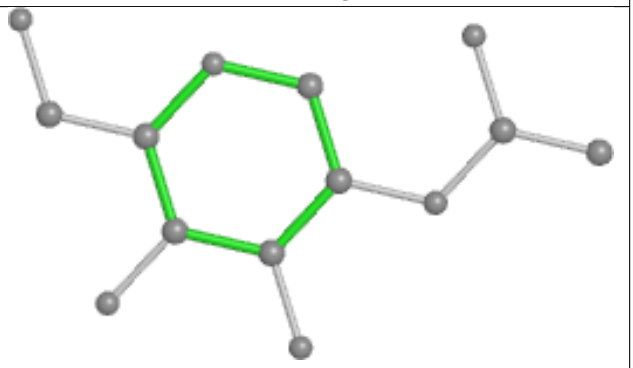
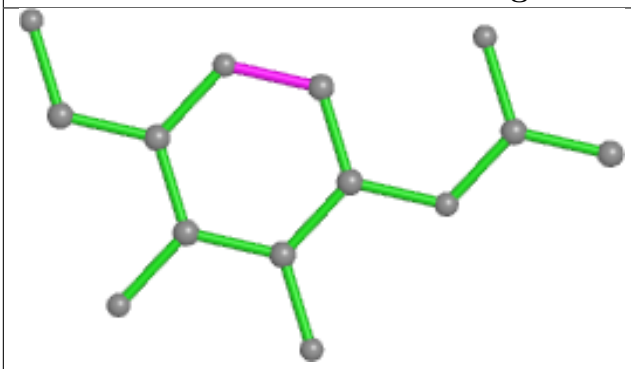
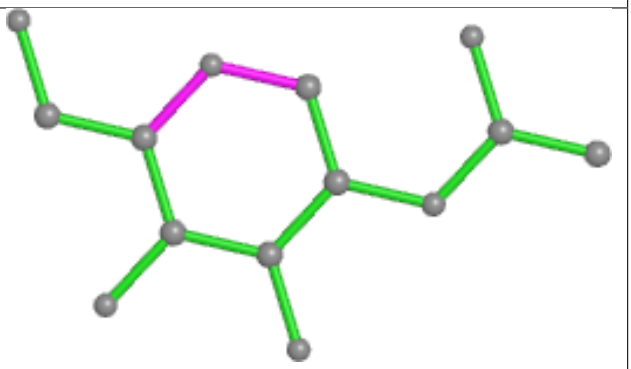
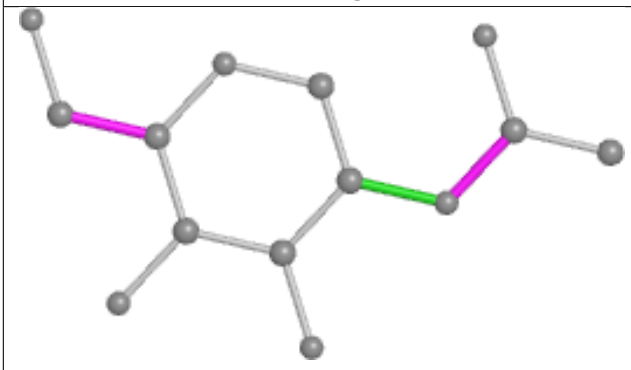
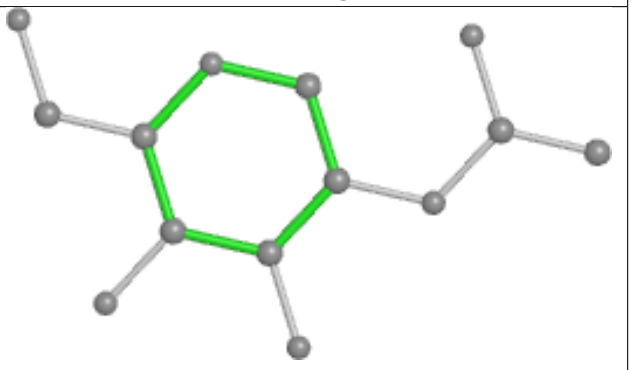
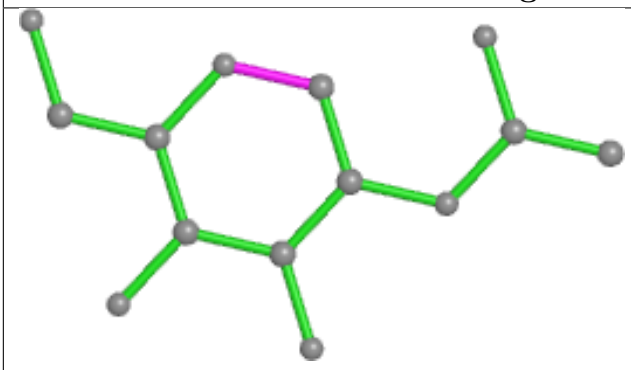
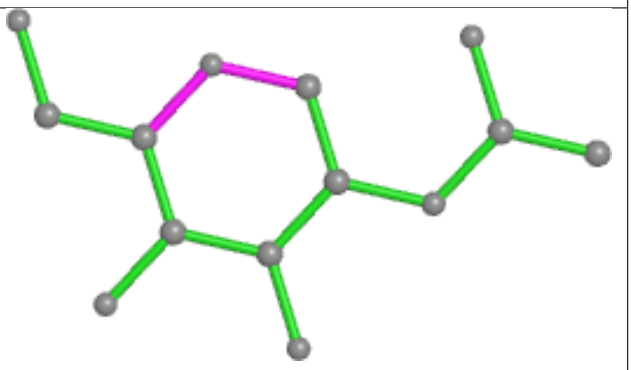
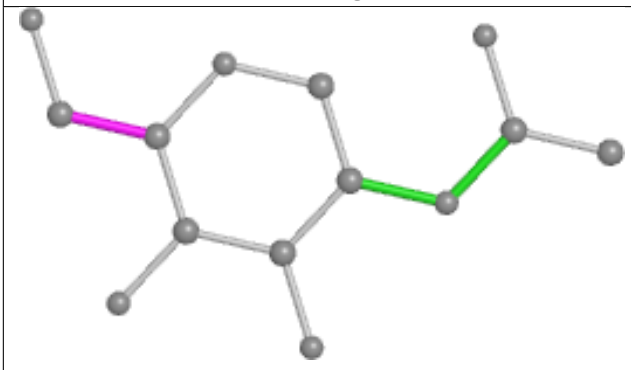
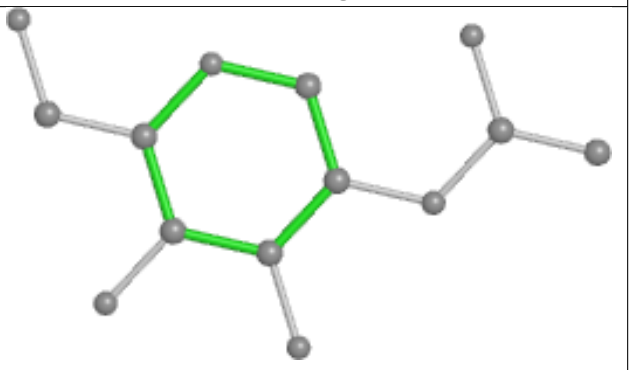


Rings

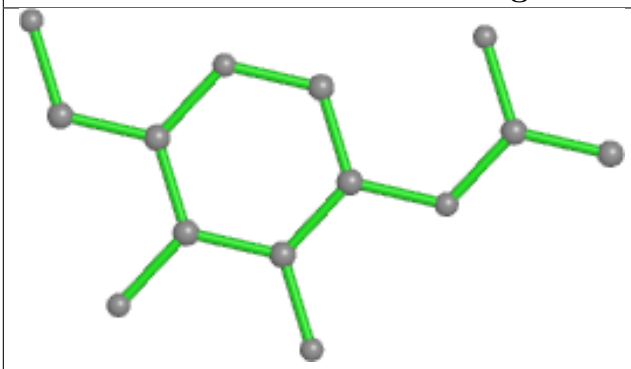
Ligand NAG F 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 1311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG D 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1309



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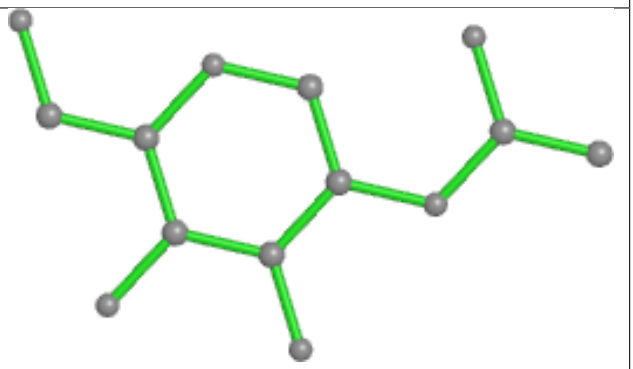
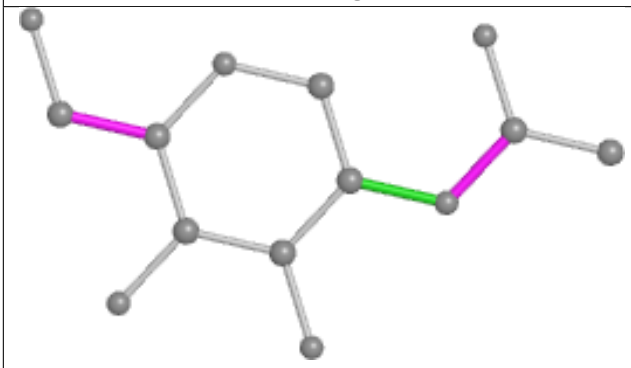
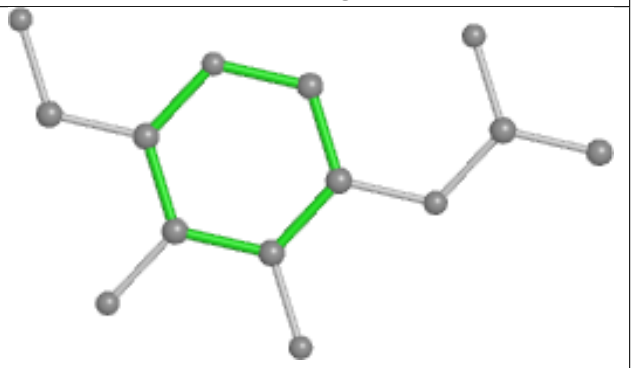


Bond angles

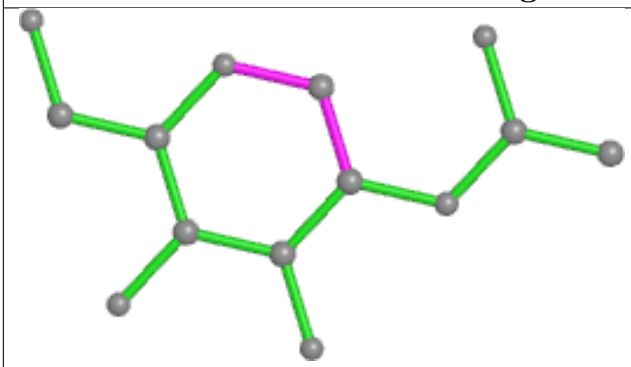


Torsions



Rings

Ligand NAG D 705



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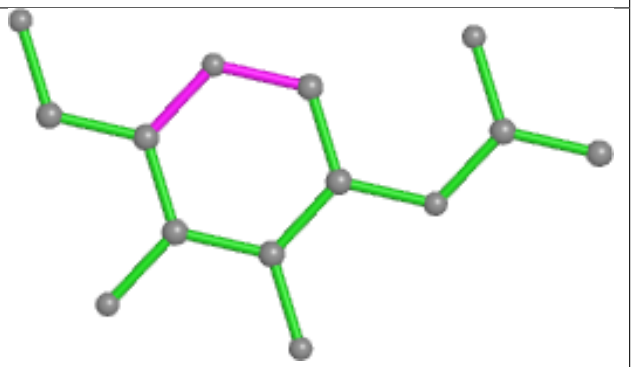
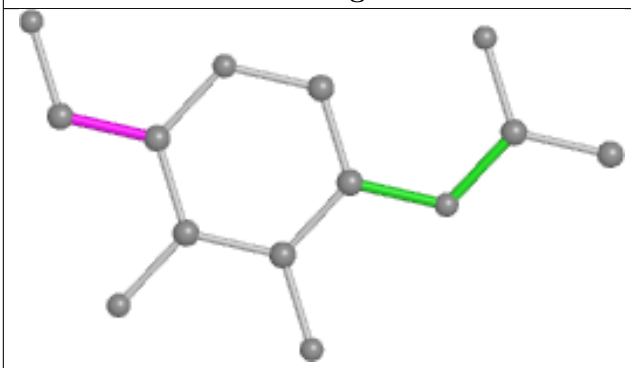


Bond angles



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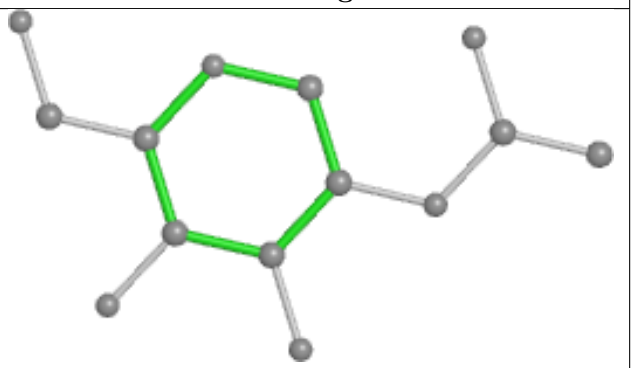
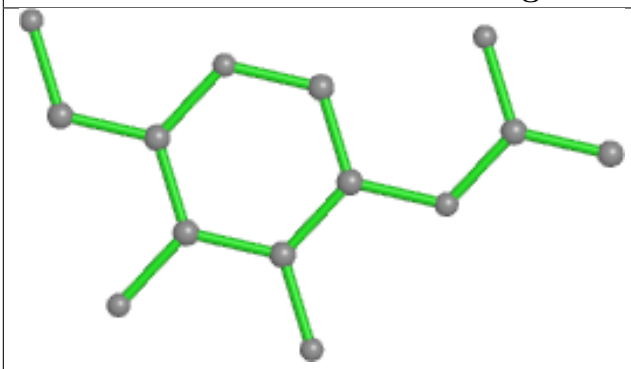


Rings

Ligand NAG F 702



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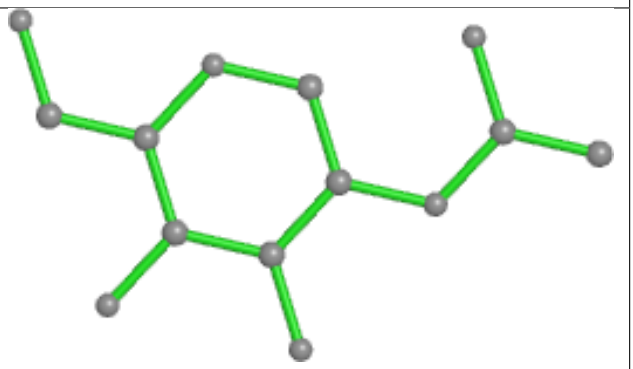
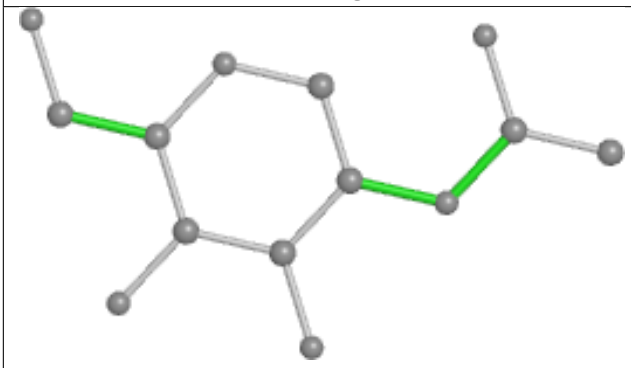


Bond angles



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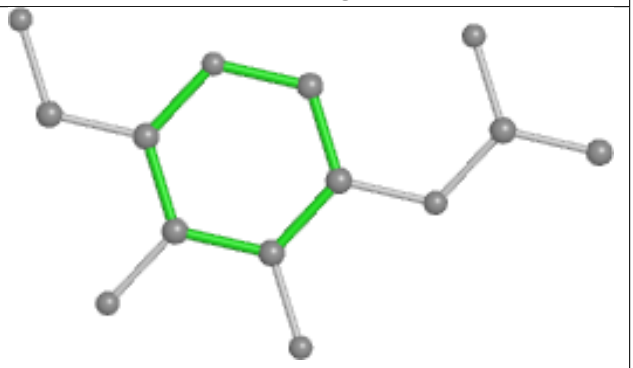
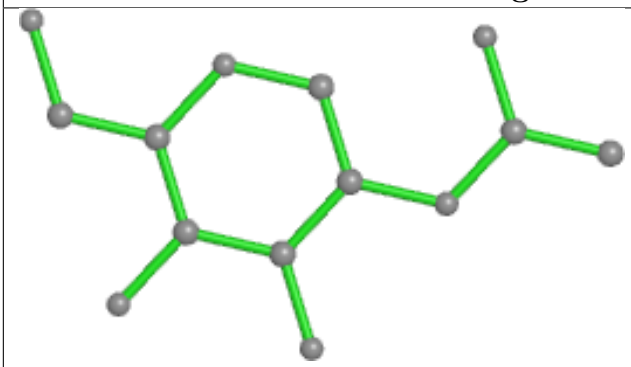


Rings

Ligand NAG B 1302



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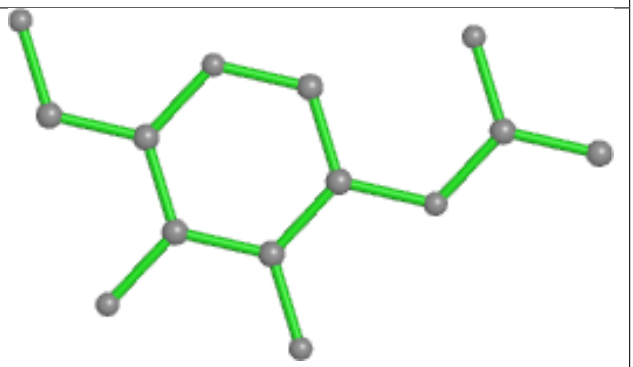

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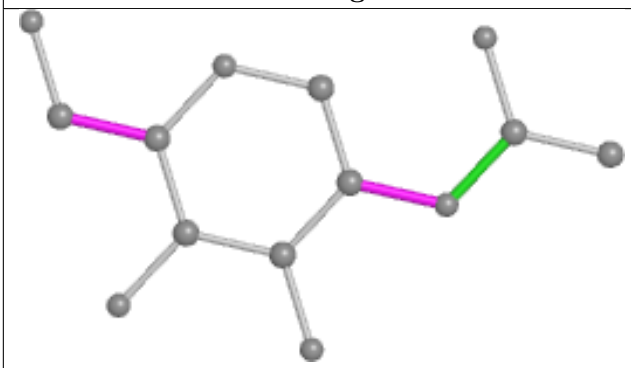

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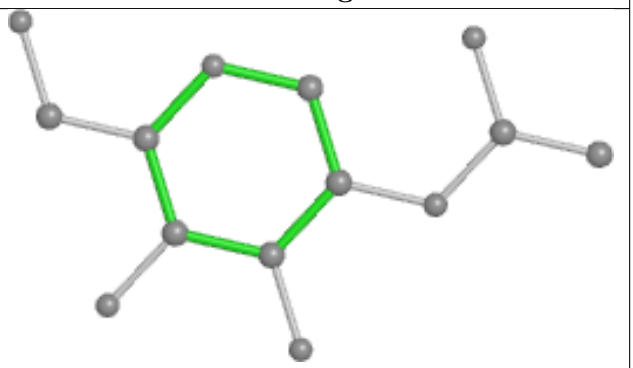
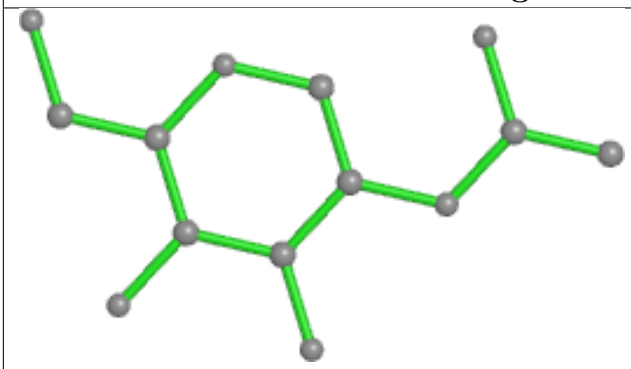


Rings

Ligand NAG C 1314



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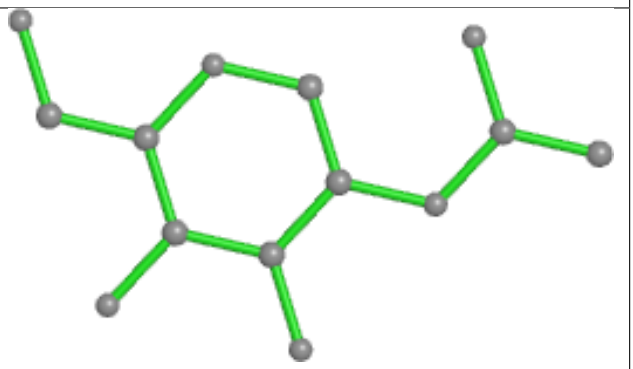
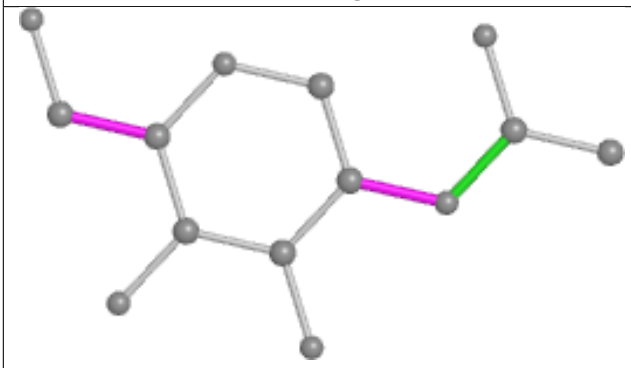


Bond angles



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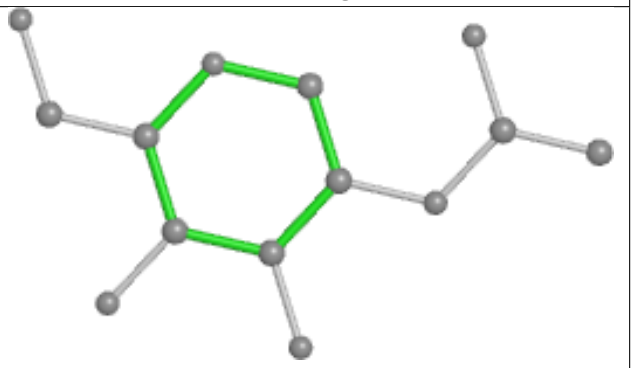
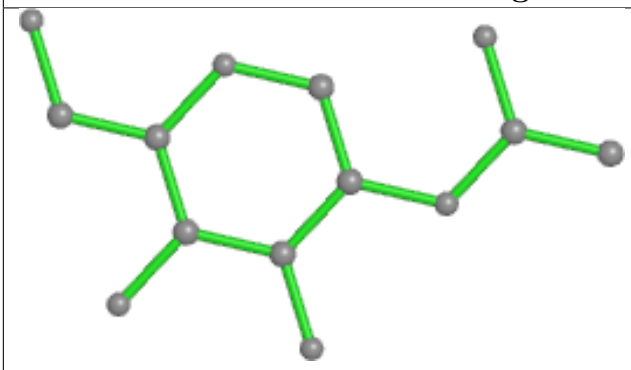


Rings

Ligand NAG B 1308



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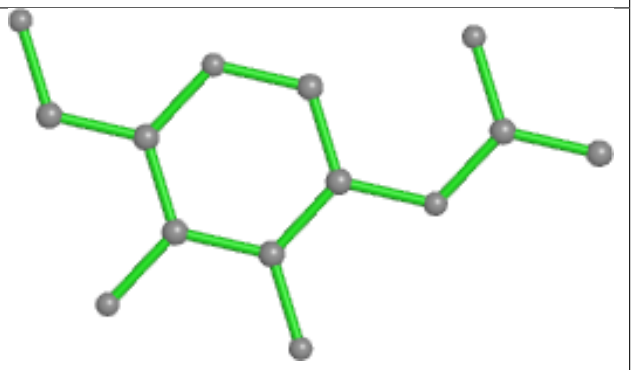

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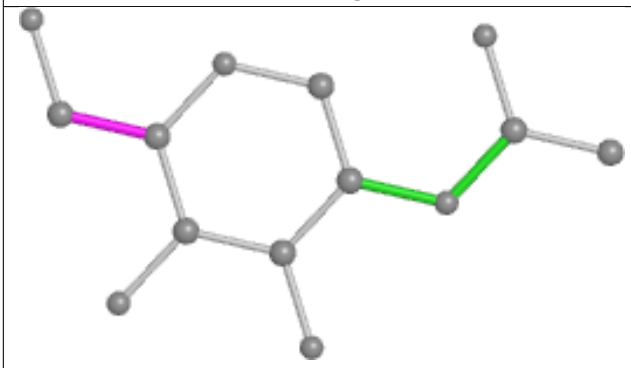

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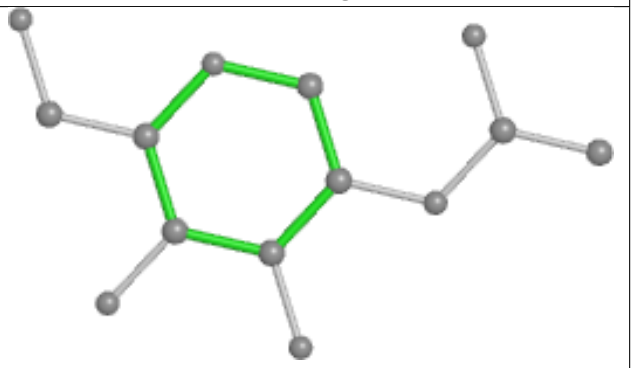
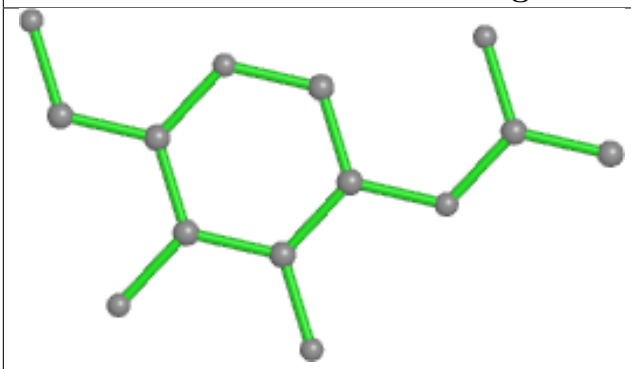


Rings

Ligand NAG B 1305



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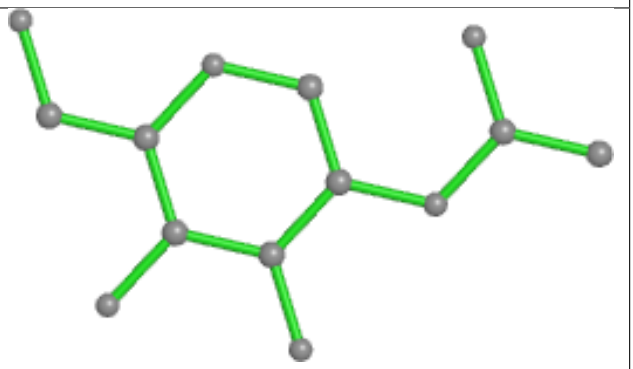
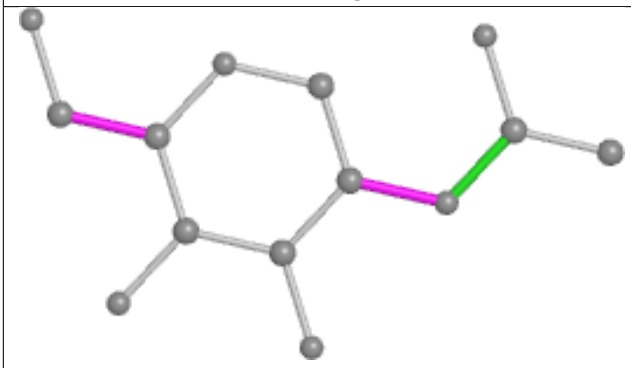


Bond angles



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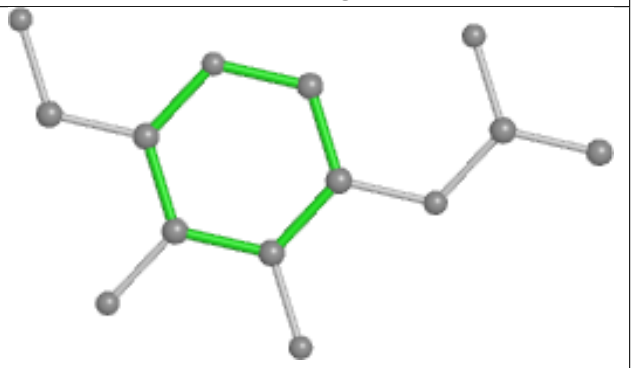
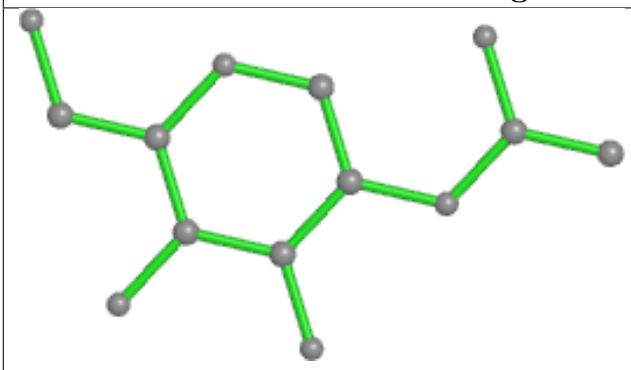
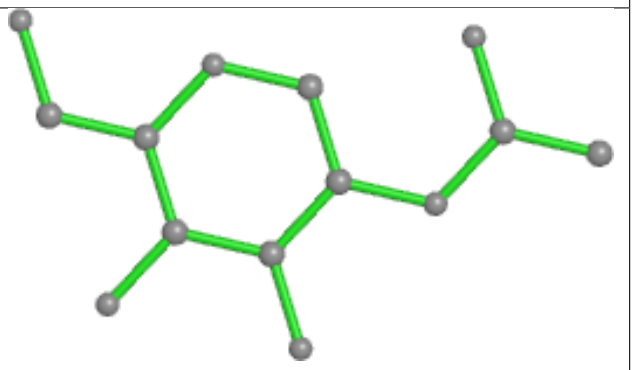


Rings

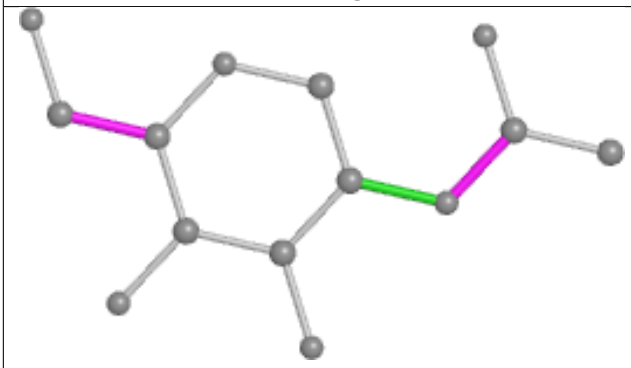
Ligand NAG A 1303



Bond lengths



Bond angles



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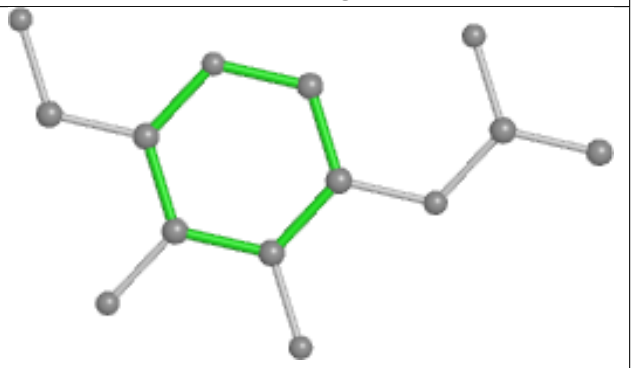
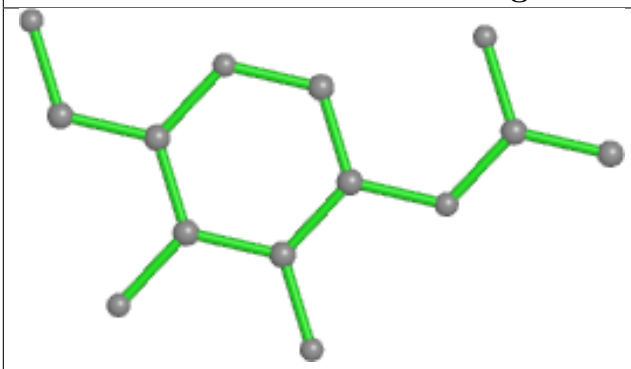
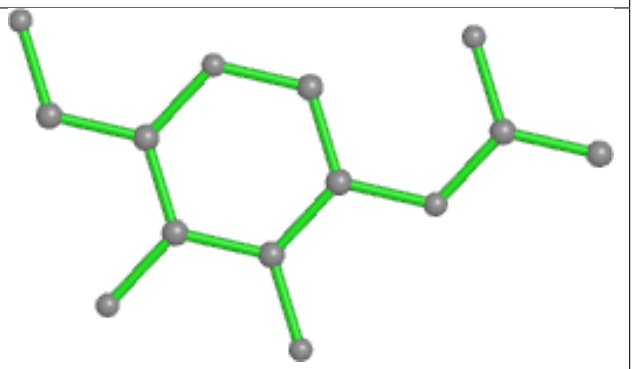


Rings

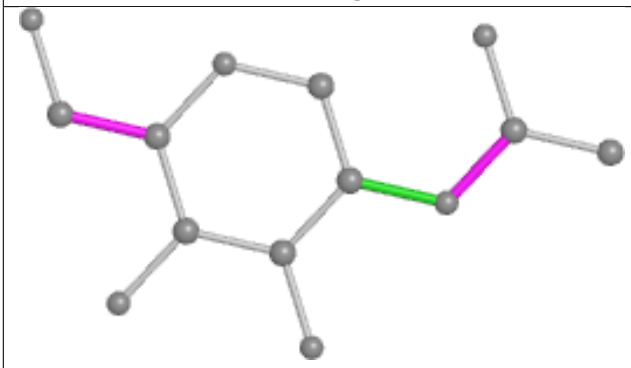
Ligand NAG A 1302



Bond lengths



Bond angles



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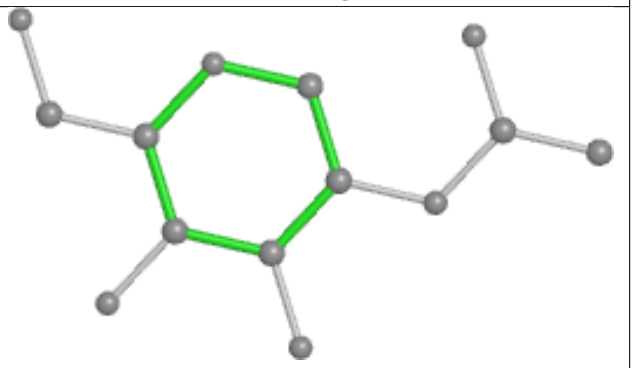
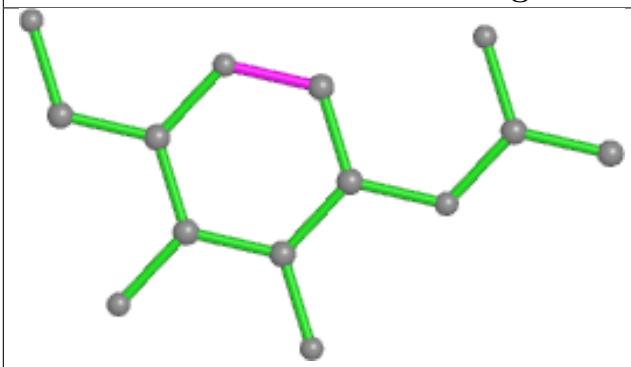


Rings

Ligand NAG C 1303



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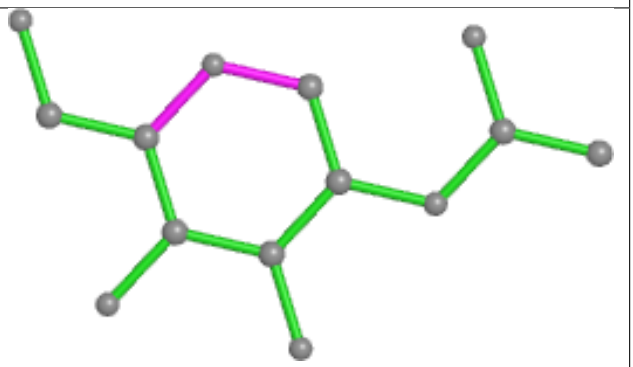

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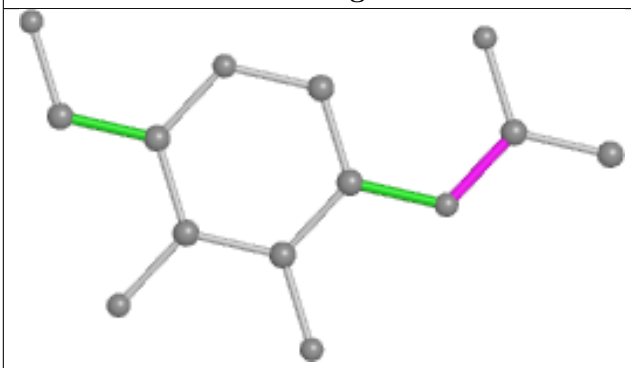

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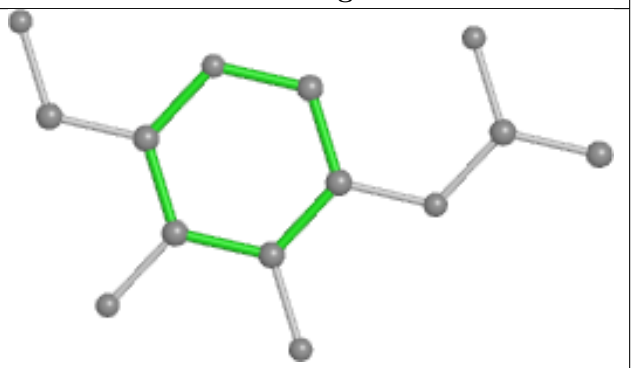
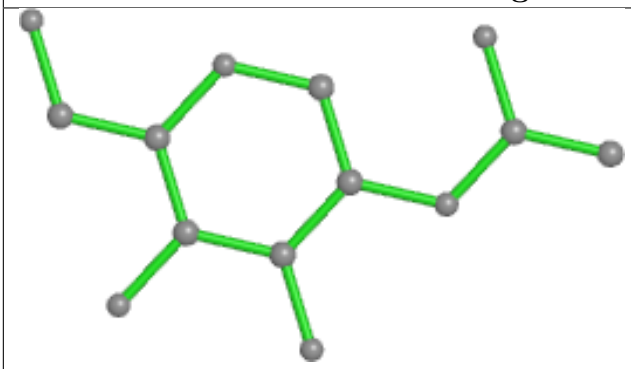
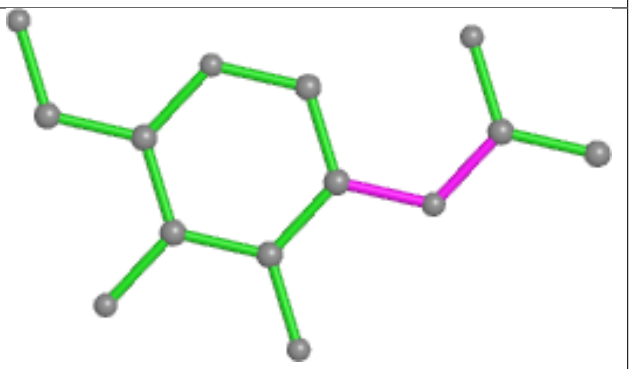
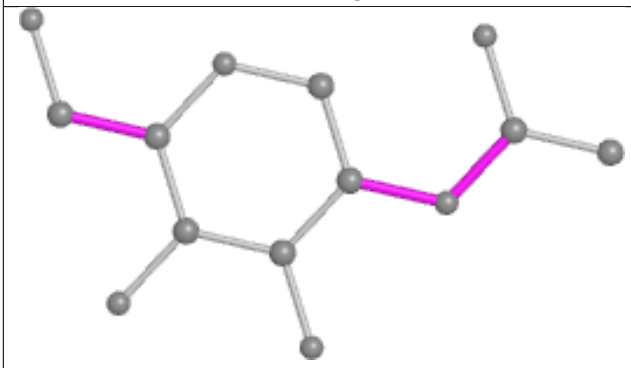
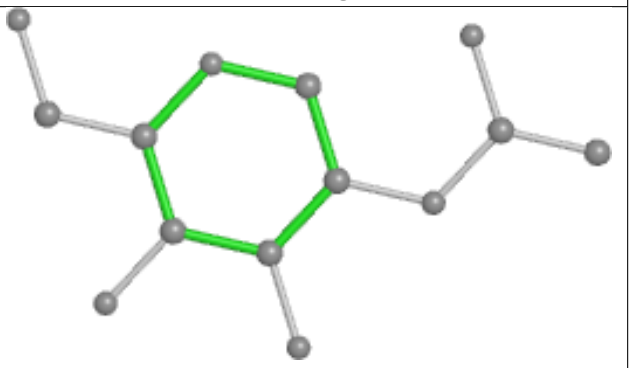
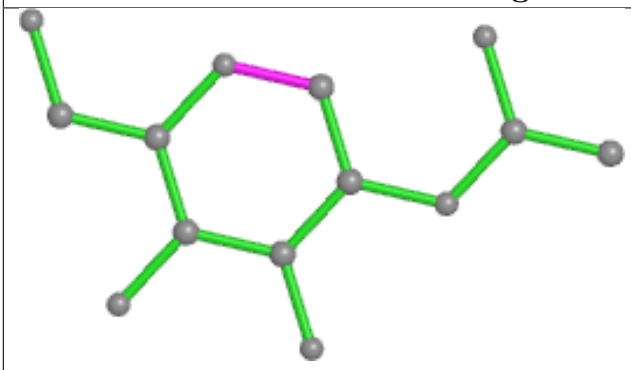
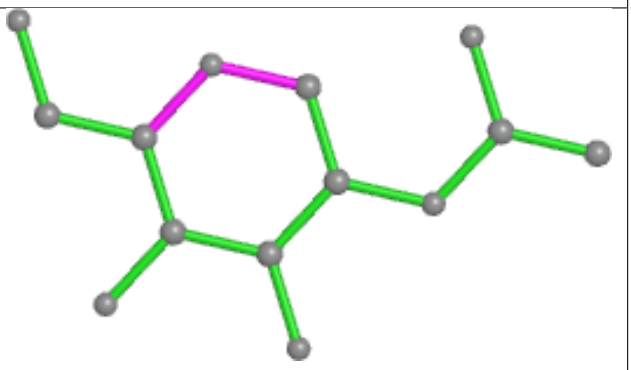
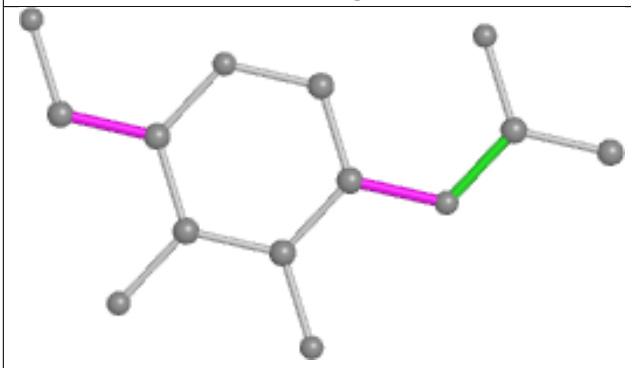
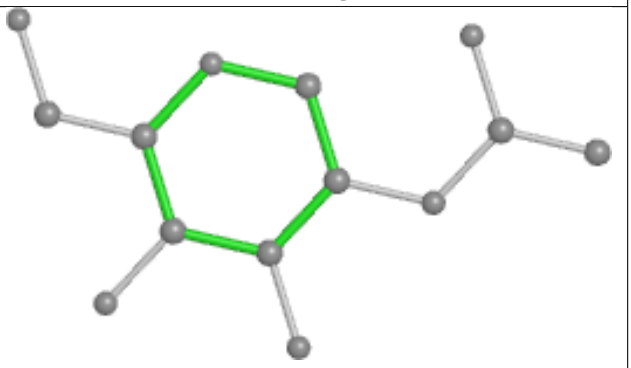
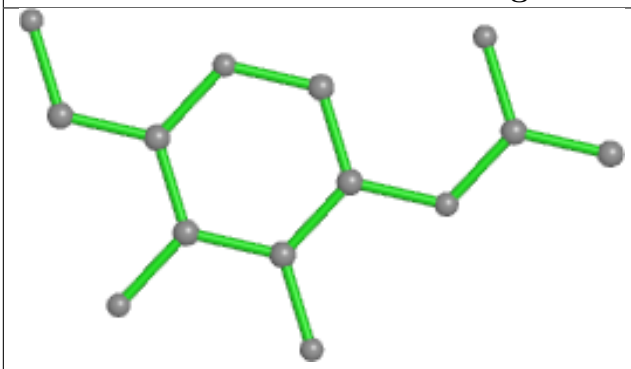


Rings

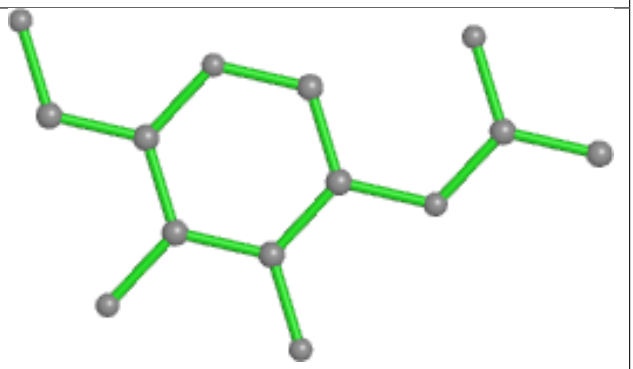
Ligand NAG C 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

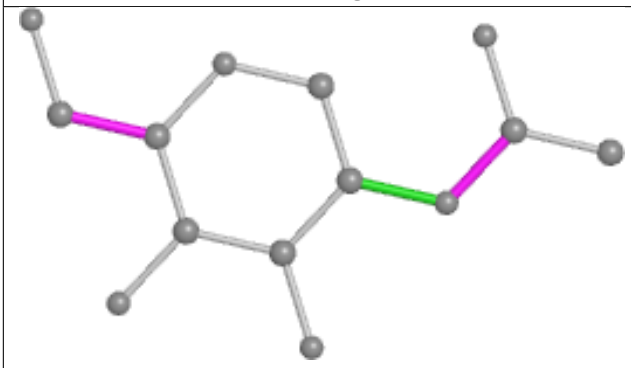
Ligand NAG A 1308



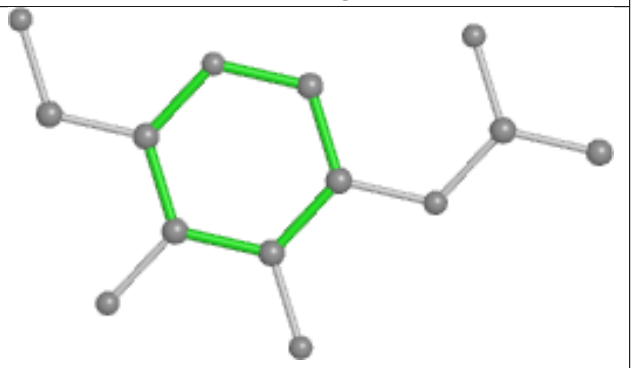
Bond lengths



Bond angles

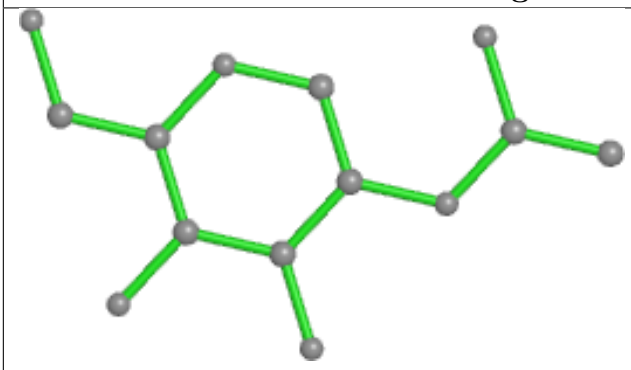


Torsions



Rings

Ligand NAG C 1307



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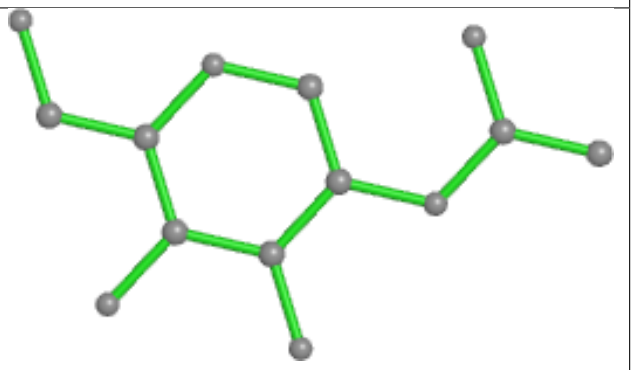
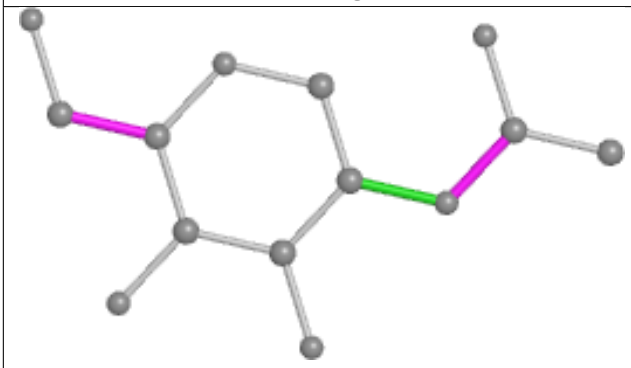
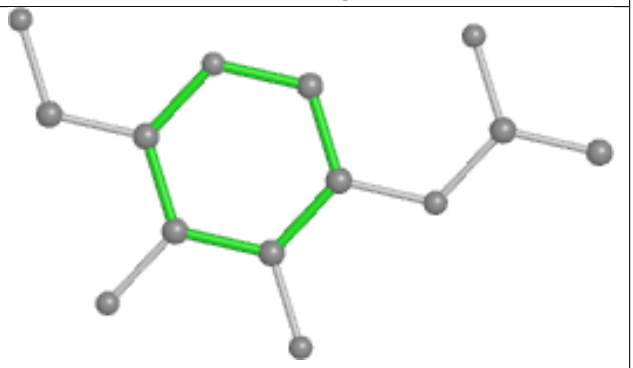


Bond angles

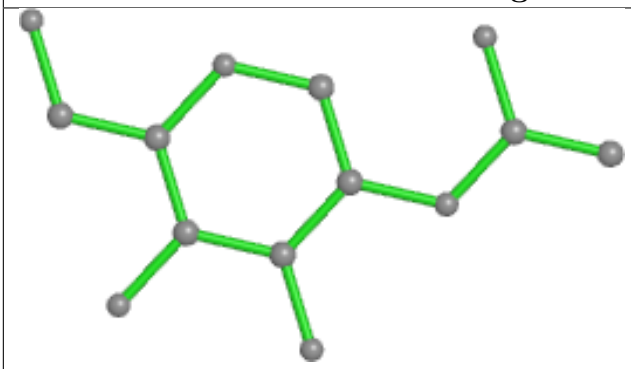


Torsions

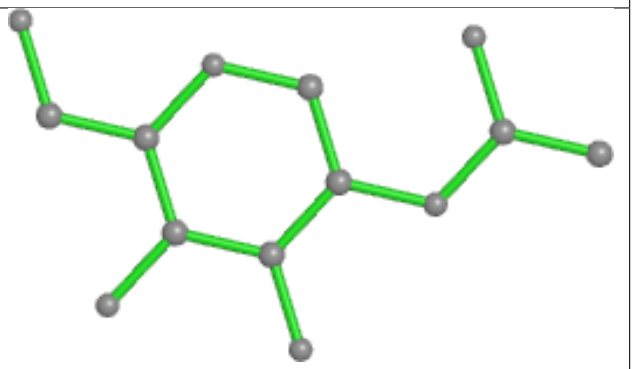


Rings

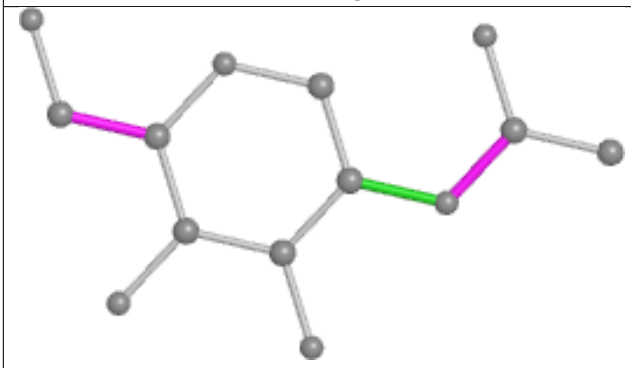
Ligand NAG A 1305



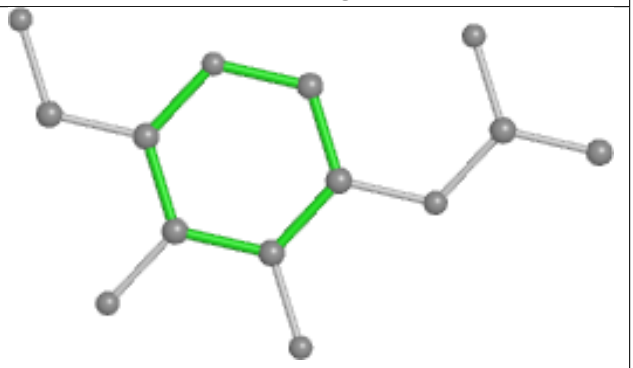
Bond lengths



Bond angles

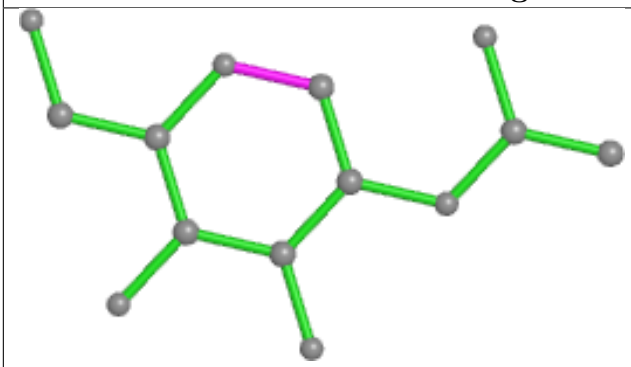


Torsions



Rings

Ligand NAG A 1311



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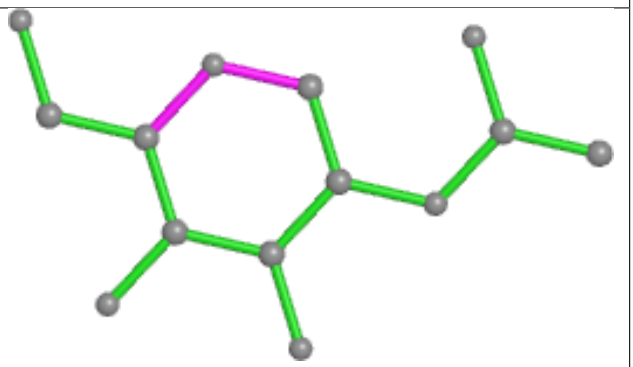
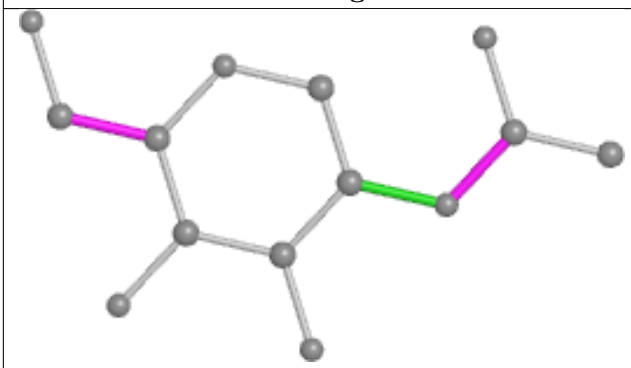


Bond angles



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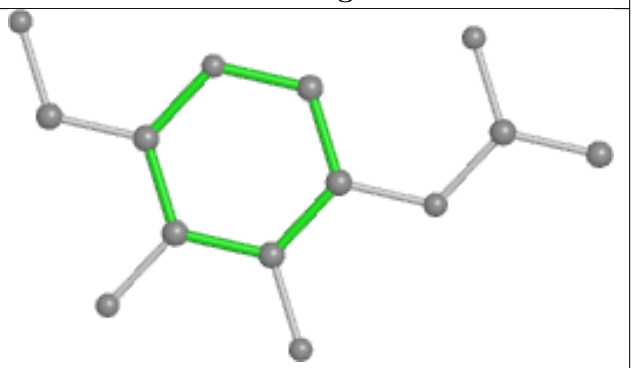
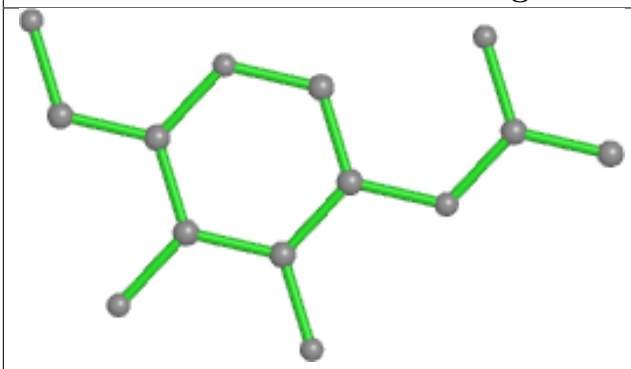
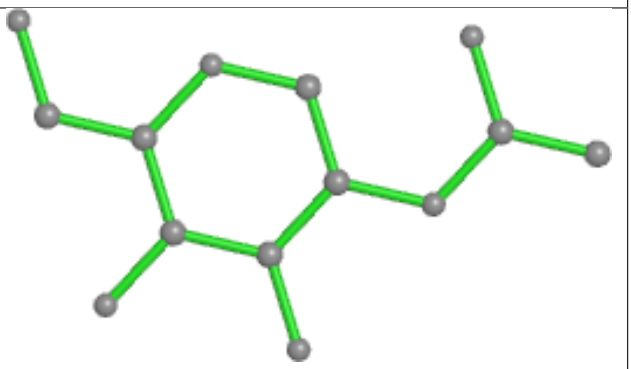
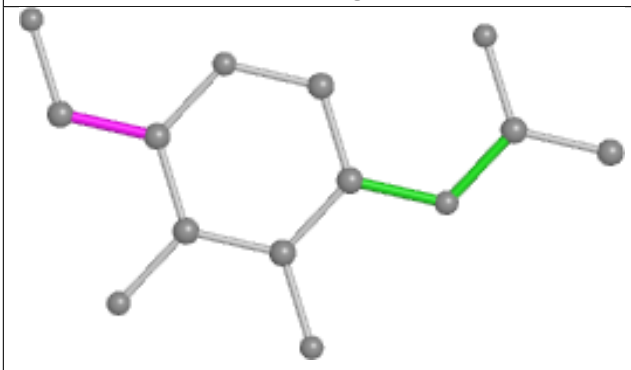
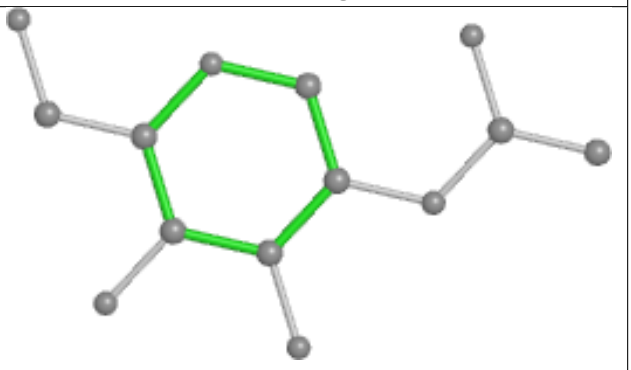
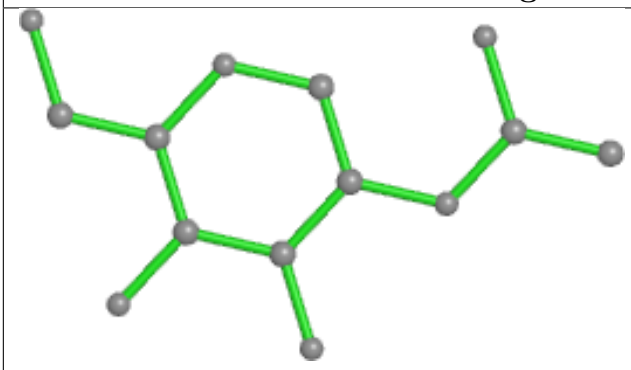
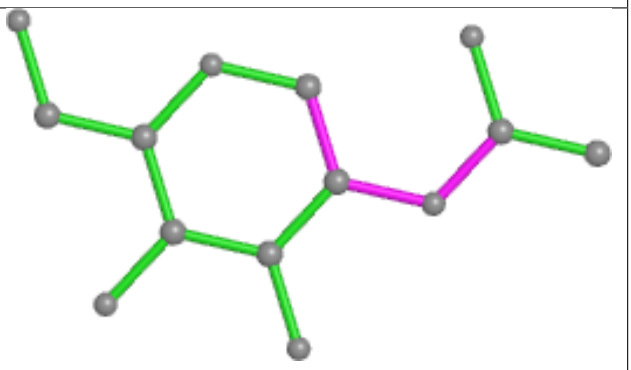
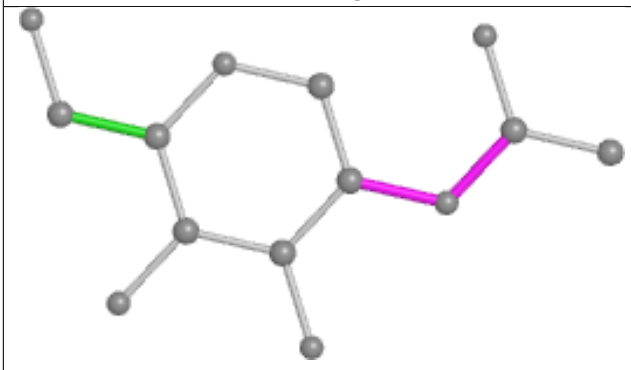
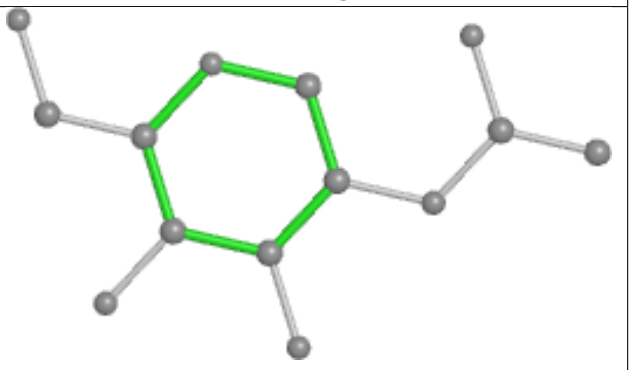
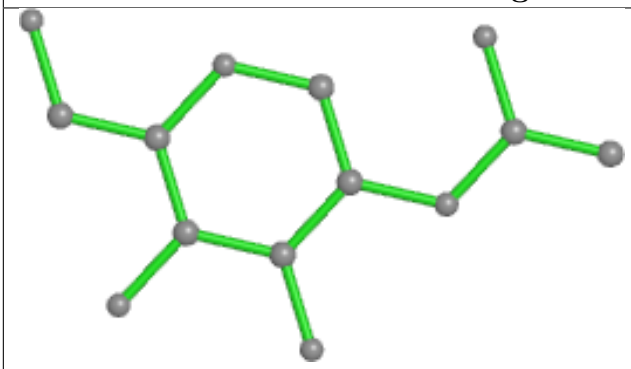


Rings

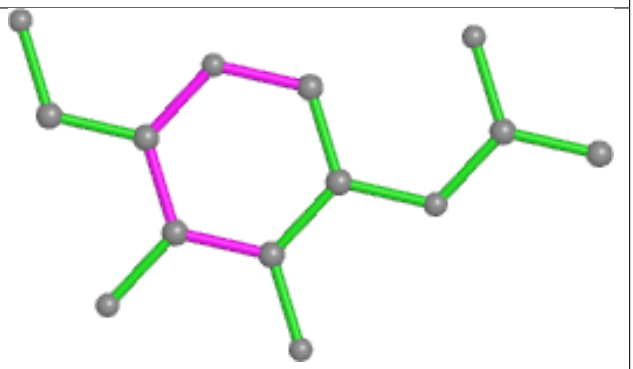
Ligand NAG C 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG D 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

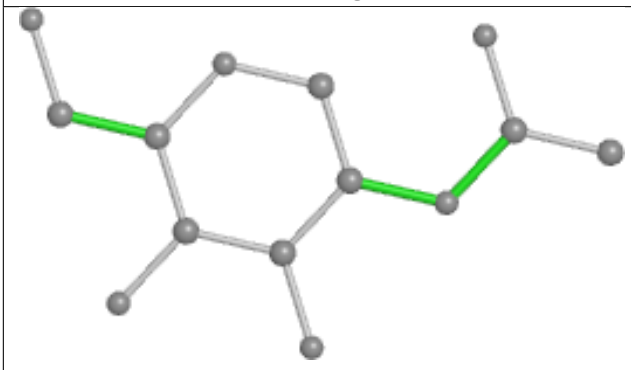
Ligand NAG C 1313



Bond lengths



Bond angles



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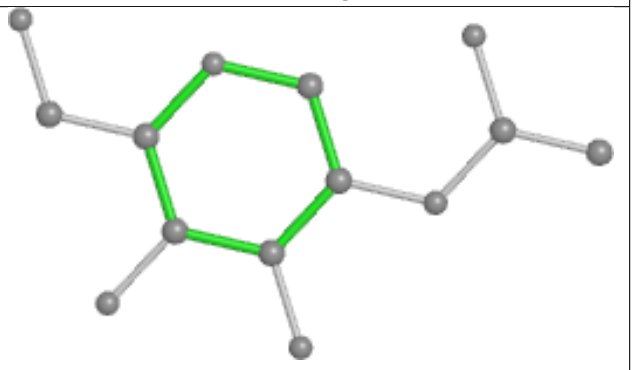
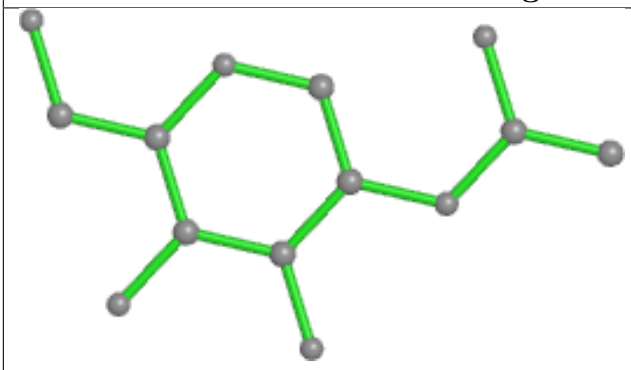


Rings

Ligand NAG F 703



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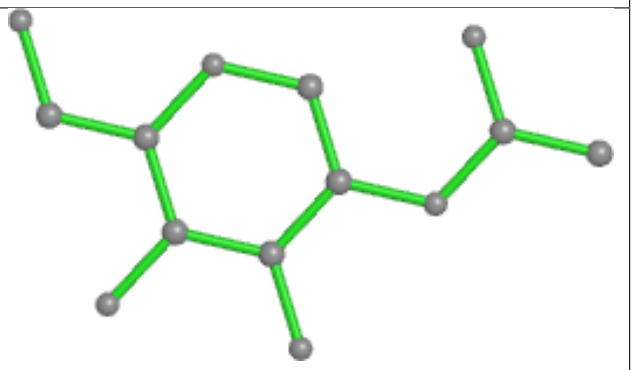
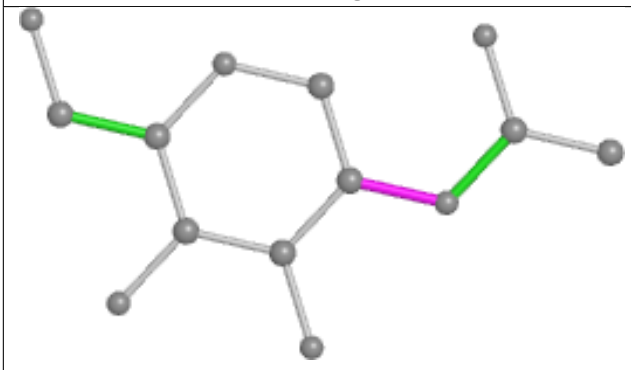


Bond angles



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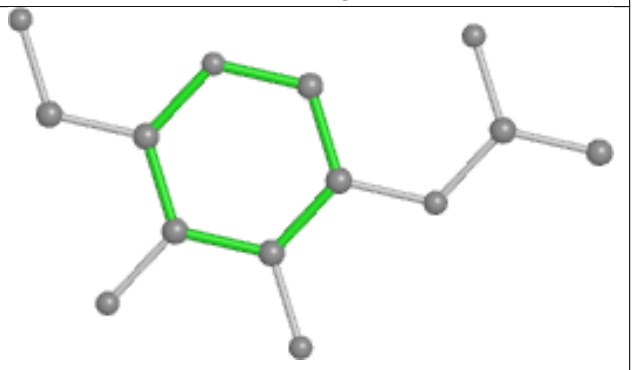
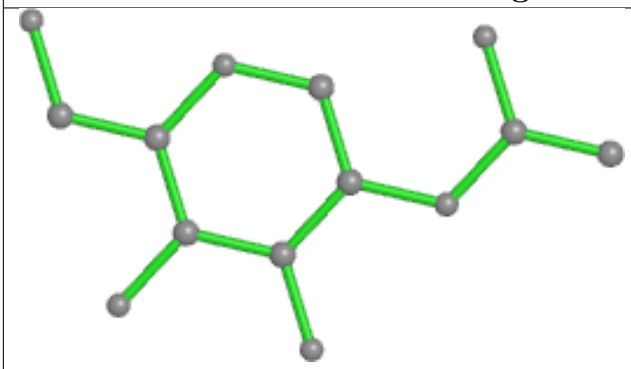


Rings

Ligand NAG B 1301



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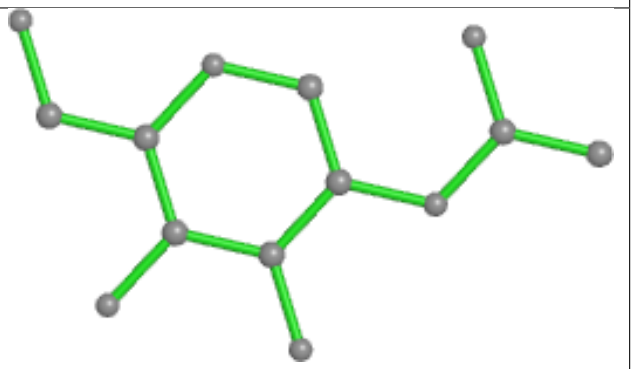
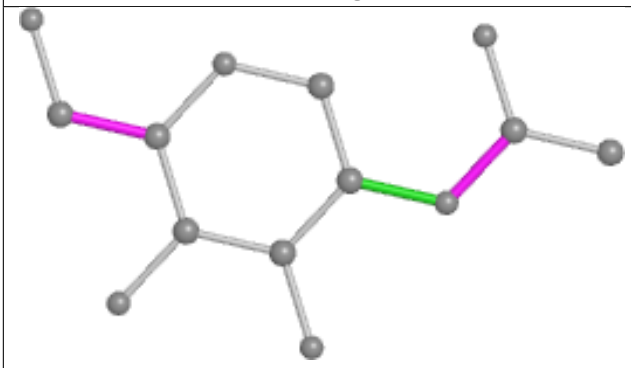


Bond angles



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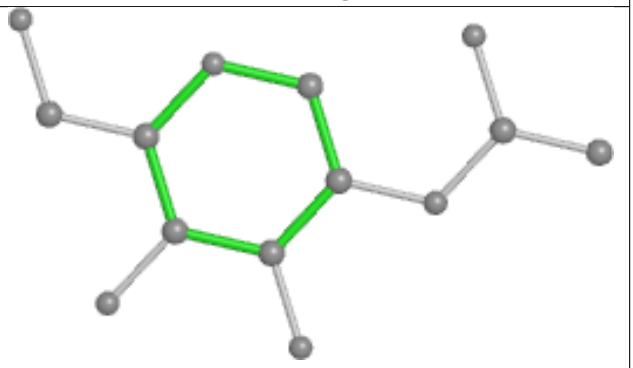
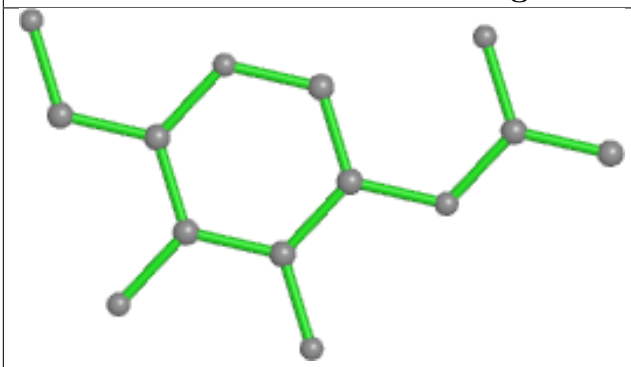


Rings

Ligand NAG A 1304



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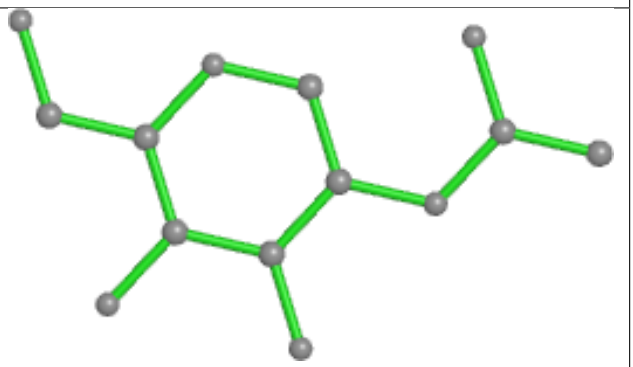
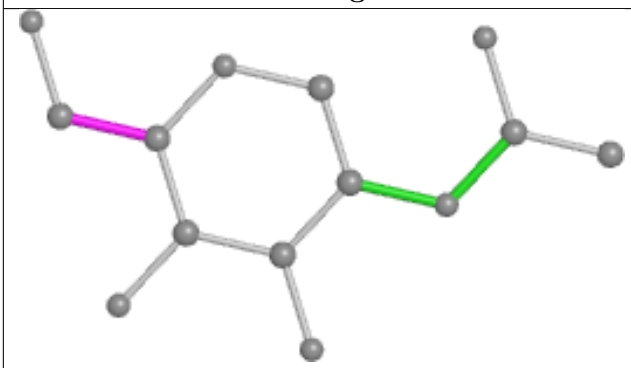


Bond angles



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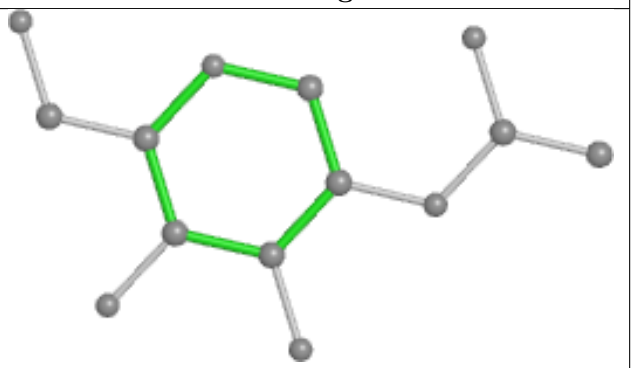
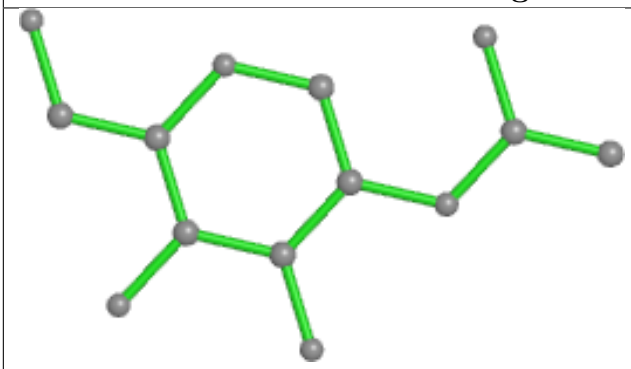


Rings

Ligand NAG C 1308



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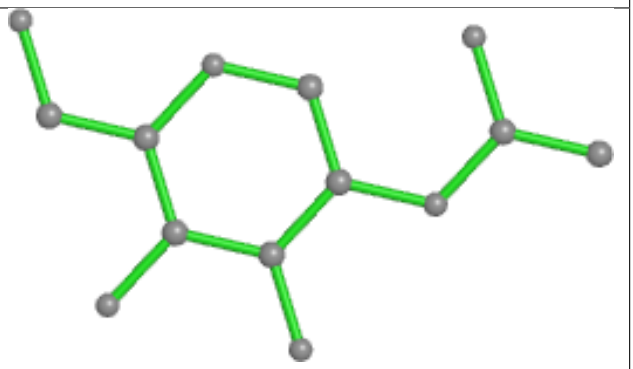
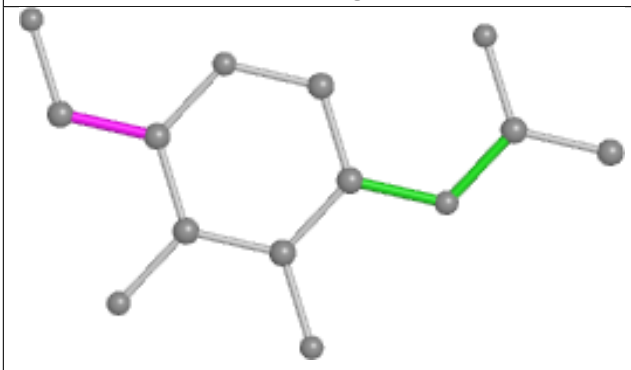


Bond angles



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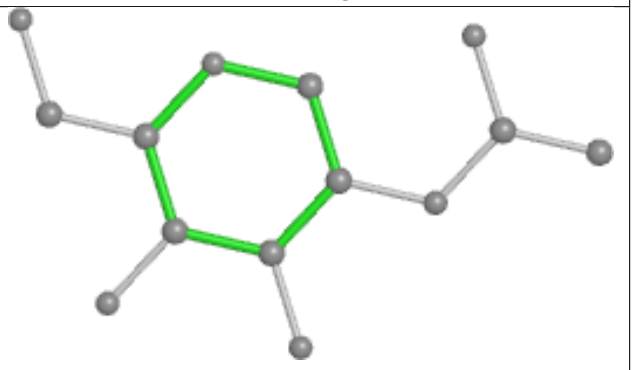
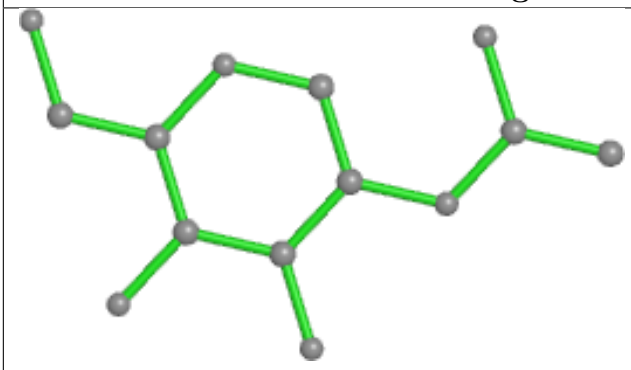


Rings

Ligand NAG B 1304



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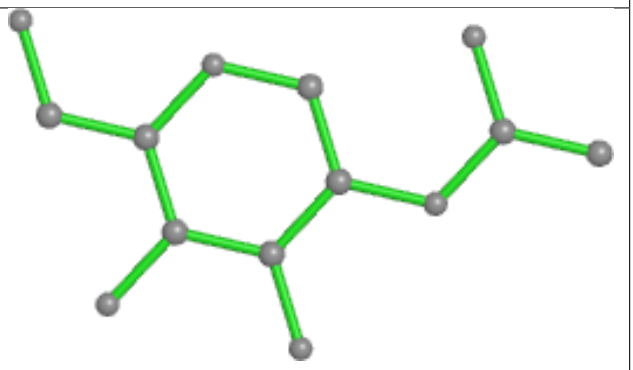
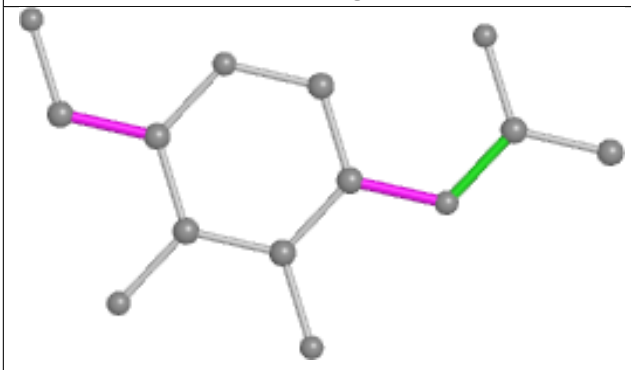


Bond angles



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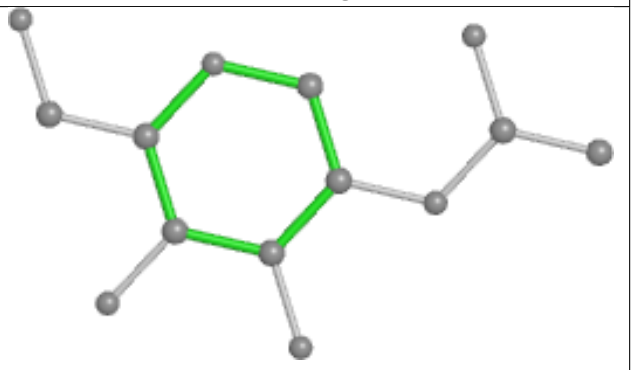
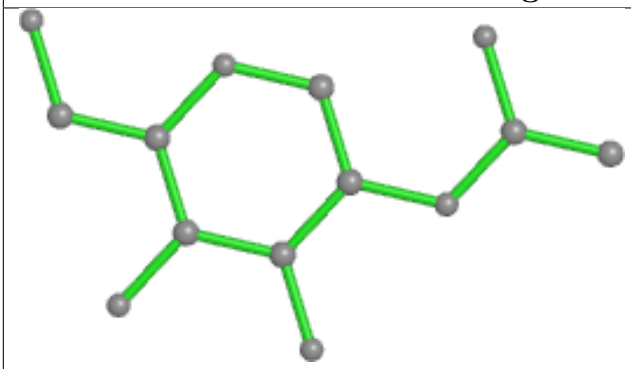
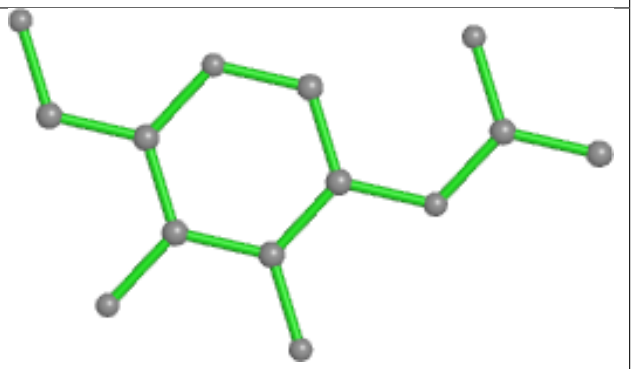


Rings

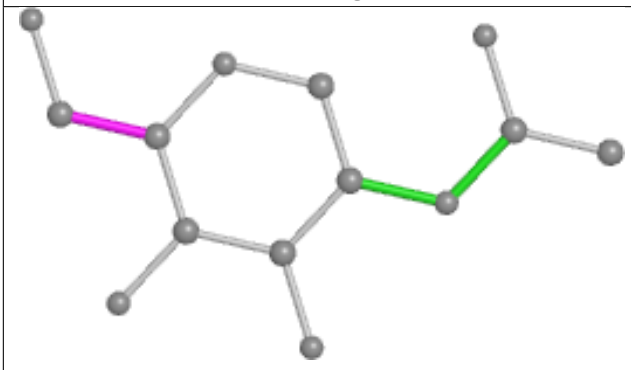
Ligand NAG E 701



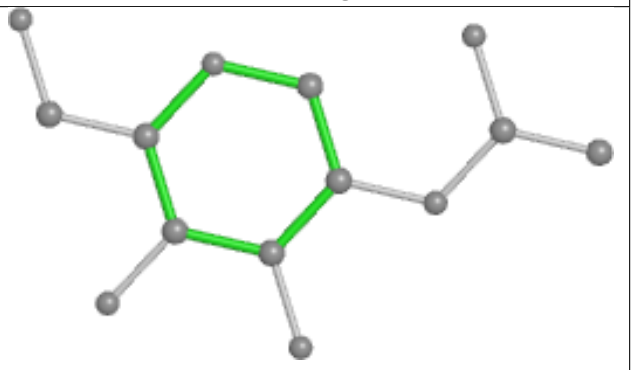
Bond lengths



Bond angles

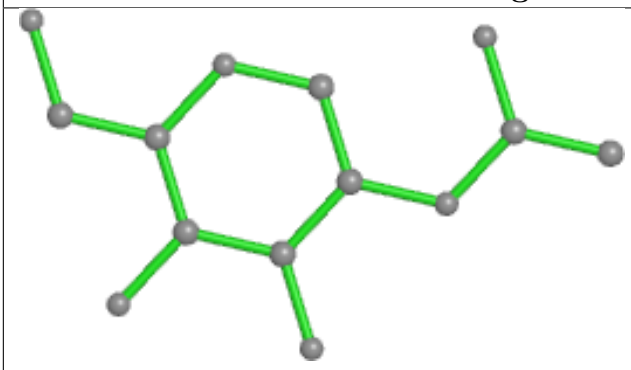


Torsions

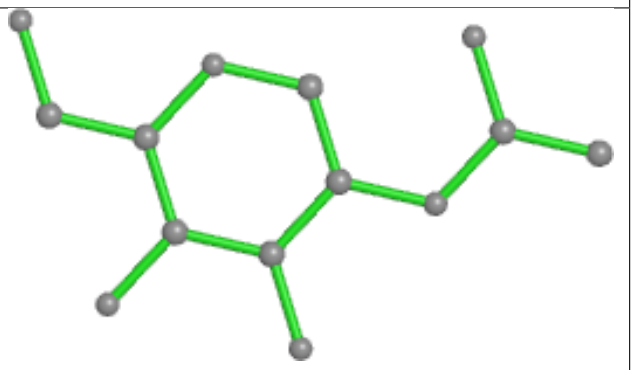


Rings

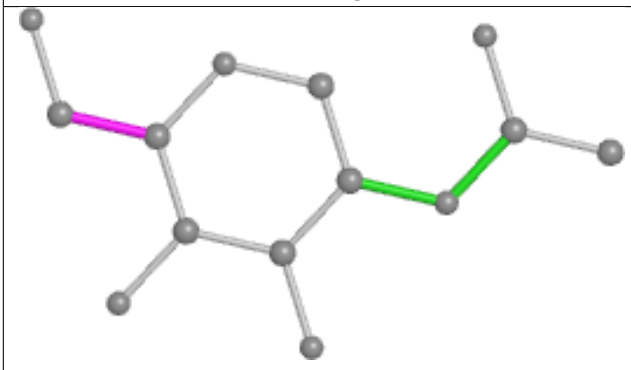
Ligand NAG C 1301



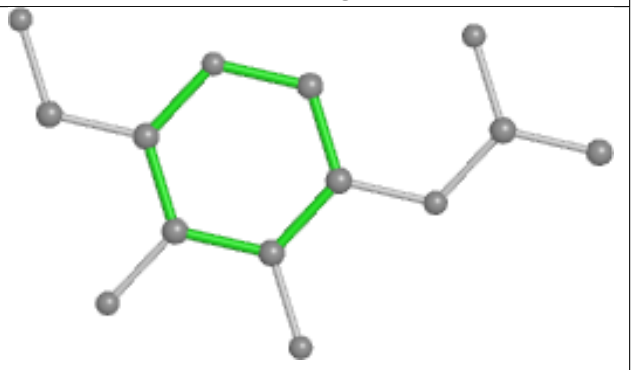
Bond lengths



Bond angles

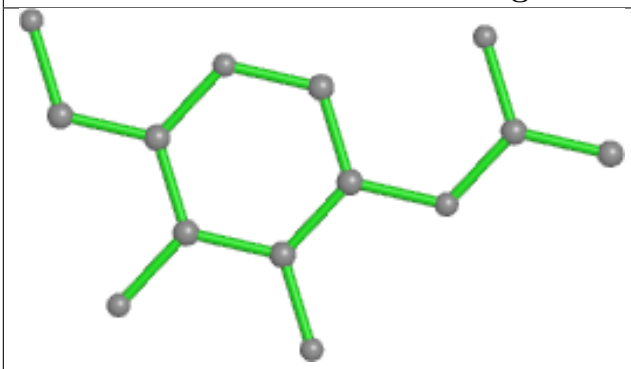


Torsions

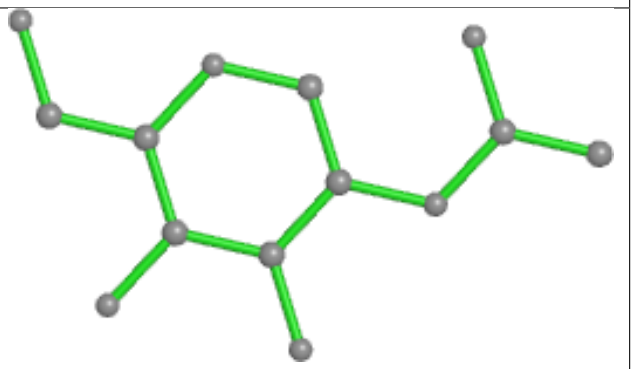


Rings

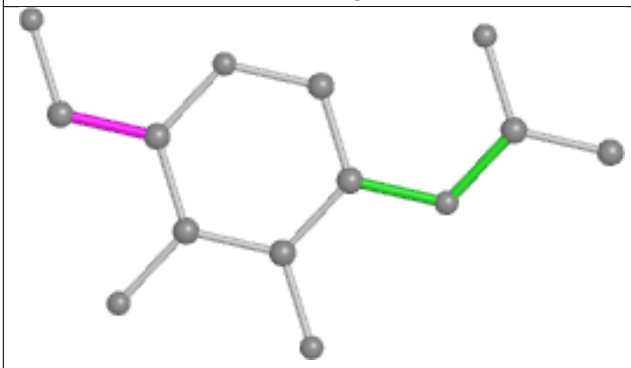
Ligand NAG C 1311



Bond lengths



Bond angles



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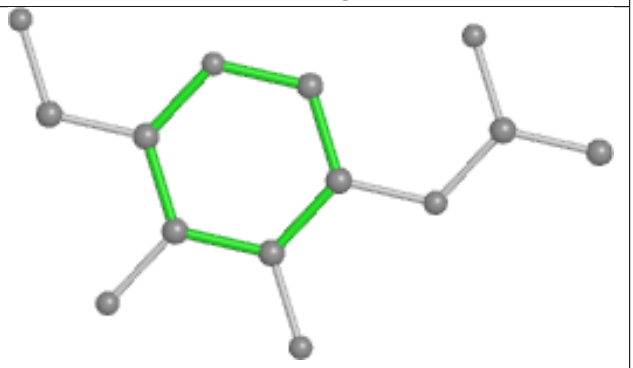
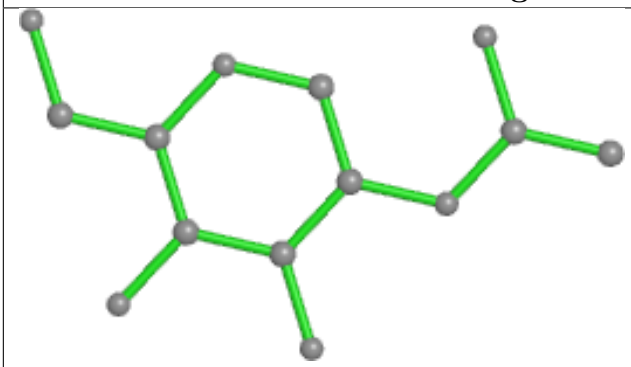
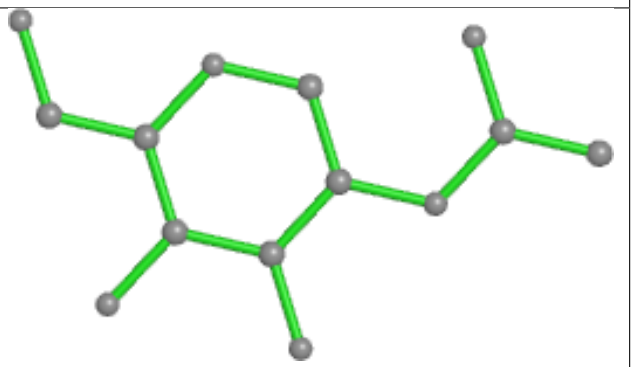


Rings

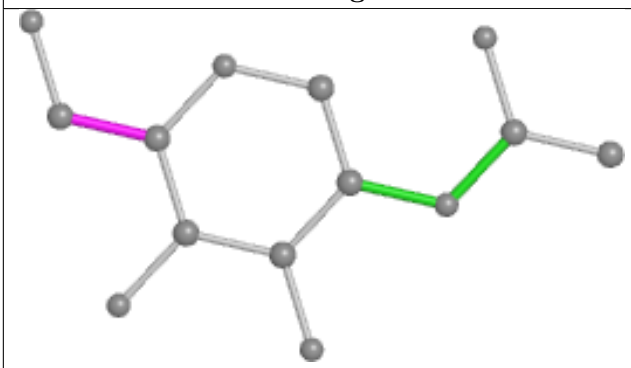
Ligand NAG A 1306



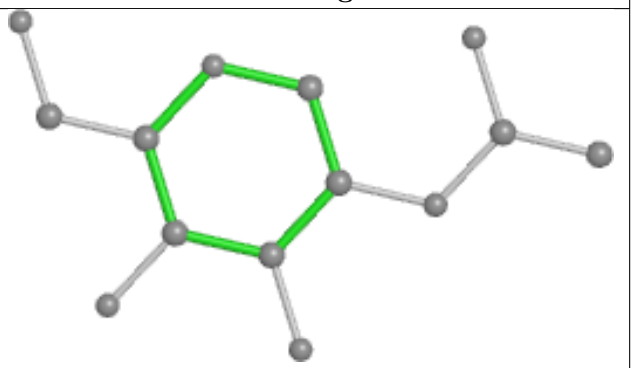
Bond lengths



Bond angles

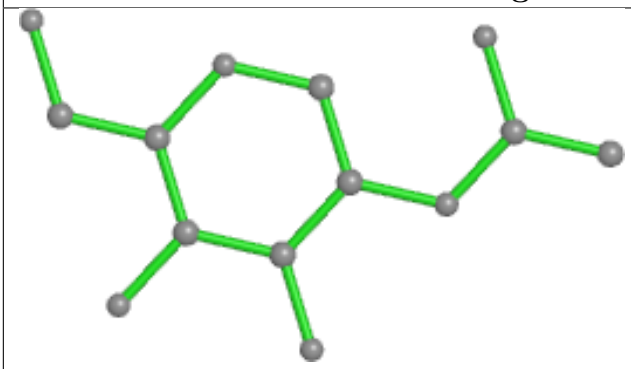


Torsions



Rings

Ligand NAG B 1307



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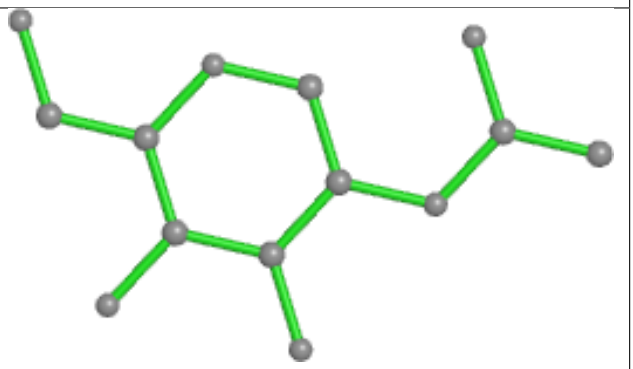
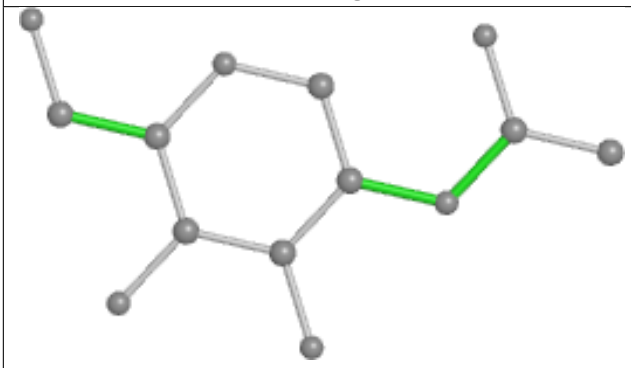
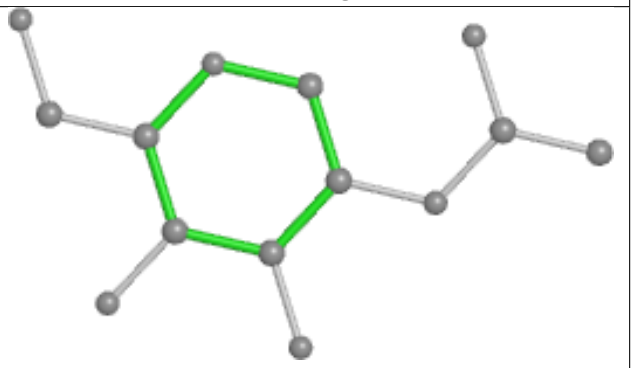


Bond angles

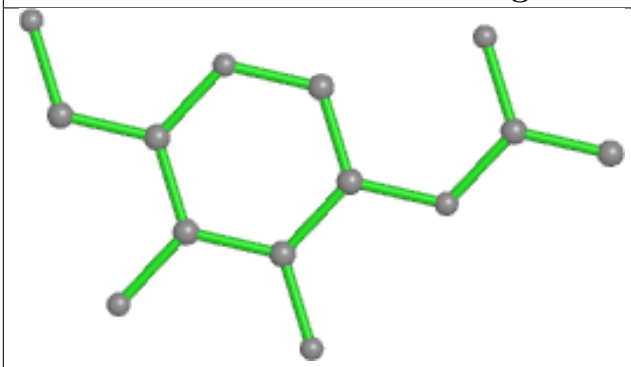


Torsions

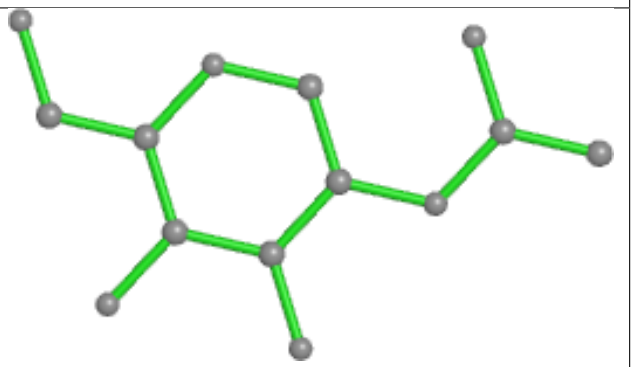


Rings

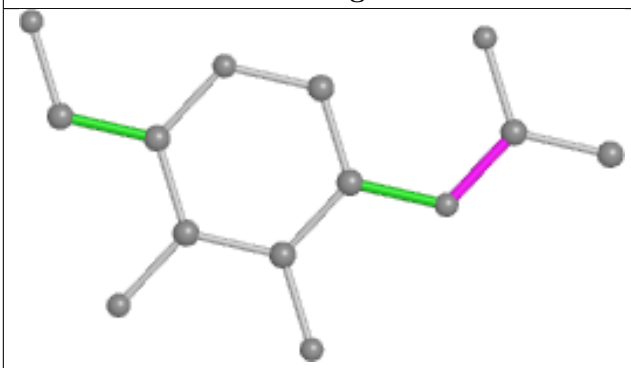
Ligand NAG C 1305



Bond lengths



Bond angles



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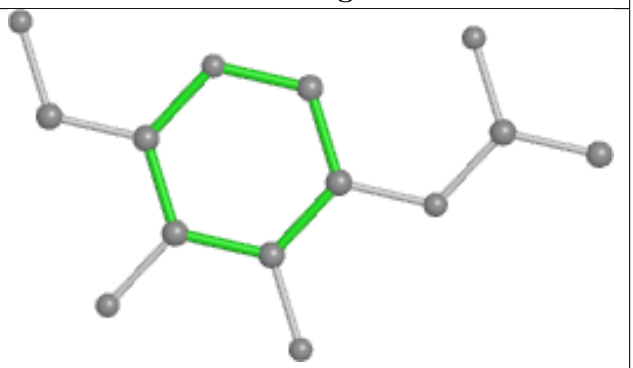
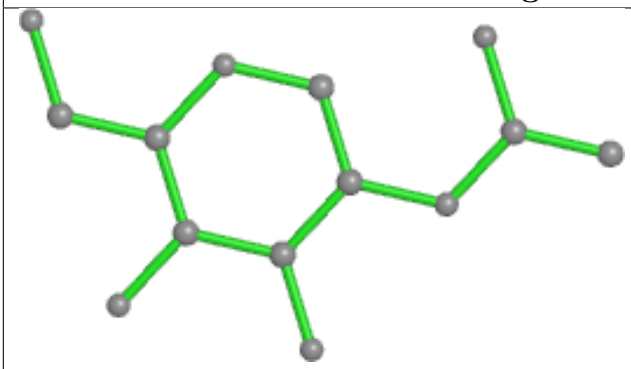


Rings

Ligand NAG E 703



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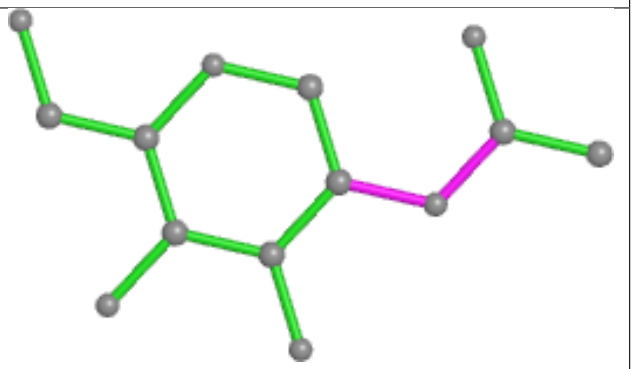
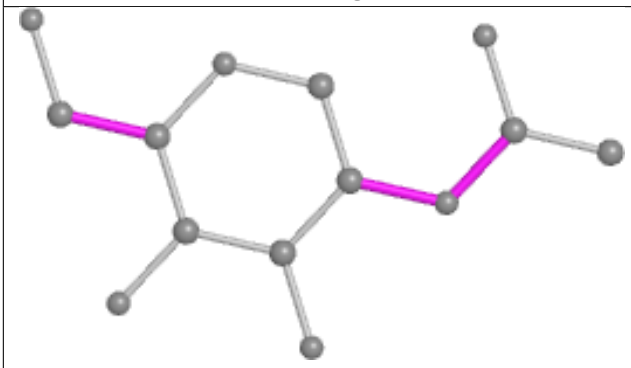


Bond angles



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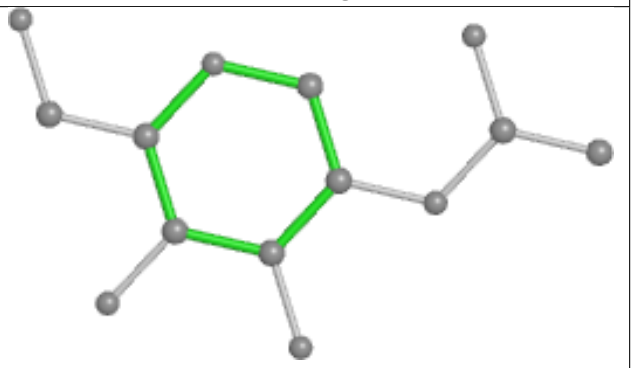
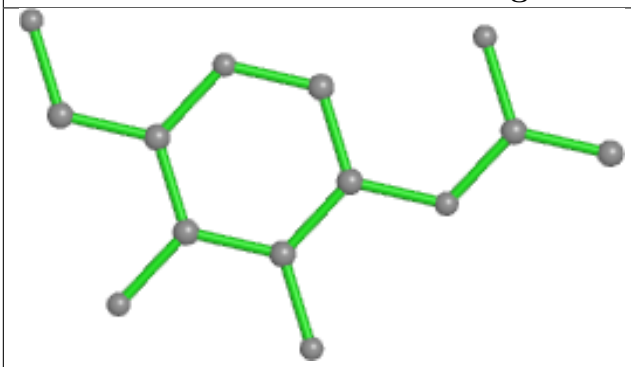
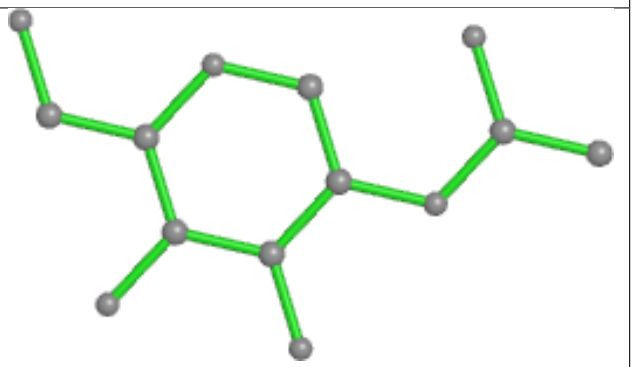


Rings

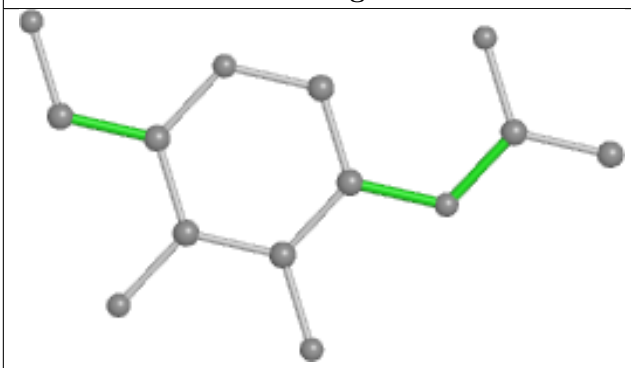
Ligand NAG A 1310



Bond lengths



Bond angles



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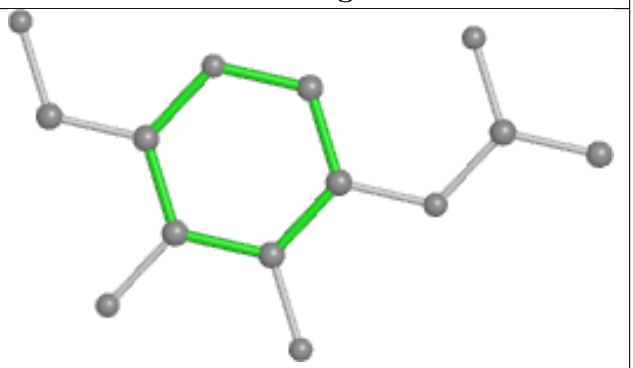
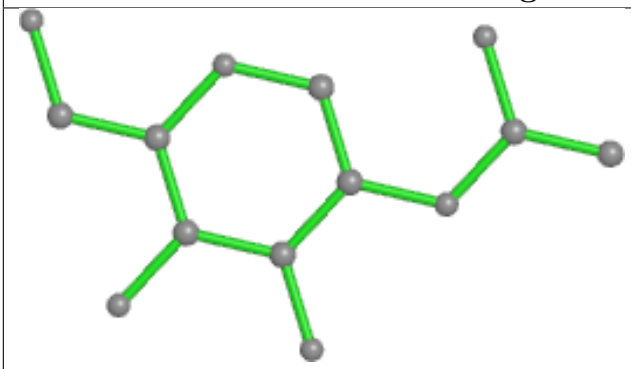
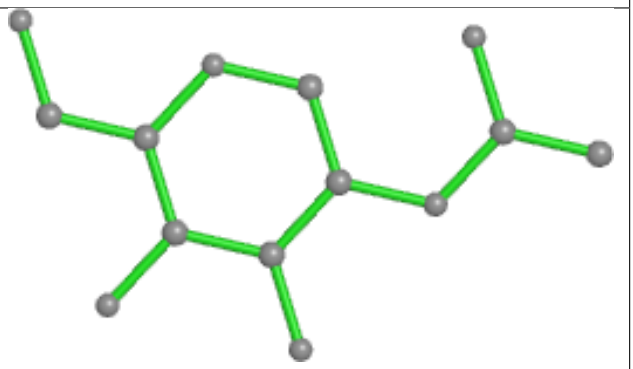


Rings

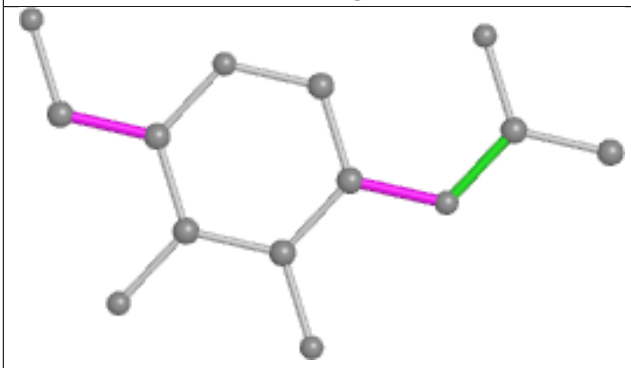
Ligand NAG D 704



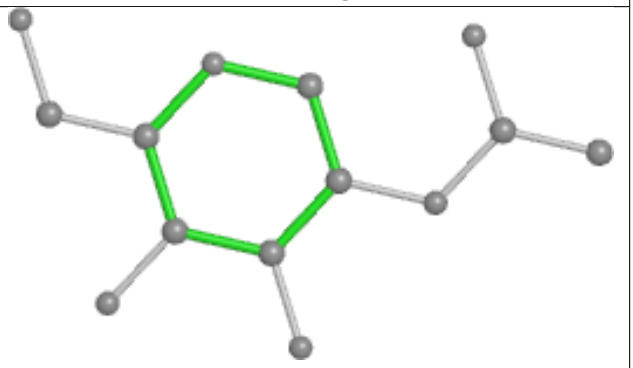
Bond lengths



Bond angles

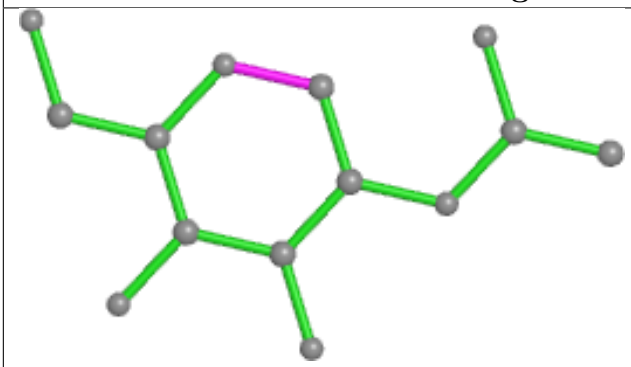


Torsions

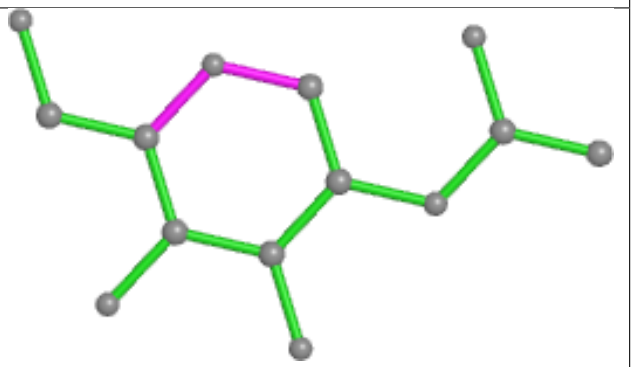


Rings

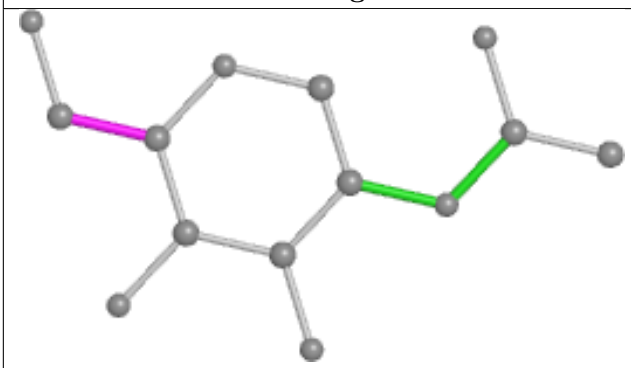
Ligand NAG C 1312



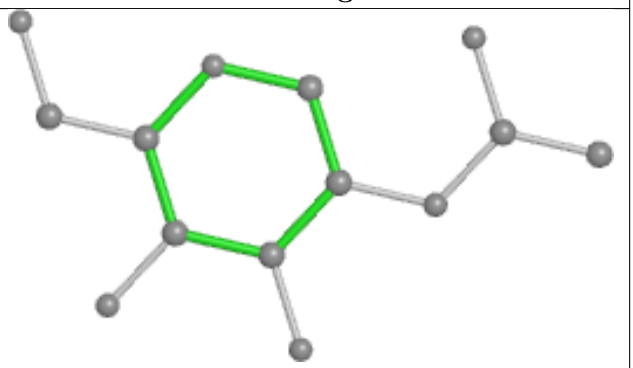
Bond lengths



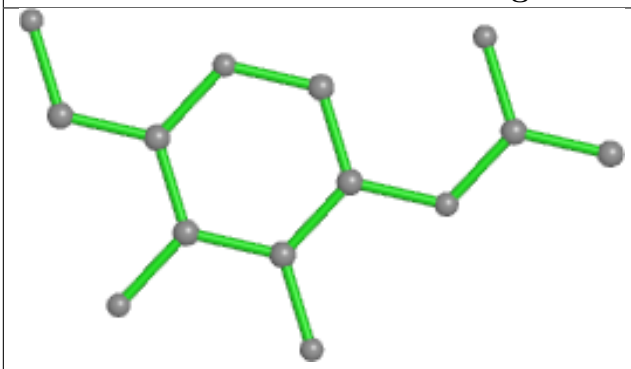
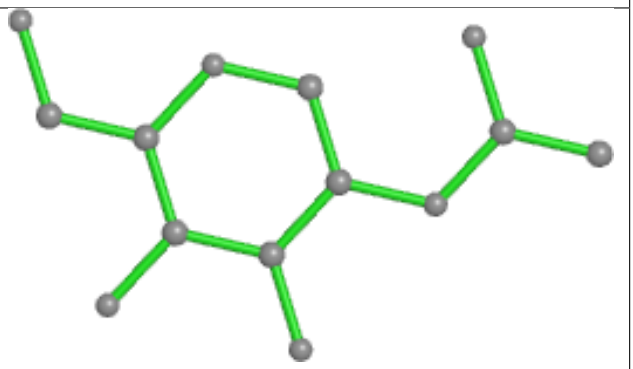
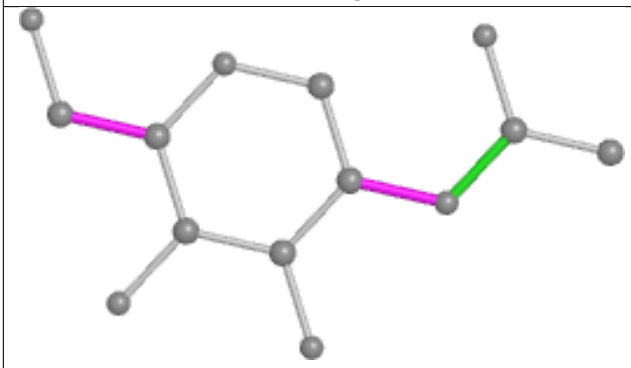
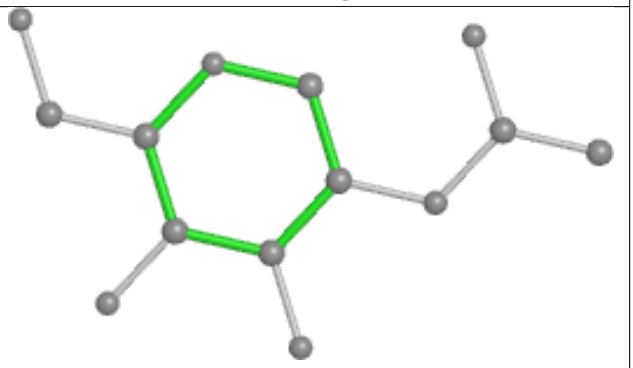
Bond angles



Torsions



Rings

Ligand NAG C 1309	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.