



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:29 AM UTC

PDB ID : 8D5A / pdb_00008d5a
EMDB ID : EMD-27207
Title : Middle 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 : 3.10 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:

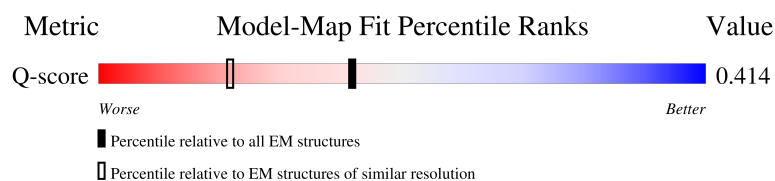
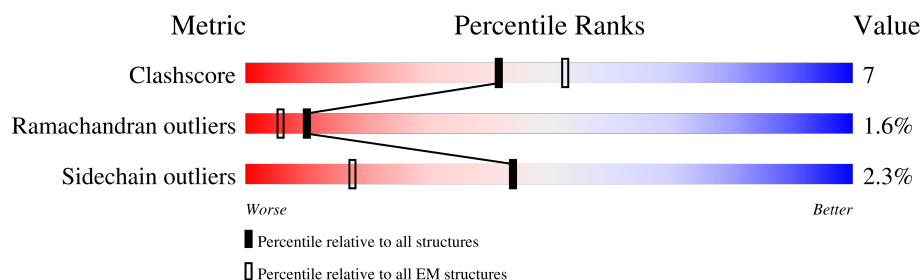
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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.



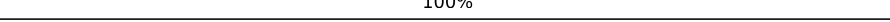
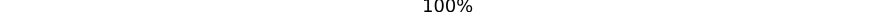
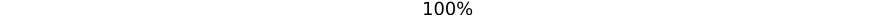
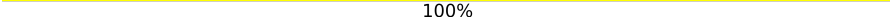
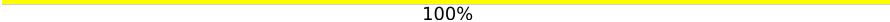
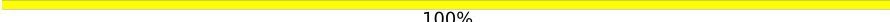
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	
1	B	1305	
1	C	1305	
2	D	3	

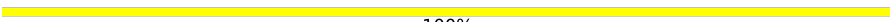
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Mol	Chain	Length	Quality of chain
2	F	3	 100%
2	H	3	 100%
2	I	3	 100%
2	K	3	 100%
2	L	3	 100%
2	M	3	 100%
2	P	3	 100%
2	R	3	 100%
2	S	3	 100%
2	U	3	 100%
2	V	3	 100%
2	W	3	 100%
2	Z	3	 100%
2	b	3	 100%
2	c	3	 100%
2	e	3	 100%
2	f	3	 100%
3	E	2	 100%
3	G	2	 100%
3	N	2	 100%
3	O	2	 100%
3	Q	2	 100%
3	X	2	 100%
3	Y	2	 100%
3	a	2	 100%

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Mol	Chain	Length	Quality of chain
4	J	3	 100%
4	T	3	 100%
4	d	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
2	NAG	D	1	-	-	X	-
2	NAG	D	2	-	-	X	-
5	NAG	C	1402	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27711 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	1118	Total	C	N	O	S	0	0
			8773	5610	1465	1658	40		
1	B	1125	Total	C	N	O	S	0	0
			8822	5639	1474	1669	40		
1	C	1122	Total	C	N	O	S	0	0
			8796	5623	1470	1663	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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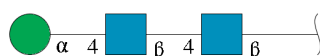
Chain	Residue	Modelled	Actual	Comment	Reference
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	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.



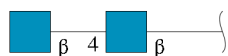
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	H	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		
2	L	3	Total	C	N	O	0	0
			39	22	2	15		
2	M	3	Total	C	N	O	0	0
			39	22	2	15		
2	P	3	Total	C	N	O	0	0
			39	22	2	15		
2	R	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	U	3	Total	C	N	O	0	0
			39	22	2	15		
2	V	3	Total	C	N	O	0	0
			39	22	2	15		
2	W	3	Total	C	N	O	0	0
			39	22	2	15		

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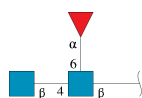
Mol	Chain	Residues	Atoms				AltConf	Trace
2	Z	3	Total	C	N	O	0	0
			39	22	2	15		
2	b	3	Total	C	N	O	0	0
			39	22	2	15		
2	c	3	Total	C	N	O	0	0
			39	22	2	15		
2	e	3	Total	C	N	O	0	0
			39	22	2	15		
2	f	3	Total	C	N	O	0	0
			39	22	2	15		

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



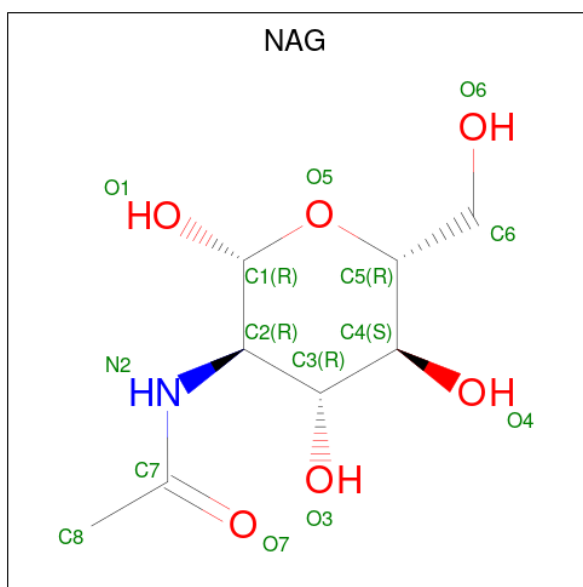
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	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	J	3	Total	C	N	O	0	0
			38	22	2	14		
4	T	3	Total	C	N	O	0	0
			38	22	2	14		
4	d	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: $C_8H_{15}NO_6$) (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	B	1	Total	C	N	O	0
			14	8	1	5	

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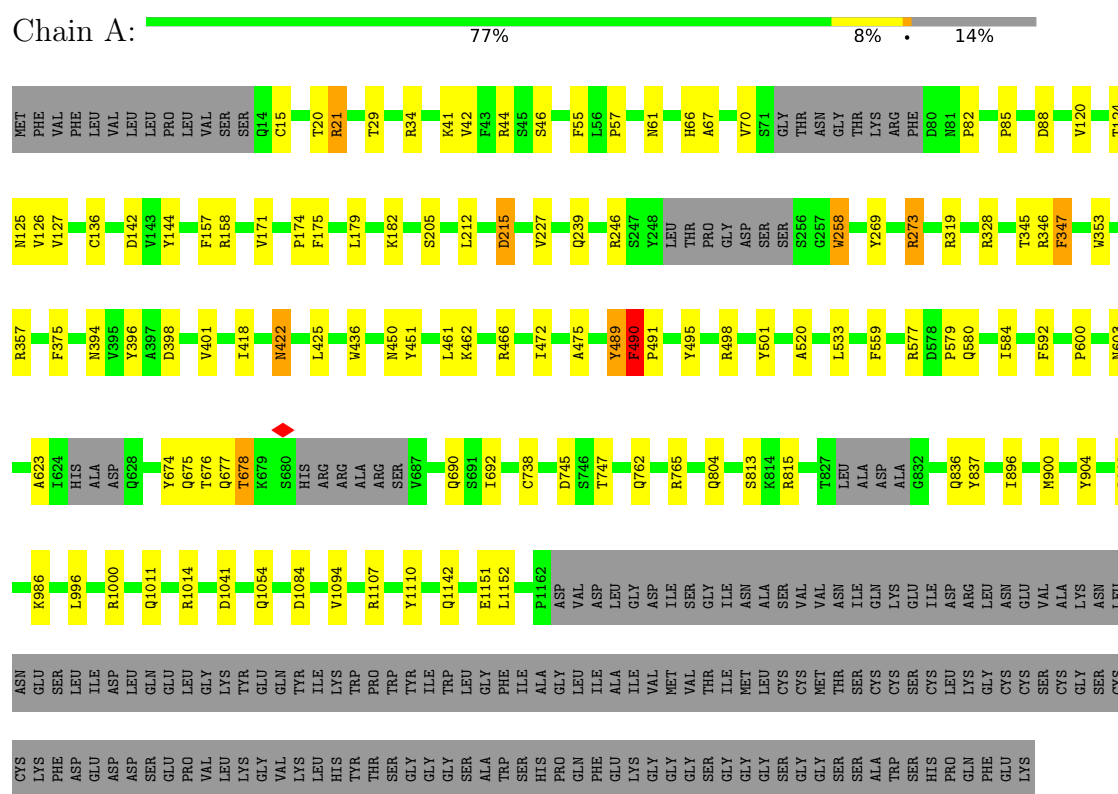
Continued from previous page...

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	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	

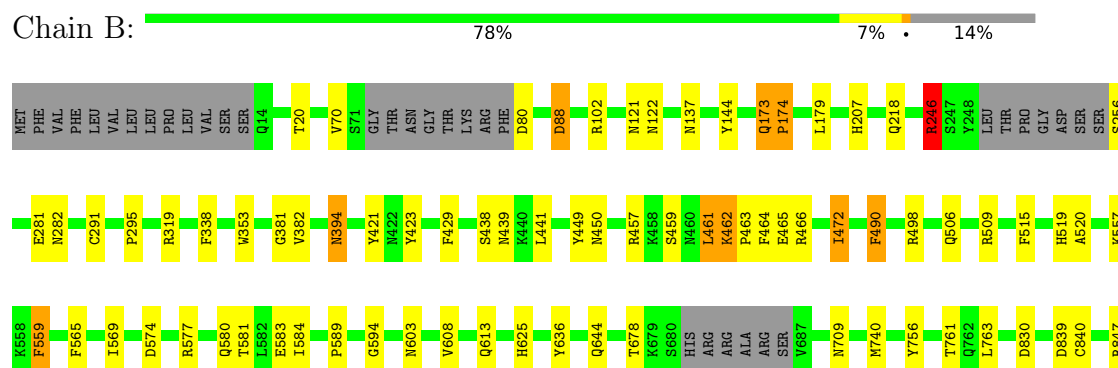
3 Residue-property plots

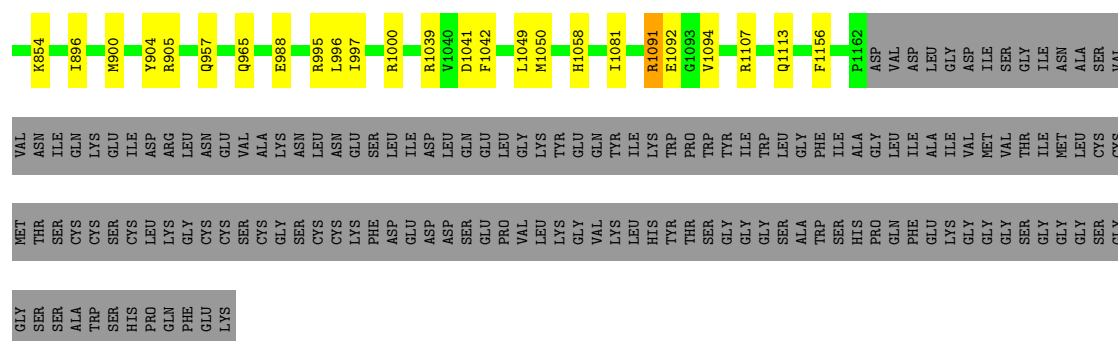
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



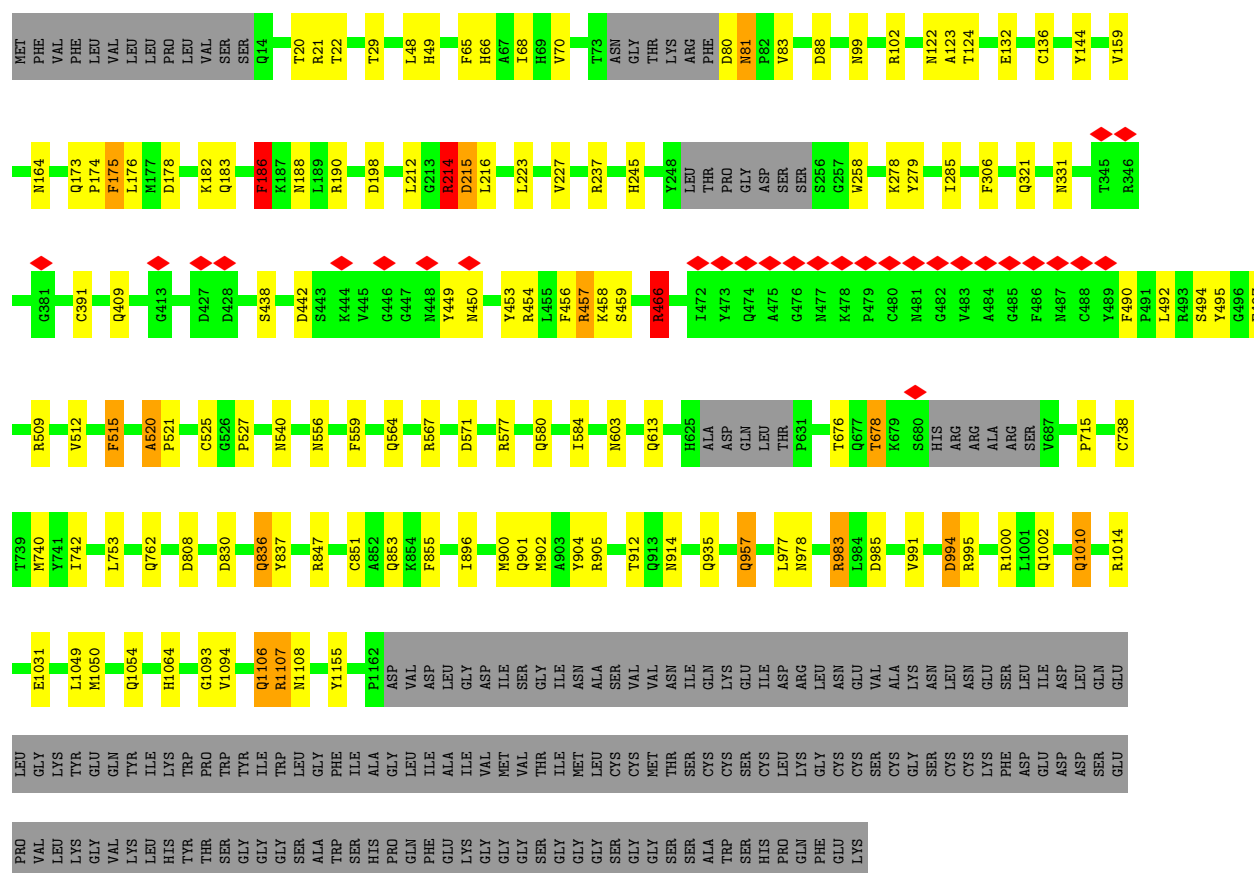
• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein

Chain C: 76% 9% 14%



• 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: 67% 33%



• 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%

NAG1
NAG2
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 H:  100%

NAG1
NAG2
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 I:  100%

NAG1
NAG2
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 K:  100%

NAG1
NAG2
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 L:  100%

NAG1
NAG2
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 M:  100%

NAG1
NAG2
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 P:  100%

NAG1
NAG2
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 R:  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 S:  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 U:  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 V:  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 W:  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:  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 b:  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 e:  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 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 G:  100%

MAG1
MAG2

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

Chain N:  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 Q:  100%

MAG1
MAG2

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

Chain X:  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 a:  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 J:  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 T:  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 d:

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	113667	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	0.508	Depositor
Minimum map value	-0.186	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	398.4, 398.4, 398.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: NAG, MAN, 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	0.85	2/8980 (0.0%)	1.38	29/12212 (0.2%)
1	B	0.85	0/9031	1.37	25/12284 (0.2%)
1	C	0.87	0/9005	1.38	32/12247 (0.3%)
All	All	0.86	2/27016 (0.0%)	1.38	86/36743 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	PHE	N-CA	6.01	1.54	1.46
1	A	490	PHE	C-N	5.32	1.40	1.33

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	ARG	N-CA-C	9.05	123.18	108.34
1	C	331	ASN	OD1-CG-ND2	-9.00	113.60	122.60
1	A	215	ASP	CA-C-N	8.70	129.94	122.28
1	A	215	ASP	C-N-CA	8.70	129.94	122.28
1	B	709	ASN	CA-CB-CG	8.00	120.60	112.60
1	A	34	ARG	N-CA-C	7.89	120.95	110.53
1	C	515	PHE	CA-CB-CG	7.49	121.29	113.80
1	C	1054	GLN	OE1-CD-NE2	-7.42	115.18	122.60
1	C	331	ASN	CB-CG-ND2	7.20	127.19	116.40
1	B	520	ALA	N-CA-CB	-7.17	103.91	111.29
1	C	122	ASN	CB-CG-ND2	7.02	126.93	116.40
1	C	122	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	B	603	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	B	1091	ARG	N-CA-C	-6.64	103.66	111.03
1	B	603	ASN	CB-CG-ND2	6.64	126.36	116.40
1	A	55	PHE	CA-CB-CG	6.38	120.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ASN	CA-CB-CG	6.30	118.90	112.60
1	B	565	PHE	CA-C-N	6.26	125.91	121.65
1	B	565	PHE	C-N-CA	6.26	125.91	121.65
1	C	68	ILE	CA-C-N	6.18	128.84	120.44
1	C	68	ILE	C-N-CA	6.18	128.84	120.44
1	C	853	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	A	175	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	559	PHE	CA-CB-CG	6.11	119.91	113.80
1	C	245	HIS	CA-CB-CG	6.02	119.82	113.80
1	C	808	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	239	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	B	957	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	B	246	ARG	N-CA-C	5.88	123.32	110.80
1	C	466	ARG	N-CA-C	5.86	118.77	108.75
1	A	490	PHE	CA-C-N	-5.82	113.97	119.85
1	A	490	PHE	C-N-CA	-5.82	113.97	119.85
1	B	515	PHE	CA-CB-CG	5.77	119.57	113.80
1	B	394	ASN	CA-CB-CG	5.77	118.37	112.60
1	C	1107	ARG	N-CA-C	5.73	117.52	111.28
1	C	580	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	B	450	ASN	CA-CB-CG	5.71	118.31	112.60
1	C	186	PHE	N-CA-C	5.71	122.96	110.80
1	C	1064	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	B	625	HIS	CB-CG-CD2	-5.69	123.81	131.20
1	C	1010	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	C	983	ARG	N-CA-C	5.62	120.13	113.28
1	A	425	LEU	CB-CA-C	5.61	117.32	108.84
1	C	321	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	A	205	SER	N-CA-C	5.50	116.62	108.60
1	A	1151	GLU	CA-C-N	5.49	127.63	120.28
1	A	1151	GLU	C-N-CA	5.49	127.63	120.28
1	B	839	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	450	ASN	CA-CB-CG	5.49	118.09	112.60
1	C	1002	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	B	88	ASP	CA-C-N	5.46	129.21	120.97
1	B	88	ASP	C-N-CA	5.46	129.21	120.97
1	B	464	PHE	N-CA-C	5.42	119.19	112.47
1	B	338	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	520	ALA	N-CA-C	5.40	112.88	108.07
1	C	409	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	C	603	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	C	978	ASN	CA-CB-CG	5.34	117.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	A	489	TYR	O-C-N	-5.31	117.30	122.99
1	A	836	GLN	CA-C-N	5.29	131.65	121.54
1	A	836	GLN	C-N-CA	5.29	131.65	121.54
1	A	1054	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	C	215	ASP	N-CA-C	5.25	121.98	110.80
1	A	475	ALA	CA-C-N	5.25	125.90	120.60
1	A	475	ALA	C-N-CA	5.25	125.90	120.60
1	C	957	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	1113	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	1142	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	422	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	1110	TYR	CA-C-N	5.20	127.61	122.00
1	A	1110	TYR	C-N-CA	5.20	127.61	122.00
1	A	462	LYS	CB-CA-C	5.19	116.33	108.86
1	B	1058	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	C	29	THR	CA-CB-CG2	5.13	119.23	110.50
1	B	218	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	745	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	490	PHE	CB-CA-C	5.10	120.22	110.17
1	B	644	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	C	564	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	762	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	498	ARG	N-CA-C	-5.04	103.83	110.39
1	A	949	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	519	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	C	613	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	C	935	GLN	OE1-CD-NE2	-5.01	117.59	122.60

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	8773	0	8560	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8822	0	8599	139	0
1	C	8796	0	8576	146	0
2	D	39	0	34	15	0
2	F	39	0	34	0	0
2	H	39	0	34	0	0
2	I	39	0	34	0	0
2	K	39	0	34	0	0
2	L	39	0	34	0	0
2	M	39	0	34	0	0
2	P	39	0	34	2	0
2	R	39	0	34	0	0
2	S	39	0	34	0	0
2	U	39	0	34	0	0
2	V	39	0	34	0	0
2	W	39	0	34	0	0
2	Z	39	0	34	0	0
2	b	39	0	34	0	0
2	c	39	0	34	0	0
2	e	39	0	34	0	0
2	f	39	0	34	0	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	Q	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	a	28	0	25	0	0
4	J	38	0	34	0	0
4	T	38	0	34	0	0
4	d	38	0	34	0	0
5	A	98	0	91	8	0
5	B	98	0	91	5	0
5	C	84	0	78	0	0
All	All	27711	0	26909	372	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 (372) 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:C:453:TYR:CZ	1:C:492:LEU:HD22	1.30	1.67
1:B:282:ASN:HD21	2:P:1:NAG:C1	1.12	1.61
1:A:61:ASN:HD22	5:A:1401:NAG:C1	1.22	1.50
1:A:603:ASN:HD22	5:A:1404:NAG:C1	1.23	1.48
1:B:594:GLY:HA3	1:B:613:GLN:NE2	1.35	1.40
1:C:905:ARG:NH1	1:C:1050:MET:HB3	1.30	1.39
1:C:851:CYS:SG	1:C:855:PHE:HE2	1.46	1.38
1:B:457:ARG:NH2	1:B:461:LEU:HB3	1.37	1.35
1:A:603:ASN:ND2	5:A:1404:NAG:C1	1.86	1.33
1:A:61:ASN:ND2	5:A:1401:NAG:C1	1.87	1.33
1:C:559:PHE:CD1	1:C:584:ILE:HG13	1.21	1.32
1:C:559:PHE:CD1	1:C:584:ILE:CG1	2.12	1.27
1:B:282:ASN:ND2	2:P:1:NAG:C1	1.98	1.24
1:C:453:TYR:OH	1:C:492:LEU:HD22	1.33	1.24
1:C:900:MET:O	1:C:904:TYR:CD2	1.93	1.22
1:C:905:ARG:NH2	1:C:1050:MET:HE3	1.53	1.20
1:B:457:ARG:HH22	1:B:461:LEU:CB	1.53	1.20
1:C:453:TYR:OH	1:C:492:LEU:CD2	1.90	1.20
1:B:246:ARG:HE	1:B:256:SER:N	1.40	1.19
1:C:851:CYS:SG	1:C:855:PHE:CE2	2.35	1.19
1:A:1107:ARG:HD3	1:B:904:TYR:CE2	1.78	1.19
1:C:453:TYR:CZ	1:C:492:LEU:CD2	2.26	1.19
1:A:171:VAL:CG2	2:D:2:NAG:O7	1.90	1.18
1:B:559:PHE:CE1	1:B:584:ILE:HG21	1.80	1.16
1:A:171:VAL:HG21	2:D:2:NAG:O7	0.98	1.14
1:B:594:GLY:CA	1:B:613:GLN:HE21	1.60	1.13
1:A:21:ARG:HB2	1:A:66:HIS:O	1.49	1.12
1:A:21:ARG:HB3	1:A:67:ALA:HA	1.21	1.12
1:A:57:PRO:HB3	1:A:273:ARG:HH12	0.99	1.11
1:A:171:VAL:HG21	2:D:2:NAG:C7	1.82	1.09
1:B:441:LEU:HD23	1:B:509:ARG:CZ	1.81	1.09
1:A:124:THR:HG22	2:D:1:NAG:H82	1.07	1.06
1:A:765:ARG:NH1	1:C:957:GLN:NE2	2.02	1.06
1:C:905:ARG:NH1	1:C:1050:MET:CB	2.18	1.05
1:B:462:LYS:HB2	1:B:463:PRO:CD	1.87	1.04
1:A:490:PHE:CD1	1:A:491:PRO:HD2	1.92	1.04
1:C:1010:GLN:HB3	1:C:1014:ARG:NH1	1.72	1.03
1:C:905:ARG:CZ	1:C:1050:MET:HB3	1.86	1.02
1:A:490:PHE:HD1	1:A:491:PRO:HD2	1.18	1.02
1:C:1010:GLN:HB3	1:C:1014:ARG:HH12	1.20	1.02
1:B:457:ARG:CZ	1:B:461:LEU:HB3	1.89	1.01
1:A:1107:ARG:HD3	1:B:904:TYR:CD2	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:900:MET:O	1:C:904:TYR:HD2	1.34	1.01
1:C:442:ASP:CG	1:C:509:ARG:HH21	1.70	1.00
1:A:124:THR:CG2	2:D:1:NAG:H82	1.92	1.00
1:C:896:ILE:HD11	1:C:904:TYR:CE2	1.96	0.99
1:C:22:THR:HG23	1:C:66:HIS:HB2	1.44	0.99
1:A:273:ARG:HG3	1:A:273:ARG:HH11	1.25	0.98
1:A:765:ARG:NH1	1:C:957:GLN:CD	2.21	0.98
1:A:57:PRO:HB3	1:A:273:ARG:NH1	1.79	0.98
1:B:905:ARG:CZ	1:B:1050:MET:HB3	1.93	0.98
1:B:353:TRP:O	1:B:466:ARG:NH1	1.97	0.97
1:A:347:PHE:HB3	1:A:401:VAL:HG23	1.46	0.97
1:C:742:ILE:O	1:C:1000:ARG:NH1	1.97	0.97
1:B:905:ARG:NH1	1:B:1050:MET:HB3	1.78	0.96
1:A:124:THR:HG22	2:D:1:NAG:C8	1.95	0.95
1:B:905:ARG:NH1	1:B:1049:LEU:O	1.99	0.95
1:B:246:ARG:NE	1:B:256:SER:N	2.14	0.94
1:B:457:ARG:HH22	1:B:461:LEU:HB3	0.86	0.94
1:A:21:ARG:CB	1:A:67:ALA:HA	1.96	0.94
1:B:457:ARG:NH2	1:B:461:LEU:CB	2.18	0.94
1:C:453:TYR:CE2	1:C:492:LEU:HD22	2.03	0.94
1:C:279:TYR:CE1	1:C:285:ILE:HG13	2.02	0.94
1:B:905:ARG:NH2	1:B:1050:MET:HE3	1.81	0.93
1:C:449:TYR:HA	1:C:494:SER:OG	1.68	0.93
1:C:214:ARG:HE	1:C:214:ARG:HA	1.32	0.93
1:A:21:ARG:HH12	1:A:82:PRO:HD2	1.33	0.92
1:B:441:LEU:HD23	1:B:509:ARG:NH1	1.83	0.91
1:B:580:GLN:O	5:B:1402:NAG:C8	2.20	0.90
1:A:1107:ARG:HD3	1:B:904:TYR:HE2	1.37	0.89
1:B:594:GLY:HA3	1:B:613:GLN:HE21	0.75	0.89
1:B:589:PRO:CG	1:C:855:PHE:HD1	1.87	0.88
1:A:57:PRO:CB	1:A:273:ARG:HH12	1.86	0.87
1:C:279:TYR:CE1	1:C:285:ILE:CG1	2.57	0.87
1:A:996:LEU:O	1:A:1000:ARG:HG3	1.75	0.86
1:A:21:ARG:HH22	1:A:82:PRO:HD2	1.40	0.85
1:B:462:LYS:HG2	1:B:465:GLU:OE2	1.76	0.84
1:C:905:ARG:HH12	1:C:1050:MET:HB3	1.40	0.84
1:B:441:LEU:HD23	1:B:509:ARG:NH2	1.93	0.84
1:A:347:PHE:HB3	1:A:401:VAL:CG2	2.07	0.83
1:B:457:ARG:HH22	1:B:461:LEU:CG	1.89	0.83
1:A:85:PRO:HG2	1:A:269:TYR:OH	1.77	0.83
1:C:1010:GLN:CB	1:C:1014:ARG:HH12	1.90	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:OD1	2:D:1:NAG:H3	1.77	0.82
1:B:295:PRO:HG2	1:B:636:TYR:CE1	2.15	0.82
1:A:21:ARG:NH1	1:A:82:PRO:HD2	1.94	0.82
1:A:21:ARG:HH22	1:A:82:PRO:CD	1.93	0.82
1:B:319:ARG:NH2	1:C:740:MET:CE	2.44	0.81
1:B:441:LEU:CD2	1:B:509:ARG:NH2	2.43	0.81
1:B:896:ILE:HD11	1:B:904:TYR:CE1	2.16	0.81
1:C:278:LYS:HB2	1:C:306:PHE:CZ	2.15	0.81
1:C:905:ARG:NH2	1:C:1050:MET:CE	2.41	0.81
1:C:466:ARG:HH21	1:C:466:ARG:HG3	1.45	0.80
1:A:490:PHE:HD1	1:A:491:PRO:CD	1.95	0.79
1:B:462:LYS:CB	1:B:463:PRO:CD	2.61	0.79
1:C:278:LYS:HB2	1:C:306:PHE:HZ	1.48	0.79
1:C:851:CYS:O	1:C:855:PHE:CD2	2.37	0.78
1:B:441:LEU:CD2	1:B:509:ARG:NH1	2.46	0.78
1:B:462:LYS:HB2	1:B:463:PRO:HD2	1.64	0.78
1:C:559:PHE:HD1	1:C:584:ILE:HG13	0.99	0.78
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.15	0.78
1:A:603:ASN:HD22	5:A:1404:NAG:C2	1.97	0.78
1:B:462:LYS:HB2	1:B:463:PRO:HD3	1.66	0.78
1:A:21:ARG:CB	1:A:66:HIS:O	2.30	0.77
1:B:580:GLN:O	5:B:1402:NAG:H82	1.84	0.77
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.17	0.77
1:A:490:PHE:HB2	1:A:491:PRO:CD	2.15	0.76
1:A:21:ARG:NH2	1:A:82:PRO:HD2	1.99	0.76
1:A:347:PHE:O	1:A:451:TYR:HE1	1.67	0.76
1:A:904:TYR:OH	1:C:1094:VAL:HB	1.86	0.76
1:A:142:ASP:HB2	1:A:158:ARG:CD	2.16	0.75
1:A:765:ARG:HH11	1:C:957:GLN:CD	1.93	0.75
1:C:214:ARG:HE	1:C:214:ARG:CA	2.00	0.75
1:B:589:PRO:CG	1:C:855:PHE:CD1	2.69	0.74
1:B:441:LEU:CD2	1:B:509:ARG:CZ	2.64	0.74
1:C:851:CYS:O	1:C:855:PHE:HD2	1.69	0.74
1:B:457:ARG:NH1	1:B:461:LEU:HB3	2.02	0.74
1:B:589:PRO:HG2	1:C:855:PHE:HD1	1.50	0.74
1:C:442:ASP:OD2	1:C:509:ARG:NE	2.21	0.74
1:C:847:ARG:O	1:C:847:ARG:HG2	1.86	0.74
1:C:449:TYR:CA	1:C:494:SER:OG	2.37	0.73
1:A:603:ASN:ND2	5:A:1404:NAG:O5	2.23	0.72
1:B:462:LYS:CG	1:B:463:PRO:HD2	2.19	0.72
1:B:900:MET:O	1:B:904:TYR:HD1	1.73	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:HD21	1:C:306:PHE:CD2	2.25	0.72
1:C:81:ASN:HD22	1:C:81:ASN:H	1.36	0.71
1:C:442:ASP:OD2	1:C:509:ARG:NH2	2.23	0.71
1:A:490:PHE:HB2	1:A:491:PRO:HD2	1.71	0.71
1:B:559:PHE:CD1	1:B:584:ILE:HG13	2.26	0.70
1:B:594:GLY:HA3	1:B:613:GLN:CD	2.17	0.70
1:C:453:TYR:CE2	1:C:492:LEU:HD13	2.27	0.70
1:B:457:ARG:NH2	1:B:461:LEU:HD22	2.07	0.69
1:B:319:ARG:NH2	1:C:740:MET:HE1	2.07	0.69
1:C:453:TYR:OH	1:C:492:LEU:HD21	1.89	0.69
1:B:462:LYS:CB	1:B:463:PRO:HD2	2.21	0.69
1:A:347:PHE:CB	1:A:401:VAL:CG2	2.69	0.69
1:B:589:PRO:HG2	1:C:855:PHE:CD1	2.27	0.69
1:C:1010:GLN:CB	1:C:1014:ARG:NH1	2.51	0.69
1:B:246:ARG:HE	1:B:256:SER:CA	2.06	0.69
1:C:559:PHE:CD1	1:C:584:ILE:CD1	2.76	0.69
1:B:608:VAL:CG2	1:B:636:TYR:OH	2.41	0.69
1:B:319:ARG:NH2	1:C:740:MET:HE2	2.08	0.68
1:A:57:PRO:CB	1:A:273:ARG:NH1	2.51	0.68
1:B:896:ILE:HD11	1:B:904:TYR:HE1	1.57	0.68
1:C:214:ARG:HA	1:C:214:ARG:NE	2.08	0.67
1:B:441:LEU:CD2	1:B:509:ARG:HH22	2.06	0.67
1:A:124:THR:CG2	2:D:1:NAG:C8	2.63	0.67
1:A:498:ARG:HB2	1:A:501:TYR:HB3	1.74	0.67
1:B:608:VAL:HG23	1:B:636:TYR:OH	1.94	0.66
1:A:273:ARG:HG3	1:A:273:ARG:NH1	1.96	0.66
1:B:900:MET:O	1:B:904:TYR:CD1	2.47	0.66
1:A:142:ASP:HB2	1:A:158:ARG:HD2	1.77	0.66
1:B:441:LEU:CD2	1:B:509:ARG:HH12	2.09	0.66
1:B:457:ARG:HH22	1:B:461:LEU:CD1	2.08	0.66
1:B:457:ARG:HH21	1:B:461:LEU:HD22	1.60	0.66
1:A:1107:ARG:CD	1:B:904:TYR:CE2	2.70	0.66
1:A:21:ARG:CZ	1:A:82:PRO:HD2	2.26	0.65
1:B:441:LEU:HG	1:B:509:ARG:NH2	2.11	0.65
1:C:905:ARG:HH22	1:C:1050:MET:HE3	1.57	0.65
1:C:22:THR:CG2	1:C:66:HIS:HB2	2.24	0.65
1:C:438:SER:OG	1:C:509:ARG:HG3	1.96	0.65
1:C:454:ARG:HD3	1:C:457:ARG:HG2	1.79	0.65
1:A:900:MET:O	1:A:904:TYR:HD1	1.80	0.64
1:B:441:LEU:HG	1:B:509:ARG:HH22	1.62	0.64
1:A:171:VAL:CG2	2:D:2:NAG:H81	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:CG	1:B:509:ARG:NH2	2.61	0.64
1:C:905:ARG:CZ	1:C:1050:MET:CB	2.70	0.64
1:B:281:GLU:OE1	1:B:847:ARG:NH2	2.30	0.64
1:A:328:ARG:NH1	1:A:533:LEU:HB2	2.11	0.64
1:B:905:ARG:NH1	1:B:1050:MET:CB	2.59	0.64
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.63	0.64
1:C:457:ARG:O	1:C:459:SER:O	2.15	0.63
1:C:896:ILE:HD11	1:C:904:TYR:CZ	2.34	0.63
1:C:896:ILE:CD1	1:C:904:TYR:CE2	2.80	0.63
1:B:589:PRO:HG3	1:C:855:PHE:HD1	1.63	0.63
1:C:48:LEU:HD21	1:C:306:PHE:CE2	2.34	0.62
1:A:896:ILE:HD11	1:A:904:TYR:CE1	2.34	0.62
1:A:158:ARG:HH12	1:A:258:TRP:NE1	1.97	0.62
1:C:457:ARG:O	1:C:459:SER:N	2.32	0.62
1:C:905:ARG:HH12	1:C:1050:MET:CB	1.96	0.62
1:A:319:ARG:HD2	1:B:740:MET:HE2	1.81	0.62
1:A:577:ARG:HB2	1:A:584:ILE:CD1	2.30	0.62
1:C:279:TYR:CD1	1:C:285:ILE:HG13	2.34	0.61
1:C:900:MET:HB3	1:C:904:TYR:HE2	1.65	0.61
1:C:454:ARG:HD3	1:C:456:PHE:O	2.00	0.61
1:C:900:MET:O	1:C:904:TYR:CE2	2.51	0.61
1:C:991:VAL:HG12	1:C:995:ARG:HH12	1.66	0.61
1:B:559:PHE:CZ	1:B:584:ILE:HG21	2.36	0.61
1:B:594:GLY:C	1:B:613:GLN:HG2	2.26	0.60
1:A:813:SER:OG	1:A:815:ARG:NH1	2.35	0.60
1:A:158:ARG:HH12	1:A:258:TRP:HE1	1.48	0.60
1:A:357:ARG:HB2	1:A:396:TYR:CE1	2.35	0.60
1:B:462:LYS:HG3	1:B:463:PRO:HD2	1.82	0.60
1:C:183:GLN:O	1:C:186:PHE:CD1	2.54	0.60
1:B:457:ARG:NH2	1:B:461:LEU:HD13	2.17	0.60
1:C:466:ARG:HH21	1:C:466:ARG:CG	2.11	0.60
1:B:441:LEU:HD21	1:B:509:ARG:HH12	1.66	0.59
1:A:353:TRP:CZ3	1:A:466:ARG:NH2	2.70	0.59
1:C:1093:GLY:HA2	1:C:1107:ARG:HG3	1.83	0.59
1:A:21:ARG:HB2	1:A:66:HIS:C	2.26	0.59
1:B:457:ARG:NH2	1:B:461:LEU:CG	2.59	0.58
1:C:442:ASP:CG	1:C:509:ARG:NH2	2.52	0.58
1:C:21:ARG:HD2	1:C:65:PHE:CD1	2.39	0.58
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.39	0.58
1:B:457:ARG:HH22	1:B:461:LEU:HD13	1.69	0.58
1:B:996:LEU:O	1:B:1000:ARG:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:ARG:CD	1:B:904:TYR:HE2	2.10	0.58
1:B:441:LEU:CG	1:B:509:ARG:HH22	2.15	0.58
1:B:457:ARG:NH2	1:B:461:LEU:CD2	2.68	0.57
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.37	0.57
1:A:490:PHE:CB	1:A:491:PRO:HD2	2.34	0.57
1:C:676:THR:HG23	1:C:676:THR:O	2.04	0.57
1:B:594:GLY:O	1:B:613:GLN:HG2	2.05	0.56
1:A:57:PRO:HG3	1:A:273:ARG:NH1	2.20	0.56
1:C:278:LYS:HG3	1:C:306:PHE:CE2	2.40	0.56
1:C:900:MET:C	1:C:904:TYR:CD2	2.78	0.56
1:A:21:ARG:HB3	1:A:67:ALA:CA	2.14	0.56
1:C:182:LYS:HA	1:C:186:PHE:CE1	2.40	0.56
1:B:462:LYS:CG	1:B:465:GLU:OE2	2.51	0.56
1:A:61:ASN:HD21	5:A:1401:NAG:C1	2.09	0.56
1:A:328:ARG:HH12	1:A:533:LEU:HB2	1.69	0.56
1:B:559:PHE:CD1	1:B:559:PHE:N	2.73	0.56
1:C:912:THR:HG22	1:C:1106:GLN:NE2	2.21	0.56
1:A:678:THR:HG23	1:A:678:THR:O	2.04	0.56
1:A:896:ILE:HD11	1:A:904:TYR:HE1	1.70	0.56
1:B:295:PRO:CG	1:B:636:TYR:CE1	2.86	0.56
1:B:905:ARG:HH21	1:B:1050:MET:HE3	1.62	0.56
1:B:559:PHE:HB2	1:B:577:ARG:NH2	2.20	0.56
1:B:559:PHE:HB2	1:B:577:ARG:HH21	1.70	0.56
1:A:347:PHE:O	1:A:451:TYR:CE1	2.55	0.56
1:A:765:ARG:CZ	1:C:957:GLN:NE2	2.69	0.56
1:A:490:PHE:CD1	1:A:491:PRO:CD	2.77	0.55
1:A:57:PRO:CG	1:A:273:ARG:NH1	2.70	0.55
1:C:83:VAL:HG13	1:C:237:ARG:HD3	1.88	0.55
1:C:902:MET:SD	1:C:905:ARG:HD2	2.46	0.55
1:B:594:GLY:CA	1:B:613:GLN:NE2	2.31	0.54
1:B:102:ARG:O	1:B:121:ASN:HB3	2.07	0.54
1:B:905:ARG:CZ	1:B:1050:MET:CB	2.79	0.54
1:B:1039:ARG:NH2	1:C:1031:GLU:OE2	2.40	0.54
1:A:21:ARG:HH12	1:A:82:PRO:CD	2.16	0.54
1:C:442:ASP:OD2	1:C:509:ARG:CZ	2.56	0.54
1:C:454:ARG:HD3	1:C:457:ARG:CG	2.38	0.54
1:A:142:ASP:CB	1:A:158:ARG:HD2	2.37	0.54
1:C:559:PHE:HB2	1:C:577:ARG:NH2	2.23	0.53
1:A:171:VAL:CG2	2:D:2:NAG:C7	2.66	0.53
1:B:580:GLN:O	5:B:1402:NAG:H81	2.04	0.53
1:C:278:LYS:CB	1:C:306:PHE:HZ	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LYS:CB	1:C:306:PHE:CZ	2.90	0.53
2:D:1:NAG:H62	2:D:2:NAG:H82	1.91	0.53
1:B:457:ARG:HH12	1:B:461:LEU:HB3	1.72	0.53
1:A:490:PHE:CG	1:A:491:PRO:HD2	2.42	0.53
1:A:21:ARG:HG3	1:A:21:ARG:HH11	1.74	0.53
1:A:1094:VAL:CG2	1:B:904:TYR:OH	2.56	0.53
1:A:171:VAL:HG22	2:D:2:NAG:H81	1.91	0.52
1:B:102:ARG:NH1	1:B:122:ASN:HA	2.24	0.52
1:A:1107:ARG:HD3	1:B:904:TYR:HD2	1.68	0.52
1:B:905:ARG:CZ	1:B:1050:MET:HE3	2.38	0.52
1:C:453:TYR:CE1	1:C:492:LEU:HD22	2.24	0.52
1:B:559:PHE:HD1	1:B:559:PHE:H	1.56	0.52
1:B:246:ARG:O	1:B:246:ARG:HG2	2.09	0.52
1:A:171:VAL:CG2	2:D:2:NAG:C8	2.88	0.52
1:B:1094:VAL:CG2	1:C:904:TYR:OH	2.58	0.52
1:A:142:ASP:CG	1:A:158:ARG:HD2	2.35	0.51
1:B:608:VAL:HG22	1:B:636:TYR:OH	2.10	0.51
1:B:319:ARG:HH21	1:C:740:MET:CE	2.23	0.51
1:A:1107:ARG:CD	1:B:904:TYR:CD2	2.82	0.51
1:A:676:THR:N	1:A:690:GLN:OE1	2.44	0.51
1:C:278:LYS:HB2	1:C:306:PHE:CE2	2.46	0.51
1:B:319:ARG:HH21	1:C:740:MET:HE1	1.75	0.51
1:A:21:ARG:HH22	1:A:82:PRO:CG	2.24	0.51
1:A:904:TYR:OH	1:C:1094:VAL:CB	2.57	0.50
1:C:22:THR:HG23	1:C:22:THR:O	2.11	0.50
1:C:81:ASN:HD22	1:C:81:ASN:N	2.00	0.50
1:C:567:ARG:NH1	1:C:571:ASP:O	2.44	0.50
1:B:438:SER:HB2	1:B:509:ARG:HG3	1.93	0.49
1:C:20:THR:HG22	1:C:80:ASP:OD2	2.11	0.49
1:C:900:MET:C	1:C:904:TYR:HD2	2.13	0.49
1:A:328:ARG:NH2	1:A:580:GLN:HB2	2.27	0.49
1:A:375:PHE:HD1	1:A:436:TRP:HA	1.75	0.49
1:A:900:MET:O	1:A:904:TYR:CD1	2.62	0.49
1:B:1094:VAL:HG21	1:C:904:TYR:OH	2.12	0.49
1:C:449:TYR:C	1:C:494:SER:HG	2.20	0.49
1:C:901:GLN:O	1:C:905:ARG:HG3	2.12	0.49
1:C:457:ARG:NE	1:C:457:ARG:HA	2.28	0.49
1:A:127:VAL:HG11	2:D:1:NAG:O6	2.13	0.48
1:B:557:LYS:HB2	1:B:559:PHE:HE1	1.78	0.48
1:B:319:ARG:HH22	1:C:740:MET:CE	2.24	0.48
1:A:85:PRO:CG	1:A:269:TYR:OH	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:CE1	1:B:584:ILE:CG2	2.74	0.48
1:B:577:ARG:HB2	1:B:584:ILE:CD1	2.42	0.48
1:C:214:ARG:CA	1:C:214:ARG:NE	2.72	0.48
1:C:900:MET:HB3	1:C:904:TYR:CE2	2.46	0.48
1:C:48:LEU:CD2	1:C:306:PHE:CE2	2.97	0.48
1:C:559:PHE:HD1	1:C:584:ILE:CG1	1.85	0.48
1:B:577:ARG:CZ	1:B:584:ILE:HD11	2.44	0.48
1:B:295:PRO:CD	1:B:636:TYR:HE1	2.27	0.48
1:C:279:TYR:CE1	1:C:285:ILE:HG12	2.43	0.48
1:A:1107:ARG:NH1	1:B:904:TYR:CD2	2.82	0.47
1:B:457:ARG:HD3	1:B:459:SER:O	2.14	0.47
1:B:20:THR:HG22	1:B:80:ASP:OD2	2.14	0.47
1:A:498:ARG:HB2	1:A:501:TYR:CB	2.43	0.47
1:A:603:ASN:ND2	5:A:1404:NAG:C2	2.68	0.47
1:B:557:LYS:CB	1:B:559:PHE:HE1	2.28	0.47
1:B:965:GLN:NE2	1:C:762:GLN:HE22	2.13	0.47
1:C:466:ARG:CG	1:C:466:ARG:NH2	2.72	0.47
1:A:42:VAL:CG1	1:C:567:ARG:HG2	2.44	0.47
1:A:346:ARG:NH1	1:A:450:ASN:HB3	2.30	0.47
1:B:995:ARG:NH2	1:C:994:ASP:OD1	2.48	0.47
1:A:319:ARG:HG2	1:A:592:PHE:HB2	1.98	0.46
1:C:81:ASN:H	1:C:81:ASN:ND2	2.09	0.46
1:C:176:LEU:CD1	1:C:190:ARG:HD3	2.45	0.46
1:A:765:ARG:HH12	1:C:957:GLN:CD	2.18	0.46
1:B:1091:ARG:NH1	1:B:1091:ARG:HG3	2.30	0.46
1:B:896:ILE:CD1	1:B:904:TYR:CE1	2.94	0.46
1:B:457:ARG:CD	1:B:459:SER:O	2.64	0.46
1:B:102:ARG:HH11	1:B:122:ASN:HA	1.81	0.46
1:A:44:ARG:HG2	1:C:567:ARG:HB2	1.97	0.45
1:A:996:LEU:O	1:A:1000:ARG:CG	2.58	0.45
1:A:171:VAL:HG21	2:D:2:NAG:C8	2.42	0.45
1:B:1107:ARG:HD3	1:C:904:TYR:CD1	2.52	0.45
1:A:1094:VAL:HG21	1:B:904:TYR:OH	2.17	0.45
1:C:278:LYS:HG3	1:C:306:PHE:HE2	1.80	0.45
1:A:765:ARG:NH1	1:C:957:GLN:CG	2.79	0.45
1:C:678:THR:HG23	1:C:678:THR:O	2.16	0.45
1:A:490:PHE:CB	1:A:491:PRO:CD	2.88	0.45
1:B:1156:PHE:CZ	1:C:1155:TYR:HB3	2.52	0.45
1:A:142:ASP:HB2	1:A:158:ARG:HD3	1.95	0.45
1:A:674:TYR:CZ	1:A:690:GLN:HB3	2.52	0.45
1:B:557:LYS:HB3	1:B:559:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:VAL:CG1	1:C:237:ARG:HD3	2.48	0.44
1:B:423:TYR:O	1:B:423:TYR:CD1	2.71	0.44
1:B:581:THR:HG22	5:B:1402:NAG:C8	2.47	0.44
1:B:569:ILE:HD12	1:B:569:ILE:H	1.83	0.44
1:B:1039:ARG:NH1	1:B:1042:PHE:CZ	2.86	0.44
1:C:183:GLN:O	1:C:186:PHE:HD1	1.96	0.43
1:C:173:GLN:HB3	1:C:174:PRO:HD2	2.00	0.43
1:C:905:ARG:HH21	1:C:1050:MET:HE3	1.63	0.43
1:C:902:MET:HA	1:C:905:ARG:HD2	1.99	0.43
1:A:765:ARG:HH12	1:C:957:GLN:CG	2.32	0.43
1:A:328:ARG:O	1:A:579:PRO:CG	2.67	0.43
1:A:577:ARG:HB2	1:A:584:ILE:HD13	2.01	0.43
1:B:678:THR:HG23	1:B:678:THR:O	2.18	0.43
1:B:756:TYR:CE1	1:B:997:ILE:HG21	2.55	0.42
1:C:520:ALA:HB3	1:C:521:PRO:HD3	2.01	0.42
1:A:21:ARG:CB	1:A:67:ALA:CA	2.84	0.42
1:A:21:ARG:NH1	1:A:21:ARG:HG3	2.34	0.42
1:B:382:VAL:HA	1:C:983:ARG:O	2.20	0.42
1:C:715:PRO:HG2	1:C:1108:ASN:O	2.19	0.42
1:A:472:ILE:HD12	1:A:490:PHE:HD2	1.83	0.42
1:A:600:PRO:HD3	1:A:692:ILE:HD11	2.02	0.42
1:A:42:VAL:HG11	1:C:567:ARG:HG2	2.02	0.42
1:B:580:GLN:O	5:B:1402:NAG:C7	2.68	0.42
1:C:99:ASN:O	1:C:102:ARG:NH1	2.27	0.42
1:A:676:THR:HG22	1:A:678:THR:HB	2.01	0.42
1:A:996:LEU:HD13	1:A:1000:ARG:HH21	1.85	0.42
1:A:21:ARG:HH22	1:A:82:PRO:HG2	1.84	0.41
1:C:1107:ARG:HG3	1:C:1107:ARG:H	1.44	0.41
1:B:457:ARG:HG2	1:B:459:SER:O	2.20	0.41
1:C:577:ARG:CZ	1:C:584:ILE:HD11	2.50	0.41
1:B:173:GLN:H	1:B:174:PRO:CD	2.33	0.41
1:B:439:ASN:ND2	1:B:506:GLN:HE21	2.18	0.41
1:C:457:ARG:NE	1:C:457:ARG:CA	2.84	0.41
1:C:900:MET:C	1:C:904:TYR:CE2	2.99	0.41
1:C:896:ILE:HD11	1:C:904:TYR:HE2	1.72	0.41
1:A:126:VAL:HG23	1:A:174:PRO:HA	2.03	0.41
1:A:158:ARG:HH22	1:A:258:TRP:HZ2	1.69	0.41
1:B:144:TYR:CD1	1:B:246:ARG:HB3	2.56	0.41
1:A:347:PHE:HB2	1:A:401:VAL:CG2	2.49	0.40
1:A:675:GLN:HA	1:A:690:GLN:OE1	2.22	0.40
1:B:559:PHE:O	1:B:577:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HB2	1:A:396:TYR:HE1	1.84	0.40
1:C:1010:GLN:O	1:C:1014:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1108/1305 (85%)	1024 (92%)	66 (6%)	18 (2%)	7	30
1	B	1117/1305 (86%)	1013 (91%)	90 (8%)	14 (1%)	9	35
1	C	1114/1305 (85%)	1025 (92%)	67 (6%)	22 (2%)	6	25
All	All	3339/3915 (85%)	3062 (92%)	223 (7%)	54 (2%)	10	30

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	VAL
1	A	490	PHE
1	A	986	LYS
1	B	70	VAL
1	B	173	GLN
1	B	246	ARG
1	B	462	LYS
1	B	490	PHE
1	C	70	VAL
1	C	212	LEU
1	C	215	ASP
1	C	258	TRP
1	C	458	LYS
1	A	136	CYS
1	A	212	LEU

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Mol	Chain	Res	Type
1	A	678	THR
1	A	1041	ASP
1	B	174	PRO
1	B	830	ASP
1	C	123	ALA
1	C	159	VAL
1	C	520	ALA
1	A	46	SER
1	A	215	ASP
1	B	1041	ASP
1	C	132	GLU
1	C	497	PHE
1	C	830	ASP
1	C	837	TYR
1	A	88	ASP
1	A	182	LYS
1	A	258	TRP
1	A	345	THR
1	A	623	ALA
1	B	137	ASN
1	B	291	CYS
1	C	88	ASP
1	C	124	THR
1	C	136	CYS
1	C	164	ASN
1	C	175	PHE
1	C	836	GLN
1	A	41	LYS
1	A	246	ARG
1	A	837	TYR
1	A	1084	ASP
1	B	88	ASP
1	C	186	PHE
1	C	490	PHE
1	B	449	TYR
1	B	472	ILE
1	C	527	PRO
1	C	678	THR
1	B	381	GLY

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	975/1130 (86%)	952 (98%)	23 (2%)	43	69
1	B	979/1130 (87%)	963 (98%)	16 (2%)	55	75
1	C	976/1130 (86%)	949 (97%)	27 (3%)	38	66
All	All	2930/3390 (86%)	2864 (98%)	66 (2%)	44	70

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	CYS
1	A	20	THR
1	A	21	ARG
1	A	29	THR
1	A	120	VAL
1	A	144	TYR
1	A	157	PHE
1	A	179	LEU
1	A	227	VAL
1	A	273	ARG
1	A	347	PHE
1	A	398	ASP
1	A	418	ILE
1	A	422	ASN
1	A	461	LEU
1	A	489	TYR
1	A	490	PHE
1	A	495	TYR
1	A	677	GLN
1	A	738	CYS
1	A	747	THR
1	A	804	GLN
1	A	1152	LEU
1	B	179	LEU
1	B	207	HIS
1	B	394	ASN

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Mol	Chain	Res	Type
1	B	429	PHE
1	B	461	LEU
1	B	472	ILE
1	B	559	PHE
1	B	574	ASP
1	B	583	GLU
1	B	761	THR
1	B	763	LEU
1	B	840	CYS
1	B	854	LYS
1	B	988	GLU
1	B	1081	ILE
1	B	1092	GLU
1	C	81	ASN
1	C	144	TYR
1	C	175	PHE
1	C	178	ASP
1	C	188	ASN
1	C	198	ASP
1	C	214	ARG
1	C	216	LEU
1	C	223	LEU
1	C	227	VAL
1	C	391	CYS
1	C	457	ARG
1	C	466	ARG
1	C	495	TYR
1	C	512	VAL
1	C	515	PHE
1	C	525	CYS
1	C	540	ASN
1	C	556	ASN
1	C	738	CYS
1	C	753	LEU
1	C	836	GLN
1	C	914	ASN
1	C	977	LEU
1	C	985	ASP
1	C	994	ASP
1	C	1106	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	66	HIS
1	A	69	HIS
1	A	87	ASN
1	A	134	GLN
1	A	149	ASN
1	A	207	HIS
1	A	211	ASN
1	A	370	ASN
1	A	394	ASN
1	A	450	ASN
1	A	540	ASN
1	A	603	ASN
1	A	677	GLN
1	A	703	ASN
1	A	755	GLN
1	A	853	GLN
1	A	907	ASN
1	A	1002	GLN
1	A	1054	GLN
1	B	49	HIS
1	B	121	ASN
1	B	134	GLN
1	B	146	HIS
1	B	148	ASN
1	B	282	ASN
1	B	317	ASN
1	B	354	ASN
1	B	394	ASN
1	B	409	GLN
1	B	506	GLN
1	B	536	ASN
1	B	607	GLN
1	B	613	GLN
1	B	755	GLN
1	B	787	GLN
1	B	856	ASN
1	B	907	ASN
1	B	913	GLN
1	B	935	GLN
1	B	965	GLN
1	B	1002	GLN
1	B	1011	GLN

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Mol	Chain	Res	Type
1	B	1048	HIS
1	B	1113	GLN
1	B	1135	ASN
1	C	81	ASN
1	C	137	ASN
1	C	146	HIS
1	C	148	ASN
1	C	188	ASN
1	C	196	ASN
1	C	218	GLN
1	C	239	GLN
1	C	370	ASN
1	C	417	ASN
1	C	448	ASN
1	C	544	ASN
1	C	564	GLN
1	C	690	GLN
1	C	824	ASN
1	C	914	ASN
1	C	957	GLN
1	C	1005	GLN
1	C	1058	HIS
1	C	1135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

79 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	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	D	2	2	14,14,15	1.34	3 (21%)	17,19,21	0.93	1 (5%)
2	MAN	D	3	2	11,11,12	1.73	3 (27%)	15,15,17	0.95	0
3	NAG	E	1	3,1	14,14,15	1.48	3 (21%)	17,19,21	0.91	0
3	NAG	E	2	3	14,14,15	1.46	3 (21%)	17,19,21	1.20	1 (5%)
2	NAG	F	1	1,2	14,14,15	1.32	2 (14%)	17,19,21	0.91	0
2	NAG	F	2	2	14,14,15	1.63	4 (28%)	17,19,21	0.82	1 (5%)
2	MAN	F	3	2	11,11,12	1.73	3 (27%)	15,15,17	0.85	1 (6%)
3	NAG	G	1	3,1	14,14,15	1.12	1 (7%)	17,19,21	0.76	0
3	NAG	G	2	3	14,14,15	1.58	4 (28%)	17,19,21	0.92	1 (5%)
2	NAG	H	1	1,2	14,14,15	1.34	3 (21%)	17,19,21	0.86	0
2	NAG	H	2	2	14,14,15	1.35	3 (21%)	17,19,21	0.86	1 (5%)
2	MAN	H	3	2	11,11,12	1.60	2 (18%)	15,15,17	1.25	1 (6%)
2	NAG	I	1	1,2	14,14,15	1.10	2 (14%)	17,19,21	0.70	0
2	NAG	I	2	2	14,14,15	1.40	3 (21%)	17,19,21	0.88	1 (5%)
2	MAN	I	3	2	11,11,12	1.34	1 (9%)	15,15,17	0.91	0
4	NAG	J	1	1,4	14,14,15	1.39	2 (14%)	17,19,21	1.27	2 (11%)
4	NAG	J	2	4	14,14,15	1.50	4 (28%)	17,19,21	1.01	1 (5%)
4	FUC	J	3	4	10,10,11	1.59	3 (30%)	14,14,16	1.08	2 (14%)
2	NAG	K	1	1,2	14,14,15	0.86	1 (7%)	17,19,21	1.04	1 (5%)
2	NAG	K	2	2	14,14,15	1.53	3 (21%)	17,19,21	0.79	1 (5%)
2	MAN	K	3	2	11,11,12	1.43	1 (9%)	15,15,17	1.14	2 (13%)
2	NAG	L	1	1,2	14,14,15	1.18	2 (14%)	17,19,21	0.87	0
2	NAG	L	2	2	14,14,15	1.46	3 (21%)	17,19,21	0.96	1 (5%)
2	MAN	L	3	2	11,11,12	1.59	2 (18%)	15,15,17	1.28	1 (6%)
2	NAG	M	1	1,2	14,14,15	1.23	1 (7%)	17,19,21	1.15	2 (11%)
2	NAG	M	2	2	14,14,15	1.62	2 (14%)	17,19,21	0.98	1 (5%)
2	MAN	M	3	2	11,11,12	1.70	2 (18%)	15,15,17	0.86	1 (6%)
3	NAG	N	1	3,1	14,14,15	1.49	4 (28%)	17,19,21	0.93	1 (5%)
3	NAG	N	2	3	14,14,15	1.26	3 (21%)	17,19,21	0.85	0
3	NAG	O	1	3,1	14,14,15	1.44	3 (21%)	17,19,21	0.97	1 (5%)
3	NAG	O	2	3	14,14,15	1.44	4 (28%)	17,19,21	0.83	1 (5%)
2	NAG	P	1	2	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	P	2	2	14,14,15	1.44	2 (14%)	17,19,21	1.08	1 (5%)
2	MAN	P	3	2	11,11,12	1.57	1 (9%)	15,15,17	1.27	2 (13%)
3	NAG	Q	1	3,1	14,14,15	1.42	2 (14%)	17,19,21	0.63	0
3	NAG	Q	2	3	14,14,15	1.26	2 (14%)	17,19,21	1.29	2 (11%)
2	NAG	R	1	1,2	14,14,15	1.22	2 (14%)	17,19,21	1.07	1 (5%)
2	NAG	R	2	2	14,14,15	1.37	2 (14%)	17,19,21	1.14	1 (5%)
2	MAN	R	3	2	11,11,12	1.65	1 (9%)	15,15,17	1.04	1 (6%)
2	NAG	S	1	1,2	14,14,15	1.08	1 (7%)	17,19,21	0.94	0
2	NAG	S	2	2	14,14,15	1.19	1 (7%)	17,19,21	1.17	1 (5%)
2	MAN	S	3	2	11,11,12	1.38	2 (18%)	15,15,17	0.51	0
4	NAG	T	1	1,4	14,14,15	1.08	1 (7%)	17,19,21	0.97	0
4	NAG	T	2	4	14,14,15	1.37	1 (7%)	17,19,21	0.79	0
4	FUC	T	3	4	10,10,11	1.71	2 (20%)	14,14,16	0.91	0
2	NAG	U	1	1,2	14,14,15	1.42	3 (21%)	17,19,21	1.11	0
2	NAG	U	2	2	14,14,15	1.21	2 (14%)	17,19,21	0.96	0
2	MAN	U	3	2	11,11,12	1.38	1 (9%)	15,15,17	0.93	0
2	NAG	V	1	1,2	14,14,15	1.17	1 (7%)	17,19,21	0.79	0
2	NAG	V	2	2	14,14,15	1.21	2 (14%)	17,19,21	0.65	0
2	MAN	V	3	2	11,11,12	1.81	2 (18%)	15,15,17	0.98	1 (6%)
2	NAG	W	1	1,2	14,14,15	1.69	5 (35%)	17,19,21	0.99	1 (5%)
2	NAG	W	2	2	14,14,15	1.35	4 (28%)	17,19,21	0.96	1 (5%)
2	MAN	W	3	2	11,11,12	1.60	2 (18%)	15,15,17	0.87	0
3	NAG	X	1	3,1	14,14,15	1.23	1 (7%)	17,19,21	0.80	0
3	NAG	X	2	3	14,14,15	1.59	4 (28%)	17,19,21	0.73	0
3	NAG	Y	1	3,1	14,14,15	1.54	3 (21%)	17,19,21	1.29	1 (5%)
3	NAG	Y	2	3	14,14,15	1.48	2 (14%)	17,19,21	0.98	1 (5%)
2	NAG	Z	1	1,2	14,14,15	1.37	3 (21%)	17,19,21	0.91	1 (5%)
2	NAG	Z	2	2	14,14,15	1.57	3 (21%)	17,19,21	0.76	1 (5%)
2	MAN	Z	3	2	11,11,12	1.88	3 (27%)	15,15,17	0.98	0
3	NAG	a	1	3,1	14,14,15	1.46	3 (21%)	17,19,21	1.02	1 (5%)
3	NAG	a	2	3	14,14,15	1.52	4 (28%)	17,19,21	1.10	2 (11%)
2	NAG	b	1	1,2	14,14,15	1.33	3 (21%)	17,19,21	1.03	1 (5%)
2	NAG	b	2	2	14,14,15	1.41	2 (14%)	17,19,21	0.98	1 (5%)
2	MAN	b	3	2	11,11,12	1.67	2 (18%)	15,15,17	1.16	2 (13%)
2	NAG	c	1	1,2	14,14,15	1.25	2 (14%)	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	c	2	2	14,14,15	1.23	2 (14%)	17,19,21	1.09	2 (11%)
2	MAN	c	3	2	11,11,12	1.44	2 (18%)	15,15,17	0.90	1 (6%)
4	NAG	d	1	1,4	14,14,15	1.51	2 (14%)	17,19,21	1.07	1 (5%)
4	NAG	d	2	4	14,14,15	1.29	2 (14%)	17,19,21	0.91	0
4	FUC	d	3	4	10,10,11	1.82	3 (30%)	14,14,16	1.11	0
2	NAG	e	1	1,2	14,14,15	1.27	2 (14%)	17,19,21	0.86	0
2	NAG	e	2	2	14,14,15	1.31	1 (7%)	17,19,21	0.90	1 (5%)
2	MAN	e	3	2	11,11,12	1.57	3 (27%)	15,15,17	1.04	1 (6%)
2	NAG	f	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	0.97	1 (5%)
2	NAG	f	2	2	14,14,15	1.35	2 (14%)	17,19,21	0.90	0
2	MAN	f	3	2	11,11,12	1.44	2 (18%)	15,15,17	1.15	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	2	-	2/6/23/26	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	3,1	-	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
2	MAN	F	3	2	-	0/2/19/22	1/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	MAN	H	3	2	-	0/2/19/22	1/1/1/1
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	-	1/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	MAN	K	3	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/2/19/22	1/1/1/1
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	-	1/2/19/22	1/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2	-	2/6/23/26	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	1/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	MAN	R	3	2	-	0/2/19/22	1/1/1/1
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	-	1/2/19/22	1/1/1/1
4	NAG	T	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	FUC	T	3	4	-	-	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	MAN	U	3	2	-	1/2/19/22	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	-	0/2/19/22	1/1/1/1
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	-	1/2/19/22	1/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
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	1/1/1/1
3	NAG	a	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	a	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	b	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	MAN	b	3	2	-	0/2/19/22	1/1/1/1
2	NAG	c	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	MAN	c	3	2	-	1/2/19/22	0/1/1/1
4	NAG	d	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	FUC	d	3	4	-	-	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	MAN	e	3	2	-	1/2/19/22	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	-	0/2/19/22	1/1/1/1

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	2	NAG	O5-C5	4.03	1.51	1.43
2	Z	3	MAN	O5-C5	3.91	1.51	1.43
2	W	3	MAN	O5-C5	3.81	1.50	1.43
4	T	2	NAG	O5-C5	3.80	1.50	1.43
2	M	2	NAG	O5-C5	3.67	1.50	1.43
3	Y	1	NAG	C1-C2	3.62	1.57	1.52
2	L	3	MAN	O5-C5	3.57	1.50	1.43
2	e	2	NAG	O5-C5	3.53	1.50	1.43
2	K	2	NAG	O5-C5	3.48	1.50	1.43
2	L	2	NAG	O5-C5	3.47	1.50	1.43
4	d	3	FUC	O5-C5	3.45	1.50	1.43
2	b	3	MAN	O5-C5	3.45	1.50	1.43
2	R	3	MAN	O5-C5	3.40	1.50	1.43
4	T	3	FUC	O5-C5	3.38	1.50	1.43
4	d	1	NAG	O5-C5	3.37	1.50	1.43
2	P	3	MAN	O5-C5	3.35	1.50	1.43
2	U	1	NAG	O5-C5	3.28	1.49	1.43
2	V	3	MAN	O5-C1	3.26	1.49	1.43
3	G	2	NAG	O5-C5	3.25	1.49	1.43
2	D	3	MAN	O5-C5	3.21	1.49	1.43
2	Z	2	NAG	O5-C5	3.20	1.49	1.43
2	D	2	NAG	O5-C5	3.20	1.49	1.43
2	V	3	MAN	O5-C5	3.19	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	2	NAG	O5-C5	3.19	1.49	1.43
3	Q	1	NAG	O5-C5	3.14	1.49	1.43
2	F	2	NAG	O5-C5	3.14	1.49	1.43
2	b	3	MAN	O5-C1	3.09	1.48	1.43
2	f	2	NAG	O4-C4	3.08	1.50	1.43
4	d	2	NAG	O5-C5	3.07	1.49	1.43
4	J	2	NAG	O5-C5	3.05	1.49	1.43
2	F	2	NAG	O5-C1	3.04	1.48	1.43
3	G	1	NAG	O5-C5	3.04	1.49	1.43
2	K	3	MAN	O5-C5	2.99	1.49	1.43
3	X	1	NAG	C1-C2	2.99	1.56	1.52
2	H	3	MAN	O5-C5	2.99	1.49	1.43
2	M	3	MAN	O5-C1	2.97	1.48	1.43
3	a	1	NAG	O5-C5	2.96	1.49	1.43
2	b	1	NAG	O5-C5	2.92	1.49	1.43
2	I	3	MAN	O5-C5	2.92	1.49	1.43
2	f	3	MAN	O5-C1	2.91	1.48	1.43
2	c	1	NAG	O5-C5	2.90	1.49	1.43
2	M	3	MAN	O5-C5	2.90	1.49	1.43
2	U	3	MAN	O5-C5	2.90	1.49	1.43
3	E	1	NAG	O5-C5	2.87	1.49	1.43
3	X	2	NAG	O5-C5	2.85	1.49	1.43
4	J	3	FUC	O5-C1	2.79	1.48	1.43
2	U	2	NAG	C1-C2	2.74	1.56	1.52
3	E	2	NAG	O4-C4	2.74	1.49	1.43
3	G	2	NAG	C1-C2	2.72	1.56	1.52
3	a	2	NAG	O5-C1	2.71	1.48	1.43
2	R	2	NAG	O5-C5	2.71	1.48	1.43
4	d	1	NAG	O5-C1	2.71	1.48	1.43
2	F	3	MAN	O5-C5	2.71	1.48	1.43
4	T	1	NAG	O5-C5	2.70	1.48	1.43
2	M	2	NAG	O5-C1	2.70	1.48	1.43
4	J	2	NAG	O5-C1	2.67	1.48	1.43
3	E	2	NAG	O5-C5	2.67	1.48	1.43
2	W	3	MAN	O5-C1	2.67	1.48	1.43
2	W	1	NAG	C8-C7	2.67	1.56	1.50
2	F	1	NAG	O5-C5	2.67	1.48	1.43
3	Y	2	NAG	O4-C4	2.66	1.49	1.43
2	c	1	NAG	C1-C2	2.66	1.56	1.52
3	X	2	NAG	C1-C2	2.66	1.56	1.52
2	D	3	MAN	O5-C1	2.65	1.48	1.43
3	O	2	NAG	C8-C7	2.64	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1	NAG	C1-C2	2.64	1.55	1.52
2	S	3	MAN	O5-C5	2.63	1.48	1.43
3	a	1	NAG	C1-C2	2.63	1.55	1.52
2	e	1	NAG	O5-C5	2.62	1.48	1.43
2	I	2	NAG	O5-C5	2.62	1.48	1.43
2	Z	2	NAG	O4-C4	2.61	1.49	1.43
3	E	1	NAG	C1-C2	2.59	1.55	1.52
2	W	1	NAG	O5-C5	2.59	1.48	1.43
2	W	1	NAG	C1-C2	2.58	1.55	1.52
2	I	2	NAG	O5-C1	2.58	1.48	1.43
2	H	1	NAG	O4-C4	2.58	1.49	1.43
2	Z	2	NAG	O5-C1	2.58	1.48	1.43
3	a	2	NAG	O5-C5	2.57	1.48	1.43
2	R	1	NAG	C1-C2	2.55	1.55	1.52
3	Y	1	NAG	O5-C5	2.55	1.48	1.43
4	J	1	NAG	C8-C7	2.53	1.55	1.50
3	N	1	NAG	O5-C5	2.53	1.48	1.43
3	O	2	NAG	O5-C5	2.53	1.48	1.43
2	M	1	NAG	O5-C1	2.50	1.47	1.43
4	J	3	FUC	O5-C5	2.50	1.48	1.43
4	d	3	FUC	O5-C1	2.49	1.47	1.43
2	b	2	NAG	O4-C4	2.49	1.49	1.43
3	O	2	NAG	O4-C4	2.49	1.49	1.43
2	F	2	NAG	C1-C2	2.48	1.55	1.52
2	W	1	NAG	O5-C1	2.48	1.47	1.43
2	f	3	MAN	O5-C5	2.48	1.48	1.43
3	Q	2	NAG	C1-C2	2.47	1.55	1.52
2	H	3	MAN	O5-C1	2.46	1.47	1.43
2	c	2	NAG	O5-C1	2.46	1.47	1.43
2	S	1	NAG	O5-C1	2.45	1.47	1.43
3	E	1	NAG	O4-C4	2.44	1.49	1.43
2	c	3	MAN	O5-C5	2.44	1.48	1.43
3	G	2	NAG	O5-C1	2.44	1.47	1.43
2	Z	1	NAG	C1-C2	2.44	1.55	1.52
3	N	1	NAG	C1-C2	2.42	1.55	1.52
2	H	1	NAG	O5-C5	2.42	1.48	1.43
2	L	1	NAG	O5-C5	2.41	1.48	1.43
3	a	2	NAG	C1-C2	2.39	1.55	1.52
3	N	1	NAG	C8-C7	2.39	1.55	1.50
2	H	2	NAG	O5-C5	2.39	1.48	1.43
3	G	2	NAG	O3-C3	2.39	1.48	1.43
3	O	1	NAG	O4-C4	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	O4-C4	2.38	1.48	1.43
2	I	1	NAG	O5-C5	2.36	1.48	1.43
3	N	2	NAG	O5-C5	2.35	1.48	1.43
2	W	2	NAG	C8-C7	2.35	1.55	1.50
3	E	2	NAG	O5-C1	2.35	1.47	1.43
3	Q	1	NAG	C8-C7	2.33	1.55	1.50
2	L	3	MAN	C2-C3	2.31	1.56	1.52
2	D	2	NAG	C8-C7	2.31	1.55	1.50
2	P	2	NAG	O4-C4	2.30	1.48	1.43
2	e	3	MAN	O5-C5	2.29	1.47	1.43
3	N	2	NAG	C8-C7	2.29	1.55	1.50
2	I	1	NAG	O5-C1	2.29	1.47	1.43
2	W	2	NAG	O5-C5	2.28	1.47	1.43
2	W	1	NAG	O4-C4	2.28	1.48	1.43
2	W	2	NAG	C1-C2	2.28	1.55	1.52
3	X	2	NAG	O5-C1	2.28	1.47	1.43
4	T	3	FUC	O5-C1	2.27	1.47	1.43
2	F	2	NAG	O4-C4	2.27	1.48	1.43
2	R	2	NAG	O4-C4	2.26	1.48	1.43
3	a	1	NAG	O5-C1	2.26	1.47	1.43
3	Y	2	NAG	O5-C5	2.25	1.47	1.43
2	F	3	MAN	C2-C3	2.25	1.55	1.52
2	K	1	NAG	O5-C5	2.24	1.47	1.43
2	R	1	NAG	O5-C5	2.24	1.47	1.43
3	O	2	NAG	O5-C1	2.23	1.47	1.43
3	N	2	NAG	O5-C1	2.22	1.47	1.43
4	J	1	NAG	O4-C4	2.22	1.48	1.43
2	V	1	NAG	O5-C5	2.21	1.47	1.43
2	b	1	NAG	C1-C2	2.21	1.55	1.52
2	V	2	NAG	O5-C5	2.19	1.47	1.43
2	Z	1	NAG	O5-C5	2.19	1.47	1.43
2	e	3	MAN	O5-C1	2.18	1.47	1.43
2	F	1	NAG	C1-C2	2.18	1.55	1.52
2	Z	1	NAG	O4-C4	2.17	1.48	1.43
3	a	2	NAG	C8-C7	2.17	1.55	1.50
2	S	3	MAN	O5-C1	2.16	1.47	1.43
2	f	2	NAG	O5-C5	2.15	1.47	1.43
2	L	2	NAG	O5-C1	2.15	1.47	1.43
2	Z	3	MAN	O5-C1	2.15	1.47	1.43
2	L	1	NAG	C1-C2	2.14	1.55	1.52
4	d	2	NAG	O5-C1	2.14	1.47	1.43
2	H	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	F	3	MAN	C1-C2	2.13	1.57	1.52
2	U	1	NAG	O4-C4	2.13	1.48	1.43
3	X	2	NAG	O3-C3	2.13	1.48	1.43
2	H	2	NAG	C8-C7	2.13	1.55	1.50
2	c	2	NAG	O5-C5	2.12	1.47	1.43
2	U	2	NAG	O5-C5	2.12	1.47	1.43
2	W	2	NAG	O4-C4	2.11	1.48	1.43
2	K	2	NAG	O5-C1	2.11	1.47	1.43
4	J	3	FUC	C1-C2	2.10	1.57	1.52
4	J	2	NAG	C1-C2	2.10	1.55	1.52
2	U	1	NAG	C8-C7	2.10	1.54	1.50
2	S	2	NAG	C1-C2	2.09	1.55	1.52
2	c	3	MAN	O5-C1	2.08	1.47	1.43
3	O	1	NAG	O5-C1	2.08	1.47	1.43
3	N	1	NAG	O4-C4	2.08	1.48	1.43
2	Z	3	MAN	O4-C4	2.06	1.48	1.43
2	D	3	MAN	O2-C2	2.06	1.47	1.43
2	f	1	NAG	O4-C4	2.06	1.48	1.43
4	J	2	NAG	C8-C7	2.05	1.54	1.50
2	K	2	NAG	C1-C2	2.04	1.55	1.52
2	b	1	NAG	O4-C4	2.04	1.48	1.43
2	L	2	NAG	C1-C2	2.03	1.55	1.52
2	H	1	NAG	C1-C2	2.03	1.55	1.52
3	Q	2	NAG	O5-C5	2.03	1.47	1.43
2	D	2	NAG	O4-C4	2.02	1.48	1.43
4	d	3	FUC	O3-C3	2.02	1.48	1.43
2	e	1	NAG	O4-C4	2.01	1.47	1.43
3	Y	1	NAG	C2-N2	2.00	1.49	1.46
2	V	2	NAG	O5-C1	2.00	1.47	1.43
2	e	3	MAN	C2-C3	2.00	1.55	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	2	NAG	C1-O5-C5	4.24	117.86	112.19
2	H	3	MAN	C1-O5-C5	4.06	117.63	112.19
2	P	3	MAN	C1-O5-C5	3.94	117.46	112.19
4	J	1	NAG	C1-O5-C5	3.84	117.33	112.19
2	S	2	NAG	C1-O5-C5	3.66	117.09	112.19
2	L	3	MAN	C1-O5-C5	3.59	117.00	112.19
2	R	3	MAN	C1-O5-C5	3.24	116.53	112.19
2	b	3	MAN	C1-O5-C5	3.22	116.51	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1	NAG	C1-O5-C5	3.21	116.48	112.19
2	M	2	NAG	C1-O5-C5	3.13	116.38	112.19
2	R	2	NAG	C3-C4-C5	3.11	115.87	110.23
2	P	2	NAG	C1-O5-C5	3.03	116.25	112.19
2	L	2	NAG	C1-O5-C5	3.02	116.24	112.19
2	W	1	NAG	C1-O5-C5	3.02	116.23	112.19
2	c	2	NAG	C1-O5-C5	2.90	116.07	112.19
2	I	2	NAG	C1-O5-C5	2.79	115.93	112.19
3	G	2	NAG	C1-O5-C5	2.74	115.85	112.19
3	E	2	NAG	C1-O5-C5	2.68	115.78	112.19
4	J	2	NAG	C1-O5-C5	2.66	115.76	112.19
2	M	1	NAG	C1-O5-C5	2.63	115.71	112.19
2	K	3	MAN	C1-C2-C3	2.61	113.44	109.64
2	F	2	NAG	C4-C3-C2	-2.60	107.21	111.02
2	H	2	NAG	O5-C1-C2	-2.56	107.33	111.29
2	M	3	MAN	C1-O5-C5	2.51	115.55	112.19
2	R	1	NAG	C1-O5-C5	2.49	115.52	112.19
2	e	2	NAG	C1-O5-C5	2.48	115.51	112.19
3	a	2	NAG	C1-O5-C5	2.44	115.46	112.19
3	Y	1	NAG	C1-O5-C5	2.41	115.42	112.19
2	D	2	NAG	C1-O5-C5	2.41	115.41	112.19
3	N	1	NAG	C1-O5-C5	2.38	115.37	112.19
4	d	1	NAG	O5-C5-C6	2.37	112.27	107.66
2	V	3	MAN	C1-O5-C5	2.36	115.35	112.19
2	M	1	NAG	O5-C1-C2	-2.35	107.65	111.29
2	b	1	NAG	O3-C3-C2	2.35	114.29	109.40
2	f	3	MAN	C1-O5-C5	2.34	115.32	112.19
2	K	3	MAN	C1-O5-C5	2.32	115.30	112.19
2	W	2	NAG	O5-C1-C2	-2.29	107.75	111.29
2	b	2	NAG	O5-C1-C2	-2.29	107.75	111.29
3	O	1	NAG	C1-O5-C5	2.27	115.23	112.19
4	J	1	NAG	O5-C5-C6	2.26	112.06	107.66
2	c	2	NAG	C4-C3-C2	-2.24	107.73	111.02
3	a	2	NAG	O5-C1-C2	-2.21	107.87	111.29
2	F	3	MAN	O5-C5-C6	2.21	111.96	107.66
3	O	2	NAG	C1-O5-C5	2.20	115.13	112.19
2	P	3	MAN	O5-C5-C6	2.19	111.92	107.66
2	f	1	NAG	C1-O5-C5	2.18	115.11	112.19
2	Z	1	NAG	C2-N2-C7	-2.18	119.98	122.90
3	Y	2	NAG	C1-O5-C5	2.18	115.11	112.19
2	e	3	MAN	O5-C5-C6	2.16	111.87	107.66
2	K	1	NAG	O4-C4-C3	-2.11	105.40	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	FUC	C1-C2-C3	2.10	112.70	109.64
4	J	3	FUC	O5-C5-C4	2.09	113.32	109.55
2	f	3	MAN	O5-C5-C6	2.09	111.73	107.66
3	Q	2	NAG	O5-C1-C2	-2.08	108.07	111.29
2	c	3	MAN	C2-C3-C4	2.08	114.51	110.86
2	Z	2	NAG	O5-C5-C6	2.05	111.66	107.66
2	K	2	NAG	C4-C3-C2	-2.00	108.08	111.02
2	b	3	MAN	O5-C5-C6	2.00	111.56	107.66

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	W	3	MAN	O5-C5-C6-O6
2	I	3	MAN	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
2	c	3	MAN	O5-C5-C6-O6
2	K	3	MAN	O5-C5-C6-O6
2	D	3	MAN	O5-C5-C6-O6
2	U	3	MAN	O5-C5-C6-O6
2	e	3	MAN	O5-C5-C6-O6
2	S	3	MAN	O5-C5-C6-O6
2	M	3	MAN	O5-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

All (13) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	V	3	MAN	C1-C2-C3-C4-C5-O5
2	W	3	MAN	C1-C2-C3-C4-C5-O5
2	b	3	MAN	C1-C2-C3-C4-C5-O5
2	F	3	MAN	C1-C2-C3-C4-C5-O5
2	Z	3	MAN	C1-C2-C3-C4-C5-O5
2	H	3	MAN	C1-C2-C3-C4-C5-O5
2	D	3	MAN	C1-C2-C3-C4-C5-O5

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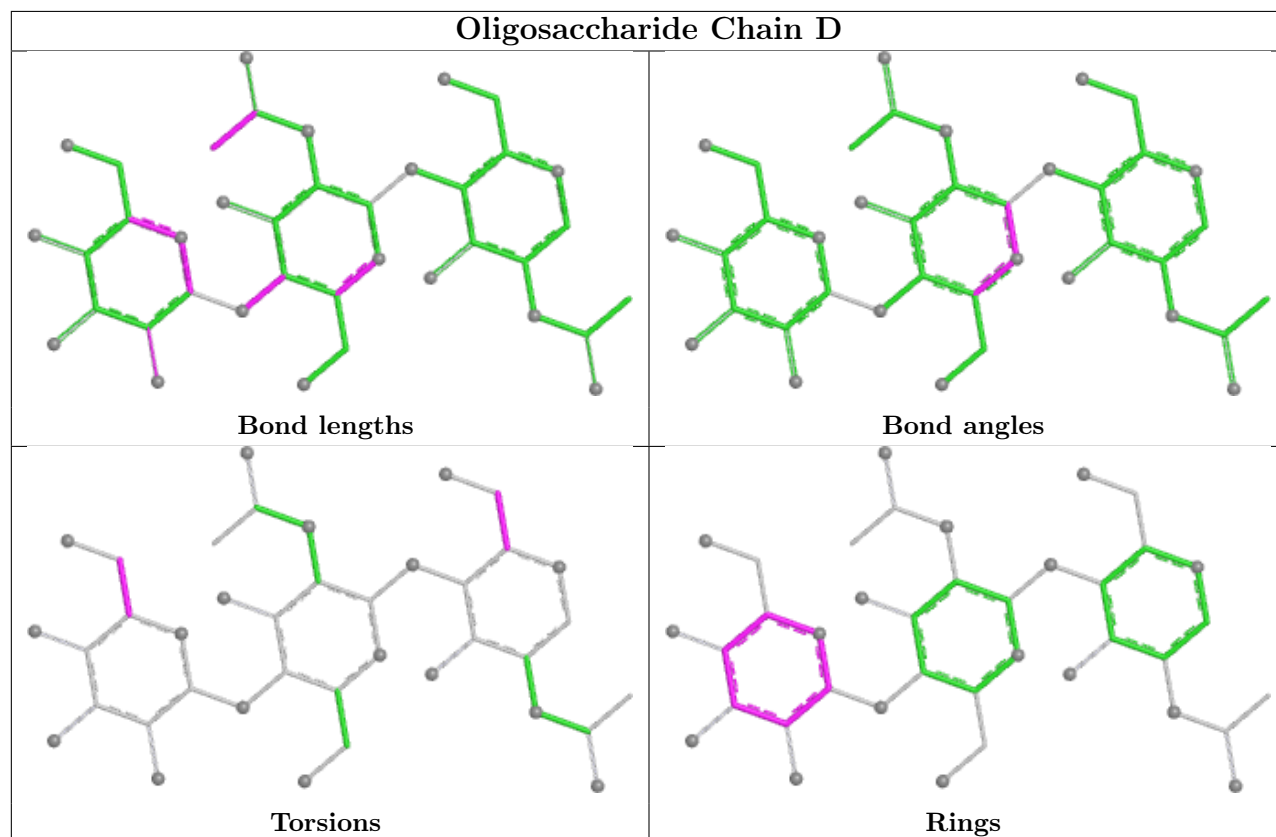
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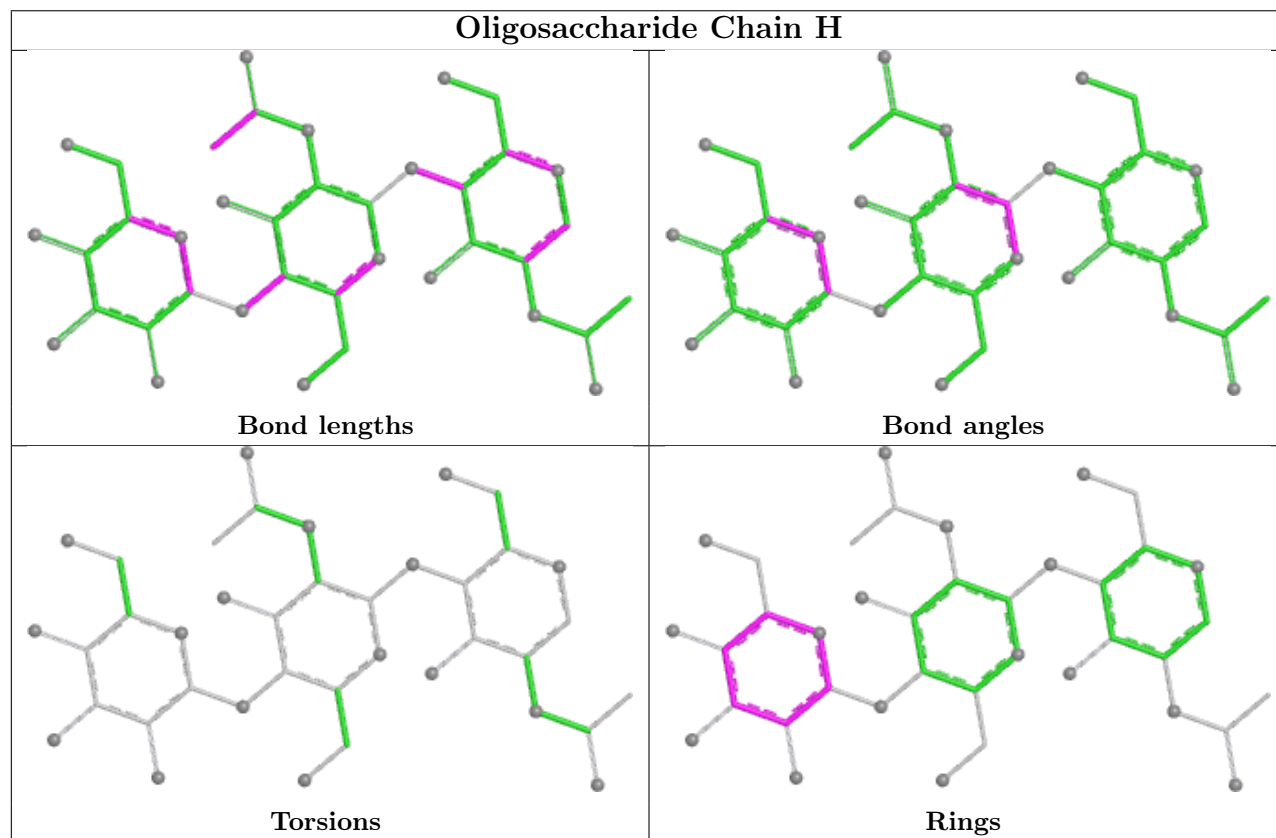
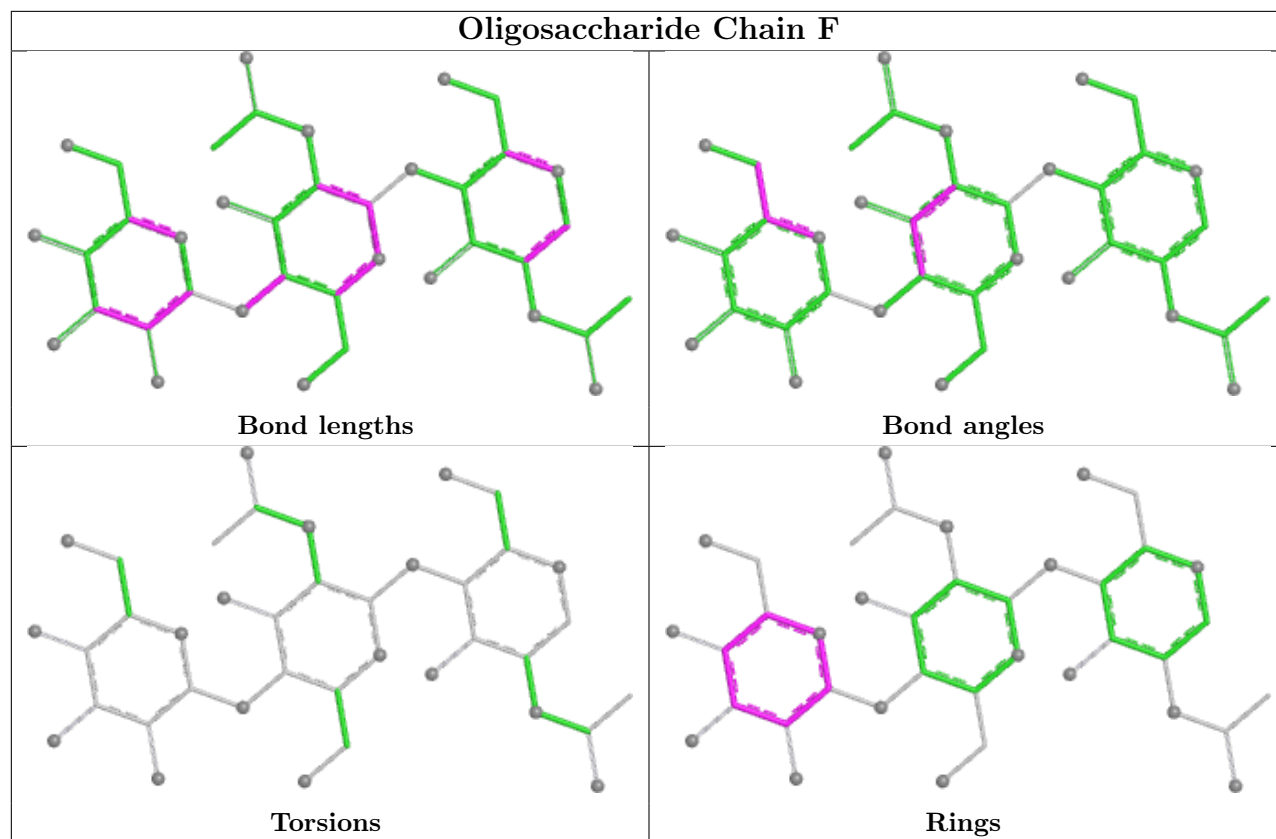
Mol	Chain	Res	Type	Atoms
2	S	3	MAN	C1-C2-C3-C4-C5-O5
2	f	3	MAN	C1-C2-C3-C4-C5-O5
2	L	3	MAN	C1-C2-C3-C4-C5-O5
2	R	3	MAN	C1-C2-C3-C4-C5-O5
2	M	3	MAN	C1-C2-C3-C4-C5-O5
2	P	3	MAN	C1-C2-C3-C4-C5-O5

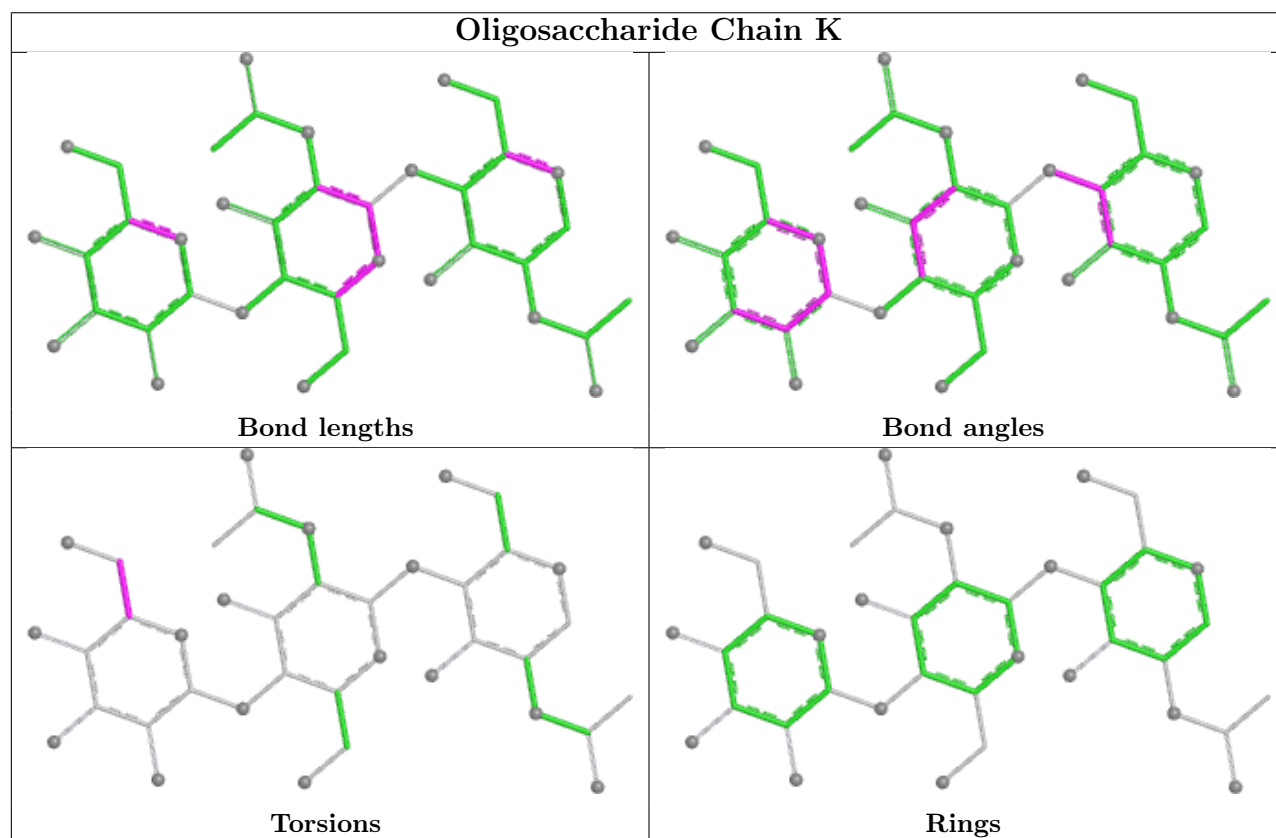
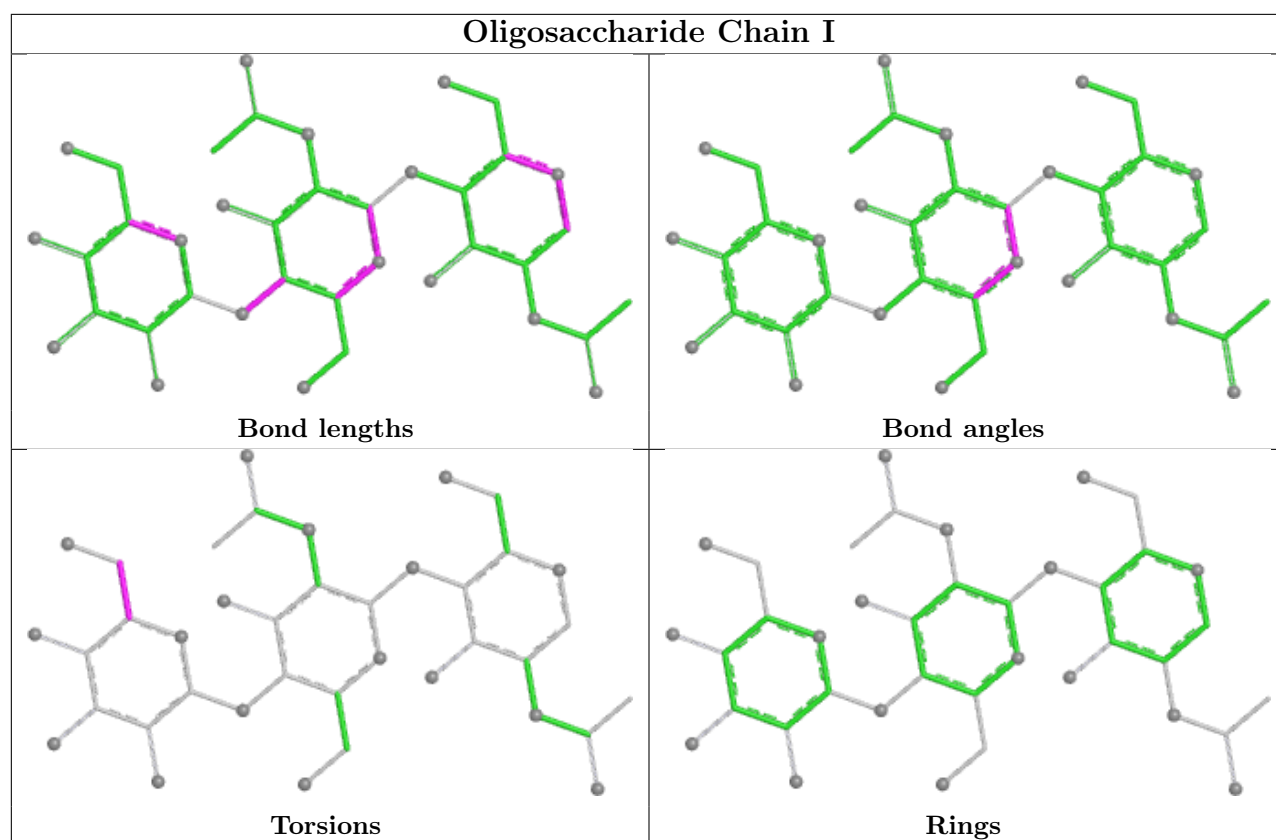
3 monomers are involved in 17 short contacts:

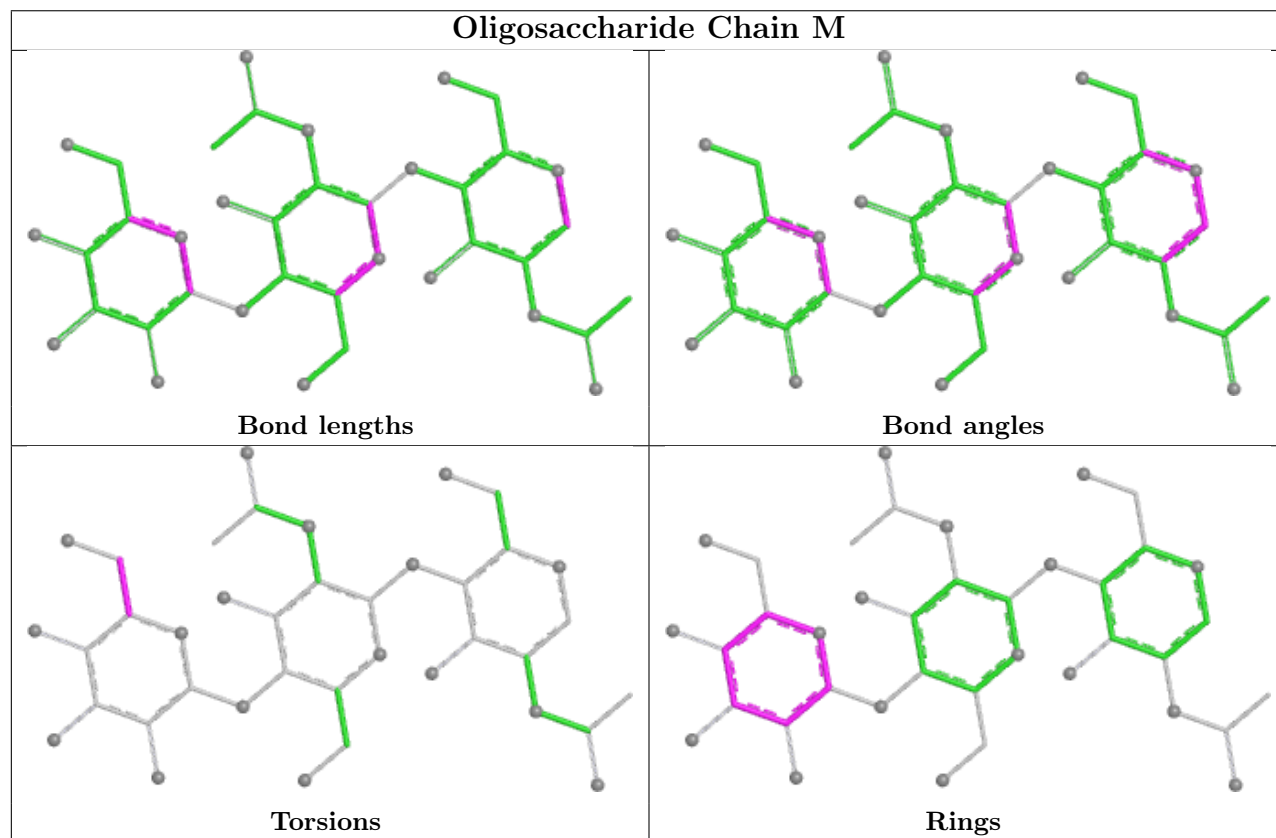
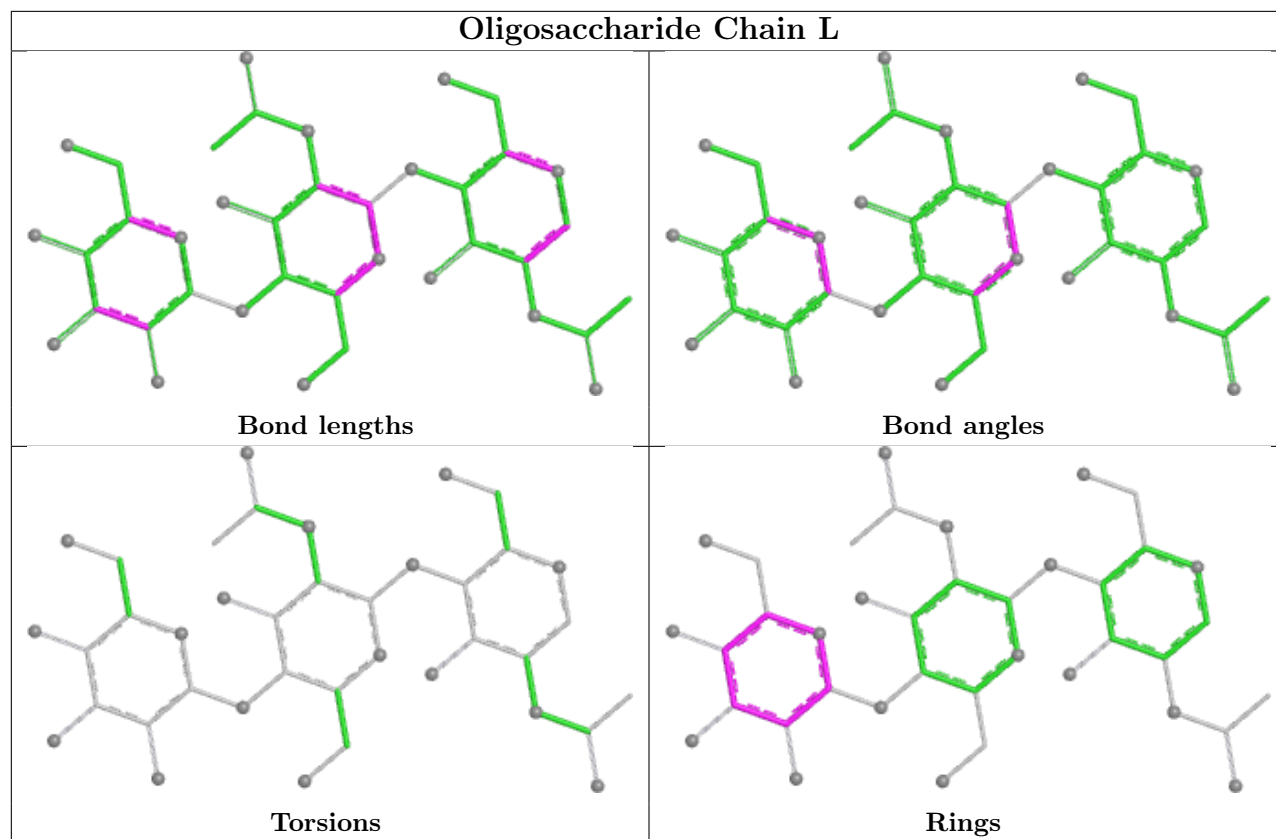
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	9	0
2	P	1	NAG	2	0
2	D	1	NAG	7	0

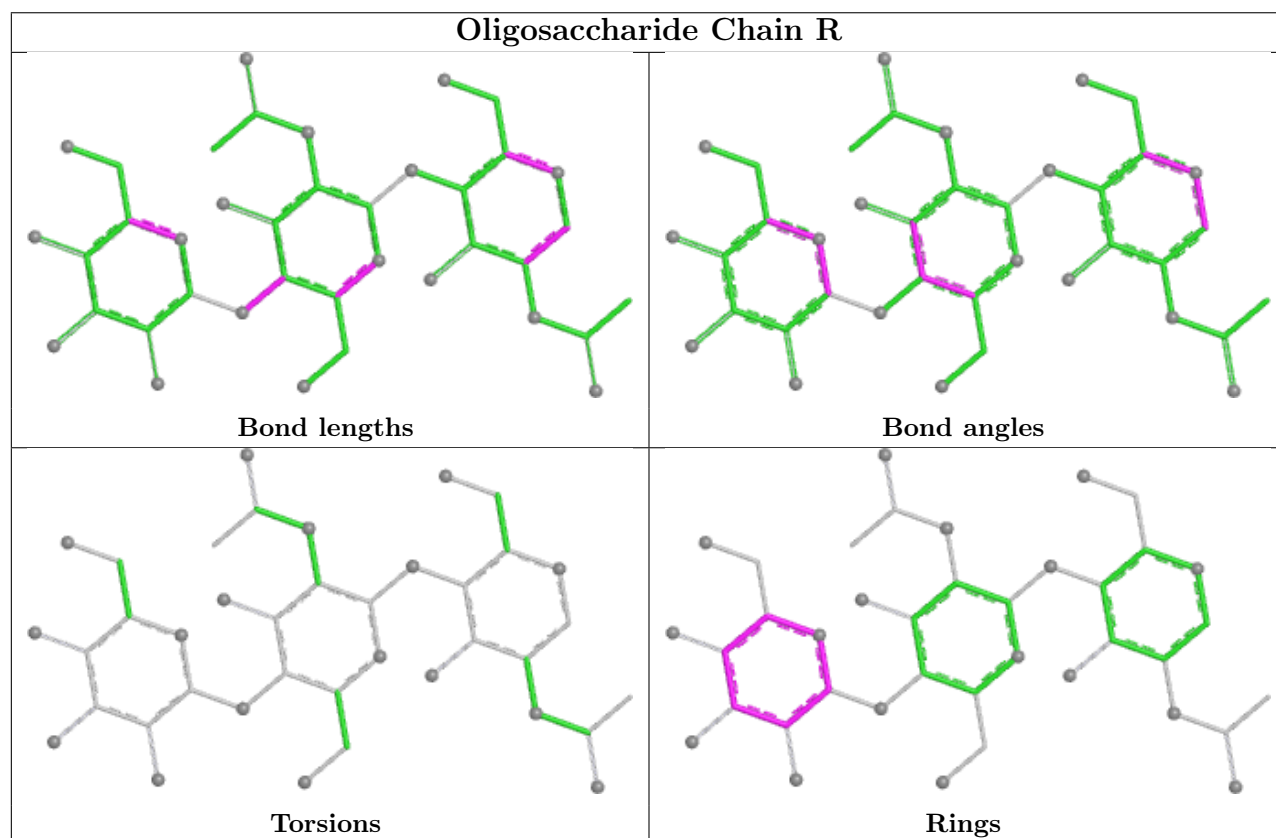
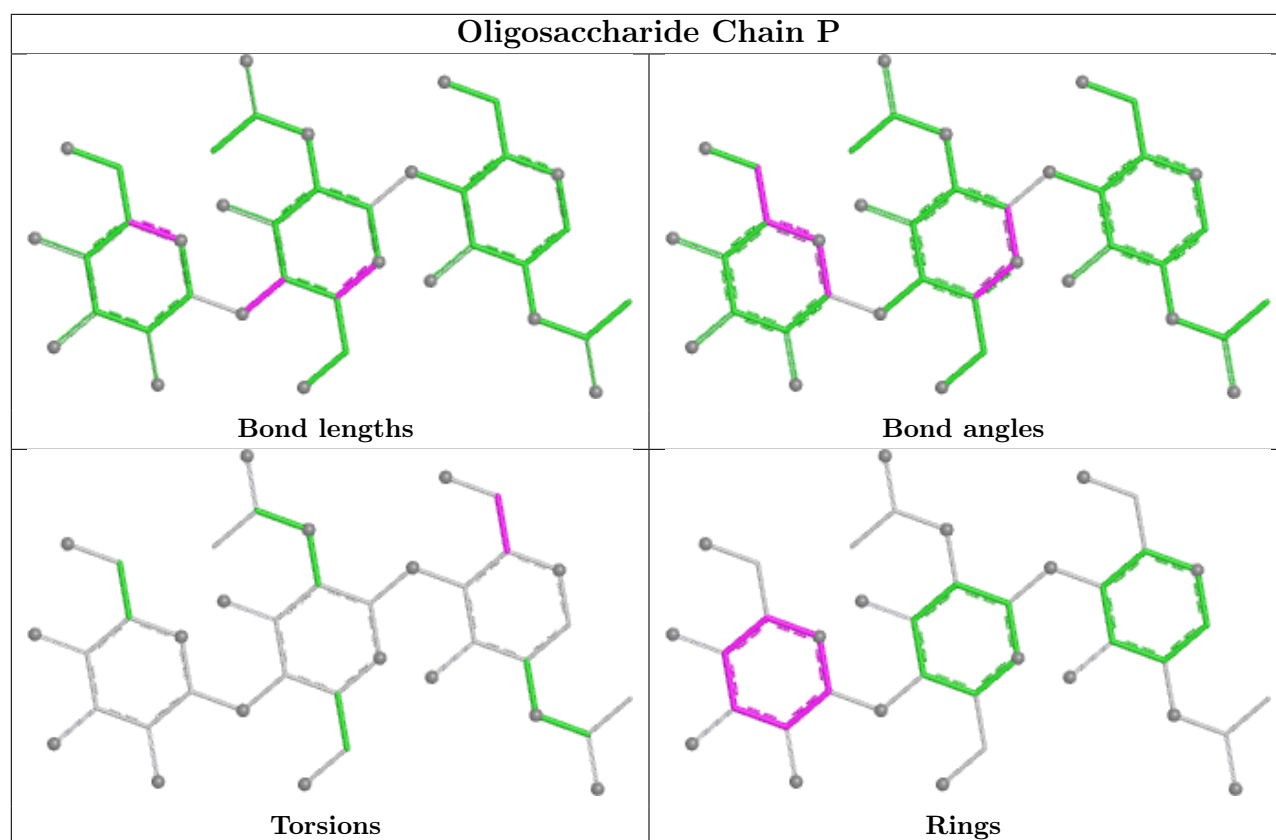
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

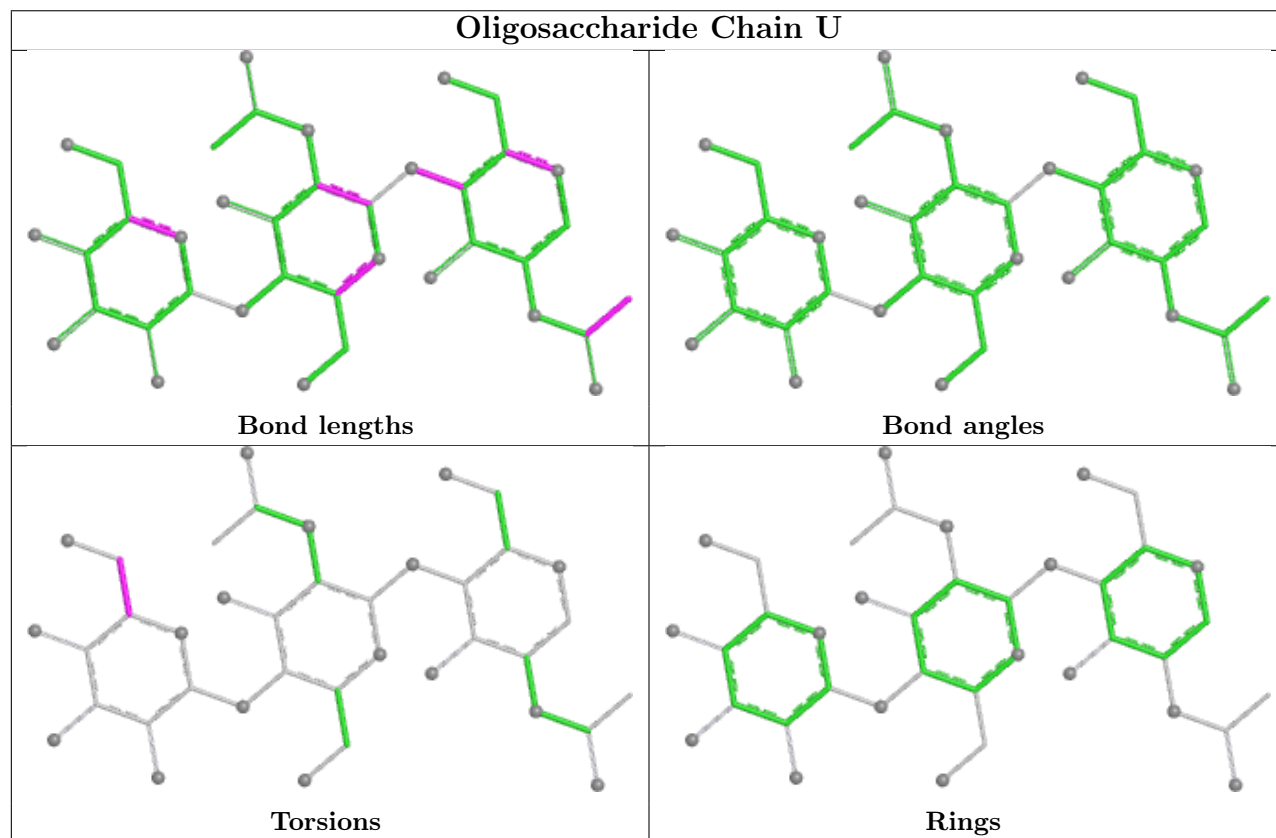
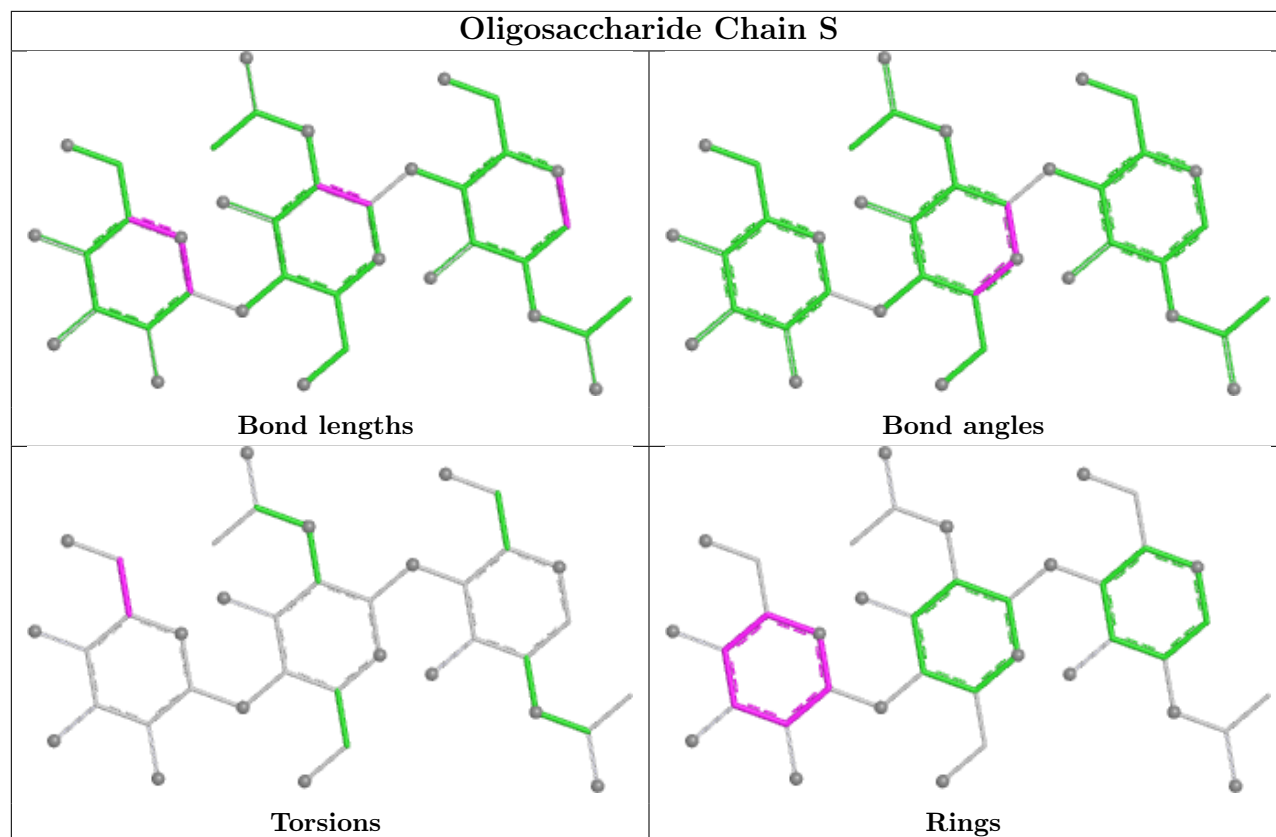


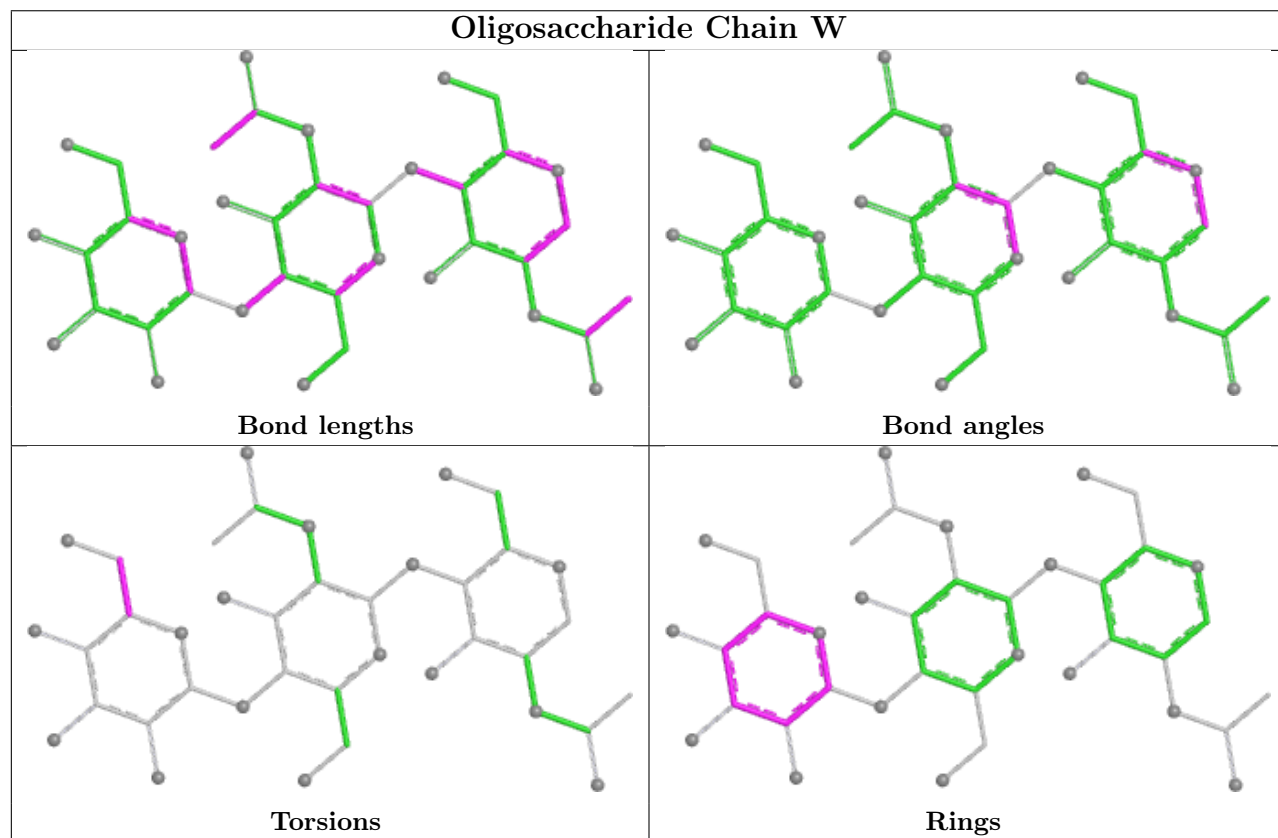
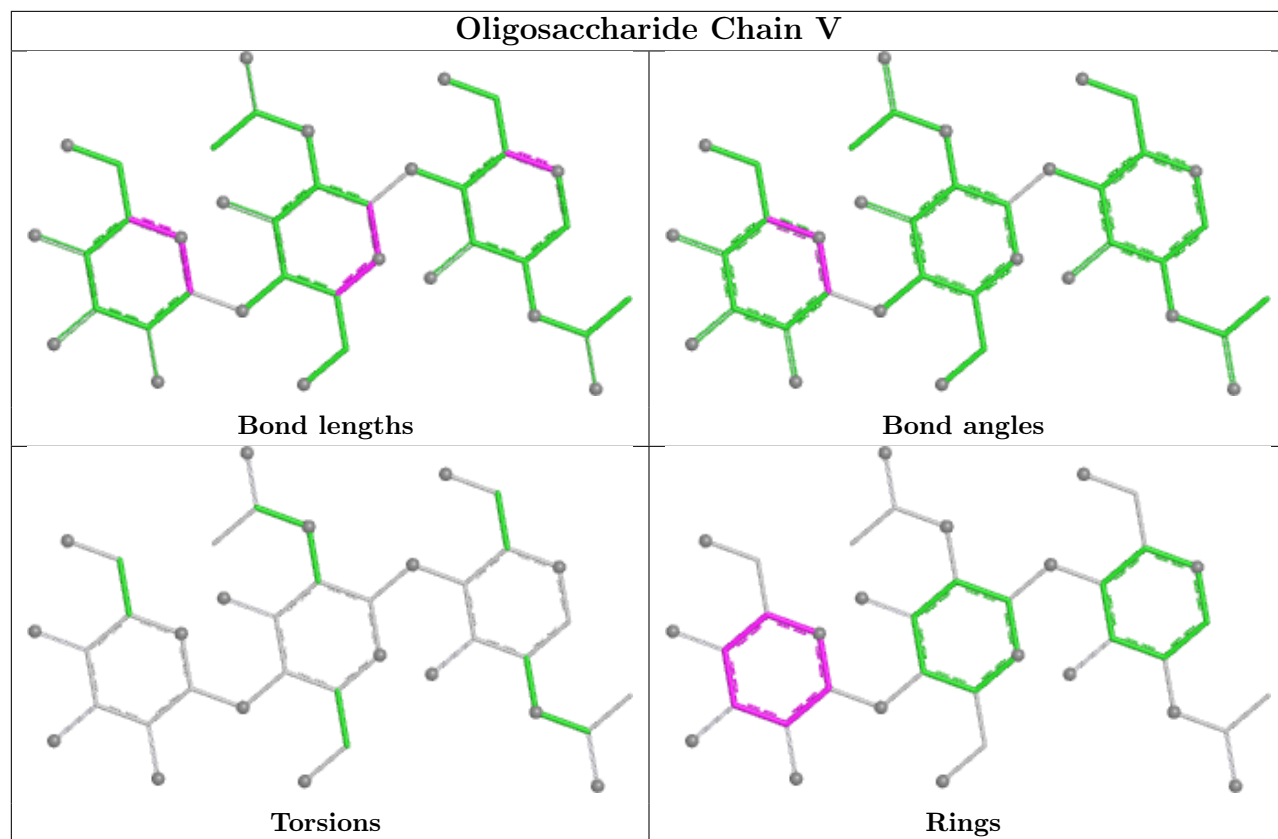


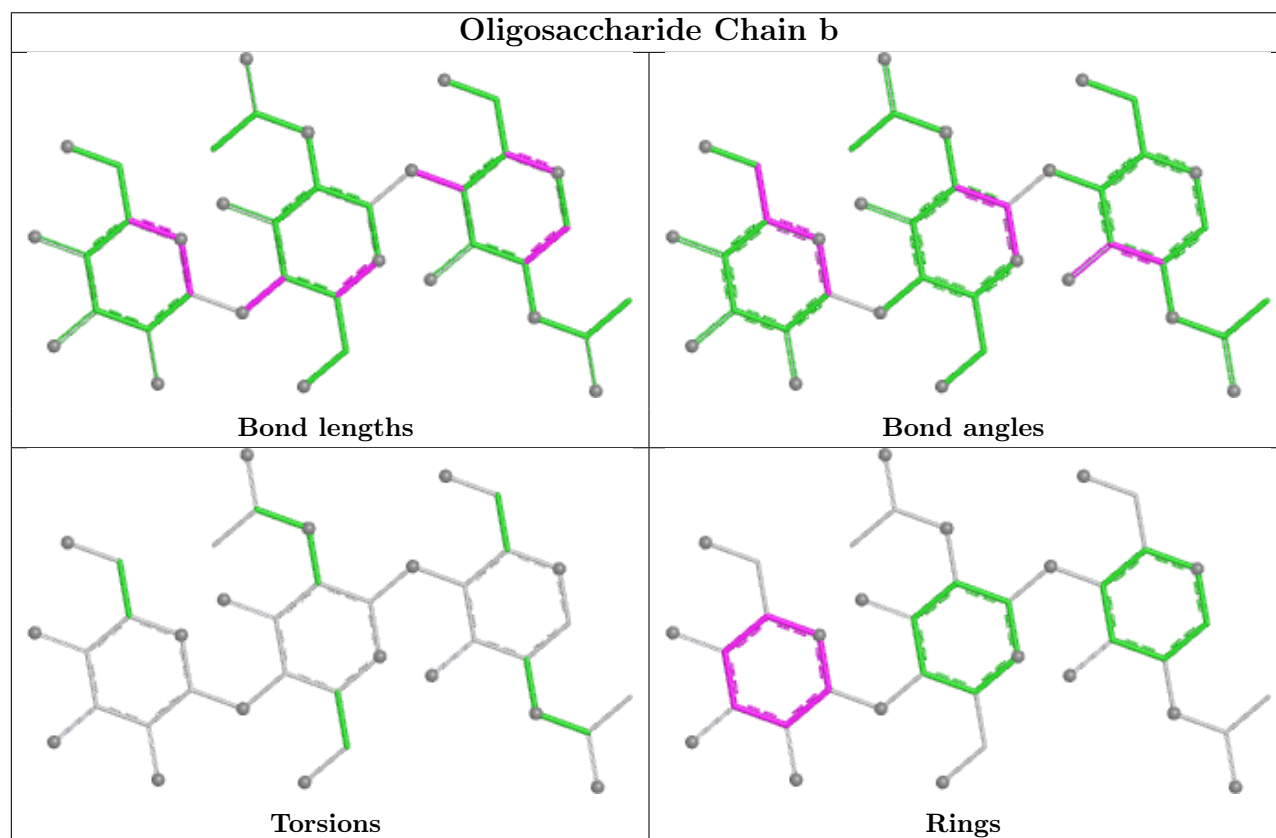
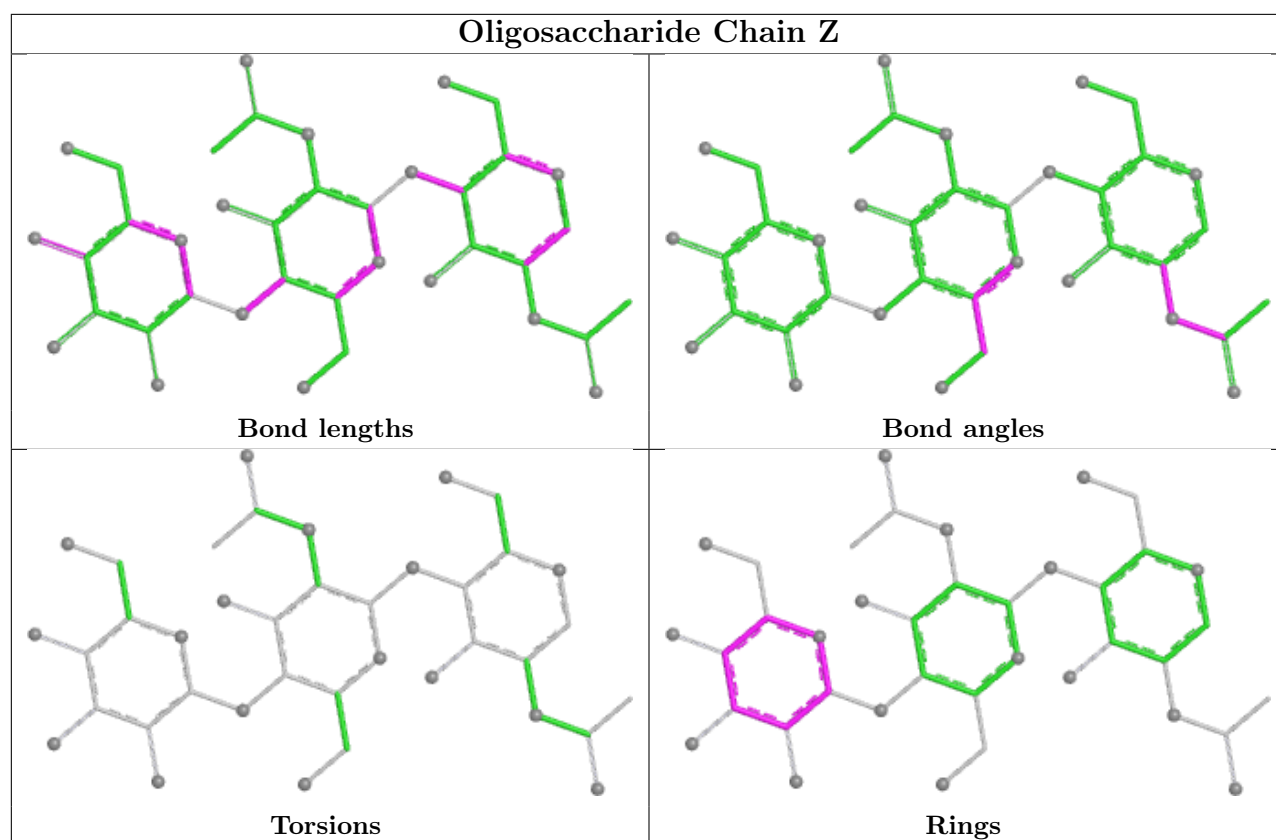


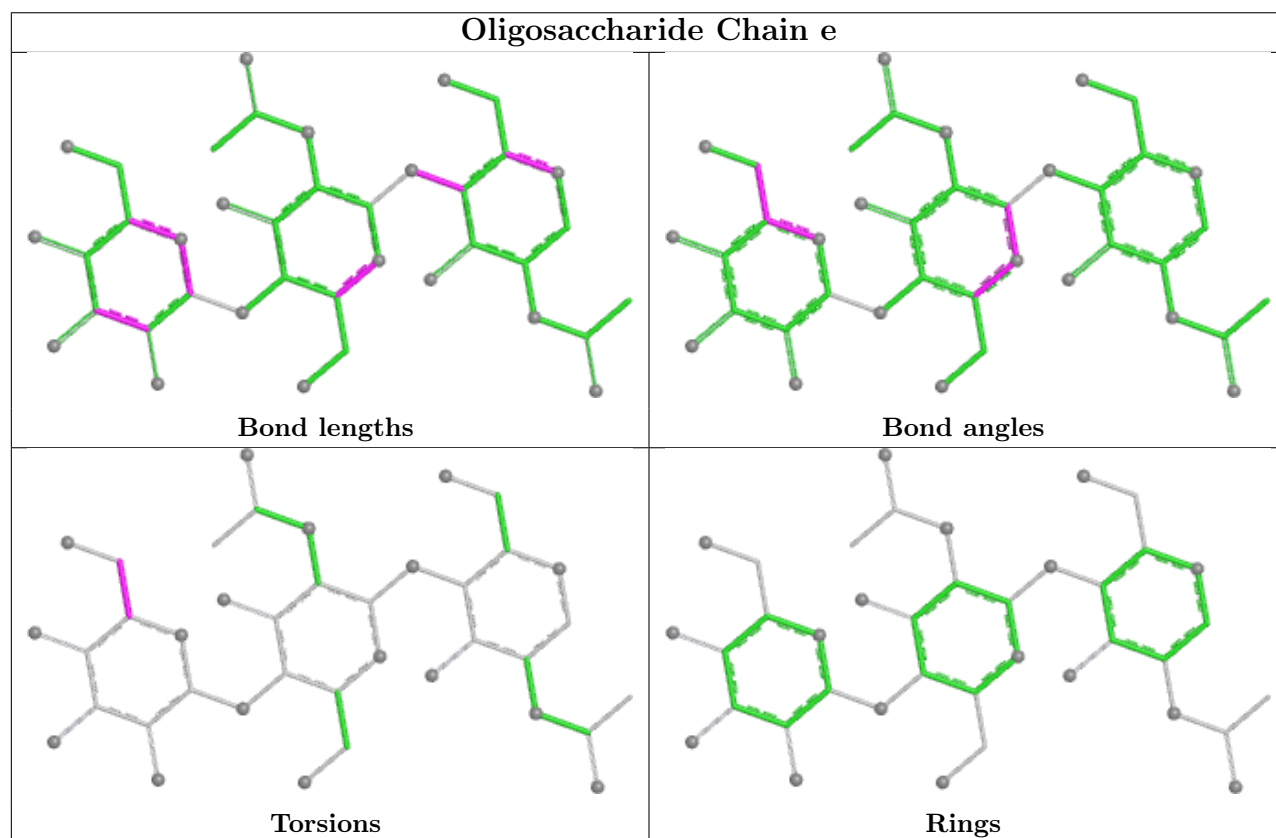
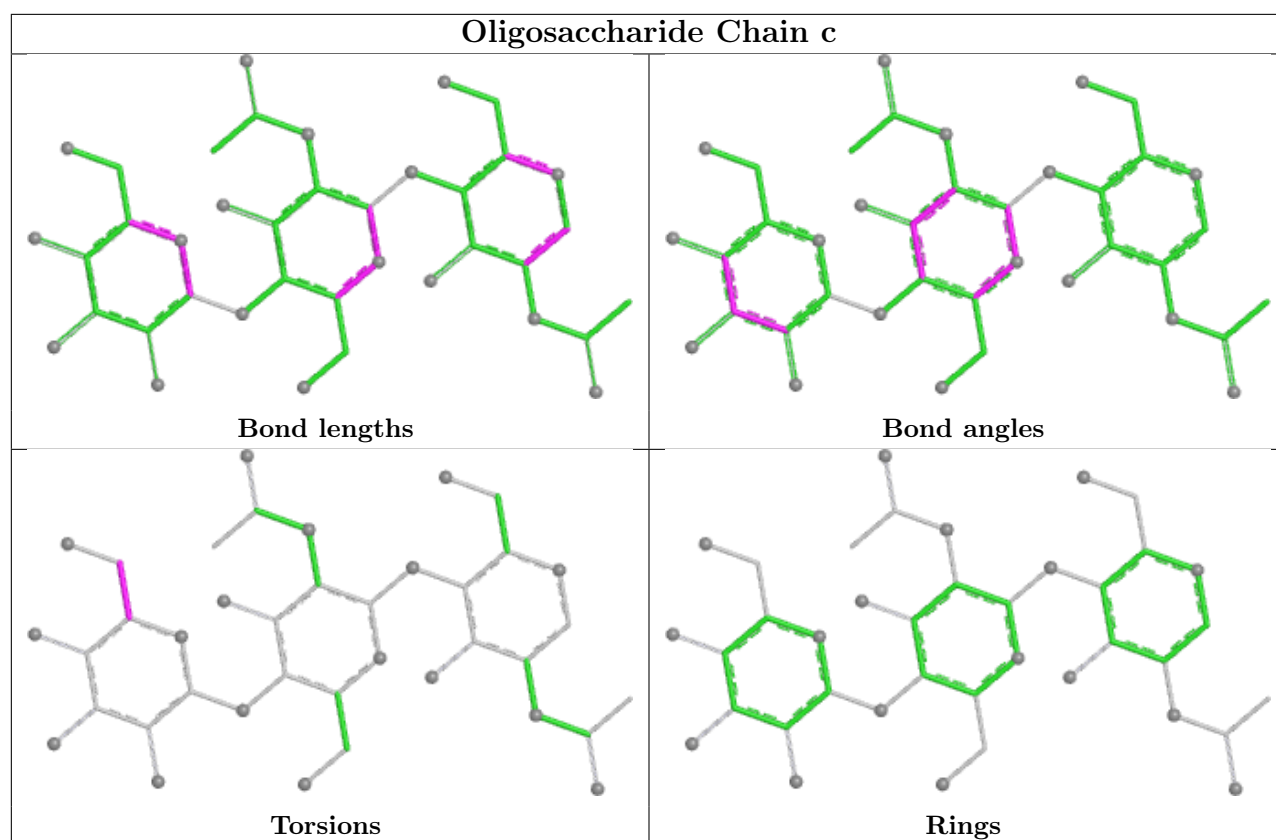


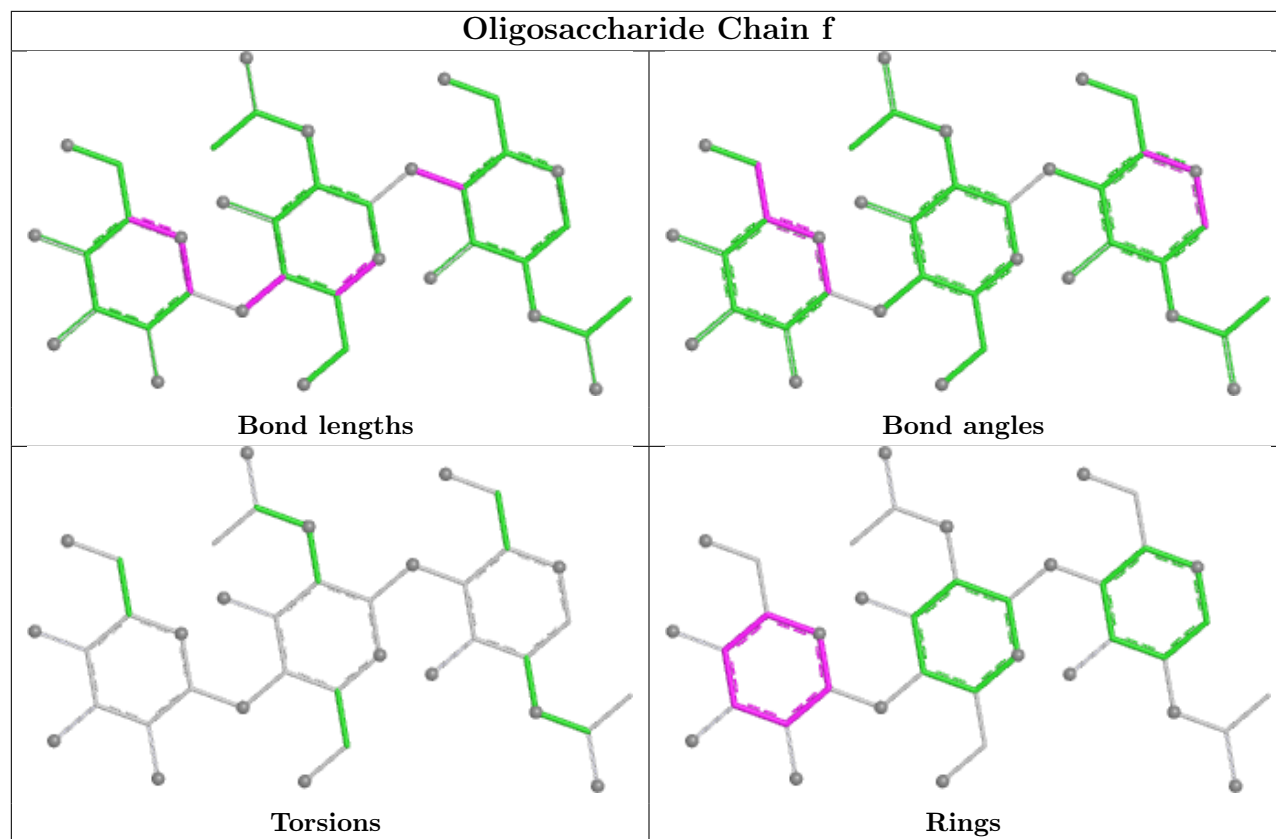


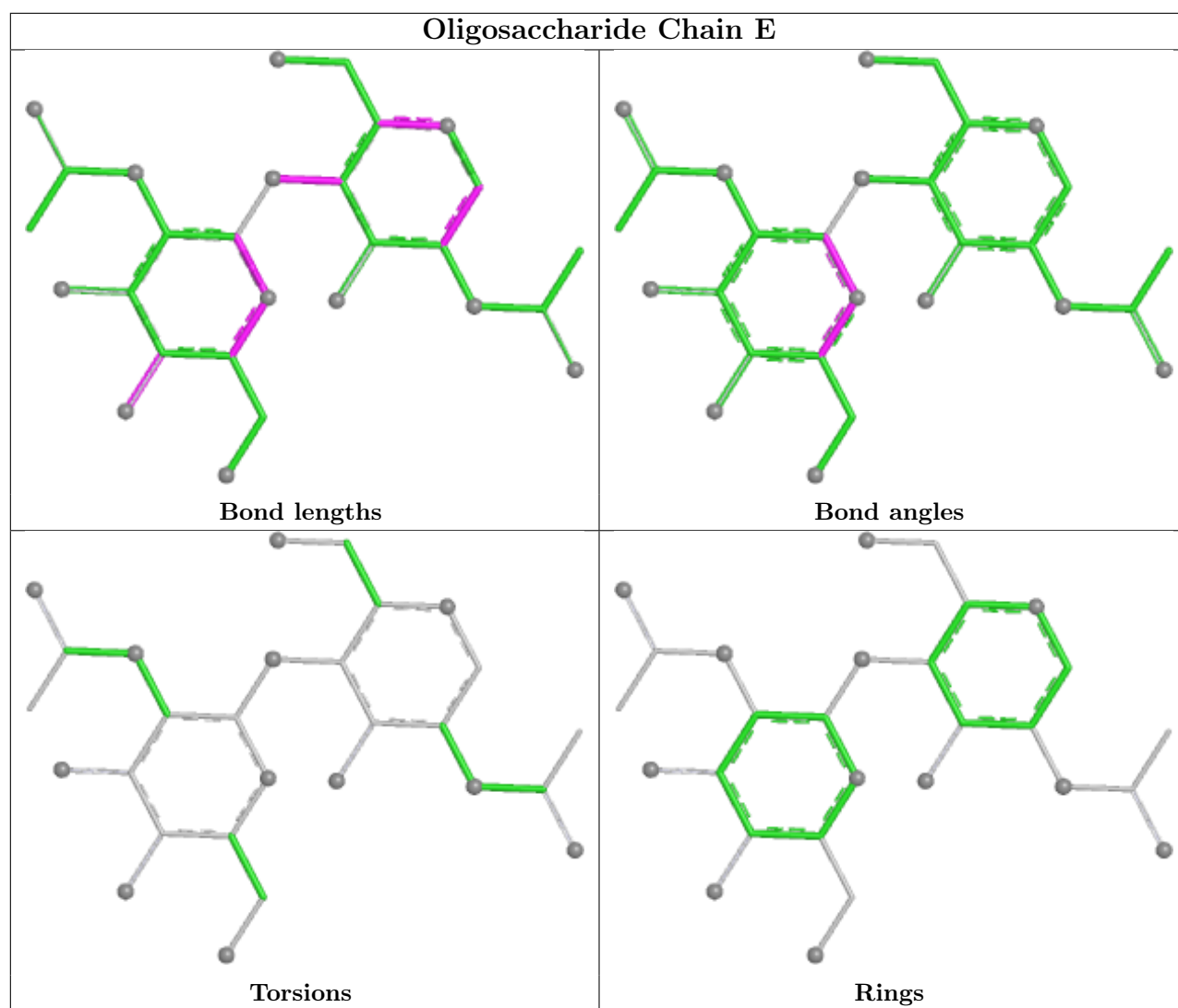


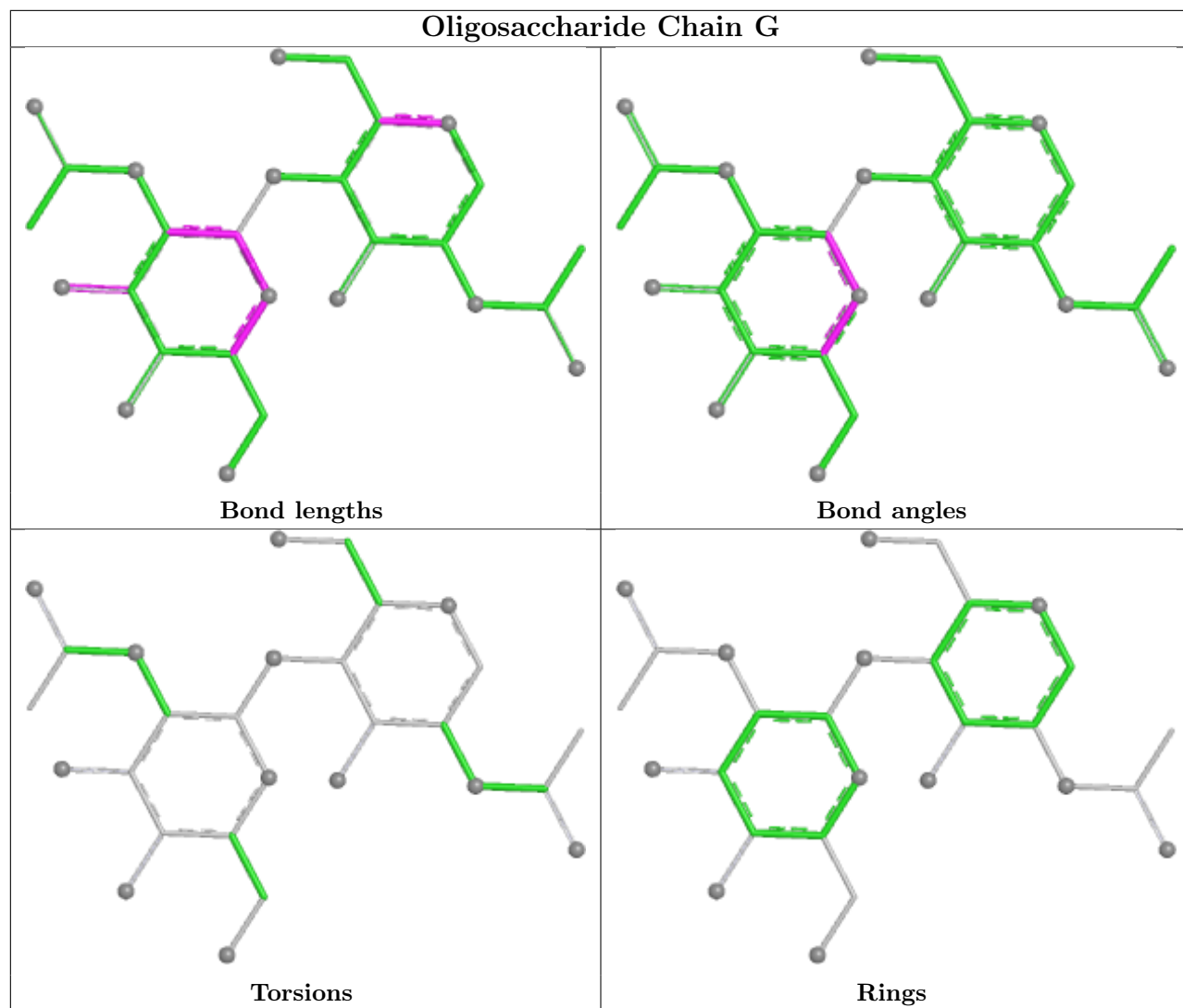


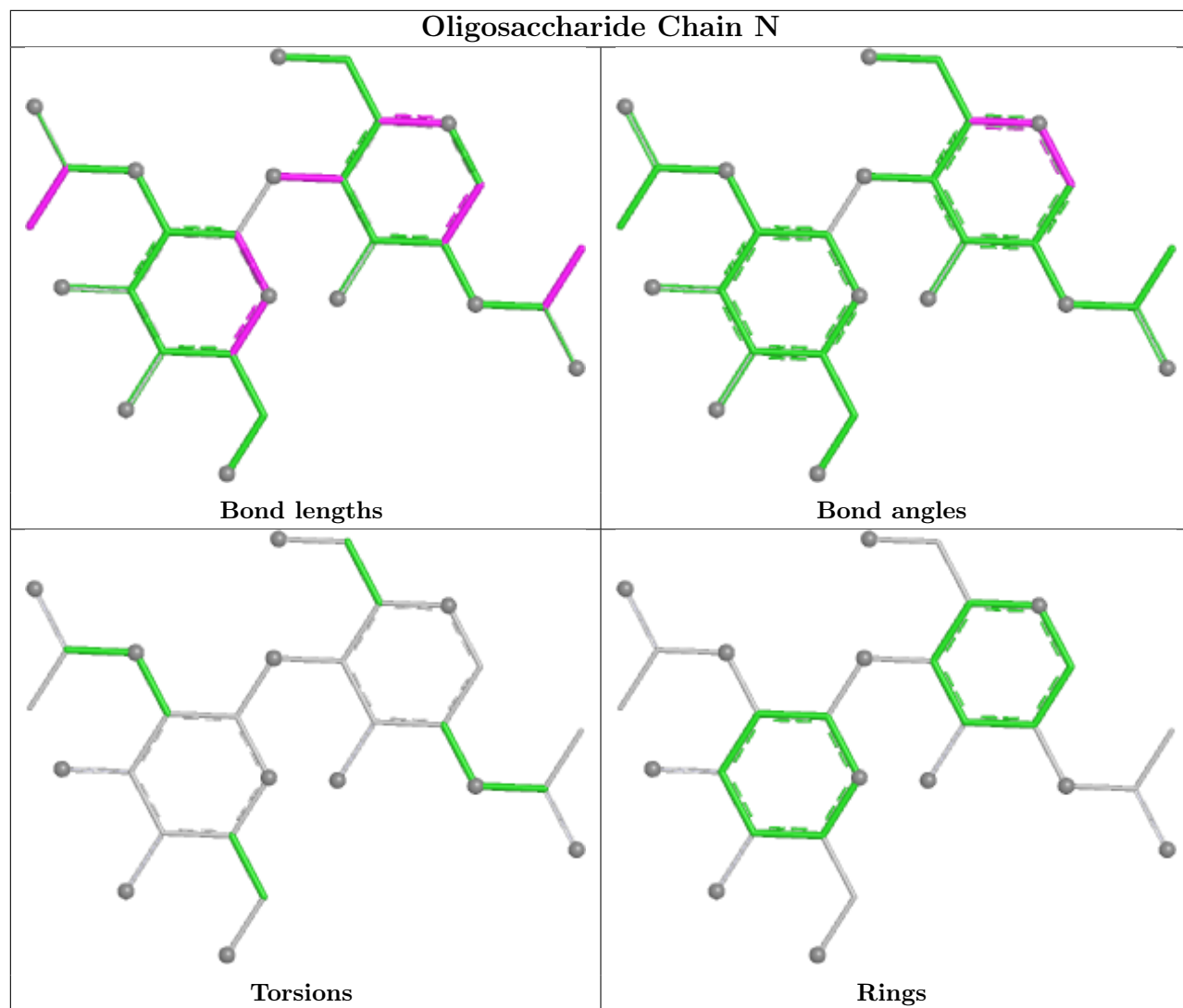


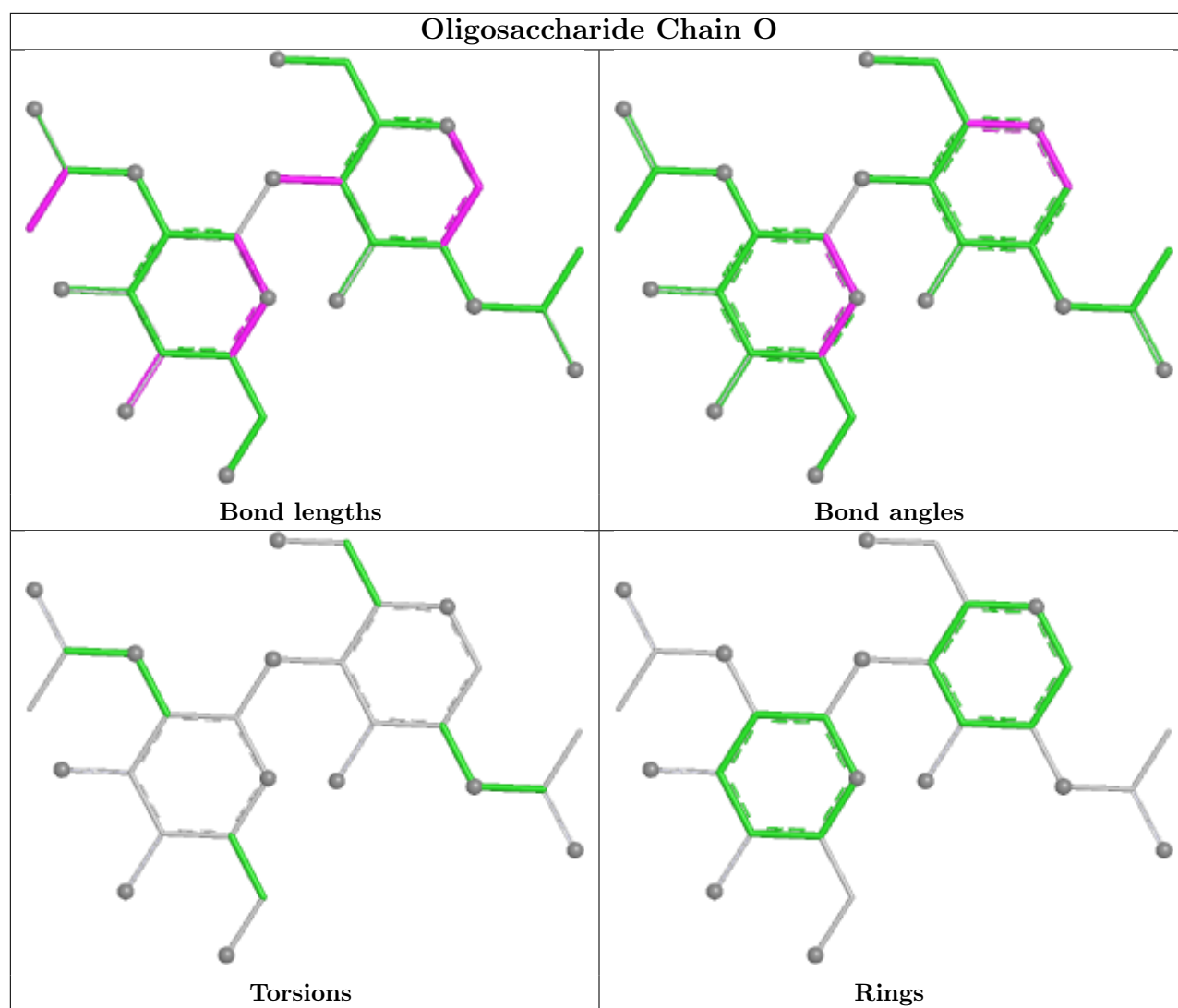


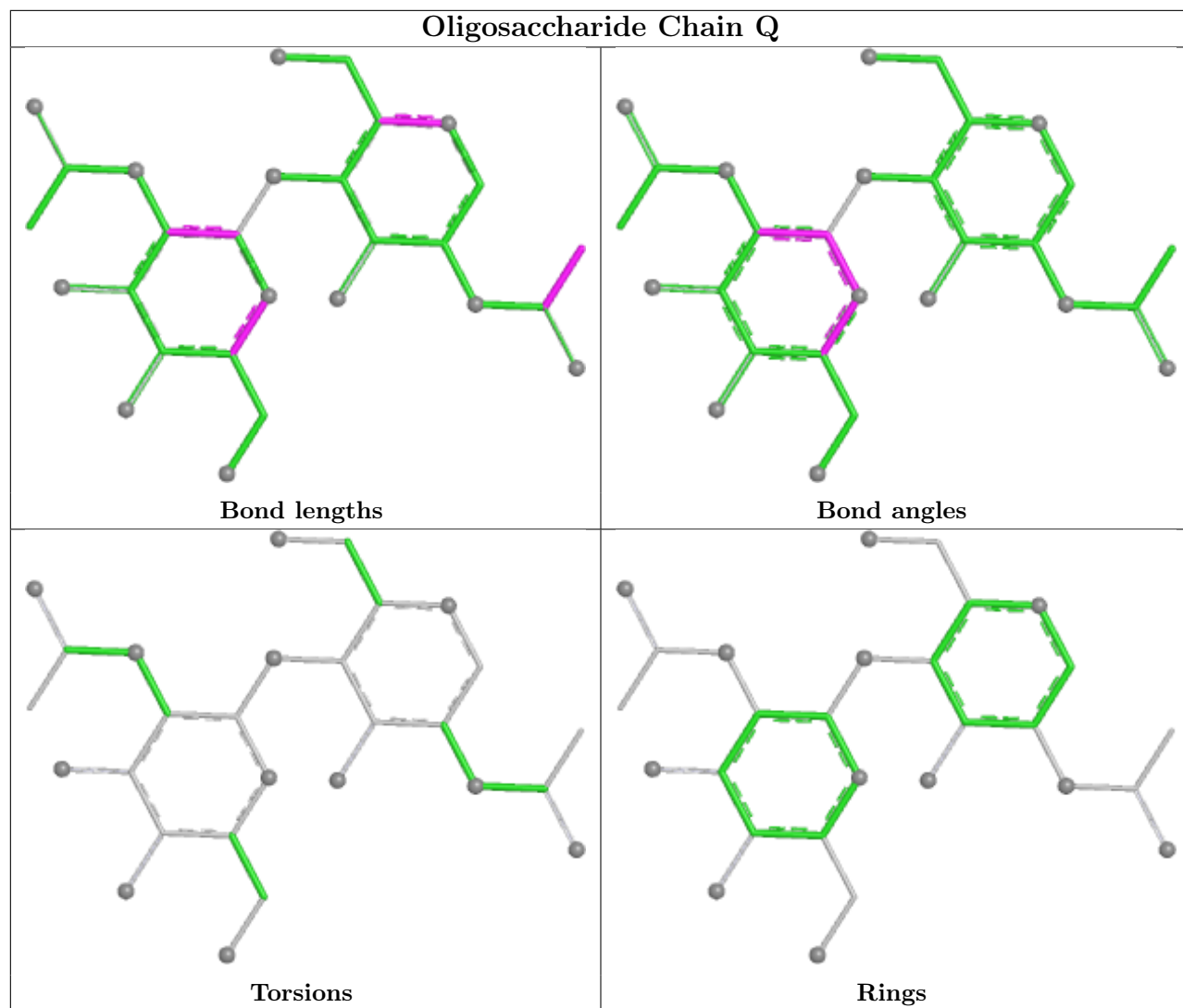


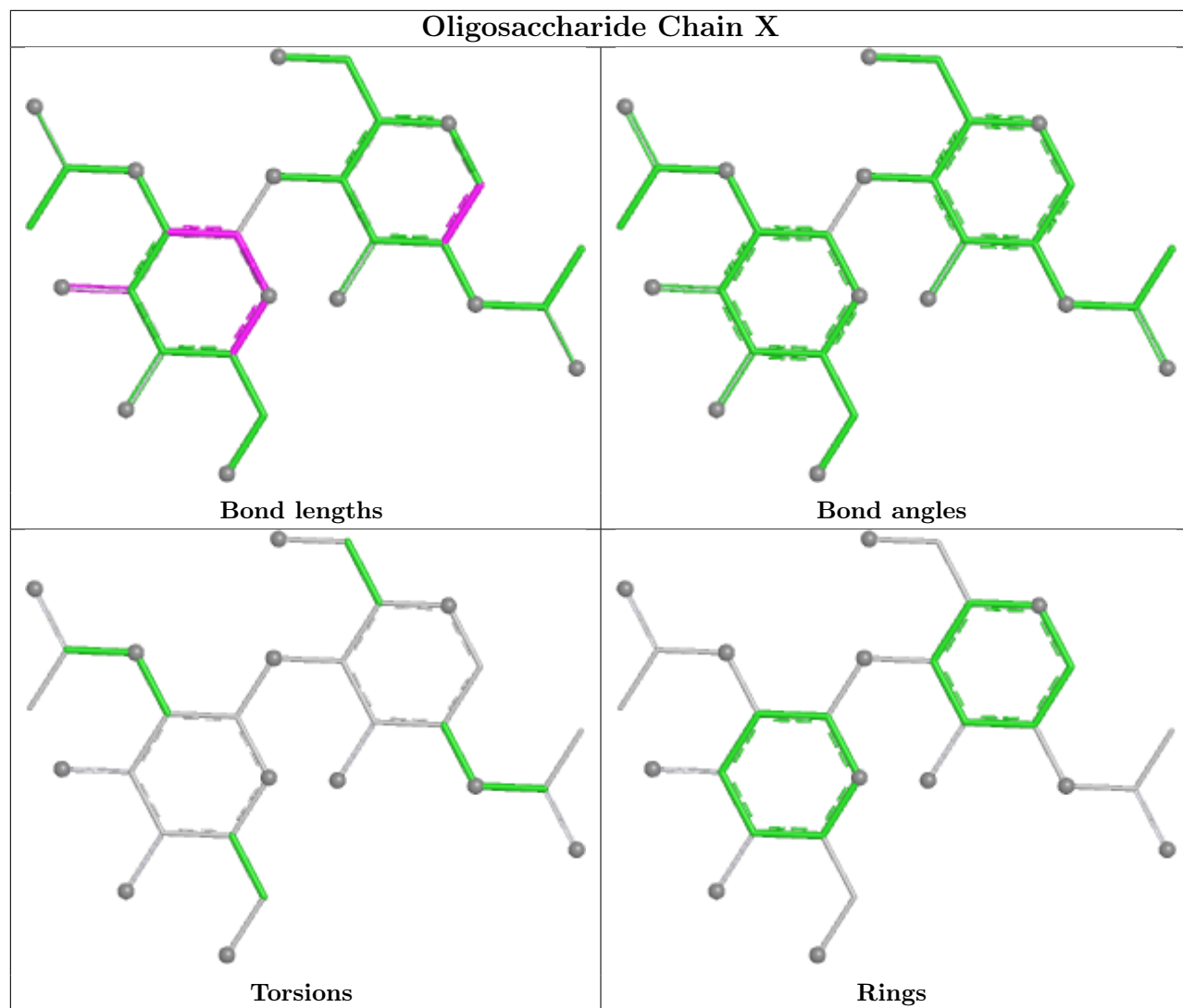


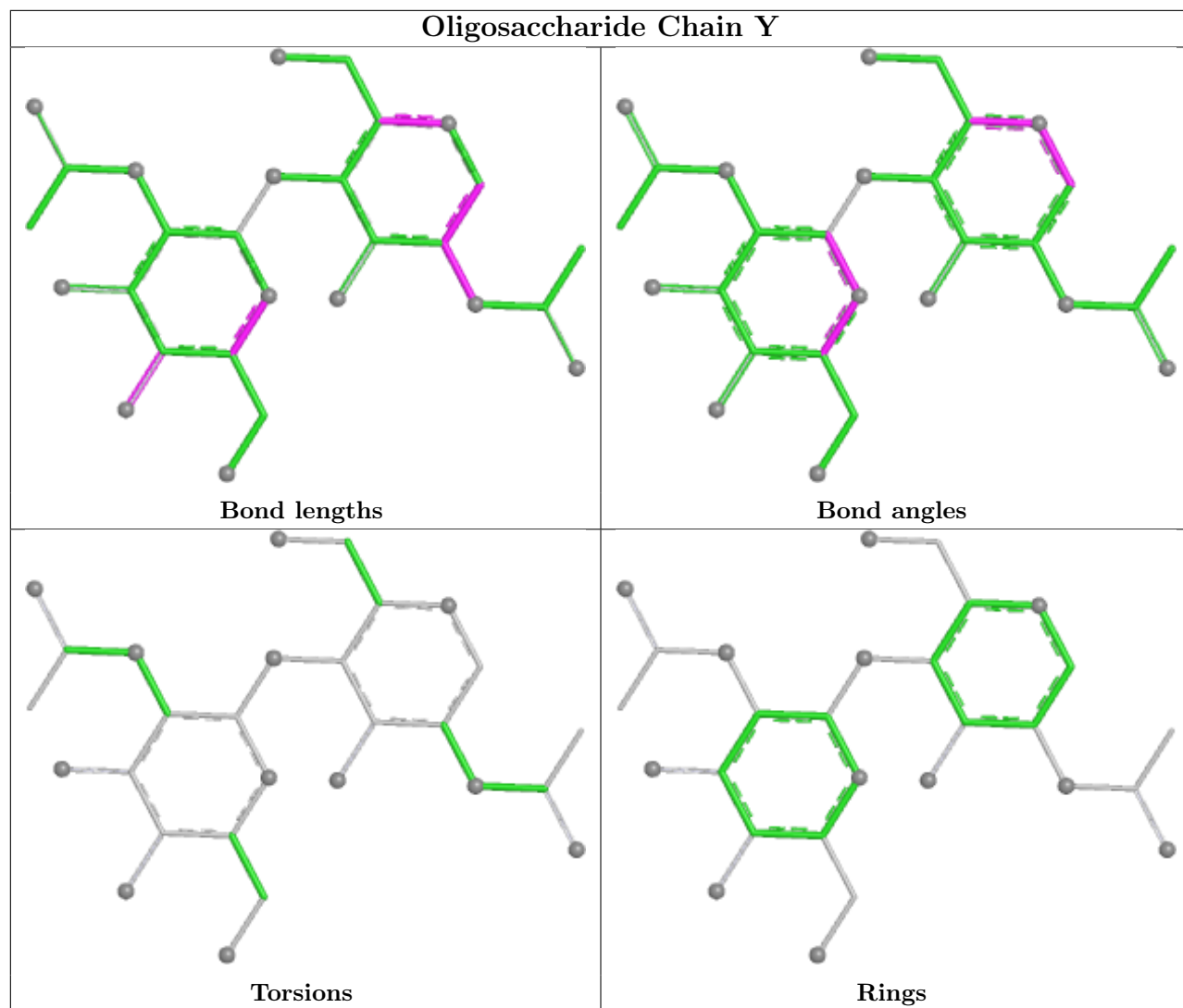


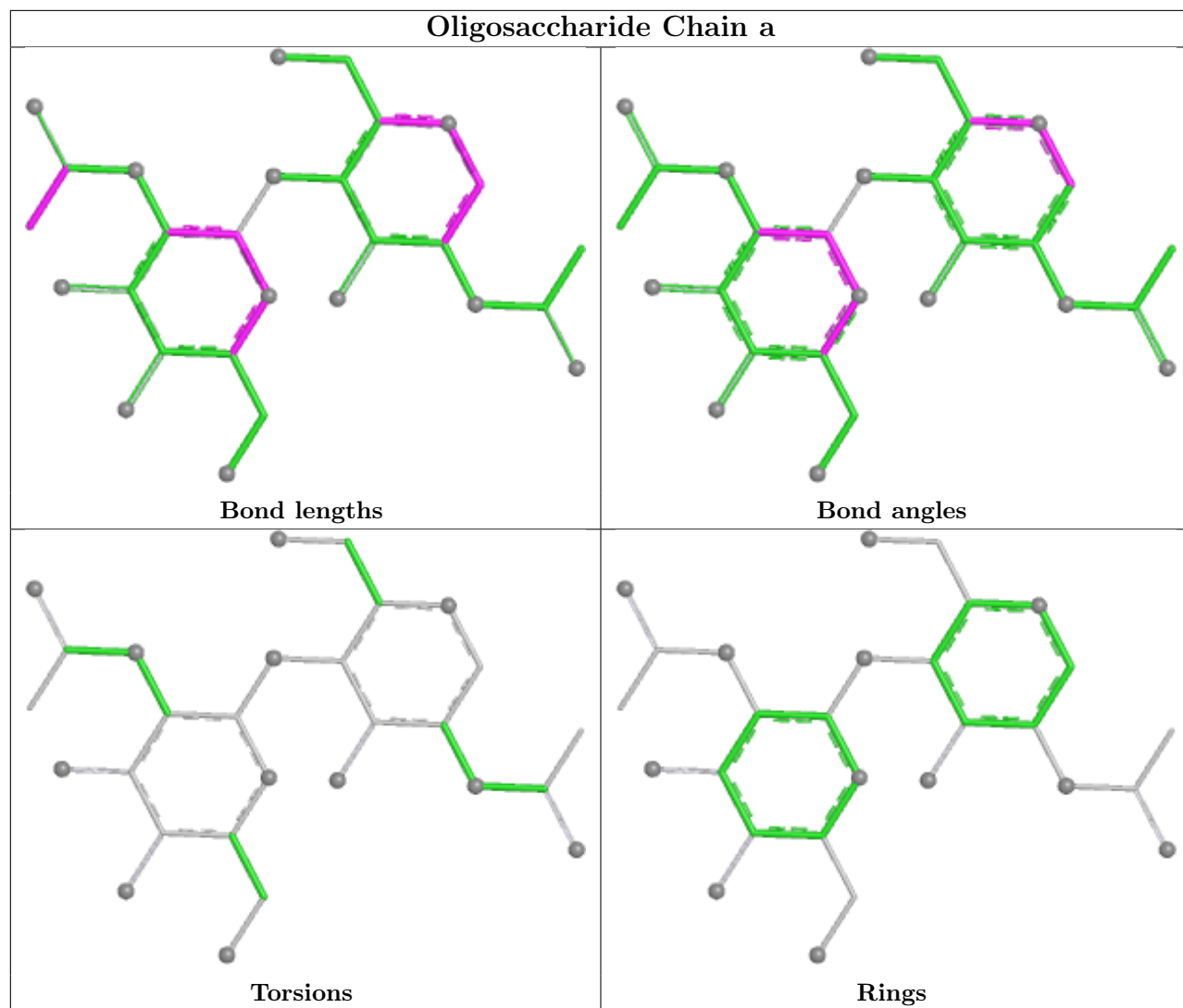


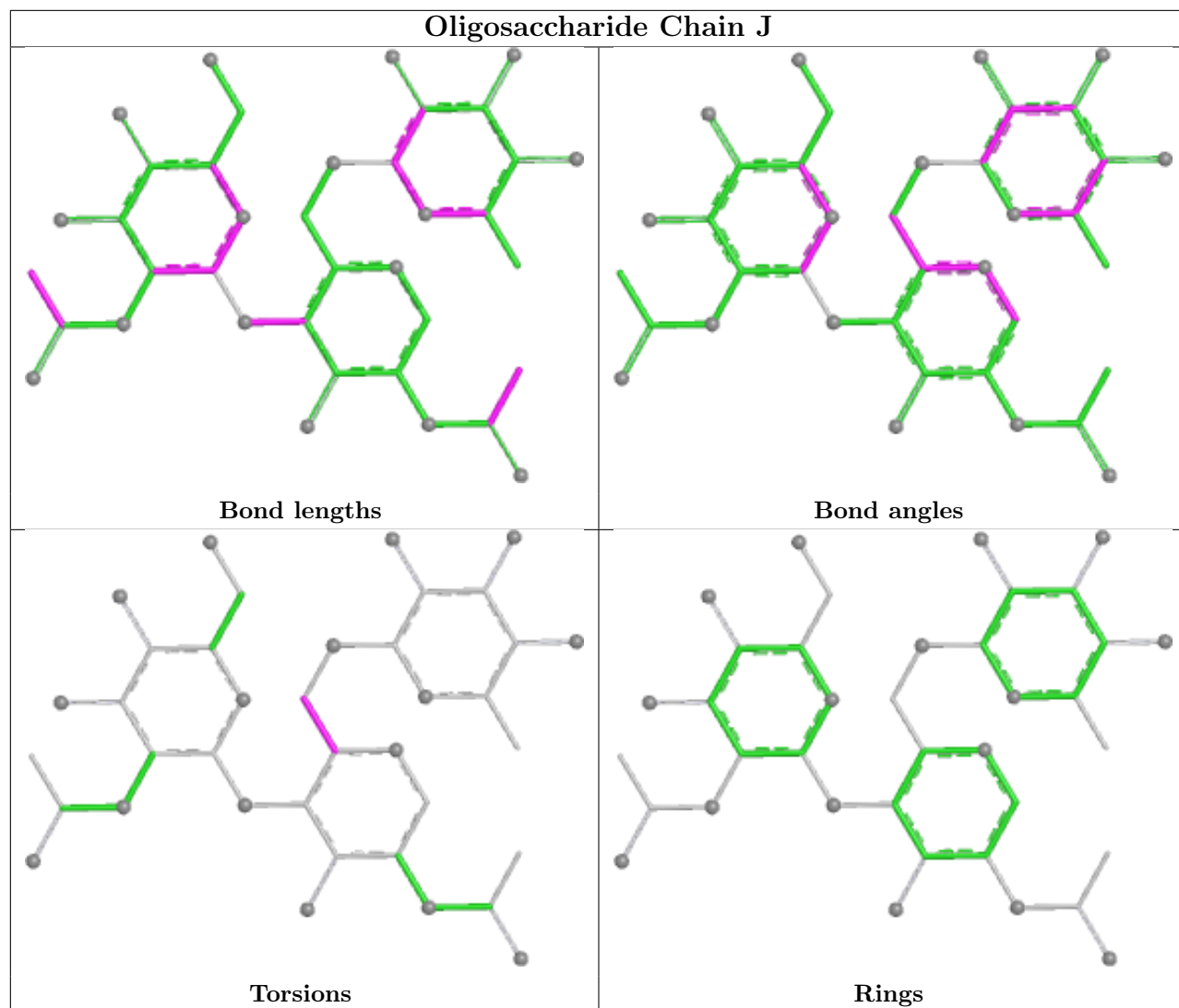


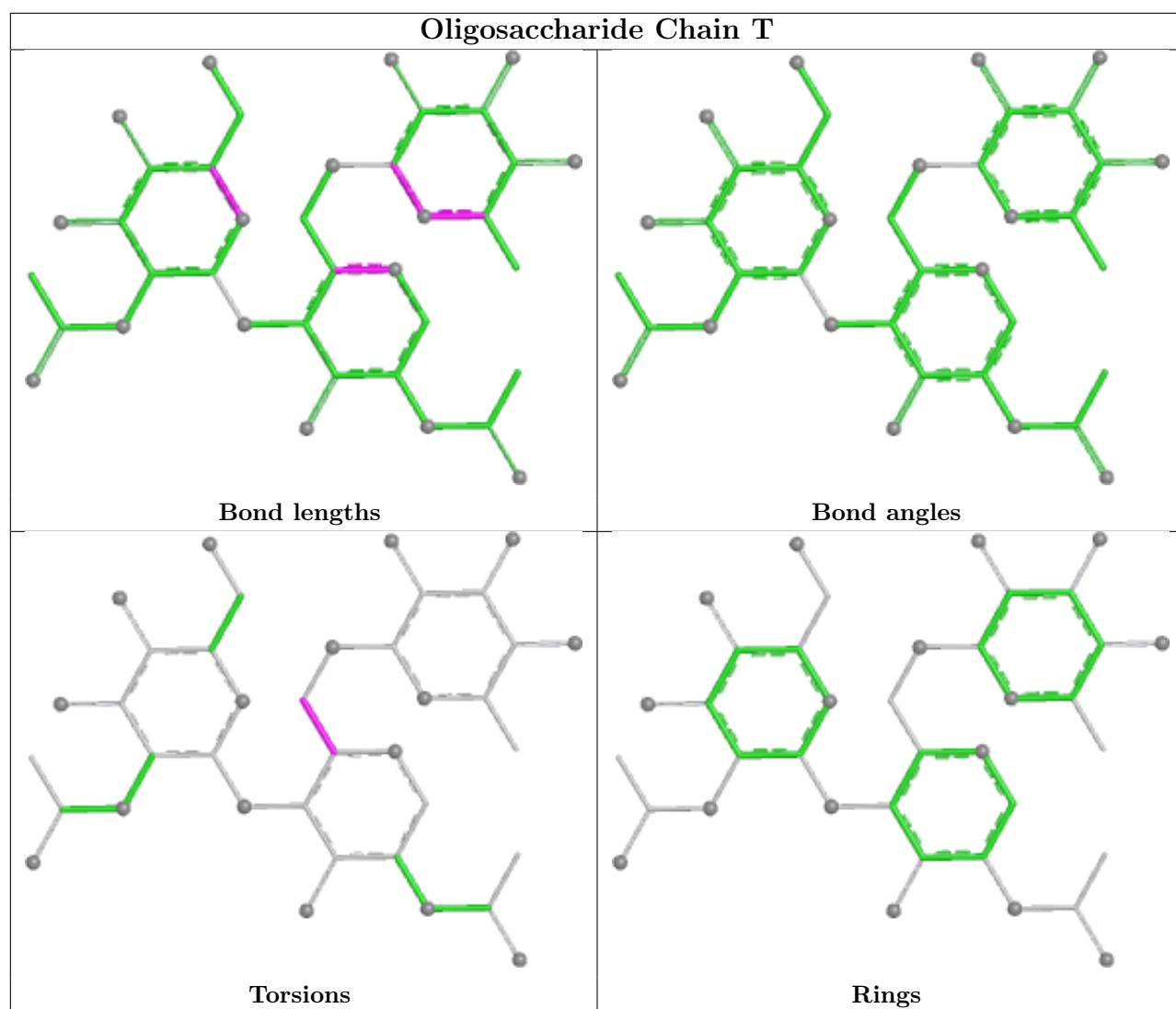


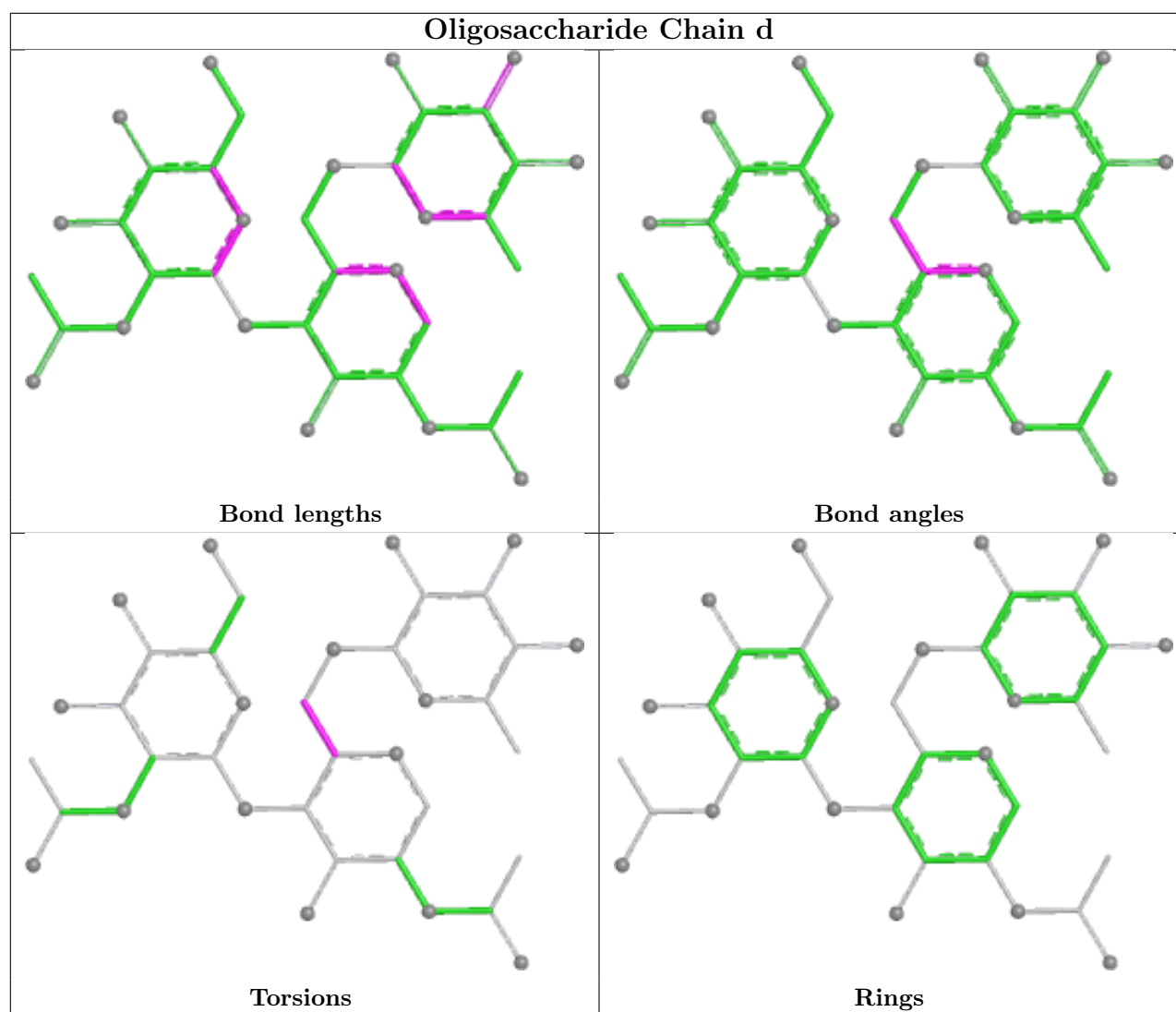












5.6 Ligand geometry [i](#)

20 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	1401	-	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	B	1403	1	14,14,15	1.46	3 (21%)	17,19,21	0.97	1 (5%)
5	NAG	A	1407	1	14,14,15	1.41	2 (14%)	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1405	1	14,14,15	1.19	2 (14%)	17,19,21	0.86	0
5	NAG	A	1404	-	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	B	1404	1	14,14,15	1.30	2 (14%)	17,19,21	0.82	0
5	NAG	A	1402	1	14,14,15	1.27	2 (14%)	17,19,21	0.60	0
5	NAG	A	1405	1	14,14,15	1.46	3 (21%)	17,19,21	0.69	0
5	NAG	C	1404	1	14,14,15	1.28	1 (7%)	17,19,21	0.76	0
5	NAG	B	1401	1	14,14,15	1.44	2 (14%)	17,19,21	1.03	1 (5%)
5	NAG	B	1407	1	14,14,15	1.63	4 (28%)	17,19,21	1.13	0
5	NAG	A	1406	1	14,14,15	1.20	1 (7%)	17,19,21	1.04	0
5	NAG	C	1403	1	14,14,15	1.42	2 (14%)	17,19,21	0.72	0
5	NAG	B	1402	1	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	B	1406	1	14,14,15	1.44	1 (7%)	17,19,21	1.04	2 (11%)
5	NAG	C	1401	1	14,14,15	1.43	3 (21%)	17,19,21	0.76	1 (5%)
5	NAG	C	1402	1	14,14,15	1.34	2 (14%)	17,19,21	1.69	1 (5%)
5	NAG	C	1406	1	14,14,15	1.40	2 (14%)	17,19,21	0.76	0
5	NAG	B	1405	1	14,14,15	1.38	2 (14%)	17,19,21	0.95	0
5	NAG	A	1403	1	14,14,15	1.42	4 (28%)	17,19,21	0.89	1 (5%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1402	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1403	1	-	0/6/23/26	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1401	NAG	O5-C5	3.89	1.51	1.43
5	B	1406	NAG	C1-C2	3.60	1.57	1.52
5	B	1407	NAG	O5-C1	3.38	1.49	1.43
5	C	1401	NAG	O5-C5	3.32	1.49	1.43
5	C	1403	NAG	C1-C2	3.22	1.56	1.52
5	C	1406	NAG	O5-C5	3.20	1.49	1.43
5	A	1405	NAG	O5-C1	3.11	1.48	1.43
5	C	1404	NAG	O5-C5	3.11	1.49	1.43
5	B	1407	NAG	O5-C5	3.10	1.49	1.43
5	B	1405	NAG	C1-C2	3.07	1.56	1.52
5	A	1403	NAG	O5-C5	2.99	1.49	1.43
5	B	1405	NAG	O5-C5	2.99	1.49	1.43
5	A	1407	NAG	O5-C5	2.82	1.48	1.43
5	C	1402	NAG	O5-C5	2.77	1.48	1.43
5	B	1404	NAG	O5-C1	2.75	1.48	1.43
5	C	1403	NAG	O5-C5	2.69	1.48	1.43
5	A	1407	NAG	C1-C2	2.68	1.56	1.52
5	A	1402	NAG	O5-C5	2.63	1.48	1.43
5	C	1405	NAG	O5-C5	2.60	1.48	1.43
5	A	1405	NAG	O5-C5	2.59	1.48	1.43
5	B	1403	NAG	O5-C5	2.51	1.48	1.43
5	A	1406	NAG	C1-C2	2.42	1.55	1.52
5	B	1403	NAG	C1-C2	2.42	1.55	1.52
5	A	1403	NAG	C1-C2	2.36	1.55	1.52
5	A	1402	NAG	C8-C7	2.35	1.55	1.50
5	C	1401	NAG	C1-C2	2.29	1.55	1.52
5	C	1401	NAG	C8-C7	2.28	1.55	1.50
5	C	1406	NAG	C1-C2	2.25	1.55	1.52
5	B	1404	NAG	O5-C5	2.21	1.47	1.43
5	C	1405	NAG	O5-C1	2.20	1.47	1.43
5	B	1401	NAG	O5-C1	2.19	1.47	1.43
5	A	1403	NAG	C8-C7	2.18	1.55	1.50
5	C	1402	NAG	C1-C2	2.15	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1407	NAG	C1-C2	2.13	1.55	1.52
5	A	1405	NAG	C1-C2	2.12	1.55	1.52
5	B	1407	NAG	C8-C7	2.08	1.54	1.50
5	B	1403	NAG	C2-N2	2.07	1.49	1.46
5	A	1403	NAG	O3-C3	2.04	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1402	NAG	C1-O5-C5	5.34	119.35	112.19
5	B	1406	NAG	C1-O5-C5	2.45	115.47	112.19
5	B	1403	NAG	C1-O5-C5	2.14	115.06	112.19
5	B	1406	NAG	O5-C5-C4	-2.06	105.82	110.83
5	A	1403	NAG	C3-C4-C5	2.05	113.94	110.23
5	C	1401	NAG	O5-C5-C4	-2.04	105.87	110.83
5	B	1401	NAG	O3-C3-C2	2.00	113.56	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	1402	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1402	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6

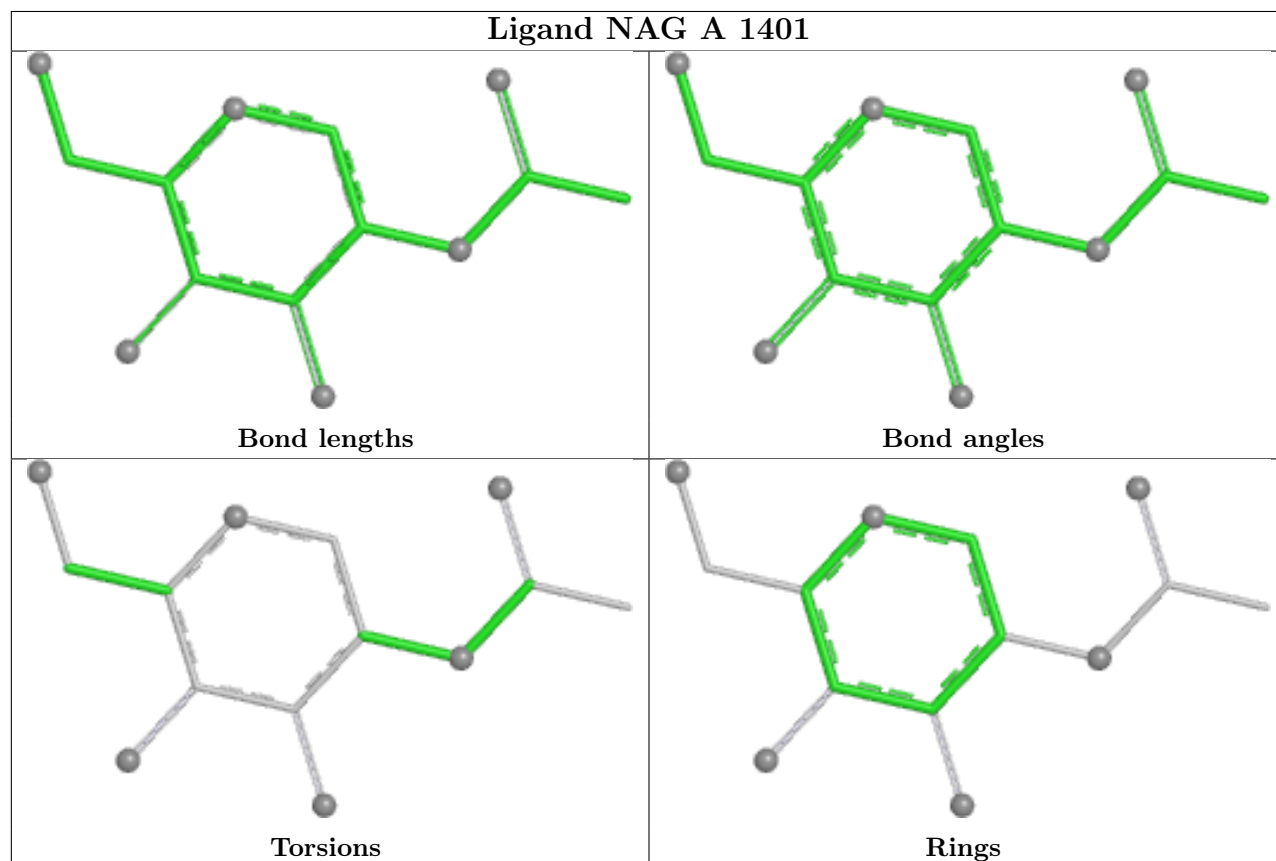
There are no ring outliers.

3 monomers are involved in 13 short contacts:

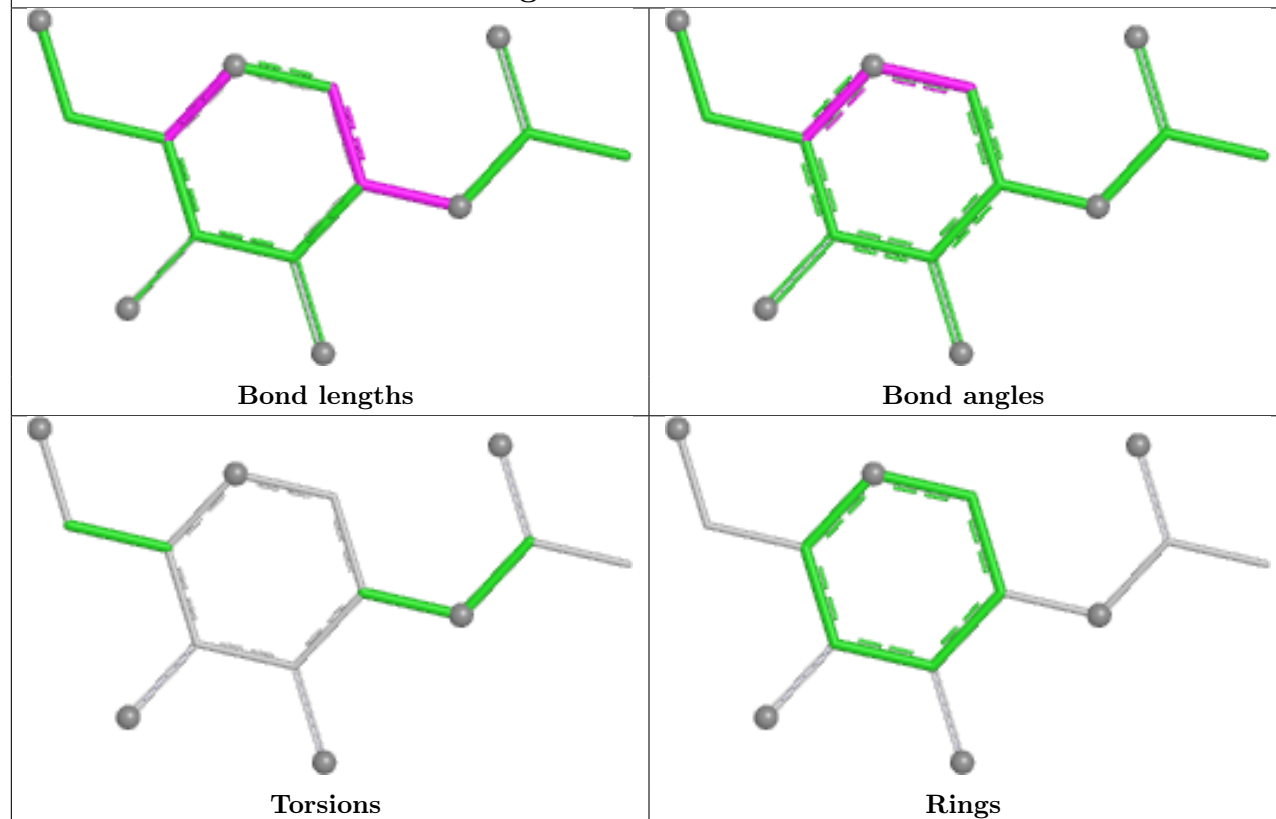
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1401	NAG	3	0
5	A	1404	NAG	5	0
5	B	1402	NAG	5	0

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.

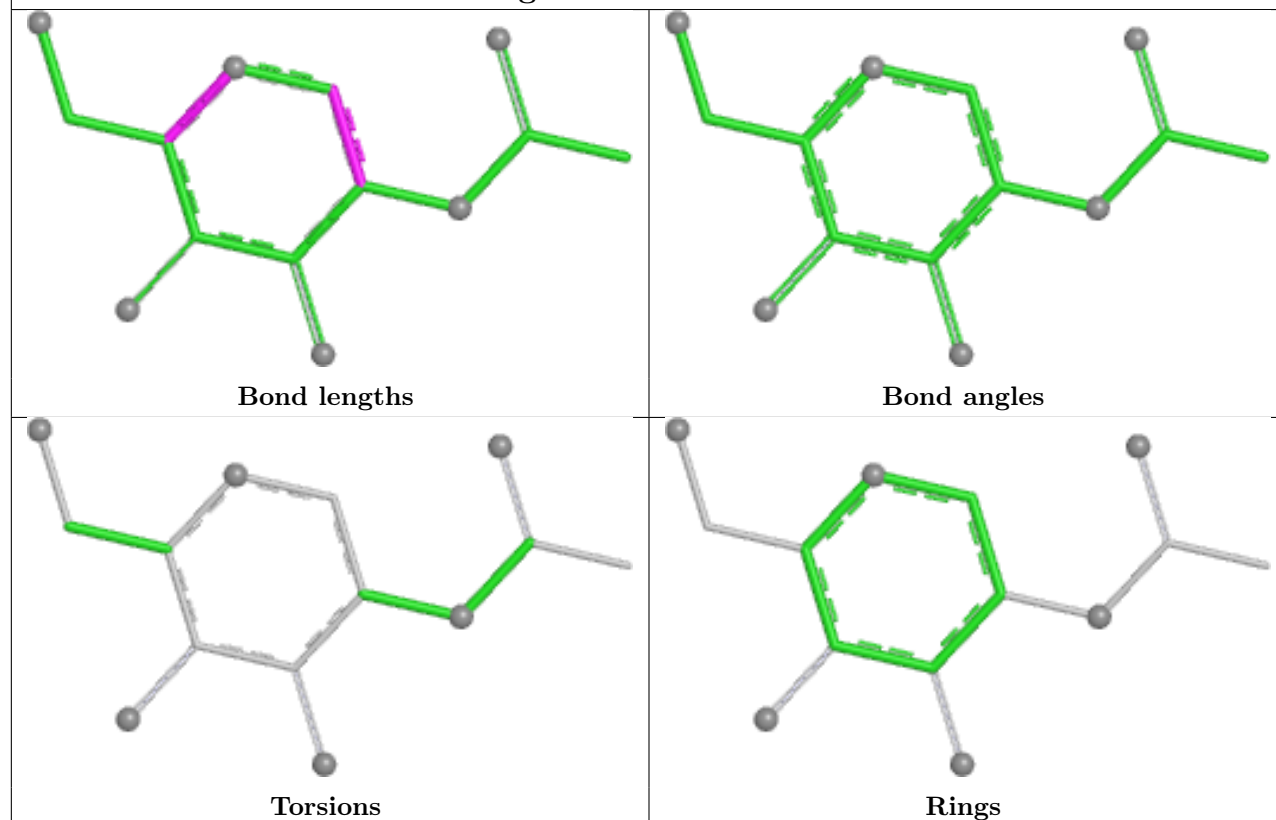
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



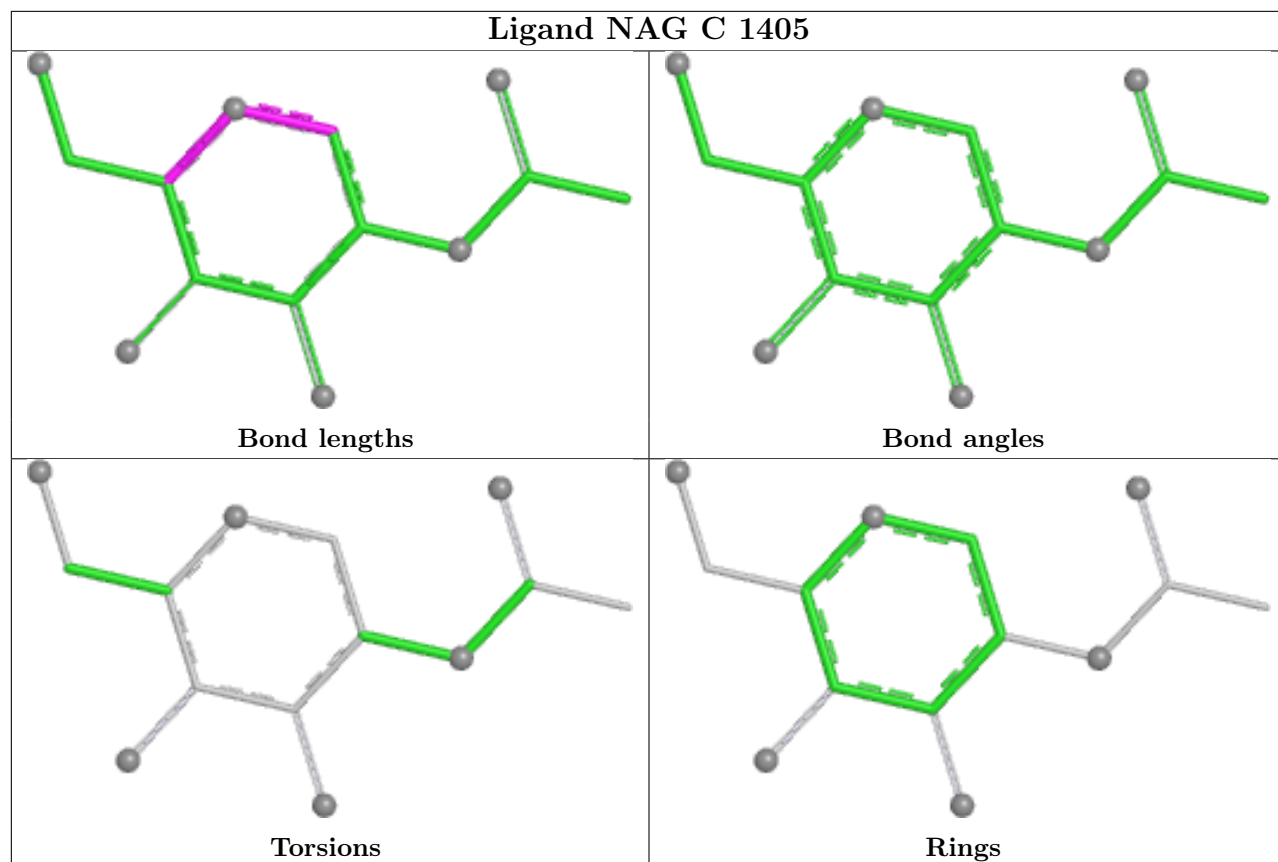
Ligand NAG B 1403



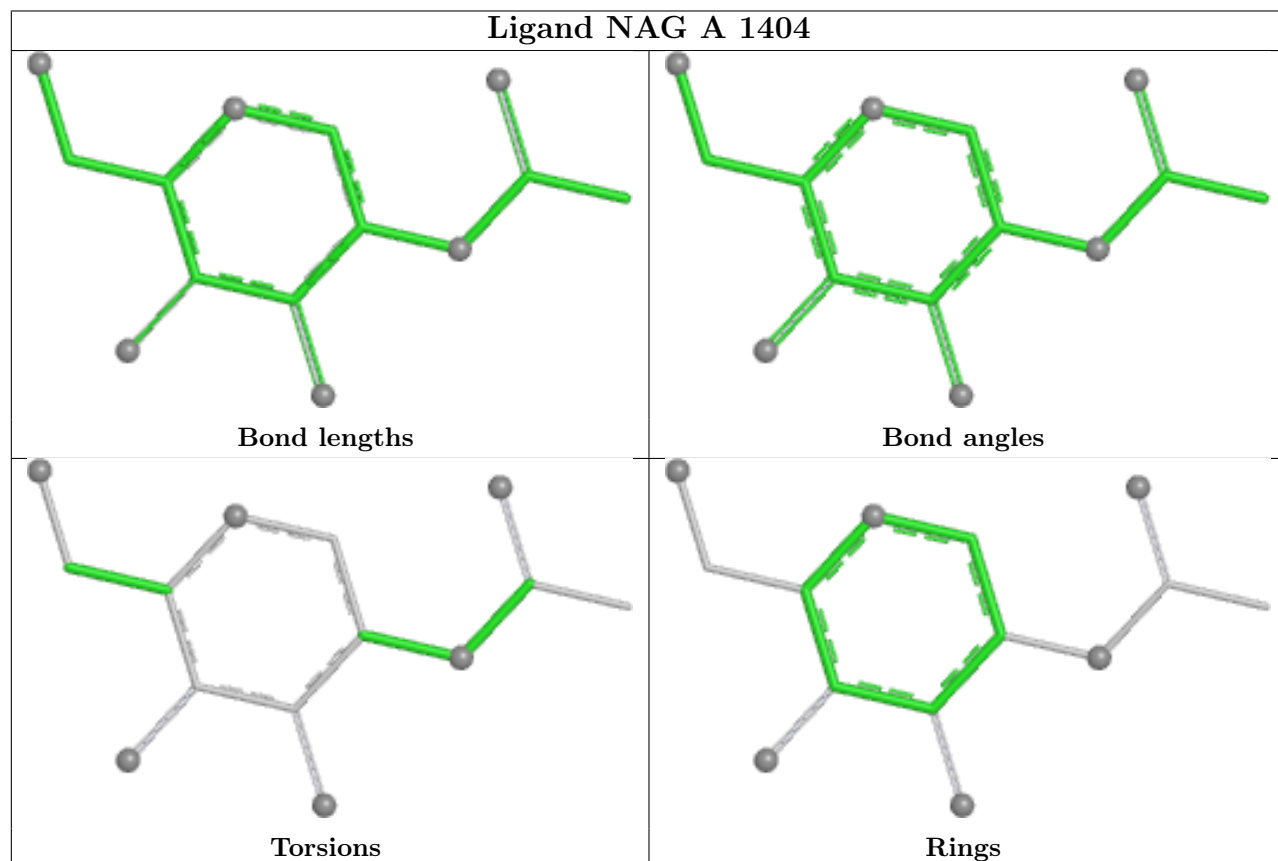
Ligand NAG A 1407

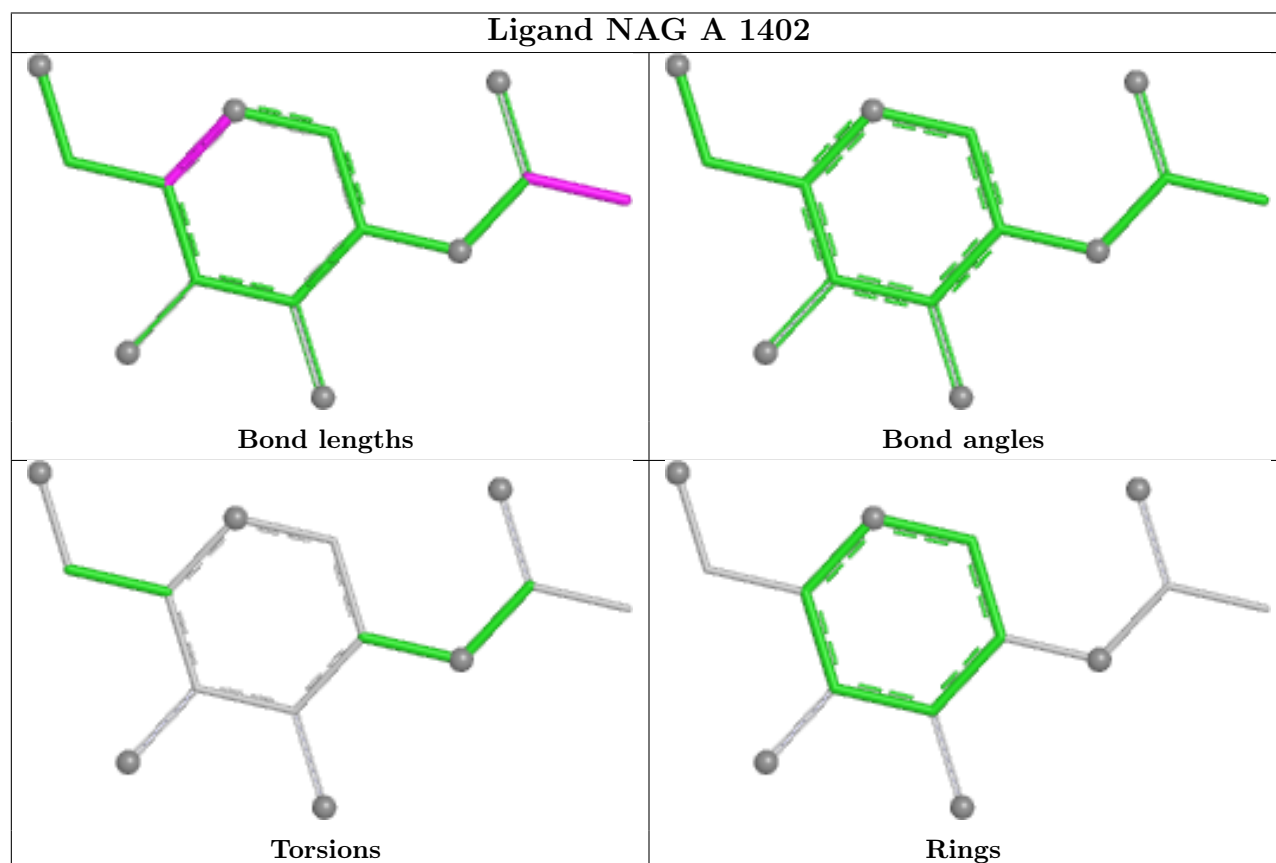
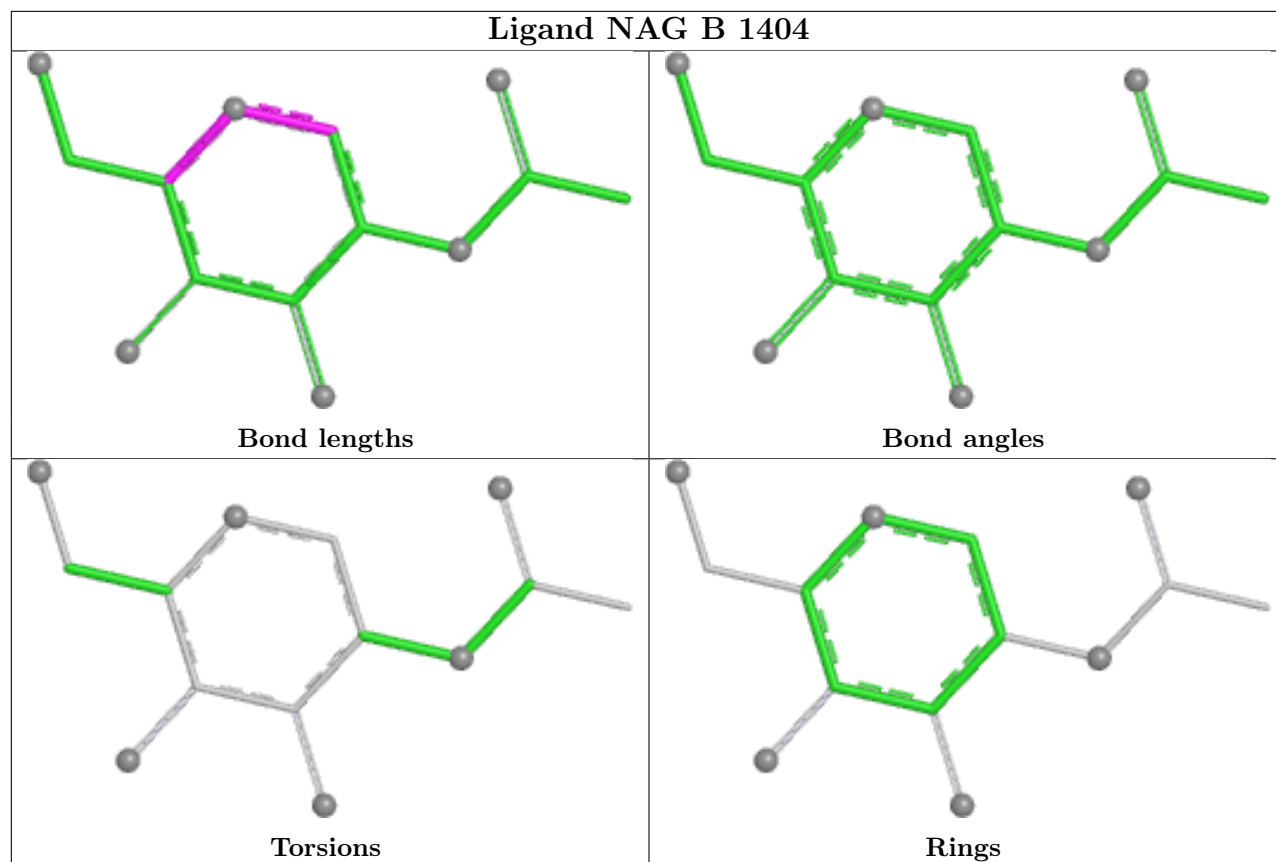


Ligand NAG C 1405

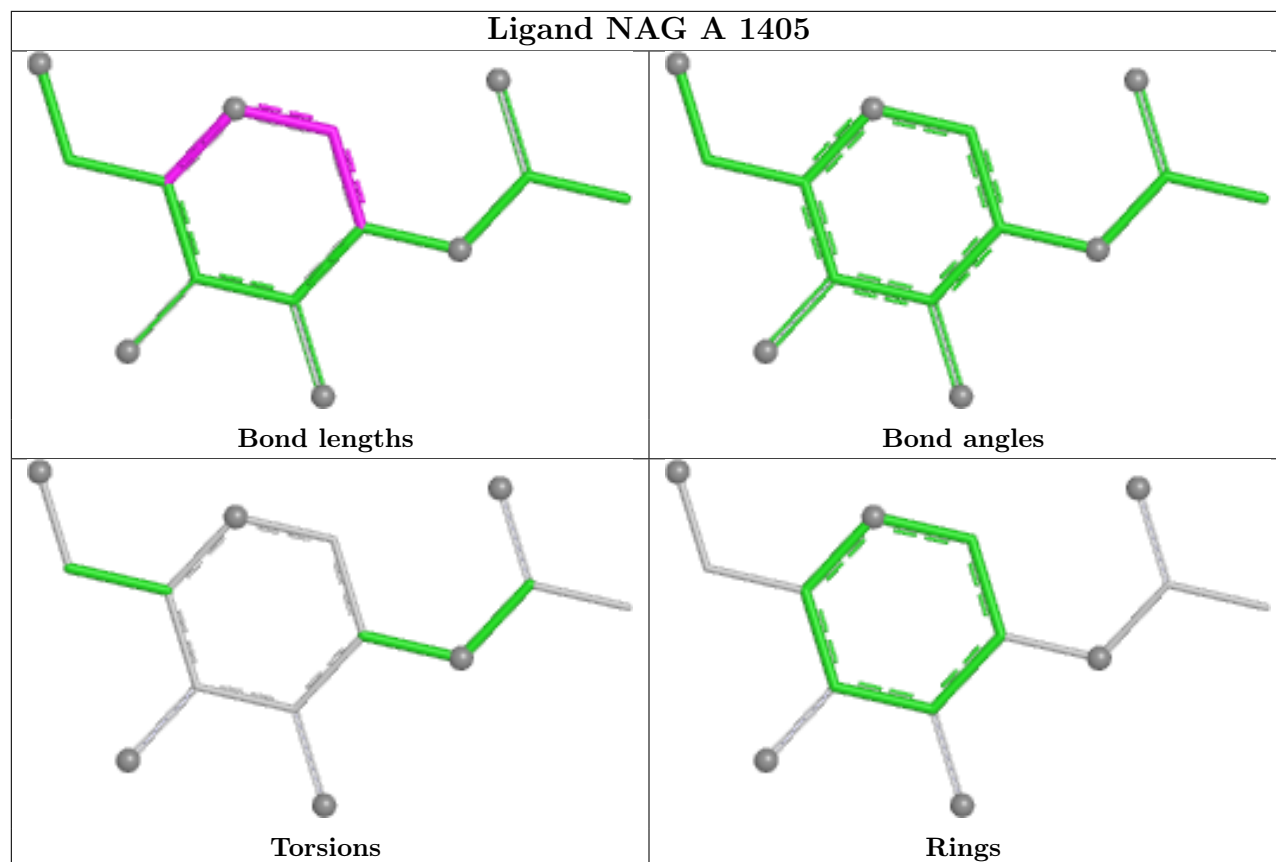


Ligand NAG A 1404

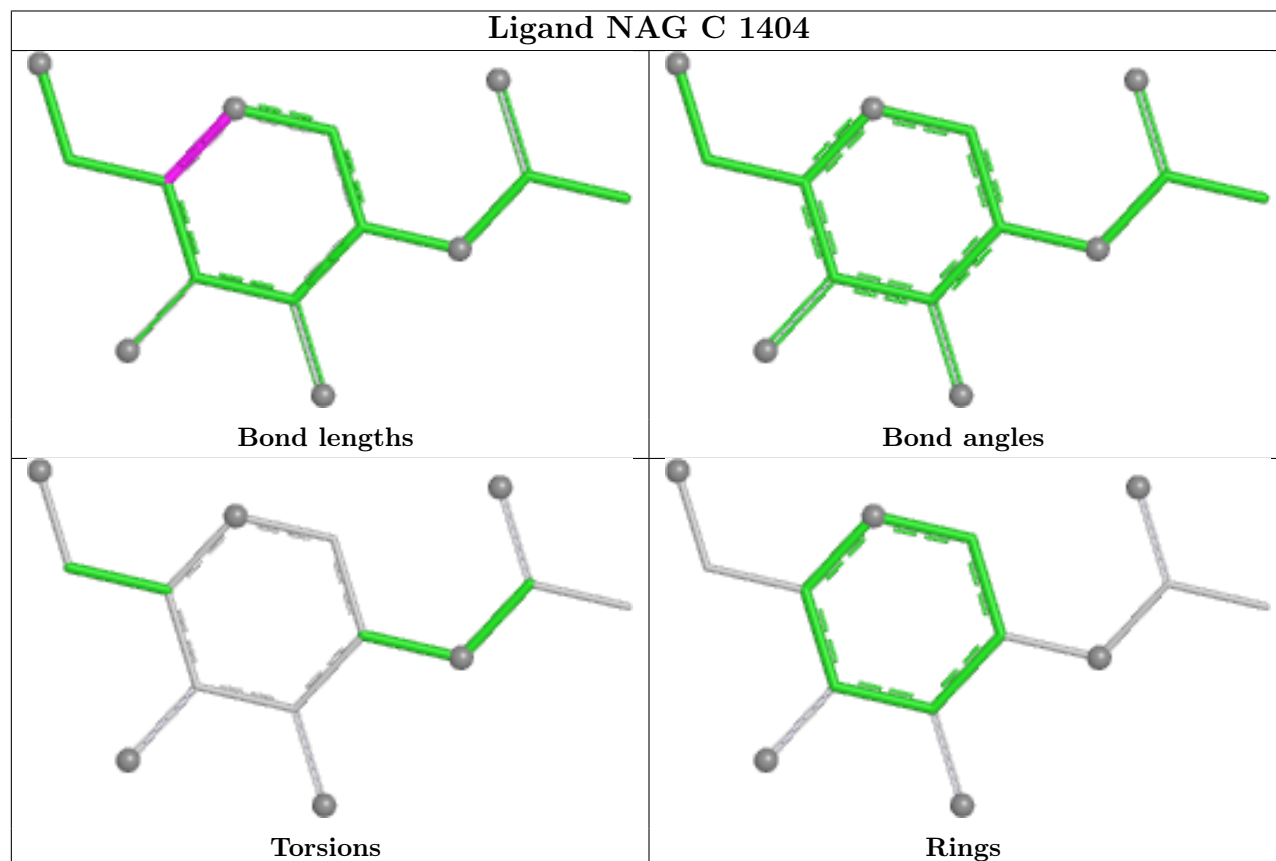


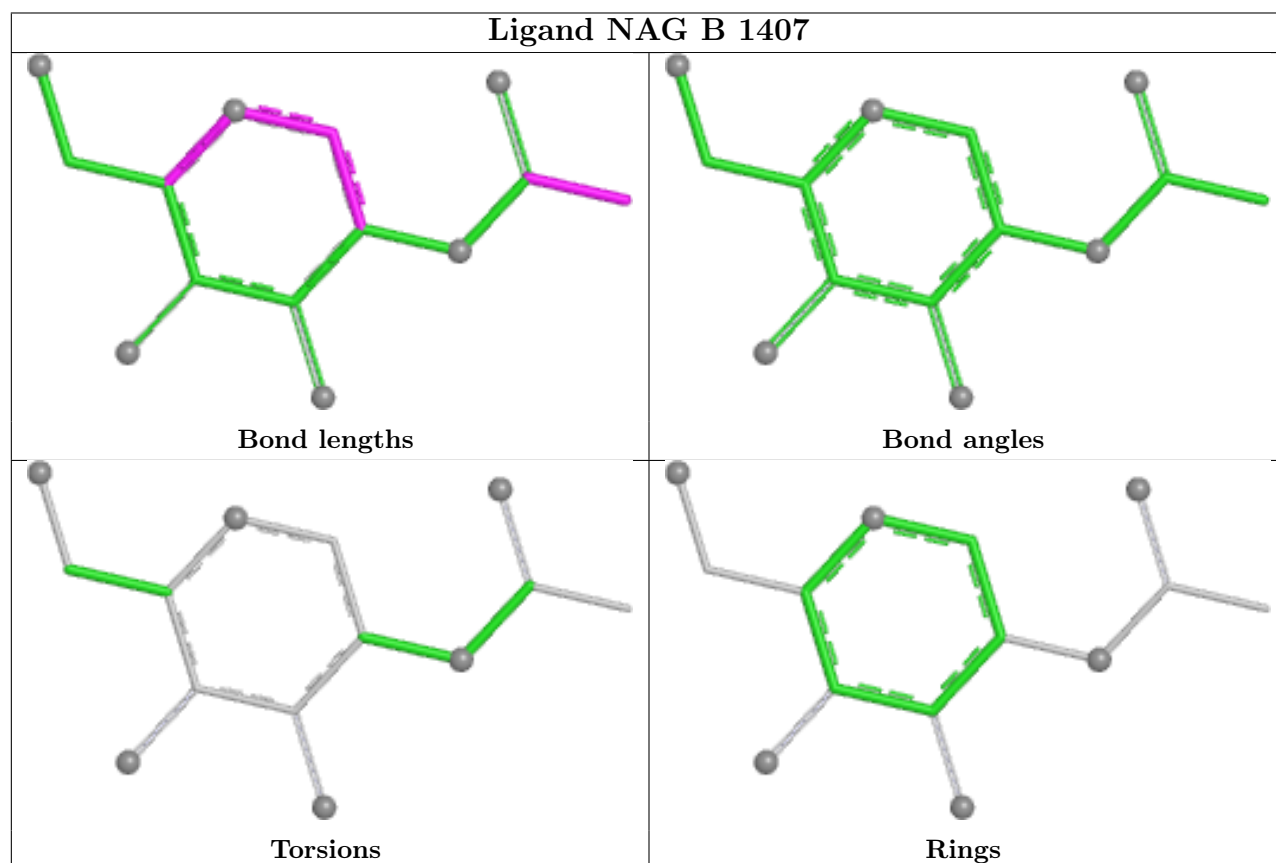
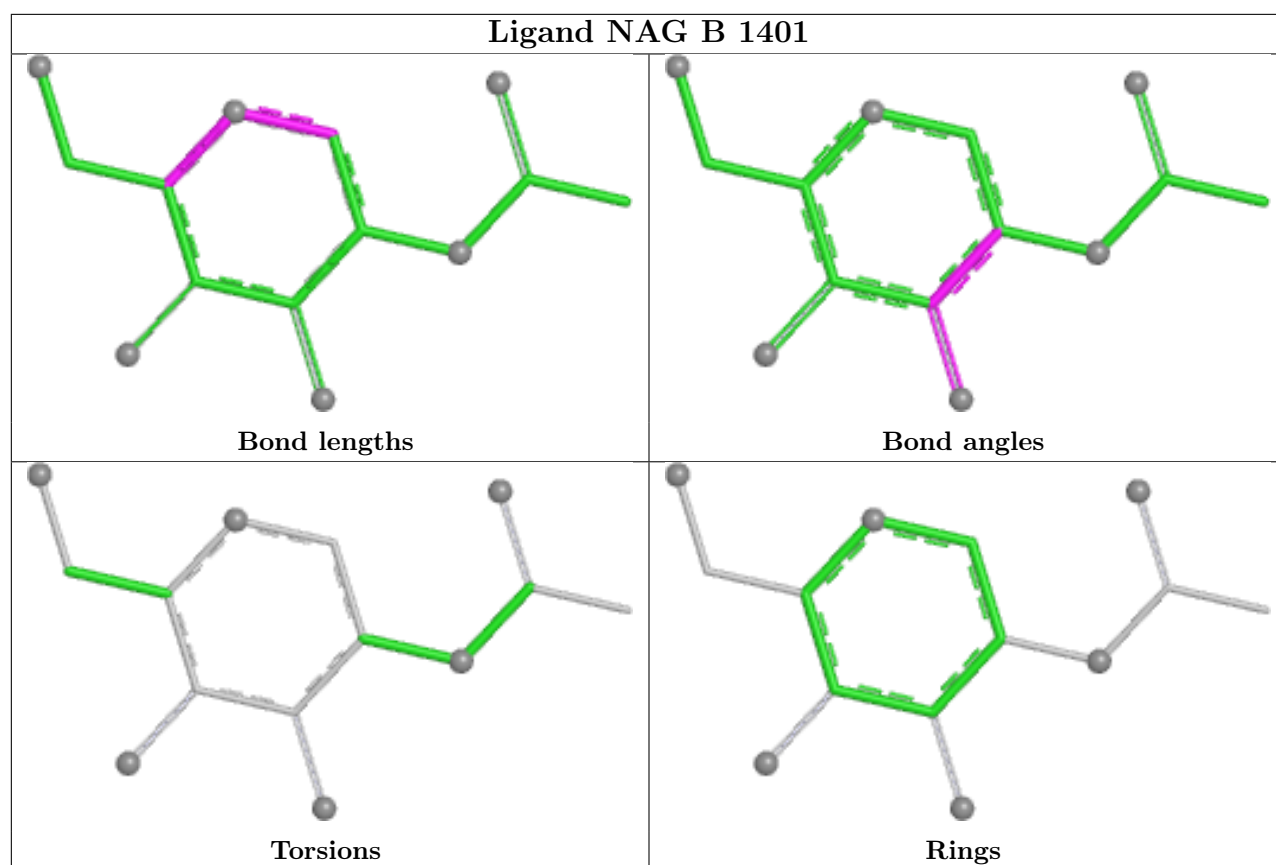


Ligand NAG A 1405

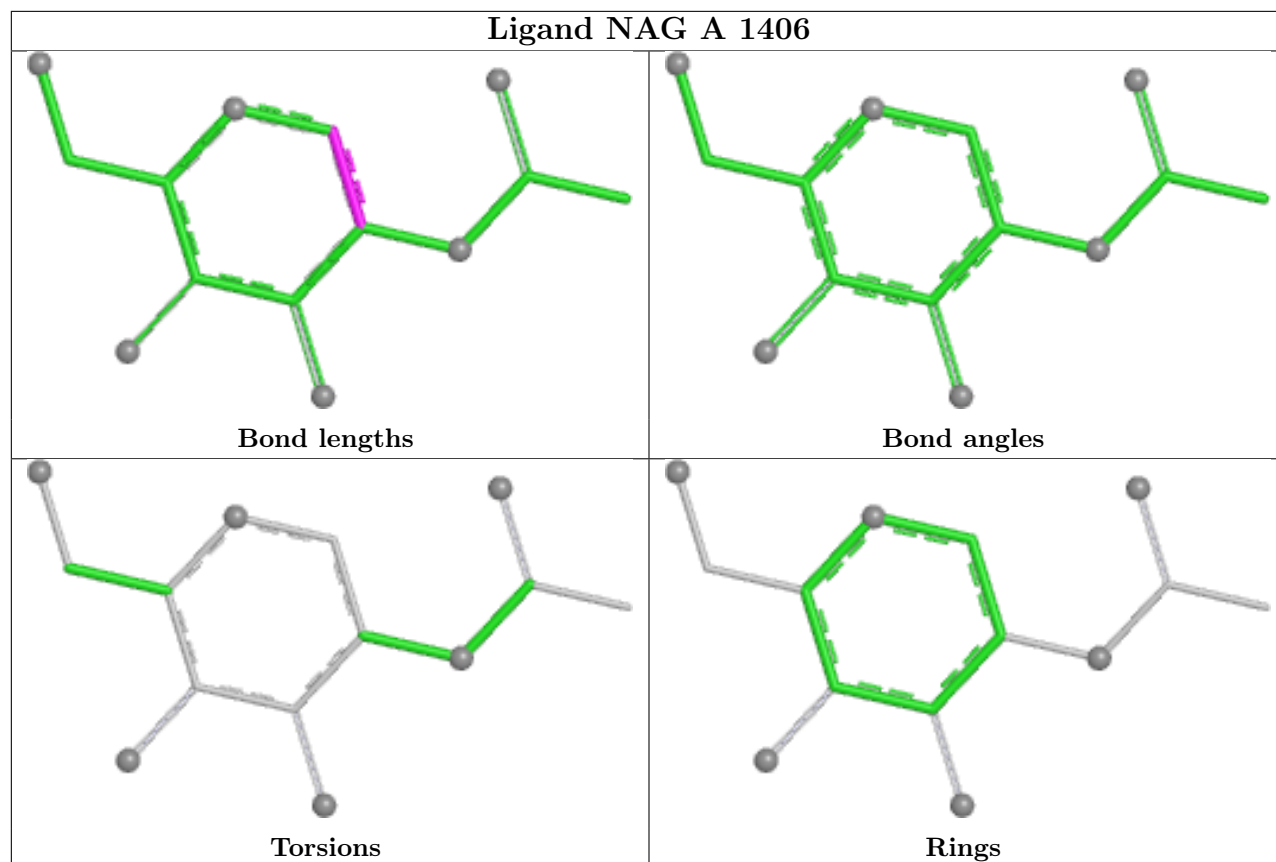


Ligand NAG C 1404

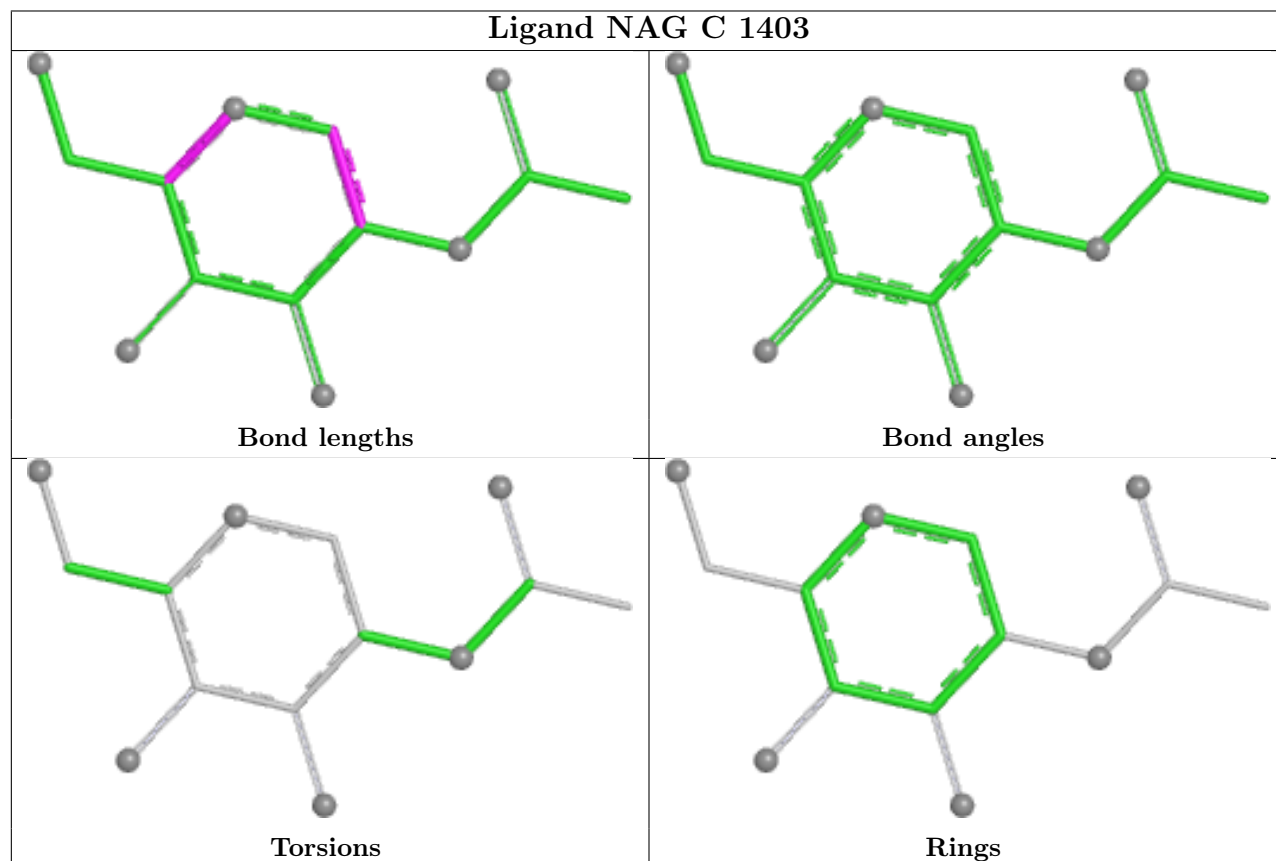




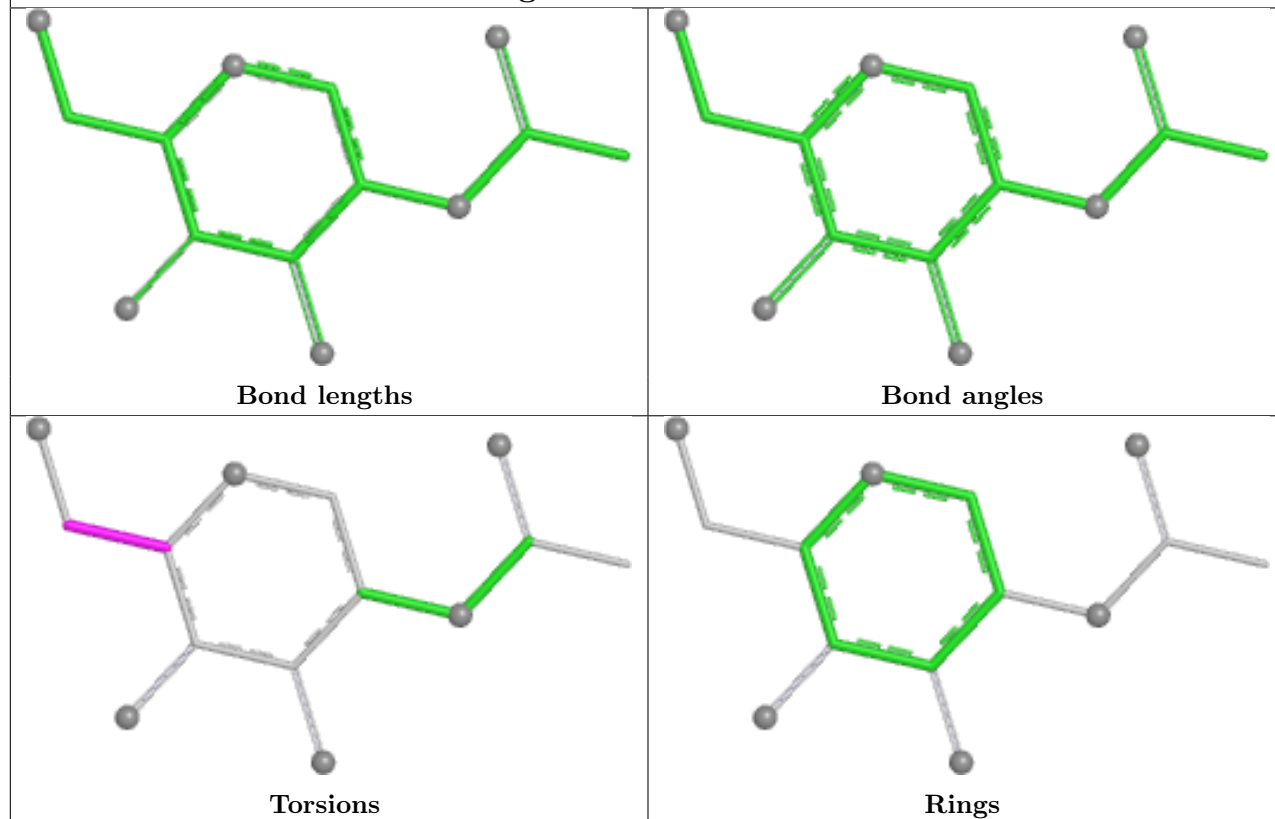
Ligand NAG A 1406



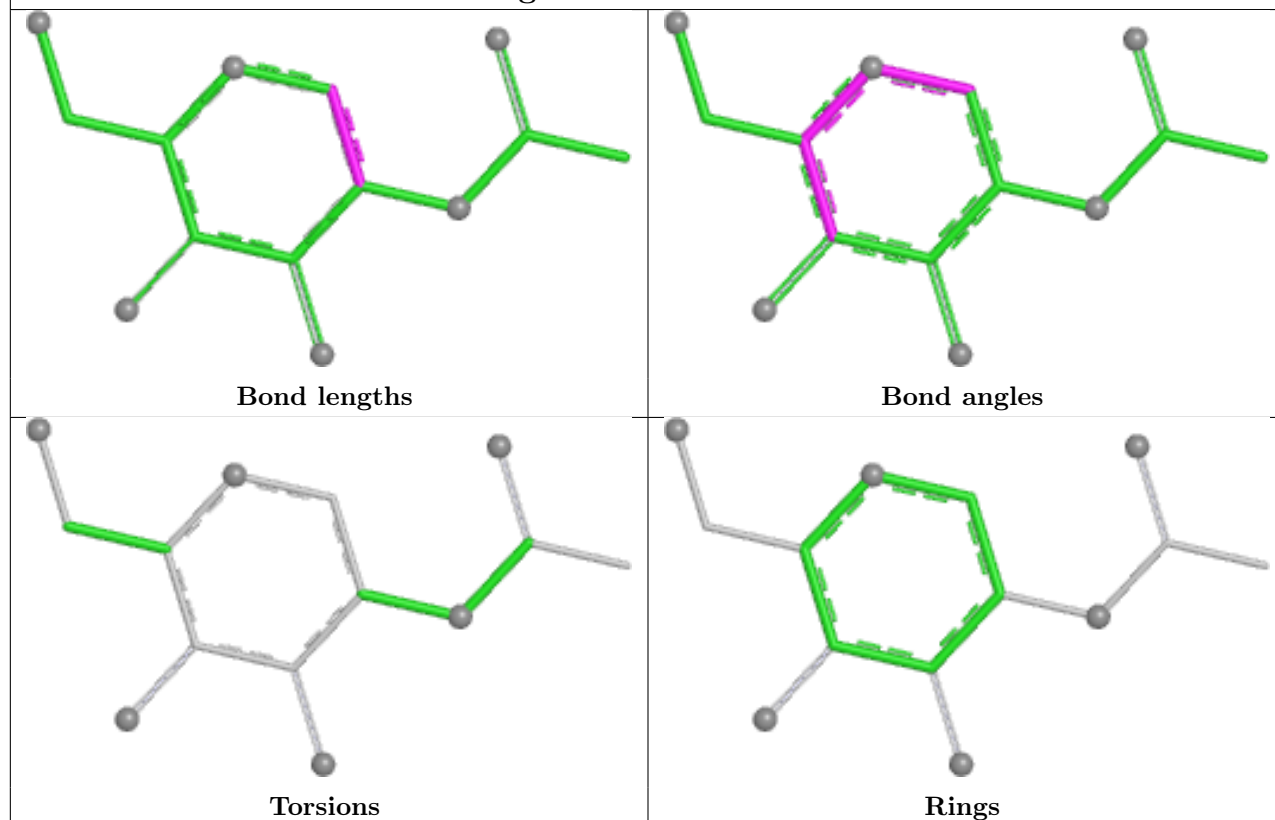
Ligand NAG C 1403



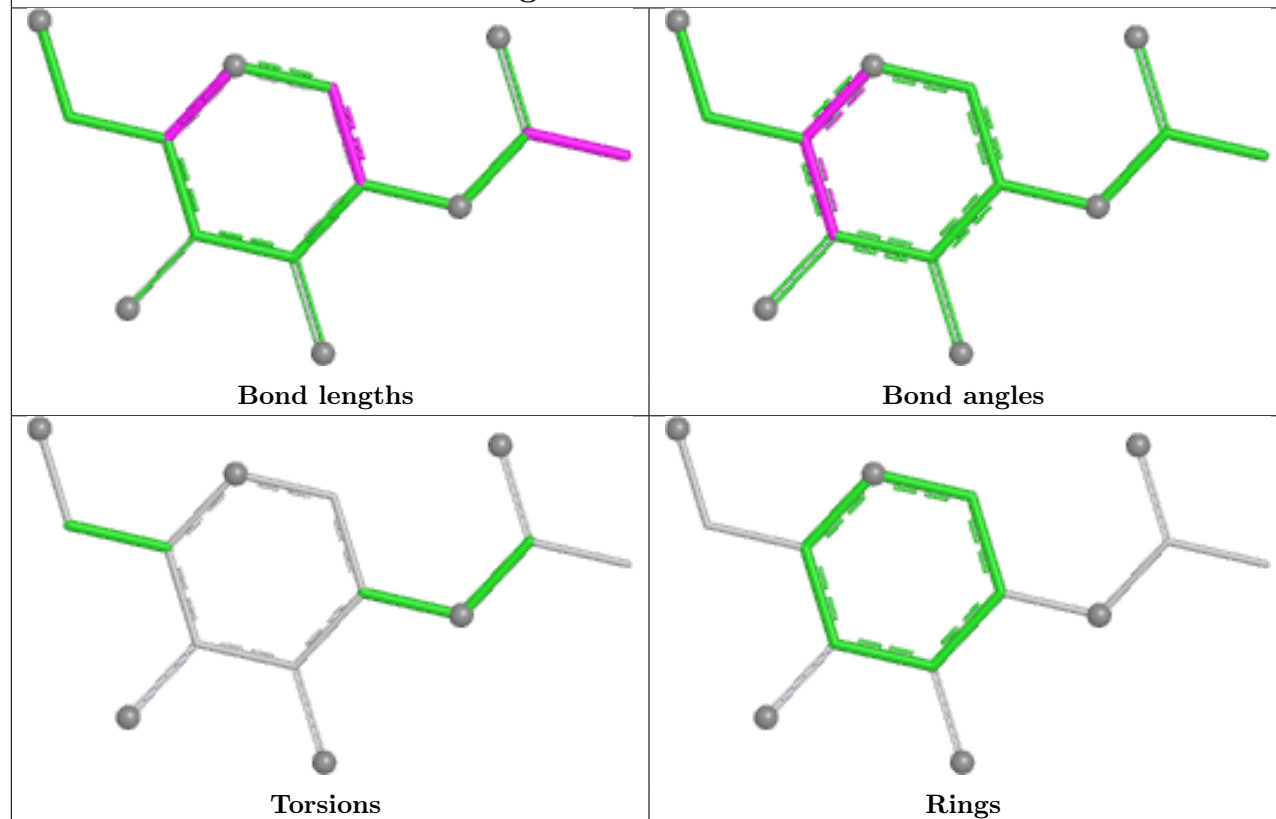
Ligand NAG B 1402



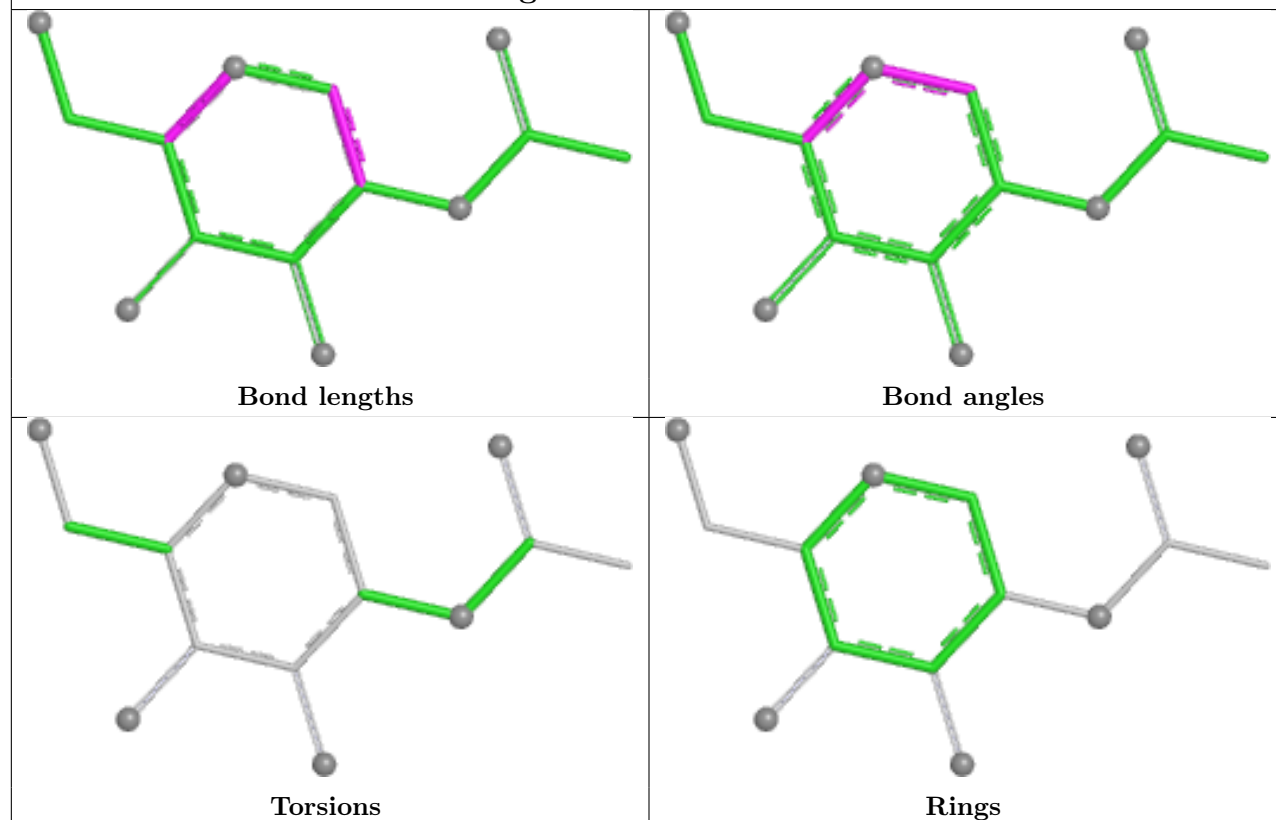
Ligand NAG B 1406



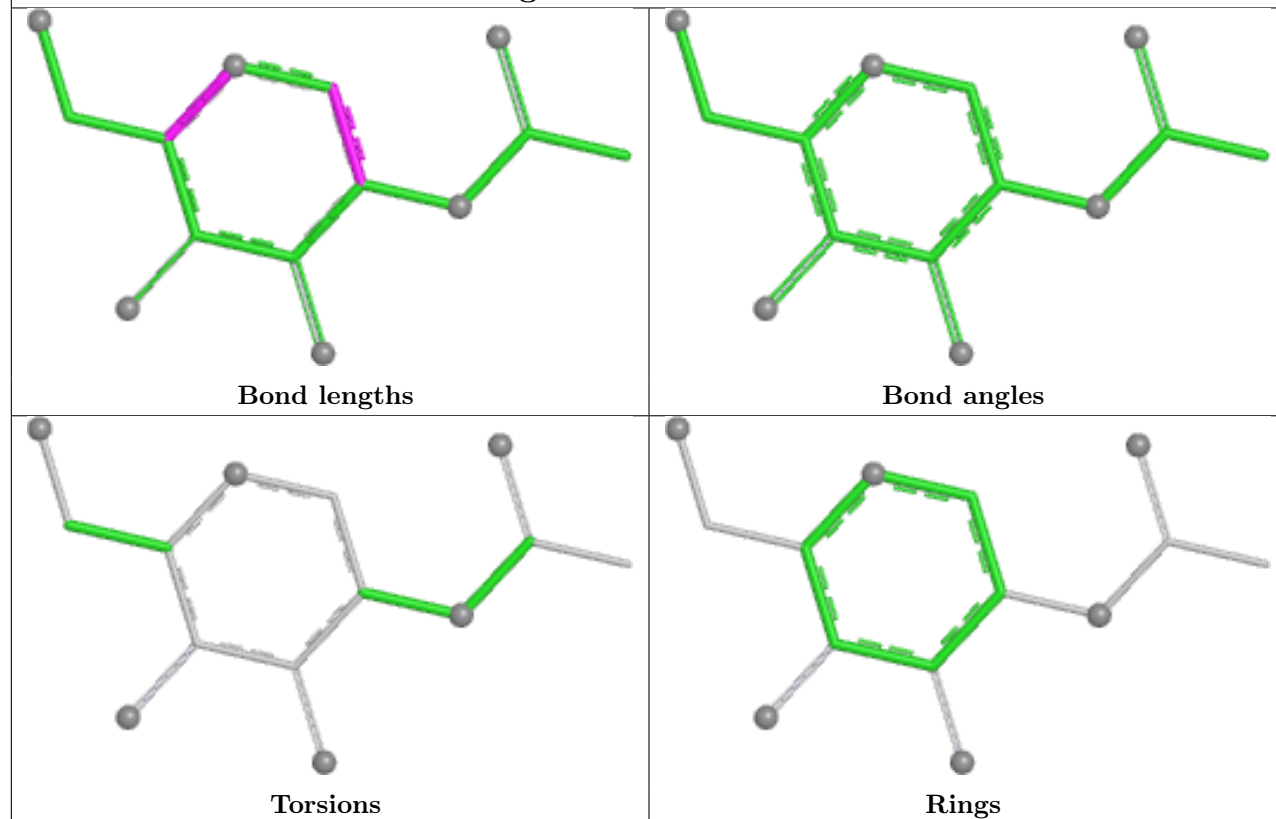
Ligand NAG C 1401



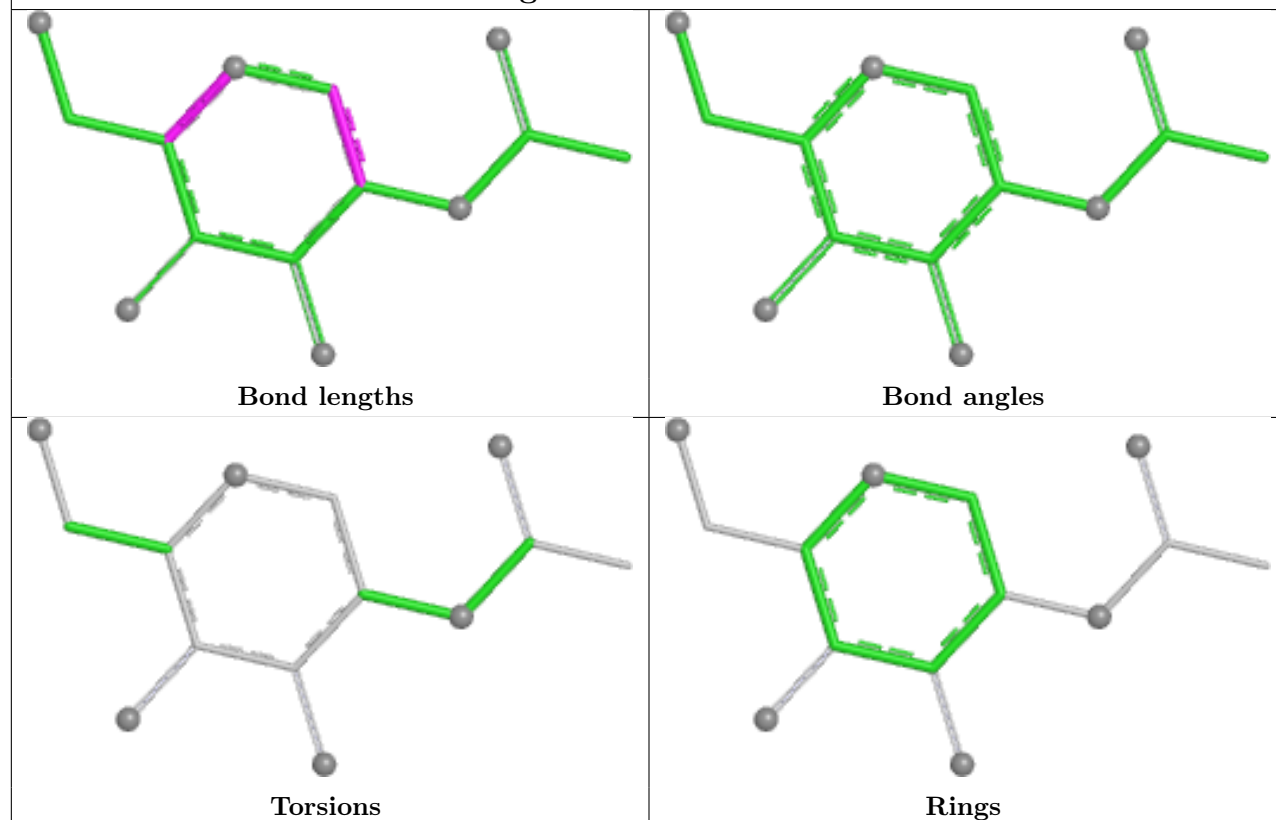
Ligand NAG C 1402

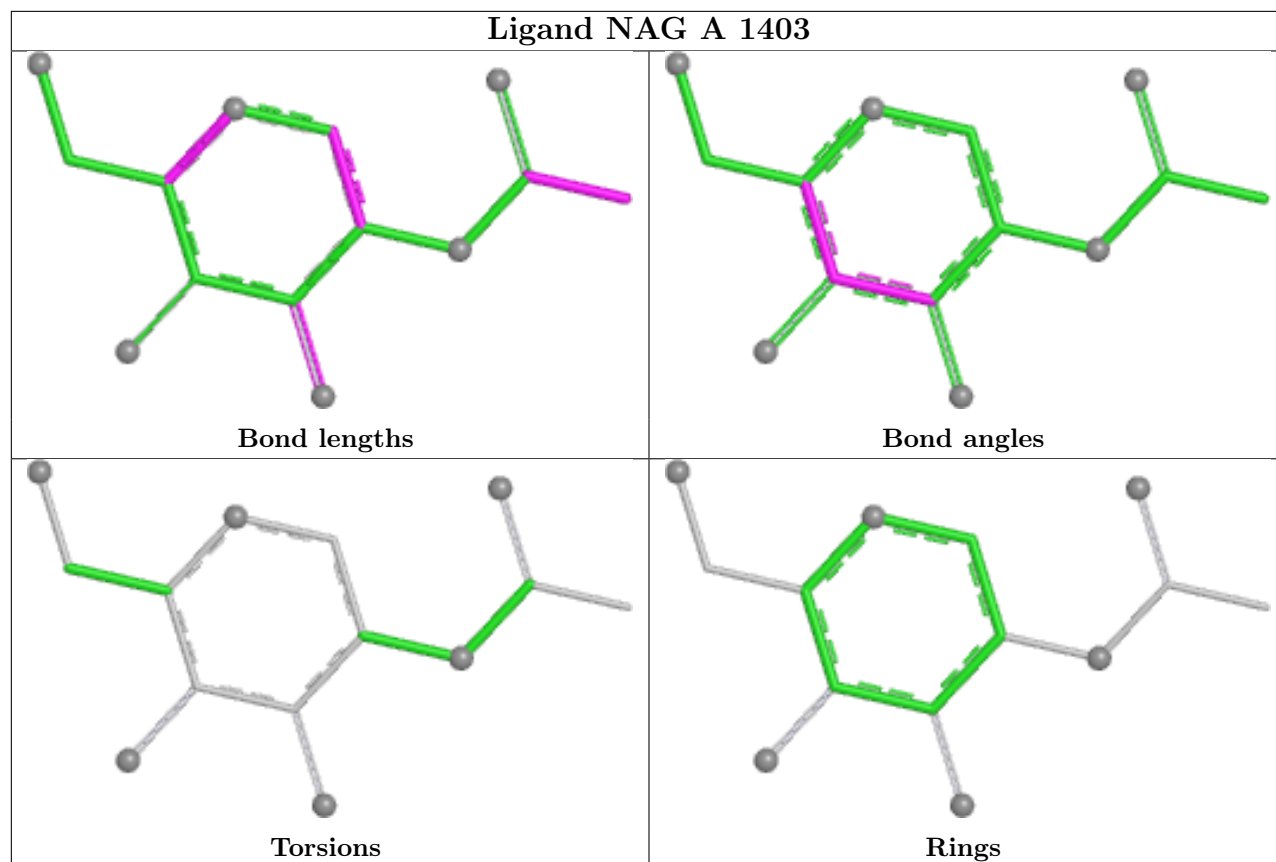


Ligand NAG C 1406



Ligand NAG B 1405





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.

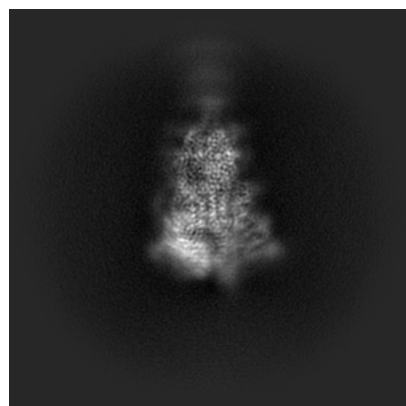
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27207. These allow visual inspection of the internal detail of the map and identification of artifacts.

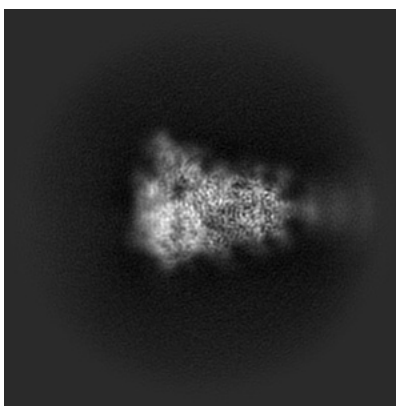
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

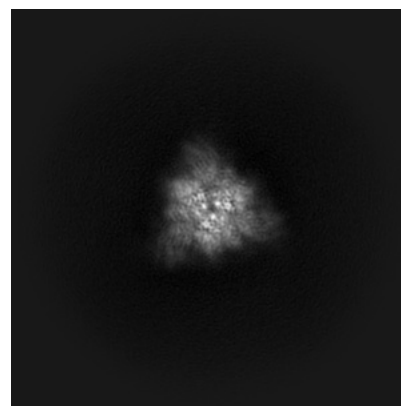
6.1.1 Primary map



X

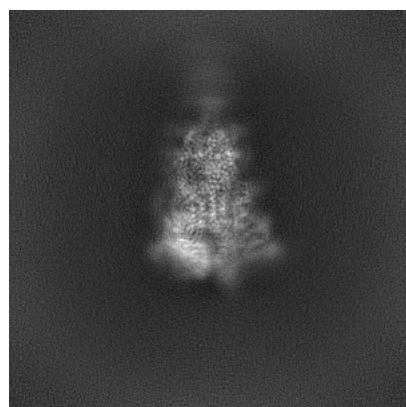


Y

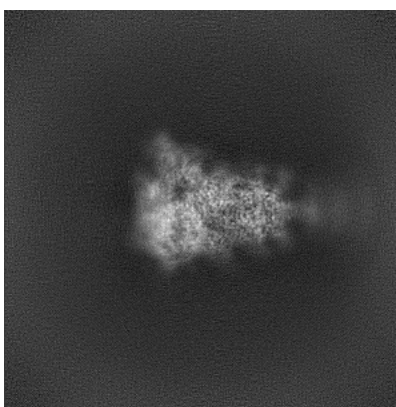


Z

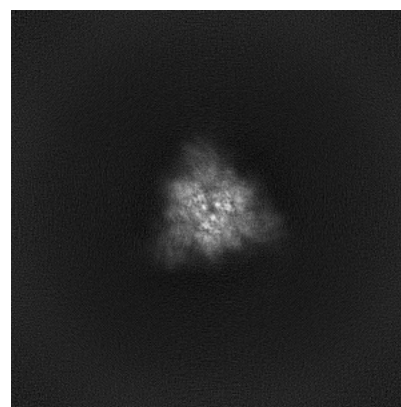
6.1.2 Raw map



X



Y

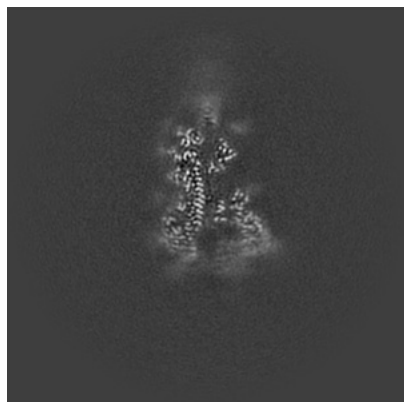


Z

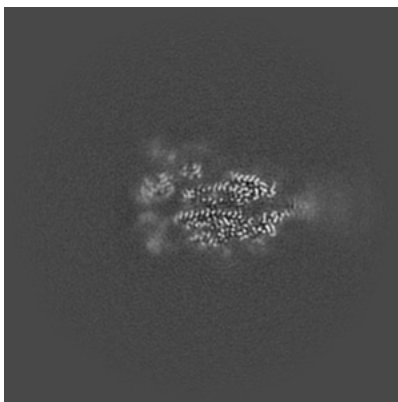
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

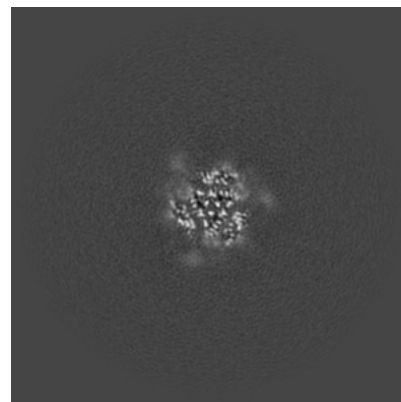
6.2.1 Primary map



X Index: 240

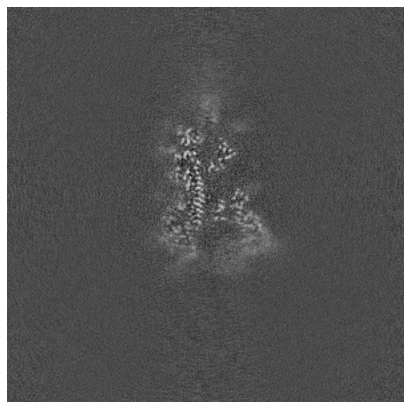


Y Index: 240

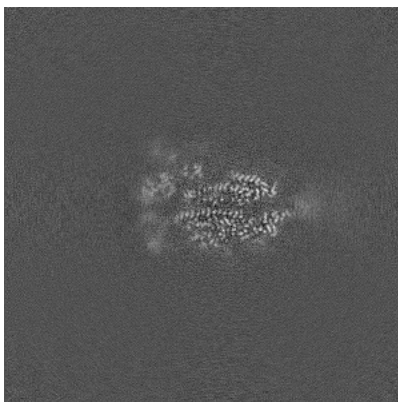


Z Index: 240

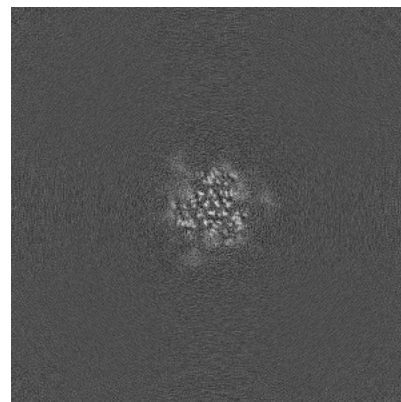
6.2.2 Raw map



X Index: 240



Y Index: 240

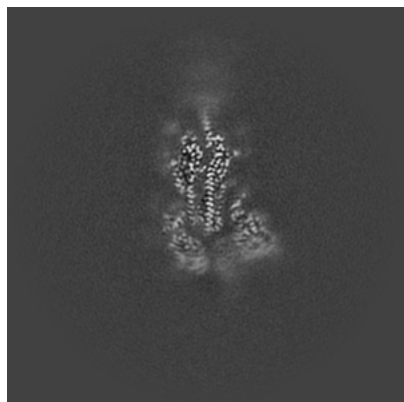


Z Index: 240

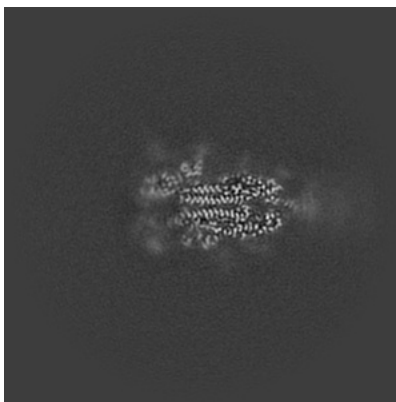
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

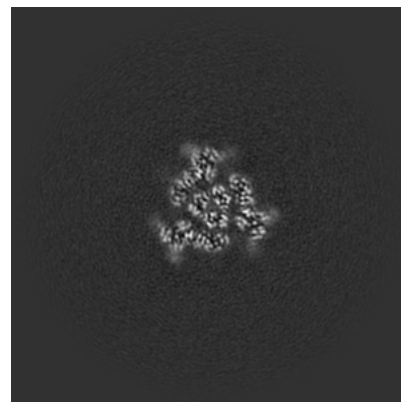
6.3.1 Primary map



X Index: 231

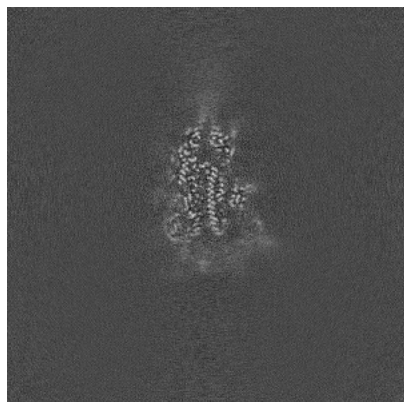


Y Index: 245

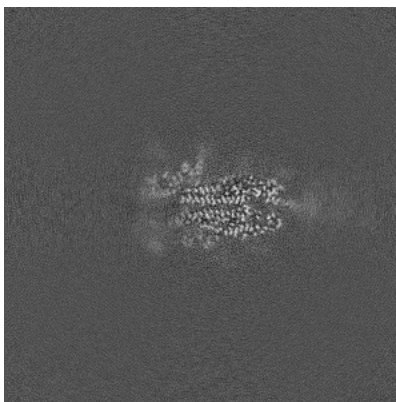


Z Index: 220

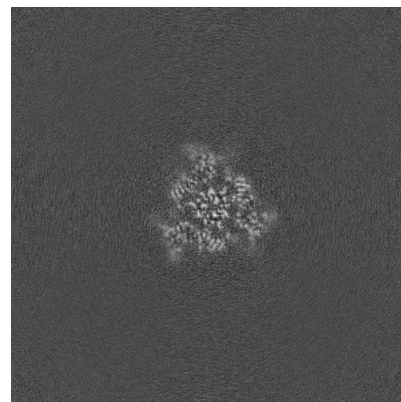
6.3.2 Raw map



X Index: 247



Y Index: 246

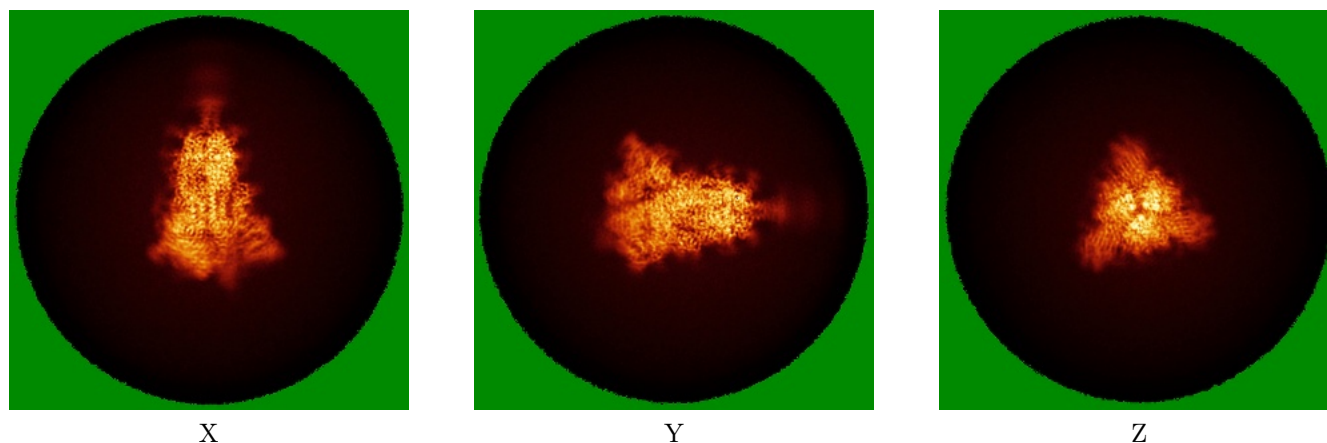


Z Index: 226

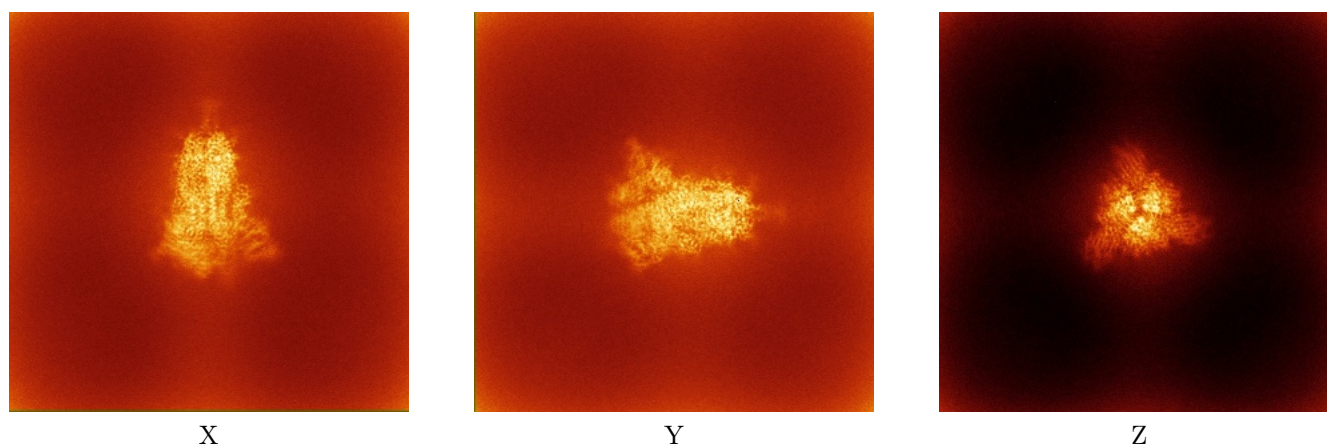
The images above show the largest variance slices of the map in three orthogonal directions.

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.

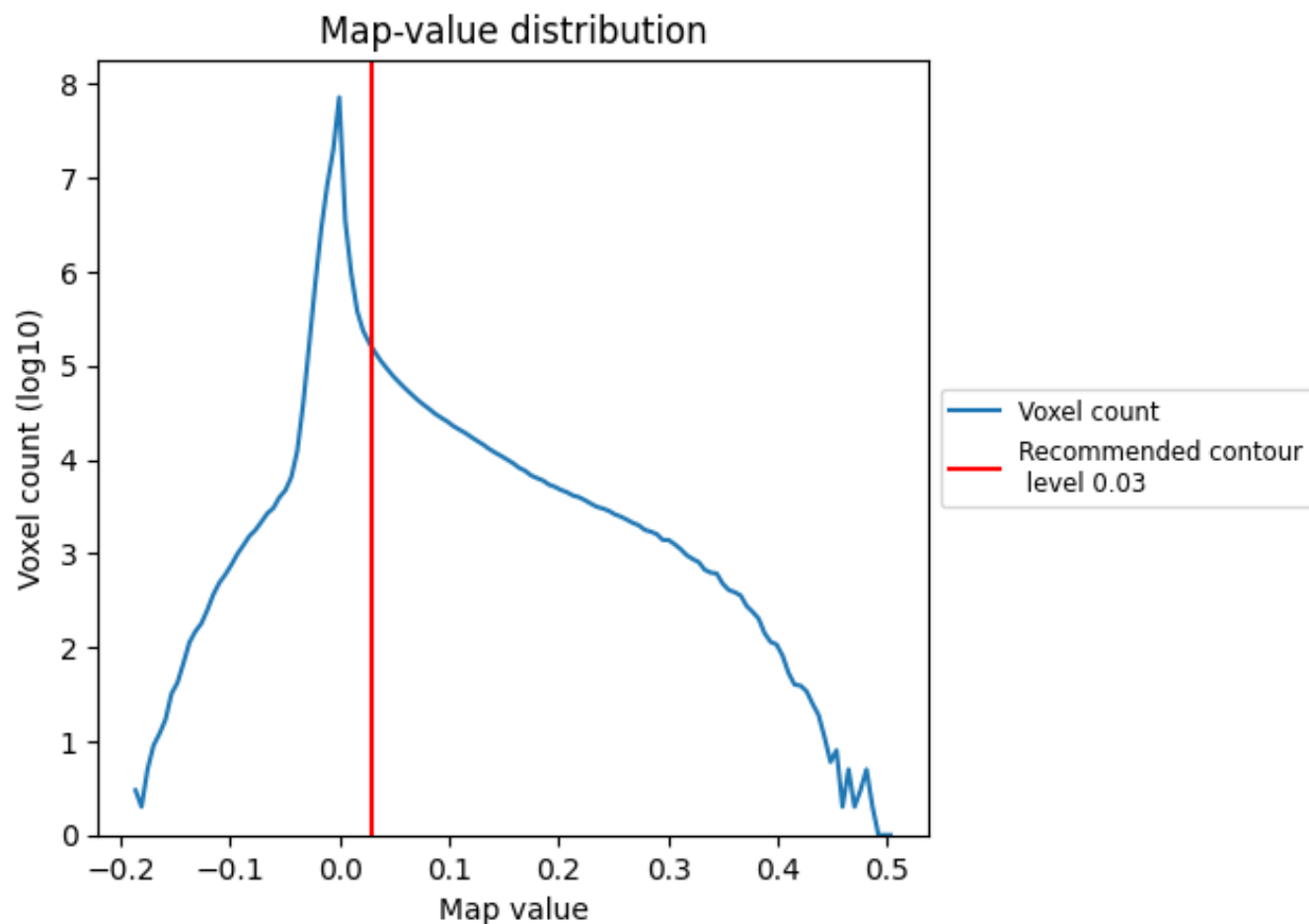
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

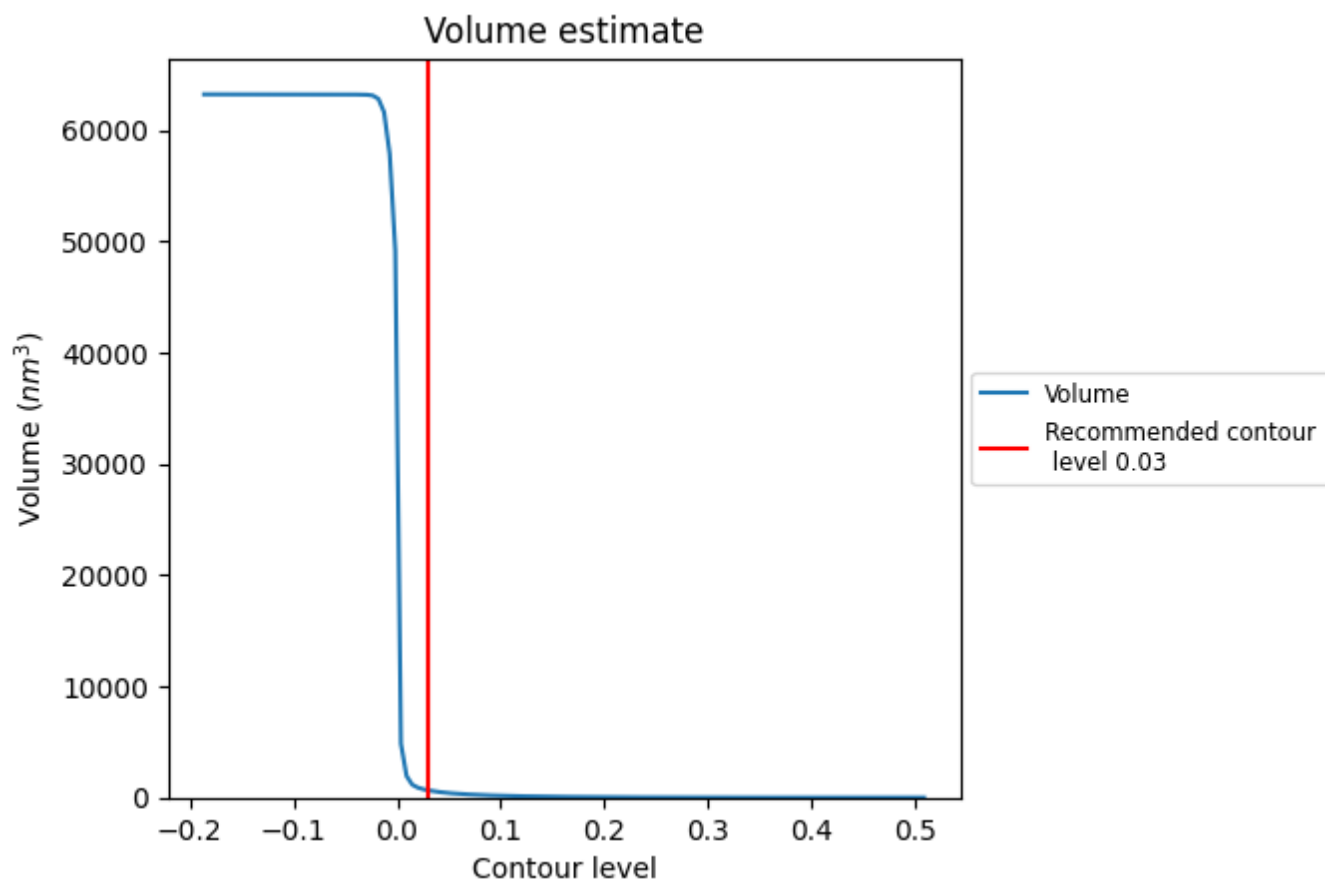
This section contains the results of statistical analysis of the map.

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.

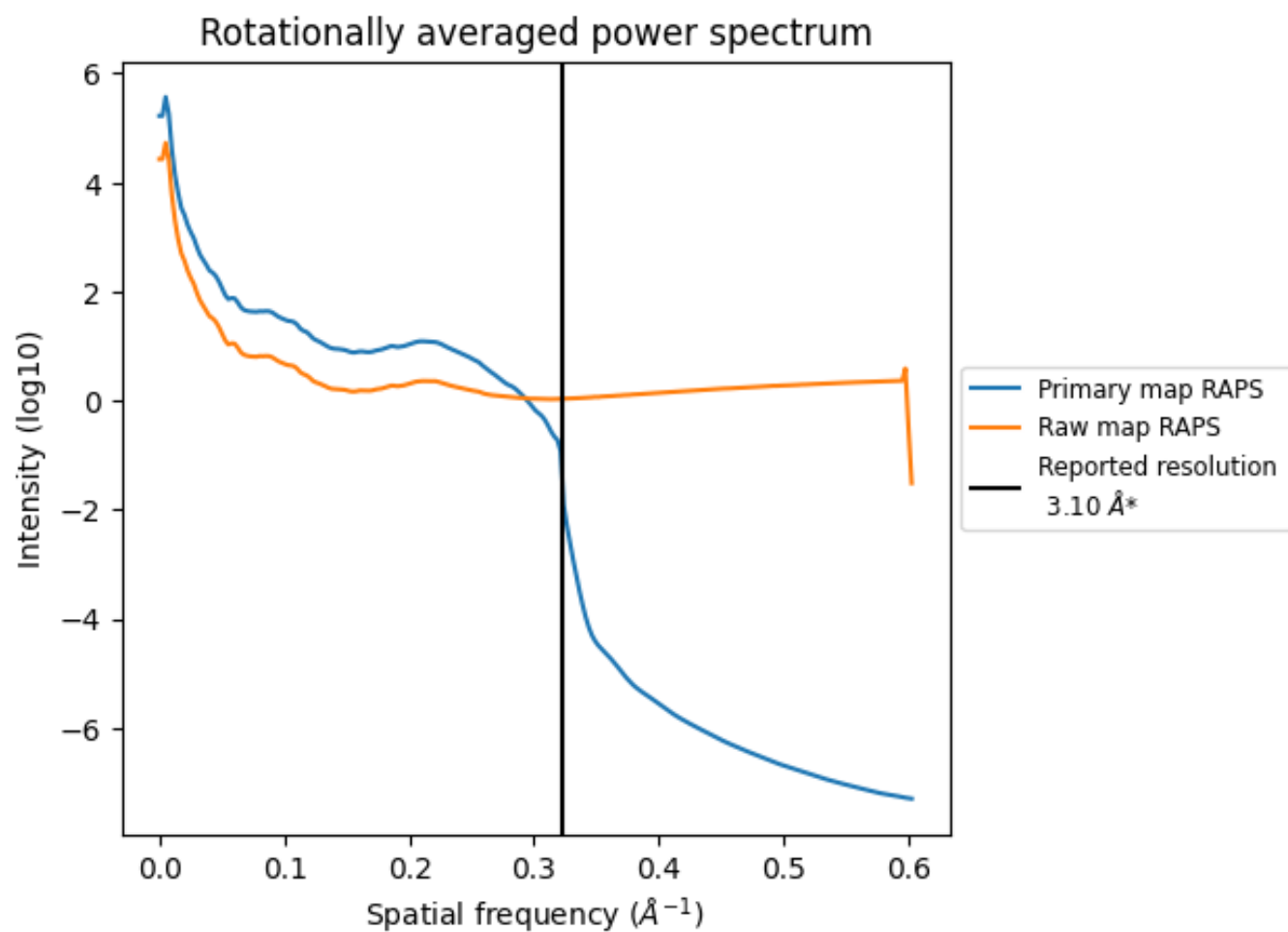
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 655 nm^3 ; this corresponds to an approximate mass of 592 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 ⓘ

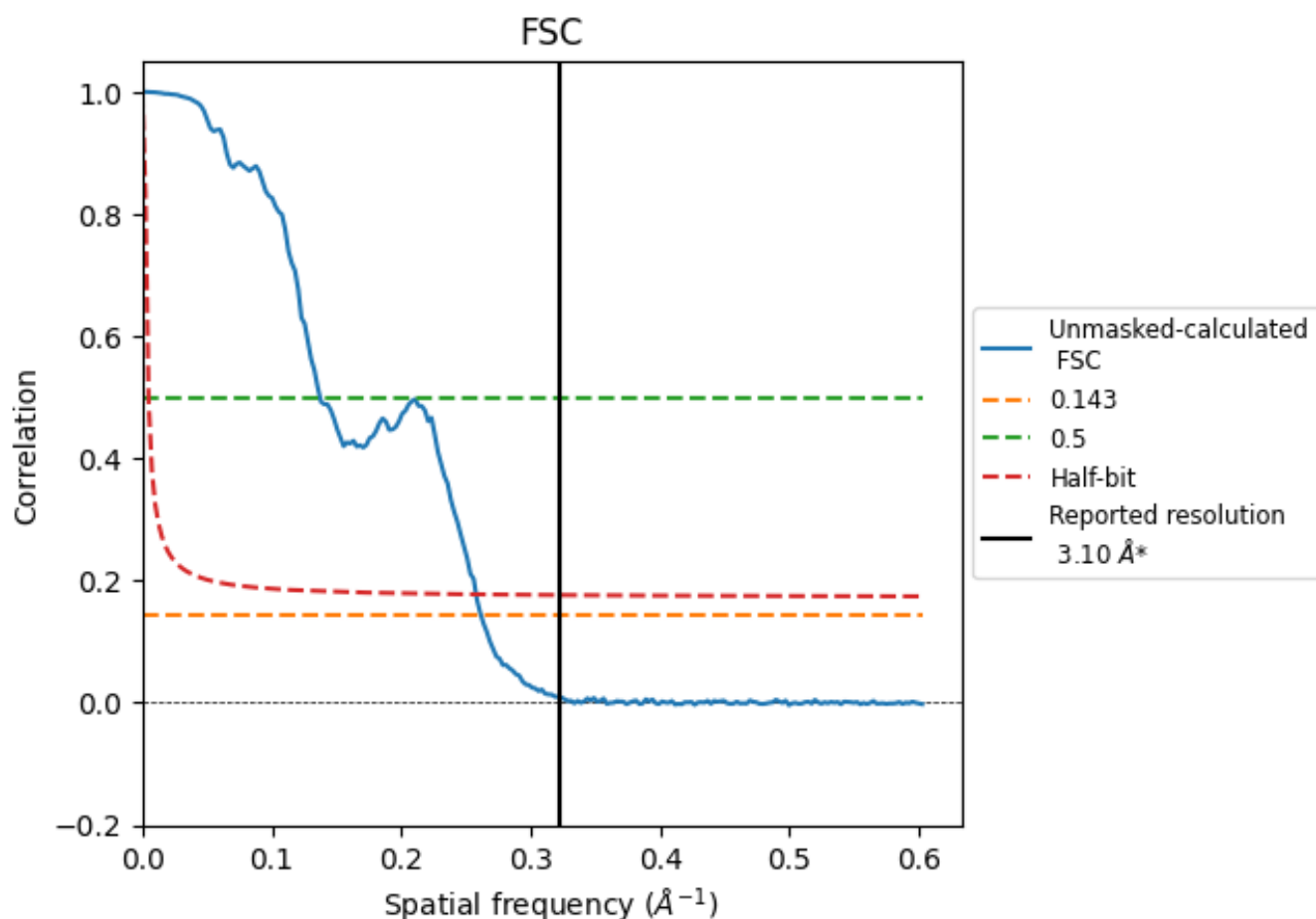


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 $0.323 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

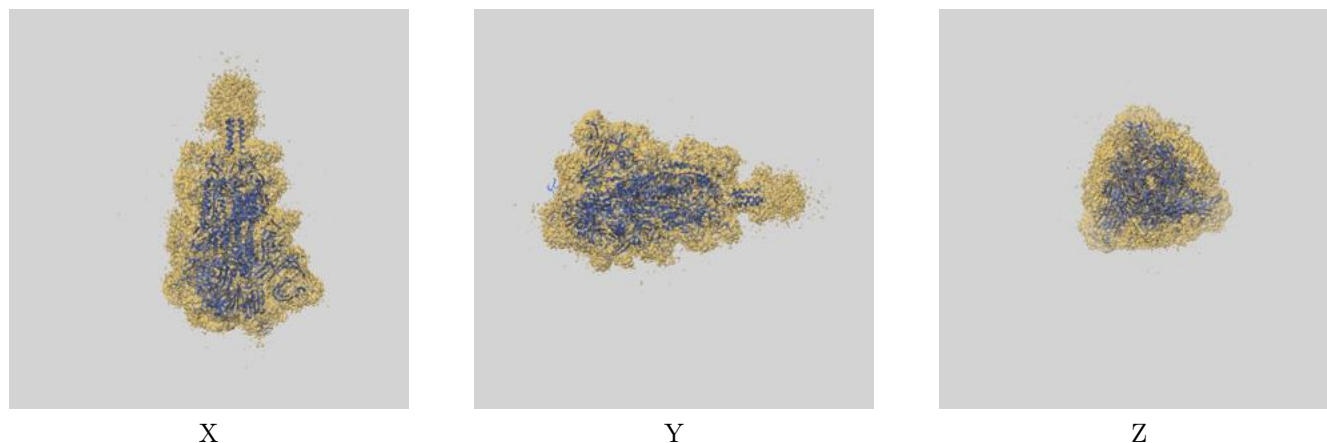
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	7.28	3.88

*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 3.82 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

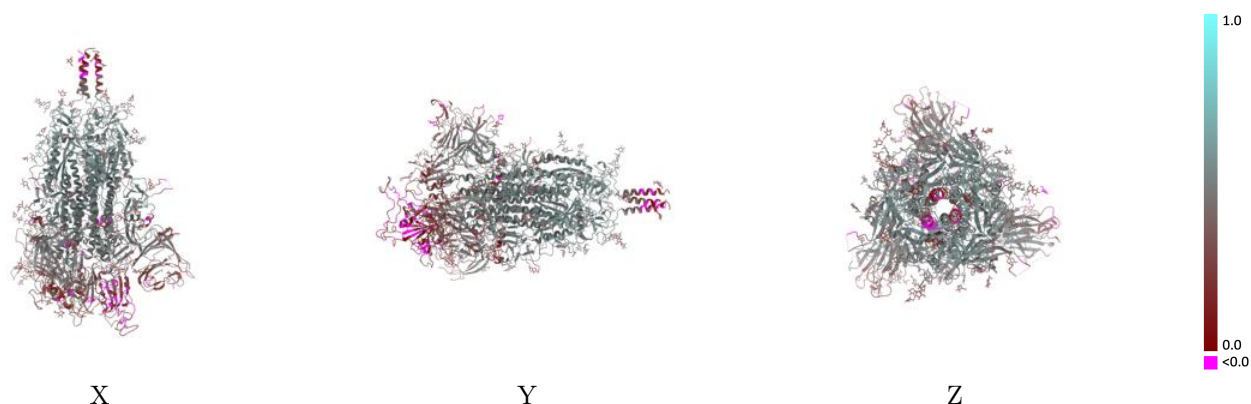
This section contains information regarding the fit between EMDB map EMD-27207 and PDB model 8D5A. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



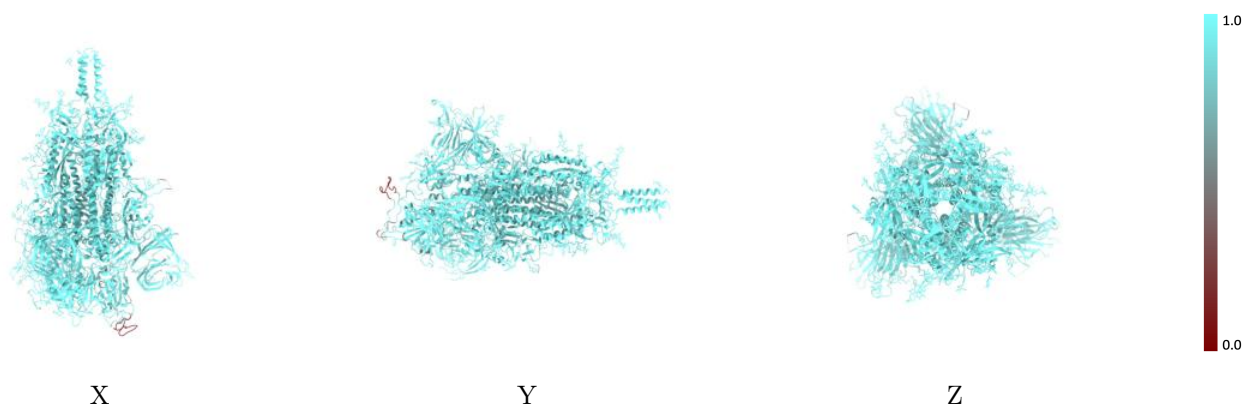
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



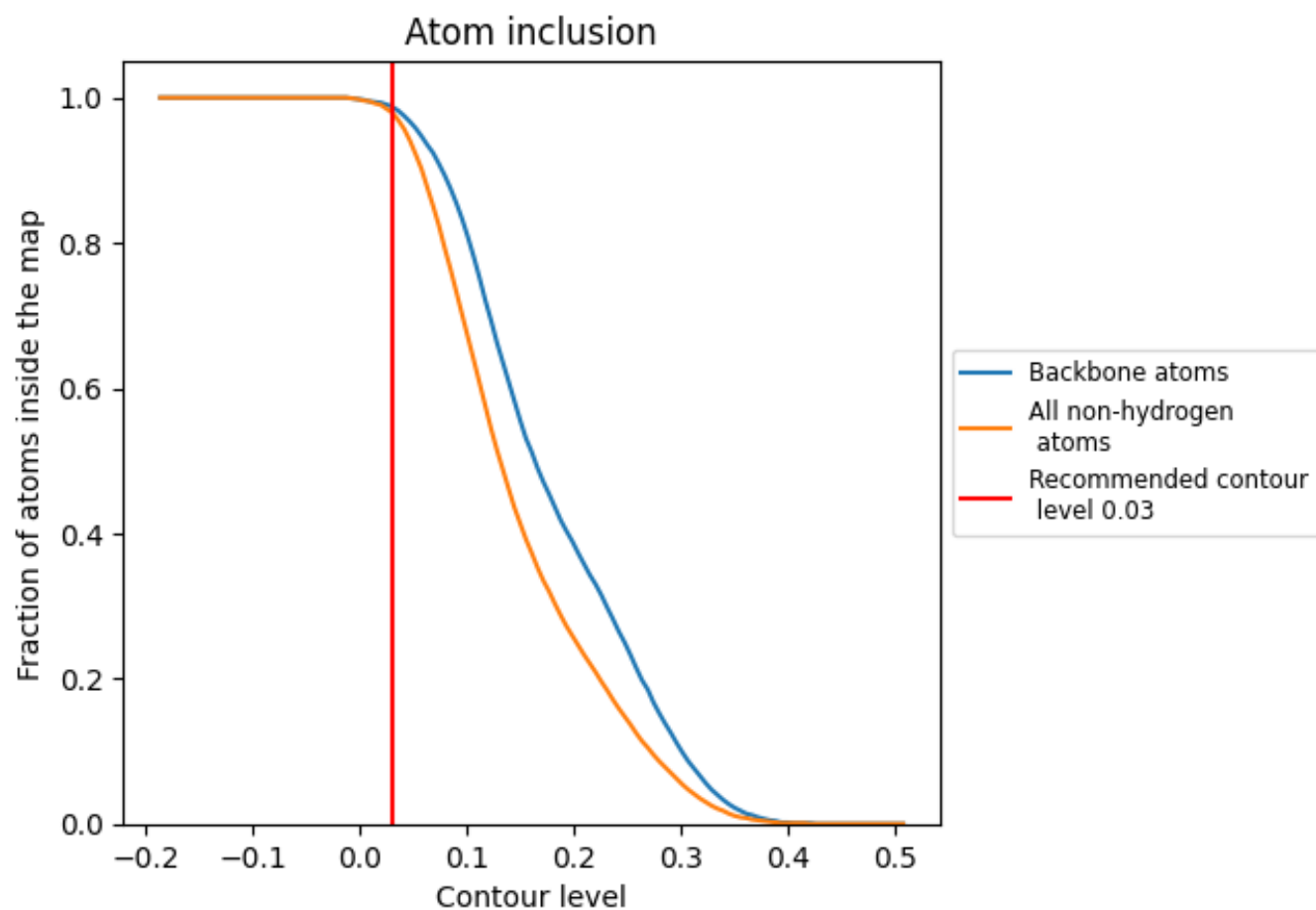
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9800	 0.4140
A	 0.9910	 0.4290
B	 0.9930	 0.4400
C	 0.9570	 0.3800
D	 0.8970	 0.1680
E	 0.8210	 0.1940
F	 1.0000	 0.2120
G	 1.0000	 0.3380
H	 1.0000	 0.4220
I	 1.0000	 0.4060
J	 0.9740	 0.4380
K	 1.0000	 0.3900
L	 1.0000	 0.4070
M	 0.9740	 0.2070
N	 1.0000	 0.3640
O	 0.9640	 0.2580
P	 1.0000	 0.1850
Q	 1.0000	 0.3350
R	 1.0000	 0.4780
S	 1.0000	 0.4200
T	 0.9740	 0.4150
U	 0.9740	 0.3960
V	 1.0000	 0.4260
W	 0.9740	 0.1910
X	 1.0000	 0.2150
Y	 0.9640	 0.2120
Z	 1.0000	 0.2940
a	 1.0000	 0.4160
b	 1.0000	 0.4780
c	 1.0000	 0.3770
d	 0.9740	 0.4640
e	 0.9740	 0.3390
f	 1.0000	 0.3670

