



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:16 PM UTC

PDB ID : 8D55 / pdb_00008d55
EMDB ID : EMD-27205
Title : Closed state of SARS-CoV-2 BA.2 variant spike protein
Authors : Zhang, J.; Tang, W.C.; Gao, H.L.; Shi, W.; Peng, H.Q.; Volloch, S.R.; Xiao, T.S.; Chen, B.
Deposited on : 2022-06-04
Resolution : 2.80 Å(reported)
Based on initial model : 7KRR

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

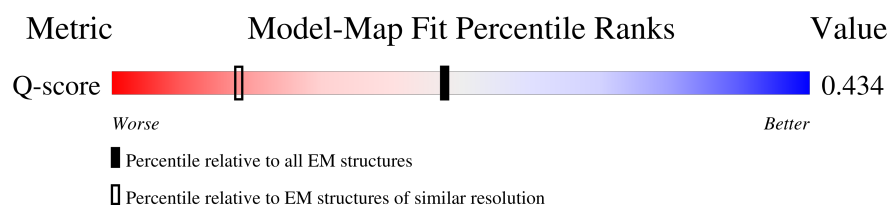
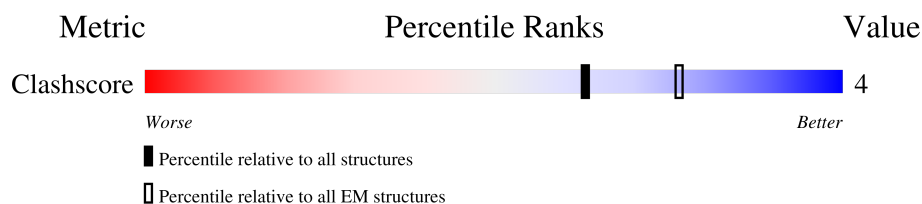
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

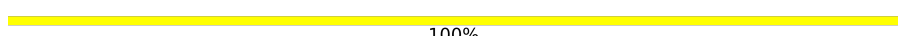
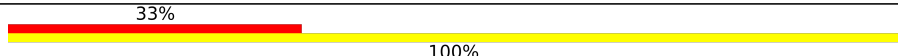
The reported resolution of this entry is 2.80 Å.

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.



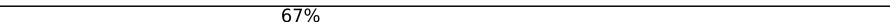
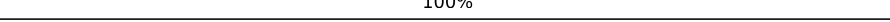
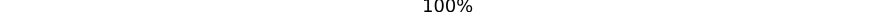
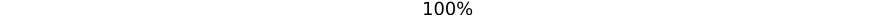
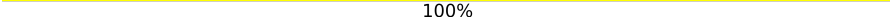
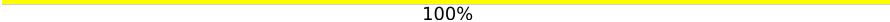
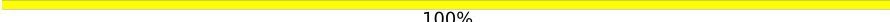
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	1305	 80% 6% • 14%
1	B	1305	 81% 5% 14%
1	C	1305	 81% • 14%
2	D	3	 100%
2	F	3	 33% 100%
2	G	3	 100%

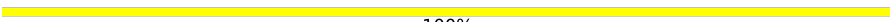
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Mol	Chain	Length	Quality of chain
2	I	3	 100%
2	J	3	 100%
2	L	3	 100%
2	M	3	 100%
2	N	3	 100%
2	P	3	 33% 100%
2	Q	3	 100%
2	S	3	 100%
2	T	3	 100%
2	V	3	 100%
2	W	3	 100%
2	X	3	 100%
2	Z	3	 67% 67% 33%
2	a	3	 100%
2	c	3	 100%
2	d	3	 100%
2	f	3	 100%
2	g	3	 100%
3	E	2	 100%
3	H	2	 100%
3	O	2	 100%
3	R	2	 100%
3	Y	2	 100%
3	b	2	 100%
4	K	3	 100%

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Mol	Chain	Length	Quality of chain
4	U	3	 100%
4	e	3	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	H	1	X	-	-	-
3	NAG	b	1	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27882 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	1126	Total	C	N	O	S	0	0
			8828	5644	1475	1669	40		
1	B	1127	Total	C	N	O	S	0	0
			8835	5648	1476	1671	40		
1	C	1125	Total	C	N	O	S	0	0
			8824	5642	1474	1668	40		

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	GLY	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	SER	-	expression tag	UNP P0DTC2
A	1279	ALA	-	expression tag	UNP P0DTC2
A	1280	TRP	-	expression tag	UNP P0DTC2
A	1281	SER	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	PRO	-	expression tag	UNP P0DTC2
A	1284	GLN	-	expression tag	UNP P0DTC2
A	1285	PHE	-	expression tag	UNP P0DTC2
A	1286	GLU	-	expression tag	UNP P0DTC2
A	1287	LYS	-	expression tag	UNP P0DTC2
A	1288	GLY	-	expression tag	UNP P0DTC2
A	1289	GLY	-	expression tag	UNP P0DTC2
A	1290	GLY	-	expression tag	UNP P0DTC2
A	1291	SER	-	expression tag	UNP P0DTC2
A	1292	GLY	-	expression tag	UNP P0DTC2
A	1293	GLY	-	expression tag	UNP P0DTC2
A	1294	GLY	-	expression tag	UNP P0DTC2
A	1295	SER	-	expression tag	UNP P0DTC2
A	1296	GLY	-	expression tag	UNP P0DTC2
A	1297	GLY	-	expression tag	UNP P0DTC2
A	1298	SER	-	expression tag	UNP P0DTC2
A	1299	SER	-	expression tag	UNP P0DTC2
A	1300	ALA	-	expression tag	UNP P0DTC2
A	1301	TRP	-	expression tag	UNP P0DTC2
A	1302	SER	-	expression tag	UNP P0DTC2
A	1303	HIS	-	expression tag	UNP P0DTC2
A	1304	PRO	-	expression tag	UNP P0DTC2
A	1305	GLN	-	expression tag	UNP P0DTC2
A	1306	PHE	-	expression tag	UNP P0DTC2
A	1307	GLU	-	expression tag	UNP P0DTC2
A	1308	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	1274	SER	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	GLY	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	SER	-	expression tag	UNP P0DTC2
B	1279	ALA	-	expression tag	UNP P0DTC2
B	1280	TRP	-	expression tag	UNP P0DTC2
B	1281	SER	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	PRO	-	expression tag	UNP P0DTC2
B	1284	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1285	PHE	-	expression tag	UNP P0DTC2
B	1286	GLU	-	expression tag	UNP P0DTC2
B	1287	LYS	-	expression tag	UNP P0DTC2
B	1288	GLY	-	expression tag	UNP P0DTC2
B	1289	GLY	-	expression tag	UNP P0DTC2
B	1290	GLY	-	expression tag	UNP P0DTC2
B	1291	SER	-	expression tag	UNP P0DTC2
B	1292	GLY	-	expression tag	UNP P0DTC2
B	1293	GLY	-	expression tag	UNP P0DTC2
B	1294	GLY	-	expression tag	UNP P0DTC2
B	1295	SER	-	expression tag	UNP P0DTC2
B	1296	GLY	-	expression tag	UNP P0DTC2
B	1297	GLY	-	expression tag	UNP P0DTC2
B	1298	SER	-	expression tag	UNP P0DTC2
B	1299	SER	-	expression tag	UNP P0DTC2
B	1300	ALA	-	expression tag	UNP P0DTC2
B	1301	TRP	-	expression tag	UNP P0DTC2
B	1302	SER	-	expression tag	UNP P0DTC2
B	1303	HIS	-	expression tag	UNP P0DTC2
B	1304	PRO	-	expression tag	UNP P0DTC2
B	1305	GLN	-	expression tag	UNP P0DTC2
B	1306	PHE	-	expression tag	UNP P0DTC2
B	1307	GLU	-	expression tag	UNP P0DTC2
B	1308	LYS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2

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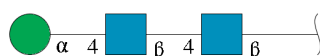
Chain	Residue	Modelled	Actual	Comment	Reference
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	1274	SER	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	GLY	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	SER	-	expression tag	UNP P0DTC2
C	1279	ALA	-	expression tag	UNP P0DTC2
C	1280	TRP	-	expression tag	UNP P0DTC2
C	1281	SER	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	PRO	-	expression tag	UNP P0DTC2
C	1284	GLN	-	expression tag	UNP P0DTC2
C	1285	PHE	-	expression tag	UNP P0DTC2
C	1286	GLU	-	expression tag	UNP P0DTC2
C	1287	LYS	-	expression tag	UNP P0DTC2
C	1288	GLY	-	expression tag	UNP P0DTC2
C	1289	GLY	-	expression tag	UNP P0DTC2
C	1290	GLY	-	expression tag	UNP P0DTC2
C	1291	SER	-	expression tag	UNP P0DTC2
C	1292	GLY	-	expression tag	UNP P0DTC2
C	1293	GLY	-	expression tag	UNP P0DTC2
C	1294	GLY	-	expression tag	UNP P0DTC2
C	1295	SER	-	expression tag	UNP P0DTC2
C	1296	GLY	-	expression tag	UNP P0DTC2
C	1297	GLY	-	expression tag	UNP P0DTC2
C	1298	SER	-	expression tag	UNP P0DTC2
C	1299	SER	-	expression tag	UNP P0DTC2
C	1300	ALA	-	expression tag	UNP P0DTC2
C	1301	TRP	-	expression tag	UNP P0DTC2
C	1302	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1303	HIS	-	expression tag	UNP P0DTC2
C	1304	PRO	-	expression tag	UNP P0DTC2
C	1305	GLN	-	expression tag	UNP P0DTC2
C	1306	PHE	-	expression tag	UNP P0DTC2
C	1307	GLU	-	expression tag	UNP P0DTC2
C	1308	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is an oligosaccharide called alpha-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
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	G	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		
2	L	3	Total	C	N	O	0	0
			39	22	2	15		
2	M	3	Total	C	N	O	0	0
			39	22	2	15		
2	N	3	Total	C	N	O	0	0
			39	22	2	15		
2	P	3	Total	C	N	O	0	0
			39	22	2	15		
2	Q	3	Total	C	N	O	0	0
			39	22	2	15		
2	S	3	Total	C	N	O	0	0
			39	22	2	15		
2	T	3	Total	C	N	O	0	0
			39	22	2	15		
2	V	3	Total	C	N	O	0	0
			39	22	2	15		

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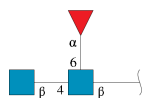
Mol	Chain	Residues	Atoms				AltConf	Trace
2	W	3	Total	C	N	O	0	0
			39	22	2	15		
2	X	3	Total	C	N	O	0	0
			39	22	2	15		
2	Z	3	Total	C	N	O	0	0
			39	22	2	15		
2	a	3	Total	C	N	O	0	0
			39	22	2	15		
2	c	3	Total	C	N	O	0	0
			39	22	2	15		
2	d	3	Total	C	N	O	0	0
			39	22	2	15		
2	f	3	Total	C	N	O	0	0
			39	22	2	15		
2	g	3	Total	C	N	O	0	0
			39	22	2	15		

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



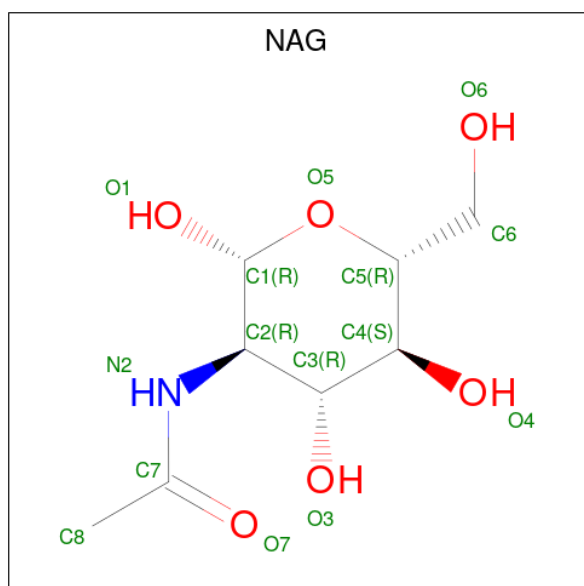
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	3	Total	C	N	O	0	0
			38	22	2	14		
4	U	3	Total	C	N	O	0	0
			38	22	2	14		
4	e	3	Total	C	N	O	0	0
			38	22	2	14		

- 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	

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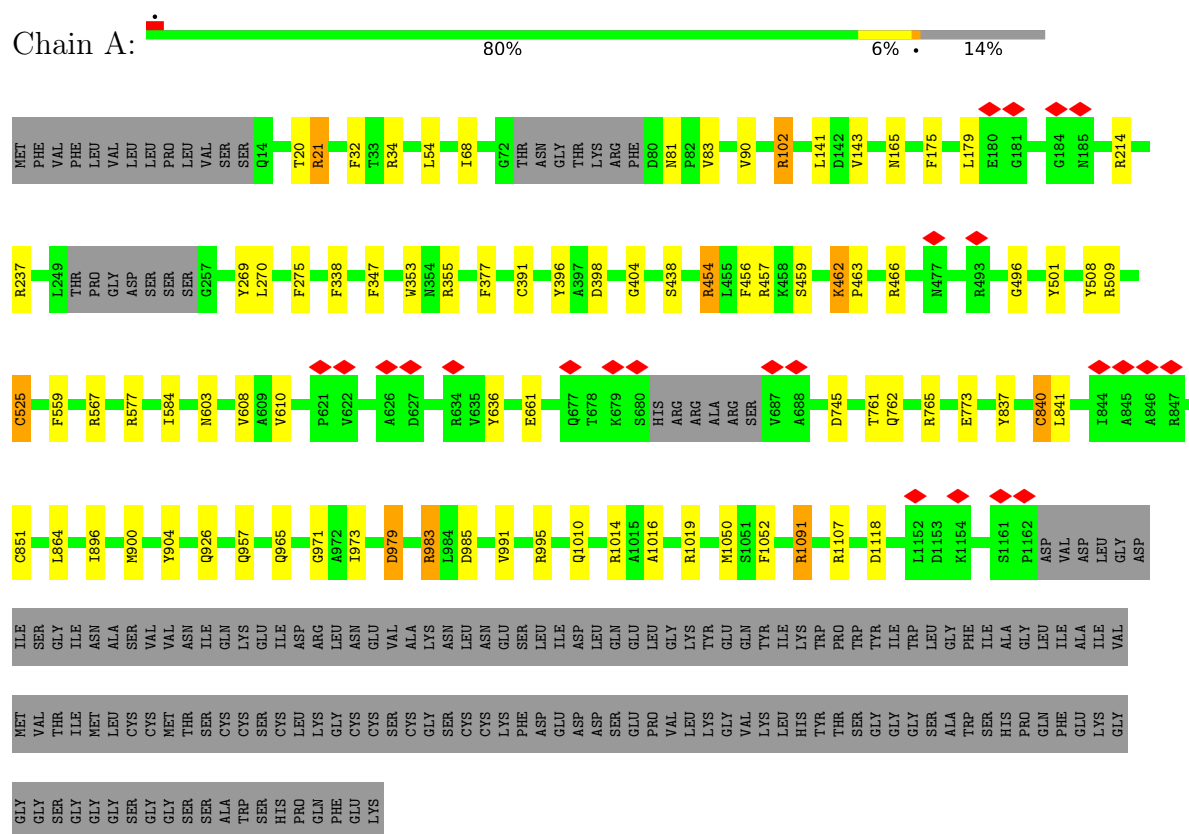
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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C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

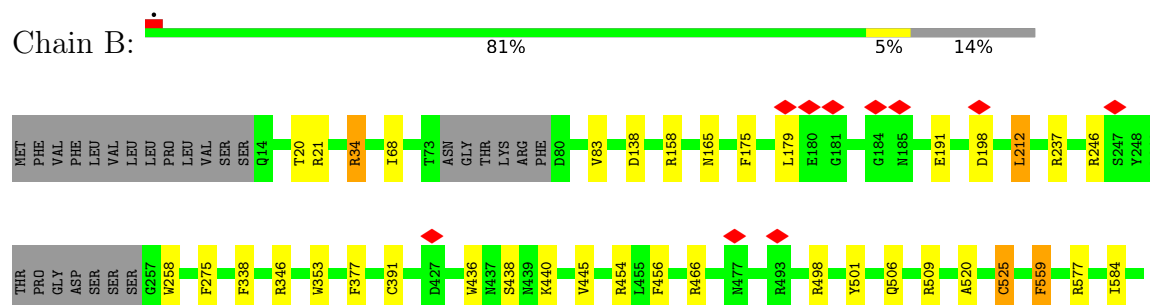
3 Residue-property plots

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

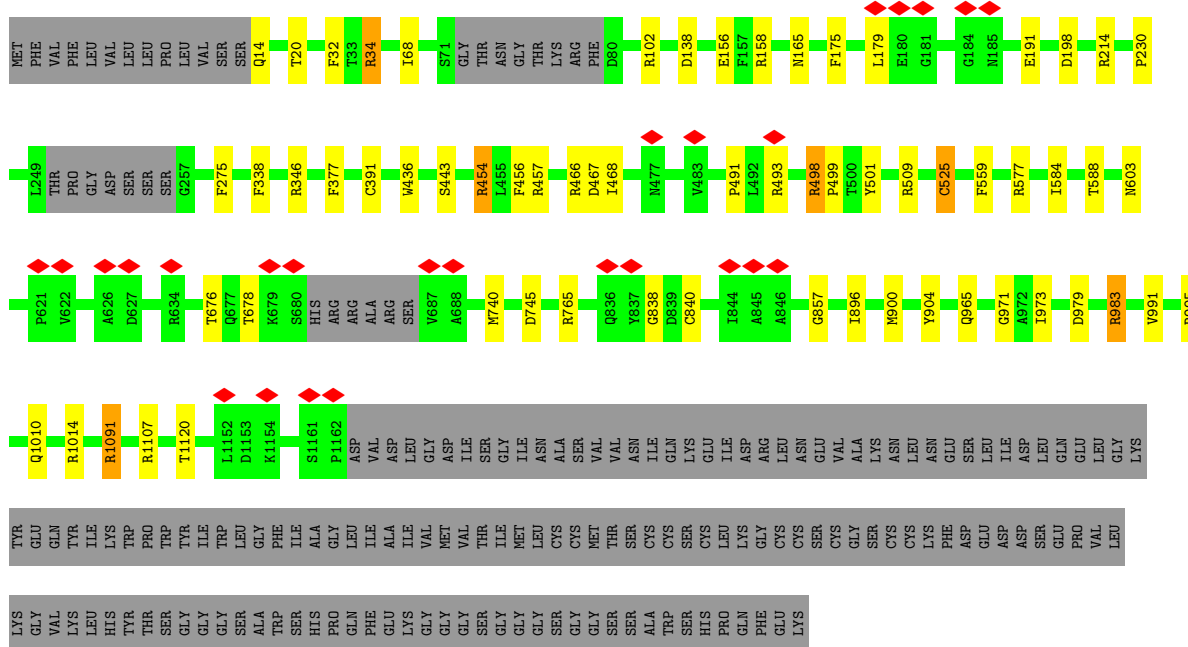
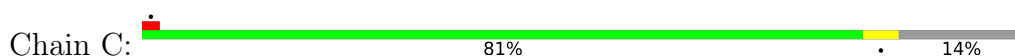
• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein



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

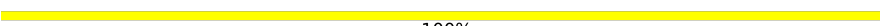


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain G:  100%

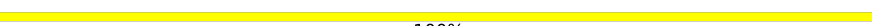


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

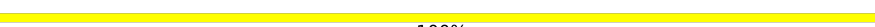


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

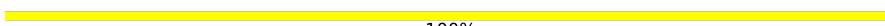


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

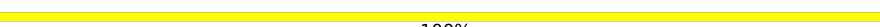


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

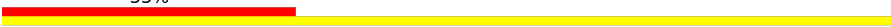


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

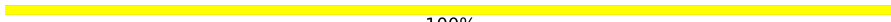


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  33% 100%

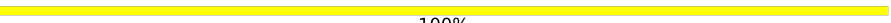


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

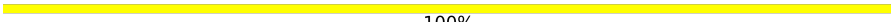


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%

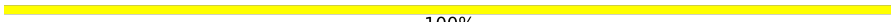


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

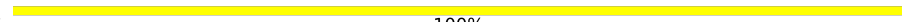


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

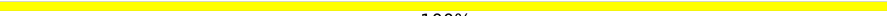


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



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

Chain X:  100%

MAG1
MAG2
MAN3

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

Chain Z:  67% 33%

MAG1
MAG2
MAN3

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

Chain a:  100%

MAG1
MAG2
MAN3

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

Chain c:  100%

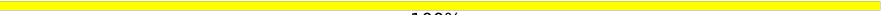
MAG1
MAG2
MAN3

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

Chain d:  100%

MAG1
MAG2
MAN3

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

Chain f:  100%

MAG1
MAG2
MAN3

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

Chain g:  100%

MAG1
MAG2
MAG3

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

Chain E:  100%MAG1
MAG2

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

Chain H:  100%MAG1
MAG2

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

Chain O:  100%MAG1
MAG2

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

Chain R:  100%MAG1
MAG2

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

Chain Y:  100%MAG1
MAG2

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

Chain b:  100%MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MAG1
MAG2
FUC3

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

MAG1
MAG2
FUC3

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

MAG1
MAG2
FUC3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.853	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.042	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: MAN, NAG, FUC

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	0.72	1/9037 (0.0%)	1.28	27/12292 (0.2%)
1	B	0.72	0/9044	1.28	27/12302 (0.2%)
1	C	0.73	0/9033	1.28	26/12287 (0.2%)
All	All	0.72	1/27114 (0.0%)	1.28	80/36881 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	ARG	CA-C	-5.04	1.49	1.52

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	840	CYS	N-CA-C	9.42	121.63	111.36
1	A	1091	ARG	N-CA-C	-8.23	101.89	111.03
1	A	525	CYS	N-CA-C	8.10	119.32	108.38
1	B	34	ARG	N-CA-C	8.08	121.89	110.50
1	C	983	ARG	N-CA-C	7.73	123.01	113.50
1	C	34	ARG	N-CA-C	7.69	120.93	110.55
1	A	34	ARG	N-CA-C	7.63	121.26	110.50
1	B	338	PHE	CA-CB-CG	7.49	121.29	113.80
1	B	165	ASN	CB-CG-ND2	7.31	127.37	116.40
1	B	165	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	B	838	GLY	N-CA-C	-7.19	104.10	112.73
1	A	983	ARG	N-CA-C	7.05	123.00	113.97
1	C	165	ASN	CB-CG-ND2	7.00	126.90	116.40
1	C	165	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	C	175	PHE	CA-CB-CG	6.82	120.61	113.80
1	C	493	ARG	N-CA-C	-6.78	98.98	109.76
1	B	983	ARG	N-CA-C	6.78	122.64	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	PRO	N-CA-CB	6.75	106.70	102.92
1	C	102	ARG	N-CA-C	6.67	122.04	113.18
1	B	175	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	165	ASN	CB-CG-ND2	6.63	126.34	116.40
1	A	165	ASN	OD1-CG-ND2	-6.61	116.00	122.60
1	C	498	ARG	CA-C-N	6.54	126.78	119.32
1	C	498	ARG	C-N-CA	6.54	126.78	119.32
1	C	840	CYS	N-CA-C	6.51	118.46	111.36
1	B	839	ASP	N-CA-C	6.39	118.32	111.36
1	A	175	PHE	CA-CB-CG	6.38	120.17	113.80
1	B	689	SER	N-CA-C	6.26	118.26	107.93
1	C	377	PHE	CA-CB-CG	6.12	119.92	113.80
1	C	525	CYS	N-CA-C	6.12	117.54	108.60
1	B	506	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	A	377	PHE	CA-CB-CG	6.01	119.81	113.80
1	B	138	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	745	ASP	CA-CB-CG	5.84	118.44	112.60
1	C	745	ASP	CA-CB-CG	5.83	118.42	112.60
1	A	567	ARG	N-CA-C	5.81	119.15	110.14
1	B	212	LEU	N-CA-C	5.80	123.16	110.80
1	C	158	ARG	CA-C-N	5.77	127.83	120.56
1	C	158	ARG	C-N-CA	5.77	127.83	120.56
1	A	454	ARG	N-CA-C	5.77	118.06	108.20
1	C	603	ASN	CB-CG-ND2	5.76	125.03	116.40
1	A	985	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	603	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	603	ASN	CB-CG-ND2	5.72	124.98	116.40
1	A	603	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	603	ASN	CB-CG-ND2	5.68	124.92	116.40
1	C	603	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	B	275	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	745	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	559	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	926	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	B	525	CYS	N-CA-C	5.57	116.73	108.60
1	A	338	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	102	ARG	CB-CA-C	-5.55	103.66	111.65
1	A	965	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	B	198	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	275	PHE	CA-CB-CG	5.38	119.18	113.80
1	C	965	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	A	462	LYS	CA-C-N	-5.27	114.30	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	LYS	C-N-CA	-5.27	114.30	119.99
1	B	158	ARG	CA-C-N	5.26	127.38	120.60
1	B	158	ARG	C-N-CA	5.26	127.38	120.60
1	B	520	ALA	N-CA-C	5.26	112.95	108.22
1	C	275	PHE	CA-CB-CG	5.25	119.05	113.80
1	B	520	ALA	N-CA-CB	-5.23	105.60	111.10
1	B	965	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	979	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	338	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	926	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	C	1091	ARG	N-CA-C	-5.16	105.56	111.14
1	B	377	PHE	CA-CB-CG	5.16	118.96	113.80
1	C	198	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	138	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	21	ARG	N-CA-C	5.11	116.74	108.41
1	A	398	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	102	ARG	N-CA-C	5.10	118.77	111.02
1	A	559	PHE	CA-CB-CG	5.10	118.90	113.80
1	C	838	GLY	N-CA-C	-5.09	106.62	112.73
1	B	21	ARG	N-CA-C	5.05	117.14	108.90
1	C	454	ARG	N-CA-C	5.05	117.14	108.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8828	0	8608	103	0
1	B	8835	0	8618	76	0
1	C	8824	0	8608	81	0
2	D	39	0	34	0	0
2	F	39	0	34	0	0
2	G	39	0	34	0	0
2	I	39	0	34	0	0
2	J	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	39	0	34	0	0
2	M	39	0	34	0	0
2	N	39	0	34	0	0
2	P	39	0	34	0	0
2	Q	39	0	34	0	0
2	S	39	0	34	0	0
2	T	39	0	34	0	0
2	V	39	0	34	0	0
2	W	39	0	34	0	0
2	X	39	0	34	0	0
2	Z	39	0	34	1	0
2	a	39	0	34	0	0
2	c	39	0	34	0	0
2	d	39	0	34	0	0
2	f	39	0	34	0	0
2	g	39	0	34	0	0
3	E	28	0	25	0	0
3	H	28	0	25	0	0
3	O	28	0	25	0	0
3	R	28	0	25	0	0
3	Y	28	0	25	0	0
3	b	28	0	25	0	0
4	K	38	0	34	0	0
4	U	38	0	34	0	0
4	e	38	0	34	0	0
5	A	98	0	91	0	0
5	B	98	0	91	2	0
5	C	98	0	91	0	0
All	All	27882	0	27073	228	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 4.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ARG:HB3	1:B:501:TYR:CE2	1.66	1.28
1:A:610:VAL:HG23	1:A:636:TYR:CE2	1.67	1.27
1:C:14:GLN:OE1	1:C:156:GLU:CG	1.83	1.25
1:A:957:GLN:NE2	1:C:765:ARG:NH2	1.84	1.25
1:B:610:VAL:HG23	1:B:636:TYR:CE2	1.71	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:904:TYR:CE2	1:C:1107:ARG:HD3	1.74	1.23
1:B:498:ARG:HB3	1:B:501:TYR:CD2	1.77	1.19
1:C:14:GLN:OE1	1:C:156:GLU:HG2	1.03	1.17
1:B:1016:ALA:HA	1:B:1019:ARG:NH1	1.60	1.15
1:A:608:VAL:HG23	1:A:636:TYR:OH	1.47	1.14
1:B:904:TYR:HE2	1:C:1107:ARG:CD	1.60	1.14
1:A:1107:ARG:HD3	1:C:904:TYR:CE2	1.83	1.13
1:A:102:ARG:NH1	1:A:141:LEU:HB3	1.61	1.13
1:B:1158:ASN:ND2	5:B:1407:NAG:C1	2.12	1.12
1:B:608:VAL:HG23	1:B:636:TYR:OH	1.49	1.11
1:B:1016:ALA:HA	1:B:1019:ARG:HH12	1.00	1.09
1:A:896:ILE:HD11	1:A:904:TYR:CE1	1.89	1.08
1:A:1016:ALA:HA	1:A:1019:ARG:NH1	1.69	1.08
1:C:34:ARG:NH2	1:C:191:GLU:OE1	1.85	1.07
1:B:904:TYR:HE2	1:C:1107:ARG:HD3	0.96	1.07
1:A:1107:ARG:HD3	1:C:904:TYR:HE2	1.06	1.06
1:B:1158:ASN:HD21	5:B:1407:NAG:C1	1.68	1.05
1:B:445:VAL:O	1:B:498:ARG:NH1	1.90	1.05
1:B:498:ARG:CB	1:B:501:TYR:CE2	2.40	1.03
1:A:1016:ALA:HA	1:A:1019:ARG:HH12	1.20	1.03
1:A:896:ILE:HD11	1:A:904:TYR:HE1	1.17	1.02
1:B:498:ARG:CB	1:B:501:TYR:HE2	1.74	1.00
1:A:1107:ARG:CD	1:C:904:TYR:HE2	1.74	0.99
1:A:102:ARG:HH11	1:A:141:LEU:HB3	1.21	0.97
1:A:32:PHE:CE2	1:A:214:ARG:NH2	2.31	0.97
1:A:462:LYS:HB3	1:A:463:PRO:HD2	1.46	0.97
1:A:610:VAL:CG2	1:A:636:TYR:CE2	2.48	0.96
1:A:102:ARG:HH11	1:A:141:LEU:CB	1.78	0.95
1:C:32:PHE:HE2	1:C:214:ARG:HH22	1.11	0.94
1:C:559:PHE:HB2	1:C:577:ARG:NH2	1.84	0.93
1:A:32:PHE:HE2	1:A:214:ARG:HH22	1.15	0.93
1:C:32:PHE:CE2	1:C:214:ARG:NH2	2.38	0.92
1:C:1010:GLN:HB3	1:C:1014:ARG:HH12	1.33	0.91
1:C:896:ILE:HD11	1:C:904:TYR:HE1	1.33	0.91
1:A:957:GLN:NE2	1:C:765:ARG:CZ	2.34	0.90
1:C:34:ARG:HH21	1:C:191:GLU:CD	1.79	0.90
1:A:608:VAL:CG2	1:A:636:TYR:OH	2.20	0.89
1:C:896:ILE:HD11	1:C:904:TYR:CE1	2.07	0.89
1:C:1010:GLN:HB3	1:C:1014:ARG:NH1	1.87	0.89
1:B:610:VAL:CG2	1:B:636:TYR:CE2	2.55	0.89
1:A:353:TRP:CZ3	1:A:466:ARG:NH2	2.42	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:GLN:CD	1:C:765:ARG:NH2	2.32	0.88
1:A:957:GLN:HE21	1:C:765:ARG:NH2	1.68	0.87
1:C:14:GLN:CD	1:C:156:GLU:HG2	2.00	0.86
1:A:896:ILE:CD1	1:A:904:TYR:CE1	2.57	0.86
1:B:1016:ALA:CA	1:B:1019:ARG:HH12	1.86	0.86
1:A:971:GLY:O	1:A:995:ARG:NH1	2.08	0.86
1:C:971:GLY:O	1:C:995:ARG:NH1	2.10	0.84
1:A:610:VAL:HG23	1:A:636:TYR:HE2	1.30	0.84
1:A:904:TYR:CE2	1:B:1107:ARG:HD3	2.11	0.84
1:A:900:MET:O	1:A:904:TYR:CD1	2.32	0.82
1:B:1010:GLN:HB3	1:B:1014:ARG:HH12	1.42	0.82
1:C:577:ARG:CZ	1:C:584:ILE:HD11	2.10	0.82
1:B:498:ARG:HB2	1:B:501:TYR:HE2	1.44	0.81
1:A:462:LYS:HB3	1:A:463:PRO:CD	2.10	0.81
1:B:608:VAL:CG2	1:B:636:TYR:OH	2.28	0.81
1:C:454:ARG:NH1	1:C:491:PRO:HD3	1.96	0.80
1:A:102:ARG:NH1	1:A:141:LEU:CB	2.39	0.80
1:C:559:PHE:HB2	1:C:577:ARG:HH21	1.44	0.79
1:B:1010:GLN:HB3	1:B:1014:ARG:NH1	1.97	0.79
1:A:904:TYR:HE2	1:B:1107:ARG:HD3	1.45	0.79
1:A:32:PHE:CZ	1:A:214:ARG:NH2	2.51	0.78
1:A:457:ARG:NH2	2:Z:1:NAG:O7	2.16	0.78
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.64	0.78
1:B:900:MET:O	1:B:904:TYR:HD1	1.67	0.78
1:A:840:CYS:HG	1:A:851:CYS:HG	1.13	0.77
1:B:34:ARG:NH2	1:B:191:GLU:OE1	2.17	0.77
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.65	0.77
1:B:973:ILE:HD12	1:B:983:ARG:NH2	2.00	0.77
1:B:904:TYR:CE2	1:C:1107:ARG:CD	2.48	0.76
1:A:1010:GLN:HB3	1:A:1014:ARG:HH12	1.48	0.76
1:A:1010:GLN:HB3	1:A:1014:ARG:NH1	2.00	0.75
1:A:1016:ALA:CA	1:A:1019:ARG:HH12	1.99	0.75
1:C:559:PHE:CB	1:C:577:ARG:HH21	2.00	0.75
1:A:762:GLN:HA	1:A:765:ARG:HH12	1.52	0.74
1:B:896:ILE:HD11	1:B:904:TYR:CE1	2.21	0.74
1:A:610:VAL:CG2	1:A:636:TYR:CD2	2.71	0.74
1:A:83:VAL:HG11	1:A:237:ARG:CZ	2.18	0.73
1:A:904:TYR:HE2	1:B:1107:ARG:CD	2.01	0.73
1:A:83:VAL:HB	1:A:237:ARG:NH1	2.03	0.73
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.70	0.73
1:B:971:GLY:O	1:B:995:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:GLN:HA	1:A:765:ARG:NH1	2.04	0.72
1:B:973:ILE:HD12	1:B:983:ARG:HH21	1.52	0.72
1:C:32:PHE:CZ	1:C:214:ARG:NH2	2.56	0.72
1:B:577:ARG:CZ	1:B:584:ILE:HD11	2.21	0.71
1:B:896:ILE:HD11	1:B:904:TYR:HE1	1.53	0.71
1:C:454:ARG:NH2	1:C:491:PRO:HG3	2.05	0.71
1:C:896:ILE:CD1	1:C:904:TYR:CE1	2.72	0.71
1:B:34:ARG:HH21	1:B:191:GLU:CD	1.99	0.70
1:B:900:MET:O	1:B:904:TYR:CD1	2.45	0.70
1:A:979:ASP:O	1:A:983:ARG:HG3	1.94	0.68
1:C:900:MET:O	1:C:904:TYR:CD1	2.47	0.67
1:C:900:MET:O	1:C:904:TYR:HD1	1.78	0.67
1:B:610:VAL:CG2	1:B:636:TYR:CD2	2.78	0.66
1:A:900:MET:O	1:A:904:TYR:HD1	1.77	0.65
1:A:457:ARG:HD2	1:A:459:SER:O	1.97	0.65
1:A:355:ARG:NH2	1:A:396:TYR:CB	2.60	0.65
1:A:957:GLN:NE2	1:C:765:ARG:HH22	1.93	0.65
1:A:761:THR:HG22	1:A:765:ARG:NH2	2.12	0.65
1:B:991:VAL:O	1:B:995:ARG:HG3	1.98	0.64
1:B:608:VAL:O	1:B:636:TYR:OH	2.15	0.64
1:A:102:ARG:HH12	1:A:141:LEU:HB3	1.58	0.64
1:A:355:ARG:NH2	1:A:396:TYR:HB2	2.14	0.63
1:A:1107:ARG:CD	1:C:904:TYR:CE2	2.60	0.62
1:C:979:ASP:O	1:C:983:ARG:HG3	1.99	0.62
1:B:346:ARG:HD3	1:B:346:ARG:N	2.14	0.62
1:B:979:ASP:O	1:B:983:ARG:HG3	1.99	0.61
1:B:773:GLU:OE1	1:B:1019:ARG:NH2	2.33	0.61
1:C:14:GLN:OE1	1:C:156:GLU:HG3	1.96	0.61
1:B:841:LEU:HB2	1:C:588:THR:HG21	1.83	0.61
1:B:904:TYR:CE2	1:C:1107:ARG:NE	2.67	0.61
1:C:1010:GLN:CB	1:C:1014:ARG:HH12	2.10	0.61
1:C:468:ILE:O	1:C:468:ILE:HG13	2.01	0.60
1:A:355:ARG:NH2	1:A:396:TYR:CG	2.70	0.60
1:C:454:ARG:HD3	1:C:456:PHE:O	2.02	0.60
1:A:957:GLN:HE21	1:C:765:ARG:CZ	2.10	0.59
1:B:212:LEU:HG	1:B:212:LEU:O	2.03	0.59
1:C:973:ILE:HD12	1:C:983:ARG:HH21	1.67	0.59
1:B:559:PHE:HB2	1:B:577:ARG:NH2	2.18	0.58
1:B:841:LEU:HD23	1:B:841:LEU:O	2.02	0.58
1:A:347:PHE:CE1	1:A:509:ARG:NH1	2.73	0.57
1:A:355:ARG:CZ	1:A:396:TYR:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:THR:HG22	1:A:765:ARG:HH22	1.69	0.55
1:A:957:GLN:CD	1:C:765:ARG:HH21	2.15	0.55
1:B:498:ARG:HB3	1:B:501:TYR:HD2	1.57	0.55
1:A:957:GLN:HE21	1:C:765:ARG:HH22	1.49	0.55
1:C:454:ARG:HH12	1:C:491:PRO:HD3	1.70	0.55
1:A:973:ILE:HD12	1:A:983:ARG:HH21	1.72	0.54
1:C:443:SER:OG	1:C:499:PRO:HD3	2.06	0.54
1:B:498:ARG:CB	1:B:501:TYR:CD2	2.70	0.54
1:C:498:ARG:HB3	1:C:501:TYR:CD1	2.43	0.54
1:B:610:VAL:HG23	1:B:636:TYR:HE2	1.56	0.53
1:B:246:ARG:HD3	1:B:258:TRP:CE3	2.44	0.53
1:A:904:TYR:CE2	1:B:1107:ARG:CD	2.83	0.53
1:B:20:THR:OG1	1:B:68:ILE:O	2.27	0.53
1:B:438:SER:CB	1:B:509:ARG:HG3	2.39	0.53
1:B:896:ILE:CD1	1:B:904:TYR:CE1	2.91	0.53
1:A:864:LEU:HG	1:B:697:MET:HE1	1.91	0.52
1:A:1091:ARG:HD2	1:A:1118:ASP:O	2.09	0.52
1:B:83:VAL:HG13	1:B:237:ARG:HD2	1.91	0.52
1:A:577:ARG:CZ	1:A:584:ILE:HD11	2.40	0.52
1:A:837:TYR:O	1:A:841:LEU:HD22	2.10	0.52
1:A:610:VAL:HG21	1:A:636:TYR:CD2	2.43	0.51
1:B:1091:ARG:HD2	1:B:1118:ASP:O	2.10	0.51
1:A:973:ILE:HD12	1:A:983:ARG:NH2	2.26	0.51
1:A:102:ARG:HH22	1:A:143:VAL:CG2	2.24	0.51
1:A:355:ARG:CZ	1:A:396:TYR:HB3	2.40	0.51
1:A:1107:ARG:HD3	1:C:904:TYR:CD2	2.43	0.51
1:C:466:ARG:HG3	1:C:466:ARG:O	2.10	0.51
1:B:904:TYR:CD2	1:C:1107:ARG:HD3	2.39	0.51
1:B:841:LEU:CB	1:C:588:THR:HG21	2.40	0.50
1:B:346:ARG:HD3	1:B:346:ARG:H	1.77	0.50
1:A:957:GLN:CG	1:C:765:ARG:NH2	2.75	0.50
1:C:973:ILE:HD12	1:C:983:ARG:NH2	2.27	0.50
1:A:102:ARG:NH1	1:A:141:LEU:CG	2.75	0.50
1:A:83:VAL:CG1	1:A:237:ARG:CZ	2.89	0.49
1:A:353:TRP:NE1	1:A:466:ARG:HB3	2.27	0.49
1:C:454:ARG:CZ	1:C:491:PRO:HD3	2.42	0.49
1:A:20:THR:OG1	1:A:68:ILE:O	2.24	0.49
1:B:671:CYS:SG	1:B:697:MET:HE2	2.53	0.49
1:C:346:ARG:HA	1:C:509:ARG:NH2	2.28	0.49
1:C:577:ARG:HB2	1:C:584:ILE:CD1	2.43	0.48
1:A:102:ARG:NH1	1:A:141:LEU:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:VAL:C	1:B:636:TYR:HH	2.17	0.48
1:C:1091:ARG:NH1	1:C:1120:THR:O	2.46	0.47
1:C:32:PHE:HE2	1:C:214:ARG:NH2	1.92	0.47
1:A:353:TRP:CE2	1:A:466:ARG:HB3	2.50	0.47
1:A:1107:ARG:NE	1:C:904:TYR:CE2	2.82	0.47
1:C:20:THR:OG1	1:C:68:ILE:O	2.31	0.47
1:A:496:GLY:O	1:A:501:TYR:CE2	2.68	0.47
1:B:577:ARG:HB2	1:B:584:ILE:CD1	2.44	0.47
1:C:346:ARG:HA	1:C:509:ARG:HH21	1.80	0.47
1:A:102:ARG:HH22	1:A:143:VAL:HG21	1.80	0.46
1:B:608:VAL:C	1:B:636:TYR:OH	2.58	0.46
1:B:454:ARG:HD3	1:B:456:PHE:O	2.15	0.46
1:A:179:LEU:HD22	1:A:179:LEU:H	1.81	0.46
1:A:353:TRP:CH2	1:A:466:ARG:NH2	2.83	0.46
1:A:355:ARG:NE	1:A:396:TYR:CD2	2.84	0.46
1:A:355:ARG:HB2	1:A:466:ARG:HH22	1.81	0.46
1:C:559:PHE:CB	1:C:577:ARG:NH2	2.63	0.45
1:A:438:SER:CB	1:A:509:ARG:HG3	2.47	0.45
1:B:346:ARG:N	1:B:346:ARG:CD	2.80	0.45
1:A:773:GLU:OE2	1:A:1019:ARG:NE	2.46	0.45
1:C:179:LEU:HD22	1:C:179:LEU:H	1.81	0.45
1:A:577:ARG:HB2	1:A:584:ILE:CD1	2.47	0.44
1:B:841:LEU:HB2	1:C:588:THR:OG1	2.16	0.44
1:A:454:ARG:HD3	1:A:456:PHE:O	2.16	0.44
1:B:179:LEU:H	1:B:179:LEU:HD22	1.82	0.44
1:C:676:THR:HG22	1:C:678:THR:HG22	1.99	0.44
1:C:454:ARG:HB2	1:C:491:PRO:HB3	1.99	0.44
1:C:457:ARG:HD2	1:C:467:ASP:OD2	2.17	0.44
1:A:90:VAL:HG22	1:A:269:TYR:HD1	1.83	0.44
1:B:353:TRP:CZ3	1:B:466:ARG:NH2	2.85	0.44
1:C:1010:GLN:CB	1:C:1014:ARG:NH1	2.71	0.44
1:A:353:TRP:O	1:A:466:ARG:NE	2.50	0.44
1:C:436:TRP:CE3	1:C:509:ARG:O	2.71	0.43
1:C:443:SER:OG	1:C:499:PRO:CD	2.66	0.43
1:C:740:MET:HE3	1:C:857:GLY:HA2	2.01	0.43
1:A:90:VAL:HG22	1:A:269:TYR:CD1	2.54	0.43
1:A:21:ARG:HD3	1:A:81:ASN:OD1	2.18	0.43
1:A:957:GLN:CG	1:C:765:ARG:HH22	2.32	0.43
1:A:1050:MET:HE2	1:A:1052:PHE:CE1	2.54	0.43
1:A:54:LEU:HD23	1:A:270:LEU:HD12	2.01	0.42
1:B:440:LYS:O	1:B:440:LYS:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:CB	1:B:577:ARG:NH2	2.82	0.42
1:A:404:GLY:HA3	1:A:508:TYR:CE1	2.54	0.42
1:A:83:VAL:CB	1:A:237:ARG:NH1	2.78	0.42
1:B:841:LEU:HB2	1:C:588:THR:CG2	2.49	0.42
1:A:904:TYR:CD2	1:B:1107:ARG:HD3	2.53	0.42
1:C:454:ARG:CZ	1:C:491:PRO:HG3	2.50	0.42
1:C:991:VAL:O	1:C:995:ARG:HG3	2.20	0.41
1:A:404:GLY:N	1:A:508:TYR:CD1	2.88	0.41
1:A:353:TRP:CE3	1:A:466:ARG:NH2	2.68	0.41
1:A:355:ARG:CZ	1:A:396:TYR:CG	3.04	0.41
1:A:991:VAL:O	1:A:995:ARG:HG3	2.21	0.41
1:A:661:GLU:CD	1:A:661:GLU:H	2.29	0.41
1:C:498:ARG:HB3	1:C:501:TYR:CE1	2.55	0.40
1:C:559:PHE:HB3	1:C:577:ARG:HH21	1.81	0.40
1:B:436:TRP:CE3	1:B:509:ARG:O	2.75	0.40
1:B:740:MET:HE3	1:B:857:GLY:HA2	2.03	0.40
1:B:840:CYS:O	1:B:845:ALA:HB2	2.22	0.40
1:C:577:ARG:NH2	1:C:584:ILE:HD11	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

84 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	1,2	14,14,15	1.34	2 (14%)	17,19,21	0.78	0
2	NAG	D	2	2	14,14,15	1.36	2 (14%)	17,19,21	0.84	1 (5%)
2	MAN	D	3	2	11,11,12	1.52	2 (18%)	15,15,17	0.84	1 (6%)
3	NAG	E	1	1,3	14,14,15	1.50	3 (21%)	17,19,21	1.87	2 (11%)
3	NAG	E	2	3	14,14,15	1.27	2 (14%)	17,19,21	0.81	1 (5%)
2	NAG	F	1	1,2	14,14,15	1.22	1 (7%)	17,19,21	0.72	0
2	NAG	F	2	2	14,14,15	1.39	2 (14%)	17,19,21	0.73	0
2	MAN	F	3	2	11,11,12	1.54	2 (18%)	15,15,17	0.94	1 (6%)
2	NAG	G	1	1,2	14,14,15	1.30	3 (21%)	17,19,21	0.62	0
2	NAG	G	2	2	14,14,15	1.42	3 (21%)	17,19,21	0.75	1 (5%)
2	MAN	G	3	2	11,11,12	1.57	2 (18%)	15,15,17	0.82	0
3	NAG	H	1	1,3	14,14,15	1.42	2 (14%)	17,19,21	1.40	3 (17%)
3	NAG	H	2	3	14,14,15	1.33	2 (14%)	17,19,21	0.93	1 (5%)
2	NAG	I	1	1,2	14,14,15	1.16	1 (7%)	17,19,21	0.72	0
2	NAG	I	2	2	14,14,15	1.28	2 (14%)	17,19,21	0.72	0
2	MAN	I	3	2	11,11,12	1.57	2 (18%)	15,15,17	0.96	1 (6%)
2	NAG	J	1	1,2	14,14,15	1.08	1 (7%)	17,19,21	0.65	0
2	NAG	J	2	2	14,14,15	1.36	3 (21%)	17,19,21	0.70	1 (5%)
2	MAN	J	3	2	11,11,12	1.43	1 (9%)	15,15,17	0.77	0
4	NAG	K	1	4,1	14,14,15	1.19	1 (7%)	17,19,21	0.86	0
4	NAG	K	2	4	14,14,15	1.24	2 (14%)	17,19,21	0.67	0
4	FUC	K	3	4	10,10,11	1.57	2 (20%)	14,14,16	0.98	0
2	NAG	L	1	1,2	14,14,15	1.21	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	L	2	2	14,14,15	1.26	1 (7%)	17,19,21	0.60	0
2	MAN	L	3	2	11,11,12	1.45	2 (18%)	15,15,17	0.67	0
2	NAG	M	1	1,2	14,14,15	1.20	1 (7%)	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	M	2	2	14,14,15	1.33	2 (14%)	17,19,21	0.85	1 (5%)
2	MAN	M	3	2	11,11,12	1.57	2 (18%)	15,15,17	0.99	1 (6%)
2	NAG	N	1	1,2	14,14,15	1.34	3 (21%)	17,19,21	0.79	0
2	NAG	N	2	2	14,14,15	1.38	2 (14%)	17,19,21	0.86	0
2	MAN	N	3	2	11,11,12	1.44	2 (18%)	15,15,17	0.94	0
3	NAG	O	1	1,3	14,14,15	1.41	3 (21%)	17,19,21	1.60	2 (11%)
3	NAG	O	2	3	14,14,15	1.28	2 (14%)	17,19,21	1.02	1 (5%)
2	NAG	P	1	1,2	14,14,15	1.28	2 (14%)	17,19,21	0.89	1 (5%)
2	NAG	P	2	2	14,14,15	1.39	3 (21%)	17,19,21	0.80	0
2	MAN	P	3	2	11,11,12	1.49	2 (18%)	15,15,17	0.94	0
2	NAG	Q	1	1,2	14,14,15	1.35	3 (21%)	17,19,21	0.59	0
2	NAG	Q	2	2	14,14,15	1.42	3 (21%)	17,19,21	0.71	1 (5%)
2	MAN	Q	3	2	11,11,12	1.49	2 (18%)	15,15,17	0.89	0
3	NAG	R	1	1,3	14,14,15	1.25	1 (7%)	17,19,21	0.64	0
3	NAG	R	2	3	14,14,15	1.28	2 (14%)	17,19,21	0.85	1 (5%)
2	NAG	S	1	1,2	14,14,15	1.17	1 (7%)	17,19,21	0.78	0
2	NAG	S	2	2	14,14,15	1.30	2 (14%)	17,19,21	0.61	0
2	MAN	S	3	2	11,11,12	1.57	2 (18%)	15,15,17	0.91	1 (6%)
2	NAG	T	1	1,2	14,14,15	1.05	1 (7%)	17,19,21	0.58	0
2	NAG	T	2	2	14,14,15	1.34	3 (21%)	17,19,21	0.75	1 (5%)
2	MAN	T	3	2	11,11,12	1.41	2 (18%)	15,15,17	0.72	0
4	NAG	U	1	4,1	14,14,15	1.20	1 (7%)	17,19,21	0.90	0
4	NAG	U	2	4	14,14,15	1.22	1 (7%)	17,19,21	0.66	0
4	FUC	U	3	4	10,10,11	1.57	2 (20%)	14,14,16	1.01	0
2	NAG	V	1	1,2	14,14,15	1.19	1 (7%)	17,19,21	1.02	1 (5%)
2	NAG	V	2	2	14,14,15	1.25	1 (7%)	17,19,21	0.64	0
2	MAN	V	3	2	11,11,12	1.44	1 (9%)	15,15,17	0.67	0
2	NAG	W	1	1,2	14,14,15	1.21	1 (7%)	17,19,21	0.74	0
2	NAG	W	2	2	14,14,15	1.31	2 (14%)	17,19,21	0.89	1 (5%)
2	MAN	W	3	2	11,11,12	1.55	2 (18%)	15,15,17	1.00	1 (6%)
2	NAG	X	1	1,2	14,14,15	1.31	2 (14%)	17,19,21	0.65	0
2	NAG	X	2	2	14,14,15	1.39	2 (14%)	17,19,21	0.75	0
2	MAN	X	3	2	11,11,12	1.51	2 (18%)	15,15,17	0.97	1 (6%)
3	NAG	Y	1	1,3	14,14,15	1.48	4 (28%)	17,19,21	1.46	1 (5%)
3	NAG	Y	2	3	14,14,15	1.31	2 (14%)	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Z	1	1,2	14,14,15	1.27	2 (14%)	17,19,21	0.87	0
2	NAG	Z	2	2	14,14,15	1.40	3 (21%)	17,19,21	0.91	2 (11%)
2	MAN	Z	3	2	11,11,12	1.47	2 (18%)	15,15,17	0.98	0
2	NAG	a	1	1,2	14,14,15	1.30	3 (21%)	17,19,21	0.59	0
2	NAG	a	2	2	14,14,15	1.40	3 (21%)	17,19,21	0.72	0
2	MAN	a	3	2	11,11,12	1.48	2 (18%)	15,15,17	0.82	0
3	NAG	b	1	1,3	14,14,15	1.44	2 (14%)	17,19,21	1.06	2 (11%)
3	NAG	b	2	3	14,14,15	1.32	2 (14%)	17,19,21	0.91	1 (5%)
2	NAG	c	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	0.73	0
2	NAG	c	2	2	14,14,15	1.26	2 (14%)	17,19,21	0.72	0
2	MAN	c	3	2	11,11,12	1.61	2 (18%)	15,15,17	1.00	1 (6%)
2	NAG	d	1	1,2	14,14,15	1.10	1 (7%)	17,19,21	0.69	0
2	NAG	d	2	2	14,14,15	1.38	3 (21%)	17,19,21	0.72	1 (5%)
2	MAN	d	3	2	11,11,12	1.42	1 (9%)	15,15,17	0.78	0
4	NAG	e	1	4,1	14,14,15	1.19	1 (7%)	17,19,21	0.88	1 (5%)
4	NAG	e	2	4	14,14,15	1.22	1 (7%)	17,19,21	0.67	0
4	FUC	e	3	4	10,10,11	1.57	2 (20%)	14,14,16	1.02	1 (7%)
2	NAG	f	1	1,2	14,14,15	1.21	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	f	2	2	14,14,15	1.25	2 (14%)	17,19,21	0.65	0
2	MAN	f	3	2	11,11,12	1.42	1 (9%)	15,15,17	0.76	0
2	NAG	g	1	1,2	14,14,15	1.23	1 (7%)	17,19,21	0.72	0
2	NAG	g	2	2	14,14,15	1.30	1 (7%)	17,19,21	0.87	1 (5%)
2	MAN	g	3	2	11,11,12	1.52	2 (18%)	15,15,17	1.03	2 (13%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	MAN	D	3	2	-	1/2/19/22	1/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	F	3	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	1/1/1/1
3	NAG	H	1	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	MAN	I	3	2	-	0/2/19/22	1/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	MAN	J	3	2	-	1/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	FUC	K	3	4	-	-	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	MAN	L	3	2	-	1/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	MAN	M	3	2	-	0/2/19/22	1/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	MAN	N	3	2	-	1/2/19/22	0/1/1/1
3	NAG	O	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	MAN	P	3	2	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
2	MAN	Q	3	2	-	0/2/19/22	1/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	MAN	S	3	2	-	0/2/19/22	1/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	MAN	T	3	2	-	1/2/19/22	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	U	3	4	-	-	0/1/1/1
2	NAG	V	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	MAN	V	3	2	-	1/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	0/6/23/26	0/1/1/1
2	MAN	W	3	2	-	0/2/19/22	1/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	0/6/23/26	0/1/1/1
2	MAN	X	3	2	-	1/2/19/22	0/1/1/1
3	NAG	Y	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	MAN	Z	3	2	-	0/2/19/22	0/1/1/1
2	NAG	a	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	MAN	a	3	2	-	0/2/19/22	0/1/1/1
3	NAG	b	1	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	0/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	MAN	c	3	2	-	0/2/19/22	1/1/1/1
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	0/6/23/26	0/1/1/1
2	MAN	d	3	2	-	1/2/19/22	0/1/1/1
4	NAG	e	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	FUC	e	3	4	-	-	0/1/1/1
2	NAG	f	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1
2	MAN	f	3	2	-	1/2/19/22	0/1/1/1
2	NAG	g	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
2	MAN	g	3	2	-	0/2/19/22	0/1/1/1

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	3	MAN	O5-C5	3.30	1.49	1.43
2	L	3	MAN	O5-C5	3.23	1.49	1.43
2	G	3	MAN	O5-C5	3.23	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	3	MAN	O5-C5	3.22	1.49	1.43
2	f	3	MAN	O5-C5	3.22	1.49	1.43
3	E	1	NAG	O5-C5	3.18	1.49	1.43
2	c	3	MAN	O5-C5	3.18	1.49	1.43
3	b	1	NAG	C1-C2	3.17	1.56	1.52
2	W	3	MAN	O5-C5	3.17	1.49	1.43
2	F	3	MAN	O5-C5	3.14	1.49	1.43
2	g	3	MAN	O5-C5	3.12	1.49	1.43
2	S	3	MAN	O5-C5	3.11	1.49	1.43
2	a	3	MAN	O5-C5	3.11	1.49	1.43
2	Q	3	MAN	O5-C5	3.10	1.49	1.43
2	D	3	MAN	O5-C5	3.08	1.49	1.43
2	T	3	MAN	O5-C5	3.07	1.49	1.43
2	I	3	MAN	O5-C5	3.05	1.49	1.43
2	P	3	MAN	O5-C5	3.03	1.49	1.43
2	Z	3	MAN	O5-C5	3.01	1.49	1.43
3	H	1	NAG	C1-C2	2.99	1.56	1.52
2	Z	2	NAG	O5-C5	2.98	1.49	1.43
2	X	2	NAG	O5-C5	2.94	1.49	1.43
2	X	3	MAN	O5-C5	2.94	1.49	1.43
4	e	3	FUC	O5-C5	2.94	1.49	1.43
4	U	3	FUC	O5-C5	2.90	1.49	1.43
2	N	2	NAG	O5-C5	2.90	1.49	1.43
4	K	3	FUC	O5-C5	2.89	1.49	1.43
2	N	3	MAN	O5-C5	2.89	1.49	1.43
2	d	3	MAN	O5-C5	2.88	1.49	1.43
3	Y	1	NAG	C1-C2	2.88	1.56	1.52
2	P	2	NAG	O5-C5	2.86	1.49	1.43
2	J	3	MAN	O5-C5	2.85	1.49	1.43
2	d	2	NAG	O5-C5	2.85	1.49	1.43
2	D	2	NAG	O5-C5	2.83	1.48	1.43
2	J	2	NAG	O5-C5	2.83	1.48	1.43
3	O	2	NAG	O5-C5	2.79	1.48	1.43
2	F	2	NAG	O5-C5	2.78	1.48	1.43
2	W	2	NAG	O5-C5	2.78	1.48	1.43
2	G	2	NAG	O5-C5	2.78	1.48	1.43
3	H	2	NAG	O5-C5	2.77	1.48	1.43
2	T	2	NAG	O5-C5	2.77	1.48	1.43
2	M	2	NAG	O5-C5	2.77	1.48	1.43
3	R	2	NAG	O5-C5	2.76	1.48	1.43
3	Y	2	NAG	O5-C5	2.75	1.48	1.43
2	Q	2	NAG	O5-C5	2.75	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	2	NAG	O5-C5	2.73	1.48	1.43
4	e	2	NAG	O5-C5	2.72	1.48	1.43
4	K	2	NAG	O5-C5	2.72	1.48	1.43
2	S	2	NAG	O5-C5	2.71	1.48	1.43
2	g	2	NAG	O5-C5	2.71	1.48	1.43
3	E	2	NAG	O5-C5	2.70	1.48	1.43
2	I	2	NAG	O5-C5	2.69	1.48	1.43
2	L	2	NAG	O5-C5	2.68	1.48	1.43
3	Y	1	NAG	O5-C5	2.68	1.48	1.43
2	c	3	MAN	O5-C1	2.68	1.48	1.43
2	c	2	NAG	O5-C5	2.67	1.48	1.43
4	U	2	NAG	O5-C5	2.67	1.48	1.43
2	f	2	NAG	O5-C5	2.66	1.48	1.43
3	O	1	NAG	O5-C5	2.65	1.48	1.43
2	V	2	NAG	O5-C5	2.63	1.48	1.43
3	O	1	NAG	C1-C2	2.63	1.55	1.52
2	N	1	NAG	O5-C5	2.62	1.48	1.43
2	a	2	NAG	O5-C5	2.62	1.48	1.43
2	M	3	MAN	O5-C1	2.60	1.48	1.43
2	Z	1	NAG	O5-C5	2.59	1.48	1.43
2	L	1	NAG	O5-C5	2.58	1.48	1.43
2	D	3	MAN	O5-C1	2.58	1.48	1.43
2	X	1	NAG	O5-C5	2.55	1.48	1.43
2	I	3	MAN	O5-C1	2.55	1.48	1.43
2	S	3	MAN	O5-C1	2.55	1.48	1.43
2	f	1	NAG	O5-C5	2.53	1.48	1.43
2	Q	1	NAG	O5-C5	2.52	1.48	1.43
4	U	3	FUC	O5-C1	2.51	1.47	1.43
2	G	3	MAN	O5-C1	2.51	1.47	1.43
3	E	1	NAG	O5-C1	2.50	1.47	1.43
2	W	3	MAN	O5-C1	2.50	1.47	1.43
2	a	1	NAG	O5-C5	2.50	1.48	1.43
2	D	1	NAG	O5-C5	2.49	1.48	1.43
3	R	1	NAG	O5-C5	2.49	1.48	1.43
2	X	3	MAN	O5-C1	2.49	1.47	1.43
2	V	1	NAG	O5-C5	2.49	1.48	1.43
2	g	3	MAN	O5-C1	2.47	1.47	1.43
2	F	3	MAN	O5-C1	2.46	1.47	1.43
2	F	1	NAG	O5-C5	2.45	1.48	1.43
4	K	3	FUC	O5-C1	2.45	1.47	1.43
4	e	3	FUC	O5-C1	2.45	1.47	1.43
2	G	1	NAG	O5-C5	2.44	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	1	NAG	O5-C5	2.42	1.48	1.43
4	K	1	NAG	O5-C5	2.40	1.48	1.43
2	g	1	NAG	O5-C5	2.39	1.48	1.43
2	P	1	NAG	O5-C5	2.36	1.48	1.43
3	Y	1	NAG	O5-C1	2.35	1.47	1.43
2	a	3	MAN	O5-C1	2.34	1.47	1.43
2	D	1	NAG	C1-C2	2.34	1.55	1.52
2	W	1	NAG	O5-C5	2.33	1.48	1.43
4	e	1	NAG	O5-C5	2.33	1.48	1.43
2	N	3	MAN	O5-C1	2.32	1.47	1.43
2	Q	3	MAN	O5-C1	2.31	1.47	1.43
2	M	1	NAG	O5-C5	2.31	1.47	1.43
2	F	2	NAG	O4-C4	2.30	1.48	1.43
3	E	1	NAG	C1-C2	2.28	1.55	1.52
2	P	1	NAG	C1-C2	2.27	1.55	1.52
2	Q	2	NAG	O4-C4	2.27	1.48	1.43
2	G	2	NAG	O5-C1	2.24	1.47	1.43
2	S	1	NAG	O5-C5	2.24	1.47	1.43
2	a	2	NAG	O5-C1	2.23	1.47	1.43
2	Q	2	NAG	O5-C1	2.22	1.47	1.43
2	Z	3	MAN	O5-C1	2.22	1.47	1.43
2	J	2	NAG	O5-C1	2.22	1.47	1.43
2	d	2	NAG	O5-C1	2.22	1.47	1.43
2	I	2	NAG	O4-C4	2.21	1.48	1.43
3	O	1	NAG	O5-C1	2.20	1.47	1.43
2	I	1	NAG	O5-C5	2.19	1.47	1.43
2	Q	1	NAG	O4-C4	2.19	1.48	1.43
2	P	3	MAN	O5-C1	2.19	1.47	1.43
2	c	2	NAG	O4-C4	2.18	1.48	1.43
2	G	2	NAG	O4-C4	2.18	1.48	1.43
2	d	2	NAG	O4-C4	2.18	1.48	1.43
2	D	2	NAG	O4-C4	2.17	1.48	1.43
3	b	2	NAG	O5-C1	2.17	1.47	1.43
2	Z	1	NAG	C1-C2	2.16	1.55	1.52
2	S	2	NAG	O4-C4	2.16	1.48	1.43
2	P	2	NAG	O4-C4	2.15	1.48	1.43
2	Q	1	NAG	C1-C2	2.15	1.55	1.52
2	G	1	NAG	O4-C4	2.15	1.48	1.43
3	Y	2	NAG	O5-C1	2.14	1.47	1.43
2	d	1	NAG	O5-C5	2.14	1.47	1.43
2	c	1	NAG	O5-C5	2.14	1.47	1.43
2	M	2	NAG	O4-C4	2.13	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	2	NAG	O5-C1	2.13	1.47	1.43
2	Z	2	NAG	O4-C4	2.13	1.48	1.43
2	X	1	NAG	C1-C2	2.12	1.55	1.52
2	J	2	NAG	O4-C4	2.11	1.48	1.43
2	P	2	NAG	O5-C1	2.11	1.47	1.43
2	a	2	NAG	O4-C4	2.10	1.48	1.43
2	a	1	NAG	C1-C2	2.08	1.55	1.52
2	N	1	NAG	O4-C4	2.08	1.48	1.43
2	N	2	NAG	O5-C1	2.08	1.47	1.43
2	a	1	NAG	O4-C4	2.08	1.48	1.43
2	T	2	NAG	O4-C4	2.08	1.48	1.43
2	N	1	NAG	C1-C2	2.08	1.55	1.52
3	H	2	NAG	O5-C1	2.05	1.47	1.43
2	W	2	NAG	O4-C4	2.05	1.48	1.43
3	O	2	NAG	O5-C1	2.05	1.47	1.43
2	X	2	NAG	O4-C4	2.05	1.48	1.43
2	f	2	NAG	O4-C4	2.05	1.48	1.43
2	T	3	MAN	O5-C1	2.05	1.47	1.43
2	Z	2	NAG	O5-C1	2.05	1.47	1.43
3	Y	1	NAG	O4-C4	2.05	1.48	1.43
2	G	1	NAG	C1-C2	2.04	1.55	1.52
4	K	2	NAG	O5-C1	2.04	1.47	1.43
3	H	1	NAG	O4-C4	2.03	1.48	1.43
3	b	1	NAG	O4-C4	2.02	1.48	1.43
2	L	3	MAN	O5-C1	2.02	1.47	1.43
3	R	2	NAG	O5-C1	2.02	1.47	1.43
2	T	1	NAG	O5-C5	2.02	1.47	1.43
2	J	1	NAG	O5-C5	2.00	1.47	1.43
3	E	2	NAG	O5-C1	2.00	1.47	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	6.61	121.05	112.19
3	O	1	NAG	C1-O5-C5	5.86	120.05	112.19
3	Y	1	NAG	C1-O5-C5	5.21	119.17	112.19
3	Y	2	NAG	C1-O5-C5	3.31	116.62	112.19
3	O	2	NAG	C1-O5-C5	3.26	116.56	112.19
3	H	1	NAG	C1-O5-C5	3.15	116.41	112.19
3	b	2	NAG	C1-O5-C5	2.95	116.14	112.19
2	W	2	NAG	C1-O5-C5	2.95	116.13	112.19
3	H	1	NAG	C4-C3-C2	2.90	115.27	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C1-O5-C5	2.89	116.06	112.19
2	g	2	NAG	C1-O5-C5	2.77	115.90	112.19
2	c	3	MAN	C1-O5-C5	2.76	115.89	112.19
2	M	2	NAG	C1-O5-C5	2.75	115.88	112.19
3	b	1	NAG	C4-C3-C2	2.74	115.04	111.02
3	H	1	NAG	C3-C4-C5	2.74	115.20	110.23
2	M	3	MAN	C1-O5-C5	2.73	115.85	112.19
3	R	2	NAG	C1-O5-C5	2.65	115.74	112.19
2	V	1	NAG	C3-C4-C5	2.62	114.98	110.23
2	W	3	MAN	C1-O5-C5	2.61	115.69	112.19
2	X	3	MAN	C1-O5-C5	2.59	115.66	112.19
3	E	1	NAG	C4-C3-C2	-2.57	107.26	111.02
2	f	1	NAG	C3-C4-C5	2.55	114.86	110.23
2	I	3	MAN	C1-O5-C5	2.51	115.54	112.19
2	D	2	NAG	C1-O5-C5	2.40	115.40	112.19
2	S	3	MAN	C1-O5-C5	2.39	115.38	112.19
2	G	2	NAG	C1-O5-C5	2.37	115.36	112.19
2	P	1	NAG	C1-O5-C5	2.31	115.28	112.19
3	b	1	NAG	C3-C4-C5	2.30	114.41	110.23
2	L	1	NAG	C3-C4-C5	2.24	114.30	110.23
2	g	3	MAN	C1-O5-C5	2.23	115.18	112.19
2	D	3	MAN	C1-O5-C5	2.18	115.11	112.19
2	Z	2	NAG	C4-C3-C2	-2.18	107.83	111.02
2	J	2	NAG	C1-O5-C5	2.13	115.04	112.19
2	Q	2	NAG	C1-O5-C5	2.12	115.02	112.19
2	Z	2	NAG	C1-O5-C5	2.11	115.02	112.19
3	O	1	NAG	O5-C1-C2	2.10	114.54	111.29
2	F	3	MAN	C1-O5-C5	2.07	114.96	112.19
4	e	1	NAG	C1-O5-C5	2.06	114.95	112.19
4	e	3	FUC	C1-C2-C3	2.03	112.60	109.64
2	d	2	NAG	C1-O5-C5	2.03	114.90	112.19
2	T	2	NAG	C1-O5-C5	2.02	114.89	112.19
2	g	3	MAN	O5-C5-C6	2.01	111.58	107.66
3	E	2	NAG	C1-O5-C5	2.00	114.87	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	1	NAG	C2
3	b	1	NAG	C2

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
2	X	3	MAN	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
2	D	3	MAN	O5-C5-C6-O6
2	N	3	MAN	O5-C5-C6-O6
2	T	3	MAN	O5-C5-C6-O6
2	L	3	MAN	O5-C5-C6-O6
2	V	3	MAN	O5-C5-C6-O6
2	f	3	MAN	O5-C5-C6-O6
2	J	3	MAN	O5-C5-C6-O6
2	d	3	MAN	O5-C5-C6-O6
2	c	1	NAG	C1-C2-N2-C7
3	O	1	NAG	C1-C2-N2-C7

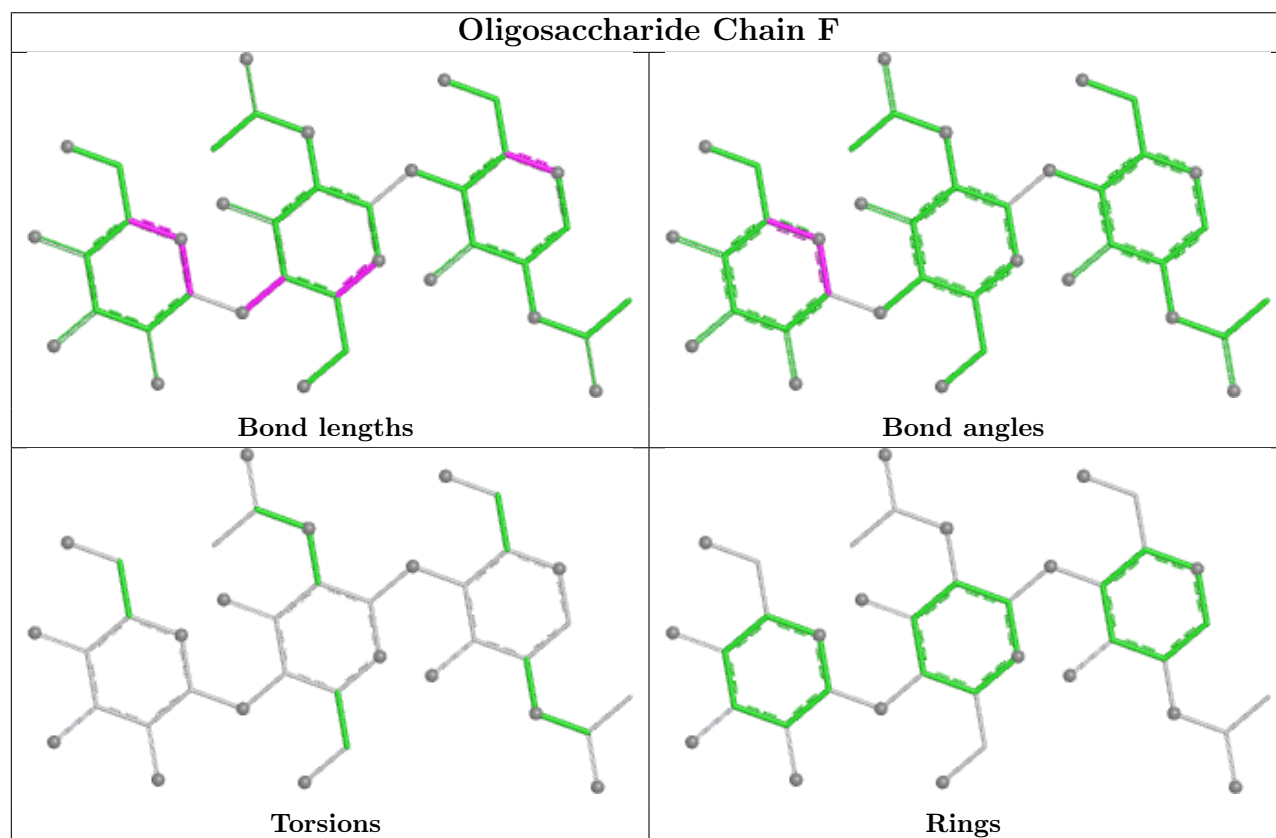
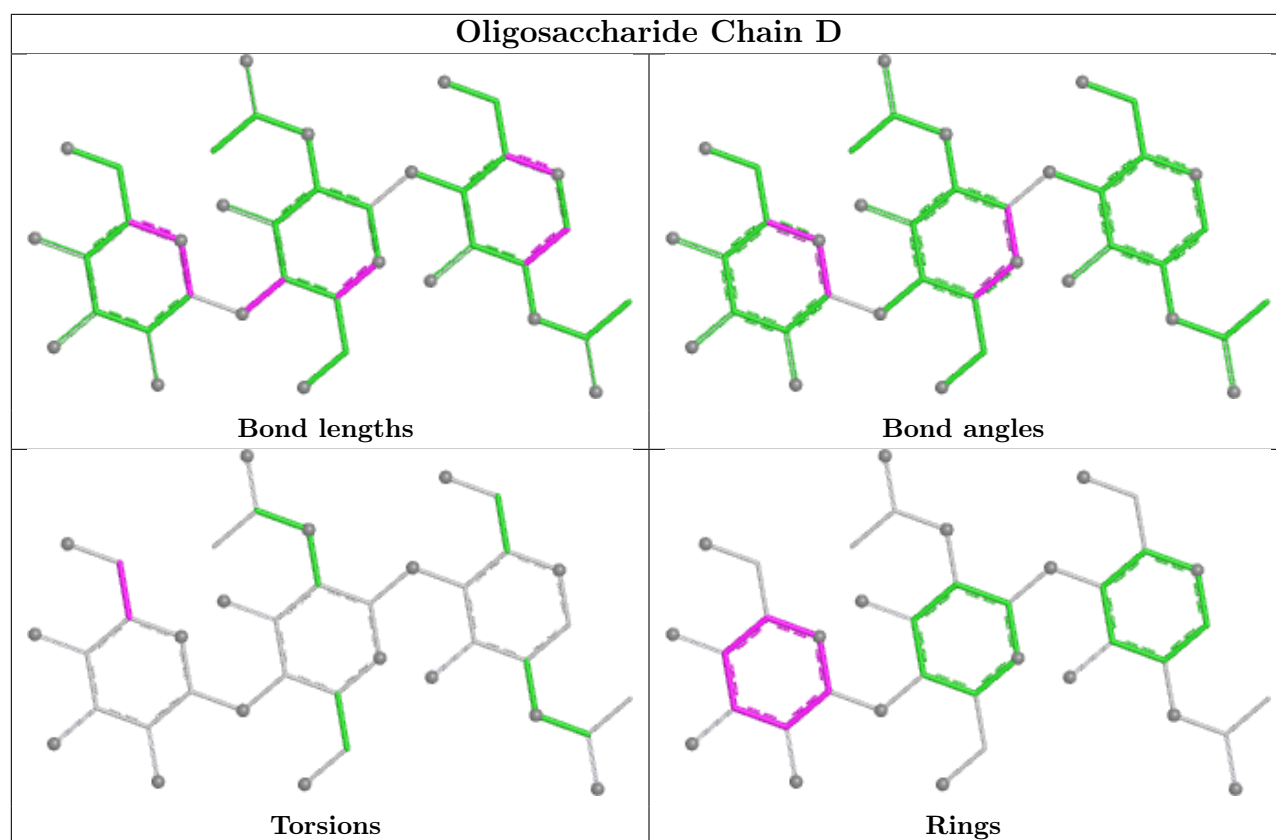
All (8) ring outliers are listed below:

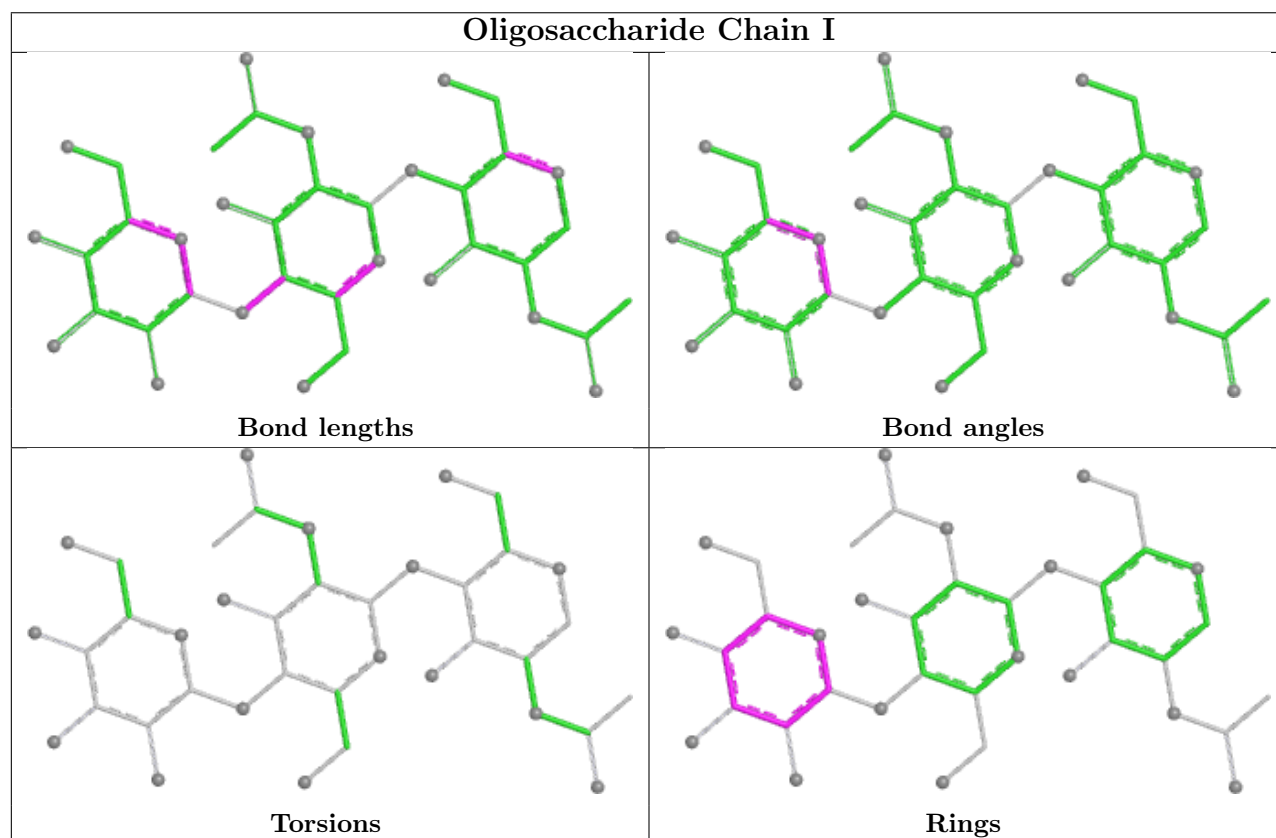
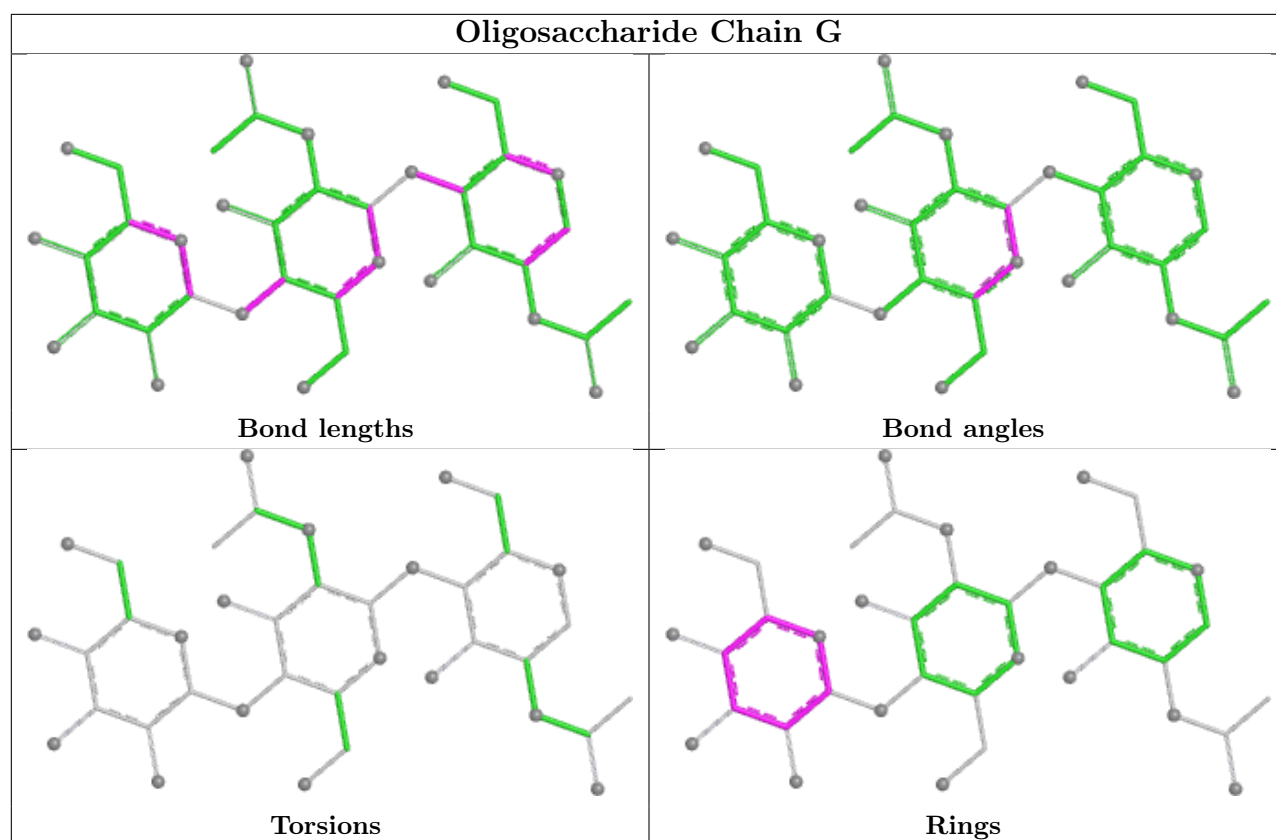
Mol	Chain	Res	Type	Atoms
2	Q	3	MAN	C1-C2-C3-C4-C5-O5
2	I	3	MAN	C1-C2-C3-C4-C5-O5
2	W	3	MAN	C1-C2-C3-C4-C5-O5
2	S	3	MAN	C1-C2-C3-C4-C5-O5
2	c	3	MAN	C1-C2-C3-C4-C5-O5
2	D	3	MAN	C1-C2-C3-C4-C5-O5
2	G	3	MAN	C1-C2-C3-C4-C5-O5
2	M	3	MAN	C1-C2-C3-C4-C5-O5

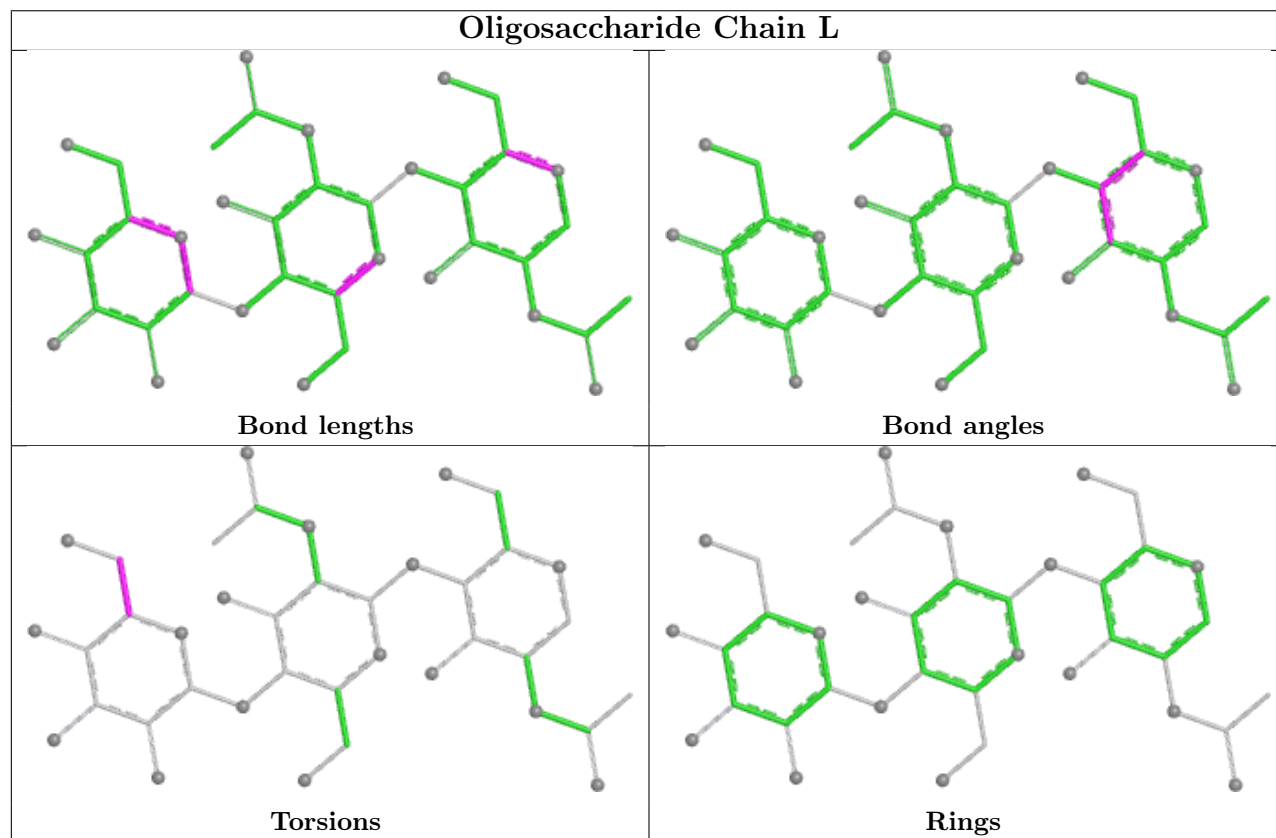
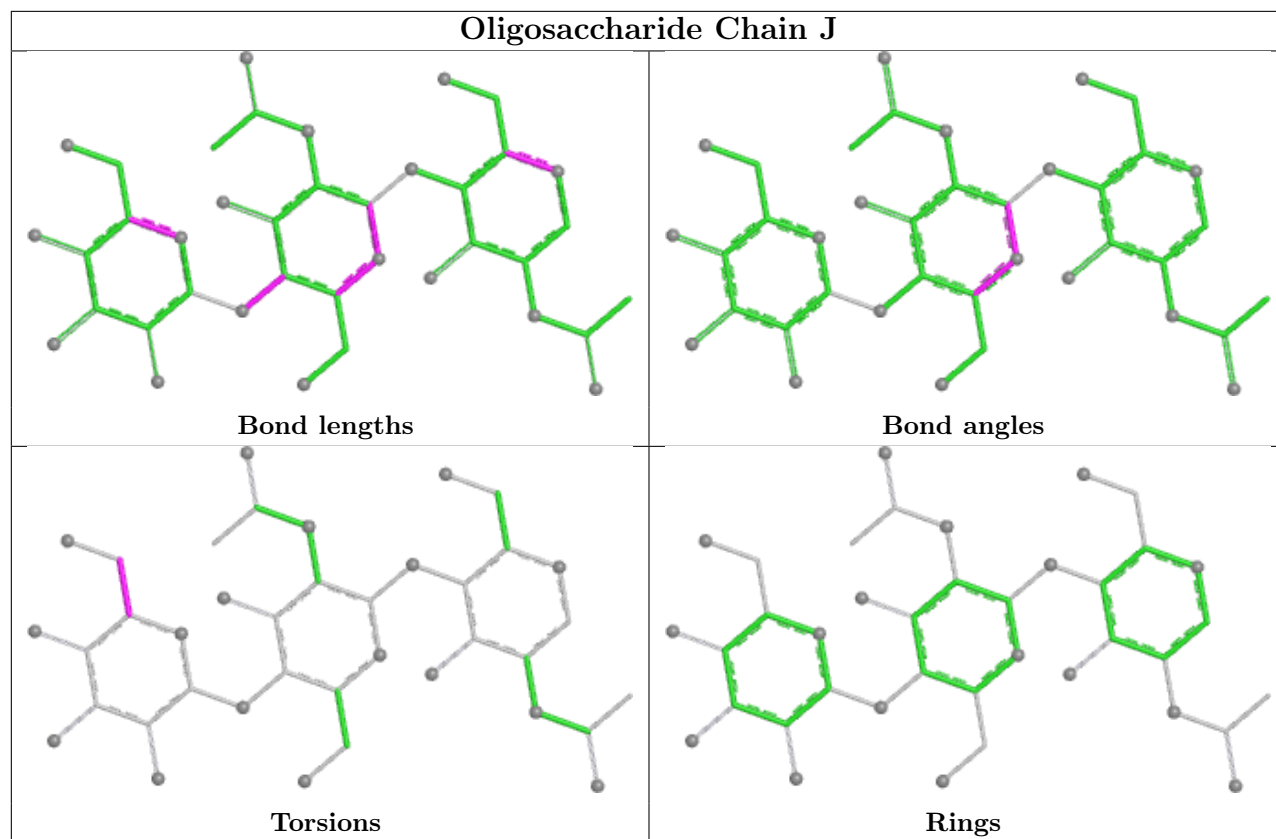
1 monomer is involved in 1 short contact:

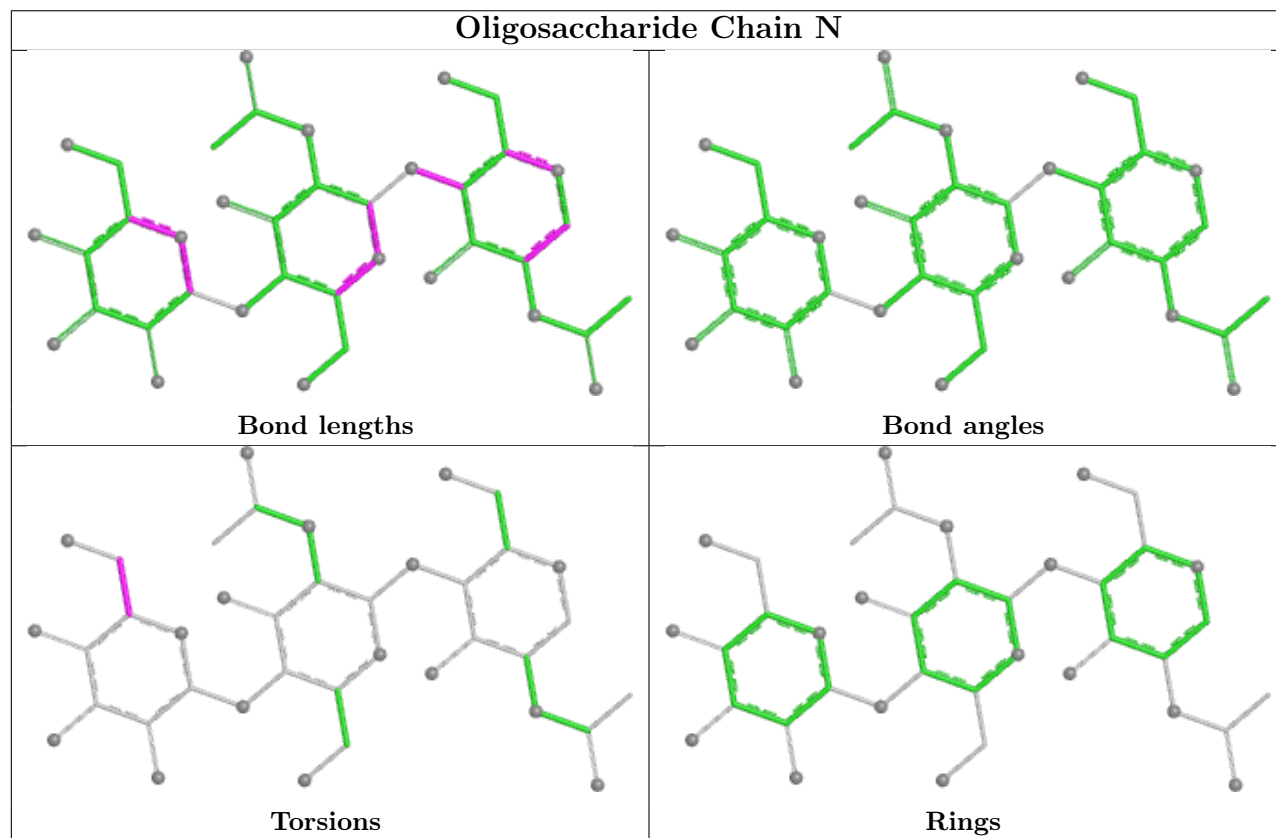
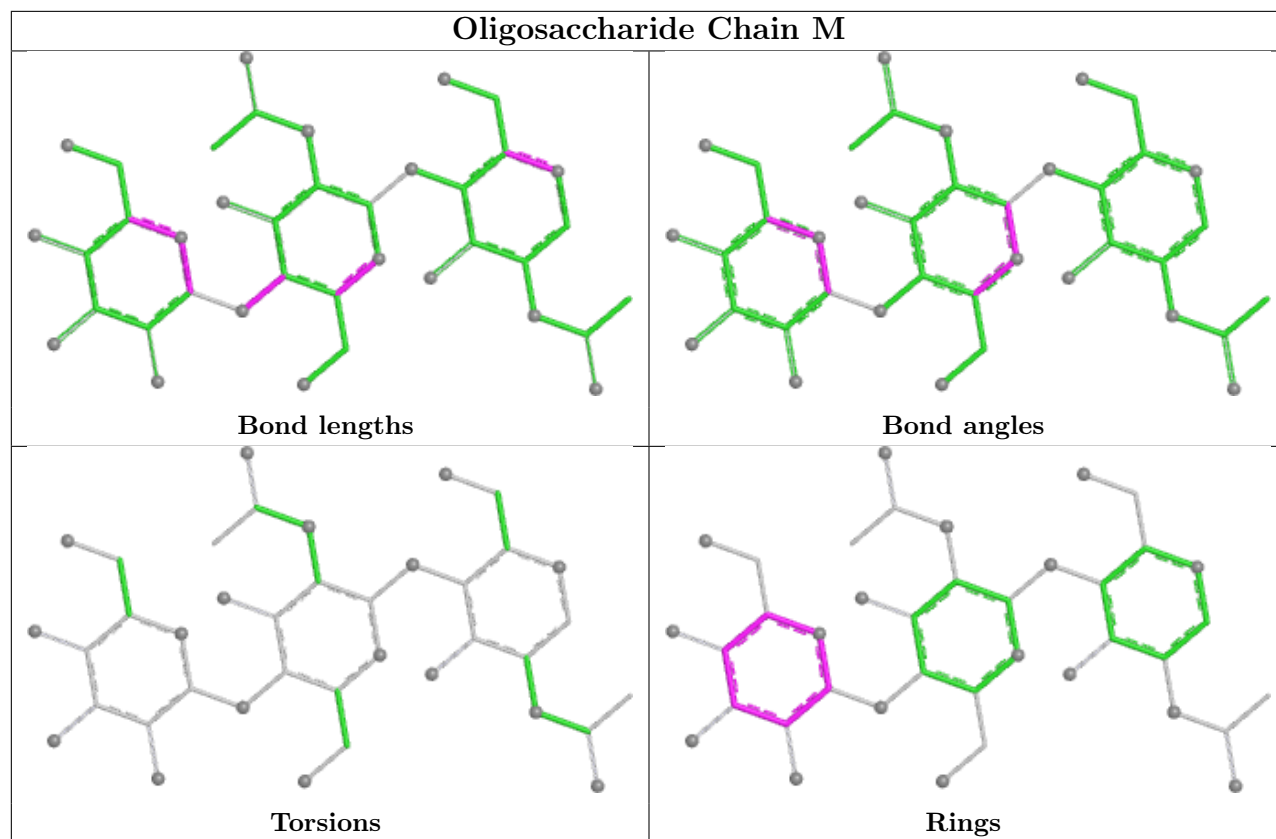
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	1	NAG	1	0

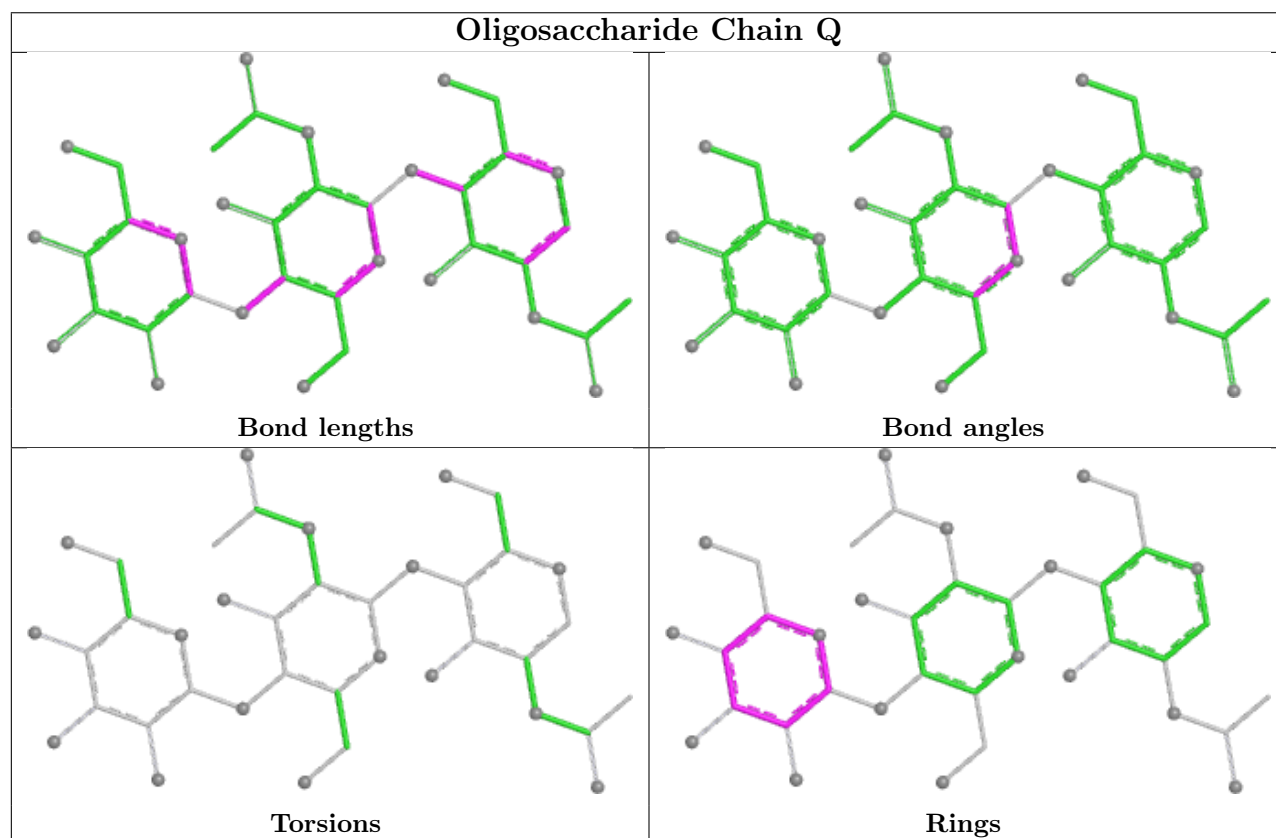
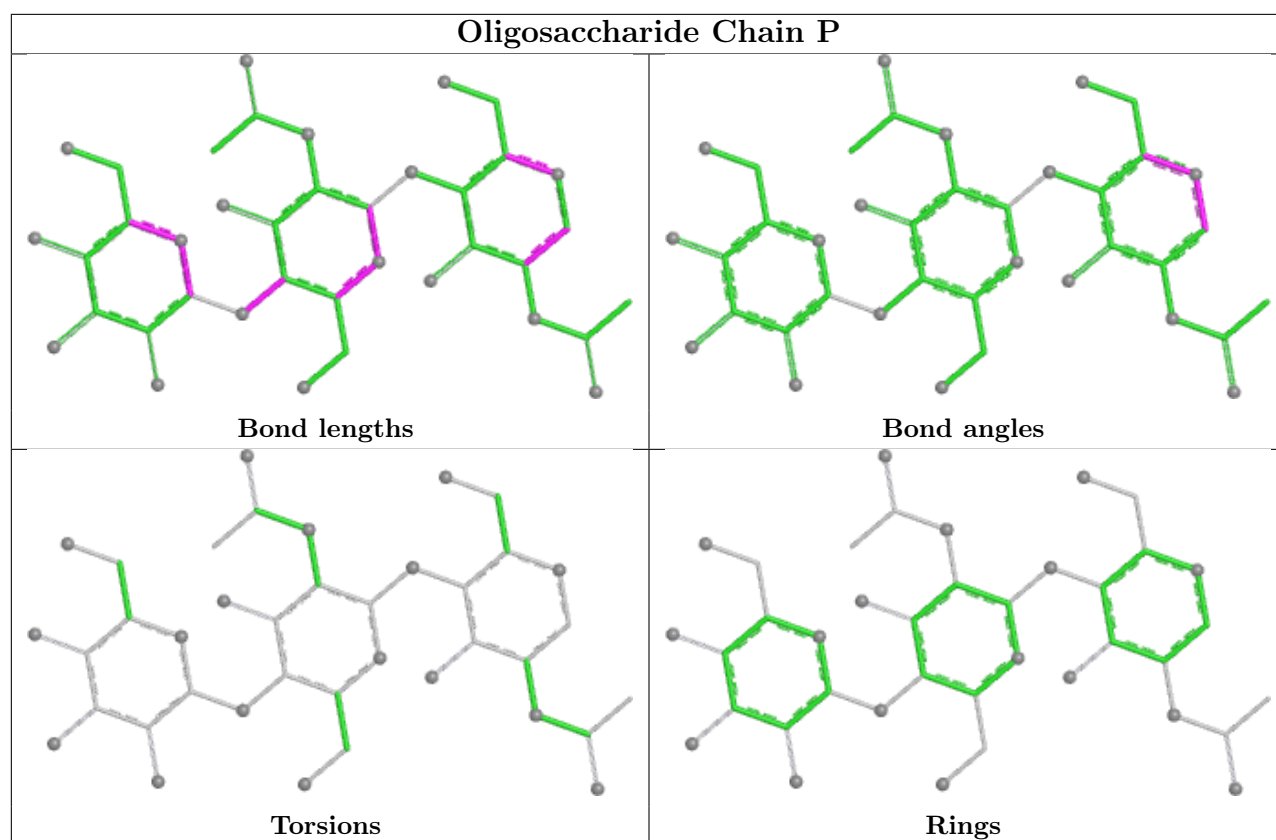
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

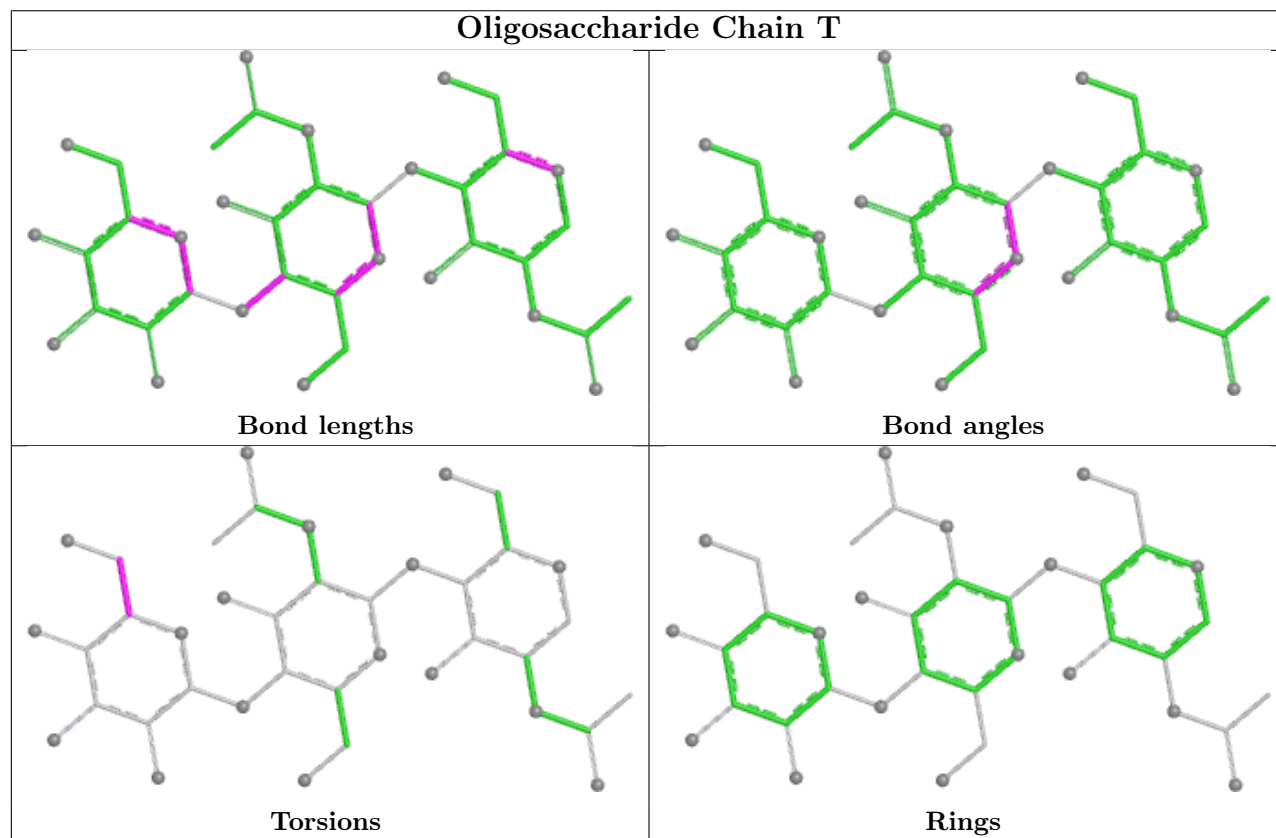
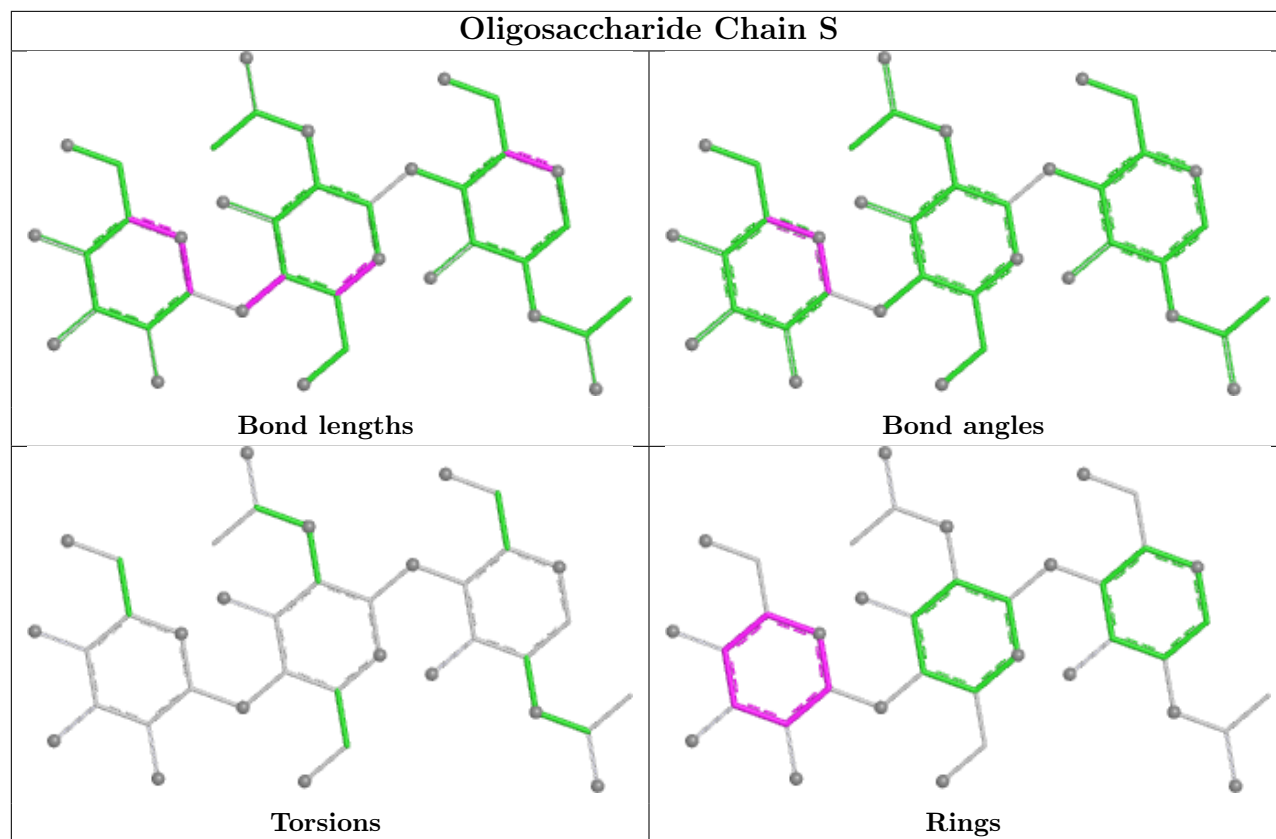


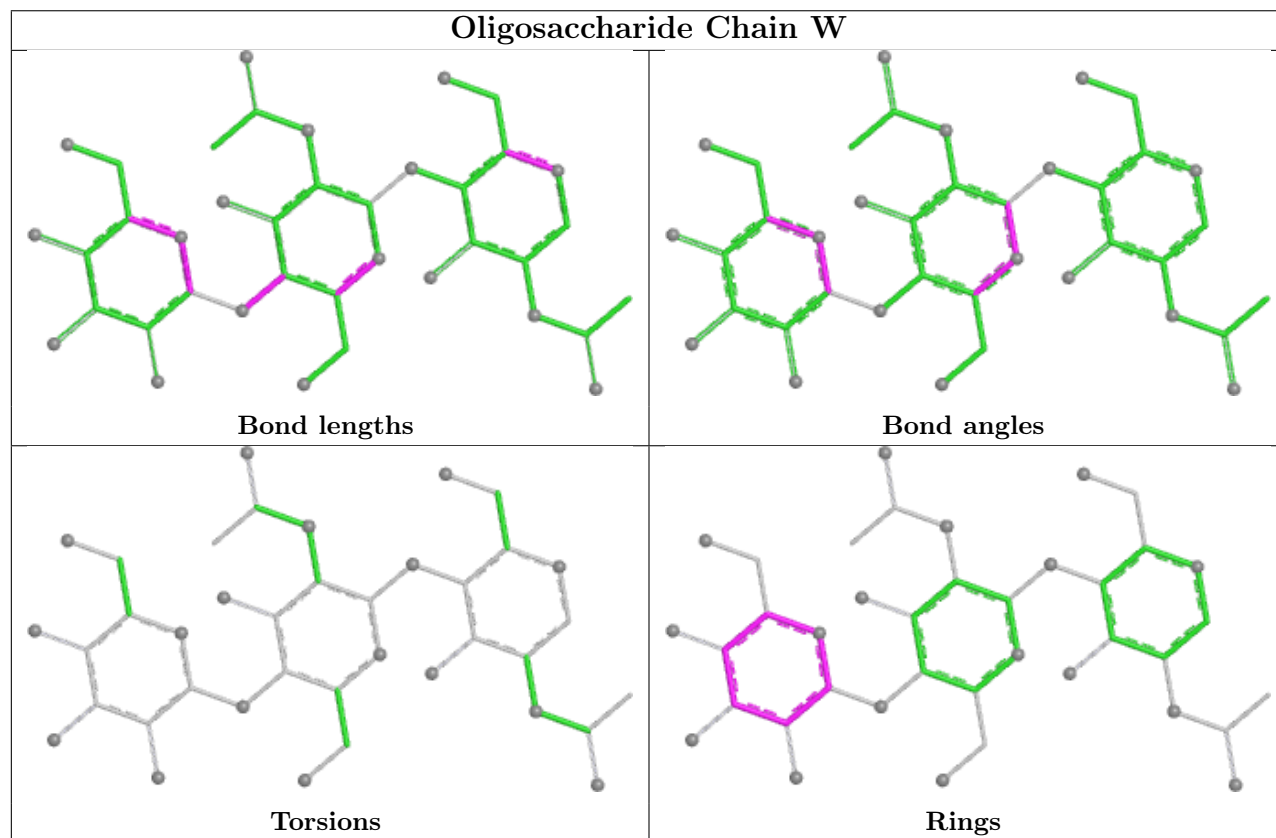
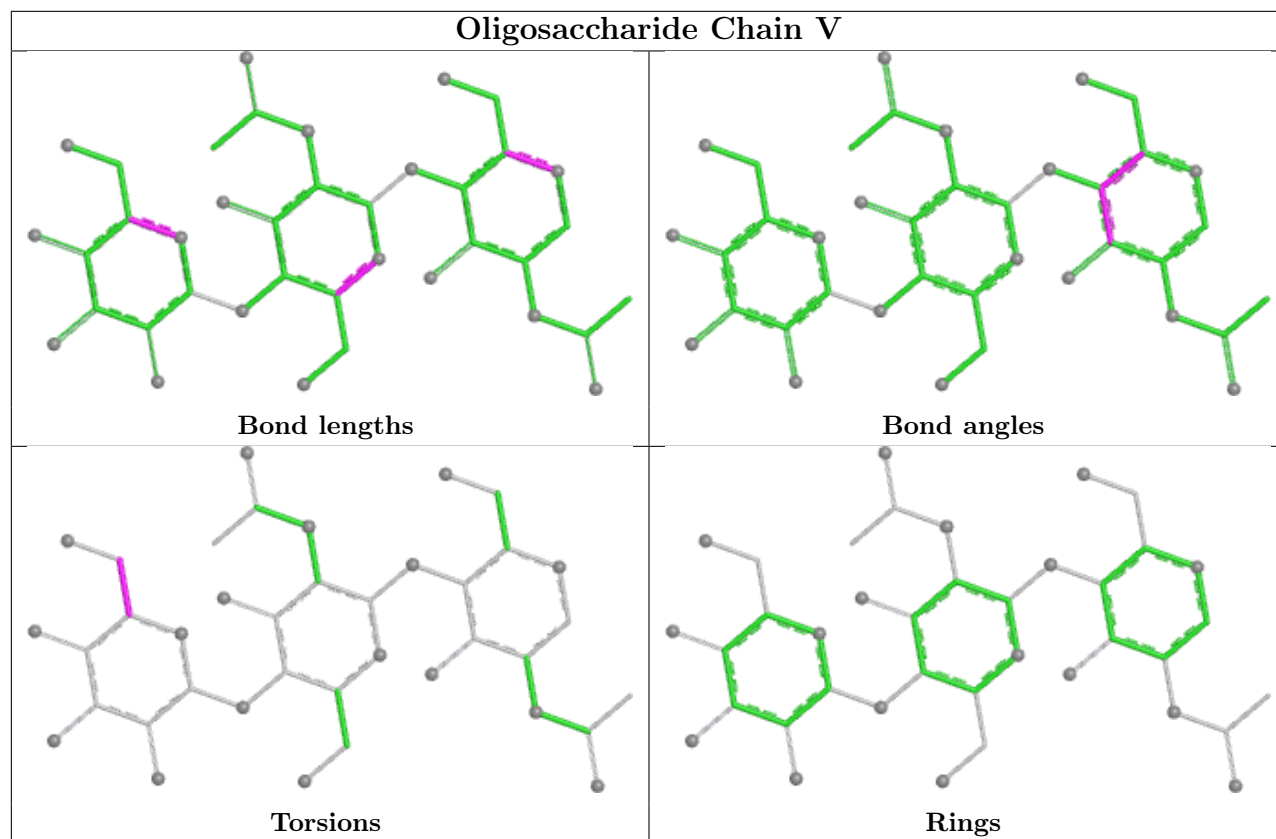


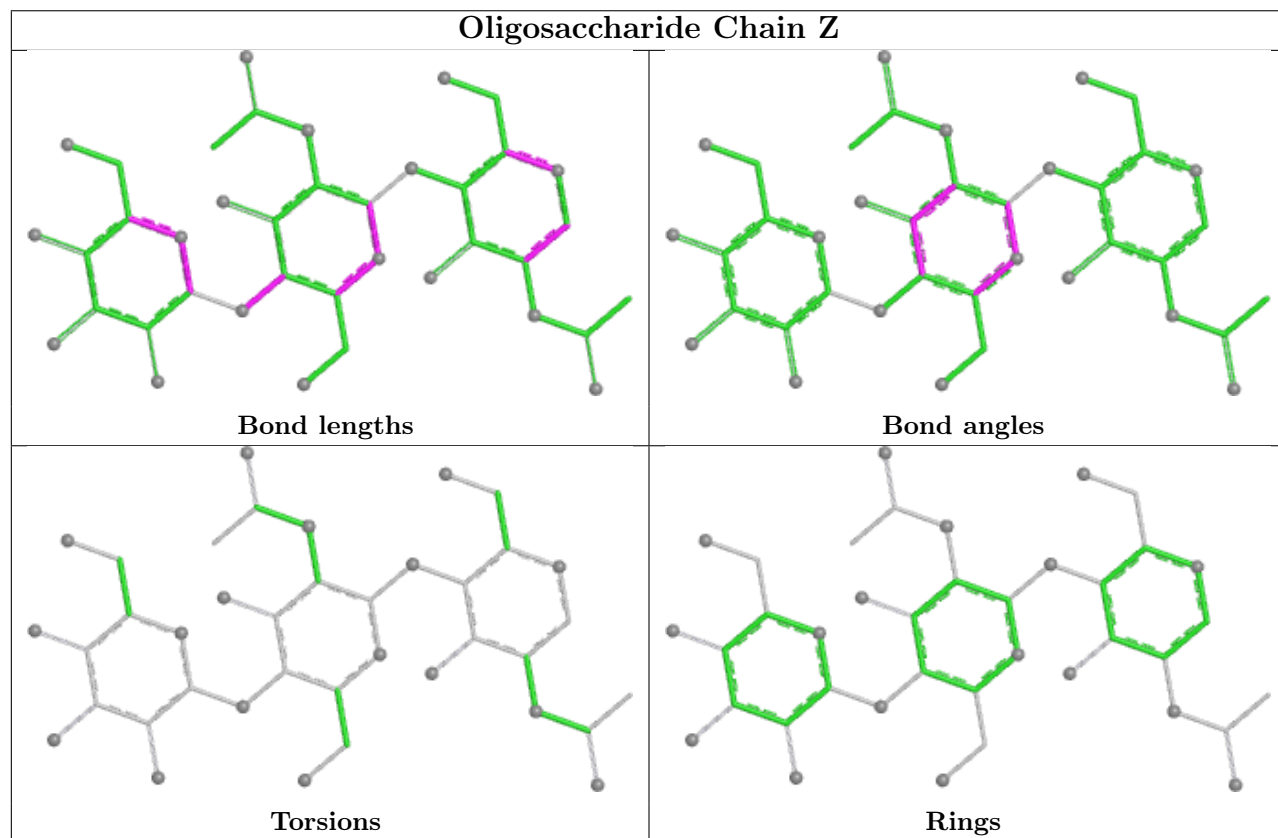
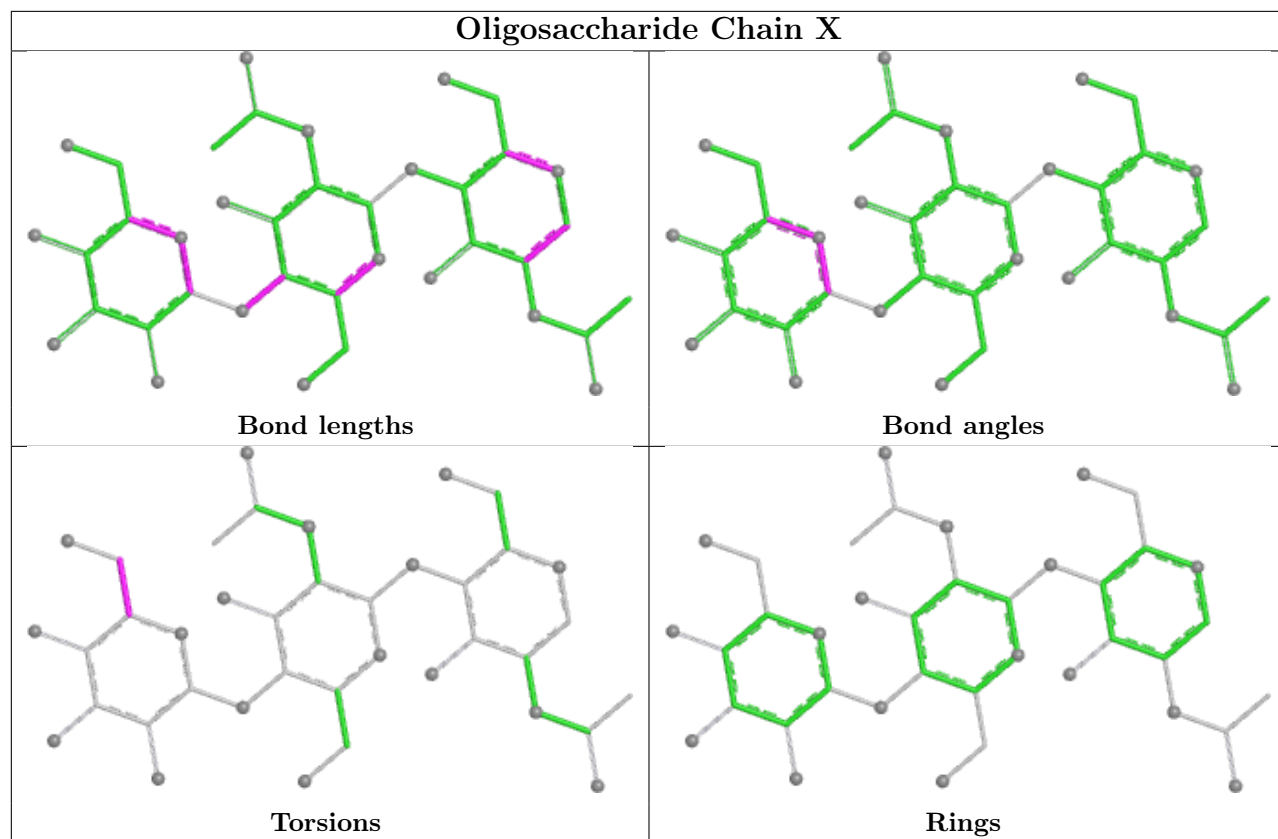


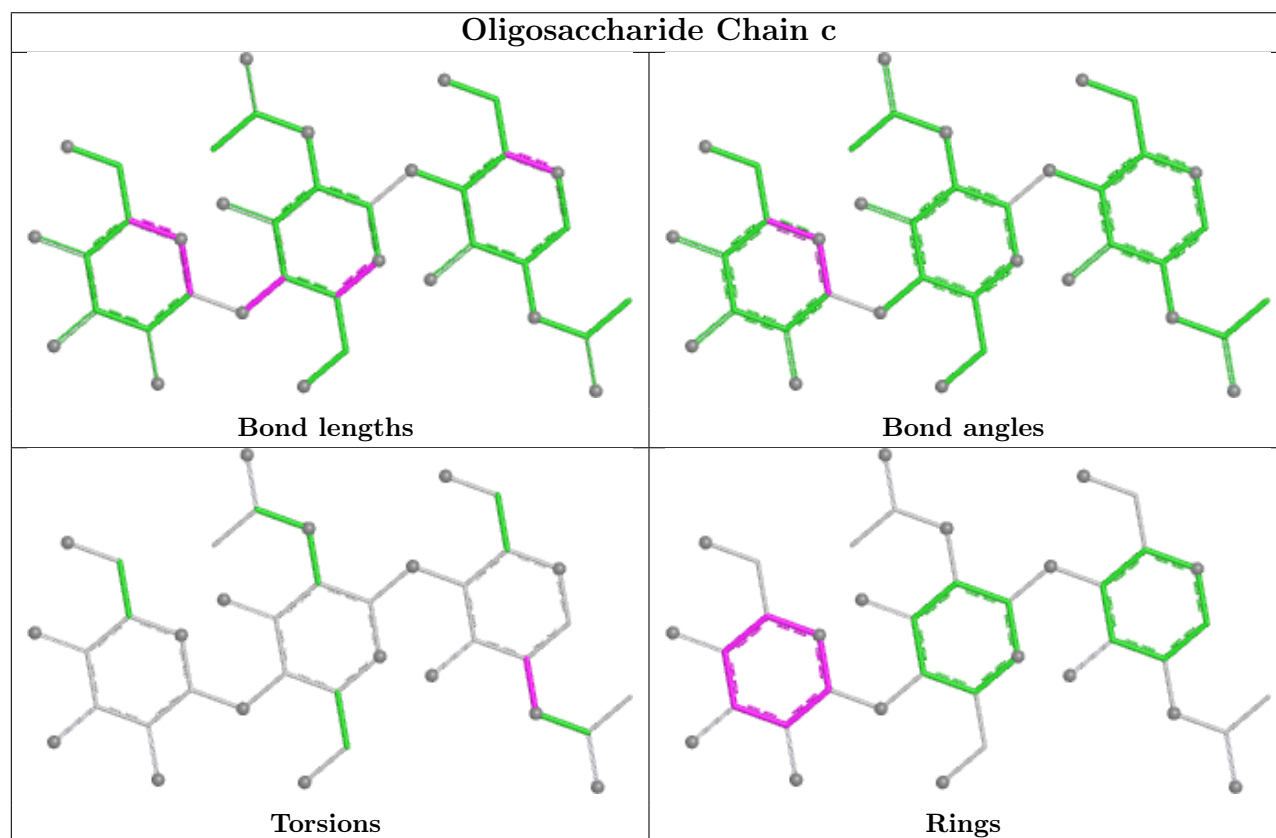
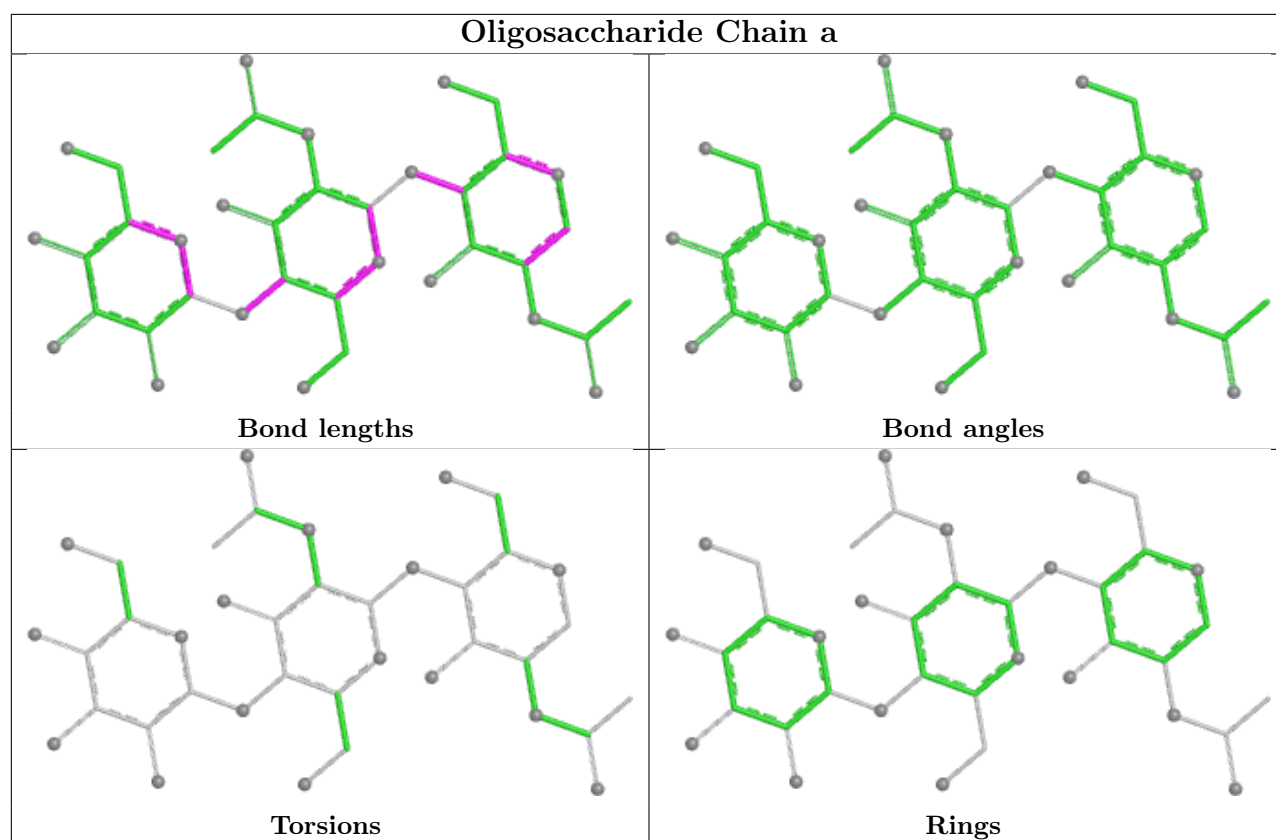


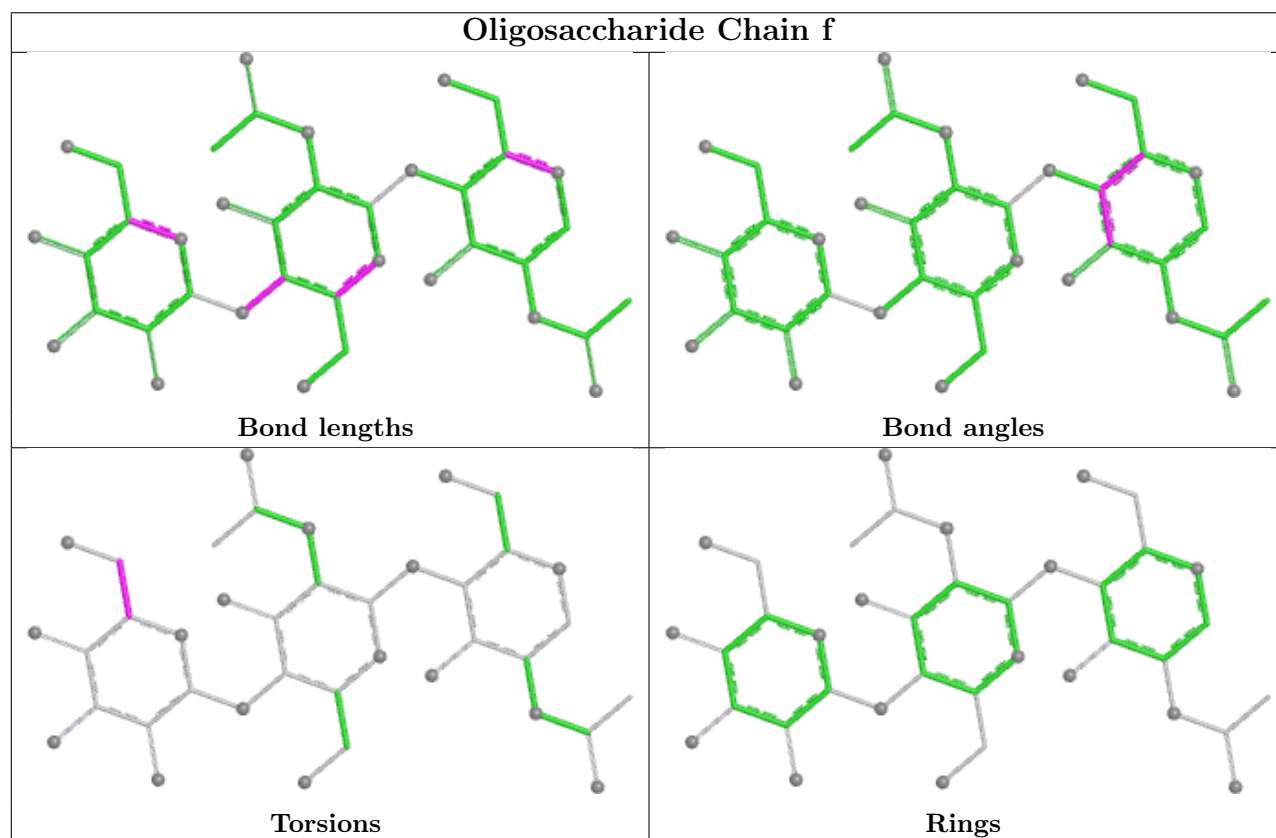
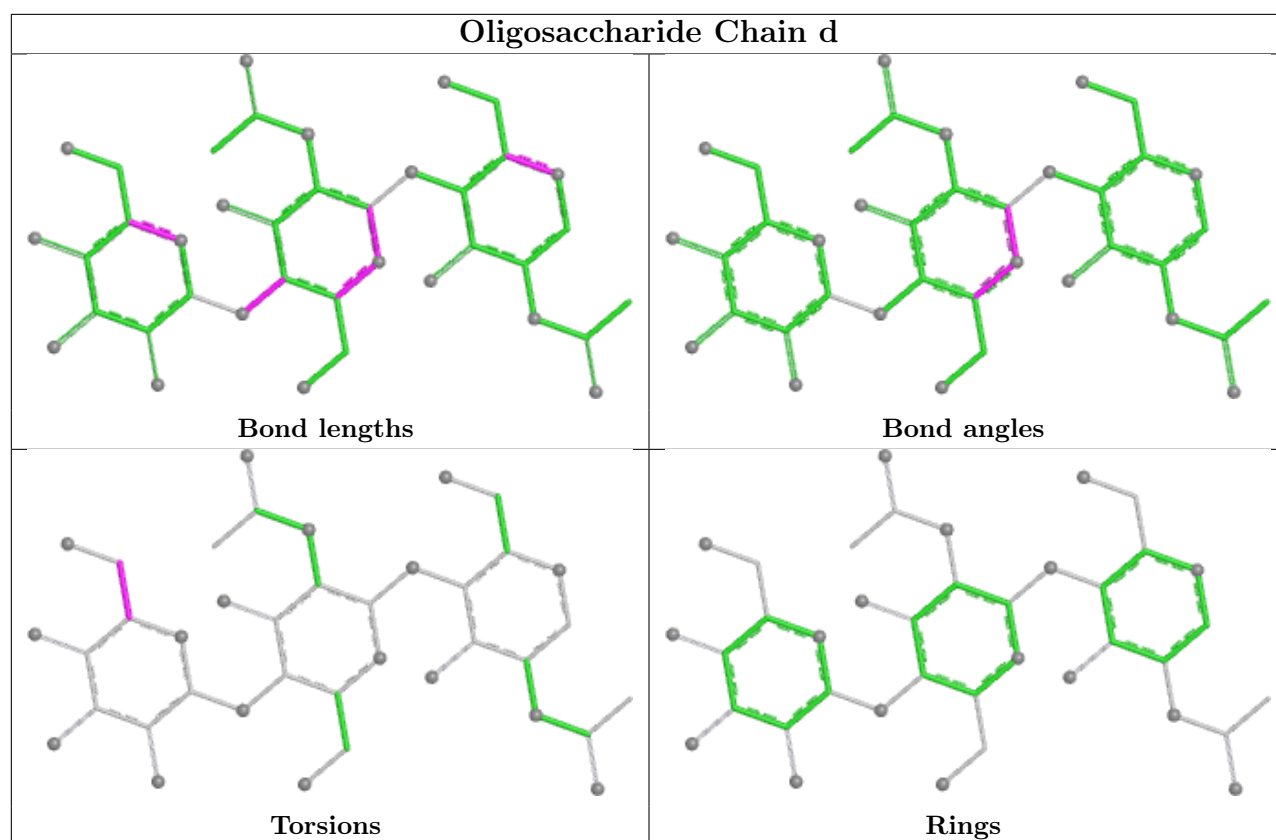


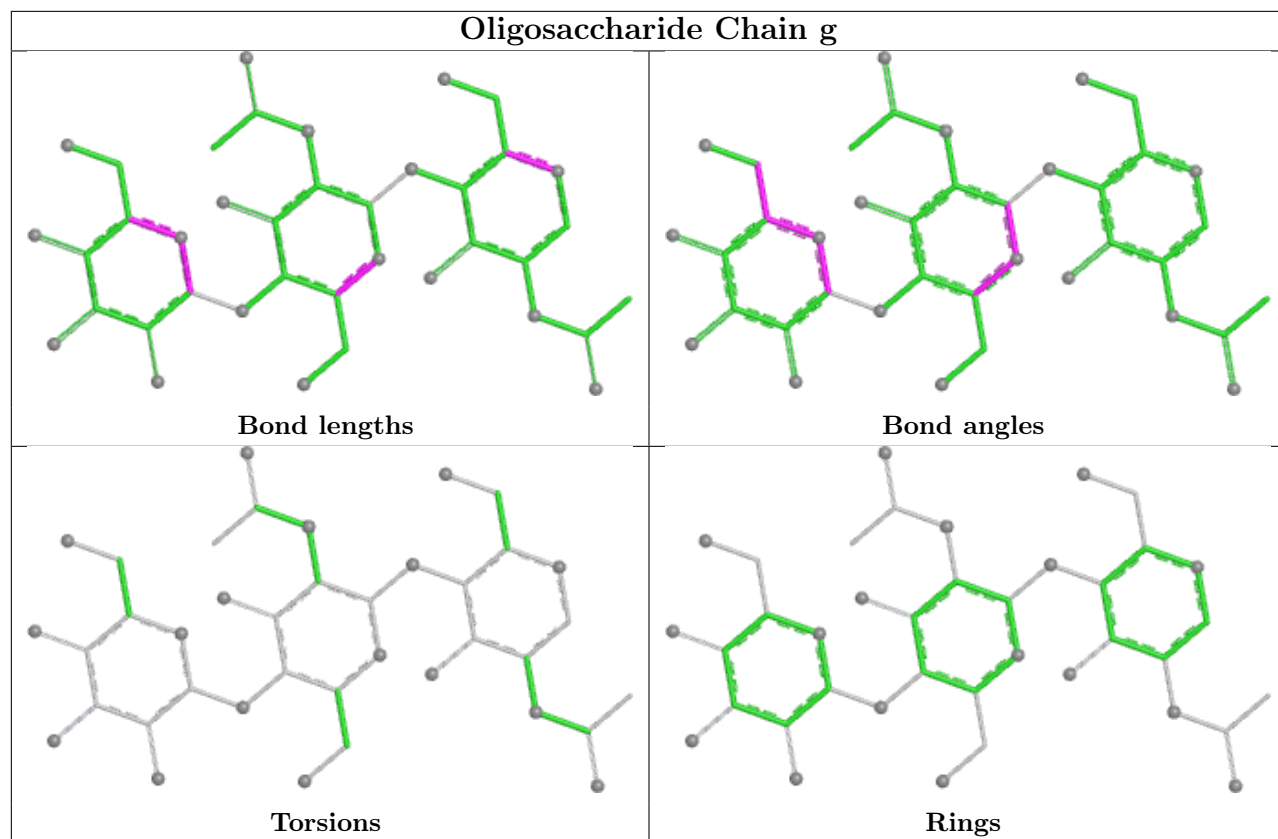


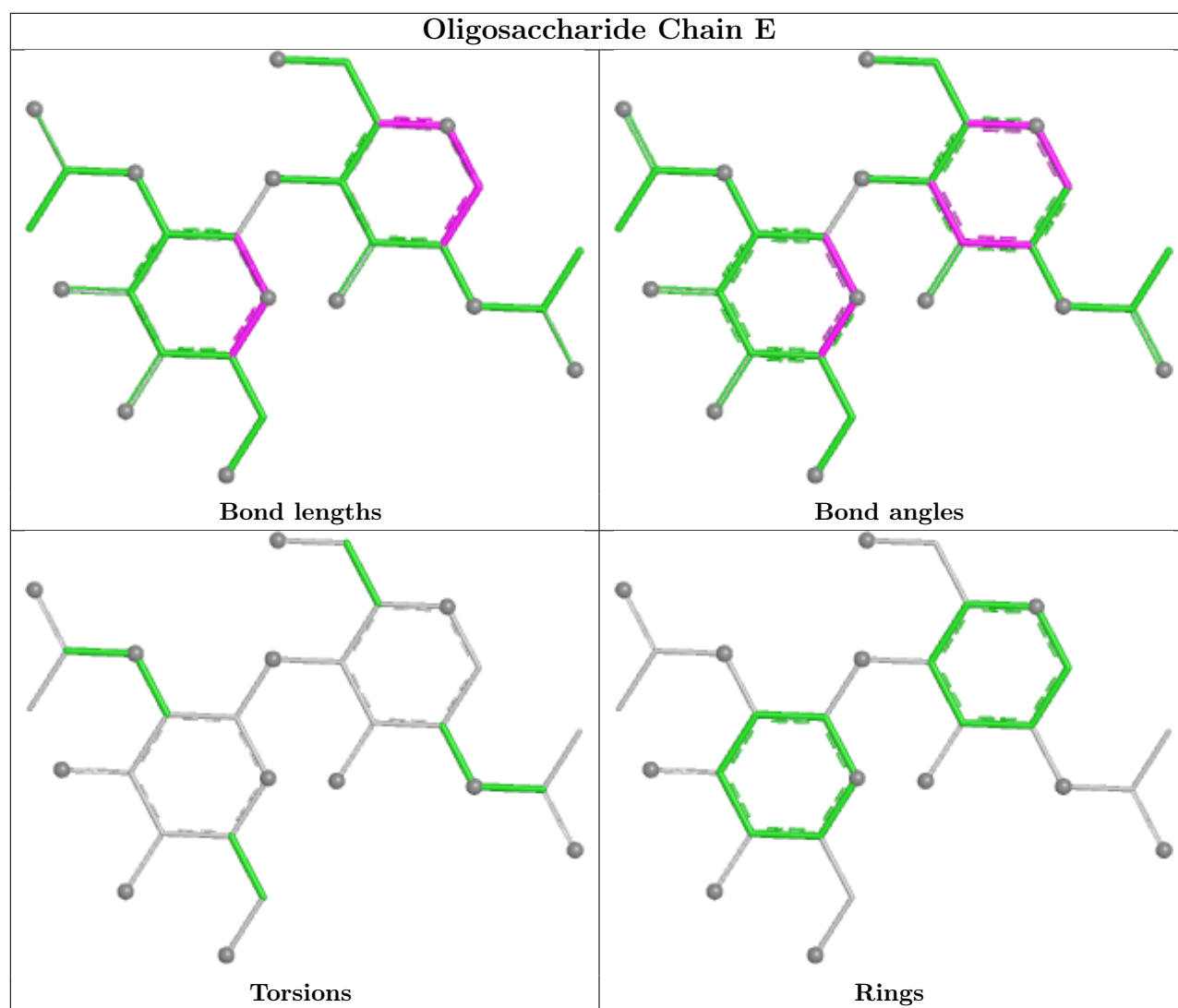


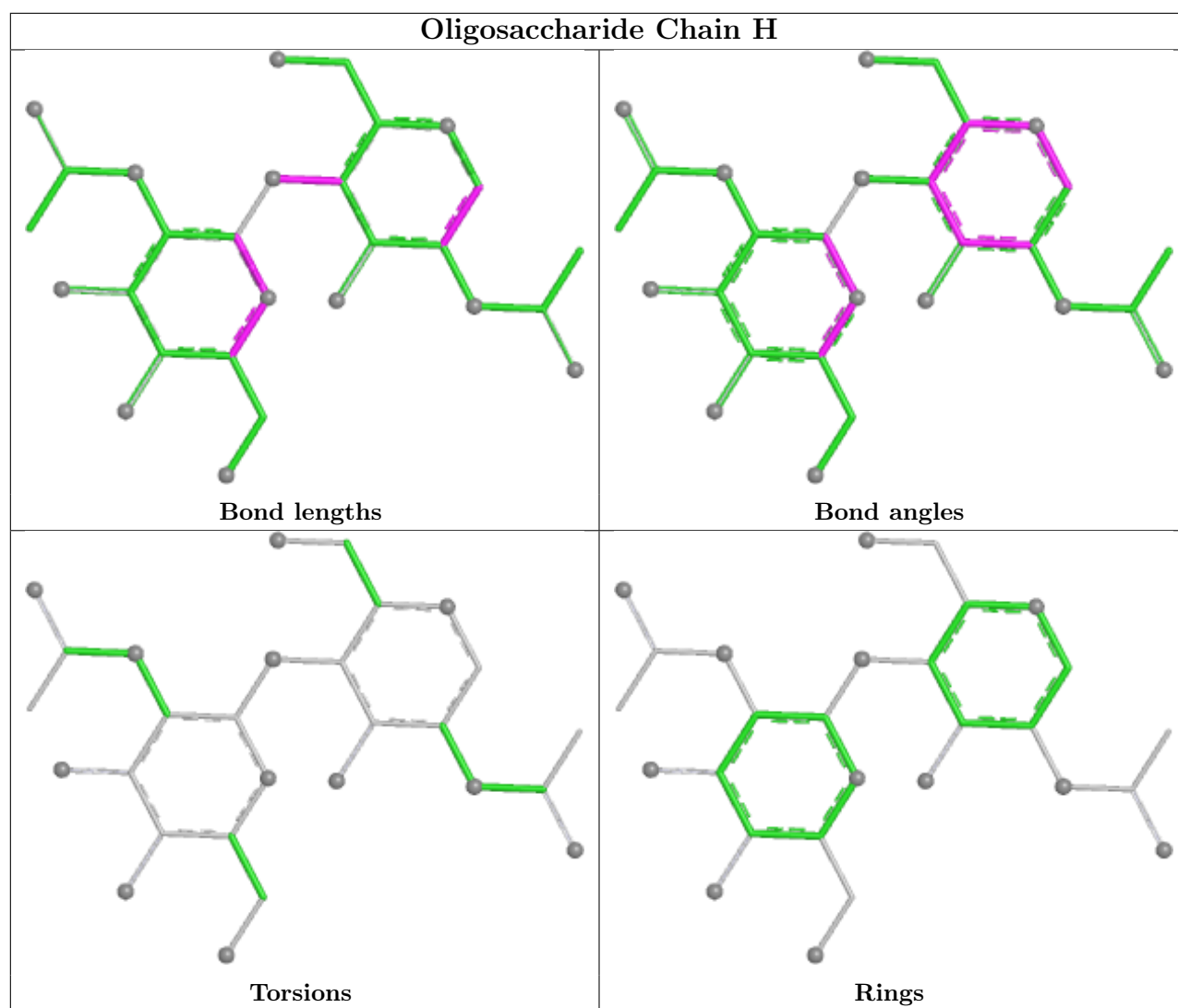


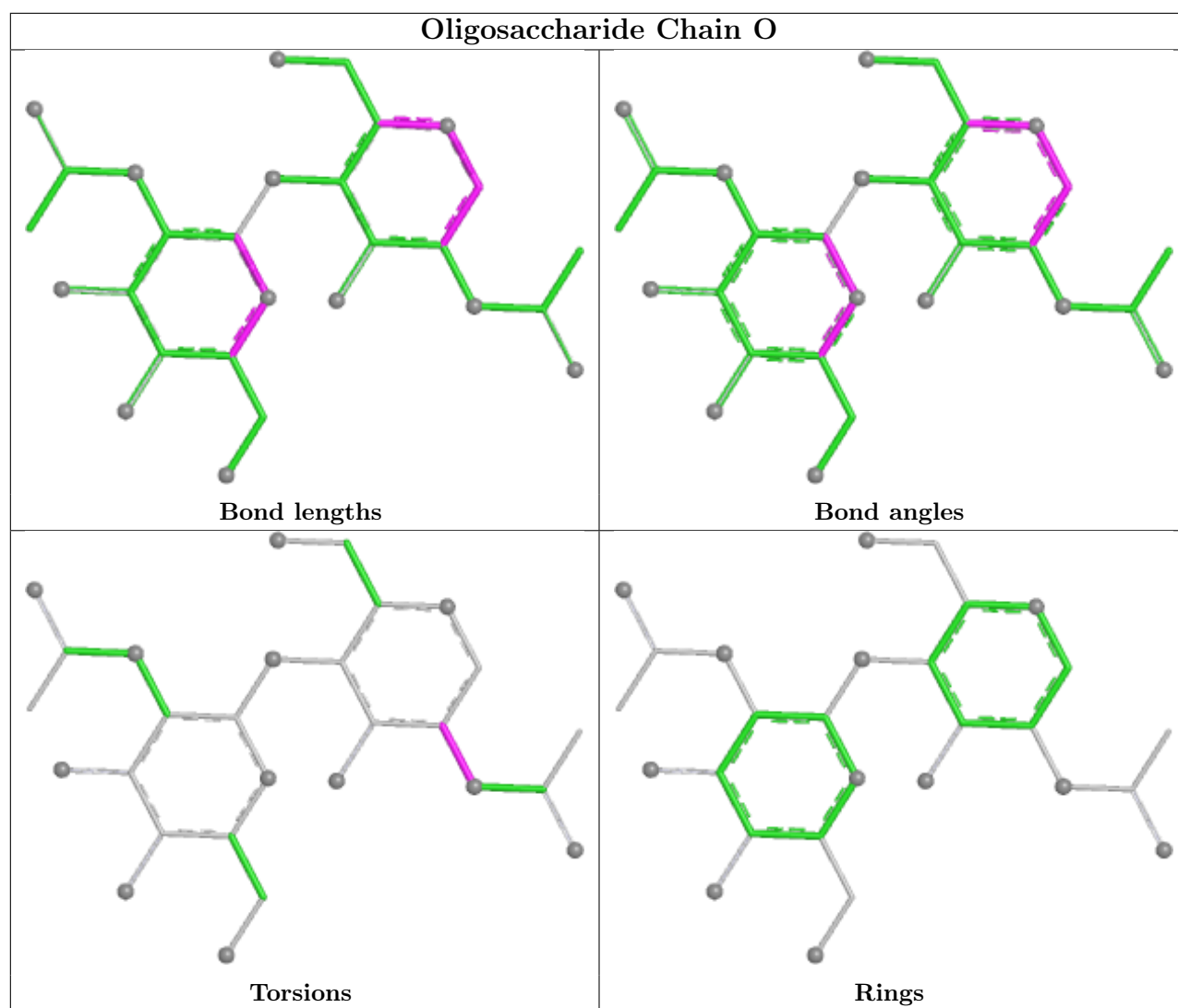


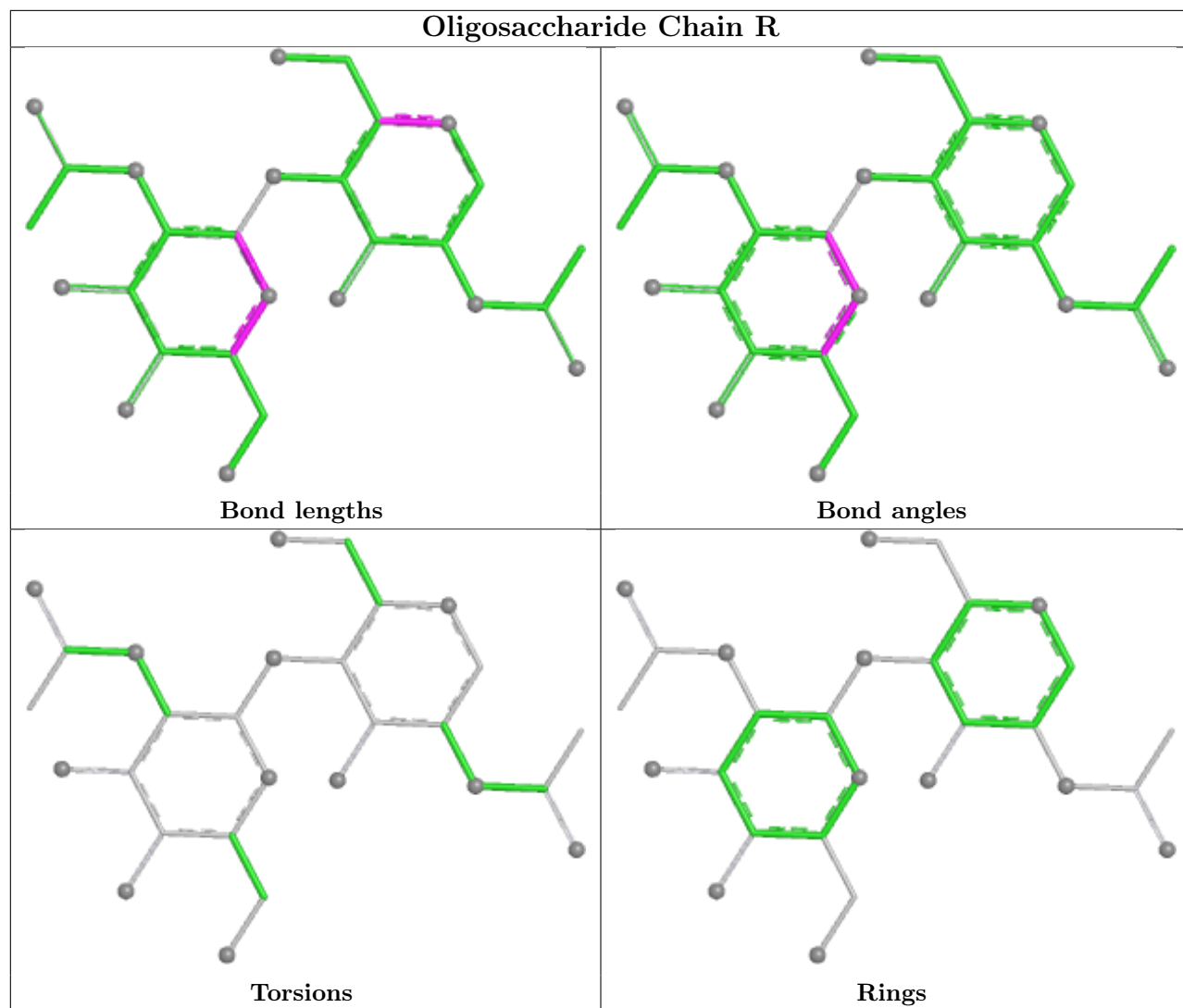


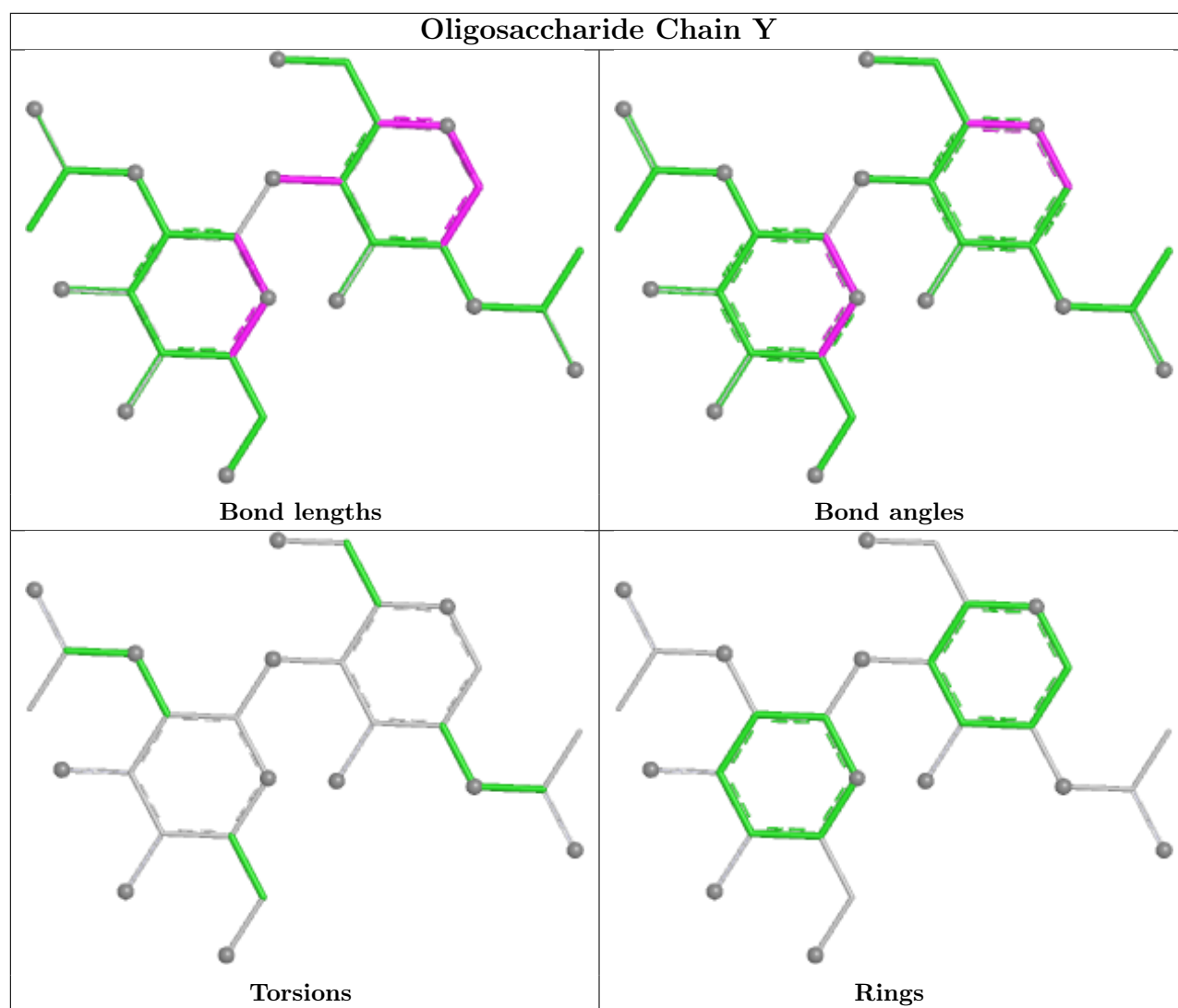


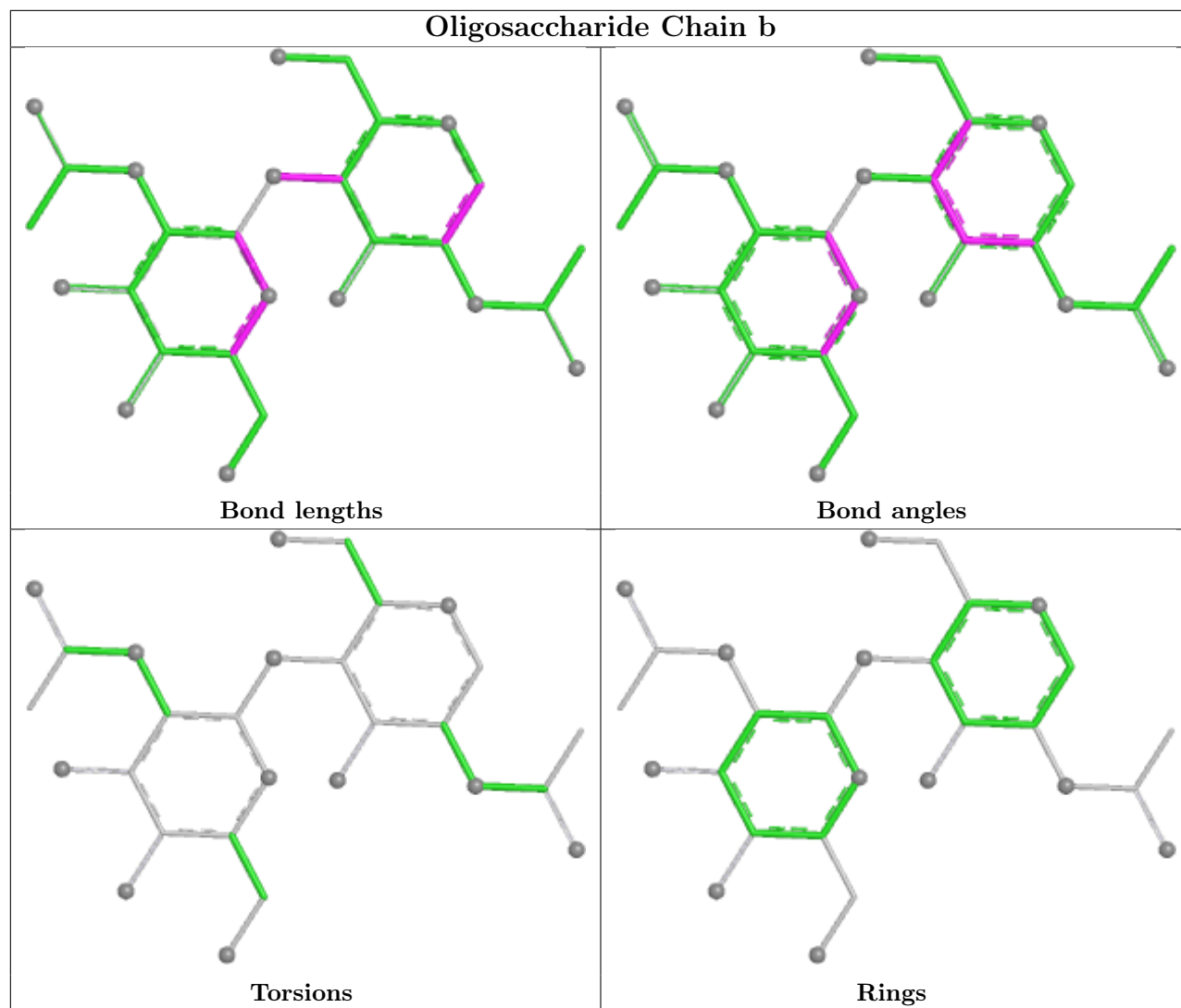


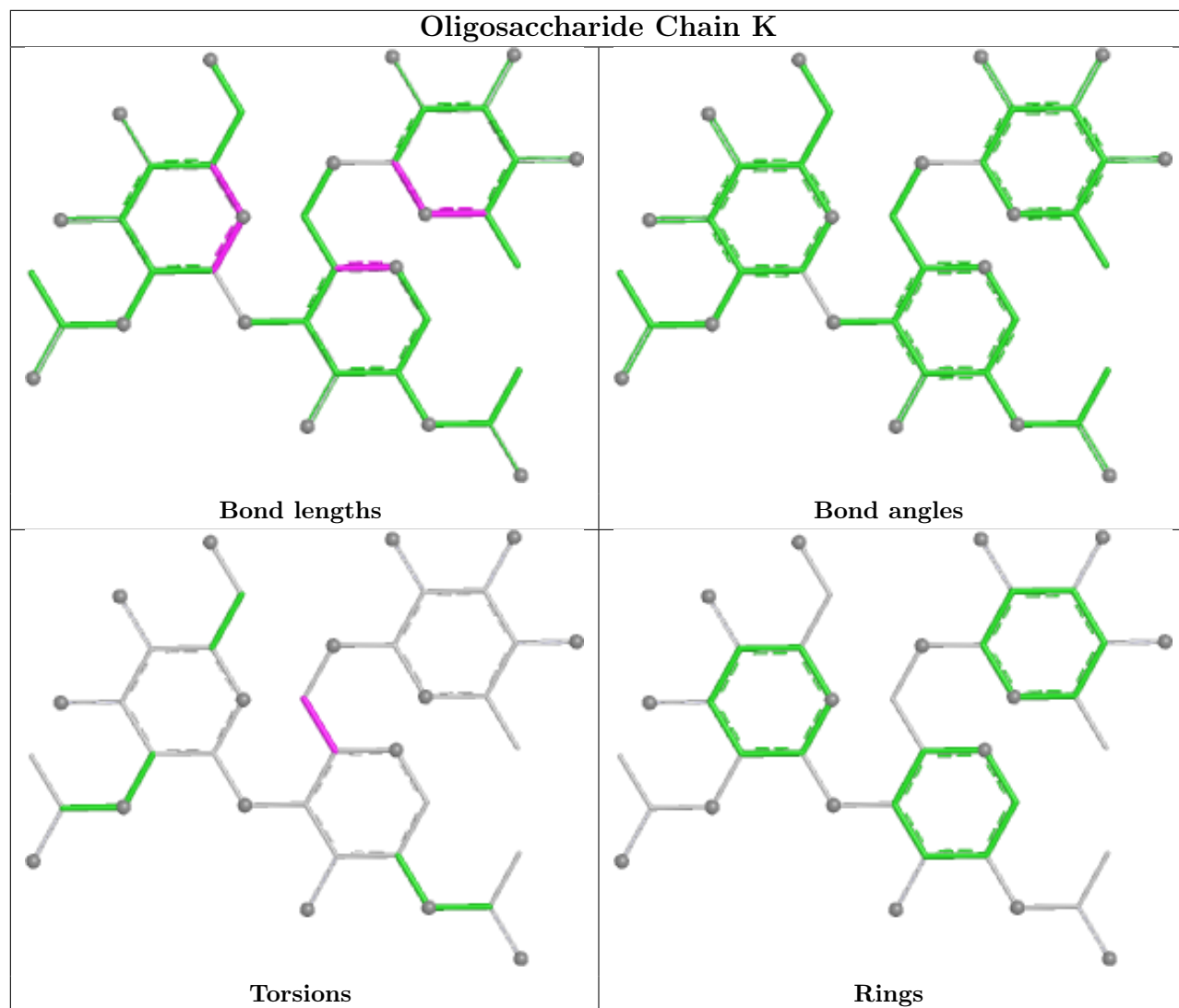


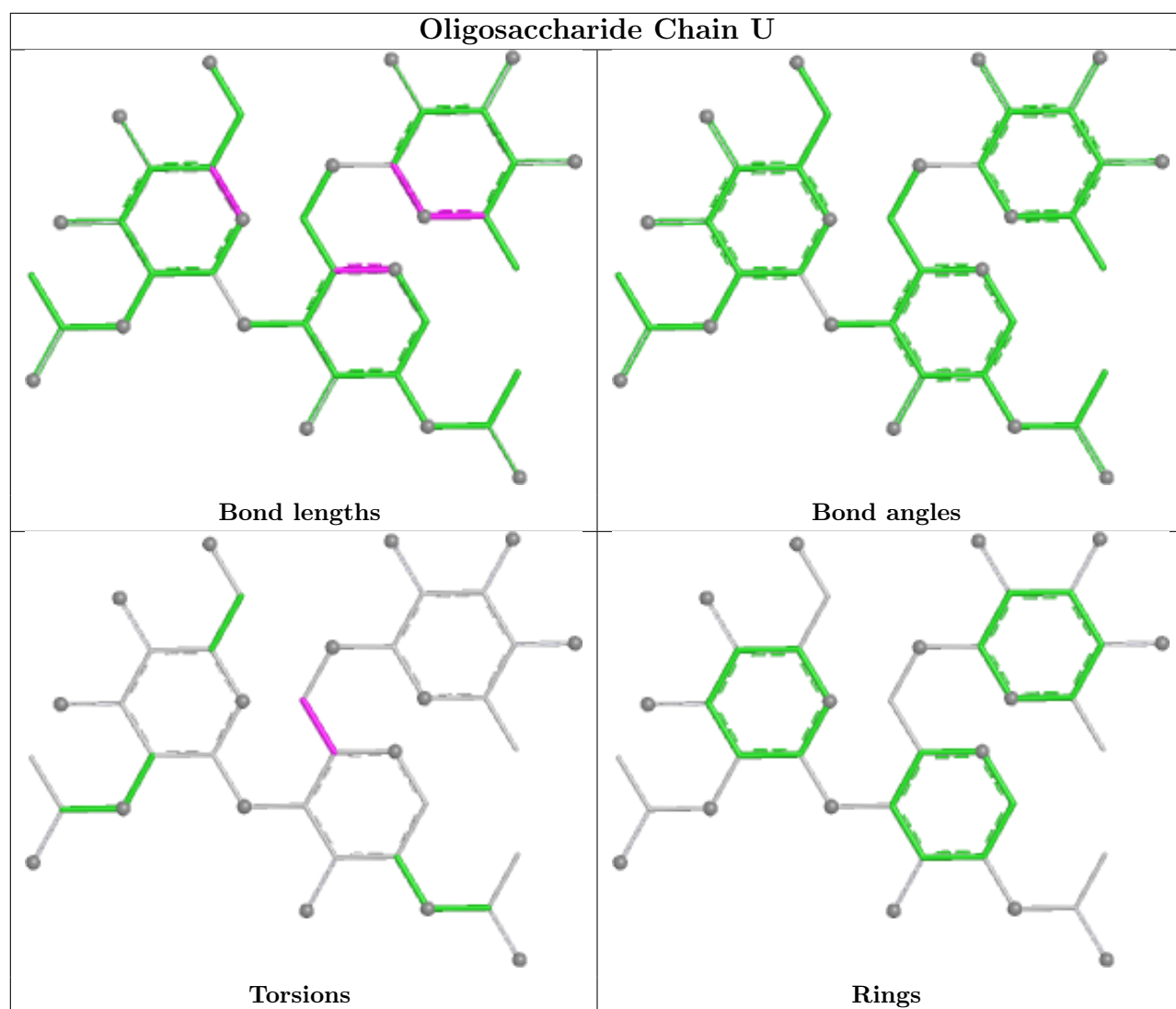


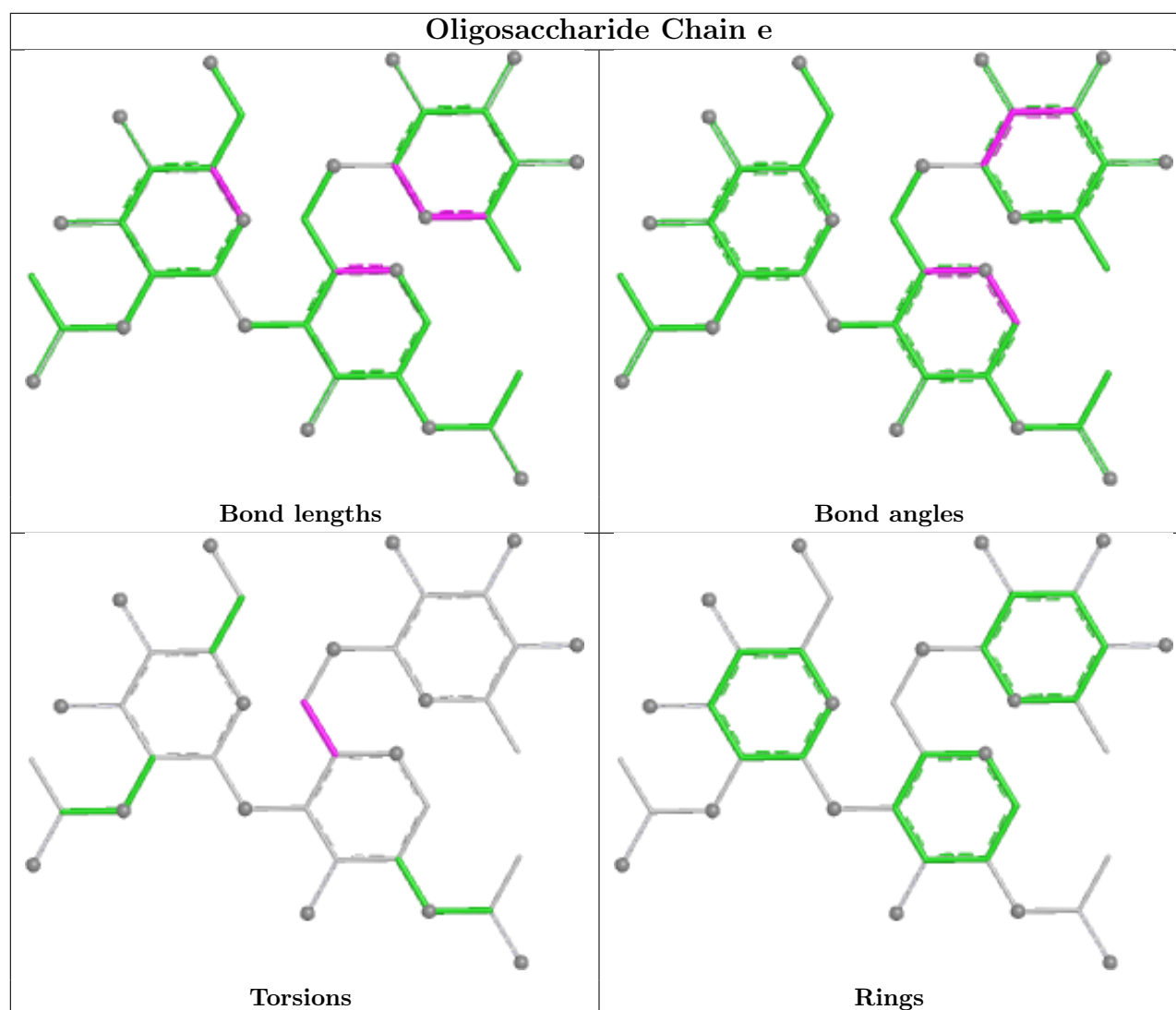












5.6 Ligand geometry [i](#)

21 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	B	1401	1	14,14,15	1.28	2 (14%)	17,19,21	0.83	0
5	NAG	B	1402	1	14,14,15	1.39	2 (14%)	17,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1403	1	14,14,15	1.28	2 (14%)	17,19,21	0.76	0
5	NAG	C	1405	1	14,14,15	1.30	2 (14%)	17,19,21	0.77	0
5	NAG	A	1405	1	14,14,15	1.30	2 (14%)	17,19,21	0.80	1 (5%)
5	NAG	C	1406	1	14,14,15	1.14	1 (7%)	17,19,21	0.62	0
5	NAG	B	1403	1	14,14,15	1.33	2 (14%)	17,19,21	0.81	0
5	NAG	C	1401	1	14,14,15	1.38	3 (21%)	17,19,21	0.95	0
5	NAG	B	1406	1	14,14,15	1.13	1 (7%)	17,19,21	0.63	0
5	NAG	C	1403	1	14,14,15	1.37	3 (21%)	17,19,21	0.87	1 (5%)
5	NAG	A	1407	1	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	B	1404	1	14,14,15	1.21	2 (14%)	17,19,21	0.70	0
5	NAG	C	1407	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	C	1404	1	14,14,15	1.26	2 (14%)	17,19,21	0.80	1 (5%)
5	NAG	A	1406	1	14,14,15	1.14	1 (7%)	17,19,21	0.67	0
5	NAG	B	1407	-	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	A	1401	1	14,14,15	1.36	3 (21%)	17,19,21	0.89	0
5	NAG	A	1404	1	14,14,15	1.22	2 (14%)	17,19,21	0.73	1 (5%)
5	NAG	A	1402	1	14,14,15	1.34	2 (14%)	17,19,21	0.74	0
5	NAG	B	1405	1	14,14,15	1.28	2 (14%)	17,19,21	0.84	0
5	NAG	C	1402	1	14,14,15	1.40	2 (14%)	17,19,21	0.80	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	B	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1401	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1407	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	1	-	0/6/23/26	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1401	NAG	O5-C5	3.17	1.49	1.43
5	A	1401	NAG	O5-C5	3.08	1.49	1.43
5	B	1401	NAG	O5-C5	2.91	1.49	1.43
5	A	1405	NAG	O5-C5	2.90	1.49	1.43
5	C	1405	NAG	O5-C5	2.87	1.49	1.43
5	B	1405	NAG	O5-C5	2.86	1.49	1.43
5	A	1406	NAG	O5-C5	2.79	1.48	1.43
5	B	1402	NAG	O5-C5	2.78	1.48	1.43
5	C	1402	NAG	O5-C5	2.78	1.48	1.43
5	B	1403	NAG	O5-C5	2.76	1.48	1.43
5	C	1406	NAG	O5-C5	2.76	1.48	1.43
5	C	1403	NAG	O5-C5	2.74	1.48	1.43
5	B	1406	NAG	O5-C5	2.70	1.48	1.43
5	A	1402	NAG	O5-C5	2.67	1.48	1.43
5	C	1402	NAG	C1-C2	2.63	1.55	1.52
5	B	1402	NAG	C1-C2	2.62	1.55	1.52
5	A	1403	NAG	O5-C5	2.56	1.48	1.43
5	A	1402	NAG	C1-C2	2.56	1.55	1.52
5	A	1404	NAG	O5-C5	2.51	1.48	1.43
5	C	1403	NAG	C1-C2	2.51	1.55	1.52
5	C	1404	NAG	O5-C5	2.46	1.48	1.43
5	B	1404	NAG	O5-C5	2.43	1.48	1.43
5	C	1404	NAG	C1-C2	2.33	1.55	1.52
5	B	1403	NAG	C1-C2	2.31	1.55	1.52
5	A	1403	NAG	C1-C2	2.29	1.55	1.52
5	A	1401	NAG	C1-C2	2.17	1.55	1.52
5	C	1401	NAG	O5-C1	2.15	1.47	1.43
5	C	1405	NAG	C1-C2	2.12	1.55	1.52
5	C	1401	NAG	C1-C2	2.10	1.55	1.52
5	A	1401	NAG	O5-C1	2.05	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1401	NAG	C1-C2	2.05	1.55	1.52
5	B	1405	NAG	C1-C2	2.04	1.55	1.52
5	A	1405	NAG	C1-C2	2.04	1.55	1.52
5	C	1403	NAG	O5-C1	2.03	1.47	1.43
5	B	1404	NAG	C1-C2	2.02	1.55	1.52
5	A	1404	NAG	C1-C2	2.01	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1405	NAG	C1-O5-C5	2.14	115.06	112.19
5	C	1404	NAG	C1-O5-C5	2.09	114.99	112.19
5	C	1403	NAG	C1-O5-C5	2.08	114.98	112.19
5	A	1404	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1407	NAG	O5-C5-C6-O6
5	B	1401	NAG	C1-C2-N2-C7
5	C	1401	NAG	C1-C2-N2-C7
5	A	1407	NAG	O5-C5-C6-O6

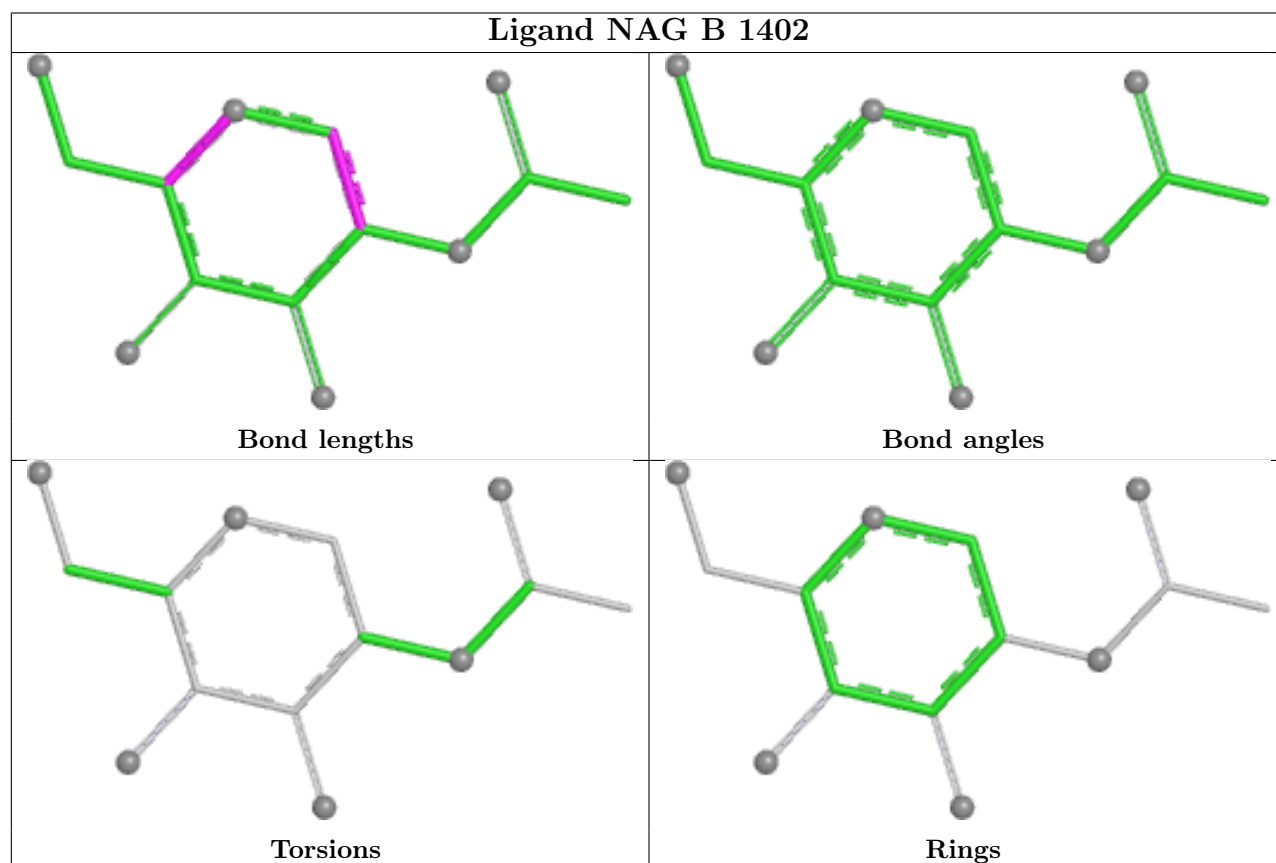
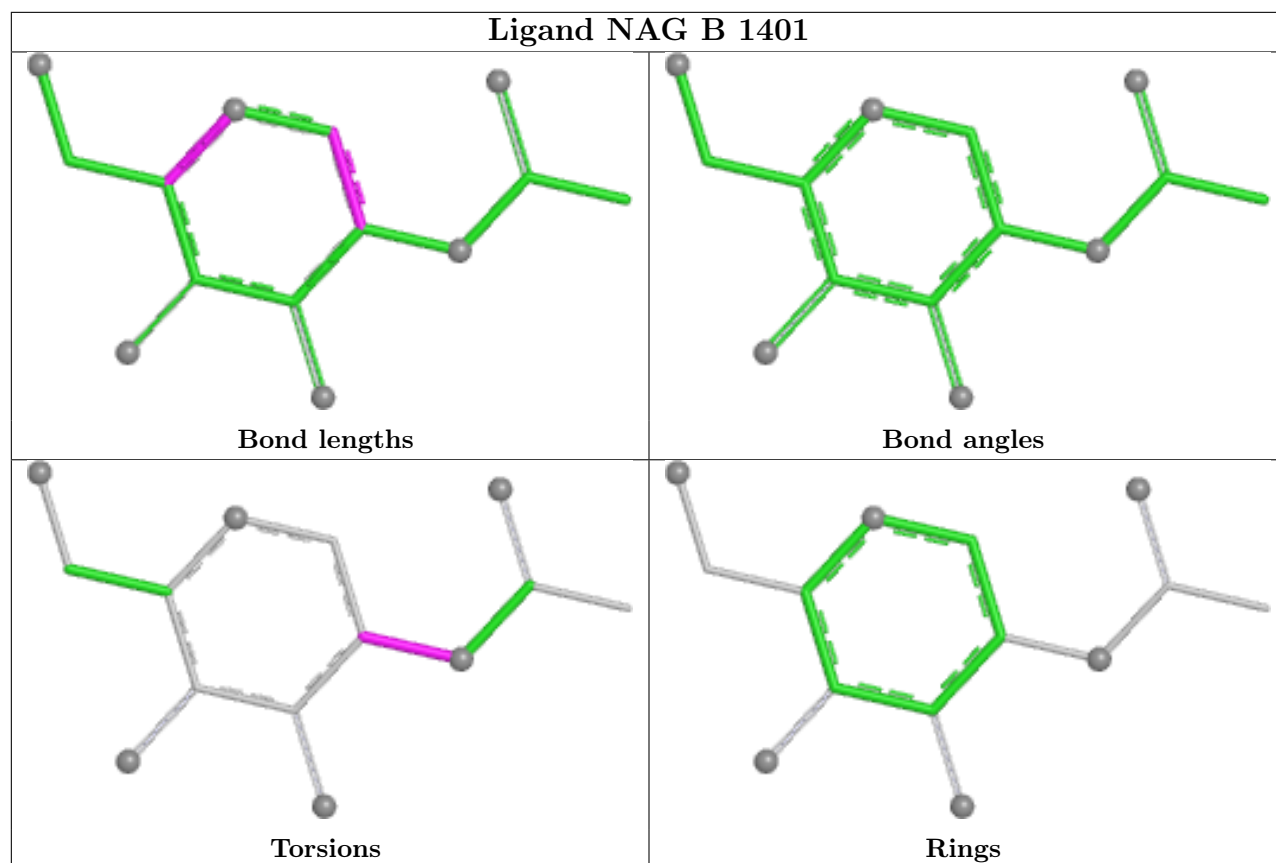
There are no ring outliers.

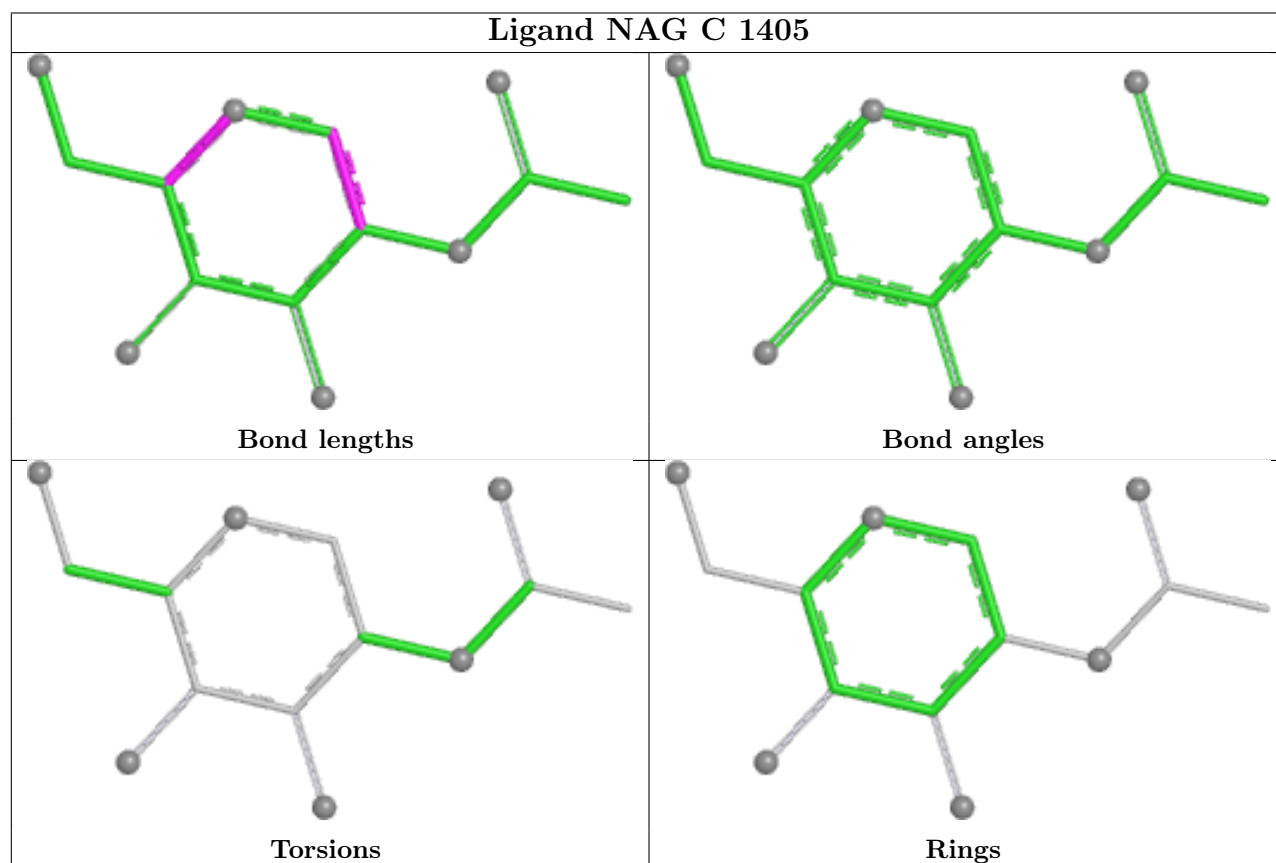
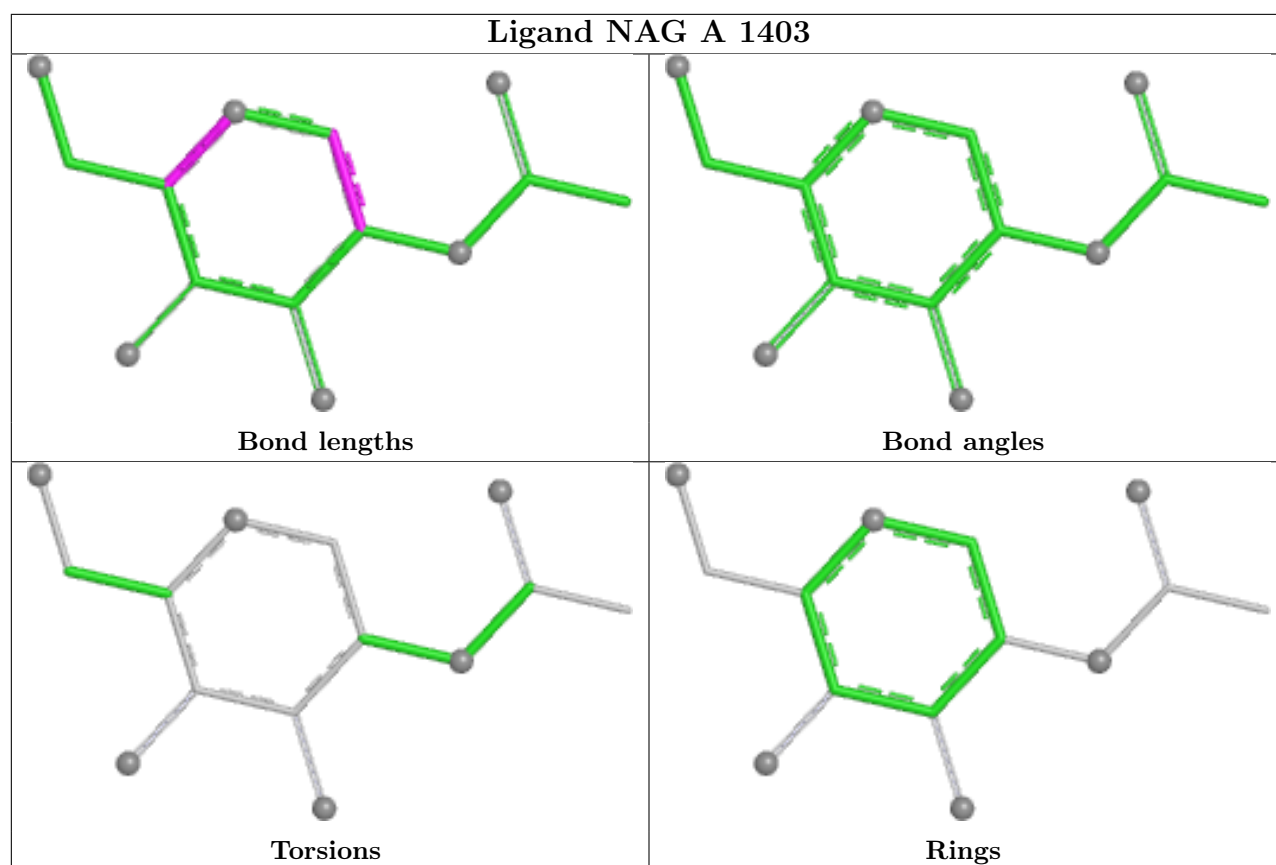
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1407	NAG	2	0

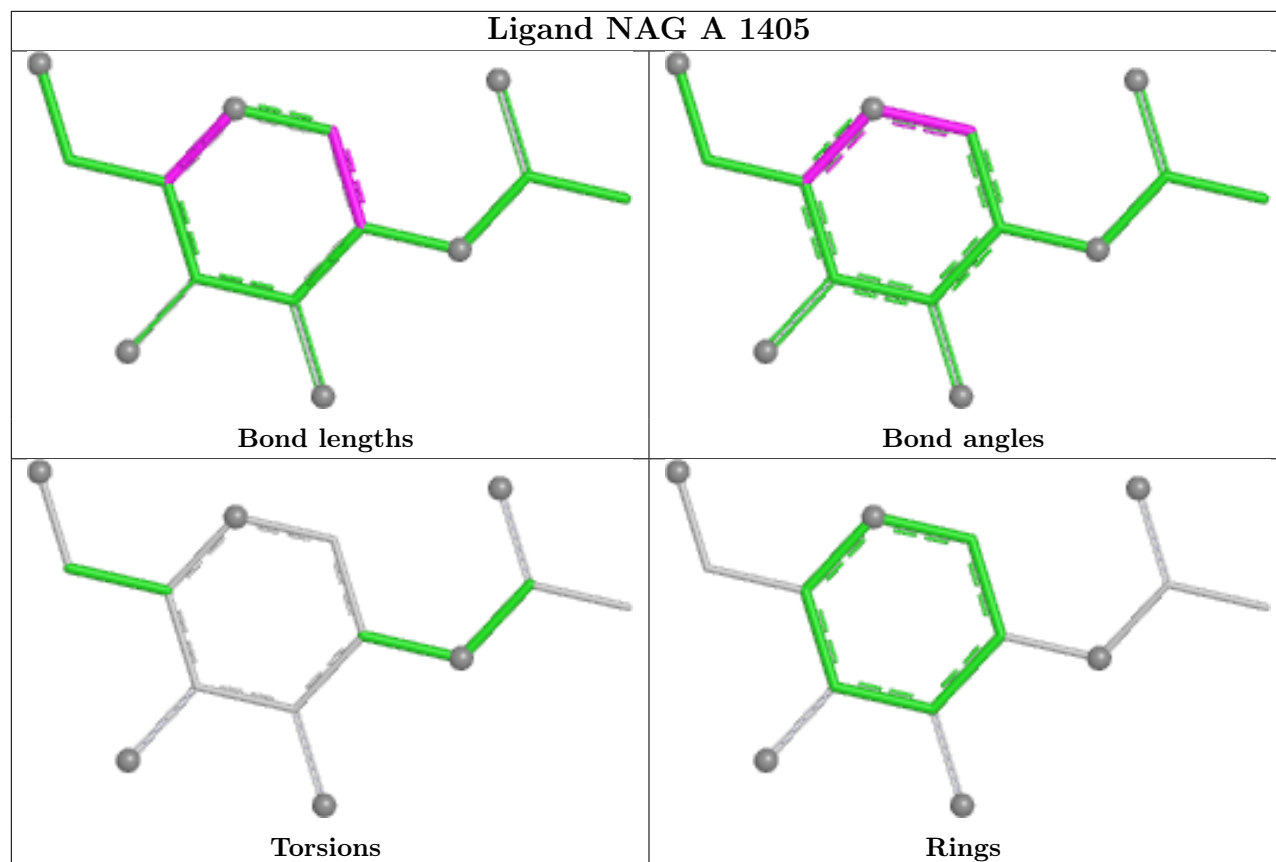
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

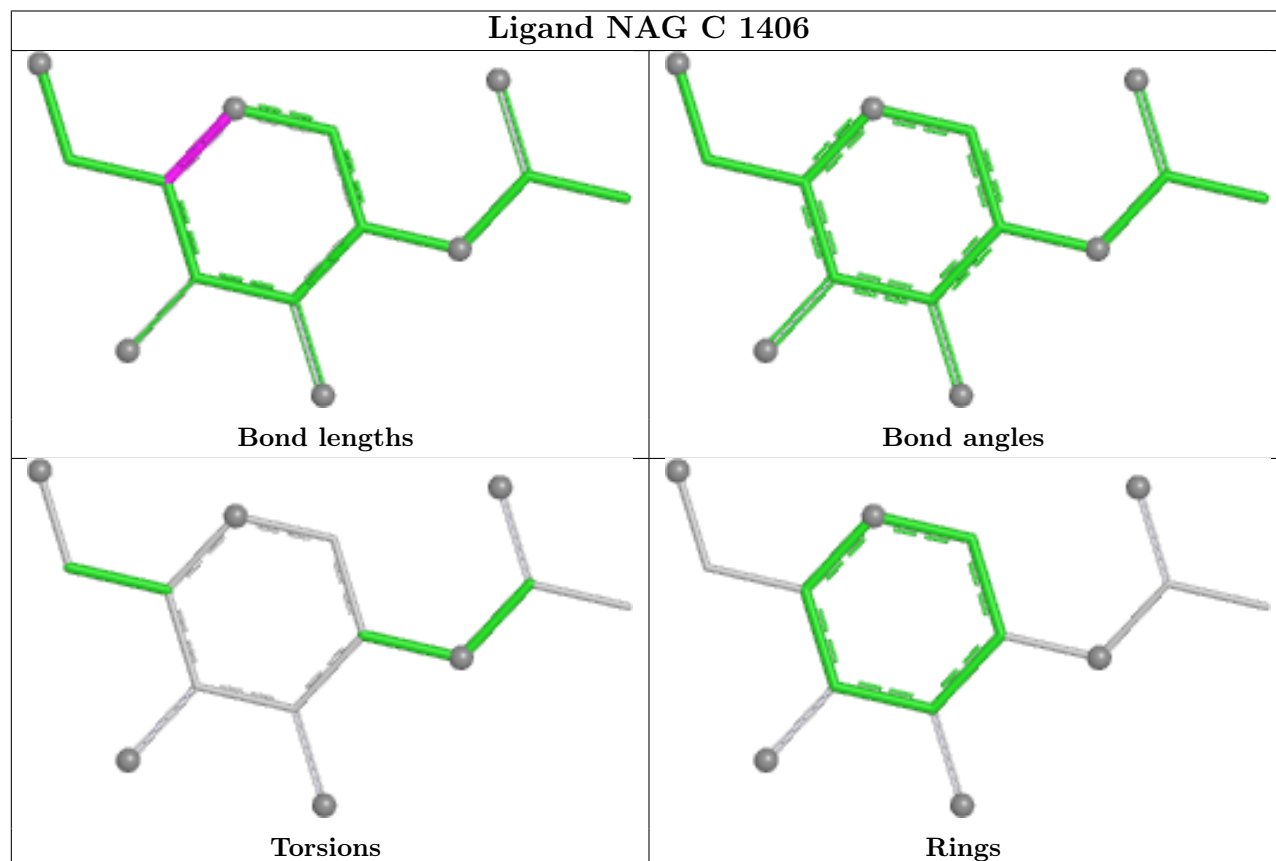


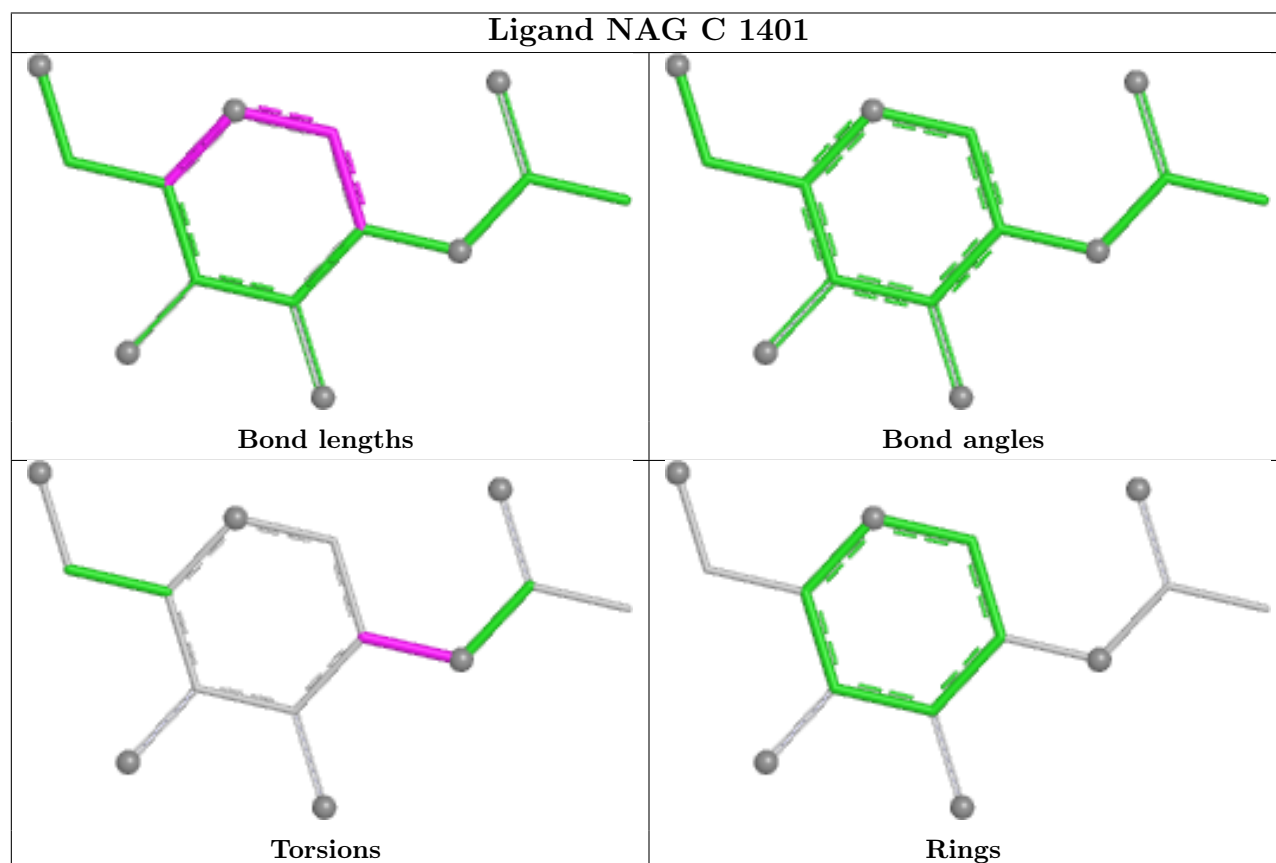
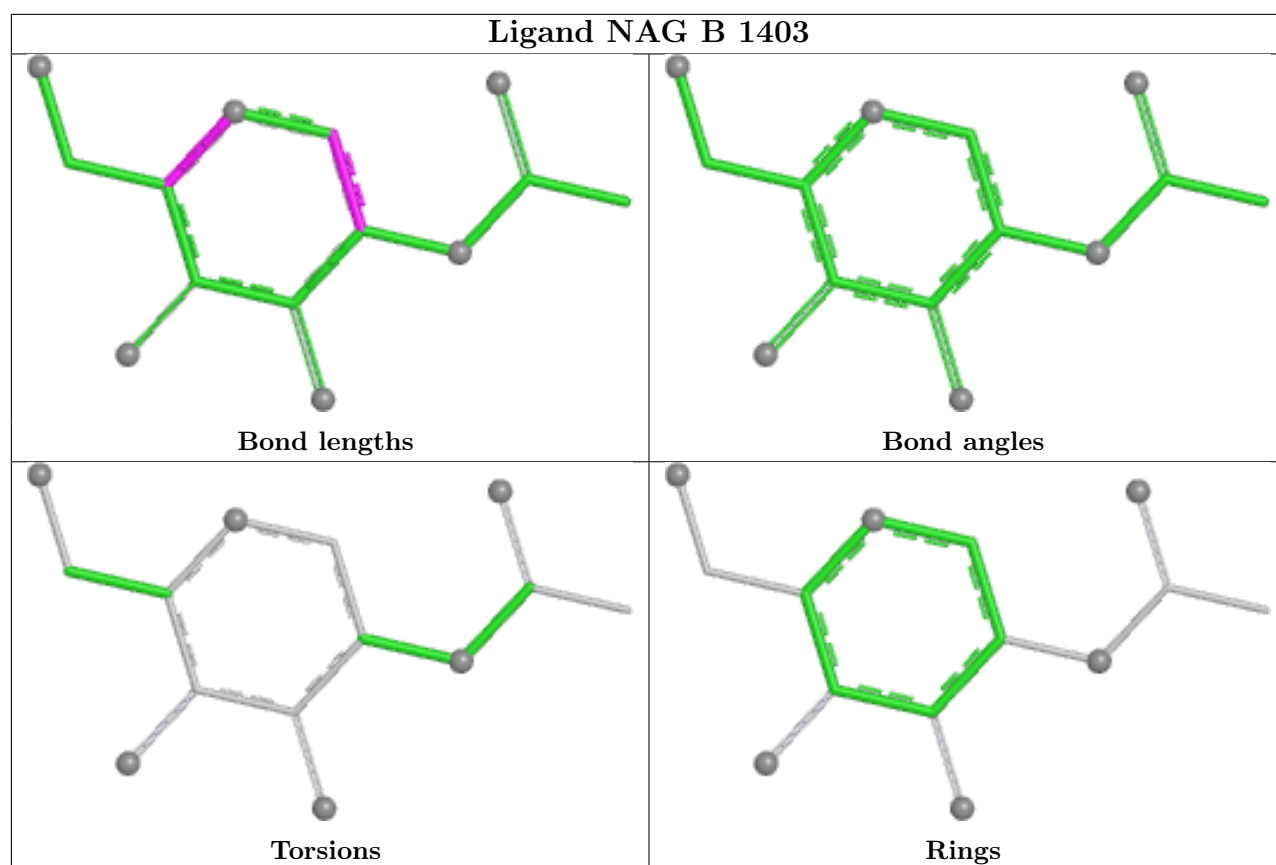


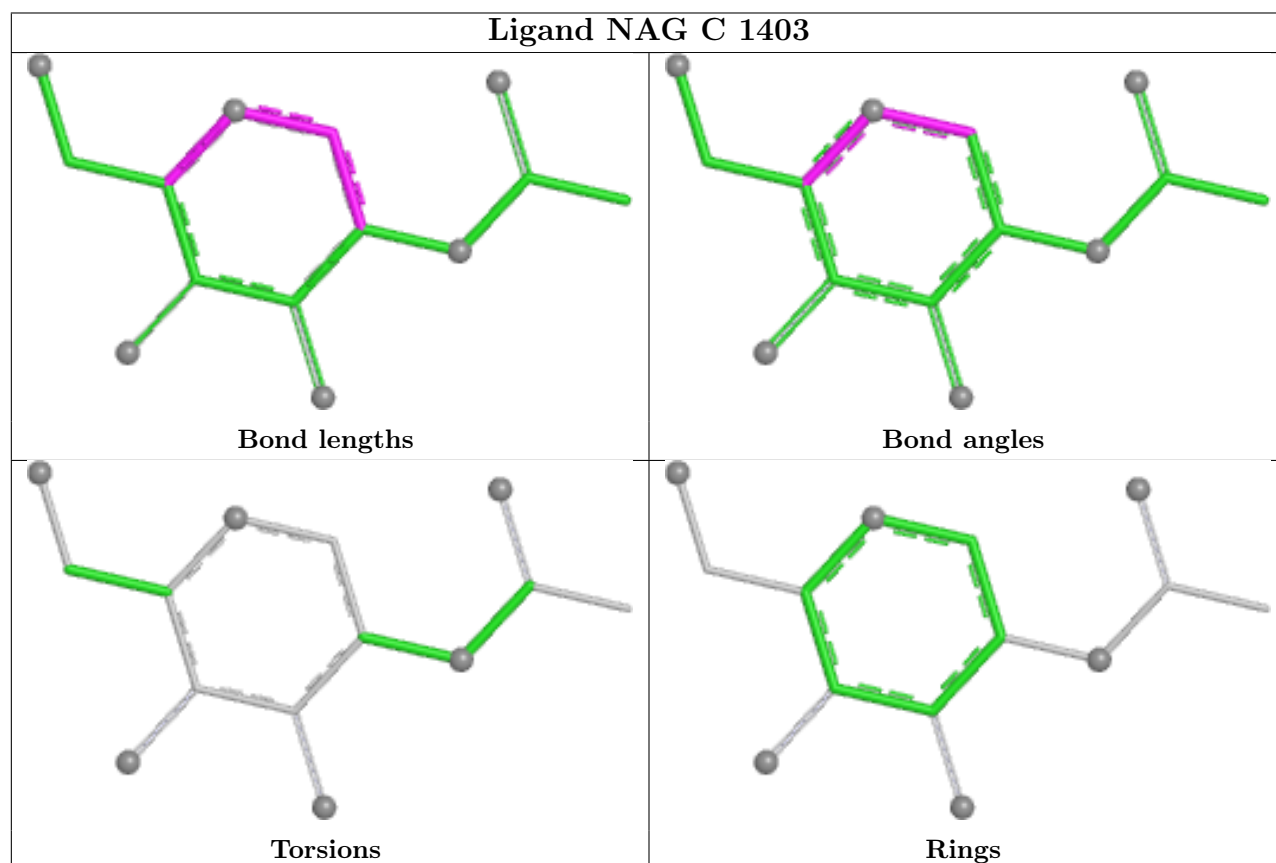
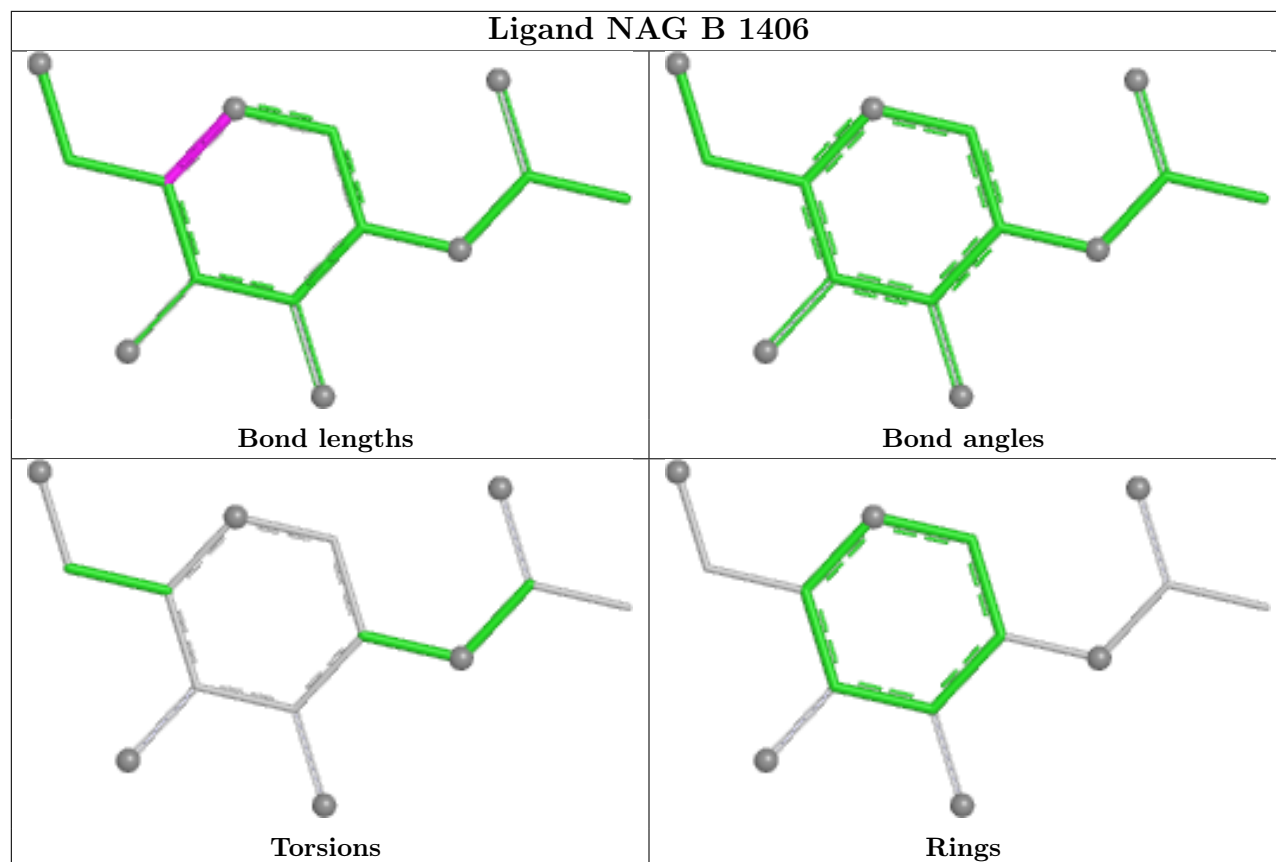
Ligand NAG A 1405

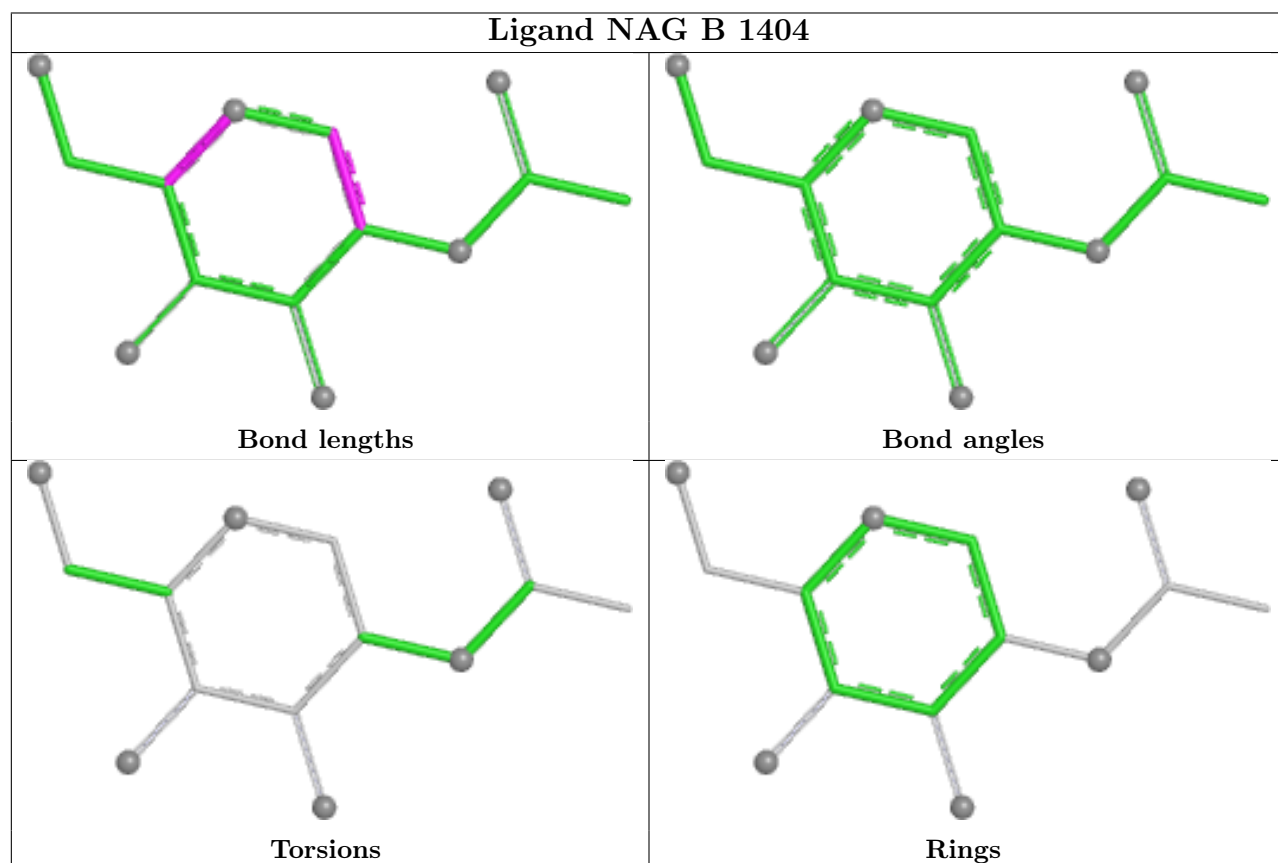
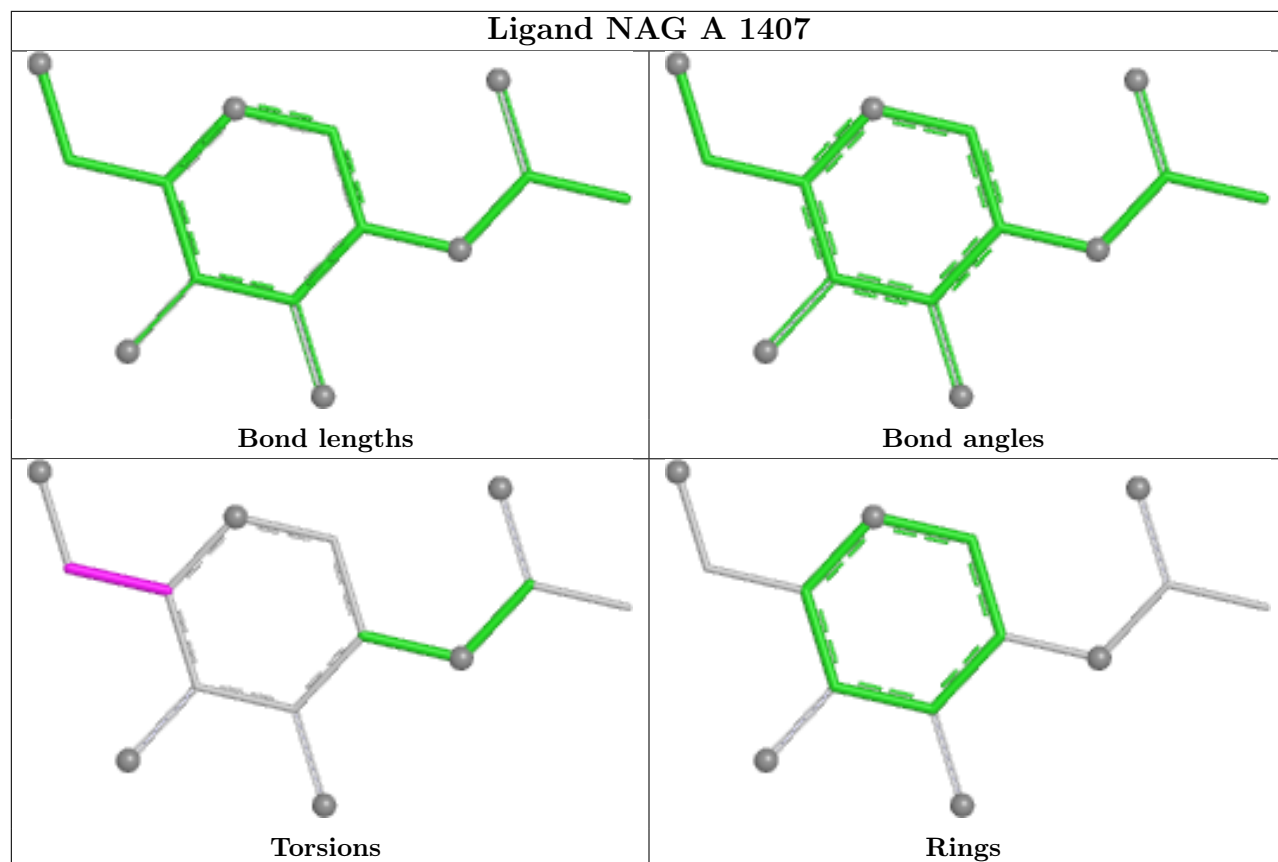


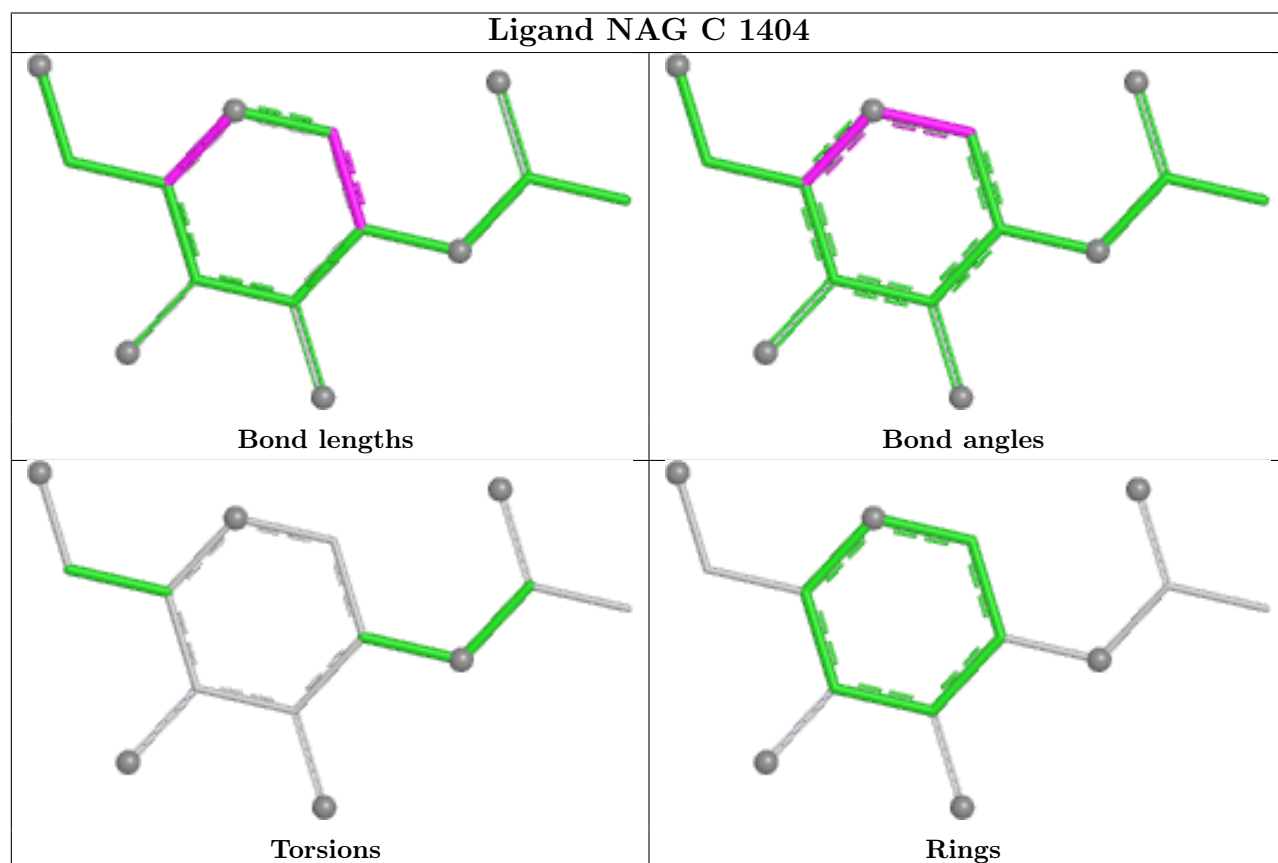
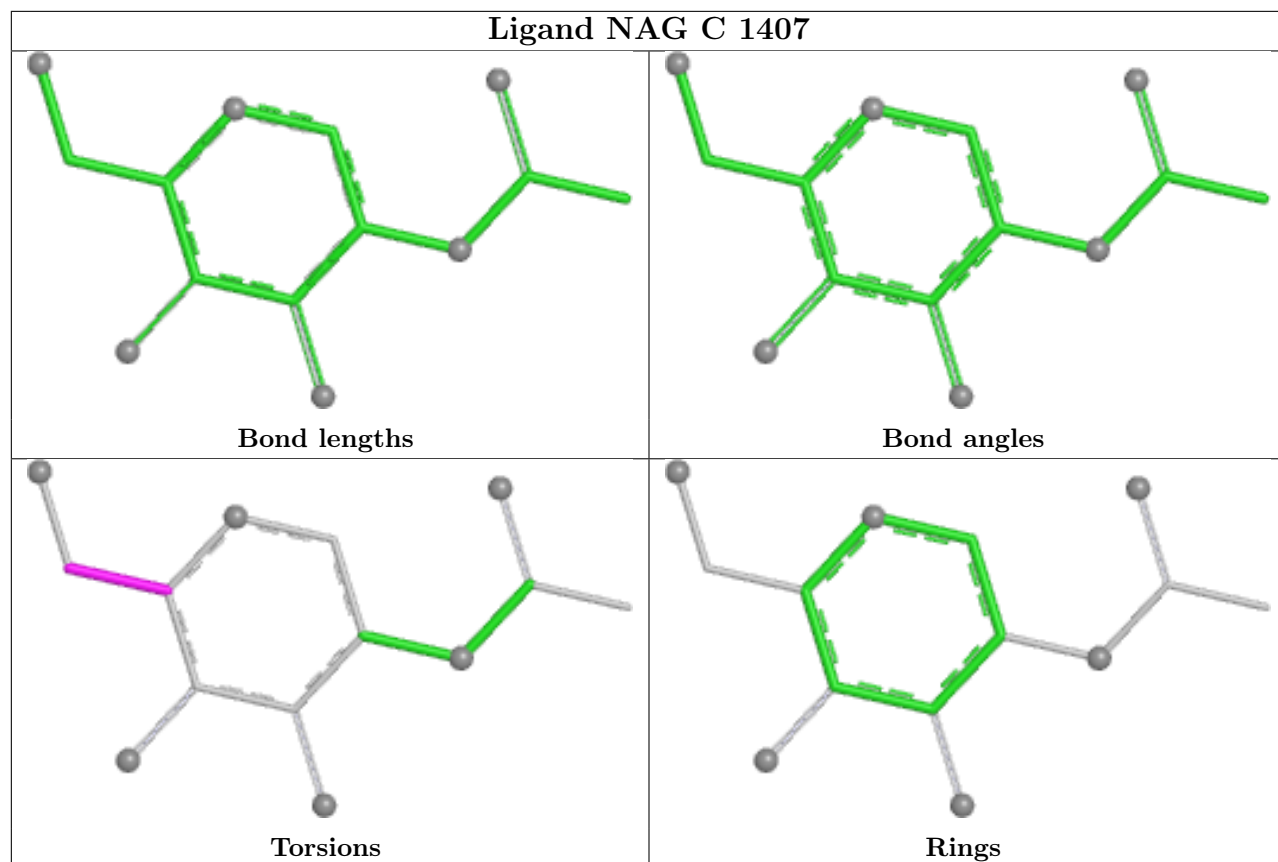
Ligand NAG C 1406

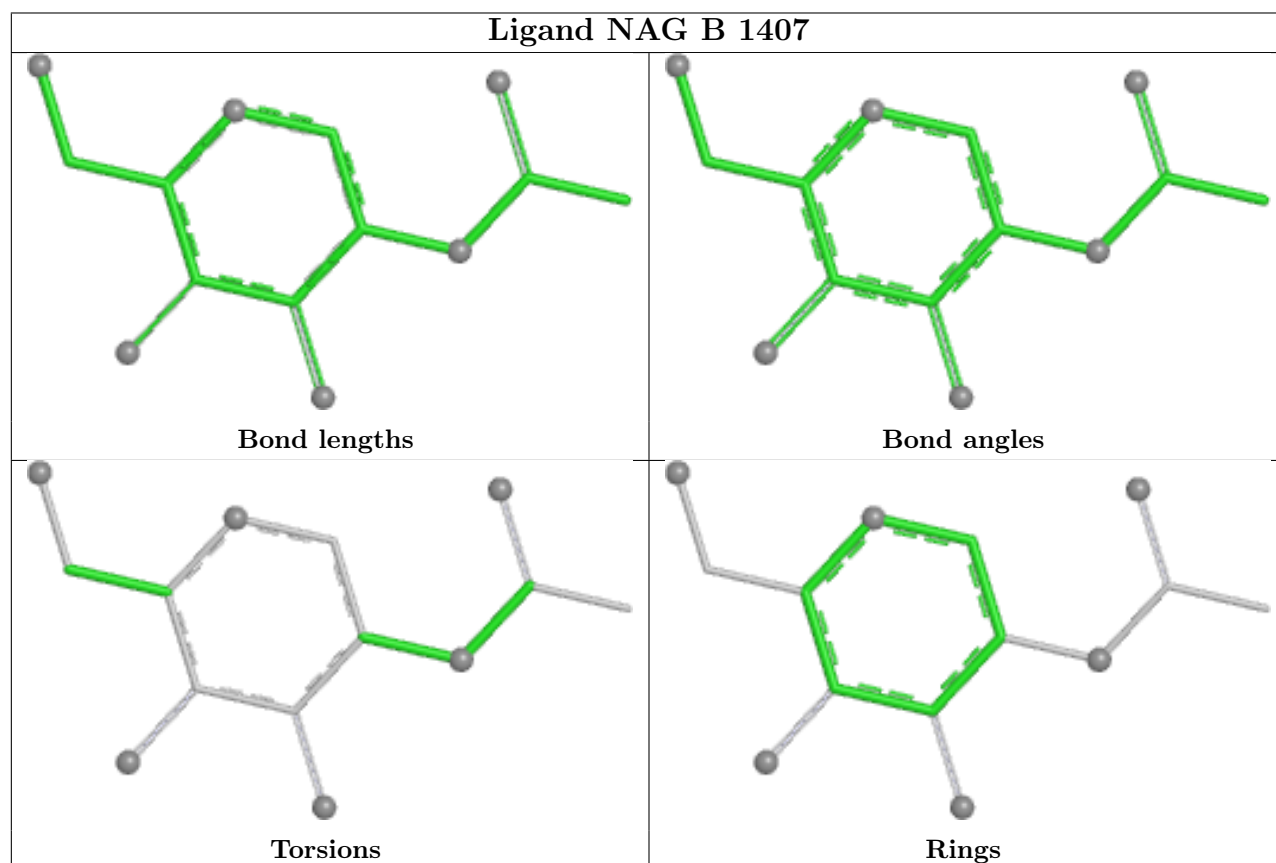
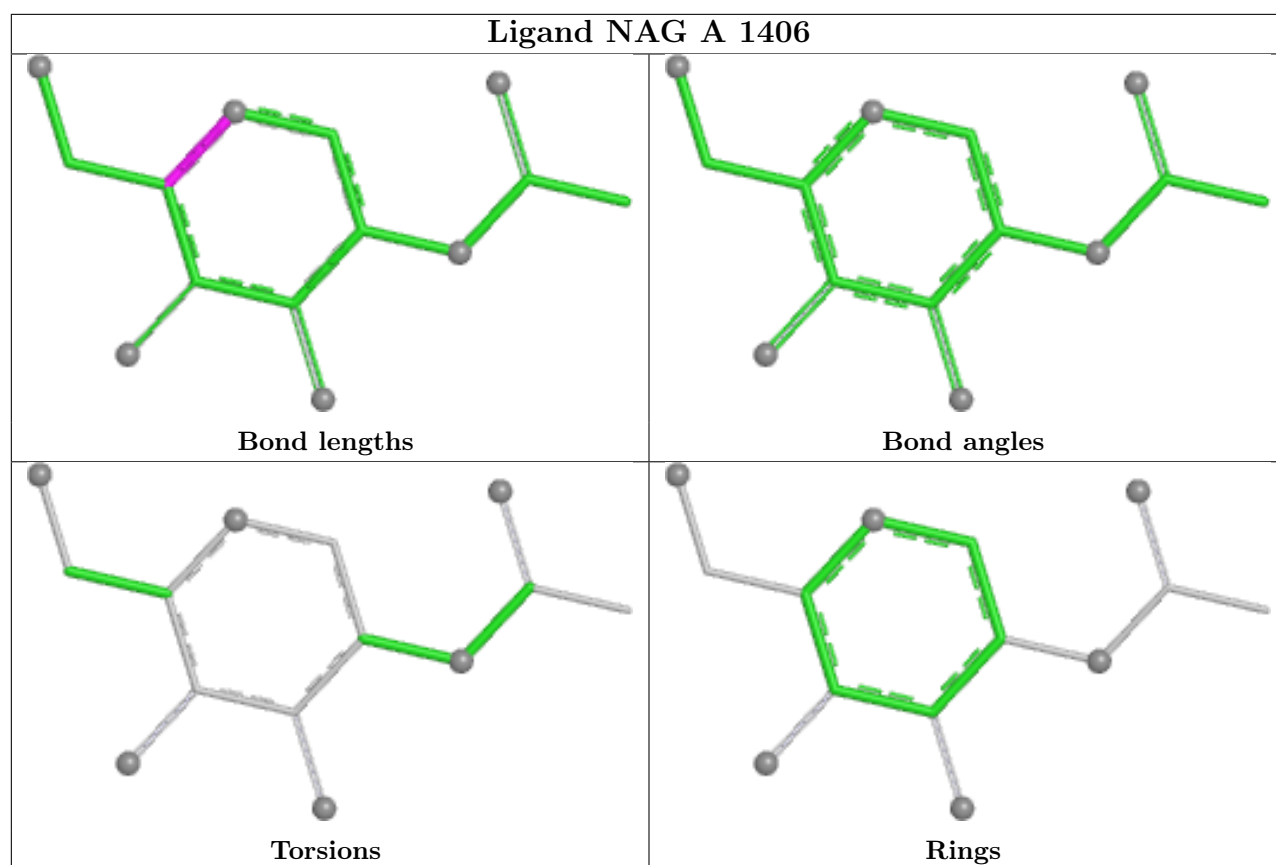


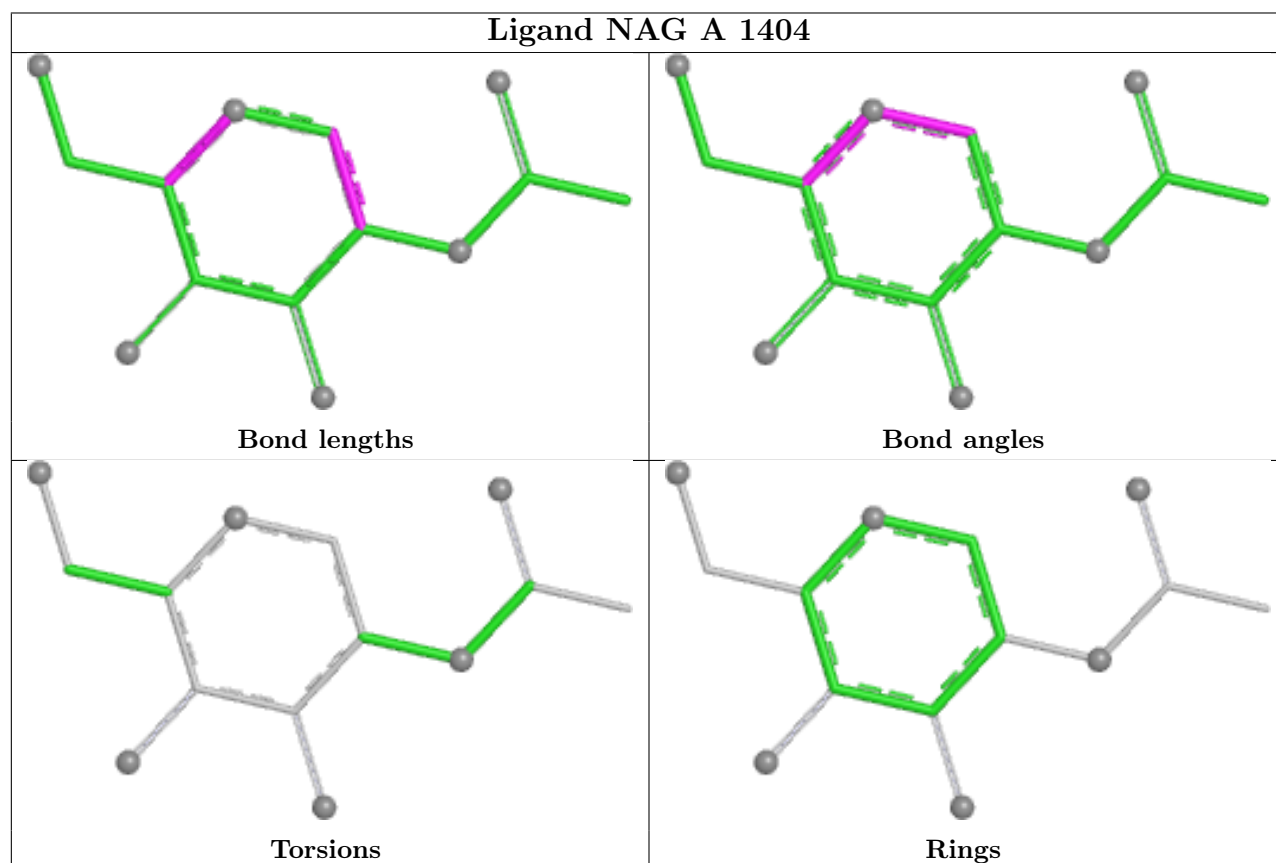
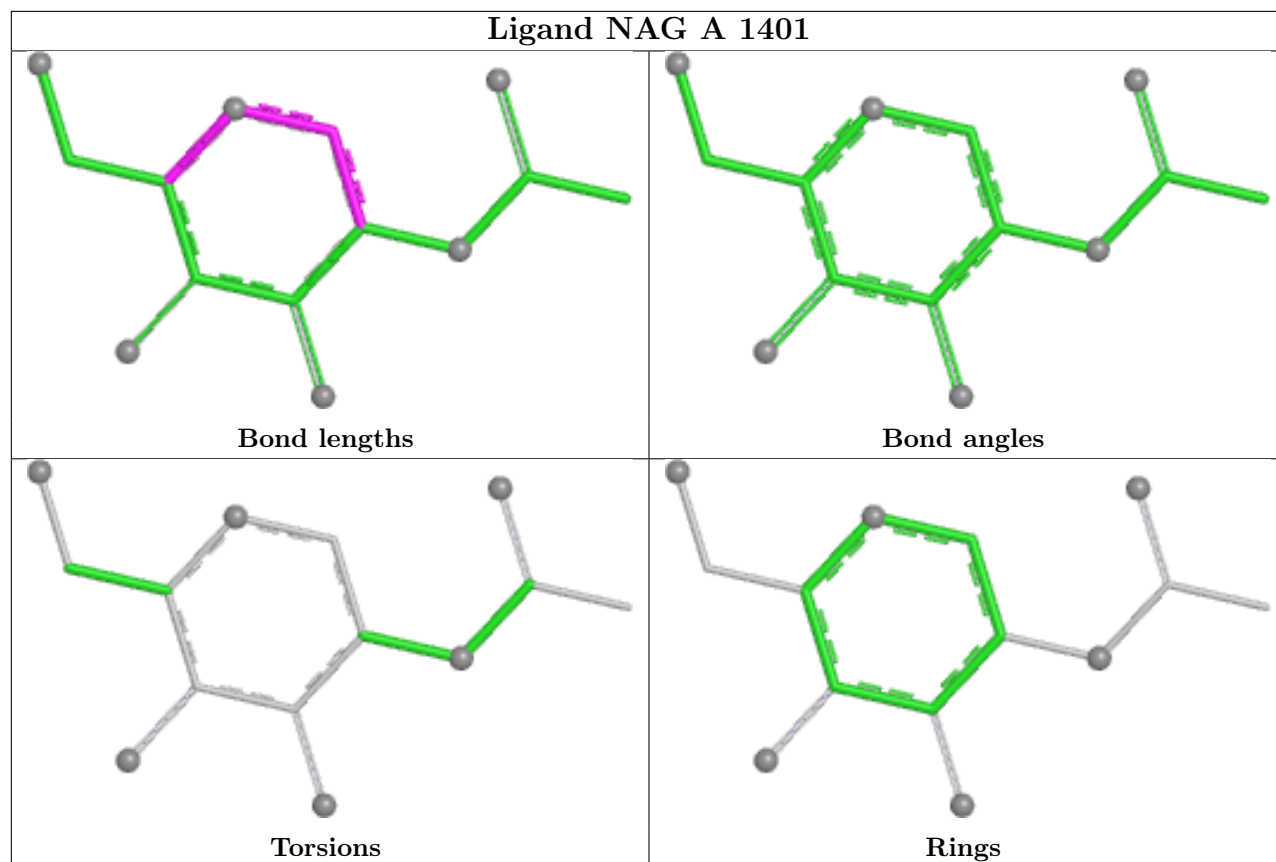


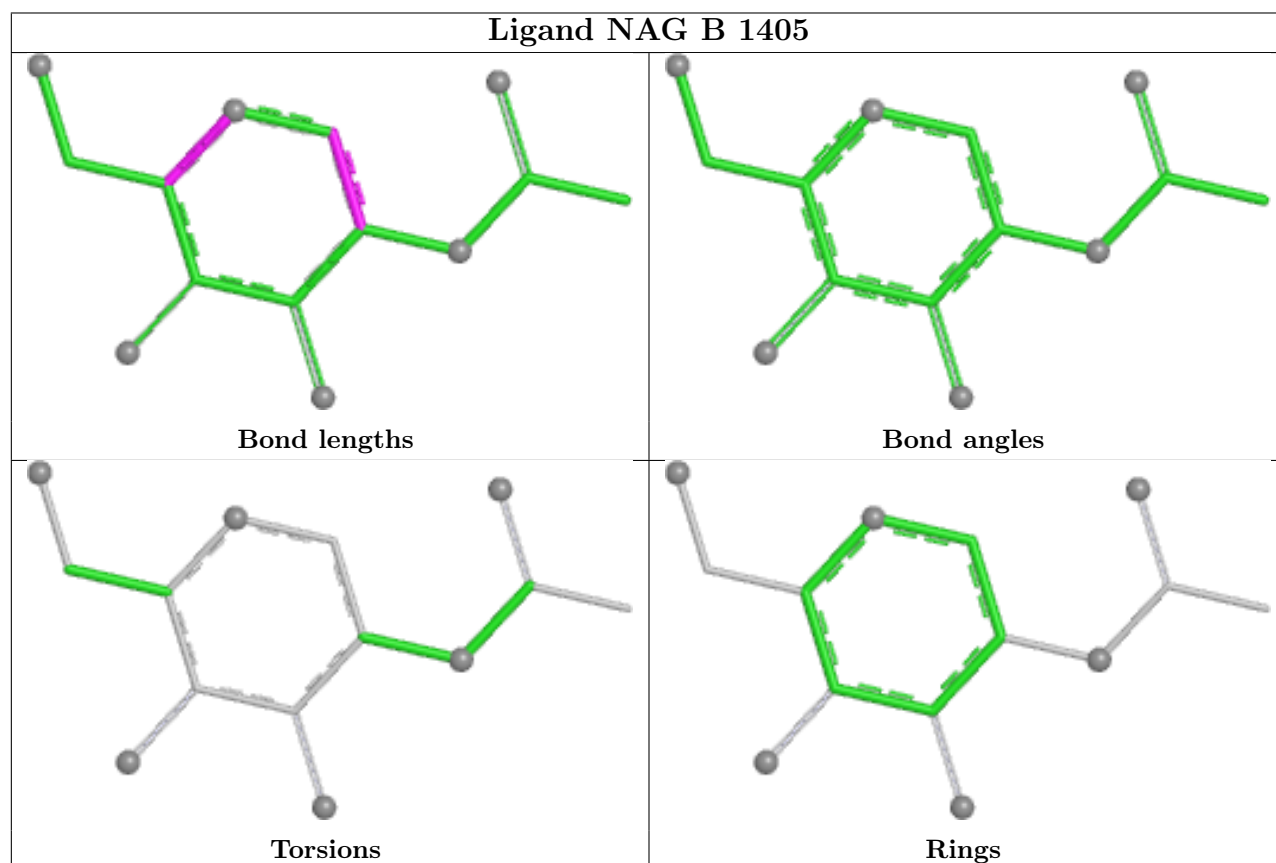
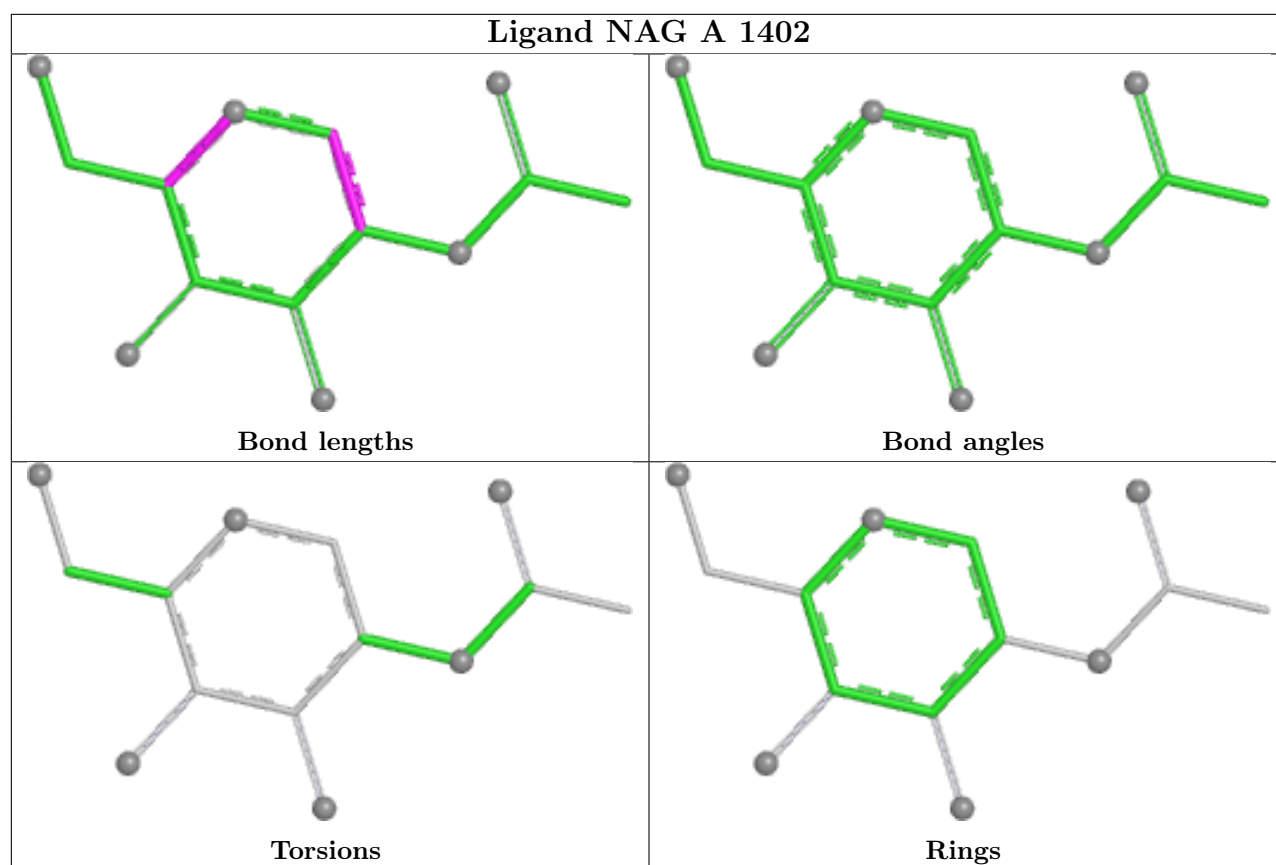


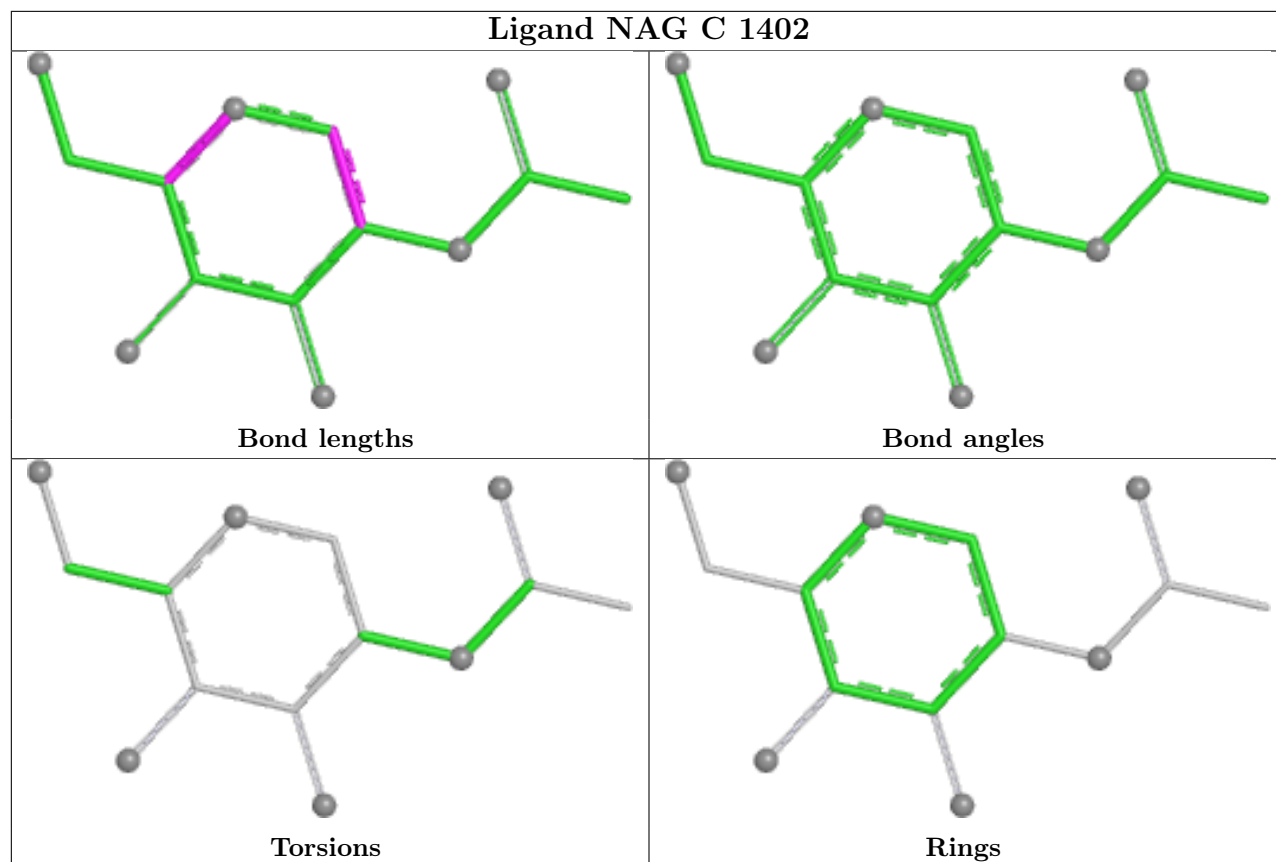












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

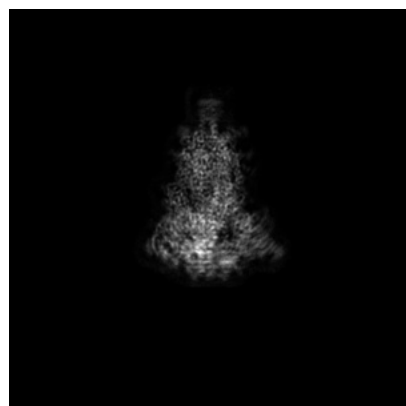
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27205. These allow visual inspection of the internal detail of the map and identification of artifacts.

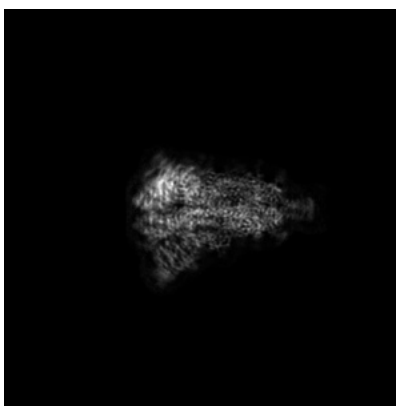
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

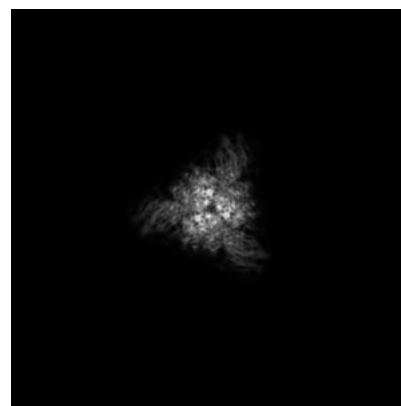
6.1.1 Primary map



X

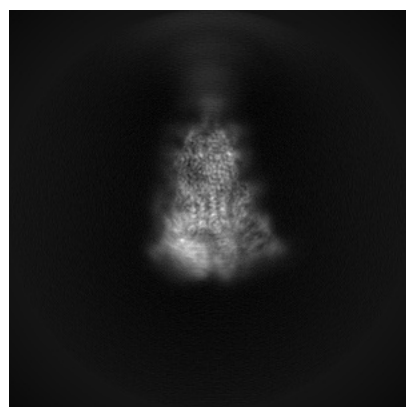


Y

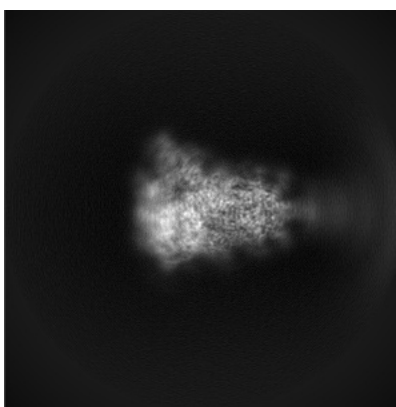


Z

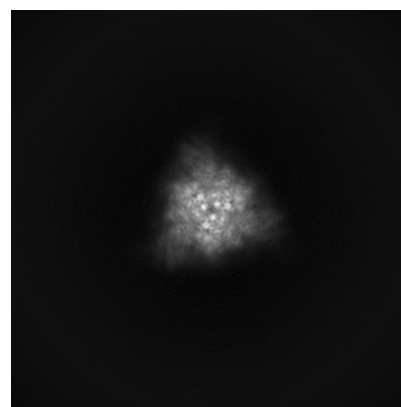
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

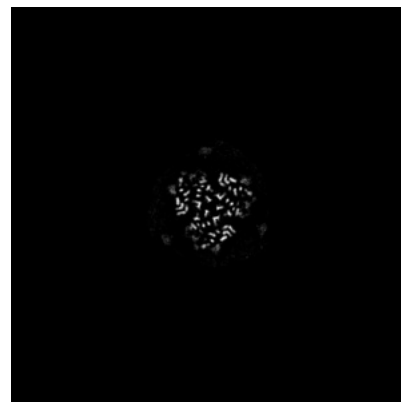
6.2.1 Primary map



X Index: 240

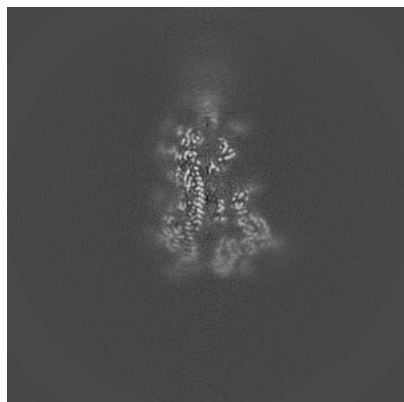


Y Index: 240

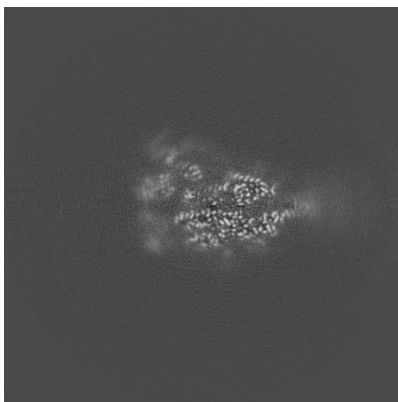


Z Index: 240

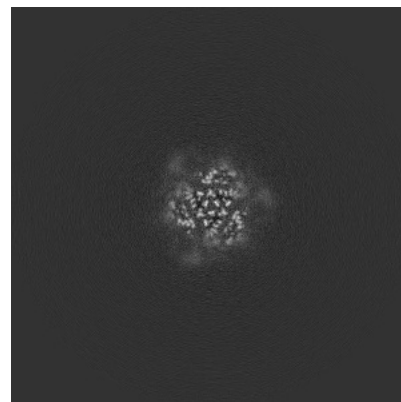
6.2.2 Raw map



X Index: 240



Y Index: 240

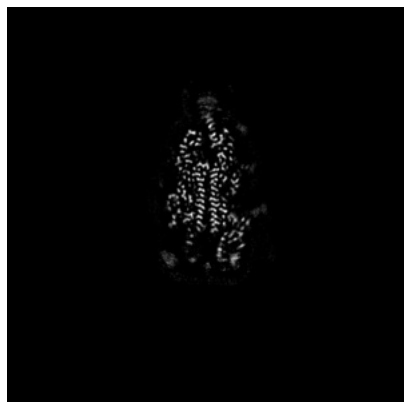


Z Index: 240

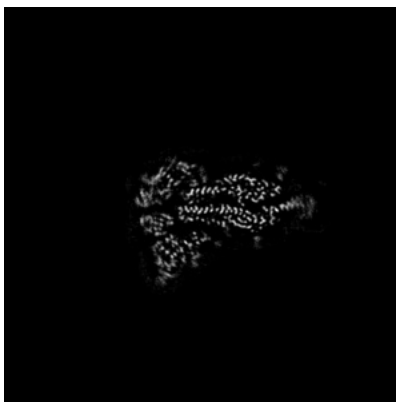
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 234

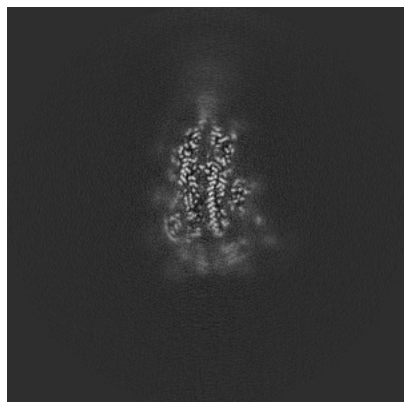


Y Index: 231

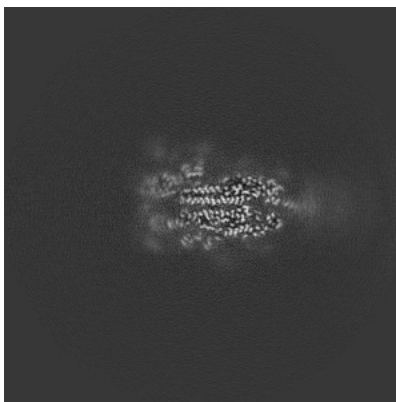


Z Index: 188

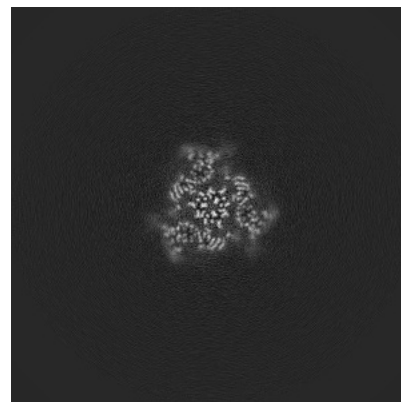
6.3.2 Raw map



X Index: 248



Y Index: 246

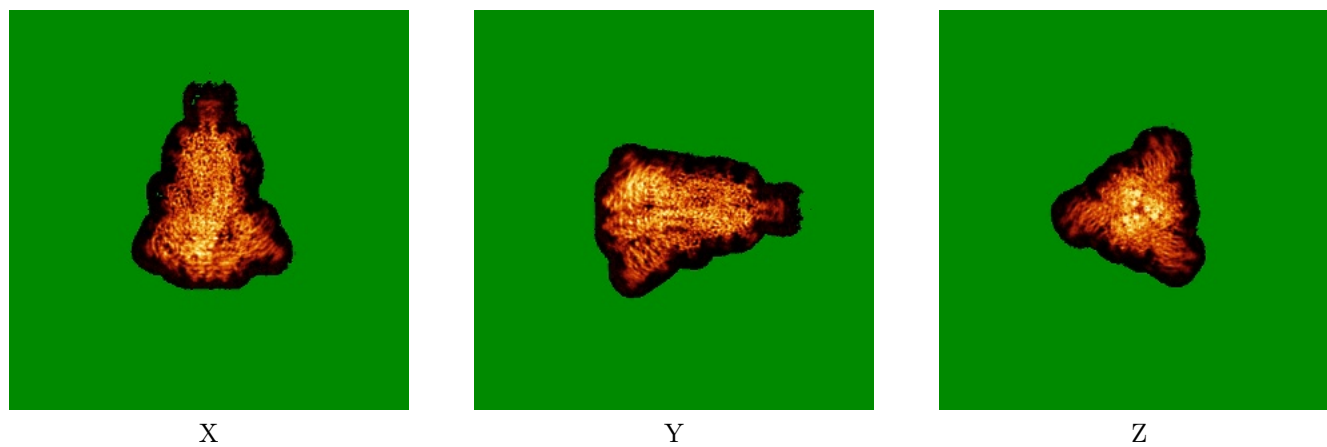


Z Index: 226

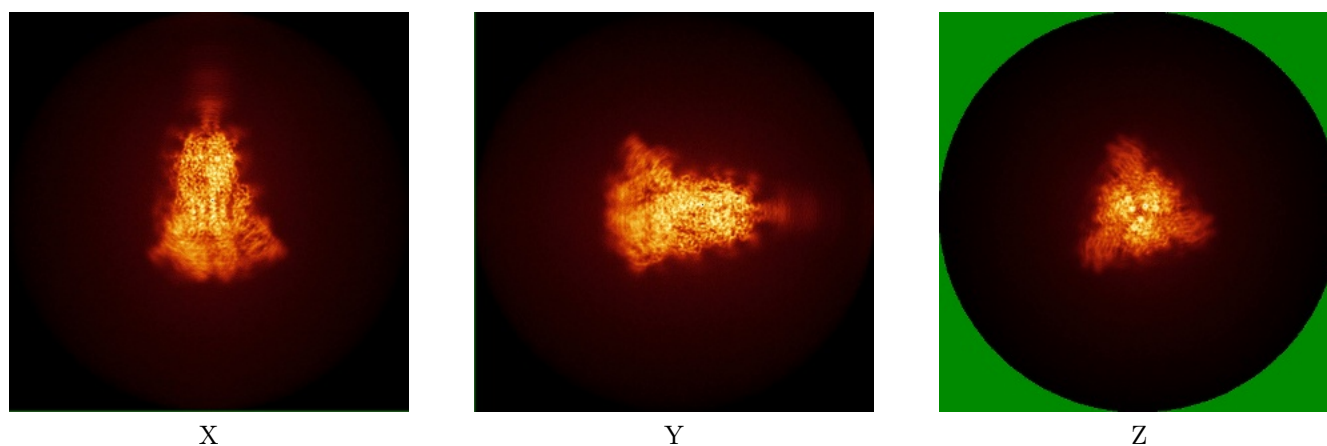
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

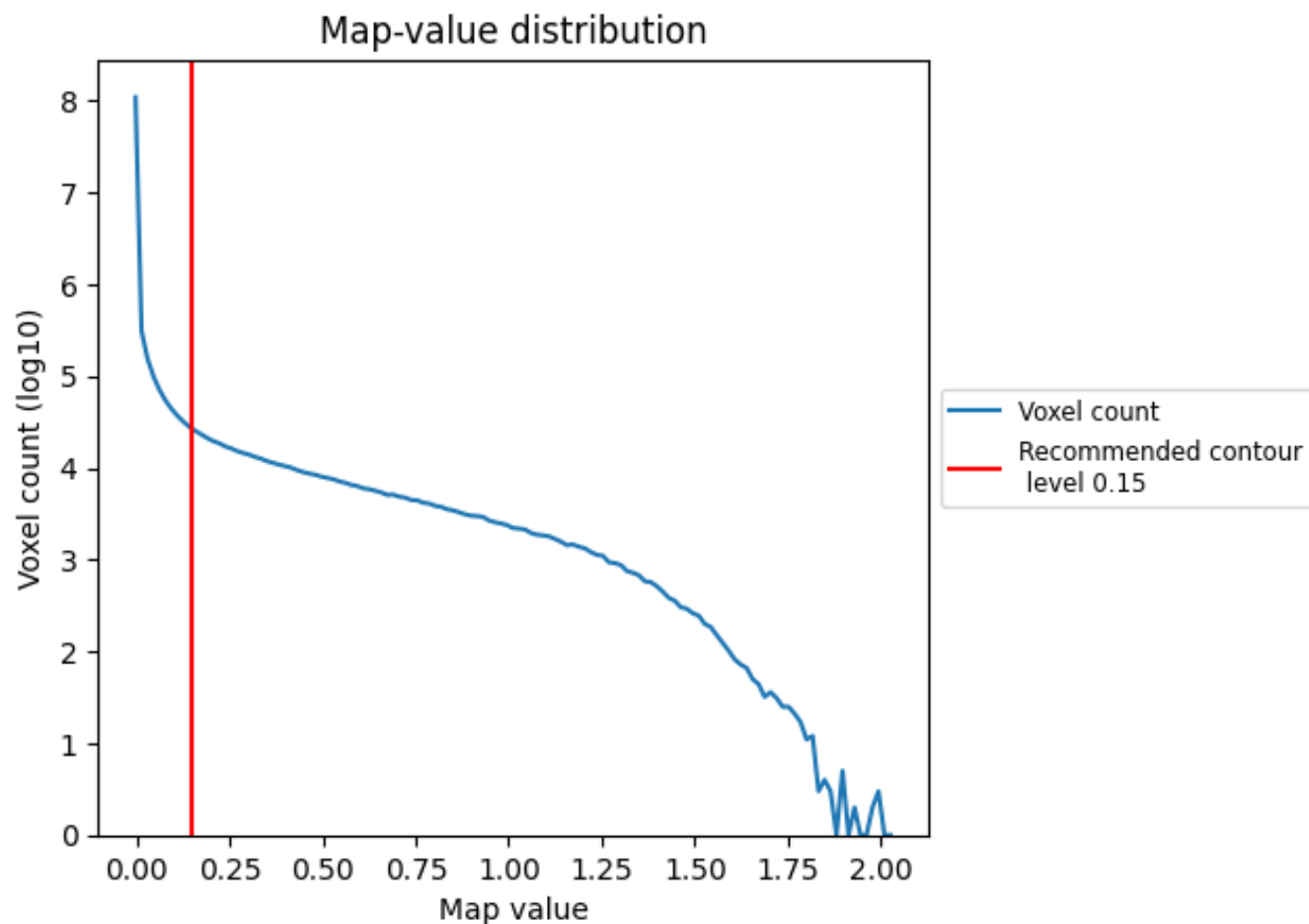
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

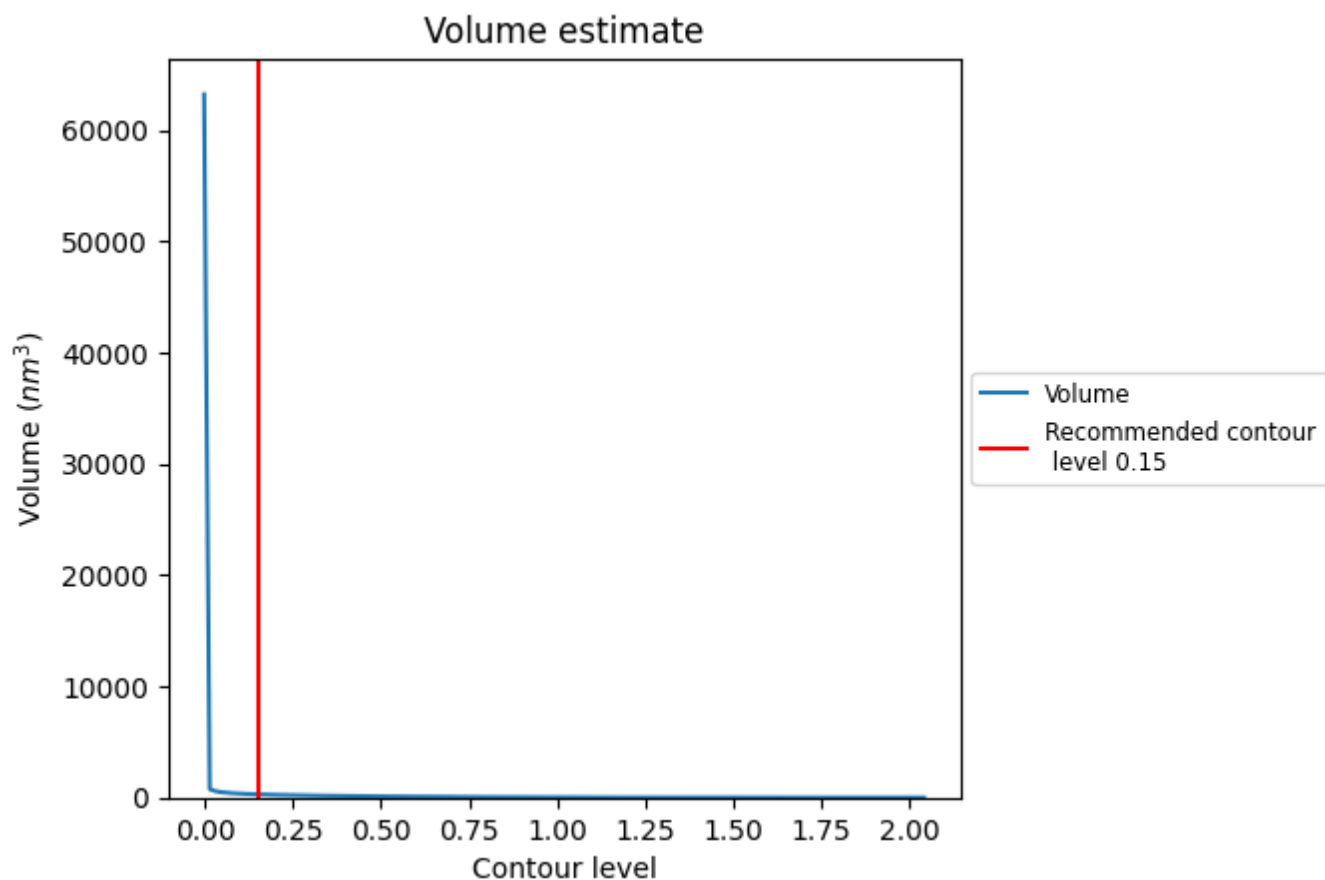
This section contains the results of statistical analysis of the map.

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.

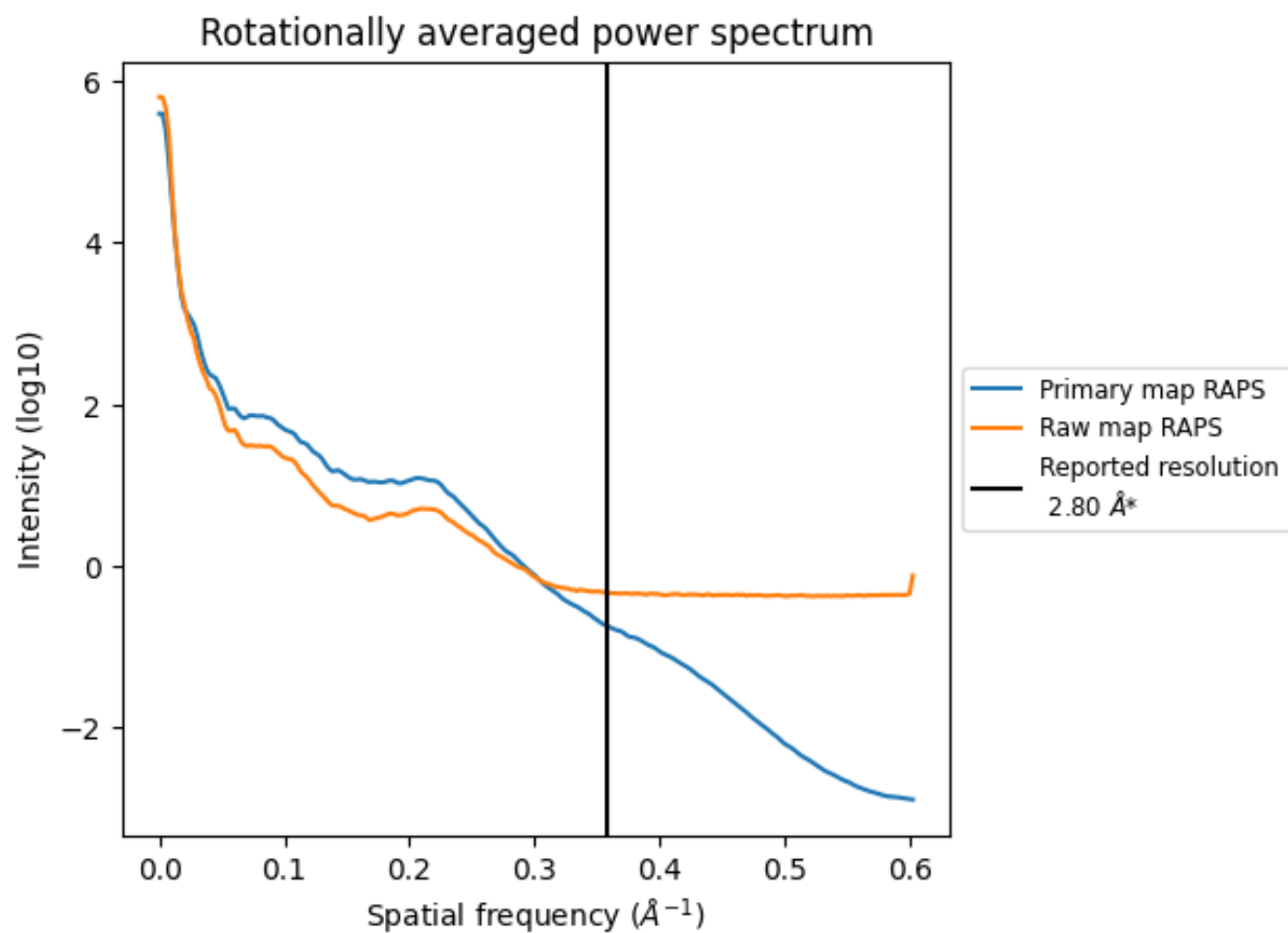
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287 nm^3 ; this corresponds to an approximate mass of 260 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 ⓘ

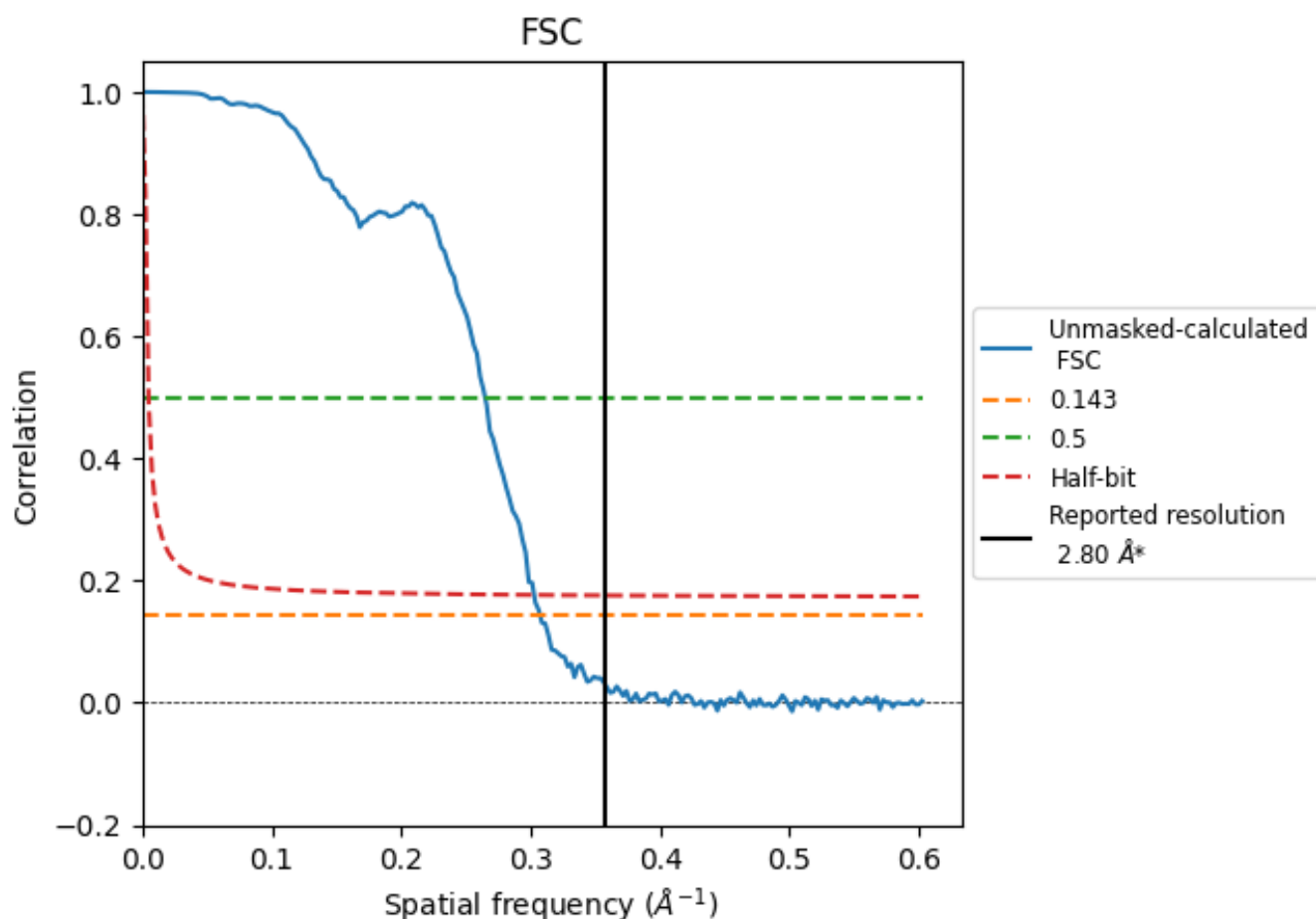


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

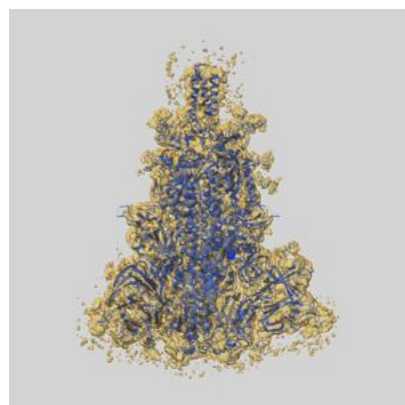
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.78	3.30

*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 3.26 differs from the reported value 2.8 by more than 10 %

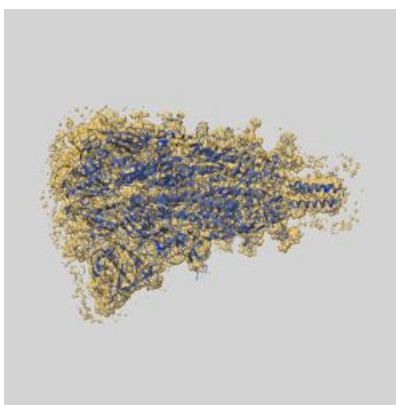
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27205 and PDB model 8D55. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

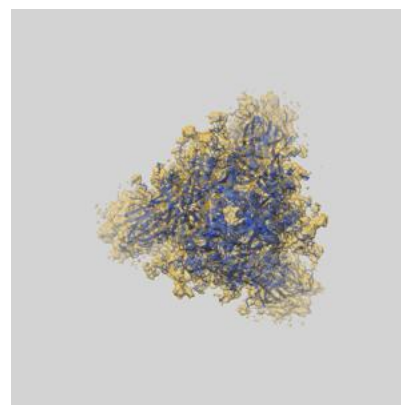
9.1 Map-model overlay [i](#)



X



Y



Z

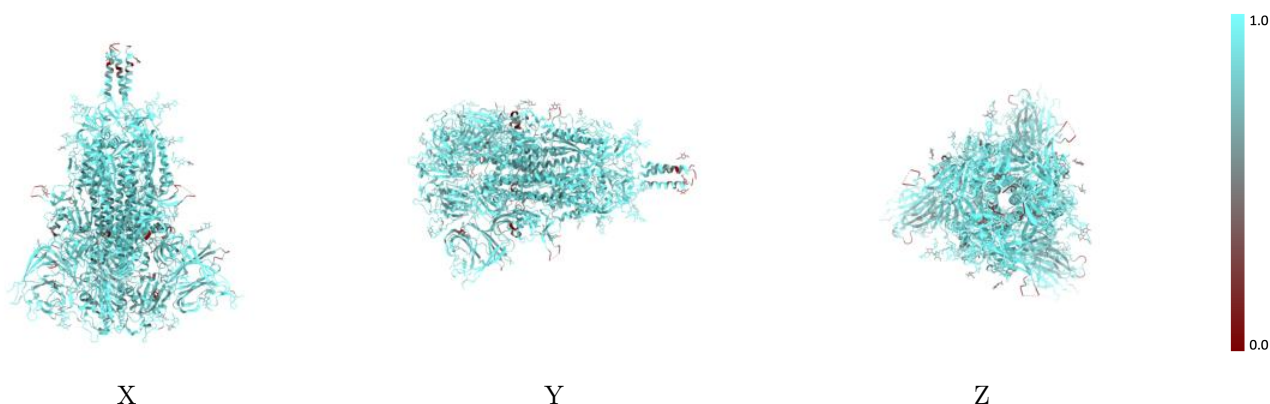
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



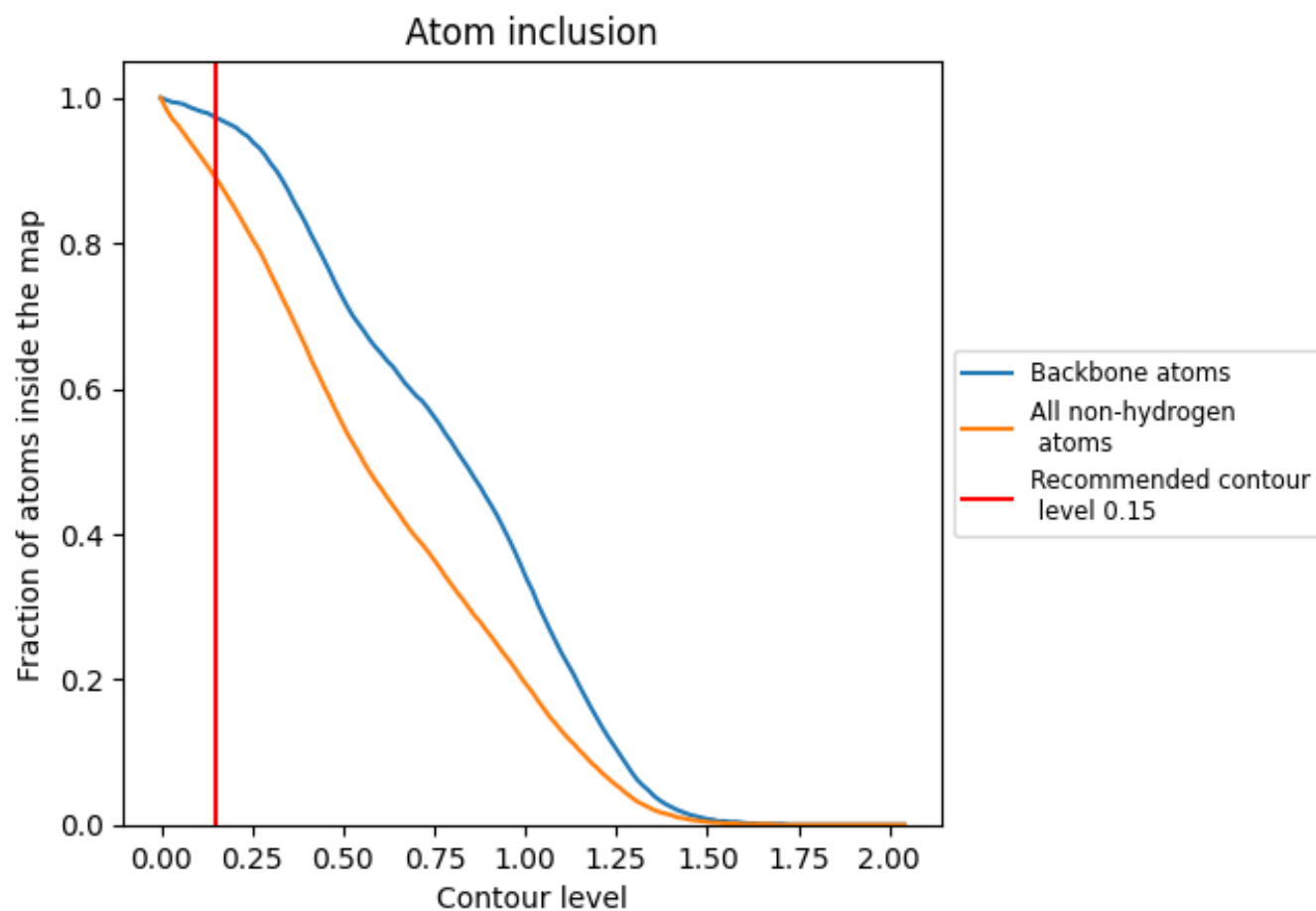
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8890	 0.4340
A	 0.8930	 0.4380
B	 0.8930	 0.4380
C	 0.8940	 0.4390
D	 0.7950	 0.2270
E	 0.8570	 0.2750
F	 0.4620	 0.2030
G	 0.7180	 0.2130
H	 0.7140	 0.2160
I	 0.8720	 0.4410
J	 0.8210	 0.4310
K	 0.7890	 0.4440
L	 0.9230	 0.4130
M	 0.8720	 0.3230
N	 0.8210	 0.2380
O	 0.7860	 0.2200
P	 0.4870	 0.1700
Q	 0.7690	 0.2340
R	 0.7140	 0.2660
S	 0.8460	 0.4340
T	 0.8460	 0.4220
U	 0.8160	 0.4450
V	 0.9490	 0.4120
W	 0.8970	 0.3290
X	 0.8210	 0.2580
Y	 0.7860	 0.2550
Z	 0.4100	 0.1540
a	 0.8460	 0.2510
b	 0.7500	 0.2210
c	 0.8720	 0.4440
d	 0.8210	 0.3870
e	 0.7890	 0.4340
f	 0.9490	 0.4170
g	 0.8970	 0.3350

