



Full wwPDB EM Validation Report ⓘ

Jul 27, 2026 – 01:24 AM JST

PDB ID : 22OV / pdb_000022ov
EMDB ID : EMD-68575
Title : SARS-CoV-2 BA.3.2.2(RE.2.2) spike protein
Authors : Li, L.J.; Qu, H.; Wu, Q.L.; Gao, G.F.
Deposited on : 2026-01-19
Resolution : 2.37 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

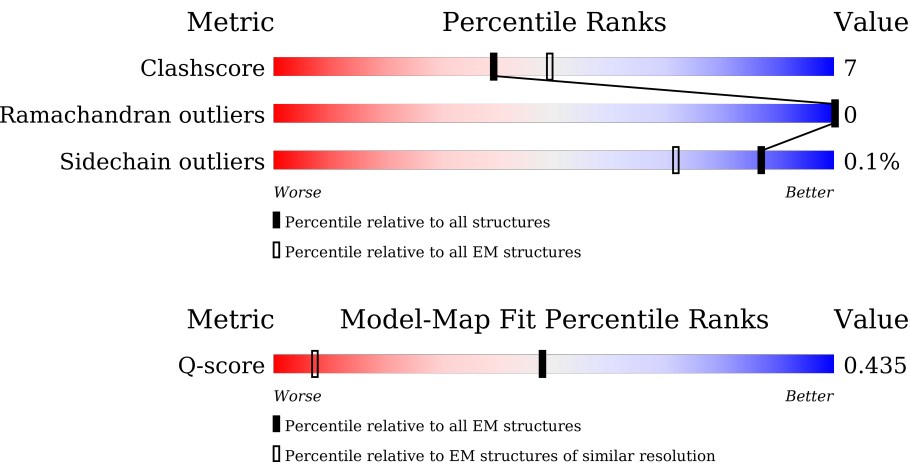
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.37 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4742 (1.87 - 2.87)

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 $\leq 5\%$. 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	1241	12% 72% 14% 14%
1	B	1241	12% 72% 14% 14%
1	C	1241	12% 72% 14% 14%
2	D	2	100% 50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	2	100%
2	J	2	100%
2	N	2	100%
2	Q	2	100%
2	R	2	100%
2	W	2	100%
2	a	2	100%
2	d	2	100%
2	e	2	100%
2	j	2	100%
2	n	2	100%
3	F	3	100%
3	H	3	67%
3	I	3	100%
3	K	3	67%
3	L	3	67%
3	M	3	100%
3	O	3	33%
3	P	3	100%
3	S	3	100%
3	U	3	67%
3	V	3	67%
3	X	3	67%
3	Y	3	67%
3	Z	3	33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	b	3	33% 100%
3	c	3	67% 100%
3	f	3	100% 100%
3	h	3	67% 100%
3	i	3	67% 67% 33%
3	k	3	100% 67% 33%
3	l	3	67% 100%
3	m	3	67% 100%
3	o	3	33% 67% 33%
3	p	3	33% 100%
4	G	5	100% 100%
4	T	5	100% 100%
4	g	5	100% 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26964 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1069	Total	C	N	O	S	0	0
			8391	5375	1392	1588	36		
1	B	1069	Total	C	N	O	S	0	0
			8391	5375	1392	1588	36		
1	C	1069	Total	C	N	O	S	0	0
			8391	5375	1392	1588	36		

There are 363 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	LEU	PRO	conflict	UNP P0DTC2
A	21	THR	ARG	conflict	UNP P0DTC2
A	26	LEU	PRO	conflict	UNP P0DTC2
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	conflict	UNP P0DTC2
A	101	THR	ILE	conflict	UNP P0DTC2
A	?	-	CYS	deletion	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	?	-	ASP	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	LYS	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	164	LYS	ASN	conflict	UNP P0DTC2
A	172	PHE	SER	conflict	UNP P0DTC2
A	187	THR	LYS	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	251	SER	PRO	conflict	UNP P0DTC2
A	326	VAL	ILE	conflict	UNP P0DTC2
A	339	TYR	GLY	conflict	UNP P0DTC2
A	348	PRO	ALA	conflict	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	435	SER	ALA	conflict	UNP P0DTC2
A	440	ARG	ASN	conflict	UNP P0DTC2
A	445	ALA	VAL	conflict	UNP P0DTC2
A	446	ASP	GLY	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	ASN	THR	conflict	UNP P0DTC2
A	484	LYS	GLU	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	529	ASN	LYS	conflict	UNP P0DTC2
A	554	ASP	GLU	conflict	UNP P0DTC2
A	575	SER	ALA	conflict	UNP P0DTC2
A	583	ASP	GLU	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	625	ARG	HIS	conflict	UNP P0DTC2
A	641	LYS	ASN	conflict	UNP P0DTC2
A	642	GLY	VAL	conflict	UNP P0DTC2
A	654	LYS	GLU	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	679	ARG	ASN	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	688	ASP	ALA	conflict	UNP P0DTC2
A	704	LEU	SER	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	764	LYS	ASN	conflict	UNP P0DTC2
A	795	THR	LYS	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	852	LYS	ALA	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1184	GLU	ASP	conflict	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	SER	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	SER	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	ILE	-	expression tag	UNP P0DTC2
A	1228	PRO	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	ALA	-	expression tag	UNP P0DTC2
A	1231	PRO	-	expression tag	UNP P0DTC2
A	1232	ARG	-	expression tag	UNP P0DTC2
A	1233	ASP	-	expression tag	UNP P0DTC2
A	1234	GLY	-	expression tag	UNP P0DTC2
A	1235	GLN	-	expression tag	UNP P0DTC2
A	1236	ALA	-	expression tag	UNP P0DTC2
A	1237	TYR	-	expression tag	UNP P0DTC2
A	1238	VAL	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	LYS	-	expression tag	UNP P0DTC2
A	1241	ASP	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2
A	1243	GLU	-	expression tag	UNP P0DTC2
A	1244	TRP	-	expression tag	UNP P0DTC2
A	1245	VAL	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1246	LEU	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	SER	-	expression tag	UNP P0DTC2
A	1249	THR	-	expression tag	UNP P0DTC2
A	1250	PHE	-	expression tag	UNP P0DTC2
A	1251	LEU	-	expression tag	UNP P0DTC2
A	1252	GLY	-	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
B	9	LEU	PRO	conflict	UNP P0DTC2
B	21	THR	ARG	conflict	UNP P0DTC2
B	26	LEU	PRO	conflict	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	conflict	UNP P0DTC2
B	101	THR	ILE	conflict	UNP P0DTC2
B	?	-	CYS	deletion	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	?	-	ASP	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	LYS	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	164	LYS	ASN	conflict	UNP P0DTC2
B	172	PHE	SER	conflict	UNP P0DTC2
B	187	THR	LYS	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	251	SER	PRO	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	326	VAL	ILE	conflict	UNP P0DTC2
B	339	TYR	GLY	conflict	UNP P0DTC2
B	348	PRO	ALA	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	conflict	UNP P0DTC2
B	408	SER	ARG	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	435	SER	ALA	conflict	UNP P0DTC2
B	440	ARG	ASN	conflict	UNP P0DTC2
B	445	ALA	VAL	conflict	UNP P0DTC2
B	446	ASP	GLY	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	ASN	THR	conflict	UNP P0DTC2
B	484	LYS	GLU	conflict	UNP P0DTC2
B	496	SER	GLY	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	529	ASN	LYS	conflict	UNP P0DTC2
B	554	ASP	GLU	conflict	UNP P0DTC2
B	575	SER	ALA	conflict	UNP P0DTC2
B	583	ASP	GLU	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	625	ARG	HIS	conflict	UNP P0DTC2
B	641	LYS	ASN	conflict	UNP P0DTC2
B	642	GLY	VAL	conflict	UNP P0DTC2
B	654	LYS	GLU	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	ARG	ASN	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	688	ASP	ALA	conflict	UNP P0DTC2
B	704	LEU	SER	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	795	THR	LYS	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	852	LYS	ALA	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1184	GLU	ASP	conflict	UNP P0DTC2
B	1218	GLY	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	SER	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	SER	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	ILE	-	expression tag	UNP P0DTC2
B	1228	PRO	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	ALA	-	expression tag	UNP P0DTC2
B	1231	PRO	-	expression tag	UNP P0DTC2
B	1232	ARG	-	expression tag	UNP P0DTC2
B	1233	ASP	-	expression tag	UNP P0DTC2
B	1234	GLY	-	expression tag	UNP P0DTC2
B	1235	GLN	-	expression tag	UNP P0DTC2
B	1236	ALA	-	expression tag	UNP P0DTC2
B	1237	TYR	-	expression tag	UNP P0DTC2
B	1238	VAL	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	LYS	-	expression tag	UNP P0DTC2
B	1241	ASP	-	expression tag	UNP P0DTC2
B	1242	GLY	-	expression tag	UNP P0DTC2
B	1243	GLU	-	expression tag	UNP P0DTC2
B	1244	TRP	-	expression tag	UNP P0DTC2
B	1245	VAL	-	expression tag	UNP P0DTC2
B	1246	LEU	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	SER	-	expression tag	UNP P0DTC2
B	1249	THR	-	expression tag	UNP P0DTC2
B	1250	PHE	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1251	LEU	-	expression tag	UNP P0DTC2
B	1252	GLY	-	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
C	9	LEU	PRO	conflict	UNP P0DTC2
C	21	THR	ARG	conflict	UNP P0DTC2
C	26	LEU	PRO	conflict	UNP P0DTC2
C	67	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	conflict	UNP P0DTC2
C	101	THR	ILE	conflict	UNP P0DTC2
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	LYS	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	164	LYS	ASN	conflict	UNP P0DTC2
C	172	PHE	SER	conflict	UNP P0DTC2
C	187	THR	LYS	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	251	SER	PRO	conflict	UNP P0DTC2
C	326	VAL	ILE	conflict	UNP P0DTC2
C	339	TYR	GLY	conflict	UNP P0DTC2
C	348	PRO	ALA	conflict	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	conflict	UNP P0DTC2
C	408	SER	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	435	SER	ALA	conflict	UNP P0DTC2
C	440	ARG	ASN	conflict	UNP P0DTC2
C	445	ALA	VAL	conflict	UNP P0DTC2
C	446	ASP	GLY	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	ASN	THR	conflict	UNP P0DTC2
C	484	LYS	GLU	conflict	UNP P0DTC2
C	496	SER	GLY	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	529	ASN	LYS	conflict	UNP P0DTC2
C	554	ASP	GLU	conflict	UNP P0DTC2
C	575	SER	ALA	conflict	UNP P0DTC2
C	583	ASP	GLU	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	625	ARG	HIS	conflict	UNP P0DTC2
C	641	LYS	ASN	conflict	UNP P0DTC2
C	642	GLY	VAL	conflict	UNP P0DTC2
C	654	LYS	GLU	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	ARG	ASN	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	688	ASP	ALA	conflict	UNP P0DTC2
C	704	LEU	SER	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	795	THR	LYS	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	852	LYS	ALA	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	969	LYS	ASN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1184	GLU	ASP	conflict	UNP P0DTC2
C	1218	GLY	-	expression tag	UNP P0DTC2
C	1219	GLY	-	expression tag	UNP P0DTC2
C	1220	SER	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	SER	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	ILE	-	expression tag	UNP P0DTC2
C	1228	PRO	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	ALA	-	expression tag	UNP P0DTC2
C	1231	PRO	-	expression tag	UNP P0DTC2
C	1232	ARG	-	expression tag	UNP P0DTC2
C	1233	ASP	-	expression tag	UNP P0DTC2
C	1234	GLY	-	expression tag	UNP P0DTC2
C	1235	GLN	-	expression tag	UNP P0DTC2
C	1236	ALA	-	expression tag	UNP P0DTC2
C	1237	TYR	-	expression tag	UNP P0DTC2
C	1238	VAL	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	LYS	-	expression tag	UNP P0DTC2
C	1241	ASP	-	expression tag	UNP P0DTC2
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	GLU	-	expression tag	UNP P0DTC2
C	1244	TRP	-	expression tag	UNP P0DTC2
C	1245	VAL	-	expression tag	UNP P0DTC2
C	1246	LEU	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	SER	-	expression tag	UNP P0DTC2
C	1249	THR	-	expression tag	UNP P0DTC2
C	1250	PHE	-	expression tag	UNP P0DTC2
C	1251	LEU	-	expression tag	UNP P0DTC2
C	1252	GLY	-	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	j	2	Total	C	N	O	0	0
			28	16	2	10		
2	n	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	P	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	Y	3	Total	C	N	O	0	0
			39	22	2	15		
3	Z	3	Total	C	N	O	0	0
			39	22	2	15		
3	b	3	Total	C	N	O	0	0
			39	22	2	15		
3	c	3	Total	C	N	O	0	0
			39	22	2	15		
3	f	3	Total	C	N	O	0	0
			39	22	2	15		
3	h	3	Total	C	N	O	0	0
			39	22	2	15		
3	i	3	Total	C	N	O	0	0
			39	22	2	15		

Continued on next page...

Continued from previous page...

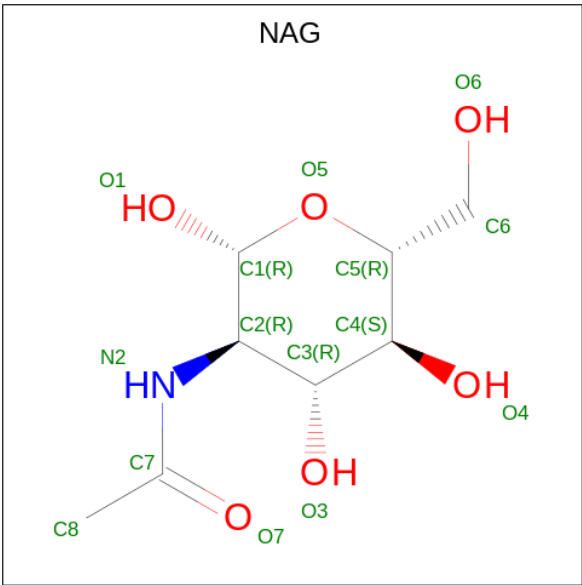
Mol	Chain	Residues	Atoms				AltConf	Trace
3	k	3	Total	C	N	O	0	0
			39	22	2	15		
3	l	3	Total	C	N	O	0	0
			39	22	2	15		
3	m	3	Total	C	N	O	0	0
			39	22	2	15		
3	o	3	Total	C	N	O	0	0
			39	22	2	15		
3	p	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	5	Total	C	N	O	0	0
			61	34	2	25		
4	T	5	Total	C	N	O	0	0
			61	34	2	25		
4	g	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

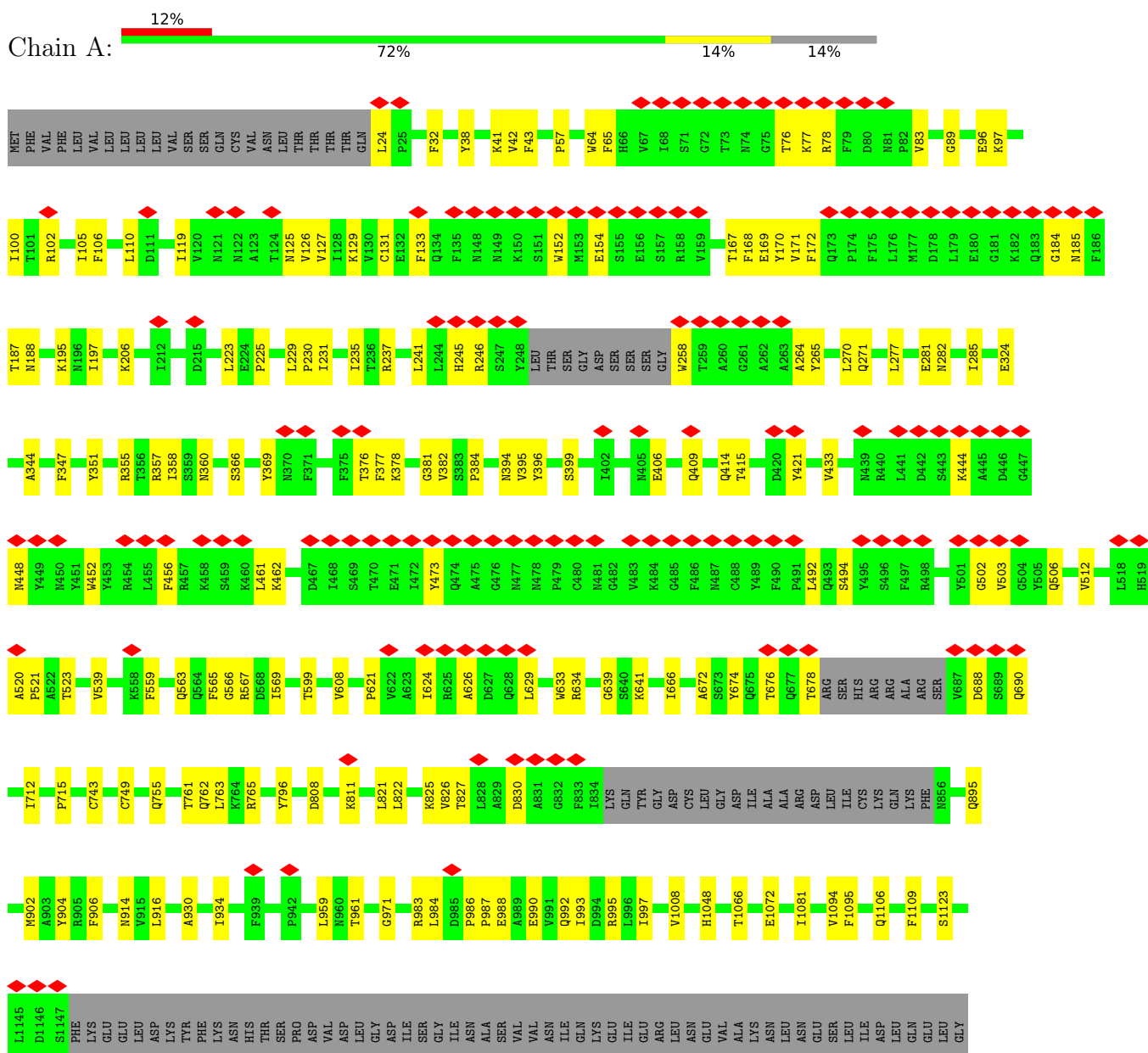
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

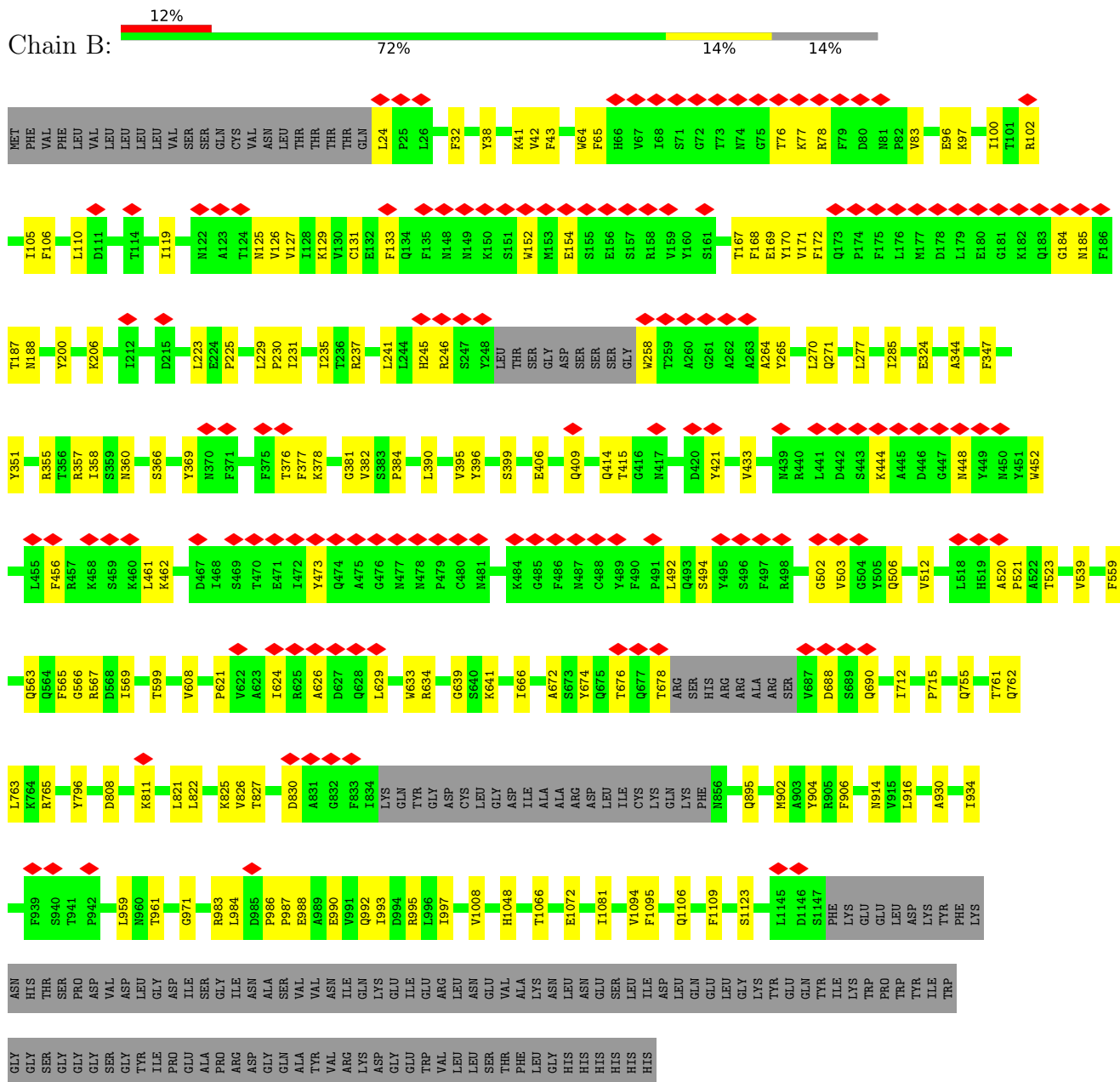
3 Residue-property plots [i](#)

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

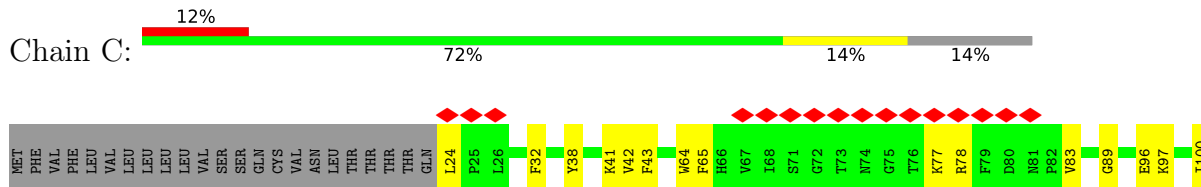
• Molecule 1: Spike glycoprotein



Chain B:



Chain C:



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



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



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



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



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



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





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



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



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



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



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



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



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



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



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



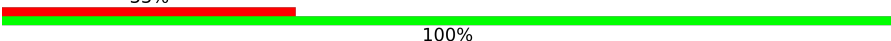
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain P:  33% 100%



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

Chain S:  100% 100%



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

Chain U:  67% 100%



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

Chain V:  67% 67% 33%

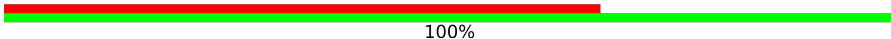


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  67% 67% 33%



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

Chain Y:  67% 100%



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



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



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



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



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



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



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



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



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



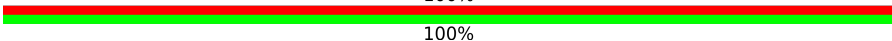
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

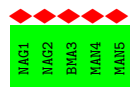


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

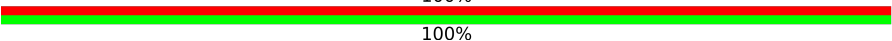


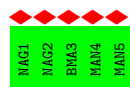
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%
100%

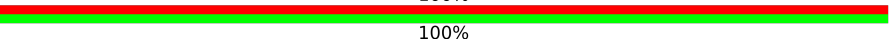


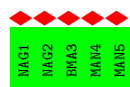
- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%
100%



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

Chain g:  100%
100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	233267	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.811	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	364.8, 364.8, 364.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.76, 0.76, 0.76	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/8598	0.47	2/11713 (0.0%)
1	B	0.23	0/8598	0.47	2/11713 (0.0%)
1	C	0.23	0/8598	0.47	2/11713 (0.0%)
All	All	0.23	0/25794	0.47	6/35139 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	PHE	CB-CA-C	-5.51	110.21	116.54
1	A	32	PHE	CB-CA-C	-5.50	110.22	116.54
1	C	32	PHE	CB-CA-C	-5.50	110.22	116.54
1	C	167	THR	O-C-N	-5.15	115.53	122.23
1	B	167	THR	O-C-N	-5.14	115.55	122.23
1	A	167	THR	O-C-N	-5.13	115.55	122.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8391	0	8179	156	0
1	B	8391	0	8179	152	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	8391	0	8179	150	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	J	28	0	25	4	0
2	N	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	1	0
2	W	28	0	25	4	0
2	a	28	0	25	0	0
2	d	28	0	25	0	0
2	e	28	0	25	1	0
2	j	28	0	25	4	0
2	n	28	0	25	0	0
3	F	39	0	34	0	0
3	H	39	0	34	0	0
3	I	39	0	34	0	0
3	K	39	0	34	5	0
3	L	39	0	34	0	0
3	M	39	0	34	0	0
3	O	39	0	34	0	0
3	P	39	0	34	0	0
3	S	39	0	34	0	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
3	X	39	0	34	4	0
3	Y	39	0	34	0	0
3	Z	39	0	34	0	0
3	b	39	0	34	0	0
3	c	39	0	34	0	0
3	f	39	0	34	0	0
3	h	39	0	34	0	0
3	i	39	0	34	0	0
3	k	39	0	34	4	0
3	l	39	0	34	0	0
3	m	39	0	34	0	0
3	o	39	0	34	1	0
3	p	39	0	34	0	0
4	G	61	0	52	0	0
4	T	61	0	52	0	0
4	g	61	0	52	0	0
5	A	112	0	104	1	0
5	B	112	0	104	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	112	0	104	1	0
All	All	26964	0	26121	383	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:2:NAG:H3	2:W:2:NAG:H83	1.30	1.11
2:j:2:NAG:H83	2:j:2:NAG:H3	1.30	1.09
2:J:2:NAG:H83	2:J:2:NAG:H3	1.30	1.08
1:A:230:PRO:HB2	1:C:357:ARG:NH1	1.75	1.00
1:C:796:TYR:CE2	3:X:1:NAG:H62	1.98	0.99
1:B:357:ARG:NH1	1:C:230:PRO:HB2	1.79	0.97
1:B:796:TYR:CE2	3:K:1:NAG:H62	1.97	0.97
1:A:796:TYR:CE2	3:k:1:NAG:H62	1.98	0.97
1:A:357:ARG:NH1	1:B:230:PRO:HB2	1.79	0.97
1:A:42:VAL:HG11	1:C:567:ARG:HD2	1.52	0.92
1:A:567:ARG:HD2	1:B:42:VAL:HG11	1.55	0.89
2:W:2:NAG:H3	2:W:2:NAG:C8	2.02	0.89
2:j:2:NAG:H3	2:j:2:NAG:C8	2.02	0.88
2:J:2:NAG:H3	2:J:2:NAG:C8	2.02	0.88
1:B:567:ARG:HD2	1:C:42:VAL:HG11	1.55	0.86
1:B:626:ALA:HB1	1:B:634:ARG:HG2	1.58	0.85
1:A:626:ALA:HB1	1:A:634:ARG:HG2	1.59	0.85
1:C:626:ALA:HB1	1:C:634:ARG:HG2	1.59	0.84
1:A:904:TYR:OH	1:C:1094:VAL:CG1	2.26	0.84
1:B:1094:VAL:CG1	1:C:904:TYR:OH	2.26	0.84
1:C:154:GLU:OE2	1:C:246:ARG:HD3	1.79	0.83
1:B:154:GLU:OE2	1:B:246:ARG:HD3	1.79	0.83
1:A:1094:VAL:CG1	1:B:904:TYR:OH	2.26	0.83
1:A:154:GLU:OE2	1:A:246:ARG:HD3	1.79	0.82
1:C:127:VAL:HG22	1:C:171:VAL:HG22	1.62	0.82
1:A:127:VAL:HG22	1:A:171:VAL:HG22	1.62	0.80
1:B:127:VAL:HG22	1:B:171:VAL:HG22	1.62	0.80
1:A:904:TYR:OH	1:C:1094:VAL:HG11	1.84	0.78
1:B:629:LEU:HD13	1:B:633:TRP:HB3	1.65	0.78
1:A:629:LEU:HD13	1:A:633:TRP:HB3	1.65	0.77
1:C:629:LEU:HD13	1:C:633:TRP:HB3	1.65	0.77
2:J:2:NAG:H83	2:J:2:NAG:C3	2.13	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.49	0.76
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.49	0.76
1:A:1094:VAL:HG11	1:B:904:TYR:OH	1.84	0.75
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.22	0.74
1:B:1094:VAL:HG11	1:C:904:TYR:OH	1.84	0.74
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.49	0.74
1:A:230:PRO:O	1:C:357:ARG:NH1	2.21	0.73
1:B:415:THR:HG23	1:C:378:LYS:HE3	1.70	0.72
1:A:357:ARG:NH1	1:B:230:PRO:O	2.21	0.72
1:A:42:VAL:HG22	1:C:565:PHE:CZ	2.24	0.71
2:W:2:NAG:H83	2:W:2:NAG:C3	2.14	0.71
1:B:563:GLN:OE1	1:C:43:PHE:HD1	1.74	0.71
1:A:415:THR:HG23	1:B:378:LYS:HE3	1.72	0.70
2:j:2:NAG:H83	2:j:2:NAG:C3	2.14	0.69
1:A:563:GLN:OE1	1:B:43:PHE:HD1	1.76	0.69
1:B:565:PHE:CZ	1:C:42:VAL:HG22	2.27	0.69
1:B:599:THR:HG22	1:B:608:VAL:HG12	1.75	0.69
1:C:599:THR:HG22	1:C:608:VAL:HG12	1.75	0.69
1:A:171:VAL:HG21	2:E:1:NAG:H62	1.75	0.68
1:B:171:VAL:HG21	2:R:1:NAG:H62	1.75	0.68
1:A:43:PHE:HD1	1:C:563:GLN:OE1	1.75	0.68
1:A:599:THR:HG22	1:A:608:VAL:HG12	1.75	0.68
1:A:378:LYS:HE3	1:C:415:THR:HG23	1.75	0.67
1:B:382:VAL:HA	1:C:983:ARG:O	1.95	0.67
1:A:521:PRO:HG3	1:B:41:LYS:HZ2	1.60	0.67
1:C:171:VAL:HG21	2:e:1:NAG:H62	1.75	0.67
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.76	0.67
1:C:83:VAL:HG11	1:C:237:ARG:HH21	1.60	0.67
1:A:433:VAL:HG22	1:A:512:VAL:HG22	1.76	0.66
1:C:433:VAL:HG22	1:C:512:VAL:HG22	1.76	0.66
1:A:762:GLN:HE21	1:C:961:THR:HG21	1.58	0.66
1:B:377:PHE:HE2	1:B:384:PRO:HB3	1.61	0.66
1:B:357:ARG:NH1	1:C:230:PRO:O	2.26	0.66
1:C:77:LYS:HE3	1:C:152:TRP:CH2	2.31	0.66
1:A:77:LYS:HE3	1:A:152:TRP:CH2	2.31	0.65
1:A:83:VAL:HG11	1:A:237:ARG:HH21	1.60	0.65
1:A:42:VAL:HG11	1:C:567:ARG:CD	2.27	0.65
1:B:83:VAL:HG11	1:B:237:ARG:HH21	1.60	0.65
1:B:77:LYS:HE3	1:B:152:TRP:CH2	2.31	0.65
1:B:961:THR:HG21	1:C:762:GLN:HE21	1.61	0.65
1:C:377:PHE:HE2	1:C:384:PRO:HB3	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:HE2	1:A:384:PRO:HB3	1.61	0.64
1:A:796:TYR:CE2	3:k:1:NAG:C6	2.80	0.64
1:A:961:THR:HG21	1:B:762:GLN:HE21	1.61	0.64
1:A:983:ARG:O	1:C:382:VAL:HA	1.98	0.64
1:A:559:PHE:CE1	1:B:43:PHE:CD2	2.86	0.64
1:B:277:LEU:HD23	1:B:285:ILE:HD13	1.80	0.64
1:C:796:TYR:CE2	3:X:1:NAG:C6	2.79	0.64
1:A:129:LYS:HG2	1:A:169:GLU:HG2	1.80	0.64
1:B:444:LYS:HE2	1:B:448:ASN:HA	1.80	0.63
1:B:796:TYR:CD2	3:K:1:NAG:H5	2.33	0.63
1:A:41:LYS:HZ2	1:C:521:PRO:HG3	1.63	0.63
1:C:277:LEU:HD23	1:C:285:ILE:HD13	1.80	0.63
1:A:277:LEU:HD23	1:A:285:ILE:HD13	1.80	0.62
1:B:621:PRO:HG3	1:B:639:GLY:H	1.64	0.62
1:B:129:LYS:HG2	1:B:169:GLU:HG2	1.80	0.62
1:C:796:TYR:CD2	3:X:1:NAG:H5	2.35	0.62
1:A:796:TYR:CD2	3:k:1:NAG:H5	2.35	0.62
1:C:129:LYS:HG2	1:C:169:GLU:HG2	1.80	0.62
1:C:621:PRO:HG3	1:C:639:GLY:H	1.64	0.62
1:A:444:LYS:HE2	1:A:448:ASN:HA	1.80	0.62
1:A:567:ARG:CD	1:B:42:VAL:HG11	2.28	0.62
1:B:796:TYR:CE2	3:K:1:NAG:C6	2.78	0.62
1:A:621:PRO:HG3	1:A:639:GLY:H	1.64	0.61
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.65	0.61
1:C:229:LEU:HB3	1:C:231:ILE:HG23	1.82	0.61
1:B:1123:SER:OG	1:C:914:ASN:ND2	2.33	0.61
1:C:444:LYS:HE2	1:C:448:ASN:HA	1.81	0.61
1:A:382:VAL:HA	1:B:983:ARG:O	2.00	0.60
1:A:229:LEU:HB3	1:A:231:ILE:HG23	1.82	0.60
1:C:65:PHE:HD2	1:C:265:TYR:HH	1.49	0.60
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.65	0.60
1:A:971:GLY:HA3	1:A:995:ARG:HH21	1.65	0.60
1:A:1123:SER:OG	1:B:914:ASN:ND2	2.34	0.60
1:B:229:LEU:HB3	1:B:231:ILE:HG23	1.82	0.60
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.84	0.60
1:B:521:PRO:HG3	1:C:41:LYS:HZ2	1.66	0.60
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.84	0.59
1:B:127:VAL:HG22	1:B:171:VAL:CG2	2.31	0.59
1:A:914:ASN:ND2	1:C:1123:SER:OG	2.34	0.59
1:A:127:VAL:HG22	1:A:171:VAL:CG2	2.31	0.59
1:B:357:ARG:HH12	1:C:230:PRO:HB2	1.65	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.84	0.59
1:C:127:VAL:HG22	1:C:171:VAL:CG2	2.31	0.59
1:C:77:LYS:HE3	1:C:152:TRP:CZ2	2.38	0.58
1:A:43:PHE:CD2	1:C:559:PHE:CE1	2.91	0.58
1:B:77:LYS:HE3	1:B:152:TRP:CZ2	2.38	0.58
1:A:77:LYS:HE3	1:A:152:TRP:CZ2	2.38	0.58
1:B:559:PHE:CE1	1:C:43:PHE:CD2	2.91	0.58
1:B:567:ARG:CD	1:C:42:VAL:HG11	2.31	0.57
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.87	0.56
1:A:762:GLN:NE2	1:C:961:THR:HG21	2.19	0.56
1:C:376:THR:HG23	1:C:378:LYS:HD3	1.88	0.56
1:B:358:ILE:HB	1:B:395:VAL:HB	1.88	0.55
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.87	0.55
1:B:761:THR:HG22	1:B:765:ARG:HH21	1.71	0.55
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.87	0.55
1:A:376:THR:HG23	1:A:378:LYS:HD3	1.88	0.55
1:A:358:ILE:HB	1:A:395:VAL:HB	1.88	0.55
1:A:930:ALA:O	1:A:934:ILE:HG12	2.07	0.55
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.89	0.55
1:C:358:ILE:HB	1:C:395:VAL:HB	1.88	0.55
1:C:761:THR:HG22	1:C:765:ARG:HH21	1.71	0.55
1:A:357:ARG:HH12	1:B:230:PRO:HB2	1.69	0.55
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.89	0.54
1:C:930:ALA:O	1:C:934:ILE:HG12	2.07	0.54
1:B:930:ALA:O	1:B:934:ILE:HG12	2.07	0.54
1:B:376:THR:HG23	1:B:378:LYS:HD3	1.88	0.54
1:A:961:THR:HG21	1:B:762:GLN:NE2	2.21	0.54
1:C:565:PHE:HE2	1:C:567:ARG:NE	2.05	0.54
1:A:761:THR:HG22	1:A:765:ARG:HH21	1.71	0.54
1:A:65:PHE:HD2	1:A:265:TYR:HH	1.56	0.54
1:A:565:PHE:CE2	1:B:42:VAL:HG22	2.41	0.54
1:B:961:THR:HG21	1:C:762:GLN:NE2	2.22	0.54
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.89	0.54
1:B:65:PHE:HD2	1:B:265:TYR:HH	1.56	0.53
1:A:565:PHE:HE2	1:A:567:ARG:NE	2.05	0.53
1:A:986:PRO:O	1:A:990:GLU:HG2	2.08	0.53
1:B:986:PRO:O	1:B:990:GLU:HG2	2.08	0.53
1:B:24:LEU:HD13	1:B:78:ARG:HH11	1.74	0.53
1:B:565:PHE:HE2	1:B:567:ARG:NE	2.05	0.53
1:A:42:VAL:HG22	1:C:565:PHE:CE2	2.44	0.53
1:C:986:PRO:O	1:C:990:GLU:HG2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD13	1:A:78:ARG:HH11	1.74	0.52
1:B:971:GLY:H	1:C:755:GLN:NE2	2.08	0.52
1:C:206:LYS:HB2	1:C:223:LEU:HG	1.92	0.52
1:C:24:LEU:HD13	1:C:78:ARG:HH11	1.74	0.52
1:B:796:TYR:CD2	3:K:1:NAG:C5	2.92	0.52
1:C:409:GLN:HA	1:C:414:GLN:HG2	1.92	0.52
1:A:206:LYS:HB2	1:A:223:LEU:HG	1.92	0.51
1:B:674:TYR:CZ	1:B:690:GLN:HB3	2.45	0.51
1:A:674:TYR:CZ	1:A:690:GLN:HB3	2.45	0.51
1:A:38:TYR:HB2	1:A:225:PRO:HD3	1.92	0.51
1:A:796:TYR:CD2	3:k:1:NAG:C5	2.93	0.51
1:C:38:TYR:HB2	1:C:225:PRO:HD3	1.93	0.51
1:C:796:TYR:CD2	3:X:1:NAG:C5	2.93	0.51
1:A:409:GLN:HA	1:A:414:GLN:HG2	1.92	0.51
1:B:993:ILE:O	1:B:997:ILE:HG13	2.11	0.51
1:C:674:TYR:CZ	1:C:690:GLN:HB3	2.45	0.51
1:C:993:ILE:O	1:C:997:ILE:HG13	2.11	0.51
1:B:38:TYR:HB2	1:B:225:PRO:HD3	1.93	0.51
1:B:206:LYS:HB2	1:B:223:LEU:HG	1.92	0.51
1:C:355:ARG:HD2	1:C:396:TYR:HB3	1.93	0.51
1:A:993:ILE:O	1:A:997:ILE:HG13	2.11	0.50
1:A:762:GLN:HE21	1:C:961:THR:CG2	2.24	0.50
1:A:184:GLY:HA3	5:A:1303:NAG:H82	1.94	0.50
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.94	0.50
1:A:755:GLN:NE2	1:C:971:GLY:H	2.10	0.50
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.76	0.50
1:A:355:ARG:HD2	1:A:396:TYR:HB3	1.93	0.49
1:B:409:GLN:HA	1:B:414:GLN:HG2	1.92	0.49
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.94	0.49
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.94	0.49
1:A:43:PHE:HB3	1:C:566:GLY:HA2	1.94	0.49
1:A:406:GLU:HA	1:A:409:GLN:HG3	1.94	0.49
1:A:559:PHE:HE1	1:B:43:PHE:CD2	2.30	0.49
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.76	0.49
1:B:406:GLU:HA	1:B:409:GLN:HG3	1.94	0.49
1:B:355:ARG:HD2	1:B:396:TYR:HB3	1.93	0.49
1:C:184:GLY:HA3	5:C:1303:NAG:H82	1.94	0.49
1:B:565:PHE:CE2	1:C:42:VAL:HG22	2.47	0.49
1:C:406:GLU:HA	1:C:409:GLN:HG3	1.94	0.49
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.76	0.48
1:C:906:PHE:CE2	1:C:916:LEU:HD12	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:PHE:HE2	1:A:473:TYR:CG	2.32	0.48
1:A:906:PHE:CE2	1:A:916:LEU:HD12	2.49	0.48
1:B:184:GLY:HA3	5:B:1303:NAG:H82	1.94	0.48
1:B:906:PHE:CE2	1:B:916:LEU:HD12	2.48	0.48
1:B:961:THR:CG2	1:C:762:GLN:HE21	2.27	0.48
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.96	0.48
1:B:83:VAL:HG21	1:B:237:ARG:CZ	2.44	0.48
1:A:971:GLY:H	1:B:755:GLN:NE2	2.12	0.47
1:B:456:PHE:HE2	1:B:473:TYR:CG	2.32	0.47
1:B:624:ILE:HG22	1:B:629:LEU:HD11	1.96	0.47
1:C:100:ILE:HD12	1:C:100:ILE:H	1.79	0.47
1:C:902:MET:HB3	1:C:916:LEU:HD11	1.96	0.47
1:A:100:ILE:HD12	1:A:100:ILE:H	1.79	0.47
1:A:988:GLU:O	1:A:992:GLN:HG2	2.15	0.47
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.96	0.47
1:A:131:CYS:HB2	1:A:133:PHE:CZ	2.50	0.47
1:A:230:PRO:HB2	1:C:357:ARG:HH12	1.64	0.47
1:B:100:ILE:HD12	1:B:100:ILE:H	1.79	0.47
1:B:131:CYS:HB2	1:B:133:PHE:CZ	2.50	0.47
1:C:119:ILE:HG22	1:C:119:ILE:O	2.15	0.47
1:A:125:ASN:HB3	1:A:172:PHE:O	2.14	0.47
1:A:168:PHE:CZ	1:A:170:TYR:HB3	2.49	0.47
1:A:357:ARG:HH11	1:B:230:PRO:HB2	1.74	0.47
1:B:119:ILE:HG22	1:B:119:ILE:O	2.15	0.47
1:B:902:MET:HB3	1:B:916:LEU:HD11	1.96	0.47
1:C:456:PHE:HE2	1:C:473:TYR:CG	2.32	0.47
1:A:624:ILE:HG22	1:A:629:LEU:HD11	1.96	0.47
1:B:168:PHE:CZ	1:B:170:TYR:HB3	2.49	0.47
1:B:827:THR:HA	1:B:830:ASP:HB2	1.97	0.47
1:C:125:ASN:HB3	1:C:172:PHE:O	2.15	0.47
1:C:324:GLU:H	1:C:539:VAL:HG12	1.80	0.47
1:A:566:GLY:HA2	1:B:43:PHE:HB3	1.96	0.47
1:A:827:THR:HA	1:A:830:ASP:HB2	1.97	0.47
1:A:1094:VAL:HG11	1:B:904:TYR:HH	1.79	0.47
1:B:125:ASN:HB3	1:B:172:PHE:O	2.14	0.47
1:B:988:GLU:O	1:B:992:GLN:HG2	2.15	0.47
1:C:83:VAL:HG21	1:C:237:ARG:CZ	2.44	0.47
1:C:131:CYS:HB2	1:C:133:PHE:CZ	2.50	0.47
1:B:502:GLY:O	1:B:506:GLN:HG3	2.15	0.47
1:C:168:PHE:CZ	1:C:170:TYR:HB3	2.49	0.47
1:C:452:TRP:CE2	1:C:494:SER:HB2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:TRP:CE2	1:A:494:SER:HB2	2.50	0.46
1:B:566:GLY:HA2	1:C:43:PHE:HB3	1.97	0.46
1:C:360:ASN:H	1:C:523:THR:HG23	1.80	0.46
1:C:827:THR:HA	1:C:830:ASP:HB2	1.97	0.46
1:C:988:GLU:O	1:C:992:GLN:HG2	2.15	0.46
1:A:666:ILE:HD11	1:A:672:ALA:HB2	1.96	0.46
1:A:83:VAL:HG21	1:A:237:ARG:CZ	2.44	0.46
1:A:119:ILE:O	1:A:119:ILE:HG22	2.15	0.46
1:A:902:MET:HB3	1:A:916:LEU:HD11	1.97	0.46
1:A:904:TYR:HH	1:C:1094:VAL:HG11	1.79	0.46
1:B:821:LEU:O	1:B:825:LYS:HG3	2.16	0.46
2:j:2:NAG:C1	2:j:2:NAG:H82	2.46	0.46
1:C:624:ILE:HG22	1:C:629:LEU:HD11	1.96	0.46
1:B:381:GLY:O	1:C:984:LEU:HD21	2.15	0.46
1:A:324:GLU:H	1:A:539:VAL:HG12	1.80	0.46
1:A:360:ASN:H	1:A:523:THR:HG23	1.80	0.46
1:B:106:PHE:HD1	1:B:235:ILE:HG21	1.81	0.46
2:J:2:NAG:C1	2:J:2:NAG:H82	2.46	0.46
1:A:381:GLY:O	1:B:984:LEU:HD21	2.17	0.45
1:B:452:TRP:CE2	1:B:494:SER:HB2	2.50	0.45
1:C:676:THR:HG22	1:C:690:GLN:OE1	2.16	0.45
1:C:986:PRO:HB2	1:C:987:PRO:HD3	1.98	0.45
1:C:821:LEU:O	1:C:825:LYS:HG3	2.16	0.45
2:W:2:NAG:H82	2:W:2:NAG:C1	2.46	0.45
1:A:821:LEU:O	1:A:825:LYS:HG3	2.16	0.45
1:B:324:GLU:H	1:B:539:VAL:HG12	1.80	0.45
1:A:502:GLY:O	1:A:506:GLN:HG3	2.15	0.45
1:C:502:GLY:O	1:C:506:GLN:HG3	2.15	0.45
1:A:106:PHE:HD1	1:A:235:ILE:HG21	1.81	0.45
1:B:360:ASN:H	1:B:523:THR:HG23	1.80	0.45
1:B:676:THR:HG22	1:B:690:GLN:OE1	2.16	0.45
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.98	0.45
1:A:961:THR:CG2	1:B:762:GLN:HE21	2.26	0.45
1:C:106:PHE:HD1	1:C:235:ILE:HG21	1.81	0.45
1:C:96:GLU:O	1:C:188:ASN:OD1	2.35	0.45
1:B:712:ILE:HD12	1:C:895:GLN:O	2.17	0.45
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.98	0.44
1:B:569:ILE:HD12	1:B:569:ILE:H	1.82	0.44
1:A:230:PRO:HB2	1:C:357:ARG:HH11	1.74	0.44
1:A:366:SER:HA	1:A:369:TYR:CE1	2.52	0.44
1:C:808:ASP:HB3	1:C:811:LYS:HE3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HD23	1:A:462:LYS:O	2.17	0.44
1:A:676:THR:HG22	1:A:690:GLN:OE1	2.16	0.44
1:B:366:SER:HA	1:B:369:TYR:CE1	2.52	0.44
1:A:569:ILE:HD12	1:A:569:ILE:H	1.83	0.44
1:A:678:THR:HA	1:A:688:ASP:HA	1.99	0.44
1:C:678:THR:HA	1:C:688:ASP:HA	1.99	0.44
1:B:96:GLU:O	1:B:188:ASN:OD1	2.35	0.44
1:C:126:VAL:O	1:C:171:VAL:HA	2.18	0.44
1:C:366:SER:HA	1:C:369:TYR:CE1	2.52	0.44
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.83	0.44
1:A:712:ILE:HD12	1:B:895:GLN:O	2.18	0.44
1:A:895:GLN:O	1:C:712:ILE:HD12	2.18	0.44
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.86	0.44
1:B:415:THR:CG2	1:C:378:LYS:HE3	2.42	0.44
1:B:461:LEU:HD23	1:B:462:LYS:O	2.17	0.44
1:A:415:THR:CG2	1:B:378:LYS:HE3	2.44	0.44
1:B:357:ARG:HH11	1:C:230:PRO:HB2	1.77	0.44
1:A:96:GLU:O	1:A:188:ASN:OD1	2.35	0.43
1:B:126:VAL:O	1:B:171:VAL:HA	2.18	0.43
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.83	0.43
1:C:102:ARG:HD3	1:C:245:HIS:HB2	2.00	0.43
1:C:569:ILE:H	1:C:569:ILE:HD12	1.83	0.43
1:A:377:PHE:CE2	1:A:384:PRO:HB3	2.48	0.43
1:A:1106:GLN:HE21	1:A:1109:PHE:HB3	1.83	0.43
1:B:97:LYS:HE2	1:B:187:THR:N	2.33	0.43
1:B:347:PHE:CE2	1:B:399:SER:HB3	2.54	0.43
1:B:808:ASP:HB3	1:B:811:LYS:HE3	2.00	0.43
1:A:97:LYS:HE2	1:A:187:THR:N	2.33	0.43
1:A:126:VAL:O	1:A:171:VAL:HA	2.18	0.43
1:B:246:ARG:HG2	1:B:258:TRP:CE3	2.53	0.43
1:C:461:LEU:HD23	1:C:462:LYS:O	2.17	0.43
1:A:102:ARG:HD3	1:A:245:HIS:HB2	2.00	0.43
1:B:102:ARG:HD3	1:B:245:HIS:HB2	2.00	0.43
1:B:678:THR:HA	1:B:688:ASP:HA	1.99	0.43
1:A:105:ILE:HG22	1:A:110:LEU:HD22	2.01	0.43
1:A:246:ARG:HG2	1:A:258:TRP:CE3	2.53	0.43
1:A:347:PHE:CE2	1:A:399:SER:HB3	2.54	0.43
1:C:246:ARG:HG2	1:C:258:TRP:CE3	2.53	0.43
1:A:41:LYS:HZ2	1:C:521:PRO:CG	2.31	0.43
1:C:97:LYS:HE2	1:C:187:THR:N	2.33	0.43
1:C:105:ILE:HG22	1:C:110:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ASP:HB3	1:A:811:LYS:HE3	1.99	0.42
1:A:521:PRO:CG	1:B:41:LYS:HZ2	2.27	0.42
1:B:822:LEU:O	1:B:826:VAL:HG23	2.19	0.42
1:B:971:GLY:HA2	1:C:755:GLN:NE2	2.34	0.42
1:C:822:LEU:O	1:C:826:VAL:HG23	2.19	0.42
1:A:378:LYS:HE3	1:C:415:THR:CG2	2.46	0.42
1:A:822:LEU:O	1:A:826:VAL:HG23	2.19	0.42
1:C:347:PHE:CE2	1:C:399:SER:HB3	2.54	0.42
1:A:984:LEU:HD21	1:C:381:GLY:O	2.20	0.42
1:B:559:PHE:HE1	1:C:43:PHE:CD2	2.36	0.42
1:B:959:LEU:HD23	1:B:959:LEU:HA	1.85	0.42
1:B:1094:VAL:HG11	1:C:904:TYR:HH	1.78	0.42
1:A:825:LYS:HB3	1:A:825:LYS:HE2	1.89	0.42
1:B:377:PHE:CE2	1:B:384:PRO:HB3	2.48	0.42
1:B:415:THR:HG21	1:C:378:LYS:HG3	2.02	0.42
1:C:421:TYR:CD2	1:C:456:PHE:HA	2.55	0.42
1:C:270:LEU:O	1:C:271:GLN:HG3	2.20	0.42
1:A:43:PHE:CD2	1:C:559:PHE:HE1	2.35	0.42
1:B:421:TYR:CD2	1:B:456:PHE:HA	2.55	0.42
1:C:503:VAL:HA	1:C:506:GLN:CD	2.45	0.42
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.55	0.42
1:A:452:TRP:HA	1:A:494:SER:HA	2.02	0.41
1:B:270:LEU:O	1:B:271:GLN:HG3	2.20	0.41
1:B:492:LEU:HD23	1:B:492:LEU:H	1.85	0.41
1:B:503:VAL:HA	1:B:506:GLN:CD	2.45	0.41
1:B:796:TYR:HE2	3:K:1:NAG:H62	1.74	0.41
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.55	0.41
1:B:1081:ILE:HG12	1:B:1095:PHE:CE2	2.55	0.41
1:A:503:VAL:HA	1:A:506:GLN:CD	2.45	0.41
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.98	0.41
1:C:377:PHE:CE2	1:C:384:PRO:HB3	2.48	0.41
1:A:421:TYR:CD2	1:A:456:PHE:HA	2.55	0.41
1:A:492:LEU:H	1:A:492:LEU:HD23	1.85	0.41
1:B:105:ILE:HG22	1:B:110:LEU:HD22	2.01	0.41
1:C:351:TYR:HE1	1:C:452:TRP:HB2	1.86	0.41
1:A:394:ASN:ND2	1:B:200:TYR:OH	2.53	0.41
1:B:351:TYR:HE1	1:B:452:TRP:HB2	1.86	0.41
1:B:390:LEU:HD21	1:C:982:SER:O	2.21	0.41
1:A:559:PHE:CE1	1:B:43:PHE:CG	3.08	0.41
1:B:105:ILE:HD11	1:B:241:LEU:HD21	2.03	0.41
1:C:452:TRP:HA	1:C:494:SER:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:THR:HG22	1:A:76:THR:O	2.21	0.41
1:A:270:LEU:O	1:A:271:GLN:HG3	2.20	0.41
1:A:89:GLY:HA3	1:A:270:LEU:HD12	2.03	0.41
1:A:105:ILE:HD11	1:A:241:LEU:HD21	2.03	0.41
1:A:281:GLU:HG3	1:A:282:ASN:OD1	2.21	0.41
1:B:641:LYS:HG3	1:B:641:LYS:O	2.21	0.41
1:C:281:GLU:HG3	1:C:282:ASN:OD1	2.21	0.41
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.85	0.41
1:A:641:LYS:O	1:A:641:LYS:HG3	2.21	0.41
1:A:351:TYR:HE1	1:A:452:TRP:HB2	1.86	0.40
1:B:76:THR:O	1:B:76:THR:HG22	2.21	0.40
1:A:57:PRO:HG2	1:A:271:GLN:OE1	2.22	0.40
1:A:195:LYS:HB3	1:A:197:ILE:CD1	2.51	0.40
1:C:89:GLY:HA3	1:C:270:LEU:HD12	2.03	0.40
1:C:127:VAL:HA	1:C:171:VAL:HG22	2.03	0.40
1:C:436:TRP:NE1	1:C:509:ARG:HD2	2.37	0.40
1:C:1103:PHE:HZ	3:o:1:NAG:H62	1.87	0.40
1:A:127:VAL:HA	1:A:171:VAL:HG22	2.03	0.40
1:A:415:THR:HG21	1:B:378:LYS:HG3	2.02	0.40
1:A:521:PRO:HG3	1:B:41:LYS:NZ	2.34	0.40
1:B:452:TRP:HA	1:B:494:SER:HA	2.03	0.40
1:C:195:LYS:HB3	1:C:197:ILE:CD1	2.51	0.40
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1061/1241 (86%)	1016 (96%)	45 (4%)	0	100	100
1	B	1061/1241 (86%)	1016 (96%)	45 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1061/1241 (86%)	1016 (96%)	45 (4%)	0	100	100
All	All	3183/3723 (86%)	3048 (96%)	135 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	938/1087 (86%)	937 (100%)	1 (0%)	88	95
1	B	938/1087 (86%)	937 (100%)	1 (0%)	88	95
1	C	938/1087 (86%)	937 (100%)	1 (0%)	88	95
All	All	2814/3261 (86%)	2811 (100%)	3 (0%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	B	185	ASN
1	C	185	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	GLN
1	A	388	ASN
1	A	394	ASN
1	A	437	ASN
1	A	755	GLN
1	A	762	GLN
1	A	926	GLN
1	A	992	GLN
1	A	1054	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1071	GLN
1	A	1142	GLN
1	B	321	GLN
1	B	388	ASN
1	B	394	ASN
1	B	437	ASN
1	B	755	GLN
1	B	762	GLN
1	B	914	ASN
1	B	926	GLN
1	B	992	GLN
1	B	1058	HIS
1	B	1071	GLN
1	B	1106	GLN
1	B	1142	GLN
1	C	321	GLN
1	C	388	ASN
1	C	394	ASN
1	C	437	ASN
1	C	755	GLN
1	C	762	GLN
1	C	914	ASN
1	C	926	GLN
1	C	992	GLN
1	C	1071	GLN
1	C	1106	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

111 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.38	0	17,19,21	0.59	0
2	NAG	D	2	2	14,14,15	0.37	0	17,19,21	1.02	2 (11%)
2	NAG	E	1	2,1	14,14,15	0.38	0	17,19,21	0.54	0
2	NAG	E	2	2	14,14,15	0.38	0	17,19,21	0.40	0
3	NAG	F	1	3,1	14,14,15	0.38	0	17,19,21	0.56	0
3	NAG	F	2	3	14,14,15	0.37	0	17,19,21	0.58	0
3	BMA	F	3	3	11,11,12	0.30	0	15,15,17	0.48	0
4	NAG	G	1	1,4	14,14,15	0.38	0	17,19,21	0.68	0
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	0.46	0
4	BMA	G	3	4	11,11,12	0.29	0	15,15,17	0.58	0
4	MAN	G	4	4	11,11,12	0.32	0	15,15,17	0.47	0
4	MAN	G	5	4	11,11,12	0.31	0	15,15,17	0.59	0
3	NAG	H	1	3,1	14,14,15	0.40	0	17,19,21	0.49	0
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	0.48	0
3	BMA	H	3	3	11,11,12	0.27	0	15,15,17	0.58	0
3	NAG	I	1	3,1	14,14,15	0.38	0	17,19,21	0.71	1 (5%)
3	NAG	I	2	3	14,14,15	0.38	0	17,19,21	0.53	0
3	BMA	I	3	3	11,11,12	0.27	0	15,15,17	0.57	0
2	NAG	J	1	2,1	14,14,15	0.38	0	17,19,21	1.15	2 (11%)
2	NAG	J	2	2	14,14,15	0.38	0	17,19,21	0.42	0
3	NAG	K	1	3,1	14,14,15	0.39	0	17,19,21	0.64	0
3	NAG	K	2	3	14,14,15	0.38	0	17,19,21	0.45	0
3	BMA	K	3	3	11,11,12	0.27	0	15,15,17	0.57	0
3	NAG	L	1	3,1	14,14,15	0.38	0	17,19,21	0.60	0
3	NAG	L	2	3	14,14,15	0.41	0	17,19,21	0.43	0
3	BMA	L	3	3	11,11,12	0.28	0	15,15,17	0.53	0
3	NAG	M	1	3,1	14,14,15	0.40	0	17,19,21	0.62	0
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	0.46	0
3	BMA	M	3	3	11,11,12	0.27	0	15,15,17	0.55	0
2	NAG	N	1	2,1	14,14,15	0.40	0	17,19,21	1.18	2 (11%)
2	NAG	N	2	2	14,14,15	0.38	0	17,19,21	0.53	0
3	NAG	O	1	3,1	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	O	2	3	14,14,15	0.38	0	17,19,21	0.52	0
3	BMA	O	3	3	11,11,12	0.28	0	15,15,17	0.55	0
3	NAG	P	1	3,1	14,14,15	0.40	0	17,19,21	0.56	0
3	NAG	P	2	3	14,14,15	0.39	0	17,19,21	0.46	0
3	BMA	P	3	3	11,11,12	0.26	0	15,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Q	1	2,1	14,14,15	0.38	0	17,19,21	0.59	0
2	NAG	Q	2	2	14,14,15	0.36	0	17,19,21	1.02	2 (11%)
2	NAG	R	1	2,1	14,14,15	0.38	0	17,19,21	0.54	0
2	NAG	R	2	2	14,14,15	0.38	0	17,19,21	0.41	0
3	NAG	S	1	3,1	14,14,15	0.39	0	17,19,21	0.57	0
3	NAG	S	2	3	14,14,15	0.37	0	17,19,21	0.58	0
3	BMA	S	3	3	11,11,12	0.29	0	15,15,17	0.47	0
4	NAG	T	1	1,4	14,14,15	0.38	0	17,19,21	0.68	0
4	NAG	T	2	4	14,14,15	0.38	0	17,19,21	0.46	0
4	BMA	T	3	4	11,11,12	0.28	0	15,15,17	0.59	0
4	MAN	T	4	4	11,11,12	0.33	0	15,15,17	0.48	0
4	MAN	T	5	4	11,11,12	0.32	0	15,15,17	0.60	0
3	NAG	U	1	3,1	14,14,15	0.39	0	17,19,21	0.49	0
3	NAG	U	2	3	14,14,15	0.40	0	17,19,21	0.48	0
3	BMA	U	3	3	11,11,12	0.26	0	15,15,17	0.58	0
3	NAG	V	1	3,1	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
3	NAG	V	2	3	14,14,15	0.38	0	17,19,21	0.53	0
3	BMA	V	3	3	11,11,12	0.28	0	15,15,17	0.57	0
2	NAG	W	1	2,1	14,14,15	0.38	0	17,19,21	1.15	2 (11%)
2	NAG	W	2	2	14,14,15	0.38	0	17,19,21	0.41	0
3	NAG	X	1	3,1	14,14,15	0.38	0	17,19,21	0.63	0
3	NAG	X	2	3	14,14,15	0.39	0	17,19,21	0.45	0
3	BMA	X	3	3	11,11,12	0.27	0	15,15,17	0.56	0
3	NAG	Y	1	3,1	14,14,15	0.37	0	17,19,21	0.60	0
3	NAG	Y	2	3	14,14,15	0.41	0	17,19,21	0.43	0
3	BMA	Y	3	3	11,11,12	0.28	0	15,15,17	0.54	0
3	NAG	Z	1	3,1	14,14,15	0.41	0	17,19,21	0.62	0
3	NAG	Z	2	3	14,14,15	0.40	0	17,19,21	0.46	0
3	BMA	Z	3	3	11,11,12	0.27	0	15,15,17	0.55	0
2	NAG	a	1	2,1	14,14,15	0.39	0	17,19,21	1.18	2 (11%)
2	NAG	a	2	2	14,14,15	0.39	0	17,19,21	0.54	0
3	NAG	b	1	3,1	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	b	2	3	14,14,15	0.38	0	17,19,21	0.53	0
3	BMA	b	3	3	11,11,12	0.26	0	15,15,17	0.55	0
3	NAG	c	1	3,1	14,14,15	0.40	0	17,19,21	0.55	0
3	NAG	c	2	3	14,14,15	0.39	0	17,19,21	0.46	0
3	BMA	c	3	3	11,11,12	0.28	0	15,15,17	0.57	0
2	NAG	d	1	2,1	14,14,15	0.38	0	17,19,21	0.59	0
2	NAG	d	2	2	14,14,15	0.38	0	17,19,21	1.02	2 (11%)
2	NAG	e	1	2,1	14,14,15	0.38	0	17,19,21	0.54	0
2	NAG	e	2	2	14,14,15	0.38	0	17,19,21	0.40	0
3	NAG	f	1	3,1	14,14,15	0.39	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	f	2	3	14,14,15	0.37	0	17,19,21	0.58	0
3	BMA	f	3	3	11,11,12	0.29	0	15,15,17	0.48	0
4	NAG	g	1	1,4	14,14,15	0.38	0	17,19,21	0.68	0
4	NAG	g	2	4	14,14,15	0.37	0	17,19,21	0.46	0
4	BMA	g	3	4	11,11,12	0.29	0	15,15,17	0.59	0
4	MAN	g	4	4	11,11,12	0.32	0	15,15,17	0.48	0
4	MAN	g	5	4	11,11,12	0.31	0	15,15,17	0.60	0
3	NAG	h	1	3,1	14,14,15	0.41	0	17,19,21	0.49	0
3	NAG	h	2	3	14,14,15	0.40	0	17,19,21	0.48	0
3	BMA	h	3	3	11,11,12	0.27	0	15,15,17	0.58	0
3	NAG	i	1	3,1	14,14,15	0.39	0	17,19,21	0.72	1 (5%)
3	NAG	i	2	3	14,14,15	0.38	0	17,19,21	0.52	0
3	BMA	i	3	3	11,11,12	0.26	0	15,15,17	0.56	0
2	NAG	j	1	2,1	14,14,15	0.38	0	17,19,21	1.15	2 (11%)
2	NAG	j	2	2	14,14,15	0.39	0	17,19,21	0.42	0
3	NAG	k	1	3,1	14,14,15	0.40	0	17,19,21	0.64	0
3	NAG	k	2	3	14,14,15	0.38	0	17,19,21	0.46	0
3	BMA	k	3	3	11,11,12	0.26	0	15,15,17	0.58	0
3	NAG	l	1	3,1	14,14,15	0.38	0	17,19,21	0.60	0
3	NAG	l	2	3	14,14,15	0.41	0	17,19,21	0.43	0
3	BMA	l	3	3	11,11,12	0.28	0	15,15,17	0.54	0
3	NAG	m	1	3,1	14,14,15	0.41	0	17,19,21	0.62	0
3	NAG	m	2	3	14,14,15	0.40	0	17,19,21	0.45	0
3	BMA	m	3	3	11,11,12	0.27	0	15,15,17	0.54	0
2	NAG	n	1	2,1	14,14,15	0.40	0	17,19,21	1.19	2 (11%)
2	NAG	n	2	2	14,14,15	0.38	0	17,19,21	0.53	0
3	NAG	o	1	3,1	14,14,15	0.38	0	17,19,21	0.49	0
3	NAG	o	2	3	14,14,15	0.38	0	17,19,21	0.53	0
3	BMA	o	3	3	11,11,12	0.28	0	15,15,17	0.54	0
3	NAG	p	1	3,1	14,14,15	0.41	0	17,19,21	0.56	0
3	NAG	p	2	3	14,14,15	0.38	0	17,19,21	0.46	0
3	BMA	p	3	3	11,11,12	0.26	0	15,15,17	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	BMA	M	3	3	-	0/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	N	2	2	-	3/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	1/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	4/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	T	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	BMA	T	3	4	-	0/2/19/22	0/1/1/1
4	MAN	T	4	4	-	0/2/19/22	0/1/1/1
4	MAN	T	5	4	-	0/2/19/22	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
3	NAG	V	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
2	NAG	W	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	W	2	2	-	3/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Y	3	3	-	0/2/19/22	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Z	3	3	-	0/2/19/22	0/1/1/1
2	NAG	a	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	a	2	2	-	3/6/23/26	0/1/1/1
3	NAG	b	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	0/6/23/26	0/1/1/1
3	BMA	b	3	3	-	1/2/19/22	0/1/1/1
3	NAG	c	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	0/6/23/26	0/1/1/1
3	BMA	c	3	3	-	0/2/19/22	0/1/1/1
2	NAG	d	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	4/6/23/26	0/1/1/1
2	NAG	e	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
3	NAG	f	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	f	2	3	-	0/6/23/26	0/1/1/1
3	BMA	f	3	3	-	1/2/19/22	0/1/1/1
4	NAG	g	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	g	2	4	-	0/6/23/26	0/1/1/1
4	BMA	g	3	4	-	0/2/19/22	0/1/1/1
4	MAN	g	4	4	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	g	5	4	-	0/2/19/22	0/1/1/1
3	NAG	h	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	h	2	3	-	0/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
3	NAG	i	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	i	2	3	-	0/6/23/26	0/1/1/1
3	BMA	i	3	3	-	0/2/19/22	0/1/1/1
2	NAG	j	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	j	2	2	-	3/6/23/26	0/1/1/1
3	NAG	k	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	k	2	3	-	0/6/23/26	0/1/1/1
3	BMA	k	3	3	-	0/2/19/22	0/1/1/1
3	NAG	l	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	l	2	3	-	0/6/23/26	0/1/1/1
3	BMA	l	3	3	-	0/2/19/22	0/1/1/1
3	NAG	m	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	m	2	3	-	0/6/23/26	0/1/1/1
3	BMA	m	3	3	-	0/2/19/22	0/1/1/1
2	NAG	n	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	n	2	2	-	3/6/23/26	0/1/1/1
3	NAG	o	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	o	2	3	-	0/6/23/26	0/1/1/1
3	BMA	o	3	3	-	1/2/19/22	0/1/1/1
3	NAG	p	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	p	2	3	-	0/6/23/26	0/1/1/1
3	BMA	p	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	1	NAG	C2-N2-C7	3.36	127.69	122.90
2	J	1	NAG	C2-N2-C7	3.31	127.62	122.90
2	j	1	NAG	C2-N2-C7	3.29	127.58	122.90
2	n	1	NAG	C1-C2-N2	3.23	116.01	110.49
2	N	1	NAG	C1-C2-N2	3.22	115.99	110.49
2	a	1	NAG	C1-C2-N2	3.21	115.97	110.49
2	Q	2	NAG	C1-C2-N2	2.77	115.21	110.49
2	D	2	NAG	C1-C2-N2	2.76	115.20	110.49
2	d	2	NAG	C1-C2-N2	2.73	115.15	110.49
2	d	2	NAG	C2-N2-C7	2.66	126.69	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C2-N2-C7	2.65	126.67	122.90
2	n	1	NAG	C2-N2-C7	2.65	126.67	122.90
2	Q	2	NAG	C2-N2-C7	2.64	126.67	122.90
2	a	1	NAG	C2-N2-C7	2.64	126.67	122.90
2	N	1	NAG	C2-N2-C7	2.64	126.66	122.90
2	j	1	NAG	C1-C2-N2	2.36	114.52	110.49
2	J	1	NAG	C1-C2-N2	2.33	114.47	110.49
2	W	1	NAG	C1-C2-N2	2.33	114.47	110.49
3	i	1	NAG	C2-N2-C7	2.04	125.81	122.90
3	I	1	NAG	C2-N2-C7	2.02	125.78	122.90
3	V	1	NAG	C2-N2-C7	2.02	125.78	122.90

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C3-C2-N2-C7
2	N	1	NAG	C3-C2-N2-C7
2	Q	2	NAG	C3-C2-N2-C7
2	a	1	NAG	C3-C2-N2-C7
2	d	2	NAG	C3-C2-N2-C7
2	n	1	NAG	C3-C2-N2-C7
2	N	1	NAG	C8-C7-N2-C2
2	a	1	NAG	C8-C7-N2-C2
2	n	1	NAG	C8-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	N	1	NAG	O7-C7-N2-C2
2	W	2	NAG	C8-C7-N2-C2
2	W	2	NAG	O7-C7-N2-C2
2	a	1	NAG	O7-C7-N2-C2
2	j	2	NAG	C8-C7-N2-C2
2	j	2	NAG	O7-C7-N2-C2
2	n	1	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	W	1	NAG	C8-C7-N2-C2
2	j	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	W	1	NAG	O7-C7-N2-C2
2	j	1	NAG	O7-C7-N2-C2
3	F	3	BMA	O5-C5-C6-O6
3	S	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

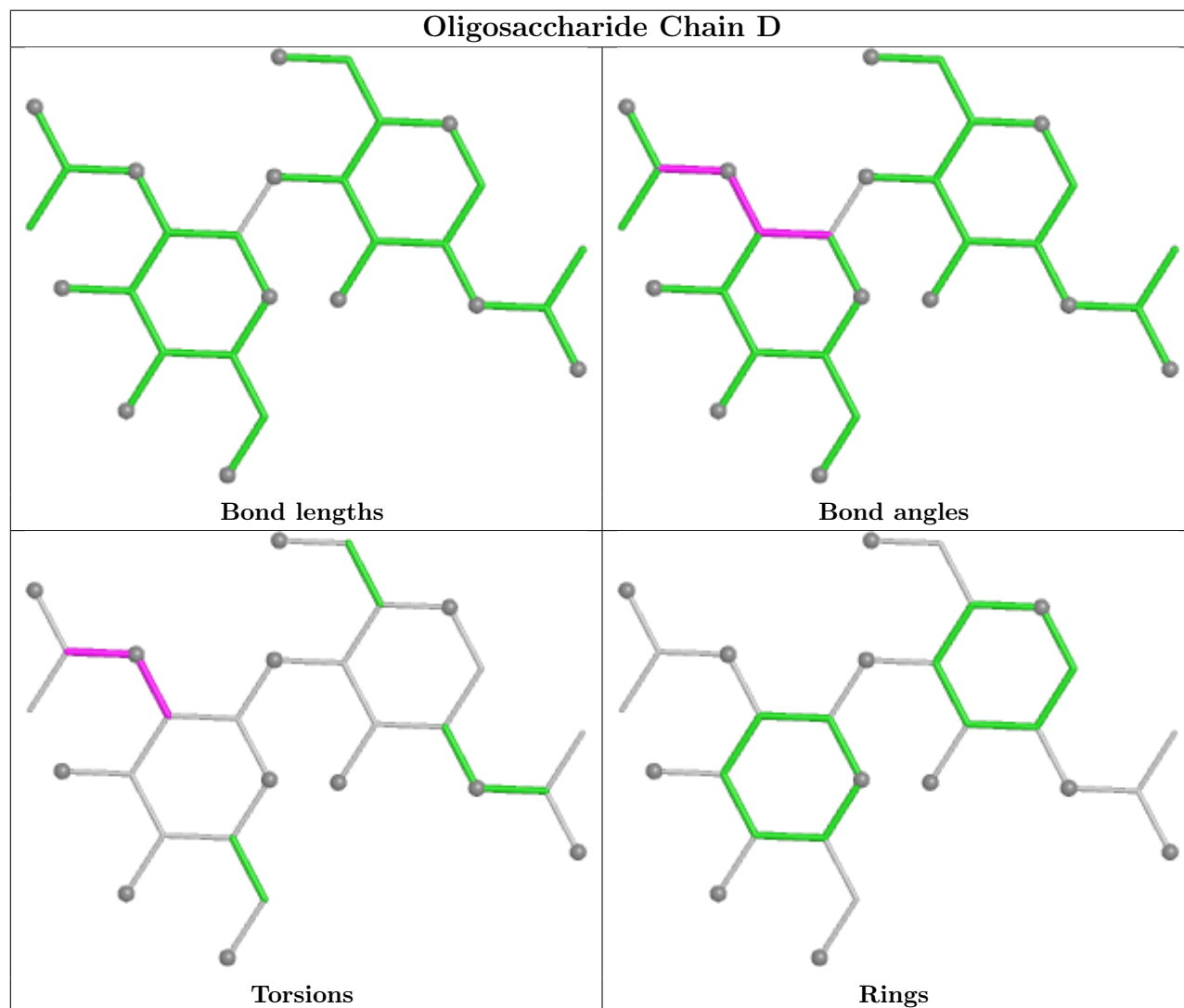
Mol	Chain	Res	Type	Atoms
3	f	3	BMA	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
3	b	3	BMA	O5-C5-C6-O6
3	o	3	BMA	O5-C5-C6-O6
2	J	1	NAG	C3-C2-N2-C7
2	J	2	NAG	C3-C2-N2-C7
2	W	1	NAG	C3-C2-N2-C7
2	W	2	NAG	C3-C2-N2-C7
2	j	1	NAG	C3-C2-N2-C7
2	j	2	NAG	C3-C2-N2-C7
2	N	2	NAG	C8-C7-N2-C2
2	a	2	NAG	C8-C7-N2-C2
2	n	2	NAG	C8-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	J	1	NAG	C1-C2-N2-C7
2	W	1	NAG	C1-C2-N2-C7
2	j	1	NAG	C1-C2-N2-C7
2	N	2	NAG	C1-C2-N2-C7
2	a	2	NAG	C1-C2-N2-C7
2	n	2	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
3	V	1	NAG	C1-C2-N2-C7
3	i	1	NAG	C1-C2-N2-C7
2	D	2	NAG	O7-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	a	2	NAG	O7-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
2	N	2	NAG	O7-C7-N2-C2
2	n	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C1-C2-N2-C7
2	Q	2	NAG	C1-C2-N2-C7
2	d	2	NAG	C1-C2-N2-C7
2	N	1	NAG	C1-C2-N2-C7
2	a	1	NAG	C1-C2-N2-C7
2	n	1	NAG	C1-C2-N2-C7

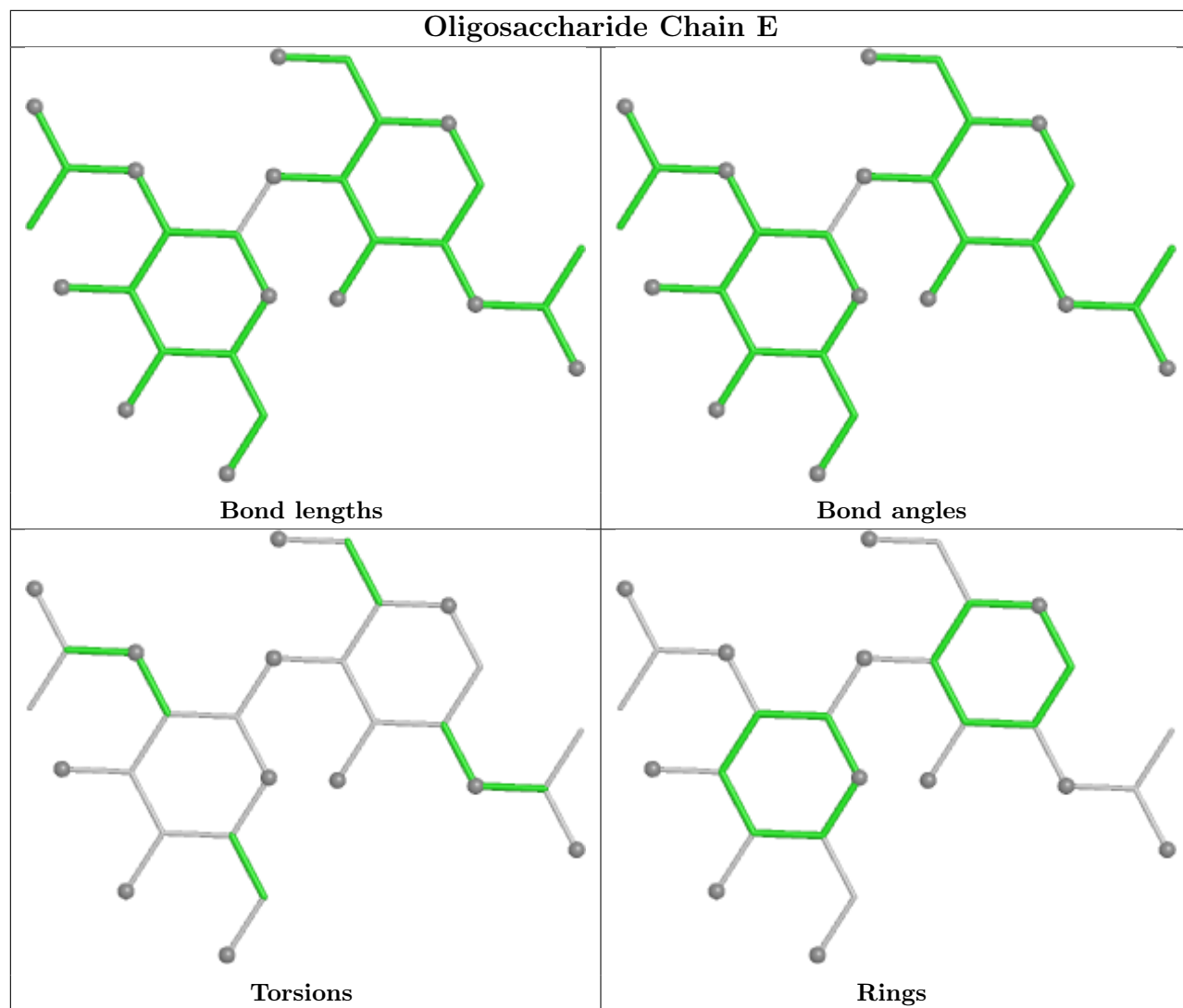
There are no ring outliers.

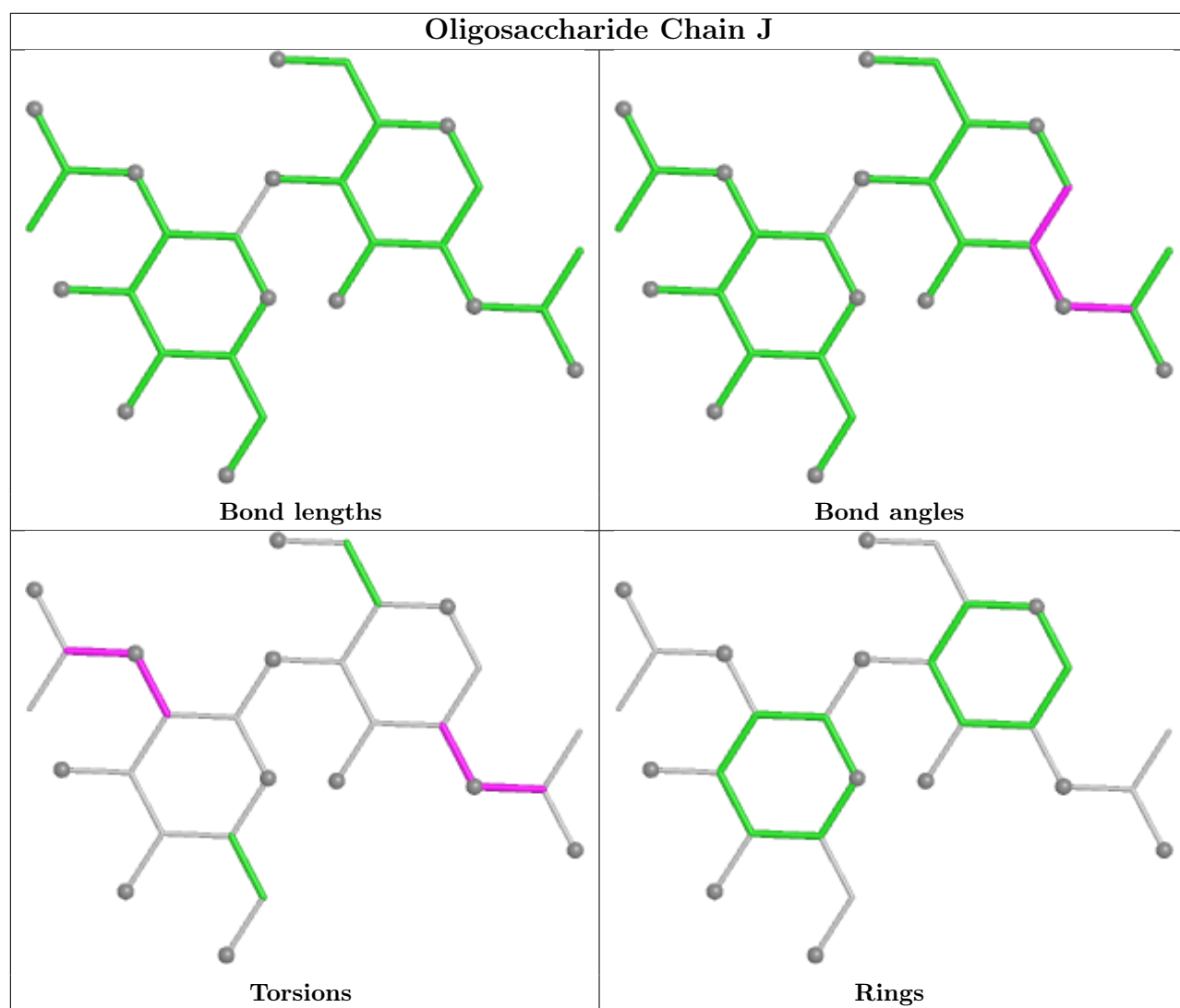
10 monomers are involved in 29 short contacts:

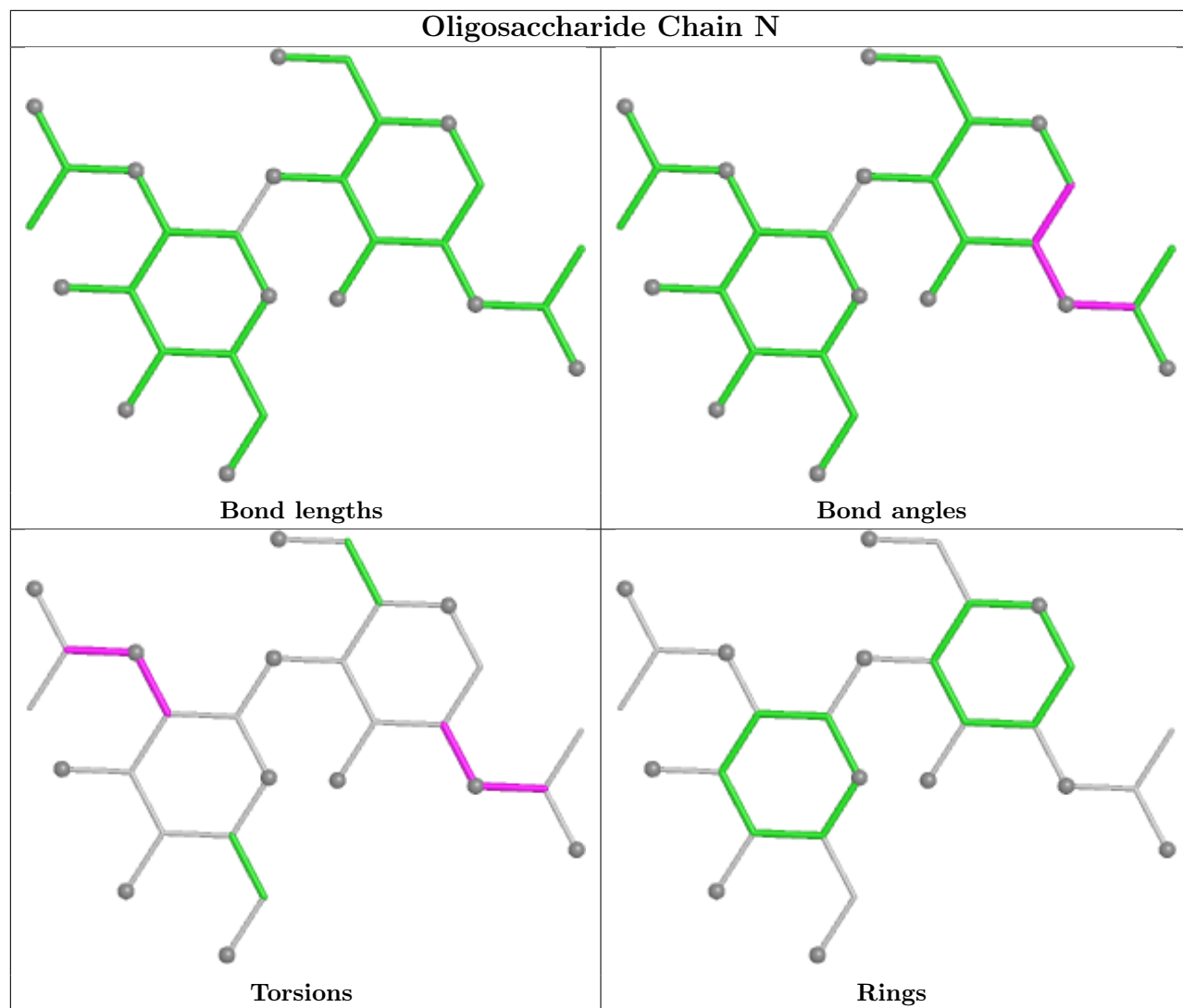
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	2	NAG	4	0
3	X	1	NAG	4	0
2	R	1	NAG	1	0
2	e	1	NAG	1	0
2	J	2	NAG	4	0
2	E	1	NAG	1	0
3	K	1	NAG	5	0
2	j	2	NAG	4	0
3	k	1	NAG	4	0
3	o	1	NAG	1	0

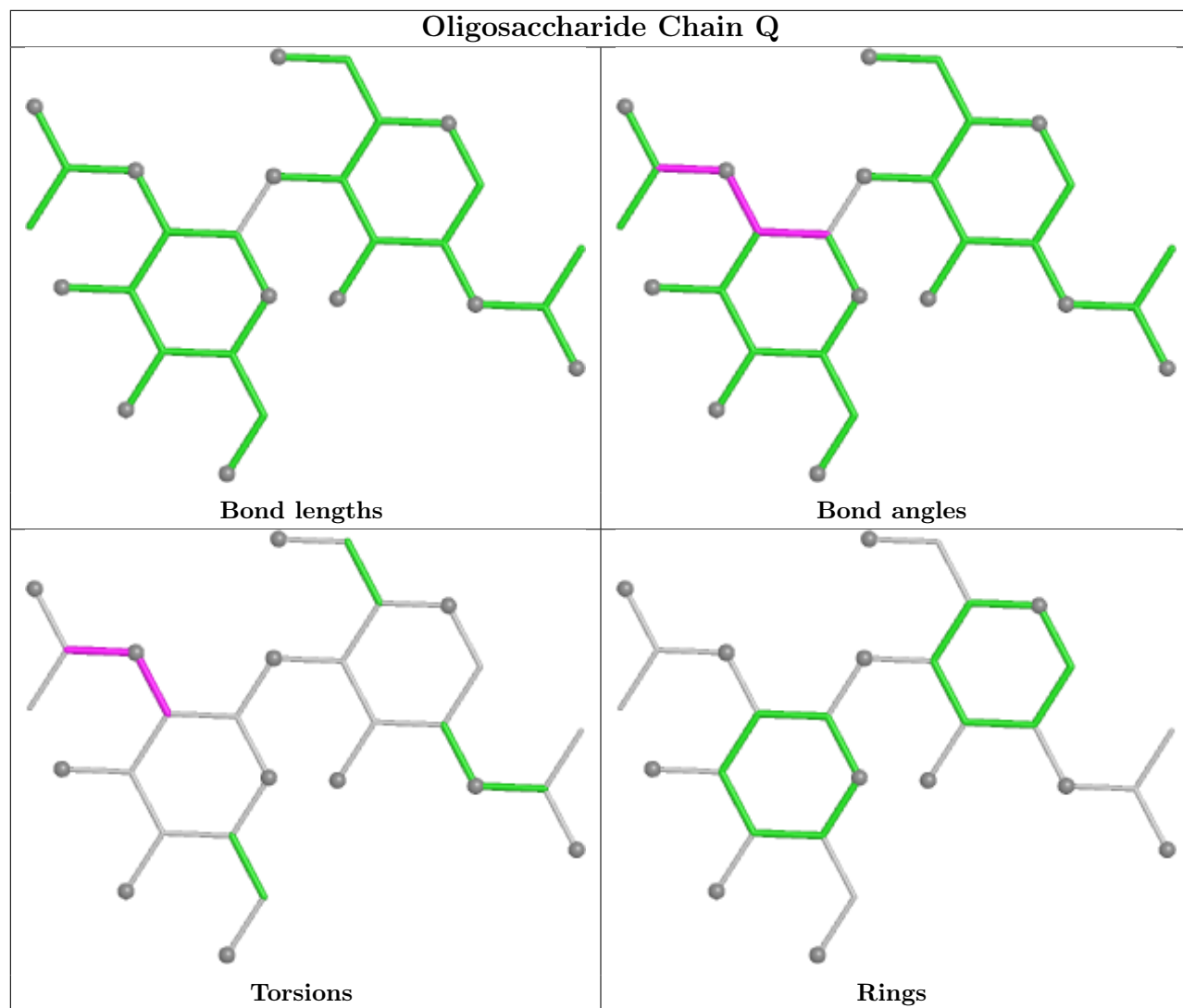
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

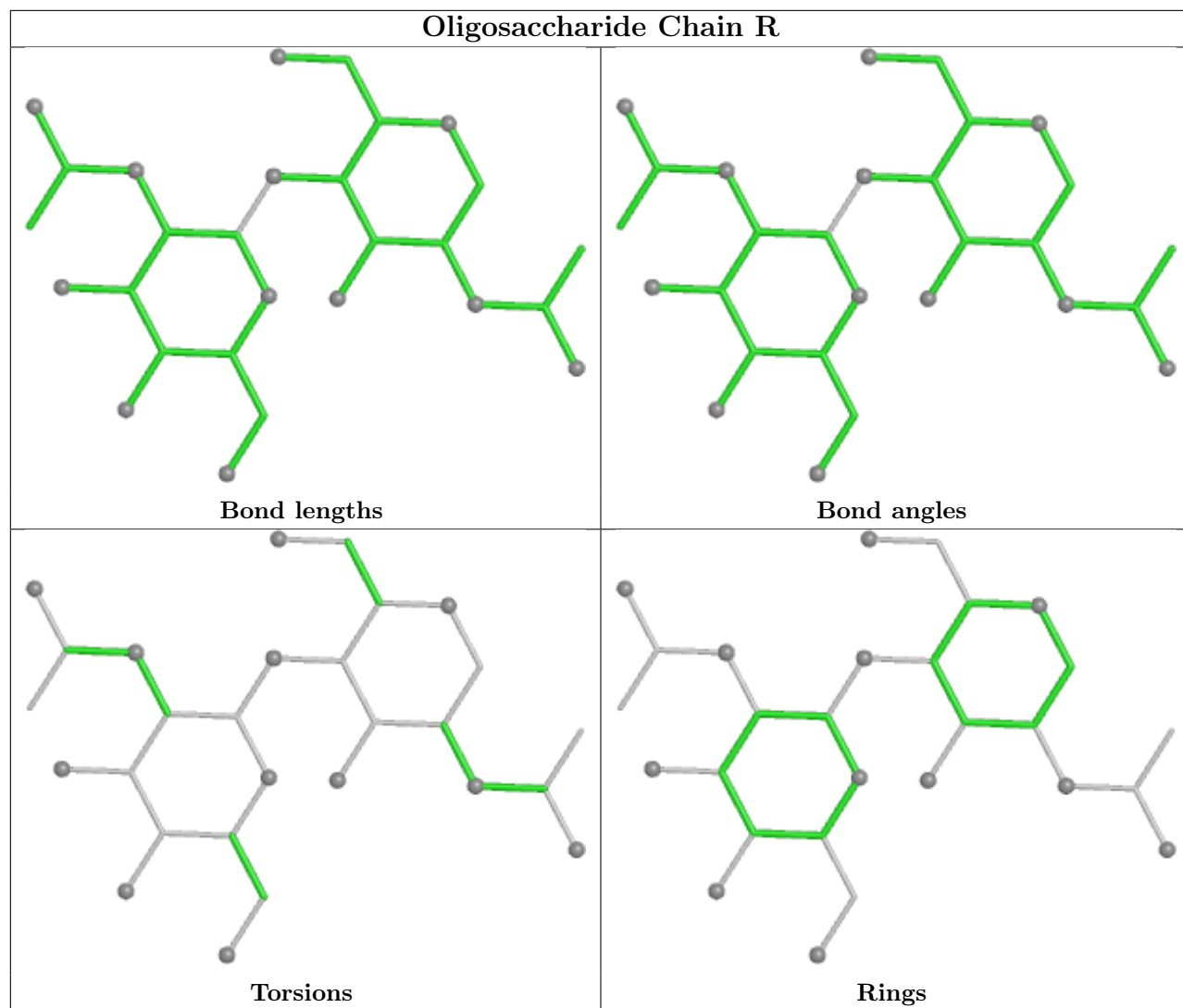


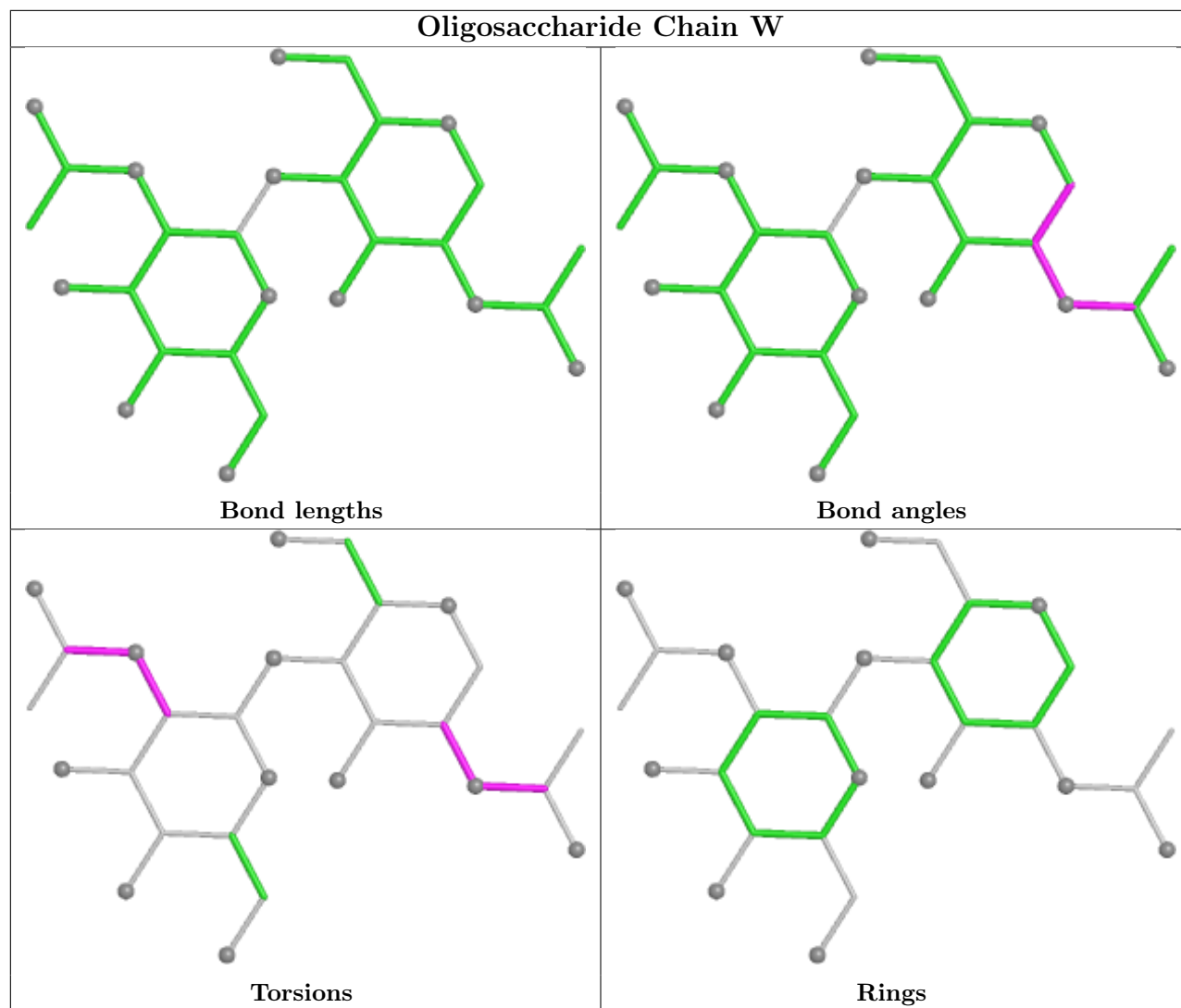


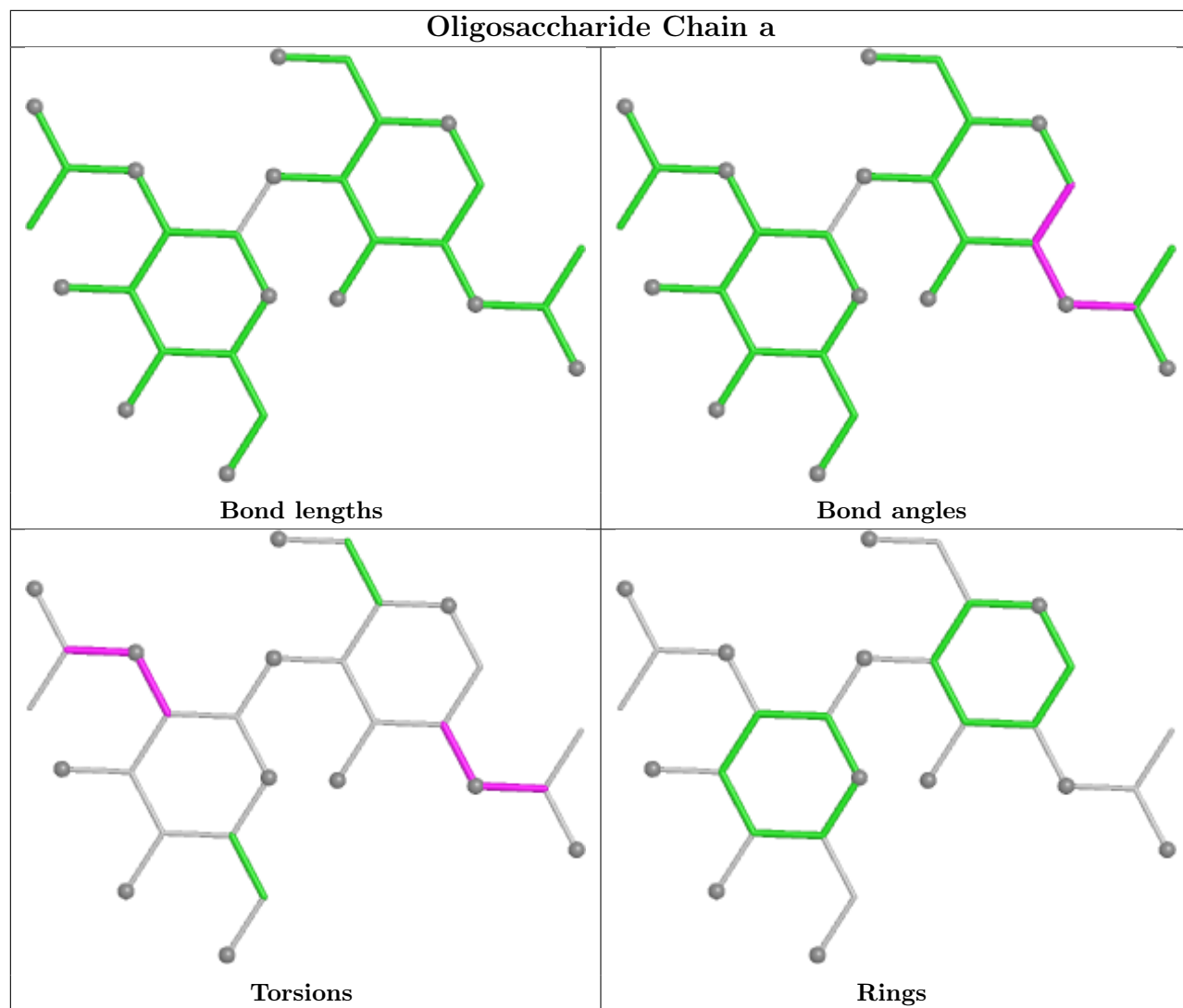


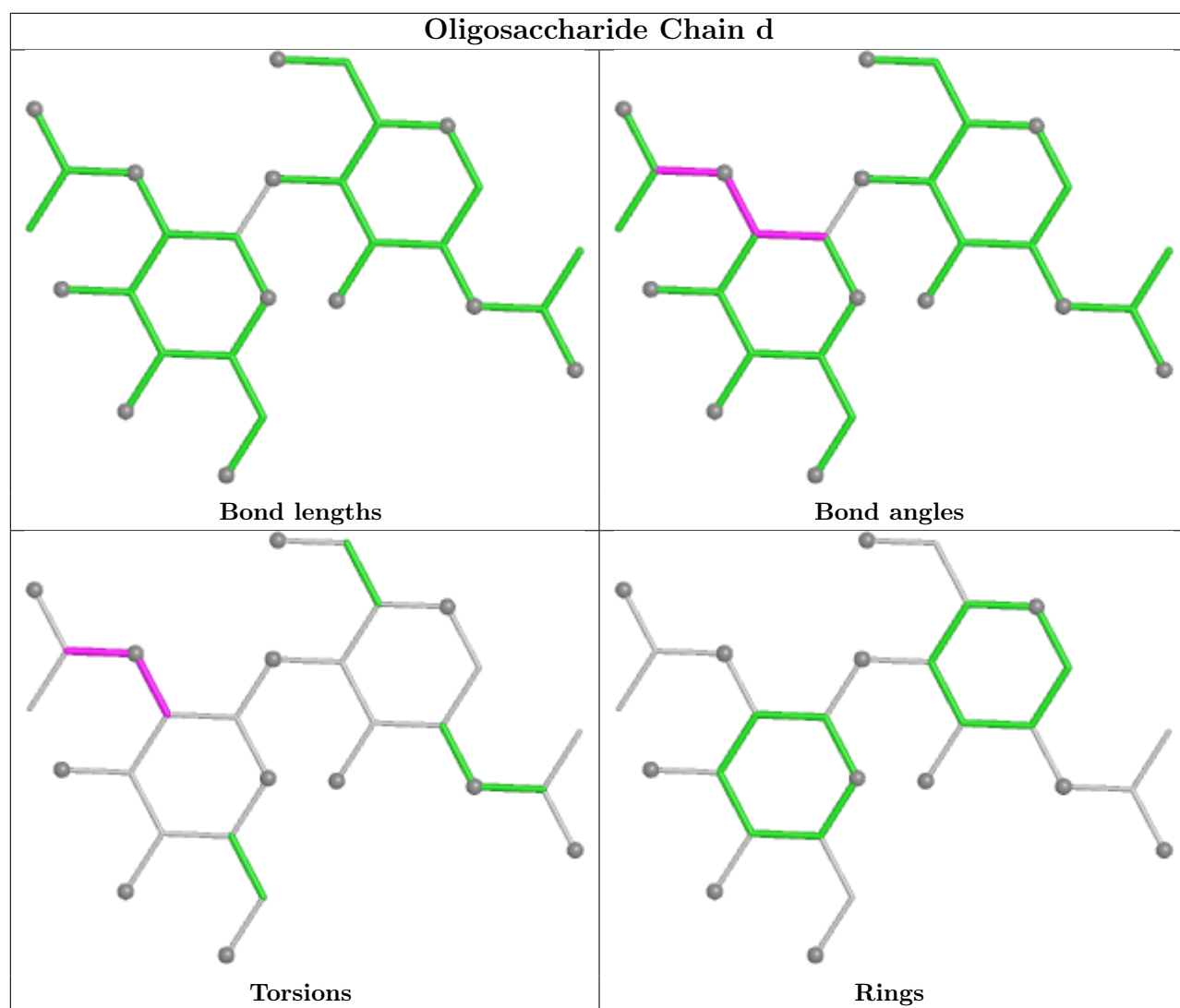


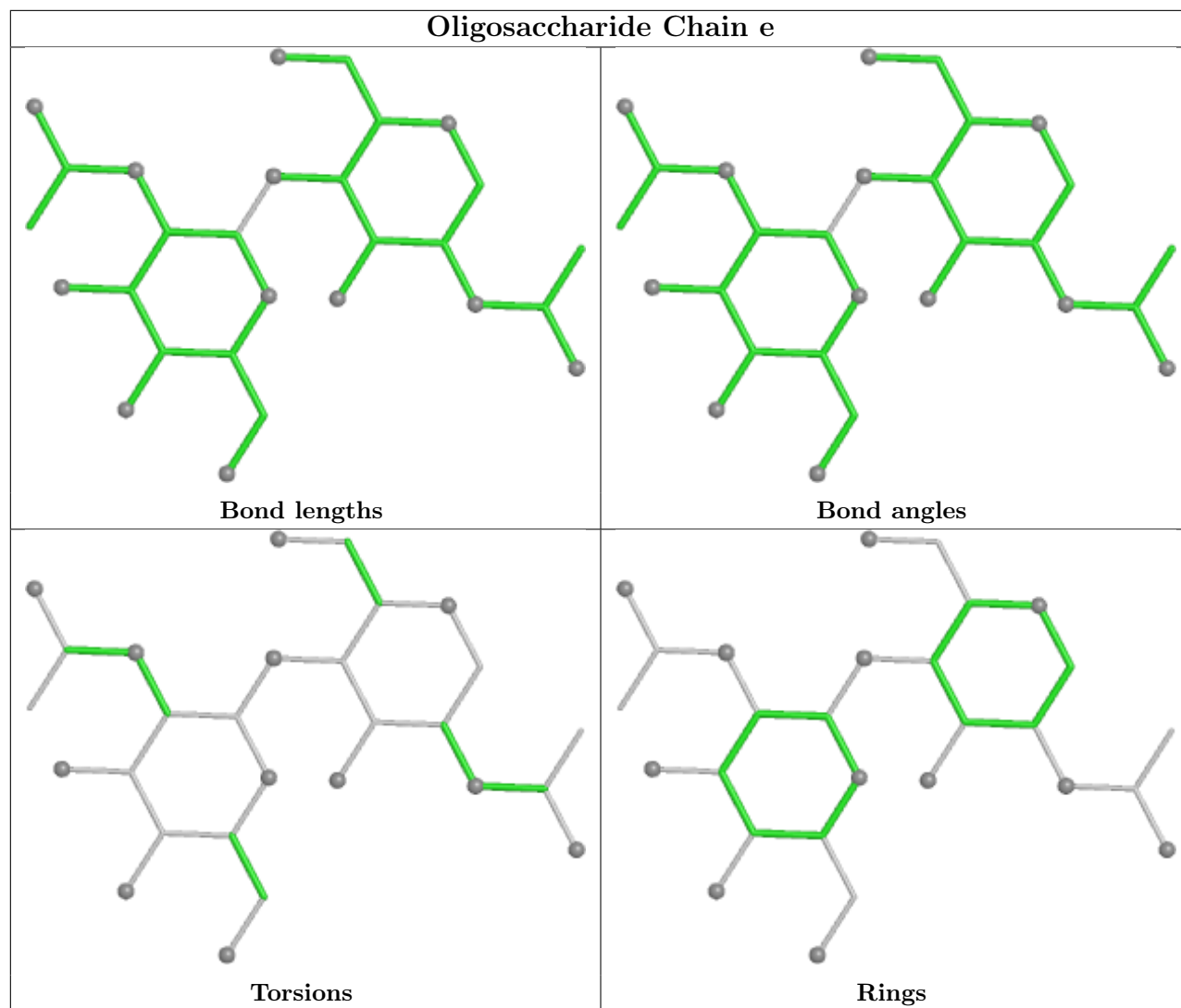


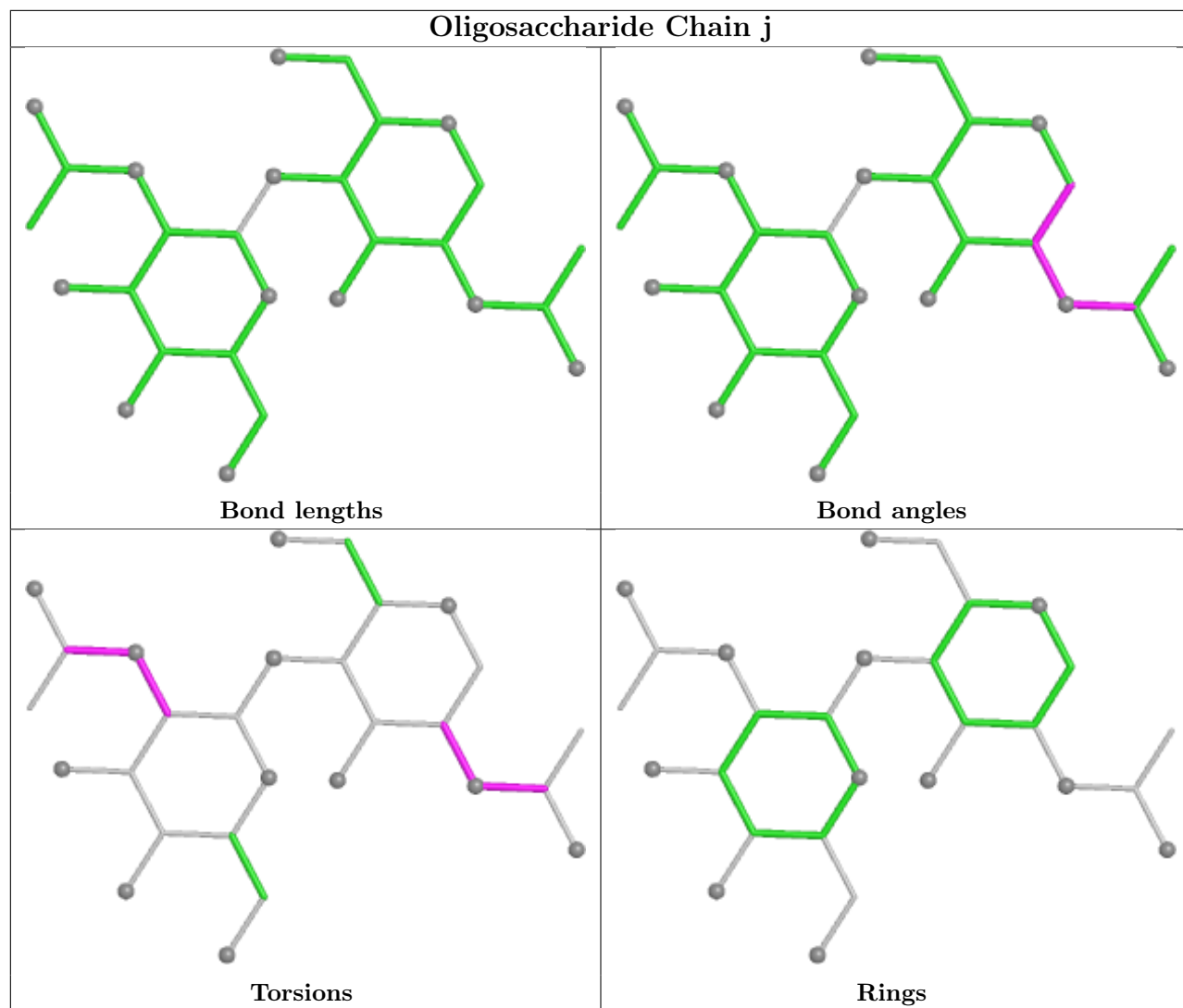


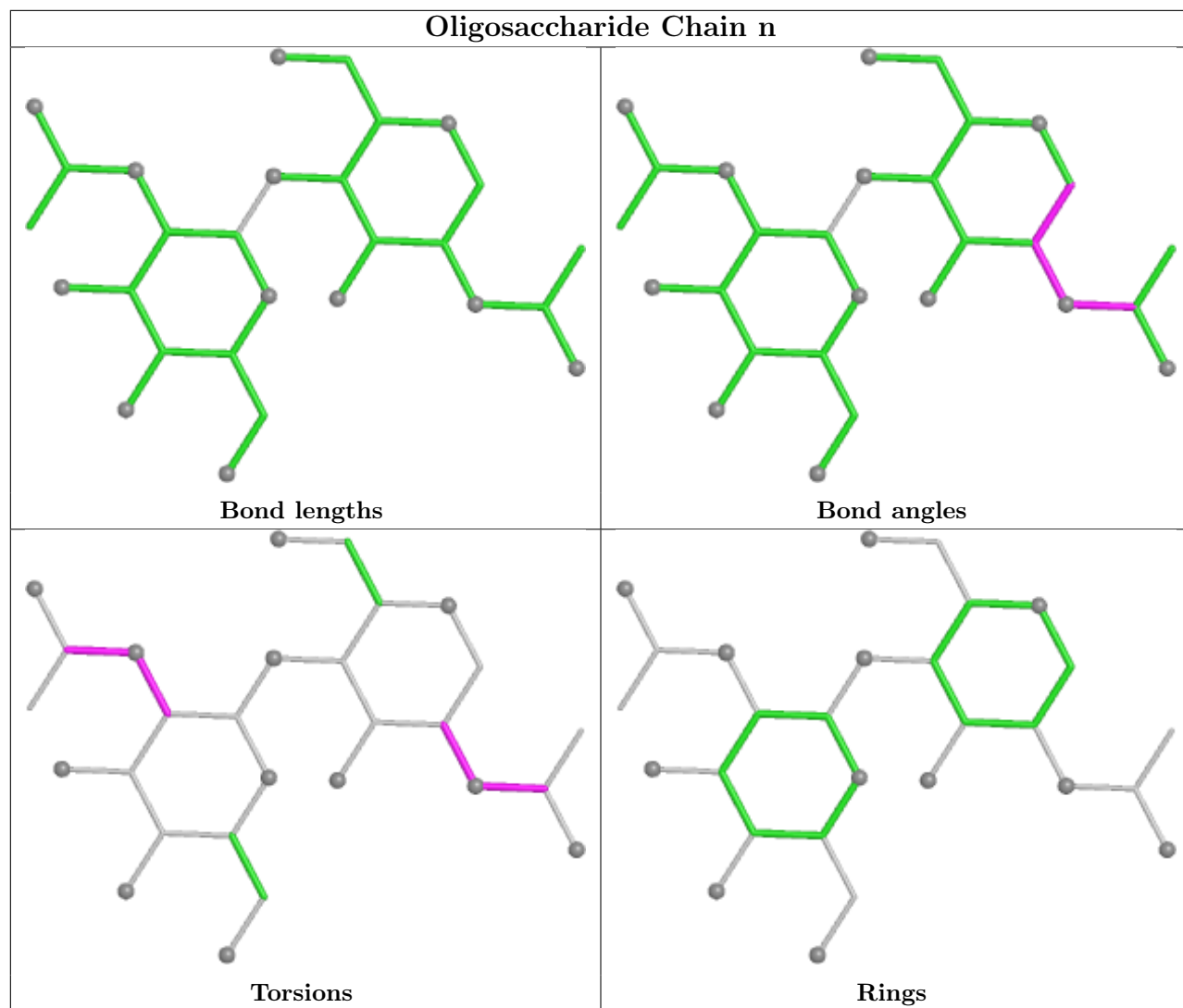


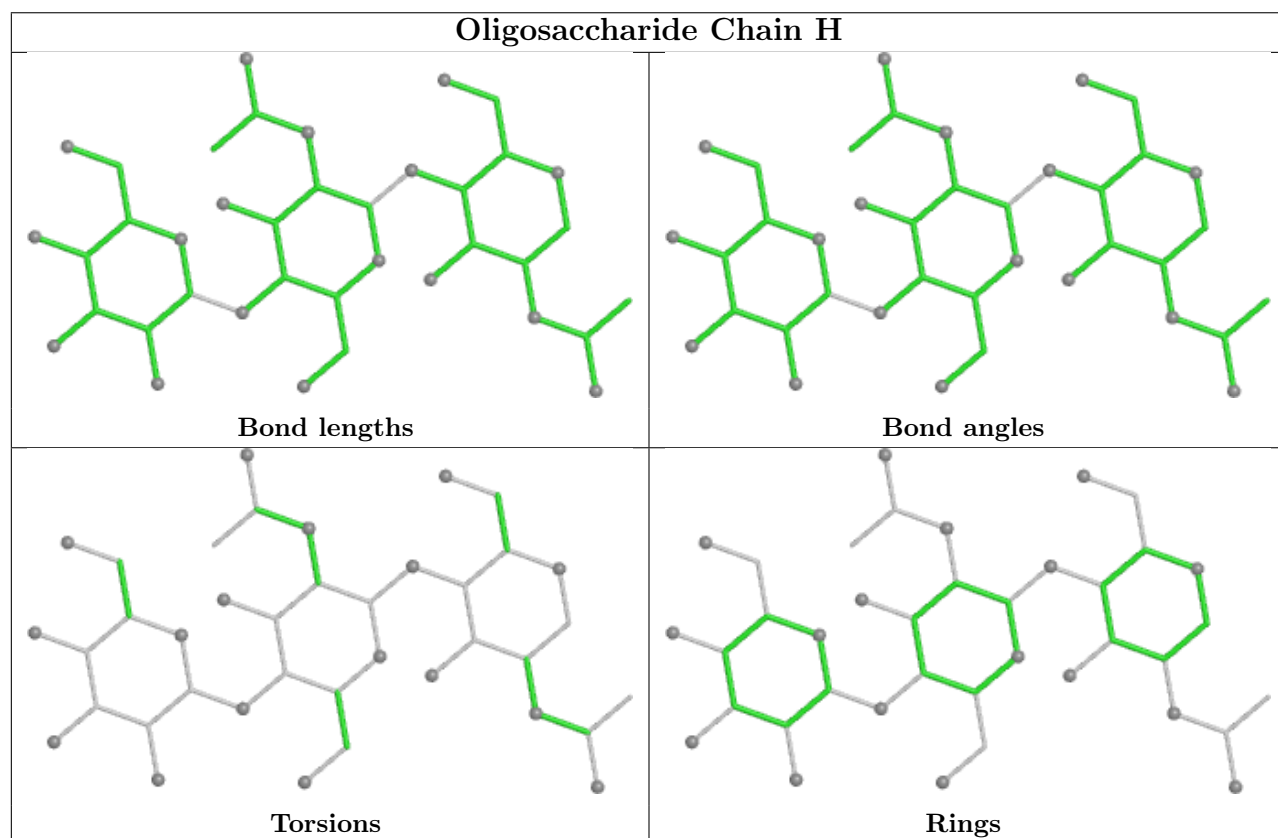
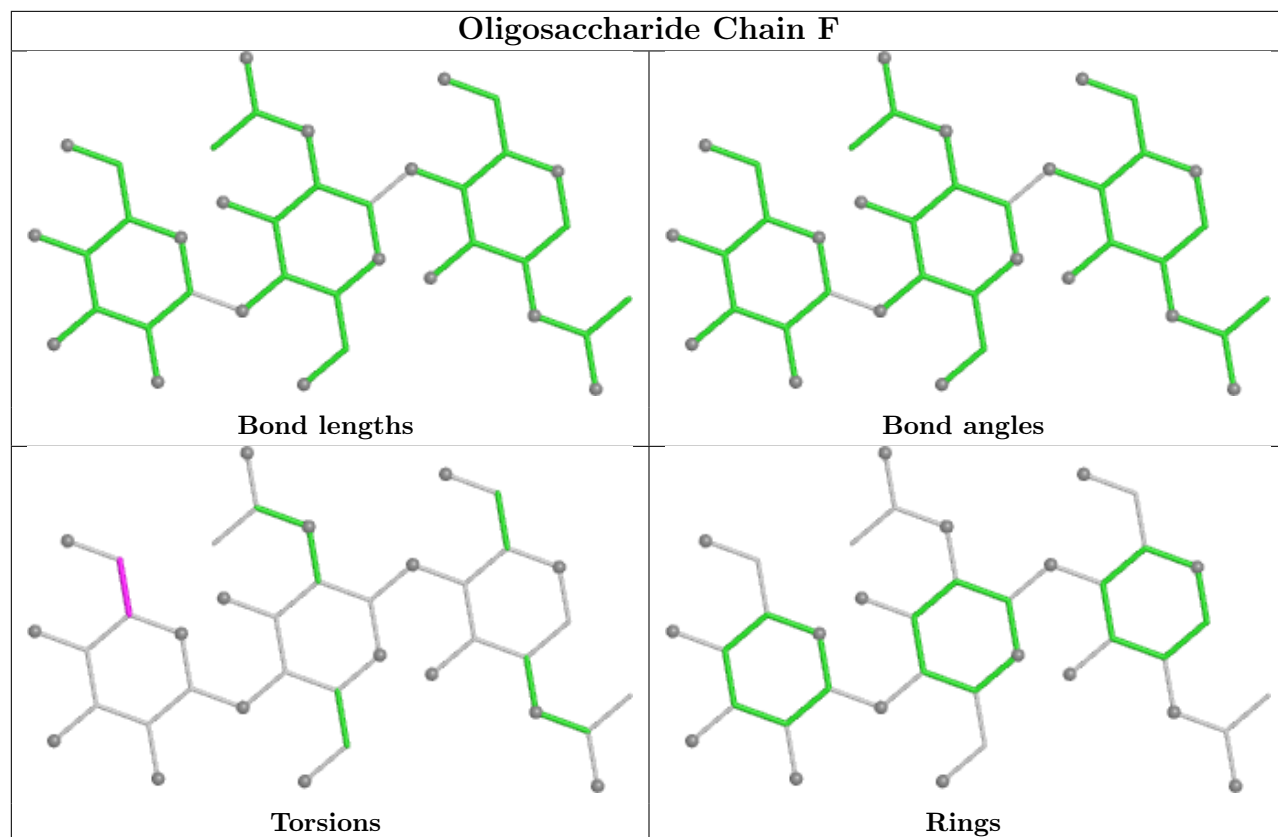


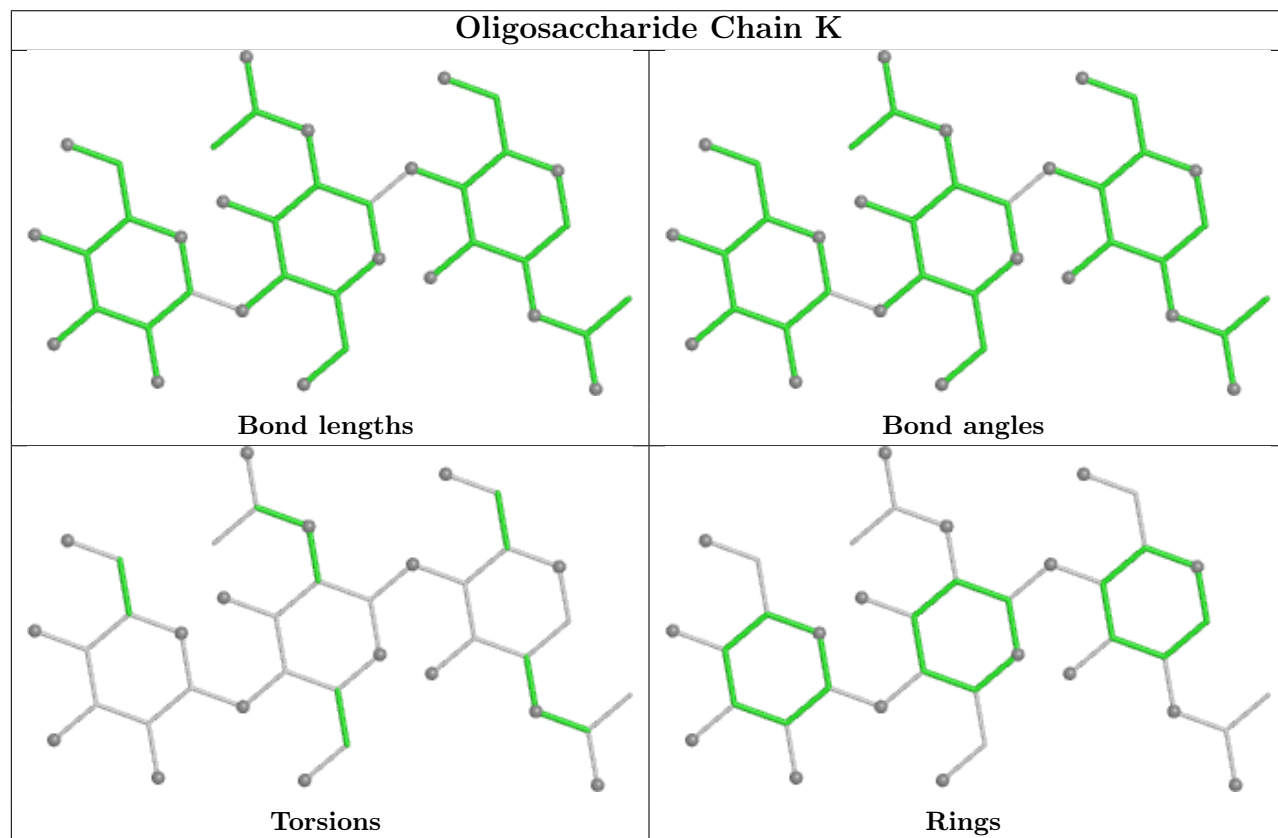
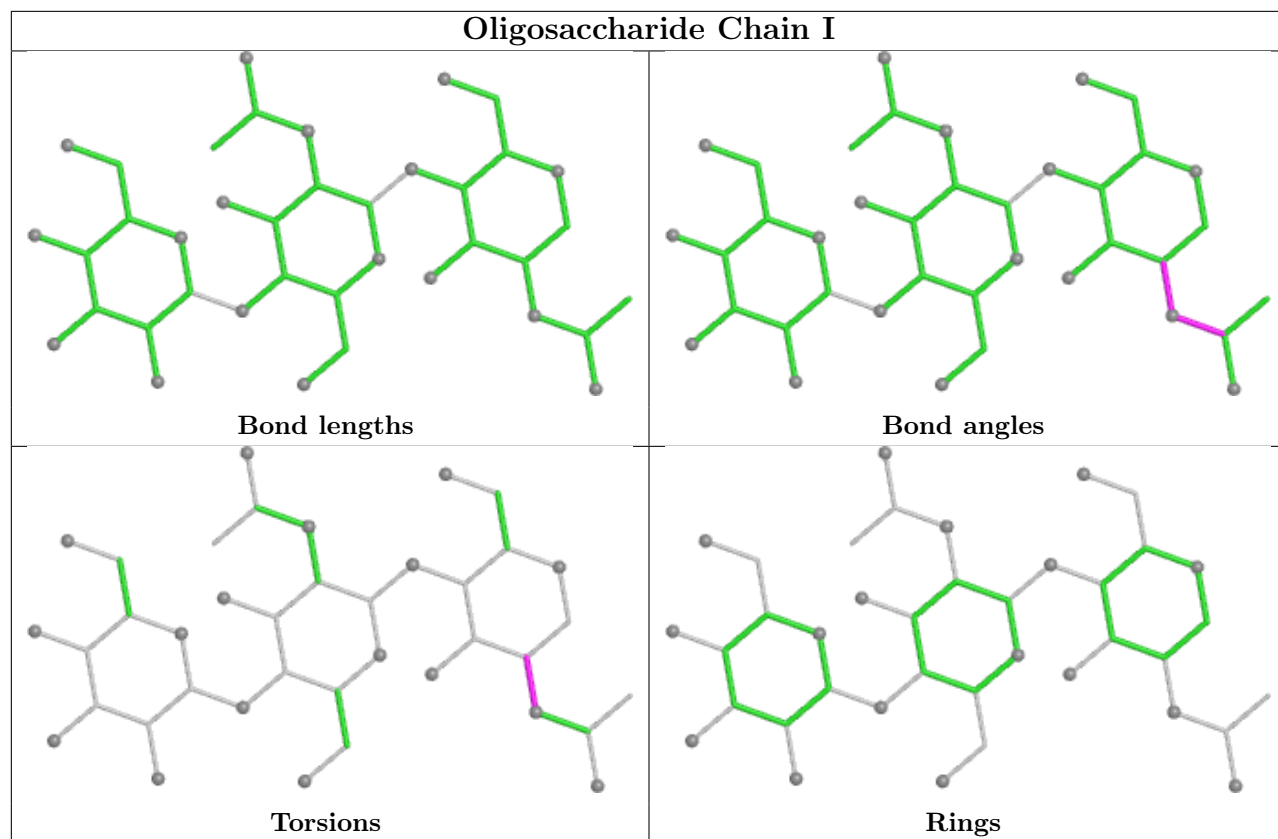


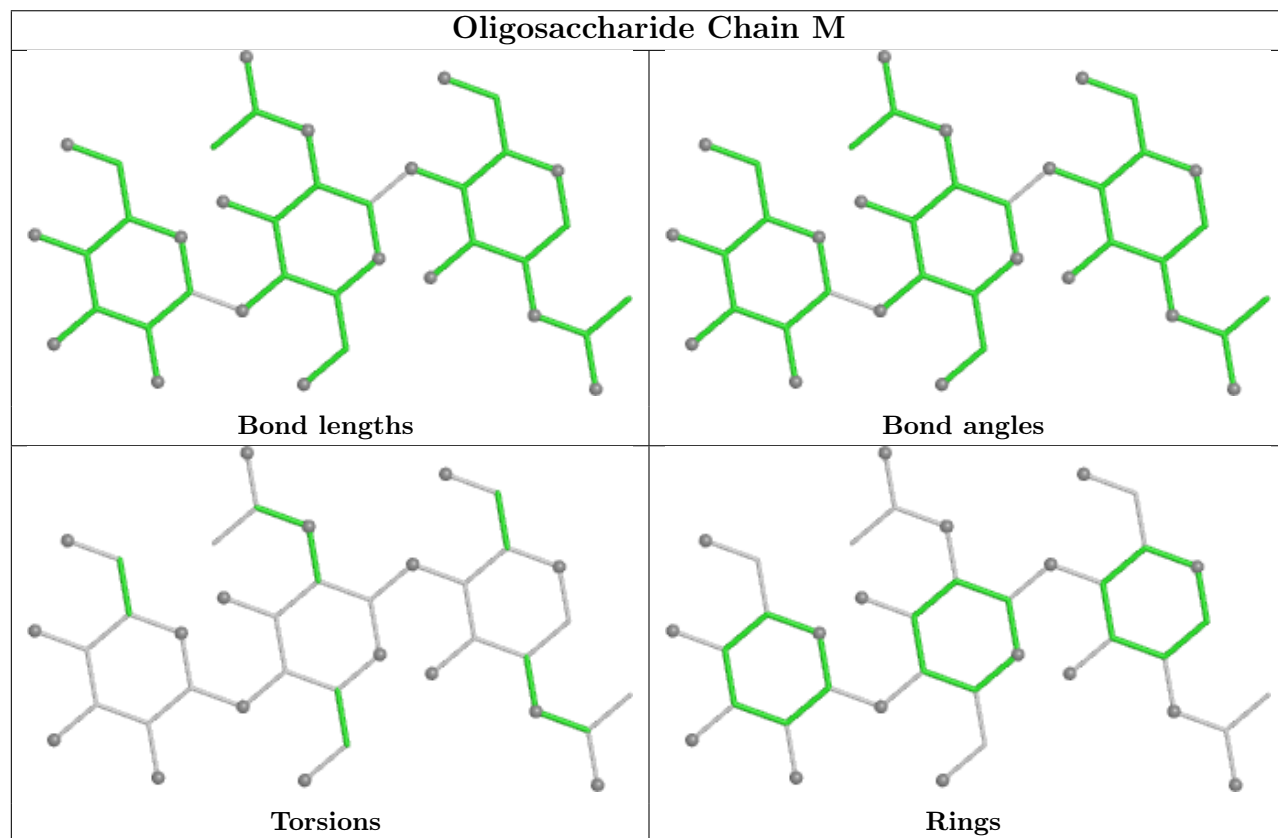
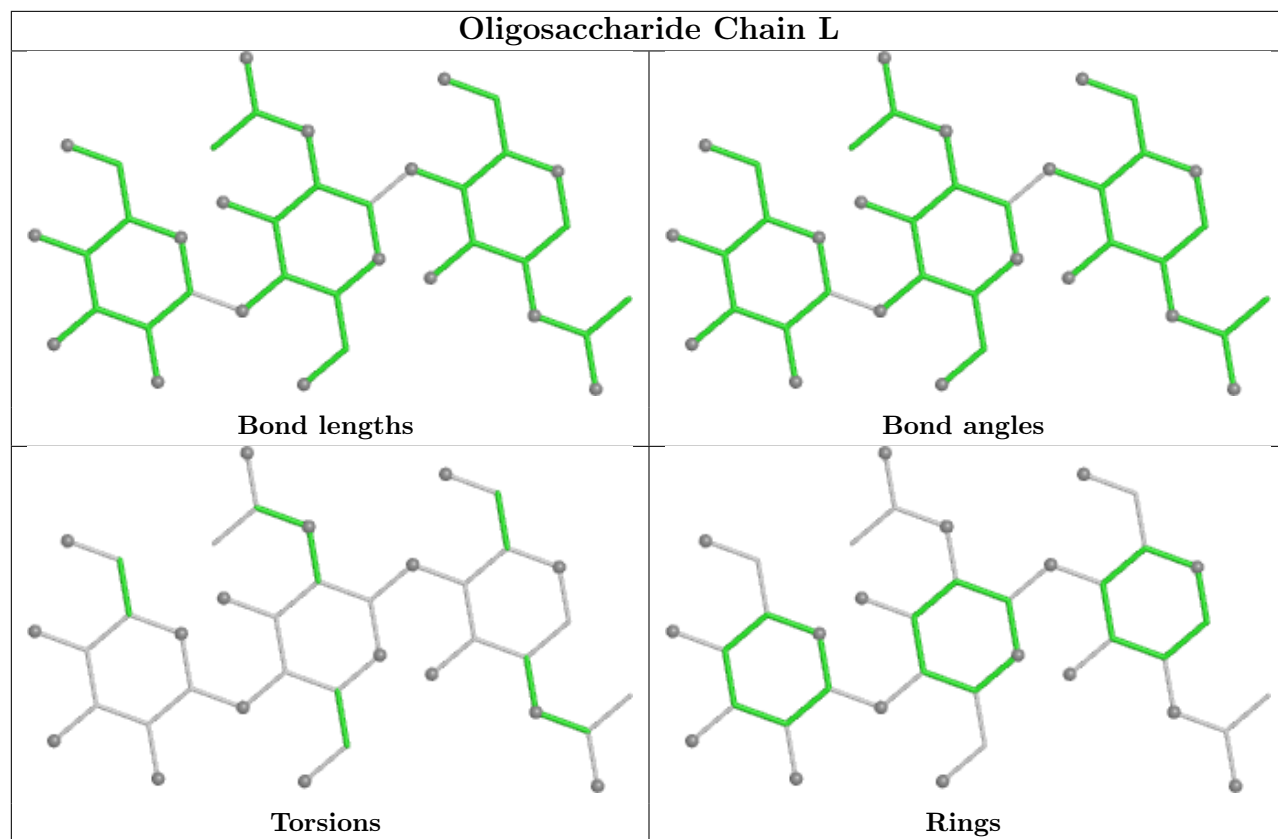


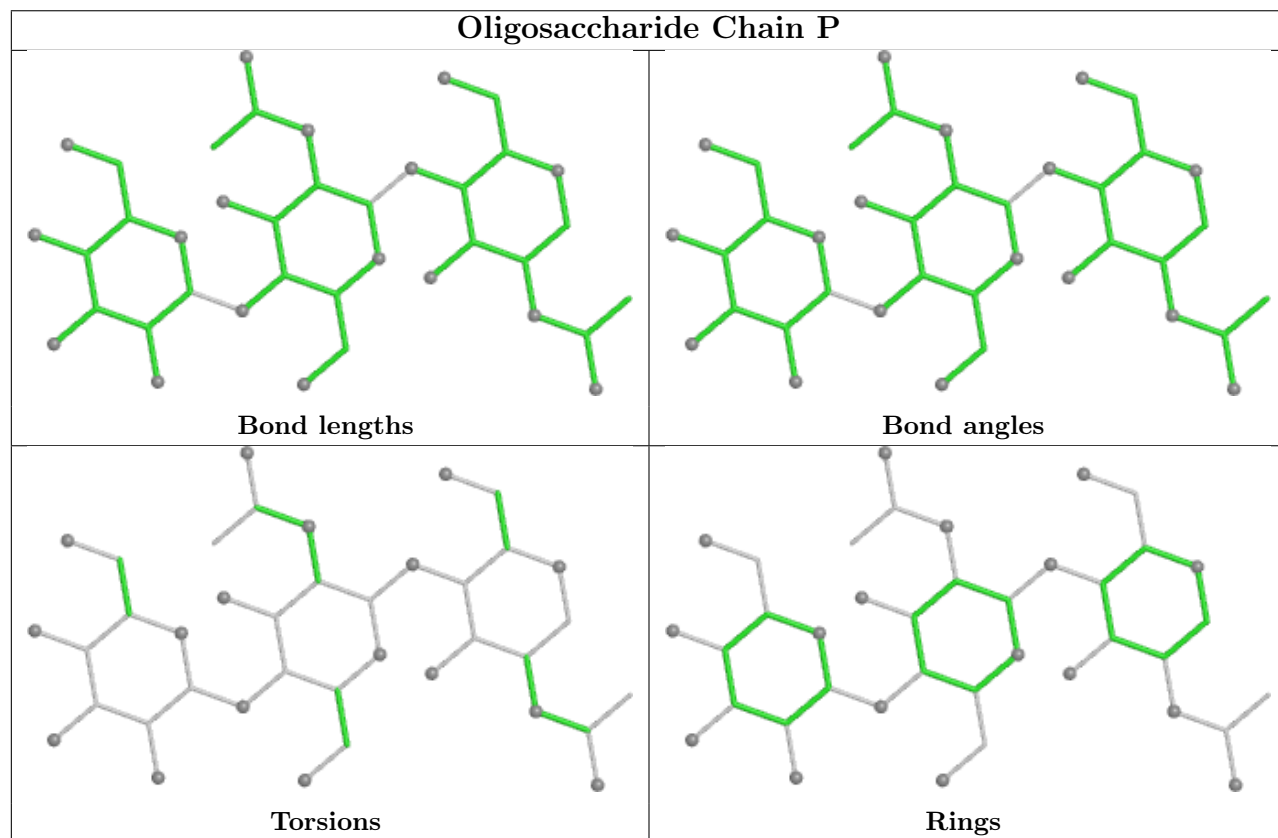
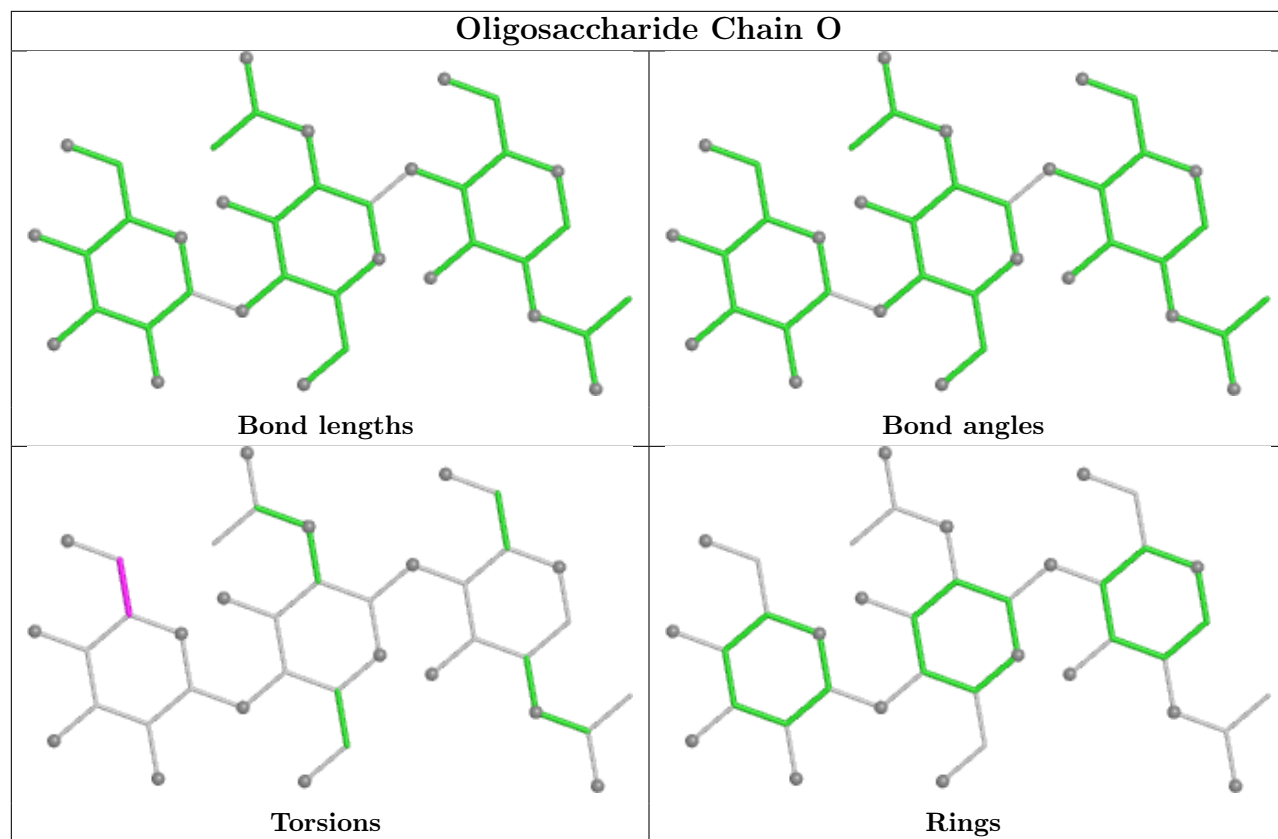


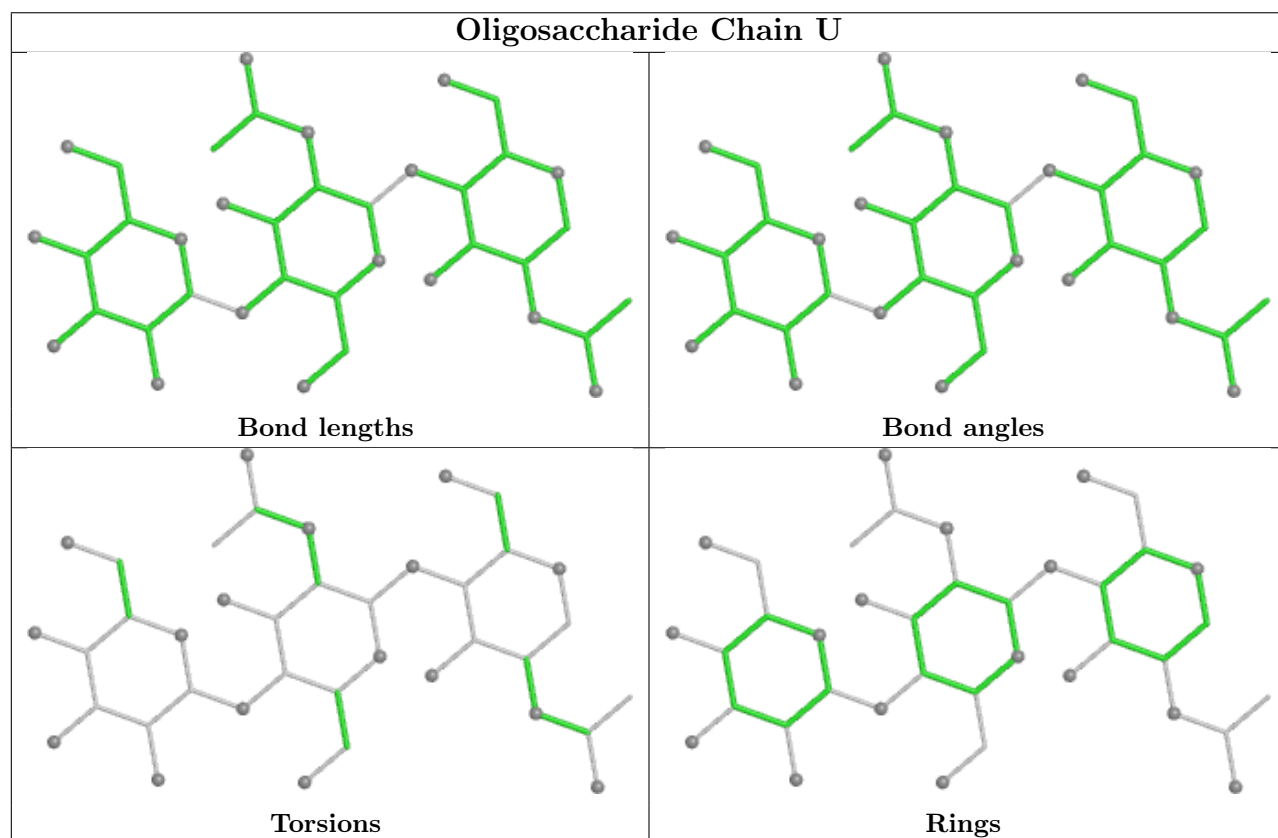
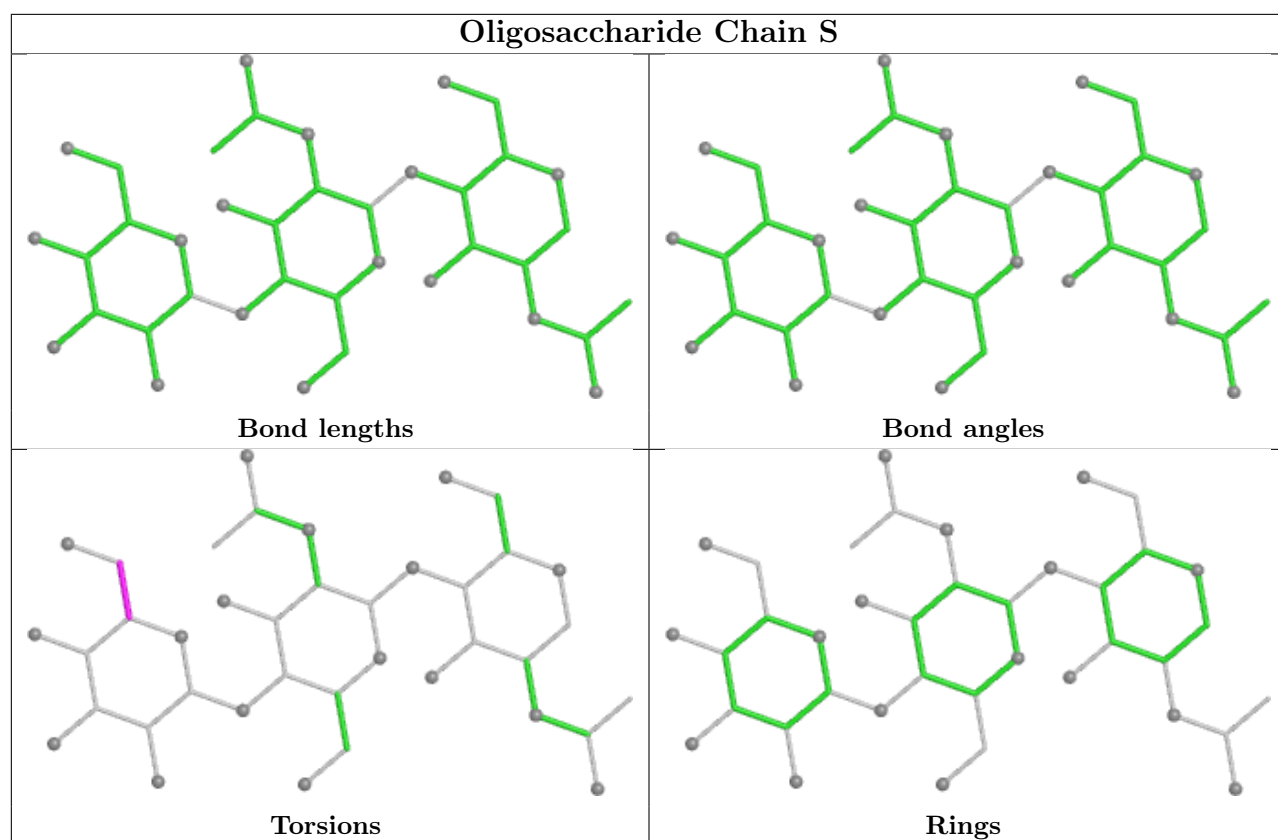


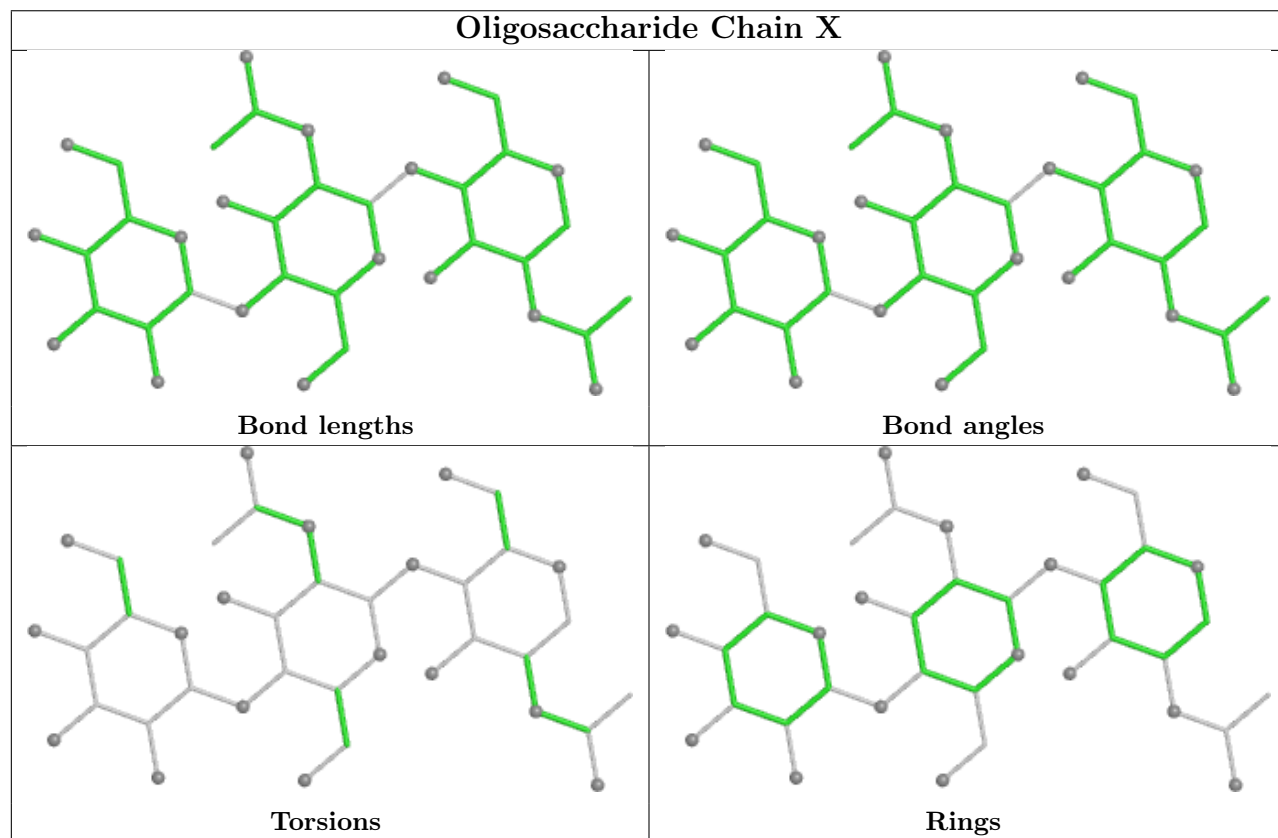
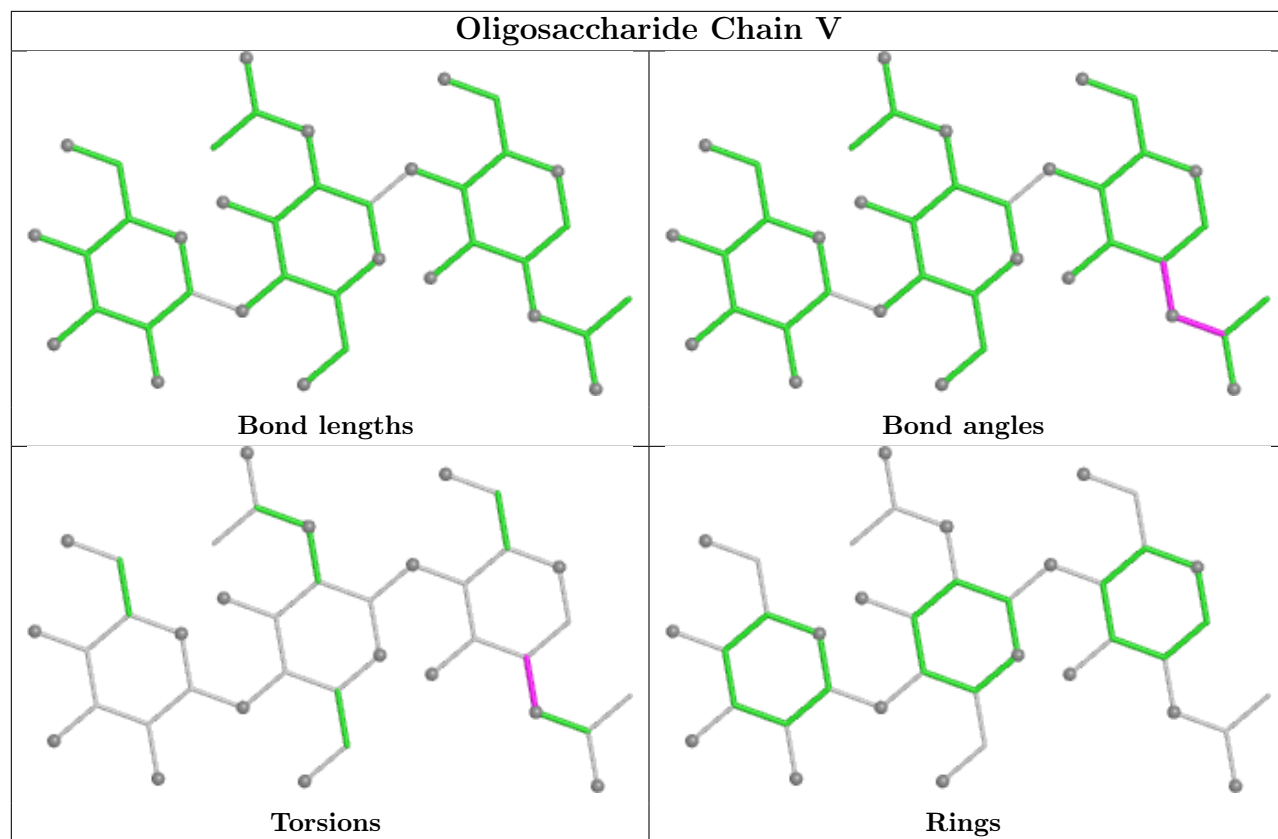


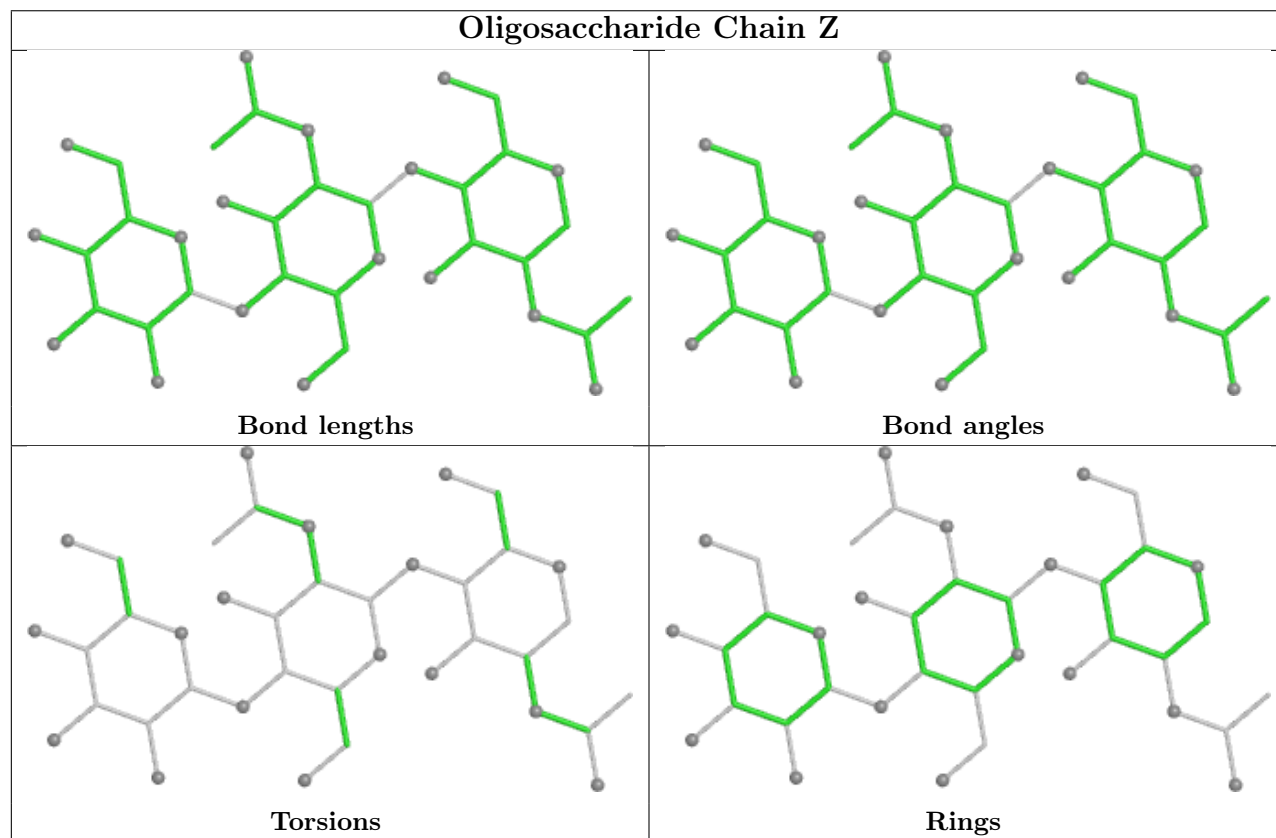
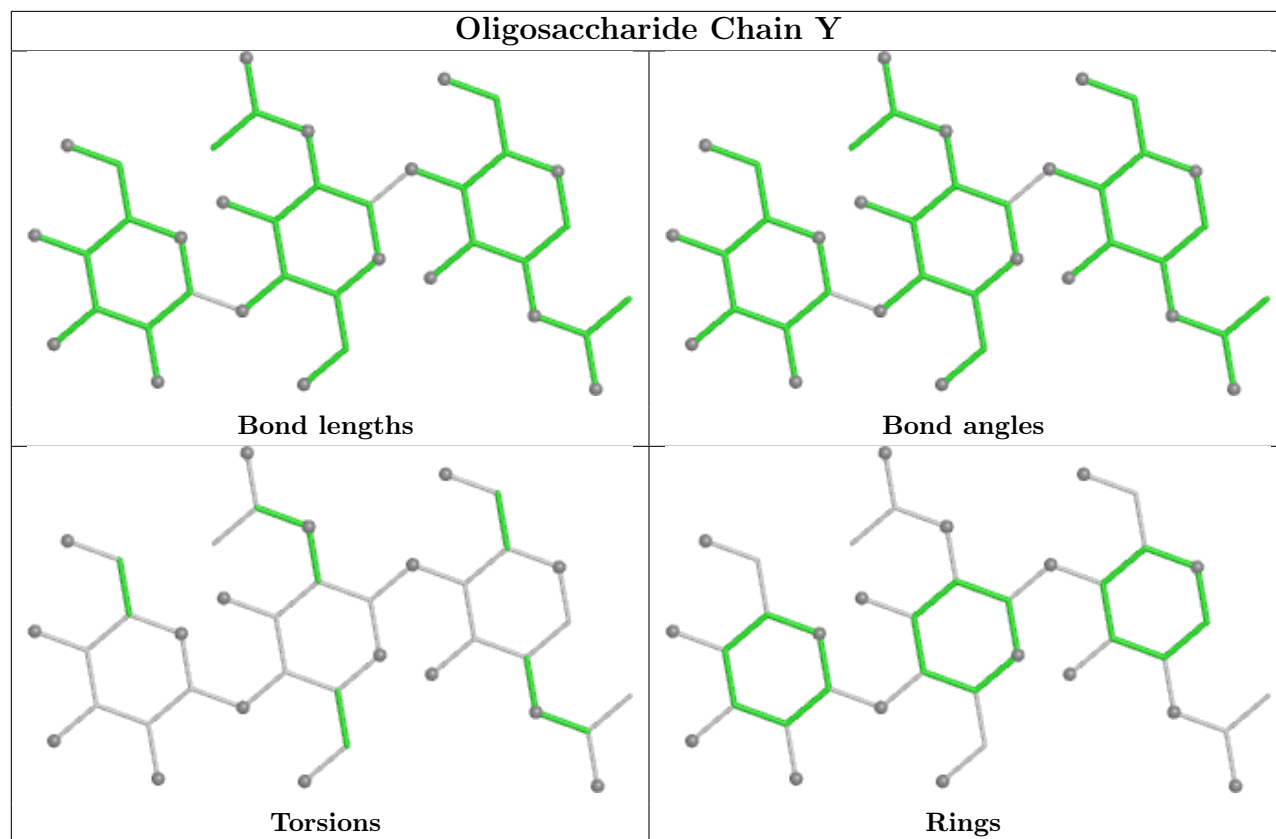


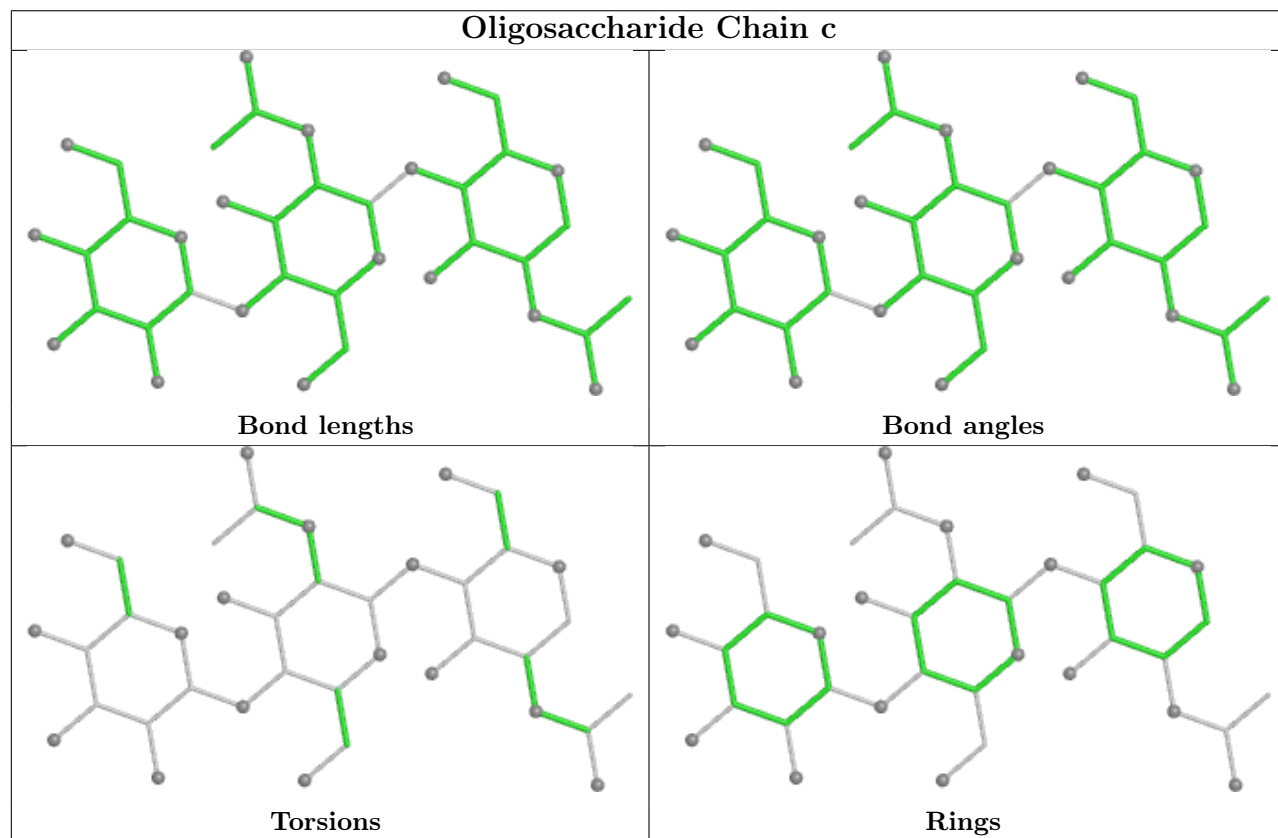
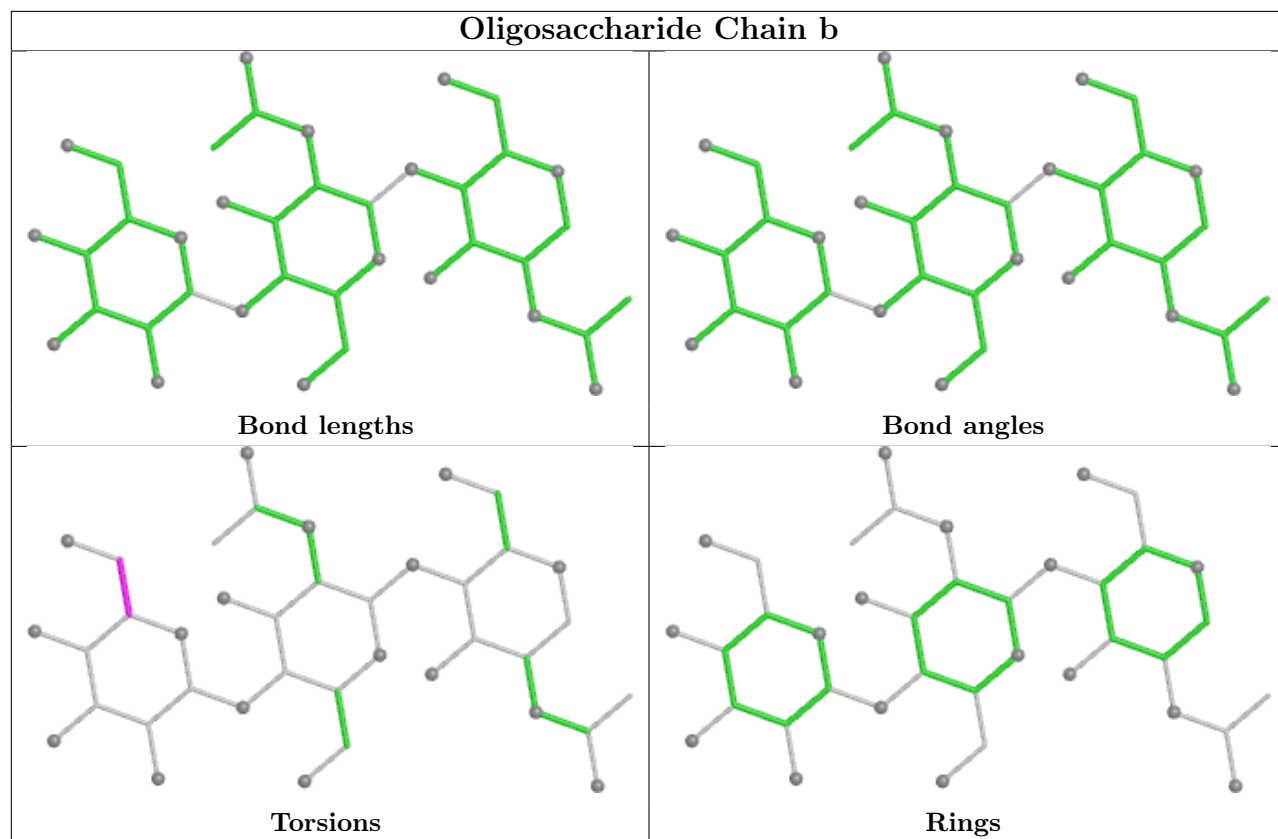


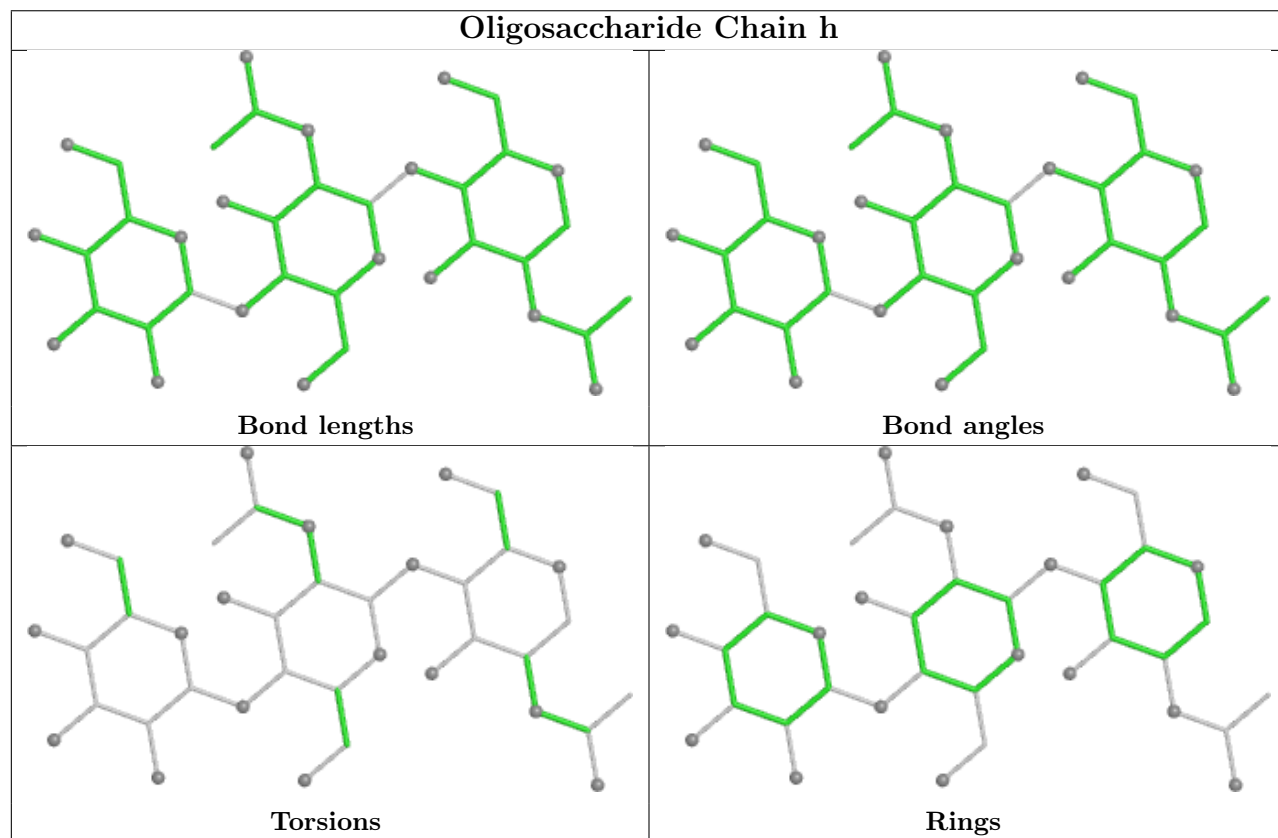
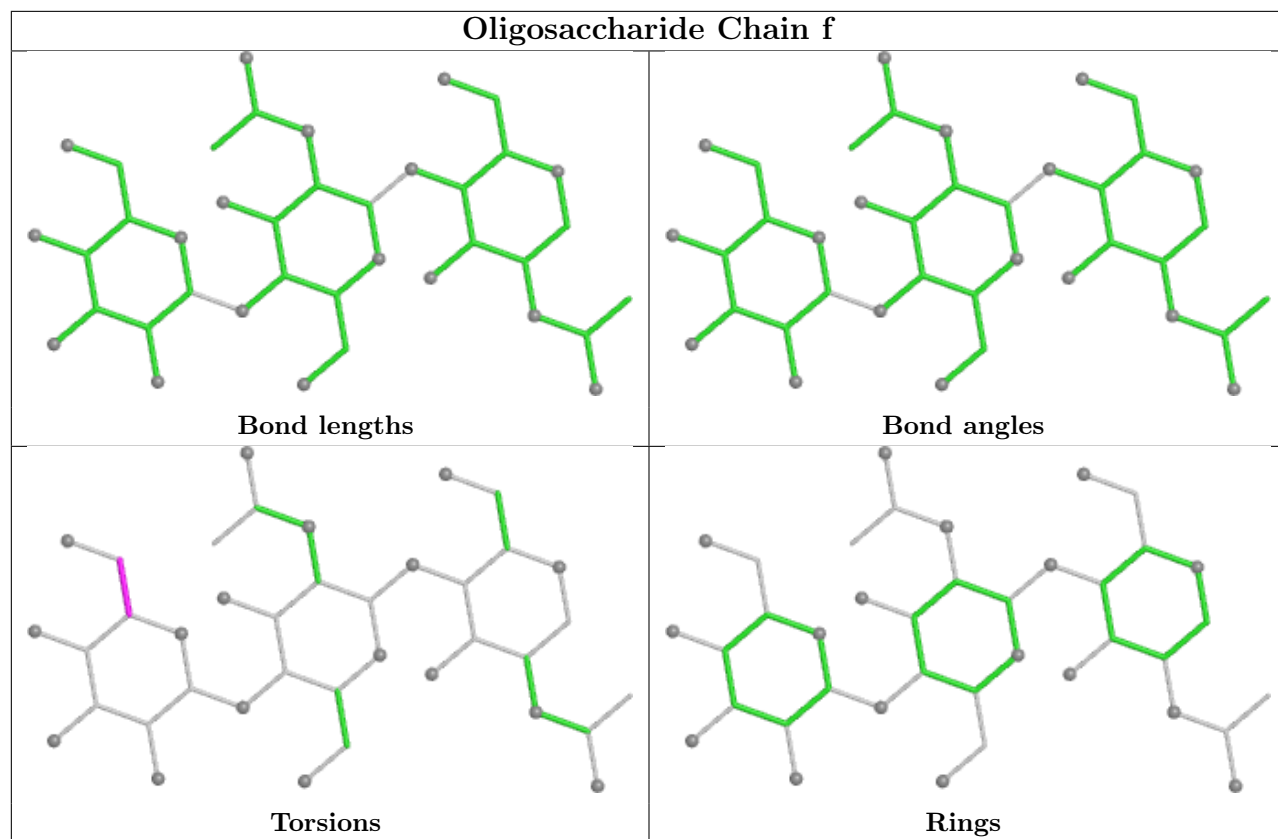


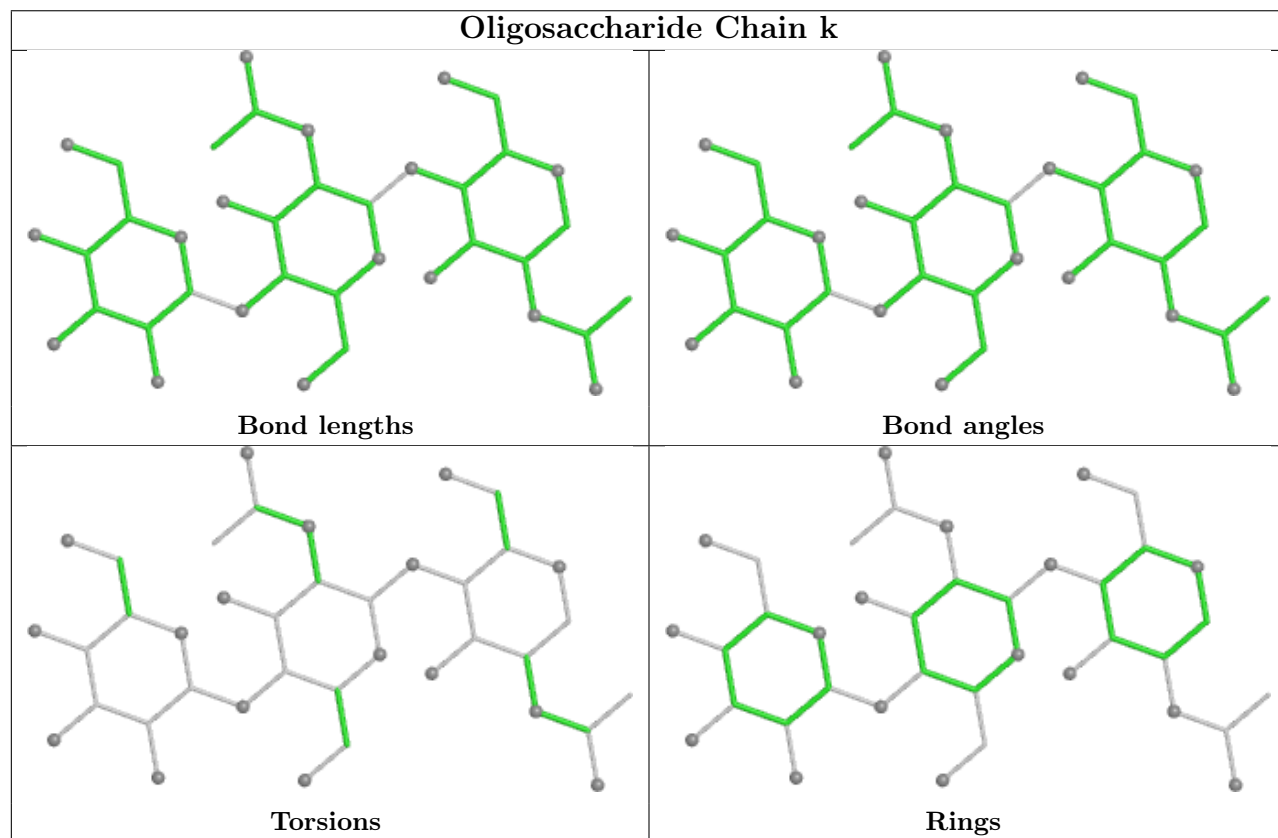
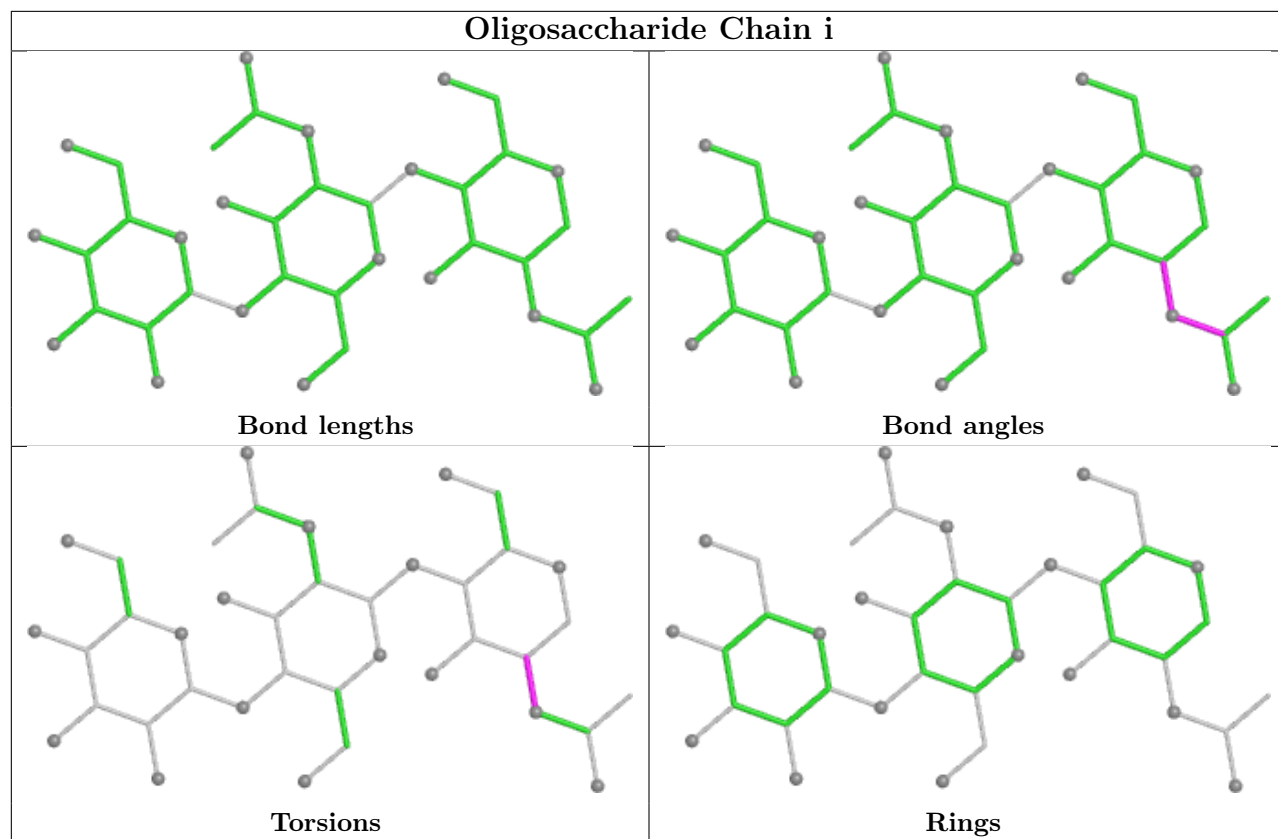


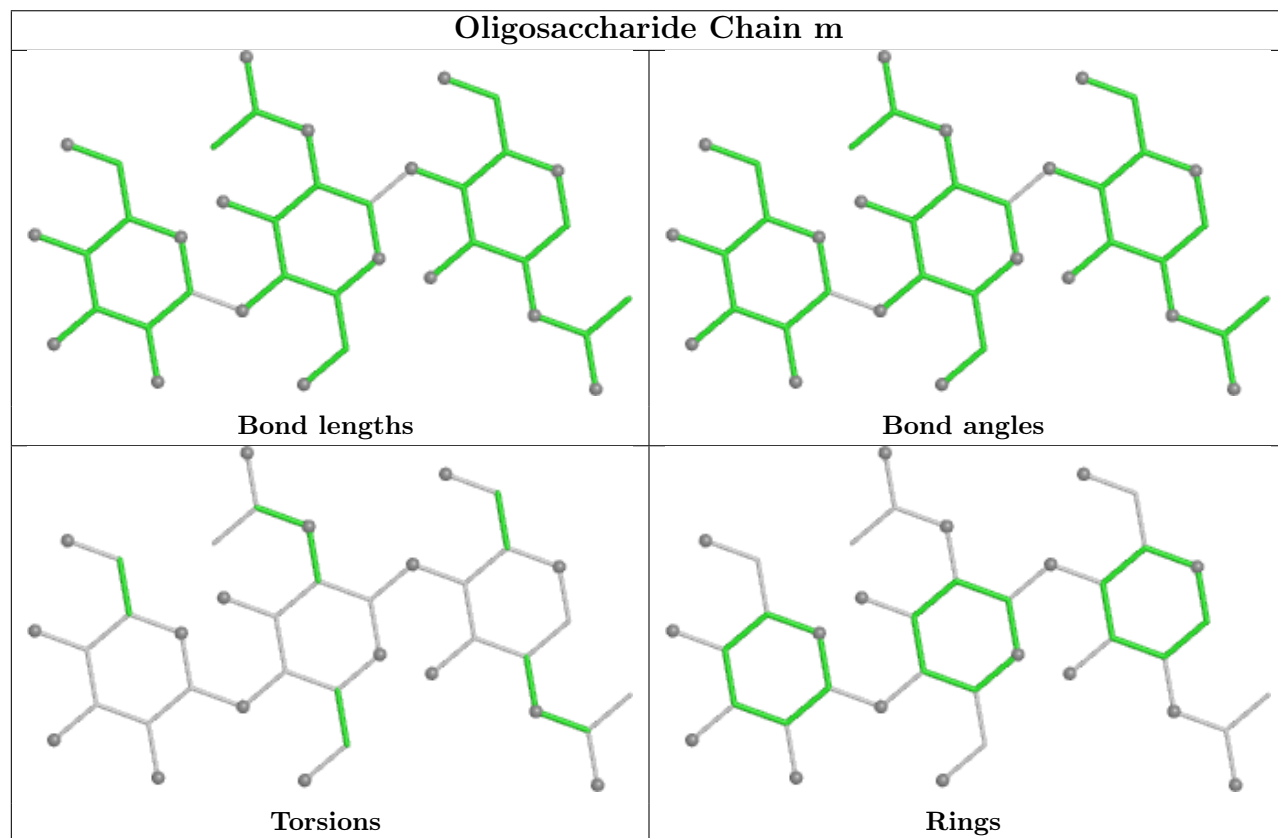
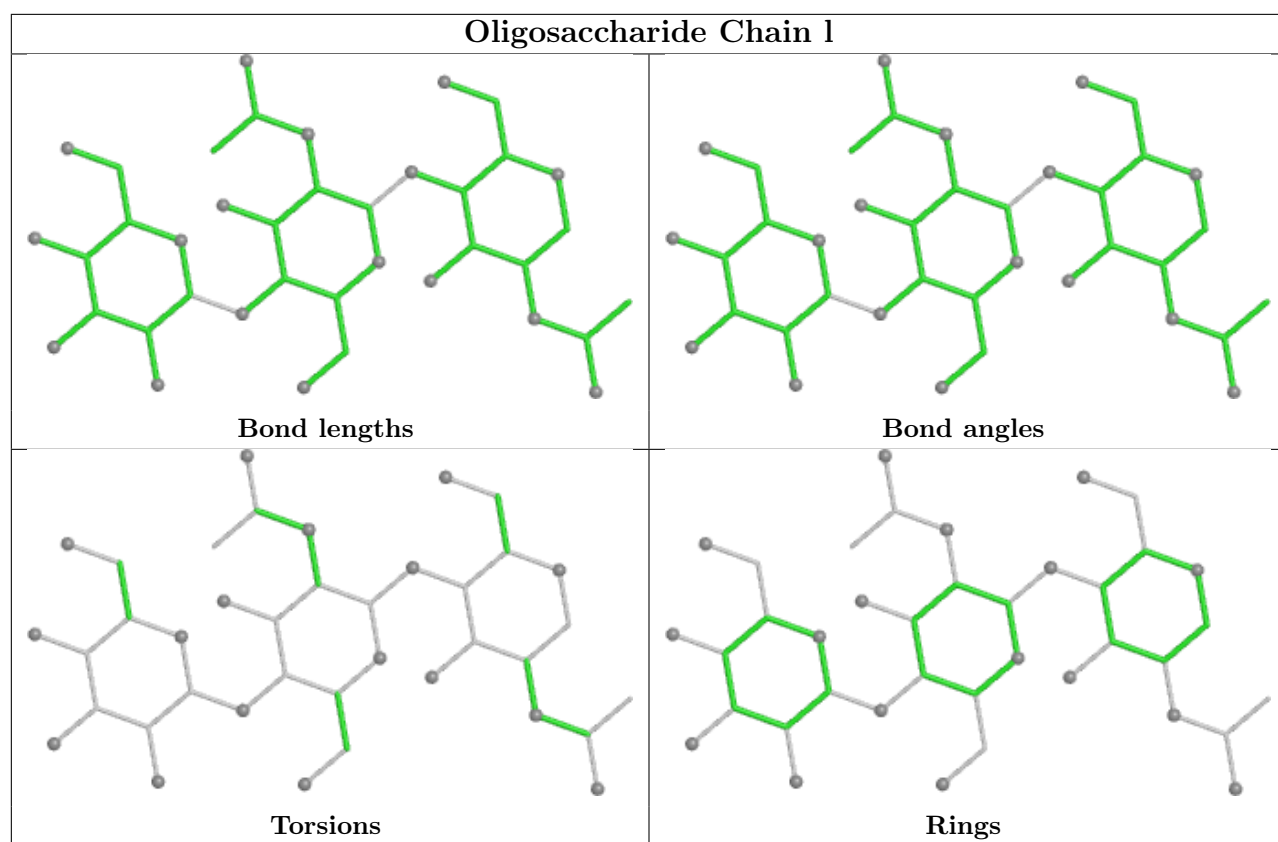


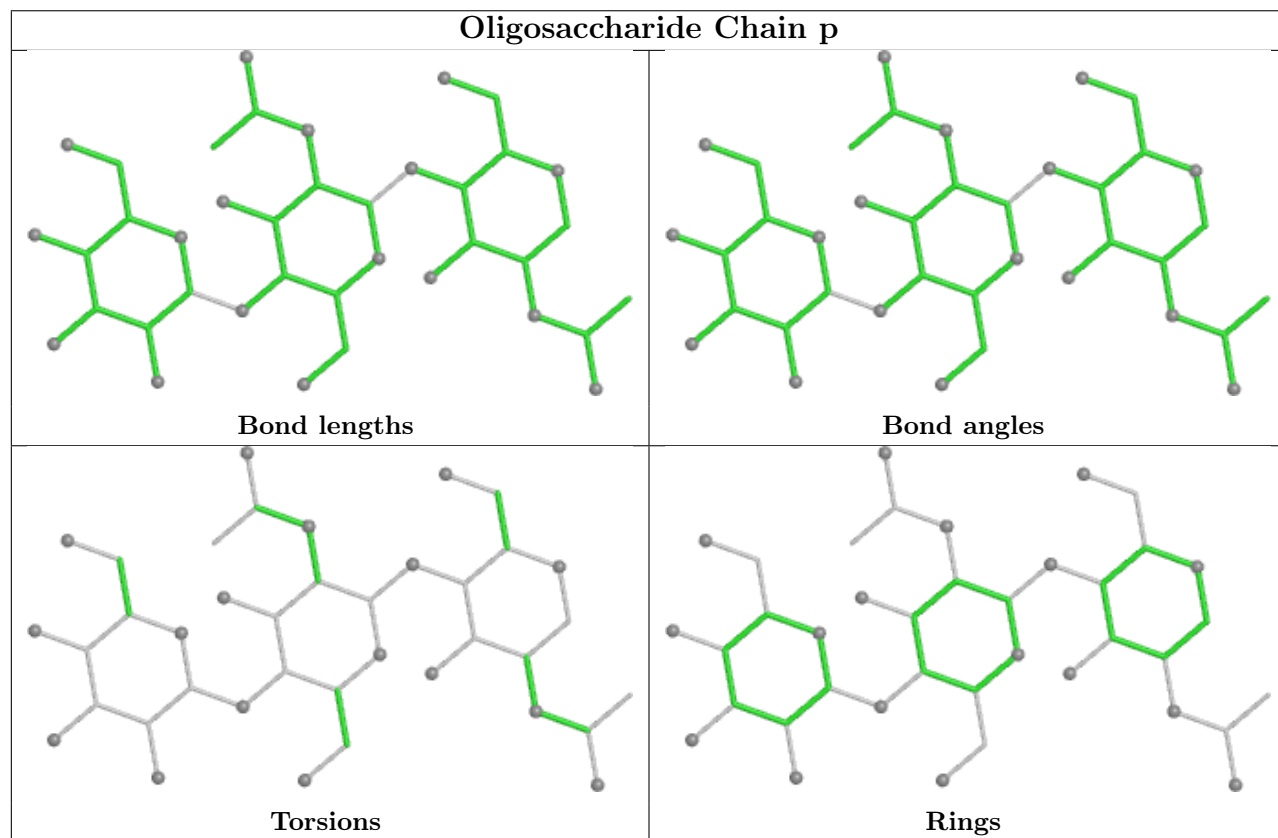
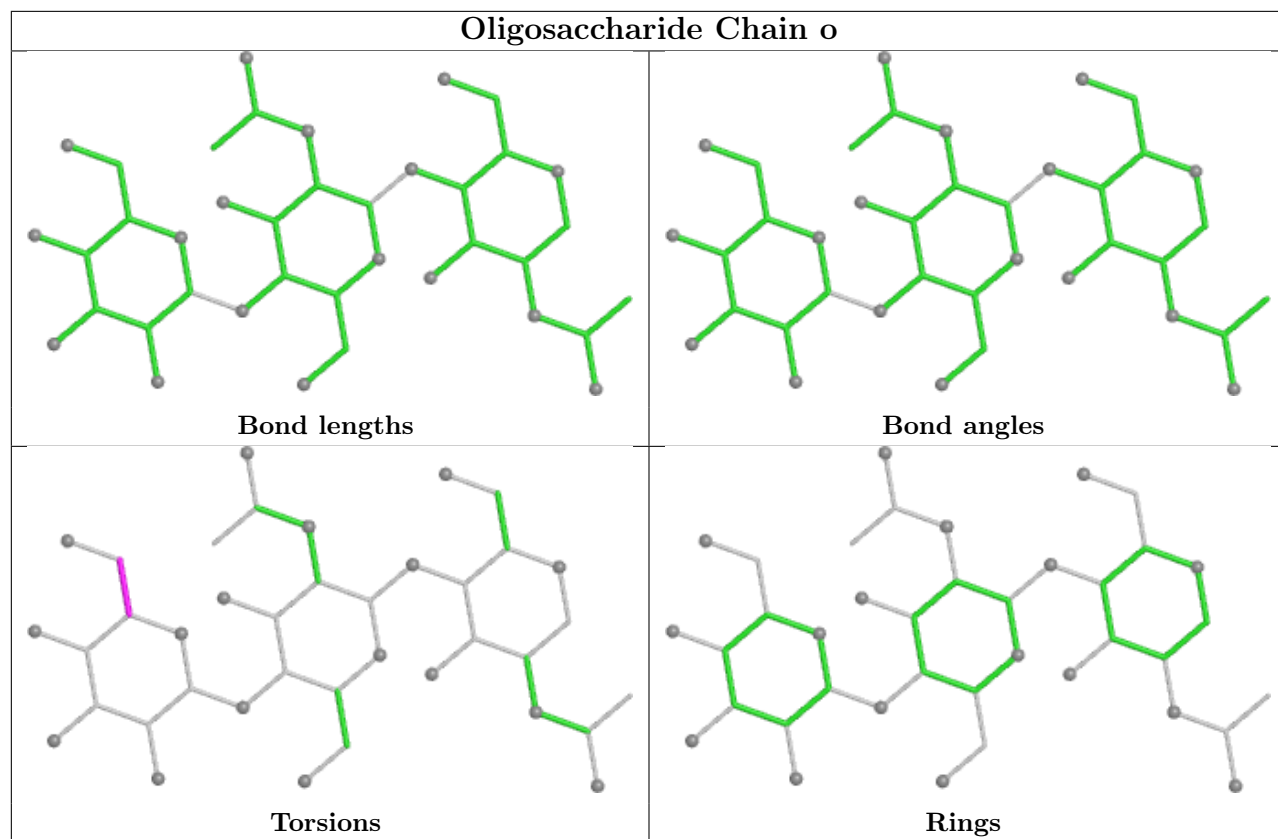


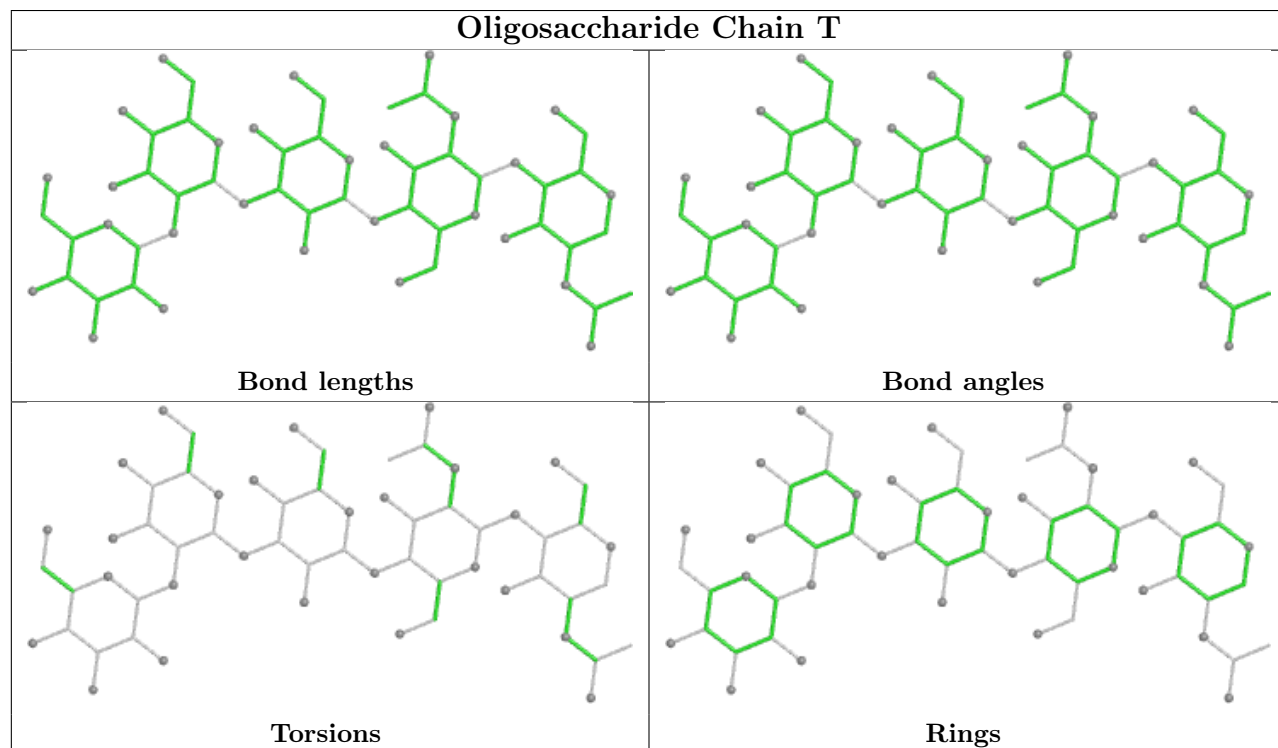
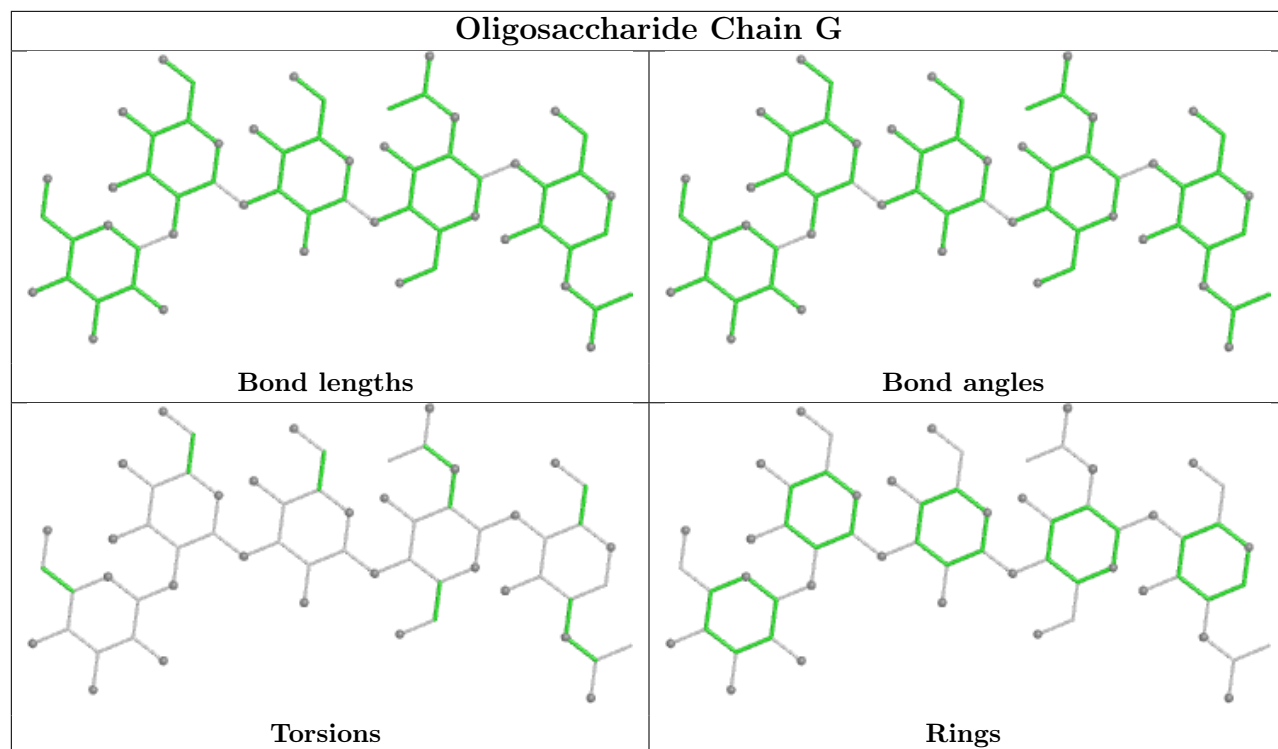


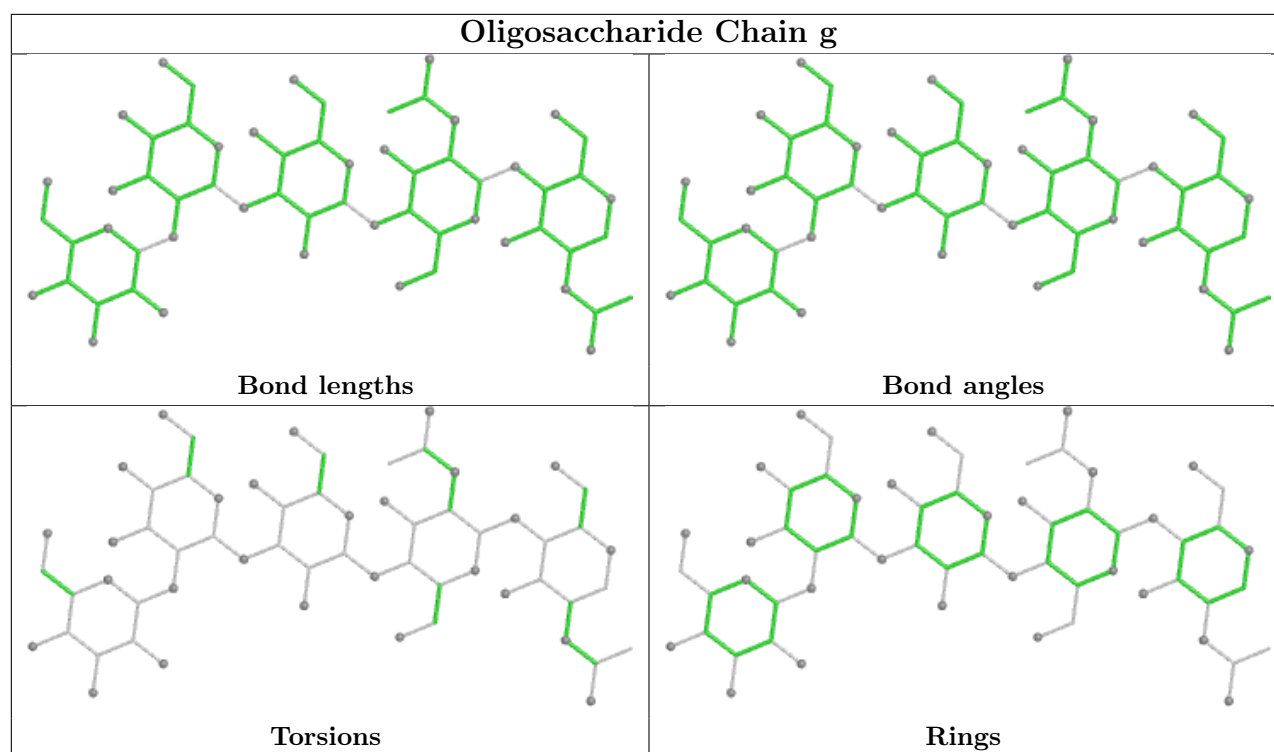












5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
5	NAG	A	1301	1	14,14,15	0.38	0	17,19,21	0.61	1 (5%)
5	NAG	C	1305	1	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	C	1302	1	14,14,15	0.38	0	17,19,21	0.46	0
5	NAG	C	1307	1	14,14,15	0.40	0	17,19,21	0.44	0
5	NAG	B	1303	1	14,14,15	0.39	0	17,19,21	0.46	0
5	NAG	C	1301	1	14,14,15	0.37	0	17,19,21	0.61	1 (5%)
5	NAG	A	1303	1	14,14,15	0.38	0	17,19,21	0.46	0
5	NAG	C	1306	1	14,14,15	0.37	0	17,19,21	0.44	0
5	NAG	B	1306	1	14,14,15	0.39	0	17,19,21	0.44	0
5	NAG	C	1304	1	14,14,15	0.38	0	17,19,21	0.51	0
5	NAG	A	1306	1	14,14,15	0.38	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1305	1	14,14,15	0.39	0	17,19,21	0.52	0
5	NAG	B	1308	1	14,14,15	0.38	0	17,19,21	0.42	0
5	NAG	B	1304	1	14,14,15	0.38	0	17,19,21	0.52	0
5	NAG	C	1308	1	14,14,15	0.38	0	17,19,21	0.42	0
5	NAG	C	1303	1	14,14,15	0.37	0	17,19,21	0.46	0
5	NAG	A	1308	1	14,14,15	0.39	0	17,19,21	0.42	0
5	NAG	B	1302	1	14,14,15	0.38	0	17,19,21	0.46	0
5	NAG	A	1305	1	14,14,15	0.38	0	17,19,21	0.51	0
5	NAG	B	1307	1	14,14,15	0.39	0	17,19,21	0.44	0
5	NAG	A	1302	1	14,14,15	0.38	0	17,19,21	0.46	0
5	NAG	A	1307	1	14,14,15	0.39	0	17,19,21	0.44	0
5	NAG	B	1301	1	14,14,15	0.39	0	17,19,21	0.61	0
5	NAG	A	1304	1	14,14,15	0.38	0	17,19,21	0.52	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
5	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1301	NAG	C1-O5-C5	2.02	114.94	112.19
5	C	1301	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1301	NAG	C8-C7-N2-C2
5	A	1301	NAG	O7-C7-N2-C2
5	B	1301	NAG	C8-C7-N2-C2
5	B	1301	NAG	O7-C7-N2-C2
5	C	1301	NAG	C8-C7-N2-C2
5	C	1301	NAG	O7-C7-N2-C2
5	A	1303	NAG	C8-C7-N2-C2
5	A	1303	NAG	O7-C7-N2-C2
5	B	1303	NAG	C8-C7-N2-C2
5	B	1303	NAG	O7-C7-N2-C2
5	C	1303	NAG	C8-C7-N2-C2
5	C	1303	NAG	O7-C7-N2-C2
5	A	1304	NAG	C8-C7-N2-C2
5	A	1304	NAG	O7-C7-N2-C2
5	B	1304	NAG	C8-C7-N2-C2
5	B	1304	NAG	O7-C7-N2-C2
5	C	1304	NAG	C8-C7-N2-C2
5	C	1304	NAG	O7-C7-N2-C2
5	A	1301	NAG	C1-C2-N2-C7
5	B	1301	NAG	C1-C2-N2-C7
5	C	1301	NAG	C1-C2-N2-C7
5	A	1303	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	A	1301	NAG	C3-C2-N2-C7
5	B	1301	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1301	NAG	C3-C2-N2-C7

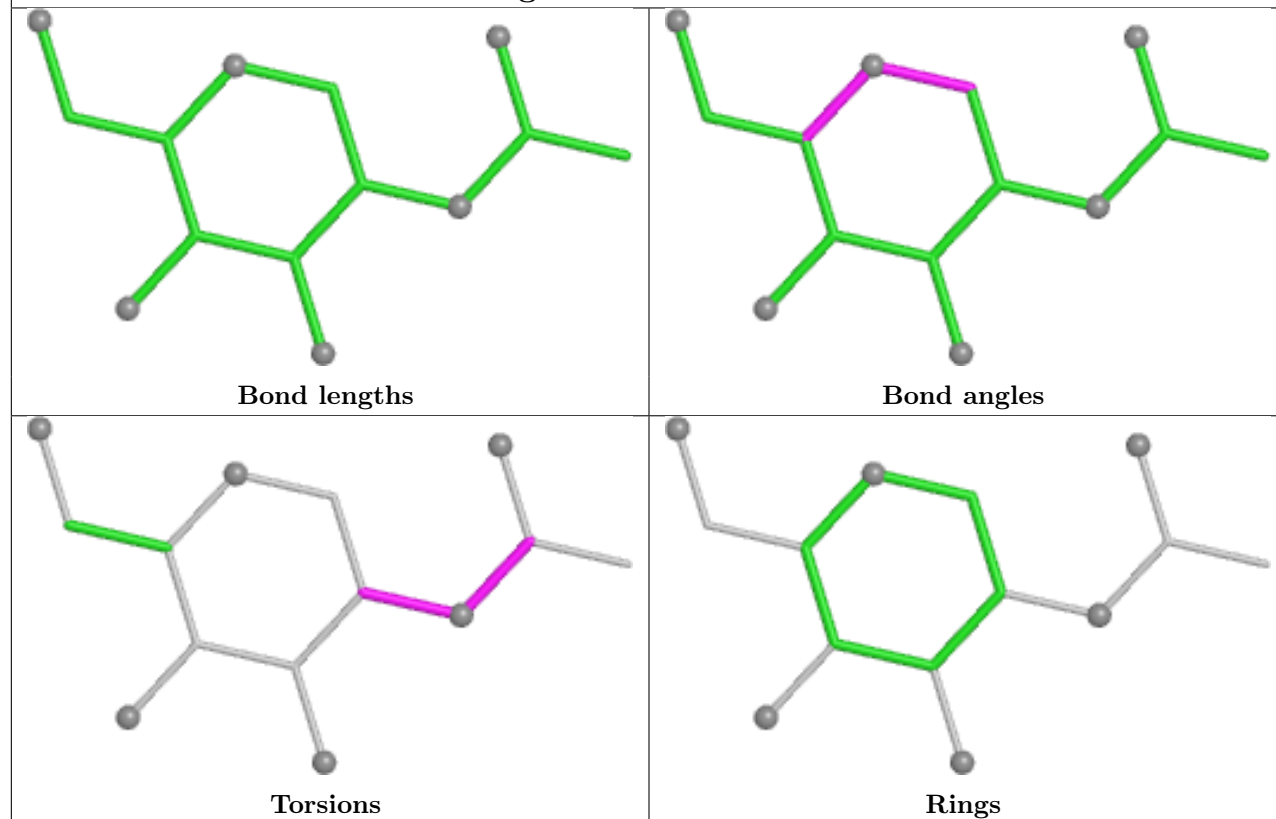
There are no ring outliers.

3 monomers are involved in 3 short contacts:

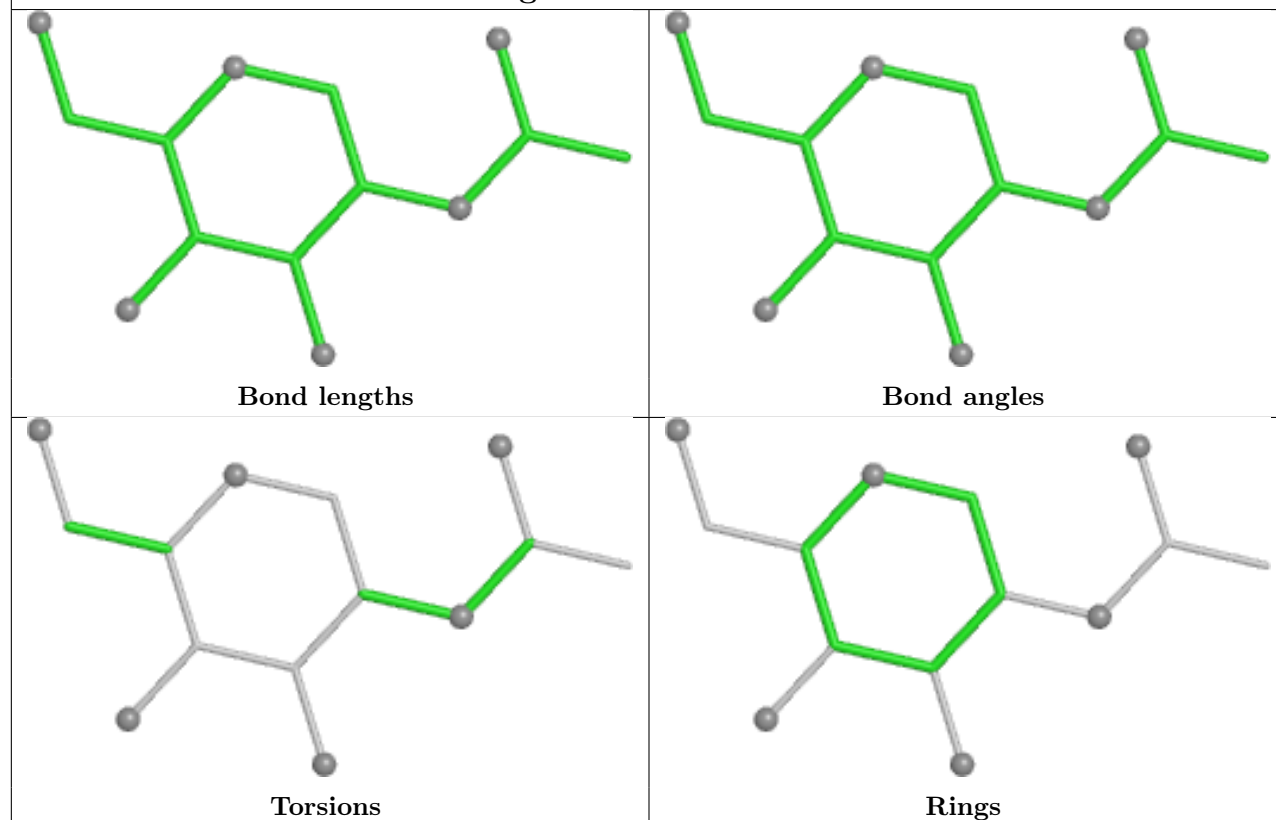
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1303	NAG	1	0
5	A	1303	NAG	1	0
5	C	1303	NAG	1	0

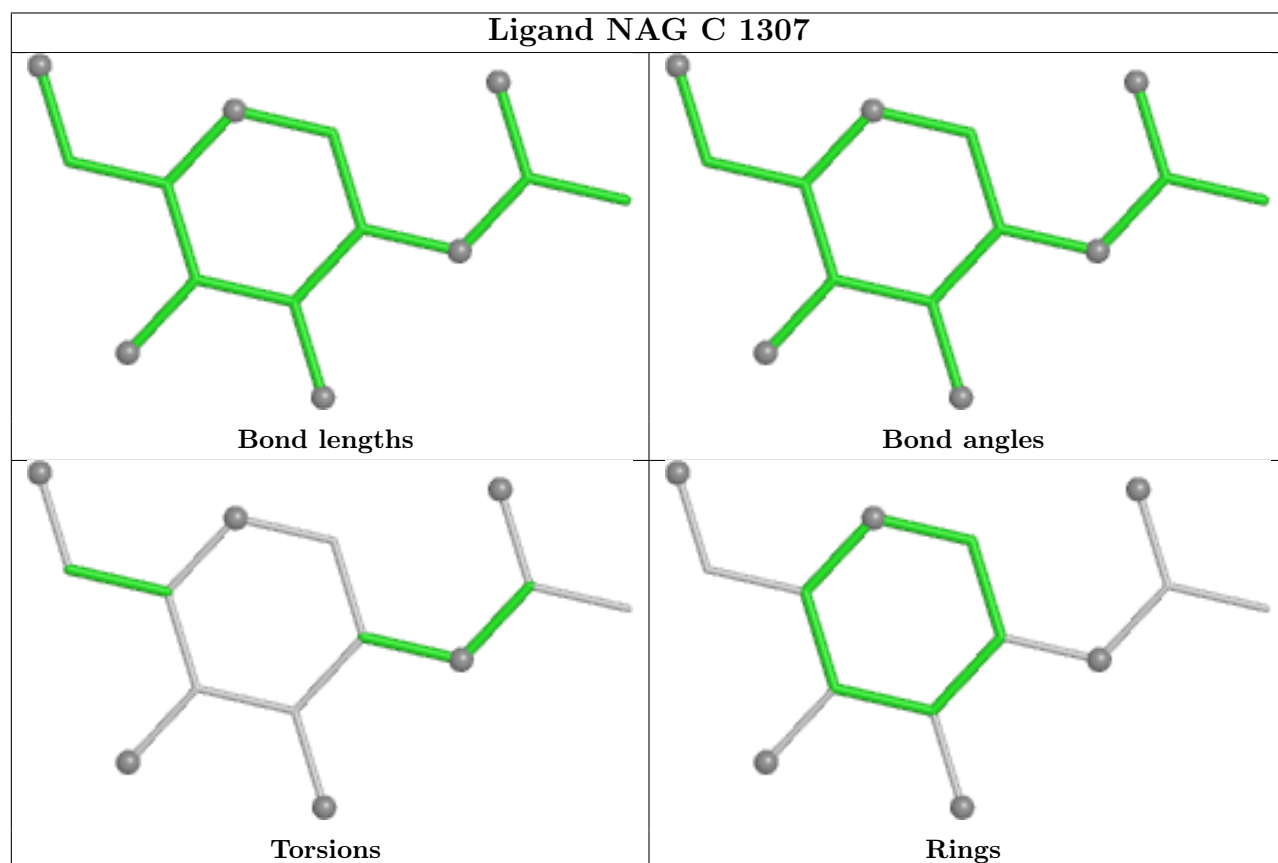
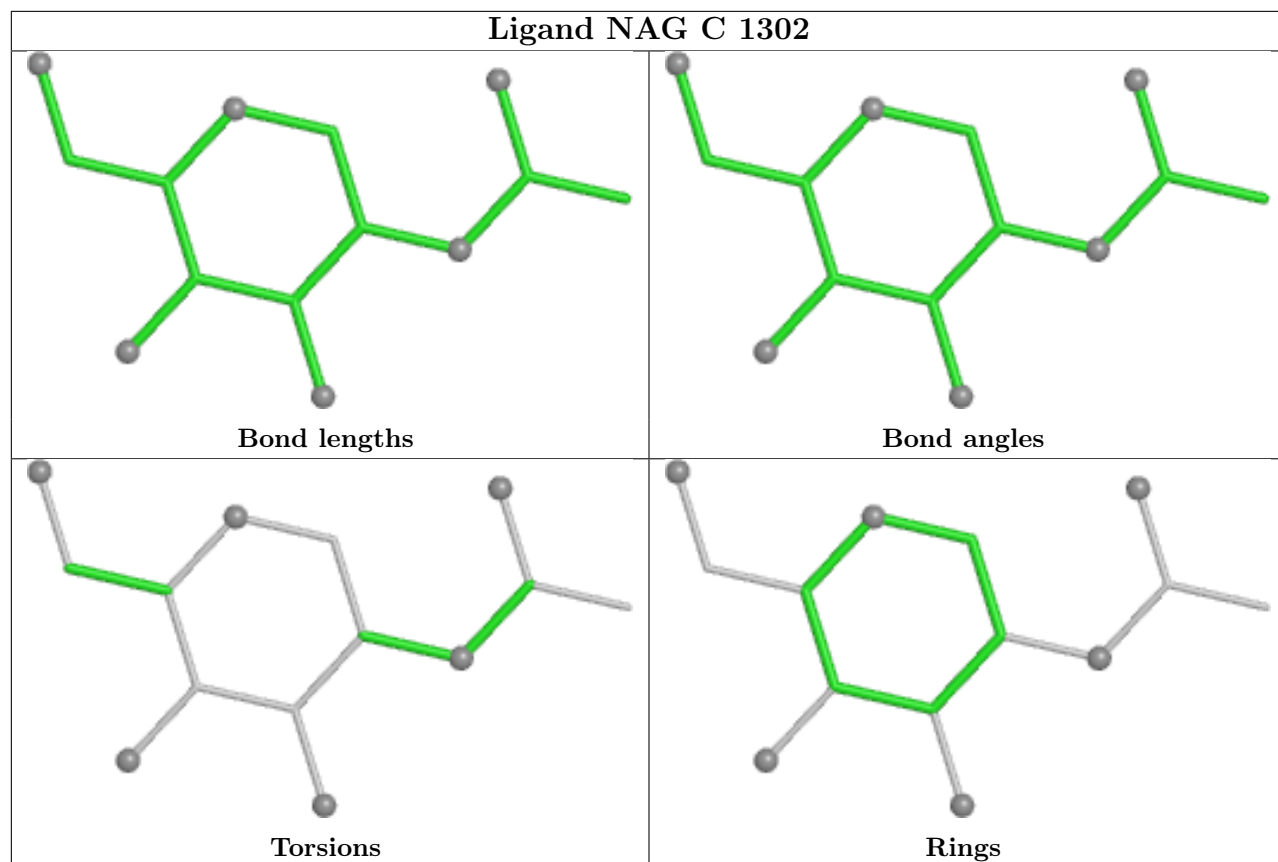
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NAG A 1301

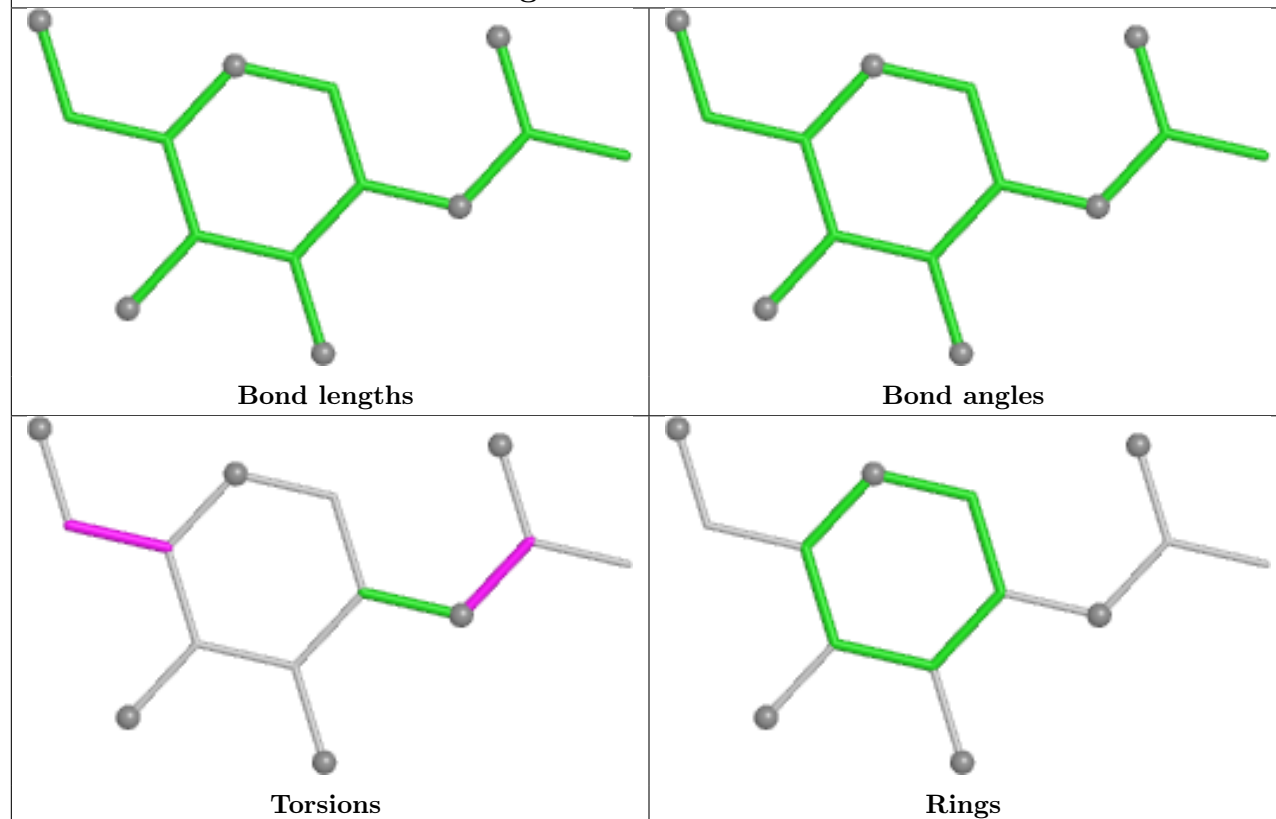


Ligand NAG C 1305

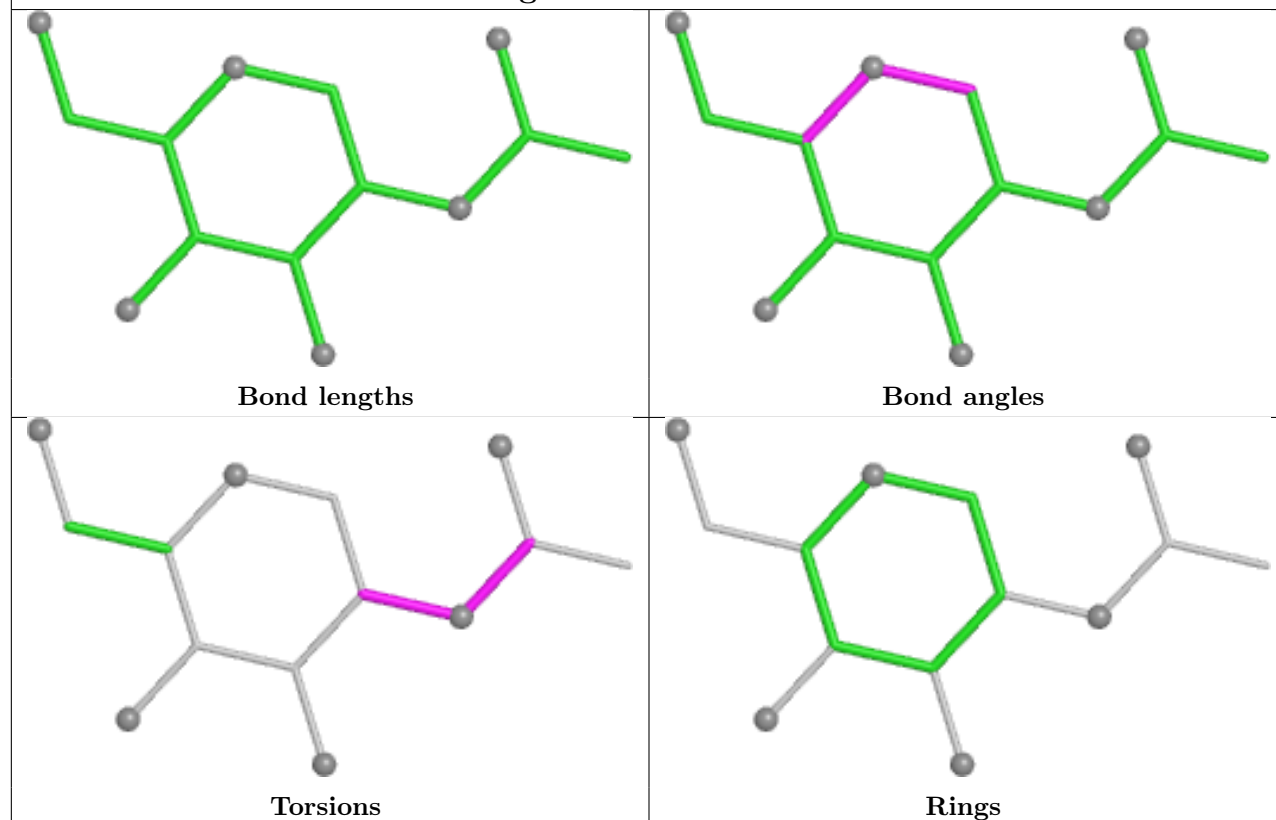




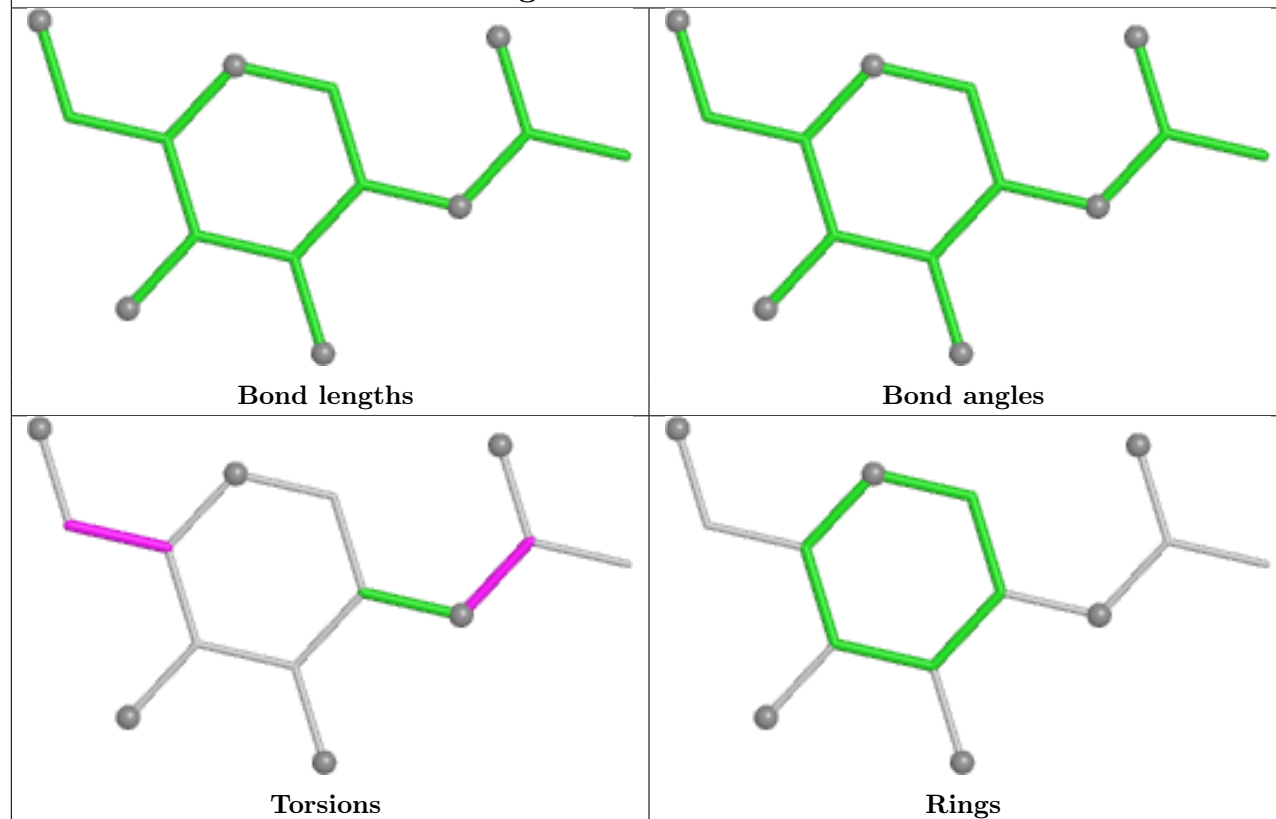
Ligand NAG B 1303



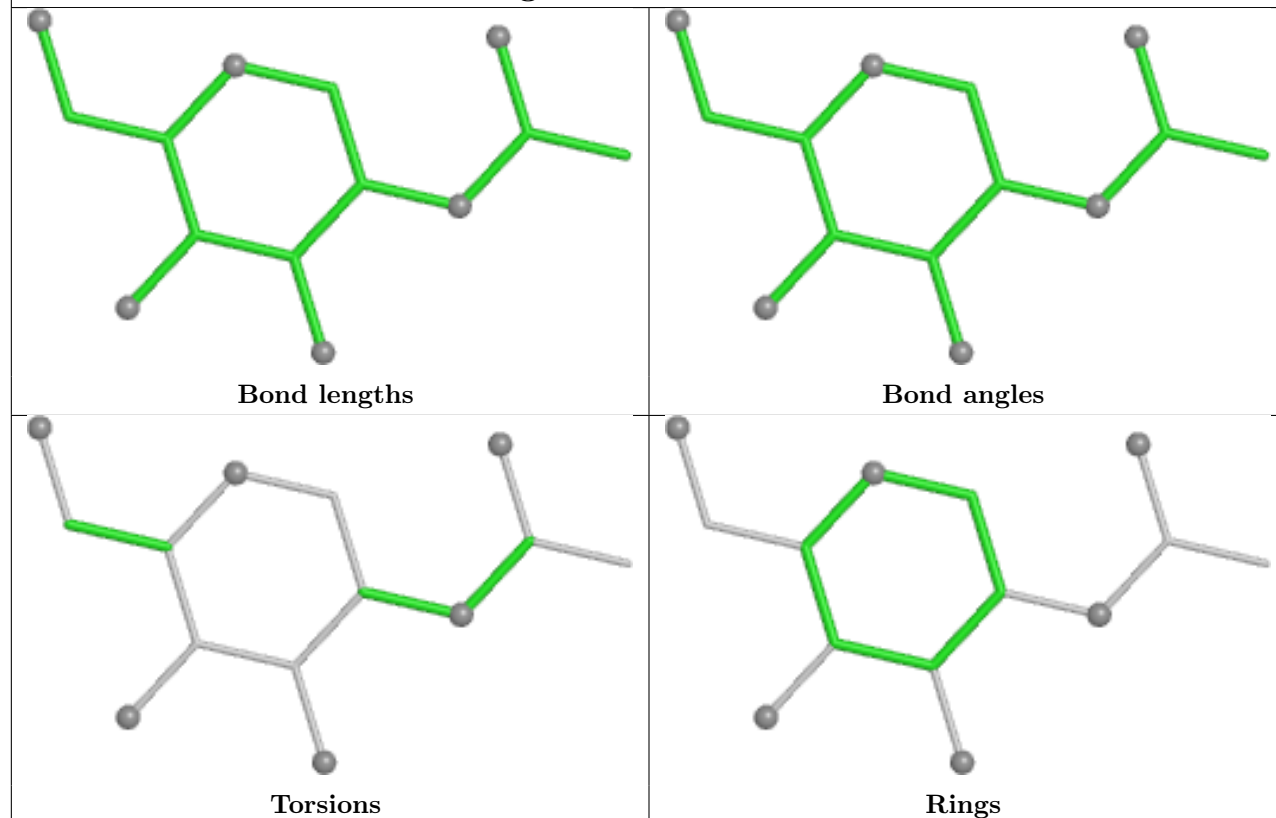
Ligand NAG C 1301



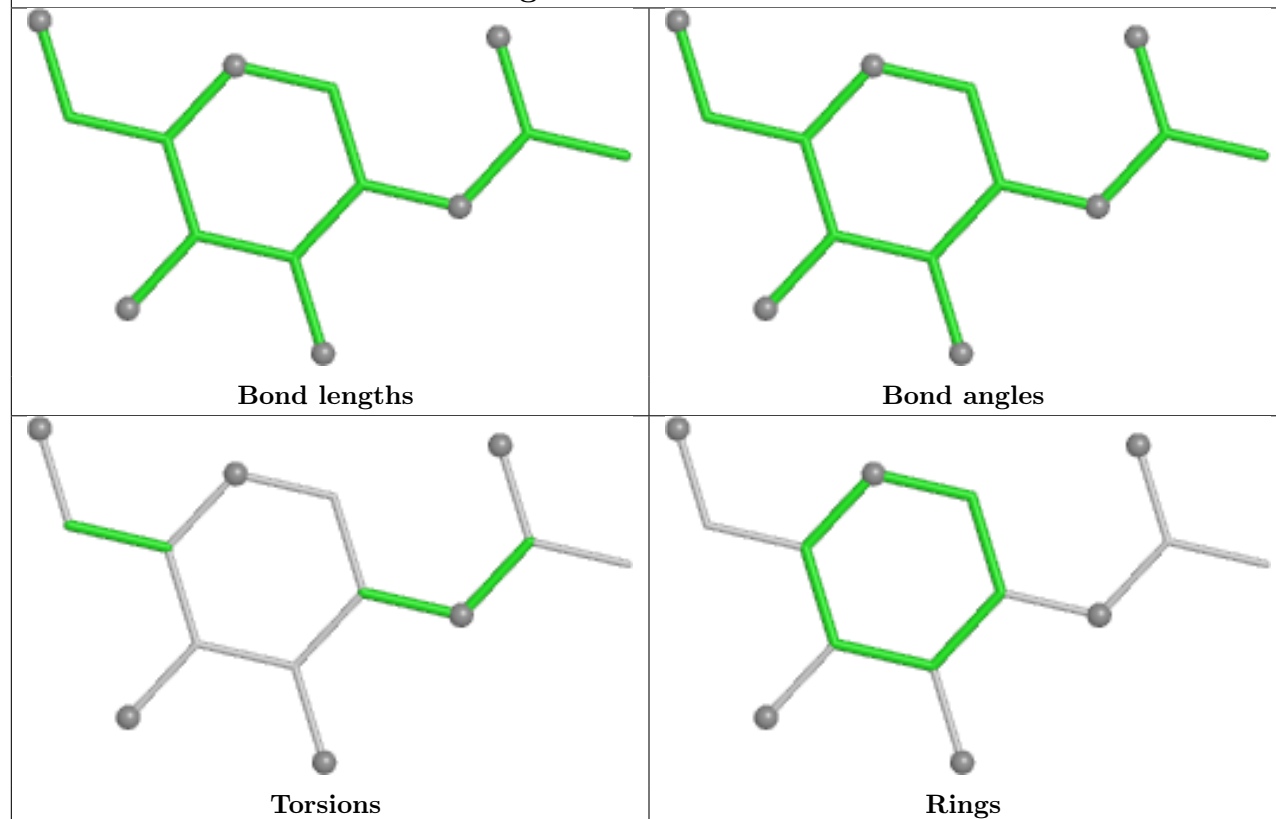
Ligand NAG A 1303



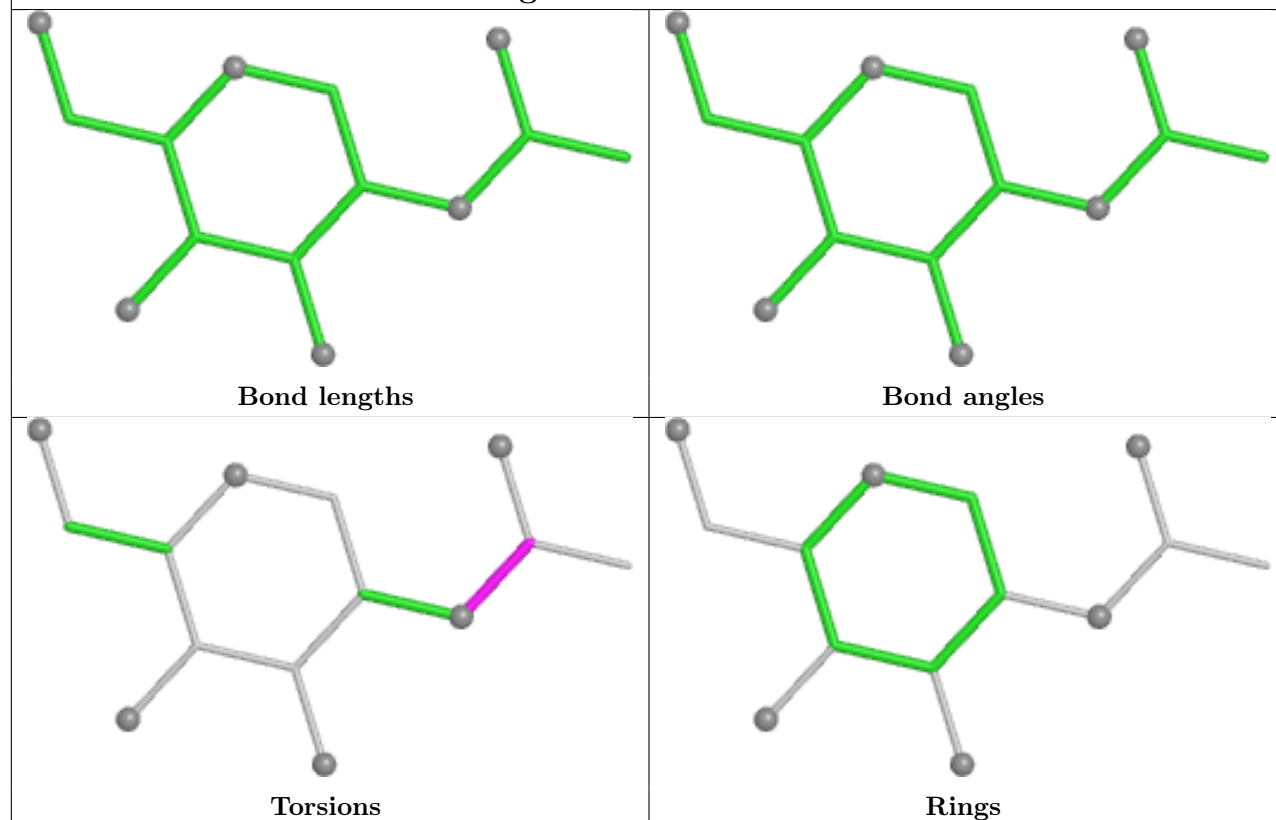
Ligand NAG C 1306



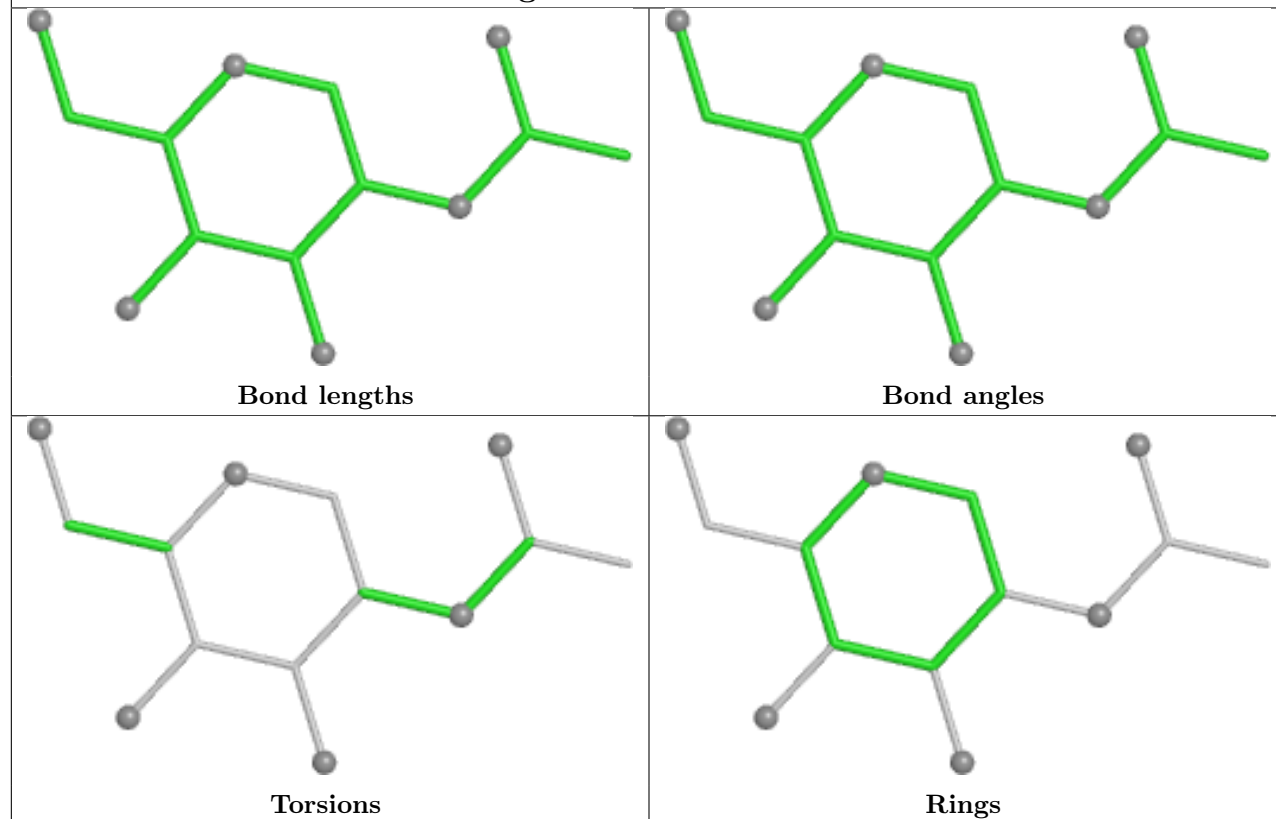
Ligand NAG B 1306



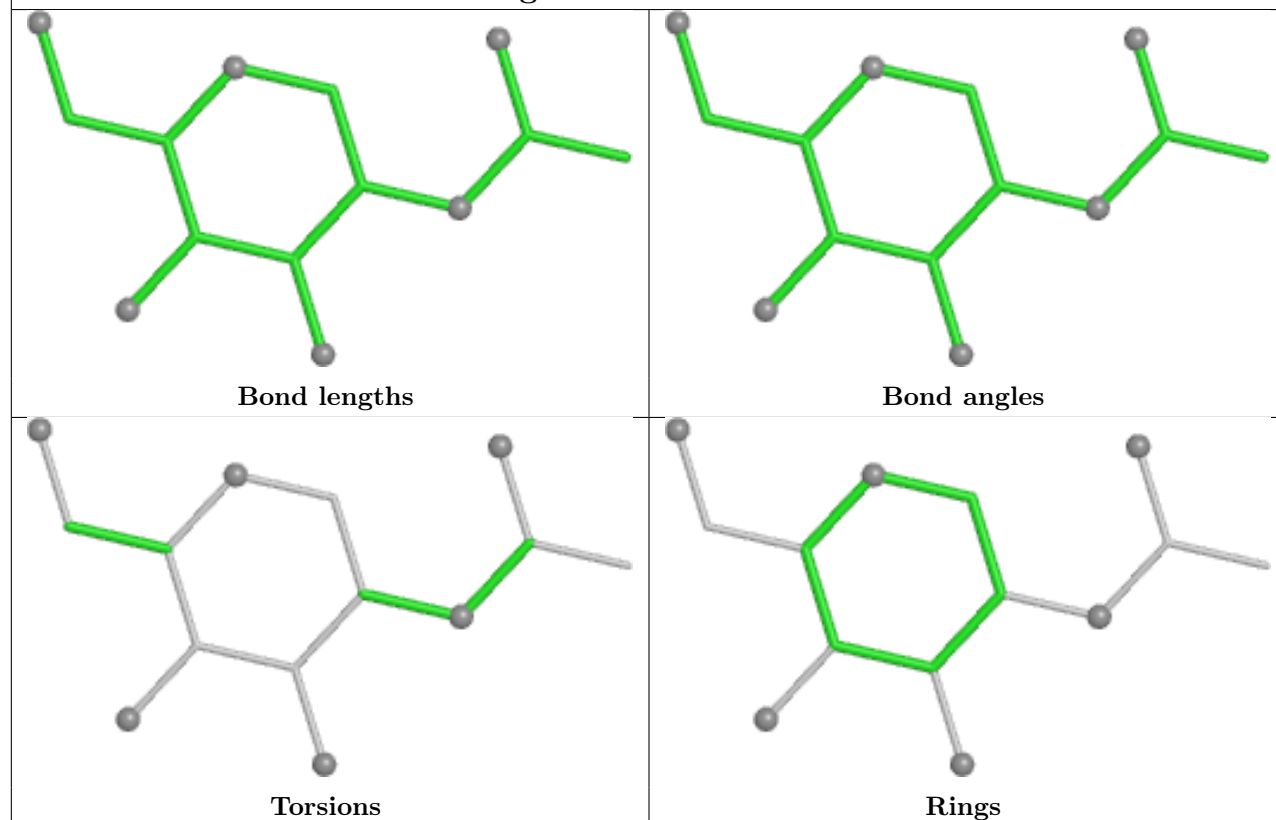
Ligand NAG C 1304

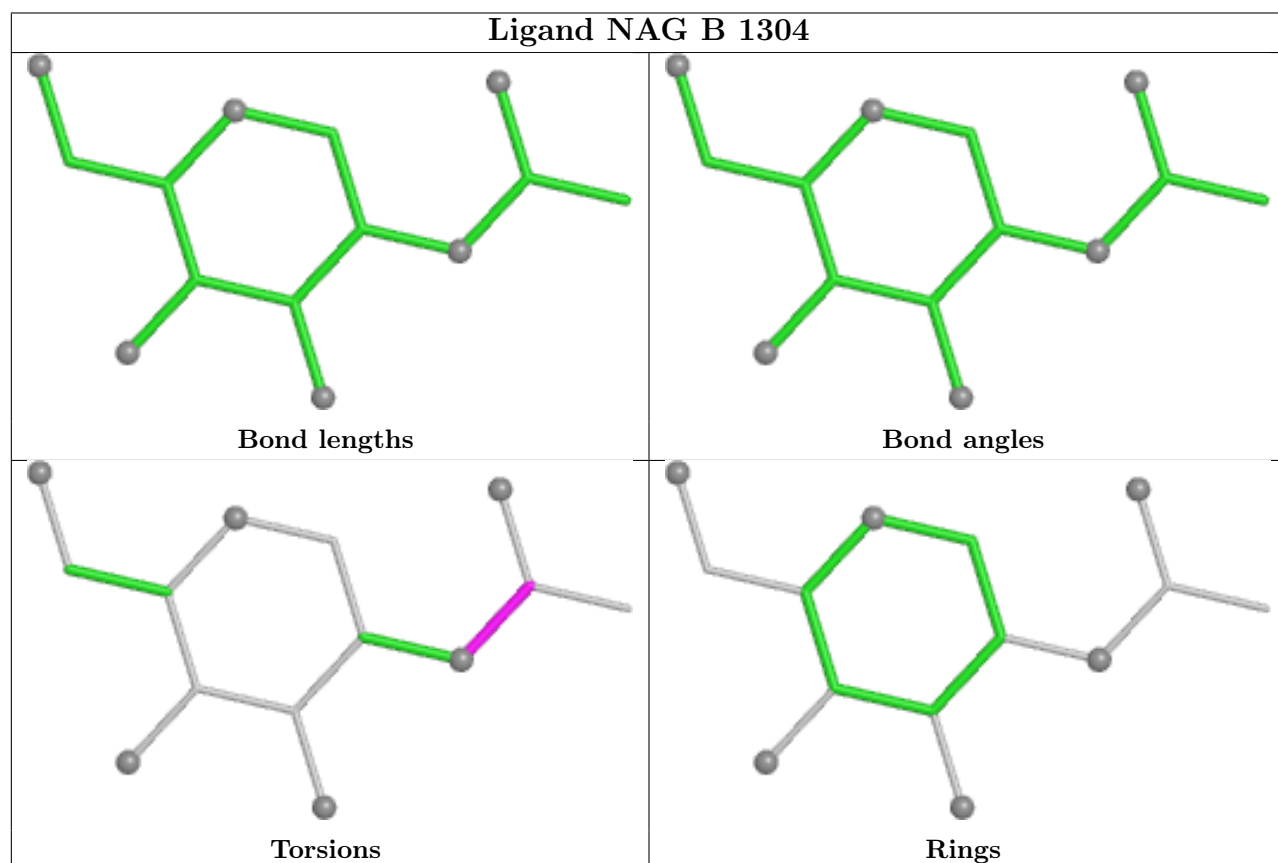
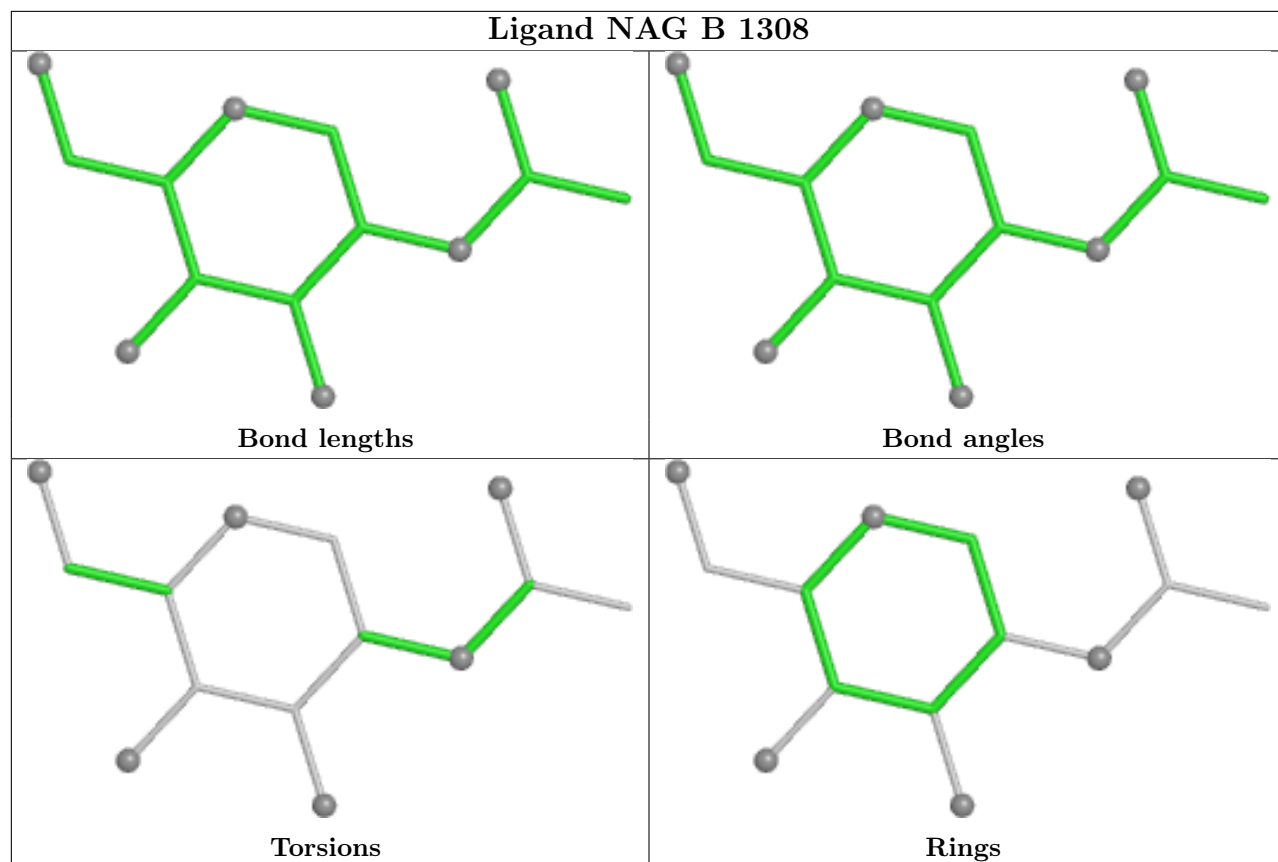


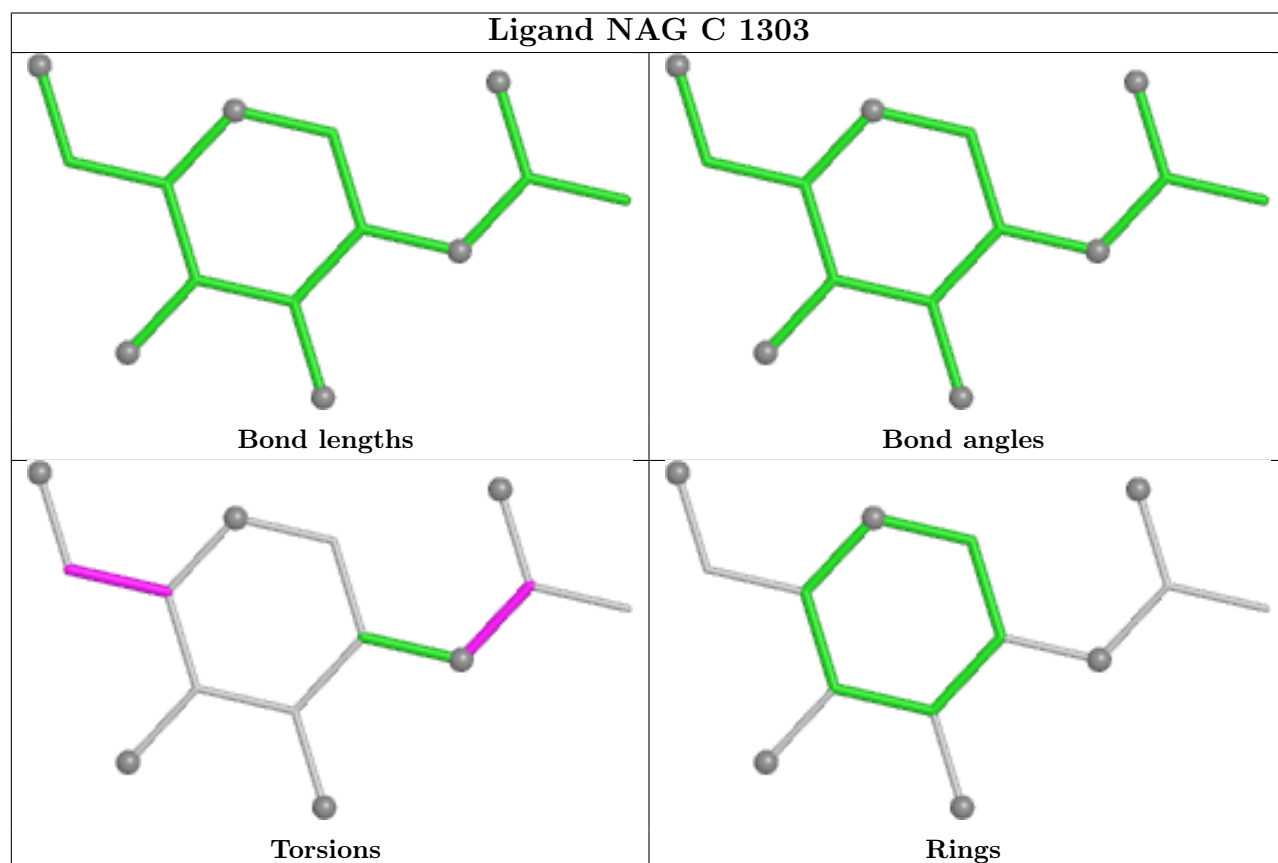
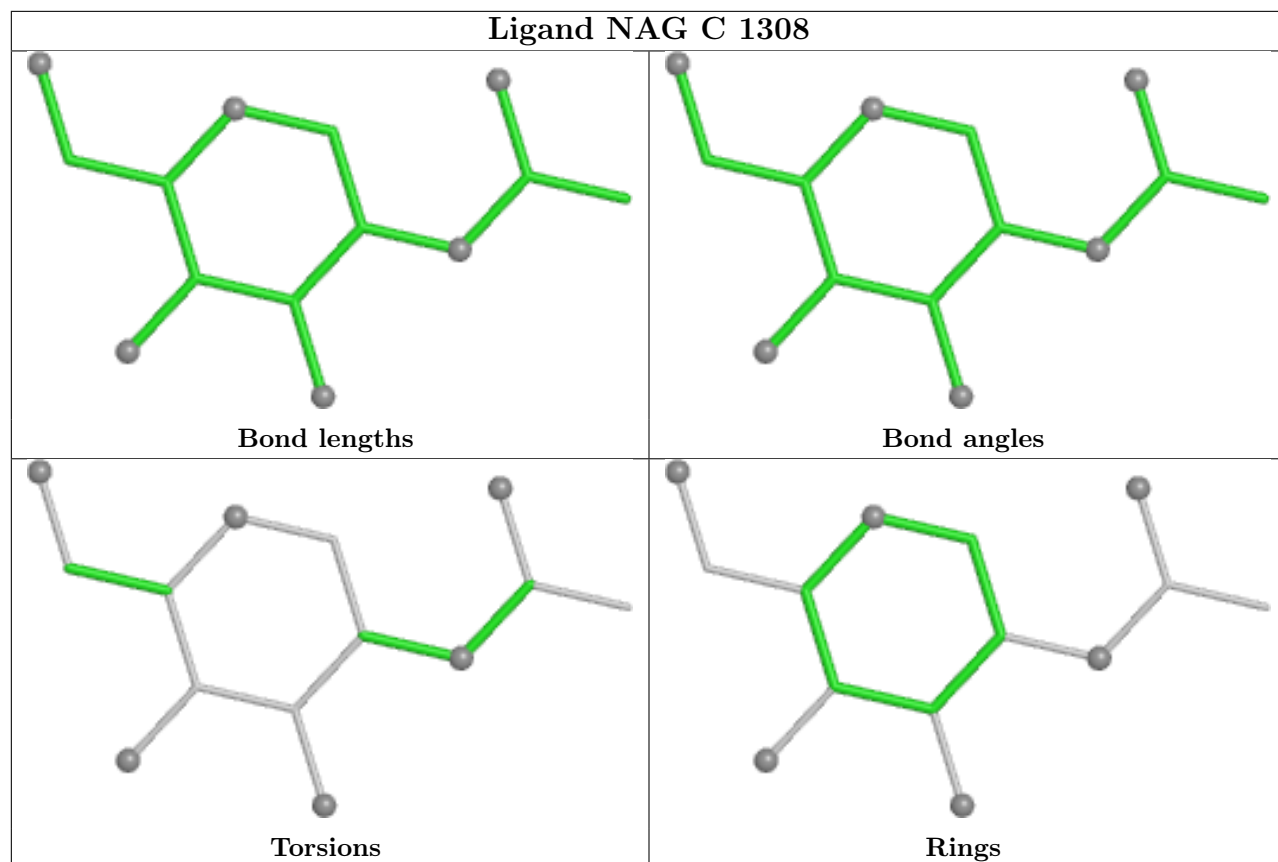
Ligand NAG A 1306



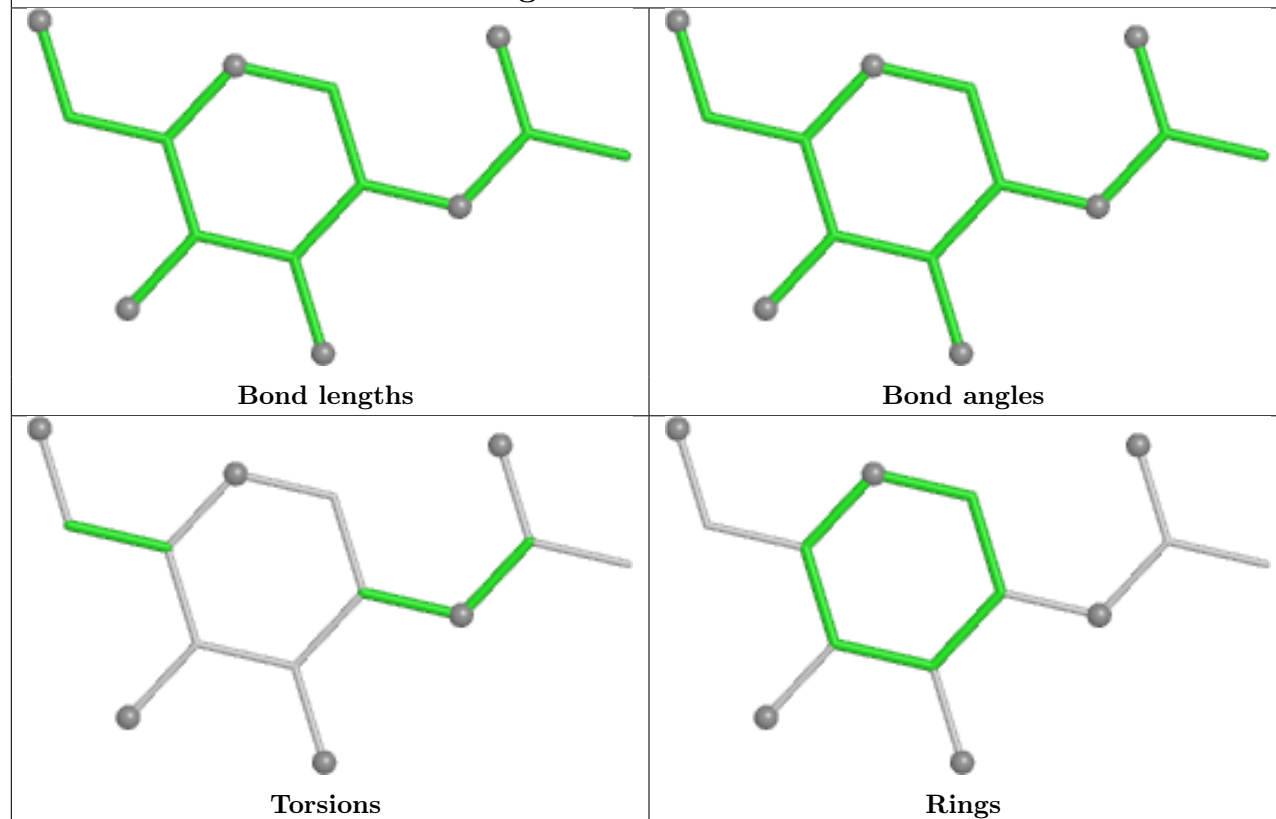
Ligand NAG B 1305



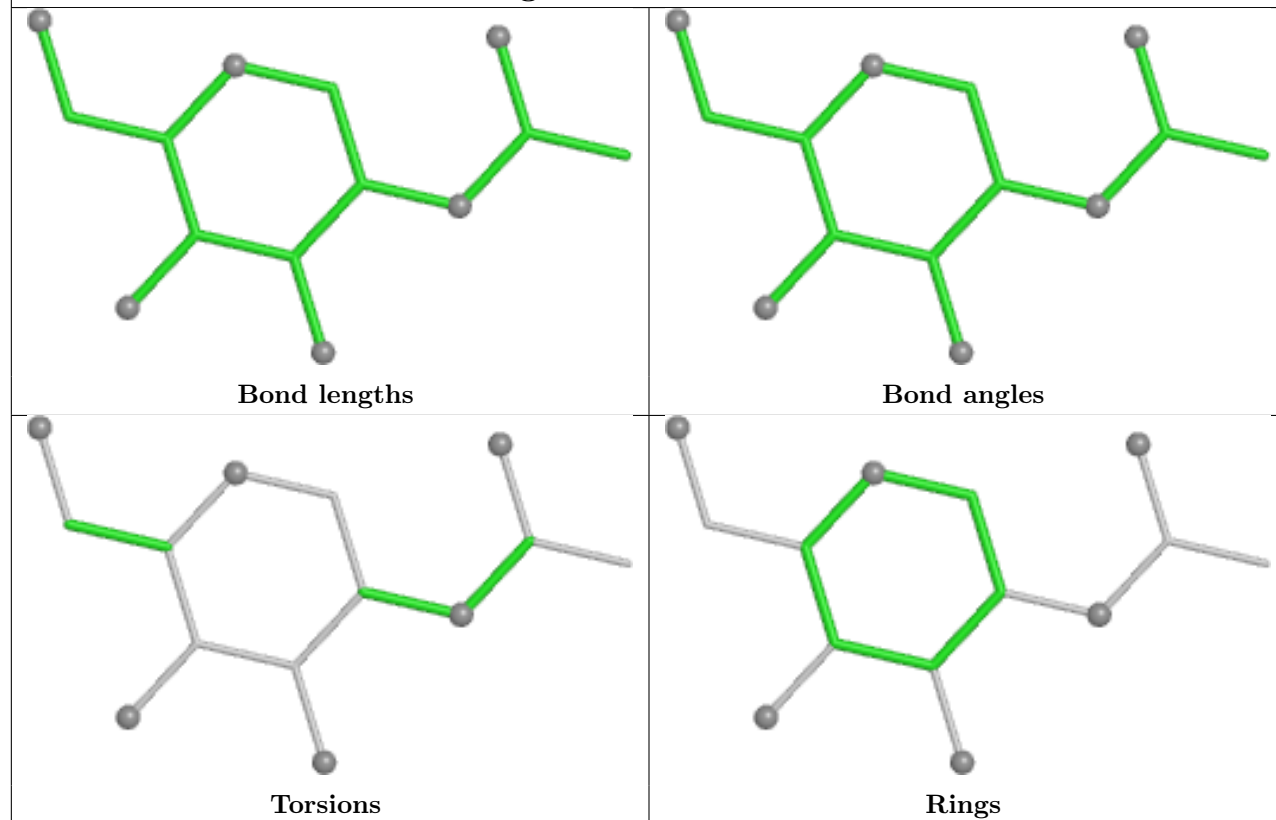




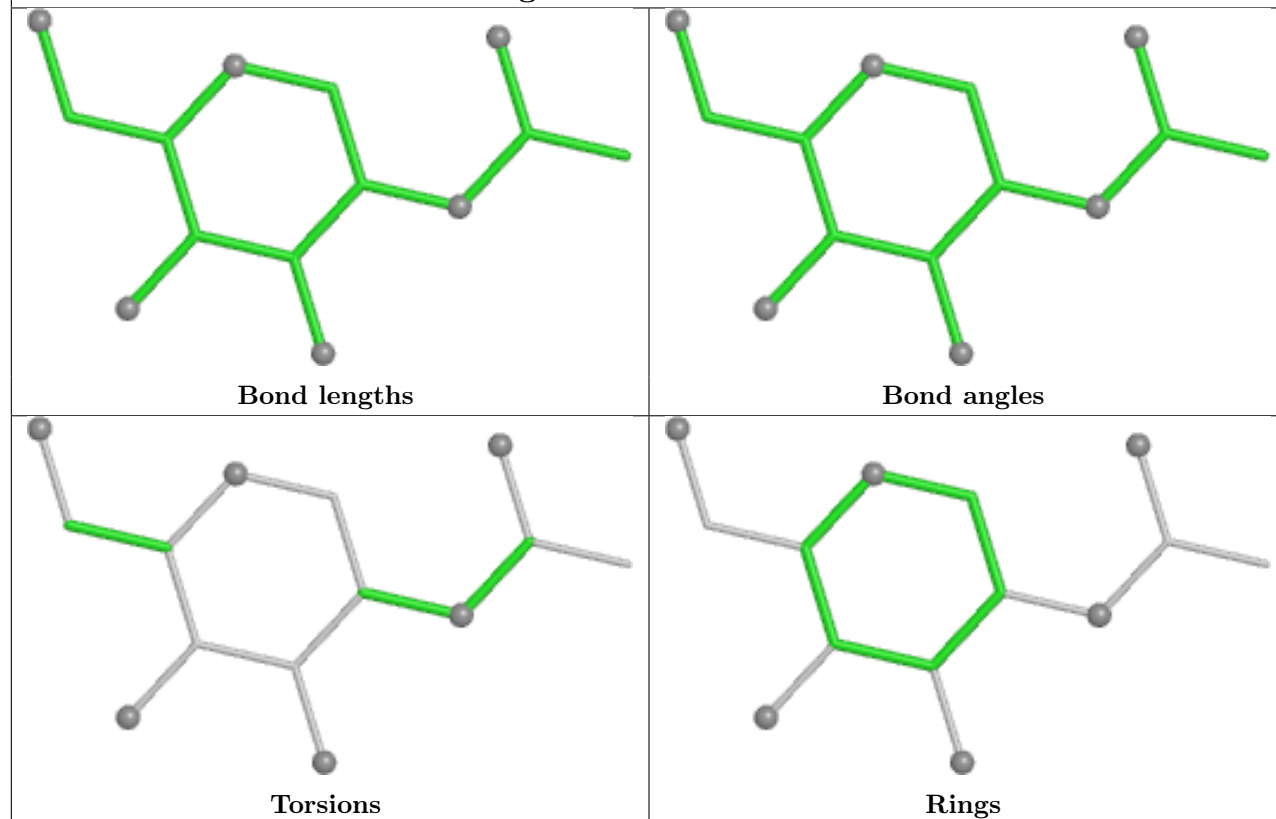
Ligand NAG A 1308



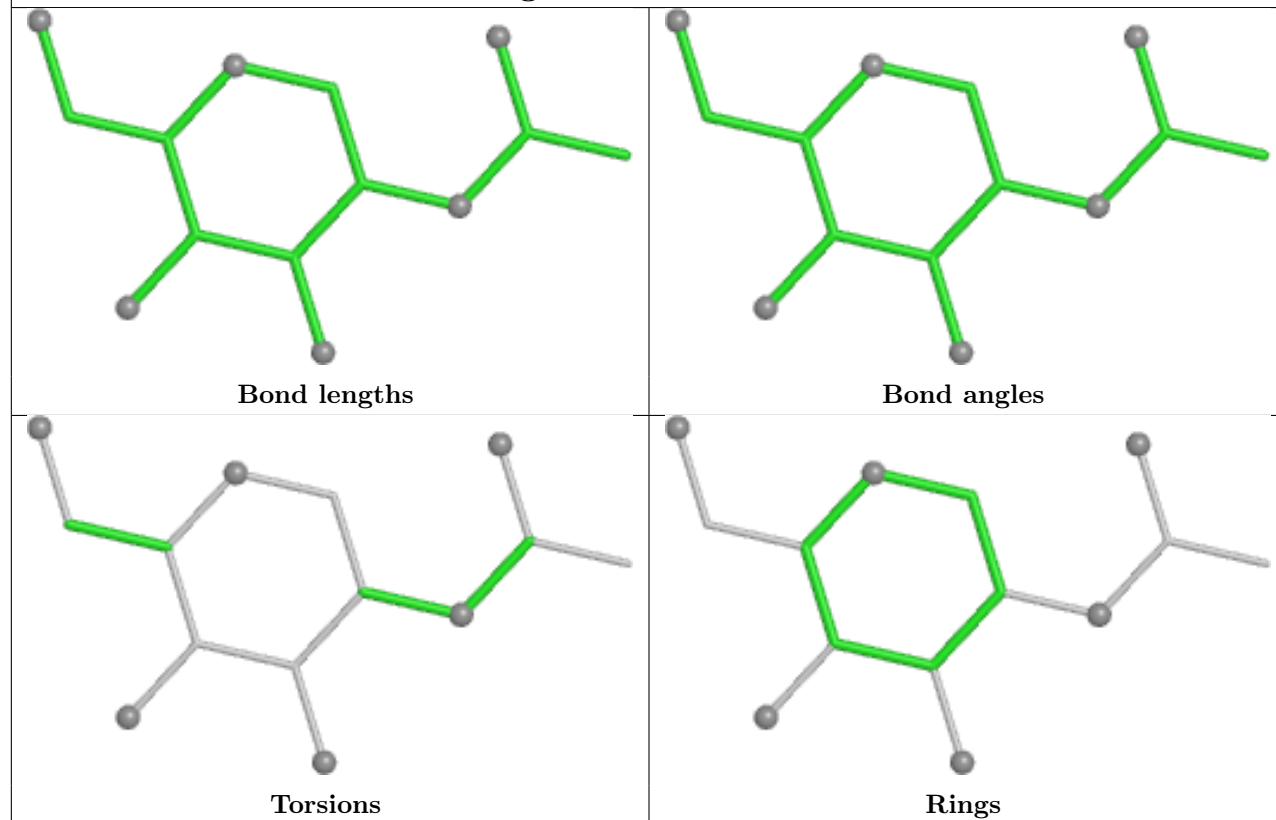
Ligand NAG B 1302



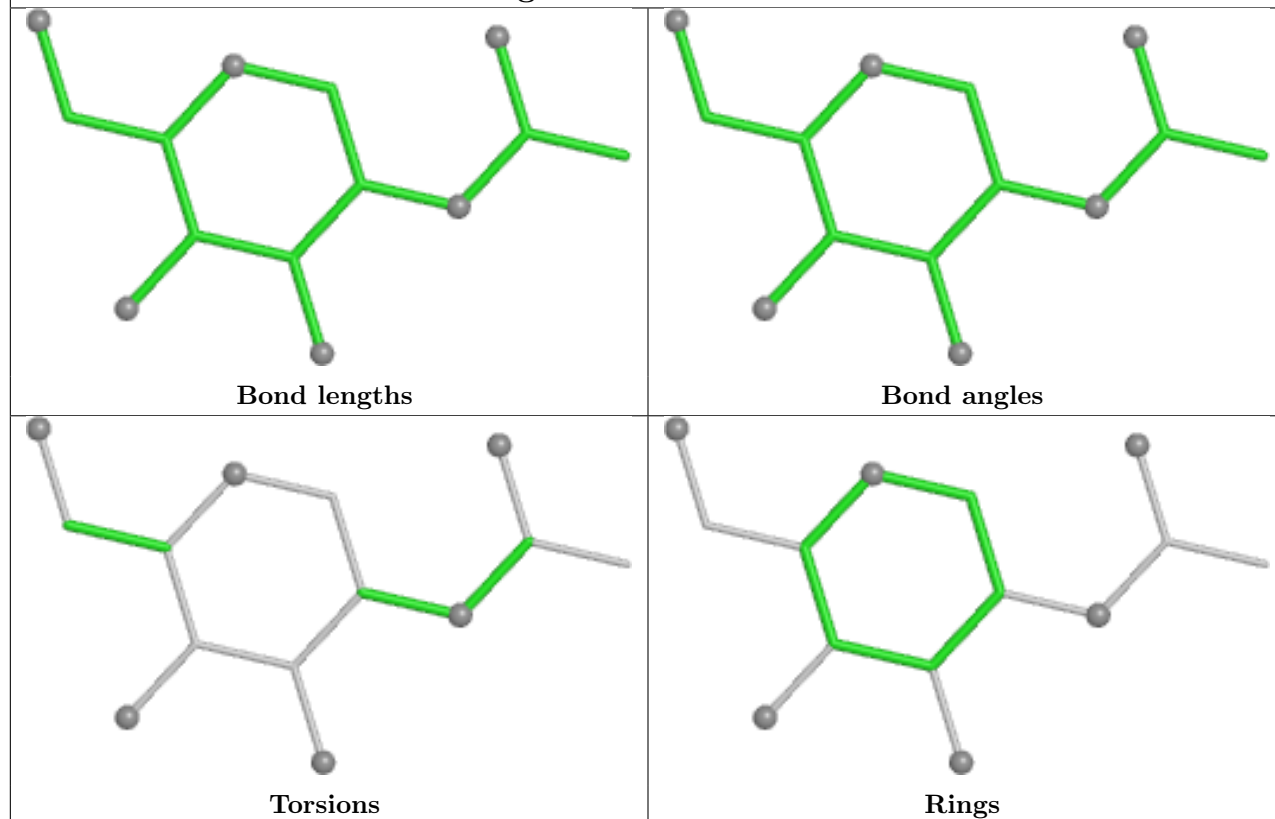
Ligand NAG A 1305



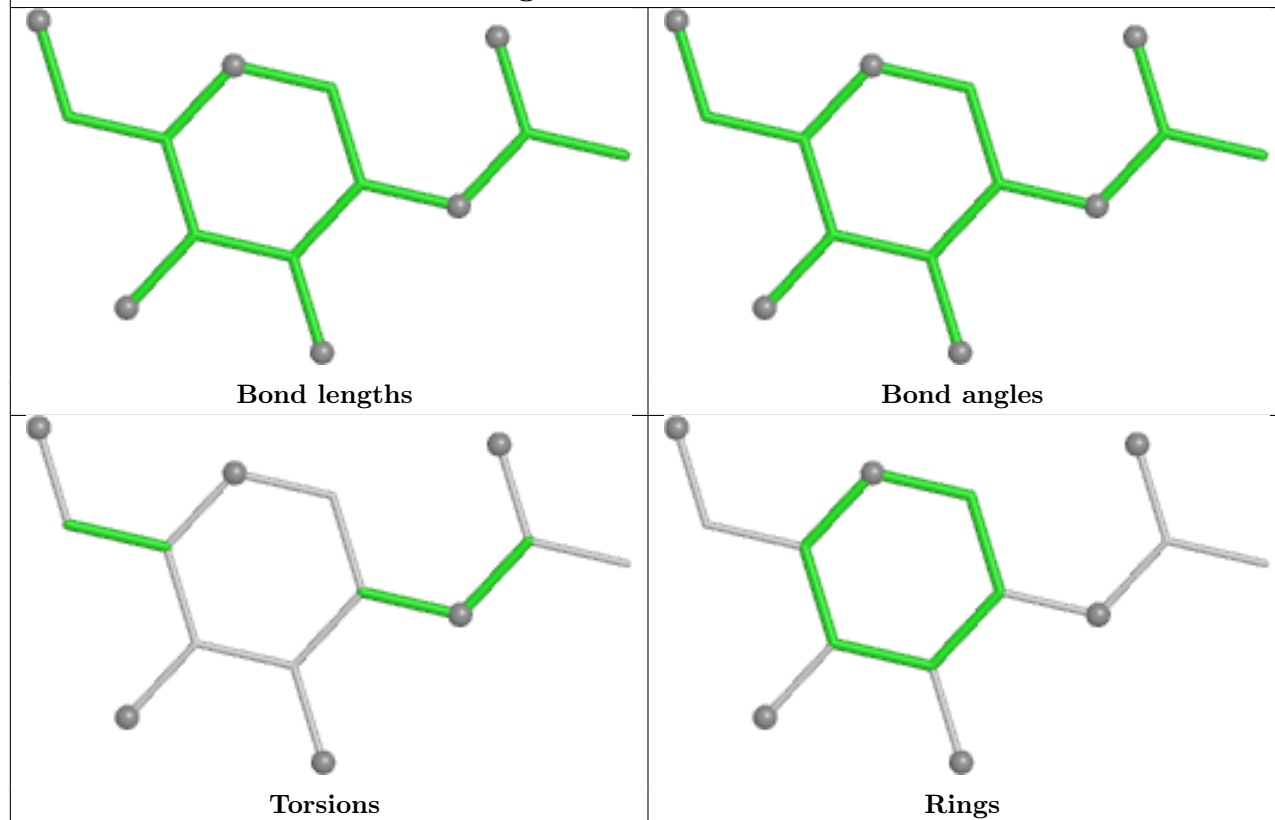
Ligand NAG B 1307



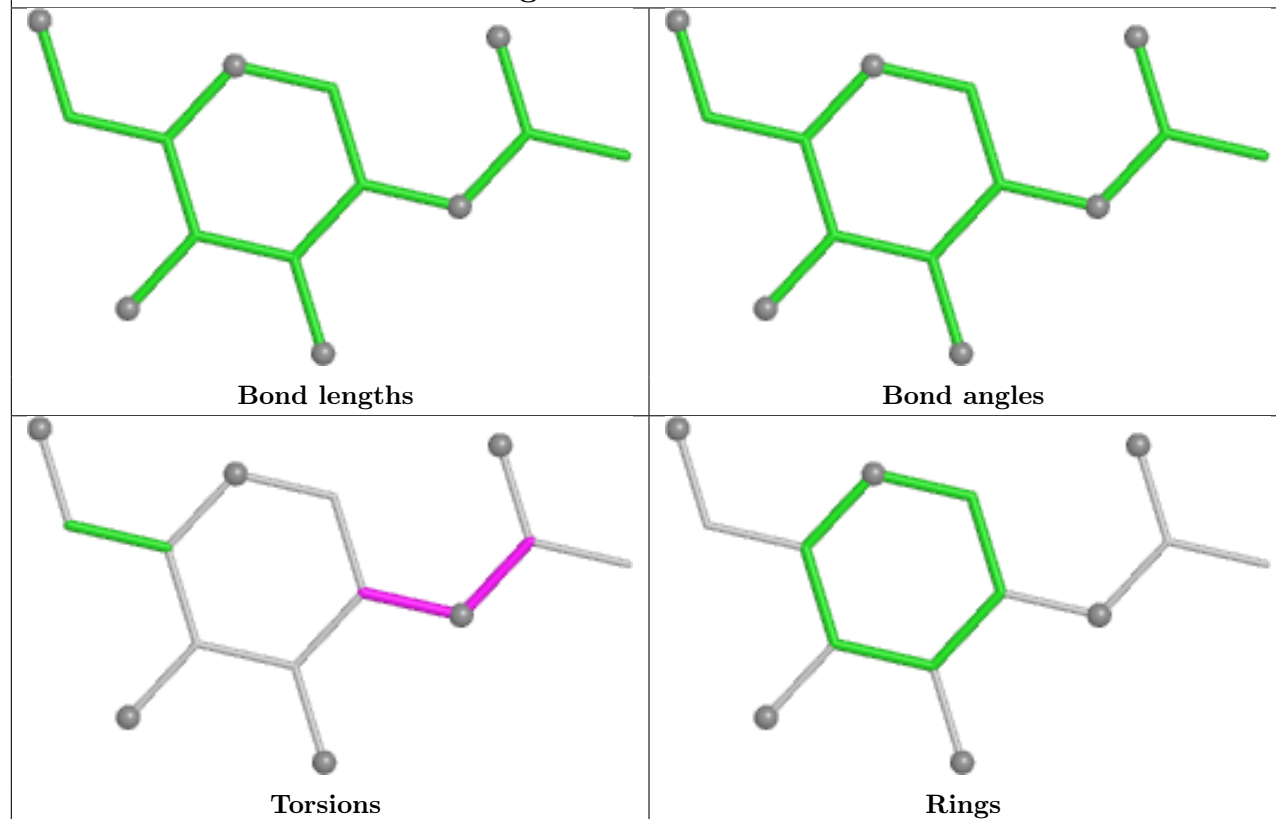
Ligand NAG A 1302



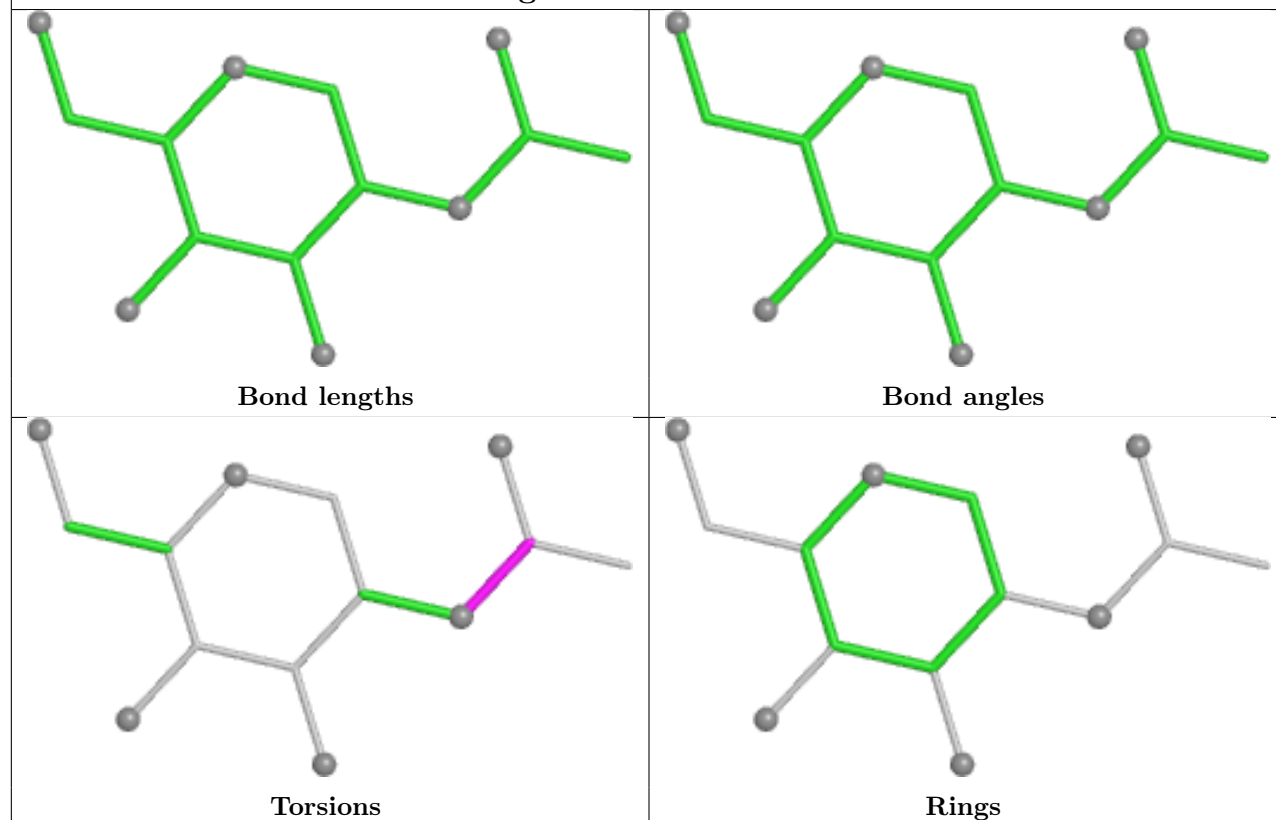
Ligand NAG A 1307



Ligand NAG B 1301



Ligand NAG A 1304



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68575. These allow visual inspection of the internal detail of the map and identification of artifacts.

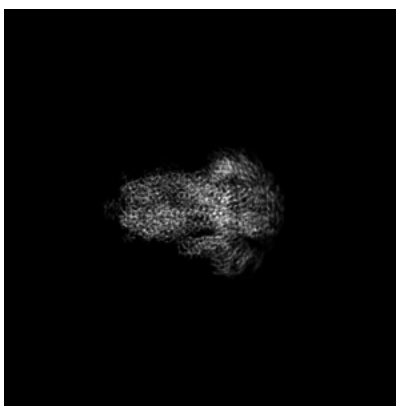
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

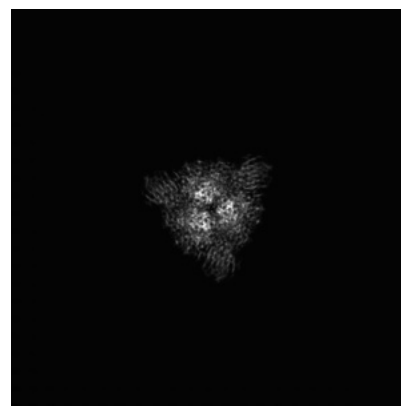
6.1.1 Primary map



X

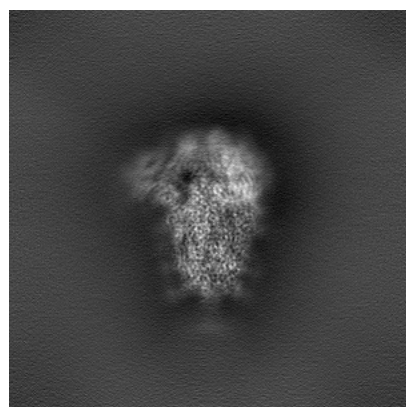


Y

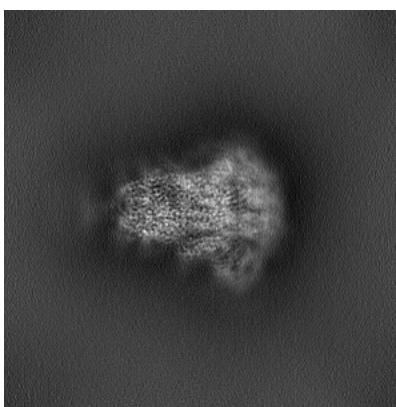


Z

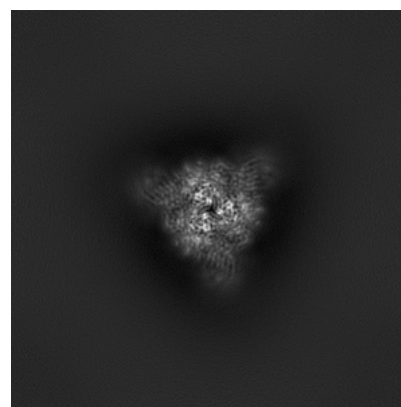
6.1.2 Raw map



X



Y

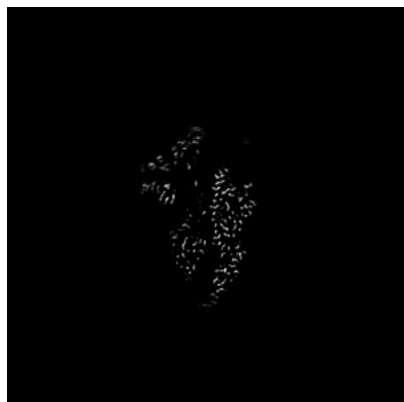


Z

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

6.2 Central slices [i](#)

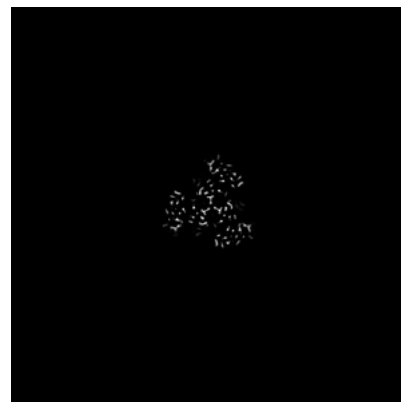
6.2.1 Primary map



X Index: 240

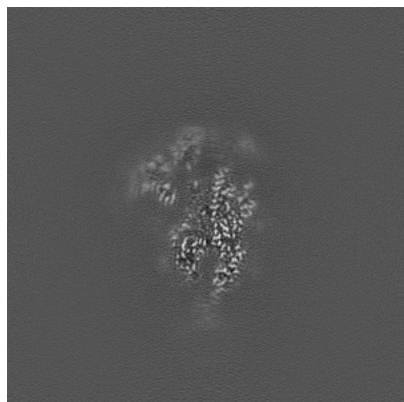


Y Index: 240

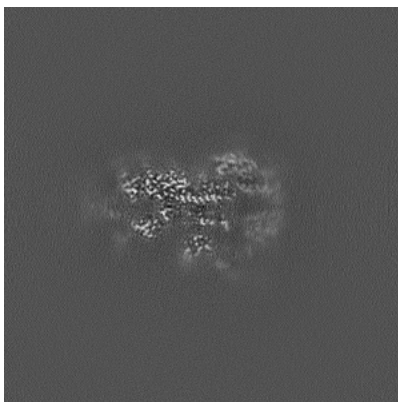


Z Index: 240

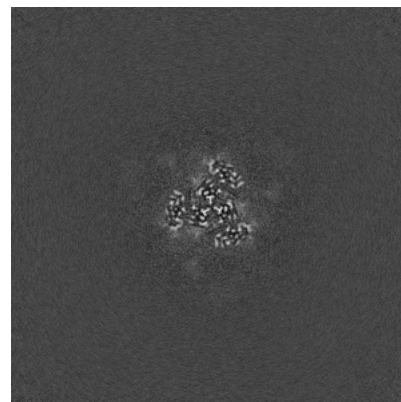
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 233

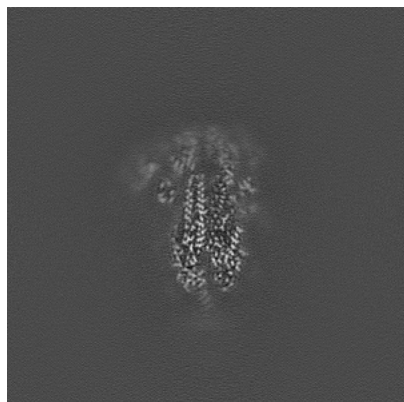


Y Index: 224

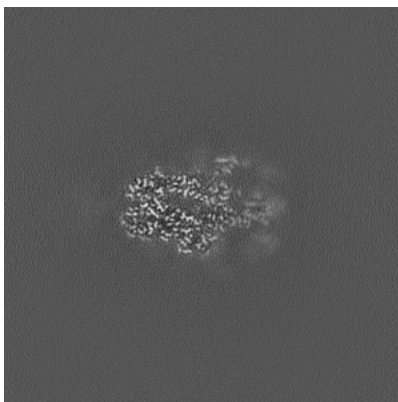


Z Index: 266

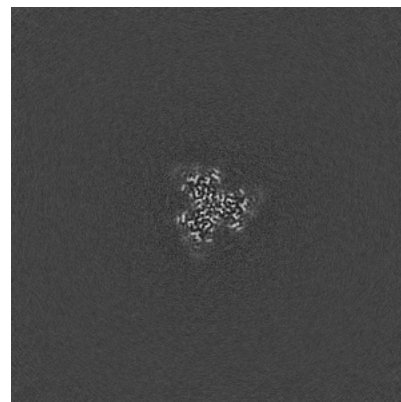
6.3.2 Raw map



X Index: 232



Y Index: 224

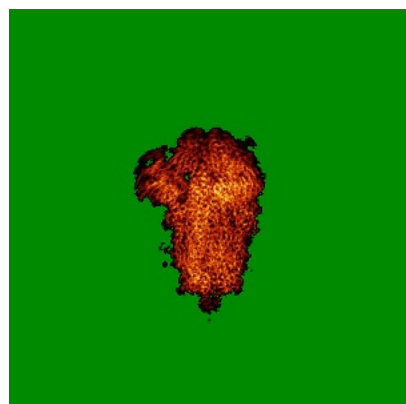


Z Index: 195

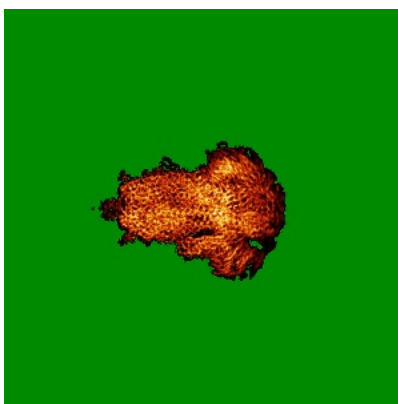
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

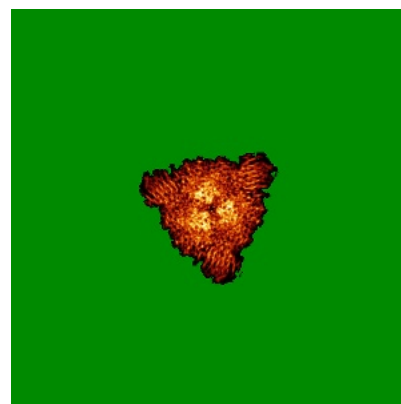
6.4.1 Primary map



X



Y

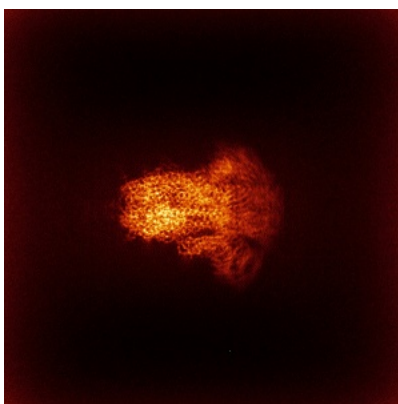


Z

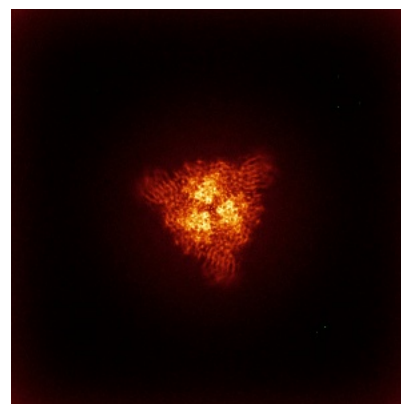
6.4.2 Raw map



X



Y

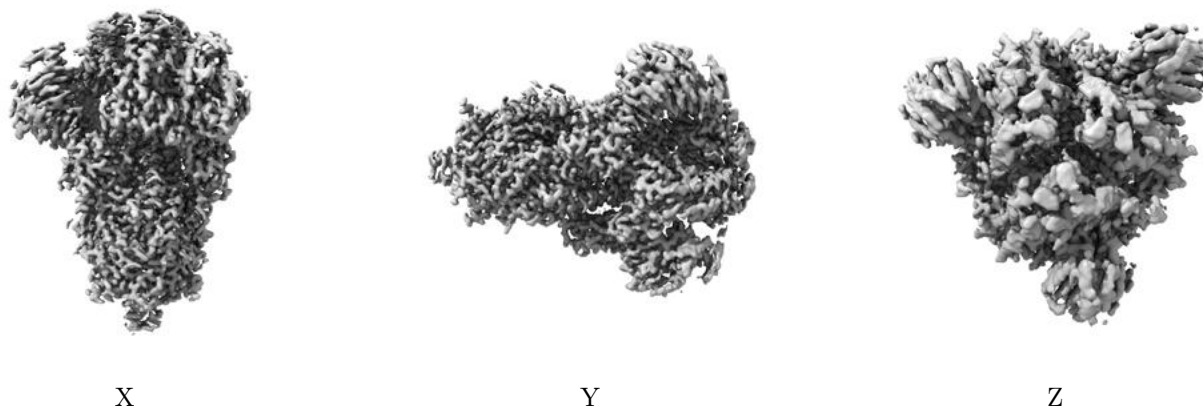


Z

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.

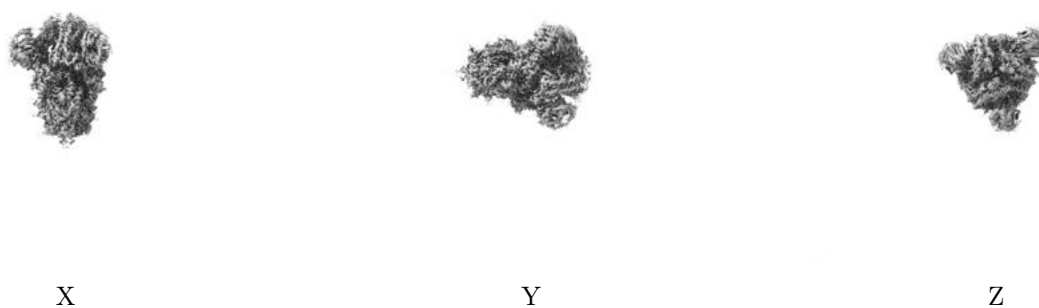
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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



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.

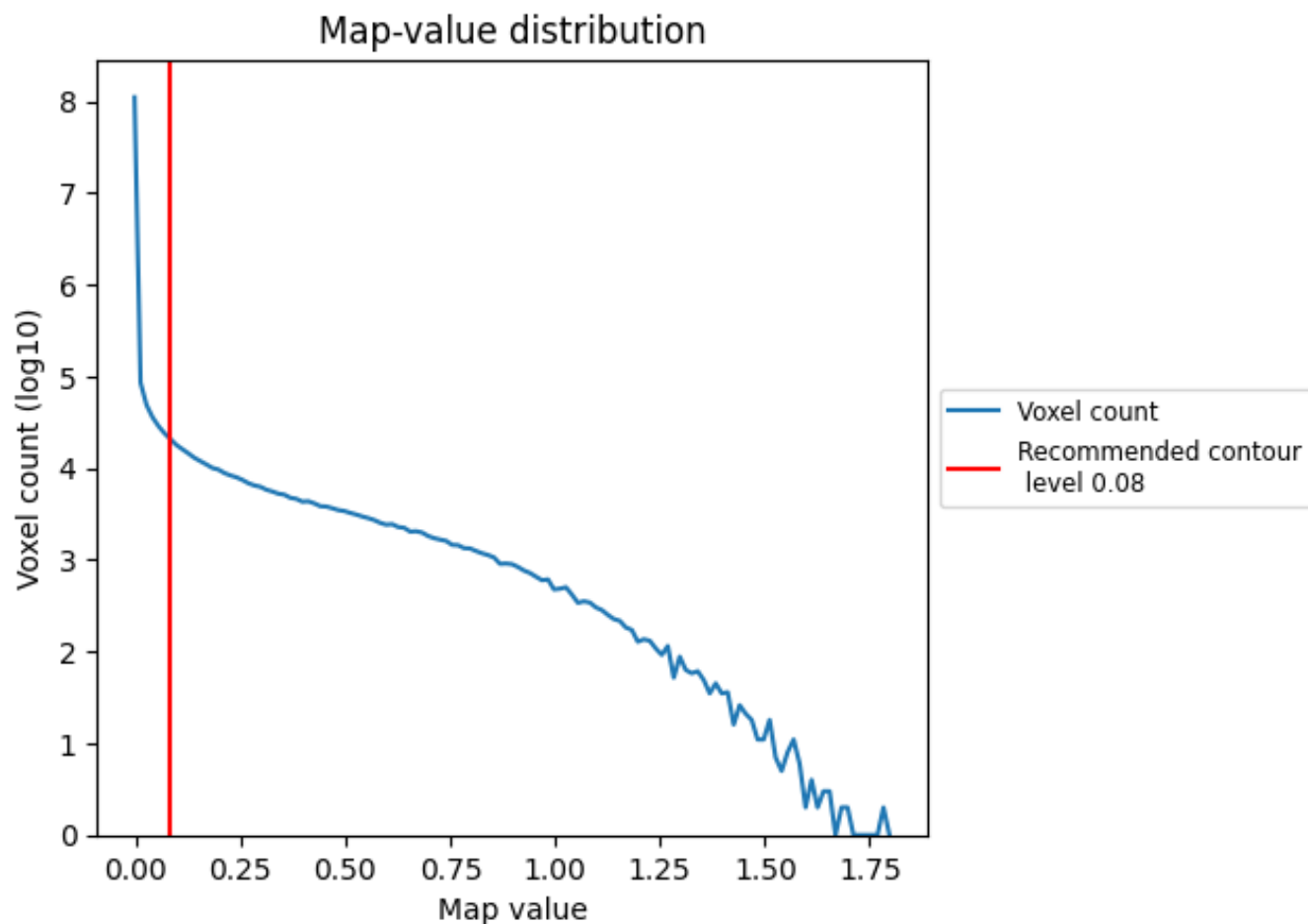
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

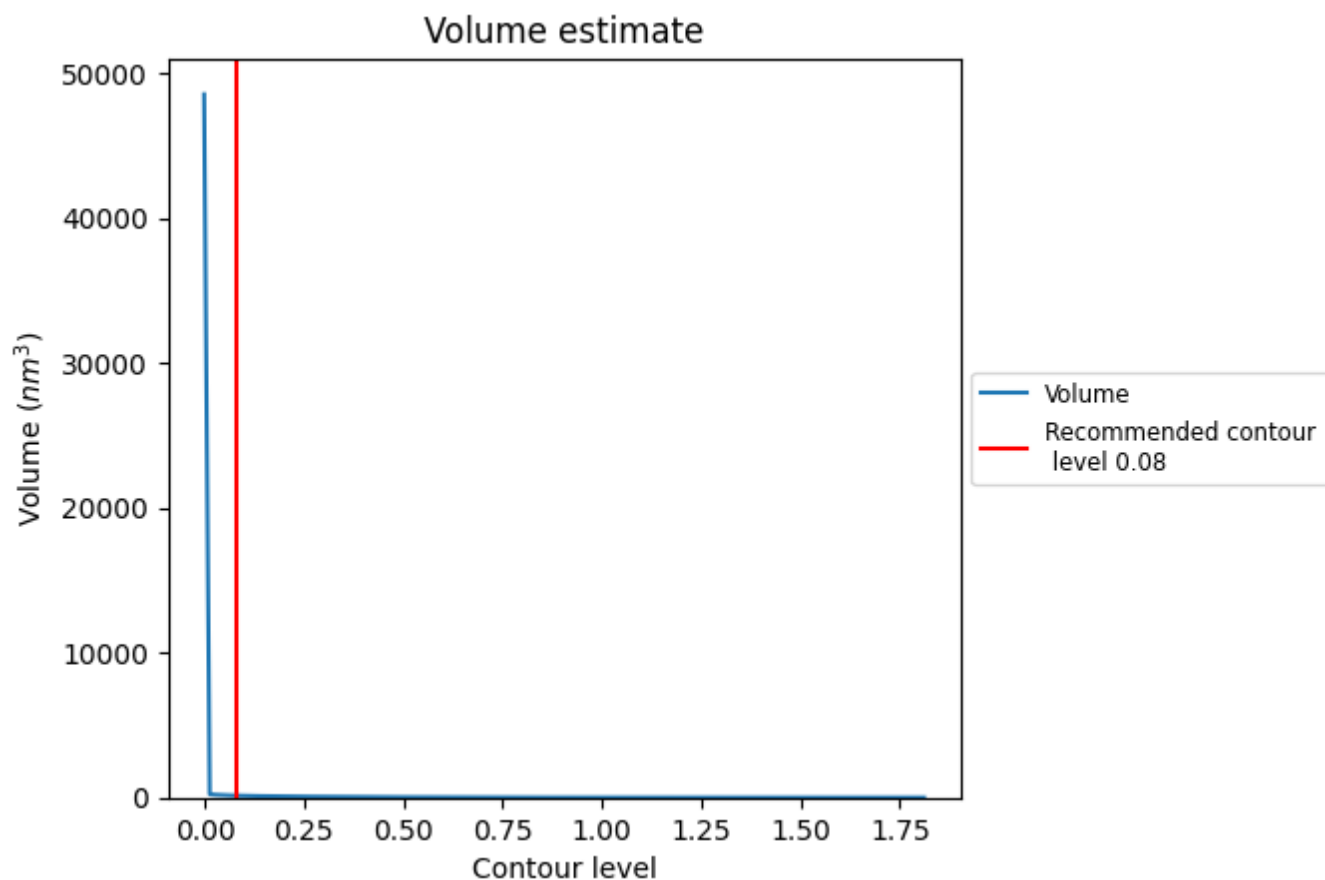
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

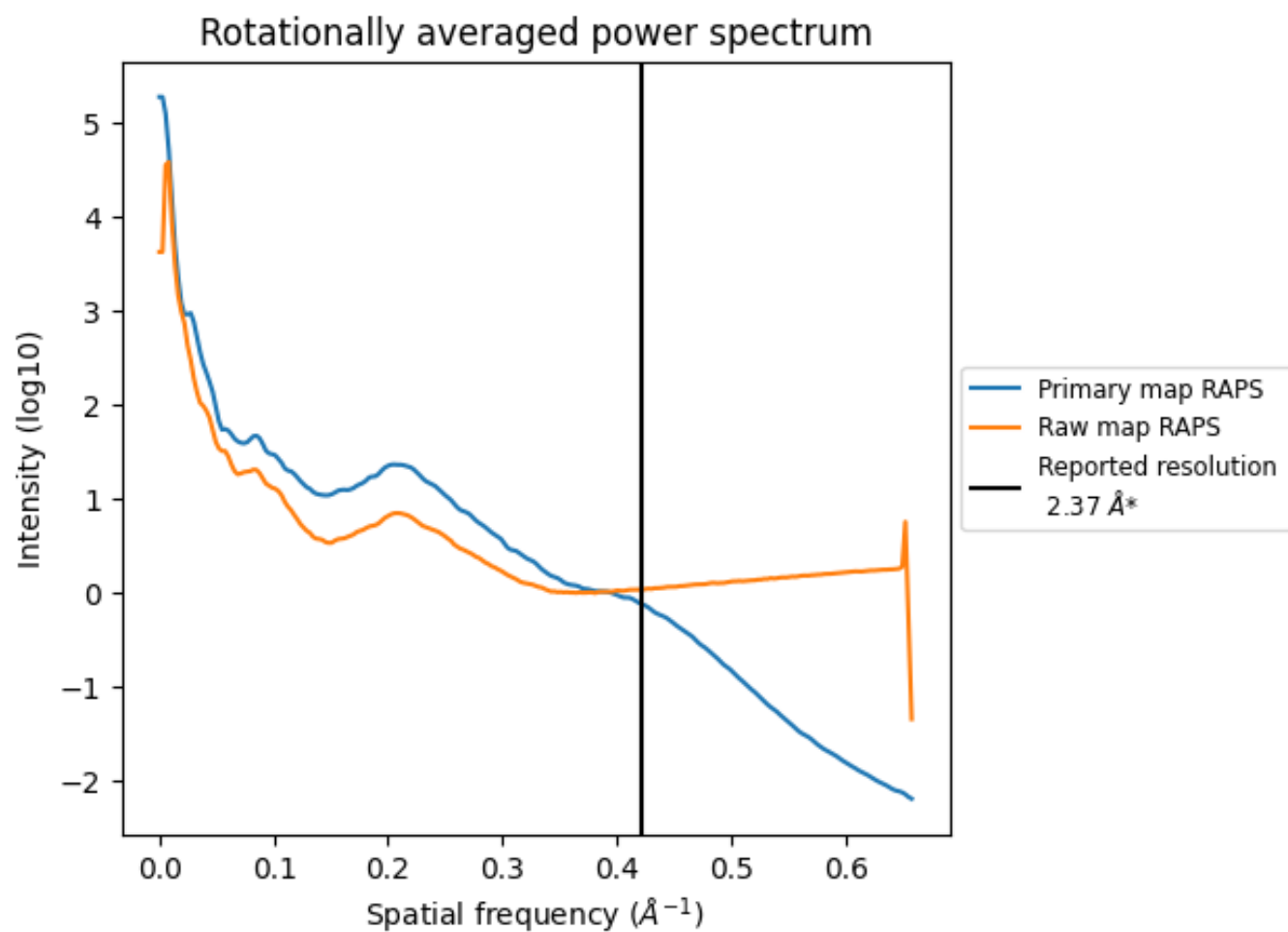
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm^3 ; this corresponds to an approximate mass of 122 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 ⓘ

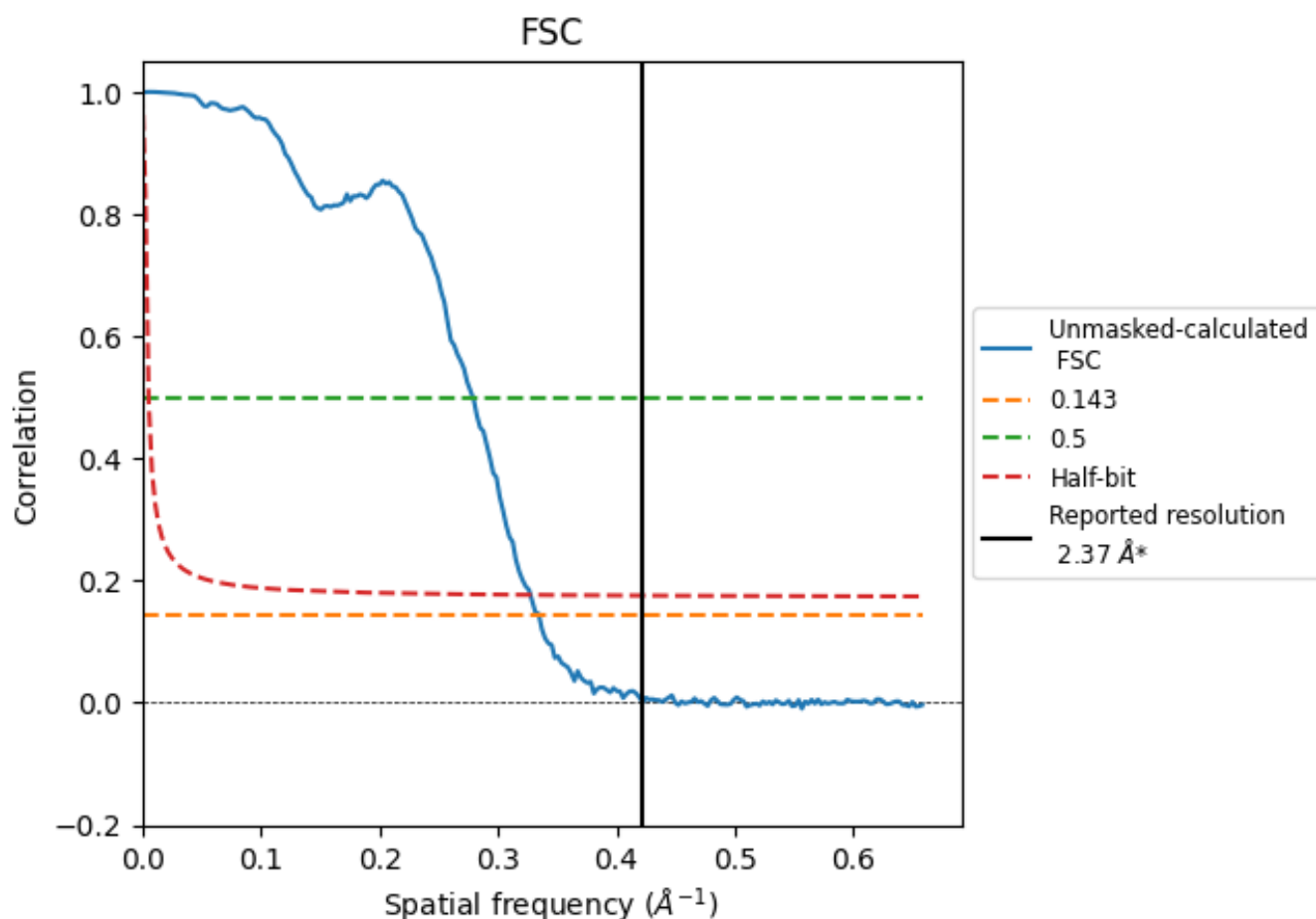


*Reported resolution corresponds to spatial frequency of 0.422 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.422 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

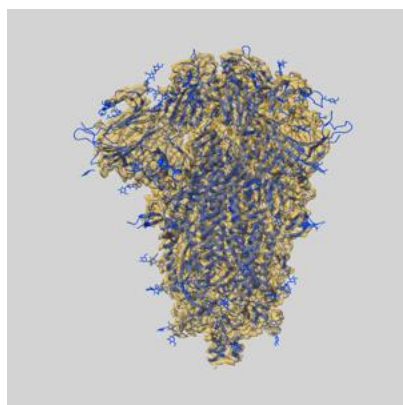
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.59	3.05

*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 2.99 differs from the reported value 2.37 by more than 10 %

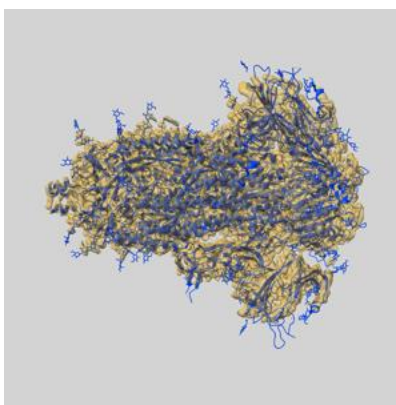
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68575 and PDB model 22OV. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

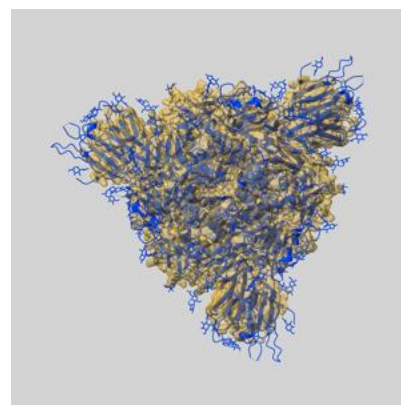
9.1 Map-model overlay [i](#)



X



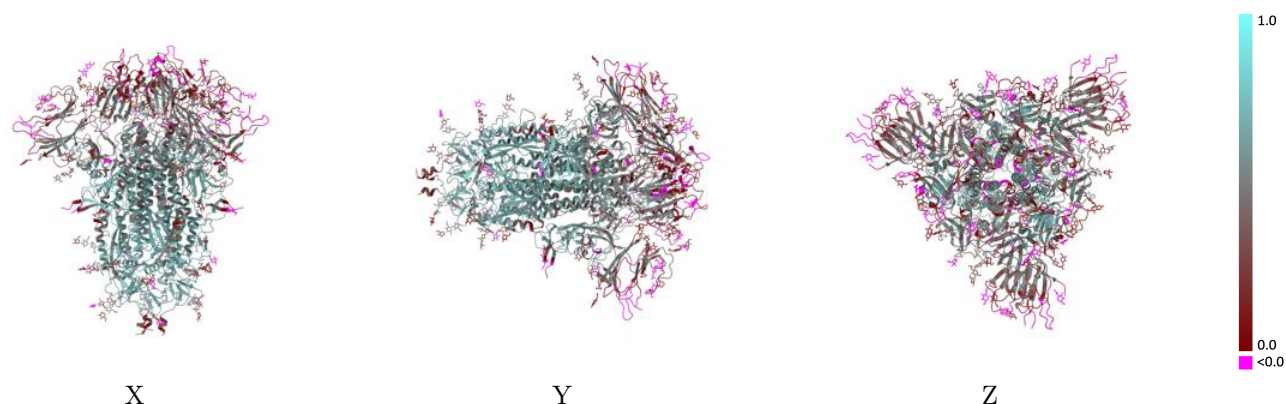
Y



Z

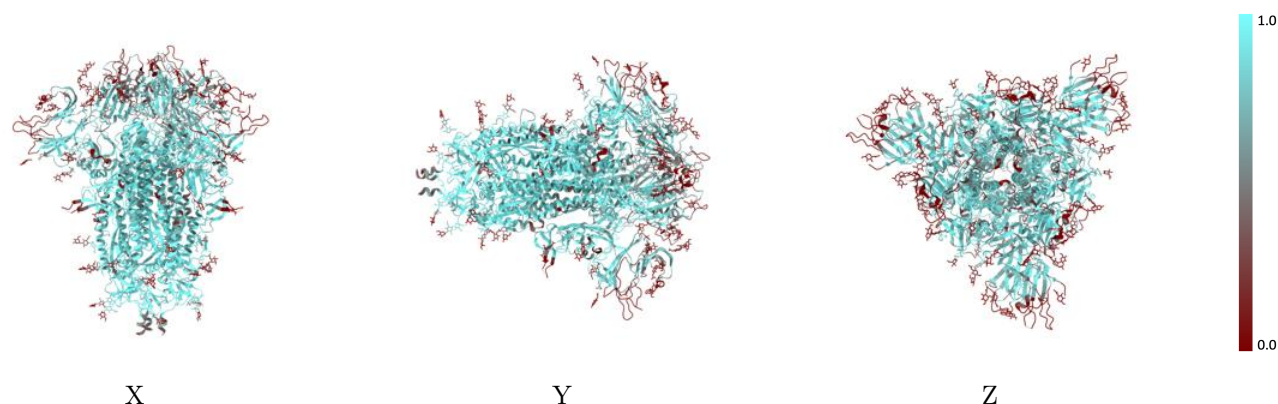
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



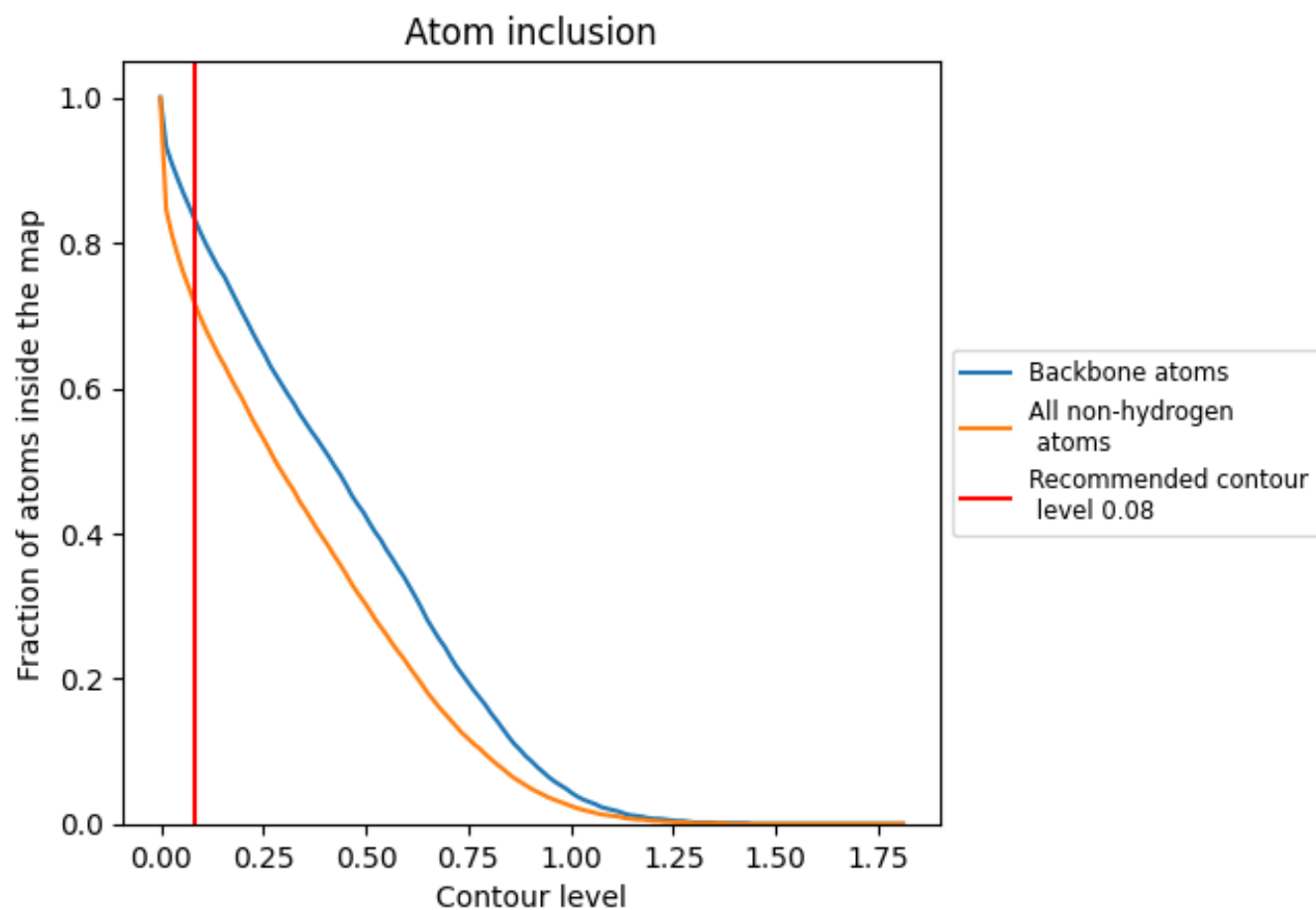
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 72% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.4350
A	 0.7470	 0.4510
B	 0.7500	 0.4500
C	 0.7520	 0.4510
D	 0.0000	 0.0180
E	 0.0000	 0.0260
F	 0.0260	 0.0020
G	 0.0490	 0.0710
H	 0.2310	 0.2370
I	 0.1280	 0.0300
J	 0.0000	 -0.0530
K	 0.1790	 0.1770
L	 0.4360	 0.3760
M	 0.4100	 0.3550
N	 0.0360	 0.0230
O	 0.5640	 0.3090
P	 0.4620	 0.2690
Q	 0.0000	 -0.0320
R	 0.0000	 -0.0100
S	 0.0260	 0.0740
T	 0.0330	 0.0530
U	 0.1790	 0.2450
V	 0.2050	 0.1490
W	 0.0360	 0.0090
X	 0.1790	 0.1160
Y	 0.4360	 0.3730
Z	 0.4620	 0.3210
a	 0.0360	 0.0260
b	 0.5640	 0.3750
c	 0.4100	 0.2160
d	 0.0000	 0.1770
e	 0.0000	 0.0340
f	 0.0260	 0.0170
g	 0.0820	 0.0800
h	 0.2050	 0.2360



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.1540	 0.0720
j	 0.0710	 0.0620
k	 0.1030	 0.1260
l	 0.3850	 0.3500
m	 0.4100	 0.3550
n	 0.0710	 0.1490
o	 0.5640	 0.3530
p	 0.4620	 0.2270