Full wwPDB EM Validation Report ⓘ

Dec 1, 2022 – 02:46 PM EST

PDB ID	:	8DXS
EMDB ID	:	EMD-27775
Title	:	Cryo-EM structure of RBD-directed neutralizing antibody P2B4 in complex with prefusion SARS-CoV-2 spike glycoprotein
Authors	:	Reddem, E.R.; Shapiro, L.
Deposited on	:	2022-08-03
Resolution	:	3.76 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

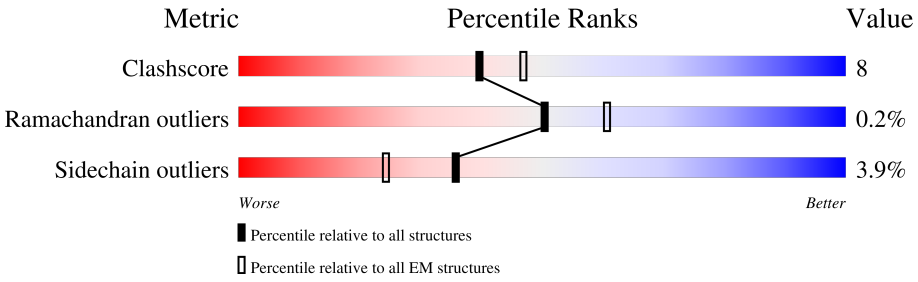
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.76 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	64% 15% 21%
1	B	1288	66% 14% 19%
1	C	1288	65% 15% 20%
2	F	231	14% 43% 10% 47%
2	G	231	15% 45% 8% 47%
2	H	231	40% 11% 47%
3	I	212	23% 43% 7% 50%
3	J	212	42% 8% 50%

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Mol	Chain	Length	Quality of chain
3	L	212	39% 9% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1315	X	-	-	-
4	NAG	B	1304	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30131 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	1021	Total	C	N	O	S	2	0
			7999	5105	1333	1526	35		
1	B	1047	Total	C	N	O	S	2	0
			8205	5234	1369	1565	37		
1	C	1033	Total	C	N	O	S	2	0
			8097	5167	1351	1543	36		

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

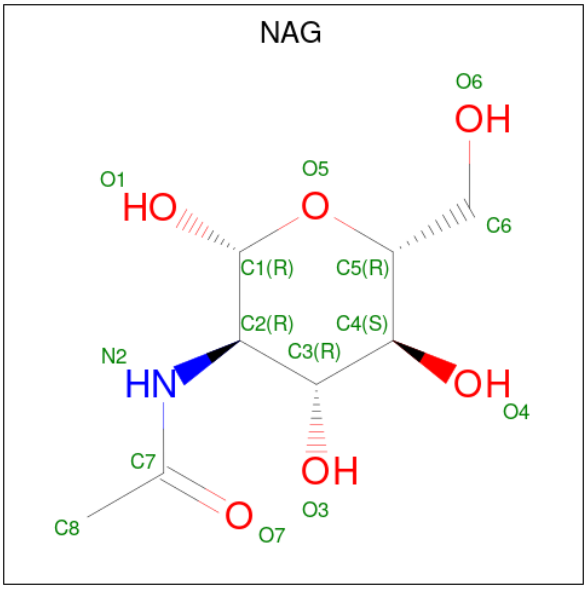
- Molecule 2 is a protein called P2B4 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	123	Total	C	N	O	S	1	0
			923	574	163	181	5		
2	F	123	Total	C	N	O	S	1	0
			923	574	163	181	5		
2	G	123	Total	C	N	O	S	1	0
			923	574	163	181	5		

- Molecule 3 is a protein called P2B4 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			815	519	133	160	3		
3	I	107	Total	C	N	O	S	0	0
			815	519	133	160	3		
3	J	107	Total	C	N	O	S	0	0
			815	519	133	160	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	

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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	A	1	Total	C	N	O	0
			224	128	16	80	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	B	1	Total	C	N	O	0
			182	104	13	65	
4	C	1	Total	C	N	O	0
			210	120	15	75	
4	C	1	Total	C	N	O	0
			210	120	15	75	
4	C	1	Total	C	N	O	0
			210	120	15	75	
4	C	1	Total	C	N	O	0
			210	120	15	75	

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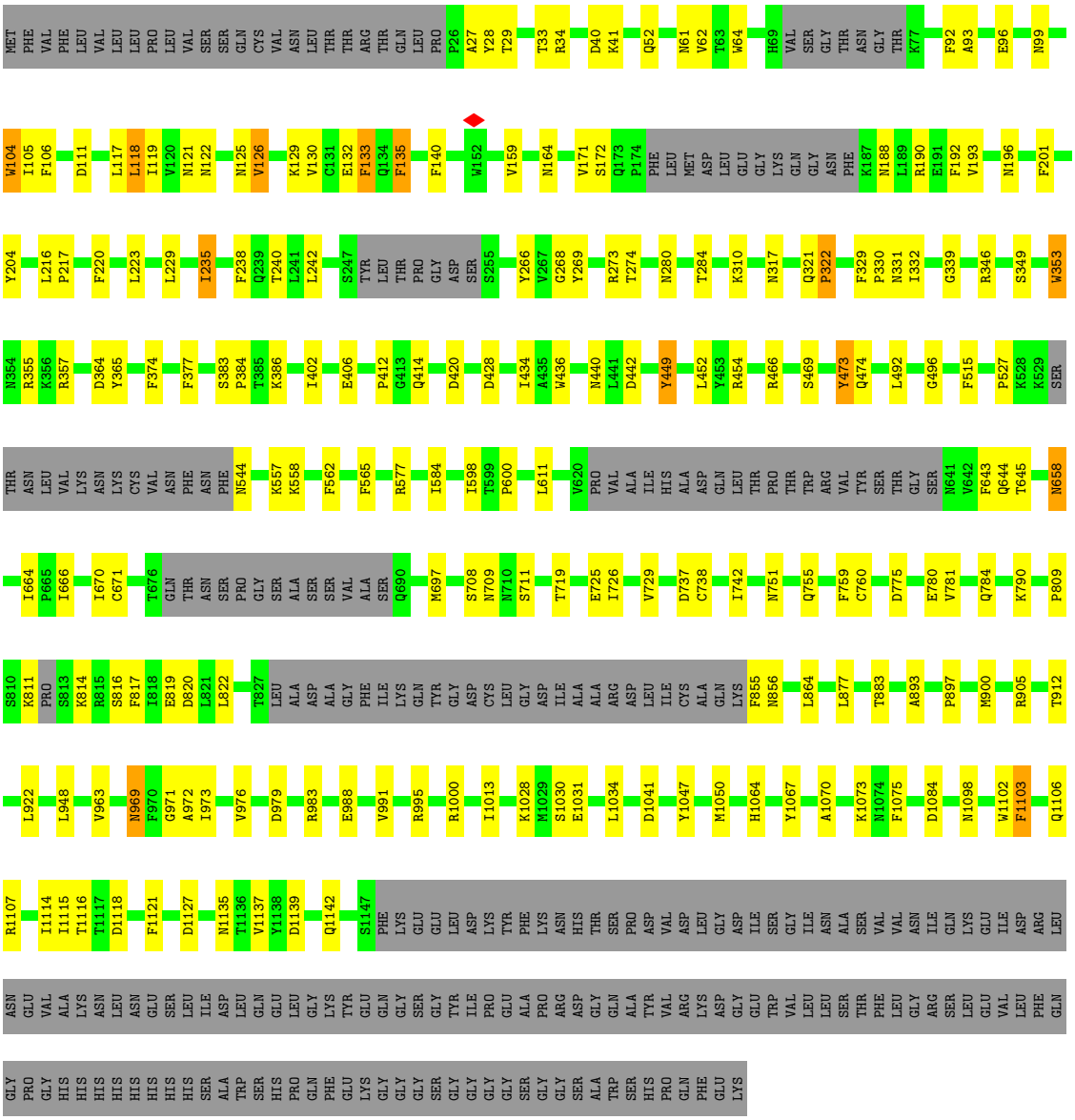
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	0
4	C	1	Total 210	C 120	N 15	O 75	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.

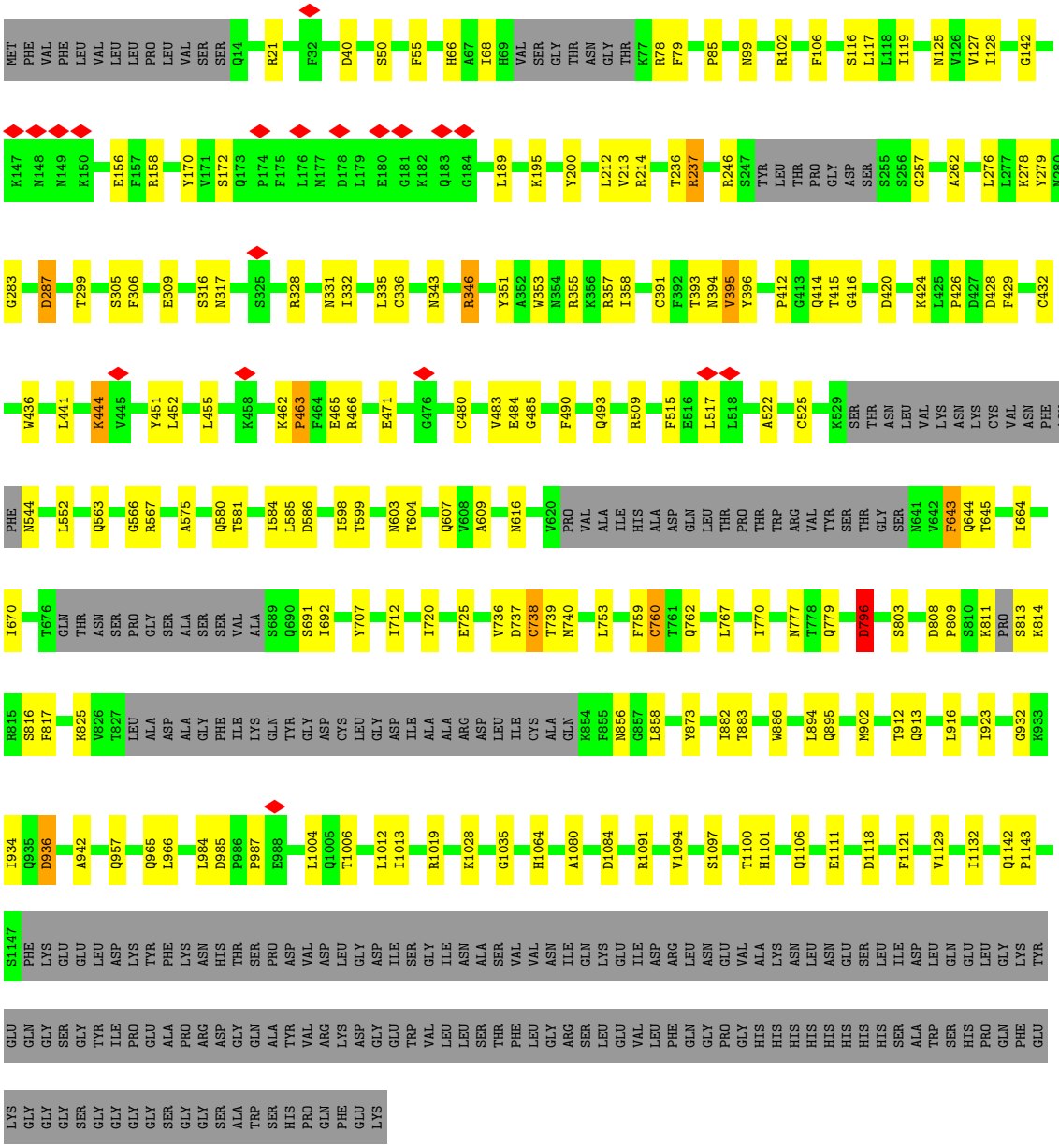
- Molecule 1: Spike glycoprotein

Chain A:



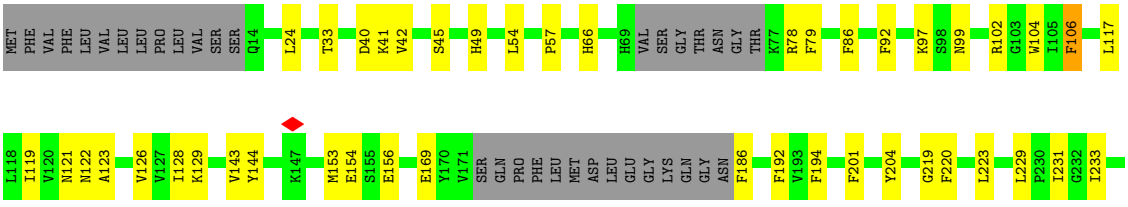
• Molecule 1: Spike glycoprotein

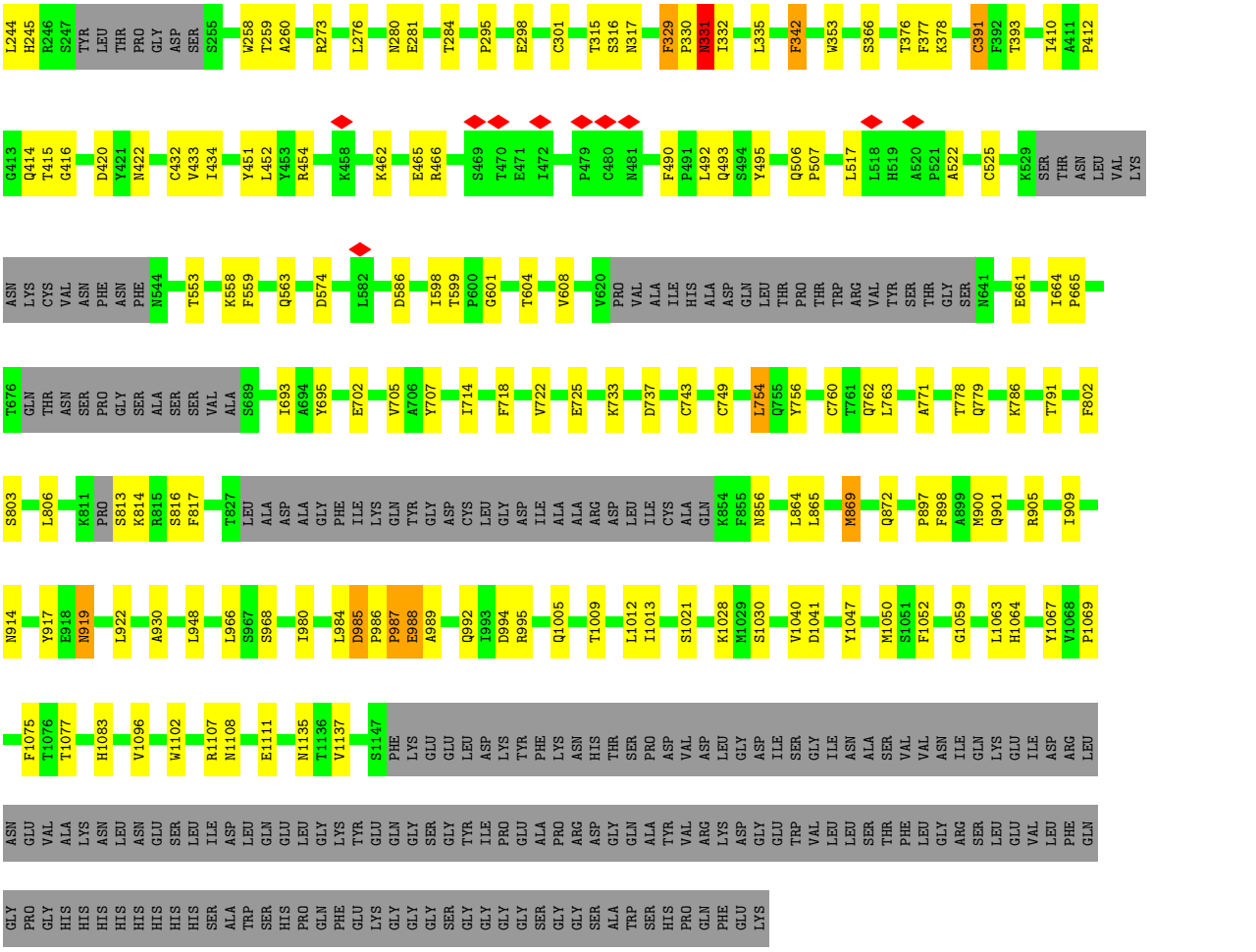
Chain B:



• Molecule 1: Spike glycoprotein

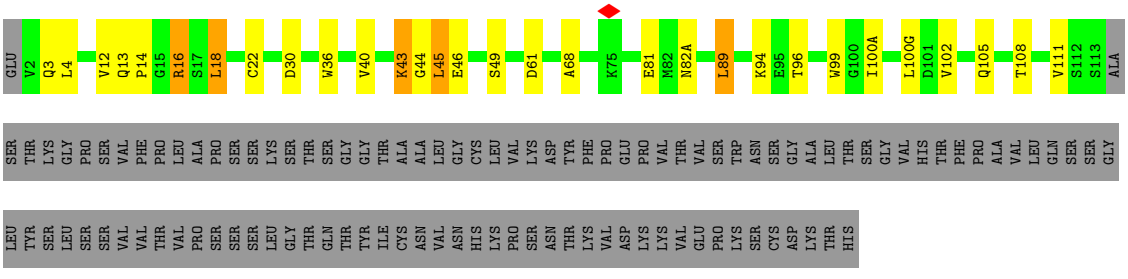
Chain C:





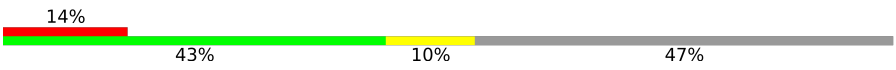
• Molecule 2: P2B4 Heavy chain

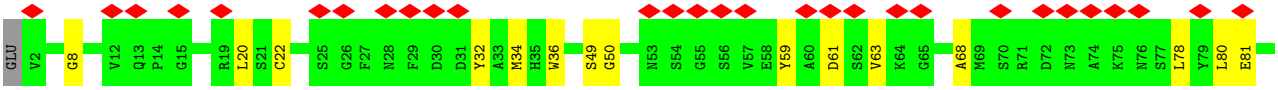
Chain H:

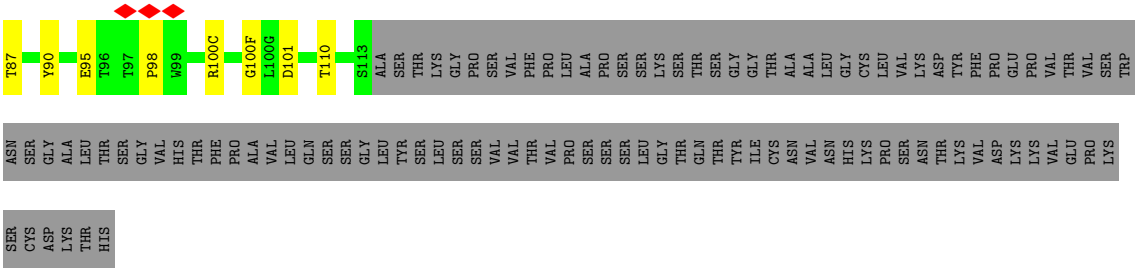


• Molecule 2: P2B4 Heavy chain

Chain F:

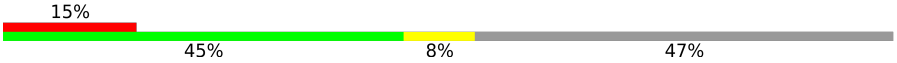


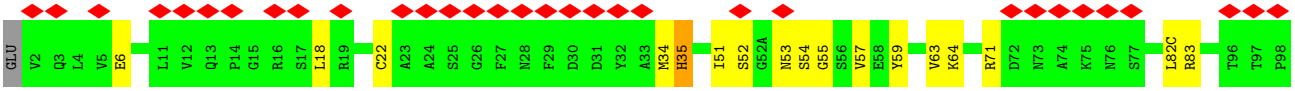


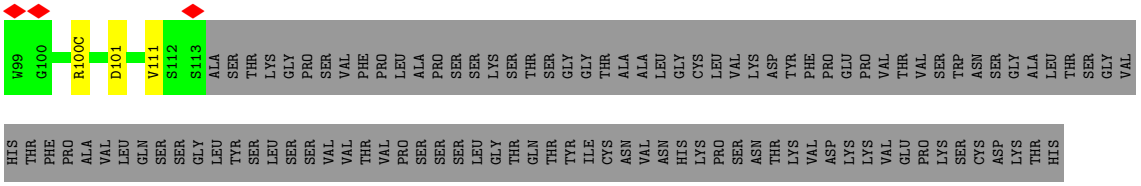


• Molecule 2: P2B4 Heavy chain

Chain G:

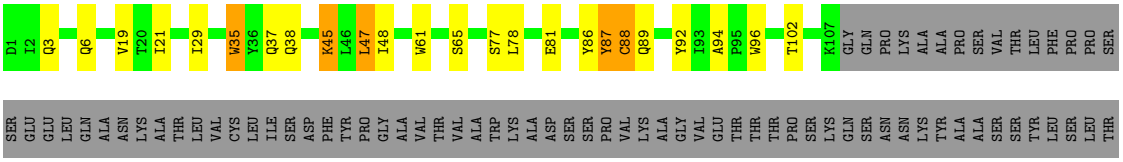






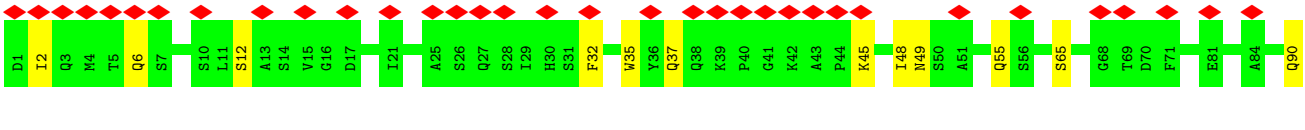
• Molecule 3: P2B4 Light chain

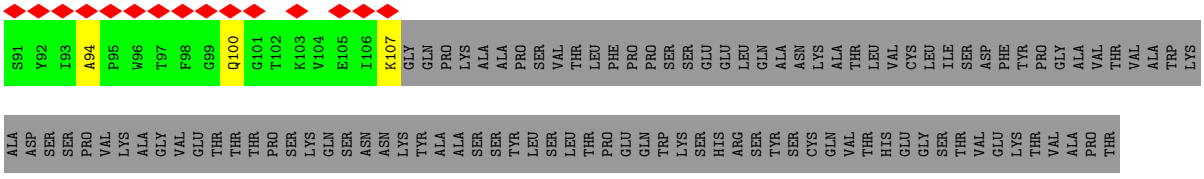
Chain L:



• Molecule 3: P2B4 Light chain

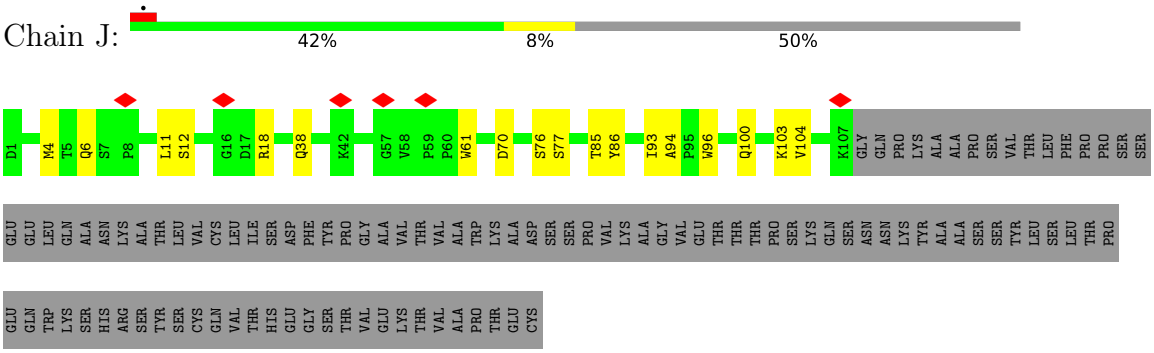
Chain I:





• Molecule 3: P2B4 Light chain

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93569	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.443	Depositor
Minimum map value	-0.247	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	365.19897, 365.19897, 365.19897	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93163, 0.93163, 0.93163	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.43	7/8187 (0.1%)	0.65	8/11137 (0.1%)
1	B	0.40	3/8396 (0.0%)	0.59	5/11419 (0.0%)
1	C	0.51	3/8286 (0.0%)	0.58	5/11272 (0.0%)
2	F	0.25	0/942	0.57	0/1275
2	G	0.26	0/942	0.55	0/1275
2	H	0.32	0/942	0.63	0/1275
3	I	0.26	0/837	0.51	0/1139
3	J	0.27	0/837	0.55	0/1139
3	L	0.32	0/837	0.61	1/1139 (0.1%)
All	All	0.42	13/30206 (0.0%)	0.60	19/41070 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
3	I	0	1
3	J	0	1
3	L	0	1
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	987	PRO	N-CD	37.16	1.99	1.47
1	B	463	PRO	N-CD	22.34	1.79	1.47
1	A	322	PRO	CB-CG	19.02	2.45	1.50
1	A	322	PRO	CG-CD	-13.10	1.07	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	760	CYS	CB-SG	-8.24	1.68	1.82
1	A	738	CYS	CB-SG	-8.04	1.68	1.82
1	C	331	ASN	CG-OD1	-6.99	1.08	1.24
1	A	322	PRO	N-CD	6.79	1.57	1.47
1	A	321	GLN	C-N	6.32	1.46	1.34
1	C	988	GLU	CD-OE2	-6.11	1.19	1.25
1	B	395	VAL	CB-CG1	-5.67	1.41	1.52
1	A	322	PRO	N-CA	-5.42	1.38	1.47
1	B	1111	GLU	CD-OE2	-5.42	1.19	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	322	PRO	CB-CG-CD	-27.29	0.05	106.50
1	C	987	PRO	CA-N-CD	-18.15	86.08	111.50
1	B	463	PRO	CA-N-CD	-14.61	91.04	111.50
1	A	322	PRO	CA-N-CD	-13.90	92.03	111.50
1	A	322	PRO	N-CA-CB	-13.71	86.84	103.30
1	B	796	ASP	CB-CG-OD1	10.74	127.97	118.30
1	A	321	GLN	C-N-CD	10.61	150.69	128.40
1	C	987	PRO	N-CD-CG	-9.22	89.36	103.20
1	A	118	LEU	CA-CB-CG	7.62	132.83	115.30
1	A	738	CYS	CA-CB-SG	7.53	127.56	114.00
1	C	986	PRO	C-N-CD	6.84	142.77	128.40
1	B	463	PRO	N-CD-CG	-6.84	92.95	103.20
1	B	796	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	C	574	ASP	CB-CG-OD1	5.86	123.58	118.30
1	C	754	LEU	CA-CB-CG	5.58	128.13	115.30
3	L	47	LEU	CB-CG-CD2	-5.46	101.73	111.00
1	B	287	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	118	LEU	CB-CG-CD1	5.24	119.91	111.00
1	A	760	CYS	CA-CB-SG	-5.08	104.85	114.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	PHE	Peptide
1	B	1097	SER	Peptide
3	I	94	ALA	Peptide
3	J	94	ALA	Peptide
3	L	94	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7999	0	7769	122	0
1	B	8205	0	7983	164	0
1	C	8097	0	7876	121	0
2	F	923	0	878	12	0
2	G	923	0	878	13	0
2	H	923	0	878	18	0
3	I	815	0	789	7	0
3	J	815	0	789	11	0
3	L	815	0	789	19	0
4	A	224	0	208	6	0
4	B	182	0	169	9	0
4	C	210	0	195	2	0
All	All	30131	0	29201	455	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 8.

All (455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASN:HD21	4:B:1304:NAG:C1	1.45	1.30
1:B:463:PRO:N	1:B:463:PRO:CD	1.79	1.28
1:B:343:ASN:ND2	4:B:1304:NAG:C1	2.02	1.22
1:C:987:PRO:N	1:C:987:PRO:CD	1.99	1.18
1:B:287:ASP:OD2	1:B:306:PHE:CE2	2.07	1.07
2:G:51:ILE:HG12	2:G:57:VAL:HG22	1.42	1.00
1:B:85:PRO:HA	1:B:237:ARG:HD3	1.45	0.96
3:L:47:LEU:N	3:L:47:LEU:HD22	1.82	0.94
1:B:343:ASN:ND2	4:B:1304:NAG:O5	1.99	0.94
1:B:236:THR:HB	1:B:237:ARG:HH22	1.33	0.94
1:B:236:THR:HB	1:B:237:ARG:NH2	1.83	0.92
1:C:987:PRO:HD2	1:C:988:GLU:CG	2.02	0.90
1:B:85:PRO:HA	1:B:237:ARG:CD	2.03	0.88
1:B:236:THR:O	1:B:237:ARG:NE	2.08	0.86
1:B:480:CYS:O	1:B:483:VAL:HG12	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1312:NAG:H5	1:B:796:ASP:OD1	1.76	0.85
1:A:52:GLN:OE1	1:A:273:ARG:C	2.15	0.85
1:B:237:ARG:HH11	1:B:237:ARG:HG2	1.42	0.83
1:B:424:LYS:HG3	1:B:463:PRO:HD3	1.61	0.83
1:C:987:PRO:HD2	1:C:988:GLU:HG3	1.61	0.82
1:B:119:ILE:HG12	1:B:128:ILE:HD12	1.63	0.81
1:B:85:PRO:CA	1:B:237:ARG:HD3	2.10	0.80
1:B:1129:VAL:CG1	1:B:1132:ILE:HD11	2.12	0.80
1:A:402:ILE:HD12	1:A:406:GLU:HG2	1.65	0.79
1:B:1129:VAL:HG12	1:B:1132:ILE:HD11	1.64	0.79
1:B:552:LEU:HD12	1:B:585:LEU:HD11	1.65	0.77
1:B:119:ILE:HG23	1:B:128:ILE:CD1	2.14	0.76
2:G:51:ILE:CG1	2:G:57:VAL:HG22	2.14	0.76
1:B:85:PRO:HA	1:B:237:ARG:NE	2.01	0.75
1:B:236:THR:O	1:B:237:ARG:CZ	2.34	0.75
1:B:343:ASN:CG	4:B:1304:NAG:C1	2.55	0.75
1:A:132:GLU:HB2	1:A:164:ASN:HB3	1.67	0.75
1:B:236:THR:C	1:B:237:ARG:CZ	2.55	0.75
1:A:473:TYR:HD1	1:A:474:GLN:NE2	1.85	0.74
1:C:985:ASP:HB2	1:C:988:GLU:HG3	1.69	0.74
1:C:987:PRO:HD2	1:C:988:GLU:HG2	1.70	0.72
1:B:1129:VAL:HG22	1:C:917:TYR:CB	2.20	0.70
1:A:52:GLN:OE1	1:A:274:THR:N	2.24	0.70
3:L:45:LYS:HD2	3:L:47:LEU:HD11	1.73	0.70
1:B:236:THR:CB	1:B:237:ARG:NH2	2.54	0.70
2:H:45:LEU:HD11	3:L:38:GLN:HE21	1.56	0.69
1:B:237:ARG:HG2	1:B:237:ARG:NH1	2.04	0.69
1:C:329:PHE:HD2	1:C:330:PRO:HD2	1.57	0.69
1:C:987:PRO:CD	1:C:988:GLU:HG3	2.23	0.69
1:C:919:ASN:HB3	1:C:922:LEU:HD23	1.75	0.68
1:B:85:PRO:HA	1:B:237:ARG:HE	1.59	0.68
1:B:1129:VAL:HG22	1:C:917:TYR:CG	2.28	0.68
3:L:3:GLN:N	3:L:3:GLN:OE1	2.27	0.68
1:B:119:ILE:HG23	1:B:128:ILE:HD11	1.75	0.67
1:B:236:THR:O	1:B:237:ARG:NH2	2.27	0.67
2:H:40:VAL:HG12	2:H:43:LYS:HE3	1.77	0.67
3:L:45:LYS:CD	3:L:47:LEU:HD11	2.25	0.66
1:B:287:ASP:OD2	1:B:306:PHE:CZ	2.48	0.66
1:B:738:CYS:HG	1:B:760:CYS:HG	0.65	0.65
1:B:309:GLU:N	1:B:309:GLU:OE2	2.29	0.65
1:C:987:PRO:HD2	1:C:988:GLU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TRP:HA	1:A:240:THR:HA	1.79	0.64
1:B:796:ASP:O	1:B:796:ASP:OD2	2.15	0.64
1:A:129:LYS:HG2	1:A:133:PHE:CZ	2.32	0.64
1:C:24:LEU:HB2	1:C:78:ARG:HG3	1.79	0.63
2:H:13:GLN:OE1	2:H:14:PRO:HD2	1.97	0.63
3:L:47:LEU:HD22	3:L:47:LEU:H	1.63	0.63
1:C:778:THR:HG22	1:C:865:LEU:HD12	1.81	0.62
1:C:987:PRO:CD	1:C:987:PRO:C	2.64	0.62
3:L:81:GLU:OE2	3:L:81:GLU:N	2.32	0.62
1:A:125:ASN:HB3	1:A:171:VAL:HG13	1.82	0.62
1:C:143:VAL:HG22	1:C:154:GLU:HG2	1.82	0.62
1:A:121:ASN:HA	1:A:126:VAL:HA	1.82	0.62
1:B:707:TYR:HE1	1:C:897:PRO:HA	1.65	0.62
1:A:922:LEU:HD11	4:A:1313:NAG:HN2	1.64	0.61
1:B:455:LEU:HD21	1:B:493:GLN:HB2	1.82	0.61
1:A:129:LYS:HD2	1:A:133:PHE:HE1	1.66	0.61
2:G:59:TYR:HB2	2:G:64:LYS:HD3	1.83	0.61
1:A:558:LYS:HE2	1:B:282:ASN:CG	2.21	0.60
2:G:51:ILE:CD1	2:G:57:VAL:HG22	2.32	0.60
1:A:92:PHE:HB3	1:A:192:PHE:HB2	1.83	0.60
1:A:897:PRO:HG2	1:A:900:MET:HG3	1.82	0.60
1:B:236:THR:CA	1:B:237:ARG:NH2	2.65	0.60
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.83	0.60
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.84	0.60
1:B:902:MET:HB3	1:B:916:LEU:HD21	1.84	0.59
1:A:1102:TRP:H	1:A:1135:ASN:ND2	2.00	0.59
1:B:236:THR:C	1:B:237:ARG:NH2	2.56	0.59
3:I:37:GLN:HB3	3:I:45:LYS:HB2	1.85	0.59
1:A:1107:ARG:HH12	1:B:894:LEU:HD23	1.68	0.59
1:C:119:ILE:HG22	1:C:128:ILE:HG23	1.85	0.58
1:C:410:ILE:HD12	1:C:433:VAL:HG21	1.85	0.58
2:H:36:TRP:HD1	2:H:49:SER:HB3	1.69	0.58
2:F:68:ALA:HB3	2:F:81:GLU:HB3	1.85	0.58
1:C:342:PHE:HZ	1:C:434:ILE:HG12	1.69	0.58
1:B:393:THR:HA	1:B:522:ALA:HA	1.84	0.58
1:A:105:ILE:HA	1:A:118:LEU:HA	1.85	0.58
1:A:645:THR:HB	1:A:670:ILE:HD13	1.85	0.57
1:B:351:TYR:HE2	1:B:452:LEU:HB3	1.68	0.57
1:C:462:LYS:HG3	1:C:465:GLU:HG3	1.85	0.57
1:A:737:ASP:OD2	1:C:317:ASN:ND2	2.38	0.57
2:H:40:VAL:CG1	2:H:43:LYS:HE3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HH22	1:B:200:TYR:HE1	1.53	0.57
2:F:87:THR:HG23	2:F:110:THR:HA	1.87	0.57
1:B:279:TYR:HB3	1:B:283:GLY:HA2	1.86	0.57
1:C:598:ILE:HG23	1:C:664:ILE:HD13	1.87	0.57
1:A:912:THR:OG1	1:A:1106:GLN:NE2	2.38	0.56
2:H:43:LYS:HD2	2:H:44:GLY:N	2.20	0.56
1:B:1129:VAL:HG22	1:C:917:TYR:HB3	1.86	0.56
1:C:987:PRO:HD2	1:C:987:PRO:C	2.25	0.56
1:C:722:VAL:HG22	1:C:930:ALA:HB1	1.87	0.56
1:B:643:PHE:CZ	1:B:645:THR:HG22	2.41	0.56
1:C:295:PRO:HB2	1:C:608:VAL:HG11	1.88	0.56
1:C:451:TYR:HB3	1:C:495:TYR:HD1	1.70	0.56
1:A:558:LYS:HE2	1:B:282:ASN:ND2	2.20	0.56
4:A:1306:NAG:H82	1:C:558:LYS:HG2	1.87	0.56
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.33	0.56
1:B:1080:ALA:HB3	1:B:1132:ILE:HD12	1.86	0.56
1:C:905:ARG:NH1	1:C:1050:MET:SD	2.78	0.56
1:A:1116:THR:HG22	1:A:1118:ASP:H	1.71	0.56
1:B:1129:VAL:HG11	1:B:1132:ILE:HD11	1.86	0.56
1:B:480:CYS:O	1:B:483:VAL:CG1	2.50	0.56
1:A:332:ILE:HD12	4:A:1307:NAG:H62	1.88	0.55
1:B:426:PRO:HA	1:B:463:PRO:HG3	1.86	0.55
1:B:607:GLN:HB3	1:B:692:ILE:HD11	1.89	0.55
1:C:987:PRO:CD	1:C:988:GLU:N	2.69	0.55
2:G:101:ASP:N	2:G:101:ASP:OD1	2.37	0.55
1:A:96:GLU:OE2	1:A:99:ASN:N	2.38	0.55
1:C:342:PHE:CZ	1:C:434:ILE:HG12	2.42	0.55
1:A:452:LEU:HB3	1:A:492:LEU:HG	1.88	0.55
2:H:12:VAL:HG23	2:H:16:ARG:HH21	1.70	0.55
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.89	0.55
1:B:932:GLY:O	1:B:936:ASP:OD1	2.25	0.55
1:C:376:THR:OG1	1:C:378:LYS:NZ	2.39	0.55
1:B:236:THR:HB	1:B:237:ARG:CZ	2.36	0.55
2:H:94:LYS:H	2:H:102:VAL:HG22	1.72	0.54
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.88	0.54
1:C:506:GLN:NE2	1:C:507:PRO:O	2.40	0.54
2:F:20:LEU:HD11	2:F:80:LEU:HD23	1.89	0.54
1:A:346:ARG:NH2	1:A:442:ASP:OD2	2.40	0.54
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.89	0.54
2:F:101:ASP:OD1	2:F:101:ASP:N	2.41	0.54
1:A:780:GLU:O	1:A:784:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:TYR:CE1	1:C:897:PRO:HA	2.43	0.54
1:C:329:PHE:HD2	1:C:330:PRO:CD	2.19	0.54
2:H:4:LEU:O	2:H:105:GLN:NE2	2.41	0.54
1:B:566:GLY:HA2	1:C:42:VAL:HG23	1.89	0.54
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.89	0.54
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.90	0.53
1:A:809:PRO:HA	1:A:814:LYS:HD2	1.89	0.53
1:C:914:ASN:ND2	1:C:1111:GLU:OE2	2.40	0.53
2:G:51:ILE:HG22	2:G:71:ARG:HH21	1.73	0.53
1:A:374:PHE:HD1	1:A:436:TRP:HB3	1.73	0.53
1:C:353:TRP:O	1:C:466:ARG:NH1	2.41	0.53
1:A:755:GLN:O	1:C:968:SER:OG	2.25	0.53
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.41	0.53
1:B:85:PRO:CA	1:B:237:ARG:HE	2.22	0.53
1:B:351:TYR:HE2	1:B:452:LEU:CB	2.22	0.53
1:B:1101:HIS:CE1	4:B:1312:NAG:H5	2.44	0.53
1:C:329:PHE:CD2	1:C:330:PRO:HD2	2.42	0.53
2:G:54:SER:OG	2:G:55:GLY:N	2.42	0.53
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.41	0.53
1:B:355:ARG:HD2	1:B:396:TYR:HD2	1.74	0.53
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.91	0.53
1:A:644:GLN:NE2	1:A:645:THR:O	2.41	0.53
1:B:886:TRP:HB3	1:B:1035:GLY:HA2	1.90	0.52
1:A:353:TRP:HZ3	1:A:355:ARG:HD2	1.73	0.52
1:B:603:ASN:O	1:B:603:ASN:ND2	2.43	0.52
1:C:816:SER:OG	1:C:817:PHE:N	2.42	0.52
1:A:819:GLU:HA	1:A:822:LEU:HD12	1.92	0.52
1:B:441:LEU:HB3	1:B:509:ARG:HH21	1.73	0.52
1:C:129:LYS:HG2	1:C:169:GLU:HA	1.91	0.52
1:C:733:LYS:HE3	1:C:771:ALA:HB1	1.91	0.52
1:C:92:PHE:HB3	1:C:192:PHE:HB2	1.91	0.52
1:C:984:LEU:HB3	1:C:989:ALA:HB2	1.91	0.52
2:H:3:GLN:OE1	2:H:105:GLN:NE2	2.43	0.52
3:I:49:ASN:HB2	3:I:55:GLN:NE2	2.24	0.52
1:B:393:THR:OG1	1:B:394:ASN:N	2.43	0.52
1:B:1013:ILE:HG21	1:C:1012:LEU:HG	1.91	0.52
1:C:104:TRP:HB2	1:C:106:PHE:HE1	1.74	0.52
1:B:50:SER:HB3	1:B:276:LEU:HD12	1.91	0.52
1:C:601:GLY:O	1:C:604:THR:OG1	2.24	0.52
2:H:68:ALA:HB3	2:H:81:GLU:HB3	1.92	0.52
3:L:37:GLN:HB3	3:L:45:LYS:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1009:THR:O	1:C:1013:ILE:HG13	2.10	0.52
1:B:127:VAL:O	1:B:128:ILE:HD13	2.10	0.51
1:B:317:ASN:ND2	1:C:737:ASP:OD2	2.44	0.51
3:J:103:LYS:NZ	3:J:104:VAL:O	2.42	0.51
1:A:117:LEU:HG	1:A:119:ILE:HG12	1.92	0.51
1:A:856:ASN:HD21	1:A:963:VAL:HG12	1.74	0.51
1:A:52:GLN:OE1	1:A:274:THR:CA	2.59	0.51
1:A:719:THR:HG23	1:A:1070:ALA:HB2	1.91	0.51
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.91	0.51
1:B:343:ASN:OD1	4:B:1304:NAG:C1	2.57	0.51
1:B:68:ILE:HG22	1:B:262:ALA:HA	1.92	0.51
1:B:213:VAL:HG12	1:B:214:ARG:HG2	1.92	0.51
1:B:738:CYS:CB	1:B:760:CYS:SG	2.98	0.51
1:B:738:CYS:HB2	1:B:760:CYS:SG	2.50	0.51
1:A:330:PRO:HG3	1:A:544:ASN:HA	1.91	0.51
1:A:62:VAL:HG12	1:A:268:GLY:HA2	1.93	0.51
1:C:40:ASP:N	1:C:40:ASP:OD1	2.44	0.51
1:C:898:PHE:HA	1:C:901:GLN:HB3	1.91	0.51
2:G:52:SER:OG	2:G:100(C):ARG:NH1	2.44	0.51
1:A:1107:ARG:HH22	1:B:894:LEU:HB3	1.74	0.51
3:L:19:VAL:HG12	3:L:78:LEU:HD11	1.93	0.51
2:F:32:TYR:HA	2:F:98:PRO:HG3	1.92	0.51
1:B:85:PRO:CA	1:B:237:ARG:CD	2.76	0.50
1:B:415:THR:OG1	1:B:416:GLY:N	2.44	0.50
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.44	0.50
2:G:6:GLU:HG3	2:G:22:CYS:HB3	1.92	0.50
1:B:712:ILE:HD11	1:B:1094:VAL:HG21	1.93	0.50
1:C:900:MET:SD	1:C:900:MET:N	2.83	0.50
3:J:6:GLN:O	3:J:100:GLN:NE2	2.44	0.50
1:A:893:ALA:HB1	1:C:705:VAL:HG23	1.93	0.50
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.92	0.50
1:C:909:ILE:O	1:C:1108:ASN:ND2	2.45	0.50
3:J:93:ILE:O	3:J:96:TRP:NE1	2.44	0.50
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.39	0.50
3:L:47:LEU:N	3:L:47:LEU:CD2	2.61	0.50
1:A:729:VAL:HG21	1:A:781:VAL:HG11	1.94	0.50
1:B:736:VAL:HG21	1:B:1004:LEU:HD11	1.93	0.50
3:L:35:TRP:HZ3	3:L:88:CYS:SG	2.35	0.50
2:G:59:TYR:HB3	2:G:63:VAL:HG23	1.93	0.50
1:B:483:VAL:HG22	1:B:484:GLU:N	2.27	0.50
1:B:738:CYS:SG	1:B:739:THR:N	2.83	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:TYR:HB3	1:C:223:LEU:HG	1.94	0.50
1:A:711:SER:HB2	1:B:895:GLN:HE21	1.76	0.50
1:A:1115:ILE:HG22	1:A:1137:VAL:HG13	1.93	0.50
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.39	0.50
1:A:364:ASP:HA	1:A:527:PRO:HG3	1.93	0.49
1:A:473:TYR:HD1	1:A:474:GLN:HE21	1.58	0.49
1:C:980:ILE:HD11	1:C:992:GLN:HB2	1.94	0.49
1:B:125:ASN:ND2	1:B:172:SER:O	2.45	0.49
1:B:811:LYS:NZ	1:B:813:SER:O	2.43	0.49
1:A:454:ARG:NH2	1:A:469:SER:O	2.46	0.49
1:A:1073:LYS:HG3	1:A:1075:PHE:CE2	2.48	0.49
1:B:462:LYS:HG3	1:B:465:GLU:HG3	1.93	0.49
1:C:201:PHE:HB3	1:C:229:LEU:HB2	1.95	0.49
1:A:991:VAL:HG12	1:C:995:ARG:NH2	2.27	0.49
1:C:244:LEU:HB3	1:C:258:TRP:HB3	1.94	0.49
1:A:196:ASN:HD21	1:A:235:ILE:HD12	1.78	0.49
1:A:473:TYR:CD1	1:A:474:GLN:N	2.81	0.49
1:B:246:ARG:NH1	1:B:257:GLY:O	2.44	0.49
1:B:353:TRP:O	1:B:466:ARG:NH1	2.46	0.49
1:A:40:ASP:OD1	1:A:40:ASP:N	2.45	0.49
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.94	0.49
1:A:883:THR:HB	1:C:707:TYR:HB2	1.95	0.49
1:B:343:ASN:OD1	4:B:1304:NAG:H2	2.12	0.49
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.38	0.49
1:B:332:ILE:HG12	1:B:580:GLN:HA	1.95	0.48
1:C:415:THR:OG1	1:C:416:GLY:N	2.45	0.48
2:H:96:THR:O	2:H:96:THR:OG1	2.22	0.48
1:A:991:VAL:HG12	1:C:995:ARG:HH22	1.77	0.48
1:A:1098:ASN:HB3	1:A:1103:PHE:HZ	1.79	0.48
1:A:1139:ASP:N	1:A:1142:GLN:HE22	2.11	0.48
1:B:643:PHE:CE2	1:B:645:THR:HG22	2.49	0.48
1:B:720:ILE:HD12	1:B:923:ILE:HB	1.96	0.48
1:A:133:PHE:HB2	1:A:135:PHE:CE1	2.48	0.48
1:B:809:PRO:HA	1:B:814:LYS:HD2	1.95	0.48
1:B:106:PHE:O	1:B:116:SER:OG	2.29	0.48
1:B:236:THR:CB	1:B:237:ARG:CZ	2.91	0.48
2:H:12:VAL:HB	2:H:18:LEU:HD13	1.95	0.48
1:A:29:THR:HA	4:A:1302:NAG:H82	1.96	0.48
1:A:188:ASN:HB3	1:A:190:ARG:HE	1.79	0.48
1:A:349:SER:OG	1:A:452:LEU:O	2.32	0.48
1:A:969:ASN:OD1	1:A:972:ALA:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1077:THR:HG22	1:C:1096:VAL:HG12	1.95	0.48
1:A:52:GLN:OE1	1:A:273:ARG:O	2.32	0.47
1:B:808:ASP:HB3	1:B:811:LYS:HG2	1.94	0.47
1:B:882:ILE:HG23	1:B:883:THR:HG23	1.94	0.47
1:C:86:PHE:HZ	1:C:194:PHE:HB2	1.79	0.47
3:I:35:TRP:HB2	3:I:48:ILE:HB	1.96	0.47
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.95	0.47
1:B:575:ALA:CB	1:B:586:ASP:OD2	2.63	0.47
1:B:643:PHE:CD1	1:B:644:GLN:N	2.82	0.47
2:G:82(C):LEU:HD11	2:G:111:VAL:HG21	1.95	0.47
1:C:377:PHE:HE2	1:C:434:ILE:HD13	1.79	0.47
1:C:422:ASN:HD21	1:C:454:ARG:H	1.63	0.47
1:C:553:THR:HG23	1:C:586:ASP:HB3	1.95	0.47
1:B:142:GLY:HA3	1:B:156:GLU:HG2	1.96	0.47
1:C:599:THR:HB	1:C:608:VAL:HG22	1.97	0.47
1:A:129:LYS:HG2	1:A:133:PHE:CE1	2.49	0.47
1:C:33:THR:OG1	1:C:219:GLY:O	2.33	0.47
1:C:99:ASN:O	1:C:102:ARG:NE	2.45	0.47
1:C:718:PHE:HA	1:C:1069:PRO:HA	1.96	0.47
1:C:97:LYS:HD2	1:C:186:PHE:HA	1.97	0.47
1:C:760:CYS:HA	1:C:763:LEU:HG	1.96	0.47
1:C:802:PHE:HB3	1:C:806:LEU:HD23	1.97	0.47
2:G:51:ILE:CD1	2:G:57:VAL:CG2	2.93	0.47
1:B:66:HIS:HB3	1:B:68:ILE:HG12	1.97	0.46
2:F:8:GLY:HA3	2:F:20:LEU:HA	1.96	0.46
1:A:129:LYS:CD	1:A:133:PHE:HE1	2.27	0.46
1:B:738:CYS:SG	1:B:753:LEU:HD21	2.55	0.46
1:B:936:ASP:OD1	1:B:936:ASP:N	2.48	0.46
3:L:47:LEU:C	3:L:48:ILE:HD13	2.36	0.46
2:F:49:SER:OG	2:F:50:GLY:N	2.48	0.46
1:B:21:ARG:NE	1:B:79:PHE:O	2.48	0.46
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.97	0.46
1:C:66:HIS:HB2	1:C:78:ARG:HD2	1.98	0.46
1:C:412:PRO:O	1:C:414:GLN:NE2	2.48	0.46
3:I:32:PHE:O	3:I:90:GLN:NE2	2.44	0.46
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.96	0.46
1:B:85:PRO:HA	1:B:237:ARG:HA	1.96	0.46
1:B:85:PRO:CA	1:B:237:ARG:NE	2.76	0.46
1:B:424:LYS:CG	1:B:463:PRO:HD3	2.40	0.46
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.47	0.46
3:L:35:TRP:CZ3	3:L:88:CYS:SG	3.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLY:HA2	4:A:1308:NAG:O7	2.15	0.46
1:A:671:CYS:SG	1:A:697:MET:HE3	2.55	0.46
1:C:280:ASN:OD1	1:C:284:THR:N	2.44	0.46
3:L:38:GLN:HG3	3:L:87:TYR:HE2	1.80	0.46
1:A:122:ASN:HD22	1:A:125:ASN:HD22	1.64	0.46
1:C:762:GLN:HE21	1:C:762:GLN:HB2	1.54	0.46
1:A:1084:ASP:OD1	1:A:1084:ASP:N	2.47	0.46
1:B:985:ASP:HB3	1:B:987:PRO:HD2	1.98	0.46
1:C:714:ILE:HG22	1:C:1107:ARG:HH12	1.80	0.46
1:B:444:LYS:HE3	1:B:444:LYS:HB3	1.75	0.46
1:C:144:TYR:HE2	1:C:156:GLU:HB2	1.80	0.46
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.97	0.46
1:A:41:LYS:HB3	1:C:563:GLN:HA	1.98	0.45
1:B:483:VAL:HG22	1:B:485:GLY:H	1.81	0.45
1:A:708:SER:OG	1:A:709:ASN:N	2.50	0.45
1:A:877:LEU:HD23	1:A:1034:LEU:HD21	1.98	0.45
1:B:40:ASP:OD1	1:B:40:ASP:N	2.49	0.45
1:B:643:PHE:HE2	1:B:670:ILE:HG21	1.80	0.45
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.72	0.45
2:F:34:MET:HE3	2:F:78:LEU:HD22	1.98	0.45
1:C:121:ASN:HA	1:C:126:VAL:HA	1.99	0.45
1:A:473:TYR:CG	1:A:474:GLN:N	2.85	0.45
1:C:452:LEU:HD12	1:C:492:LEU:HB3	1.98	0.45
1:A:384:PRO:HD2	1:B:985:ASP:OD2	2.17	0.45
1:C:393:THR:HA	1:C:522:ALA:HA	1.98	0.45
1:A:976:VAL:HB	1:A:979:ASP:HB2	1.99	0.45
1:C:661:GLU:O	1:C:695:TYR:OH	2.29	0.45
2:H:99:TRP:HD1	2:H:100(A):ILE:H	1.65	0.45
1:B:357:ARG:C	1:B:358:ILE:HD13	2.37	0.45
1:B:483:VAL:HG22	1:B:485:GLY:N	2.32	0.45
1:B:598:ILE:HG23	1:B:664:ILE:HG21	1.99	0.45
1:B:965:GLN:NE2	1:C:756:TYR:O	2.49	0.45
1:B:328:ARG:O	1:B:544:ASN:N	2.50	0.45
1:C:281:GLU:HG2	4:C:1304:NAG:H82	1.99	0.45
1:C:331:ASN:C	1:C:331:ASN:OD1	2.56	0.45
1:C:420:ASP:OD1	1:C:420:ASP:N	2.48	0.45
2:F:59:TYR:HB3	2:F:63:VAL:HG23	1.99	0.45
1:A:33:THR:HB	1:A:220:PHE:HD1	1.83	0.44
2:H:89:LEU:HA	2:H:108:THR:HA	1.98	0.44
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.50	0.44
3:J:11:LEU:HD23	3:J:11:LEU:HA	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:HD12	1:A:983:ARG:HH12	1.82	0.44
1:B:99:ASN:O	1:B:102:ARG:NE	2.46	0.44
2:F:36:TRP:CZ3	2:F:90:TYR:HB3	2.52	0.44
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.99	0.44
1:A:105:ILE:HG23	1:A:118:LEU:HB3	2.00	0.44
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.84	0.44
1:B:412:PRO:O	1:B:414:GLN:NE2	2.50	0.44
1:B:1091:ARG:HG2	1:B:1121:PHE:HD1	1.83	0.44
1:C:693:ILE:HD12	1:C:693:ILE:HA	1.81	0.44
3:J:18:ARG:HH21	3:J:76:SER:HA	1.82	0.44
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.50	0.44
1:C:791:THR:HG21	1:C:806:LEU:HD11	2.00	0.44
2:H:14:PRO:HD3	2:H:111:VAL:HG12	2.00	0.44
3:I:6:GLN:O	3:I:100:GLN:NE2	2.51	0.44
3:I:12:SER:HB3	3:I:107:LYS:HB3	2.00	0.44
1:A:449:TYR:HD2	1:A:496:GLY:HA2	1.82	0.44
1:A:905:ARG:NE	1:A:1050:MET:HB3	2.33	0.44
1:B:584:ILE:HD12	1:B:584:ILE:HA	1.81	0.44
1:B:604:THR:HA	4:B:1305:NAG:H83	1.98	0.44
1:A:658:ASN:OD1	1:A:658:ASN:N	2.48	0.44
1:B:195:LYS:HD2	1:B:195:LYS:HA	1.70	0.44
1:B:299:THR:HG21	1:B:599:THR:HG21	1.99	0.44
1:A:864:LEU:HD22	1:C:665:PRO:HB3	1.99	0.44
1:B:128:ILE:HG12	1:B:170:TYR:HD2	1.82	0.44
1:B:343:ASN:OD1	4:B:1304:NAG:C2	2.66	0.43
1:B:391:CYS:HA	1:B:525:CYS:HA	2.00	0.43
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.98	0.43
1:B:575:ALA:HB2	1:B:586:ASP:OD2	2.18	0.43
2:F:34:MET:CE	2:F:78:LEU:HD22	2.48	0.43
1:A:611:LEU:HD13	1:A:666:ILE:HD12	2.00	0.43
1:C:244:LEU:HD23	1:C:260:ALA:HB2	2.00	0.43
3:L:29:ILE:HD12	3:L:29:ILE:HA	1.87	0.43
1:A:317:ASN:ND2	1:B:737:ASP:OD1	2.51	0.43
1:B:236:THR:C	1:B:237:ARG:NE	2.66	0.43
1:C:786:LYS:H	1:C:786:LYS:HG2	1.54	0.43
1:B:281:GLU:OE1	1:B:282:ASN:OD1	2.36	0.43
1:B:68:ILE:HG13	1:B:78:ARG:H	1.84	0.43
1:B:739:THR:OG1	1:B:740:MET:SD	2.77	0.43
1:C:869:MET:HA	1:C:872:GLN:HB2	2.01	0.43
1:A:111:ASP:OD1	1:A:111:ASP:N	2.50	0.43
1:B:346:ARG:HA	1:B:346:ARG:NE	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1083:HIS:HB2	1:C:1137:VAL:HG23	2.00	0.43
2:H:46:GLU:N	2:H:46:GLU:OE2	2.51	0.43
3:L:6:GLN:OE1	3:L:102:THR:OG1	2.31	0.43
3:J:11:LEU:N	3:J:103:LYS:O	2.49	0.43
1:A:280:ASN:ND2	1:A:284:THR:OG1	2.48	0.43
1:C:129:LYS:HE2	1:C:129:LYS:HB3	1.87	0.43
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.81	0.43
1:A:1114:ILE:HD12	1:A:1114:ILE:HA	1.90	0.43
2:F:95:GLU:HB3	2:F:100(F):GLY:HA3	2.00	0.43
1:A:971:GLY:HA3	1:A:995:ARG:HH21	1.84	0.42
1:A:1013:ILE:HD13	1:B:1012:LEU:HB3	2.01	0.42
1:C:33:THR:HB	1:C:220:PHE:HD1	1.83	0.42
1:C:276:LEU:HD11	1:C:301:CYS:HA	2.01	0.42
1:A:584:ILE:HD13	1:A:584:ILE:HA	1.80	0.42
1:B:106:PHE:HB2	1:B:117:LEU:HB3	2.00	0.42
1:C:231:ILE:HG13	1:C:233:ILE:H	1.84	0.42
3:I:2:ILE:HG12	3:I:90:GLN:HB3	2.01	0.42
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.48	0.42
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	2.01	0.42
1:B:825:LYS:HE3	1:B:942:ALA:HA	2.01	0.42
2:G:34:MET:SD	2:G:35:HIS:N	2.93	0.42
1:A:1031:GLU:HA	1:C:1040:VAL:HG23	2.02	0.42
1:B:483:VAL:CG2	1:B:484:GLU:N	2.82	0.42
3:J:93:ILE:H	3:J:96:TRP:HE1	1.68	0.42
3:J:103:LYS:HA	3:J:103:LYS:HD2	1.77	0.42
1:A:34:ARG:HH21	1:A:217:PRO:HB2	1.84	0.42
1:A:988:GLU:OE1	1:A:988:GLU:N	2.53	0.42
1:B:856:ASN:OD1	1:B:856:ASN:N	2.52	0.42
1:B:331:ASN:HD22	1:B:331:ASN:HA	1.59	0.42
1:C:298:GLU:HG2	1:C:315:THR:HB	2.01	0.42
1:C:864:LEU:HD12	1:C:864:LEU:HA	1.88	0.42
1:A:28:TYR:HB3	1:A:61:ASN:HD22	1.83	0.42
1:B:335:LEU:HD12	1:B:336:CYS:H	1.85	0.42
1:B:358:ILE:HB	1:B:395:VAL:CG1	2.50	0.42
1:A:565:PHE:N	1:A:577:ARG:HH21	2.17	0.41
1:C:245:HIS:ND1	1:C:259:THR:O	2.53	0.41
1:C:1102:TRP:HB2	1:C:1135:ASN:HD22	1.85	0.41
3:J:38:GLN:HE21	3:J:85:THR:HG23	1.85	0.41
1:A:52:GLN:OE1	1:A:274:THR:HA	2.20	0.41
1:A:126:VAL:HG23	1:A:172:SER:OG	2.19	0.41
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:ILE:H	1:B:934:ILE:HG13	1.71	0.41
1:C:57:PRO:HB3	1:C:273:ARG:NH1	2.35	0.41
1:B:1100:THR:HG1	1:B:1101:HIS:CE1	2.38	0.41
3:J:6:GLN:H	3:J:100:GLN:HE22	1.69	0.41
1:C:331:ASN:OD1	4:C:1305:NAG:H2	2.20	0.41
3:J:93:ILE:N	3:J:96:TRP:HE1	2.18	0.41
1:C:106:PHE:HB2	1:C:117:LEU:HB3	2.03	0.41
2:H:36:TRP:CD1	2:H:49:SER:HB3	2.53	0.41
1:A:434:ILE:HD12	1:A:434:ILE:HA	1.94	0.41
3:L:35:TRP:O	3:L:47:LEU:HD23	2.20	0.41
1:A:386:LYS:NZ	1:B:984:LEU:O	2.50	0.41
3:L:21:ILE:HD13	3:L:21:ILE:HA	1.89	0.41
1:A:216:LEU:HA	1:A:217:PRO:HD3	1.92	0.40
1:A:412:PRO:O	1:A:414:GLN:NE2	2.54	0.40
1:B:580:GLN:OE1	1:B:581:THR:OG1	2.37	0.40
1:B:816:SER:OG	1:B:817:PHE:N	2.54	0.40
1:B:913:GLN:H	1:B:913:GLN:HG2	1.57	0.40
1:A:726:ILE:HD11	1:A:948:LEU:HD21	2.02	0.40
1:B:563:GLN:HA	1:C:41:LYS:HB3	2.02	0.40
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	2.02	0.40
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.96	0.40
1:B:643:PHE:CD1	1:B:643:PHE:C	2.94	0.40
1:B:912:THR:OG1	1:B:1106:GLN:OE1	2.28	0.40
1:C:813:SER:OG	1:C:814:LYS:N	2.53	0.40
1:A:353:TRP:O	1:A:466:ARG:NH2	2.54	0.40
1:A:816:SER:OG	1:A:817:PHE:N	2.55	0.40
1:B:85:PRO:N	1:B:237:ARG:HD3	2.35	0.40
1:B:1006:THR:HG23	1:C:1005:GLN:HE22	1.87	0.40
1:C:856:ASN:OD1	1:C:966:LEU:HD21	2.20	0.40
3:L:89:GLN:OE1	3:L:96:TRP:HB3	2.22	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	1005/1288 (78%)	947 (94%)	53 (5%)	5 (0%)	29 65
1	B	1031/1288 (80%)	980 (95%)	51 (5%)	0	100 100
1	C	1017/1288 (79%)	975 (96%)	40 (4%)	2 (0%)	47 78
2	F	121/231 (52%)	113 (93%)	8 (7%)	0	100 100
2	G	121/231 (52%)	112 (93%)	9 (7%)	0	100 100
2	H	121/231 (52%)	111 (92%)	10 (8%)	0	100 100
3	I	105/212 (50%)	97 (92%)	8 (8%)	0	100 100
3	J	105/212 (50%)	98 (93%)	7 (7%)	0	100 100
3	L	105/212 (50%)	95 (90%)	10 (10%)	0	100 100
All	All	3731/5193 (72%)	3528 (95%)	196 (5%)	7 (0%)	50 78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	159	VAL
1	A	331	ASN
1	C	123	ALA
1	C	332	ILE
1	A	235	ILE
1	A	322	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	892/1113 (80%)	861 (96%)	31 (4%)	36 63
1	B	916/1113 (82%)	881 (96%)	35 (4%)	33 61
1	C	904/1113 (81%)	874 (97%)	30 (3%)	38 64
2	F	96/192 (50%)	93 (97%)	3 (3%)	40 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	96/192 (50%)	92 (96%)	4 (4%)	30 59
2	H	96/192 (50%)	86 (90%)	10 (10%)	7 31
3	I	92/183 (50%)	91 (99%)	1 (1%)	73 85
3	J	92/183 (50%)	86 (94%)	6 (6%)	17 49
3	L	92/183 (50%)	83 (90%)	9 (10%)	8 33
All	All	3276/4464 (73%)	3147 (96%)	129 (4%)	36 61

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	TRP
1	A	133	PHE
1	A	135	PHE
1	A	140	PHE
1	A	238	PHE
1	A	242	LEU
1	A	269	TYR
1	A	353	TRP
1	A	365[A]	TYR
1	A	365[B]	TYR
1	A	377	PHE
1	A	383	SER
1	A	420	ASP
1	A	428	ASP
1	A	440	ASN
1	A	449	TYR
1	A	473	TYR
1	A	515	PHE
1	A	562	PHE
1	A	643	PHE
1	A	658	ASN
1	A	751	ASN
1	A	759	PHE
1	A	775	ASP
1	A	855	PHE
1	A	969	ASN
1	A	1030	SER
1	A	1041	ASP
1	A	1103	PHE
1	A	1121	PHE

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Mol	Chain	Res	Type
1	A	1127	ASP
1	B	55	PHE
1	B	158	ARG
1	B	189	LEU
1	B	237	ARG
1	B	278	LYS
1	B	305	SER
1	B	316	SER
1	B	346	ARG
1	B	420	ASP
1	B	428	ASP
1	B	432	CYS
1	B	436	TRP
1	B	444	LYS
1	B	451	TYR
1	B	471	GLU
1	B	490	PHE
1	B	515	PHE
1	B	517	LEU
1	B	567	ARG
1	B	616	ASN
1	B	643	PHE
1	B	691	SER
1	B	738	CYS
1	B	759	PHE
1	B	760	CYS
1	B	762	GLN
1	B	779	GLN
1	B	796	ASP
1	B	803	SER
1	B	858	LEU
1	B	873	TYR
1	B	936	ASP
1	B	957	GLN
1	B	966	LEU
1	B	1118	ASP
1	C	45	SER
1	C	49	HIS
1	C	54	LEU
1	C	79	PHE
1	C	106	PHE
1	C	122	ASN

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Mol	Chain	Res	Type
1	C	153	MET
1	C	316	SER
1	C	329	PHE
1	C	331	ASN
1	C	335	LEU
1	C	342	PHE
1	C	366	SER
1	C	391	CYS
1	C	432	CYS
1	C	490	PHE
1	C	493	GLN
1	C	517	LEU
1	C	559	PHE
1	C	754	LEU
1	C	779	GLN
1	C	803	SER
1	C	869	MET
1	C	919	ASN
1	C	985	ASP
1	C	994	ASP
1	C	1021	SER
1	C	1030	SER
1	C	1041	ASP
1	C	1075	PHE
2	H	16	ARG
2	H	18	LEU
2	H	22	CYS
2	H	30	ASP
2	H	43	LYS
2	H	45	LEU
2	H	61	ASP
2	H	82(A)	ASN
2	H	89	LEU
2	H	100(G)	LEU
3	L	35	TRP
3	L	45	LYS
3	L	61	TRP
3	L	65	SER
3	L	77	SER
3	L	86	TYR
3	L	87	TYR
3	L	88	CYS

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Mol	Chain	Res	Type
3	L	92	TYR
2	F	22	CYS
2	F	61	ASP
2	F	100(C)	ARG
3	I	65	SER
2	G	18	LEU
2	G	35	HIS
2	G	53	ASN
2	G	83	ARG
3	J	4	MET
3	J	12	SER
3	J	61	TRP
3	J	70	ASP
3	J	77	SER
3	J	86	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	755	GLN
3	L	38	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

44 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1313	1	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	A	1316	1	14,14,15	0.34	0	17,19,21	0.49	0
4	NAG	A	1315	1	14,14,15	1.38	1 (7%)	17,19,21	1.12	1 (5%)
4	NAG	A	1304	1	14,14,15	0.91	2 (14%)	17,19,21	1.30	1 (5%)
4	NAG	C	1313	1	14,14,15	0.51	0	17,19,21	0.54	0
4	NAG	C	1303	1	14,14,15	0.36	0	17,19,21	0.48	0
4	NAG	C	1305	1	14,14,15	3.50	2 (14%)	17,19,21	2.48	3 (17%)
4	NAG	B	1304	-	14,14,15	1.26	2 (14%)	17,19,21	1.26	2 (11%)
4	NAG	C	1315	1	14,14,15	0.61	0	17,19,21	1.94	2 (11%)
4	NAG	B	1312	1	14,14,15	0.83	1 (7%)	17,19,21	0.62	0
4	NAG	C	1304	1	14,14,15	0.40	0	17,19,21	0.48	0
4	NAG	C	1308	1	14,14,15	0.29	0	17,19,21	0.43	0
4	NAG	B	1307	1	14,14,15	0.68	1 (7%)	17,19,21	1.96	2 (11%)
4	NAG	A	1314	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	B	1311	1	14,14,15	0.38	0	17,19,21	0.46	0
4	NAG	C	1301	1	14,14,15	0.33	0	17,19,21	0.48	0
4	NAG	A	1308	1	14,14,15	0.60	0	17,19,21	1.38	2 (11%)
4	NAG	C	1311	1	14,14,15	0.32	0	17,19,21	0.43	0
4	NAG	A	1307	1	14,14,15	0.48	0	17,19,21	0.87	1 (5%)
4	NAG	B	1308	1	14,14,15	0.45	0	17,19,21	0.80	1 (5%)
4	NAG	A	1303	1	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	B	1303	1	14,14,15	0.31	0	17,19,21	0.54	0
4	NAG	B	1313	1	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	C	1310	1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	C	1302	1	14,14,15	0.60	0	17,19,21	0.58	0
4	NAG	C	1314	1	14,14,15	0.30	0	17,19,21	0.46	0
4	NAG	C	1309	1	14,14,15	0.41	0	17,19,21	0.65	1 (5%)
4	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.74	1 (5%)
4	NAG	A	1301	1	14,14,15	0.36	0	17,19,21	0.56	0
4	NAG	B	1306	1	14,14,15	0.46	0	17,19,21	0.84	1 (5%)
4	NAG	B	1305	1	14,14,15	0.58	0	17,19,21	0.78	1 (5%)
4	NAG	B	1301	1	14,14,15	0.39	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1310	1	14,14,15	0.26	0	17,19,21	0.82	1 (5%)
4	NAG	A	1311	1	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	A	1302	1	14,14,15	0.97	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	B	1310	1	14,14,15	0.36	0	17,19,21	0.45	0
4	NAG	A	1309	1	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	B	1302	1	14,14,15	0.39	0	17,19,21	0.40	0
4	NAG	B	1309	1	14,14,15	0.52	0	17,19,21	0.55	0
4	NAG	A	1306	1	14,14,15	0.47	0	17,19,21	0.53	0
4	NAG	A	1305	1	14,14,15	0.27	0	17,19,21	0.53	0
4	NAG	C	1307	1	14,14,15	0.56	0	17,19,21	0.40	0
4	NAG	C	1312	1	14,14,15	0.27	0	17,19,21	0.43	0
4	NAG	A	1312	1	14,14,15	0.41	0	17,19,21	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1315	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1315	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1305	NAG	C1-C2	12.13	1.70	1.52
4	A	1315	NAG	O5-C1	-4.70	1.36	1.43
4	C	1305	NAG	O5-C1	-4.42	1.36	1.43
4	B	1304	NAG	C1-C2	4.12	1.58	1.52
4	A	1302	NAG	C1-C2	3.05	1.56	1.52
4	B	1312	NAG	O5-C1	-2.90	1.39	1.43
4	A	1304	NAG	C1-C2	2.63	1.56	1.52
4	B	1304	NAG	O5-C1	2.09	1.47	1.43
4	A	1304	NAG	O5-C1	2.01	1.46	1.43
4	B	1307	NAG	C1-C2	2.01	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1305	NAG	C2-N2-C7	8.16	134.52	122.90
4	C	1315	NAG	C2-N2-C7	6.88	132.69	122.90
4	B	1307	NAG	C2-N2-C7	6.87	132.69	122.90
4	A	1304	NAG	C1-O5-C5	4.90	118.83	112.19
4	A	1308	NAG	C1-O5-C5	4.41	118.16	112.19
4	C	1305	NAG	C1-C2-N2	4.00	117.31	110.49
4	B	1304	NAG	C1-O5-C5	3.59	117.06	112.19
4	A	1315	NAG	C3-C4-C5	3.20	115.95	110.24
4	B	1307	NAG	C1-C2-N2	3.12	115.81	110.49
4	C	1315	NAG	C1-C2-N2	3.10	115.78	110.49
4	A	1302	NAG	C1-O5-C5	2.80	115.99	112.19
4	B	1304	NAG	C2-N2-C7	2.65	126.68	122.90
4	A	1308	NAG	C1-C2-N2	2.54	114.82	110.49
4	A	1310	NAG	C2-N2-C7	2.50	126.46	122.90
4	C	1306	NAG	C1-O5-C5	2.43	115.49	112.19
4	B	1308	NAG	C2-N2-C7	2.43	126.36	122.90
4	B	1306	NAG	C2-N2-C7	2.38	126.30	122.90
4	A	1307	NAG	C2-N2-C7	2.38	126.29	122.90
4	B	1305	NAG	C2-N2-C7	2.35	126.25	122.90
4	C	1305	NAG	O3-C3-C2	-2.24	104.83	109.47
4	C	1309	NAG	C1-O5-C5	2.14	115.09	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1315	NAG	C1

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1312	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	A	1309	NAG	C8-C7-N2-C2
4	A	1309	NAG	O7-C7-N2-C2
4	A	1314	NAG	C8-C7-N2-C2
4	A	1314	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	B	1307	NAG	C8-C7-N2-C2
4	B	1307	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	1312	NAG	C8-C7-N2-C2
4	B	1312	NAG	O7-C7-N2-C2
4	B	1313	NAG	C8-C7-N2-C2
4	B	1313	NAG	O7-C7-N2-C2
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	C	1313	NAG	C8-C7-N2-C2
4	C	1313	NAG	O7-C7-N2-C2
4	C	1315	NAG	C8-C7-N2-C2
4	C	1315	NAG	O7-C7-N2-C2
4	B	1312	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	C	1313	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	C	1314	NAG	C4-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	B	1313	NAG	O5-C5-C6-O6
4	A	1313	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1313	NAG	C4-C5-C6-O6
4	C	1315	NAG	O5-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	C	1311	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	C	1312	NAG	O5-C5-C6-O6
4	C	1314	NAG	O5-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	A	1302	NAG	C1-C2-N2-C7
4	A	1307	NAG	C3-C2-N2-C7
4	B	1304	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	B	1305	NAG	C3-C2-N2-C7
4	B	1306	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	C	1305	NAG	C1-C2-N2-C7
4	A	1308	NAG	C3-C2-N2-C7
4	A	1310	NAG	C3-C2-N2-C7
4	B	1308	NAG	C3-C2-N2-C7
4	C	1315	NAG	C3-C2-N2-C7

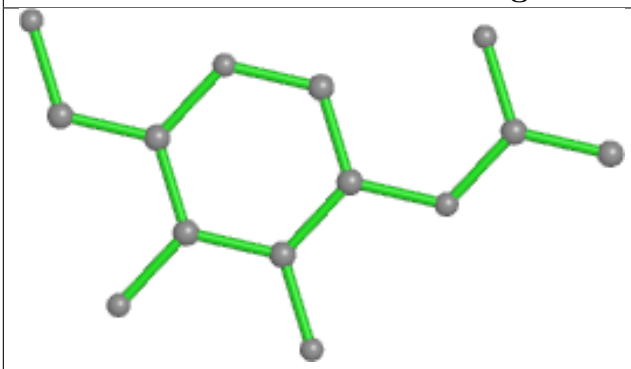
There are no ring outliers.

11 monomers are involved in 17 short contacts:

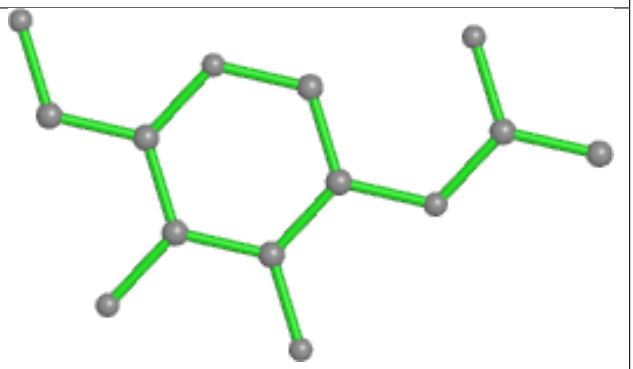
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1313	NAG	1	0
4	C	1305	NAG	1	0
4	B	1304	NAG	7	0
4	B	1312	NAG	1	0
4	C	1304	NAG	1	0
4	A	1308	NAG	1	0
4	A	1307	NAG	1	0
4	B	1305	NAG	1	0
4	A	1302	NAG	1	0
4	A	1306	NAG	1	0
4	A	1312	NAG	1	0

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

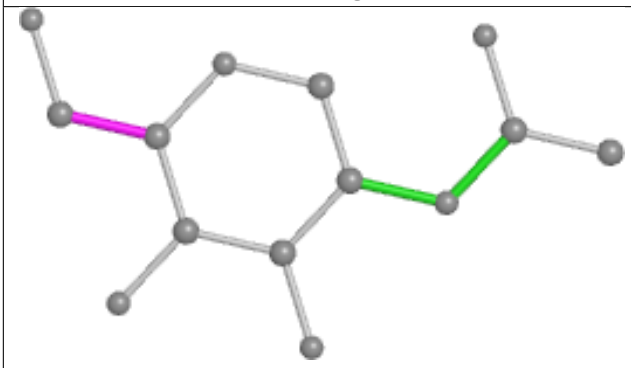
Ligand NAG A 1313



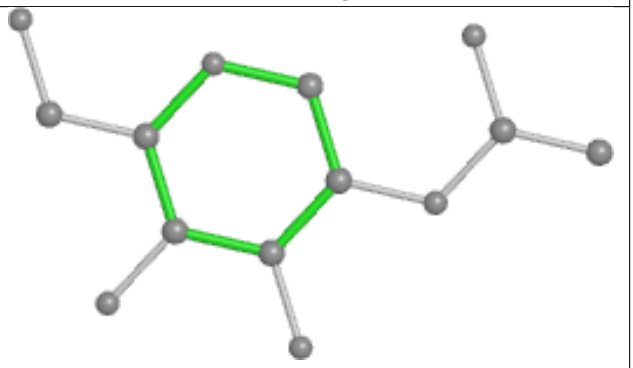
Bond lengths



Bond angles

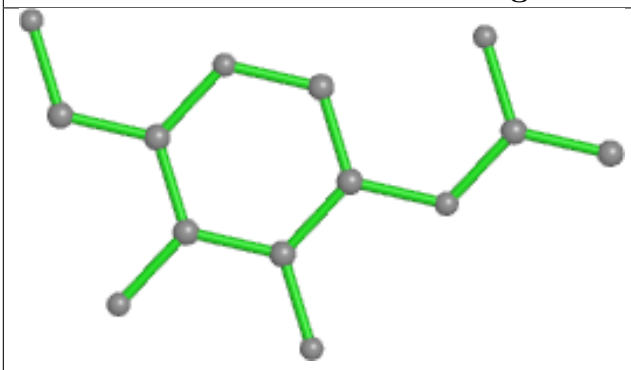


Torsions

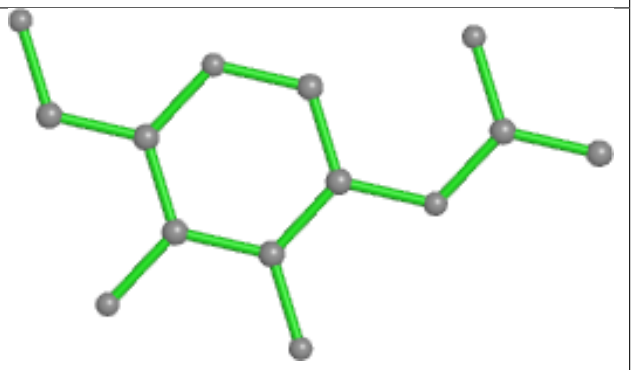


Rings

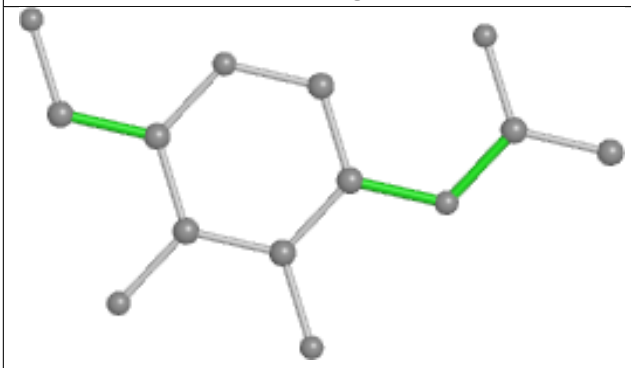
Ligand NAG A 1316



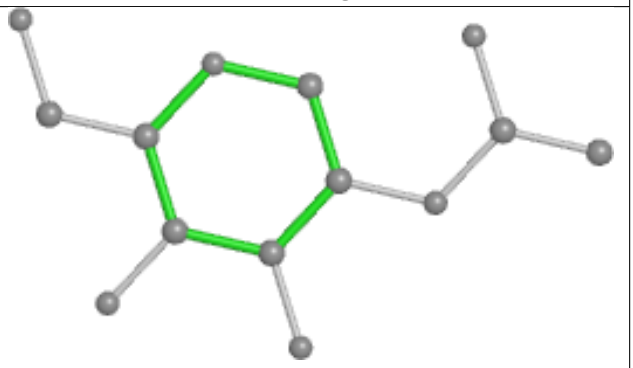
Bond lengths



Bond angles

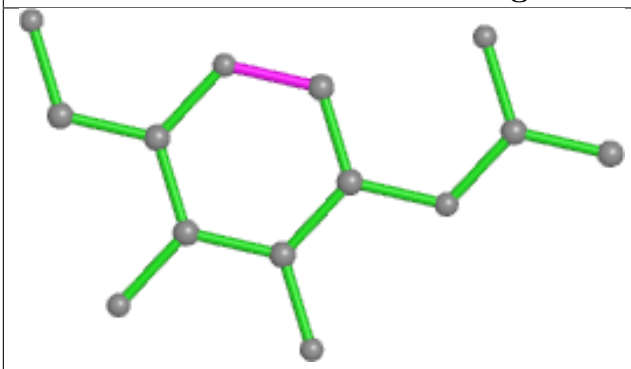


Torsions

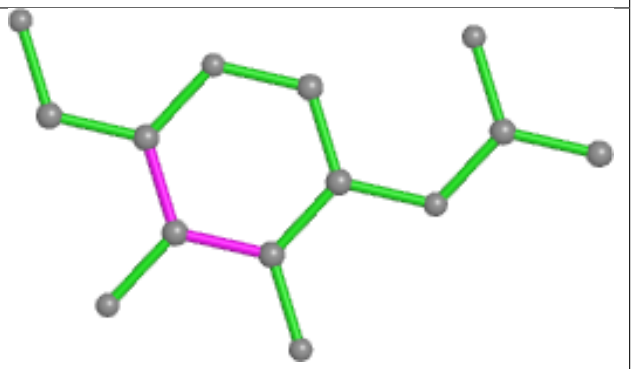


Rings

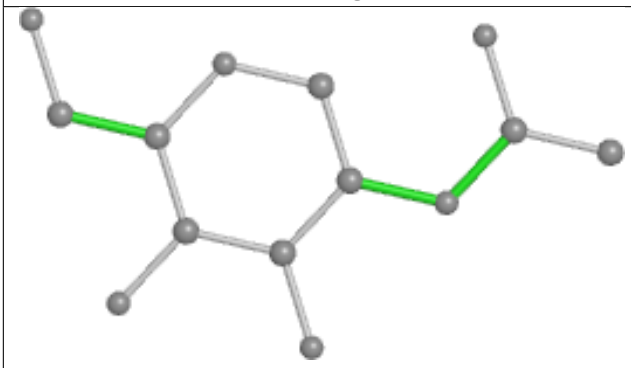
Ligand NAG A 1315



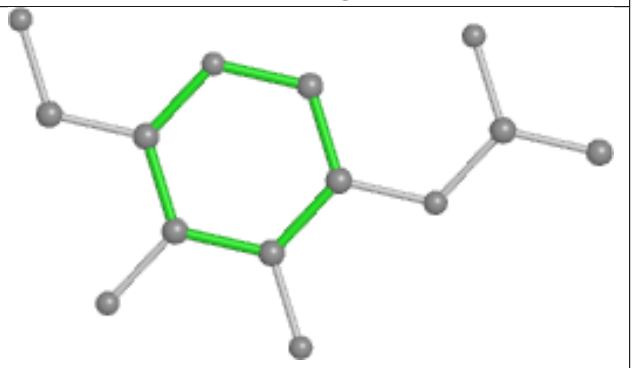
Bond lengths



Bond angles

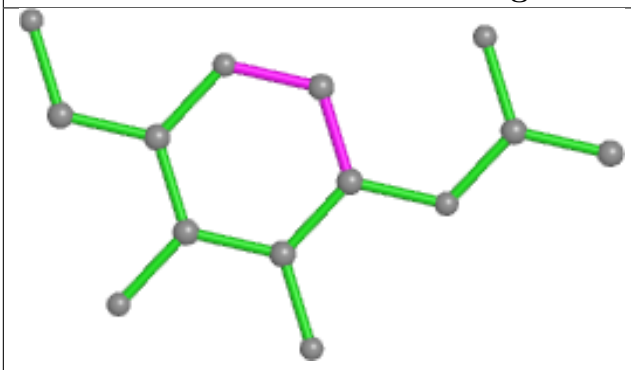


Torsions

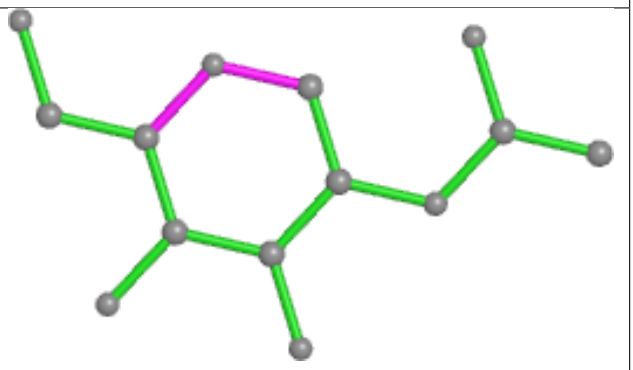


Rings

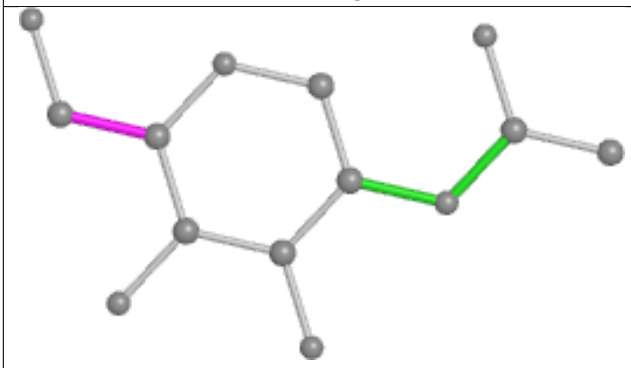
Ligand NAG A 1304



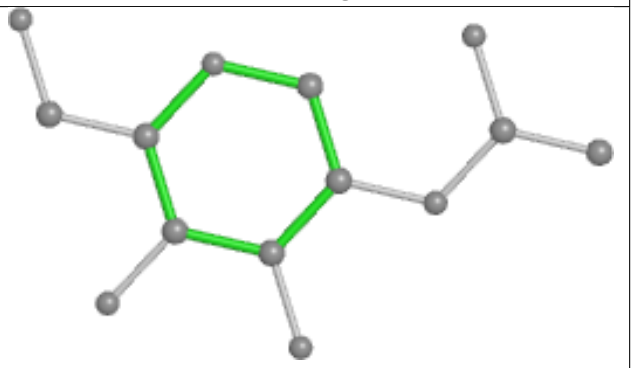
Bond lengths



Bond angles

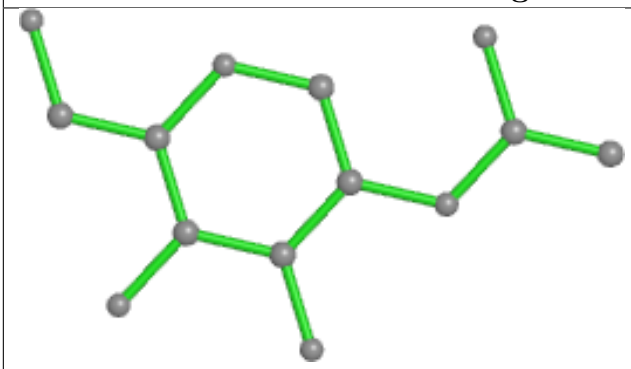


Torsions

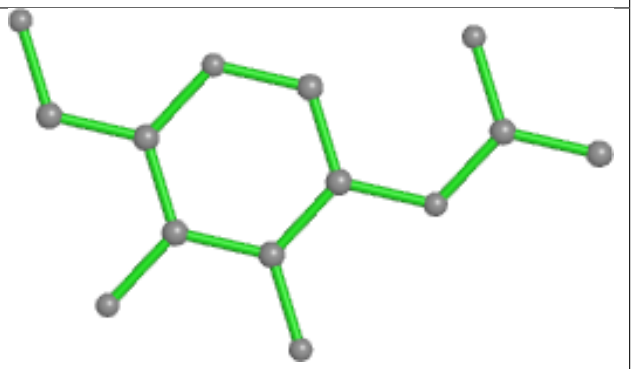


Rings

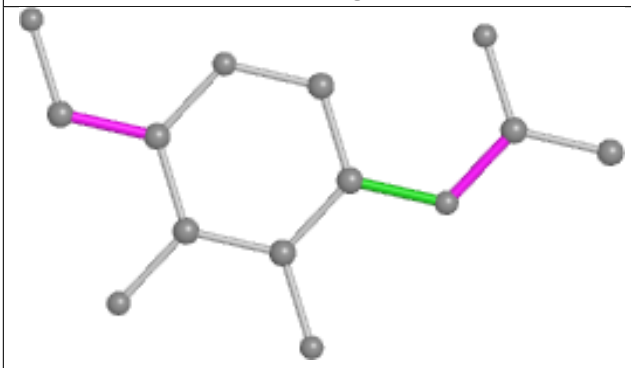
Ligand NAG C 1313



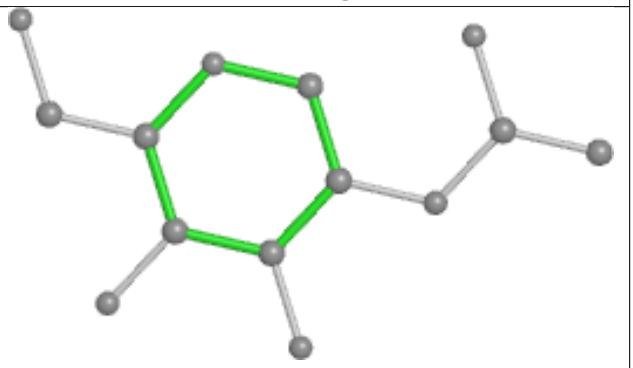
Bond lengths



Bond angles

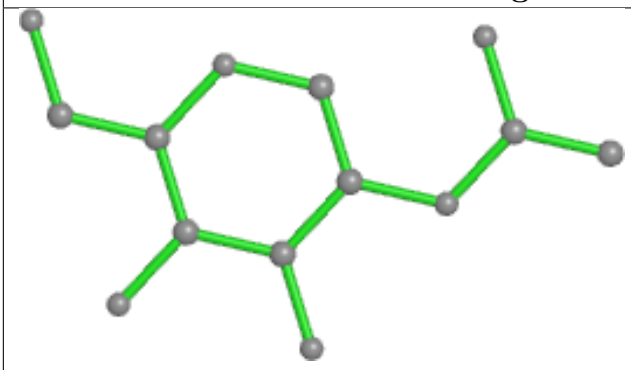


Torsions

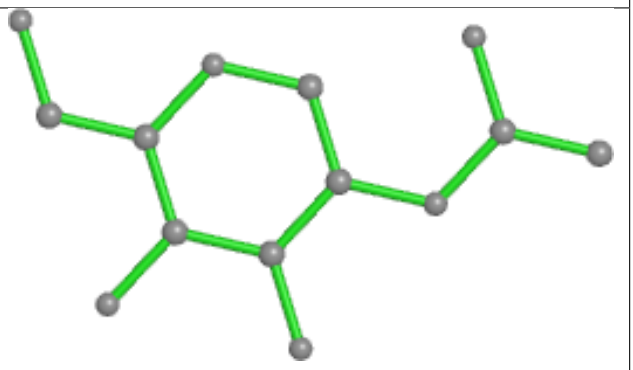


Rings

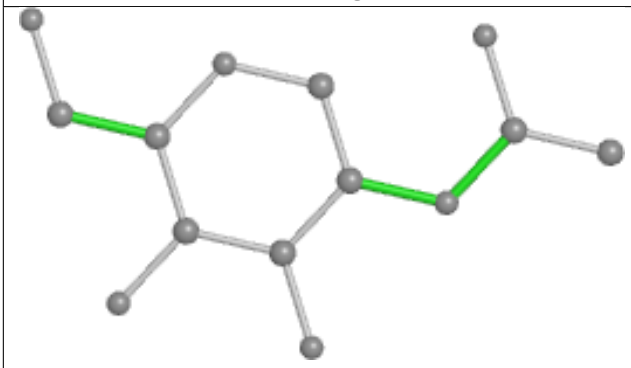
Ligand NAG C 1303



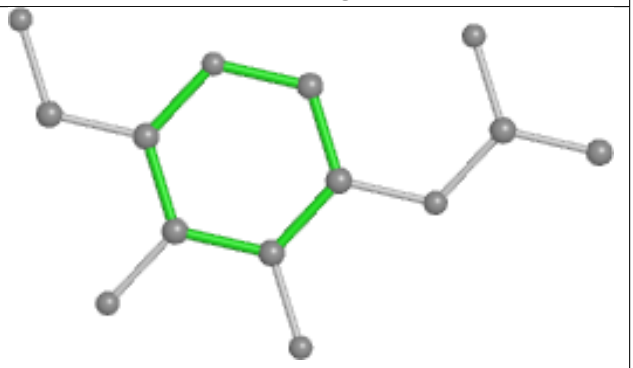
Bond lengths



Bond angles

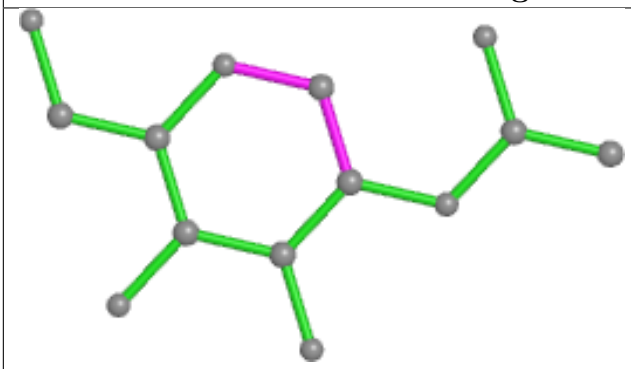


Torsions



Rings

Ligand NAG C 1305



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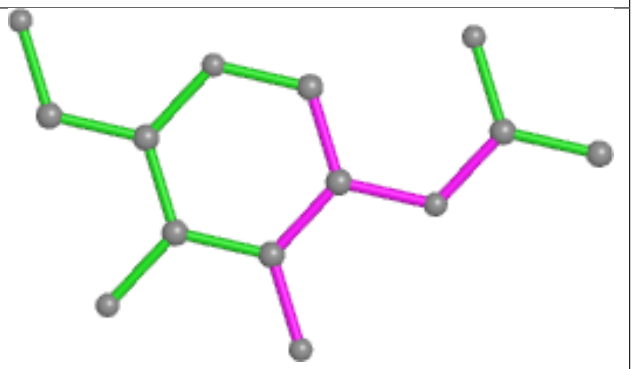
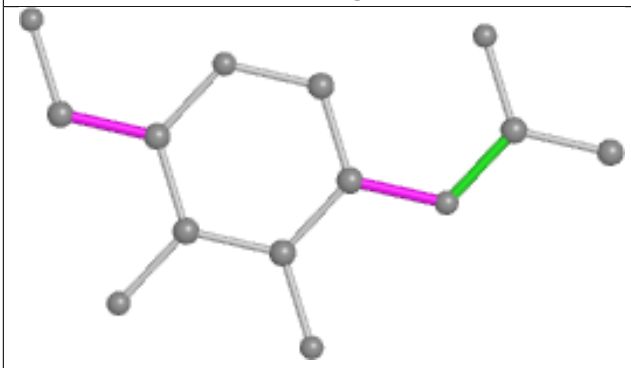
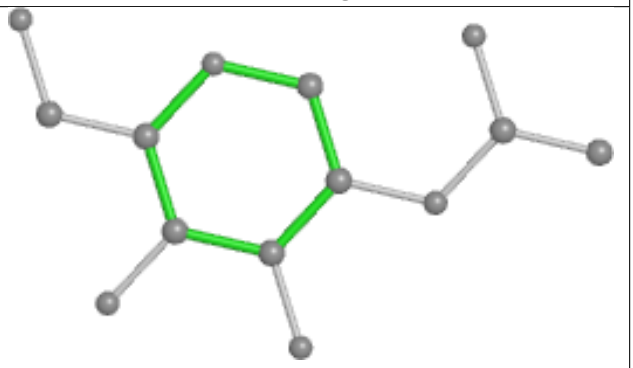


Bond angles

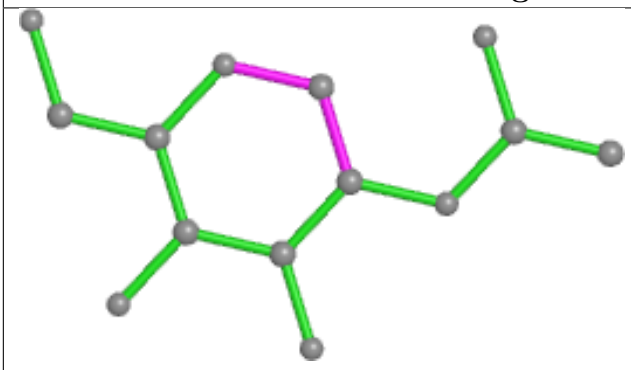


Torsions



Rings

Ligand NAG B 1304



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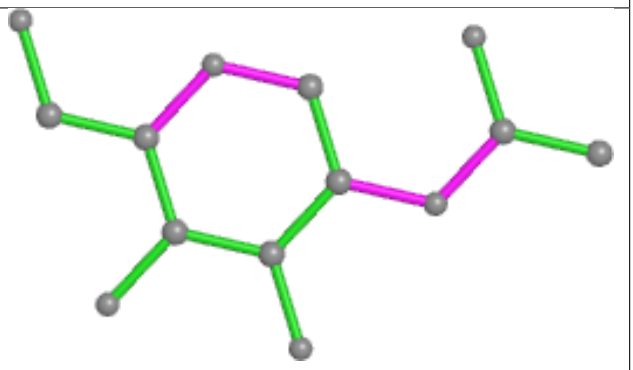
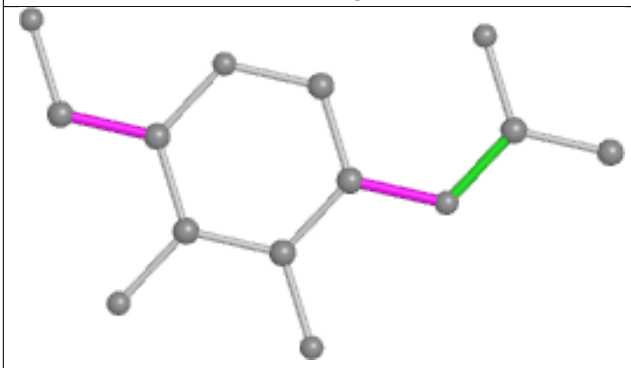


Bond angles



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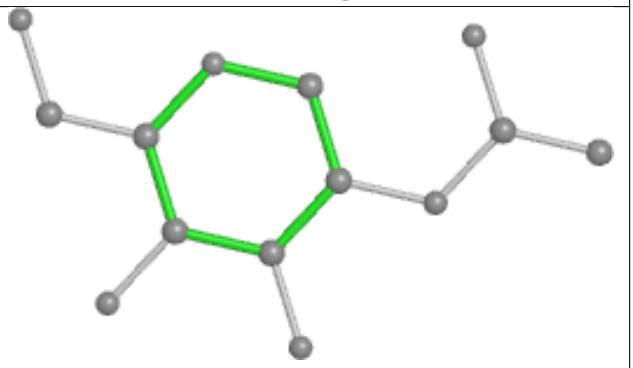
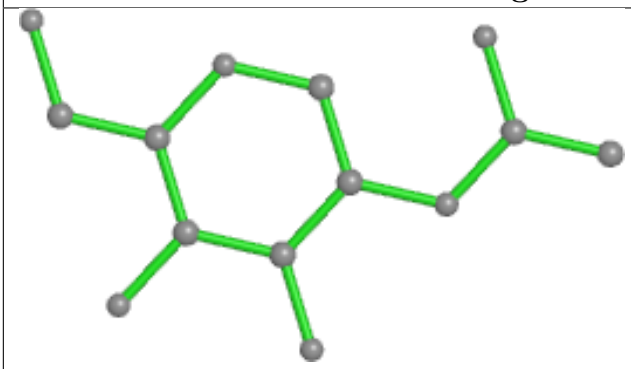


Rings

Ligand NAG C 1315



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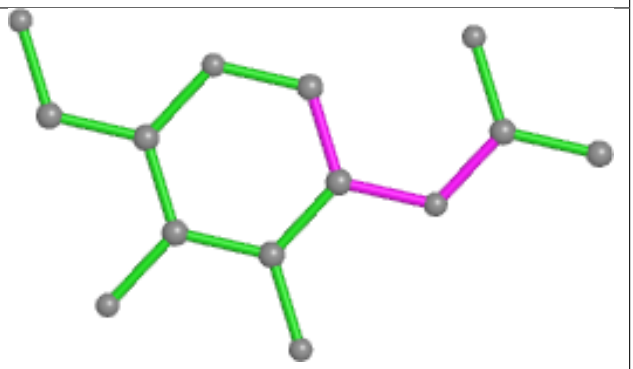
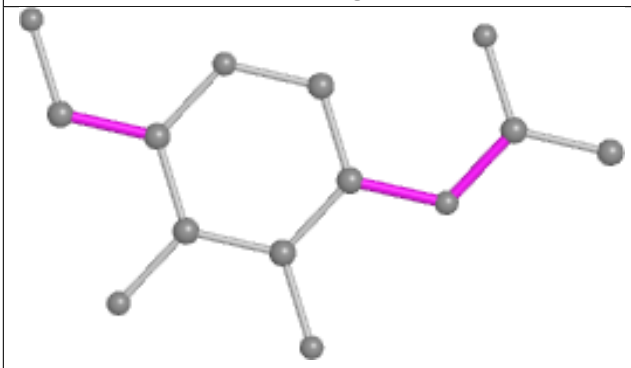


Bond angles



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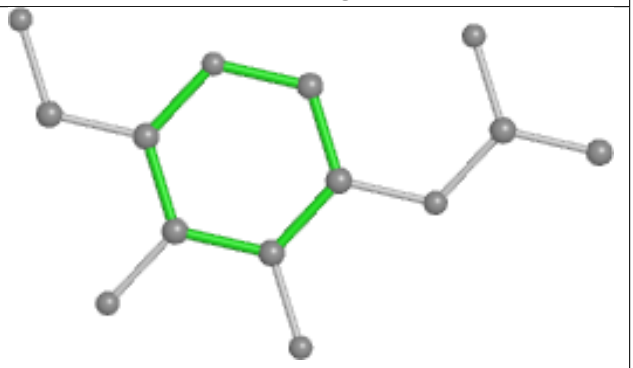
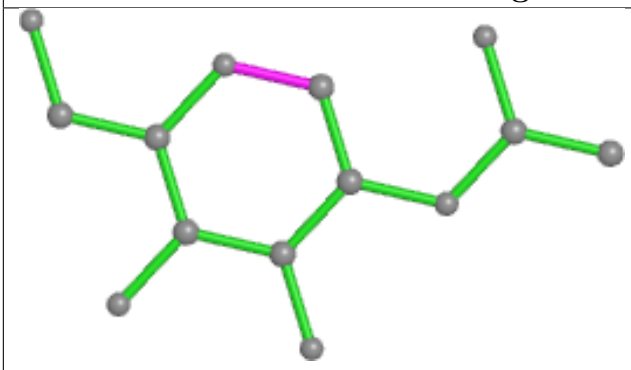


Rings

Ligand NAG B 1312



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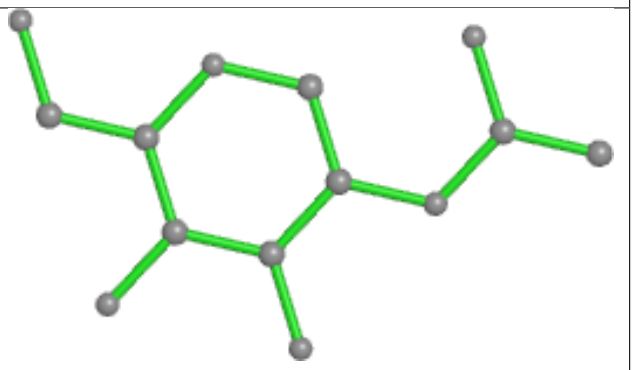
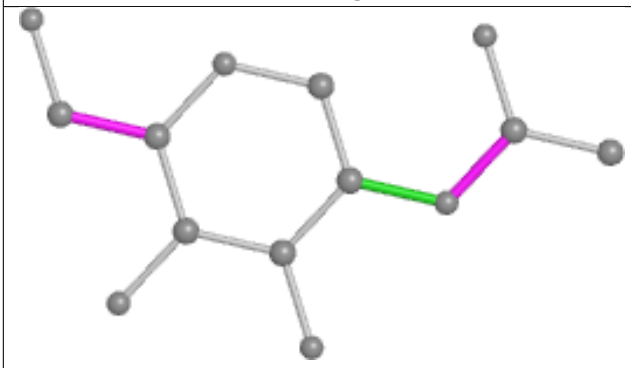


Bond angles



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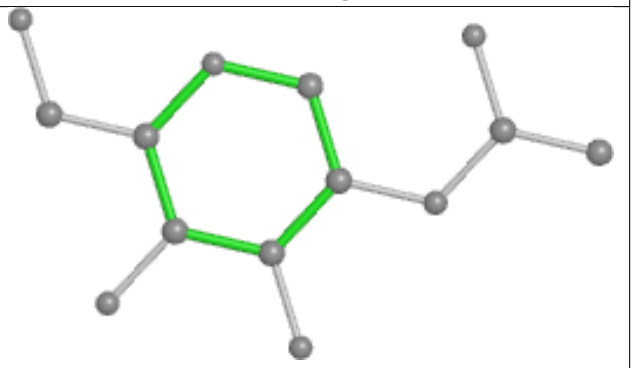
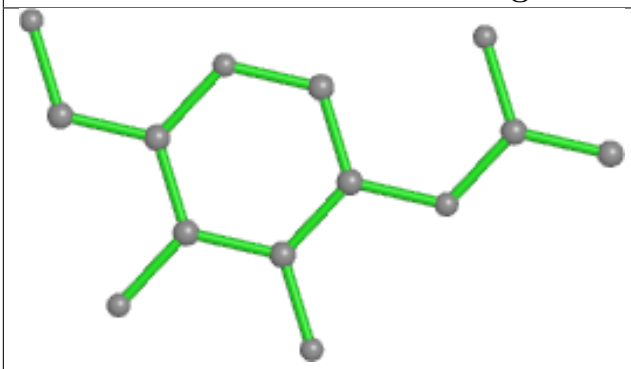


Rings

Ligand NAG C 1304



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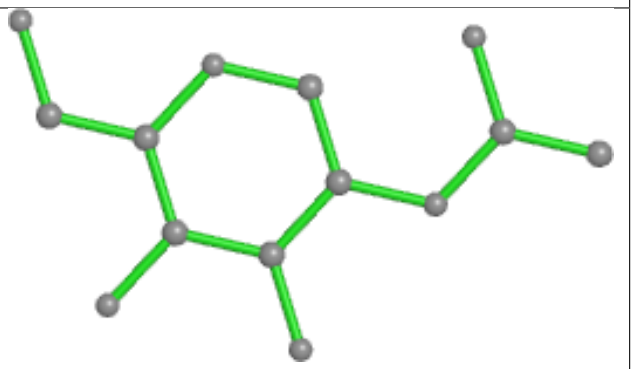

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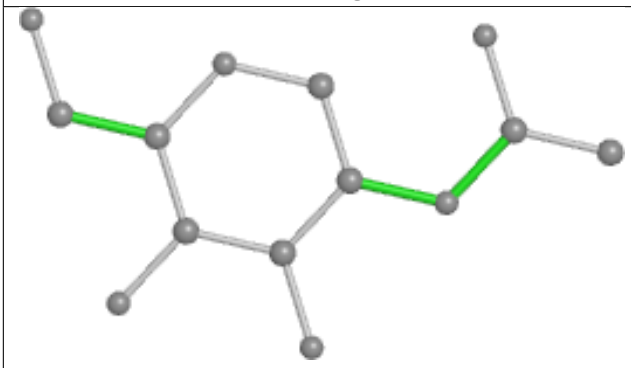

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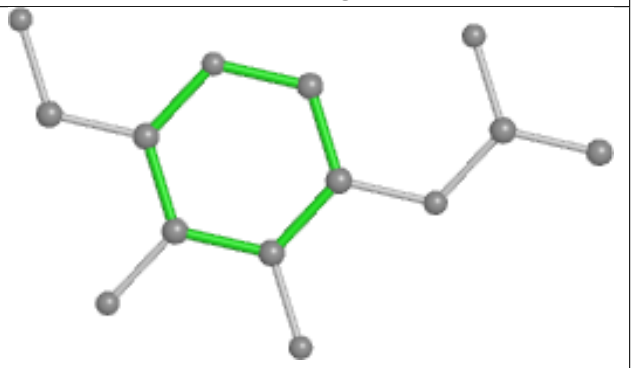
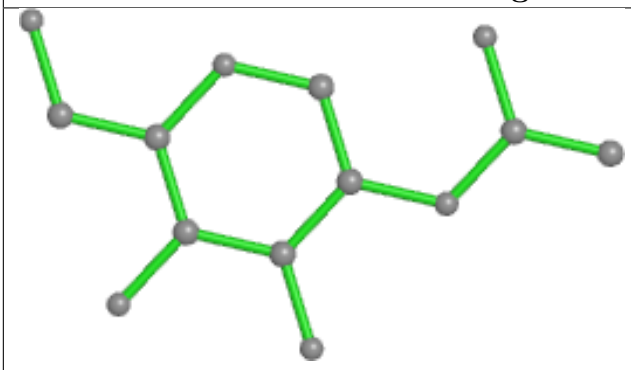


Rings

Ligand NAG C 1308



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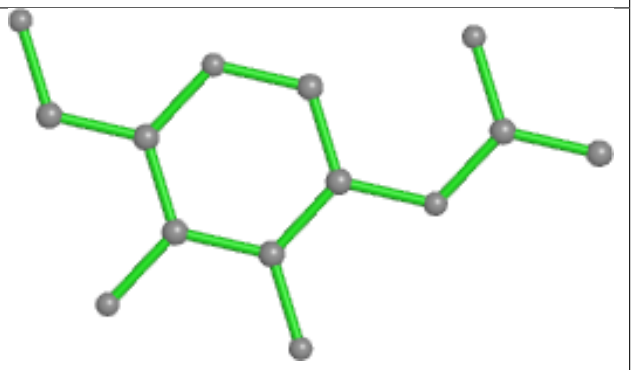
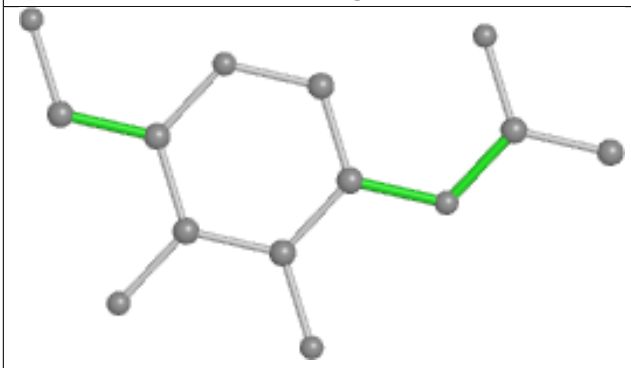


Bond angles



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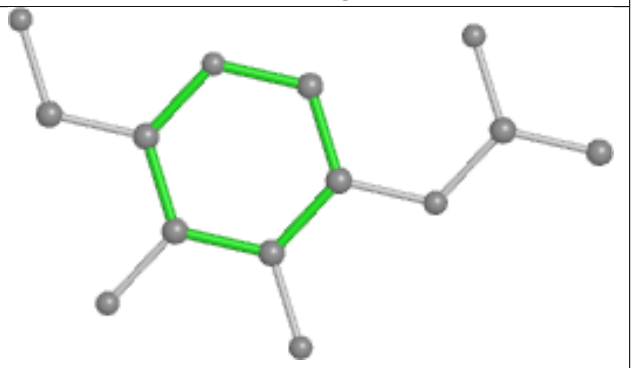
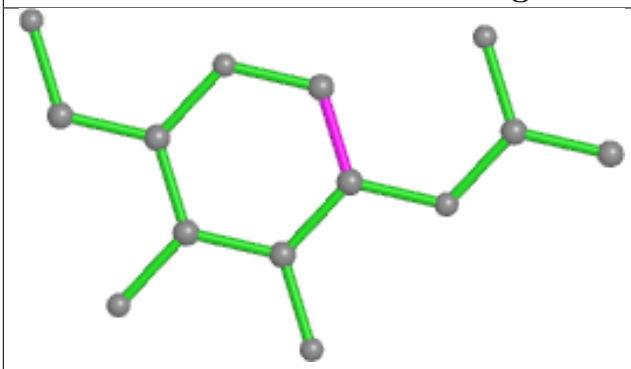


Rings

Ligand NAG B 1307



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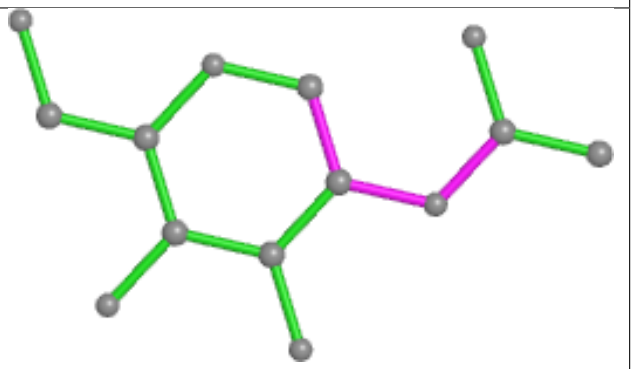
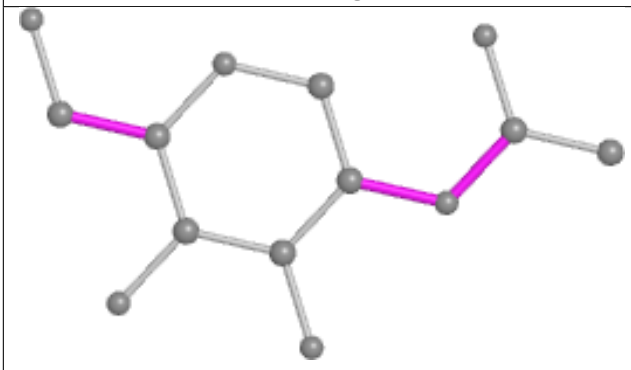


Bond angles



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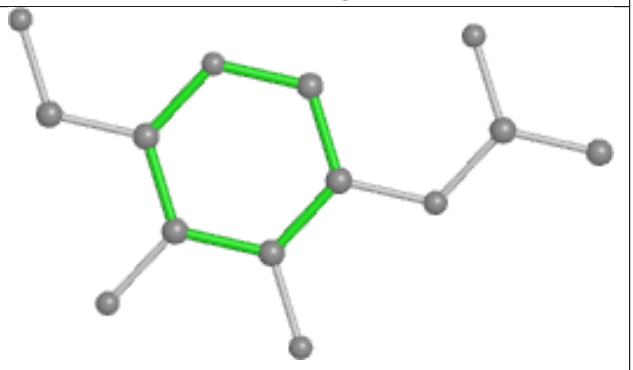
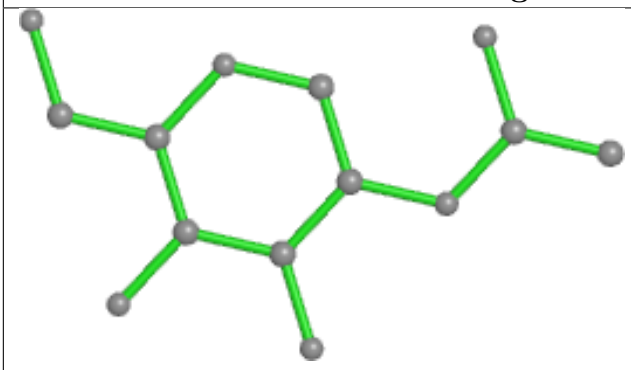
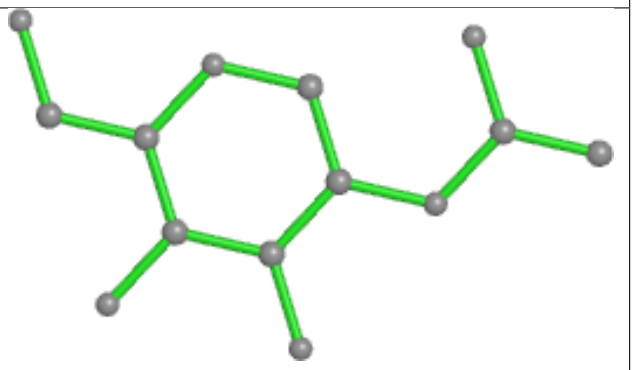


Rings

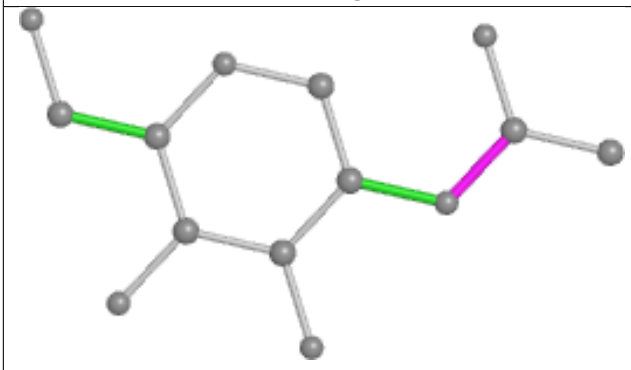
Ligand NAG A 1314



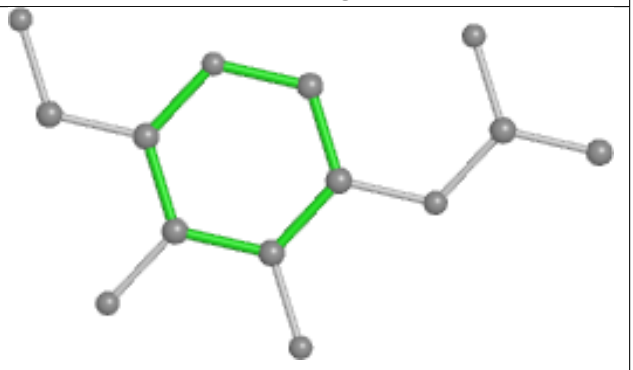
Bond lengths



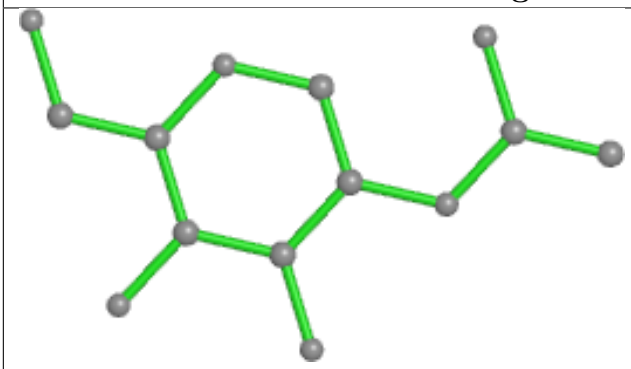
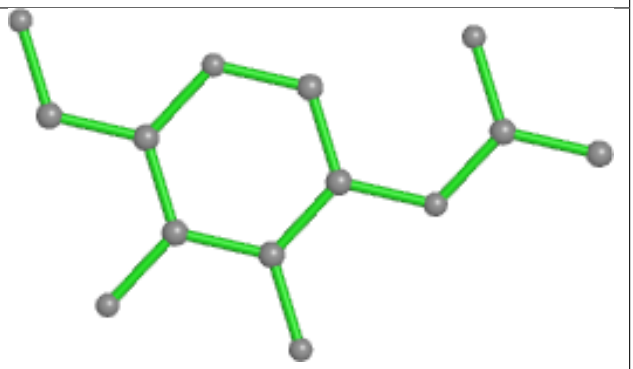
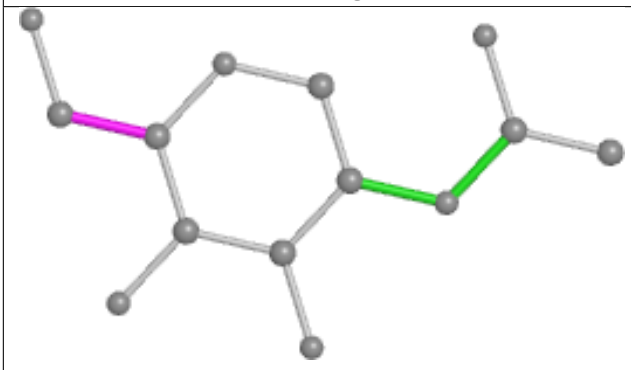
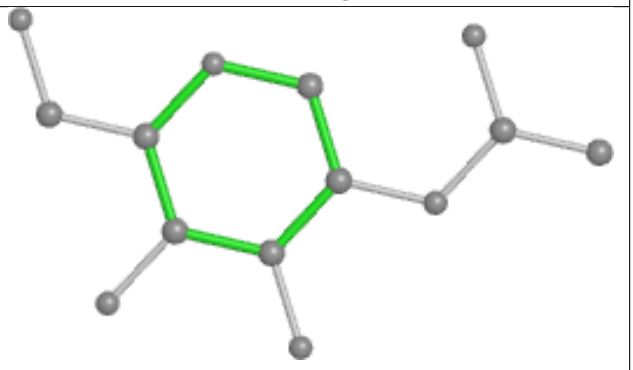
Bond angles

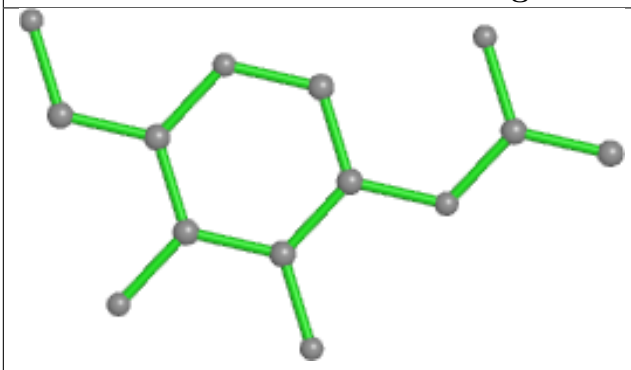
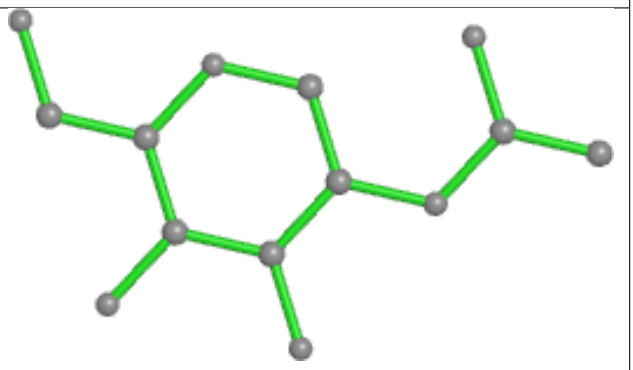
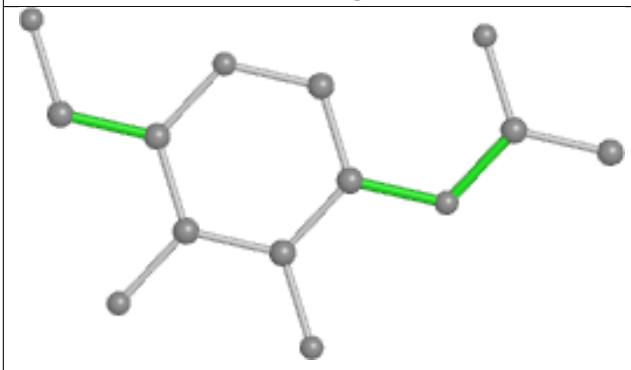
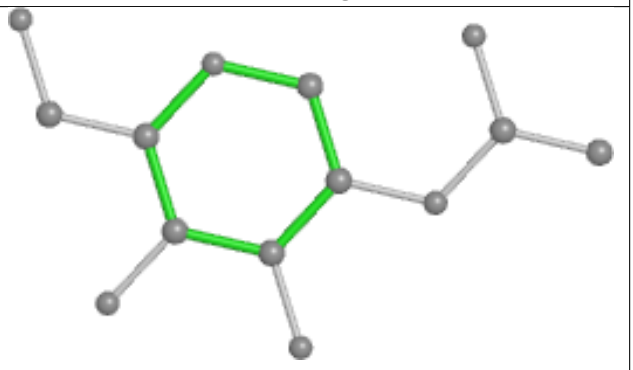


Torsions

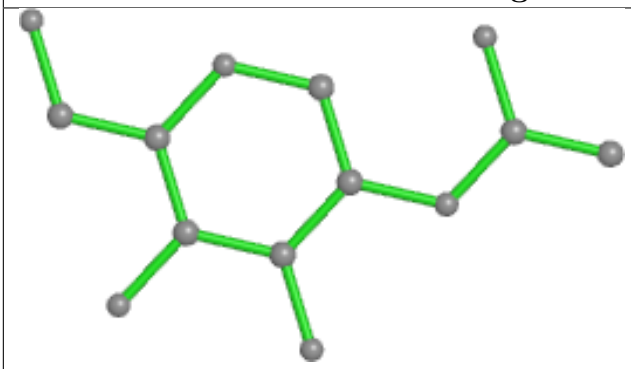


Rings

Ligand NAG B 1311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1308



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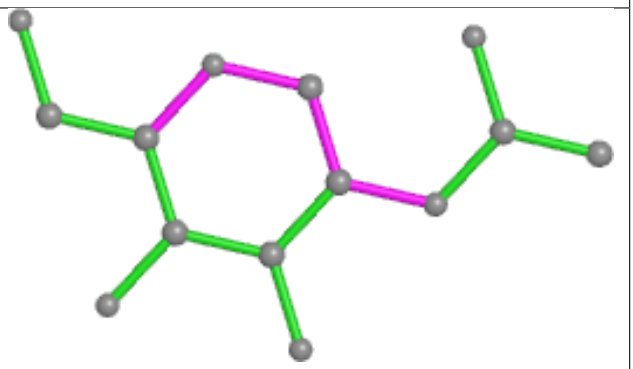
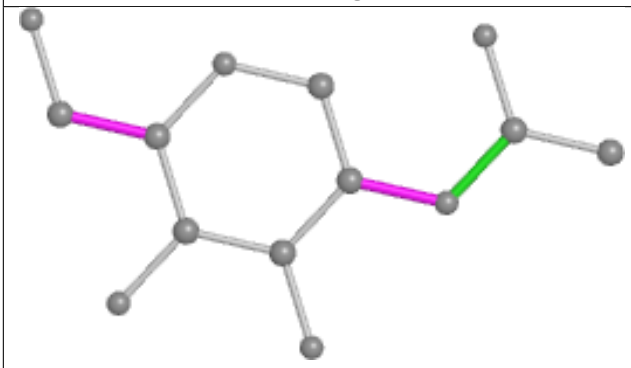
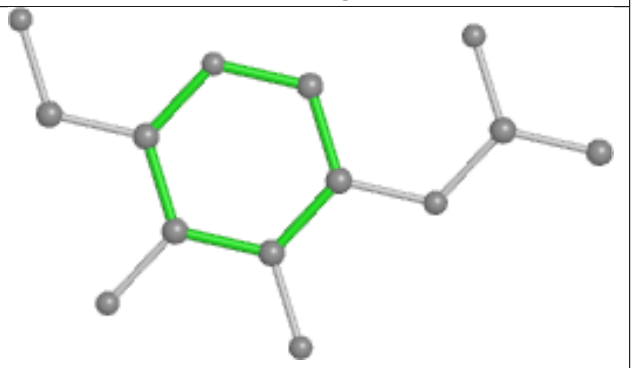


Bond angles

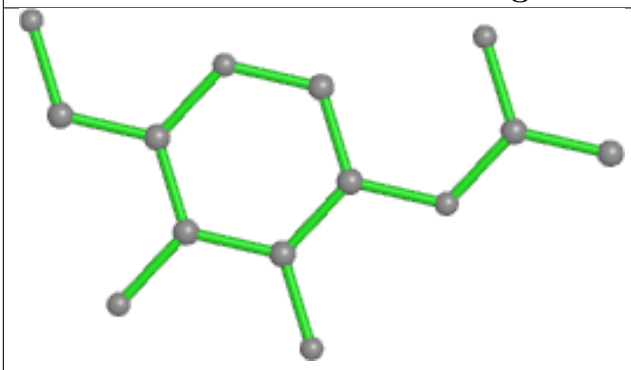


Torsions



Rings

Ligand NAG C 1311



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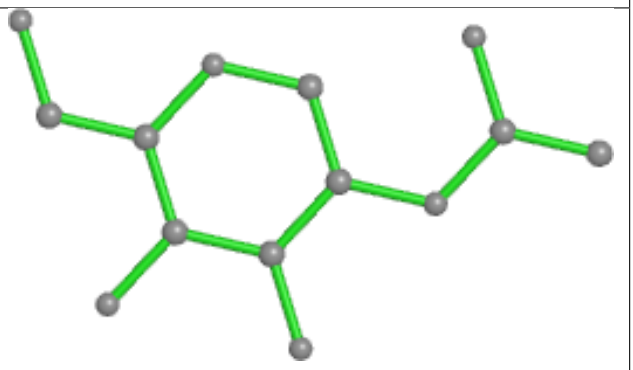
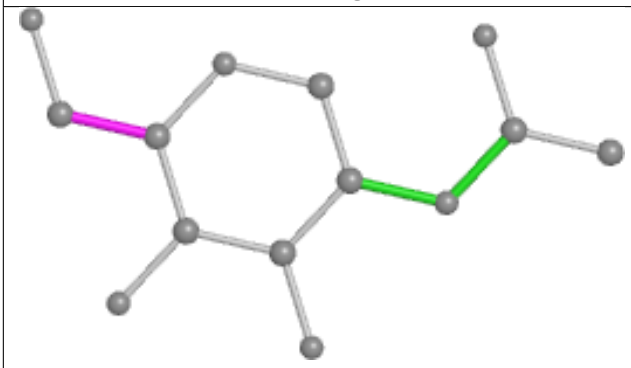
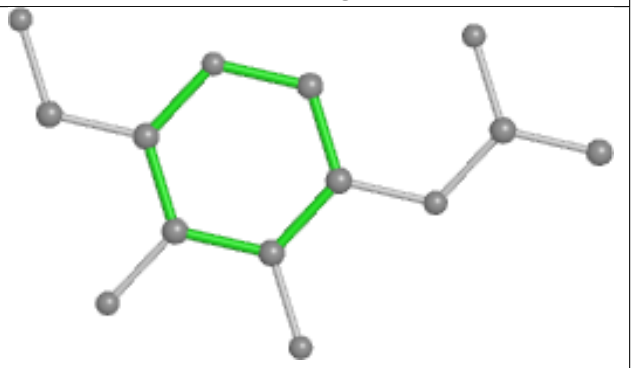


Bond angles

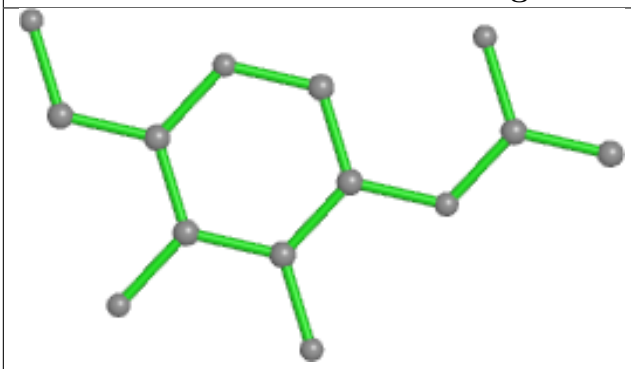


Torsions



Rings

Ligand NAG A 1307



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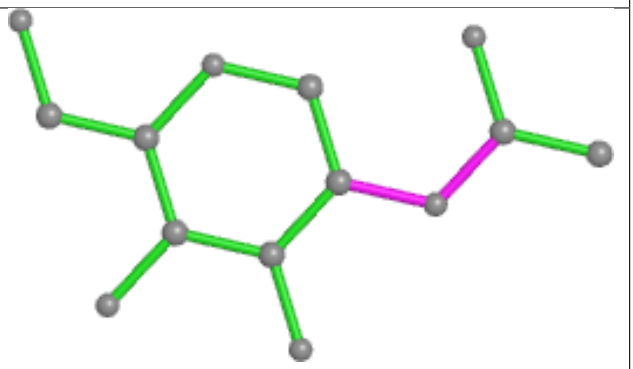
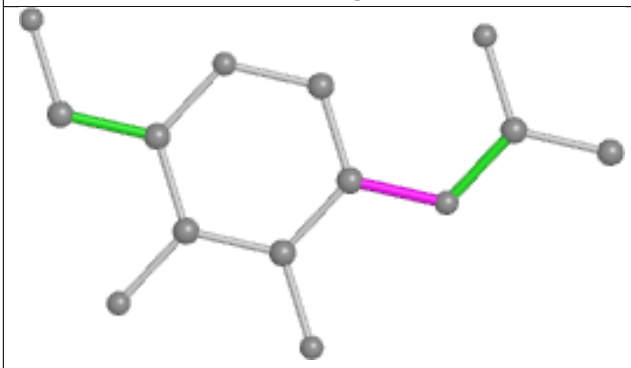
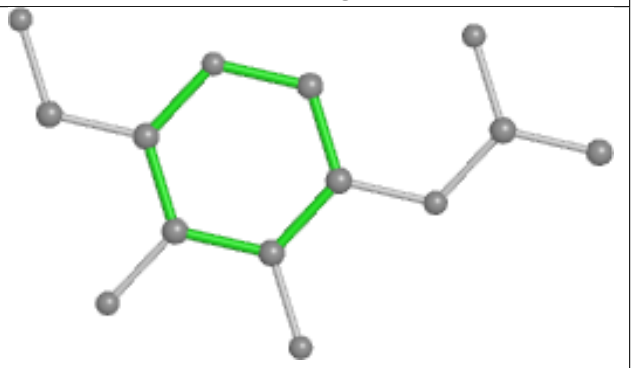


Bond angles

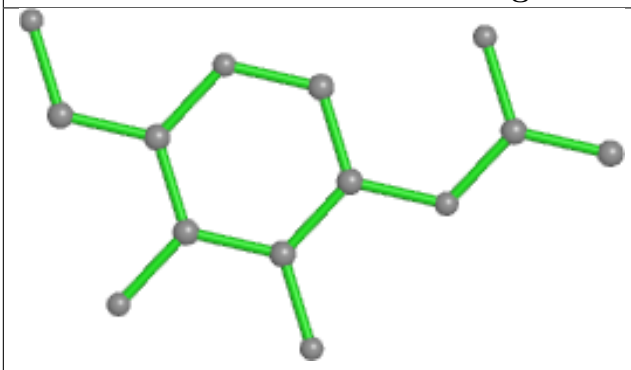


Torsions

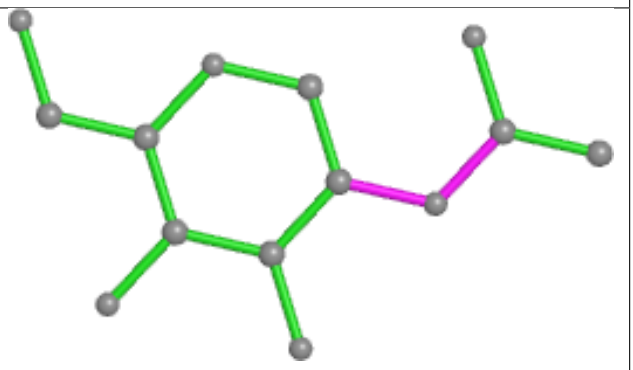


Rings

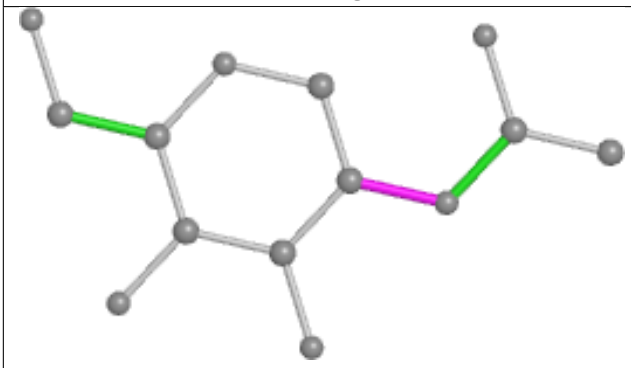
Ligand NAG B 1308



Bond lengths



Bond angles



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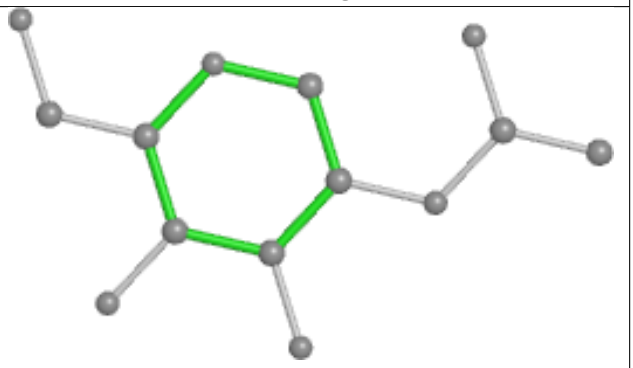
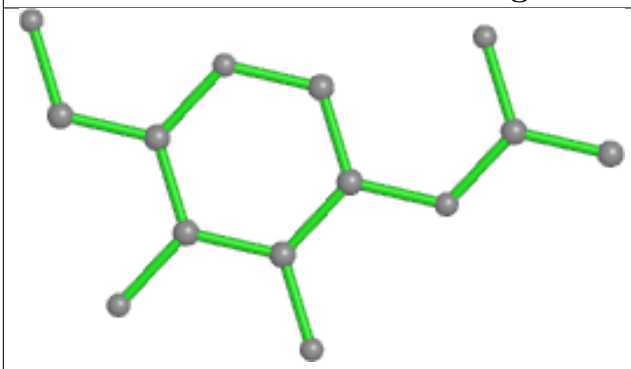
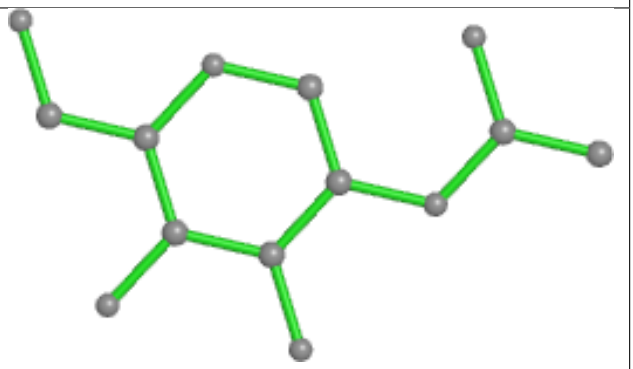


Rings

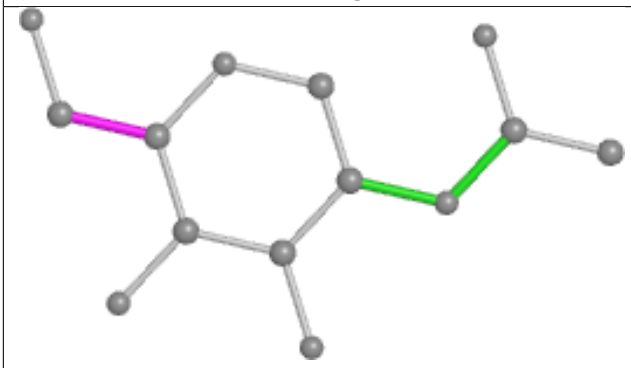
Ligand NAG A 1303



Bond lengths



Bond angles



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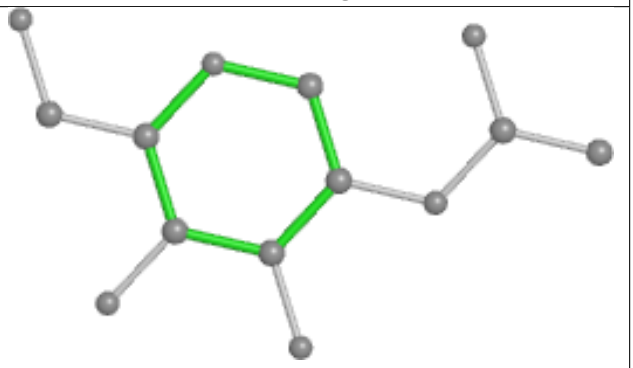
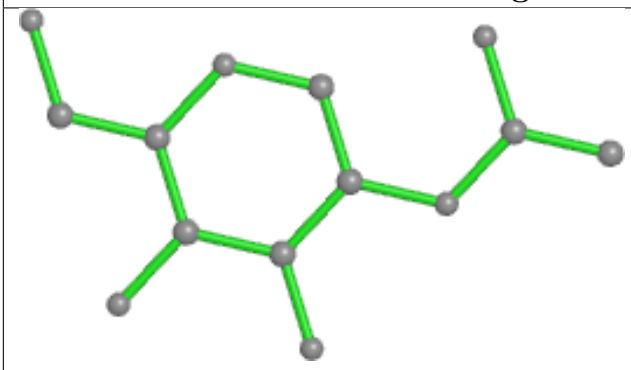


Rings

Ligand NAG B 1303



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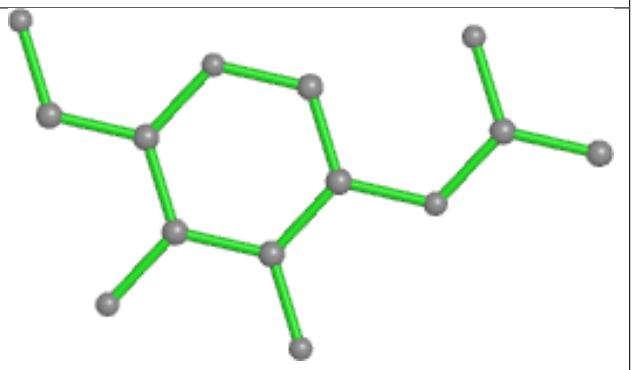
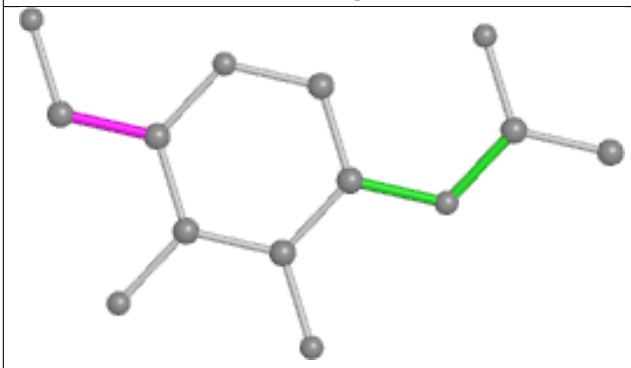


Bond angles



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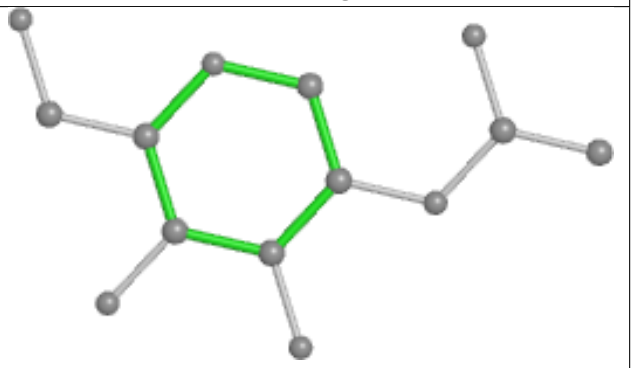
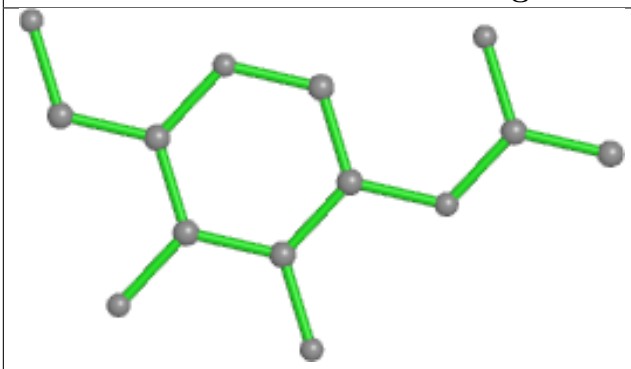
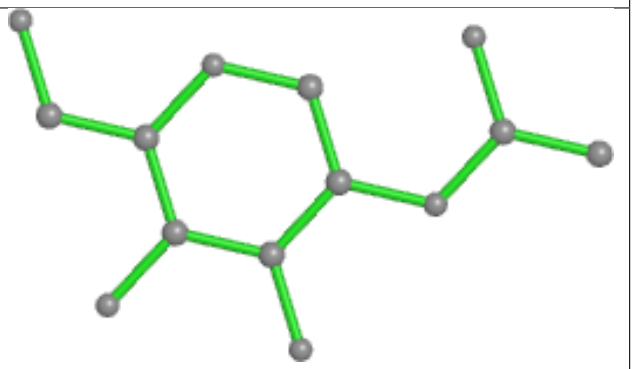


Rings

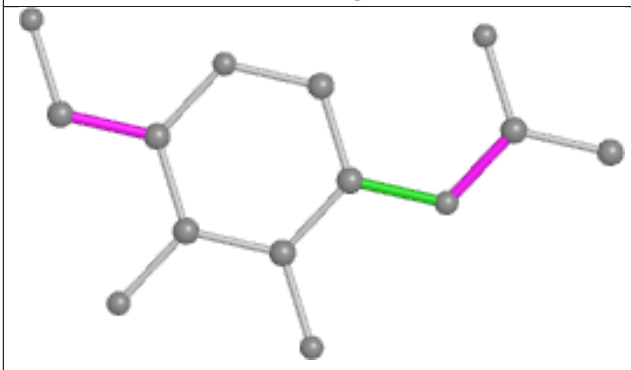
Ligand NAG B 1313



Bond lengths



Bond angles



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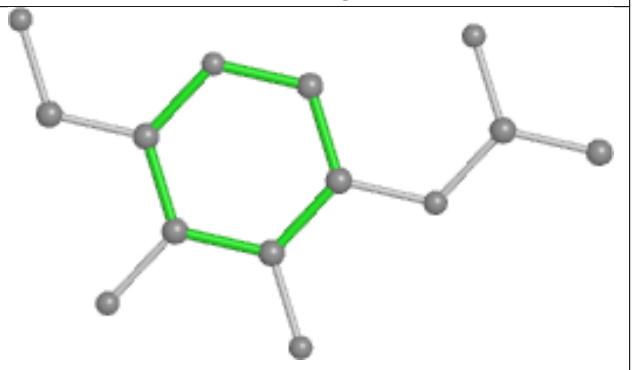
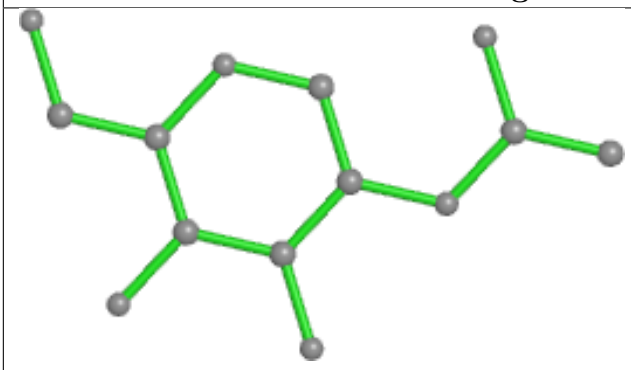


Rings

Ligand NAG C 1310



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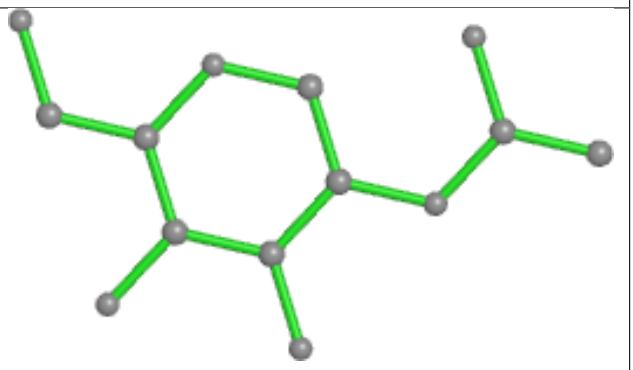
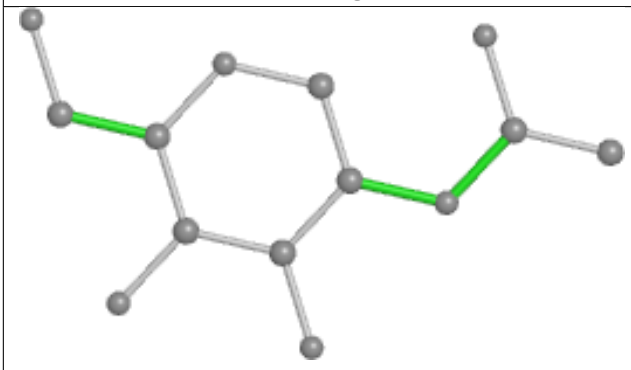


Bond angles



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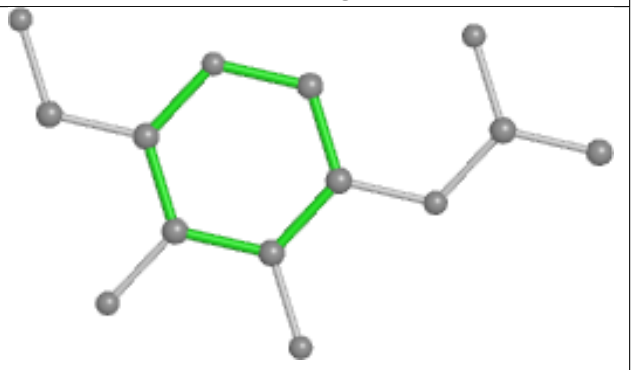
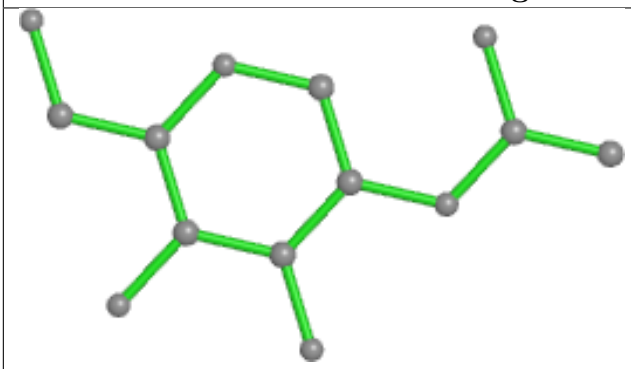


Rings

Ligand NAG C 1302



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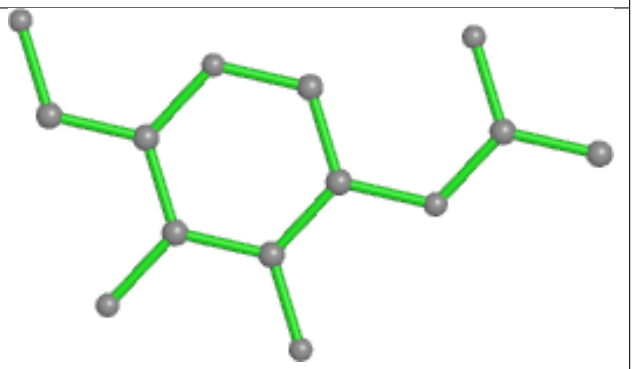

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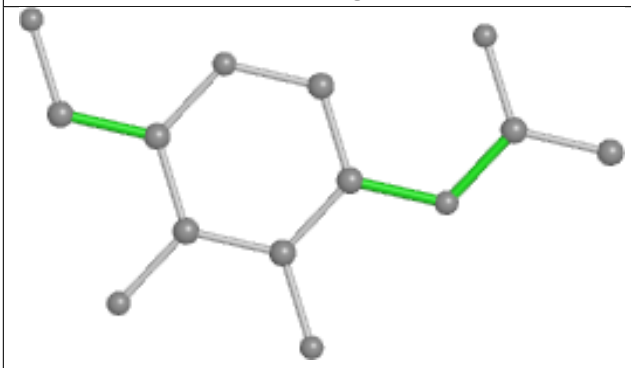

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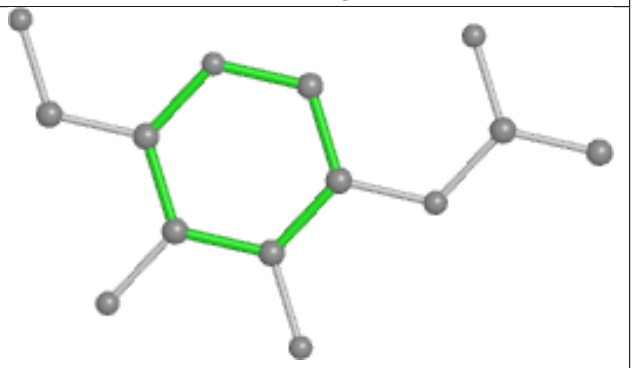
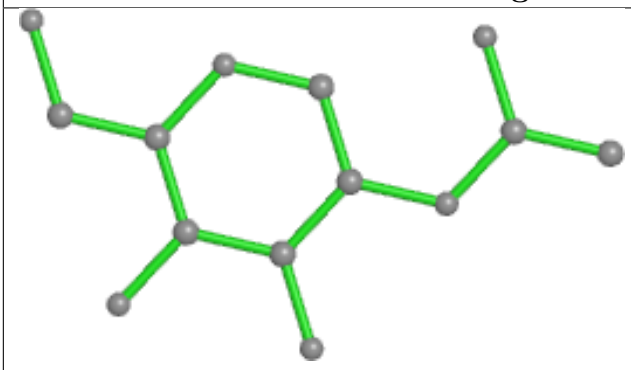


Rings

Ligand NAG C 1314



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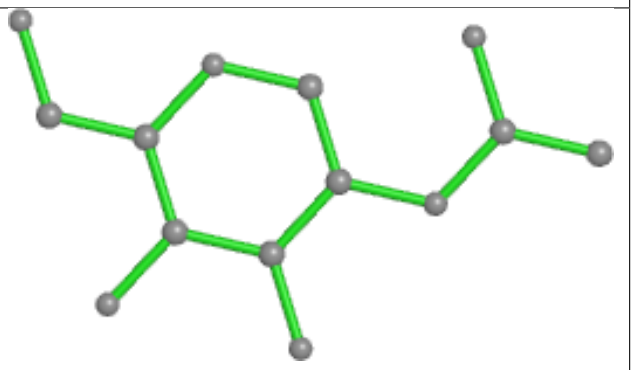
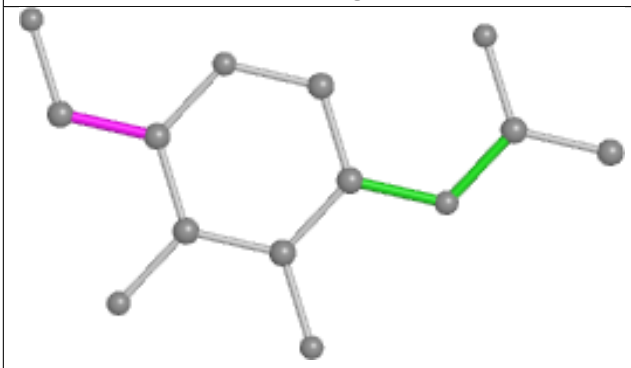


Bond angles



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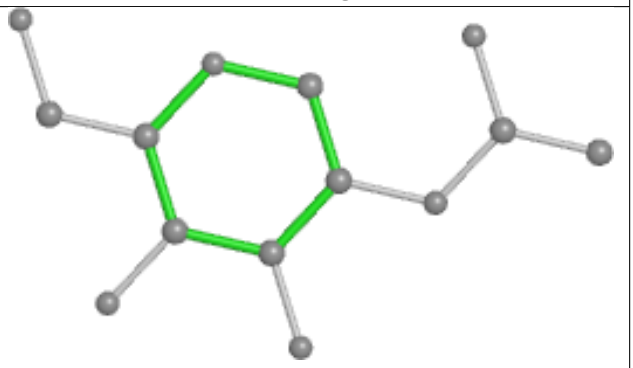
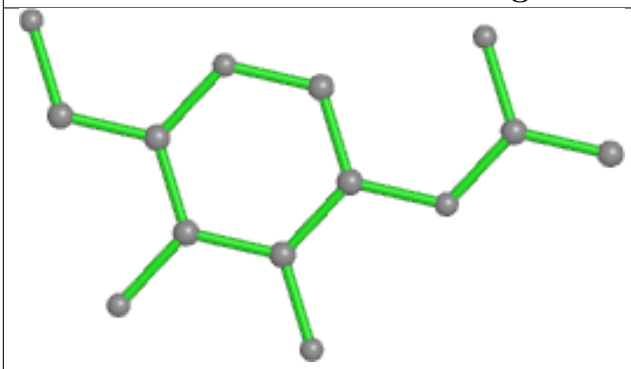


Rings

Ligand NAG C 1309



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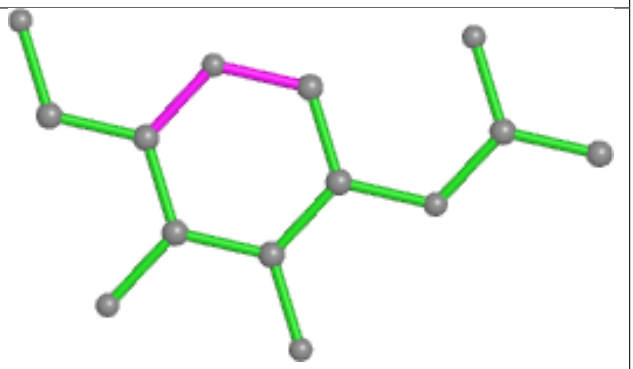
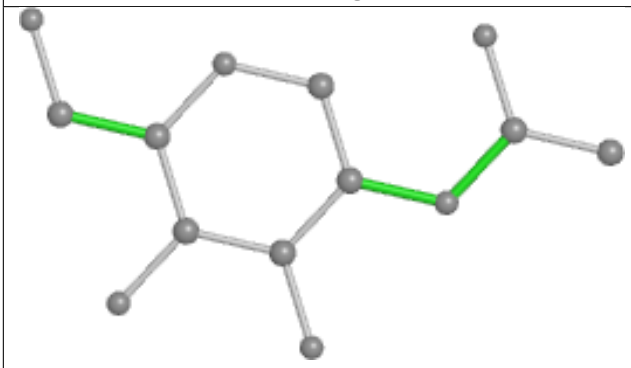


Bond angles



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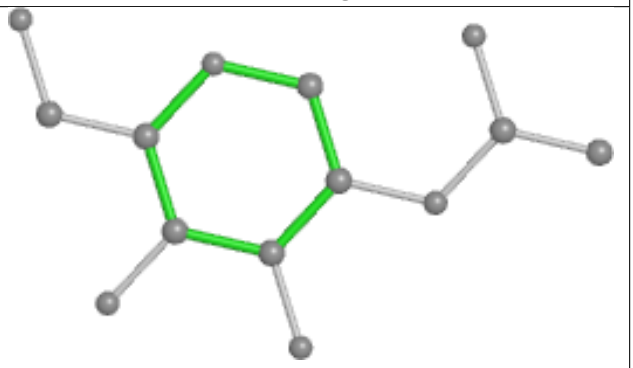
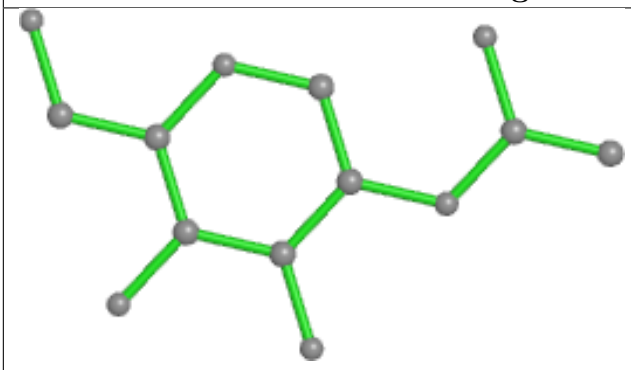


Rings

Ligand NAG C 1306



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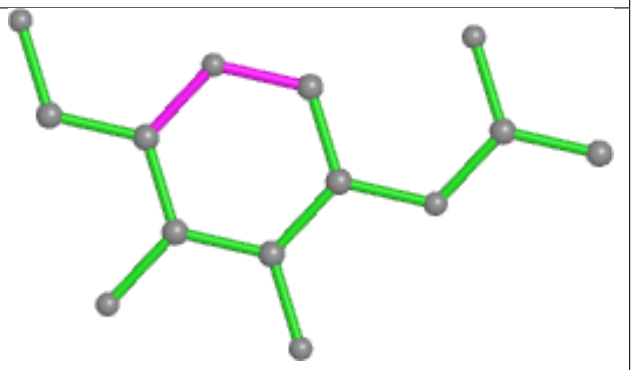
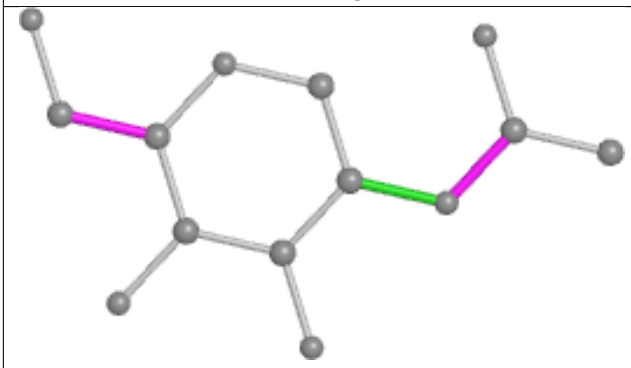


Bond angles



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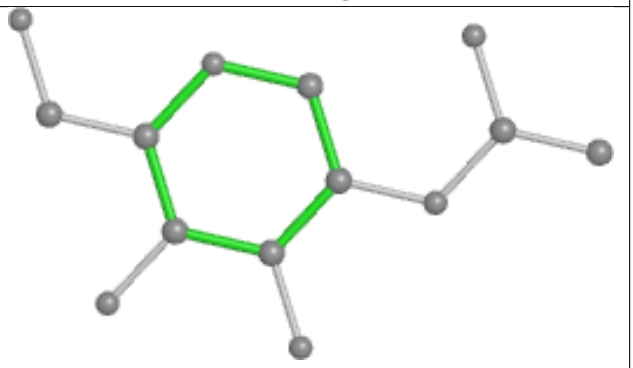
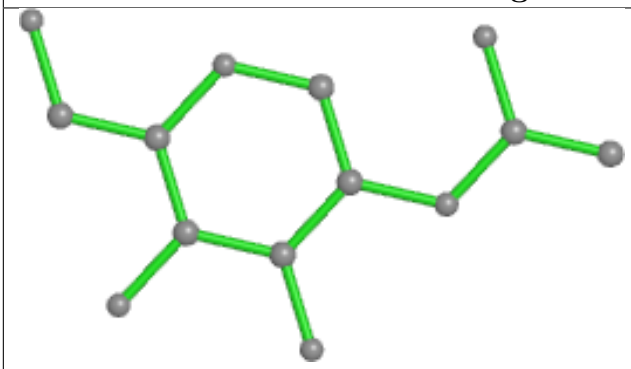


Rings

Ligand NAG A 1301



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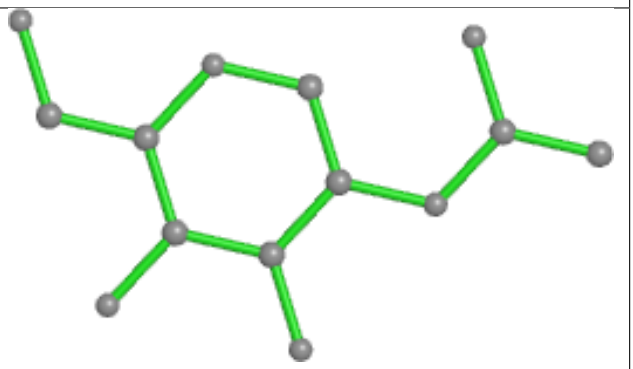
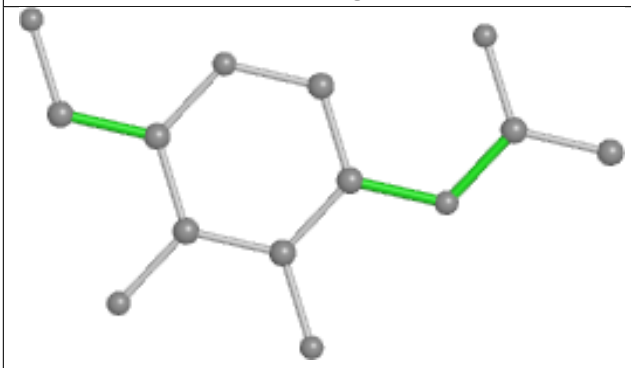


Bond angles



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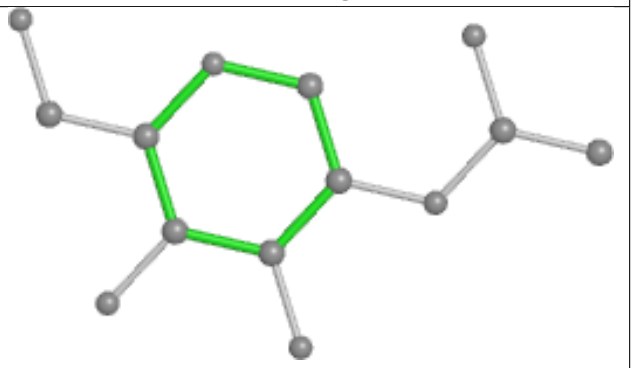
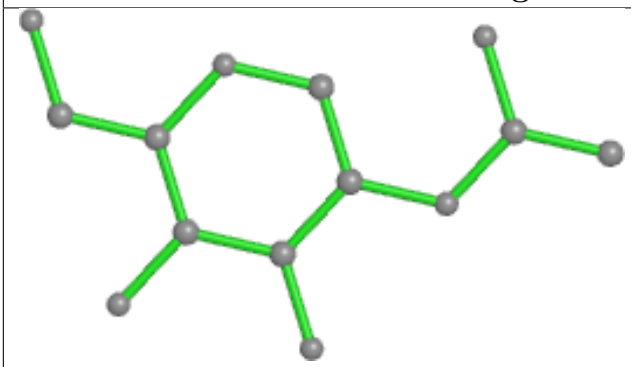


Rings

Ligand NAG B 1306



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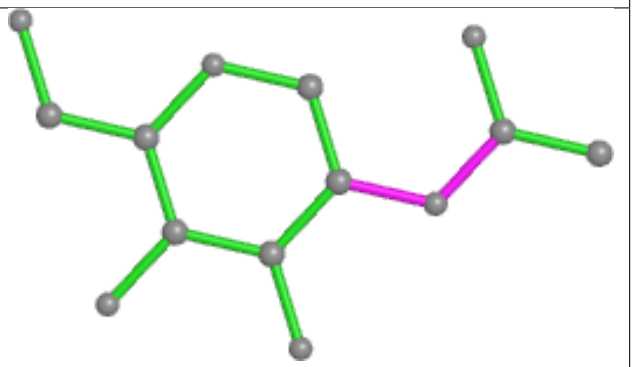
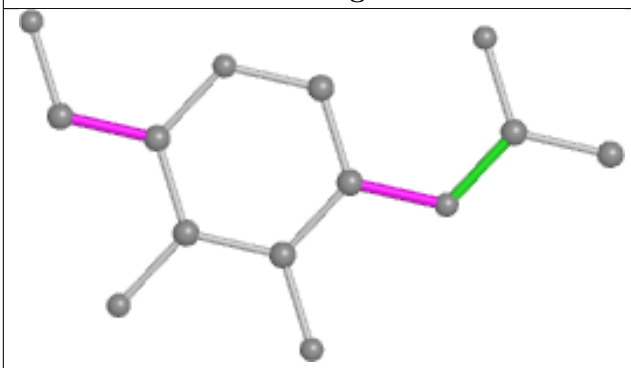


Bond angles



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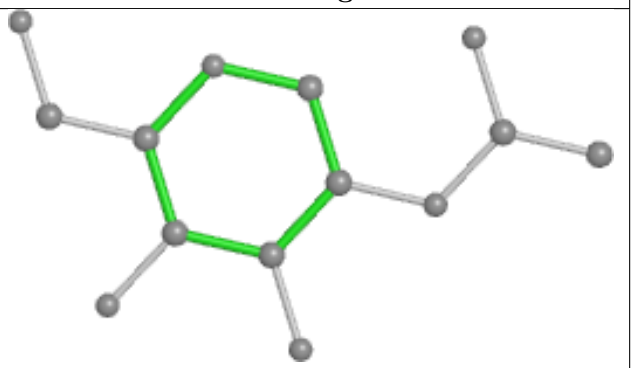
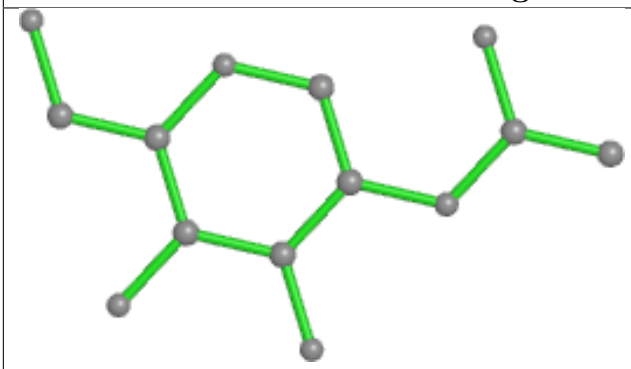


Rings

Ligand NAG B 1305



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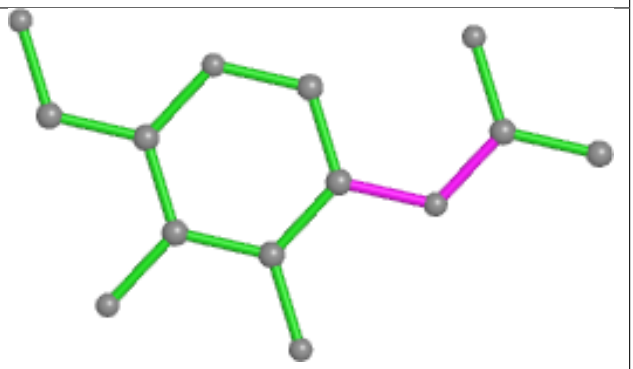
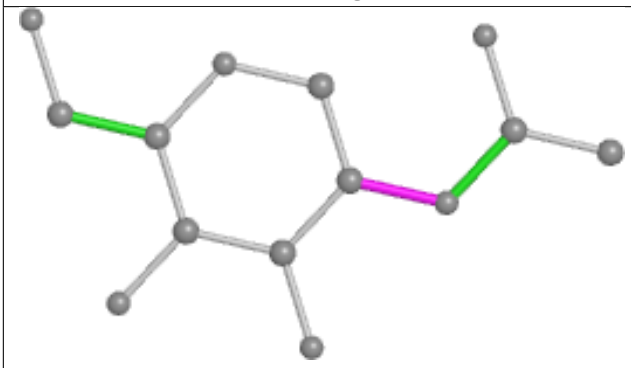


Bond angles



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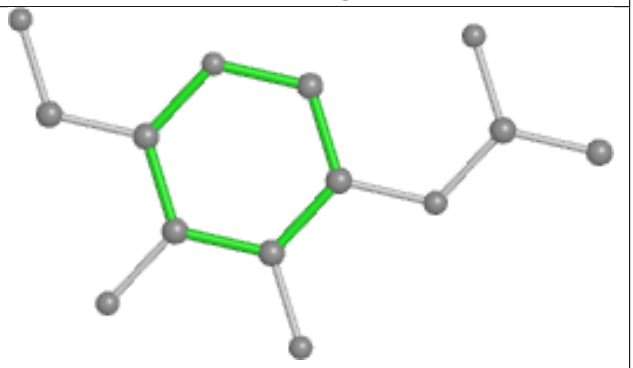
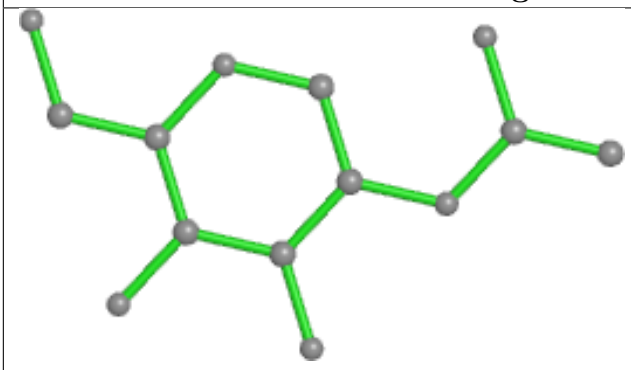
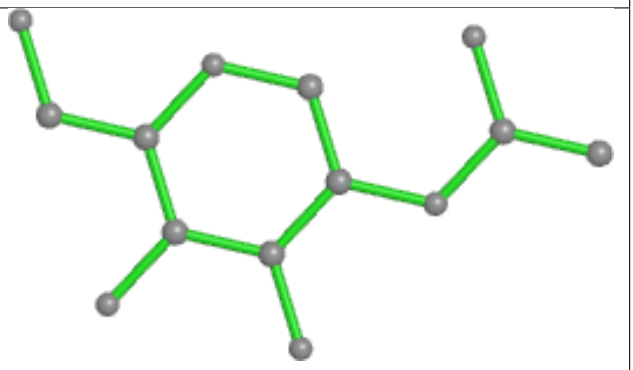


Rings

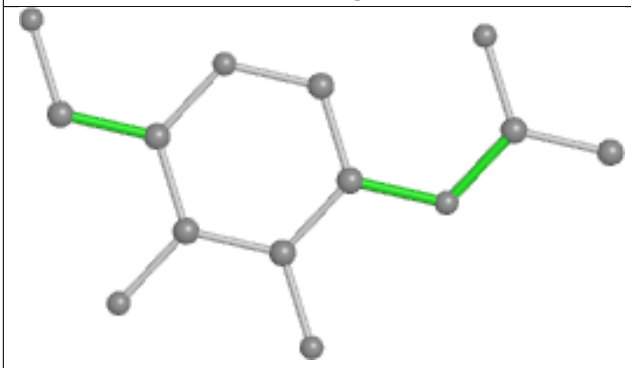
Ligand NAG B 1301



Bond lengths



Bond angles



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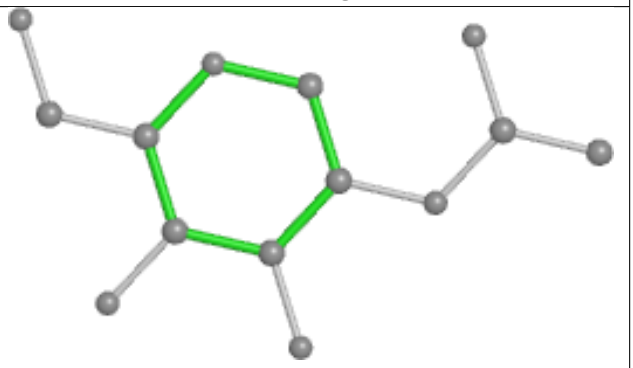
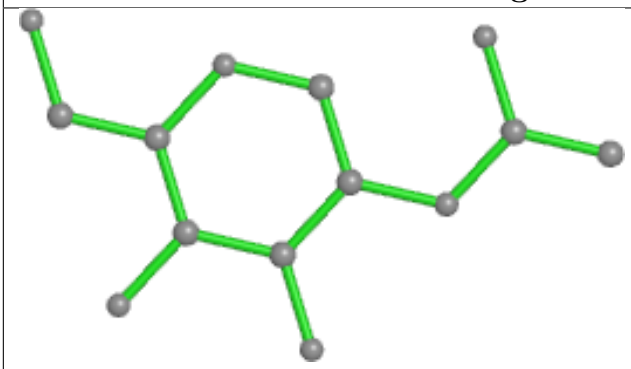
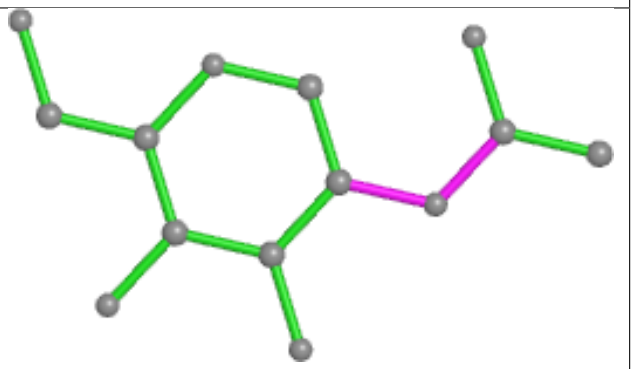


Rings

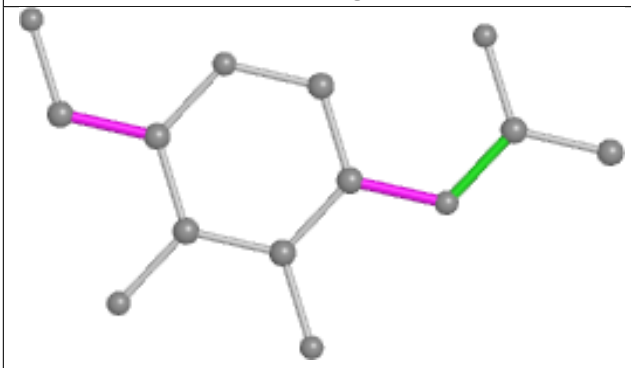
Ligand NAG A 1310



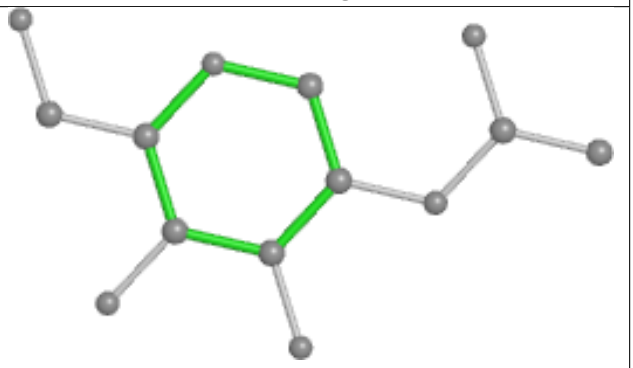
Bond lengths



Bond angles

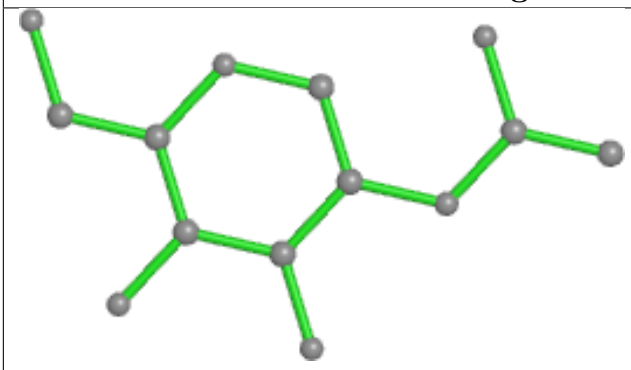


Torsions



Rings

Ligand NAG A 1311



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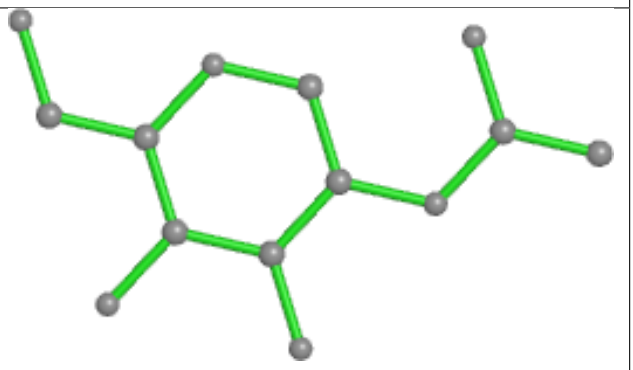
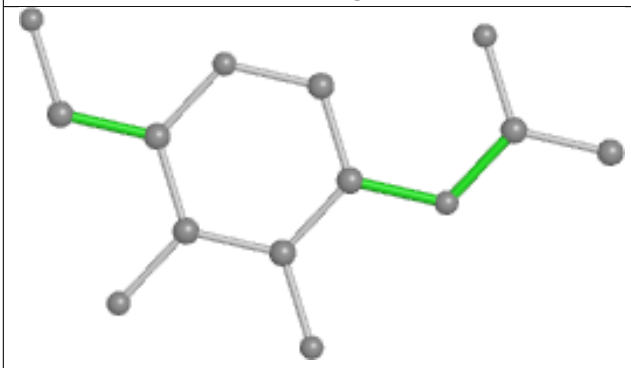


Bond angles



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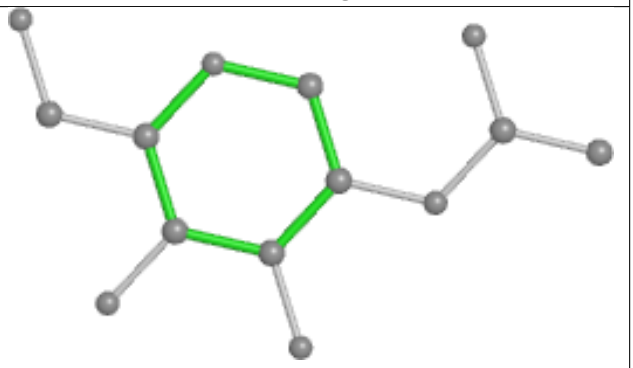
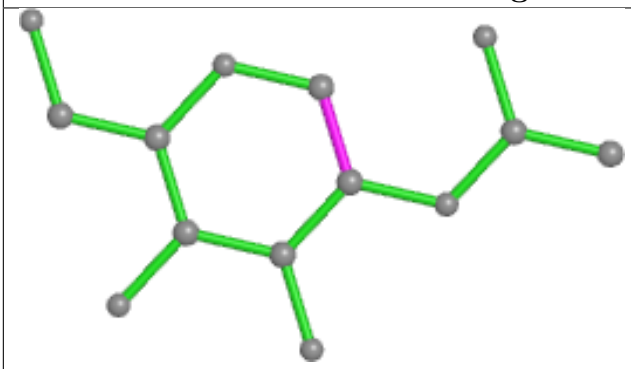
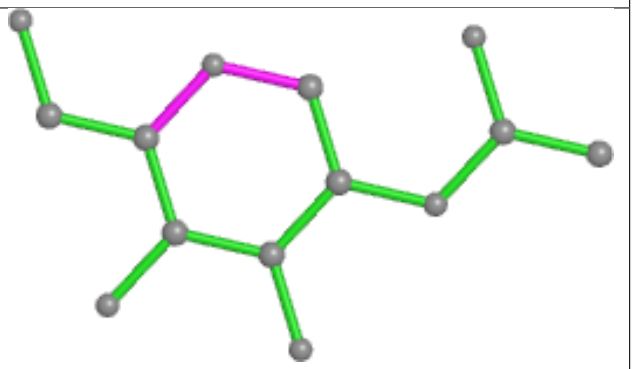


Rings

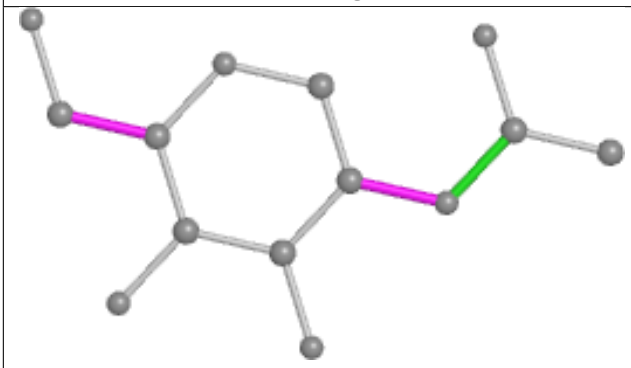
Ligand NAG A 1302



Bond lengths



Bond angles



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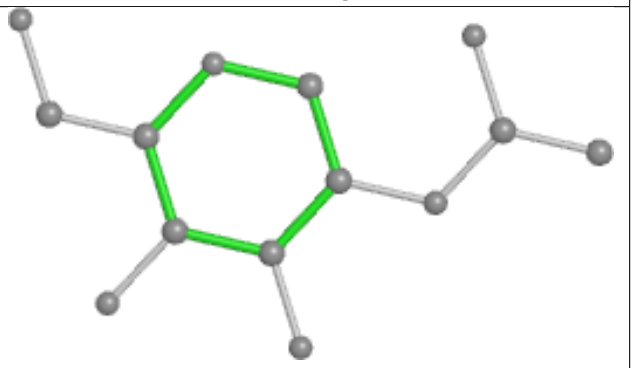
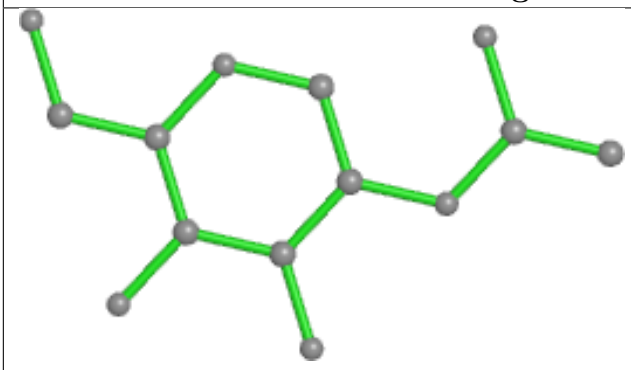
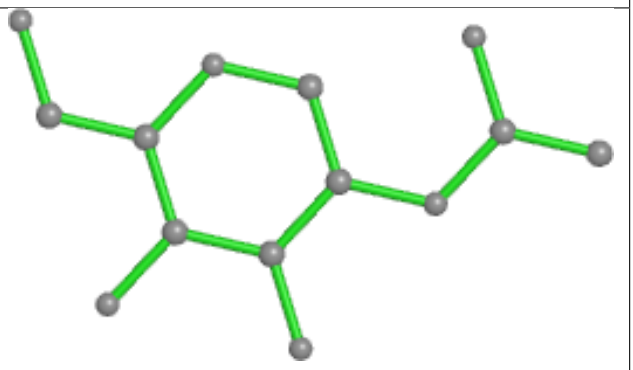


Rings

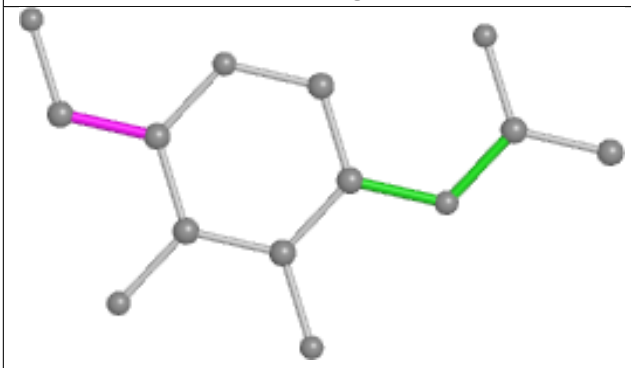
Ligand NAG B 1310



Bond lengths



Bond angles



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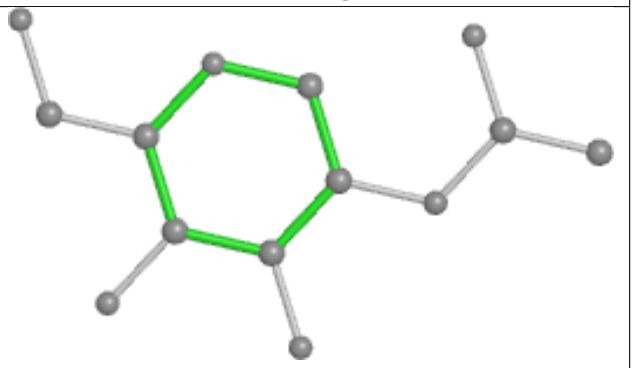
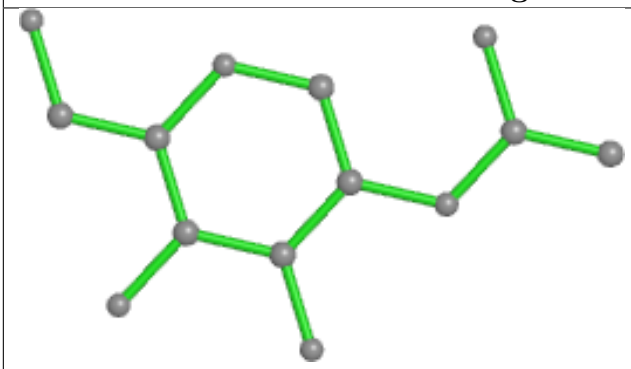
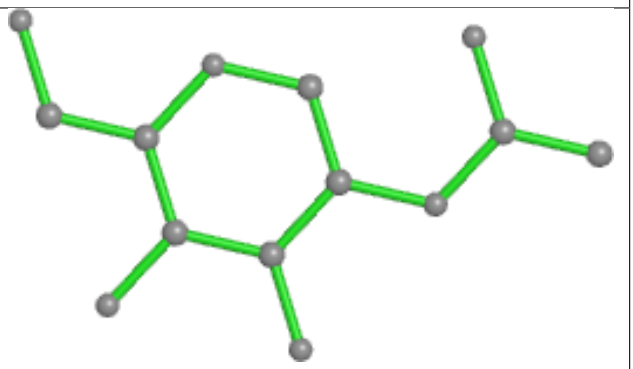


Rings

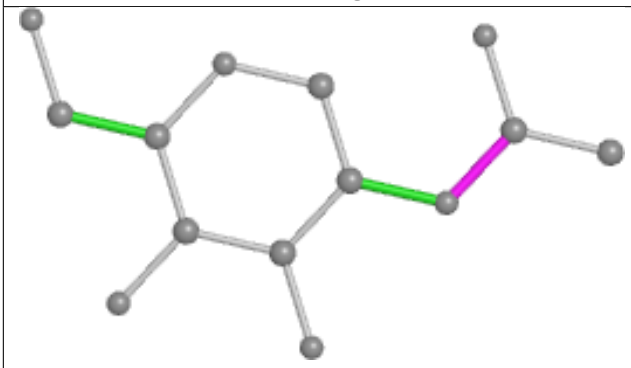
Ligand NAG A 1309



Bond lengths



Bond angles



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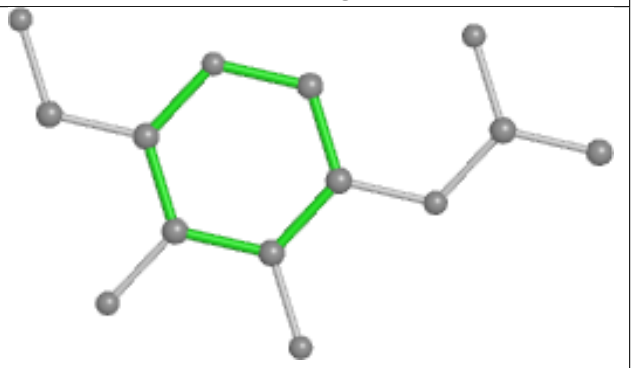
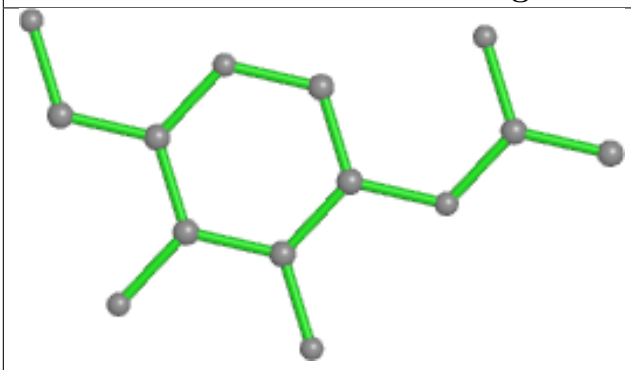


Rings

Ligand NAG B 1302



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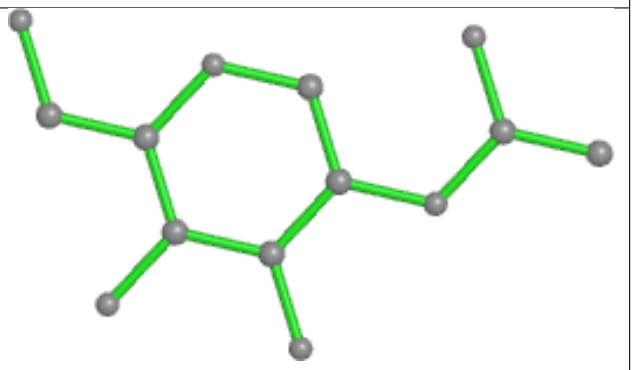
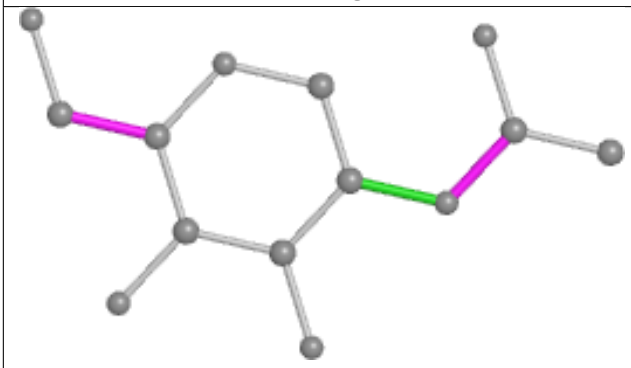


Bond angles



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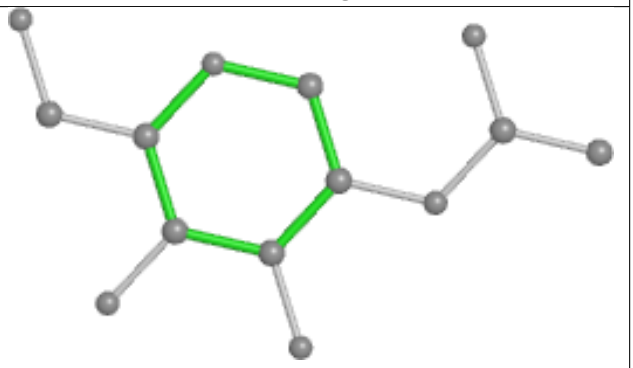
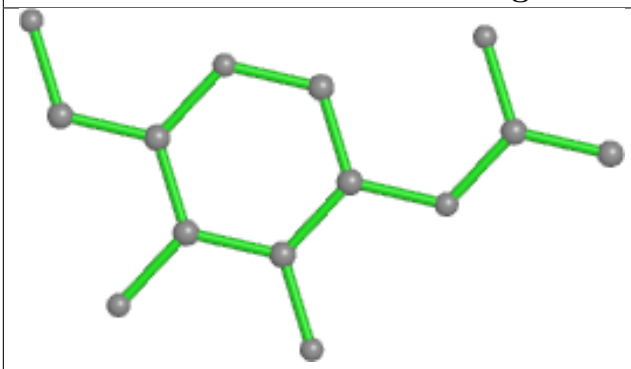


Rings

Ligand NAG B 1309



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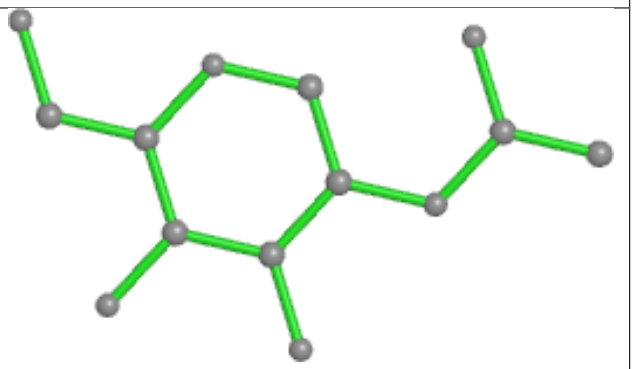
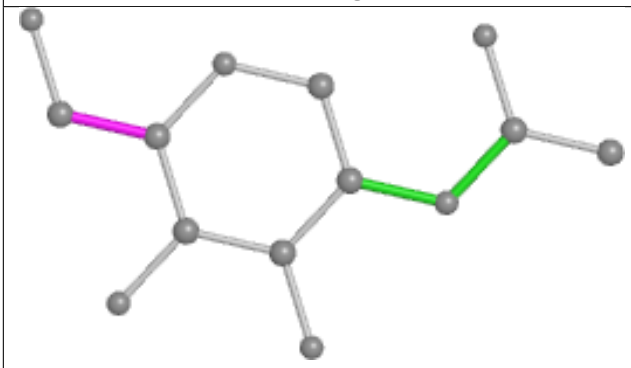


Bond angles



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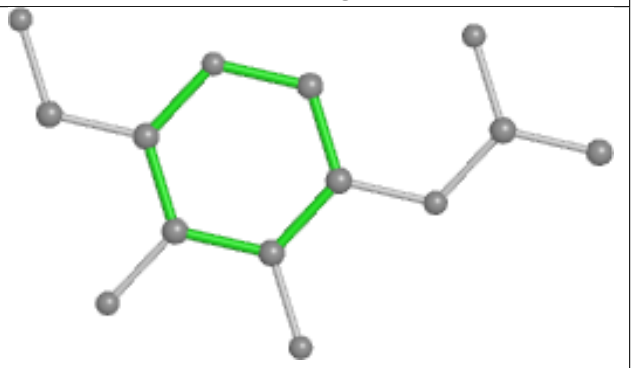
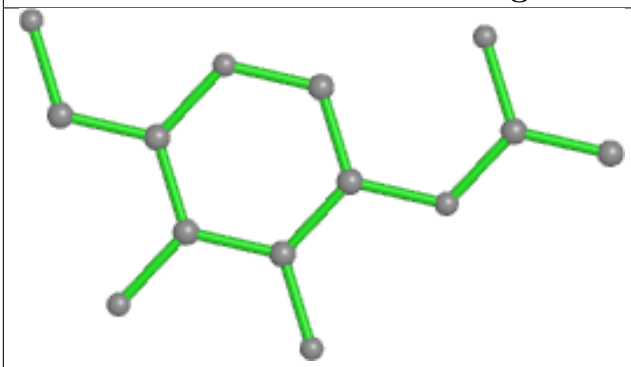
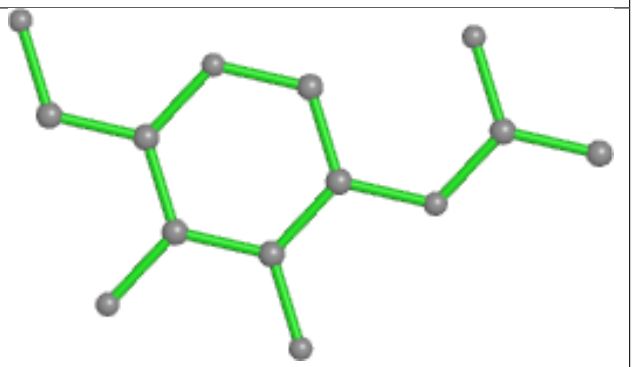


Rings

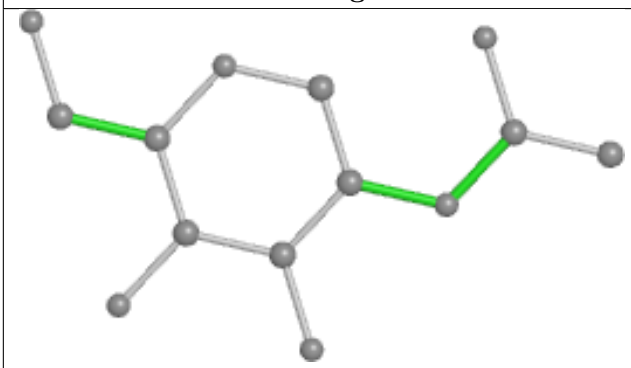
Ligand NAG A 1306



Bond lengths



Bond angles



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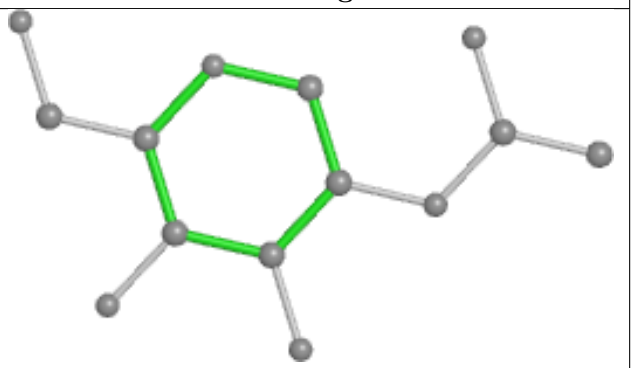
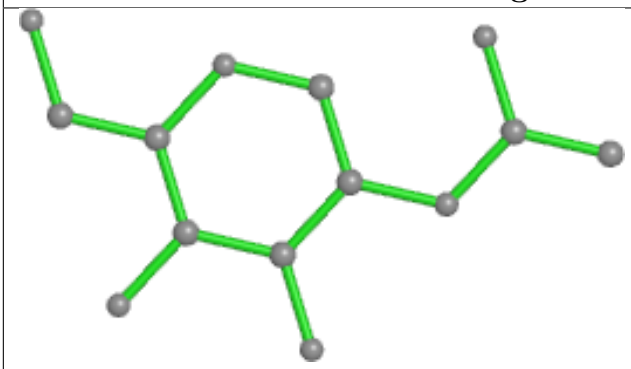


Rings

Ligand NAG A 1305



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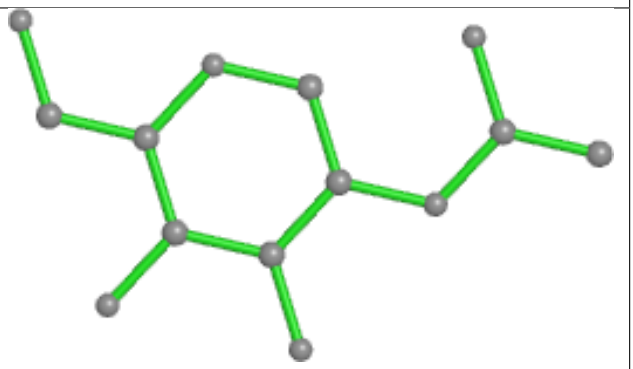
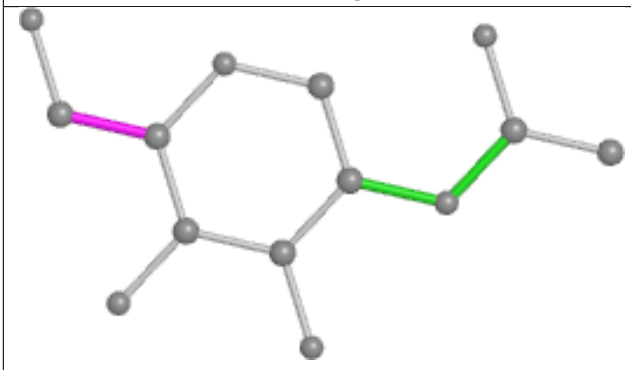
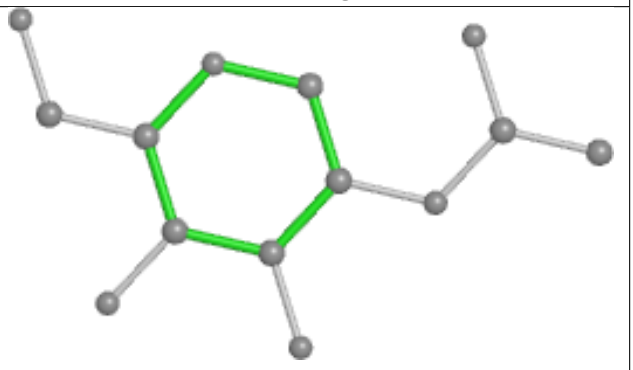


Bond angles

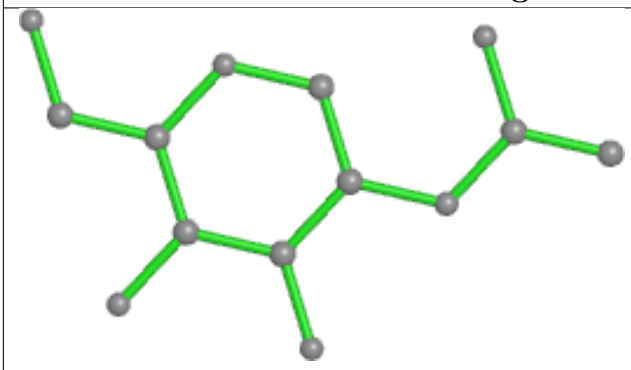


Torsions



Rings

Ligand NAG C 1307



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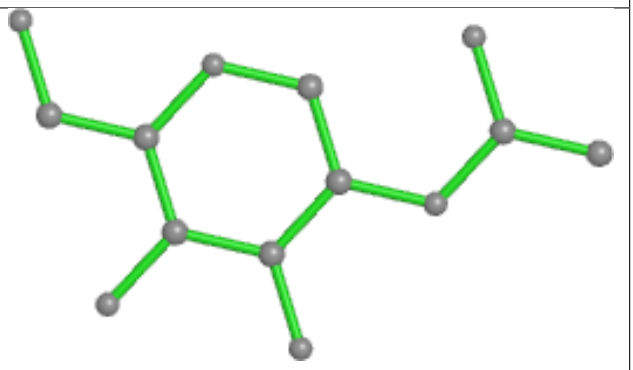
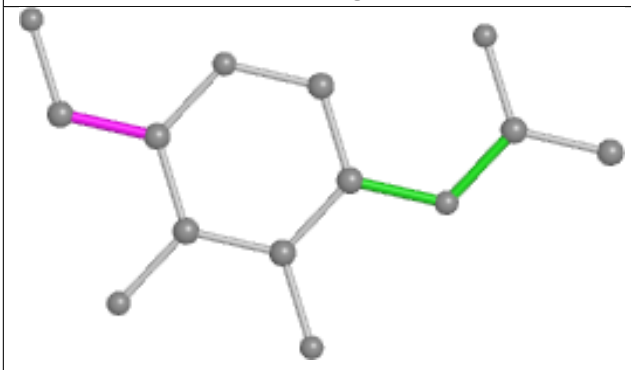


Bond angles



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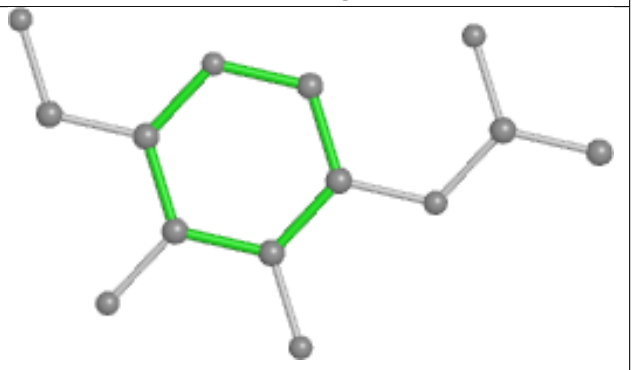
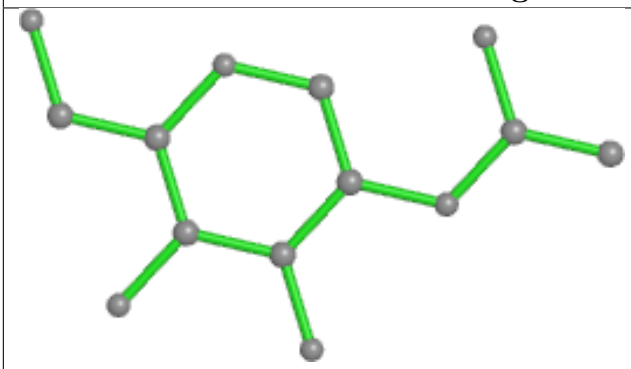


Rings

Ligand NAG C 1312



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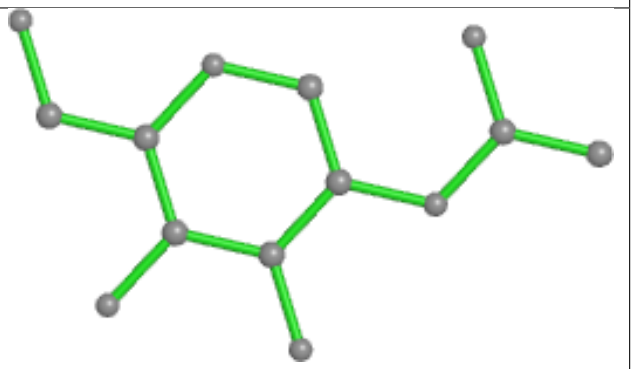
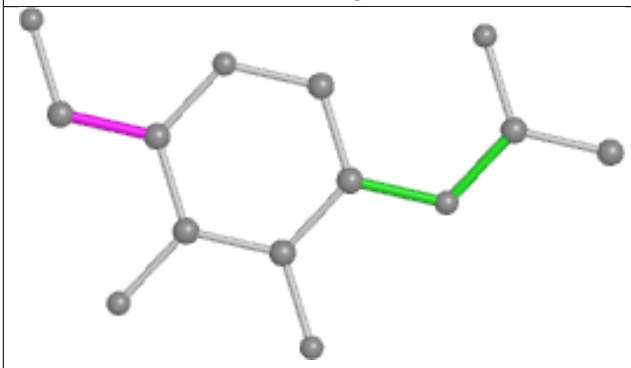
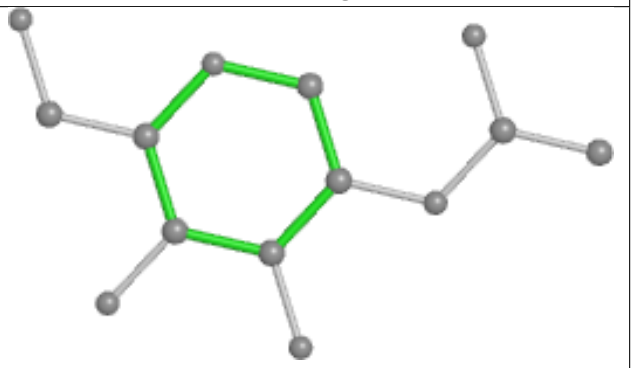


Bond angles

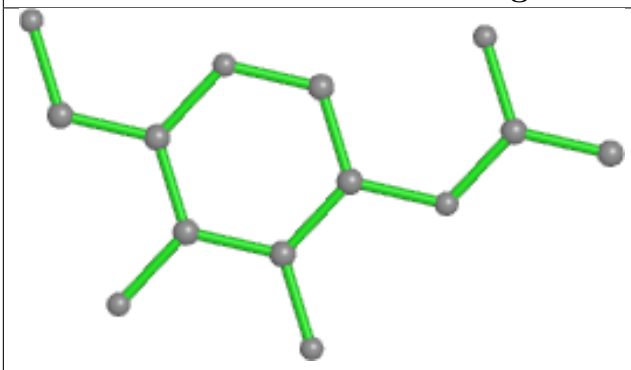


Torsions

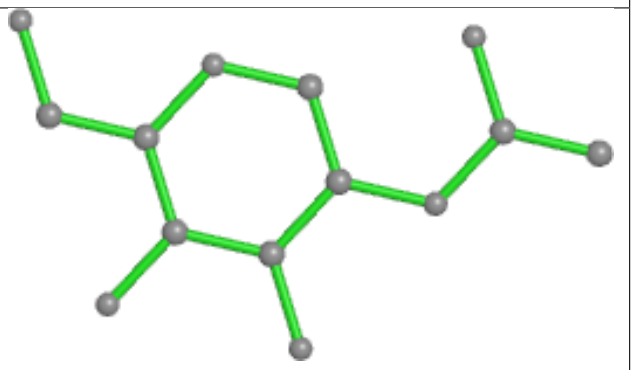


Rings

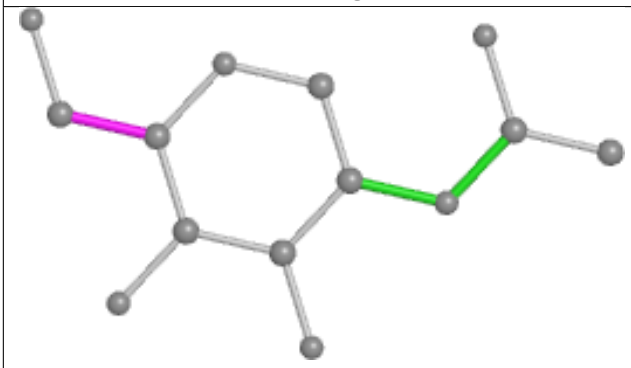
Ligand NAG A 1312



Bond lengths



Bond angles



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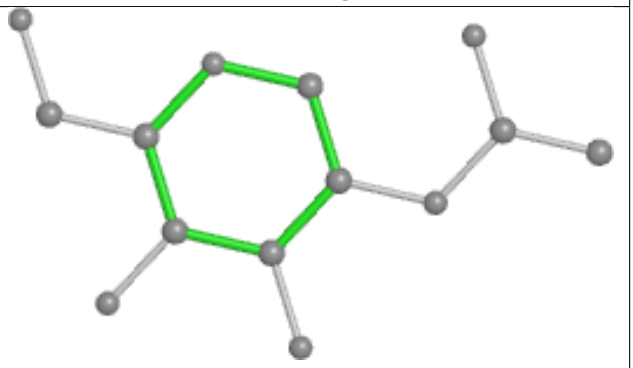


Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	328:ARG	C	329:PHE	N	4.86

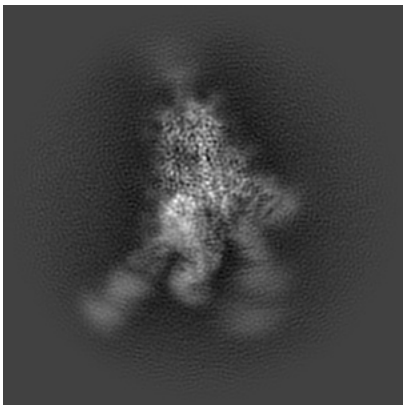
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27775. These allow visual inspection of the internal detail of the map and identification of artifacts.

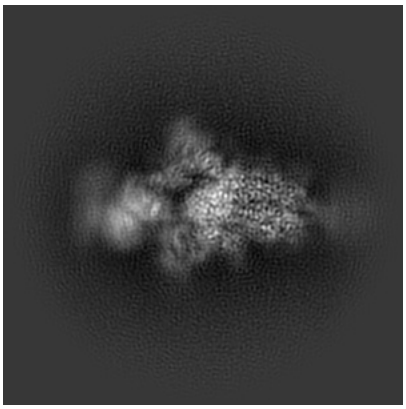
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

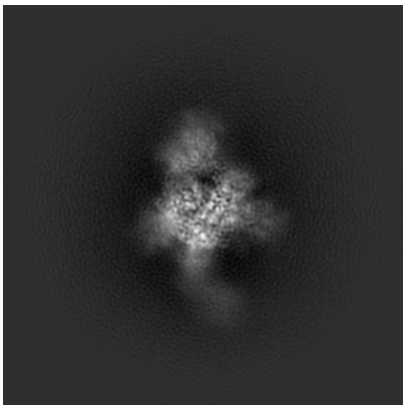
6.1.1 Primary map



X

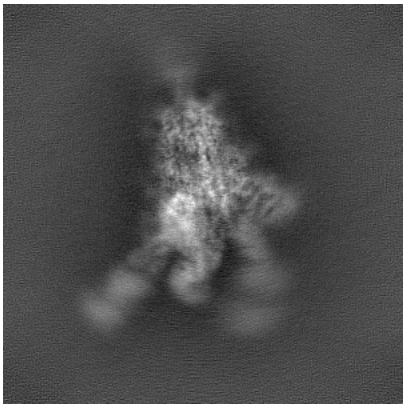


Y



Z

6.1.2 Raw map



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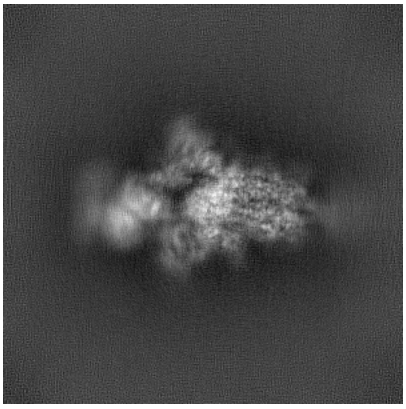
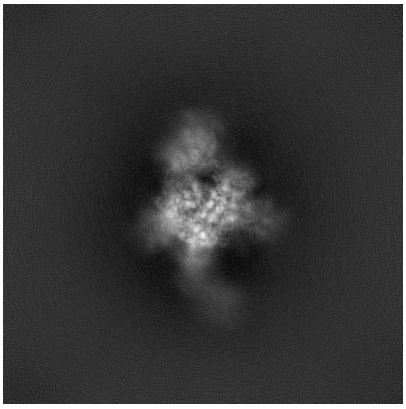


Y

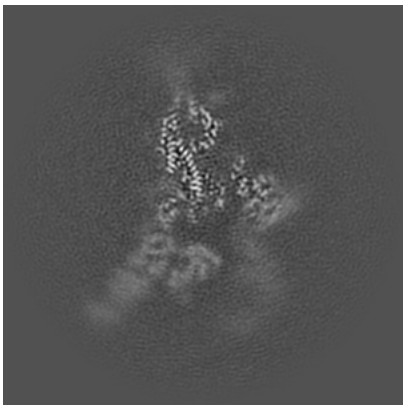


Z

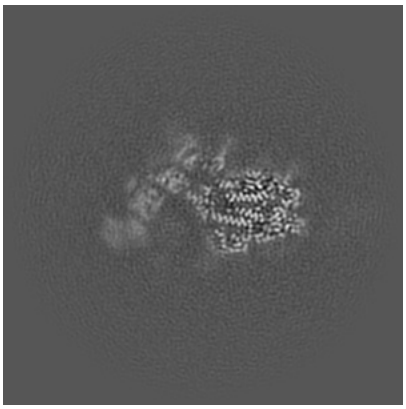
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

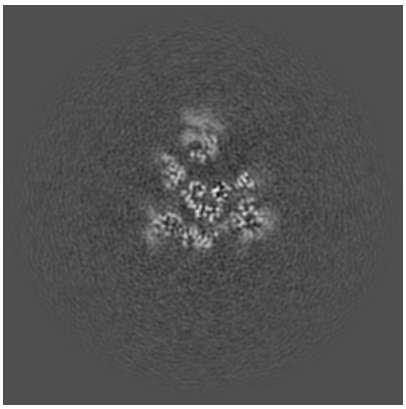
6.2.1 Primary map



X Index: 196

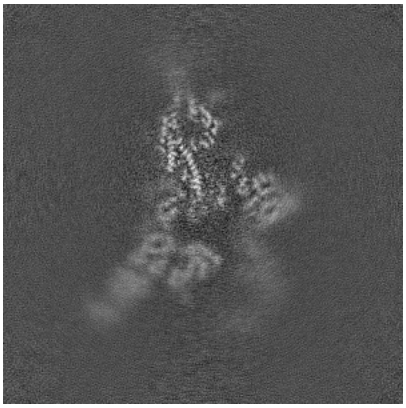


Y Index: 196

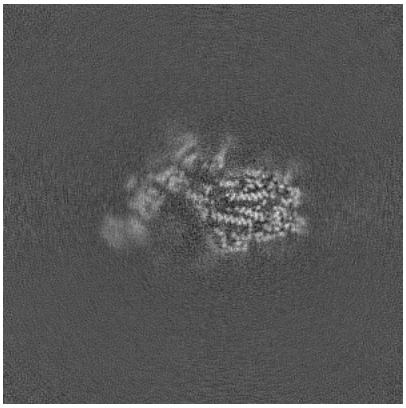


Z Index: 196

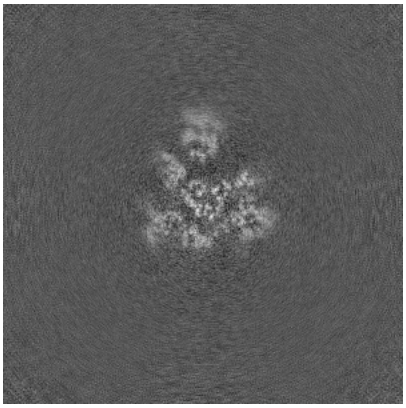
6.2.2 Raw map



X Index: 196



Y Index: 196

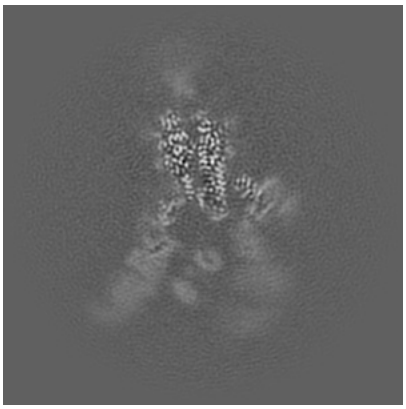


Z Index: 196

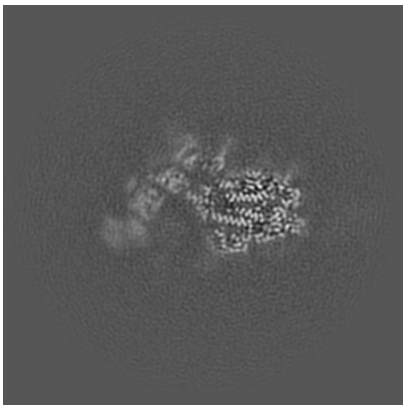
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

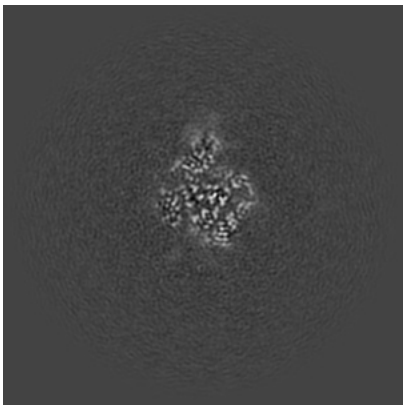
6.3.1 Primary map



X Index: 187

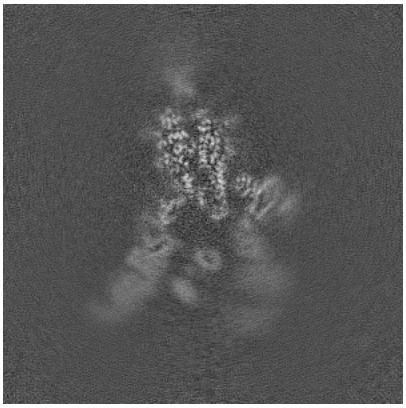


Y Index: 196

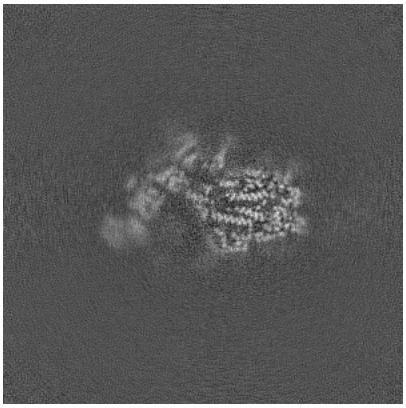


Z Index: 213

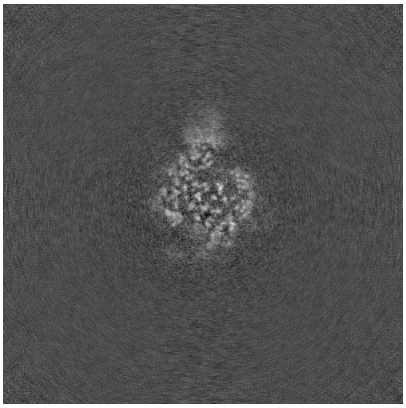
6.3.2 Raw map



X Index: 187



Y Index: 196

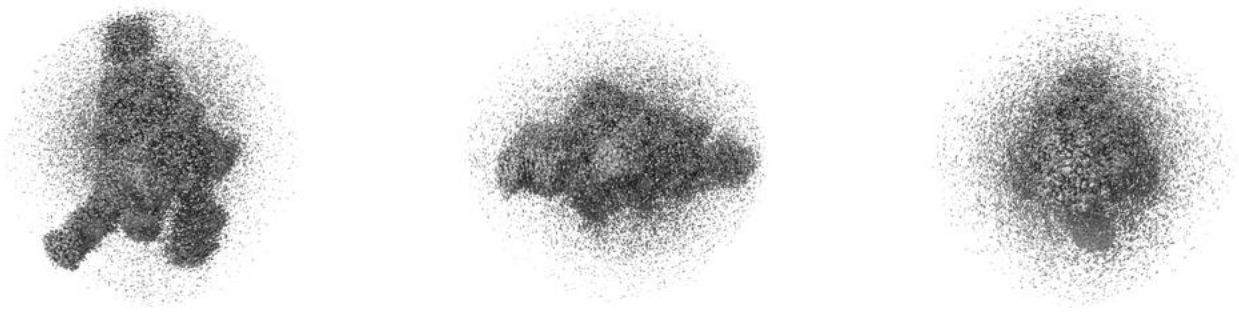


Z Index: 210

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

6.4 Orthogonal surface views (i)

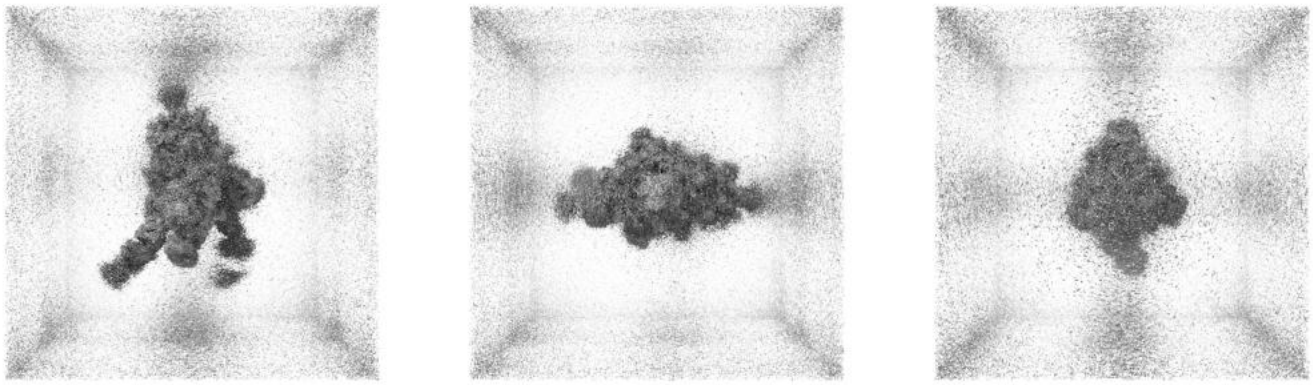
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

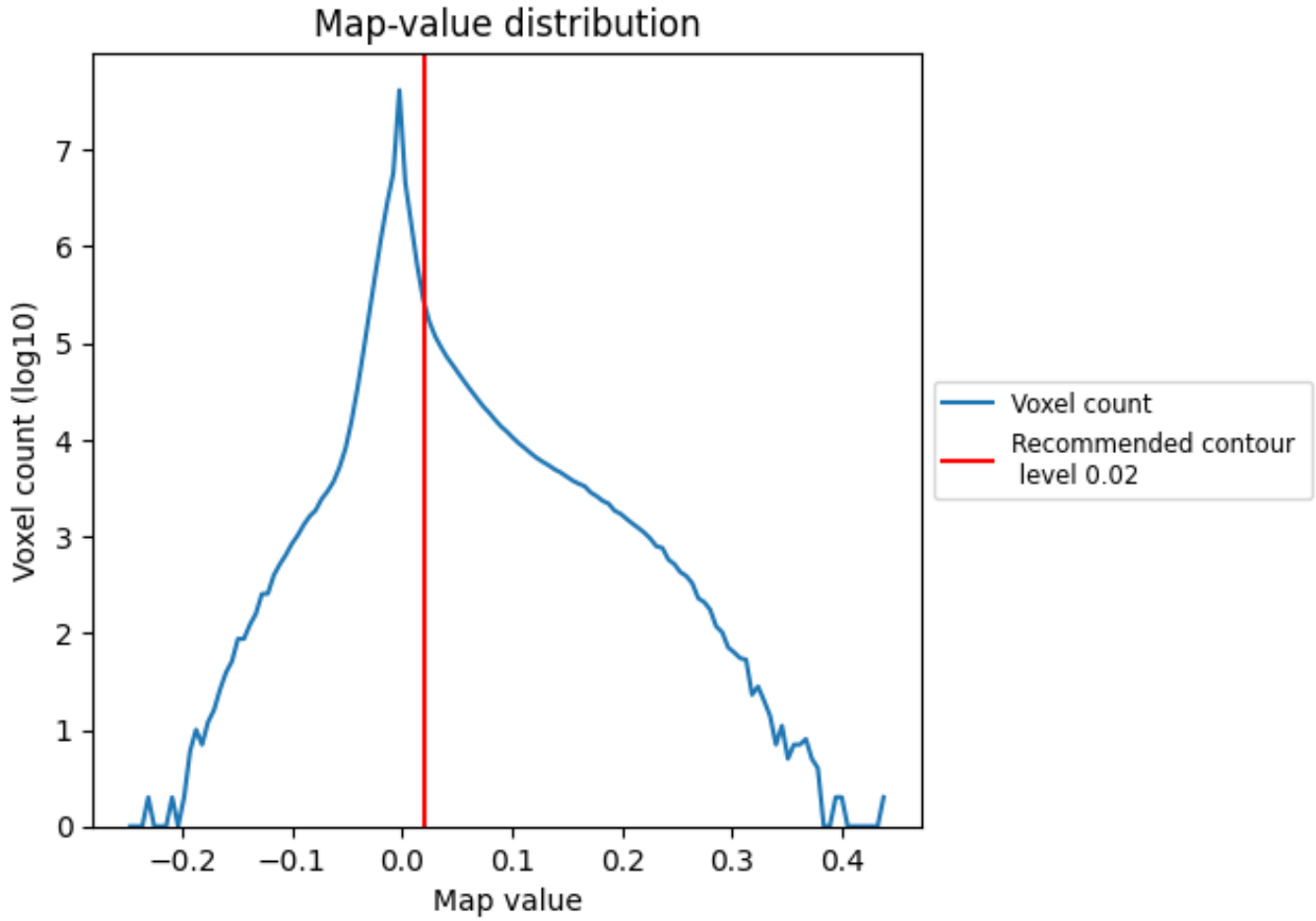
6.5 Mask visualisation (i)

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

7 Map analysis

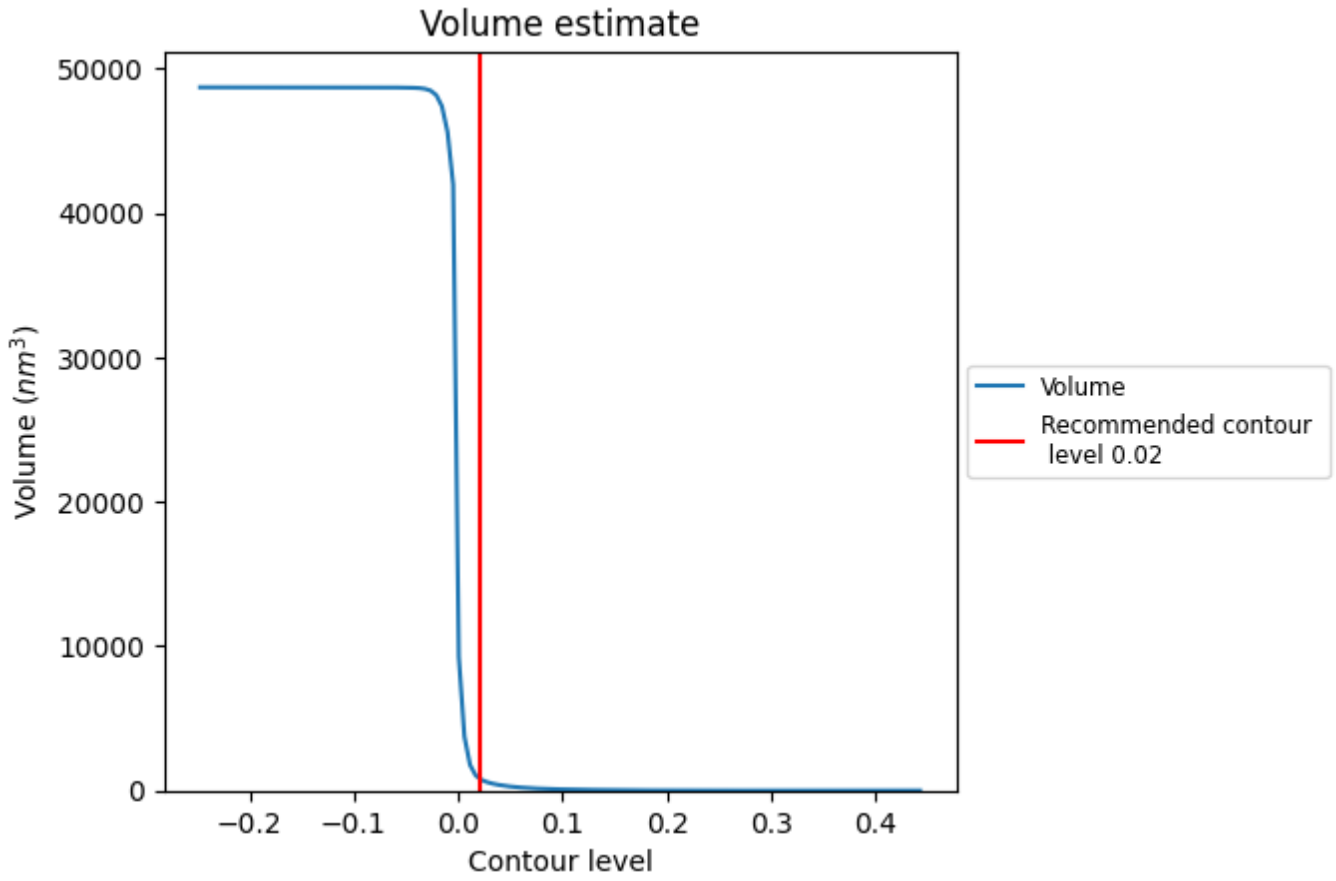
This section contains the results of statistical analysis of the map.

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.

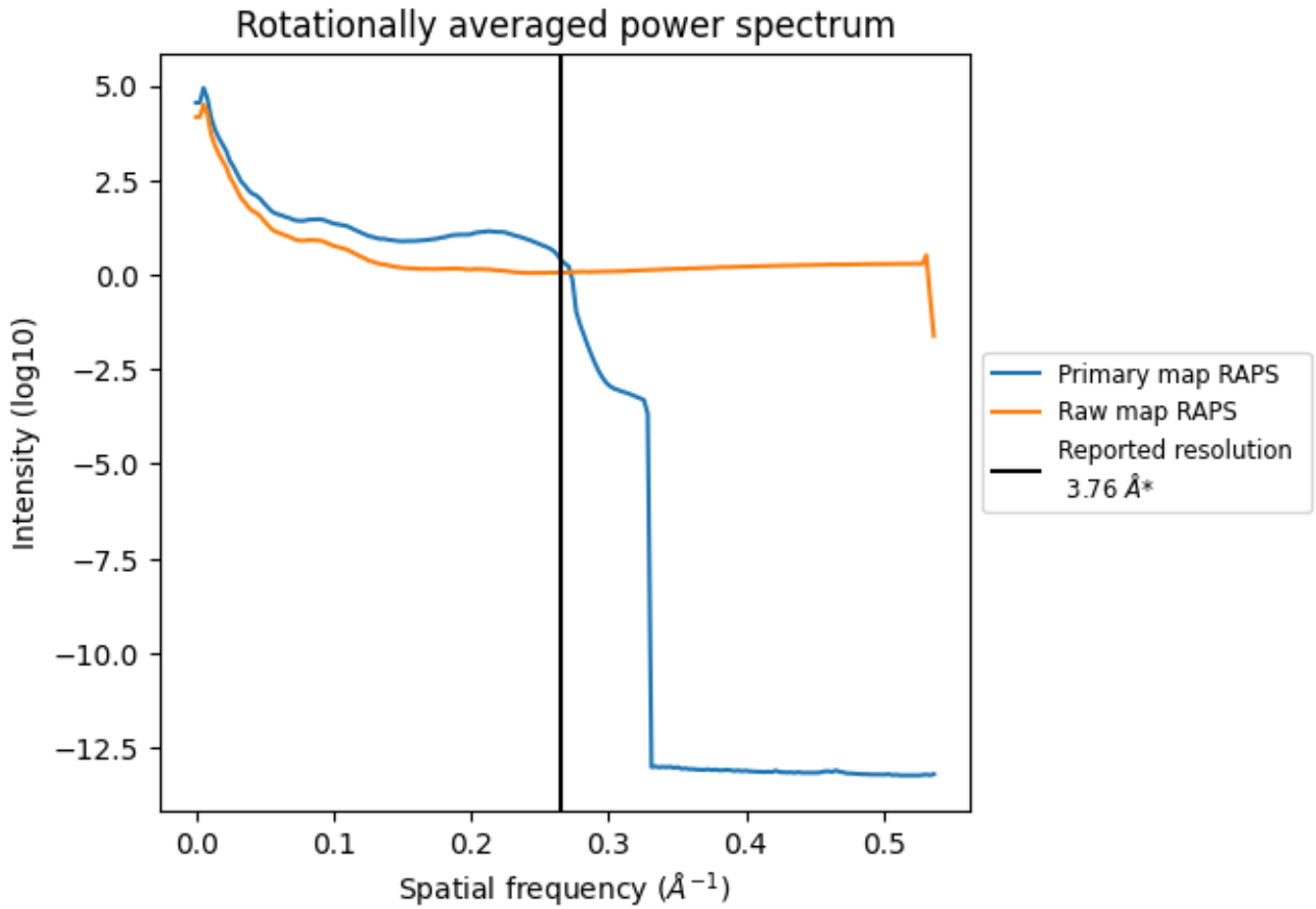
7.2 Volume estimate



The volume at the recommended contour level is 873 nm^3; this corresponds to an approximate mass of 788 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)

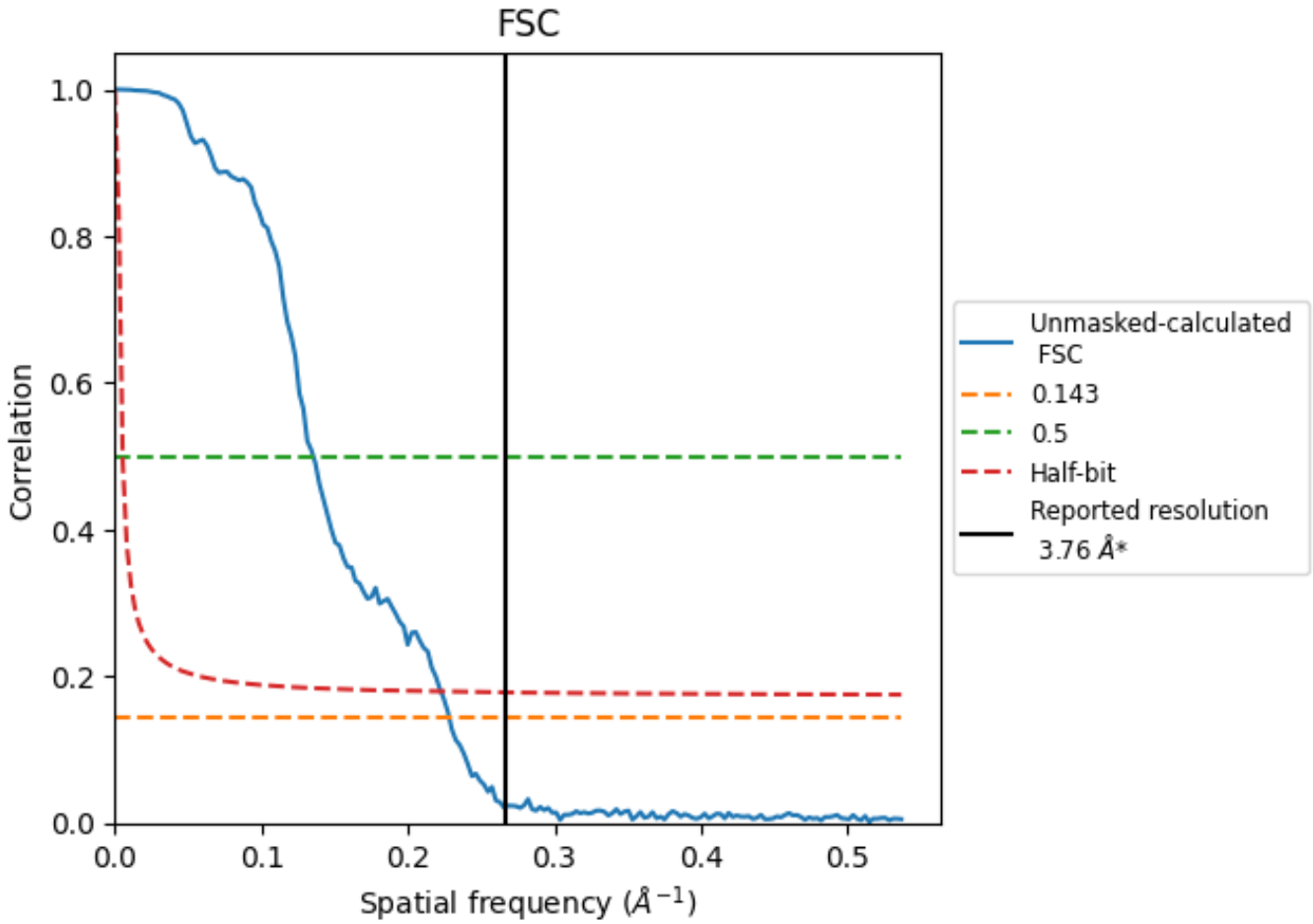


*Reported resolution corresponds to spatial frequency of 0.266 $Å^{-1}$

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 0.266 Å^{-1}

8.2 Resolution estimates (i)

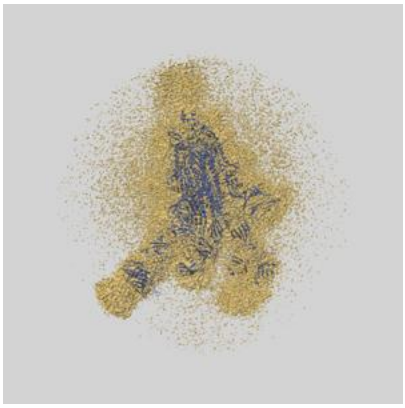
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.38	7.39	4.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.38 differs from the reported value 3.76 by more than 10 %

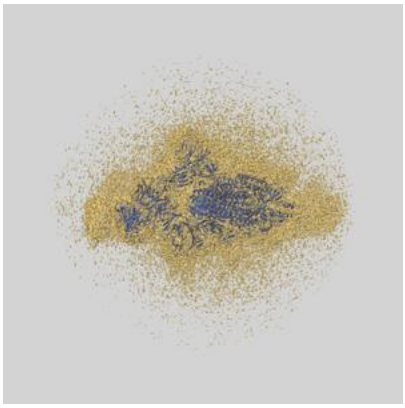
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27775 and PDB model 8DXS. Per-residue inclusion information can be found in section 3 on page 14.

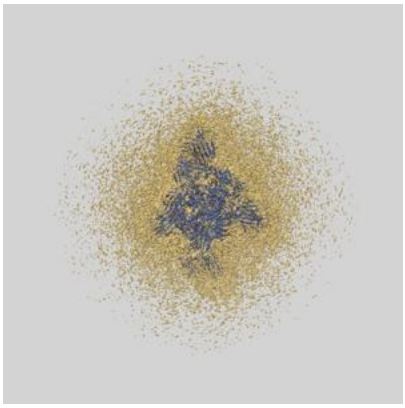
9.1 Map-model overlay



X



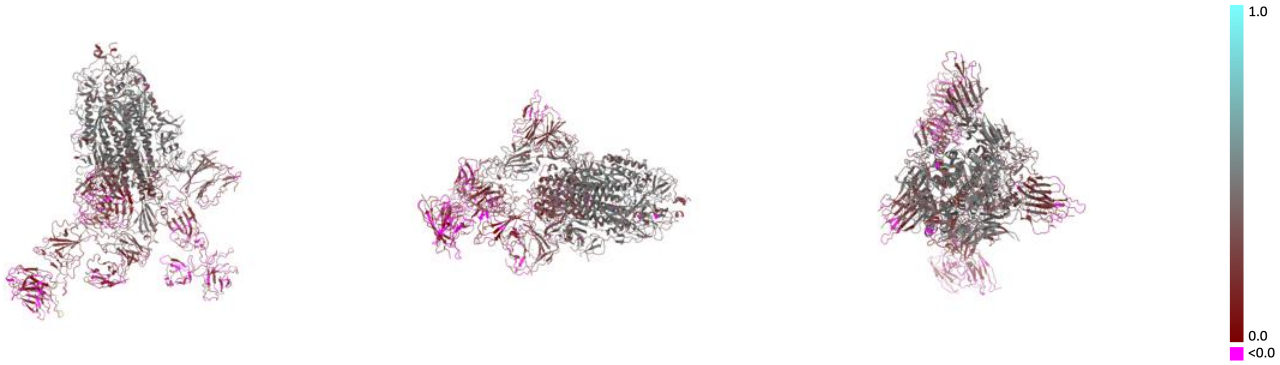
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

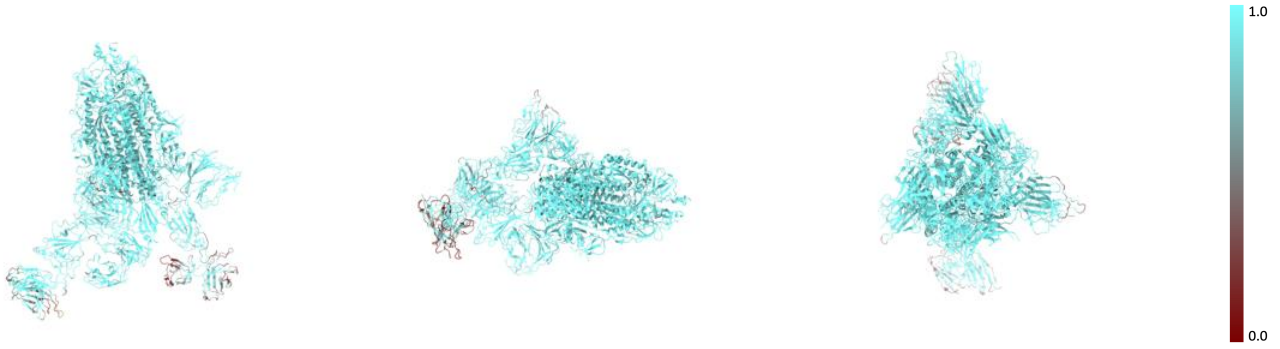
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

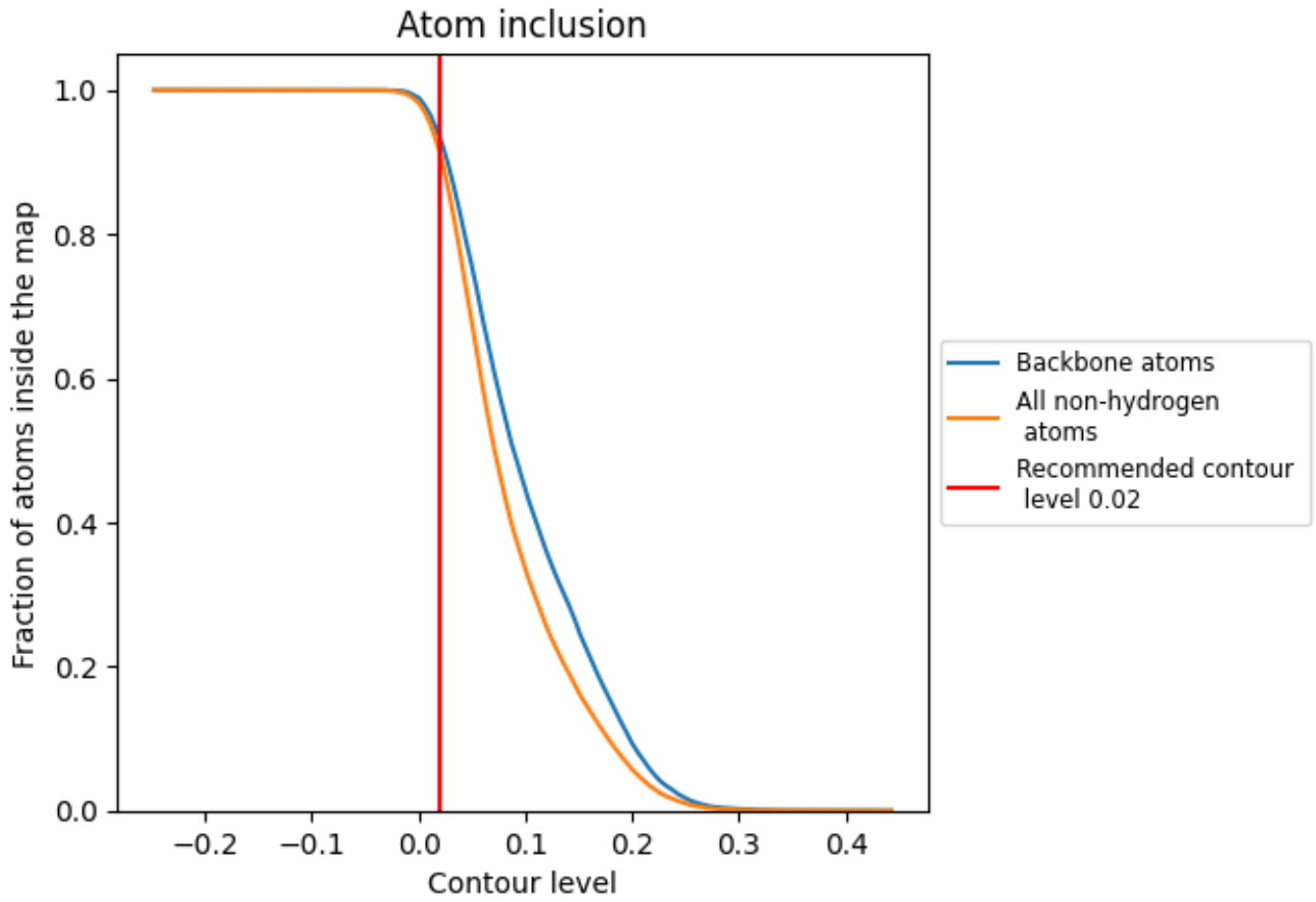
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.2910
A	0.9644	0.3740
B	0.9412	0.3140
C	0.9437	0.3060
F	0.5900	0.0920
G	0.6267	0.0260
H	0.9400	0.1530
I	0.4565	0.0220
J	0.8831	0.0700
L	0.9689	0.2450