Full wwPDB EM Validation Report ⓘ

Mar 10, 2022 – 01:45 am GMT

PDB ID	:	7Q1Z
EMDB ID	:	EMD-13776
Title	:	Structure of formaldehyde cross-linked SARS-CoV-2 S glycoprotein
Authors	:	Sulbaran, G.; Effantin, G.; Schoehn, G.; Weissenhorn, W.
Deposited on	:	2021-10-22
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

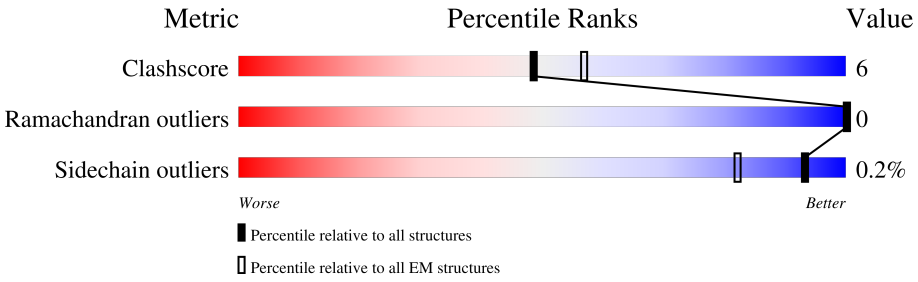
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1288	37% 63% 12% 25%
1	B	1288	38% 63% 12% 25%
1	C	1288	35% 63% 12% 25%
2	D	2	100% 100%
2	E	2	50% 50% 50%
2	F	2	100% 50% 50%
2	G	2	100% 100%
2	H	2	50% 100%

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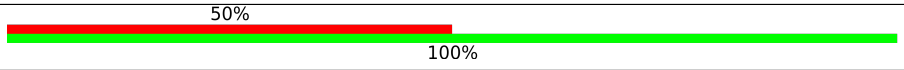
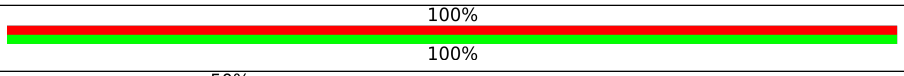
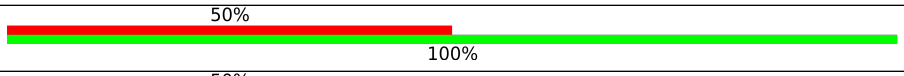
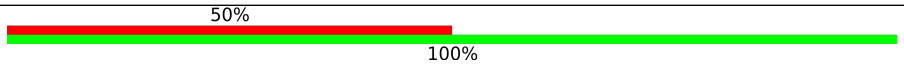
Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23694 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	972	Total 7604	C 4861	N 1262	O 1448	S 33	0	0
1	B	972	Total 7604	C 4861	N 1262	O 1448	S 33	0	0
1	C	972	Total 7604	C 4861	N 1262	O 1448	S 33	0	0

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		

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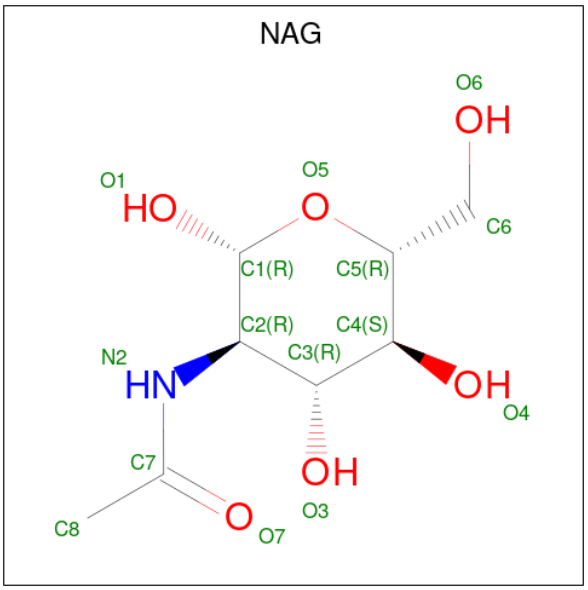
Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	A	1	Total	C	N	O	0
			154	88	11	55	
3	A	1	Total	C	N	O	0
			154	88	11	55	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 154	C 88	N 11	O 55	0
3	A	1	Total 154	C 88	N 11	O 55	0
3	A	1	Total 154	C 88	N 11	O 55	0
3	A	1	Total 154	C 88	N 11	O 55	0
3	A	1	Total 154	C 88	N 11	O 55	0
3	A	1	Total 154	C 88	N 11	O 55	0
3	A	1	Total 154	C 88	N 11	O 55	0
3	A	1	Total 154	C 88	N 11	O 55	0
3	A	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	B	1	Total 154	C 88	N 11	O 55	0
3	C	1	Total 154	C 88	N 11	O 55	0

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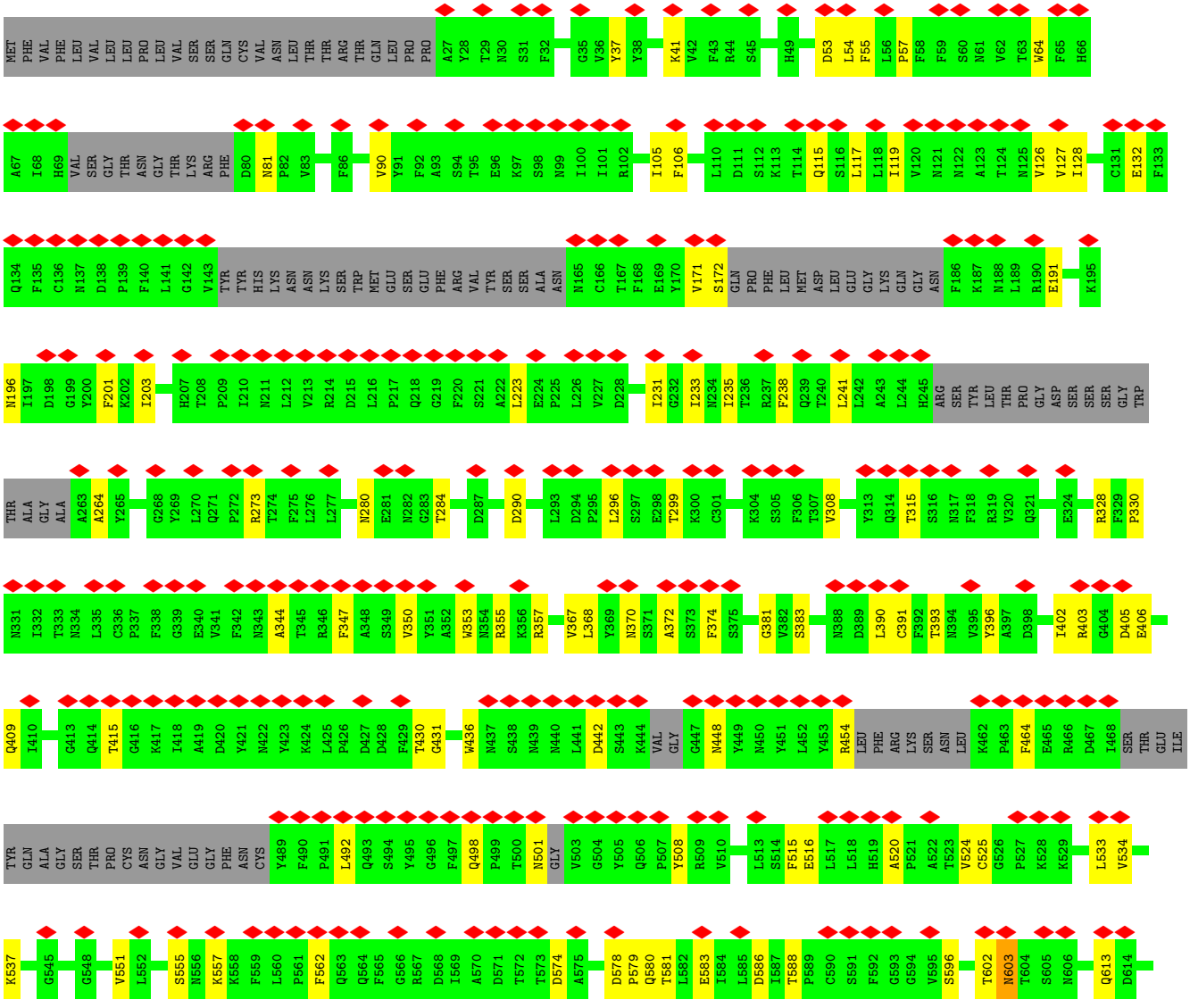
Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0
3	C	1	Total C N O 154 88 11 55	0

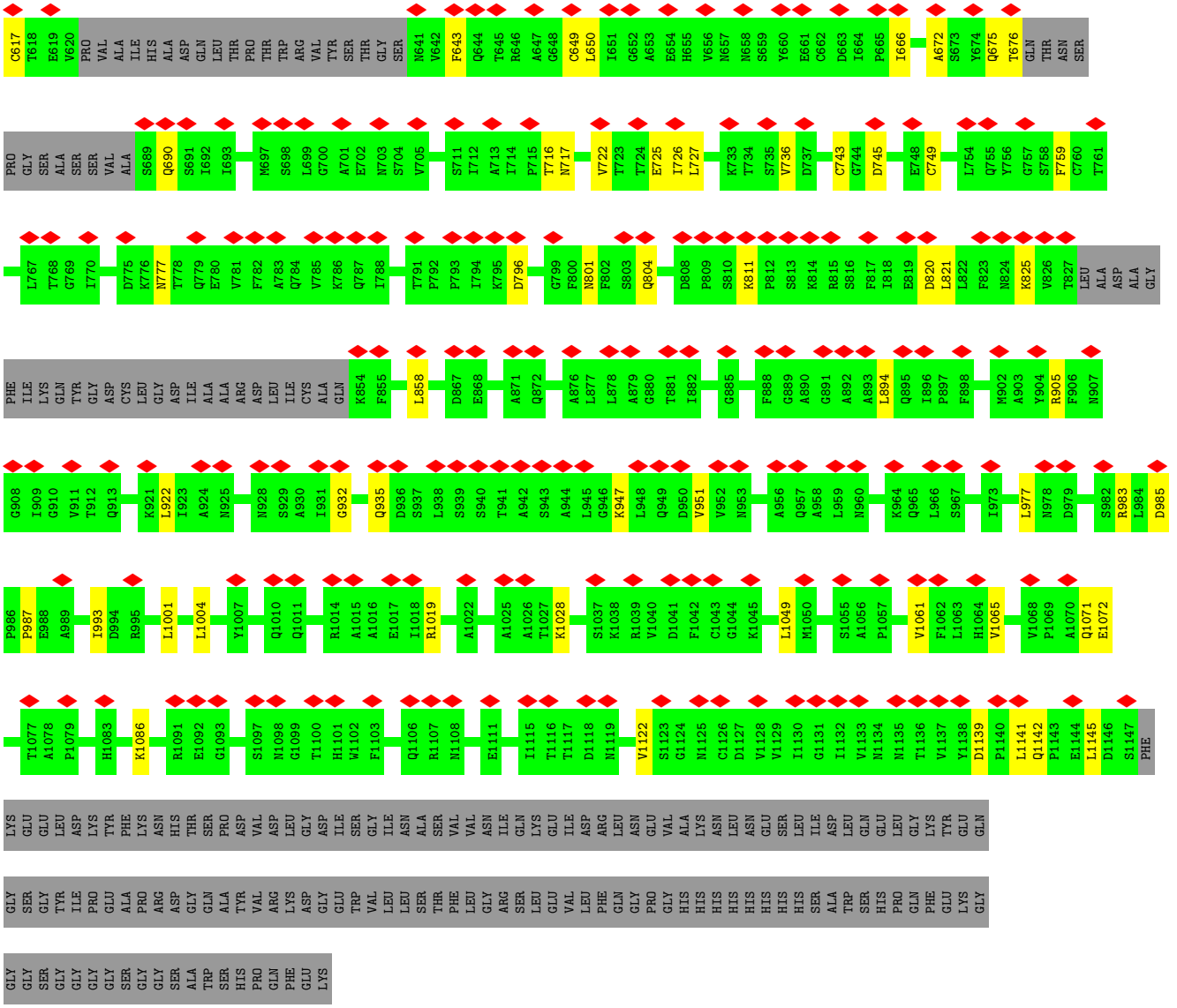
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

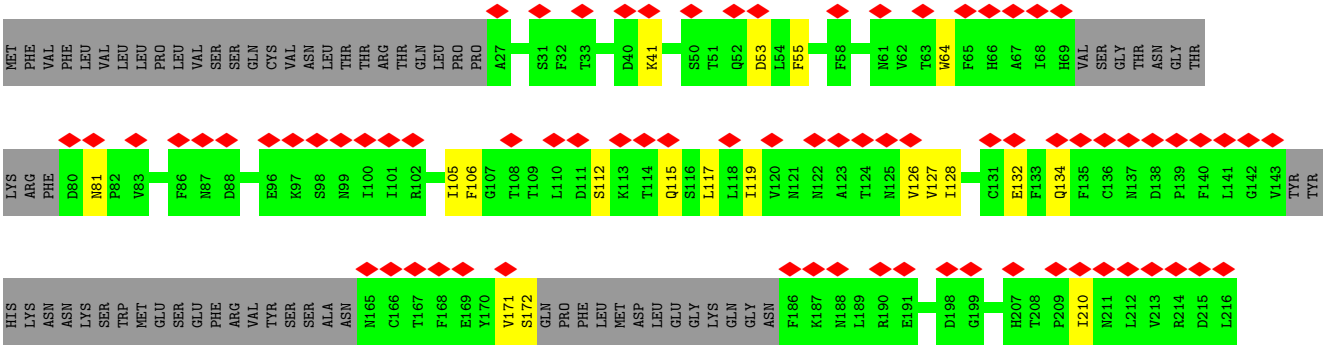
Chain A:

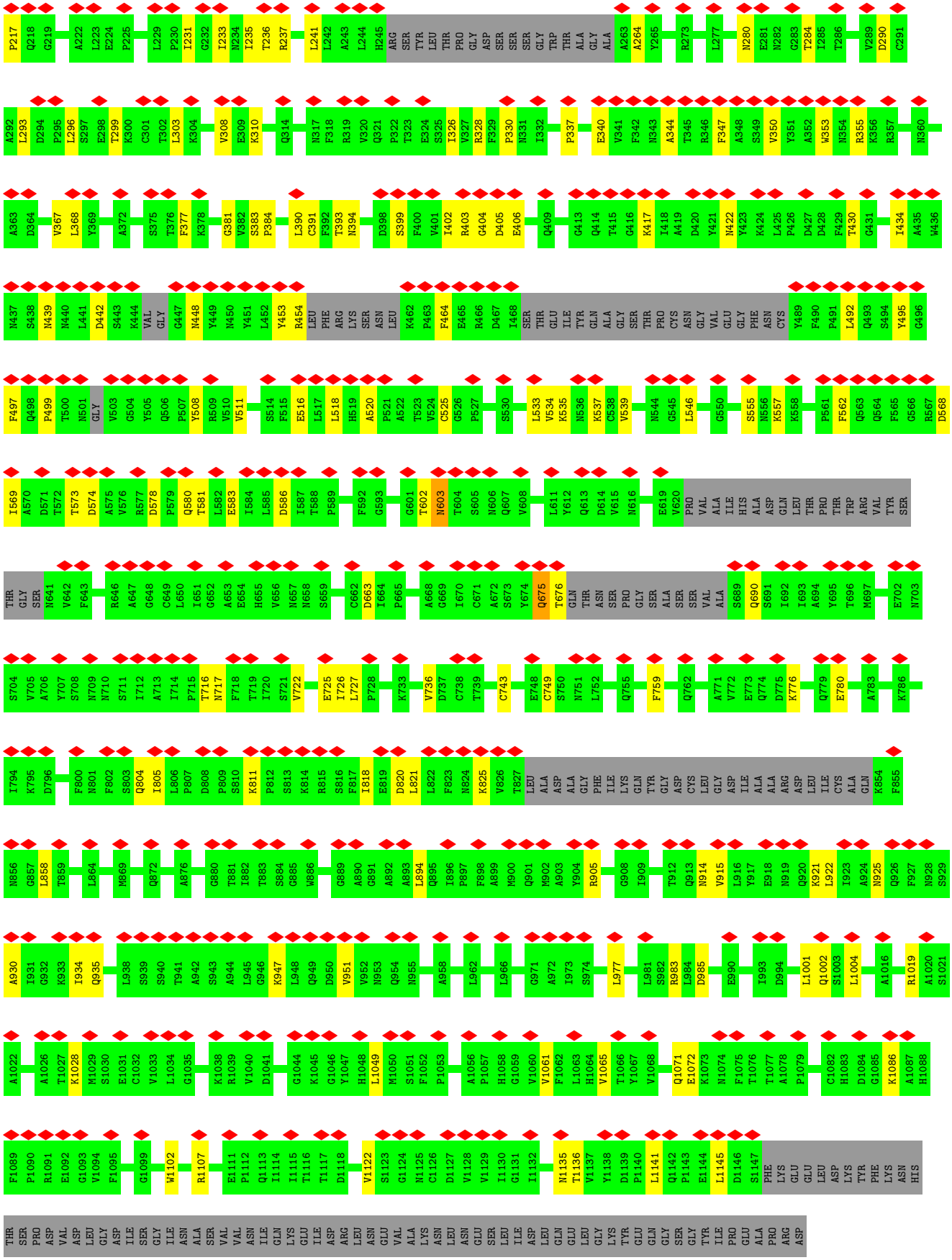




• Molecule 1: Spike glycoprotein

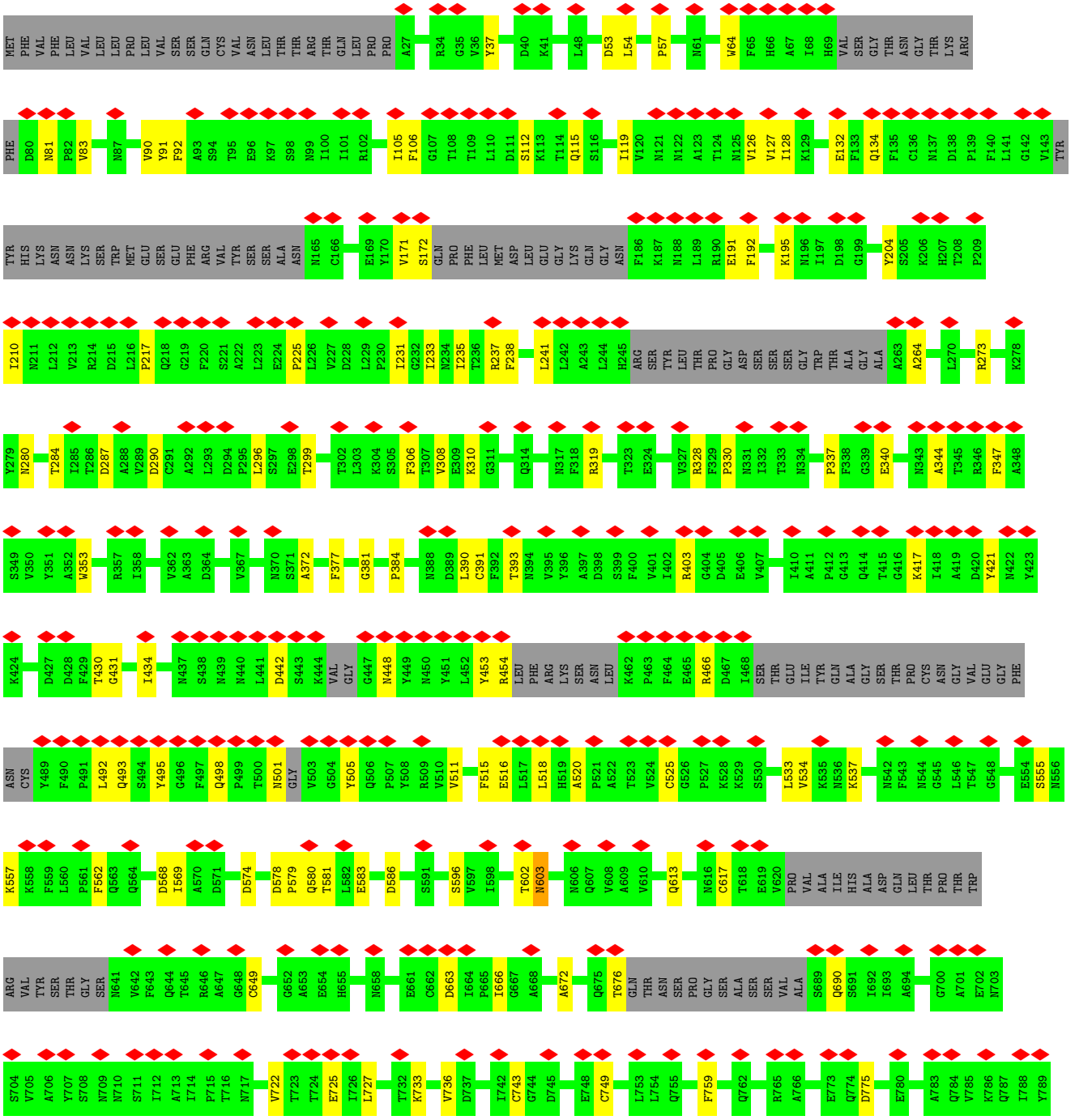
Chain B:

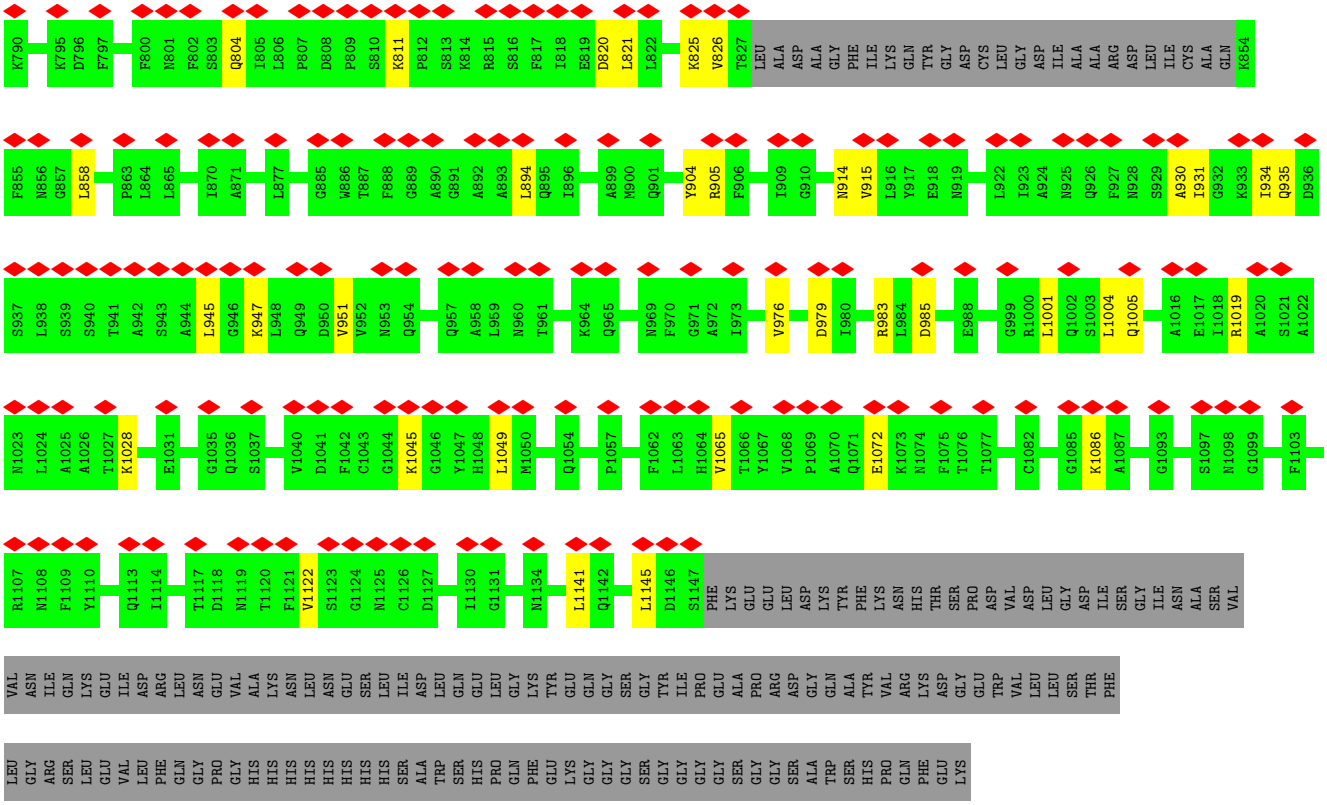



P217 Q218 G219 A222 L223 E224 P225 L229 P230 I231 G232 I233 N234 I235 T236 R237 L241 L242 A243 L244 H245 ARG SER TYR LEU THR PRO GLY ASP SER SER SER GLY TRP THR ALA GLY ALA A263 A264 Y265 R273 L277 N280 E281 N282 G283 T284 I285 T286 V289 D290 C291
A292 L293 D294 P295 L296 S297 E298 T299 K300 C301 T302 L303 K304 V308 E309 K310 Q314 N317 F318 R319 V320 Q321 P322 T323 E324 S325 I326 V327 R328 F329 P330 N331 I332 P337 E340 V341 F342 N343 A344 T345 R346 F347 A348 S349 V350 Y351 A352 W353 N354 R355 K356 R357 N360
A363 D364 V367 L368 Y369 A372 S375 T376 F377 K378 G381 V382 S383 P384 L390 C391 F392 T393 N394 D398 S399 F400 V401 I402 R403 G404 D405 E406 Q409 G413 Q414 T415 G416 K417 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 G431 I434 A435 W436
N437 S438 N439 N440 L441 D442 S443 K444 VAL GLY G447 N448 Y449 N450 Y451 L452 Y453 R454 LEU PHE ARG LYS SER ASN LEU K462 P463 F464 E465 R466 D467 I468 SER THR GLU ILE TYR GLN ALA GLY SER THR PRO CYS ASN GLY VAL GLU GLY PHE ASN CYS Y489 F490 P491 L492 Q493 S494 Y495 G496
F497 Q498 P499 T500 N501 GLY V503 G504 Y505 Q506 P507 Y508 R509 V510 V511 S514 F515 E516 L517 L518 H519 A520 P521 A522 T523 V524 C525 G526 P527 S530 L533 V534 K535 N536 K537 C538 V539 N544 G545 L546 G550 S555 N556 K557 K558 P561 F562 Q563 Q564 F565 G566 R567 D568
I569 A570 D571 T572 T573 D574 A575 V576 R577 D578 P579 Q580 T581 L582 E583 I584 L585 D586 I587 T588 P589 F592 G593 G601 T602 N603 T604 S605 N606 Q607 V608 L611 Y612 Q613 D614 V615 N616 E619 V620 PRO VAL ALA ILE HIS ALA ASP GLN LEU THR PRO THR TRP ARG VAL TYR SER
THR GLY SER N641 V642 F643 R646 A647 G648 C649 L650 I651 G652 A653 E654 H655 V656 N657 N658 S659 C662 D663 I664 P665 A668 G669 I670 C671 A672 S673 Y674 Q675 T676 GLN THR ASN SER PRO GLY SER ALA SER SER VAL ALA S689 Q690 S691 I692 I693 A694 Y695 T696 M697 E702 N703
S704 V705 A706 Y707 S708 N709 N710 S711 I712 A713 I714 P715 T716 N717 F718 T719 I720 S721 V722 E725 I726 L727 P728 K733 V736 D737 C738 T739 C743 E748 C749 S750 N751 L752 Q755 F759 Q762 A771 V772 E773 Q774 D775 K776 Q779 E780 A783 K786
I794 K795 D796 F800 N801 F802 S803 Q804 I805 L806 P807 D808 P809 S810 K811 P812 S813 K814 R815 S816 F817 I818 E819 D820 L821 L822 F823 N824 K825 V826 T827 LEU ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ARG ASP LEU ILE CYS ALA GLN K854 F855
N856 G857 L858 T859 L864 M969 Q872 A876 G880 T881 I882 T883 S884 G885 W886 G889 A890 G891 A892 A893 L894 Q895 I896 P897 F898 A899 M900 Q901 M902 A903 Y904 R905 G908 I909 T912 Q913 N914 V915 L916 Y917 E918 N919 Q920 K921 L922 I923 A924 N925 Q926 F927 N928 S929
A930 I931 G932 K933 I934 Q935 L938 S939 S940 T941 A942 S943 A944 L945 G946 K947 L948 Q949 D950 V951 V952 N953 Q954 N955 A958 L962 L966 G971 A972 I973 S974 L977 L981 S982 R983 L984 D985 E990 I993 D994 L1001 Q1002 S1003 L1004 A1016 R1019 A1020 S1021
A1022 A1026 T1027 K1028 M1029 S1030 E1031 C1032 V1033 L1034 G1035 K1038 R1039 V1040 D1041 G1044 K1045 G1046 Y1047 H1048 L1049 M1050 S1051 F1052 P1053 A1056 P1057 H1058 G1059 V1060 V1061 F1062 L1063 H1064 V1065 T1066 Y1067 V1068 Q1071 E1072 K1073 N1074 F1075 T1076 T1077 A1078 P1079 C1082 H1083 D1084 G1085 K1086 A1087 H1088
F1089 P1090 R1091 E1092 G1093 V1094 F1095 G1099 W1102 R1107 E1111 P1112 Q1113 I1114 I1115 T1116 T1117 D1118 V1122 S1123 G1124 N1125 C1126 D1127 V1128 V1129 I1130 G1131 I1132 N1135 T1136 V1137 Y1138 D1139 P1140 L1141 Q1142 P1143 E1144 L1145 D1146 S1147 PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS
THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP

• Molecule 1: Spike glycoprotein

Chain C:





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

Chain D:

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

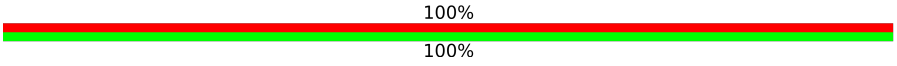
Chain E:

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

Chain F:

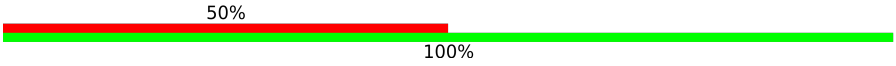
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



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

Chain I:

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

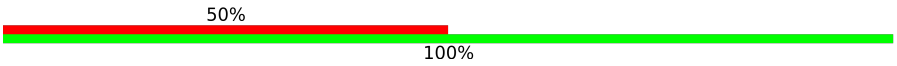
Chain J:

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

Chain K:

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

Chain L:



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

Chain M:

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

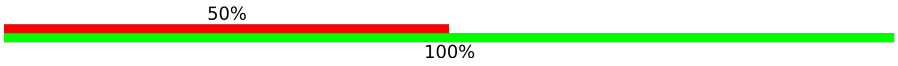
Chain N:

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

Chain O:

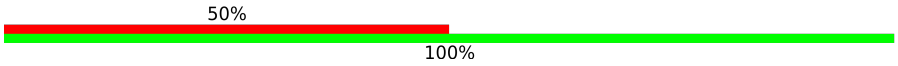
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



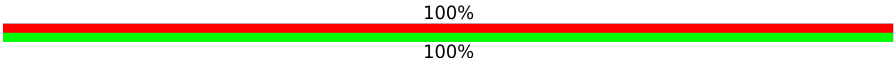
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



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

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126719	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.770	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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	0/7772	0.48	0/10572
1	B	0.28	0/7772	0.48	0/10572
1	C	0.27	0/7772	0.48	0/10572
All	All	0.28	0/23316	0.48	0/31716

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7604	0	7419	105	0
1	B	7604	0	7419	107	0
1	C	7604	0	7417	102	0
2	D	28	0	25	0	0
2	E	28	0	25	3	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
3	A	154	0	142	1	0
3	B	154	0	142	1	0
3	C	154	0	142	1	0
All	All	23694	0	23056	289	0

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

All (289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.53	0.90
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.54	0.89
1:A:196:ASN:HD21	1:A:235:ILE:HD12	1.54	0.72
1:A:393:THR:OG1	1:A:516:GLU:OE2	2.07	0.72
1:A:191:GLU:HG2	1:A:223:LEU:HD21	1.70	0.72
1:C:557:LYS:NZ	1:C:574:ASP:OD2	2.23	0.71
1:B:355:ARG:HH22	1:B:464:PHE:HB3	1.54	0.71
1:B:557:LYS:NZ	1:B:574:ASP:OD2	2.26	0.69
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.25	0.68
1:C:83:VAL:HB	1:C:237:ARG:HH21	1.60	0.67
1:A:390:LEU:HD22	1:B:983:ARG:HG2	1.76	0.67
1:B:403:ARG:HE	1:B:495:TYR:HB2	1.58	0.67
1:A:355:ARG:HH12	1:A:464:PHE:HB3	1.59	0.66
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.77	0.65
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.29	0.65
1:C:454:ARG:HH21	1:C:492:LEU:HD21	1.62	0.65
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.29	0.65
1:B:328:ARG:HH21	1:B:533:LEU:HB3	1.63	0.64
1:B:555:SER:HB3	1:B:586:ASP:HB2	1.79	0.64
1:A:983:ARG:HG2	1:C:390:LEU:HD22	1.79	0.64
1:B:328:ARG:NH1	1:B:580:GLN:OE1	2.30	0.64
1:B:390:LEU:HD22	1:C:983:ARG:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:OH	1:C:191:GLU:OE2	2.15	0.63
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.81	0.62
1:A:403:ARG:HD2	1:A:403:ARG:N	2.14	0.62
1:A:894:LEU:HD22	1:C:1072:GLU:HG2	1.81	0.62
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.82	0.62
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.80	0.61
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.82	0.61
1:C:826:VAL:HG23	1:C:945:LEU:HD13	1.82	0.61
1:A:357:ARG:HG3	1:A:396:TYR:HE2	1.66	0.61
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.16	0.61
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.66	0.61
1:C:759:PHE:HD2	1:C:1001:LEU:HD21	1.65	0.61
1:A:454:ARG:HH21	1:A:492:LEU:HD21	1.66	0.60
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.83	0.60
1:A:115:GLN:NE2	1:A:132:GLU:OE2	2.35	0.59
1:B:377:PHE:HE2	1:B:384:PRO:HB3	1.67	0.59
1:A:562:PHE:HD2	1:B:41:LYS:HG2	1.68	0.59
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.67	0.58
1:A:328:ARG:HH21	1:A:533:LEU:HB3	1.69	0.58
1:B:236:THR:HG23	1:B:237:ARG:HG3	1.85	0.58
1:C:393:THR:HG21	1:C:520:ALA:HB3	1.86	0.58
1:A:1072:GLU:HG2	1:B:894:LEU:HD22	1.85	0.58
1:B:568:ASP:OD1	1:B:569:ILE:N	2.35	0.57
1:C:328:ARG:HH21	1:C:533:LEU:HB3	1.68	0.57
1:B:759:PHE:HD2	1:B:1001:LEU:HD21	1.70	0.57
1:B:1072:GLU:HG2	1:C:894:LEU:HD22	1.87	0.57
1:C:330:PRO:HB3	3:C:1304:NAG:H82	1.87	0.56
1:B:115:GLN:NE2	1:B:132:GLU:OE2	2.37	0.56
1:B:717:ASN:ND2	2:J:1:NAG:O7	2.39	0.56
1:B:1107:ARG:HG2	1:C:904:TYR:OH	2.06	0.56
1:A:372:ALA:HA	1:C:417:LYS:HE2	1.87	0.56
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.70	0.56
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.87	0.56
1:B:330:PRO:HB3	3:B:1304:NAG:H82	1.88	0.55
1:A:105:ILE:HD11	1:A:241:LEU:HD21	1.88	0.55
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.87	0.55
1:C:115:GLN:NE2	1:C:132:GLU:OE2	2.37	0.55
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.06	0.55
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.39	0.55
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.06	0.55
1:C:442:ASP:O	1:C:448:ASN:ND2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:H	1:B:172:SER:HB2	1.72	0.54
1:C:37:TYR:OH	1:C:53:ASP:OD2	2.23	0.54
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.07	0.54
1:C:377:PHE:HE2	1:C:384:PRO:HB3	1.72	0.54
1:C:105:ILE:HD11	1:C:241:LEU:HD21	1.88	0.54
1:B:454:ARG:HH21	1:B:492:LEU:HD21	1.73	0.54
1:B:947:LYS:NZ	1:C:1019:ARG:HH22	2.05	0.54
1:B:546:LEU:HD21	1:B:573:THR:HG21	1.90	0.54
1:A:409:GLN:NE2	1:A:415:THR:O	2.40	0.54
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.73	0.54
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.90	0.53
1:C:231:ILE:HD12	1:C:233:ILE:HD12	1.91	0.53
1:A:1141:LEU:HG	1:A:1145:LEU:HD13	1.90	0.53
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.90	0.53
1:A:330:PRO:HB3	3:A:1304:NAG:H82	1.91	0.53
1:C:568:ASP:OD1	1:C:569:ILE:N	2.36	0.53
1:A:126:VAL:H	1:A:172:SER:HB2	1.73	0.52
1:C:1141:LEU:HG	1:C:1145:LEU:HD13	1.90	0.52
1:B:442:ASP:O	1:B:448:ASN:ND2	2.37	0.52
1:C:126:VAL:H	1:C:172:SER:HB2	1.74	0.52
1:B:231:ILE:HD12	1:B:233:ILE:HD12	1.92	0.52
1:B:280:ASN:OD1	1:B:284:THR:N	2.38	0.52
1:B:417:LYS:HE2	1:C:372:ALA:HA	1.91	0.52
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.91	0.52
1:A:736:VAL:HG22	1:A:858:LEU:HG	1.92	0.52
1:B:105:ILE:HD11	1:B:241:LEU:HD21	1.91	0.52
1:A:759:PHE:HD2	1:A:1001:LEU:HD21	1.74	0.51
1:B:404:GLY:HA2	1:B:508:TYR:HD1	1.73	0.51
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	1.92	0.51
1:A:596:SER:OG	1:A:613:GLN:OE1	2.24	0.51
1:A:1139:ASP:HB3	1:A:1142:GLN:HG2	1.92	0.51
1:A:725:GLU:OE1	1:A:1028:LYS:HE3	2.11	0.51
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	1.92	0.51
1:C:337:PRO:HB2	1:C:340:GLU:HG2	1.92	0.51
1:B:1141:LEU:HG	1:B:1145:LEU:HD13	1.93	0.50
1:B:603:ASN:O	1:B:603:ASN:ND2	2.45	0.50
1:C:596:SER:OG	1:C:613:GLN:OE1	2.29	0.50
1:A:391:CYS:CB	1:A:525:CYS:HA	2.40	0.50
1:A:717:ASN:ND2	2:E:1:NAG:O7	2.45	0.50
1:C:676:THR:HA	1:C:690:GLN:HA	1.94	0.50
1:B:377:PHE:CD1	1:B:434:ILE:HG12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:603:ASN:O	1:C:603:ASN:ND2	2.45	0.49
1:A:745:ASP:HB2	1:C:319:ARG:NH2	2.28	0.49
1:B:117:LEU:HD12	1:B:231:ILE:HD13	1.95	0.49
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.45	0.49
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.46	0.49
1:A:804:GLN:NE2	1:A:935:GLN:HB2	2.28	0.49
1:B:326:ILE:HD12	1:B:539:VAL:HG21	1.94	0.49
1:A:383:SER:OG	1:B:985:ASP:N	2.45	0.48
1:B:404:GLY:HA2	1:B:508:TYR:CD1	2.47	0.48
1:C:377:PHE:CD1	1:C:434:ILE:HG12	2.49	0.48
1:C:37:TYR:OH	1:C:54:LEU:O	2.31	0.48
1:A:442:ASP:O	1:A:448:ASN:ND2	2.38	0.48
1:A:676:THR:HA	1:A:690:GLN:HA	1.96	0.48
1:A:603:ASN:O	1:A:603:ASN:ND2	2.45	0.47
1:B:676:THR:HA	1:B:690:GLN:HA	1.95	0.47
1:C:534:VAL:HG11	1:C:537:LYS:HE2	1.96	0.47
1:C:725:GLU:OE2	1:C:1028:LYS:HE3	2.13	0.47
1:A:796:ASP:OD1	1:A:796:ASP:N	2.45	0.47
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.80	0.47
1:C:119:ILE:HG12	1:C:128:ILE:HG12	1.95	0.47
1:B:736:VAL:HG11	1:B:1004:LEU:HD21	1.96	0.47
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.80	0.47
1:A:1086:LYS:HD2	1:A:1122:VAL:HG11	1.97	0.47
1:A:273:ARG:HH21	1:A:290:ASP:CG	2.18	0.47
1:B:337:PRO:HB2	1:B:340:GLU:HG2	1.97	0.47
1:A:119:ILE:HG12	1:A:128:ILE:HG12	1.95	0.47
1:A:41:LYS:HZ1	1:C:562:PHE:HB2	1.80	0.47
1:B:922:LEU:HD11	2:J:1:NAG:H5	1.97	0.47
1:B:804:GLN:NE2	1:B:935:GLN:HB2	2.30	0.46
1:A:391:CYS:HB2	1:A:524:VAL:O	2.15	0.46
1:A:617:CYS:HB3	1:A:649:CYS:HB3	1.85	0.46
1:A:381:GLY:HA3	1:A:430:THR:HG23	1.97	0.46
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.98	0.46
1:B:381:GLY:HA3	1:B:430:THR:HG23	1.97	0.46
1:B:562:PHE:CE1	1:C:225:PRO:HD2	2.50	0.46
1:B:725:GLU:OE2	1:B:1028:LYS:HE3	2.15	0.46
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.82	0.46
1:A:367:VAL:HG13	1:A:368:LEU:HD22	1.98	0.46
1:B:776:LYS:NZ	1:B:780:GLU:OE2	2.47	0.46
1:B:350:VAL:O	1:B:353:TRP:HD1	1.99	0.46
1:A:922:LEU:HD11	2:E:1:NAG:H5	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:VAL:HG13	1:B:368:LEU:HD22	1.98	0.46
1:B:1086:LYS:HB3	1:B:1122:VAL:HG13	1.98	0.46
1:B:399:SER:HA	1:B:511:VAL:HG12	1.98	0.45
1:C:106:PHE:HB3	1:C:235:ILE:HD12	1.98	0.45
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.81	0.45
1:A:117:LEU:HD12	1:A:231:ILE:HD13	1.98	0.45
1:A:280:ASN:OD1	1:A:284:THR:N	2.38	0.45
1:B:736:VAL:HG22	1:B:858:LEU:HG	1.98	0.45
1:C:310:LYS:NZ	1:C:663:ASP:OD1	2.36	0.45
1:A:821:LEU:O	1:A:825:LYS:HG2	2.16	0.45
1:A:1086:LYS:HB3	1:A:1122:VAL:HG13	1.98	0.45
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	1.97	0.45
1:C:308:VAL:HB	1:C:602:THR:HG23	1.98	0.45
1:A:431:GLY:HA2	1:A:515:PHE:HD1	1.80	0.45
1:C:287:ASP:HB3	1:C:306:PHE:CE2	2.52	0.45
1:C:381:GLY:HA3	1:C:430:THR:HG23	1.98	0.45
1:A:308:VAL:HB	1:A:602:THR:HG23	1.98	0.45
1:B:127:VAL:HG22	1:B:171:VAL:HG13	1.98	0.45
1:C:516:GLU:HG2	1:C:518:LEU:H	1.81	0.45
1:A:804:GLN:HE22	1:A:935:GLN:HB2	1.82	0.45
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.49	0.45
1:B:434:ILE:HB	1:B:511:VAL:HG23	1.98	0.45
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.98	0.45
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.50	0.45
1:C:287:ASP:HB3	1:C:306:PHE:HE2	1.81	0.45
1:B:308:VAL:HB	1:B:602:THR:HG23	1.99	0.45
1:B:516:GLU:HG2	1:B:518:LEU:H	1.82	0.45
1:C:403:ARG:HD3	1:C:495:TYR:CD2	2.51	0.45
1:B:112:SER:HB2	1:B:134:GLN:HA	1.98	0.45
1:B:1002:GLN:NE2	1:C:1005:GLN:OE1	2.50	0.45
1:C:403:ARG:HH12	1:C:505:TYR:HD1	1.65	0.45
1:A:41:LYS:NZ	1:C:562:PHE:HB2	2.33	0.44
1:A:357:ARG:HG3	1:A:396:TYR:CE2	2.51	0.44
1:A:581:THR:HG23	1:A:583:GLU:HG2	1.98	0.44
1:A:717:ASN:HD21	2:E:1:NAG:C1	2.31	0.44
1:A:745:ASP:HB2	1:C:319:ARG:HH22	1.81	0.44
1:A:977:LEU:HD11	1:A:993:ILE:HG12	1.99	0.44
1:C:617:CYS:HB3	1:C:649:CYS:HB3	1.85	0.44
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.85	0.44
1:C:976:VAL:HG12	1:C:979:ASP:H	1.81	0.44
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:947:LYS:O	1:C:951:VAL:HG23	2.17	0.44
1:B:326:ILE:HD11	1:B:534:VAL:H	1.81	0.44
1:B:422:ASN:HD22	1:B:453:TYR:HB2	1.83	0.44
1:C:578:ASP:HB3	1:C:581:THR:O	2.17	0.44
1:C:1086:LYS:HB3	1:C:1122:VAL:HG13	2.00	0.44
1:B:106:PHE:HB3	1:B:235:ILE:HD12	2.00	0.44
1:C:273:ARG:HH21	1:C:290:ASP:CG	2.21	0.44
1:C:736:VAL:HG11	1:C:1004:LEU:HD21	1.99	0.44
1:B:439:ASN:HD21	1:B:499:PRO:HA	1.82	0.44
1:C:127:VAL:HG22	1:C:171:VAL:HG13	1.99	0.44
1:C:434:ILE:HB	1:C:511:VAL:HG23	2.00	0.44
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.51	0.43
1:C:821:LEU:O	1:C:825:LYS:HG2	2.18	0.43
1:A:498:GLN:H	1:A:501:ASN:ND2	2.16	0.43
1:B:383:SER:OG	1:C:985:ASP:N	2.51	0.43
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.42	0.43
1:C:498:GLN:HB2	1:C:501:ASN:ND2	2.33	0.43
1:A:350:VAL:O	1:A:353:TRP:HD1	2.02	0.43
1:A:374:PHE:HA	1:A:436:TRP:HB3	2.00	0.43
1:A:777:ASN:OD1	1:A:1019:ARG:HD2	2.17	0.43
1:B:578:ASP:HB3	1:B:581:THR:O	2.19	0.43
1:A:727:LEU:HD11	1:A:1028:LYS:HD2	2.01	0.43
1:B:947:LYS:O	1:B:951:VAL:HG23	2.19	0.43
1:C:280:ASN:OD1	1:C:284:THR:N	2.42	0.43
1:A:370:ASN:OD1	1:C:421:TYR:OH	2.25	0.43
1:B:310:LYS:NZ	1:B:663:ASP:OD1	2.36	0.43
1:C:296:LEU:O	1:C:299:THR:OG1	2.29	0.43
1:A:947:LYS:O	1:A:951:VAL:HG23	2.18	0.43
1:B:231:ILE:HG13	1:B:233:ILE:H	1.84	0.43
1:B:717:ASN:HD21	2:J:1:NAG:C1	2.31	0.43
1:A:947:LYS:NZ	1:B:1019:ARG:HH22	2.16	0.43
1:C:112:SER:HB2	1:C:134:GLN:HA	2.00	0.43
1:C:431:GLY:HA2	1:C:515:PHE:HD1	1.82	0.43
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	2.01	0.43
1:A:736:VAL:HG11	1:A:1004:LEU:HD21	2.00	0.43
1:B:921:LYS:NZ	1:B:925:ASN:OD1	2.51	0.43
1:C:90:VAL:HG21	1:C:238:PHE:CE1	2.53	0.43
1:A:643:PHE:O	1:A:650:LEU:N	2.47	0.43
1:C:328:ARG:HG3	1:C:579:PRO:HG2	2.01	0.42
1:C:453:TYR:CE1	1:C:493:GLN:HB2	2.54	0.42
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASP:HB3	1:B:293:LEU:HB2	2.01	0.42
1:B:581:THR:HG23	1:B:583:GLU:HG2	2.00	0.42
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.54	0.42
1:B:534:VAL:HG11	1:B:537:LYS:HE2	2.01	0.42
1:B:821:LEU:O	1:B:825:LYS:HG2	2.19	0.42
1:A:231:ILE:HG13	1:A:233:ILE:H	1.85	0.42
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.54	0.42
1:A:299:THR:HG22	1:A:315:THR:HG21	2.01	0.42
1:A:551:VAL:HG12	1:A:588:THR:HB	2.01	0.42
1:A:578:ASP:HB3	1:A:581:THR:O	2.19	0.42
1:C:727:LEU:HD11	1:C:1028:LYS:HD2	2.01	0.42
1:B:930:ALA:O	1:B:934:ILE:HG12	2.19	0.42
1:A:405:ASP:OD1	1:A:406:GLU:HG3	2.20	0.42
1:A:666:ILE:HD11	1:A:672:ALA:HB2	2.02	0.41
1:B:210:ILE:HG21	1:B:217:PRO:HG2	2.02	0.41
1:C:736:VAL:HG22	1:C:858:LEU:HG	2.01	0.41
1:C:92:PHE:O	1:C:192:PHE:N	2.41	0.41
1:B:675:GLN:HE21	1:B:675:GLN:HB3	1.74	0.41
1:B:716:THR:N	1:B:1071:GLN:O	2.44	0.41
1:A:37:TYR:OH	1:A:54:LEU:O	2.39	0.41
1:B:296:LEU:O	1:B:299:THR:OG1	2.30	0.41
1:B:805:ILE:HG22	1:B:818:ILE:HD12	2.03	0.41
1:C:195:LYS:HE2	1:C:204:TYR:CE1	2.55	0.41
1:C:914:ASN:OD1	1:C:915:VAL:N	2.53	0.41
1:C:1045:LYS:HB3	1:C:1045:LYS:HE3	1.80	0.41
1:A:1142:GLN:HA	1:A:1142:GLN:OE1	2.21	0.41
1:B:914:ASN:OD1	1:B:915:VAL:N	2.54	0.41
1:B:350:VAL:HG21	1:B:402:ILE:HD11	2.01	0.41
1:B:1107:ARG:HG2	1:C:904:TYR:CZ	2.55	0.41
1:B:81:ASN:N	1:B:81:ASN:OD1	2.54	0.41
1:A:231:ILE:HD12	1:A:233:ILE:HB	2.03	0.41
1:A:1072:GLU:HG2	1:B:894:LEU:CD2	2.51	0.41
1:B:535:LYS:HE2	1:B:535:LYS:HB3	1.71	0.41
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	2.01	0.41
1:B:1072:GLU:HG2	1:C:894:LEU:CD2	2.51	0.41
1:C:127:VAL:HG13	1:C:171:VAL:HG22	2.03	0.41
1:A:127:VAL:HG22	1:A:171:VAL:HG13	2.03	0.41
1:A:296:LEU:O	1:A:299:THR:OG1	2.29	0.41
1:A:534:VAL:HG11	1:A:537:LYS:HE2	2.02	0.41
1:A:801:ASN:HD21	2:F:1:NAG:C1	2.34	0.41
1:A:932:GLY:O	1:A:935:GLN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:CYS:HB2	1:B:977:LEU:HD21	2.03	0.41
1:C:581:THR:HG23	1:C:583:GLU:HG2	2.02	0.41
1:A:81:ASN:OD1	1:A:81:ASN:N	2.54	0.40
1:C:930:ALA:O	1:C:934:ILE:HG12	2.21	0.40
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.56	0.40
1:B:303:LEU:HD12	1:B:308:VAL:HG22	2.03	0.40
1:B:377:PHE:HD1	1:B:434:ILE:HG12	1.86	0.40
1:A:716:THR:N	1:A:1071:GLN:O	2.40	0.40
1:B:405:ASP:OD1	1:B:406:GLU:HG3	2.21	0.40
1:C:115:GLN:HA	1:C:132:GLU:HG2	2.02	0.40
1:C:353:TRP:O	1:C:466:ARG:NE	2.55	0.40
1:C:403:ARG:HD3	1:C:495:TYR:CG	2.56	0.40
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.43	0.40
1:A:328:ARG:HG3	1:A:579:PRO:HG2	2.04	0.40
1:A:1019:ARG:HH22	1:C:947:LYS:NZ	2.19	0.40
1:C:210:ILE:HG21	1:C:217:PRO:HG2	2.04	0.40
1:A:201:PHE:HE1	1:A:203:ILE:HD11	1.87	0.40
1:A:402:ILE:O	1:A:508:TYR:HB2	2.22	0.40
1:A:985:ASP:CG	1:A:987:PRO:HD2	2.42	0.40
1:C:81:ASN:OD1	1:C:81:ASN:N	2.55	0.40
1:C:804:GLN:HG2	1:C:931:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	948/1288 (74%)	929 (98%)	19 (2%)	0	100	100
1	B	948/1288 (74%)	923 (97%)	25 (3%)	0	100	100
1	C	948/1288 (74%)	930 (98%)	18 (2%)	0	100	100
All	All	2844/3864 (74%)	2782 (98%)	62 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	852/1113 (76%)	850 (100%)	2 (0%)	93	98
1	B	852/1113 (76%)	849 (100%)	3 (0%)	91	95
1	C	852/1113 (76%)	851 (100%)	1 (0%)	93	98
All	All	2556/3339 (76%)	2550 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	603	ASN
1	A	675	GLN
1	B	394	ASN
1	B	603	ASN
1	B	675	GLN
1	C	603	ASN

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

Mol	Chain	Res	Type
1	A	196	ASN
1	B	949	GLN
1	B	1002	GLN
1	C	804	GLN
1	C	935	GLN
1	C	1005	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.45	0
2	NAG	E	1	2	14,14,15	0.46	0	17,19,21	0.43	0
2	NAG	E	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	F	1	2	14,14,15	0.36	0	17,19,21	0.37	0
2	NAG	F	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	G	1	2,1	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	G	2	2	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	H	1	2,1	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	H	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	I	1	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	J	1	2	14,14,15	0.45	0	17,19,21	0.42	0
2	NAG	J	2	2	14,14,15	0.18	0	17,19,21	0.42	0
2	NAG	K	1	2	14,14,15	0.32	0	17,19,21	0.37	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	L	1	2,1	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	L	2	2	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	M	1	2,1	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	M	2	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	N	1	2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	N	2	2	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	O	1	2,1	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	O	2	2	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	P	1	2,1	14,14,15	0.24	0	17,19,21	0.39	0
2	NAG	P	2	2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	Q	1	2,1	14,14,15	0.25	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	Q	2	2	14,14,15	0.27	0	17,19,21	0.41	0
2	NAG	R	1	2,1	14,14,15	0.17	0	17,19,21	0.45	0
2	NAG	R	2	2	14,14,15	0.24	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2	-	1/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	1/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6

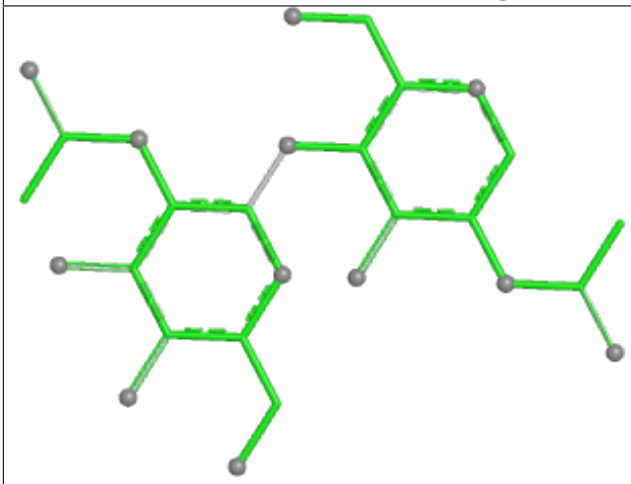
There are no ring outliers.

3 monomers are involved in 7 short contacts:

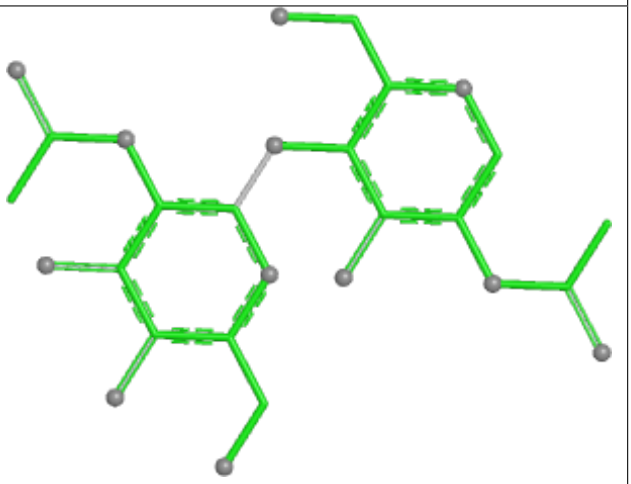
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	E	1	NAG	3	0
2	J	1	NAG	3	0

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

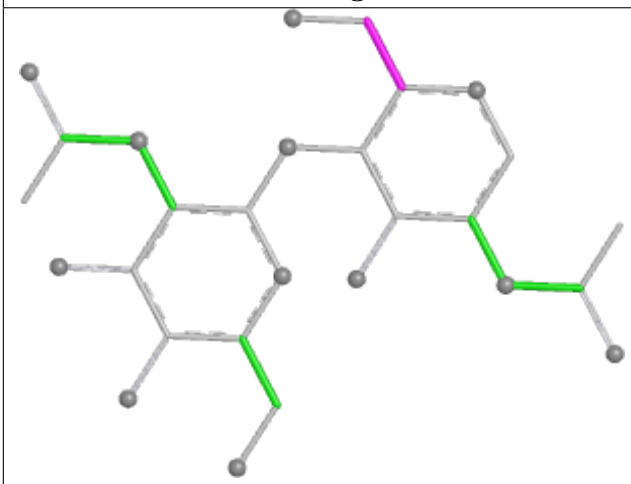
Oligosaccharide Chain D



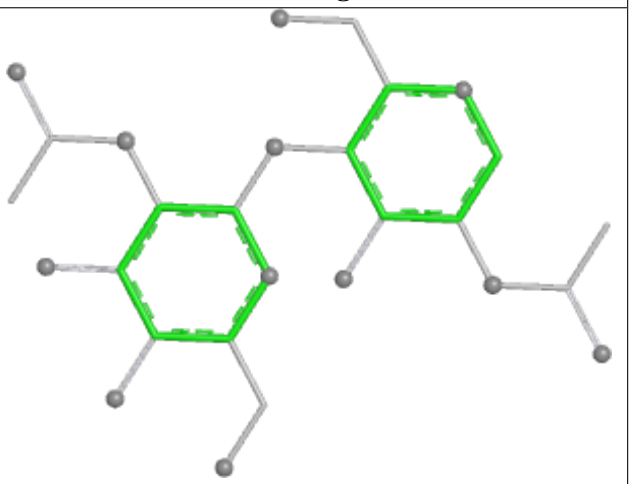
Bond lengths



Bond angles

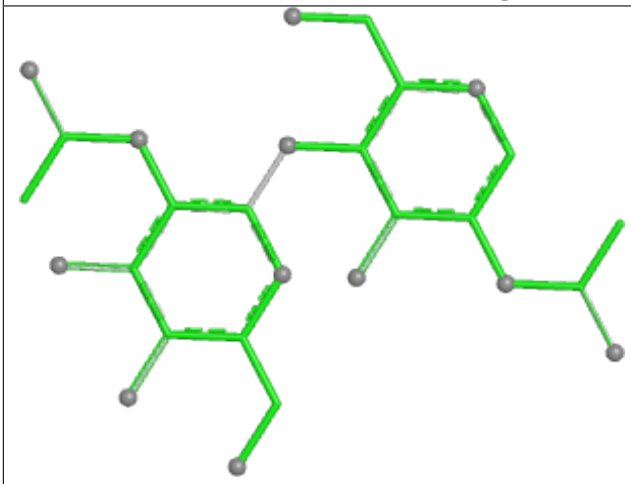


Torsions

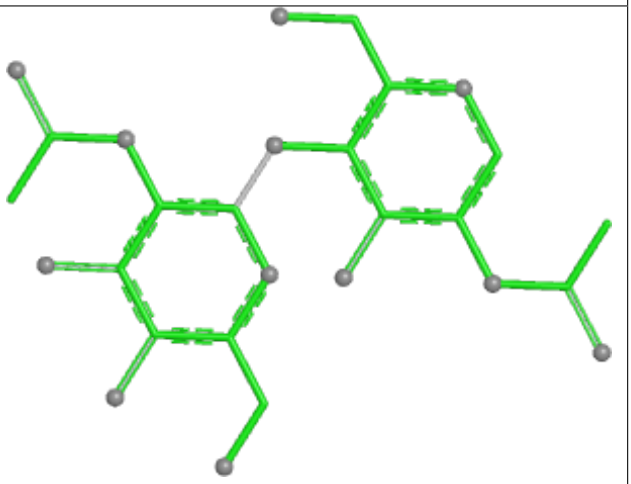


Rings

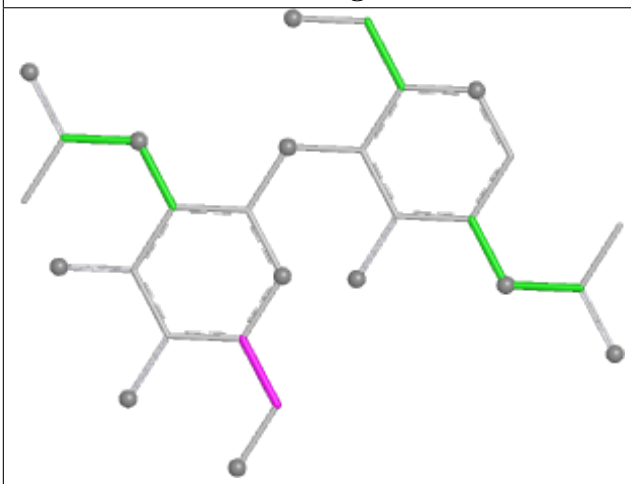
Oligosaccharide Chain E



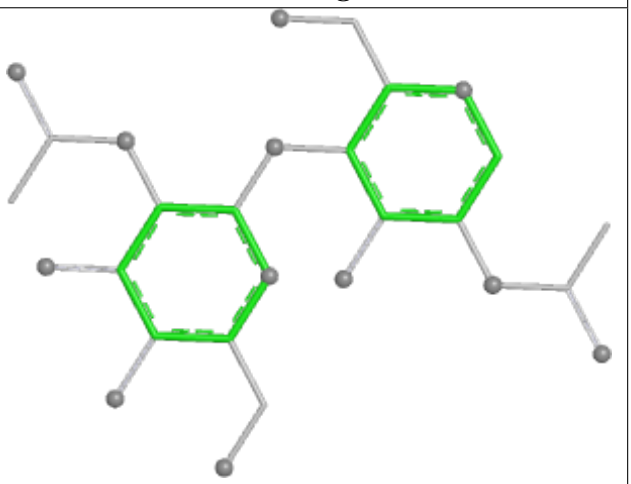
Bond lengths



Bond angles

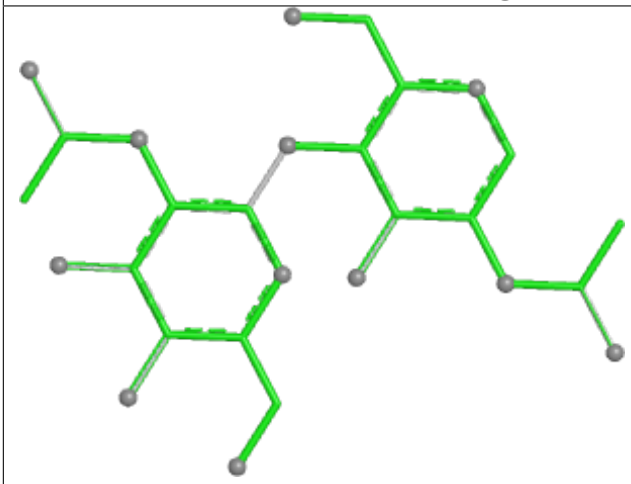


Torsions

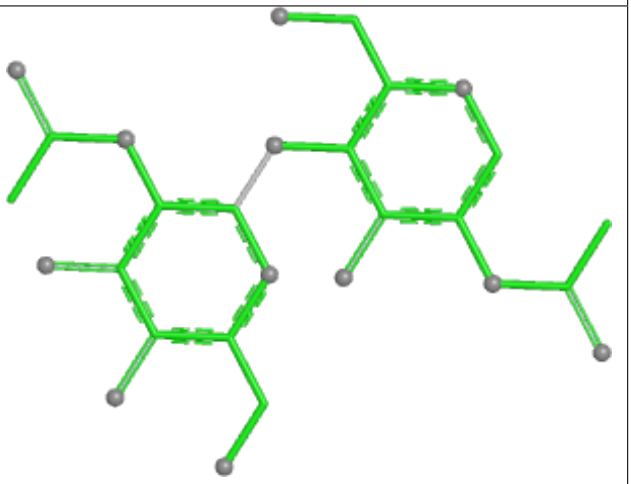


Rings

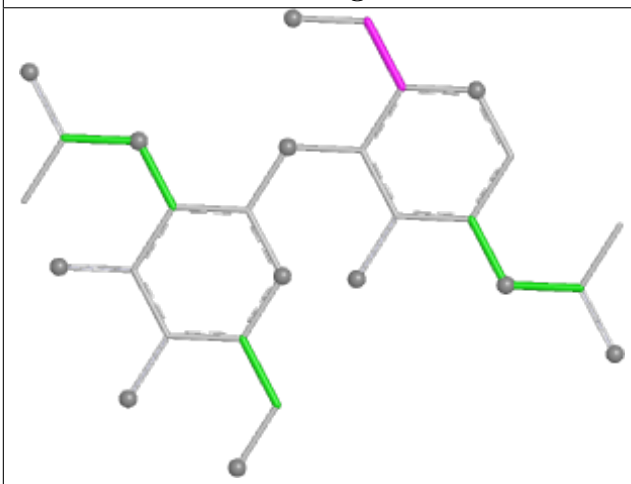
Oligosaccharide Chain F



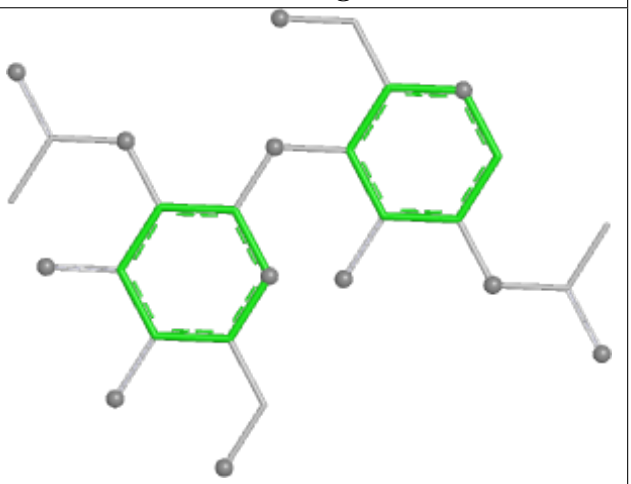
Bond lengths



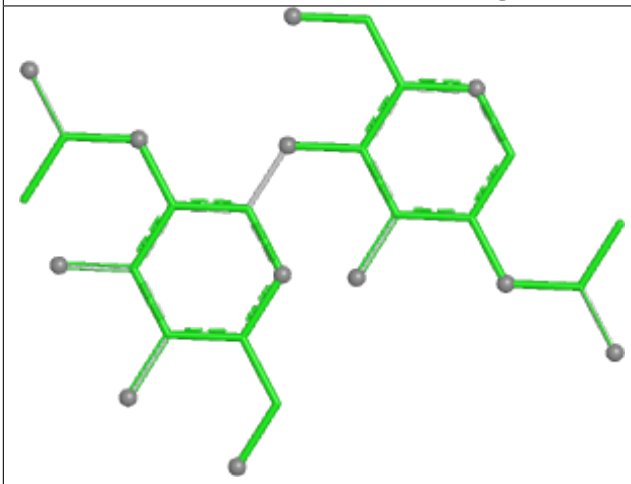
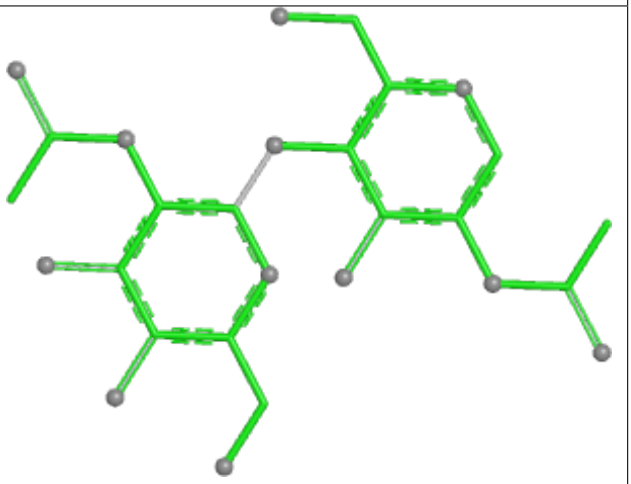
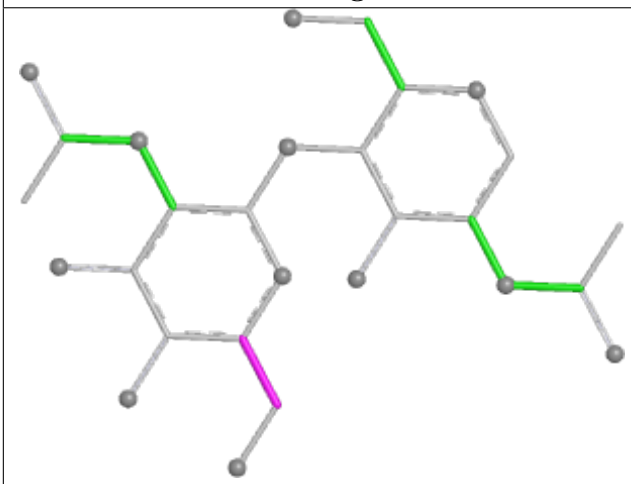
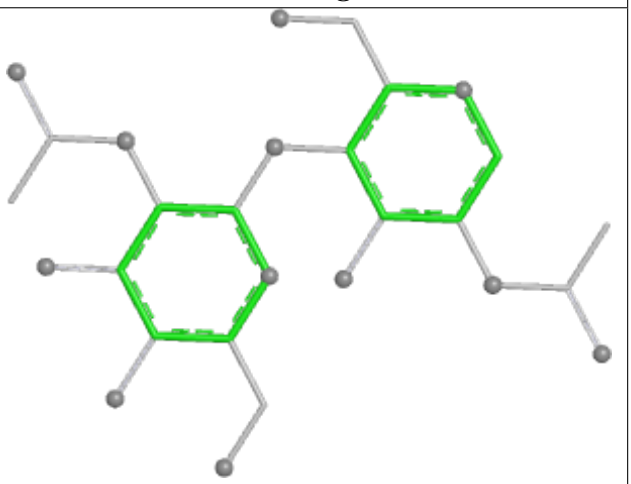
Bond angles



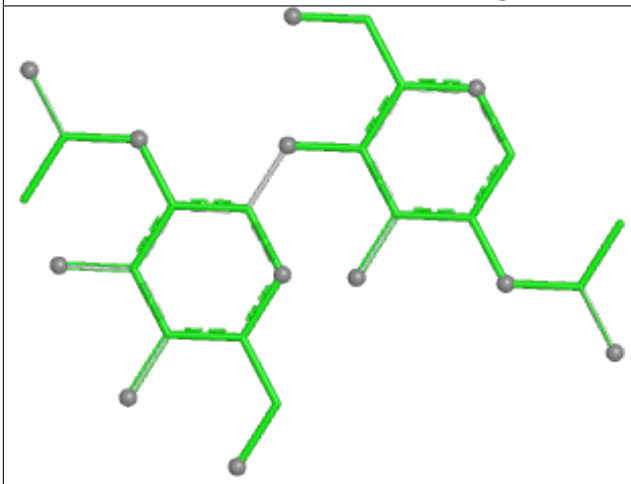
Torsions



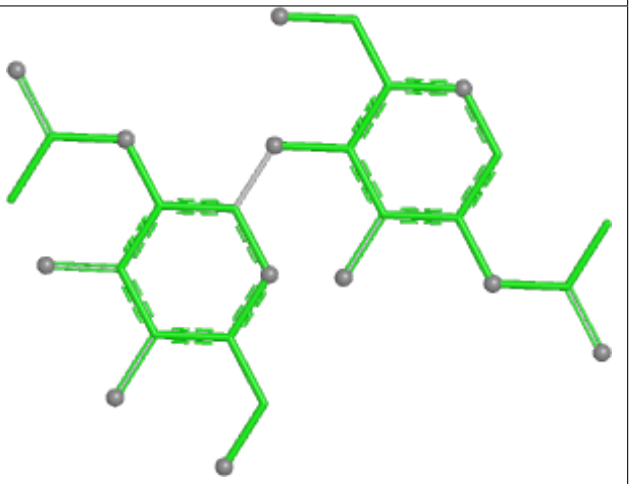
Rings

Oligosaccharide Chain G	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

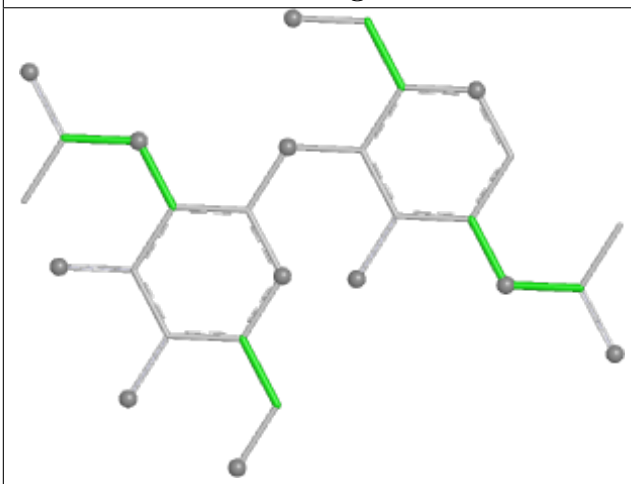
Oligosaccharide Chain H



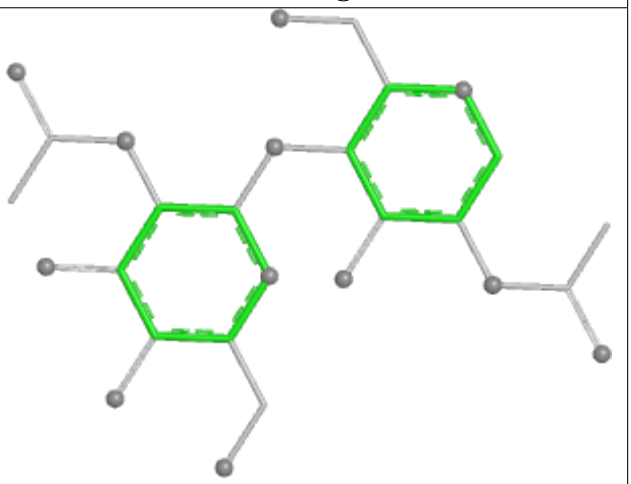
Bond lengths



Bond angles

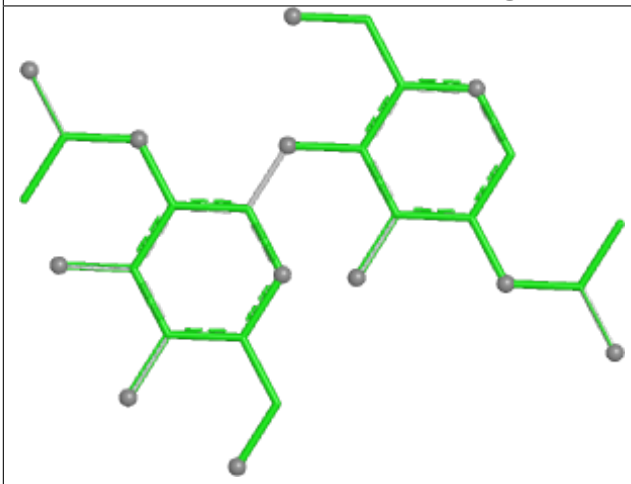


Torsions

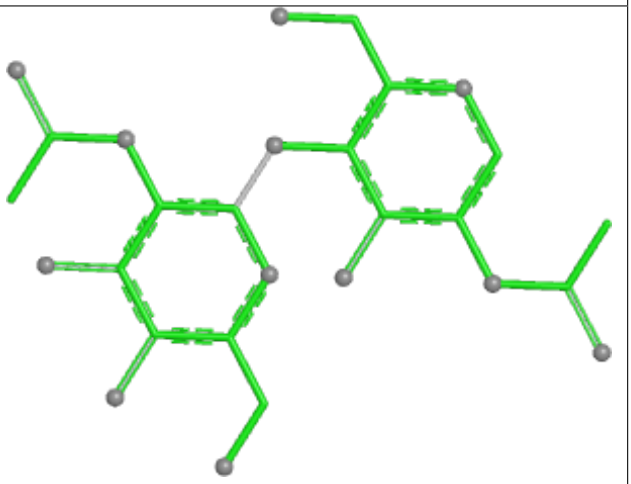


Rings

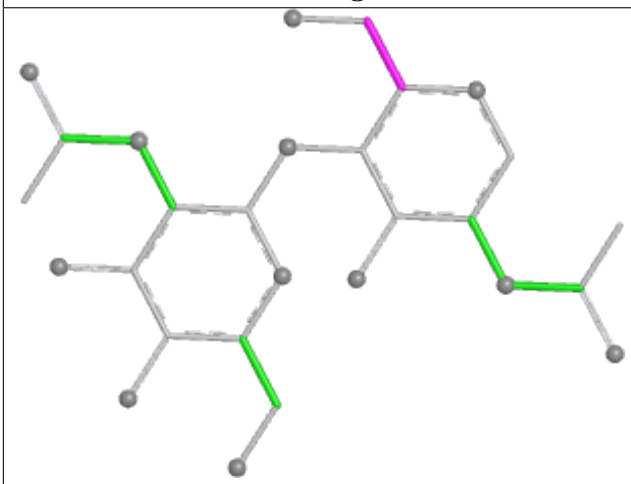
Oligosaccharide Chain I



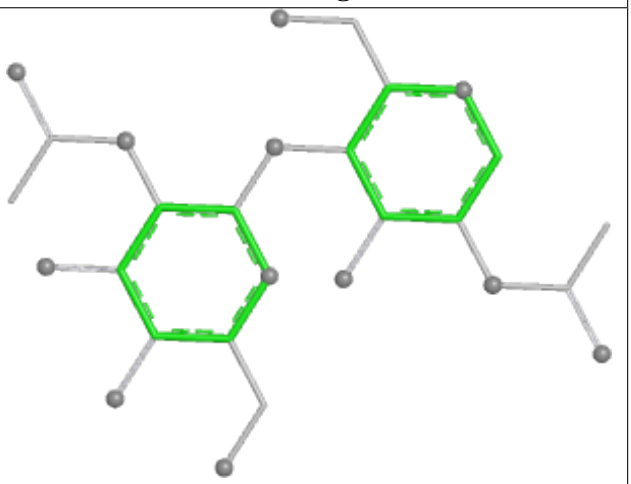
Bond lengths



Bond angles

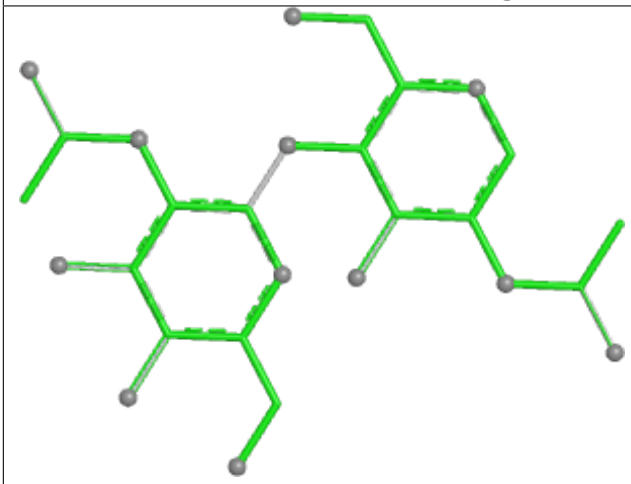


Torsions

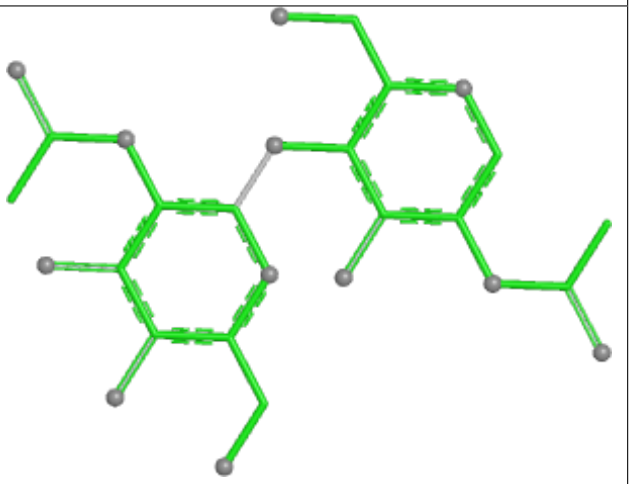


Rings

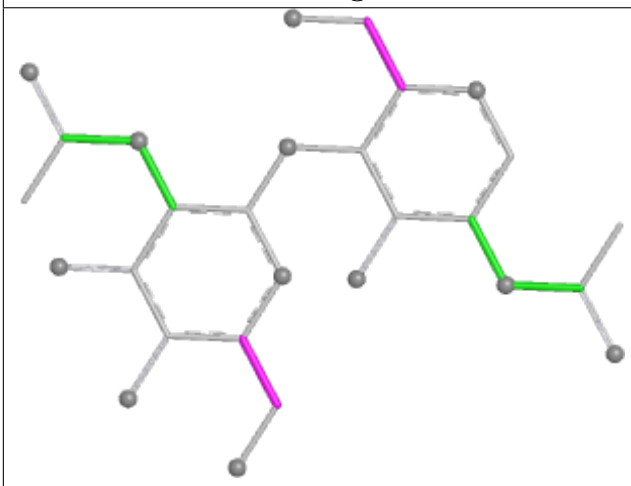
Oligosaccharide Chain J



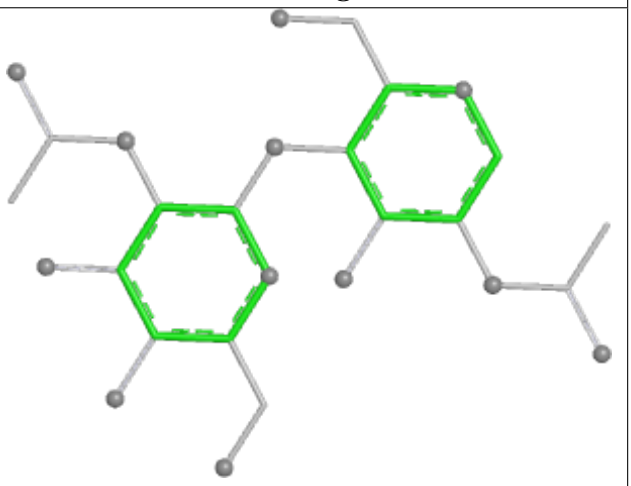
Bond lengths



Bond angles

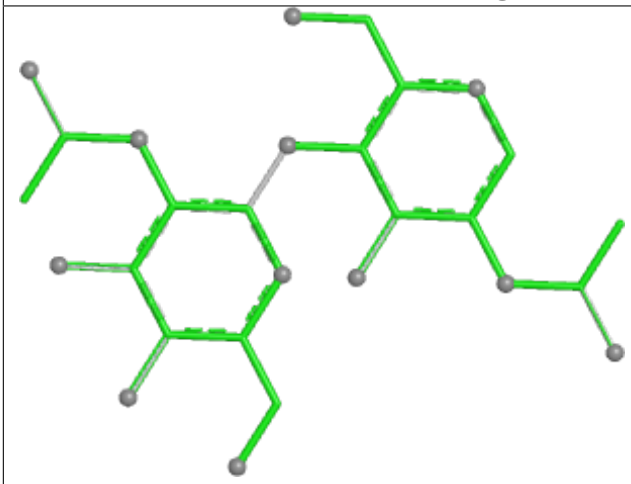


Torsions

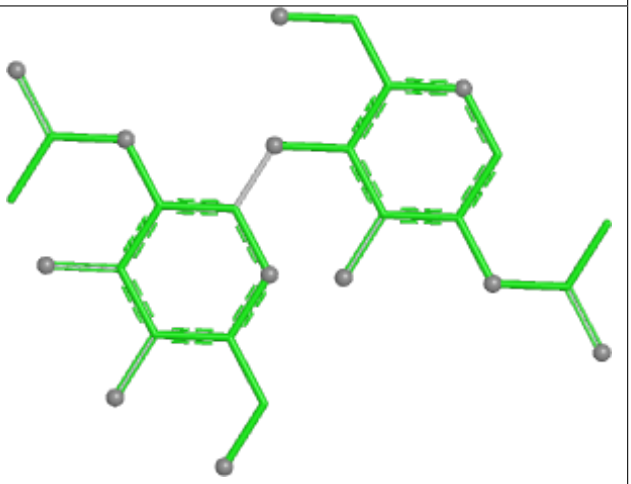


Rings

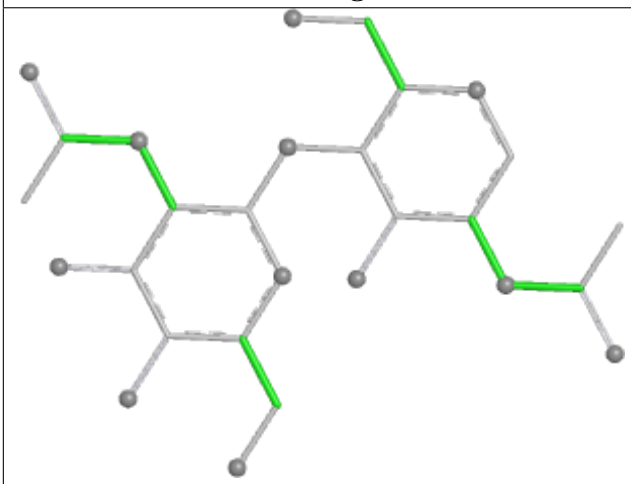
Oligosaccharide Chain K



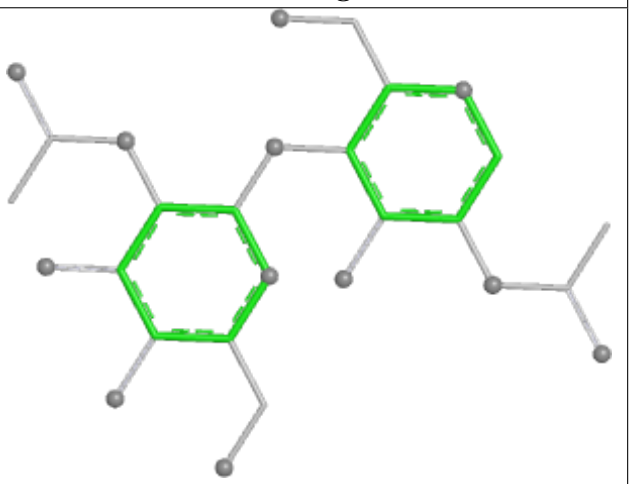
Bond lengths



Bond angles

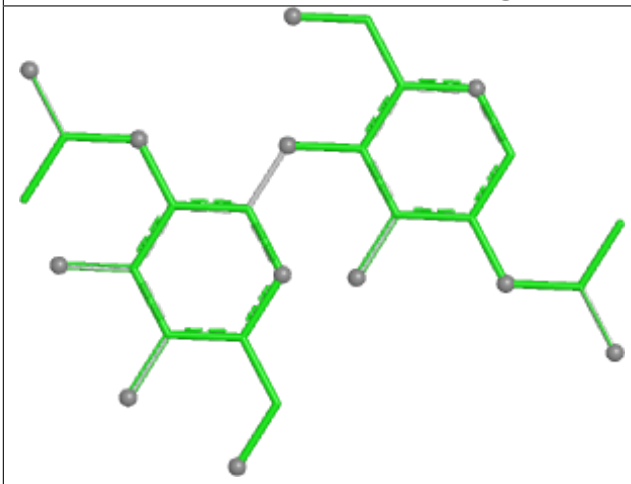


Torsions

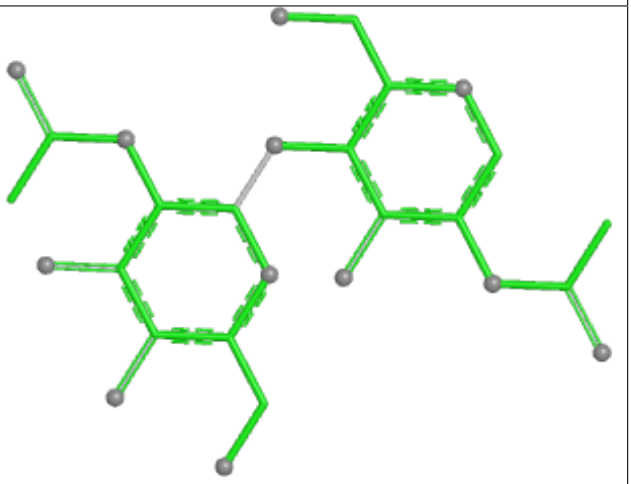


Rings

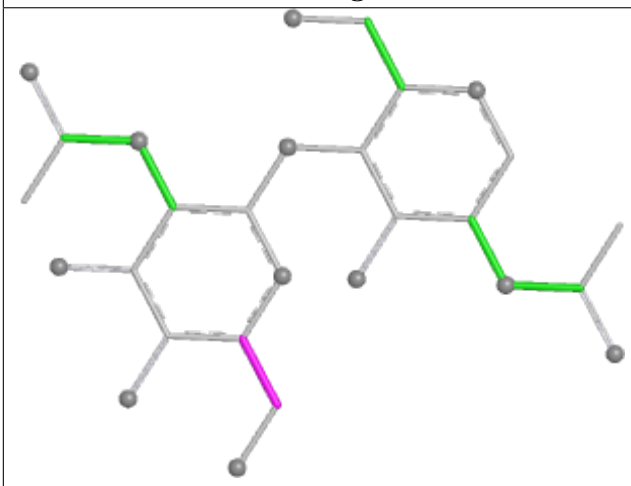
Oligosaccharide Chain L



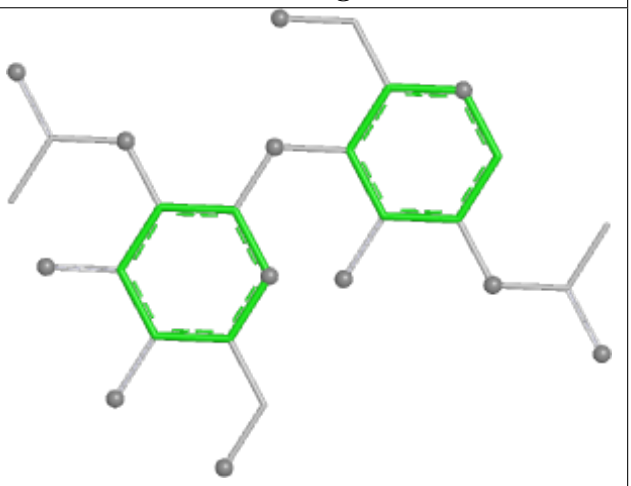
Bond lengths



Bond angles

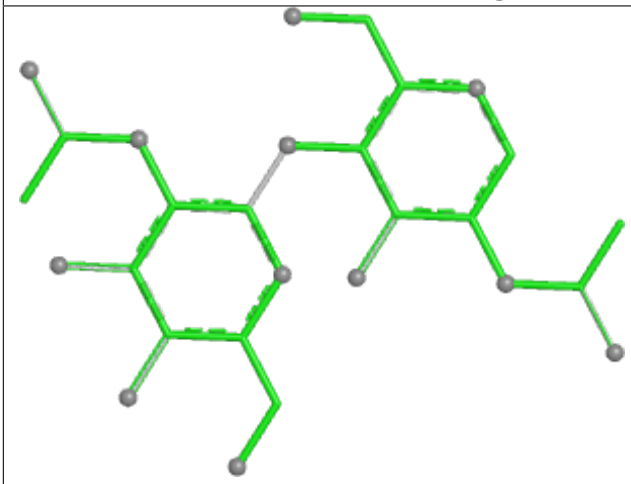


Torsions

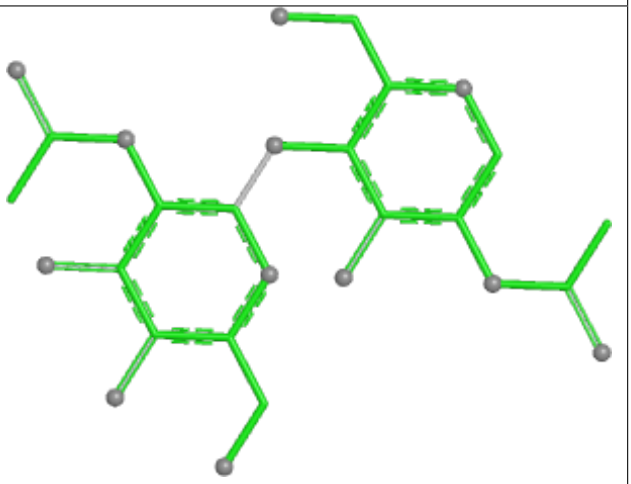


Rings

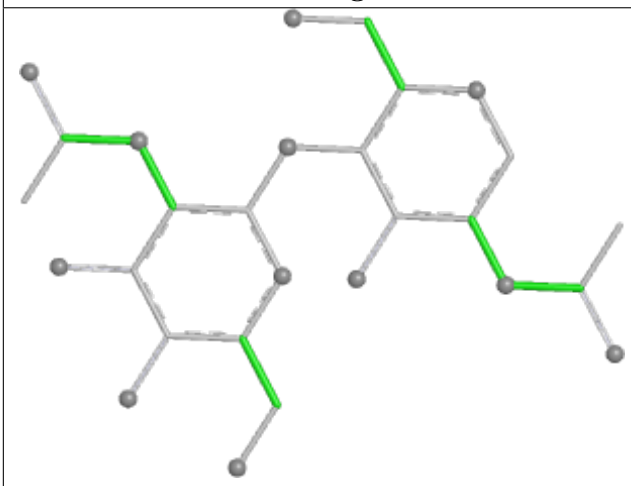
Oligosaccharide Chain M



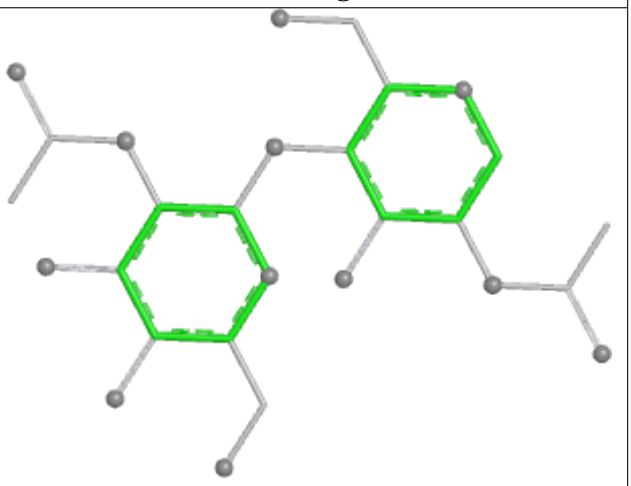
Bond lengths



Bond angles

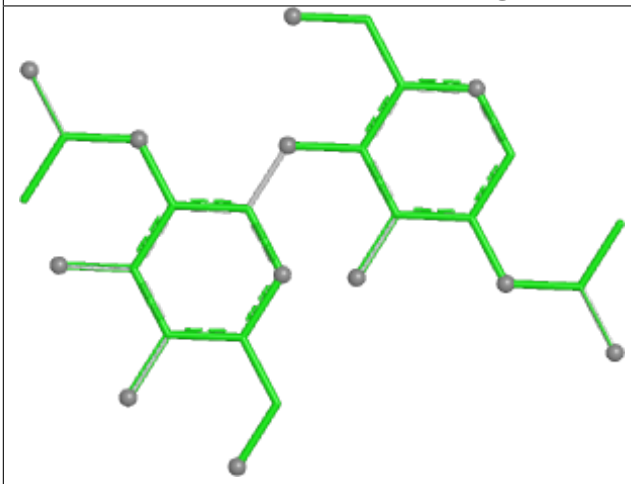


Torsions

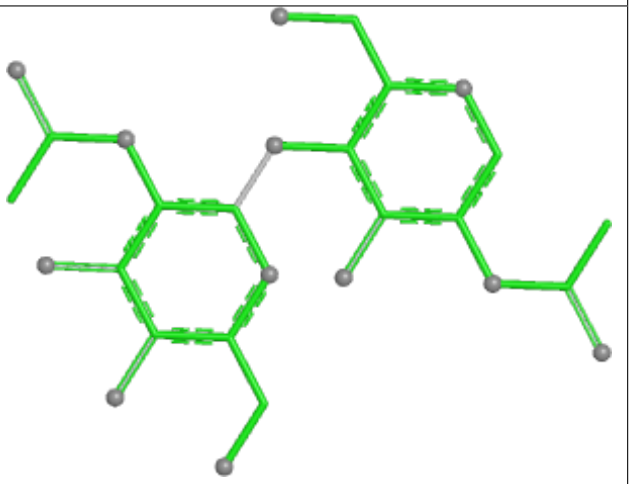


Rings

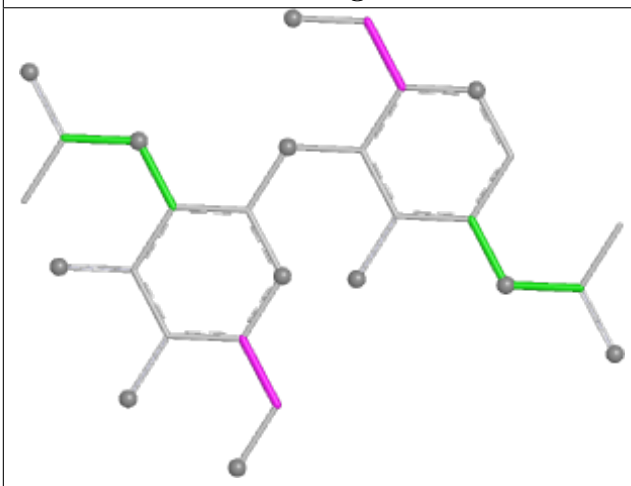
Oligosaccharide Chain N



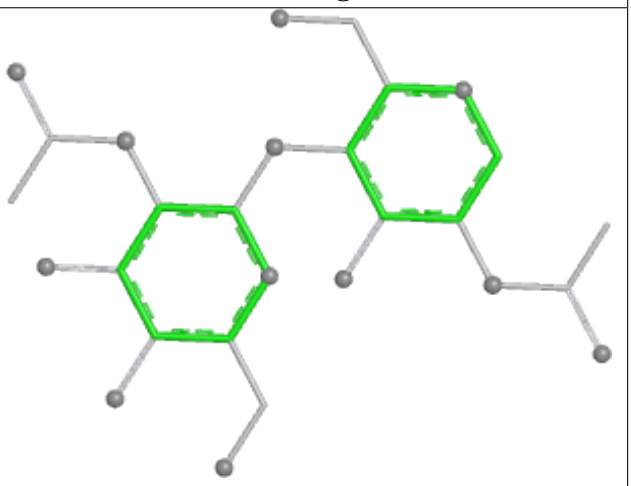
Bond lengths



Bond angles

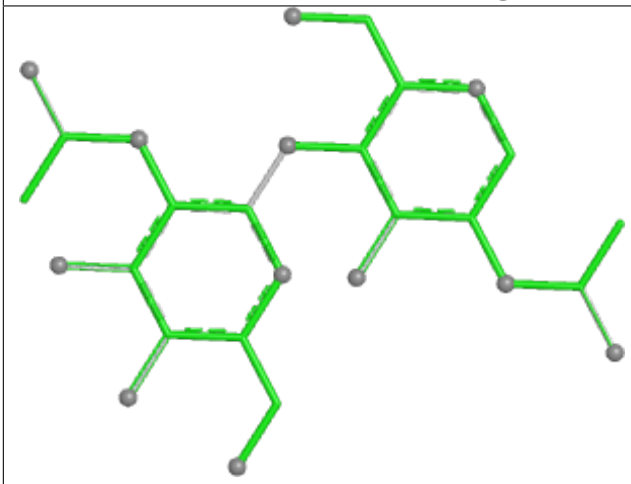


Torsions

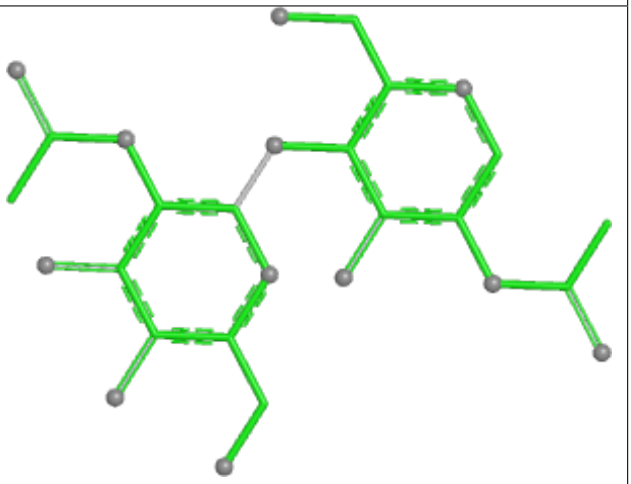


Rings

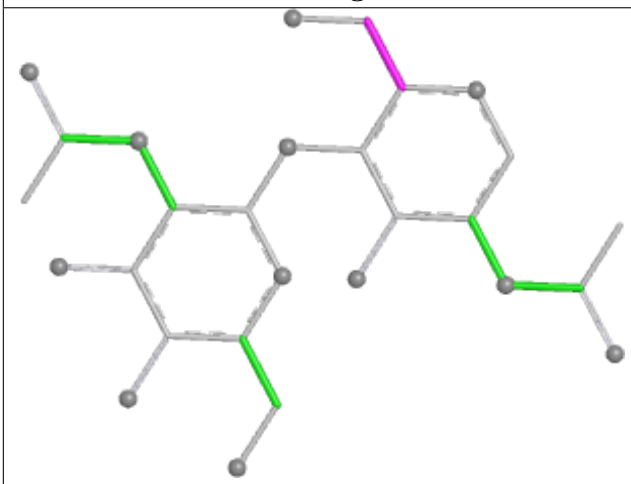
Oligosaccharide Chain O



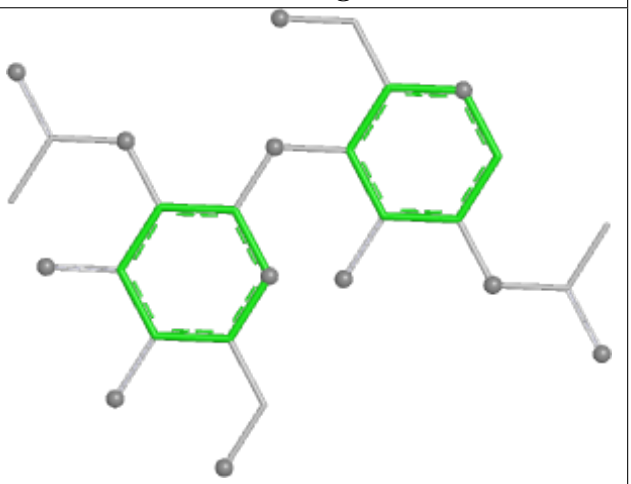
Bond lengths



Bond angles

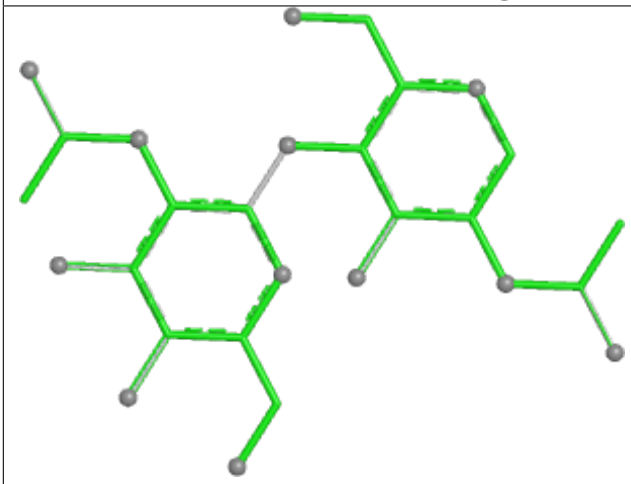


Torsions

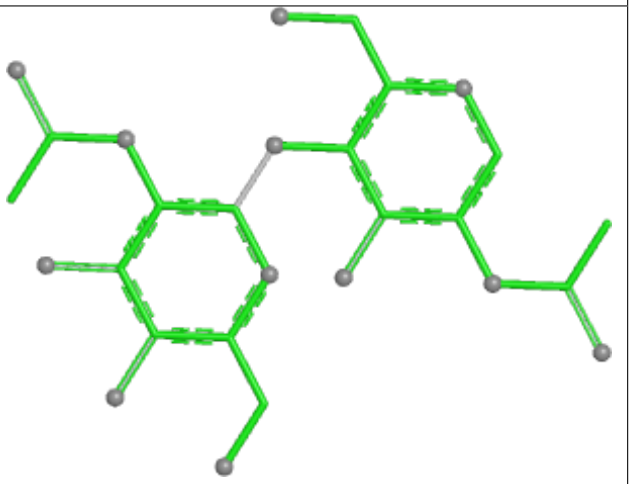


Rings

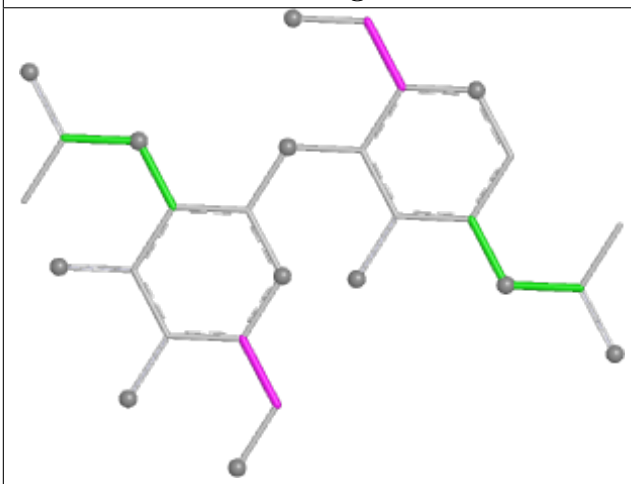
Oligosaccharide Chain P



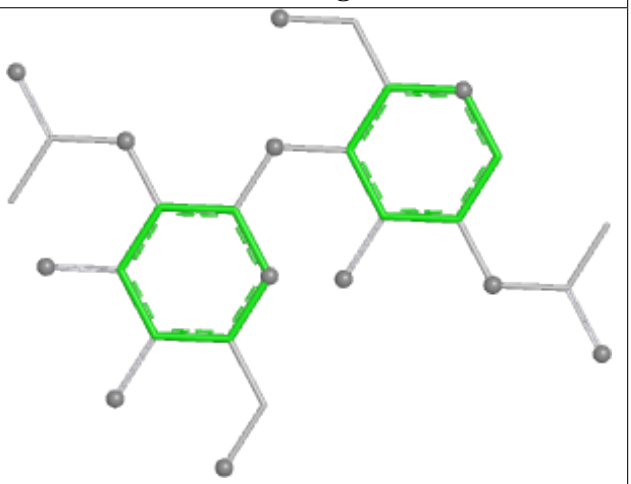
Bond lengths



Bond angles

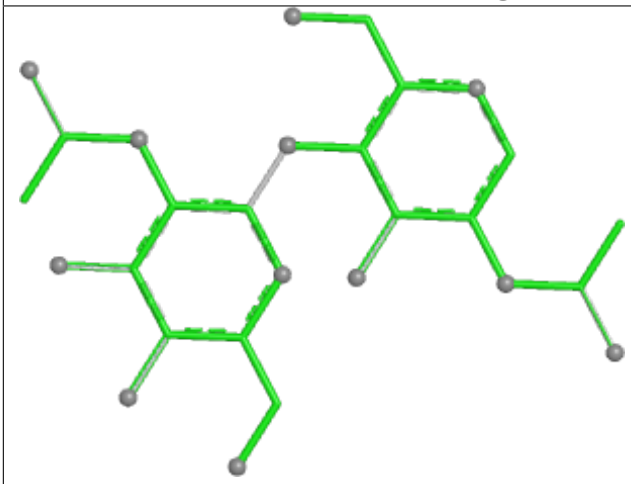


Torsions

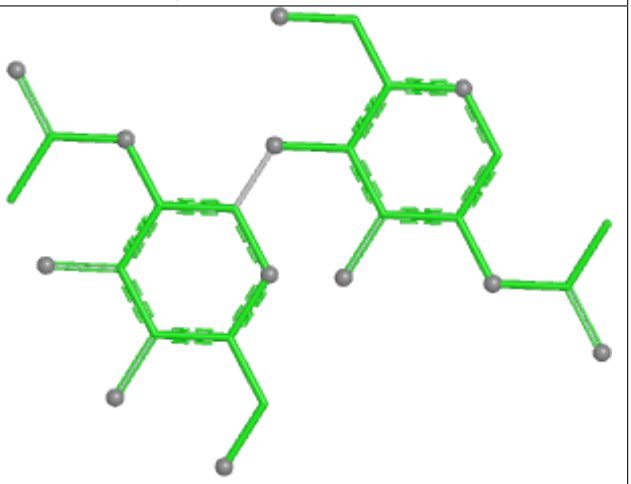


Rings

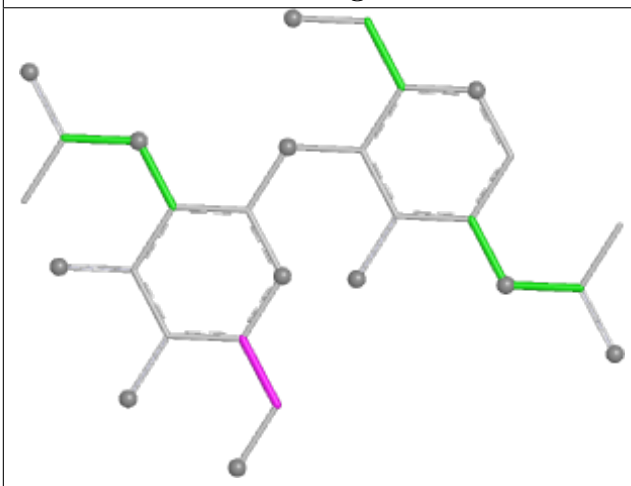
Oligosaccharide Chain Q



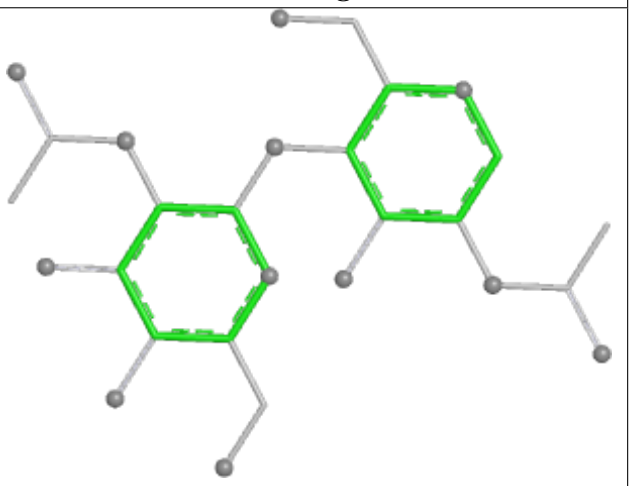
Bond lengths



Bond angles

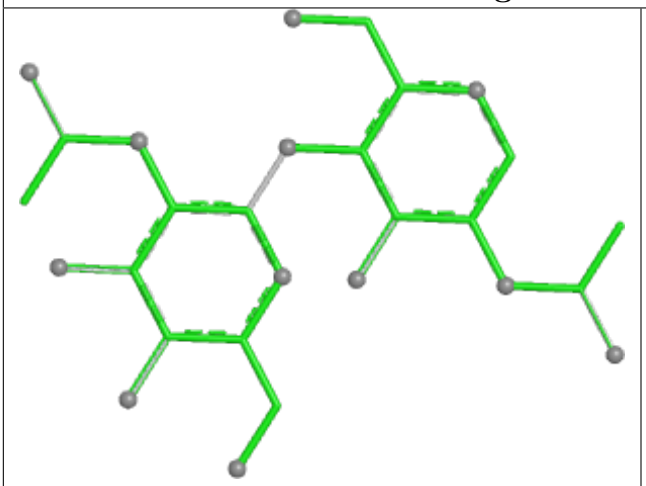


Torsions

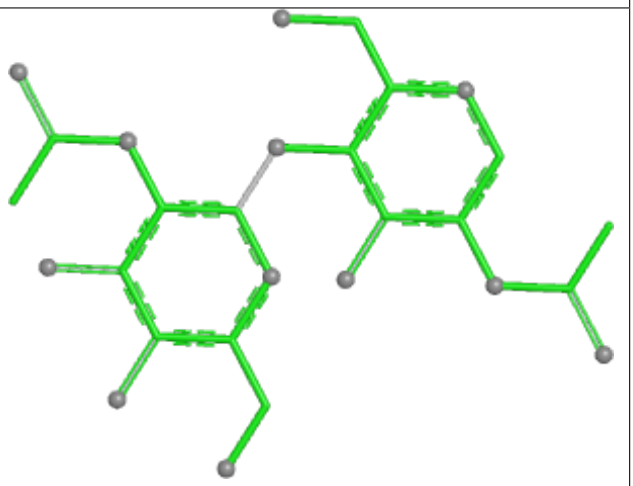


Rings

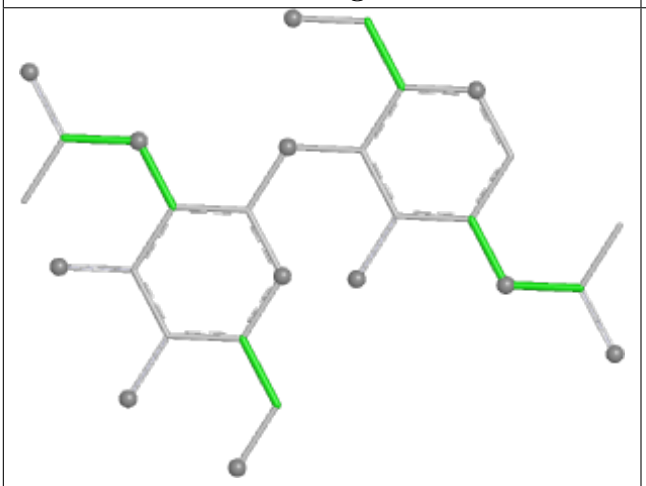
Oligosaccharide Chain R



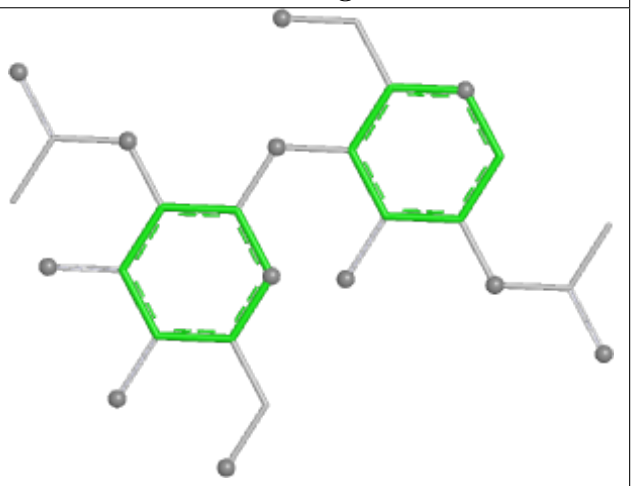
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1306	-	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	A	1304	1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	C	1306	-	14,14,15	0.19	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	C	1311	-	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	B	1311	-	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	B	1305	1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	C	1309	1	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	C	1302	-	14,14,15	0.24	0	17,19,21	0.53	0
3	NAG	C	1307	1	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	A	1307	1	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	A	1311	-	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	C	1305	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	A	1301	1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	B	1307	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	B	1308	1	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	B	1302	-	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	B	1303	1	14,14,15	0.30	0	17,19,21	0.43	0
3	NAG	A	1309	1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	A	1302	-	14,14,15	0.25	0	17,19,21	0.53	0
3	NAG	A	1310	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	C	1301	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.44	0
3	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.50	0
3	NAG	B	1309	1	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	C	1303	1	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	B	1310	1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	A	1306	-	14,14,15	0.20	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1302	-	-	1/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1311	-	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	-	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1302	-	-	1/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1308	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1304	NAG	1	0
3	C	1304	NAG	1	0

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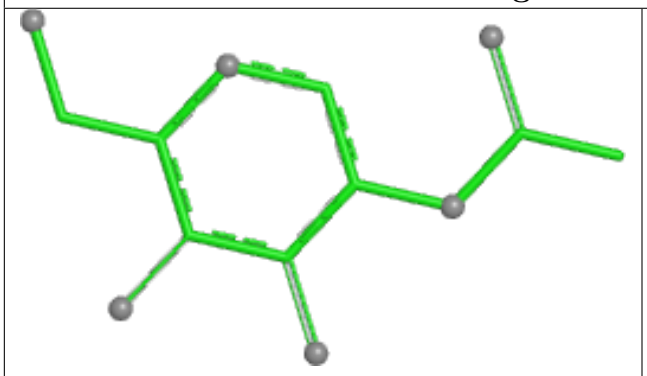
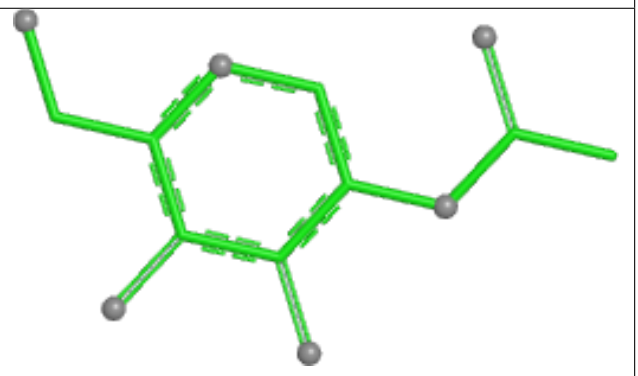
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1304	NAG	1	0

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

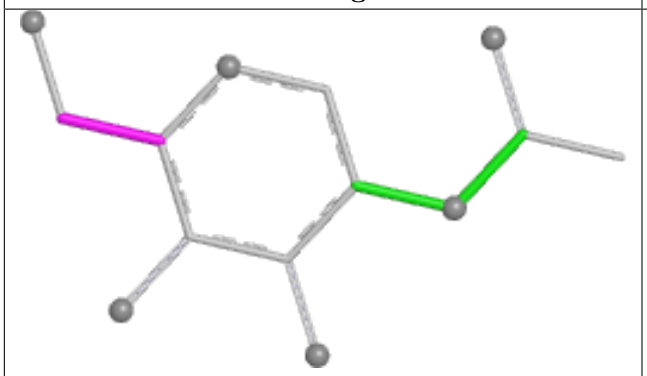
Ligand NAG B 1306



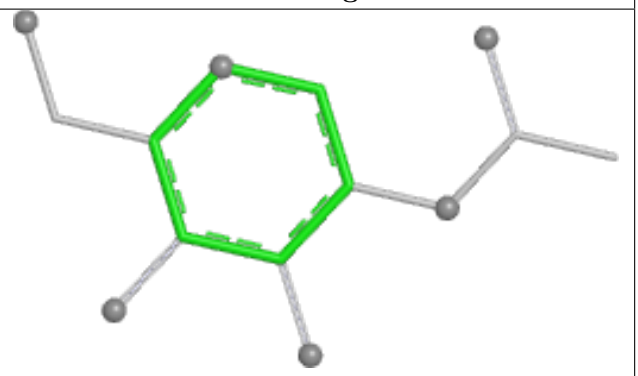
Bond lengths



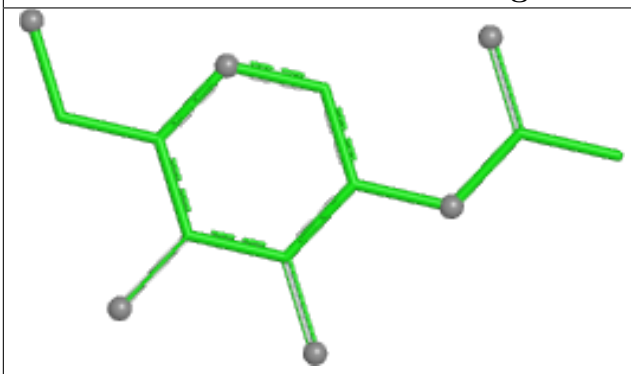
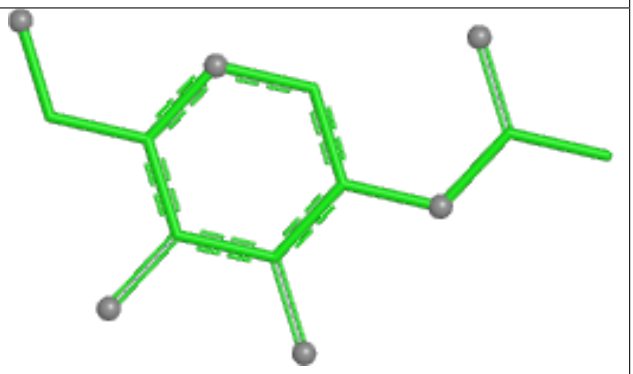
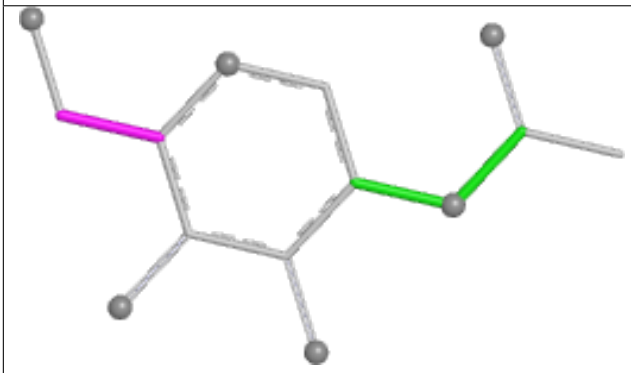
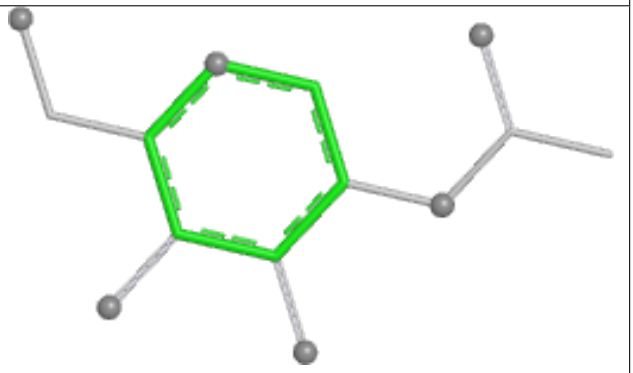
Bond angles

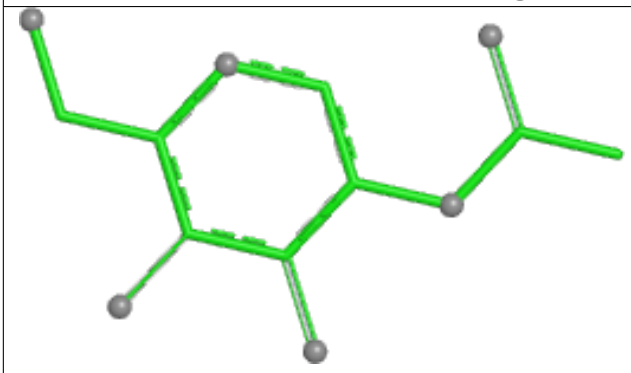
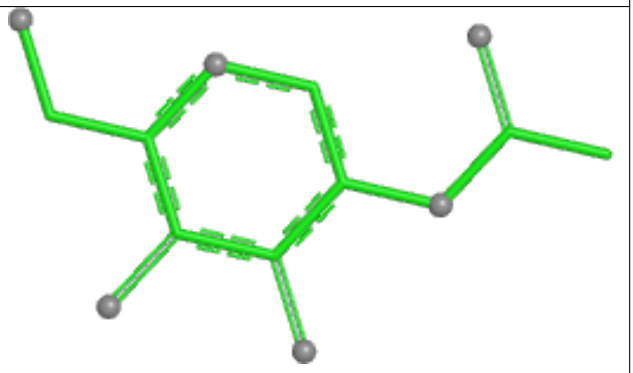
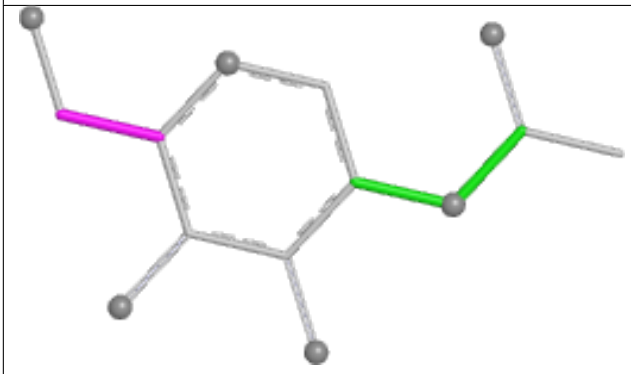
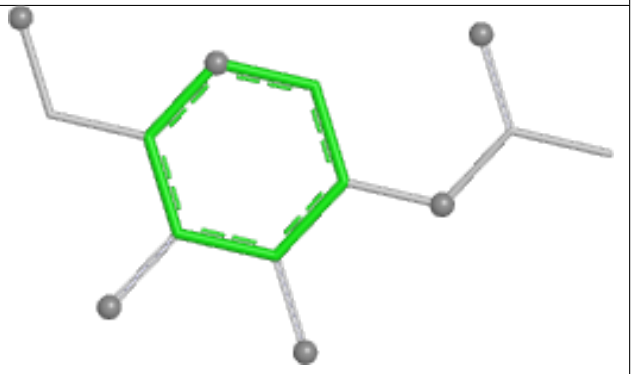


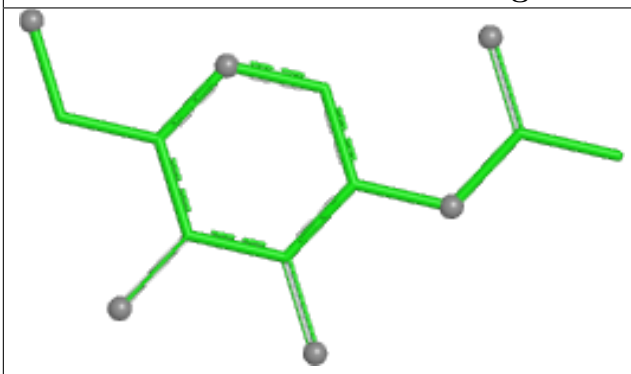
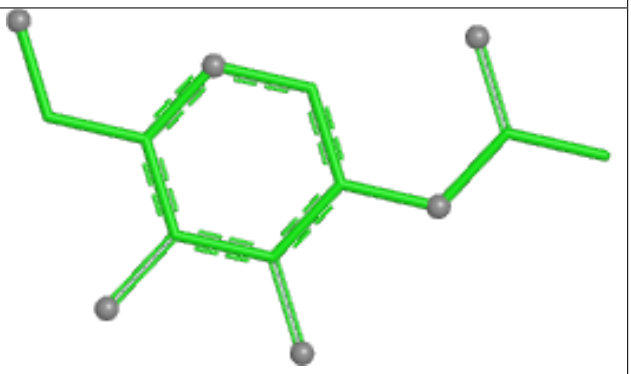
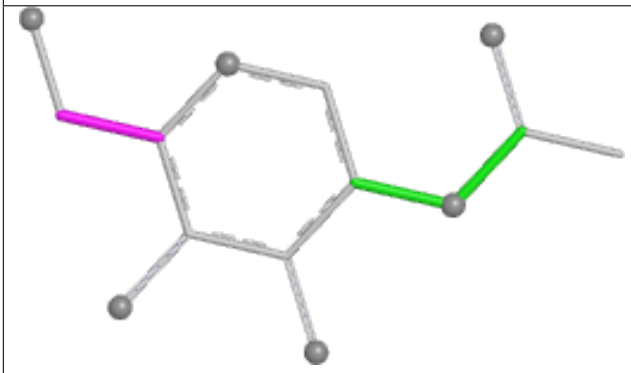
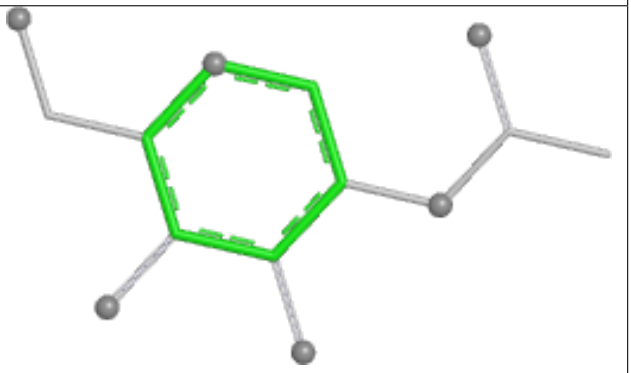
Torsions

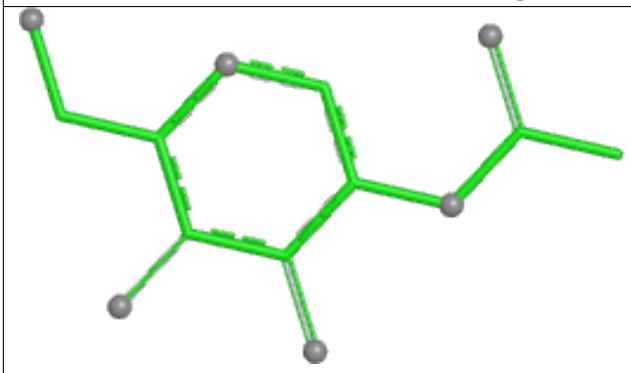
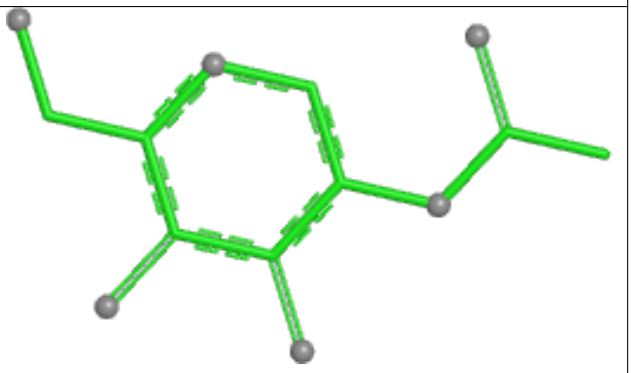
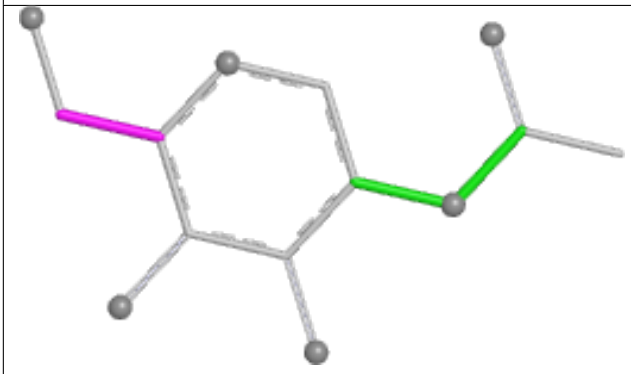
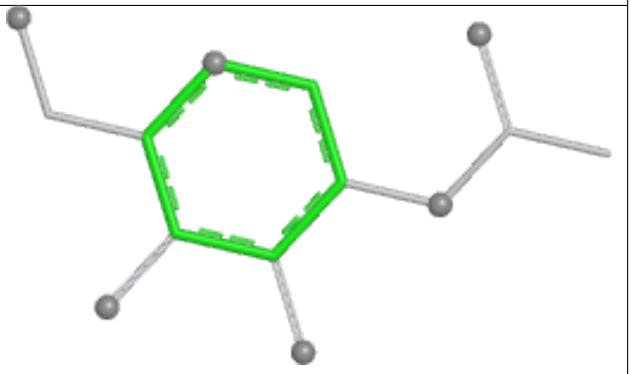


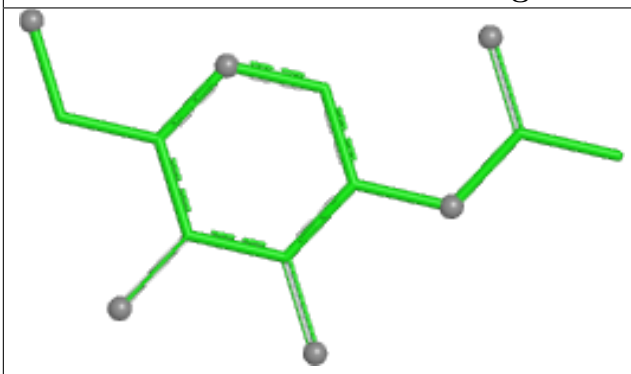
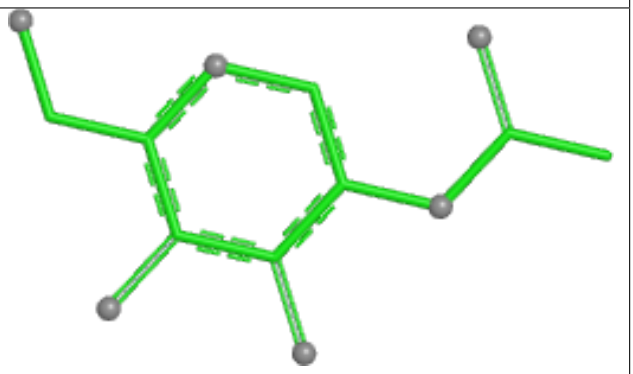
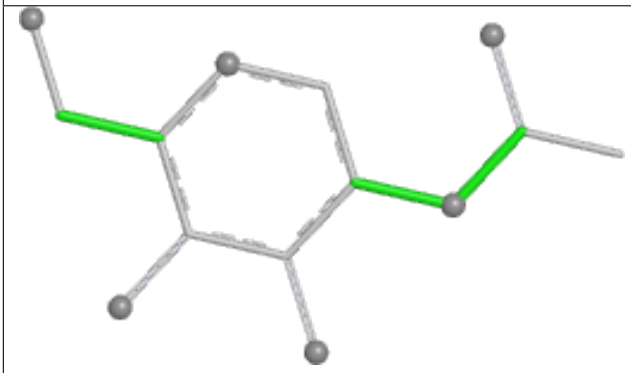
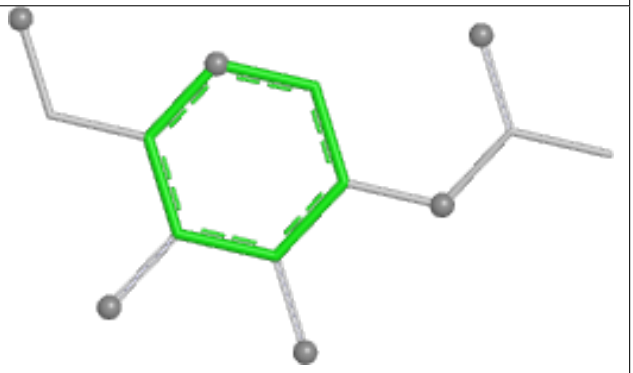
Rings

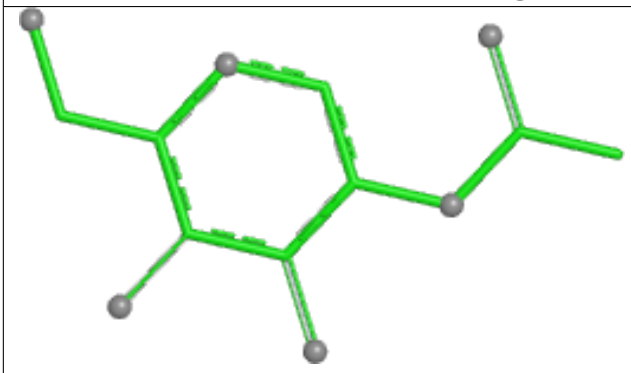
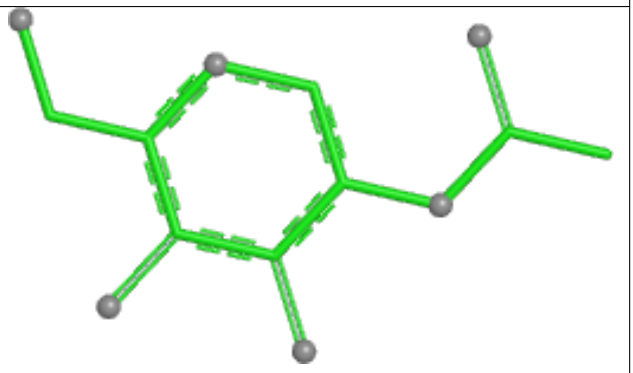
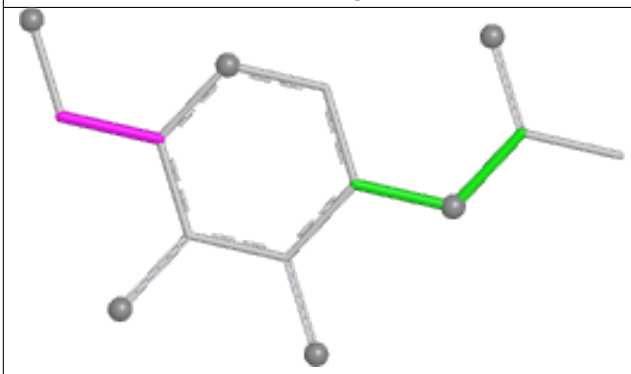
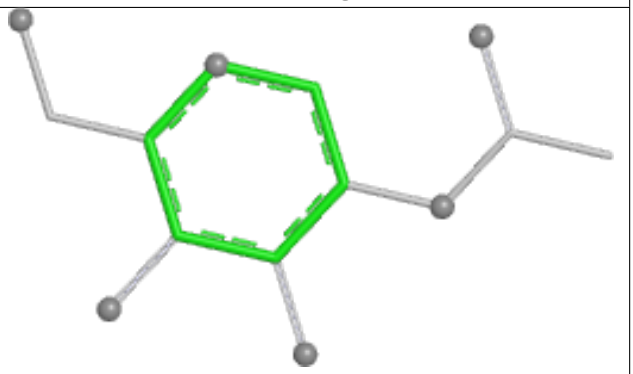
Ligand NAG A 1304	
	
Bond lengths	Bond angles
	
Torsions	Rings

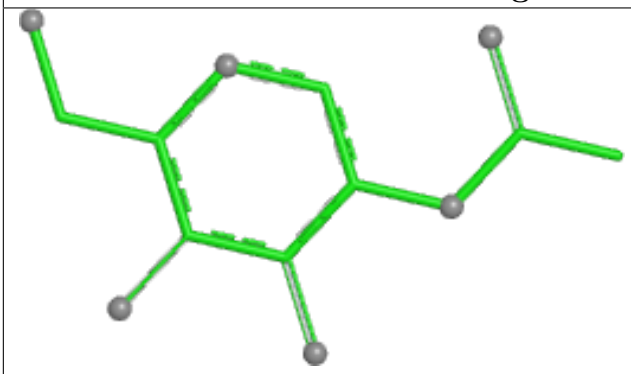
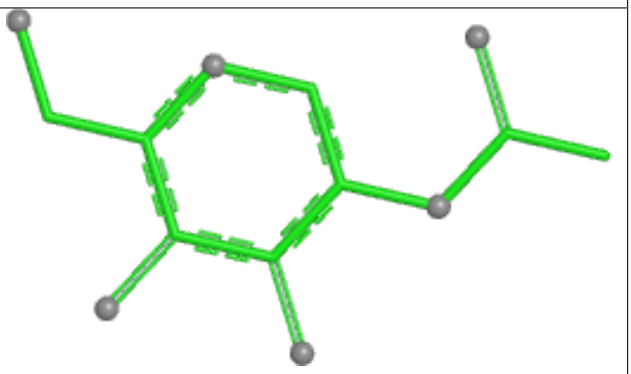
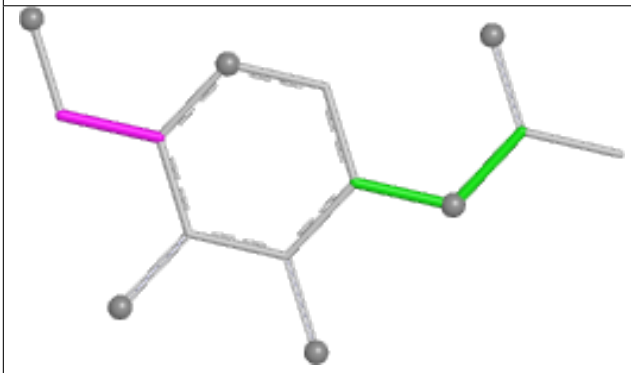
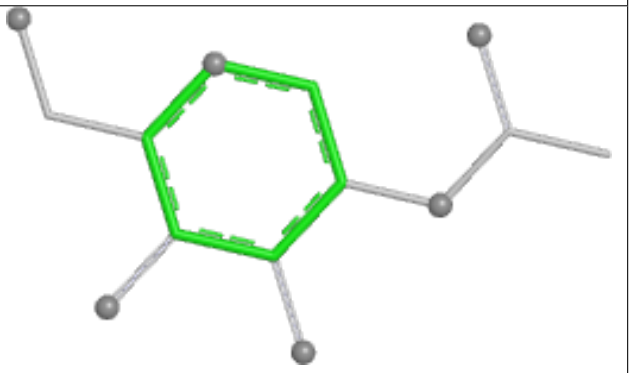
Ligand NAG C 1306	
	
Bond lengths	Bond angles
	
Torsions	Rings

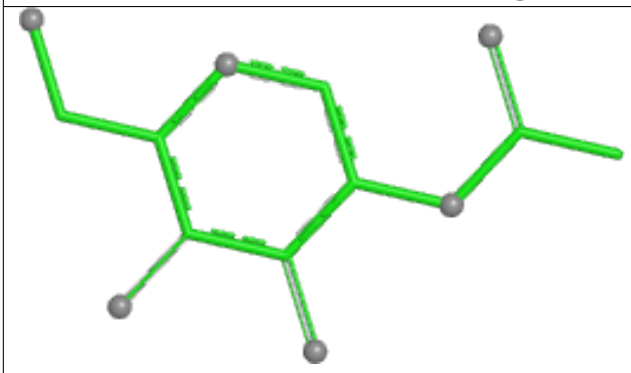
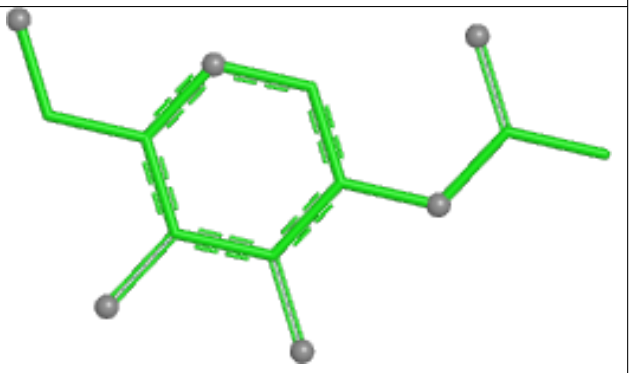
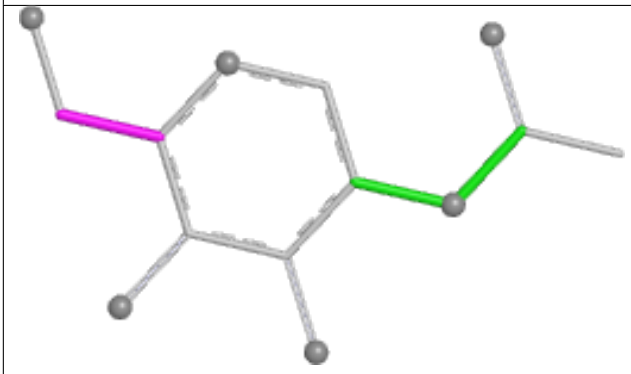
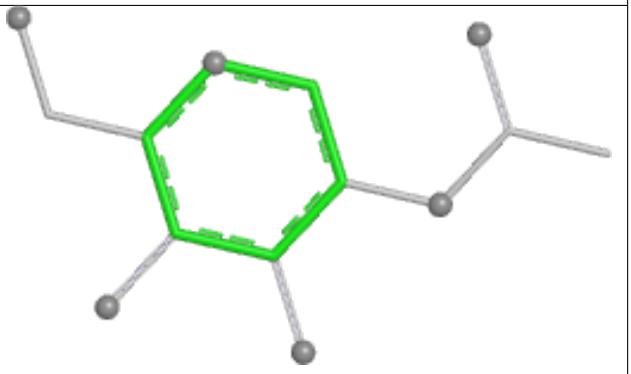
Ligand NAG C 1311	
 Bond lengths	 Bond angles
 Torsions	 Rings

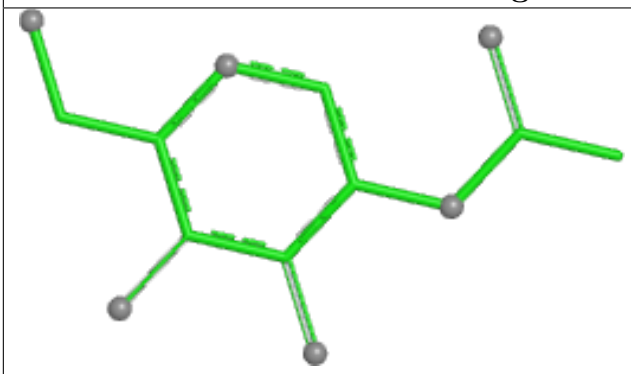
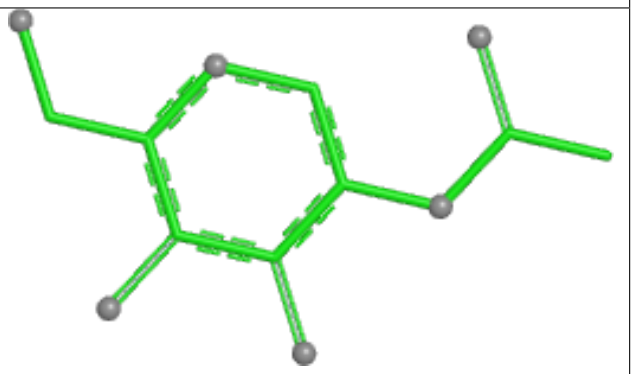
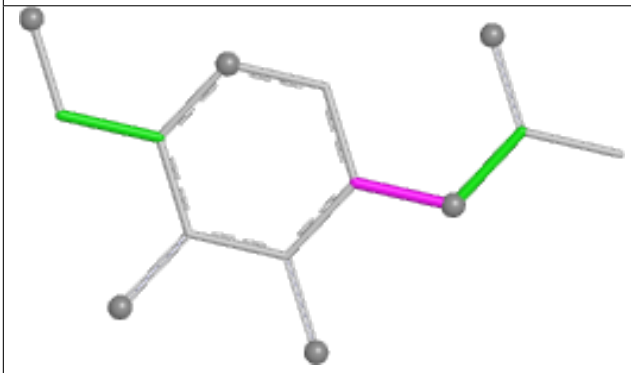
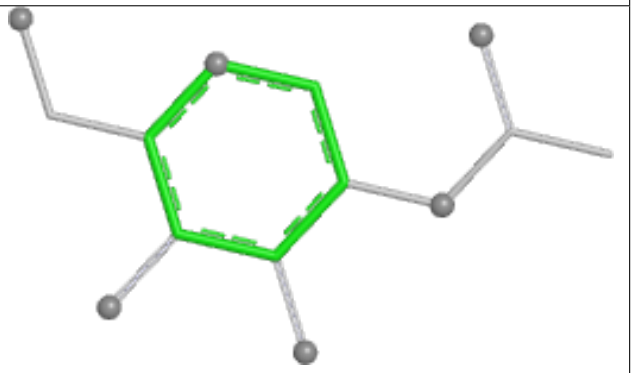
Ligand NAG B 1311	
 Bond lengths	 Bond angles
 Torsions	 Rings

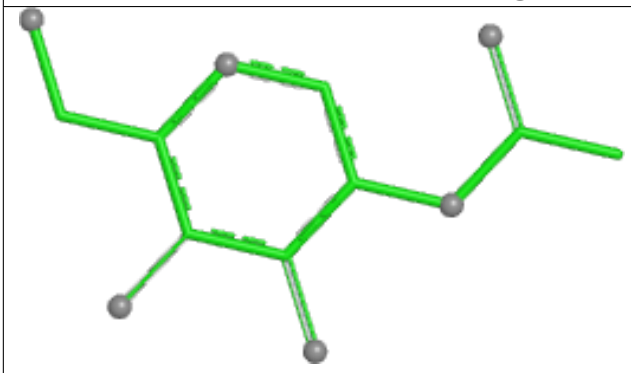
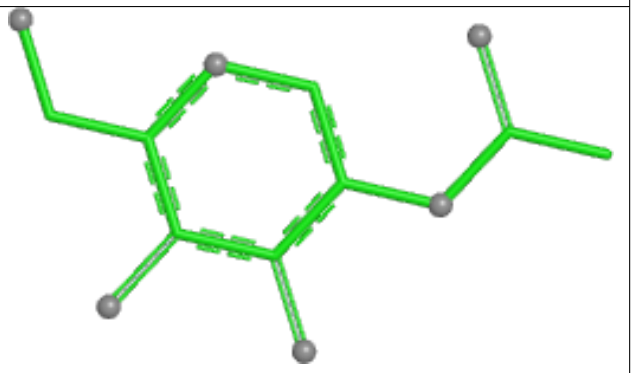
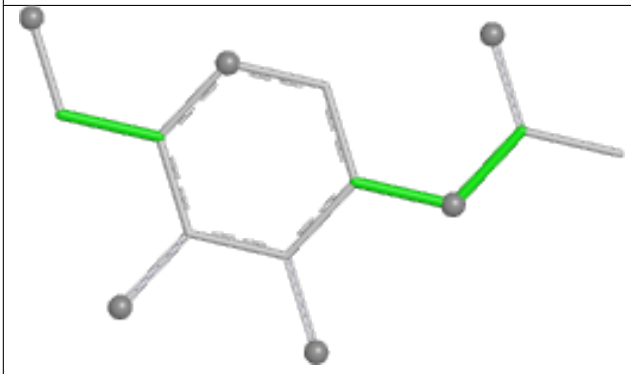
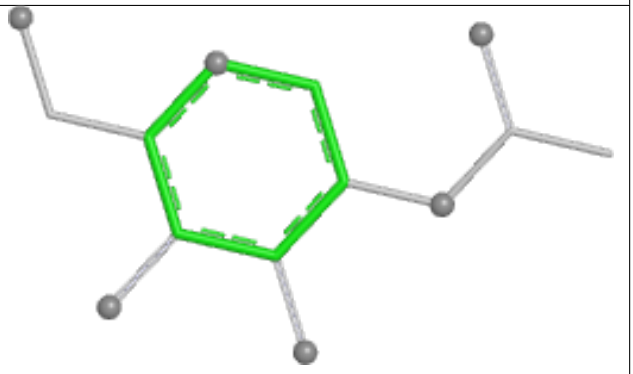
Ligand NAG B 1305	
	
Bond lengths	Bond angles
	
Torsions	Rings

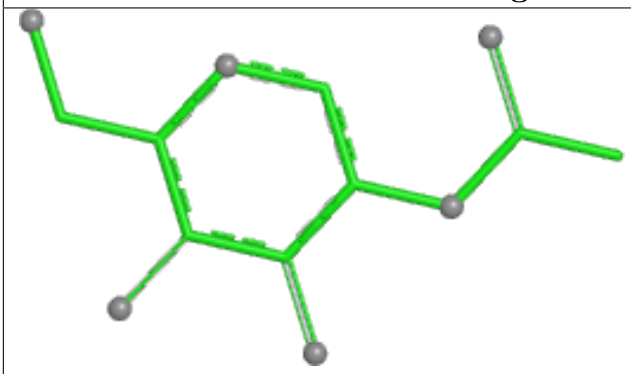
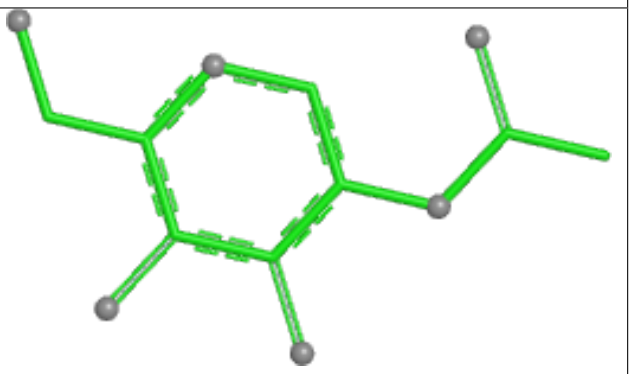
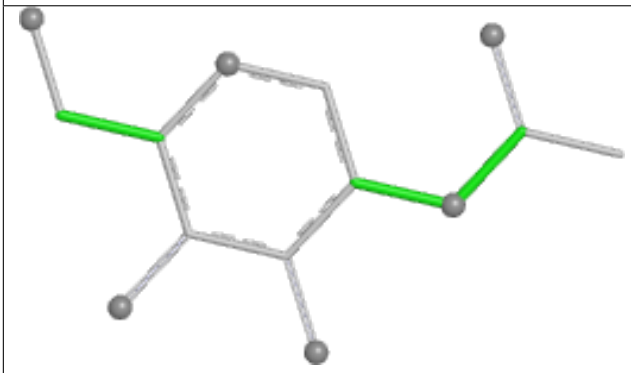
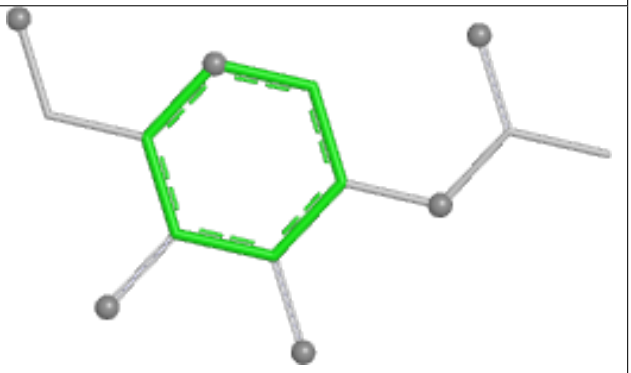
Ligand NAG C 1304	
	
Bond lengths	Bond angles
	
Torsions	Rings

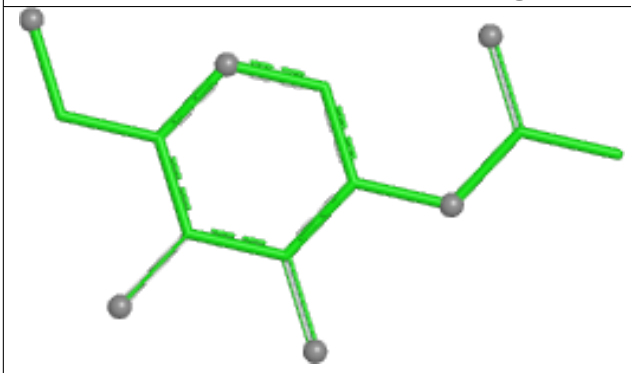
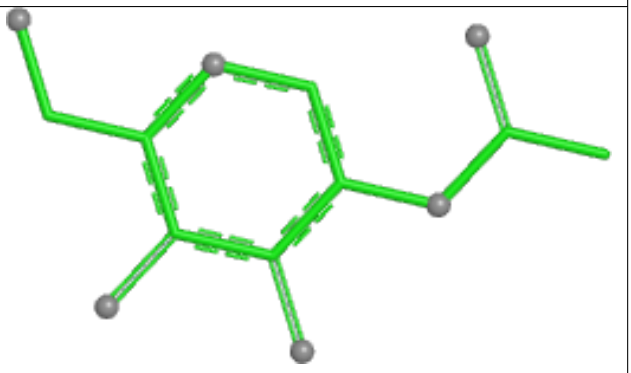
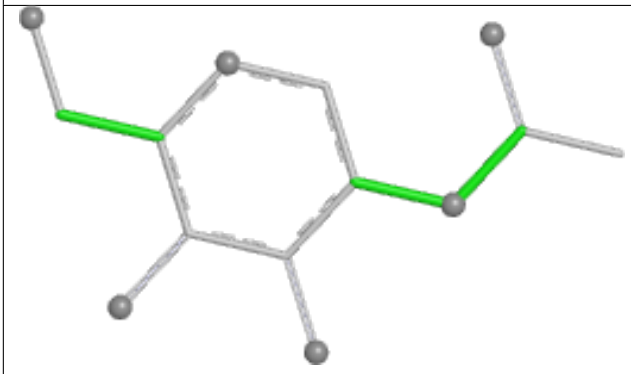
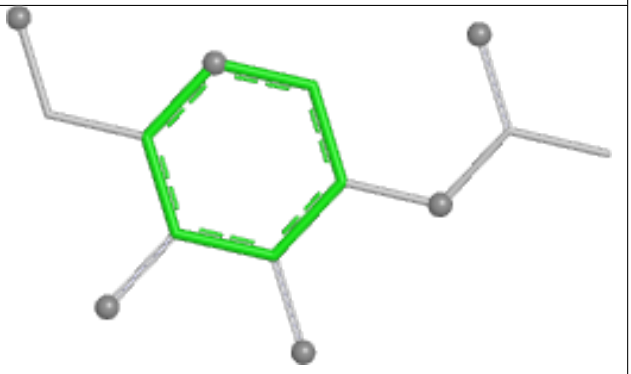
Ligand NAG B 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

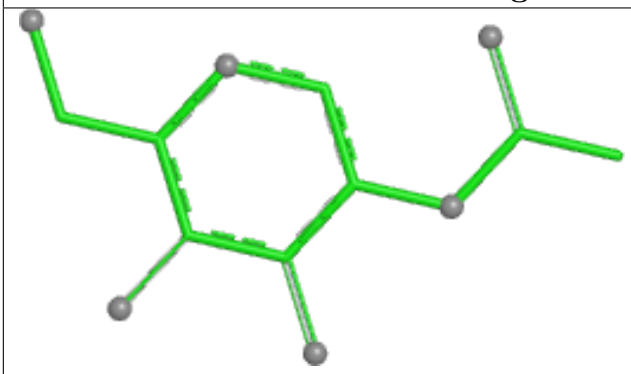
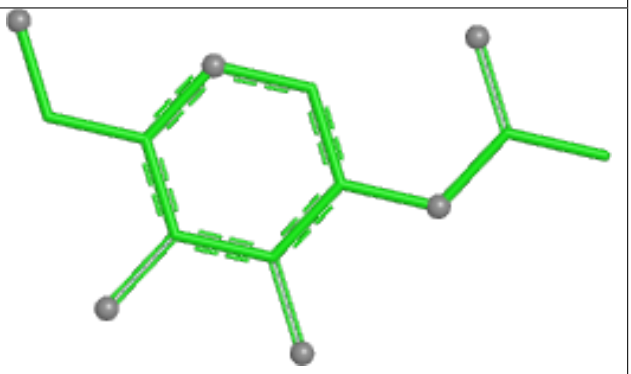
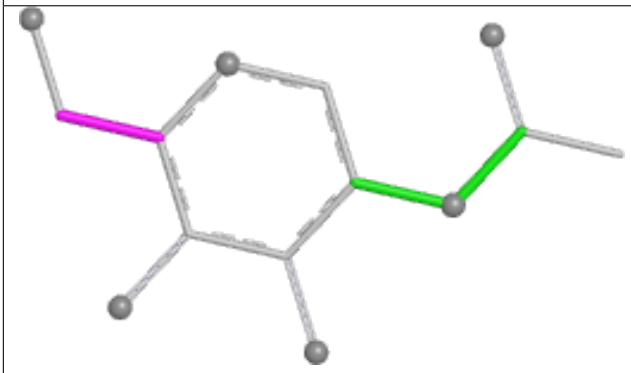
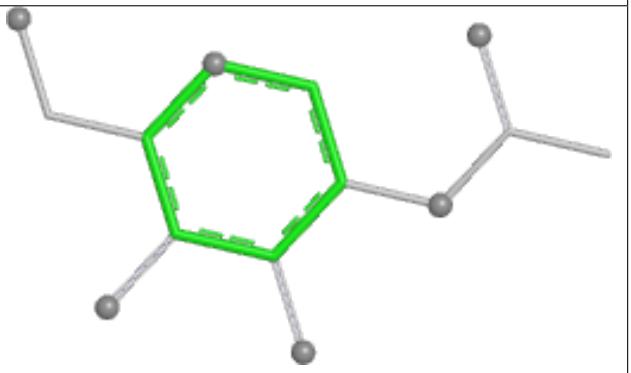
Ligand NAG C 1309	
 Bond lengths	 Bond angles
 Torsions	 Rings

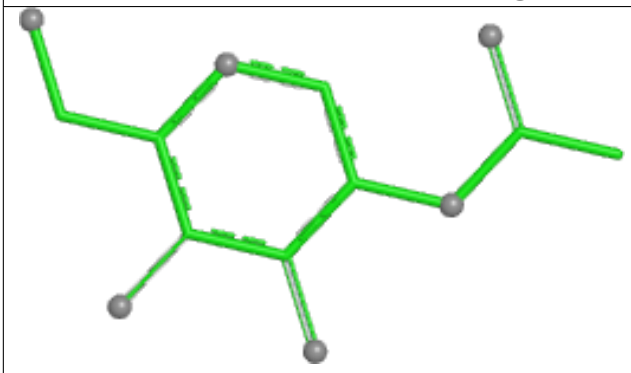
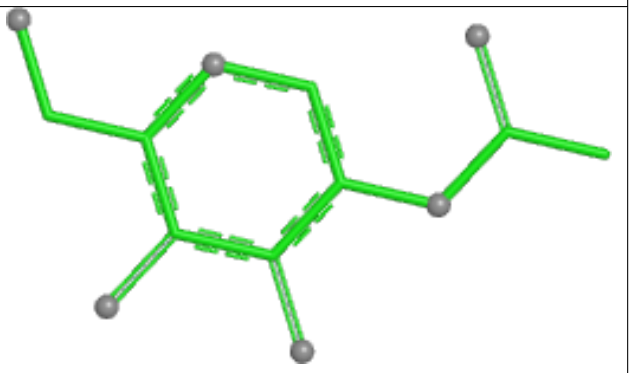
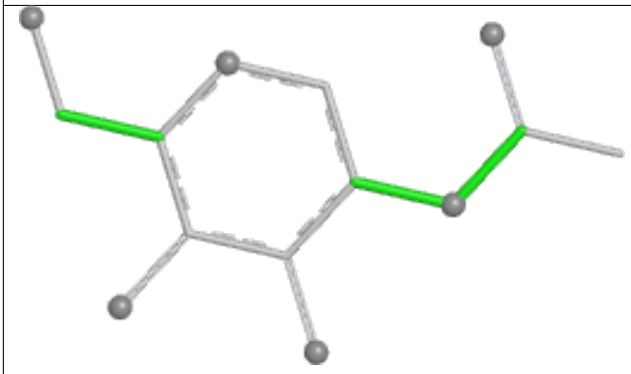
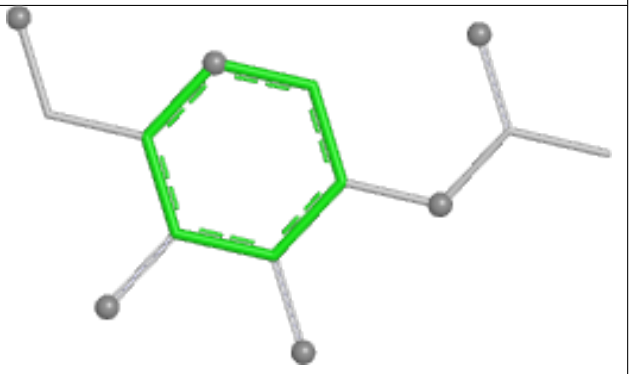
Ligand NAG C 1302	
	
Bond lengths	Bond angles
	
Torsions	Rings

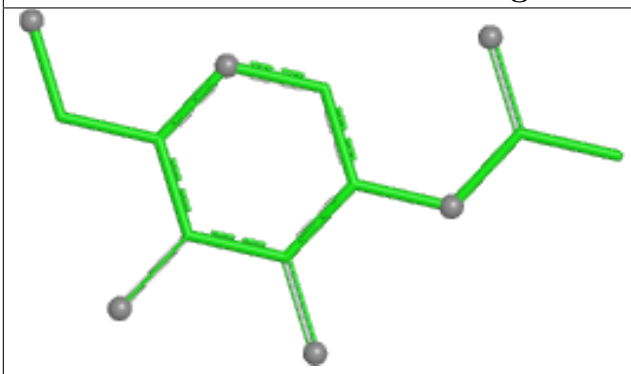
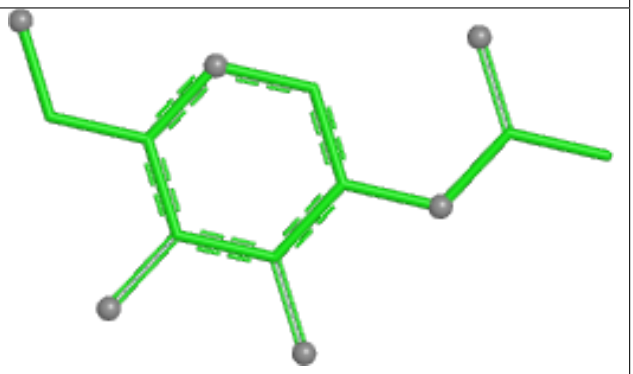
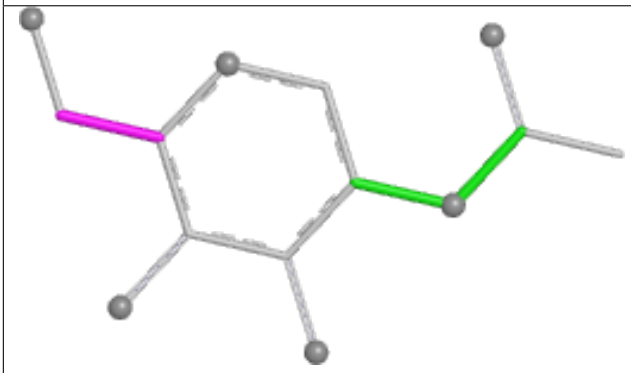
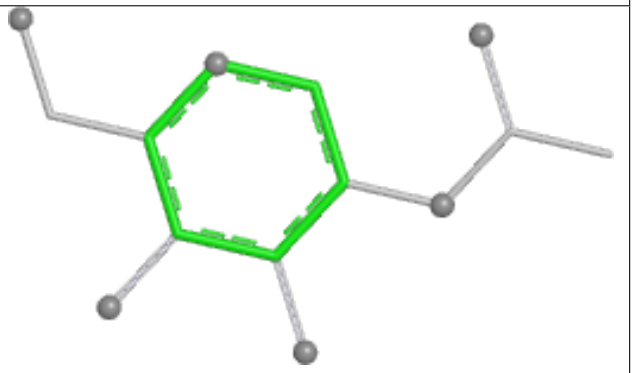
Ligand NAG C 1307	
	
Bond lengths	Bond angles
	
Torsions	Rings

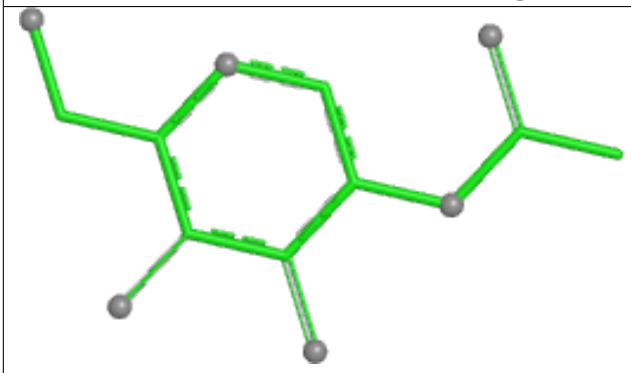
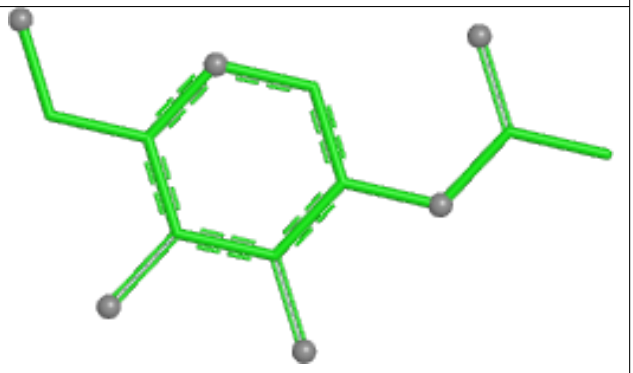
Ligand NAG A 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG C 1308	
	
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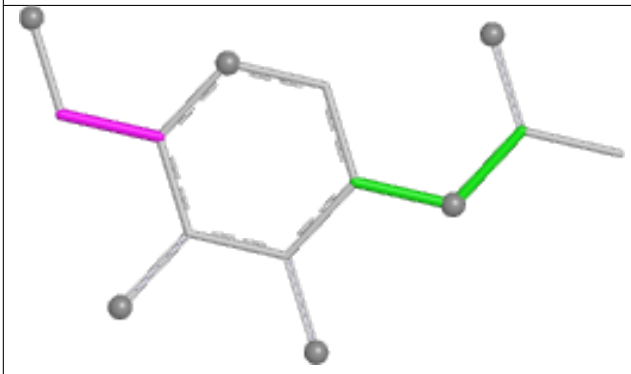
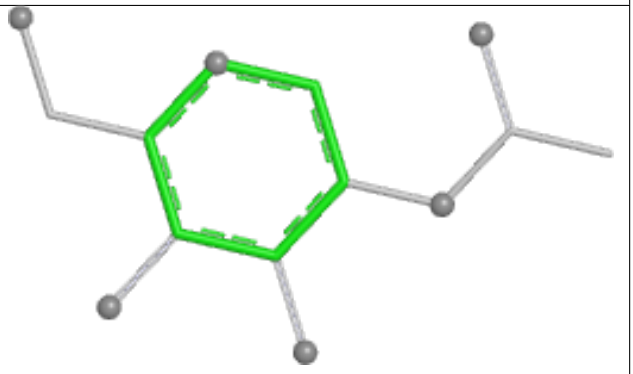
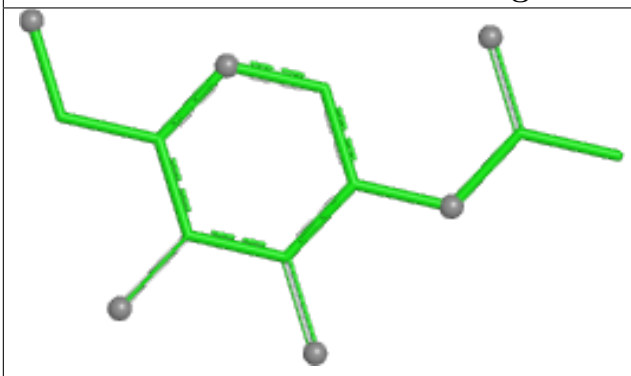
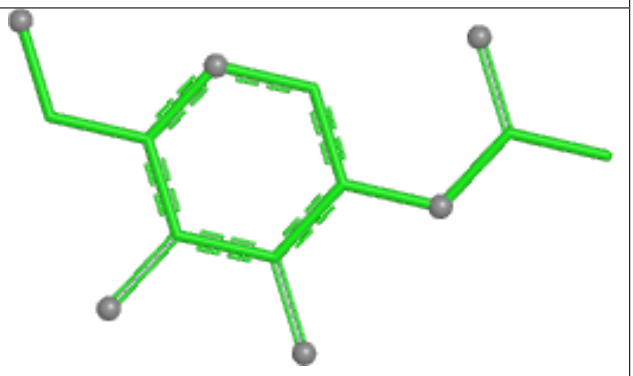
	
Torsions	Rings

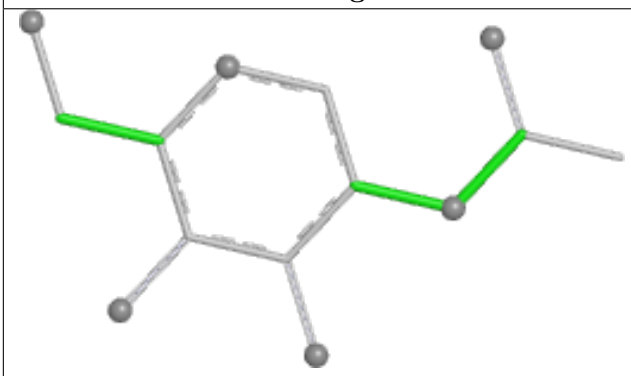
Ligand NAG B 1307



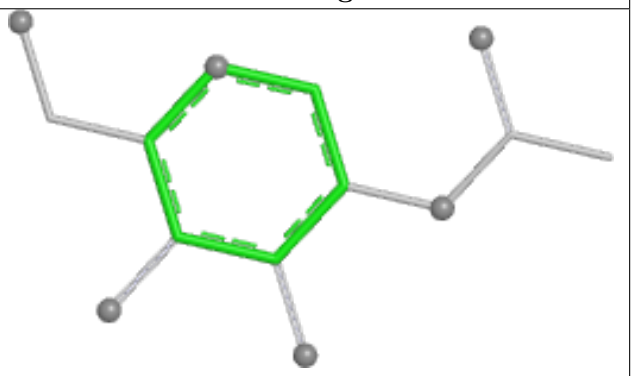
Bond lengths



Bond angles

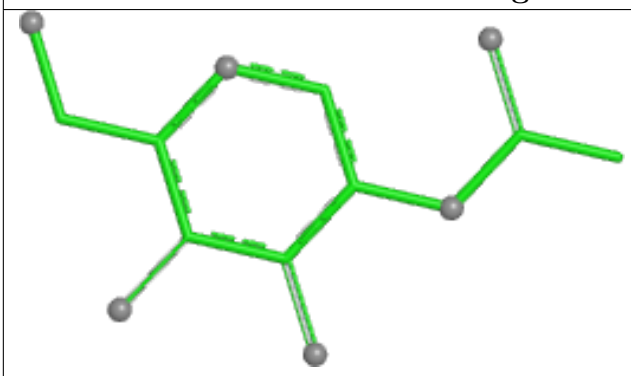


Torsions

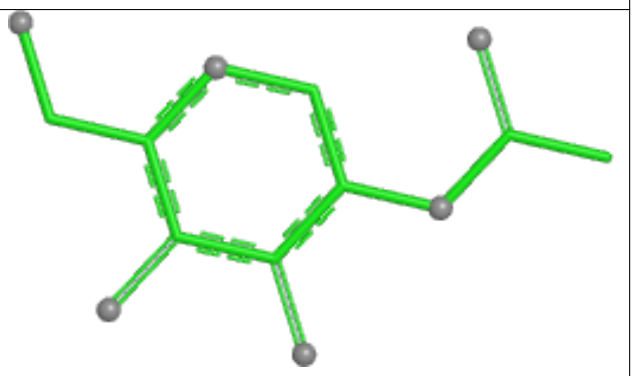


Rings

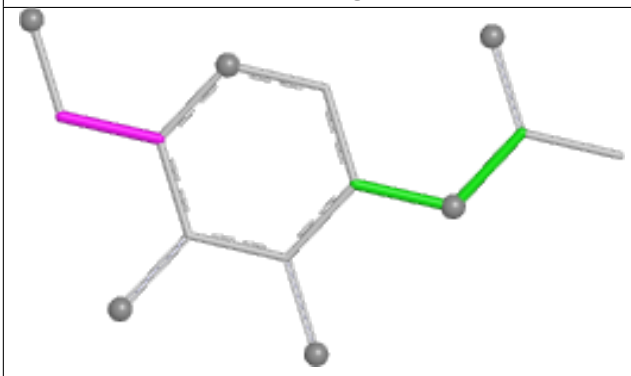
Ligand NAG B 1308



Bond lengths



Bond angles



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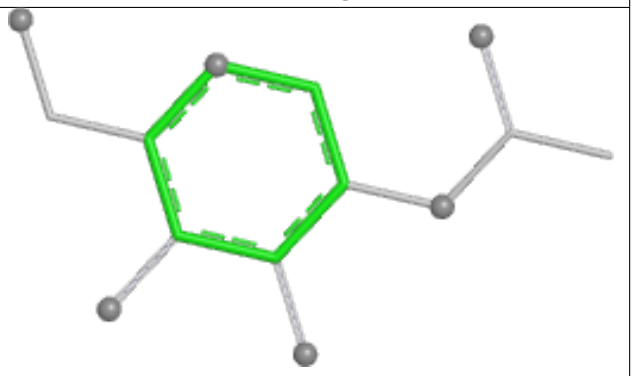
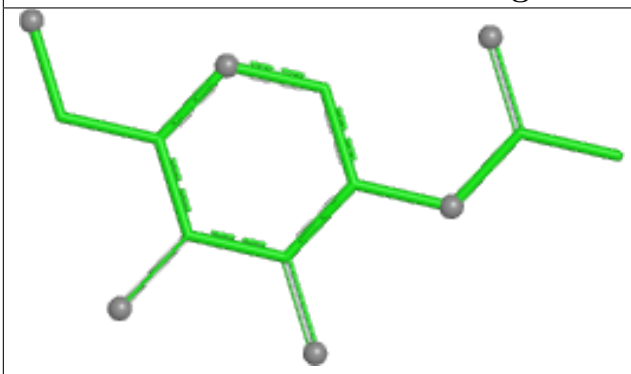
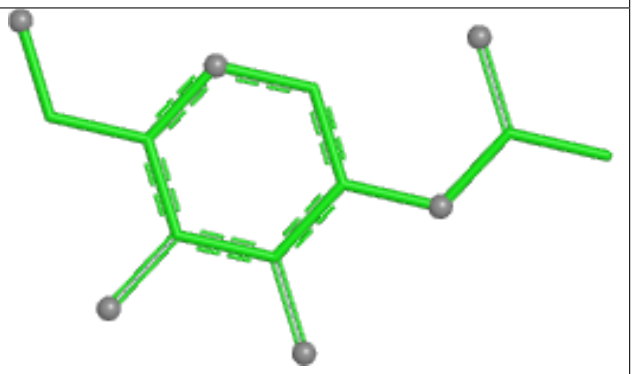
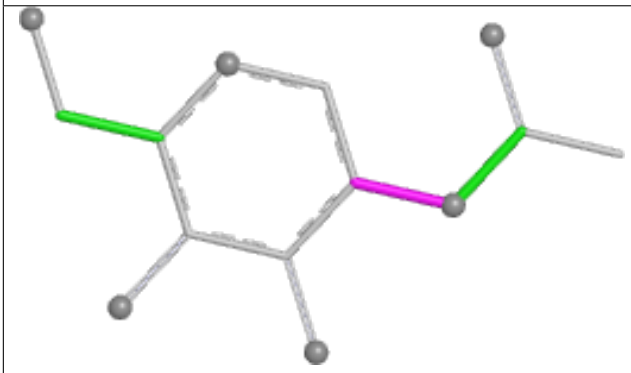
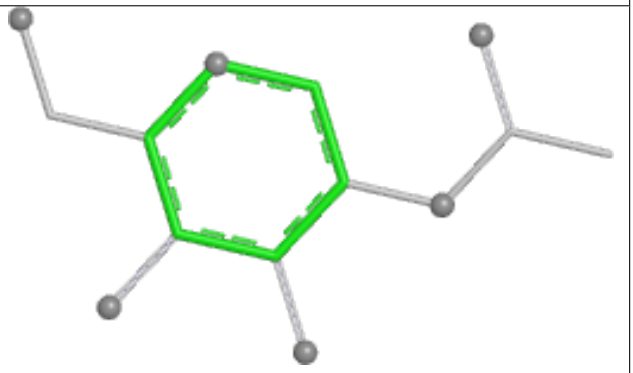
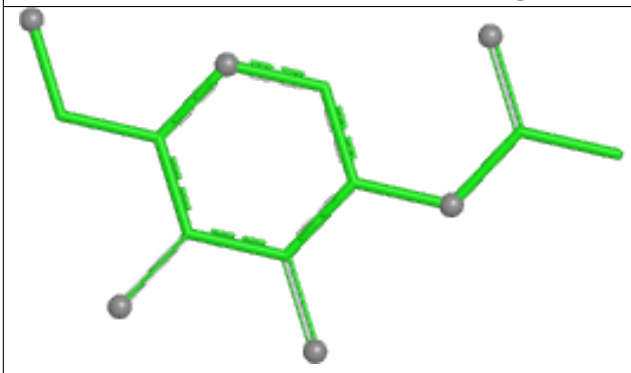
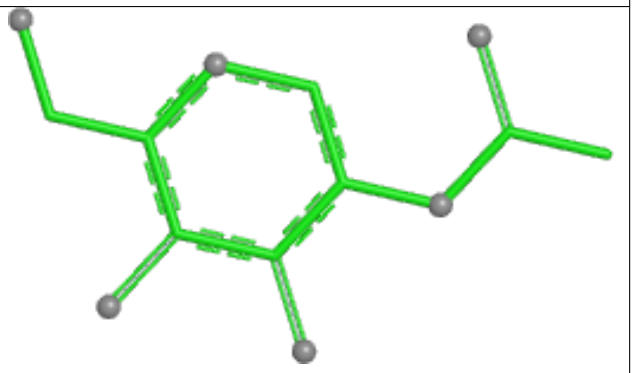
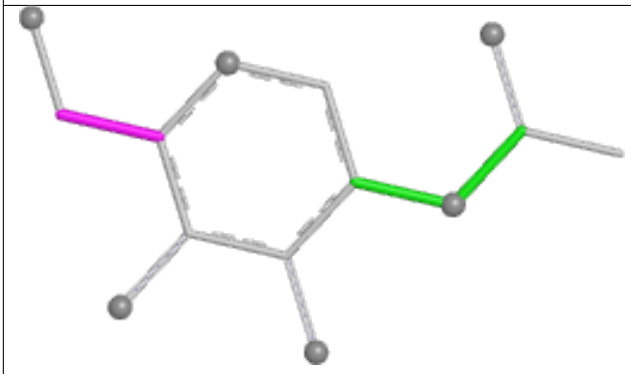
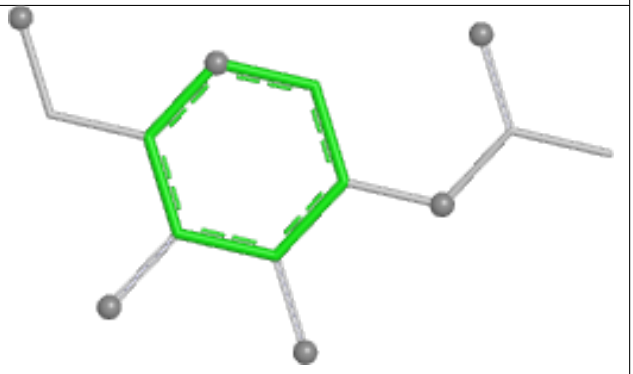
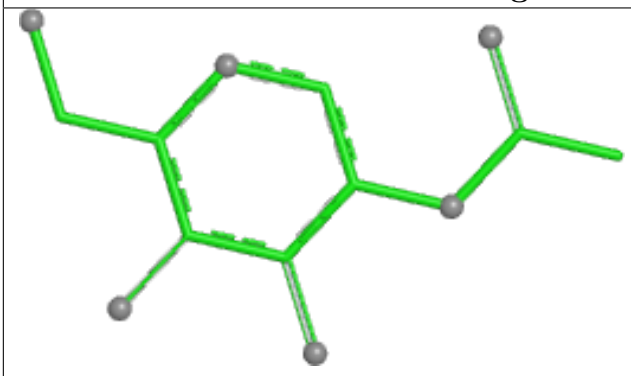


Rings

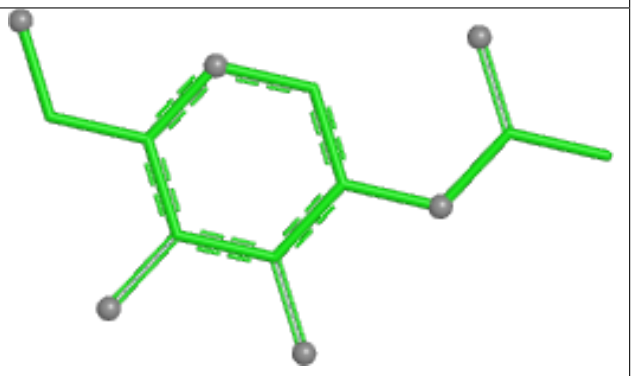
Ligand NAG B 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

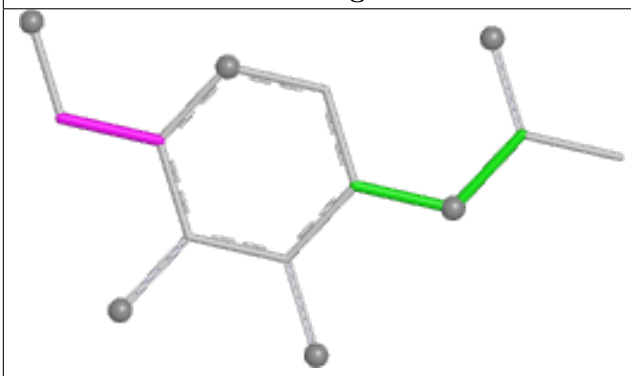
Ligand NAG A 1309



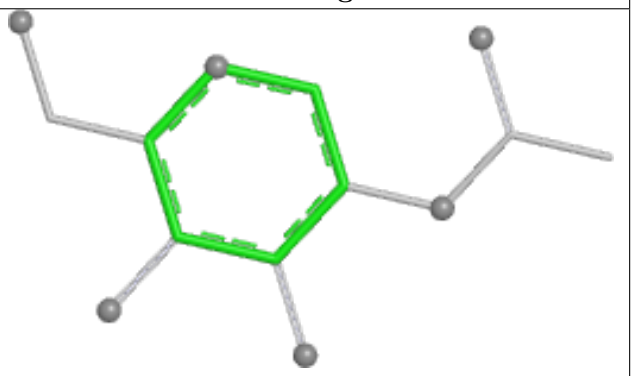
Bond lengths



Bond angles

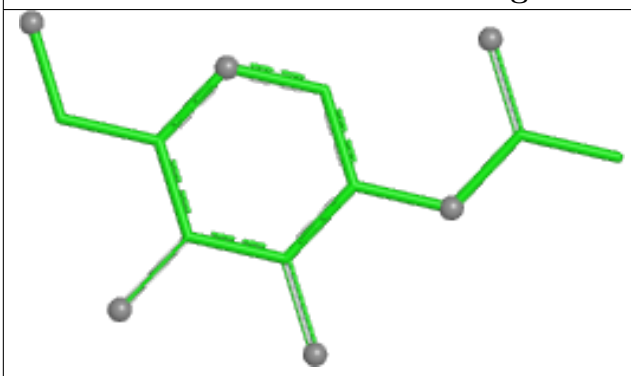


Torsions

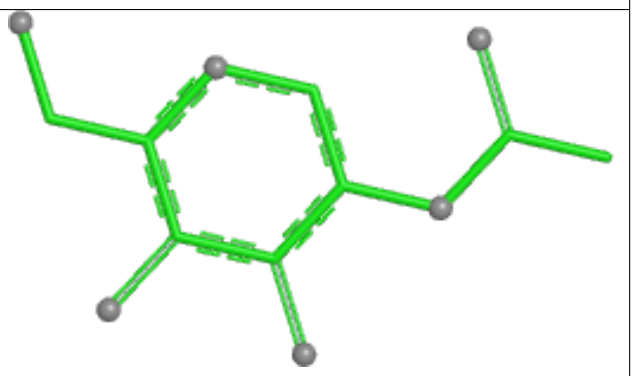


Rings

Ligand NAG A 1302



Bond lengths



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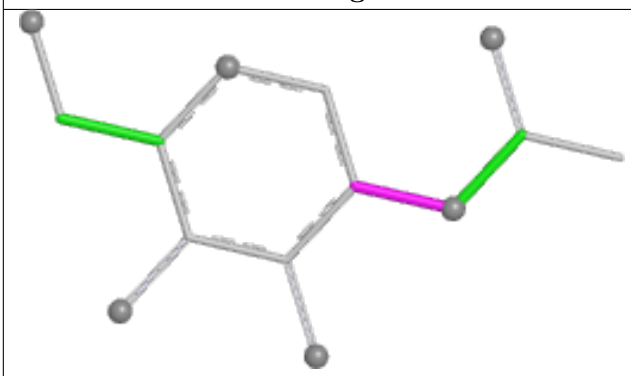
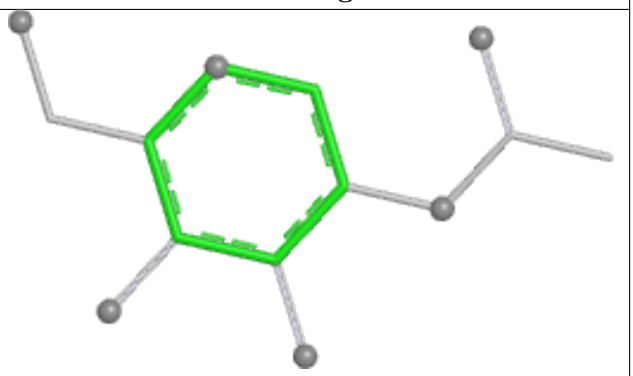
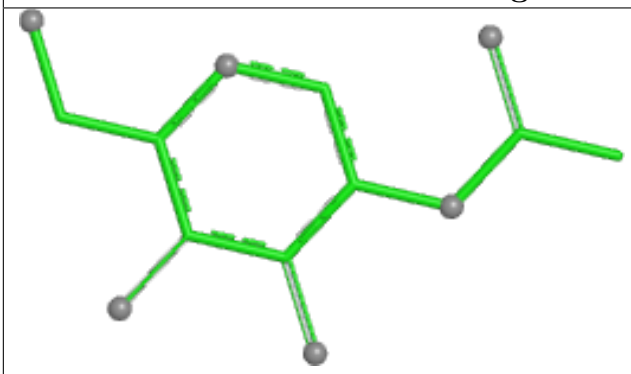
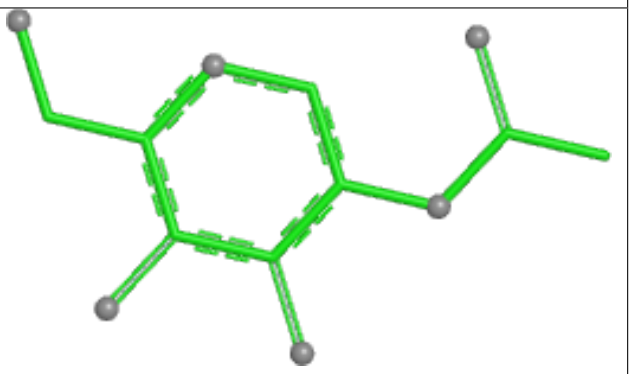
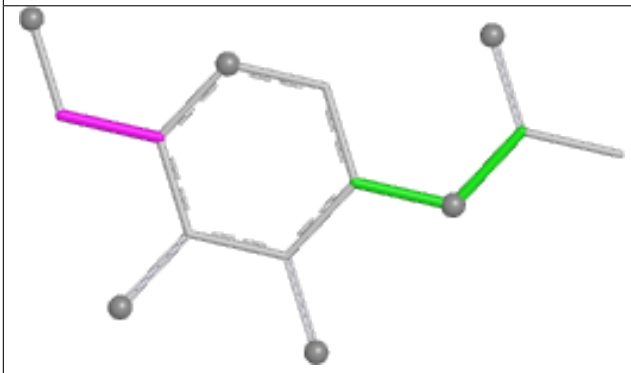
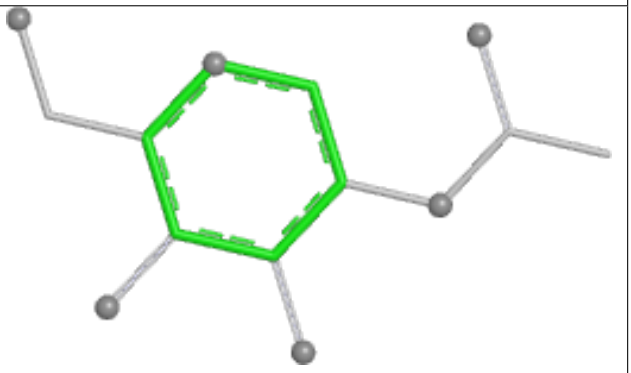
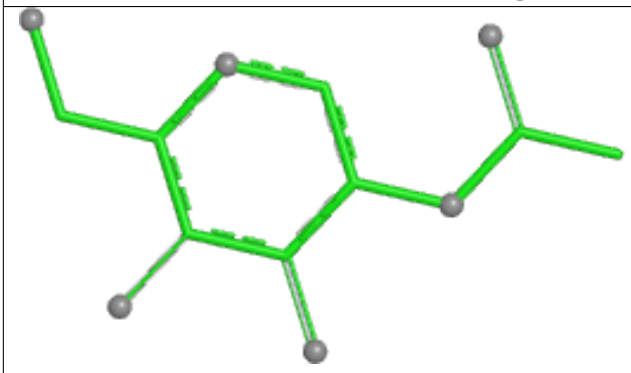
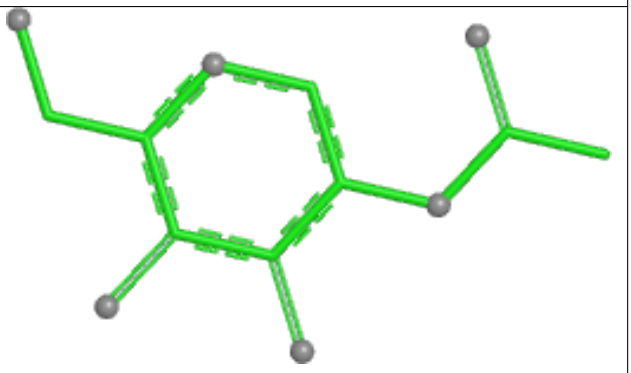
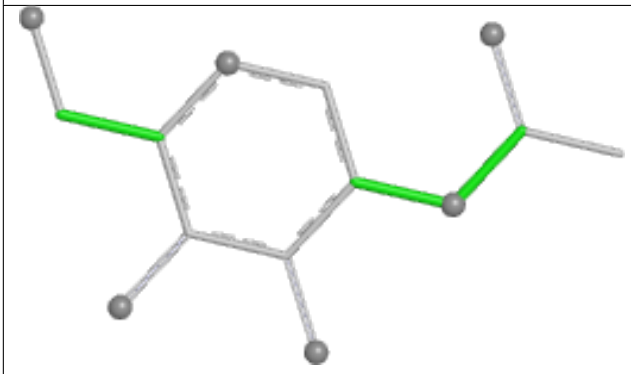
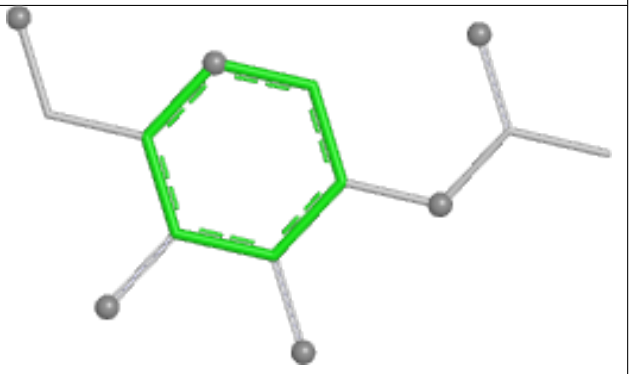


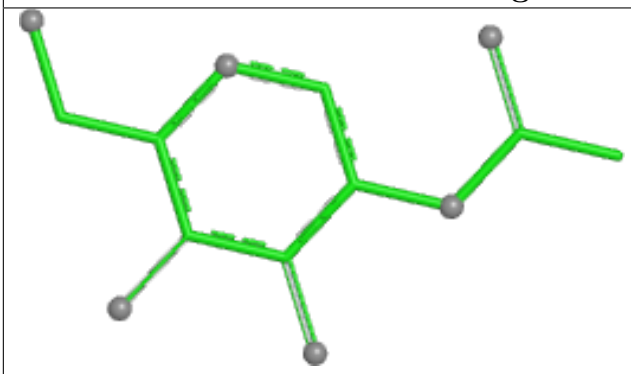
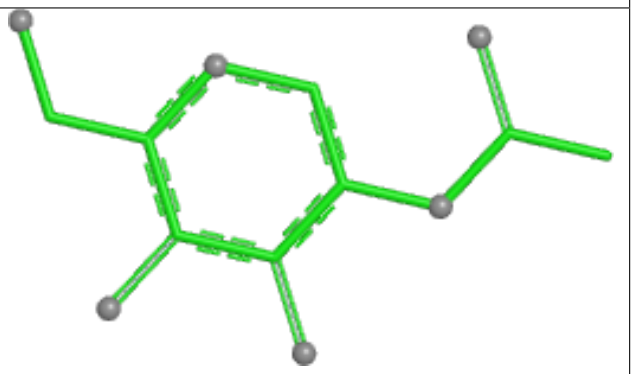
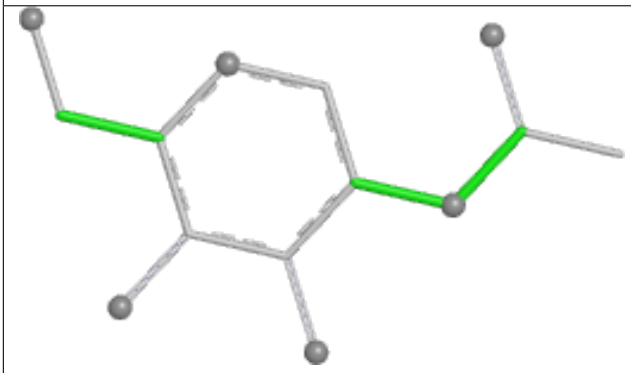
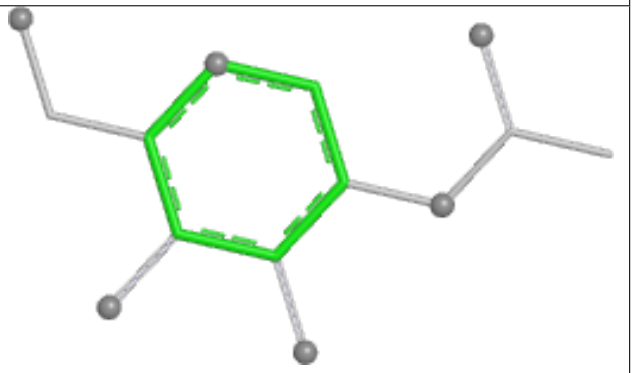
Torsions

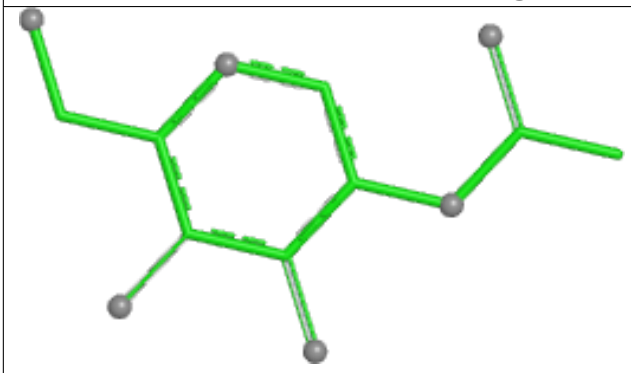
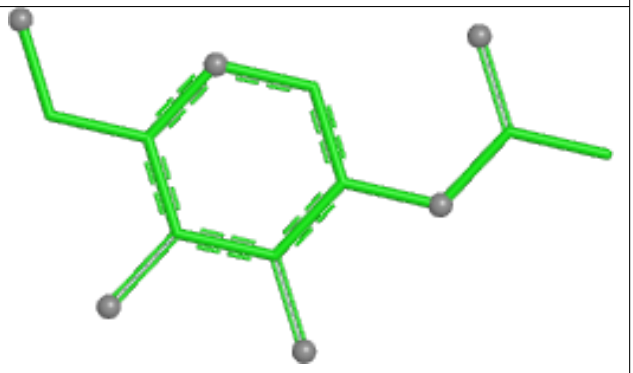
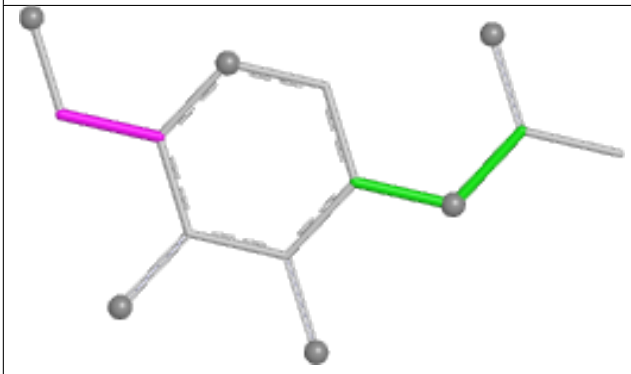
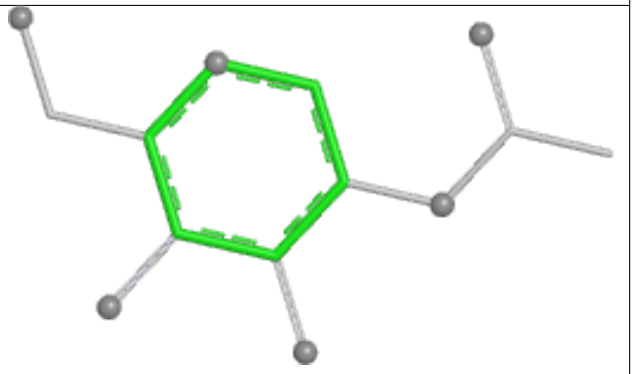


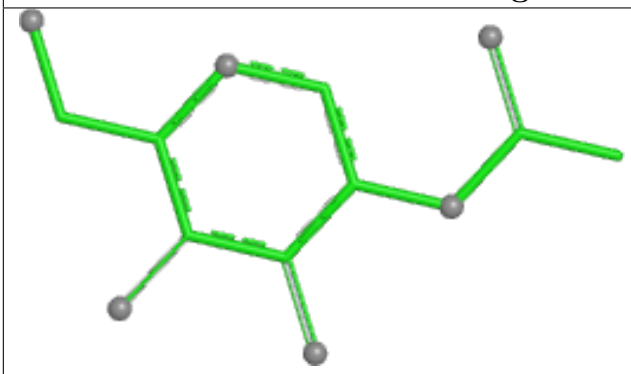
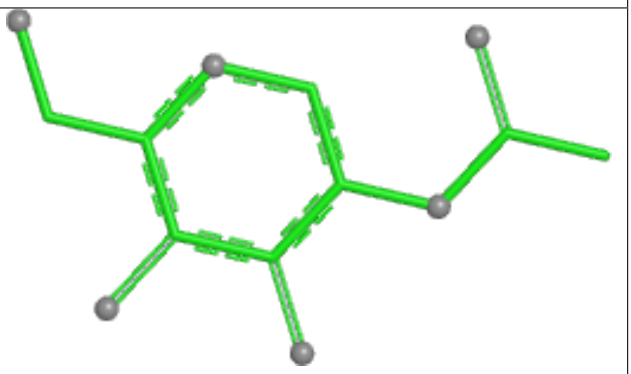
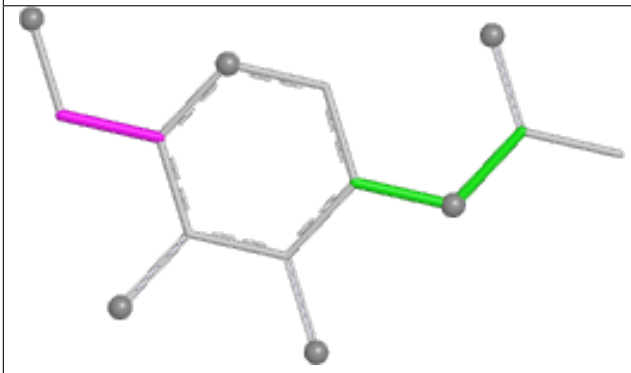
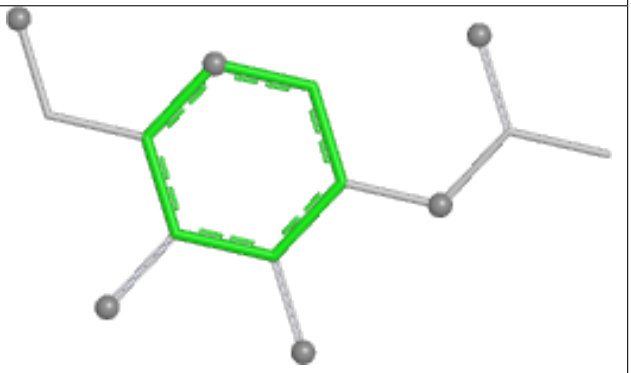
Rings

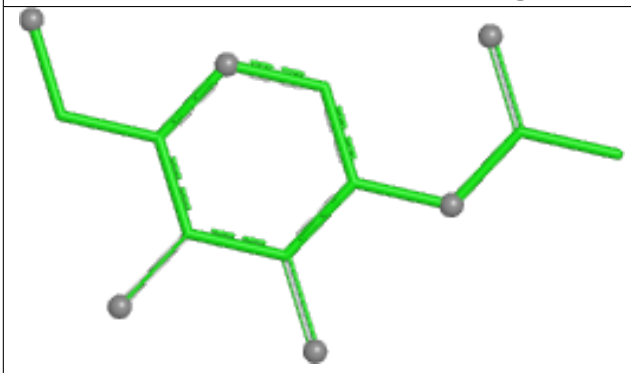
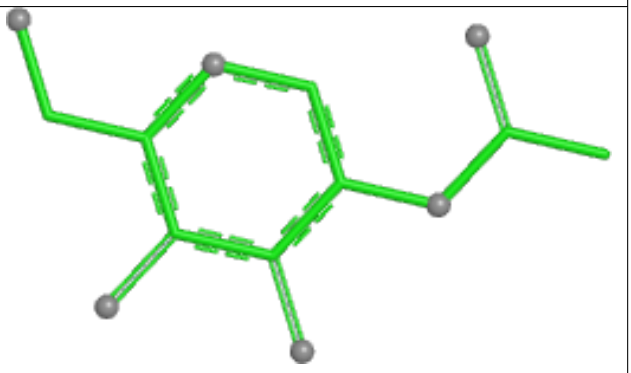
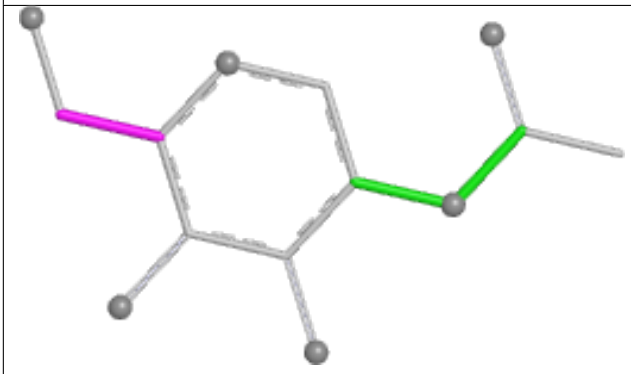
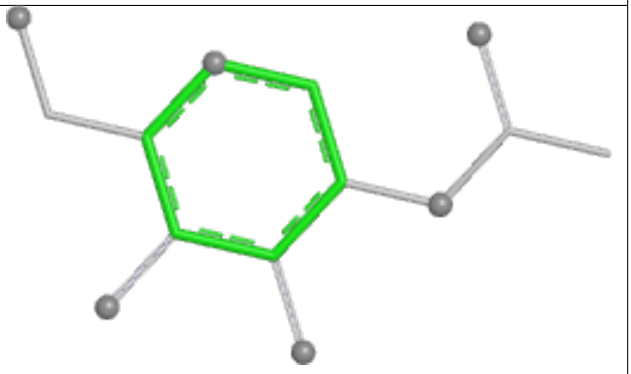
Ligand NAG A 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

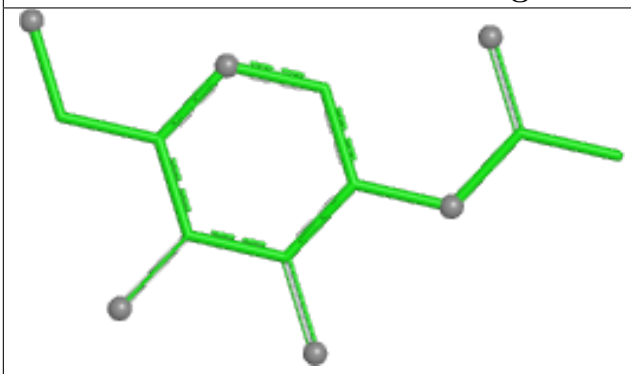
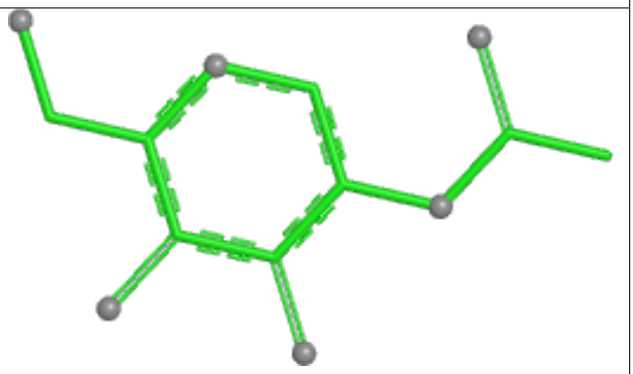
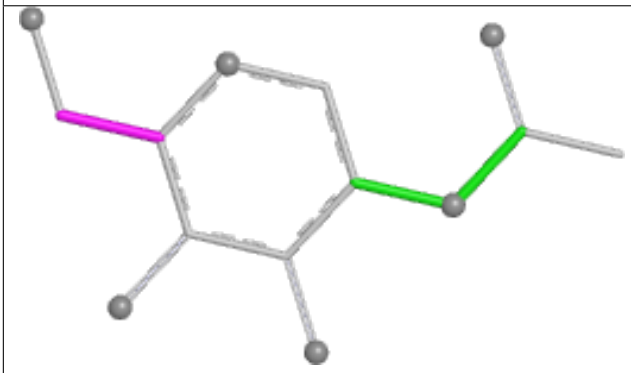
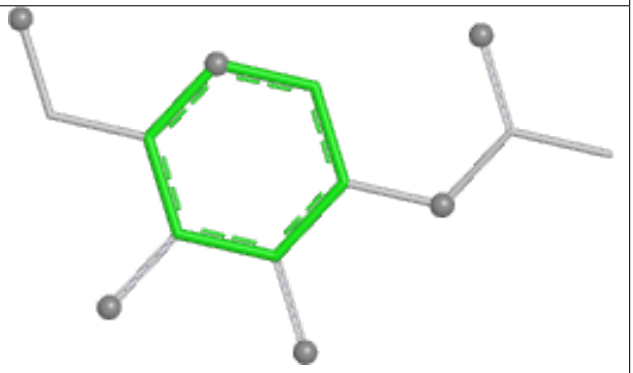
Ligand NAG C 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

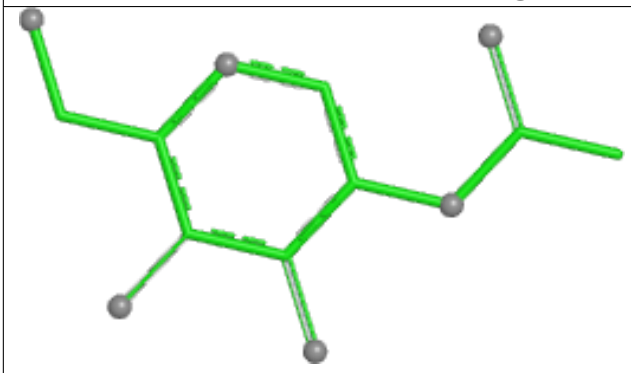
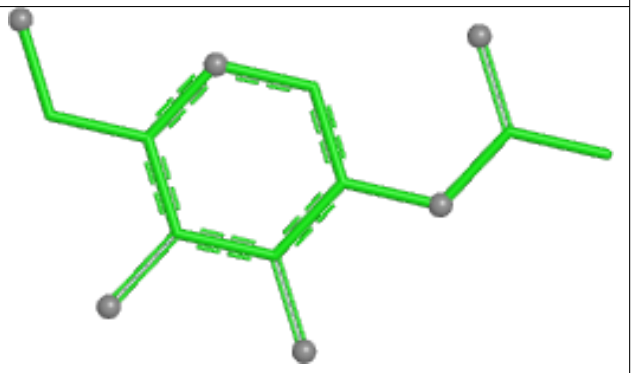
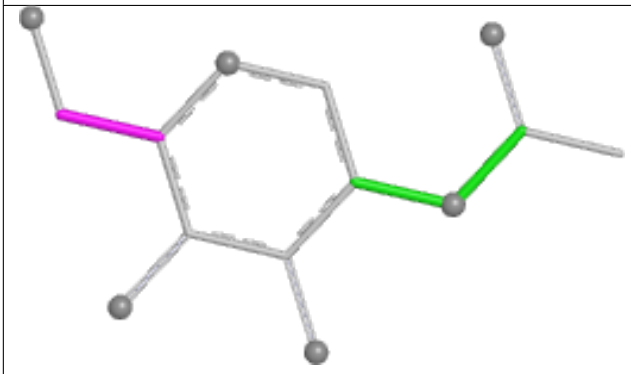
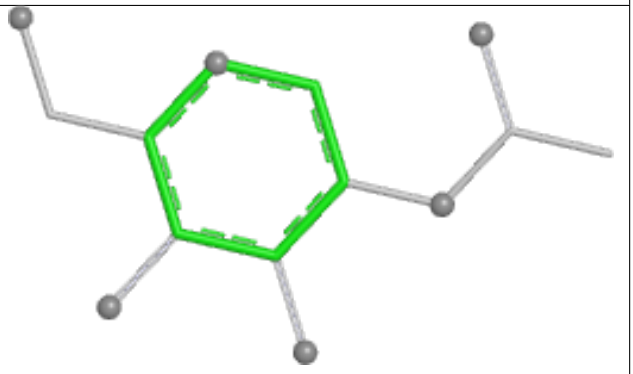
Ligand NAG B 1304	
	
Bond lengths	Bond angles
	
Torsions	Rings

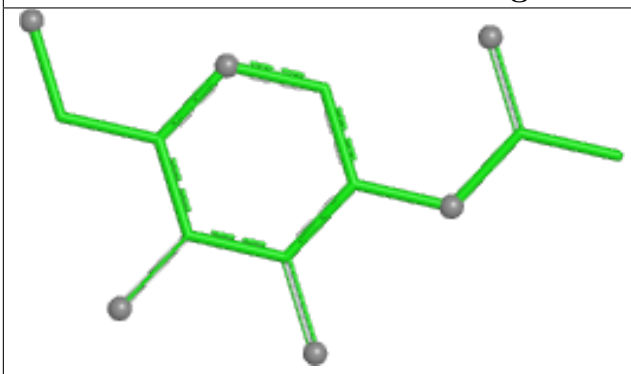
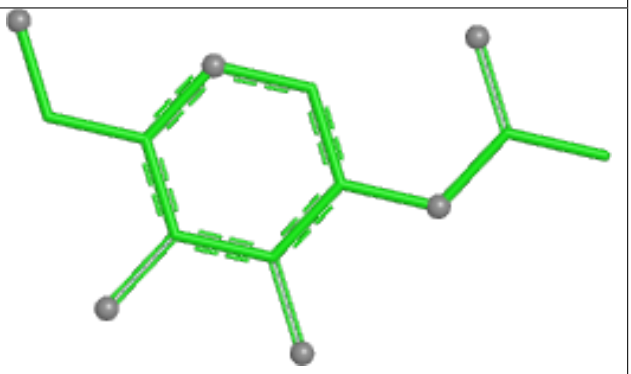
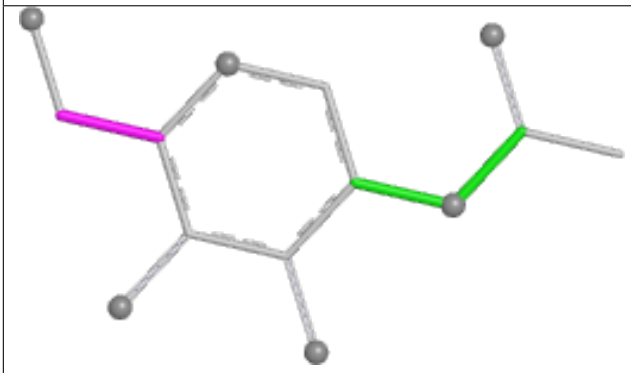
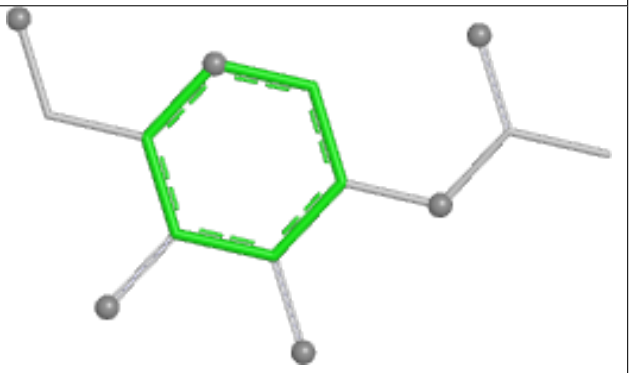
Ligand NAG A 1303	
	
Bond lengths	Bond angles
	
Torsions	Rings

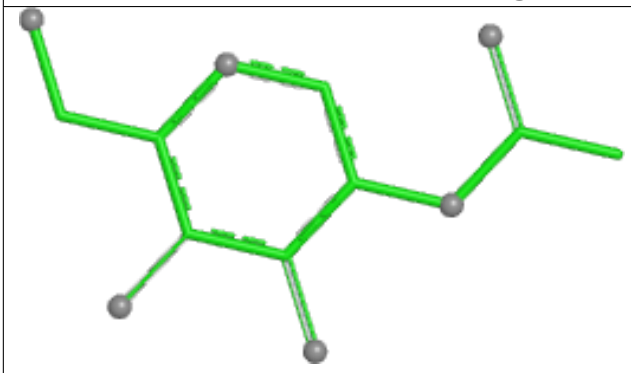
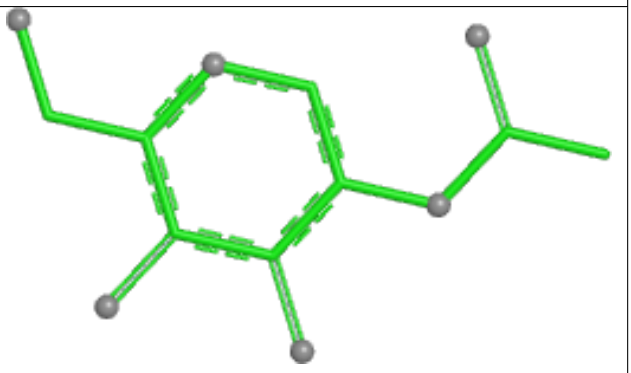
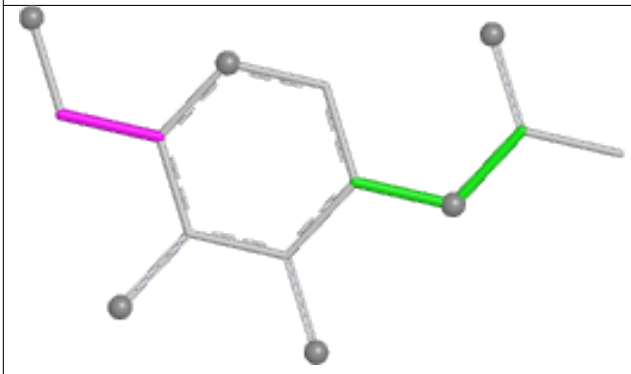
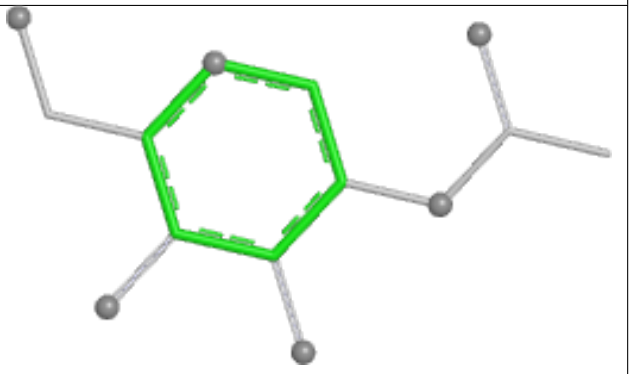
Ligand NAG C 1310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 1310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG A 1308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

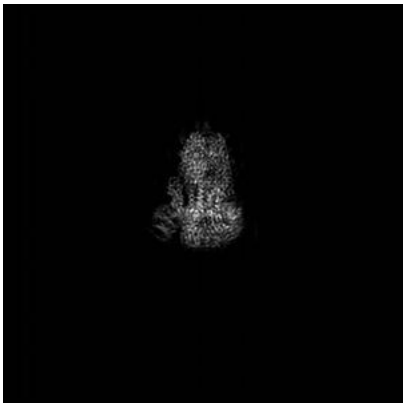
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13776. These allow visual inspection of the internal detail of the map and identification of artifacts.

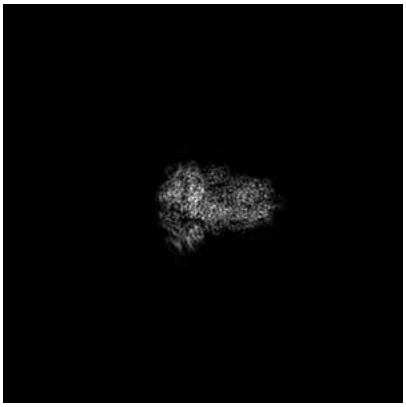
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

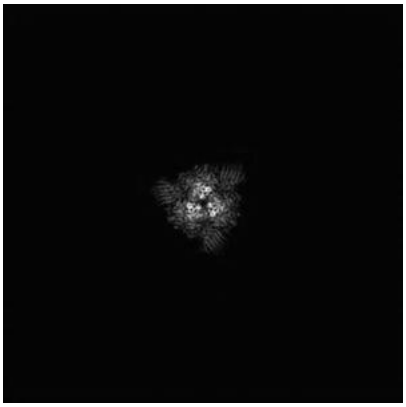
6.1.1 Primary map



X



Y

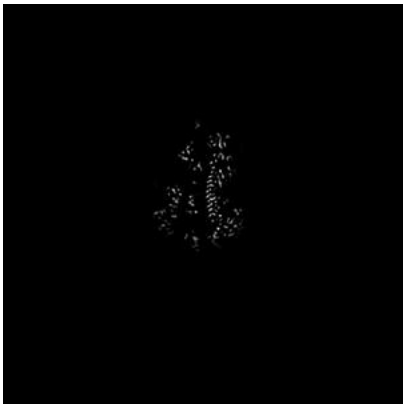


Z

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

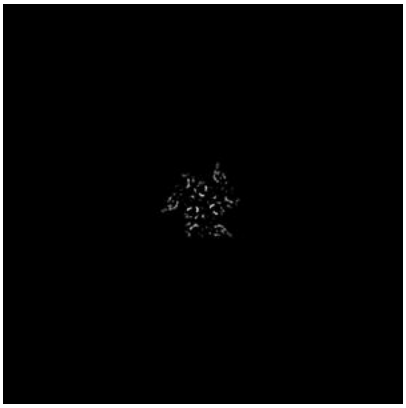
6.2 Central slices

6.2.1 Primary map



X Index: 200

Y Index: 200



Z Index: 200

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

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 194

Y Index: 195

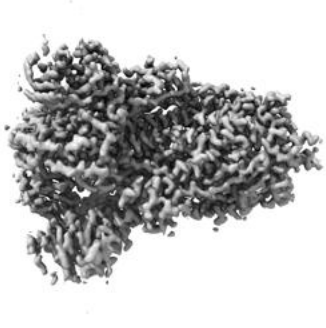
Z Index: 192

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

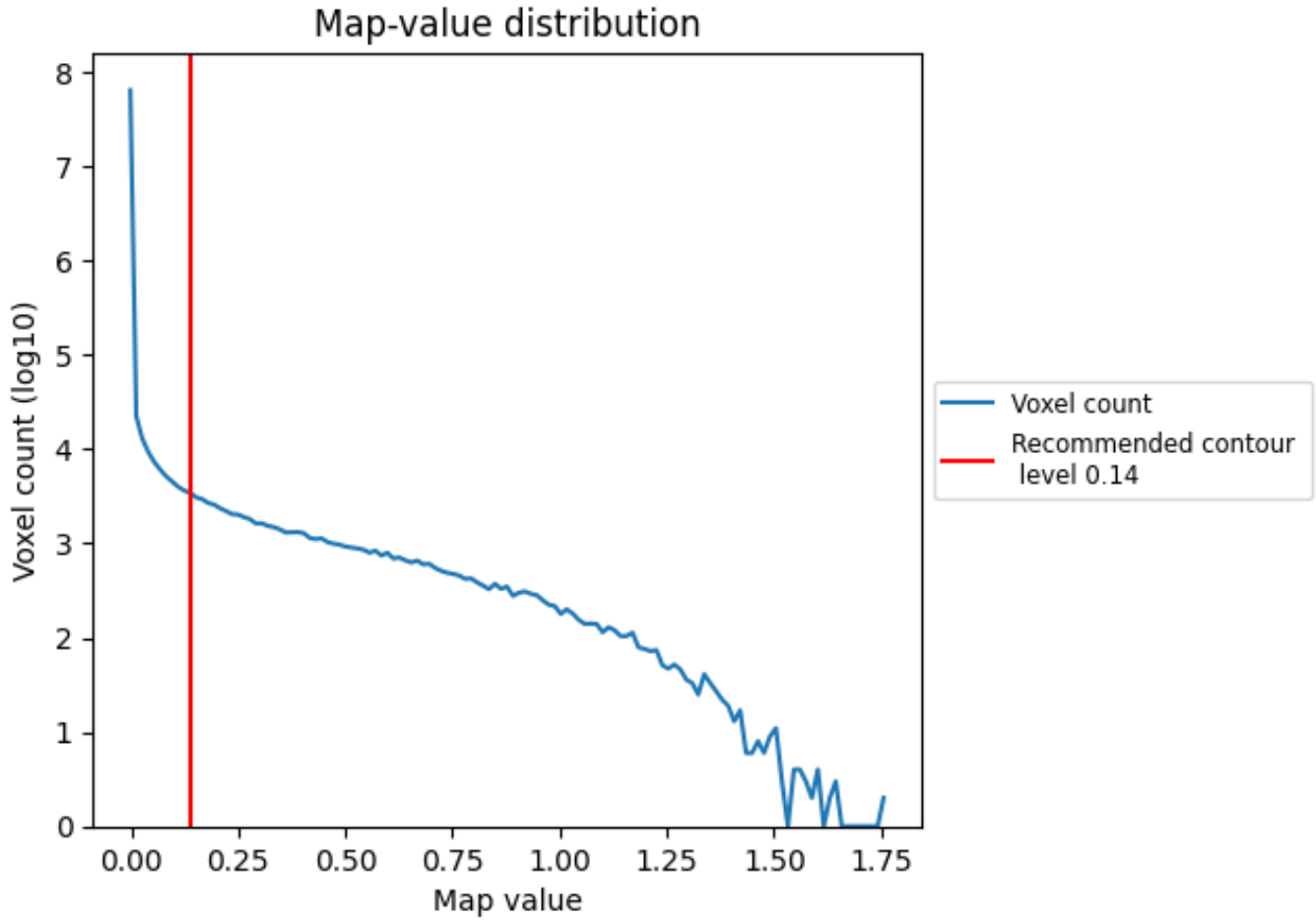
6.5 Mask visualisation (i)

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

7 Map analysis

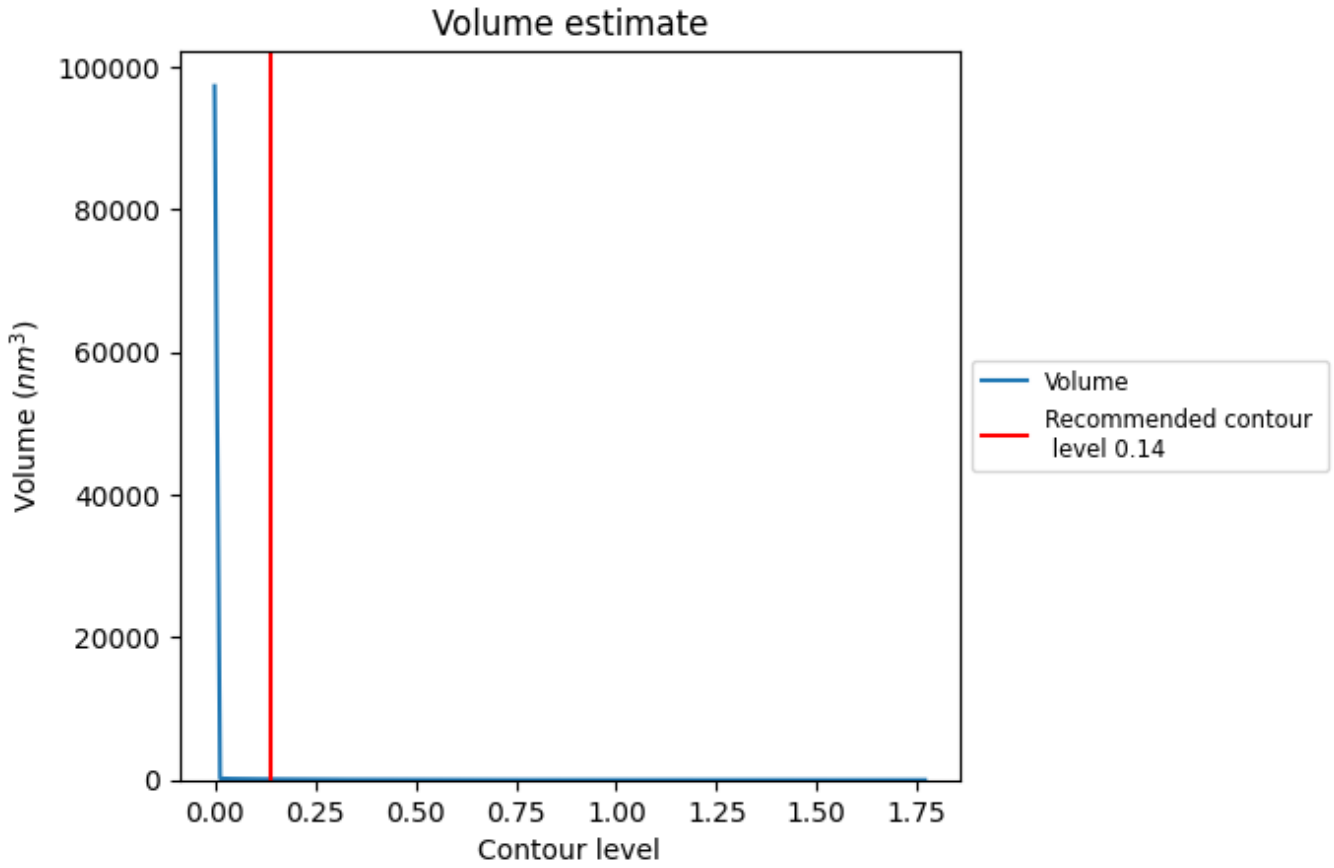
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

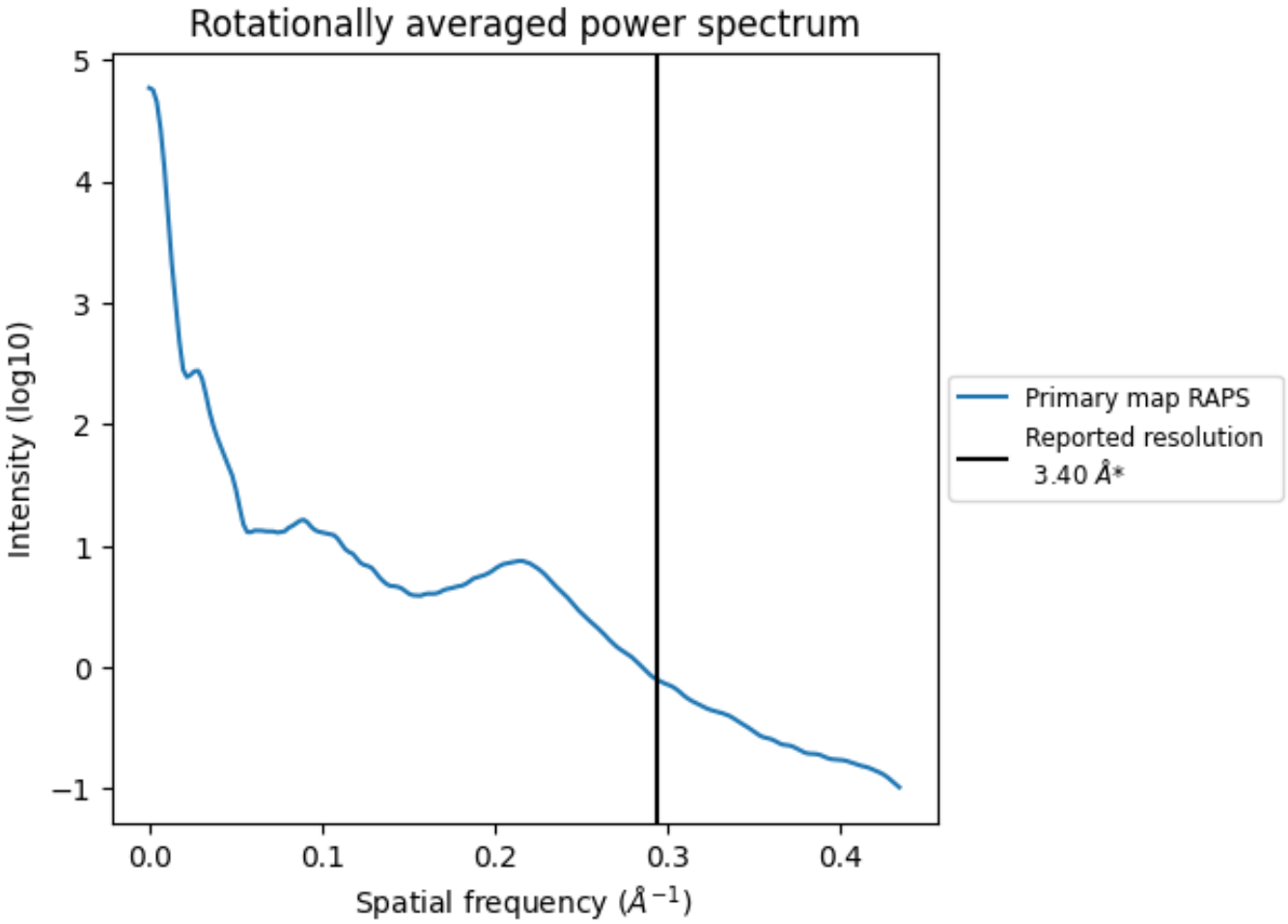
7.2 Volume estimate



The volume at the recommended contour level is 102 nm^3; this corresponds to an approximate mass of 93 kDa.

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

7.3 Rotationally averaged power spectrum (i)

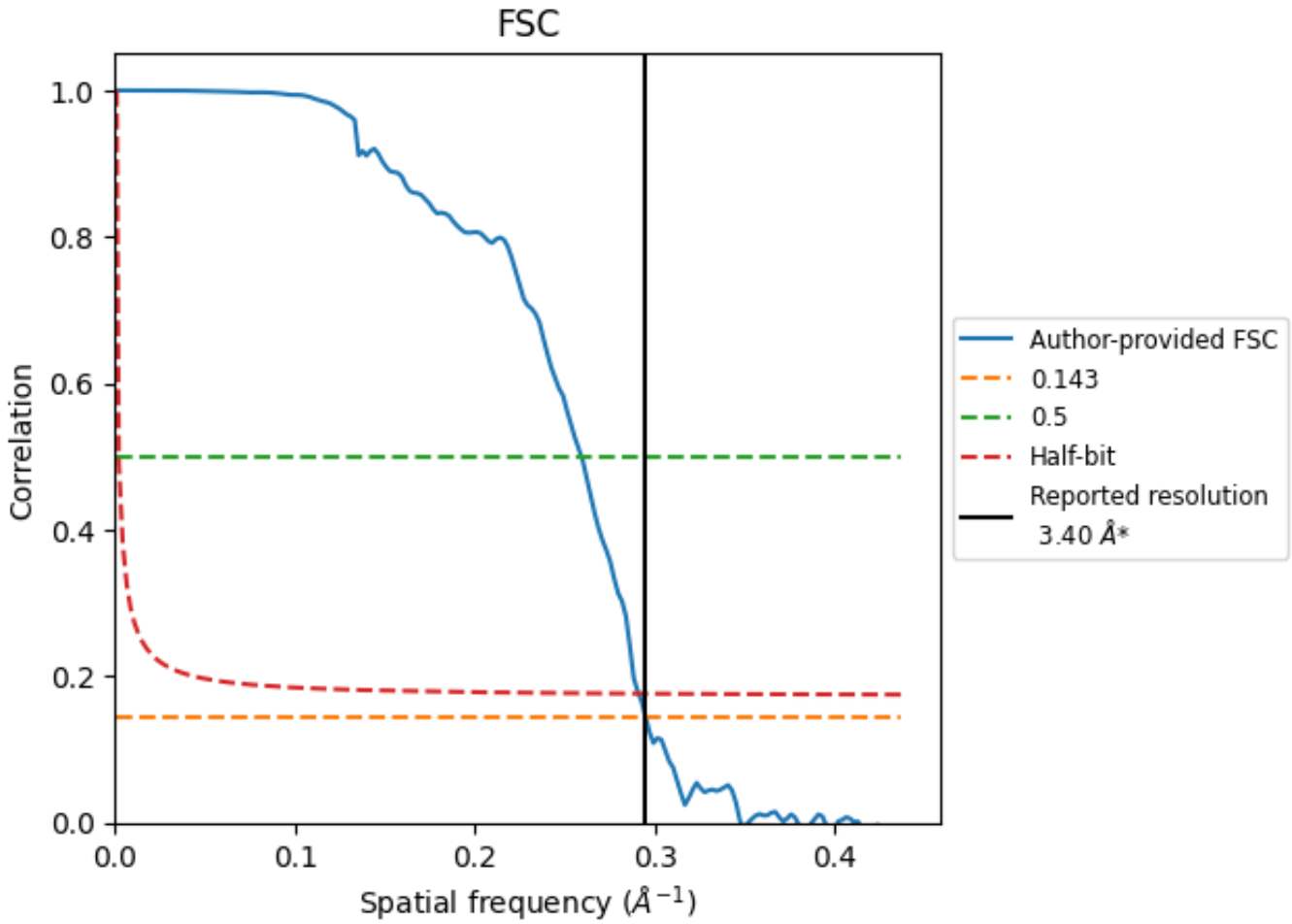


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

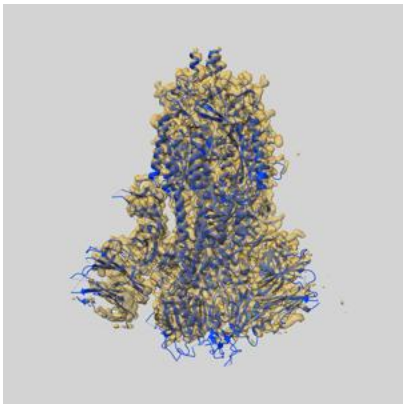
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.86	3.44
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

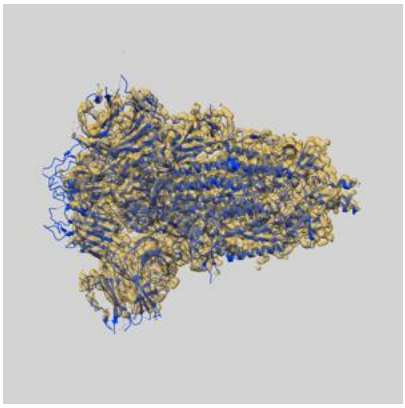
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13776 and PDB model 7Q1Z. Per-residue inclusion information can be found in section 3 on page 14.

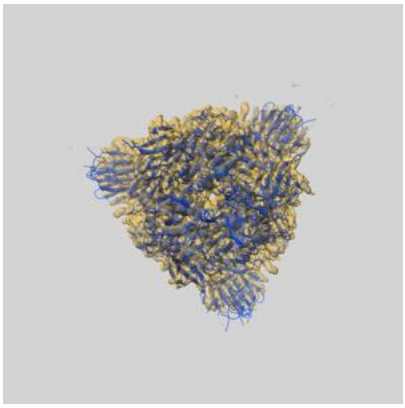
9.1 Map-model overlay



X



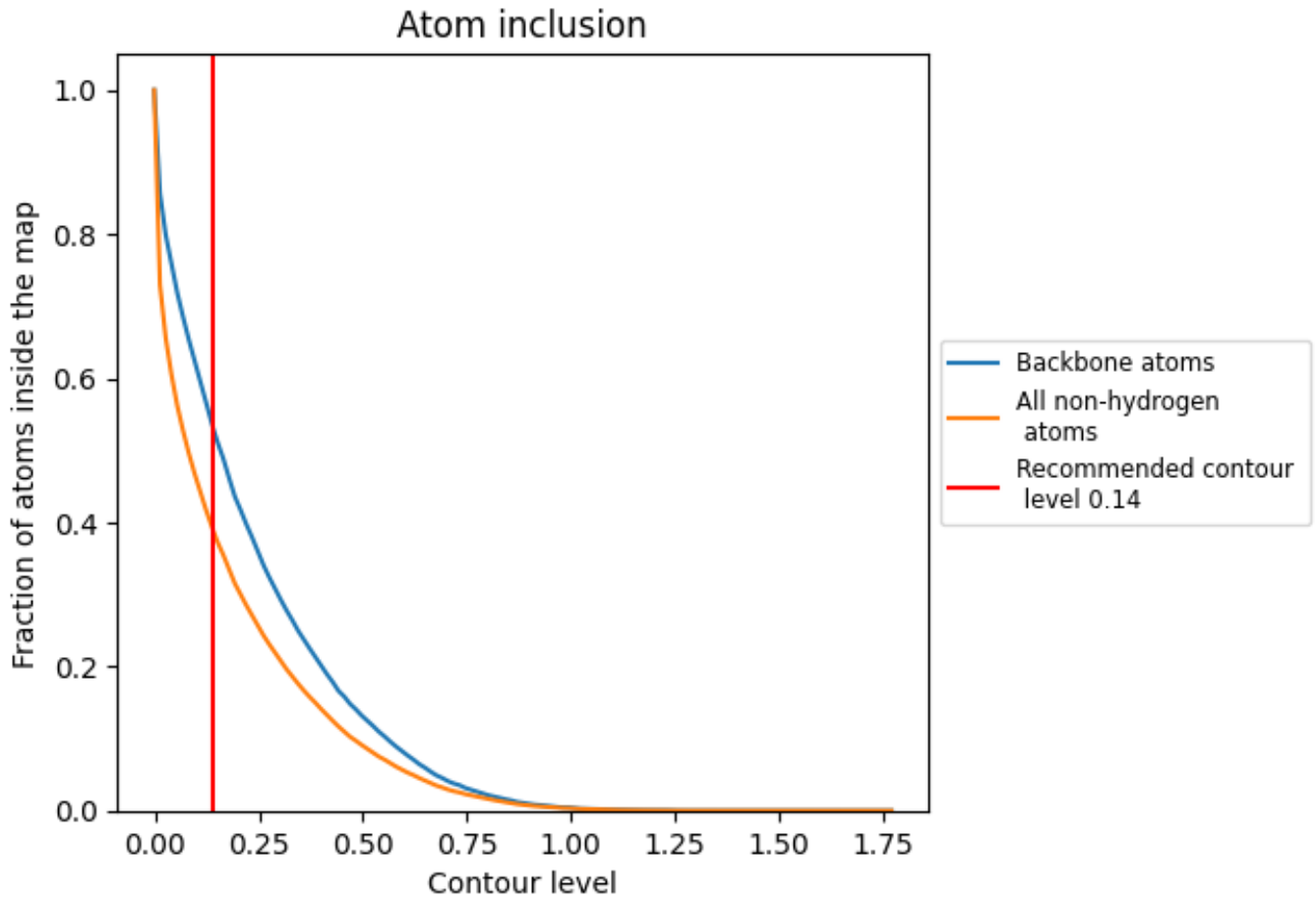
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 39% of all non-hydrogen atoms, are inside the map.