wwPDB EM Validation Summary Report ⓘ

Nov 30, 2022 – 12:22 AM JST

PDB ID : 7XID
EMDB ID : EMD-33203
Title : S-ECD (Omicron) in complex with PD of ACE2
Authors : Li, Y.N.; Shen, Y.P.; Zhang, Y.Y.; Yan, R.H.
Deposited on : 2022-04-12
Resolution : 3.30 Å(reported)

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

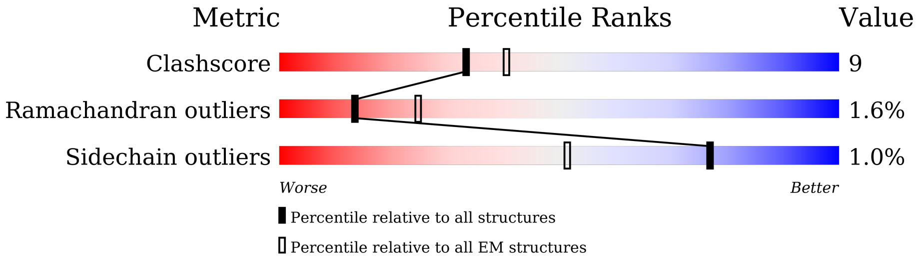
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance ⓘ

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

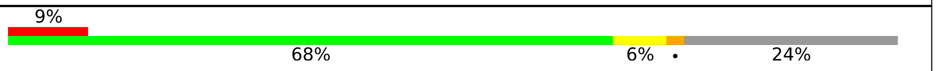
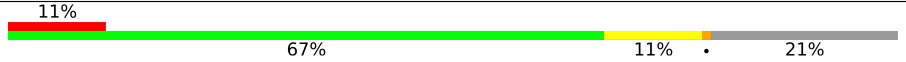
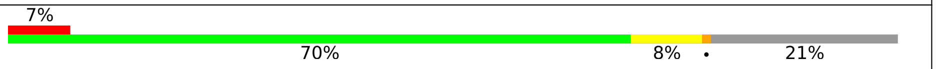
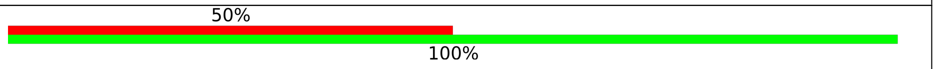
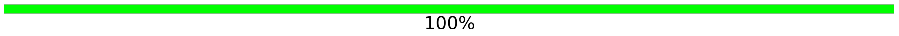
The reported resolution of this entry is 3.30 Å.

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	1267	
1	B	1267	
1	C	1267	
2	D	817	
2	E	817	
3	F	2	
3	G	2	
3	H	2	

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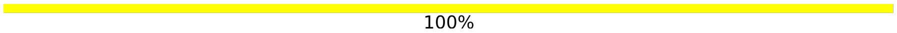
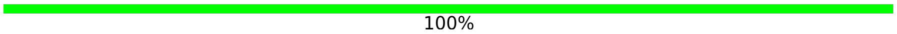
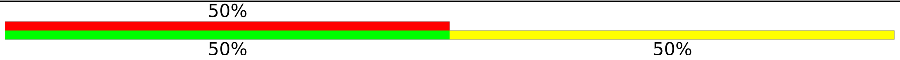
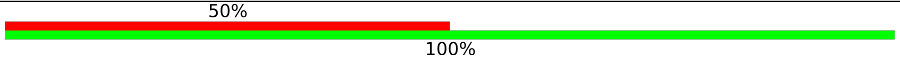
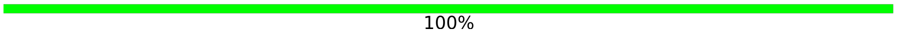
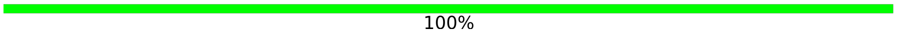
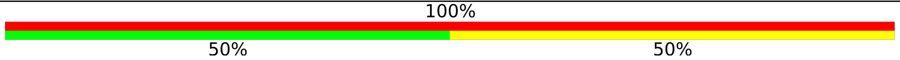
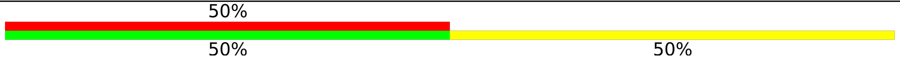
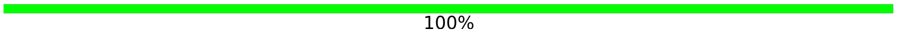
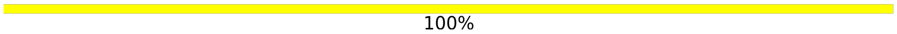
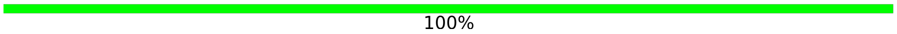
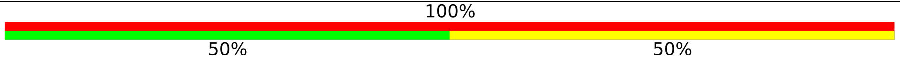
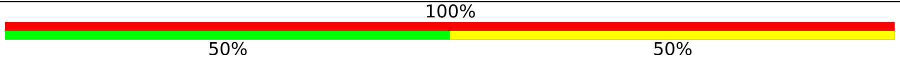
Mol	Chain	Length	Quality of chain
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	

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	D	902	-	-	X	-
4	NAG	E	902	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 34256 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	963	Total 7558	C 4842	N 1255	O 1427	S 34	0	0
1	B	998	Total 7842	C 5025	N 1304	O 1477	S 36	0	0
1	C	998	Total 7842	C 5025	N 1304	O 1477	S 36	0	0

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	145	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	211	ILE	LEU	variant	UNP P0DTC2
A	214	GLU	-	insertion	UNP P0DTC2
A	214A	PRO	-	insertion	UNP P0DTC2
A	214B	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	SER	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLU	-	expression tag	UNP P0DTC2
A	1244	VAL	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	ALA	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	SER	-	expression tag	UNP P0DTC2
A	1249	HIS	-	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	HIS	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	SER	-	expression tag	UNP P0DTC2
A	1261	VAL	-	expression tag	UNP P0DTC2
A	1262	GLU	-	expression tag	UNP P0DTC2
A	1263	ASP	-	expression tag	UNP P0DTC2
A	1264	TYR	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	ASP	-	expression tag	UNP P0DTC2
A	1267	ASP	-	expression tag	UNP P0DTC2
A	1268	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1269	ASP	-	expression tag	UNP P0DTC2
A	1270	LYS	-	expression tag	UNP P0DTC2
B	69	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	145	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	211	ILE	LEU	variant	UNP P0DTC2
B	214	GLU	-	insertion	UNP P0DTC2
B	214A	PRO	-	insertion	UNP P0DTC2
B	214B	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	GLU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	SER	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1243	GLU	-	expression tag	UNP P0DTC2
B	1244	VAL	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	ALA	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	SER	-	expression tag	UNP P0DTC2
B	1249	HIS	-	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	HIS	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	SER	-	expression tag	UNP P0DTC2
B	1261	VAL	-	expression tag	UNP P0DTC2
B	1262	GLU	-	expression tag	UNP P0DTC2
B	1263	ASP	-	expression tag	UNP P0DTC2
B	1264	TYR	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	ASP	-	expression tag	UNP P0DTC2
B	1267	ASP	-	expression tag	UNP P0DTC2
B	1268	ASP	-	expression tag	UNP P0DTC2
B	1269	ASP	-	expression tag	UNP P0DTC2
B	1270	LYS	-	expression tag	UNP P0DTC2
C	69	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	145	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	211	ILE	LEU	variant	UNP P0DTC2
C	214	GLU	-	insertion	UNP P0DTC2
C	214A	PRO	-	insertion	UNP P0DTC2
C	214B	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	SER	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLU	-	expression tag	UNP P0DTC2
C	1244	VAL	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	ALA	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	SER	-	expression tag	UNP P0DTC2
C	1249	HIS	-	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	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	SER	-	expression tag	UNP P0DTC2
C	1261	VAL	-	expression tag	UNP P0DTC2
C	1262	GLU	-	expression tag	UNP P0DTC2
C	1263	ASP	-	expression tag	UNP P0DTC2
C	1264	TYR	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	ASP	-	expression tag	UNP P0DTC2
C	1267	ASP	-	expression tag	UNP P0DTC2
C	1268	ASP	-	expression tag	UNP P0DTC2
C	1269	ASP	-	expression tag	UNP P0DTC2
C	1270	LYS	-	expression tag	UNP P0DTC2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total 4870	C 3115	N 806	O 920	S 29	0	0
2	E	597	Total 4870	C 3115	N 806	O 920	S 29	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP Q9BYF1
D	-10	ALA	-	expression tag	UNP Q9BYF1
D	-9	SER	-	expression tag	UNP Q9BYF1
D	-8	GLY	-	expression tag	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1
E	-11	MET	-	expression tag	UNP Q9BYF1
E	-10	ALA	-	expression tag	UNP Q9BYF1
E	-9	SER	-	expression tag	UNP Q9BYF1
E	-8	GLY	-	expression tag	UNP Q9BYF1
E	-7	ARG	-	expression tag	UNP Q9BYF1

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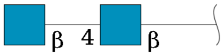
Chain	Residue	Modelled	Actual	Comment	Reference
E	10	TRP	-	insertion	UNP Q9BYF1
E	11	SER	-	insertion	UNP Q9BYF1
E	12	HIS	-	insertion	UNP Q9BYF1
E	13	PRO	-	insertion	UNP Q9BYF1
E	14	GLN	-	insertion	UNP Q9BYF1
E	15	PHE	-	insertion	UNP Q9BYF1
E	16	GLU	-	insertion	UNP Q9BYF1
E	17	LYS	-	insertion	UNP Q9BYF1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
3	F	2	Total C N O 28 16 2 10	0	0
3	G	2	Total C N O 28 16 2 10	0	0
3	H	2	Total C N O 28 16 2 10	0	0
3	I	2	Total C N O 28 16 2 10	0	0
3	J	2	Total C N O 28 16 2 10	0	0
3	K	2	Total C N O 28 16 2 10	0	0
3	L	2	Total C N O 28 16 2 10	0	0
3	M	2	Total C N O 28 16 2 10	0	0
3	N	2	Total C N O 28 16 2 10	0	0
3	O	2	Total C N O 28 16 2 10	0	0
3	P	2	Total C N O 28 16 2 10	0	0
3	Q	2	Total C N O 28 16 2 10	0	0

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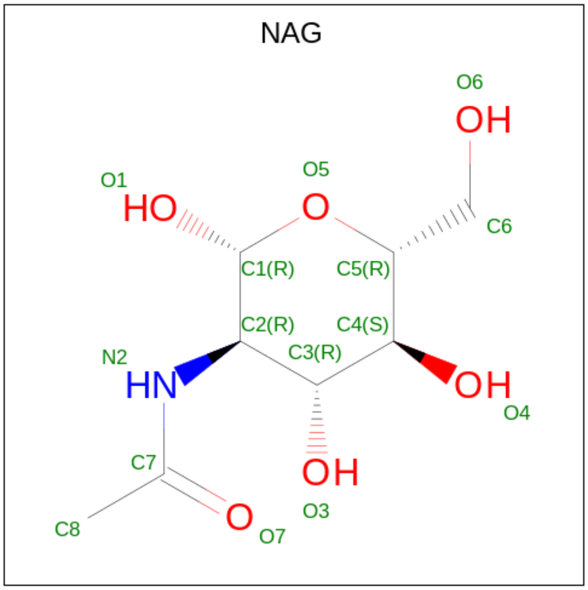
Mol	Chain	Residues	Atoms	AltConf	Trace
3	R	2	Total C N O 28 16 2 10	0	0
3	S	2	Total C N O 28 16 2 10	0	0
3	T	2	Total C N O 28 16 2 10	0	0
3	U	2	Total C N O 28 16 2 10	0	0
3	V	2	Total C N O 28 16 2 10	0	0
3	W	2	Total C N O 28 16 2 10	0	0
3	X	2	Total C N O 28 16 2 10	0	0
3	Y	2	Total C N O 28 16 2 10	0	0
3	Z	2	Total C N O 28 16 2 10	0	0
3	a	2	Total C N O 28 16 2 10	0	0
3	b	2	Total C N O 28 16 2 10	0	0

- 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 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	A	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0
4	B	1	Total C N O 154 88 11 55	0

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Mol	Chain	Residues	Atoms	AltConf
4	C	1	Total C N O 126 72 9 45	0
4	C	1	Total C N O 126 72 9 45	0
4	C	1	Total C N O 126 72 9 45	0
4	C	1	Total C N O 126 72 9 45	0
4	C	1	Total C N O 126 72 9 45	0
4	C	1	Total C N O 126 72 9 45	0
4	C	1	Total C N O 126 72 9 45	0
4	C	1	Total C N O 126 72 9 45	0
4	C	1	Total C N O 126 72 9 45	0
4	D	1	Total C N O 98 56 7 35	0
4	D	1	Total C N O 98 56 7 35	0
4	D	1	Total C N O 98 56 7 35	0
4	D	1	Total C N O 98 56 7 35	0
4	D	1	Total C N O 98 56 7 35	0
4	D	1	Total C N O 98 56 7 35	0
4	D	1	Total C N O 98 56 7 35	0
4	E	1	Total C N O 98 56 7 35	0
4	E	1	Total C N O 98 56 7 35	0
4	E	1	Total C N O 98 56 7 35	0
4	E	1	Total C N O 98 56 7 35	0
4	E	1	Total C N O 98 56 7 35	0

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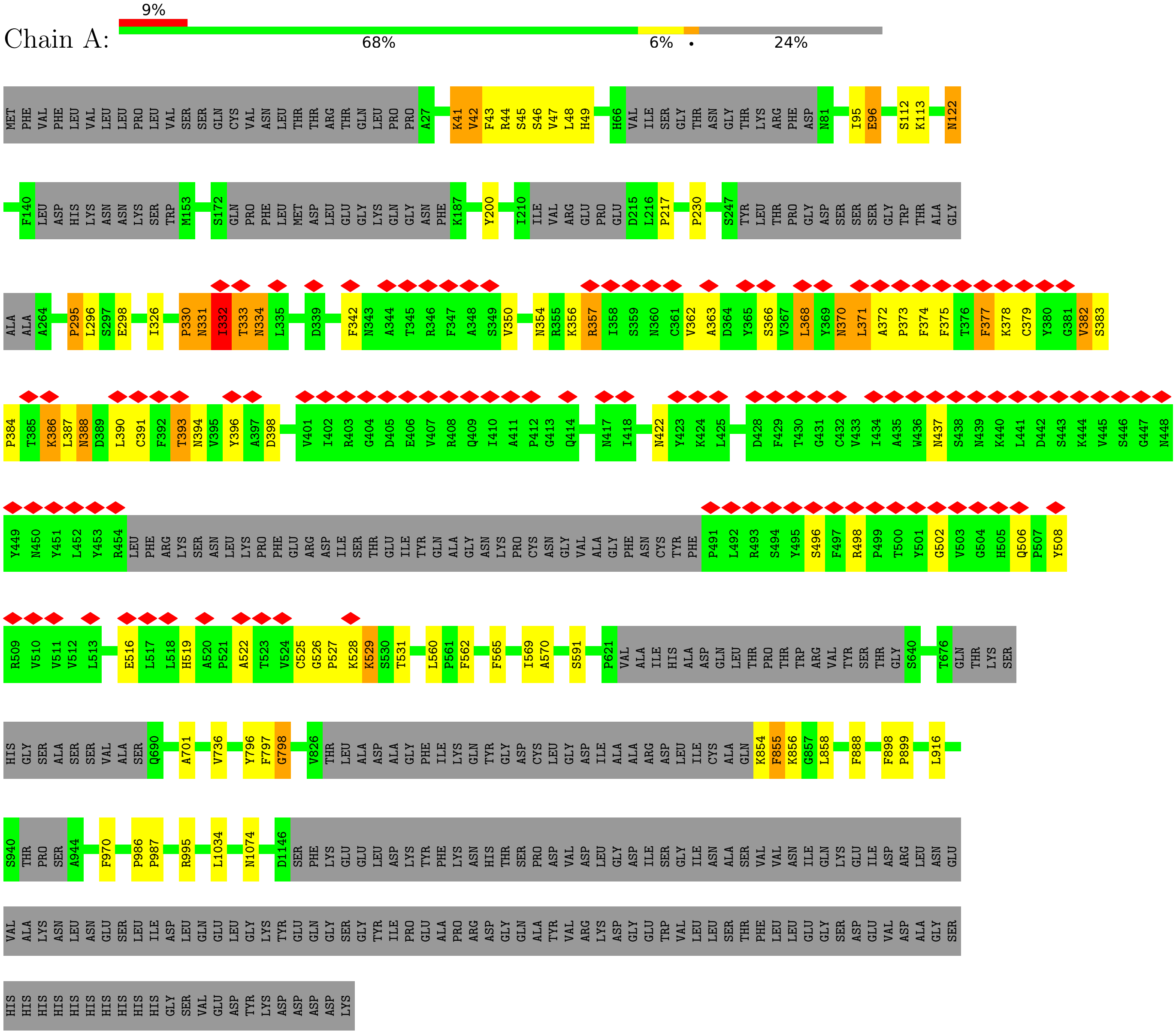
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	E	1	98	56	7	35	0
4	E	1	98	56	7	35	0

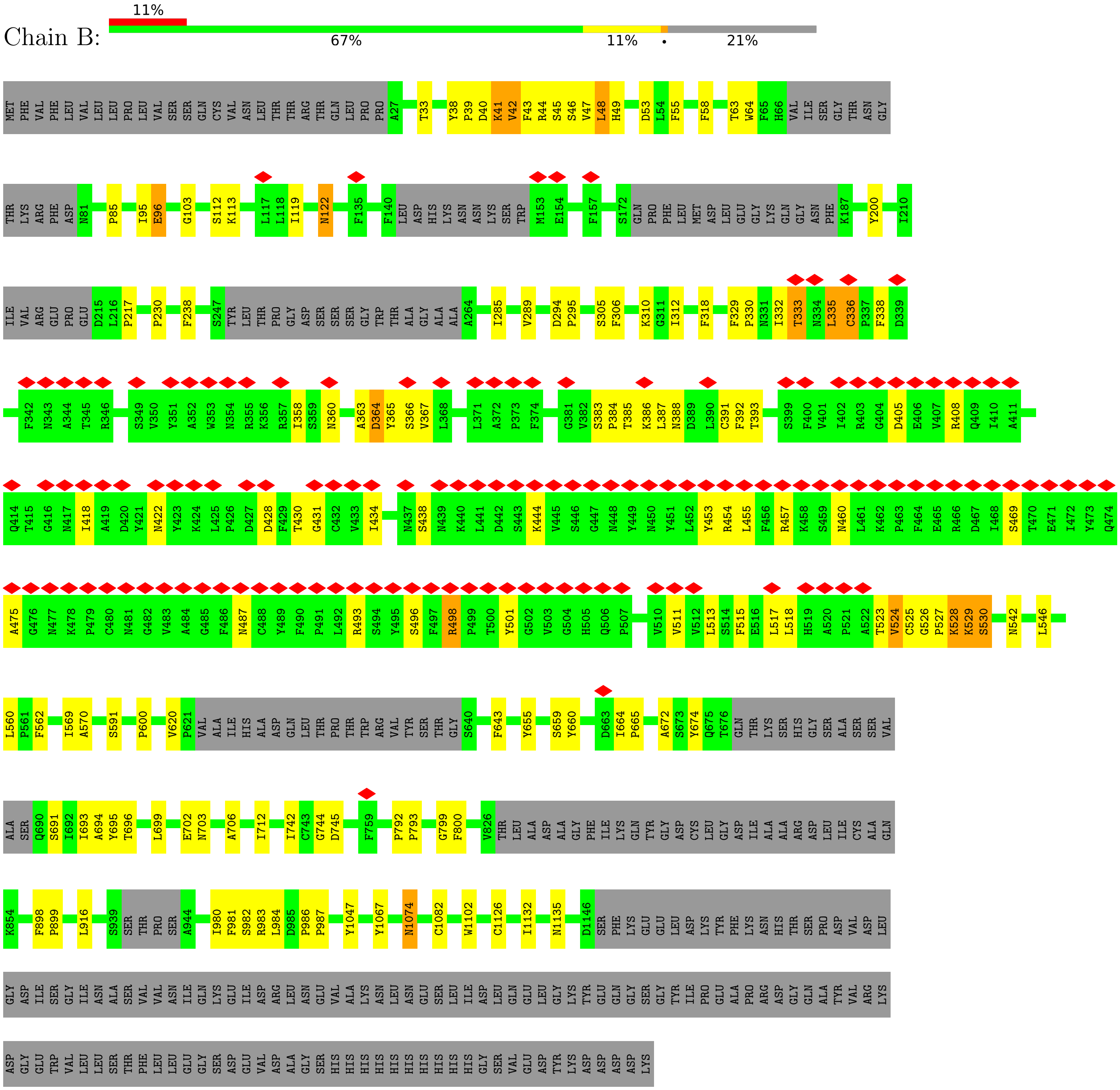
3 Residue-property plots ⓘ

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.

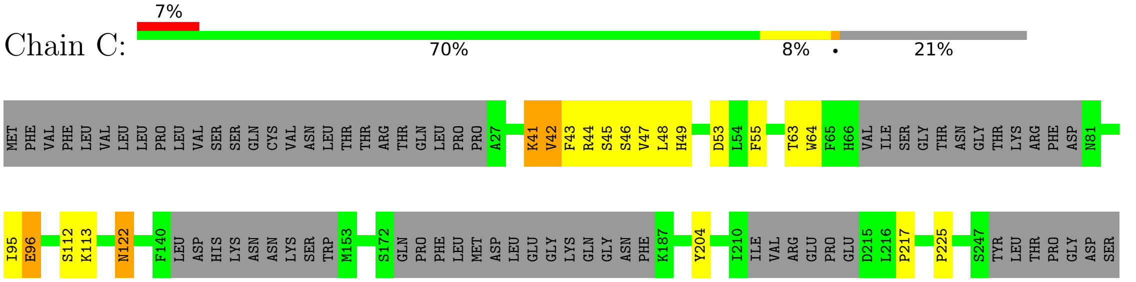
- Molecule 1: Spike glycoprotein

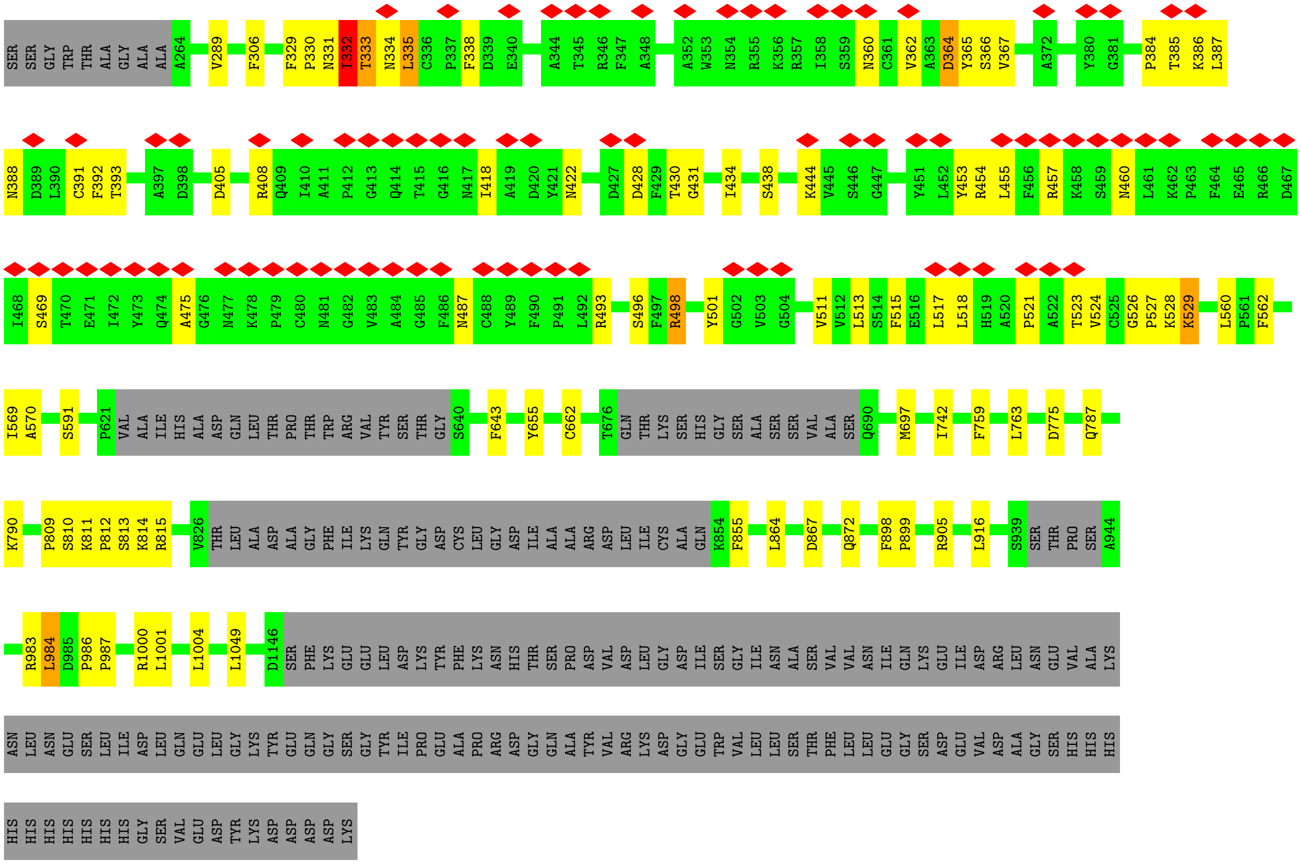


- Molecule 1: Spike glycoprotein



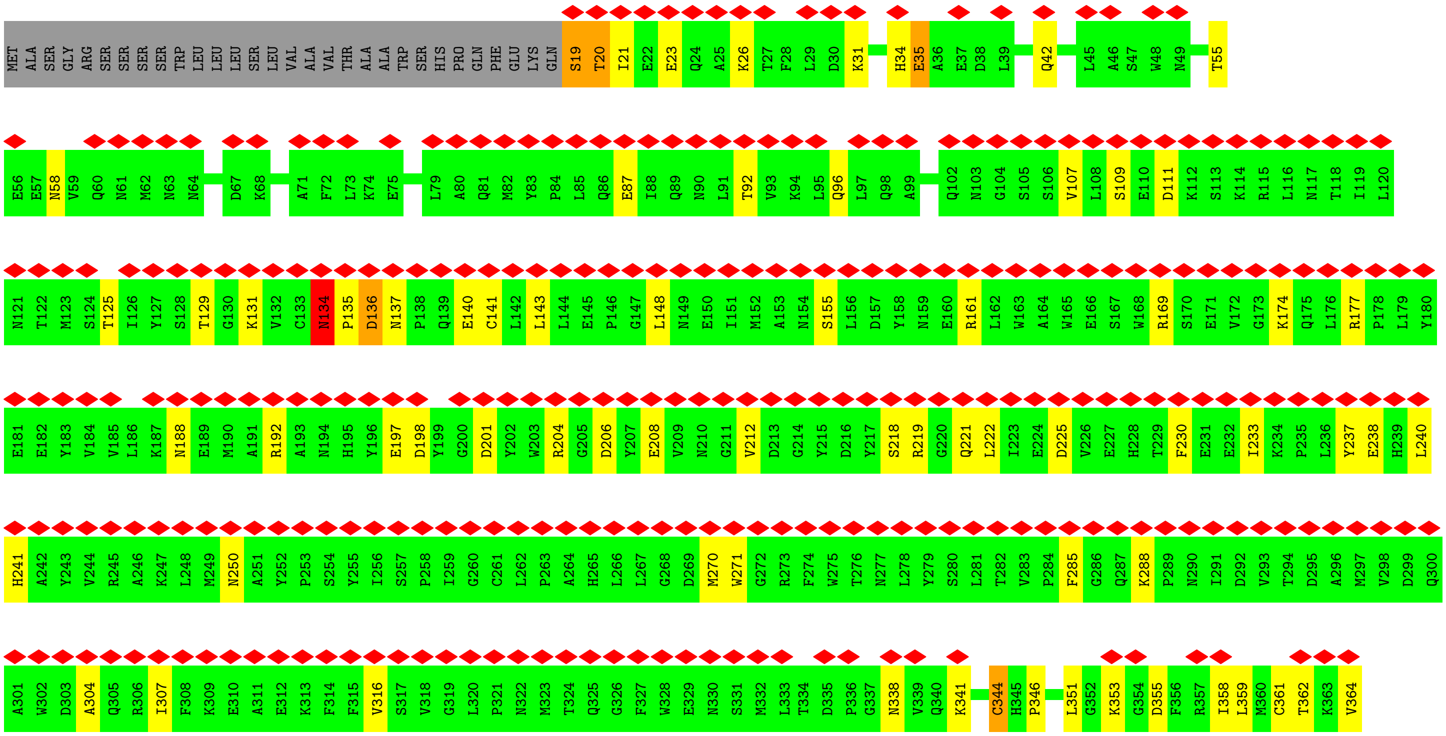
- Molecule 1: Spike glycoprotein

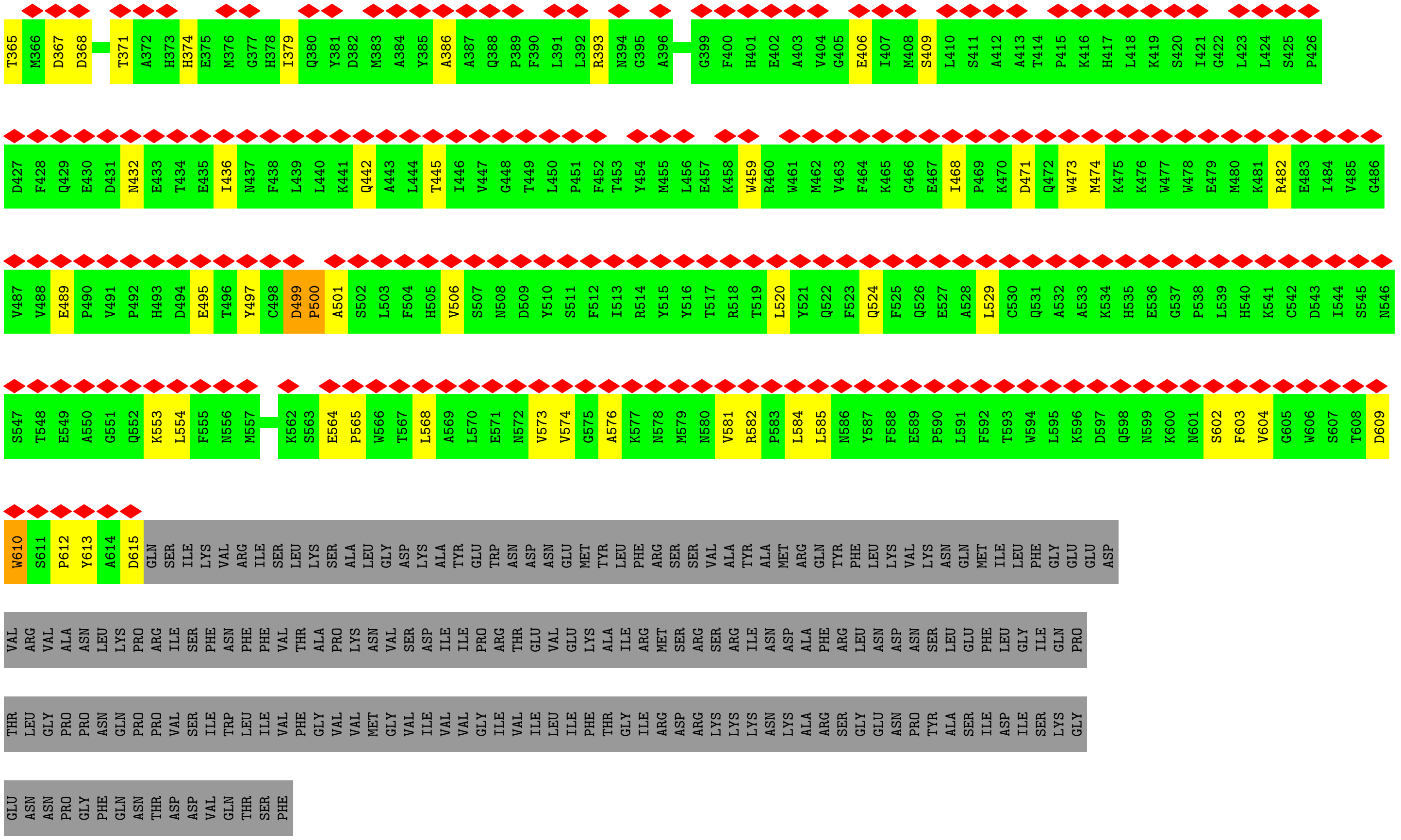




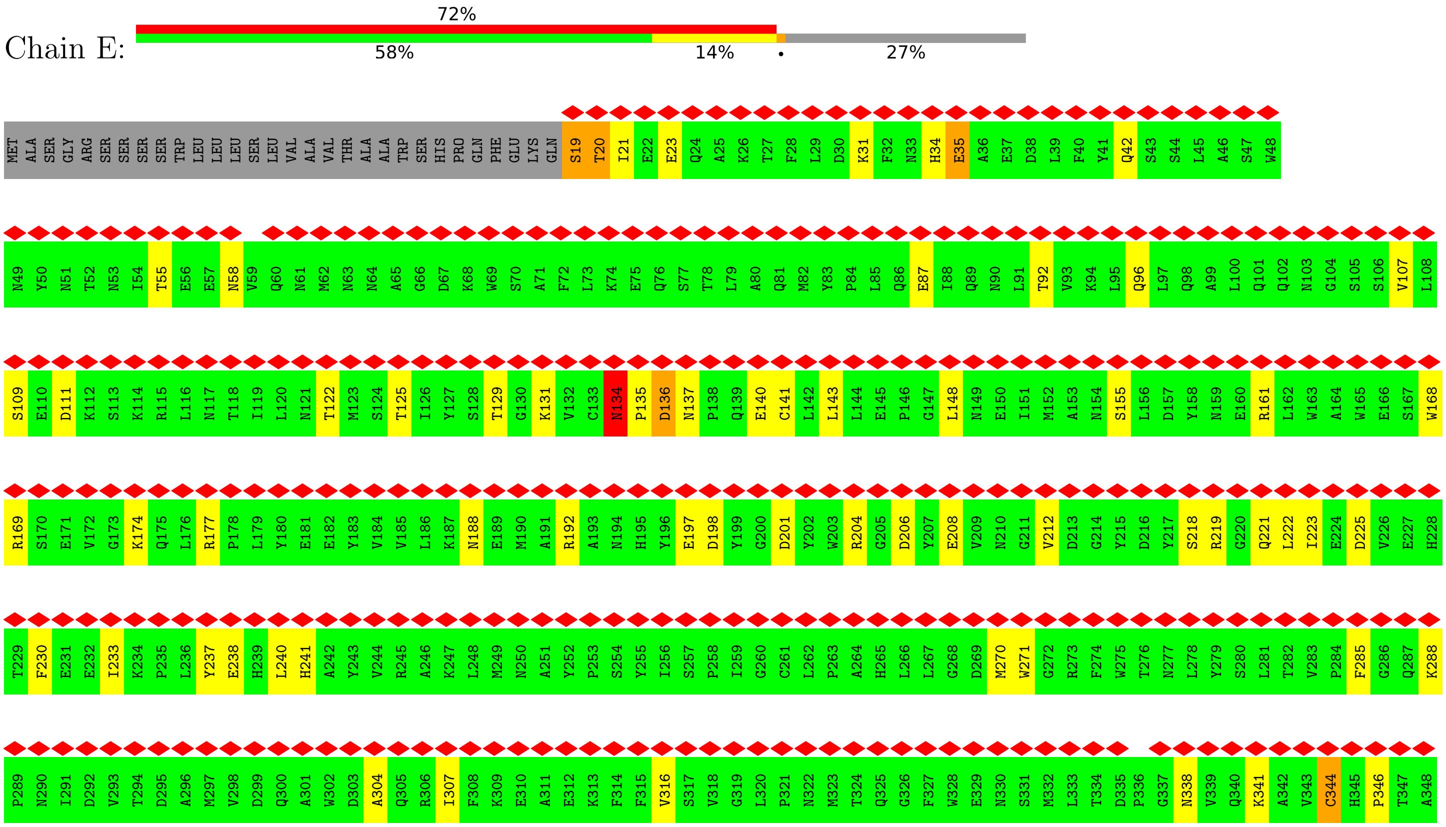
- Molecule 2: Angiotensin-converting enzyme 2

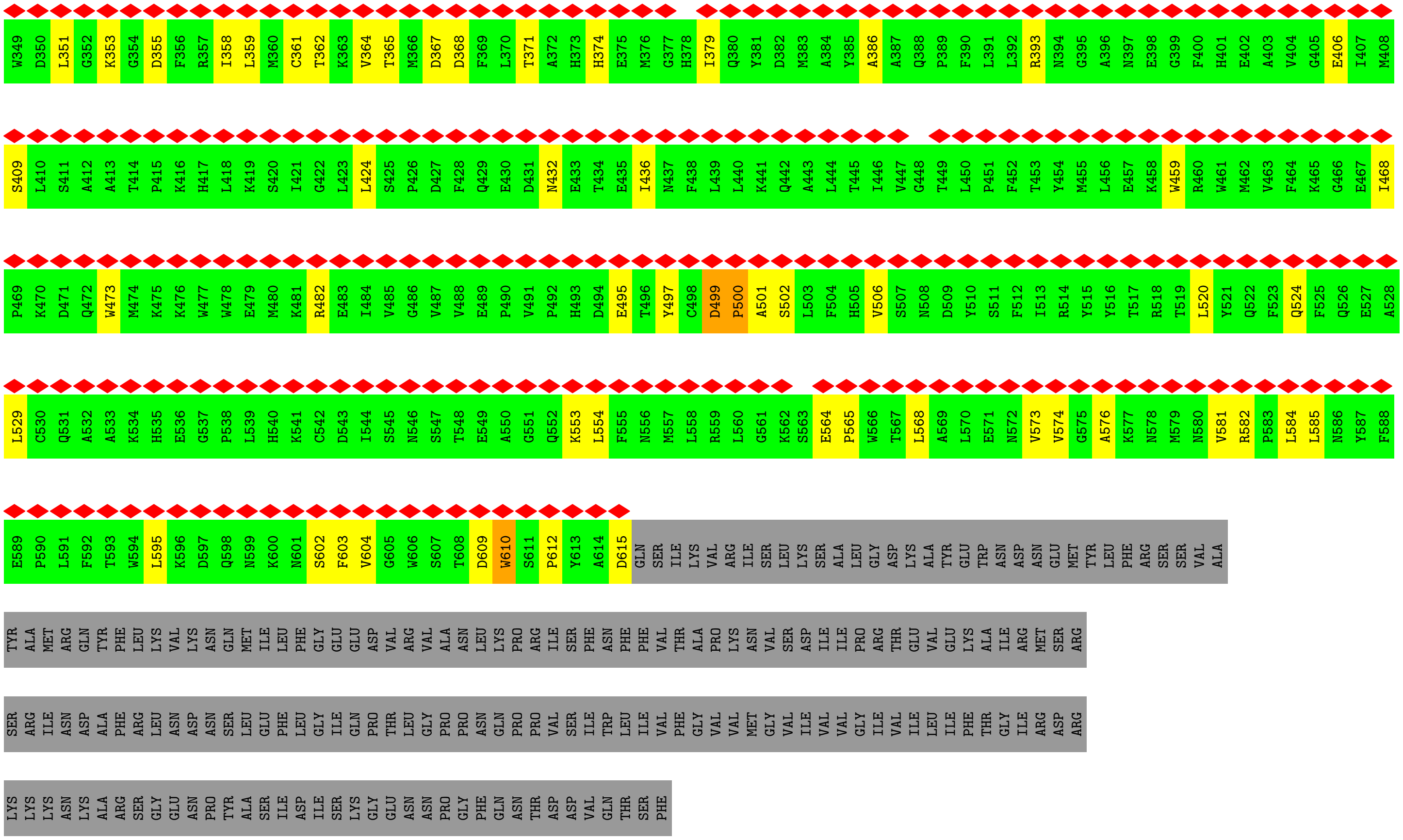
Chain D:





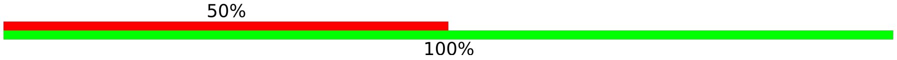
- Molecule 2: Angiotensin-converting enzyme 2





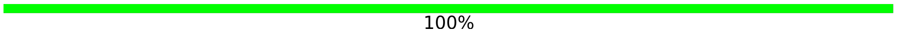
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain G:

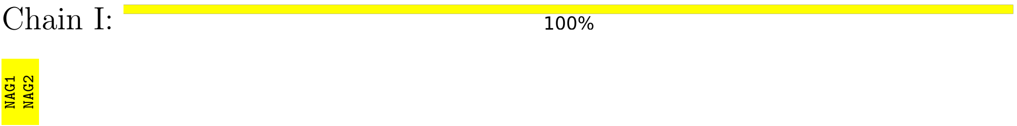


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain I:



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

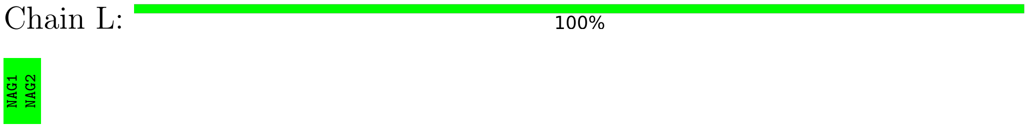
Chain J:

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

Chain K:

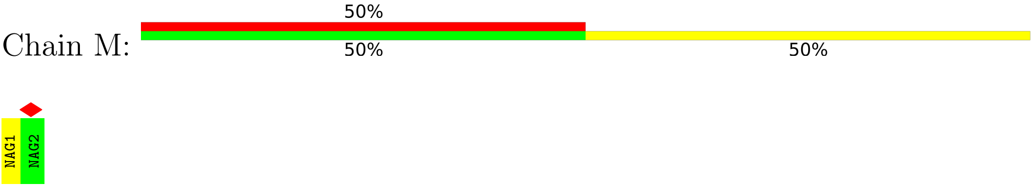
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



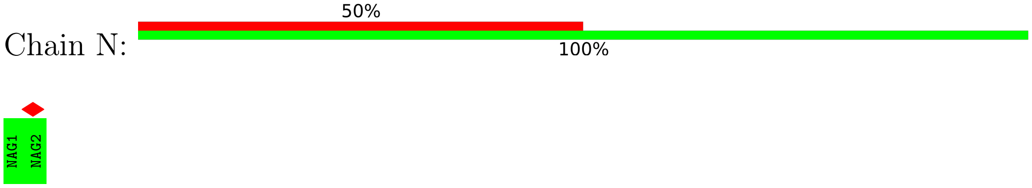
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain N:



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

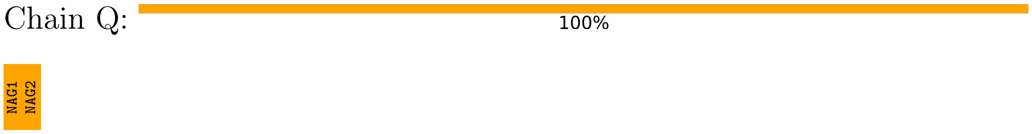
Chain O:

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

Chain P:

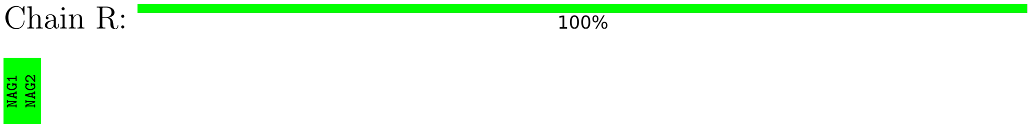
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



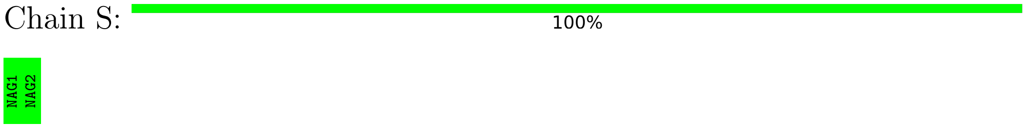
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



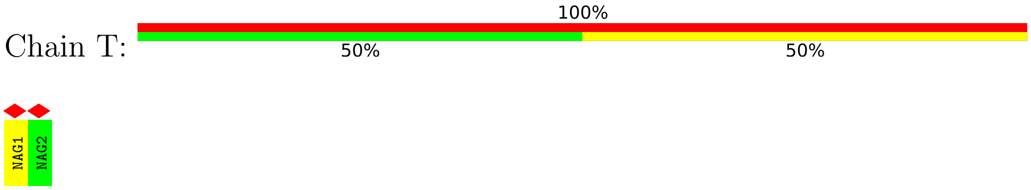
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain T:



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

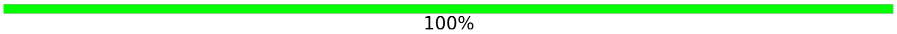
Chain U:

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

Chain V:

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

Chain W:

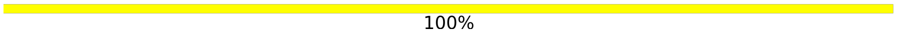


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

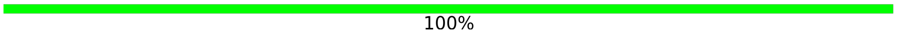
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



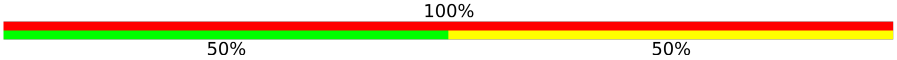
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



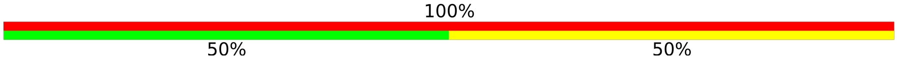
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



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

Chain b:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97021	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 ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.014	Depositor
Minimum map value	-1.616	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.58	0/7732	0.57	0/10514
1	B	0.56	0/8025	0.56	0/10911
1	C	0.56	0/8025	0.56	0/10911
2	D	0.37	0/5007	0.55	0/6803
2	E	0.37	0/5007	0.55	0/6803
All	All	0.52	0/33796	0.56	0/45942

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7558	0	7394	125	0
1	B	7842	0	7665	196	0
1	C	7842	0	7665	130	0
2	D	4870	0	4633	112	0
2	E	4870	0	4633	110	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	24	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	1	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	24	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
4	A	154	0	142	0	0
4	B	154	0	142	6	0
4	C	126	0	117	0	0
4	D	98	0	89	12	0
4	E	98	0	89	12	0
All	All	34256	0	33142	609	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 9.

The worst 5 of 609 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)
4:B:1410:NAG:O4	4:B:1411:NAG:C1	1.63	1.43
4:D:905:NAG:O4	4:D:906:NAG:C1	1.65	1.43
4:E:905:NAG:O4	4:E:906:NAG:C1	1.65	1.42
1:A:230:PRO:HB3	1:C:521:PRO:CG	1.57	1.33
1:A:230:PRO:CB	1:C:521:PRO:HG2	1.59	1.32

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	941/1267 (74%)	868 (92%)	52 (6%)	21 (2%)	6	30
1	B	978/1267 (77%)	904 (92%)	61 (6%)	13 (1%)	12	40
1	C	978/1267 (77%)	899 (92%)	62 (6%)	17 (2%)	9	35
2	D	595/817 (73%)	553 (93%)	35 (6%)	7 (1%)	13	42
2	E	595/817 (73%)	553 (93%)	35 (6%)	7 (1%)	13	42
All	All	4087/5435 (75%)	3777 (92%)	245 (6%)	65 (2%)	13	36

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	46	SER
1	A	332	ILE
1	A	591	SER
1	A	855	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	848/1108 (76%)	835 (98%)	13 (2%)	65	81
1	B	878/1108 (79%)	871 (99%)	7 (1%)	81	89
1	C	878/1108 (79%)	872 (99%)	6 (1%)	84	90
2	D	527/721 (73%)	521 (99%)	6 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	527/721 (73%)	521 (99%)	6 (1%)	73	85
All	All	3658/4766 (77%)	3620 (99%)	38 (1%)	77	86

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	134	ASN
2	E	344	CYS
2	D	344	CYS
2	E	19	SER
2	E	610	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	61	ASN
2	E	98	GLN
2	E	61	ASN
1	C	360	ASN
1	C	1005	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

46 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	F	1	3,1	14,14,15	0.54	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	G	1	3,1	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	G	2	3	14,14,15	0.54	0	17,19,21	0.48	0
3	NAG	H	1	3,1	14,14,15	0.37	0	17,19,21	0.72	0
3	NAG	H	2	3	14,14,15	0.28	0	17,19,21	1.31	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
3	NAG	I	2	3	14,14,15	0.38	0	17,19,21	1.41	3 (17%)
3	NAG	J	1	3,1	14,14,15	0.71	1 (7%)	17,19,21	0.66	0
3	NAG	J	2	3	14,14,15	0.28	0	17,19,21	0.65	0
3	NAG	K	1	3,1	14,14,15	0.24	0	17,19,21	0.68	1 (5%)
3	NAG	K	2	3	14,14,15	0.17	0	17,19,21	0.47	0
3	NAG	L	1	3,1	14,14,15	0.54	0	17,19,21	0.50	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.57	0
3	NAG	M	1	3,1	14,14,15	0.60	1 (7%)	17,19,21	0.57	0
3	NAG	M	2	3	14,14,15	0.30	0	17,19,21	0.45	0
3	NAG	N	1	3,1	14,14,15	0.31	0	17,19,21	0.40	0
3	NAG	N	2	3	14,14,15	0.36	0	17,19,21	0.36	0
3	NAG	O	1	3,1	14,14,15	0.33	0	17,19,21	1.14	1 (5%)
3	NAG	O	2	3	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	P	1	3,1	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
3	NAG	P	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	Q	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	Q	2	3	14,14,15	0.35	0	17,19,21	0.71	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	R	2	3	14,14,15	0.28	0	17,19,21	0.38	0
3	NAG	S	1	3,1	14,14,15	0.53	0	17,19,21	0.50	0
3	NAG	S	2	3	14,14,15	0.24	0	17,19,21	0.58	0
3	NAG	T	1	3,1	14,14,15	0.60	1 (7%)	17,19,21	0.57	0
3	NAG	T	2	3	14,14,15	0.29	0	17,19,21	0.45	0
3	NAG	U	1	3,1	14,14,15	0.23	0	17,19,21	1.37	1 (5%)
3	NAG	U	2	3	14,14,15	0.16	0	17,19,21	0.49	0
3	NAG	V	1	3,1	14,14,15	0.53	0	17,19,21	0.70	1 (5%)
3	NAG	V	2	3	14,14,15	0.39	0	17,19,21	0.47	0
3	NAG	W	1	3,1	14,14,15	0.39	0	17,19,21	0.41	0
3	NAG	W	2	3	14,14,15	0.21	0	17,19,21	0.74	0
3	NAG	X	1	3,1	14,14,15	0.37	0	17,19,21	0.48	0
3	NAG	X	2	3	14,14,15	0.57	0	17,19,21	1.30	1 (5%)
3	NAG	Y	1	3,1	14,14,15	0.64	1 (7%)	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	Y	2	3	14,14,15	0.33	0	17,19,21	1.35	2 (11%)
3	NAG	Z	1	3,1	14,14,15	0.40	0	17,19,21	0.45	0
3	NAG	Z	2	3	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	a	1	3,2	14,14,15	0.60	1 (7%)	17,19,21	0.73	0
3	NAG	a	2	3	14,14,15	0.53	0	17,19,21	0.38	0
3	NAG	b	1	3,2	14,14,15	0.62	1 (7%)	17,19,21	0.73	0
3	NAG	b	2	3	14,14,15	0.53	0	17,19,21	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	T	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	4/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	O5-C1	-2.73	1.39	1.43
3	J	1	NAG	O5-C1	-2.58	1.39	1.43
3	I	1	NAG	O5-C1	-2.31	1.40	1.43
3	b	1	NAG	O5-C1	-2.19	1.40	1.43
3	Y	1	NAG	O5-C1	-2.17	1.40	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	1	NAG	C2-N2-C7	4.72	129.62	122.90
3	I	2	NAG	C2-N2-C7	4.45	129.24	122.90
3	Y	2	NAG	C2-N2-C7	4.32	129.06	122.90
3	X	2	NAG	C2-N2-C7	4.31	129.04	122.90
3	H	2	NAG	C2-N2-C7	4.25	128.96	122.90

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

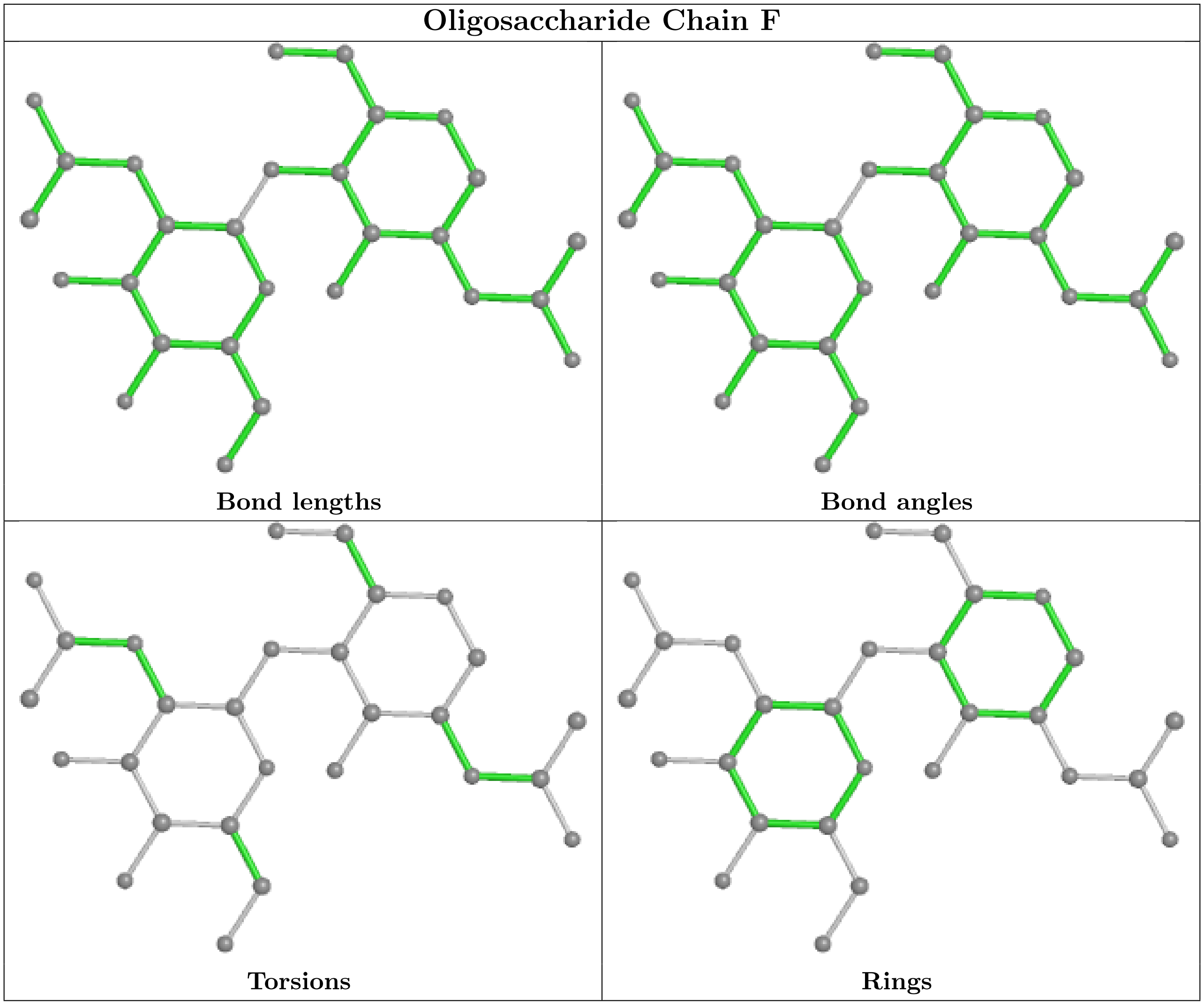
Mol	Chain	Res	Type	Atoms
3	a	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6

There are no ring outliers.

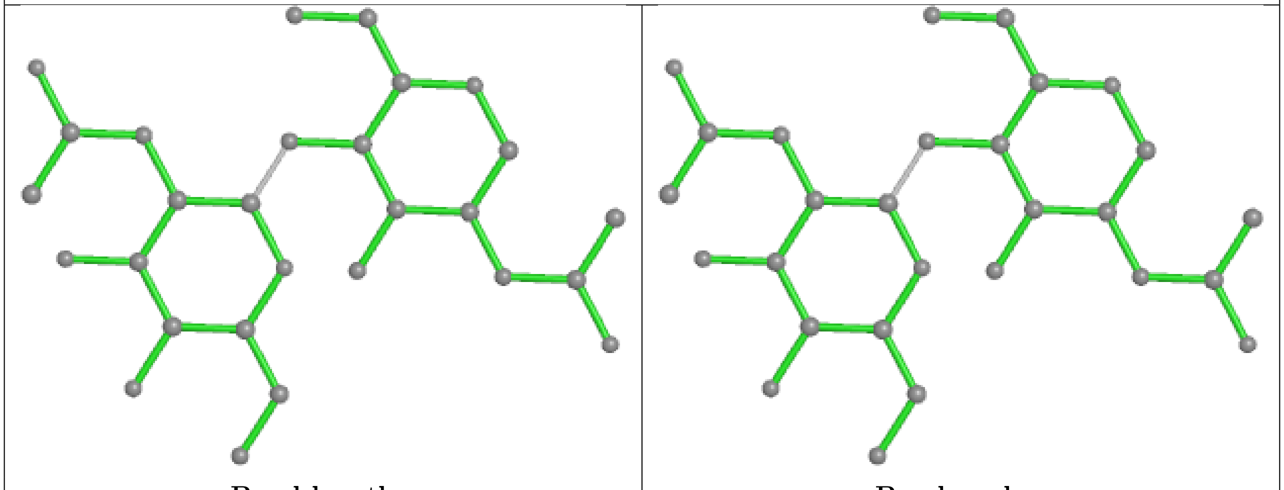
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	2	NAG	1	0
3	Q	1	NAG	1	0

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

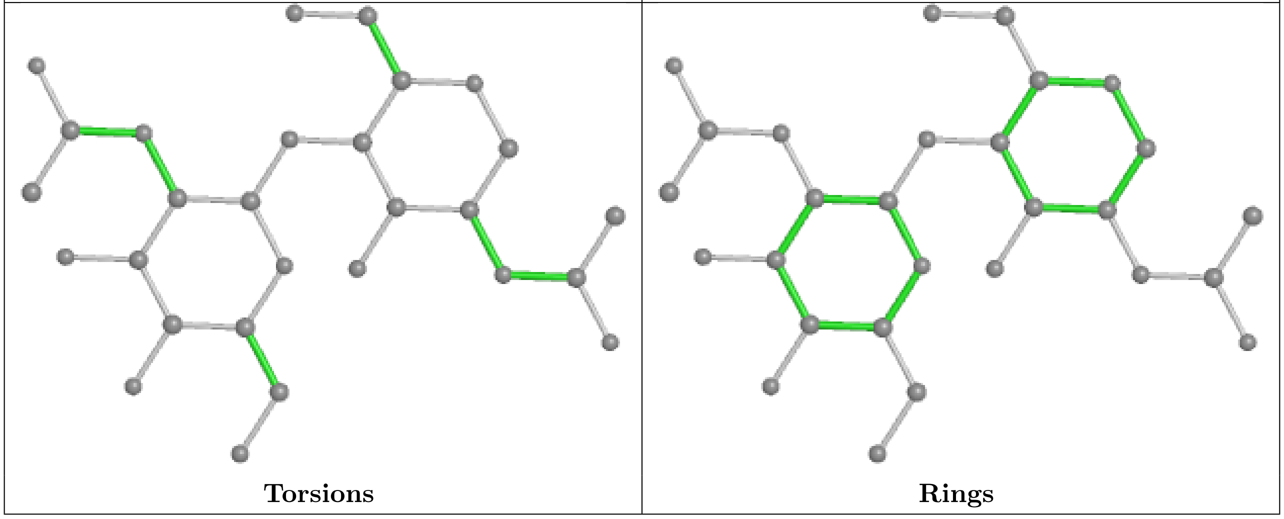

Oligosaccharide Chain F

Oligosaccharide Chain G



Bond lengths

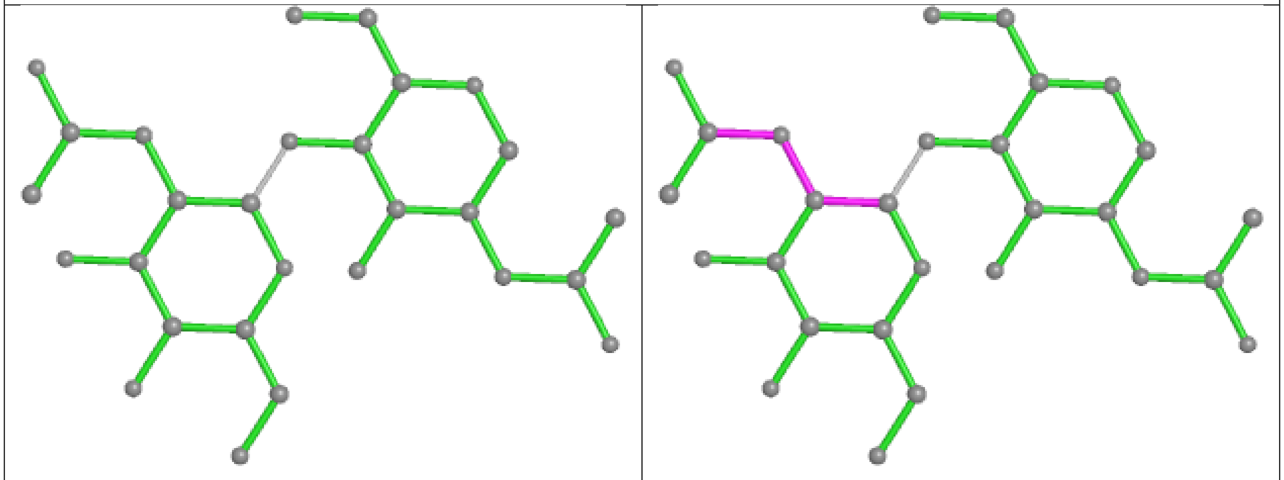
Bond angles



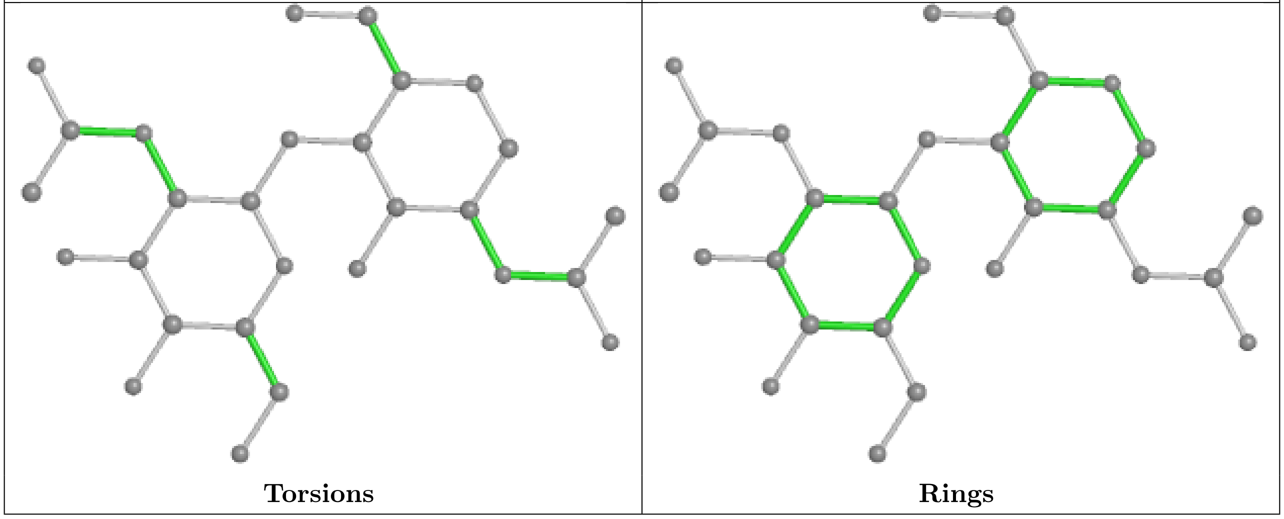
Torsions

Rings

Oligosaccharide Chain H

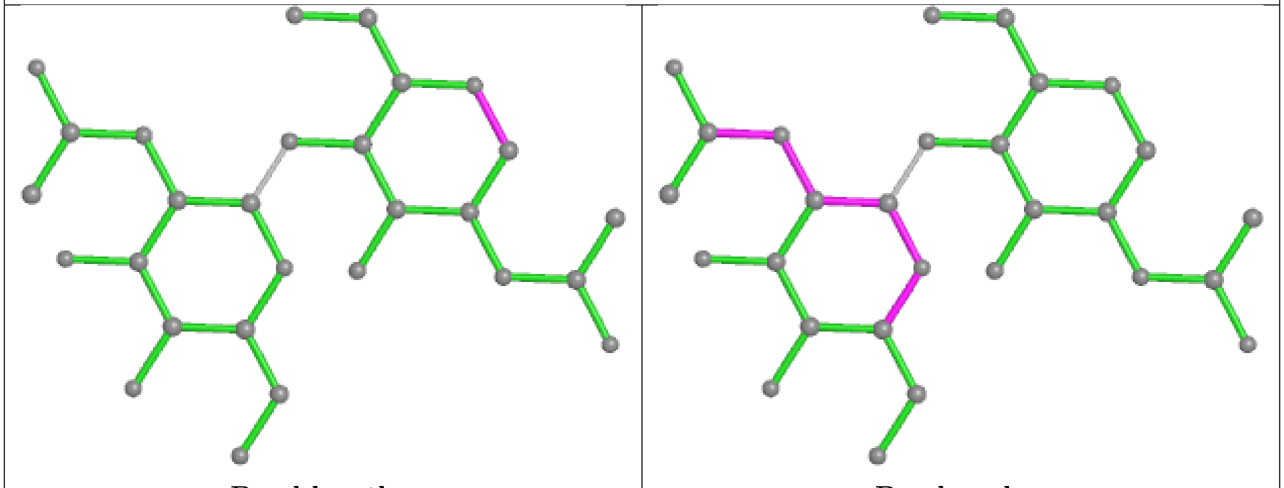


Bond lengths **Bond angles**

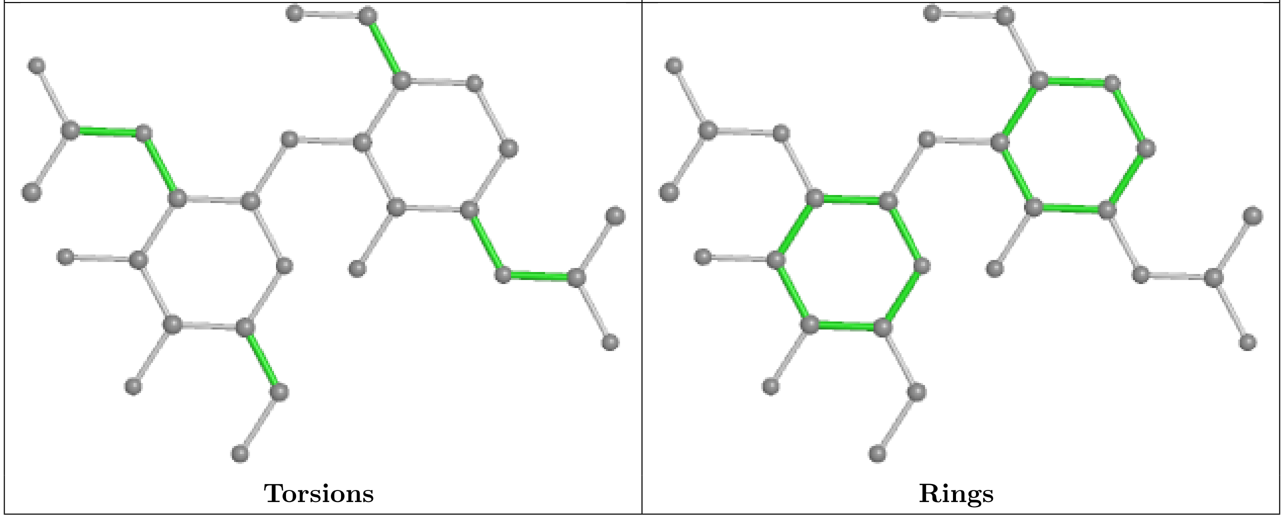


Torsions **Rings**

Oligosaccharide Chain I

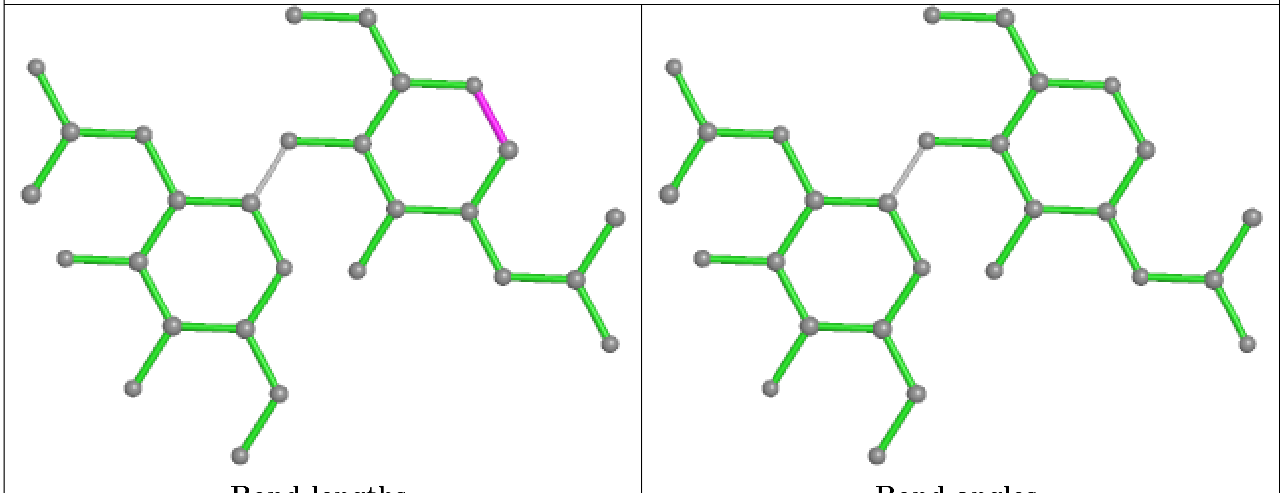


Bond lengths **Bond angles**

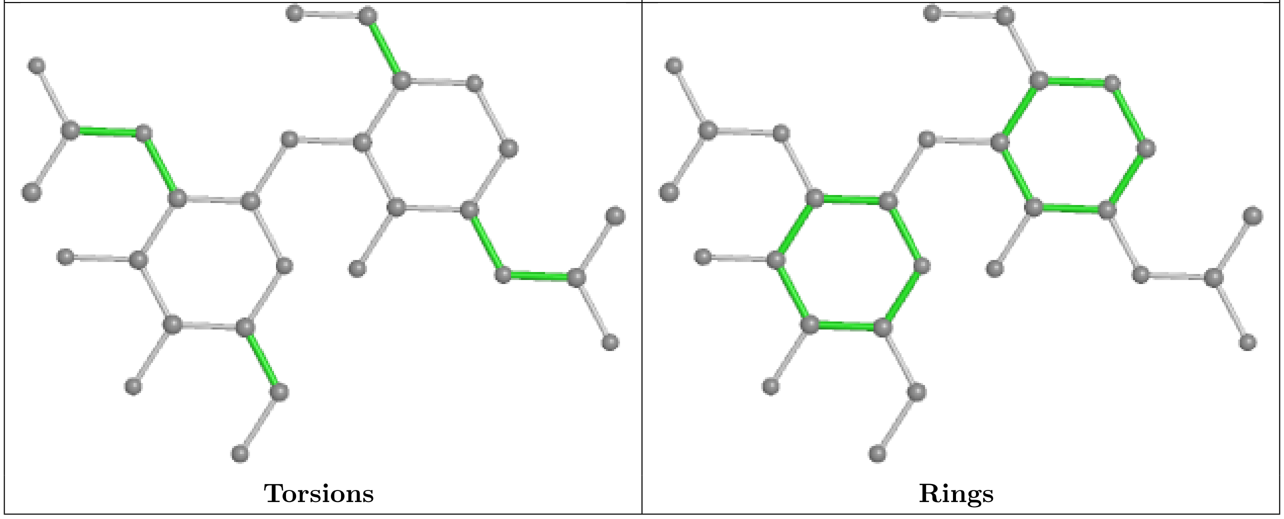


Torsions **Rings**

Oligosaccharide Chain J

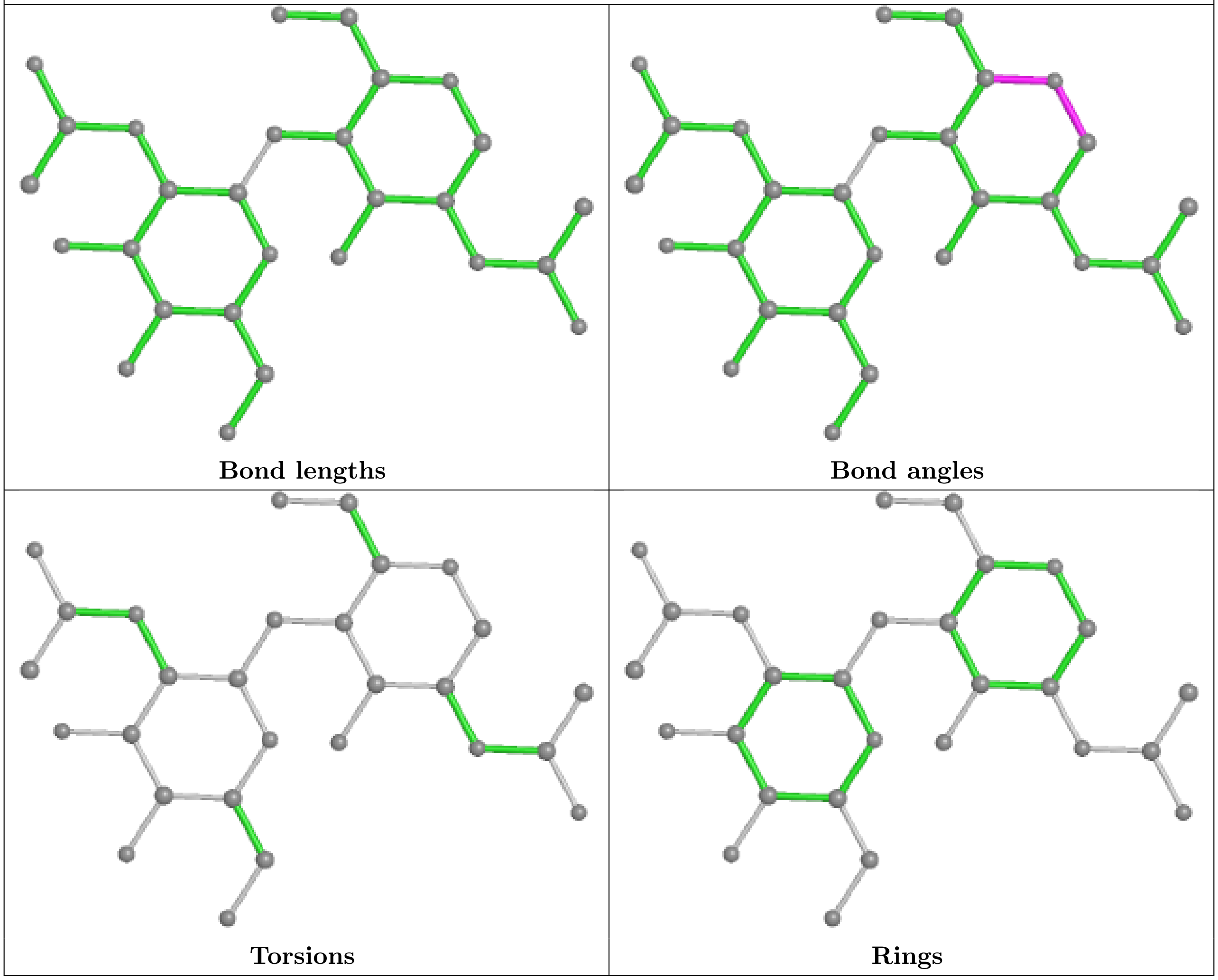


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain K



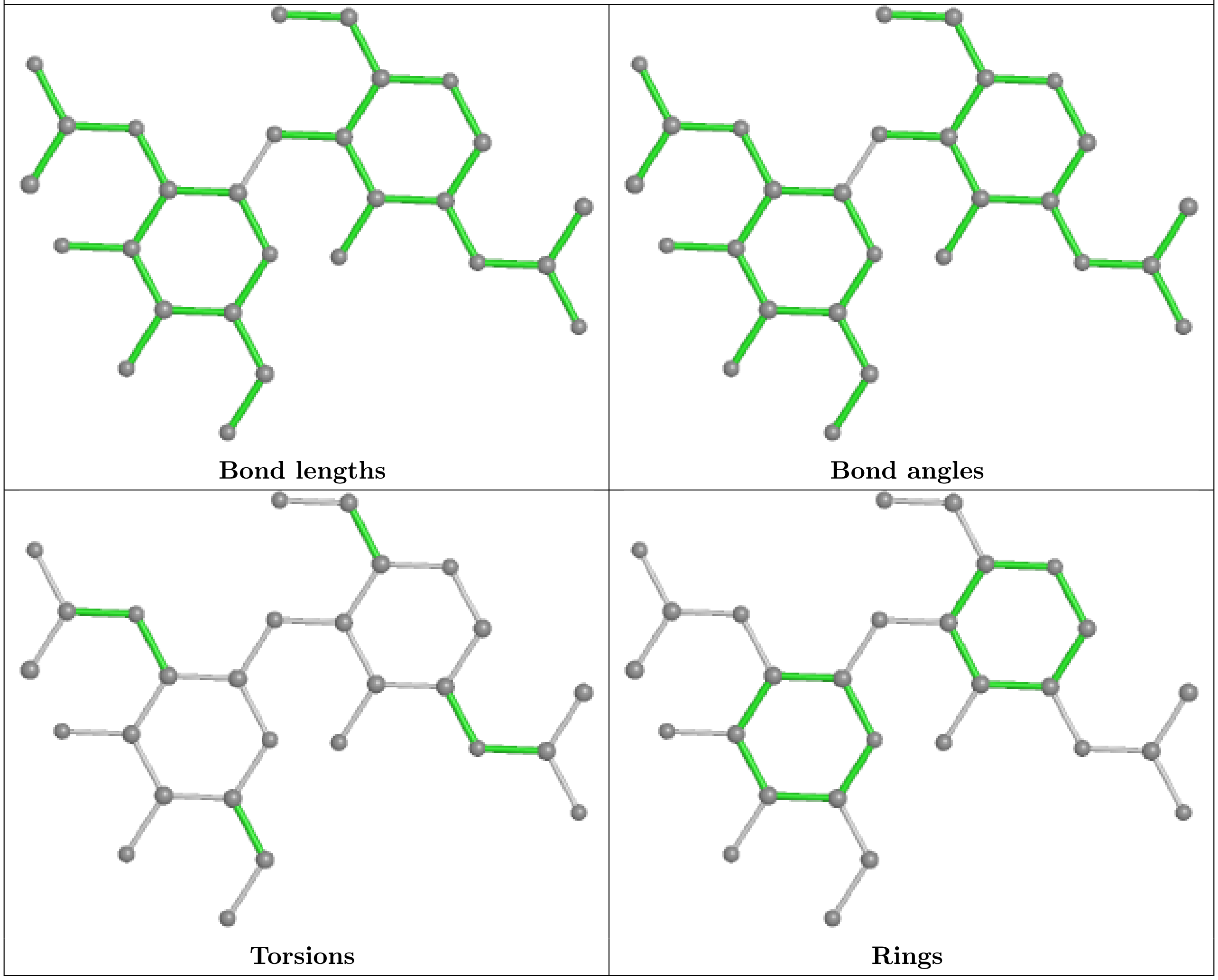
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L



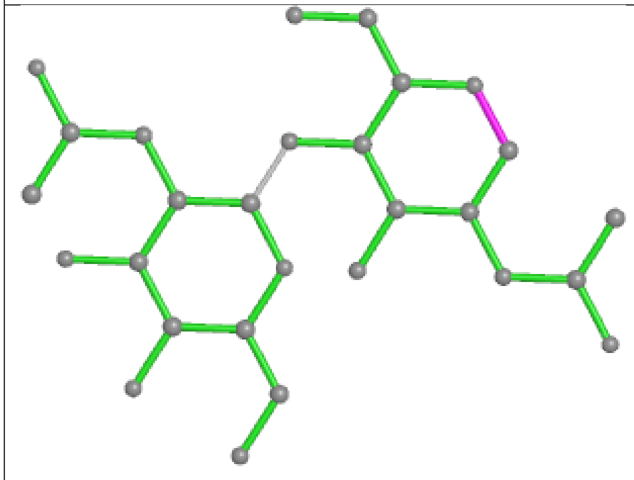
Bond lengths

Bond angles

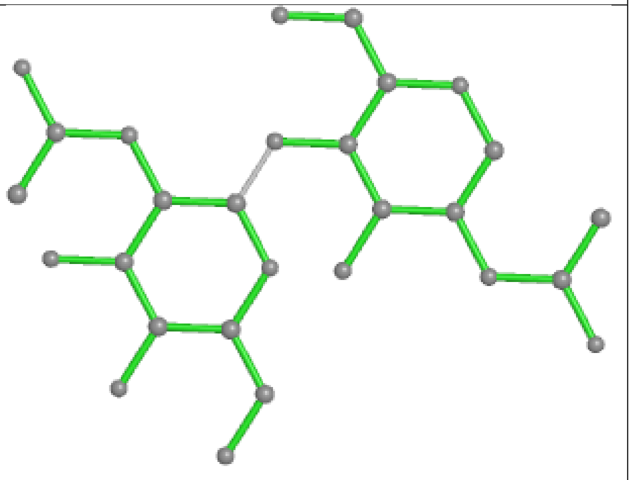
Torsions

Rings

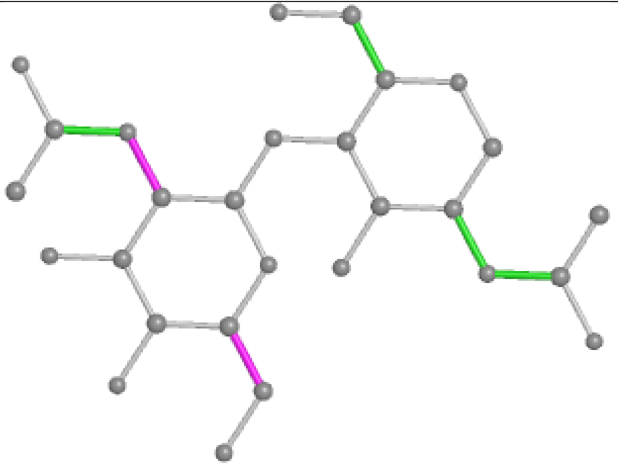
Oligosaccharide Chain M



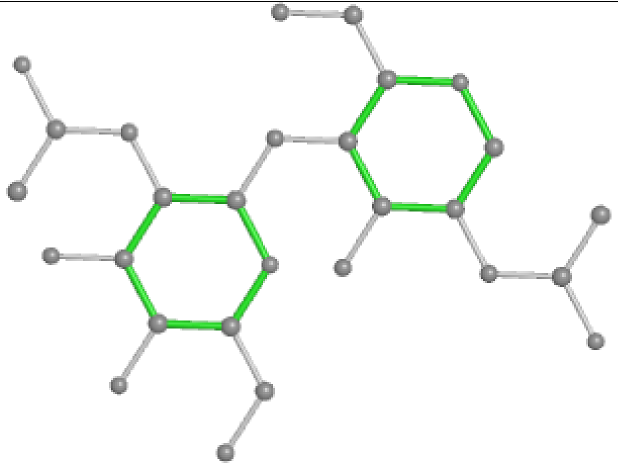
Bond lengths



Bond angles

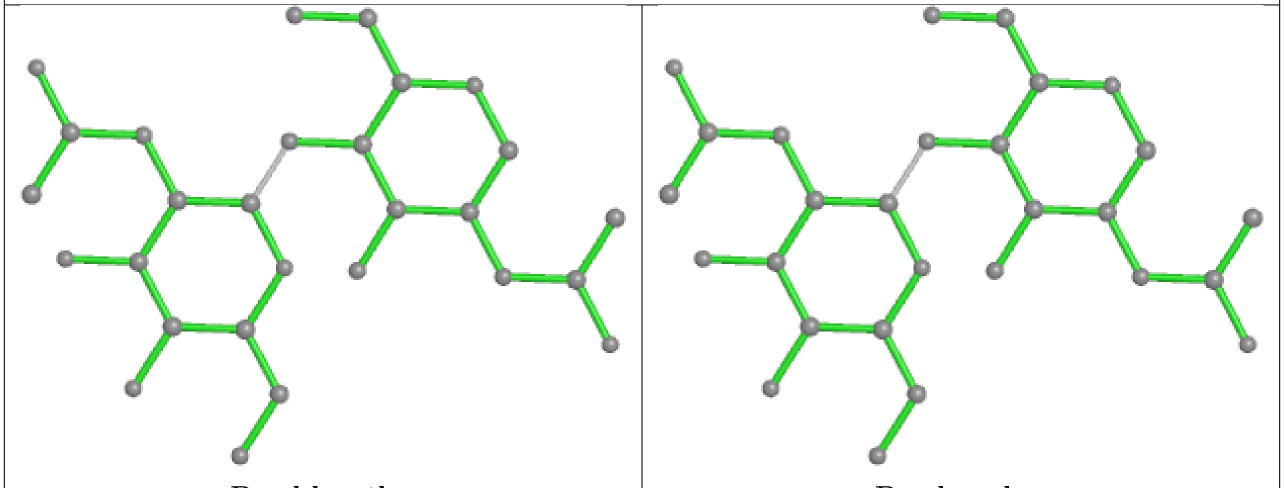


Torsions

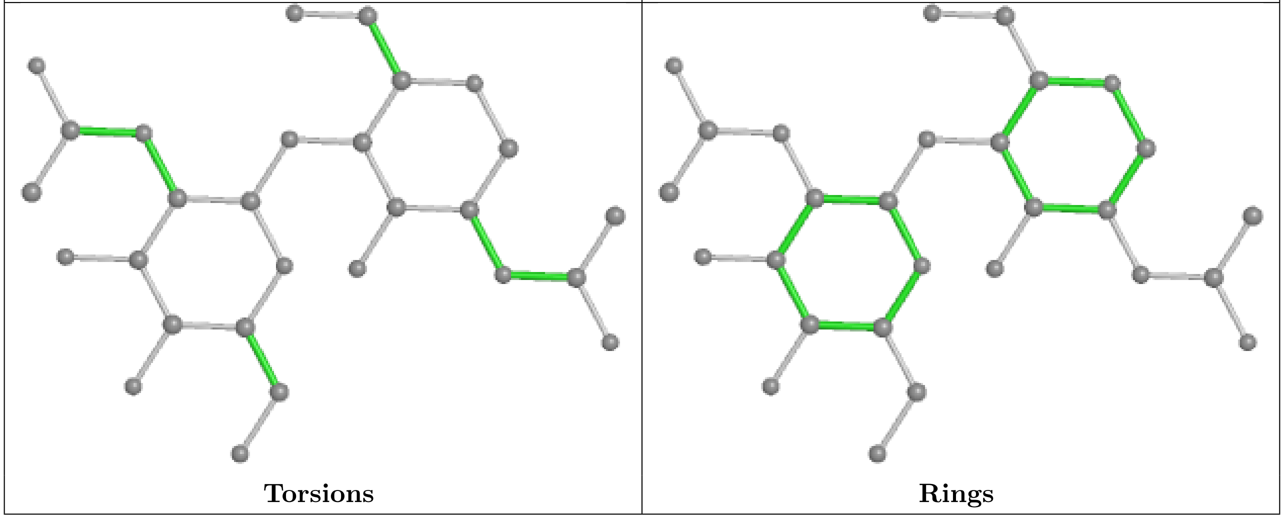


Rings

Oligosaccharide Chain N

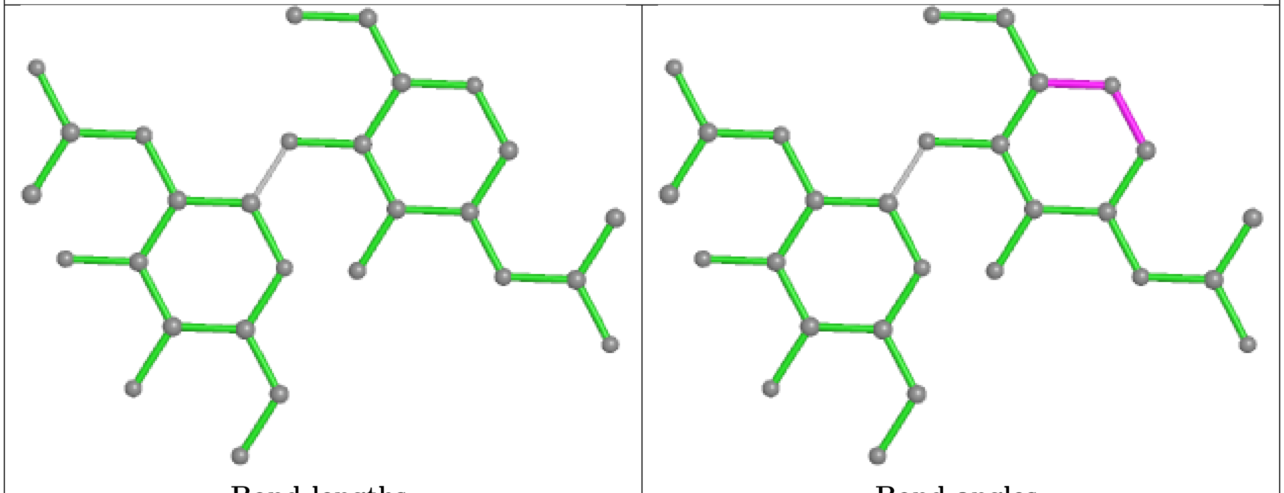


Bond lengths **Bond angles**

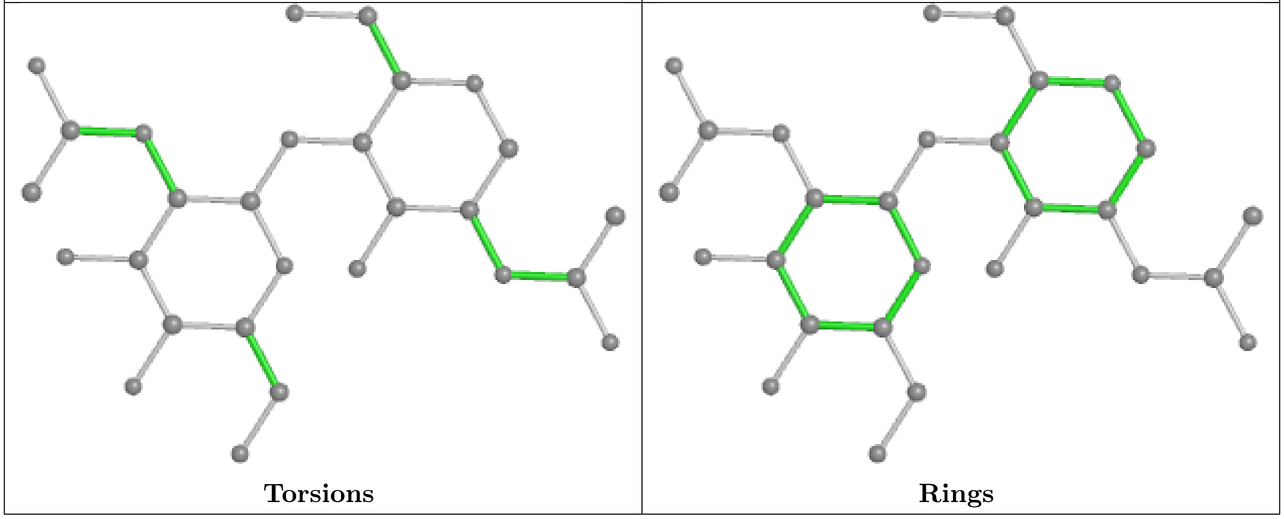


Torsions **Rings**

Oligosaccharide Chain O

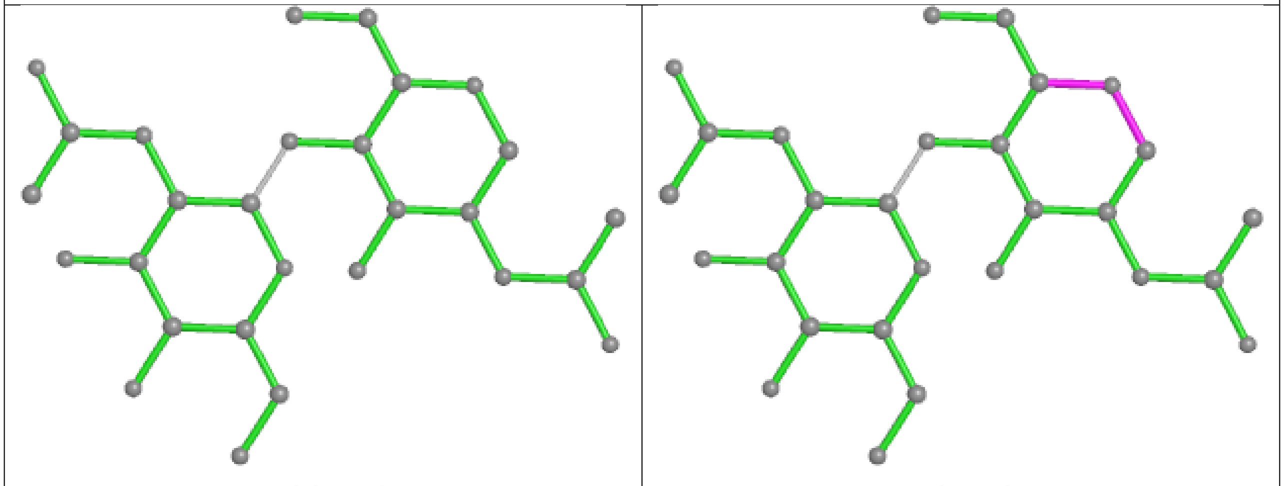


Bond lengths **Bond angles**



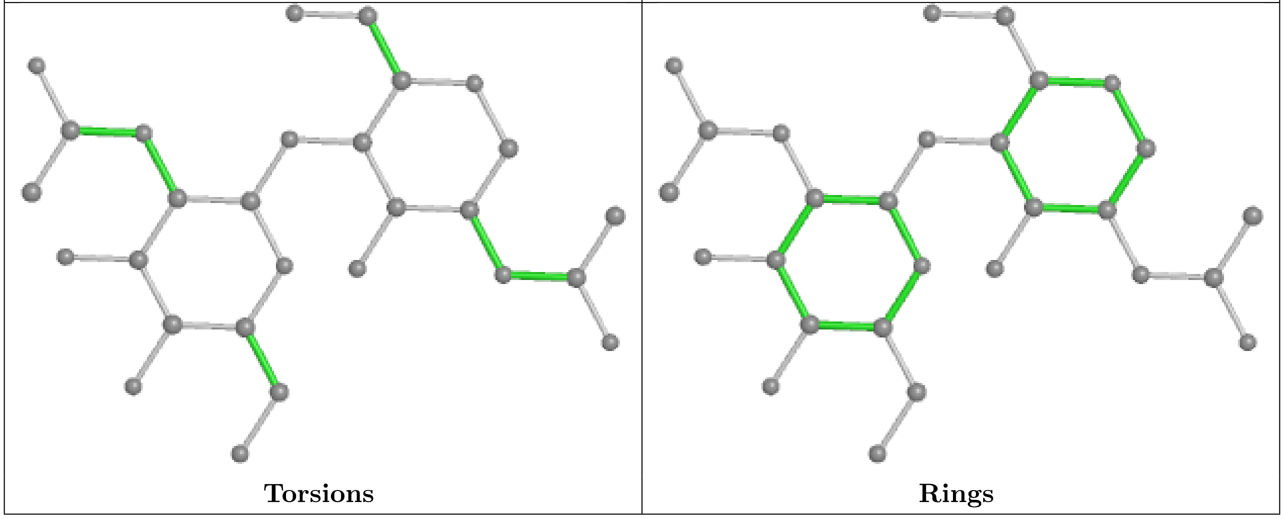
Torsions **Rings**

Oligosaccharide Chain P



Bond lengths

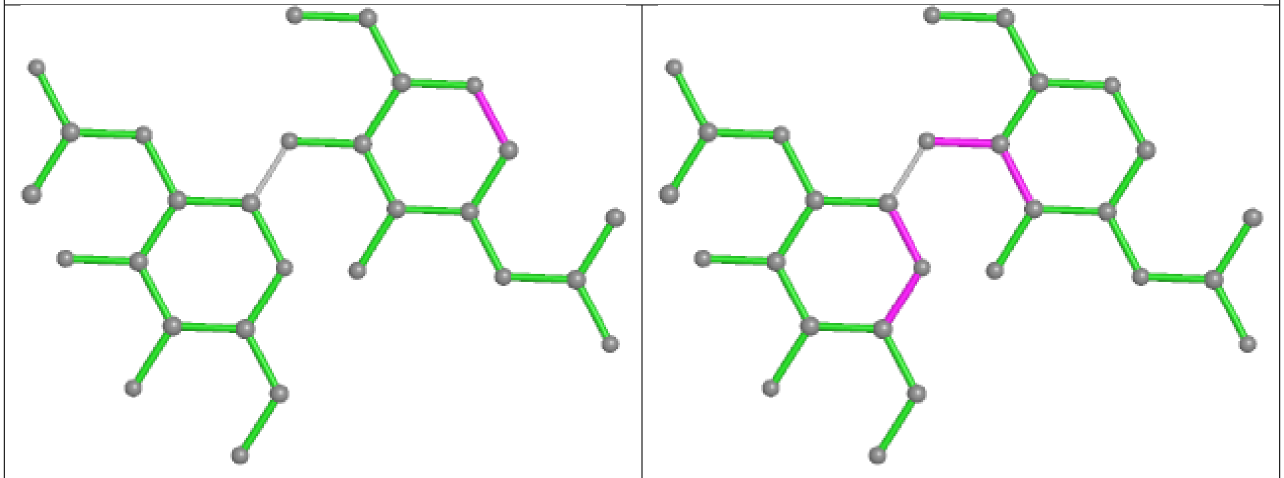
Bond angles



Torsions

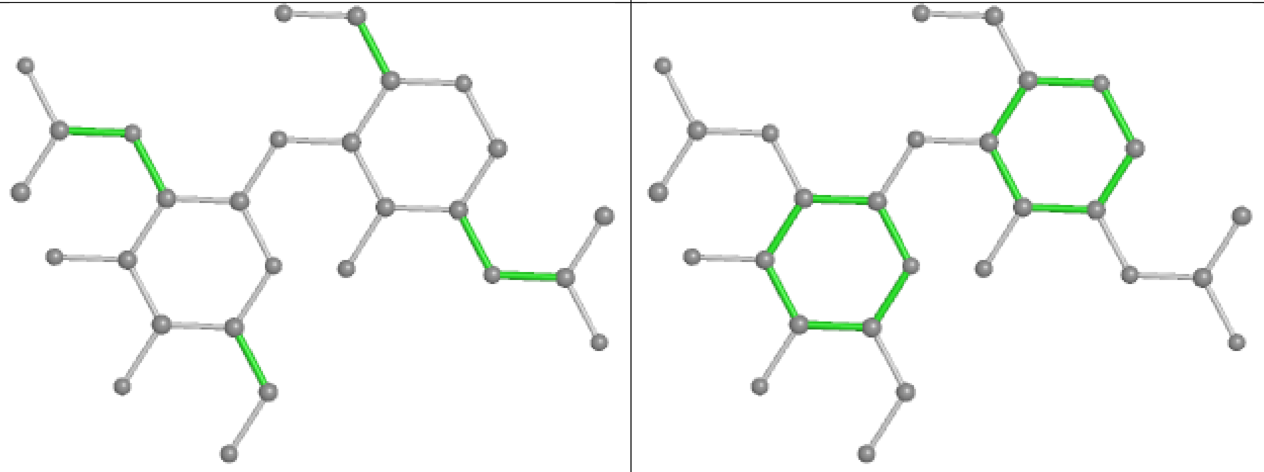
Rings

Oligosaccharide Chain Q



Bond lengths

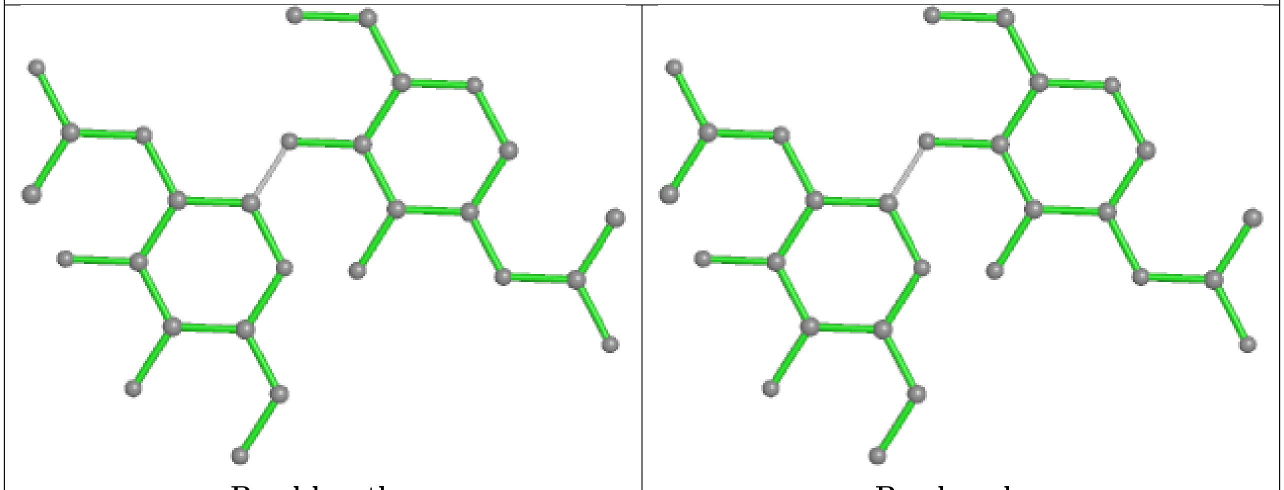
Bond angles



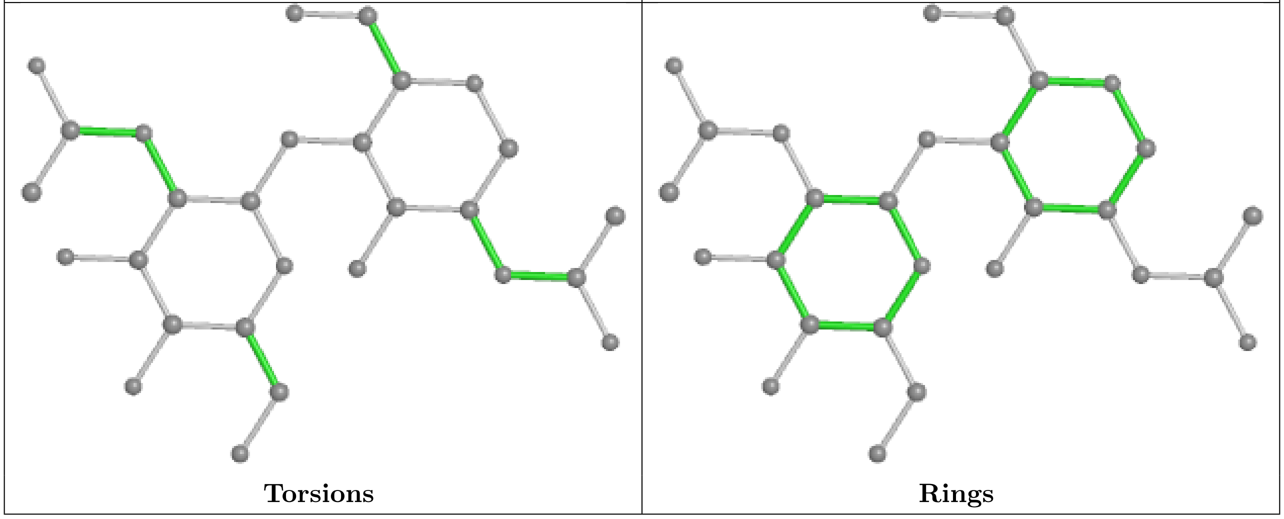
Torsions

Rings

Oligosaccharide Chain R

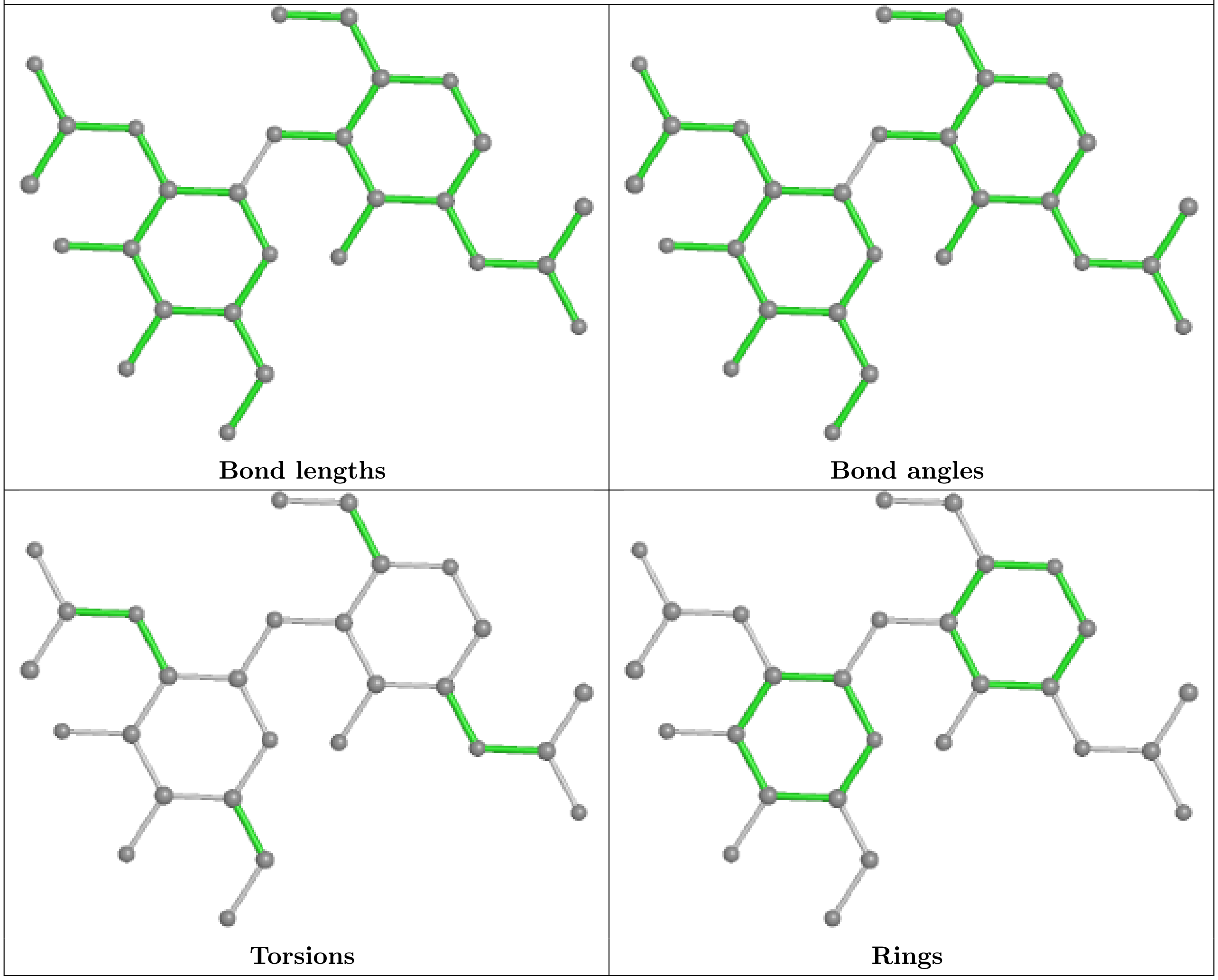


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain S



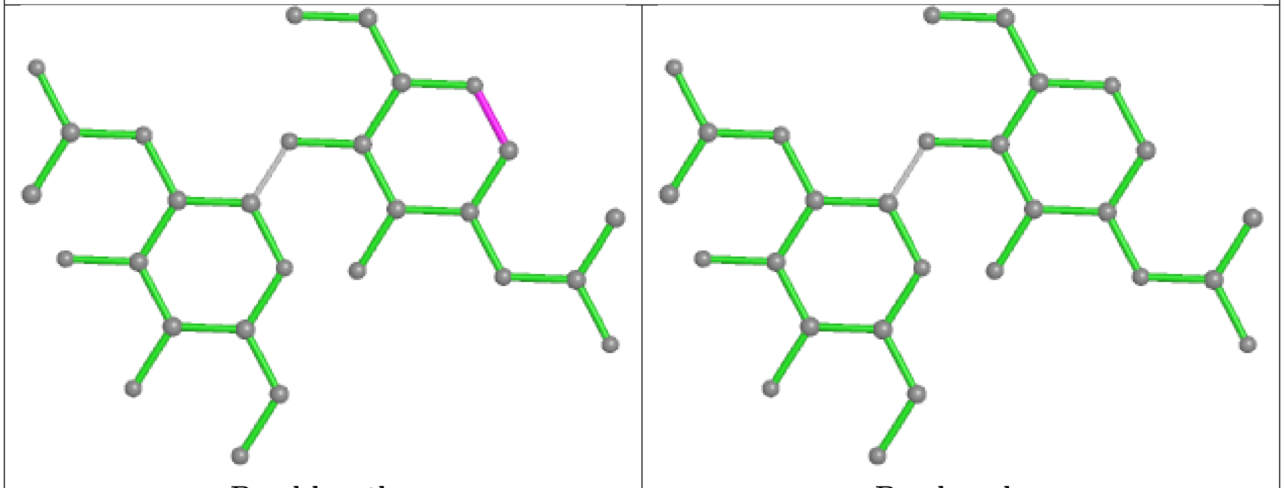
Bond lengths

Bond angles

Torsions

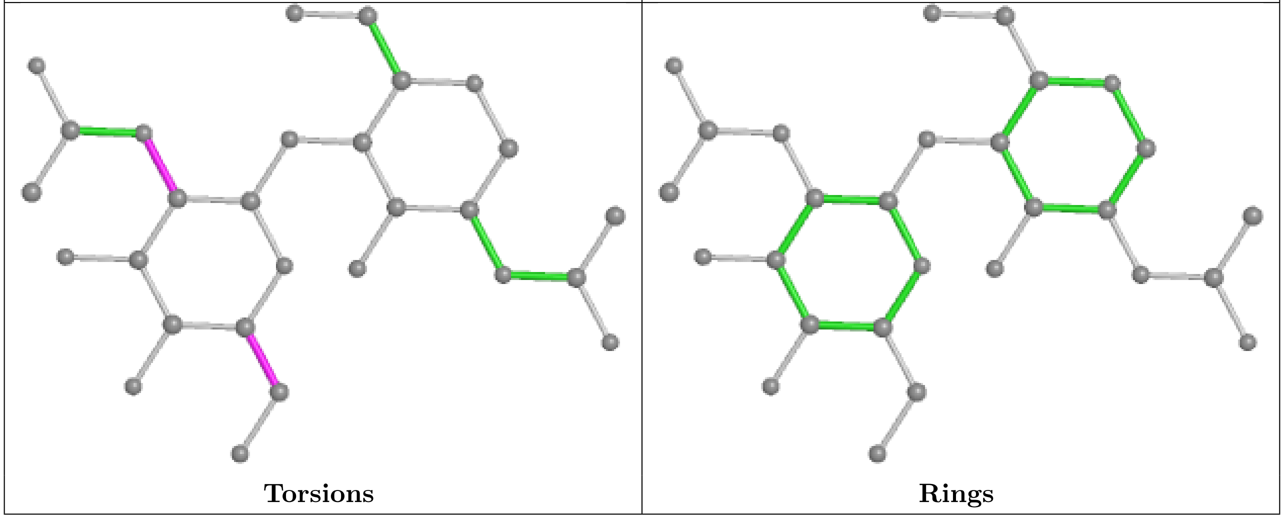
Rings

Oligosaccharide Chain T



Bond lengths

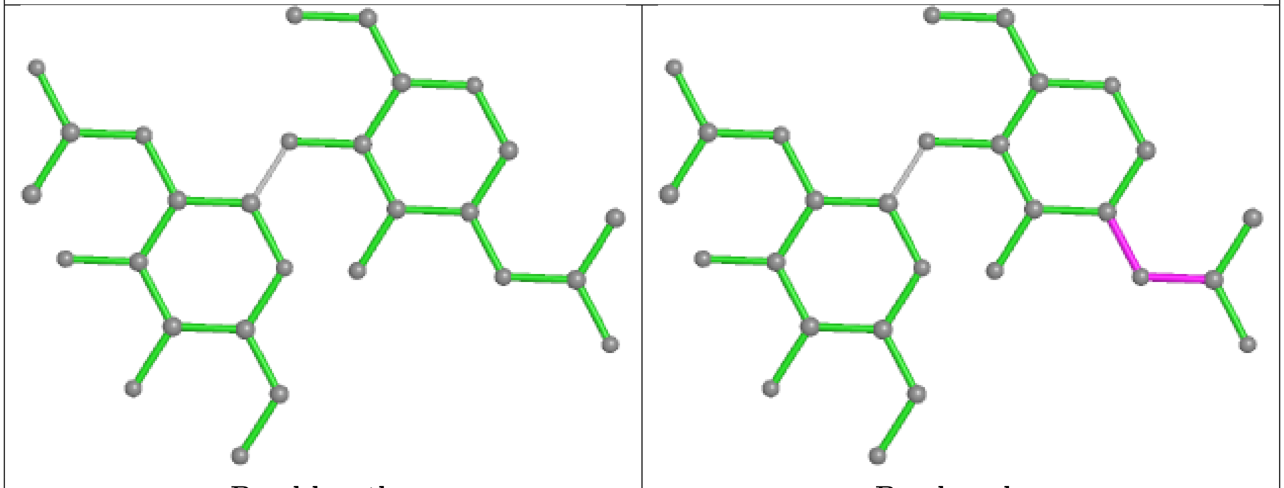
Bond angles



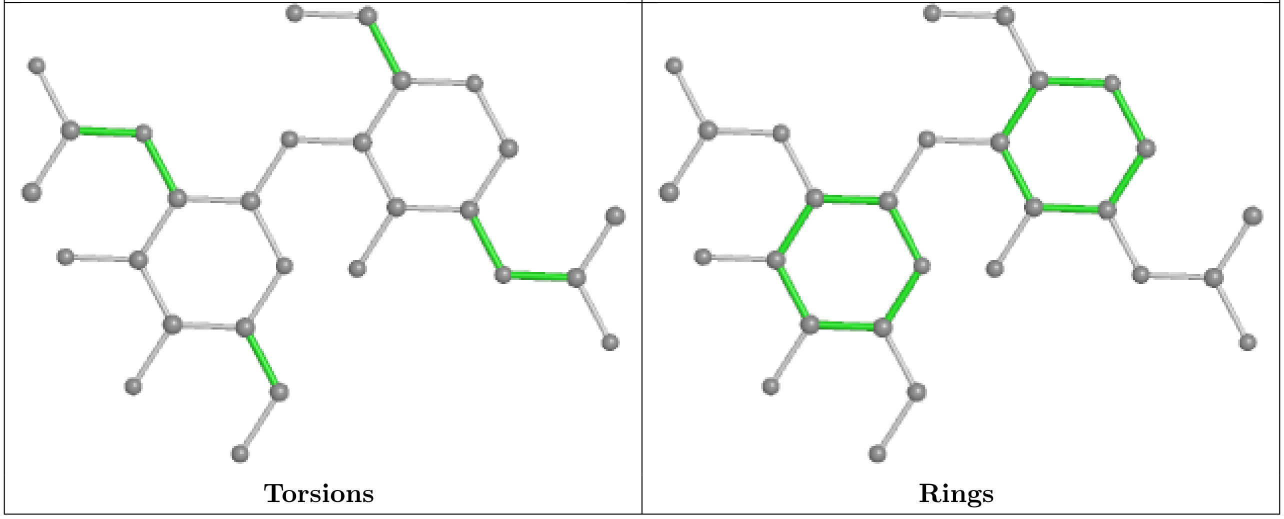
Torsions

Rings

Oligosaccharide Chain U

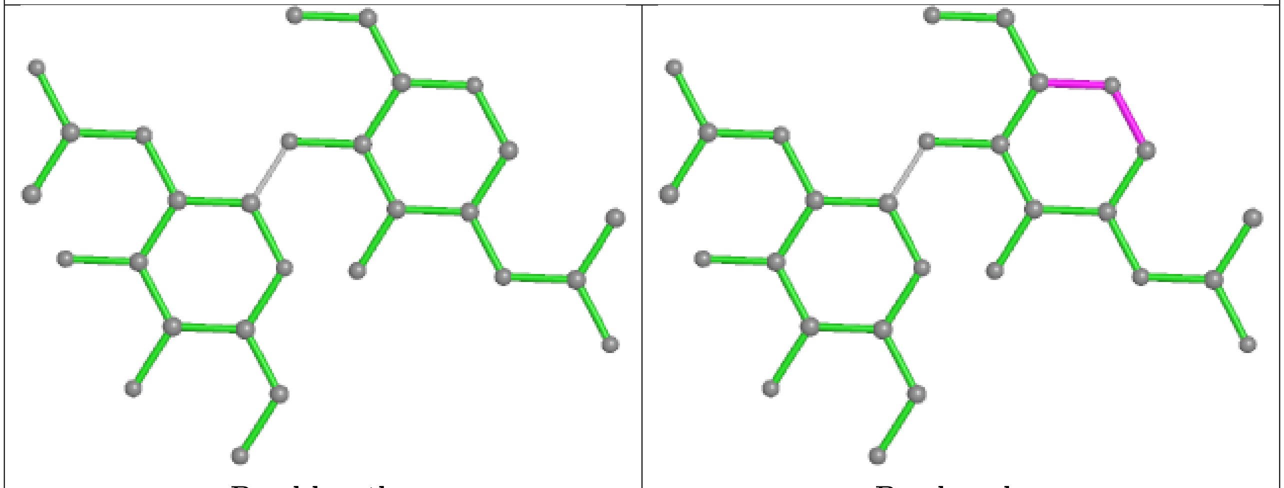


Bond lengths Bond angles



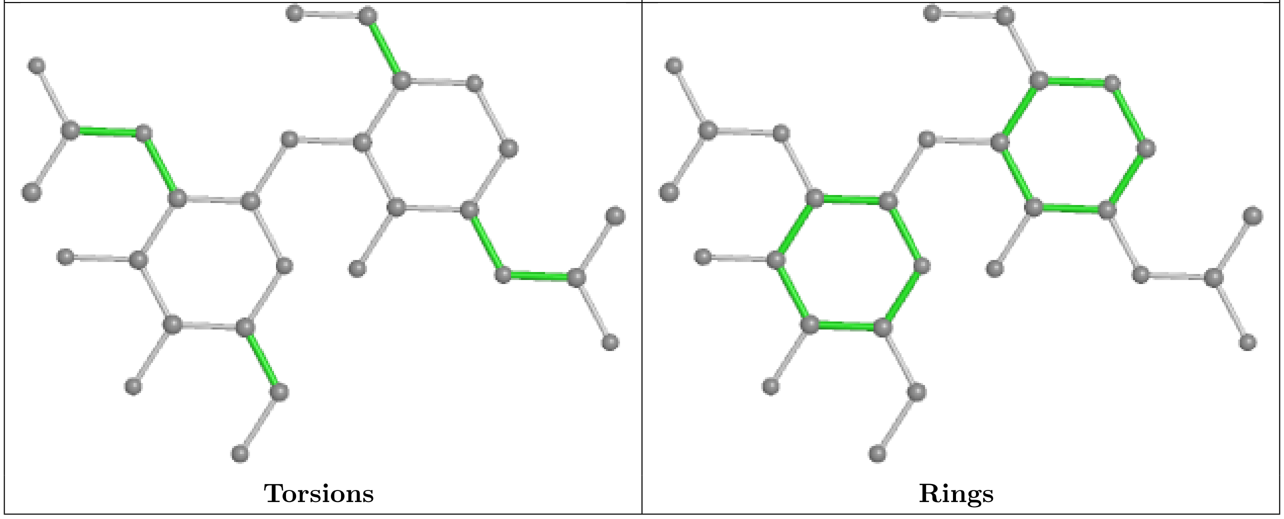
Torsions Rings

Oligosaccharide Chain V



Bond lengths

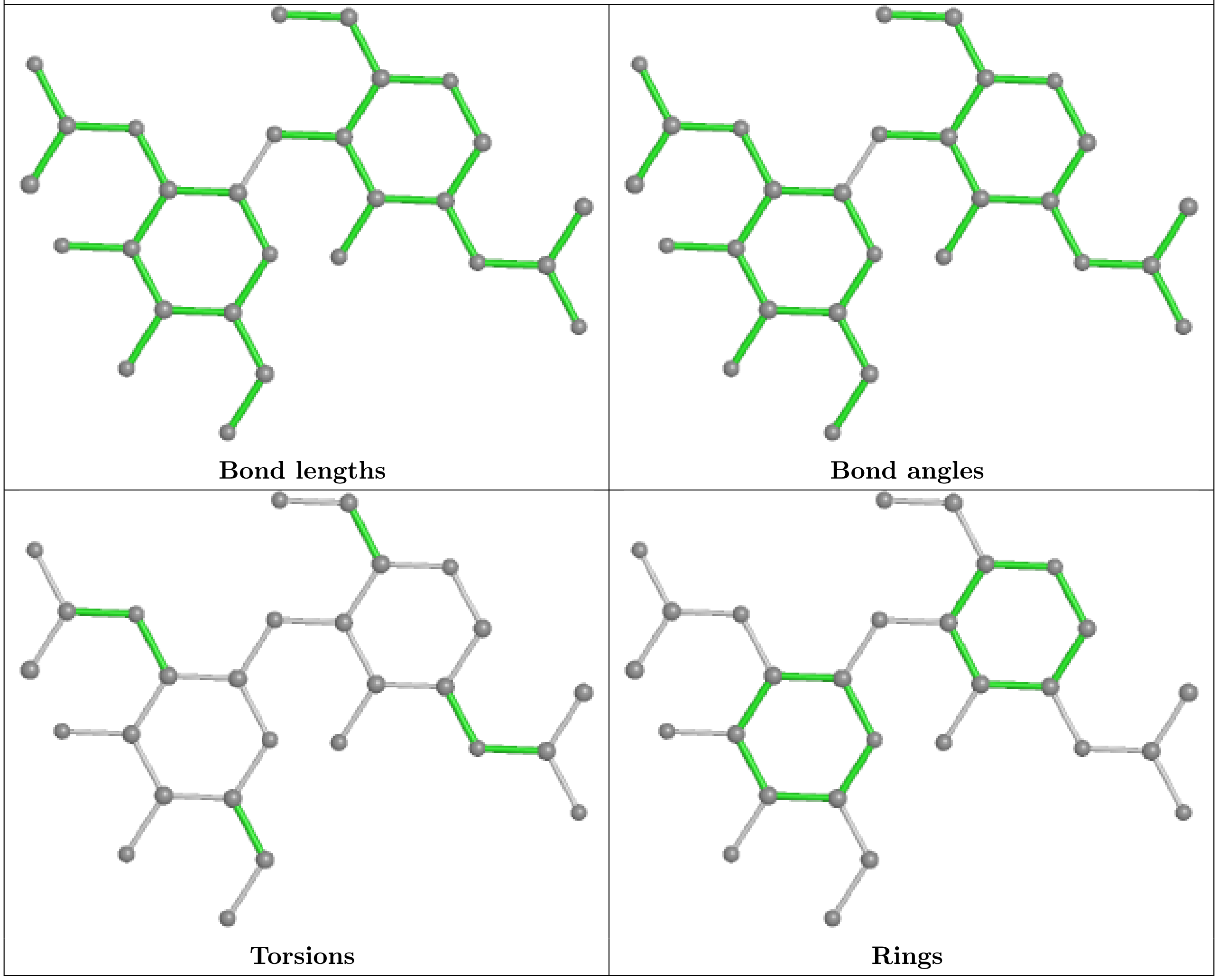
Bond angles



Torsions

Rings

Oligosaccharide Chain W



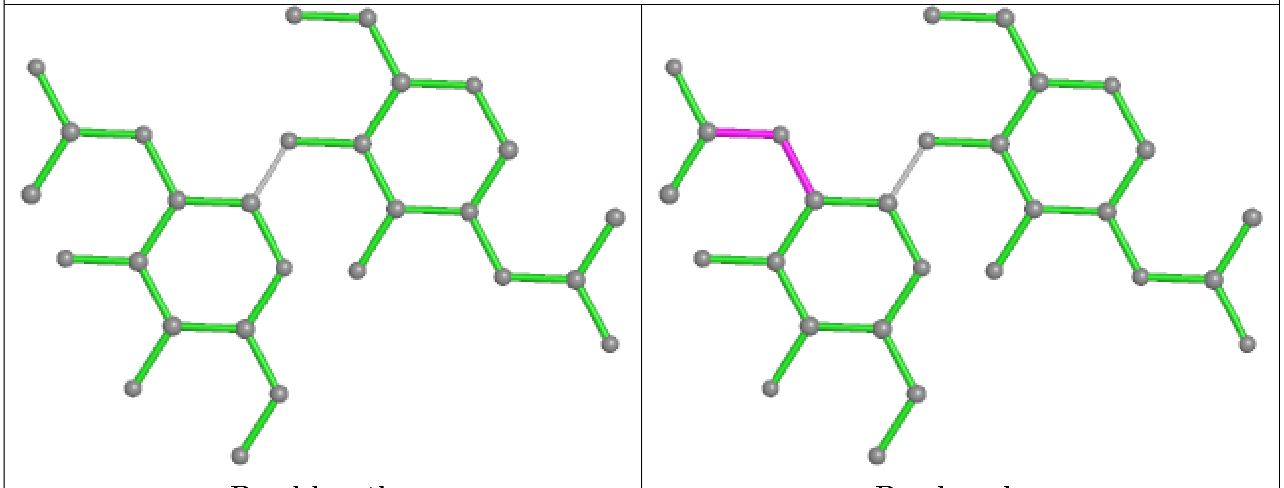
Bond lengths

Bond angles

Torsions

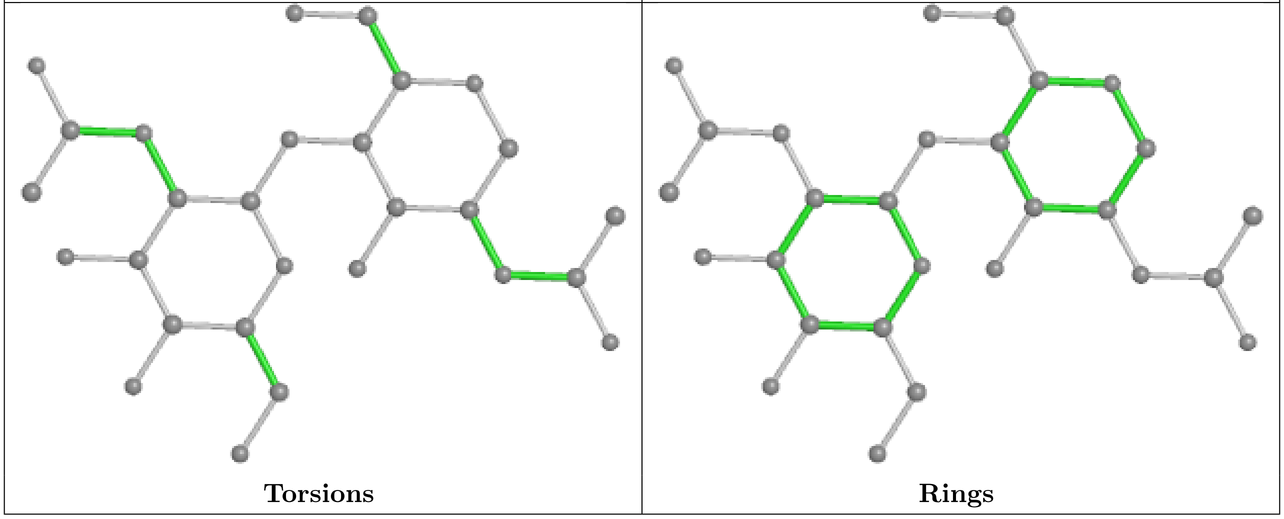
Rings

Oligosaccharide Chain X



Bond lengths

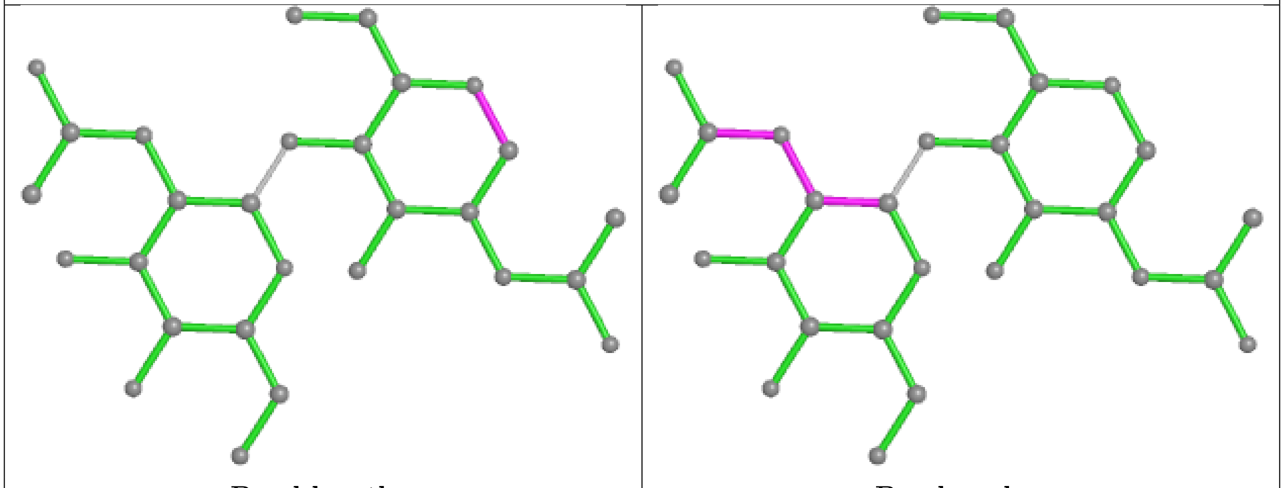
Bond angles



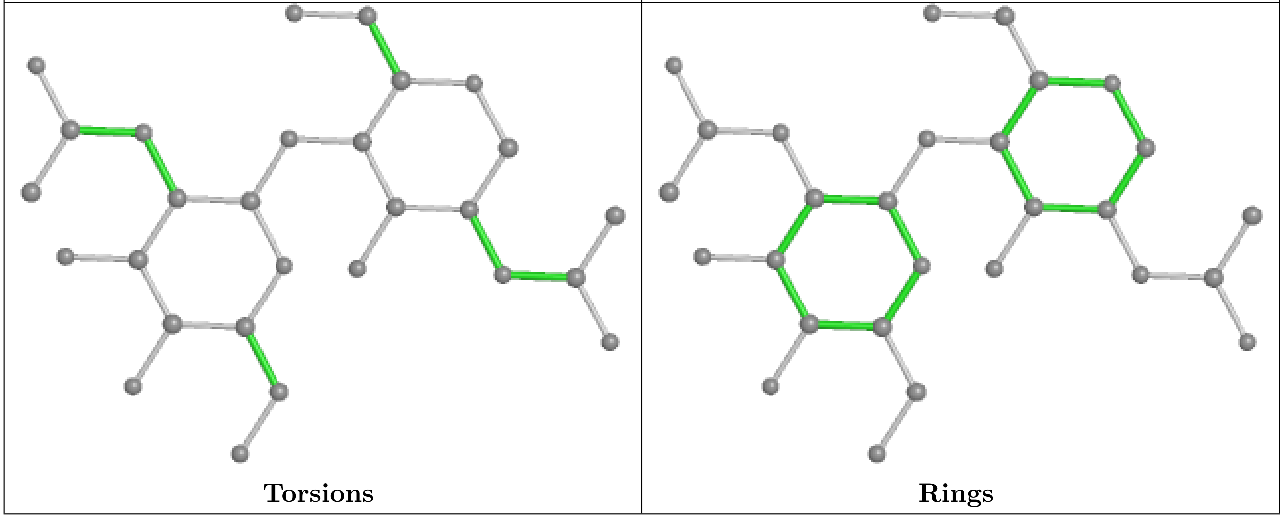
Torsions

Rings

Oligosaccharide Chain Y

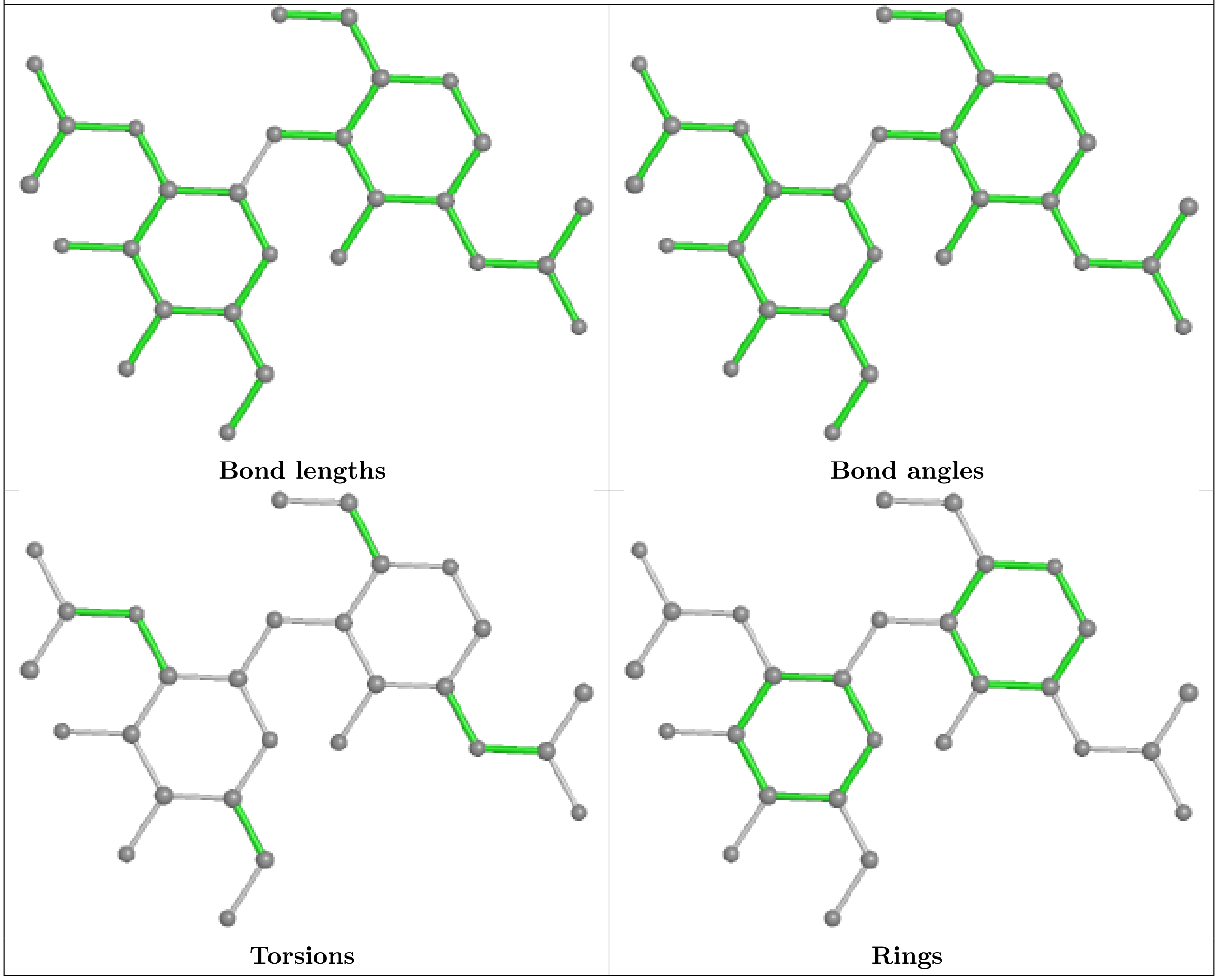


Bond lengths Bond angles



Torsions Rings

Oligosaccharide Chain Z



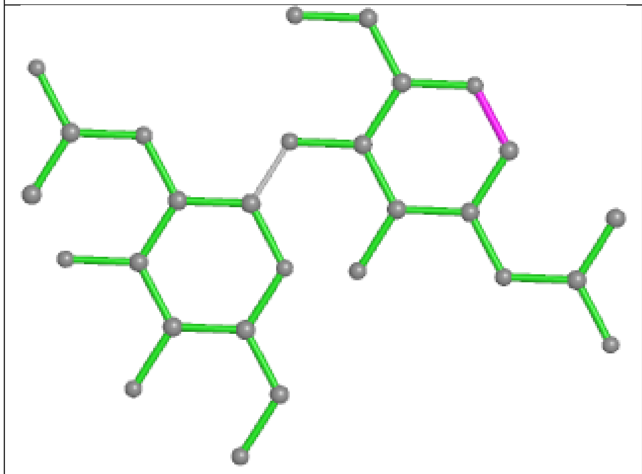
Bond lengths

Bond angles

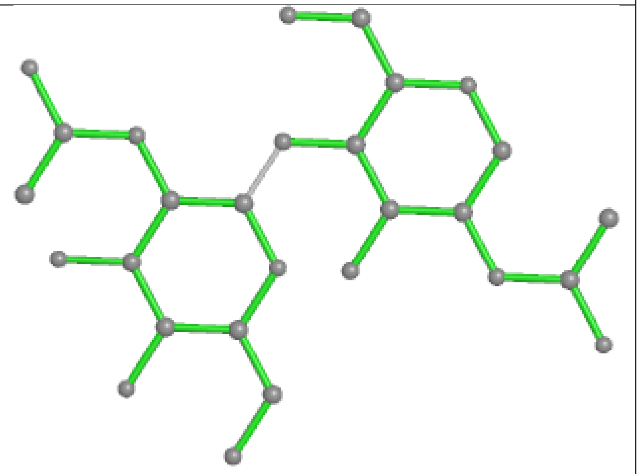
Torsions

Rings

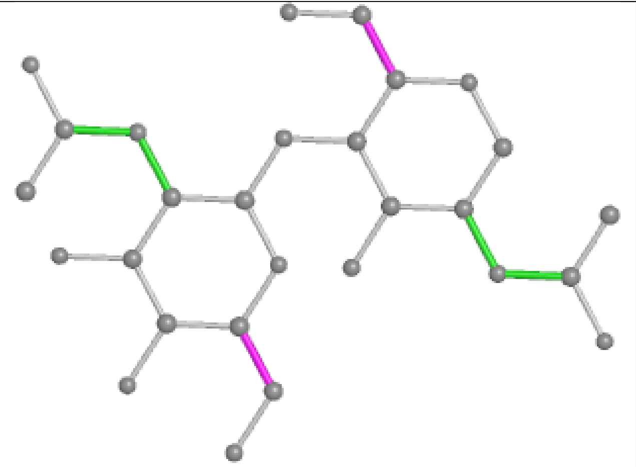
Oligosaccharide Chain a



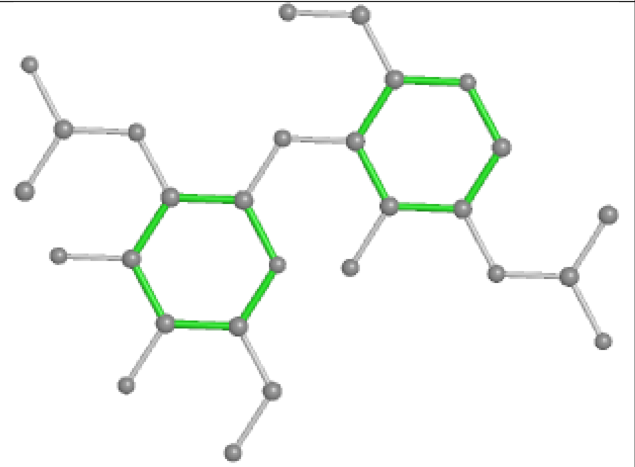
Bond lengths



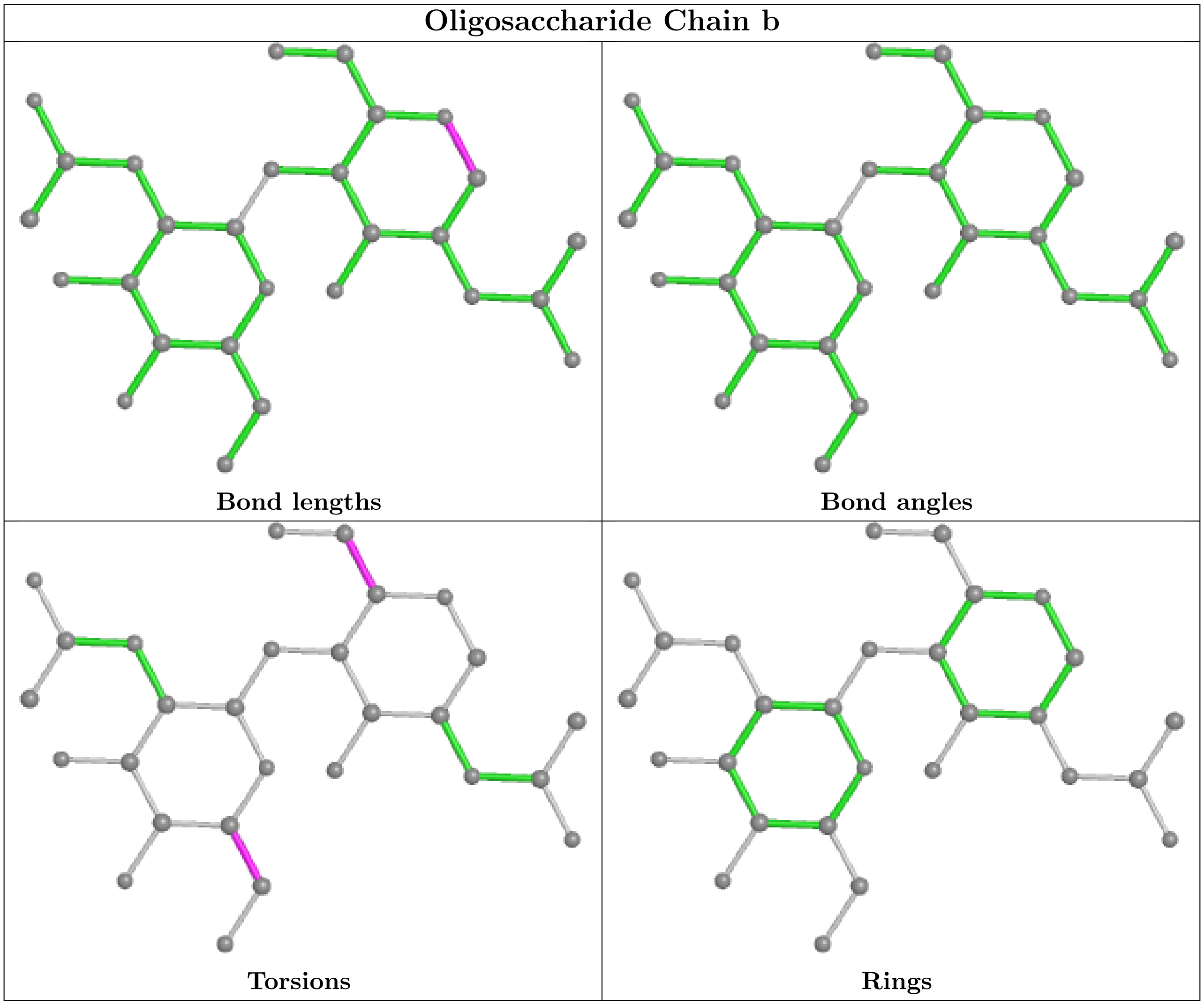
Bond angles



Torsions



Rings



Oligosaccharide Chain b

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

45 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	B	1405	1	14,14,15	0.59	0	17,19,21	1.27	1 (5%)
4	NAG	D	905	-	14,14,15	0.34	0	17,19,21	0.47	0
4	NAG	A	1409	1	14,14,15	0.23	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	B	1410	1	14,14,15	0.41	0	17,19,21	1.13	2 (11%)
4	NAG	E	904	2	14,14,15	0.31	0	17,19,21	0.51	0
4	NAG	D	904	2	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	B	1403	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1404	1	14,14,15	0.48	0	17,19,21	0.53	0
4	NAG	A	1405	1	14,14,15	0.58	0	17,19,21	1.26	1 (5%)
4	NAG	C	1406	-	14,14,15	0.41	0	17,19,21	1.18	1 (5%)
4	NAG	D	902	-	14,14,15	0.29	0	17,19,21	0.63	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
4	NAG	B	1407	1	14,14,15	0.28	0	17,19,21	0.39	0
4	NAG	B	1411	-	14,14,15	0.36	0	17,19,21	0.41	0
4	NAG	E	902	-	14,14,15	0.28	0	17,19,21	0.63	0
4	NAG	B	1408	1	14,14,15	0.23	0	17,19,21	0.48	0
4	NAG	A	1403	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	E	903	2	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
4	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.34	0
4	NAG	E	905	-	14,14,15	0.34	0	17,19,21	0.48	0
4	NAG	C	1409	1	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	A	1407	-	14,14,15	0.32	0	17,19,21	0.46	0
4	NAG	A	1410	1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	D	903	2	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
4	NAG	A	1411	1	14,14,15	0.50	0	17,19,21	0.36	0
4	NAG	A	1401	1	14,14,15	0.30	0	17,19,21	0.33	0
4	NAG	C	1403	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	A	1408	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	D	906	-	14,14,15	0.23	0	17,19,21	0.62	0
4	NAG	D	907	-	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
4	NAG	C	1407	1	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	B	1406	-	14,14,15	0.41	0	17,19,21	1.17	1 (5%)
4	NAG	B	1402	1	14,14,15	0.21	0	17,19,21	0.63	0
4	NAG	C	1408	1	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	E	901	2	14,14,15	0.41	0	17,19,21	0.65	0
4	NAG	E	906	-	14,14,15	0.23	0	17,19,21	0.63	0
4	NAG	C	1401	1	14,14,15	0.28	0	17,19,21	0.33	0
4	NAG	B	1409	1	14,14,15	0.30	0	17,19,21	0.39	0
4	NAG	A	1404	1	14,14,15	0.47	0	17,19,21	0.54	0
4	NAG	A	1406	1	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
4	NAG	E	907	-	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
4	NAG	D	901	2	14,14,15	0.42	0	17,19,21	0.65	0
4	NAG	A	1402	1	14,14,15	0.20	0	17,19,21	0.63	0
4	NAG	B	1404	1	14,14,15	0.47	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	C	1405	1	14,14,15	0.60	0	17,19,21	1.27	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	D	905	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	E	904	2	-	0/6/23/26	0/1/1/1
4	NAG	D	904	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1406	-	-	0/6/23/26	0/1/1/1
4	NAG	D	902	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1411	-	-	0/6/23/26	0/1/1/1
4	NAG	E	902	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	E	903	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	E	905	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	D	903	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1411	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	D	906	-	-	0/6/23/26	0/1/1/1
4	NAG	D	907	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1406	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	E	906	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	E	907	-	-	2/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1406	NAG	O5-C1	-2.02	1.40	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1405	NAG	C2-N2-C7	4.39	129.16	122.90
4	C	1405	NAG	C2-N2-C7	4.38	129.14	122.90
4	A	1405	NAG	C2-N2-C7	4.35	129.09	122.90
4	C	1406	NAG	C8-C7-N2	2.36	120.09	116.10
4	B	1406	NAG	C8-C7-N2	2.35	120.08	116.10

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	902	NAG	O7-C7-N2-C2
4	E	902	NAG	O7-C7-N2-C2
4	D	902	NAG	C8-C7-N2-C2
4	E	902	NAG	C8-C7-N2-C2
4	D	907	NAG	O5-C5-C6-O6

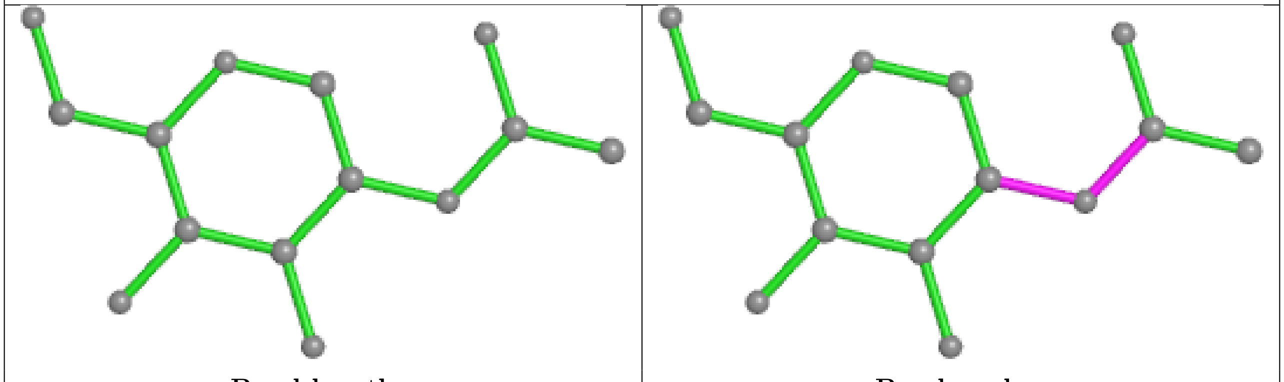
There are no ring outliers.

12 monomers are involved in 30 short contacts:

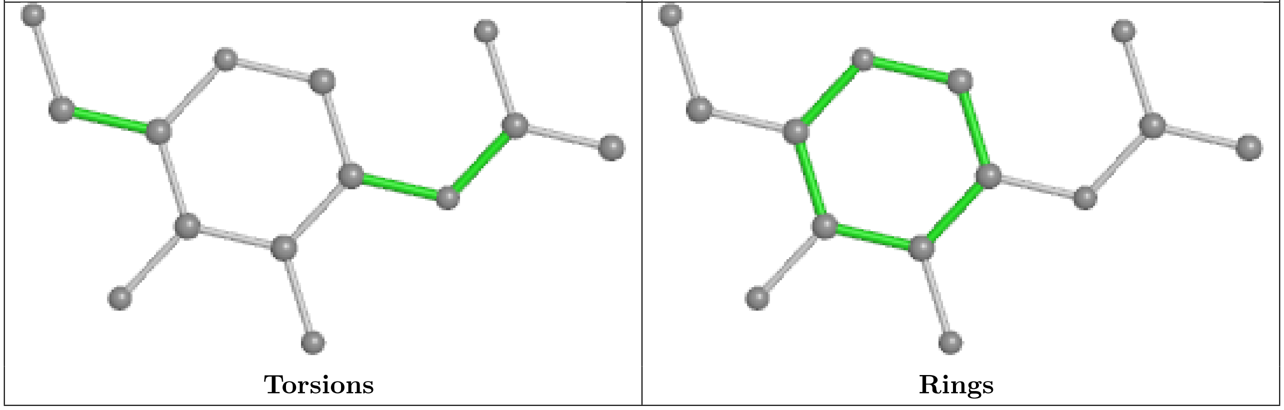
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	905	NAG	2	0
4	B	1410	NAG	6	0
4	E	904	NAG	1	0
4	D	904	NAG	1	0
4	D	902	NAG	8	0
4	B	1411	NAG	4	0
4	E	902	NAG	8	0
4	E	903	NAG	1	0
4	E	905	NAG	2	0
4	D	903	NAG	1	0
4	D	906	NAG	2	0
4	E	906	NAG	2	0

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

Ligand NAG B 1405

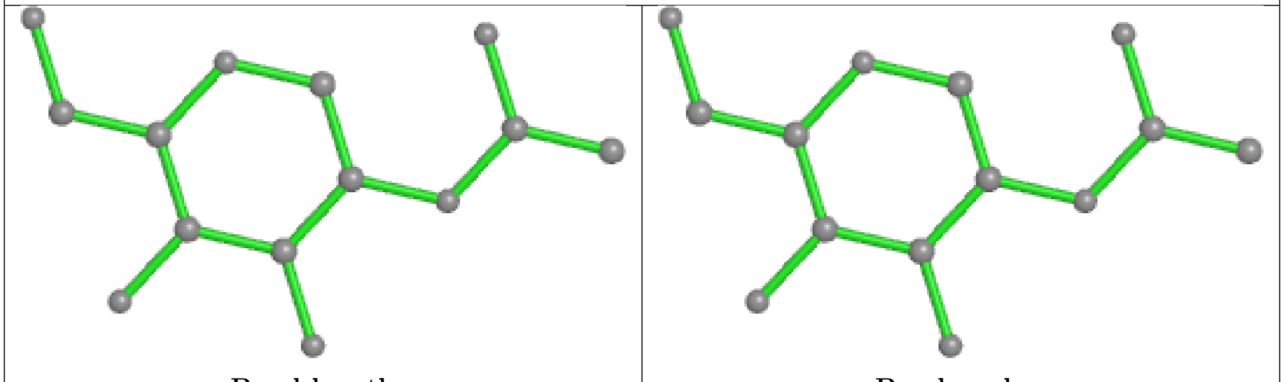


Bond lengths Bond angles

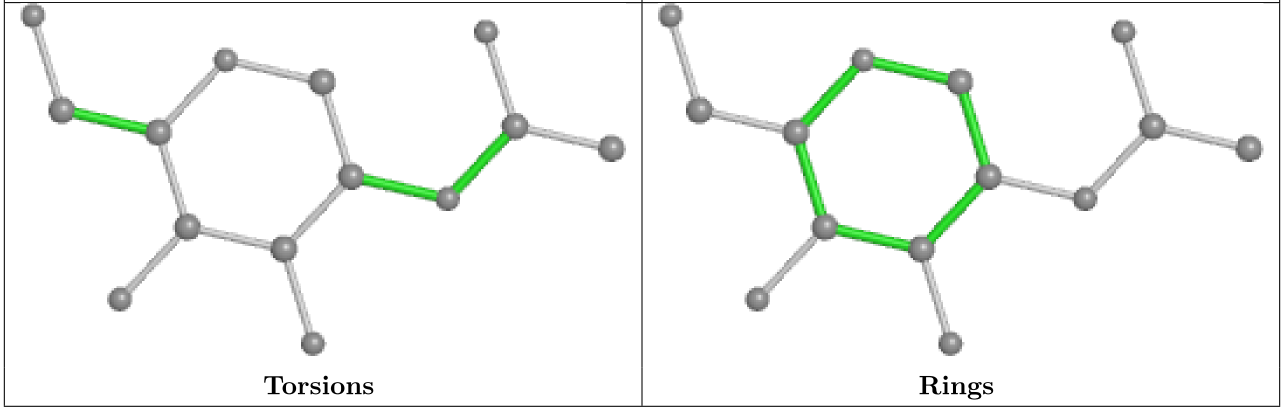


Torsions Rings

Ligand NAG D 905

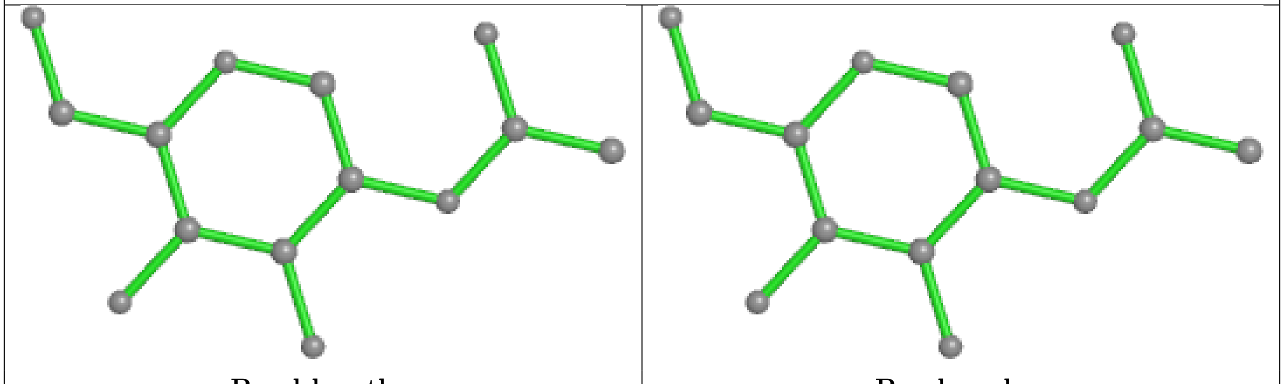


Bond lengths Bond angles

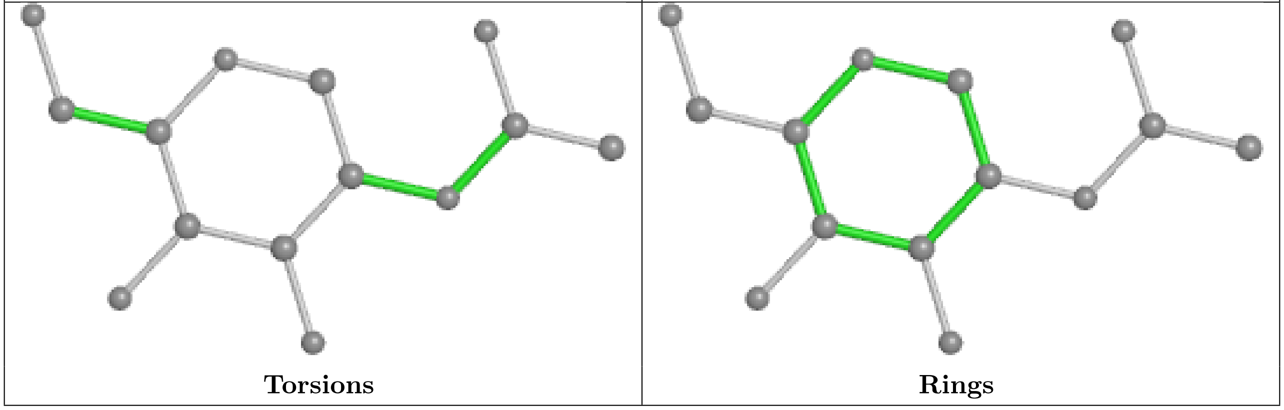


Torsions Rings

Ligand NAG A 1409



Bond lengths Bond angles



Torsions Rings

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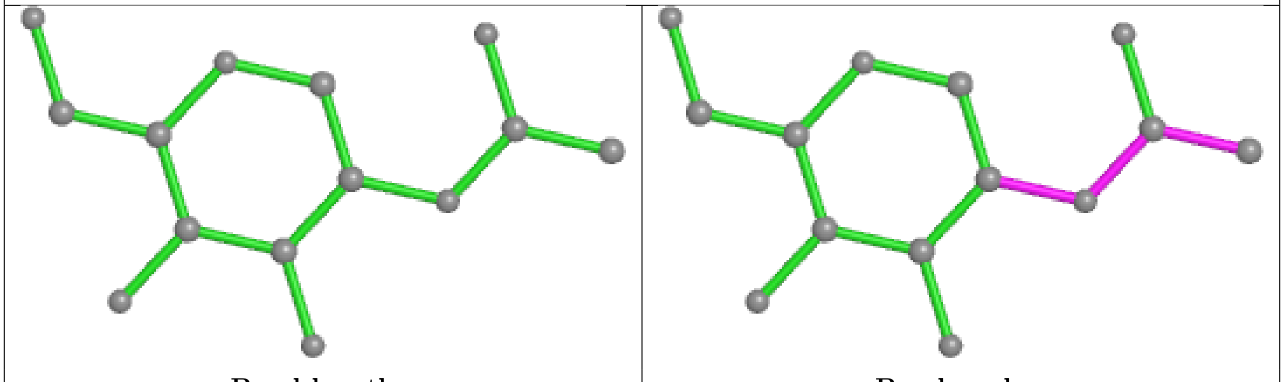
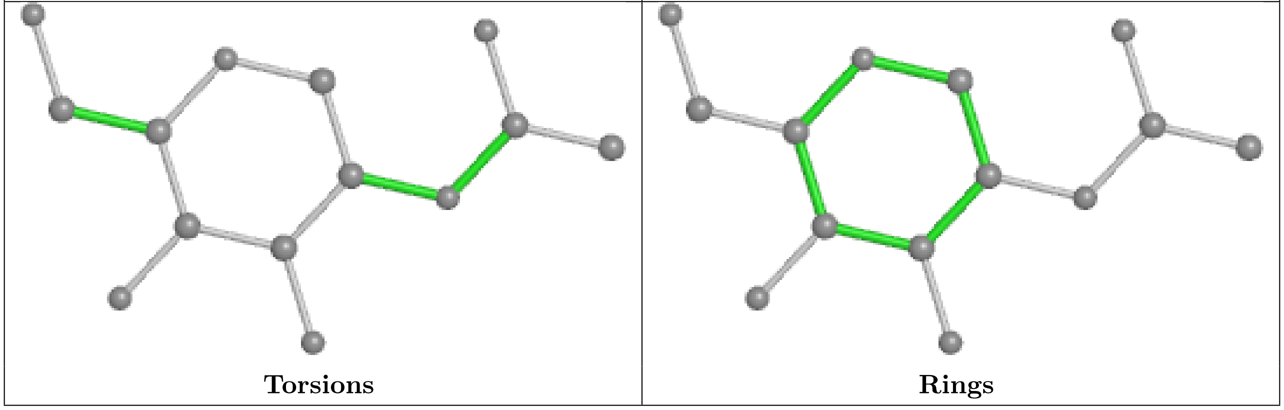
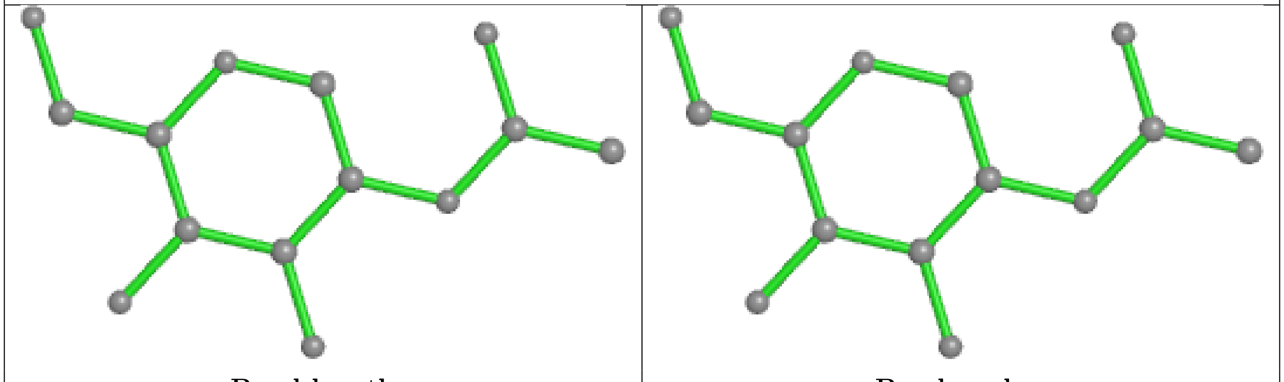


Bond lengths Bond angles



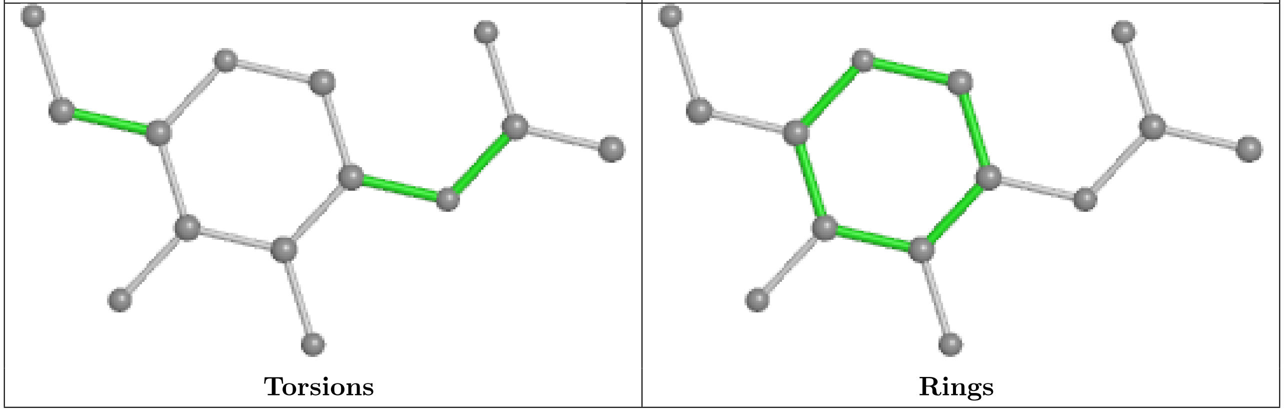
Torsions Rings

Ligand NAG E 904



Bond lengths

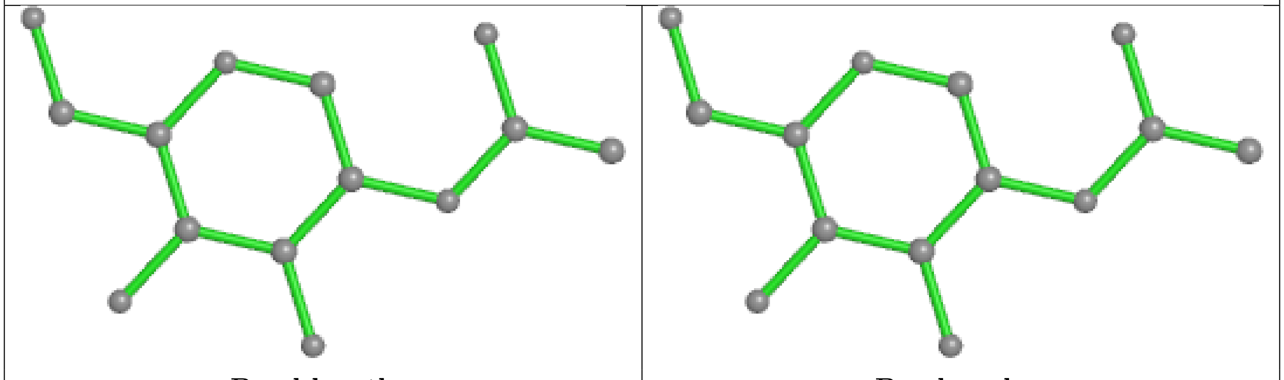
Bond angles



Torsions

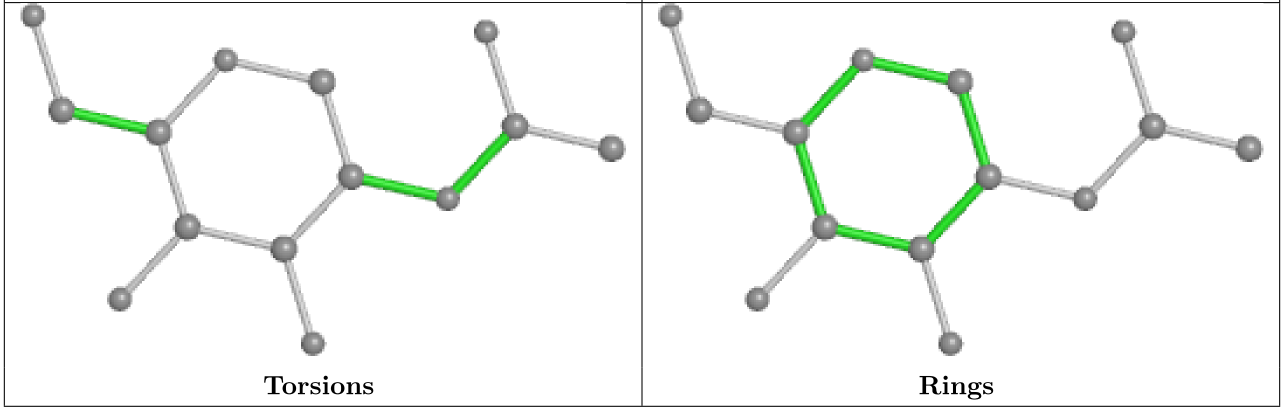
Rings

Ligand NAG D 904



Bond lengths

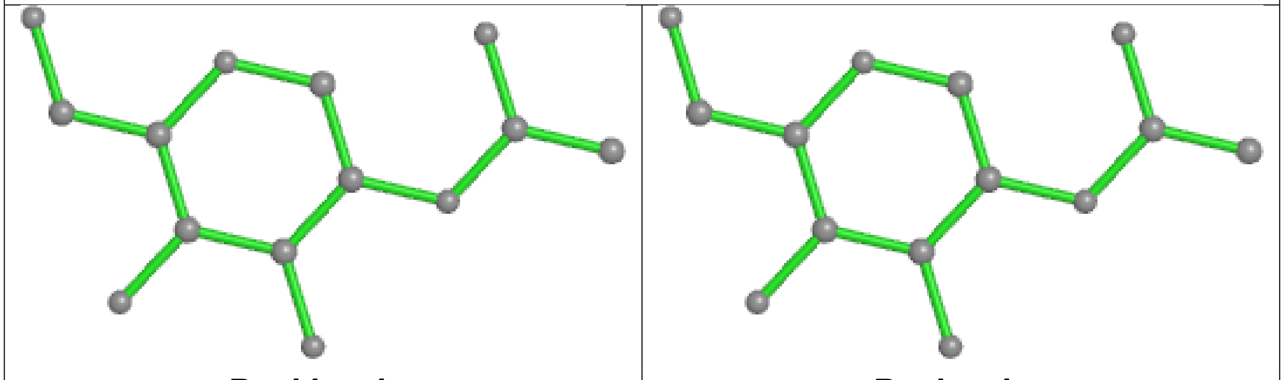
Bond angles



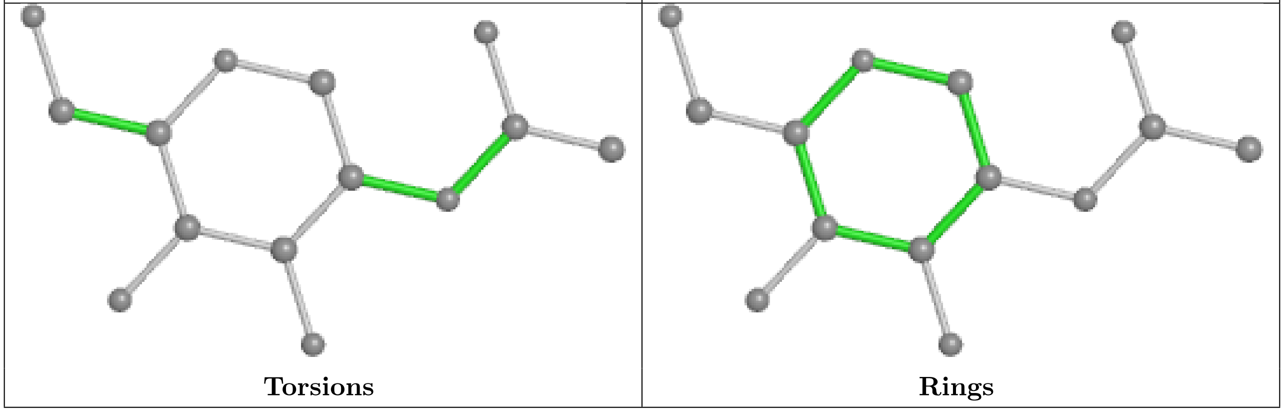
Torsions

Rings

Ligand NAG B 1403

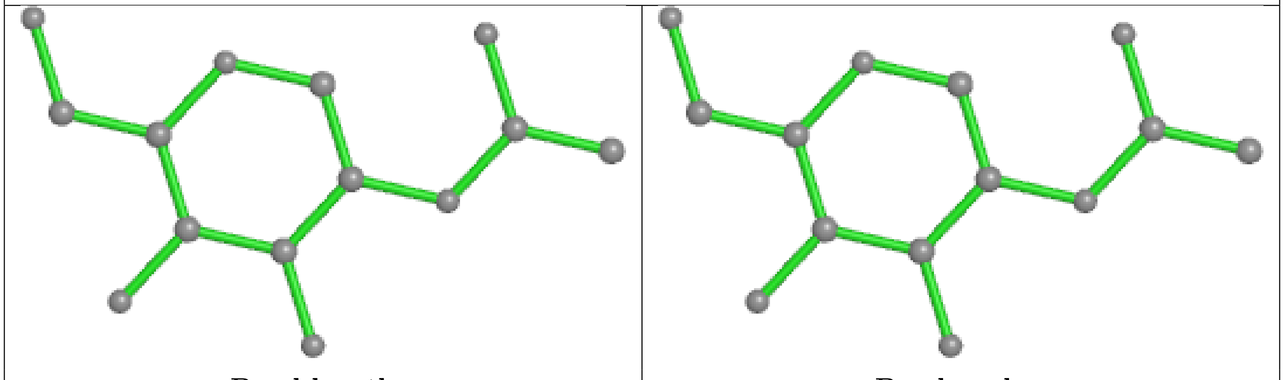


Bond lengths Bond angles

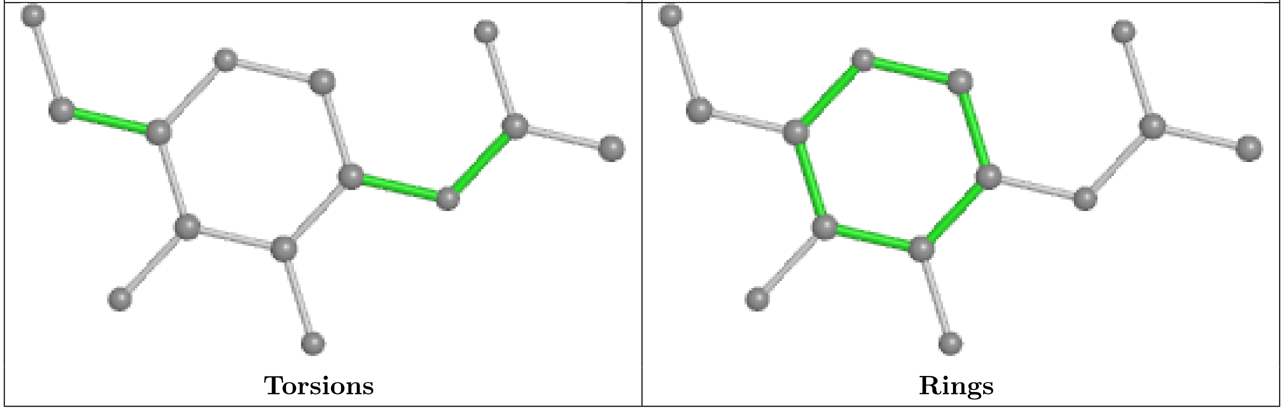


Torsions Rings

Ligand NAG C 1404

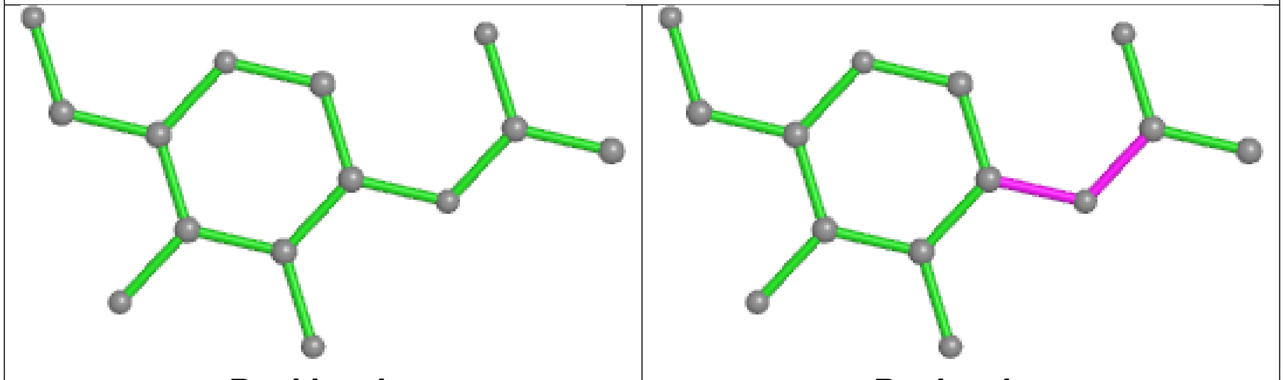


Bond lengths Bond angles

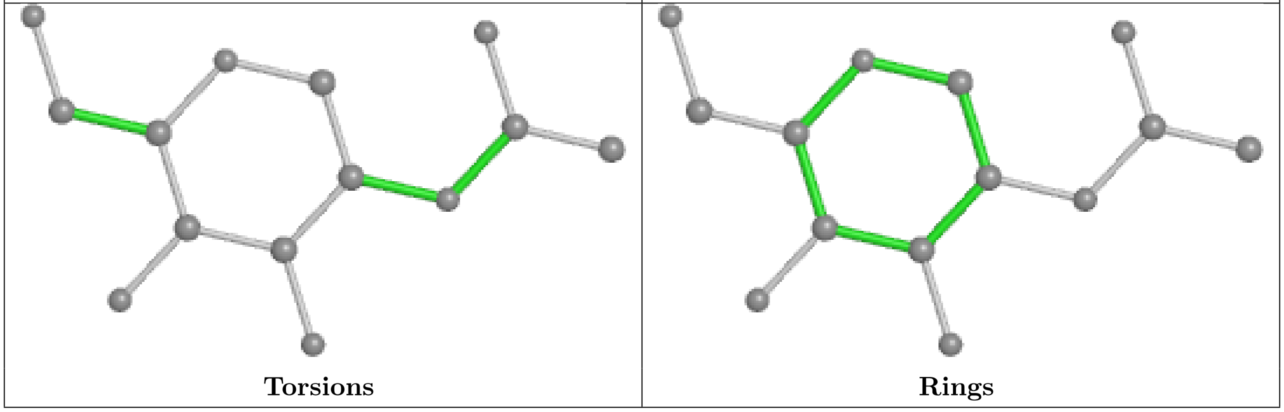


Torsions Rings

Ligand NAG A 1405



Bond lengths Bond angles



Torsions Rings

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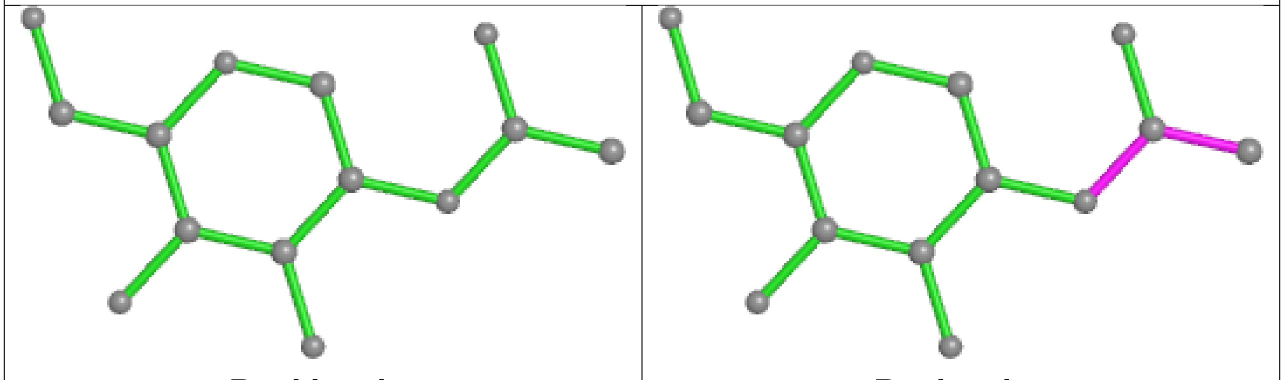
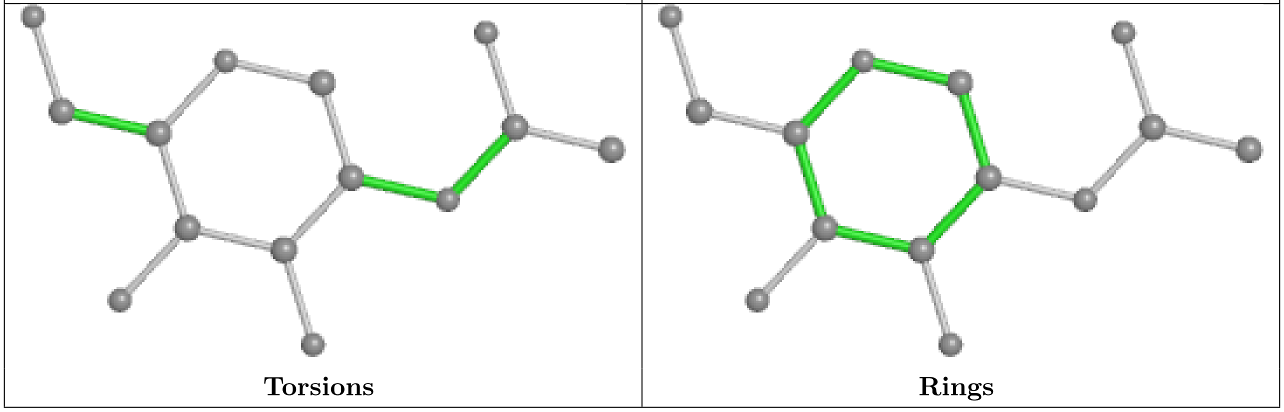
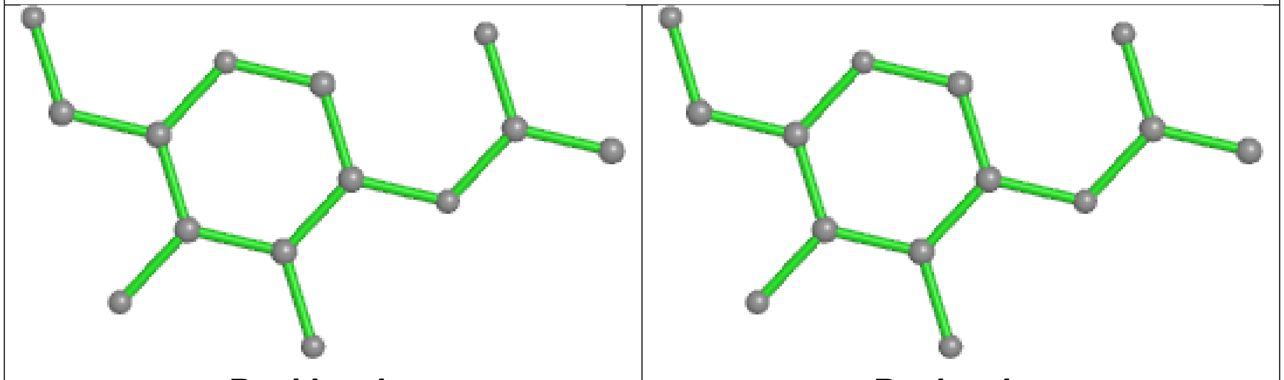


Bond lengths Bond angles



Torsions Rings

Ligand NAG D 902



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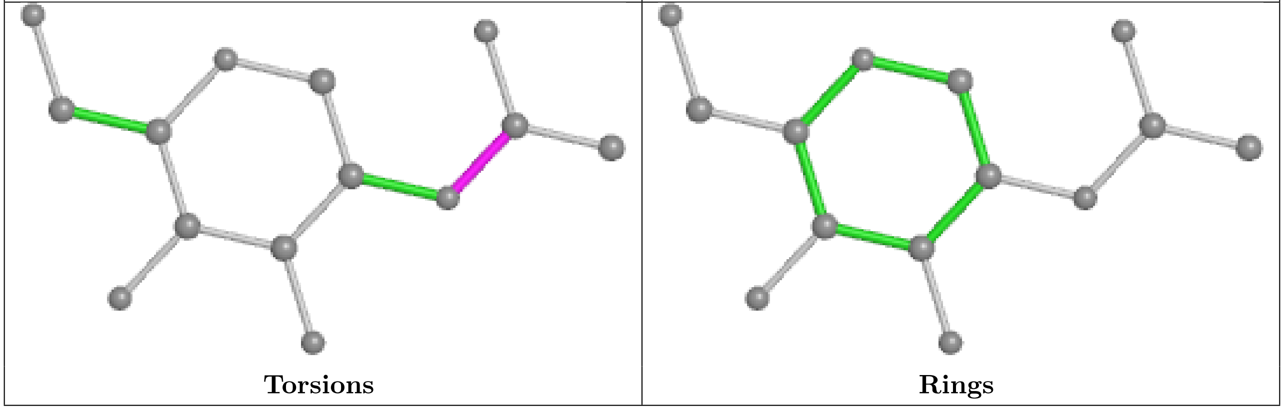

Torsions Rings

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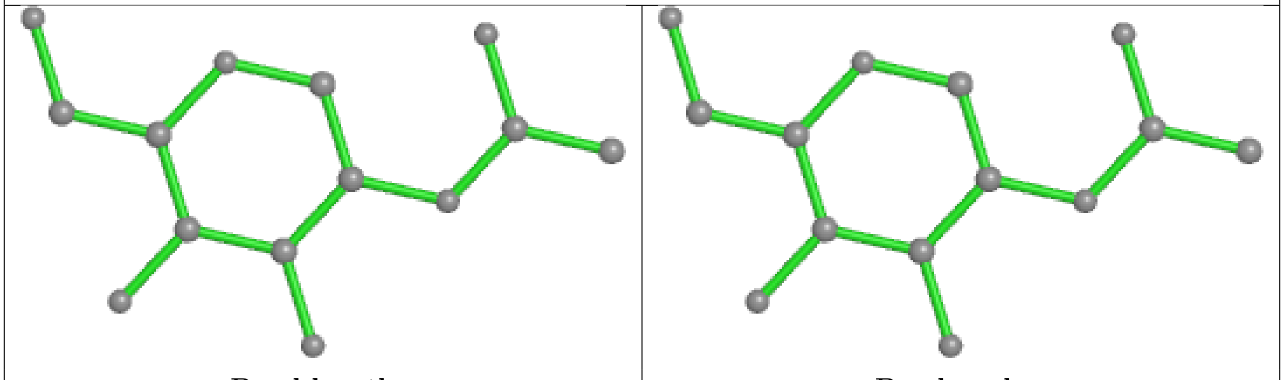

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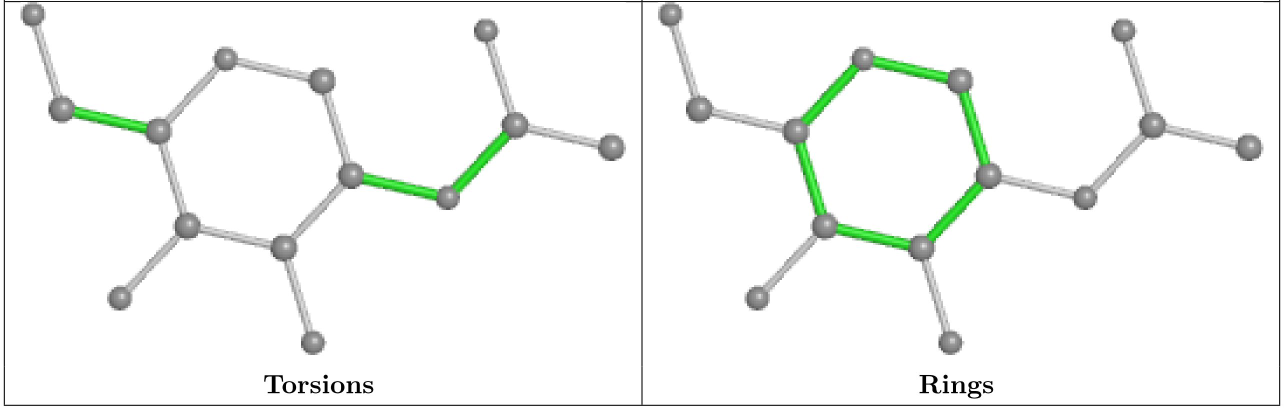

Torsions Rings

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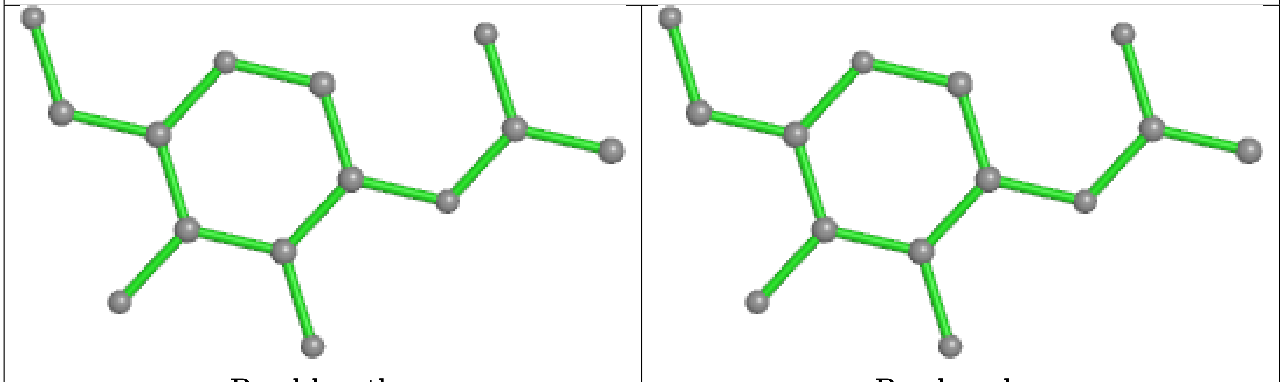

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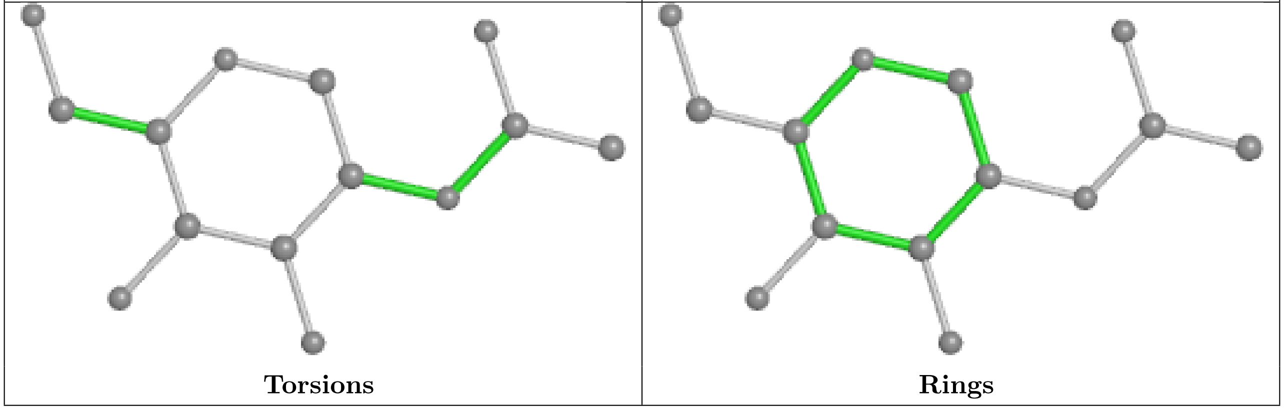

Torsions Rings

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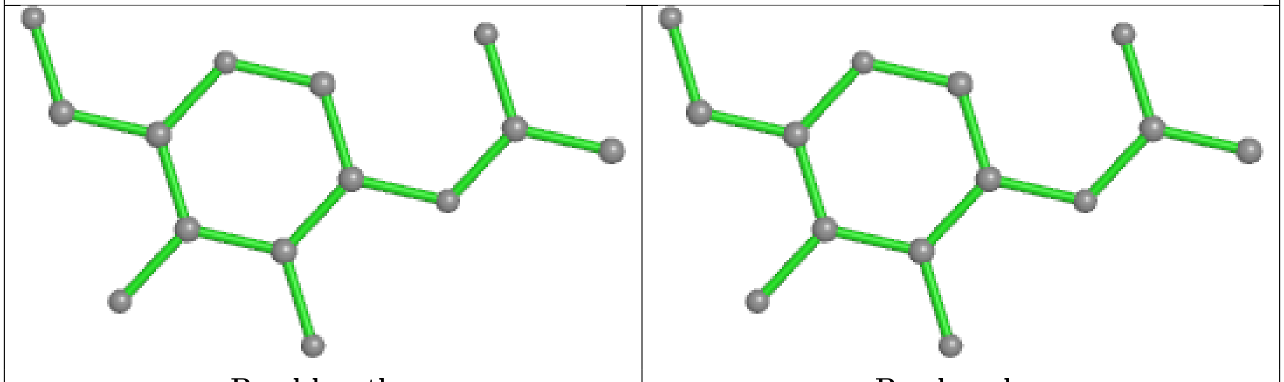
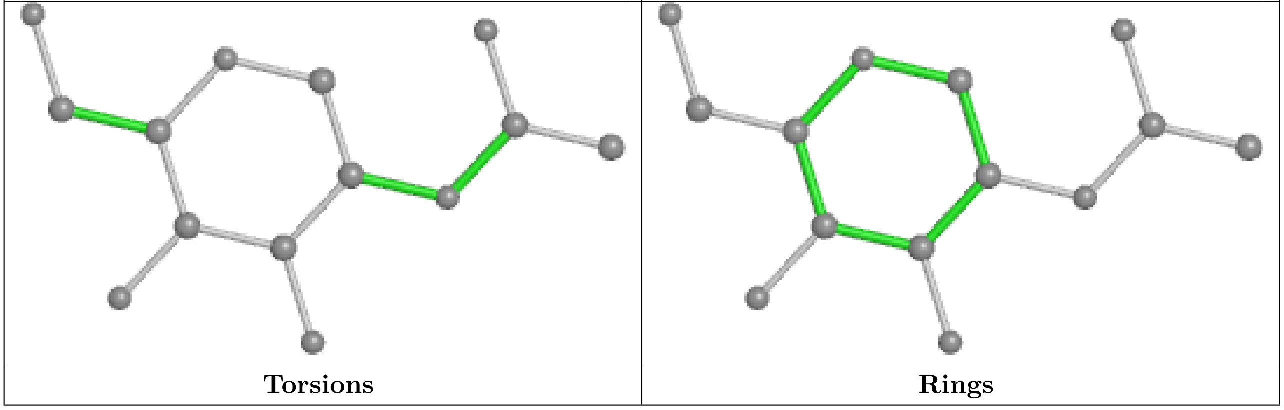
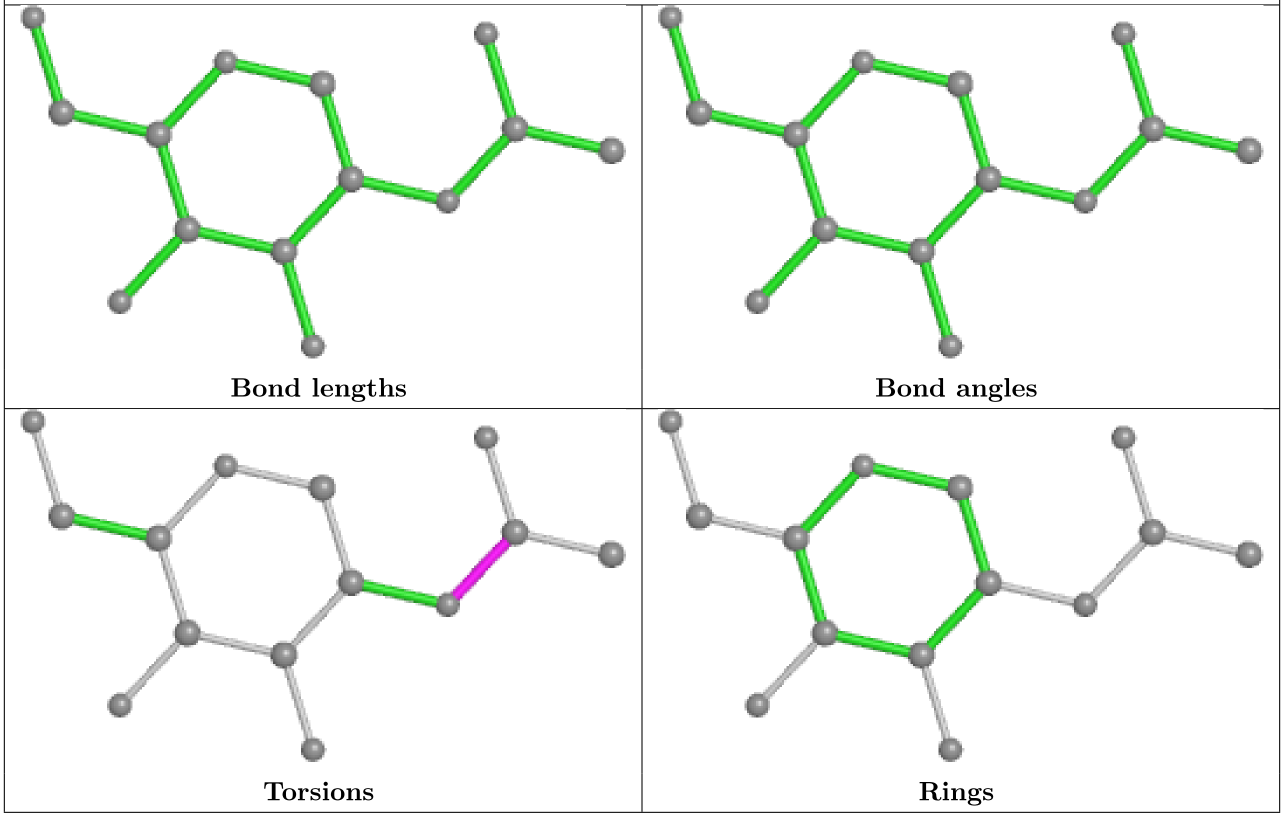


Bond lengths Bond angles



Torsions Rings

Ligand NAG E 902



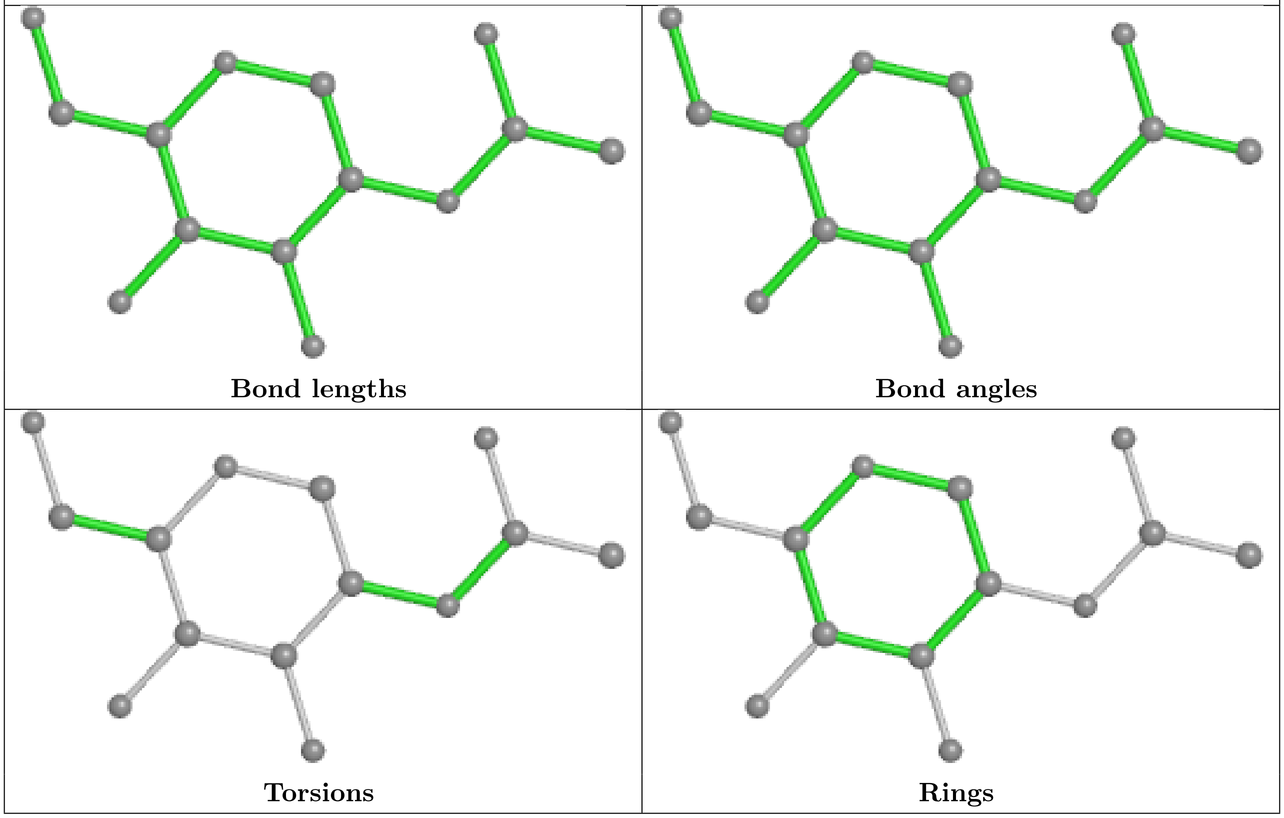
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1408



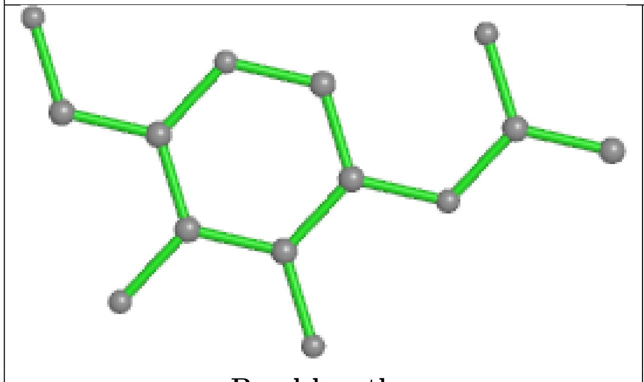
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1403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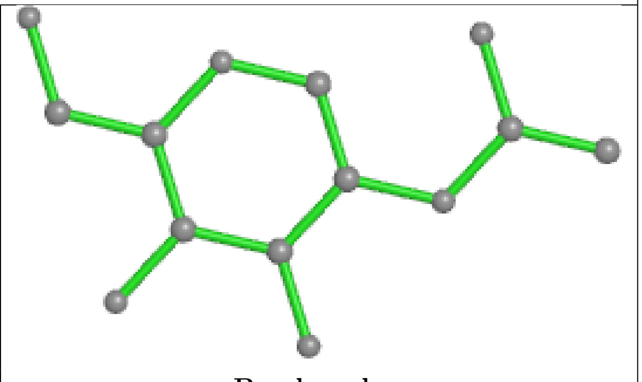
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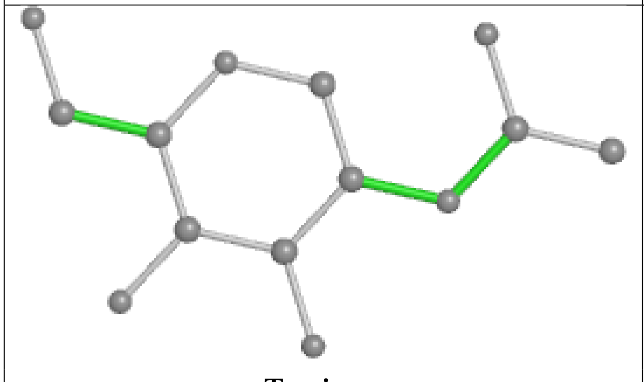
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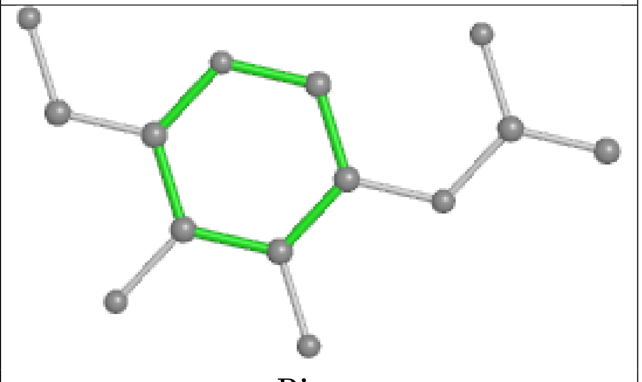
Rings

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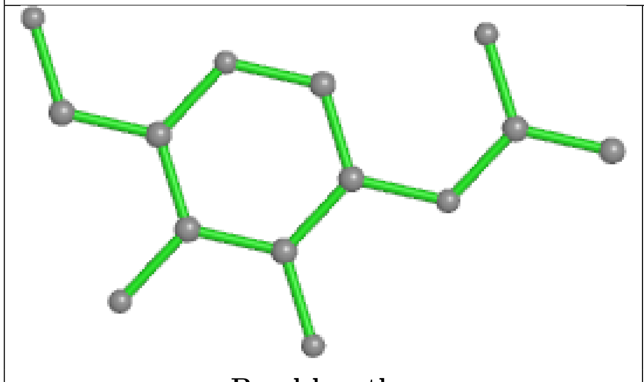
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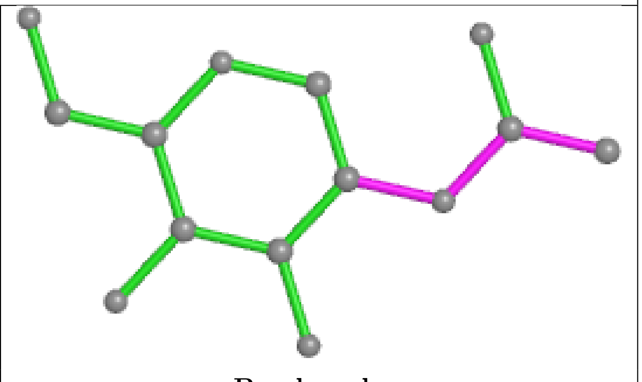
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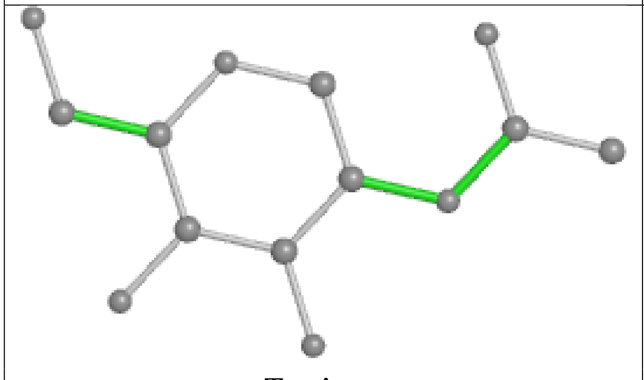
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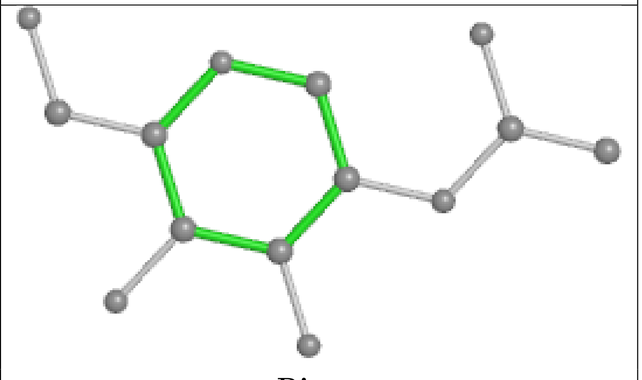
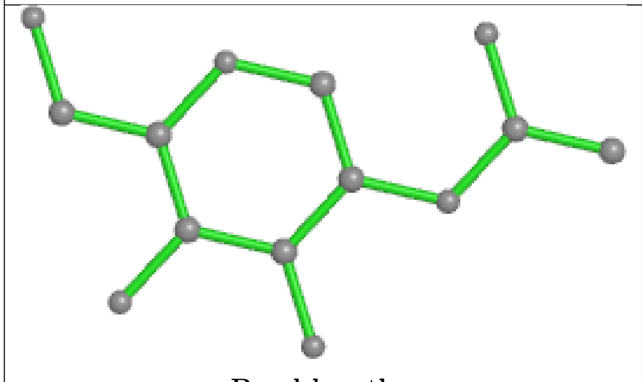

Rings

Ligand NAG B 1401



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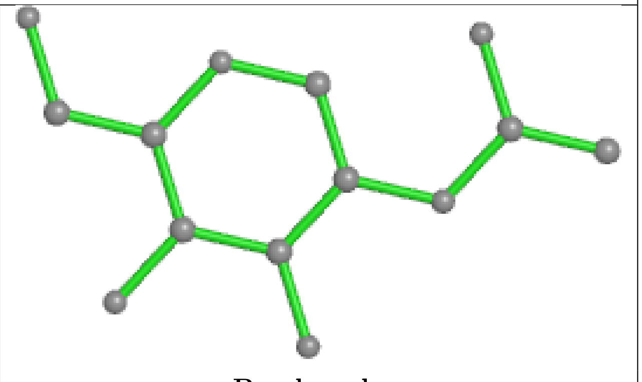

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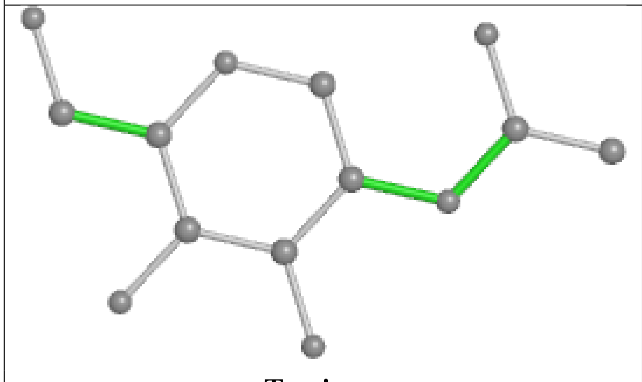

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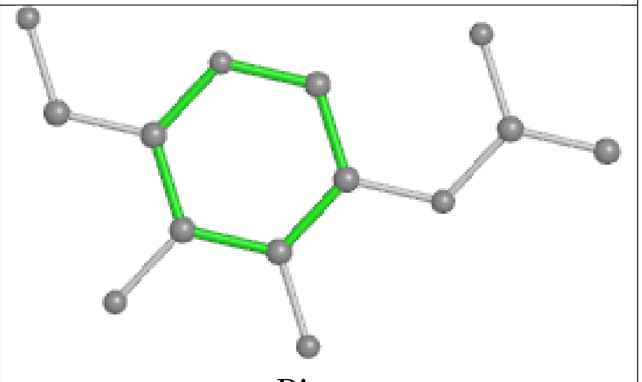

Rings

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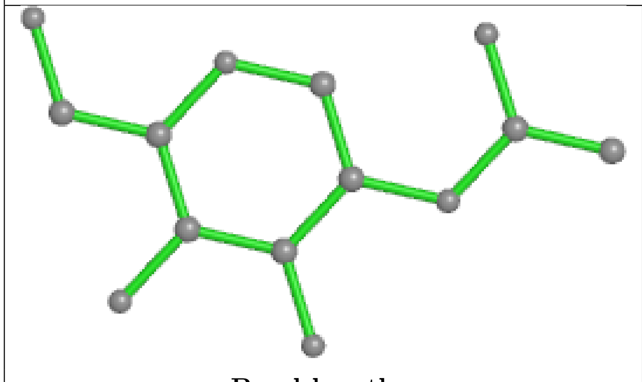

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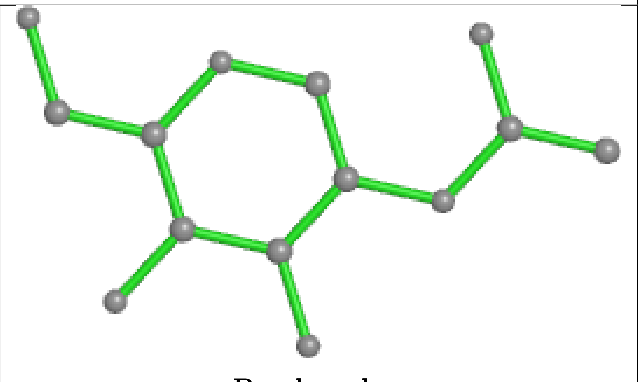

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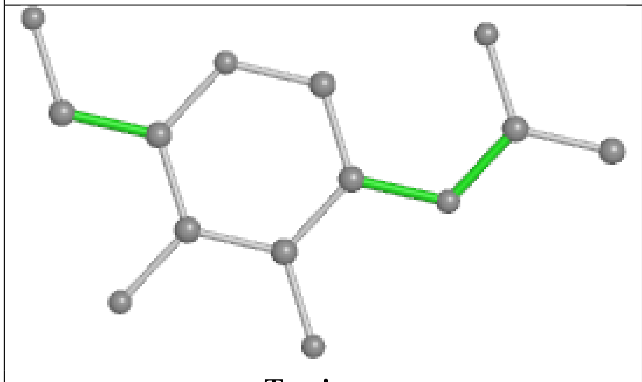

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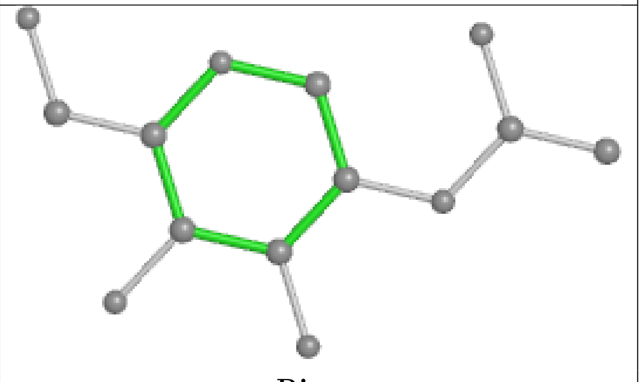
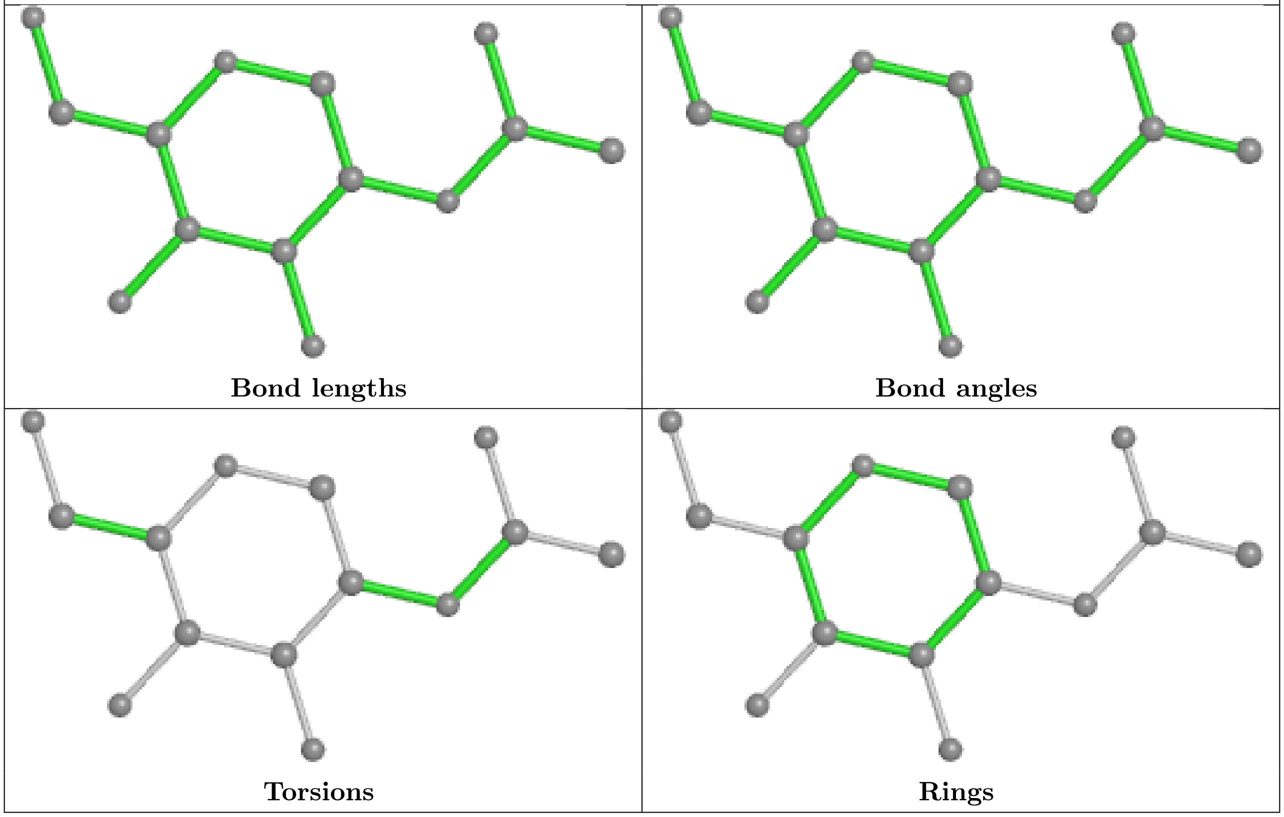


Rings

Ligand NAG C 1409



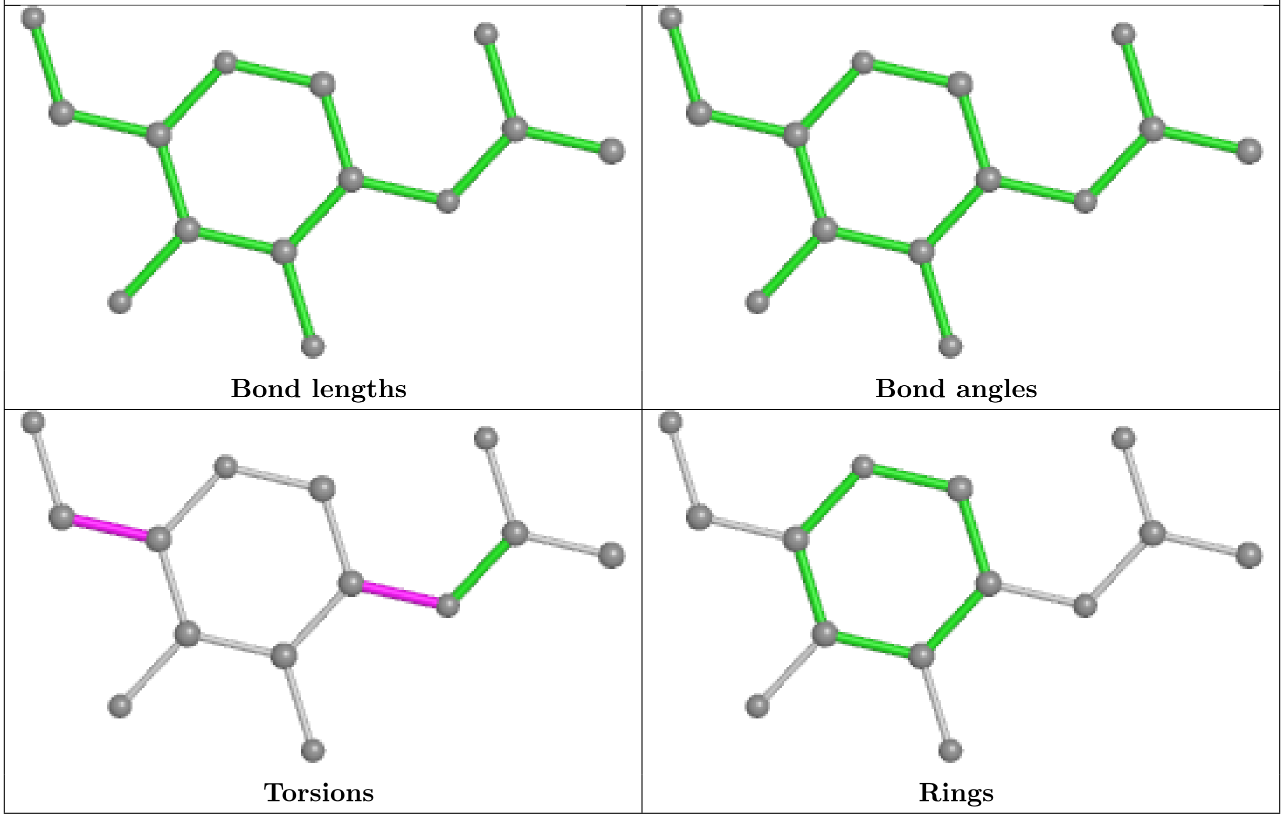
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1407



Bond lengths

Bond angles

Torsions

Rings

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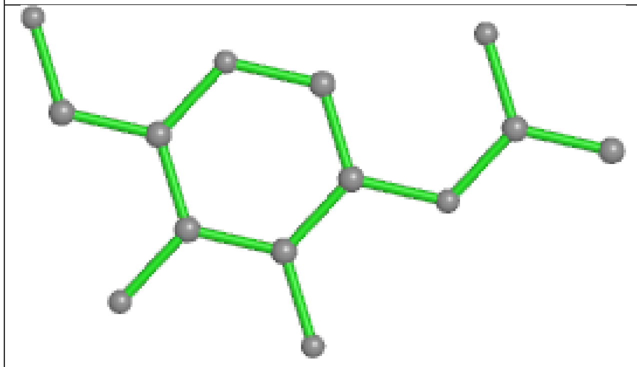

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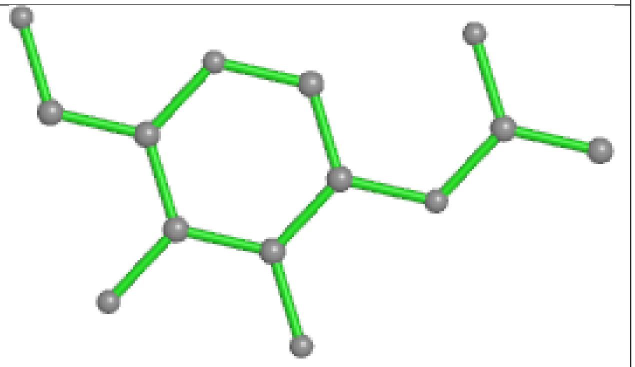

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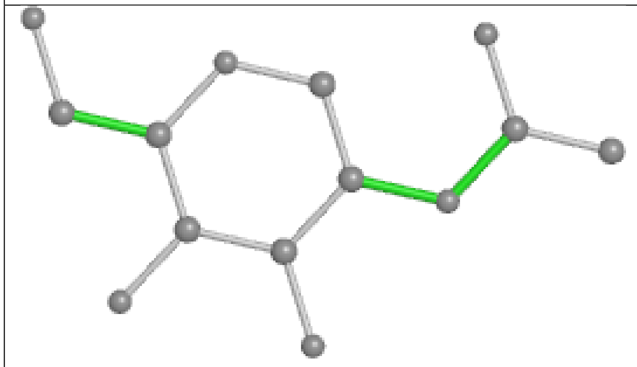

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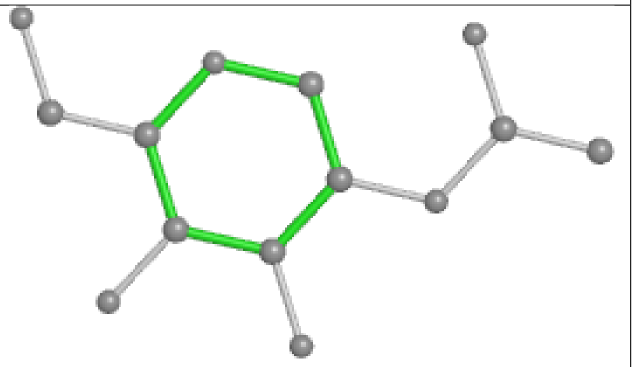
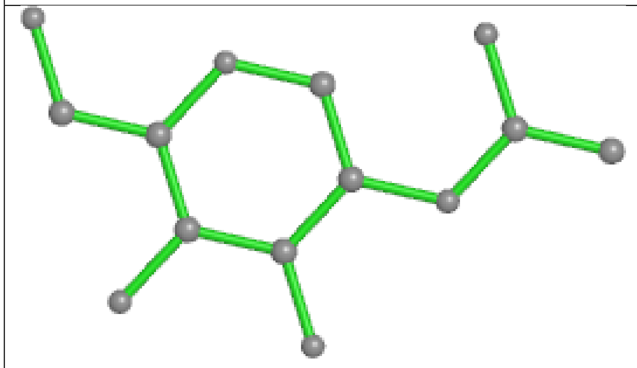


Rings

Ligand NAG D 903



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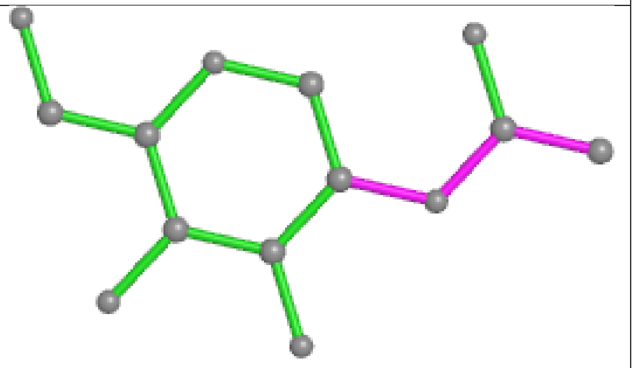

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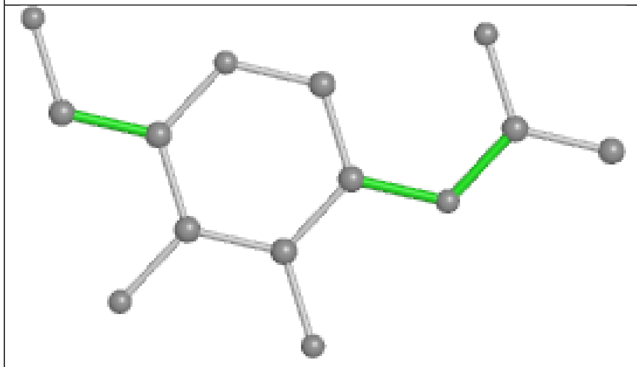

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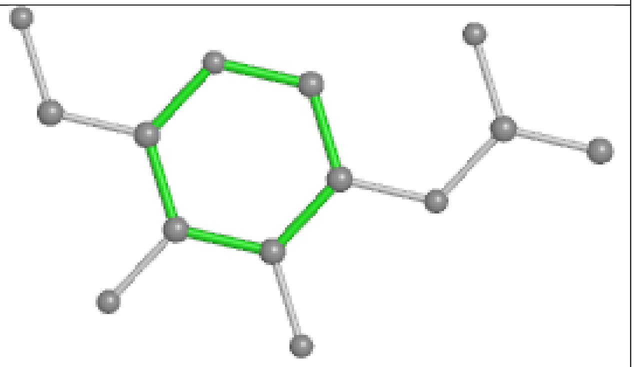
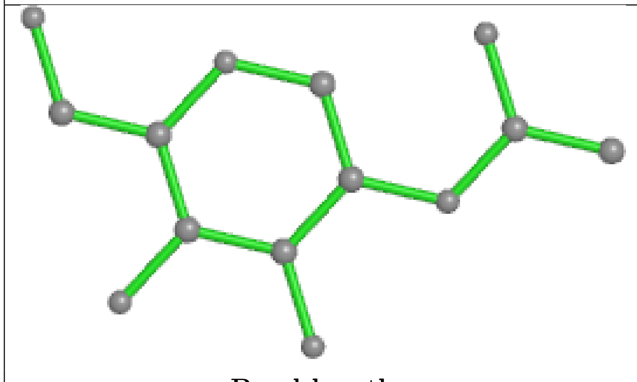
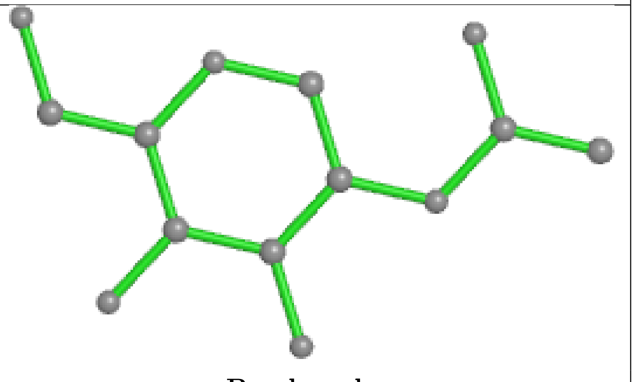


Rings

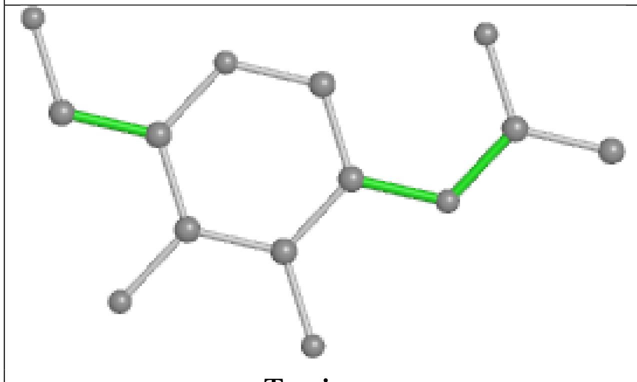
Ligand NAG A 1411



Bond lengths



Bond angles



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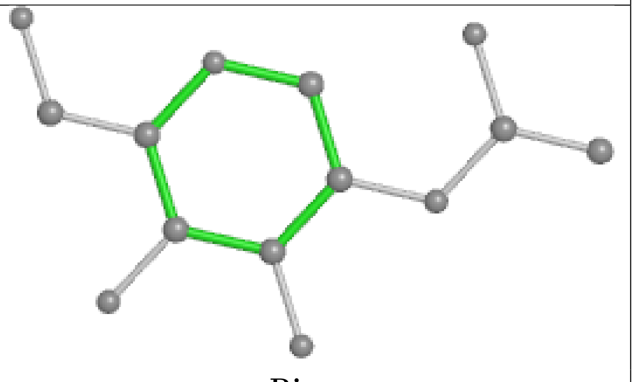
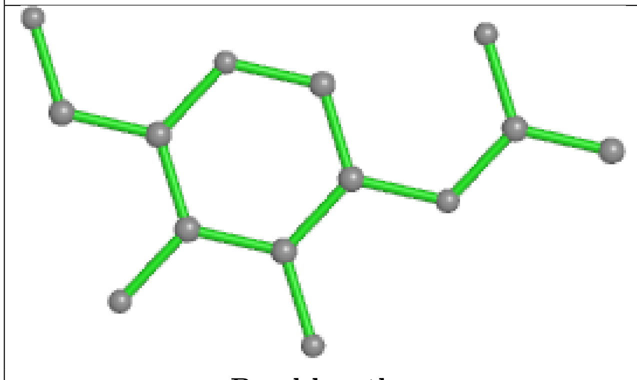


Rings

Ligand NAG A 1401



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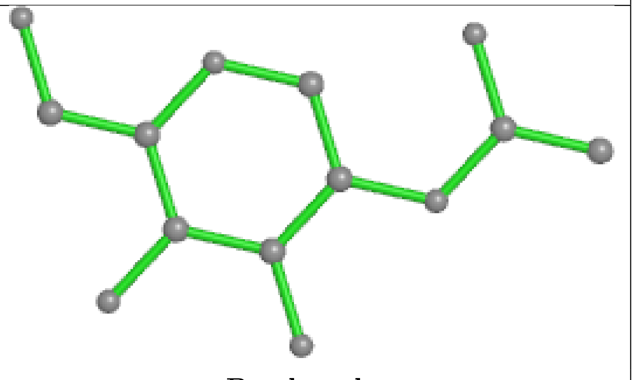
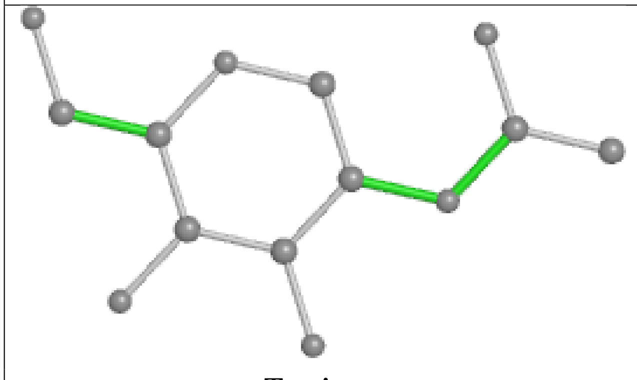
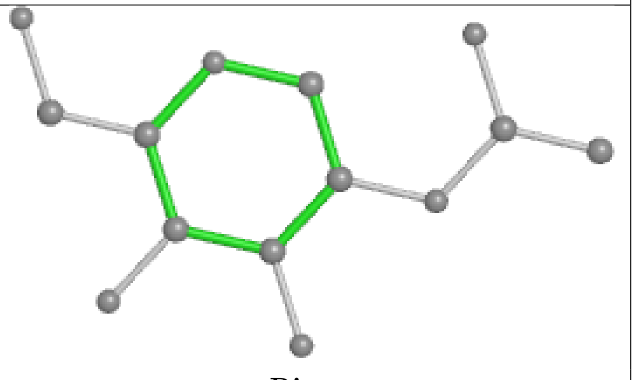


Bond angles

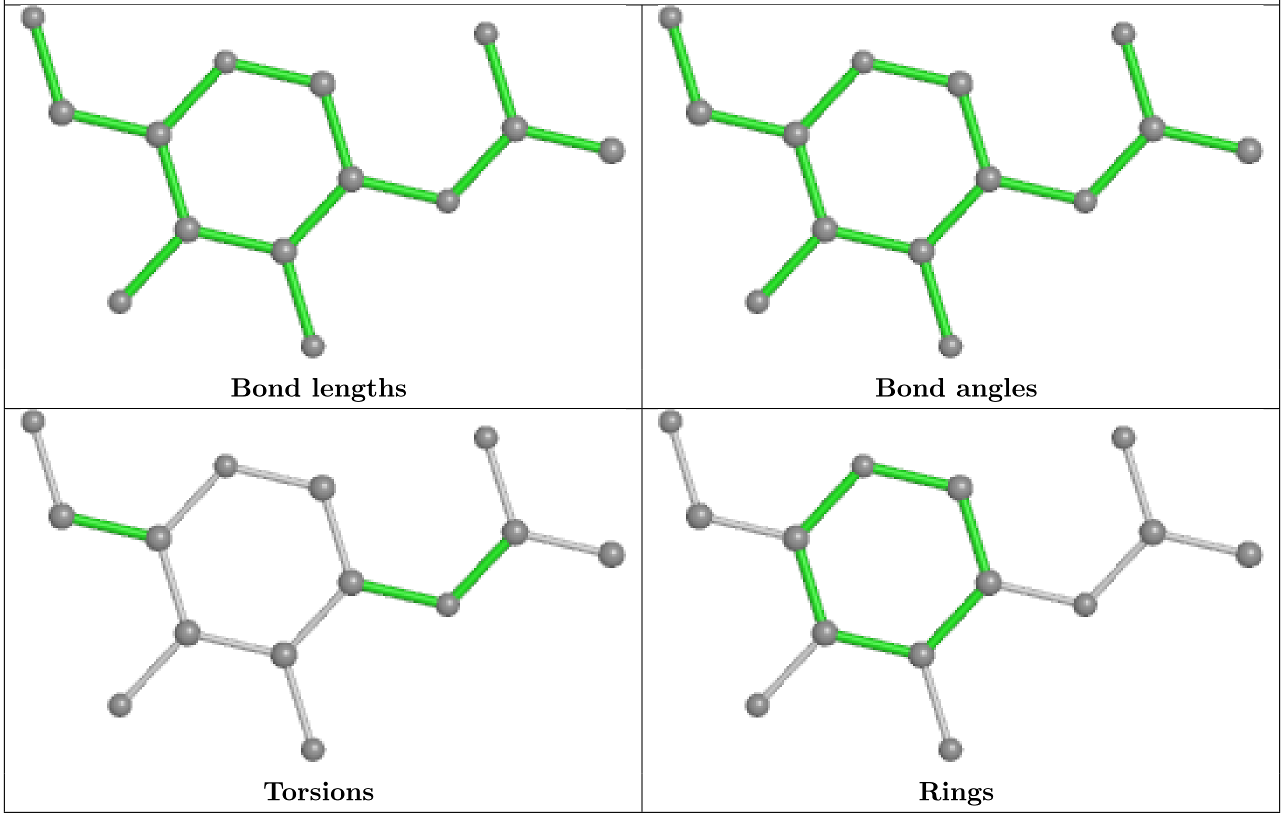


Torsions



Rings

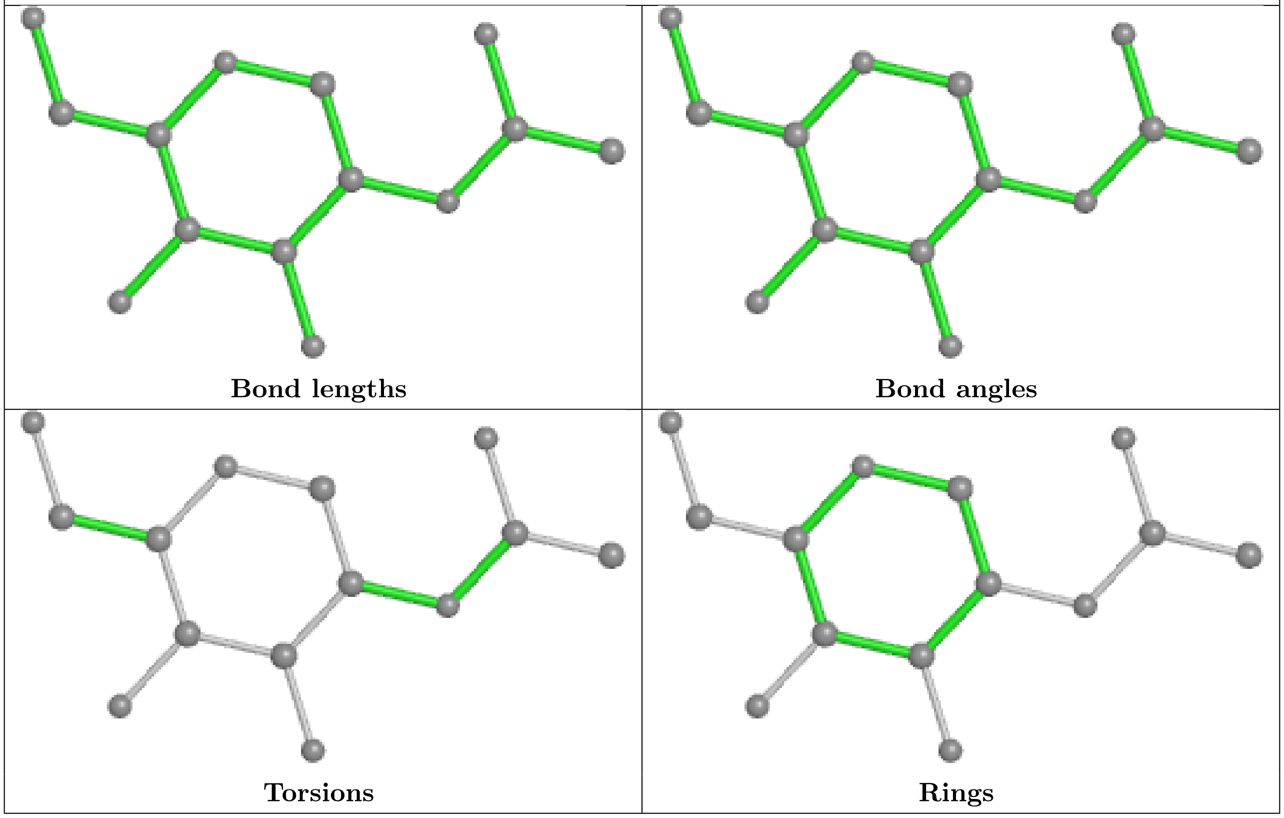
Ligand NAG C 1403



Bond lengths Bond angles

Torsions Rings

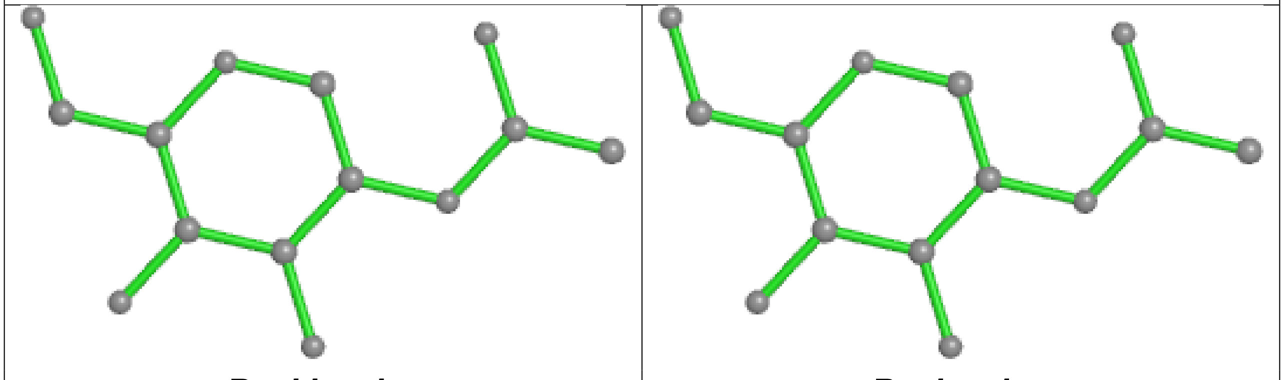
Ligand NAG A 1408



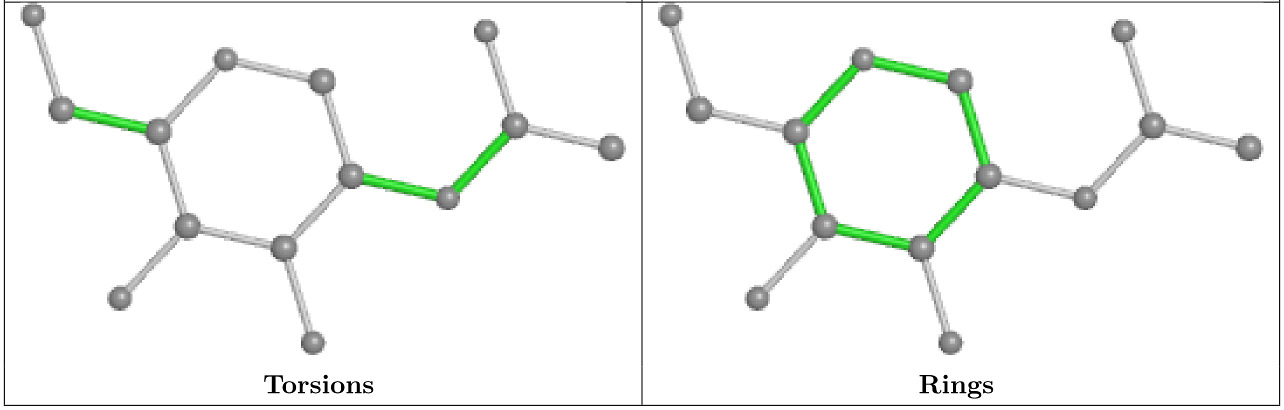
Bond lengths Bond angles

Torsions Rings

Ligand NAG D 906

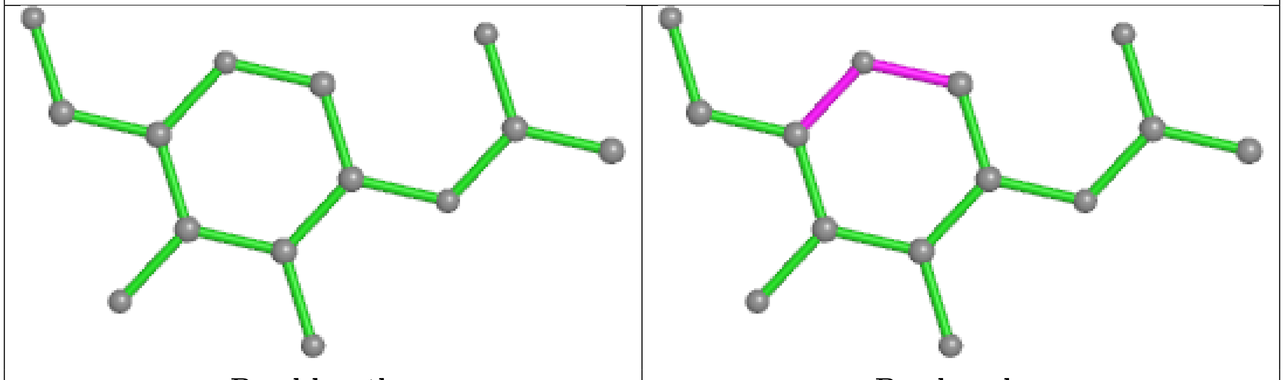


Bond lengths Bond angles

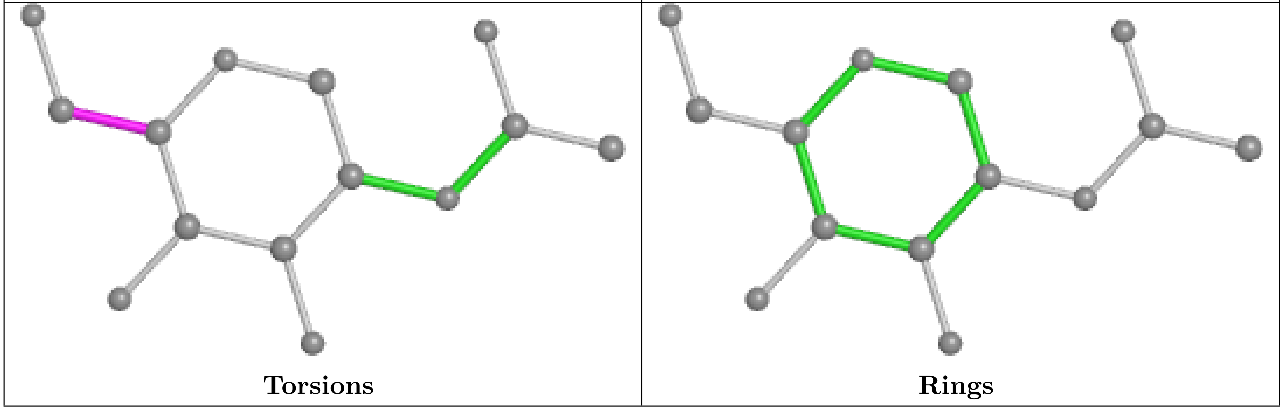


Torsions Rings

Ligand NAG D 907

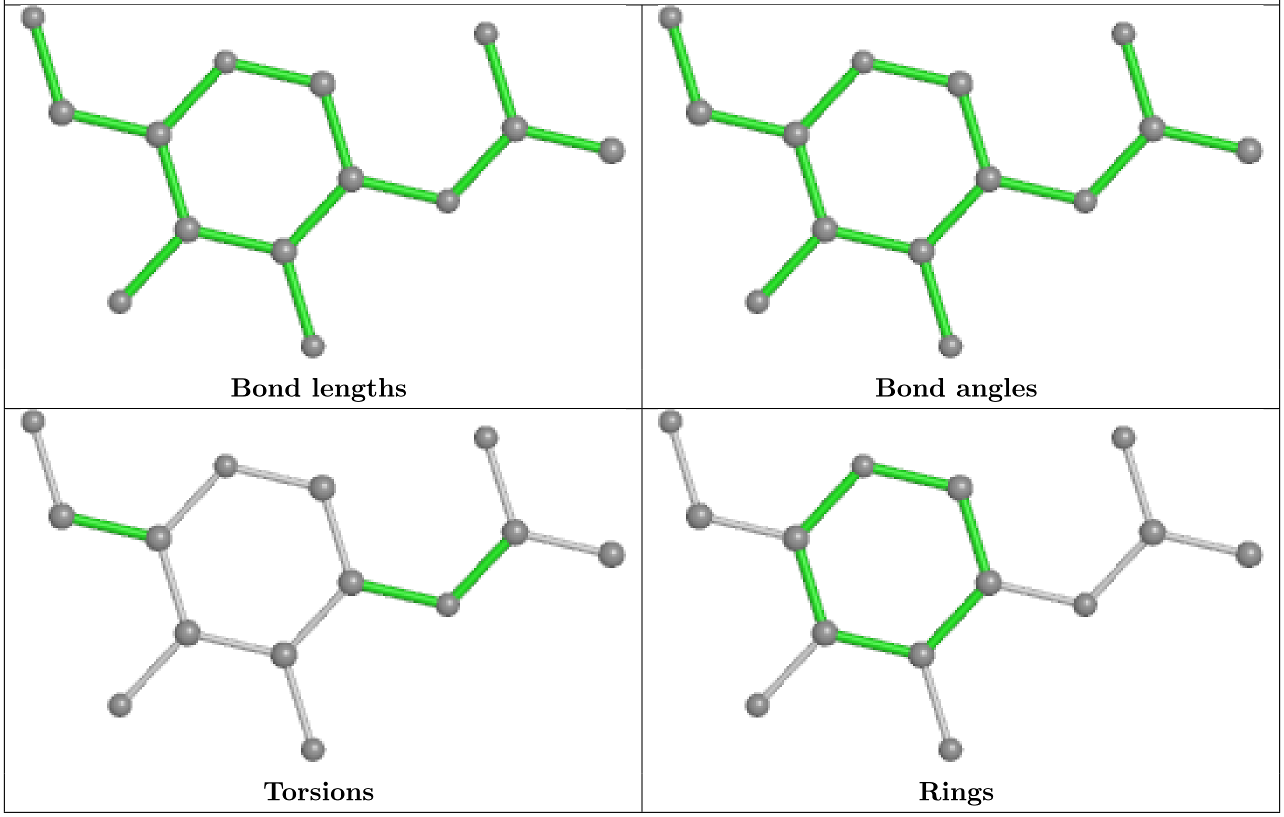


Bond lengths Bond angles



Torsions Rings

Ligand NAG C 1407



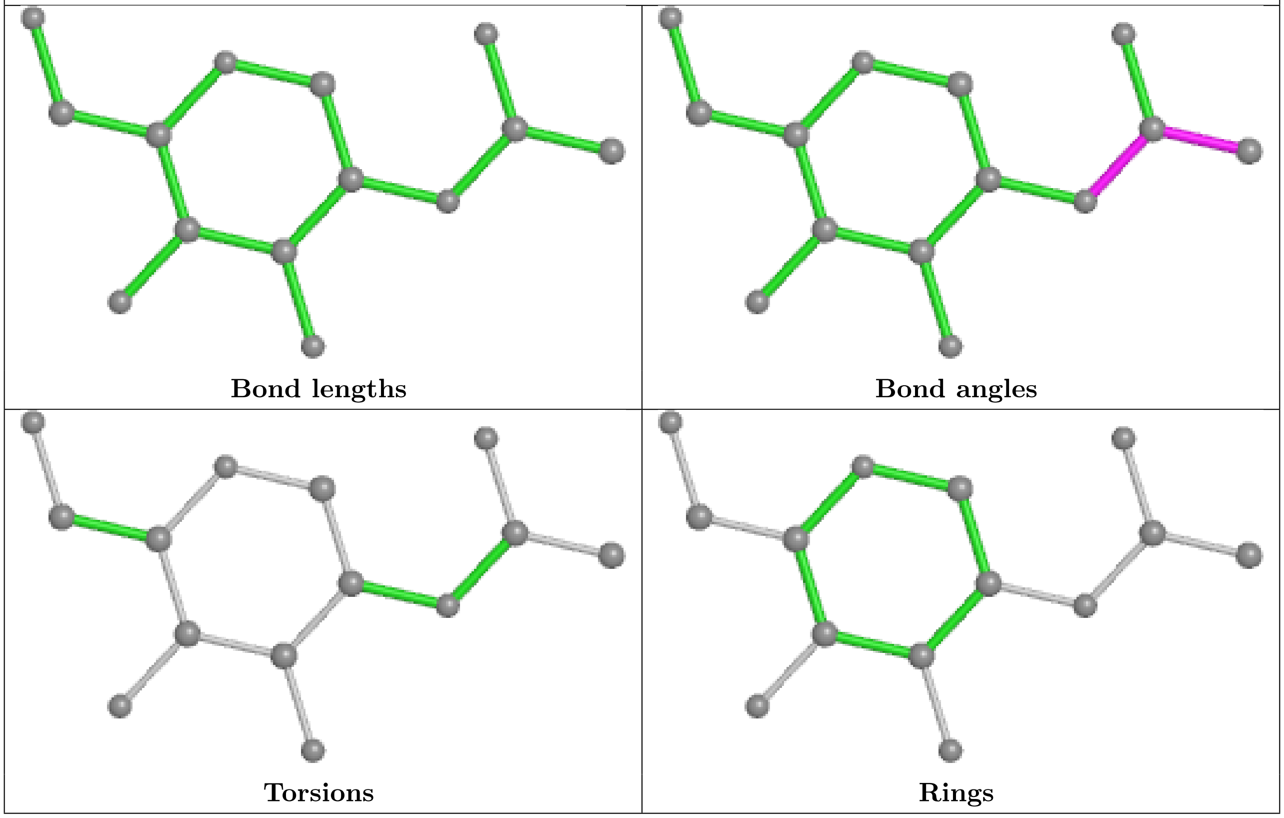
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1406



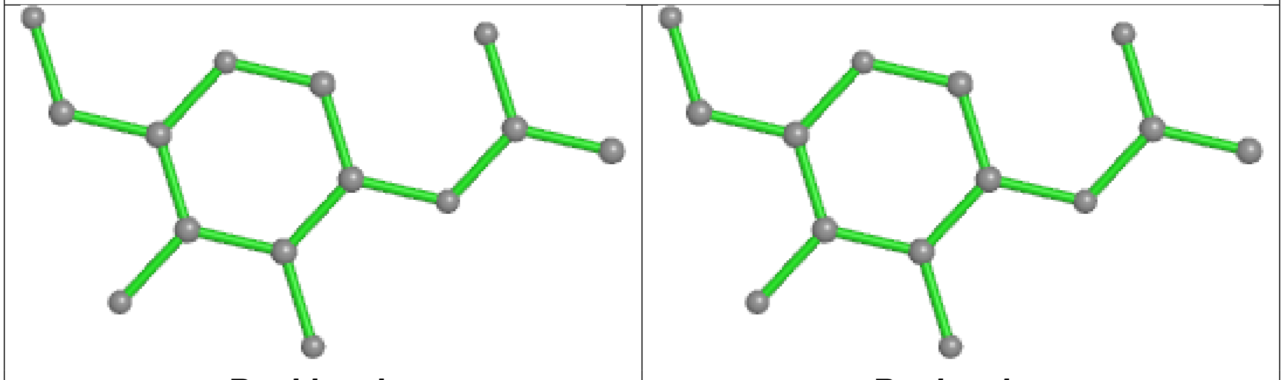
Bond lengths

Bond angles

Torsions

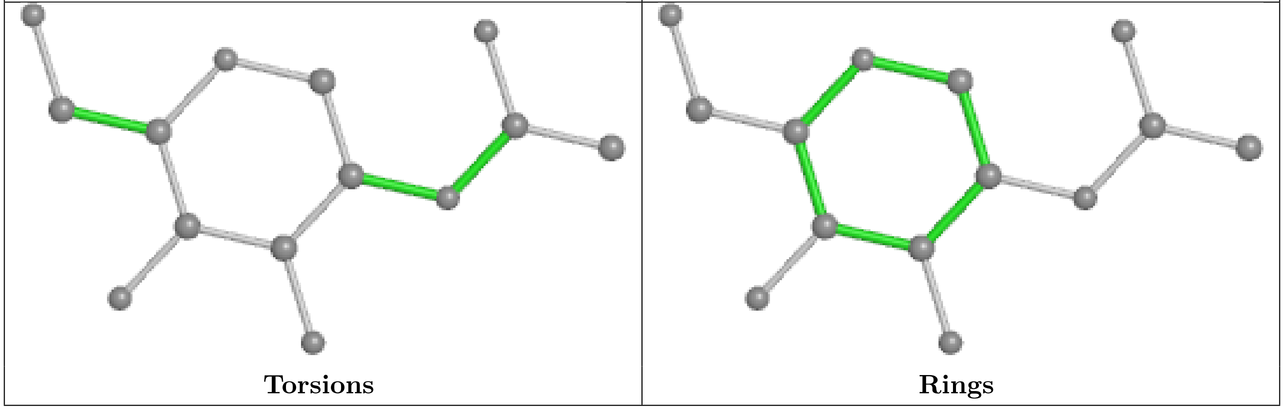
Rings

Ligand NAG B 1402



Bond lengths

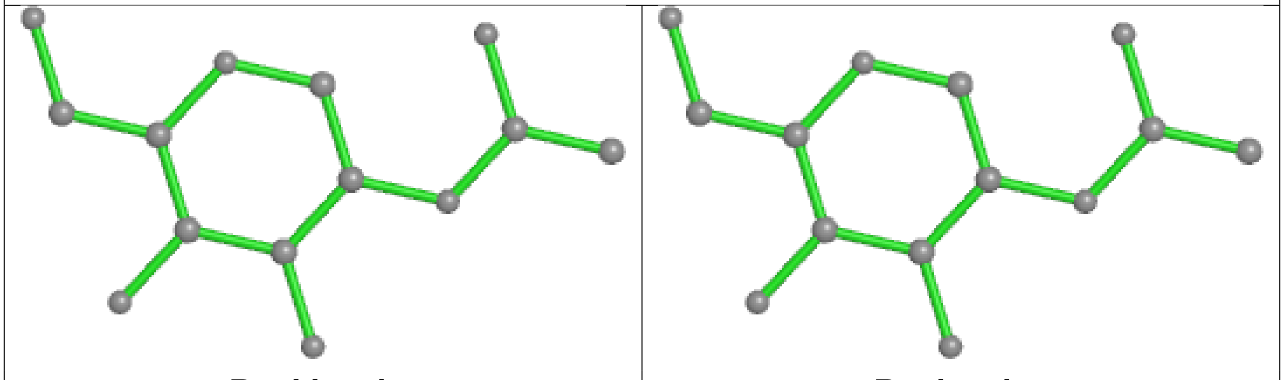
Bond angles



Torsions

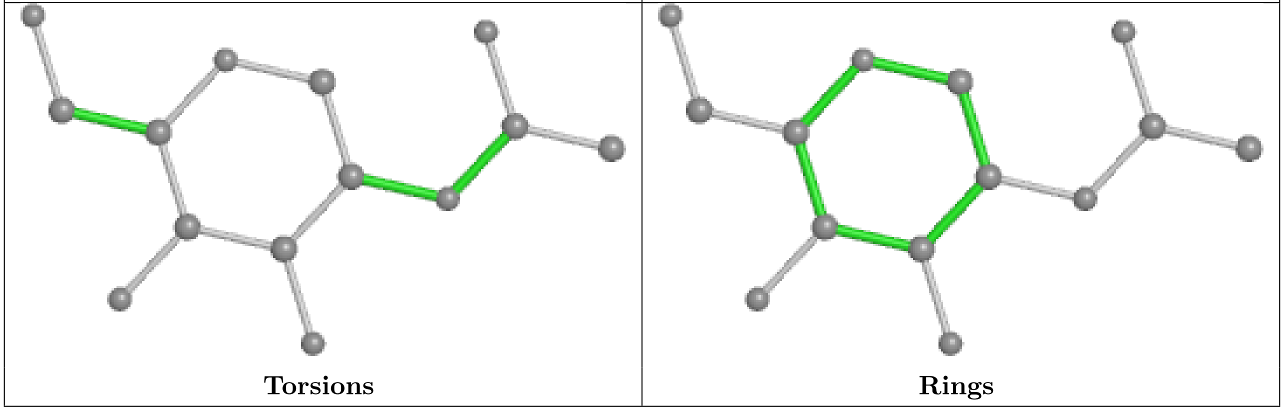
Rings

Ligand NAG C 1408



Bond lengths

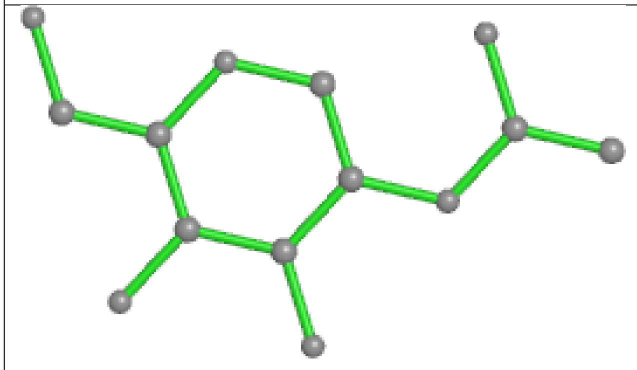
Bond angles

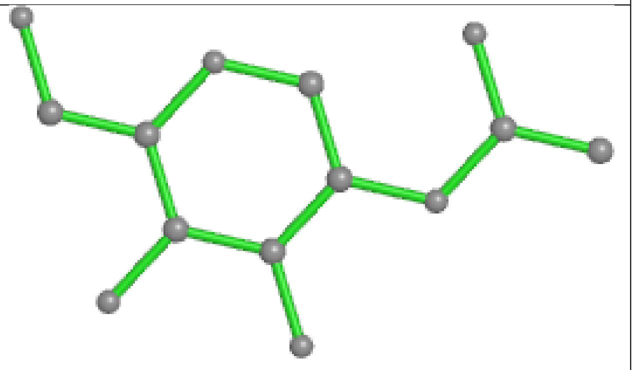


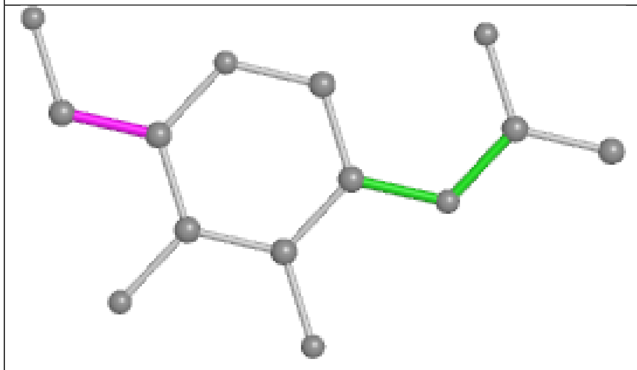
Torsions

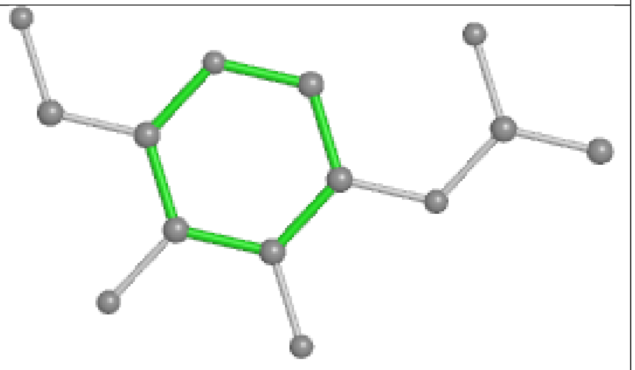
Rings

Ligand NAG E 901

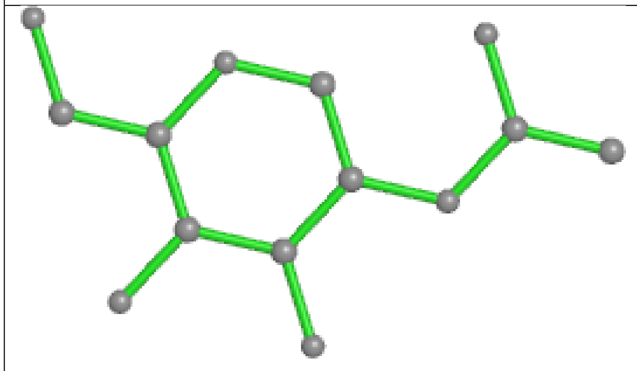

Bond lengths

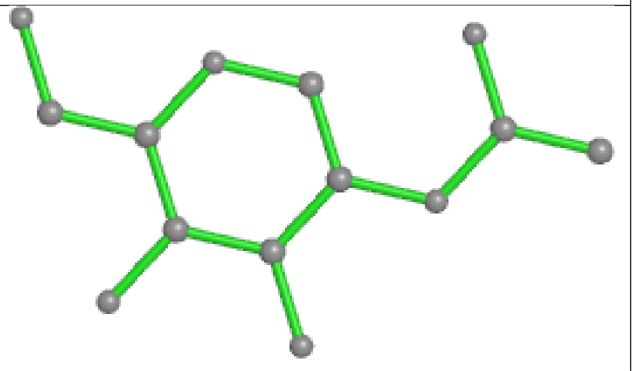

Bond angles

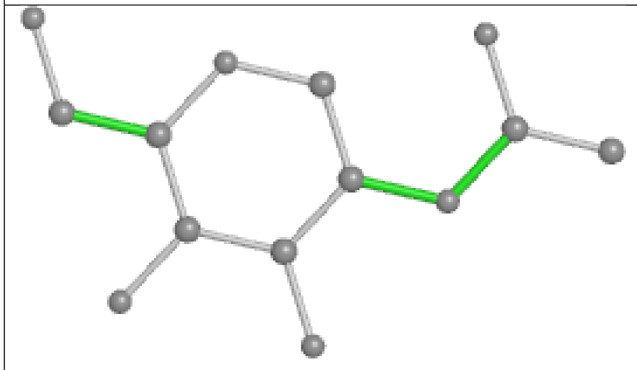

Torsions

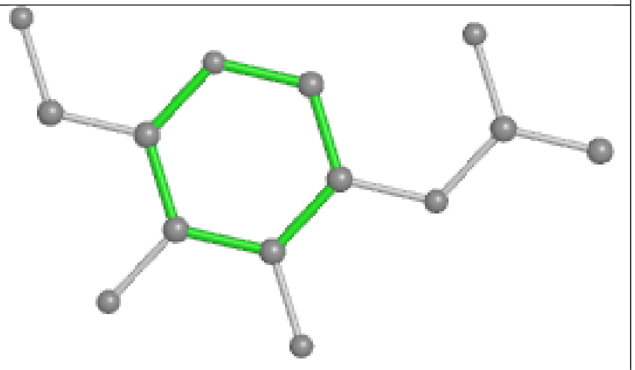

Rings

Ligand NAG E 906

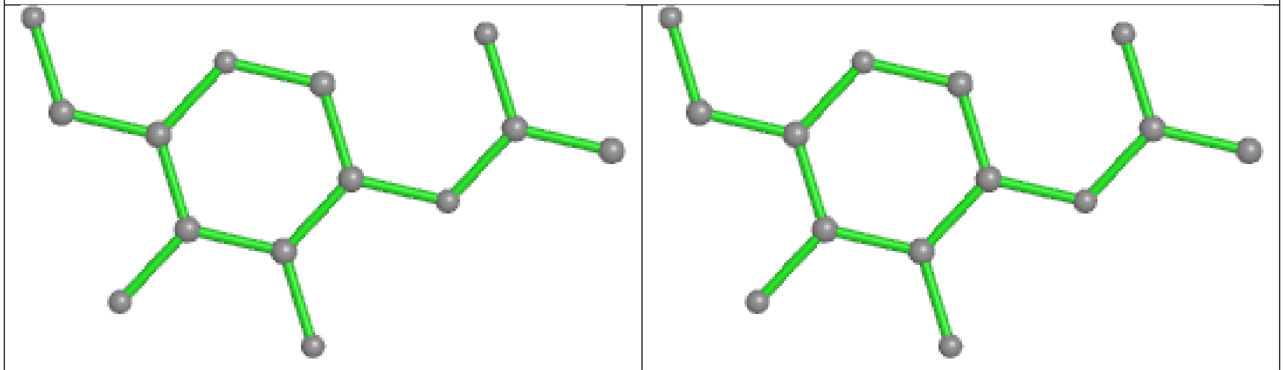

Bond lengths


Bond angles


Torsions

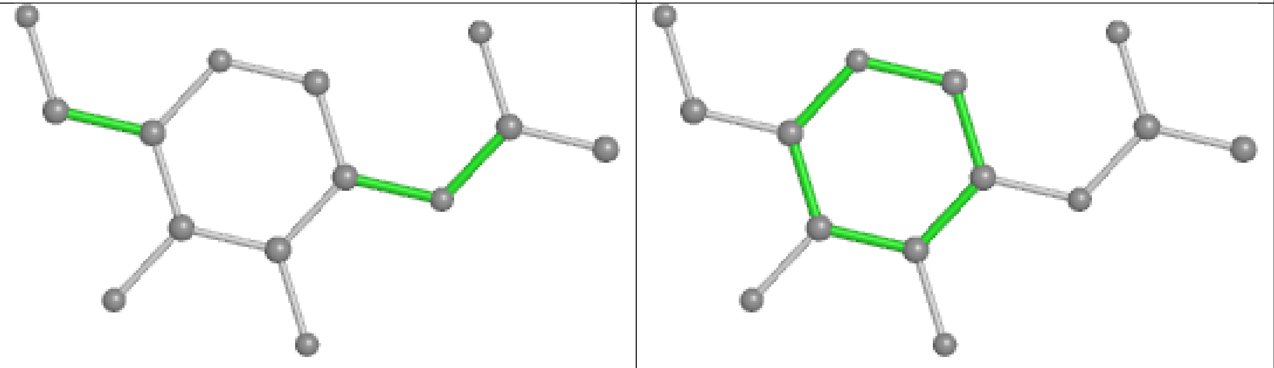

Rings

Ligand NAG C 1401



Bond lengths

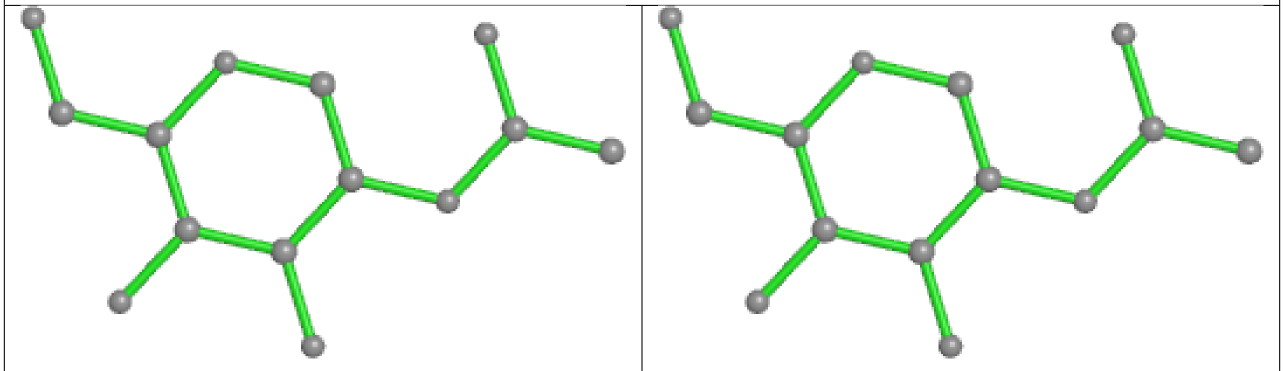
Bond angles



Torsions

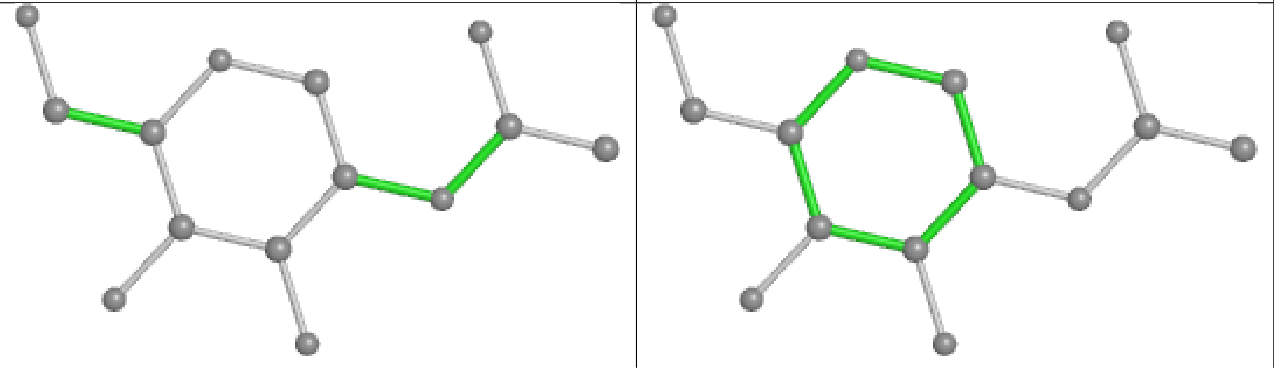
Rings

Ligand NAG B 1409



Bond lengths

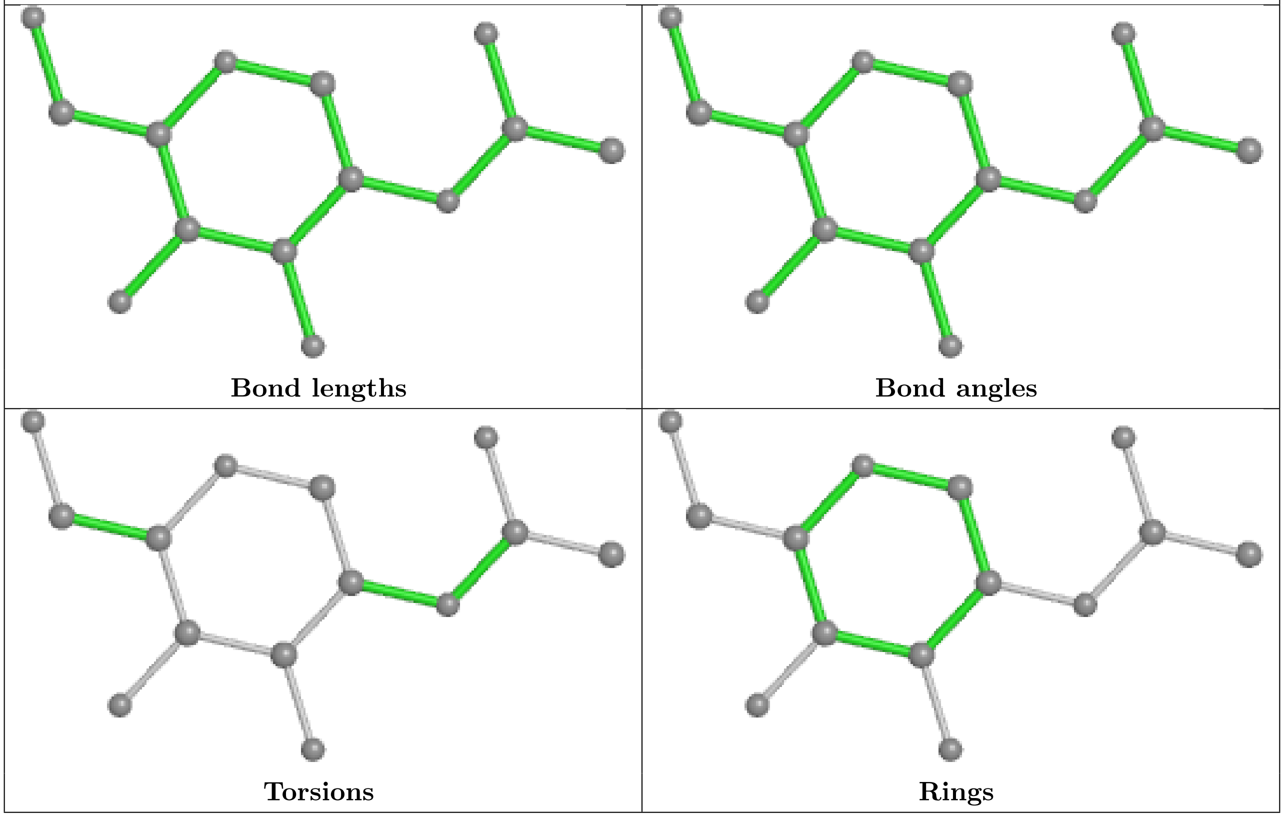
Bond angles



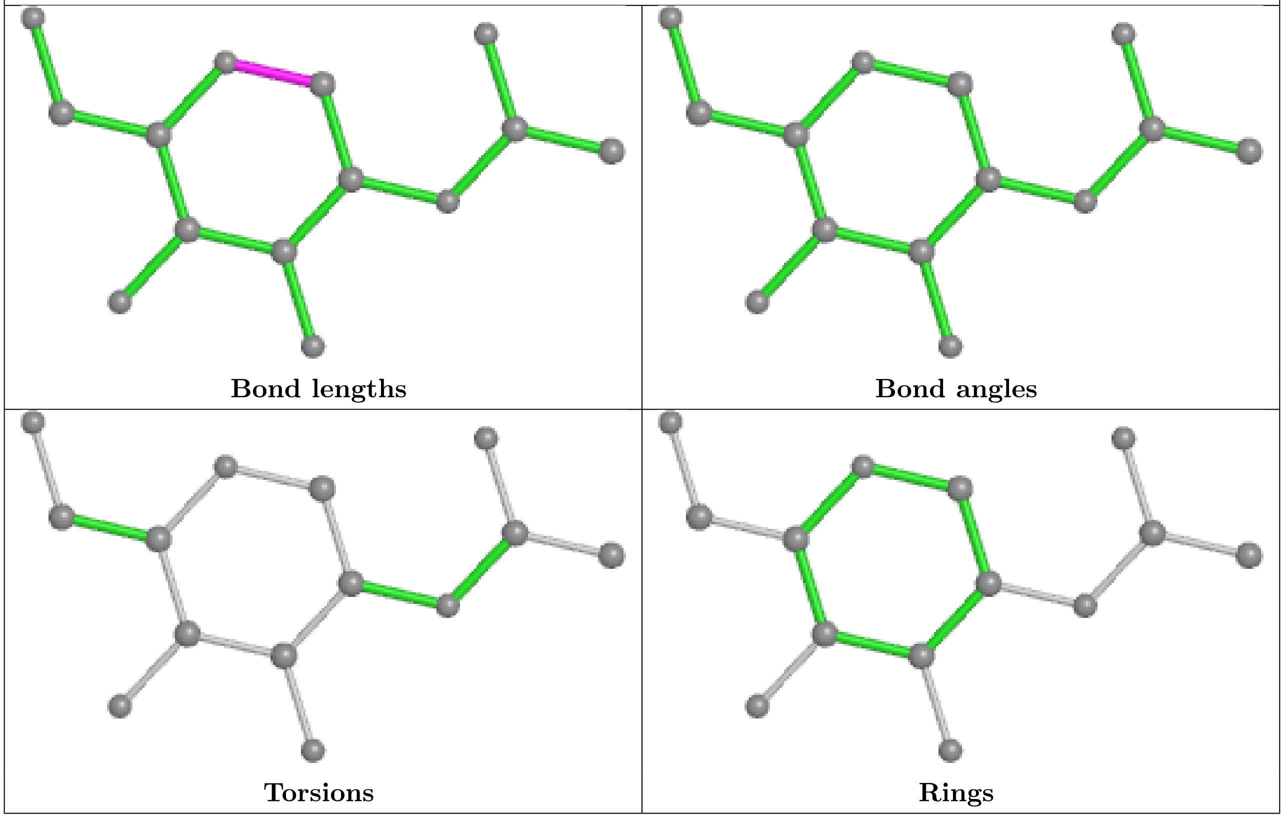
Torsions

Rings

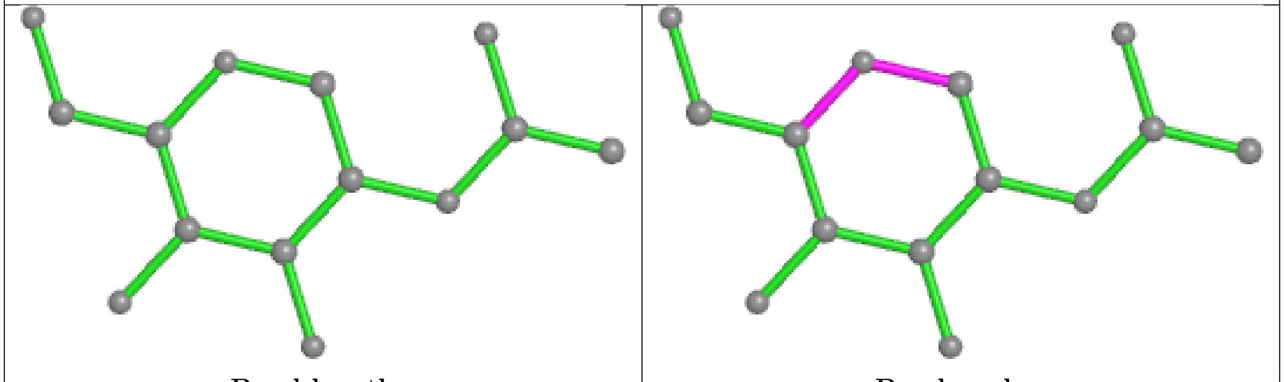
Ligand NAG A 1404


Bond lengths
Bond angles
Torsions
Rings

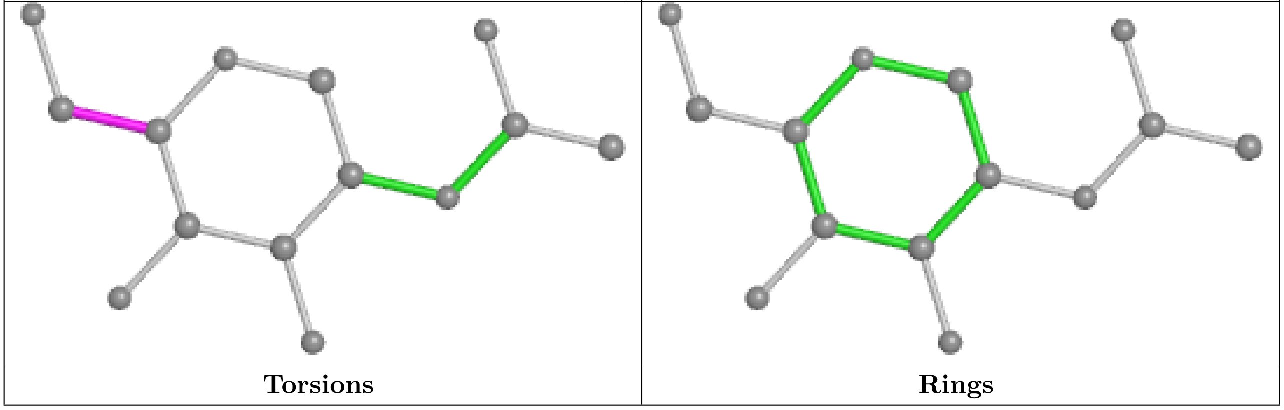
Ligand NAG A 1406


Bond lengths
Bond angles
Torsions
Rings

Ligand NAG E 907

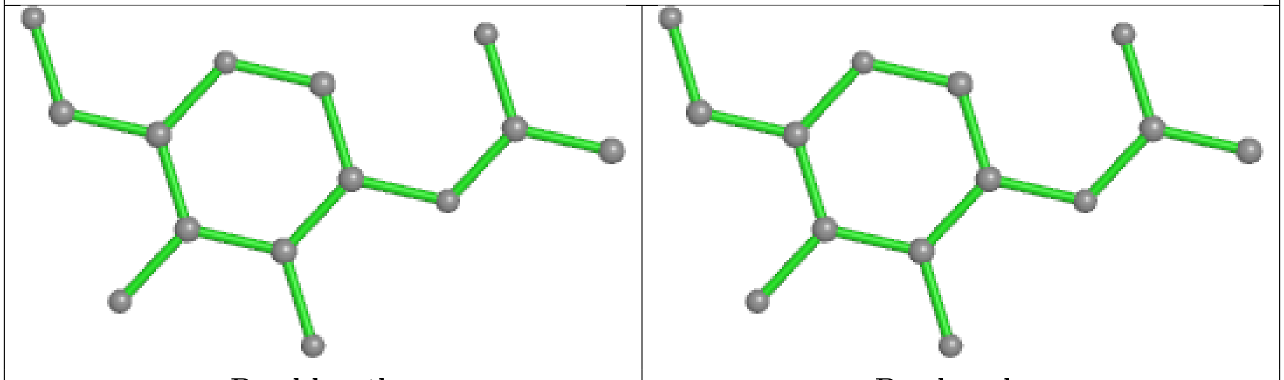


Bond lengths **Bond angles**

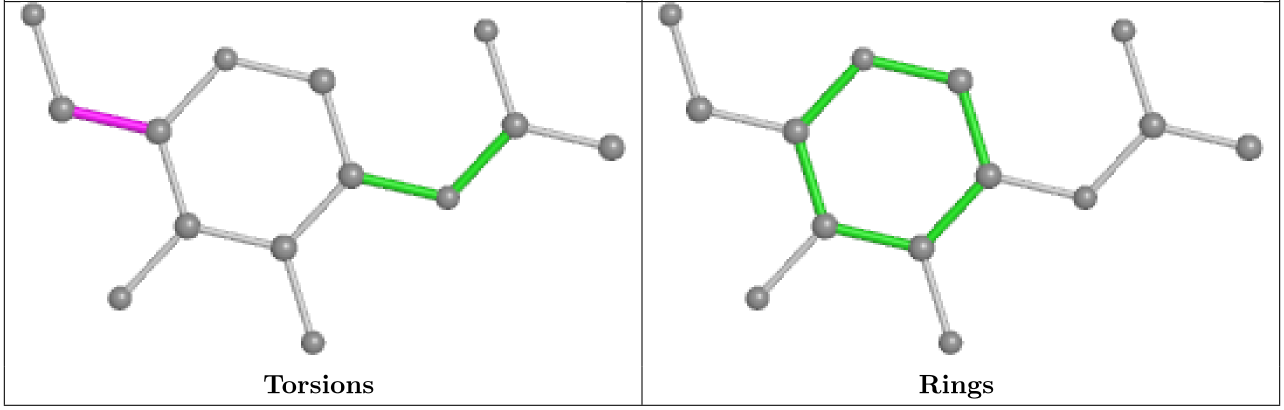


Torsions **Rings**

Ligand NAG D 901

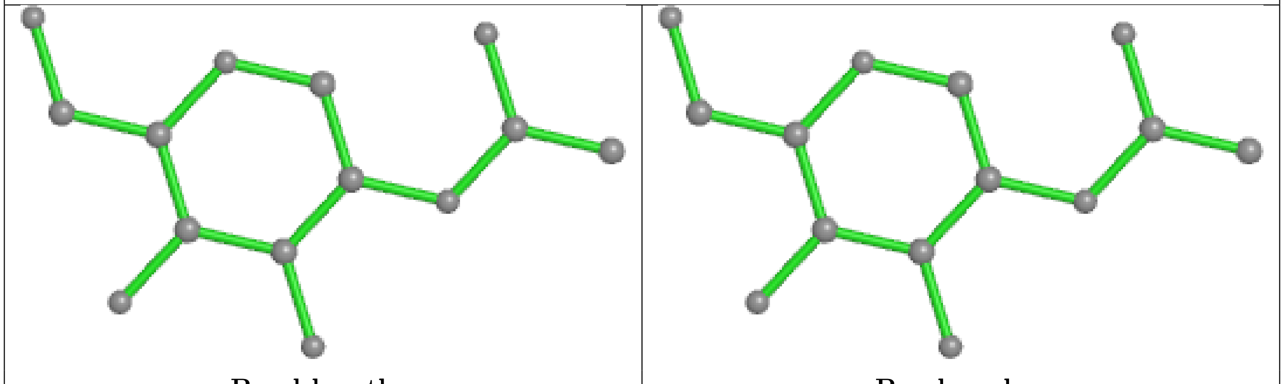


Bond lengths **Bond angles**



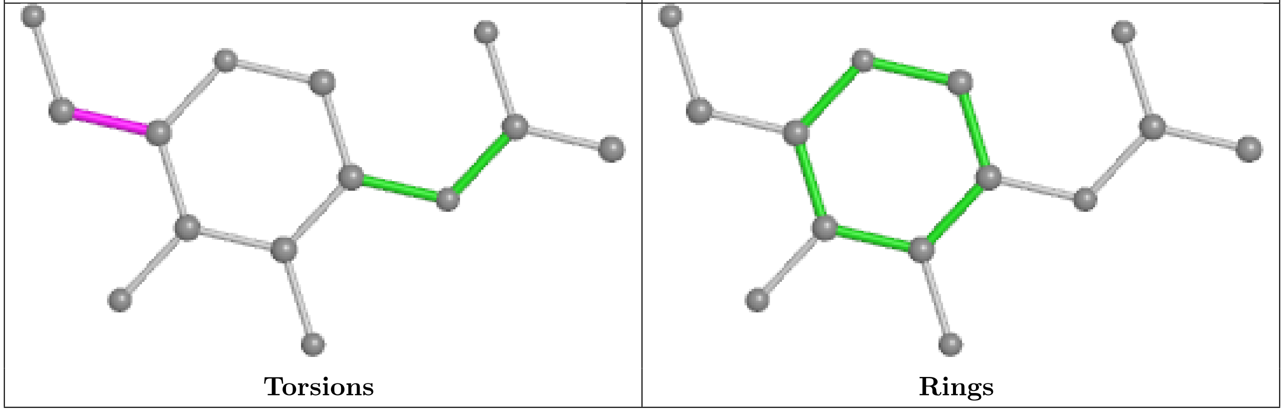
Torsions **Rings**

Ligand NAG A 1402



Bond lengths

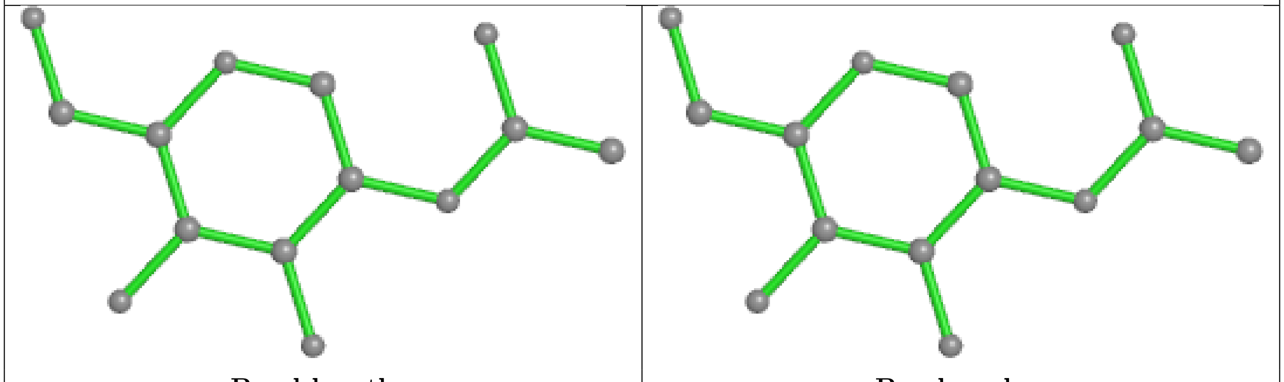
Bond angles



Torsions

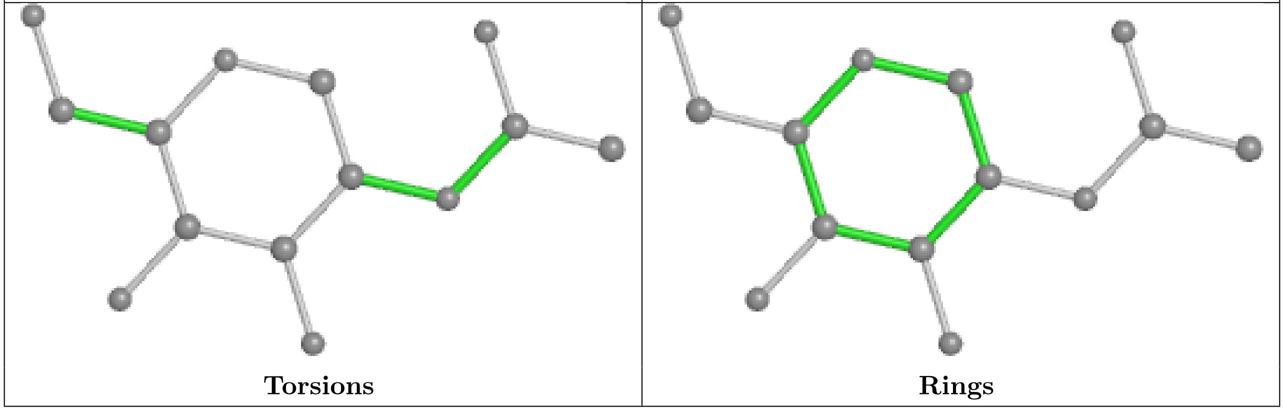
Rings

Ligand NAG B 1404



Bond lengths

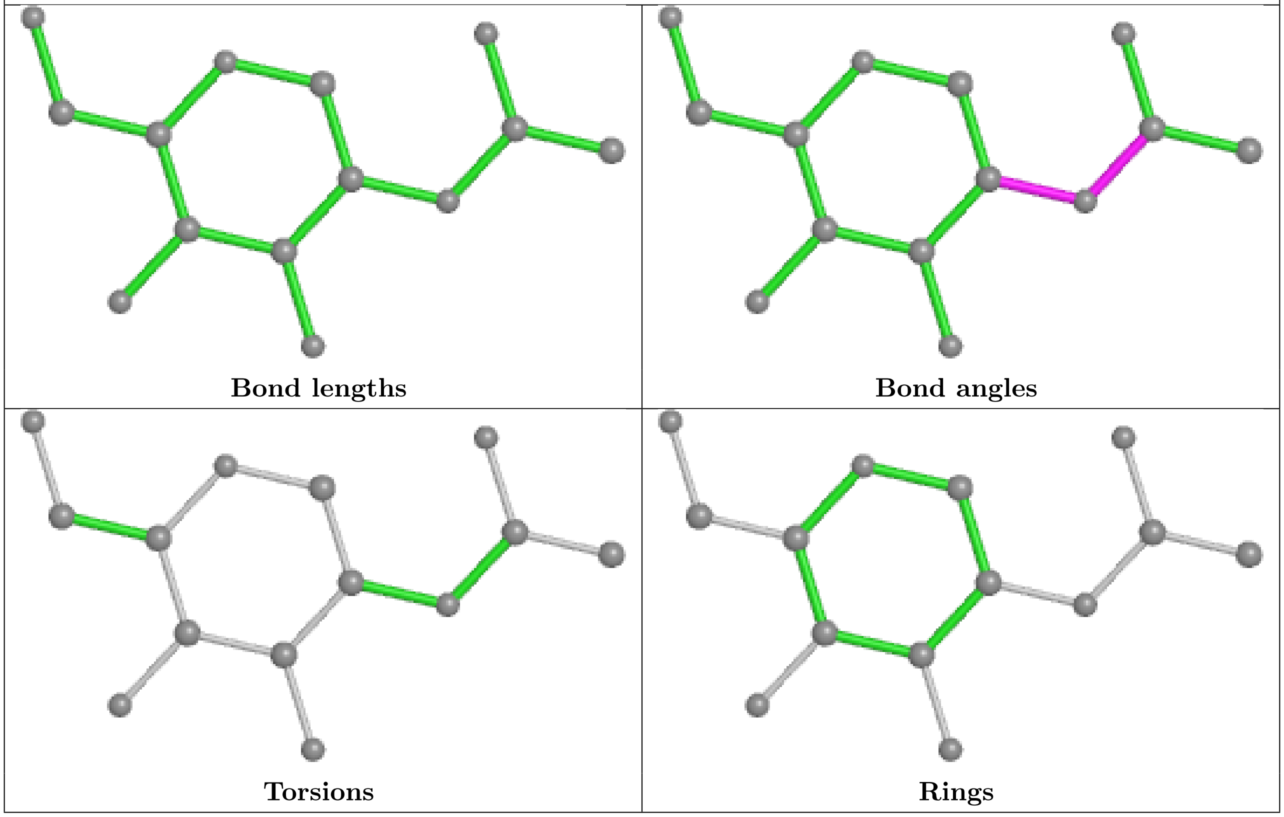
Bond angles



Torsions

Rings

Ligand NAG C 1405



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

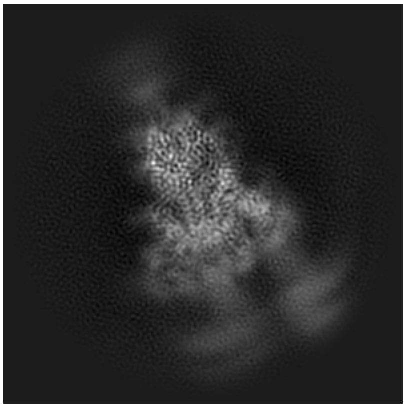
6 Map visualisation

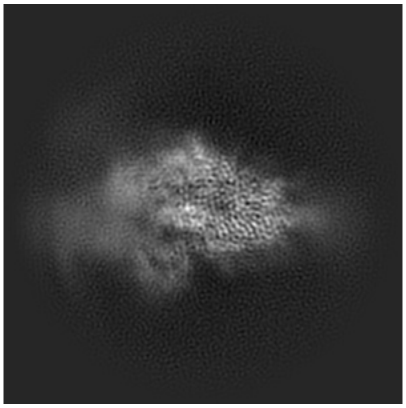
This section contains visualisations of the EMDB entry EMD-33203. These allow visual inspection of the internal detail of the map and identification of artifacts.

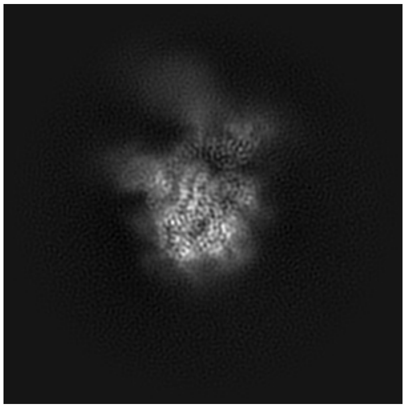
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

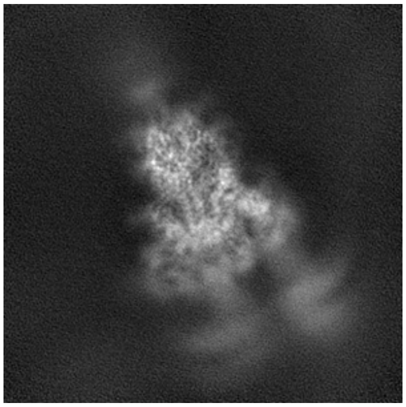
6.1.1 Primary map

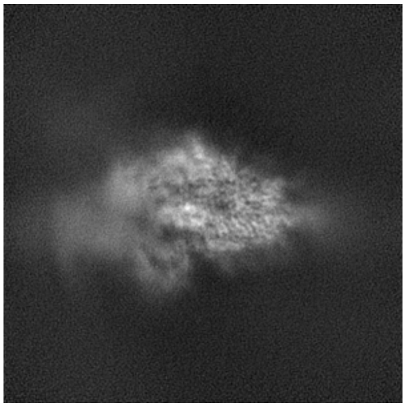

X

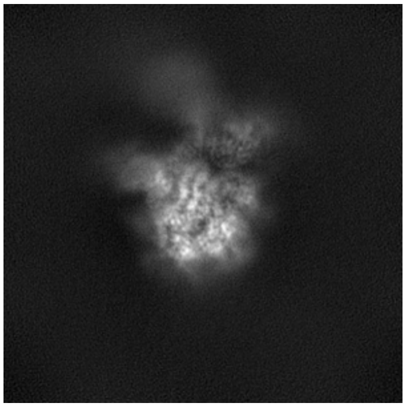

Y


Z

6.1.2 Raw map


X

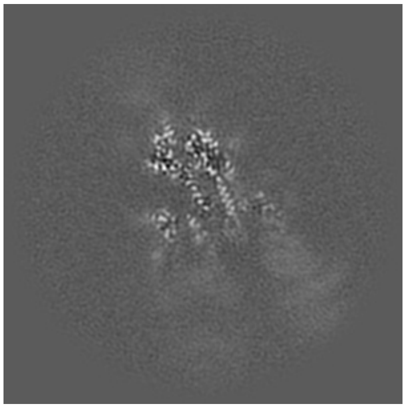

Y


Z

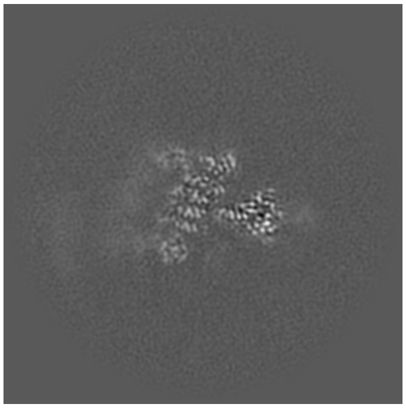
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

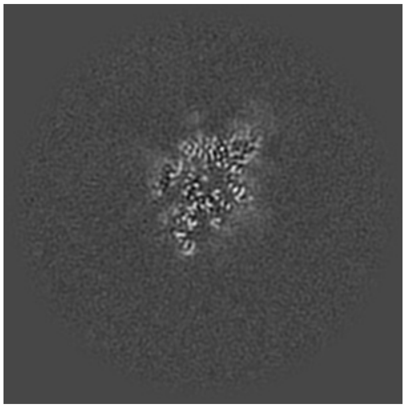
6.2.1 Primary map



X Index: 144

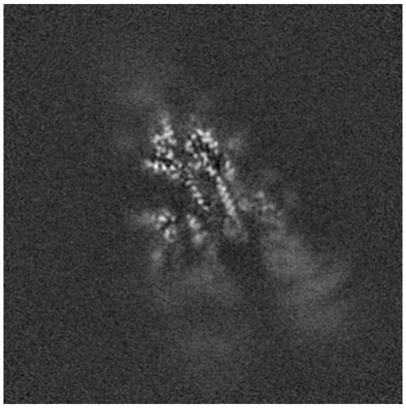


Y Index: 144

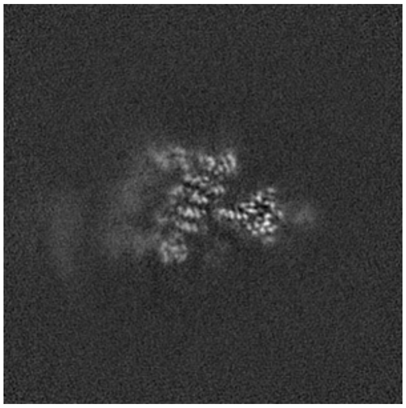


Z Index: 144

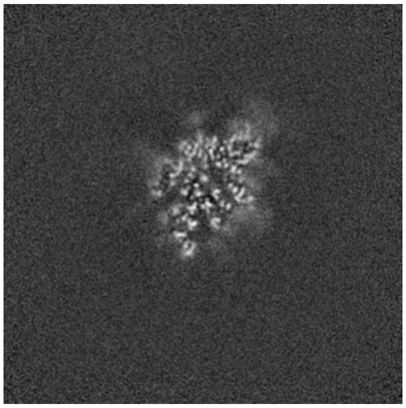
6.2.2 Raw map



X Index: 144



Y Index: 144

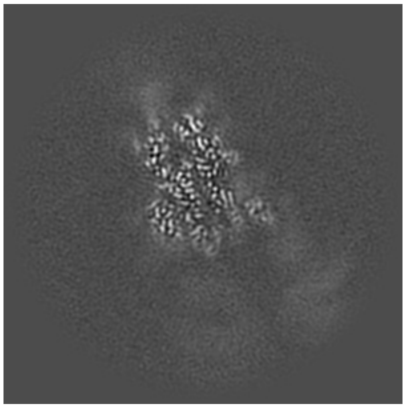


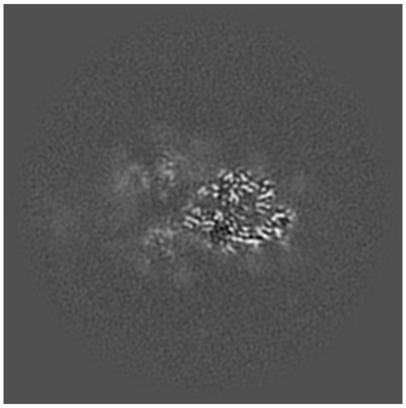
Z Index: 144

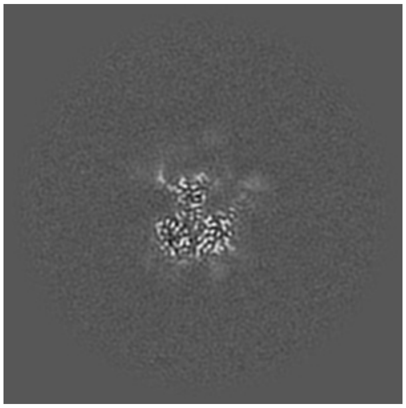
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

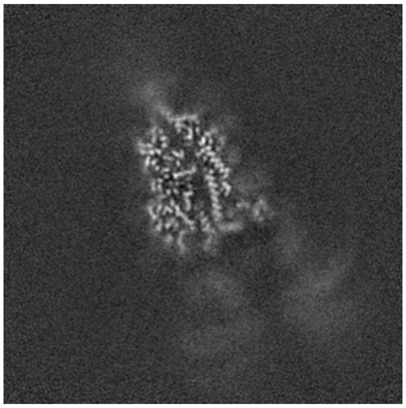
6.3.1 Primary map

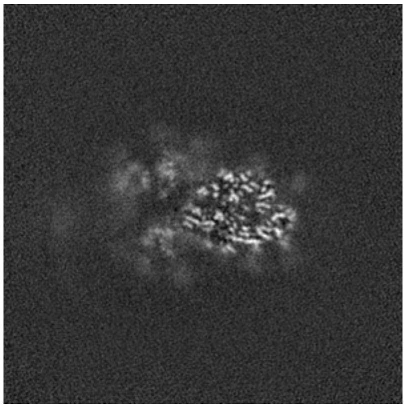

X Index: 133

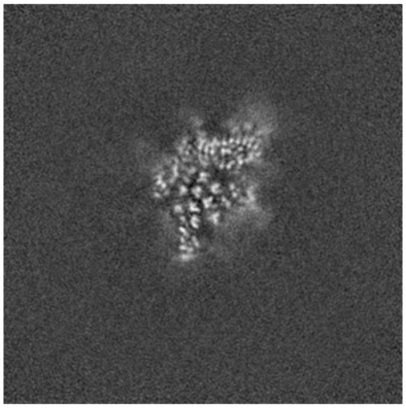

Y Index: 132


Z Index: 168

6.3.2 Raw map


X Index: 129


Y Index: 132


Z Index: 141

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

6.4 Orthogonal surface views

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

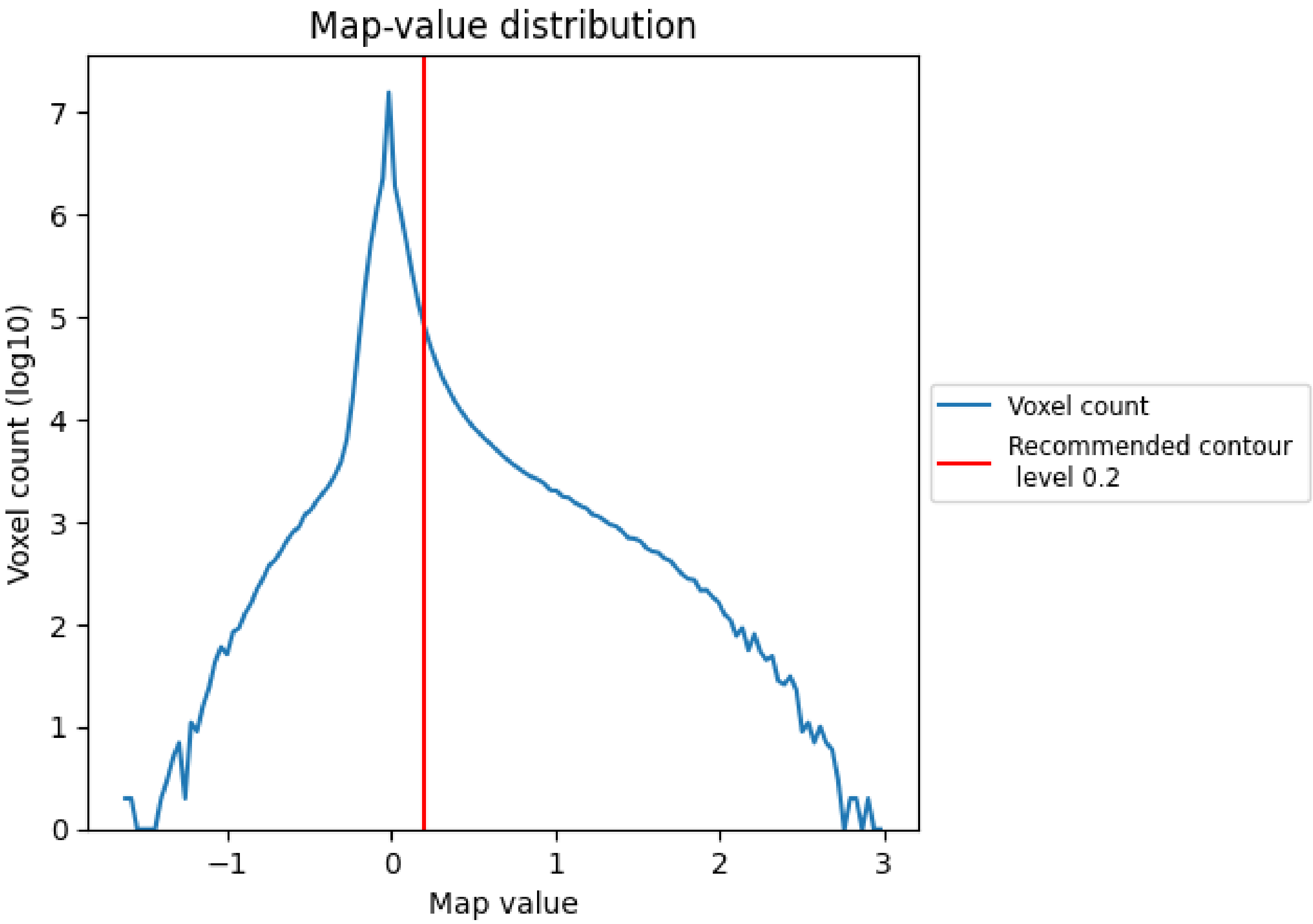
6.5 Mask visualisation

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

7 Map analysis ⓘ

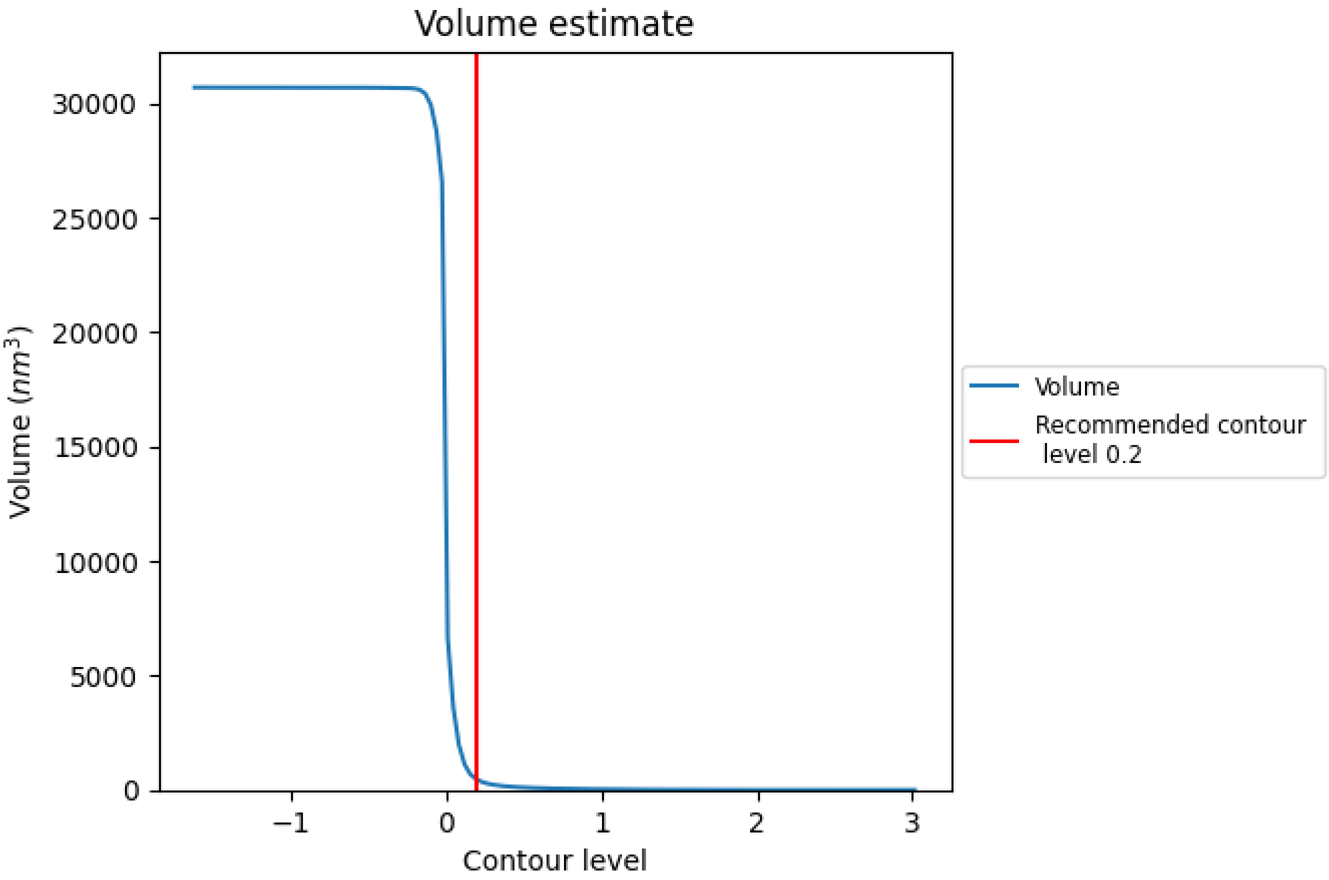
This section contains the results of statistical analysis of the map.

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.

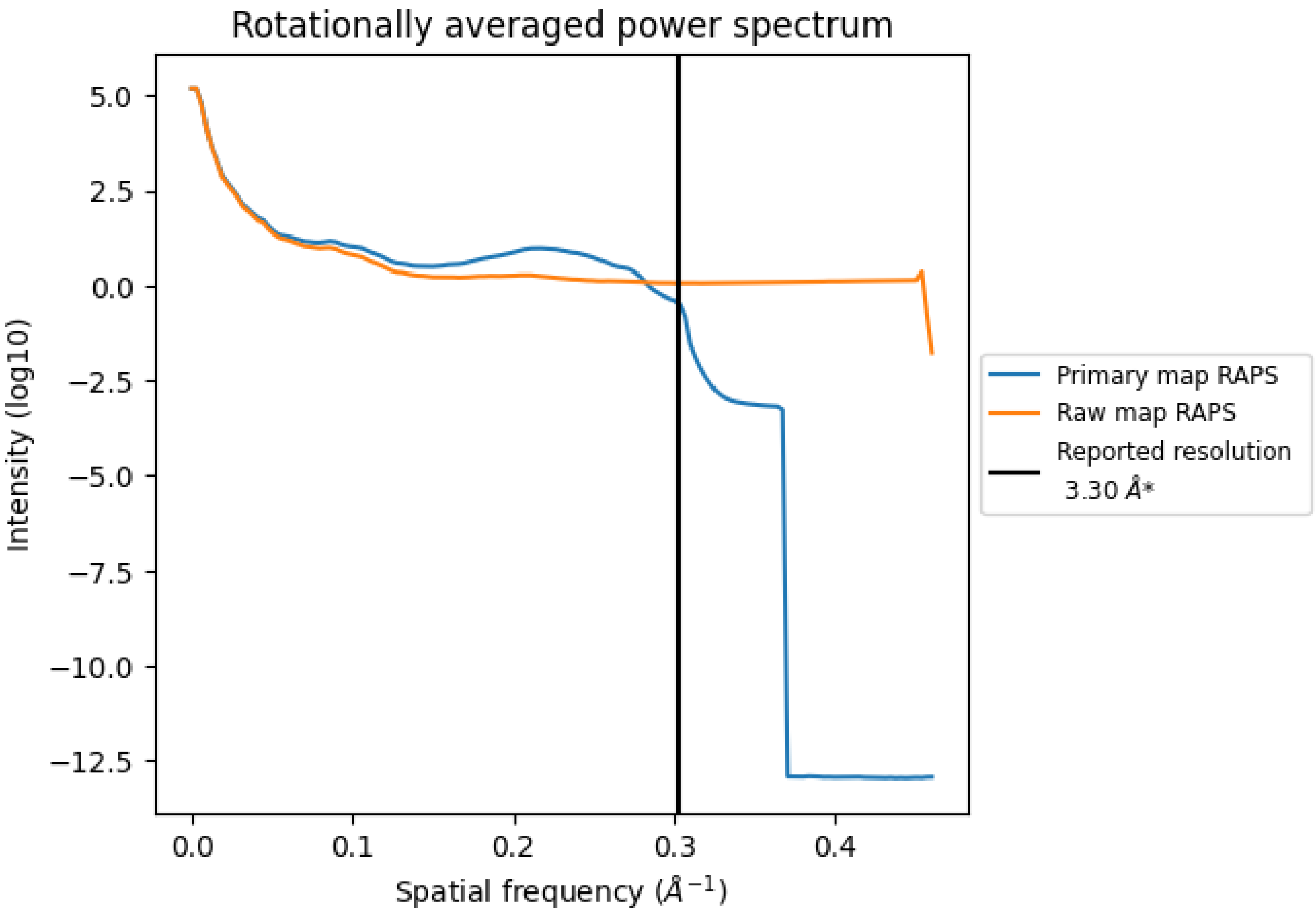
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 452 nm^3; this corresponds to an approximate mass of 408 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 ⓘ

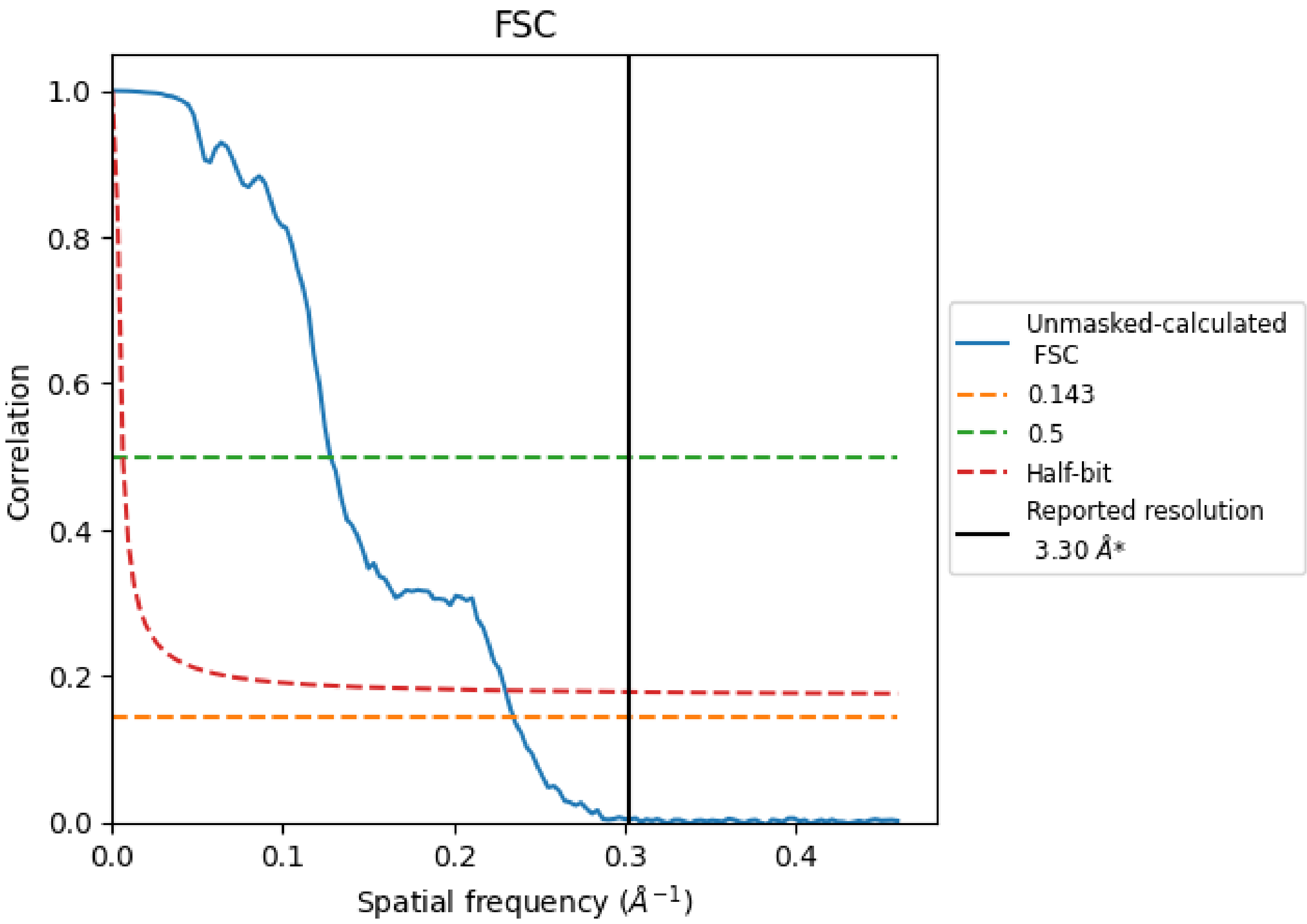


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 $Å^{-1}$

8.2 Resolution estimates ⓘ

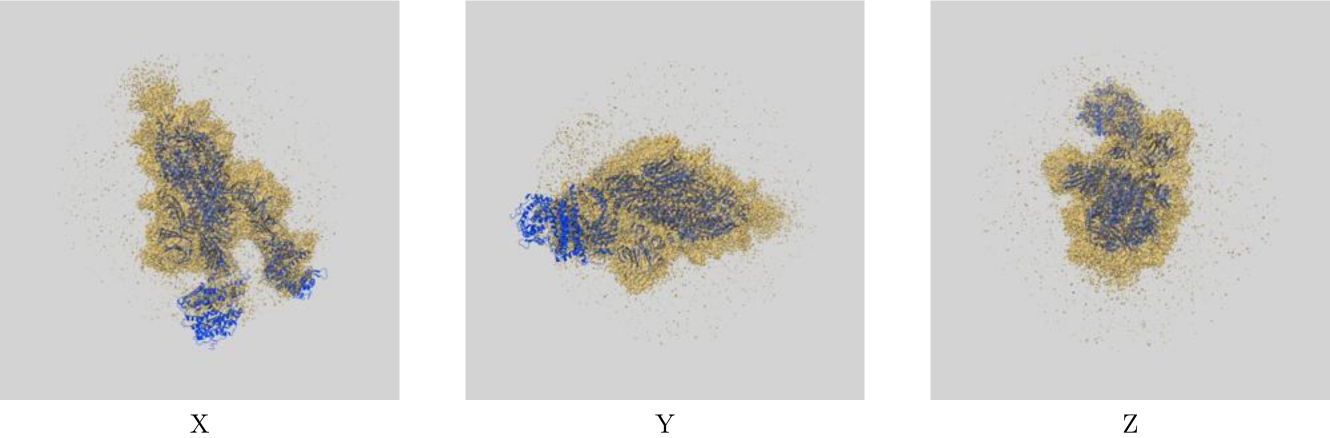
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.25	7.83	4.34

*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 4.25 differs from the reported value 3.3 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-33203 and PDB model 7XID. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay ⓘ



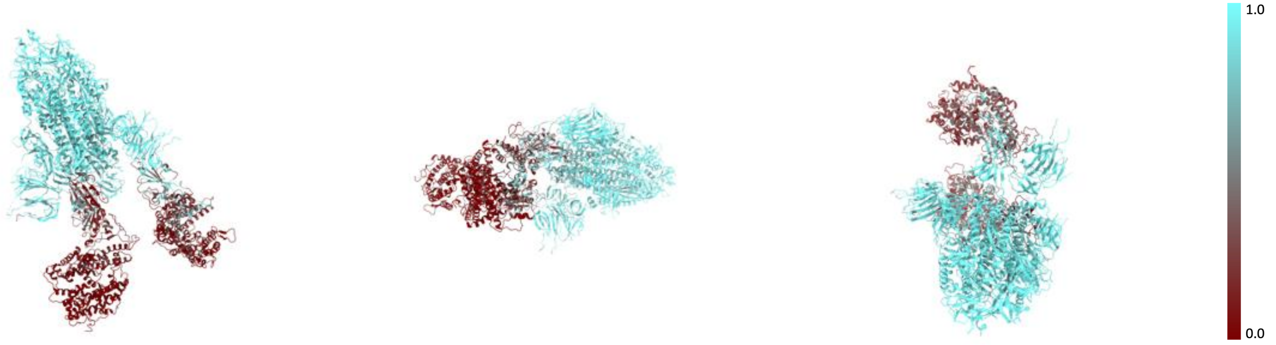
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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.

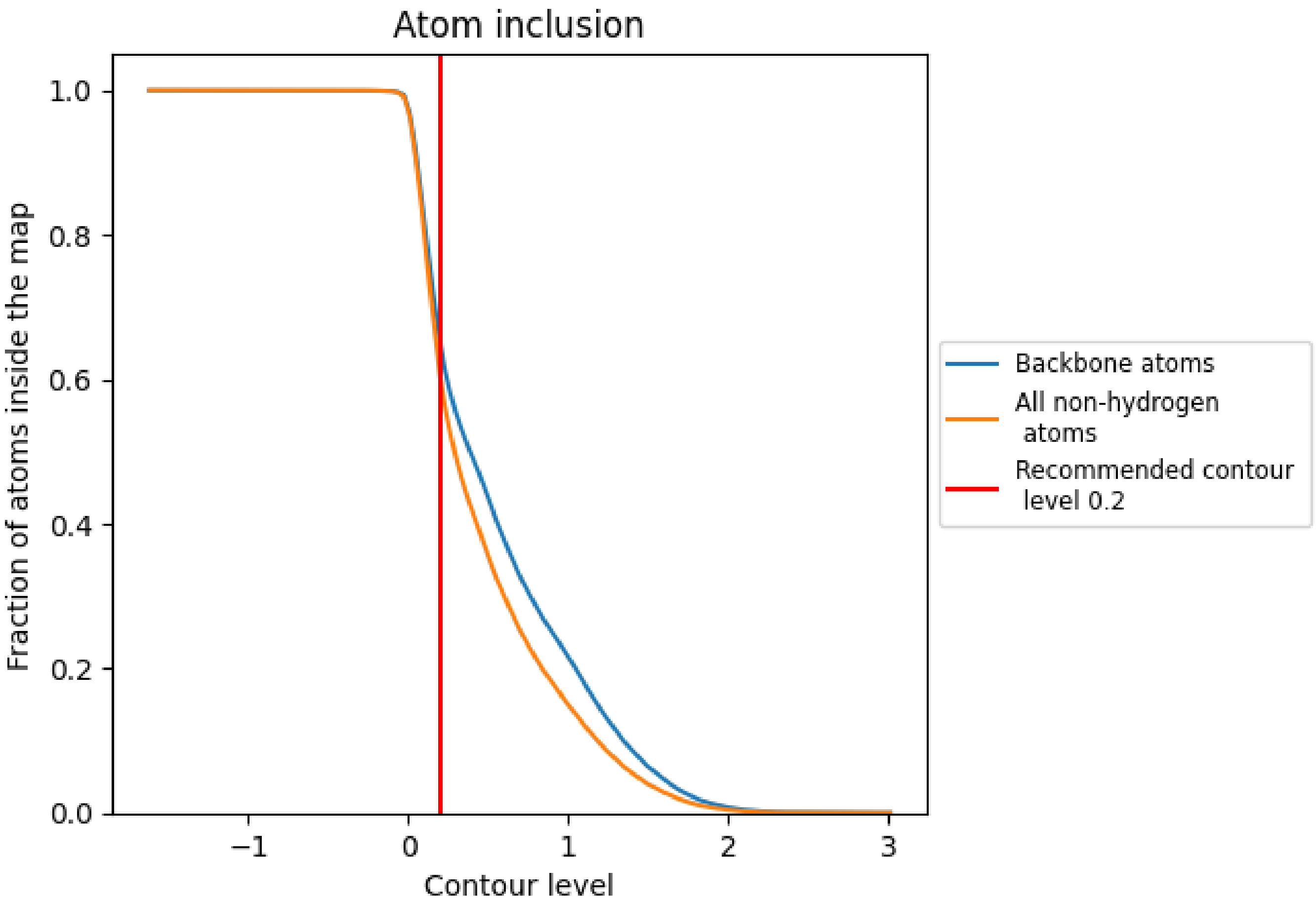
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 65% of all backbone atoms, 60% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6049	0.2340
A	0.8245	0.3430
B	0.7819	0.2950
C	0.8351	0.3350
D	0.1556	0.0170
E	0.0397	0.0150
F	0.5000	0.0540
G	0.9643	0.4330
H	0.9286	0.3310
I	0.8571	0.3310
J	1.0000	0.4650
K	0.9643	0.4130
L	0.8571	0.2420
M	0.3929	0.1630
N	0.4286	0.0570
O	0.9286	0.3700
P	0.9286	0.3030
Q	0.9643	0.3670
R	0.8571	0.3030
S	0.8929	0.3210
T	0.3214	-0.0170
U	0.5357	0.1110
V	1.0000	0.4560
W	0.8214	0.3020
X	0.9286	0.3490
Y	0.8929	0.3180
Z	0.8929	0.2670
a	0.1071	-0.0600
b	0.0714	0.0160