Full wwPDB EM Validation Report ⓘ

Jan 30, 2024 – 02:24 PM JST

PDB ID	:	8I9D
EMDB ID	:	EMD-35267
Title	:	S-ECD (Omicron XBB.1) in complex with PD of ACE2
Authors	:	Li, Y.N.; Shen, Y.P.; Zhang, Y.Y.; Yan, R.H.
Deposited on	:	2023-02-06
Resolution	:	3.95 Å(reported)

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

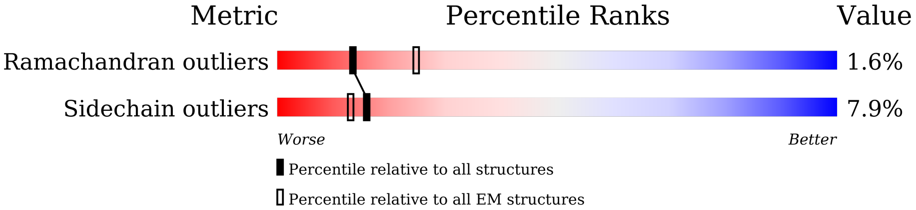
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

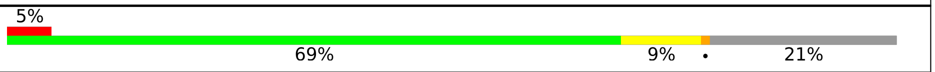
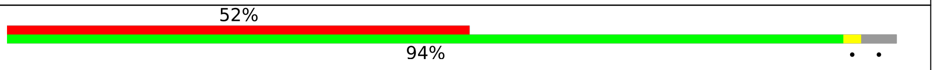
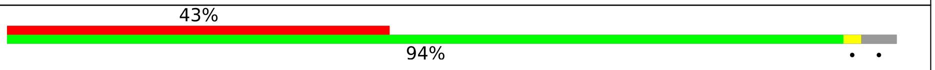
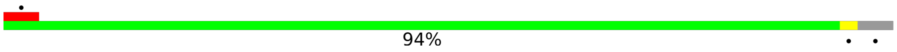
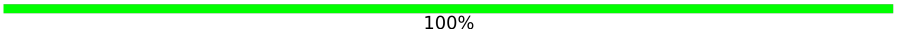
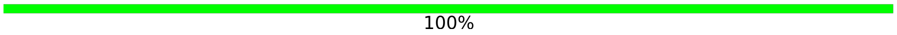
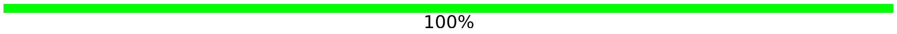
The reported resolution of this entry is 3.95 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1266	
1	B	1266	
1	C	1266	
2	D	624	
2	E	624	
2	F	624	
3	G	2	
3	H	2	
3	I	2	

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Mol	Chain	Length	Quality of chain
3	J	2	🟩 50% 🟨 50%
3	K	2	🟨 100%
3	L	2	🟩 50% 🟨 50%
3	M	2	🟩 50% 🟨 50%
3	N	2	🟩 100%
3	O	2	🟥 50% 🟩 100%
3	P	2	🟩 100%
3	Q	2	🟩 50% 🟨 50%
3	R	2	🟩 50% 🟨 50%
3	S	2	🟩 50% 🟨 50%
3	T	2	🟨 100%
3	U	2	🟩 100%
3	V	2	🟩 100%
3	W	2	🟥 50% 🟩 100%
3	X	2	🟥 50% 🟩 50% 🟨 50%
3	Y	2	🟩 50% 🟨 50%
3	Z	2	🟩 100%
3	a	2	🟩 50% 🟨 50%
3	b	2	🟨 100%
3	c	2	🟩 50% 🟨 50%
3	d	2	🟩 100%
3	e	2	🟥 50% 🟩 100%
3	f	2	🟨 100%
3	g	2	🟥 100% 🟩 100%
3	h	2	🟩 100%

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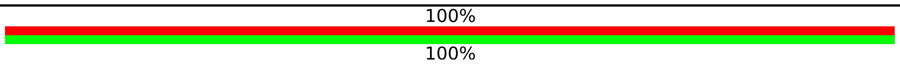
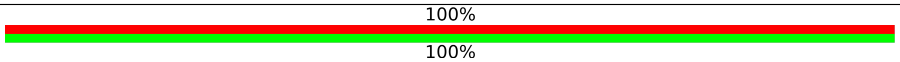
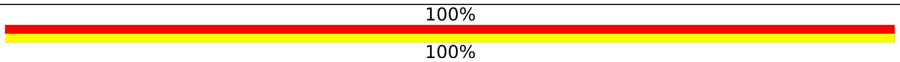
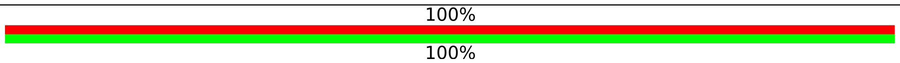
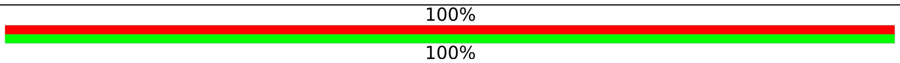
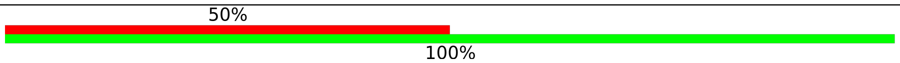
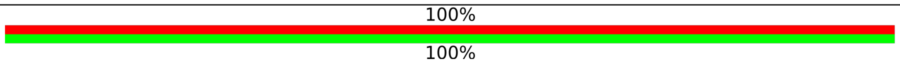
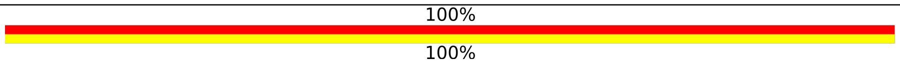
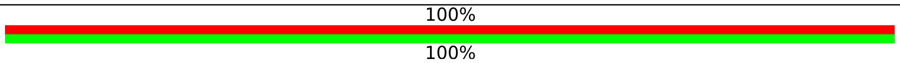
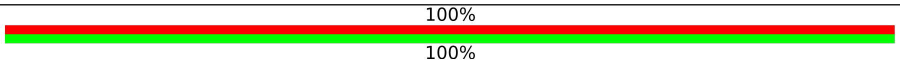
Mol	Chain	Length	Quality of chain
3	i	2	 100% 100%
3	j	2	 100% 100%
3	k	2	 100% 100%
3	l	2	 100% 100%
3	m	2	 100% 100%
3	n	2	 50% 100%
3	o	2	 100% 100%
3	p	2	 100% 100%
3	q	2	 100% 100%
3	r	2	 100% 100%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 39517 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
			Total	C	N	O	S		
1	A	999	7821	5004	1299	1482	36	0	0
1	B	998	7815	5001	1298	1480	36	0	0
1	C	998	7815	5001	1298	1480	36	0	0

There are 339 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	83	ALA	VAL	variant	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	SER	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1266	ASP	-	expression tag	UNP P0DTC2
A	1267	ASP	-	expression tag	UNP P0DTC2
A	1268	ASP	-	expression tag	UNP P0DTC2
A	1269	ASP	-	expression tag	UNP P0DTC2
A	1270	LYS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	83	ALA	VAL	variant	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	SER	PHE	variant	UNP P0DTC2
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	SER	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	597	Total 4870	C 3115	N 806	O 920	S 29	0	0
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 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	initiating methionine	UNP Q9BYF1
F	1	GLY	-	expression tag	UNP Q9BYF1
F	2	VAL	-	expression tag	UNP Q9BYF1
F	3	LYS	-	expression tag	UNP Q9BYF1
F	4	VAL	-	expression tag	UNP Q9BYF1
F	5	LEU	-	expression tag	UNP Q9BYF1
F	6	PHE	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	7	ALA	-	expression tag	UNP Q9BYF1
F	8	LEU	-	expression tag	UNP Q9BYF1
F	9	ILE	-	expression tag	UNP Q9BYF1
F	10	CYS	-	expression tag	UNP Q9BYF1
F	11	ILE	-	expression tag	UNP Q9BYF1
F	12	ALA	-	expression tag	UNP Q9BYF1
F	13	VAL	-	expression tag	UNP Q9BYF1
F	14	ALA	-	expression tag	UNP Q9BYF1
F	15	GLU	-	expression tag	UNP Q9BYF1
F	16	ALA	-	expression tag	UNP Q9BYF1
F	17	GLY	-	expression tag	UNP Q9BYF1
F	18	THR	-	expression tag	UNP Q9BYF1
F	616	ASP	-	expression tag	UNP Q9BYF1
F	617	TYR	-	expression tag	UNP Q9BYF1
F	618	LYS	-	expression tag	UNP Q9BYF1
F	619	ASP	-	expression tag	UNP Q9BYF1
F	620	ASP	-	expression tag	UNP Q9BYF1
F	621	ASP	-	expression tag	UNP Q9BYF1
F	622	ASP	-	expression tag	UNP Q9BYF1
F	623	LYS	-	expression tag	UNP Q9BYF1
D	0	MET	-	initiating methionine	UNP Q9BYF1
D	1	GLY	-	expression tag	UNP Q9BYF1
D	2	VAL	-	expression tag	UNP Q9BYF1
D	3	LYS	-	expression tag	UNP Q9BYF1
D	4	VAL	-	expression tag	UNP Q9BYF1
D	5	LEU	-	expression tag	UNP Q9BYF1
D	6	PHE	-	expression tag	UNP Q9BYF1
D	7	ALA	-	expression tag	UNP Q9BYF1
D	8	LEU	-	expression tag	UNP Q9BYF1
D	9	ILE	-	expression tag	UNP Q9BYF1
D	10	CYS	-	expression tag	UNP Q9BYF1
D	11	ILE	-	expression tag	UNP Q9BYF1
D	12	ALA	-	expression tag	UNP Q9BYF1
D	13	VAL	-	expression tag	UNP Q9BYF1
D	14	ALA	-	expression tag	UNP Q9BYF1
D	15	GLU	-	expression tag	UNP Q9BYF1
D	16	ALA	-	expression tag	UNP Q9BYF1
D	17	GLY	-	expression tag	UNP Q9BYF1
D	18	THR	-	expression tag	UNP Q9BYF1
D	616	ASP	-	expression tag	UNP Q9BYF1
D	617	TYR	-	expression tag	UNP Q9BYF1
D	618	LYS	-	expression tag	UNP Q9BYF1

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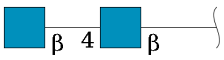
Chain	Residue	Modelled	Actual	Comment	Reference
D	619	ASP	-	expression tag	UNP Q9BYF1
D	620	ASP	-	expression tag	UNP Q9BYF1
D	621	ASP	-	expression tag	UNP Q9BYF1
D	622	ASP	-	expression tag	UNP Q9BYF1
D	623	LYS	-	expression tag	UNP Q9BYF1
E	0	MET	-	initiating methionine	UNP Q9BYF1
E	1	GLY	-	expression tag	UNP Q9BYF1
E	2	VAL	-	expression tag	UNP Q9BYF1
E	3	LYS	-	expression tag	UNP Q9BYF1
E	4	VAL	-	expression tag	UNP Q9BYF1
E	5	LEU	-	expression tag	UNP Q9BYF1
E	6	PHE	-	expression tag	UNP Q9BYF1
E	7	ALA	-	expression tag	UNP Q9BYF1
E	8	LEU	-	expression tag	UNP Q9BYF1
E	9	ILE	-	expression tag	UNP Q9BYF1
E	10	CYS	-	expression tag	UNP Q9BYF1
E	11	ILE	-	expression tag	UNP Q9BYF1
E	12	ALA	-	expression tag	UNP Q9BYF1
E	13	VAL	-	expression tag	UNP Q9BYF1
E	14	ALA	-	expression tag	UNP Q9BYF1
E	15	GLU	-	expression tag	UNP Q9BYF1
E	16	ALA	-	expression tag	UNP Q9BYF1
E	17	GLY	-	expression tag	UNP Q9BYF1
E	18	THR	-	expression tag	UNP Q9BYF1
E	616	ASP	-	expression tag	UNP Q9BYF1
E	617	TYR	-	expression tag	UNP Q9BYF1
E	618	LYS	-	expression tag	UNP Q9BYF1
E	619	ASP	-	expression tag	UNP Q9BYF1
E	620	ASP	-	expression tag	UNP Q9BYF1
E	621	ASP	-	expression tag	UNP Q9BYF1
E	622	ASP	-	expression tag	UNP Q9BYF1
E	623	LYS	-	expression tag	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	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
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

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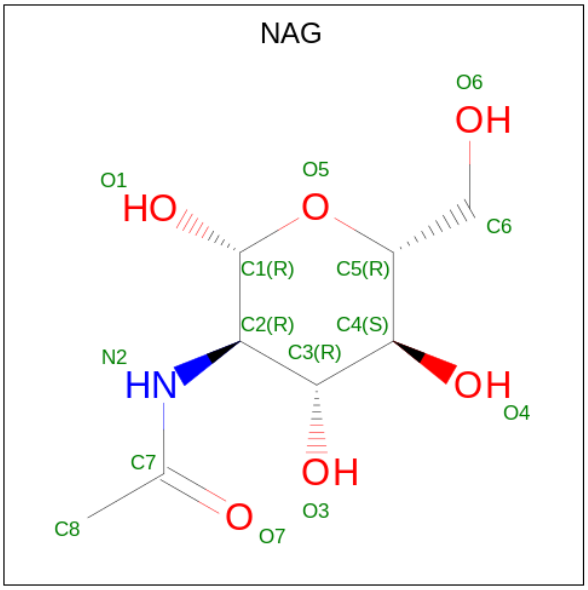
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	c	2	28	16	2	10	0	0
3	d	2	28	16	2	10	0	0
3	e	2	28	16	2	10	0	0
3	f	2	28	16	2	10	0	0
3	g	2	28	16	2	10	0	0
3	h	2	28	16	2	10	0	0
3	i	2	28	16	2	10	0	0
3	j	2	28	16	2	10	0	0
3	k	2	28	16	2	10	0	0
3	l	2	28	16	2	10	0	0
3	m	2	28	16	2	10	0	0
3	n	2	28	16	2	10	0	0
3	o	2	28	16	2	10	0	0
3	p	2	28	16	2	10	0	0
3	q	2	28	16	2	10	0	0
3	r	2	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 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0

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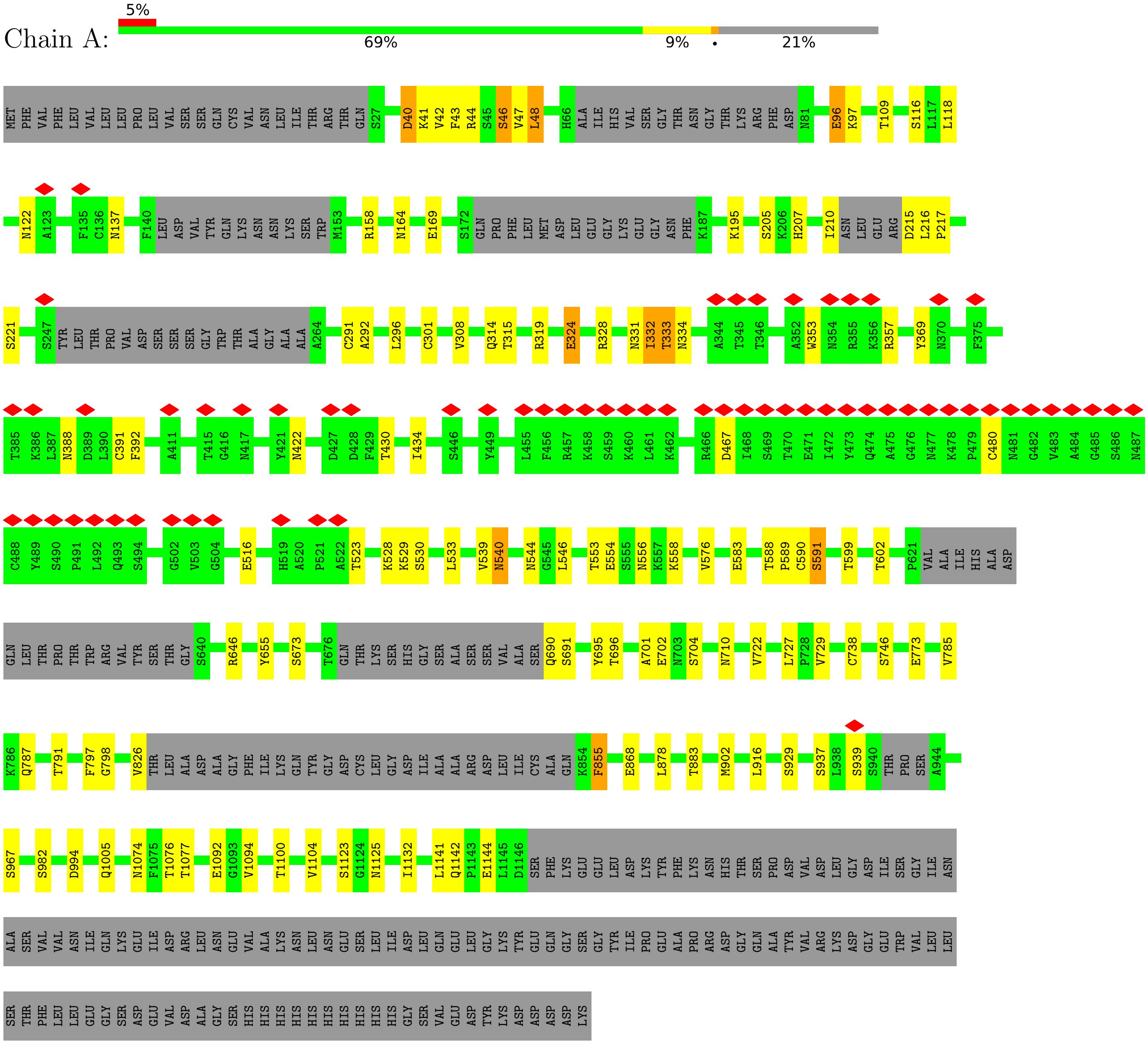
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total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

3 Residue-property plots ⓘ

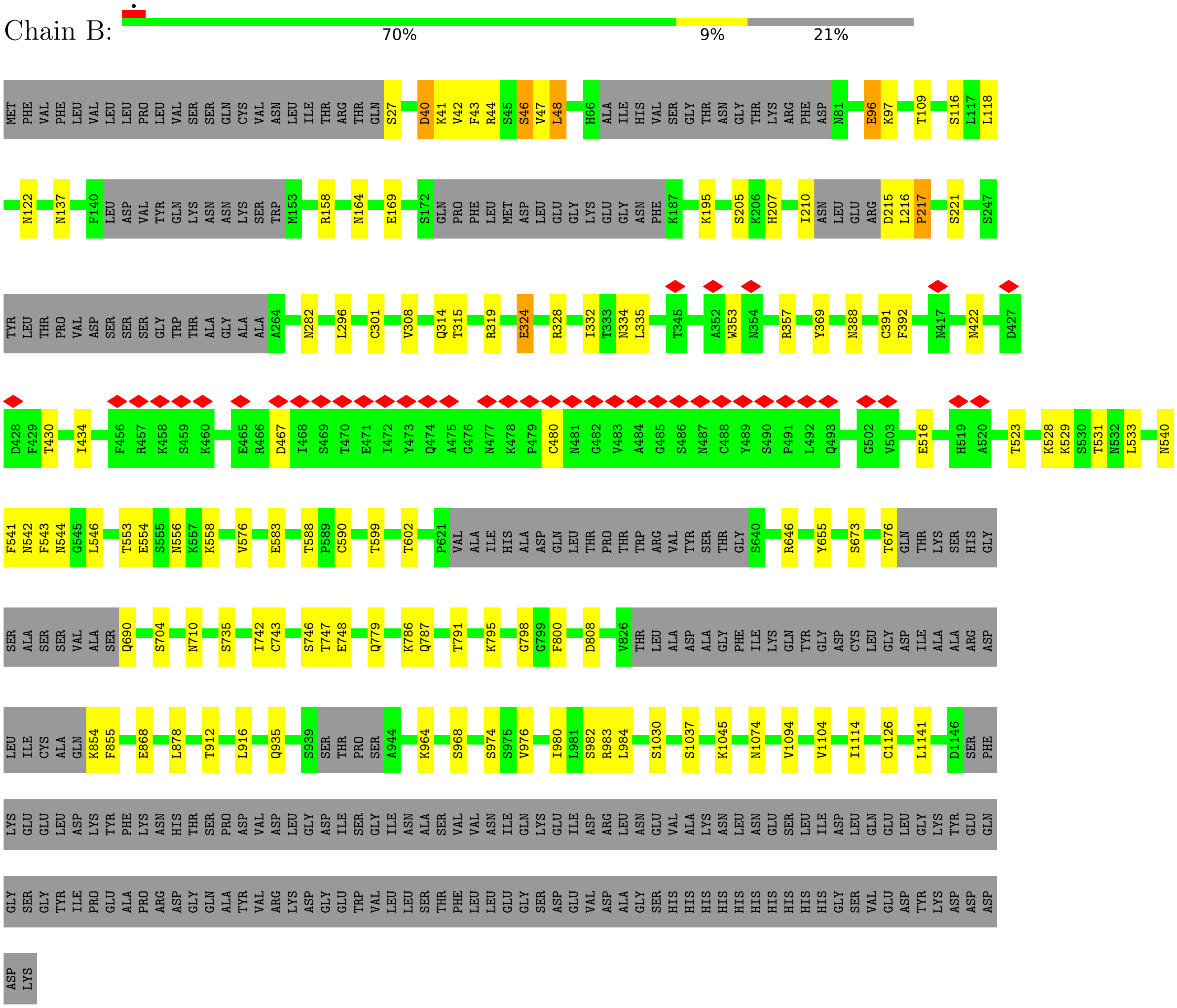
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



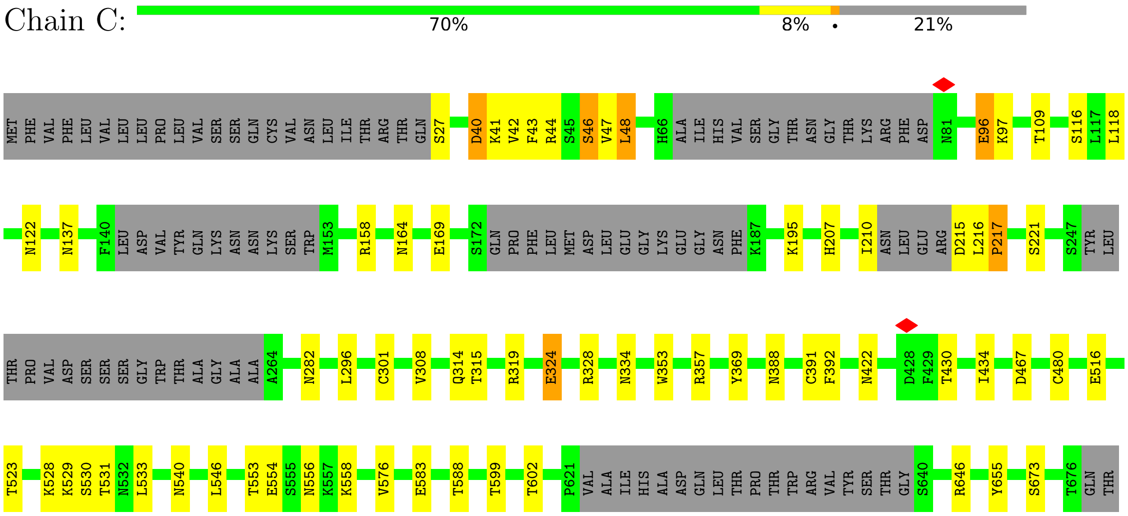
- Molecule 1: Spike glycoprotein

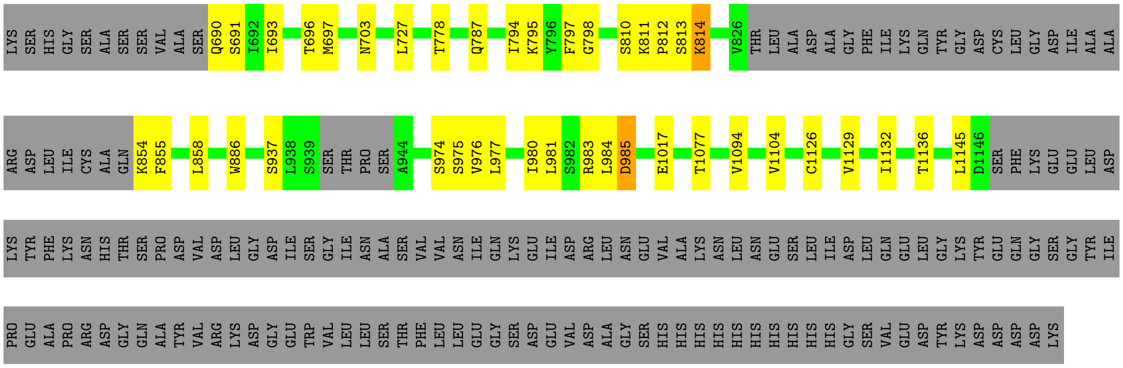
Chain B:



- Molecule 1: Spike glycoprotein

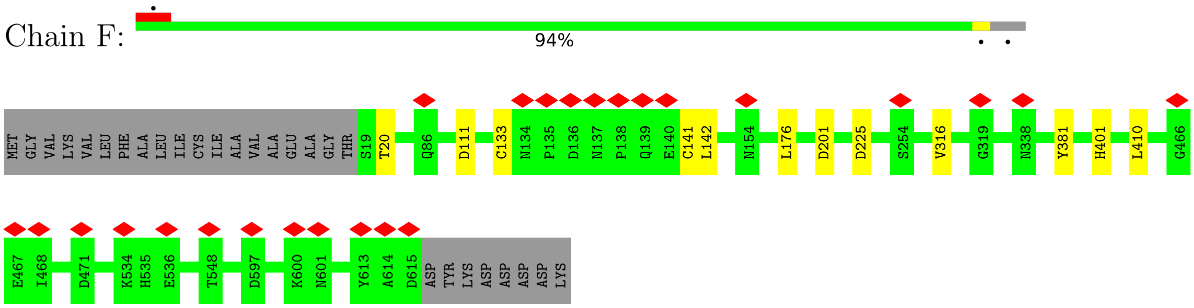
Chain C:





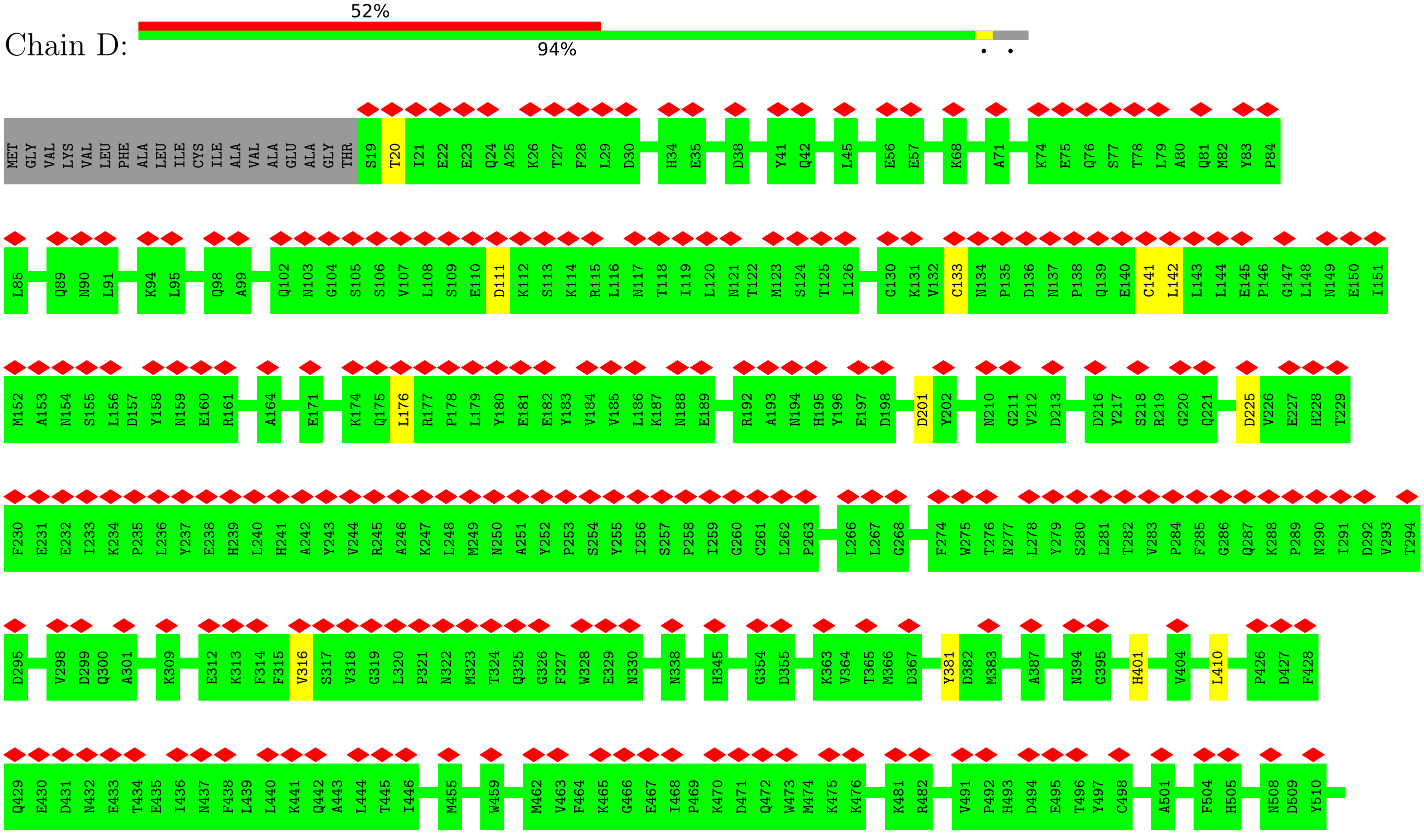
- Molecule 2: Processed angiotensin-converting enzyme 2

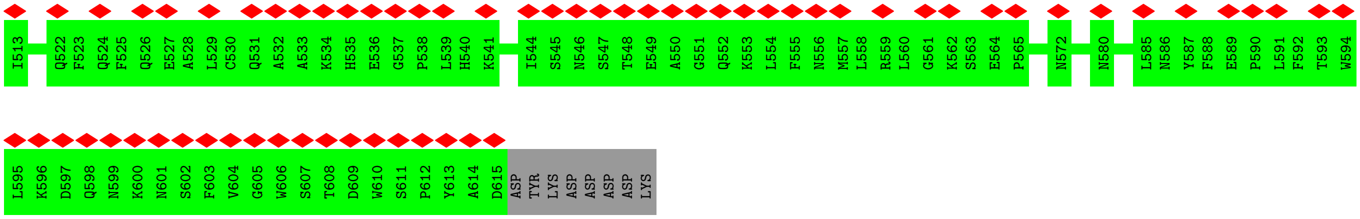
Chain F:



- Molecule 2: Processed angiotensin-converting enzyme 2

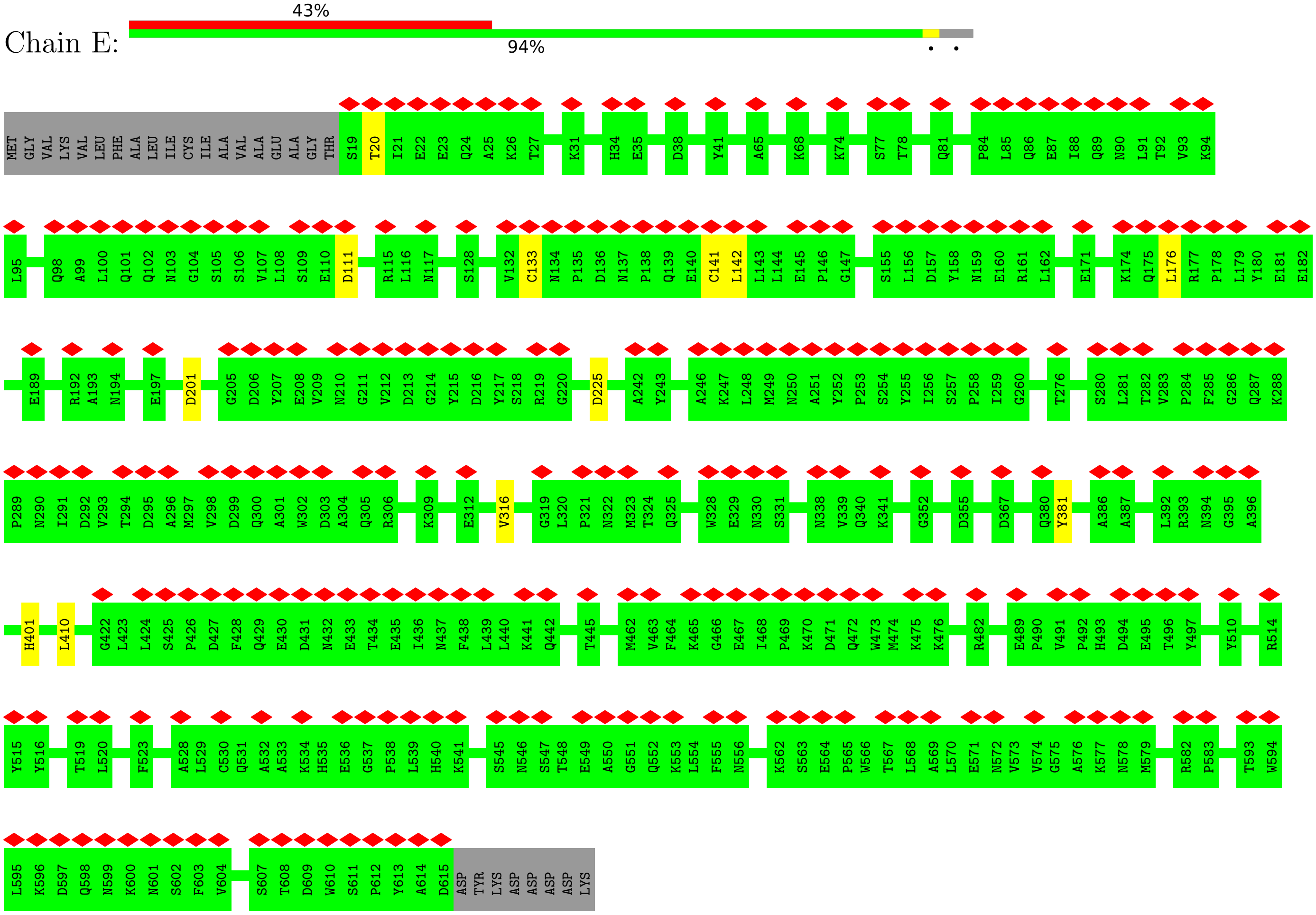
Chain D:





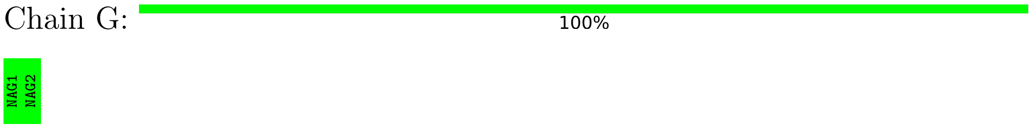
- Molecule 2: Processed angiotensin-converting enzyme 2

Chain E:



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

Chain G:

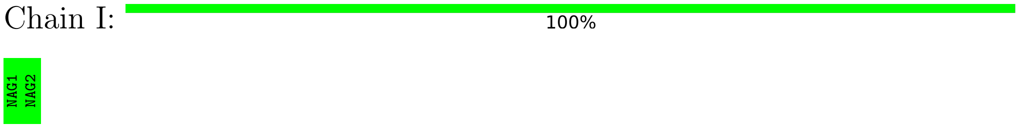


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain I:

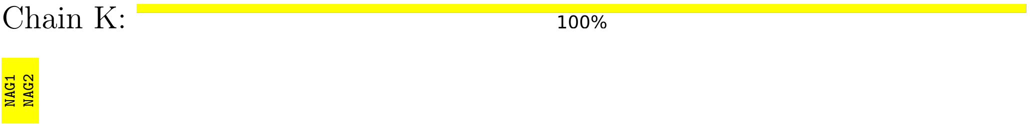


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

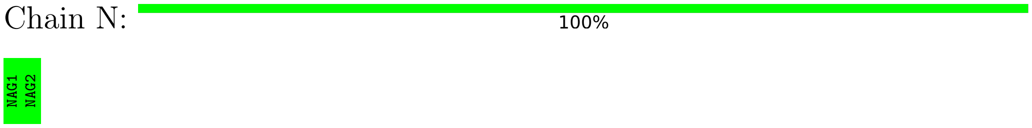
Chain L:

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

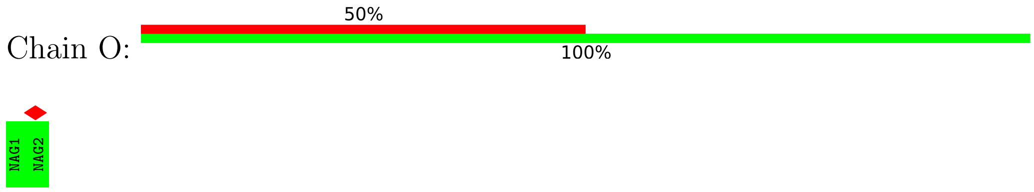
Chain M:

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

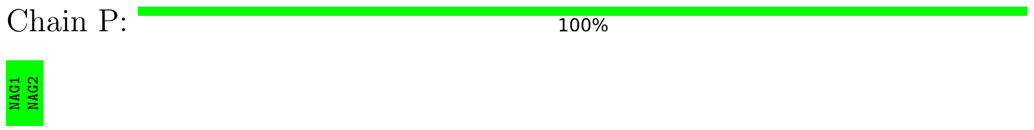
Chain N:



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



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

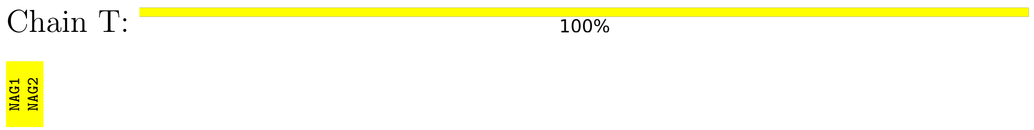


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

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

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



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

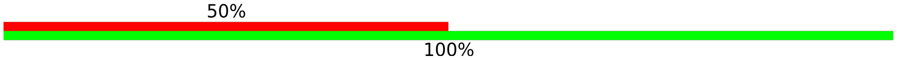
Chain U:

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

Chain V:

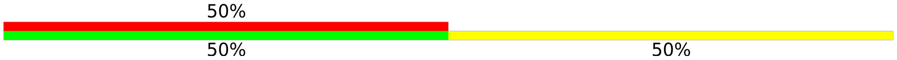
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



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

Chain X:

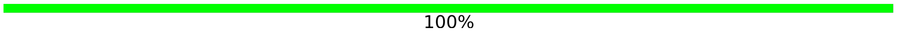


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

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

Chain Z:

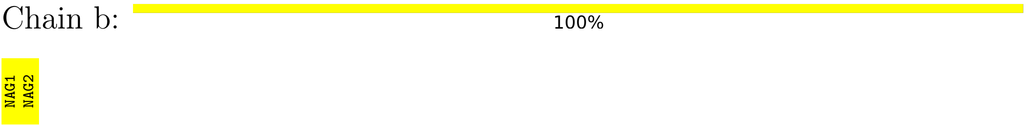


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

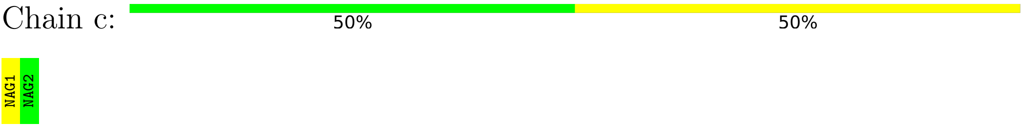
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



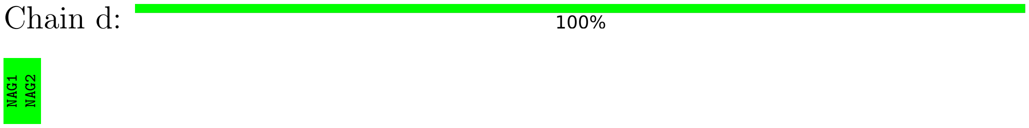
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



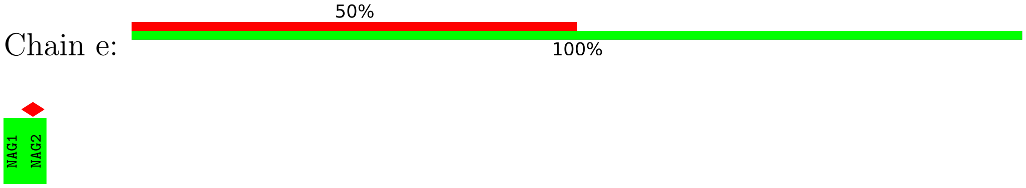
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



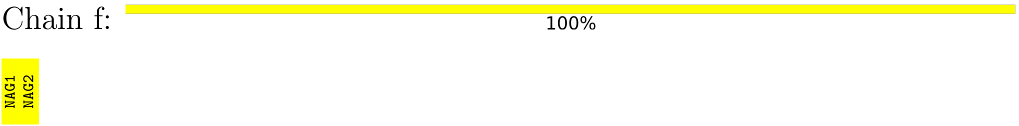
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



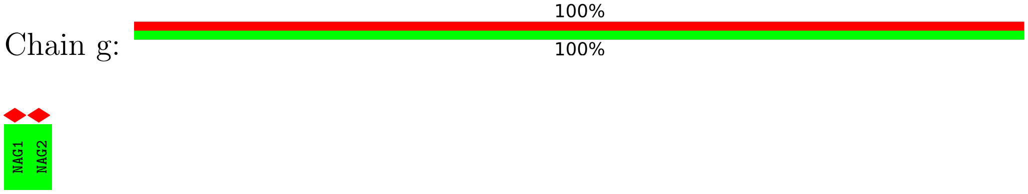
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:

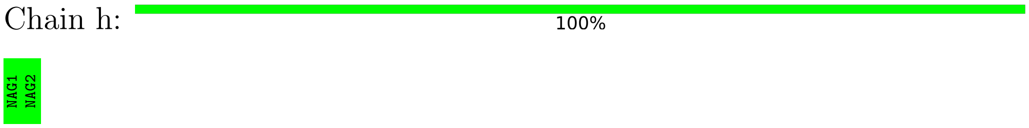


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

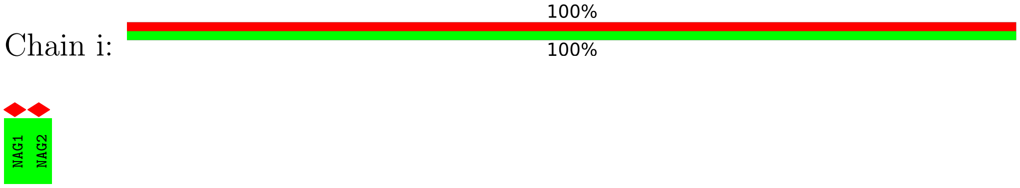
Chain g:



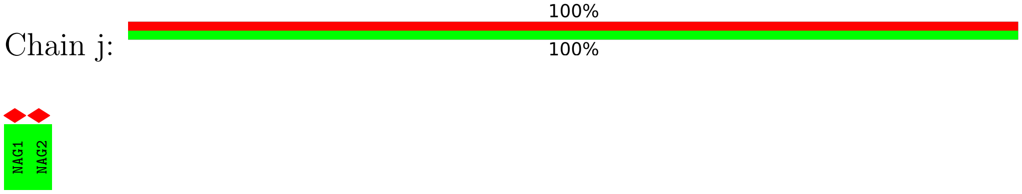
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



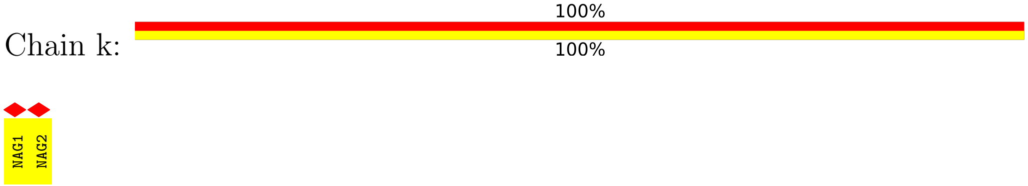
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



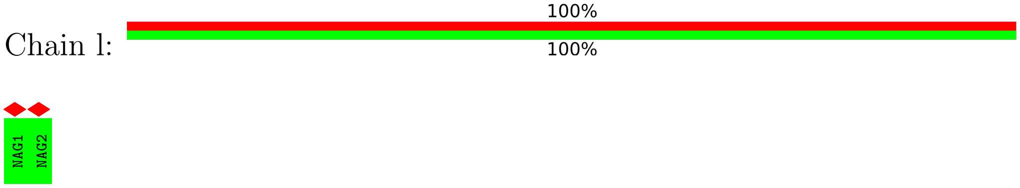
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



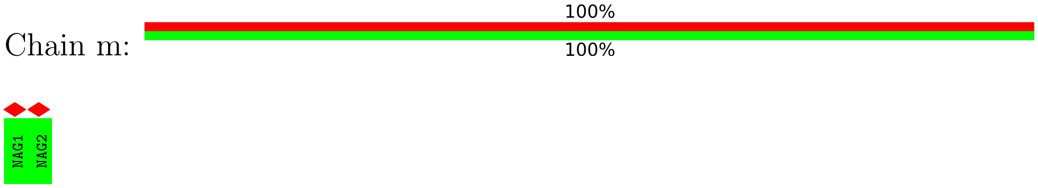
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

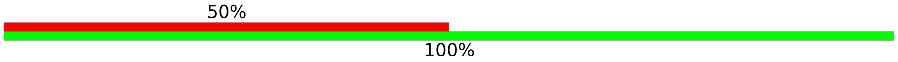


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain n:

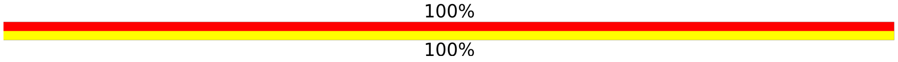


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	804338	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	1.337	Depositor
Minimum map value	-0.623	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.12	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	0.48	0/8004	0.54	0/10887
1	B	0.48	0/7998	0.53	0/10879
1	C	0.48	0/7998	0.53	0/10879
2	D	0.27	0/5007	0.42	0/6803
2	E	0.27	0/5007	0.42	0/6803
2	F	0.27	0/5007	0.42	0/6803
All	All	0.41	0/39021	0.49	0/53054

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 ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	979/1266 (77%)	864 (88%)	85 (9%)	30 (3%)	4	31
1	B	978/1266 (77%)	867 (89%)	91 (9%)	20 (2%)	7	39
1	C	978/1266 (77%)	865 (88%)	88 (9%)	25 (3%)	5	35
2	D	595/624 (95%)	563 (95%)	32 (5%)	0	100	100
2	E	595/624 (95%)	563 (95%)	32 (5%)	0	100	100
2	F	595/624 (95%)	563 (95%)	32 (5%)	0	100	100
All	All	4720/5670 (83%)	4285 (91%)	360 (8%)	75 (2%)	13	44

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	217	PRO
1	A	291	CYS
1	A	292	ALA
1	A	331	ASN
1	A	332	ILE
1	A	333	THR
1	A	539	VAL
1	A	544	ASN
1	A	591	SER
1	A	691	SER
1	A	701	ALA
1	A	797	PHE
1	A	855	PHE
1	B	48	LEU
1	B	217	PRO
1	B	544	ASN
1	B	800	PHE
1	C	48	LEU
1	C	217	PRO
1	C	814	LYS
1	C	855	PHE
1	C	984	LEU
1	A	41	LYS
1	A	46	SER
1	A	96	GLU
1	A	334	ASN
1	B	41	LYS
1	B	46	SER
1	B	96	GLU

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Mol	Chain	Res	Type
1	B	590	CYS
1	B	742	ILE
1	B	743	CYS
1	B	798	GLY
1	B	982	SER
1	C	41	LYS
1	C	46	SER
1	C	96	GLU
1	C	697	MET
1	C	798	GLY
1	C	810	SER
1	A	43	PHE
1	A	589	PRO
1	A	695	TYR
1	A	710	ASN
1	B	43	PHE
1	C	43	PHE
1	A	44	ARG
1	A	324	GLU
1	B	44	ARG
1	B	324	GLU
1	B	543	PHE
1	B	746	SER
1	C	44	ARG
1	C	324	GLU
1	C	813	SER
1	C	858	LEU
1	A	40	ASP
1	A	42	VAL
1	A	47	VAL
1	A	798	GLY
1	B	40	ASP
1	B	42	VAL
1	B	47	VAL
1	C	40	ASP
1	C	42	VAL
1	C	47	VAL
1	C	691	SER
1	C	812	PRO
1	C	985	ASP
1	A	530	SER
1	A	540	ASN

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Mol	Chain	Res	Type
1	C	811	LYS
1	C	981	LEU
1	C	980	ILE

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	877/1105 (79%)	775 (88%)	102 (12%)	5	25
1	B	876/1105 (79%)	773 (88%)	103 (12%)	5	24
1	C	876/1105 (79%)	784 (90%)	92 (10%)	7	28
2	D	527/548 (96%)	515 (98%)	12 (2%)	50	70
2	E	527/548 (96%)	515 (98%)	12 (2%)	50	70
2	F	527/548 (96%)	515 (98%)	12 (2%)	50	70
All	All	4210/4959 (85%)	3877 (92%)	333 (8%)	16	40

All (333) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	46	SER
1	A	48	LEU
1	A	96	GLU
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	137	ASN
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU
1	A	195	LYS
1	A	205	SER

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Mol	Chain	Res	Type
1	A	207	HIS
1	A	210	ILE
1	A	215	ASP
1	A	216	LEU
1	A	221	SER
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	319	ARG
1	A	324	GLU
1	A	328	ARG
1	A	332	ILE
1	A	333	THR
1	A	353	TRP
1	A	357	ARG
1	A	369	TYR
1	A	388	ASN
1	A	391	CYS
1	A	392	PHE
1	A	422	ASN
1	A	430	THR
1	A	434	ILE
1	A	467	ASP
1	A	480	CYS
1	A	516	GLU
1	A	523	THR
1	A	528	LYS
1	A	529	LYS
1	A	533	LEU
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	558	LYS
1	A	576	VAL
1	A	583	GLU
1	A	588	THR
1	A	590	CYS
1	A	591	SER

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Mol	Chain	Res	Type
1	A	599	THR
1	A	602	THR
1	A	646	ARG
1	A	655	TYR
1	A	673	SER
1	A	690	GLN
1	A	696	THR
1	A	702	GLU
1	A	704	SER
1	A	722	VAL
1	A	727	LEU
1	A	729	VAL
1	A	738	CYS
1	A	746	SER
1	A	773	GLU
1	A	785	VAL
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	855	PHE
1	A	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU
1	A	929	SER
1	A	937	SER
1	A	939	SER
1	A	967	SER
1	A	982	SER
1	A	994	ASP
1	A	1005	GLN
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1123	SER
1	A	1125	ASN
1	A	1132	ILE

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Mol	Chain	Res	Type
1	A	1141	LEU
1	A	1142	GLN
1	A	1144	GLU
1	B	27	SER
1	B	40	ASP
1	B	46	SER
1	B	48	LEU
1	B	96	GLU
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	137	ASN
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	195	LYS
1	B	205	SER
1	B	207	HIS
1	B	210	ILE
1	B	215	ASP
1	B	216	LEU
1	B	217	PRO
1	B	221	SER
1	B	282	ASN
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL
1	B	314	GLN
1	B	315	THR
1	B	319	ARG
1	B	324	GLU
1	B	328	ARG
1	B	332	ILE
1	B	334	ASN
1	B	335	LEU
1	B	353	TRP
1	B	357	ARG
1	B	369	TYR
1	B	388	ASN
1	B	391	CYS

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Mol	Chain	Res	Type
1	B	392	PHE
1	B	422	ASN
1	B	430	THR
1	B	434	ILE
1	B	467	ASP
1	B	480	CYS
1	B	516	GLU
1	B	523	THR
1	B	528	LYS
1	B	529	LYS
1	B	531	THR
1	B	533	LEU
1	B	540	ASN
1	B	541	PHE
1	B	542	ASN
1	B	546	LEU
1	B	553	THR
1	B	554	GLU
1	B	556	ASN
1	B	558	LYS
1	B	576	VAL
1	B	583	GLU
1	B	588	THR
1	B	599	THR
1	B	602	THR
1	B	646	ARG
1	B	655	TYR
1	B	673	SER
1	B	676	THR
1	B	690	GLN
1	B	704	SER
1	B	710	ASN
1	B	735	SER
1	B	747	THR
1	B	748	GLU
1	B	779	GLN
1	B	786	LYS
1	B	787	GLN
1	B	791	THR
1	B	795	LYS
1	B	808	ASP
1	B	854	LYS

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Mol	Chain	Res	Type
1	B	855	PHE
1	B	868	GLU
1	B	878	LEU
1	B	912	THR
1	B	916	LEU
1	B	935	GLN
1	B	964	LYS
1	B	968	SER
1	B	974	SER
1	B	976	VAL
1	B	980	ILE
1	B	983	ARG
1	B	984	LEU
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1141	LEU
1	C	27	SER
1	C	40	ASP
1	C	46	SER
1	C	48	LEU
1	C	96	GLU
1	C	97	LYS
1	C	109	THR
1	C	116	SER
1	C	118	LEU
1	C	122	ASN
1	C	137	ASN
1	C	158	ARG
1	C	164	ASN
1	C	169	GLU
1	C	195	LYS
1	C	207	HIS
1	C	210	ILE
1	C	215	ASP
1	C	216	LEU
1	C	217	PRO

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Mol	Chain	Res	Type
1	C	221	SER
1	C	282	ASN
1	C	296	LEU
1	C	301	CYS
1	C	308	VAL
1	C	314	GLN
1	C	315	THR
1	C	319	ARG
1	C	324	GLU
1	C	328	ARG
1	C	334	ASN
1	C	353	TRP
1	C	357	ARG
1	C	369	TYR
1	C	388	ASN
1	C	391	CYS
1	C	392	PHE
1	C	422	ASN
1	C	430	THR
1	C	434	ILE
1	C	467	ASP
1	C	480	CYS
1	C	516	GLU
1	C	523	THR
1	C	528	LYS
1	C	529	LYS
1	C	530	SER
1	C	531	THR
1	C	533	LEU
1	C	540	ASN
1	C	546	LEU
1	C	553	THR
1	C	554	GLU
1	C	556	ASN
1	C	558	LYS
1	C	576	VAL
1	C	583	GLU
1	C	588	THR
1	C	599	THR
1	C	602	THR
1	C	646	ARG
1	C	655	TYR

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Mol	Chain	Res	Type
1	C	673	SER
1	C	690	GLN
1	C	693	ILE
1	C	696	THR
1	C	703	ASN
1	C	727	LEU
1	C	778	THR
1	C	787	GLN
1	C	794	ILE
1	C	795	LYS
1	C	797	PHE
1	C	814	LYS
1	C	854	LYS
1	C	886	TRP
1	C	937	SER
1	C	974	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	983	ARG
1	C	985	ASP
1	C	1017	GLU
1	C	1077	THR
1	C	1094	VAL
1	C	1104	VAL
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU
2	F	20	THR
2	F	111	ASP
2	F	133	CYS
2	F	141	CYS
2	F	142	LEU
2	F	176	LEU
2	F	201	ASP
2	F	225	ASP
2	F	316	VAL
2	F	381	TYR
2	F	401	HIS
2	F	410	LEU

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Mol	Chain	Res	Type
2	D	20	THR
2	D	111	ASP
2	D	133	CYS
2	D	141	CYS
2	D	142	LEU
2	D	176	LEU
2	D	201	ASP
2	D	225	ASP
2	D	316	VAL
2	D	381	TYR
2	D	401	HIS
2	D	410	LEU
2	E	20	THR
2	E	111	ASP
2	E	133	CYS
2	E	141	CYS
2	E	142	LEU
2	E	176	LEU
2	E	201	ASP
2	E	225	ASP
2	E	316	VAL
2	E	381	TYR
2	E	401	HIS
2	E	410	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	239	GLN
1	A	317	ASN
1	A	334	ASN
1	A	339	HIS
1	A	542	ASN
1	A	556	ASN
1	A	644	GLN
1	A	658	ASN
1	A	703	ASN
1	A	762	GLN
1	A	787	GLN

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Mol	Chain	Res	Type
1	A	901	GLN
1	A	914	ASN
1	A	919	ASN
1	A	926	GLN
1	A	954	HIS
1	A	955	ASN
1	A	992	GLN
1	A	1125	ASN
1	A	1142	GLN
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	239	GLN
1	B	317	ASN
1	B	334	ASN
1	B	339	HIS
1	B	540	ASN
1	B	542	ASN
1	B	556	ASN
1	B	580	GLN
1	B	644	GLN
1	B	658	ASN
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	920	GLN
1	B	926	GLN
1	B	992	GLN
1	B	1054	GLN
1	C	134	GLN
1	C	137	ASN
1	C	188	ASN
1	C	239	GLN
1	C	317	ASN
1	C	339	HIS
1	C	540	ASN
1	C	542	ASN
1	C	556	ASN
1	C	644	GLN
1	C	658	ASN

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Mol	Chain	Res	Type
1	C	703	ASN
1	C	784	GLN
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	926	GLN
1	C	935	GLN
1	C	954	HIS
1	C	992	GLN
1	C	1010	GLN
1	C	1071	GLN
1	C	1101	HIS
1	C	1106	GLN
2	F	42	GLN
2	F	96	GLN
2	F	102	GLN
2	F	239	HIS
2	F	305	GLN
2	F	340	GLN
2	F	374	HIS
2	F	472	GLN
2	F	505	HIS
2	F	599	ASN
2	D	42	GLN
2	D	96	GLN
2	D	102	GLN
2	D	239	HIS
2	D	305	GLN
2	D	340	GLN
2	D	374	HIS
2	D	472	GLN
2	D	505	HIS
2	D	526	GLN
2	D	599	ASN
2	E	42	GLN
2	E	96	GLN
2	E	102	GLN
2	E	239	HIS
2	E	305	GLN
2	E	340	GLN
2	E	374	HIS

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Mol	Chain	Res	Type
2	E	472	GLN
2	E	505	HIS
2	E	599	ASN

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 ⓘ

76 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	1	1,3	14,14,15	0.53	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	H	1	1,3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	H	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	I	1	1,3	14,14,15	0.33	0	17,19,21	0.61	0
3	NAG	I	2	3	14,14,15	0.55	0	17,19,21	0.47	0
3	NAG	J	1	1,3	14,14,15	0.37	0	17,19,21	0.72	0
3	NAG	J	2	3	14,14,15	0.28	0	17,19,21	1.31	2 (11%)
3	NAG	K	1	1,3	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
3	NAG	K	2	3	14,14,15	0.41	0	17,19,21	1.40	3 (17%)
3	NAG	L	1	1,3	14,14,15	0.72	1 (7%)	17,19,21	0.66	0
3	NAG	L	2	3	14,14,15	0.31	0	17,19,21	0.65	0
3	NAG	M	1	1,3	14,14,15	0.24	0	17,19,21	0.68	1 (5%)
3	NAG	M	2	3	14,14,15	0.19	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	N	1	1,3	14,14,15	0.52	0	17,19,21	0.51	0
3	NAG	N	2	3	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	O	1	1,3	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	O	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	P	1	1,3	14,14,15	0.31	0	17,19,21	0.40	0
3	NAG	P	2	3	14,14,15	0.35	0	17,19,21	0.36	0
3	NAG	Q	1	1,3	14,14,15	0.33	0	17,19,21	1.14	1 (5%)
3	NAG	Q	2	3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	R	1	1,3	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
3	NAG	R	2	3	14,14,15	0.23	0	17,19,21	0.39	0
3	NAG	S	1	1,3	14,14,15	0.41	0	17,19,21	1.14	2 (11%)
3	NAG	S	2	3	14,14,15	0.35	0	17,19,21	0.41	0
3	NAG	T	1	1,3	14,14,15	0.75	1 (7%)	17,19,21	0.92	1 (5%)
3	NAG	T	2	3	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
3	NAG	U	1	1,3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	U	2	3	14,14,15	0.29	0	17,19,21	0.37	0
3	NAG	V	1	1,3	14,14,15	0.56	0	17,19,21	0.51	0
3	NAG	V	2	3	14,14,15	0.26	0	17,19,21	0.56	0
3	NAG	W	1	1,3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	W	2	3	14,14,15	0.26	0	17,19,21	0.43	0
3	NAG	X	1	1,3	14,14,15	0.24	0	17,19,21	1.37	1 (5%)
3	NAG	X	2	3	14,14,15	0.19	0	17,19,21	0.49	0
3	NAG	Y	1	1,3	14,14,15	0.55	0	17,19,21	0.71	1 (5%)
3	NAG	Y	2	3	14,14,15	0.38	0	17,19,21	0.47	0
3	NAG	Z	1	1,3	14,14,15	0.40	0	17,19,21	0.41	0
3	NAG	Z	2	3	14,14,15	0.20	0	17,19,21	0.74	0
3	NAG	a	1	1,3	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	a	2	3	14,14,15	0.57	0	17,19,21	1.30	1 (5%)
3	NAG	b	1	1,3	14,14,15	0.62	1 (7%)	17,19,21	0.42	0
3	NAG	b	2	3	14,14,15	0.34	0	17,19,21	1.35	2 (11%)
3	NAG	c	1	1,3	14,14,15	0.40	0	17,19,21	1.16	1 (5%)
3	NAG	c	2	3	14,14,15	0.35	0	17,19,21	0.78	0
3	NAG	d	1	2,3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	d	2	3	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	e	1	2,3	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	e	2	3	14,14,15	0.20	0	17,19,21	0.47	0
3	NAG	f	1	2,3	14,14,15	0.64	0	17,19,21	1.03	1 (5%)
3	NAG	f	2	3	14,14,15	0.48	0	17,19,21	1.31	2 (11%)
3	NAG	g	1	2,3	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	g	2	3	14,14,15	0.23	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	h	1	2,3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	h	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	i	1	2,3	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	i	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	j	1	2,3	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	j	2	3	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	k	1	2,3	14,14,15	0.64	0	17,19,21	1.03	1 (5%)
3	NAG	k	2	3	14,14,15	0.47	0	17,19,21	1.31	2 (11%)
3	NAG	l	1	2,3	14,14,15	0.20	0	17,19,21	0.47	0
3	NAG	l	2	3	14,14,15	0.23	0	17,19,21	0.55	0
3	NAG	m	1	2,3	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	m	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	n	1	2,3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	n	2	3	14,14,15	0.24	0	17,19,21	0.38	0
3	NAG	o	1	2,3	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	o	2	3	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	p	1	2,3	14,14,15	0.65	0	17,19,21	1.02	1 (5%)
3	NAG	p	2	3	14,14,15	0.47	0	17,19,21	1.31	2 (11%)
3	NAG	q	1	2,3	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	q	2	3	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	r	1	2,3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	r	2	3	14,14,15	0.22	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	5/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	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	1,3	-	6/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	1/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	5/6/23/26	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	4/6/23/26	0/1/1/1
3	NAG	c	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	1/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	e	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	f	2	3	-	3/6/23/26	0/1/1/1
3	NAG	g	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	NAG	j	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1
3	NAG	k	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	k	2	3	-	3/6/23/26	0/1/1/1
3	NAG	l	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	NAG	m	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	2/6/23/26	0/1/1/1
3	NAG	n	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	2/6/23/26	0/1/1/1
3	NAG	o	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	o	2	3	-	2/6/23/26	0/1/1/1
3	NAG	p	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	p	2	3	-	3/6/23/26	0/1/1/1
3	NAG	q	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	r	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	NAG	O5-C1	-2.73	1.39	1.43
3	L	1	NAG	O5-C1	-2.59	1.39	1.43
3	K	1	NAG	O5-C1	-2.24	1.40	1.43
3	b	1	NAG	O5-C1	-2.09	1.40	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	1	NAG	C2-N2-C7	4.72	129.62	122.90
3	K	2	NAG	C2-N2-C7	4.43	129.21	122.90
3	b	2	NAG	C2-N2-C7	4.31	129.04	122.90
3	f	2	NAG	C2-N2-C7	4.29	129.02	122.90
3	p	2	NAG	C2-N2-C7	4.26	128.97	122.90
3	J	2	NAG	C2-N2-C7	4.26	128.97	122.90
3	k	2	NAG	C2-N2-C7	4.23	128.93	122.90
3	a	2	NAG	C2-N2-C7	4.23	128.92	122.90
3	Q	1	NAG	C1-O5-C5	3.34	116.72	112.19
3	f	1	NAG	C1-O5-C5	3.04	116.32	112.19
3	k	1	NAG	C1-O5-C5	2.99	116.25	112.19
3	p	1	NAG	C1-O5-C5	2.98	116.23	112.19
3	T	1	NAG	O4-C4-C3	-2.41	104.77	110.35
3	J	2	NAG	C1-C2-N2	2.36	114.52	110.49
3	K	2	NAG	C1-C2-N2	2.35	114.49	110.49
3	c	1	NAG	C8-C7-N2	2.30	120.00	116.10
3	R	1	NAG	C1-O5-C5	2.28	115.28	112.19
3	Y	1	NAG	C1-O5-C5	2.27	115.27	112.19
3	b	2	NAG	C1-C2-N2	2.25	114.33	110.49
3	S	1	NAG	C8-C7-N2	2.23	119.87	116.10
3	S	1	NAG	C2-N2-C7	-2.11	119.91	122.90
3	M	1	NAG	C1-O5-C5	2.08	115.01	112.19
3	p	2	NAG	C1-C2-N2	2.06	114.01	110.49
3	k	2	NAG	C1-C2-N2	2.05	114.00	110.49
3	K	2	NAG	C1-O5-C5	2.02	114.94	112.19
3	f	2	NAG	C1-C2-N2	2.01	113.93	110.49
3	T	2	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	d	2	NAG	C4-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	n	2	NAG	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	m	2	NAG	C4-C5-C6-O6
3	r	2	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	e	1	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	j	1	NAG	O5-C5-C6-O6
3	n	2	NAG	O5-C5-C6-O6
3	o	1	NAG	O5-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	l	2	NAG	C4-C5-C6-O6
3	q	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	m	2	NAG	O5-C5-C6-O6
3	r	2	NAG	O5-C5-C6-O6
3	e	2	NAG	O5-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	e	1	NAG	C4-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
3	o	1	NAG	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
3	q	2	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	e	2	NAG	C4-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
3	o	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
3	R	2	NAG	C8-C7-N2-C2
3	R	2	NAG	O7-C7-N2-C2
3	X	1	NAG	C8-C7-N2-C2
3	X	1	NAG	O7-C7-N2-C2
3	a	2	NAG	C8-C7-N2-C2
3	a	2	NAG	O7-C7-N2-C2
3	b	2	NAG	C8-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
3	f	2	NAG	C8-C7-N2-C2
3	f	2	NAG	O7-C7-N2-C2
3	k	2	NAG	C8-C7-N2-C2
3	k	2	NAG	O7-C7-N2-C2
3	p	2	NAG	C8-C7-N2-C2
3	p	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C4-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	r	1	NAG	C4-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
3	m	1	NAG	C4-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	m	1	NAG	O5-C5-C6-O6
3	r	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6

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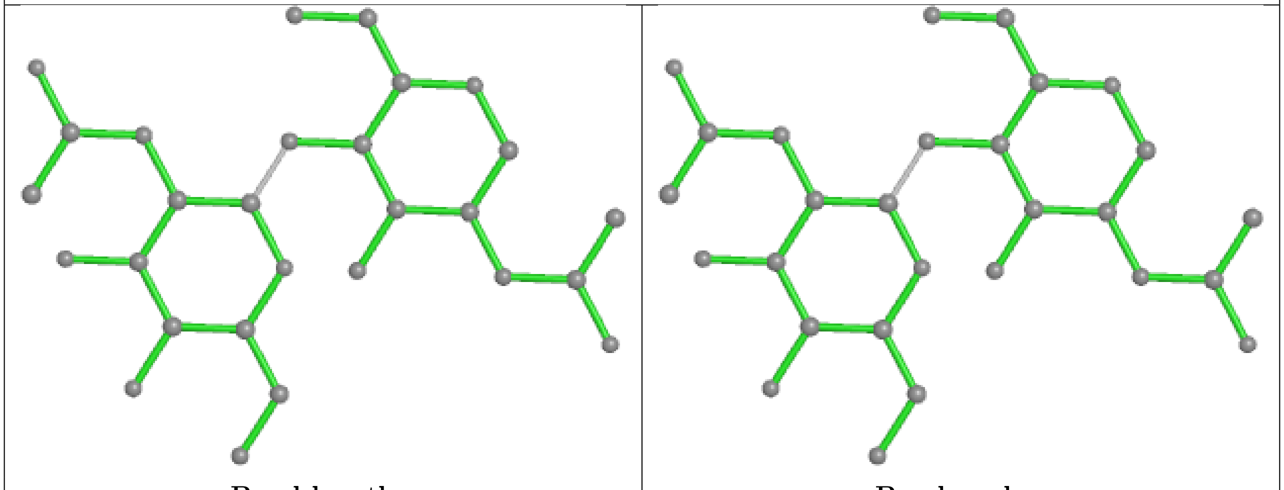
Mol	Chain	Res	Type	Atoms
3	g	1	NAG	O5-C5-C6-O6
3	l	1	NAG	O5-C5-C6-O6
3	q	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
3	Q	1	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
3	Z	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C4-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	X	1	NAG	C1-C2-N2-C7
3	R	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C3-C2-N2-C7
3	K	2	NAG	C3-C2-N2-C7
3	X	1	NAG	C3-C2-N2-C7
3	a	2	NAG	C3-C2-N2-C7
3	b	2	NAG	C3-C2-N2-C7
3	f	2	NAG	C3-C2-N2-C7
3	k	2	NAG	C3-C2-N2-C7
3	p	2	NAG	C3-C2-N2-C7
3	j	1	NAG	C1-C2-N2-C7
3	o	1	NAG	C1-C2-N2-C7
3	e	1	NAG	C1-C2-N2-C7

There are no ring outliers.

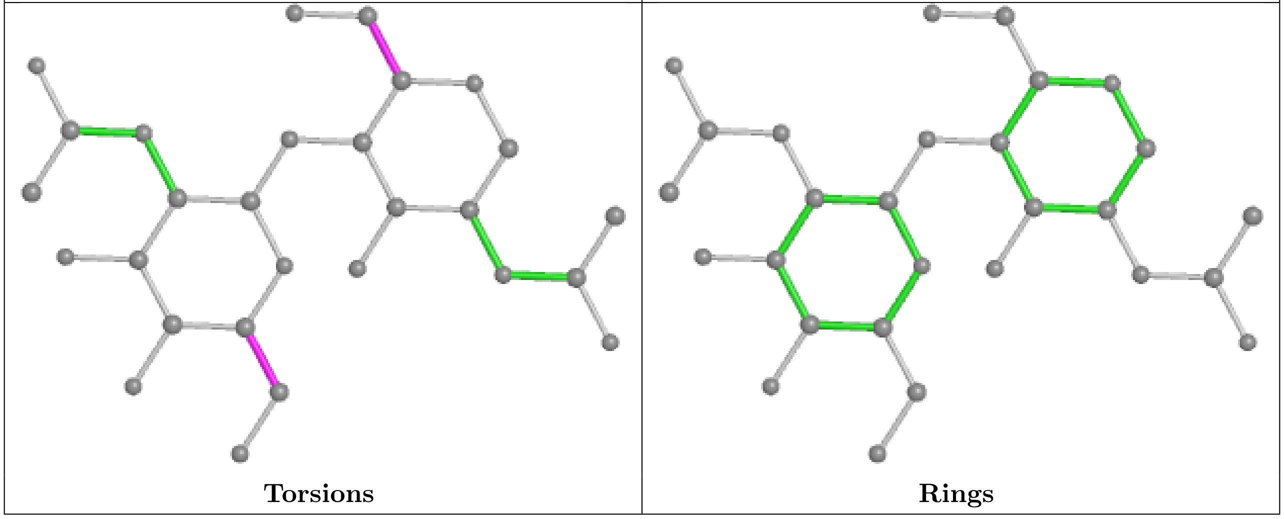
No monomer is involved in short contacts.

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

Oligosaccharide Chain G

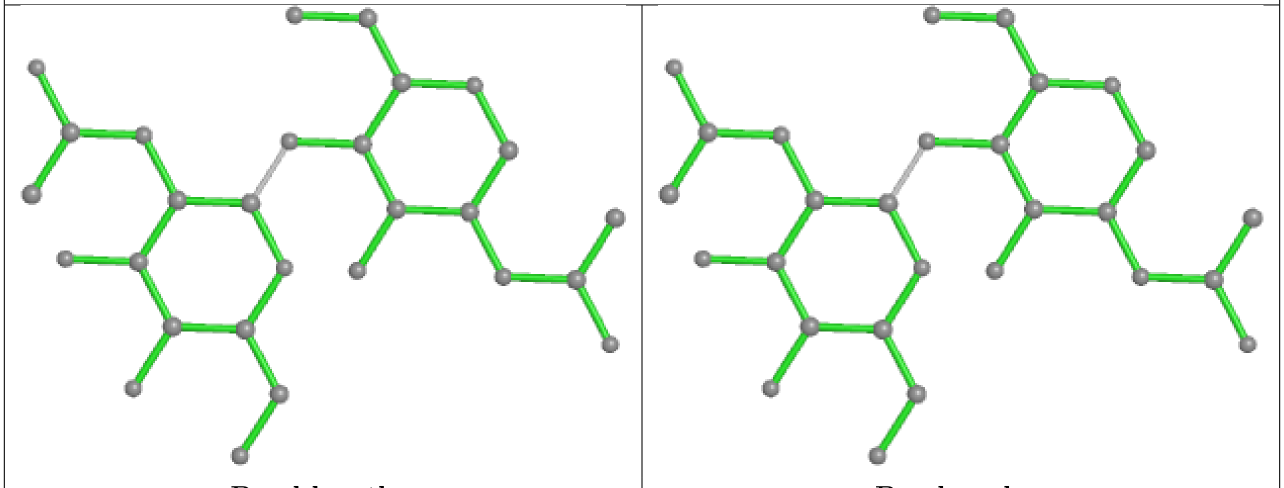


Bond lengths **Bond angles**

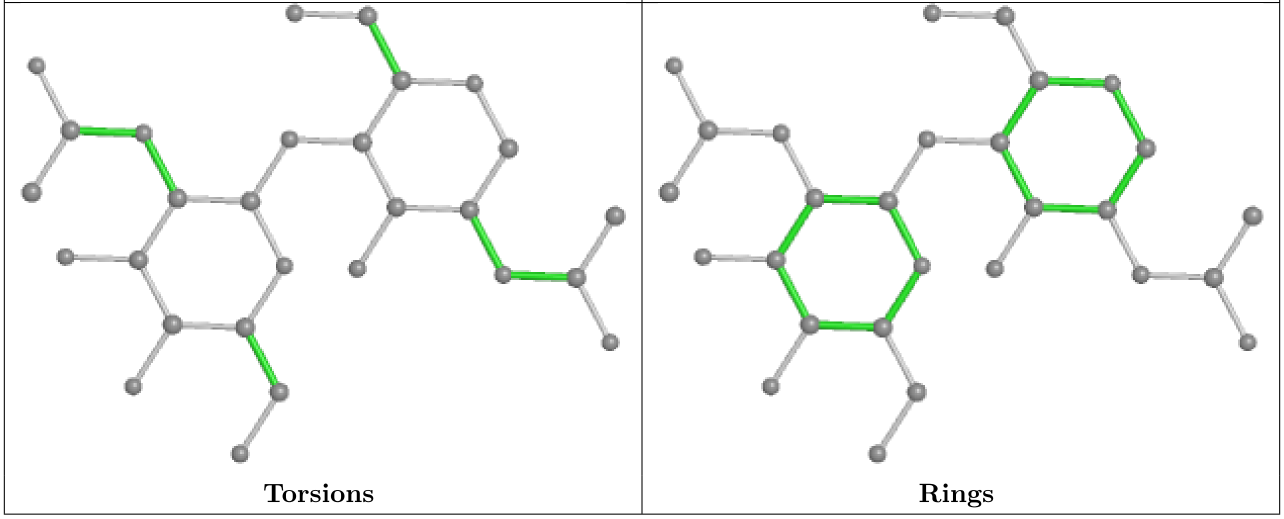


Torsions **Rings**

Oligosaccharide Chain H

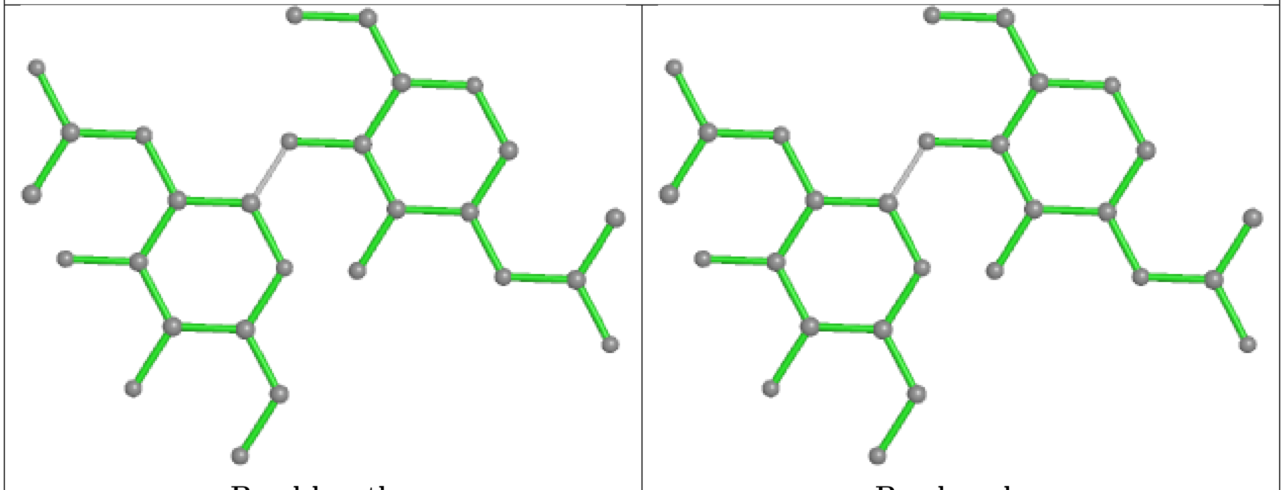


Bond lengths **Bond angles**

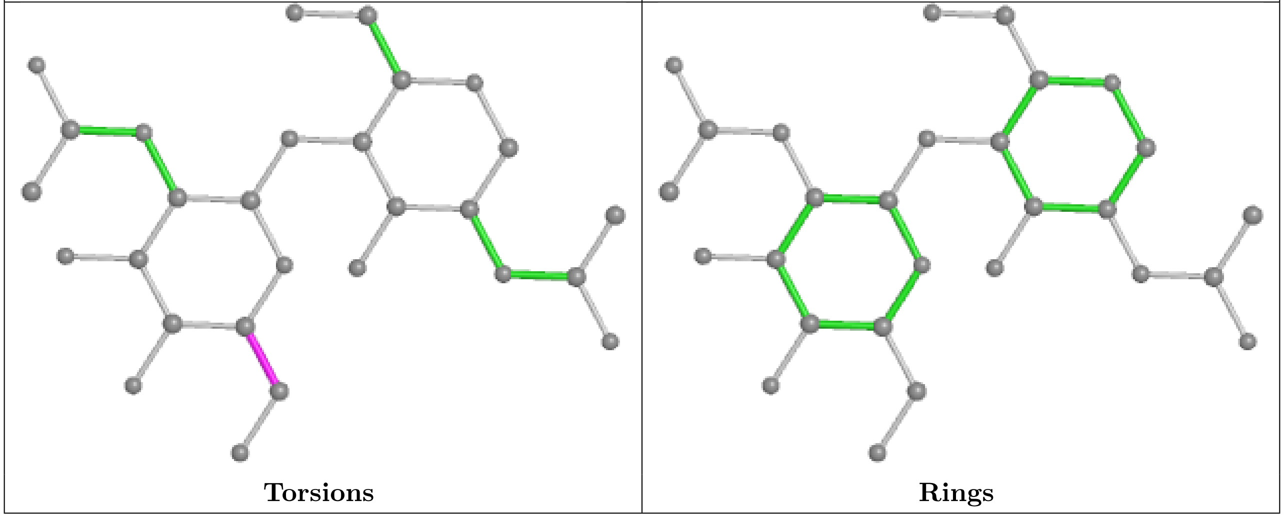


Torsions **Rings**

Oligosaccharide Chain I

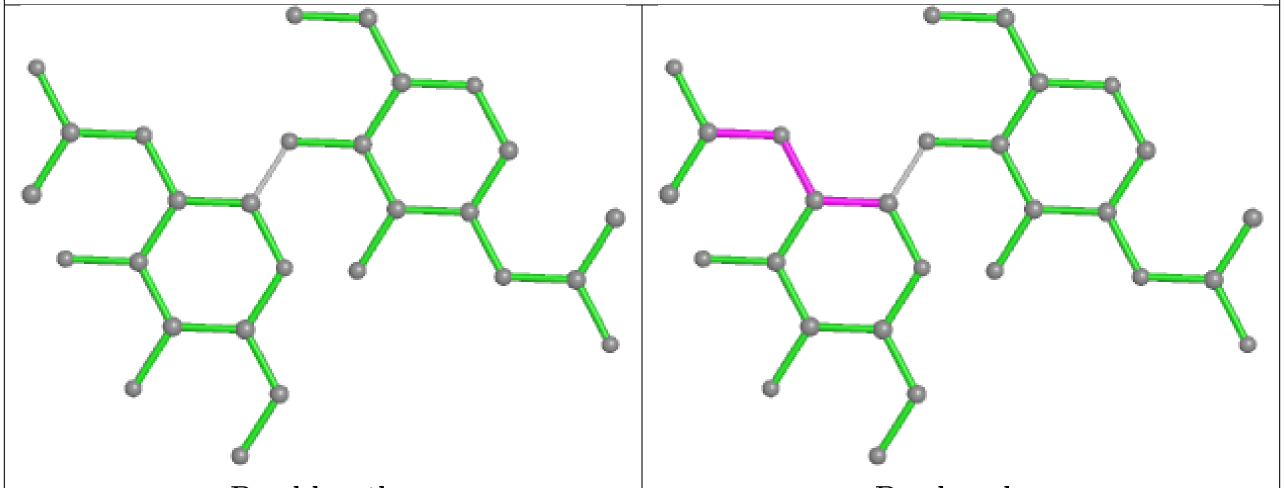


Bond lengths **Bond angles**

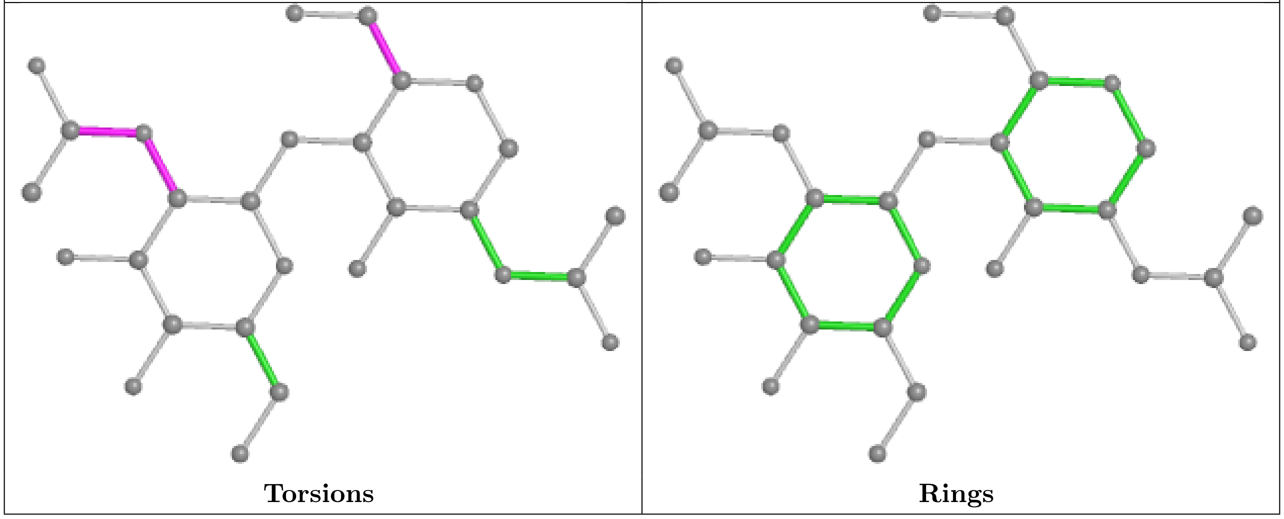


Torsions **Rings**

Oligosaccharide Chain J

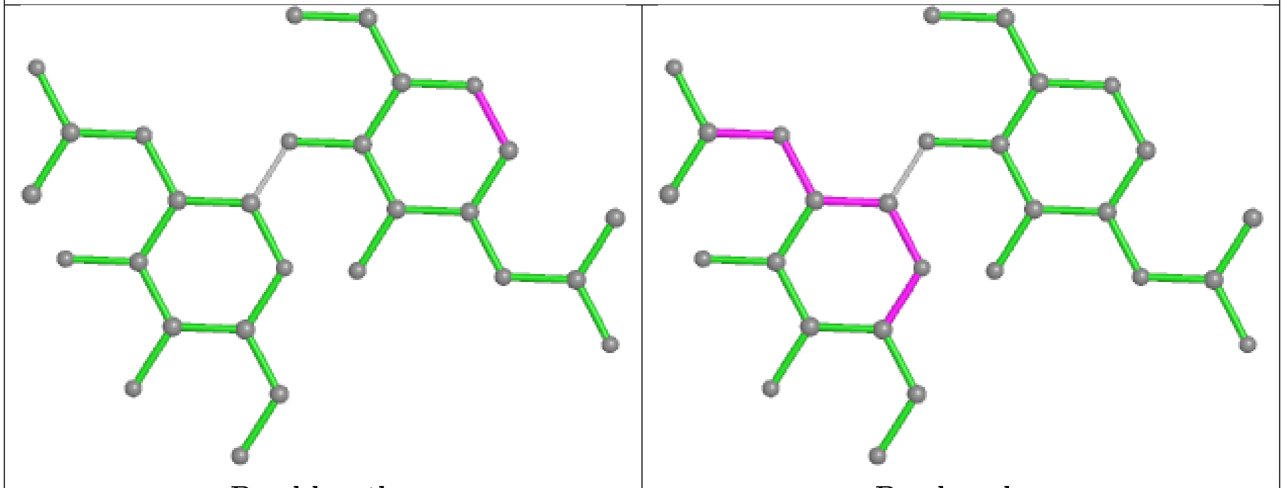


Bond lengths **Bond angles**



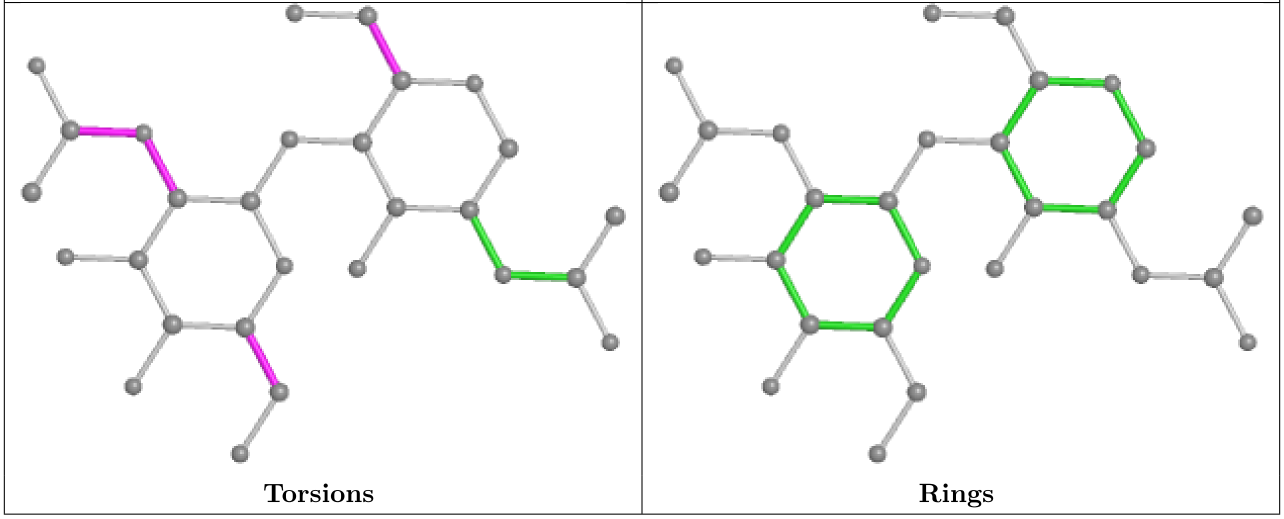
Torsions **Rings**

Oligosaccharide Chain K



Bond lengths

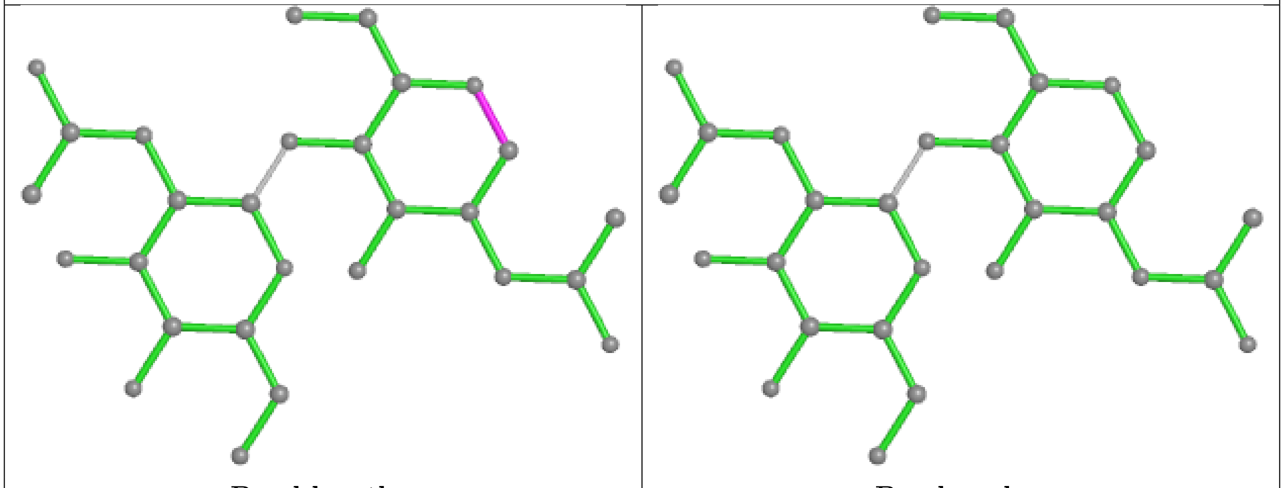
Bond angles



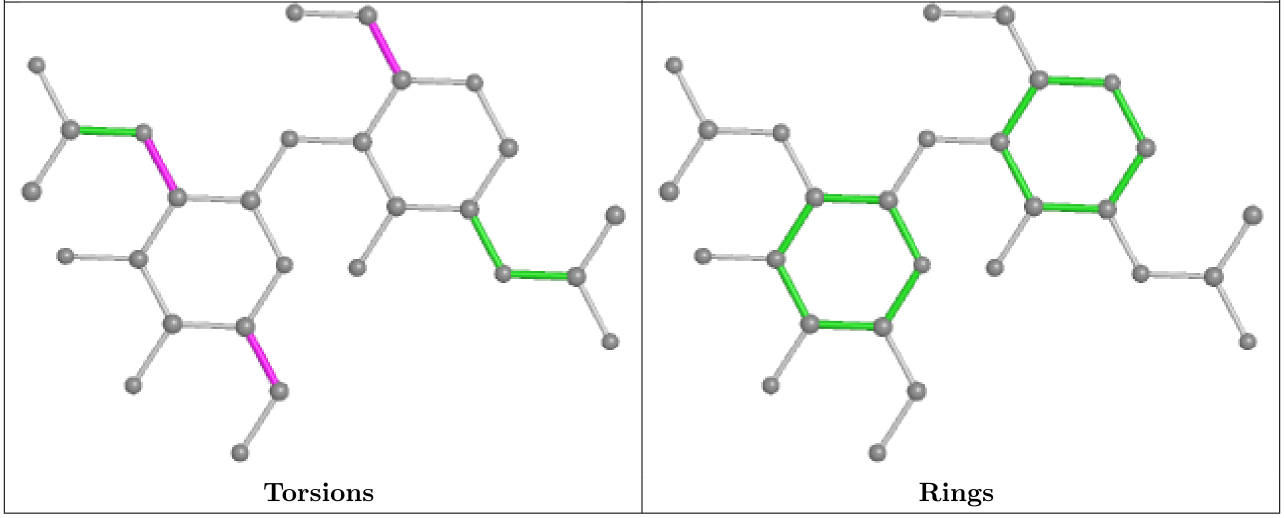
Torsions

Rings

Oligosaccharide Chain L

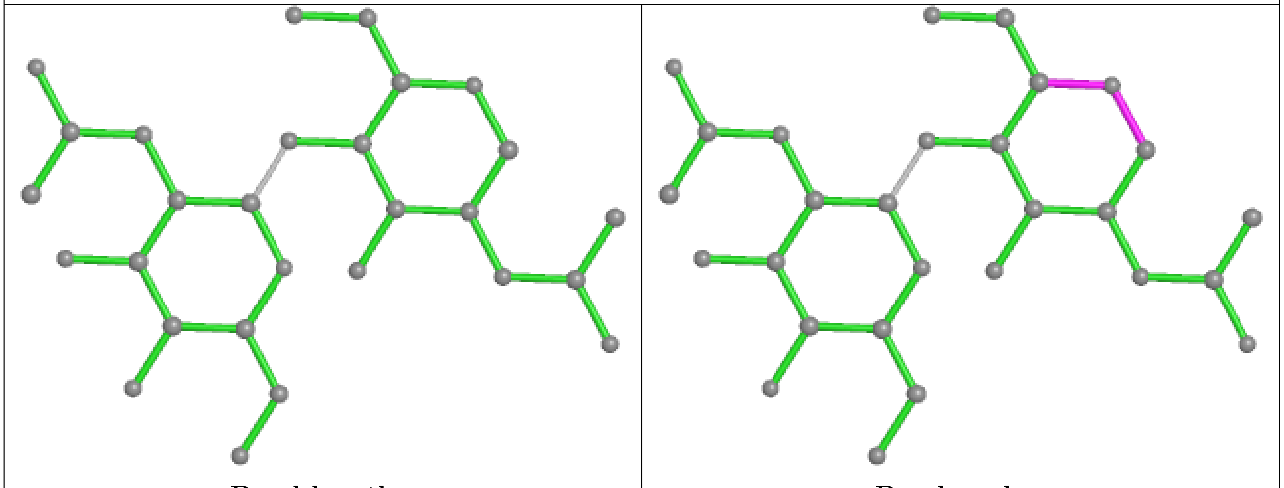


Bond lengths **Bond angles**

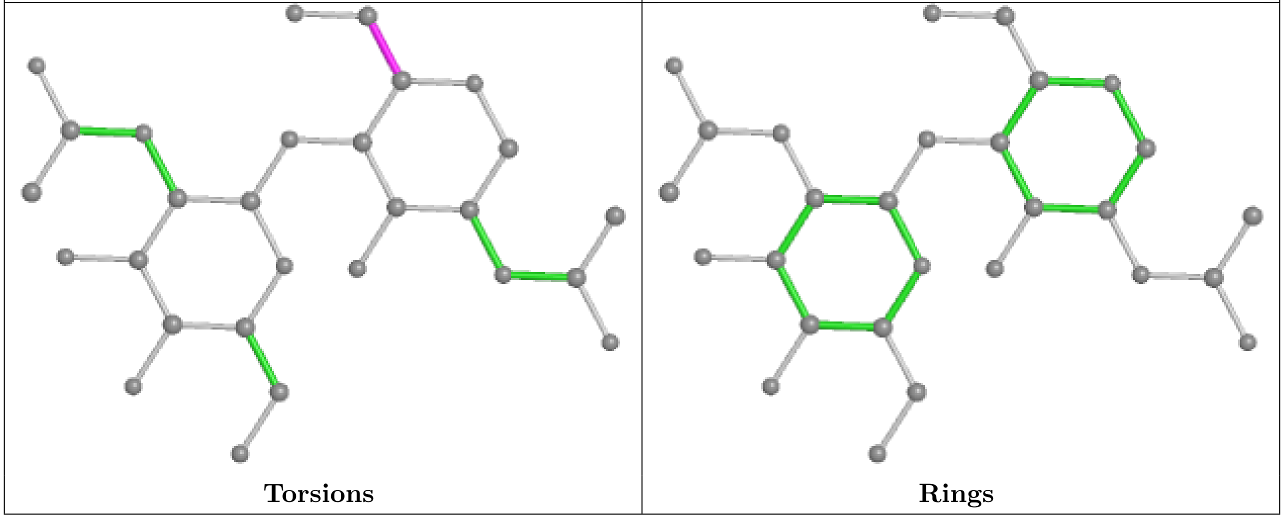


Torsions **Rings**

Oligosaccharide Chain M

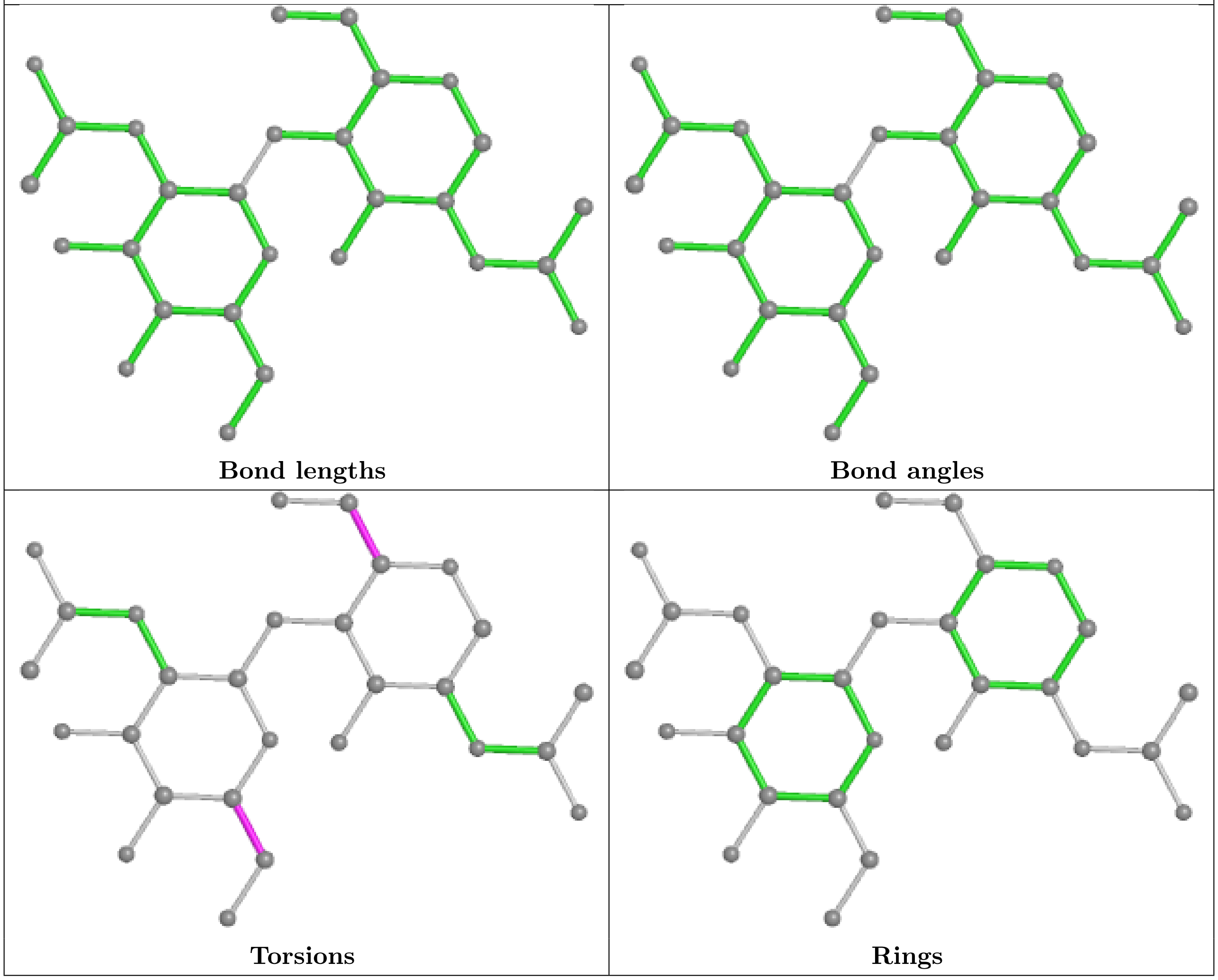


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain N



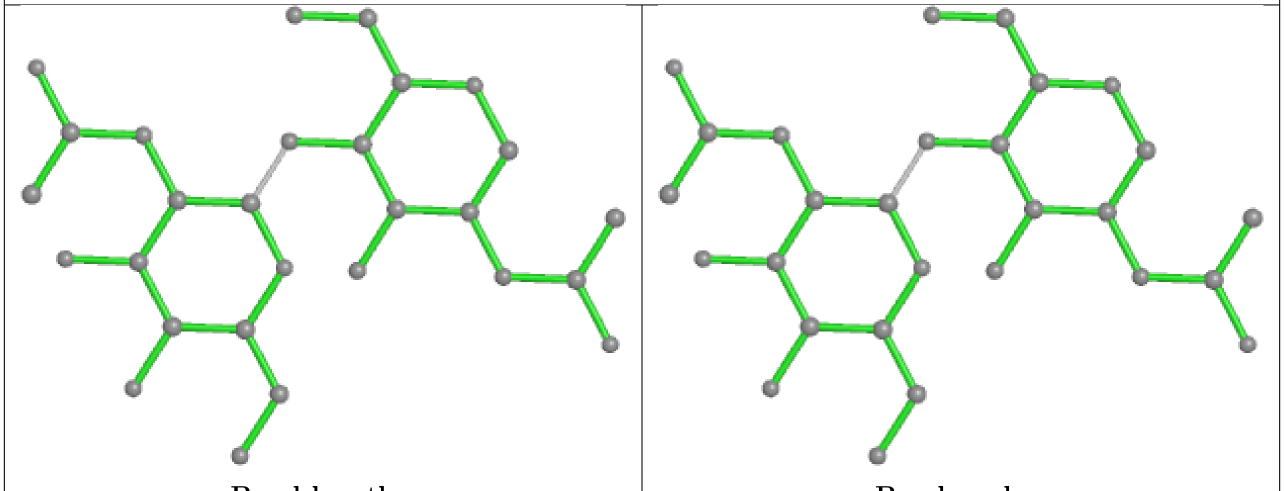
Bond lengths

Bond angles

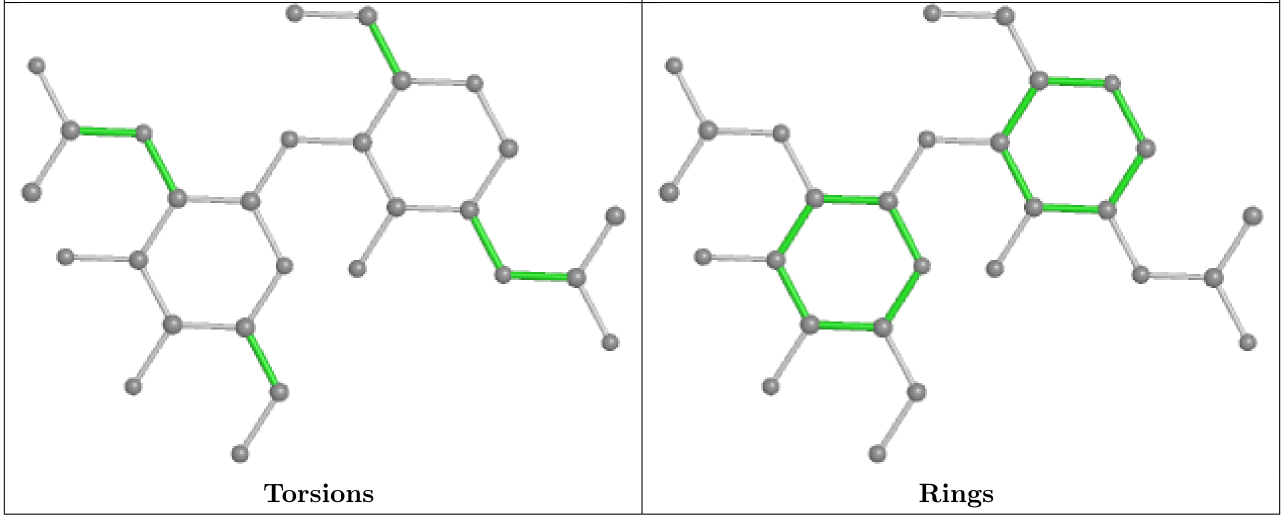
Torsions

Rings

Oligosaccharide Chain O

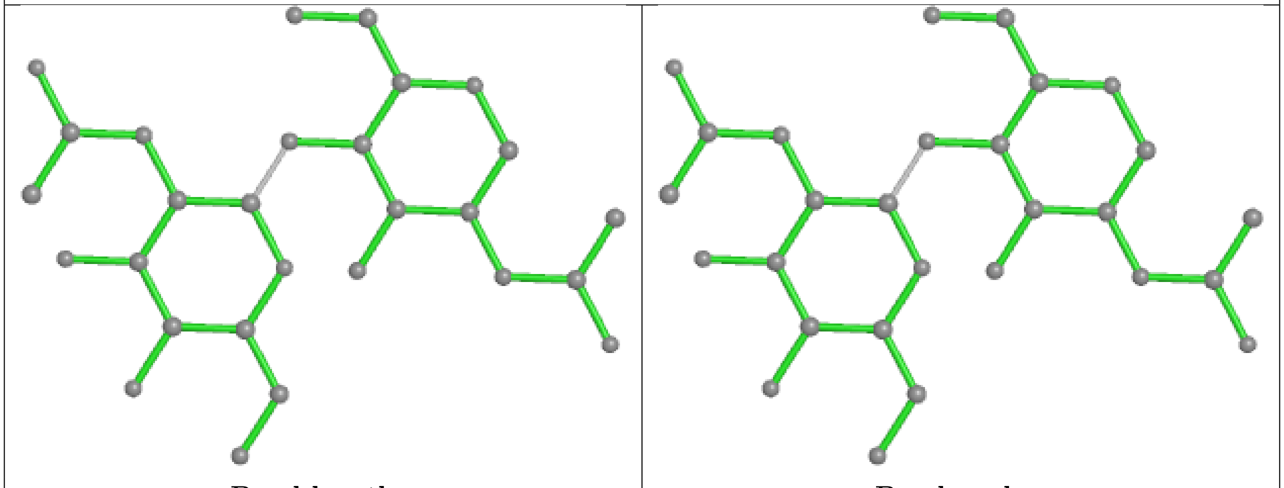


Bond lengths **Bond angles**

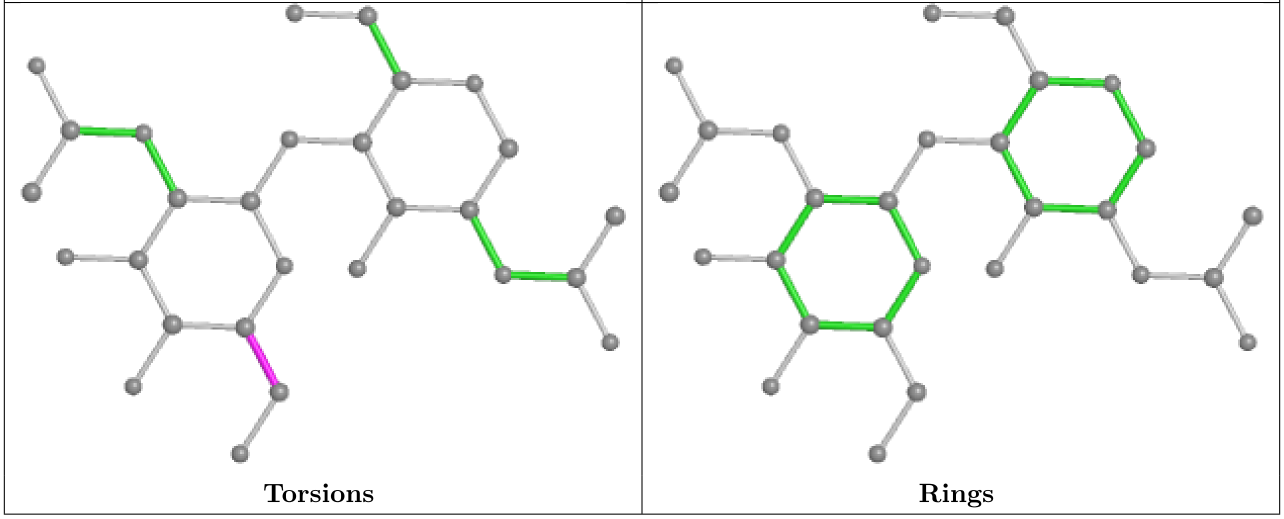


Torsions **Rings**

Oligosaccharide Chain P

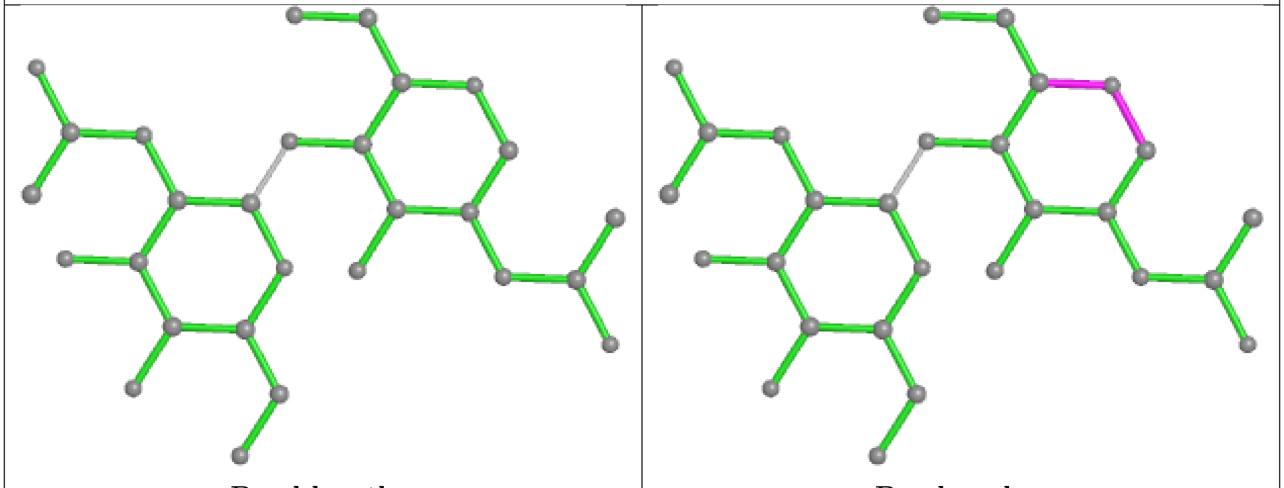


Bond lengths **Bond angles**

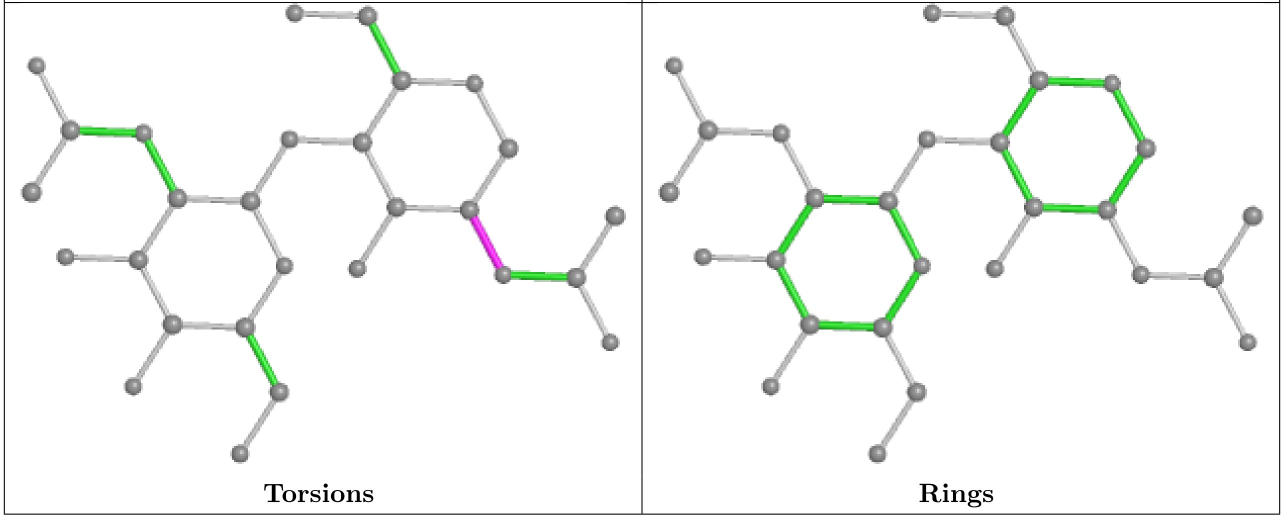


Torsions **Rings**

Oligosaccharide Chain Q

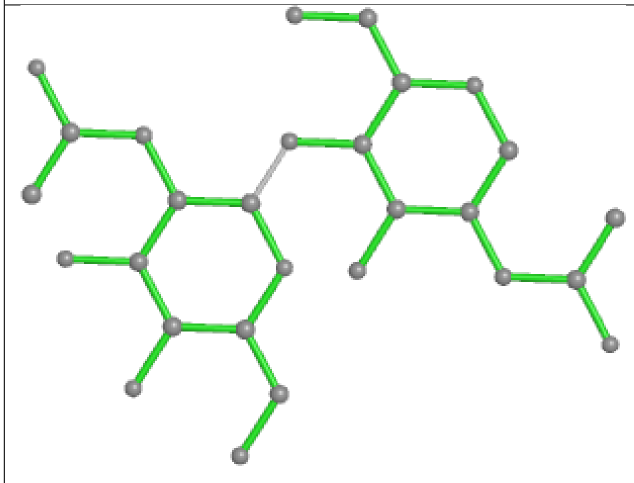


Bond lengths **Bond angles**

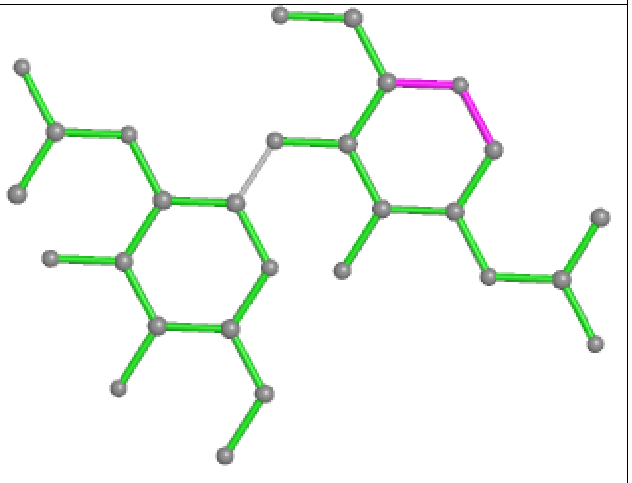


Torsions **Rings**

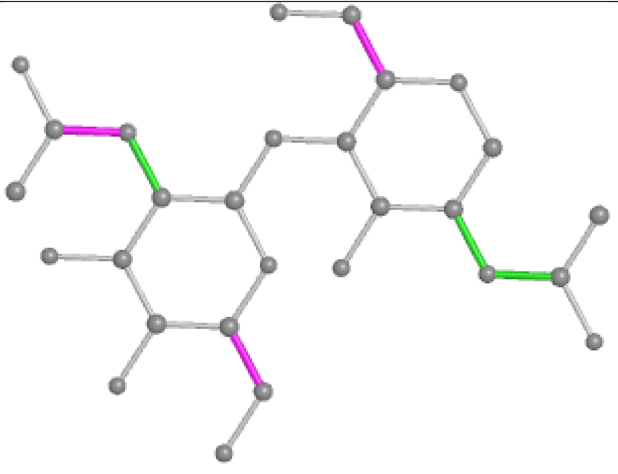
Oligosaccharide Chain R



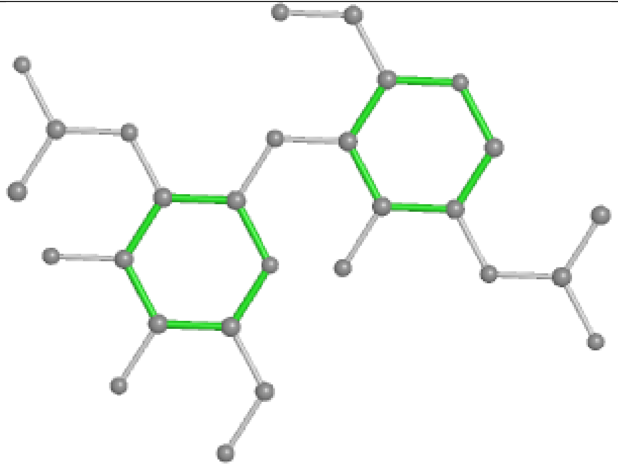
Bond lengths



Bond angles

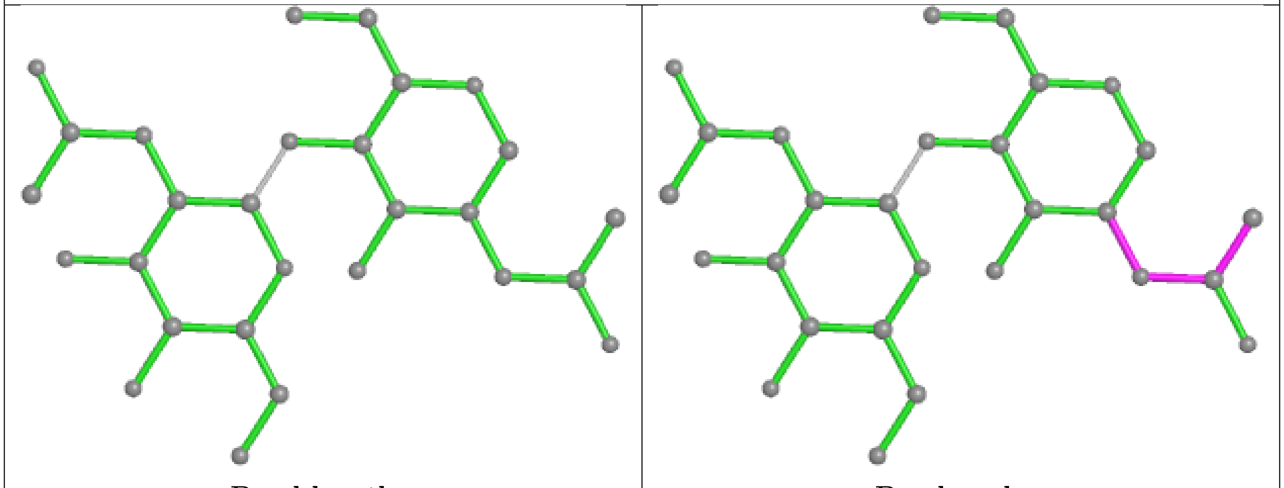


Torsions



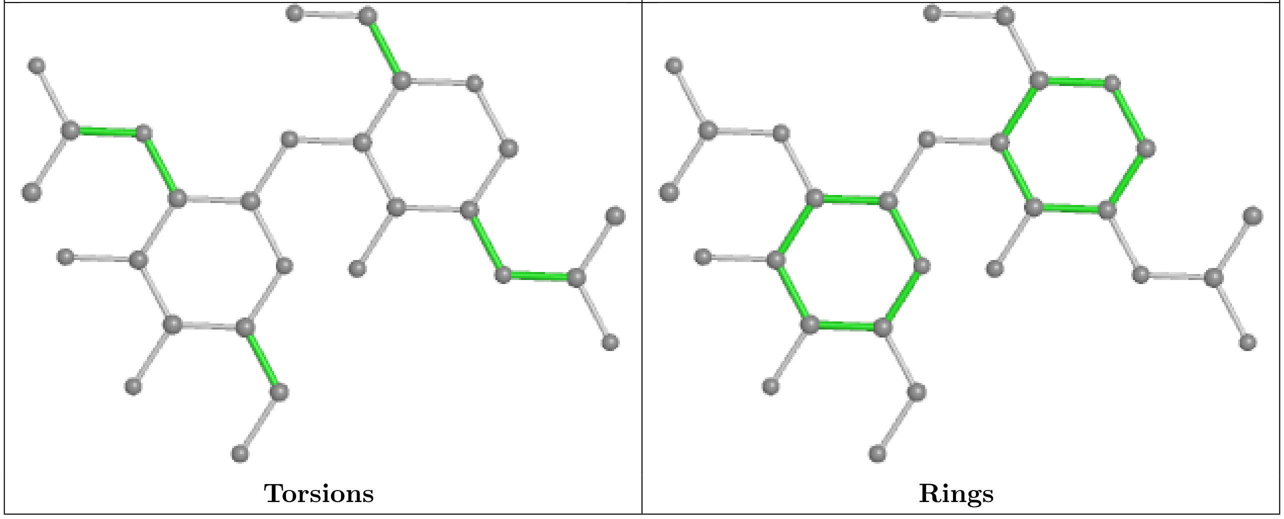
Rings

Oligosaccharide Chain S



Bond lengths

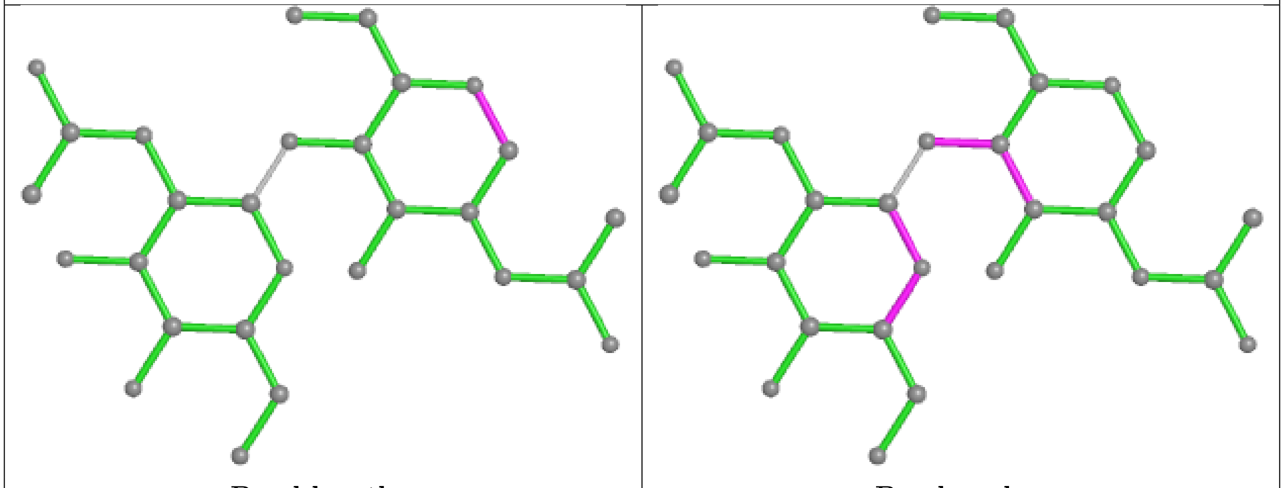
Bond angles



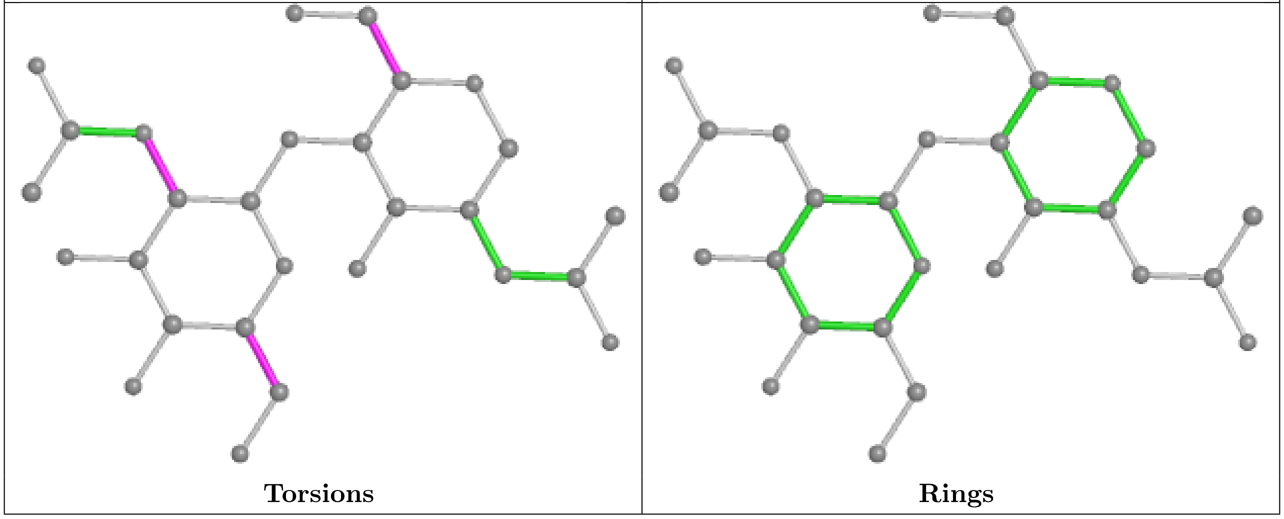
Torsions

Rings

Oligosaccharide Chain T

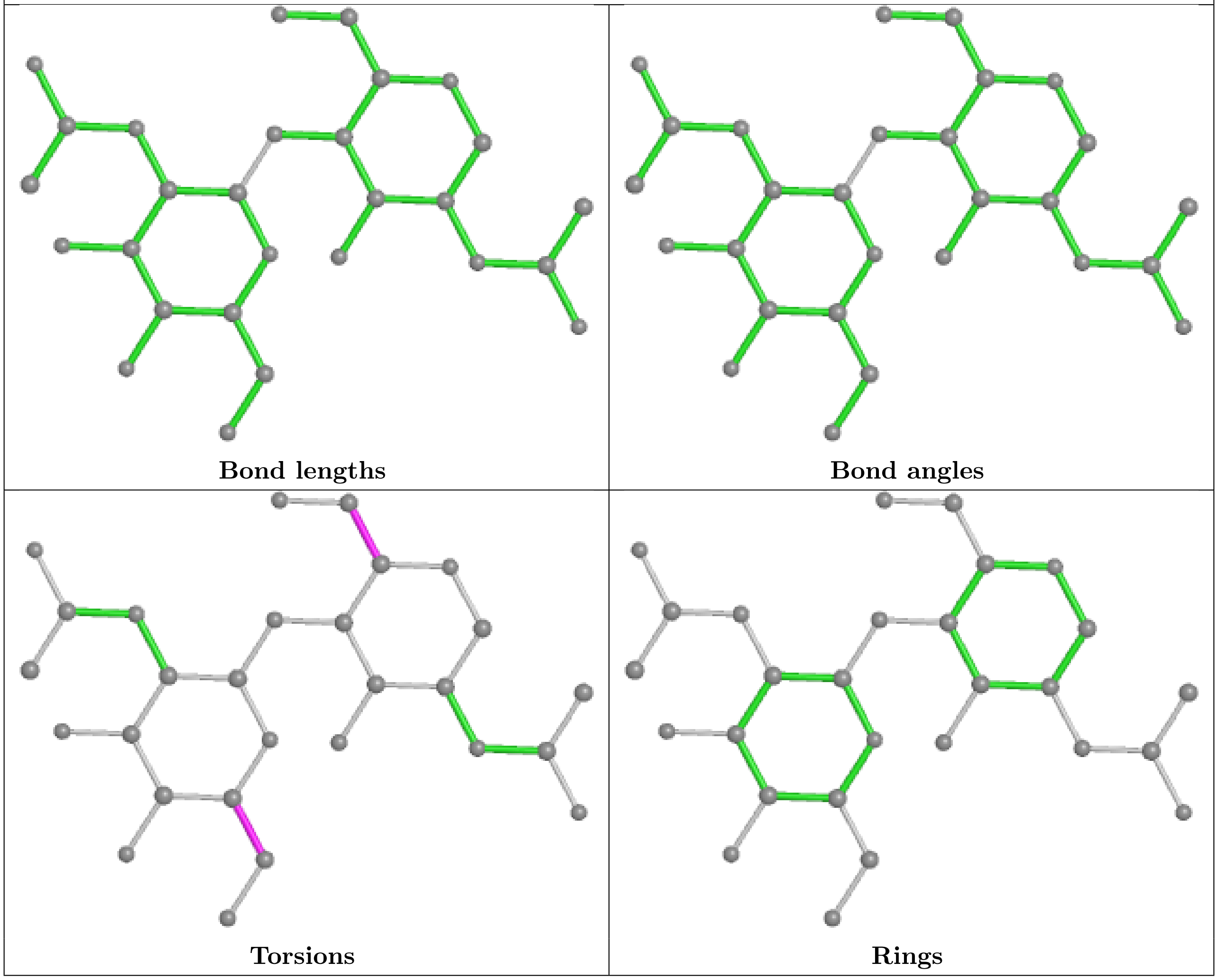


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain U



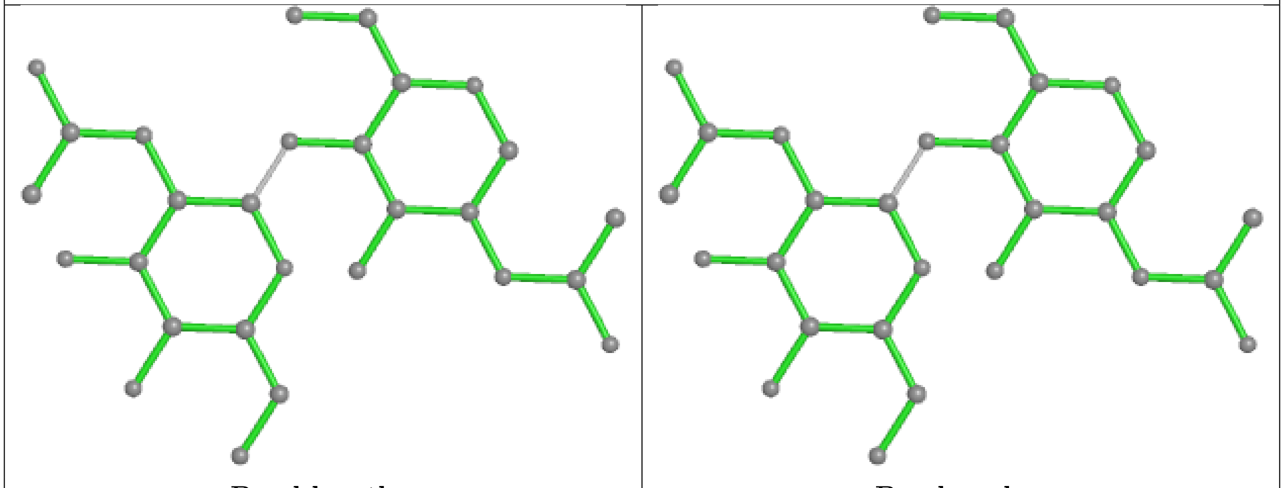
Bond lengths

Bond angles

Torsions

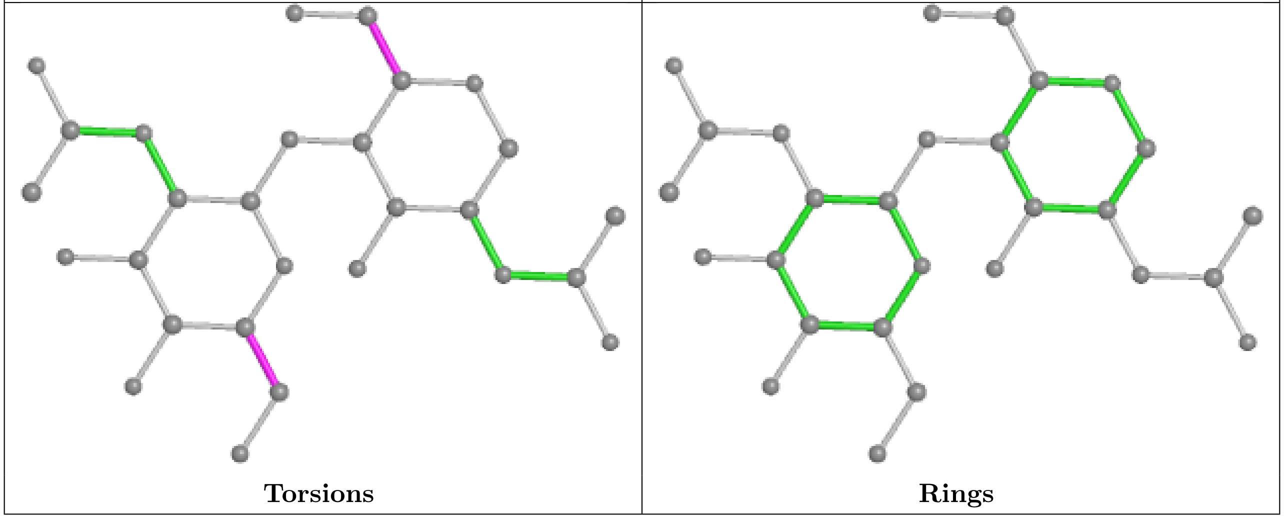
Rings

Oligosaccharide Chain V



Bond lengths

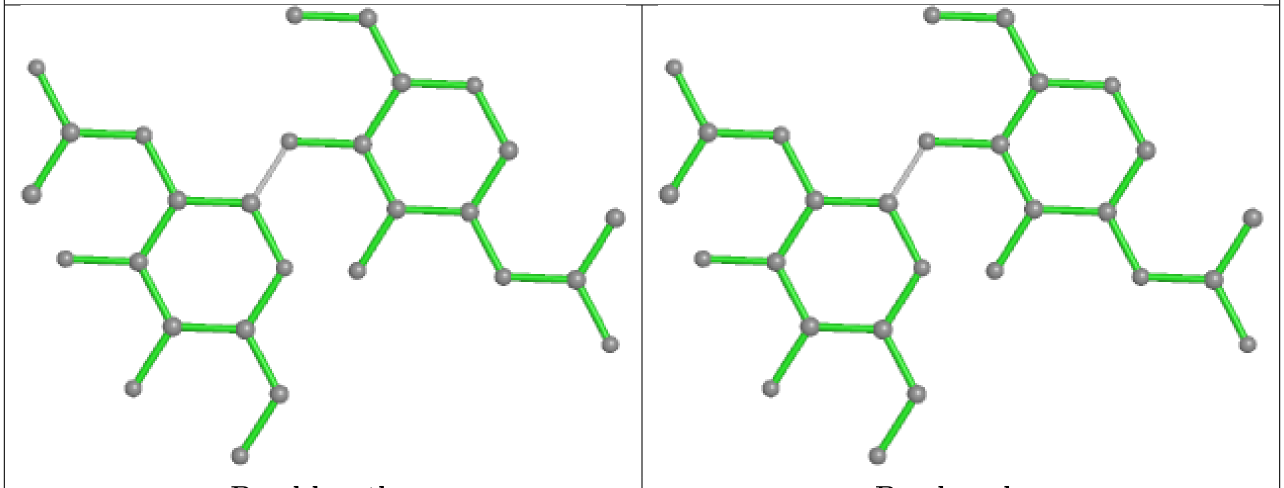
Bond angles



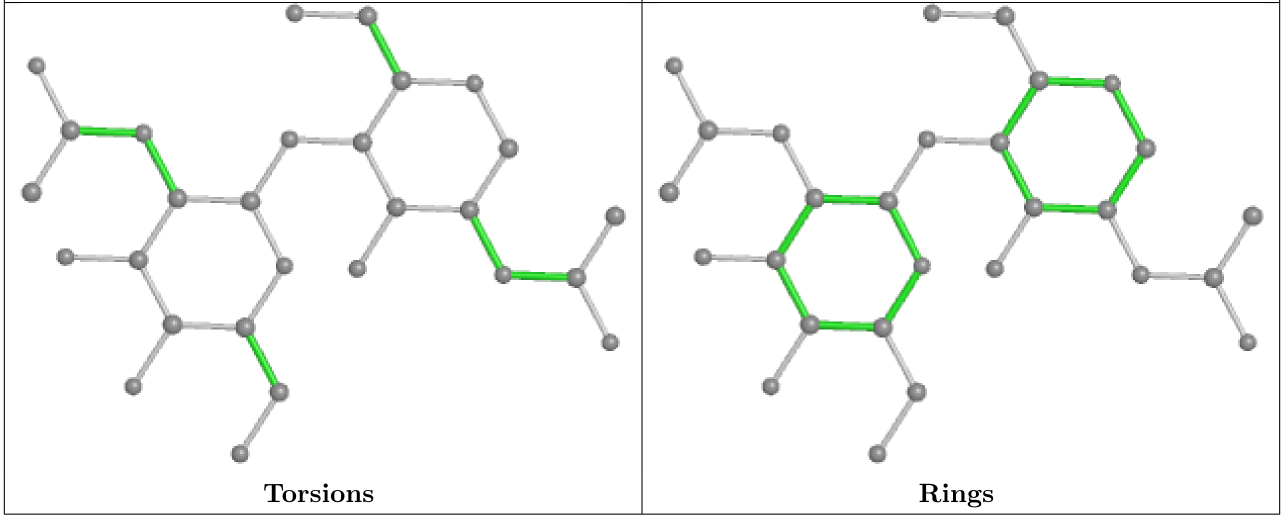
Torsions

Rings

Oligosaccharide Chain W

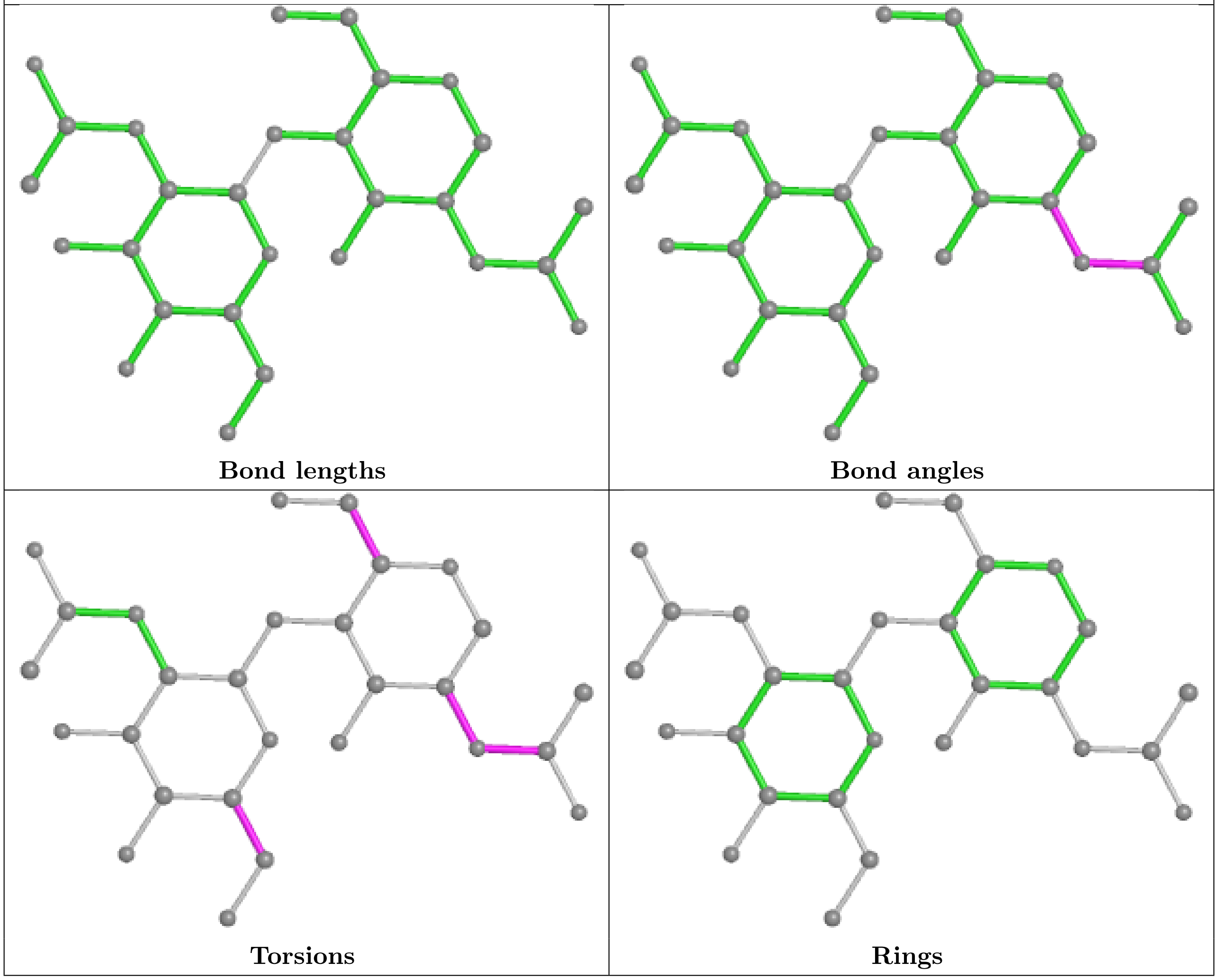


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain X



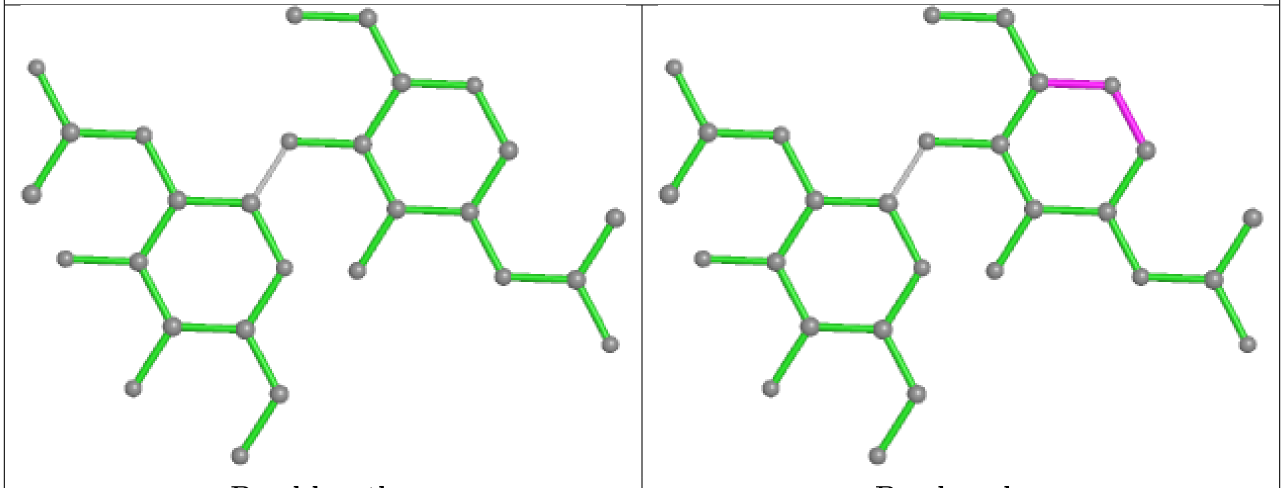
Bond lengths

Bond angles

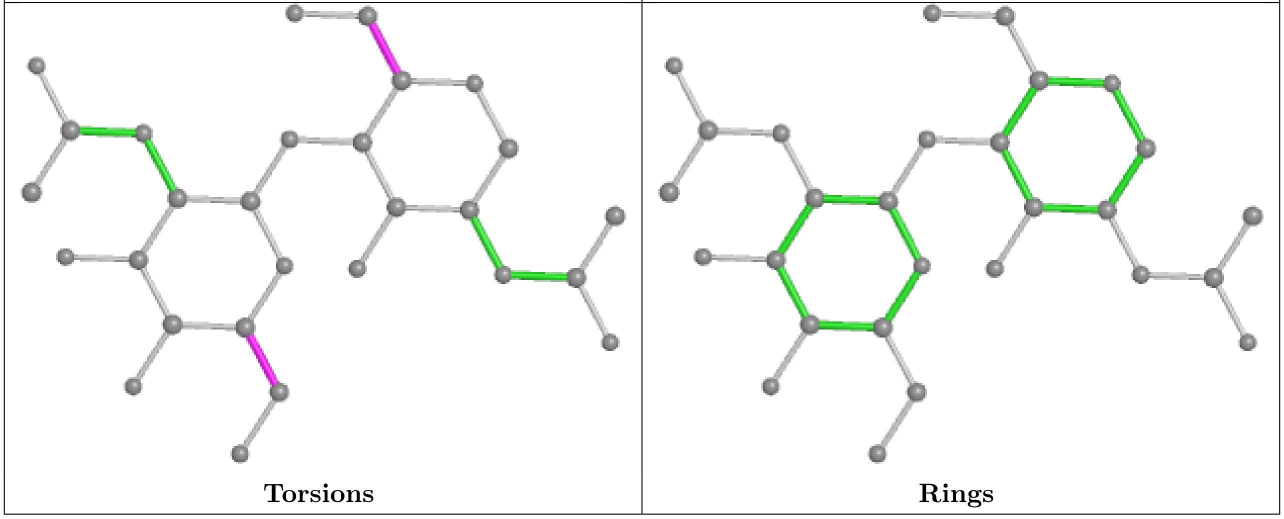
Torsions

Rings

Oligosaccharide Chain Y

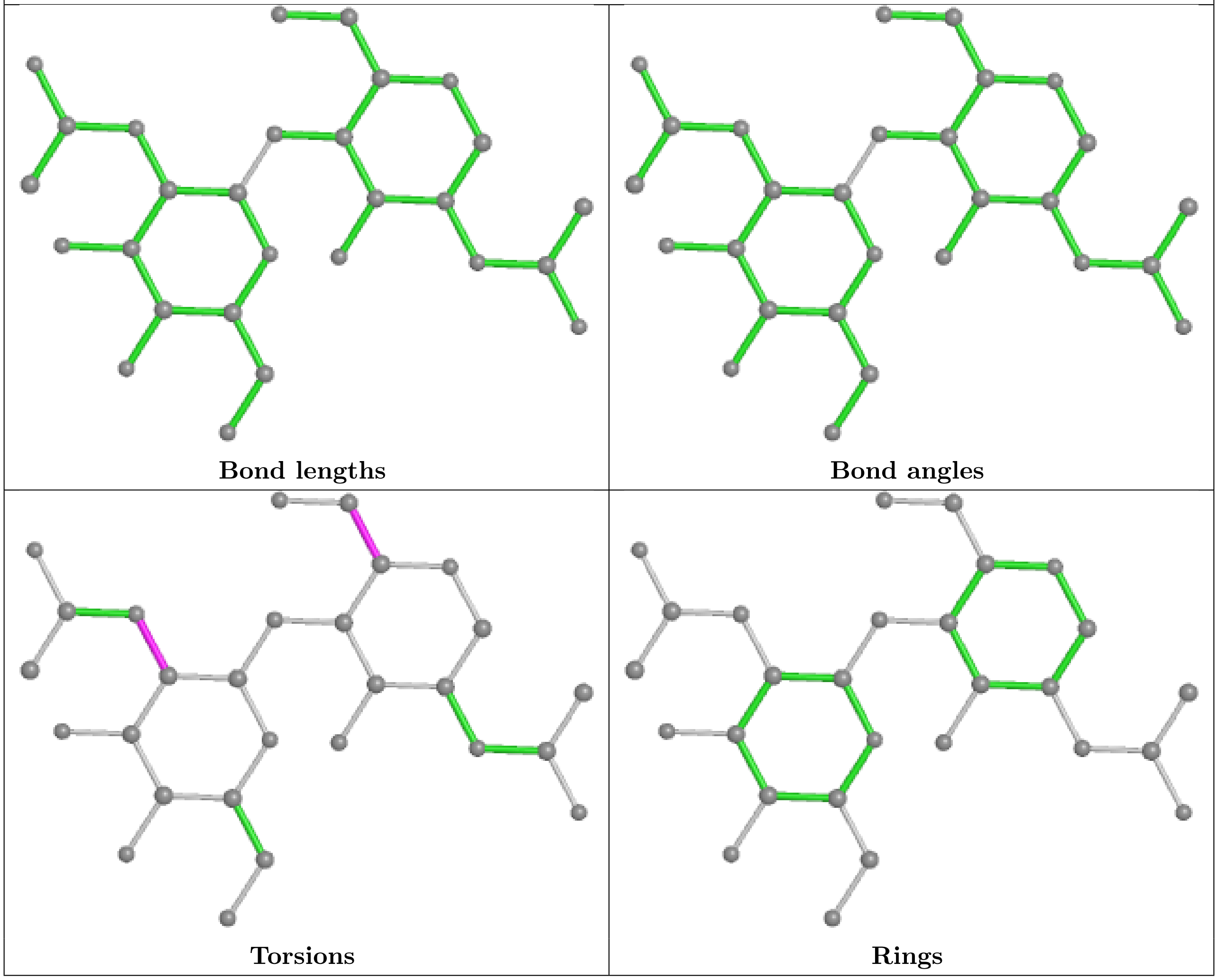


Bond lengths Bond angles



Torsions Rings

Oligosaccharide Chain Z



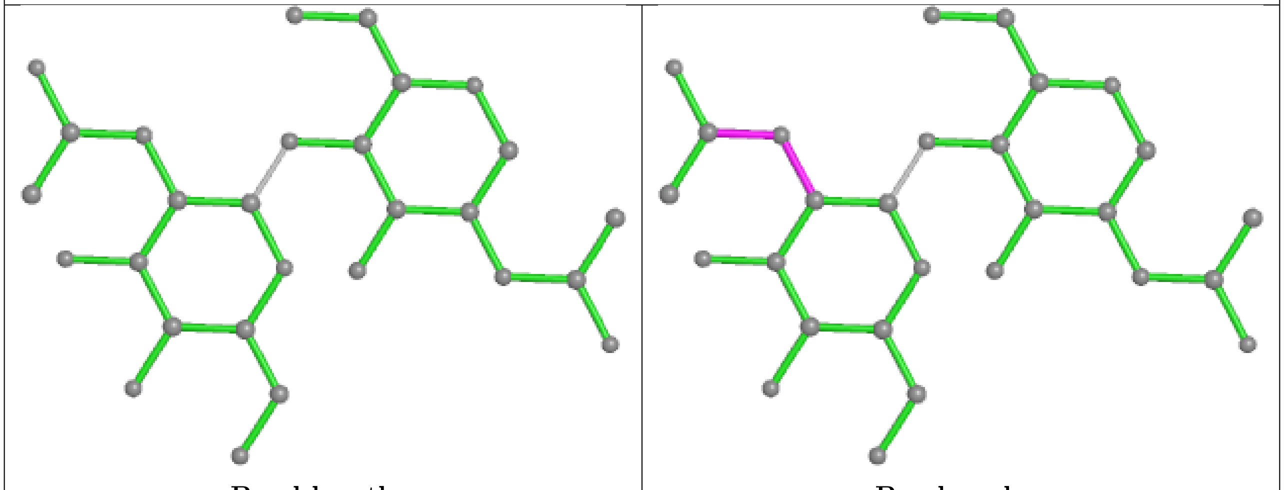
Bond lengths

Bond angles

Torsions

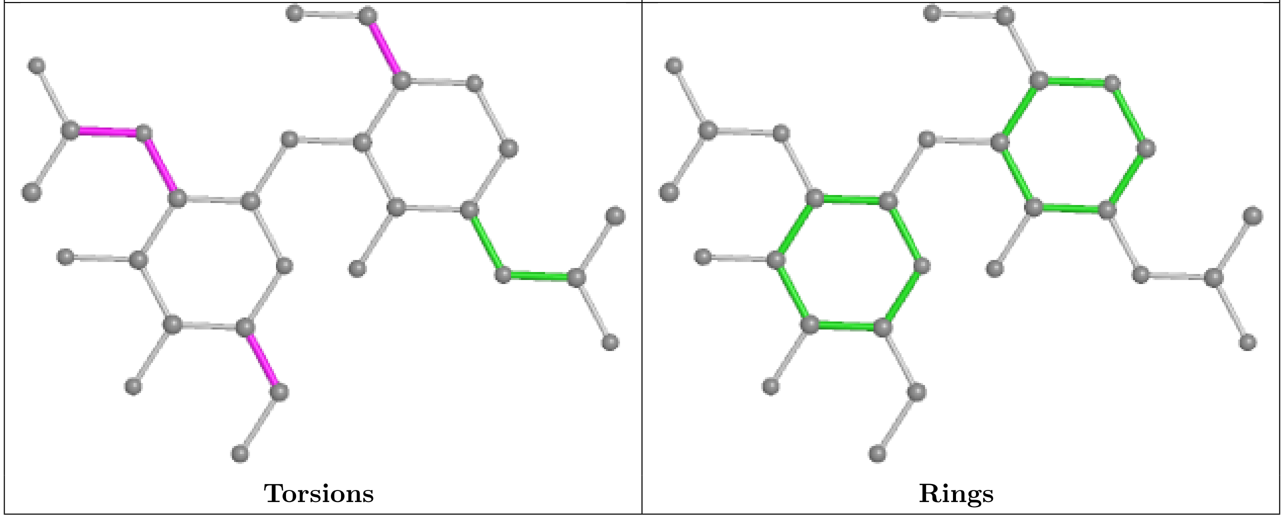
Rings

Oligosaccharide Chain a



Bond lengths

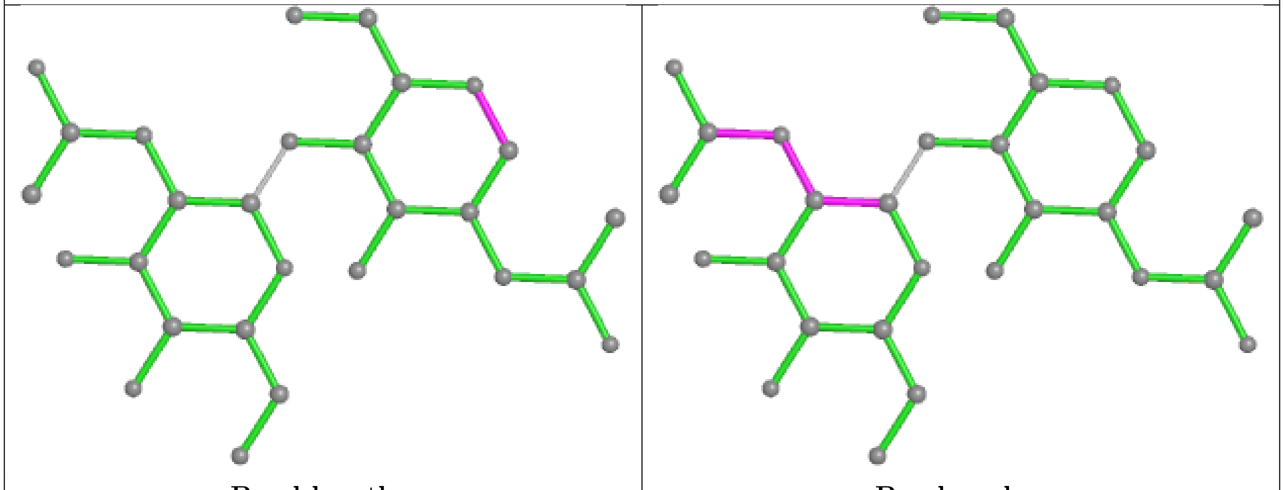
Bond angles



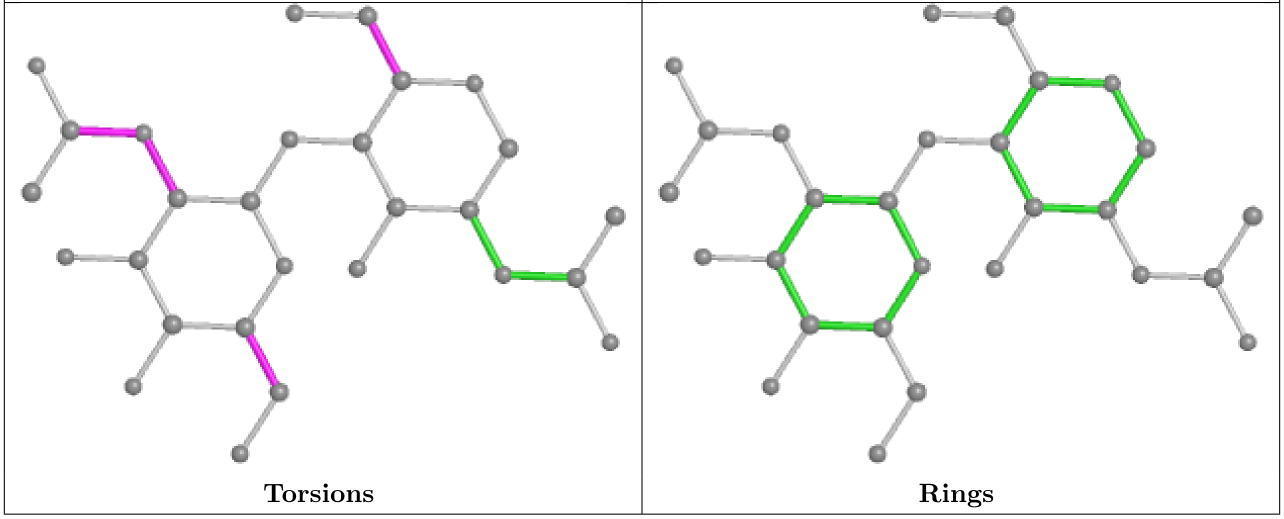
Torsions

Rings

Oligosaccharide Chain b

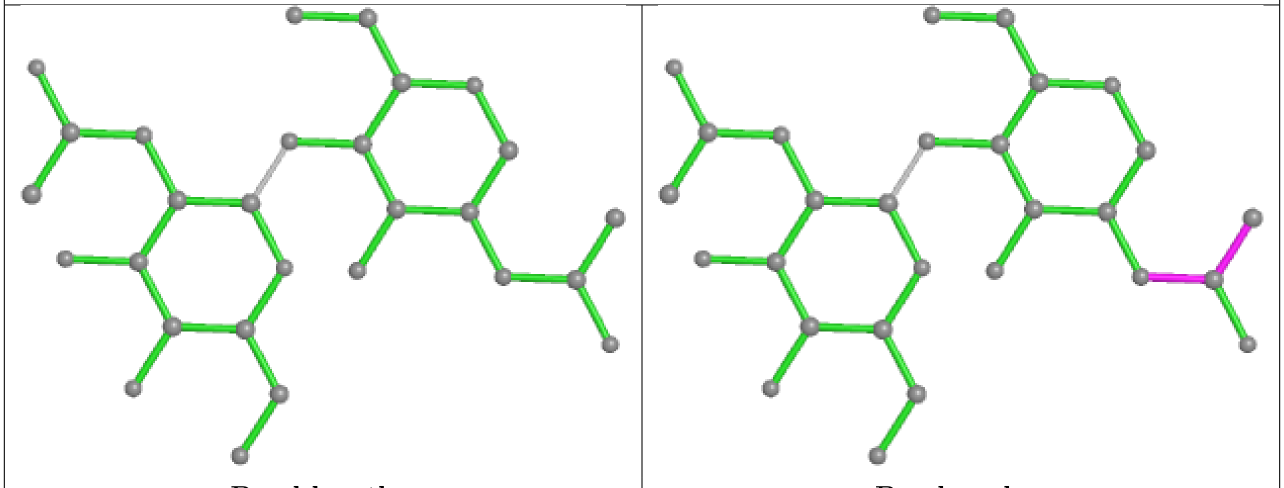


Bond lengths **Bond angles**



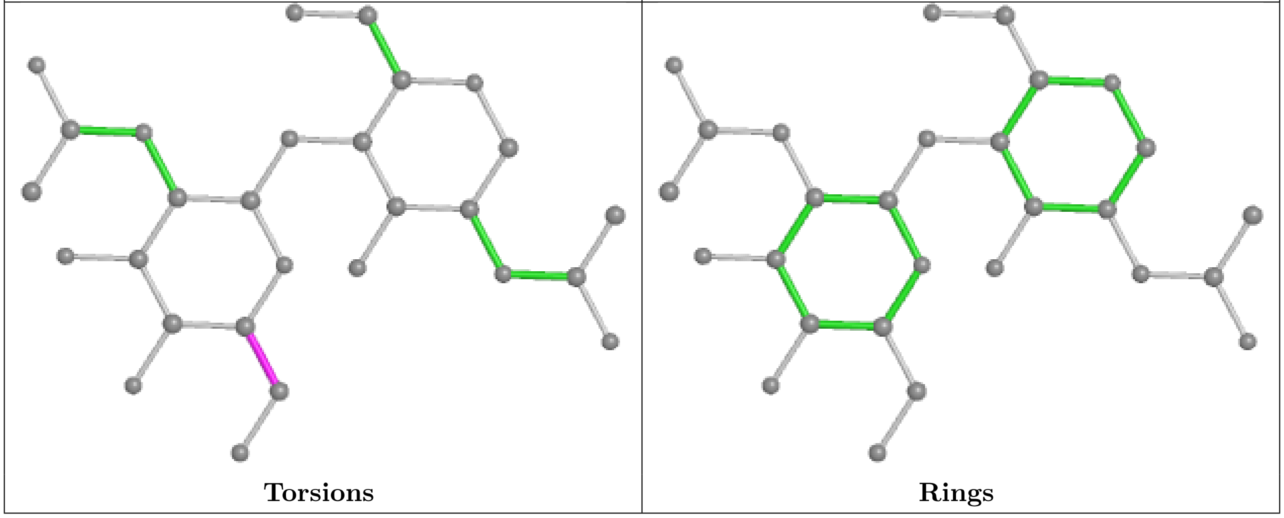
Torsions **Rings**

Oligosaccharide Chain c



Bond lengths

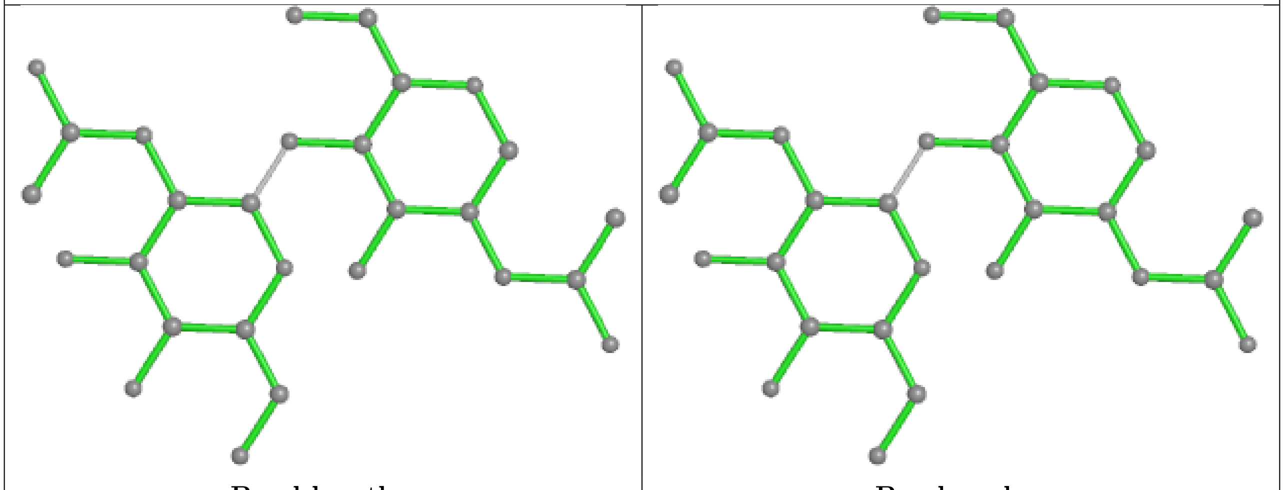
Bond angles



Torsions

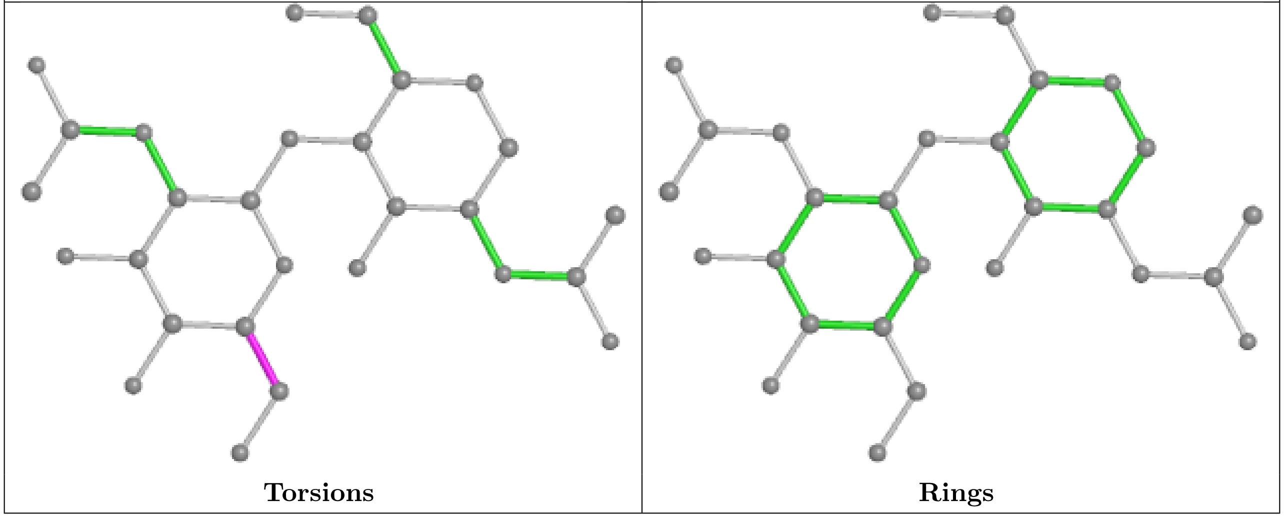
Rings

Oligosaccharide Chain d



Bond lengths

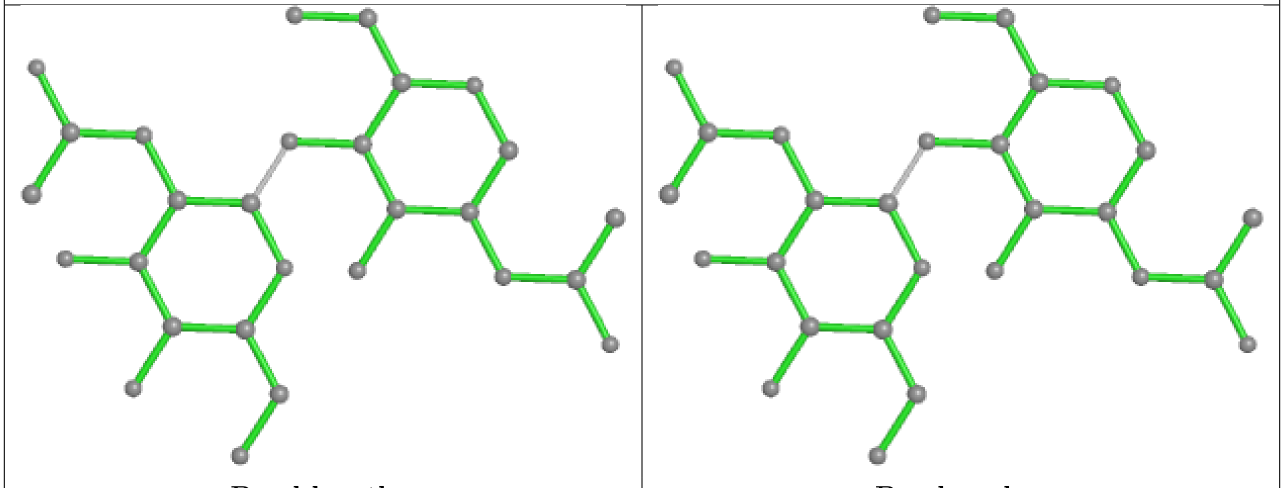
Bond angles



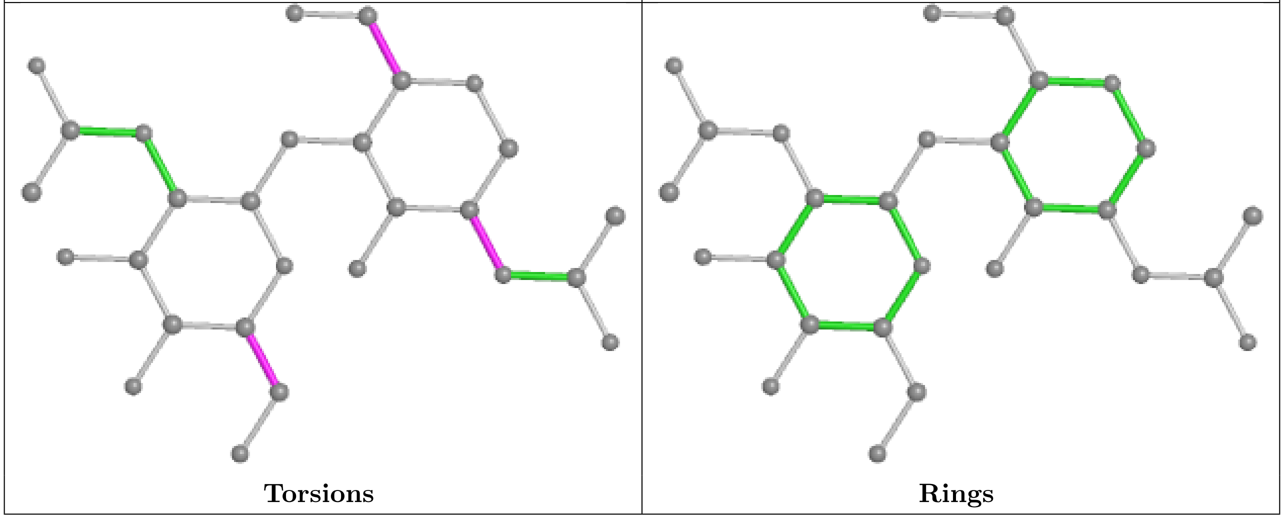
Torsions

Rings

Oligosaccharide Chain e

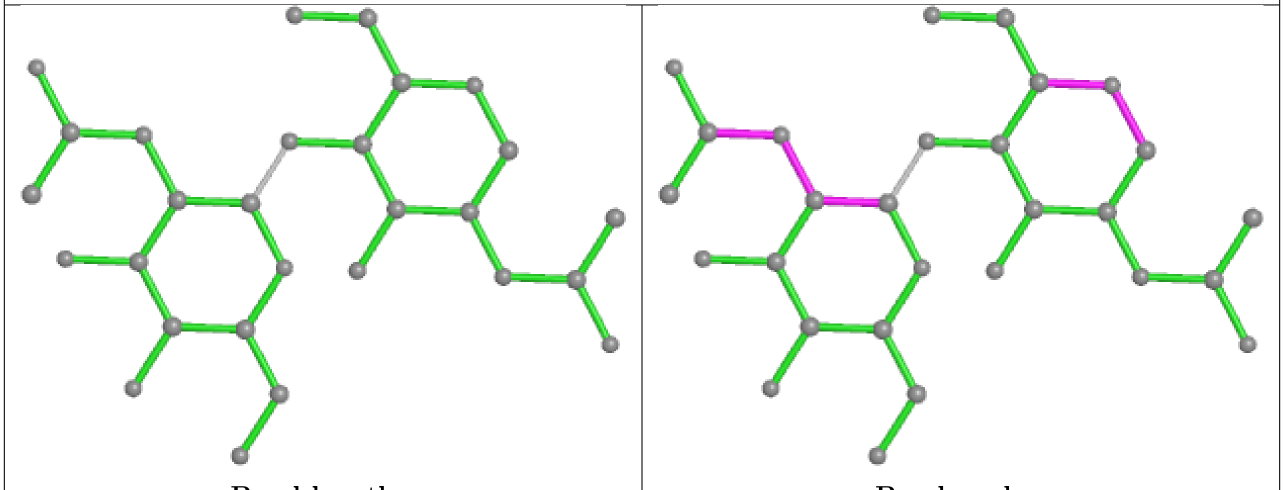


Bond lengths **Bond angles**

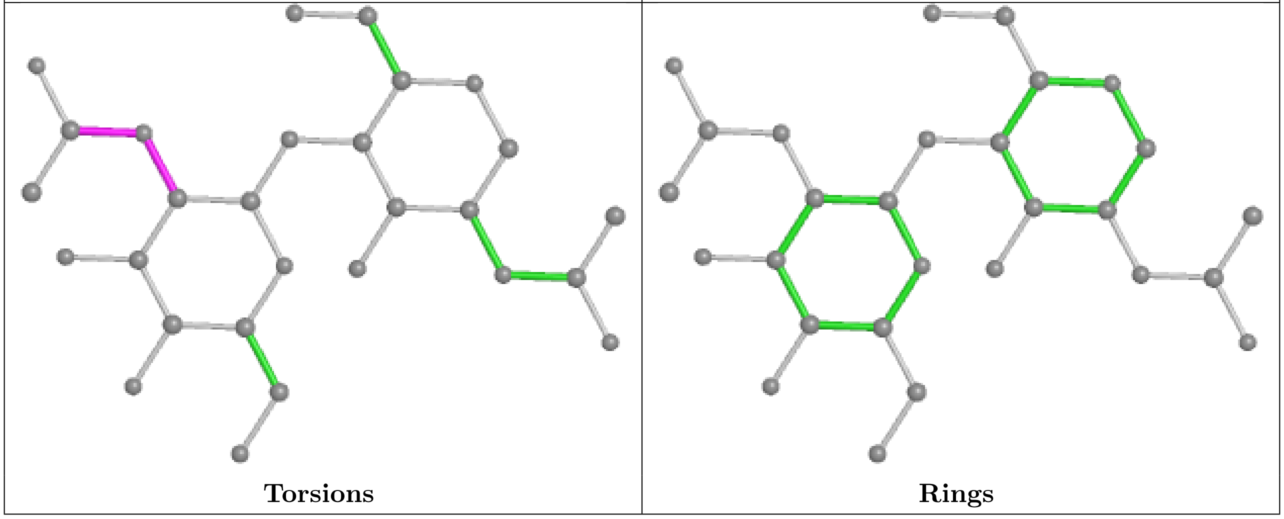


Torsions **Rings**

Oligosaccharide Chain f

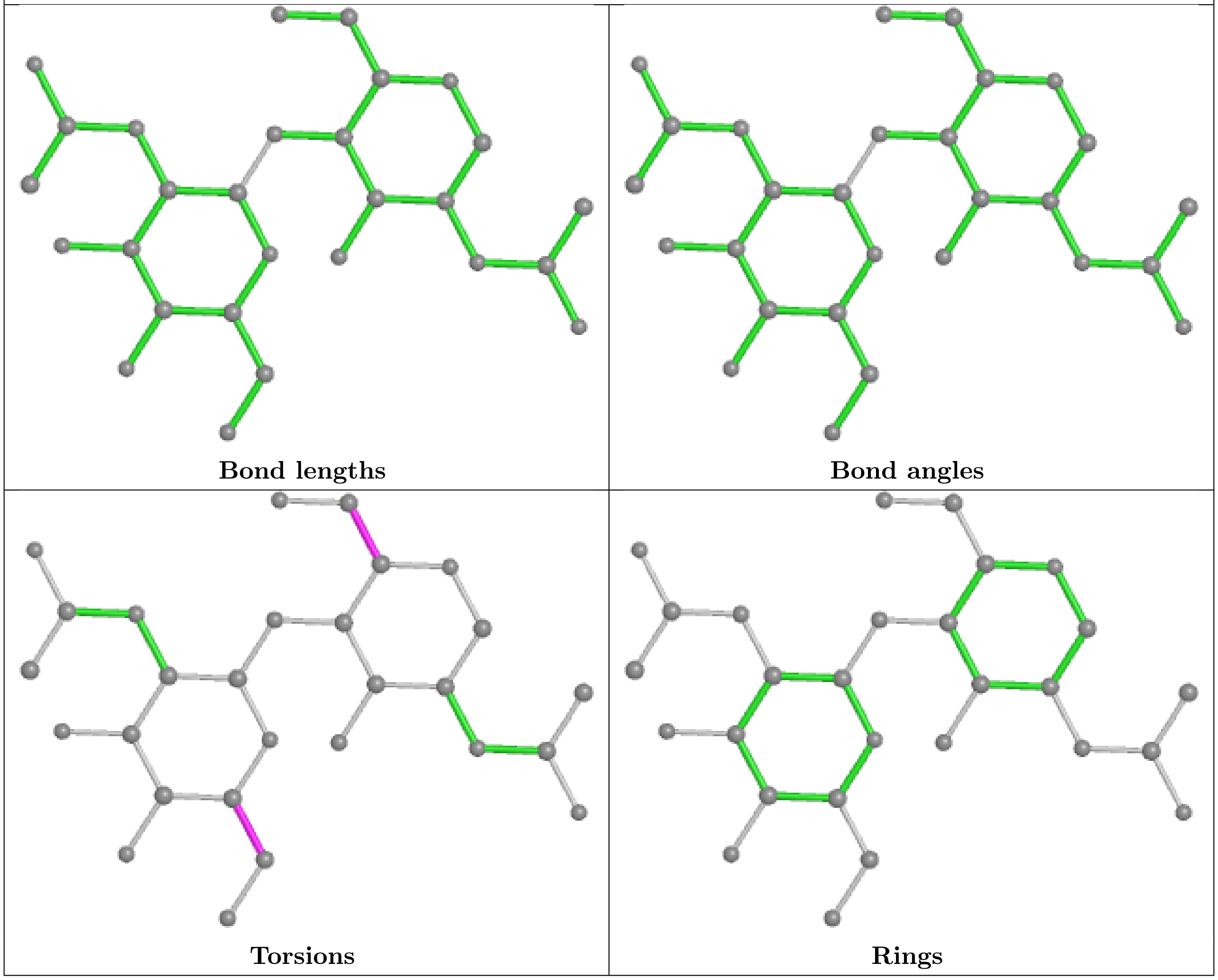


Bond lengths Bond angles



Torsions Rings

Oligosaccharide Chain g



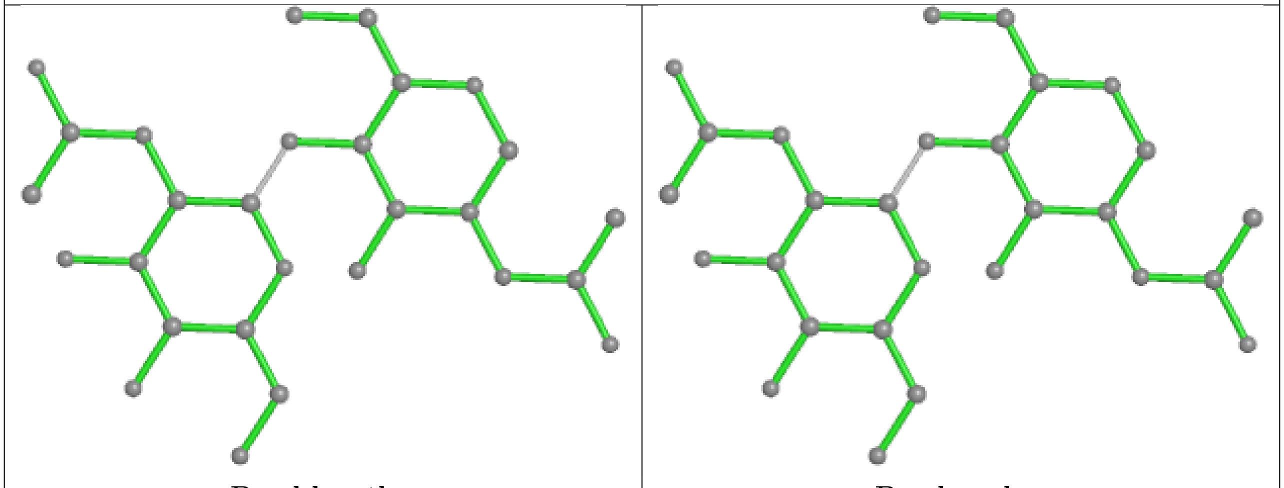
Bond lengths

Bond angles

Torsions

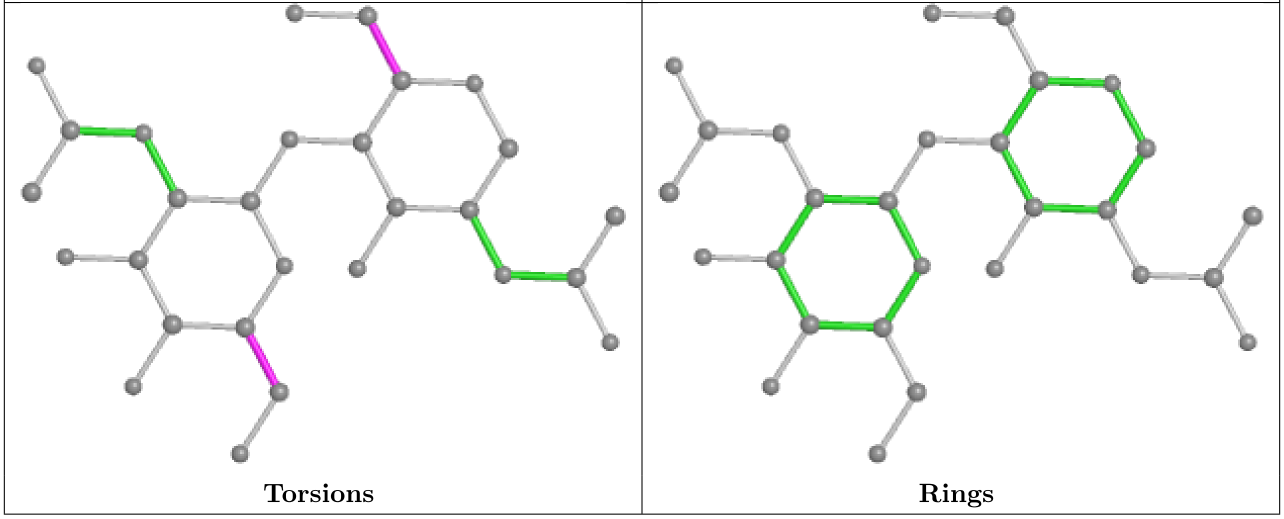
Rings

Oligosaccharide Chain h



Bond lengths

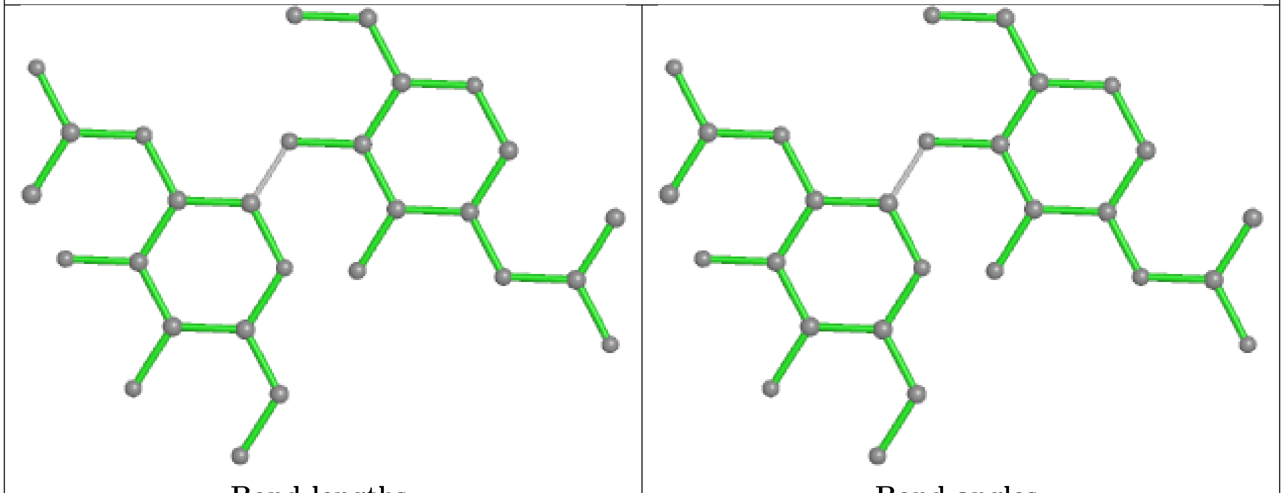
Bond angles



Torsions

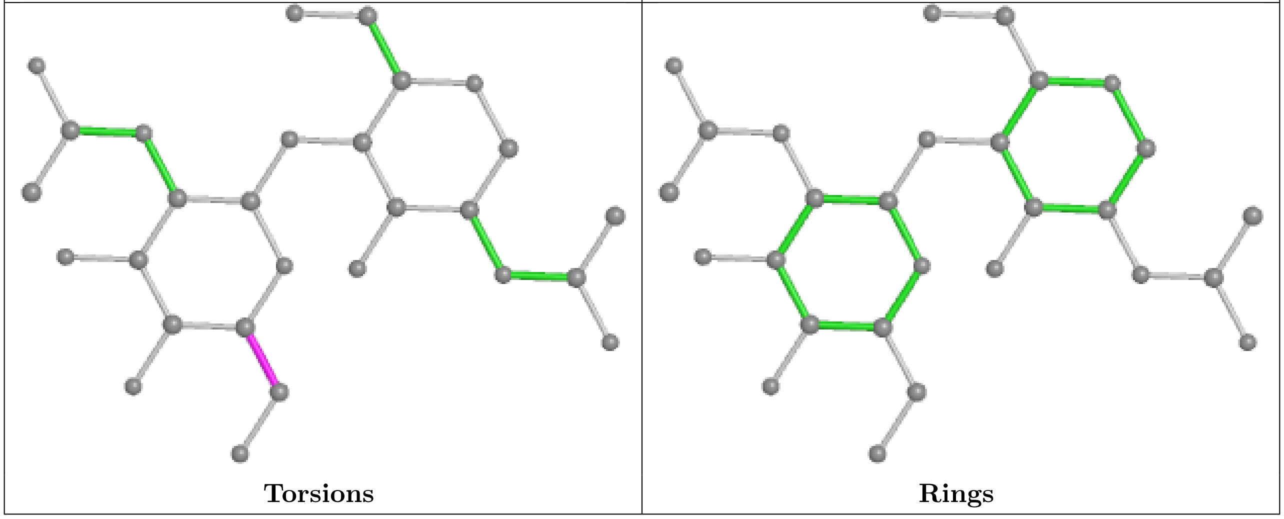
Rings

Oligosaccharide Chain i



Bond lengths

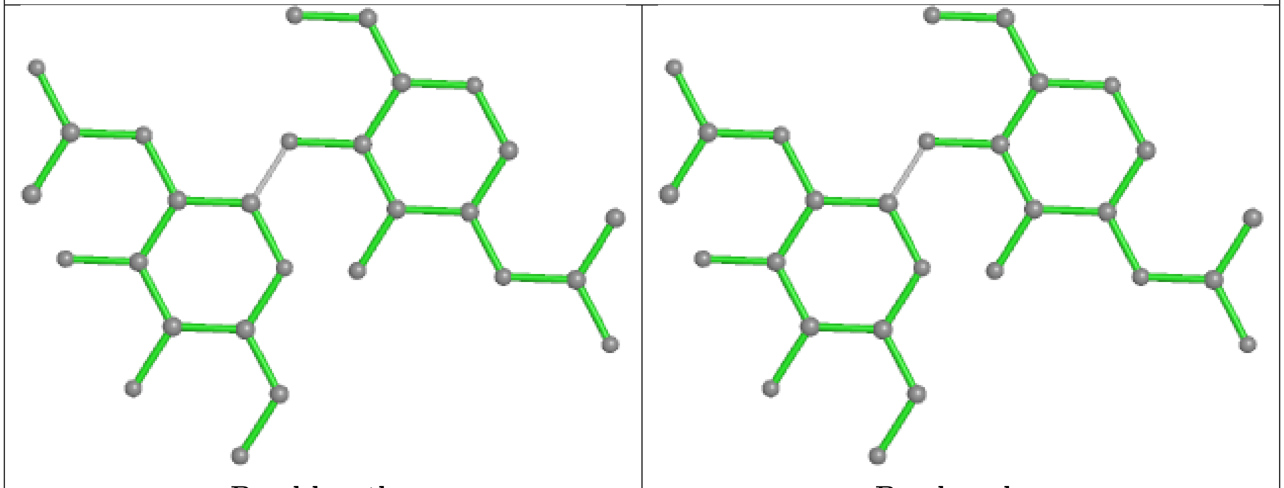
Bond angles



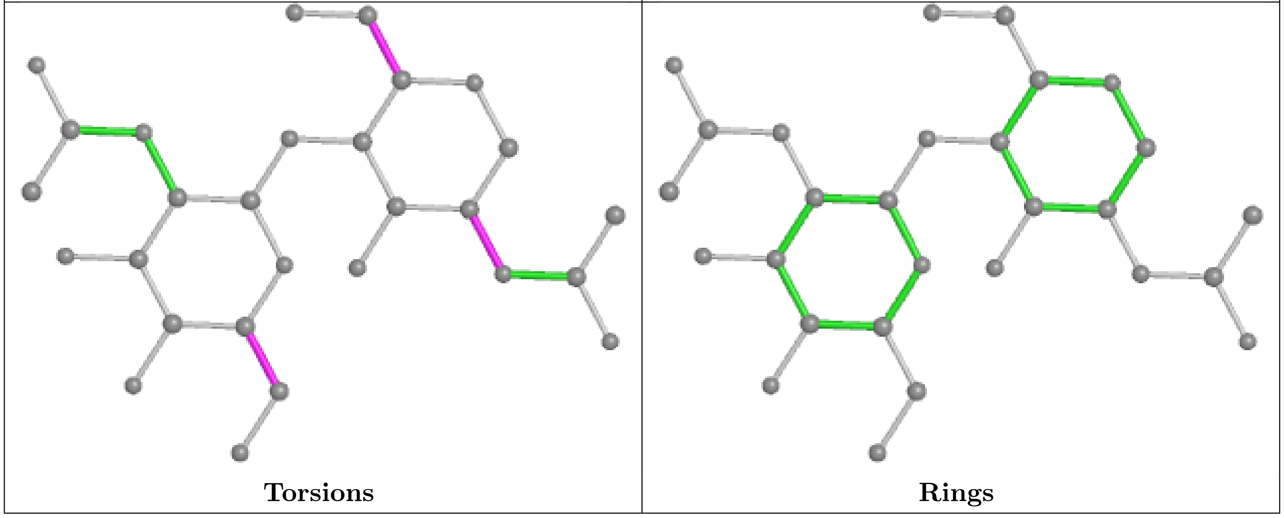
Torsions

Rings

Oligosaccharide Chain j

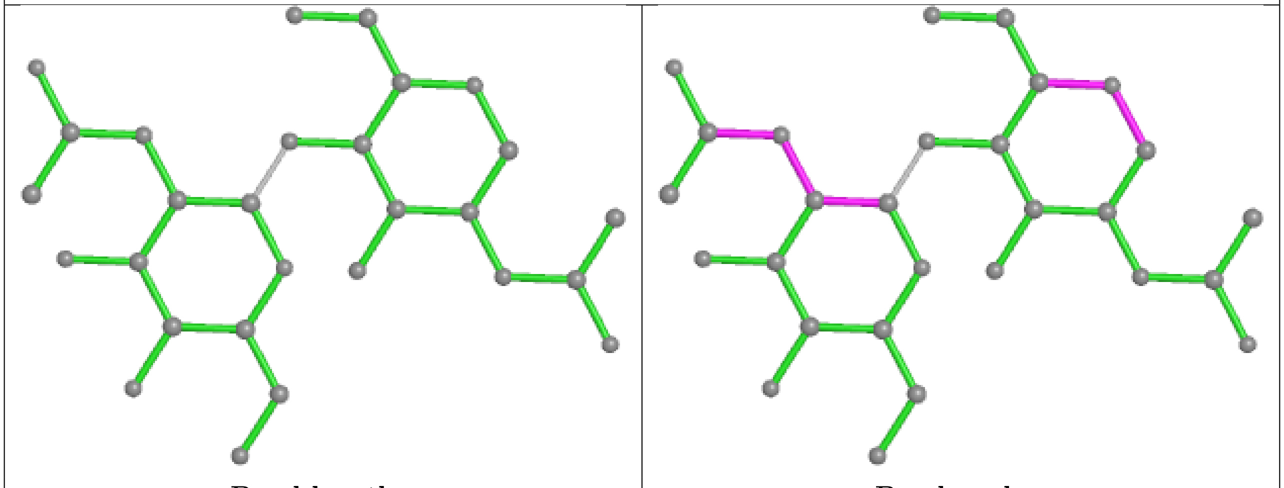


Bond lengths Bond angles



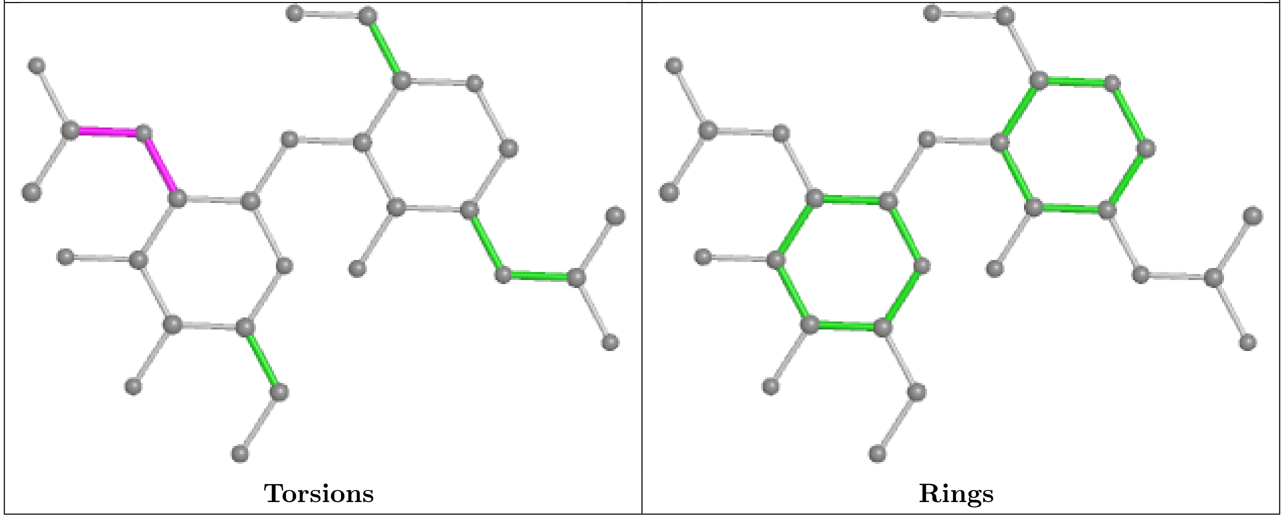
Torsions Rings

Oligosaccharide Chain k



Bond lengths

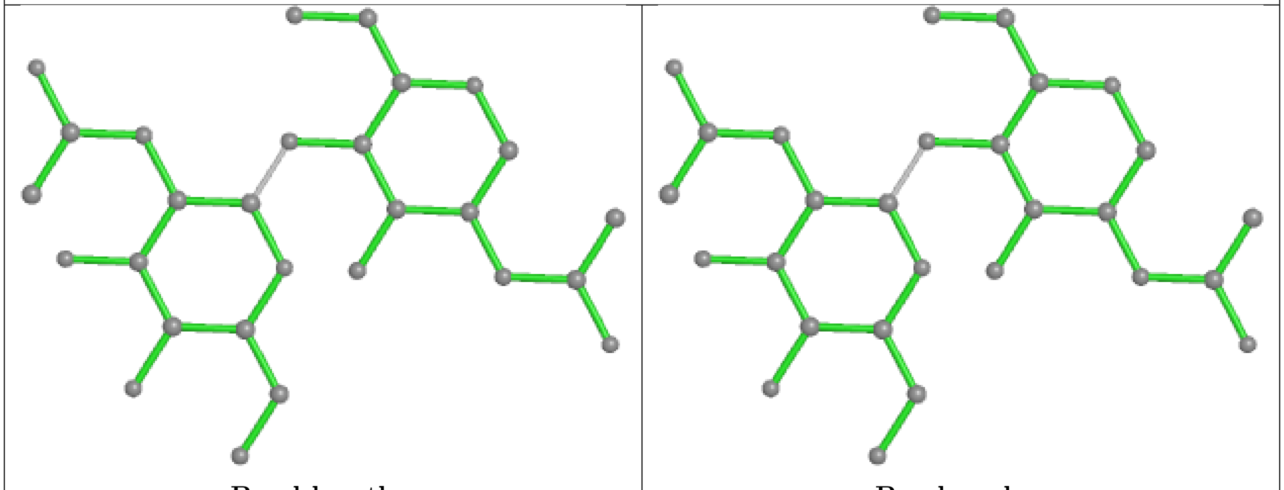
Bond angles



Torsions

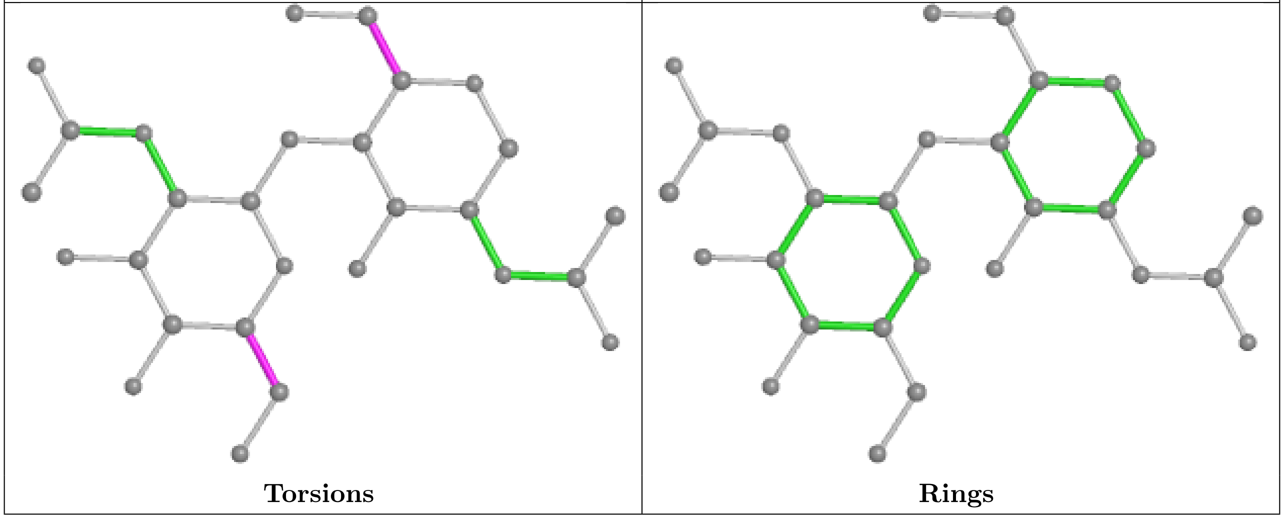
Rings

Oligosaccharide Chain l



Bond lengths

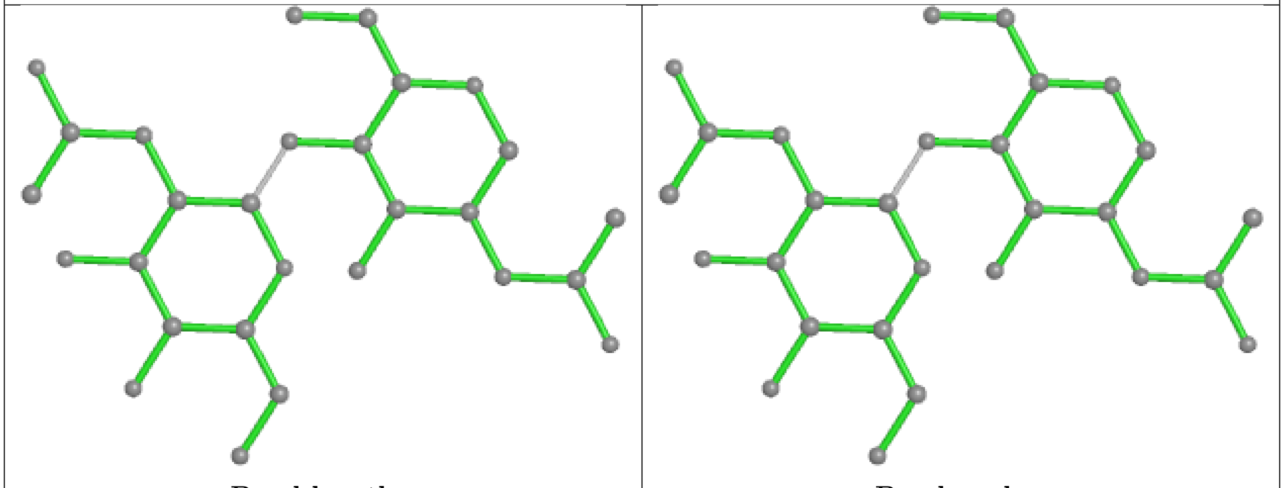
Bond angles



Torsions

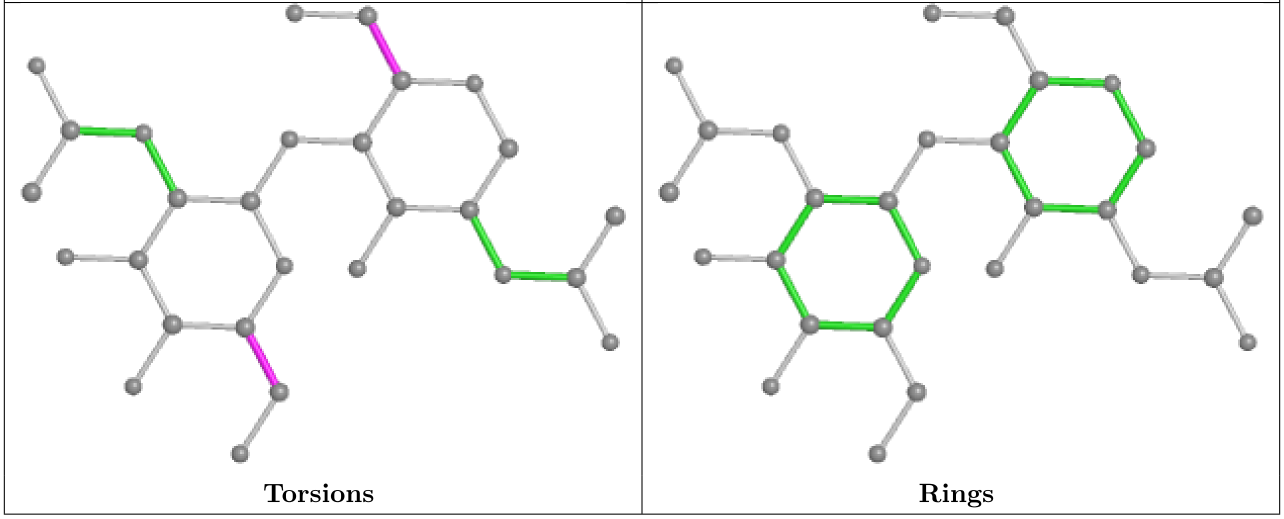
Rings

Oligosaccharide Chain m



Bond lengths

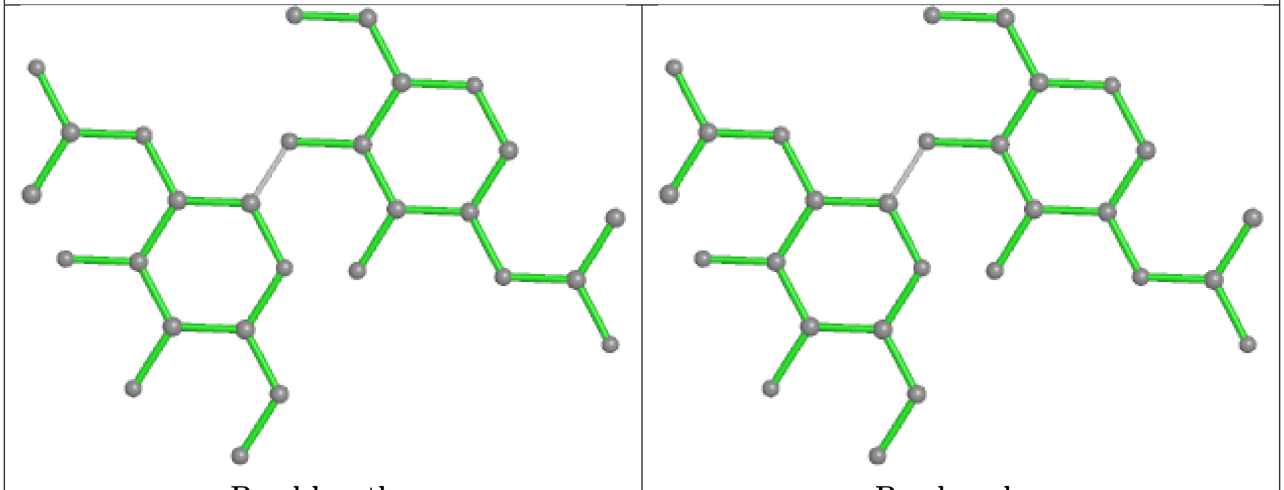
Bond angles



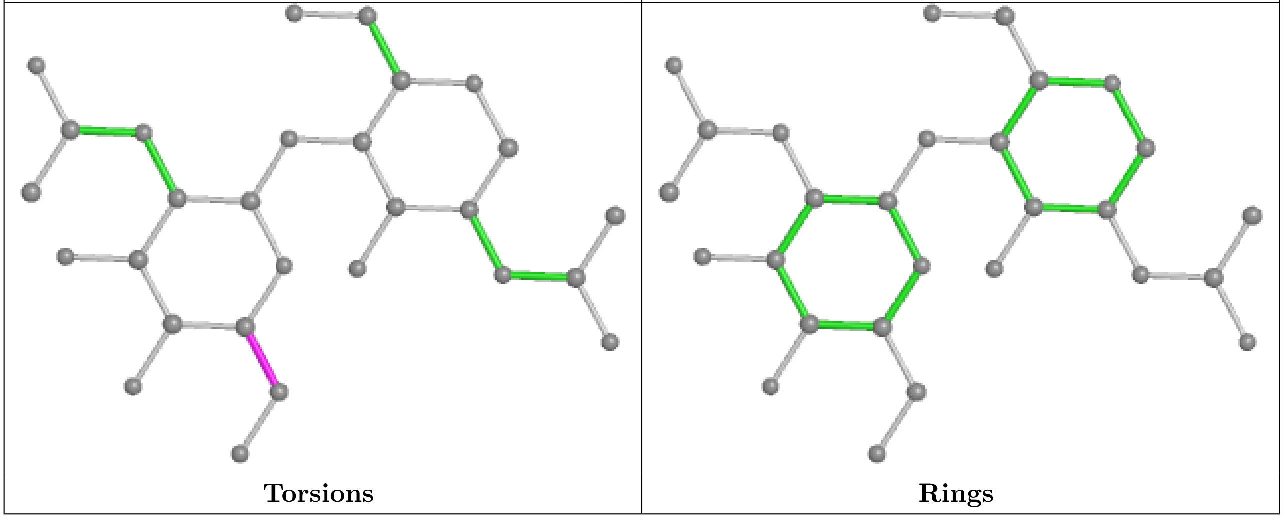
Torsions

Rings

Oligosaccharide Chain n

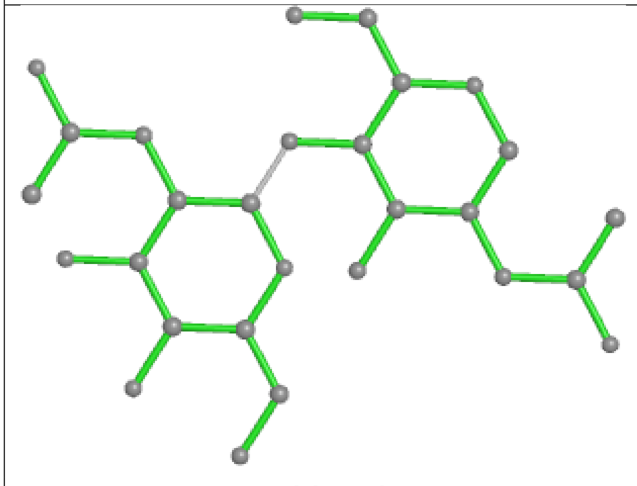


Bond lengths Bond angles

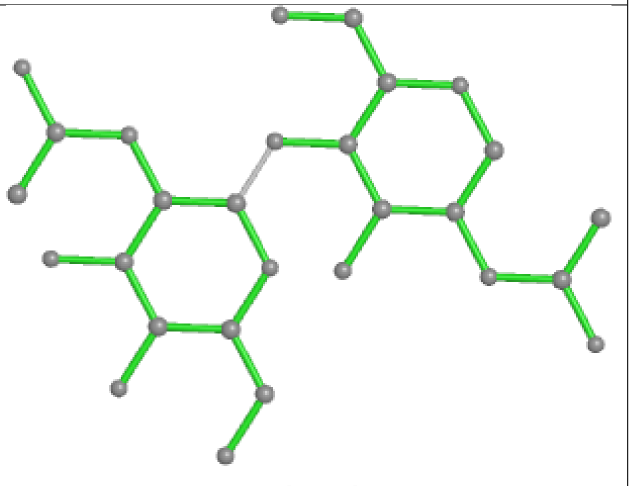


Torsions Rings

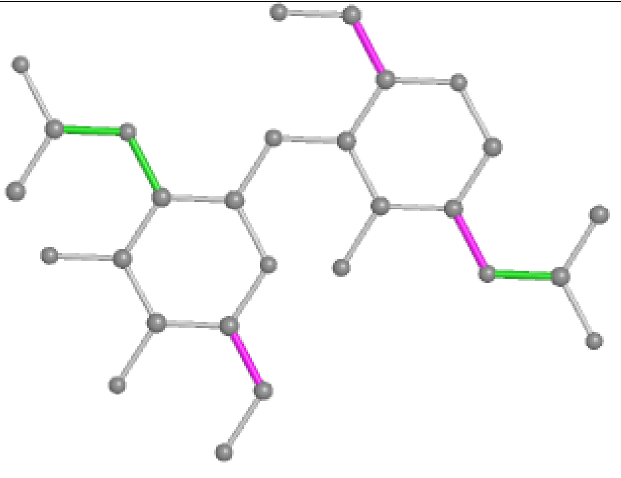
Oligosaccharide Chain o



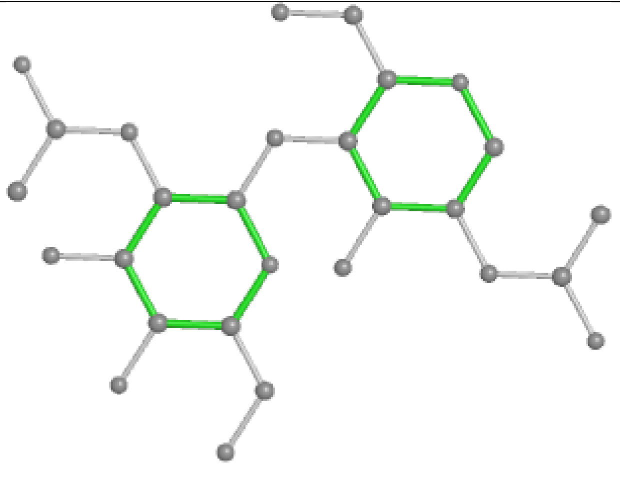
Bond lengths



Bond angles

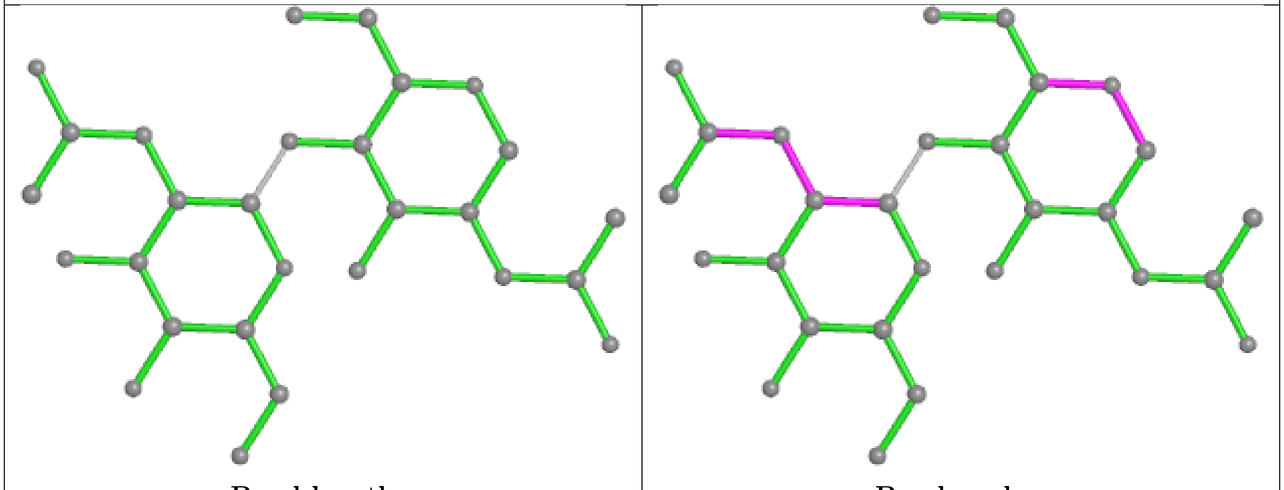


Torsions



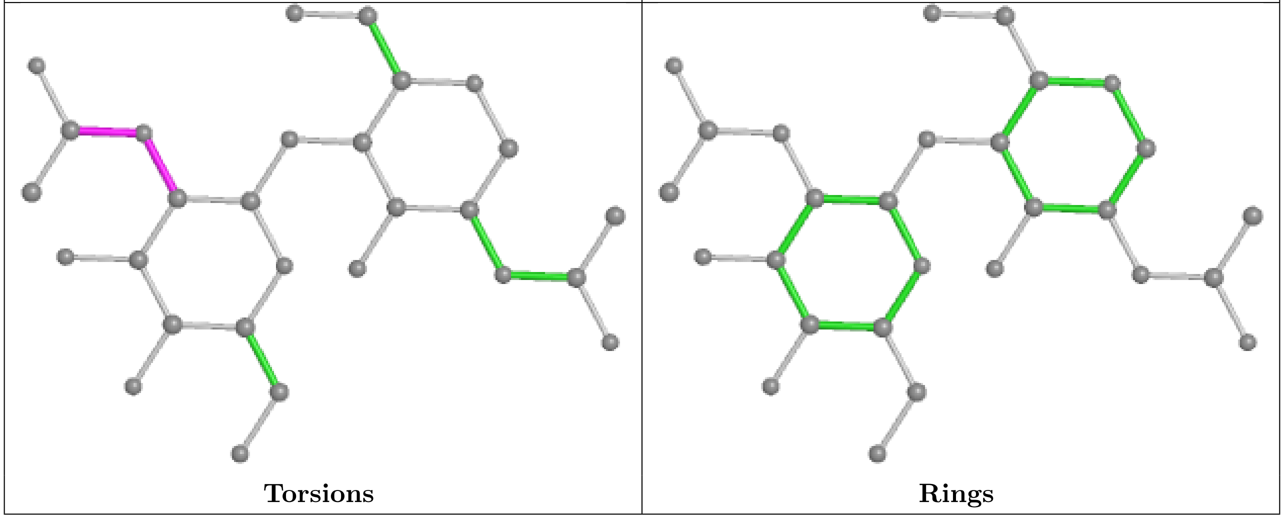
Rings

Oligosaccharide Chain p



Bond lengths

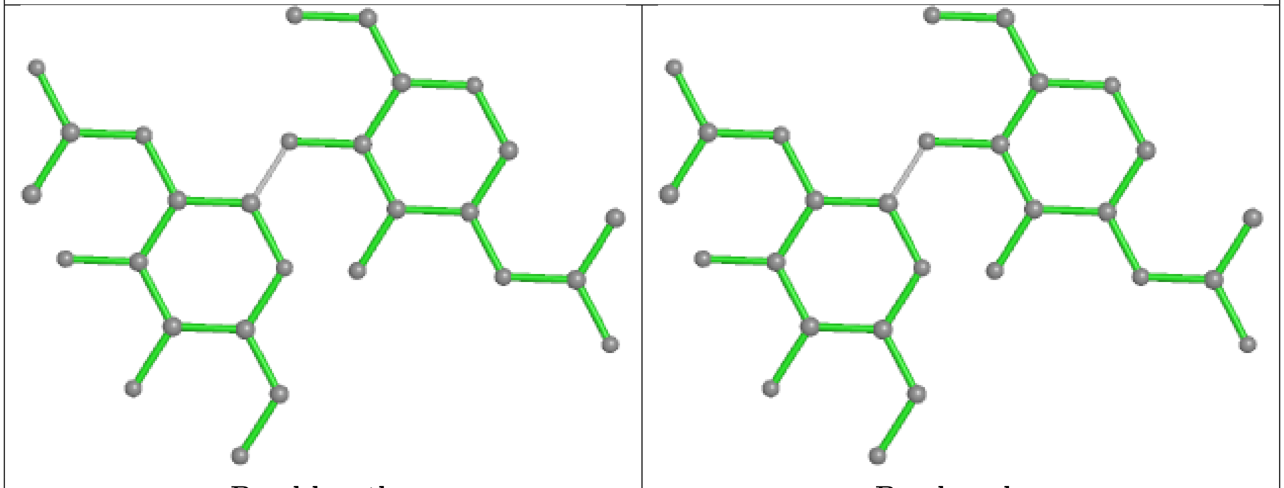
Bond angles



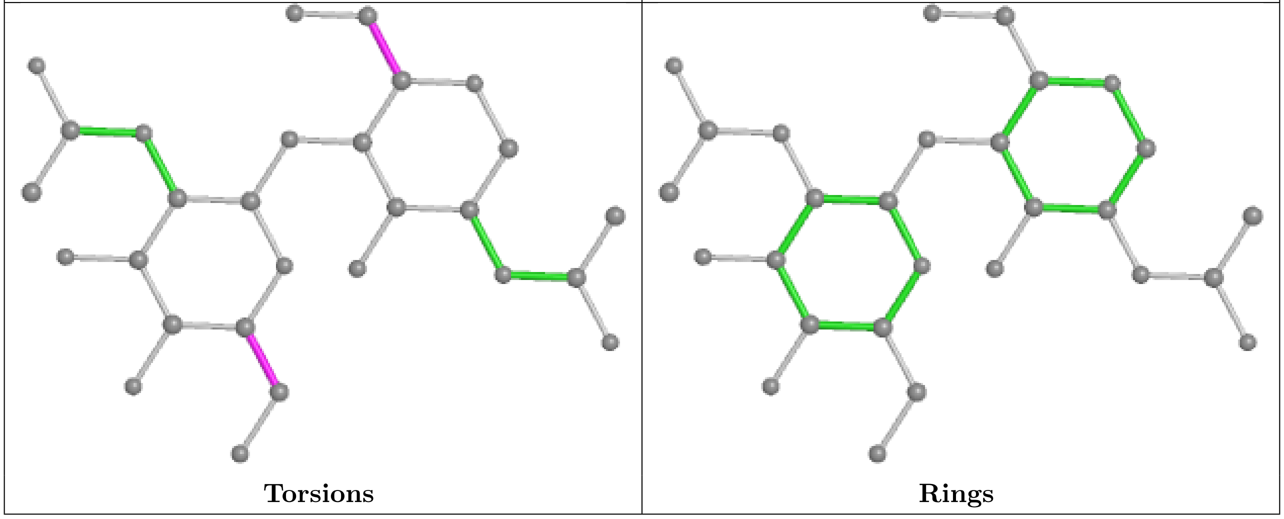
Torsions

Rings

Oligosaccharide Chain q

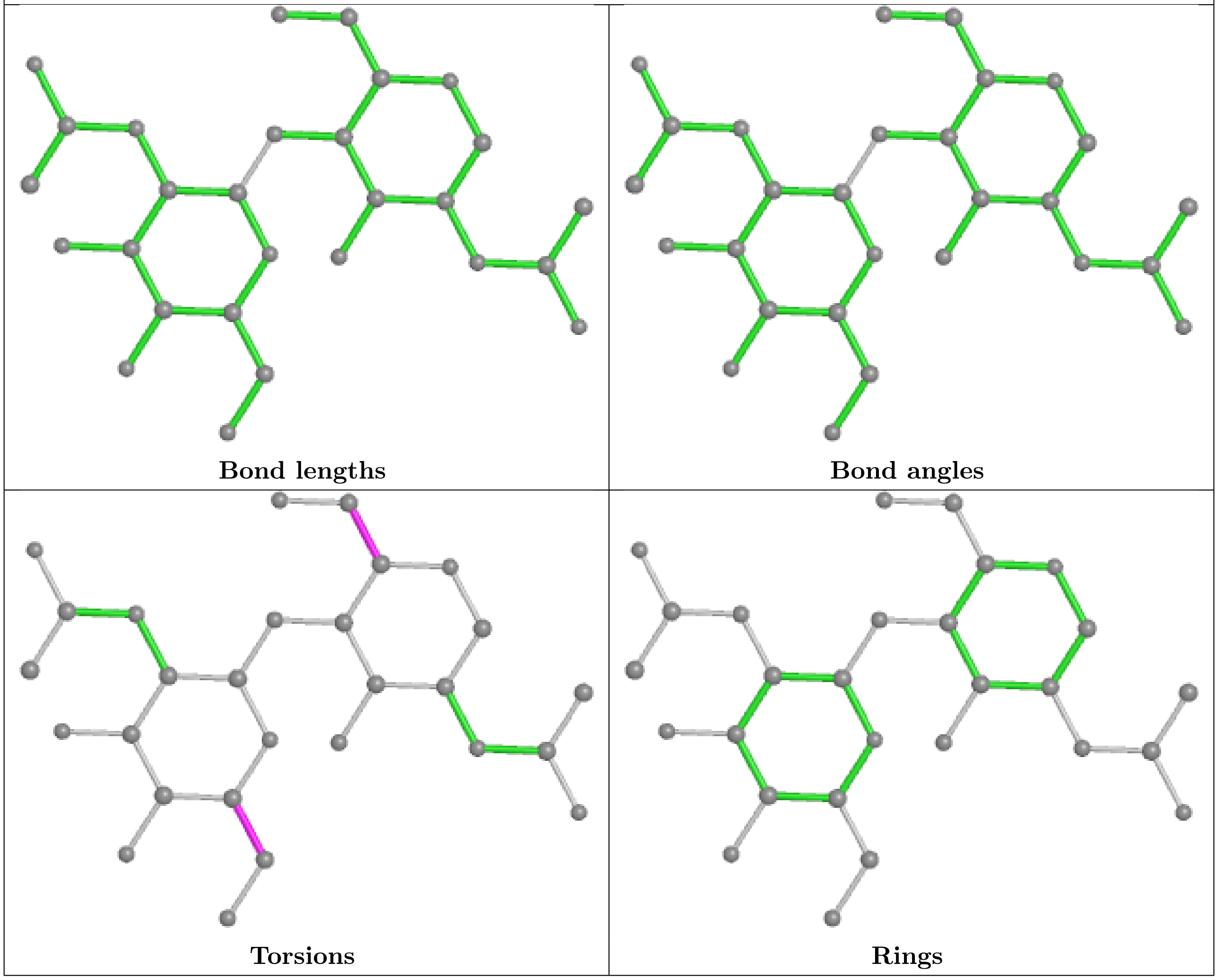


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain r



5.6 Ligand geometry ⓘ

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	E	701	2	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	C	1405	1	14,14,15	0.57	0	17,19,21	1.27	1 (5%)
4	NAG	A	1409	1	14,14,15	0.52	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	A	1404	1	14,14,15	0.48	0	17,19,21	0.53	0
4	NAG	B	1403	1	14,14,15	0.22	0	17,19,21	0.42	0
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	0.31	0	17,19,21	0.39	0
4	NAG	C	1403	1	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	A	1403	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1402	1	14,14,15	0.20	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	D	701	2	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	B	1405	1	14,14,15	0.60	0	17,19,21	1.27	1 (5%)
4	NAG	F	701	2	14,14,15	0.23	0	17,19,21	0.47	0
4	NAG	B	1404	1	14,14,15	0.47	0	17,19,21	0.54	0
4	NAG	C	1404	1	14,14,15	0.47	0	17,19,21	0.54	0
4	NAG	A	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	A	1401	1	14,14,15	0.30	0	17,19,21	0.33	0
4	NAG	B	1401	1	14,14,15	0.29	0	17,19,21	0.34	0
4	NAG	C	1406	1	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	B	1406	1	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.63	0
4	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	A	1408	1	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	C	1407	1	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	A	1407	1	14,14,15	0.26	0	17,19,21	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	701	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	D	701	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	F	701	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1405	NAG	C2-N2-C7	4.37	129.13	122.90
4	A	1405	NAG	C2-N2-C7	4.36	129.11	122.90
4	C	1405	NAG	C2-N2-C7	4.36	129.10	122.90

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	701	NAG	O5-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	E	701	NAG	O5-C5-C6-O6
4	A	1406	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1402	NAG	C4-C5-C6-O6
4	B	1402	NAG	C4-C5-C6-O6
4	C	1402	NAG	C4-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	B	1402	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	C	1402	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	F	701	NAG	C4-C5-C6-O6
4	D	701	NAG	C4-C5-C6-O6
4	E	701	NAG	C4-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	A	1405	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	A	1409	NAG	C4-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	A	1405	NAG	C4-C5-C6-O6
4	B	1405	NAG	C4-C5-C6-O6
4	C	1405	NAG	C4-C5-C6-O6
4	A	1405	NAG	C8-C7-N2-C2
4	A	1405	NAG	O7-C7-N2-C2
4	B	1405	NAG	C8-C7-N2-C2
4	B	1405	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	A	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
4	B	1406	NAG	C4-C5-C6-O6
4	C	1406	NAG	C4-C5-C6-O6
4	A	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	A	1403	NAG	O5-C5-C6-O6
4	B	1403	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

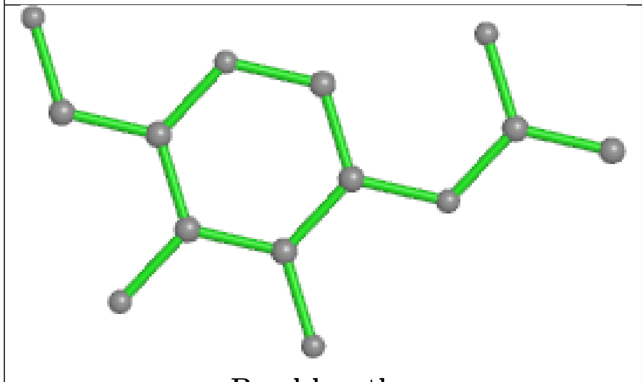
Mol	Chain	Res	Type	Atoms
4	C	1403	NAG	O5-C5-C6-O6
4	A	1403	NAG	C4-C5-C6-O6
4	B	1403	NAG	C4-C5-C6-O6
4	C	1403	NAG	C4-C5-C6-O6
4	A	1408	NAG	C4-C5-C6-O6
4	B	1408	NAG	C4-C5-C6-O6
4	C	1408	NAG	C4-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
4	A	1401	NAG	C4-C5-C6-O6
4	B	1401	NAG	C4-C5-C6-O6
4	A	1407	NAG	C1-C2-N2-C7
4	C	1407	NAG	C1-C2-N2-C7
4	B	1407	NAG	C1-C2-N2-C7
4	A	1405	NAG	C3-C2-N2-C7
4	B	1405	NAG	C3-C2-N2-C7
4	C	1405	NAG	C3-C2-N2-C7

There are no ring outliers.

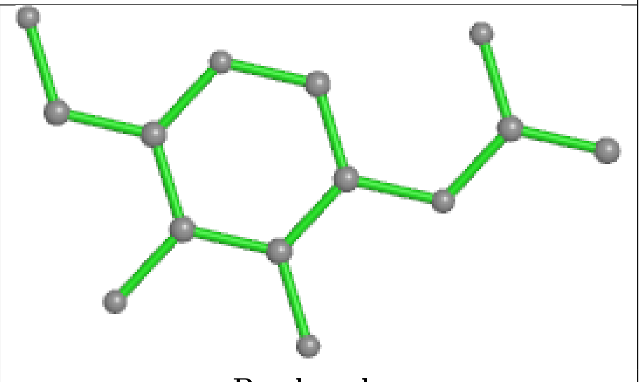
No monomer is involved in short contacts.

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

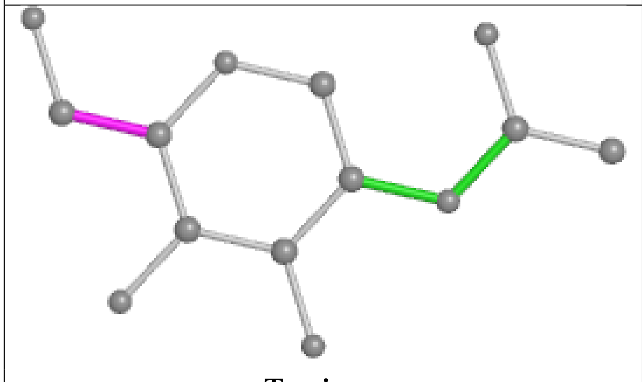
Ligand NAG E 701



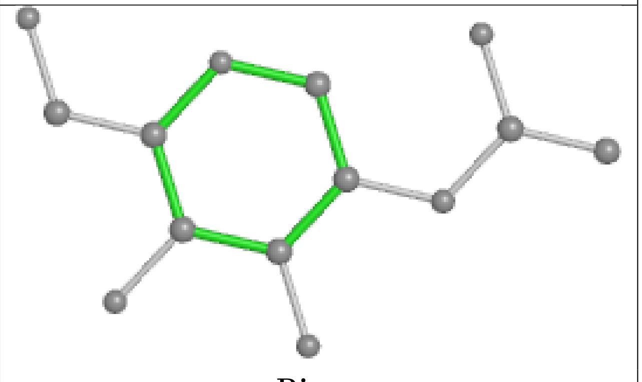
Bond lengths



Bond angles

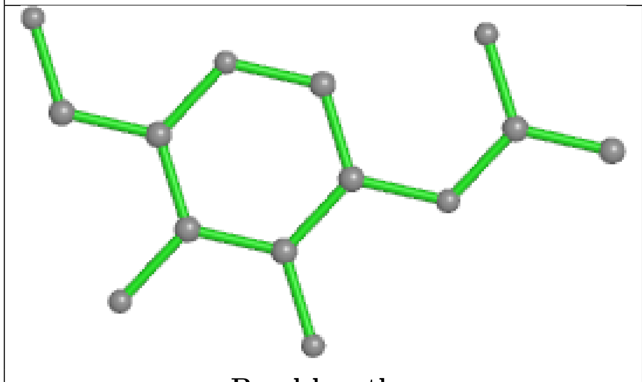


Torsions

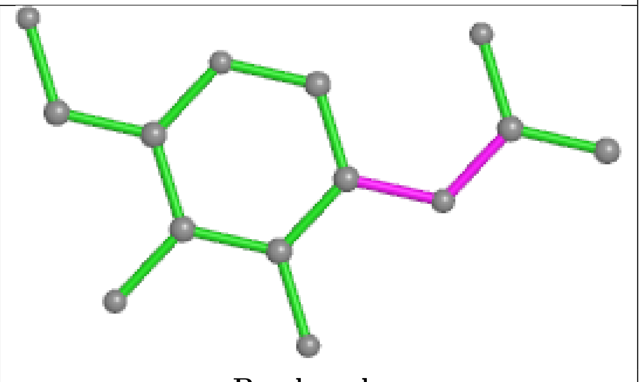


Rings

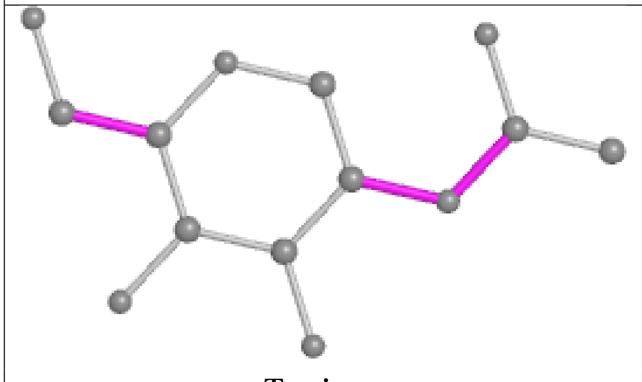
Ligand NAG C 1405



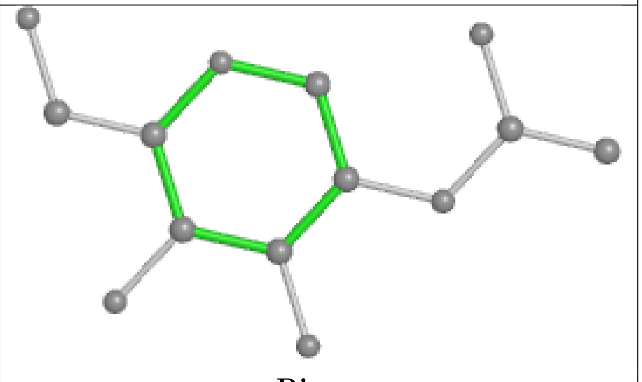
Bond lengths



Bond angles

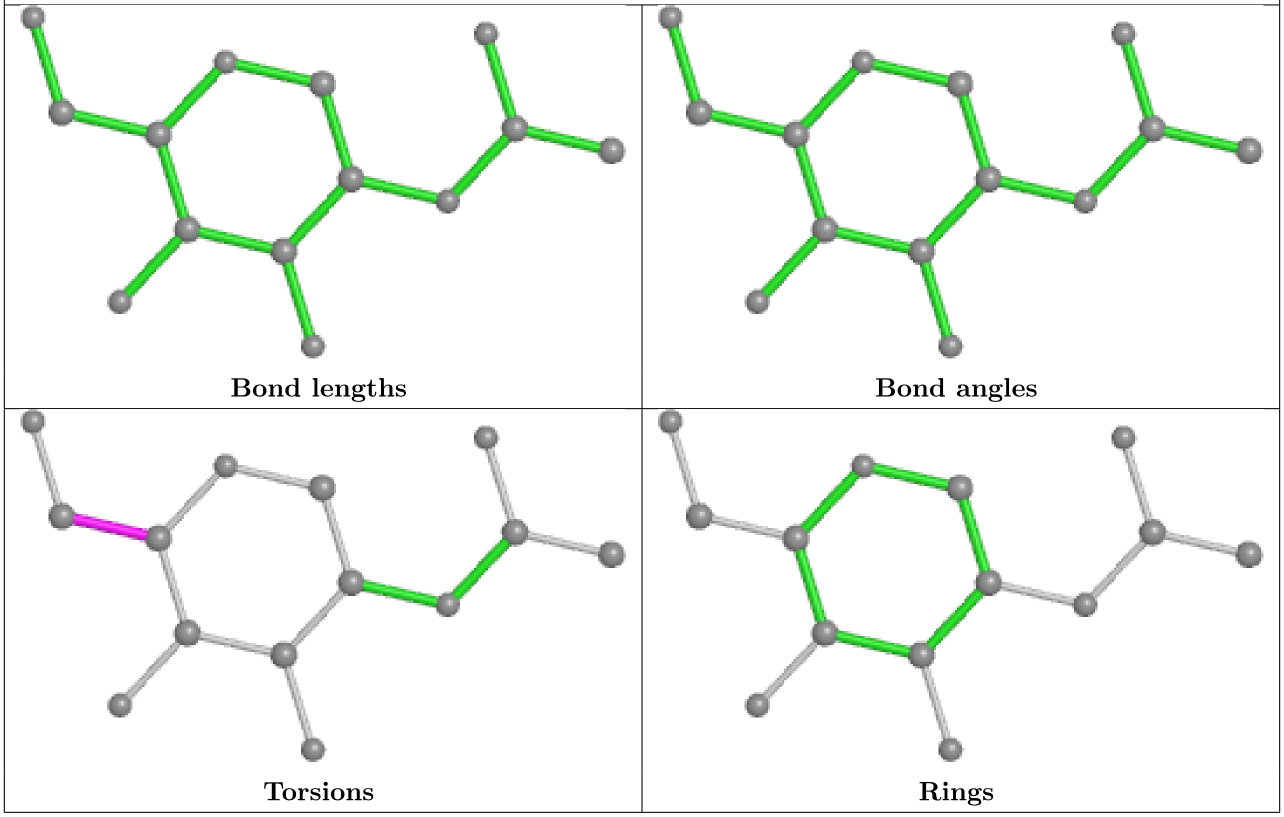


Torsions



Rings

Ligand NAG A 1409



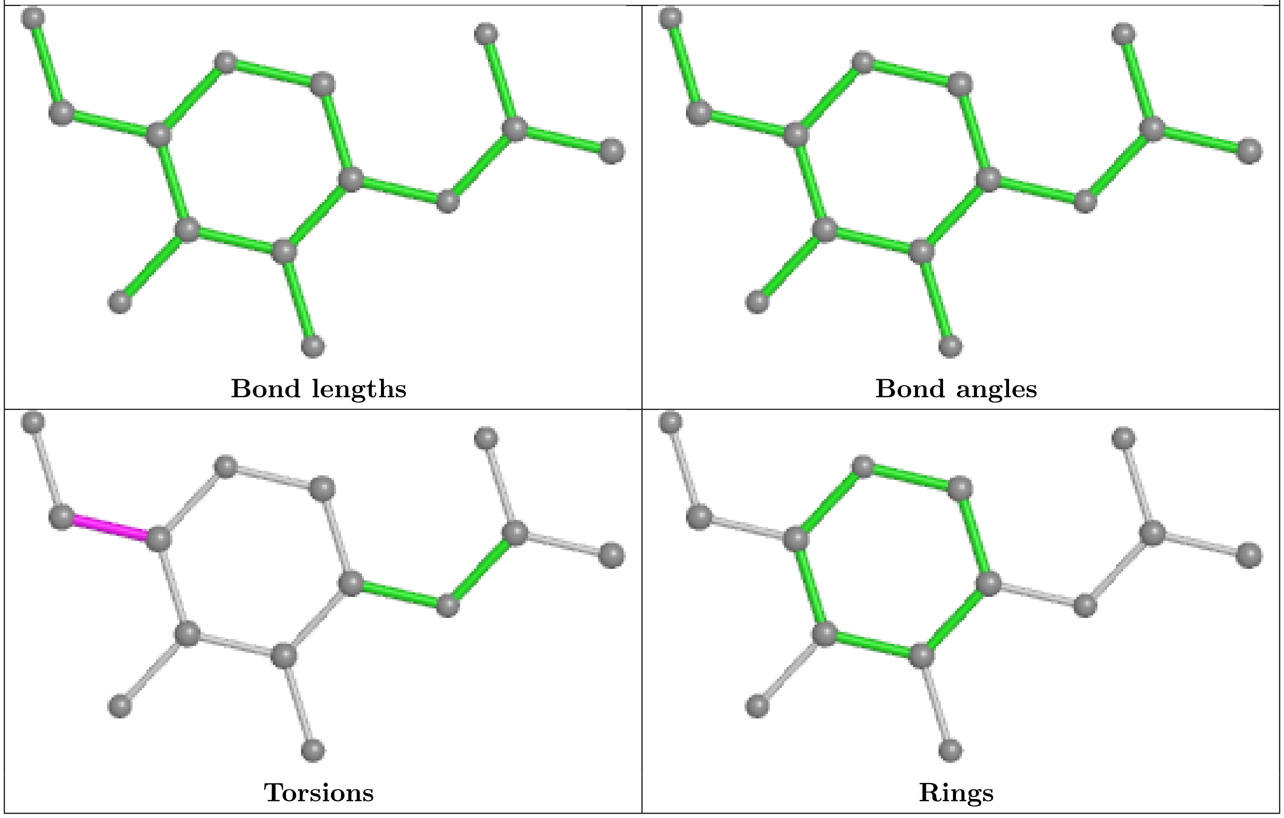
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1404



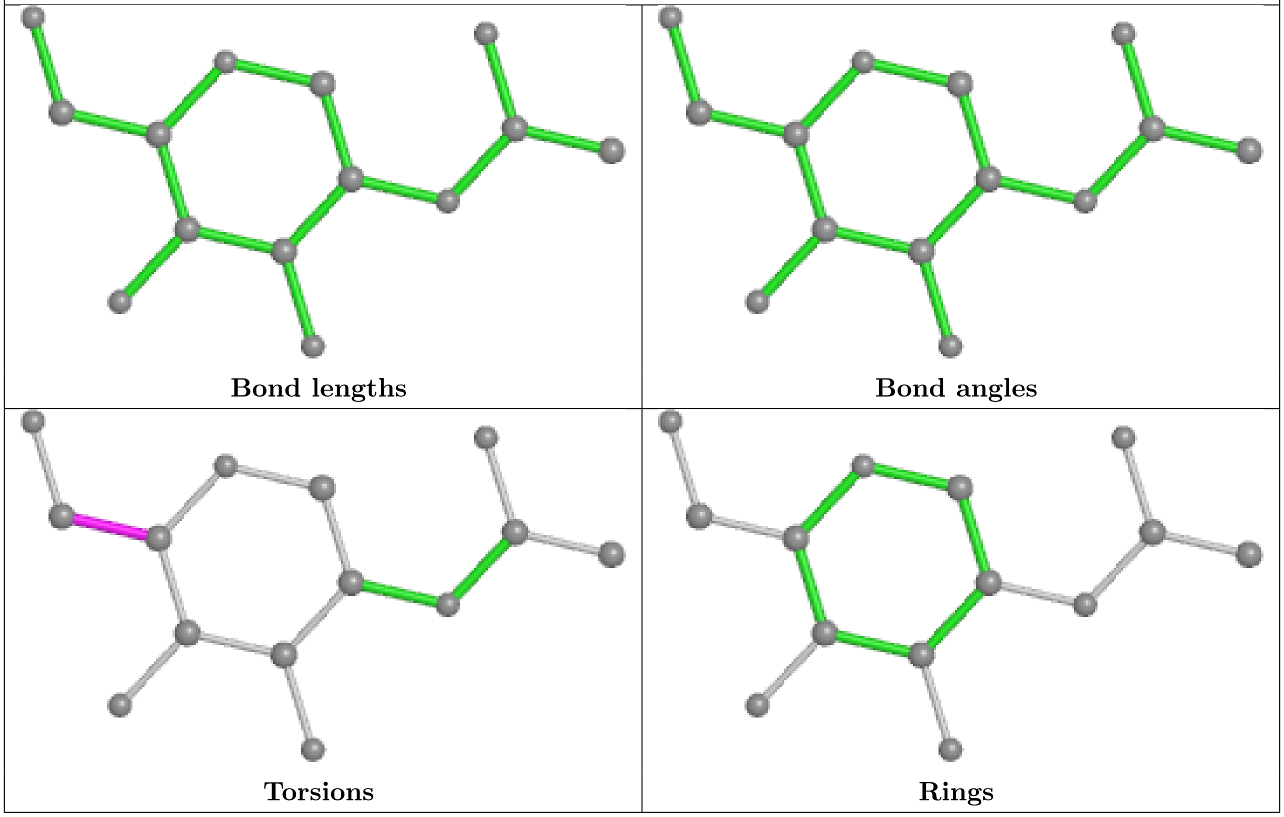
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1403



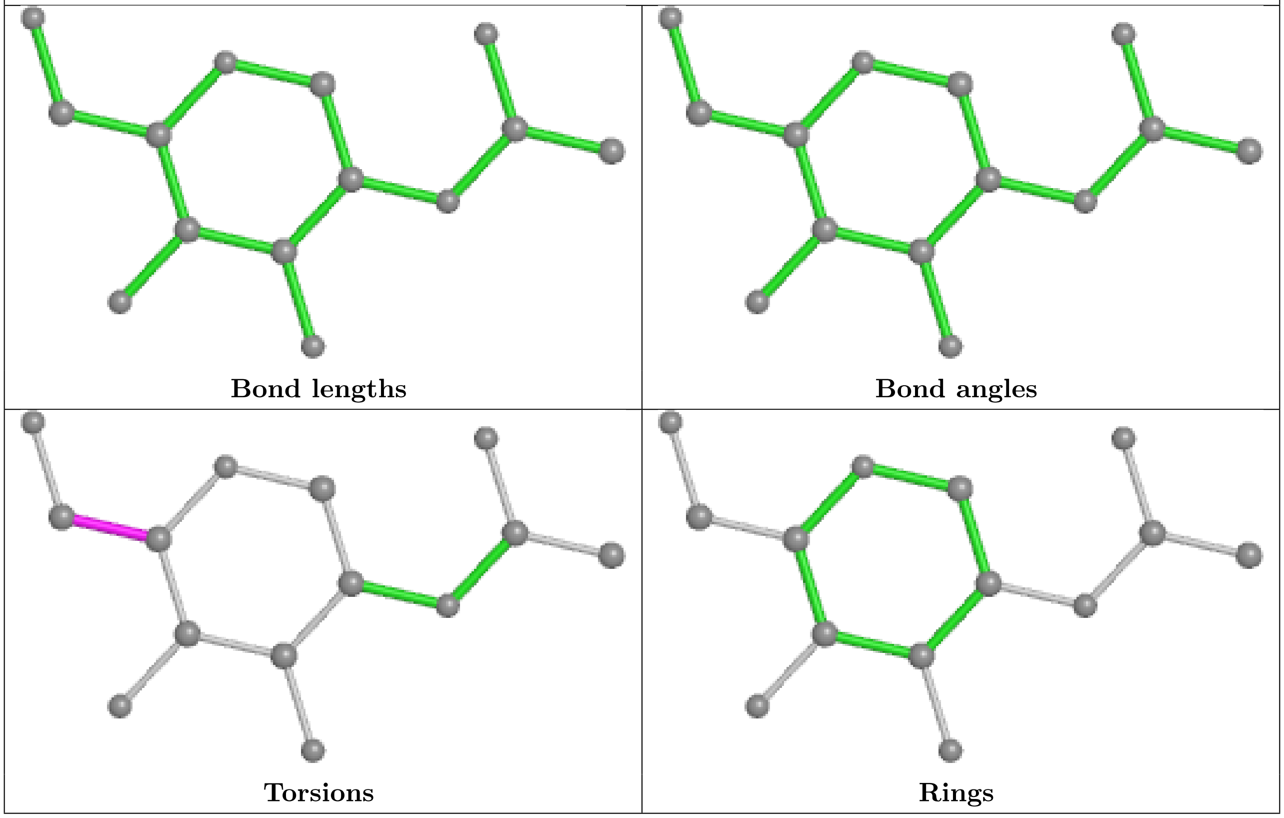
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1402



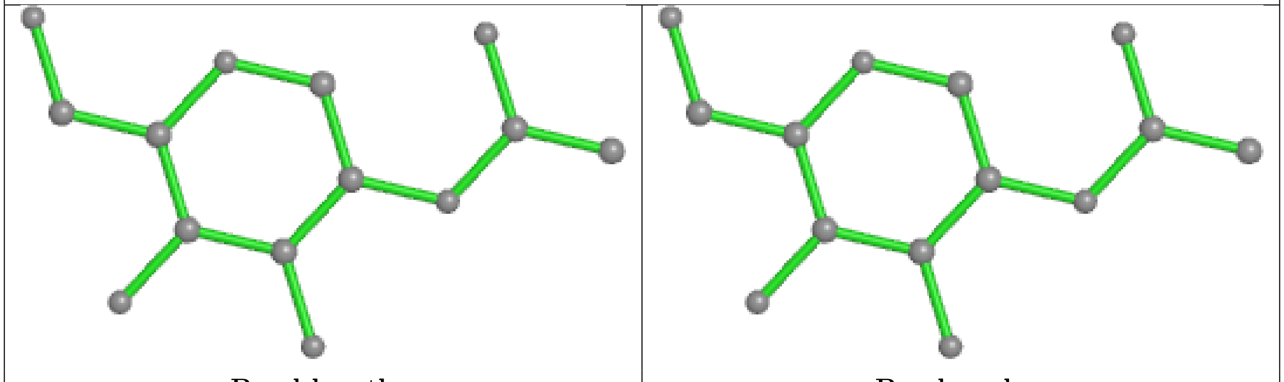
Bond lengths

Bond angles

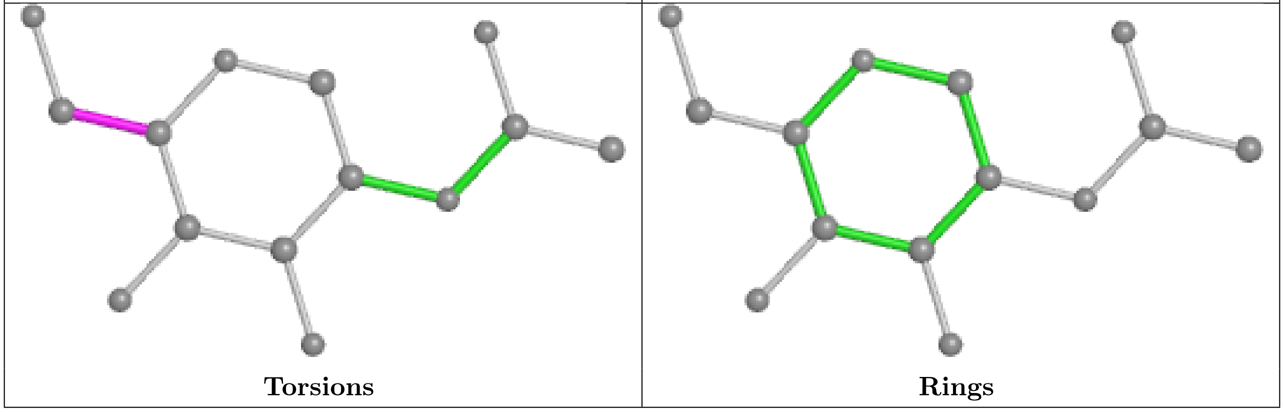
Torsions

Rings

Ligand NAG C 1408

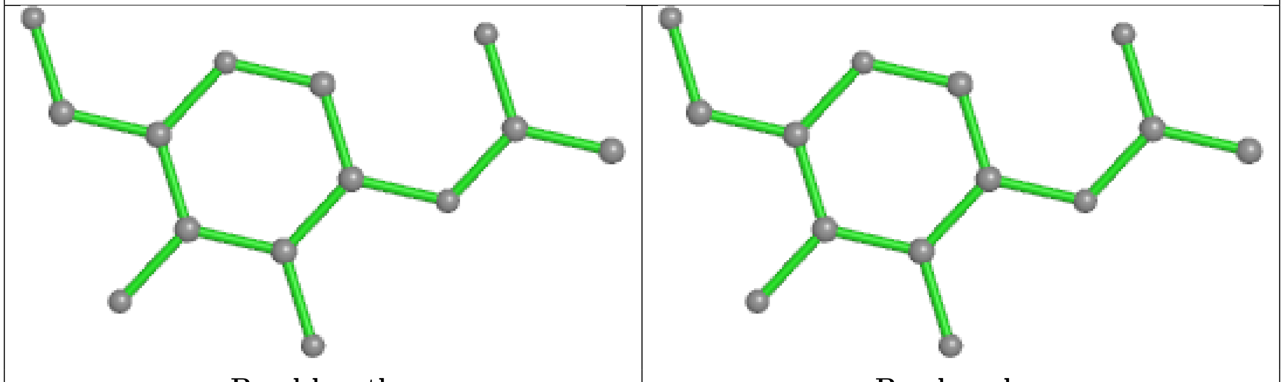


Bond lengths Bond angles

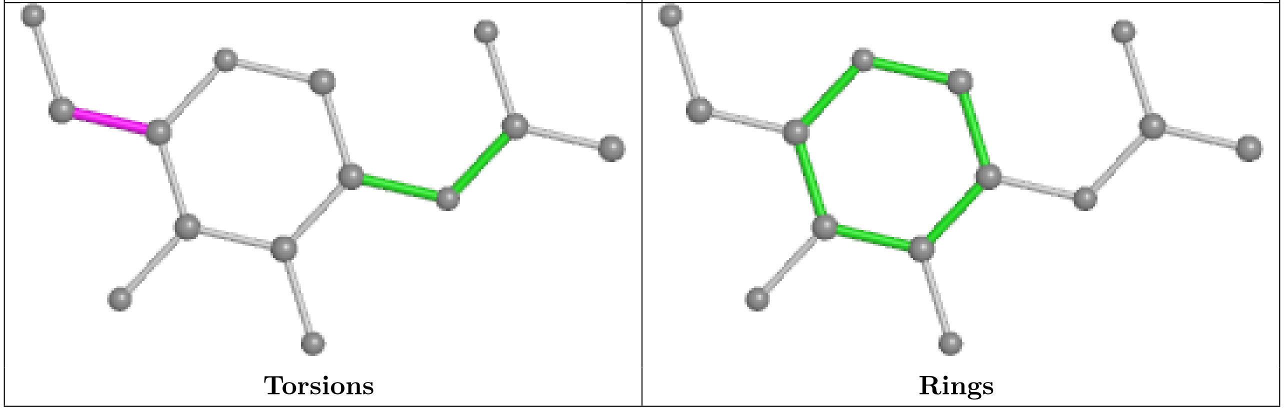


Torsions Rings

Ligand NAG C 1403

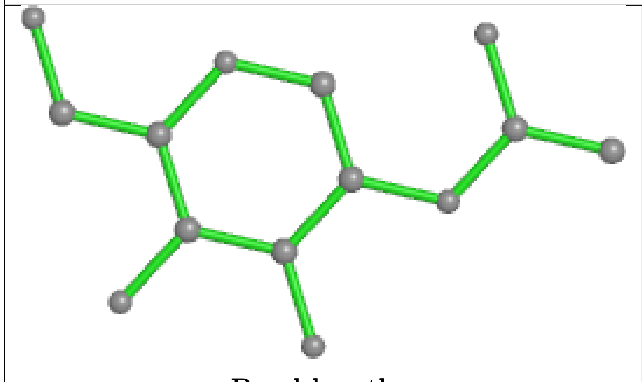


Bond lengths Bond angles

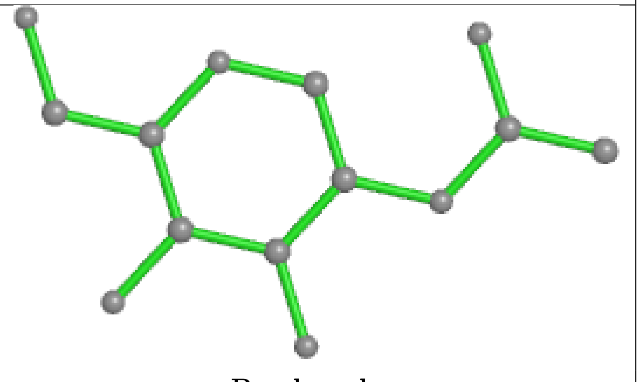


Torsions Rings

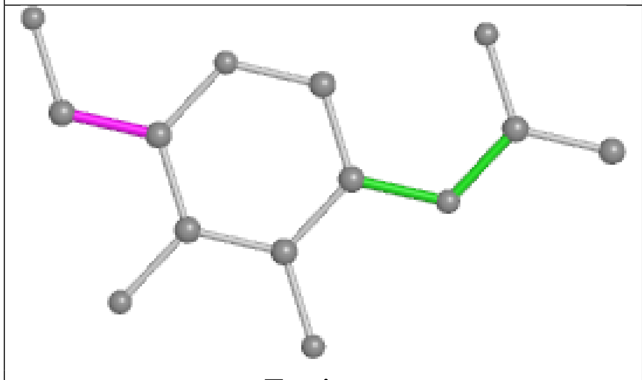
Ligand NAG A 1403



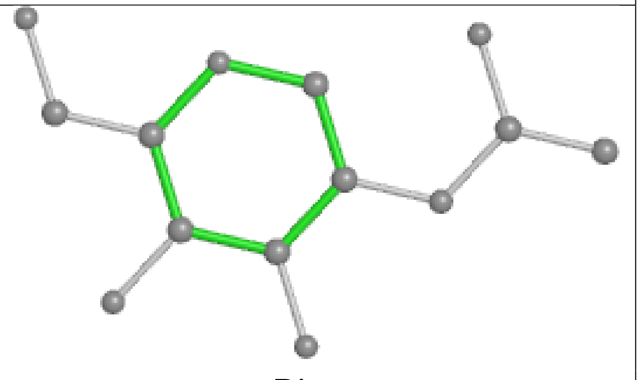
Bond lengths



Bond angles

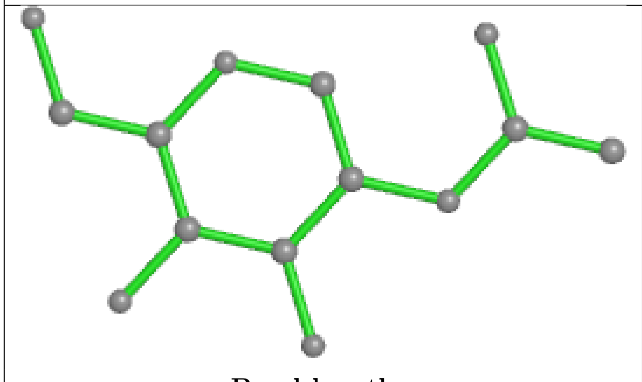


Torsions

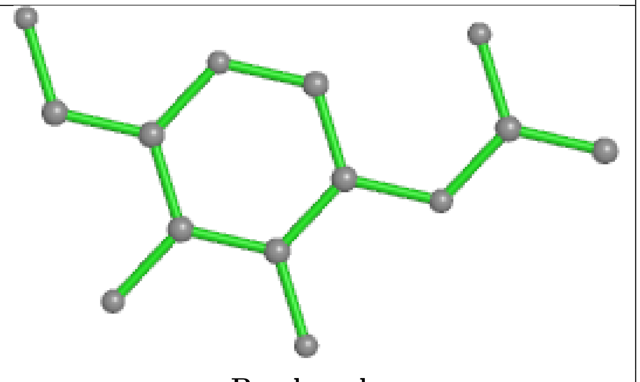


Rings

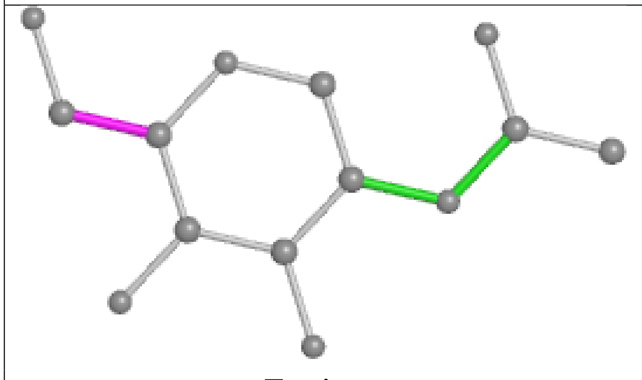
Ligand NAG A 1402



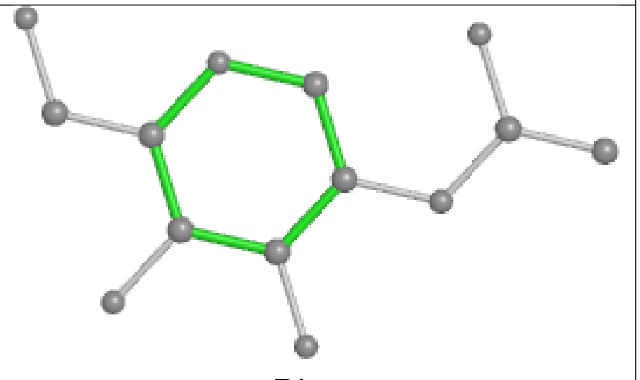
Bond lengths



Bond angles

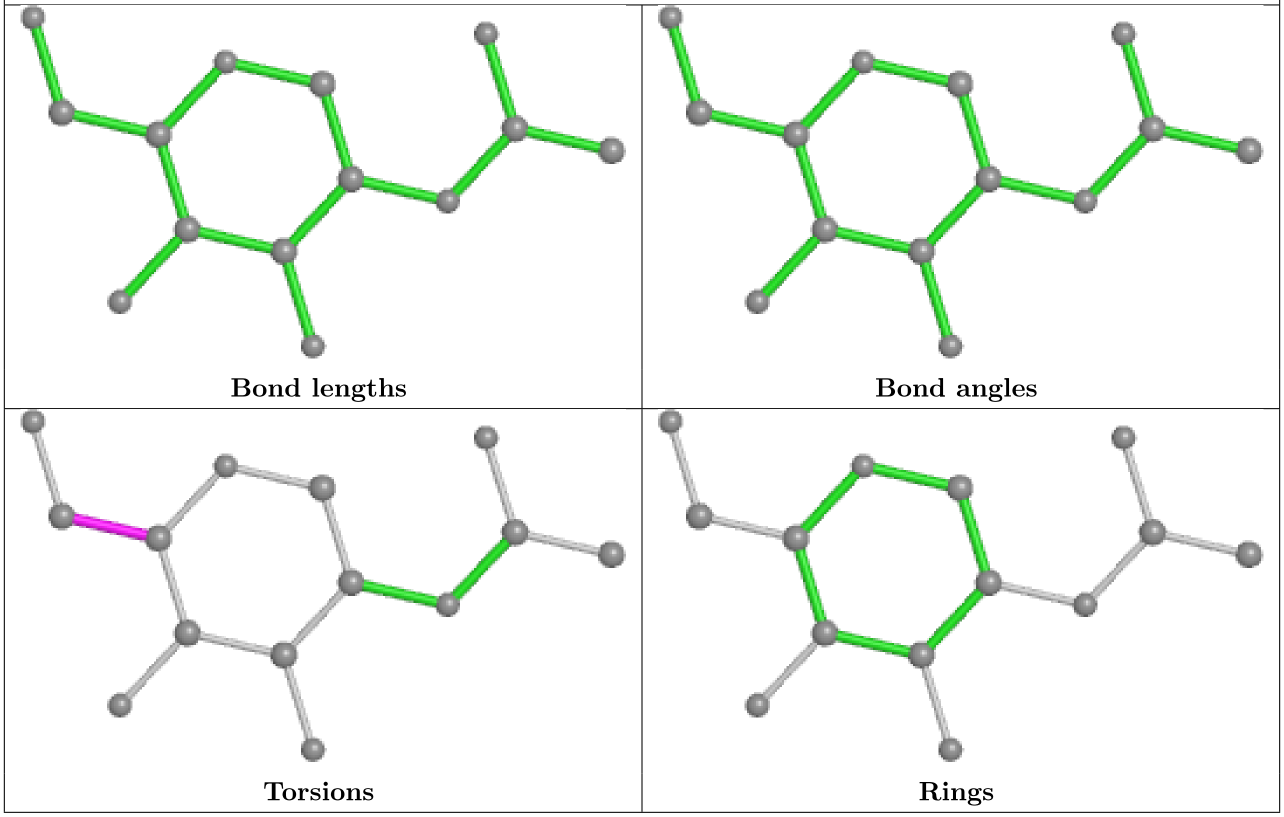


Torsions



Rings

Ligand NAG C 1401



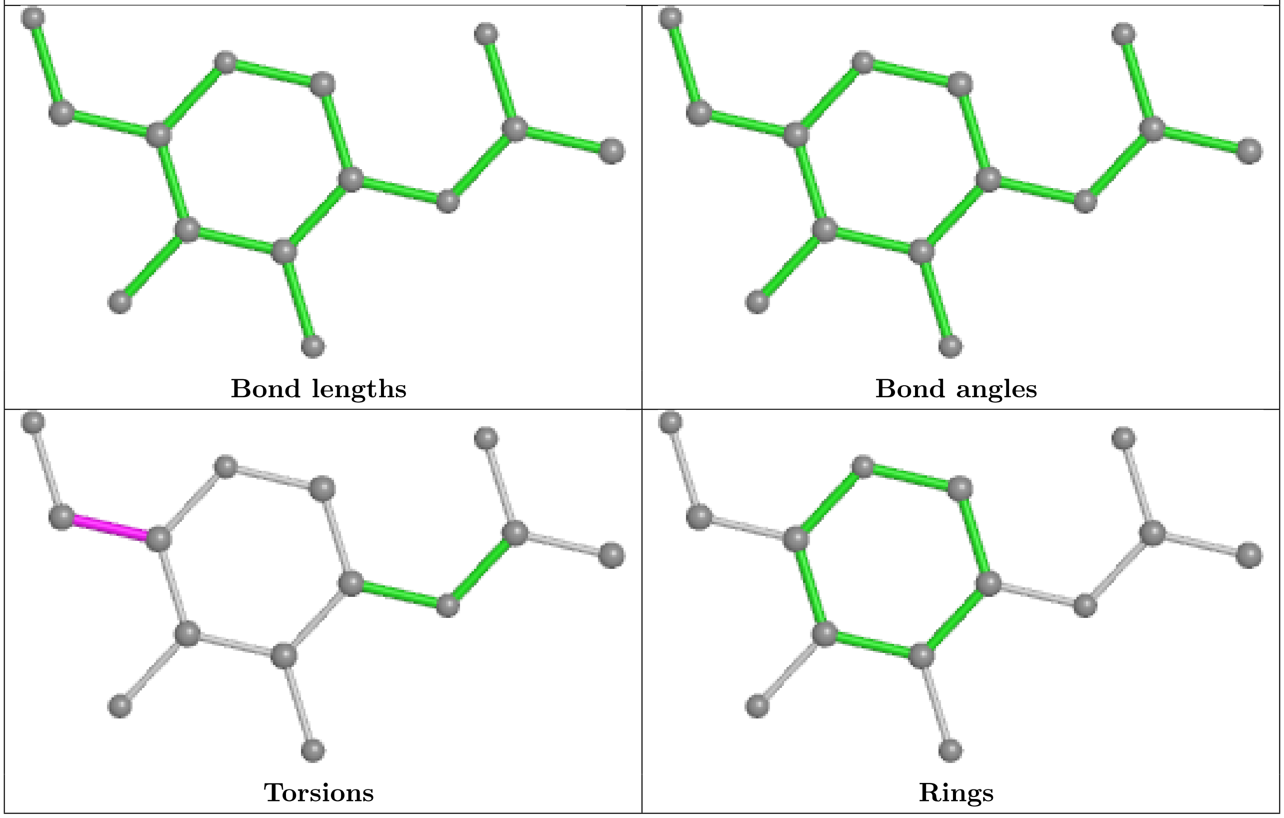
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG D 701



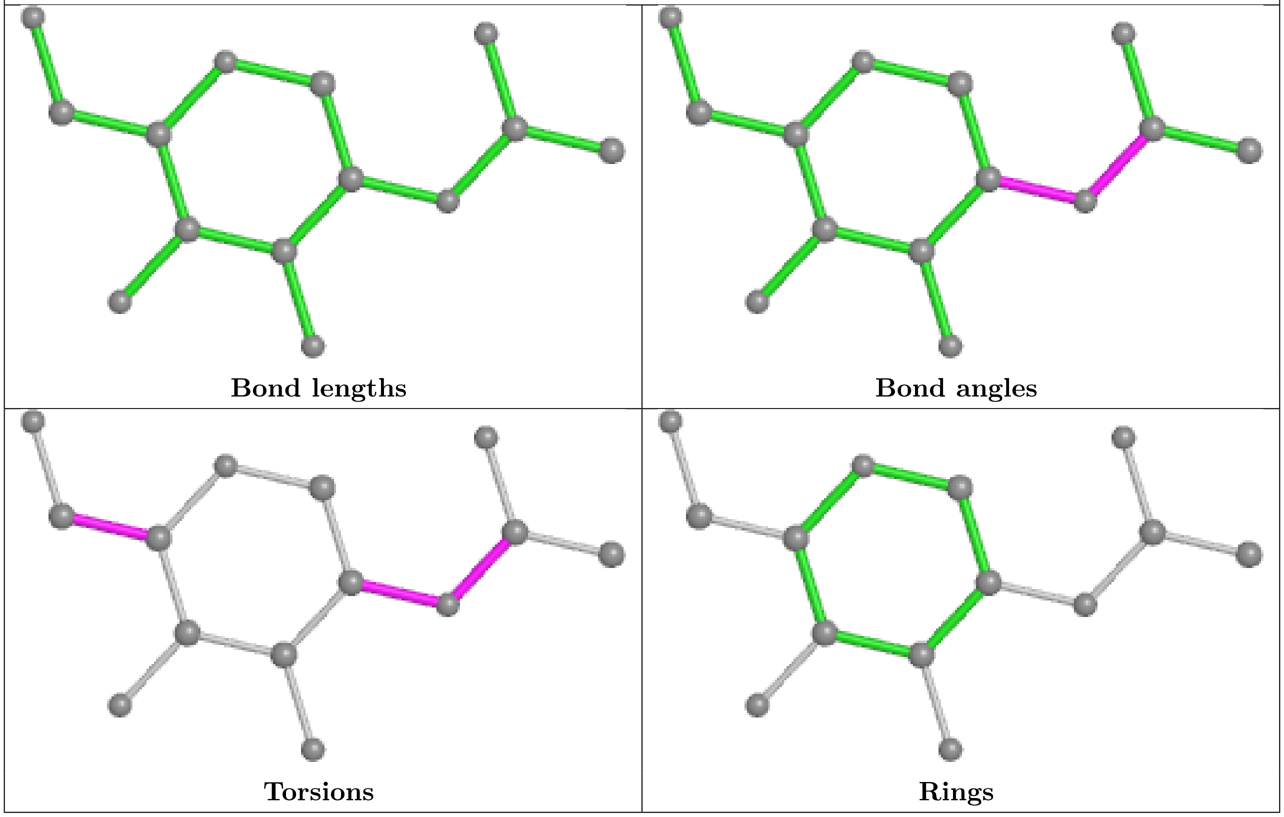
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 1405



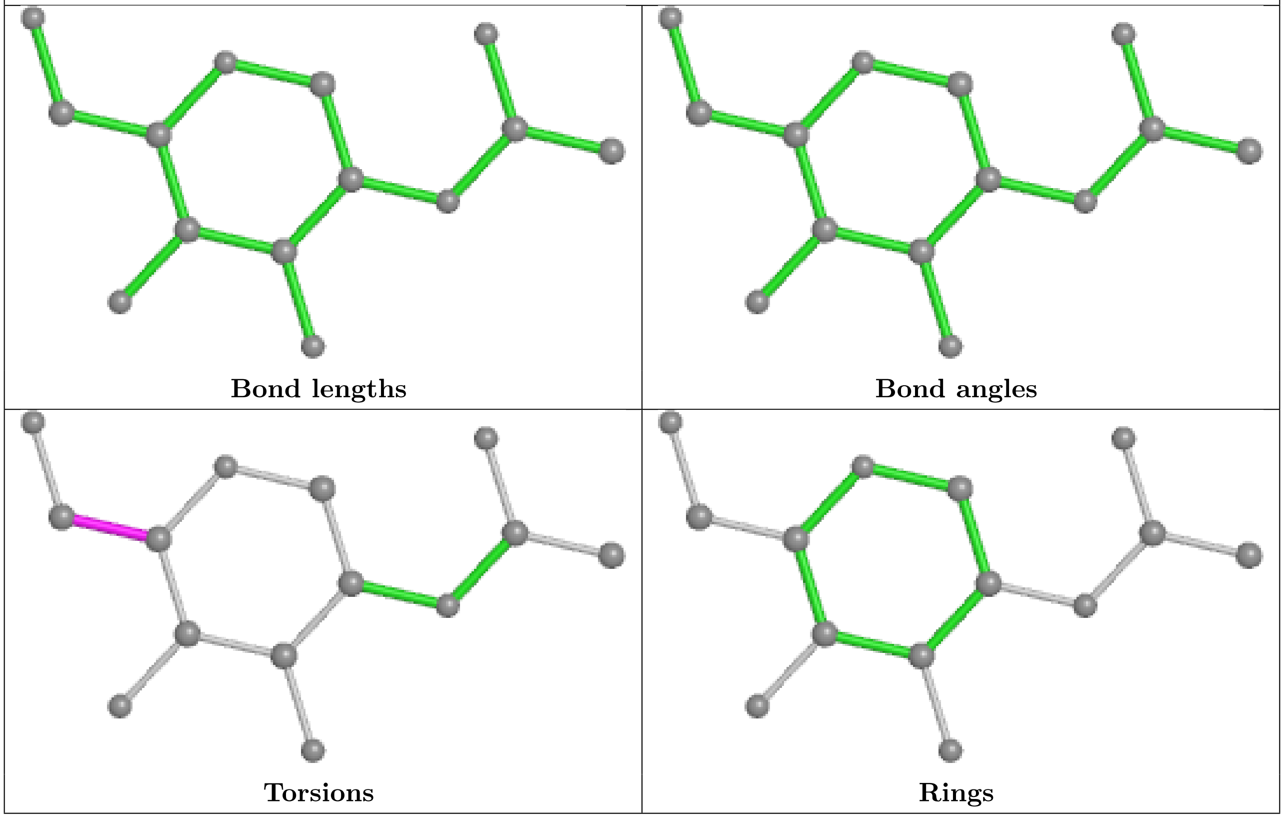
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG F 701



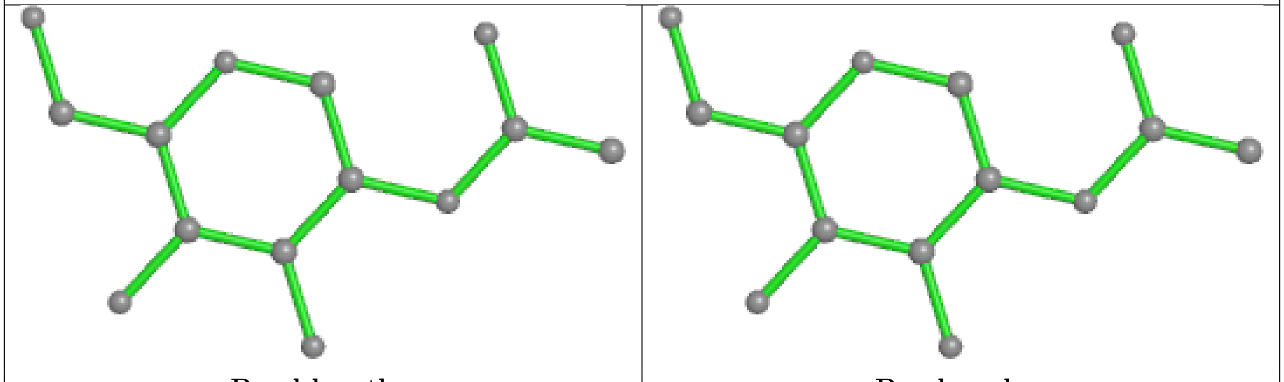
Bond lengths

Bond angles

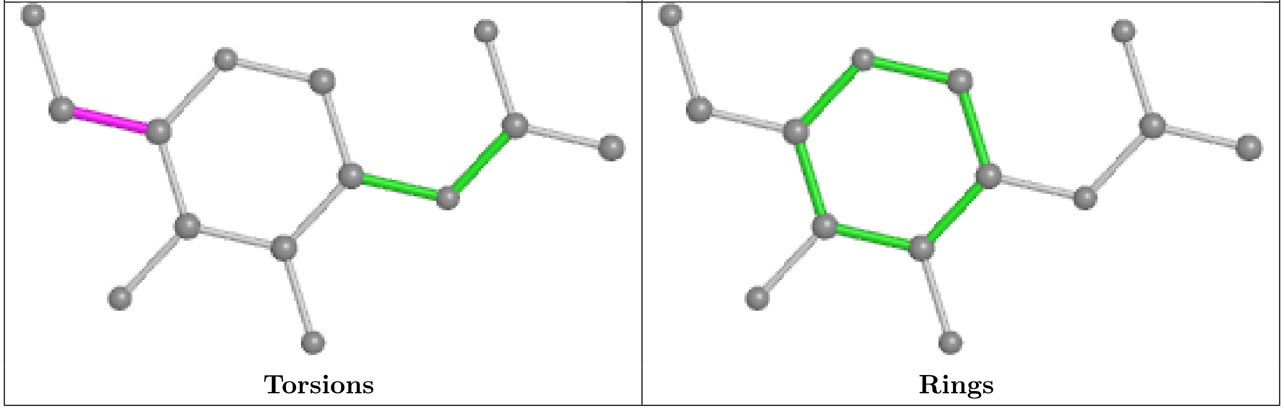
Torsions

Rings

Ligand NAG B 1404

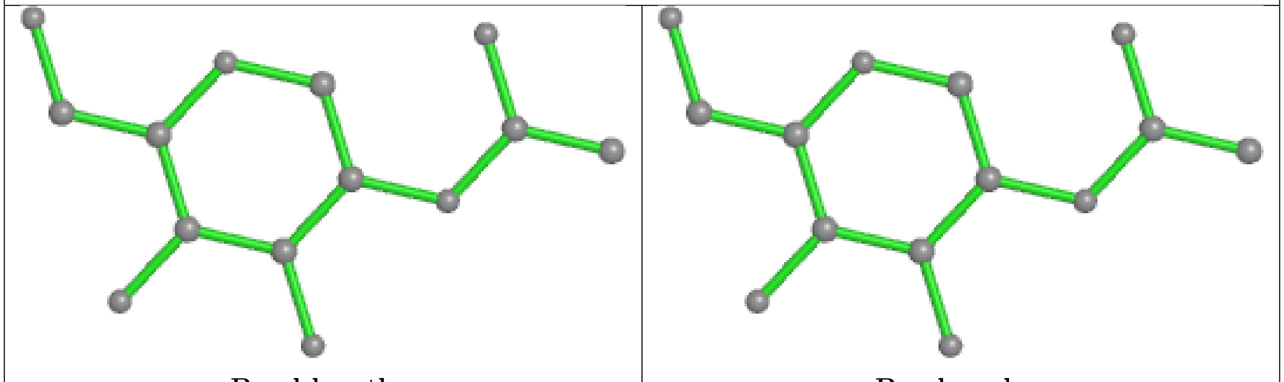


Bond lengths Bond angles

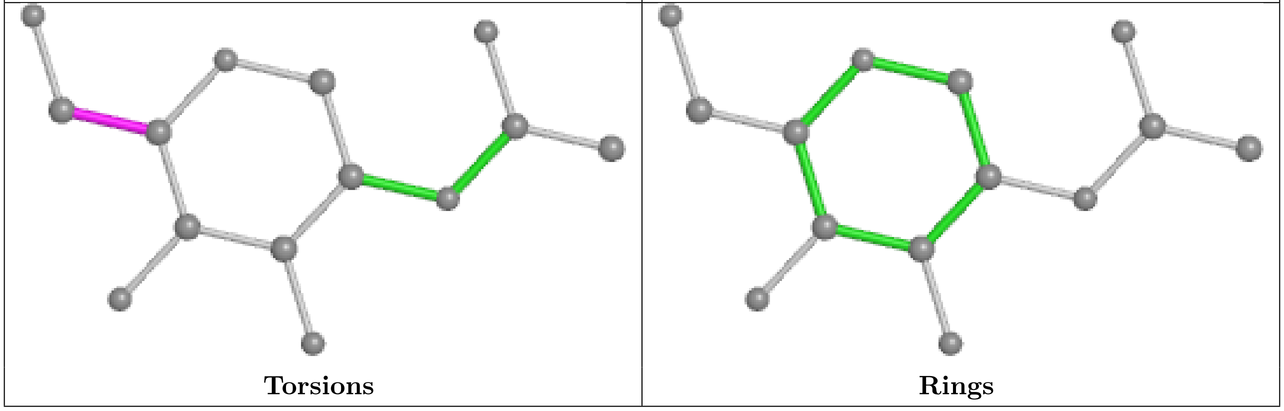


Torsions Rings

Ligand NAG C 1404

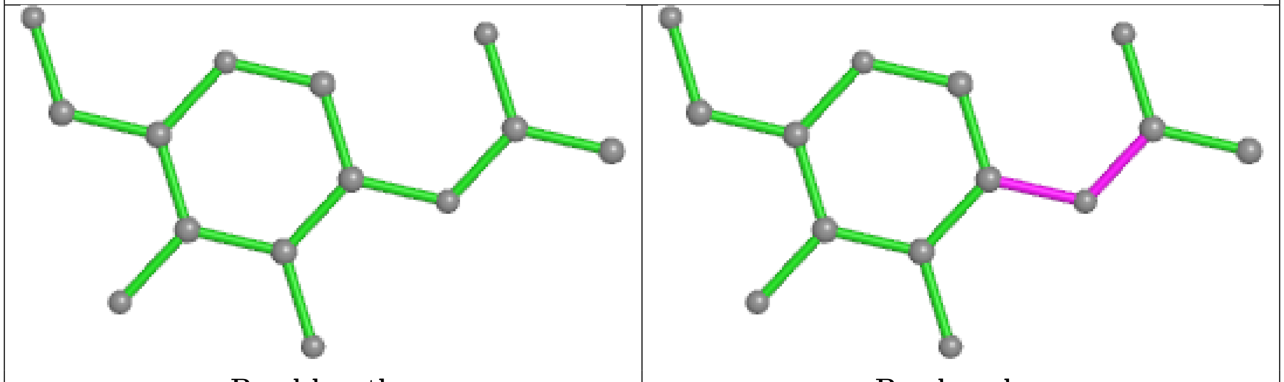


Bond lengths Bond angles



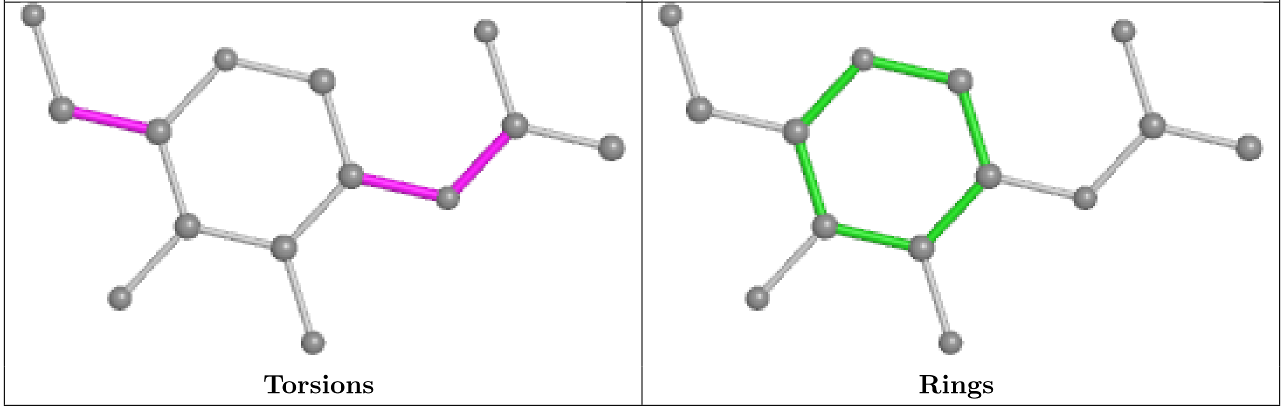
Torsions Rings

Ligand NAG A 1405



Bond lengths

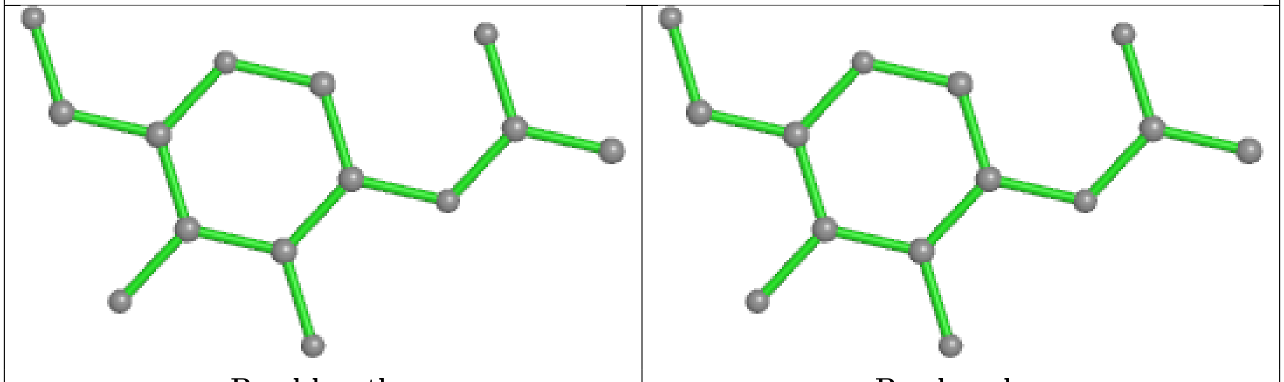
Bond angles



Torsions

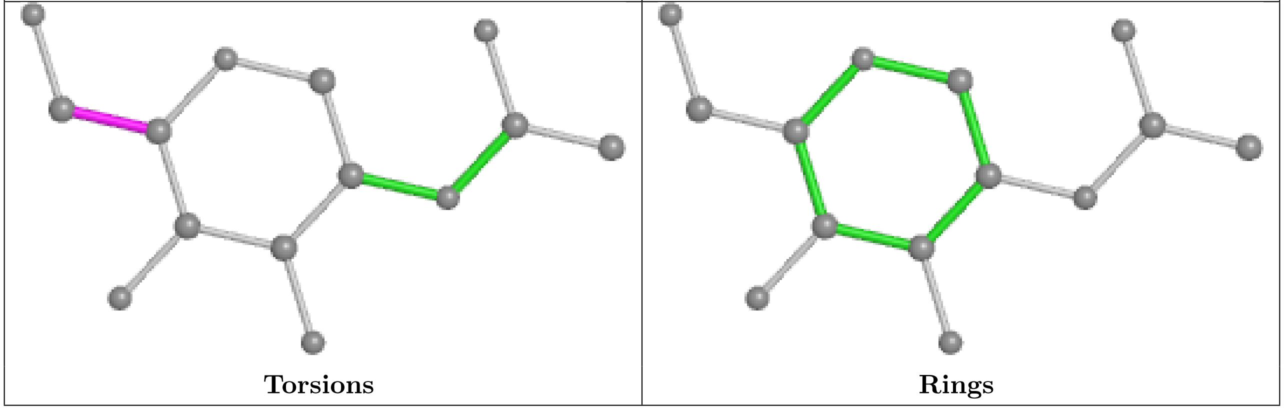
Rings

Ligand NAG A 1401



Bond lengths

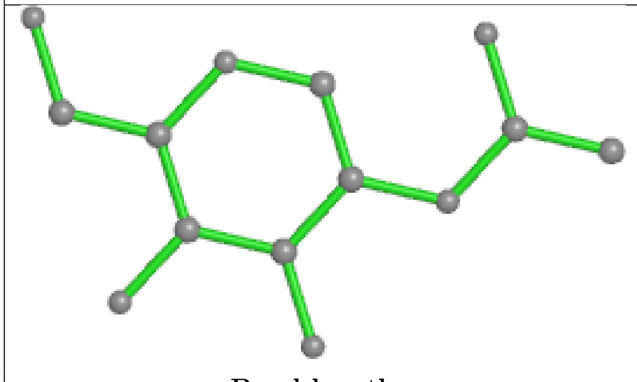
Bond angles



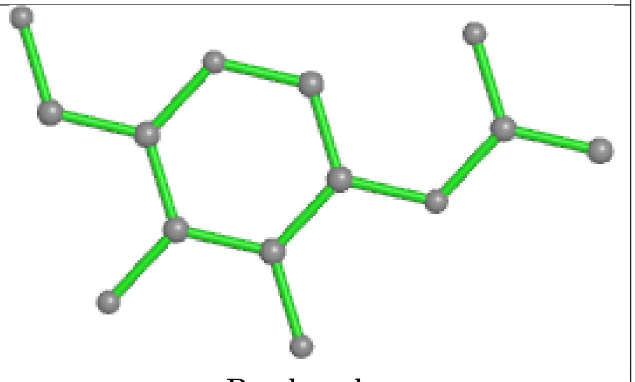
Torsions

Rings

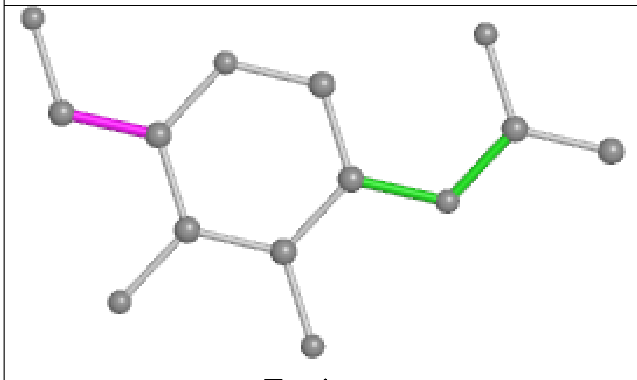
Ligand NAG B 1401



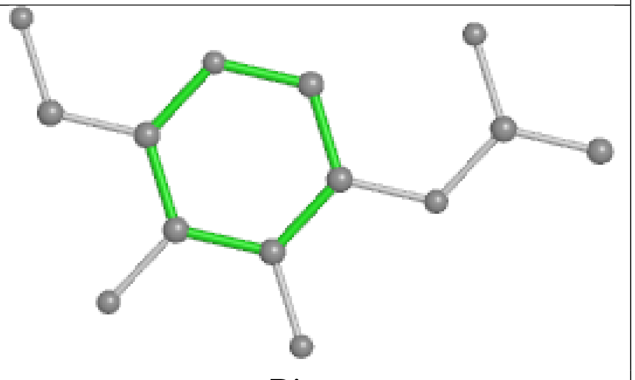
Bond lengths



Bond angles

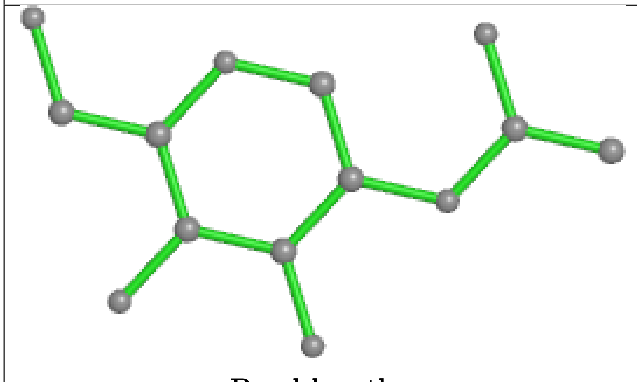


Torsions

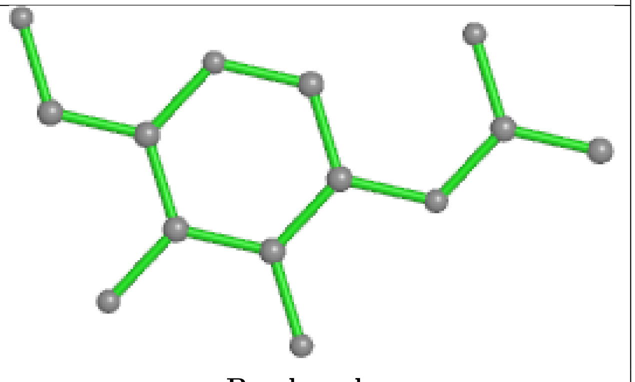


Rings

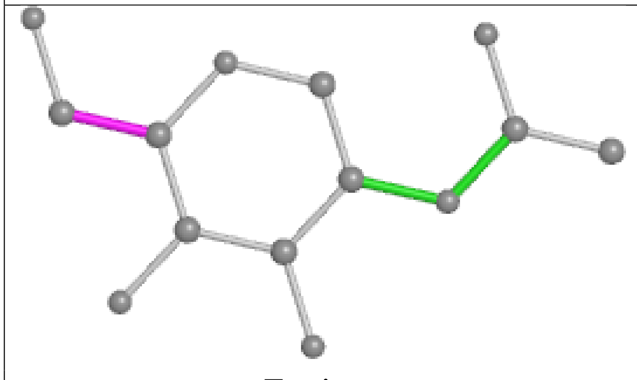
Ligand NAG C 1406



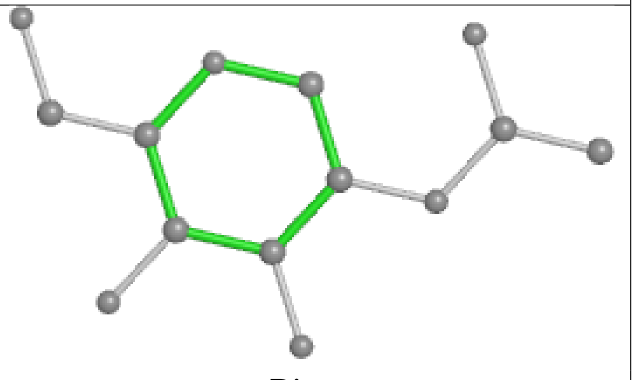
Bond lengths



Bond angles

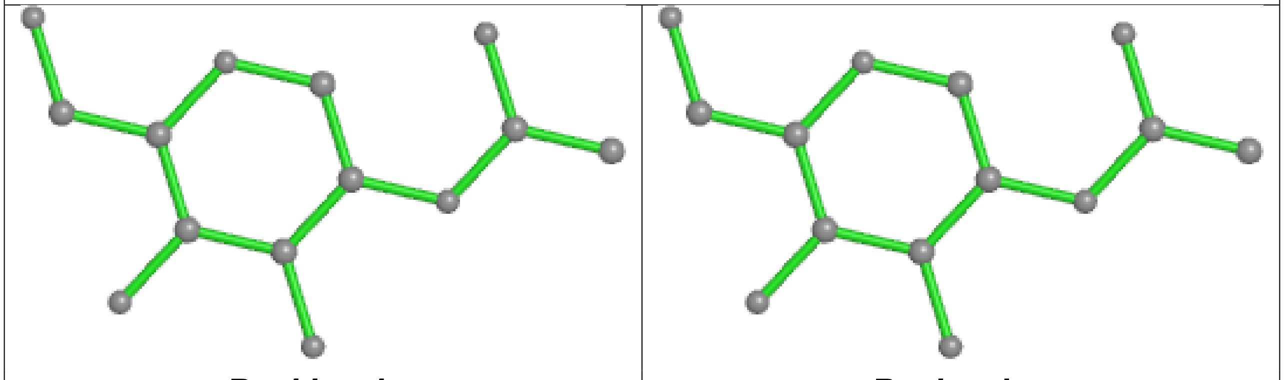


Torsions

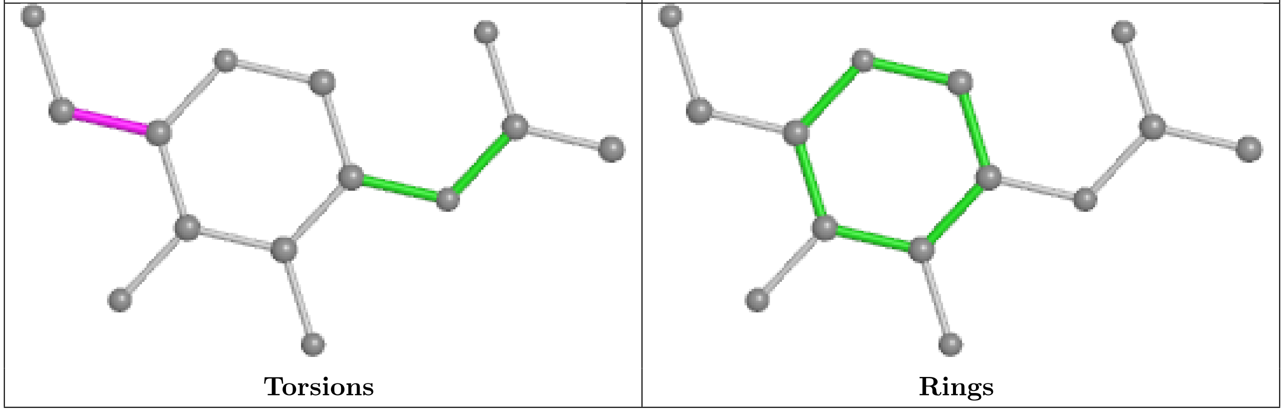


Rings

Ligand NAG B 1406

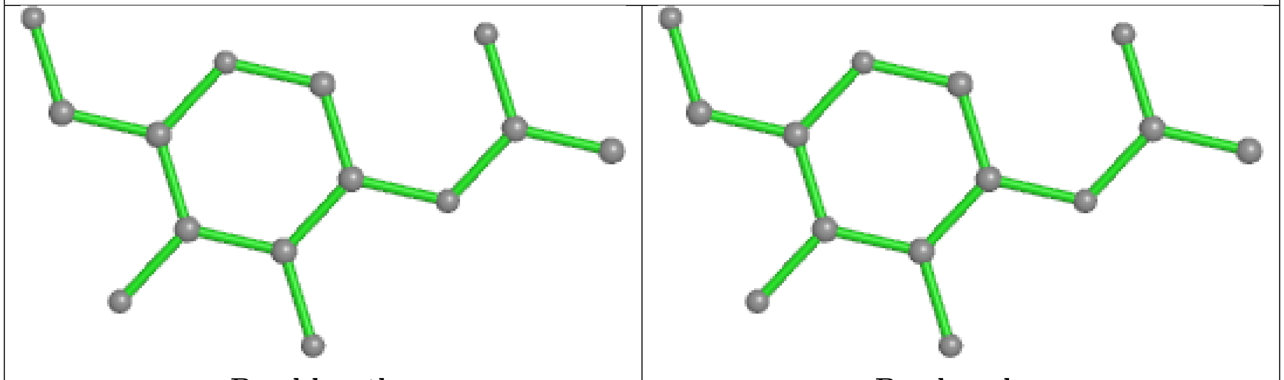


Bond lengths Bond angles

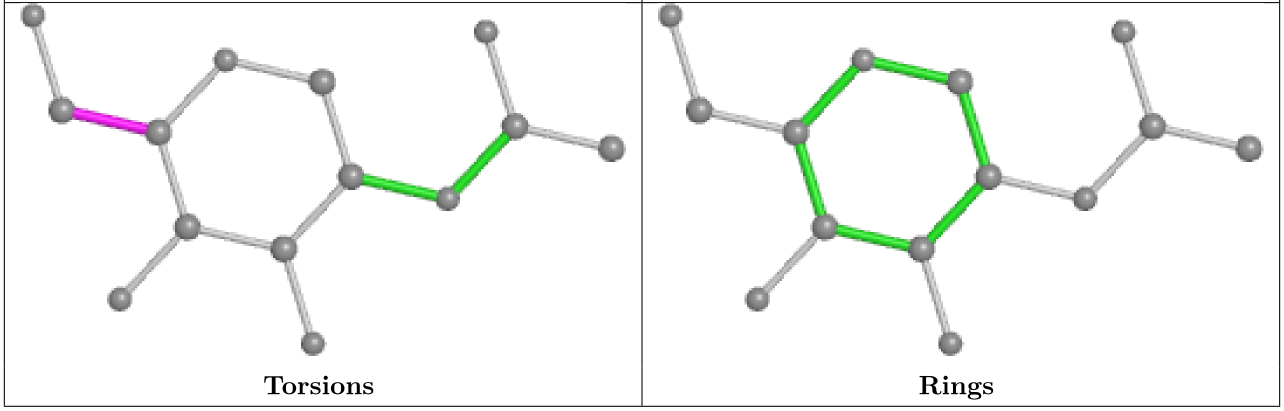


Torsions Rings

Ligand NAG A 1406

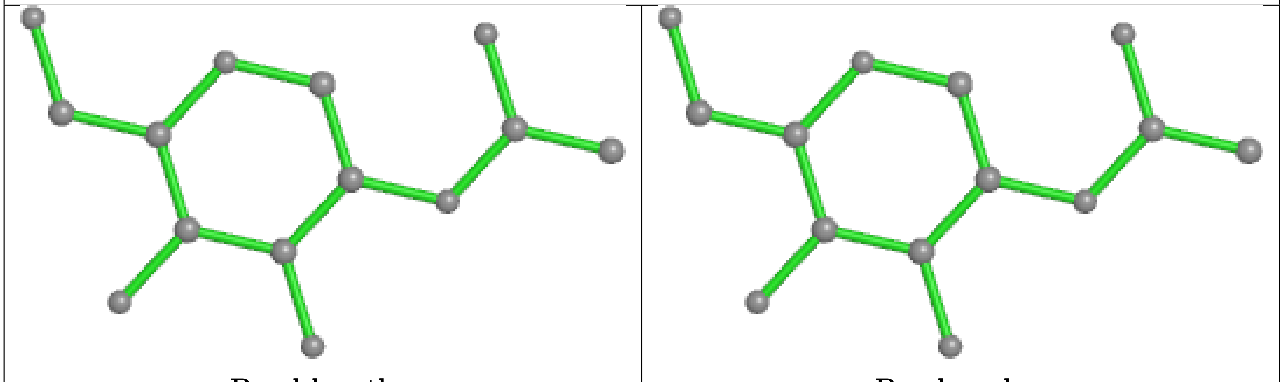


Bond lengths Bond angles

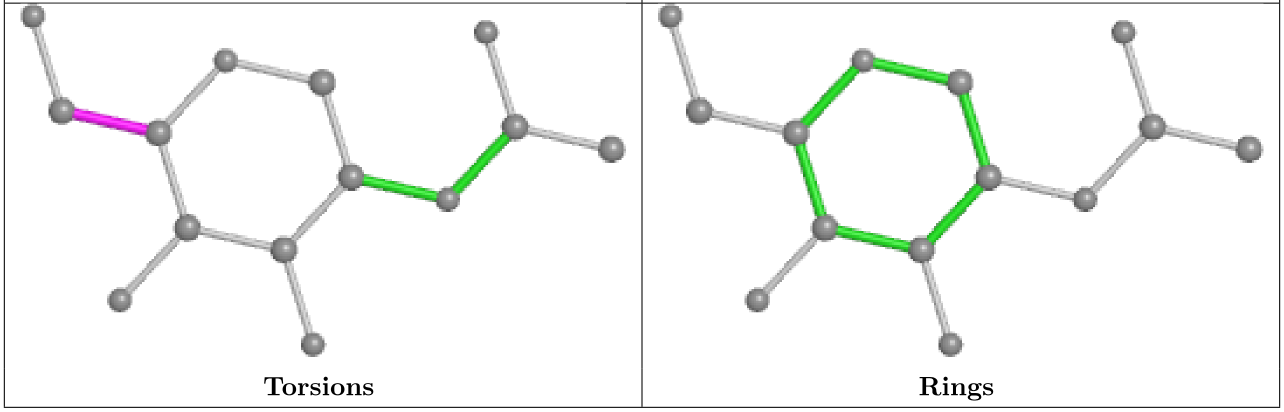


Torsions Rings

Ligand NAG C 1402

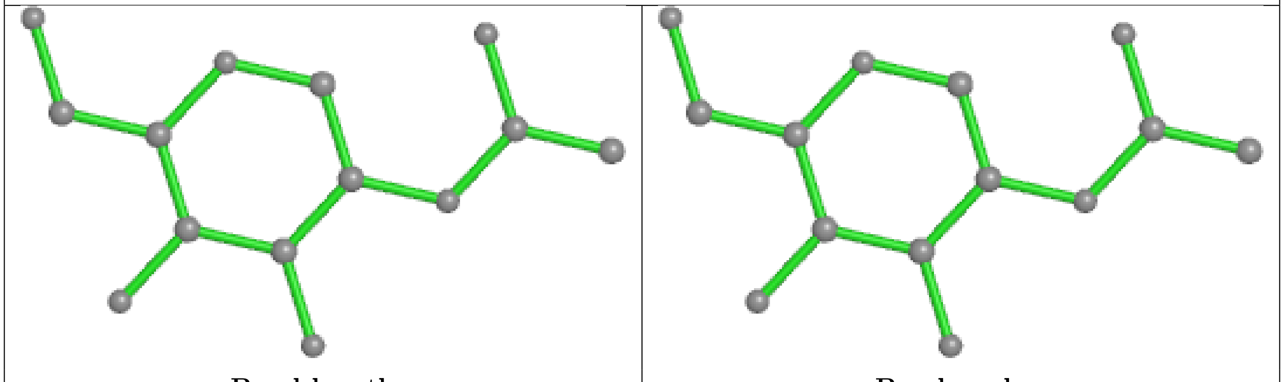


Bond lengths Bond angles

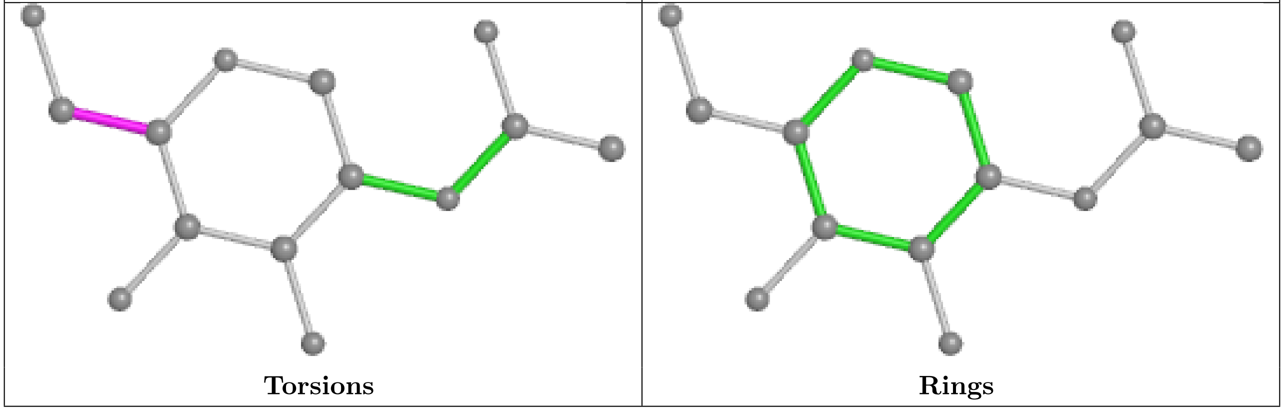


Torsions Rings

Ligand NAG B 1408

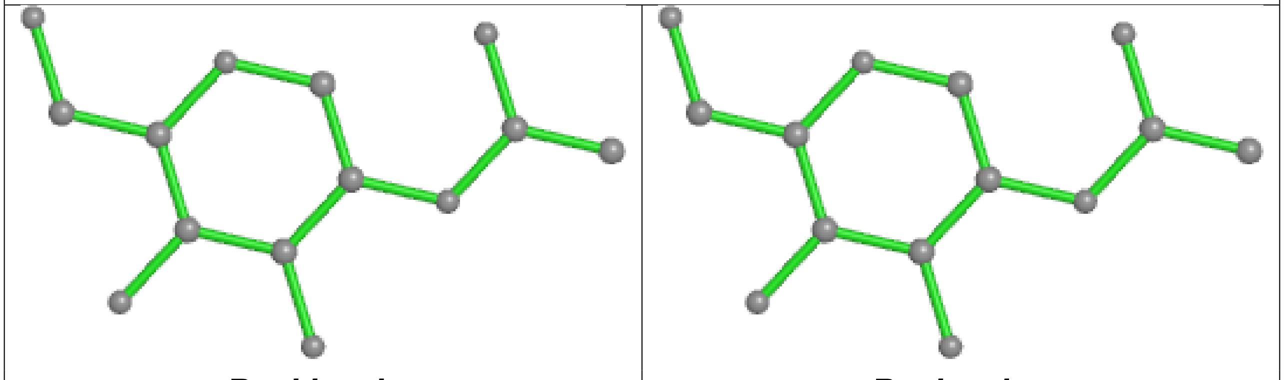


Bond lengths Bond angles

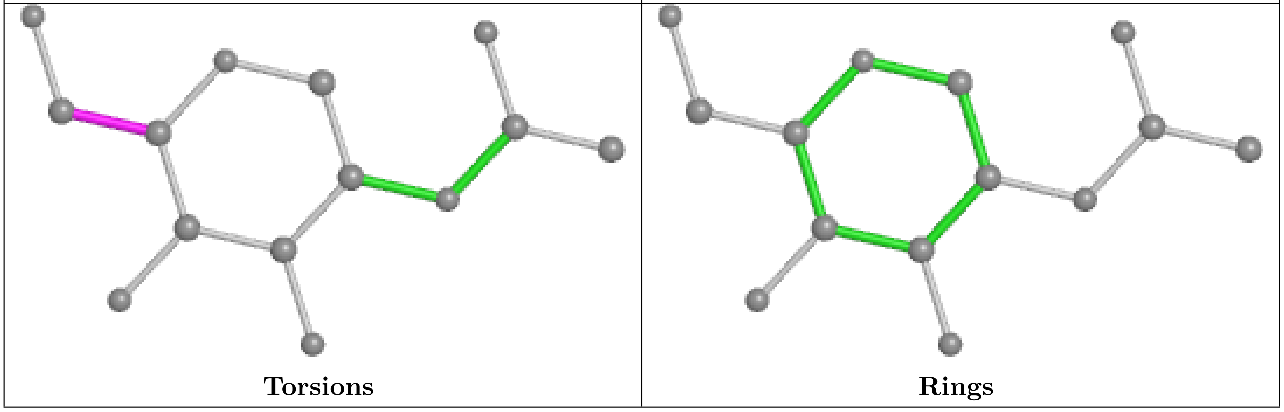


Torsions Rings

Ligand NAG A 1408

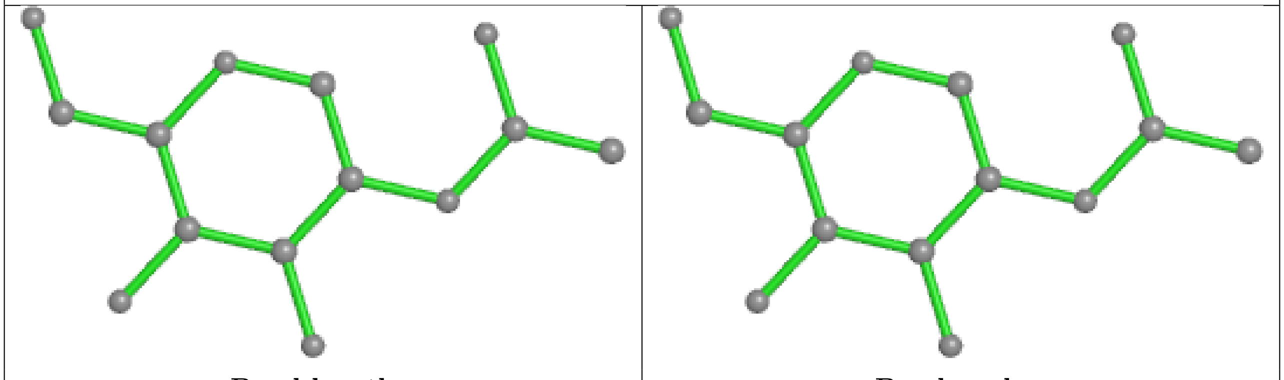


Bond lengths Bond angles

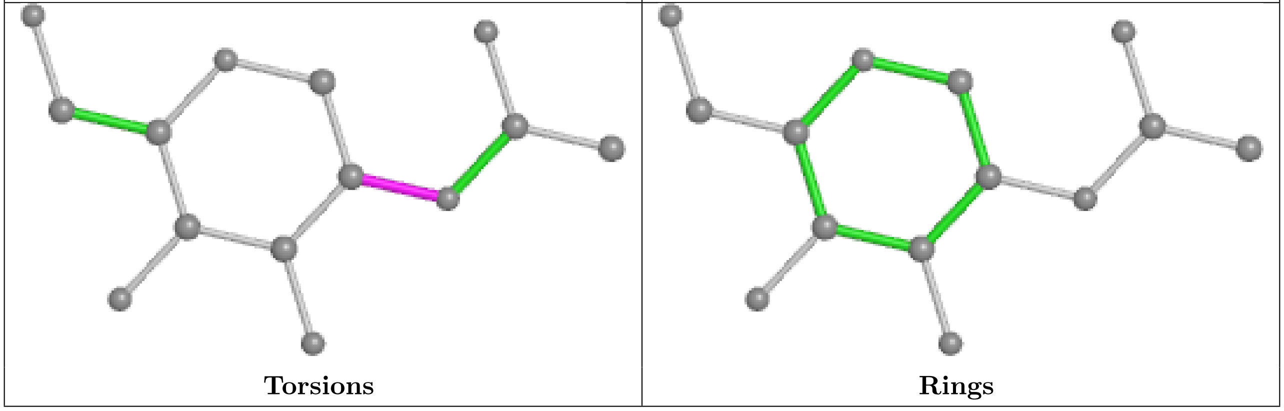


Torsions Rings

Ligand NAG C 1407



Bond lengths Bond angles



Torsions Rings

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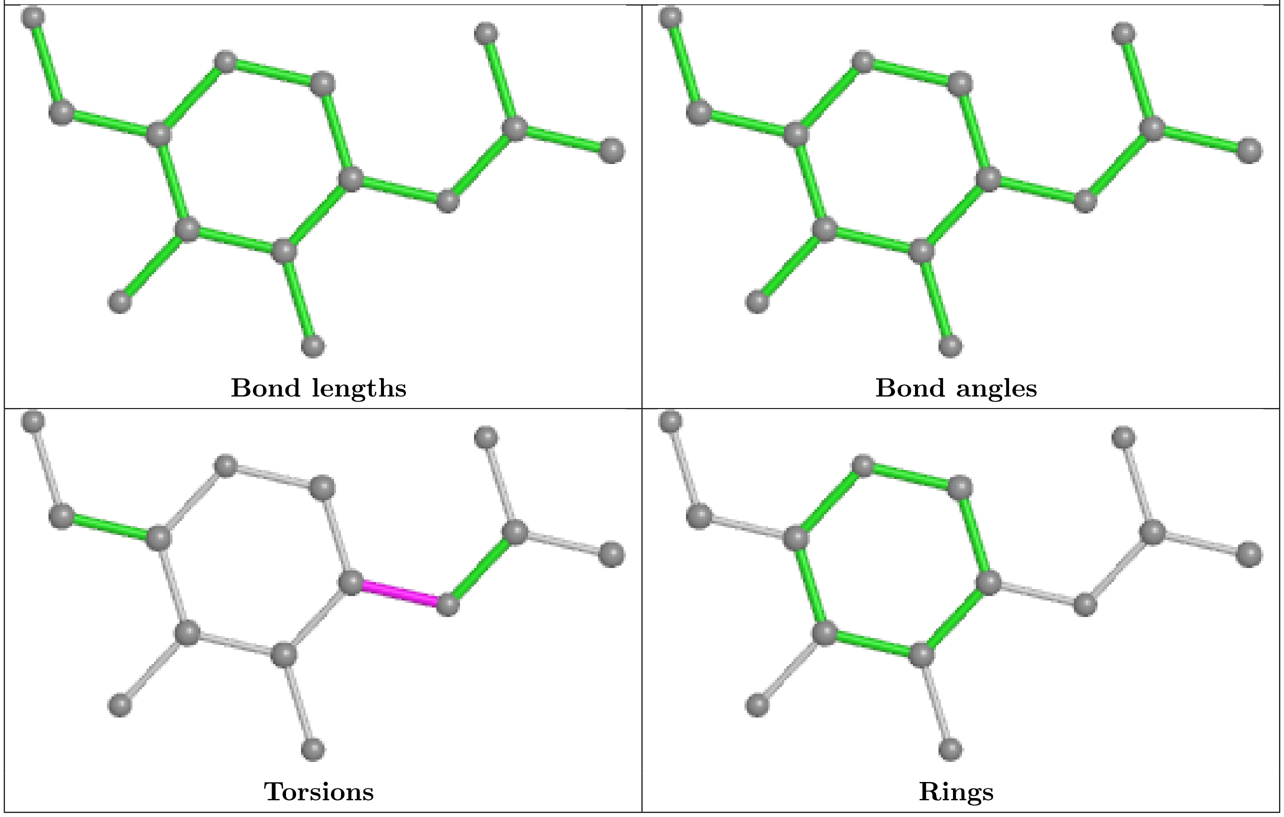


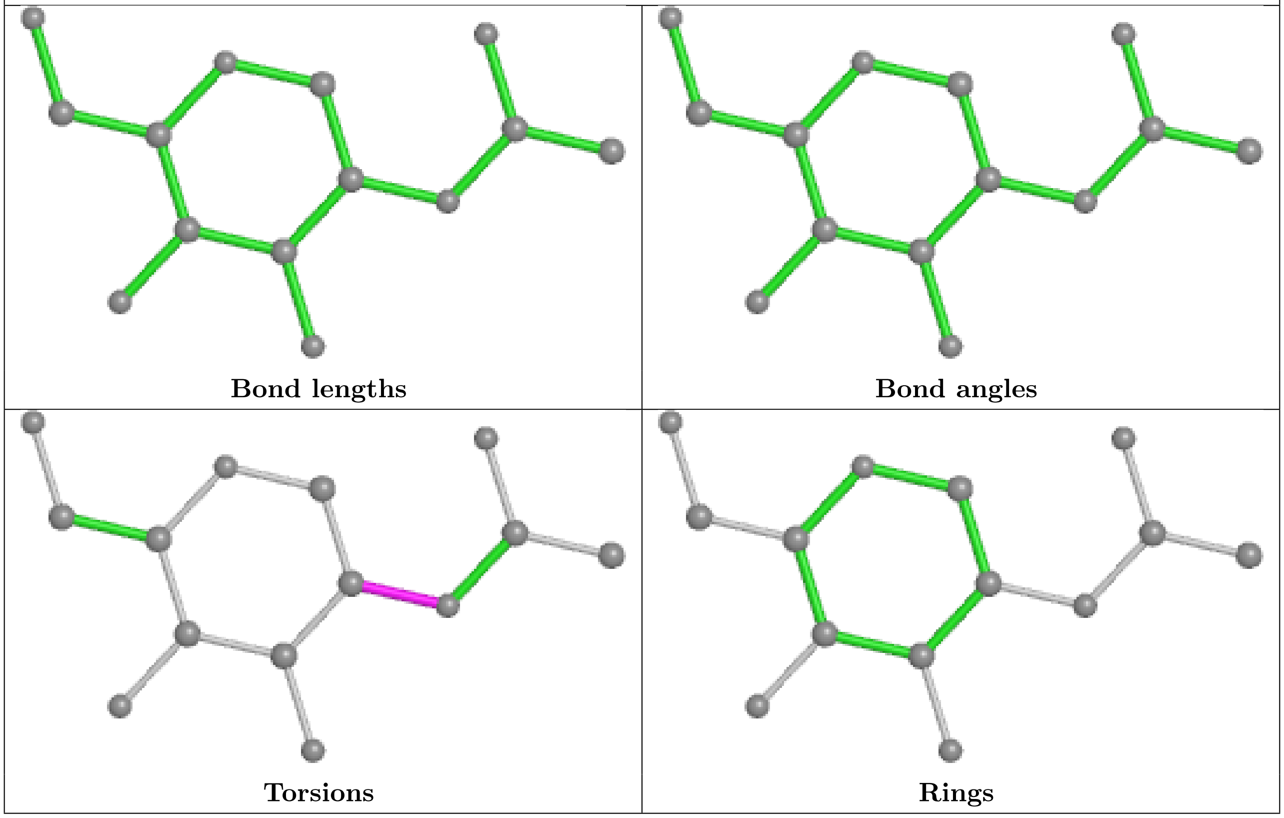
Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 1407



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.

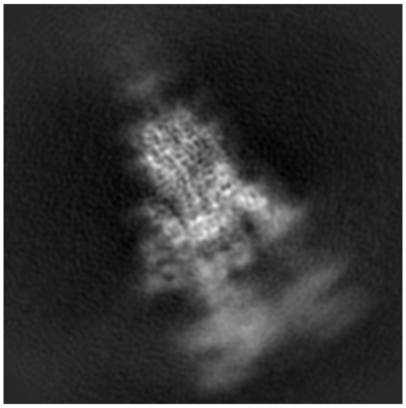
6 Map visualisation ⓘ

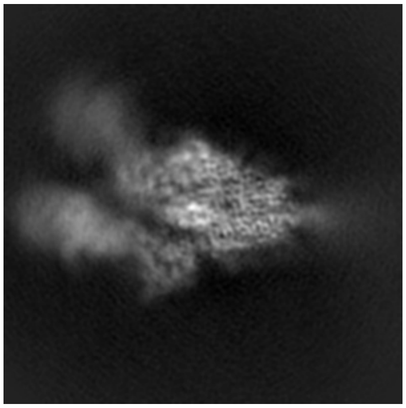
This section contains visualisations of the EMDB entry EMD-35267. These allow visual inspection of the internal detail of the map and identification of artifacts.

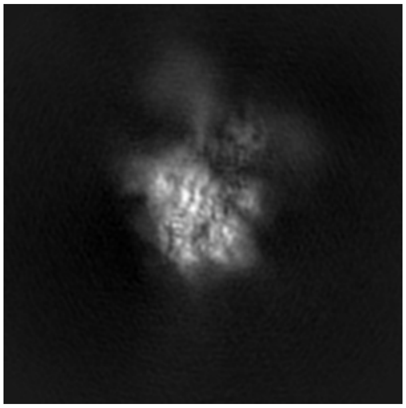
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

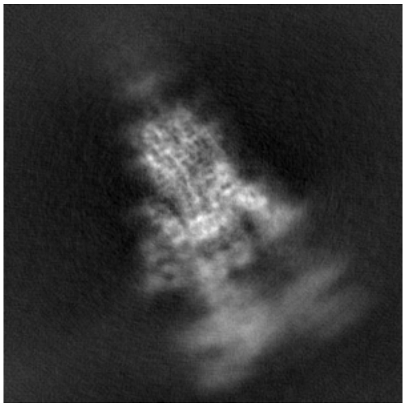
6.1.1 Primary map

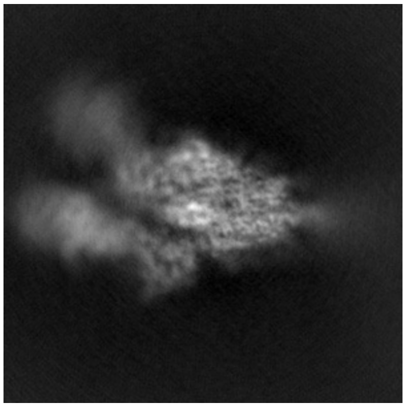

X

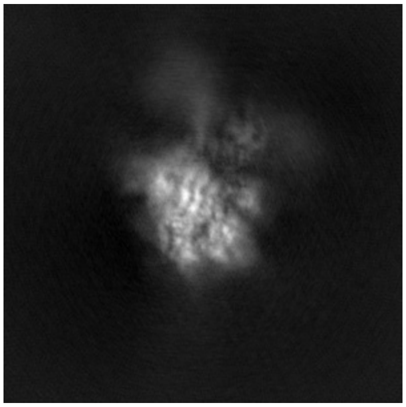

Y


Z

6.1.2 Raw map


X

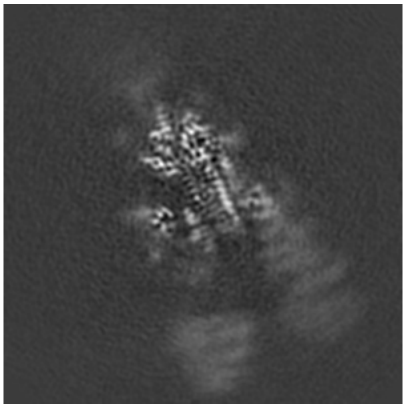

Y

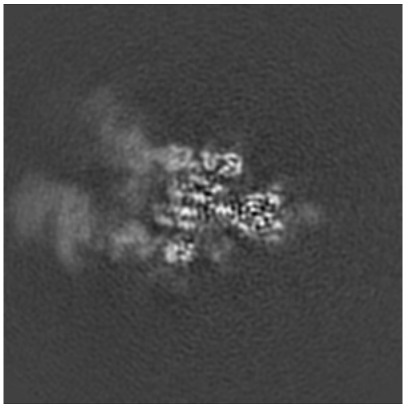

Z

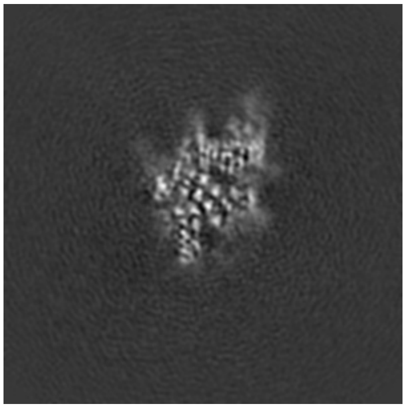
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

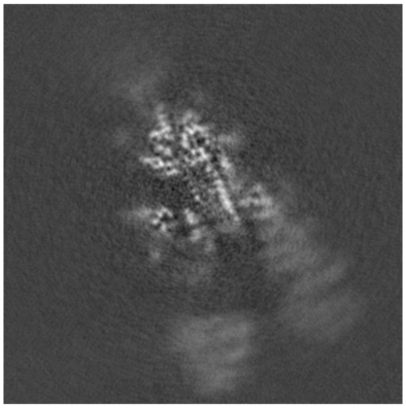
6.2.1 Primary map

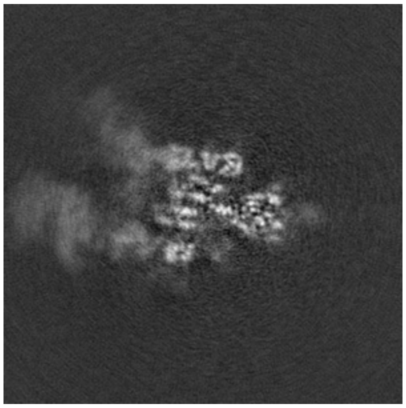

X Index: 144

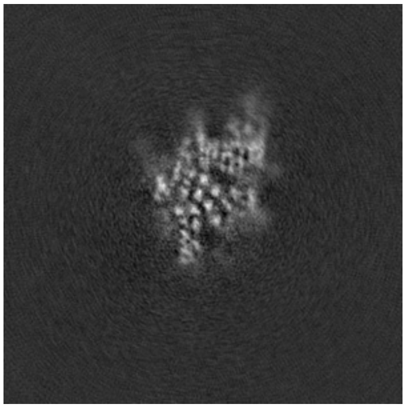

Y Index: 144


Z Index: 144

6.2.2 Raw map


X Index: 144

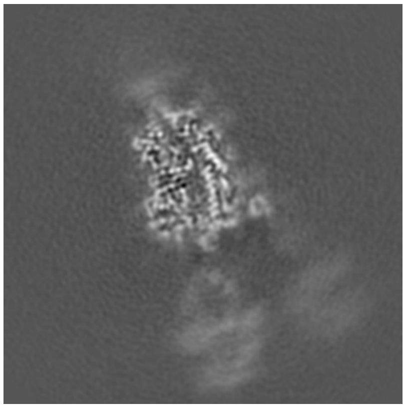

Y Index: 144


Z Index: 144

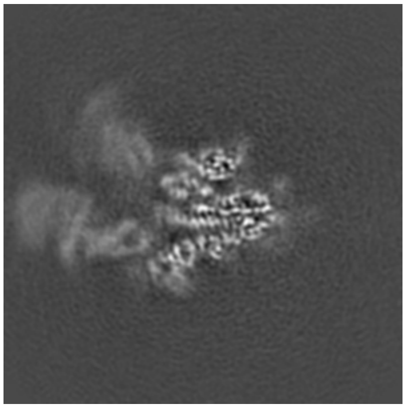
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

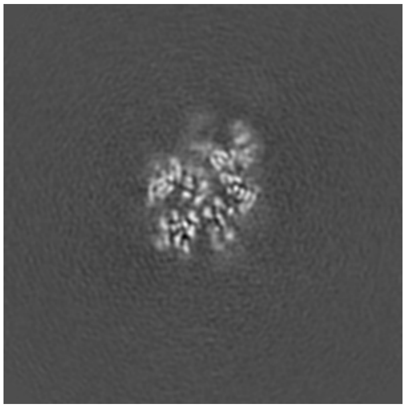
6.3.1 Primary map



X Index: 131

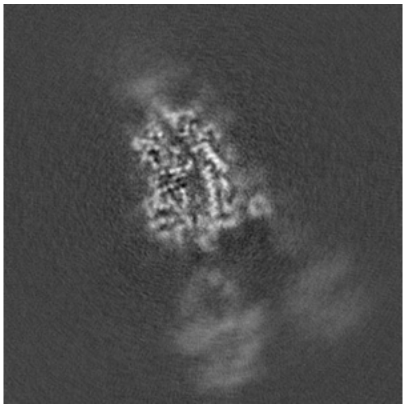


Y Index: 152

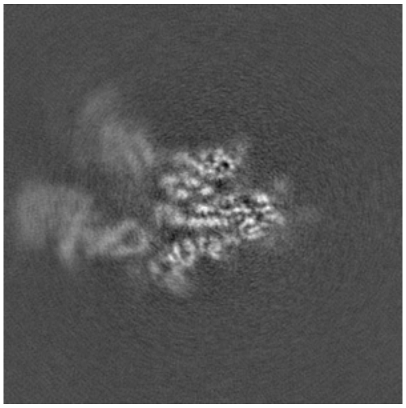


Z Index: 153

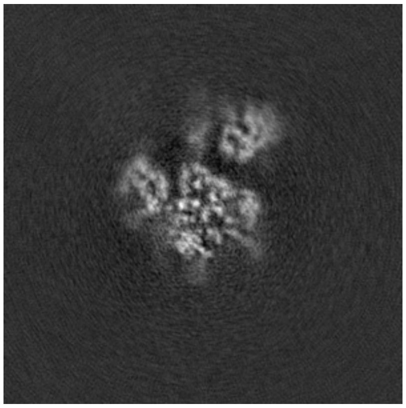
6.3.2 Raw map



X Index: 131



Y Index: 151

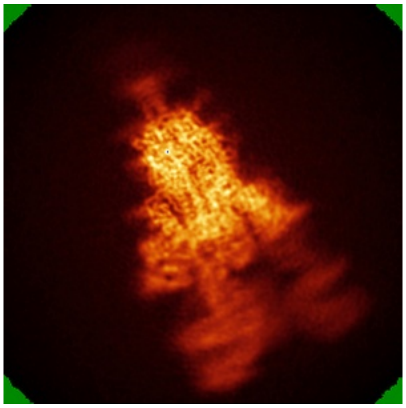


Z Index: 132

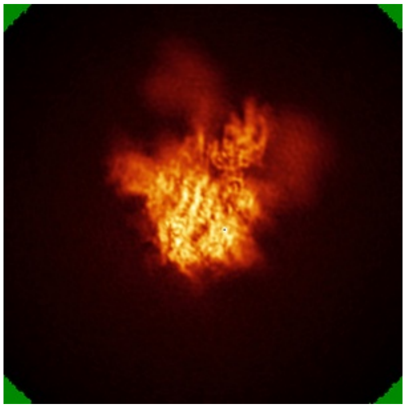
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

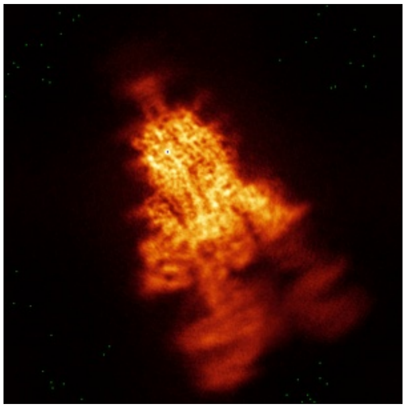
6.4.1 Primary map


X


Y


Z

6.4.2 Raw map


X


Y


Z

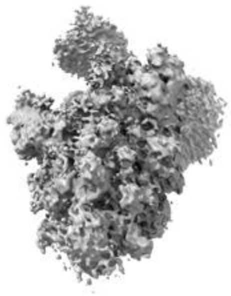
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

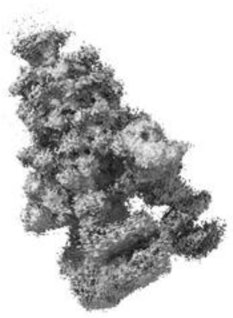

X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

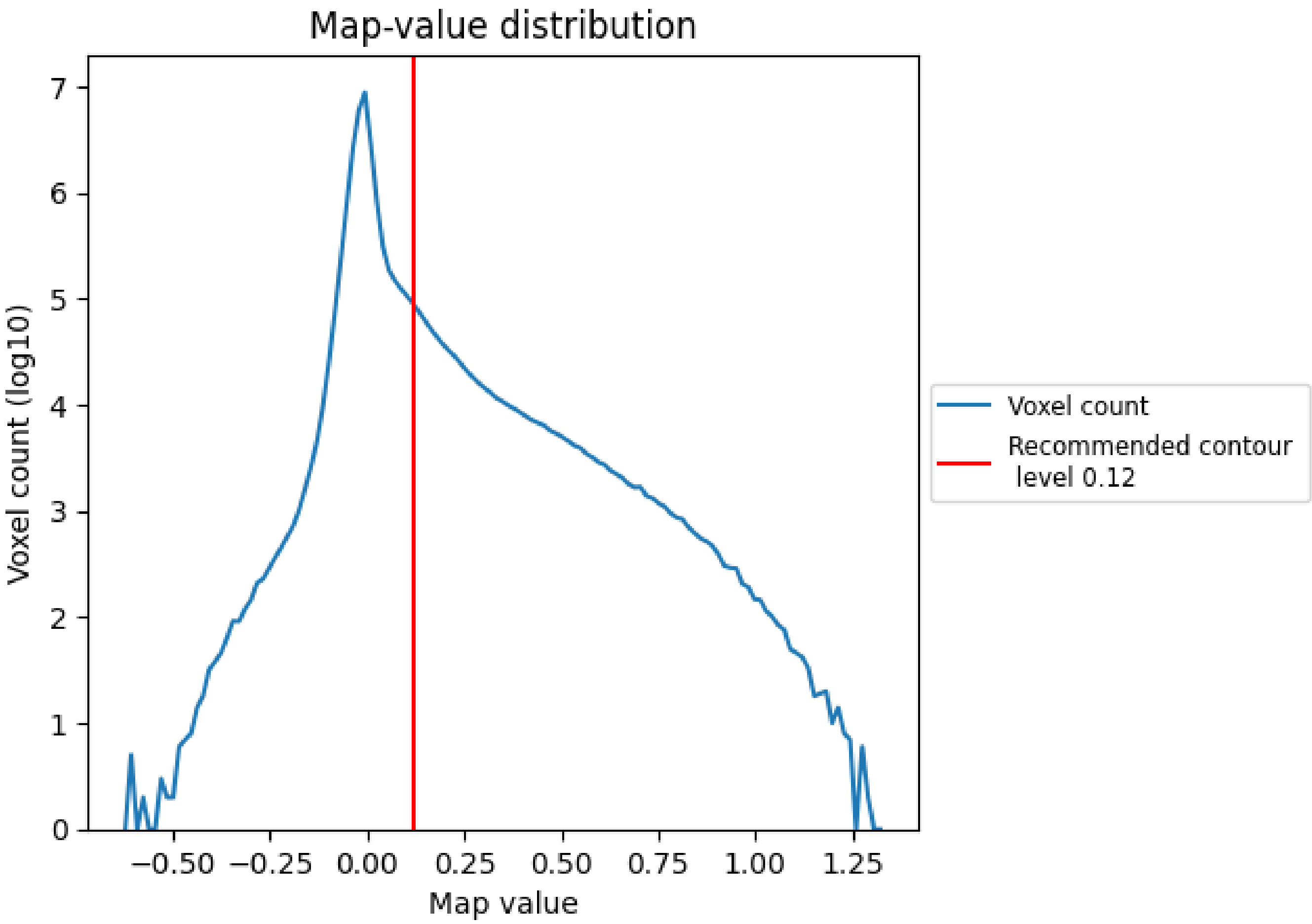
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

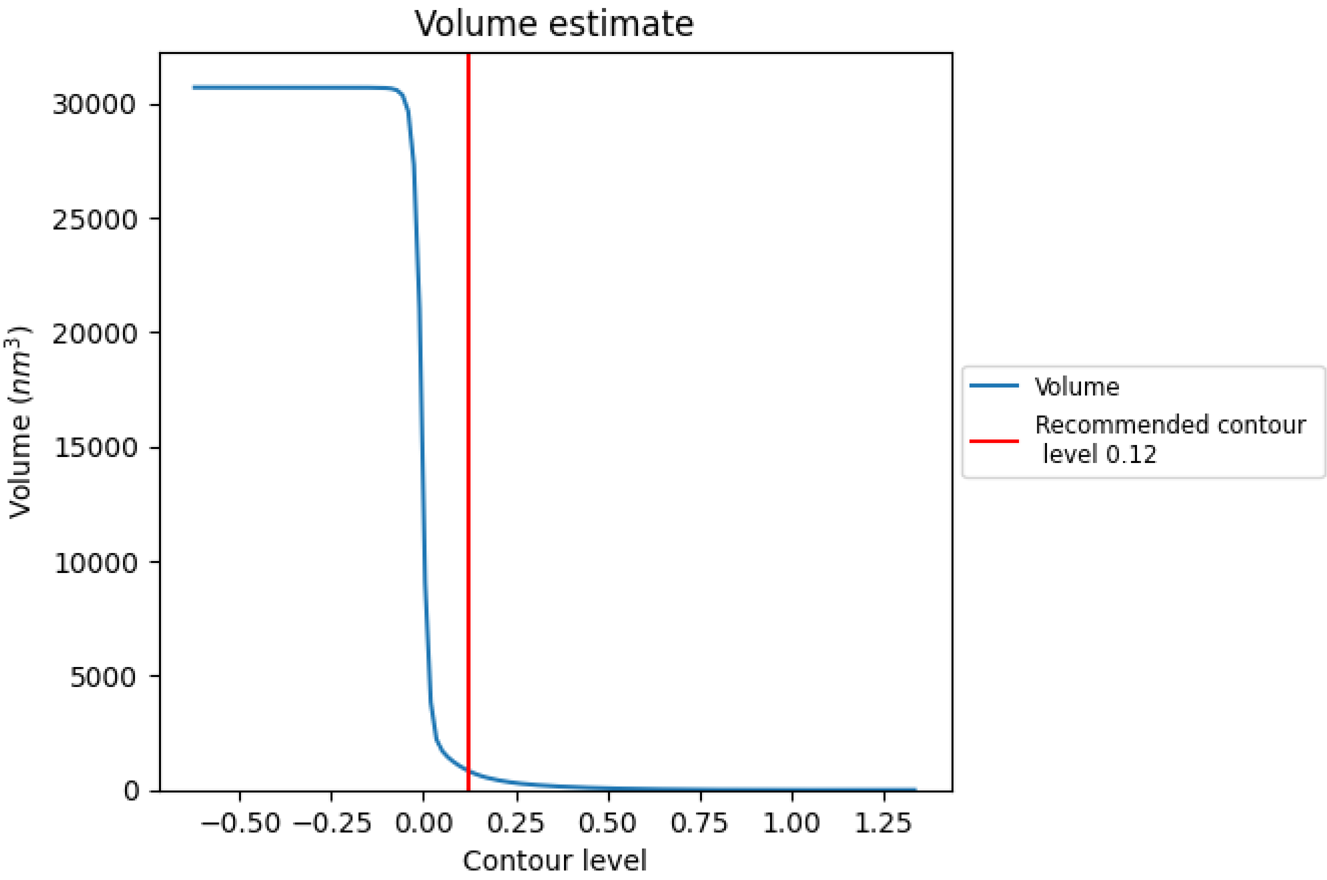
This section contains the results of statistical analysis of the map.

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.

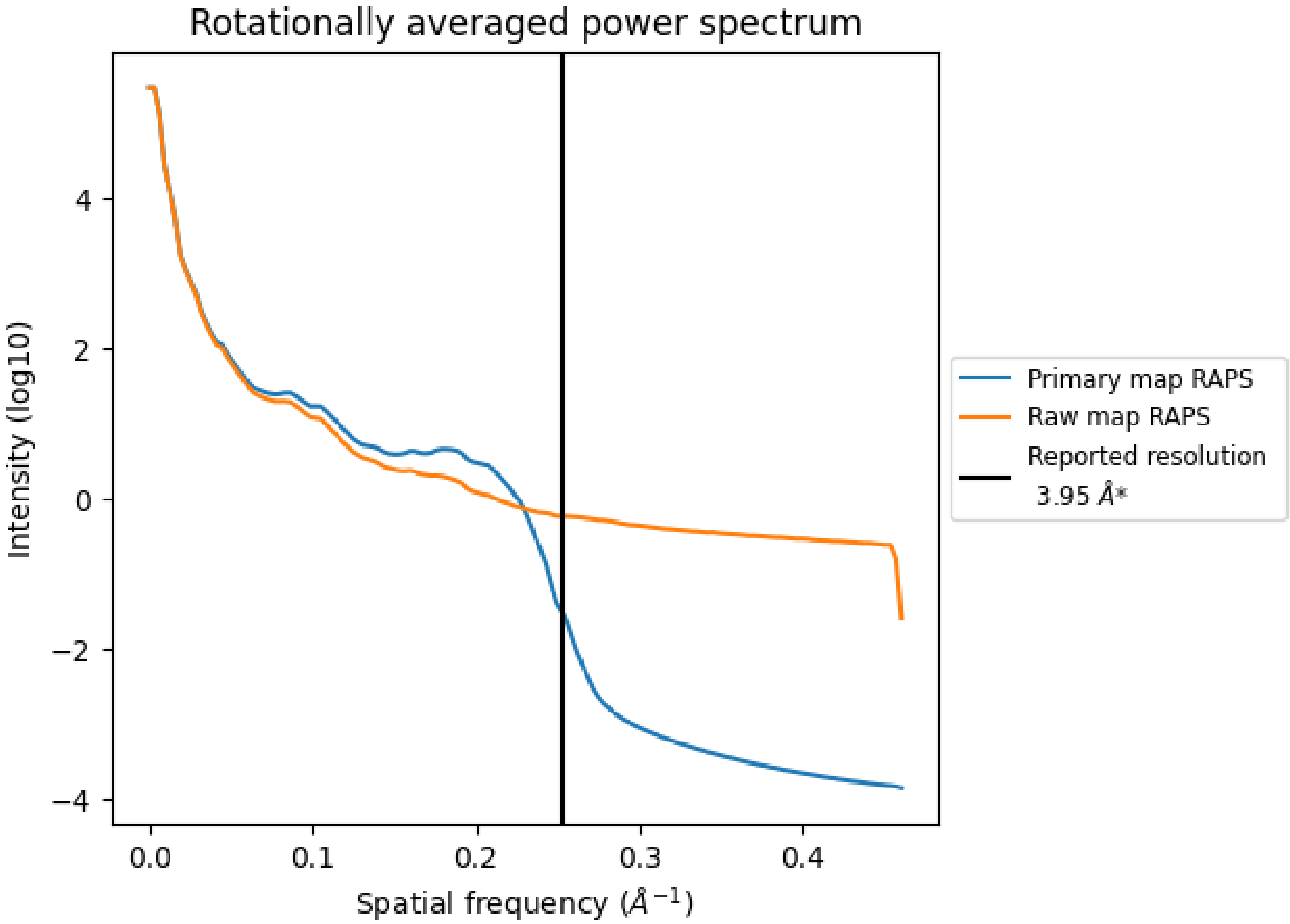
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 852 nm^3; this corresponds to an approximate mass of 770 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 ⓘ

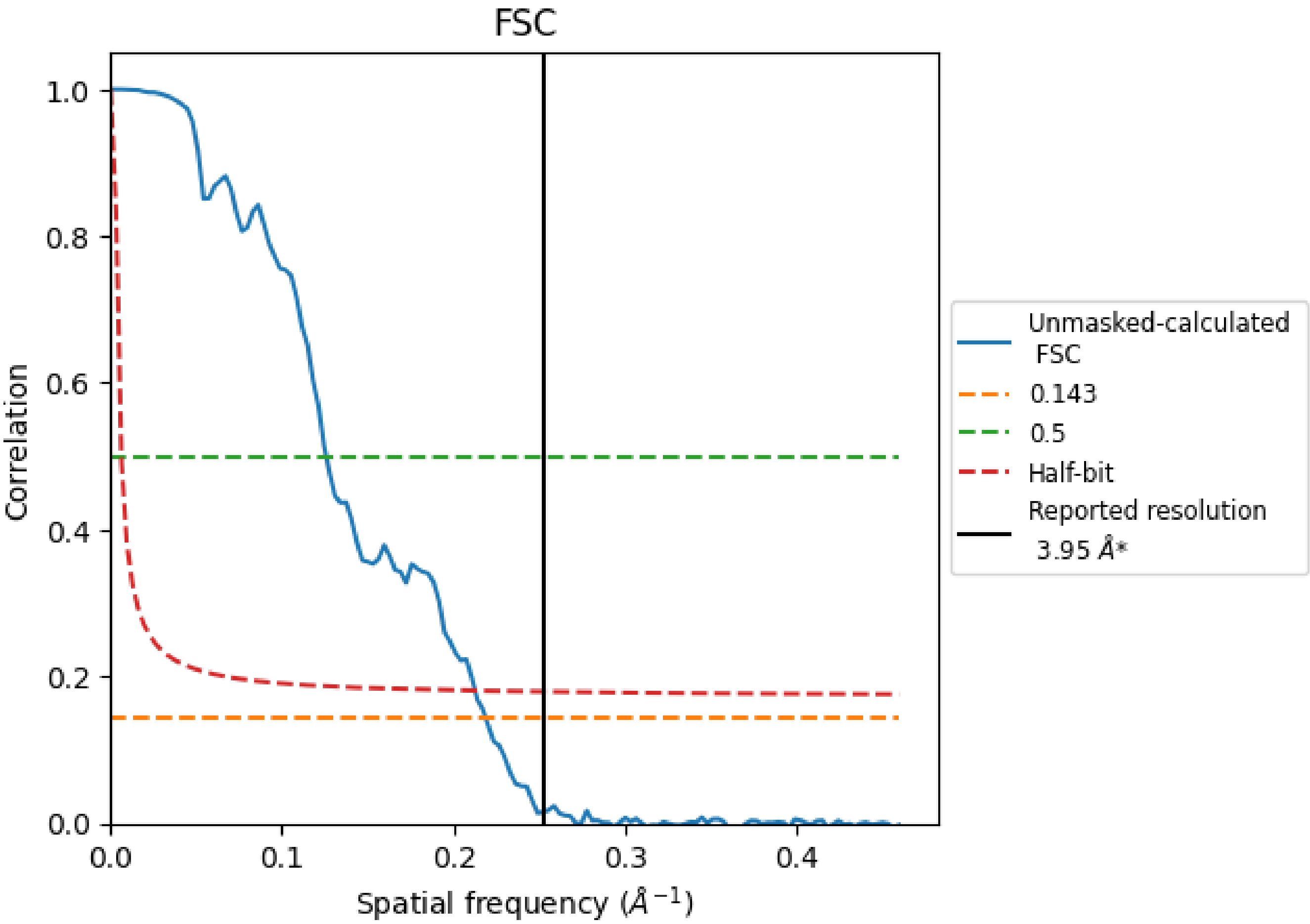


*Reported resolution corresponds to spatial frequency of 0.253 $Å^{-1}$

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 0.253 $Å^{-1}$

8.2 Resolution estimates ⓘ

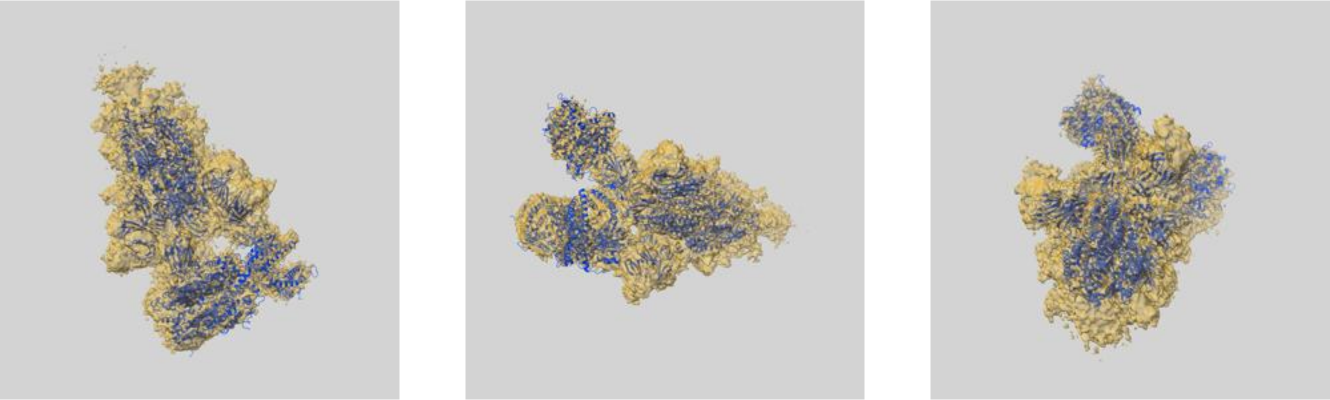
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.57	7.95	4.70

*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 4.57 differs from the reported value 3.95 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-35267 and PDB model 8I9D. Per-residue inclusion information can be found in section 3 on page 20.

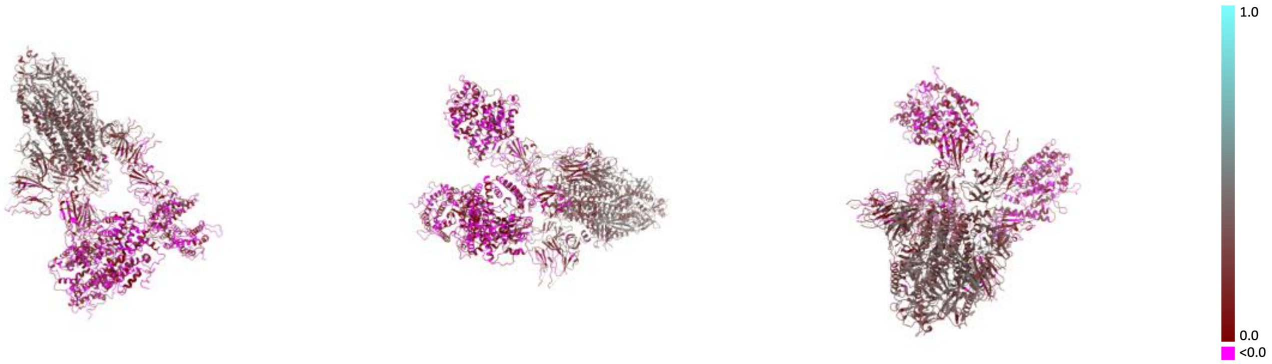
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

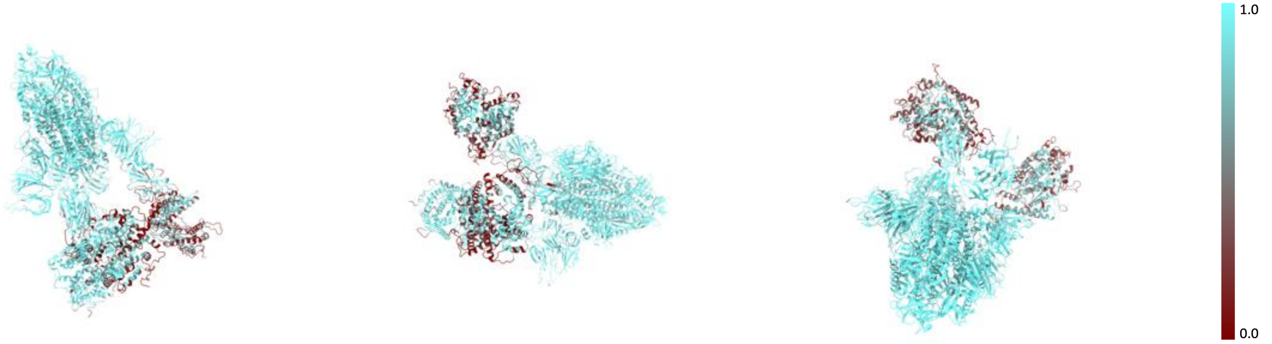
9.2 Q-score mapped to coordinate model



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.

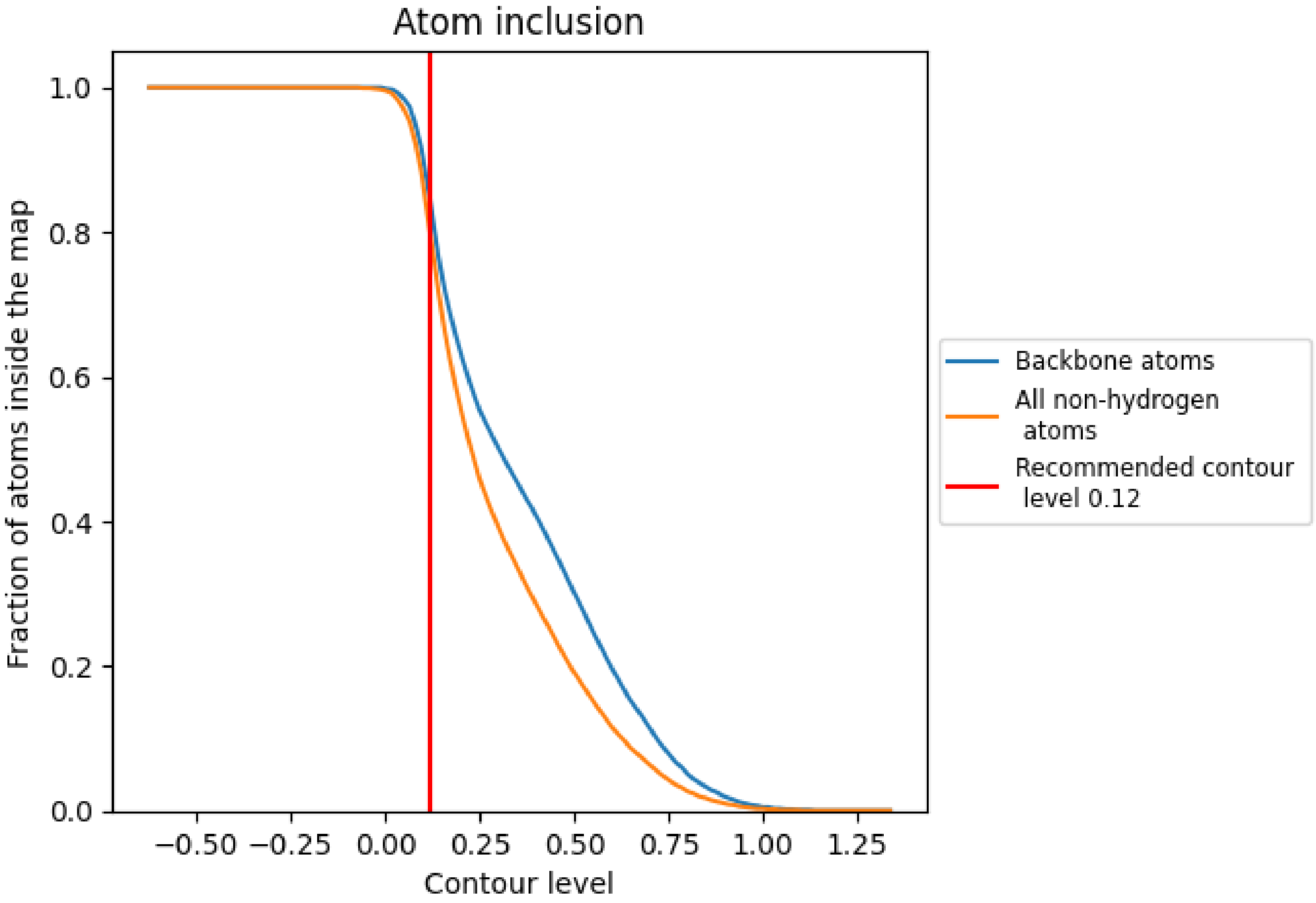
9.3 Atom inclusion mapped to coordinate model



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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.1700
A	0.8860	0.2370
B	0.9220	0.2480
C	0.9540	0.2540
D	0.4210	0.0390
E	0.5050	0.0370
F	0.9150	0.0650
G	0.9640	0.2200
H	0.8210	0.0860
I	0.8570	0.3600
J	0.9290	0.2370
K	0.9290	0.1680
L	1.0000	0.3070
M	1.0000	0.3390
N	1.0000	0.2980
O	0.6790	0.0960
P	0.8210	0.1430
Q	0.9640	0.3300
R	0.9290	0.3170
S	0.9290	0.2640
T	0.9640	0.2340
U	1.0000	0.3220
V	0.9640	0.2690
W	0.5360	0.0390
X	0.3930	-0.0810
Y	0.9640	0.3530
Z	1.0000	0.3520
a	0.8570	0.1540
b	1.0000	0.2350
c	0.9290	0.2810
d	0.6790	0.0720
e	0.4640	0.0240
f	0.8930	0.0700
g	0.1790	0.1210
h	0.7140	-0.0680

Continued on next page...

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Chain	Atom inclusion	Q-score
i	🟥 0.1070	🟥 0.0420
j	🟥 0.0000	🟥 0.1120
k	🟥 0.0000	🟥 0.0490
l	🟥 0.0000	🟥 0.0740
m	🟥 0.1790	🟥 0.1520
n	⬛ 0.4290	🟥 0.0840
o	🟥 0.0000	🟪 -0.0540
p	🟥 0.0000	🟪 -0.1430
q	🟥 0.0000	🟥 0.0840
r	🟥 0.0360	🟪 -0.0180